

Supplementary Information

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Table S1. ^1H and ^{13}C NMR data for okadaic acid in CD_3OD (J in Hz).

C	δ_{C}	δ_{H}	$^3J_{\text{H,H}}$	C	δ_{C}	δ_{H}	$^3J_{\text{H,H}}$
1	182.2	-	-	23	78.1	3.28	9.8, 9.8
2	76.0	-	-	24	71.8	3.92	9.8
3	46.1	1.79 ^S 1.65 ^R	2.0, 12.0 11.0, 12.0	25	146.7	-	-
4	68.2	3.92	2.0, 2.5, 9.0, 11.0	26	86.2	3.80	8.8
5	33.1	1.72 ^R 1.30 ^S	4.0, 9.0, 10.0, 13.0 2.5, 2.5, 5.0, 13.0	27	65.8	3.94	2.0, 8.8, 10.0
6	28.2	1.82 ^R 1.51 ^S	4.0, 4.8, 5.0, 13.0 2.5, 9.5, 10.0, 13.0	28	36.3	1.28 ^R 0.82 ^S	2.6, 10.0, 12.0 2.0, 11.0, 12.0
7	73.2	3.22	4.8, 9.5	29	32.0	1.78	2.6, 6.4, 10.5, 11.0
8	97.1	-	-	30	76.7	3.13	2.2, 10.5
9	123.5	5.13	-	31	28.5	1.69	2.2, 2.5, 6.5, 6.9
10	138.8	-	-	32	27.5	1.88 ^S 1.25 ^R	2.5, 2.5, 12.0, 12.0 2.0, 6.5, 6.5, 12.0
11	33.4	1.90 ^R 1.69 ^S	11.0, 16.0 4.0, 16.0	33	30.6	1.22(2H)	-
12	71.4	3.71	4.0, 8.0, 11.0	34	96.5	-	-
13	42.9	2.20	7.0, 8.0, 8.5	35	36.6	1.49 ^R 1.26 ^S	2.5, 4.3, 13.0 2.5, 13.0, 13.0
14	137.2	5.81	8.5, 15.4	36	19.4	1.79 ^S 1.40 ^R	2.5, 2.5, 4.3, 4.3, 13.0 2.5, 2.5, 13.0, 13.0, 13.0
15	131.9	5.34	7.9, 15.4	37	26.1	1.37(2H)	-
16	80.2	4.52	7.5, 7.5, 7.9	38	60.9	3.57 ^S 3.39 ^R	3.0, 11.5, 12.0 2.5, 3.0, 12.0
17	31.0	2.04 ^R 1.43 ^S	6.2, 7.5, 9.5, 12.0 5.0, 5.5, 7.5, 12.0	39	10.6	0.79	6.9
18	37.7	1.88 ^S 1.72 ^R	5.0, 9.5, 12.5 5.5, 6.2, 12.5	40	16.8	0.91	6.4
19	106.5	-	-	41	112.6	5.25 4.91	-
20	33.4	1.75(2H) 1.75 ^R	- 4.0, 13.0	42	16.9	0.98	7.0
21	27.5	1.65 ^S	10.0, 13.0	43	22.9	1.59	-
22	71.1	3.50	4.0, 9.8, 10.0	44	27.5	1.16	-

Table S2. ^1H and ^{13}C NMR data for okadaic acid in CDCl_3 .

C	δ_{C}	δ_{H}	C	δ_{C}	δ_{H}
1	176.7	-	23	76.5	3.35
2	77.2	-	24	71.1	4.07
3	42.6	2.12 ^S 1.62 ^R	25	144.7	-
4	69.3	3.96	26	84.9	3.90
5	31.6	1.72 ^S 1.31 ^R	27	64.7	4.04
6	32.8	1.83 ^S 1.79 ^R	28	35.3	1.28 ^R 0.95 ^S
7	71.5	3.34	29	31.1	1.91
8	96.5	-	30	75.0	3.25
9	121.5	5.29	31	27.4	1.75
10	139.4	-	32	26.6	1.96 ^S 1.86 ^R
11	33.2	1.91 ^S 1.87 ^R	33	30.3	1.52 ^R 1.34 ^S
12	71.5	3.35	34	95.6	
13	42.2	2.21	35	25.4	1.48 1.31
14	136.3	5.63	36	18.7	1.39 ^R 1.61 ^S
15	131.4	5.42	37	35.9	1.84 ^R 1.51 ^S
16	79.1	4.51	38	60.3	3.62 ^S 3.53 ^R
17	30.6	2.14 ^R 1.54 ^S	39	10.7	0.88
18	37.3	2.04 ^S 1.80 ^R	40	16.2	1.01
19	105.7	-	41	112.5	5.39 5.02
20	26.4	1.47 1.32	42	15.9	0.97
21	27.1	1.81 ^S 1.72 ^R	43	23.1	1.73
22	69.7	3.57	44	27.3	1.36

Figure S1. ^1H NMR spectrum of okadaic acid in CD_3OD .

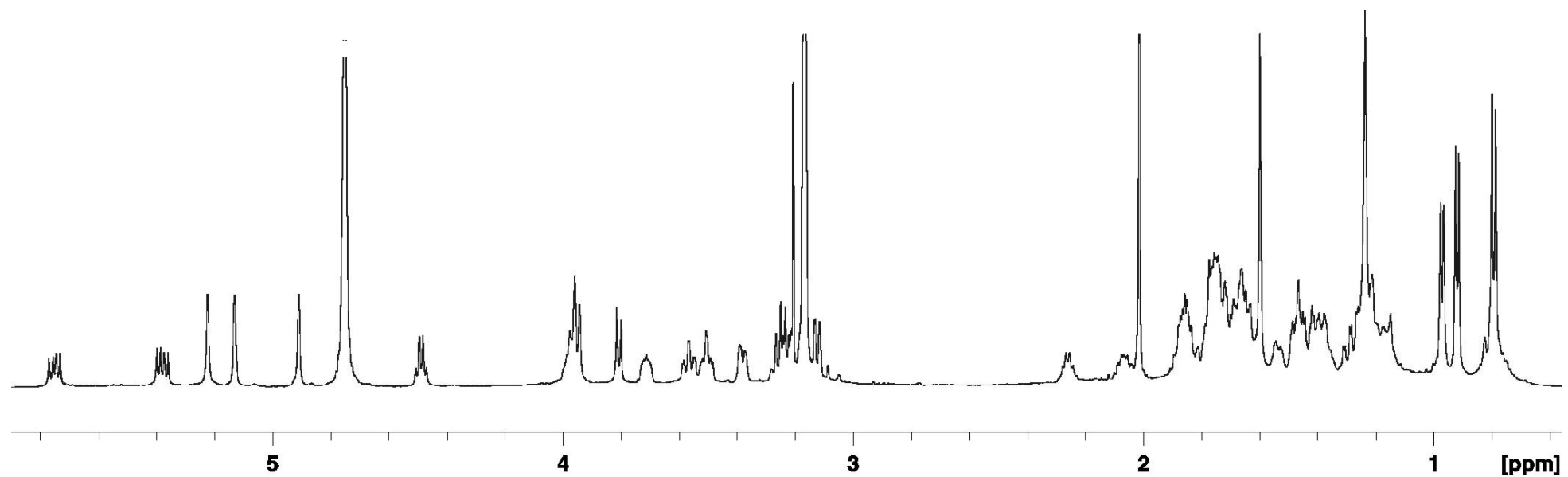


Figure S2. ^{13}C NMR spectrum of okadaic acid in CD_3OD .

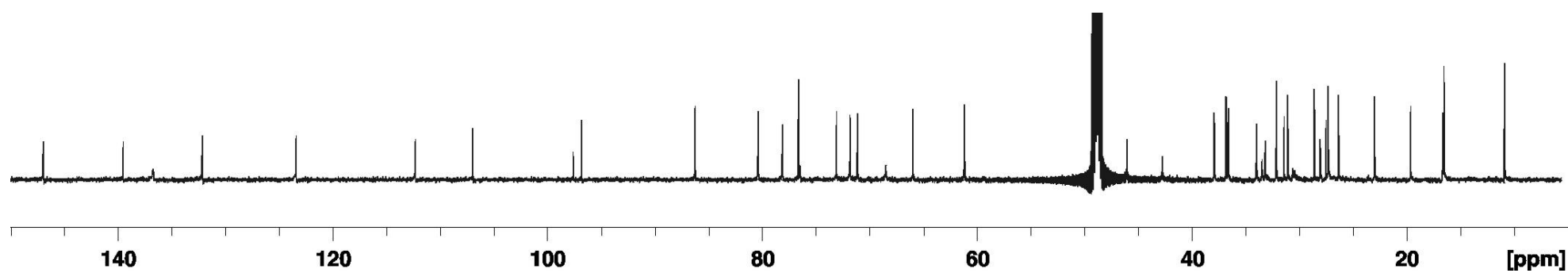


Figure S3. ROESY spectrum of okadaic acid in CD₃OD.

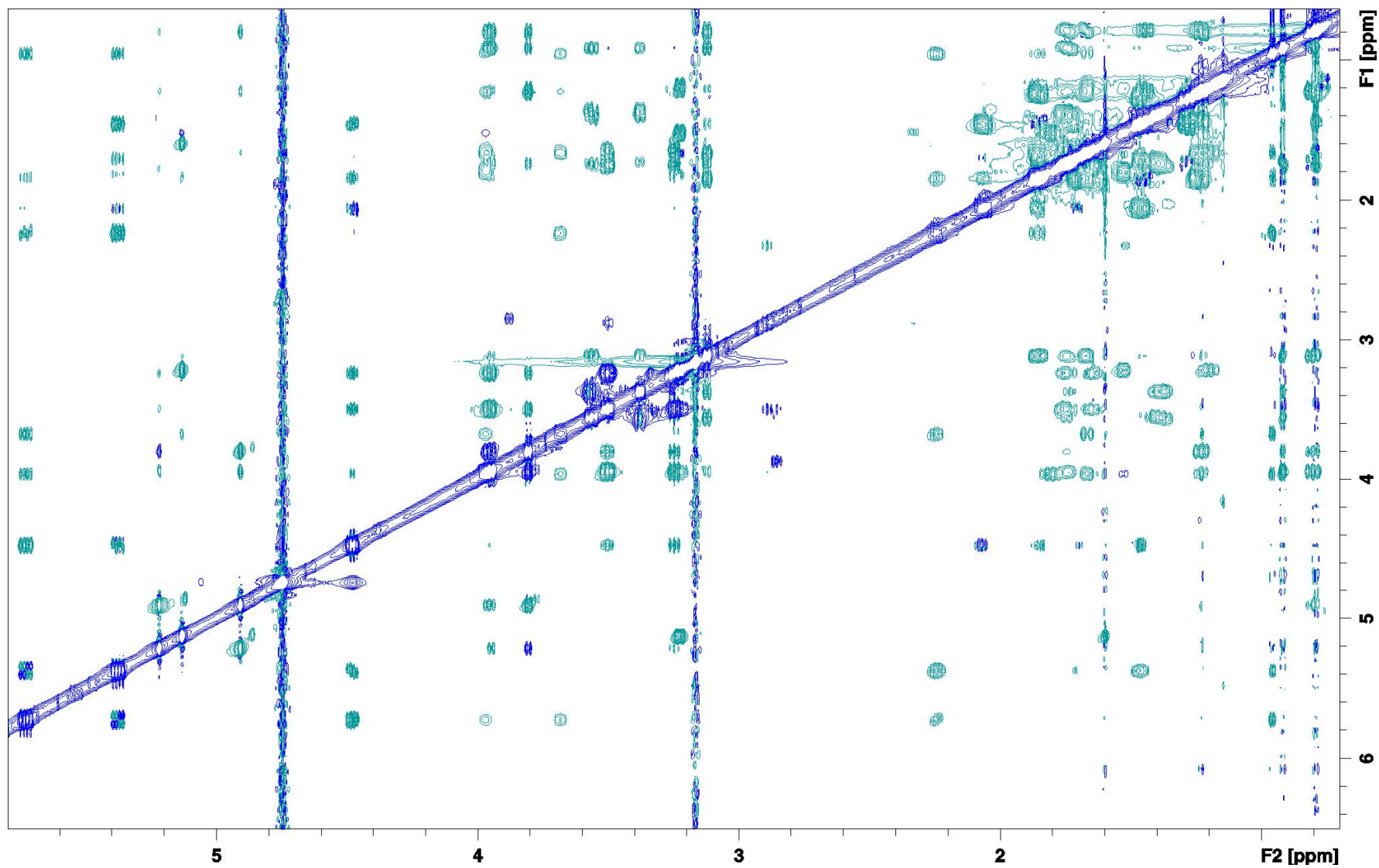


Figure S4. HSQC spectrum of okadaic acid in CD₃OD.

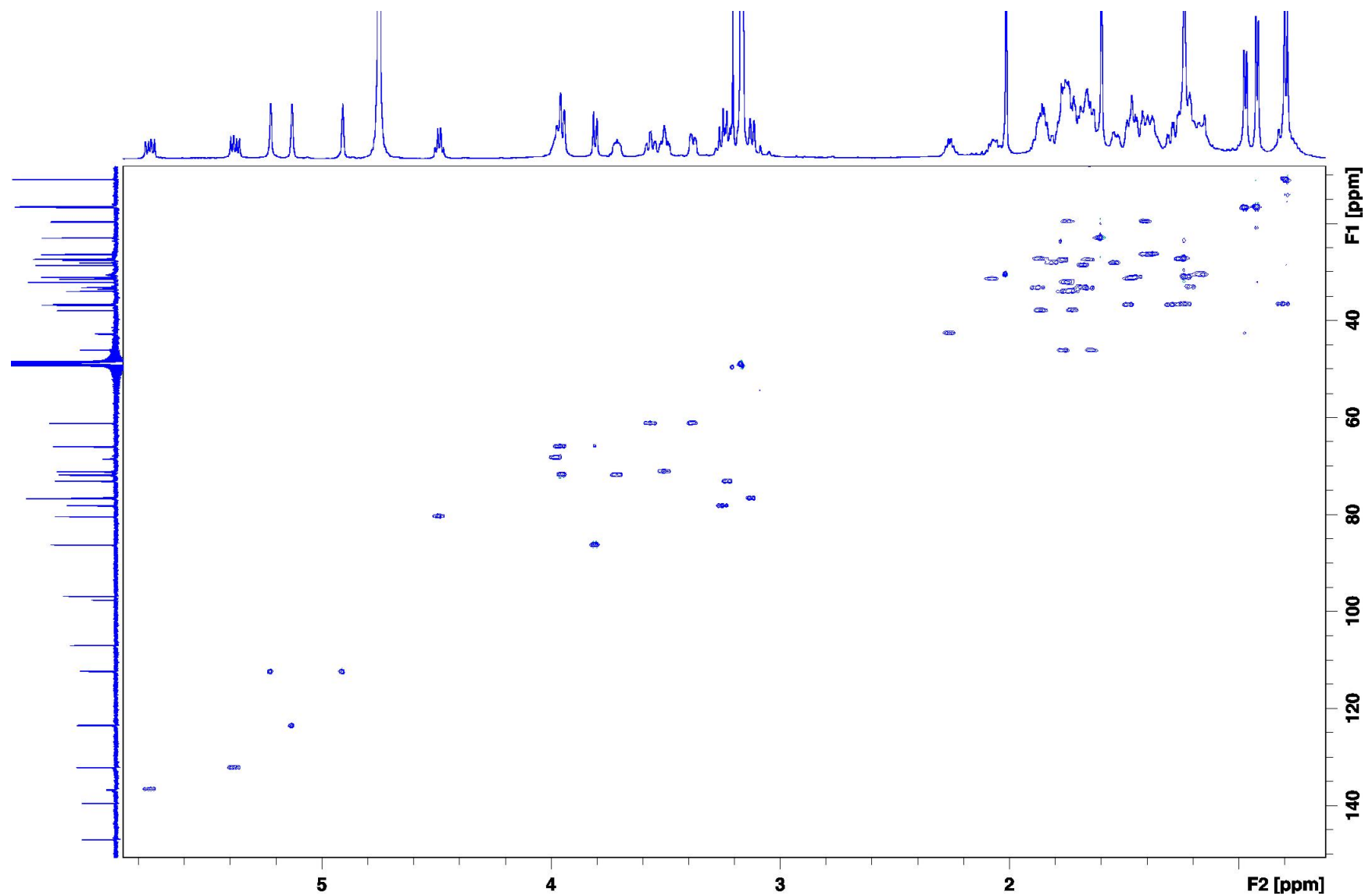


Figure S5. 1D-TOCSY spectrum of okadaic acid in CD₃OD with selective excitation (*purple*) H-14 (δ_{H} 5.81), (*green*) H-15 (δ_{H} 5.34) and (*red*) H-16 (δ_{H} 4.52).

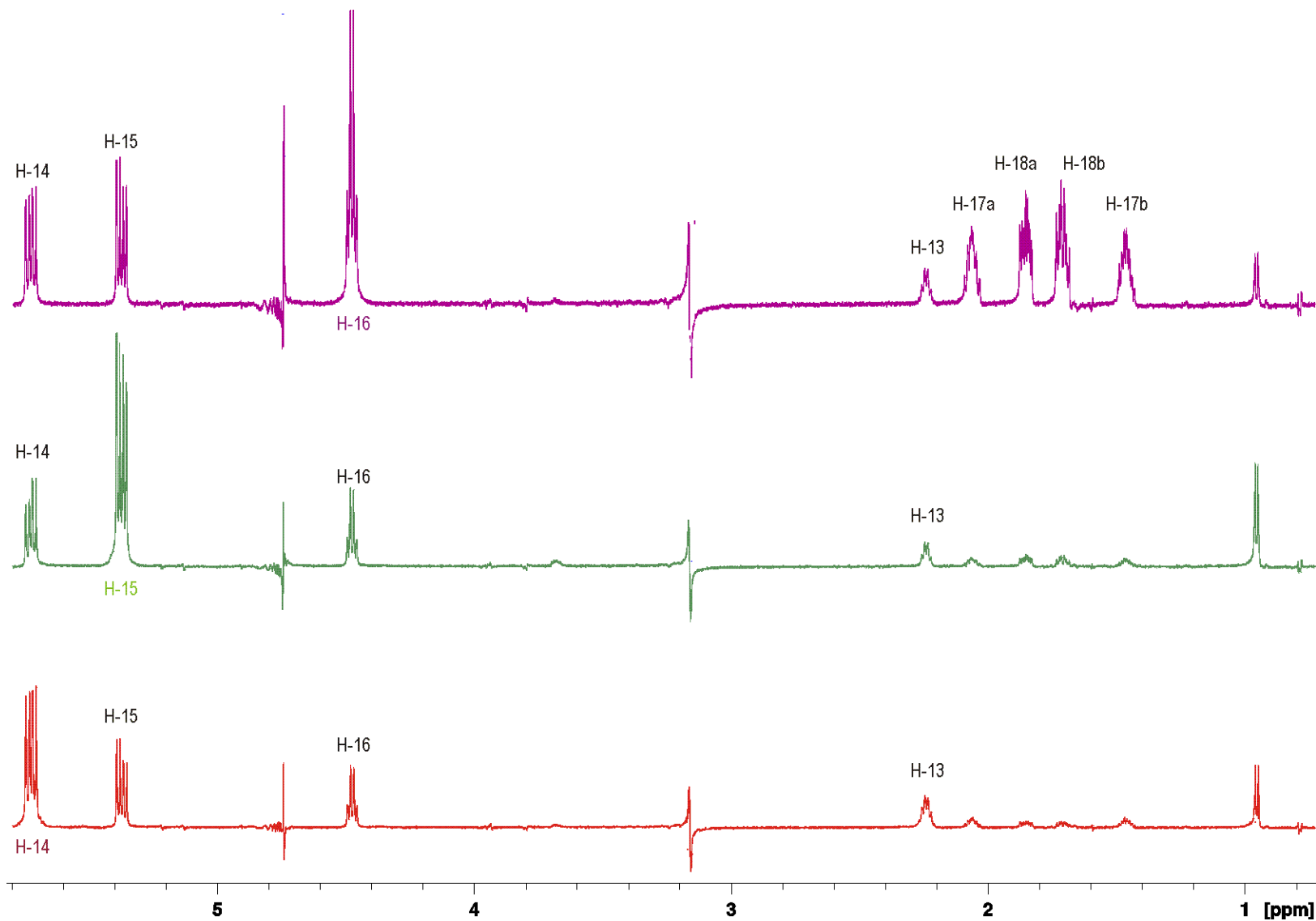


Figure S6. 1D-TOCSY spectrum of okadaic acid in CD₃OD with selective excitation (*purple*) H-27/H-24 (δ_{H} 3.94/3.92), (*green*) H-26 (δ_{H} 3.80) and (*red*) H-12 (δ_{H} 3.71).

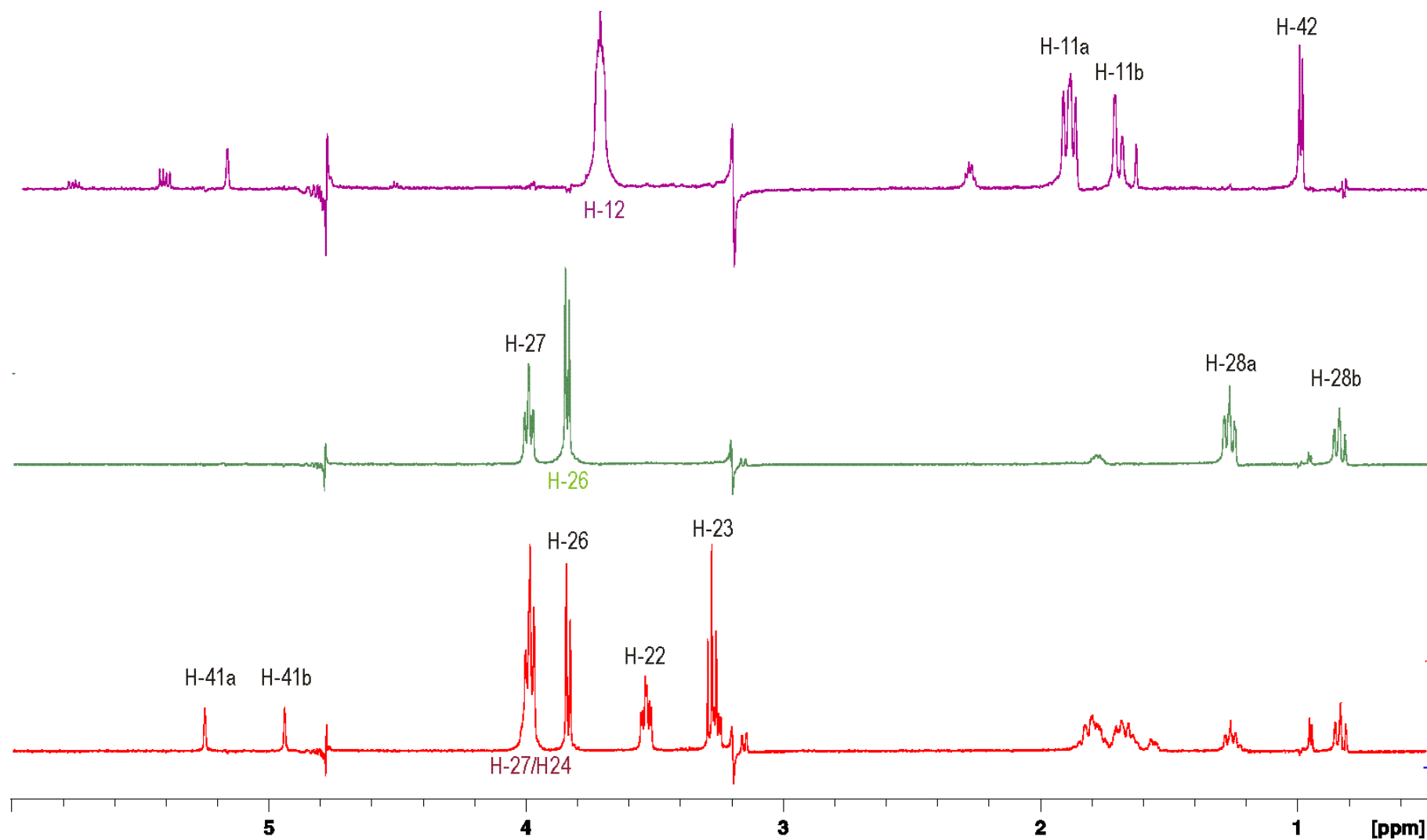


Figure S7. 1D-TOCSY spectrum of okadaic acid in CD₃OD with selective excitation (*purple*) H-38 α (δ_{H} 3.57), (*green*) H-22 (δ_{H} 3.50) and (*red*) H-38 β (δ_{H} 3.39).

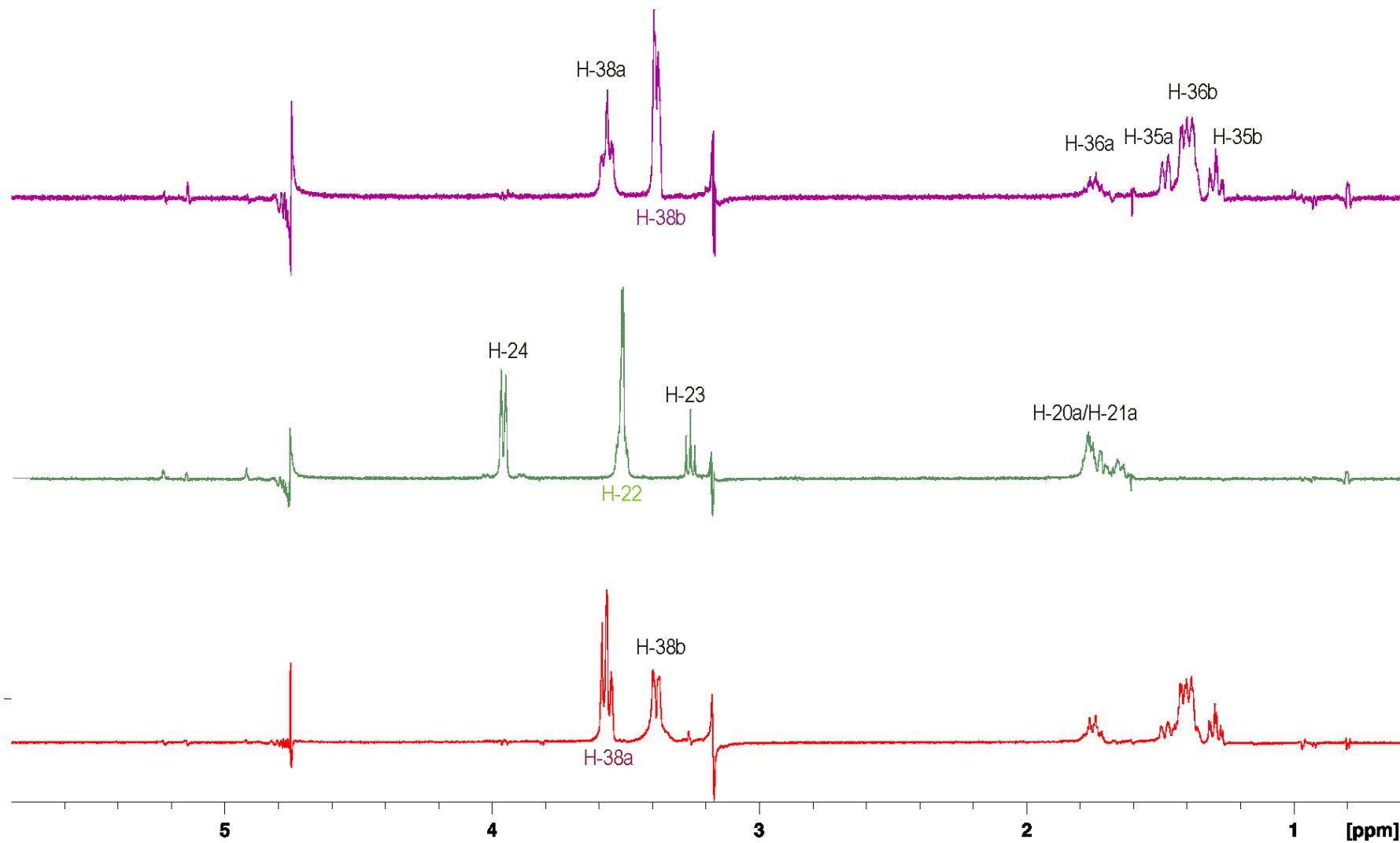


Figure S8. 1D-TOCSY spectrum of okadaic acid in CD₃OD with selective excitation (*purple*) H-30 (δ_{H} 3.13), (*green*) H-13 (δ_{H} 2.20) and (*red*) H-17 α (δ_{H} 2.04).

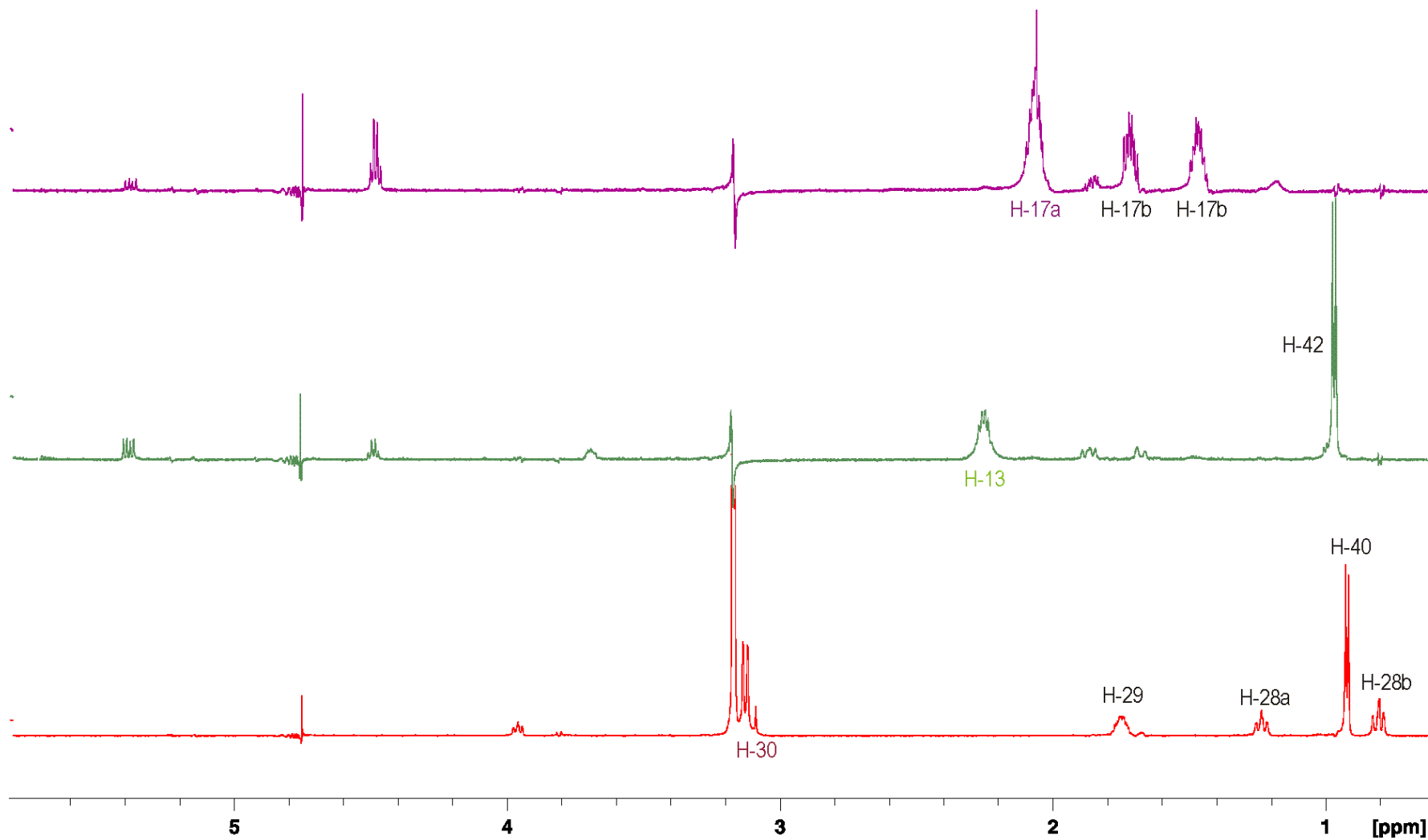


Table S3. Computed ^{13}C and ^1H chemical shifts for okadaic acid (**1**) and the studied diastereoisomer (**2**) on B3LYP-6-31G + (d).

C	1 (Gas)	1 (CHCl ₃)	1 (CH ₃ OH)	2 (Gas)	2 (CHCl ₃)	2 (CH ₃ OH)	CS I	CS II
1	14.1	13.3	13.4	23.4	23.0	21.2	7.8	14.3
2	114.1	114.0	114.0	116.6	115.7	115.5	114.9	111.5
3	147.4	147.5	147.8	145.5	145.9	146.2	143.6	146.8
4	123.3	122.7	122.7	121.8	122.1	123.0	122.6	119.2
5	158.1	158.1	158.3	157.1	157.4	157.7	155.6	155.7
6	158.0	158.1	158.1	152.9	152.8	152.9	157.6	160.7
7	117.1	118.0	118.1	119.0	119.3	119.8	117.6	119.4
8	95.9	96.5	96.4	97.2	97.8	99.3	90.9	89.7
9	67.9	71.3	72.7	70.1	72.6	75.1	68.2	69.9
10	53.6	51.0	49.2	55.9	52.2	51.3	54.5	51.5
11	154.8	154.8	154.8	156.4	156.9	157.0	154.5	154.5
12	120.0	120.6	120.3	122.6	121.8	123.2	120.8	118.3
13	143.3	143.8	144.0	142.6	143.3	143.3	142.4	146.0
14	55.5	55.0	53.8	60.0	58.6	59.5	51.6	57.1
15	57.5	58.4	59.2	54.7	55.2	56.8	62.5	61.6
16	113.7	114.0	114.2	115.6	115.3	115.9	112.5	115.4
17	158.6	158.7	159.1	158.8	159.2	159.4	157.4	156.5
18	152.7	152.6	152.6	155.0	155.1	155.2	151.7	151.0
19	89.1	89.2	89.2	88.2	88.5	88.7	90.4	94.5
20	153.4	153.9	154.0	152.5	152.9	153.0	152.4	153.8
21	162.8	163.1	163.2	161.2	161.4	161.4	160.2	162.1
22	117.8	117.9	118.2	117.5	120.1	120.6	117.9	116.6
23	114.8	115.1	115.1	117.3	117.9	117.7	114.4	114.4
24	117.5	118.0	117.9	117.5	117.6	117.3	115.5	115.9
25	39.9	40.8	41.4	46.1	44.6	43.2	47.6	33.3
26	103.0	103.7	103.9	100.6	101.6	101.3	105.0	105.0
27	127.0	127.0	127.1	118.1	119.2	119.1	123.6	112.8
28	155.4	155.3	155.4	149.9	148.8	148.2	154.7	152.0
29	155.6	155.6	155.5	146.7	147.1	147.3	154.9	152.3
30	116.1	116.0	116.0	117.9	115.9	115.9	113.3	117.3
31	159.3	159.5	159.7	153.9	153.8	153.9	159.1	160.0
32	162.5	162.4	162.5	164.0	163.0	163.1	162.6	161.6
33	157.5	157.4	157.5	158.5	158.7	158.7	157.5	157.2
34	99.1	98.6	98.5	98.0	97.5	97.5	98.5	100.0
35	151.2	150.9	150.9	150.9	150.9	150.8	150.4	152.3
36	167.3	167.3	167.4	166.3	165.7	165.8	168.0	167.3
37	161.8	161.4	161.5	162.3	161.6	161.6	163.7	162.5
38	129.3	129.4	129.3	131.4	131.1	130.9	129.9	129.3
39	178.1	178.4	178.6	174.9	175.0	175.0	175.7	175.6
40	173.7	174.2	174.4	173.9	174.9	174.7	173.8	172.8
41	81.3	80.8	80.3	75.5	74.4	74.9	83.7	83.6
42	172.9	173.4	173.5	174.4	175.4	175.2	172.4	174.2
43	166.7	167.0	167.3	167.0	167.7	167.8	165.6	166.1
44	164.5	164.1	164.2	167.0	167.8	168.6	162.8	164.2

Table S3. Cont.

H	1 (Gas)	1 (CHCl ₃)	1 (CH ₃ OH)	2 (Gas)	2 (CHCl ₃)	2 (CH ₃ OH)	CS I	CS II
H3	30.77	30.60	30.56	30.62	30.62	30.71	30.33	31.23
H3	30.36	30.32	30.29	30.76	30.57	30.17	29.97	29.64
H4	27.94	27.86	27.83	28.38	27.99	28.28	28.55	27.39
H5	30.75	30.79	30.79	31.02	30.85	30.93	30.63	31.17
H5	31.04	30.79	30.70	30.23	30.20	30.19	30.75	29.73
H6	30.50	30.49	30.50	30.33	30.59	30.65	30.31	30.27
H6	30.02	30.06	30.11	30.32	30.07	30.33	30.13	29.98
H7	28.77	28.46	28.35	29.02	28.80	28.94	28.88	28.81
H9	26.40	26.48	26.55	26.48	26.26	26.56	26.39	26.66
H11	30.66	30.53	30.39	30.49	30.36	30.13	30.49	30.46
H11	30.54	30.35	30.24	30.76	30.40	30.60	30.77	30.79
H12	28.42	28.75	28.71	28.10	27.89	27.78	27.93	28.05
H13	30.54	30.30	30.16	30.70	29.96	30.39	30.45	30.00
H14	26.85	26.85	26.73	26.62	26.51	26.66	25.90	25.25
H15	27.02	26.91	26.82	26.37	26.06	26.56	26.70	26.54
H16	27.61	27.61	27.68	27.92	27.90	27.98	27.73	27.65
H17	30.72	30.54	30.53	30.28	30.23	30.30	30.47	30.48
H17	30.22	30.12	30.15	30.92	30.71	30.63	30.85	30.86
H18	30.13	30.19	30.26	30.22	30.15	30.20	30.24	30.14
H18	30.34	30.19	30.12	30.44	30.25	30.07	30.53	30.80
H20	30.35	30.27	30.20	30.45	30.41	30.33	30.84	30.70
H20	30.29	30.18	30.20	30.46	30.47	30.44	30.08	30.35
H21	30.41	30.32	30.26	29.89	30.15	30.21	30.40	30.86
H21	30.01	30.09	30.15	30.41	30.63	30.71	30.03	30.07
H22	28.59	28.56	28.44	27.45	27.75	27.71	28.23	28.28
H23	28.47	28.40	28.40	28.31	28.35	28.28	29.08	29.29
H24	27.70	27.74	27.63	27.99	27.93	27.72	27.47	26.89
H26	28.28	28.18	28.02	27.90	27.56	27.12	28.43	28.26
H27	27.84	27.75	27.67	26.19	26.30	26.15	27.20	28.15
H28	31.09	31.08	30.98	30.37	30.54	30.40	30.84	30.12
H28	31.47	31.56	31.53	31.41	31.15	30.88	30.81	30.75
H29	29.62	29.90	29.97	30.62	30.56	30.38	29.70	30.16
H30	28.63	28.63	28.58	28.89	28.54	28.53	28.51	28.23
H31	30.44	30.42	30.36	30.81	30.61	30.56	30.21	30.44
H32	31.11	30.97	30.93	31.41	31.19	31.26	30.84	31.25
H32	29.96	30.09	30.15	30.53	30.53	30.77	30.12	29.91
H33	30.65	30.52	30.48	30.71	30.59	30.52	30.66	30.82
H33	31.18	31.02	31.03	31.75	31.35	31.44	31.39	31.30
H35	30.67	30.65	30.66	30.14	30.43	30.36	30.72	30.70
H35	30.92	30.71	30.66	31.56	31.16	31.14	31.28	31.05
H36	30.90	30.83	30.79	29.52	29.82	29.76	30.04	30.00
H36	29.97	30.11	30.15	30.65	30.78	30.71	31.20	30.94
H37	30.76	30.82	30.78	31.06	30.70	30.76	31.12	30.80
H37	30.72	30.57	30.56	30.71	30.86	30.80	30.96	30.87
H38	28.26	28.36	28.33	28.36	28.45	28.41	28.27	28.38

Table S3. *Cont.*

H	1 (Gas)	1 (CHCl₃)	1 (CH₃OH)	2 (Gas)	2 (CHCl₃)	2 (CH₃OH)	CS I	CS II
H38	28.71	28.57	28.52	29.49	28.88	28.83	28.87	28.71
H39	31.22	31.24	31.25	31.01	31.02	30.95	30.99	31.11
H40	31.10	31.21	31.18	30.10	30.56	30.50	31.11	31.13
H41	27.52	27.28	27.11	27.71	27.44	27.15	27.00	26.86
H41	26.89	26.97	26.90	26.76	26.62	26.71	27.23	26.52
H42	31.41	31.34	31.30	31.35	31.54	31.18	31.18	31.17
H43	30.51	30.45	30.40	30.55	30.39	30.40	30.57	30.63
H44	30.92	30.88	30.87	30.70	30.80	30.78	31.01	30.80

Table S4. Computed ¹³C and ¹H chemical shifts for okadaic acid (**1**) and the studied diastereoisomer (**2**) on mPW1Pw91-6-31G + (d).

H	1 (Gas)	1 (CHCl₃)	1 (CH₃OH)	2 (Gas)	2 (CHCl₃)	2 (CH₃OH)	CS I	CS II
1	16.6	16.3	16.1	26.0	26.7	25.7	10.3	17.3
2	118.5	118.5	118.4	121.2	120.4	120.3	119.4	116.1
3	152.4	152.7	152.7	150.7	150.8	151.0	148.4	152.3
4	127.8	127.4	127.5	127.2	127.1	127.3	128.2	124.2
5	163.2	163.3	163.3	162.2	162.5	162.7	160.7	160.7
6	162.7	162.9	163.0	158.7	158.6	158.7	163.4	167.1
7	122.1	122.9	123.1	124.0	124.4	124.8	123.2	124.8
8	100.7	101.0	101.3	102.4	101.9	102.5	96.3	94.7
9	70.8	74.0	75.7	72.9	75.5	76.7	70.2	72.2
10	57.1	54.3	52.7	59.2	55.5	53.8	58.3	55.3
11	159.5	159.6	159.5	161.3	161.8	161.9	159.2	159.0
12	124.9	125.0	125.2	127.6	126.4	126.5	125.8	123.7
13	148.8	149.2	149.4	148.7	149.4	149.7	148.5	151.6
14	59.1	58.5	57.2	63.2	61.4	60.8	55.3	60.0
15	61.0	61.6	62.5	58.2	58.4	59.1	65.0	64.0
16	118.5	118.7	118.6	120.8	120.6	120.6	117.0	119.7
17	163.3	163.6	163.8	163.4	163.9	164.2	162.2	161.1
18	156.9	157.0	157.0	158.9	159.2	159.3	156.6	156.0
19	94.2	94.2	94.1	93.5	93.7	93.4	95.4	99.1
20	158.2	158.6	158.6	156.5	156.9	157.1	157.2	159.5
21	167.4	167.7	167.9	166.3	166.4	166.4	165.2	166.6
22	123.1	123.1	123.2	123.0	124.8	125.0	123.0	121.4
23	119.3	119.7	119.7	122.1	122.5	122.4	118.9	119.7
24	122.3	122.5	122.7	122.1	122.6	122.3	120.9	120.9
25	43.8	44.7	45.5	49.7	49.1	49.0	51.6	37.9
26	108.0	108.6	109.1	106.1	107.1	107.1	109.7	110.6
27	131.5	131.5	131.6	123.4	124.4	124.5	128.5	117.9
28	160.4	160.4	160.6	154.6	153.8	153.6	160.2	157.5
29	160.8	160.8	160.7	152.0	152.6	152.9	159.8	157.8
30	121.1	121.0	121.0	122.2	120.6	120.5	118.8	122.5
31	164.7	164.9	165.1	159.7	159.7	159.8	164.9	165.4

Table S4. Cont.

H	1 (Gas)	1 (CHCl ₃)	1 (CH ₃ OH)	2 (Gas)	2 (CHCl ₃)	2 (CH ₃ OH)	CS I	CS II
32	167.6	167.6	167.7	169.1	168.3	168.4	167.8	166.7
33	162.6	162.6	162.6	163.7	164.1	164.1	162.4	162.2
34	103.6	103.2	103.2	102.9	102.6	102.6	103.0	104.2
35	156.3	156.3	156.2	155.7	155.9	155.9	156.2	157.3
36	172.0	172.0	172.1	170.6	170.2	170.2	172.7	171.8
37	166.8	166.6	166.6	167.4	166.8	166.9	168.9	167.5
38	134.0	134.0	133.9	135.2	135.1	135.0	134.3	134.0
39	182.2	182.6	182.8	178.5	178.9	179.1	180.1	179.1
40	177.3	177.9	178.2	177.6	178.4	178.4	177.7	176.9
41	83.2	82.6	82.1	78.0	76.6	76.6	84.1	85.1
42	176.8	177.3	177.5	178.4	179.2	179.2	176.0	178.2
43	170.3	170.7	170.9	170.9	171.5	171.8	168.8	169.4
44	169.2	169.1	169.0	171.5	172.1	172.5	167.0	168.0
H3	30.71	30.55	30.47	30.56	30.40	30.39	30.22	31.10
H3	30.36	30.32	30.31	30.70	30.59	30.47	29.97	29.68
H4	27.81	27.72	27.77	28.28	27.75	27.76	28.42	27.40
H5	30.66	30.69	30.73	31.02	30.77	30.76	30.59	31.10
H5	30.97	30.73	30.61	30.39	30.32	30.30	30.83	29.78
H6	30.45	30.43	30.41	30.34	30.52	30.56	30.25	30.18
H6	29.95	29.97	30.02	30.23	29.96	30.02	30.00	30.02
H7	28.66	28.34	28.24	29.00	28.71	28.68	28.70	28.68
H9	26.30	26.36	26.42	26.32	26.16	26.14	26.28	26.51
H11	30.56	30.42	30.36	30.49	30.31	30.17	30.42	30.35
H11	30.47	30.29	30.17	30.63	30.27	30.27	30.68	30.70
H12	28.46	28.68	28.76	28.13	27.92	27.85	27.96	28.14
H13	30.29	30.07	29.95	30.28	29.58	29.58	30.26	29.95
H14	26.79	26.72	26.64	26.66	26.36	26.24	25.88	25.37
H15	26.80	26.69	26.69	26.08	25.76	25.78	26.43	26.41
H16	27.56	27.58	27.55	27.81	27.71	27.71	27.69	27.62
H17	30.64	30.49	30.41	30.24	30.08	30.07	30.42	30.41
H17	30.20	30.11	30.06	30.69	30.55	30.50	30.71	30.77
H18	30.08	30.12	30.15	30.24	30.12	30.13	30.15	30.06
H18	30.29	30.13	30.01	30.35	30.25	30.16	30.41	30.72
H20	30.30	30.22	30.11	30.38	30.32	30.25	30.79	30.63
H20	30.24	30.15	30.08	30.40	30.39	30.36	30.03	30.33
H21	30.34	30.24	30.14	29.93	30.06	30.05	30.38	30.70
H21	29.90	29.99	30.02	30.37	30.52	30.57	29.90	30.06
H22	28.54	28.49	28.35	27.54	27.71	27.63	28.34	28.31
H23	28.27	28.22	28.20	28.26	28.27	28.21	28.92	29.12
H24	27.63	27.61	27.54	27.87	27.84	27.72	27.51	27.10
H26	28.18	28.03	27.98	27.74	27.57	27.39	28.11	28.10
H27	27.79	27.72	27.64	26.28	26.37	26.28	27.32	28.22
H28	31.08	31.04	31.03	30.35	30.53	30.47	30.78	30.01

Table S4. Cont.

H	1 (Gas)	1 (CHCl ₃)	1 (CH ₃ OH)	2 (Gas)	2 (CHCl ₃)	2 (CH ₃ OH)	CS I	CS II
H28	31.45	31.54	31.56	31.40	31.23	31.14	30.81	30.69
H29	29.55	29.80	29.91	30.52	30.48	30.37	29.60	30.06
H30	28.57	28.58	28.56	28.77	28.47	28.48	28.48	28.20
H31	30.44	30.42	30.37	30.72	30.52	30.48	30.19	30.41
H32	31.06	30.92	30.86	31.37	31.11	31.09	30.77	31.17
H32	29.94	30.05	30.12	30.50	30.43	30.56	30.12	29.95
H33	30.62	30.50	30.45	30.70	30.64	30.57	30.68	30.72
H33	31.11	30.95	30.94	31.59	31.24	31.26	31.39	31.24
H35	30.63	30.62	30.62	30.19	30.48	30.45	30.65	30.65
H35	30.90	30.66	30.60	31.47	31.09	31.05	31.19	31.03
H36	30.85	30.77	30.73	29.53	29.87	29.88	29.97	30.06
H36	29.90	30.08	30.13	30.68	30.78	30.74	31.11	30.88
H37	30.73	30.79	30.75	30.96	30.59	30.60	31.05	30.80
H37	30.70	30.53	30.51	30.68	30.80	30.75	30.89	30.83
H38	28.23	28.35	28.33	28.43	28.49	28.46	28.22	28.43
H38	28.66	28.50	28.45	29.35	28.79	28.73	28.80	28.69
H39	31.18	31.20	31.22	31.00	31.03	31.01	30.95	31.03
H40	31.07	31.16	31.16	30.16	30.59	30.59	31.05	31.08
H41	27.33	27.09	26.99	27.50	27.29	27.12	26.84	26.76
H41	26.73	26.76	26.76	26.54	26.33	26.36	27.06	26.38
H42	31.34	31.26	31.23	31.35	31.56	31.49	31.13	31.08
H43	30.44	30.36	30.34	30.47	30.30	30.27	30.49	30.52
H44	30.86	30.82	30.78	30.67	30.73	30.67	31.01	30.75

S1. Correlation Graphs

B3LYP-6-31G + (d)

S1.1. Use of $CHCl_3$ as Solvent

1_{gas} (A); 2_{gas} (B); 1_{CHCl₃} (C); 2_{CHCl₃} (D); 1_{CH₃OH} (E); 2_{CH₃OH} (F); CS I (G) CS II (H).

S1.2. Use of CH_3OH as Solvent

1_{gas} (I); 2_{gas} (J); 1_{CH₃OH} (K); 2_{CH₃OH} (L); 1_{CHCl₃} (M); 2_{CHCl₃} (N); CS I (O); CS II (P).

Figure S9. Correlations graphs for calculated vs. experimental data.

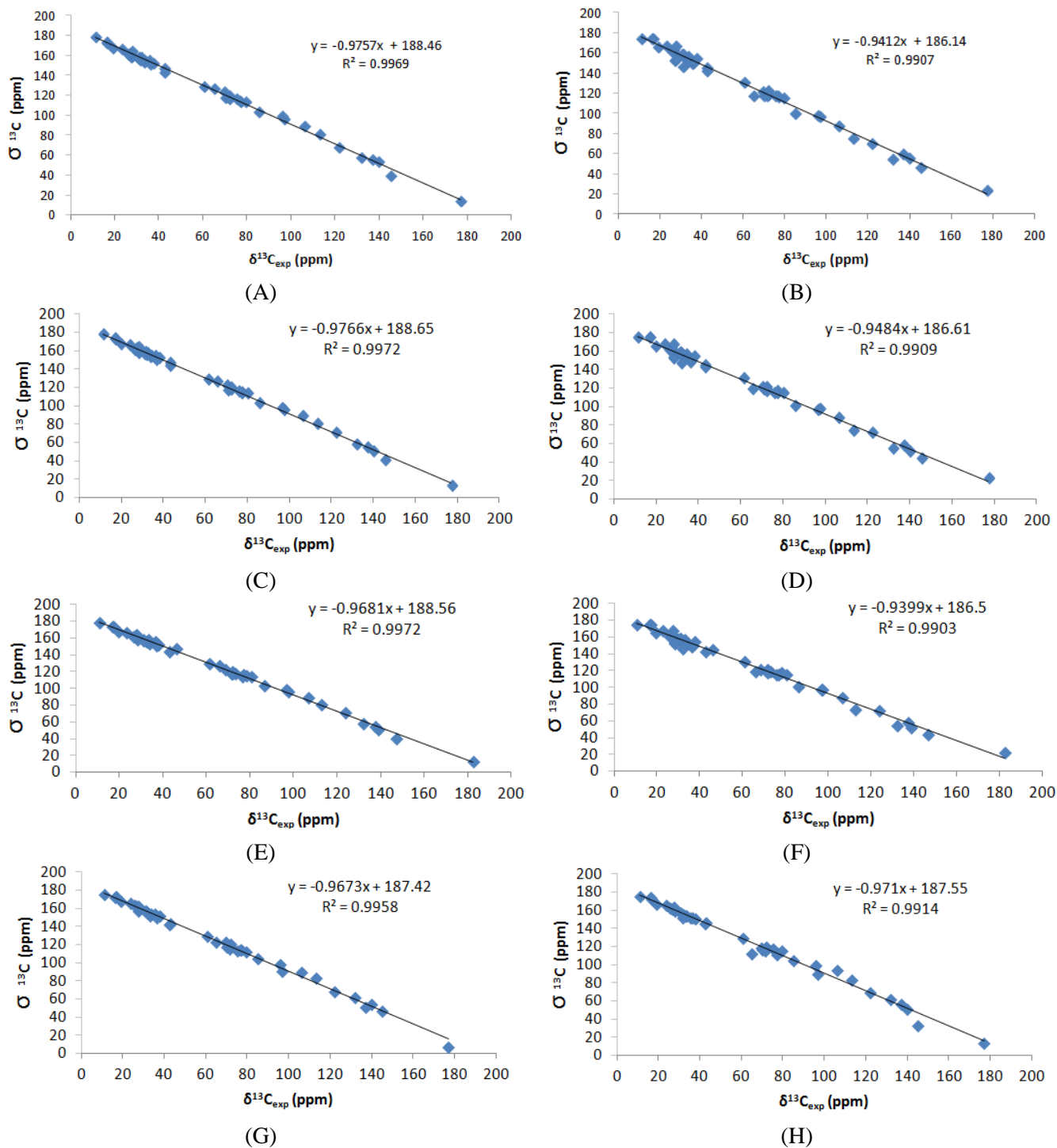


Figure S10. Correlations graphs for calculated vs. experimental data.

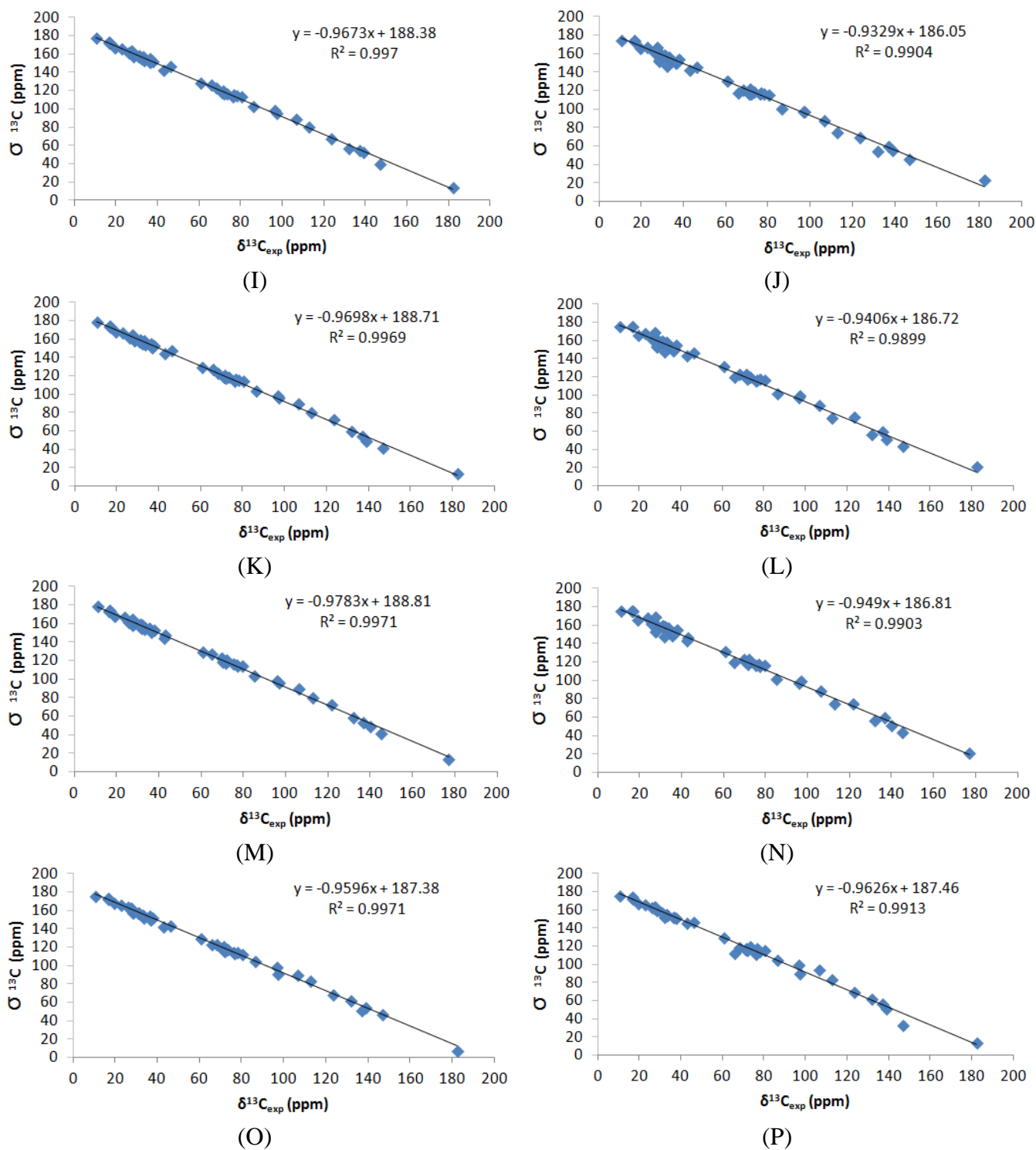


Figure S11. Correlations graphs for calculated vs experimental data.

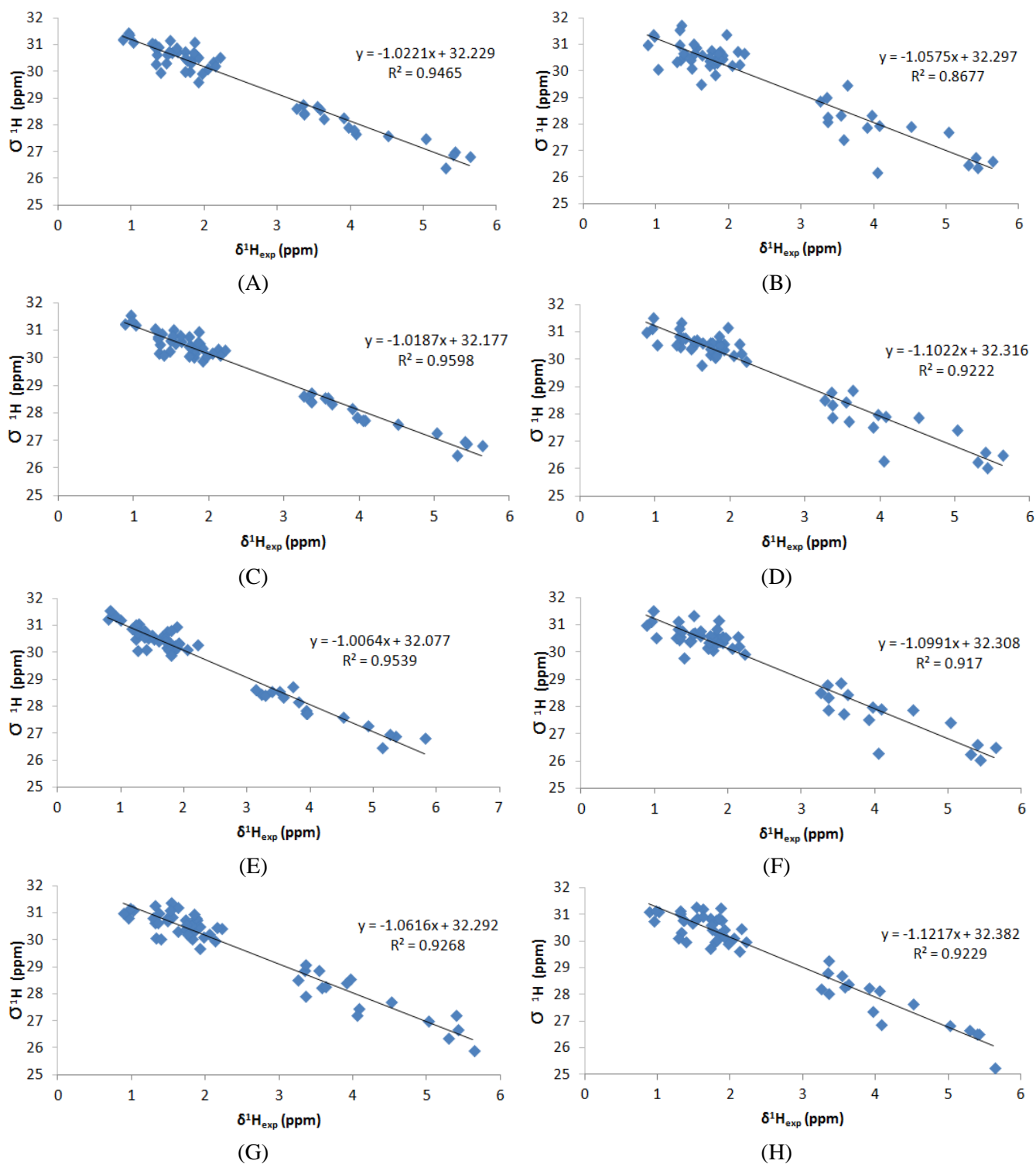
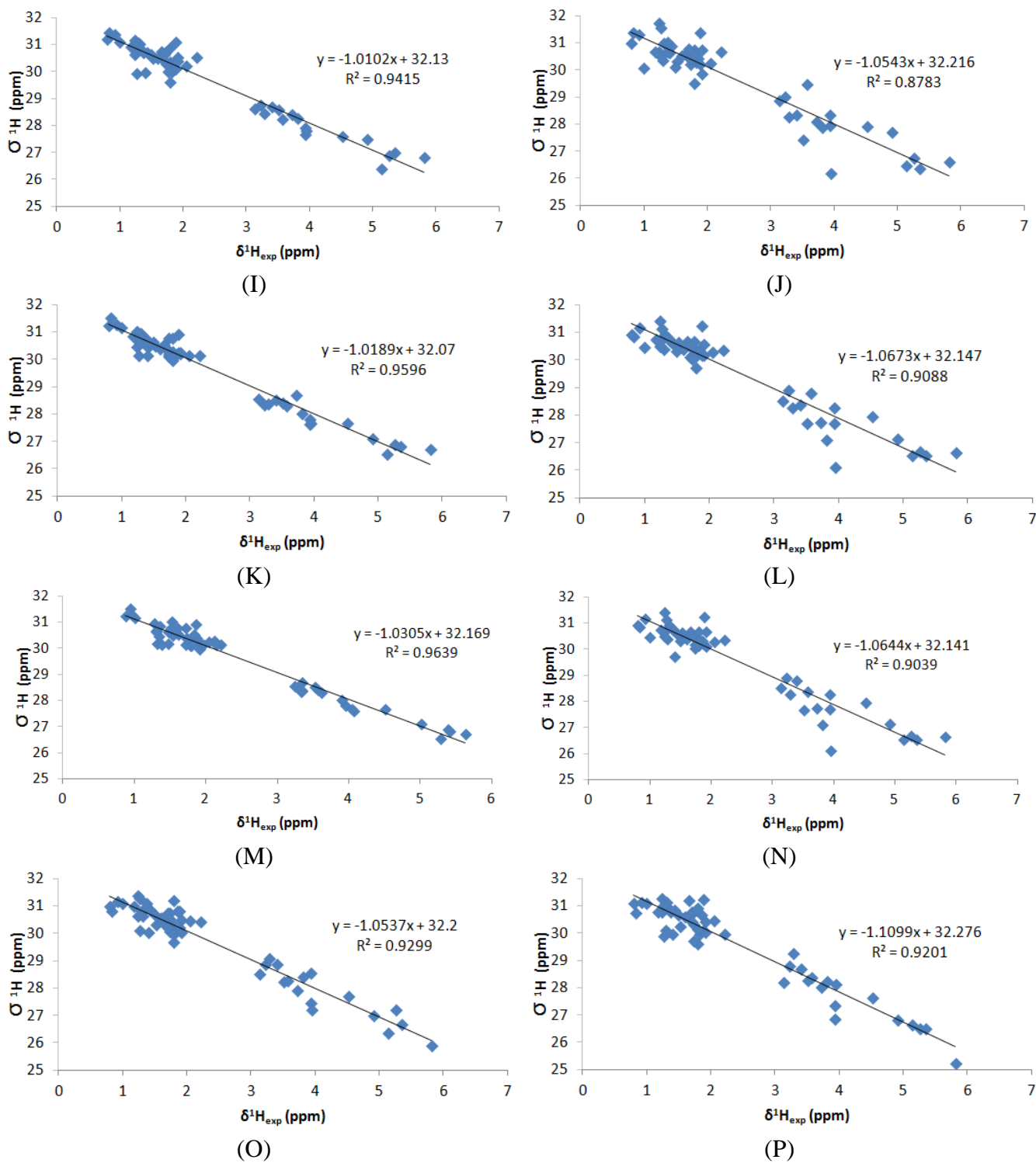


Figure S12. Correlations graphs for calculated vs experimental data.



S2. Correlation Graphs

mPW1Pw91-6-31G + (d)

S2.1. Use of $CHCl_3$ as Solvent

1_{gas} (A); 2_{gas} (B); 1_{CHCl₃} (C); 2_{CHCl₃} (D); 1_{CH₃OH} (E); 2_{CH₃OH} (F); CS I (G) CS II (H)

S2.2. Use of CH_3OH as Solvent

1_{gas} (I); 2_{gas} (J); 1_{CH₃OH} (K); 2_{CH₃OH} (L); 1_{CHCl₃} (M); 2_{CHCl₃} (N); CS I (O); CS II (P)

Figure S13. Correlations graphs for calculated vs. experimental data.

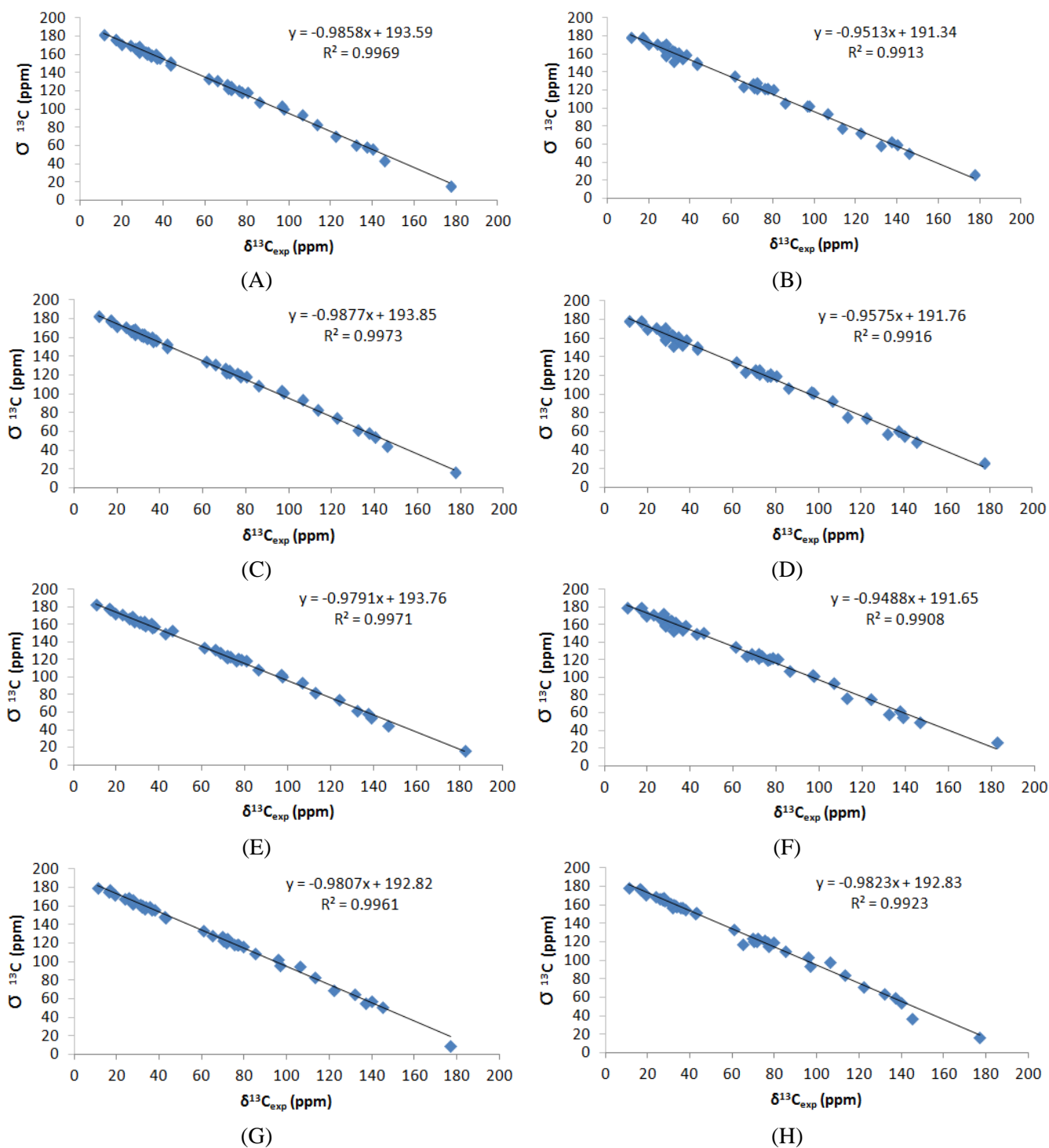


Figure S14. Correlations graphs for calculated vs. experimental data.

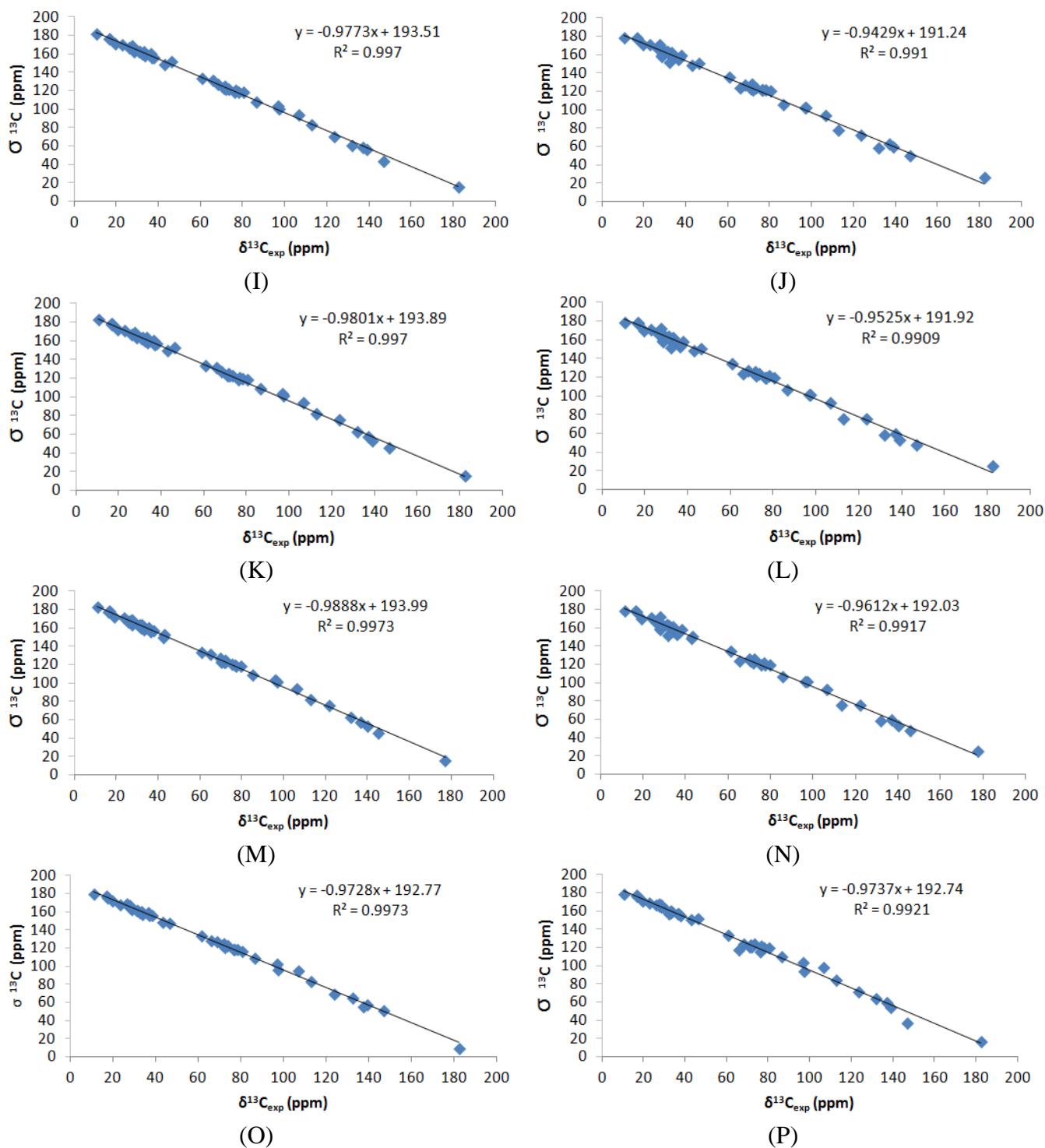


Figure S15. Correlations graphs for calculated vs experimental data.

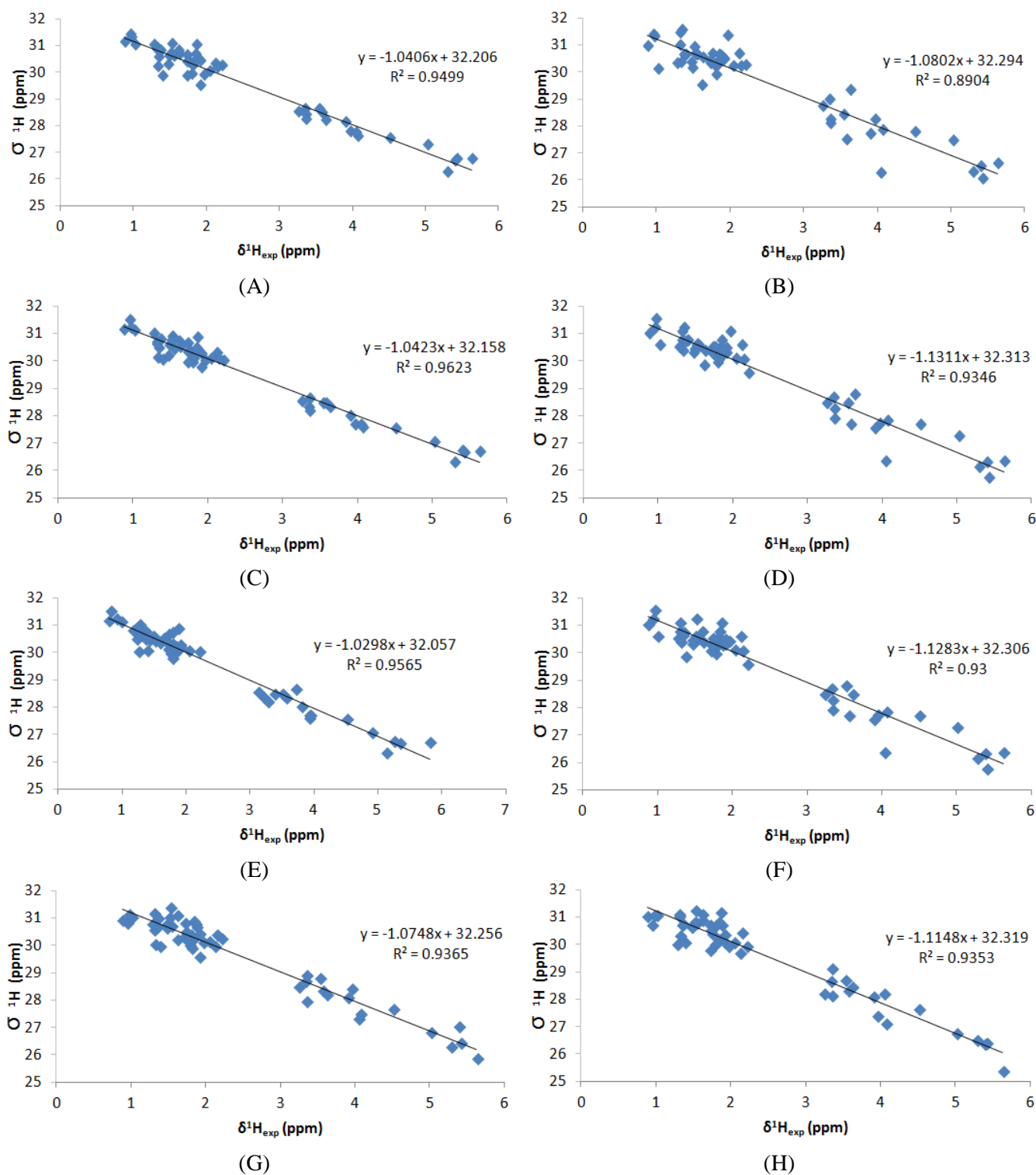
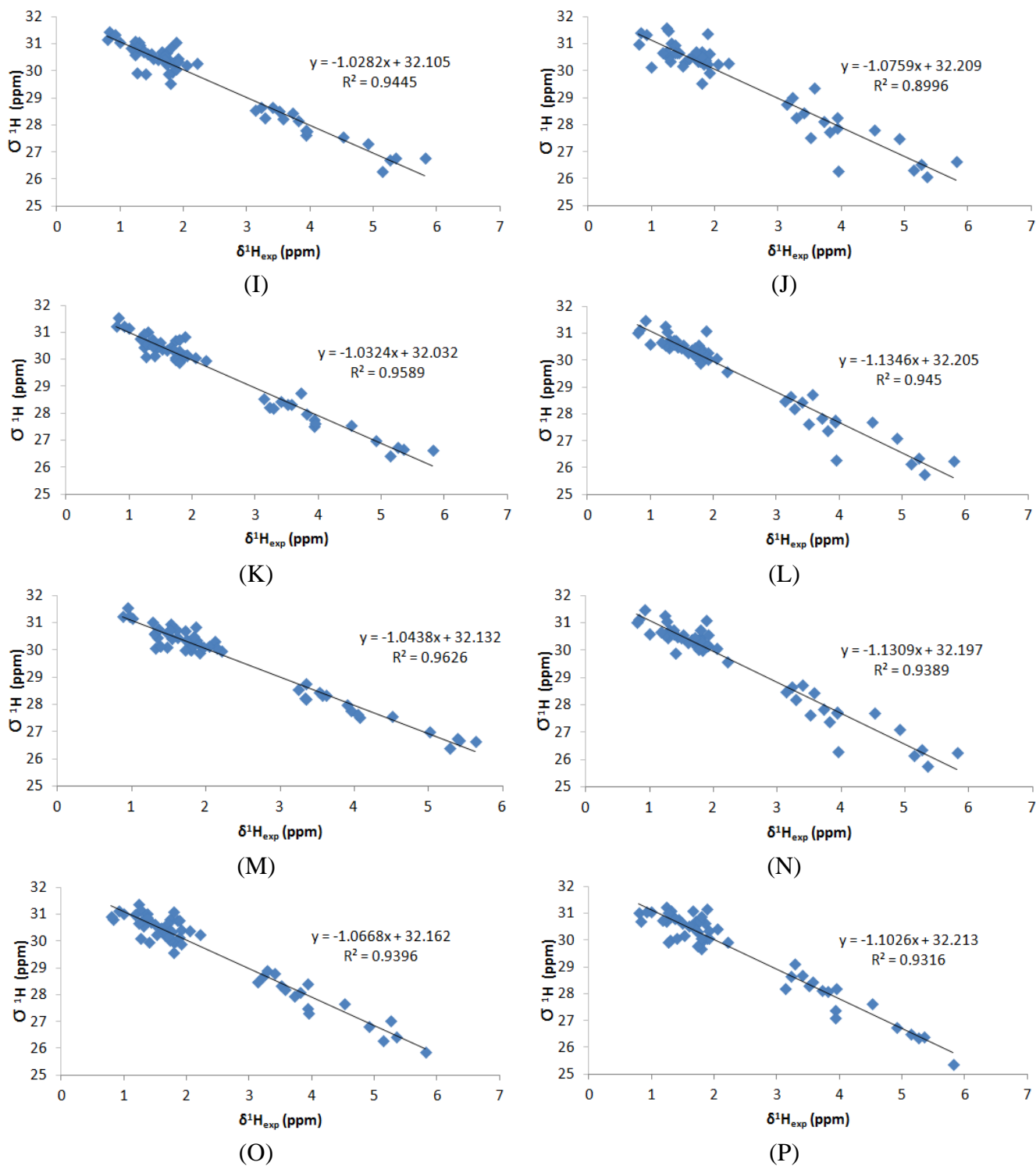
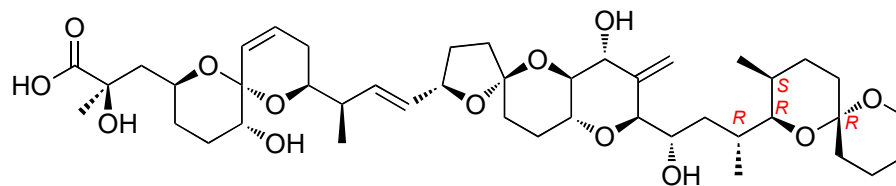


Figure S16. Correlations graphs for calculated vs. experimental data.



S3. Energies and Coordinates

Figure S17. Studied diastereoisomer of okadaic acid (**2**). Gas phase energy -2695.5434021131 hartrees.



Okadaic acid 29-32 diastereoisomer (**2**)

Table S5. Structural coordinates.

	Center		Coordinates		
	Number		X	Y	Z
1	C1		84.111168	50.706711	25.452652
2	C2		84.569450	50.336964	26.878521
3	C3		86.049271	50.719624	27.141647
4	C4		86.453064	52.212521	27.066313
5	C5		87.971275	52.351387	27.286291
6	C6		88.352135	53.823807	27.406681
7	C7		87.549423	54.434280	28.561356
8	C8		86.036255	54.280807	28.270906
9	C9		85.213867	54.795223	29.442688
10	C10		84.194481	55.656734	29.293772
11	C11		83.793610	56.137955	27.913450
12	C12		84.414833	55.262589	26.803734
13	C13		84.379234	55.931839	25.412613
14	C14		85.175659	55.102440	24.425243
15	C15		86.354111	55.461567	23.893171
16	C16		87.152122	54.571793	22.969793
17	C17		87.600609	55.236305	21.668802
18	C18		88.942505	54.571815	21.368023
19	C19		89.148048	53.632244	22.561241
20	C20		90.616982	53.522858	23.026472
21	C21		90.721100	52.493526	24.163731
22	C22		90.101562	51.175564	23.693445
23	C23		88.641785	51.435474	23.283344
24	C24		87.954483	50.139030	22.836945
25	C25		88.170837	49.048931	23.886366
26	C26		89.607170	48.915943	24.396290
27	C27		90.552406	48.173565	23.417315
28	C28		90.155930	46.700756	23.161081
29	C29		90.807404	46.029861	21.923105
30	C30		90.094727	44.687622	21.596380
31	O31		90.680389	43.635422	22.364664

Table S5. *Cont.*

Center		Coordinates		
Number		X	Y	Z
32	C32	90.005676	42.407364	22.344997
33	C33	89.922409	41.904999	20.887642
34	C34	89.249680	42.966602	20.004866
35	C35	90.806839	41.412422	23.213621
36	C36	92.331757	45.860352	22.109474
37	C37	87.176369	48.296246	24.397663
38	C38	82.950027	56.149242	24.892761
39	C39	83.407585	56.218822	30.461561
40	C40	84.356705	48.832565	27.134996
41	O41	83.815460	52.026081	25.329220
42	O42	84.003120	49.896599	24.536442
43	O43	83.749283	50.999065	27.820791
44	O44	85.745148	52.920490	28.091942
45	O45	87.890564	55.793686	28.706728
46	O46	85.785103	55.034733	27.118515
47	O47	88.378242	54.193047	23.570438
48	O48	88.681152	52.362568	22.198915
49	O49	90.161705	50.197285	24.726454
50	O50	86.572433	50.410881	22.657864
51	O51	91.808601	48.210762	24.059958
52	C52	90.007942	44.299297	20.098160
53	O53	88.699608	42.490490	22.850510
54	H54	86.333282	50.339264	28.123478
55	H55	86.668495	50.171185	26.431437
56	H56	86.200981	52.633137	26.092199
57	H57	88.269814	51.824951	28.193848
58	H58	88.517792	51.885452	26.466759
59	H59	89.421394	53.918850	27.595942
60	H60	88.150208	54.341377	26.467031
61	H61	87.783318	53.913967	29.491819
62	H62	83.899315	54.301678	26.762352
63	H63	84.864586	56.906067	25.489885
64	H64	86.575798	53.670700	22.746561
65	H65	86.872444	55.090221	20.870790
66	H66	87.742798	56.308842	21.804970
67	H67	88.954659	54.012646	20.431881
68	H68	89.736809	55.318512	21.344118
69	H69	91.229828	53.219292	22.176924
70	H70	90.965218	54.503040	23.353600
71	H71	91.763275	52.346546	24.446087
72	H72	90.201996	52.863209	25.048258
73	H73	90.669670	50.833321	22.828732
74	H74	88.084137	51.843391	24.128347

Table S5. *Cont.*

Center		Coordinates		
Number		X	Y	Z
75	H75	88.384071	49.802094	21.892485
76	H76	89.579605	48.347851	25.328142
77	H77	90.613678	48.695683	22.463161
78	H78	90.337334	46.099056	24.052914
79	H79	89.077415	46.675266	23.011967
80	H80	90.642036	46.695164	21.075048
81	H81	89.058197	44.787342	21.921312
82	H82	90.927528	41.681141	20.530481
83	H83	89.357536	40.972553	20.866545
84	H84	92.839638	46.823589	22.135321
85	H85	92.554741	45.347065	23.045341
86	H86	92.795830	45.284130	21.314009
87	H87	82.959930	56.591686	23.896093
88	H88	82.400185	55.209396	24.835022
89	H89	82.388596	56.824135	25.538750
90	H90	82.352356	55.960987	30.367887
91	H91	83.769310	55.825420	31.412176
92	H92	83.494972	57.305283	30.488779
93	H93	84.596390	48.567059	28.164793
94	H94	83.320381	48.542191	26.956467
95	H95	84.983955	48.223568	26.483643
96	H96	83.528610	52.162209	24.441505
97	H97	83.975571	51.920898	27.756470
98	H98	87.388588	56.241985	28.036694
99	H99	86.142975	49.626049	22.352432
100	H100	91.847290	49.044250	24.515341
101	H101	82.706703	56.129211	27.827446
102	H102	84.757889	54.142712	24.166992
103	H103	86.791862	56.417255	24.140842
104	H104	87.375031	47.558117	25.160955
105	H105	86.149849	48.397522	24.078188
106	H106	89.403000	45.053524	19.592585
107	C107	91.353195	44.241768	19.352644
108	H108	89.198418	42.622536	18.971785
109	H109	88.217789	43.105591	20.330845
110	H110	91.798187	45.232716	19.266016
111	H111	92.069412	43.594204	19.858271
112	H112	91.224106	43.864391	18.338161
113	C113	90.790962	41.871494	24.677481
114	H114	91.828842	41.353699	22.837666
115	C115	88.588509	42.945984	24.199028
116	H116	91.304405	42.829464	24.774235
117	C117	89.340828	42.001106	25.145294

Table S5. Cont.

Center		Coordinates		
Number		X	Y	Z
118	H118	91.329857	41.159924	25.303045
119	H119	88.973053	43.962822	24.286367
120	H120	87.533424	42.986008	24.469910
121	H121	88.858932	41.022606	25.150194
122	H122	89.301437	42.378227	26.167719
123	H123	90.361908	40.421181	23.118170
124	H124	85.510338	54.457653	30.424559
125	H125	84.115982	57.174664	27.811586

S4. Representative NMR Compatible Conformational Search (CS I)

Figure S18. Crystallographic structure of okadaic acid (blue) superimposed with the energetically representative structures obtained from conformational search. Structures of an NMR compatible search (CS I) are in greenish.

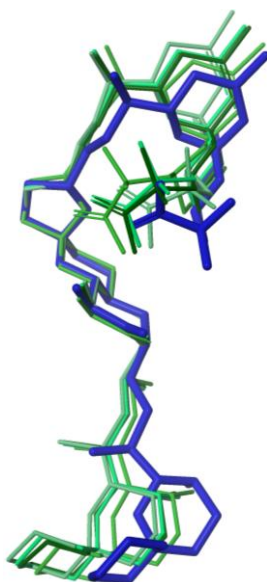


Table S6. CS I, Conformer 1. Gas phase energy and Boltzmann Populations
−2695.56653455841 hartrees, 58.61%.

Center		Coordinates		
Number		X	Y	Z
1	C1	85.938423	59.391159	20.347820
2	C2	86.392860	60.592625	21.191975
3	C3	87.774376	60.391079	21.869789
4	C4	88.951302	59.979923	20.953747
5	C5	89.218025	58.461964	20.917515
6	C6	90.453751	58.182812	20.060827
7	C7	91.644516	58.968315	20.629108
8	C8	91.288322	60.474541	20.686728
9	C9	92.408371	61.278221	21.330400
10	C10	92.879913	62.416512	20.792999
11	C11	92.270668	62.974224	19.518822
12	C12	90.923485	62.293095	19.192814
13	C13	90.438103	62.522362	17.745958
14	C14	89.198853	61.685757	17.483696
15	C15	89.166595	60.615349	16.674168
16	C16	87.952621	59.741291	16.455696
17	C17	87.635223	59.512947	14.983790
18	C18	86.835953	58.230499	15.057970
19	C19	87.548485	57.466137	16.178650
20	C20	88.614578	56.474808	15.654953
21	C21	89.231659	55.713634	16.839275
22	C22	88.106422	55.037701	17.621374
23	C23	87.094421	56.110638	18.057440
24	C24	85.944130	55.453075	18.817022
25	C25	86.515106	54.658474	19.986126
26	C26	87.665611	53.720581	19.612938
27	C27	87.195999	52.411205	18.933592
28	C28	86.266716	51.555794	19.821550
29	C29	85.761269	50.238968	19.177412
30	C30	85.045074	49.318207	20.202232
31	C31	85.880455	48.889973	21.437641
32	C32	85.029259	47.939415	22.292288
33	C33	84.542709	46.751320	21.453449
34	C34	83.784851	47.266834	20.214048
35	C35	83.424500	46.092525	19.277086
36	C36	82.577942	46.603386	18.104137
37	C37	81.332611	47.300915	18.652786
38	C38	81.762192	48.408169	19.624062
39	C39	87.248627	48.279404	21.075542
40	C40	84.825584	50.531094	17.984020
41	C41	86.107628	54.807781	21.261488

Table S6. *Cont.*

Center		Coordinates		
Number		X	Y	Z
42	C42	90.153862	64.000816	17.440260
43	C43	94.036507	63.196060	21.387562
44	C44	85.313530	60.939682	22.232323
45	O45	85.827042	58.247368	21.070648
46	O46	85.673103	59.492287	19.150784
47	O47	86.469421	61.704109	20.322102
48	O48	90.128426	60.619358	21.458162
49	O49	92.780785	58.759079	19.822449
50	O50	91.095932	60.888828	19.362513
51	O51	88.194199	58.432640	16.953829
52	O52	86.576347	56.766281	16.902910
53	O53	88.627876	54.373516	18.769985
54	O54	85.077492	56.489895	19.243832
55	O55	88.377335	51.676975	18.691595
56	O56	84.622169	48.140945	19.508362
57	O57	82.596870	47.871960	20.650900
58	H58	88.034248	61.336681	22.347324
59	H59	87.687187	59.677975	22.690208
60	H60	88.756210	60.345993	19.945763
61	H61	89.374237	58.083241	21.928223
62	H62	88.366226	57.922165	20.513056
63	H63	90.671425	57.114635	20.053175
64	H64	90.256805	58.471233	19.026707
65	H65	91.863335	58.622890	21.640902
66	H66	90.155647	62.647152	19.884382
67	H67	91.220833	62.180714	17.066999
68	H68	87.082794	60.155460	16.967625
69	H69	87.081711	60.338558	14.536098
70	H70	88.547485	59.355301	14.406977
71	H71	85.812523	58.447521	15.368058
72	H72	86.809341	57.663166	14.127451
73	H73	88.141617	55.781960	14.957982
74	H74	89.379814	57.024723	15.106452
75	H75	89.947792	54.973236	16.483629
76	H76	89.780357	56.401066	17.484564
77	H77	87.622574	54.318043	16.961044
78	H78	87.583344	56.834087	18.710278
79	H79	85.398216	54.775757	18.158175
80	H80	88.190903	53.454411	20.532137
81	H81	86.705376	52.628151	17.987442
82	H82	86.813232	51.341206	20.738115
83	H83	85.400314	52.143269	20.126476

Table S6. *Cont.*

Center		Coordinates		
Number		X	Y	Z
84	H84	86.620529	49.693756	18.785835
85	H85	84.161385	49.851463	20.556786
86	H86	86.071068	49.765858	22.057217
87	H87	85.594208	47.586575	23.155155
88	H88	84.167252	48.477154	22.689888
89	H89	85.381599	46.136238	21.127892
90	H90	83.879120	46.111652	22.036030
91	H91	84.343361	45.627857	18.917908
92	H92	82.875328	45.341679	19.846518
93	H93	83.160866	47.296932	17.496445
94	H94	82.294197	45.775848	17.454006
95	H95	80.739388	47.719772	17.839298
96	H96	80.696587	46.581852	19.170544
97	H97	82.283051	49.204353	19.091175
98	H98	80.885696	48.862370	20.086201
99	H99	87.756104	47.893665	21.959623
100	H100	87.149742	47.461975	20.361343
101	H101	87.907806	49.023327	20.627371
102	H102	84.462227	49.609028	17.529850
103	H103	83.954132	51.108387	18.293219
104	H104	85.332031	51.079674	17.191727
105	H105	89.785194	64.125122	16.421621
106	H106	89.402832	64.408554	18.117861
107	H107	91.053459	64.608833	17.534466
108	H108	93.720490	64.207504	21.644150
109	H109	94.415054	62.719273	22.292328
110	H110	94.855545	63.263065	20.671030
111	H111	85.559074	61.859779	22.763214
112	H112	84.336441	61.079521	21.767925
113	H113	85.212395	60.149151	22.977018
114	H114	85.528122	57.542999	20.488194
115	H115	86.072945	61.400196	19.511171
116	H116	92.672752	59.359585	19.094614
117	H117	84.934128	57.030109	18.469141
118	H118	89.039284	52.311874	18.443222
119	H119	92.126320	64.049614	19.625711
120	H120	88.305870	61.977985	18.018335
121	H121	90.062546	60.321247	16.147848
122	H122	86.563820	54.244980	22.062572
123	H123	85.310249	55.484222	21.531557
124	H124	92.841423	60.870438	22.231379
125	H125	92.983070	62.823223	18.707310

Table S7. CS I, Conformer 2. Gas phase energy and Boltzmann Populations
−2695.56555785124 hartrees, 20.83%.

Center		Coordinates		
Number		X	Y	Z
1	C1	86.176521	59.402092	20.591660
2	C2	86.654037	60.332878	21.718271
3	C3	88.057289	59.935188	22.238607
4	C4	89.169022	59.791603	21.169176
5	C5	89.716805	58.358089	21.046959
6	C6	90.876930	58.337139	20.048229
7	C7	91.942162	59.354698	20.487354
8	C8	91.294914	60.756691	20.611015
9	C9	92.288124	61.788704	21.121283
10	C10	92.406883	63.008549	20.568670
11	C11	91.515251	63.419041	19.409948
12	C12	90.342278	62.432777	19.210299
13	C13	89.672829	62.554909	17.824179
14	C14	88.737564	61.383816	17.581375
15	C15	88.934509	60.448284	16.638229
16	C16	88.046036	59.244446	16.419600
17	C17	87.475525	59.165829	15.003479
18	C18	87.540100	57.685749	14.646619
19	C19	88.127106	57.031250	15.899818
20	C20	89.126129	55.898071	15.576921
21	C21	89.612053	55.254974	16.883104
22	C22	88.385994	54.767204	17.647429
23	C23	87.455498	55.961273	17.912962
24	C24	86.198982	55.475433	18.639511
25	C25	86.586906	54.684200	19.886814
26	C26	87.688515	53.643913	19.673159
27	C27	87.176895	52.332344	19.030041
28	C28	86.133667	51.581089	19.882542
29	C29	85.544266	50.317333	19.206173
30	C30	84.808853	49.382771	20.202698
31	C31	85.642288	48.875317	21.409264
32	C32	84.773598	47.906883	22.224667
33	C33	84.252586	46.772915	21.334391
34	C34	83.497543	47.364498	20.127445
35	C35	83.106148	46.247078	19.136433
36	C36	82.266426	46.834286	17.994564
37	C37	81.041130	47.530388	18.584084
38	C38	81.499741	48.577187	19.606064
39	C39	86.992447	48.250843	21.007404
40	C40	84.596184	50.707718	18.051495
41	C41	86.055573	54.901630	21.104803

Table S7. Cont.

Center		Coordinates		
Number		X	Y	Z
42	C42	88.919151	63.882767	17.650194
43	C43	93.424904	64.032661	21.031172
44	C44	85.624855	60.376694	22.860867
45	O45	86.012253	58.125778	21.015785
46	O46	86.008438	59.791103	19.436468
47	O47	86.707344	61.642368	21.194597
48	O48	90.240913	60.665222	21.527151
49	O49	92.996574	59.374432	19.553127
50	O50	90.853706	61.107487	19.328154
51	O51	88.799988	58.051937	16.555159
52	O52	87.063316	56.529564	16.664160
53	O53	88.764809	54.167431	18.881681
54	O54	85.421043	56.621155	18.947660
55	O55	88.320290	51.512463	18.910337
56	O56	84.347633	48.252262	19.458263
57	O57	82.327080	47.973438	20.600729
58	H58	88.367867	60.673332	22.977434
59	H59	87.973129	59.004276	22.796984
60	H60	88.785110	60.107941	20.200432
61	H61	90.061684	58.004940	22.018551
62	H62	88.931564	57.674988	20.723589
63	H63	91.307632	57.337711	19.994013
64	H64	90.507614	58.571362	19.048386
65	H65	92.343018	59.069454	21.460808
66	H66	89.588829	62.591187	19.984776
67	H67	90.455025	62.508148	17.064795
68	H68	87.234390	59.227993	17.147907
69	H69	86.458344	59.558147	14.963836
70	H70	88.080139	59.738373	14.298585
71	H71	86.569183	57.251461	14.401868
72	H72	88.212814	57.534073	13.800322
73	H73	88.631050	55.161541	14.943235
74	H74	89.963936	56.308846	15.013496
75	H75	90.285439	54.425060	16.670189
76	H76	90.172195	55.977501	17.478603
77	H77	87.878372	54.038265	17.016949
78	H78	87.969101	56.705944	18.524910
79	H79	85.624908	54.819405	17.983110
80	H80	88.112350	53.399082	20.648933
81	H81	86.767029	52.524132	18.041546
82	H82	86.614838	51.327477	20.824850
83	H83	85.311028	52.245743	20.145645

Table S7. *Cont.*

Center		Coordinates		
Number		X	Y	Z
84	H84	86.364563	49.746590	18.770493
85	H85	83.945229	49.926666	20.588652
86	H86	85.858994	49.714855	22.068953
87	H87	85.335442	47.499466	23.064981
88	H88	83.928452	48.446484	22.654202
89	H89	85.073822	46.155514	20.972328
90	H90	83.579849	46.120838	21.891195
91	H91	84.012039	45.781460	18.749327
92	H92	82.543915	45.481819	19.671486
93	H93	82.862305	47.542709	17.418972
94	H94	81.960632	46.048729	17.305140
95	H95	80.453987	48.001186	17.794436
96	H96	80.392502	46.801487	19.069780
97	H97	82.033035	49.388031	19.110216
98	H98	80.635628	49.024185	20.096310
99	H99	87.497498	47.811222	21.866899
100	H100	86.868813	47.472023	20.255796
101	H101	87.665634	48.999523	20.589428
102	H102	84.192444	49.825207	17.555367
103	H103	83.750778	51.292919	18.412580
104	H104	85.101425	51.286404	17.280781
105	H105	88.447304	63.937717	16.668718
106	H106	88.137360	63.996819	18.402878
107	H107	89.590225	64.737846	17.736046
108	H108	92.922508	64.939529	21.370613
109	H109	94.029770	63.650593	21.854925
110	H110	94.094398	64.296288	20.211250
111	H111	85.909378	61.103672	23.621048
112	H112	84.637093	60.654774	22.494133
113	H113	85.532310	59.409348	23.354132
114	H114	85.748177	57.560219	20.283035
115	H115	86.641968	61.524078	20.235332
116	H116	92.680672	59.919842	18.842766
117	H117	85.315926	57.085308	18.121000
118	H118	89.040977	52.091984	18.693117
119	H119	91.130043	64.423965	19.585329
120	H120	87.879662	61.310665	18.234602
121	H121	89.793289	60.522667	15.984978
122	H122	86.378128	54.333652	21.964808
123	H123	85.281395	55.636238	21.268661
124	H124	92.924583	61.486752	21.939465
125	H125	92.133583	63.463707	18.512917

Table S8. CS I, Conformer 3. Gas phase energy and Boltzmann Populations
−2695.56509557079 hartrees, 12.77%.

Center		Coordinates		
Number		X	Y	Z
1	C1	86.193192	59.313828	20.594460
2	C2	86.677666	60.290848	21.679338
3	C3	88.115227	59.989704	22.178545
4	C4	89.206650	59.852951	21.089464
5	C5	89.725784	58.411724	20.920134
6	C6	90.873489	58.393982	19.907120
7	C7	91.964630	59.379581	20.357172
8	C8	91.344696	60.788845	20.522987
9	C9	92.365280	61.796055	21.030281
10	C10	92.503586	63.017311	20.484138
11	C11	91.603531	63.457951	19.341259
12	C12	90.399666	62.506039	19.169872
13	C13	89.674751	62.641331	17.812672
14	C14	88.717758	61.476269	17.637423
15	C15	88.862137	60.507092	16.719923
16	C16	87.981369	59.282410	16.630825
17	C17	87.232109	59.147091	15.299958
18	C18	87.653061	57.784580	14.773096
19	C19	88.187294	57.090630	16.021074
20	C20	89.241280	56.005585	15.705320
21	C21	89.681610	55.319931	17.006390
22	C22	88.437798	54.772034	17.701015
23	C23	87.469330	55.937302	17.963573
24	C24	86.205673	55.416782	18.651148
25	C25	86.582031	54.612167	19.892883
26	C26	87.702316	53.591091	19.684086
27	C27	87.223160	52.281387	19.011099
28	C28	86.161659	51.518600	19.832872
29	C29	85.646126	50.203579	19.192905
30	C30	84.779060	49.370075	20.174946
31	C31	85.461098	48.953217	21.504799
32	C32	84.475082	48.089592	22.305033
33	C33	84.005791	46.893032	21.468365
34	C34	83.406403	47.392445	20.138876
35	C35	83.073326	46.198292	19.216986
36	C36	82.378960	46.700756	17.944672
37	C37	81.127937	47.488407	18.335697
38	C38	81.522415	48.613503	19.301355
39	C39	86.820442	48.253738	21.308050
40	C40	84.852257	50.492138	17.900043
41	C41	86.028358	54.807983	21.105421
42	C42	88.930237	63.976742	17.671322

Table S8. Cont.

Center		Coordinates		
Number		X	Y	Z
43	C43	93.553894	64.012131	20.938194
44	C44	85.678795	60.307644	22.849529
45	O45	86.242950	58.019039	20.995081
46	O46	85.773232	59.696842	19.503740
47	O47	86.650665	61.589241	21.120775
48	O48	90.304848	60.693413	21.455662
49	O49	93.004105	59.403873	19.406134
50	O50	90.888977	61.170666	19.255840
51	O51	88.781204	58.112309	16.743433
52	O52	87.106377	56.523113	16.712812
53	O53	88.789948	54.145939	18.930407
54	O54	85.407318	56.544857	18.971544
55	O55	88.376183	51.471939	18.918198
56	O56	84.359276	48.187428	19.488373
57	O57	82.218155	48.079937	20.428225
58	H58	88.402924	60.789478	22.862091
59	H59	88.103027	59.090233	22.795233
60	H60	88.807198	60.204964	20.139854
61	H61	90.075668	58.024513	21.877815
62	H62	88.925591	57.751034	20.587532
63	H63	91.283295	57.387375	19.823704
64	H64	90.495598	58.660404	18.918444
65	H65	92.374367	59.063911	21.318073
66	H66	89.679108	62.673779	19.973572
67	H67	90.419823	62.579105	17.018166
68	H68	87.263077	59.279617	17.449762
69	H69	86.156418	59.175606	15.476455
70	H70	87.473831	59.940945	14.592482
71	H71	86.848068	57.213768	14.309361
72	H72	88.466713	57.900425	14.056028
73	H73	88.804909	55.282040	15.015588
74	H74	90.093071	56.467068	15.204517
75	H75	90.385803	54.516254	16.792219
76	H76	90.196617	56.031452	17.653723
77	H77	87.973213	54.046974	17.033031
78	H78	87.948280	56.678993	18.606503
79	H79	85.654747	54.765083	17.970818
80	H80	88.108101	53.336361	20.665026
81	H81	86.840126	52.483086	18.013355
82	H82	86.600822	51.315826	20.807997
83	H83	85.305199	52.165379	20.024647
84	H84	86.506432	49.595215	18.912373

Table S8. *Cont.*

Center		Coordinates		
Number		X	Y	Z
85	H85	83.897156	49.965778	20.416489
86	H86	85.640060	49.844440	22.105709
87	H87	84.929863	47.745853	23.234119
88	H88	83.610710	48.690575	22.591366
89	H89	84.835518	46.219372	21.254414
90	H90	83.251312	46.317112	22.005022
91	H91	83.994728	45.668983	18.971909
92	H92	82.427406	45.504574	19.756559
93	H93	83.058846	47.333782	17.372761
94	H94	82.113663	45.861282	17.302074
95	H95	80.643990	47.901566	17.450148
96	H96	80.402802	46.828720	18.813841
97	H97	82.139137	49.355644	18.793394
98	H98	80.632187	49.134644	19.653528
99	H99	87.214211	47.881344	22.253670
100	H100	86.745377	47.411465	20.620285
101	H101	87.563217	48.939861	20.900248
102	H102	84.482498	49.571644	17.447823
103	H103	83.989647	51.129097	18.096115
104	H104	85.466133	50.976185	17.142420
105	H105	88.415627	64.037910	16.711987
106	H106	88.184586	64.099838	18.457743
107	H107	89.615944	64.822105	17.727459
108	H108	93.080948	64.930687	21.286551
109	H109	94.156761	63.610783	21.753481
110	H110	94.221466	64.260689	20.112770
111	H111	85.943588	61.069992	23.582674
112	H112	84.663391	60.516777	22.510208
113	H113	85.659714	59.347927	23.367615
114	H114	85.908279	57.451527	20.293346
115	H115	86.079636	61.520462	20.362936
116	H116	92.685448	59.972836	18.715590
117	H117	85.273827	57.009819	18.150080
118	H118	89.097969	52.057667	18.720984
119	H119	91.250053	64.473122	19.523605
120	H120	87.897003	61.427494	18.338907
121	H121	89.674149	60.558071	16.009808
122	H122	86.345154	54.232613	21.962898
123	H123	85.244370	55.532784	21.267246
124	H124	93.006935	61.472569	21.835981
125	H125	92.203033	63.484474	18.430937

Table S9. CS I, Conformer 4. Gas phase energy and Boltzmann Populations
−2695.56407862476 hartrees, 4.35%.

Center		Coordinates		
Number		X	Y	Z
1	C1	85.736389	58.924442	20.079184
2	C2	86.005821	60.136490	20.985167
3	C3	87.334167	60.036224	21.781301
4	C4	88.619820	59.755844	20.967699
5	C5	89.024467	58.268673	20.925571
6	C6	90.353790	58.122803	20.183258
7	C7	91.411751	58.994877	20.874958
8	C8	90.917122	60.461575	20.925570
9	C9	91.897285	61.344852	21.683113
10	C10	92.310181	62.533699	21.210798
11	C11	91.769890	63.067242	19.895790
12	C12	90.524582	62.277924	19.436039
13	C13	90.152199	62.499485	17.954903
14	C14	89.020714	61.564919	17.566380
15	C15	89.155937	60.516624	16.738710
16	C16	88.048195	59.547192	16.393957
17	C17	87.882431	59.335197	14.895021
18	C18	87.194008	57.988220	14.869953
19	C19	87.868416	57.255024	16.034281
20	C20	89.056175	56.369938	15.587824
21	C21	89.629509	55.629337	16.806650
22	C22	88.501556	54.841164	17.470793
23	C23	87.368332	55.814472	17.836929
24	C24	86.215721	55.043110	18.476580
25	C25	86.747757	54.266235	19.675377
26	C26	88.001007	53.436417	19.386778
27	C27	87.705299	52.112339	18.641260
28	C28	86.763000	51.167702	19.416246
29	C29	86.443573	49.823467	18.716503
30	C30	85.694611	48.878029	19.694056
31	C31	85.963982	47.360645	19.530203
32	C32	85.149452	46.624458	20.604340
33	C33	83.665894	47.009274	20.507793
34	C34	83.509201	48.540283	20.630518
35	C35	82.039474	48.951706	20.391853
36	C36	81.877953	50.459908	20.621771
37	C37	82.347183	50.803783	22.036005
38	C38	83.785995	50.305588	22.225376
39	C39	85.699089	46.791645	18.124971
40	C40	85.669151	50.059242	17.398684
41	C41	86.220085	54.346458	20.912300
42	C42	89.765930	63.954628	17.649118

Table S9. Cont.

Center		Coordinates		
Number		X	Y	Z
43	C43	93.333328	63.397400	21.922234
44	C44	84.811981	60.359135	21.930134
45	O45	85.665169	57.755207	20.765469
46	O46	85.567871	59.036186	18.865671
47	O47	86.060005	61.274593	20.148643
48	O48	89.684425	60.482895	21.589760
49	O49	92.632225	58.908085	20.175961
50	O50	90.807678	60.890701	19.596647
51	O51	88.359962	58.250031	16.883226
52	O52	86.899559	56.457558	16.654572
53	O53	88.975060	54.189289	18.647055
54	O54	85.230438	55.992565	18.845387
55	O55	88.958755	51.477203	18.502117
56	O56	84.294243	49.158783	19.647867
57	O57	83.870003	48.910404	21.934561
58	H58	87.465057	60.986580	22.300371
59	H59	87.238472	59.294750	22.575205
60	H60	88.482742	60.131229	19.953615
61	H61	89.120796	57.876297	21.938557
62	H62	88.265144	57.668266	20.431864
63	H63	90.666870	57.078606	20.176346
64	H64	90.227074	58.420078	19.140676
65	H65	91.566528	58.643852	21.896608
66	H66	89.668915	62.544960	20.060314
67	H67	91.019897	62.244255	17.344719
68	H68	87.103569	59.869717	16.834263
69	H69	87.300858	60.123558	14.416769
70	H70	88.852127	59.271847	14.399577
71	H71	86.132248	58.109066	15.090666
72	H72	87.298897	57.447514	13.929172
73	H73	88.706223	55.660206	14.837280
74	H74	89.817108	56.996201	15.121320
75	H75	90.434189	54.960899	16.501341
76	H76	90.059341	56.341370	17.512611
77	H77	88.139671	54.103531	16.754608
78	H78	87.735428	56.557037	18.545904
79	H79	85.788795	54.341396	17.758055
80	H80	88.463890	53.188435	20.343821
81	H81	87.290276	52.313423	17.655914
82	H82	87.212563	50.975227	20.391260
83	H83	85.819885	51.675034	19.622158
84	H84	87.395615	49.348709	18.475216

Table S9. Cont.

Center		Coordinates		
Number		X	Y	Z
85	H85	86.042763	49.120384	20.699209
86	H86	87.019455	47.185390	19.744225
87	H87	85.267944	45.545261	20.507193
88	H88	85.526039	46.884098	21.594828
89	H89	83.239861	46.682751	19.559284
90	H90	83.091698	46.530064	21.301237
91	H91	81.754570	48.682533	19.374254
92	H92	81.399780	48.389942	21.073633
93	H93	82.462807	51.014820	19.886648
94	H94	80.837486	50.754189	20.484751
95	H95	82.293549	51.879677	22.205463
96	H96	81.694107	50.334435	22.772783
97	H97	84.473129	50.865700	21.590164
98	H98	84.107094	50.469376	23.254000
99	H99	85.806732	45.707008	18.113888
100	H100	84.695053	47.029034	17.773903
101	H101	86.411697	47.186192	17.401035
102	H102	85.332657	49.133675	16.939611
103	H103	84.780350	50.667698	17.568239
104	H104	86.284744	50.565590	16.656610
105	H105	89.480225	64.071342	16.603292
106	H106	88.923988	64.278557	18.262041
107	H107	90.595764	64.636261	17.835073
108	H108	92.905251	64.370064	22.165987
109	H109	93.670654	62.933327	22.849646
110	H110	94.204018	63.554806	21.285141
111	H111	84.926842	61.281586	22.499882
112	H112	83.871338	60.426994	21.381910
113	H113	84.715820	59.541977	22.646204
114	H114	85.481087	57.044582	20.144176
115	H115	85.762314	60.961330	19.299889
116	H116	92.538086	59.514759	19.451338
117	H117	85.107529	56.538227	18.071051
118	H118	89.588516	52.167210	18.328146
119	H119	91.519775	64.122589	20.007360
120	H120	88.061066	61.764931	18.022152
121	H121	90.117928	60.314552	16.291544
122	H122	86.650581	53.800629	21.738916
123	H123	85.348114	54.947380	21.123960
124	H124	92.282776	60.954334	22.612898
125	H125	92.563004	63.000477	19.150545

Table S10. CS I, Conformer 5. Gas phase energy and Boltzmann Populations
−2695.56290872663 hartrees, 1.26%.

Center		Coordinates		
Number		X	Y	Z
1	C1	86.125305	59.076077	20.963697
2	C2	86.633011	60.396461	21.564951
3	C3	88.127510	60.357292	21.981575
4	C4	89.142906	59.901501	20.907084
5	C5	89.515221	58.407688	20.988312
6	C6	90.588905	58.093571	19.945488
7	C7	91.799675	59.007751	20.182634
8	C8	91.344475	60.487606	20.140989
9	C9	92.498444	61.425209	20.463409
10	C10	92.772217	62.512985	19.722698
11	C11	91.895912	62.874905	18.536579
12	C12	90.568863	62.085117	18.554083
13	C13	89.807518	62.107216	17.211895
14	C14	88.610672	61.176487	17.287382
15	C15	88.512848	60.015068	16.621279
16	C16	87.351898	59.053921	16.738791
17	C17	86.785553	58.629749	15.390203
18	C18	86.116386	57.323524	15.757735
19	C19	87.081650	56.743206	16.796709
20	C20	88.104828	55.754269	16.189537
21	C21	88.988190	55.179977	17.308779
22	C22	88.083290	54.545784	18.364008
23	C23	87.090851	55.607643	18.866297
24	C24	86.154976	54.986252	19.900324
25	C25	86.990257	54.369583	21.017431
26	C26	88.121368	53.457752	20.534588
27	C27	87.637283	52.053501	20.097580
28	C28	87.014175	51.225845	21.248558
29	C29	86.245598	49.935913	20.853706
30	C30	85.068100	50.172005	19.873930
31	C31	84.027733	51.231121	20.317028
32	C32	82.943390	51.309124	19.232655
33	C33	82.323868	49.924797	18.994621
34	C34	83.431488	48.904827	18.656717
35	C35	82.845497	47.477165	18.587225
36	C36	83.932426	46.490021	18.142735
37	C37	84.497734	46.942257	16.795809
38	C38	84.998741	48.387039	16.919781
39	C39	83.429848	50.966461	21.713821
40	C40	87.188591	48.832829	20.338335
41	C41	86.815529	54.651608	22.323086
42	C42	89.356529	63.518623	16.806204

Table S10. Cont.

Center		Coordinates		
Number		X	Y	Z
43	C43	93.954727	63.422695	19.992884
44	C44	85.741066	60.809959	22.748684
45	O45	86.238441	58.026585	21.817499
46	O46	85.636810	59.012424	19.836365
47	O47	86.460701	61.393799	20.578241
48	O48	90.339859	60.662128	21.101030
49	O49	92.779541	58.763584	19.199877
50	O50	90.878563	60.724186	18.841312
51	O51	87.783882	57.831562	17.320372
52	O52	86.318130	56.086269	17.768702
53	O53	88.857994	54.058651	19.457132
54	O54	85.306511	56.018822	20.370743
55	O55	88.804855	51.403801	19.644478
56	O56	84.393234	48.927925	19.677135
57	O57	83.954453	49.235916	17.397572
58	H58	88.396812	61.367764	22.291704
59	H59	88.249519	59.747753	22.877552
60	H60	88.736916	60.129040	19.921444
61	H61	89.884735	58.165813	21.985477
62	H62	88.647766	57.775955	20.818085
63	H63	90.883713	57.046299	20.014265
64	H64	90.182152	58.240818	18.943356
65	H65	92.228333	58.802395	21.164986
66	H66	89.917213	62.478531	19.337509
67	H67	90.475372	61.729252	16.436329
68	H68	86.562492	59.477852	17.361189
69	H69	86.095901	59.362228	14.970302
70	H70	87.584373	58.453674	14.668621
71	H71	85.154320	57.519566	16.233837
72	H72	85.962196	56.645824	14.917856
73	H73	87.565224	54.955925	15.678640
74	H74	88.709976	56.273071	15.445549
75	H75	89.680504	54.441380	16.905386
76	H76	89.592773	55.970749	17.755159
77	H77	87.542130	53.724304	17.894243
78	H78	87.635178	56.431427	19.328619
79	H79	85.549065	54.208645	19.433205
80	H80	88.826546	53.330395	21.358124
81	H81	86.931221	52.140720	19.274914
82	H82	87.790924	50.976299	21.972563
83	H83	86.322754	51.859234	21.801645
84	H84	85.819260	49.542385	21.776745

Table S10. Cont.

Center		Coordinates		
Number		X	Y	Z
85	H85	85.491333	50.479759	18.917425
86	H86	84.511726	52.206650	20.353657
87	H87	82.170631	52.026005	19.510662
88	H88	83.379639	51.674149	18.301653
89	H89	81.783676	49.584076	19.877810
90	H90	81.607986	49.957088	18.172749
91	H91	82.452454	47.204594	19.567253
92	H92	82.012161	47.470806	17.883585
93	H93	84.727257	46.447868	18.888933
94	H94	83.520340	45.484100	18.063162
95	H95	85.309906	46.285542	16.482332
96	H96	83.727539	46.882950	16.025785
97	H97	85.861031	48.437397	17.585505
98	H98	85.331764	48.753120	15.948592
99	H99	82.622955	51.665169	21.935280
100	H100	83.029633	49.956074	21.798170
101	H101	84.176308	51.083561	22.498510
102	H102	86.665146	47.881695	20.238224
103	H103	87.599167	49.081463	19.359997
104	H104	88.024757	48.675816	21.019623
105	H105	88.797157	63.496002	15.870474
106	H106	88.714195	63.963650	17.567003
107	H107	90.207520	64.183151	16.657660
108	H108	93.613976	64.438927	20.192661
109	H109	94.530441	63.082569	20.854334
110	H110	94.618958	63.446396	19.128603
111	H111	86.008163	61.801064	23.116228
112	H112	84.687042	60.836777	22.468918
113	H113	85.841301	60.113762	23.582346
114	H114	85.892921	57.240147	21.385508
115	H115	85.943138	60.971375	19.899422
116	H116	92.492714	59.263462	18.444958
117	H117	84.986076	56.456894	19.584490
118	H118	89.342430	52.077366	19.242847
119	H119	91.690559	63.945595	18.550003
120	H120	87.812309	61.481216	17.949520
121	H121	89.315773	59.709774	15.966801
122	H122	87.453522	54.216484	23.078299
123	H123	86.032967	55.312267	22.665876
124	H124	93.121315	61.156155	21.303188
125	H125	92.455223	62.664902	17.624464

S5. Representative NMR Incompatible Conformational Search (CS II)

Figure S19. Crystallographic structure of okadaic acid (blue) superimposed with the energetically representative structures obtained from conformational search. Structures of an NMR incompatible search (CS II) are in reddish.

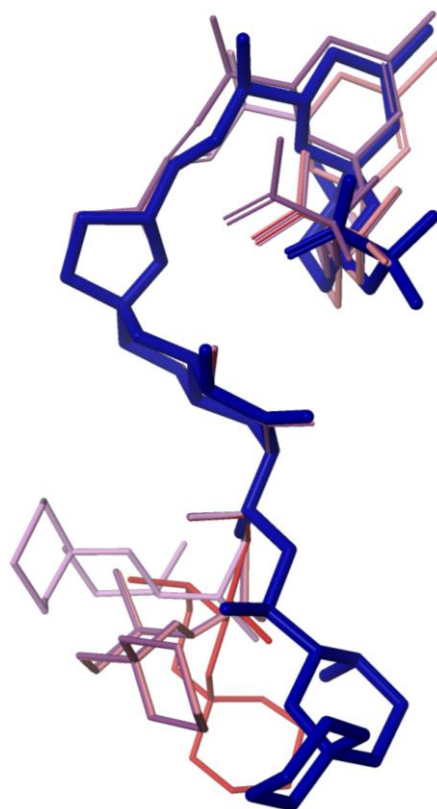


Table S11. CS II, Conformer 1. Gas phase energy and Boltzmann Populations -2695.556258 hartrees, 49.92%.

Center		Coordinates		
Number		X	Y	Z
1	C1	76.108307	57.051773	13.750768
2	C2	75.429855	58.363914	14.170176
3	C3	74.437378	58.179733	15.341824
4	C4	75.022827	57.547798	16.623804
5	C5	73.951668	57.380959	17.714109
6	C6	74.608322	56.832005	18.978533
7	C7	75.720596	57.795208	19.409668
8	C8	76.744438	57.968029	18.257376
9	C9	77.787117	59.010006	18.638943
10	C10	79.108200	58.785065	18.546137
11	C11	79.621376	57.467831	17.999399
12	C12	78.510857	56.713223	17.239944
13	C13	78.848022	55.240070	16.924829
14	C14	77.715454	54.636383	16.120249
15	C15	76.835739	53.731888	16.575811

Table S11. Cont.

Center		Coordinates		
Number		X	Y	Z
16	C16	75.674141	53.221558	15.755466
17	C17	75.568810	51.708580	15.674277
18	C18	74.126579	51.540218	15.226770
19	C19	73.432053	52.788177	15.803410
20	C20	72.401237	52.447525	16.900993
21	C21	71.726028	53.737736	17.382313
22	C22	71.109398	54.437626	16.173166
23	C23	72.208061	54.707359	15.126352
24	C24	71.608162	55.397099	13.892622
25	C25	70.787636	56.615200	14.323368
26	C26	69.877159	56.393219	15.532850
27	C27	68.469101	55.832832	15.190156
28	C28	67.655487	55.469902	16.451273
29	C29	66.107574	55.435360	16.307262
30	C30	65.463570	54.317921	15.434609
31	C31	65.423157	52.866890	15.986176
32	C32	64.641068	52.013367	14.976174
33	C33	65.275459	52.119820	13.582923
34	C34	65.324104	53.596909	13.141768
35	C35	66.097092	53.736790	11.811905
36	C36	66.053688	55.194866	11.336917
37	C37	64.594818	55.633678	11.202279
38	C38	63.870186	55.399796	12.534517
39	C39	66.792381	52.240955	16.307014
40	C40	65.442276	55.495792	17.694809
41	C41	70.905571	57.829014	13.749936
42	C42	80.170998	55.071873	16.160881
43	C43	80.153801	59.789085	18.990238
44	C44	74.743706	58.992775	12.948071
45	O45	77.408821	57.321247	13.480883
46	O46	75.555595	55.959755	13.657129
47	O47	76.444305	59.277065	14.575750
48	O48	76.064102	58.406437	17.110668
49	O49	76.354858	57.300713	20.566484
50	O50	77.340363	56.715534	18.055521
51	O51	74.445923	53.558487	16.369848
52	O52	72.800461	53.462475	14.749808
53	O53	70.524529	55.666550	16.581560
54	O54	72.676163	55.777962	13.038436
55	O55	68.546272	54.718143	14.328876
56	O56	66.008812	54.339535	14.115639
57	O57	64.008926	54.038456	12.943127

Table S11. Cont.

Center		Coordinates		
Number		X	Y	Z
58	H58	73.990303	59.143097	15.589536
59	H59	73.610176	57.559288	14.996874
60	H60	75.435562	56.564980	16.391291
61	H61	73.473900	58.338184	17.926580
62	H62	73.162125	56.707710	17.382320
63	H63	73.866989	56.729080	19.771109
64	H64	75.008026	55.834545	18.786991
65	H65	75.288483	58.770378	19.641142
66	H66	78.297371	57.236324	16.305279
67	H67	78.928200	54.695034	17.866661
68	H68	75.702156	53.644321	14.750332
69	H69	76.286629	51.267860	14.982249
70	H70	75.713646	51.261459	16.658510
71	H71	74.055977	51.558052	14.138186
72	H72	73.672691	50.617878	15.589911
73	H73	71.662689	51.758118	16.489866
74	H74	72.907616	51.941956	17.723717
75	H75	70.957512	53.512146	18.121140
76	H76	72.454491	54.387505	17.868404
77	H77	70.349640	53.776974	15.757547
78	H78	72.969894	55.357929	15.555001
79	H79	70.959061	54.698822	13.363420
80	H80	69.700310	57.376362	15.971578
81	H81	67.937859	56.611401	14.640248
82	H82	68.049843	54.561047	16.896490
83	H83	67.879501	56.241833	17.188786
84	H84	65.839226	56.371746	15.815718
85	H85	64.420395	54.624687	15.337218
86	H86	64.847107	52.863308	16.912289
87	H87	64.604279	50.971855	15.295983
88	H88	63.604900	52.352070	14.929430
89	H89	66.287567	51.714409	13.585257
90	H90	64.700279	51.550301	12.852210
91	H91	67.126892	53.407822	11.957623
92	H92	65.643860	53.079201	11.068956
93	H93	66.577614	55.837204	12.046294
94	H94	66.569778	55.295952	10.382098
95	H95	64.536346	56.684944	10.918287
96	H96	64.104012	55.065323	10.411174
97	H97	64.259468	56.066422	13.305314
98	H98	62.809525	55.628281	12.429527
99	H99	66.712044	51.161369	16.434416

Table S11. *Cont.*

Center		Coordinates		
Number		X	Y	Z
100	H100	67.522858	52.427517	15.519726
101	H101	67.191856	52.626747	17.243059
102	H102	64.355110	55.522594	17.613152
103	H103	65.709618	54.632000	18.304033
104	H104	65.745995	56.388577	18.242207
105	H105	80.342560	54.025936	15.904432
106	H106	80.169060	55.644821	15.232762
107	H107	81.023544	55.399296	16.755669
108	H108	80.796921	60.063904	18.153765
109	H109	79.694122	60.698994	19.377598
110	H110	80.776993	59.362881	19.776924
111	H111	74.293610	59.954639	13.194332
112	H112	75.445724	59.157600	12.129434
113	H113	73.950623	58.345753	12.569774
114	H114	77.420509	58.253006	13.715962
115	H115	76.519165	59.175243	15.526061
116	H116	76.972359	56.652126	20.250748
117	H117	73.430481	55.246925	13.273880
118	H118	67.640495	54.464680	14.146080
119	H119	80.463219	57.658867	17.333239
120	H120	77.616226	54.998119	15.107305
121	H121	76.919792	53.354340	17.584005
122	H122	70.335190	58.675194	14.101346
123	H123	71.566696	57.992874	12.912091
124	H124	77.415474	59.941650	19.039204
125	H125	79.995270	56.870209	18.831408

Table S12. CS II, Conformer 2. Gas phase energy and Boltzmann Populations
−2695.555664 hartrees, 26.61%.

Center		Coordinates		
Number		X	Y	Z
1	C1	76.679565	57.083557	14.014741
2	C2	75.993996	58.427334	14.294632
3	C3	74.684105	58.262936	15.102359
4	C4	74.834404	57.612045	16.494566
5	C5	73.474121	57.443493	17.190573
6	C6	73.688347	56.927303	18.613255
7	C7	74.609932	57.900974	19.359800
8	C8	75.948029	58.040981	18.591066
9	C9	76.844437	59.074860	19.254337
10	C10	78.140831	58.844788	19.519381
11	C11	78.782600	57.528740	19.123833
12	C12	77.899879	56.739285	18.131910

Table S12. Cont.

Center		Coordinates		
Number		X	Y	Z
13	C13	78.311714	55.257053	17.981783
14	C14	77.275505	54.519310	17.143671
15	C15	77.476547	53.832798	16.003962
16	C16	76.367012	53.180557	15.204565
17	C17	76.429428	51.661335	15.155599
18	C18	74.991142	51.276173	14.826412
19	C19	74.192970	52.554558	15.138440
20	C20	72.975540	52.311642	16.055592
21	C21	72.225716	53.634445	16.265236
22	C22	71.853302	54.209091	14.898273
23	C23	73.132736	54.383587	14.058359
24	C24	72.784248	54.941875	12.670822
25	C25	71.925232	56.198635	12.821101
26	C26	70.797478	56.095783	13.850586
27	C27	69.466194	55.518291	13.295045
28	C28	68.404976	55.318970	14.396938
29	C29	67.002632	54.865612	13.914270
30	C30	66.052963	54.542171	15.098755
31	C31	66.546646	53.460644	16.095234
32	C32	65.451645	53.240894	17.149340
33	C33	64.122353	52.876366	16.476387
34	C34	63.743954	53.963020	15.450235
35	C35	62.494102	53.534622	14.649531
36	C36	62.063313	54.668659	13.710460
37	C37	61.809456	55.931202	14.535032
38	C38	63.065041	56.259560	15.353296
39	C39	66.972420	52.143272	15.416993
40	C40	66.358788	55.925064	12.993842
41	C41	72.174927	57.350311	12.167266
42	C42	79.746208	55.100342	17.440271
43	C43	79.029541	59.843033	20.235088
44	C44	75.739639	59.150398	12.963075
45	O45	78.012611	57.240734	14.198514
46	O46	76.105362	56.065853	13.639646
47	O47	76.897598	59.246719	15.028807
48	O48	75.669083	58.467503	17.284851
49	O49	74.836266	57.434593	20.669746
50	O50	76.555580	56.778927	18.608038
51	O51	75.091141	53.393326	15.785621
52	O52	73.762405	53.107841	13.927160
53	O53	71.216599	55.469227	15.066699
54	O54	73.985184	55.221794	11.964080

Table S12. Cont.

Center		Coordinates		
Number		X	Y	Z
55	O55	69.654419	54.304138	12.590844
56	O56	64.804657	54.115528	14.546799
57	O57	63.444073	55.139336	16.153366
58	H58	74.205437	59.236565	15.214181
59	H59	73.987083	57.662514	14.515414
60	H60	75.301384	56.631126	16.393984
61	H61	72.942703	58.395645	17.219118
62	H62	72.844963	56.752365	16.630651
63	H63	72.731003	56.842289	19.127794
64	H64	74.121300	55.926228	18.585255
65	H65	74.136131	58.882553	19.417593
66	H66	77.940201	57.214603	17.149847
67	H67	78.277039	54.794357	18.969000
68	H68	76.378342	53.582893	14.190787
69	H69	77.148209	51.292553	14.423738
70	H70	76.703094	51.266144	16.134674
71	H71	74.864174	51.008282	13.776711
72	H72	74.652657	50.443066	15.442946
73	H73	72.326202	51.570221	15.588340
74	H74	73.318489	51.903332	17.006685
75	H75	71.330200	53.473366	16.864843
76	H76	72.854332	54.336124	16.813795
77	H77	71.177406	53.507446	14.410799
78	H78	73.798515	55.085510	14.562951
79	H79	72.215599	54.200726	12.108788
80	H80	70.564377	57.116959	14.155984
81	H81	69.102150	56.243134	12.567011
82	H82	68.806351	54.588345	15.097375
83	H83	68.302986	56.243526	14.966803
84	H84	67.112289	53.953106	13.328830
85	H85	65.894119	55.469208	15.652419
86	H86	67.414223	53.844425	16.632124
87	H87	65.744827	52.462132	17.853495
88	H88	65.320801	54.150944	17.736780
89	H89	64.195221	51.915253	15.967487
90	H90	63.324837	52.791332	17.215122
91	H91	62.724388	52.630543	14.084874
92	H92	61.692696	53.292080	15.348522
93	H93	62.839752	54.854359	12.967046
94	H94	61.164028	54.385475	13.163515
95	H95	61.551945	56.767521	13.884328
96	H96	60.961933	55.778652	15.204452

Table S12. *Cont.*

Center		Coordinates		
Number		X	Y	Z
97	H97	63.885674	56.549133	14.696188
98	H98	62.873974	57.109608	16.008324
99	H99	67.203064	51.376106	16.156210
100	H100	66.191803	51.754406	14.763110
101	H101	67.867531	52.280300	14.810291
102	H102	65.365158	55.616989	12.667253
103	H103	66.250153	56.881695	13.505477
104	H104	66.937431	56.091225	12.086661
105	H105	80.020912	54.049232	17.347979
106	H106	79.854301	55.566021	16.459753
107	H107	80.478050	55.556786	18.106058
108	H108	79.875465	60.119370	19.605099
109	H109	78.484360	60.752888	20.488607
110	H110	79.416039	59.411205	21.158693
111	H111	75.308212	60.138939	13.122230
112	H112	76.660461	59.282764	12.392897
113	H113	75.047539	58.586739	12.335752
114	H114	78.017738	58.153805	14.497914
115	H115	76.642838	59.158169	15.949044
116	H116	75.523033	56.784077	20.588125
117	H117	74.695000	55.279148	12.599669
118	H118	68.838379	54.073872	12.171689
119	H119	79.758438	57.724892	18.678802
120	H120	76.266418	54.580666	17.525967
121	H121	78.466011	53.734921	15.584064
122	H122	71.565971	58.228203	12.321176
123	H123	72.984810	57.430222	11.456911
124	H124	76.379166	60.004974	19.545694
125	H125	78.953262	56.948433	20.031210

Table S13. CS II, Conformer 3. Gas phase energy and Boltzmann Populations
−2695.554772 hartrees, 10.35%.

Center		Coordinates		
Number		X	Y	Z
1	C1	75.953598	57.063057	13.812674
2	C2	75.426163	58.435211	14.251992
3	C3	74.365150	58.326965	15.373464
4	C4	74.840797	57.659088	16.682007
5	C5	73.702652	57.554550	17.710096
6	C6	74.254082	57.017731	19.030720
7	C7	75.387062	57.937683	19.504711
8	C8	76.483459	58.014709	18.412474
9	C9	77.573914	58.996197	18.812452

Table S13. Cont.

Center		Coordinates		
Number		X	Y	Z
10	C10	78.880920	58.697781	18.731808
11	C11	79.328598	57.353378	18.191044
12	C12	78.178391	56.617889	17.468267
13	C13	78.459618	55.117535	17.225134
14	C14	77.204781	54.441353	16.687885
15	C15	77.068283	53.753441	15.539480
16	C16	75.756989	53.167011	15.057623
17	C17	75.723740	51.647251	15.002251
18	C18	74.230377	51.343060	15.051254
19	C19	73.609367	52.656746	15.558966
20	C20	72.662903	52.464542	16.762966
21	C21	72.063828	53.820873	17.159521
22	C22	71.376686	54.429192	15.936838
23	C23	72.399193	54.549763	14.790947
24	C24	71.731239	55.143181	13.541498
25	C25	71.003586	56.437725	13.909659
26	C26	70.181168	56.377422	15.199308
27	C27	68.725876	55.864189	15.019760
28	C28	67.996971	55.674377	16.367638
29	C29	66.442627	55.711189	16.340946
30	C30	65.680214	54.549713	15.637591
31	C31	65.613358	53.165478	16.338133
32	C32	64.715820	52.259880	15.481054
33	C33	65.245064	52.191475	14.042261
34	C34	65.329597	53.612152	13.447900
35	C35	66.003197	53.575569	12.058452
36	C36	65.992386	54.978973	11.438933
37	C37	64.549934	55.481812	11.364981
38	C38	63.920280	55.422688	12.763083
39	C39	66.971848	52.499977	16.622900
40	C40	65.891113	55.946072	17.759474
41	C41	71.130096	57.583588	13.211611
42	C42	79.694893	54.891003	16.331642
43	C43	79.975777	59.643696	19.184662
44	C44	74.867981	59.176327	13.027371
45	O45	77.294113	57.158817	13.641146
46	O46	75.256256	56.074280	13.607692
47	O47	76.525841	59.208363	14.720929
48	O48	75.895493	58.464928	17.221867
49	O49	75.923302	57.450855	20.713091
50	O50	77.008553	56.723019	18.278065
51	O51	74.687851	53.440918	15.947822

Table S13. *Cont.*

Center		Coordinates		
Number		X	Y	Z
52	O52	72.907234	53.245979	14.501328
53	O53	70.873177	55.717907	16.264086
54	O54	72.722328	55.375439	12.549129
55	O55	68.683990	54.665966	14.277204
56	O56	66.122078	54.409481	14.287581
57	O57	64.025459	54.103516	13.299876
58	H58	73.979149	59.321365	15.600872
59	H59	73.511604	57.764778	14.991077
60	H60	75.214622	56.656525	16.468767
61	H61	73.246117	58.532116	17.870476
62	H62	72.914932	56.900299	17.338053
63	H63	73.461113	56.977806	19.777775
64	H64	74.612907	55.996113	18.896864
65	H65	74.995644	58.941727	19.677931
66	H66	77.985916	57.097965	16.506771
67	H67	78.657516	54.649422	18.190315
68	H68	75.527031	53.576706	14.073262
69	H69	76.212051	51.246864	14.113721
70	H70	76.215363	51.229820	15.881855
71	H71	73.825783	51.099361	14.068052
72	H72	74.014847	50.518879	15.731703
73	H73	71.876213	51.762897	16.482796
74	H74	73.220665	52.027733	17.591805
75	H75	71.349289	53.698250	17.973000
76	H76	72.849472	54.483631	17.522739
77	H77	70.562149	53.767059	15.645674
78	H78	73.208885	55.211002	15.103603
79	H79	71.001381	54.437382	13.144415
80	H80	70.085518	57.405399	15.552076
81	H81	68.190567	56.611374	14.431593
82	H82	68.381187	54.793835	16.874439
83	H83	68.314156	56.502270	17.003185
84	H84	66.181549	56.607357	15.776015
85	H85	64.648476	54.902561	15.584469
86	H86	65.110992	53.286251	17.298643
87	H87	64.654327	51.259136	15.908966
88	H88	63.696438	52.648930	15.474149
89	H89	66.233917	51.733128	14.013756
90	H90	64.588768	51.584393	13.417886
91	H91	67.024437	53.206612	12.162909
92	H92	65.463219	52.872925	11.422428
93	H93	66.599533	55.659176	12.038090

Table S13. *Cont.*

Center		Coordinates		
Number		X	Y	Z
94	H94	66.437294	54.955399	10.444072
95	H95	64.519585	56.500977	10.978215
96	H96	63.973000	54.865028	10.674691
97	H97	64.399254	56.140598	13.430352
98	H98	62.866722	55.697636	12.711704
99	H99	66.850166	51.444695	16.867376
100	H100	67.647331	52.565941	15.769910
101	H101	67.460464	52.954891	17.482483
102	H102	64.803383	56.024525	17.754681
103	H103	66.163727	55.133747	18.433708
104	H104	66.278557	56.870777	18.188116
105	H105	79.881187	53.827850	16.177412
106	H106	79.569595	55.358261	15.353928
107	H107	80.596901	55.303551	16.782633
108	H108	80.641327	59.880665	18.354164
109	H109	79.563263	60.578556	19.565691
110	H110	80.566849	59.185829	19.978315
111	H111	74.537544	60.182442	13.286615
112	H112	75.614304	59.270000	12.236962
113	H113	74.012161	58.647839	12.604788
114	H114	77.418152	58.069164	13.922536
115	H115	76.517365	59.122822	15.676013
116	H116	76.530197	56.766300	20.459064
117	H117	73.574524	55.376129	12.978751
118	H118	67.756134	54.444790	14.186909
119	H119	80.163574	57.502316	17.505919
120	H120	76.333183	54.553165	17.317169
121	H121	77.909241	53.606373	14.879135
122	H122	70.626244	58.487549	13.518216
123	H123	71.728600	57.632301	12.313748
124	H124	77.249321	59.946877	19.209078
125	H125	79.699501	56.758316	19.026217

Table S14. CS II, Conformer 4. Gas phase energy and Boltzmann Populations
−2695.554695 hartrees, 9.54%.

Center		Coordinates		
Number		X	Y	Z
1	C1	76.033676	57.383125	13.781252
2	C2	75.513123	58.689163	14.398239
3	C3	74.450546	58.451412	15.496490
4	C4	74.890709	57.546078	16.667879
5	C5	73.756294	57.339962	17.684395
6	C6	74.279701	56.504890	18.850527

Table S14. Cont.

Center		Coordinates		
Number		X	Y	Z
7	C7	75.479843	57.229675	19.471411
8	C8	76.570908	57.464035	18.393890
9	C9	77.710930	58.287601	18.977356
10	C10	78.998810	57.918228	18.880869
11	C11	79.377014	56.658630	18.127438
12	C12	78.221214	56.186512	17.221451
13	C13	78.395760	54.756016	16.668289
14	C14	77.235130	54.437355	15.748568
15	C15	76.230659	53.594688	16.031992
16	C16	75.053246	53.370403	15.112164
17	C17	74.763718	51.913174	14.796431
18	C18	73.331985	52.000259	14.295819
19	C19	72.774040	53.227940	15.039486
20	C20	71.664230	52.865143	16.049200
21	C21	71.129921	54.146503	16.701122
22	C22	70.665367	55.094749	15.597732
23	C23	71.834908	55.369667	14.633391
24	C24	71.384911	56.311680	13.507080
25	C25	70.709641	57.550327	14.102010
26	C26	69.722168	57.273285	15.237571
27	C27	68.275154	56.956692	14.768746
28	C28	67.355217	56.516953	15.924918
29	C29	65.927757	56.099449	15.486600
30	C30	65.712227	54.561245	15.413899
31	C31	65.389610	53.821617	16.741716
32	C32	65.146118	52.345222	16.404375
33	C33	66.354340	51.764629	15.659117
34	C34	66.641418	52.594025	14.389535
35	C35	67.936386	52.079391	13.715927
36	C36	68.149109	52.748730	12.351790
37	C37	66.901718	52.561653	11.488951
38	C38	65.678650	53.081909	12.252862
39	C39	66.437218	53.978176	17.860979
40	C40	64.836403	56.815006	16.303955
41	C41	71.009590	58.809635	13.727809
42	C42	79.721169	54.55497	15.916602
43	C43	80.134300	58.694145	19.518984
44	C44	74.974480	59.597157	13.282463
45	O45	77.368217	57.515541	13.585978
46	O46	75.348984	56.404137	13.498984
47	O47	76.617546	59.376690	14.976639
48	O48	76.003944	58.171028	17.322170

Table S14. Cont.

Center		Coordinates		
Number		X	Y	Z
49	O49	75.993744	56.466976	20.538694
50	O50	77.022232	56.198605	17.994638
51	O51	73.850357	53.769039	15.739714
52	O52	72.274689	54.125427	14.086259
53	O53	70.225471	56.316288	16.174736
54	O54	72.528870	56.670815	12.747477
55	O55	68.247597	55.989277	13.741638
56	O56	66.824944	53.940895	14.753215
57	O57	65.569374	52.40958	13.506447
58	H58	74.118835	59.412346	15.891354
59	H59	73.568375	58.011536	15.031030
60	H60	75.190933	56.570217	16.283350
61	H61	73.391594	58.30188	18.046923
62	H62	72.906303	56.841328	17.220270
63	H63	73.494507	56.365578	19.593761
64	H64	74.563164	55.511242	18.498762
65	H65	75.159348	58.198162	19.859484
66	H66	78.115112	56.880459	16.384809
67	H67	78.371117	54.056980	17.505733
68	H68	75.179779	53.931900	14.185503
69	H69	75.449982	51.491997	14.061522
70	H70	74.810394	51.308647	15.703072
71	H71	73.310303	52.188026	13.221271
72	H72	72.752495	51.100494	14.503682
73	H73	70.867752	52.338943	15.523409
74	H74	72.071037	52.186733	16.799709
75	H75	70.304100	53.915417	17.373602
76	H76	71.908745	54.615509	17.303152
77	H77	69.847221	54.610542	15.066191
78	H78	72.654076	55.841000	15.176002
79	H79	70.676147	55.795132	12.859124
80	H80	69.646065	58.192841	15.819720
81	H81	67.865753	57.867004	14.327682
82	H82	67.834366	55.70195	16.461275
83	H83	67.302795	57.335728	16.643465
84	H84	65.790024	56.465202	14.467479
85	H85	64.838905	54.431057	14.771917
86	H86	64.449516	54.213387	17.132036
87	H87	64.946823	51.769756	17.308556
88	H88	64.255615	52.250576	15.781002
89	H89	67.241318	51.761444	16.292393
90	H90	66.162994	50.730595	15.370293

Table S14. Cont.

Center		Coordinates		
Number		X	Y	Z
91	H91	68.781860	52.268795	14.376613
92	H92	67.856628	50.999046	13.588325
93	H93	68.361015	53.808338	12.474131
94	H94	69.019196	52.319042	11.855204
95	H95	67.010834	53.091503	10.541988
96	H96	66.765282	51.506702	11.247858
97	H97	65.745613	54.160503	12.403852
98	H98	64.771439	52.899921	11.676616
99	H99	66.183136	53.361294	18.723112
100	H100	67.434578	53.688141	17.531101
101	H101	66.490913	55.006527	18.216316
102	H102	63.840401	56.527813	15.965155
103	H103	64.905777	56.586021	17.367163
104	H104	64.915176	57.897373	16.197678
105	H105	79.779587	53.552658	15.490972
106	H106	79.826050	55.269104	15.098864
107	H107	80.580139	54.672539	16.577034
108	H108	80.843956	59.023621	18.759602
109	H109	79.768318	59.575855	20.046188
110	H110	80.664955	58.066753	20.235689
111	H111	74.638756	60.556732	13.676093
112	H112	75.731712	59.799294	12.523561
113	H113	74.125641	59.133324	12.777552
114	H114	77.491257	58.386395	13.973159
115	H115	76.633018	59.113235	15.898235
116	H116	76.544518	55.810532	20.129492
117	H117	73.212715	56.037235	12.941386
118	H118	67.798798	55.217346	14.086383
119	H119	80.265282	56.852871	17.525585
120	H120	77.227638	54.961704	14.804208
121	H121	76.222046	53.058548	16.969322
122	H122	70.53685	59.661953	14.191514
123	H123	71.723228	59.007923	12.942192
124	H124	77.434311	59.177353	19.523373
125	H125	79.639038	55.887653	18.852779

Table S15. CS II, Conformer 5. Gas phase energy and Boltzmann Populations
−2695.553772 hartrees, 3.59%.

Center		Coordinates		
Number		X	Y	Z
1	C1	75.890556	57.383163	13.848571
2	C2	75.523041	58.725010	14.495579
3	C3	74.394081	58.582329	15.544791
4	C4	74.705727	57.653561	16.738420
5	C5	73.506783	57.534351	17.692944
6	C6	73.911423	56.718246	18.920511
7	C7	75.121185	57.389496	19.584583
8	C8	76.278954	57.502151	18.560778
9	C9	77.456894	58.254303	19.159861
10	C10	78.720474	57.807774	19.071852
11	C11	79.030602	56.526138	18.322475
12	C12	77.839722	56.073250	17.448908
13	C13	77.950935	54.609932	16.963610
14	C14	76.651100	54.192635	16.287844
15	C15	76.487068	53.725315	15.036680
16	C16	75.139244	53.391056	14.430634
17	C17	74.930916	51.914566	14.125496
18	C18	73.411690	51.777874	14.118857
19	C19	72.927635	53.076397	14.786735
20	C20	71.898605	52.845150	15.913271
21	C21	71.445206	54.200317	16.474419
22	C22	70.919594	55.062267	15.325928
23	C23	72.015434	55.200214	14.253289
24	C24	71.509026	56.051193	13.079323
25	C25	70.943108	57.371632	13.606651
26	C26	70.040314	57.247353	14.836775
27	C27	68.546288	56.969433	14.515411
28	C28	67.703056	56.703598	15.778321
29	C29	66.229240	56.314533	15.494909
30	C30	65.944908	54.790417	15.613015
31	C31	65.687881	54.221287	17.035467
32	C32	65.356010	52.731239	16.886494
33	C33	66.481247	52.009453	16.135015
34	C34	66.715767	52.676933	14.763121
35	C35	67.938293	52.025154	14.073311
36	C36	68.087532	52.527111	12.631272
37	C37	66.777435	52.309639	11.874915
38	C38	65.632271	52.972111	12.649562
39	C39	66.821098	54.447716	18.055058
40	C40	65.235878	57.170998	16.301706
41	C41	71.267838	58.574757	13.093816
42	C42	79.190857	54.380352	16.077417

Table S15. Cont.

Center		Coordinates		
Number		X	Y	Z
43	C43	79.895775	58.516060	19.716465
44	C44	75.138634	59.726955	13.396097
45	O45	77.239693	57.318153	13.743106
46	O46	75.082405	56.547279	13.455462
47	O47	76.685822	59.251278	15.126298
48	O48	75.818993	58.214748	17.444395
49	O49	75.523903	56.642574	20.709105
50	O50	76.649414	56.193291	18.226366
51	O51	74.070511	53.651932	15.325438
52	O52	72.362175	53.891094	13.799306
53	O53	70.572411	56.350540	15.817247
54	O54	72.578491	56.275948	12.170374
55	O55	68.387306	55.906067	13.601954
56	O56	66.981392	54.045189	14.956956
57	O57	65.579178	52.449532	13.976109
58	H58	74.126137	59.569908	15.922248
59	H59	73.498810	58.210087	15.043915
60	H60	74.963829	56.658455	16.372948
61	H61	73.168892	58.524345	18.002089
62	H62	72.665146	57.062016	17.187468
63	H63	73.078613	56.660271	19.621618
64	H64	74.147942	55.694599	18.626266
65	H65	74.847755	58.393448	19.914183
66	H66	77.758316	56.725357	16.577114
67	H67	78.046387	53.968708	17.840874
68	H68	75.005074	53.978928	13.521594
69	H69	75.390411	51.611588	13.184563
70	H70	75.352516	51.303631	14.924659
71	H71	73.003792	51.705418	13.109824
72	H72	73.092583	50.904709	14.688554
73	H73	71.052826	52.291275	15.506478
74	H74	72.352501	52.233425	16.693485
75	H75	70.670380	54.060642	17.227890
76	H76	72.282166	54.695580	16.966860
77	H77	70.044395	54.566620	14.907831
78	H78	72.883850	55.693508	14.692658
79	H79	70.715492	55.519783	12.553537
80	H80	70.055725	58.217453	15.335706
81	H81	68.147797	57.852291	14.012828
82	H82	68.187317	55.926796	16.364782
83	H83	67.742393	57.595875	16.404175
84	H84	66.027954	56.572289	14.453582

Table S15. Cont.

Center		Coordinates		
Number		X	Y	Z
85	H85	65.023399	54.632710	15.049306
86	H86	64.796791	54.701962	17.441034
87	H87	65.196510	52.271259	17.861877
88	H88	64.420151	52.613987	16.337900
89	H89	67.409431	52.029671	16.705828
90	H90	66.224045	50.961254	15.978923
91	H91	68.833763	52.243092	14.654455
92	H92	67.802795	50.942841	14.074979
93	H93	68.354378	53.581249	12.618521
94	H94	68.902237	52.000763	12.133783
95	H95	66.845131	52.725513	10.869021
96	H96	66.579437	51.242809	11.763961
97	H97	65.755394	54.056072	12.672008
98	H98	64.681198	52.773094	12.155547
99	H99	66.604378	53.945580	18.998047
100	H100	67.777679	54.071033	17.693588
101	H101	66.946465	55.505211	18.284283
102	H102	64.205368	56.899281	16.070396
103	H103	65.377174	57.058151	17.376368
104	H104	65.352264	58.229446	16.066944
105	H105	79.256744	53.341927	15.751645
106	H106	79.167534	55.013123	15.189141
107	H107	80.113403	54.598019	16.614763
108	H108	80.629158	58.800526	18.961435
109	H109	79.579620	59.419514	20.239082
110	H110	80.383125	57.860085	20.438337
111	H111	75.935028	59.843616	12.659428
112	H112	74.929466	60.713295	13.810926
113	H113	74.246414	59.399727	12.860421
114	H114	77.465958	58.144314	14.178555
115	H115	76.609421	59.017864	16.053257
116	H116	76.057465	55.937691	20.362774
117	H117	73.399284	56.157944	12.643105
118	H118	67.952484	55.191284	14.066560
119	H119	79.912201	56.679073	17.699427
120	H120	75.771072	54.306110	16.904930
121	H121	77.334091	53.586613	14.382244
122	H122	70.872780	59.488808	13.510451
123	H123	71.921852	58.664364	12.238818
124	H124	77.228973	59.159286	19.703493
125	H125	79.283089	55.758308	19.054516