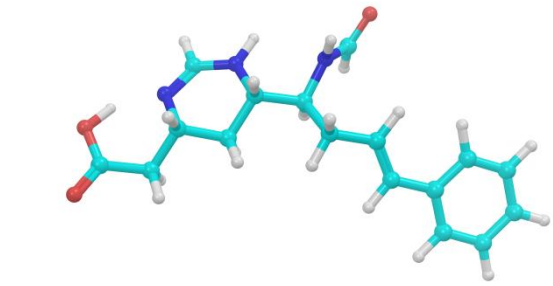
Nuevos compuestos citotóxicos de esponjas de Indonesia con naturaleza estructural diversa. Uso de técnicas avanzadas en la determinación de su estereoquímica relativa y absoluta.

CONTENIDO

- Resultados obtenidos mediante cálculos computacionales DFT para **6**.
- Resultados obtenidos mediante cálculos computacionales DFT para **10-12**.

Ácido lanesoico (6)



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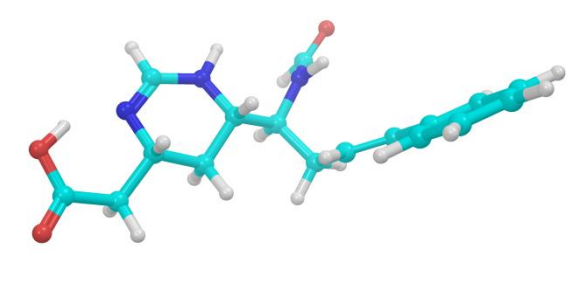

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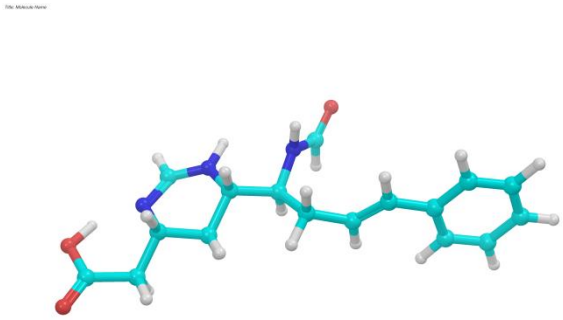

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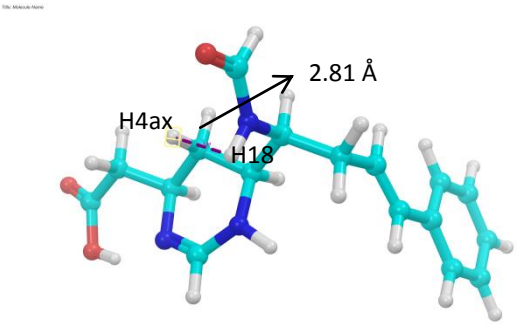

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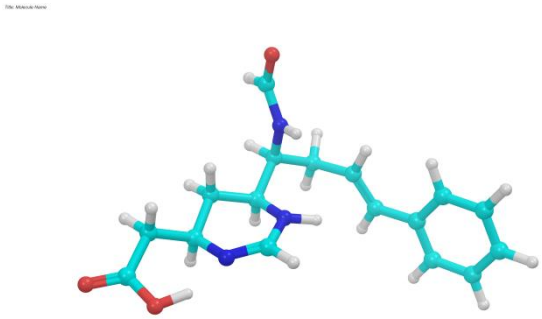

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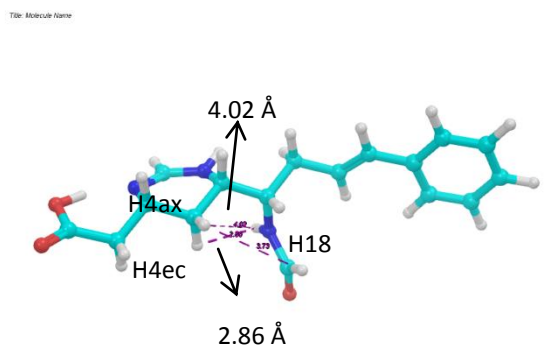

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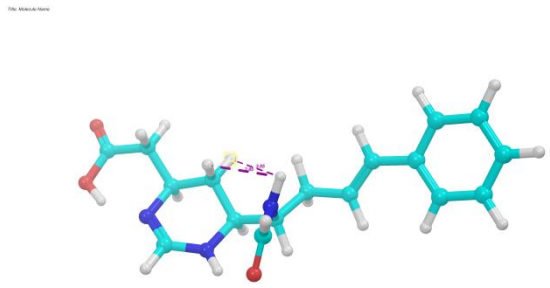
Principales confórmeros encontrados en el estudio DFT del modelo *sin-cis*, contabilizando el 82.9% de la población conformacional.



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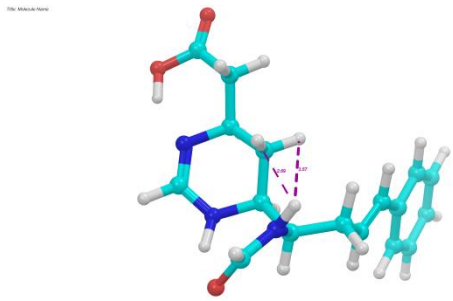

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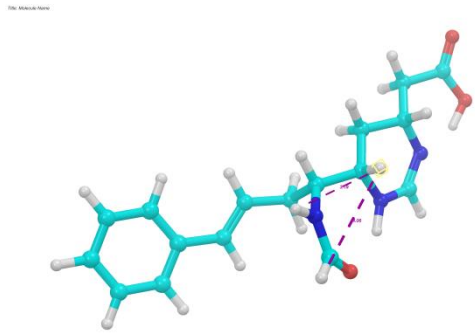

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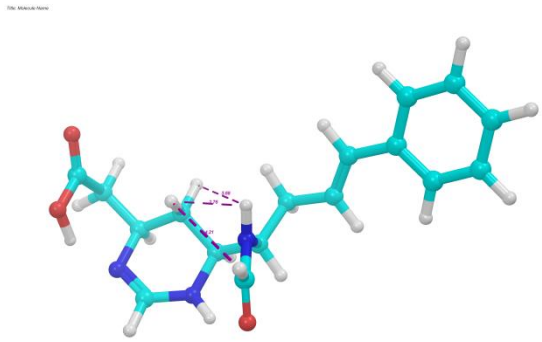

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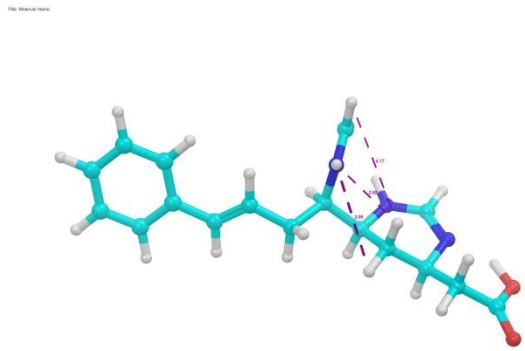

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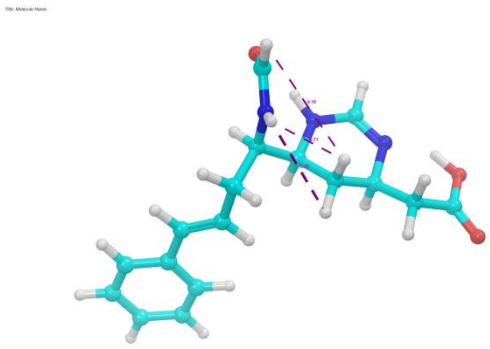
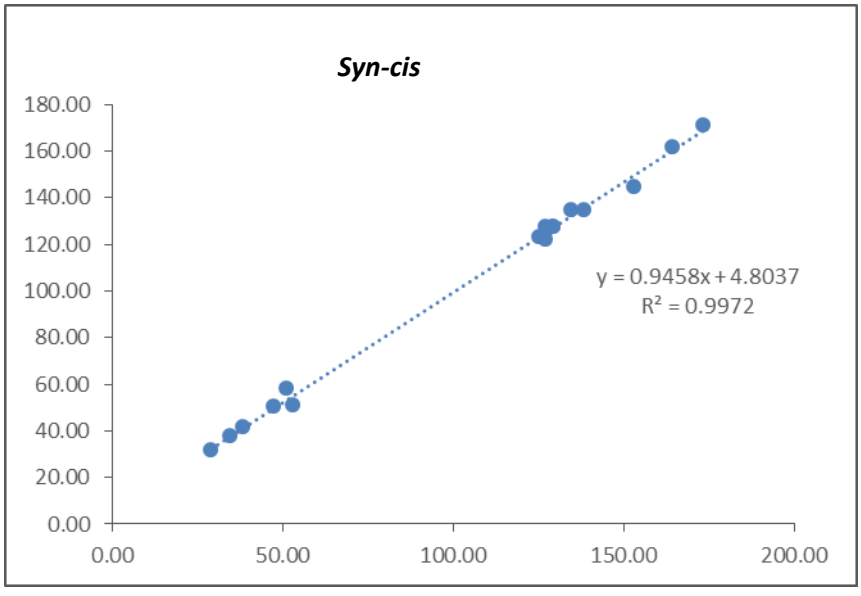


1b17

Principales confórmeros encontrados en el estudio DFT del modelo *anti-cis*, contabilizando el 100% de la población conformacional.

Comparación entre los desplazamientos químicos de ^{13}C calculados (MP1WMP91/6-311+G(2d,p)) y experimentales en methanol-d_4 para los diasteroisómeros *sin-cis*.

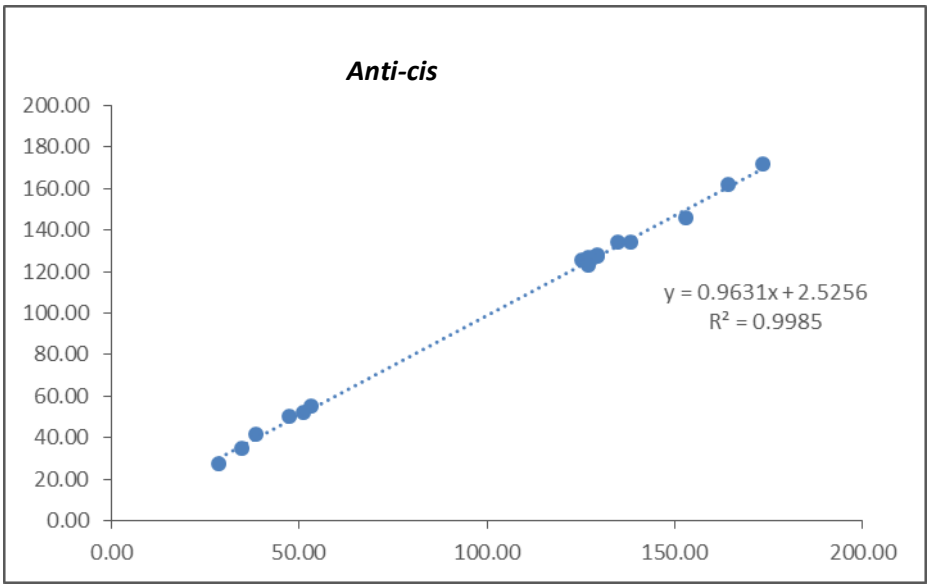
Número en la molécula	$\delta_{C\ exp}$ CD_3OD	$\delta_{C\ calc}$	$\Delta\delta_{C\ calc}$	$\delta_{C\ escal}$	$\Delta\delta_{C\ escal}$
1	173.49	171.07	2.01	2.42	175.43
2	38.60	41.61	2.97	3.01	40.54
3	47.64	50.17	2.55	2.53	49.49
4	28.91	31.60	1.85	2.69	25.48
5	53.30	50.89	1.93	2.41	54.72
6	51.26	58.17	0.84	6.91	51.48
7	34.80	37.58	0.01	2.78	33.52
8	125.52	122.99	0.36	2.53	127.34
9	134.88	134.67	1.26	0.21	136.12
10	138.43	134.88	4.37	3.55	136.58
11	127.23	121.98	4.19	5.25	125.13
12	129.57	127.31	2.32	2.26	129.51
13	128.52	126.76	2.01	1.76	128.74
14	129.57	127.64	2.14	1.93	129.69
15	127.23	127.75	0.57	0.52	128.89
16	153.01	144.35	7.30	8.66	148.67
17	164.39	161.86	2.99	2.53	164.96
		MAD	3.06	MAD	2.74



Regresión lineal de los δ_C calculados vs los experimentales en methanol-d_4 para los diasteroisómeros *sin-cis*.

Comparación entre los desplazamientos químicos de ^{13}C calculados (MP1WMP91/6-311+G(2d,p)) y experimentales en methanol-d_4 para los diasteroisómeros *anti-cis*.

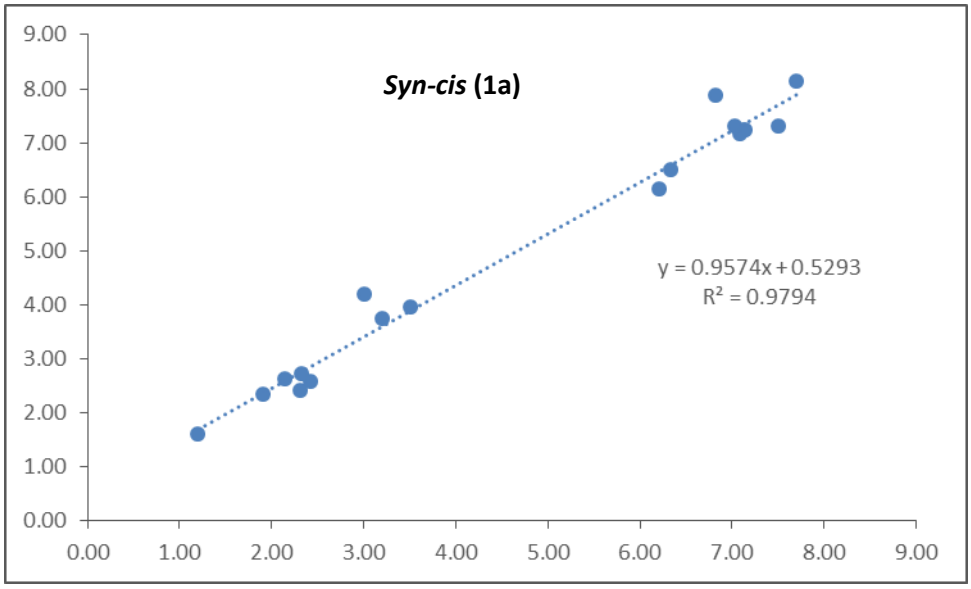
Número en la molécula	$\delta_{C\ exp}$ CD_3OD	$\delta_{C\ calc}$	$\Delta\delta_{C\ calc}$	$\delta_{C\ escal}$	$\Delta\delta_{C\ escal}$
1	173.49	171.48	171.07	2.01	2.42
2	38.60	41.57	41.61	2.97	3.01
3	47.64	50.19	50.17	2.55	2.53
4	28.91	27.06	31.60	1.85	2.69
5	53.30	55.23	50.89	1.93	2.41
6	51.26	52.10	58.17	0.84	6.91
7	34.80	34.81	37.58	0.01	2.78
8	125.52	125.16	122.99	0.36	2.53
9	134.88	133.62	134.67	1.26	0.21
10	138.43	134.06	134.88	4.37	3.55
11	127.23	123.04	121.98	4.19	5.25
12	129.57	127.25	127.31	2.32	2.26
13	128.52	126.51	126.76	2.01	1.76
14	129.57	127.43	127.64	2.14	1.93
15	127.23	126.66	127.75	0.57	0.52
16	153.01	145.71	144.35	7.30	8.66
17	164.39	161.40	161.86	2.99	2.53
		MAD	2.33	MAD	1.53



Regresión lineal de los δ_C calculados vs los experimentales en methanol-d_4 para los diasteroisómeros *anti-cis*.

Comparación entre los desplazamientos químicos de ^{1}H calculados (MP1WMP91/6-311+G(2d,p)) y experimentales en methanol-d_4 para los diasteroisómeros *sin-cis*.

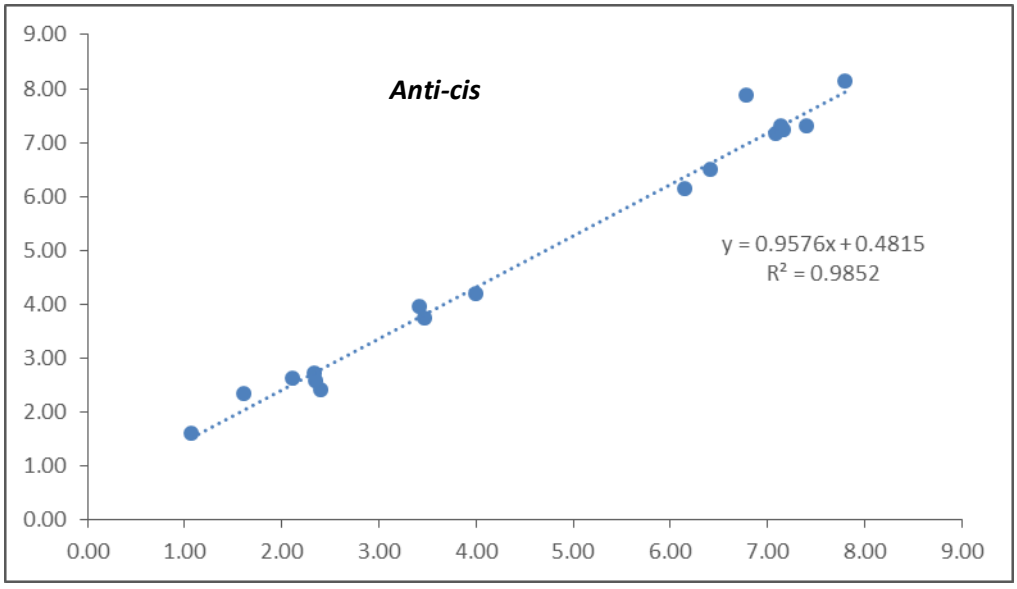
Número en la molécula	$\delta_{H\ exp}$ CD_3OD	$\delta_{H\ calc}$	$\Delta\delta_{H\ calc}$	$\delta_{H\ escal}$	$\Delta\delta_{H\ escal}$
H2h	2.62	2.15	0.47	1.62	1.00
H2l	2.71	2.33	0.38	1.81	0.90
H3	3.94	3.51	0.43	3.05	0.89
H4ax	1.60	1.21	0.39	0.63	0.97
H4ec	2.33	1.91	0.42	1.37	0.96
H5	3.73	3.21	0.52	2.73	1.00
H6	4.19	3.02	1.17	2.53	1.66
H7h	2.40	2.31	0.09	1.79	0.61
H7l	2.56	2.42	0.14	1.90	0.66
H8	6.14	6.21	0.07	5.87	0.27
H9	6.49	6.34	0.15	6.01	0.48
H11	7.31	7.50	0.19	7.23	0.08
H12	7.23	7.13	0.10	6.84	0.39
H13	7.15	7.09	0.06	6.80	0.35
H14	7.23	7.15	0.08	6.85	0.38
H15	7.31	7.04	0.27	6.74	0.57
H16	7.88	6.82	1.06	6.51	1.37
H17	8.13	7.70	0.43	7.43	0.70
		MAD	0.357	MAD	0.737



Regresión lineal de los δ_H calculados vs los experimentales en methanol-d_4 para los diasteroisómeros *sin-cis*.

Comparación entre los desplazamientos químicos de ^{1}H calculados (MP1WMP91/6-311+G(2d,p)) y experimentales en methanol-d_4 para los diasteroisómeros anti-*cis*.

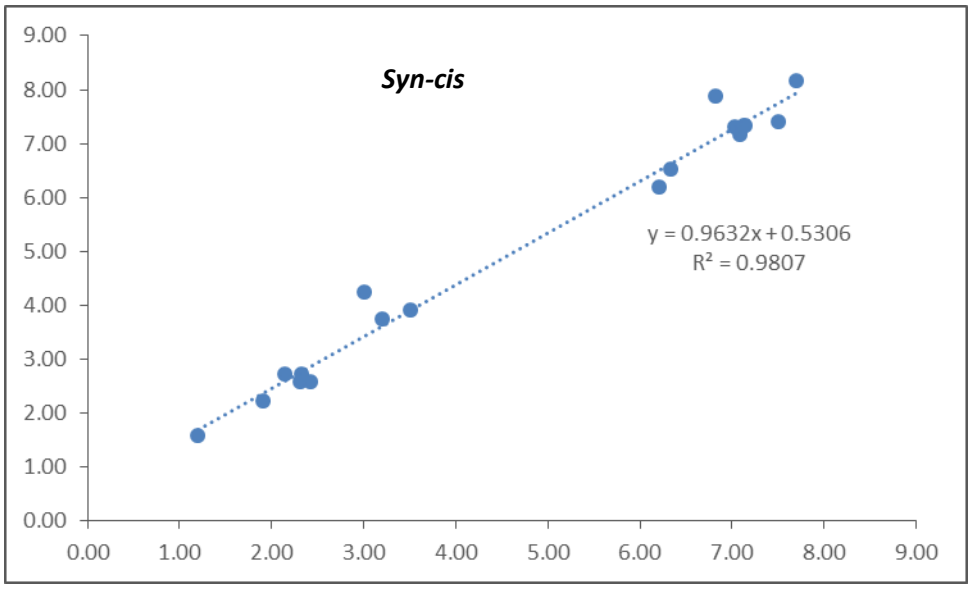
Número en la molécula	$\delta_{H\ exp}$ CD_3OD	$\delta_{H\ calc}$	$\Delta\delta_{H\ calc}$	$\delta_{H\ escal}$	$\Delta\delta_{H\ escal}$
H2h	2.62	2.12	0.50	1.63	0.99
H2l	2.71	2.34	0.37	1.87	0.84
H3	3.94	3.42	0.52	3.02	0.92
H4ax	1.60	1.08	0.52	0.52	1.08
H4ec	2.33	1.61	0.72	1.08	1.25
H5	3.73	3.47	0.26	3.07	0.66
H6	4.19	4.00	0.19	3.64	0.55
H7h	2.40	2.41	0.01	1.94	0.46
H7l	2.56	2.35	0.21	1.88	0.68
H8	6.14	6.15	0.01	5.94	0.20
H9	6.49	6.42	0.07	6.22	0.27
H11	7.31	7.41	0.10	7.28	0.03
H12	7.23	7.17	0.06	7.02	0.21
H13	7.15	7.10	0.05	6.95	0.20
H14	7.23	7.15	0.08	7.01	0.22
H15	7.31	7.14	0.17	6.99	0.32
H16	7.88	6.79	1.09	6.62	1.26
H17	8.13	7.80	0.33	7.70	0.43
		MAD	0.292	MAD	0.588



Regresión lineal de los δ_H calculados vs los experimentales en methanol-d_4 para los diasteroisómeros *anti-cis*.

Comparación entre los desplazamientos químicos de ^{1}H calculados (MP1WMP91/6-311+G(2d,p)) y experimentales en acetonitrilo-d_3 para los diasteroisómeros *sin-cis*.

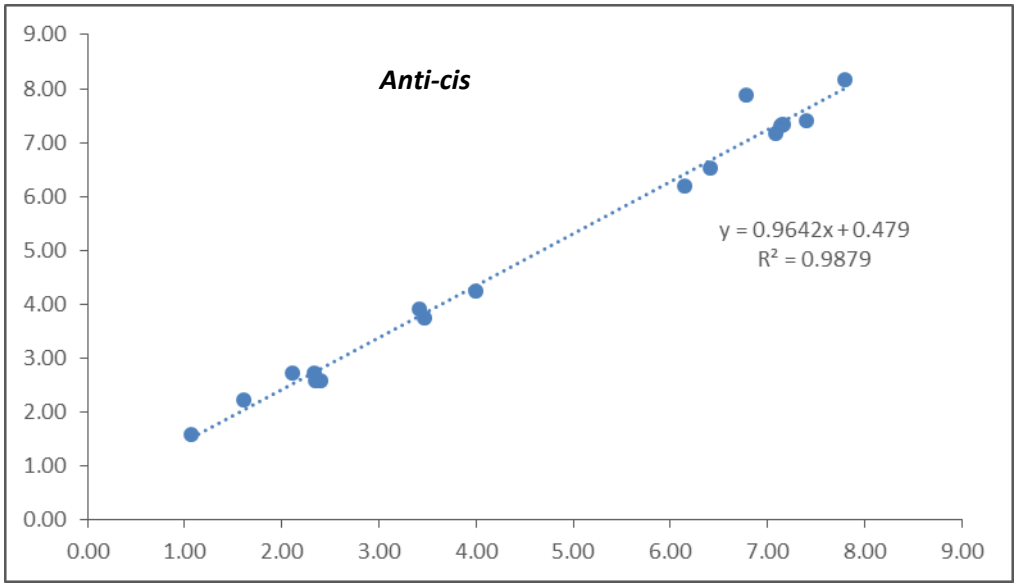
Número en la molécula	$\delta_{H\ exp}$ CD_3CN	$\delta_{H\ calc}$	$\Delta\delta_{H\ calc}$	$\delta_{H\ escal}$	$\Delta\delta_{H\ escal}$
H2h	2.72	2.15	0.57	1.68	1.04
H2l	2.71	2.33	0.38	1.87	0.84
H3	3.91	3.51	0.40	3.10	0.81
H4ax	1.57	1.21	0.36	0.70	0.87
H4ec	2.22	1.91	0.31	1.44	0.78
H5	3.74	3.21	0.53	2.78	0.96
H6	4.24	3.02	1.22	2.58	1.66
H7h	2.56	2.31	0.25	1.85	0.71
H7l	2.56	2.42	0.14	1.96	0.60
H8	6.19	6.21	0.02	5.90	0.29
H9	6.52	6.34	0.18	6.03	0.49
H11	7.39	7.50	0.11	7.24	0.15
H12	7.32	7.13	0.19	6.85	0.47
H13	7.15	7.09	0.06	6.81	0.34
H14	7.32	7.15	0.17	6.87	0.45
H15	7.31	7.04	0.27	6.76	0.55
H16	7.88	6.82	1.06	6.53	1.35
H17	8.16	7.70	0.46	7.44	0.72
		MAD	0.372	MAD	0.727



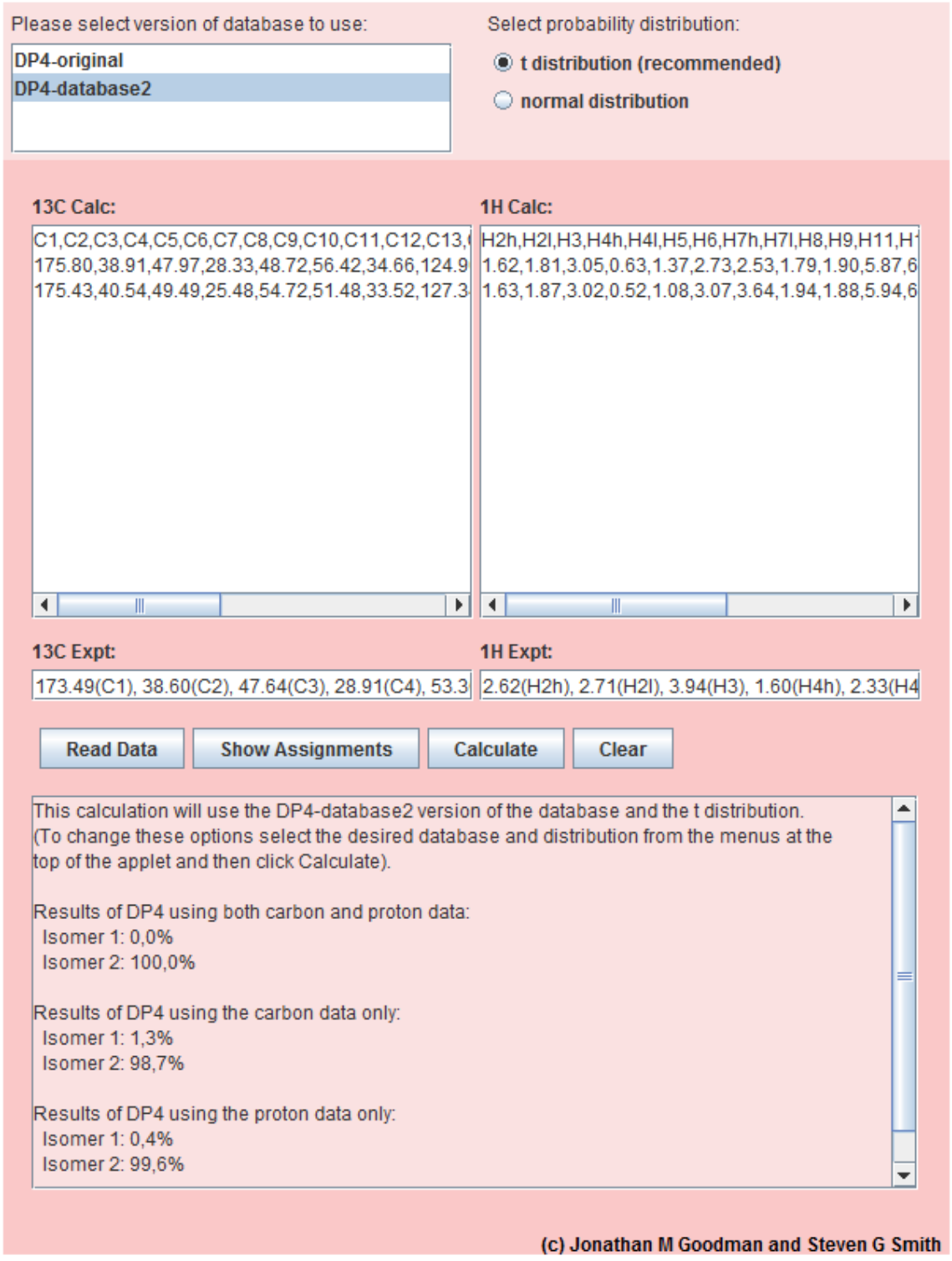
Regresión lineal de los δ_H calculados vs los experimentales en acetonitrilo-d_3 para los diasteroisómeros *sin-cis*.

Comparación entre los desplazamientos químicos de ^{1}H calculados (MP1WMP91/6-311+G(2d,p)) y experimentales en acetonitrilo-d_3 para los diasteroisómeros anti-*cis*.

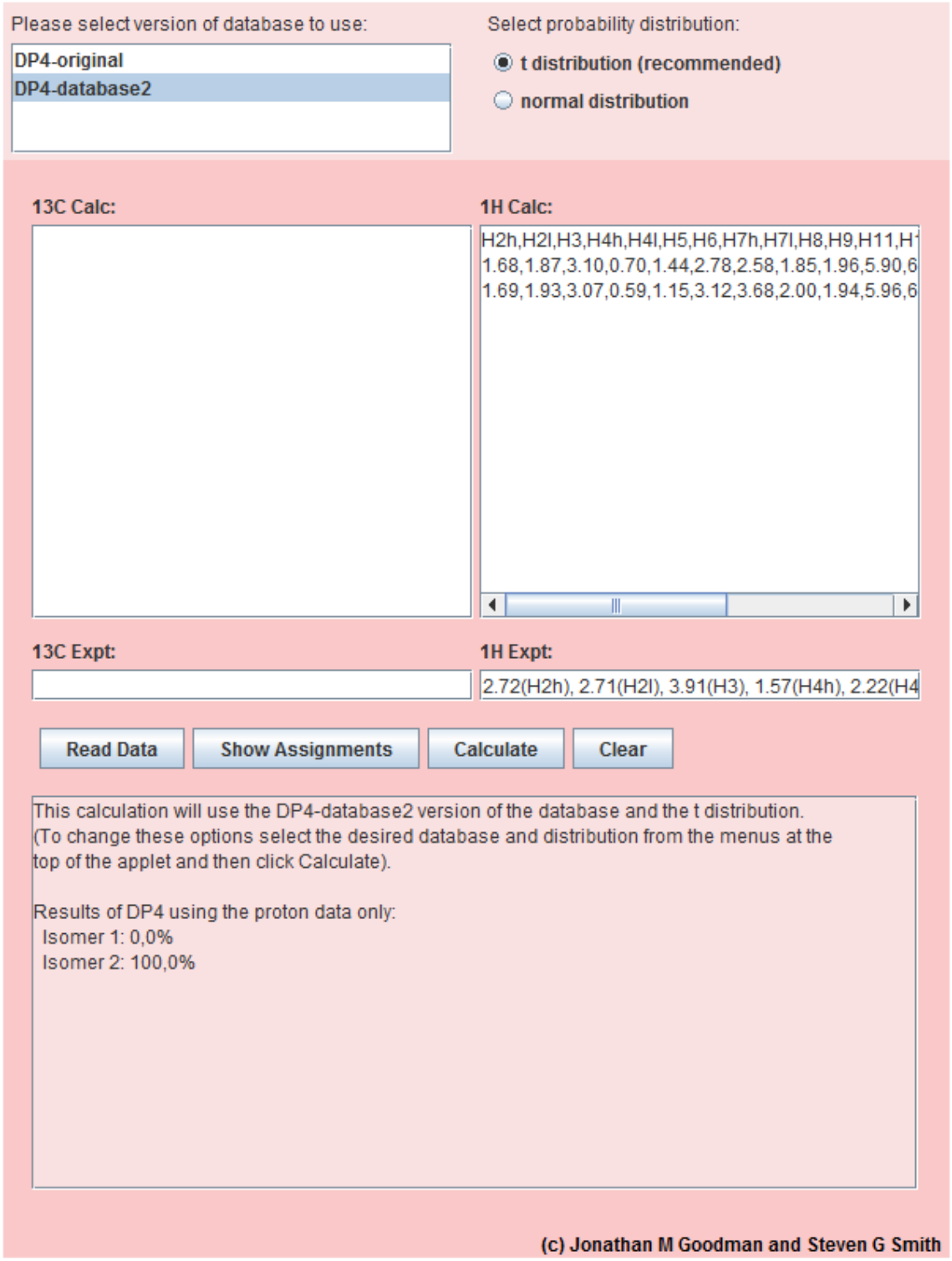
Número en la molécula	$\delta_{H\ exp}$ CD_3CN	$\delta_{H\ calc}$	$\Delta\delta_{H\ calc}$	$\delta_{H\ escal}$	$\Delta\delta_{H\ escal}$
H2h	2.72	2.12	0.60	1.69	1.03
H2l	2.71	2.34	0.37	1.93	0.78
H3	3.91	3.42	0.49	3.07	0.84
H4ax	1.57	1.08	0.49	0.59	0.98
H4ec	2.22	1.61	0.61	1.15	1.07
H5	3.74	3.47	0.27	3.12	0.62
H6	4.24	4.00	0.24	3.68	0.56
H7h	2.56	2.41	0.15	2.00	0.56
H7l	2.56	2.35	0.21	1.94	0.62
H8	6.19	6.15	0.04	5.96	0.23
H9	6.52	6.42	0.10	6.25	0.27
H11	7.39	7.41	0.02	7.29	0.10
H12	7.32	7.17	0.15	7.04	0.28
H13	7.15	7.10	0.05	6.96	0.19
H14	7.32	7.15	0.17	7.02	0.30
H15	7.31	7.14	0.17	7.01	0.30
H16	7.88	6.79	1.09	6.64	1.24
H17	8.16	7.80	0.36	7.71	0.45
		MAD	0.310	MAD	0.578



Regresión lineal de los δ_H calculados vs los experimentales en acetonitrilo-d_3 para los diasteroisómeros *anti-cis*.



Correlaciones DP4 de los diasteroisómeros de **6**. Desplazamientos químicos experimentales de $^{13}C/^{1}H$ en metanol-d_4 de **6**. Isómero 1: *sin-cis*, isómero 2: *anti-cis*.



Correlaciones DP4 de los diasteroisómeros de **6**. Desplazamientos químicos experimentales de ^{1}H en acetonitrilo-d_3 de **6**. Isómero 1: *sin-cis*, isómero 2: *anti-cis*.

DP4+

AJUSTE PROTON (en CD_3CN)

Functional	Solvent?	Basis Set	Type o
mPW1PW91	PCM	6-311G(d,p)	Unscale

	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5
sDP4+ (H data)	2.24%	97.76%	-	-	-
sDP4+ (C data)	-	-	-	-	-
sDP4+ (all data)	2.24%	97.76%	-	-	-
uDP4+ (H data)	4.58%	95.42%	-	-	-
uDP4+ (C data)	-	-	-	-	-
uDP4+ (all data)	4.58%	95.42%	-	-	-
DP4+ (H data)	0.11%	99.89%	-	-	-
DP4+ (C data)	-	-	-	-	-
DP4+ (all data)	0.11%	99.89%	-	-	-

AJSTE CARBONO (en CD_3CN)

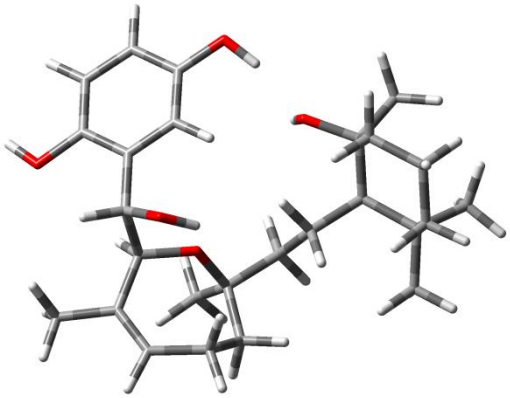
Functional	Solvent?	Basis Set
mPW1PW91	PCM	6-311G(d,p)

		DP4+	2.24%	97.76%	-
Nuclei	sp2?	Experimental	Isomer 1	Isomer 2	Isomer 3
C	x	173.49	171.07	171.48	
C		38.60	41.61	41.57	
C		47.64	50.17	50.19	
C		28.91	31.60	27.06	
C		53.30	50.89	55.23	
C		51.26	58.17	52.10	
C		34.80	37.58	34.81	
C	x	125.52	122.99	125.16	
C	x	134.88	134.67	133.62	
C	x	138.43	134.88	134.06	
C	x	127.23	121.98	123.04	
C	x	129.57	127.31	127.25	
C	x	128.52	126.76	126.51	
C	x	129.57	127.64	127.43	
C	x	127.23	127.75	126.66	
C	x	153.01	144.35	145.71	
C	x	164.39	161.86	161.40	

Halioxepinas

Energías DFT calculadas para diasteroisómero 7*S**10*S** deducido por búsqueda DFT search of **11**.

Confórmeros 7*S**10*S**	B3LYP/6-31G(d) DFT Energía (hartree)	Δ (DFT Energía) (kcal/mol)	% Población
12	-1390.376822	-872474.5128	33.00
6	-1390.37637	-872474.2292	20.43
10	-1390.376202	-872474.1238	17.10
8	-1390.375972	-872473.9795	13.40
5	-1390.375006	-872473.3733	4.81
11	-1390.374867	-872473.2861	4.15
2	-1390.374853	-872473.2773	4.09
7	-1390.373687	-872472.5456	1.19
9	-1390.373248	-872472.2701	0.75
1	-1390.372932	-872472.0718	0.53
4	-1390.372886	-872472.043	0.51
3	-1390.370384	-872470.4729	0.04



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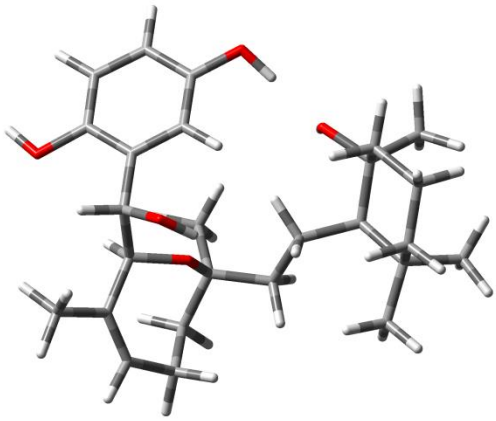

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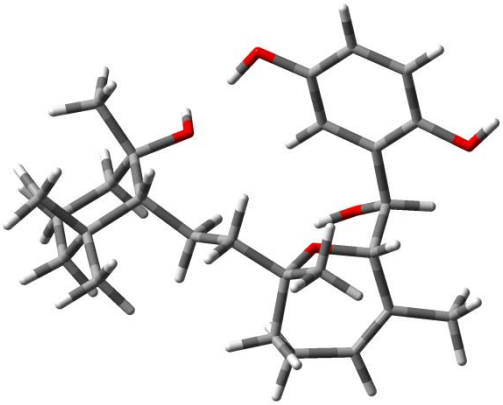

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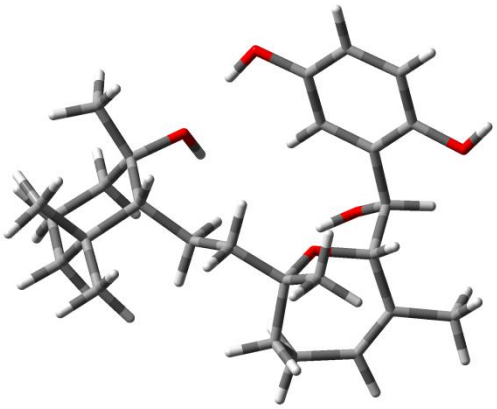

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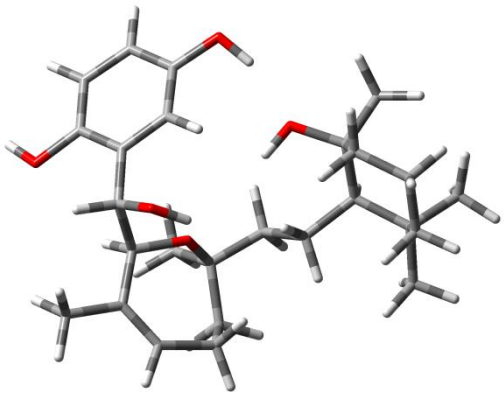

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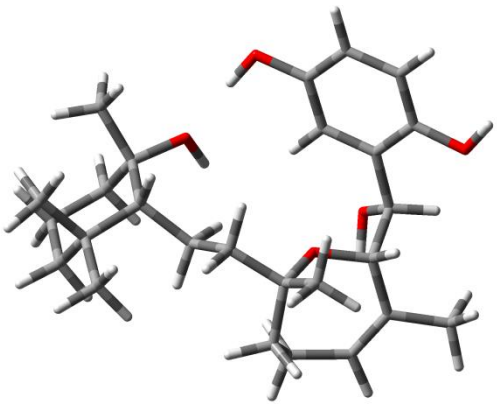

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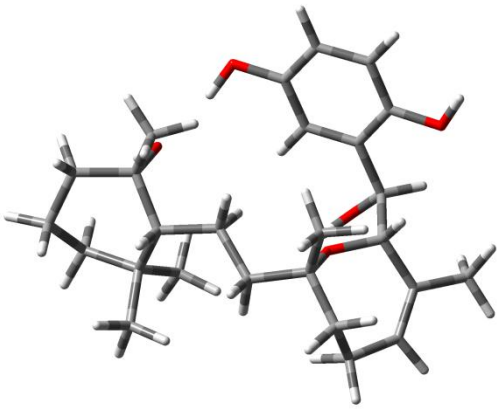

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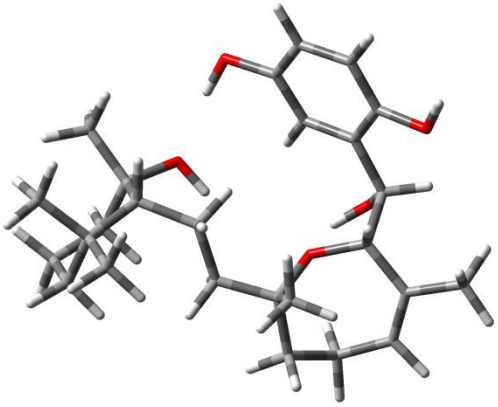

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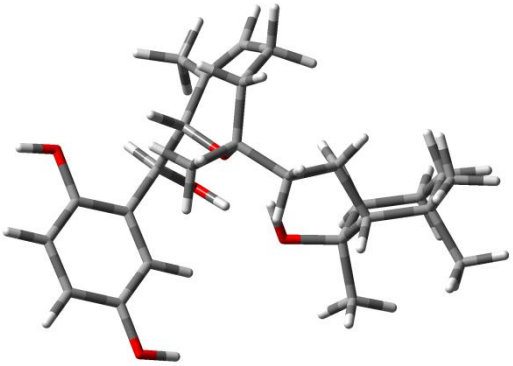

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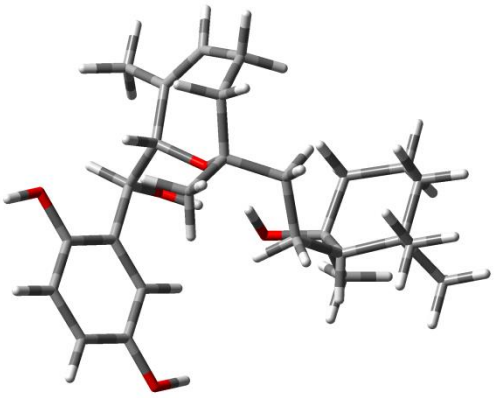

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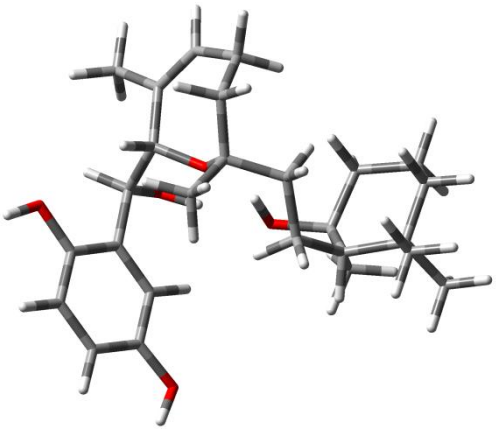

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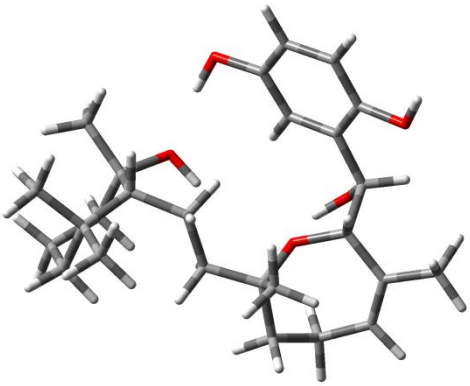

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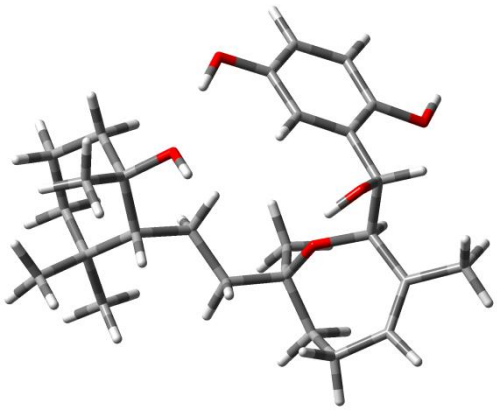
Energías DFT calculadas para diasteroisómero 7*R**10*S** deducido por búsqueda DFT search of **11**.

Confórmeros 7*R**10*S**	B3LYP/6-31G(d) DFT Energía (hartree)	Δ (DFT Energía) (kcal/mol)	% Población
1	-1390.378243	-872475.4045	63.52
6	-1390.377381	-872474.8636	25.47
2	-1390.375837	-872473.8947	4.95
3	-1390.37577	-872473.8527	4.61
7	-1390.373695	-872472.5506	0.51
5	-1390.373476	-872472.4132	0.41
8	-1390.37344	-872472.3906	0.39
4	-1390.372403	-872471.7399	0.13
9	-1390.368789	-872469.4721	0.003



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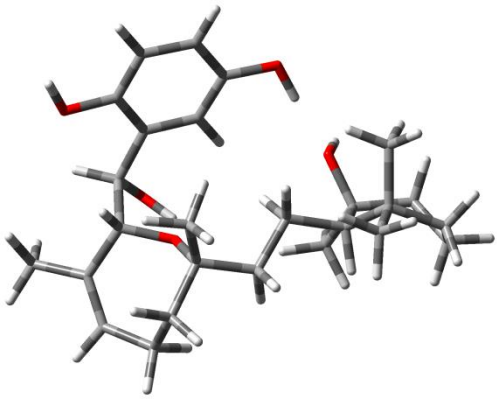

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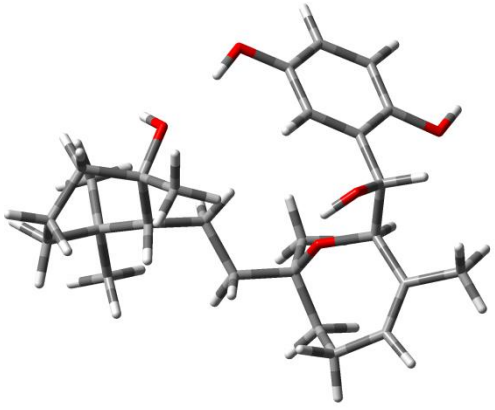

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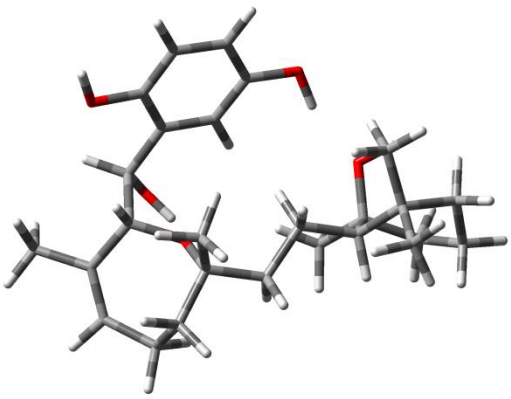

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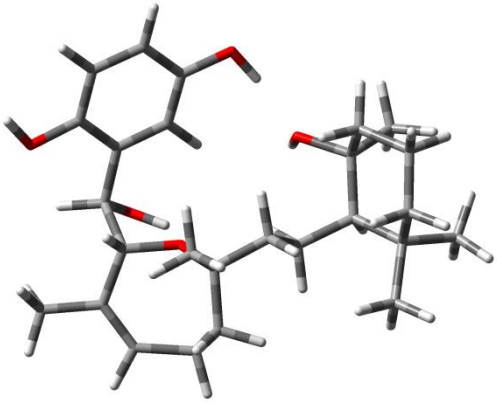

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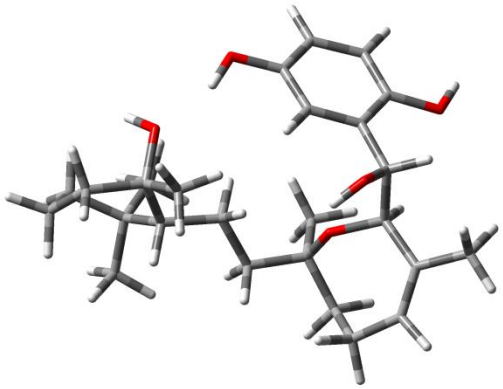

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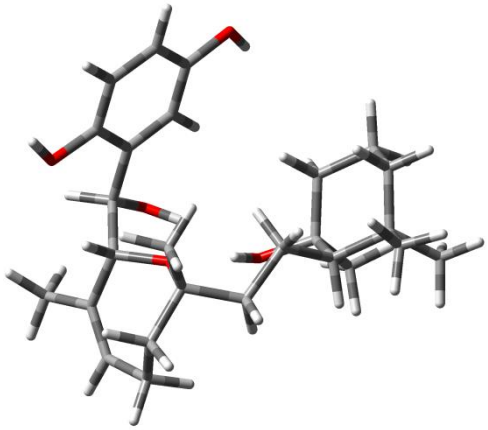

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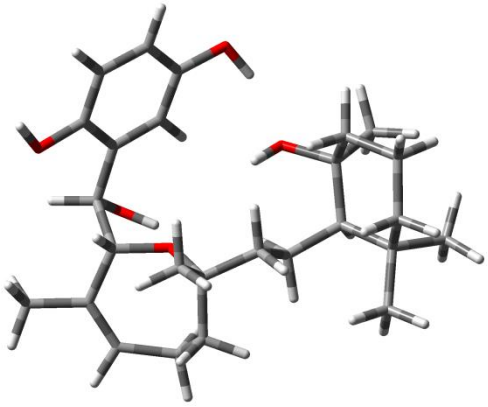

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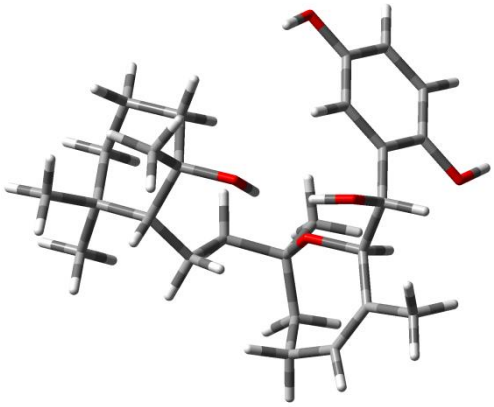
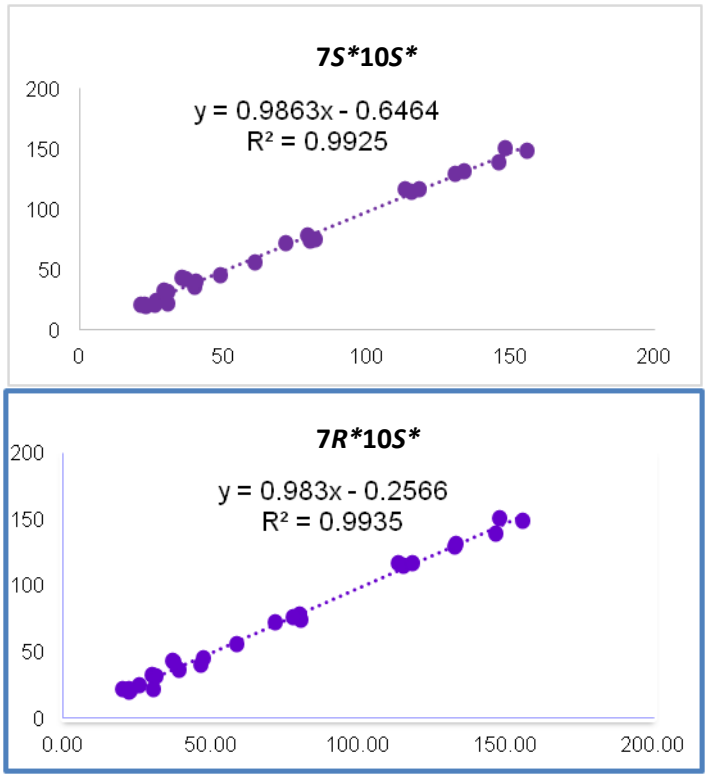


9

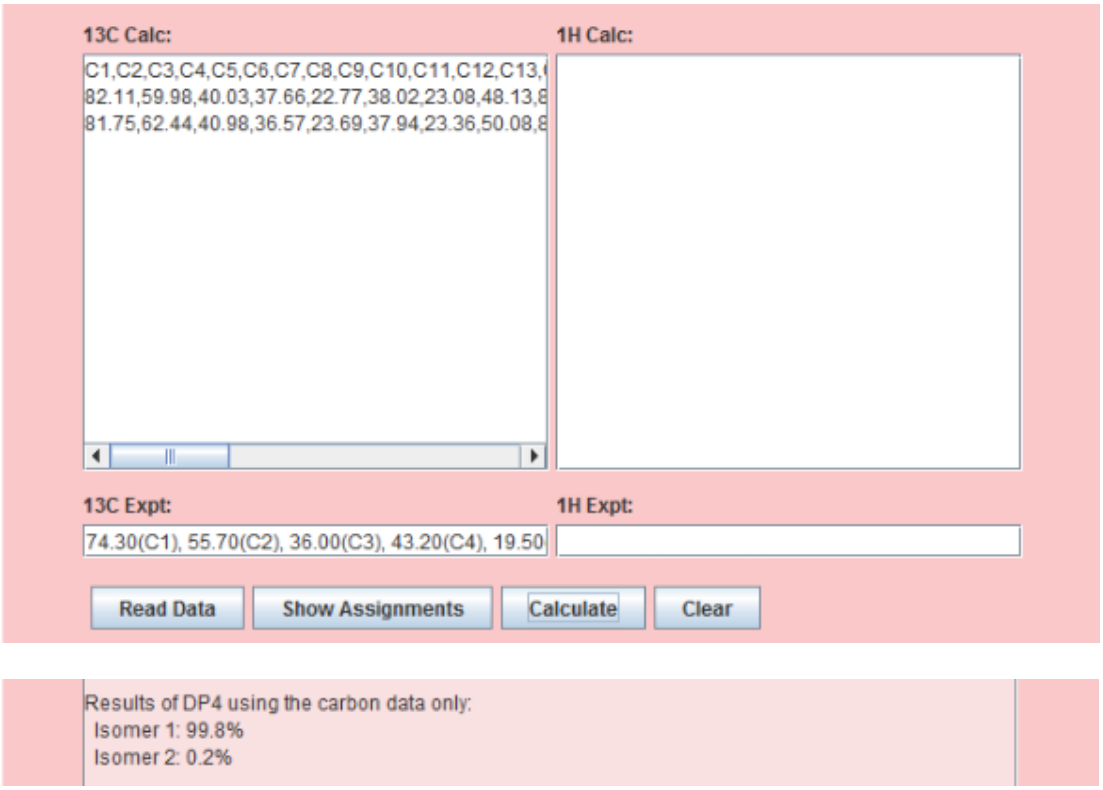
Comparación entre desplazamientos químicos calculados y experimentales de ^{13}C para **11**.

7*S10*S****	**7*R**10*S****	**EXP**
79.98	80.46	74.3
60.94	58.70	55.7
39.77	39.10	36.0
35.42	36.76	43.2
22.71	22.12	19.5
36.78	37.11	42.0
22.39	22.43	21.1
48.74	47.06	44.8
79.14	79.81	78.0
40.39	46.44	40.0
26.34	25.54	24.4
130.69	132.25	129.6
145.63	146.42	138.7
81.78	77.74	75.4
71.68	71.48	72.0
133.55	133.01	131.3
147.87	147.66	150.8
113.21	113.39	116.4
115.36	115.00	114.8
155.39	155.40	148.2
118.11	118.28	116.3
30.53	30.26	22.0
29.05	29.88	32.5
30.37	30.99	31.6
26.01	19.87	21.3
21.22	21.94	21.2

R^2-gráfico de correlación de ambos diasteroisómeros **11**.



Correlación DP4 de ambos diasteroisómeros de **11**.



Correlación DP4 de los diasteroisómeros ***7R*10S****, ***7S*10S**** y desplazamientos químicos en metanol-d_4 de **11**. Isómero 1: ***7R*10S****, isómero 2: ***7S*10S****.

Correlación DP4+ de los diasteroisómeros ***7R*10S****, ***7S*10S****

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCM		6-31+G(d,p)		Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	100.00%	0.00%	-	-	-	-
sDP4+ (C data)	99.91%	0.09%	-	-	-	-
sDP4+ (all data)	100.00%	0.00%	-	-	-	-
uDP4+ (H data)	100.00%	0.00%	-	-	-	-
uDP4+ (C data)	93.59%	6.41%	-	-	-	-
uDP4+ (all data)	100.00%	0.00%	-	-	-	-
DP4+ (H data)	100.00%	0.00%	-	-	-	-
DP4+ (C data)	99.99%	0.01%	-	-	-	-
DP4+ (all data)	100.00%	0.00%	-	-	-	-

Energías DFT calculadas para diasteroisómero 7*R**10*R** y 7*R**10*S** deducido por búsqueda DFT search of **11**.

Confórmeros 7*R**10*R**	B3LYP/6-31G(d) DFT Energía (hartree)	Δ (DFT Energía) (kcal/mol)	% Población
11	-1312.85805	-823830.752	51.21
10	-1312.85728	-823830.275	22.85
4	-1312.85680	-823829.968	13.61
14	-1312.85618	-823829.583	7.10
6	-1312.85548	-823829.143	3.37
19	-1312.85483	-823828.732	1.69
3	-1312.85212	-823827.033	0.10
16	-1312.85175	-823826.799	0.06

Confórmeros 7*R**10*S**	B3LYP/6-31G(d) DFT Energía (hartree)	Δ (DFT Energía) (kcal/mol)	% Población
8	-1312.85757	-823830.457	96.51
31	-1312.85396	-823828.189	2.09
34	-1312.85235	-823827.177	0.38
18	-1312.85149	-823826.638	0.15
23	-1312.85148	-823826.63	0.15
15	-1312.85109	-823826.388	0.1
20	-1312.85108	-823826.382	0.1
27	-1312.85108	-823826.38	0.1
28	-1312.85108	-823826.383	0.1
33	-1312.85108	-823826.382	0.1
35	-1312.85108	-823826.383	0.1
29	-1312.85025	-823825.863	0.04
11	-1312.84972	-823825.529	0.02
16	-1312.84948	-823825.375	0.02
25	-1312.84945	-823825.359	0.02
9	-1312.84945	-823825.358	0.02
13	-1312.84902	-823825.092	0.01
26	-1312.84418	-823822.051	0
32	-1312.84385	-823821.847	0

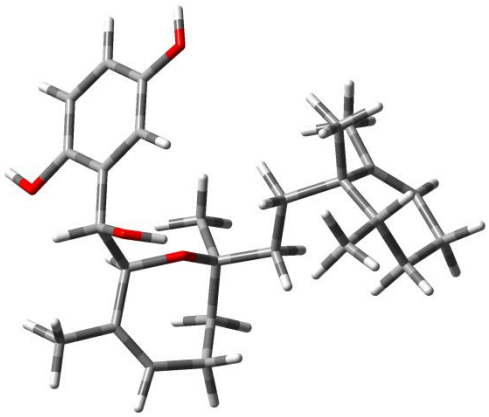
Correlación DP4+ de ambos diasteroisómeros de **12**.

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCM		6-311+G(d,p)		Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	-	-	-	-	-	-
sDP4+ (C data)	30.14%	69.86%	-	-	-	-
sDP4+ (all data)	30.14%	69.86%	-	-	-	-
uDP4+ (H data)	-	-	-	-	-	-
uDP4+ (C data)	27.62%	72.38%	-	-	-	-
uDP4+ (all data)	27.62%	72.38%	-	-	-	-
DP4+ (H data)	-	-	-	-	-	-
DP4+ (C data)	14.13%	85.87%	-	-	-	-
DP4+ (all data)	14.13%	85.87%	-	-	-	-

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCM		6-311+G(d,p)		Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.00%	100.00%	-	-	-	-
sDP4+ (C data)	30.14%	69.86%	-	-	-	-
sDP4+ (all data)	0.00%	100.00%	-	-	-	-
uDP4+ (H data)	0.00%	100.00%	-	-	-	-
uDP4+ (C data)	#¡REF!	#¡REF!	-	-	-	-
uDP4+ (all data)	#¡REF!	#¡REF!	-	-	-	-
DP4+ (H data)	0.00%	100.00%	-	-	-	-
DP4+ (C data)	#¡REF!	#¡REF!	-	-	-	-
DP4+ (all data)	#¡REF!	#¡REF!	-	-	-	-

Energías DFT calculadas para diasteroisómero 7*R**10*S** deducido por búsqueda DFT search of **10**.

Confórmeros 7*R**10*S**	B3LYP/6-31G(d) DFT Energía (hartree)	Δ (DFT Energía) (kcal/mol)	% Población
2	-1313.96973	-824528.3451	37.22
16	-1313.969244	-824528.0401	22.23
8	-1313.968812	-824527.769	14.06
10	-1313.968347	-824527.4772	8.59
1	-1313.968167	-824527.3643	7.10
11	-1313.967182	-824526.7462	2.50
17	-1313.966874	-824526.5529	1.80
6	-1313.966852	-824526.5391	1.76
12	-1313.966733	-824526.4644	1.55
13	-1313.9665	-824526.3182	1.21
9	-1313.965501	-824525.6913	0.42
14	-1313.965494	-824525.6869	0.42
3	-1313.96548	-824525.6781	0.41
5	-1313.965447	-824525.6574	0.40
4	-1313.965194	-824525.4987	0.30
7	-1313.962941	-824524.0849	0.03
15	-1313.962028	-824523.512	0.01
18	-1313.960461	-824522.5287	0.00



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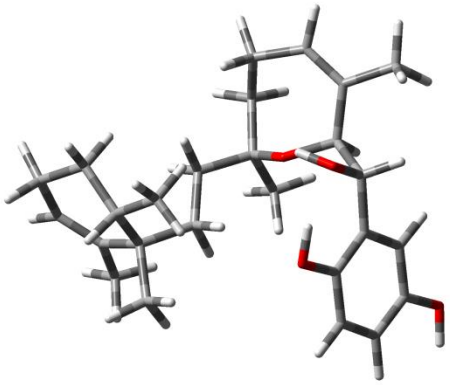

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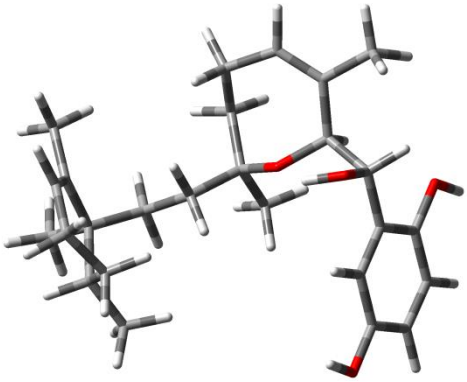

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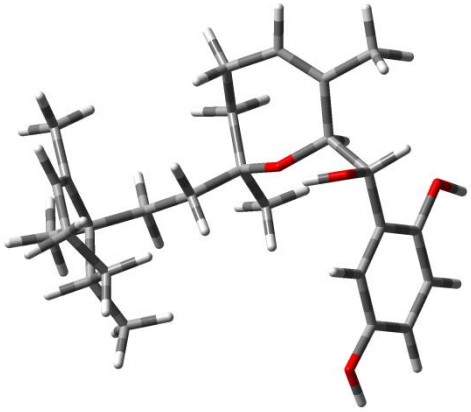

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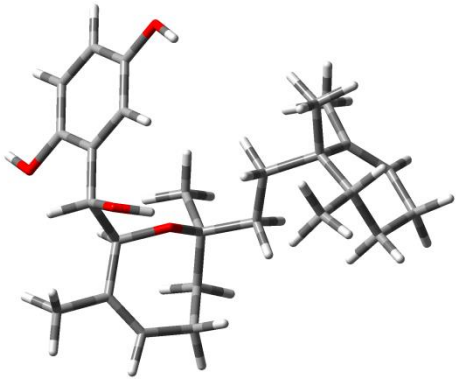

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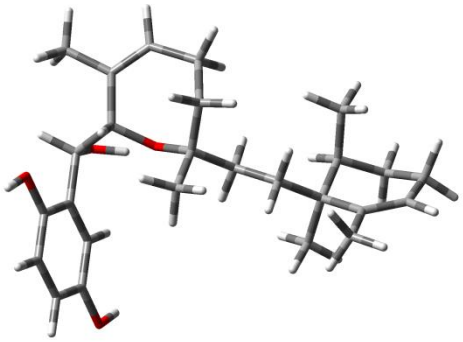

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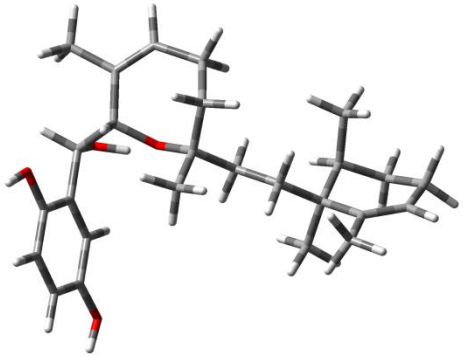

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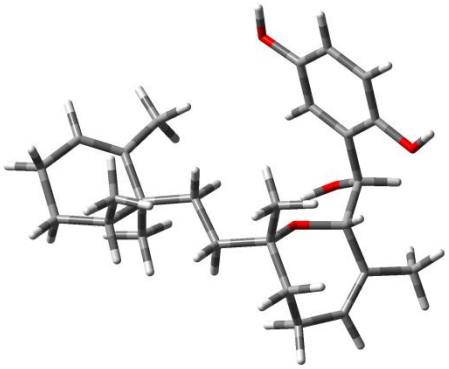

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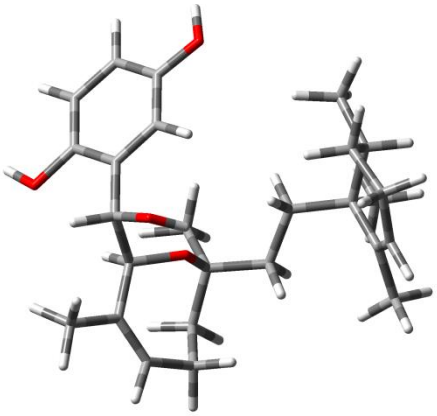

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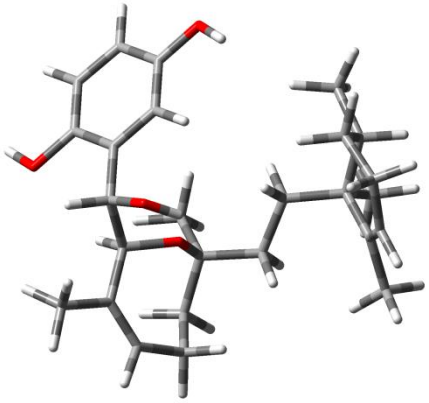

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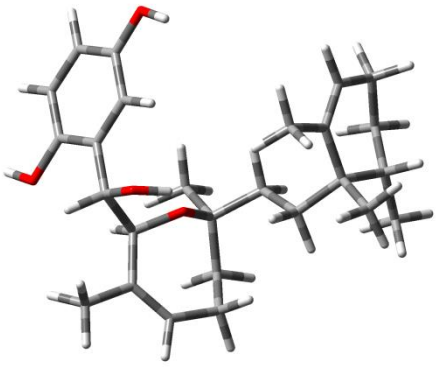

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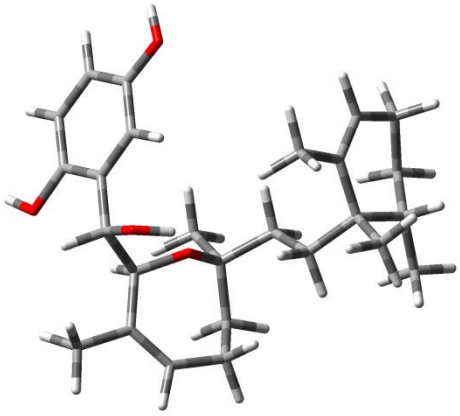

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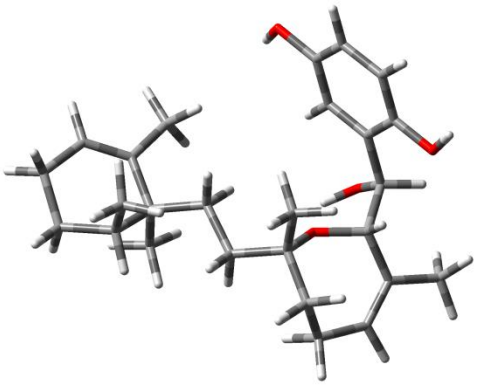

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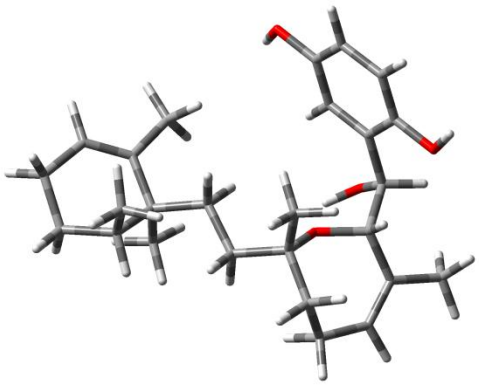

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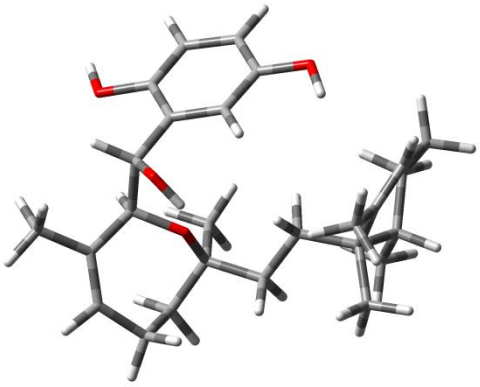

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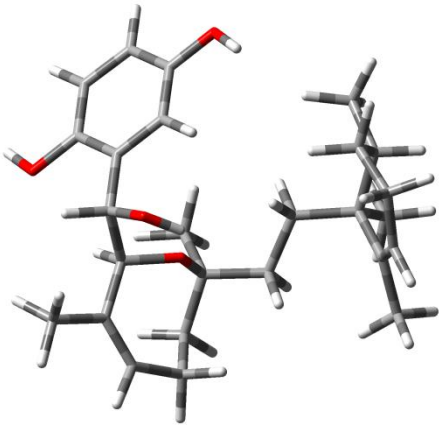

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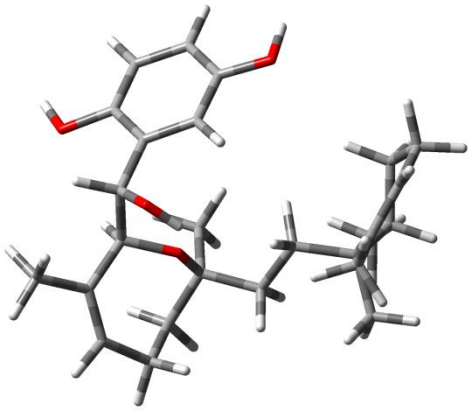

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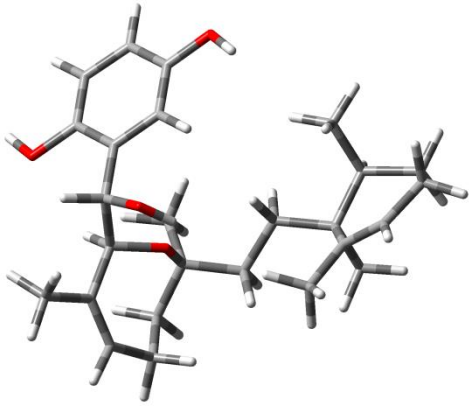
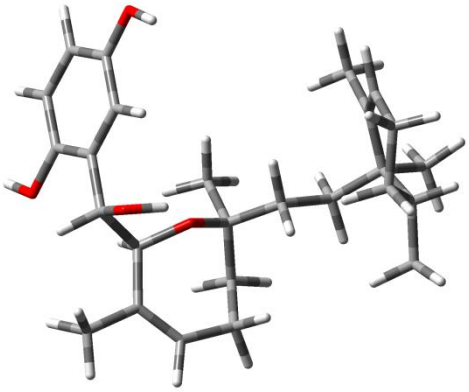


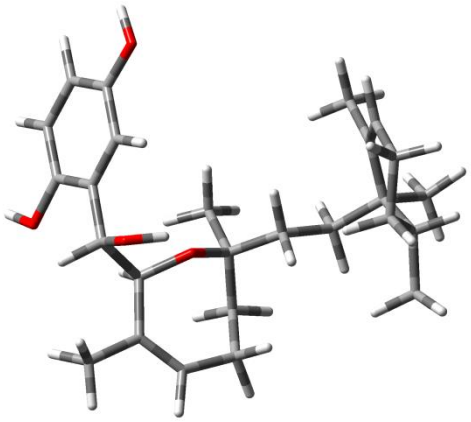
18

Energías DFT calculadas para diasteroisómero 7*R**10*R** deducido por búsqueda DFT search of **10**.

Confórmeros 7*R**10*S**	B3LYP/6-31G(d) DFT Energía (hartree)	Δ (DFT Energía) (kcal/mol)	% Población
6	-1313.968999	-824527.8864	28.57
11	-1313.96848	-824527.5607	16.48
1	-1313.968323	-824527.4622	13.95
8	-1313.968147	-824527.3517	11.58
13	-1313.967869	-824527.1773	8.62
3	-1313.967817	-824527.1446	8.16
12	-1313.967511	-824526.9526	5.90
2	-1313.966567	-824526.3603	2.17
9	-1313.966482	-824526.3069	1.98
5	-1313.965958	-824525.9781	1.14
4	-1313.965765	-824525.857	0.93
7	-1313.964965	-824525.355	0.40
10	-1313.963933	-824524.7074	0.13



6



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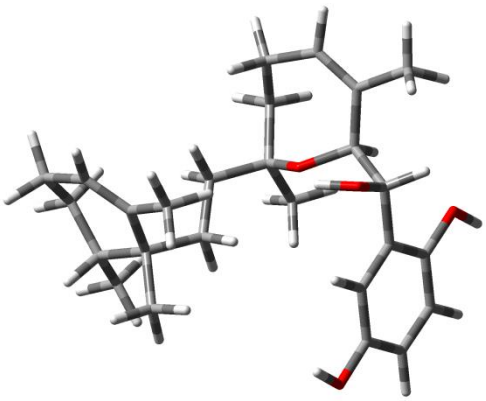

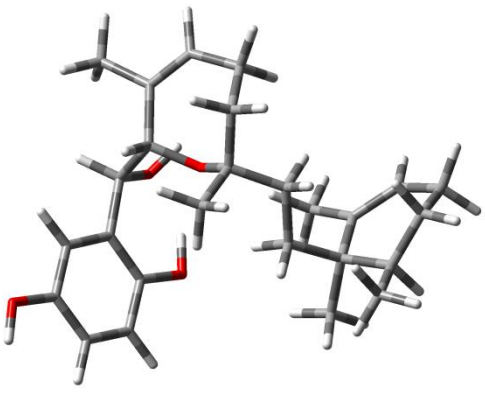

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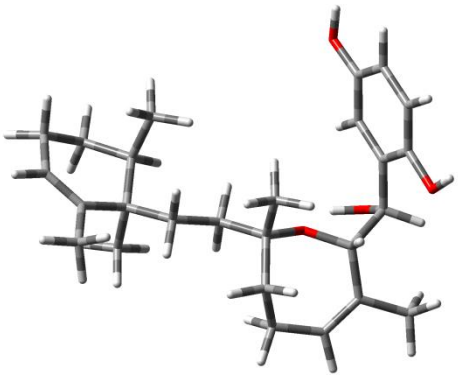

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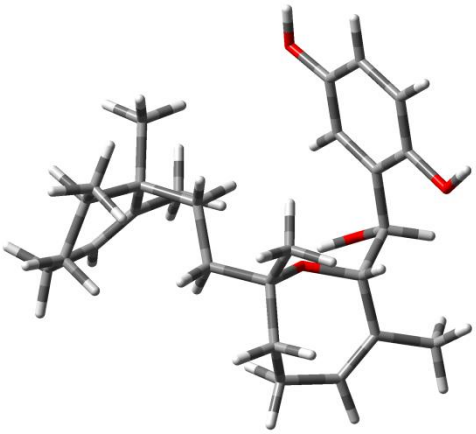

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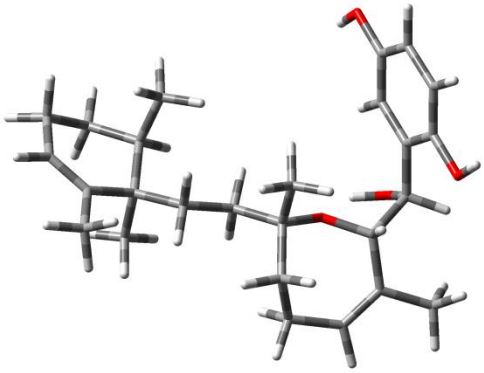

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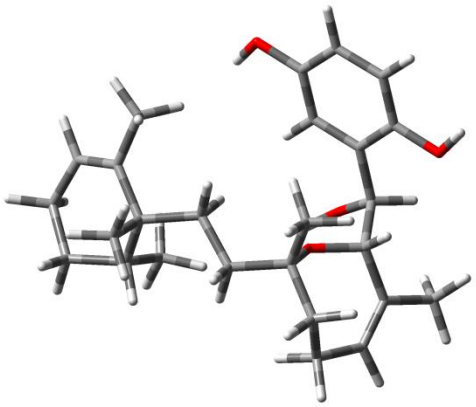

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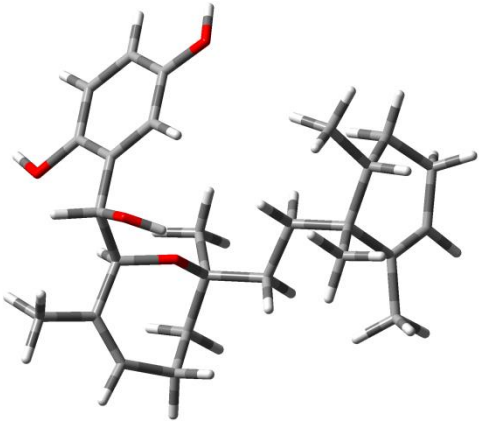

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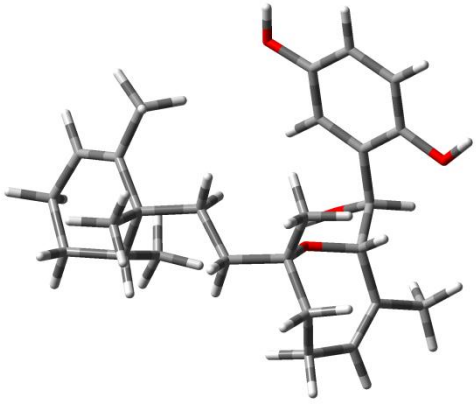

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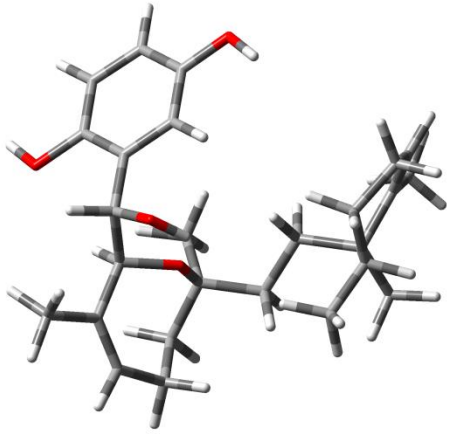
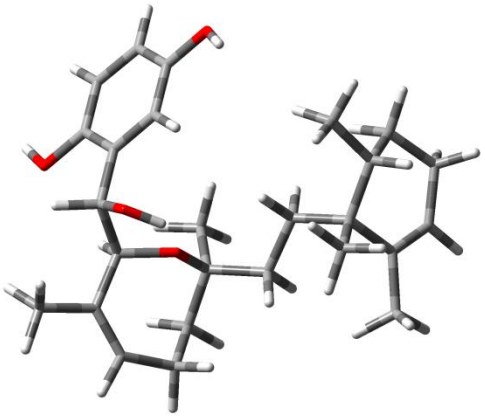


4



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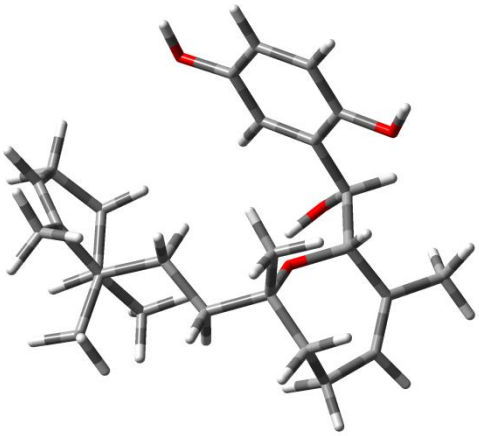


10

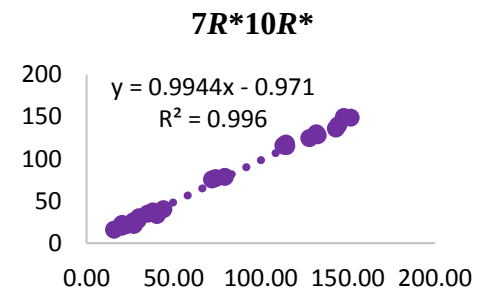
Comparación entre desplazamientos químicos calculados y experimentales de ^{13}C para **10**.

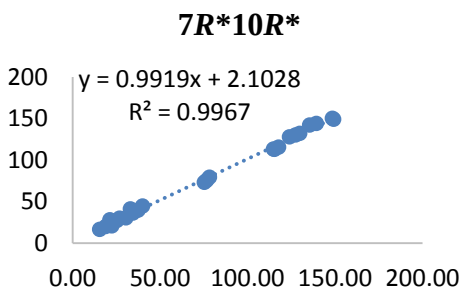
	B3LYP_6_31_G_NMR MPW_6311_plus_plus_2d_p		**B3LYP_6_31_plus_G_d_p_NMR MPW_6311_plus_plus_2d_p**		**B3LYP_6_31_plus_G_d_p_NMR MPW_6311_plus_plus_2d_p_Scaled**	
EXP	**7*R**10*S****	**7*R**10*R****	**7*R**10*S****	**7*R**10*R****	**7*R**10*S****	**7*R**10*R****
75.60	72.17	72.02	73.90	73.20	72.07	71.68
77.00	74.53	74.05	75.73	75.21	73.90	73.71
135.70	141.28	143.15	141.70	141.87	139.99	140.91
130.10	130.77	132.04	132.15	131.71	130.42	130.67
23.40	25.86	26.29	26.18	26.50	24.25	24.59
37.50	39.87	38.05	40.99	39.54	39.10	37.75
78.60	78.75	79.49	79.60	79.33	77.77	77.86
34.70	35.51	35.18	36.09	36.06	34.18	34.23
30.70	30.17	30.17	30.12	30.17	28.21	28.30
40.30	42.97	44.13	43.66	44.36	41.77	42.60
139.60	142.85	144.52	143.43	143.87	141.73	142.93
124.30	126.67	127.91	127.59	127.66	125.86	126.58
25.60	27.47	26.90	27.41	27.23	25.49	25.34
27.10	30.03	29.46	30.14	29.81	28.22	27.93
33.30	40.52	40.56	40.40	41.07	38.50	39.29
21.30	22.48	22.79	22.84	23.03	20.91	21.09
22.60	19.72	20.36	20.14	20.61	18.20	18.65
21.40	27.09	27.18	27.47	27.93	25.55	26.04
19.20	19.73	20.02	19.61	19.93	17.68	17.97
15.70	16.06	15.86	15.77	16.45	13.82	14.46
127.70	130.57	132.70	149.48	148.85	147.79	147.94
149.40	147.01	147.75	129.44	130.10	127.71	129.04
118.10	113.30	114.54	112.87	113.14	111.11	111.94
115.70	111.35	112.98	149.60	149.83	147.91	148.93
148.70	149.48	151.57	112.40	112.71	110.64	111.52
115.10	113.53	114.79	115.54	115.26	113.79	114.09
$\Delta\delta$	**1.9913**	2.2671	**2.4904**	2.6092	**2.1900**	2.2531

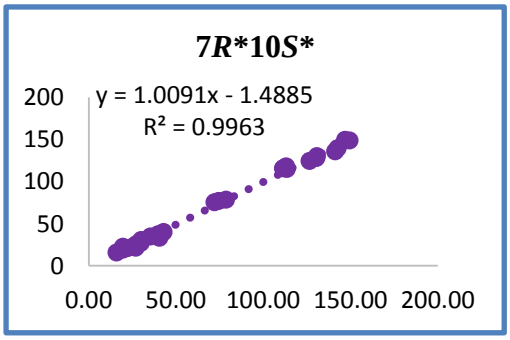
R^2-gráfico de correlación de ambos diasteroisómeros **10**.

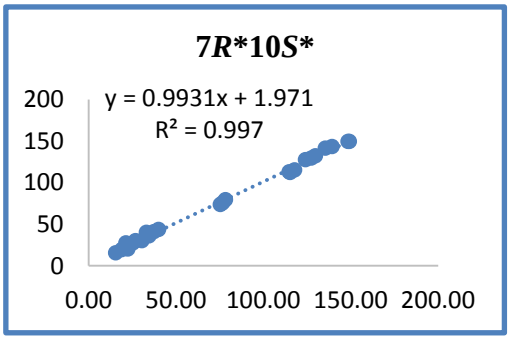
B3LYP_6_31_G_NMR
MPW_6311_plus_plus_2d_p

B3LYP_6_31_plus_G_d_p_NMR
MPW_6311_plus_plus_2d_p







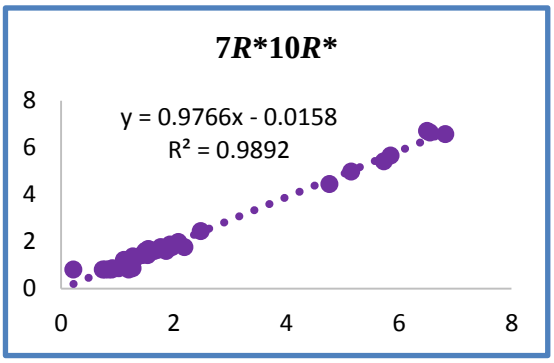


Comparación entre desplazamientos químicos calculados y experimentales de ^{1}H para **10**.

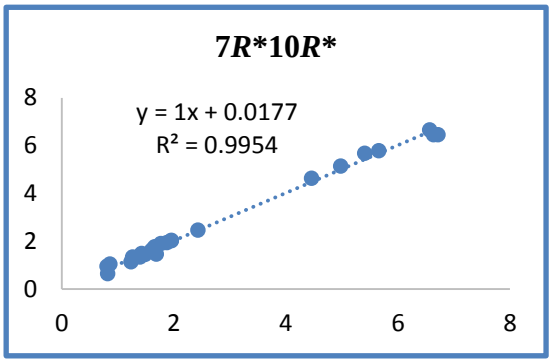
	B3LYP_6_31_G_NMR MPW_6311_plus_plus_2d_p		**B3LYP_6_31_plus_G_d_p_NMR MPW_6311_plus_plus_2d_p**		**B3LYP_6_31_plus_G_d_p_NMR MPW_6311_plus_plus_2d_p_Scaled**	
EXP	**7*R**10*S****	**7*R**10*R****	**7*R**10*S****	**7*R**10*R****	**7*R**10*S****	**7*R**10*R****
4.45	4.61	4.77	4.66	4.62	4.64	4.60
4.98	5.17	5.15	5.17	5.14	5.15	5.12
5.66	5.79	5.85	5.77	5.78	5.75	5.76
1.88	1.91	1.94	1.96	1.94	1.93	1.92
2.44	2.51	2.48	2.50	2.46	2.48	2.44
1.66	1.52	1.57	1.51	1.55	1.49	1.53
1.66	1.77	1.73	1.81	1.76	1.78	1.74
1.25	1.70	1.30	1.69	1.44	1.67	1.42
1.45	1.00	1.45	0.97	1.34	0.94	1.32
1.22	1.18	1.12	1.17	1.14	1.14	1.12
1.37	1.52	1.28	1.37	1.34	1.34	1.32
5.41	5.70	5.73	5.73	5.68	5.72	5.66
1.92	2.05	2.07	2.01	2.02	1.98	2.00
1.98	2.11	2.09	2.06	2.03	2.04	2.01
1.42	1.53	1.54	1.51	1.48	1.48	1.46
1.42	1.53	1.44	1.51	1.43	1.48	1.41
1.68	1.54	1.55	1.46	1.46	1.43	1.44
1.77	1.96	1.98	1.87	1.90	1.84	1.88
0.81	0.61	0.60	0.70	0.63	0.67	0.61
0.86	1.11	1.07	1.01	1.04	0.98	1.02
1.60	1.61	1.68	1.56	1.62	1.53	1.61
0.81	1.08	0.96	0.99	0.95	0.96	0.93
6.71	6.39	6.50	6.43	6.45	6.42	6.43
6.64	6.43	6.55	6.40	6.44	6.38	6.42
6.57	6.73	6.82	6.59	6.64	6.58	6.63
$\Delta\delta$	0.1743	**0.1490**	0.1423	**0.1153**	0.1365	**0.1107**

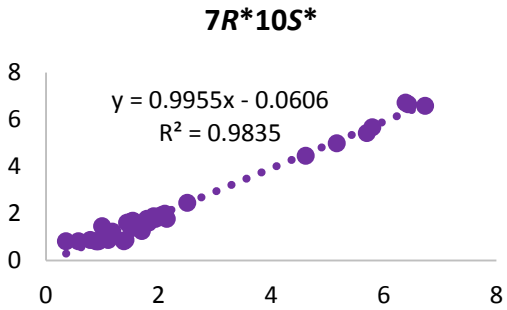
R^2-gráfico de correlación de ambos diasteroisómeros **10**.

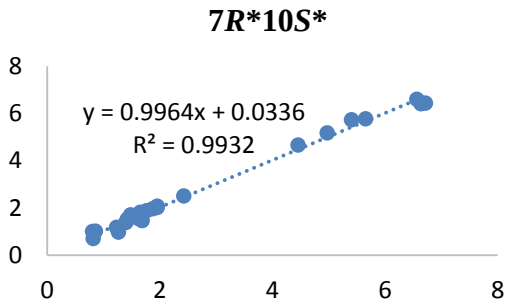
B3LYP_6_31_G_NMR
MPW_6311_plus_plus_2d_p



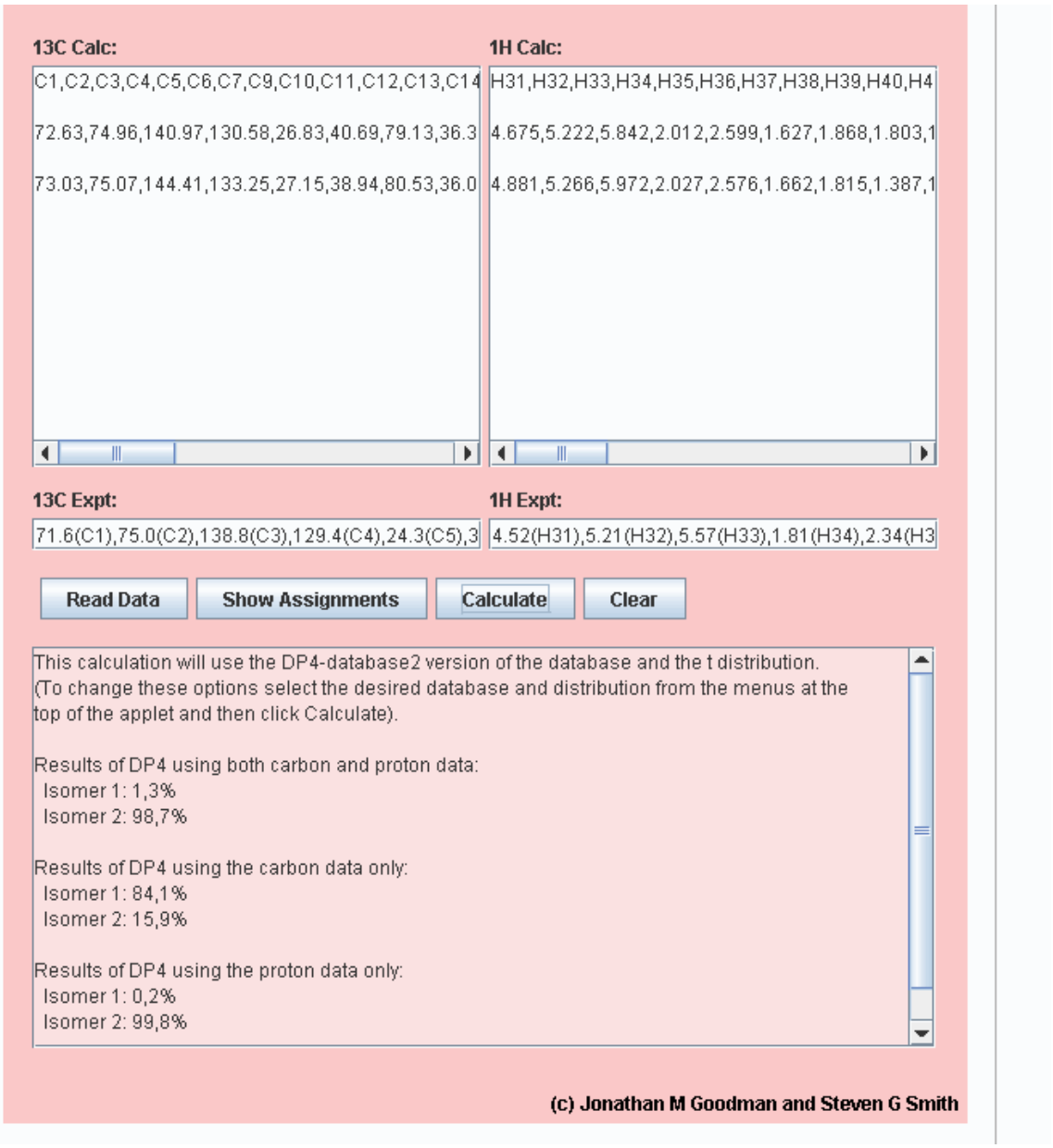
B3LYP_6_31_plus_G_d_p_NMR
MPW_6311_plus_plus_2d_p







Correlación DP4 de ambos diasteroisómeros de **10**.



Correlación DP4 de los diasteroisómeros ***7R*10S****, ***7R*10R**** y desplazamientos químicos en cloroformo-d de **10**. Isómero 1: ***7R*10S****, isómero 2: ***7R*10R****.

Correlaciones DP4+ de ambos diasteroisómeros de **10**.

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCM		6-31+G(d,p)		Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.71%	99.29%	-	-	-	-
sDP4+ (C data)	93.04%	6.96%	-	-	-	-
sDP4+ (all data)	8.69%	91.31%	-	-	-	-
uDP4+ (H data)	0.04%	99.96%	-	-	-	-
uDP4+ (C data)	99.39%	0.61%	-	-	-	-
uDP4+ (all data)	5.66%	94.34%	-	-	-	-
DP4+ (H data)	0.00%	100.00%	-	-	-	-
DP4+ (C data)	99.95%	0.05%	-	-	-	-
DP4+ (all data)	0.57%	99.43%	-	-	-	-

Correlación DP4+ de los diasteroisómeros ***7R*10S****, ***7R*10R**** y desplazamientos químicos en cloroformo-d de **10**. Isómero 1: ***7R*10S****, isómero 2: ***7R*10R****.