Determinación de la estereoquímica de telepamida y enigmazol C mediante cálculos computacionales, reacciones de cicloisomerización de 1,5-eninos catalizadas por indio(III), y síntesis total de ircinialactama J

Ramón Eduardo Millán Álvarez

Tesis doctoral UDC / 2022

Directores: José Pérez Sestelo

Jaime Rodríguez González

Programa de doctorado en: Química Ambiental y Fundamental RD 99/2011

UNIVERSIDADE DA CORUÑA

ANEXO B

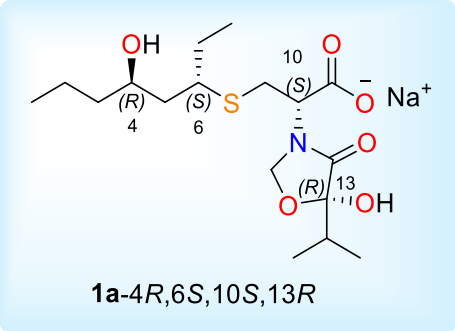
CÁLCULOS COMPUTACIONALES

Índice

CÁLCULOS COMPUTACIONALES TELEPAMIDA

Computational details. Conformational searches were performed by using the corresponding module implemented in the Maestro Quantum mechanical software. OPLS 2005 force field with methanol as solvent was used, and torsional enhanced sampling with 1000 or 10000 steps were fixed using an energy window of 3 kcal/mol. So 51 conformers for **1a**-4*R*,6*S*,10*S*,13*R*, 67 for **1b**-4*R*,6*S*,10*S*,13*S*, 90 for **1c**-4*R*,6*S*,10*R*,13*S* and 85 for **1d**-4*R*,6*S*,10*R*,13*R* were found. Molecular geometry optimizations were performed at the DFT theoretical level using the Gaussian 09W package with B3LYP[1]/6-31+G(d,p) for energy and frequencies calculation and the MPW1PW91[2]/6-311++G(2d,p) with the IEF-PCM solvent continum model, as implemented in Gaussian (methanol as solvent), was used for proton and chemical shifts calculations. Chemical shifts were calculated following Tantillo and coworkers recommendations,[3] using the scaling factor protocol with the combination B3LYP/6-31+G(d,p) (gas phase)// MPW1PW91/6-311+G(2d,p)(giao, scrf) slope: -1.0754, intercept: 31.8463 for ^{1}H, and slope: -1.0399, intercept: 186.5993 for ^{13}C.[4] To calculate Boltzmann populations, saddle points and final chemical shifts, Hoye et al. Phyton scripts were used.[5] The DP4+ statistical parameters were computed using the Excel file recommended by Sarotti and coworkers.[6]

[1] Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648.
[2] Adamo, C.; Barone, V. *J. Chem. Phys.* **1998**, *108*, 664.
[3] http://www.cheshirenmr.info
[4] Lodewyk, M. W.; Siebert, M. R.; Tantillo, D. J. *Chem. Rev.* **2012**, *112*, 1839.
[5] Manna, M. S.; Mukherjee, S. *Chem. Eur. J.* **2012**, *18*, 15277.
[6] Grimblat, N.; Zanardi, M. M.; Sarotti, A. M. *J. Org. Chem.* **2015**, *80*, 12526.



1a-4*R*,6*S*,10*S*,13*R*

Calculated DFT energies of the 1a-diasteroisomer

Conformers **1a**	OPLS2008 Force Field Conformational Search Relative Energy (kcal/mol)	B3LYP/6-31+G(d,p) DFT Energy (hartree)	Δ (DFT Energy) (kcal/mol)	% Population
1a51	2.977441146	-1732.255354	0	15.28
1a20	1.951914201	-1732.255121	0.146209688	11.94
1a40	2.703731474	-1732.254907	0.280496698	9.52
1a49	2.926963078	-1732.254805	0.344502656	8.54
1a39	2.656312684	-1732.254439	0.574171093	5.79
1a11	1.570795233	-1732.254387	0.606801581	5.48
1a2	0.339364619	-1732.254332	0.641314598	5.17
1a15	1.728037281	-1732.25419	0.730420931	4.45
1a36	2.54699134	-1732.254147	0.757403835	4.25
1a26	2.193238559	-1732.254032	0.829567415	3.76
1a8	1.201507063	-1732.253844	0.94753918	3.08
1a34	2.488410969	-1732.253816	0.965109443	2.99
1a19	1.933319534	-1732.25351	1.157127317	2.16
1a33	2.456647072	-1732.253422	1.212348143	1.97
1a37	2.575409153	-1732.253314	1.280119158	1.76
1a48	2.923162883	-1732.253071	1.432603939	1.36
1a4	0.573733903	-1732.252945	1.511670123	1.19
1a21	2.008630325	-1732.252888	1.547438158	1.12
1a38	2.652249582	-1732.252804	1.600148947	1.02
1a22	2.063601705	-1732.252716	1.655369774	0.93
1a27	2.193788273	-1732.25269	1.671685018	0.91
1a1	0	-1732.252611	1.72125826	0.83
1a43	2.770031739	-1732.252515	1.781499161	0.75
1a14	1.68219593	-1732.25237	1.872488023	0.65
1a18	1.888577611	-1732.252342	1.890058286	0.63
1a9	1.426340007	-1732.25222	1.966614431	0.55
1a24	2.159156303	-1732.252091	2.047563143	0.48
1a12	1.63958116	-1732.252039	2.080193631	0.45
1a44	2.78363118	-1732.251789	2.237070979	0.35
1a28	2.237024458	-1732.251738	2.269073958	0.33
1a42	2.753612027	-1732.251696	2.295429352	0.32

1a41	2.713482919	-1732.25165	2.324294784	0.30
1a13	1.681717918	-1732.25156	2.38077063	0.27
1a31	2.402273207	-1732.251214	2.597888879	0.19
1a30	2.359323828	-1732.251103	2.667542421	0.17
1a7	1.193595964	-1732.251019	2.72025321	0.15
1a50	2.953612247	-1732.250953	2.76166883	0.14
1a10	1.437644991	-1732.250803	2.855795238	0.12
1a16	1.832865312	-1732.250729	2.902230933	0.11

39 conformers counting for the 99.49% of the DFT conformational population

DFT COORDINATES FOR CONFORMATIONAL SEARCH OF 1a (4*R*, 6*S*, 10*S*, 13*R*)

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 51

C	5.04833	-2.53058	-0.55461
C	4.78201	-1.17643	0.11329
C	3.52455	-0.46158	-0.40838
C	3.34939	0.92482	0.24709
C	2.53955	1.97636	-0.5363
S	0.72642	1.59767	-0.73634
C	0.0376	1.81733	0.96978
C	-0.82551	0.66163	1.52122
C	-0.03215	-0.68981	1.5512
O	1.0968	-0.60978	2.098
O	-0.54692	-1.68362	0.9783
N	-2.16079	0.56823	0.91543
C	-3.33396	0.73109	1.77066
O	-4.45099	0.62286	0.9157
C	-4.06619	0.05194	-0.34999
C	-2.51755	0.09899	-0.30106
O	-1.78944	-0.19839	-1.25213
C	-4.67501	-1.35617	-0.51431
C	-4.2298	-2.30885	0.60633
C	-4.41832	-1.96022	-1.90404
O	-4.57698	0.84837	-1.38053
C	2.80161	3.4025	-0.0117

C	2.22155	4.53273	-0.86746
O	2.37225	-1.30472	-0.24206
C	6.30624	-3.22392	-0.01864
H	4.17681	-3.17795	-0.40945
H	5.1472	-2.38237	-1.63988
H	5.64773	-0.5172	-0.04271
H	4.68379	-1.31129	1.2004
H	3.62719	-0.33487	-1.49623
H	2.93658	0.79104	1.25414
H	4.35434	1.34835	0.37834
H	2.85855	1.9441	-1.58822
H	0.88142	1.92342	1.65158
H	-0.54256	2.74447	0.98282
H	-1.00731	0.92258	2.57122
H	-3.33758	1.71806	2.24954
H	-3.35116	-0.05135	2.54401
H	-5.75388	-1.17725	-0.41214
H	-4.7037	-3.28578	0.46707
H	-4.5288	-1.93915	1.59197
H	-3.14446	-2.46111	0.60942
H	-4.98185	-2.89438	-2.0032
H	-4.73362	-1.28033	-2.69854
H	-3.35803	-2.18605	-2.05039
H	-4.26898	1.7581	-1.26208
H	2.43735	3.48858	1.02042
H	3.89122	3.52679	0.05059
H	2.48787	5.50788	-0.44632
H	2.61364	4.49313	-1.89063
H	1.13124	4.47384	-0.9311
H	2.09362	-1.2737	0.70613
H	6.47337	-4.18537	-0.51637
H	7.20073	-2.60869	-0.17523
H	6.22233	-3.41777	1.05723

Na	0.22164	-1.27571	-1.1105

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 20

C	5.1308	-2.44413	-0.58682
C	4.84299	-1.08135	0.05398
C	3.54567	-0.42137	-0.44213
C	3.34584	0.97442	0.18524
C	2.47693	1.97883	-0.59648
S	0.67346	1.53562	-0.74569
C	0.0095	1.78222	0.96722
C	-0.78178	0.6089	1.58844
C	0.06806	-0.70762	1.63384
O	-0.41965	-1.73915	1.10762
O	1.20933	-0.56267	2.14203
N	-2.13209	0.43266	1.03896
C	-3.29319	0.69001	1.88707
O	-4.39547	0.13981	1.19271
C	-4.05798	0.00543	-0.18668
C	-2.51094	-0.02252	-0.17426
O	-1.80426	-0.35949	-1.12748
C	-4.77253	-1.2463	-0.73128
C	-4.35263	-2.5187	0.02146
C	-4.60743	-1.40874	-2.25103
O	-4.39428	1.18304	-0.89558
C	2.7009	3.4238	-0.10668
C	2.06711	4.51658	-0.97309
O	2.42897	-1.29692	-0.21531
C	6.42414	-3.08588	-0.07136
H	4.28356	-3.11232	-0.39864
H	5.19327	-2.32207	-1.67806
H	5.68118	-0.39942	-0.14828
H	4.78508	-1.18998	1.14691

H	3.60748	-0.31884	-1.53569
H	2.96987	0.85284	1.20817
H	4.34001	1.43345	0.27249
H	2.77066	1.93703	-1.65548
H	0.86177	1.96116	1.62314
H	-0.61804	2.67791	0.95544
H	-0.93592	0.89831	2.63507
H	-3.42723	1.76968	2.05076
H	-3.19239	0.17664	2.84979
H	-5.83807	-1.0645	-0.51623
H	-4.91625	-3.37785	-0.35675
H	-4.54303	-2.43072	1.09373
H	-3.28661	-2.72839	-0.11718
H	-5.22844	-2.24103	-2.59891
H	-4.90605	-0.50768	-2.79319
H	-3.5669	-1.62106	-2.50921
H	-5.35913	1.26805	-0.89892
H	2.35354	3.51898	0.9304
H	3.78668	3.58557	-0.06816
H	2.31077	5.50831	-0.57754
H	2.43969	4.46782	-2.00316
H	0.97823	4.42256	-1.01296
H	2.17553	-1.24166	0.73915
H	6.60528	-4.05519	-0.54865
H	7.29497	-2.44939	-0.27077
H	6.37764	-3.25293	1.01126
Na	0.2493	-1.35838	-1.0097

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 40

C	5.1502	-2.70182	0.03694
C	4.87289	-1.26036	0.49216
C	3.65205	-0.5923	-0.16626

C	3.4571	0.84275	0.36669
C	2.67736	1.8296	-0.52344
S	0.86852	1.44639	-0.75012
C	0.12808	1.79378	0.91388
C	-0.75127	0.68265	1.52985
C	0.03713	-0.66342	1.68049
O	-0.46002	-1.69551	1.16367
O	1.14917	-0.54421	2.2552
N	-2.06968	0.5351	0.90104
C	-3.27287	0.86853	1.66189
O	-4.34968	0.31155	0.93291
C	-3.93152	0.08846	-0.41141
C	-2.39147	0.0265	-0.30696
O	-1.65206	-0.38181	-1.20521
C	-4.57336	-1.19864	-0.95441
C	-6.09459	-1.0548	-1.13022
C	-4.23594	-2.4142	-0.0765
O	-4.18697	1.22392	-1.21542
C	2.93068	3.29214	-0.10488
C	2.38423	4.35328	-1.06496
O	2.48692	-1.41551	0.00781
C	5.55613	-2.8338	-1.43703
H	5.95239	-3.1095	0.66517
H	4.26193	-3.31306	0.23105
H	5.75786	-0.63902	0.29304
H	4.72096	-1.24795	1.58052
H	3.80905	-0.55026	-1.25242
H	4.45894	1.27416	0.49739
H	3.01089	0.78977	1.3668
H	3.02887	1.71351	-1.55902
H	0.95098	1.95673	1.61043
H	-0.45348	2.71656	0.83418
H	-0.95783	1.02233	2.55197

H	-3.3842	1.95864	1.75946
H	-3.24424	0.40594	2.65462
H	-4.11528	-1.33871	-1.94126
H	-6.51277	-1.99238	-1.51008
H	-6.36683	-0.27689	-1.85343
H	-6.58418	-0.8337	-0.17571
H	-4.57846	-3.33256	-0.56495
H	-3.16035	-2.50804	0.10188
H	-4.73225	-2.34168	0.8963
H	-5.14475	1.32946	-1.30109
H	2.53335	3.45959	0.9047
H	4.01846	3.41774	-0.01707
H	2.64484	5.35764	-0.71468
H	2.80662	4.23034	-2.06931
H	1.29601	4.2946	-1.15691
H	2.17419	-1.31997	0.94109
H	5.80457	-3.8719	-1.68345
H	4.75104	-2.52409	-2.11273
H	6.43632	-2.21961	-1.66525
Na	0.35826	-1.43029	-0.92393

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 49

C	5.99028	-1.15239	-0.49771
C	4.61916	-1.65506	-0.023
C	3.4132	-0.83071	-0.50937
C	3.31029	0.53575	0.19952
C	2.54529	1.65485	-0.53376
S	0.70757	1.39227	-0.69048
C	0.08305	1.57735	1.0457
C	-0.80352	0.43912	1.60101
C	-0.07488	-0.94796	1.54073
O	-0.64853	-1.88432	0.92954

O	1.0705	-0.94875	2.05923
N	-2.17103	0.41766	1.06734
C	-3.29598	0.67445	1.96263
O	-4.44547	0.25649	1.25282
C	-4.14402	0.20752	-0.14041
C	-2.60171	0.08544	-0.16823
O	-1.9354	-0.21612	-1.16151
C	-4.94436	-0.95527	-0.75857
C	-4.58581	-2.3043	-0.11515
C	-4.8238	-1.00927	-2.29011
O	-4.42253	1.45299	-0.75146
C	2.90461	3.04888	0.01929
C	2.37418	4.23334	-0.79449
O	2.2161	-1.61492	-0.36685
C	7.14181	-2.05861	-0.04469
H	5.98988	-1.08646	-1.59518
H	6.17329	-0.13422	-0.13051
H	4.59735	-1.70668	1.0751
H	4.46813	-2.67956	-0.38465
H	3.52048	-0.67127	-1.59224
H	2.89343	0.37613	1.20106
H	4.33237	0.9085	0.34408
H	2.83294	1.63401	-1.59503
H	0.95461	1.63331	1.69881
H	-0.46163	2.52377	1.10433
H	-0.9174	0.67028	2.66694
H	-3.35596	1.74254	2.21929
H	-3.20984	0.07524	2.87592
H	-5.99195	-0.72893	-0.50164
H	-5.20588	-3.09745	-0.54557
H	-4.75193	-2.28942	0.96464
H	-3.53655	-2.56396	-0.29222
H	-5.4952	-1.7805	-2.6824

H	-5.08838	-0.05576	-2.75467
H	-3.80205	-1.25237	-2.59234
H	-5.3802	1.59528	-0.72379
H	2.56911	3.12993	1.06147
H	4.00093	3.10639	0.05822
H	2.71264	5.17971	-0.35957
H	2.73582	4.19354	-1.8289
H	1.28116	4.24432	-0.8288
H	1.96216	-1.62307	0.5882
H	8.10769	-1.68482	-0.40142
H	7.19031	-2.11882	1.04877
H	7.01623	-3.07845	-0.4264
Na	0.03731	-1.38936	-1.15907

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 39

C	5.15213	-2.41552	-0.60446
C	4.8543	-1.05529	0.03717
C	3.54812	-0.40789	-0.4521
C	3.33877	0.98559	0.1773
C	2.45353	1.98256	-0.59568
S	0.65259	1.52209	-0.72477
C	0.00654	1.75819	0.99635
C	-0.77874	0.57584	1.60688
C	0.08114	-0.73385	1.64322
O	-0.40248	-1.7677	1.11861
O	1.22476	-0.58049	2.14351
N	-2.12488	0.39416	1.04756
C	-3.29225	0.77095	1.84339
O	-4.4096	0.27569	1.13311
C	-4.0464	0.01839	-0.20364
C	-2.5051	-0.07226	-0.15768
O	-1.80657	-0.42083	-1.11927

C	-4.80616	-1.23426	-0.68117
C	-4.39178	-2.48232	0.11442
C	-4.69085	-1.4706	-2.19596
O	-4.38084	1.1819	-0.96194
C	2.66851	3.429	-0.10626
C	2.01602	4.5174	-0.96416
O	2.441	-1.29393	-0.21899
C	6.45344	-3.04485	-0.09378
H	4.31195	-3.09151	-0.41254
H	5.20916	-2.29333	-1.69599
H	5.68481	-0.36535	-0.16947
H	4.80299	-1.16407	1.13041
H	3.60265	-0.30441	-1.54595
H	2.97298	0.85951	1.20338
H	4.32877	1.45476	0.25663
H	2.73655	1.9441	-1.65765
H	0.86444	1.92904	1.64702
H	-0.61945	2.65517	0.99908
H	-0.9408	0.85284	2.65577
H	-3.35011	1.86352	1.95612
H	-3.26311	0.29476	2.82985
H	-5.85519	-1.0047	-0.45019
H	-5.01429	-3.33457	-0.17705
H	-4.51316	-2.32784	1.18969
H	-3.3464	-2.75068	-0.0735
H	-5.28274	-2.3486	-2.47457
H	-5.07944	-0.62502	-2.77267
H	-3.65401	-1.65167	-2.49423
H	-3.94722	1.11894	-1.82584
H	2.33107	3.51918	0.9345
H	3.75305	3.60063	-0.07891
H	2.25778	5.51058	-0.57126
H	2.3758	4.47179	-1.99892

H	0.92732	4.41645	-0.98977
H	2.19235	-1.24125	0.73707
H	6.64172	-4.0126	-0.57138
H	7.31745	-2.40034	-0.29688
H	6.41268	-3.21185	0.98905
Na	0.26161	-1.39634	-0.9956

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 11

C	5.23974	-2.42576	-0.5915
C	4.93434	-1.05992	0.03453
C	3.62446	-0.42471	-0.46102
C	3.40912	0.97434	0.15389
C	2.51824	1.95849	-0.62872
S	0.72061	1.48662	-0.75925
C	0.06596	1.74048	0.95634
C	-0.69381	0.56062	1.60404
C	0.17959	-0.73973	1.65579
O	-0.29602	-1.78515	1.14621
O	1.3236	-0.5697	2.14988
N	-2.0486	0.35215	1.07763
C	-3.19911	0.55383	1.95326
O	-4.29051	-0.03882	1.2777
C	-3.98777	-0.10858	-0.11535
C	-2.4373	-0.1087	-0.13007
O	-1.73374	-0.43234	-1.09053
C	-4.66911	-1.36532	-0.69368
C	-4.47162	-1.49339	-2.21267
C	-6.16442	-1.407	-0.32954
O	-4.35586	1.09099	-0.76978
C	2.72513	3.41041	-0.15188
C	2.0655	4.48784	-1.01818
O	2.5221	-1.31379	-0.21705

C	6.54293	-3.04309	-0.07114
H	4.40225	-3.10341	-0.39372
H	5.29839	-2.3155	-1.6842
H	5.76117	-0.36791	-0.17996
H	4.88378	-1.1566	1.12896
H	3.67742	-0.33292	-1.55596
H	3.04383	0.85714	1.18115
H	4.39709	1.44882	0.22779
H	2.80336	1.91286	-1.6899
H	0.92047	1.94785	1.60101
H	-0.58127	2.62187	0.93815
H	-0.8385	0.86262	2.64843
H	-3.37566	1.62536	2.1291
H	-3.05657	0.03604	2.90781
H	-4.18022	-2.21522	-0.20084
H	-4.90511	-2.43772	-2.55906
H	-3.41509	-1.47028	-2.48408
H	-4.9721	-0.67769	-2.7451
H	-6.60393	-2.34035	-0.69554
H	-6.32326	-1.35083	0.74956
H	-6.72332	-0.58983	-0.80556
H	-5.3216	1.15738	-0.76718
H	2.38816	3.50765	0.88843
H	3.80869	3.58873	-0.12666
H	2.30221	5.48571	-0.63394
H	2.42424	4.43538	-2.05296
H	0.97743	4.38041	-1.04204
H	2.27835	-1.25378	0.73954
H	6.73707	-4.01517	-0.53753
H	7.40427	-2.3966	-0.2794
H	6.50051	-3.19815	1.01342
Na	0.33188	-1.41503	-0.98284

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 2

C	5.52658	-0.51771	-1.27883
C	4.74313	0.14715	-0.14013
C	3.261	0.3874	-0.45524
C	2.53891	1.11654	0.69807
C	1.13131	1.60549	0.30915
S	-0.05864	1.73204	1.74072
C	-0.06674	0.10634	2.59785
C	-0.67959	-1.14225	1.90034
C	0.36041	-2.01067	1.1153
O	1.56024	-1.87492	1.47369
O	-0.08439	-2.76525	0.21313
N	-1.88621	-0.83328	1.13536
C	-3.14497	-0.638	1.85387
O	-4.08343	-0.26462	0.87231
C	-3.39686	0.23837	-0.27917
C	-1.98488	-0.37552	-0.13167
O	-1.11723	-0.35429	-1.01549
C	-4.21832	-0.14345	-1.52174
C	-4.36452	-1.66632	-1.66114
C	-3.6817	0.49264	-2.81326
O	-3.28149	1.64203	-0.23748
C	1.19281	2.99686	-0.35389
C	-0.10466	3.4962	-0.99996
O	2.59909	-0.85752	-0.76627
C	7.00179	-0.74818	-0.93144
H	5.05089	-1.47224	-1.52999
H	5.45667	0.11015	-2.1788
H	5.20461	1.11426	0.10411
H	4.81303	-0.46906	0.76793
H	3.18975	0.97969	-1.37738
H	2.49906	0.42247	1.54162

H	3.14307	1.97448	1.01848
H	0.67451	0.90296	-0.3906
H	0.94249	-0.16647	2.90858
H	-0.63686	0.34157	3.50265
H	-1.00689	-1.80657	2.71258
H	-3.03608	0.14262	2.62296
H	-3.47022	-1.5727	2.32484
H	-5.21063	0.28128	-1.31787
H	-5.02492	-1.90048	-2.50233
H	-4.79116	-2.11454	-0.76028
H	-3.3973	-2.14381	-1.85775
H	-4.36539	0.27093	-3.63993
H	-3.59746	1.57706	-2.71654
H	-2.69546	0.09459	-3.06916
H	-2.58025	1.89959	0.38522
H	1.55045	3.72709	0.38447
H	1.97226	2.94073	-1.12568
H	0.08026	4.41733	-1.56282
H	-0.51865	2.75366	-1.69009
H	-0.87302	3.7198	-0.25402
H	2.45585	-1.34936	0.08499
H	7.5377	-1.22009	-1.76212
H	7.51035	0.19578	-0.70089
H	7.10409	-1.40106	-0.05662
Na	0.6124	-1.67291	-1.58478

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 15

C	5.88839	0.25495	-0.65871
C	4.77257	-0.79507	-0.55495
C	3.34975	-0.25534	-0.76529
C	2.86011	0.63722	0.39336
C	1.51753	1.33113	0.09908

S	0.55271	1.79319	1.61858
C	0.19339	0.23876	2.52409
C	-0.69289	-0.86287	1.88503
C	0.10634	-1.94275	1.07614
O	-0.53462	-2.61546	0.22599
O	1.32585	-2.04707	1.36617
N	-1.87005	-0.36194	1.17294
C	-3.07961	-0.02964	1.92271
O	-4.08878	0.14956	0.94673
C	-3.47313	0.44518	-0.30448
C	-2.02492	-0.06648	-0.13179
O	-1.21613	-0.15743	-1.06242
C	-4.24516	-0.25148	-1.4402
C	-5.65791	0.33101	-1.61363
C	-4.30405	-1.77402	-1.23844
O	-3.34681	1.83813	-0.49534
C	1.71358	2.62953	-0.71158
C	0.44127	3.22728	-1.32461
O	2.44158	-1.3611	-0.9717
C	7.28903	-0.35993	-0.54723
H	5.79958	0.78443	-1.61805
H	5.76863	1.01517	0.12308
H	4.82167	-1.29754	0.42165
H	4.93739	-1.57164	-1.31273
H	3.32631	0.30485	-1.70954
H	2.78135	0.00047	1.27975
H	3.61534	1.40063	0.61433
H	0.8706	0.66238	-0.4716
H	1.11689	-0.25052	2.83731
H	-0.2969	0.62361	3.42514
H	-1.0957	-1.43678	2.73228
H	-2.9344	0.88634	2.51295
H	-3.36573	-0.85895	2.5786

H	-3.66149	-0.03606	-2.34379
H	-6.17664	-0.18986	-2.42482
H	-5.64792	1.39397	-1.88128
H	-6.25086	0.20425	-0.70167
H	-4.73878	-2.25204	-2.12263
H	-3.31275	-2.20817	-1.07398
H	-4.92745	-2.02778	-0.37537
H	-4.23385	2.22009	-0.54955
H	2.21177	3.37364	-0.07465
H	2.42367	2.40249	-1.51831
H	0.68684	4.10555	-1.93198
H	-0.06757	2.50001	-1.96616
H	-0.27355	3.53527	-0.55706
H	2.2546	-1.77637	-0.09012
H	8.0678	0.40659	-0.62325
H	7.41939	-0.87367	0.41238
H	7.4641	-1.09448	-1.34201
Na	0.28094	-1.73647	-1.64448

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 36

C	6.08289	-1.0897	-0.53288
C	4.72713	-1.61748	-0.04189
C	3.49916	-0.81997	-0.518
C	3.37612	0.54742	0.1858
C	2.58077	1.64713	-0.54437
S	0.74914	1.34083	-0.68914
C	0.13128	1.52309	1.04961
C	-0.72656	0.37027	1.61954
C	0.03	-1.00196	1.56324
O	1.17895	-0.97642	2.07317
O	-0.52958	-1.9534	0.96229
N	-2.09739	0.31652	1.09739

C	-3.22194	0.51051	2.00753
O	-4.35658	0.04559	1.30369
C	-4.07619	0.07128	-0.09556
C	-2.52868	-0.01581	-0.13763
O	-1.85673	-0.29642	-1.1335
C	-4.83394	-1.09693	-0.75902
C	-4.66785	-1.11219	-2.28688
C	-6.32329	-1.08966	-0.36897
O	-4.38503	1.33743	-0.64674
C	2.91168	3.05004	0.0039
C	2.34625	4.22022	-0.80694
O	2.32078	-1.62862	-0.3582
C	7.25647	-1.97207	-0.0894
H	6.06965	-1.02735	-1.63048
H	6.25016	-0.06699	-0.17072
H	4.71806	-1.6654	1.05658
H	4.59276	-2.64624	-0.39804
H	3.59042	-0.66324	-1.60272
H	2.97381	0.38452	1.19283
H	4.39198	0.94152	0.31731
H	2.86229	1.63063	-1.60737
H	1.00578	1.6021	1.69629
H	-0.43345	2.45781	1.10622
H	-0.83693	0.60749	2.68449
H	-3.32974	1.57156	2.27719
H	-3.09958	-0.09561	2.9115
H	-4.38379	-2.00828	-0.34541
H	-5.16161	-1.99873	-2.69914
H	-3.61612	-1.12809	-2.57688
H	-5.12729	-0.22824	-2.74165
H	-6.81712	-1.96884	-0.79489
H	-6.46121	-1.10761	0.71433
H	-6.84606	-0.2112	-0.771

H	-5.34489	1.45925	-0.61555
H	2.58301	3.12465	1.04876
H	4.00661	3.13375	0.0338
H	2.66301	5.17518	-0.37445
H	2.70233	4.18916	-1.84357
H	1.25309	4.20283	-0.83452
H	2.07562	-1.63529	0.59915
H	8.21121	-1.58066	-0.45707
H	7.31735	-2.02818	1.00367
H	7.1468	-2.99528	-0.46702
Na	0.12591	-1.46042	-1.13286

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 26

C	5.06948	-1.91559	0.52384
C	4.81451	-1.32249	-0.86943
C	3.51473	-0.51053	-1.02343
C	3.45356	0.70703	-0.0759
C	2.60921	1.90819	-0.54425
S	0.77663	1.59508	-0.66213
C	0.22538	1.49402	1.10517
C	-0.60142	0.25393	1.51228
C	0.16113	-1.08056	1.20506
O	-0.42544	-1.941	0.50153
O	1.33787	-1.11343	1.64705
N	-1.98917	0.26864	1.03458
C	-3.08515	0.3584	1.99794
O	-4.25295	0.0117	1.27846
C	-4.00237	0.16701	-0.11637
C	-2.46266	0.10385	-0.21777
O	-1.8418	-0.03223	-1.27444
C	-4.72608	-0.93596	-0.90637
C	-6.25468	-0.77154	-0.85709

C	-4.31132	-2.33809	-0.43281
O	-4.33316	1.47269	-0.54763
C	2.9539	3.18712	0.24513
C	2.33381	4.47991	-0.29405
O	2.37379	-1.3771	-0.89732
C	6.32972	-2.78875	0.5633
H	5.16548	-1.11054	1.26338
H	4.20408	-2.51376	0.83265
H	4.77753	-2.13699	-1.60467
H	5.66021	-0.67973	-1.15543
H	3.47784	-0.14841	-2.06055
H	3.12887	0.37842	0.91756
H	4.48072	1.08008	0.03905
H	2.83715	2.09921	-1.603
H	1.12266	1.484	1.72403
H	-0.3449	2.40017	1.32817
H	-0.67405	0.3117	2.60505
H	-3.16212	1.37597	2.40882
H	-2.94628	-0.36274	2.81106
H	-4.38889	-0.79877	-1.94115
H	-6.73111	-1.57755	-1.42418
H	-6.5958	0.16874	-1.30631
H	-6.62494	-0.82391	0.17237
H	-4.72737	-3.09615	-1.10478
H	-3.22438	-2.46325	-0.41541
H	-4.68767	-2.53487	0.57585
H	-5.2928	1.58042	-0.49036
H	2.68369	3.05395	1.30078
H	4.04795	3.28513	0.2328
H	2.67213	5.34048	0.29276
H	2.62555	4.65179	-1.33687
H	1.24116	4.45126	-0.25926
H	2.17945	-1.51351	0.06141

H	6.49609	-3.20191	1.56393
H	6.24894	-3.63014	-0.13512
H	7.22238	-2.21407	0.28702
Na	0.14814	-1.12704	-1.52548

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 8

C	5.45345	-0.8844	-1.17609
C	4.67913	0.00361	-0.19408
C	3.19653	0.18232	-0.54589
C	2.48849	1.15084	0.42715
C	1.0505	1.48075	-0.00823
S	-0.0898	1.96826	1.38451
C	-0.15779	0.53285	2.53154
C	-0.79303	-0.80765	2.06054
C	0.24098	-1.82679	1.47414
O	-0.21029	-2.74822	0.74746
O	1.44199	-1.62913	1.79883
N	-1.97444	-0.61047	1.22125
C	-3.22306	-0.19376	1.86129
O	-4.1278	0.03267	0.80613
C	-3.39323	0.28009	-0.39816
C	-2.03649	-0.40438	-0.11376
O	-1.17004	-0.62261	-0.97139
C	-4.23073	-0.24432	-1.57513
C	-4.47396	-1.75727	-1.46586
C	-3.64545	0.13845	-2.94294
O	-3.15978	1.6571	-0.58876
C	0.95587	2.58459	-1.08546
C	1.39286	3.99746	-0.67291
O	2.52463	-1.09511	-0.58158
C	6.93094	-1.04262	-0.79905
H	4.97467	-1.86896	-1.22122

H	5.37786	-0.45588	-2.18587
H	5.14626	0.99785	-0.15469
H	4.75082	-0.41462	0.82025
H	3.12453	0.56416	-1.57302
H	2.49179	0.67988	1.41474
H	3.08091	2.06835	0.51334
H	0.59944	0.58592	-0.43473
H	0.84213	0.29844	2.89874
H	-0.73058	0.94443	3.36879
H	-1.1559	-1.30388	2.97178
H	-3.0669	0.71791	2.45869
H	-3.61311	-0.99129	2.50361
H	-5.1949	0.2691	-1.45937
H	-5.14975	-2.08445	-2.26255
H	-4.9256	-2.02351	-0.50683
H	-3.53894	-2.31944	-1.57333
H	-4.32838	-0.1865	-3.73541
H	-3.50822	1.21848	-3.02726
H	-2.67656	-0.34223	-3.10703
H	-2.45204	1.95987	0.00882
H	1.56963	2.25438	-1.93435
H	-0.07439	2.61704	-1.45872
H	1.31644	4.6771	-1.52814
H	0.76526	4.40069	0.12769
H	2.43068	4.02398	-0.32482
H	2.36817	-1.38983	0.35404
H	7.45911	-1.6797	-1.51676
H	7.44324	-0.07319	-0.77499
H	7.03922	-1.49857	0.19212
Na	0.53575	-2.06915	-1.2275

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 34

C	-5.5953	0.1641	1.32436
C	-4.77899	0.34457	0.03846
C	-3.28651	0.60982	0.27547
C	-2.52772	0.85149	-1.04694
C	-1.09918	1.38229	-0.82575
S	0.1029	0.9382	-2.18306
C	0.01939	-0.88273	-2.42153
C	0.56048	-1.84189	-1.32187
C	-0.52594	-2.33028	-0.30549
O	-0.12363	-2.74606	0.8109
O	-1.71623	-2.2671	-0.71264
N	1.78302	-1.35042	-0.69068
C	3.05162	-1.49084	-1.40444
O	4.00899	-0.87032	-0.58099
C	3.35167	0.08647	0.25982
C	1.90953	-0.47648	0.33228
O	1.04428	-0.1086	1.13877
C	4.13811	0.18178	1.57785
C	3.55388	1.22964	2.53814
C	5.62615	0.46341	1.3042
O	3.29949	1.36091	-0.34112
C	-1.09297	2.91975	-0.6998
C	0.21959	3.55445	-0.22613
O	-2.6883	-0.47673	1.01462
C	-7.07941	-0.10858	1.05384
H	-5.16706	-0.65923	1.90683
H	-5.49597	1.0671	1.94376
H	-5.19055	1.18313	-0.54073
H	-4.87997	-0.54947	-0.59373
H	-3.18503	1.48402	0.93282
H	-2.5201	-0.09724	-1.58975
H	-3.0881	1.56743	-1.66103

H	-0.6828	0.953	0.0876
H	-1.00337	-1.19183	-2.64005
H	0.60306	-1.00709	-3.33961
H	0.84981	-2.76287	-1.84753
H	2.99624	-1.00897	-2.39332
H	3.31453	-2.5474	-1.52467
H	4.05485	-0.80988	2.04192
H	4.10726	1.206	3.48323
H	2.49833	1.04547	2.7478
H	3.64621	2.23355	2.11332
H	6.17369	0.49162	2.25223
H	6.07316	-0.30628	0.67098
H	5.75198	1.4317	0.80984
H	2.57525	1.39569	-0.99043
H	-1.39749	3.35665	-1.66029
H	-1.88648	3.17712	0.01461
H	0.07899	4.6244	-0.03921
H	0.57424	3.09186	0.70084
H	1.01524	3.45608	-0.97022
H	-2.57633	-1.24348	0.39285
H	-7.63888	-0.23103	1.98759
H	-7.54156	0.71384	0.49445
H	-7.21132	-1.024	0.46504
Na	-0.74897	-1.06152	2.10523

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 19

C	5.49018	-1.39315	-0.99535
C	4.79923	-0.29612	-0.17604
C	3.33515	-0.05207	-0.56373
C	2.71751	1.12289	0.22329
C	1.307	1.49941	-0.26354
S	0.2624	2.37457	0.99992

C	-0.02375	1.16262	2.34672
C	-0.77736	-0.1644	2.06202
C	0.15868	-1.36369	1.68138
O	-0.37444	-2.34526	1.09994
O	1.36727	-1.23796	2.00793
N	-1.93176	-0.02895	1.17098
C	-3.19546	0.47382	1.70645
O	-4.15106	0.24748	0.68698
C	-3.47358	0.13498	-0.56168
C	-2.01837	-0.19732	-0.16273
O	-1.15079	-0.54263	-0.97294
C	-4.14431	-0.95217	-1.42155
C	-5.56892	-0.55219	-1.84076
C	-4.14604	-2.31759	-0.71641
O	-3.39402	1.38448	-1.21471
C	1.28973	2.36073	-1.54678
C	1.87798	3.77471	-1.43542
O	2.55699	-1.25755	-0.38838
C	6.95224	-1.61054	-0.58848
H	4.93088	-2.32885	-0.88373
H	5.44369	-1.12899	-2.06178
H	5.34837	0.64855	-0.29512
H	4.84132	-0.54807	0.89337
H	3.2899	0.15419	-1.64138
H	2.68723	0.83257	1.27812
H	3.38576	1.98854	0.15433
H	0.75702	0.58824	-0.49694
H	0.9183	0.88605	2.82297
H	-0.59429	1.76171	3.06484
H	-1.19861	-0.4742	3.02957
H	-3.11918	1.54413	1.94547
H	-3.48854	-0.09175	2.59751
H	-3.51831	-1.01843	-2.32006

H	-6.01168	-1.34491	-2.45225
H	-5.59051	0.36014	-2.44794
H	-6.21149	-0.40648	-0.96593
H	-4.51913	-3.08961	-1.39762
H	-3.14502	-2.61482	-0.38805
H	-4.79566	-2.30022	0.1643
H	-4.2925	1.67747	-1.42121
H	1.83887	1.80572	-2.31992
H	0.25377	2.4251	-1.89797
H	1.82944	4.27899	-2.40652
H	1.32604	4.38705	-0.71571
H	2.92787	3.76281	-1.12428
H	2.35405	-1.35922	0.57818
H	7.42145	-2.39593	-1.19109
H	7.54254	-0.69518	-0.71704
H	7.02949	-1.90843	0.46385
Na	0.48835	-2.08679	-0.93442

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 33

C	5.433	-0.30891	-1.27687
C	4.63612	0.07324	-0.02341
C	3.17097	0.43833	-0.3001
C	2.45135	0.901	0.98827
C	1.03023	1.45352	0.76178
S	-0.15188	1.12135	2.17381
C	-0.16486	-0.68152	2.52236
C	-0.80253	-1.66663	1.49886
C	0.23342	-2.30625	0.51585
O	-0.21003	-2.77875	-0.56129
O	1.43082	-2.29254	0.90845
N	-1.98407	-1.11289	0.8393
C	-3.2387	-1.04692	1.5897

O	-4.13748	-0.3536	0.75628
C	-3.39681	0.43301	-0.18415
C	-2.03619	-0.2992	-0.23932
O	-1.15732	-0.08022	-1.08408
C	-4.22257	0.52321	-1.47728
C	-4.47398	-0.86289	-2.09013
C	-3.62105	1.49459	-2.50437
O	-3.17231	1.73827	0.29734
C	0.96478	2.98771	0.5974
C	1.73076	3.54539	-0.61016
O	2.47997	-0.66804	-0.91271
C	6.89013	-0.67296	-0.96954
H	4.93755	-1.15095	-1.77306
H	5.40807	0.52885	-1.98853
H	5.11966	0.92893	0.46872
H	4.66099	-0.75538	0.69899
H	3.14362	1.23177	-1.0546
H	2.42673	0.03877	1.66144
H	3.06315	1.66496	1.48476
H	0.58409	0.98653	-0.1182
H	0.84662	-1.03836	2.72082
H	-0.71752	-0.71512	3.46708
H	-1.16408	-2.5217	2.08699
H	-3.09021	-0.52124	2.54598
H	-3.62942	-2.0527	1.78043
H	-5.1858	0.93226	-1.1432
H	-5.13691	-0.77121	-2.95654
H	-4.94412	-1.541	-1.37349
H	-3.54008	-1.32148	-2.43615
H	-4.30232	1.59101	-3.35679
H	-3.46827	2.48534	-2.07138
H	-2.65812	1.13141	-2.8754
H	-2.4653	1.72483	0.96825

H	-0.08713	3.2827	0.50357
H	1.34122	3.45935	1.51462
H	1.55309	4.62226	-0.69899
H	2.8118	3.40145	-0.51821
H	1.40169	3.07795	-1.54518
H	2.32944	-1.36799	-0.22312
H	7.43554	-0.93638	-1.88227
H	7.41952	0.16228	-0.4952
H	6.94836	-1.53058	-0.28904
Na	0.53666	-1.24793	-1.98031

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 37

C	5.10155	-2.66942	0.12788
C	4.82905	-1.20721	0.51445
C	3.5929	-0.57616	-0.152
C	3.40156	0.88169	0.31649
C	2.60003	1.82235	-0.6036
S	0.79081	1.41626	-0.78492
C	0.07586	1.8362	0.87415
C	-0.78575	0.75341	1.56262
C	0.0098	-0.58205	1.76216
O	-0.49251	-1.63857	1.30394
O	1.13236	-0.4317	2.30915
N	-2.11869	0.57437	0.97401
C	-3.30291	0.9408	1.74678
O	-4.39348	0.35499	1.06309
C	-4.00939	0.09122	-0.28497
C	-2.46522	0.02193	-0.20816
O	-1.73354	-0.4194	-1.0977
C	-4.74138	-1.18307	-0.74785
C	-4.3852	-2.39768	0.12396
C	-4.5289	-1.47814	-2.24139

O	-4.28199	1.21171	-1.10521
C	2.84656	3.30411	-0.25396
C	2.28828	4.3163	-1.25909
O	2.43513	-1.39401	0.08351
C	5.47613	-2.87656	-1.34566
H	5.91833	-3.04242	0.75887
H	4.21958	-3.2717	0.37233
H	5.70772	-0.59459	0.26632
H	4.69896	-1.14	1.60365
H	3.72939	-0.58524	-1.24174
H	2.97494	0.87362	1.32657
H	4.40352	1.32297	0.4072
H	2.93733	1.66388	-1.63828
H	0.91113	2.0363	1.54612
H	-0.51226	2.75135	0.76156
H	-0.96928	1.14297	2.57126
H	-3.41169	2.03421	1.8021
H	-3.25381	0.51909	2.75677
H	-5.80785	-0.95573	-0.58789
H	-4.96425	-3.26915	-0.19859
H	-4.60527	-2.21215	1.17792
H	-3.3227	-2.64957	0.03904
H	-5.15776	-2.32363	-2.5399
H	-4.78711	-0.62069	-2.86841
H	-3.48557	-1.73372	-2.44299
H	-5.24289	1.32324	-1.15446
H	2.4532	3.51548	0.74884
H	3.93395	3.44026	-0.17824
H	2.5468	5.33726	-0.95885
H	2.70404	4.14767	-2.25961
H	1.19973	4.24903	-1.34003
H	2.13637	-1.25075	1.01557
H	5.72101	-3.92579	-1.54372

H	4.65615	-2.60238	-2.01884
H	6.35022	-2.27439	-1.6239
Na	0.2864	-1.45788	-0.80575

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 48

C	5.05998	-2.74901	0.34947
C	4.80235	-1.25383	0.59389
C	3.58078	-0.67318	-0.14153
C	3.40297	0.82437	0.18777
C	2.60976	1.67828	-0.81766
S	0.79092	1.29588	-0.93383
C	0.104	1.87814	0.68818
C	-0.75528	0.87439	1.49054
C	0.02564	-0.45048	1.79434
O	-0.4957	-1.53405	1.42952
O	1.15605	-0.27227	2.31592
N	-2.10325	0.66118	0.94925
C	-3.26721	1.06283	1.73376
O	-4.3667	0.41017	1.1302
C	-4.02919	0.09308	-0.21981
C	-2.4807	0.02435	-0.1794
O	-1.76735	-0.4852	-1.04744
C	-4.74934	-1.21605	-0.60256
C	-4.52215	-1.60245	-2.07257
C	-6.25307	-1.14144	-0.2802
O	-4.32334	1.17828	-1.0791
C	2.85225	3.19365	-0.64804
C	4.27126	3.65082	-1.01961
O	2.40991	-1.45088	0.15795
C	5.45309	-3.09785	-1.09212
H	5.86227	-3.0719	1.02515
H	4.16632	-3.31476	0.63509

H	5.69089	-0.67766	0.29834
H	4.66282	-1.08311	1.6705
H	3.72553	-0.78533	-1.22436
H	2.9672	0.91424	1.19012
H	4.40914	1.25724	0.24698
H	2.9244	1.40403	-1.83518
H	0.95303	2.1346	1.32271
H	-0.4784	2.78331	0.49635
H	-0.9119	1.3579	2.46233
H	-3.39515	2.15527	1.71444
H	-3.17889	0.71385	2.76807
H	-4.3075	-1.9895	0.03835
H	-4.98084	-2.57754	-2.26903
H	-3.4595	-1.65801	-2.31348
H	-4.98151	-0.87232	-2.74726
H	-6.72216	-2.10628	-0.49751
H	-6.43336	-0.89853	0.76927
H	-6.76737	-0.39602	-0.90185
H	-5.28469	1.28318	-1.12245
H	2.13343	3.72736	-1.27934
H	2.63656	3.48603	0.38797
H	4.34893	4.741	-0.94995
H	5.03599	3.22829	-0.3604
H	4.52045	3.36679	-2.04896
H	2.11932	-1.22791	1.07646
H	5.68284	-4.16469	-1.18806
H	4.64807	-2.8746	-1.80119
H	6.34165	-2.53805	-1.41019
Na	0.23698	-1.5474	-0.69996

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 4

C	5.52772	-1.1714	-0.95523
C	4.80216	-0.08601	-0.15055
C	3.33076	0.10642	-0.53946
C	2.67478	1.26617	0.23776
C	1.27156	1.62553	-0.28383
S	0.17761	2.43731	0.97915
C	-0.01404	1.24845	2.36177
C	-0.72329	-0.11467	2.13609
C	0.24712	-1.28629	1.75824
O	-0.2574	-2.29297	1.19556
O	1.45422	-1.11497	2.07062
N	-1.913	-0.04643	1.28446
C	-3.17148	0.42415	1.85678
O	-4.14915	0.16265	0.86874
C	-3.51054	0.07343	-0.40325
C	-2.03288	-0.22213	-0.04691
O	-1.17107	-0.54259	-0.87385
C	-4.2533	-1.00049	-1.2257
C	-4.21079	-2.37926	-0.54849
C	-3.77422	-1.07302	-2.68418
O	-3.49169	1.33261	-1.04252
C	1.34164	2.58539	-1.49002
C	0.04184	2.74149	-2.28851
O	2.59101	-1.12071	-0.35048
C	6.99539	-1.33694	-0.54428
H	4.99823	-2.12284	-0.8318
H	5.47395	-0.92276	-2.02501
H	5.32059	0.87409	-0.28298
H	4.8534	-0.32168	0.9222
H	3.27727	0.30037	-1.61928
H	2.63385	0.97222	1.29061
H	3.32048	2.15149	0.17809

H	0.74804	0.71884	-0.59338
H	0.95182	1.02089	2.81533
H	-0.58513	1.84309	3.08311
H	-1.09901	-0.41398	3.12543
H	-3.11834	1.49799	2.0868
H	-3.42117	-0.14267	2.76029
H	-5.30116	-0.65979	-1.2249
H	-4.79546	-3.09867	-1.13113
H	-4.62532	-2.34254	0.46175
H	-3.18517	-2.75915	-0.48112
H	-4.41831	-1.75636	-3.24779
H	-3.80128	-0.09498	-3.1712
H	-2.74686	-1.4425	-2.74118
H	-4.40808	1.59697	-1.21124
H	1.6911	3.56724	-1.14165
H	2.12691	2.20825	-2.15908
H	0.19894	3.40389	-3.14704
H	-0.30938	1.77448	-2.66398
H	-0.76258	3.1609	-1.6785
H	2.40885	-1.22532	0.62018
H	7.49026	-2.11449	-1.13641
H	7.55645	-0.40493	-0.68365
H	7.08051	-1.61898	0.51181
Na	0.53946	-2.01074	-0.85708

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 21

C	5.64355	0.40771	-0.62899
C	4.58135	-0.70154	-0.62717
C	3.13328	-0.22062	-0.80546
C	2.60068	0.55997	0.41569
C	1.20555	1.16224	0.17364
S	0.2033	1.42894	1.72398

C	-0.00345	-0.22636	2.49569
C	-0.84474	-1.31905	1.77235
C	0.00707	-2.28971	0.88654
O	-0.60201	-2.93998	-0.00055
O	1.23645	-2.33413	1.15731
N	-2.02065	-0.7741	1.09467
C	-3.16206	-0.35538	1.90964
O	-4.07153	0.23	1.00785
C	-3.36339	0.6598	-0.15989
C	-2.10821	-0.24355	-0.14633
O	-1.3188	-0.35739	-1.0937
C	-4.3176	0.54931	-1.35954
C	-4.79902	-0.89386	-1.57268
C	-3.72838	1.14506	-2.64749
O	-2.9422	2.00023	-0.04443
C	1.22036	2.49965	-0.60017
C	1.87023	3.70134	0.10041
O	2.28326	-1.35153	-1.09672
C	7.07245	-0.14579	-0.56312
H	5.5312	1.016	-1.53779
H	5.48524	1.08772	0.2173
H	4.65002	-1.28314	0.30325
H	4.79049	-1.40078	-1.44656
H	3.082	0.4073	-1.70459
H	2.57622	-0.13996	1.25666
H	3.30995	1.34931	0.68386
H	0.61819	0.46265	-0.41935
H	0.97256	-0.66545	2.70624
H	-0.46614	0.02921	3.45434
H	-1.2361	-1.97085	2.56621
H	-2.84337	0.36301	2.68093
H	-3.63582	-1.22059	2.38666
H	-5.18091	1.16057	-1.06331

H	-5.54308	-0.92248	-2.37529
H	-5.25855	-1.30231	-0.66913
H	-3.9722	-1.55163	-1.8655
H	-4.48762	1.12907	-3.43694
H	-3.40872	2.17818	-2.49617
H	-2.86518	0.56723	-2.99026
H	-2.17682	2.05628	0.55604
H	1.74239	2.3134	-1.5485
H	0.18907	2.75189	-0.87335
H	1.84035	4.57756	-0.5557
H	1.35015	3.96304	1.02697
H	2.91976	3.51568	0.3511
H	2.13146	-1.85228	-0.25306
H	7.81287	0.66126	-0.56798
H	7.22618	-0.73414	0.34897
H	7.28387	-0.79909	-1.41768
Na	0.157	-1.90035	-1.8055

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 38

C	5.72129	0.6185	-0.45891
C	4.66826	-0.47662	-0.68383
C	3.21776	0.02235	-0.76889
C	2.66786	0.52371	0.58291
C	1.31179	1.24151	0.4485
S	0.24135	1.14046	1.97349
C	0.09145	-0.63456	2.42465
C	-0.71972	-1.60644	1.51987
C	0.14631	-2.36844	0.46079
O	-0.44989	-2.82672	-0.54707
O	1.37344	-2.45875	0.72867
N	-1.9275	-0.99634	0.96728
C	-3.09629	-0.84481	1.83334

O	-4.04847	-0.15215	1.06132
C	-3.38628	0.5406	-0.00291
C	-2.05728	-0.23824	-0.14338
O	-1.26021	-0.0955	-1.08069
C	-4.33674	0.56294	-1.21144
C	-4.6764	-0.85528	-1.69391
C	-3.82452	1.44367	-2.3613
O	-3.08749	1.87025	0.35479
C	1.50738	2.73834	0.13103
C	0.24665	3.52285	-0.25157
O	2.37662	-1.026	-1.29712
C	7.15478	0.07454	-0.49852
H	5.60646	1.39538	-1.22822
H	5.55424	1.11453	0.50527
H	4.73875	-1.23243	0.1113
H	4.88451	-0.99579	-1.62607
H	3.16854	0.82475	-1.51695
H	2.59188	-0.34855	1.23752
H	3.38895	1.20765	1.04523
H	0.72723	0.78421	-0.35215
H	1.07781	-1.07895	2.5632
H	-0.37976	-0.56804	3.41077
H	-1.07198	-2.40721	2.18537
H	-2.83352	-0.28462	2.74428
H	-3.50204	-1.82464	2.10976
H	-5.25285	1.01986	-0.81295
H	-5.42126	-0.80683	-2.4948
H	-5.08608	-1.46802	-0.88695
H	-3.79163	-1.36298	-2.09564
H	-4.58618	1.49615	-3.14685
H	-3.61142	2.45867	-2.01959
H	-2.91056	1.03109	-2.79869
H	-2.31338	1.88969	0.94342

H	2.0046	3.21982	0.9838
H	2.22012	2.79037	-0.70292
H	0.51442	4.52898	-0.59152
H	-0.30323	3.02757	-1.05861
H	-0.43752	3.63772	0.59418
H	2.23648	-1.69868	-0.58043
H	7.88774	0.8721	-0.33638
H	7.31099	-0.68458	0.27672
H	7.3754	-0.39075	-1.46628
Na	0.25403	-1.40874	-2.0964

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 22

C	5.04269	-1.86474	0.50778
C	4.75367	-1.30606	-0.89308
C	3.44441	-0.50765	-1.0385
C	3.39279	0.73057	-0.1176
C	2.52332	1.91168	-0.59132
S	0.69154	1.57822	-0.65581
C	0.1865	1.5062	1.12673
C	-0.61833	0.26713	1.57944
C	0.14794	-1.06618	1.2769
O	-0.44714	-1.944	0.60338
O	1.33556	-1.08001	1.69041
N	-2.01975	0.2623	1.14297
C	-3.08443	0.36877	2.13719
O	-4.27113	0.00816	1.45812
C	-4.06724	0.14531	0.05252
C	-2.52847	0.07823	-0.09361
O	-1.92674	-0.07049	-1.16007
C	-4.88151	-0.95593	-0.65378
C	-4.44513	-2.36261	-0.21403
C	-4.86937	-0.81339	-2.18441

O	-4.41699	1.44802	-0.37374
C	2.87357	3.21239	0.15905
C	2.22848	4.48589	-0.3965
O	2.31355	-1.37994	-0.8701
C	6.30647	-2.7331	0.53881
H	5.15317	-1.04182	1.22527
H	4.18685	-2.45783	0.85107
H	4.70731	-2.13779	-1.60824
H	5.58813	-0.66408	-1.21196
H	3.38377	-0.1692	-2.08248
H	3.09881	0.42134	0.89157
H	4.41821	1.11752	-0.03852
H	2.72249	2.08019	-1.65967
H	1.09964	1.515	1.72195
H	-0.38547	2.41186	1.34742
H	-0.66022	0.34499	2.67257
H	-3.15032	1.39343	2.53237
H	-2.92053	-0.3376	2.9587
H	-5.91317	-0.79816	-0.29964
H	-5.07783	-3.11544	-0.69544
H	-4.5293	-2.48747	0.86815
H	-3.40677	-2.5644	-0.49785
H	-5.54915	-1.55054	-2.62483
H	-5.18835	0.18173	-2.50543
H	-3.86648	-0.98473	-2.58365
H	-5.37401	1.55341	-0.26815
H	2.62906	3.10243	1.22363
H	3.96602	3.32038	0.1189
H	2.57061	5.36344	0.16228
H	2.49564	4.63596	-1.44923
H	1.13719	4.44734	-0.33695
H	2.14195	-1.49928	0.09546
H	6.49793	-3.12083	1.54512

H	6.21176	-3.59179	-0.13642
H	7.19047	-2.16312	0.2272
Na	0.06974	-1.15686	-1.44624

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 27

C	5.21303	-2.63868	0.14561
C	4.92345	-1.17243	0.50322
C	3.67253	-0.57317	-0.16517
C	3.46511	0.89151	0.27455
C	2.63956	1.8005	-0.65585
S	0.83456	1.36401	-0.80856
C	0.13138	1.80773	0.84954
C	-0.69965	0.72714	1.5781
C	0.12068	-0.59018	1.79602
O	1.24747	-0.41098	2.32529
O	-0.37016	-1.66356	1.36534
N	-2.03949	0.51092	1.01875
C	-3.21638	0.82658	1.82308
O	-4.29518	0.18462	1.17273
C	-3.94526	-0.03143	-0.19415
C	-2.39558	-0.06129	-0.15078
O	-1.66562	-0.49368	-1.04642
C	-4.63038	-1.32943	-0.66778
C	-4.38754	-1.60973	-2.15923
C	-6.13693	-1.31356	-0.35038
O	-4.26536	1.10164	-0.97912
C	2.86804	3.29286	-0.34027
C	2.2875	4.27546	-1.36201
O	2.52854	-1.40162	0.09849
C	5.57826	-2.87218	-1.32633
H	6.04015	-2.98685	0.77735
H	4.34158	-3.24764	0.41044

H	5.79113	-0.5532	0.23375
H	4.8022	-1.08352	1.59186
H	3.79935	-0.60379	-1.25569
H	4.46143	1.34905	0.34455
H	3.04946	0.89863	1.28919
H	2.96787	1.62528	-1.69074
H	0.97185	2.03998	1.50455
H	-0.47596	2.70837	0.72345
H	-0.87245	1.13935	2.57959
H	-3.37544	1.91386	1.87573
H	-3.12065	0.41249	2.83244
H	-4.17225	-2.1332	-0.07766
H	-4.82598	-2.57765	-2.42483
H	-3.32269	-1.6279	-2.39621
H	-4.85752	-0.84363	-2.78494
H	-6.58132	-2.27102	-0.64021
H	-6.32784	-1.15174	0.71271
H	-6.66616	-0.53736	-0.91975
H	-5.22906	1.18487	-1.01795
H	2.48017	3.52063	0.6611
H	3.95402	3.44551	-0.27688
H	2.53614	5.30595	-1.08699
H	2.69568	4.08978	-2.36263
H	1.19917	4.19331	-1.43058
H	2.23911	-1.24399	1.03112
H	5.83526	-3.92212	-1.5043
H	4.74928	-2.62288	-1.99818
H	6.44213	-2.26479	-1.62449
Na	0.36641	-1.51508	-0.75906

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 1

C	5.5994	-1.03317	-1.10232
C	4.86163	-0.00816	-0.23221
C	3.37892	0.16559	-0.58537
C	2.70869	1.26473	0.26435
C	1.28677	1.61419	-0.21131
S	0.19703	2.32688	1.11414
C	0.07393	1.06537	2.43838
C	-0.60373	-0.30488	2.16314
C	0.38781	-1.42863	1.7033
O	1.59765	-1.23895	1.99429
O	-0.10354	-2.41975	1.10287
N	-1.81806	-0.23033	1.34739
C	-3.08057	0.14624	1.97553
O	-4.06967	-0.1291	1.00371
C	-3.46796	-0.07557	-0.28944
C	-1.96739	-0.33559	0.01161
O	-1.11275	-0.57982	-0.84833
C	-4.16392	-1.12824	-1.18054
C	-3.65647	-1.10379	-2.63086
C	-5.69496	-0.96956	-1.1371
O	-3.51651	1.23315	-0.81797
C	1.30907	2.63825	-1.36557
C	-0.01016	2.80411	-2.1296
O	2.67455	-1.089	-0.44871
C	7.07703	-1.18357	-0.72241
H	5.09455	-2.00224	-1.01969
H	5.52244	-0.7321	-2.1571
H	5.35393	0.97022	-0.32454
H	4.93814	-0.29577	0.82632
H	3.29963	0.41475	-1.65212
H	2.69628	0.91319	1.30014
H	3.33046	2.1687	0.24108

H	0.78045	0.7116	-0.55899
H	1.05746	0.84386	2.85546
H	-0.49404	1.60686	3.20277
H	-0.94404	-0.66295	3.14564
H	-3.07849	1.21119	2.24912
H	-3.27387	-0.47106	2.85891
H	-3.91592	-2.10009	-0.73458
H	-4.12591	-1.91545	-3.19709
H	-2.57278	-1.22076	-2.68092
H	-3.9117	-0.15864	-3.12114
H	-6.16261	-1.77124	-1.7176
H	-6.08079	-1.01249	-0.11636
H	-6.0183	-0.02357	-1.59162
H	-4.44409	1.46888	-0.96308
H	1.64169	3.60876	-0.97191
H	2.08944	2.31694	-2.06878
H	0.11278	3.51661	-2.95285
H	-0.34458	1.85045	-2.5518
H	-0.81214	3.16828	-1.48206
H	2.51897	-1.25073	0.5187
H	7.58027	-1.91812	-1.3606
H	7.61388	-0.23245	-0.82272
H	7.18594	-1.51628	0.3166
Na	0.63186	-2.00729	-0.94832

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 43

C	5.04452	-1.85693	0.50402
C	4.75569	-1.29705	-0.8965
C	3.44482	-0.50146	-1.04243
C	3.3891	0.73523	-0.1198
C	2.51249	1.91288	-0.58946
S	0.68189	1.57015	-0.64343

C	0.18778	1.49086	1.14184
C	-0.61628	0.24843	1.58592
C	0.15332	-1.08054	1.27441
O	-0.44034	-1.95521	0.59563
O	1.34095	-1.09336	1.68694
N	-2.01572	0.24244	1.14227
C	-3.08521	0.44348	2.11806
O	-4.28437	0.13936	1.43398
C	-4.06133	0.15819	0.04255
C	-2.5265	0.04951	-0.08859
O	-1.93361	-0.08957	-1.16721
C	-4.8964	-0.96886	-0.59667
C	-4.44179	-2.35374	-0.10845
C	-4.93454	-0.90012	-2.13202
O	-4.44032	1.45217	-0.42787
C	2.85985	3.21501	0.15974
C	2.20749	4.48579	-0.39337
O	2.31547	-1.37619	-0.87651
C	6.30954	-2.72348	0.5349
H	5.1533	-1.03475	1.22259
H	4.18949	-2.45184	0.84621
H	4.71198	-2.1279	-1.61278
H	5.58908	-0.65292	-1.21368
H	3.38458	-0.16152	-2.08596
H	3.09996	0.42313	0.88988
H	4.41263	1.12743	-0.04311
H	2.70555	2.0822	-1.65876
H	1.10386	1.49343	1.73255
H	-0.3807	2.3964	1.37211
H	-0.66313	0.31687	2.67948
H	-3.09163	1.48209	2.47974
H	-2.97704	-0.24593	2.96307
H	-5.91186	-0.7822	-0.2219

H	-5.10071	-3.12769	-0.51549
H	-4.47498	-2.42247	0.98192
H	-3.41924	-2.57975	-0.43012
H	-5.58159	-1.69532	-2.51649
H	-5.34577	0.04956	-2.48912
H	-3.93854	-1.03519	-2.56387
H	-4.0936	1.56438	-1.32543
H	2.61974	3.10379	1.22515
H	3.9516	3.32759	0.11541
H	2.5485	5.36471	0.16378
H	2.46975	4.6368	-1.4472
H	1.1166	4.44328	-0.32881
H	2.14738	-1.50285	0.08871
H	6.50063	-3.11209	1.54089
H	6.21657	-3.58152	-0.14136
H	7.19296	-2.15188	0.22474
Na	0.07154	-1.17509	-1.45071

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 14

C	5.15439	-1.83503	0.47348
C	4.84875	-1.2614	-0.91773
C	3.52381	-0.48643	-1.04618
C	3.45375	0.73935	-0.10981
C	2.56378	1.91089	-0.56904
S	0.73896	1.54417	-0.64161
C	0.23252	1.44451	1.13917
C	-0.54675	0.18589	1.5832
C	0.24459	-1.12987	1.26869
O	-0.33465	-2.01103	0.58553
O	1.43164	-1.12683	1.68367
N	-1.94874	0.15473	1.15062
C	-3.01309	0.16979	2.1496

O	-4.17811	-0.23651	1.45906
C	-3.99707	0.00777	0.06449
C	-2.45451	-0.01025	-0.08952
O	-1.84465	-0.11635	-1.15679
C	-4.76246	-1.07814	-0.71903
C	-4.70892	-0.8514	-2.23815
C	-6.21835	-1.197	-0.23244
O	-4.38155	1.32841	-0.26781
C	2.88972	3.20779	0.19869
C	2.2223	4.47637	-0.34157
O	2.41004	-1.38135	-0.88349
C	6.44036	-2.67061	0.48906
H	5.24434	-1.02141	1.20433
H	4.31471	-2.45581	0.80765
H	4.81631	-2.08314	-1.64509
H	5.66909	-0.5983	-1.23
H	3.45172	-0.13595	-2.08549
H	3.16627	0.41327	0.89599
H	4.47267	1.14243	-0.02733
H	2.76183	2.09684	-1.63472
H	1.14536	1.46585	1.73455
H	-0.35739	2.33643	1.36811
H	-0.58751	0.25585	2.67685
H	-3.13595	1.17604	2.5769
H	-2.80947	-0.55319	2.94673
H	-4.25275	-2.02118	-0.48424
H	-5.19446	-1.68911	-2.75013
H	-3.68149	-0.7679	-2.59581
H	-5.23674	0.06639	-2.5181
H	-6.71561	-2.01507	-0.7633
H	-6.2752	-1.39673	0.83984
H	-6.79592	-0.28747	-0.44642
H	-5.3406	1.40453	-0.16015

H	2.64562	3.07971	1.26131
H	3.98007	3.33609	0.16189
H	2.54688	5.35276	0.22937
H	2.48875	4.64508	-1.39167
H	1.13178	4.41673	-0.28508
H	2.24435	-1.5161	0.08096
H	6.64211	-3.07134	1.48824
H	6.36809	-3.51914	-0.20163
H	7.30913	-2.0722	0.18811
Na	0.15846	-1.19619	-1.45536

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 18

C	-5.53727	-1.1992	0.64165
C	-4.72782	-0.17652	-0.172
C	-3.27891	0.02778	0.29462
C	-2.55194	1.0839	-0.56684
C	-1.15311	1.42642	-0.02615
S	0.04709	2.04465	-1.31359
C	0.22446	0.6934	-2.54686
C	0.88576	-0.65324	-2.13307
C	-0.1378	-1.74631	-1.67471
O	0.30956	-2.69926	-0.98727
O	-1.32686	-1.56859	-2.05086
N	2.01092	-0.47478	-1.21671
C	3.27625	0.02723	-1.75373
O	4.11262	0.2113	-0.63555
C	3.30797	0.33461	0.54292
C	1.99074	-0.36152	0.13014
O	1.08416	-0.66306	0.91827
C	4.09827	-0.2648	1.71711
C	4.41079	-1.75141	1.48775
C	3.42069	-0.03343	3.07643

O	3.0223	1.68374	0.83494
C	-1.15702	2.45294	1.12893
C	-1.61617	3.87824	0.7899
O	-2.56389	-1.2267	0.28783
C	-5.81876	-0.77879	2.09035
H	-6.49258	-1.36519	0.12785
H	-5.00966	-2.15977	0.63118
H	-5.23768	0.79704	-0.14588
H	-4.70423	-0.48793	-1.22535
H	-3.27706	0.34418	1.34444
H	-2.48379	0.68424	-1.58307
H	-3.17109	1.98603	-0.6246
H	-0.69675	0.51734	0.36299
H	-0.74739	0.44971	-2.97797
H	0.82056	1.17928	-3.32603
H	1.31631	-1.07176	-3.05375
H	3.11924	0.97187	-2.29717
H	3.73093	-0.71047	-2.42459
H	5.04479	0.29244	1.70664
H	5.05213	-2.12543	2.29229
H	4.9282	-1.91169	0.53853
H	3.49571	-2.35526	1.48673
H	4.07598	-0.39553	3.87612
H	3.22258	1.0269	3.24634
H	2.47154	-0.57319	3.14084
H	2.34558	2.02	0.22017
H	-1.80626	2.04578	1.91586
H	-0.15093	2.48827	1.56272
H	-1.6008	4.50058	1.69081
H	-0.96375	4.3507	0.04924
H	-2.6367	3.90076	0.39371
H	-2.34574	-1.45524	-0.65398
H	-6.44695	-1.51895	2.59777

H	-4.89781	-0.67919	2.67585
H	-6.3433	0.18393	2.13065
Na	-0.57824	-2.17961	0.97804

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 9

C	5.80671	0.30208	-0.66594
C	4.70136	-0.76099	-0.58609
C	3.27129	-0.22546	-0.75348
C	2.78983	0.61004	0.44999
C	1.44005	1.30858	0.20282
S	0.48949	1.68895	1.75369
C	0.14115	0.08833	2.57994
C	-0.75202	-0.97827	1.89161
C	0.04247	-2.02116	1.03179
O	-0.60422	-2.6613	0.16177
O	1.2654	-2.13269	1.30621
N	-1.92908	-0.43524	1.20989
C	-3.11057	-0.08558	1.99384
O	-4.1266	0.16494	1.04211
C	-3.52056	0.50439	-0.20363
C	-2.08801	-0.07081	-0.07799
O	-1.28505	-0.14484	-1.01552
C	-4.4017	-0.07899	-1.32807
C	-4.52489	-1.60769	-1.22837
C	-3.94832	0.36112	-2.72896
O	-3.35079	1.90211	-0.3131
C	1.6189	2.64682	-0.54487
C	0.33703	3.25507	-1.12634
O	2.36942	-1.32864	-0.99758
C	7.21407	-0.30388	-0.59922
H	5.69872	0.86693	-1.60287
H	5.69276	1.03094	0.14609

H	4.77001	-1.3011	0.36902
H	4.86052	-1.50572	-1.37636
H	3.23056	0.37618	-1.67126
H	2.7253	-0.06686	1.30735
H	3.5432	1.36717	0.69749
H	0.79258	0.66386	-0.3943
H	1.06846	-0.41644	2.8551
H	-0.33834	0.42416	3.50604
H	-1.15604	-1.59062	2.71096
H	-2.91976	0.80316	2.61225
H	-3.41733	-0.92598	2.62584
H	-5.39849	0.35015	-1.13774
H	-5.2004	-1.97918	-2.00584
H	-4.9214	-1.91447	-0.25755
H	-3.5539	-2.09608	-1.36734
H	-4.67291	0.01617	-3.47418
H	-3.86506	1.44801	-2.80788
H	-2.97146	-0.06379	-2.97426
H	-4.22844	2.31181	-0.31646
H	2.10839	3.36587	0.12662
H	2.33043	2.46835	-1.36244
H	0.56622	4.17334	-1.67843
H	-0.15407	2.55774	-1.81327
H	-0.387	3.49997	-0.34478
H	2.19117	-1.78211	-0.13314
H	7.98499	0.47207	-0.65739
H	7.36357	-0.85284	0.33783
H	7.38318	-1.00575	-1.42425
Na	0.20911	-1.7027	-1.66695

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 24

C	-5.96805	-0.01761	-0.2933
C	-4.78879	0.95056	-0.49864
C	-3.39849	0.31358	-0.65916
C	-2.89606	-0.37369	0.62624
C	-1.57856	-1.14666	0.42892
S	-0.58713	-1.35002	1.9869
C	-0.16107	0.33535	2.56929
C	0.74666	1.25901	1.71192
C	-0.04	2.20967	0.74421
O	-1.24633	2.41091	1.03987
O	0.59736	2.69708	-0.22632
N	1.87071	0.5778	1.06601
C	3.07227	0.27701	1.8422
O	4.03463	-0.14322	0.89288
C	3.35645	-0.61038	-0.27022
C	1.95798	0.03894	-0.16535
O	1.12811	0.02425	-1.08148
C	4.13759	-0.1982	-1.53129
C	5.4905	-0.92313	-1.62957
C	4.32576	1.32466	-1.61444
O	3.11683	-2.00032	-0.19786
C	-1.82547	-2.56407	-0.12908
C	-0.58604	-3.28639	-0.6707
O	-2.46439	1.33081	-1.08843
C	-6.23322	-0.95873	-1.47658
H	-5.82003	-0.60819	0.61957
H	-6.86687	0.58556	-0.11321
H	-4.74519	1.65456	0.34368
H	-4.97209	1.55354	-1.39732
H	-3.42143	-0.40534	-1.48654
H	-2.77751	0.4068	1.38406
H	-3.66136	-1.06481	0.99929

H	-0.93215	-0.60964	-0.26734
H	-1.06204	0.90952	2.79136
H	0.33498	0.11748	3.52149
H	1.20847	1.95764	2.42472
H	2.87195	-0.51389	2.57908
H	3.44207	1.17671	2.34551
H	3.50367	-0.52201	-2.36605
H	6.01563	-0.6062	-2.53626
H	5.38244	-2.01191	-1.6953
H	6.12966	-0.68493	-0.7727
H	4.7729	1.59368	-2.57728
H	3.37753	1.86386	-1.52238
H	4.99127	1.67867	-0.82101
H	3.96982	-2.45662	-0.19257
H	-2.30907	-3.17266	0.64769
H	-2.56321	-2.46925	-0.93748
H	-0.86319	-4.26292	-1.08323
H	-0.10551	-2.70462	-1.46434
H	0.16402	-3.44673	0.10824
H	-2.2366	1.89286	-0.30314
H	-7.13362	-1.55853	-1.3056
H	-6.38188	-0.39289	-2.40433
H	-5.40523	-1.65646	-1.6434
Na	-0.3279	1.54334	-1.88578

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 12

C	5.18209	-0.69728	0.05257
C	4.60421	0.10705	-1.12094
C	3.07944	0.30632	-1.12123
C	2.55144	1.03327	0.13564
C	1.08178	1.46239	-0.0179
S	0.1511	1.64229	1.58814

C	0.20485	0.00072	2.41336
C	-0.52241	-1.21645	1.77111
C	0.39301	-2.09018	0.84915
O	1.63204	-1.96323	1.03737
O	-0.17895	-2.84122	0.01879
N	-1.80314	-0.85495	1.16423
C	-2.93887	-0.57853	2.04533
O	-3.97364	-0.14086	1.19651
C	-3.40416	0.35538	-0.02044
C	-2.04113	-0.37245	-0.07677
O	-1.3065	-0.40527	-1.07328
C	-4.4099	0.09078	-1.1521
C	-4.67762	-1.41105	-1.3327
C	-4.01002	0.75813	-2.47685
O	-3.16104	1.74204	0.0499
C	0.88613	2.77775	-0.80488
C	1.43098	4.06025	-0.16003
O	2.39762	-0.9527	-1.31408
C	6.69265	-0.92351	-0.08582
H	4.98201	-0.17874	0.99835
H	4.67553	-1.66756	0.12089
H	4.86843	-0.39175	-2.06284
H	5.07634	1.09989	-1.1513
H	2.82822	0.8943	-2.01292
H	2.66043	0.35542	0.98573
H	3.1846	1.90386	0.34068
H	0.54534	0.68539	-0.56134
H	1.23949	-0.29994	2.58268
H	-0.23766	0.22773	3.38862
H	-0.76865	-1.89123	2.60321
H	-2.67467	0.19171	2.78652
H	-3.25939	-1.49051	2.56128
H	-5.33429	0.56522	-0.79566

H	-5.46624	-1.56154	-2.07697
H	-4.99969	-1.8777	-0.39828
H	-3.78276	-1.93504	-1.68851
H	-4.80467	0.60626	-3.21545
H	-3.85824	1.83205	-2.35013
H	-3.08638	0.32723	-2.87439
H	-2.37077	1.91457	0.59317
H	1.36488	2.63876	-1.78351
H	-0.18308	2.90105	-1.01293
H	1.26027	4.91408	-0.82406
H	0.93962	4.27808	0.79313
H	2.50796	4.00256	0.02895
H	2.3634	-1.4316	-0.44593
H	7.08702	-1.49772	0.75928
H	6.92818	-1.47655	-1.00289
H	7.23627	0.02834	-0.12458
Na	0.30833	-1.76767	-1.85703

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 44

C	4.88336	-1.9754	0.56211
C	4.63461	-1.44344	-0.85696
C	3.35799	-0.6015	-1.04217
C	3.33597	0.65863	-0.14974
C	2.50029	1.84995	-0.6534
S	0.65889	1.57465	-0.70195
C	0.1532	1.54958	1.08299
C	-0.68208	0.3398	1.55953
C	0.04597	-1.0186	1.27617
O	-0.57407	-1.88975	0.61671
O	1.23393	-1.05923	1.68744
N	-2.08531	0.36658	1.12904
C	-3.14107	0.522	2.12618

O	-4.34169	0.18779	1.45828
C	-4.14086	0.29789	0.05017
C	-2.60565	0.17867	-0.10231
O	-2.01451	-0.00614	-1.16901
C	-4.99504	-0.78533	-0.63654
C	-4.60775	-2.19936	-0.17509
C	-4.98176	-0.66789	-2.16924
O	-4.44954	1.60531	-0.39359
C	2.84899	3.17751	0.05277
C	4.24932	3.7178	-0.27605
O	2.19341	-1.42794	-0.87122
C	6.11003	-2.89315	0.63389
H	5.01828	-1.13846	1.25879
H	3.99988	-2.52344	0.91001
H	4.5669	-2.29145	-1.55098
H	5.49692	-0.8416	-1.18003
H	3.32524	-0.28535	-2.09425
H	3.02327	0.38097	0.86302
H	4.37201	1.01097	-0.07021
H	2.69697	1.98529	-1.72692
H	1.06632	1.54988	1.67807
H	-0.39706	2.47279	1.28386
H	-0.71687	0.43674	2.6514
H	-3.17311	1.55434	2.50526
H	-2.99514	-0.17633	2.95789
H	-6.01969	-0.58581	-0.28306
H	-5.26567	-2.93711	-0.64598
H	-4.69732	-2.30518	0.90869
H	-3.57675	-2.44125	-0.45471
H	-5.68908	-1.38669	-2.5964
H	-5.2651	0.333	-2.5054
H	-3.98677	-0.88189	-2.56769
H	-5.40246	1.74293	-0.28809

H	2.10476	3.92592	-0.24085
H	2.75536	3.05149	1.13921
H	4.39934	4.69494	0.1952
H	5.04832	3.05972	0.07954
H	4.37795	3.84905	-1.35711
H	2.01494	-1.52827	0.09531
H	6.27292	-3.25973	1.65309
H	5.98844	-3.76608	-0.01834
H	7.02051	-2.36872	0.31855
Na	-0.04379	-1.14676	-1.44659

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 28

C	5.2526	-0.55445	-0.01074
C	4.66424	0.42936	-1.03285
C	3.13688	0.60457	-1.00203
C	2.59628	1.07815	0.36431
C	1.14737	1.59418	0.27408
S	0.16916	1.41907	1.85394
C	0.29907	-0.3332	2.39426
C	-0.39643	-1.45919	1.57529
C	0.53068	-2.14765	0.51753
O	-0.03038	-2.752	-0.43155
O	1.76773	-2.03636	0.72683
N	-1.6984	-1.05774	1.04664
C	-2.8447	-1.01954	1.95471
O	-3.91065	-0.50688	1.19056
C	-3.38679	0.21816	0.07226
C	-1.97239	-0.38589	-0.09314
O	-1.237	-0.19092	-1.07075
C	-4.37698	0.06562	-1.09391
C	-4.55452	-1.40485	-1.50153
C	-4.02077	0.9477	-2.30038

O	-3.25172	1.58988	0.36519
C	1.11349	3.08686	-0.11414
C	-0.26191	3.66075	-0.47299
O	2.47414	-0.60894	-1.42104
C	6.76423	-0.7424	-0.18872
H	5.05214	-0.20104	1.00834
H	4.75341	-1.52665	-0.102
H	4.93431	0.10062	-2.04511
H	5.12306	1.41897	-0.89323
H	2.8758	1.34089	-1.77276
H	2.67232	0.23851	1.05839
H	3.2411	1.87593	0.75448
H	0.59833	1.02215	-0.47683
H	1.34503	-0.62085	2.50606
H	-0.13682	-0.28291	3.39744
H	-0.60504	-2.26406	2.29426
H	-2.62906	-0.37907	2.82425
H	-3.10088	-2.02857	2.29694
H	-5.32758	0.42457	-0.67656
H	-5.3338	-1.48676	-2.26609
H	-4.84699	-2.02583	-0.65108
H	-3.63117	-1.81613	-1.9262
H	-4.80731	0.86346	-3.0582
H	-3.93149	1.99725	-2.01239
H	-3.07496	0.63505	-2.75226
H	-2.4628	1.73624	0.91562
H	1.56709	3.67475	0.69509
H	1.77951	3.2	-0.98013
H	-0.15981	4.68001	-0.86045
H	-0.76002	3.05526	-1.23739
H	-0.92492	3.70801	0.39585
H	2.45901	-1.23918	-0.65492
H	7.16684	-1.44311	0.55044

H	6.99962	-1.13702	-1.1843
H	7.30032	0.20761	-0.07408
Na	0.40072	-1.34694	-2.08988

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 42

C	5.80652	0.00244	-0.69688
C	4.6716	-1.00707	-0.46955
C	3.25852	-0.47582	-0.75456
C	2.79186	0.58975	0.25871
C	1.43372	1.21589	-0.10548
S	0.51245	1.94363	1.3353
C	0.12874	0.53685	2.44588
C	-0.78959	-0.61821	1.96081
C	-0.01688	-1.82315	1.31891
O	-0.67707	-2.60003	0.57957
O	1.20233	-1.91021	1.61705
N	-1.94478	-0.1873	1.17003
C	-3.13009	0.33174	1.85034
O	-4.12821	0.41628	0.85007
C	-3.49403	0.49512	-0.4238
C	-2.07919	-0.06985	-0.16511
O	-1.2766	-0.33826	-1.06645
C	-4.30151	-0.30888	-1.45888
C	-5.66808	0.33511	-1.74683
C	-4.46609	-1.77753	-1.0375
O	-3.28261	1.83734	-0.80825
C	1.50917	2.30605	-1.19843
C	2.26826	3.5917	-0.83965
O	2.33046	-1.5838	-0.79253
C	7.19522	-0.62214	-0.5125
H	5.72643	0.4165	-1.71215
H	5.70197	0.85113	-0.0099

H	4.70791	-1.38277	0.56301
H	4.82629	-1.8759	-1.12195
H	3.24109	-0.06161	-1.7712
H	2.73097	0.10129	1.23646
H	3.55324	1.3715	0.34398
H	0.77551	0.43801	-0.49101
H	1.04646	0.06969	2.80681
H	-0.3396	1.04581	3.29531
H	-1.21711	-1.05545	2.87478
H	-2.92702	1.31877	2.28973
H	-3.46562	-0.36444	2.62644
H	-3.6949	-0.26892	-2.37213
H	-6.21463	-0.26707	-2.47964
H	-5.57886	1.34107	-2.17292
H	-6.27862	0.39137	-0.83921
H	-4.92241	-2.35098	-1.85129
H	-3.50787	-2.2465	-0.79187
H	-5.1141	-1.86075	-0.15939
H	-4.14465	2.26221	-0.91837
H	1.97654	1.85042	-2.08233
H	0.48498	2.5601	-1.494
H	2.27014	4.27705	-1.69408
H	1.80461	4.1136	0.00309
H	3.31261	3.39591	-0.5748
H	2.13801	-1.85942	0.14108
H	7.98897	0.11419	-0.67851
H	7.31704	-1.02124	0.50122
H	7.35376	-1.44905	-1.21461
Na	0.16434	-2.03855	-1.39965

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 41

C	5.7998	-0.86952	-1.00331
C	4.94782	0.06675	-0.12527
C	3.47671	0.22985	-0.5358
C	2.78437	1.35361	0.26574
C	1.379	1.69649	-0.26032
S	0.25965	2.45667	1.01283
C	0.07706	1.2285	2.36208
C	-0.60656	-0.13952	2.09358
C	0.38662	-1.28203	1.68438
O	-0.09675	-2.27715	1.08308
O	1.5883	-1.10129	2.01086
N	-1.79166	-0.06992	1.23611
C	-3.07322	0.3347	1.81101
O	-4.03575	0.05727	0.8111
C	-3.38341	0.02636	-0.45564
C	-1.89934	-0.21669	-0.09854
O	-1.03101	-0.48713	-0.93589
C	-4.00006	-1.07873	-1.33245
C	-5.4527	-0.75717	-1.72204
C	-3.9062	-2.4582	-0.66194
O	-3.40363	1.29693	-1.07154
C	1.43966	2.68587	-1.44309
C	0.14236	2.83764	-2.24661
O	2.74688	-1.01087	-0.40191
C	5.58657	-2.37259	-0.77917
H	5.62358	-0.62494	-2.06097
H	6.85633	-0.63643	-0.81628
H	5.39989	1.06725	-0.15043
H	4.98764	-0.26192	0.92309
H	3.44041	0.45949	-1.60933
H	2.73854	1.02928	1.30948
H	3.40836	2.25562	0.23851

H	0.87554	0.78787	-0.59593
H	1.04314	1.00576	2.81769
H	-0.51045	1.79364	3.0939
H	-0.98159	-0.47448	3.07163
H	-3.06516	1.40418	2.06574
H	-3.30399	-0.26321	2.69915
H	-3.38557	-1.0848	-2.24128
H	-5.85787	-1.56436	-2.34057
H	-5.53763	0.16214	-2.31294
H	-6.08887	-0.66429	-0.83536
H	-4.23727	-3.23549	-1.35873
H	-2.88428	-2.69822	-0.35163
H	-4.54494	-2.50394	0.22564
H	-4.32375	1.53111	-1.25692
H	1.76881	3.66537	-1.0692
H	2.23623	2.33898	-2.11521
H	0.29317	3.52257	-3.08843
H	-0.19007	1.87381	-2.6466
H	-0.67298	3.22884	-1.63237
H	2.55833	-1.15407	0.56241
H	6.27098	-2.95825	-1.40375
H	5.77785	-2.64245	0.26637
H	4.56222	-2.67219	-1.01248
Na	0.70867	-1.91254	-0.95587

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 13

C	5.42053	-1.45907	-0.85088
C	4.72806	-0.3025	-0.11946
C	3.2667	-0.08371	-0.53213
C	2.6484	1.14485	0.16788
C	1.24099	1.48983	-0.35014
S	0.18885	2.44541	0.84818

C	-0.08235	1.33702	2.28296
C	-0.83538	-0.00895	2.10316
C	0.09957	-1.23176	1.80622
O	-0.43423	-2.25355	1.30033
O	1.30932	-1.08159	2.11898
N	-1.99911	0.06203	1.21601
C	-3.24539	0.62983	1.72314
O	-4.21145	0.35423	0.72742
C	-3.55002	0.14014	-0.51799
C	-2.0951	-0.18983	-0.10494
O	-1.22846	-0.59521	-0.88835
C	-4.32031	-0.96489	-1.2717
C	-4.35146	-2.28479	-0.485
C	-3.81237	-1.17595	-2.70665
O	-3.46345	1.34241	-1.25323
C	1.2317	2.26858	-1.68539
C	1.82337	3.68526	-1.6606
O	2.48485	-1.27181	-0.27517
C	6.8774	-1.65327	-0.41476
H	4.85533	-2.38167	-0.67705
H	5.38525	-1.27277	-1.93401
H	5.2808	0.62942	-0.30441
H	4.7635	-0.47494	0.9659
H	3.22731	0.04575	-1.62195
H	2.61291	0.9281	1.23995
H	3.31897	2.00211	0.04167
H	0.69129	0.56591	-0.52788
H	0.86332	1.09864	2.77236
H	-0.64908	1.98651	2.95901
H	-1.24791	-0.24686	3.09459
H	-3.14299	1.71223	1.8864
H	-3.54473	0.13511	2.65357
H	-5.35226	-0.58243	-1.32464

H	-4.95091	-3.02589	-1.02371
H	-4.78886	-2.14939	0.50707
H	-3.34428	-2.69765	-0.35845
H	-4.47388	-1.87426	-3.23031
H	-3.78339	-0.24046	-3.27097
H	-2.80191	-1.59357	-2.7063
H	-4.36392	1.63295	-1.46011
H	1.78266	1.6642	-2.41914
H	0.19743	2.31327	-2.04475
H	1.78047	4.12781	-2.66162
H	1.27028	4.34283	-0.98295
H	2.87191	3.69019	-1.34481
H	2.28612	-1.3074	0.69706
H	7.34822	-2.48244	-0.95415
H	7.47411	-0.75249	-0.60291
H	6.94257	-1.87473	0.65708
Na	0.4132	-2.13449	-0.74998

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 31

C	4.99863	-1.94161	0.53291
C	4.73197	-1.39923	-0.87889
C	3.43812	-0.58075	-1.04866
C	3.39593	0.66947	-0.14315
C	2.53954	1.85095	-0.63494
S	0.70441	1.54084	-0.69212
C	0.19411	1.49391	1.0912
C	-0.61549	0.26479	1.56278
C	0.13836	-1.07768	1.27078
O	1.32629	-1.10006	1.68306
O	-0.46591	-1.95463	0.6041
N	-2.01987	0.26283	1.1365
C	-3.07834	0.32482	2.13989

O	-4.25717	-0.0637	1.46274
C	-4.07678	0.14765	0.0627
C	-2.53598	0.08781	-0.09806
O	-1.93468	-0.05366	-1.16614
C	-4.87209	-0.93528	-0.69485
C	-4.82409	-0.73863	-2.21833
C	-6.32672	-1.01271	-0.19642
O	-4.43039	1.47024	-0.29508
C	2.86263	3.17658	0.08713
C	4.25317	3.74652	-0.23349
O	2.29056	-1.43141	-0.88132
C	6.24508	-2.83346	0.58852
H	5.11894	-1.10985	1.23846
H	4.12875	-2.51245	0.87851
H	4.67796	-2.24069	-1.58201
H	5.58042	-0.77661	-1.19935
H	3.39401	-0.25441	-2.09721
H	3.08857	0.37635	0.86692
H	4.42576	1.03886	-0.06057
H	2.73646	2.00196	-1.70632
H	1.10632	1.5102	1.68744
H	-0.37583	2.40407	1.29631
H	-0.64939	0.35693	2.65503
H	-3.17265	1.34182	2.54857
H	-2.88963	-0.38818	2.9496
H	-4.38179	-1.88486	-0.44554
H	-5.33011	-1.57573	-2.71109
H	-3.79756	-0.68298	-2.58387
H	-5.33518	0.18426	-2.51224
H	-6.8451	-1.83055	-0.70708
H	-6.38023	-1.18933	0.88006
H	-6.88649	-0.0956	-0.42495
H	-5.38705	1.57154	-0.18708

H	2.10505	3.91465	-0.19852
H	2.77059	3.03629	1.17195
H	4.38549	4.71956	0.25134
H	5.0637	3.09787	0.1133
H	4.37967	3.89498	-1.31256
H	2.11685	-1.54449	0.08447
H	6.42088	-3.20812	1.60262
H	6.13914	-3.70125	-0.07326
H	7.14245	-2.28587	0.27498
Na	0.04371	-1.18679	-1.45209

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 30

C	5.74784	0.05981	-0.27879
C	4.60362	-0.93974	-0.52784
C	3.19497	-0.34364	-0.68527
C	2.65924	0.28676	0.61868
C	1.30219	0.98629	0.42484
S	0.25816	1.08691	1.96699
C	-0.07052	-0.64462	2.48577
C	-0.93683	-1.57211	1.58427
C	-0.10038	-2.45212	0.59494
O	-0.70652	-2.9358	-0.39483
O	1.11407	-2.60141	0.89408
N	-2.05384	-0.87019	0.95261
C	-3.21394	-0.52017	1.77336
O	-4.05117	0.24074	0.93414
C	-3.26933	0.79935	-0.12735
C	-2.0624	-0.1647	-0.20115
O	-1.23976	-0.18586	-1.12645
C	-4.17086	0.92391	-1.36582
C	-4.70332	-0.44247	-1.82277
C	-3.49871	1.68394	-2.51973

O	-2.7879	2.08217	0.20505
C	1.40447	2.4165	-0.15066
C	2.07701	3.47386	0.73656
O	2.29877	-1.37234	-1.16001
C	5.98967	1.05032	-1.42624
H	5.57376	0.61247	0.65319
H	6.66502	-0.51884	-0.11204
H	4.57449	-1.67175	0.29089
H	4.81564	-1.50709	-1.44312
H	3.20496	0.4044	-1.48639
H	2.57332	-0.51973	1.35351
H	3.39508	0.99465	1.01355
H	0.70592	0.40489	-0.27682
H	0.86954	-1.16741	2.66684
H	-0.56112	-0.49854	3.45357
H	-1.39359	-2.30786	2.26122
H	-2.90245	0.05612	2.65845
H	-3.74912	-1.42169	2.09199
H	-5.01995	1.52338	-1.01039
H	-5.42039	-0.30774	-2.63902
H	-5.20955	-0.9697	-1.01018
H	-3.89431	-1.08102	-2.19655
H	-4.21899	1.8219	-3.33349
H	-3.15044	2.66734	-2.19727
H	-2.64123	1.12912	-2.91125
H	-2.05136	2.00632	0.8383
H	1.954	2.34191	-1.09884
H	0.39645	2.75435	-0.41788
H	2.11359	4.43458	0.21241
H	1.52995	3.62688	1.67185
H	3.10552	3.2026	0.99607
H	2.08852	-1.97665	-0.40099
H	6.86715	1.67442	-1.22608

H	6.1656	0.52285	-2.37153
H	5.13928	1.72434	-1.57693
Na	0.18044	-1.69824	-2.0078

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 7

C	-5.8373	-0.68217	-0.49491
C	-4.77424	0.38082	-0.80875
C	-3.3231	-0.12287	-0.7849
C	-2.81891	-0.46042	0.63265
C	-1.44216	-1.15154	0.63955
S	-0.4861	-0.92035	2.21569
C	-0.21243	0.88147	2.4197
C	0.64003	1.67624	1.39403
C	-0.19147	2.31871	0.23027
O	0.43411	2.63777	-0.81463
O	-1.41926	2.4719	0.45916
N	1.84607	0.98402	0.93453
C	3.05159	1.01887	1.75657
O	4.07783	0.51475	0.9247
C	3.49158	-0.31819	-0.07502
C	2.02664	0.19035	-0.13965
O	1.2174	-0.11201	-1.02481
C	4.31457	-0.15276	-1.37198
C	3.83104	-1.07657	-2.50062
C	5.81738	-0.35862	-1.10704
O	3.39942	-1.65575	0.36861
C	-1.57191	-2.67332	0.41902
C	-0.2688	-3.40736	0.08088
O	-2.46381	0.85899	-1.40743
C	-7.2672	-0.14678	-0.64051
H	-5.70074	-1.54061	-1.16789
H	-5.70151	-1.06621	0.52365

H	-4.87031	1.22363	-0.10933
H	-4.95716	0.78715	-1.81168
H	-3.25097	-1.00733	-1.43195
H	-2.78746	0.47784	1.19477
H	-3.54475	-1.10946	1.13679
H	-0.81381	-0.73945	-0.15211
H	-1.16319	1.41012	2.50405
H	0.27261	0.91576	3.40146
H	1.00983	2.5534	1.9446
H	2.93079	0.39982	2.65712
H	3.29976	2.04793	2.03659
H	4.16953	0.8906	-1.68067
H	4.39879	-0.86755	-3.41371
H	2.76851	-0.93908	-2.70749
H	3.98571	-2.12868	-2.24009
H	6.38046	-0.17081	-2.02683
H	6.19061	0.31294	-0.33091
H	6.03986	-1.39185	-0.80829
H	4.29648	-1.99978	0.48687
H	-2.03908	-3.12159	1.30692
H	-2.2866	-2.82104	-0.40193
H	-0.46577	-4.46915	-0.1045
H	0.19979	-2.98648	-0.81511
H	0.46124	-3.33373	0.8913
H	-2.31291	1.59546	-0.75962
H	-8.00767	-0.92132	-0.41335
H	-7.44507	0.69422	0.03977
H	-7.45594	0.20746	-1.66072
Na	-0.31847	1.06499	-2.18373

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 50

C	6.11572	-1.33263	0.02151
C	4.69914	-1.77377	0.43229
C	3.5228	-0.99309	-0.18551
C	3.42613	0.44713	0.35736
C	2.69211	1.48413	-0.51489
S	0.86261	1.20227	-0.72232
C	0.158	1.60898	0.94435
C	-0.75827	0.55505	1.6068
C	-0.04283	-0.83205	1.75341
O	-0.60694	-1.83609	1.25004
O	1.08361	-0.77269	2.30835
N	-2.10495	0.47214	1.02957
C	-3.26407	0.79142	1.85718
O	-4.37753	0.27406	1.15584
C	-4.03224	0.13258	-0.22184
C	-2.48768	0.00681	-0.17783
O	-1.77773	-0.40436	-1.09947
C	-4.78907	-1.08743	-0.7854
C	-4.55675	-1.2762	-2.29289
C	-6.29338	-1.00866	-0.46709
O	-4.2809	1.33373	-0.92747
C	3.03306	2.9266	-0.08867
C	2.52865	4.02612	-1.02831
O	2.31263	-1.74301	0.02322
C	6.43751	-1.52095	-1.46784
H	6.28805	-0.28556	0.30346
H	6.83152	-1.91711	0.61318
H	4.60422	-1.7256	1.52592
H	4.55843	-2.82621	0.15643
H	3.64673	-0.96145	-1.27587
H	2.99097	0.41262	1.36331
H	4.45063	0.82254	0.477

H	3.02311	1.35809	-1.55601
H	0.99848	1.75323	1.62348
H	-0.38487	2.55391	0.85319
H	-0.9086	0.92255	2.62901
H	-3.35607	1.87811	2.00129
H	-3.19896	0.28878	2.82816
H	-4.37943	-1.95541	-0.25338
H	-5.04511	-2.19864	-2.62502
H	-3.4936	-1.33449	-2.53124
H	-4.98321	-0.44486	-2.8641
H	-6.78983	-1.91791	-0.82075
H	-6.47844	-0.90868	0.60462
H	-6.77631	-0.16728	-0.98228
H	-5.23767	1.47764	-0.95932
H	2.66425	3.10577	0.92954
H	4.12761	2.99072	-0.02004
H	2.8557	5.01039	-0.67672
H	2.91998	3.8874	-2.0431
H	1.43708	4.03238	-1.09561
H	2.03382	-1.63028	0.96407
H	7.48498	-1.27745	-1.67605
H	6.26914	-2.5592	-1.77829
H	5.8219	-0.88094	-2.10959
Na	0.16367	-1.61651	-0.85411

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 10

C	5.5065	-1.33077	-0.98386
C	4.79392	-0.21477	-0.21003
C	3.31829	-0.03152	-0.58745
C	2.67836	1.16117	0.15399
C	1.25063	1.47326	-0.32765
S	0.19014	2.36257	0.91251

C	-0.00312	1.21876	2.33236
C	-0.711	-0.15163	2.15167
C	0.25769	-1.33269	1.7995
O	-0.25262	-2.35866	1.27827
O	1.46883	-1.1481	2.08774
N	-1.90884	-0.11154	1.30961
C	-3.17218	0.34213	1.88291
O	-4.15027	0.02376	0.91286
C	-3.52288	-0.03373	-0.36771
C	-2.03743	-0.31543	-0.01676
O	-1.17585	-0.65379	-0.83722
C	-4.23266	-1.12658	-1.19739
C	-3.70292	-1.20915	-2.63745
C	-5.75968	-0.92899	-1.18862
O	-3.52074	1.23461	-0.989
C	1.19049	2.28481	-1.64209
C	1.73488	3.71966	-1.59115
O	2.57794	-1.24854	-0.34335
C	6.97684	-1.49086	-0.58036
H	4.97297	-2.2744	-0.82326
H	5.44433	-1.1184	-2.06098
H	5.31381	0.73823	-0.38248
H	4.85732	-0.4124	0.86975
H	3.25172	0.12229	-1.67279
H	2.67195	0.91862	1.221
H	3.31941	2.04158	0.03398
H	0.72724	0.53675	-0.51843
H	0.96362	1.00705	2.79197
H	-0.57481	1.83532	3.03454
H	-1.07702	-0.42225	3.15275
H	-3.14651	1.42324	2.08137
H	-3.39882	-0.20558	2.80354
H	-4.01548	-2.07268	-0.68475

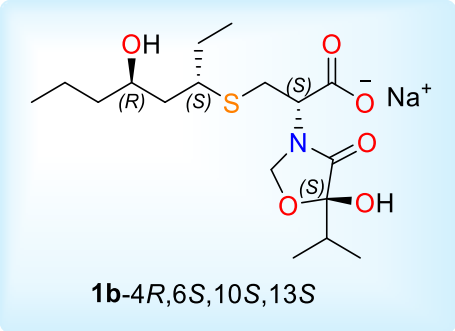
H	-4.1798	-2.04767	-3.15635
H	-2.62102	-1.34907	-2.66146
H	-3.93159	-0.29389	-3.19305
H	-6.23844	-1.75144	-1.72963
H	-6.16157	-0.90335	-0.17352
H	-6.05301	-0.00305	-1.70117
H	-4.43791	1.48932	-1.16503
H	1.74764	1.71823	-2.40102
H	0.14874	2.30411	-1.98173
H	1.65777	4.18596	-2.57927
H	1.17336	4.34034	-0.88626
H	2.78863	3.75225	-1.29484
H	2.40603	-1.31521	0.63264
H	7.46214	-2.29094	-1.14999
H	7.54201	-0.56747	-0.75594
H	7.06955	-1.73755	0.48392
Na	0.51499	-2.15133	-0.79225

Compound 1a: Isomer 4R, 6S, 10S, 13R conformer 16

C	5.69965	-0.3132	-1.14586
C	4.80031	0.38485	-0.1071
C	3.3113	0.49551	-0.46762
C	2.54093	1.34369	0.56911
C	1.11835	1.71108	0.10852
S	-0.08494	1.99039	1.50789
C	-0.03857	0.49314	2.57354
C	-0.59632	-0.8607	2.04559
C	0.48485	-1.78539	1.39213
O	0.07985	-2.67021	0.59578
O	1.6739	-1.55719	1.73922
N	-1.80609	-0.7031	1.24047
C	-3.07511	-0.45125	1.92325

O	-4.01969	-0.25572	0.89766
C	-3.34077	0.1252	-0.30406
C	-1.91218	-0.42335	-0.07712
O	-1.04162	-0.49387	-0.95545
C	-4.14348	-0.42415	-1.49445
C	-4.25791	-1.95531	-1.44783
C	-3.60837	0.06241	-2.85005
O	-3.26291	1.5268	-0.42869
C	1.12994	2.99488	-0.74692
C	-0.17664	3.3432	-1.46944
O	2.69793	-0.80357	-0.61255
C	5.65749	-1.84724	-1.13549
H	5.44356	0.05768	-2.14887
H	6.73408	0.00691	-0.96512
H	5.16881	1.40893	0.03931
H	4.89363	-0.11732	0.86648
H	3.23025	0.95385	-1.46256
H	2.51961	0.77044	1.49945
H	3.10047	2.26457	0.7745
H	0.6969	0.89604	-0.48328
H	0.97779	0.30405	2.921
H	-0.62492	0.82334	3.43734
H	-0.90693	-1.4222	2.93806
H	-2.99644	0.43541	2.57155
H	-3.37074	-1.31931	2.52319
H	-5.1461	0.00089	-1.35002
H	-4.90315	-2.30428	-2.26056
H	-4.68692	-2.29865	-0.50311
H	-3.27961	-2.4337	-1.57469
H	-4.27776	-0.27497	-3.64877
H	-3.55068	1.15229	-2.88535
H	-2.61013	-0.33901	-3.04715
H	-2.56734	1.87334	0.1568

H	1.44752	3.83743	-0.11798
H	1.92174	2.86259	-1.49649
H	-0.02085	4.18746	-2.1495
H	-0.5463	2.4971	-2.05792
H	-0.96754	3.63076	-0.77079
H	2.56791	-1.18407	0.2958
H	6.36488	-2.25954	-1.86414
H	5.93252	-2.23809	-0.14855
H	4.65935	-2.2229	-1.37206
Na	0.74706	-1.80037	-1.3283



1b-4*R*,6*S*,10*S*,13*S*

Calculated DFT energies of the 1b-diasteroisomer

Conformers **1b**	OPLS2008 Force Field Conformational Search Relative Energy (kcal/mol)	B3LYP/6-31+G(d,p) DFT Energy (hartree)	Δ (DFT Energy) (kcal/mol)	% Population
1b19	1.456622067	-1732.258964	0	58.02
1b39	2.214892503	-1732.257811	0.723518328	17.09
1b41	2.288912661	-1732.257674	0.809487114	14.78
1b21	1.566995038	-1732.256081	1.809109574	2.73
1b46	2.399978749	-1732.255872	1.940259037	2.19
1b42	2.312526454	-1732.255688	2.055720765	1.80
1b13	1.125288049	-1732.254458	2.827557316	0.49
1b34	2.065035741	-1732.254192	2.994474814	0.37
1b11	0.988074705	-1732.25398	3.127506805	0.29
1b58	2.714247738	-1732.253966	3.136291936	0.29
1b35	2.097875165	-1732.253916	3.167667406	0.27
1b25	1.73121606	-1732.253812	3.232928382	0.25
1b30	1.960040405	-1732.253598	3.367215392	0.20
1b10	0.918619561	-1732.253582	3.377255542	0.19
1b1	0	-1732.253532	3.408631012	0.18
1b52	2.506025711	-1732.252641	3.967741879	0.07
1b51	2.492497972	-1732.252579	4.006647462	0.07
1b57	2.709754426	-1732.252409	4.113324058	0.06
1b54	2.638889147	-1732.252383	4.129639302	0.05
1b7	0.841038213	-1732.252382	4.130266812	0.05
1b26	1.769815529	-1732.25221	4.238198427	0.05
1b37	2.17696225	-1732.252112	4.299694347	0.04

22 conformers counting for the 99.52% of the DFT conformational population

DFT COORDINATES FOR CONFORMATIONAL SEARCH OF 1b (4*R*, 6*S*, 10*S*, 13*S*)

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 19

C	4.97881	-2.54433	-0.65365
C	4.74222	-1.19395	0.03304
C	3.48319	-0.45888	-0.45445
C	3.33551	0.92274	0.21812
C	2.53321	1.99319	-0.54717
S	0.71572	1.63666	-0.75189
C	0.00825	1.90305	0.94086
C	-0.81244	0.76297	1.58431
C	-0.03578	-0.5995	1.59308
O	-0.5917	-1.59107	1.02685
O	1.10699	-0.56069	2.09803
N	-2.18152	0.59974	1.08297
C	-3.21441	0.24664	2.06851
O	-4.29603	-0.23648	1.30977
C	-3.77541	-0.79911	0.09702
C	-2.4859	0.02186	-0.11214
O	-1.80444	0.04469	-1.14142
C	-4.87758	-0.73374	-0.96871
C	-5.32499	0.71129	-1.23804
C	-4.48381	-1.4521	-2.26852
O	-3.3712	-2.13532	0.27632
C	2.82111	3.41019	-0.01202
C	2.2392	4.55689	-0.84429
O	2.32388	-1.29358	-0.27312
C	6.24196	-3.25505	-0.15399
H	4.10463	-3.18483	-0.49453
H	5.05371	-2.38644	-1.7394
H	5.61163	-0.54292	-0.1354
H	4.66678	-1.33798	1.12086
H	3.56301	-0.32327	-1.54289
H	2.92998	0.78631	1.22759

H	4.34828	1.32915	0.34342
H	2.84644	1.96825	-1.60124
H	0.84942	2.09122	1.60839
H	-0.61104	2.80266	0.90304
H	-0.92089	1.06548	2.63287
H	-3.54252	1.12629	2.6314
H	-2.82788	-0.51773	2.76095
H	-5.71732	-1.27821	-0.51578
H	-4.51941	1.29614	-1.69785
H	-6.17113	0.71563	-1.93288
H	-5.63755	1.21328	-0.31881
H	-5.33541	-1.45325	-2.95754
H	-4.19592	-2.48784	-2.0754
H	-3.64817	-0.94536	-2.7607
H	-2.48292	-2.15428	0.68908
H	2.47842	3.49024	1.02789
H	3.91318	3.52039	0.03145
H	2.60723	4.52068	-1.87642
H	1.14703	4.51602	-0.88409
H	2.53016	5.52376	-0.42047
H	2.07103	-1.2713	0.67989
H	6.38775	-4.21301	-0.66483
H	7.13843	-2.64687	-0.32572
H	6.1816	-3.45883	0.92163
Na	0.1656	-1.17467	-1.11347

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 39

C	4.81835	-2.72031	-0.51434
C	4.62971	-1.31983	0.08112
C	3.39397	-0.57645	-0.45053
C	3.29419	0.85034	0.13065
C	2.52245	1.89291	-0.69921

S	0.69641	1.57565	-0.88438
C	-0.00151	1.97872	0.78674
C	-0.86364	0.91563	1.50282
C	-0.13704	-0.46998	1.60732
O	-0.73079	-1.47888	1.11567
O	1.00932	-0.43572	2.10504
N	-2.23788	0.76943	1.01058
C	-3.28471	0.53228	2.01633
O	-4.38479	0.03854	1.29213
C	-3.88619	-0.63468	0.12718
C	-2.56524	0.11722	-0.13944
O	-1.88422	0.03703	-1.16606
C	-4.98467	-0.60777	-0.94405
C	-5.38066	0.82903	-1.31762
C	-4.61461	-1.43037	-2.188
O	-3.53464	-1.9678	0.40936
C	2.80608	3.34552	-0.26007
C	4.23091	3.82972	-0.56977
O	2.20734	-1.35668	-0.21089
C	6.06363	-3.43455	0.02354
H	3.92635	-3.321	-0.30642
H	4.88854	-2.63823	-1.60877
H	5.51951	-0.71117	-0.13346
H	4.55539	-1.38823	1.17639
H	3.47341	-0.51578	-1.54564
H	2.88257	0.79351	1.14549
H	4.32008	1.22439	0.23372
H	2.83364	1.7999	-1.74991
H	0.84729	2.1776	1.441
H	-0.58587	2.89652	0.68781
H	-0.96095	1.29246	2.52819
H	-3.57684	1.46376	2.51155
H	-2.92958	-0.19373	2.76454

H	-5.84324	-1.08904	-0.45625
H	-4.55391	1.35131	-1.81377
H	-6.22429	0.81297	-2.01533
H	-5.67744	1.40558	-0.43784
H	-5.46572	-1.45297	-2.87723
H	-4.36091	-2.45856	-1.92052
H	-3.76274	-0.98751	-2.71268
H	-2.64549	-1.99058	0.82002
H	2.09203	4.00248	-0.76874
H	2.61572	3.44847	0.81599
H	4.99386	3.27109	-0.01857
H	4.45455	3.73934	-1.63942
H	4.34081	4.88466	-0.29732
H	1.95733	-1.25879	0.73805
H	6.17519	-4.42916	-0.42166
H	6.97654	-2.86763	-0.19601
H	6.00715	-3.56246	1.11099
Na	0.04963	-1.23382	-1.04511

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 41

C	4.83792	-2.81421	-0.50692
C	4.68654	-1.42482	0.12412
C	3.48975	-0.62278	-0.41175
C	3.42914	0.78894	0.20957
C	2.71243	1.88514	-0.60322
S	0.87887	1.64336	-0.83313
C	0.15984	2.01359	0.83534
C	-0.74933	0.95619	1.50089
C	-0.06712	-0.4536	1.57721
O	-0.67786	-1.42759	1.03748
O	1.0664	-0.47126	2.10366
N	-2.11819	0.86646	0.98081

C	-3.1875	0.62703	1.96131
O	-4.28863	0.19576	1.20153
C	-3.78801	-0.47204	0.03182
C	-2.44399	0.25782	-0.19386
O	-1.7449	0.19569	-1.20942
C	-4.86335	-0.38347	-1.05982
C	-4.4185	-1.03262	-2.37967
C	-6.18603	-0.99529	-0.56573
O	-3.46842	-1.81782	0.28947
C	3.08429	3.2956	-0.10356
C	2.59325	4.45414	-0.97704
O	2.2712	-1.36642	-0.22148
C	6.04478	-3.58758	0.03661
H	3.92049	-3.38728	-0.33485
H	4.93498	-2.70459	-1.59685
H	5.60188	-0.84301	-0.05419
H	4.58585	-1.52082	1.21518
H	3.59562	-0.53306	-1.50267
H	3.00131	0.71675	1.2164
H	4.46567	1.12946	0.33708
H	3.04173	1.80789	-1.64978
H	0.99946	2.16495	1.51394
H	-0.39437	2.95204	0.75544
H	-0.85493	1.30496	2.53529
H	-3.45979	1.54861	2.48505
H	-2.86791	-0.13647	2.68793
H	-5.02163	0.6894	-1.23126
H	-4.24356	-2.1041	-2.24066
H	-5.20854	-0.91146	-3.1287
H	-3.50308	-0.58038	-2.76736
H	-6.95551	-0.87711	-1.33613
H	-6.53696	-0.51179	0.34906
H	-6.06635	-2.0645	-0.36518

H	-2.57984	-1.87061	0.69948
H	2.73105	3.42818	0.92724
H	4.18046	3.33438	-0.04384
H	2.96712	4.36025	-2.00337
H	1.50143	4.49059	-1.02789
H	2.94857	5.41042	-0.57902
H	2.00701	-1.2927	0.72561
H	6.1308	-4.57276	-0.43441
H	6.98179	-3.04798	-0.14734
H	5.95984	-3.74358	1.11852
Na	0.14872	-1.12853	-1.10183

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 21

C	-4.91521	-2.00429	-0.37629
C	-4.64213	-1.35226	0.987
C	-3.36997	-0.48971	1.07412
C	-3.37921	0.69761	0.08679
C	-2.57496	1.94601	0.49863
S	-0.72933	1.70597	0.60585
C	-0.18173	1.61063	-1.16286
C	0.64375	0.38629	-1.61652
C	-0.05563	-0.97089	-1.25974
O	-1.23968	-1.08035	-1.64516
O	0.6017	-1.79795	-0.55525
N	2.05781	0.38437	-1.22512
C	3.01877	-0.13565	-2.21001
O	4.18522	-0.41329	-1.47458
C	3.80231	-0.72029	-0.12639
C	2.49603	0.08569	0.02956
O	1.90675	0.30534	1.09198
C	4.98931	-0.39684	0.7907
C	5.39822	1.08123	0.69681

C	4.74015	-0.81903	2.24703
O	3.4522	-2.07575	0.01753
C	-2.98533	3.18289	-0.32522
C	-2.39856	4.51491	0.152
O	-2.20035	-1.32014	0.9394
C	-6.1546	-2.90718	-0.35226
H	-5.04738	-1.23081	-1.1435
H	-4.04373	-2.59493	-0.68314
H	-4.55643	-2.13717	1.74971
H	-5.50148	-0.72874	1.27418
H	-3.31276	-0.09397	2.09757
H	-3.0628	0.35133	-0.9033
H	-4.42298	1.02486	-0.01681
H	-2.79451	2.16399	1.55403
H	-1.08563	1.61295	-1.77201
H	0.38648	2.51786	-1.38253
H	0.64659	0.45409	-2.71117
H	3.2514	0.61568	-2.97136
H	2.61351	-1.0407	-2.68918
H	5.80833	-1.00984	0.39061
H	4.60761	1.73631	1.08205
H	6.29379	1.25828	1.30132
H	5.62015	1.37302	-0.33285
H	5.65005	-0.65655	2.83491
H	4.47295	-1.8762	2.31109
H	3.93492	-0.22911	2.69522
H	2.531	-2.20917	-0.28901
H	-2.7393	3.02236	-1.38299
H	-4.08155	3.24231	-0.28651
H	-2.66648	4.71173	1.19671
H	-1.30696	4.52496	0.086
H	-2.78494	5.34198	-0.45283
H	-2.03932	-1.4886	-0.01774

H	-6.33363	-3.3622	-1.33221
H	-6.0382	-3.71913	0.37534
H	-7.05398	-2.34281	-0.07714
Na	0.00782	-0.94687	1.50785

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 46

C	4.80119	-2.20617	0.44783
C	4.59651	-1.57285	-0.93614
C	3.38902	-0.62603	-1.06641
C	3.4647	0.57638	-0.10015
C	2.73228	1.86259	-0.52969
S	0.87563	1.73018	-0.63583
C	0.32191	1.67849	1.13273
C	-0.58209	0.51188	1.58898
C	0.02978	-0.88944	1.24313
O	-0.67782	-1.67888	0.54457
O	1.2054	-1.06958	1.62914
N	-1.99147	0.59983	1.19157
C	-2.99091	0.16131	2.1765
O	-4.17298	-0.02222	1.43814
C	-3.80731	-0.39286	0.09913
C	-2.44529	0.319	-0.06195
O	-1.835	0.48884	-1.1215
C	-4.95744	0.00839	-0.83513
C	-4.66177	-0.32151	-2.30638
C	-6.2755	-0.64218	-0.3797
O	-3.54886	-1.7719	-0.01376
C	3.21119	3.08479	0.27907
C	2.70999	4.44198	-0.22418
O	2.16252	-1.3707	-0.93817
C	5.97388	-3.19408	0.46993
H	4.97543	-1.42366	1.19724

H	3.88517	-2.72511	0.75434
H	4.46745	-2.36943	-1.6804
H	5.50204	-1.01872	-1.22373
H	3.37854	-0.24774	-2.09794
H	3.13144	0.26417	0.89572
H	4.5256	0.84518	-0.00251
H	2.96432	2.05414	-1.58755
H	1.22288	1.62587	1.74401
H	-0.18813	2.62082	1.34752
H	-0.58522	0.58578	2.68331
H	-3.16511	0.93048	2.93535
H	-2.66072	-0.77242	2.65838
H	-5.05583	1.09703	-0.73153
H	-4.55173	-1.40191	-2.44203
H	-5.49577	0.01721	-2.93051
H	-3.74907	0.1658	-2.6561
H	-7.09324	-0.30758	-1.02693
H	-6.52077	-0.37616	0.65123
H	-6.21193	-1.73269	-0.447
H	-2.63452	-1.95956	0.28422
H	2.94607	2.95572	1.33653
H	4.3093	3.07775	0.25013
H	3.00456	4.60852	-1.26699
H	1.61991	4.51588	-0.17551
H	3.13478	5.25366	0.37573
H	1.98049	-1.5155	0.01977
H	6.10375	-3.63387	1.46449
H	5.81296	-4.01533	-0.23853
H	6.91542	-2.70177	0.19741
Na	-0.015	-0.88188	-1.52259

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 42

C	4.7596	-2.10033	0.41173
C	4.52249	-1.4696	-0.96826
C	3.28348	-0.5633	-1.08625
C	3.32421	0.64058	-0.11931
C	2.5497	1.89999	-0.54988
S	0.69841	1.70852	-0.64266
C	0.15324	1.6516	1.12988
C	-0.7016	0.45445	1.60155
C	-0.0419	-0.92493	1.2553
O	1.14111	-1.06292	1.63525
O	-0.72497	-1.74057	0.56213
N	-2.11737	0.48739	1.2176
C	-3.08713	0.00425	2.21264
O	-4.26571	-0.24448	1.48639
C	-3.89864	-0.57822	0.14016
C	-2.57113	0.18902	-0.03169
O	-1.98238	0.38143	-1.09967
C	-5.0809	-0.23302	-0.77505
C	-5.44571	1.25763	-0.69994
C	-4.85236	-0.68235	-2.22663
O	-3.5867	-1.94466	0.01138
C	2.95315	3.16064	0.24414
C	4.37528	3.66203	-0.05062
O	2.08315	-1.34842	-0.94891
C	5.96266	-3.05134	0.41886
H	4.91631	-1.31512	1.16225
H	3.86332	-2.64882	0.72515
H	4.41445	-2.26773	-1.71423
H	5.40673	-0.88462	-1.26107
H	3.25133	-0.18469	-2.11714
H	2.99539	0.31972	0.87543
H	4.37655	0.93419	-0.01932

H	2.76619	2.09539	-1.61027
H	1.05835	1.64251	1.73689
H	-0.39288	2.57511	1.33605
H	-0.69643	0.5339	2.69543
H	-3.29272	0.7683	2.9691
H	-2.70606	-0.90861	2.69681
H	-5.91519	-0.81622	-0.36211
H	-4.6386	1.88314	-1.09979
H	-6.33978	1.45246	-1.3012
H	-5.65194	1.57074	0.32673
H	-5.76061	-0.50211	-2.81189
H	-4.61578	-1.7475	-2.27735
H	-4.03326	-0.12192	-2.68739
H	-2.66721	-2.09939	0.31305
H	2.24161	3.95838	0.00424
H	2.85499	2.96593	1.31989
H	5.14529	2.94767	0.25712
H	4.50961	3.86182	-1.12033
H	4.56691	4.59691	0.48651
H	1.91557	-1.50175	0.00988
H	6.11676	-3.48955	1.41065
H	5.81956	-3.87522	-0.29033
H	6.88547	-2.52933	0.13762
Na	-0.11723	-0.92613	-1.51304

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 13

C	5.31869	-2.04627	-0.90157
C	4.9329	-0.78654	-0.11742
C	3.57687	-0.18709	-0.52728
C	3.275	1.10782	0.25631
C	2.29477	2.10836	-0.38678
S	0.53647	1.51412	-0.56035

C	-0.11529	1.50823	1.17653
C	-0.75944	0.2008	1.69085
C	0.22138	-1.01461	1.57108
O	1.35406	-0.81607	2.07999
O	-0.17342	-2.01791	0.92667
N	-2.10549	-0.05572	1.16048
C	-3.20546	-0.29465	2.09417
O	-4.35793	-0.38385	1.27946
C	-3.96274	-0.81667	-0.02288
C	-2.46394	-0.43338	-0.0869
O	-1.77193	-0.47013	-1.1075
C	-4.8945	-0.14232	-1.05035
C	-4.8034	1.39067	-0.99562
C	-4.67346	-0.66331	-2.47944
O	-3.98374	-2.22535	-0.10845
C	2.39421	3.50235	0.26475
C	1.65547	4.62358	-0.47287
O	2.5411	-1.17403	-0.39134
C	6.66547	-2.63285	-0.46285
H	4.52952	-2.79608	-0.78102
H	5.35666	-1.80509	-1.97389
H	5.7097	-0.02056	-0.25317
H	4.9035	-1.0147	0.95808
H	3.61015	0.04188	-1.60273
H	2.94623	0.84136	1.26777
H	4.22725	1.64379	0.37008
H	2.56174	2.21707	-1.4482
H	0.72757	1.71515	1.83617
H	-0.83637	2.32571	1.26408
H	-0.90537	0.36756	2.76501
H	-3.32928	0.54689	2.78343
H	-3.03551	-1.22408	2.65712
H	-5.9075	-0.43029	-0.72622

H	-3.81283	1.73752	-1.31152
H	-5.53856	1.83211	-1.67631
H	-5.00183	1.76895	0.01048
H	-5.4291	-0.23488	-3.14652
H	-4.74823	-1.75249	-2.53195
H	-3.68467	-0.37748	-2.84803
H	-4.89826	-2.51986	0.01415
H	2.04953	3.44738	1.30543
H	3.46127	3.75676	0.32126
H	2.01901	4.7231	-1.50258
H	0.57891	4.43679	-0.52103
H	1.81396	5.58336	0.03016
H	2.31176	-1.25183	0.56699
H	6.917	-3.52894	-1.04072
H	7.48028	-1.91087	-0.59733
H	6.64623	-2.91611	0.59622
Na	0.34797	-1.3531	-1.15201

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 34

C	5.65148	-0.36231	-1.28416
C	4.84805	0.17678	-0.09417
C	3.37705	0.4753	-0.41157
C	2.63898	1.08568	0.79881
C	1.2317	1.59771	0.44285
S	0.0278	1.61732	1.8606
C	-0.06008	-0.08482	2.54662
C	-0.60335	-1.26977	1.70697
C	0.48542	-2.01767	0.86302
O	0.0893	-2.65056	-0.15001
O	1.66457	-1.92305	1.29068
N	-1.82421	-0.97343	0.95362
C	-3.12275	-1.36683	1.49698

O	-4.08077	-0.79585	0.62641
C	-3.46477	-0.54341	-0.63326
C	-1.95506	-0.51288	-0.30339
O	-1.08174	-0.15041	-1.10069
C	-4.0149	0.76321	-1.23146
C	-5.48581	0.62491	-1.65984
C	-3.8365	1.9488	-0.27121
O	-3.60486	-1.65111	-1.50251
C	1.28842	3.03493	-0.11575
C	0.0047	3.55056	-0.77666
O	2.70467	-0.71769	-0.87237
C	7.11266	-0.66193	-0.92983
H	5.16771	-1.27076	-1.66023
H	5.61686	0.36965	-2.10402
H	5.31552	1.10116	0.27337
H	4.88687	-0.54264	0.73639
H	3.33508	1.1655	-1.26512
H	2.59153	0.31444	1.57216
H	3.23417	1.91298	1.20577
H	0.78163	0.9486	-0.30993
H	0.91548	-0.39546	2.92367
H	-0.71402	0.07294	3.41136
H	-0.90328	-2.02556	2.44707
H	-3.27434	-0.95496	2.50029
H	-3.20475	-2.46335	1.52159
H	-3.40291	0.93735	-2.12515
H	-6.12518	0.37544	-0.80599
H	-5.84032	1.57407	-2.07414
H	-5.63044	-0.13035	-2.44094
H	-4.10832	2.88189	-0.77557
H	-2.80338	2.04511	0.07542
H	-4.47913	1.83653	0.60756
H	-4.54664	-1.77741	-1.68396

H	1.59617	3.71672	0.68881
H	2.09943	3.05771	-0.85602
H	-0.33301	2.87081	-1.56685
H	-0.81124	3.64923	-0.05544
H	0.17501	4.53528	-1.22562
H	2.55571	-1.30155	-0.08297
H	7.66315	-1.04363	-1.79666
H	7.63099	0.23769	-0.57628
H	7.17941	-1.41513	-0.1359
Na	0.69601	-1.35144	-1.82395

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 11

C	5.30721	-2.20263	-0.83998
C	4.96643	-0.90609	-0.09625
C	3.6291	-0.27638	-0.52178
C	3.37221	1.05379	0.2178
C	2.43255	2.0675	-0.46361
S	0.65451	1.53294	-0.62401
C	-0.00219	1.61407	1.10886
C	-0.69209	0.34989	1.67037
C	0.24462	-0.90367	1.60149
O	1.38341	-0.72669	2.10477
O	-0.18626	-1.91771	0.99778
N	-2.04581	0.12187	1.14608
C	-3.15493	-0.05098	2.08186
O	-4.30737	-0.10903	1.2654
C	-3.93087	-0.60124	-0.02349
C	-2.41438	-0.28129	-0.0902
O	-1.71397	-0.37948	-1.10088
C	-4.81324	0.10357	-1.07697
C	-4.51674	-0.37075	-2.508
C	-6.30833	-0.05419	-0.74416

O	-4.00762	-2.00933	-0.07203
C	2.58385	3.47837	0.14023
C	1.88365	4.60017	-0.63319
O	2.56229	-1.22351	-0.34867
C	6.63473	-2.82046	-0.38564
H	4.49349	-2.92097	-0.69365
H	5.3499	-1.99755	-1.9196
H	5.76719	-0.1707	-0.25906
H	4.93372	-1.09787	0.98622
H	3.66494	-0.08539	-1.60454
H	3.02752	0.83274	1.23487
H	4.34296	1.55771	0.32072
H	2.70609	2.12979	-1.52703
H	0.84493	1.81879	1.7638
H	-0.69587	2.45783	1.16224
H	-0.83423	0.56281	2.73686
H	-3.24621	0.80957	2.75207
H	-3.02479	-0.97439	2.66495
H	-4.56568	1.17051	-1.00121
H	-4.74821	-1.43484	-2.62281
H	-5.13857	0.18926	-3.21474
H	-3.46804	-0.22441	-2.77192
H	-6.90506	0.52505	-1.45599
H	-6.54155	0.29478	0.26448
H	-6.63704	-1.09785	-0.83677
H	-4.93261	-2.26844	0.04686
H	2.24077	3.47087	1.18295
H	3.6596	3.69569	0.18622
H	2.24829	4.65292	-1.66596
H	0.80106	4.44998	-0.6744
H	2.07694	5.56976	-0.16213
H	2.33127	-1.25786	0.61156
H	6.85318	-3.74311	-0.93444

H	7.47345	-2.13191	-0.54591
H	6.60971	-3.06808	0.6822
Na	0.36256	-1.36062	-1.10357

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 58

C	5.42993	-1.10832	-1.22933
C	4.7663	-0.24449	-0.14974
C	3.33409	0.19102	-0.48226
C	2.7429	1.11975	0.59745
C	1.41211	1.76202	0.1666
S	0.2767	2.21317	1.56556
C	0.02108	0.71201	2.58659
C	-0.7695	-0.51311	2.06977
C	0.08934	-1.6003	1.33194
O	-0.51158	-2.33564	0.48625
O	1.30082	-1.65697	1.64125
N	-2.00568	-0.23312	1.33297
C	-3.27769	-0.72025	1.88192
O	-4.19179	-0.65768	0.81234
C	-3.45805	-0.7524	-0.41205
C	-2.08378	-0.17594	-0.01976
O	-1.18243	0.11511	-0.81524
C	-4.2756	-0.06273	-1.51152
C	-4.51221	1.42159	-1.19261
C	-3.66571	-0.24539	-2.91018
O	-3.21773	-2.09705	-0.77471
C	1.64644	3.05268	-0.64599
C	0.4215	3.60011	-1.38923
O	2.48369	-0.96307	-0.68271
C	6.86525	-1.51009	-0.87063
H	4.82384	-2.00631	-1.39412
H	5.43189	-0.55685	-2.18054

H	5.36832	0.66032	0.01382
H	4.75642	-0.78683	0.80686
H	3.33887	0.70066	-1.45489
H	2.61822	0.52315	1.50604
H	3.46866	1.90801	0.83365
H	0.84706	1.06374	-0.45146
H	0.97469	0.33393	2.95945
H	-0.51738	1.13475	3.44134
H	-1.0942	-1.02846	2.98488
H	-3.63852	-0.07691	2.6907
H	-3.15262	-1.75042	2.25048
H	-5.24296	-0.58251	-1.48947
H	-3.5712	1.98375	-1.20619
H	-5.1719	1.86378	-1.94622
H	-4.97896	1.55271	-0.21324
H	-4.34148	0.17771	-3.66108
H	-3.51525	-1.30247	-3.14173
H	-2.7049	0.27219	-2.99072
H	-2.46366	-2.44178	-0.25491
H	2.0578	3.82331	0.0201
H	2.43553	2.83476	-1.37861
H	-0.00223	2.84491	-2.0606
H	-0.36975	3.90543	-0.69903
H	0.69768	4.47214	-1.99197
H	2.29537	-1.36147	0.20304
H	7.31591	-2.12365	-1.6582
H	7.50295	-0.62907	-0.72945
H	6.89287	-2.09039	0.05919
Na	0.36229	-1.44468	-1.41001

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 35

C	-6.05352	-0.69109	0.75971
C	-4.75408	-1.38292	0.32325
C	-3.45986	-0.60986	0.63665
C	-3.27289	0.61636	-0.28103
C	-2.39643	1.76771	0.24819
S	-0.58965	1.36165	0.45169
C	0.04082	1.24364	-1.28867
C	0.80644	-0.03978	-1.68212
C	-0.05155	-1.32598	-1.42879
O	-1.20073	-1.28989	-1.93711
O	0.44506	-2.21862	-0.69731
N	2.17391	-0.11502	-1.14976
C	3.28254	-0.37279	-2.06827
O	4.44451	-0.27856	-1.26736
C	4.09493	-0.58517	0.08288
C	2.56965	-0.32432	0.12567
O	1.88691	-0.31018	1.15306
C	4.97249	0.282	1.00881
C	4.7568	1.78473	0.77042
C	4.80093	-0.07689	2.49336
O	4.2358	-1.96689	0.33481
C	-2.63891	3.07296	-0.53636
C	-1.98747	4.3261	0.05653
O	-2.34396	-1.51474	0.58022
C	-7.29926	-1.53872	0.4731
H	-6.00217	-0.47244	1.83595
H	-6.15978	0.27856	0.25594
H	-4.78761	-1.59924	-0.75434
H	-4.67579	-2.35181	0.83142
H	-3.50159	-0.277	1.68402
H	-2.90546	0.26972	-1.25425
H	-4.26646	1.04696	-0.45999

H	-2.66769	1.95522	1.29736
H	-0.82643	1.29274	-1.94759
H	0.67335	2.11583	-1.47516
H	0.92942	0.03379	-2.76949
H	3.33441	0.39143	-2.85045
H	3.18243	-1.37106	-2.51874
H	6.00426	0.0395	0.70756
H	3.7444	2.08818	1.06066
H	5.45979	2.36327	1.37853
H	4.91426	2.05188	-0.27765
H	5.52244	0.48874	3.09253
H	4.96412	-1.14211	2.67566
H	3.79403	0.17184	2.83928
H	5.17111	-2.19718	0.23356
H	-2.31902	2.94192	-1.57828
H	-3.72614	3.22398	-0.57997
H	-2.32609	4.49675	1.08535
H	-0.89717	4.24371	0.07891
H	-2.25162	5.2109	-0.53233
H	-2.12094	-1.67683	-0.36814
H	-8.21245	-1.02934	0.79947
H	-7.39743	-1.74614	-0.59884
H	-7.25008	-2.5027	0.99276
Na	-0.12614	-1.41502	1.31339

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 25

C	5.16264	-2.39405	-0.7287
C	4.8595	-1.04734	-0.06175
C	3.5369	-0.40933	-0.51827
C	3.3194	0.97216	0.13577
C	2.41097	1.96505	-0.61205
S	0.61865	1.47476	-0.73657

C	-0.03553	1.69448	0.9855
C	-0.76275	0.49163	1.62819
C	0.13597	-0.7913	1.64558
O	-0.32785	-1.83279	1.11797
O	1.28197	-0.61275	2.13197
N	-2.12272	0.27131	1.11654
C	-3.24004	0.20868	2.05636
O	-4.39223	0.14085	1.24029
C	-4.03321	-0.45052	-0.01156
C	-2.50435	-0.20037	-0.091
O	-1.80636	-0.39762	-1.08883
C	-4.88101	0.22212	-1.11364
C	-4.60364	-0.35737	-2.50918
C	-6.38223	0.1539	-0.77779
O	-4.17071	-1.85403	0.03093
C	2.56684	3.41893	-0.11712
C	3.92698	4.0553	-0.44311
O	2.44533	-1.31318	-0.27869
C	6.47929	-3.01585	-0.24899
H	4.33335	-3.08241	-0.53356
H	5.20033	-2.25474	-1.81899
H	5.6777	-0.34394	-0.27256
H	4.82887	-1.17286	1.03048
H	3.57017	-0.2892	-1.6112
H	2.95962	0.82597	1.16132
H	4.30553	1.44546	0.21638
H	2.68152	1.94831	-1.67798
H	0.81738	1.91673	1.6268
H	-0.70323	2.56016	0.97927
H	-0.89895	0.77833	2.6781
H	-3.29752	1.11639	2.66539
H	-3.14931	-0.67652	2.70277
H	-4.58587	1.27957	-1.10649

H	-4.8874	-1.41396	-2.55739
H	-5.19457	0.18605	-3.25437
H	-3.54808	-0.27991	-2.77495
H	-6.95181	0.70614	-1.53207
H	-6.60147	0.58403	0.20222
H	-6.75638	-0.87834	-0.79647
H	-5.10686	-2.06534	0.15682
H	1.7763	4.02296	-0.57596
H	2.40157	3.45756	0.96731
H	4.75771	3.55497	0.06429
H	4.12679	4.03018	-1.52098
H	3.93938	5.10451	-0.12936
H	2.21596	-1.27531	0.68197
H	6.67129	-3.9737	-0.74482
H	7.33234	-2.35789	-0.45557
H	6.4581	-3.20034	0.83159
Na	0.2375	-1.44444	-1.01556

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 30

C	5.58186	-0.69349	-1.25785
C	4.78985	0.03658	-0.16601
C	3.31886	0.28924	-0.52096
C	2.59599	1.10749	0.57103
C	1.16288	1.49681	0.17117
S	0.00839	1.82244	1.59158
C	-0.13763	0.24483	2.5205
C	-0.71151	-1.03067	1.85064
C	0.36262	-1.92264	1.1376
O	1.54621	-1.77553	1.53816
O	-0.04881	-2.70901	0.24561
N	-1.91211	-0.80482	1.0418
C	-3.23258	-0.99968	1.63793

O	-4.15141	-0.51238	0.67862
C	-3.52911	-0.53157	-0.6027
C	-2.01921	-0.5494	-0.2747
O	-1.13032	-0.37795	-1.11764
C	-3.9877	0.68383	-1.42753
C	-5.47229	0.58463	-1.81806
C	-3.70141	2.00851	-0.70408
O	-3.75462	-1.76294	-1.26219
C	1.08368	2.72073	-0.76961
C	1.52644	4.07073	-0.18718
O	2.63517	-0.95923	-0.76947
C	7.04401	-0.94181	-0.86979
H	5.08931	-1.64712	-1.4785
H	5.54518	-0.10335	-2.185
H	5.26542	1.00498	0.04454
H	4.82962	-0.53924	0.7698
H	3.27741	0.82479	-1.47889
H	2.58203	0.50067	1.48091
H	3.18571	2.00333	0.796
H	0.70631	0.66524	-0.3635
H	0.82799	-0.03761	2.9429
H	-0.78779	0.54432	3.34985
H	-1.04537	-1.66505	2.6845
H	-3.34392	-0.41338	2.55597
H	-3.39779	-2.06653	1.84825
H	-3.37971	0.64242	-2.33975
H	-6.11313	0.54027	-0.93079
H	-5.76249	1.46901	-2.39412
H	-5.68692	-0.28447	-2.45072
H	-3.91662	2.85049	-1.37035
H	-2.65663	2.08918	-0.38892
H	-4.3306	2.10963	0.18579
H	-4.70337	-1.84799	-1.43082

H	1.69899	2.49324	-1.65095
H	0.05342	2.8048	-1.13454
H	0.90394	4.36972	0.66173
H	2.56619	4.05122	0.15588
H	1.4478	4.85317	-0.94967
H	2.46455	-1.39256	0.10835
H	7.58601	-1.46025	-1.6683
H	7.56943	-0.00044	-0.66798
H	7.11339	-1.55911	0.03365
Na	0.62219	-1.72664	-1.61277

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 10

C	5.40508	-1.56216	-0.98429
C	4.80147	-0.44	-0.1303
C	3.38906	-0.01687	-0.55167
C	2.86611	1.1682	0.28588
C	1.54356	1.74588	-0.24916
S	0.48898	2.57969	1.03187
C	0.16733	1.3566	2.36063
C	-0.69989	0.0967	2.1285
C	0.08432	-1.17408	1.64776
O	-0.57465	-2.05198	1.00535
O	1.29992	-1.22263	1.94183
N	-1.93195	0.27787	1.35423
C	-3.21846	0.01835	2.0119
O	-4.14959	-0.10581	0.96436
C	-3.45318	-0.5526	-0.20447
C	-2.03779	0.01827	0.02658
O	-1.13604	0.05973	-0.81895
C	-4.24793	-0.09526	-1.43518
C	-3.5772	-0.49826	-2.75757
C	-5.69262	-0.62159	-1.37191

O	-3.29505	-1.95671	-0.22471
C	1.78855	2.7833	-1.36474
C	0.55226	3.18714	-2.17783
O	2.47864	-1.13952	-0.47434
C	6.81094	-1.96773	-0.52704
H	4.74003	-2.43262	-0.95415
H	5.44175	-1.236	-2.03365
H	5.45258	0.44416	-0.17602
H	4.77425	-0.75018	0.92444
H	3.40431	0.25183	-1.61613
H	2.75195	0.81433	1.31479
H	3.62691	1.9587	0.30628
H	0.92525	0.94404	-0.65225
H	1.10534	1.01175	2.79989
H	-0.32919	1.98634	3.10634
H	-1.03789	-0.18539	3.13591
H	-3.51957	0.85427	2.65096
H	-3.1511	-0.90475	2.60881
H	-4.27618	1.00041	-1.37537
H	-3.52447	-1.5882	-2.84493
H	-4.17031	-0.1194	-3.59672
H	-2.56667	-0.09232	-2.84069
H	-6.26016	-0.24028	-2.22739
H	-6.19674	-0.30516	-0.45585
H	-5.70836	-1.71522	-1.41273
H	-2.53505	-2.20595	0.33948
H	2.25771	3.67446	-0.92579
H	2.53563	2.35502	-2.04688
H	0.06876	2.30989	-2.62174
H	-0.1935	3.69257	-1.55805
H	0.83356	3.86706	-2.98935
H	2.28551	-1.31203	0.48064
H	7.21884	-2.76698	-1.15526

H	7.50631	-1.1209	-0.573
H	6.80035	-2.33102	0.50734
Na	0.32406	-1.67441	-1.0454

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 1

C	5.61135	-0.01778	-1.38484
C	4.83513	0.24517	-0.08857
C	3.35173	0.57518	-0.30007
C	2.63848	0.89847	1.03013
C	1.21395	1.44522	0.82676
S	0.05146	1.12776	2.24398
C	0.0056	-0.68527	2.5279
C	-0.57225	-1.64865	1.45769
C	0.48994	-2.19614	0.44368
O	0.06287	-2.6155	-0.66285
O	1.68369	-2.17582	0.84231
N	-1.80179	-1.17275	0.82104
C	-3.09609	-1.58844	1.35061
O	-4.04338	-0.77806	0.68485
C	-3.48065	-0.32088	-0.54497
C	-1.95456	-0.44585	-0.30089
O	-1.08171	0.02532	-1.04025
C	-4.01176	1.10533	-0.80675
C	-3.51854	1.68544	-2.14101
C	-5.54908	1.14681	-0.7279
O	-3.75079	-1.22725	-1.59615
C	1.22508	2.9713	0.59844
C	-0.08521	3.57755	0.08154
O	2.68434	-0.50385	-0.99036
C	7.08689	-0.35279	-1.13832
H	5.1305	-0.83857	-1.9286
H	5.54082	0.86745	-2.03339

H	5.30007	1.08126	0.45268
H	4.908	-0.63135	0.57138
H	3.27726	1.43176	-0.98397
H	2.62283	-0.02004	1.62322
H	3.23252	1.63176	1.59026
H	0.7562	0.96686	-0.04065
H	0.99943	-1.06017	2.77705
H	-0.60579	-0.74167	3.43526
H	-0.86999	-2.54991	2.01279
H	-3.16697	-1.39416	2.42582
H	-3.26389	-2.65636	1.14747
H	-3.61715	1.71951	0.01237
H	-3.89451	1.09961	-2.98647
H	-3.8855	2.71145	-2.25115
H	-2.4289	1.69747	-2.19571
H	-5.89329	2.17938	-0.84421
H	-5.91963	0.76575	0.22625
H	-6.01402	0.56854	-1.53772
H	-4.70708	-1.24477	-1.74512
H	1.52685	3.4681	1.53059
H	2.02232	3.18204	-0.12712
H	-0.40098	3.09469	-0.84966
H	-0.89723	3.46258	0.80519
H	0.03951	4.64768	-0.11701
H	2.54974	-1.24256	-0.33962
H	7.61782	-0.53208	-2.07964
H	7.60071	0.46397	-0.61694
H	7.18938	-1.25409	-0.52243
Na	0.67817	-0.98869	-2.02389

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 52

C	-5.17004	-2.5071	0.11235
C	-4.82652	-1.0791	-0.33983
C	-3.53484	-0.49654	0.26239
C	-3.27593	0.92934	-0.26967
C	-2.389	1.8528	0.58489
S	-0.60252	1.34486	0.72094
C	0.08636	1.6665	-0.97216
C	0.84041	0.50571	-1.65837
C	-0.05718	-0.77158	-1.78514
O	-1.18636	-0.55875	-2.29696
O	0.38703	-1.84522	-1.30861
N	2.18143	0.25536	-1.11103
C	3.33712	0.2945	-2.00654
O	4.45908	0.15848	-1.15644
C	4.05528	-0.53582	0.02482
C	2.52466	-0.30688	0.06919
O	1.80109	-0.58738	1.02806
C	4.87238	0.02657	1.2062
C	4.62863	1.52949	1.41382
C	4.64892	-0.75905	2.50823
O	4.21348	-1.9289	-0.1353
C	-2.52146	3.34229	0.20049
C	-3.89139	3.95936	0.52236
O	-2.43372	-1.38807	0.0226
C	-5.50659	-2.63566	1.60397
H	-6.02761	-2.85468	-0.47771
H	-4.33302	-3.16925	-0.13517
H	-5.65993	-0.40723	-0.08848
H	-4.72935	-1.06028	-1.43435
H	-3.63491	-0.4568	1.35532
H	-2.87866	0.85787	-1.28942
H	-4.25417	1.41876	-0.35134

H	-2.69309	1.75383	1.63721
H	-0.75589	1.9096	-1.62036
H	0.74245	2.53841	-0.90527
H	1.01372	0.85415	-2.68387
H	3.4047	1.2576	-2.52289
H	3.28346	-0.52443	-2.73876
H	5.9213	-0.10376	0.89479
H	3.60046	1.71923	1.7425
H	5.29792	1.91195	2.19128
H	4.81287	2.09622	0.49758
H	5.32917	-0.38703	3.28184
H	4.83297	-1.8283	2.37583
H	3.62202	-0.63768	2.86303
H	5.15778	-2.1138	-0.24578
H	-1.74762	3.90357	0.73568
H	-2.31261	3.46407	-0.87018
H	-4.70264	3.50807	-0.05735
H	-4.13511	3.8474	1.58563
H	-3.88718	5.0308	0.29564
H	-2.16608	-1.29995	-0.9253
H	-5.80887	-3.6593	1.85065
H	-4.64878	-2.38885	2.23951
H	-6.33187	-1.96961	1.8858
Na	-0.25372	-1.58237	0.8243

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 51

C	5.31542	-1.60209	-0.96515
C	4.68637	-0.50132	-0.10174
C	3.27807	-0.08309	-0.54115
C	2.73339	1.08835	0.30308
C	1.3984	1.63754	-0.22846
S	0.32177	2.46735	1.03775

C	-0.01347	1.22548	2.34588
C	-0.85194	-0.04682	2.08028
C	-0.03663	-1.29495	1.59209
O	1.17292	-1.32901	1.91157
O	-0.66723	-2.17098	0.91933
N	-2.077	0.1227	1.29151
C	-3.3653	-0.18425	1.92755
O	-4.28075	-0.31976	0.86659
C	-3.55666	-0.70957	-0.30356
C	-2.16008	-0.11225	-0.04241
O	-1.25374	-0.03416	-0.88054
C	-4.35487	-0.25277	-1.53136
C	-4.55157	1.27093	-1.545
C	-3.7507	-0.75303	-2.85267
O	-3.36653	-2.10892	-0.35879
C	1.55362	2.62588	-1.40743
C	2.25537	3.95837	-1.10795
O	2.37546	-1.21396	-0.49481
C	6.71734	-2.00242	-0.49149
H	4.65846	-2.4792	-0.96206
H	5.36661	-1.25667	-2.00773
H	5.3303	0.38914	-0.1195
H	4.64289	-0.8309	0.94651
H	3.30992	0.20009	-1.60138
H	2.618	0.72462	1.32863
H	3.4856	1.88415	0.33685
H	0.79318	0.81049	-0.59512
H	0.92073	0.89199	2.80188
H	-0.53771	1.83755	3.08723
H	-1.19814	-0.35086	3.0784
H	-3.69737	0.63235	2.57649
H	-3.27875	-1.1145	2.5106
H	-5.33615	-0.72918	-1.40195

H	-3.59525	1.7931	-1.66515
H	-5.19116	1.55589	-2.38669
H	-5.02379	1.62319	-0.62465
H	-4.41432	-0.48554	-3.68186
H	-3.63055	-1.83898	-2.84697
H	-2.77524	-0.29286	-3.03827
H	-2.6182	-2.35643	0.22157
H	2.10627	2.10178	-2.19947
H	0.55678	2.82646	-1.81707
H	1.70804	4.54686	-0.36574
H	3.27307	3.81367	-0.73042
H	2.32752	4.55788	-2.02177
H	2.16986	-1.40217	0.45483
H	7.1435	-2.78649	-1.12668
H	7.405	-1.14827	-0.5109
H	6.69312	-2.38399	0.53606
Na	0.23246	-1.74903	-1.11911

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 57

C	5.73141	-0.66344	-1.0047
C	4.8966	-0.12483	0.16817
C	3.4597	0.28582	-0.18567
C	2.70193	0.81788	1.04914
C	1.33841	1.43657	0.69249
S	0.08167	1.38845	2.06254
C	-0.11497	-0.36224	2.58309
C	-0.68288	-1.43552	1.61898
C	0.39823	-2.15777	0.74325
O	0.00956	-2.67024	-0.33842
O	1.5636	-2.16777	1.2164
N	-1.85913	-1.00923	0.85733
C	-3.19442	-1.38982	1.31369

O	-4.09018	-0.69754	0.46482
C	-3.41403	-0.36947	-0.74518
C	-1.91918	-0.43211	-0.35642
O	-0.99929	-0.03856	-1.08344
C	-3.88968	1.00167	-1.25597
C	-5.34857	0.95853	-1.74215
C	-3.69942	2.10272	-0.20224
O	-3.56009	-1.39701	-1.7076
C	1.48928	2.91489	0.27668
C	0.26174	3.55444	-0.38269
O	2.75014	-0.82163	-0.78413
C	6.04674	0.3746	-2.08993
H	6.67456	-1.05413	-0.60196
H	5.20843	-1.51692	-1.45119
H	5.40328	0.74563	0.60874
H	4.84592	-0.8875	0.95736
H	3.48307	1.05565	-0.9667
H	2.58298	-0.01958	1.74166
H	3.31973	1.56988	1.55644
H	0.88595	0.8867	-0.1347
H	0.82877	-0.75626	2.96319
H	-0.79382	-0.25014	3.43562
H	-1.04559	-2.23959	2.27546
H	-3.36947	-1.0645	2.34454
H	-3.32443	-2.47904	1.23352
H	-3.23961	1.21779	-2.11283
H	-6.02804	0.67302	-0.93172
H	-5.64959	1.95031	-2.09425
H	-5.49465	0.27071	-2.58293
H	-3.93017	3.07994	-0.63904
H	-2.67262	2.13901	0.17292
H	-4.36714	1.94451	0.65037
H	-4.49889	-1.47585	-1.92719

H	1.79233	3.50161	1.1546
H	2.33298	2.96505	-0.4247
H	-0.06982	2.97051	-1.24841
H	-0.58059	3.62315	0.31117
H	0.49614	4.56799	-0.72613
H	2.54068	-1.47002	-0.06152
H	6.68947	-0.05355	-2.86696
H	5.13943	0.73963	-2.58413
H	6.56862	1.24366	-1.67024
Na	0.74762	-1.25069	-1.85522

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 54

C	5.65284	-1.02081	-0.88236
C	4.83275	-0.2042	0.12962
C	3.39371	0.11606	-0.30097
C	2.65652	0.95067	0.76889
C	1.26674	1.41853	0.30475
S	0.0562	1.7734	1.67052
C	-0.19605	0.19586	2.57658
C	-0.79069	-1.05049	1.87144
C	0.27626	-1.98192	1.19903
O	1.44525	-1.88864	1.65448
O	-0.12681	-2.74273	0.28133
N	-1.94476	-0.77097	1.01321
C	-3.29682	-0.92235	1.54762
O	-4.15331	-0.39648	0.55159
C	-3.47388	-0.42692	-0.7001
C	-1.98242	-0.50122	-0.30405
O	-1.04959	-0.35452	-1.10316
C	-3.85011	0.81158	-1.53188
C	-5.31938	0.77279	-1.98548
C	-3.54351	2.11777	-0.78373

O	-3.71279	-1.64352	-1.38185
C	1.29845	2.66541	-0.60849
C	1.78095	3.97736	0.02718
O	2.67103	-1.09971	-0.59702
C	5.96013	-0.2847	-2.19333
H	6.59909	-1.30549	-0.40493
H	5.12215	-1.95504	-1.0989
H	5.34778	0.74492	0.33588
H	4.78915	-0.74793	1.08326
H	3.41438	0.66545	-1.2499
H	2.56737	0.32861	1.66426
H	3.27707	1.81173	1.04126
H	0.799	0.6222	-0.2728
H	0.73723	-0.12891	3.03927
H	-0.87037	0.51574	3.3786
H	-1.18641	-1.67581	2.68479
H	-3.42863	-0.3378	2.46409
H	-3.50929	-1.98379	1.74216
H	-3.20611	0.75393	-2.41817
H	-5.99887	0.7509	-1.12661
H	-5.54962	1.66975	-2.56913
H	-5.54076	-0.08515	-2.6309
H	-3.69949	2.97358	-1.44881
H	-2.50991	2.15525	-0.42628
H	-4.20364	2.2346	0.08145
H	-4.6559	-1.69432	-1.59115
H	1.94539	2.42442	-1.4631
H	0.29436	2.81242	-1.02304
H	1.12887	4.29535	0.84639
H	2.79674	3.89244	0.42705
H	1.78911	4.77688	-0.72146
H	2.44623	-1.53722	0.26604
H	6.596	-0.89378	-2.84514

H	5.04928	-0.0505	-2.75563
H	6.48641	0.65957	-2.00598
Na	0.66403	-1.76956	-1.53407

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 7

C	5.80835	0.80558	-0.2937
C	4.77262	-0.24745	-0.71426
C	3.31401	0.2352	-0.71392
C	2.75641	0.48391	0.70314
C	1.37034	1.15536	0.69502
S	0.33527	0.80195	2.19926
C	0.14201	-1.01915	2.32447
C	-0.61559	-1.82216	1.23451
C	0.29645	-2.35946	0.07884
O	-0.26697	-2.64006	-1.01063
O	1.51794	-2.47494	0.35803
N	-1.84734	-1.18554	0.76406
C	-3.12056	-1.5288	1.38898
O	-4.04276	-0.58127	0.88953
C	-3.55794	-0.07442	-0.35377
C	-2.03432	-0.35129	-0.27489
O	-1.19355	0.10771	-1.05778
C	-3.973	1.40932	-0.4557
C	-3.55721	2.05047	-1.78868
C	-5.4844	1.58013	-0.21513
O	-4.01087	-0.8639	-1.43616
C	1.49079	2.69003	0.59037
C	0.19409	3.43962	0.26173
O	2.4919	-0.7204	-1.42036
C	7.24992	0.29668	-0.41767
H	5.68555	1.7035	-0.916
H	5.62931	1.1226	0.74118

H	4.85407	-1.13155	-0.06589
H	4.99856	-0.58755	-1.73294
H	3.25074	1.15475	-1.31108
H	2.71781	-0.48631	1.20652
H	3.45448	1.11133	1.26988
H	0.78812	0.79237	-0.15333
H	1.11356	-1.5012	2.444
H	-0.39119	-1.10846	3.27734
H	-0.94586	-2.74391	1.73506
H	-3.07082	-1.42466	2.47772
H	-3.41075	-2.55509	1.12002
H	-3.4442	1.91846	0.35982
H	-4.06589	1.57013	-2.6312
H	-3.83422	3.11009	-1.78628
H	-2.48159	1.97199	-1.95413
H	-5.73616	2.64543	-0.21283
H	-5.79666	1.15017	0.73903
H	-6.07902	1.11967	-1.01556
H	-4.97428	-0.7854	-1.48797
H	1.92307	3.07731	1.52316
H	2.22955	2.90204	-0.19415
H	-0.24722	3.07073	-0.67063
H	-0.55339	3.31979	1.05113
H	0.38985	4.51097	0.14316
H	2.35983	-1.50526	-0.82685
H	7.97083	1.06405	-0.11558
H	7.41395	-0.58271	0.21595
H	7.48108	0.00833	-1.44982
Na	0.36916	-0.95659	-2.29031

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 26

C	5.58317	-0.23763	-1.29119
C	4.7821	0.16132	-0.04577
C	3.30947	0.48873	-0.32486
C	2.57369	0.97014	0.94314
C	1.16934	1.52418	0.64148
S	-0.0355	1.40344	2.05229
C	-0.1336	-0.35881	2.56189
C	-0.67973	-1.45261	1.60837
C	0.40471	-2.11613	0.69165
O	0.00421	-2.64653	-0.37699
O	1.58549	-2.06628	1.1225
N	-1.90313	-1.08188	0.89257
C	-3.19732	-1.53939	1.39122
O	-4.15692	-0.88379	0.58589
C	-3.54726	-0.50105	-0.64484
C	-2.03495	-0.49804	-0.31311
O	-1.154	-0.06239	-1.06453
C	-4.17829	0.83357	-1.08954
C	-4.00582	1.93638	-0.03406
C	-3.68321	1.2935	-2.4701
O	-3.69513	-1.51901	-1.61644
C	1.23596	3.01242	0.23848
C	-0.03841	3.59996	-0.37894
O	2.6361	-0.65121	-0.90375
C	7.04822	-0.56419	-0.9791
H	5.10318	-1.10196	-1.76381
H	5.53975	0.58077	-2.02434
H	5.24786	1.04047	0.42142
H	4.8259	-0.64638	0.69887
H	3.26405	1.26301	-1.10267
H	2.52108	0.12142	1.62993
H	3.17128	1.74715	1.4365

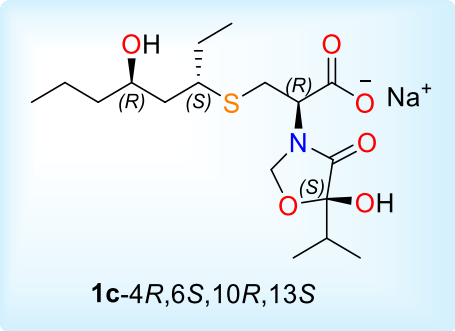
H	0.71636	0.96008	-0.17586
H	0.83869	-0.71055	2.91024
H	-0.79082	-0.28464	3.43529
H	-0.979	-2.27755	2.27083
H	-3.35116	-1.23827	2.43292
H	-3.27258	-2.63289	1.29914
H	-5.25419	0.60742	-1.16641
H	-2.94826	2.17344	0.12258
H	-4.50738	2.851	-0.36689
H	-4.43567	1.64138	0.92614
H	-4.26176	2.16502	-2.79399
H	-3.79325	0.50915	-3.22365
H	-2.62812	1.5765	-2.43115
H	-4.63983	-1.61714	-1.80624
H	1.53535	3.60378	1.11453
H	2.05565	3.11161	-0.48578
H	-0.36236	3.01409	-1.24623
H	-0.8654	3.61668	0.33624
H	0.13685	4.62886	-0.71181
H	2.48367	-1.3105	-0.17681
H	7.59695	-0.84052	-1.88611
H	7.56166	0.29369	-0.52812
H	7.1253	-1.40213	-0.27629
Na	0.6227	-1.18231	-1.90499

Compound 1b: Isomer 4R, 6S, 10S, 13S conformer 37

C	5.93961	-0.20187	-0.60103
C	4.64078	-0.85972	-1.10171
C	3.33762	-0.096	-0.8175
C	2.97263	-0.04644	0.67959
C	1.78308	0.88634	0.97204
S	0.80255	0.44319	2.48657

C	0.26696	-1.30118	2.3071
C	-0.77961	-1.7363	1.25379
C	-0.18889	-2.17336	-0.13288
O	-0.95551	-2.07763	-1.14326
O	0.99274	-2.58561	-0.13008
N	-1.93901	-0.8572	1.07632
C	-3.27354	-1.38101	1.3904
O	-4.17272	-0.4887	0.77754
C	-3.51216	0.11876	-0.33869
C	-2.03397	0.08368	0.10348
O	-1.10526	0.68161	-0.45327
C	-4.17882	1.476	-0.60171
C	-3.53085	2.24094	-1.7662
C	-5.68942	1.29815	-0.83621
O	-3.57839	-0.68646	-1.4981
C	2.24237	2.34798	1.15279
C	1.12574	3.39942	1.14365
O	2.2623	-0.69801	-1.57847
C	6.26331	1.14833	-1.2557
H	5.90976	-0.08328	0.48951
H	6.76371	-0.89818	-0.80061
H	4.55076	-1.8649	-0.66724
H	4.70409	-0.9959	-2.18896
H	3.41731	0.92063	-1.21922
H	2.75609	-1.0729	0.99144
H	3.84061	0.28299	1.2628
H	1.07284	0.84756	0.14661
H	1.13026	-1.95661	2.17813
H	-0.14289	-1.49547	3.30381
H	-1.19254	-2.67274	1.65512
H	-3.46146	-1.383	2.4686
H	-3.37597	-2.4019	0.98982
H	-4.03748	2.05524	0.31987

H	-3.64178	1.68345	-2.70179
H	-4.02897	3.20874	-1.88773
H	-2.468	2.42204	-1.59157
H	-6.15787	2.27845	-0.97363
H	-6.17226	0.80127	0.00848
H	-5.87357	0.70289	-1.73595
H	-2.89142	-1.38206	-1.44964
H	2.82582	2.42692	2.08028
H	2.94303	2.56985	0.33622
H	0.53016	3.33371	0.22634
H	0.44192	3.27245	1.98751
H	1.54924	4.40803	1.2017
H	2.0221	-1.55465	-1.14771
H	7.23882	1.51991	-0.92425
H	6.29538	1.05923	-2.34835
H	5.52267	1.9164	-1.0074
Na	0.07343	-0.31115	-2.12943



1c-4*R*,6*S*,10*R*,13*S*

Calculated DFT energies of the 1c-diasteroisomer

Conformers **1c**	OPLS2008 Force Field Conformational Search Relative Energy (kcal/mol)	B3LYP/6-31+G(d,p) DFT Energy (hartree)	Δ (DFT Energy) (kcal/mol)	% Population
1c29	1.515441444	-1732.26022	0	66.77
1c22	1.232625644	-1732.258396	1.144577129	9.65
1c26	1.371846639	-1732.257831	1.499119935	5.30
1c12	0.903227575	-1732.257399	1.770203992	3.35
1c54	2.348377354	-1732.257246	1.866212929	2.85
1c78	2.810686659	-1732.256942	2.056975784	2.07
1c51	2.24029884	-1732.256602	2.270328977	1.44
1c64	2.605284903	-1732.256371	2.415283646	1.13
1c34	1.658486535	-1732.256288	2.467366925	1.03
1c70	2.674309836	-1732.256286	2.468621944	1.03
1c4	0.235659916	-1732.256139	2.560865825	0.88
1c21	1.2109478	-1732.255993	2.652482196	0.76
1c7	0.698184327	-1732.255733	2.815634637	0.57
1c19	1.185971673	-1732.25542	3.012045077	0.41
1c30	1.543333444	-1732.255348	3.057225753	0.38
1c42	2.01639802	-1732.255135	3.190885253	0.30
1c36	1.714581243	-1732.254724	3.448791613	0.20
1c15	1.027534595	-1732.254579	3.539780475	0.17
1c28	1.51529804	-1732.254468	3.609434017	0.15
1c56	2.374691914	-1732.254291	3.720503179	0.12
1c6	0.429135273	-1732.254288	3.722385707	0.12
1c47	2.167736619	-1732.254231	3.758153743	0.12
1c75	2.771322371	-1732.254069	3.859810264	0.10
1c3	0.22029183	-1732.253979	3.916286109	0.09
1c1	0	-1732.253954	3.931973844	0.09
1c17	1.094360673	-1732.253892	3.970879426	0.08
1c85	2.883822495	-1732.253664	4.113951567	0.06
1c9	0.815631876	-1732.253419	4.267691368	0.05
1c10	0.858055441	-1732.253371	4.297811819	0.05
1c79	2.815968692	-1732.25329	4.34864008	0.04
1c43	2.056455425	-1732.25327	4.361190268	0.04

1c27	1.444934674	-1732.253262	4.366210343	0.04
1c83	2.852727815	-1732.253183	4.415783585	0.04

33 conformers counting for the 99.49% of the DFT conformational population

DFT COORDINATES FOR CONFORMATIONAL SEARCH OF 1c (4*R*, 6*S*, 10*R*, 13*S*)

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 29

C	4.91389	2.81599	0.41056
C	4.54542	1.68256	-0.55462
C	3.66279	0.59557	0.06471
C	3.5033	-0.61132	-0.87991
C	2.58478	-1.74169	-0.36134
S	0.88255	-1.47481	-1.07422
C	-0.20019	-2.26525	0.19898
C	-0.97747	-1.3307	1.16187
C	-0.09632	-0.14083	1.67361
O	-0.53634	1.02431	1.50633
O	1.02291	-0.48144	2.13795
N	-2.27543	-0.89989	0.63039
C	-3.50886	-1.28731	1.31066
O	-4.52058	-0.46487	0.76075
C	-4.06601	0.07408	-0.47873
C	-2.53043	-0.06182	-0.39375
O	-1.73827	0.48485	-1.16604
C	-4.55379	1.52481	-0.63031
C	-6.07888	1.60543	-0.81057
C	-4.0946	2.40145	0.54599
O	-4.43844	-0.75809	-1.55953
C	3.10188	-3.1509	-0.70439
C	4.34697	-3.56022	0.09627
O	2.40361	1.18943	0.41824
C	5.76613	3.90709	-0.24733
H	3.99382	3.25217	0.81484

H	5.45773	2.39457	1.26736
H	5.46224	1.21396	-0.93832
H	4.02051	2.09648	-1.4288
H	4.13762	0.24046	0.99197
H	3.15916	-0.26408	-1.86506
H	4.5073	-1.0208	-1.04696
H	2.46048	-1.64673	0.72214
H	-0.91049	-2.90195	-0.33501
H	0.44831	-2.90957	0.79532
H	-1.21428	-1.94019	2.04206
H	-3.43772	-1.087	2.38567
H	-3.7306	-2.3515	1.14187
H	-4.07043	1.88282	-1.54775
H	-6.38416	2.6521	-0.90848
H	-6.42718	1.09356	-1.71544
H	-6.60243	1.18504	0.05482
H	-4.3222	3.45238	0.33849
H	-3.01891	2.31775	0.72942
H	-4.61274	2.11751	1.46733
H	-5.40141	-0.7333	-1.64828
H	2.30536	-3.87886	-0.50894
H	3.30579	-3.20743	-1.78174
H	4.6558	-4.57769	-0.1663
H	5.20099	-2.90169	-0.09583
H	4.1471	-3.5389	1.1738
H	2.03308	0.71656	1.20439
H	6.01655	4.70002	0.46558
H	6.70769	3.50009	-0.63596
H	5.23639	4.37213	-1.08765
Na	0.29355	1.3612	-0.57287

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 22

C	4.9095	2.73156	0.5145
C	4.49836	1.65672	-0.49903
C	3.61827	0.54728	0.08297
C	3.41826	-0.60042	-0.92599
C	2.49353	-1.74656	-0.45592
S	0.77985	-1.40584	-1.10423
C	-0.28213	-2.26336	0.14281
C	-1.02217	-1.38066	1.18111
C	-0.11105	-0.23789	1.7444
O	-0.53756	0.94078	1.66126
O	1.01391	-0.62279	2.15808
N	-2.32698	-0.90446	0.70712
C	-3.54908	-1.34667	1.3712
O	-4.57254	-0.51033	0.86748
C	-4.14145	0.06877	-0.36274
C	-2.59941	-0.02733	-0.28007
O	-1.81045	0.56271	-1.02407
C	-4.7524	1.47917	-0.4654
C	-4.31869	2.38174	0.70046
C	-4.48204	2.14439	-1.82491
O	-4.49583	-0.76252	-1.45223
C	2.97682	-3.13861	-0.90184
C	4.23053	-3.6209	-0.15685
O	2.37782	1.13551	0.5062
C	5.76004	3.84416	-0.10863
H	4.0075	3.15819	0.96683
H	5.47017	2.25801	1.33239
H	5.3977	1.19885	-0.93374
H	3.95549	2.12435	-1.33443
H	4.11353	0.13279	0.97423
H	3.05898	-0.19114	-1.88146
H	4.41193	-1.01397	-1.13896

H	2.39855	-1.7204	0.6344
H	-1.01378	-2.85678	-0.41183
H	0.37193	-2.95121	0.68158
H	-1.24755	-2.04015	2.02769
H	-3.47731	-1.20128	2.45484
H	-3.75568	-2.40396	1.1477
H	-5.8376	1.31066	-0.37288
H	-4.81344	3.35524	0.62023
H	-4.58169	1.9442	1.66642
H	-3.23703	2.55348	0.68977
H	-5.03586	3.08712	-1.88641
H	-4.79146	1.50958	-2.65929
H	-3.41762	2.35903	-1.9498
H	-5.46176	-0.77095	-1.52391
H	2.17096	-3.8639	-0.73744
H	3.15759	-3.12753	-1.98474
H	4.51728	-4.62268	-0.49411
H	5.09127	-2.96357	-0.32137
H	4.0524	-3.66998	0.92362
H	2.02252	0.62213	1.27353
H	6.04561	4.59239	0.63853
H	6.68214	3.44462	-0.54826
H	5.21339	4.36342	-0.90529
Na	0.24173	1.39208	-0.40911

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 26

C	4.64875	2.58801	-0.10335
C	3.53529	1.86473	-0.87194
C	3.09182	0.54107	-0.24493
C	2.01345	-0.16918	-1.08886
C	1.84036	-1.66683	-0.74493
S	0.08087	-2.25225	-1.01343

C	-0.49527	-2.71746	0.67222
C	-1.09954	-1.60696	1.56784
C	-0.05096	-0.74585	2.34453
O	-0.50155	0.24517	2.97433
O	1.15135	-1.11808	2.26868
N	-2.05788	-0.78046	0.8281
C	-3.35302	-1.34851	0.44978
O	-3.98485	-0.36183	-0.33444
C	-3.00181	0.55123	-0.83011
C	-1.82884	0.36743	0.1541
O	-0.85252	1.12413	0.21332
C	-3.58782	1.96543	-0.90223
C	-4.69243	2.05717	-1.96678
C	-4.08769	2.44729	0.46741
O	-2.54908	0.19123	-2.11787
C	2.81559	-2.54998	-1.54297
C	2.94211	-3.99096	-1.04141
O	2.60582	0.83812	1.08193
C	5.0677	3.90653	-0.76414
H	4.31838	2.77403	0.92464
H	5.52028	1.92335	-0.027
H	3.87447	1.65959	-1.89591
H	2.65694	2.52122	-0.96592
H	3.97563	-0.10812	-0.14255
H	1.07364	0.37056	-0.94678
H	2.27476	-0.0782	-2.15178
H	1.99384	-1.81836	0.32565
H	-1.24767	-3.49053	0.48656
H	0.32987	-3.18243	1.21409
H	-1.67955	-2.11357	2.35272
H	-3.96264	-1.54452	1.33928
H	-3.21947	-2.28184	-0.11737
H	-2.74638	2.59695	-1.21275

H	-5.04795	3.09032	-2.04304
H	-4.32803	1.74459	-2.94785
H	-5.54522	1.42463	-1.69901
H	-4.42056	3.48801	0.39646
H	-3.30596	2.40069	1.23331
H	-4.93446	1.84379	0.80885
H	-1.88744	-0.51882	-2.05519
H	2.52335	-2.54438	-2.60203
H	3.80273	-2.0676	-1.50031
H	3.66412	-4.55123	-1.6449
H	3.28461	-4.01761	-0.00024
H	1.98194	-4.51344	-1.09607
H	2.33114	0.0129	1.54839
H	5.86551	4.39958	-0.19843
H	5.43561	3.74311	-1.7842
H	4.22462	4.60535	-0.8268
Na	0.6187	1.76565	1.78485

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 12

C	4.97609	2.74948	0.59614
C	4.56083	1.71038	-0.45226
C	3.68938	0.57664	0.09538
C	3.48685	-0.5337	-0.9541
C	2.56724	-1.6996	-0.52427
S	0.84817	-1.32981	-1.14082
C	-0.20518	-2.24083	0.07445
C	-0.93131	-1.40884	1.16308
C	-0.01569	-0.28788	1.76289
O	-0.44552	0.8924	1.7274
O	1.11351	-0.68526	2.15163
N	-2.24348	-0.91321	0.73319
C	-3.44717	-1.30908	1.45569

O	-4.45394	-0.41757	1.01713
C	-4.072	0.13012	-0.24437
C	-2.52808	-0.00712	-0.22318
O	-1.74354	0.58096	-0.9742
C	-4.61941	1.56918	-0.33214
C	-4.3366	2.22051	-1.69537
C	-6.1222	1.61751	-0.00138
O	-4.49646	-0.70627	-1.30435
C	3.04695	-3.07072	-1.03452
C	4.30694	-3.58348	-0.32113
O	2.45045	1.14431	0.55012
C	5.81837	3.88667	0.00698
H	4.07611	3.1565	1.06999
H	5.54433	2.24897	1.39243
H	5.45838	1.27243	-0.91059
H	4.00957	2.20611	-1.26569
H	4.19327	0.1315	0.96683
H	3.12238	-0.09055	-1.89235
H	4.48066	-0.93625	-1.18662
H	2.48301	-1.72163	0.56695
H	-0.94475	-2.80465	-0.5
H	0.45134	-2.95596	0.57302
H	-1.14206	-2.10801	1.98093
H	-3.3131	-1.18093	2.53516
H	-3.71505	-2.35191	1.23018
H	-4.08741	2.13168	0.44561
H	-4.66699	3.26463	-1.67706
H	-3.27413	2.19094	-1.94215
H	-4.88061	1.70916	-2.49648
H	-6.46441	2.65726	-0.00644
H	-6.338	1.18842	0.9796
H	-6.72277	1.08629	-0.75215
H	-5.46341	-0.68284	-1.34489

H	2.2429	-3.80321	-0.89494
H	3.21869	-3.01284	-2.11741
H	4.59261	-4.5688	-0.70459
H	5.16541	-2.91786	-0.46261
H	4.13697	-3.68067	0.75739
H	2.10515	0.60203	1.30169
H	6.10662	4.6091	0.77814
H	6.73872	3.5064	-0.4529
H	5.26435	4.43182	-0.76701
Na	0.30089	1.42802	-0.33239

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 54

C	4.46801	2.48225	-0.78506
C	3.44131	2.19928	0.3205
C	3.04826	0.72632	0.47765
C	2.14066	0.21896	-0.66076
C	2.03641	-1.3212	-0.74202
S	0.37083	-1.87149	-1.3983
C	-0.37176	-2.79861	0.00851
C	-1.15556	-1.99563	1.07688
C	-0.27404	-1.34151	2.19036
O	0.9495	-1.64465	2.1918
O	-0.8668	-0.5687	2.98634
N	-2.07719	-1.03506	0.46283
C	-3.28138	-1.52599	-0.20988
O	-3.89269	-0.38586	-0.77084
C	-2.92778	0.66357	-0.88035
C	-1.85792	0.26197	0.15586
O	-0.94941	1.00988	0.53599
C	-3.59774	2.02138	-0.64417
C	-4.58253	2.36202	-1.77379
C	-4.27567	2.09321	0.73156

O	-2.3158	0.68651	-2.15253
C	3.16613	-1.92685	-1.59293
C	3.32786	-3.44405	-1.46597
O	2.38344	0.62186	1.75609
C	4.86346	3.96212	-0.85704
H	5.36569	1.87423	-0.60768
H	4.07265	2.16949	-1.75944
H	2.53262	2.79335	0.14179
H	3.85204	2.52991	1.28302
H	3.96842	0.12388	0.52595
H	1.15296	0.66342	-0.51222
H	2.51745	0.59548	-1.6203
H	2.06079	-1.74685	0.26334
H	-1.04154	-3.51641	-0.47568
H	0.41245	-3.36484	0.51381
H	-1.78716	-2.71812	1.61385
H	-3.96786	-1.98236	0.51244
H	-3.02244	-2.26167	-0.98622
H	-2.77198	2.74317	-0.66841
H	-4.9932	3.36515	-1.61662
H	-4.09321	2.33882	-2.75001
H	-5.41738	1.65354	-1.79066
H	-4.66258	3.10315	0.90272
H	-3.58245	1.86032	1.54701
H	-5.11629	1.39477	0.79067
H	-1.62046	0.00909	-2.20276
H	3.01266	-1.65115	-2.64531
H	4.10297	-1.43965	-1.28695
H	4.1613	-3.79988	-2.08091
H	3.53096	-3.73309	-0.42806
H	2.42303	-3.96612	-1.79253
H	2.11562	-0.30998	1.9415
H	5.59969	4.13863	-1.6483

H	3.99281	4.59497	-1.06567
H	5.30202	4.30184	0.08854
Na	0.27591	1.25911	2.40683

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 78

C	-5.15874	-2.60538	0.50115
C	-4.71016	-1.54864	-0.51599
C	-3.76118	-0.4927	0.06017
C	-3.50384	0.64277	-0.94757
C	-2.59986	1.80122	-0.45931
S	-0.84445	1.44174	-0.98413
C	0.17306	2.17079	0.38206
C	0.88346	1.19335	1.34892
C	-0.06782	0.04385	1.81885
O	0.32998	-1.13843	1.67308
O	-1.1936	0.43512	2.22647
N	2.1815	0.71714	0.85789
C	3.39995	1.03392	1.59551
O	4.39027	0.17579	1.06321
C	3.98811	-0.23936	-0.24167
C	2.44555	-0.09397	-0.1861
O	1.64824	-0.60087	-0.98097
C	4.52376	-1.66538	-0.4829
C	4.21762	-2.17203	-1.9012
C	6.03067	-1.75464	-0.18073
O	4.40491	0.69804	-1.21702
C	-3.10336	3.15162	-1.00369
C	-2.3284	4.39325	-0.55462
O	-2.5548	-1.15198	0.46948
C	-6.07554	-3.67135	-0.10915
H	-4.27205	-3.07909	0.93638
H	-5.68009	-2.10652	1.33001

H	-5.59179	-1.04183	-0.93195
H	-4.20689	-2.04033	-1.36223
H	-4.22615	-0.0527	0.95587
H	-3.10824	0.21941	-1.88212
H	-4.4839	1.06459	-1.20658
H	-2.58007	1.81797	0.63563
H	0.91543	2.82458	-0.08386
H	-0.50323	2.78826	0.97182
H	1.11583	1.78499	2.24266
H	3.2795	0.80956	2.6607
H	3.67649	2.09023	1.4616
H	3.99858	-2.30119	0.24112
H	4.54382	-3.21335	-1.99617
H	3.15169	-2.11425	-2.12696
H	4.75158	-1.5817	-2.65325
H	6.36621	-2.79005	-0.29701
H	6.26231	-1.42828	0.83542
H	6.62363	-1.15223	-0.88222
H	5.37117	0.67423	-1.27173
H	-3.11824	3.10619	-2.10086
H	-4.15048	3.25385	-0.68406
H	-2.79609	5.29959	-0.95334
H	-2.31309	4.48289	0.53825
H	-1.29417	4.37127	-0.91194
H	-2.19241	-0.69083	1.26858
H	-6.38587	-4.4058	0.64188
H	-6.98359	-3.22456	-0.53228
H	-5.56949	-4.21598	-0.91562
Na	-0.4254	-1.42746	-0.43667

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 51

C	-4.74611	-2.37394	-0.15202
C	-3.64984	-1.58571	-0.88023
C	-3.12975	-0.3678	-0.11353
C	-2.07424	0.41669	-0.92016
C	-1.81033	1.83734	-0.36903
S	-0.04576	2.40436	-0.65171
C	0.5981	2.63436	1.05843
C	1.20288	1.40512	1.78216
C	0.16152	0.47949	2.49329
O	-1.02918	0.89259	2.53009
O	0.60621	-0.59769	2.9662
N	2.10737	0.6531	0.90843
C	3.40641	1.22678	0.55268
O	3.98315	0.31864	-0.35907
C	2.95683	-0.49994	-0.92581
C	1.81827	-0.39647	0.10934
O	0.8167	-1.12139	0.10948
C	3.49277	-1.91388	-1.17753
C	4.57231	-1.91351	-2.27131
C	4.00303	-2.56915	0.11406
O	2.48286	0.02018	-2.14959
C	-2.80387	2.89665	-0.88805
C	-2.72962	3.22774	-2.38387
O	-2.58743	-0.84719	1.13608
C	-5.25524	-3.57166	-0.96237
H	-4.3658	-2.71334	0.8179
H	-5.58443	-1.69917	0.06978
H	-4.03478	-1.23827	-1.84815
H	-2.80053	-2.24747	-1.10839
H	-3.98486	0.28567	0.12007
H	-1.15227	-0.17104	-0.91788
H	-2.40421	0.47999	-1.9639

H	-1.87518	1.80889	0.71963
H	1.36334	3.40875	0.9465
H	-0.19547	3.04291	1.68665
H	1.82759	1.79541	2.5986
H	4.04957	1.30563	1.43663
H	3.28291	2.22147	0.09841
H	2.62461	-2.47787	-1.5399
H	4.88672	-2.94142	-2.48153
H	4.20137	-1.47029	-3.19815
H	5.45346	-1.34927	-1.94842
H	4.30518	-3.6021	-0.0874
H	3.23633	-2.59328	0.89588
H	4.87229	-2.03278	0.50712
H	1.85386	0.74292	-1.98498
H	-3.81643	2.54179	-0.64589
H	-2.65802	3.81685	-0.31046
H	-3.47167	3.99099	-2.64066
H	-1.74362	3.62017	-2.65322
H	-2.92976	2.35465	-3.01428
H	-2.2763	-0.09743	1.6963
H	-6.03663	-4.11568	-0.42097
H	-5.6771	-3.25333	-1.92327
H	-4.44595	-4.28014	-1.1775
Na	-0.61644	-1.91714	1.64343

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 64

C	4.64552	2.76707	0.04252
C	3.6755	1.93869	-0.80942
C	3.20078	0.64176	-0.15036
C	2.27595	-0.1759	-1.07322
C	2.1152	-1.65401	-0.64583
S	0.41604	-2.30454	-1.07083

C	-0.29878	-2.76186	0.56092
C	-1.01799	-1.66581	1.38011
C	-0.08558	-0.6837	2.16068
O	-0.63352	0.34615	2.63563
O	1.12654	-1.01238	2.25213
N	-2.03462	-0.96624	0.58909
C	-3.36952	-1.54123	0.45451
O	-3.98805	-0.82068	-0.58734
C	-3.31428	0.44145	-0.77315
C	-1.94544	0.19853	-0.07979
O	-0.97789	0.96241	-0.17667
C	-4.14105	1.59053	-0.15084
C	-3.48434	2.96723	-0.33755
C	-5.57448	1.58873	-0.70902
O	-3.1719	0.68908	-2.13554
C	3.20705	-2.54448	-1.26467
C	3.31466	-3.94648	-0.65897
O	2.52456	1.00408	1.07357
C	5.11201	4.04635	-0.662
H	4.16782	3.0181	0.99608
H	5.51817	2.1484	0.29345
H	4.1586	1.67834	-1.76052
H	2.79455	2.54515	-1.07083
H	4.0858	0.04401	0.11777
H	1.30124	0.32042	-1.09671
H	2.67232	-0.14373	-2.09716
H	2.15421	-1.7259	0.44303
H	-1.01401	-3.55542	0.31918
H	0.47981	-3.19967	1.18818
H	-1.57428	-2.18957	2.1725
H	-3.92359	-1.43591	1.40069
H	-3.32033	-2.60012	0.17736
H	-4.1894	1.37069	0.92525

H	-4.09005	3.73318	0.15845
H	-2.47628	3.00072	0.08203
H	-3.41411	3.21886	-1.39977
H	-6.16866	2.35444	-0.19912
H	-6.06112	0.62121	-0.56478
H	-5.57264	1.81486	-1.77948
H	-2.63253	-0.00919	-2.53441
H	3.04162	-2.61633	-2.34847
H	4.16827	-2.02479	-1.13879
H	4.11768	-4.51767	-1.13697
H	3.53244	-3.89715	0.41447
H	2.38163	-4.50332	-0.79092
H	2.26517	0.19916	1.5847
H	5.80628	4.6158	-0.03486
H	5.62521	3.81892	-1.60412
H	4.26522	4.70202	-0.89911
Na	0.41431	1.84185	1.36315

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 34

C	4.81822	3.08018	0.00482
C	4.44342	1.887	-0.88931
C	3.65468	0.77455	-0.18977
C	3.45311	-0.43846	-1.11828
C	2.60668	-1.59014	-0.52816
S	0.85003	-1.36694	-1.11191
C	-0.11755	-2.18337	0.23623
C	-0.84013	-1.2693	1.25941
C	0.05021	-0.0611	1.70908
O	-0.4289	1.09295	1.57883
O	1.20894	-0.37635	2.08679
N	-2.18463	-0.86712	0.83011
C	-3.34692	-1.23737	1.63028

O	-4.40273	-0.42795	1.15016
C	-4.08536	0.01575	-0.16879
C	-2.53752	-0.06408	-0.19359
O	-1.80432	0.48046	-1.02488
C	-4.68934	1.42139	-0.36395
C	-4.47846	1.95645	-1.78931
C	-6.18104	1.44706	0.01649
O	-4.51383	-0.92752	-1.13284
C	3.13301	-2.98687	-0.90503
C	4.44409	-3.35962	-0.19705
O	2.4126	1.33287	0.26658
C	5.85444	2.75733	1.08933
H	5.212	3.8791	-0.63678
H	3.90717	3.47257	0.4706
H	5.35477	1.45123	-1.32201
H	3.83839	2.24301	-1.73555
H	4.21244	0.43142	0.69306
H	3.02287	-0.10325	-2.07333
H	4.45109	-0.82244	-1.36419
H	2.56186	-1.49338	0.56142
H	-0.85155	-2.83462	-0.24554
H	0.58769	-2.81448	0.78001
H	-0.99646	-1.88744	2.15137
H	-3.18119	-1.00433	2.68758
H	-3.58083	-2.30572	1.51176
H	-4.15282	2.06957	0.34054
H	-4.85013	2.98483	-1.85272
H	-3.42453	1.9445	-2.07156
H	-5.02759	1.35416	-2.52069
H	-6.56227	2.46978	-0.06647
H	-6.34774	1.099	1.0383
H	-6.78565	0.831	-0.6629
H	-5.4818	-0.94038	-1.14003

H	2.37252	-3.73446	-0.64943
H	3.25844	-3.04307	-1.99436
H	4.7615	-4.3688	-0.4805
H	5.26283	-2.67773	-0.45133
H	4.3226	-3.34064	0.89219
H	2.11753	0.84662	1.07576
H	6.11817	3.65624	1.6569
H	5.48008	2.02	1.80754
H	6.77814	2.35873	0.65136
Na	0.22282	1.44617	-0.55299

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 70

C	-5.06774	-2.70081	0.40415
C	-4.67737	-1.51668	-0.48902
C	-3.73174	-0.51706	0.18345
C	-3.54376	0.75193	-0.66985
C	-2.58612	1.80917	-0.07264
S	-0.87656	1.54459	-0.77383
C	0.20413	2.17776	0.58725
C	0.94521	1.13602	1.46407
C	0.02505	-0.0708	1.85118
O	-1.08809	0.25694	2.33964
O	0.43074	-1.22579	1.56916
N	2.23942	0.72242	0.91085
C	3.4655	0.96692	1.66251
O	4.44752	0.15726	1.04596
C	4.02898	-0.15113	-0.2833
C	2.48879	0.00558	-0.20345
O	1.6803	-0.42009	-1.03391
C	4.54238	-1.56245	-0.63493
C	4.22722	-1.95579	-2.08692
C	6.048	-1.69912	-0.34399

O	4.45106	0.85138	-1.18839
C	-3.07357	3.25592	-0.28252
C	-3.28397	3.69034	-1.73783
O	-2.49204	-1.1875	0.45654
C	-5.98424	-3.70639	-0.30189
H	-4.15645	-3.20214	0.74813
H	-5.56882	-2.31992	1.30492
H	-5.58308	-0.98428	-0.81088
H	-4.1932	-1.88736	-1.40501
H	-4.16787	-0.214	1.14763
H	-3.23265	0.46966	-1.68553
H	-4.53581	1.20965	-0.78008
H	-2.47754	1.62559	1.00036
H	0.93554	2.84912	0.1298
H	-0.43973	2.772	1.23785
H	1.18535	1.65488	2.39957
H	3.35357	0.64826	2.70444
H	3.74536	2.03009	1.62208
H	4.00798	-2.24334	0.03968
H	4.53073	-2.99416	-2.25795
H	3.16319	-1.85877	-2.30856
H	4.7755	-1.32409	-2.79367
H	6.36753	-2.72651	-0.54588
H	6.28595	-1.46158	0.69507
H	6.64995	-1.05012	-0.99435
H	5.41649	0.81983	-1.25267
H	-4.01813	3.3611	0.27142
H	-2.36508	3.94119	0.20019
H	-3.61738	4.73249	-1.78166
H	-2.35552	3.60904	-2.31159
H	-4.04441	3.08173	-2.23958
H	-2.10484	-0.81299	1.28685
H	-6.24775	-4.53778	0.3608

H	-6.91841	-3.23476	-0.63064
H	-5.49917	-4.13099	-1.18928
Na	-0.37623	-1.32094	-0.54052

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 4

C	-4.62602	-2.46352	0.07944
C	-3.52241	-1.77753	-0.73639
C	-3.03244	-0.45293	-0.14745
C	-1.96899	0.22181	-1.03829
C	-1.75618	1.72105	-0.7257
S	0.00289	2.26884	-1.06423
C	0.64519	2.74917	0.59284
C	1.25685	1.64182	1.48763
C	0.21961	0.81611	2.31529
O	0.67325	-0.16931	2.95153
O	-0.97781	1.20927	2.27254
N	2.17647	0.78536	0.73191
C	3.46478	1.32799	0.30108
O	4.05251	0.31913	-0.48761
C	3.03881	-0.58426	-0.94349
C	1.90411	-0.36906	0.08322
O	0.91304	-1.1006	0.19573
C	3.66646	-1.98446	-1.04117
C	4.18549	-2.47178	0.32015
C	2.73009	-3.01457	-1.69141
O	2.55765	-0.22207	-2.21806
C	-2.74245	2.60985	-1.50375
C	-2.82618	4.06018	-1.02071
O	-2.50899	-0.73696	1.16809
C	-5.09401	-3.78322	-0.54486
H	-4.267	-2.63951	1.09959
H	-5.48012	-1.77855	0.17164

H	-3.88959	-1.58311	-1.75278
H	-2.66138	-2.45423	-0.84578
H	-3.89932	0.21572	-0.02756
H	-1.03532	-0.33356	-0.91794
H	-2.26703	0.11852	-2.09037
H	-1.86869	1.89249	0.347
H	1.40652	3.50306	0.36868
H	-0.15131	3.24077	1.15365
H	1.87168	2.15077	2.24404
H	4.10795	1.52909	1.16564
H	3.32598	2.25454	-0.27603
H	4.52842	-1.83804	-1.70617
H	4.70036	-3.43046	0.20017
H	4.89007	-1.7617	0.76057
H	3.36306	-2.62538	1.02883
H	3.26347	-3.96294	-1.81829
H	2.38851	-2.67657	-2.67191
H	1.84985	-3.19695	-1.06824
H	1.91654	0.5055	-2.14305
H	-2.48682	2.58311	-2.57193
H	-3.73595	2.14623	-1.42013
H	-3.55879	4.62427	-1.60765
H	-3.13183	4.10867	0.03111
H	-1.85954	4.56455	-1.11651
H	-2.20365	0.09073	1.61038
H	-5.88472	-4.24818	0.05364
H	-5.48953	-3.62881	-1.55595
H	-4.26911	-4.50212	-0.62077
Na	-0.51706	-1.68569	1.82764

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 21

C	4.43404	2.38301	-0.69167
C	3.37316	2.12052	0.38626
C	2.96995	0.65178	0.55673
C	2.10249	0.12571	-0.60374
C	1.98232	-1.41507	-0.65376
S	0.34096	-1.95977	-1.37197
C	-0.49167	-2.83224	0.02078
C	-1.31537	-1.98799	1.02526
C	-0.48309	-1.32802	2.17167
O	0.7376	-1.63733	2.23421
O	-1.10716	-0.54285	2.93049
N	-2.17931	-1.02291	0.34
C	-3.35231	-1.5044	-0.38828
O	-3.9087	-0.36396	-1.00175
C	-2.92772	0.67778	-1.06475
C	-1.91901	0.26623	0.03094
O	-1.01039	0.99113	0.45386
C	-3.65763	2.02128	-0.90069
C	-4.38384	2.11287	0.44996
C	-2.74204	3.2327	-1.13368
O	-2.25983	0.68449	-2.30615
C	3.1394	-2.05091	-1.44405
C	3.2763	-3.5674	-1.2849
O	2.25839	0.57482	1.81184
C	4.83514	3.86089	-0.77435
H	5.32426	1.77577	-0.4778
H	4.0675	2.05635	-1.67273
H	2.47219	2.71359	0.16967
H	3.75487	2.4665	1.35535
H	3.88556	0.04758	0.65043
H	1.11577	0.58596	-0.50638
H	2.5228	0.47386	-1.55585

H	1.95956	-1.81855	0.36091
H	-1.14807	-3.55151	-0.47936
H	0.25391	-3.39864	0.58116
H	-1.99225	-2.6843	1.5412
H	-4.08599	-1.93538	0.30305
H	-3.06612	-2.25948	-1.13592
H	-4.41346	2.00542	-1.69766
H	-4.96795	3.03769	0.49564
H	-5.0675	1.27307	0.5982
H	-3.67345	2.13012	1.28492
H	-3.33718	4.15165	-1.09703
H	-2.25176	3.17769	-2.1078
H	-1.96663	3.29587	-0.3647
H	-1.59225	-0.02136	-2.33185
H	3.03422	-1.79238	-2.50674
H	4.06852	-1.56928	-1.10739
H	4.13054	-3.94331	-1.85795
H	3.43162	-3.84149	-0.23475
H	2.37955	-4.08385	-1.64123
H	1.96347	-0.34828	1.99604
H	5.59454	4.02414	-1.5463
H	3.97233	4.49208	-1.01778
H	5.24658	4.2141	0.17844
Na	0.13315	1.23566	2.38231

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 7

C	-4.70134	-2.76491	-0.00567
C	-3.74734	-1.91475	-0.85426
C	-3.24022	-0.6484	-0.16047
C	-2.33749	0.19921	-1.07737
C	-2.15201	1.65896	-0.5972
S	-0.45025	2.29785	-1.02309

C	0.28613	2.70591	0.61117
C	1.01182	1.58518	1.3895
C	0.08016	0.57093	2.13123
O	0.61942	-0.489	2.54626
O	-1.12557	0.91061	2.25864
N	2.04586	0.91563	0.59237
C	3.36511	1.52888	0.45235
O	4.1813	0.53149	-0.13292
C	3.34399	-0.39907	-0.81448
C	1.96748	-0.21754	-0.13345
O	1.0221	-0.99955	-0.27216
C	3.92556	-1.81737	-0.68484
C	5.24775	-1.96952	-1.45575
C	4.1014	-2.23039	0.78497
O	3.1331	-0.00626	-2.15485
C	-3.24201	2.58274	-1.16921
C	-3.32022	3.96596	-0.51775
O	-2.52979	-1.06559	1.02591
C	-5.19645	-4.01661	-0.73953
H	-4.20077	-3.05067	0.92609
H	-5.56224	-2.14879	0.28847
H	-4.2538	-1.61506	-1.78126
H	-2.88034	-2.51963	-1.16246
H	-4.1109	-0.05452	0.15857
H	-1.367	-0.30088	-1.15349
H	-2.76403	0.21037	-2.08952
H	-2.17907	1.69117	0.49379
H	1.00135	3.50449	0.38625
H	-0.48204	3.12613	1.26302
H	1.55645	2.08583	2.20451
H	3.77499	1.78953	1.43407
H	3.31877	2.4229	-0.18586
H	3.1718	-2.46642	-1.14752

H	5.62971	-2.98875	-1.33867
H	5.13074	-1.80196	-2.53254
H	6.00969	-1.28165	-1.07372
H	4.38743	-3.28574	0.84564
H	3.182	-2.09751	1.36403
H	4.88633	-1.63773	1.26471
H	3.9805	-0.04	-2.62028
H	-3.0922	2.687	-2.25269
H	-4.20862	2.07241	-1.04428
H	-4.12267	4.5633	-0.96391
H	-3.52099	3.88532	0.55718
H	-2.38125	4.51324	-0.64764
H	-2.2593	-0.28435	1.56856
H	-5.88029	-4.60063	-0.11422
H	-5.73039	-3.75453	-1.66091
H	-4.36163	-4.67122	-1.01859
Na	-0.41343	-1.91777	1.19392

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 19

C	4.66219	2.46332	0.04116
C	3.49705	1.85041	-0.74698
C	3.04982	0.47571	-0.24562
C	1.91696	-0.11742	-1.10843
C	1.71974	-1.63911	-0.91839
S	-0.06419	-2.15729	-1.16637
C	-0.58412	-2.77677	0.48829
C	-1.1224	-1.75156	1.51767
C	-0.02244	-1.00533	2.3393
O	-0.4219	-0.0846	3.09693
O	1.16683	-1.38853	2.16786
N	-2.08619	-0.82972	0.9096
C	-3.41293	-1.32167	0.5395

O	-4.05328	-0.22986	-0.07734
C	-3.06168	0.6778	-0.57453
C	-1.85257	0.37654	0.34455
O	-0.84836	1.09033	0.45339
C	-3.64908	2.09818	-0.52396
C	-2.68676	3.15445	-1.08967
C	-5.0049	2.15298	-1.25004
O	-2.69287	0.37689	-1.90238
C	2.63501	-2.45014	-1.85271
C	2.74884	-3.93937	-1.51695
O	2.63239	0.63672	1.12712
C	5.08408	3.83715	-0.49237
H	4.38336	2.54232	1.09784
H	5.51919	1.77673	0.00363
H	3.78405	1.75172	-1.80223
H	2.63201	2.53065	-0.72686
H	3.92085	-0.19838	-0.25605
H	0.99917	0.4243	-0.8669
H	2.13425	0.07996	-2.16678
H	1.91624	-1.9101	0.12123
H	-1.36349	-3.51001	0.25784
H	0.25008	-3.3125	0.94417
H	-1.68657	-2.32481	2.26747
H	-3.98077	-1.61299	1.43006
H	-3.33706	-2.17975	-0.14564
H	-3.81993	2.30747	0.54039
H	-3.12302	4.1509	-0.96006
H	-1.71654	3.13089	-0.58963
H	-2.52182	2.99011	-2.15858
H	-5.42121	3.16294	-1.17184
H	-5.72263	1.45039	-0.82061
H	-4.88469	1.91667	-2.31194
H	-2.03804	-0.34223	-1.91836

H	2.2943	-2.32305	-2.88947
H	3.63467	-1.99457	-1.80652
H	3.42905	-4.44373	-2.21145
H	3.13744	-4.08684	-0.50241
H	1.77489	-4.43432	-1.58232
H	2.3514	-0.22733	1.51238
H	5.91922	4.24849	0.08463
H	5.40096	3.77863	-1.54055
H	4.25758	4.55623	-0.43847
Na	0.70399	1.51894	2.02475

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 30

C	2.37123	3.37682	-0.46047
C	3.53268	2.38164	-0.32371
C	3.15569	0.95144	0.08169
C	2.19816	0.25657	-0.91111
C	2.22465	-1.28576	-0.80447
S	0.5699	-2.05085	-1.2354
C	0.024	-2.83568	0.33764
C	-0.75286	-1.96107	1.35372
C	0.14507	-1.08372	2.2863
O	-0.45366	-0.25485	3.01844
O	1.38815	-1.28415	2.22018
N	-1.80463	-1.17803	0.69716
C	-2.99516	-1.86106	0.18737
O	-3.74588	-0.86805	-0.47527
C	-2.89165	0.2311	-0.80207
C	-1.72583	0.07375	0.19505
O	-0.86654	0.94022	0.39468
C	-3.6699	1.54798	-0.7063
C	-4.74947	1.63845	-1.79619
C	-4.2652	1.75838	0.69331

O	-2.36528	0.12015	-2.1075
C	3.33182	-1.89991	-1.67892
C	3.64349	-3.37053	-1.38871
O	2.58736	1.00993	1.40777
C	2.84127	4.7673	-0.90485
H	1.62879	2.99855	-1.17313
H	1.85628	3.47079	0.50561
H	4.24785	2.76306	0.41654
H	4.07206	2.32567	-1.2791
H	4.09154	0.37615	0.14516
H	1.1883	0.63157	-0.73241
H	2.46896	0.54562	-1.93596
H	2.37137	-1.57683	0.23795
H	-0.60654	-3.66842	0.0101
H	0.89312	-3.25851	0.84402
H	-1.2708	-2.65117	2.03532
H	-3.58974	-2.27005	1.01219
H	-2.71477	-2.67239	-0.50097
H	-2.91833	2.3256	-0.89023
H	-5.24527	2.61377	-1.74577
H	-4.32019	1.52125	-2.79368
H	-5.51096	0.86404	-1.65644
H	-4.74143	2.74266	0.75077
H	-3.5024	1.71226	1.47806
H	-5.02446	1.00141	0.91302
H	-1.60945	-0.49156	-2.11395
H	3.06795	-1.77321	-2.73785
H	4.24171	-1.30306	-1.52152
H	4.45163	-3.73194	-2.03344
H	3.95912	-3.50882	-0.34785
H	2.76662	-4.00165	-1.56386
H	2.41107	0.10006	1.74836
H	2.00203	5.46669	-0.98232

H	3.56375	5.18793	-0.19559
H	3.32836	4.72336	-1.88597
Na	0.46333	1.56154	2.09664

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 42

C	4.60993	2.50897	0.01957
C	3.57544	1.73443	-0.80716
C	3.08037	0.44258	-0.15108
C	2.0827	-0.31125	-1.05954
C	1.83374	-1.79358	-0.67936
S	0.0439	-2.2966	-0.93807
C	-0.55429	-2.73001	0.74629
C	-1.16418	-1.59472	1.6036
C	-0.11444	-0.71544	2.35662
O	-0.55142	0.32321	2.91564
O	1.07564	-1.13064	2.33847
N	-2.12387	-0.79626	0.83418
C	-3.42367	-1.37759	0.49325
O	-4.06264	-0.42477	-0.32594
C	-3.08551	0.46764	-0.86773
C	-1.89806	0.31875	0.10548
O	-0.91878	1.07327	0.11489
C	-3.67184	1.87935	-0.98174
C	-4.79378	1.9331	-2.03076
C	-4.14984	2.41134	0.37718
O	-2.6536	0.06192	-2.14935
C	2.70623	-2.79097	-1.46857
C	4.22112	-2.59933	-1.30772
O	2.48055	0.80553	1.10863
C	5.09242	3.78667	-0.677
H	4.18217	2.75562	0.99773
H	5.46927	1.85467	0.2209

H	4.01011	1.47775	-1.78236
H	2.70745	2.37722	-1.01938
H	3.95002	-0.19266	0.06548
H	1.14261	0.24723	-1.03742
H	2.44816	-0.26946	-2.09431
H	1.98733	-1.93093	0.3936
H	-1.3074	-3.50394	0.56768
H	0.26144	-3.18511	1.31059
H	-1.74636	-2.07674	2.40246
H	-4.02456	-1.53498	1.39629
H	-3.29665	-2.33459	-0.03479
H	-2.83555	2.49843	-1.32888
H	-5.14943	2.9633	-2.13972
H	-4.44598	1.58356	-3.00536
H	-5.64269	1.31247	-1.72546
H	-4.48842	3.44736	0.27265
H	-3.35498	2.3965	1.13081
H	-4.98786	1.81798	0.75584
H	-1.97643	-0.63109	-2.07277
H	2.43965	-3.8051	-1.1518
H	2.44372	-2.72579	-2.53349
H	4.75757	-3.38788	-1.84626
H	4.56455	-1.64075	-1.71014
H	4.5235	-2.65242	-0.25544
H	2.20167	0.00119	1.61271
H	5.83119	4.31791	-0.06735
H	5.55876	3.56264	-1.64393
H	4.26036	4.47608	-0.86561
Na	0.51323	1.81936	1.66462

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 36

C	4.63362	2.47442	-0.84778
C	3.49513	2.31429	0.16912
C	3.11174	0.86551	0.49152
C	2.33998	0.17401	-0.64801
C	2.28226	-1.36829	-0.53501
S	0.70192	-2.03207	-1.27594
C	-0.18354	-2.78967	0.14646
C	-1.06615	-1.88818	1.03999
C	-0.29484	-1.04226	2.10536
O	0.91716	-1.33361	2.28161
O	-0.9576	-0.15159	2.70066
N	-2.02336	-1.08074	0.27625
C	-3.25763	-1.68971	-0.21469
O	-4.05984	-0.60916	-0.65361
C	-3.21479	0.50425	-0.93405
C	-1.92941	0.20044	-0.13018
O	-1.02885	1.02286	0.06506
C	-3.91775	1.80816	-0.51605
C	-5.14241	2.10823	-1.39658
C	-4.30635	1.79497	0.97086
O	-2.80318	0.50362	-2.28457
C	3.50537	-2.02977	-1.19517
C	3.68595	-3.51592	-0.87517
O	2.31317	0.92349	1.69481
C	5.00079	3.94297	-1.09347
H	5.5187	1.93363	-0.48583
H	4.35799	2.00867	-1.80203
H	2.60248	2.84719	-0.19237
H	3.78869	2.79088	1.11316
H	4.03066	0.30508	0.72262
H	1.32771	0.58921	-0.66436
H	2.79896	0.43624	-1.60995

H	2.22772	-1.66105	0.51566
H	-0.81174	-3.55593	-0.32072
H	0.53283	-3.30037	0.79274
H	-1.68296	-2.57157	1.64332
H	-3.7787	-2.21091	0.5957
H	-3.0514	-2.38651	-1.0396
H	-3.16648	2.59076	-0.67957
H	-5.61695	3.03769	-1.06611
H	-4.87996	2.24883	-2.45138
H	-5.88728	1.30861	-1.32331
H	-4.68045	2.78028	1.26848
H	-3.45882	1.54743	1.61788
H	-5.09591	1.06126	1.16054
H	-3.58458	0.62312	-2.84219
H	3.44861	-1.88509	-2.28299
H	4.39835	-1.48007	-0.86345
H	4.5793	-3.91558	-1.36721
H	3.79808	-3.67658	0.20367
H	2.82411	-4.09745	-1.21701
H	2.04622	0.01821	1.98794
H	5.8168	4.0333	-1.81825
H	4.14448	4.50493	-1.48486
H	5.32266	4.43187	-0.1664
Na	0.14229	1.60878	1.89841

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 15

C	-4.28375	-2.99269	-0.25917
C	-3.28597	-2.09142	-1.00599
C	-2.9449	-0.7705	-0.30985
C	-1.92808	0.05767	-1.12227
C	-1.8547	1.54254	-0.69883
S	-0.14341	2.26054	-0.9501

C	0.42006	2.67558	0.75271
C	1.10893	1.56494	1.58477
C	0.13137	0.59581	2.32506
O	-1.09519	0.88457	2.27479
O	0.65638	-0.38913	2.90466
N	2.117	0.84625	0.79926
C	3.3658	1.5235	0.45147
O	4.06327	0.62395	-0.37903
C	3.15118	-0.33858	-0.92
C	1.96695	-0.28282	0.07146
O	1.03988	-1.10095	0.10021
C	3.90606	-1.67061	-1.06567
C	4.42243	-2.18387	0.28672
C	3.09071	-2.74335	-1.80378
O	2.68517	0.04814	-2.19292
C	-2.89871	2.39847	-1.43736
C	-3.11521	3.79811	-0.85593
O	-2.42772	-1.09943	0.99761
C	-5.6952	-2.40528	-0.13241
H	-4.34179	-3.95043	-0.79238
H	-3.89159	-3.21439	0.74006
H	-3.68405	-1.85628	-2.00209
H	-2.34829	-2.64145	-1.1722
H	-3.86809	-0.18912	-0.1702
H	-0.95148	-0.42204	-1.01715
H	-2.19516	0.0054	-2.18646
H	-2.00479	1.62411	0.37988
H	1.11589	3.50692	0.60168
H	-0.42794	3.05348	1.32617
H	1.66043	2.07057	2.39064
H	3.96189	1.7194	1.3504
H	3.1652	2.47196	-0.06908
H	4.77268	-1.41078	-1.68887

H	5.03126	-3.08112	0.13543
H	5.03983	-1.4369	0.79208
H	3.59523	-2.45547	0.9532
H	3.71541	-3.62863	-1.96526
H	2.74671	-2.38184	-2.77497
H	2.21448	-3.04407	-1.22202
H	1.98798	0.72008	-2.10715
H	-2.62135	2.47021	-2.49803
H	-3.85009	1.84787	-1.41144
H	-3.88022	4.34085	-1.42125
H	-3.44603	3.74479	0.18804
H	-2.19256	4.38582	-0.88953
H	-2.20304	-0.28146	1.50217
H	-6.37318	-3.11881	0.34805
H	-5.70356	-1.49194	0.47169
H	-6.11417	-2.16078	-1.11635
Na	-0.37729	-1.91732	1.64759

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 28

C	4.73655	2.63065	-0.06009
C	3.79254	1.70314	-0.83653
C	3.24434	0.53068	-0.01991
C	2.35926	-0.40716	-0.86464
C	2.12285	-1.79263	-0.21518
S	0.43379	-2.47479	-0.63514
C	-0.37243	-2.65229	1.00775
C	-1.11141	-1.4334	1.60444
C	-0.19714	-0.35065	2.26675
O	-0.73795	0.75561	2.53227
O	0.99663	-0.68537	2.48693
N	-2.08747	-0.84745	0.67935
C	-3.41676	-1.43991	0.54999

O	-4.17484	-0.50355	-0.19381
C	-3.28344	0.33934	-0.92015
C	-1.94318	0.1937	-0.16341
O	-0.96822	0.93006	-0.34135
C	-3.82824	1.77896	-0.94033
C	-5.11288	1.89939	-1.77709
C	-4.05104	2.32222	0.48003
O	-3.03087	-0.17745	-2.20896
C	3.23054	-2.81654	-0.53996
C	3.33192	-3.27076	-2.0017
O	2.50317	1.0929	1.08523
C	5.26219	3.79286	-0.91049
H	4.21796	3.01807	0.82387
H	5.58351	2.04165	0.31806
H	4.31986	1.29482	-1.7087
H	2.94439	2.28084	-1.23568
H	4.09566	-0.031	0.39536
H	1.40251	0.09554	-1.03731
H	2.82108	-0.53611	-1.85083
H	2.08004	-1.67128	0.86807
H	-1.09062	-3.4654	0.85671
H	0.36098	-2.99444	1.74085
H	-1.70791	-1.82203	2.44382
H	-3.87909	-1.56599	1.53517
H	-3.36993	-2.40817	0.03129
H	-3.03737	2.36539	-1.42426
H	-5.4711	2.93374	-1.75873
H	-4.95661	1.64197	-2.83095
H	-5.90875	1.26386	-1.37404
H	-4.29507	3.38903	0.43875
H	-3.16516	2.20255	1.11183
H	-4.88119	1.80339	0.96931
H	-3.85882	-0.16649	-2.70912

H	4.18988	-2.37482	-0.23097
H	3.08123	-3.69608	0.09727
H	4.14342	-3.9969	-2.11927
H	2.40435	-3.75099	-2.32948
H	3.53926	-2.43795	-2.68249
H	2.19432	0.38461	1.70159
H	5.93889	4.43365	-0.33498
H	5.81301	3.42953	-1.78645
H	4.44103	4.42152	-1.27623
Na	0.40332	1.99847	1.08409

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 56

C	2.64231	3.10516	-0.43129
C	3.72309	2.04016	-0.19423
C	3.22703	0.66197	0.26156
C	2.2744	-0.01687	-0.74738
C	2.16776	-1.54656	-0.5456
S	0.48889	-2.2248	-1.03261
C	-0.18815	-2.8647	0.55646
C	-0.95038	-1.87854	1.47609
C	-0.04263	-1.01505	2.41193
O	1.18308	-1.30996	2.43573
O	-0.61748	-0.10224	3.0584
N	-1.90538	-1.06328	0.72079
C	-3.12071	-1.68551	0.19369
O	-3.76988	-0.67745	-0.5487
C	-2.82755	0.3437	-0.88638
C	-1.71319	0.15076	0.16194
O	-0.8006	0.96224	0.35574
C	-3.51183	1.71523	-0.87285
C	-4.55162	1.83069	-1.9984
C	-4.13018	2.0299	0.49712

O	-2.26497	0.13973	-2.16521
C	3.28642	-2.34237	-1.24893
C	3.27765	-2.32104	-2.78282
O	2.59742	0.83265	1.54982
C	3.22955	4.43545	-0.91853
H	1.90547	2.74433	-1.15867
H	2.09537	3.28318	0.50487
H	4.43119	2.40876	0.55921
H	4.2974	1.89924	-1.11988
H	4.11542	0.02903	0.40492
H	1.29001	0.44547	-0.64905
H	2.62149	0.19733	-1.76555
H	2.20874	-1.76213	0.52336
H	-0.85906	-3.67165	0.24549
H	0.62149	-3.31377	1.13421
H	-1.55273	-2.49002	2.16357
H	-3.77561	-2.00821	1.01116
H	-2.87333	-2.54927	-0.44157
H	-2.70185	2.42917	-1.06647
H	-4.9766	2.84013	-2.00765
H	-4.10511	1.63594	-2.97603
H	-5.37051	1.11989	-1.84622
H	-4.53739	3.04631	0.4969
H	-3.39531	1.96682	1.30691
H	-4.94693	1.33811	0.7255
H	-1.56161	-0.52965	-2.11874
H	4.24696	-1.94697	-0.88742
H	3.23674	-3.38225	-0.90593
H	4.10838	-2.91686	-3.17522
H	2.34953	-2.74578	-3.17905
H	3.38512	-1.30835	-3.18593
H	2.33572	-0.04074	1.92782
H	2.44681	5.18607	-1.0714

H	3.94681	4.84153	-0.19559
H	3.75715	4.30712	-1.87095
Na	0.49084	1.57936	2.0921

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 6

C	4.6335	2.70185	0.12428
C	3.67896	1.87816	-0.74932
C	3.16646	0.59371	-0.09438
C	2.26239	-0.22114	-1.03888
C	2.06722	-1.69337	-0.60433
S	0.37062	-2.31298	-1.07573
C	-0.39614	-2.75817	0.53443
C	-1.12787	-1.65381	1.33087
C	-0.20364	-0.67543	2.12777
O	-0.74781	0.36386	2.58554
O	1.00152	-1.01948	2.25177
N	-2.1356	-0.94747	0.53123
C	-3.44109	-1.56287	0.30903
O	-4.23954	-0.54334	-0.26005
C	-3.38595	0.42291	-0.87035
C	-2.03187	0.21429	-0.14669
O	-1.07504	0.99189	-0.21699
C	-4.05454	1.80391	-0.71375
C	-4.27018	2.17812	0.76096
C	-3.31513	2.91429	-1.47687
O	-3.13735	0.08654	-2.21958
C	3.16254	-2.60466	-1.18601
C	3.22991	-4.00342	-0.56717
O	2.45492	0.97568	1.10363
C	5.14093	3.96632	-0.57867
H	4.12969	2.97006	1.05957
H	5.48865	2.07349	0.40916

H	4.18739	1.60264	-1.68277
H	2.81476	2.49388	-1.04327
H	4.03435	-0.01268	0.20817
H	1.29492	0.28642	-1.10095
H	2.69138	-0.20374	-2.04989
H	2.07706	-1.75724	0.48554
H	-1.11199	-3.54614	0.27644
H	0.35802	-3.20068	1.1879
H	-1.69804	-2.17369	2.11586
H	-3.88847	-1.87394	1.25929
H	-3.36062	-2.4245	-0.36908
H	-5.04765	1.67391	-1.17317
H	-4.79776	3.13509	0.82972
H	-4.86288	1.42341	1.28319
H	-3.31561	2.28394	1.2884
H	-3.9039	3.83715	-1.44296
H	-3.15099	2.64901	-2.52426
H	-2.33724	3.11203	-1.03001
H	-3.97694	0.13202	-2.70047
H	3.02568	-2.68239	-2.27338
H	4.12862	-2.09986	-1.03711
H	4.03575	-4.59231	-1.0184
H	3.41871	-3.94905	0.51156
H	2.29104	-4.54487	-0.72057
H	2.17062	0.17763	1.61278
H	5.82418	4.5323	0.0636
H	5.67935	3.72095	-1.50205
H	4.312	4.632	-0.84892
Na	0.34207	1.82907	1.31808

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 47

C	4.40287	2.47409	-0.67786
C	3.4182	2.09058	0.43547
C	3.01889	0.6113	0.46203
C	2.04907	0.2265	-0.67313
C	1.91668	-1.29789	-0.89396
S	0.21558	-1.76673	-1.52212
C	-0.47572	-2.82076	-0.17876
C	-1.20609	-2.12357	0.99716
C	-0.27083	-1.59919	2.1345
O	-0.82285	-0.93061	3.04506
O	0.95344	-1.88754	2.03772
N	-2.13363	-1.09213	0.52376
C	-3.36314	-1.491	-0.15939
O	-3.97114	-0.2859	-0.56087
C	-2.97534	0.74226	-0.63994
C	-1.89237	0.2256	0.33814
O	-0.95385	0.89992	0.77869
C	-3.65029	2.08271	-0.30379
C	-2.6836	3.27285	-0.40555
C	-4.88601	2.30741	-1.19353
O	-2.40371	0.82203	-1.9269
C	2.99815	-1.83417	-1.84783
C	3.13951	-3.35854	-1.87379
O	2.42071	0.37823	1.75624
C	4.80739	3.95222	-0.62435
H	5.30176	1.84787	-0.59457
H	3.96735	2.25717	-1.66122
H	2.50903	2.70456	0.35348
H	3.87074	2.32194	1.40814
H	3.93455	0.0031	0.39959
H	1.07717	0.66622	-0.43411
H	2.38541	0.68898	-1.60992

H	1.97631	-1.81573	0.06539
H	-1.17033	-3.48668	-0.70034
H	0.32484	-3.43573	0.23538
H	-1.8286	-2.89005	1.48077
H	-4.0346	-2.01902	0.52686
H	-3.14143	-2.13422	-1.02458
H	-3.98856	1.98865	0.73667
H	-3.20032	4.18846	-0.0979
H	-1.80518	3.13891	0.22878
H	-2.3422	3.40301	-1.4367
H	-5.3733	3.24695	-0.91205
H	-5.61214	1.49802	-1.0891
H	-4.59745	2.37691	-2.24703
H	-1.71184	0.14617	-2.03319
H	2.80425	-1.45714	-2.86136
H	3.95553	-1.3907	-1.53895
H	3.93789	-3.66369	-2.55851
H	3.38499	-3.74918	-0.87918
H	2.21223	-3.83564	-2.20619
H	2.14264	-0.56344	1.8518
H	5.51699	4.19893	-1.42112
H	3.93526	4.60618	-0.74146
H	5.28146	4.19917	0.33283
Na	0.35534	0.92194	2.6094

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 75

C	2.40559	3.40628	-0.52944
C	3.57997	2.46699	-0.21563
C	3.20804	1.04621	0.22823
C	2.41528	0.25179	-0.83163
C	2.49153	-1.28194	-0.63969
S	0.92899	-2.12215	-1.22779

C	0.20728	-2.84711	0.3006
C	-0.68779	-1.95705	1.19151
C	0.07275	-0.97337	2.13871
O	-0.62483	-0.08631	2.69827
O	1.31066	-1.16317	2.26539
N	-1.7512	-1.29705	0.42873
C	-2.98923	-2.01695	0.14387
O	-3.66179	-1.24392	-0.82428
C	-3.1667	0.11075	-0.78995
C	-1.79509	-0.05136	-0.0786
O	-0.93242	0.83374	-0.03185
C	-4.15733	1.02862	-0.03595
C	-3.69318	2.49259	0.01451
C	-5.56556	0.92127	-0.64552
O	-3.03191	0.58288	-2.09176
C	3.71862	-1.88016	-1.35066
C	4.05227	-3.32221	-0.95952
O	2.46826	1.15999	1.46294
C	2.8706	4.78361	-1.01824
H	1.74846	2.95601	-1.28334
H	1.79944	3.54382	0.37723
H	4.19658	2.91698	0.57305
H	4.21962	2.38345	-1.10449
H	4.14794	0.51817	0.44741
H	1.37266	0.57806	-0.80724
H	2.80051	0.50066	-1.83023
H	2.53251	-1.51676	0.42639
H	-0.38235	-3.69244	-0.07021
H	1.00815	-3.25104	0.92254
H	-1.20699	-2.63946	1.88181
H	-3.5868	-2.11996	1.06353
H	-2.7852	-3.01011	-0.27122
H	-4.19597	0.64072	0.992

H	-4.40309	3.08303	0.6035
H	-2.70386	2.5934	0.46676
H	-3.64596	2.91631	-0.9929
H	-6.26919	1.51512	-0.05261
H	-5.91725	-0.11299	-0.6644
H	-5.57401	1.3046	-1.67017
H	-2.39364	0.03277	-2.56861
H	3.57383	-1.81013	-2.4377
H	4.58075	-1.23757	-1.11928
H	4.94101	-3.67536	-1.49347
H	4.25369	-3.40251	0.11526
H	3.22439	-3.99622	-1.20069
H	2.29521	0.26702	1.84968
H	2.02074	5.44295	-1.22433
H	3.50401	5.27645	-0.27145
H	3.45494	4.6956	-1.94152
Na	0.25076	1.69088	1.68753

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 3

C	2.2646	3.36252	-0.337
C	3.43448	2.3803	-0.18064
C	3.06465	0.94155	0.20042
C	2.14994	0.24075	-0.82819
C	2.2075	-1.30199	-0.74347
S	0.58635	-2.09685	-1.24392
C	-0.02052	-2.88401	0.30546
C	-0.85241	-2.01879	1.2857
C	-0.00692	-1.13934	2.26299
O	-0.647	-0.32515	2.97643
O	1.24012	-1.32494	2.24993
N	-1.88162	-1.2449	0.58404
C	-3.04017	-1.94165	0.02568

O	-3.77257	-0.95709	-0.66726
C	-2.92249	0.15847	-0.95608
C	-1.79864	0.01231	0.09425
O	-0.95394	0.88141	0.3419
C	-3.78697	1.42955	-0.91922
C	-4.43586	1.63868	0.45719
C	-3.02859	2.68261	-1.38315
O	-2.34643	0.05118	-2.2386
C	3.35577	-1.87727	-1.59114
C	3.69399	-3.34431	-1.31274
O	2.4524	0.98183	1.50743
C	2.72763	4.7625	-0.75829
H	1.54359	2.98127	-1.06985
H	1.72677	3.44253	0.6179
H	4.12521	2.76281	0.58195
H	3.99927	2.34106	-1.12205
H	4.00612	0.37901	0.29006
H	1.12731	0.58999	-0.6718
H	2.44115	0.55041	-1.84135
H	2.32768	-1.60612	0.29877
H	-0.62538	-3.72486	-0.04852
H	0.83001	-3.2954	0.85108
H	-1.39472	-2.71633	1.94029
H	-3.66378	-2.35774	0.82543
H	-2.7227	-2.75018	-0.64979
H	-4.58308	1.22297	-1.64747
H	-5.116	2.49584	0.42068
H	-5.01086	0.76307	0.76886
H	-3.68295	1.84824	1.22628
H	-3.72113	3.52987	-1.4334
H	-2.58959	2.53674	-2.37229
H	-2.22454	2.93833	-0.68699
H	-1.5895	-0.55872	-2.21826

H	3.12183	-1.74063	-2.6559
H	4.24558	-1.26122	-1.39711
H	4.5292	-3.67667	-1.93835
H	3.98243	-3.49061	-0.26513
H	2.83816	-3.99347	-1.52244
H	2.27031	0.06714	1.83171
H	1.88187	5.45234	-0.84916
H	3.42813	5.18537	-0.0286
H	3.23791	4.73334	-1.72808
Na	0.29407	1.50422	2.11081

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 1

C	4.61869	2.78174	0.1267
C	3.62729	1.99317	-0.73843
C	3.18558	0.65554	-0.14028
C	2.2396	-0.11793	-1.07889
C	2.10396	-1.621	-0.73705
S	0.40175	-2.25453	-1.16886
C	-0.29143	-2.79604	0.44583
C	-0.98463	-1.74893	1.34709
C	-0.02735	-0.8163	2.15945
O	1.18424	-1.15657	2.20236
O	-0.55583	0.18565	2.71015
N	-2.03756	-1.00228	0.64976
C	-3.36668	-1.58746	0.50526
O	-4.19152	-0.52291	0.07379
C	-3.3756	0.44544	-0.58506
C	-1.97392	0.19638	0.03541
O	-1.01783	0.97483	-0.04297
C	-3.98357	1.84027	-0.3242
C	-3.24523	2.95289	-1.08527
C	-5.4888	1.86463	-0.64735

O	-3.23227	0.13574	-1.95554
C	3.18963	-2.45979	-1.43412
C	3.32482	-3.89445	-0.91691
O	2.54361	0.94197	1.12216
C	5.03758	4.11149	-0.51133
H	4.17623	2.96292	1.11258
H	5.50973	2.16336	0.30218
H	4.07908	1.79372	-1.71911
H	2.73252	2.60439	-0.93411
H	4.08394	0.05345	0.06703
H	1.25931	0.36703	-1.0428
H	2.59978	-0.02004	-2.11202
H	2.16962	-1.75753	0.34426
H	-1.02103	-3.56495	0.16908
H	0.49027	-3.28086	1.03369
H	-1.50957	-2.32391	2.12503
H	-3.73647	-1.95043	1.46985
H	-3.36179	-2.40563	-0.22908
H	-3.87124	2.01263	0.75413
H	-3.6532	3.92767	-0.79685
H	-2.17418	2.94191	-0.87663
H	-3.37371	2.84053	-2.16677
H	-5.90126	2.84704	-0.39602
H	-6.03883	1.10576	-0.08678
H	-5.67719	1.70893	-1.71782
H	-4.09874	0.21683	-2.37966
H	2.9985	-2.46837	-2.51608
H	4.14886	-1.93821	-1.30012
H	4.11969	-4.42853	-1.44873
H	3.56991	-3.90735	0.15174
H	2.39279	-4.45079	-1.05789
H	2.29872	0.10619	1.58958
H	5.74943	4.65096	0.12265

H	5.51381	3.95409	-1.48657
H	4.17223	4.76662	-0.67022
Na	0.43681	1.75396	1.49493

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 17

C	4.59024	2.51007	-0.75231
C	3.47479	2.28149	0.27712
C	3.09889	0.81343	0.50809
C	2.29275	0.2052	-0.65496
C	2.23874	-1.34122	-0.65482
S	0.63272	-1.94765	-1.3891
C	-0.19281	-2.82481	-0.0005
C	-1.03603	-2.00621	1.00323
C	-0.22498	-1.23793	2.09709
O	-0.86643	-0.39858	2.78308
O	0.99336	-1.53625	2.20478
N	-2.04065	-1.15782	0.35197
C	-3.30533	-1.73851	-0.08708
O	-4.13669	-0.6316	-0.37564
C	-3.30884	0.48575	-0.6984
C	-1.97434	0.14771	0.02077
O	-1.05883	0.95181	0.22618
C	-4.02513	1.76489	-0.21421
C	-3.27093	3.04522	-0.60625
C	-5.48062	1.81382	-0.71418
O	-2.99299	0.49875	-2.07496
C	3.43905	-1.94971	-1.40134
C	3.62798	-3.45549	-1.19965
O	2.33557	0.78289	1.73516
C	4.94527	3.99276	-0.91731
H	5.48549	1.95397	-0.44238
H	4.29664	2.10066	-1.72687

H	2.57445	2.83656	-0.02756
H	3.78981	2.69394	1.24417
H	4.02356	0.23871	0.67161
H	1.27957	0.61609	-0.60735
H	2.72068	0.53966	-1.60881
H	2.21818	-1.70993	0.37285
H	-0.84248	-3.54909	-0.50395
H	0.54981	-3.38903	0.56711
H	-1.61556	-2.74324	1.57972
H	-3.76349	-2.32274	0.71767
H	-3.16369	-2.36756	-0.97751
H	-4.05141	1.68973	0.88071
H	-3.77541	3.91538	-0.17256
H	-2.23694	3.02669	-0.25796
H	-3.2525	3.17306	-1.69344
H	-5.97926	2.69763	-0.30349
H	-6.04517	0.92859	-0.41365
H	-5.53286	1.9034	-1.80751
H	-3.80997	0.64207	-2.57415
H	3.34784	-1.72416	-2.47293
H	4.34271	-1.42526	-1.05782
H	4.50657	-3.81554	-1.74586
H	3.77083	-3.69706	-0.13968
H	2.75636	-4.01091	-1.55972
H	2.09012	-0.14395	1.97593
H	5.7468	4.13061	-1.65076
H	4.07888	4.57166	-1.25867
H	5.28247	4.42791	0.03081
Na	0.16772	1.42767	2.06393

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 85

C	-3.95995	-3.22481	-0.06837
C	-4.154	-1.814	-0.6398
C	-3.16066	-0.78028	-0.10237
C	-3.4308	0.62338	-0.66435
C	-2.64707	1.76772	0.01243
S	-0.91607	1.83473	-0.68414
C	0.04211	2.49657	0.7496
C	1.02156	1.52811	1.43658
C	0.35726	0.34561	2.21688
O	1.13512	-0.54158	2.65125
O	-0.90144	0.3384	2.28103
N	2.05342	1.0236	0.52359
C	3.30045	1.75238	0.31434
O	4.16874	0.83463	-0.32668
C	3.39199	-0.2019	-0.92486
C	2.05276	-0.14149	-0.1587
O	1.17829	-1.00788	-0.20794
C	4.12185	-1.54919	-0.79162
C	5.40656	-1.59608	-1.63559
C	4.4196	-1.88958	0.6774
O	3.05713	0.12315	-2.25886
C	-3.36083	3.1292	-0.09018
C	-3.66504	3.62135	-1.50962
O	-1.82837	-1.25261	-0.40203
C	-4.99296	-4.22814	-0.59467
H	-2.95149	-3.57546	-0.31771
H	-4.02092	-3.1815	1.029
H	-5.17036	-1.46755	-0.40604
H	-4.06908	-1.84683	-1.73477
H	-3.25762	-0.72687	0.99401
H	-3.27483	0.61949	-1.75168
H	-4.49925	0.82496	-0.51007

H	-2.50224	1.51087	1.06553
H	0.59277	3.36575	0.37603
H	-0.67205	2.84924	1.49682
H	1.55978	2.11464	2.19526
H	3.74136	2.04492	1.27384
H	3.14027	2.64155	-0.31248
H	3.4116	-2.28559	-1.18744
H	5.89666	-2.56671	-1.50876
H	5.21414	-1.48259	-2.70898
H	6.11438	-0.82129	-1.32195
H	4.80813	-2.91081	0.75138
H	3.52626	-1.82239	1.30588
H	5.17224	-1.20981	1.08915
H	3.86933	0.13322	-2.78419
H	-4.29882	3.04777	0.47895
H	-2.75578	3.88057	0.43279
H	-4.13844	4.60839	-1.48008
H	-2.74763	3.70496	-2.101
H	-4.34729	2.9465	-2.03804
H	-1.25647	-0.48774	-0.61513
H	-4.83012	-5.22677	-0.17506
H	-6.01347	-3.92104	-0.33658
H	-4.9388	-4.31331	-1.68633
Na	-0.35927	-1.81396	1.31927

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 9

C	2.42777	3.41193	-0.55581
C	3.5995	2.47742	-0.21816
C	3.22333	1.0607	0.2355
C	2.4447	0.25464	-0.82536
C	2.51481	-1.27743	-0.61511
S	0.9591	-2.11479	-1.22041

C	0.20517	-2.81966	0.3008
C	-0.69738	-1.9187	1.17303
C	0.05838	-0.9258	2.11656
O	-0.63673	-0.02383	2.65539
O	1.29214	-1.12655	2.26417
N	-1.76562	-1.26221	0.41153
C	-2.98156	-2.001	0.0784
O	-3.8949	-1.02663	-0.39131
C	-3.16201	0.11175	-0.83744
C	-1.80053	-0.02344	-0.11706
O	-0.95383	0.87435	-0.07009
C	-3.92884	1.39719	-0.47893
C	-5.23415	1.53034	-1.2813
C	-4.2048	1.49434	1.02991
O	-2.85535	0.01279	-2.21209
C	3.75104	-1.88439	-1.3028
C	4.0754	-3.32338	-0.89303
O	2.46838	1.18778	1.45983
C	2.89673	4.78429	-1.0548
H	1.77978	2.9521	-1.31177
H	1.81192	3.55984	0.34291
H	4.20604	2.93656	0.5731
H	4.24937	2.38565	-1.09869
H	4.16089	0.53593	0.4719
H	1.40194	0.58217	-0.82347
H	2.84433	0.49096	-1.82131
H	2.54151	-1.50107	0.45375
H	-0.38633	-3.66254	-0.07308
H	0.98992	-3.22654	0.94142
H	-1.21623	-2.59608	1.86826
H	-3.40037	-2.47741	0.97143
H	-2.78361	-2.75863	-0.69331
H	-3.25287	2.21107	-0.76893

H	-5.75166	2.45228	-0.99735
H	-5.0612	1.5891	-2.36201
H	-5.90996	0.69261	-1.07835
H	-4.62579	2.47618	1.27094
H	-3.29655	1.36185	1.6265
H	-4.92333	0.73098	1.34392
H	-3.68436	0.0215	-2.71062
H	3.62111	-1.82492	-2.39235
H	4.61182	-1.24176	-1.06595
H	4.96975	-3.68493	-1.41197
H	4.26256	-3.39343	0.18509
H	3.24795	-3.99656	-1.13795
H	2.28512	0.29862	1.85125
H	2.0487	5.44094	-1.27688
H	3.52226	5.28572	-0.30704
H	3.49045	4.68653	-1.97107
Na	0.25251	1.73357	1.6249

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 10

C	4.56272	2.4144	0.2153
C	3.54499	1.67466	-0.66284
C	3.01349	0.37337	-0.05619
C	2.03479	-0.34365	-1.01399
C	1.75741	-1.83238	-0.68173
S	-0.02995	-2.30664	-1.0041
C	-0.68531	-2.77191	0.64997
C	-1.3095	-1.65045	1.51554
C	-0.27503	-0.80503	2.32489
O	-0.71843	0.22034	2.90283
O	0.91096	-1.23248	2.33021
N	-2.23602	-0.82241	0.73579
C	-3.52579	-1.3855	0.33702

O	-4.12475	-0.41143	-0.48605
C	-3.12384	0.48883	-0.9746
C	-1.97373	0.30791	0.04182
O	-0.98344	1.04507	0.11191
C	-3.76482	1.8817	-1.09545
C	-4.27114	2.39512	0.26098
C	-2.84711	2.90543	-1.78115
O	-2.65783	0.10302	-2.24791
C	2.63984	-2.8183	-1.47441
C	4.15183	-2.6498	-1.26732
O	2.37992	0.71157	1.19377
C	5.08396	3.70178	-0.43367
H	4.10704	2.64319	1.18518
H	5.40641	1.74339	0.42762
H	4.00695	1.43702	-1.63031
H	2.69233	2.33428	-0.88522
H	3.86781	-0.27919	0.17006
H	1.10124	0.22589	-1.00543
H	2.43197	-0.27882	-2.03579
H	1.88061	-2.00099	0.39076
H	-1.44082	-3.53257	0.42945
H	0.10709	-3.24992	1.22822
H	-1.92265	-2.14532	2.28279
H	-4.16098	-1.55505	1.21428
H	-3.38808	-2.33377	-0.20397
H	-4.634	1.71253	-1.74556
H	-4.79426	3.34739	0.12643
H	-4.96544	1.69012	0.72522
H	-3.44164	2.56984	0.9565
H	-3.39237	3.84453	-1.92538
H	-2.51243	2.54702	-2.75675
H	-1.96192	3.11307	-1.17295
H	-2.00103	-0.60886	-2.16606

H	2.35281	-3.83749	-1.1938
H	2.40757	-2.72023	-2.54385
H	4.69359	-3.42939	-1.81353
H	4.51713	-1.68459	-1.63297
H	4.42511	-2.73623	-0.20928
H	2.07474	-0.10201	1.6667
H	5.80908	4.20784	0.21267
H	5.57888	3.49499	-1.39016
H	4.26748	4.40689	-0.63203
Na	0.40829	1.73035	1.72539

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 79

C	-3.92363	-3.23198	0.01191
C	-4.14683	-1.87287	-0.66478
C	-3.13969	-0.79646	-0.25097
C	-3.42198	0.54684	-0.93976
C	-2.70909	1.78303	-0.35058
S	-0.91677	1.77983	-0.87876
C	-0.0442	2.46426	0.60056
C	0.89937	1.51024	1.35171
C	0.19173	0.34228	2.11432
O	-1.0678	0.33212	2.0981
O	0.94454	-0.53116	2.61749
N	1.98241	0.99477	0.50669
C	3.23099	1.73323	0.34549
O	4.14124	0.81113	-0.22714
C	3.40754	-0.24609	-0.84277
C	2.0289	-0.18394	-0.15002
O	1.16669	-1.06048	-0.22695
C	4.14207	-1.58217	-0.64243
C	5.46953	-1.63294	-1.4173
C	4.36509	-1.88862	0.84718

O	3.14051	0.04725	-2.19924
C	-3.42962	3.07707	-0.76995
C	-2.87337	4.37266	-0.17263
O	-1.81964	-1.30171	-0.54872
C	-4.98129	-4.27257	-0.37464
H	-2.9293	-3.6067	-0.25896
H	-3.92914	-3.09681	1.10361
H	-5.15494	-1.51086	-0.41986
H	-4.1054	-1.99535	-1.75597
H	-3.20617	-0.64005	0.83714
H	-3.21479	0.457	-2.01565
H	-4.50101	0.72897	-0.85164
H	-2.68312	1.68933	0.73981
H	0.5199	3.33486	0.25038
H	-0.80042	2.81559	1.30346
H	1.39297	2.11136	2.12915
H	3.61779	2.05329	1.31945
H	3.09421	2.60579	-0.30965
H	3.46087	-2.33433	-1.05912
H	5.9619	-2.5954	-1.24477
H	5.33191	-1.5439	-2.50135
H	6.15263	-0.84421	-1.08411
H	4.75635	-2.90473	0.96407
H	3.43919	-1.81583	1.4261
H	5.08984	-1.19378	1.283
H	3.97931	0.05755	-2.68092
H	-3.42601	3.14744	-1.86575
H	-4.48212	2.97316	-0.46934
H	-3.47696	5.22985	-0.48893
H	-2.88591	4.34523	0.92349
H	-1.84461	4.5543	-0.499
H	-1.23165	-0.54445	-0.74505
H	-4.7974	-5.23233	0.12029

H	-5.98751	-3.94023	-0.09302
H	-4.98178	-4.45105	-1.45631
Na	-0.43679	-1.85487	1.2393

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 43

C	4.78326	2.18621	0.08357
C	3.61359	1.57204	-0.69694
C	3.08429	0.25991	-0.11409
C	1.95296	-0.34088	-0.97468
C	1.66044	-1.82685	-0.66341
S	-0.13814	-2.28069	-0.94009
C	-0.72036	-2.75665	0.74041
C	-1.23881	-1.63828	1.67929
C	-0.129	-0.88429	2.48113
O	1.04507	-1.33407	2.38006
O	-0.5061	0.10793	3.15523
N	-2.14081	-0.71974	0.97798
C	-3.47334	-1.18208	0.59172
O	-4.04258	-0.11281	-0.12582
C	-2.99638	0.71882	-0.64402
C	-1.83083	0.42744	0.33267
O	-0.79444	1.09729	0.4188
C	-3.52262	2.16305	-0.70055
C	-2.4983	3.14167	-1.29611
C	-4.85149	2.2287	-1.47385
O	-2.60001	0.3204	-1.93765
C	2.57981	-2.80868	-1.41855
C	2.41209	-2.86574	-2.94224
O	2.63121	0.54179	1.22786
C	5.28366	3.49896	-0.52997
H	4.47841	2.35207	1.12286
H	5.60806	1.46128	0.12075

H	3.9269	1.38336	-1.73228
H	2.78266	2.29147	-0.75443
H	3.92163	-0.45182	-0.04381
H	1.05838	0.26559	-0.81197
H	2.21873	-0.23114	-2.03272
H	1.78253	-1.99365	0.40784
H	-1.5247	-3.47198	0.54223
H	0.0786	-3.29272	1.25576
H	-1.84985	-2.13071	2.44946
H	-4.08577	-1.38493	1.47727
H	-3.40886	-2.08983	-0.02738
H	-3.71748	2.44504	0.34271
H	-2.89757	4.16061	-1.24714
H	-1.54804	3.11354	-0.7593
H	-2.30261	2.9014	-2.34527
H	-5.22701	3.25751	-1.46915
H	-5.61122	1.58278	-1.02801
H	-4.70862	1.92427	-2.51539
H	-1.98158	-0.42895	-1.88828
H	3.61772	-2.53502	-1.17856
H	2.4263	-3.81189	-1.00441
H	3.10895	-3.59184	-3.37382
H	1.39852	-3.17587	-3.21674
H	2.61121	-1.90038	-3.41984
H	2.30383	-0.27766	1.66865
H	6.12131	3.91159	0.04245
H	5.62562	3.3532	-1.56164
H	4.49068	4.25645	-0.55033
Na	0.72547	1.57391	2.00472

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 27

C	4.57129	2.42094	-0.74919
C	3.42222	2.25063	0.25418
C	3.03234	0.7986	0.553
C	2.27123	0.12514	-0.6041
C	2.20188	-1.4178	-0.51047
S	0.63128	-2.06028	-1.29007
C	-0.28858	-2.82701	0.10514
C	-1.18353	-1.92911	0.99071
C	-0.42981	-1.10951	2.08821
O	-1.10254	-0.23417	2.69433
O	0.78026	-1.4031	2.27604
N	-2.11119	-1.09924	0.21385
C	-3.31984	-1.69839	-0.3446
O	-4.09569	-0.60873	-0.80492
C	-3.23598	0.50567	-1.03749
C	-1.99071	0.187	-0.17282
O	-1.08797	0.99259	0.07678
C	-4.02097	1.78525	-0.68254
C	-4.48563	1.79194	0.78223
C	-3.25705	3.07014	-1.03947
O	-2.7682	0.50531	-2.3699
C	3.43242	-2.08085	-1.15488
C	3.59673	-3.57129	-0.84606
O	2.22094	0.84127	1.7485
C	4.94311	3.89159	-0.97433
H	5.4519	1.87459	-0.38469
H	4.30473	1.96676	-1.71159
H	2.53448	2.7903	-0.10919
H	3.70743	2.71413	1.20728
H	3.9476	0.23306	0.78629
H	1.26187	0.54687	-0.62769
H	2.74395	0.39593	-1.55693

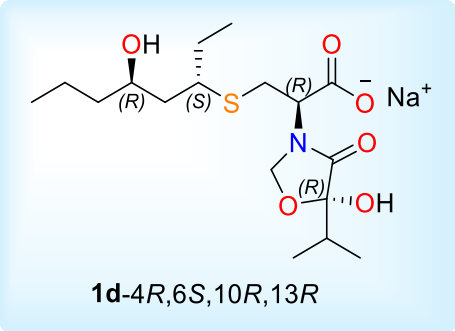
H	2.12471	-1.72238	0.53536
H	-0.91188	-3.58385	-0.38341
H	0.41086	-3.34996	0.75997
H	-1.82412	-2.61388	1.56704
H	-3.88113	-2.23025	0.4314
H	-3.07527	-2.38387	-1.16864
H	-4.92059	1.73222	-1.31664
H	-5.09535	2.6805	0.976
H	-5.08543	0.90917	1.01582
H	-3.63403	1.81526	1.47137
H	-3.90512	3.93857	-0.88056
H	-2.92822	3.07236	-2.08176
H	-2.36829	3.18224	-0.41301
H	-3.52941	0.62912	-2.95591
H	3.3966	-1.92529	-2.24207
H	4.32286	-1.54066	-0.80148
H	4.4959	-3.97284	-1.32581
H	3.68828	-3.74297	0.23302
H	2.73703	-4.14326	-1.20881
H	1.94139	-0.06668	2.01949
H	5.76673	3.98873	-1.68959
H	4.09176	4.45928	-1.36825
H	5.25612	4.36949	-0.03856
Na	0.04759	1.52121	1.954

Compound 1c: Isomer 4R, 6S, 10R, 13S conformer 83

C	3.73414	3.26985	0.2071
C	3.94719	1.96897	-0.57847
C	3.00809	0.832	-0.16684
C	3.29059	-0.46154	-0.94602
C	2.57907	-1.72501	-0.41801
S	0.82368	-1.73311	-1.04976

C	-0.06988	-2.61952	0.30263
C	-1.03995	-1.78373	1.15713
C	-0.37418	-0.70714	2.07611
O	-1.15651	0.07701	2.6704
O	0.88557	-0.66287	2.08669
N	-2.11765	-1.18489	0.36028
C	-3.33803	-1.92757	0.06687
O	-4.25087	-0.96252	-0.42329
C	-3.52427	0.17128	-0.89651
C	-2.16941	0.06205	-0.15749
O	-1.31908	0.9519	-0.09623
C	-4.36925	1.42863	-0.61418
C	-4.66135	1.60072	0.8849
C	-3.75659	2.70156	-1.22023
O	-3.20602	0.01862	-2.2657
C	3.29855	-3.03081	-0.80392
C	4.63312	-3.2475	-0.07446
O	1.65216	1.29902	-0.33837
C	4.71633	4.37719	-0.19265
H	2.70707	3.61885	0.0474
H	3.83746	3.06299	1.28246
H	4.98228	1.6282	-0.43636
H	3.81672	2.1627	-1.65209
H	3.15644	0.61604	0.90348
H	3.0678	-0.30866	-2.0119
H	4.3714	-0.63414	-0.88349
H	2.48405	-1.64992	0.66971
H	-0.62001	-3.43599	-0.17595
H	0.67744	-3.0645	0.96316
H	-1.53671	-2.48651	1.84167
H	-3.74925	-2.37233	0.98006
H	-3.15646	-2.7122	-0.68215
H	-5.32699	1.22952	-1.1219

H	-5.31189	2.46786	1.0392
H	-5.16117	0.72157	1.29862
H	-3.74021	1.76699	1.45392
H	-4.45005	3.53905	-1.08907
H	-3.55317	2.58814	-2.28817
H	-2.81299	2.95231	-0.72902
H	-4.03253	0.03106	-2.7705
H	2.63481	-3.87338	-0.57661
H	3.45193	-3.05162	-1.89095
H	5.06487	-4.2164	-0.34718
H	5.37534	-2.48133	-0.32222
H	4.49479	-3.23774	1.01291
H	1.08979	0.54872	-0.6201
H	4.54022	5.29356	0.38109
H	5.75455	4.07022	-0.01876
H	4.61809	4.62649	-1.25569
Na	0.24583	1.58169	1.49535



1d-4*R*,6*S*,10*R*,13*R*

Calculated DFT energies of the 1d-diasteroisomer

Conformers **1d**	OPLS2008 Force Field Conformational Search Relative Energy (kcal/mol)	B3LYP/6-31+G(d,p) DFT Energy (hartree)	Δ (DFT Energy) (kcal/mol)	% Population
1d83	2.941016631	-1732.26171	0	80.20
1d40	2.031288093	-1732.259496	1.389305792	7.67
1d22	1.457171781	-1732.25886	1.788401764	3.91
1d73	2.747708578	-1732.258037	2.304841993	1.63
1d84	2.954090259	-1732.257984	2.338099991	1.54
1d13	0.892950317	-1732.257485	2.651227177	0.91
1d69	2.688458991	-1732.257329	2.749118642	0.77
1d77	2.788435201	-1732.257034	2.934233912	0.56
1d60	2.527775257	-1732.256764	3.103661448	0.42
1d48	2.342330502	-1732.256629	3.188375216	0.37
1d32	1.810781158	-1732.256623	3.192140272	0.36
1d71	2.714534546	-1732.256283	3.405493465	0.25
1d5	0.545865803	-1732.255845	3.680342578	0.16
1d27	1.591947264	-1732.255693	3.775724006	0.14
1d11	0.787429168	-1732.255631	3.814629588	0.13
1d29	1.651555361	-1732.255627	3.817139625	0.13
1d25	1.534657526	-1732.255218	4.073790966	0.08
1d20	1.221201157	-1732.255043	4.18360511	0.07
1d54	2.408893673	-1732.254931	4.253886162	0.06
1d50	2.365203376	-1732.254919	4.261416274	0.06
1d23	1.463027428	-1732.254838	4.312244535	0.05
1d65	2.614510535	-1732.254817	4.325422232	0.05

22 conformers counting for the 99.53% of the DFT conformational population

DFT COORDINATES FOR CONFORMATIONAL SEARCH OF 1d (4*R*, 6*S*, 10*R*, 13*R*)

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 83

C	4.74804	2.81225	0.56997
C	4.4065	1.72846	-0.45988
C	3.54372	0.58951	0.08964
C	3.41491	-0.56345	-0.92404
C	2.51317	-1.74123	-0.48713
S	0.81196	-1.4403	-1.18557
C	-0.27143	-2.36008	-0.00638
C	-1.04234	-1.55508	1.07232
C	-0.20066	-0.36859	1.65828
O	0.93047	-0.67115	2.09964
O	-0.6939	0.79709	1.56183
N	-2.3707	-1.09917	0.64962
C	-3.43553	-1.07699	1.66178
O	-4.44182	-0.25795	1.11541
C	-3.82204	0.68587	0.23044
C	-2.56561	-0.08162	-0.23243
O	-1.8153	0.25051	-1.1562
C	-4.85949	1.10907	-0.81813
C	-5.35992	-0.08962	-1.63834
C	-4.35252	2.23943	-1.72705
O	-3.36183	1.82167	0.92271
C	3.05151	-3.1136	-0.93179
C	4.29815	-3.56567	-0.15688
O	2.26845	1.13724	0.47
C	5.58777	3.9513	-0.01903
H	3.81788	3.21139	0.98923
H	5.29176	2.35308	1.40727
H	5.3344	1.30087	-0.86414
H	3.87827	2.18133	-1.31249
H	4.01912	0.19163	0.99873

H	3.07535	-0.16528	-1.89139
H	4.42827	-0.94357	-1.10265
H	2.39067	-1.72822	0.60076
H	-0.99179	-2.92101	-0.60584
H	0.3743	-3.08019	0.49934
H	-1.21964	-2.258	1.89465
H	-3.04646	-0.66958	2.60809
H	-3.84654	-2.07782	1.82819
H	-5.69691	1.4965	-0.22212
H	-6.15768	0.23038	-2.3166
H	-5.75714	-0.87969	-0.99588
H	-4.55582	-0.51144	-2.2532
H	-5.16205	2.56639	-2.38853
H	-4.01924	3.09867	-1.14072
H	-3.51975	1.90004	-2.35056
H	-2.51948	1.60539	1.37308
H	2.26468	-3.86558	-0.79725
H	3.26138	-3.08581	-2.0091
H	4.62302	-4.55552	-0.49457
H	5.14372	-2.88262	-0.29254
H	4.09244	-3.63003	0.91787
H	1.91704	0.62218	1.2345
H	5.81935	4.70713	0.73901
H	6.53895	3.58131	-0.42071
H	5.05764	4.45416	-0.83699
Na	0.15946	1.29763	-0.52445

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 40

C	4.03904	2.88569	-0.35649
C	4.45627	1.78604	0.63132
C	3.53409	0.56002	0.70334
C	3.52445	-0.27376	-0.59254

C	2.64744	-1.54754	-0.5473
S	0.98573	-1.11128	-1.2695
C	-0.14407	-2.31333	-0.43924
C	-1.03009	-1.80616	0.72769
C	-0.28066	-0.7851	1.65166
O	-0.80331	0.36296	1.79471
O	0.81989	-1.17018	2.10513
N	-2.3358	-1.28211	0.31356
C	-3.47924	-1.52905	1.20319
O	-4.46537	-0.61206	0.79345
C	-3.80762	0.53281	0.23234
C	-2.4957	-0.0794	-0.3037
O	-1.68832	0.47929	-1.0536
C	-4.77382	1.20006	-0.75528
C	-5.17661	0.24733	-1.89113
C	-4.23089	2.52934	-1.30256
O	-3.43795	1.45787	1.22636
C	3.27158	-2.74122	-1.29341
C	4.48732	-3.34684	-0.57663
O	2.21885	1.00161	1.08851
C	4.98421	4.09304	-0.32047
H	4.00715	2.48747	-1.37878
H	3.02158	3.2171	-0.11353
H	4.50648	2.21816	1.63864
H	5.47117	1.44208	0.38714
H	3.91171	-0.08927	1.506
H	3.23005	0.3507	-1.44635
H	4.56338	-0.56791	-0.78713
H	2.45447	-1.82484	0.4944
H	-0.79024	-2.73321	-1.21326
H	0.49223	-3.1161	-0.06244
H	-1.24733	-2.69032	1.3382
H	-3.18239	-1.36836	2.25142

H	-3.86771	-2.5448	1.07815
H	-5.66511	1.4156	-0.15048
H	-5.93427	0.72173	-2.5233
H	-5.59318	-0.68626	-1.50442
H	-4.3185	0.00801	-2.53057
H	-4.992	3.00371	-1.93147
H	-3.97775	3.21637	-0.49194
H	-3.33718	2.3676	-1.91297
H	-2.61932	1.14878	1.66736
H	2.5112	-3.52222	-1.41416
H	3.54513	-2.42695	-2.30919
H	4.87639	-4.20336	-1.13718
H	5.30775	-2.62907	-0.46883
H	4.21933	-3.69784	0.42659
H	1.8183	0.3123	1.66944
H	4.66875	4.86834	-1.0269
H	5.01229	4.5432	0.67859
H	6.00868	3.80211	-0.58138
Na	0.19756	1.37317	-0.02689

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 22

C	3.95769	3.00928	-0.25277
C	4.39413	1.91842	0.73652
C	3.52401	0.6534	0.77087
C	3.59375	-0.16982	-0.53043
C	2.7683	-1.47812	-0.52527
S	1.11817	-1.11024	-1.30954
C	0.01185	-2.36166	-0.52155
C	-0.93978	-1.89663	0.61052
C	-0.27001	-0.85307	1.56978
O	0.82785	-1.19616	2.0621
O	-0.84614	0.27038	1.70172

N	-2.24851	-1.42476	0.14702
C	-3.41845	-1.73765	0.97769
O	-4.42654	-0.86627	0.52663
C	-3.79831	0.32314	0.02205
C	-2.43671	-0.22355	-0.46485
O	-1.62126	0.3746	-1.17436
C	-4.74253	0.95837	-1.00812
C	-4.15503	2.23073	-1.6381
C	-6.11818	1.2402	-0.3791
O	-3.51217	1.24374	1.04744
C	3.46951	-2.64172	-1.25032
C	4.68325	-3.19928	-0.49203
O	2.17871	1.03439	1.11456
C	4.85507	4.25134	-0.18657
H	3.96423	2.61829	-1.27834
H	2.92311	3.29975	-0.03076
H	4.3981	2.34232	1.74854
H	5.42899	1.62011	0.51756
H	3.90277	0.01464	1.58137
H	3.30668	0.44973	-1.39034
H	4.65003	-0.42081	-0.68897
H	2.54602	-1.76842	0.50683
H	-0.58556	-2.80859	-1.31927
H	0.66863	-3.13574	-0.12064
H	-1.14486	-2.79261	1.20799
H	-3.18148	-1.57455	2.04077
H	-3.75058	-2.76927	0.82469
H	-4.87054	0.20353	-1.7952
H	-4.84651	2.61486	-2.39586
H	-3.19157	2.03911	-2.1155
H	-4.01727	3.00704	-0.87896
H	-6.79341	1.64736	-1.13923
H	-6.56756	0.33242	0.03052

H	-6.03082	1.97437	0.42781
H	-2.69035	0.97327	1.5072
H	2.74783	-3.45397	-1.39968
H	3.76562	-2.31288	-2.25509
H	5.12515	-4.0389	-1.03889
H	5.47075	-2.45005	-0.35592
H	4.39517	-3.5624	0.50129
H	1.78852	0.32512	1.67814
H	4.52611	5.01979	-0.89433
H	4.84359	4.69425	0.81606
H	5.89545	4.00159	-0.42625
Na	0.1907	1.32928	-0.07243

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 73

C	-5.13526	-2.48711	0.3067
C	-4.59747	-1.43336	-0.66938
C	-3.65849	-0.4093	-0.02578
C	-3.31924	0.73961	-0.99474
C	-2.35033	1.8101	-0.4415
S	-0.62677	1.36099	-0.98907
C	0.41358	2.09693	0.35105
C	1.03006	1.12966	1.39312
C	0.00298	0.04557	1.86443
O	-1.11018	0.50171	2.23489
O	0.34437	-1.15818	1.75531
N	2.32015	0.57115	0.96734
C	3.47837	0.65253	1.85547
O	4.55695	0.15395	1.08618
C	4.04013	-0.73313	0.09307
C	2.55768	-0.30711	-0.03001
O	1.77661	-0.71062	-0.89686
C	4.90689	-0.58264	-1.17462

C	4.86358	0.84713	-1.73583
C	4.55709	-1.61691	-2.25633
O	4.00301	-2.05883	0.57588
C	-2.70964	3.24138	-0.88109
C	-3.97921	3.78791	-0.21134
O	-2.48948	-1.10381	0.43682
C	-6.04634	-3.51814	-0.3689
H	-4.29012	-2.99238	0.78691
H	-5.68914	-1.98159	1.10999
H	-5.43841	-0.89829	-1.13184
H	-4.0573	-1.92963	-1.48977
H	-4.1595	0.02537	0.85263
H	-2.92903	0.32288	-1.93463
H	-4.26703	1.22494	-1.25878
H	-2.32769	1.75518	0.65166
H	1.21282	2.66432	-0.13253
H	-0.22729	2.80238	0.88252
H	1.26057	1.7458	2.27048
H	3.31273	0.04742	2.75855
H	3.69512	1.69005	2.12974
H	5.93381	-0.7754	-0.82499
H	5.56331	0.94126	-2.57257
H	5.13891	1.58477	-0.97768
H	3.86415	1.09	-2.11465
H	5.26685	-1.53337	-3.08623
H	4.59918	-2.63871	-1.87068
H	3.54929	-1.44713	-2.6449
H	4.9131	-2.34072	0.7499
H	-1.87169	3.90698	-0.64121
H	-2.8137	3.26778	-1.97382
H	-4.17861	4.81273	-0.54223
H	-4.86559	3.19026	-0.45039
H	-3.87407	3.80321	0.87962

H	-2.14093	-0.64302	1.23928
H	-6.42109	-4.25148	0.35329
H	-6.91498	-3.03928	-0.8373
H	-5.51107	-4.06859	-1.15224
Na	-0.32017	-1.51654	-0.35984

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 84

C	-5.26864	-2.44835	-0.09132
C	-4.75562	-1.17761	-0.77987
C	-3.77124	-0.36393	0.06517
C	-3.45879	0.99823	-0.58496
C	-2.44254	1.87612	0.18219
S	-0.74231	1.57341	-0.52472
C	0.35037	1.91574	0.92762
C	0.99082	0.69983	1.64222
C	-0.04015	-0.45946	1.85021
O	0.2712	-1.59408	1.41123
O	-1.12957	-0.10698	2.37366
N	2.24864	0.26186	1.02285
C	3.4464	0.09969	1.84671
O	4.48124	-0.19733	0.92712
C	3.8989	-0.80169	-0.22674
C	2.42628	-0.33438	-0.17519
O	1.61288	-0.49276	-1.08967
C	4.66033	-0.36171	-1.48982
C	6.10955	-0.8768	-1.49025
C	4.62168	1.1613	-1.68511
O	3.82935	-2.20556	-0.0881
C	-2.80985	3.37284	0.18467
C	-2.93861	4.03629	-1.19141
O	-2.59583	-1.16158	0.27316
C	-6.21371	-3.2683	-0.9769

H	-4.41127	-3.06113	0.20809
H	-5.78709	-2.16906	0.83644
H	-5.60584	-0.53486	-1.04715
H	-4.25953	-1.44374	-1.72542
H	-4.22491	-0.1726	1.04972
H	-3.13428	0.84172	-1.6233
H	-4.40953	1.54399	-0.64964
H	-2.38014	1.52712	1.21712
H	1.13847	2.59389	0.59024
H	-0.26509	2.4475	1.65466
H	1.27105	1.05542	2.64099
H	3.30564	-0.71531	2.57132
H	3.69817	1.02951	2.36666
H	4.11634	-0.83308	-2.3174
H	6.61499	-0.56159	-2.40858
H	6.16873	-1.97092	-1.46018
H	6.67224	-0.47378	-0.64161
H	5.10839	1.42937	-2.62852
H	3.59519	1.5386	-1.72712
H	5.14735	1.67452	-0.87357
H	4.73039	-2.54948	-0.01288
H	-3.76093	3.47034	0.72882
H	-2.06652	3.91804	0.78057
H	-3.19588	5.09527	-1.08346
H	-1.99901	3.97244	-1.74887
H	-3.72217	3.56862	-1.79767
H	-2.20651	-0.93326	1.15345
H	-6.56665	-4.1657	-0.45744
H	-7.09546	-2.68529	-1.26984
H	-5.71275	-3.59341	-1.89688
Na	-0.47382	-1.38103	-0.69959

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 13

C	-4.81767	-2.46823	-0.04982
C	-3.73333	-1.75656	-0.86913
C	-3.18245	-0.48408	-0.22112
C	-2.1418	0.22125	-1.11382
C	-1.88955	1.70099	-0.73512
S	-0.11478	2.18949	-1.0509
C	0.5318	2.63593	0.6113
C	1.05727	1.51312	1.53143
C	-0.03969	0.66463	2.25621
O	-1.20729	1.1354	2.24896
O	0.34854	-0.40594	2.79228
N	2.07738	0.68347	0.87985
C	3.48935	1.03936	1.00333
O	4.16778	0.18896	0.098
C	3.36102	-0.96122	-0.13871
C	1.93849	-0.49525	0.24487
O	0.91295	-1.14208	0.00882
C	3.50937	-1.41475	-1.60107
C	4.92761	-1.93117	-1.89829
C	3.11326	-0.30618	-2.58791
O	3.65232	-1.9889	0.79017
C	-2.85189	2.6451	-1.47745
C	-2.89267	4.07718	-0.93786
O	-2.60779	-0.86324	1.04777
C	-5.35428	-3.72794	-0.73938
H	-4.41699	-2.72358	0.93745
H	-5.64536	-1.76841	0.13004
H	-4.1388	-1.48883	-1.85386
H	-2.89656	-2.44615	-1.06092
H	-4.02505	0.19644	-0.02107
H	-1.20987	-0.34853	-1.05646

H	-2.47684	0.17609	-2.15917
H	-2.01011	1.82921	0.34239
H	1.35252	3.32659	0.38856
H	-0.2303	3.1933	1.15926
H	1.5826	2.01917	2.35566
H	3.83016	0.88188	2.03712
H	3.66603	2.0776	0.70377
H	2.80115	-2.24604	-1.70501
H	4.99403	-2.24745	-2.94411
H	5.19882	-2.80296	-1.2912
H	5.67511	-1.14693	-1.73805
H	3.12013	-0.69809	-3.61034
H	2.11038	0.08287	-2.38727
H	3.81936	0.52889	-2.53997
H	4.56321	-2.2807	0.64507
H	-2.59629	2.65392	-2.54611
H	-3.8591	2.20796	-1.41068
H	-3.60746	4.6869	-1.50106
H	-3.19616	4.09289	0.11562
H	-1.91019	4.55362	-1.01479
H	-2.32928	-0.06328	1.55958
H	-6.12877	-4.21326	-0.13578
H	-5.79334	-3.49216	-1.71632
H	-4.55598	-4.46154	-0.90649
Na	-0.60668	-1.90931	1.48426

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 69

C	-4.53746	-2.93284	0.2481
C	-3.70509	-2.05969	-0.70011
C	-3.21315	-0.74826	-0.08499
C	-2.45734	0.13067	-1.09897
C	-2.28761	1.6003	-0.64342

S	-0.66497	2.30825	-1.23474
C	0.16643	2.82899	0.31724
C	1.00749	1.81371	1.11402
C	0.21782	0.74414	1.94273
O	-0.98467	0.98605	2.19172
O	0.87198	-0.28792	2.29817
N	2.08617	1.16959	0.35135
C	3.47889	1.4283	0.74115
O	4.23355	0.39953	0.14041
C	3.37618	-0.72415	-0.05462
C	1.98809	-0.07436	-0.18454
O	0.96769	-0.66658	-0.54881
C	3.8632	-1.5679	-1.23263
C	5.22119	-2.21979	-0.92823
C	3.90287	-0.75609	-2.53551
O	3.2942	-1.53956	1.10221
C	-3.47031	2.47158	-1.1038
C	-3.54251	3.85502	-0.45221
O	-2.36426	-1.09464	1.03439
C	-5.01175	-4.23637	-0.40438
H	-3.94969	-3.15601	1.14551
H	-5.40839	-2.357	0.5902
H	-4.30199	-1.81592	-1.58872
H	-2.83455	-2.62712	-1.06422
H	-4.08232	-0.19993	0.30969
H	-1.47941	-0.32424	-1.28278
H	-2.99676	0.11538	-2.05557
H	-2.21332	1.63895	0.44558
H	0.82818	3.64068	-0.00243
H	-0.57552	3.25673	0.99501
H	1.52076	2.41479	1.87971
H	3.56665	1.40741	1.8385
H	3.83297	2.3904	0.35774

H	3.11001	-2.35871	-1.3389
H	5.50764	-2.88232	-1.75192
H	5.18436	-2.8085	-0.00853
H	6.00167	-1.45989	-0.8179
H	4.18275	-1.40689	-3.37028
H	2.92905	-0.3146	-2.77236
H	4.64076	0.04962	-2.4717
H	2.69999	-1.11257	1.75275
H	-3.43571	2.57404	-2.19707
H	-4.39575	1.92052	-0.87932
H	-4.41425	4.41157	-0.81262
H	-3.62468	3.77403	0.63825
H	-2.64913	4.44385	-0.68323
H	-2.12724	-0.29426	1.55761
H	-5.6073	-4.83595	0.29229
H	-5.63185	-4.03897	-1.28704
H	-4.16335	-4.85103	-0.72918
Na	-0.20063	-1.8189	1.02031

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 77

C	-5.29451	-2.32428	0.21409
C	-4.7376	-1.23619	-0.7119
C	-3.72579	-0.30412	-0.03656
C	-3.35259	0.88002	-0.94631
C	-2.3821	1.9252	-0.34321
S	-0.64228	1.46256	-0.83741
C	0.381	2.00992	0.60582
C	0.97808	0.9142	1.52173
C	-0.08104	-0.18256	1.87204
O	-1.18401	0.26671	2.28148
O	0.22458	-1.37726	1.63504
N	2.25208	0.37027	1.03424

C	3.40466	0.30714	1.93147
O	4.47039	-0.1421	1.11573
C	3.92894	-0.89827	0.03192
C	2.46387	-0.40585	-0.05035
O	1.67387	-0.68604	-0.95652
C	4.81186	-0.64938	-1.20841
C	4.83162	0.83257	-1.61431
C	4.42864	-1.54647	-2.39609
O	3.83715	-2.26523	0.37203
C	-2.76084	3.34656	-0.79962
C	-1.91401	4.48928	-0.23286
O	-2.58528	-1.08525	0.34692
C	-6.27987	-3.26307	-0.4913
H	-4.45986	-2.90021	0.62827
H	-5.79366	-1.84656	1.06868
H	-5.56573	-0.63234	-1.10791
H	-4.2507	-1.70382	-1.58103
H	-4.18025	0.10209	0.88016
H	-2.95837	0.49769	-1.89893
H	-4.28924	1.39413	-1.19896
H	-2.40302	1.85942	0.74999
H	1.187	2.63689	0.21537
H	-0.26702	2.63195	1.22187
H	1.22576	1.42293	2.46119
H	3.20839	-0.38965	2.75915
H	3.65731	1.29802	2.32229
H	5.82689	-0.92108	-0.87693
H	5.54586	0.98694	-2.4295
H	5.1245	1.4739	-0.77913
H	3.84741	1.15318	-1.97484
H	5.14762	-1.4044	-3.20998
H	4.42541	-2.60472	-2.12277
H	3.4319	-1.29328	-2.76722

H	4.734	-2.59767	0.52444
H	-2.73692	3.38352	-1.89698
H	-3.8087	3.50609	-0.50735
H	-2.30412	5.45552	-0.56976
H	-1.92678	4.49267	0.86369
H	-0.8731	4.4213	-0.56429
H	-2.21816	-0.71809	1.19034
H	-6.6653	-4.02413	0.19576
H	-7.13939	-2.71301	-0.89362
H	-5.80099	-3.78506	-1.32872
Na	-0.44586	-1.47545	-0.51351

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 60

C	-5.2098	-2.4331	0.0242
C	-4.69089	-1.196	-0.71904
C	-3.70661	-0.34784	0.09123
C	-3.39194	0.98494	-0.61596
C	-2.37619	1.89322	0.11568
S	-0.67638	1.562	-0.57947
C	0.41915	1.97516	0.85175
C	1.04352	0.79946	1.64576
C	0.00933	-0.34824	1.89765
O	0.32274	-1.50106	1.50927
O	-1.08317	0.02637	2.39782
N	2.31186	0.32505	1.07701
C	3.47272	0.14683	1.94723
O	4.52553	-0.21235	1.07222
C	3.9667	-0.82853	-0.08857
C	2.5041	-0.32229	-0.09277
O	1.69933	-0.4942	-1.01296
C	4.83895	-0.43876	-1.29959
C	4.87311	1.08096	-1.52428

C	4.43563	-1.18273	-2.58255
O	3.8681	-2.22624	0.08469
C	-2.74424	3.38854	0.05902
C	-2.87489	3.99827	-1.34155
O	-2.53142	-1.13641	0.33483
C	-6.15998	-3.28539	-0.82459
H	-4.35534	-3.03673	0.34943
H	-5.72608	-2.11117	0.93926
H	-5.53868	-0.56351	-1.0169
H	-4.1933	-1.50563	-1.6504
H	-4.16094	-0.11415	1.06624
H	-3.06566	0.78411	-1.64611
H	-4.34206	1.52823	-0.70559
H	-2.31345	1.58574	1.16363
H	1.217	2.61935	0.47359
H	-0.1893	2.56217	1.54151
H	1.30553	1.21077	2.62784
H	3.27785	-0.64077	2.68944
H	3.73942	1.08252	2.44908
H	5.85416	-0.75846	-1.01476
H	5.57785	1.32348	-2.32623
H	5.1876	1.61346	-0.62307
H	3.88896	1.45597	-1.82795
H	5.15022	-0.95208	-3.37986
H	4.42227	-2.26587	-2.43722
H	3.43929	-0.87668	-2.91308
H	4.76324	-2.57822	0.19854
H	-3.69489	3.5064	0.59987
H	-2.00121	3.95736	0.63278
H	-3.13732	5.05933	-1.27406
H	-1.93486	3.91804	-1.89616
H	-3.65585	3.50404	-1.92988
H	-2.1475	-0.87228	1.2069

H	-6.51499	-4.15921	-0.26769
H	-7.0403	-2.71152	-1.13906
H	-5.66267	-3.64999	-1.73165
Na	-0.39734	-1.37618	-0.61588

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 48

C	-5.16983	-2.5754	0.16861
C	-4.70707	-1.35992	-0.64416
C	-3.7511	-0.43132	0.11027
C	-3.4966	0.87351	-0.66894
C	-2.51217	1.85946	0.00179
S	-0.80422	1.55493	-0.6847
C	0.28132	2.09108	0.71268
C	0.95311	0.98883	1.57218
C	-0.03132	-0.1864	1.89131
O	0.32857	-1.34419	1.56236
O	-1.13717	0.16891	2.37599
N	2.24125	0.53834	1.0299
C	3.4094	0.45842	1.90311
O	4.47675	0.11764	1.0398
C	3.94963	-0.5945	-0.08306
C	2.4618	-0.15717	-0.1065
O	1.6587	-0.40954	-1.00947
C	4.78415	-0.20811	-1.32365
C	4.32125	-0.93492	-2.59561
C	6.28643	-0.43601	-1.07421
O	3.91469	-1.98323	0.16455
C	-2.9382	3.33359	-0.13889
C	-3.10463	3.8536	-1.57161
O	-2.54328	-1.15838	0.38255
C	-6.09426	-3.50665	-0.6239
H	-4.28951	-3.1279	0.51496

H	-5.68963	-2.22603	1.07155
H	-5.58228	-0.77888	-0.96652
H	-4.20465	-1.69877	-1.56264
H	-4.20662	-0.16525	1.07636
H	-3.17304	0.63205	-1.69119
H	-4.46842	1.37371	-0.77517
H	-2.43227	1.61567	1.06528
H	1.05349	2.73972	0.29122
H	-0.34444	2.69655	1.37054
H	1.19606	1.46603	2.52899
H	3.25688	-0.30513	2.67963
H	3.62891	1.42731	2.36261
H	4.62824	0.87043	-1.45755
H	4.90972	-0.58607	-3.45099
H	3.26457	-0.75465	-2.80047
H	4.46714	-2.01622	-2.50301
H	6.85975	-0.076	-1.93445
H	6.63666	0.08967	-0.18283
H	6.52257	-1.50284	-0.96482
H	4.82392	-2.29723	0.27171
H	-3.88796	3.44715	0.40444
H	-2.21267	3.96327	0.39187
H	-3.40226	4.90745	-1.56397
H	-2.1683	3.77172	-2.13235
H	-3.87469	3.29938	-2.11961
H	-2.16584	-0.83564	1.23747
H	-6.40905	-4.36393	-0.01909
H	-6.99973	-2.98433	-0.95632
H	-5.59235	-3.89779	-1.51727
Na	-0.40028	-1.35172	-0.56594

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 32

C	4.7336	2.28691	-0.65727
C	3.63255	2.06992	0.39018
C	3.12698	0.6274	0.50568
C	2.23556	0.20182	-0.67717
C	2.04495	-1.32808	-0.80865
S	0.35521	-1.73778	-1.49192
C	-0.44937	-2.6997	-0.147
C	-1.14494	-1.93521	1.00076
C	-0.19379	-1.34147	2.09229
O	-0.70786	-0.50967	2.88483
O	0.99385	-1.75877	2.0881
N	-2.12586	-0.95891	0.51242
C	-3.51618	-1.36311	0.31555
O	-4.12448	-0.28244	-0.36683
C	-3.37068	0.89904	-0.11047
C	-1.98203	0.36353	0.30538
O	-0.97892	1.0731	0.43249
C	-3.3575	1.79644	-1.35984
C	-4.75456	2.35604	-1.67773
C	-2.76665	1.07407	-2.58009
O	-3.84547	1.56665	1.04406
C	3.14848	-1.96618	-1.67043
C	3.21674	-3.49414	-1.60055
O	2.39955	0.55285	1.75157
C	5.23428	3.73583	-0.69598
H	5.57562	1.61644	-0.43721
H	4.37029	2.00627	-1.65371
H	2.78029	2.73129	0.17166
H	4.01483	2.36121	1.37679
H	3.99843	-0.04087	0.58203
H	1.26631	0.69326	-0.55177

H	2.6644	0.58317	-1.61302
H	2.04311	-1.78451	0.1832
H	-1.19459	-3.30422	-0.67558
H	0.27857	-3.38291	0.29454
H	-1.73478	-2.68532	1.54922
H	-3.99718	-1.54867	1.28715
H	-3.58647	-2.25582	-0.31449
H	-2.69567	2.62952	-1.09239
H	-4.7039	2.99245	-2.56687
H	-5.15591	2.97948	-0.87018
H	-5.4661	1.54946	-1.88424
H	-2.66111	1.77718	-3.41293
H	-1.77769	0.65502	-2.37098
H	-3.42045	0.25886	-2.90623
H	-4.7477	1.86967	0.87101
H	3.02402	-1.64369	-2.71351
H	4.11011	-1.54911	-1.33714
H	4.03435	-3.87763	-2.22047
H	3.38833	-3.83386	-0.57234
H	2.28502	-3.94544	-1.95592
H	2.11564	-0.37615	1.93894
H	6.02365	3.86403	-1.44427
H	4.42249	4.42889	-0.94684
H	5.64242	4.0405	0.27485
Na	0.30758	1.35235	2.26116

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 71

C	-4.77885	-2.35945	0.14734
C	-3.70494	-1.69054	-0.72061
C	-3.12118	-0.40508	-0.12974
C	-2.09371	0.25444	-1.07144
C	-1.80526	1.74025	-0.74729

S	-0.03217	2.18544	-1.12874
C	0.66863	2.6755	0.49895
C	1.19933	1.57643	1.44471
C	0.10914	0.77168	2.22714
O	-1.05104	1.26014	2.23392
O	0.49592	-0.28486	2.79183
N	2.19124	0.70826	0.79928
C	3.61206	1.02695	0.906
O	4.25844	0.1313	0.02206
C	3.4192	-1.00307	-0.18321
C	2.01295	-0.48804	0.20696
O	0.96219	-1.11033	0.01902
C	3.61192	-1.48093	-1.63669
C	3.25639	-0.38871	-2.65745
C	2.86243	-2.78946	-1.93465
O	3.70484	-2.0146	0.76472
C	-2.77275	2.67761	-1.49152
C	-2.77232	4.12717	-0.99922
O	-2.52019	-0.75037	1.1369
C	-5.34536	-3.63562	-0.48548
H	-4.35879	-2.58528	1.13376
H	-5.59404	-1.64354	0.3209
H	-4.13034	-1.4507	-1.70411
H	-2.88221	-2.39797	-0.90831
H	-3.94925	0.29361	0.06808
H	-1.17047	-0.32972	-1.02143
H	-2.4585	0.18247	-2.10525
H	-1.89152	1.90401	0.32866
H	1.49569	3.34163	0.22993
H	-0.06775	3.26586	1.04761
H	1.7527	2.10304	2.237
H	3.95412	0.88929	1.94225
H	3.81746	2.05082	0.57619

H	4.69389	-1.67542	-1.71428
H	3.46359	-0.74676	-3.67121
H	3.84069	0.51992	-2.49243
H	2.19341	-0.12876	-2.60649
H	3.1344	-3.14711	-2.93334
H	3.10701	-3.57276	-1.21232
H	1.78089	-2.63237	-1.90833
H	4.6102	-2.32268	0.6114
H	-2.54938	2.64651	-2.56701
H	-3.78506	2.26171	-1.38053
H	-3.49453	4.73048	-1.55987
H	-3.0418	4.18304	0.06213
H	-1.78515	4.58358	-1.1228
H	-2.21589	0.06159	1.61339
H	-6.11152	-4.08993	0.15193
H	-5.80367	-3.42881	-1.46012
H	-4.55947	-4.38427	-0.64424
Na	-0.52418	-1.81012	1.5603

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 5

C	4.72356	2.54307	0.17013
C	3.65606	1.87351	-0.7052
C	3.15456	0.52784	-0.17548
C	2.13388	-0.12885	-1.12672
C	1.9285	-1.64332	-0.88268
S	0.17127	-2.16131	-1.25
C	-0.46265	-2.76595	0.36758
C	-1.02353	-1.74181	1.37851
C	0.04332	-0.92929	2.18335
O	-0.38158	0.07347	2.81487
O	1.22609	-1.35837	2.13874
N	-2.06407	-0.88954	0.79234

C	-3.46424	-1.28996	0.87735
O	-4.14941	-0.4112	0.00727
C	-3.38174	0.78361	-0.14374
C	-1.94961	0.33516	0.24474
O	-0.93149	1.0184	0.09267
C	-3.56243	1.28168	-1.59411
C	-2.80395	2.58831	-1.87296
C	-5.05436	1.42741	-1.94657
O	-3.73545	1.74271	0.83358
C	2.9237	-2.48542	-1.70075
C	3.0067	-3.95962	-1.29654
O	2.57402	0.77099	1.12376
C	5.19321	3.89079	-0.38968
H	4.32963	2.67583	1.18386
H	5.58359	1.86584	0.26429
H	4.05996	1.71488	-1.71385
H	2.79376	2.54793	-0.8242
H	4.02155	-0.13769	-0.03998
H	1.18499	0.40404	-1.01881
H	2.46414	0.02051	-2.16384
H	2.04781	-1.86306	0.18022
H	-1.26141	-3.4605	0.0852
H	0.31664	-3.34312	0.86895
H	-1.5386	-2.33185	2.15158
H	-3.82352	-1.19605	1.91278
H	-3.60998	-2.31524	0.52199
H	-3.14326	0.49004	-2.22805
H	-2.93938	2.87164	-2.92212
H	-1.73597	2.48306	-1.67579
H	-3.18571	3.40479	-1.25073
H	-5.15654	1.69655	-3.00265
H	-5.60799	0.50172	-1.77338
H	-5.53199	2.2319	-1.37122

H	-4.65048	2.01606	0.67555
H	2.67432	-2.40255	-2.7678
H	3.91635	-2.02545	-1.5859
H	3.74328	-4.4915	-1.90847
H	3.30523	-4.06447	-0.24676
H	2.04011	-4.4568	-1.42549
H	2.31688	-0.07988	1.55872
H	5.95909	4.34246	0.24996
H	5.62138	3.77971	-1.3932
H	4.36159	4.60224	-0.46403
Na	0.54267	1.70872	1.65146

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 27

C	-4.5195	-2.79652	0.35537
C	-3.66754	-1.96947	-0.61657
C	-3.14913	-0.65073	-0.04015
C	-2.36971	0.179	-1.07766
C	-2.17284	1.65925	-0.67075
S	-0.53818	2.31731	-1.2861
C	0.3115	2.85891	0.24863
C	1.13248	1.84758	1.07113
C	0.32266	0.82377	1.93708
O	-0.87479	1.09755	2.17787
O	0.95701	-0.20755	2.3288
N	2.19279	1.15482	0.3256
C	3.591	1.39892	0.70064
O	4.32012	0.33548	0.13192
C	3.44126	-0.78139	-0.01821
C	2.06446	-0.10512	-0.16663
O	1.02344	-0.679	-0.50189
C	3.97346	-1.66075	-1.15656
C	4.02255	-0.89289	-2.48663

C	3.19865	-2.98014	-1.30051
O	3.3577	-1.54558	1.1701
C	-3.33902	2.53715	-1.15974
C	-3.38628	3.94151	-0.55205
O	-2.31268	-0.98062	1.09343
C	-5.02172	-4.10743	-0.26032
H	-3.93737	-3.00673	1.25954
H	-5.37783	-2.19221	0.67984
H	-4.25792	-1.73981	-1.51326
H	-2.80855	-2.5656	-0.96186
H	-4.00744	-0.07133	0.33314
H	-1.3996	-0.30025	-1.23896
H	-2.90313	0.14232	-2.03703
H	-2.0966	1.7324	0.41632
H	0.99024	3.64637	-0.09518
H	-0.41746	3.32162	0.91757
H	1.66362	2.45974	1.81558
H	3.68352	1.41398	1.7978
H	3.96256	2.34039	0.28361
H	5.00187	-1.89841	-0.85282
H	4.48079	-1.51743	-3.26032
H	4.60991	0.02461	-2.39965
H	3.01485	-0.62929	-2.82868
H	3.6781	-3.60395	-2.06233
H	3.18687	-3.53761	-0.36083
H	2.16638	-2.79702	-1.61446
H	2.77446	-1.08484	1.80737
H	-3.30172	2.60469	-2.25564
H	-4.27479	2.01072	-0.91953
H	-4.24667	4.50274	-0.932
H	-3.47222	3.89643	0.54019
H	-2.48149	4.50595	-0.79906
H	-2.0539	-0.16889	1.58804

H	-5.63146	-4.67331	0.45209
H	-5.63606	-3.92167	-1.1495
H	-4.1868	-4.7499	-0.56565
Na	-0.16554	-1.75243	1.10997

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 11

C	2.74199	3.24397	-0.39435
C	3.80009	2.14545	-0.21435
C	3.27124	0.75087	0.14605
C	2.32051	0.15343	-0.9136
C	2.2046	-1.3886	-0.83655
S	0.49803	-1.97161	-1.32287
C	-0.15502	-2.76976	0.1993
C	-0.8181	-1.88385	1.27629
C	0.16756	-1.08686	2.19395
O	1.37354	-1.44739	2.16532
O	-0.33775	-0.1653	2.88631
N	-1.88924	-1.04173	0.73011
C	-3.2662	-1.53131	0.71856
O	-3.98352	-0.60327	-0.07382
C	-3.28149	0.63676	-0.06678
C	-1.83746	0.23652	0.31138
O	-0.87038	1.002	0.24557
C	-3.41232	1.32319	-1.43733
C	-4.85833	1.7644	-1.72083
C	-2.87648	0.43972	-2.57409
O	-3.70628	1.4584	1.00494
C	3.27613	-2.08003	-1.69811
C	3.44156	-3.57977	-1.43877
O	2.62559	0.85176	1.43294
C	3.35724	4.5909	-0.79368
H	2.0064	2.94202	-1.14975

H	2.19098	3.37578	0.54744
H	4.50433	2.45179	0.56985
H	4.38248	2.05422	-1.14116
H	4.14535	0.09231	0.25906
H	1.33496	0.6088	-0.7905
H	2.67614	0.43188	-1.91547
H	2.3057	-1.70835	0.20257
H	-0.89581	-3.48081	-0.18261
H	0.64029	-3.34475	0.67776
H	-1.32087	-2.57485	1.96974
H	-3.66089	-1.57413	1.74423
H	-3.33487	-2.51739	0.2478
H	-2.77938	2.21585	-1.35975
H	-4.91028	2.25264	-2.69914
H	-5.23183	2.49103	-0.98968
H	-5.53776	0.90561	-1.73951
H	-2.88606	0.99852	-3.51577
H	-1.84817	0.11404	-2.39017
H	-3.49926	-0.45136	-2.70165
H	-4.6329	1.69478	0.85878
H	3.05268	-1.90545	-2.75979
H	4.2335	-1.57455	-1.50351
H	4.22627	-4.00241	-2.07553
H	3.71797	-3.77079	-0.3951
H	2.5119	-4.11846	-1.64751
H	2.39837	-0.04764	1.77804
H	2.59025	5.36508	-0.9038
H	4.07661	4.93661	-0.04209
H	3.88963	4.51199	-1.74878
Na	0.51343	1.62783	1.91078

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 29

C	4.91664	2.25901	-0.22443
C	3.85094	1.42926	-0.95137
C	3.21932	0.32396	-0.10095
C	2.2036	-0.51664	-0.90127
C	1.86475	-1.87715	-0.24346
S	0.08589	-2.37313	-0.53731
C	-0.61526	-2.47927	1.16036
C	-1.13927	-1.19134	1.83288
C	-0.0434	-0.23804	2.41471
O	-0.41523	0.92926	2.70297
O	1.1071	-0.72932	2.5561
N	-2.1254	-0.48462	1.00642
C	-3.55114	-0.74932	1.18679
O	-4.19018	-0.08589	0.11213
C	-3.33772	0.9587	-0.34938
C	-1.93759	0.53487	0.14805
O	-0.88733	1.08822	-0.19277
C	-3.45397	1.0959	-1.87708
C	-4.8462	1.59172	-2.30321
C	-3.09291	-0.21189	-2.59783
O	-3.59671	2.17031	0.33539
C	2.82905	-3.00936	-0.65488
C	2.7677	-3.45859	-2.12052
O	2.59366	0.96252	1.03232
C	5.52938	3.35045	-1.10978
H	4.47589	2.70881	0.67216
H	5.71046	1.58775	0.13126
H	4.29617	0.96316	-1.84044
H	3.05107	2.08963	-1.32129
H	4.02453	-0.32437	0.27847
H	1.29481	0.08087	-1.02076

H	2.60122	-0.6839	-1.90959
H	1.91337	-1.76511	0.8405
H	-1.44524	-3.18558	1.05013
H	0.11923	-2.93452	1.82798
H	-1.69569	-1.52178	2.72306
H	-3.88794	-0.35899	2.15837
H	-3.77076	-1.81962	1.11546
H	-2.71077	1.85803	-2.14213
H	-4.88814	1.68415	-3.39309
H	-5.08648	2.58104	-1.89644
H	-5.62749	0.88794	-1.99705
H	-3.07113	-0.04665	-3.68008
H	-2.10949	-0.58676	-2.29818
H	-3.83358	-0.99018	-2.38815
H	-4.49519	2.45615	0.11917
H	3.85061	-2.67291	-0.42213
H	2.6394	-3.87454	-0.00882
H	3.49323	-4.25809	-2.30478
H	1.77476	-3.84517	-2.37183
H	2.99804	-2.6433	-2.81506
H	2.2801	0.29003	1.68717
H	6.28815	3.92423	-0.56678
H	6.00937	2.92256	-1.99821
H	4.76537	4.05689	-1.45697
Na	0.60597	2.11164	1.14175

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 25

C	4.79157	2.42724	0.04489
C	3.79938	1.6484	-0.82816
C	3.20277	0.40731	-0.1586
C	2.27105	-0.36486	-1.11702
C	1.90121	-1.80284	-0.66616

S	0.09471	-2.16559	-0.99053
C	-0.57412	-2.62716	0.65819
C	-1.11755	-1.49958	1.56012
C	-0.02998	-0.62153	2.2605
O	-0.41564	0.47833	2.73434
O	1.13335	-1.10305	2.29596
N	-2.15402	-0.70336	0.89109
C	-3.55956	-1.07254	1.04679
O	-4.2606	-0.27103	0.11469
C	-3.47442	0.88115	-0.17536
C	-2.03998	0.45225	0.2082
O	-1.02971	1.10465	-0.07054
C	-3.64514	1.27472	-1.65258
C	-5.07762	1.74564	-1.95665
C	-3.22946	0.13881	-2.59952
O	-3.77222	1.93965	0.71604
C	2.74792	-2.89695	-1.34579
C	4.25731	-2.79957	-1.08009
O	2.49778	0.85154	1.01763
C	5.37253	3.65512	-0.66593
H	4.29593	2.73193	0.97333
H	5.60881	1.75608	0.34297
H	4.30099	1.33203	-1.75234
H	2.97593	2.31007	-1.13889
H	4.02615	-0.24207	0.17011
H	1.3619	0.23301	-1.23746
H	2.74712	-0.41234	-2.10575
H	1.99912	-1.88401	0.41837
H	-1.38818	-3.3227	0.42715
H	0.18406	-3.17877	1.21774
H	-1.63282	-1.99785	2.39545
H	-3.89099	-0.87595	2.07698
H	-3.72473	-2.12499	0.79376

H	-2.95757	2.11757	-1.7943
H	-5.15891	2.02563	-3.01173
H	-5.36662	2.62995	-1.37635
H	-5.80419	0.94899	-1.76483
H	-3.26164	0.48817	-3.63678
H	-2.21222	-0.21051	-2.39773
H	-3.90945	-0.71414	-2.50784
H	-4.68925	2.2111	0.57028
H	2.38692	-3.87258	-1.00181
H	2.56451	-2.8695	-2.42879
H	4.77912	-3.64229	-1.54652
H	4.69292	-1.88181	-1.48955
H	4.47703	-2.82667	-0.0064
H	2.22008	0.079	1.57252
H	6.0811	4.18919	-0.02374
H	5.90331	3.37187	-1.5829
H	4.58303	4.36231	-0.94859
Na	0.50656	1.92436	1.34023

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 20

C	-4.50612	-2.83148	-0.28868
C	-3.50818	-1.95109	-1.05937
C	-3.04478	-0.68666	-0.32877
C	-2.03527	0.12254	-1.1675
C	-1.86383	1.5893	-0.70331
S	-0.11085	2.18324	-0.95923
C	0.48513	2.56914	0.73697
C	1.06196	1.42669	1.60064
C	0.00648	0.47774	2.25778
O	-1.18592	0.88214	2.25881
O	0.4478	-0.59909	2.73748
N	2.13747	0.69574	0.92013

C	3.52523	1.10783	1.11025
O	4.26548	0.35988	0.16522
C	3.5225	-0.8049	-0.18983
C	2.07065	-0.44378	0.20531
O	1.07917	-1.12348	-0.08029
C	3.78597	-1.09684	-1.68111
C	3.36287	0.07494	-2.58081
C	3.15556	-2.41833	-2.14884
O	3.86444	-1.89162	0.6489
C	-2.86118	2.52487	-1.40928
C	-2.97511	3.92381	-0.79791
O	-2.46341	-1.10721	0.92376
C	-5.86917	-2.1726	-0.04039
H	-4.65577	-3.75746	-0.85912
H	-4.06322	-3.1222	0.6708
H	-3.95475	-1.64548	-2.01496
H	-2.61735	-2.54448	-1.31434
H	-3.92091	-0.06166	-0.10226
H	-1.07532	-0.40047	-1.13086
H	-2.35809	0.11899	-2.21772
H	-2.00746	1.65042	0.37744
H	1.2673	3.31761	0.56908
H	-0.31596	3.04879	1.30274
H	1.54614	1.91359	2.46072
H	3.84729	0.89001	2.1392
H	3.65802	2.17308	0.89356
H	4.88188	-1.19279	-1.74635
H	3.62408	-0.14259	-3.62158
H	3.86385	1.00181	-2.29091
H	2.28092	0.24095	-2.53531
H	3.4762	-2.6333	-3.17365
H	3.45129	-3.25821	-1.51441
H	2.06432	-2.35426	-2.13595

H	4.79259	-2.11599	0.48679
H	-2.59402	2.60109	-2.47243
H	-3.84737	2.03855	-1.37918
H	-3.71056	4.52839	-1.33962
H	-3.29167	3.87143	0.25055
H	-2.01467	4.44735	-0.83646
H	-2.23039	-0.32434	1.48299
H	-6.55577	-2.86958	0.45208
H	-5.78365	-1.29104	0.60342
H	-6.3357	-1.85682	-0.98181
Na	-0.41333	-2.06414	1.32387

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 54

C	-4.19501	-3.23216	-0.05712
C	-3.44896	-2.21496	-0.93688
C	-3.06285	-0.90269	-0.24831
C	-2.30789	0.04424	-1.19957
C	-2.21718	1.50319	-0.69081
S	-0.60693	2.29387	-1.20603
C	0.16139	2.78705	0.38713
C	1.0132	1.77492	1.17654
C	0.23867	0.65281	1.94812
O	-0.97893	0.8427	2.16619
O	0.92044	-0.36441	2.29511
N	2.13761	1.19433	0.42879
C	3.50559	1.48911	0.87362
O	4.31376	0.50771	0.26568
C	3.50635	-0.64412	0.01429
C	2.0993	-0.03617	-0.1465
O	1.10528	-0.6427	-0.55837
C	4.12848	-1.42058	-1.15289
C	4.1877	-0.56862	-2.43014

C	3.43209	-2.76624	-1.40963
O	3.42445	-1.48452	1.1501
C	-3.41959	2.33996	-1.16353
C	-3.5676	3.70032	-0.4772
O	-2.24892	-1.24698	0.89715
C	-5.57982	-2.76726	0.41144
H	-4.3053	-4.16129	-0.6311
H	-3.57879	-3.4755	0.81613
H	-4.06641	-1.96734	-1.81045
H	-2.53204	-2.67639	-1.33319
H	-3.97216	-0.40846	0.12212
H	-1.30478	-0.36247	-1.35887
H	-2.80892	0.03934	-2.1771
H	-2.17922	1.50888	0.40081
H	0.80451	3.62998	0.11355
H	-0.61342	3.16832	1.05577
H	1.48119	2.36813	1.97659
H	3.55848	1.43511	1.97216
H	3.83749	2.47538	0.53392
H	5.15565	-1.62413	-0.82136
H	4.7055	-1.12034	-3.2214
H	4.72366	0.36897	-2.2631
H	3.18139	-0.33312	-2.79608
H	3.97537	-3.31637	-2.18527
H	3.41105	-3.38082	-0.5064
H	2.40549	-2.61668	-1.75795
H	2.79187	-1.09841	1.79033
H	-3.35606	2.47507	-2.25196
H	-4.3281	1.74621	-0.98346
H	-4.45127	4.23055	-0.84808
H	-3.67703	3.58567	0.60783
H	-2.69324	4.33103	-0.66625
H	-2.06117	-0.45255	1.44812

H	-6.08647	-3.55774	0.9753
H	-5.51519	-1.89164	1.06584
H	-6.22026	-2.50415	-0.43946
Na	-0.06055	-1.89133	0.94089

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 50

C	4.59223	2.66805	0.35738
C	3.7813	1.75636	-0.57245
C	3.17233	0.53153	0.11288
C	2.44099	-0.39182	-0.88012
C	2.13839	-1.79818	-0.30753
S	0.51051	-2.46652	-0.93571
C	-0.40459	-2.82551	0.61595
C	-1.2273	-1.71585	1.29896
C	-0.42474	-0.61718	2.07556
O	-1.04305	0.46826	2.31664
O	0.75273	-0.8913	2.40132
N	-2.25174	-1.09337	0.4484
C	-3.66435	-1.26021	0.8128
O	-4.35317	-0.25962	0.0985
C	-3.44495	0.81352	-0.15886
C	-2.08029	0.09822	-0.182
O	-1.01703	0.60858	-0.54768
C	-3.92592	1.55616	-1.4119
C	-3.95391	0.6316	-2.63886
C	-3.12266	2.83544	-1.69415
O	-3.37789	1.71539	0.92942
C	3.28506	-2.80672	-0.53033
C	3.55901	-3.21691	-1.98271
O	2.27014	1.01654	1.13452
C	5.19555	3.87527	-0.36983
H	3.95292	3.00828	1.17965

H	5.39683	2.08045	0.82057
H	4.42568	1.40323	-1.38831
H	2.97312	2.33197	-1.04973
H	3.97892	-0.02409	0.61508
H	1.51032	0.10032	-1.17862
H	3.04967	-0.48396	-1.78732
H	1.97311	-1.70972	0.76721
H	-1.09172	-3.62924	0.33223
H	0.28942	-3.23328	1.35471
H	-1.79178	-2.23516	2.08804
H	-3.7838	-1.13767	1.90064
H	-4.0486	-2.2378	0.50467
H	-4.95747	1.84615	-1.17047
H	-4.38053	1.16337	-3.49553
H	-4.55912	-0.25985	-2.45645
H	-2.94254	0.31364	-2.91809
H	-3.57404	3.36982	-2.53688
H	-3.12132	3.50269	-0.82879
H	-2.08759	2.5997	-1.96024
H	-2.82633	1.32343	1.63673
H	4.19858	-2.37091	-0.09804
H	3.07002	-3.70586	0.05918
H	4.38423	-3.93562	-2.02596
H	2.67903	-3.69096	-2.42896
H	3.83777	-2.36354	-2.61059
H	1.97084	0.28069	1.71753
H	5.76842	4.50746	0.31697
H	5.87167	3.56084	-1.17392
H	4.41482	4.49929	-0.82157
Na	0.15116	1.83445	0.95802

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 23

C	4.64565	2.39025	-0.5637
C	3.55452	2.08587	0.47212
C	3.09817	0.6233	0.52023
C	2.21939	0.22208	-0.68056
C	2.07736	-1.30569	-0.87945
S	0.40511	-1.73748	-1.59185
C	-0.38235	-2.77045	-0.29071
C	-1.10796	-2.0694	0.87967
C	-0.18389	-1.50202	2.00695
O	-0.73005	-0.72817	2.83615
O	1.01677	-1.88033	1.99196
N	-2.1037	-1.09562	0.41782
C	-3.47821	-1.52294	0.18241
O	-4.09027	-0.43881	-0.48741
C	-3.37069	0.7587	-0.19071
C	-1.98224	0.23606	0.25882
O	-0.99155	0.94848	0.45283
C	-3.38039	1.6402	-1.45864
C	-2.66441	2.98432	-1.25492
C	-4.81661	1.85687	-1.97035
O	-3.90094	1.40169	0.95144
C	3.20367	-1.87254	-1.76131
C	3.32252	-3.39902	-1.74929
O	2.3758	0.46822	1.7618
C	5.09657	3.85562	-0.53253
H	5.51052	1.73924	-0.37631
H	4.29017	2.14553	-1.57239
H	2.67975	2.72726	0.28518
H	3.92812	2.34305	1.47149
H	3.99167	-0.01808	0.56642
H	1.2344	0.67411	-0.53275

H	2.63377	0.65848	-1.59869
H	2.08512	-1.80358	0.09217
H	-1.10704	-3.37409	-0.8481
H	0.35991	-3.45065	0.13107
H	-1.68839	-2.85366	1.38879
H	-3.97658	-1.74187	1.13837
H	-3.51767	-2.40136	-0.47002
H	-2.83711	1.06383	-2.21815
H	-2.6674	3.54534	-2.19551
H	-1.63017	2.84571	-0.93575
H	-3.17497	3.59012	-0.49865
H	-4.78973	2.4117	-2.91355
H	-5.33591	0.91148	-2.14317
H	-5.41203	2.45845	-1.27034
H	-4.79906	1.69795	0.74527
H	3.0701	-1.51477	-2.79167
H	4.15027	-1.43668	-1.40964
H	4.14931	-3.73193	-2.38606
H	3.51007	-3.77127	-0.73521
H	2.40434	-3.8673	-2.11781
H	2.11251	-0.475	1.90148
H	5.87908	4.04689	-1.27449
H	4.26087	4.53183	-0.74852
H	5.4966	4.12656	0.45159
Na	0.26263	1.17781	2.3116

Compound 1d: Isomer 4R, 6S, 10R, 13R conformer 65

C	2.5361	3.45262	-0.38701
C	3.64426	2.50834	0.10206
C	3.22	1.06681	0.40921
C	2.61353	0.32482	-0.79852
C	2.61555	-1.21456	-0.63823

S	1.12795	-1.98047	-1.46551
C	0.27621	-2.85792	-0.09512
C	-0.71347	-2.09951	0.80947
C	-0.09314	-1.12822	1.8717
O	-0.8779	-0.25477	2.3619
O	1.11509	-1.2882	2.15645
N	-1.82146	-1.44086	0.10326
C	-3.19214	-1.91389	0.34287
O	-4.0316	-0.87442	-0.10868
C	-3.30246	0.34949	-0.03129
C	-1.84389	-0.11404	-0.18562
O	-0.88317	0.64012	-0.36566
C	-3.82727	1.34886	-1.062
C	-5.25866	1.7967	-0.72721
C	-3.72445	0.79765	-2.49151
O	-3.36974	0.93037	1.25998
C	3.91973	-1.83617	-1.16932
C	4.1406	-3.29941	-0.77697
O	2.28796	1.11498	1.51444
C	3.06223	4.85761	-0.70548
H	2.04963	3.03702	-1.27764
H	1.75903	3.53704	0.38631
H	4.09867	2.9269	1.00923
H	4.43841	2.46745	-0.65552
H	4.11626	0.52985	0.75255
H	1.59159	0.67991	-0.95238
H	3.17952	0.5892	-1.70248
H	2.49475	-1.47155	0.41654
H	-0.27343	-3.65707	-0.60334
H	1.02252	-3.3293	0.54821
H	-1.19079	-2.8829	1.4173
H	-3.33351	-2.11161	1.41676
H	-3.41397	-2.81722	-0.23397

H	-3.1588	2.21466	-0.97497
H	-5.58322	2.56442	-1.43765
H	-5.32136	2.21111	0.28178
H	-5.95586	0.95528	-0.79596
H	-4.02678	1.56726	-3.20917
H	-2.70169	0.49571	-2.74076
H	-4.38111	-0.06759	-2.62531
H	-2.75928	0.45222	1.85802
H	3.94627	-1.73331	-2.26282
H	4.75594	-1.23222	-0.78695
H	5.08916	-3.6728	-1.17754
H	4.1689	-3.41573	0.31298
H	3.33834	-3.93448	-1.16583
H	2.11807	0.21005	1.86516
H	2.25714	5.51976	-1.0413
H	3.52821	5.31578	0.17464
H	3.8173	4.82316	-1.49945
Na	0.06107	1.60207	1.46176

Comparison between calculated (MP1WMP91/6-311++ G(2d,p)) and experimental ^{1}H NMR data for 1a-diasteroisomer.

H	Calc **1a**(ppm)	Exp(ppm)	DD	Scaled	ΔΔ scaled
1	0.94046318	0.94	0.00046318	0.853	0.08691927
2h	1.25003094	1.33	0.07996906	1.199	0.13114941
2l	1.74229282	1.45	0.29229282	1.749	0.29867957
3h	1.23016289	1.36	0.12983711	1.177	0.1833409
3l	1.34718398	1.38	0.03281602	1.307	0.07263489
4	3.66913546	3.65	0.01913546	3.901	0.25085497
5h	1.23252003	1.6	0.36747997	1.179	0.42070811
5l	1.52499428	1.77	0.24500572	1.506	0.26403074
6	3.2236897	2.86	0.3636897	3.403	0.54331698
7h	1.40201473	1.47	0.06798527	1.369	0.10139201
7l	1.78519699	1.69	0.09519699	1.797	0.10660113
8	0.98215668	0.89	0.09215668	0.900	0.00965004
9h	2.98743066	2.70	0.28743066	3.139	0.43942887
9l	3.33363085	3.28	0.05363085	3.526	0.2461151
10	3.94820583	4.69	0.74179417	4.213	0.47743904
14h	4.61744218	4.94	0.32255782	4.960	0.02006051
14l	4.71620081	5.26	0.54379919	5.070	0.18963162
15	2.07315459	2.18	0.10684541	2.118	0.06176635
16	1.03611043	0.98	0.05611043	0.960	0.02008664
17	1.24721454	1.1	0.14721454	1.196	0.09570484
		AVERAGE	0.20227055		0.20097555

^{1}H chemical shifts for the diasteroisomer **1a.**

Comparison between calculated (MP1WMP91/6-311++ G(2d,p)) and experimental ^{13}C NMR data for 1a-diasteroisomer.

C	Calc. **1a**(ppm)	Exp (ppm)	DD	Scaled	DD Scaled
1	14.53828487	14.50	0.04	12.13	2.37
2	22.3065874	19.90	2.41	19.84	0.06
3	40.05146031	41.00	0.95	37.46	3.54
4	73.86423333	69.60	4.26	71.04	1.44
5	41.17221497	43.70	2.53	38.58	5.12
6	54.61594789	44.80	9.82	51.93	7.13
7	33.31564436	27.60	5.72	30.78	3.18
8	12.56424668	11.30	1.26	10.17	1.13
9	40.0666136	31.00	9.07	37.48	6.48
10	64.21909645	56.90	7.32	61.46	4.56
11	175.3316894	175.00	0.33	171.79	3.21
12	178.0690039	171.40	6.67	174.51	3.11
13	104.2248194	104.70	0.48	101.18	3.52
14	79.91531853	77.30	2.62	77.05	0.25
15	36.46357274	35.00	1.46	33.90	1.10
16	16.44911434	17.70	1.25	14.03	3.67
17	15.9988804	15.50	0.50	13.58	1.92
		AVERAGE	3.33		3.05

Comparison between calculated (MP1WMP91/6-311++ G(2d,p)) and experimental ^{1}H NMR data for 1b-diasteroisomer.

H	Calc. **1b**(ppm)	Exp (ppm)	ΔΔ	scaled	ΔΔ scaled
1	0.954857556	0.94	0.01485756	0.786	0.15397704
2h	1.221220925	1.33	0.10877908	1.105	0.22474961
2l	1.755269259	1.45	0.30526926	1.745	0.29528914
3h	1.314197885	1.36	0.04580211	1.217	0.14331989
3l	1.325635964	1.38	0.05436404	1.230	0.14961174
4	3.304630974	3.65	0.34536903	3.602	0.04785358
5h	1.415362728	1.6	0.18463727	1.338	0.26207727
5l	2.340591096	1.77	0.5705911	2.447	0.67677744
6	2.353222701	2.86	0.5067773	2.462	0.39808401
7h	1.587939138	1.47	0.11793914	1.545	0.07474969
7l	1.61619763	1.69	0.07380237	1.579	0.11138347
8	1.071806452	0.89	0.18180645	0.926	0.03618223
9h	2.960018061	2.7	0.26001806	3.189	0.48913957
9l	3.193917666	3.28	0.08608233	3.469	0.18946029
10	3.803043675	4.69	0.88695632	4.199	0.49052292
14h	4.628609587	4.94	0.31139041	5.189	0.24888973
14l	4.73020061	5.26	0.52979939	5.311	0.05064311
15	2.07067209	2.18	0.10932791	2.123	0.0567113
16	1.073962606	0.98	0.09396261	0.929	0.05123369
17	1.239604831	1.1	0.13960483	1.127	0.02728287
		AVERAGE	0.24635683		0.20889693

Comparison between calculated (MP1WMP91/6-311++ G(2d,p)) and experimental ^{13}C NMR data for 1b-diasteroisomer.

C	Calc. **1b**(ppm)	Exp (ppm)	ΔΔ	Scaled	ΔΔ Scaled
1	14.37669197	14.50	0.12	12.38	2.12
2	22.36881707	19.90	2.47	20.28	0.38
3	43.39250891	41.00	2.39	41.05	0.05
4	76.51512005	69.60	6.92	73.78	4.18
5	41.02494514	43.70	2.68	38.71	4.99
6	57.01119262	44.80	12.21	54.51	9.71
7	30.1257825	27.60	2.53	27.95	0.35
8	12.33423601	11.30	1.03	10.36	0.94
9	32.77135717	31.00	1.77	30.56	0.44
10	63.84971556	56.90	6.95	61.27	4.37
11	174.8804943	175.00	0.12	170.98	4.02
12	178.4112237	171.40	7.01	174.47	3.07
13	103.8312271	104.70	0.87	100.78	3.92
14	79.57793927	77.30	2.28	76.81	0.49
15	36.83373685	35.00	1.83	34.57	0.43
16	16.45741474	17.70	1.24	14.44	3.26
17	15.99531174	15.50	0.50	13.98	1.52
		AVERAGE	3.11		2.60

Comparison between calculated (MP1WMP91/6-311++ G(2d,p)) and experimental ^{1}H NMR data for 1c-diasteroisomer.

H	Calc. **1c**(ppm)	Exp (ppm)	ΔΔ	scaled	ΔΔ
1	0.946267344	0.94	0.00626734	0.89491659	0.04508341
2h	1.238246456	1.33	0.09175354	1.2085354	0.1214646
2l	1.768041181	1.45	0.31804118	1.77759525	0.32759525
3h	1.232237063	1.36	0.12776294	1.20208063	0.15791937
3l	1.312039727	1.38	0.06796027	1.28779777	0.09220223
4	3.609596044	3.65	0.04040396	3.75563485	0.10563485
5h	1.339196085	1.6	0.26080392	1.31696679	0.28303321
5l	1.536814982	1.77	0.23318502	1.52923199	0.24076801
6	3.402719153	2.86	0.54271915	3.53342551	0.67342551
7h	1.459767963	1.47	0.01023204	1.44647472	0.02352528
7l	1.696470207	1.69	0.00647021	1.70071988	0.01071988
8	0.999092113	0.89	0.10909211	0.95165641	0.06165641
9h	2.907606274	2.7	0.20760627	3.00161791	0.30161791
9l	3.260779176	3.28	0.01922082	3.38096582	0.10096582
10	3.987010482	4.69	0.70298952	4.16102093	0.52897907
14h	4.621660512	4.94	0.31833949	4.84270732	0.09729268
14l	5.103661257	5.26	0.15633874	5.360431	0.100431
15	2.141602426	2.18	0.03839757	2.17884256	0.00115744
16	1.072846459	0.98	0.09284646	1.03087697	0.05087697
17	1.007669635	1.1	0.09233037	0.96086964	0.13913036
		AVERAGE	0.17213805		0.17317396

Comparison between calculated (MP1WMP91/6-311++ G(2d,p)) and experimental ^{13}C NMR data for 1c-diasteroisomer.

C	Calc. **1c**(ppm)	Exp (ppm)	ΔΔ	Scaled	ΔΔ Scaled
1	14.41	14.50	0.09	11.25	3.25
2	22.87	19.90	2.97	19.87	0.03
3	40.16	41.00	0.84	37.50	3.50
4	73.76	69.60	4.16	71.77	2.17
5	42.12	43.70	1.58	39.50	4.20
6	55.75	44.80	10.95	53.40	8.60
7	33.44	27.60	5.84	30.65	3.05
8	12.57	11.30	1.27	9.37	1.93
9	41.67	31.00	10.67	39.04	8.04
10	62.21	56.90	5.31	59.98	3.08
11	173.96	175.00	1.04	173.95	1.05
12	169.69	171.40	1.71	169.60	1.80
13	105.26	104.70	0.56	103.89	0.81
14	80.47	77.30	3.17	78.61	1.31
15	36.92	35.00	1.92	34.20	0.80
16	16.71	17.70	0.99	13.58	4.12
17	13.89	15.50	1.61	10.71	4.79
		AVERAGE	3.22		3.09

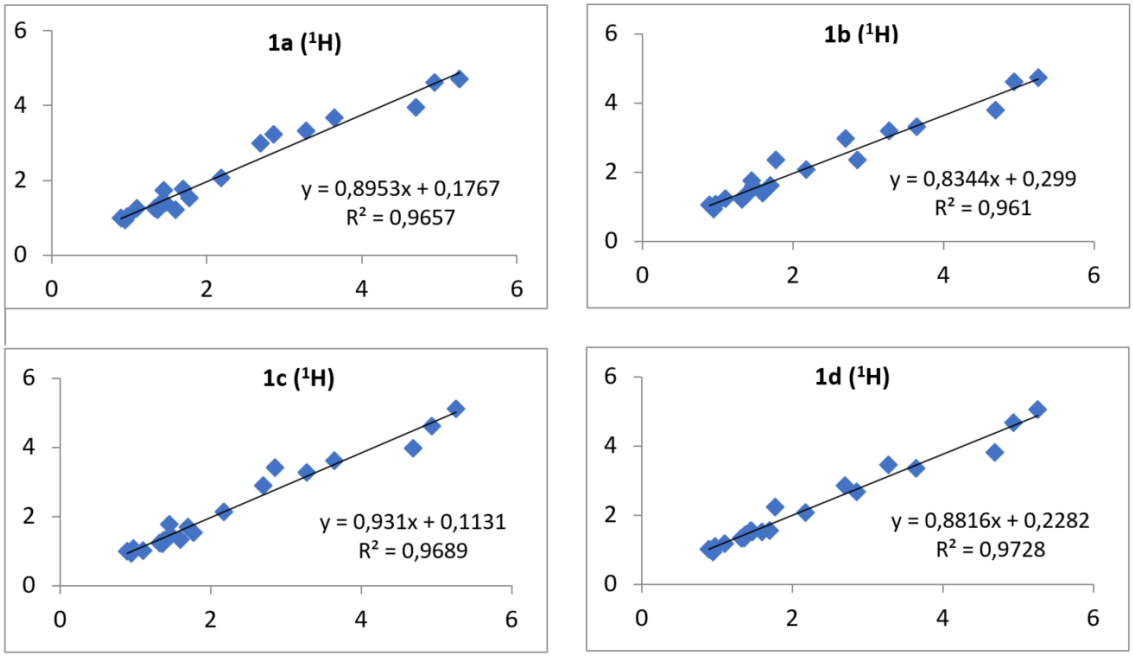
Comparison between calculated (MP1WMP91/6-311++ G(2d,p)) and experimental ^{1}H NMR data for 1d-diasteroisomer.

H	Calc. **1d**(ppm)	Exp (ppm)	ΔΔ	Scaled	ΔΔ scaled
2l	1.574997514	1.45	0.12499751	1.52767413	0.07767413
2h	1.326772664	1.33	0.00322734	1.24611237	0.08388763
3l	1.416773919	1.38	0.03677392	1.34820091	0.03179909
3h	1.336012838	1.36	0.02398716	1.25659351	0.10340649
4	3.346764271	3.65	0.30323573	3.53739142	0.11260858
5l	2.236484147	1.77	0.46648415	2.27799926	0.50799926
5h	1.51243747	1.6	0.08756253	1.45671219	0.14328781
6	2.660454802	2.86	0.1995452	2.75890971	0.10109029
9l	3.45840845	3.28	0.17840845	3.66402955	0.38402955
9h	2.863735234	2.7	0.16373523	2.98949096	0.28949096
10	3.828833071	4.69	0.86116693	4.08420267	0.60579733
14l	5.055493324	5.26	0.20450668	5.47560495	0.21560495
14h	4.669850714	4.94	0.27014929	5.03817005	0.09817005
15	2.081993148	2.18	0.09800685	2.10275992	0.07724008
16	1.10353097	0.98	0.12353097	0.99288903	0.01288903
17	1.164331855	1.1	0.06433185	1.06185555	0.03814445
7l	1.559644927	1.69	0.13035507	1.51025967	0.17974033
7h	1.515940717	1.47	0.04594072	1.46068593	0.00931407
8	1.025816206	0.89	0.13581621	0.90473708	0.01473708
1	0.954622209	0.94	0.01462221	0.82398163	0.11601837
		AVERAGE	0.1768192		0.16014648

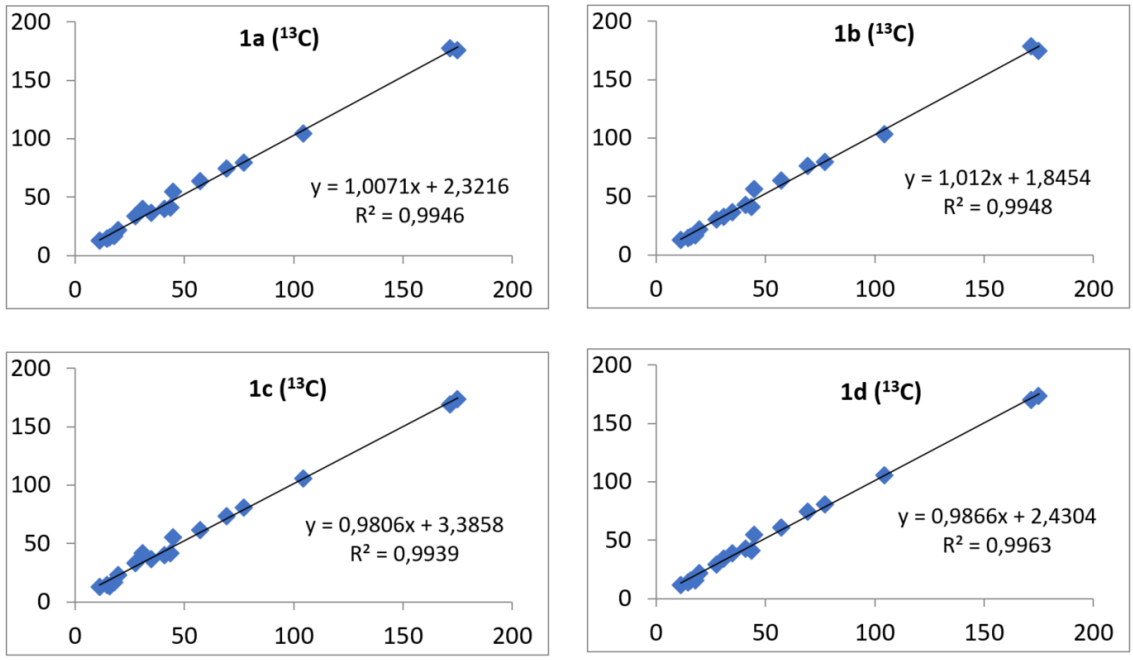
Comparison between calculated (MP1WMP91/6-311++ G(2d,p)) and experimental ^{13}C NMR data for 1d-diasteroisomer.

C	Calc. **1d**(ppm)	Exp (ppm)	ΔΔ	Scaled	ΔΔ Scaled
1	14.12543245	14.50	0.37	11.85	2.65
2	21.73886264	19.90	1.84	19.57	0.33
3	42.76503697	41.00	1.77	40.88	0.12
4	74.39168448	69.60	4.79	72.94	3.34
5	40.83128581	43.70	2.87	38.92	4.78
6	54.66869365	44.80	9.87	52.95	8.15
7	29.44015179	27.60	1.84	27.38	0.22
8	11.92007781	11.30	0.62	9.62	1.68
9	34.77044208	31.00	3.77	32.78	1.78
10	61.19143223	56.90	4.29	59.56	2.66
11	173.2036111	175.00	1.80	173.09	1.91
12	170.1357676	171.40	1.26	169.98	1.42
13	105.2267935	104.70	0.53	104.19	0.51
14	80.48004248	77.30	3.18	79.11	1.81
15	38.89450007	35.00	3.89	36.96	1.96
16	16.08990311	17.70	1.61	13.85	3.85
17	15.4743591	15.50	0.03	13.22	2.28
			2.61		2.32

*R^2-correlation graphs of diasteroisomers **1a**, **1b**, **1c**, and **1d** and the experimental ^1H chemical shifts of **1**.*



*R^2-correlation graphs of diasteroisomers **1a**, **1b**, **1c**, and **1d** and the experimental ^{13}C chemical shifts of **1**.*



DP4+ statistical comparation between the experimental and calculated values of diastereisomers **1a**, **1b**, **1c**, and **1d**

Position	sp2 carbon?	δ experimental (CD_3OD)	δ calc. **1a**	δ calc. **1b**	δ calc. **1c**	δ calc. **1d**
C1		14.5	12.1	12.4	11.2	11.9
C2		19.9	19.8	20.3	19.9	19.6
C3		41.0	37.5	41.1	37.5	40.9
C4		69.6	71.0	73.8	71.8	72.9
C5		43.7	38.6	38.7	39.5	38.9
C6		44.8	51.9	54.5	53.4	52.9
C7		27.6	30.8	27.9	30.6	27.4
C8		11.3	10.2	10.4	9.4	9.6
C9		31.0	37.5	30.6	39.0	32.8
C10		56.9	61.5	61.3	60.0	59.6
C11	x	175.0	171.8	171.0	173.9	173.1
C12	x	171.4	174.5	174.5	169.6	170.0
C13		104.7	101.2	100.8	103.9	104.2
C14		77.3	77.0	76.8	78.6	79.1
C15		35.0	33.9	34.6	34.2	37.0
C16		17.7	14.0	14.4	13.6	13.8
C17		15.5	13.6	14.0	10.7	13.2
H1		0.94	0.85	0.79	0.89	0.82
H2h		1.33	1.20	1.11	1.21	1.25
H2l		1.45	1.75	1.75	1.78	1.53
H3h		1.36	1.18	1.22	1.20	1.26
H3l		1.38	1.31	1.23	1.29	1.35
H4		3.65	3.90	3.60	3.76	3.54
H5h		1.60	1.18	1.34	1.32	1.46
H5l		1.77	1.51	2.45	1.53	2.28
H6		2.86	3.40	2.46	3.53	2.76
H7h		1.47	1.37	1.54	1.45	1.46
H7l		1.69	1.80	1.58	1.70	1.51
H8		0.89	0.90	0.93	0.95	0.90
H9h		2.70	3.14	3.19	3.00	2.99
H9l		3.28	3.53	3.47	3.38	3.66
H10		4.69	4.21	4.20	4.16	4.08
H14h		4.94	4.96	5.19	4.84	5.04
H14l		5.26	5.07	5.31	5.36	5.48
H15		2.18	2.12	2.12	2.18	2.10
H16		0.98	0.96	0.93	1.03	0.99
H17		1.10	1.20	1.13	0.96	1.06

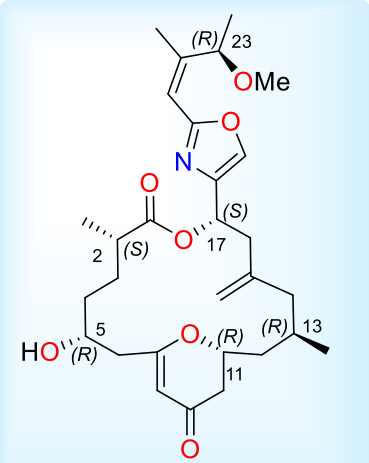
	1a	*1b*	*1c*	*1d*
	Isomer 1	Isomer 2	Isomer 3	Isomer 4
sDP4+ (H data)	0.15%	0.09%	14.87%	84.89%
sDP4+ (C data)	0.00%	1.52%	0.00%	98.47%
sDP4+ (all data)	0.00%	0.00%	0.00%	100.00%
uDP4+ (H data)	0.20%	0.13%	11.45%	88.22%
uDP4+ (C data)	2.54%	1.43%	0.04%	95.99%
uDP4+ (all data)	0.01%	0.00%	0.01%	99.99%
DP4+ (H data)	0.00%	0.00%	2.22%	97.78%
DP4+ (C data)	0.00%	0.02%	0.00%	99.98%
DP4+ (all data)	0.00%	0.00%	0.00%	100.00%

DP4+ statistical correlations of diasteroisomers **1a**, **1b**, **1c**, and **1d**

CÁLCULOS COMPUTACIONALES ENIGMAZOL C

Computational details. Conformational searches were performed by using the Macromodel program using the protocol of Daranas, Sarotti et al.[7] to all diasteroisomers. Thus 58 conformers for **2a-**2*S*5*R*11*R*13*R*17*S*23*R*, 64 for **2b-**2*S*5*R*11*S*13*S*17*S*23*S*, 60 for **2c-**2*S*5*R*11*S*13*S*17*S*23*R* and 62 for **2d-**2S5*R*11*R*13*R*17*S*23*S* were found within a 5.0 kcal/mol window, which were further classified by energy and frequencies using the B3LYP/6-31G(d) functional. Once the duplicates and conformers with imaginary frequencies were removed, a combination of MPW1PW91/6-31G(d,p) and polarizable continuum model was used for proton and carbon chemical shift calculations using acetonitrile as solvent. The sets of ^{1}H and ^{13}C chemical shifts were compared by the statistical DP4+ parameter developed by Sarotti and co-workers.[6,7] i*J*-DP4 was computed using the suggested combination MMFF-5 Kcal/mol conformational search, and B3LYP/6-31G(d,p) for chemical shifts and coupling constants (just the Contact Fermi contribution).

[6] Grimblat, N.; Zanardi, M. M.; Sarotti, A. M. *J. Org. Chem.* **2015**, *80*, 12526.
[7] Grimblat, N.; Gavín, J. A.; Hernández Daranas, A.; Sarotti, A. M. *Org. Lett.* **2019**, *21*, 4003.



2a-2*S*,5*R*,11*R*,13*R*,17*S*,23*R*

Calculated DFT energies of the 2a-diasteroisomer

Conformers **2a**	OPLS2008 Force Field Conformotional Search Relative Energy (kcal/mol)	B3LYP/6-31+G(d,p) DFT Energy (hartree)	Δ (DFT Energy) (kcal/mol)	% Population
2a6	0.858102294	-1710.461923	0	64.40
2a29	3.018642447	-1710.460565	0.852157753	15.26
2a1	0	-1710.459781	1.344125116	6.65
2a21	2.317638623	-1710.459393	1.587598759	4.40
2a31	3.215033461	-1710.459381	1.595128872	4.35
2a13	1.829134799	-1710.45839	2.216990678	1.52
2a11	1.531763862	-1710.458116	2.388928252	1.14
2a3	0.107002868	-1710.457939	2.499997414	0.94
2a22	2.380234226	-1710.456575	3.355920223	0.22
2a16	2.030736138	-1710.456348	3.498364855	0.17
2a2	0.080807839	-1710.456243	3.564253341	0.16
2a34	3.28166826	-1710.456065	3.675950012	0.13
2a4	0.739268642	-1710.455876	3.794549287	0.11
2a12	1.58874283	-1710.45573	3.886165658	0.09

14 conformers counting for the 99.54% of the DFT conformational population

DFT COORDINATES FOR CONFORMATIONAL SEARCH OF 2a

(2*S*, 5*R*, 11*R*, 13*R* , 17*S*, 23*R*)

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 1

C	-2.81439	1.21179	1.55029
C	-4.03916	1.38349	2.11606
C	-5.13199	2.03955	1.39955
C	-4.76046	2.52652	-0.00188
C	-3.68677	1.64237	-0.63154
O	-2.54456	1.52002	0.26034
C	-1.6505	0.54101	2.21751
C	-1.69819	-0.98207	1.92485
C	-0.42229	-1.70245	2.35852
C	-0.49393	-3.23245	2.19811
C	-0.90184	-3.78355	0.80356
C	0.15406	-3.47406	-0.24678
C	-1.14516	-5.2966	0.87114
O	0.07152	-2.1901	-0.6833
O	0.9892	-4.25826	-0.64907
C	1.09517	-1.76347	-1.63468
C	0.56498	-0.50076	-2.32164
C	2.39787	-1.52258	-0.92756
C	-0.71762	-0.7036	-3.12034
C	-3.18685	2.15557	-1.98003
C	-1.90611	1.50885	-2.55141
C	-1.97637	-0.03884	-2.5996
C	-0.72033	-1.43433	-4.24019
C	-1.6138	2.11051	-3.93416
O	-6.24015	2.2308	1.88059
O	-2.79123	-1.59409	2.60448
C	3.45239	-2.3683	-0.78175
O	4.41864	-1.72471	-0.06632

C	3.89783	-0.48361	0.20163
N	2.69327	-0.32605	-0.28376
C	4.76022	0.40124	0.95939
C	4.58526	1.71597	1.21116
C	3.38569	2.51866	0.72214
C	5.59143	2.46482	2.04648
C	2.30502	2.62682	1.80105
O	3.76402	3.85324	0.37957
C	4.42124	3.94982	-0.86961
H	-4.1991	1.1076	3.15302
H	-5.66016	2.55156	-0.62435
H	-4.38938	3.55849	0.08199
H	-4.0866	0.62287	-0.73759
H	-1.68166	0.69582	3.30046
H	-0.71942	0.96299	1.82314
H	-1.81198	-1.10305	0.83801
H	-0.23263	-1.48153	3.41773
H	0.41365	-1.28501	1.78674
H	-1.23189	-3.61527	2.91035
H	0.47445	-3.66783	2.47836
H	-1.82872	-3.28427	0.50131
H	-1.44555	-5.69588	-0.1029
H	-1.93849	-5.51622	1.59312
H	-0.23698	-5.82426	1.17785
H	1.22222	-2.57464	-2.35485
H	1.3642	-0.14255	-2.98194
H	0.43828	0.2671	-1.5536
H	-3.01368	3.23718	-1.89915
H	-4.0142	2.02946	-2.69325
H	-1.08534	1.78577	-1.8787
H	-2.16474	-0.41276	-1.58465
H	-2.82993	-0.34343	-3.22075

H	-1.62733	-1.59285	-4.81807
H	0.1814	-1.90928	-4.622
H	-0.67152	1.73505	-4.3445
H	-1.5491	3.20384	-3.88262
H	-2.40764	1.8563	-4.64891
H	-3.60503	-1.14689	2.31745
H	3.6453	-3.38786	-1.07193
H	5.64407	-0.09573	1.3522
H	2.95037	2.0238	-0.15461
H	6.38336	1.80293	2.40876
H	6.0491	3.28258	1.47918
H	5.10893	2.93222	2.91448
H	1.47262	3.22859	1.42262
H	1.93556	1.63121	2.06413
H	2.69381	3.111	2.70298
H	4.63401	5.00931	-1.03597
H	5.36896	3.38985	-0.88999
H	3.78595	3.57909	-1.68911

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 2

C	2.9488	-2.13843	-0.37577
C	4.01704	-2.67306	0.27003
C	5.3326	-2.04634	0.23379
C	5.4022	-0.79609	-0.64375
C	4.07484	-0.04111	-0.64365
O	2.97555	-0.92884	-0.98709
C	1.59779	-2.79225	-0.45598
C	0.75144	-2.63079	0.83723
C	0.47851	-1.16091	1.18958
C	-0.22303	-0.9906	2.54639
C	-0.09961	0.41505	3.19514

C	-0.90178	1.48221	2.45947
C	-0.51378	0.38516	4.67151
O	-0.38762	1.73373	1.22545
O	-1.87137	2.06119	2.89818
C	-1.07393	2.71836	0.4164
C	-0.16392	2.99812	-0.79444
C	-2.42761	2.22594	-0.00956
C	1.20277	3.56043	-0.43078
C	4.05273	1.12317	-1.62928
C	2.75435	1.95161	-1.73192
C	2.37953	2.60719	-0.37613
C	1.34491	4.86361	-0.16434
C	2.91825	2.9947	-2.84811
O	6.32174	-2.497	0.79711
O	-0.42754	-3.41587	0.75035
C	-3.60526	2.90032	-0.07592
O	-4.5496	2.05728	-0.59183
C	-3.89149	0.87668	-0.80317
N	-2.62353	0.94071	-0.48993
C	-4.69178	-0.20744	-1.35183
C	-4.45347	-1.53341	-1.2748
C	-3.29185	-2.1187	-0.48552
C	-5.36891	-2.51193	-1.96485
C	-3.74785	-3.13693	0.56034
O	-2.36078	-2.81634	-1.34637
C	-1.81031	-2.01844	-2.3926
H	3.92084	-3.63174	0.76847
H	6.21275	-0.15239	-0.28896
H	5.65418	-1.11	-1.66742
H	3.86988	0.30824	0.37897
H	1.71295	-3.86565	-0.63603
H	1.05219	-2.36045	-1.30342

H	1.32232	-3.08	1.66028
H	-0.10412	-0.68721	0.39104
H	1.44105	-0.63376	1.21789
H	0.22157	-1.69767	3.25979
H	-1.28012	-1.27106	2.46872
H	0.95531	0.71562	3.12234
H	-0.41616	1.37217	5.13313
H	0.11562	-0.32033	5.22412
H	-1.55806	0.07518	4.77834
H	-1.19482	3.62844	1.01226
H	-0.70183	3.71152	-1.42948
H	-0.07321	2.06978	-1.36838
H	4.29121	0.72233	-2.62374
H	4.88348	1.79065	-1.35846
H	1.94806	1.26426	-2.01838
H	2.15116	1.81417	0.34741
H	3.25453	3.15104	0.00588
H	2.30448	5.28958	0.11757
H	0.50681	5.5563	-0.21272
H	1.99923	3.56731	-3.00491
H	3.18492	2.51447	-3.79689
H	3.71201	3.71205	-2.60154
H	-0.93889	-3.17609	-0.05016
H	-3.93268	3.89203	0.19191
H	-5.59087	0.13482	-1.86044
H	-2.75462	-1.30574	0.00791
H	-6.07349	-2.00536	-2.63067
H	-4.78517	-3.23065	-2.55272
H	-5.94831	-3.09838	-1.24069
H	-2.88782	-3.46353	1.15121
H	-4.48317	-2.68297	1.23344
H	-4.19716	-4.01615	0.08898

H	-1.04413	-2.63091	-2.87525
H	-2.57137	-1.7504	-3.13658
H	-1.36373	-1.09435	-2.00479

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 3

C	-2.87036	1.16771	1.53203
C	-4.07766	1.40864	2.09838
C	-5.14858	2.07901	1.36943
C	-4.77235	2.5054	-0.05066
C	-3.72402	1.57659	-0.6597
O	-2.58558	1.4412	0.23402
C	-1.71415	0.49941	2.21724
C	-1.69416	-1.01997	1.91832
C	-0.38722	-1.68783	2.3672
C	-0.40241	-3.22274	2.24226
C	-0.78535	-3.82167	0.86115
C	0.26045	-3.49605	-0.19452
C	-0.97035	-5.34091	0.96363
O	0.13901	-2.22114	-0.64536
O	1.1159	-4.26174	-0.58941
C	1.14208	-1.77825	-1.6116
C	0.56562	-0.54476	-2.31313
C	2.44086	-1.48624	-0.9174
C	-0.71891	-0.80095	-3.09404
C	-3.21619	2.0585	-2.01841
C	-1.92977	1.40906	-2.57201
C	-1.98561	-0.13921	-2.58866
C	-0.71557	-1.57151	-4.18681
C	-1.63691	1.98479	-3.96584
O	-6.24547	2.33263	1.85015
O	-2.84427	-1.6651	2.46477

C	3.52868	-2.29026	-0.78125
O	4.47647	-1.60888	-0.07602
C	3.91053	-0.38852	0.19595
N	2.69588	-0.27856	-0.27716
C	4.74606	0.53084	0.94273
C	4.52567	1.83995	1.18811
C	3.2942	2.59577	0.7031
C	5.51069	2.63068	2.00975
C	2.21933	2.67486	1.79036
O	3.62247	3.93977	0.34664
C	4.26454	4.04884	-0.90952
H	-4.25693	1.13183	3.13076
H	-5.67544	2.53124	-0.66838
H	-4.37713	3.53096	-0.00497
H	-4.15186	0.56722	-0.74656
H	-1.77254	0.65874	3.30106
H	-0.78	0.95021	1.86114
H	-1.79724	-1.14926	0.83768
H	-0.19477	-1.43554	3.42212
H	0.4379	-1.25448	1.79112
H	-1.12916	-3.62156	2.95883
H	0.5786	-3.61648	2.5393
H	-1.73004	-3.36584	0.54623
H	-1.25234	-5.77223	-0.00197
H	-1.75811	-5.57489	1.68732
H	-0.04381	-5.82719	1.28381
H	1.28975	-2.59716	-2.31885
H	1.34602	-0.17155	-2.98774
H	0.42229	0.23077	-1.55596
H	-3.04674	3.14232	-1.96198
H	-4.03954	1.91442	-2.7329
H	-1.11391	1.7068	-1.9022

H	-2.17402	-0.49222	-1.56633
H	-2.83452	-0.46574	-3.20479
H	-1.62341	-1.76565	-4.75228
H	0.19163	-2.04458	-4.55793
H	-0.68996	1.60948	-4.36584
H	-1.58182	3.07949	-3.93639
H	-2.42604	1.70953	-4.67801
H	-2.7839	-1.61029	3.43287
H	3.75856	-3.3018	-1.07279
H	5.65078	0.06855	1.33039
H	2.86939	2.07839	-0.16569
H	6.32963	2.001	2.36943
H	5.93257	3.46076	1.43279
H	5.01849	3.08611	2.87864
H	1.36283	3.24315	1.41407
H	1.88785	1.66893	2.06472
H	2.59815	3.18036	2.68485
H	3.6348	3.64991	-1.71995
H	4.43921	5.11362	-1.08597
H	5.23069	3.52151	-0.93429

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 4

C	-1.12248	1.99234	1.33796
C	-1.37007	3.18039	1.94856
C	-1.94065	4.31122	1.21884
C	-2.18873	4.03327	-0.26463
C	-2.57052	2.57142	-0.48512
O	-1.55097	1.70003	0.08449
C	-0.37562	0.84412	1.95106
C	-1.30011	-0.34443	2.29873
C	-0.49765	-1.59421	2.66577

C	-1.32005	-2.89226	2.7257
C	-2.05052	-3.31722	1.42051
C	-1.08794	-3.39479	0.24091
C	-2.76415	-4.66137	1.61113
O	-0.9048	-2.17197	-0.31979
O	-0.53898	-4.40126	-0.15707
C	0.02887	-2.07008	-1.43834
C	-0.28604	-0.75272	-2.16722
C	1.44953	-2.1302	-0.95415
C	-1.64925	-0.71049	-2.83106
C	-2.75609	2.20035	-1.95854
C	-3.57957	0.93259	-2.29595
C	-2.87575	-0.41105	-1.97581
C	-1.76494	-0.93696	-4.14521
C	-4.98016	0.96629	-1.66189
O	-2.15163	5.40727	1.71943
O	-2.14486	-0.04416	3.41035
C	2.26127	-3.21738	-0.86696
O	3.47263	-2.80784	-0.39615
C	3.34718	-1.45335	-0.21145
N	2.15401	-1.01188	-0.51841
C	4.54769	-0.79191	0.26419
C	4.80917	0.5299	0.34695
C	3.82253	1.62063	-0.05171
C	6.14392	0.99904	0.86728
C	3.21265	2.30988	1.17123
O	4.4724	2.64278	-0.81214
C	4.76276	2.25969	-2.14327
H	-1.03515	3.34494	2.96679
H	-2.9785	4.69881	-0.62523
H	-1.27198	4.27287	-0.82335
H	-3.48919	2.37012	0.08429

H	0.1401	1.17834	2.85694
H	0.37713	0.50518	1.22837
H	-1.90871	-0.55188	1.41024
H	-0.04231	-1.42294	3.64993
H	0.32377	-1.70451	1.9508
H	-2.08389	-2.79712	3.50601
H	-0.6568	-3.71299	3.02913
H	-2.79117	-2.54689	1.17813
H	-3.33887	-4.93857	0.72119
H	-3.45375	-4.60524	2.46012
H	-2.04069	-5.45977	1.80096
H	-0.15959	-2.92474	-2.09302
H	0.49503	-0.62304	-2.92499
H	-0.17716	0.06774	-1.45091
H	-1.7652	2.14197	-2.42639
H	-3.26478	3.05262	-2.42865
H	-3.71818	0.96352	-3.38552
H	-2.60911	-0.43997	-0.91739
H	-3.61327	-1.20991	-2.13155
H	-2.73033	-0.93523	-4.64719
H	-0.89935	-1.13531	-4.77314
H	-5.60947	0.17029	-2.07571
H	-5.4849	1.92197	-1.84988
H	-4.94394	0.81563	-0.57602
H	-2.65052	0.75584	3.19293
H	2.13039	-4.27029	-1.05478
H	5.32047	-1.49458	0.56752
H	3.01625	1.17797	-0.64861
H	6.80396	0.15834	1.09897
H	6.639	1.65038	0.13926
H	6.0216	1.59799	1.77915
H	2.48837	3.06308	0.84624

H	2.70328	1.58015	1.80768
H	3.98464	2.81361	1.76165
H	5.21137	3.12853	-2.63236
H	5.47124	1.41855	-2.19215
H	3.85017	1.97264	-2.68851

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 6

C	-5.15153	-0.2362	0.5308
C	-5.91413	-0.42719	-0.57305
C	-6.08427	0.61384	-1.58352
C	-5.37976	1.92864	-1.24948
C	-4.09164	1.68556	-0.46939
O	-4.35931	0.85925	0.70686
C	-5.0998	-1.16864	1.70886
C	-3.69398	-1.71412	2.06036
C	-3.01154	-2.43301	0.88571
C	-1.7395	-3.17629	1.31829
C	-0.85681	-3.65282	0.14439
C	-0.41047	-2.46565	-0.69849
C	0.35728	-4.45884	0.64128
O	0.26832	-1.56642	0.05216
O	-0.64829	-2.31431	-1.87996
C	0.62049	-0.30233	-0.58905
C	0.55113	0.76106	0.51941
C	1.95851	-0.42314	-1.25244
C	0.41286	2.16895	-0.0292
C	-3.4282	2.96876	0.02565
C	-2.00445	2.82799	0.60657
C	-0.96199	2.58396	-0.51729
C	1.46173	2.99633	-0.09055
C	-1.64658	4.07024	1.43418

O	-6.77996	0.48588	-2.58096
O	-2.86472	-0.68886	2.60382
C	2.22134	-0.74673	-2.54657
O	3.5746	-0.79429	-2.70696
C	4.08982	-0.49193	-1.47071
N	3.16169	-0.27202	-0.57586
C	5.53651	-0.49163	-1.38611
C	6.30807	-0.12318	-0.34141
C	5.75159	0.37149	0.98842
C	7.80792	-0.23335	-0.43682
C	5.62356	-0.76845	2.00218
O	6.6078	1.35571	1.57192
C	6.48269	2.6335	0.9794
H	-6.49261	-1.33786	-0.67904
H	-5.16949	2.46881	-2.17728
H	-6.0675	2.54759	-0.65484
H	-3.40611	1.0976	-1.09642
H	-5.78475	-2.00139	1.52079
H	-5.47032	-0.63085	2.59206
H	-3.83059	-2.43229	2.87924
H	-2.77357	-1.68624	0.11557
H	-3.71806	-3.13455	0.42025
H	-2.01739	-4.05416	1.91785
H	-1.14726	-2.52163	1.96531
H	-1.45039	-4.27687	-0.53348
H	0.97859	-4.80004	-0.19405
H	0.02045	-5.34272	1.1941
H	0.98052	-3.85362	1.30685
H	-0.13239	-0.12135	-1.35977
H	1.4436	0.67494	1.14465
H	-0.31187	0.50343	1.14496
H	-4.09289	3.40755	0.78115

H	-3.40371	3.6779	-0.81351
H	-1.99689	1.96385	1.28459
H	-1.34665	1.81168	-1.19933
H	-0.87816	3.50222	-1.11355
H	1.37496	4.00041	-0.49943
H	2.44569	2.69367	0.25768
H	-0.62778	4.00306	1.82725
H	-2.3322	4.19042	2.28071
H	-1.70915	4.97903	0.82087
H	-2.98907	0.09205	2.03842
H	1.61111	-0.98368	-3.40305
H	6.01739	-0.84805	-2.2939
H	4.75559	0.8019	0.82731
H	8.117	-0.66471	-1.39337
H	8.28871	0.74427	-0.32161
H	8.205	-0.86215	0.37028
H	5.25979	-0.36833	2.9537
H	4.91414	-1.51683	1.63798
H	6.59111	-1.24943	2.18053
H	7.15779	3.30304	1.51942
H	6.76077	2.63235	-0.08602
H	5.45404	3.01844	1.06449

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 11

C	-2.81354	1.11231	1.56476
C	-4.04488	1.24737	2.126
C	-5.15354	1.87319	1.40653
C	-4.79224	2.37021	0.00584
C	-3.69088	1.51766	-0.61945
O	-2.54825	1.43119	0.27612
C	-1.63294	0.47469	2.23501

C	-1.63085	-1.04742	1.9332
C	-0.33494	-1.72979	2.36883
C	-0.36014	-3.26096	2.20681
C	-0.74987	-3.82247	0.81137
C	0.29806	-3.48352	-0.23817
C	-0.95074	-5.34183	0.87799
O	0.18262	-2.20188	-0.67355
O	1.15251	-4.24615	-0.6416
C	1.19034	-1.75197	-1.63264
C	0.6217	-0.50889	-2.32443
C	2.49027	-1.47151	-0.93492
C	-0.66131	-0.75119	-3.11124
C	-3.2027	2.04295	-1.96749
C	-1.90474	1.42966	-2.53677
C	-1.93406	-0.11942	-2.58331
C	-0.65319	-1.48659	-4.22798
C	-1.62658	2.03755	-3.91975
O	-6.26771	2.03381	1.88476
O	-2.70725	-1.69736	2.60404
C	3.55749	-2.29719	-0.76879
O	4.51573	-1.61988	-0.07364
C	3.97777	-0.37953	0.16094
N	2.76985	-0.25262	-0.3261
C	4.82815	0.54084	0.88717
C	4.62689	1.85736	1.10677
C	3.3944	2.60055	0.62367
C	5.63215	2.65765	1.89081
C	2.26795	2.53268	1.669
O	3.78828	3.95122	0.36503
C	2.93508	4.64388	-0.52126
H	-4.20096	0.96455	3.16169
H	-5.69038	2.36803	-0.61936

H	-4.4525	3.41293	0.08998
H	-4.05985	0.48659	-0.72492
H	-1.67521	0.62187	3.31862
H	-0.71323	0.92819	1.84896
H	-1.73545	-1.16564	0.84512
H	-0.15311	-1.50398	3.42837
H	0.48904	-1.28782	1.79816
H	-1.08668	-3.66684	2.91799
H	0.62084	-3.6667	2.48772
H	-1.69008	-3.34955	0.5078
H	-1.23882	-5.74881	-0.09656
H	-1.73834	-5.58397	1.59905
H	-0.02839	-5.84396	1.18525
H	1.33481	-2.56396	-2.34849
H	1.40605	-0.13483	-2.99366
H	0.4812	0.2614	-1.5613
H	-3.05857	3.12894	-1.88733
H	-4.0255	1.89447	-2.68165
H	-1.09224	1.72823	-1.8632
H	-2.1067	-0.49725	-1.56695
H	-2.78287	-0.44704	-3.19923
H	-1.56028	-1.67252	-4.79749
H	0.25813	-1.93823	-4.61518
H	-0.67319	1.68839	-4.32753
H	-1.59336	3.13245	-3.86987
H	-2.41119	1.75987	-4.63588
H	-3.53347	-1.27479	2.31534
H	3.76525	-3.32095	-1.03256
H	5.73189	0.07793	1.27508
H	3.03455	2.13821	-0.30447
H	6.45104	2.02809	2.25071
H	6.04251	3.46402	1.27427

H	5.1609	3.14396	2.75481
H	1.39114	3.09619	1.33153
H	1.96428	1.49307	1.82231
H	2.5989	2.95413	2.62412
H	3.38632	5.62541	-0.69073
H	2.84384	4.12202	-1.48725
H	1.9247	4.79115	-0.11103

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 12

C	-2.86076	1.05832	1.54703
C	-4.07548	1.2589	2.1131
C	-5.16813	1.89316	1.38392
C	-4.8075	2.32877	-0.03754
C	-3.72823	1.43478	-0.64465
O	-2.58529	1.34203	0.24887
C	-1.68375	0.42704	2.23181
C	-1.61508	-1.09041	1.92952
C	-0.28755	-1.71744	2.37663
C	-0.25457	-3.25175	2.25031
C	-0.61631	-3.86083	0.8682
C	0.41963	-3.50129	-0.18657
C	-0.7529	-5.38538	0.96878
O	0.25923	-2.23075	-0.6371
O	1.29815	-4.24055	-0.58142
C	1.24433	-1.76067	-1.61048
C	0.62447	-0.55203	-2.31806
C	2.53604	-1.42164	-0.92436
C	-0.65765	-0.85409	-3.08628
C	-3.23836	1.92883	-2.00546
C	-1.9332	1.31846	-2.55948
C	-1.94094	-0.23092	-2.57336

C	-0.63911	-1.6299	-4.17513
C	-1.65938	1.90039	-3.95466
O	-6.27215	2.11202	1.86525
O	-2.744	-1.77277	2.47465
C	3.63864	-2.20031	-0.76274
O	4.57184	-1.48023	-0.07642
C	3.9828	-0.26317	0.1577
N	2.76723	-0.18987	-0.32119
C	4.79767	0.69565	0.87483
C	4.54542	2.00523	1.08323
C	3.28484	2.69587	0.59447
C	5.51944	2.85053	1.85936
C	2.16256	2.59539	1.64173
O	3.62682	4.05769	0.322
C	2.74556	4.70951	-0.56821
H	-4.24581	0.97583	3.14529
H	-5.7113	2.322	-0.65469
H	-4.44791	3.36752	0.00531
H	-4.121	0.41102	-0.72779
H	-1.74789	0.58206	3.31592
H	-0.76416	0.90817	1.87753
H	-1.71401	-1.22039	0.84856
H	-0.10143	-1.45969	3.43131
H	0.52301	-1.25898	1.79938
H	-0.96898	-3.67427	2.9657
H	0.73813	-3.6143	2.54828
H	-1.57485	-3.43566	0.55204
H	-1.02207	-5.82397	0.0028
H	-1.53218	-5.64527	1.69283
H	0.18892	-5.84254	1.28722
H	1.41483	-2.57954	-2.31252
H	1.38789	-0.16116	-3.00199

H	0.46335	0.22582	-1.56703
H	-3.1033	3.01773	-1.95245
H	-4.05805	1.75683	-2.71795
H	-1.12627	1.64202	-1.89076
H	-2.1119	-0.58809	-1.54935
H	-2.78322	-0.58455	-3.18358
H	-1.54511	-1.85622	-4.73155
H	0.27962	-2.07567	-4.55157
H	-0.70048	1.55566	-4.35359
H	-1.6409	2.99647	-3.92817
H	-2.43866	1.59727	-4.66627
H	-2.68378	-1.72064	3.44291
H	3.88862	-3.21509	-1.0248
H	5.71981	0.27201	1.26441
H	2.94208	2.21081	-0.32851
H	6.36236	2.25614	2.22355
H	5.89783	3.66712	1.23586
H	5.0301	3.32532	2.71969
H	1.26461	3.12151	1.29975
H	1.89906	1.54635	1.80494
H	2.47811	3.03853	2.5923
H	3.15972	5.70526	-0.74889
H	2.67074	4.17491	-1.52856
H	1.73187	4.82321	-0.15576

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 13

C	-2.99356	-1.72242	-1.32555
C	-4.26873	-1.74369	-1.79086
C	-5.41559	-1.78886	-0.89134
C	-5.04397	-1.88266	0.58922
C	-3.73014	-1.16218	0.88487

O	-2.67905	-1.61576	-0.01181
C	-1.77211	-1.75769	-2.20137
C	-1.44323	-0.38718	-2.85437
C	-1.27513	0.73248	-1.8241
C	-1.00801	2.10695	-2.45306
C	-1.1328	3.3155	-1.48638
C	0.00779	3.37874	-0.47506
C	-1.22242	4.63958	-2.25386
O	0.02084	2.2883	0.33258
O	0.81115	4.28308	-0.38119
C	1.09935	2.20597	1.31168
C	0.6704	1.17026	2.36013
C	2.38841	1.83565	0.63809
C	-0.64487	1.49085	3.0556
C	-3.24471	-1.37818	2.31587
C	-1.89435	-0.74919	2.72219
C	-1.89968	0.794	2.56569
C	-0.67976	2.36453	4.06775
C	-1.55997	-1.17778	4.15914
O	-6.57981	-1.81114	-1.2687
O	-0.30161	-0.51762	-3.69858
C	3.4142	2.64696	0.26793
O	4.37623	1.87799	-0.31679
C	3.88138	0.59865	-0.28051
N	2.69666	0.53048	0.27067
C	4.73981	-0.41613	-0.85831
C	4.59133	-1.75689	-0.80422
C	3.43517	-2.44961	-0.09281
C	5.57923	-2.6543	-1.50397
C	2.30002	-2.78466	-1.06415
O	3.85234	-3.6819	0.49519
C	4.57053	-3.51575	1.70329

H	-4.45318	-1.79985	-2.85843
H	-5.85739	-1.46589	1.19076
H	-4.95274	-2.94706	0.85092
H	-3.8606	-0.0903	0.67461
H	-1.90482	-2.4857	-3.00756
H	-0.91762	-2.07733	-1.59291
H	-2.2608	-0.13127	-3.53904
H	-0.47084	0.46275	-1.13068
H	-2.18962	0.7892	-1.21987
H	-1.73938	2.2709	-3.25603
H	-0.02476	2.11925	-2.93882
H	-2.05435	3.17522	-0.90255
H	-1.31288	5.48958	-1.57176
H	-2.09357	4.63096	-2.91735
H	-0.32635	4.80005	-2.86181
H	1.20031	3.19433	1.7666
H	1.48016	1.12218	3.09791
H	0.63583	0.19116	1.87364
H	-3.189	-2.46151	2.48889
H	-4.03272	-0.99964	2.98299
H	-1.12765	-1.16175	2.05423
H	-2.04186	1.03875	1.50526
H	-2.76335	1.20111	3.10955
H	-1.60821	2.62189	4.57135
H	0.21824	2.86117	4.43016
H	-0.57947	-0.80736	4.47311
H	-1.55487	-2.27017	4.25121
H	-2.30008	-0.78578	4.86923
H	0.47081	-0.65225	-3.12449
H	3.58788	3.7096	0.31149
H	5.59284	-0.00316	-1.39138
H	3.03827	-1.78629	0.68547

H	6.33773	-2.0742	-2.03722
H	6.08132	-3.32317	-0.79665
H	5.07167	-3.30533	-2.22736
H	1.50323	-3.30919	-0.52742
H	1.89384	-1.86223	-1.49089
H	2.64931	-3.42987	-1.87668
H	4.80488	-4.51723	2.07385
H	5.51049	-2.96106	1.55954
H	3.97036	-2.98507	2.45867

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 16

C	-3.01764	1.78456	1.03523
C	-4.12859	2.35154	1.57267
C	-5.28349	2.69913	0.74194
C	-5.11485	2.37747	-0.7466
C	-4.21571	1.15859	-0.93882
O	-2.95329	1.37224	-0.2522
C	-1.75806	1.43517	1.77301
C	-1.72921	-0.08525	2.06846
C	-0.3554	-0.58209	2.51522
C	-0.32924	-2.08548	2.84433
C	-0.76114	-3.06615	1.71711
C	0.27933	-3.15053	0.60817
C	-1.02098	-4.46532	2.29031
O	0.26993	-2.05263	-0.19466
O	1.04281	-4.08034	0.44609
C	1.27815	-2.03491	-1.25491
C	0.84178	-1.01501	-2.31634
C	2.62296	-1.6991	-0.67837
C	-0.55735	-1.2142	-2.88345
C	-3.90937	0.82215	-2.39661

C	-3.0685	-0.45039	-2.68755
C	-1.59149	-0.2851	-2.27911
C	-0.7816	-2.10132	-3.85795
C	-3.70098	-1.7129	-2.07858
O	-6.289	3.24267	1.17652
O	-2.66525	-0.41802	3.09152
C	3.6473	-2.53463	-0.3623
O	4.66727	-1.78524	0.14605
C	4.20626	-0.49272	0.12207
N	2.99162	-0.39864	-0.35372
C	5.12528	0.50621	0.62969
C	4.99775	1.84943	0.5819
C	3.80534	2.56338	-0.04388
C	6.05043	2.72941	1.205
C	2.75093	2.9221	1.00645
O	4.20465	3.78559	-0.66683
C	4.82823	3.5999	-1.92297
H	-4.14063	2.64593	2.61655
H	-6.10228	2.21462	-1.18872
H	-4.66982	3.25301	-1.24167
H	-4.68781	0.29819	-0.44176
H	-1.69071	1.99017	2.71358
H	-0.89974	1.70157	1.1445
H	-1.99683	-0.59908	1.13382
H	-0.05685	-0.02822	3.41542
H	0.36952	-0.34499	1.72916
H	-1.00442	-2.25943	3.68847
H	0.67765	-2.36249	3.18368
H	-1.68717	-2.68952	1.26772
H	-1.32168	-5.16831	1.50731
H	-1.81807	-4.41923	3.0395
H	-0.11948	-4.86624	2.76357

H	1.3089	-3.04001	-1.6812
H	1.58494	-1.07926	-3.12041
H	0.93689	-0.01333	-1.88465
H	-3.42222	1.69275	-2.85593
H	-4.88178	0.71197	-2.89597
H	-3.09793	-0.55716	-3.78152
H	-1.27099	0.74189	-2.51534
H	-1.50203	-0.35349	-1.19018
H	-1.76496	-2.2666	-4.28751
H	0.02462	-2.70426	-4.27033
H	-3.1585	-2.61152	-2.38565
H	-4.74699	-1.82701	-2.38897
H	-3.67769	-1.68271	-0.98238
H	-3.53518	-0.08243	2.81817
H	3.78806	-3.60233	-0.39935
H	6.00625	0.07824	1.10205
H	3.34028	1.90651	-0.78913
H	6.83501	2.13649	1.68387
H	6.51228	3.38803	0.46142
H	5.60788	3.39075	1.96097
H	1.93064	3.46518	0.52617
H	2.35518	2.01243	1.46736
H	3.17259	3.56286	1.78804
H	5.0586	4.59457	-2.31422
H	5.763	3.02317	-1.84655
H	4.16244	3.08185	-2.63079

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 21

C	-5.34662	0.66707	0.27596
C	-5.75507	0.7912	1.56222
C	-5.80335	-0.35161	2.471
C	-5.41017	-1.67983	1.82467
C	-4.35122	-1.47853	0.74576
O	-4.79673	-0.47686	-0.22212
C	-5.47385	1.73834	-0.7712
C	-4.15073	2.15617	-1.45814
C	-3.07683	2.63857	-0.4694
C	-1.87096	3.26296	-1.18591
C	-0.64413	3.49755	-0.27826
C	-0.165	2.18064	0.31765
C	0.49515	4.19912	-1.04019
O	0.14695	1.29332	-0.65471
O	-0.09361	1.93247	1.50506
C	0.46193	-0.06916	-0.23024
C	-0.02193	-0.98262	-1.36749
C	1.92633	-0.1872	0.0733
C	-0.2196	-2.41934	-0.92069
C	-4.02975	-2.7485	-0.03913
C	-2.79067	-2.69182	-0.95851
C	-1.47788	-2.72611	-0.13172
C	0.68644	-3.3626	-1.19964
C	-2.83476	-3.83946	-1.97698
O	-6.18606	-0.2822	3.63031
O	-3.65988	1.11826	-2.30362
C	2.55491	0.04987	1.25536
O	3.89518	-0.14896	1.07018
C	4.02151	-0.49921	-0.24986
N	2.87444	-0.53694	-0.8764
C	5.31033	-0.81428	-0.83185

C	6.55387	-0.68203	-0.32313
C	6.87065	-0.13574	1.06639
C	7.74282	-1.12749	-1.1377
C	7.05892	-1.26064	2.08811
O	8.08273	0.6196	1.05713
C	7.93766	1.91221	0.49993
H	-6.1457	1.73869	1.91574
H	-5.04296	-2.36061	2.59828
H	-6.31212	-2.13228	1.38714
H	-3.44853	-1.05953	1.21299
H	-5.94811	2.61284	-0.31474
H	-6.14693	1.37256	-1.5585
H	-4.39655	2.9831	-2.13696
H	-2.75762	1.78265	0.1415
H	-3.51687	3.36334	0.23002
H	-2.16679	4.22853	-1.61897
H	-1.57878	2.61549	-2.01872
H	-0.93355	4.11198	0.582
H	1.36006	4.37466	-0.39108
H	0.15298	5.1695	-1.41653
H	0.82328	3.59605	-1.89248
H	-0.10008	-0.24603	0.68991
H	0.69736	-0.93012	-2.18841
H	-0.96555	-0.55759	-1.73007
H	-4.91923	-2.99808	-0.63209
H	-3.90112	-3.56564	0.68446
H	-2.8256	-1.74781	-1.51907
H	-1.5615	-2.00912	0.69819
H	-1.38795	-3.71825	0.33028
H	0.55973	-4.39089	-0.86854
H	1.59137	-3.13315	-1.75543
H	-1.94924	-3.83216	-2.61961

H	-3.72186	-3.7657	-2.61643
H	-2.86919	-4.81165	-1.46739
H	-3.74202	0.29175	-1.7983
H	2.23113	0.36033	2.23541
H	5.19819	-1.21775	-1.83492
H	6.05248	0.51086	1.40505
H	7.4315	-1.56675	-2.08968
H	8.42289	-0.29347	-1.34236
H	8.3345	-1.87342	-0.59171
H	7.31404	-0.83038	3.06156
H	6.13805	-1.8429	2.18675
H	7.8703	-1.93166	1.78805
H	8.91313	2.40059	0.57212
H	7.6322	1.88142	-0.55715
H	7.1967	2.50896	1.05466

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 22

C	2.91005	-1.90614	1.02439
C	4.14748	-2.0041	1.57422
C	5.35854	-1.83577	0.7791
C	5.09984	-1.61516	-0.71192
C	3.78819	-0.86918	-0.94844
O	2.68999	-1.52469	-0.25567
C	1.62748	-2.15521	1.76924
C	1.20617	-0.97354	2.68392
C	1.04596	0.33443	1.91594
C	0.70945	1.53446	2.81291
C	0.89212	2.92646	2.14928
C	-0.16696	3.2103	1.08912
C	0.8991	4.04943	3.19283
O	-0.08668	2.3306	0.05956

O	-0.9842	4.10548	1.13656
C	-1.10044	2.43816	-0.9829
C	-0.57736	1.65014	-2.19226
C	-2.41413	1.91403	-0.48414
C	0.76832	2.1308	-2.71559
C	3.4143	-0.775	-2.42494
C	2.07351	-0.09979	-2.78543
C	2.00997	1.3702	-2.29265
C	0.84027	3.19543	-3.52216
C	1.85702	-0.20462	-4.30284
O	6.49145	-1.92008	1.23485
O	-0.05016	-1.2588	3.29975
C	-3.51029	2.6139	-0.09053
O	-4.4658	1.72388	0.29912
C	-3.89245	0.48699	0.12927
N	-2.67053	0.55688	-0.33109
C	-4.74142	-0.63108	0.4926
C	-4.49862	-1.95235	0.36304
C	-3.21063	-2.52975	-0.21057
C	-5.52984	-2.95264	0.81949
C	-2.27814	-3.04566	0.88821
O	-3.48888	-3.6425	-1.06692
C	-4.00757	-3.26702	-2.32828
H	4.2563	-2.28554	2.6163
H	5.9408	-1.065	-1.14464
H	5.06353	-2.59943	-1.20165
H	3.86769	0.13253	-0.50165
H	1.73688	-3.05323	2.39033
H	0.82447	-2.33767	1.04892
H	1.98081	-0.84407	3.4583
H	0.27865	0.19766	1.14935
H	1.98744	0.53613	1.39054

H	1.37389	1.51768	3.68817
H	-0.31002	1.43809	3.2038
H	1.85914	2.91683	1.62518
H	1.0282	5.02843	2.72263
H	1.7157	3.89561	3.90634
H	-0.04465	4.07371	3.74698
H	-1.2035	3.49763	-1.23069
H	-1.33802	1.74366	-2.97643
H	-0.54367	0.59213	-1.91595
H	3.41041	-1.79427	-2.83433
H	4.2333	-0.24267	-2.93008
H	1.2778	-0.66614	-2.28528
H	2.06356	1.37727	-1.19649
H	2.89531	1.9051	-2.66368
H	1.79044	3.56866	-3.8961
H	-0.04823	3.7396	-3.83661
H	0.88742	0.20545	-4.60035
H	1.90036	-1.24886	-4.63411
H	2.62917	0.35245	-4.84984
H	0.05839	-2.04092	3.86331
H	-3.7434	3.66214	0.00083
H	-5.68702	-0.31542	0.92714
H	-2.68681	-1.7531	-0.77981
H	-6.41428	-2.45832	1.23161
H	-5.84001	-3.60199	-0.00628
H	-5.11855	-3.61703	1.59037
H	-1.39644	-3.49756	0.42141
H	-1.953	-2.23321	1.5449
H	-2.76998	-3.81643	1.49134
H	-4.1404	-4.18712	-2.90407
H	-4.97908	-2.75536	-2.24735
H	-3.3145	-2.60311	-2.86826

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 29

C	-5.53223	0.55021	-0.23423
C	-6.17648	0.76053	0.93877
C	-6.27878	-0.27716	1.9606
C	-5.66301	-1.6172	1.5595
C	-4.46662	-1.44036	0.62839
O	-4.82338	-0.5825	-0.50296
C	-5.50887	1.51361	-1.38876
C	-4.09103	2.01296	-1.76829
C	-3.35485	2.64243	-0.57625
C	-1.98102	3.21729	-0.95398
C	-1.00013	3.33732	0.24508
C	-0.65898	1.9277	0.7064
C	0.2316	4.17873	-0.1148
O	0.39312	1.41522	0.02809
O	-1.29626	1.30296	1.53474
C	0.68672	0.00209	0.24508
C	0.06317	-0.80365	-0.91549
C	2.17214	-0.14182	0.34021
C	-0.13008	-2.2609	-0.54223
C	-3.97055	-2.76067	0.04188
C	-2.65359	-2.71487	-0.763
C	-1.42147	-2.60018	0.17613
C	0.80434	-3.17972	-0.81023
C	-2.54936	-3.95035	-1.66833
O	-6.86055	-0.12619	3.02591
O	-3.32585	0.96738	-2.36717
C	2.92675	-0.3695	1.44681
O	4.23912	-0.42352	1.06474
C	4.21837	-0.21469	-0.29124
N	3.00965	-0.05166	-0.76136
C	5.43445	-0.21127	-1.07884

C	6.72723	-0.25097	-0.6919
C	7.19855	-0.31694	0.75837
C	7.81559	-0.27287	-1.736
C	7.49406	-1.75572	1.19182
O	8.40537	0.42397	0.94208
C	8.20612	1.82413	0.99208
H	-6.69361	1.69762	1.11125
H	-5.3663	-2.158	2.4631
H	-6.44101	-2.21345	1.06009
H	-3.6672	-0.90828	1.16306
H	-6.15185	2.36545	-1.14618
H	-5.93234	1.01758	-2.27207
H	-4.21319	2.76497	-2.55841
H	-3.23613	1.87895	0.20085
H	-3.98252	3.42884	-0.13393
H	-2.10088	4.21507	-1.39654
H	-1.52036	2.58431	-1.72098
H	-1.53095	3.79895	1.08616
H	0.93614	4.23839	0.72173
H	-0.07748	5.19843	-0.37038
H	0.76242	3.75397	-0.97133
H	0.22978	-0.27894	1.19584
H	0.70625	-0.69756	-1.79353
H	-0.89955	-0.33902	-1.15779
H	-4.77529	-3.15165	-0.59443
H	-3.85886	-3.47362	0.87075
H	-2.67831	-1.83024	-1.41364
H	-1.61873	-1.82843	0.93386
H	-1.3124	-3.55035	0.71607
H	0.68755	-4.21808	-0.5086
H	1.71992	-2.92414	-1.33749
H	-1.60733	-3.95477	-2.22444

H	-3.3726	-3.97775	-2.39136
H	-2.59401	-4.87383	-1.07557
H	-3.4847	0.1724	-1.83026
H	2.71956	-0.51489	2.49528
H	5.20944	-0.17157	-2.14147
H	6.42586	0.09538	1.41791
H	7.39776	-0.28555	-2.7466
H	8.47823	0.59421	-1.64124
H	8.45505	-1.15693	-1.61703
H	7.85671	-1.75818	2.22441
H	6.58783	-2.36563	1.13115
H	8.26513	-2.20555	0.55807
H	9.18545	2.27828	1.16482
H	7.78929	2.22226	0.05435
H	7.5308	2.10549	1.8153

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 31

C	-3.08183	2.18749	-0.30501
C	-4.13593	2.97274	0.04557
C	-5.4724	2.75888	-0.50705
C	-5.55898	1.61076	-1.51389
C	-4.53721	0.51995	-1.20373
O	-3.20484	1.09104	-1.08883
C	-1.68775	2.34198	0.2267
C	-1.54022	1.52617	1.53882
C	-0.09238	1.46015	2.02154
C	0.07733	0.7263	3.3647
C	-0.50403	-0.71198	3.46536
C	0.21782	-1.65915	2.51939
C	-0.41033	-1.2342	4.90449
O	-0.25656	-1.55712	1.24909

O	1.12426	-2.40373	2.83032
C	0.44821	-2.32685	0.23101
C	-0.47077	-2.39315	-0.99437
C	1.76023	-1.67338	-0.09054
C	-1.81768	-3.06278	-0.74715
C	-4.49485	-0.58969	-2.25367
C	-3.28748	-1.55137	-2.21857
C	-3.04976	-2.18339	-0.8235
C	-1.89884	-4.37141	-0.48523
C	-3.46483	-2.62245	-3.30531
O	-6.43959	3.45615	-0.2336
O	-2.31694	2.0996	2.58735
C	3.01405	-2.07076	0.24659
O	3.90033	-1.16603	-0.27084
C	3.12278	-0.22839	-0.89986
N	1.84446	-0.49571	-0.82202
C	3.70648	0.9057	-1.58682
C	4.9842	1.34074	-1.62246
C	6.15078	0.67286	-0.89917
C	5.33746	2.54767	-2.45522
C	6.92029	-0.27381	-1.82511
O	7.088	1.64284	-0.43116
C	6.66314	2.32156	0.73591
H	-3.97815	3.83409	0.68602
H	-6.57553	1.20563	-1.51173
H	-5.37051	2.02093	-2.51688
H	-4.76124	0.0973	-0.21297
H	-1.46809	3.39363	0.43607
H	-0.97475	1.96712	-0.51584
H	-1.88383	0.50335	1.32849
H	0.28351	2.48497	2.14523
H	0.50736	0.98939	1.23538

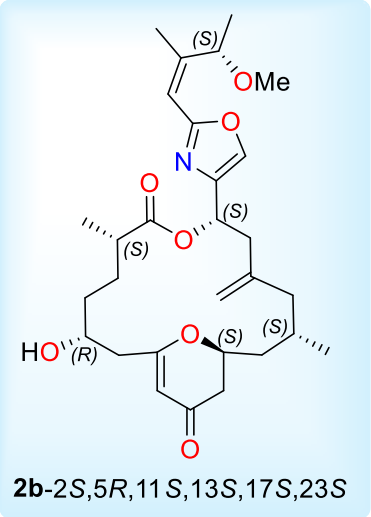
H	-0.41462	1.31708	4.14427
H	1.14501	0.68849	3.61895
H	-1.55622	-0.67508	3.16277
H	-0.83907	-2.2378	4.99314
H	-0.95372	-0.5673	5.58193
H	0.63262	-1.29061	5.23048
H	0.63144	-3.32321	0.64008
H	0.08131	-2.93533	-1.77209
H	-0.59815	-1.3723	-1.36497
H	-4.52988	-0.12856	-3.25002
H	-5.4277	-1.16205	-2.14775
H	-2.40273	-0.9543	-2.47012
H	-2.93818	-1.37738	-0.08664
H	-3.93371	-2.76845	-0.53467
H	-2.85239	-4.86026	-0.30235
H	-1.01624	-5.0063	-0.4364
H	-2.59498	-3.28389	-3.36024
H	-3.60617	-2.16449	-4.29143
H	-4.34255	-3.24904	-3.09884
H	-3.24175	2.12561	2.28966
H	3.42304	-2.88611	0.82064
H	2.95325	1.45423	-2.14657
H	5.77731	0.09862	-0.04326
H	4.4671	2.92718	-2.99786
H	5.74418	3.35442	-1.83579
H	6.11952	2.30337	-3.18531
H	7.76614	-0.7069	-1.28232
H	6.26859	-1.08135	-2.17175
H	7.31128	0.26204	-2.69604
H	7.46669	3.00867	1.01386
H	5.74082	2.89992	0.57252
H	6.48736	1.62128	1.56739

Compound 2a: Isomer 2S, 5R, 11R, 13R, 17S, 23R conformer 34

C	-2.95152	-1.90326	-1.06289
C	-4.10899	-1.95372	-1.77485
C	-5.4062	-1.70198	-1.15624
C	-5.33485	-1.4191	0.34518
C	-4.02939	-0.71285	0.69851
O	-2.89064	-1.47446	0.21572
C	-1.61813	-2.332	-1.60931
C	-0.53281	-1.23449	-1.72373
C	-1.08964	0.11019	-2.22403
C	-0.0347	1.04297	-2.85373
C	-0.33235	2.56003	-2.66954
C	0.34802	3.0717	-1.40305
C	0.09781	3.40404	-3.87412
O	0.10046	2.25227	-0.34586
O	1.05931	4.04963	-1.33131
C	0.94566	2.42497	0.82418
C	0.27421	1.67026	1.98118
C	2.31751	1.90143	0.51784
C	-1.05067	2.27582	2.42559
C	-3.82878	-0.49918	2.19438
C	-2.49504	0.14779	2.62396
C	-2.32181	1.56371	2.01541
C	-1.07439	3.3993	3.15108
C	-2.41581	0.17068	4.15756
O	-6.47192	-1.76348	-1.75605
O	0.08848	-1.12367	-0.44747
C	3.49775	2.56967	0.50959
O	4.48642	1.68475	0.19378
C	3.8542	0.48307	0.01163
N	2.55703	0.57073	0.18018

C	4.74715	-0.61419	-0.31425
C	4.53244	-1.94565	-0.25567
C	3.22797	-2.5937	0.19145
C	5.64541	-2.89349	-0.62495
C	2.54252	-3.36041	-0.94002
O	3.48317	-3.54654	1.22923
C	3.73358	-2.95915	2.49302
H	-4.09454	-2.27209	-2.81123
H	-6.19831	-0.81503	0.64004
H	-5.40089	-2.37683	0.88196
H	-3.9994	0.24669	0.16178
H	-1.78838	-2.76486	-2.60012
H	-1.20844	-3.1218	-0.96759
H	0.20026	-1.61171	-2.45818
H	-1.55925	0.59424	-1.36269
H	-1.88597	-0.06918	-2.95809
H	0.03213	0.83389	-3.92847
H	0.96154	0.82455	-2.44754
H	-1.41577	2.67951	-2.52361
H	-0.08917	4.46712	-3.70092
H	-0.4541	3.09161	-4.76698
H	1.16854	3.28627	-4.07257
H	1.01102	3.49269	1.04723
H	0.98519	1.67916	2.81586
H	0.1511	0.62749	1.67439
H	-3.92152	-1.47462	2.6908
H	-4.66763	0.11408	2.55439
H	-1.68961	-0.49048	2.24118
H	-2.32921	1.47986	0.92082
H	-3.18575	2.18125	2.29788
H	-2.00814	3.85849	3.46561
H	-0.1618	3.90797	3.45641

H	-1.46202	0.57809	4.50635
H	-2.52435	-0.8393	4.57011
H	-3.2134	0.79326	4.58477
H	0.83868	-0.49841	-0.48113
H	3.78699	3.596	0.66782
H	5.73394	-0.26435	-0.60968
H	2.53889	-1.82804	0.56323
H	6.58815	-2.36599	-0.79576
H	5.78883	-3.63979	0.16326
H	5.39913	-3.44996	-1.53894
H	1.58463	-3.7462	-0.58271
H	2.35698	-2.70299	-1.79521
H	3.15793	-4.20349	-1.26944
H	3.8689	-3.78077	3.20149
H	4.64132	-2.33678	2.49248
H	2.88703	-2.33741	2.82221



2b-2*S*,5*R*,11*S*,13*S*,17*S*,23*S*

Calculated DFT energies of the 2b-diasteroisomer

Conformers **2b**	OPLS2008 Force Field Conformotional Search Relative Energy (kcal/mol)	B3LYP/6-31+G(d,p) DFT Energy (hartree)	Δ (DFT Energy) (kcal/mol)	% Population
2b4	1.495960803	-1710.456029	0	19.95
2b3	1.322944551	-1710.455954	0.0470632	18.43
2b1	0	-1710.455935	0.05898588	18.06
2b18	2.732791587	-1710.455096	0.58546626	7.42
2b8	1.785062141	-1710.454916	0.69841795	6.13
2b2	0.431716061	-1710.454814	0.76242391	5.50
2b22	3.070650096	-1710.454601	0.89608341	4.39
2b17	2.713217017	-1710.454415	1.01280016	3.60
2b21	2.994502868	-1710.454414	1.01342767	3.60
2b27	3.242160612	-1710.453776	1.41377866	1.83
2b12	2.148183556	-1710.453697	1.4633519	1.68
2b10	2.04292543	-1710.453516	1.5769311	1.39
2b11	2.075262906	-1710.453341	1.68674524	1.15
2b6	1.530640535	-1710.453309	1.70682554	1.12
2b19	2.852868069	-1710.453155	1.80346199	0.95
2b56	4.674689293	-1710.452849	1.99547986	0.68
2b42	4.111089866	-1710.45258	2.16427989	0.51
2b32	3.536567878	-1710.452455	2.24271856	0.45
2b37	3.785994264	-1710.452396	2.27974162	0.42
2b55	4.660994264	-1710.45214	2.44038402	0.32
2b47	4.423064054	-1710.452031	2.50878255	0.29
2b23	3.084799235	-1710.451875	2.60667401	0.24
2b46	4.35250956	-1710.451748	2.6863677	0.21
2b52	4.594144359	-1710.451529	2.82379226	0.17
2b15	2.470960803	-1710.451487	2.85014765	0.16
2b28	3.356046845	-1710.451399	2.90536848	0.15

2b5	1.508819312	-1710.451364	2.92733131	0.14
2b63	4.930760038	-1710.451278	2.98129712	0.13
2b16	2.509703633	-1710.451185	3.03965549	0.12
2b9	1.942853728	-1710.451176	3.04530307	0.12
2b57	4.736304971	-1710.451132	3.07291349	0.11
2b13	2.355066922	-1710.451021	3.14256703	0.10

32 conformers counting for the 99.54% of the DFT conformational population

DFT COORDINATES FOR CONFORMATIONAL SEARCH OF 2b

(2*S*, 5*R*, 11*S*, 13*S* , 17*S*, 23*S*)

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 1

C	-2.7622	1.47339	0.93925
C	-3.73055	2.32989	1.35375
C	-5.02562	2.40471	0.67885
C	-5.20834	1.39109	-0.45396
C	-3.88435	1.08016	-1.14898
O	-2.87568	0.70807	-0.17165
C	-1.47093	1.19493	1.65369
C	-1.42775	-0.25262	2.19889
C	-0.02543	-0.66238	2.64639
C	0.07092	-2.12399	3.1162
C	-0.28689	-3.21873	2.07283
C	0.71631	-3.24607	0.92742
C	-0.35465	-4.59943	2.73863
O	0.45508	-2.28699	0.00019
O	1.64775	-4.01942	0.83824
C	1.37386	-2.22347	-1.13629
C	0.66047	-1.48268	-2.27808
C	2.6547	-1.55016	-0.73799
C	-0.66458	-2.10069	-2.69273
C	-3.99053	-0.04051	-2.18409
C	-2.68874	-0.5075	-2.88788

C	-1.9234	-1.56028	-2.03703
C	-0.71036	-3.07892	-3.6041
C	-1.81353	0.67013	-3.34197
O	-5.92419	3.16194	1.01863
O	-2.29582	-0.40011	3.32177
C	3.83859	-2.12124	-0.39136
O	4.72965	-1.12495	-0.12173
C	4.03033	0.04058	-0.31204
N	2.7934	-0.16766	-0.684
C	4.78523	1.25905	-0.09841
C	4.32864	2.52954	-0.09821
C	2.87008	2.90304	-0.33419
C	5.28751	3.67516	0.09831
C	2.60639	3.23188	-1.80586
O	2.50338	4.05748	0.42331
C	2.27764	3.78636	1.79282
H	-3.57203	2.94733	2.23092
H	-5.62901	0.47081	-0.02217
H	-5.94053	1.78093	-1.1673
H	-3.51118	1.99887	-1.62362
H	-0.6464	1.33217	0.94258
H	-1.33922	1.89646	2.48349
H	-1.7494	-0.917	1.3857
H	0.27583	-0.01042	3.47734
H	0.66883	-0.47768	1.81985
H	-0.60504	-2.25895	3.96748
H	1.08723	-2.31616	3.48477
H	-1.2658	-2.98057	1.6421
H	-0.6248	-5.3772	2.01707
H	-1.10465	-4.59454	3.53642
H	0.61327	-4.87154	3.17
H	1.58677	-3.25403	-1.4293
H	1.35966	-1.48277	-3.12304

H	0.53018	-0.43819	-1.97998
H	-4.47836	-0.90545	-1.71446
H	-4.68877	0.32861	-2.94782
H	-3.01372	-1.03274	-3.79755
H	-1.67102	-1.1263	-1.06818
H	-2.61539	-2.39015	-1.84213
H	-1.64753	-3.55177	-3.88975
H	0.18507	-3.44936	-4.09883
H	-2.39704	1.39116	-3.92795
H	-1.37557	1.20439	-2.49098
H	-0.99285	0.32048	-3.97617
H	-3.18635	-0.12551	3.0493
H	4.17923	-3.13678	-0.27384
H	5.8451	1.08188	0.06767
H	2.23012	2.0586	-0.04904
H	6.3189	3.32212	0.18781
H	5.23444	4.37651	-0.74425
H	5.03794	4.25825	0.99144
H	3.23996	4.05773	-2.14608
H	1.56069	3.53068	-1.93
H	2.8009	2.35343	-2.42758
H	1.47308	3.04655	1.93001
H	3.17823	3.40964	2.30185
H	1.977	4.72863	2.25886

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 2

C	1.93844	-2.17962	0.71187
C	3.01649	-2.88212	1.15156
C	4.0314	-3.37844	0.22732
C	3.69727	-3.15818	-1.25017
C	2.90355	-1.87012	-1.48395
O	1.7672	-1.79169	-0.5719

C	0.83847	-1.65717	1.59021
C	1.16278	-0.22159	2.07575
C	-0.05366	0.47944	2.67874
C	0.23884	1.89811	3.19935
C	0.88708	2.89804	2.20256
C	-0.01915	3.16984	1.00869
C	1.22647	4.2173	2.90902
O	0.11553	2.21778	0.0484
O	-0.78149	4.10906	0.90949
C	-0.73956	2.34823	-1.13015
C	-0.09874	1.49724	-2.23186
C	-2.14399	1.92085	-0.81833
C	1.22869	2.00968	-2.78459
C	3.76066	-0.60021	-1.36758
C	2.99572	0.73718	-1.4408
C	2.36105	1.00313	-2.83138
C	1.37122	3.25583	-3.24778
C	3.91258	1.89861	-1.03268
O	5.03661	-3.98151	0.57819
O	2.19245	-0.23842	3.06221
C	-3.21945	2.70775	-0.55029
O	-4.30396	1.90152	-0.37193
C	-3.82913	0.62391	-0.5339
N	-2.54916	0.59037	-0.80458
C	-4.82276	-0.425	-0.41885
C	-4.62004	-1.75849	-0.3672
C	-3.24039	-2.40427	-0.40205
C	-5.79631	-2.69881	-0.30899
C	-2.8463	-2.82147	-1.82068
O	-3.20284	-3.58297	0.40453
C	-3.14766	-3.31877	1.79309
H	3.09731	-3.15007	2.19972
H	4.62337	-3.1553	-1.83243

H	3.10591	-4.02341	-1.58097
H	2.42481	-1.90489	-2.46587
H	-0.09102	-1.64661	1.01029
H	0.70517	-2.30333	2.4637
H	1.48895	0.35537	1.20242
H	-0.43129	-0.1225	3.51644
H	-0.84105	0.50157	1.91683
H	0.92192	1.81944	4.05156
H	-0.69374	2.33788	3.57696
H	1.80954	2.44727	1.82091
H	1.72388	4.91703	2.2294
H	1.89418	4.02859	3.75617
H	0.31925	4.70386	3.27934
H	-0.7509	3.4058	-1.40211
H	-0.82554	1.43029	-3.052
H	0.00965	0.47847	-1.84711
H	4.31656	-0.6353	-0.42118
H	4.5175	-0.64557	-2.16415
H	2.17935	0.68737	-0.7139
H	3.14165	1.3449	-3.52365
H	1.96638	0.0645	-3.24487
H	2.31004	3.60053	-3.67347
H	0.56072	3.98124	-3.22906
H	4.28199	1.77259	-0.00783
H	4.78612	1.96482	-1.69481
H	3.37847	2.85266	-1.08513
H	2.97507	-0.65243	2.66194
H	-3.36685	3.76946	-0.43873
H	-5.84185	-0.04709	-0.38599
H	-2.49647	-1.68515	-0.03604
H	-6.74467	-2.15578	-0.35456
H	-5.76586	-3.41062	-1.1439
H	-5.78236	-3.30408	0.60377

H	-3.57115	-3.52673	-2.24062
H	-1.8671	-3.30986	-1.79592
H	-2.78716	-1.94126	-2.46687
H	-2.2583	-2.72509	2.05611
H	-4.03684	-2.7802	2.15524
H	-3.09102	-4.2864	2.29892

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 3

C	1.68675	2.21305	-0.99075
C	2.69087	3.02325	-1.41999
C	3.49482	3.80213	-0.48325
C	3.01475	3.72926	0.96837
C	2.40341	2.36925	1.31492
O	1.41745	1.97669	0.3126
C	0.79836	1.3983	-1.88652
C	1.40954	-0.00518	-2.13165
C	0.40117	-0.98122	-2.73546
C	0.96338	-2.3944	-2.96993
C	1.57245	-3.12015	-1.73822
C	0.53189	-3.31819	-0.64364
C	2.16486	-4.47497	-2.14825
O	0.43643	-2.23102	0.1623
O	-0.14914	-4.31391	-0.50197
C	-0.56378	-2.28385	1.23112
C	-0.15383	-1.2261	2.25864
C	-1.94103	-2.04669	0.67727
C	1.14825	-1.49312	3.00782
C	3.45008	1.25743	1.48613
C	2.8898	-0.16528	1.68871
C	2.13724	-0.34465	3.03499
C	1.38657	-2.64719	3.6393
C	4.0101	-1.2059	1.55308

O	4.43306	4.51294	-0.81746
O	2.52582	0.07018	-3.0151
C	-2.818	-2.96007	0.1793
O	-3.95076	-2.30151	-0.19611
C	-3.71103	-0.98159	0.0943
N	-2.52751	-0.7869	0.61702
C	-4.80485	-0.07747	-0.19925
C	-4.83825	1.26526	-0.06279
C	-3.67076	2.093	0.4616
C	-6.10156	2.02236	-0.38205
C	-3.77056	2.29868	1.97574
O	-3.64932	3.39189	-0.13249
C	-3.12758	3.40524	-1.44652
H	2.86021	3.15916	-2.48295
H	3.8496	3.96148	1.63605
H	2.26164	4.51867	1.10032
H	1.80338	2.45507	2.22429
H	-0.17721	1.28968	-1.39952
H	0.66173	1.89656	-2.85161
H	1.72701	-0.39822	-1.15844
H	0.05532	-0.5817	-3.69821
H	-0.46951	-1.02083	-2.07154
H	1.75374	-2.33498	-3.72572
H	0.1691	-3.02747	-3.38682
H	2.36831	-2.48901	-1.32867
H	2.63811	-4.97692	-1.29783
H	2.92165	-4.33417	-2.92706
H	1.38526	-5.13885	-2.53335
H	-0.52089	-3.28984	1.65336
H	-0.97556	-1.13859	2.98123
H	-0.10978	-0.26132	1.74407
H	4.10851	1.25375	0.60729
H	4.08545	1.53813	2.33871

H	2.169	-0.34959	0.88634
H	2.86857	-0.4929	3.84019
H	1.5865	0.57442	3.27963
H	2.30394	-2.80917	4.19941
H	0.67933	-3.47374	3.63127
H	4.47655	-1.16102	0.56151
H	4.79877	-1.03931	2.29878
H	3.61963	-2.21848	1.69752
H	3.18556	0.65419	-2.60564
H	-2.78338	-4.02449	0.01697
H	-5.69538	-0.58989	-0.55508
H	-2.7287	1.5736	0.24578
H	-6.91304	1.34445	-0.66213
H	-6.42848	2.61647	0.48075
H	-5.94574	2.7365	-1.19811
H	-4.70863	2.79539	2.24512
H	-2.94098	2.92872	2.31147
H	-3.71652	1.33552	2.49085
H	-2.08948	3.03815	-1.47123
H	-3.72381	2.79522	-2.14275
H	-3.14395	4.44456	-1.78575

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 4

C	2.13043	-2.14392	0.39905
C	2.49396	-3.38098	-0.02555
C	3.56162	-3.56701	-1.00781
C	4.25772	-2.27395	-1.44624
C	3.30316	-1.08367	-1.40771
O	2.64889	-1.00477	-0.11344
C	1.15591	-1.82941	1.49586
C	1.85895	-1.19417	2.72274
C	0.89864	-0.47453	3.67543

C	0.1197	0.70511	3.06633
C	0.99338	1.87865	2.53278
C	0.17412	2.665	1.51865
C	1.50794	2.78846	3.6519
O	0.13331	2.00309	0.33274
O	-0.39963	3.71328	1.72473
C	-0.7763	2.52016	-0.68717
C	-0.31672	1.93777	-2.0311
C	-2.18251	2.12886	-0.3411
C	0.94582	2.54992	-2.63273
C	3.97068	0.27132	-1.62959
C	3.02386	1.48888	-1.52922
C	2.15438	1.64948	-2.80497
C	0.95544	3.82249	-3.04581
C	3.8274	2.76648	-1.25014
O	3.92473	-4.66248	-1.41339
O	2.51529	-2.19576	3.49684
C	-3.14422	2.87619	0.2624
O	-4.26664	2.11017	0.38018
C	-3.92791	0.89565	-0.16287
N	-2.69873	0.86638	-0.60925
C	-4.97845	-0.10242	-0.15894
C	-4.88151	-1.40718	-0.49209
C	-3.58885	-2.06863	-0.95545
C	-6.10428	-2.28716	-0.45751
C	-3.48646	-2.08885	-2.4828
O	-3.5187	-3.42574	-0.51444
C	-3.16394	-3.55946	0.84759
H	2.01899	-4.263	0.38948
H	5.10454	-2.09604	-0.76699
H	4.66836	-2.41316	-2.45078
H	2.49923	-1.24995	-2.14015
H	0.41974	-1.13005	1.08376

H	0.63532	-2.73564	1.82139
H	2.60058	-0.47279	2.35101
H	1.49055	-0.14323	4.53728
H	0.18164	-1.2101	4.06352
H	-0.56299	1.10501	3.82696
H	-0.51798	0.3371	2.25507
H	1.83911	1.45766	1.97794
H	2.1724	3.565	3.25904
H	2.06615	2.20927	4.39469
H	0.67391	3.28827	4.15376
H	-0.69288	3.6091	-0.68096
H	-1.14588	2.077	-2.73507
H	-0.2088	0.85613	-1.90481
H	4.76662	0.37164	-0.87958
H	4.46681	0.25535	-2.6103
H	2.35274	1.31857	-0.68124
H	2.79079	2.03823	-3.61139
H	1.80504	0.66121	-3.13585
H	1.83223	4.26709	-3.50937
H	0.08679	4.47007	-2.94306
H	4.37257	2.68974	-0.30195
H	4.56404	2.95229	-2.04345
H	3.17085	3.64035	-1.19177
H	3.12594	-2.66924	2.90851
H	-3.18468	3.87891	0.65552
H	-5.94337	0.2909	0.15172
H	-2.7319	-1.5093	-0.56007
H	-7.00016	-1.71704	-0.1953
H	-6.26947	-2.76305	-1.43246
H	-5.98673	-3.10557	0.26116
H	-2.5684	-2.60632	-2.77819
H	-3.45903	-1.06661	-2.87059
H	-4.33531	-2.61755	-2.92899

H	-3.11497	-4.63073	1.06061
H	-2.18021	-3.10841	1.05392
H	-3.90073	-3.09642	1.52231

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 5

C	-1.44485	2.62473	1.37115
C	-0.24764	3.25658	1.2719
C	0.21273	3.83461	0.01283
C	-0.76265	3.66387	-1.15051
C	-1.57884	2.38495	-0.99221
O	-2.24186	2.37106	0.30378
C	-2.03846	2.12195	2.65366
C	-2.20031	0.58309	2.73535
C	-0.86568	-0.16445	2.64572
C	-0.95484	-1.6617	2.98796
C	-1.88789	-2.54108	2.10765
C	-1.21836	-2.96768	0.80667
C	-2.35931	-3.78096	2.87776
O	-0.99618	-1.91169	-0.02037
O	-0.92004	-4.10757	0.51797
C	-0.40088	-2.21938	-1.31986
C	-0.80058	-1.09686	-2.29347
C	1.0822	-2.3825	-1.18874
C	-2.29745	-1.00814	-2.54557
C	-2.62526	2.19402	-2.08741
C	-3.7046	1.11879	-1.85283
C	-3.17392	-0.30491	-1.51601
C	-2.81792	-1.60392	-3.62657
C	-4.68836	1.11949	-3.03196
O	1.26472	4.45031	-0.10748
O	-2.79652	0.23986	3.98759
C	1.79326	-3.53997	-1.21405

O	3.11283	-3.23092	-1.0784
C	3.14879	-1.8618	-0.96061
N	1.96149	-1.31686	-1.031
C	4.47794	-1.30644	-0.79388
C	4.82984	-0.05471	-0.43259
C	3.8373	1.0581	-0.12041
C	6.28852	0.30864	-0.32095
C	3.72275	2.06412	-1.26835
O	4.25643	1.79043	1.03416
C	4.01646	1.11235	2.25072
H	0.36267	3.40688	2.15512
H	-1.43344	4.53536	-1.17141
H	-0.20409	3.65702	-2.09157
H	-0.88785	1.53281	-0.9685
H	-1.42915	2.45651	3.49877
H	-3.03582	2.5728	2.76723
H	-2.85369	0.26455	1.90982
H	-0.16333	0.2988	3.35244
H	-0.44865	-0.02194	1.64363
H	-1.31387	-1.749	4.01779
H	0.05643	-2.08901	2.97395
H	-2.76607	-1.94417	1.83026
H	-2.9969	-4.41859	2.2584
H	-2.92536	-3.47296	3.76288
H	-1.50723	-4.38638	3.20329
H	-0.82943	-3.16758	-1.65256
H	-0.2816	-1.30853	-3.23536
H	-0.38493	-0.15761	-1.91575
H	-3.13587	3.15304	-2.24962
H	-2.07849	1.97798	-3.01597
H	-4.26379	1.42515	-0.95904
H	-2.6353	-0.25335	-0.56722
H	-4.0593	-0.92733	-1.33005

H	-3.88779	-1.62408	-3.81557
H	-2.19146	-2.10728	-4.35995
H	-5.12491	2.11516	-3.17572
H	-4.19445	0.83303	-3.96703
H	-5.51255	0.41698	-2.85922
H	-3.67761	0.64387	4.02095
H	1.53368	-4.58308	-1.29404
H	5.26362	-2.0346	-0.98227
H	2.84739	0.62196	0.06248
H	6.93466	-0.53876	-0.56796
H	6.53746	1.1383	-0.99488
H	6.52932	0.65649	0.68918
H	4.69437	2.51446	-1.49703
H	3.03535	2.8654	-0.98236
H	3.34596	1.5662	-2.16778
H	4.57759	0.16746	2.32413
H	4.34065	1.77856	3.055
H	2.94619	0.88664	2.38222

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 6

C	-1.64397	-2.01349	-2.067
C	-0.34154	-2.31301	-2.30832
C	0.47562	-3.02258	-1.33311
C	-0.27507	-3.44566	-0.07274
C	-1.37785	-2.44311	0.25801
O	-2.26198	-2.26774	-0.88972
C	-2.55004	-1.32528	-3.04381
C	-2.91169	0.12935	-2.64335
C	-1.68739	1.0485	-2.57827
C	-2.02093	2.53222	-2.34845
C	-2.66656	2.90034	-0.98519
C	-1.64021	2.85741	0.14012

C	-3.29734	4.2991	-1.04531
O	-1.53962	1.61888	0.68964
O	-0.9846	3.80642	0.51701
C	-0.64224	1.48827	1.83583
C	-1.09489	0.27706	2.68116
C	0.77127	1.33508	1.35961
C	-2.59467	0.13832	2.87509
C	-2.21574	-2.84624	1.46981
C	-3.51971	-2.06268	1.73836
C	-3.41105	-0.50966	1.76728
C	-3.17322	0.59672	3.99182
C	-4.19561	-2.61077	3.00366
O	1.65923	-3.29666	-1.50938
O	-3.80114	0.67997	-3.61579
C	1.77784	2.24594	1.34455
O	2.87995	1.65052	0.79393
C	2.48224	0.37368	0.48694
N	1.23263	0.14827	0.8061
C	3.37157	-0.57311	-0.1527
C	4.69586	-0.48866	-0.40382
C	5.58122	0.69577	-0.02949
C	5.37553	-1.6169	-1.13996
C	5.7539	1.66639	-1.20123
O	6.89115	0.26426	0.343
C	6.95141	-0.30228	1.63756
H	0.1069	-2.05093	-3.25985
H	-0.70519	-4.4443	-0.2402
H	0.43468	-3.52412	0.75606
H	-0.90666	-1.4658	0.40823
H	-2.08984	-1.31235	-4.03659
H	-3.48408	-1.90107	-3.11576
H	-3.4023	0.09921	-1.65942
H	-1.1513	0.96562	-3.53344

H	-1.00872	0.67738	-1.80269
H	-2.71301	2.85197	-3.13388
H	-1.10728	3.12836	-2.47007
H	-3.44381	2.16406	-0.75231
H	-3.75781	4.57246	-0.09013
H	-4.06971	4.32779	-1.82087
H	-2.54049	5.05455	-1.27642
H	-0.73697	2.41036	2.41338
H	-0.60213	0.389	3.65439
H	-0.67722	-0.62515	2.23111
H	-2.48458	-3.90665	1.36651
H	-1.55373	-2.78948	2.34509
H	-4.18374	-2.27419	0.88963
H	-3.02854	-0.17409	0.80043
H	-4.43995	-0.13418	1.84099
H	-4.24741	0.5333	4.14805
H	-2.59627	1.05597	4.79175
H	-4.34872	-3.6943	2.93266
H	-3.59137	-2.41242	3.89627
H	-5.17618	-2.14515	3.15903
H	-4.62312	0.16571	-3.59558
H	1.86939	3.28114	1.63031
H	2.84176	-1.46663	-0.47212
H	5.13609	1.24006	0.8125
H	5.89022	-1.24471	-2.03508
H	6.1481	-2.08812	-0.52192
H	4.65351	-2.3785	-1.44563
H	6.19425	1.16094	-2.06668
H	6.42116	2.48198	-0.90523
H	4.78648	2.08564	-1.49298
H	6.33263	-1.20793	1.72873
H	7.99616	-0.56823	1.81995
H	6.62584	0.41556	2.40725

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 8

C	-1.30813	2.36179	0.73763
C	-1.38994	3.71158	0.63625
C	-2.54415	4.36444	0.02249
C	-3.66677	3.41135	-0.40285
C	-3.12208	2.04597	-0.81379
O	-2.23345	1.52576	0.20817
C	-0.19897	1.58623	1.39737
C	-0.70077	0.4182	2.27339
C	0.42593	-0.54195	2.65526
C	-0.05773	-1.85685	3.29185
C	-1.01169	-2.74126	2.43948
C	-0.37451	-3.13418	1.11212
C	-1.42013	-3.99911	3.21739
O	-0.54101	-2.16506	0.17402
O	0.22111	-4.16995	0.90005
C	0.09744	-2.38243	-1.12294
C	-0.56875	-1.4026	-2.09624
C	1.58252	-2.18257	-1.03341
C	-1.95866	-1.77521	-2.60368
C	-4.19858	0.98195	-1.03269
C	-3.6746	-0.45573	-1.24131
C	-2.97581	-0.65051	-2.6162
C	-2.25221	-2.9969	-3.0612
C	-4.81321	-1.47017	-1.06553
O	-2.65428	5.57712	-0.0975
O	-1.28958	0.88547	3.48994
C	2.55047	-3.13575	-1.00272
O	3.76256	-2.51327	-0.98938
C	3.47543	-1.1713	-1.00082
N	2.18892	-0.92969	-1.03124
C	4.63133	-0.29605	-1.02749
C	4.67101	1.03814	-0.82822

C	3.44426	1.87437	-0.48994
C	5.97355	1.7835	-0.96388
C	2.83389	2.52478	-1.7335
O	3.77198	2.93111	0.41366
C	3.97592	2.49852	1.74541
H	-0.6089	4.33707	1.05383
H	-4.35429	3.29847	0.44846
H	-4.23257	3.86805	-1.22042
H	-2.50267	2.16853	-1.71454
H	0.42048	1.16343	0.59372
H	0.42816	2.26068	1.98907
H	-1.44416	-0.12894	1.68526
H	1.08595	-0.03159	3.36963
H	1.02251	-0.75228	1.76188
H	-0.58555	-1.62482	4.22393
H	0.81739	-2.46133	3.56441
H	-1.90808	-2.15589	2.20677
H	-2.13821	-4.60242	2.65216
H	-1.88218	-3.71977	4.17023
H	-0.54813	-4.6271	3.42223
H	-0.09211	-3.42001	-1.40523
H	0.09793	-1.28773	-2.9609
H	-0.59085	-0.42247	-1.60952
H	-4.85935	0.99061	-0.15514
H	-4.81491	1.29117	-1.88878
H	-2.93338	-0.65004	-0.45854
H	-3.74095	-0.83927	-3.38038
H	-2.46627	0.27705	-2.91126
H	-3.23208	-3.22906	-3.47016
H	-1.53285	-3.81261	-3.05706
H	-5.24267	-1.41338	-0.05828
H	-5.62253	-1.28717	-1.78494
H	-4.45141	-2.49213	-1.21911

H	-2.10074	1.3659	3.26208
H	2.54594	-4.21296	-0.96951
H	5.55761	-0.82095	-1.24912
H	2.68741	1.22525	-0.03227
H	6.78843	1.11459	-1.25535
H	5.89036	2.57482	-1.71999
H	6.24799	2.28574	-0.03015
H	3.55838	3.17527	-2.23443
H	1.97399	3.13489	-1.43901
H	2.50039	1.75422	-2.43424
H	3.08531	1.98972	2.14592
H	4.832	1.81292	1.83941
H	4.17312	3.39268	2.34279

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 9

C	-1.81954	-2.6245	-1.46403
C	-0.6657	-2.84629	-2.14348
C	0.56398	-3.23287	-1.46234
C	0.42352	-3.38807	0.05053
C	-0.64731	-2.44919	0.59946
O	-1.9032	-2.6446	-0.11162
C	-3.1313	-2.29022	-2.10806
C	-3.61248	-0.8417	-1.83481
C	-2.62985	0.21618	-2.34875
C	-3.15905	1.65726	-2.27388
C	-3.44007	2.22578	-0.85477
C	-2.16365	2.6985	-0.16776
C	-4.44265	3.38589	-0.9239
O	-1.4245	1.67346	0.32536
O	-1.83691	3.86335	-0.05476
C	-0.2848	2.04492	1.17488
C	-0.02695	0.88526	2.14963

C	0.92583	2.39003	0.34945
C	-1.22614	0.51245	3.00542
C	-0.89341	-2.62477	2.09647
C	-2.14075	-1.94353	2.69725
C	-2.28325	-0.41722	2.42721
C	-1.35325	1.03447	4.23198
C	-2.23548	-2.27741	4.193
O	1.61676	-3.46132	-2.04707
O	-4.85704	-0.62348	-2.49945
C	1.15023	3.50856	-0.39387
O	2.39911	3.41621	-0.93138
C	2.9012	2.22338	-0.47515
N	2.05414	1.57971	0.28753
C	4.26554	1.94053	-0.87121
C	5.01317	0.85329	-0.585
C	4.51515	-0.33017	0.23901
C	6.45236	0.79722	-1.02793
C	4.74632	-0.09167	1.73501
O	5.20977	-1.5266	-0.09897
C	4.75218	-2.14337	-1.29381
H	-0.65328	-2.78613	-3.22574
H	0.1535	-4.43222	0.26671
H	1.3897	-3.1944	0.52664
H	-0.35278	-1.41635	0.37477
H	-3.06242	-2.43834	-3.19003
H	-3.89477	-2.98253	-1.72421
H	-3.74133	-0.7258	-0.74856
H	-2.40278	-0.00911	-3.39953
H	-1.69044	0.12366	-1.7941
H	-4.09887	1.70227	-2.83245
H	-2.45634	2.32473	-2.78943
H	-3.86277	1.42645	-0.23466
H	-4.63994	3.80557	0.06742

H	-5.38885	3.03263	-1.3468
H	-4.05918	4.19473	-1.55325
H	-0.6035	2.92921	1.7319
H	0.80181	1.20541	2.7905
H	0.34977	0.0314	1.58148
H	-0.96613	-3.70017	2.30888
H	0.01247	-2.27557	2.61151
H	-3.00998	-2.39628	2.20223
H	-2.34448	-0.26195	1.34704
H	-3.25881	-0.1242	2.83653
H	-2.21828	0.8282	4.8575
H	-0.59933	1.69425	4.65619
H	-2.22408	-3.36191	4.35454
H	-1.40019	-1.84417	4.75442
H	-3.16433	-1.88665	4.62527
H	-5.51176	-1.22901	-2.1183
H	0.56858	4.38446	-0.62672
H	4.71582	2.74893	-1.44213
H	3.43814	-0.46187	0.07027
H	6.75537	1.72807	-1.51628
H	7.1145	0.62164	-0.17073
H	6.62916	-0.03338	-1.71977
H	5.80918	0.06978	1.94428
H	4.41815	-0.97148	2.29773
H	4.17826	0.77975	2.07146
H	4.85247	-1.48198	-2.16815
H	5.37945	-3.02539	-1.4495
H	3.70424	-2.46275	-1.21978

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 10

C	2.27138	-2.31289	0.0209
C	2.95704	-3.29105	-0.62467
C	4.23248	-3.03237	-1.2849
C	4.74015	-1.59881	-1.12869
C	3.58722	-0.60312	-1.03067
O	2.64244	-1.01089	0.00123
C	1.01828	-2.5559	0.81621
C	1.11952	-2.34468	2.35208
C	1.30984	-0.8957	2.81802
C	0.1762	0.05385	2.40512
C	0.47099	1.54449	2.71923
C	-0.35293	2.44904	1.80556
C	0.25836	1.91692	4.18882
O	-0.09837	2.15146	0.504
O	-1.12137	3.31758	2.15487
C	-0.89029	2.80311	-0.52164
C	-0.16953	2.53662	-1.85389
C	-2.28472	2.25103	-0.52062
C	1.19618	3.19692	-2.01642
C	4.04021	0.81386	-0.68923
C	2.92625	1.87891	-0.59446
C	2.4328	2.31591	-1.99877
C	1.28495	4.5147	-2.23169
C	3.42429	3.08523	0.2137
O	4.88298	-3.8899	-1.86742
O	-0.0832	-2.81372	2.9699
C	-3.454	2.88688	-0.25062
O	-4.47133	1.99019	-0.40117
C	-3.85789	0.81338	-0.75064
N	-2.55838	0.92731	-0.84402
C	-4.74328	-0.31229	-0.97261
C	-4.40844	-1.61562	-1.07844

C	-2.9801	-2.13488	-0.95763
C	-5.47159	-2.64637	-1.35912
C	-2.31734	-2.28323	-2.32937
O	-2.95439	-3.42305	-0.33975
C	-3.14999	-3.38341	1.0642
H	2.58968	-4.31105	-0.61205
H	5.35342	-1.55149	-0.21667
H	5.39074	-1.35401	-1.97361
H	3.02091	-0.62109	-1.97368
H	0.21381	-1.92474	0.42235
H	0.71807	-3.59618	0.64586
H	1.97667	-2.93392	2.71585
H	2.26082	-0.53135	2.4143
H	1.40799	-0.92128	3.91013
H	-0.75601	-0.24447	2.89868
H	0.00937	-0.03657	1.32988
H	1.51951	1.73448	2.4452
H	0.50183	2.96776	4.3711
H	0.88899	1.30013	4.83737
H	-0.78638	1.76501	4.47897
H	-0.92473	3.87383	-0.30142
H	-0.83714	2.89587	-2.64625
H	-0.09932	1.45092	-1.97709
H	4.57098	0.76191	0.27102
H	4.78658	1.11704	-1.4373
H	2.08298	1.43532	-0.0585
H	3.25459	2.84461	-2.50106
H	2.22679	1.41992	-2.60191
H	2.24247	5.00914	-2.37382
H	0.40397	5.15209	-2.27774
H	3.71295	2.78626	1.22865
H	4.3044	3.54314	-0.2583
H	2.65185	3.8558	0.29409

H	-0.17759	-3.75831	2.77007
H	-3.72056	3.88569	0.05524
H	-5.78965	-0.02876	-1.05817
H	-2.38781	-1.42792	-0.36269
H	-6.45104	-2.18076	-1.50229
H	-5.22745	-3.22177	-2.26123
H	-5.54577	-3.37669	-0.5462
H	-1.30992	-2.69368	-2.20579
H	-2.24557	-1.30732	-2.81734
H	-2.88598	-2.96432	-2.97125
H	-3.17512	-4.42246	1.40666
H	-2.33075	-2.85618	1.57469
H	-4.10039	-2.90224	1.3406

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 11

C	2.39057	-2.28419	0.05881
C	3.09646	-3.24806	-0.58547
C	4.34218	-2.95363	-1.28646
C	4.79557	-1.49769	-1.17614
C	3.60612	-0.54703	-1.06688
O	2.70927	-0.96777	0.00123
C	1.16367	-2.55915	0.88282
C	1.2844	-2.29918	2.40018
C	1.44383	-0.82936	2.82658
C	0.28513	0.08071	2.39801
C	0.52417	1.58259	2.69863
C	-0.34719	2.4534	1.79436
C	0.32095	1.95804	4.16904
O	-0.14216	2.1272	0.49296
O	-1.10791	3.32404	2.15612
C	-0.9725	2.75844	-0.51798
C	-0.29153	2.47857	-1.86804

C	-2.36115	2.19626	-0.46021
C	1.05928	3.15373	-2.08529
C	4.01281	0.89428	-0.77216
C	2.86554	1.92313	-0.67529
C	2.31237	2.29524	-2.0762
C	1.12019	4.46612	-2.34021
C	3.34817	3.17199	0.07564
O	5.01161	-3.79697	-1.86818
O	0.0902	-2.87378	2.94573
C	-3.51858	2.818	-0.11624
O	-4.53572	1.91564	-0.22723
C	-3.93368	0.74969	-0.63121
N	-2.64189	0.87628	-0.79205
C	-4.82255	-0.37853	-0.8217
C	-4.48501	-1.67403	-0.99551
C	-3.04713	-2.18149	-1.01295
C	-5.55756	-2.70815	-1.22147
C	-2.49804	-2.25624	-2.44036
O	-2.95998	-3.49587	-0.46419
C	-3.01913	-3.52861	0.95255
H	2.77013	-4.28082	-0.53937
H	5.43115	-1.40478	-0.28306
H	5.41245	-1.24703	-2.04436
H	3.01485	-0.61036	-1.99243
H	0.32709	-1.97342	0.48448
H	0.89975	-3.61382	0.76728
H	2.16182	-2.85782	2.7656
H	2.38433	-0.44993	2.41091
H	1.56104	-0.81208	3.92101
H	-0.64485	-0.24383	2.88126
H	0.13231	-0.02877	1.3229
H	1.56034	1.81236	2.40774
H	0.51686	3.02082	4.33696

H	0.99264	1.37975	4.81216
H	-0.71042	1.76084	4.48015
H	-1.00671	3.83165	-0.31084
H	-0.98892	2.81745	-2.64344
H	-0.21253	1.39206	-1.97761
H	4.56856	0.88642	0.17531
H	4.72898	1.20523	-1.54611
H	2.05571	1.47017	-0.0974
H	3.10548	2.81887	-2.62762
H	2.10317	1.37262	-2.63618
H	2.06541	4.97146	-2.52108
H	0.22766	5.08756	-2.38124
H	3.67962	2.91781	1.08984
H	4.19668	3.64189	-0.44031
H	2.55314	3.91925	0.15511
H	0.09879	-2.7187	3.90351
H	-3.77482	3.80919	0.22148
H	-5.87484	-0.10436	-0.81724
H	-2.41398	-1.49577	-0.43537
H	-6.54996	-2.25066	-1.27139
H	-5.38034	-3.25416	-2.15685
H	-5.55762	-3.46236	-0.42724
H	-1.48227	-2.66352	-2.41745
H	-2.47164	-1.25805	-2.88603
H	-3.11359	-2.91169	-3.06547
H	-2.96903	-4.58126	1.24423
H	-2.17351	-2.99581	1.41037
H	-3.95646	-3.09923	1.33942

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 12

C	-1.6503	-2.03011	-2.04984
C	-0.3477	-2.32941	-2.29286
C	0.47589	-3.02409	-1.31299
C	-0.26951	-3.43649	-0.04633
C	-1.37393	-2.43383	0.27928
O	-2.26183	-2.26747	-0.86706
C	-2.56348	-1.36189	-3.03439
C	-2.93221	0.0975	-2.66101
C	-1.70887	1.0265	-2.57975
C	-2.05746	2.5082	-2.35965
C	-2.68892	2.8772	-0.9907
C	-1.64696	2.85011	0.12132
C	-3.33386	4.26953	-1.04974
O	-1.53702	1.61842	0.68241
O	-0.99036	3.80559	0.47942
C	-0.63561	1.502	1.82702
C	-1.08432	0.29814	2.68491
C	0.77692	1.34762	1.34853
C	-2.58362	0.16	2.88476
C	-2.20756	-2.83147	1.49587
C	-3.51175	-2.04862	1.76504
C	-3.4048	-0.49546	1.78474
C	-3.15762	0.62552	4.00092
C	-4.18135	-2.59051	3.03632
O	1.66017	-3.29514	-1.49055
O	-3.91427	0.58399	-3.57662
C	1.78384	2.25802	1.32965
O	2.88552	1.66017	0.78068
C	2.48712	0.38227	0.47869
N	1.23753	0.15867	0.79911
C	3.37577	-0.56771	-0.15717
C	4.7002	-0.48536	-0.40828

C	5.58638	0.70003	-0.03888
C	5.37929	-1.61749	-1.13896
C	5.7593	1.66589	-1.21455
O	6.89614	0.26936	0.33482
C	6.95672	-0.29175	1.63182
H	0.09579	-2.08071	-3.25039
H	-0.69761	-4.43774	-0.20296
H	0.44281	-3.5052	0.7811
H	-0.90471	-1.45443	0.42169
H	-2.09299	-1.37468	-4.02536
H	-3.50119	-1.92626	-3.10132
H	-3.44833	0.07777	-1.69649
H	-1.14963	0.94266	-3.52511
H	-1.03236	0.66565	-1.79688
H	-2.77024	2.81297	-3.1339
H	-1.15633	3.11845	-2.50175
H	-3.45606	2.13495	-0.74496
H	-3.78342	4.54246	-0.0894
H	-4.11842	4.28622	-1.81325
H	-2.58779	5.03141	-1.29474
H	-0.73127	2.42971	2.39542
H	-0.58862	0.4195	3.65551
H	-0.66714	-0.60774	2.24175
H	-2.47497	-3.89279	1.39873
H	-1.54248	-2.76934	2.36851
H	-4.17898	-2.2654	0.92038
H	-3.0279	-0.16566	0.81383
H	-4.43361	-0.12071	1.86091
H	-4.23112	0.56264	4.16184
H	-2.57756	1.08988	4.79568
H	-4.333	-3.67467	2.97211
H	-3.57384	-2.38604	3.92538
H	-5.16212	-2.12578	3.19264

H	-3.49118	0.65486	-4.44854
H	1.87627	3.29405	1.6122
H	2.84536	-1.46243	-0.47233
H	5.14172	1.24796	0.80101
H	5.89506	-1.24985	-2.03535
H	6.15093	-2.08668	-0.51826
H	4.65676	-2.37985	-1.44152
H	6.19892	1.15664	-2.07815
H	6.42733	2.48214	-0.92211
H	4.79205	2.08475	-1.50748
H	6.33729	-1.19651	1.72714
H	8.00136	-0.55772	1.81468
H	6.63215	0.42963	2.39858

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 13

C	2.52474	-2.22618	-0.33131
C	3.43618	-3.0325	-0.93359
C	4.79523	-2.5845	-1.21765
C	5.10478	-1.17023	-0.72714
C	3.86362	-0.28157	-0.75782
O	2.75704	-0.91879	-0.05768
C	1.14936	-2.67946	0.07133
C	0.85807	-2.82493	1.58935
C	0.90988	-1.51725	2.40537
C	-0.1123	-0.45688	1.97752
C	0.07085	0.92034	2.66788
C	-0.67144	2.00072	1.88368
C	-0.35196	0.93443	4.13923
O	-0.22604	2.033	0.59894
O	-1.53275	2.73741	2.30902
C	-0.91342	2.86915	-0.35991
C	-0.0538	2.84336	-1.63887

C	-2.29471	2.33212	-0.60363
C	1.31728	3.50545	-1.53703
C	4.09296	1.08059	-0.10708
C	2.88886	2.04485	-0.05745
C	2.55742	2.62987	-1.45567
C	1.41515	4.83946	-1.58484
C	3.16811	3.16057	0.9595
O	5.645	-3.2841	-1.75304
O	-0.37874	-3.50967	1.76793
C	-3.49433	2.96963	-0.58593
O	-4.46667	2.05502	-0.87645
C	-3.79935	0.87018	-1.04556
N	-2.50488	0.99691	-0.91269
C	-4.63238	-0.29026	-1.3088
C	-4.28184	-1.5931	-1.25069
C	-2.87936	-2.05744	-0.88565
C	-5.29203	-2.66756	-1.56548
C	-2.18177	-2.73302	-2.06693
O	-2.89452	-3.0223	0.18677
C	-3.51595	-2.56072	1.38406
H	3.17994	-4.05943	-1.16841
H	5.48641	-1.2414	0.30201
H	5.90184	-0.74304	-1.34312
H	3.53109	-0.17232	-1.80088
H	0.42038	-1.98631	-0.36821
H	0.9756	-3.66545	-0.37035
H	1.6202	-3.49703	2.00427
H	1.922	-1.10089	2.32801
H	0.75323	-1.79412	3.45486
H	-1.1259	-0.82236	2.18249
H	-0.04062	-0.29923	0.89869
H	1.13711	1.18058	2.59403
H	-0.19399	1.91996	4.58706

H	0.22256	0.20006	4.71231
H	-1.41572	0.69463	4.23944
H	-0.98133	3.88546	0.04031
H	-0.63819	3.35325	-2.41393
H	0.03666	1.79745	-1.95213
H	4.43601	0.89435	0.91967
H	4.93394	1.55925	-0.62942
H	2.02082	1.47846	0.28735
H	3.42243	3.2167	-1.79425
H	2.4439	1.80309	-2.17126
H	2.37531	5.34653	-1.53411
H	0.53925	5.47882	-1.6779
H	3.3459	2.74528	1.95883
H	4.05899	3.73942	0.67969
H	2.32774	3.85725	1.02632
H	-1.02399	-3.24275	1.08621
H	-3.81821	3.97833	-0.38577
H	-5.65979	-0.03452	-1.55782
H	-2.29217	-1.19209	-0.56587
H	-6.30477	-2.2606	-1.63736
H	-5.05897	-3.1571	-2.52056
H	-5.27884	-3.45476	-0.80399
H	-2.73727	-3.61296	-2.40497
H	-1.17918	-3.05936	-1.77637
H	-2.08966	-2.02997	-2.90084
H	-3.15621	-1.56241	1.66663
H	-4.6085	-2.52133	1.28587
H	-3.24762	-3.27334	2.16684

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 15

C	-1.68707	-2.08744	-1.95739
C	-0.40005	-2.4944	-2.10642
C	0.30509	-3.21052	-1.05071
C	-0.54473	-3.50607	0.18294
C	-1.57736	-2.40328	0.39773
O	-2.38448	-2.22907	-0.80538
C	-2.48808	-1.3973	-3.02089
C	-2.77438	0.09791	-2.72225
C	-1.49812	0.94227	-2.64567
C	-1.74663	2.45491	-2.51756
C	-2.43411	2.94472	-1.21426
C	-1.46971	2.9081	-0.03547
C	-2.97064	4.37283	-1.38901
O	-1.47798	1.70158	0.58858
O	-0.77272	3.83574	0.31979
C	-0.63801	1.57799	1.77778
C	-1.19982	0.44371	2.66385
C	0.77927	1.31227	1.36774
C	-2.712	0.40637	2.80006
C	-2.50563	-2.66909	1.58194
C	-3.75694	-1.77628	1.73297
C	-3.52334	-0.23811	1.68609
C	-3.30397	0.94907	3.87113
C	-4.54074	-2.2006	2.98309
O	1.47081	-3.58316	-1.14391
O	-3.57782	0.64311	-3.77004
C	1.8448	2.15286	1.35826
O	2.92307	1.46441	0.8711
C	2.44977	0.20596	0.594
N	1.17745	0.07681	0.87512
C	3.29602	-0.82247	0.02852
C	4.62471	-0.82048	-0.21261

C	5.54499	0.35633	0.06851
C	5.26182	-2.03414	-0.8387
C	5.61352	1.30408	-1.14203
O	6.83286	-0.17973	0.38408
C	7.6701	0.70073	1.10212
H	0.11857	-2.32092	-3.04254
H	-1.0469	-4.4742	0.03855
H	0.10988	-3.59761	1.05467
H	-1.03798	-1.45764	0.51954
H	-1.97343	-1.47075	-3.98383
H	-3.45328	-1.91533	-3.11756
H	-3.31359	0.15784	-1.76569
H	-0.92444	0.77089	-3.56667
H	-0.8814	0.57593	-1.81773
H	-2.37689	2.76852	-3.35578
H	-0.79136	2.98511	-2.62449
H	-3.26731	2.27303	-0.97984
H	-3.463	4.7299	-0.47834
H	-3.69743	4.40161	-2.20745
H	-2.15618	5.06623	-1.61867
H	-0.69642	2.53368	2.30322
H	-0.73997	0.57824	3.65025
H	-0.82149	-0.50504	2.27909
H	-2.84924	-3.71129	1.52385
H	-1.88727	-2.6081	2.48841
H	-4.38804	-1.98393	0.85855
H	-3.06526	0.00775	0.72544
H	-4.51969	0.22279	1.68148
H	-4.3854	0.95989	3.98394
H	-2.73104	1.40646	4.675
H	-4.77513	-3.27153	2.95745
H	-3.97098	-2.00126	3.8978
H	-5.4881	-1.65361	3.05784

H	-4.43094	0.18198	-3.7642
H	1.99654	3.18972	1.6103
H	2.72818	-1.7116	-0.23091
H	5.17327	0.91754	0.93514
H	4.51128	-2.79055	-1.0824
H	5.80139	-1.76549	-1.75629
H	6.00765	-2.46647	-0.16318
H	5.96115	0.76677	-2.03046
H	6.30336	2.13337	-0.9516
H	4.62666	1.72771	-1.35016
H	7.95944	1.587	0.51741
H	7.1946	1.04247	2.03573
H	8.57549	0.14066	1.35195

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 16

C	2.73325	-2.14587	-0.09569
C	3.5902	-2.98828	-0.72683
C	4.82884	-2.51434	-1.33655
C	5.0885	-1.01995	-1.14811
C	3.78475	-0.22796	-1.08282
O	2.88565	-0.79929	-0.0892
C	1.50656	-2.60121	0.64352
C	1.54022	-2.45872	2.18064
C	1.5757	-1.02023	2.726
C	0.3745	-0.15742	2.31642
C	0.50769	1.32986	2.72598
C	-0.42021	2.21649	1.89436
C	0.29217	1.58225	4.2214
O	-0.27419	1.94791	0.57208
O	-1.16742	3.06636	2.32675
C	-1.12733	2.6482	-0.37243
C	-0.49204	2.44485	-1.75978

C	-2.52559	2.11278	-0.30267
C	0.81512	3.19058	-2.0108
C	3.99582	1.23827	-0.71518
C	2.73411	2.12111	-0.61051
C	2.12383	2.41834	-2.00543
C	0.78813	4.49827	-2.29565
C	3.07976	3.41958	0.1328
O	5.63106	-3.24467	-1.90276
O	0.36801	-3.15744	2.61664
C	-3.65899	2.76228	0.06819
O	-4.70554	1.89639	-0.05551
C	-4.14504	0.72223	-0.49402
N	-2.85085	0.81077	-0.6648
C	-5.0737	-0.37083	-0.69535
C	-4.78758	-1.67756	-0.87352
C	-3.37231	-2.22671	-0.90231
C	-5.89859	-2.67287	-1.07767
C	-2.8031	-2.21668	-2.3312
O	-3.42839	-3.55275	-0.37058
C	-2.20237	-4.02268	0.15511
H	3.39407	-4.05451	-0.73636
H	5.65311	-0.88598	-0.21357
H	5.71957	-0.65931	-1.96597
H	3.26242	-0.3247	-2.04575
H	0.63458	-2.06309	0.25522
H	1.35193	-3.66335	0.43399
H	2.43941	-2.98304	2.5439
H	2.5037	-0.54673	2.38455
H	1.64833	-1.0829	3.82232
H	-0.54808	-0.57221	2.74158
H	0.26298	-0.20021	1.23181
H	1.52499	1.65187	2.45355
H	0.41097	2.6417	4.46411

H	1.01067	1.0101	4.81758
H	-0.71869	1.28755	4.52324
H	-1.13746	3.708	-0.10259
H	-1.23505	2.78181	-2.49181
H	-0.37227	1.3672	-1.91415
H	4.52234	1.2581	0.24874
H	4.68926	1.66794	-1.45251
H	1.9893	1.57791	-0.02338
H	2.86579	2.98145	-2.58824
H	1.96633	1.46948	-2.53747
H	1.69576	5.06034	-2.50065
H	-0.14372	5.05888	-2.33776
H	3.45694	3.20776	1.14074
H	3.85794	3.98447	-0.39838
H	2.20551	4.07001	0.22699
H	0.32396	-3.08884	3.58341
H	-3.8799	3.75231	0.4333
H	-6.11561	-0.06103	-0.67835
H	-2.72926	-1.60145	-0.26879
H	-6.87638	-2.18278	-1.09412
H	-5.76715	-3.21963	-2.02052
H	-5.88552	-3.42654	-0.28396
H	-1.8033	-2.6639	-2.34998
H	-2.7214	-1.18858	-2.69492
H	-3.44517	-2.78942	-3.00884
H	-1.42138	-4.11497	-0.61526
H	-1.82215	-3.37652	0.95972
H	-2.39869	-5.01724	0.56532

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 17

C	2.25333	-2.15792	0.52584
C	2.56711	-3.4029	0.09215
C	3.55226	-3.61461	-0.96573
C	4.22171	-2.33337	-1.47338
C	3.26868	-1.14449	-1.39709
O	2.7152	-1.02961	-0.05962
C	1.35207	-1.81898	1.67828
C	2.05392	-0.95666	2.75615
C	1.07079	-0.21217	3.67588
C	0.20625	0.86681	2.99715
C	0.9989	2.07588	2.42122
C	0.1315	2.7727	1.38068
C	1.45239	3.05912	3.50402
O	0.08607	2.04155	0.23826
O	-0.46852	3.81484	1.53871
C	-0.85308	2.477	-0.79356
C	-0.40101	1.82625	-2.10727
C	-2.24444	2.07747	-0.39913
C	0.84949	2.41948	-2.75145
C	3.90926	0.20567	-1.7075
C	2.94635	1.41235	-1.62702
C	2.06176	1.5199	-2.89789
C	0.84537	3.67237	-3.22098
C	3.73191	2.71015	-1.39435
O	3.87324	-4.71878	-1.38455
O	2.97484	-1.73738	3.51387
C	-3.20307	2.83261	0.19994
O	-4.3093	2.05438	0.37584
C	-3.96445	0.82529	-0.12946
N	-2.74662	0.79799	-0.60576
C	-4.99815	-0.18789	-0.05915
C	-4.89244	-1.50115	-0.35392

C	-3.6065	-2.15887	-0.84075
C	-6.10015	-2.39638	-0.25044
C	-3.56226	-2.23984	-2.36876
O	-3.49526	-3.49565	-0.34812
C	-3.08243	-3.56609	1.00172
H	2.1388	-4.27437	0.57425
H	5.10741	-2.14207	-0.85011
H	4.56711	-2.49224	-2.49933
H	2.41207	-1.33401	-2.06189
H	0.49664	-1.26587	1.27012
H	0.96545	-2.73776	2.1355
H	2.68755	-0.22787	2.2451
H	1.66448	0.22873	4.48557
H	0.39976	-0.94588	4.14942
H	-0.52049	1.24881	3.72575
H	-0.38149	0.41032	2.19335
H	1.87166	1.69154	1.88071
H	2.04966	3.87072	3.07635
H	2.06277	2.55198	4.25832
H	0.58767	3.51058	3.99986
H	-0.79321	3.56582	-0.85289
H	-1.23834	1.91678	-2.80965
H	-0.27854	0.75454	-1.92298
H	4.73214	0.34823	-0.99475
H	4.36631	0.15165	-2.70561
H	2.2879	1.25597	-0.76604
H	2.68832	1.87994	-3.7251
H	1.71631	0.5167	-3.18566
H	1.71413	4.10157	-3.71334
H	-0.02641	4.31856	-3.13756
H	4.28977	2.66855	-0.45139
H	4.45632	2.88424	-2.2015
H	3.06261	3.57537	-1.35363

H	2.46293	-2.38444	4.02625
H	-3.25	3.84908	0.5551
H	-5.95857	0.20142	0.27004
H	-2.74527	-1.5701	-0.50184
H	-6.99224	-1.83321	0.0384
H	-6.3001	-2.89307	-1.20852
H	-5.9407	-3.19953	0.47728
H	-2.64639	-2.75252	-2.67875
H	-3.56936	-1.234	-2.79834
H	-4.41728	-2.80103	-2.76002
H	-3.00759	-4.62656	1.25742
H	-2.09806	-3.09279	1.14729
H	-3.79802	-3.08487	1.68667

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 18

C	3.96007	0.4291	1.58591
C	3.86152	-0.06145	2.84865
C	3.88168	-1.49602	3.11858
C	4.07381	-2.35945	1.87108
C	3.41123	-1.71435	0.6588
O	3.8941	-0.34677	0.479
C	4.21155	1.87665	1.26538
C	3.17432	2.58402	0.36151
C	1.76464	2.5663	0.95629
C	0.73272	3.45785	0.23844
C	0.67352	3.36044	-1.30462
C	0.60327	1.92257	-1.79058
C	-0.49524	4.19392	-1.86046
O	-0.53201	1.30168	-1.39449
O	1.47125	1.37444	-2.44518
C	-0.62095	-0.12393	-1.70434
C	0.13658	-0.89399	-0.60337

C	-2.0703	-0.47331	-1.78668
C	0.49099	-2.32572	-0.95066
C	3.66916	-2.45243	-0.65256
C	2.90941	-1.93193	-1.89606
C	1.49785	-2.55773	-2.06157
C	-0.06929	-3.34684	-0.29132
C	3.72791	-2.21531	-3.16666
O	3.82342	-1.97929	4.24159
O	3.5517	3.95719	0.20982
C	-2.79234	-0.83599	-2.87916
O	-4.07367	-1.08323	-2.48148
C	-4.075	-0.84771	-1.12834
N	-2.90093	-0.49511	-0.67465
C	-5.34789	-1.03924	-0.46313
C	-5.6703	-0.7186	0.80826
C	-4.69729	-0.08154	1.79392
C	-7.04876	-1.02215	1.33527
C	-4.02635	-1.13438	2.68008
O	-5.37169	0.82798	2.66527
C	-5.65678	2.07697	2.06518
H	3.87728	0.61596	3.69495
H	5.15296	-2.48147	1.69557
H	3.65421	-3.35314	2.05365
H	2.33606	-1.63414	0.85681
H	4.29524	2.43964	2.20015
H	5.18926	1.93701	0.76308
H	3.16023	2.09026	-0.61809
H	1.8169	2.88607	2.00556
H	1.41742	1.52606	0.97245
H	0.94624	4.50548	0.476
H	-0.25936	3.23116	0.64784
H	1.61292	3.74851	-1.70871
H	-0.50954	4.1816	-2.95607

H	-0.39665	5.23603	-1.53704
H	-1.45571	3.8113	-1.50138
H	-0.14747	-0.27474	-2.6765
H	-0.46793	-0.86056	0.30786
H	1.0572	-0.33405	-0.41257
H	4.75009	-2.40297	-0.83887
H	3.43198	-3.51299	-0.49086
H	2.80382	-0.84422	-1.81538
H	1.08543	-2.16621	-3.00358
H	1.61127	-3.64019	-2.21065
H	0.18152	-4.3806	-0.51791
H	-0.80554	-3.18559	0.4921
H	4.70715	-1.72553	-3.12049
H	3.89823	-3.29226	-3.29861
H	3.21179	-1.84637	-4.0603
H	4.37686	3.98396	-0.29919
H	-2.57203	-0.9691	-3.92659
H	-6.10174	-1.49736	-1.09889
H	-3.91519	0.45147	1.23974
H	-7.65829	-1.53915	0.5885
H	-6.99263	-1.65176	2.23236
H	-7.56796	-0.10735	1.64097
H	-4.76856	-1.70775	3.2455
H	-3.36247	-0.63724	3.394
H	-3.43696	-1.8222	2.06704
H	-6.13703	2.6947	2.82895
H	-4.73833	2.57897	1.72346
H	-6.33731	1.98401	1.20448

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 19

C	1.56184	-2.51281	1.76967
C	0.25202	-2.88483	1.78961
C	-0.43976	-3.32442	0.58516
C	0.45091	-3.41465	-0.6504
C	1.54476	-2.34907	-0.61257
O	2.29514	-2.42937	0.63782
C	2.3137	-2.06254	2.99034
C	1.99117	-0.58589	3.37294
C	2.35095	0.40993	2.26318
C	2.1337	1.87337	2.66761
C	2.58182	2.92699	1.6177
C	1.63103	3.02216	0.42614
C	2.74277	4.31161	2.25788
O	1.65383	1.89425	-0.3299
O	0.94789	3.98712	0.15497
C	0.83654	1.89767	-1.53987
C	1.38766	0.82463	-2.50661
C	-0.5967	1.6341	-1.1843
C	2.90098	0.72848	-2.58883
C	2.52116	-2.46037	-1.78321
C	3.80873	-1.60781	-1.74515
C	3.62884	-0.07721	-1.52299
C	3.56337	1.3559	-3.56831
C	4.65462	-1.90685	-2.99177
O	-1.62713	-3.63438	0.55699
O	0.63647	-0.44828	3.78683
C	-1.63784	2.50118	-1.10068
O	-2.74644	1.79681	-0.71691
C	-2.31817	0.5014	-0.57688
N	-1.04306	0.36433	-0.8422
C	-3.20498	-0.56113	-0.15177
C	-4.53892	-0.55355	0.06075

C	-5.44435	0.66107	-0.1207
C	-5.20802	-1.81212	0.55483
C	-5.68887	1.38716	1.20518
O	-6.7262	0.28007	-0.62243
C	-6.72146	-0.03118	-2.00228
H	-0.28145	-2.92091	2.73312
H	0.8995	-4.41862	-0.6829
H	-0.16641	-3.29813	-1.54594
H	1.05852	-1.36681	-0.59124
H	2.04166	-2.68966	3.84478
H	3.38866	-2.16823	2.80869
H	2.57628	-0.35849	4.27243
H	1.75369	0.18157	1.37464
H	3.40093	0.2575	1.97701
H	2.70672	2.07395	3.58335
H	1.08163	2.0338	2.93116
H	3.55072	2.60236	1.21223
H	3.0508	5.05861	1.52076
H	3.49788	4.2729	3.05018
H	1.79888	4.65139	2.69555
H	0.93098	2.89264	-1.98052
H	0.97331	1.06624	-3.49271
H	0.95706	-0.13701	-2.22195
H	2.82608	-3.51218	-1.87259
H	1.94818	-2.23651	-2.69383
H	4.37775	-1.94785	-0.86958
H	3.13422	0.07322	-0.56159
H	4.64035	0.33573	-1.41594
H	4.64797	1.32471	-3.63804
H	3.04708	1.92772	-4.33647
H	4.85462	-2.98088	-3.08599
H	4.14909	-1.57559	-3.90602
H	5.62102	-1.39106	-2.94317

H	0.07936	-0.6266	3.00913
H	-1.75297	3.56436	-1.23457
H	-2.66362	-1.48803	0.01726
H	-4.98448	1.36443	-0.82532
H	-5.96641	-2.16512	-0.1528
H	-4.47782	-2.60896	0.71844
H	-5.73869	-1.62637	1.49781
H	-6.15456	0.7192	1.93677
H	-6.36145	2.23453	1.03912
H	-4.74528	1.75735	1.617
H	-6.07424	-0.89008	-2.23627
H	-7.7506	-0.27889	-2.27596
H	-6.38702	0.82648	-2.60751

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 21

C	-4.67497	0.3207	-1.17096
C	-5.77745	-0.12428	-1.8259
C	-6.42225	-1.38791	-1.48305
C	-5.77763	-2.11453	-0.30299
C	-4.27519	-1.85294	-0.2523
O	-4.00047	-0.42144	-0.25801
C	-4.08365	1.68715	-1.37135
C	-4.14789	2.59368	-0.11591
C	-2.86976	2.59166	0.74333
C	-1.65096	3.23178	0.06177
C	-0.41607	3.36848	0.97933
C	0.02939	2.00763	1.49587
C	0.73639	4.09559	0.26377
O	0.43631	1.20691	0.48282
O	0.00271	1.66239	2.66026
C	0.7831	-0.17117	0.8378
C	0.45431	-1.02458	-0.39981

C	2.21696	-0.23813	1.2711
C	0.1896	-2.48668	-0.07008
C	-3.6028	-2.45474	0.97834
C	-2.08636	-2.21822	1.12963
C	-1.26523	-2.90678	0.01051
C	1.19056	-3.35582	0.10624
C	-1.6288	-2.69009	2.51817
O	-7.42648	-1.81377	-2.03757
O	-4.44269	3.9052	-0.60946
C	2.71639	-0.13045	2.53131
O	4.07525	-0.22182	2.46018
C	4.35217	-0.37923	1.12499
N	3.2739	-0.40139	0.38484
C	5.75673	-0.5031	0.79043
C	6.32035	-0.4975	-0.43645
C	5.5289	-0.35962	-1.73192
C	7.81085	-0.66603	-0.58121
C	5.23761	-1.72382	-2.36243
O	6.25787	0.39744	-2.70029
C	6.22669	1.79209	-2.46507
H	-6.25027	0.50144	-2.57423
H	-6.25253	-1.75876	0.62312
H	-5.9805	-3.18656	-0.38562
H	-3.82339	-2.24333	-1.17558
H	-3.04771	1.58732	-1.71694
H	-4.64706	2.19188	-2.15965
H	-4.98283	2.2469	0.51315
H	-2.65639	1.55806	1.04245
H	-3.08501	3.13729	1.67503
H	-1.92711	4.23063	-0.29474
H	-1.3602	2.65587	-0.82464
H	-0.69661	3.93284	1.87605
H	1.60345	4.21373	0.92296

H	0.41224	5.09377	-0.05049
H	1.05651	3.54191	-0.62404
H	0.15192	-0.44291	1.68447
H	1.27718	-0.93204	-1.11418
H	-0.43518	-0.58408	-0.86308
H	-4.1111	-2.05636	1.86679
H	-3.80628	-3.53521	0.96432
H	-1.92574	-1.13517	1.06128
H	-1.32859	-3.99551	0.14121
H	-1.72718	-2.68184	-0.96201
H	1.00251	-4.40006	0.34487
H	2.23029	-3.05459	0.01123
H	-2.13599	-2.13319	3.31432
H	-1.85201	-3.75582	2.65941
H	-0.54942	-2.56282	2.64955
H	-4.5279	4.49425	0.15737
H	2.27858	0.02038	3.50455
H	6.39722	-0.60998	1.66267
H	4.5731	0.13594	-1.52244
H	8.2921	-0.82121	0.38874
H	8.04628	-1.52341	-1.22466
H	8.26489	0.2065	-1.06341
H	4.6254	-2.32939	-1.68798
H	6.1648	-2.2633	-2.58243
H	4.69461	-1.58099	-3.30183
H	6.78337	2.2645	-3.27904
H	5.19535	2.17778	-2.46506
H	6.69595	2.0673	-1.5077

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 22

C	0.43668	2.33816	-1.28348
C	-0.1082	3.56324	-1.48873
C	0.38289	4.7485	-0.78982
C	1.60612	4.5047	0.10022
C	1.61686	3.09249	0.68017
O	1.40845	2.10916	-0.36823
C	0.04342	1.06597	-1.98907
C	1.24681	0.17385	-2.35913
C	0.81632	-1.22332	-2.80493
C	1.97729	-2.22538	-2.9319
C	2.83136	-2.46872	-1.65467
C	1.95545	-2.91559	-0.49121
C	3.92273	-3.51279	-1.9247
O	1.47942	-1.85775	0.21057
O	1.68563	-4.06981	-0.22477
C	0.5424	-2.14314	1.30132
C	0.50595	-0.88306	2.1676
C	-0.81585	-2.49103	0.75252
C	1.73587	-0.58146	3.01485
C	2.92778	2.71591	1.37354
C	3.05348	1.23658	1.79903
C	2.16258	0.87395	3.02179
C	2.36725	-1.511	3.73899
C	4.52025	0.88251	2.08174
O	-0.08932	5.86752	-0.93722
O	2.01649	0.74076	-3.42319
C	-1.26703	-3.68933	0.29104
O	-2.566	-3.53431	-0.09439
C	-2.8621	-2.21878	0.1572
N	-1.84765	-1.5623	0.65949
C	-4.221	-1.82132	-0.15275
C	-4.81339	-0.62778	0.06609

C	-4.12385	0.55124	0.74494
C	-6.26131	-0.42887	-0.29934
C	-4.33539	0.50932	2.26197
O	-4.65163	1.79537	0.2876
C	-4.11854	2.2157	-0.95389
H	-0.89548	3.69217	-2.22306
H	2.50503	4.66285	-0.51398
H	1.62215	5.25292	0.89836
H	0.76339	2.98203	1.36524
H	-0.60248	0.49829	-1.30324
H	-0.54108	1.3022	-2.8842
H	1.86454	0.07841	-1.46201
H	0.31759	-1.13927	-3.77949
H	0.06956	-1.60178	-2.09833
H	2.66168	-1.87882	-3.71438
H	1.575	-3.1914	-3.26365
H	3.3009	-1.52222	-1.3665
H	4.57298	-3.6448	-1.05337
H	4.54431	-3.19951	-2.77026
H	3.47782	-4.48434	-2.15874
H	0.94004	-3.00317	1.84377
H	-0.36753	-0.95834	2.82805
H	0.29312	-0.0398	1.50324
H	3.74758	2.95357	0.6819
H	3.05462	3.37625	2.24304
H	2.72364	0.62567	0.95205
H	2.70856	1.10855	3.94445
H	1.26091	1.50207	3.02871
H	3.20754	-1.25693	4.37995
H	2.07248	-2.55775	3.73312
H	5.1429	1.0262	1.19073
H	4.93234	1.5102	2.88299
H	4.61443	-0.16361	2.39164

H	2.45852	1.53215	-3.07865
H	-0.8221	-4.66187	0.1637
H	-4.80807	-2.62467	-0.59109
H	-3.04654	0.51063	0.54455
H	-6.70777	-1.35174	-0.68075
H	-6.84087	-0.0942	0.57013
H	-6.37675	0.35432	-1.05688
H	-5.40174	0.52974	2.51056
H	-3.8617	1.38387	2.7187
H	-3.89052	-0.39729	2.68219
H	-3.02885	2.36124	-0.89449
H	-4.33026	1.50106	-1.76479
H	-4.58973	3.17227	-1.19496

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 23

C	-1.68796	-2.1051	-1.93937
C	-0.40109	-2.51587	-2.08292
C	0.30374	-3.21837	-1.01842
C	-0.54775	-3.50016	0.21695
C	-1.57946	-2.39413	0.42001
O	-2.38421	-2.22713	-0.78584
C	-2.48977	-1.4333	-3.01447
C	-2.77909	0.06653	-2.74655
C	-1.50164	0.91728	-2.64358
C	-1.76057	2.42952	-2.53207
C	-2.44332	2.92523	-1.2292
C	-1.47061	2.903	-0.05639
C	-2.98968	4.34856	-1.41156
O	-1.47523	1.70381	0.58
O	-0.77282	3.83548	0.28406
C	-0.63578	1.59254	1.77082
C	-1.1993	0.4666	2.66639

C	0.78162	1.3237	1.36367
C	-2.71195	0.43238	2.80099
C	-2.51047	-2.65056	1.60428
C	-3.76077	-1.75528	1.74745
C	-3.52419	-0.21807	1.69098
C	-3.30333	0.9837	3.868
C	-4.54689	-2.17028	2.99922
O	1.4701	-3.59089	-1.10619
O	-3.67083	0.55946	-3.74745
C	1.8486	2.16243	1.35341
O	2.92646	1.47076	0.86977
C	2.45134	0.2123	0.59556
N	1.17839	0.0862	0.87513
C	3.29646	-0.81945	0.03447
C	4.62489	-0.81944	-0.20818
C	5.54605	0.35858	0.06514
C	5.26066	-2.03696	-0.82808
C	5.61102	1.3012	-1.14966
O	6.83497	-0.17581	0.37884
C	7.67364	0.7072	1.09216
H	0.11754	-2.35832	-3.02198
H	-1.05091	-4.46906	0.08163
H	0.1054	-3.58361	1.09057
H	-1.03926	-1.44821	0.53586
H	-1.9619	-1.5343	-3.97082
H	-3.45876	-1.93731	-3.11193
H	-3.35014	0.13984	-1.81631
H	-0.89681	0.73971	-3.54704
H	-0.89652	0.56142	-1.80212
H	-2.40539	2.7299	-3.36537
H	-0.8131	2.96989	-2.65472
H	-3.27096	2.25033	-0.98585
H	-3.47672	4.709	-0.49953

H	-3.72457	4.36594	-2.22299
H	-2.18159	5.04554	-1.653
H	-0.69516	2.55334	2.28683
H	-0.74045	0.60953	3.65208
H	-0.82138	-0.48589	2.29045
H	-2.85521	-3.69267	1.55215
H	-1.89344	-2.58462	2.51136
H	-4.39086	-1.96706	0.87352
H	-3.06558	0.01975	0.72869
H	-4.51947	0.2447	1.68239
H	-4.38478	0.99741	3.98007
H	-2.72991	1.44533	4.66913
H	-4.78318	-3.24092	2.97993
H	-3.97818	-1.96618	3.91361
H	-5.49343	-1.62131	3.06866
H	-3.19339	0.55026	-4.59373
H	2.00204	3.19959	1.60327
H	2.72784	-1.70977	-0.21921
H	5.1769	0.92353	0.93043
H	5.79924	-1.77396	-1.7479
H	6.00724	-2.46561	-0.15105
H	4.50949	-2.79454	-1.06614
H	5.95539	0.75989	-2.03695
H	6.30211	2.13074	-0.96496
H	4.62375	1.7247	-1.35618
H	7.20059	1.05099	2.02623
H	8.58017	0.14847	1.34078
H	7.96059	1.59215	0.50426

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 27

C	0.38974	2.33013	-1.2863
C	-0.14154	3.56238	-1.48836
C	0.39069	4.74661	-0.81843
C	1.64257	4.49282	0.0277
C	1.64831	3.08841	0.62628
O	1.38596	2.0953	-0.39979
C	-0.04651	1.05674	-1.96289
C	1.13207	0.15689	-2.39197
C	0.67656	-1.25196	-2.77183
C	1.82849	-2.25737	-2.9424
C	2.74542	-2.48408	-1.70608
C	1.92973	-2.92635	-0.49784
C	3.82982	-3.52306	-2.01998
O	1.46549	-1.86458	0.20735
O	1.69248	-4.08009	-0.20117
C	0.56824	-2.15004	1.33113
C	0.53895	-0.88054	2.18446
C	-0.79832	-2.52757	0.82837
C	1.78452	-0.56292	3.00345
C	2.97453	2.69644	1.28049
C	3.08715	1.22037	1.72019
C	2.22107	0.88889	2.96886
C	2.42105	-1.47868	3.74066
C	4.55463	0.84641	1.97146
O	-0.07329	5.87056	-0.95585
O	1.8247	0.69733	-3.52075
C	-1.25735	-3.75476	0.46271
O	-2.55927	-3.62465	0.07913
C	-2.84817	-2.29187	0.23078
N	-1.82725	-1.60288	0.67442
C	-4.20443	-1.91408	-0.10923
C	-4.78389	-0.69794	-0.02116

C	-4.07522	0.52829	0.52759
C	-6.22246	-0.518	-0.42595
C	-4.19292	0.57457	2.06206
O	-4.67166	1.66996	-0.08849
C	-3.91737	2.86009	0.02483
H	-0.9513	3.69519	-2.19714
H	2.5205	4.62563	-0.62178
H	1.70242	5.25103	0.81428
H	0.81698	3.00337	1.34174
H	-0.65655	0.49615	-1.23965
H	-0.67768	1.28971	-2.82642
H	1.81104	0.08653	-1.53733
H	0.11918	-1.19317	-3.7159
H	-0.02472	-1.60997	-2.01062
H	2.47274	-1.92351	-3.76365
H	1.40956	-3.22763	-3.23942
H	3.22182	-1.53205	-1.44862
H	4.52127	-3.64473	-1.17941
H	4.40852	-3.21204	-2.89624
H	3.38106	-4.49922	-2.22577
H	0.99563	-2.99667	1.87182
H	-0.31956	-0.9577	2.86428
H	0.3053	-0.04608	1.51614
H	3.77546	2.91081	0.55979
H	3.14162	3.36418	2.1375
H	2.72649	0.60456	0.8894
H	2.78849	1.13941	3.87432
H	1.32355	1.52288	2.98174
H	3.27425	-1.21534	4.36045
H	2.11807	-2.52282	3.76641
H	5.15732	0.97023	1.06392
H	4.99585	1.47661	2.75508
H	4.64003	-0.19745	2.29122

H	2.27176	1.50865	-3.23378
H	-0.81597	-4.73547	0.40225
H	-4.80055	-2.74918	-0.46786
H	-3.0104	0.48404	0.26355
H	-6.67067	-1.46565	-0.73814
H	-6.81498	-0.10501	0.40046
H	-6.30103	0.20414	-1.24526
H	-5.24427	0.58871	2.36872
H	-3.70652	1.46951	2.46419
H	-3.70486	-0.29952	2.50239
H	-3.87888	3.24147	1.05573
H	-2.88484	2.72409	-0.33294
H	-4.41262	3.60703	-0.60128

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 28

C	2.92299	-2.16422	-0.65628
C	3.92555	-2.81814	-1.2965
C	5.27679	-2.2721	-1.37443
C	5.46152	-0.94772	-0.63318
C	4.17821	-0.12104	-0.63971
O	3.056	-0.91139	-0.15556
C	1.55044	-2.73739	-0.44529
C	1.19181	-3.12413	1.00622
C	1.06116	-1.96031	2.00439
C	-0.02102	-0.93103	1.64909
C	-0.02467	0.31043	2.57641
C	-0.7326	1.48983	1.91029
C	-0.61951	0.04258	3.96219
O	-0.20127	1.7257	0.68223
O	-1.62186	2.1546	2.39203
C	-0.7916	2.74977	-0.14467
C	0.14614	2.90688	-1.36105

C	-2.18992	2.37202	-0.55214
C	1.48058	3.59579	-1.09017
C	4.26522	1.12695	0.2348
C	3.00546	2.01543	0.31224
C	2.74922	2.76341	-1.02206
C	1.52514	4.92919	-0.98009
C	3.14699	2.99775	1.48392
O	6.20872	-2.838	-1.93031
O	-0.03426	-3.84986	0.8739
C	-3.25442	3.19059	-0.75937
O	-4.30296	2.42459	-1.18245
C	-3.82075	1.14207	-1.19586
N	-2.56116	1.06878	-0.84817
C	-4.77802	0.12348	-1.58587
C	-4.72503	-1.20189	-1.33742
C	-3.60763	-1.8722	-0.54813
C	-5.82322	-2.10575	-1.83652
C	-2.6603	-2.67661	-1.43897
O	-4.14928	-2.78725	0.41158
C	-4.74986	-2.14982	1.52281
H	3.74945	-3.80247	-1.71537
H	5.75483	-1.17332	0.40272
H	6.28369	-0.39065	-1.09235
H	3.93137	0.13969	-1.67941
H	0.80269	-2.03079	-0.82248
H	1.46171	-3.65084	-1.03984
H	1.98212	-3.79873	1.37546
H	2.03439	-1.46064	2.07769
H	0.86492	-2.39546	2.99621
H	-1.01082	-1.40361	1.67104
H	0.13552	-0.58958	0.62454
H	1.02155	0.63326	2.69176
H	-0.58998	0.94015	4.58614

H	-0.06539	-0.75087	4.47433
H	-1.66743	-0.2659	3.88048
H	-0.82876	3.68431	0.42478
H	-0.4065	3.49382	-2.10321
H	0.29303	1.91096	-1.79449
H	4.5259	0.79601	1.24942
H	5.11778	1.72274	-0.12213
H	2.14711	1.36828	0.51058
H	3.60905	3.41961	-1.21553
H	2.72585	2.03218	-1.84228
H	2.45755	5.45986	-0.80543
H	0.63118	5.54444	-1.0629
H	3.2767	2.46153	2.43181
H	4.0212	3.64964	1.35123
H	2.26641	3.63993	1.5754
H	-0.36192	-4.05729	1.76306
H	-3.43497	4.24884	-0.65738
H	-5.63763	0.52334	-2.11943
H	-3.02503	-1.10326	-0.02683
H	-6.60666	-1.5418	-2.35099
H	-5.42603	-2.85323	-2.53578
H	-6.27217	-2.66855	-1.01134
H	-1.88949	-3.14222	-0.81767
H	-2.18278	-2.01614	-2.16999
H	-3.19723	-3.46633	-1.97503
H	-5.07574	-2.94029	2.20474
H	-4.03656	-1.49436	2.04742
H	-5.62358	-1.54362	1.23893

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 32

C	-0.44416	2.35696	1.25478
C	0.08458	3.59268	1.43546
C	-0.43793	4.75886	0.73062
C	-1.67674	4.47974	-0.12614
C	-1.66457	3.06499	-0.69972
O	-1.40566	2.0895	0.34286
C	-0.01282	1.10579	1.97479
C	-1.18551	0.22024	2.41671
C	-0.73517	-1.20252	2.78148
C	-1.8874	-2.20978	2.94673
C	-2.7792	-2.45685	1.69565
C	-1.92838	-2.91601	0.51702
C	-3.86797	-3.49443	1.99822
O	-1.46902	-1.8658	-0.20227
O	-1.66569	-4.07406	0.26101
C	-0.54284	-2.15956	-1.30258
C	-0.52125	-0.90851	-2.18185
C	0.82122	-2.49663	-0.76324
C	-1.76336	-0.62313	-3.01719
C	-2.98356	2.65611	-1.35934
C	-3.08724	1.17315	-1.77606
C	-2.21421	0.82453	-3.01535
C	-2.38474	-1.56166	-3.73851
C	-4.55149	0.78691	-2.02808
O	0.01824	5.88847	0.84933
O	-1.80458	0.88408	3.52526
C	1.2872	-3.6929	-0.31172
O	2.58508	-3.52574	0.07201
C	2.86526	-2.20458	-0.17046
N	1.84213	-1.5565	-0.66575
C	4.21908	-1.79277	0.14273
C	4.79959	-0.59343	-0.07673

C	4.10212	0.576	-0.76448
C	6.24312	-0.37787	0.29608
C	4.31442	0.52226	-2.28122
O	4.62269	1.82652	-0.31781
C	4.07734	2.26179	0.91364
H	0.87147	3.74568	2.16541
H	-2.56207	4.61512	0.51223
H	-1.73345	5.22253	-0.92754
H	-0.8267	2.97534	-1.40726
H	0.61305	0.52436	1.28362
H	0.59998	1.37011	2.84273
H	-1.88667	0.16856	1.57791
H	-0.17113	-1.15294	3.72181
H	-0.04342	-1.56706	2.01424
H	-2.54988	-1.88373	3.76129
H	-1.4729	-3.17462	3.26538
H	-3.24998	-1.51141	1.40423
H	-4.53804	-3.62927	1.14271
H	-4.47044	-3.17572	2.85587
H	-3.42072	-4.46591	2.22756
H	-0.94444	-3.02644	-1.83082
H	0.34471	-0.98871	-2.85154
H	-0.30441	-0.05772	-1.52871
H	-3.79047	2.87797	-0.64792
H	-3.1468	3.30924	-2.22834
H	-2.72706	0.57382	-0.93316
H	-2.78102	1.04975	-3.9278
H	-1.3232	1.46717	-3.0385
H	-3.23582	-1.32079	-4.37024
H	-2.07028	-2.60281	-3.73983
H	-5.15916	0.92238	-1.12548
H	-4.9925	1.40254	-2.8233
H	-4.63041	-0.26227	-2.33237

H	-2.68123	0.49334	3.6573
H	0.85418	-4.67166	-0.19049
H	4.81302	-2.58899	0.58476
H	3.0251	0.53021	-0.56388
H	6.69818	-1.29521	0.68069
H	6.82321	-0.03655	-0.57038
H	6.34482	0.40719	1.05365
H	5.3808	0.54827	-2.52924
H	3.83475	1.3896	-2.7453
H	3.8764	-0.39101	-2.69413
H	2.98873	2.40807	0.84154
H	4.28084	1.55645	1.73481
H	4.54714	3.22065	1.14811

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 37

C	1.70988	-2.55687	1.65043
C	0.41912	-2.99071	1.65189
C	-0.25594	-3.39867	0.42664
C	0.63346	-3.38097	-0.81296
C	1.67855	-2.27102	-0.71992
O	2.4356	-2.38176	0.52397
C	2.44252	-2.13239	2.89194
C	2.04778	-0.69488	3.34869
C	2.35555	0.37229	2.29062
C	2.06138	1.80086	2.76475
C	2.45484	2.92441	1.76676
C	1.50212	3.02795	0.57717
C	2.54478	4.28393	2.47137
O	1.58329	1.94077	-0.23253
O	0.77249	3.9699	0.34945
C	0.7772	1.96776	-1.44978
C	1.38891	0.9751	-2.46461

C	-0.64496	1.61594	-1.1284
C	2.90564	0.96142	-2.53878
C	2.65433	-2.28005	-1.89608
C	3.90625	-1.37864	-1.81875
C	3.6689	0.13102	-1.51817
C	3.53983	1.68216	-3.47161
C	4.75604	-1.57929	-3.08234
O	-1.42695	-3.76353	0.38452
O	0.68911	-0.64579	3.76928
C	-1.73104	2.42349	-1.02641
O	-2.80965	1.64457	-0.70408
C	-2.31676	0.36674	-0.61808
N	-1.03088	0.30929	-0.85947
C	-3.16024	-0.75868	-0.27854
C	-4.49817	-0.82469	-0.10675
C	-5.43661	0.3653	-0.22336
C	-5.12827	-2.14271	0.26284
C	-5.587	1.08528	1.1285
O	-6.6939	-0.13124	-0.69064
C	-7.51825	0.84618	-1.28835
H	-0.10927	-3.10103	2.59251
H	1.12646	-4.36062	-0.89931
H	0.0088	-3.24459	-1.70056
H	1.14882	-1.31425	-0.64801
H	2.20502	-2.81466	3.71382
H	3.5208	-2.17482	2.70431
H	2.62315	-0.48392	4.25845
H	1.77258	0.15847	1.38917
H	3.41246	0.28924	2.00147
H	2.62247	1.98776	3.69074
H	1.00216	1.89296	3.03234
H	3.43933	2.66908	1.3493
H	2.81768	5.07866	1.77123

H	3.29843	4.2457	3.26507
H	1.58377	4.55605	2.91896
H	0.82656	2.98794	-1.83686
H	0.9687	1.24555	-3.4407
H	1.00599	-0.02022	-2.23302
H	3.00316	-3.31215	-2.0394
H	2.06846	-2.03575	-2.7931
H	4.4932	-1.73987	-0.96371
H	3.17447	0.21476	-0.54818
H	4.66468	0.57619	-1.39475
H	4.62497	1.71231	-3.53353
H	2.99841	2.27342	-4.20709
H	4.99307	-2.63885	-3.23575
H	4.23465	-1.21675	-3.97563
H	5.70411	-1.03324	-3.00902
H	0.13925	-0.81668	2.98474
H	-1.89889	3.48466	-1.11163
H	-2.58341	-1.67113	-0.15677
H	-5.04185	1.0764	-0.9601
H	-5.83613	-2.4581	-0.51105
H	-4.3693	-2.91764	0.39796
H	-5.71004	-2.05374	1.18966
H	-5.95691	0.39327	1.89205
H	-6.2935	1.91865	1.05025
H	-4.62419	1.48898	1.45518
H	-7.01039	1.34701	-2.12846
H	-8.40009	0.32404	-1.6697
H	-7.85033	1.61696	-0.57664

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 42

C	1.55529	-2.22485	0.98573
C	1.40653	-3.56401	0.82897
C	2.11474	-4.29077	-0.22214
C	3.07546	-3.43073	-1.04976
C	2.56121	-2.00072	-1.18289
O	2.25426	-1.45253	0.12638
C	0.96037	-1.38926	2.08364
C	2.01439	-0.54969	2.84178
C	1.4012	0.58565	3.68029
C	0.67858	1.68859	2.88542
C	1.60473	2.5447	1.9703
C	0.75951	3.11402	0.83955
C	2.32237	3.65648	2.74078
O	0.53552	2.16611	-0.10467
O	0.30055	4.23604	0.79232
C	-0.44079	2.48542	-1.14624
C	-0.17143	1.52655	-2.30922
C	-1.82417	2.33094	-0.58514
C	1.11968	1.75627	-3.08901
C	3.54116	-1.02386	-1.8278
C	3.00455	0.42016	-1.95822
C	2.06988	0.57912	-3.18919
C	1.37094	2.9213	-3.69603
C	4.16148	1.42652	-2.0227
O	2.00669	-5.49598	-0.40619
O	2.85035	-1.38192	3.64287
C	-2.62832	3.27799	-0.03325
O	-3.7844	2.67318	0.36644
C	-3.62794	1.34962	0.03665
N	-2.47721	1.10472	-0.53545
C	-4.74216	0.48781	0.37191
C	-4.83714	-0.84888	0.20598

C	-3.74782	-1.68912	-0.43761
C	-6.08839	-1.57411	0.62341
C	-3.91891	-1.7106	-1.96736
O	-3.83519	-2.99773	0.12877
C	-2.69097	-3.80187	-0.07783
H	0.80782	-4.13306	1.53139
H	4.05267	-3.43011	-0.54519
H	3.21108	-3.89029	-2.03335
H	1.60708	-2.01607	-1.73202
H	0.22932	-0.71704	1.61681
H	0.41644	-2.02931	2.78877
H	2.69806	-0.12224	2.10438
H	2.21579	1.01789	4.2745
H	0.68949	0.15211	4.40015
H	0.17525	2.36406	3.58859
H	-0.11576	1.23836	2.27988
H	2.34143	1.88313	1.50139
H	3.02948	4.19254	2.09939
H	2.88078	3.24142	3.58646
H	1.60013	4.3847	3.12179
H	-0.27961	3.52524	-1.43757
H	-1.02353	1.60793	-2.99602
H	-0.20846	0.50816	-1.91093
H	4.45278	-1.02354	-1.21592
H	3.82645	-1.41556	-2.81419
H	2.42	0.63749	-1.05791
H	2.69108	0.67448	-4.08963
H	1.47658	-0.33722	-3.31905
H	2.26967	3.07402	-4.28789
H	0.6896	3.76743	-3.63371
H	4.76973	1.38796	-1.11127
H	4.82213	1.21442	-2.87401
H	3.78674	2.4492	-2.13509

H	2.29994	-1.76143	4.34741
H	-2.53003	4.33457	0.15495
H	-5.58211	1.02111	0.80944
H	-2.7668	-1.25419	-0.20563
H	-6.84116	-0.88141	1.01063
H	-6.52233	-2.12712	-0.21955
H	-5.85834	-2.32152	1.38982
H	-3.15217	-2.33553	-2.43722
H	-3.81925	-0.69842	-2.36909
H	-4.90143	-2.10971	-2.24126
H	-2.83627	-4.71252	0.50949
H	-2.55652	-4.0864	-1.13138
H	-1.77169	-3.30009	0.26342

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 46

C	-1.23075	2.74529	1.43531
C	-0.00734	3.33445	1.47046
C	0.53849	4.02608	0.30654
C	-0.4065	4.05998	-0.8981
C	-1.20128	2.76264	-0.95634
O	-1.92917	2.56575	0.29274
C	-2.00013	2.31044	2.65116
C	-2.69815	0.93517	2.58197
C	-1.71833	-0.24052	2.56787
C	-2.41385	-1.61239	2.59758
C	-3.13205	-2.04159	1.28388
C	-2.11966	-2.66868	0.3383
C	-4.26612	-3.03416	1.56859
O	-1.41788	-1.7373	-0.34972
O	-1.92328	-3.86373	0.2331
C	-0.35798	-2.24563	-1.22784
C	-0.11491	-1.16634	-2.27838

C	0.87424	-2.55678	-0.42346
C	-1.26357	-0.88348	-3.23934
C	-2.24157	2.63878	-2.06839
C	-2.57663	1.16245	-2.38756
C	-1.58422	0.58308	-3.44261
C	-1.91317	-1.85071	-3.89489
C	-4.02707	0.9854	-2.85275
O	1.62839	4.58547	0.29544
O	-3.51776	0.77467	3.74408
C	1.13418	-3.65597	0.33615
O	2.37157	-3.50569	0.88916
C	2.82727	-2.29593	0.42718
N	1.96625	-1.6992	-0.35642
C	4.15916	-1.92993	0.86268
C	4.8667	-0.82443	0.5448
C	4.36681	0.26803	-0.39657
C	6.26873	-0.65647	1.0699
C	4.6763	-0.08791	-1.85515
O	5.00966	1.51148	-0.1308
C	4.42383	2.2515	0.92758
H	0.53418	3.40479	2.40704
H	-1.08165	4.92248	-0.7994
H	0.17978	4.19798	-1.81137
H	-0.48379	1.93022	-1.01605
H	-1.34594	2.34382	3.52821
H	-2.78369	3.06703	2.81643
H	-3.32094	0.90803	1.67651
H	-1.07784	-0.15425	3.45572
H	-1.06684	-0.1558	1.6909
H	-3.15859	-1.59674	3.39929
H	-1.68425	-2.38694	2.86589
H	-3.54135	-1.15087	0.79284
H	-4.75954	-3.35507	0.6453

H	-5.01538	-2.56935	2.21795
H	-3.88061	-3.92943	2.06543
H	-0.73756	-3.1659	-1.67526
H	0.773	-1.45942	-2.85358
H	0.17628	-0.25234	-1.75163
H	-3.13683	3.18411	-1.74526
H	-1.87427	3.14618	-2.96992
H	-2.45716	0.5917	-1.45776
H	-2.00374	0.74814	-4.4433
H	-0.64371	1.15031	-3.40892
H	-2.6933	-1.6223	-4.61658
H	-1.69259	-2.90555	-3.74847
H	-4.73351	1.30107	-2.07595
H	-4.2298	1.58072	-3.75275
H	-4.2347	-0.06388	-3.09035
H	-4.23367	1.42706	3.69881
H	0.5845	-4.55034	0.57775
H	4.61722	-2.67829	1.50473
H	3.28006	0.37594	-0.2887
H	6.59092	-1.53569	1.6356
H	6.97469	-0.49066	0.24669
H	6.35021	0.22429	1.71668
H	5.75268	-0.22855	-2.00151
H	4.34719	0.72926	-2.50467
H	4.15399	-1.0047	-2.14169
H	3.40263	2.57467	0.68335
H	4.40104	1.68181	1.87008
H	5.04247	3.14153	1.06949

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 47

C	3.07992	-1.86512	-0.18172
C	4.17267	-2.63845	-0.4096
C	5.50231	-2.06141	-0.57467
C	5.53906	-0.53873	-0.44995
C	4.23656	0.08769	-0.94403
O	3.09738	-0.51127	-0.25563
C	1.73767	-2.42015	0.21158
C	1.56278	-2.62349	1.73262
C	1.53049	-1.32856	2.56388
C	0.30782	-0.44422	2.28583
C	0.38372	0.95708	2.93601
C	-0.61142	1.91933	2.28502
C	0.20509	0.94799	4.45738
O	-0.53442	1.83249	0.93591
O	-1.34766	2.68442	2.86958
C	-1.41306	2.66695	0.13312
C	-0.81007	2.70223	-1.28278
C	-2.79356	2.08325	0.14391
C	0.62999	3.18512	-1.37018
C	4.19446	1.60251	-0.73683
C	3.13935	2.44206	-1.49992
C	1.70085	2.1572	-1.02951
C	0.88237	4.45082	-1.72324
C	3.28729	2.31589	-3.02466
O	6.51841	-2.72371	-0.73862
O	0.3499	-3.37222	1.86489
C	-3.9238	2.54983	0.73505
O	-4.92865	1.65761	0.49524
C	-4.34493	0.65436	-0.23869
N	-3.0796	0.8759	-0.48043
C	-5.21257	-0.44703	-0.60257
C	-4.85401	-1.62905	-1.14865

C	-3.41795	-1.99896	-1.50548
C	-5.90577	-2.65672	-1.47647
C	-3.10377	-1.65756	-2.96516
O	-3.19311	-3.39949	-1.34674
C	-2.95821	-3.78838	-0.00391
H	4.08422	-3.71914	-0.38439
H	5.70295	-0.28011	0.60684
H	6.39212	-0.15505	-1.01726
H	4.10899	-0.16756	-2.00552
H	0.94281	-1.77542	-0.17429
H	1.61586	-3.40535	-0.24927
H	2.41253	-3.23304	2.07956
H	2.45154	-0.76665	2.35951
H	1.57159	-1.60415	3.62788
H	-0.60394	-0.95216	2.62389
H	0.20272	-0.31257	1.20791
H	1.37549	1.37359	2.69693
H	0.25338	1.9611	4.86505
H	0.98406	0.34563	4.93604
H	-0.77012	0.5297	4.73031
H	-1.42868	3.66607	0.57735
H	-1.45714	3.35629	-1.87871
H	-0.90169	1.69473	-1.70485
H	4.10194	1.7885	0.3419
H	5.18525	1.97711	-1.02767
H	3.37989	3.48014	-1.23098
H	1.38066	1.18224	-1.42034
H	1.70096	2.02358	0.05845
H	1.88812	4.852	-1.80459
H	0.07585	5.14476	-1.94839
H	4.30879	2.54971	-3.34879
H	3.04993	1.30221	-3.3699
H	2.60586	3.00053	-3.53838

H	0.19668	-3.52245	2.81111
H	-4.16517	3.41404	1.33248
H	-6.26215	-0.2617	-0.38728
H	-2.7274	-1.43757	-0.86445
H	-6.91189	-2.27917	-1.27178
H	-5.85202	-2.9469	-2.53342
H	-5.75276	-3.57763	-0.90325
H	-2.08089	-1.9699	-3.19796
H	-3.19268	-0.57976	-3.12787
H	-3.78348	-2.17938	-3.64731
H	-2.82862	-4.87425	-0.00913
H	-2.04675	-3.32565	0.40262
H	-3.80398	-3.53719	0.65565

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 52

C	0.07107	-2.71796	1.17567
C	-1.03572	-3.18034	0.53624
C	-0.93489	-3.87721	-0.74472
C	0.50062	-4.05154	-1.2496
C	1.30767	-2.82171	-0.86123
O	1.28708	-2.65777	0.58704
C	0.11951	-2.32864	2.62795
C	0.94334	-1.07635	3.00075
C	0.28525	0.23631	2.57034
C	1.07809	1.48564	2.99555
C	2.36977	1.78793	2.18091
C	1.99633	2.50037	0.89035
C	3.34854	2.64855	2.98934
O	1.5996	1.62687	-0.06996
O	2.00568	3.70383	0.73296
C	1.08521	2.21435	-1.30425
C	1.22879	1.1456	-2.38716

C	-0.33566	2.64949	-1.10687
C	2.65595	0.75253	-2.75598
C	2.7783	-2.78603	-1.27268
C	3.30204	-1.33652	-1.39173
C	2.93704	-0.73509	-2.7838
C	3.58718	1.65689	-3.07602
C	4.81081	-1.24138	-1.13748
O	-1.89612	-4.33415	-1.35128
O	1.07198	-1.01768	4.42586
C	-0.81434	3.91312	-0.96581
O	-2.16845	3.84185	-0.8282
C	-2.46272	2.50026	-0.88001
N	-1.40076	1.75675	-1.0523
C	-3.87309	2.18354	-0.75736
C	-4.45686	0.98175	-0.56496
C	-3.69403	-0.32946	-0.42118
C	-5.95993	0.88594	-0.49177
C	-3.77642	-1.18036	-1.69054
O	-4.24287	-1.1177	0.6428
C	-3.9809	-0.59303	1.92975
H	-2.00665	-3.1363	1.01678
H	0.93634	-4.95757	-0.80412
H	0.48588	-4.18508	-2.33528
H	0.78567	-1.94155	-1.26607
H	-0.90021	-2.22819	3.01354
H	0.56841	-3.18108	3.16264
H	1.93644	-1.16336	2.53765
H	-0.70546	0.27748	3.04258
H	0.12514	0.22629	1.48664
H	1.3625	1.36442	4.04555
H	0.42555	2.36684	2.94996
H	2.85155	0.83986	1.91331
H	4.24976	2.87978	2.41199

H	3.64766	2.12037	3.90079
H	2.88532	3.59847	3.27255
H	1.69515	3.09201	-1.52667
H	0.71472	1.51741	-3.28364
H	0.65723	0.27022	-2.06298
H	3.34967	-3.35117	-0.52615
H	2.90497	-3.31084	-2.22874
H	2.79711	-0.74228	-0.61911
H	3.75368	-0.95545	-3.48328
H	2.0494	-1.24664	-3.18152
H	4.58676	1.35894	-3.38201
H	3.39423	2.72707	-3.05322
H	5.0629	-1.57148	-0.12281
H	5.37164	-1.86813	-1.8433
H	5.16063	-0.20956	-1.25303
H	1.62096	-1.76526	4.70862
H	-0.36329	4.89144	-0.92762
H	-4.50806	3.06332	-0.83366
H	-2.63937	-0.11778	-0.20727
H	-6.43121	1.86848	-0.5866
H	-6.34852	0.24228	-1.29134
H	-6.28123	0.42762	0.44945
H	-4.81696	-1.38629	-1.96203
H	-3.27403	-2.13839	-1.52927
H	-3.29363	-0.6573	-2.52224
H	-2.89958	-0.49318	2.11243
H	-4.44423	0.39327	2.0858
H	-4.40242	-1.298	2.65188

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 55

C	-2.51548	2.15526	0.63899
C	-3.06862	3.30755	0.1809
C	-4.05809	3.31611	-0.89132
C	-4.466	1.9259	-1.37748
C	-3.31315	0.93083	-1.27082
O	-2.73679	0.9464	0.06832
C	-1.58168	2.09422	1.81658
C	-2.06543	1.29907	3.06178
C	-2.19143	-0.22462	2.87936
C	-0.88777	-0.92836	2.47408
C	-1.06312	-2.44019	2.17612
C	0.04757	-2.94273	1.25453
C	-1.15675	-3.30646	3.43505
O	0.11101	-2.18414	0.13221
O	0.77099	-3.89292	1.46431
C	1.15693	-2.48344	-0.83908
C	0.73429	-1.81511	-2.15468
C	2.47599	-1.97127	-0.33933
C	-0.51301	-2.38498	-2.82279
C	-3.73688	-0.50714	-1.55928
C	-2.61472	-1.56754	-1.53379
C	-1.77324	-1.5378	-2.83711
C	-0.46778	-3.57502	-3.43313
C	-3.21687	-2.96065	-1.30224
O	-4.57205	4.33406	-1.33562
O	-1.22587	1.62641	4.16974
C	3.45799	-2.64889	0.31158
O	4.4707	-1.77558	0.58044
C	4.04762	-0.5715	0.07448
N	2.86799	-0.64568	-0.48616
C	4.96743	0.53374	0.24457
C	4.76734	1.83327	-0.0618

C	3.49109	2.35049	-0.70173
C	5.85333	2.84496	0.18938
C	3.5713	2.24796	-2.23473
O	3.32071	3.70292	-0.26978
C	2.00437	4.19556	-0.40308
H	-2.8221	4.25192	0.65279
H	-5.31214	1.58392	-0.76337
H	-4.81906	1.99566	-2.4107
H	-2.504	1.24892	-1.94487
H	-0.61942	1.68546	1.47781
H	-1.39713	3.11621	2.15848
H	-3.04868	1.69068	3.34564
H	-2.95288	-0.42057	2.11647
H	-2.56606	-0.62885	3.82764
H	-0.12969	-0.81871	3.26365
H	-0.48837	-0.45175	1.57594
H	-1.98994	-2.54848	1.59357
H	-1.31667	-4.3579	3.18017
H	-1.98522	-2.97591	4.06966
H	-0.23103	-3.24612	4.01676
H	1.20429	-3.5698	-0.94702
H	1.58484	-1.91348	-2.83979
H	0.62209	-0.74353	-1.96312
H	-4.50153	-0.77151	-0.81653
H	-4.24069	-0.5196	-2.53636
H	-1.95283	-1.33751	-0.69446
H	-2.4158	-1.86604	-3.66557
H	-1.48951	-0.49867	-3.05845
H	-1.33422	-3.9928	-3.93946
H	0.43806	-4.17796	-3.45482
H	-3.75263	-3.00476	-0.34621
H	-3.93397	-3.21749	-2.09377
H	-2.44134	-3.73237	-1.29369

H	-0.33522	1.29351	3.97501
H	3.57485	-3.66416	0.65352
H	5.9192	0.23945	0.67915
H	2.64149	1.74588	-0.35787
H	6.75546	2.37157	0.58748
H	6.11663	3.37716	-0.73383
H	5.50812	3.60972	0.89279
H	2.66804	2.65674	-2.70009
H	3.65939	1.20018	-2.53491
H	4.43427	2.80435	-2.61564
H	1.99475	5.1941	0.04222
H	1.6842	4.27868	-1.45212
H	1.27761	3.56103	0.13002

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 56

C	2.21206	2.32299	-1.56363
C	1.9058	3.53712	-1.03635
C	2.65446	4.10055	0.08456
C	3.80011	3.21326	0.58143
C	3.42619	1.7465	0.41676
O	3.08838	1.47215	-0.97442
C	1.68391	1.81321	-2.87765
C	0.72596	0.5882	-2.85985
C	1.38297	-0.69841	-2.34535
C	0.53153	-1.9622	-2.53688
C	1.05507	-3.20449	-1.75128
C	0.53395	-3.17756	-0.31842
C	0.66161	-4.52248	-2.42647
O	1.0121	-2.09679	0.36128
O	-0.23802	-3.97189	0.16976
C	0.3434	-1.72433	1.59515
C	1.09807	-0.50298	2.1515

C	-1.07858	-1.34667	1.29177
C	2.47376	-0.70821	2.7639
C	4.50553	0.7444	0.81831
C	4.08823	-0.74311	0.67816
C	3.58453	-1.39588	1.99358
C	2.69733	-0.26017	4.00681
C	5.25554	-1.58042	0.12966
O	2.44201	5.20965	0.55737
O	-0.47719	0.89963	-2.17094
C	-2.23676	-1.76931	1.85533
O	-3.27095	-1.10352	1.25039
C	-2.68402	-0.29119	0.32205
N	-1.37704	-0.40399	0.31724
C	-3.45891	0.54798	-0.56837
C	-4.77146	0.86365	-0.5268
C	-5.75134	0.37382	0.536
C	-5.3571	1.73562	-1.60827
C	-6.53147	-0.85602	0.06269
O	-6.7154	1.37814	0.85013
C	-6.21017	2.40737	1.68047
H	1.16399	4.16325	-1.51848
H	4.7041	3.4452	-0.0006
H	4.00902	3.44869	1.62931
H	2.50972	1.56914	0.99239
H	1.15211	2.6361	-3.36405
H	2.54788	1.56309	-3.51026
H	0.43631	0.43882	-3.91075
H	1.60547	-0.56664	-1.28589
H	2.3513	-0.83224	-2.84667
H	0.50905	-2.22641	-3.60234
H	-0.50675	-1.75632	-2.25175
H	2.15111	-3.13551	-1.70144
H	1.01163	-5.38588	-1.85283

H	1.0952	-4.57326	-3.43085
H	-0.42631	-4.60548	-2.51435
H	0.36649	-2.57142	2.28715
H	0.4512	-0.05128	2.9112
H	1.13805	0.21741	1.32625
H	5.38523	0.94162	0.19212
H	4.80148	0.96591	1.85205
H	3.27985	-0.79648	-0.05498
H	3.26277	-2.41479	1.73816
H	4.44192	-1.5054	2.67121
H	3.66898	-0.36125	4.48404
H	1.92057	0.22307	4.59493
H	5.57451	-1.21284	-0.85231
H	6.12385	-1.53817	0.80039
H	4.97366	-2.63452	0.01953
H	-0.45543	0.54221	-1.26011
H	-2.49879	-2.49242	2.61055
H	-2.84425	0.94762	-1.37145
H	-5.20473	0.11043	1.44978
H	-5.77147	2.66044	-1.19289
H	-4.6071	1.99299	-2.36077
H	-6.1913	1.22885	-2.11011
H	-7.09695	-0.63503	-0.84822
H	-7.2405	-1.15808	0.8397
H	-5.84864	-1.68659	-0.13874
H	-5.38901	2.96512	1.20535
H	-7.03843	3.09393	1.87426
H	-5.84504	2.00749	2.63959

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 57

C	-2.23629	2.4214	0.49289
C	-2.91479	3.53541	0.11615
C	-4.20037	3.461	-0.5686
C	-4.75034	2.04284	-0.72811
C	-3.63488	1.00948	-0.87028
O	-2.64389	1.16945	0.18375
C	-0.93325	2.46128	1.25362
C	-0.73692	1.45688	2.41946
C	-0.47752	0.03636	1.92725
C	-0.20423	-0.99657	3.03116
C	-0.49519	-2.46883	2.62425
C	0.35248	-2.95034	1.44798
C	-0.32287	-3.41924	3.81434
O	0.01419	-2.30953	0.29975
O	1.21003	-3.80613	1.50338
C	0.78751	-2.61195	-0.89789
C	0.02091	-1.99246	-2.07657
C	2.18163	-2.06493	-0.7967
C	-1.3235	-2.62801	-2.41824
C	-4.14449	-0.42907	-0.78844
C	-3.08913	-1.55319	-0.87506
C	-2.5574	-1.75038	-2.31823
C	-1.39601	-3.89319	-2.84664
C	-3.67876	-2.86073	-0.32674
O	-4.8333	4.44192	-0.93677
O	0.40708	1.84805	3.18686
C	3.34132	-2.74328	-0.59551
O	4.37044	-1.85028	-0.63477
C	3.77659	-0.6319	-0.85126
N	2.47549	-0.71592	-0.96153
C	4.68551	0.4923	-0.95796
C	4.38097	1.80684	-0.93347

C	2.96613	2.34177	-0.74868
C	5.46489	2.83691	-1.12143
C	2.30492	2.66394	-2.0911
O	2.96807	3.54819	0.01542
C	3.19949	3.34336	1.40077
H	-2.52545	4.51758	0.35981
H	-5.35651	1.81467	0.16098
H	-5.41774	2.01263	-1.59456
H	-3.09671	1.18833	-1.81265
H	-0.10696	2.30681	0.54508
H	-0.81689	3.4789	1.64401
H	-1.63209	1.46645	3.06353
H	0.35752	0.06387	1.21895
H	-1.35402	-0.26707	1.35554
H	-0.84634	-0.78496	3.89718
H	0.82704	-0.9092	3.39189
H	-1.53826	-2.50531	2.27884
H	-0.57039	-4.44946	3.54149
H	-0.97527	-3.11289	4.63916
H	0.71189	-3.41348	4.17049
H	0.83925	-3.70004	-0.99024
H	0.68005	-2.06277	-2.95075
H	-0.09225	-0.92372	-1.87074
H	-4.68372	-0.52465	0.16362
H	-4.89518	-0.56195	-1.58085
H	-2.24214	-1.27662	-0.24077
H	-3.36195	-2.17814	-2.93161
H	-2.32071	-0.76926	-2.75488
H	-2.34253	-4.35019	-3.12373
H	-0.51351	-4.52297	-2.94228
H	-3.97728	-2.74882	0.72263
H	-4.56989	-3.16125	-0.89436
H	-2.95234	-3.67646	-0.38804

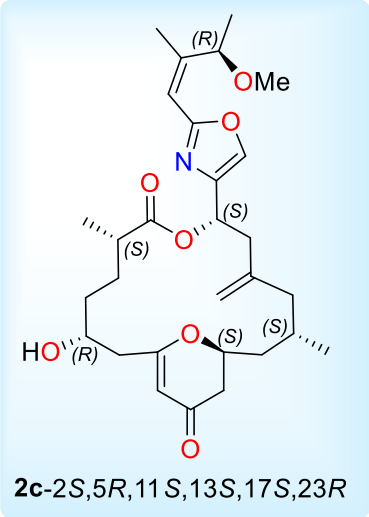
H	0.22395	2.71268	3.58708
H	3.58866	-3.77404	-0.40086
H	5.72486	0.1949	-1.07627
H	2.35994	1.58324	-0.23726
H	6.43649	2.36707	-1.29982
H	5.23583	3.48944	-1.97377
H	5.5468	3.49532	-0.25025
H	2.8884	3.4014	-2.65222
H	1.30819	3.08223	-1.91669
H	2.20838	1.7537	-2.68947
H	2.41844	2.71829	1.85639
H	4.17747	2.87717	1.59533
H	3.18686	4.33258	1.86803

Compound 2b: Isomer 2S, 5R, 11S, 13S, 17S, 23S conformer 63

C	-0.40192	2.3504	1.26978
C	0.12411	3.58867	1.44432
C	-0.42466	4.75602	0.76161
C	-1.68872	4.47536	-0.05689
C	-1.68085	3.06612	-0.64356
O	-1.38653	2.08406	0.38268
C	0.05745	1.09647	1.9669
C	-1.09706	0.19943	2.43315
C	-0.63022	-1.22707	2.76062
C	-1.77331	-2.23994	2.95186
C	-2.71005	-2.47221	1.73108
C	-1.90611	-2.92676	0.51804
C	-3.7935	-3.50593	2.06467
O	-1.45432	-1.87255	-0.20136
O	-1.67155	-4.08445	0.23566
C	-0.56443	-2.16524	-1.33134
C	-0.54768	-0.90283	-2.19502

C	0.80628	-2.53389	-0.83499
C	-1.80349	-0.59879	-3.00383
C	-3.01188	2.65018	-1.27315
C	-3.10856	1.17053	-1.70314
C	-2.25797	0.84702	-2.96426
C	-2.43374	-1.52261	-3.73649
C	-4.57355	0.7711	-1.92861
O	0.03268	5.88655	0.86844
O	-1.68256	0.84504	3.57028
C	1.27587	-3.75863	-0.4748
O	2.57781	-3.61964	-0.09474
C	2.85574	-2.28369	-0.24285
N	1.82813	-1.60158	-0.68134
C	4.20932	-1.89589	0.0961
C	4.77819	-0.67445	0.01081
C	4.05922	0.54748	-0.53439
C	6.21525	-0.48351	0.41558
C	4.17424	0.59668	-2.06911
O	4.64802	1.69194	0.08277
C	3.88768	2.87878	-0.03233
H	0.93098	3.74078	2.15236
H	-2.55438	4.59622	0.61065
H	-1.77745	5.22501	-0.84895
H	-0.86079	2.99026	-1.37346
H	0.66661	0.52486	1.25297
H	0.69391	1.35682	2.81866
H	-1.82481	0.15735	1.61656
H	-0.03298	-1.18997	3.68079
H	0.03446	-1.57673	1.96344
H	-2.40708	-1.92761	3.7943
H	-1.34584	-3.20804	3.24226
H	-3.18559	-1.52177	1.46442
H	-4.49377	-3.63166	1.23229

H	-4.36364	-3.18954	2.94498
H	-3.34413	-4.48139	2.27192
H	-0.9944	-3.01776	-1.86047
H	0.30444	-0.98358	-2.88237
H	-0.31088	-0.0622	-1.53569
H	-3.80278	2.85548	-0.53917
H	-3.20448	3.31001	-2.13104
H	-2.72384	0.56587	-0.87496
H	-2.84214	1.08855	-3.86151
H	-1.36884	1.49216	-2.99128
H	-3.29586	-1.27038	-4.34849
H	-2.1162	-2.56242	-3.76659
H	-5.16328	0.89092	-1.01202
H	-5.03776	1.39001	-2.70793
H	-4.64777	-0.27571	-2.24196
H	-2.54591	0.43722	3.73476
H	0.84279	-4.74323	-0.41676
H	4.81285	-2.72692	0.45175
H	2.9951	0.49463	-0.26899
H	6.67162	-1.42801	0.72557
H	6.80389	-0.06343	-0.40998
H	6.28758	0.23759	1.23635
H	5.22504	0.62102	-2.37713
H	3.679	1.48769	-2.46899
H	3.6937	-0.2812	-2.51019
H	3.854	3.26216	-1.06257
H	2.85385	2.73697	0.31869
H	4.37543	3.62657	0.59855



2c-2*S*,5*R*,11*S*,13*S*,17*S*,23*R*

Calculated DFT energies of the 2c-diasteroisomer

Conformers **2c**	OPLS2008 Force Field Conformotional Search Relative Energy (kcal/mol)	B3LYP/6-31+G(d,p) DFT Energy (hartree)	Δ (DFT Energy) (kcal/mol)	% Population
2c27	3.033771511	-1710.457316	0	31.66
2c3	0.665033461	-1710.456605	0.44615918	14.90
2c10	1.587858509	-1710.456251	0.6682975	10.24
2c1	0	-1710.456055	0.79128934	8.31
2c49	4.037237094	-1710.455728	0.99648491	5.88
2c38	3.522538241	-1710.455608	1.07178604	5.18
2c23	2.803417782	-1710.455529	1.12135928	4.76
2c7	1.343140535	-1710.455497	1.14143958	4.60
2c30	3.134942639	-1710.454966	1.47464707	2.62
2c16	2.067710325	-1710.454909	1.5104151	2.47
2c22	2.673087954	-1710.454587	1.71247313	1.75
2c51	4.068618547	-1710.454511	1.76016384	1.62
2c52	4.156716061	-1710.454278	1.90637353	1.26
2c13	1.850860421	-1710.454269	1.91202111	1.25
2c42	3.694694073	-1710.453716	2.25903381	0.70
2c46	3.740248566	-1710.453422	2.44352157	0.51
2c57	4.662165392	-1710.453352	2.48744723	0.47
2c11	1.756835564	-1710.453154	2.61169409	0.38
2c55	4.470984704	-1710.452868	2.79116177	0.28
2c29	3.091037285	-1710.452806	2.83006735	0.27
2c31	3.143283939	-1710.452093	3.27748155	0.12
2c58	4.684369025	-1710.452083	3.28375664	0.12
2c19	2.379732314	-1710.452035	3.31387709	0.12
2c12	1.842997132	-1710.451995	3.33897747	0.11

24 conformers counting for the 99.58% of the DFT conformational population

DFT COORDINATES FOR CONFORMATIONAL SEARCH OF 2c

(2*S*, 5*R*, 11*S*, 13*S* , 17*S*, 23*R*)

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 1

C	-2.78941	1.3837	1.26069
C	-3.719	2.19976	1.82011
C	-4.92354	2.59881	1.09399
C	-5.07342	1.95431	-0.28648
C	-3.71604	1.6918	-0.93558
O	-2.85075	0.96248	-0.02468
C	-1.60595	0.78632	1.96638
C	-1.7275	-0.75212	2.07559
C	-0.41494	-1.40686	2.503
C	-0.47684	-2.94303	2.5511
C	-0.80364	-3.67487	1.21944
C	0.3051	-3.48493	0.19306
C	-1.03276	-5.17153	1.46749
O	0.20625	-2.28942	-0.44625
O	1.18577	-4.28867	-0.03541
C	1.24332	-1.99936	-1.43554
C	0.70312	-0.91046	-2.37544
C	2.51377	-1.58387	-0.75301
C	-0.61251	-1.26401	-3.04904
C	-3.80923	0.90525	-2.24382
C	-2.48369	0.51452	-2.95062
C	-1.89013	-0.80057	-2.37073
C	-0.63374	-1.95145	-4.19649
C	-1.48023	1.67678	-2.9921
O	-5.78341	3.33394	1.55945
O	-2.72085	-1.1189	3.03247
C	3.60545	-2.34131	-0.46571

O	4.51967	-1.54968	0.16385
C	3.92989	-0.31256	0.23805
N	2.73181	-0.29189	-0.28702
C	4.72791	0.7156	0.87598
C	4.48196	2.04149	0.93867
C	3.25451	2.70446	0.32549
C	5.43147	2.94946	1.67695
C	2.14842	2.9059	1.36457
O	3.57224	3.99599	-0.19621
C	4.2466	3.95191	-1.43914
H	-3.60167	2.5365	2.84411
H	-5.61885	1.00699	-0.16222
H	-5.6877	2.6032	-0.91782
H	-3.21623	2.65516	-1.11092
H	-0.70291	1.03177	1.3933
H	-1.50935	1.21272	2.96972
H	-2.00549	-1.12933	1.08231
H	-0.15639	-1.03971	3.50526
H	0.37481	-1.07389	1.82128
H	-1.2466	-3.23458	3.2738
H	0.47815	-3.32862	2.932
H	-1.7158	-3.23782	0.79792
H	-1.28555	-5.69551	0.54002
H	-1.85449	-5.3125	2.17734
H	-0.13291	-5.64047	1.87661
H	1.41985	-2.92373	-1.99025
H	1.48302	-0.74406	-3.12844
H	0.61291	0.01919	-1.80599
H	-4.40698	0.00072	-2.06722
H	-4.39753	1.53422	-2.92602
H	-2.75521	0.2899	-3.99214
H	-1.70844	-0.67467	-1.30209
H	-2.65713	-1.5796	-2.47254

H	-1.56777	-2.23711	-4.67547
H	0.27912	-2.25944	-4.70213
H	-1.94536	2.58386	-3.39798
H	-1.0933	1.91536	-1.99486
H	-0.62747	1.43125	-3.63297
H	-3.55328	-0.688	2.77954
H	3.85666	-3.38072	-0.59853
H	5.6266	0.32623	1.34847
H	2.86319	2.06965	-0.47882
H	6.24956	2.38565	2.13429
H	5.8566	3.70742	1.01004
H	4.909	3.50211	2.46834
H	1.29705	3.4103	0.89652
H	1.81988	1.93897	1.75691
H	2.49631	3.52669	2.19678
H	5.22419	3.45023	-1.36918
H	3.64833	3.43243	-2.20389
H	4.40339	4.98754	-1.75273

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 3

C	1.8576	2.12526	-1.24422
C	2.90328	2.88424	-1.66826
C	3.59038	3.80602	-0.76921
C	2.94392	3.93462	0.61219
C	2.30164	2.62653	1.08077
O	1.44006	2.07371	0.0408
C	1.07889	1.17618	-2.10896
C	1.71141	-0.23828	-2.0751
C	0.78088	-1.30434	-2.65111
C	1.37052	-2.7258	-2.62988
C	1.85565	-3.26772	-1.25696
C	0.71017	-3.34601	-0.25653

C	2.50182	-4.64988	-1.42146
O	0.51724	-2.16302	0.37962
O	0.03017	-4.33096	-0.05011
C	-0.59404	-2.09556	1.33008
C	-0.31945	-0.88742	2.22919
C	-1.9043	-1.98204	0.60236
C	0.89036	-1.00056	3.15208
C	3.3273	1.57438	1.53138
C	2.75788	0.18017	1.86454
C	1.85037	0.17233	3.12402
C	1.07066	-2.04414	3.968
C	3.89525	-0.84009	2.01191
O	4.55932	4.47958	-1.093
O	2.92792	-0.27351	-2.81805
C	-2.72234	-2.9795	0.1704
O	-3.80416	-2.41092	-0.43409
C	-3.59591	-1.05758	-0.34109
N	-2.47117	-0.75999	0.25674
C	-4.6389	-0.22746	-0.9114
C	-4.80421	1.10593	-0.77925
C	-3.86897	1.99766	0.02869
C	-5.94957	1.7965	-1.4736
C	-2.85043	2.70649	-0.8671
O	-4.59663	3.01869	0.71462
C	-5.27523	2.55173	1.86493
H	3.19423	2.86922	-2.71333
H	3.69388	4.27869	1.33048
H	2.17727	4.71863	0.53915
H	1.60003	2.83055	1.89375
H	0.05291	1.12496	-1.7284
H	1.05679	1.5289	-3.14496
H	1.90627	-0.48574	-1.0247
H	0.54662	-1.04408	-3.6921

H	-0.16072	-1.26783	-2.09166
H	2.23465	-2.75321	-3.30215
H	0.62728	-3.4247	-3.03567
H	2.59806	-2.56882	-0.85702
H	2.89292	-5.02317	-0.4692
H	3.33116	-4.59427	-2.13431
H	1.77228	-5.37772	-1.78868
H	-0.58387	-3.02863	1.89717
H	-1.22019	-0.72164	2.83464
H	-0.2306	-0.00735	1.58495
H	4.08852	1.46377	0.74747
H	3.85194	1.98694	2.40541
H	2.14129	-0.13064	1.01572
H	2.48153	0.16678	4.02228
H	1.26	1.09857	3.16293
H	1.91748	-2.09496	4.64757
H	0.3825	-2.88607	3.99845
H	4.47851	-0.92242	1.08683
H	4.58546	-0.55	2.81515
H	3.49879	-1.83209	2.25123
H	3.53174	0.37717	-2.42299
H	-2.66874	-4.05541	0.18512
H	-5.35656	-0.78925	-1.50472
H	-3.32317	1.38449	0.75588
H	-6.55022	1.09091	-2.05482
H	-6.60056	2.3059	-0.75497
H	-5.58181	2.57584	-2.15373
H	-2.19247	3.32869	-0.25271
H	-2.24294	1.97058	-1.40187
H	-3.34971	3.35219	-1.59695
H	-6.04267	1.80024	1.62331
H	-4.57765	2.10802	2.59245
H	-5.76139	3.41841	2.321

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 7

C	-1.83637	-2.14743	-1.2671
C	-2.8184	-3.00451	-1.64015
C	-3.4011	-3.95222	-0.69881
C	-2.72637	-3.97239	0.67555
C	-2.18226	-2.60029	1.08028
O	-1.3803	-2.0298	0.00359
C	-1.12827	-1.18676	-2.1795
C	-1.70131	0.24758	-2.08485
C	-0.74207	1.29408	-2.6691
C	-1.30526	2.7263	-2.67519
C	-1.80679	3.29328	-1.3196
C	-0.67879	3.37784	-0.29984
C	-2.43699	4.67859	-1.51612
O	-0.50394	2.20049	0.35
O	-0.00185	4.36353	-0.08751
C	0.57021	2.14575	1.34249
C	0.25555	0.95326	2.2485
C	1.90729	2.01986	0.6693
C	-0.98734	1.08697	3.1238
C	-3.27653	-1.60828	1.50189
C	-2.78638	-0.18157	1.82257
C	-1.92489	-0.10373	3.11284
C	-1.21542	2.16174	3.88546
C	-3.97266	0.78884	1.90513
O	-4.30693	-4.72647	-0.98039
O	-3.00669	0.32258	-2.65742
C	2.76746	3.00911	0.30679
O	3.86582	2.43219	-0.25904
C	3.62214	1.08194	-0.21663
N	2.46267	0.79494	0.31648
C	4.67506	0.24366	-0.75541
C	4.77866	-1.10126	-0.69606

C	3.74083	-2.00135	-0.03608
C	5.95305	-1.79653	-1.33484
C	2.76555	-2.57856	-1.06501
O	4.36072	-3.11169	0.6154
C	4.95096	-2.77804	1.85714
H	-3.16479	-3.01961	-2.66709
H	-3.43691	-4.34462	1.41947
H	-1.90123	-4.69641	0.6216
H	-1.45556	-2.71623	1.88907
H	-0.06959	-1.16709	-1.8952
H	-1.19057	-1.53822	-3.21667
H	-1.85538	0.47928	-1.03035
H	-0.49006	1.01981	-3.7057
H	0.19619	1.24856	-2.10357
H	-2.16029	2.76375	-3.35982
H	-0.54514	3.40691	-3.08049
H	-2.56225	2.60668	-0.92377
H	-2.8343	5.07151	-0.57461
H	-3.26019	4.61871	-2.23581
H	-1.69674	5.39347	-1.88756
H	0.54192	3.08814	1.89307
H	1.13191	0.78974	2.88976
H	0.1842	0.065	1.61309
H	-4.02662	-1.5511	0.70276
H	-3.78957	-2.03663	2.37529
H	-2.15511	0.13784	0.98803
H	-2.5878	-0.07213	3.98725
H	-1.32078	-1.01646	3.21364
H	-2.087	2.2244	4.53188
H	-0.54569	3.01872	3.90296
H	-4.51838	0.82773	0.95512
H	-4.68108	0.48077	2.68561
H	-3.63157	1.80205	2.14251

H	-2.92343	0.15075	-3.61004
H	2.73744	4.0853	0.34951
H	5.45811	0.80889	-1.25534
H	3.16714	-1.41903	0.69481
H	6.61681	-1.08516	-1.83471
H	6.53254	-2.35754	-0.59359
H	5.61669	-2.53335	-2.07564
H	2.02164	-3.20028	-0.55758
H	2.25037	-1.76789	-1.58863
H	3.28977	-3.19865	-1.79975
H	5.76412	-2.04324	1.75148
H	4.20812	-2.36886	2.55955
H	5.36231	-3.70208	2.27238

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 10

C	2.21585	-2.08652	0.78186
C	2.52339	-3.39761	0.61015
C	3.4612	-3.83187	-0.42452
C	4.10263	-2.692	-1.22304
C	3.16289	-1.49566	-1.34518
O	2.66583	-1.10853	-0.03671
C	1.38259	-1.50445	1.886
C	2.22258	-0.60651	2.83021
C	1.37638	0.34183	3.68592
C	0.53943	1.371	2.90639
C	1.35381	2.38183	2.04595
C	0.43209	2.94441	0.97293
C	1.97854	3.50251	2.88161
O	0.25559	2.03288	-0.01952
O	-0.11202	4.0278	0.99607
C	-0.78026	2.3188	-1.00831
C	-0.49288	1.43109	-2.22719

C	-2.12546	2.04512	-0.40349
C	0.69432	1.84184	-3.09451
C	3.80405	-0.24527	-1.94224
C	2.87932	0.99113	-2.01479
C	1.86712	0.88401	-3.18621
C	0.6651	2.98337	-3.7918
C	3.71438	2.27398	-2.12844
O	3.76831	-5.00102	-0.61279
O	2.97383	-1.40476	3.7427
C	-3.01688	2.93017	0.11549
O	-4.09337	2.22956	0.57482
C	-3.80091	0.91413	0.31244
N	-2.63526	0.75984	-0.26068
C	-4.81104	-0.04075	0.72233
C	-4.85943	-1.363	0.45371
C	-3.80376	-2.10074	-0.36162
C	-5.98508	-2.20203	1.00122
C	-2.75966	-2.76391	0.54061
O	-4.39302	-3.1383	-1.14732
C	-5.04623	-2.66394	-2.30896
H	2.10411	-4.14826	1.27087
H	5.02579	-2.39127	-0.70572
H	4.38882	-3.06585	-2.21071
H	2.27784	-1.79807	-1.92464
H	0.59038	-0.91181	1.41427
H	0.91886	-2.29874	2.47901
H	2.90982	-0.01295	2.21048
H	2.0615	0.84624	4.37789
H	0.7041	-0.26243	4.30931
H	-0.06789	1.94181	3.62045
H	-0.1719	0.84511	2.26043
H	2.13878	1.83234	1.51446
H	2.59791	4.16104	2.26389

H	2.61062	3.08782	3.67369
H	1.19915	4.11671	3.3427
H	-0.70914	3.3777	-1.26658
H	-1.39979	1.44165	-2.84397
H	-0.38331	0.40237	-1.87036
H	4.68237	-0.00261	-1.32909
H	4.18278	-0.49563	-2.94336
H	2.31229	1.03754	-1.07961
H	2.40731	1.05342	-4.12747
H	1.4738	-0.14119	-3.23546
H	1.4846	3.27825	-4.44199
H	-0.18023	3.66735	-3.74591
H	4.36454	2.39947	-1.2545
H	4.35593	2.25139	-3.01978
H	3.0722	3.15738	-2.20079
H	3.51516	-2.0195	3.22099
H	-3.02608	3.99917	0.25291
H	-5.60435	0.40386	1.31843
H	-3.29002	-1.38885	-1.01913
H	-6.65804	-1.60939	1.62756
H	-6.56806	-2.66069	0.19523
H	-5.59536	-3.03308	1.60287
H	-2.04325	-3.31471	-0.0768
H	-2.22311	-2.00379	1.11598
H	-3.22784	-3.47072	1.23358
H	-5.89056	-1.99756	-2.07348
H	-4.35216	-2.11871	-2.96749
H	-5.42641	-3.54045	-2.84057

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 11

C	-1.39546	-1.94654	-2.15565
C	-0.1021	-2.36063	-2.16974
C	0.46368	-3.14762	-1.08162
C	-0.53462	-3.51026	0.01551
C	-1.58398	-2.41301	0.16913
O	-2.23279	-2.15262	-1.11167
C	-2.05137	-1.1779	-3.2639
C	-2.36502	0.29946	-2.90722
C	-1.10702	1.11432	-2.59011
C	-1.36179	2.61793	-2.38788
C	-2.21031	3.0256	-1.15251
C	-1.40139	2.90347	0.13293
C	-2.72009	4.46671	-1.29772
O	-1.48761	1.65798	0.66853
O	-0.75366	3.79877	0.63374
C	-0.79875	1.44449	1.93777
C	-1.46628	0.25518	2.66429
C	0.65636	1.19349	1.68127
C	-2.98451	0.22995	2.61718
C	-2.65338	-2.74599	1.20822
C	-3.90863	-1.84866	1.26775
C	-3.66397	-0.31494	1.36939
C	-3.69462	0.70179	3.64932
C	-4.8465	-2.35301	2.37408
O	1.63105	-3.52586	-1.05107
O	-3.0049	0.92707	-4.01941
C	1.72471	2.00075	1.90272
O	2.84843	1.34026	1.48505
C	2.39838	0.13874	0.99951
N	1.09979	0.00996	1.1076
C	3.29422	-0.8539	0.44429
C	4.62097	-0.79446	0.1978

C	5.51134	0.40846	0.49625
C	5.31297	-2.00561	-0.37674
C	6.23312	0.25819	1.83872
O	6.525	0.56415	-0.49808
C	6.04394	1.10819	-1.71222
H	0.53012	-2.13417	-3.02081
H	-1.01616	-4.46288	-0.25067
H	0.00552	-3.66232	0.95467
H	-1.06287	-1.48255	0.41835
H	-1.41858	-1.19617	-4.15654
H	-2.99911	-1.67506	-3.51662
H	-3.03628	0.30473	-2.03591
H	-0.40951	0.99958	-3.43108
H	-0.61683	0.67869	-1.71286
H	-1.87561	2.99823	-3.27645
H	-0.3982	3.14079	-2.33218
H	-3.06652	2.34665	-1.07055
H	-3.32391	4.76693	-0.43488
H	-3.33689	4.55653	-2.19794
H	-1.88253	5.1663	-1.37514
H	-0.91824	2.36044	2.52075
H	-1.12692	0.30983	3.70556
H	-1.04964	-0.66768	2.25664
H	-2.99306	-3.77669	1.03499
H	-2.15155	-2.7567	2.18587
H	-4.42598	-1.98074	0.30807
H	-3.09771	-0.00047	0.48974
H	-4.65124	0.15799	1.28731
H	-4.78167	0.72305	3.63557
H	-3.21664	1.08874	4.54678
H	-5.07605	-3.4172	2.24269
H	-4.39892	-2.22393	3.36614
H	-5.79552	-1.8038	2.36572

H	-3.85405	0.48249	-4.16715
H	1.85731	2.99647	2.29354
H	2.765	-1.76933	0.19426
H	4.90355	1.32049	0.52584
H	4.60151	-2.81303	-0.56766
H	5.83008	-1.76055	-1.31044
H	6.08679	-2.37591	0.3091
H	6.87996	1.1253	2.00529
H	5.50833	0.19269	2.65584
H	6.85721	-0.64114	1.84912
H	5.29648	0.46023	-2.19473
H	5.59091	2.10024	-1.55735
H	6.90536	1.21101	-2.37769

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 12

C	0.62154	-2.32543	1.88626
C	-0.47976	-2.8835	1.31209
C	-0.41786	-3.55285	0.02082
C	0.98805	-3.64719	-0.56272
C	1.81042	-2.41861	-0.1776
O	1.82543	-2.25308	1.27538
C	0.59078	-1.65976	3.23346
C	0.05788	-0.19476	3.17579
C	0.97864	0.74647	2.38963
C	0.56658	2.22108	2.49073
C	1.48258	3.21884	1.72589
C	1.22374	3.17246	0.22345
C	1.30119	4.6518	2.24012
O	1.6658	2.00963	-0.31806
O	0.68379	4.04545	-0.42269
C	1.36485	1.77379	-1.72712
C	2.29264	0.6463	-2.24278

C	-0.08635	1.40613	-1.8383
C	3.69884	0.63605	-1.66732
C	3.24553	-2.49002	-0.69994
C	4.28061	-1.47346	-0.17192
C	3.90111	0.03161	-0.28372
C	4.71357	1.16663	-2.36038
C	5.64802	-1.77062	-0.80525
O	-1.396	-4.02901	-0.54903
O	-1.28018	-0.1508	2.68789
C	-1.15256	2.16104	-2.20738
O	-2.28494	1.41075	-2.03423
C	-1.84698	0.21106	-1.53854
N	-0.54486	0.16305	-1.42005
C	-2.75976	-0.8651	-1.19874
C	-4.06577	-0.81607	-0.86021
C	-4.88975	0.4637	-0.76405
C	-4.78326	-2.09958	-0.52204
C	-5.92042	0.57669	-1.88915
O	-5.61658	0.5049	0.46564
C	-4.80922	0.7952	1.59437
H	-1.42103	-2.88428	1.85016
H	1.46802	-4.55923	-0.17823
H	0.92085	-3.74158	-1.65066
H	1.29149	-1.53009	-0.55435
H	-0.07079	-2.22437	3.89738
H	1.5983	-1.6638	3.6634
H	-0.0171	0.15066	4.2142
H	0.98435	0.43432	1.341
H	2.00809	0.62776	2.75559
H	0.57966	2.51946	3.5481
H	-0.47106	2.3384	2.15583
H	2.52424	2.90498	1.87979
H	1.93933	5.35431	1.69572

H	1.55576	4.7053	3.30401
H	0.26577	4.98271	2.11357
H	1.56021	2.70837	-2.25748
H	2.33408	0.75739	-3.33265
H	1.79882	-0.30814	-2.04907
H	3.63601	-3.49498	-0.48823
H	3.17968	-2.41854	-1.79505
H	4.36951	-1.65426	0.90774
H	3.00294	0.1983	0.31212
H	4.70491	0.58714	0.21666
H	5.72511	1.19832	-1.96319
H	4.5709	1.59549	-3.34995
H	5.94585	-2.81171	-0.63222
H	5.6321	-1.60025	-1.88783
H	6.4266	-1.12662	-0.37933
H	-1.2588	-0.44277	1.75953
H	-1.28262	3.17129	-2.55923
H	-2.26341	-1.83157	-1.18753
H	-4.22428	1.33422	-0.81003
H	-5.53877	-2.33706	-1.28352
H	-4.08588	-2.93938	-0.45923
H	-5.32147	-2.00018	0.42619
H	-6.48382	1.50804	-1.77598
H	-5.42319	0.57872	-2.86439
H	-6.62919	-0.25656	-1.85636
H	-4.04642	0.02589	1.78181
H	-4.29853	1.76466	1.48377
H	-5.47989	0.84431	2.45621

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 13

C	-1.93528	-2.03967	-1.29909
C	-3.01994	-2.73925	-1.72667
C	-3.75251	-3.63129	-0.83333
C	-3.11258	-3.80219	0.54673
C	-2.40439	-2.53134	1.02256
O	-1.51317	-2.02051	-0.01402
C	-1.10746	-1.12737	-2.1573
C	-1.64797	0.3237	-2.09418
C	-0.64953	1.34057	-2.64509
C	-1.16091	2.79205	-2.6246
C	-1.65149	3.349	-1.25975
C	-0.52628	3.38164	-0.23375
C	-2.24056	4.75536	-1.43305
O	-0.37685	2.18489	0.38849
O	0.17194	4.34645	0.00432
C	0.70524	2.08101	1.36972
C	0.37759	0.86876	2.24574
C	2.03547	1.94912	0.68276
C	-0.83863	1.01045	3.15643
C	-3.37575	-1.42955	1.47479
C	-2.73662	-0.07022	1.82556
C	-1.84574	-0.12103	3.0953
C	-0.98581	2.04346	3.99232
C	-3.82105	1.00694	1.96951
O	-4.75442	-4.25269	-1.16076
O	-2.8579	0.44992	-2.83852
C	2.88892	2.93469	0.29499
O	3.98248	2.35127	-0.27386
C	3.7444	1.00161	-0.20562
N	2.59161	0.71963	0.34569
C	4.79234	0.15539	-0.73841
C	4.89853	-1.18733	-0.64733

C	3.85693	-2.05644	0.03371
C	6.07164	-1.89888	-1.26628
C	2.76215	-2.47791	-0.96092
O	4.5385	-3.19104	0.57622
C	3.8408	-3.84169	1.61678
H	-3.31193	-2.70045	-2.7708
H	-3.87862	-4.11254	1.26337
H	-2.38689	-4.62378	0.46767
H	-1.71627	-2.77396	1.83638
H	-0.07626	-1.14996	-1.78876
H	-1.11857	-1.46291	-3.19908
H	-1.83035	0.56204	-1.03953
H	-0.40862	1.07535	-3.68334
H	0.2767	1.24887	-2.06658
H	-2.00515	2.87168	-3.31751
H	-0.3712	3.45252	-3.00638
H	-2.42904	2.67868	-0.87792
H	-2.63026	5.14394	-0.48641
H	-3.06099	4.73184	-2.15786
H	-1.4782	5.45445	-1.78932
H	0.69738	3.00678	1.94853
H	1.26406	0.66255	2.85947
H	0.26653	0.00235	1.58638
H	-4.12335	-1.27257	0.68578
H	-3.92906	-1.82066	2.34101
H	-2.09456	0.21508	0.98679
H	-2.48789	-0.10406	3.98566
H	-1.29506	-1.07181	3.12587
H	-1.83793	2.11511	4.66332
H	-0.26397	2.8553	4.04816
H	-4.38726	1.12826	1.0382
H	-4.53559	0.74521	2.76109
H	-3.37669	1.97446	2.2241

H	-3.50266	-0.16942	-2.45816
H	2.85645	4.01119	0.3216
H	5.57378	0.70836	-1.25331
H	3.38678	-1.48707	0.84575
H	6.73467	-1.19998	-1.78433
H	6.64151	-2.43418	-0.49983
H	5.73734	-2.65894	-1.98442
H	2.00866	-3.10448	-0.47162
H	2.25749	-1.59066	-1.35335
H	3.19304	-3.04321	-1.79415
H	3.60956	-3.15116	2.44355
H	2.90055	-4.30049	1.27599
H	4.49695	-4.63292	1.98989

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 16

C	0.75335	2.29315	-1.3455
C	0.33555	3.56035	-1.58824
C	0.92527	4.70726	-0.90198
C	2.09411	4.36488	0.02837
C	1.94436	2.97297	0.63619
O	1.67627	1.99232	-0.39992
C	0.25515	1.04805	-2.03283
C	1.37268	0.03355	-2.35286
C	0.81502	-1.32648	-2.77373
C	1.86729	-2.44731	-2.82932
C	2.64174	-2.74614	-1.51403
C	1.68554	-3.06872	-0.37281
C	3.6266	-3.90472	-1.71978
O	1.29364	-1.94567	0.28084
O	1.29584	-4.181	-0.08011
C	0.30165	-2.10579	1.34497
C	0.35844	-0.82141	2.17477

C	-1.06459	-2.34835	0.76679
C	1.5833	-0.61975	3.05953
C	3.18386	2.48207	1.38604
C	3.13526	1.01017	1.85039
C	2.16327	0.7813	3.04359
C	2.08734	-1.58684	3.83278
C	4.54381	0.5106	2.20157
O	0.57163	5.86421	-1.08577
O	2.2172	0.49183	-3.4125
C	-1.66449	-3.53714	0.49122
O	-2.91057	-3.2817	0.0019
C	-3.02293	-1.9137	-0.0002
N	-1.94076	-1.31945	0.43374
C	-4.30266	-1.40812	-0.46016
C	-4.79408	-0.15347	-0.37634
C	-4.03746	1.01883	0.23647
C	-6.16818	0.1517	-0.91521
C	-3.51169	1.97889	-0.8335
O	-4.89192	1.78764	1.08727
C	-5.16016	1.16749	2.33065
H	-0.42236	3.74849	-2.34037
H	3.02126	4.41721	-0.56145
H	2.16282	5.12664	0.81081
H	1.06045	2.96346	1.29107
H	-0.45682	0.56252	-1.34957
H	-0.28355	1.31789	-2.94711
H	1.95979	-0.09599	-1.43934
H	0.36225	-1.22166	-3.76851
H	0.00806	-1.60183	-2.0861
H	2.61444	-2.19508	-3.59038
H	1.37897	-3.37443	-3.15677
H	3.1977	-1.84665	-1.22866
H	4.23012	-4.08027	-0.82292

H	4.30475	-3.67956	-2.54965
H	3.09059	-4.8308	-1.94731
H	0.59526	-2.98145	1.92732
H	-0.53962	-0.79401	2.80619
H	0.25208	0.01802	1.48079
H	4.04815	2.61321	0.72078
H	3.34894	3.14796	2.24484
H	2.77467	0.41399	1.0054
H	2.69544	0.98444	3.98167
H	1.33538	1.50213	2.99493
H	2.92791	-1.40139	4.49637
H	1.68395	-2.59663	3.84601
H	5.21172	0.56226	1.33348
H	4.99002	1.11363	3.00352
H	4.51404	-0.53052	2.54005
H	2.71676	1.25453	-3.082
H	-1.35501	-4.56731	0.5523
H	-4.9228	-2.18122	-0.90814
H	-3.18965	0.63704	0.81761
H	-6.65404	-0.74465	-1.311
H	-6.80425	0.58745	-0.13744
H	-6.11742	0.89629	-1.72029
H	-2.93978	2.78256	-0.36009
H	-2.86154	1.44962	-1.53659
H	-4.33769	2.43189	-1.39108
H	-5.70114	0.21563	2.21618
H	-4.23316	0.97085	2.89162
H	-5.78204	1.86097	2.90309

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 19

C	1.39845	-1.97502	2.12917
C	0.10633	-2.39364	2.14433
C	-0.46458	-3.16399	1.04748
C	0.53041	-3.51432	-0.0565
C	1.57536	-2.41178	-0.2034
O	2.22871	-2.1614	1.07607
C	2.06172	-1.23261	3.25085
C	2.38342	0.23958	2.91909
C	1.12621	1.06611	2.59622
C	1.37681	2.57369	2.41703
C	2.22113	3.00631	1.18606
C	1.40106	2.90591	-0.09639
C	2.72967	4.44597	1.35043
O	1.48994	1.67427	-0.65494
O	0.74749	3.8112	-0.57049
C	0.79501	1.47731	-1.92519
C	1.46042	0.29546	-2.66561
C	-0.65901	1.22415	-1.66652
C	2.97869	0.26682	-2.61804
C	2.64132	-2.73126	-1.25075
C	3.89803	-1.83537	-1.30104
C	3.65632	-0.2998	-1.37898
C	3.68992	0.75431	-3.6421
C	4.83206	-2.32484	-2.41722
O	-1.63372	-3.53719	1.0132
O	3.06041	0.72765	4.08155
C	-1.73017	2.02806	-1.88673
O	-2.85146	1.36233	-1.47124
C	-2.39722	0.16109	-0.98823
N	-1.0981	0.0378	-1.09589
C	-3.28898	-0.83722	-0.43685
C	-4.61673	-0.78575	-0.1938

C	-5.51312	0.41265	-0.4922
C	-5.30302	-2.00249	0.37566
C	-6.22991	0.26097	-1.83722
O	-6.53066	0.5604	0.49922
C	-6.05654	1.10339	1.7165
H	-0.52104	-2.18227	3.00283
H	1.01676	-4.46709	0.20015
H	-0.01239	-3.66046	-0.99509
H	1.04949	-1.48094	-0.44193
H	1.42622	-1.26259	4.14158
H	3.00861	-1.72579	3.50154
H	3.06716	0.25036	2.05752
H	0.419	0.93858	3.4267
H	0.64412	0.65217	1.7035
H	1.877	2.95667	3.31706
H	0.41374	3.09766	2.37368
H	3.07614	2.32797	1.07974
H	3.33025	4.75869	0.49013
H	3.35035	4.52952	2.24941
H	1.89098	5.14242	1.44001
H	0.9146	2.40037	-2.49692
H	1.12096	0.36316	-3.70605
H	1.04203	-0.631	-2.26812
H	2.98061	-3.76445	-1.09263
H	2.1366	-2.72819	-2.22702
H	4.41746	-1.98202	-0.34481
H	3.09053	0.00058	-0.49415
H	4.64459	0.16964	-1.28911
H	4.77701	0.77279	-3.62772
H	3.21311	1.15608	-4.53368
H	5.0608	-3.39094	-2.30123
H	4.38202	-2.18161	-3.40629
H	5.78184	-1.77703	-2.40366

H	3.46993	1.5761	3.85664
H	-1.86692	3.02364	-2.2766
H	-2.7555	-1.75058	-0.1882
H	-4.91054	1.32831	-0.51799
H	-4.58721	-2.80602	0.56665
H	-5.82466	-1.76291	1.30826
H	-6.07237	-2.3756	-0.31366
H	-6.88133	1.1246	-2.00392
H	-5.50234	0.20136	-2.65232
H	-6.84864	-0.64198	-1.85132
H	-5.30776	0.4577	2.19999
H	-5.60773	2.09806	1.56587
H	-6.9208	1.20031	2.37914

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 22

C	2.906	-2.13185	0.39122
C	3.70354	-3.21367	0.58751
C	5.09609	-3.22984	0.14391
C	5.58127	-1.91092	-0.46379
C	4.4521	-1.1744	-1.18128
O	3.29665	-1.04215	-0.31048
C	1.53117	-1.94194	0.96442
C	1.52499	-0.82965	2.04062
C	0.10883	-0.43361	2.45449
C	0.05713	0.77097	3.41013
C	0.63019	2.11099	2.87041
C	-0.17027	2.59899	1.67091
C	0.63297	3.18177	3.96932
O	0.27358	2.04637	0.5103
O	-1.10489	3.37124	1.72428
C	-0.47298	2.39183	-0.69563
C	0.41474	2.07982	-1.91228

C	-1.7599	1.62149	-0.73611
C	1.79638	2.71075	-1.86505
C	4.85021	0.21957	-1.66936
C	3.75608	1.0889	-2.34435
C	2.91757	1.86592	-1.28776
C	2.00535	3.95077	-2.32098
C	2.91188	0.28659	-3.34568
O	5.84618	-4.18421	0.2969
O	2.2097	-1.25082	3.21978
C	-3.02446	2.06055	-0.50838
O	-3.87596	0.99974	-0.65566
C	-3.06678	-0.06508	-0.9569
N	-1.80176	0.26243	-1.02051
C	-3.60904	-1.38646	-1.19906
C	-4.86396	-1.85751	-1.03687
C	-6.04404	-1.0311	-0.53152
C	-5.17628	-3.28676	-1.40397
C	-6.87902	-0.47362	-1.68782
O	-6.92288	-1.82469	0.26588
C	-6.43902	-2.0627	1.57443
H	3.32626	-4.07608	1.12569
H	5.97913	-1.2863	0.34978
H	6.40794	-2.11677	-1.1502
H	4.11477	-1.7884	-2.02838
H	0.84787	-1.65453	0.15552
H	1.17689	-2.87689	1.40984
H	2.02802	0.04446	1.60573
H	-0.35353	-1.29491	2.95474
H	-0.47418	-0.23444	1.54946
H	0.61826	0.52176	4.31757
H	-0.98352	0.94172	3.71585
H	1.65752	1.93903	2.53177
H	1.07149	4.11944	3.61199

H	1.21625	2.83616	4.82927
H	-0.38653	3.39818	4.30203
H	-0.69034	3.46138	-0.64577
H	-0.13844	2.43641	-2.78986
H	0.48856	0.99275	-2.00658
H	5.28694	0.77407	-0.82769
H	5.66555	0.05963	-2.38819
H	4.29374	1.85277	-2.92454
H	2.49938	1.15915	-0.56927
H	3.61031	2.51176	-0.73222
H	2.98423	4.42236	-2.26831
H	1.20838	4.54563	-2.76247
H	3.55306	-0.244	-4.06074
H	2.28	-0.45561	-2.84529
H	2.25909	0.95038	-3.921
H	3.10252	-1.53317	2.96294
H	-3.46071	3.0061	-0.2306
H	-2.84319	-2.06203	-1.57136
H	-5.67715	-0.19261	0.0721
H	-4.29945	-3.79369	-1.81652
H	-5.53345	-3.85248	-0.53672
H	-5.98215	-3.33235	-2.1476
H	-7.73201	0.08216	-1.28636
H	-6.27506	0.19799	-2.30507
H	-7.26375	-1.28163	-2.3183
H	-5.49517	-2.62922	1.576
H	-6.2757	-1.12064	2.12082
H	-7.20291	-2.64713	2.09402

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 23

C	0.18187	2.81215	-1.65089
C	-0.79801	3.68324	-1.29475
C	-0.62963	4.62333	-0.19073
C	0.75084	4.56806	0.46681
C	1.29009	3.14331	0.45073
O	1.29816	2.61691	-0.90905
C	0.18645	2.05011	-2.94869
C	0.27867	0.50192	-2.92198
C	1.59808	-0.04667	-2.36666
C	1.81121	-1.53472	-2.68117
C	2.94715	-2.20259	-1.85091
C	2.38442	-2.718	-0.53214
C	3.63377	-3.34144	-2.61172
O	1.86119	-1.70912	0.21289
O	2.35625	-3.88009	-0.18654
C	1.07413	-2.09924	1.3778
C	0.98201	-0.86756	2.27893
C	-0.27132	-2.58001	0.92264
C	2.29462	-0.36546	2.87
C	2.71313	2.98455	0.98238
C	3.09028	1.52617	1.32176
C	2.54521	1.12017	2.72127
C	3.14525	-1.17127	3.5134
C	4.60587	1.3036	1.24514
O	-1.47871	5.43674	0.14914
O	-0.85689	-0.09065	-2.2958
C	-0.71676	-3.85806	0.82127
O	-1.99358	-3.8265	0.34533
C	-2.28157	-2.4969	0.16942
N	-1.27572	-1.71864	0.48419
C	-3.62272	-2.23037	-0.31696
C	-4.3445	-1.09404	-0.22624

C	-3.86042	0.17773	0.45861
C	-5.73546	-1.04486	-0.80472
C	-3.61369	1.3142	-0.5335
O	-4.84451	0.64736	1.38656
C	-4.92347	-0.11867	2.57311
H	-1.69199	3.76825	-1.90143
H	1.42874	5.23653	-0.08402
H	0.67741	4.94271	1.49213
H	0.59332	2.50512	1.01604
H	-0.724	2.31953	-3.49196
H	1.03544	2.4204	-3.54284
H	0.19686	0.20117	-3.97604
H	1.61422	0.11231	-1.28629
H	2.43511	0.53681	-2.77293
H	2.05804	-1.64541	-3.74517
H	0.87138	-2.07947	-2.52909
H	3.69048	-1.43008	-1.60801
H	4.40561	-3.81994	-2.00201
H	4.10019	-2.95488	-3.52418
H	2.91116	-4.11404	-2.8932
H	1.59781	-2.91976	1.8722
H	0.28796	-1.11266	3.09433
H	0.49315	-0.07341	1.70548
H	3.39361	3.39028	0.2231
H	2.82893	3.6149	1.87461
H	2.62408	0.87837	0.57009
H	3.25217	1.46545	3.48677
H	1.60096	1.65016	2.9135
H	4.05694	-0.7893	3.96543
H	2.96935	-2.23913	3.62231
H	4.9807	1.4872	0.23141
H	5.13903	1.97975	1.92661
H	4.86448	0.27568	1.52117

H	-0.68884	-0.22593	-1.34586
H	-0.2784	-4.82582	1.00298
H	-4.07991	-3.10065	-0.78269
H	-2.9283	-0.03455	0.99709
H	-6.05976	-2.02569	-1.16408
H	-6.4502	-0.67929	-0.06035
H	-5.78034	-0.34388	-1.64854
H	-3.25955	2.19773	0.00591
H	-2.86223	1.0223	-1.27309
H	-4.53937	1.58499	-1.05166
H	-5.24305	-1.15502	2.38428
H	-3.95653	-0.14728	3.1
H	-5.66287	0.3677	3.21512

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 27

C	-2.14792	2.65372	1.24769
C	-1.92057	3.80776	0.56744
C	-2.77686	4.23197	-0.53494
C	-3.95014	3.28699	-0.80905
C	-3.5434	1.8469	-0.52554
O	-3.03917	1.71999	0.83543
C	-1.51176	2.31975	2.56819
C	-0.57136	1.08789	2.64677
C	-1.26856	-0.26037	2.42323
C	-0.39935	-1.45608	2.84234
C	-0.91716	-2.83795	2.34185
C	-0.37696	-3.10992	0.94437
C	-0.52713	-3.9788	3.28723
O	-0.87804	-2.22473	0.0405
O	0.42759	-3.96692	0.65139
C	-0.26217	-2.20813	-1.27054
C	-1.19426	-1.39282	-2.17313

C	1.09908	-1.57979	-1.17939
C	-2.59393	-1.95377	-2.39337
C	-4.65513	0.80876	-0.66785
C	-4.12518	-0.63555	-0.8052
C	-3.71155	-0.94004	-2.27528
C	-2.81812	-3.23254	-2.71068
C	-5.14389	-1.6675	-0.30534
O	-2.63176	5.27977	-1.15146
O	0.55758	1.25762	1.80138
C	2.27754	-1.99934	-1.70299
O	3.23437	-1.06673	-1.39849
C	2.58663	-0.10946	-0.67107
N	1.30851	-0.37146	-0.52802
C	3.27005	1.05152	-0.14064
C	4.57657	1.39029	-0.19797
C	5.66358	0.57471	-0.89359
C	5.02944	2.68935	0.41964
C	5.9033	1.06564	-2.32477
O	6.91007	0.68449	-0.20728
C	6.98055	-0.10336	0.96655
H	-1.16008	4.49722	0.91538
H	-4.79428	3.57847	-0.16699
H	-4.26997	3.40198	-1.84909
H	-2.69776	1.59582	-1.18467
H	-0.93506	3.19303	2.88645
H	-2.31994	2.17914	3.30093
H	-0.17924	1.10272	3.67533
H	-1.53873	-0.3437	1.36778
H	-2.21244	-0.28077	2.98433
H	-0.34816	-1.49328	3.93845
H	0.62943	-1.30095	2.49564
H	-2.01205	-2.78525	2.26562
H	-0.87177	-4.94623	2.90972

H	-0.96883	-3.81434	4.27589
H	0.56011	-4.03781	3.39884
H	-0.16025	-3.23814	-1.62175
H	-0.69327	-1.27932	-3.1443
H	-1.25422	-0.3839	-1.74998
H	-5.30429	0.89949	0.21205
H	-5.27219	1.06335	-1.54012
H	-3.23432	-0.72172	-0.17129
H	-4.59685	-1.28266	-2.82623
H	-3.38716	-0.00972	-2.76378
H	-3.82199	-3.59926	-2.90837
H	-2.01832	-3.96501	-2.79221
H	-5.35941	-1.52527	0.76004
H	-6.09202	-1.58477	-0.853
H	-4.76537	-2.68673	-0.44014
H	0.45767	0.73064	0.98268
H	2.60069	-2.86317	-2.26113
H	2.58177	1.71247	0.379
H	5.37148	-0.48114	-0.92945
H	5.54174	3.31617	-0.32126
H	4.18496	3.25275	0.82517
H	5.75418	2.51779	1.22297
H	6.70708	0.47967	-2.78118
H	4.99535	0.95311	-2.9248
H	6.20127	2.11897	-2.3323
H	6.23303	0.19487	1.71734
H	6.83672	-1.17213	0.74333
H	7.97983	0.04086	1.38578

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 29

C	5.24545	0.35129	0.23434
C	5.78352	-0.03132	-0.95027
C	5.78144	-1.4265	-1.37508
C	5.2492	-2.39888	-0.32007
C	4.1092	-1.77767	0.48604
O	4.53896	-0.4889	1.03767
C	5.39301	1.72221	0.83765
C	4.07522	2.41007	1.27479
C	3.06735	2.55951	0.12299
C	1.76651	3.24255	0.56174
C	0.68604	3.30471	-0.53945
C	0.29455	1.90977	-1.00852
C	-0.54807	4.09799	-0.07445
O	-0.33513	1.20485	-0.03663
O	0.5195	1.46517	-2.11703
C	-0.79703	-0.13128	-0.40469
C	-0.9347	-0.93826	0.89588
C	-2.09338	-0.03187	-1.15612
C	0.35629	-1.23523	1.6429
C	2.79758	-1.60209	-0.31287
C	1.71345	-2.67692	-0.05454
C	1.06448	-2.54498	1.3483
C	0.80943	-0.39958	2.58495
C	2.20963	-4.11343	-0.28497
O	6.22863	-1.81634	-2.44542
O	3.51002	1.76566	2.41084
C	-2.28054	0.07206	-2.49943
O	-3.62102	0.15686	-2.73579
C	-4.20633	0.09931	-1.49526
N	-3.33205	-0.00451	-0.52816
C	-5.65317	0.17728	-1.48518
C	-6.48426	0.00437	-0.4354

C	-6.0077	-0.31044	0.97772
C	-7.97165	0.16288	-0.6178
C	-5.86146	0.96177	1.81644
O	-6.93744	-1.15571	1.65829
C	-6.84988	-2.51378	1.27337
H	6.29274	0.69441	-1.57411
H	4.92358	-3.31952	-0.80987
H	6.08391	-2.65529	0.34745
H	3.92367	-2.36396	1.38911
H	6.02175	1.63489	1.73418
H	5.92806	2.35618	0.12298
H	4.34561	3.41238	1.6309
H	2.84826	1.56878	-0.29621
H	3.5379	3.13052	-0.69026
H	1.98447	4.27147	0.88027
H	1.36634	2.72216	1.43721
H	1.10901	3.78614	-1.42867
H	-1.31054	4.14788	-0.85962
H	-0.25882	5.12345	0.18059
H	-0.99998	3.63793	0.80945
H	-0.04223	-0.55676	-1.06756
H	-1.43474	-1.87904	0.63274
H	-1.62902	-0.39419	1.54302
H	2.37424	-0.62856	-0.04866
H	3.01937	-1.56925	-1.3861
H	0.92789	-2.49455	-0.80048
H	0.33954	-3.36629	1.45335
H	1.82772	-2.71842	2.11842
H	1.70693	-0.61689	3.1599
H	0.29372	0.52407	2.83116
H	2.65026	-4.22818	-1.28199
H	2.9648	-4.41117	0.4533
H	1.38089	-4.82606	-0.20361

H	3.43149	0.8234	2.18484
H	-1.62073	0.12742	-3.34966
H	-6.07716	0.41104	-2.45882
H	-5.0296	-0.80463	0.92963
H	-8.21906	0.46555	-1.63943
H	-8.50316	-0.76739	-0.38928
H	-8.37134	0.91649	0.07269
H	-5.55654	0.69298	2.83265
H	-5.10078	1.61426	1.37866
H	-6.80907	1.50739	1.87689
H	-7.08292	-2.66475	0.20779
H	-5.84595	-2.92341	1.4661
H	-7.57947	-3.06309	1.87469

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 30

C	-1.52704	2.67842	1.32865
C	-1.21378	3.78064	0.59823
C	-2.1221	4.31723	-0.41072
C	-3.44498	3.55471	-0.52332
C	-3.22052	2.07219	-0.25617
O	-2.58568	1.88276	1.0424
C	-0.79504	2.26094	2.57434
C	0.00909	0.93343	2.54424
C	-0.85179	-0.32573	2.37773
C	-0.07211	-1.61719	2.66615
C	-0.78173	-2.92164	2.19512
C	-0.45584	-3.17114	0.72891
C	-0.37953	-4.13519	3.03923
O	-0.99972	-2.21277	-0.06624
O	0.23594	-4.07107	0.3028
C	-0.55796	-2.1823	-1.4519
C	-1.56347	-1.31424	-2.20977

C	0.82217	-1.59631	-1.51193
C	-3.01666	-1.76864	-2.19636
C	-4.47773	1.20317	-0.24799
C	-4.17741	-0.30104	-0.43619
C	-4.01613	-0.65936	-1.9451
C	-3.38692	-3.03325	-2.41847
C	-5.24876	-1.18415	0.21566
O	-1.89618	5.32542	-1.06726
O	1.06788	0.98754	1.59654
C	1.9962	-2.18352	-1.85283
O	2.98683	-1.24257	-1.75703
C	2.35953	-0.1044	-1.33427
N	1.06926	-0.26703	-1.183
C	3.08273	1.13625	-1.12202
C	4.38382	1.33317	-0.82689
C	5.39119	0.21759	-0.56655
C	4.90164	2.73769	-0.64632
C	6.56756	0.22953	-1.54255
O	5.94055	0.37186	0.7455
C	5.05175	-0.01858	1.78239
H	-0.32851	4.35621	0.8433
H	-4.15475	3.97103	0.20649
H	-3.8661	3.7099	-1.52114
H	-2.50056	1.6976	-1.
H	-0.09623	3.06158	2.83289
H	-1.5333	2.19543	3.38642
H	0.51164	0.88355	3.52035
H	-1.247	-0.34749	1.35922
H	-1.72292	-0.26535	3.04409
H	0.09871	-1.69919	3.74781
H	0.92103	-1.55214	2.20503
H	-1.86694	-2.76738	2.26999
H	-0.86074	-5.04955	2.67912

H	-0.66955	-3.97874	4.08376
H	0.70244	-4.29586	3.00018
H	-0.53541	-3.20847	-1.82541
H	-1.21471	-1.24067	-3.24947
H	-1.48472	-0.30145	-1.80198
H	-4.99216	1.37855	0.70515
H	-5.15711	1.5496	-1.03841
H	-3.22812	-0.51264	0.07086
H	-4.99931	-0.92976	-2.35087
H	-3.69003	0.23209	-2.50003
H	-4.43496	-3.32034	-2.44438
H	-2.66778	-3.83214	-2.58426
H	-5.29487	-1.01614	1.29798
H	-6.24282	-0.97194	-0.19957
H	-5.03392	-2.24542	0.04787
H	0.73059	0.73769	0.71435
H	2.29115	-3.17614	-2.15206
H	2.4242	1.9997	-1.17585
H	4.89181	-0.75525	-0.63028
H	5.61061	3.00009	-1.443
H	4.09172	3.47205	-0.66283
H	5.4448	2.82408	0.30033
H	7.24163	-0.60074	-1.31109
H	6.21413	0.12108	-2.5734
H	7.13646	1.1607	-1.46116
H	4.11096	0.5494	1.7691
H	4.80978	-1.09107	1.71469
H	5.57191	0.16767	2.72568

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 31

C	1.4311	-2.46552	1.81841
C	0.18605	-2.9663	1.58771
C	-0.20795	-3.47024	0.27871
C	0.91396	-3.46545	-0.75558
C	1.85995	-2.28935	-0.5225
O	2.35954	-2.3019	0.84963
C	1.88348	-1.95637	3.15764
C	1.36205	-0.51728	3.45597
C	1.85358	0.5194	2.43808
C	1.45041	1.9559	2.79501
C	2.00907	3.05844	1.85356
C	1.29655	3.09825	0.50326
C	1.93522	4.44058	2.51439
O	1.55557	1.98788	-0.23392
O	0.5959	4.00671	0.10983
C	0.94786	1.9181	-1.55853
C	1.73768	0.89363	-2.40631
C	-0.49386	1.52772	-1.4238
C	3.24659	0.92179	-2.23483
C	3.048	-2.28684	-1.48481
C	4.21521	-1.31412	-1.20707
C	3.84651	0.18927	-1.04335
C	4.01129	1.5921	-3.10528
C	5.31102	-1.52212	-2.26299
O	-1.32896	-3.89908	0.02173
O	-0.05504	-0.50126	3.58394
C	-1.61202	2.28306	-1.56655
O	-2.69688	1.48614	-1.31609
C	-2.1744	0.2555	-1.00793
N	-0.86623	0.23787	-1.06822
C	-3.01594	-0.87115	-0.66717
C	-4.34659	-0.92892	-0.44306

C	-5.28607	0.26079	-0.55827
C	-4.97568	-2.25127	-0.08802
C	-5.82335	0.40276	-1.99344
O	-6.34956	0.05623	0.37512
C	-7.02325	1.2373	0.75524
H	-0.5163	-3.05736	2.40893
H	1.46399	-4.41496	-0.67777
H	0.47786	-3.41597	-1.75767
H	1.27707	-1.36462	-0.60472
H	1.50481	-2.61192	3.9477
H	2.97823	-1.9641	3.19362
H	1.72972	-0.25153	4.45474
H	1.45856	0.26038	1.45067
H	2.94779	0.45088	2.36192
H	1.81956	2.18373	3.80446
H	0.35799	2.03168	2.85056
H	3.05999	2.81529	1.64171
H	2.32665	5.21983	1.85409
H	2.51835	4.44496	3.44147
H	0.90024	4.70298	2.75495
H	1.02351	2.91597	-1.99655
H	1.47447	1.09906	-3.45073
H	1.34624	-0.10039	-2.18161
H	3.46591	-3.30272	-1.51144
H	2.63917	-2.10459	-2.48865
H	4.63348	-1.6031	-0.23371
H	3.17205	0.28459	-0.1908
H	4.77431	0.70253	-0.75908
H	5.09114	1.65127	-2.99266
H	3.58739	2.11166	-3.96206
H	5.62795	-2.57112	-2.30207
H	4.96167	-1.23747	-3.26204
H	6.1956	-0.91518	-2.03624

H	-0.42586	-0.71275	2.70939
H	-1.80577	3.31786	-1.79733
H	-2.44196	-1.78856	-0.57397
H	-4.75084	1.18029	-0.28939
H	-5.75003	-2.52731	-0.81627
H	-4.22662	-3.04652	-0.05178
H	-5.47966	-2.18374	0.8816
H	-6.5274	1.23885	-2.06552
H	-5.002	0.59147	-2.69099
H	-6.34364	-0.51058	-2.29981
H	-7.75345	0.95177	1.51739
H	-6.33089	1.97857	1.18575
H	-7.55933	1.70994	-0.08151

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 38

C	-1.96066	2.36044	0.76331
C	-2.17945	3.69382	0.64622
C	-3.41179	4.2222	0.06868
C	-4.45168	3.15865	-0.30192
C	-3.79313	1.84507	-0.71406
O	-2.82138	1.43051	0.28114
C	-0.75275	1.71278	1.38918
C	-1.09395	0.46261	2.2261
C	0.15165	-0.33713	2.60884
C	-0.15054	-1.72084	3.21069
C	-0.97197	-2.70363	2.32865
C	-0.30373	-2.91367	0.97633
C	-1.15176	-4.0499	3.0429
O	-0.73847	-2.00593	0.06401
O	0.52846	-3.76165	0.72834
C	-0.09028	-2.01316	-1.24473
C	-0.99237	-1.19449	-2.17202

C	1.28735	-1.42339	-1.14672
C	-2.33164	-1.80876	-2.56185
C	-4.77034	0.6795	-0.87648
C	-4.11901	-0.70084	-1.11187
C	-3.50697	-0.85083	-2.53459
C	-2.46212	-3.08356	-2.94271
C	-5.12927	-1.82474	-0.84133
O	-3.64383	5.41675	-0.06347
O	-1.76839	0.80402	3.44153
C	2.48486	-2.06313	-1.11675
O	3.4706	-1.11766	-1.03938
C	2.81067	0.08294	-1.01005
N	1.51076	-0.0536	-1.07702
C	3.52449	1.34182	-0.94566
C	4.8354	1.59072	-0.73877
C	5.89884	0.51874	-0.51506
C	5.33444	3.01375	-0.75845
C	6.62466	0.16344	-1.81605
O	6.89533	0.96712	0.40315
C	6.47797	0.92819	1.7551
H	-1.44941	4.39939	1.02687
H	-5.09464	2.9952	0.57562
H	-5.08752	3.54506	-1.10422
H	-3.221	2.00942	-1.6393
H	-0.08742	1.40111	0.57046
H	-0.21591	2.44391	2.00259
H	-1.73814	-0.17017	1.60924
H	0.72541	0.24473	3.34246
H	0.78478	-0.43995	1.72119
H	-0.70766	-1.58648	4.14464
H	0.79846	-2.20766	3.47107
H	-1.95566	-2.26048	2.14096
H	-1.78991	-4.72677	2.46472

H	-1.61536	-3.89812	4.02343
H	-0.18564	-4.543	3.18554
H	-0.00841	-3.05404	-1.56515
H	-0.42179	-0.98459	-3.08709
H	-1.14742	-0.22237	-1.69444
H	-5.38159	0.62967	0.03493
H	-5.45815	0.92272	-1.6987
H	-3.3064	-0.80485	-0.38521
H	-4.28954	-1.18676	-3.22691
H	-3.16876	0.12809	-2.90148
H	-3.41936	-3.48339	-3.26711
H	-1.6265	-3.7796	-2.95459
H	-5.48322	-1.79933	0.19612
H	-6.00599	-1.73584	-1.49654
H	-4.67585	-2.80607	-1.01687
H	-2.64811	1.13722	3.20585
H	2.79247	-3.09596	-1.11867
H	2.85258	2.18248	-1.09869
H	5.43137	-0.38933	-0.11607
H	4.52866	3.71614	-0.98913
H	5.78014	3.29379	0.20208
H	6.12657	3.13973	-1.50747
H	7.39682	-0.58407	-1.60962
H	5.92	-0.24481	-2.5465
H	7.10963	1.04489	-2.24777
H	5.62126	1.59165	1.94892
H	6.19933	-0.09229	2.06103
H	7.32633	1.26102	2.35884

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 42

C	-0.5658	2.26511	1.42417
C	-0.0333	3.48346	1.69276
C	-0.52023	4.69481	1.03726
C	-1.7213	4.48055	0.10969
C	-1.69369	3.09712	-0.5341
O	-1.51561	2.0713	0.47754
C	-0.17432	0.96469	2.07633
C	-1.36863	0.03475	2.37345
C	-0.91686	-1.37624	2.75199
C	-2.05169	-2.41489	2.77151
C	-2.83829	-2.61457	1.44494
C	-1.90395	-2.97383	0.2962
C	-3.91001	-3.69997	1.61157
O	-1.4144	-1.86442	-0.3127
O	-1.60885	-4.10359	-0.03767
C	-0.44567	-2.06755	-1.39207
C	-0.40587	-0.75473	-2.17723
C	0.90165	-2.44479	-0.84152
C	-1.60883	-0.43518	-3.05738
C	-2.96667	2.73392	-1.29957
C	-3.03444	1.27734	-1.80823
C	-2.07753	1.0061	-3.00479
C	-2.18502	-1.3389	-3.85647
C	-4.47639	0.90266	-2.17821
O	-0.05884	5.80981	1.24087
O	-2.17009	0.52704	3.45112
C	1.38675	-3.68985	-0.5891
O	2.66483	-3.5643	-0.13338
C	2.91469	-2.2146	-0.12861
N	1.88546	-1.51068	-0.5278
C	4.25425	-1.84509	0.28422
C	4.85663	-0.63972	0.20761

C	4.16193	0.6111	-0.29689
C	6.28298	-0.47746	0.66147
C	3.58094	1.42103	0.87501
O	5.13538	1.36543	-1.02492
C	4.5857	2.31844	-1.91087
H	0.7418	3.58421	2.44425
H	-2.63706	4.59594	0.70819
H	-1.72888	5.26561	-0.65243
H	-0.81101	3.02745	-1.1872
H	0.49308	0.44096	1.37675
H	0.38812	1.1629	2.99449
H	-1.96779	-0.02184	1.46023
H	-0.46051	-1.33662	3.74987
H	-0.13142	-1.69192	2.05677
H	-2.78178	-2.12853	3.53704
H	-1.63702	-3.38556	3.07321
H	-3.32266	-1.66732	1.18487
H	-4.5179	-3.80374	0.70656
H	-4.57567	-3.44707	2.44361
H	-3.44806	-4.67033	1.81563
H	-0.81734	-2.89453	-2.00024
H	0.49471	-0.76975	-2.80517
H	-0.24304	0.05105	-1.45454
H	-3.81982	2.91504	-0.63169
H	-3.0734	3.43688	-2.1378
H	-2.72693	0.62947	-0.98043
H	-2.58725	1.27661	-3.93825
H	-1.19559	1.65788	-2.93468
H	-3.00613	-1.07089	-4.51631
H	-1.8624	-2.37657	-3.89613
H	-5.14303	0.98386	-1.31142
H	-4.86814	1.56122	-2.96479
H	-4.52747	-0.12774	-2.54549

H	-2.61615	1.33131	3.14352
H	0.97458	-4.68334	-0.6499
H	4.82339	-2.68555	0.67351
H	3.34212	0.32481	-0.96751
H	6.68763	-1.41468	1.05421
H	6.90811	-0.13692	-0.17047
H	6.36538	0.28998	1.44194
H	3.04782	2.30792	0.517
H	2.87287	0.80908	1.44113
H	4.37915	1.7496	1.54889
H	3.89547	1.85084	-2.63128
H	4.04907	3.12404	-1.38835
H	5.4233	2.75853	-2.4589

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 46

C	-0.84672	2.31585	1.31059
C	-0.48887	3.607	1.51916
C	-1.14527	4.70518	0.81748
C	-2.31406	4.27837	-0.07679
C	-2.09292	2.88927	-0.66876
O	-1.74252	1.93983	0.36982
C	-0.2719	1.11962	2.02427
C	-1.32141	0.06429	2.39557
C	-0.68532	-1.28615	2.75932
C	-1.68572	-2.45156	2.86291
C	-2.49513	-2.79568	1.57941
C	-1.55984	-3.1078	0.41667
C	-3.43661	-3.98059	1.83179
O	-1.21597	-1.98439	-0.25817
O	-1.15039	-4.21472	0.13157
C	-0.23882	-2.13018	-1.34041
C	-0.34846	-0.85936	-2.18564

C	1.14267	-2.32902	-0.78413
C	-1.59018	-0.71596	-3.05881
C	-3.31922	2.31623	-1.38181
C	-3.19603	0.84298	-1.82622
C	-2.23878	0.65397	-3.03751
C	-2.05177	-1.7072	-3.82818
C	-4.58019	0.25695	-2.13825
O	-0.84734	5.88362	0.96288
O	-2.08248	0.60492	3.48265
C	1.78864	-3.49888	-0.53331
O	3.0318	-3.20533	-0.05886
C	3.09495	-1.83385	-0.03959
N	1.98606	-1.27345	-0.45037
C	4.36262	-1.29	0.40974
C	4.80547	-0.01618	0.34652
C	3.99435	1.14146	-0.22322
C	6.1773	0.3274	0.86764
C	3.45169	2.05226	0.88097
O	4.80439	1.96346	-1.06725
C	5.07118	1.38763	-2.33204
H	0.25841	3.85	2.26612
H	-3.22558	4.27981	0.5386
H	-2.45032	5.0215	-0.86827
H	-1.2265	2.92514	-1.3463
H	0.45699	0.65045	1.34902
H	0.26223	1.44626	2.92251
H	-1.9666	-0.07003	1.52166
H	-0.17356	-1.17522	3.7241
H	0.08335	-1.53018	2.01812
H	-2.41409	-2.24159	3.65925
H	-1.14867	-3.3548	3.17941
H	-3.08634	-1.91965	1.28959
H	-4.05835	-4.18927	0.95494

H	-4.09956	-3.76569	2.67694
H	-2.86496	-4.8854	2.05762
H	-0.5197	-3.02072	-1.90606
H	0.54095	-0.8112	-2.82779
H	-0.26392	-0.00716	-1.50441
H	-4.17272	2.40711	-0.69659
H	-3.5434	2.95759	-2.24602
H	-2.78245	0.28238	-0.98112
H	-2.79912	0.82431	-3.96574
H	-1.44736	1.41552	-3.00906
H	-2.90726	-1.56425	-4.48311
H	-1.59707	-2.69499	-3.84732
H	-5.2317	0.28709	-1.25671
H	-5.07752	0.81875	-2.94011
H	-4.49866	-0.78691	-2.45987
H	-2.89722	0.08712	3.56424
H	1.51584	-4.53882	-0.60426
H	5.01885	-2.04886	0.82979
H	3.15145	0.74274	-0.80004
H	6.7018	-0.55851	1.23676
H	6.78333	0.80063	0.08776
H	6.11465	1.05408	1.68803
H	2.83326	2.84004	0.44045
H	2.8428	1.47815	1.58574
H	4.27001	2.52856	1.43042
H	5.65817	2.118	-2.89532
H	5.64676	0.45248	-2.25378
H	4.14147	1.17417	-2.88223

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 49

C	-2.32167	2.65158	1.16352
C	-2.13369	3.80825	0.47586
C	-2.97846	4.17678	-0.65484
C	-4.09475	3.17132	-0.95046
C	-3.62705	1.7563	-0.63593
O	-3.15541	1.67097	0.73972
C	-1.70425	2.36331	2.50361
C	-0.72296	1.16741	2.62348
C	-1.36948	-0.20818	2.41526
C	-0.47439	-1.36621	2.88262
C	-0.94499	-2.7747	2.40973
C	-0.35836	-3.07494	1.037
C	-0.557	-3.87781	3.39968
O	-0.84573	-2.22282	0.09437
O	0.46861	-3.92552	0.79193
C	-0.18223	-2.22309	-1.19318
C	-1.09463	-1.44579	-2.14824
C	1.16383	-1.56942	-1.06304
C	-2.47001	-2.04634	-2.41341
C	-4.6852	0.66572	-0.79361
C	-4.08854	-0.75563	-0.89101
C	-3.61953	-1.06437	-2.34302
C	-2.64674	-3.33388	-2.72558
C	-5.07577	-1.82302	-0.40274
O	-2.86854	5.22376	-1.28014
O	0.41112	1.36517	1.79128
C	2.36583	-1.97019	-1.54569
O	3.29692	-1.02176	-1.20926
C	2.60872	-0.07449	-0.50517
N	1.33058	-0.35718	-0.40688
C	3.25907	1.08878	0.05812
C	4.56202	1.44479	0.04112

C	5.65858	0.65737	-0.65946
C	4.99013	2.7223	0.7144
C	5.77589	1.0744	-2.13655
O	6.8764	0.90369	0.04681
C	7.87027	-0.08067	-0.14785
H	-1.4171	4.538	0.83458
H	-4.97128	3.42817	-0.33762
H	-4.38857	3.25789	-2.0009
H	-2.7525	1.53769	-1.26843
H	-1.16643	3.26228	2.81847
H	-2.52278	2.20669	3.22155
H	-0.35127	1.21526	3.65893
H	-1.61233	-0.32352	1.35626
H	-2.32521	-0.24653	2.95494
H	-0.44369	-1.37294	3.98007
H	0.55641	-1.19166	2.55164
H	-2.03815	-2.75041	2.30082
H	-0.86715	-4.86387	3.041
H	-1.03214	-3.69546	4.36953
H	0.52745	-3.9069	3.54516
H	-0.0503	-3.25826	-1.51822
H	-0.55673	-1.33838	-3.10011
H	-1.19666	-0.43114	-1.74746
H	-5.36412	0.74045	0.06506
H	-5.28646	0.87914	-1.68772
H	-3.21351	-0.79293	-0.23089
H	-4.47658	-1.43897	-2.91739
H	-3.30679	-0.13024	-2.83185
H	-3.63249	-3.73123	-2.95303
H	-1.8239	-4.04379	-2.7713
H	-5.33062	-1.67135	0.65262
H	-6.0091	-1.79264	-0.98047
H	-4.6485	-2.82645	-0.50617

H	0.37123	0.78442	1.00457
H	2.72207	-2.8295	-2.09046
H	2.5511	1.72797	0.57805
H	5.43231	-0.41483	-0.61086
H	5.50613	3.38584	0.00846
H	4.1334	3.25629	1.13365
H	5.70862	2.51023	1.51287
H	6.59079	0.53413	-2.63018
H	4.84889	0.8509	-2.67284
H	5.97843	2.14742	-2.21689
H	7.50732	-1.08317	0.12979
H	8.23389	-0.11875	-1.18556
H	8.70749	0.18501	0.50315

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 51

C	0.88478	2.30319	-1.28625
C	0.57817	3.6043	-1.51549
C	1.27801	4.68533	-0.82898
C	2.43293	4.22458	0.06584
C	2.16282	2.85374	0.6806
O	1.76067	1.90406	-0.3394
C	0.27753	1.11825	-1.99015
C	1.31326	0.04176	-2.37373
C	0.65626	-1.2903	-2.76197
C	1.64792	-2.4606	-2.87636
C	2.4466	-2.82041	-1.59126
C	1.5077	-3.12195	-0.43003
C	3.37149	-4.01746	-1.84759
O	1.17686	-1.99333	0.24718
O	1.0811	-4.22205	-0.14325
C	0.19917	-2.12907	1.32838
C	0.32551	-0.8637	2.18021

C	-1.18544	-2.30662	0.77173
C	1.56538	-0.74479	3.05999
C	3.37588	2.24255	1.38541
C	3.21274	0.77382	1.83196
C	2.2454	0.60987	3.03862
C	1.99916	-1.74403	3.83518
C	4.58088	0.15462	2.15048
O	1.02487	5.87213	-0.99036
O	2.21963	0.50308	-3.37675
C	-1.84806	-3.46653	0.51825
O	-3.08737	-3.15446	0.04489
C	-3.13114	-1.78249	0.02899
N	-2.01421	-1.23852	0.44028
C	-4.39158	-1.21944	-0.41727
C	-4.8175	0.05978	-0.34742
C	-3.99031	1.2035	0.22718
C	-6.18553	0.42403	-0.86469
C	-3.43267	2.11	-0.87325
O	-4.78883	2.03491	1.07266
C	-5.06317	1.46029	2.33658
H	-0.16142	3.86668	-2.26379
H	3.33973	4.18055	-0.55482
H	2.6039	4.97301	0.84544
H	1.30735	2.93335	1.36809
H	-0.44888	0.65992	-1.30403
H	-0.27909	1.45853	-2.87241
H	1.94182	-0.11848	-1.49825
H	0.14437	-1.16845	-3.72938
H	-0.12652	-1.52821	-2.0335
H	2.3849	-2.22596	-3.6535
H	1.10728	-3.35677	-3.20734
H	3.051	-1.95284	-1.30637
H	3.99115	-4.23674	-0.97173

H	4.03623	-3.80589	-2.69176
H	2.78862	-4.91457	-2.07622
H	0.46668	-3.02563	1.89104
H	-0.56591	-0.80419	2.81861
H	0.25862	-0.00683	1.50295
H	4.22637	2.30566	0.69365
H	3.62586	2.87788	2.24708
H	2.79024	0.2224	0.98546
H	2.80469	0.7697	3.96936
H	1.47156	1.3891	3.00438
H	2.85432	-1.61929	4.49421
H	1.52154	-2.72098	3.85415
H	5.23595	0.16782	1.27141
H	5.08824	0.70455	2.95438
H	4.47228	-0.88673	2.47215
H	1.70491	0.66947	-4.18361
H	-1.58942	-4.51028	0.58612
H	-5.05857	-1.9675	-0.83981
H	-3.15376	0.79057	0.8033
H	-6.72112	-0.45281	-1.23953
H	-6.78519	0.89871	-0.08077
H	-6.11547	1.1559	-1.6799
H	-2.80239	2.88645	-0.42935
H	-2.83222	1.52854	-1.57931
H	-4.24301	2.60101	-1.42167
H	-5.65018	0.53251	2.2564
H	-4.13633	1.23451	2.88657
H	-5.64128	2.19695	2.90081

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 52

C	2.93583	-2.10803	0.57774
C	3.69035	-3.22144	0.74947
C	5.06582	-3.29301	0.26447
C	5.57263	-1.9995	-0.37943
C	4.43939	-1.26006	-1.08581
O	3.32954	-1.05341	-0.17247
C	1.5835	-1.86292	1.18476
C	1.57044	-0.61116	2.08951
C	0.15135	-0.22927	2.52907
C	0.09521	1.05057	3.38059
C	0.63947	2.34773	2.72199
C	-0.17821	2.7212	1.49333
C	0.6346	3.50775	3.72627
O	0.26178	2.07553	0.38112
O	-1.11928	3.48751	1.48936
C	-0.48538	2.32474	-0.84833
C	0.40527	1.92287	-2.03581
C	-1.77146	1.55204	-0.83046
C	1.78631	2.55738	-2.03072
C	4.85028	0.09636	-1.65925
C	3.76249	0.92733	-2.39081
C	2.90727	1.7579	-1.3908
C	1.99441	3.76154	-2.57471
C	2.93003	0.07081	-3.35676
O	5.78841	-4.27067	0.40738
O	2.45694	-0.75725	3.1993
C	-3.03523	2.00561	-0.62729
O	-3.88787	0.93835	-0.70454
C	-3.08007	-0.14391	-0.94099
N	-1.81495	0.17756	-1.02748
C	-3.62519	-1.47589	-1.10675
C	-4.88178	-1.93303	-0.91989

C	-6.05795	-1.07593	-0.45865
C	-5.20048	-3.37766	-1.21387
C	-6.8842	-0.56548	-1.64258
O	-6.94593	-1.82538	0.37091
C	-6.47031	-2.00455	1.69148
H	3.30806	-4.05523	1.32761
H	5.99728	-1.36593	0.41281
H	6.37818	-2.23947	-1.07978
H	4.04981	-1.90496	-1.88657
H	0.85409	-1.7117	0.37748
H	1.26975	-2.74599	1.75523
H	1.99656	0.21224	1.51336
H	-0.27481	-1.05648	3.11857
H	-0.47772	-0.13127	1.63735
H	0.68248	0.88897	4.2917
H	-0.94118	1.22957	3.69552
H	1.66681	2.16192	2.39169
H	1.05468	4.41753	3.28496
H	1.23253	3.24663	4.60579
H	-0.38497	3.73702	4.05004
H	-0.70453	3.3946	-0.88002
H	-0.14575	2.21208	-2.93919
H	0.48025	0.83184	-2.04807
H	5.29145	0.69836	-0.8535
H	5.66287	-0.11431	-2.36793
H	4.30536	1.65958	-3.00594
H	2.48771	1.08922	-0.63787
H	3.58783	2.44007	-0.86481
H	2.97238	4.23745	-2.55342
H	1.19792	4.32139	-3.06068
H	3.579	-0.50225	-4.03076
H	2.28764	-0.6405	-2.82513
H	2.28723	0.70174	-3.97866

H	2.13483	-1.49721	3.74027
H	-3.46973	2.96731	-0.40847
H	-2.86166	-2.1728	-1.44265
H	-5.68705	-0.21328	0.10753
H	-4.32518	-3.90983	-1.59688
H	-5.56444	-3.8968	-0.32073
H	-6.00378	-3.45651	-1.95753
H	-7.73303	0.01647	-1.27046
H	-6.27186	0.07085	-2.28819
H	-7.27483	-1.39834	-2.23603
H	-5.5297	-2.5757	1.72462
H	-6.30433	-1.03891	2.19422
H	-7.24017	-2.55989	2.23372

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 55

C	-2.38803	2.32716	1.43987
C	-2.26244	3.51798	0.79827
C	-3.14674	3.89738	-0.30066
C	-4.21397	2.85061	-0.63616
C	-3.66445	1.45262	-0.3863
O	-3.2	1.3383	0.9905
C	-1.71087	1.99194	2.74123
C	-0.62427	0.87896	2.7374
C	-1.17024	-0.51239	2.39507
C	-0.16866	-1.65577	2.61764
C	-0.60152	-3.01073	1.97652
C	-0.1885	-3.05378	0.50902
C	-0.01398	-4.2145	2.72053
O	-0.83897	-2.10109	-0.21746
O	0.63713	-3.79672	0.0277
C	-0.31127	-1.77686	-1.53041
C	-1.24005	-0.70002	-2.12147

C	1.07819	-1.22346	-1.38644
C	-2.62418	-1.10895	-2.59712
C	-4.64986	0.31007	-0.62048
C	-4.06296	-1.10713	-0.3868
C	-3.59169	-1.82912	-1.67755
C	-2.98513	-0.81458	-3.8535
C	-5.08676	-2.00167	0.3318
O	-3.09733	4.97824	-0.87348
O	0.47366	1.2514	1.91668
C	2.22023	-1.54377	-2.04267
O	3.21665	-0.71917	-1.58777
C	2.62858	0.07152	-0.64275
N	1.35006	-0.18881	-0.50213
C	3.3625	1.07658	0.09686
C	4.67628	1.38989	0.06642
C	5.71727	0.7144	-0.82254
C	5.18576	2.51667	0.92935
C	5.94916	1.5027	-2.11526
O	6.97952	0.62686	-0.16205
C	7.03934	-0.40258	0.80765
H	-1.56568	4.26056	1.16955
H	-5.09675	3.03223	-0.00568
H	-4.5197	2.97038	-1.67985
H	-2.77652	1.32519	-1.01711
H	-1.2412	2.90585	3.11628
H	-2.49105	1.70603	3.46148
H	-0.23674	0.8588	3.76743
H	-1.48956	-0.50638	1.35227
H	-2.07415	-0.70024	2.99043
H	-0.04187	-1.82183	3.6955
H	0.8175	-1.36669	2.23589
H	-1.699	-3.06456	2.00903
H	-0.30159	-5.15749	2.24614

H	-0.36828	-4.22428	3.75677
H	1.07971	-4.17117	2.72904
H	-0.29078	-2.68251	-2.14399
H	-0.70732	-0.25281	-2.96748
H	-1.30216	0.08404	-1.35802
H	-5.50385	0.47111	0.04995
H	-5.03446	0.40372	-1.64439
H	-3.20079	-1.00758	0.27672
H	-3.14085	-2.77984	-1.3612
H	-4.48025	-2.09162	-2.26739
H	-3.97078	-1.06541	-4.23783
H	-2.31193	-0.3144	-4.54582
H	-5.36516	-1.57589	1.30253
H	-6.0046	-2.11074	-0.26082
H	-4.68502	-3.00689	0.50764
H	0.44324	0.77652	1.0615
H	2.4951	-2.27475	-2.78566
H	2.70765	1.6279	0.76677
H	5.3837	-0.29653	-1.08368
H	4.3715	2.99634	1.47876
H	5.93355	2.16228	1.64714
H	5.68874	3.27815	0.31983
H	6.72022	1.00511	-2.71154
H	5.02656	1.55802	-2.70091
H	6.28875	2.52036	-1.89799
H	6.32026	-0.24945	1.62671
H	6.84531	-1.3895	0.35923
H	8.05194	-0.392	1.21945

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 57

C	-0.22278	2.36953	1.80271
C	0.83157	2.92592	1.14991
C	0.65048	3.72055	-0.05757
C	-0.81563	3.99409	-0.40238
C	-1.64736	2.75494	-0.08516
O	-1.48462	2.38179	1.31924
C	-0.09865	1.64495	3.11282
C	0.10372	0.10993	2.97263
C	-1.12306	-0.62063	2.41289
C	-1.00242	-2.14629	2.52351
C	-2.10076	-2.94211	1.7614
C	-1.74193	-3.01653	0.28387
C	-2.27582	-4.35413	2.33079
O	-1.93684	-1.82557	-0.33722
O	-1.29973	-3.99577	-0.28031
C	-1.46176	-1.72882	-1.71156
C	-2.15834	-0.52668	-2.35714
C	0.02655	-1.51911	-1.69564
C	-3.66085	-0.37525	-2.18393
C	-3.15436	2.87731	-0.31771
C	-3.87533	1.50529	-0.42999
C	-4.09432	1.05223	-1.91623
C	-4.52643	-1.38773	-2.28261
C	-5.21294	1.50204	0.32399
O	1.57805	4.16236	-0.72835
O	1.27961	-0.18606	2.22351
C	1.04003	-2.37489	-1.98234
O	2.22418	-1.7071	-1.80653
C	1.86839	-0.45048	-1.39647
N	0.57093	-0.29643	-1.31979
C	2.84123	0.59032	-1.11919
C	4.15226	0.50021	-0.81216

C	4.92279	-0.80808	-0.66772
C	4.93166	1.76555	-0.55332
C	5.96643	-0.9948	-1.77076
O	5.62604	-0.83516	0.57567
C	4.78892	-1.09041	1.69368
H	1.82919	2.82971	1.5626
H	-1.16838	4.8566	0.18166
H	-0.89404	4.25071	-1.46287
H	-1.22998	1.91579	-0.65795
H	0.7643	2.04685	3.65164
H	-0.99649	1.83689	3.71235
H	0.31853	-0.26698	3.98053
H	-1.25835	-0.33038	1.36692
H	-2.02266	-0.28329	2.94587
H	-1.05764	-2.43342	3.58242
H	-0.01219	-2.46119	2.17221
H	-3.04617	-2.38981	1.84439
H	-3.03423	-4.91693	1.77764
H	-2.58259	-4.30104	3.38088
H	-1.33884	-4.91587	2.26941
H	-1.70169	-2.6688	-2.21254
H	-1.91566	-0.55361	-3.42959
H	-1.66502	0.36967	-1.97584
H	-3.56379	3.46215	0.5154
H	-3.32536	3.4715	-1.22417
H	-3.23469	0.76081	0.05787
H	-5.15177	1.17927	-2.17797
H	-3.53206	1.7149	-2.58911
H	-5.59805	-1.22867	-2.19123
H	-4.20683	-2.41254	-2.45686
H	-5.06697	1.71224	1.38992
H	-5.89688	2.2606	-0.07869
H	-5.70589	0.52677	0.23653

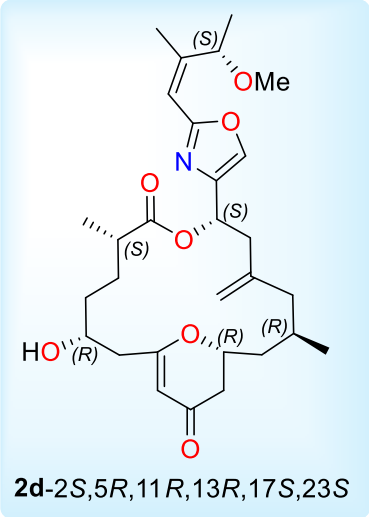
H	1.11941	0.08434	1.30191
H	1.10047	-3.40733	-2.28593
H	2.38637	1.57742	-1.14664
H	4.22469	-1.65277	-0.69945
H	4.27744	2.64195	-0.5402
H	5.46836	1.69591	0.39861
H	5.69378	1.92147	-1.32882
H	6.4825	-1.94902	-1.62683
H	5.4885	-0.99518	-2.75585
H	6.71382	-0.19605	-1.74195
H	4.00479	-0.33156	1.82123
H	4.30034	-2.07371	1.61006
H	5.43587	-1.08968	2.57502

Compound 2c: Isomer 2S, 5R, 11S, 13S, 17S, 23R conformer 58

C	2.79859	-2.23324	0.91023
C	3.14633	-3.26152	0.09367
C	4.13078	-3.09789	-0.97071
C	4.74003	-1.69588	-1.04883
C	3.72344	-0.64426	-0.62027
O	3.19997	-0.95959	0.70265
C	1.98109	-2.39599	2.16255
C	0.63595	-1.62515	2.20157
C	0.77679	-0.10744	2.36105
C	-0.53417	0.58535	2.75638
C	-0.44084	2.14219	2.77002
C	-0.99015	2.74242	1.47893
C	-1.15183	2.76415	3.97726
O	-0.39399	2.20013	0.38692
O	-1.85564	3.58837	1.40988
C	-0.93599	2.56808	-0.90953
C	0.11223	2.13119	-1.94308

C	-2.26209	1.90058	-1.13474
C	1.38381	2.97309	-1.999
C	4.26439	0.78089	-0.53723
C	3.17052	1.87248	-0.4916
C	2.6997	2.22589	-1.92866
C	1.33908	4.29954	-2.16546
C	3.66423	3.12081	0.25018
O	4.49696	-4.00486	-1.70729
O	-0.10997	-1.84153	1.01001
C	-3.43911	2.44927	-1.53584
O	-4.35297	1.44297	-1.67363
C	-3.67714	0.3022	-1.32285
N	-2.42991	0.52998	-1.00941
C	-4.44725	-0.93105	-1.38875
C	-4.18004	-2.11315	-0.79436
C	-3.01097	-2.31232	0.16052
C	-5.08498	-3.29768	-1.0174
C	-3.4886	-2.58487	1.58864
O	-2.19658	-3.4425	-0.20941
C	-1.52088	-3.26842	-1.45377
H	2.76655	-4.25895	0.28395
H	5.62153	-1.66072	-0.39177
H	5.08327	-1.5104	-2.07111
H	2.86111	-0.69412	-1.30246
H	1.7803	-3.46558	2.2896
H	2.59085	-2.08445	3.02264
H	0.08431	-2.01513	3.07425
H	1.13476	0.29583	1.41199
H	1.54691	0.10846	3.11421
H	-0.82731	0.25368	3.76184
H	-1.32866	0.26327	2.07523
H	0.62354	2.41781	2.80872
H	-1.08585	3.8555	3.96063

H	-0.70037	2.40007	4.90656
H	-2.21433	2.49907	3.98344
H	-1.07946	3.65144	-0.9261
H	-0.37038	2.1549	-2.92875
H	0.34558	1.07983	-1.74421
H	4.89802	0.83666	0.35693
H	4.92441	0.95814	-1.39743
H	2.31277	1.47349	0.0627
H	3.4894	2.81738	-2.41122
H	2.60639	1.29927	-2.51375
H	2.24552	4.8932	-2.25022
H	0.40191	4.84822	-2.23023
H	3.91618	2.88379	1.29049
H	4.56451	3.5333	-0.22516
H	2.89909	3.90355	0.25492
H	-0.52251	-2.72292	0.99718
H	-3.7819	3.45096	-1.73984
H	-5.353	-0.83787	-1.98457
H	-2.38143	-1.4217	0.15372
H	-5.61803	-3.57122	-0.09738
H	-5.83031	-3.09781	-1.79262
H	-4.4995	-4.17754	-1.30835
H	-2.62645	-2.62667	2.26174
H	-4.15178	-1.78394	1.93146
H	-4.02173	-3.53828	1.65606
H	-2.22845	-3.18632	-2.29017
H	-0.88394	-2.37578	-1.43558
H	-0.90173	-4.15777	-1.59793



2d-2*S*,5*R*,11*R*,13*R*,17*S*,23*S*

Calculated DFT energies of the 2d-diasteroisomer

Conformers **2d**	OPLS2008 Force Field Conformotional Search Relative Energy (kcal/mol)	B3LYP/6-31+G(d,p) DFT Energy (hartree)	Δ (DFT Energy) (kcal/mol)	% Population
2d4	0.675979924	-1710.462343	0	60.29
2d25	2.917853728	-1710.461345	0.62625437	20.92
2d15	2.413838432	-1710.460657	1.05798083	10.09
2d1	0	-1710.459641	1.69553037	3.44
2d22	2.878847992	-1710.458274	2.55333571	0.81
2d28	3.050454111	-1710.458268	2.55710077	0.80
2d45	3.916849904	-1710.457978	2.73907849	0.59
2d20	2.781477055	-1710.457663	2.93674395	0.42
2d6	1.353608987	-1710.457538	3.01518262	0.37
2d2	0.363957935	-1710.457466	3.0603633	0.34
2d17	2.638432122	-1710.457395	3.10491647	0.32
2d3	0.483843212	-1710.457216	3.21724065	0.26
2d33	3.420458891	-1710.457205	3.22414325	0.26
2d39	3.690774379	-1710.456651	3.57178345	0.14
2d55	4.390869981	-1710.456577	3.61821915	0.13
2d57	4.408819312	-1710.456514	3.65775224	0.12
2d11	1.783699809	-1710.456114	3.908756	0.08
2d49	4.078967495	-1710.456082	3.9288363	0.08
2d16	2.592638623	-1710.455898	4.04429803	0.06

19 conformers counting for the 99.53% of the DFT conformational population

DFT COORDINATES FOR CONFORMATIONAL SEARCH OF 2d

(2*S*, 5*R*, 11*R*, 13*R* , 17*S*, 23*S*)

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 1

C	-2.71147	1.51437	1.11078
C	-3.87926	1.81271	1.74062
C	-5.11957	2.03067	0.99687
C	-4.96889	1.91817	-0.52103
C	-3.86493	0.93351	-0.89822
O	-2.62631	1.27878	-0.21907
C	-1.40309	1.27155	1.80327
C	-1.27705	-0.23433	2.15522
C	0.1226	-0.60754	2.64153
C	0.2402	-2.06575	3.12184
C	-0.22323	-3.17713	2.13989
C	0.66763	-3.23929	0.90815
C	-0.24422	-4.54213	2.83963
O	0.36161	-2.26218	0.01409
O	1.55844	-4.04449	0.7305
C	1.2047	-2.1897	-1.17644
C	0.43197	-1.37922	-2.22272
C	2.53001	-1.56851	-0.84402
C	-0.89199	-1.99883	-2.65611
C	-3.58582	0.87317	-2.39831
C	-2.29788	0.14968	-2.84951
C	-2.16402	-1.27695	-2.25857
C	-0.91962	-3.13107	-3.36697
C	-2.23933	0.14124	-4.38448
O	-6.18391	2.32261	1.52393
O	-2.20007	-0.59314	3.17997
C	3.72069	-2.18455	-0.62017
O	4.65744	-1.22484	-0.37365
C	3.97807	-0.03484	-0.45063

N	2.7106	-0.19406	-0.73369
C	4.781	1.15239	-0.23629
C	4.36052	2.43009	-0.12158
C	2.89781	2.84939	-0.20403
C	5.36366	3.54039	0.05661
C	2.51458	3.27479	-1.62377
O	2.63045	3.96259	0.6508
C	2.52119	3.61313	2.01688
H	-3.88785	1.98083	2.81235
H	-5.92679	1.6174	-0.9563
H	-4.72657	2.91591	-0.91546
H	-4.13753	-0.06391	-0.52254
H	-1.33681	1.85845	2.72478
H	-0.58568	1.56277	1.13405
H	-1.48768	-0.80339	1.23832
H	0.39337	0.04806	3.48056
H	0.82919	-0.4038	1.82977
H	-0.36657	-2.17667	4.0262
H	1.2811	-2.26401	3.4103
H	-1.23671	-2.93111	1.80468
H	-0.58531	-5.33146	2.16213
H	-0.91996	-4.51134	3.70063
H	0.75553	-4.81731	3.18904
H	1.36612	-3.21413	-1.51906
H	1.09572	-1.27224	-3.08934
H	0.2882	-0.37142	-1.82417
H	-3.5523	1.89927	-2.78874
H	-4.45973	0.3954	-2.86416
H	-1.45474	0.7456	-2.47957
H	-2.18847	-1.20523	-1.16318
H	-3.03142	-1.87831	-2.56384
H	-1.85515	-3.58845	-3.67894
H	-0.00982	-3.65062	-3.66143

H	-2.31714	1.15812	-4.787
H	-3.06388	-0.44883	-4.8059
H	-1.30469	-0.29632	-4.74784
H	-3.09162	-0.36524	2.867
H	4.0412	-3.21258	-0.57941
H	5.84617	0.94275	-0.1749
H	2.26173	2.00352	0.0856
H	6.38879	3.15936	0.03774
H	5.25977	4.29099	-0.7374
H	5.20521	4.07509	0.99935
H	1.47122	3.60546	-1.63426
H	2.6273	2.43179	-2.31128
H	3.13959	4.10465	-1.96996
H	1.71333	2.88301	2.18315
H	3.45372	3.18785	2.41881
H	2.28786	4.53121	2.56291

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 2

C	-2.77561	1.42462	1.15819
C	-3.93767	1.77674	1.75988
C	-5.15212	2.03561	0.99411
C	-4.98024	1.9087	-0.52047
C	-3.89594	0.89611	-0.88254
O	-2.66285	1.19852	-0.17467
C	-1.48065	1.16043	1.87004
C	-1.29463	-0.35072	2.15224
C	0.12504	-0.6861	2.63014
C	0.2963	-2.14715	3.08535
C	-0.12728	-3.25797	2.08589
C	0.76109	-3.26425	0.85079
C	-0.09337	-4.63454	2.76168
O	0.42594	-2.27146	-0.01337

O	1.67013	-4.04265	0.64803
C	1.25371	-2.15029	-1.21129
C	0.44584	-1.33826	-2.22819
C	2.5656	-1.50226	-0.87742
C	-0.86799	-1.98371	-2.65639
C	-3.59481	0.85425	-2.38077
C	-2.29713	0.14872	-2.8302
C	-2.15167	-1.28337	-2.25745
C	-0.87667	-3.11682	-3.36628
C	-2.22509	0.16114	-4.36468
O	-6.2153	2.37482	1.49714
O	-2.29369	-0.83059	3.05155
C	3.77356	-2.0923	-0.6772
O	4.68762	-1.1146	-0.4165
C	3.97741	0.05902	-0.46127
N	2.712	-0.12646	-0.7373
C	4.752	1.26111	-0.22632
C	4.30209	2.52652	-0.08896
C	2.83028	2.91388	-0.16546
C	5.27946	3.65632	0.10875
C	2.43887	3.35796	-1.5772
O	2.5374	4.00432	0.71056
C	2.43074	3.62509	2.06826
H	-3.97416	1.90869	2.83507
H	-5.93911	1.62943	-0.96808
H	-4.70956	2.89864	-0.91655
H	-4.20386	-0.09748	-0.52587
H	-1.44936	1.7155	2.81586
H	-0.65251	1.5154	1.24448
H	-1.48429	-0.89103	1.22104
H	0.38549	-0.03405	3.47908
H	0.82748	-0.44231	1.8255
H	-0.30588	-2.30222	3.98757

H	1.3427	-2.31205	3.37441
H	-1.15036	-3.04448	1.75844
H	-0.40166	-5.42388	2.06902
H	-0.7717	-4.64785	3.62118
H	0.91629	-4.87611	3.10774
H	1.43852	-3.16245	-1.57754
H	1.09374	-1.19305	-3.10135
H	0.28071	-0.34421	-1.8044
H	-3.56291	1.88519	-2.75862
H	-4.46003	0.37785	-2.86402
H	-1.4638	0.74886	-2.44508
H	-2.18712	-1.2243	-1.16178
H	-3.0091	-1.89151	-2.5767
H	-1.80474	-3.59039	-3.67625
H	0.04126	-3.62106	-3.66231
H	-2.31123	1.18227	-4.75459
H	-3.03934	-0.43255	-4.80073
H	-1.28258	-0.26112	-4.7262
H	-2.15261	-0.39971	3.91082
H	4.12072	-3.11238	-0.66297
H	5.82194	1.07562	-0.17021
H	2.21291	2.04876	0.10715
H	6.31314	3.29965	0.08297
H	5.15776	4.41824	-0.67181
H	5.1094	4.17069	1.06079
H	1.3879	3.66354	-1.58311
H	2.57265	2.53172	-2.28109
H	3.04436	4.20914	-1.90586
H	1.63609	2.87641	2.21647
H	3.36986	3.20897	2.46472
H	2.1783	4.52705	2.63244

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 3

C	2.92859	-2.11991	-0.24281
C	4.04635	-2.58196	0.37437
C	5.34307	-1.93861	0.20345
C	5.33109	-0.76452	-0.77584
C	3.99001	-0.03404	-0.75608
O	2.89042	-0.96575	-0.95233
C	1.58976	-2.80096	-0.17745
C	0.82328	-2.53187	1.14632
C	0.51674	-1.04217	1.36047
C	-0.10525	-0.74847	2.73487
C	0.03128	0.7141	3.24003
C	-0.82771	1.70078	2.45636
C	-0.2989	0.81673	4.73418
O	-0.39512	1.83609	1.17499
O	-1.77478	2.31304	2.9008
C	-1.14398	2.74279	0.3216
C	-0.29182	2.96405	-0.93959
C	-2.48697	2.16774	-0.01785
C	1.08471	3.55568	-0.67548
C	3.88316	1.03983	-1.8347
C	2.56543	1.83871	-1.9238
C	2.27064	2.61351	-0.61178
C	1.23051	4.87445	-0.5055
C	2.63276	2.7739	-3.14081
O	6.37458	-2.3246	0.73803
O	-0.32533	-3.36228	1.23202
C	-3.72762	2.69135	0.16237
O	-4.63993	1.8093	-0.34295
C	-3.89533	0.75543	-0.80368
N	-2.61031	0.93899	-0.64807
C	-4.64475	-0.3604	-1.3529
C	-4.19955	-1.61464	-1.57946

C	-2.77754	-2.05361	-1.26273
C	-5.11686	-2.65583	-2.16834
C	-1.98064	-2.37685	-2.52668
O	-2.75618	-3.24254	-0.44911
C	-3.408	-3.09594	0.81145
H	4.00199	-3.49719	0.955
H	6.14708	-0.07982	-0.52585
H	5.52803	-1.15797	-1.78399
H	3.84066	0.39942	0.24372
H	1.71882	-3.88434	-0.26357
H	0.98394	-2.46035	-1.02594
H	1.46457	-2.87067	1.97015
H	-0.12697	-0.67229	0.55366
H	1.45881	-0.48657	1.27116
H	0.39317	-1.37819	3.48416
H	-1.16017	-1.04788	2.75138
H	1.07547	1.01859	3.07934
H	-0.19504	1.84383	5.09582
H	0.37356	0.17463	5.31278
H	-1.32945	0.50313	4.9279
H	-1.27855	3.68329	0.86351
H	-0.86652	3.63703	-1.58679
H	-0.22059	2.00662	-1.46547
H	4.06521	0.55639	-2.80406
H	4.71712	1.7392	-1.67765
H	1.75546	1.1166	-2.08878
H	2.09558	1.88749	0.19255
H	3.16306	3.19224	-0.33596
H	2.19962	5.32249	-0.30069
H	0.38597	5.55872	-0.56048
H	2.84636	2.21015	-4.05652
H	3.42453	3.52454	-3.01749
H	1.6929	3.31425	-3.28861

H	-0.90353	-3.23165	0.45576
H	-4.11505	3.59224	0.61013
H	-5.68309	-0.12164	-1.5718
H	-2.27273	-1.25066	-0.71836
H	-6.15052	-2.30147	-2.21688
H	-4.80456	-2.92164	-3.18715
H	-5.08629	-3.58247	-1.585
H	-0.96503	-2.68708	-2.26123
H	-1.91593	-1.49207	-3.16746
H	-2.44373	-3.19189	-3.09123
H	-3.18325	-3.99922	1.38172
H	-3.02813	-2.22444	1.36106
H	-4.49478	-2.99573	0.69614

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 4

C	5.12942	-0.56206	-0.50222
C	5.87754	-0.69138	0.62025
C	6.13656	0.43786	1.50997
C	5.53812	1.76063	1.0314
C	4.23314	1.53783	0.27391
O	4.43104	0.56947	-0.80368
C	4.9915	-1.61406	-1.56735
C	3.54152	-2.07127	-1.86214
C	2.8074	-2.5997	-0.61929
C	1.47092	-3.26557	-0.97667
C	0.55606	-3.54307	0.23621
C	0.22322	-2.24143	0.95275
C	-0.72624	-4.28512	-0.18164
O	-0.3953	-1.37297	0.11833
O	0.49917	-1.98592	2.10778
C	-0.62079	-0.02016	0.62178
C	-0.48965	0.90697	-0.59754

C	-1.94661	0.05158	1.31635
C	-0.22253	2.3494	-0.2103
C	3.67206	2.8076	-0.36221
C	2.2361	2.71692	-0.92315
C	1.18915	2.6957	0.22278
C	-1.19526	3.26663	-0.23941
C	1.9727	3.87633	-1.89395
O	6.82445	0.36454	2.51828
O	2.79948	-1.04344	-2.51515
C	-2.20468	-0.11253	2.64108
O	-3.55043	0.00137	2.8297
C	-4.0668	0.22932	1.5781
N	-3.14523	0.27367	0.65134
C	-5.50712	0.38284	1.52141
C	-6.29254	0.46697	0.42663
C	-5.76285	0.42789	-1.0021
C	-7.78148	0.64328	0.579
C	-5.60969	1.83642	-1.58192
O	-6.65923	-0.27818	-1.8628
C	-6.58331	-1.68406	-1.72215
H	6.37796	-1.62969	0.831
H	5.37306	2.41208	1.89463
H	6.27169	2.25646	0.37891
H	3.50385	1.07799	0.9562
H	5.60176	-2.47677	-1.28219
H	5.40349	-1.21441	-2.50392
H	3.61113	-2.88257	-2.59833
H	2.64474	-1.75946	0.0699
H	3.45174	-3.31087	-0.08344
H	1.66625	-4.21961	-1.48547
H	0.93546	-2.6281	-1.68738
H	1.09659	-4.14563	0.97509
H	-1.36823	-4.48913	0.68232

H	-0.47082	-5.24397	-0.64617
H	-1.30028	-3.69562	-0.90322
H	0.16458	0.17551	1.35549
H	-1.40115	0.83078	-1.19584
H	0.33424	0.51133	-1.20371
H	4.36347	3.10377	-1.16182
H	3.71127	3.60586	0.39203
H	2.15091	1.78083	-1.49159
H	1.51484	1.97636	0.98837
H	1.19168	3.68047	0.70863
H	-1.0165	4.2988	0.053
H	-2.20619	3.01302	-0.54676
H	2.65989	3.84013	-2.74698
H	2.11151	4.8436	-1.39291
H	0.94907	3.845	-2.27906
H	2.99819	-0.21867	-2.0405
H	-1.59716	-0.3177	3.50758
H	-5.97027	0.42929	2.50419
H	-4.78137	-0.06091	-1.01304
H	-8.07079	0.71751	1.63129
H	-8.12302	1.54962	0.06259
H	-8.32822	-0.18864	0.12187
H	-5.24865	1.76871	-2.61284
H	-4.89188	2.41269	-0.99051
H	-6.56814	2.36597	-1.58924
H	-7.28153	-2.11423	-2.44538
H	-5.56971	-2.05651	-1.93694
H	-6.86562	-2.02039	-0.7124

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 6

C	-2.76752	1.24087	1.345
C	-3.97585	1.41785	1.94325
C	-5.16213	1.80475	1.18064
C	-4.90834	2.01275	-0.31314
C	-3.77723	1.11919	-0.81665
O	-2.58951	1.29493	0.00415
C	-1.51294	0.82945	2.05682
C	-1.42198	-0.71952	2.08329
C	-0.06243	-1.21878	2.5706
C	0.00962	-2.7489	2.7273
C	-0.40095	-3.60775	1.49928
C	0.57198	-3.42217	0.34465
C	-0.48439	-5.09121	1.8805
O	0.34443	-2.26448	-0.32892
O	1.46396	-4.19348	0.0547
C	1.28153	-1.95259	-1.40856
C	0.59956	-0.91784	-2.30906
C	2.58018	-1.45169	-0.84419
C	-0.68725	-1.40049	-2.96859
C	-3.3959	1.38289	-2.27196
C	-2.07917	0.75838	-2.78368
C	-1.9859	-0.76486	-2.51328
C	-0.66091	-2.34266	-3.91702
C	-1.91595	1.08617	-4.27537
O	-6.26035	1.99344	1.68472
O	-2.4171	-1.26965	2.94203
C	3.70628	-2.15824	-0.55935
O	4.63883	-1.293	-0.06813
C	4.02436	-0.06595	-0.06911
N	2.79919	-0.11525	-0.5267
C	4.83543	1.0333	0.41134
C	4.47281	2.3217	0.58623

C	3.08788	2.84814	0.25423
C	5.47286	3.32614	1.09311
C	3.00182	3.2659	-1.22386
O	2.83421	3.95257	1.12756
C	1.46752	4.26513	1.28684
H	-4.05958	1.35271	3.02293
H	-5.83333	1.82046	-0.86533
H	-4.64471	3.06885	-0.47097
H	-4.07177	0.06744	-0.68445
H	-1.50834	1.20311	3.08546
H	-0.64709	1.23824	1.52371
H	-1.57148	-1.07308	1.0532
H	0.1528	-0.76638	3.54802
H	0.70113	-0.85917	1.87228
H	-0.65553	-3.04048	3.54635
H	1.02747	-3.03025	3.02839
H	-1.38669	-3.26811	1.16304
H	-0.79148	-5.70495	1.02761
H	-1.2134	-5.23033	2.68561
H	0.48748	-5.46162	2.22025
H	1.46109	-2.88237	-1.95237
H	1.33183	-0.6391	-3.07649
H	0.428	-0.01695	-1.71415
H	-3.33873	2.46903	-2.42531
H	-4.2353	1.02979	-2.88818
H	-1.26369	1.24604	-2.23551
H	-2.0899	-0.93398	-1.43345
H	-2.82804	-1.27228	-3.00372
H	-1.57002	-2.70188	-4.39262
H	0.26895	-2.79809	-4.25217
H	-1.96726	2.16757	-4.44906
H	-2.70964	0.61476	-4.86986
H	-0.95825	0.72674	-4.66358

H	-3.28338	-0.96515	2.62353
H	3.97707	-3.19929	-0.61961
H	5.85503	0.74146	0.64931
H	2.34712	2.05845	0.43629
H	6.45546	2.86958	1.24315
H	5.58018	4.16311	0.39098
H	5.13143	3.76327	2.03708
H	2.01436	3.68036	-1.45422
H	3.16043	2.39696	-1.8684
H	3.75497	4.0267	-1.45485
H	0.99786	4.61123	0.35416
H	0.89544	3.40085	1.6619
H	1.41151	5.07128	2.02353

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 11

C	-1.8569	1.27538	1.61962
C	-2.51787	2.27858	2.25274
C	-3.49415	3.11173	1.54808
C	-3.66383	2.76289	0.0652
C	-3.47954	1.26309	-0.13941
O	-2.17879	0.85834	0.37185
C	-0.72142	0.4702	2.18295
C	-1.09655	-1.02045	2.34568
C	0.12752	-1.89685	2.60697
C	-0.15958	-3.4077	2.58152
C	-0.77456	-3.98145	1.27453
C	0.09934	-3.67711	0.06358
C	-0.99416	-5.49454	1.39952
O	-0.15351	-2.43997	-0.42899
O	0.92556	-4.43015	-0.41245
C	0.64185	-1.99372	-1.57453
C	-0.11509	-0.82436	-2.20079

C	2.02424	-1.5986	-1.13245
C	-1.42627	-1.12219	-2.90012
C	-3.58249	0.69903	-1.55714
C	-2.54405	1.21352	-2.58306
C	-2.09407	0.07931	-3.54546
C	-1.97084	-2.34057	-2.99359
C	-3.07656	2.39673	-3.40763
O	-4.08866	4.04561	2.0677
O	-1.99627	-1.21243	3.43881
C	3.12322	-2.38716	-0.98545
O	4.15891	-1.60103	-0.57559
C	3.63643	-0.33529	-0.48763
N	2.36902	-0.28995	-0.80995
C	4.57658	0.69331	-0.08965
C	4.35052	2.01416	0.0753
C	2.99981	2.67934	-0.16385
C	5.48535	2.9298	0.4548
C	2.87905	3.18099	-1.6061
O	2.82227	3.81313	0.68531
C	2.44559	3.47896	2.00697
H	-2.25491	2.54747	3.2698
H	-4.65282	3.08965	-0.26973
H	-2.91272	3.32663	-0.50473
H	-4.22149	0.74533	0.48898
H	-0.40692	0.8824	3.14702
H	0.12162	0.54385	1.48291
H	-1.56659	-1.33454	1.40645
H	0.53389	-1.63618	3.59321
H	0.89606	-1.64593	1.86823
H	-0.85422	-3.64973	3.39365
H	0.77362	-3.94766	2.7897
H	-1.73905	-3.48972	1.10644
H	-1.48665	-5.90156	0.51017

H	-1.6231	-5.71294	2.26903
H	-0.03985	-6.01609	1.51813
H	0.71715	-2.83957	-2.26218
H	0.56164	-0.34233	-2.92047
H	-0.27532	-0.07501	-1.41767
H	-4.60154	0.88889	-1.92077
H	-3.48553	-0.38834	-1.45864
H	-1.65996	1.55638	-2.0311
H	-2.96764	-0.26175	-4.1166
H	-1.40035	0.52266	-4.27635
H	-2.90185	-2.49792	-3.53268
H	-1.52276	-3.22398	-2.5503
H	-3.40767	3.22425	-2.77164
H	-3.93369	2.08943	-4.02093
H	-2.30665	2.78552	-4.08455
H	-2.7836	-0.66849	3.27591
H	3.31341	-3.44098	-1.10227
H	5.58279	0.31126	0.06451
H	2.19829	1.95268	0.01755
H	6.43419	2.38839	0.50919
H	5.59095	3.74339	-0.27395
H	5.30328	3.41327	1.42096
H	1.91723	3.68718	-1.7351
H	2.93604	2.34095	-2.30413
H	3.67519	3.89489	-1.84217
H	3.19695	2.85268	2.51259
H	2.34209	4.41872	2.55597
H	1.48203	2.94618	2.02853

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 15

C	-5.36749	0.3516	0.38565
C	-5.74278	0.34868	1.68783
C	-5.66504	-0.85561	2.51097
C	-5.18099	-2.09533	1.75893
C	-4.1776	-1.72628	0.67124
O	-4.739	-0.70219	-0.20893
C	-5.61972	1.47902	-0.57653
C	-4.35939	2.06105	-1.2622
C	-3.30251	2.56299	-0.26496
C	-2.17144	3.33365	-0.96073
C	-0.94562	3.60887	-0.06285
C	-0.34852	2.29757	0.42915
C	0.11216	4.45386	-0.79607
O	0.0269	1.51593	-0.60974
O	-0.24567	1.96616	1.59361
C	0.46021	0.15745	-0.29236
C	0.03704	-0.70587	-1.49125
C	1.93302	0.14244	-0.01048
C	-0.02926	-2.18376	-1.15362
C	-3.77186	-2.90319	-0.21279
C	-2.57069	-2.66974	-1.15538
C	-1.23533	-2.65646	-0.36451
C	0.94512	-3.02187	-1.52336
C	-2.55021	-3.73401	-2.26122
O	-6.01546	-0.90262	3.68156
O	-3.80702	1.13521	-2.19523
C	2.55449	0.31324	1.1865
O	3.90454	0.26971	0.97314
C	4.04282	0.06599	-0.3762
N	2.89489	-0.00903	-0.99791
C	5.34667	-0.02163	-1.00162
C	6.579	-0.05776	-0.45126

C	6.86322	-0.01014	1.04774
C	7.79363	-0.10579	-1.34443
C	7.17458	1.41346	1.51863
O	7.99703	-0.81151	1.38297
C	7.72009	-2.19871	1.4098
H	-6.20083	1.2311	2.11999
H	-4.73396	-2.7949	2.47139
H	-6.05479	-2.59164	1.31181
H	-3.29991	-1.26327	1.14447
H	-6.15376	2.27315	-0.0454
H	-6.28218	1.11177	-1.37207
H	-4.6962	2.91032	-1.87074
H	-2.89787	1.69728	0.27766
H	-3.78191	3.19889	0.49264
H	-2.55719	4.2975	-1.32057
H	-1.84845	2.76958	-1.84138
H	-1.26342	4.13625	0.84381
H	0.97669	4.65554	-0.1541
H	-0.3178	5.41614	-1.09529
H	0.46587	3.94048	-1.69544
H	-0.07147	-0.1364	0.61567
H	0.73508	-0.5299	-2.31353
H	-0.94594	-0.33817	-1.80919
H	-4.65421	-3.18754	-0.80073
H	-3.54978	-3.75572	0.44401
H	-2.70129	-1.69129	-1.63747
H	-1.35411	-2.01664	0.52237
H	-1.04977	-3.67053	0.0139
H	0.91448	-4.07963	-1.27166
H	1.812	-2.67414	-2.07848
H	-3.45858	-3.68518	-2.8725
H	-2.48997	-4.74262	-1.83102
H	-1.68737	-3.60177	-2.9209

H	-3.8032	0.26957	-1.75286
H	2.21856	0.49228	2.19493
H	5.25845	-0.05024	-2.08464
H	5.99259	-0.3791	1.60221
H	7.51362	-0.07165	-2.40104
H	8.46372	0.73865	-1.1383
H	8.38449	-1.0108	-1.1665
H	7.40204	1.40216	2.5891
H	6.3159	2.06846	1.34412
H	8.04213	1.82046	0.98921
H	6.92945	-2.4376	2.13835
H	7.40904	-2.5839	0.42655
H	8.64339	-2.70131	1.71019

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 16

C	2.73464	-2.24733	-0.11873
C	3.79251	-2.81657	0.51274
C	5.15641	-2.34145	0.30537
C	5.2784	-1.21865	-0.72656
C	4.03354	-0.33406	-0.74741
O	2.83161	-1.13879	-0.88913
C	1.31313	-2.72693	-0.01715
C	0.61497	-2.33093	1.31055
C	0.73453	-0.83725	1.60733
C	0.00205	-0.39833	2.88172
C	0.20851	1.09118	3.2721
C	-0.5937	2.03984	2.38517
C	-0.13943	1.33971	4.74448
O	-0.21384	1.94535	1.08475
O	-1.45901	2.79718	2.76828
C	-0.93773	2.75506	0.11916
C	-0.0851	2.77038	-1.16056

C	-2.31291	2.20766	-0.12281
C	1.30395	3.36443	-0.97076
C	4.04355	0.68261	-1.88598
C	2.78799	1.56128	-2.07606
C	2.47462	2.41333	-0.81831
C	1.47128	4.69112	-0.93517
C	2.97839	2.43232	-3.32711
O	6.13779	-2.82532	0.85376
O	-0.77675	-2.63031	1.2386
C	-3.50812	2.81963	0.08252
O	-4.49595	1.97847	-0.33645
C	-3.84142	0.85382	-0.7743
N	-2.54102	0.9538	-0.67824
C	-4.69801	-0.20218	-1.28225
C	-4.39782	-1.50719	-1.4479
C	-3.05416	-2.11447	-1.06758
C	-5.41441	-2.44225	-2.05294
C	-2.17205	-2.33644	-2.29702
O	-3.22397	-3.39614	-0.44354
C	-3.83145	-3.32344	0.84067
H	3.64424	-3.6885	1.14094
H	6.17096	-0.62501	-0.50726
H	5.42513	-1.68018	-1.7142
H	3.94158	0.17043	0.22547
H	1.28374	-3.81949	-0.11771
H	0.74281	-2.2908	-0.84334
H	1.07856	-2.90655	2.12968
H	0.35157	-0.28523	0.74628
H	1.8	-0.59143	1.70835
H	0.36244	-1.00359	3.72499
H	-1.06879	-0.61042	2.78756
H	1.26828	1.33613	3.10712
H	-0.00604	2.3912	5.01379

H	0.50153	0.73002	5.39016
H	-1.18301	1.07864	4.94764
H	-1.02494	3.76538	0.52859
H	-0.64313	3.35614	-1.9004
H	-0.03573	1.74635	-1.54412
H	4.22663	0.13575	-2.82085
H	4.91855	1.33063	-1.73161
H	1.94077	0.88684	-2.25362
H	2.26568	1.73815	0.02111
H	3.36967	2.99293	-0.55286
H	2.44839	5.14202	-0.78065
H	0.637	5.37988	-1.05413
H	3.18505	1.81332	-4.20815
H	3.8214	3.12455	-3.20036
H	2.09024	3.03517	-3.53795
H	-0.92288	-3.46413	0.76427
H	-3.81242	3.76676	0.49815
H	-5.69507	0.14396	-1.54594
H	-2.52844	-1.44794	-0.37652
H	-6.35511	-1.92708	-2.26801
H	-5.03875	-2.86864	-2.9925
H	-5.61903	-3.29233	-1.39405
H	-1.23264	-2.80907	-1.99412
H	-1.94507	-1.37746	-2.77174
H	-2.6599	-2.99082	-3.02694
H	-3.89176	-4.34942	1.21537
H	-3.22896	-2.71971	1.5308
H	-4.84752	-2.90596	0.79485

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 17

C	-2.7476	-2.10758	-0.59778
C	-3.92832	-2.40476	-1.19791
C	-5.20854	-2.07586	-0.58134
C	-5.09137	-1.45198	0.81021
C	-3.8167	-0.6221	0.95184
O	-2.65123	-1.3915	0.5485
C	-1.39534	-2.47389	-1.14365
C	-0.92156	-1.54857	-2.29936
C	-1.02808	-0.06414	-1.94554
C	-0.5563	0.8772	-3.06117
C	-0.74525	2.38995	-2.76254
C	0.26544	2.90137	-1.74011
C	-0.66674	3.23106	-4.04147
O	0.1214	2.27581	-0.54395
O	1.10066	3.75642	-1.94514
C	1.06914	2.62541	0.5068
C	0.45164	2.15933	1.83331
C	2.40591	1.99466	0.24692
C	-0.91608	2.75936	2.12787
C	-3.57987	-0.13693	2.38013
C	-2.269	0.62401	2.67403
C	-2.14315	1.91938	1.82975
C	-1.01839	3.99434	2.63143
C	-2.189	0.91401	4.18053
O	-6.29444	-2.32194	-1.08975
O	0.40797	-1.90697	-2.68148
C	3.53558	2.58587	-0.22287
O	4.52483	1.64933	-0.25692
C	3.93928	0.49388	0.19766
N	2.67741	0.65481	0.50772
C	4.82923	-0.6455	0.29792
C	4.52388	-1.92197	0.61402

C	3.10992	-2.40804	0.91197
C	5.62209	-2.94533	0.74861
C	2.78871	-2.30382	2.40555
O	2.9428	-3.77649	0.54816
C	2.80537	-3.99395	-0.84495
H	-3.93698	-2.95748	-2.13137
H	-5.97583	-0.83739	1.00327
H	-5.09008	-2.26682	1.54909
H	-3.86859	0.22777	0.25512
H	-1.39836	-3.50337	-1.51483
H	-0.66761	-2.4129	-0.32626
H	-1.53111	-1.76188	-3.18561
H	-0.45819	0.11868	-1.02892
H	-2.07507	0.1641	-1.7079
H	-1.12568	0.65514	-3.97386
H	0.49373	0.6785	-3.30823
H	-1.73863	2.51764	-2.30811
H	-0.78884	4.29602	-3.82499
H	-1.45198	2.92512	-4.74076
H	0.30291	3.10488	-4.53371
H	1.17881	3.71262	0.49609
H	1.16024	2.43956	2.62162
H	0.41503	1.06596	1.82495
H	-3.62633	-1.01247	3.04177
H	-4.43563	0.49885	2.64987
H	-1.43902	-0.04278	2.40861
H	-2.12731	1.64632	0.76683
H	-3.03949	2.53373	1.99213
H	-1.98289	4.453	2.83464
H	-0.1415	4.59844	2.85628
H	-2.27105	-0.01103	4.76314
H	-3.00193	1.5812	4.49632
H	-1.24575	1.39951	4.44811

H	1.00935	-1.53687	-2.01362
H	3.7793	3.57696	-0.56923
H	5.86893	-0.38789	0.11132
H	2.38952	-1.78669	0.36126
H	6.60761	-2.4928	0.60617
H	5.59546	-3.41254	1.74126
H	5.50511	-3.76161	0.02784
H	1.78463	-2.69885	2.58952
H	2.82555	-1.25932	2.72593
H	3.50008	-2.88711	2.99959
H	2.69308	-5.07222	-0.98609
H	1.91621	-3.49137	-1.25322
H	3.68506	-3.65387	-1.41248

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 20

C	2.93644	-2.04926	0.42014
C	4.1562	-2.29594	0.9632
C	5.38856	-1.84386	0.32739
C	5.17544	-1.14713	-1.01637
C	3.84681	-0.39475	-1.05259
O	2.74744	-1.26759	-0.66845
C	1.642	-2.56679	0.9862
C	1.15026	-1.75974	2.217
C	0.88463	-0.29334	1.89133
C	0.46322	0.53566	3.11379
C	0.58349	2.0739	2.94772
C	-0.43965	2.64955	1.97299
C	0.47556	2.79124	4.29852
O	-0.26463	2.16291	0.71895
O	-1.30012	3.45564	2.25863
C	-1.19425	2.63252	-0.30279
C	-0.54889	2.33102	-1.66261

C	-2.52975	1.96694	-0.15302
C	0.81418	2.97583	-1.86579
C	3.52749	0.17726	-2.4307
C	2.18228	0.91227	-2.6113
C	2.04604	2.11948	-1.64673
C	0.91096	4.25987	-2.22746
C	2.04102	1.33311	-4.08207
O	6.50611	-2.04772	0.7831
O	-0.07019	-2.31429	2.71163
C	-3.68096	2.48159	0.35314
O	-4.65137	1.52829	0.25914
C	-4.02937	0.44177	-0.30448
N	-2.76873	0.66369	-0.57286
C	-4.87258	-0.71632	-0.52264
C	-4.48669	-1.96683	-0.85312
C	-3.03178	-2.38034	-1.04234
C	-5.5204	-3.03851	-1.08537
C	-2.61778	-2.3221	-2.51491
O	-2.818	-3.72195	-0.60196
C	-2.76502	-3.85046	0.80939
H	4.23806	-2.90683	1.85603
H	6.01033	-0.4655	-1.20455
H	5.19193	-1.91383	-1.80487
H	3.87227	0.40259	-0.29545
H	1.77454	-3.61312	1.28869
H	0.86815	-2.53516	0.21266
H	1.9262	-1.81883	2.99796
H	0.12569	-0.2381	1.1057
H	1.804	0.12997	1.46897
H	1.10767	0.26473	3.96155
H	-0.55733	0.2712	3.4136
H	1.57176	2.28029	2.51085
H	0.56783	3.87469	4.18182

H	1.26645	2.44518	4.97259
H	-0.49226	2.59355	4.77032
H	-1.31124	3.71006	-0.16341
H	-1.2497	2.69174	-2.42478
H	-0.49859	1.24437	-1.77753
H	3.57336	-0.64811	-3.15409
H	4.34842	0.86123	-2.69085
H	1.38443	0.19498	-2.3812
H	2.02847	1.74369	-0.61561
H	2.93842	2.75344	-1.74452
H	1.87377	4.74593	-2.36423
H	0.03129	4.87789	-2.39681
H	2.14908	0.46963	-4.74903
H	2.81024	2.06685	-4.35682
H	1.06756	1.79204	-4.2789
H	0.11214	-3.21338	3.02718
H	-3.95321	3.4222	0.80333
H	-5.9325	-0.50754	-0.39779
H	-2.38581	-1.69939	-0.47416
H	-6.53559	-2.6401	-1.00028
H	-5.40524	-3.48037	-2.08336
H	-5.40647	-3.86405	-0.37455
H	-1.58178	-2.66149	-2.61465
H	-2.69266	-1.29599	-2.88562
H	-3.25013	-2.97169	-3.12944
H	-2.57921	-4.90793	1.02032
H	-1.95629	-3.24445	1.24293
H	-3.71136	-3.55839	1.29065

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 22

C	5.03239	0.77026	0.43854
C	5.83036	0.73198	-0.65909
C	6.1425	-0.51701	-1.34134
C	5.56524	-1.75743	-0.66086
C	4.23669	-1.45979	0.02982
O	4.3571	-0.30152	0.91436
C	4.80046	2.01991	1.24568
C	3.58777	2.86735	0.7779
C	2.23857	2.25668	1.17636
C	1.02256	2.97855	0.5719
C	0.79002	2.72775	-0.94243
C	0.62154	1.23365	-1.16611
C	-0.38979	3.55851	-1.46749
O	-0.63157	0.81565	-0.87455
O	1.52143	0.48484	-1.49974
C	-0.84355	-0.62941	-0.86223
C	-0.57155	-1.15206	0.56747
C	-2.23904	-0.8839	-1.33097
C	-0.15912	-2.60999	0.57864
C	3.74725	-2.62257	0.8926
C	2.29082	-2.53555	1.39623
C	1.29507	-2.89527	0.25967
C	-1.04291	-3.581	0.83388
C	2.09331	-3.44555	2.61647
O	6.85988	-0.5959	-2.33029
O	3.70905	4.2073	1.25829
C	-2.64915	-1.43835	-2.50177
O	-4.01241	-1.48715	-2.4972
C	-4.38145	-0.94137	-1.29247
N	-3.35676	-0.58158	-0.56471
C	-5.80797	-0.87818	-1.04657
C	-6.44393	-0.24551	-0.03748

C	-5.72708	0.5362	1.0577
C	-7.94514	-0.31846	0.06982
C	-5.51126	-0.31928	2.30873
O	-6.49054	1.67542	1.45867
C	-6.40774	2.75666	0.54993
H	6.3179	1.63747	-1.00368
H	5.43729	-2.54757	-1.40687
H	6.30061	-2.11623	0.07474
H	3.49285	-1.17263	-0.72507
H	5.684	2.65961	1.16555
H	4.6739	1.74475	2.30148
H	3.65084	2.96462	-0.31087
H	2.16665	2.29432	2.27478
H	2.23561	1.19454	0.91179
H	1.14194	4.05817	0.72116
H	0.11423	2.67839	1.109
H	1.69716	2.9994	-1.49242
H	-0.55763	3.38481	-2.53591
H	-0.18435	4.62536	-1.32708
H	-1.31334	3.31139	-0.93596
H	-0.13521	-1.06496	-1.56934
H	-1.46662	-0.98536	1.17317
H	0.23071	-0.53881	0.99152
H	4.43078	-2.69749	1.74845
H	3.87336	-3.54958	0.3156
H	2.11052	-1.49923	1.71238
H	1.5774	-2.33385	-0.64165
H	1.41741	-3.96015	0.02024
H	-0.76006	-4.63092	0.81597
H	-2.08183	-3.36075	1.06706
H	2.74199	-3.13884	3.44516
H	2.33752	-4.48771	2.37024
H	1.05693	-3.42208	2.96754

H	3.6045	4.18076	2.22392
H	-2.14905	-1.83135	-3.37284
H	-6.39689	-1.4169	-1.785
H	-4.74671	0.86226	0.68945
H	-8.37244	-0.95086	-0.71369
H	-8.24709	-0.72401	1.04395
H	-8.39809	0.67672	0.00402
H	-5.02678	0.28514	3.08187
H	-4.87132	-1.17487	2.07449
H	-6.46342	-0.68485	2.7074
H	-6.99734	3.57421	0.97364
H	-5.36797	3.09452	0.41917
H	-6.81336	2.50342	-0.44189

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 25

C	5.09547	-0.59792	-0.53721
C	5.8613	-0.7083	0.57523
C	6.14349	0.43821	1.43538
C	5.54652	1.75478	0.93817
C	4.22798	1.52576	0.20643
O	4.40106	0.53242	-0.85247
C	4.92915	-1.67269	-1.57522
C	3.46995	-2.12827	-1.82451
C	2.76386	-2.62197	-0.55157
C	1.41353	-3.28549	-0.85807
C	0.52475	-3.51833	0.38382
C	0.22169	-2.1911	1.06605
C	-0.77229	-4.26182	0.01812
O	-0.42542	-1.35058	0.22402
O	0.54338	-1.89481	2.19897
C	-0.62895	0.01998	0.68477
C	-0.50748	0.90434	-0.5679

C	-1.94349	0.1303	1.3936
C	-0.22719	2.35736	-0.23415
C	3.66698	2.78562	-0.44916
C	2.22282	2.69329	-0.98823
C	1.19141	2.70773	0.17211
C	-1.19314	3.28077	-0.28556
C	1.9551	3.83166	-1.98246
O	6.84796	0.3818	2.43325
O	2.71834	-1.11083	-2.48331
C	-2.17827	0.0888	2.73155
O	-3.52285	0.20193	2.93175
C	-4.06201	0.30164	1.67314
N	-3.15587	0.27058	0.73027
C	-5.50402	0.42771	1.62158
C	-6.30179	0.37205	0.53419
C	-5.77245	0.18676	-0.87633
C	-7.79217	0.52664	0.68039
C	-5.46539	1.54374	-1.532
O	-6.76703	-0.53439	-1.61022
C	-6.2702	-1.20975	-2.74655
H	6.35762	-1.64583	0.79868
H	5.39985	2.4255	1.78989
H	6.27311	2.23131	0.26387
H	3.50606	1.08702	0.91013
H	5.54178	-2.53188	-1.28465
H	5.32087	-1.29626	-2.52988
H	3.51658	-2.95701	-2.54279
H	2.62509	-1.76511	0.12195
H	3.41646	-3.32557	-0.01574
H	1.58794	-4.25603	-1.3428
H	0.86657	-2.6642	-1.57441
H	1.07838	-4.1021	1.12805
H	-1.39696	-4.43225	0.90175

H	-0.53496	-5.23722	-0.4209
H	-1.35723	-3.6904	-0.70913
H	0.16842	0.23305	1.4005
H	-1.42748	0.81216	-1.15096
H	0.3063	0.48323	-1.17065
H	4.34917	3.05933	-1.26452
H	3.72231	3.59973	0.2869
H	2.12228	1.74497	-1.53346
H	1.52336	2.00675	0.95173
H	1.20556	3.70489	0.63176
H	-1.004	4.32079	-0.02987
H	-2.20884	3.02624	-0.57626
H	2.62944	3.76896	-2.84417
H	2.10964	4.8093	-1.50682
H	0.92573	3.80018	-2.35192
H	2.93361	-0.27676	-2.03267
H	-1.55524	-0.02329	3.60421
H	-5.95991	0.57109	2.59793
H	-4.84522	-0.3992	-0.84006
H	-8.07435	0.7085	1.72144
H	-8.16382	1.35913	0.06868
H	-8.30631	-0.37011	0.31964
H	-5.10897	1.40686	-2.55864
H	-4.6838	2.06287	-0.96994
H	-6.36195	2.17209	-1.56209
H	-7.10731	-1.77155	-3.17027
H	-5.88684	-0.52255	-3.5156
H	-5.46619	-1.914	-2.4803

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 28

C	5.02726	0.75077	0.43457
C	5.82059	0.7151	-0.66708
C	6.12464	-0.53012	-1.35889
C	5.54617	-1.77219	-0.68289
C	4.22252	-1.47436	0.01739
O	4.35011	-0.31993	0.90617
C	4.80323	1.99653	1.24977
C	3.59959	2.85805	0.78066
C	2.25202	2.27606	1.2065
C	1.03476	2.99648	0.60282
C	0.79138	2.74746	-0.91035
C	0.62715	1.25382	-1.13842
C	-0.39552	3.57509	-1.42461
O	-0.62518	0.83144	-0.84948
O	1.52907	0.50866	-1.47505
C	-0.83533	-0.61364	-0.84644
C	-0.57132	-1.14352	0.58171
C	-2.22735	-0.86812	-1.32569
C	-0.17067	-2.60472	0.58849
C	3.73639	-2.63936	0.87902
C	2.28389	-2.54934	1.39293
C	1.27948	-2.90131	0.26176
C	-1.06062	-3.56916	0.84706
C	2.09101	-3.46312	2.61101
O	6.83699	-0.60485	-2.35202
O	3.67309	4.16078	1.3637
C	-2.62818	-1.4165	-2.50255
O	-3.99134	-1.46937	-2.50733
C	-4.36978	-0.93221	-1.30159
N	-3.35096	-0.57383	-0.56499
C	-5.79806	-0.87507	-1.06451
C	-6.44255	-0.25028	-0.05593

C	-5.73558	0.52775	1.04825
C	-7.94418	-0.32874	0.04114
C	-5.5254	-0.33357	2.29621
O	-6.50569	1.66232	1.4498
C	-6.41898	2.74907	0.54808
H	6.31248	1.61952	-1.00868
H	5.4109	-2.55738	-1.43283
H	6.28452	-2.13826	0.0461
H	3.47437	-1.18207	-0.73111
H	5.70555	2.61504	1.18054
H	4.66555	1.72991	2.30382
H	3.64751	2.93229	-0.3165
H	2.20208	2.35216	2.30052
H	2.237	1.20967	0.96184
H	1.15015	4.07548	0.756
H	0.13052	2.69285	1.1451
H	1.69303	3.02309	-1.46775
H	-0.57087	3.40482	-2.49247
H	-0.19425	4.6424	-1.28096
H	-1.31402	3.32234	-0.88714
H	-0.12199	-1.04421	-1.55162
H	-1.46664	-0.97214	1.1857
H	0.23454	-0.53788	1.00997
H	4.42566	-2.71925	1.72979
H	3.85594	-3.56449	0.29756
H	2.10947	-1.51367	1.71406
H	1.56143	-2.34206	-0.64106
H	1.39231	-3.967	0.0212
H	-0.78593	-4.62122	0.82674
H	-2.0966	-3.34109	1.08565
H	2.74508	-3.16094	3.43708
H	2.33076	-4.50514	2.35974
H	1.05672	-3.43764	2.96803

H	4.43409	4.62123	0.97727
H	-2.1212	-1.80281	-3.37264
H	-6.38045	-1.41149	-1.80977
H	-4.75382	0.85891	0.68843
H	-8.36435	-0.95765	-0.74903
H	-8.25113	-0.74127	1.01076
H	-8.39981	0.66543	-0.02138
H	-5.048	0.26834	3.07565
H	-4.88107	-1.18582	2.06178
H	-6.47899	-0.70435	2.68657
H	-7.01405	3.5625	0.97207
H	-5.37921	3.09055	0.42727
H	-6.8164	2.50049	-0.44829

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 33

C	5.01932	-0.38132	0.08736
C	5.61308	-0.15452	1.2876
C	5.69724	1.17996	1.86801
C	5.13355	2.28012	0.97013
C	3.95922	1.77254	0.13864
O	4.32182	0.56105	-0.59075
C	5.08952	-1.70098	-0.63142
C	3.83168	-2.6067	-0.52303
C	2.70722	-2.18659	-1.4704
C	1.48046	-3.11465	-1.46548
C	0.77061	-3.28413	-0.1018
C	0.48299	-1.92794	0.52103
C	-0.50876	-4.12725	-0.24221
O	-0.37512	-1.20775	-0.23969
O	0.98893	-1.51115	1.54523
C	-0.6063	0.17753	0.16921
C	-0.72098	0.99647	-1.12553

C	-1.81252	0.25152	1.0532
C	-0.44586	2.47477	-0.92754
C	3.4715	2.7854	-0.8968
C	2.08417	2.50514	-1.5123
C	0.95744	2.8796	-0.51452
C	-1.41022	3.38299	-1.1104
C	1.91978	3.26103	-2.83808
O	6.23254	1.42753	2.94048
O	4.17994	-3.94622	-0.88171
C	-1.85558	0.23344	2.41215
O	-3.16241	0.29066	2.79725
C	-3.87627	0.3367	1.62514
N	-3.11037	0.32249	0.56543
C	-5.31598	0.40248	1.77669
C	-6.25512	0.32247	0.81015
C	-5.93314	0.15695	-0.67071
C	-7.71485	0.43826	1.16533
C	-5.90596	1.50779	-1.39084
O	-6.91857	-0.64383	-1.32609
C	-6.76702	-2.02997	-1.08734
H	6.12653	-0.962	1.79769
H	4.82416	3.12702	1.58986
H	5.93935	2.6321	0.30913
H	3.14887	1.47515	0.81999
H	5.93562	-2.25753	-0.21332
H	5.30973	-1.52638	-1.69186
H	3.4708	-2.57309	0.51558
H	3.115	-2.15953	-2.48955
H	2.41709	-1.15816	-1.22654
H	1.78559	-4.1092	-1.80709
H	0.75283	-2.73114	-2.19091
H	1.44899	-3.78345	0.59722
H	-0.99313	-4.28358	0.72805

H	-0.26376	-5.11025	-0.65919
H	-1.22747	-3.64006	-0.90826
H	0.2672	0.47391	0.75153
H	-1.71591	0.84837	-1.55319
H	0.00388	0.57299	-1.83121
H	4.22975	2.82536	-1.68933
H	3.46278	3.77848	-0.42633
H	2.03104	1.42928	-1.72621
H	1.18822	2.43095	0.46279
H	0.98227	3.96622	-0.35778
H	-1.22618	4.44703	-0.98132
H	-2.42002	3.0935	-1.38959
H	2.67054	2.94192	-3.57004
H	2.03719	4.34259	-2.68843
H	0.92811	3.09536	-3.27137
H	4.77422	-4.29526	-0.19956
H	-1.11154	0.17376	3.19021
H	-5.63299	0.53367	2.80849
H	-4.94783	-0.31247	-0.77819
H	-7.8536	0.62043	2.23497
H	-8.18798	1.25883	0.61089
H	-8.2644	-0.46818	0.88908
H	-5.70355	1.34878	-2.45464
H	-5.12105	2.14291	-0.96968
H	-6.86765	2.02361	-1.29914
H	-7.54918	-2.53853	-1.65764
H	-5.78373	-2.39214	-1.42552
H	-6.87962	-2.28769	-0.0227

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 39

C	4.86318	-0.97567	-0.3385
C	5.13358	-1.31825	-1.62421
C	4.48034	-2.44552	-2.27564
C	3.54865	-3.23724	-1.35916
C	2.88877	-2.34613	-0.30945
O	3.88755	-1.54852	0.40138
C	5.61671	0.09412	0.40643
C	5.00807	1.51587	0.27086
C	3.77154	1.71777	1.14652
C	3.03418	3.0457	0.90573
C	2.28082	3.16404	-0.44782
C	1.3041	2.00687	-0.56353
C	1.62495	4.54371	-0.59888
O	0.13488	2.25562	0.07742
O	1.56168	0.94791	-1.10132
C	-0.78605	1.13912	0.20482
C	-0.5312	0.4719	1.58298
C	-2.16842	1.6866	0.03007
C	-0.9925	-0.96794	1.66901
C	2.13234	-3.14322	0.75265
C	1.20448	-2.32772	1.67839
C	-0.13131	-1.9931	0.95826
C	-2.0877	-1.30828	2.357
C	0.95452	-3.08575	2.98948
O	4.69968	-2.78914	-3.43011
O	5.95683	2.499	0.69029
C	-2.6215	2.96209	0.15642
O	-3.96532	2.9583	-0.0983
C	-4.27242	1.65087	-0.36828
N	-3.22885	0.86273	-0.31274
C	-5.66156	1.38078	-0.67822
C	-6.25043	0.17691	-0.84312

C	-5.51001	-1.15105	-0.73028
C	-7.71241	0.09521	-1.1991
C	-5.05572	-1.65646	-2.10216
O	-6.3527	-2.16176	-0.17088
C	-6.49474	-2.06103	1.23244
H	5.91191	-0.79651	-2.17067
H	2.78715	-3.73501	-1.96699
H	4.14195	-4.02309	-0.86809
H	2.23832	-1.61697	-0.81015
H	6.63819	0.12826	0.01041
H	5.68274	-0.17015	1.46798
H	4.74812	1.66901	-0.78735
H	4.10935	1.68777	2.19067
H	3.09945	0.8658	1.00616
H	3.75639	3.86787	0.96279
H	2.3077	3.2036	1.71323
H	2.99455	3.01427	-1.2647
H	1.08287	4.62977	-1.54679
H	2.39309	5.32439	-0.57678
H	0.91916	4.73757	0.21448
H	-0.57446	0.43104	-0.5982
H	-1.00231	1.08135	2.36102
H	0.55195	0.51397	1.75132
H	2.88414	-3.67189	1.35296
H	1.54344	-3.91858	0.2428
H	1.72188	-1.3905	1.92352
H	0.09667	-1.63174	-0.05371
H	-0.69821	-2.92531	0.83469
H	-2.42422	-2.34038	2.41935
H	-2.69066	-0.5676	2.87625
H	1.89149	-3.24661	3.53512
H	0.50957	-4.07052	2.79316
H	0.26987	-2.53574	3.64267

H	6.68488	2.50791	0.0497
H	-2.16709	3.91368	0.37596
H	-6.262	2.28069	-0.78773
H	-4.62245	-1.02282	-0.09937
H	-8.14866	1.08947	-1.33241
H	-7.85583	-0.47293	-2.12706
H	-8.28095	-0.43742	-0.42895
H	-4.56775	-2.62924	-1.98656
H	-4.34396	-0.95376	-2.54453
H	-5.90634	-1.77861	-2.78104
H	-7.12302	-2.89775	1.55029
H	-5.52083	-2.12958	1.74194
H	-6.97632	-1.11945	1.53975

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 45

C	2.87806	-2.43016	-0.25443
C	3.87862	-3.1479	0.31786
C	5.28209	-2.85959	0.05119
C	5.51282	-1.75429	-0.98195
C	4.39889	-0.70876	-0.95803
O	3.09465	-1.34066	-1.03237
C	1.40878	-2.68623	-0.0752
C	0.81812	-2.20551	1.29063
C	1.42823	-0.87839	1.76561
C	0.7617	-0.306	3.02616
C	1.0468	1.20454	3.27578
C	0.16931	2.0552	2.36503
C	0.81991	1.59517	4.73949
O	0.52089	1.89306	1.05917
O	-0.74672	2.76453	2.7165
C	-0.33853	2.46919	0.05119
C	0.42961	2.36337	-1.28036

C	-1.65499	1.74531	0.00087
C	1.79655	3.03609	-1.25768
C	4.49509	0.29007	-2.11161
C	3.30007	1.24278	-2.33468
C	3.01558	2.14643	-1.10695
C	1.8986	4.36552	-1.36294
C	3.55053	2.07356	-3.60256
O	6.21431	-3.47482	0.55318
O	-0.59552	-2.12139	1.17154
C	-2.9055	2.26715	-0.0607
O	-3.79828	1.23121	-0.1444
C	-3.03702	0.09859	-0.12473
N	-1.75319	0.35929	-0.04116
C	-3.62794	-1.22355	-0.15392
C	-4.90975	-1.59011	-0.37144
C	-6.05696	-0.62355	-0.6524
C	-5.28466	-3.04878	-0.30037
C	-6.8296	-0.28113	0.62492
O	-6.99717	-1.19133	-1.5637
C	-6.56273	-1.17232	-2.91022
H	3.64087	-3.99344	0.9546
H	6.48549	-1.28815	-0.79724
H	5.55872	-2.22604	-1.9746
H	4.42179	-0.18724	0.0102
H	1.18646	-3.75191	-0.18992
H	0.87763	-2.14951	-0.86793
H	1.00292	-2.98318	2.04214
H	1.34669	-0.15909	0.94754
H	2.49954	-1.02399	1.95314
H	1.11011	-0.86113	3.90686
H	-0.32116	-0.4655	2.97488
H	2.09174	1.40572	3.00109
H	0.9977	2.6628	4.90026

H	1.49661	1.02912	5.38828
H	-0.20991	1.38345	5.04394
H	-0.51591	3.51867	0.30467
H	-0.2053	2.81999	-2.04869
H	0.51844	1.3019	-1.53451
H	4.64926	-0.2795	-3.03804
H	5.41135	0.87785	-1.95632
H	2.41774	0.61407	-2.50767
H	2.87284	1.5135	-0.22242
H	3.89783	2.77255	-0.91562
H	2.86023	4.87115	-1.32655
H	1.02482	5.00307	-1.48437
H	3.70311	1.42579	-4.47381
H	4.44621	2.6993	-3.49181
H	2.70975	2.73974	-3.81765
H	-0.80447	-1.28402	0.70392
H	-3.31788	3.26286	-0.0349
H	-2.89157	-1.99662	0.05087
H	-5.66291	0.30504	-1.08262
H	-4.4282	-3.66674	-0.01799
H	-6.08409	-3.20956	0.43394
H	-5.67799	-3.40695	-1.258
H	-7.65891	0.3896	0.37984
H	-6.17333	0.21277	1.34739
H	-7.24476	-1.18343	1.08514
H	-7.37077	-1.59846	-3.51061
H	-6.36455	-0.14509	-3.25464
H	-5.65111	-1.76936	-3.06574

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 49

C	-5.00604	0.36123	0.07376
C	-5.60298	0.09985	1.26533
C	-5.67844	-1.24926	1.81202
C	-5.10129	-2.32207	0.88988
C	-3.92768	-1.78408	0.07663
O	-4.29788	-0.55831	-0.62446
C	-5.08413	1.69769	-0.61245
C	-3.83304	2.60912	-0.47804
C	-2.70193	2.21673	-1.42906
C	-1.4783	3.14829	-1.39448
C	-0.77768	3.28921	-0.02226
C	-0.49796	1.91868	0.57205
C	0.50216	4.13514	-0.13556
O	0.38178	1.2221	-0.18599
O	-1.0291	1.47198	1.57056
C	0.60909	-0.17234	0.1923
C	0.76103	-0.9558	-1.1206
C	1.79104	-0.26499	1.10609
C	0.49019	-2.44054	-0.97051
C	-3.42629	-2.76642	-0.98145
C	-2.03552	-2.46197	-1.57803
C	-0.91515	-2.86438	-0.58393
C	1.45979	-3.33914	-1.17237
C	-1.85809	-3.17484	-2.92571
O	-6.21658	-1.52808	2.87537
O	-4.18858	3.95392	-0.80918
C	1.79396	-0.31288	2.46463
O	3.09013	-0.36149	2.88583
C	3.8388	-0.33363	1.7351
N	3.10396	-0.28393	0.65416
C	5.27397	-0.36609	1.92652
C	6.23744	-0.21323	0.99363

C	5.94118	-0.01151	-0.48155
C	7.68907	-0.27374	1.38717
C	5.83645	-1.36377	-1.20757
O	6.99634	0.79129	-1.02002
C	6.65474	1.47206	-2.20895
H	-6.12497	0.89035	1.793
H	-4.78749	-3.18145	1.48991
H	-5.90103	-2.66432	0.21651
H	-3.12306	-1.49623	0.76876
H	-5.9355	2.23775	-0.18359
H	-5.29975	1.54764	-1.67761
H	-3.47647	2.55511	0.56106
H	-3.10401	2.21367	-2.45086
H	-2.40978	1.18355	-1.2093
H	-1.78431	4.14947	-1.71536
H	-0.74454	2.78364	-2.12353
H	-1.46181	3.7736	0.68156
H	0.97929	4.27143	0.84124
H	0.2598	5.12652	-0.53385
H	1.22636	3.66218	-0.80579
H	-0.27773	-0.48834	0.74319
H	1.76561	-0.79041	-1.51865
H	0.05152	-0.51741	-1.83299
H	-4.17812	-2.78921	-1.78073
H	-3.41553	-3.77175	-0.53787
H	-1.98467	-1.37967	-1.75739
H	-1.15614	-2.44986	0.40579
H	-0.93641	-3.95576	-0.464
H	1.27869	-4.40737	-1.07867
H	2.47123	-3.03792	-1.43266
H	-2.60382	-2.83492	-3.65344
H	-1.97317	-4.26092	-2.81129
H	-0.86335	-2.99237	-3.34506

H	-4.78505	4.28538	-0.12021
H	1.0268	-0.30652	3.22222
H	5.56751	-0.52303	2.96125
H	4.98549	0.51659	-0.5901
H	7.80547	-0.47855	2.45536
H	8.21812	-1.0531	0.8234
H	8.18931	0.66959	1.14504
H	5.659	-1.21683	-2.27849
H	5.0012	-1.94199	-0.80197
H	6.76084	-1.9392	-1.08965
H	7.51158	2.09925	-2.47046
H	6.45457	0.78852	-3.0477
H	5.77149	2.11516	-2.06848

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 55

C	3.50777	-2.30004	-0.4896
C	4.63516	-2.78247	0.09886
C	5.94198	-2.17441	-0.12195
C	5.92179	-0.98946	-1.08842
C	4.5954	-0.2401	-0.99801
O	3.48003	-1.14952	-1.19605
C	2.17531	-2.99318	-0.42621
C	1.03069	-2.21868	0.27359
C	1.50836	-1.4465	1.5187
C	0.40232	-1.14403	2.54866
C	0.65796	0.13796	3.39887
C	-0.02897	1.32552	2.73429
C	0.18584	-0.00152	4.84948
O	0.34672	1.44186	1.43121
O	-0.84841	2.05103	3.25293
C	-0.47987	2.28195	0.58609
C	0.27223	2.44895	-0.74461

C	-1.81111	1.61579	0.38675
C	1.59347	3.19555	-0.62433
C	4.45379	0.8814	-2.02097
C	3.11479	1.64868	-2.02375
C	2.8689	2.38121	-0.6781
C	1.6109	4.52478	-0.4766
C	3.09104	2.6205	-3.21284
O	6.9828	-2.59402	0.36859
O	0.44333	-1.37317	-0.70406
C	-3.06568	2.10014	0.56168
O	-3.95569	1.11621	0.21259
C	-3.18673	0.053	-0.16275
N	-1.9045	0.30759	-0.06931
C	-3.75791	-1.20497	-0.59395
C	-5.04718	-1.55343	-0.7944
C	-6.2422	-0.628	-0.57796
C	-5.37877	-2.96174	-1.21803
C	-6.84432	-0.80867	0.81879
O	-7.28176	-0.90309	-1.51527
C	-7.0366	-0.37333	-2.80498
H	4.5923	-3.693	0.68609
H	6.76148	-0.32525	-0.86211
H	6.06822	-1.37258	-2.10908
H	4.48743	0.14988	0.02474
H	2.32392	-3.95006	0.0841
H	1.83379	-3.20861	-1.44616
H	0.29942	-2.98426	0.59117
H	1.9522	-0.51486	1.15573
H	2.31025	-2.00548	2.01902
H	0.30573	-1.99625	3.23281
H	-0.5699	-1.05147	2.04846
H	1.73832	0.34053	3.39307
H	0.34478	0.92382	5.41027

H	0.73388	-0.80948	5.34581
H	-0.88371	-0.23255	4.89311
H	-0.62111	3.2474	1.07893
H	-0.40123	2.98932	-1.42048
H	0.41896	1.45032	-1.16721
H	4.61144	0.44892	-3.0182
H	5.28134	1.58614	-1.85385
H	2.31976	0.90598	-2.16263
H	2.83519	1.63769	0.12891
H	3.72241	3.04163	-0.47095
H	2.54133	5.07747	-0.37467
H	0.69575	5.11344	-0.44767
H	3.24937	2.08703	-4.15747
H	3.88151	3.37739	-3.12001
H	2.13701	3.15226	-3.28115
H	-0.31505	-0.88076	-0.32689
H	-3.48248	3.02872	0.91649
H	-2.98231	-1.94693	-0.76677
H	-5.92833	0.4163	-0.69185
H	-4.47994	-3.58057	-1.28758
H	-6.06788	-3.43131	-0.50456
H	-5.89089	-2.9762	-2.18605
H	-7.71449	-0.15402	0.92686
H	-6.1093	-0.55352	1.58794
H	-7.17224	-1.8416	0.97323
H	-7.90637	-0.6195	-3.41956
H	-6.91801	0.72101	-2.7743
H	-6.1376	-0.80406	-3.27176

Compound 2d: Isomer 2S, 5R, 11R, 13R, 17S, 23S conformer 57

C	2.95366	-2.39186	-0.41162
C	3.96261	-3.13259	0.11496
C	5.36282	-2.80739	-0.12497
C	5.58181	-1.63042	-1.07832
C	4.45235	-0.60554	-0.98998
O	3.15782	-1.24953	-1.11371
C	1.48755	-2.68049	-0.25686
C	0.88306	-2.29331	1.13291
C	1.46807	-0.98744	1.68961
C	0.79069	-0.50581	2.98233
C	1.04774	0.99099	3.32443
C	0.15774	1.87948	2.46356
C	0.80984	1.28771	4.80843
O	0.5232	1.81113	1.15361
O	-0.77713	2.54343	2.85237
C	-0.33979	2.43449	0.17734
C	0.44026	2.42863	-1.15163
C	-1.64167	1.6913	0.06667
C	1.79712	3.11659	-1.07205
C	4.54175	0.46908	-2.07429
C	3.33503	1.41714	-2.24738
C	3.02676	2.23532	-0.96655
C	1.88228	4.4512	-1.09167
C	3.58655	2.33139	-3.45617
O	6.3018	-3.44301	0.33759
O	-0.53124	-2.22628	1.01225
C	-2.90033	2.19413	0.02141
O	-3.77279	1.15026	-0.14534
C	-2.99067	0.03222	-0.18967
N	-1.71304	0.30957	-0.06966
C	-3.55516	-1.29333	-0.32855
C	-4.82918	-1.66859	-0.57389

C	-5.99136	-0.70199	-0.73668
C	-5.16811	-3.1334	-0.66203
C	-6.65145	-0.40155	0.62088
O	-6.91562	-1.30458	-1.64545
C	-7.80183	-0.39372	-2.2617
H	3.73544	-4.02346	0.69084
H	6.5464	-1.1637	-0.85636
H	5.63968	-2.03206	-2.10073
H	4.46318	-0.14942	0.0109
H	1.28248	-3.74041	-0.43768
H	0.9517	-2.10426	-1.0181
H	1.07859	-3.11191	1.83675
H	1.37377	-0.22133	0.91663
H	2.54172	-1.12438	1.87
H	1.14922	-1.10783	3.82746
H	-0.28906	-0.68181	2.91975
H	2.08964	1.2272	3.06677
H	0.97221	2.34583	5.03534
H	1.49222	0.69244	5.42433
H	-0.21794	1.0438	5.09526
H	-0.53892	3.4621	0.49602
H	-0.19524	2.92679	-1.89316
H	0.54564	1.38776	-1.47524
H	4.71328	-0.03589	-3.03453
H	5.44735	1.05893	-1.87144
H	2.46364	0.78886	-2.46994
H	2.8853	1.54396	-0.12658
H	3.89858	2.85946	-0.727
H	2.83686	4.9653	-1.01331
H	1.00132	5.08401	-1.18148
H	3.76318	1.7431	-4.36429
H	4.4687	2.96473	-3.29269
H	2.7364	2.99457	-3.6417

H	-0.75234	-1.36579	0.59495
H	-3.33127	3.17859	0.10647
H	-2.8019	-2.06648	-0.20275
H	-5.63131	0.23941	-1.17038
H	-4.2925	-3.75679	-0.46254
H	-5.95556	-3.39851	0.05501
H	-5.56502	-3.37408	-1.65364
H	-7.51003	0.26696	0.49641
H	-5.93923	0.0855	1.29324
H	-7.00312	-1.32626	1.08976
H	-8.39041	-0.96698	-2.98296
H	-8.4907	0.07914	-1.54628
H	-7.25812	0.40114	-2.79717

*DP4+ statistical comparation between the experimental and calculated values of diastereisomers **2a**, **2b**, **2c**, and **2d***

Position	sp^2 carbon?	δ experimental (CD_3CN)	δ calc. **2a**	δ calc. **2b**	δ calc. **2c**	δ calc. **2d**
C7	x	175.5	23.1	24.0	23.2	23.2
C8	x	106.8	90.9	92.1	91.3	90.9
C9	x	193.6	10.1	10.0	10.1	10.1
C10		42.2	154.1	154.3	154.6	154.2
C11		77.8	118.3	119.0	118.5	118.4
C6		44.6	152.9	150.5	150.3	153.1
C5		69.5	125.5	128.1	126.6	125.0
C4		34.5	161.0	162.5	160.3	160.6
C3		30.8	162.7	164.0	163.2	162.4
C2		39.9	152.9	157.5	157.3	152.2
C1	x	175.6	24.0	22.9	23.0	23.9
C26		17.6	176.9	177.8	177.4	176.8
C17		66.7	128.1	124.5	125.7	128.6
C16		42.2	158.6	156.5	156.1	158.7
C18	x	141.7	58.3	57.8	57.9	58.3
C15	x	143.9	54.4	51.0	51.7	54.9
C12		42.9	153.4	155.1	154.8	153.4
C13		25.8	166.1	166.0	165.3	165.9
C14		40.2	154.0	151.3	150.2	154.5
C28	x	113.9	79.3	82.4	84.5	78.7
C27		21.2	175.1	175.8	175.7	175.2
C19	x	135.9	59.5	60.1	60.8	59.5
C20	x	161.2	39.3	39.3	38.5	39.5
C21	x	113.6	84.6	85.0	84.5	85.4
C22	x	152.7	41.2	40.7	41.1	41.2
C23		75.5	120.0	119.9	120.4	120.1
C25		17.7	174.7	174.6	174.8	174.6
C24		19.5	175.2	175.5	175.1	176.2
C29		56.6	139.8	139.8	140.0	140.1
H8	x	5.30	26.3	26.2	26.2	26.3
H10h		2.23	29.7	29.4	29.5	29.8
H10l		2.41	29.2	29.3	29.3	29.2
H11		4.48	26.9	26.7	26.8	26.9
H6h		2.27	29.3	29.4	29.4	29.3
H6l		2.49	28.8	28.9	29.0	28.8
H5		3.74	27.8	27.0	27.4	27.9
H4h		1.31	30.4	30.3	30.2	30.5
H4l		1.43	30.1	30.1	29.6	30.1
H3h		1.63	30.1	30.2	30.2	30.2
H3l		1.69	29.7	30.0	30.1	29.5
H2		2.49	29.2	28.9	29.0	29.3
H26		1.10	30.6	30.6	30.6	30.6
H17		5.92	25.7	25.8	25.8	25.7
H16l		2.72	28.3	28.6	28.7	28.1
H16h		2.62	29.1	28.9	29.1	29.1
H12l		1.81	29.7	29.7	29.7	29.7
H12h		1.46	30.3	30.2	30.3	30.3
H13		2.2	29.7	29.2	29.4	29.7
H14l		2.49	29.0	29.3	29.4	29.0
H14h		1.59	30.0	29.5	29.6	30.1
H28h	x	4.86	26.5	26.3	26.2	26.5
H28l	x	4.91	26.4	26.3	26.2	26.4
H27		0.95	30.7	30.6	30.6	30.7
H19	x	7.63	23.8	23.8	23.7	23.8
H21	x	6.20	25.3	25.3	25.2	25.3
H23		5.20	26.3	26.3	26.5	26.2
H25		1.86	29.6	29.6	29.7	29.6
H24		1.23	30.3	30.4	30.4	30.3
H29		3.15	28.3	28.4	28.4	28.3

	2a	*2b*	*2c*	*2d*
	Isomer 1	Isomer 2	Isomer 3	Isomer 4
sDP4+ (H data)	99.66%	0.01%	0.00%	0.32%
sDP4+ (C data)	69.96%	0.12%	26.64%	3.28%
sDP4+ (all data)	99.98%	0.00%	0.00%	0.02%
uDP4+ (H data)	98.67%	0.13%	0.25%	0.95%
uDP4+ (C data)	74.63%	0.01%	23.10%	2.26%
uDP4+ (all data)	99.89%	0.00%	0.08%	0.03%
DP4+ (H data)	100.00%	0.00%	0.00%	0.00%
DP4+ (C data)	89.34%	0.00%	10.53%	0.13%
DP4+ (all data)	100.00%	0.00%	0.00%	0.00%

DP4+ statistical correlations of diasteroisomers **2a**, **2b**, **2c**, and **2d**

*J-DP4+ statistical comparation between the experimental and calculated values of diastereisomers **2a**, **2b**, **2c**, and **2d***

Position	δ experimental $(CD_3)_2CO$	δ calc. **2a**	δ calc. **2b**	δ calc. **2c**	δ calc. **2d**
C7	174.8	24.2	25.2	25.9	24.3
C8	106.8	82.8	81.8	83.3	82.7
C9	192.4	5.5	5.2	6.1	5.5
C10	42.3	149.0	149.1	150.5	149.0
C11	77.4	116.6	116.2	117.7	116.4
C6	44.9	145.0	143.4	143.8	145.3
C5	69.6	121.6	125.6	124.8	121.5
C4	34.5	154.5	156.0	157.0	153.6
C3	30.8	158.2	159.2	158.9	157.9
C2	39.7	152.8	154.8	154.6	152.3
C1	174.9	20.2	19.6	19.4	20.3
C26	17.6	171.1	171.1	171.1	171.3
C17	66.3	119.4	119.4	120.4	120.3
C16	42.3	151.7	147.6	148.9	152.8
C18	142.0	52.7	52.8	53.1	52.8
C15	143.8	46.2	43.9	45.1	46.9
C12	43.1	145.8	147.4	149.2	145.2
C13	25.6	161.0	153.8	157.5	161.5
C14	40.0	147.6	146.3	146.5	147.4
C28	113.5	79.4	80.3	80.5	78.8
C27	21.2	170.0	174.3	172.5	169.9
C19	135.6	60.2	58.5	59.2	59.3
C20	161.0	32.6	33.2	32.7	33.0
C21	113.5	83.2	84.1	83.3	84.2
C22	152.4	41.9	39.6	42.0	40.0
C23	75.3	118.5	114.7	118.7	115.2
C25	17.5	170.1	169.4	170.0	169.6
C24	19.4	170.6	172.0	170.2	172.0
C29	56.5	135.9	136.0	135.6	136.0
H8	5.28	26.00	25.93	26.00	26.02
H10h	2.26	29.82	29.82	29.57	29.80
H10l	2.41	29.45	29.45	29.41	29.45
H11	4.53	27.38	27.20	27.04	27.39
H6h	2.31	29.48	29.38	29.51	29.50
H6l	2.59	29.14	28.85	29.01	29.17
H5	3.83	27.47	26.75	26.97	27.55
H4h	1.38	30.25	30.37	30.36	30.36
H4l	1.51	29.79	29.84	29.98	29.89
H3h	1.68	30.22	30.53	30.52	30.11
H3l	1.79	29.92	29.66	29.70	29.99
H2	2.53	29.05	28.91	28.91	29.09
H26	1.11	30.67	30.69	30.69	30.65
H17	6.00	26.11	26.11	26.04	26.06
H16l	2.75	28.55	28.46	28.52	28.50
H16h	2.67	29.44	29.32	29.31	29.35
H12l	1.85	29.80	29.84	29.71	29.83
H12h	1.54	30.48	30.17	30.46	30.48
H13	2.29	29.36	29.74	29.53	29.31
H14l	2.27	28.85	28.62	29.22	28.89
H14h	1.61	30.00	29.34	29.37	30.10
H28h	4.88	26.58	26.49	26.49	26.63
H28l	4.94	26.49	26.48	26.46	26.49
H27	0.98	30.88	30.62	30.70	30.88
H19	7.77	24.15	24.05	24.09	24.11
H21	6.21	25.63	25.61	25.63	25.61
H23	5.29	25.65	26.36	25.62	26.28
H25	1.88	29.81	29.81	29.81	29.80
H24	1.24	30.54	30.41	30.53	30.36
H29	3.17	28.25	28.55	28.33	28.56

Type	Experimental $(CD_3)_2CO$	Calc. **2a**	Calc. **2b**	Calc. **2c**	Calc. **2d**
$^3JH2\text{-}H3_l$	3.4	2.7	2.7	2.8	2.7
$^3JH2\text{-}H3_h$	10.6	12.1	12.4	12.3	12.1
$^3JH5\text{-}H4_l$	2.2	1.8	1.5	1.8	1.7
$^3JH5\text{-}H4_h$	10.4	10.0	10.4	10.6	10.0
$^3JH11\text{-}H12_h$	2.7	2.3	1.7	1.9	2.4
$^3JH11\text{-}H12_l$	11.0	9.7	9.8	10.4	9.7

		2a	*2b*	*2c*	*2d*
Isomer №		**1**	**2**	**3**	**4**
DP4 (%)	H	0.00	0.00	0.00	100.00
	C	80.72	0.00	0.00	19.27
	H+C	*0.00*	*0.00*	*0.00*	*100.00*
	J	36.17	8.56	19.57	35.70
	all data	**0.00**	**0.00**	**0.00**	**100.00**

J-DP4+ statistical correlations of diasteroisomers **2a**, **2b**, **2c**, and **2d**