SUPPORTING INFORMATION

Lignanamides from the roots of *Metternichia macrocalyx* and their anti-inflammatory activity

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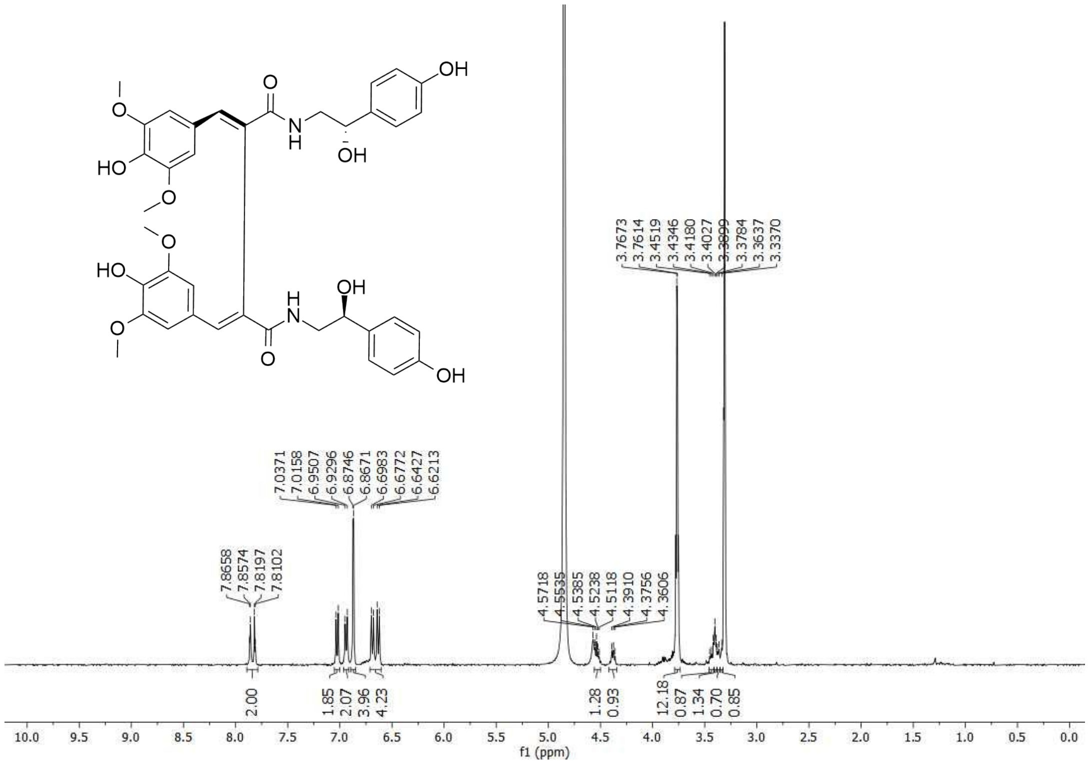

Figure S1. [1]H NMR spectrum of compound **1 (**400 MHz, MeOD).

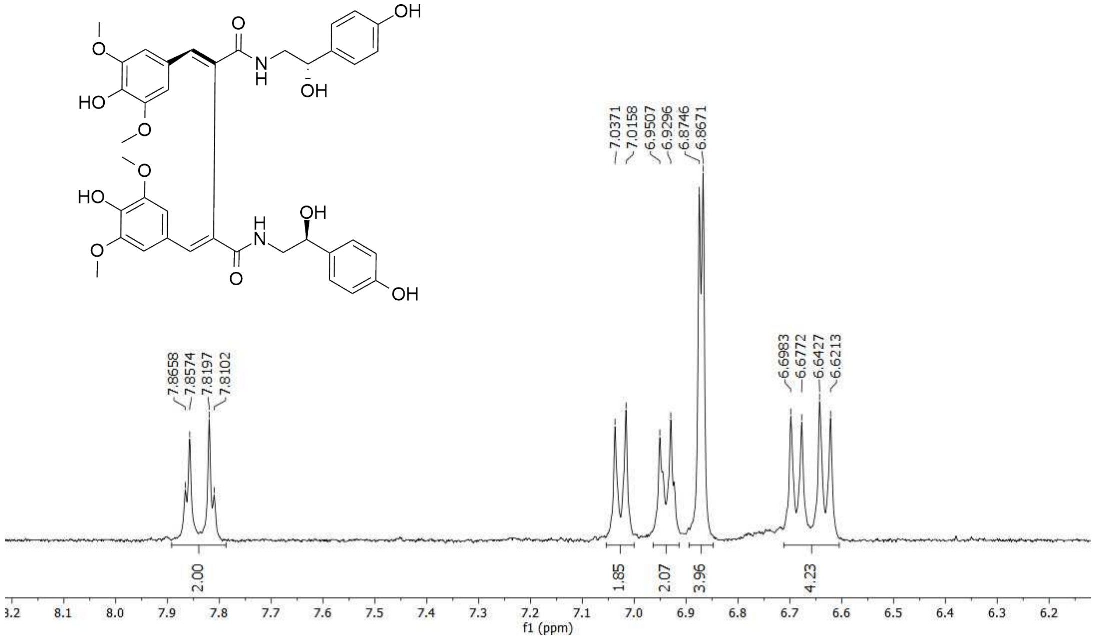

Figure S2. Amplification of the [1]H NMR spectrum of compound **1 (**400 MHz, MeOD).

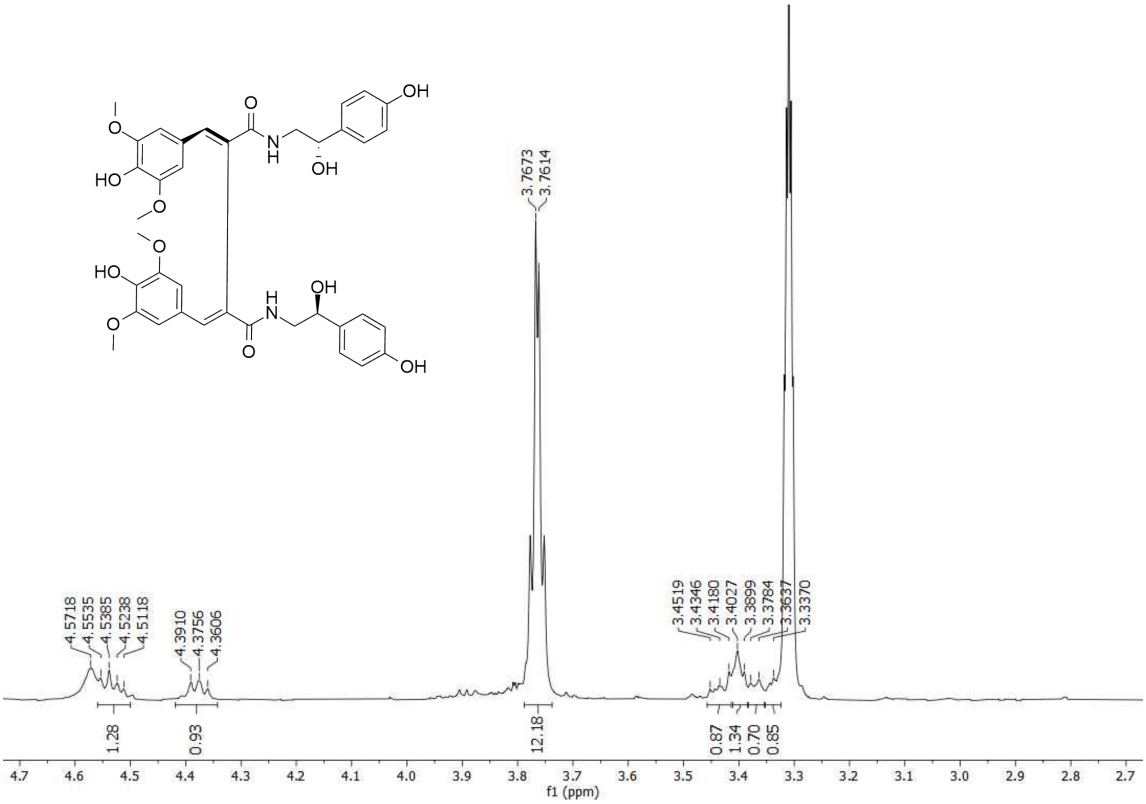

Figure S3. Amplification of the [1]H NMR spectrum of compound **1 (**400 MHz, MeOD).

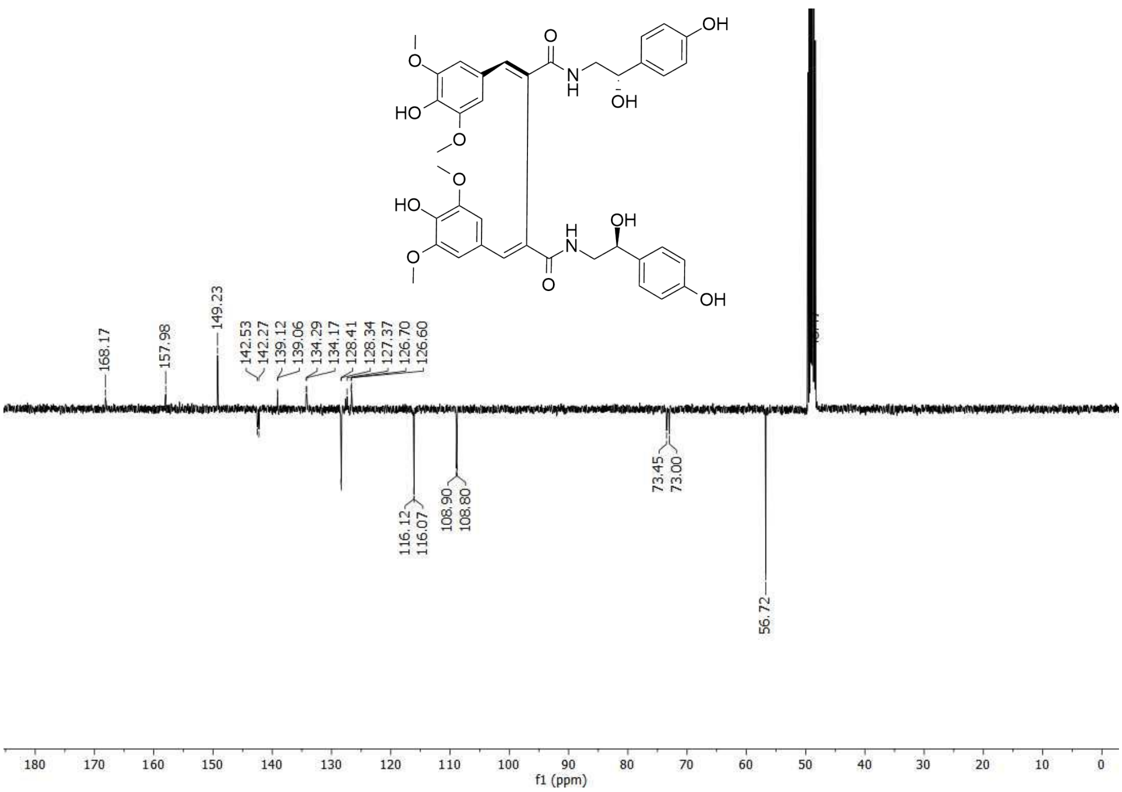

Figure S4. [13]C-APT NMR spectrum of compound **1** (100 MHz, MeOD).

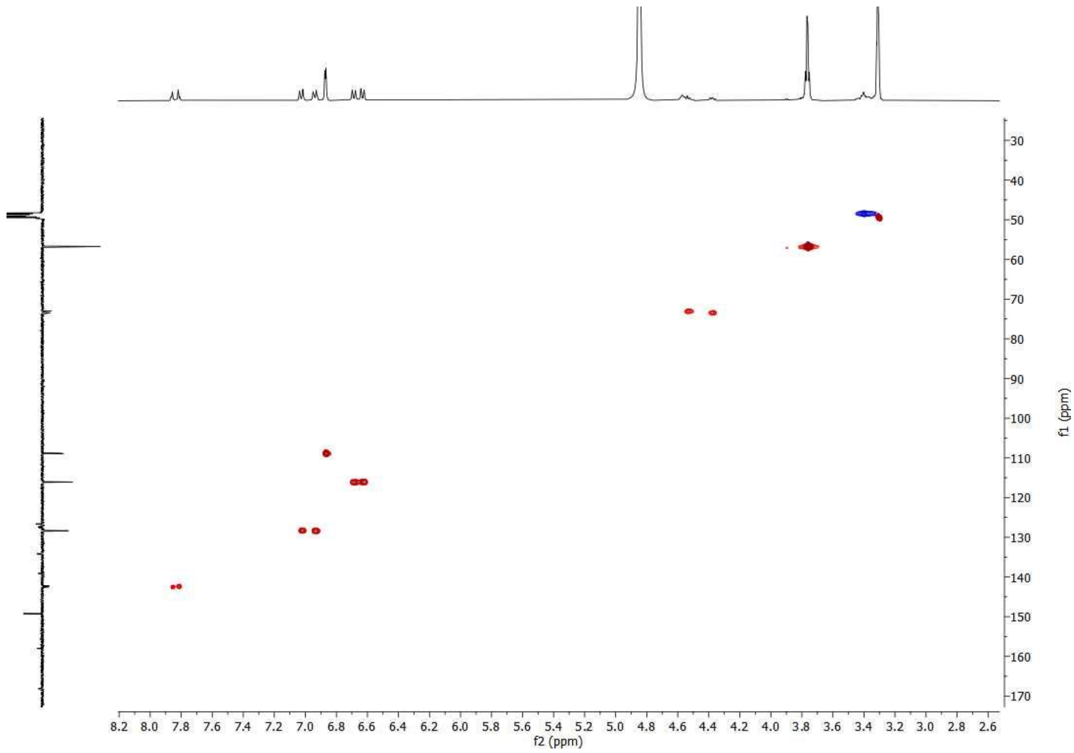

Figure S5. HSQC spectrum of compound **1 (**400/100 MHz, MeOD).

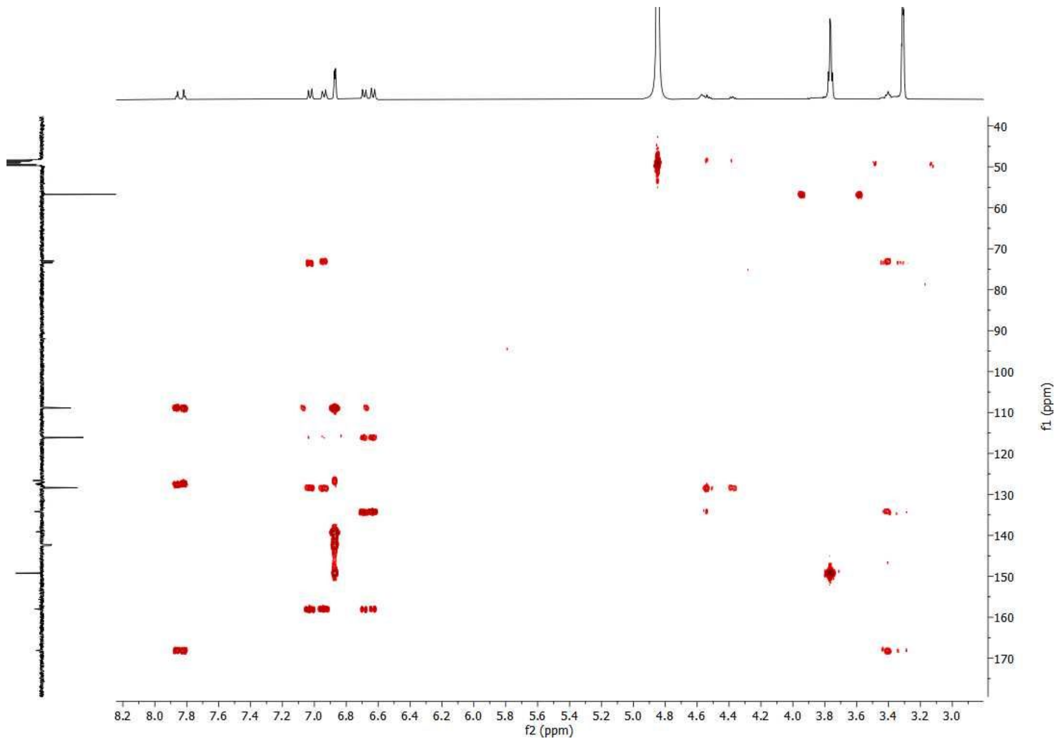

Figure S6. HMBC spectrum of compound **1 (**400/100 MHz, MeOD).

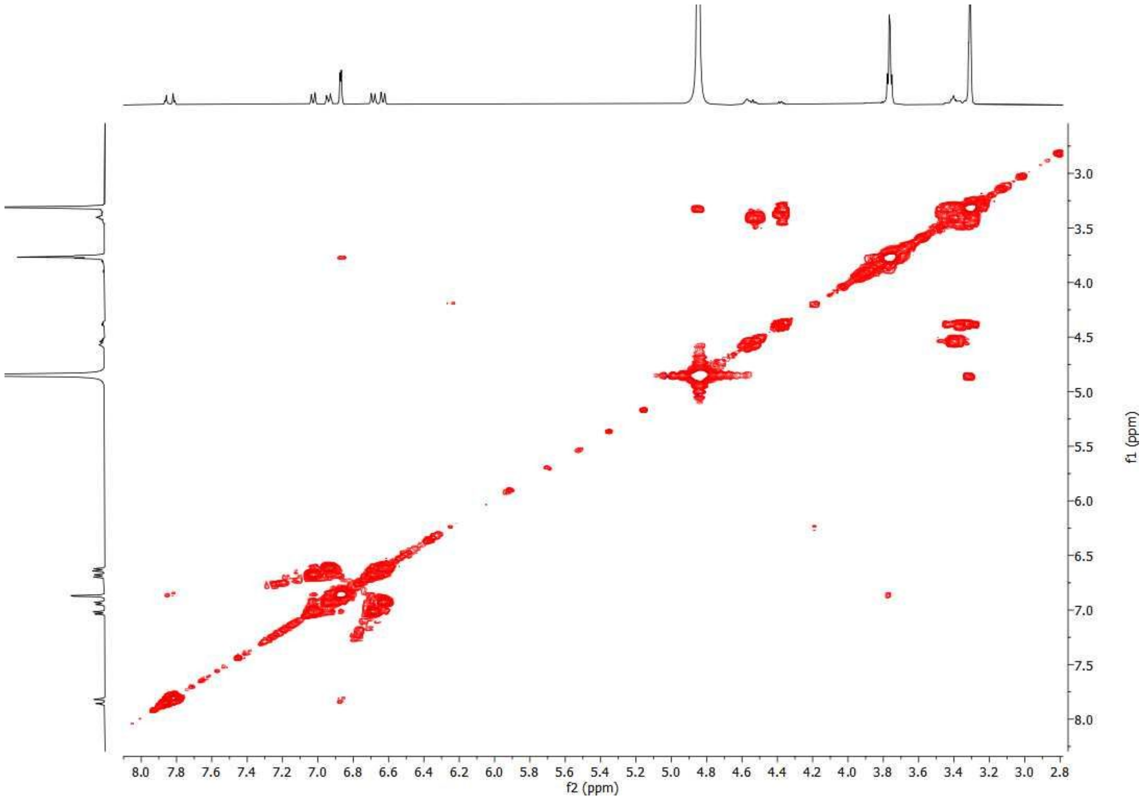

Figure S7. COSY spectrum of compound **1 (**400 MHz, MeOD).

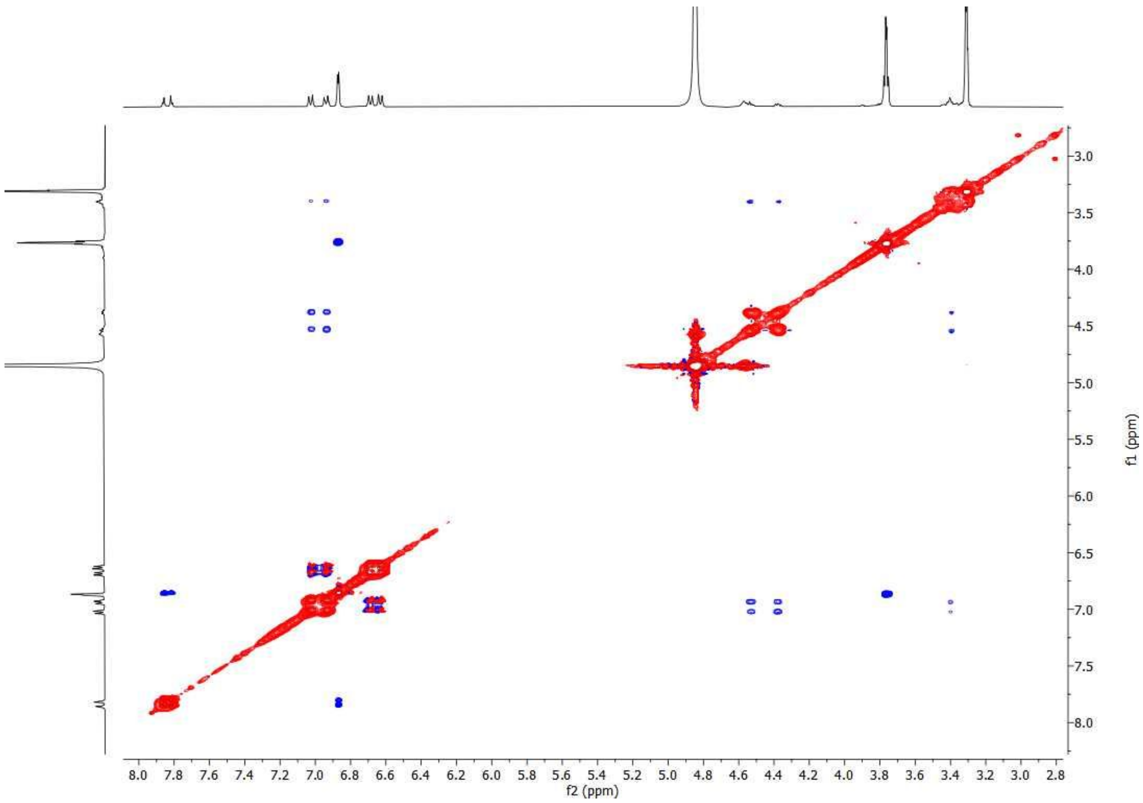

Figure S8. NOESY spectrum of compound **1 (**400 MHz, MeOD).

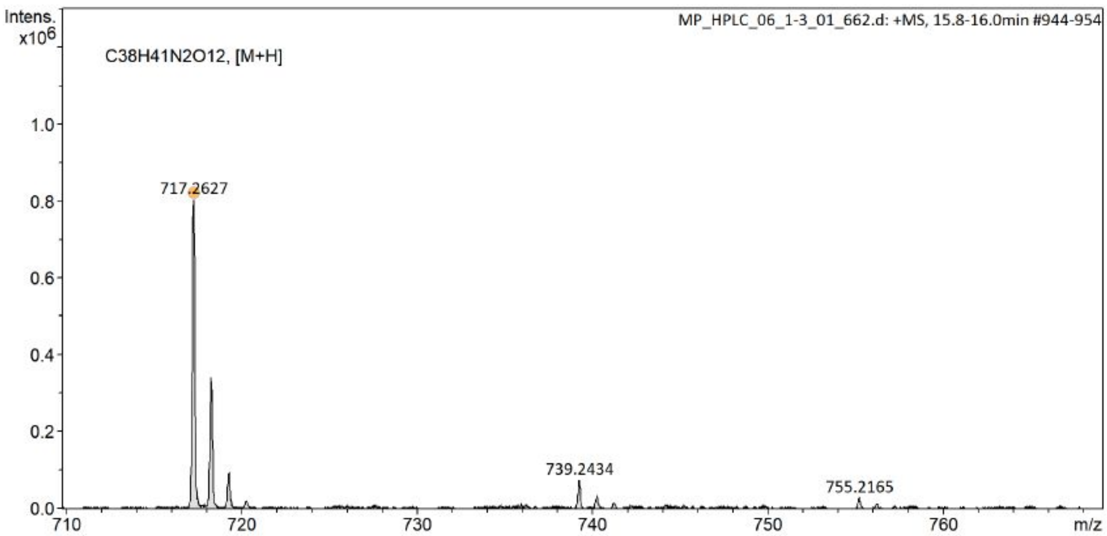

Figure S9. HRESIMS spectrum of compound **1** ($[M + H]^+$, positive mode).

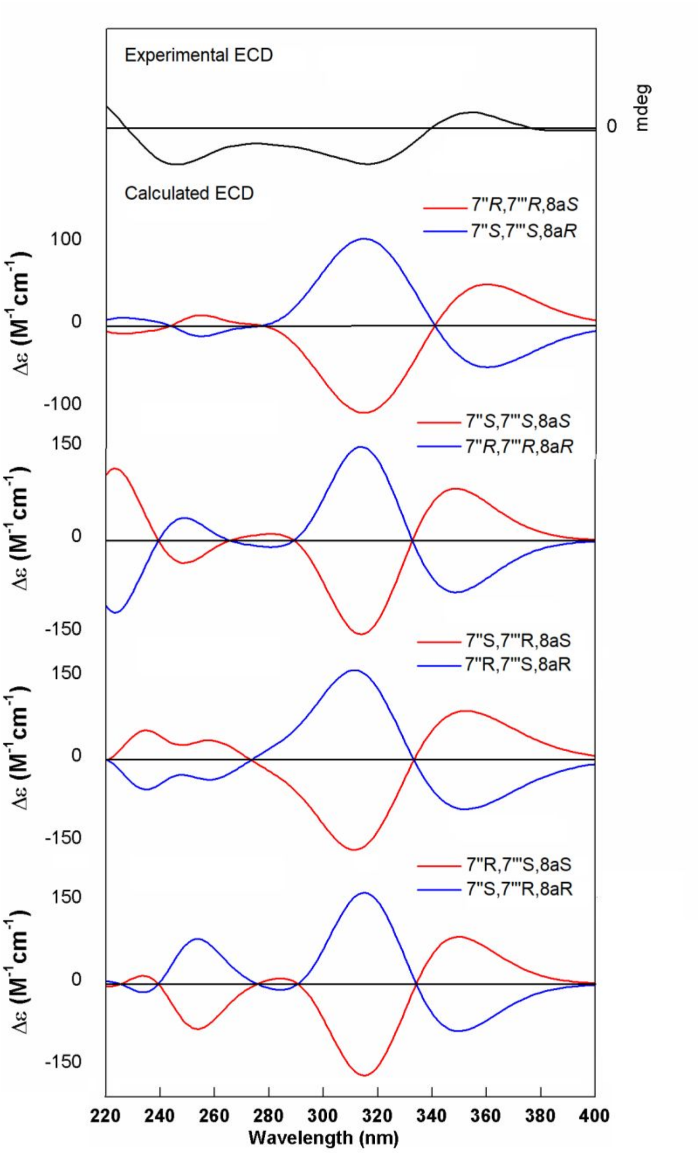

Figure S10. Experimental (top) and calculated (bottom) ECD spectra of all possible stereoisomers of compound **1**. a*S* atropisomers are marked in red and a*R* atropisomers are marked in blue.

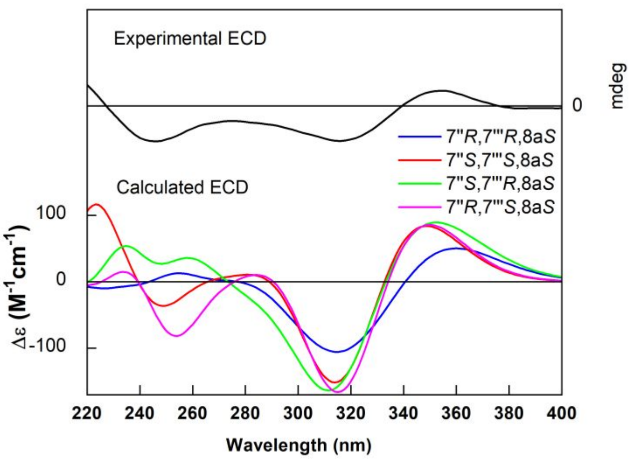

Figure S11. Experimental (top) and calculated (bottom) ECD spectra of a*S* atropoisomers of compound **1**.

2 Spectroscopic data for compound 2

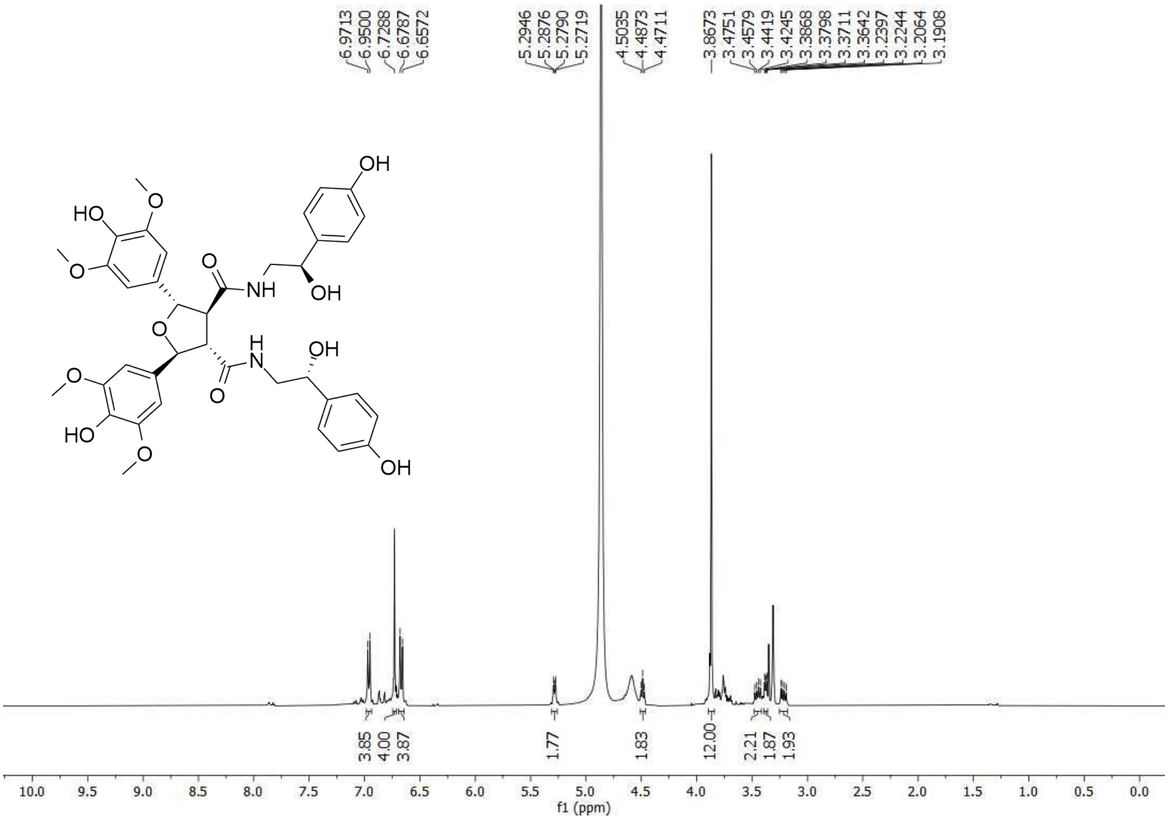

Figure S12. ^{1}H NMR spectrum of compound **2 (**400 MHz, MeOD).

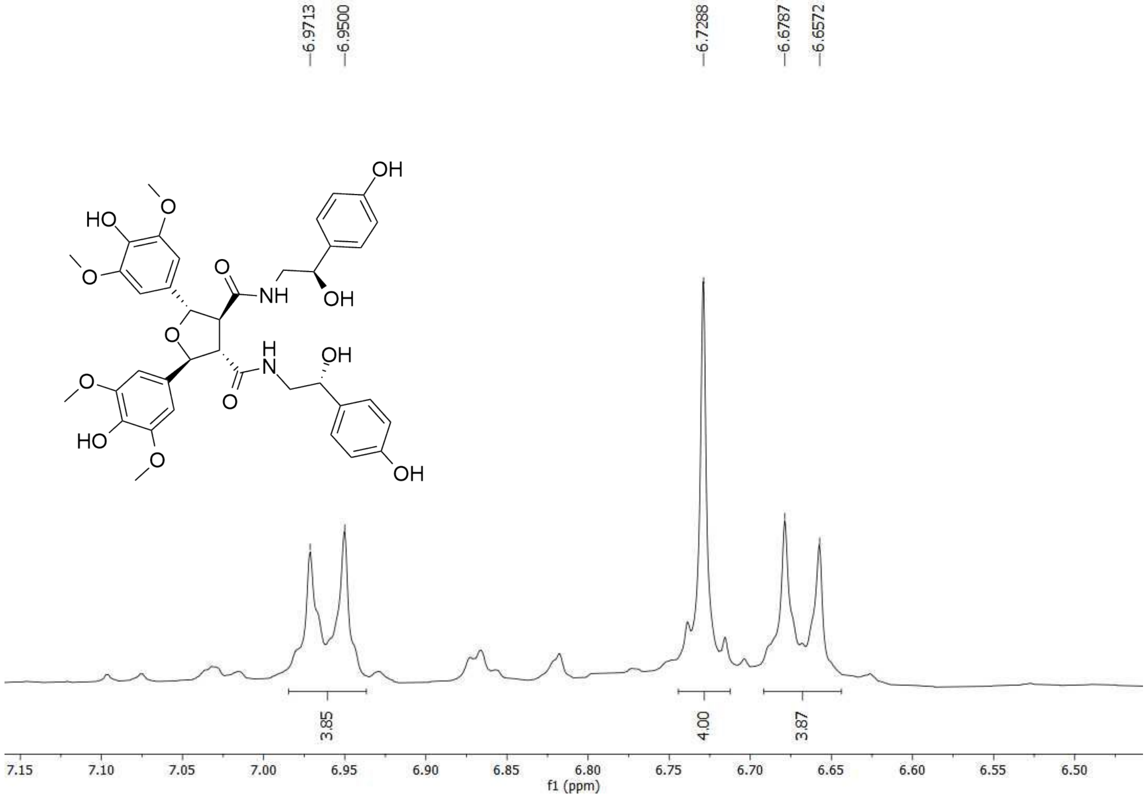

Figure S13. Amplification of the ^{1}H NMR spectrum of compound **2 (**400 MHz, MeOD).

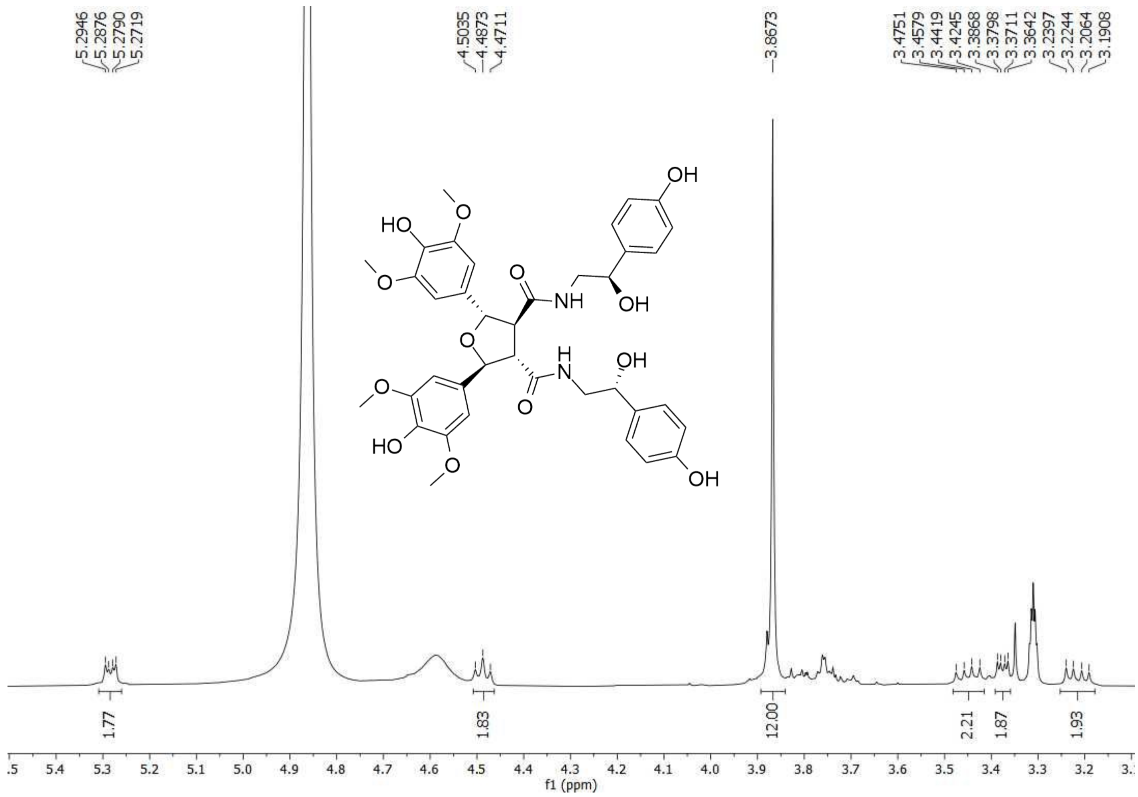

Figure S14. Amplification of the ^{1}H NMR spectrum of compound **2 (**400 MHz, MeOD).

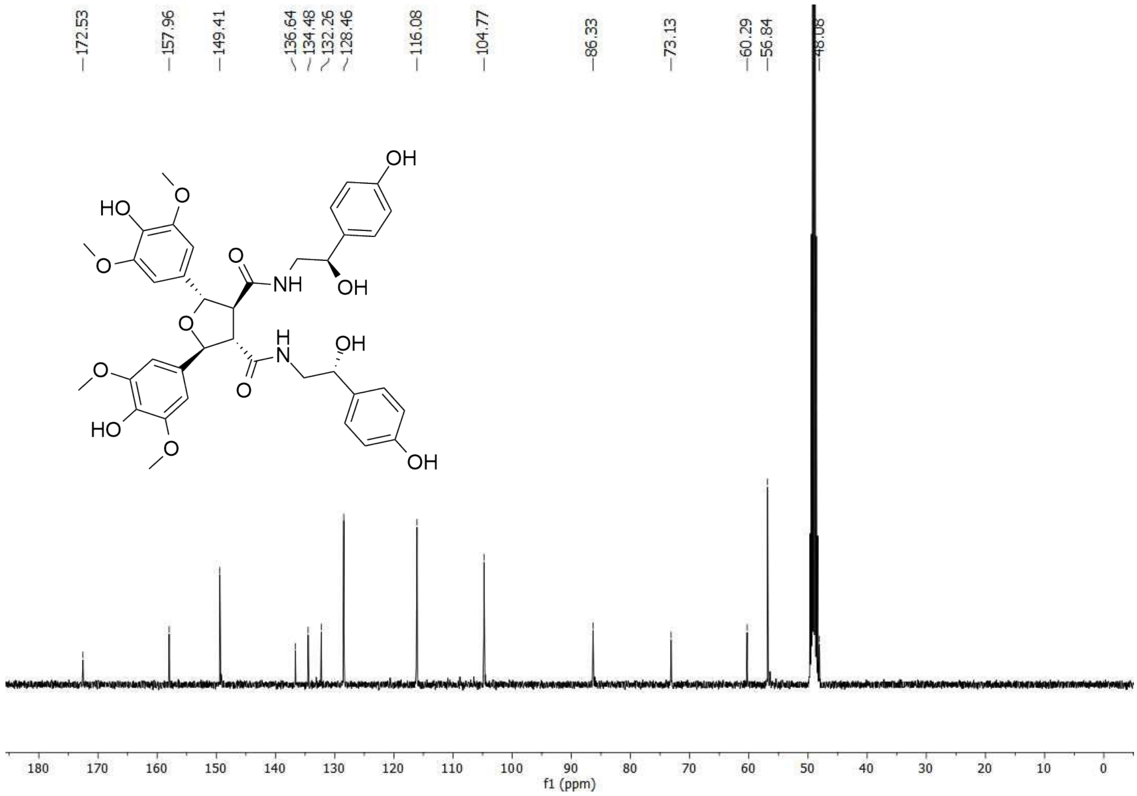

Figure S15. ^{13}C-BB NMR spectrum of compound **2** (100 MHz, MeOD).

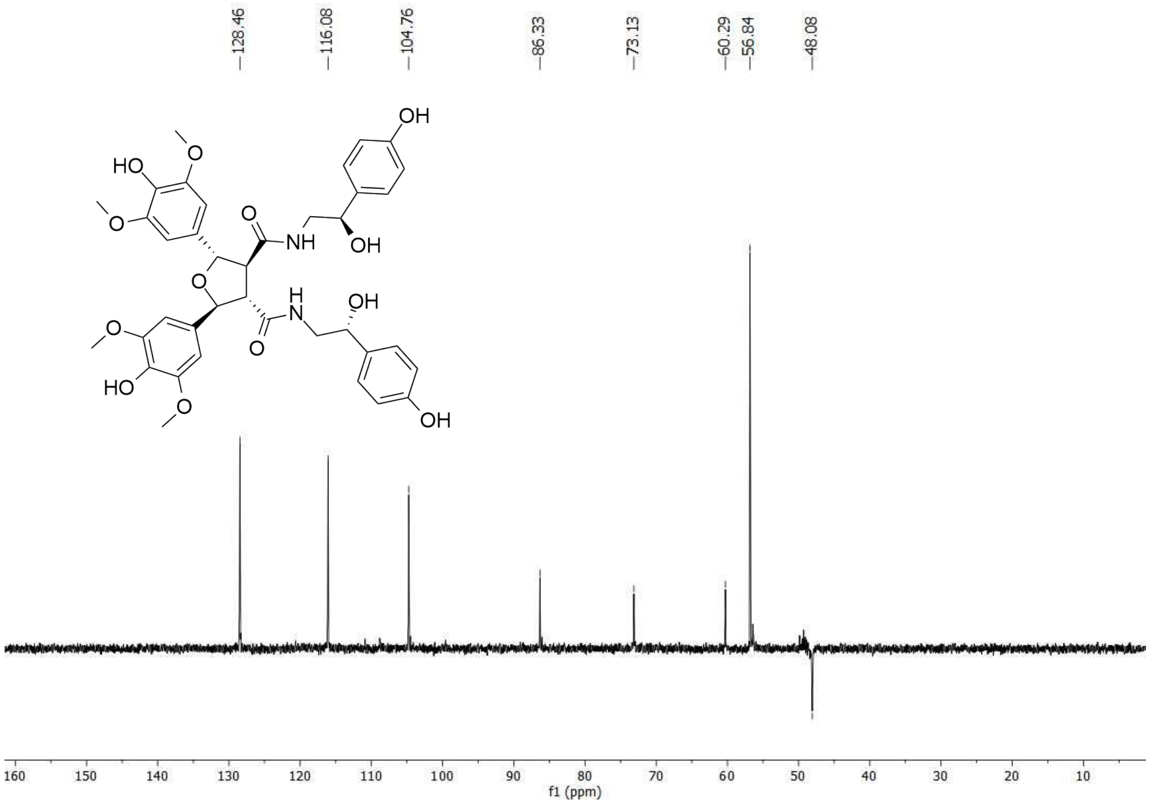

Figure S16. ^{13}C-DEPT135 NMR spectrum of compound **2** (100 MHz, MeOD).

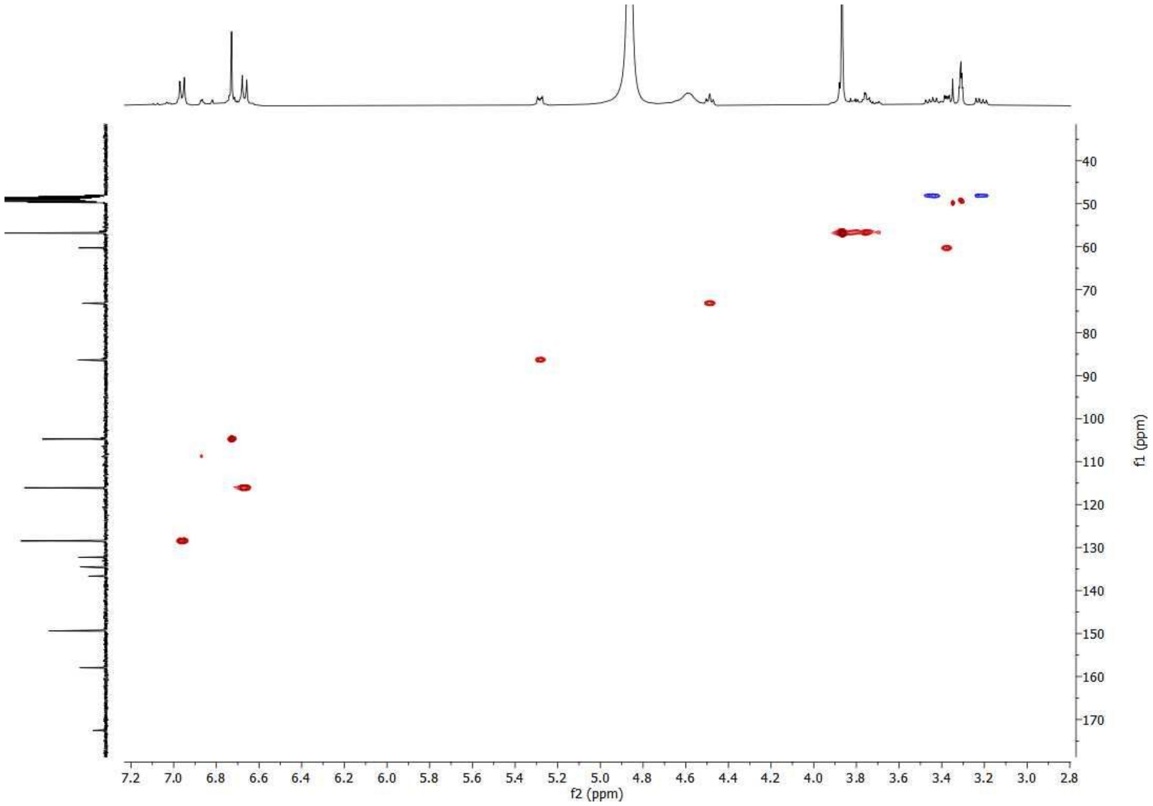

Figure S17. HSQC spectrum of compound **2** (400/100 MHz, MeOD).

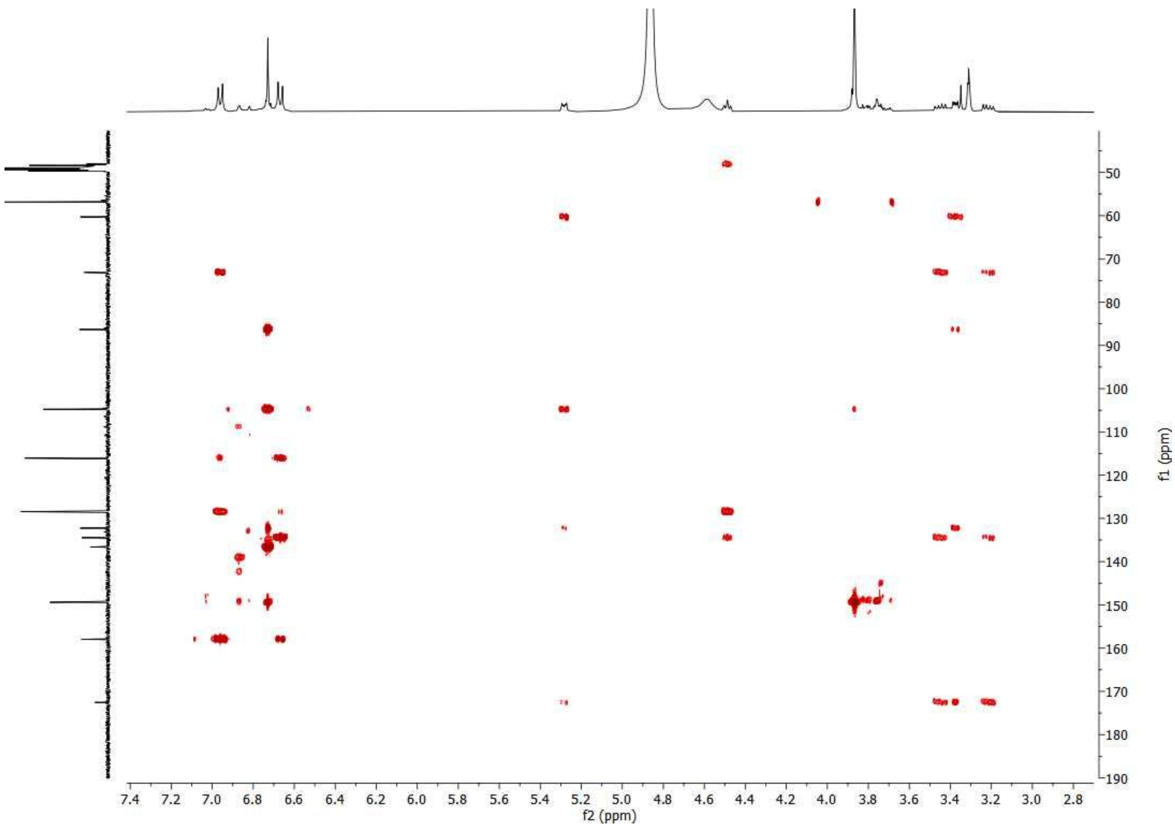

Figure S18. HMBC spectrum of compound **2** (400/100 MHz, MeOD).

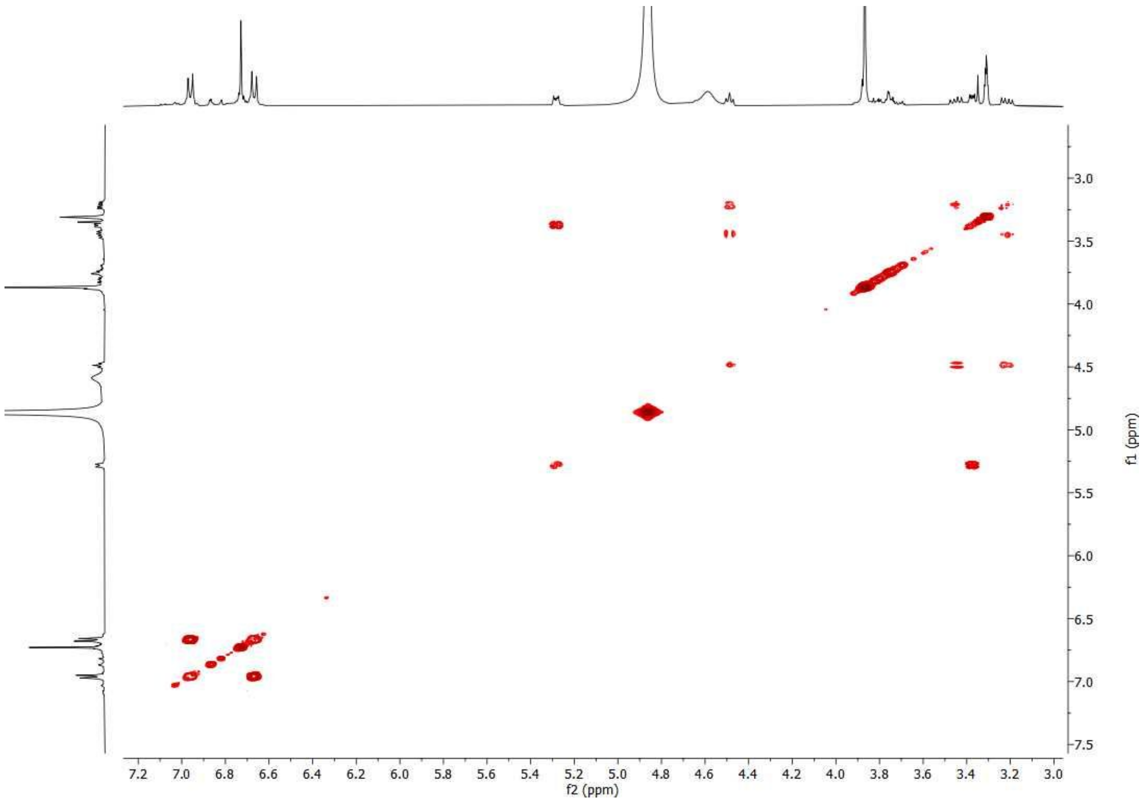

Figure S19. COSY spectrum of compound **2 (**400 MHz, MeOD).

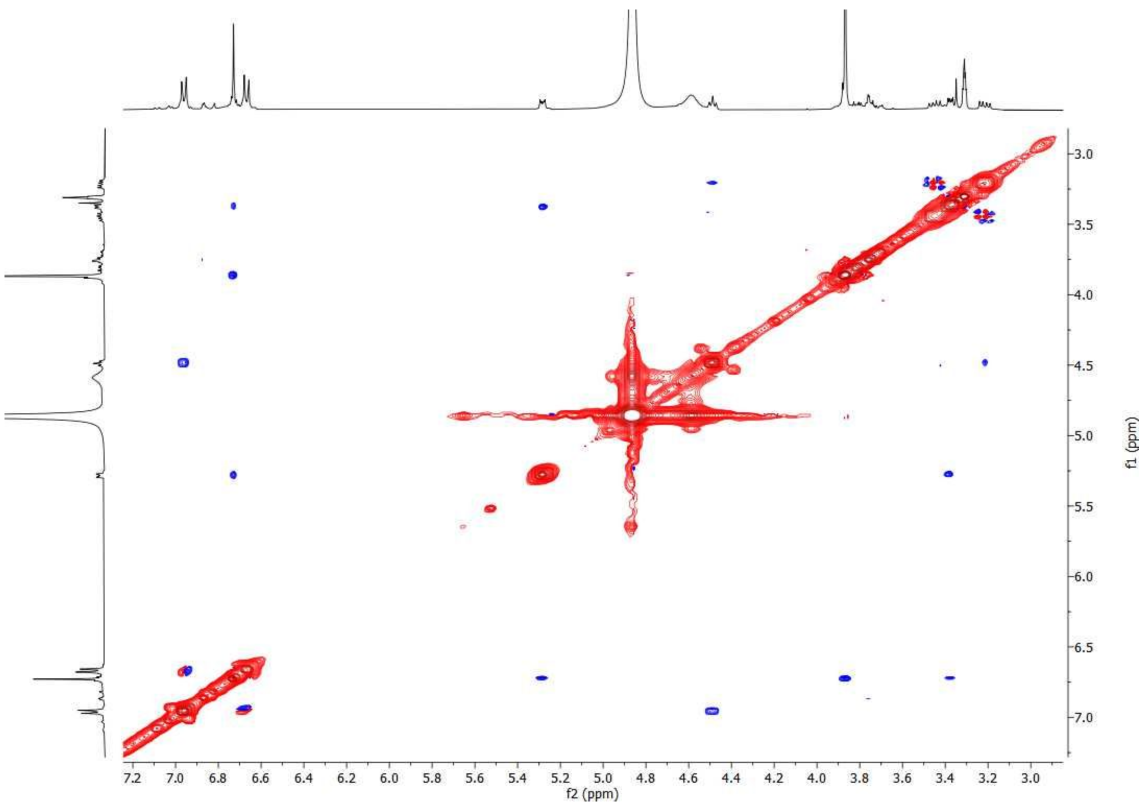

Figure S20. NOESY spectrum of compound **2 (**400 MHz, MeOD).

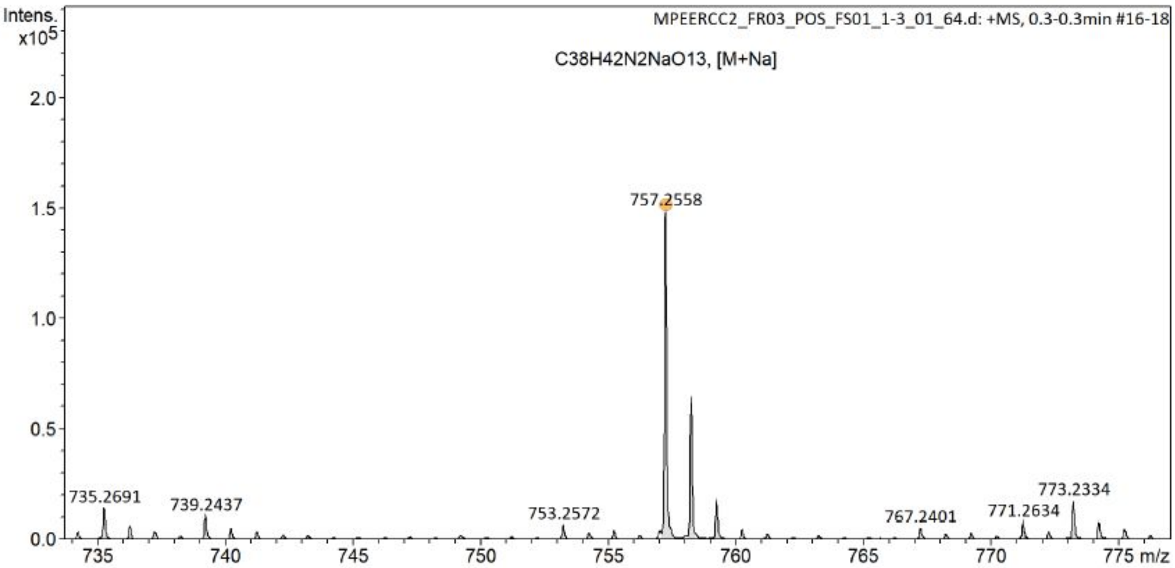

Figure S21. HRESIMS spectrum of compound **2** ($[M + Na]^+$, positive mode).

3 Spectroscopic data for Compound 3

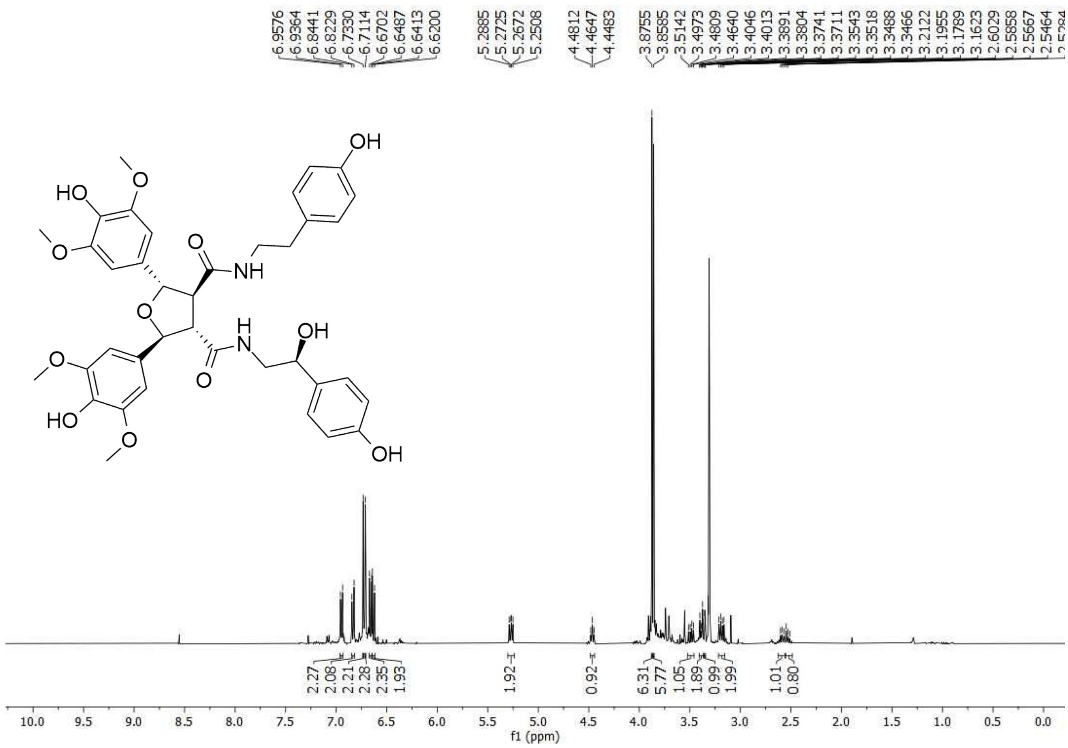

Figure S22. ^{1}H NMR spectrum of compound **3** (400 MHz, MeOD).

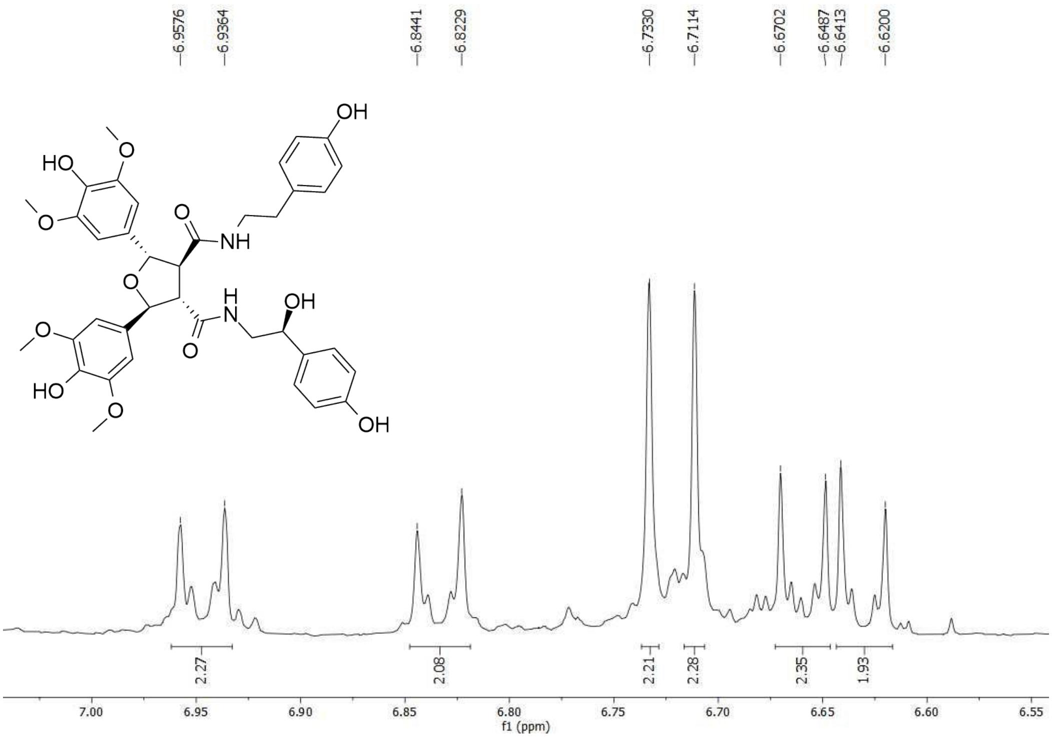

Figure S23. Amplification of the ¹H NMR spectrum of compound **3** (400 MHz, MeOD).

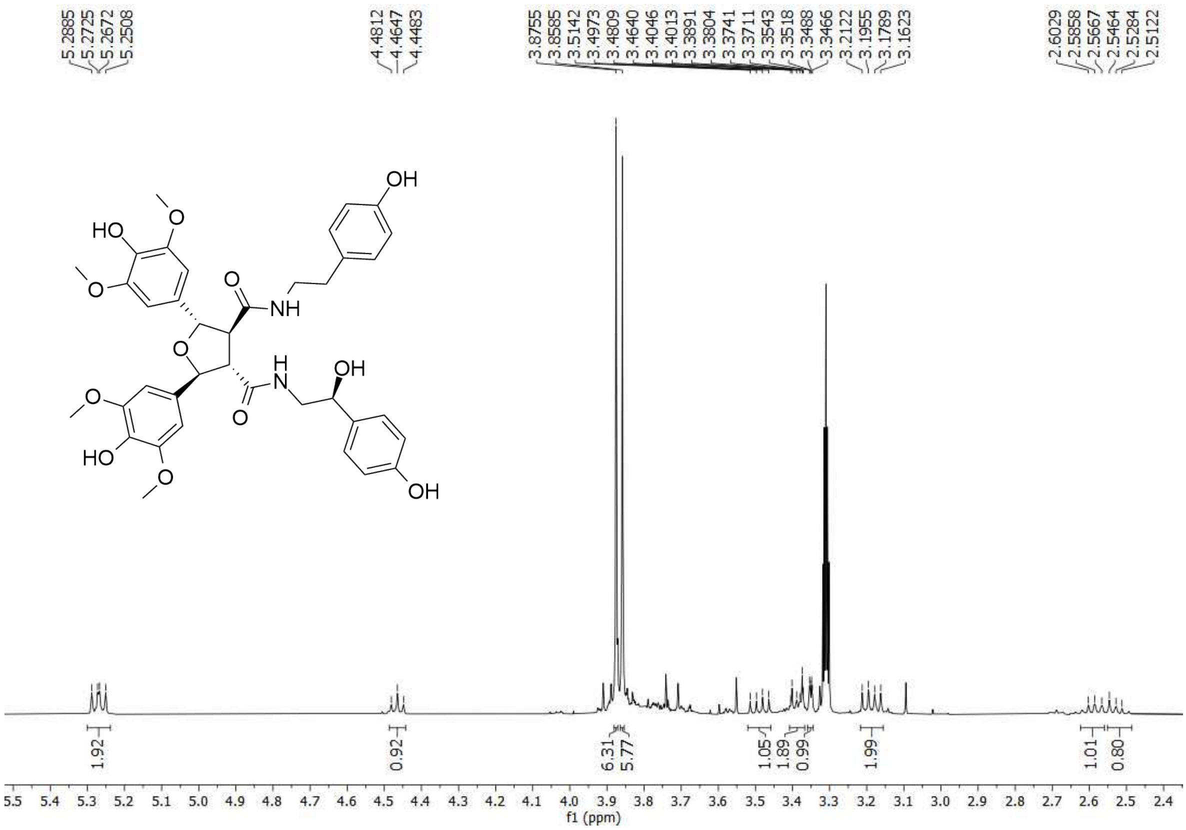

Figure S24. Amplification of the ¹H NMR spectrum of compound **3** (400 MHz, MeOD).

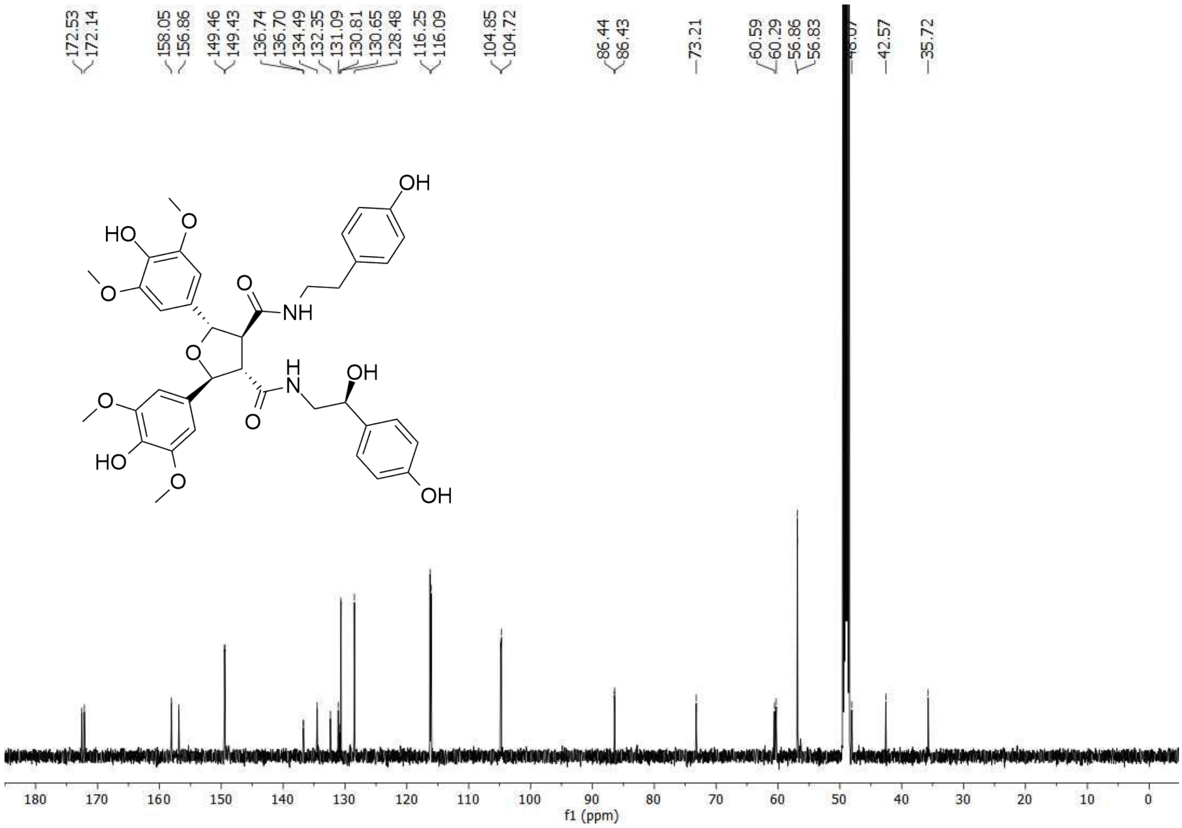

Figure S25. [13]C-BB NMR spectrum of compound **3** (100 MHz, MeOD).

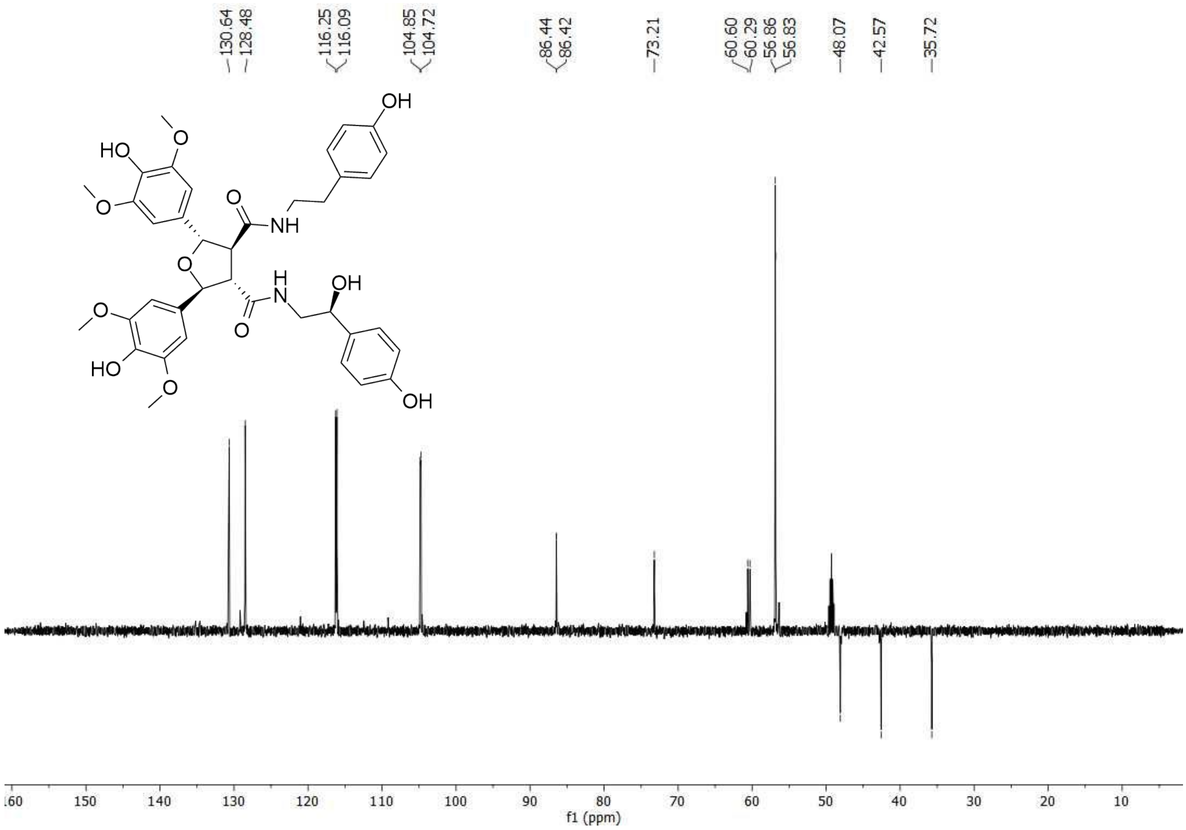

Figure S26. [13]C-DEPT135 NMR spectrum of compound **3** (100 MHz, MeOD).

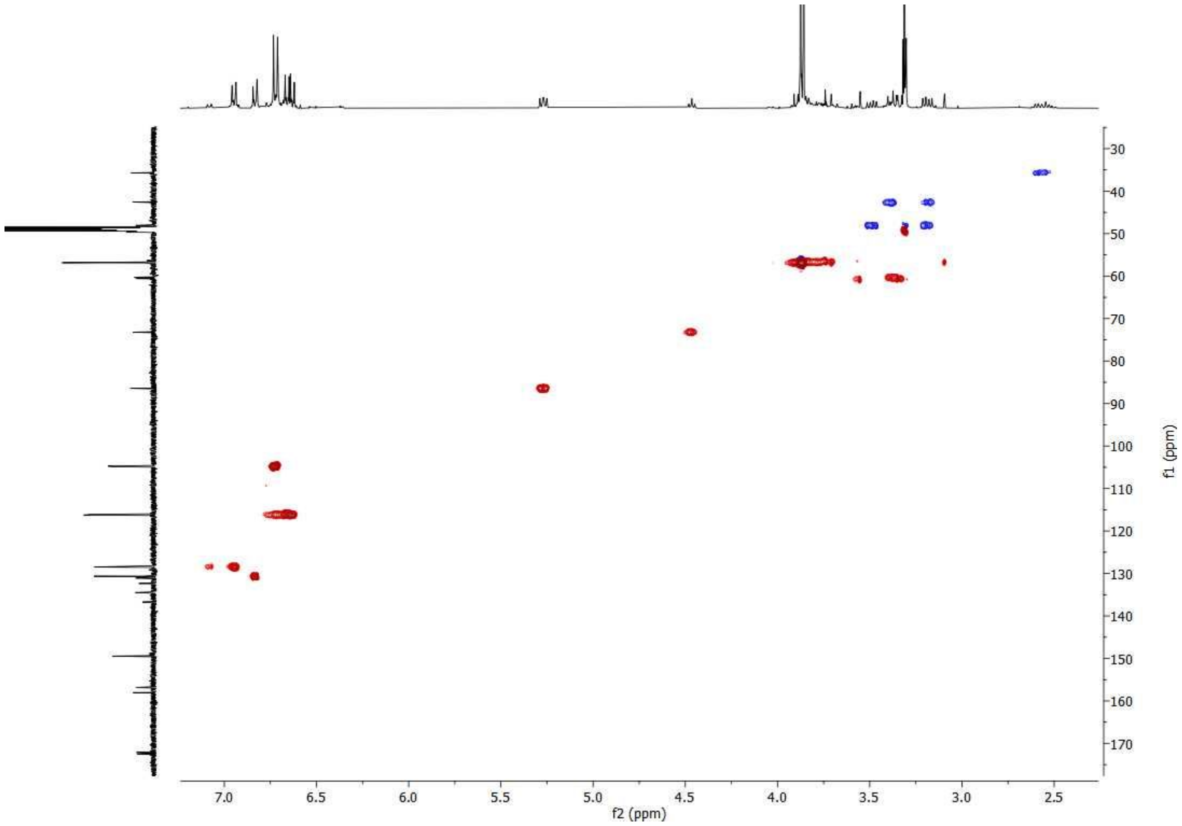

Figure S27. HSQC spectrum of compound **3** (400/100 MHz, MeOD).

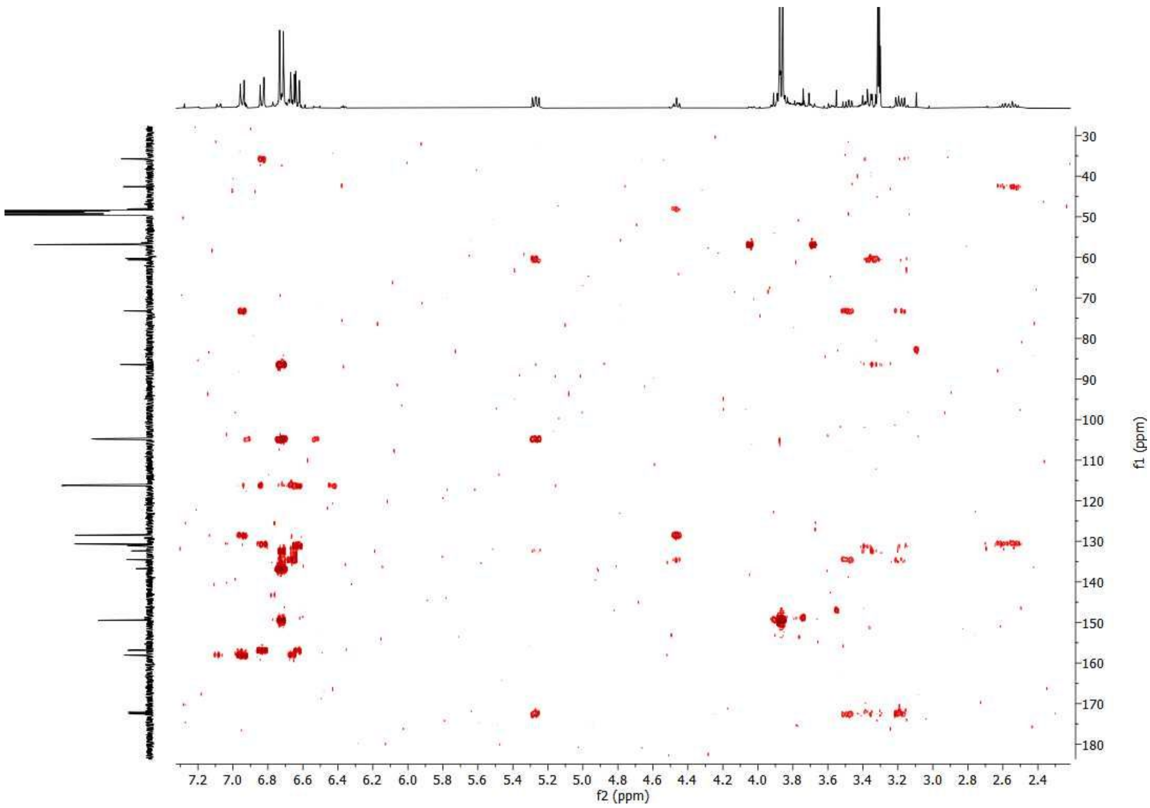

Figure S28. HMBC spectrum of compound **3** (400/100 MHz, MeOD).

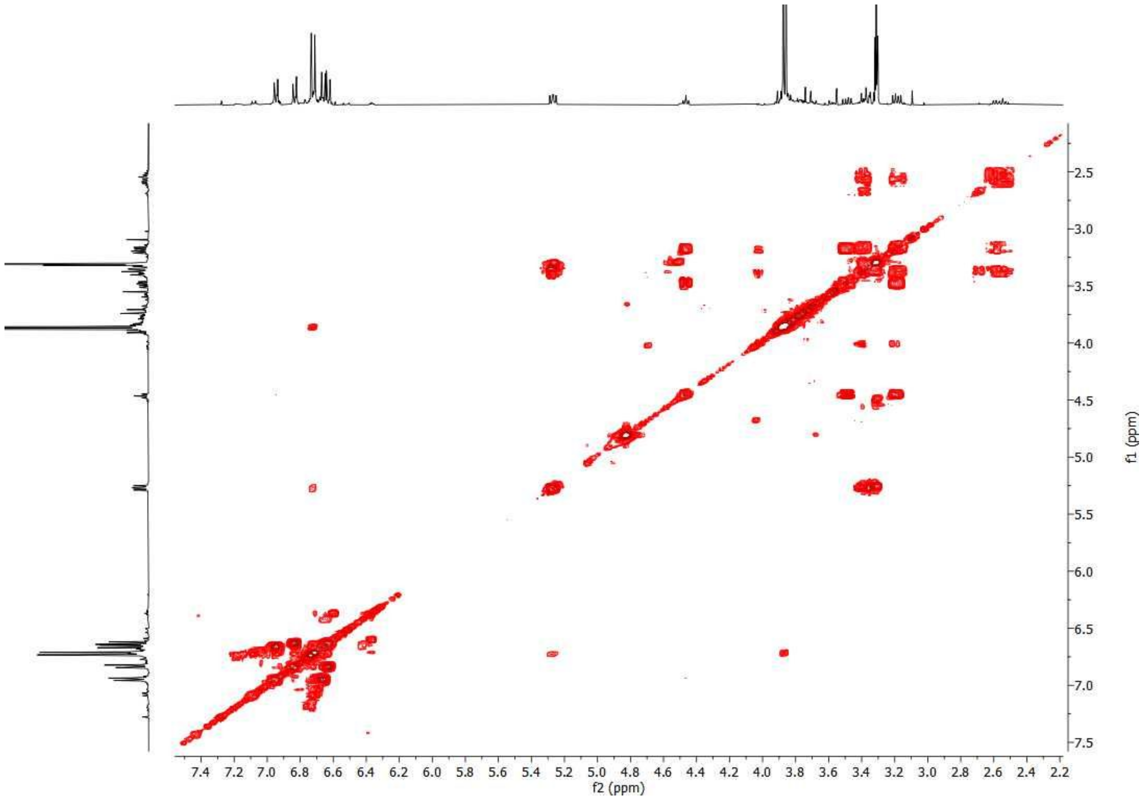

Figure S29. COSY spectrum of compound **3** (400 MHz, MeOD).

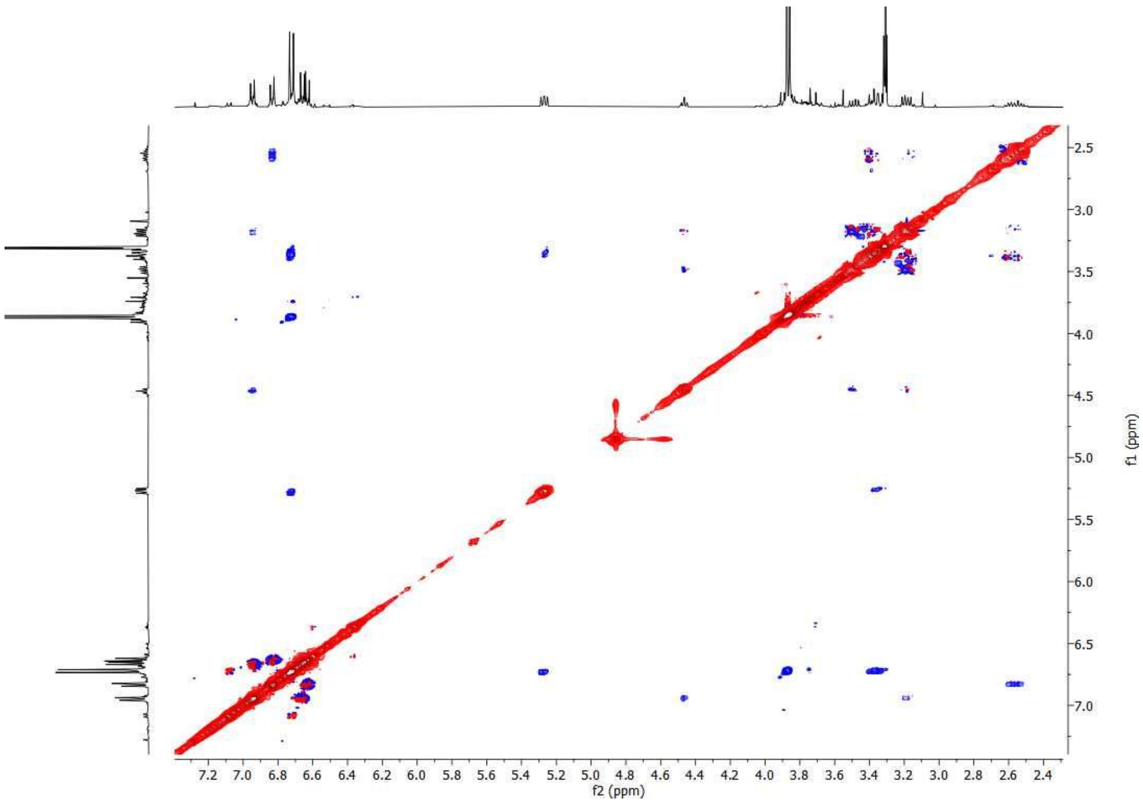

Figure S30. NOESY spectrum of compound **3** (400 MHz, MeOD).

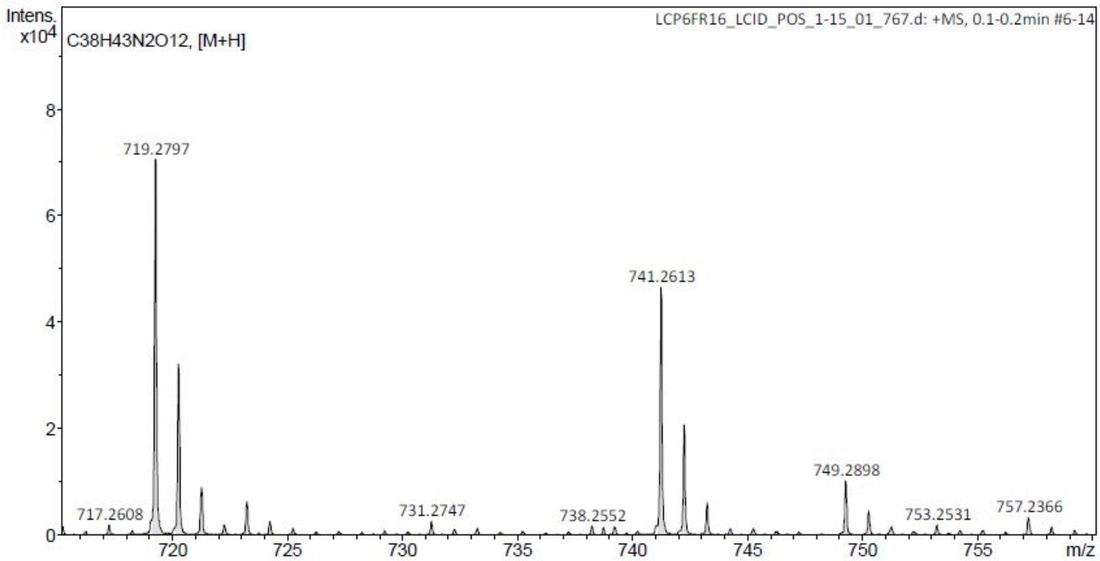

Figure S31. HRESIMS spectrum of compound **3** ($[M + H]^+$, positive mode).

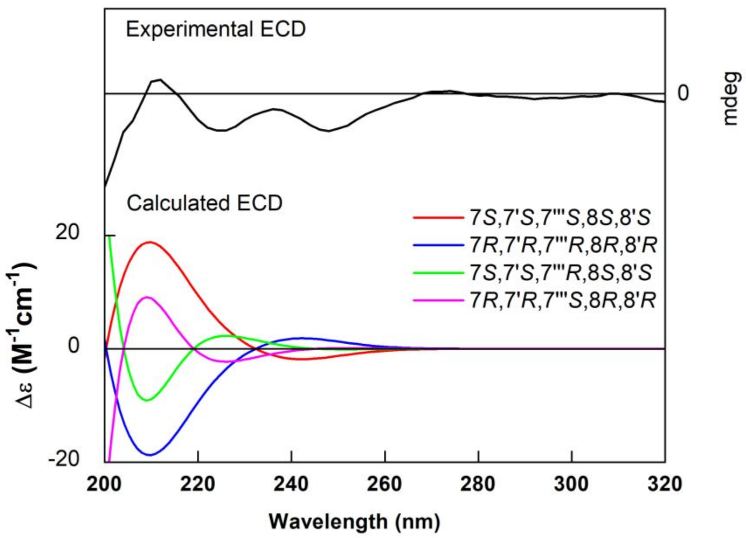

Figure S32. Experimental (top) and calculated (bottom) ECD spectra of all possible stereoisomers of compound **3**.

4 Spectroscopic data for Compound 4

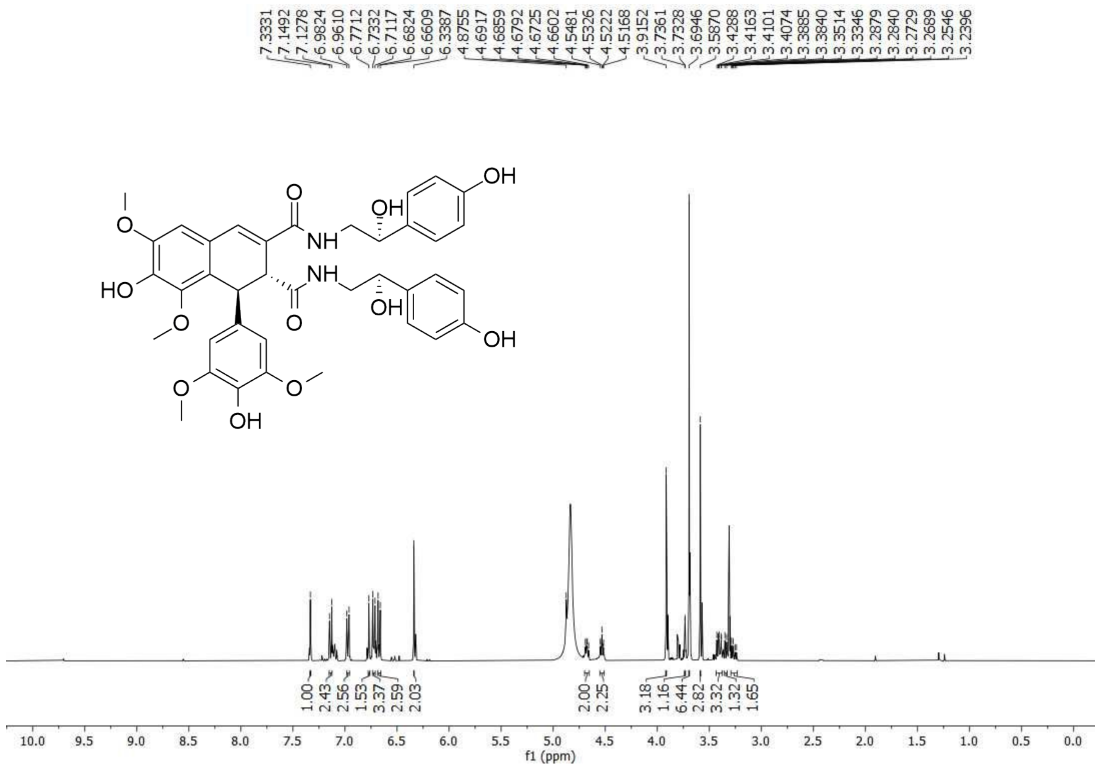

Figure S33. [1]H NMR spectrum of compound **4** (400 MHz, MeOD).

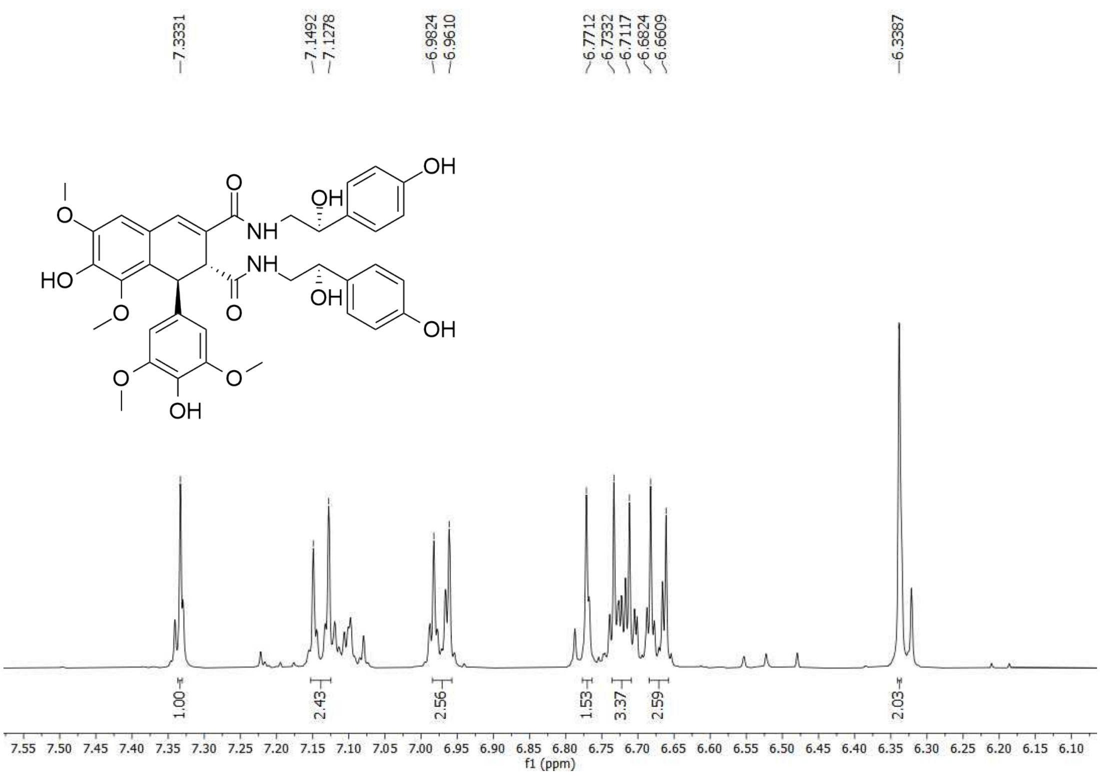

Figure S34. Amplification of the [1]H NMR spectrum of compound **4** (400 MHz, MeOD).

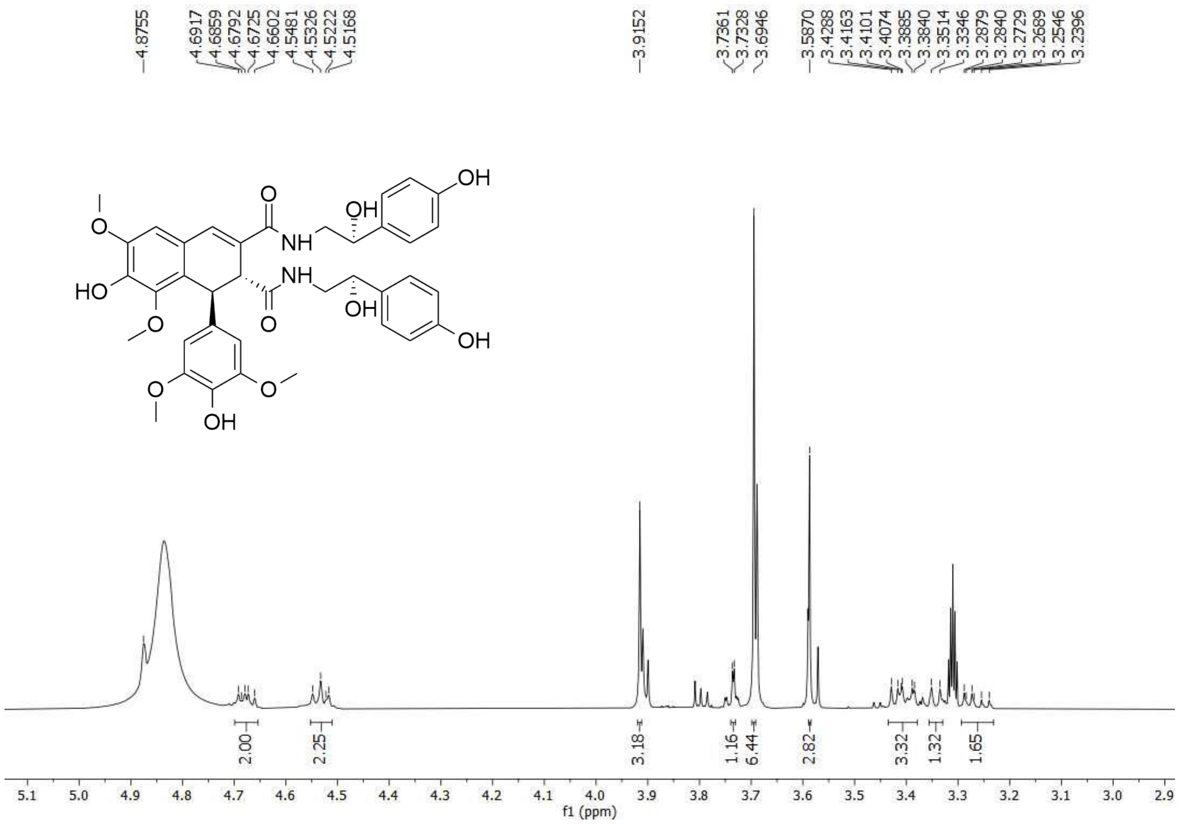

Figure S35. Amplification of the ^{1}H NMR spectrum of compound **4** (400 MHz, MeOD).

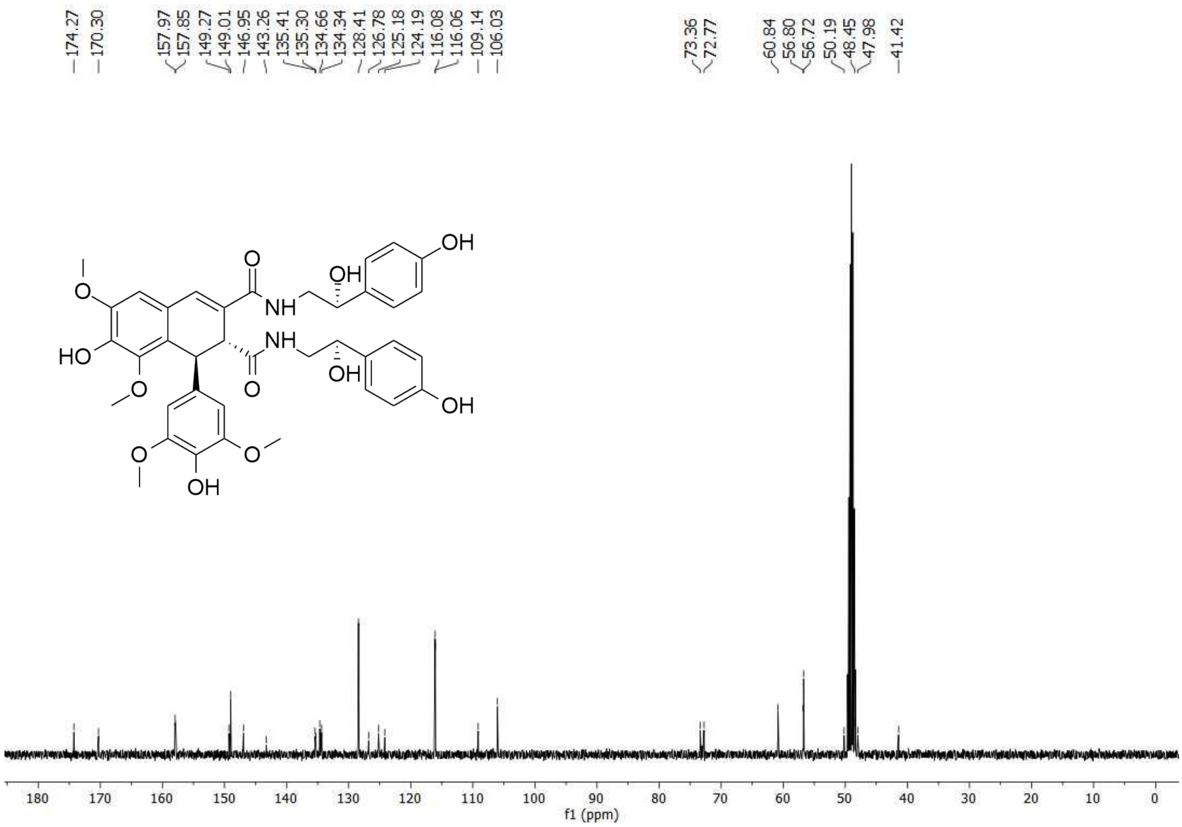

Figure S36. ^{13}C-BB NMR spectrum of compound **4** (100 MHz, MeOD).

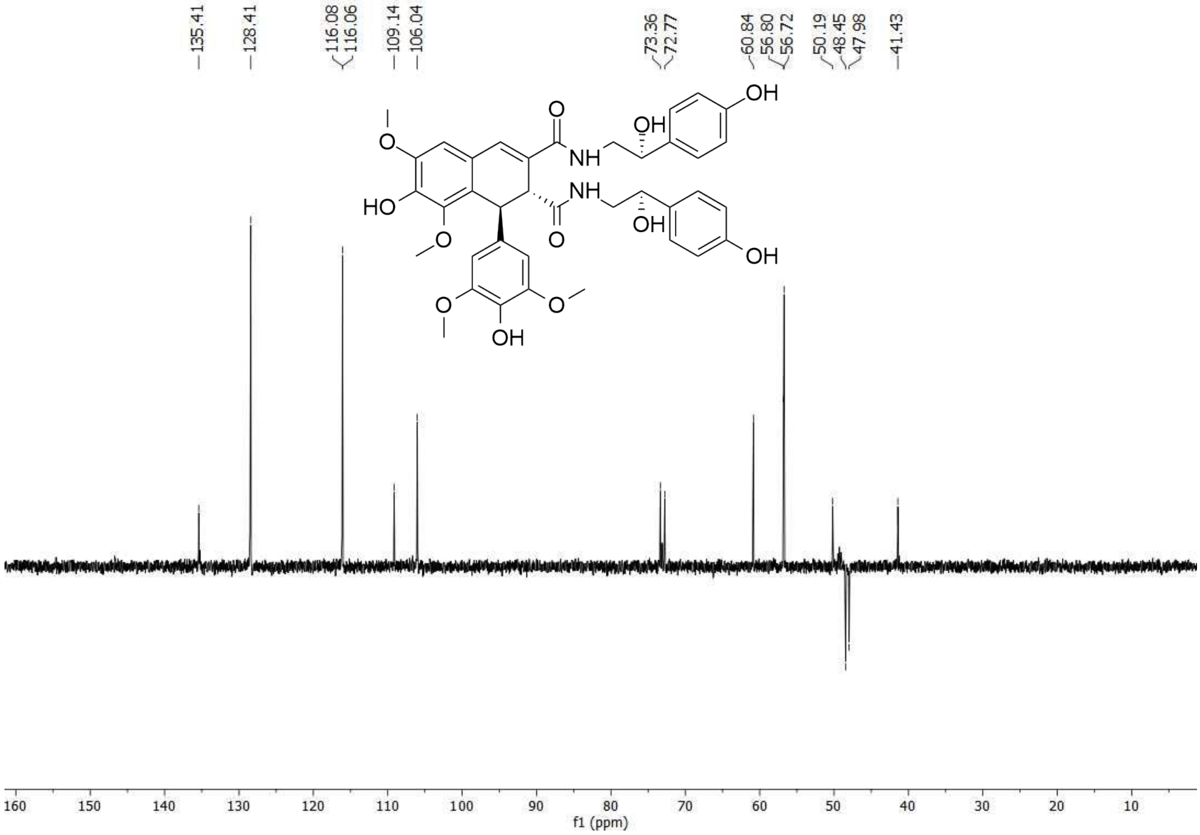

Figure S37. [13]C-DEPT135 NMR spectrum of compound **4** (100 MHz, MeOD).

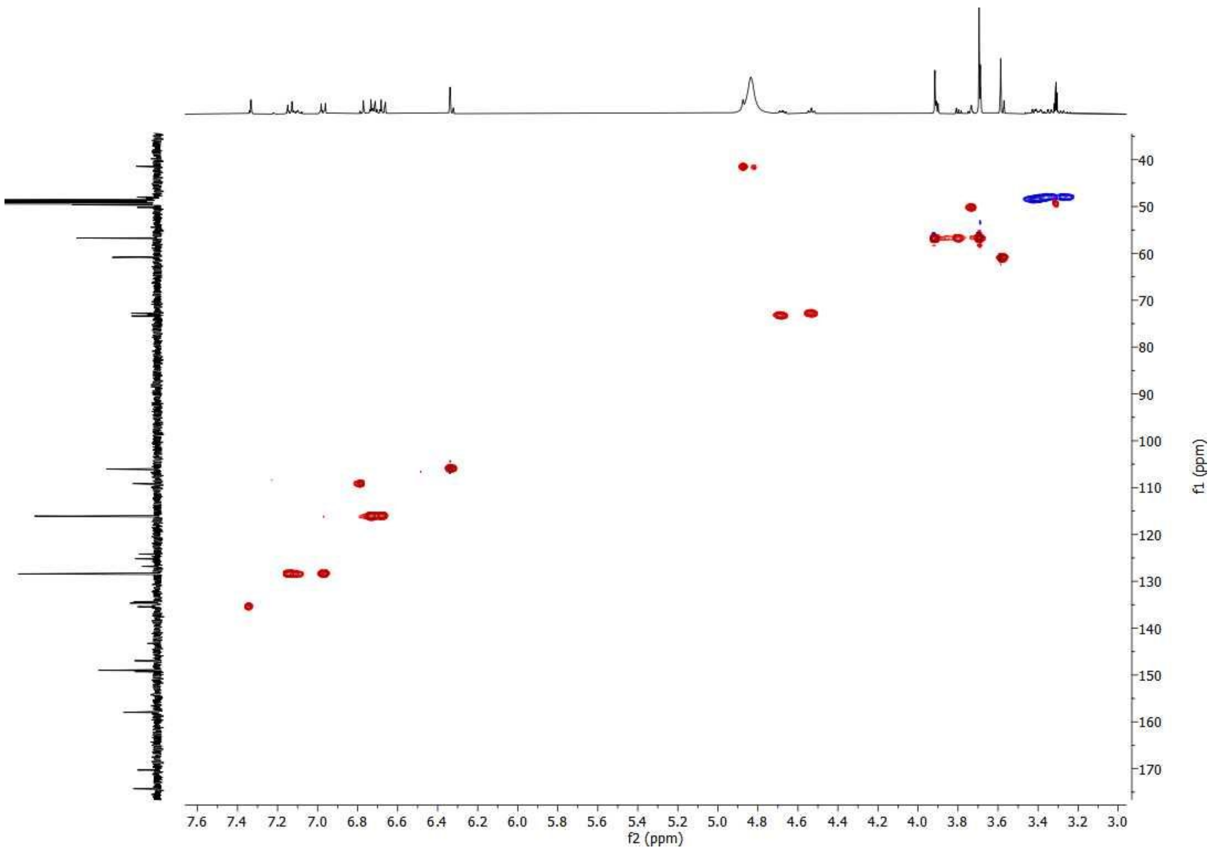

Figure S38. HSQC spectrum of compound **4** (400/100 MHz, MeOD).

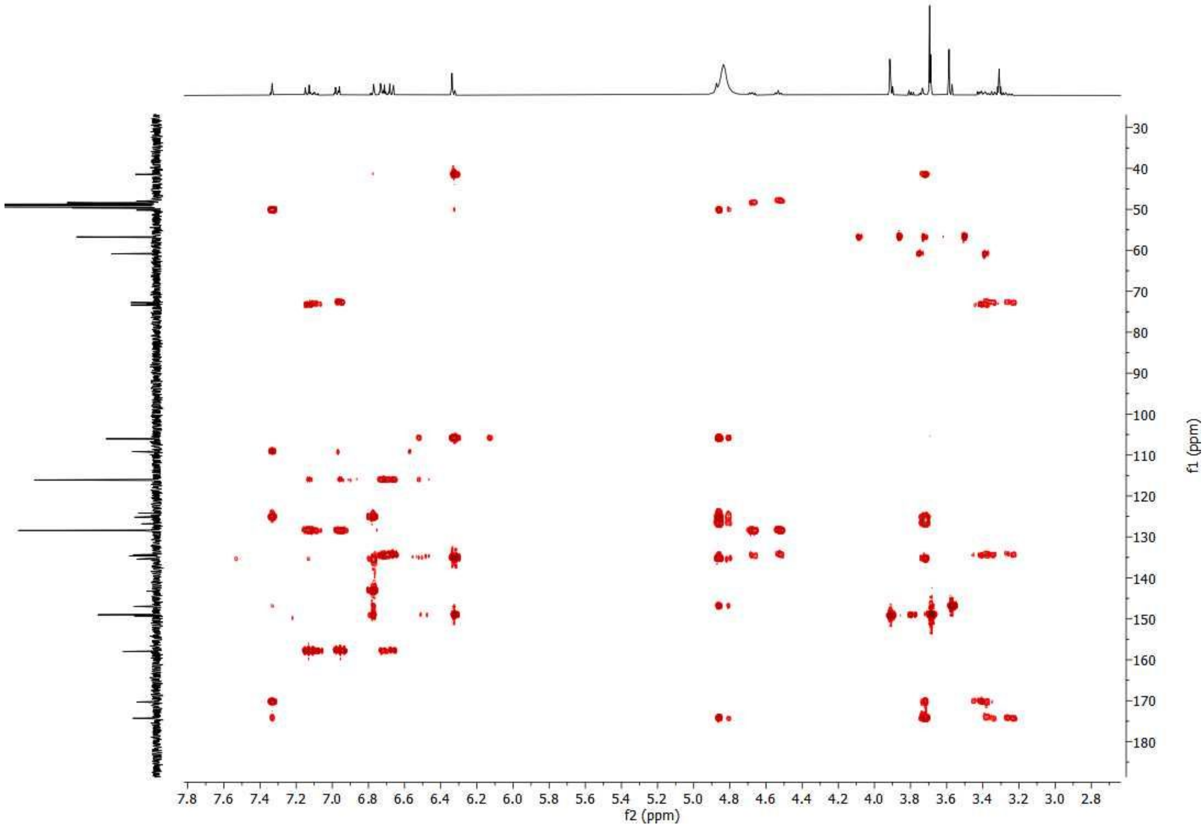

Figure S39. HMBC spectrum of compound **4 (**400/100 MHz, MeOD).

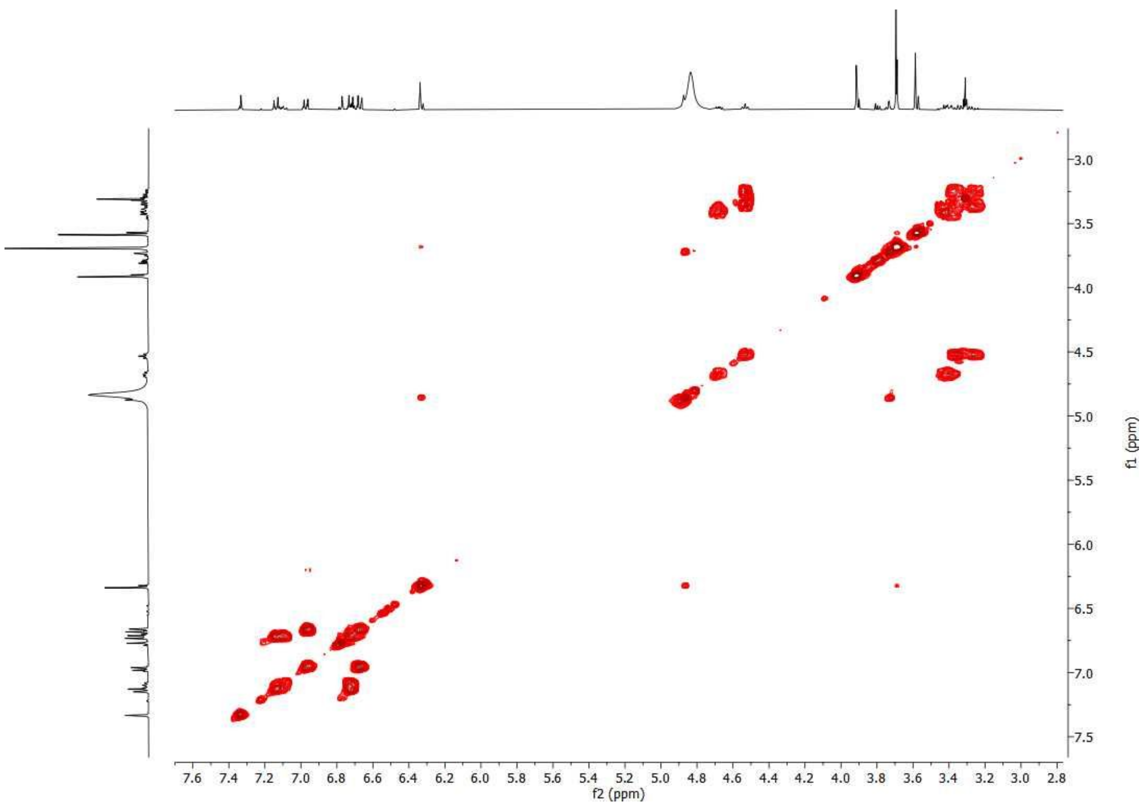

Figure S40. COSY spectrum of compound **4 (**400 MHz, MeOD).

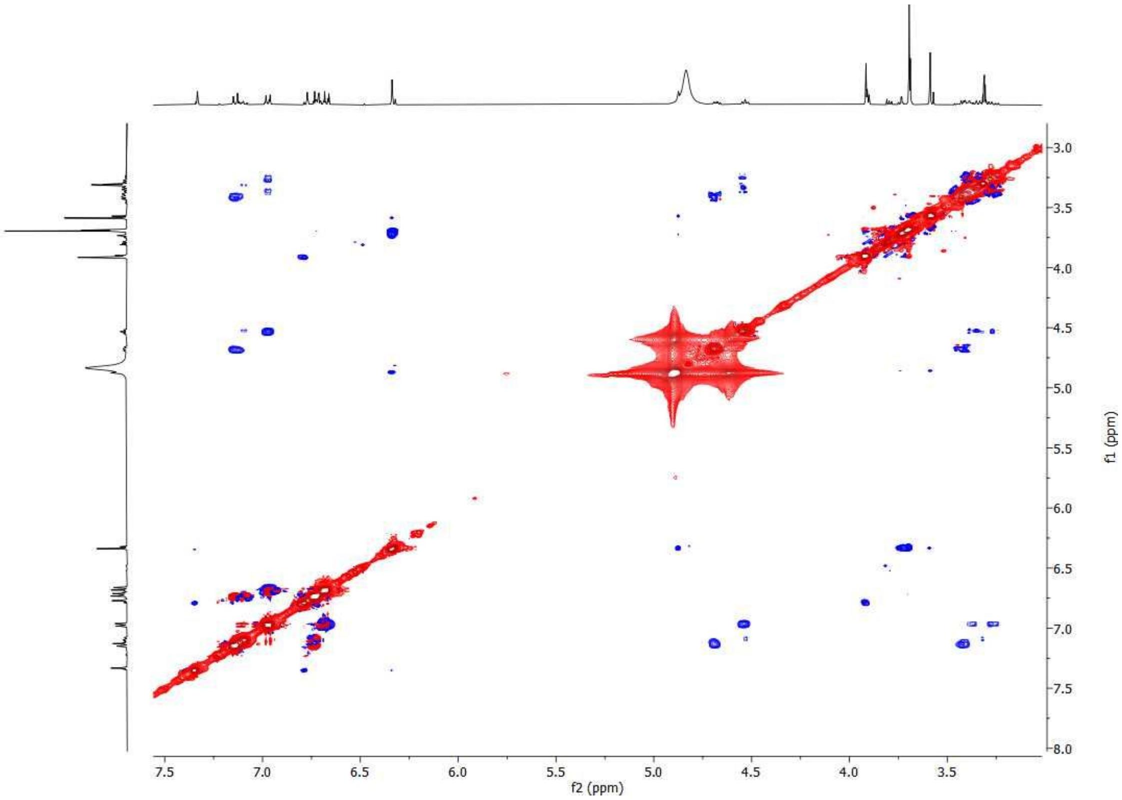

Figure S41. NOESY spectrum of compound **4 (**400 MHz, MeOD).

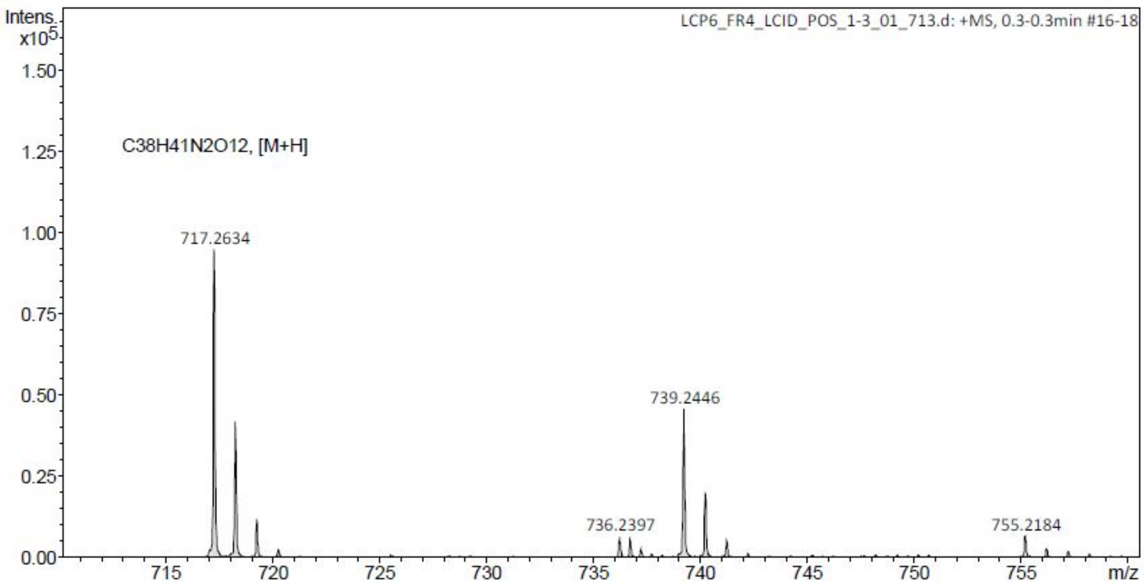

Figure S42. HRESIMS spectrum of compound **4** ($[M + H]^+$, positive mode).

5 Spectroscopic data for compound 5

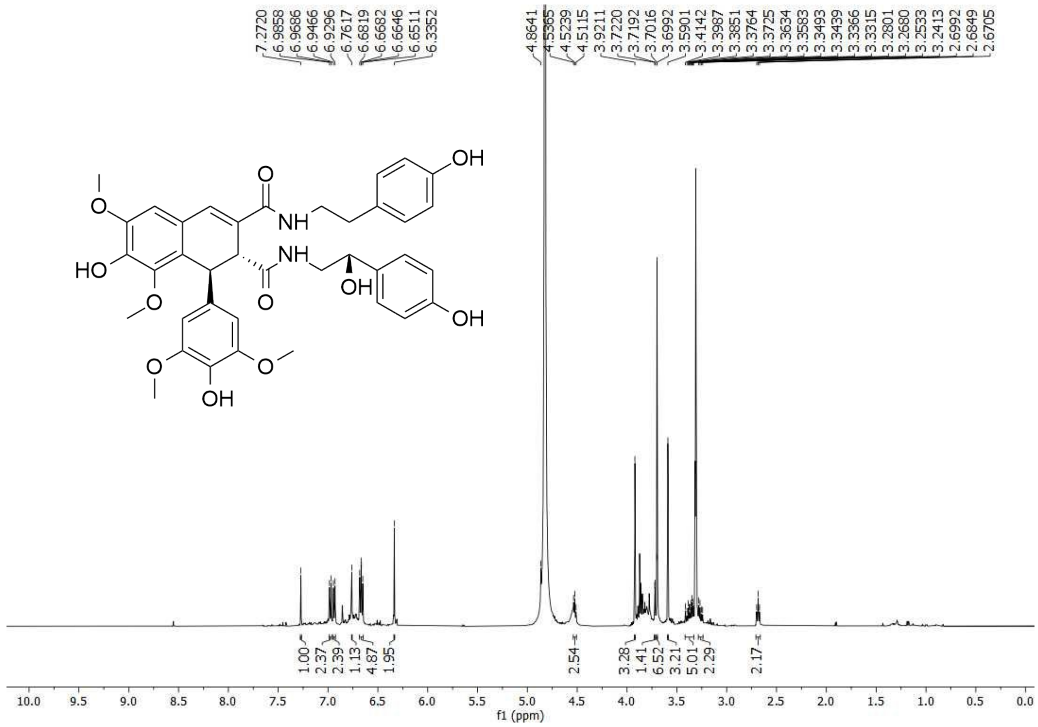

Figure S43. [1]H NMR spectrum of compound **5 (**500 MHz, MeOD).

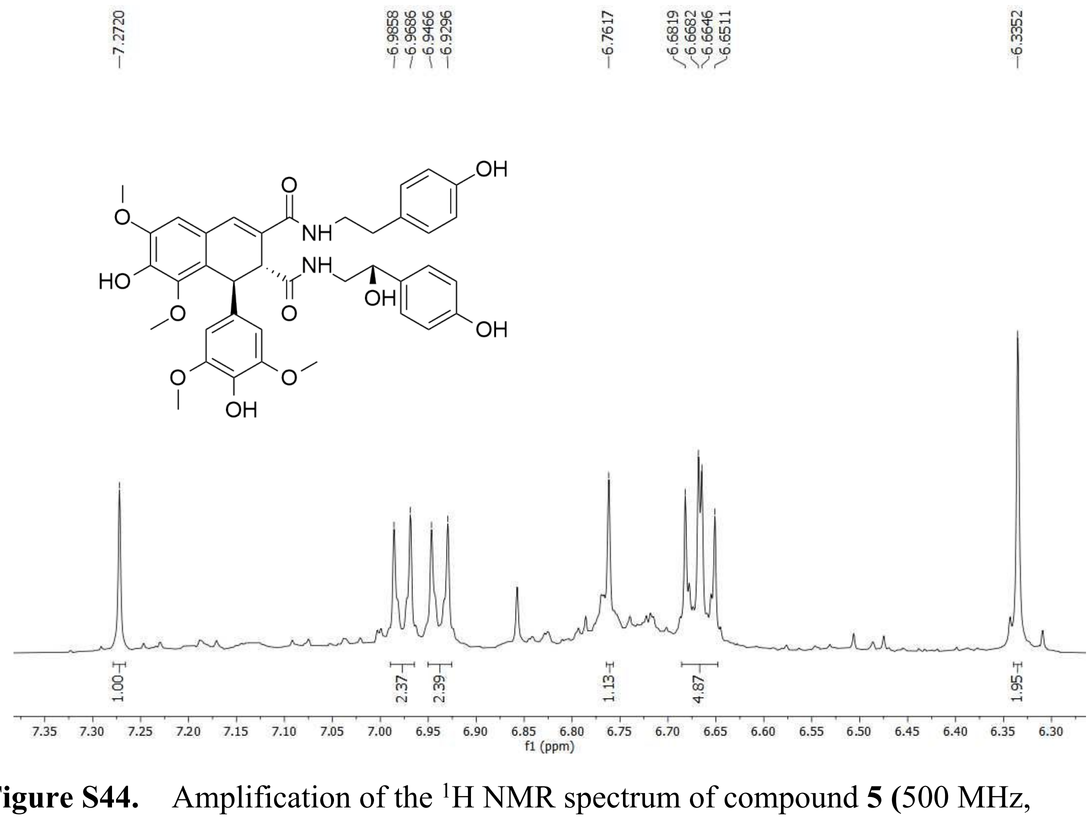

Figure S44. Amplification of the [1]H NMR spectrum of compound **5 (**500 MHz, MeOD).

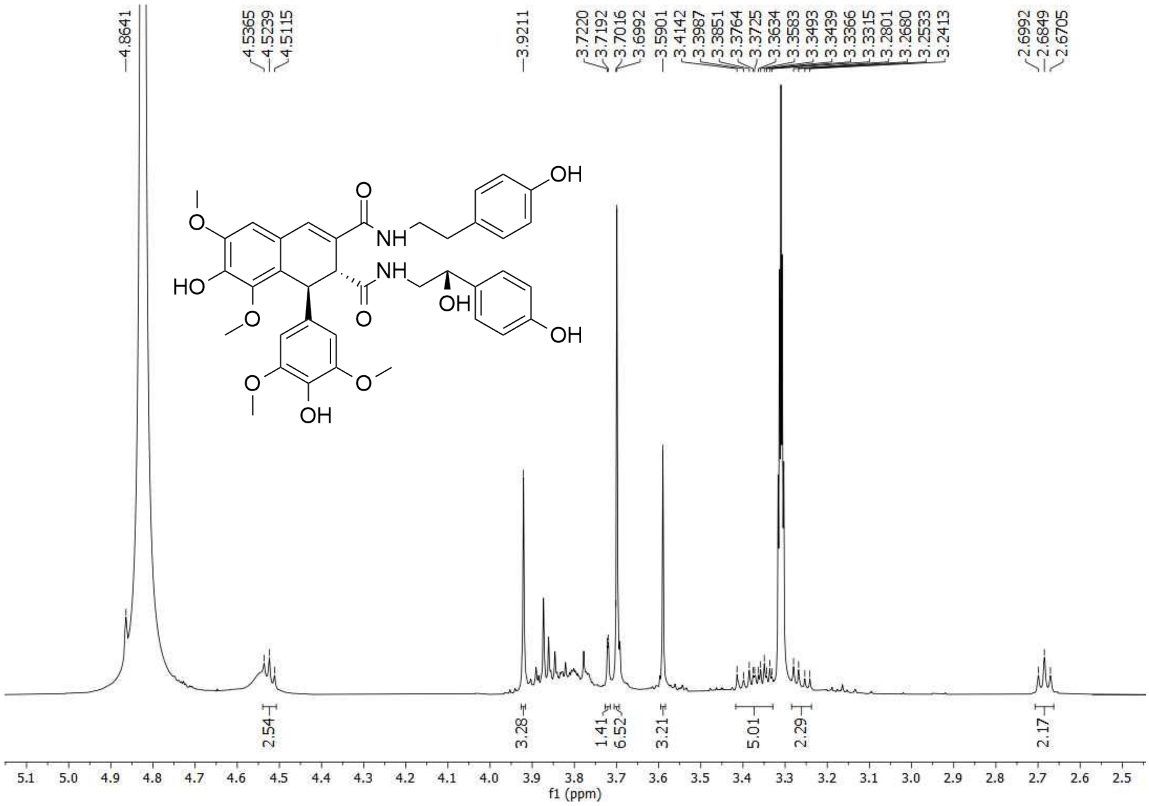

Figure S45. Amplification of the [1]H NMR spectrum of compound **5 (**500 MHz, MeOD).

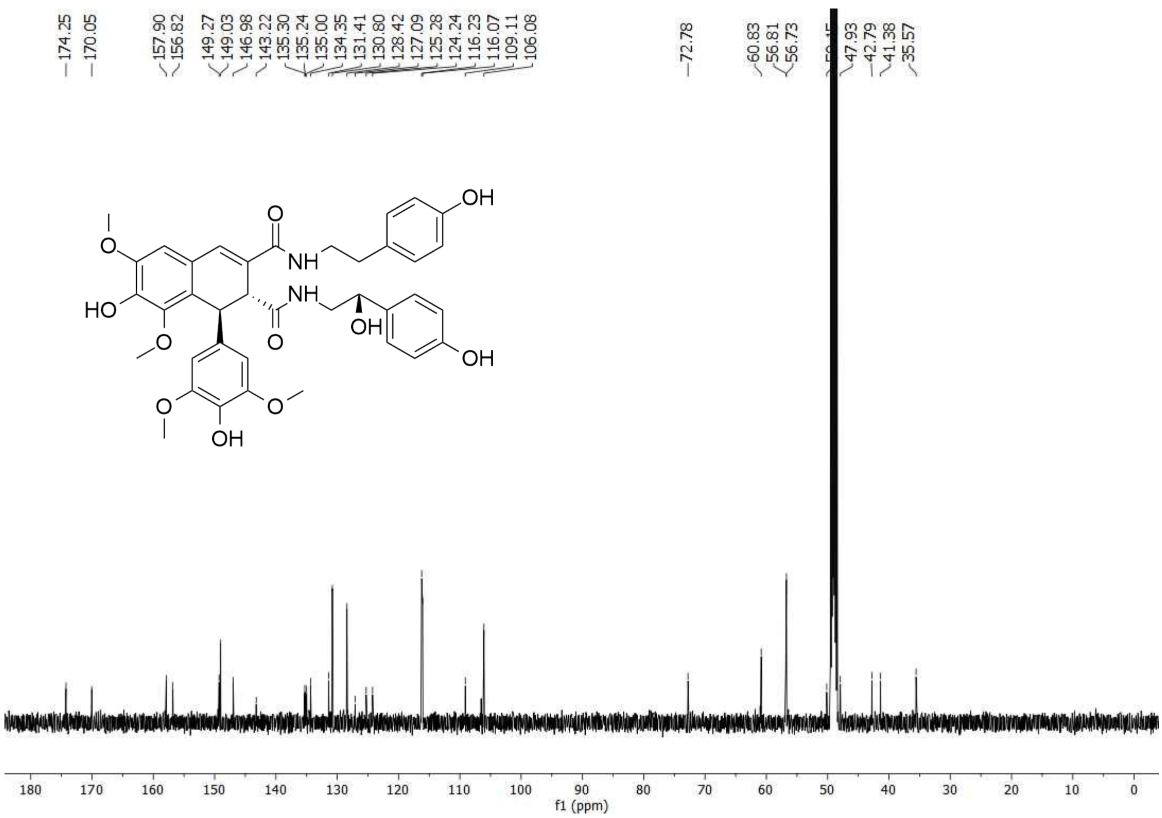

Figure S46. ^{13}C-BB NMR spectrum of compound **5** (125 MHz, MeOD).

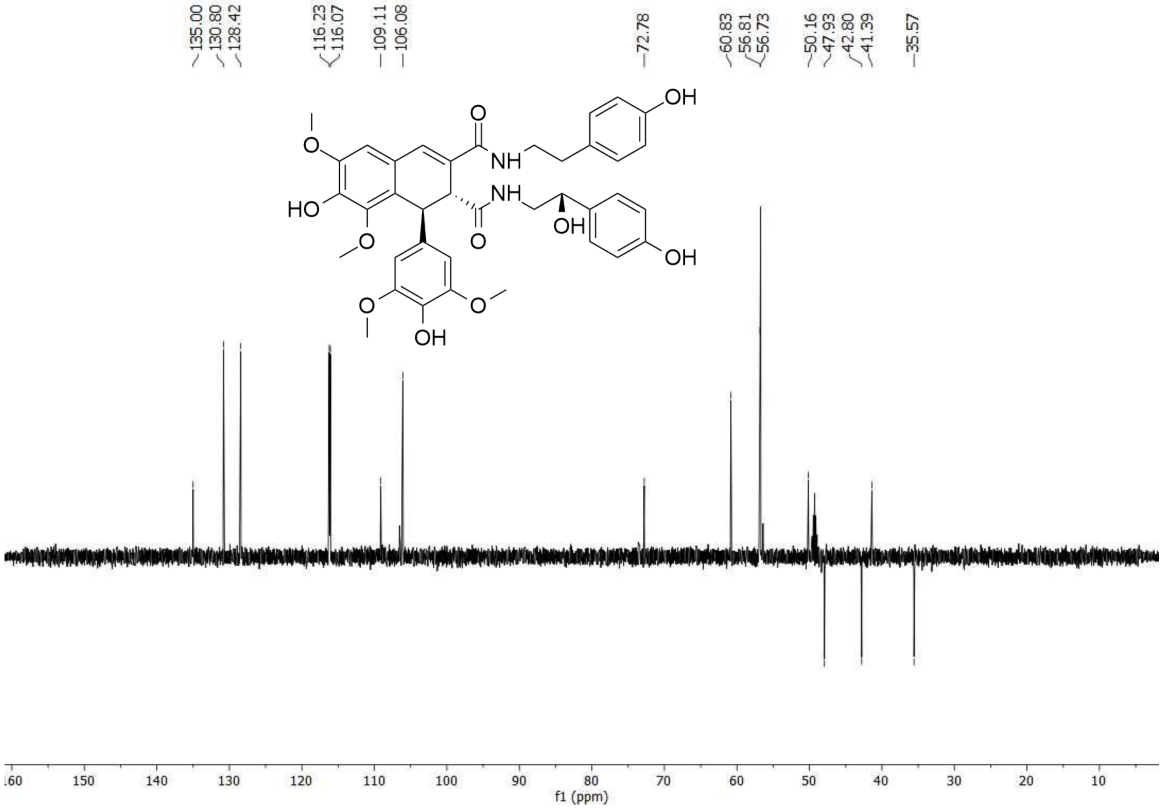

Figure S47. [13]C-DEPT135 NMR spectrum of compound **5** (125 MHz, MeOD).

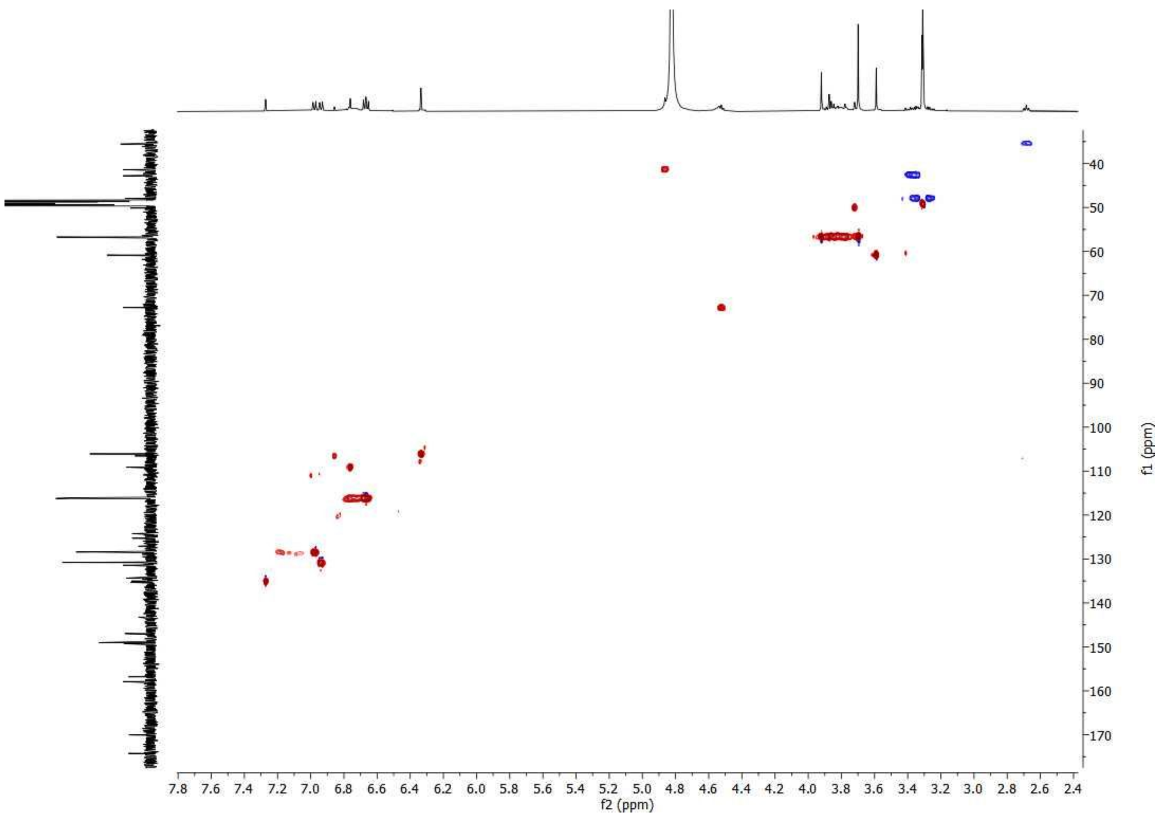

Figure S48. HSQC spectrum of compound **5** (500/125 MHz, MeOD).

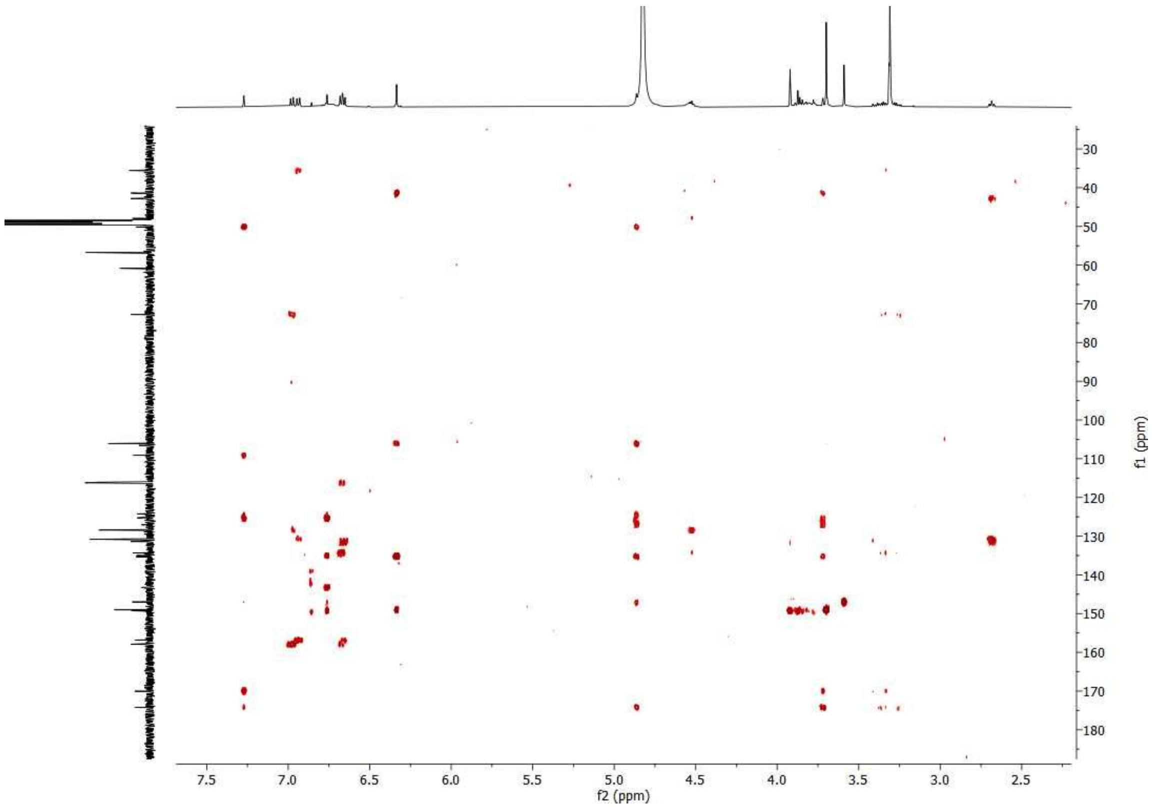

Figure S49. HMBC spectrum of compound **5 (**500/125 MHz, MeOD).

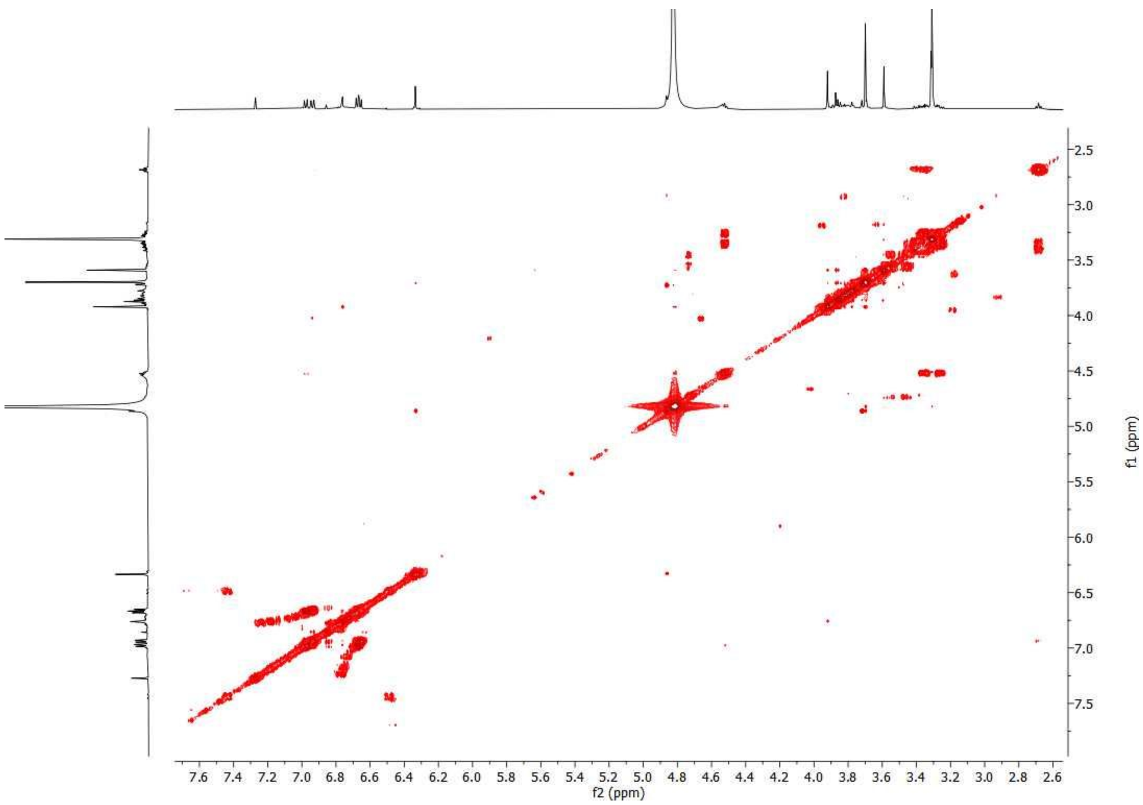

Figure S50. COSY spectrum of compound **5 (**500 MHz, MeOD).

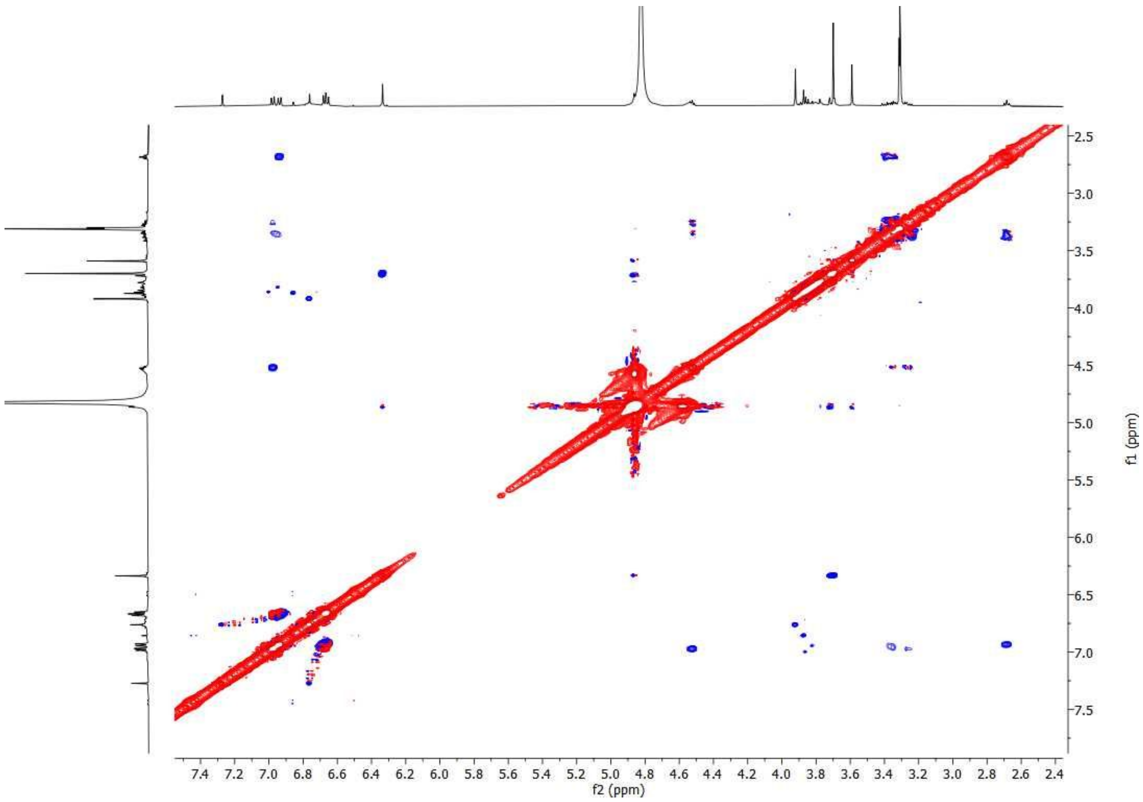

Figure S51. NOESY spectrum of compound **5 (**500 MHz, MeOD).

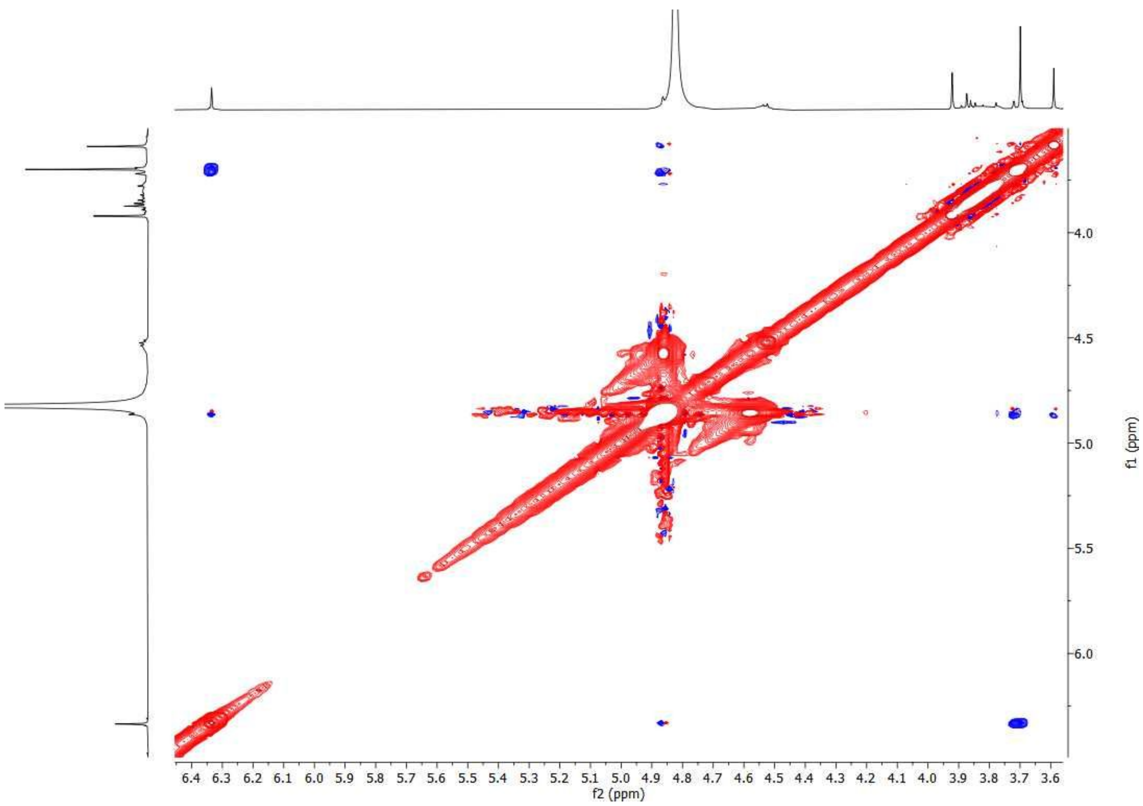

Figure S52. Amplification of the NOESY spectrum of compound **5 (**500 MHz, MeOD).

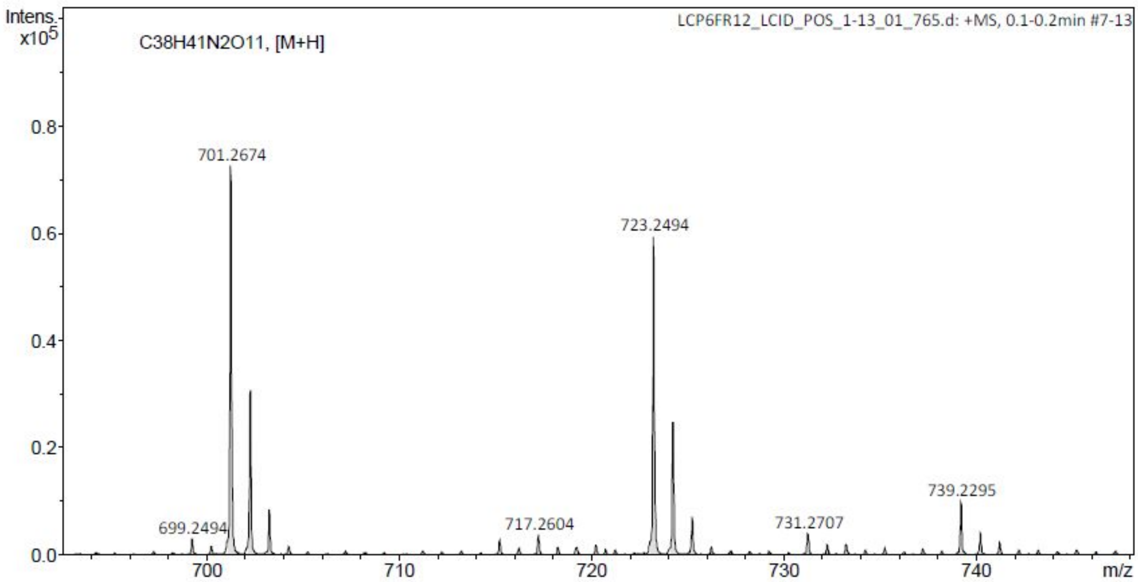

Figure S53. HRESIMS spectrum of compound **5** ($[M + H]^+$, positive mode).

6 Spectroscopic data for compound 6

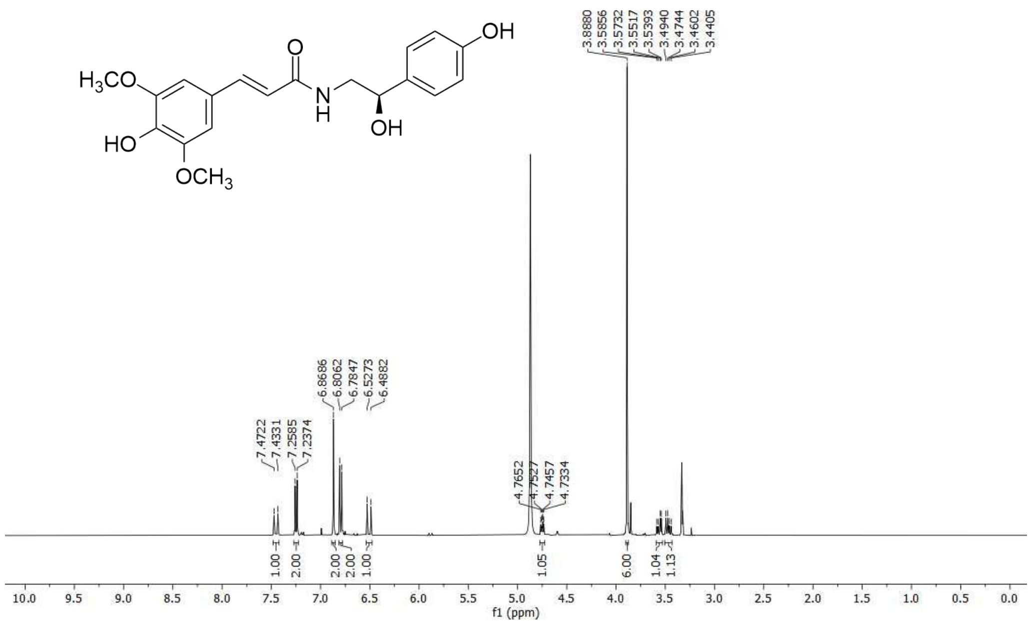

Figure S54. ^{1}H NMR spectrum of compound **6 (**400 MHz, MeOD).

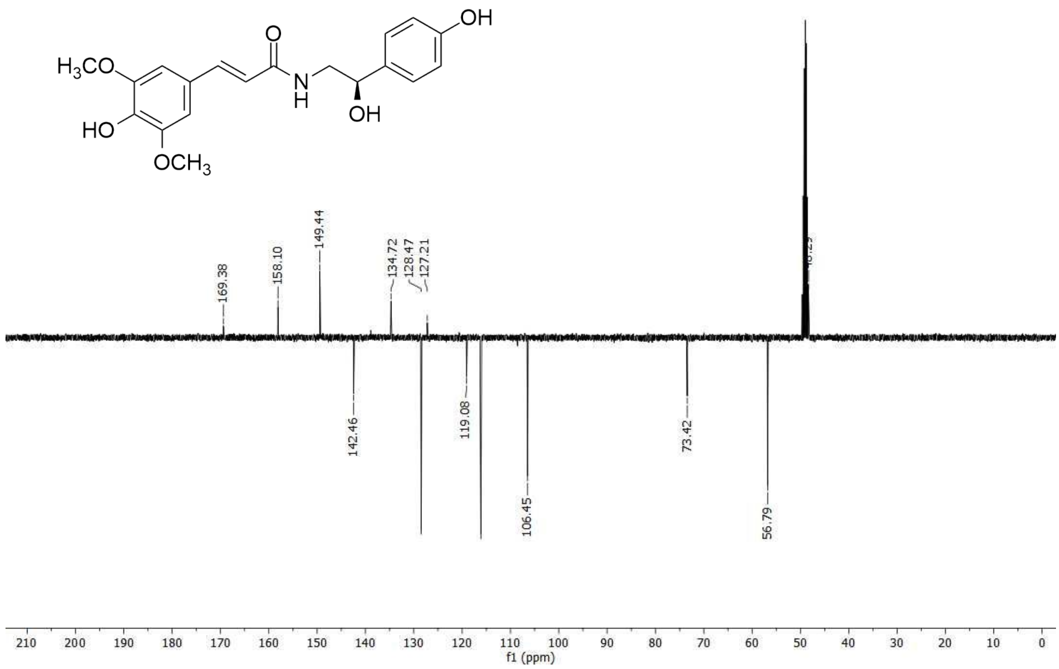

Figure S55. ^{13}C-APT NMR spectrum of compound **6** (100 MHz, MeOD).

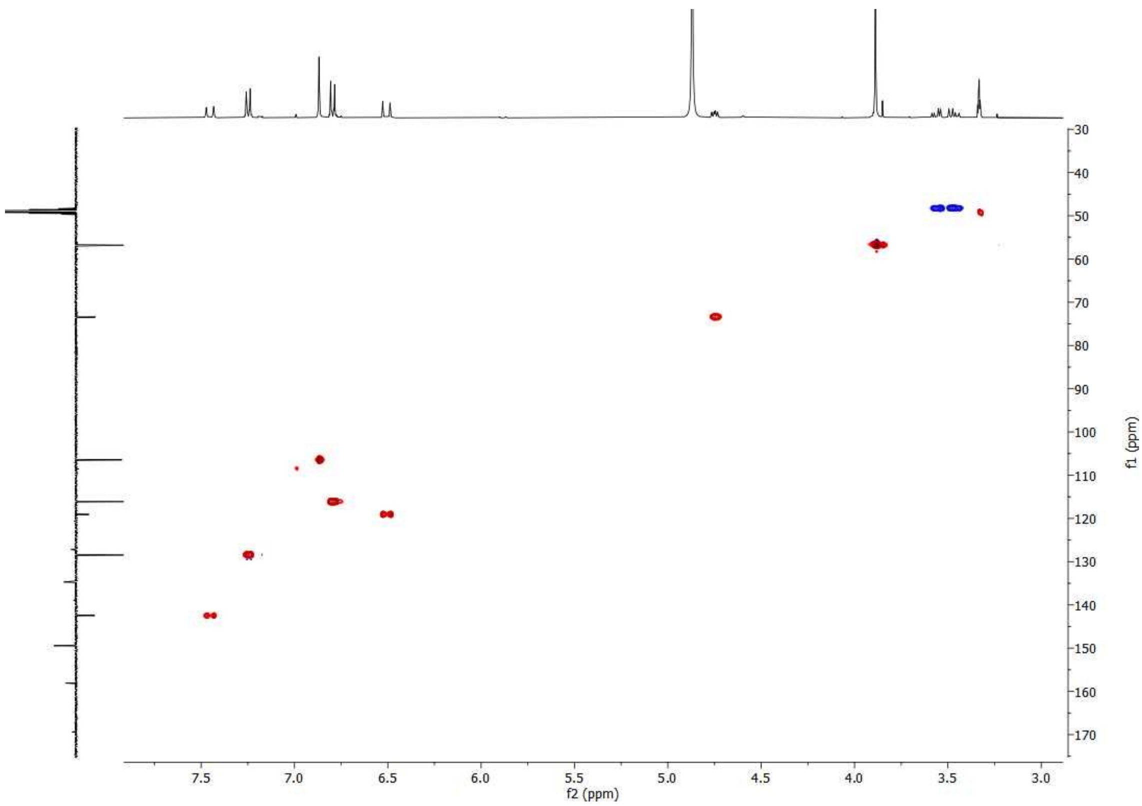

Figure S56. HSQC spectrum of compound **6 (**400/100 MHz, MeOD).

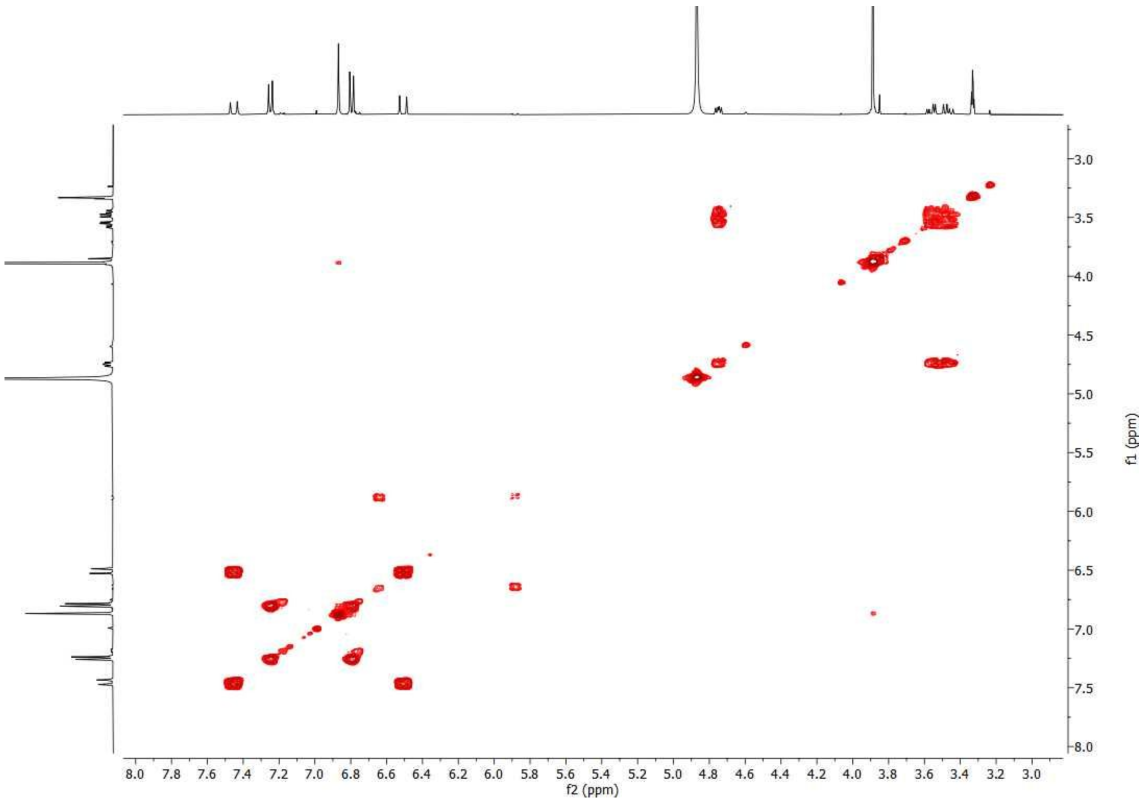

Figure S57. COSY spectrum of compound **6 (**400 MHz, MeOD).

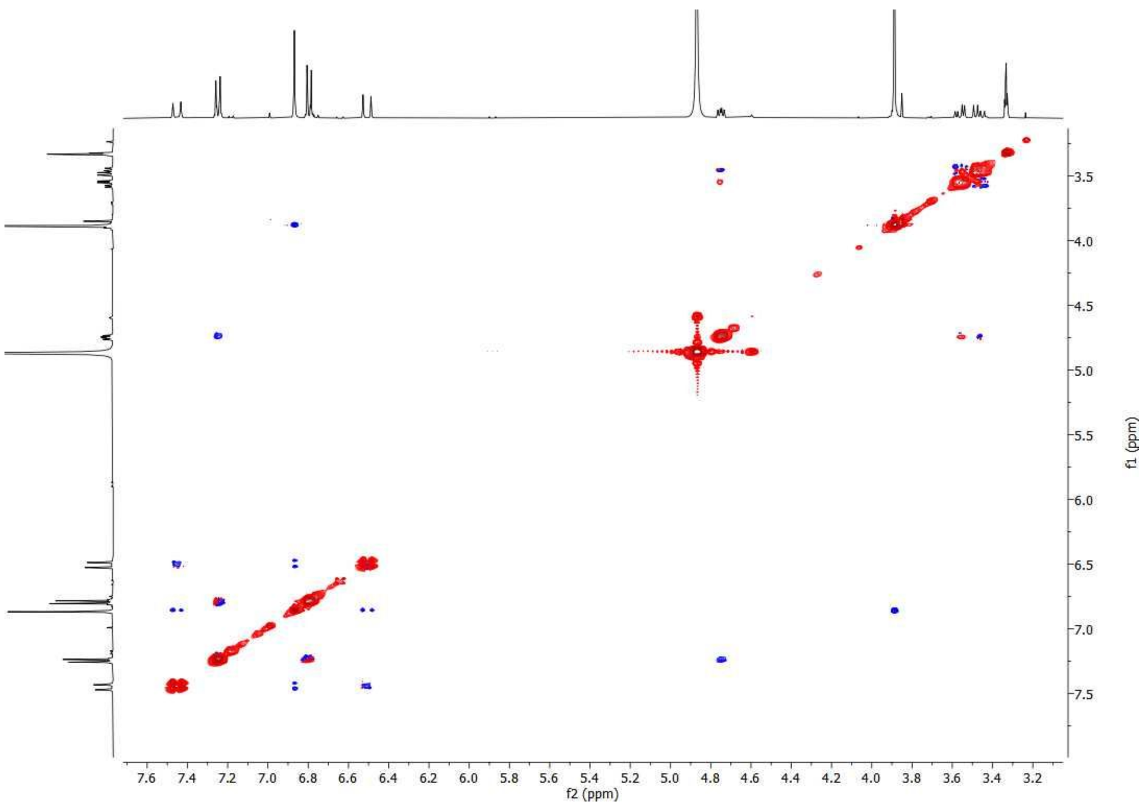

Figure S58. NOESY spectrum of compound **6 (**400 MHz, MeOD).

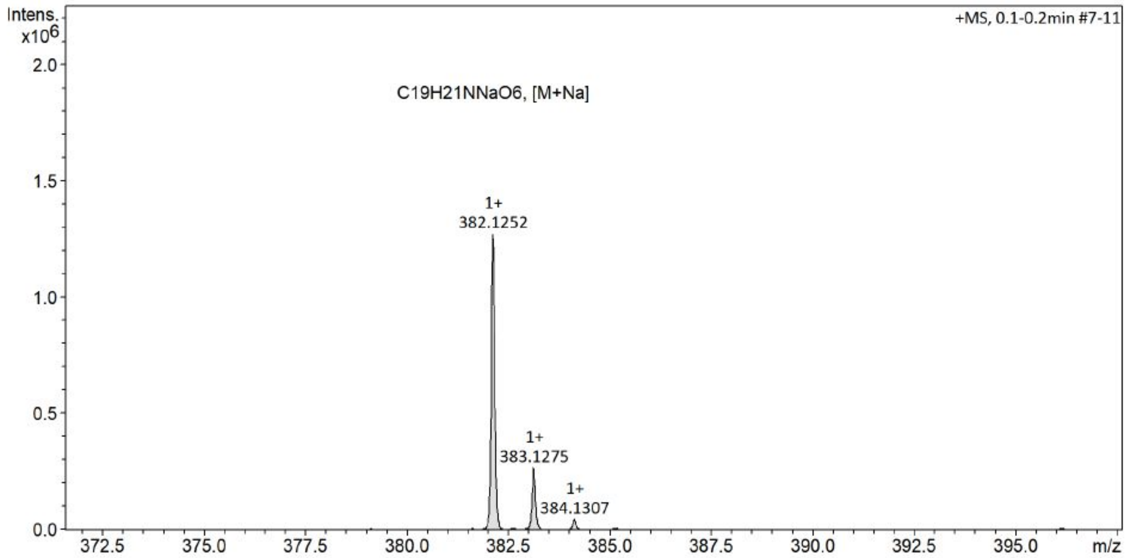

Figure S59. HRESIMS spectrum of compound **6** ([M + Na]$^+$, positive mode).

7 Spectroscopic data for compound 7

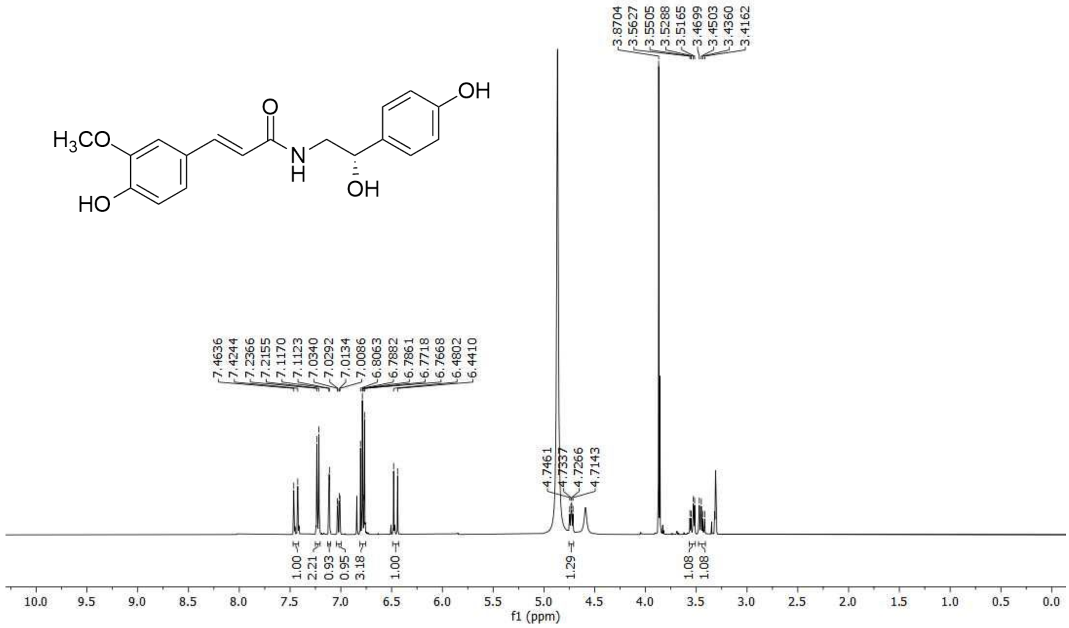

Figure S60. ^{1}H NMR spectrum of compound **7 (**400 MHz, MeOD).

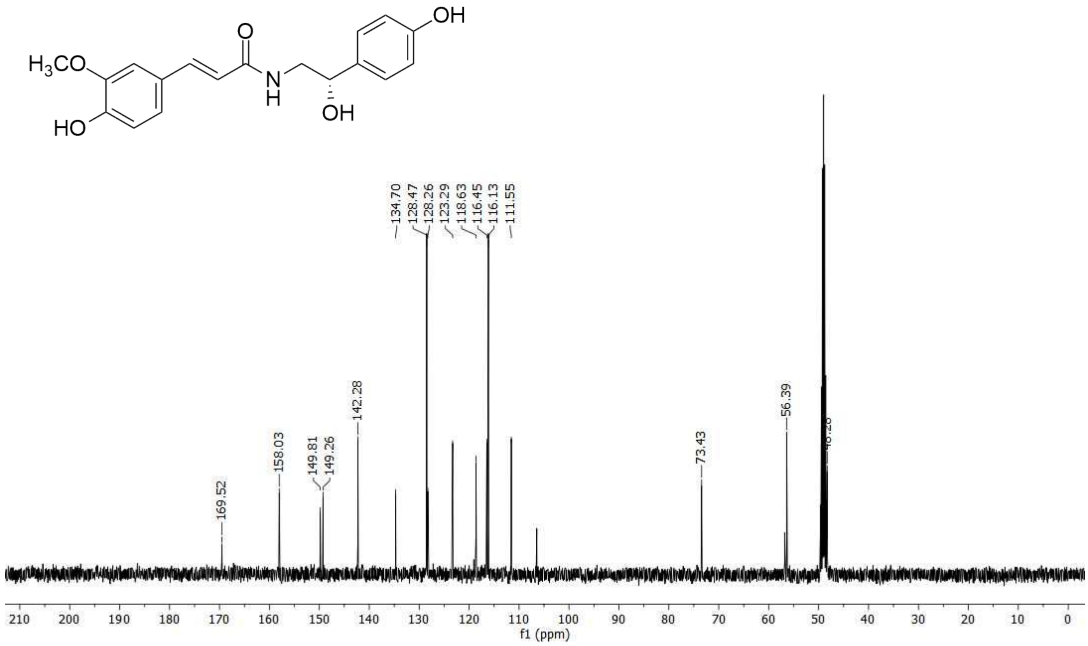

Figure S61. [13]C-BB NMR spectrum of compound **7** (100 MHz, MeOD).

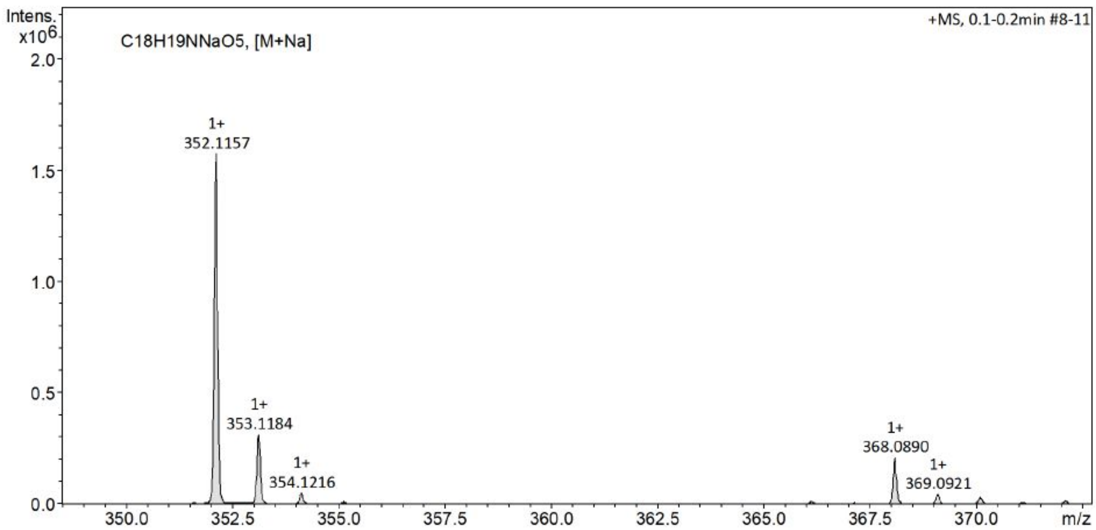

Figure S62. HRESIMS spectrum of compound **7** ($[M + Na]^+$, positive mode).

8 Spectroscopic data for compound 8

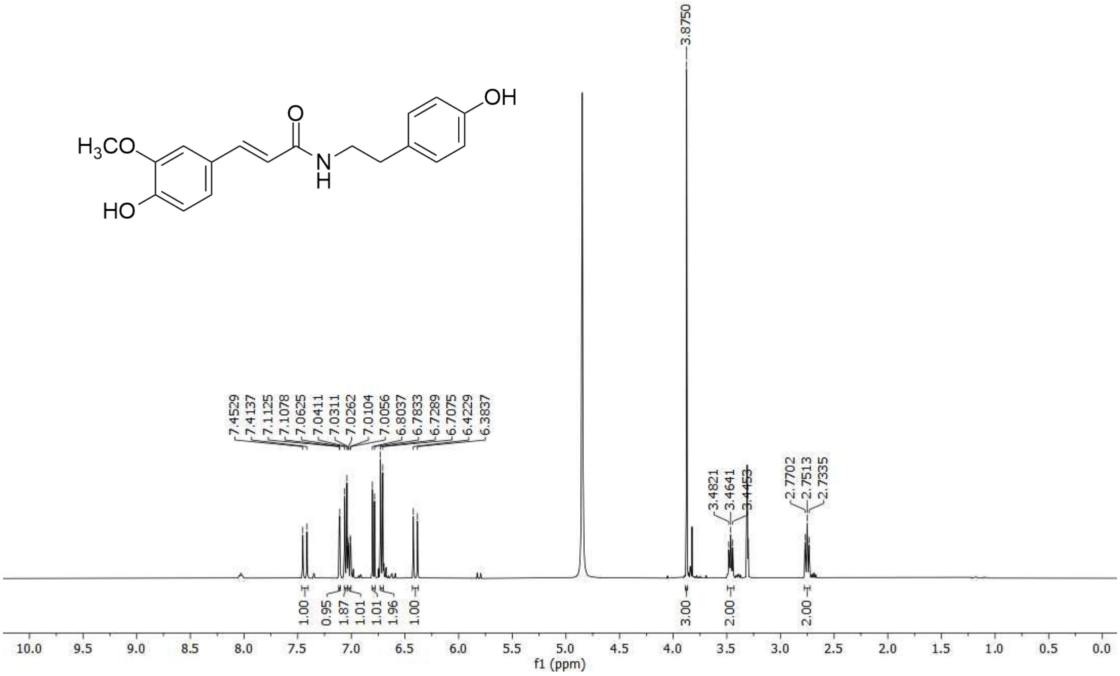

Figure S63. ^{1}H NMR spectrum of compound **8** **(**400 MHz, MeOD).

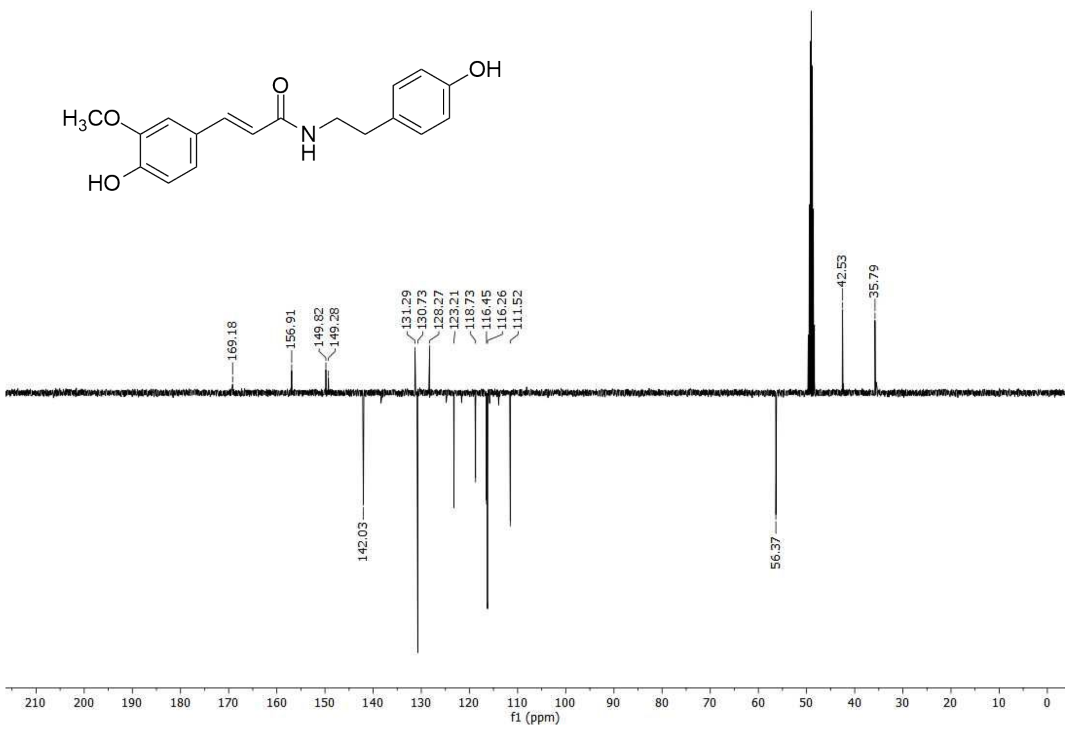

Figure S64. ^{13}C-APT NMR spectrum of compound **8** (100 MHz, MeOD).

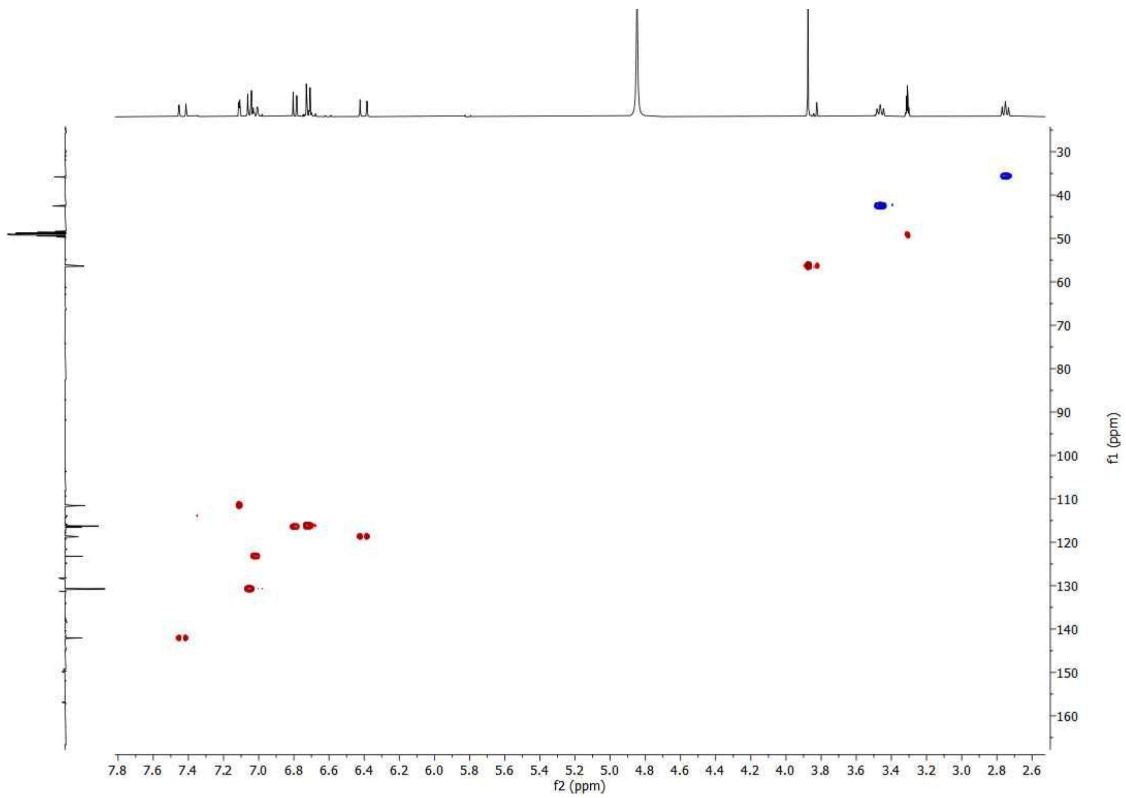

Figure S65. HSQC spectrum of compound **8 (**400/100 MHz, MeOD).

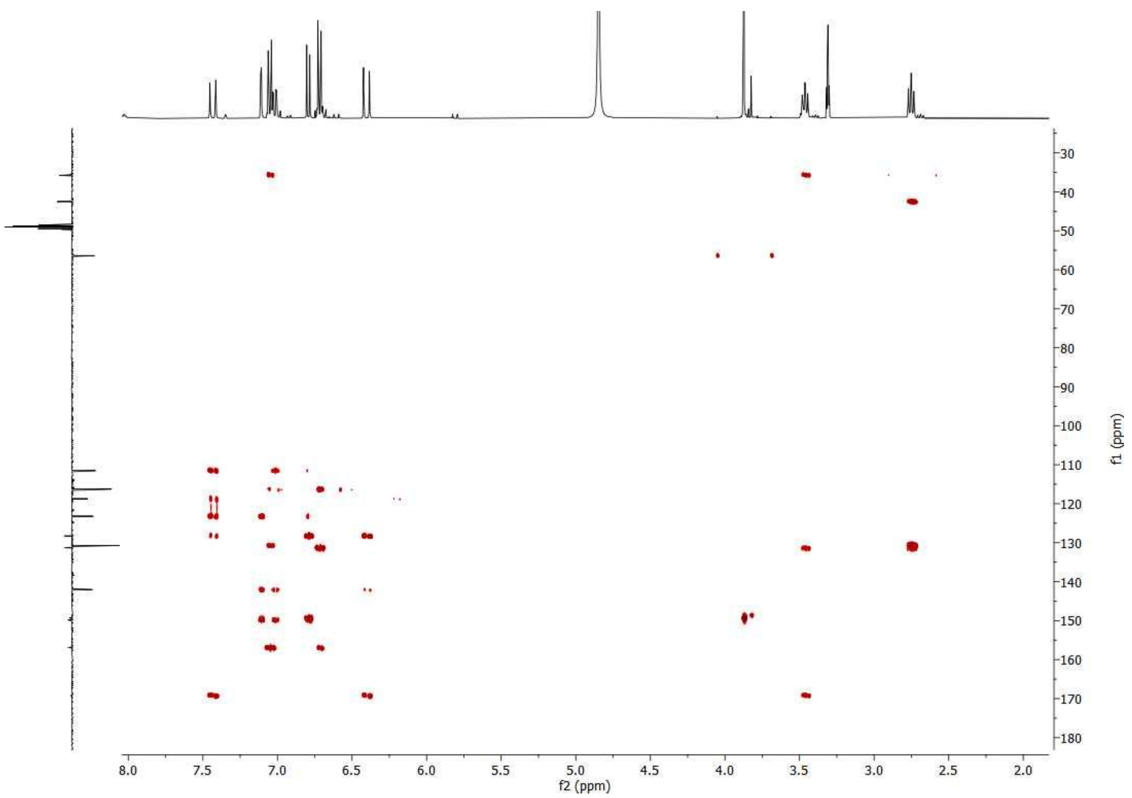

Figure S66. HMBC spectrum of compound **8 (**400/100 MHz, MeOD).

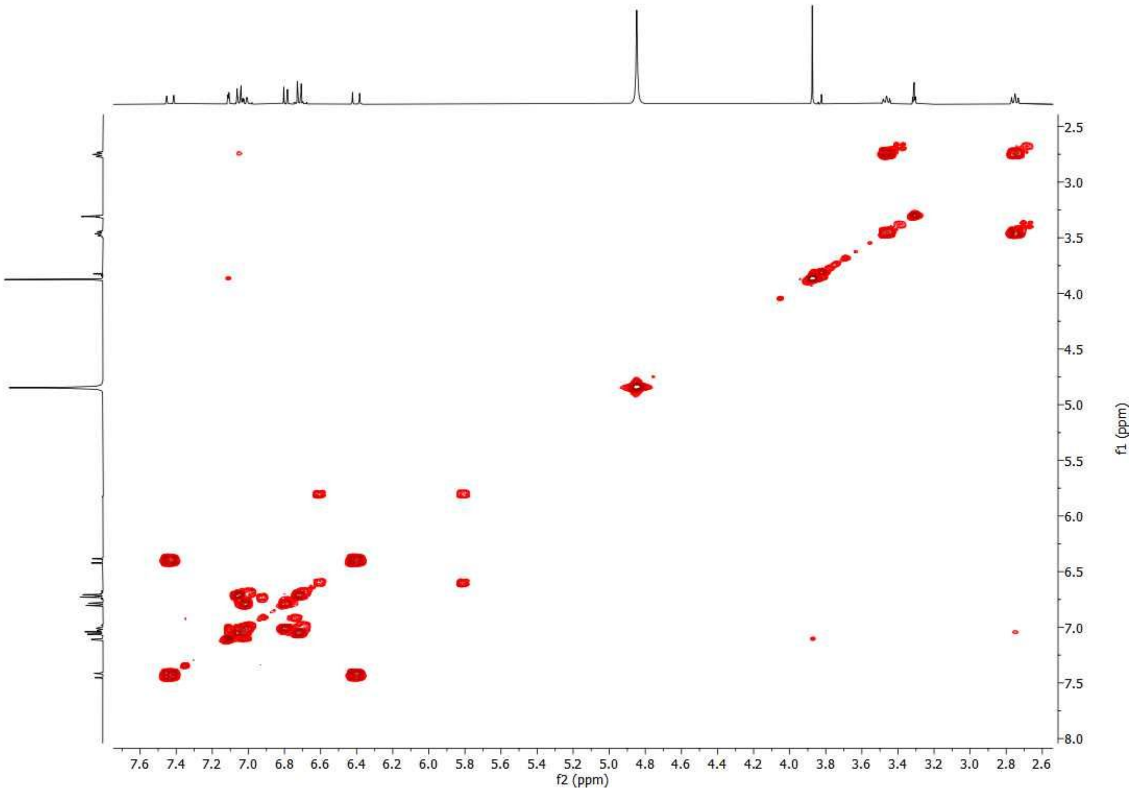

Figure S67. COSY spectrum of compound **8 (**400 MHz, MeOD).

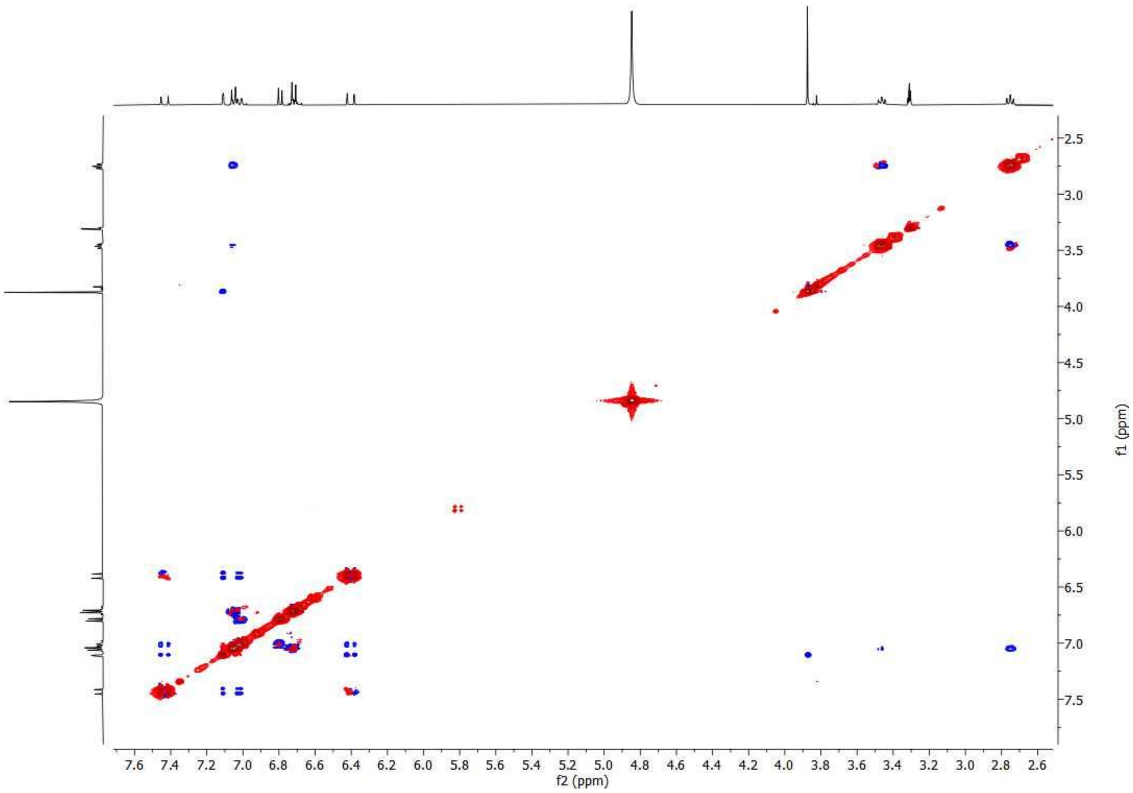

Figure S68. NOESY spectrum of compound **8 (**400 MHz, MeOD).

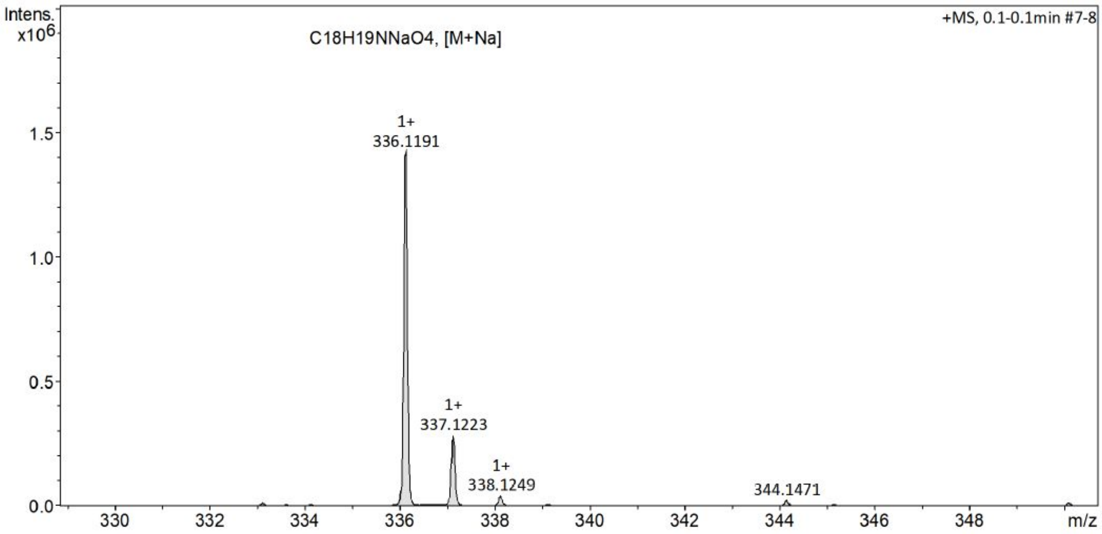

Figure S69. HRESIMS spectrum of compound **8** ([M + Na]$^+$, positive mode).

9 Spectroscopic data for compound 9

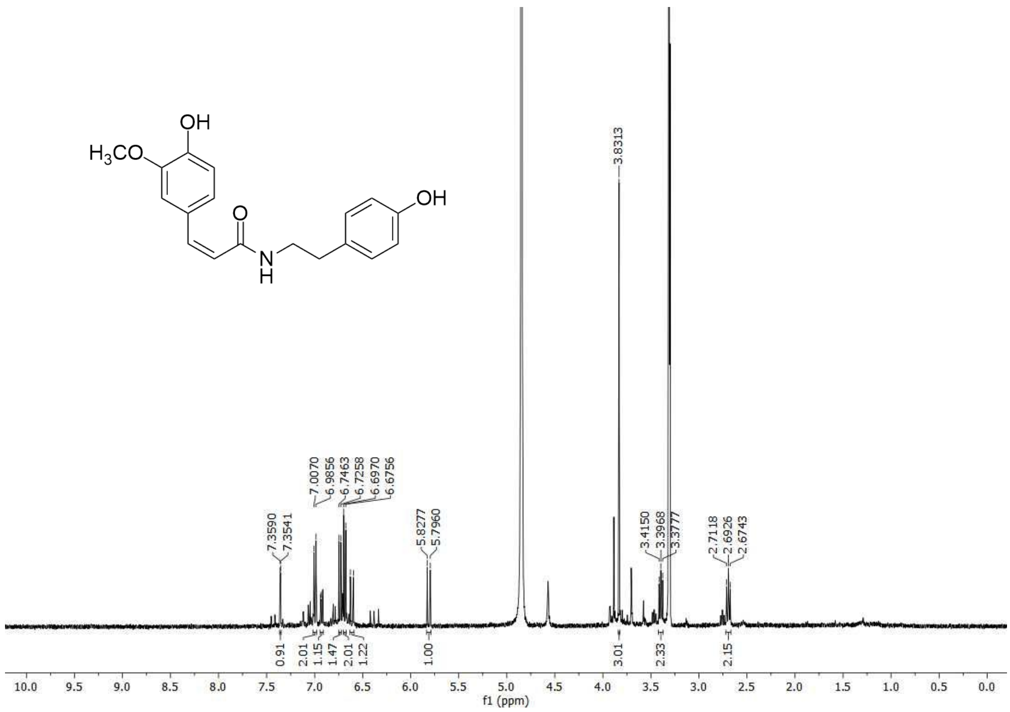

Figure S70. ^{1}H NMR spectrum of compound **9** (400 MHz, MeOD).

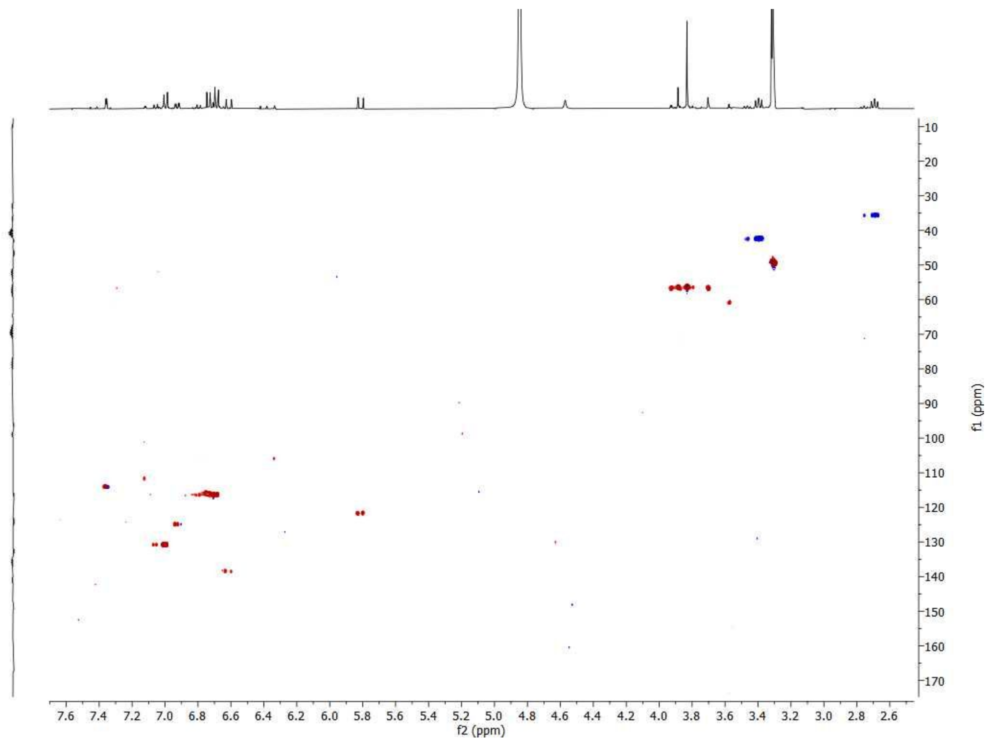

Figure S71. HSQC spectrum of compound **9 (**400/100 MHz, MeOD).

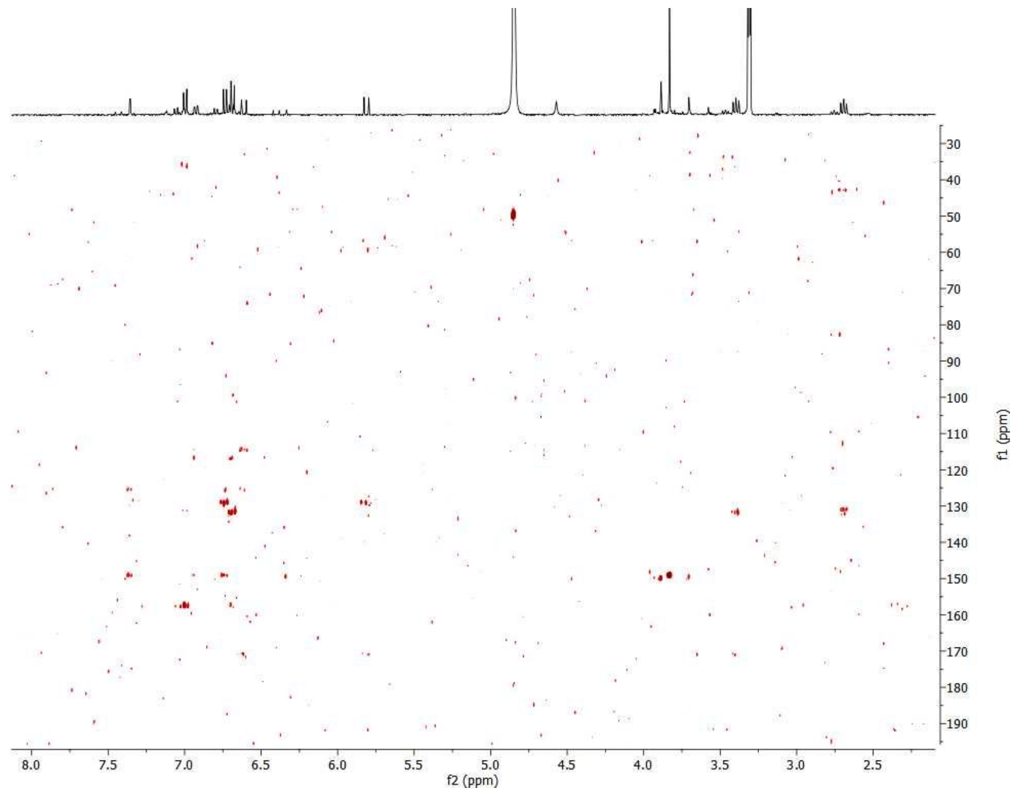

Figure S72. HMBC spectrum of compound **9 (**400/100 MHz, MeOD).

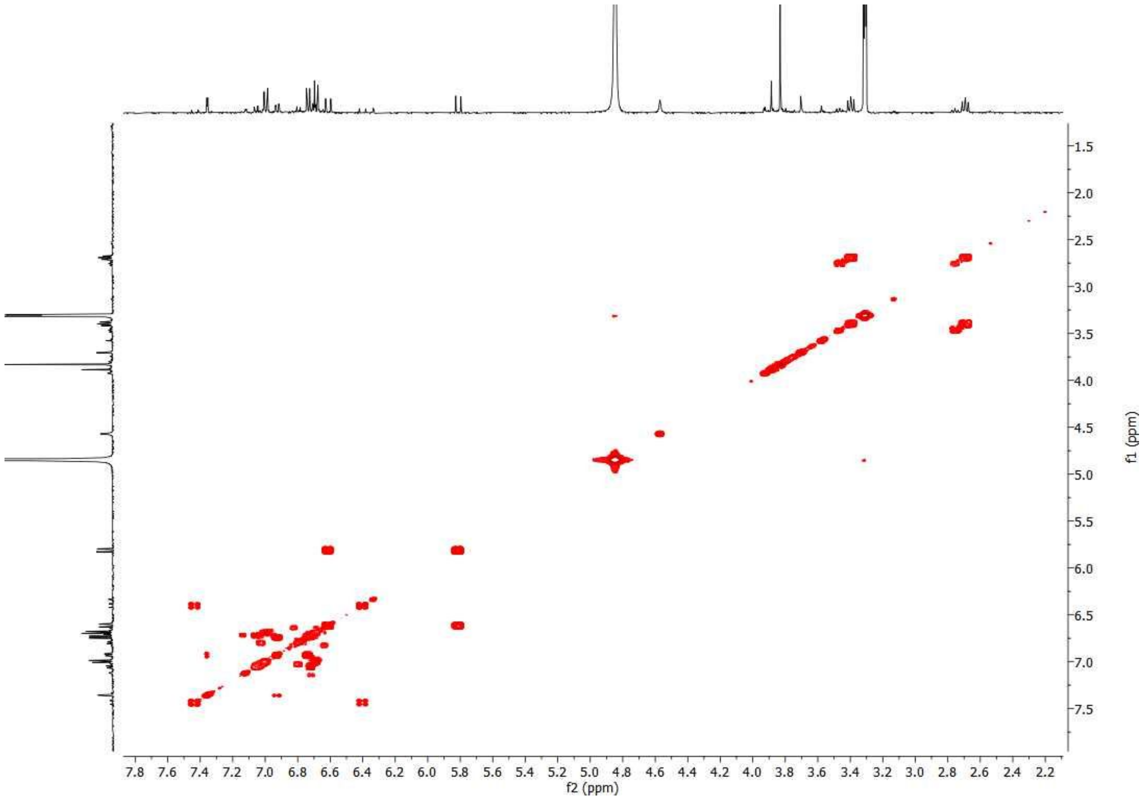

Figure S73. COSY spectrum of compound **9 (**400 MHz, MeOD).

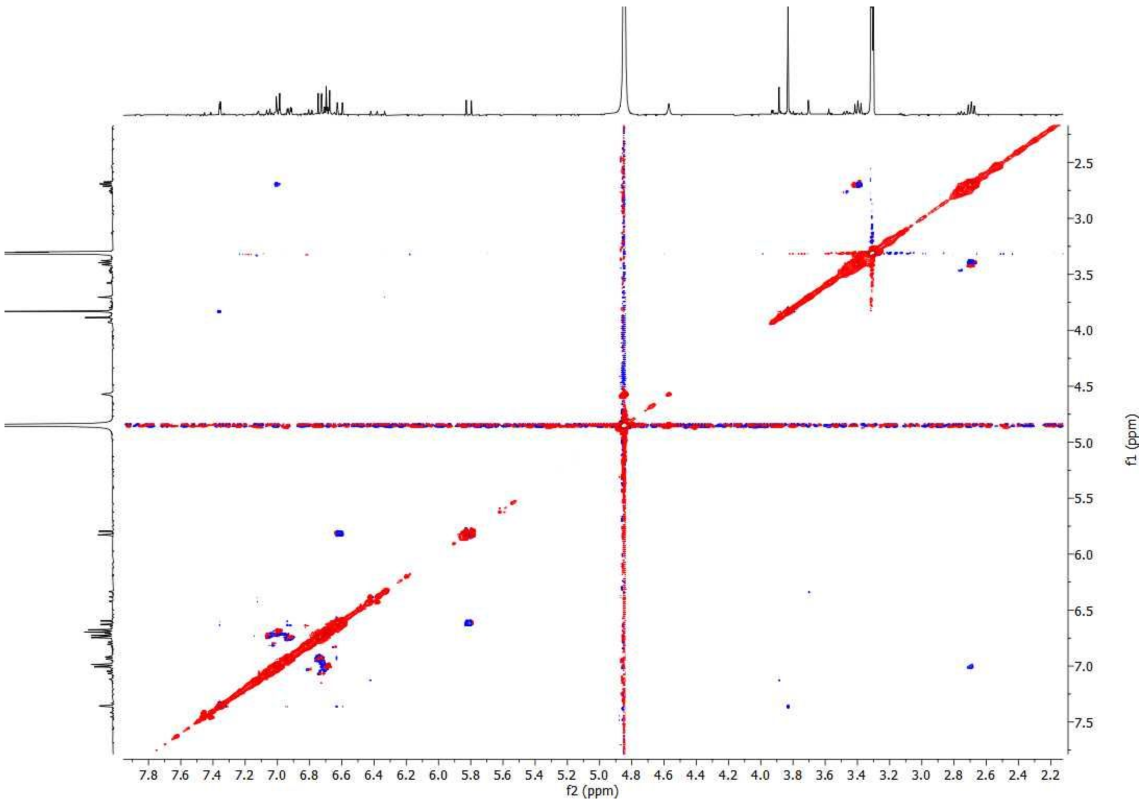

Figure S74. NOESY spectrum of compound **9 (**400 MHz, MeOD).

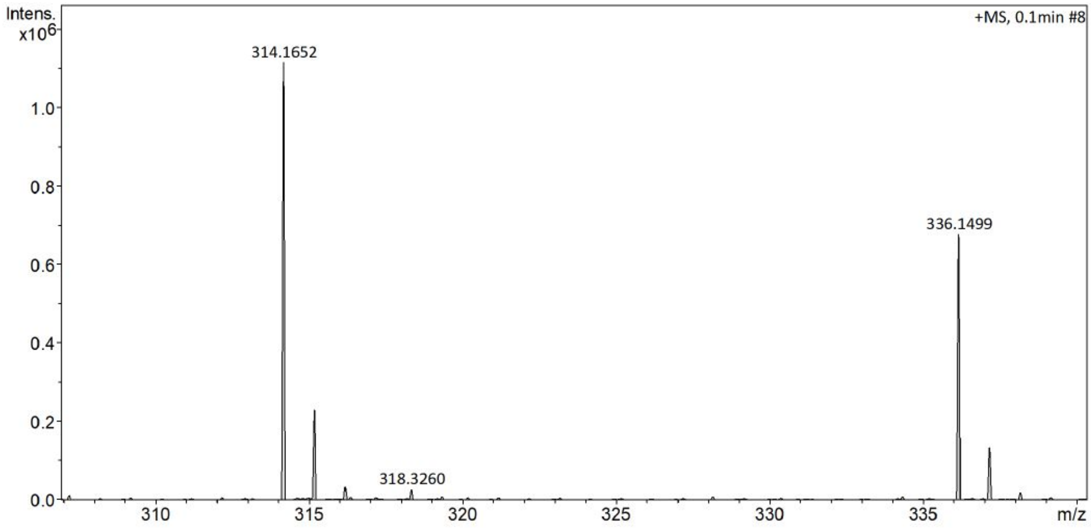

Figure S75. HRESIMS spectrum of compound **9** ([M + H]$^+$, positive mode).

10 Spectroscopic data for compound 10

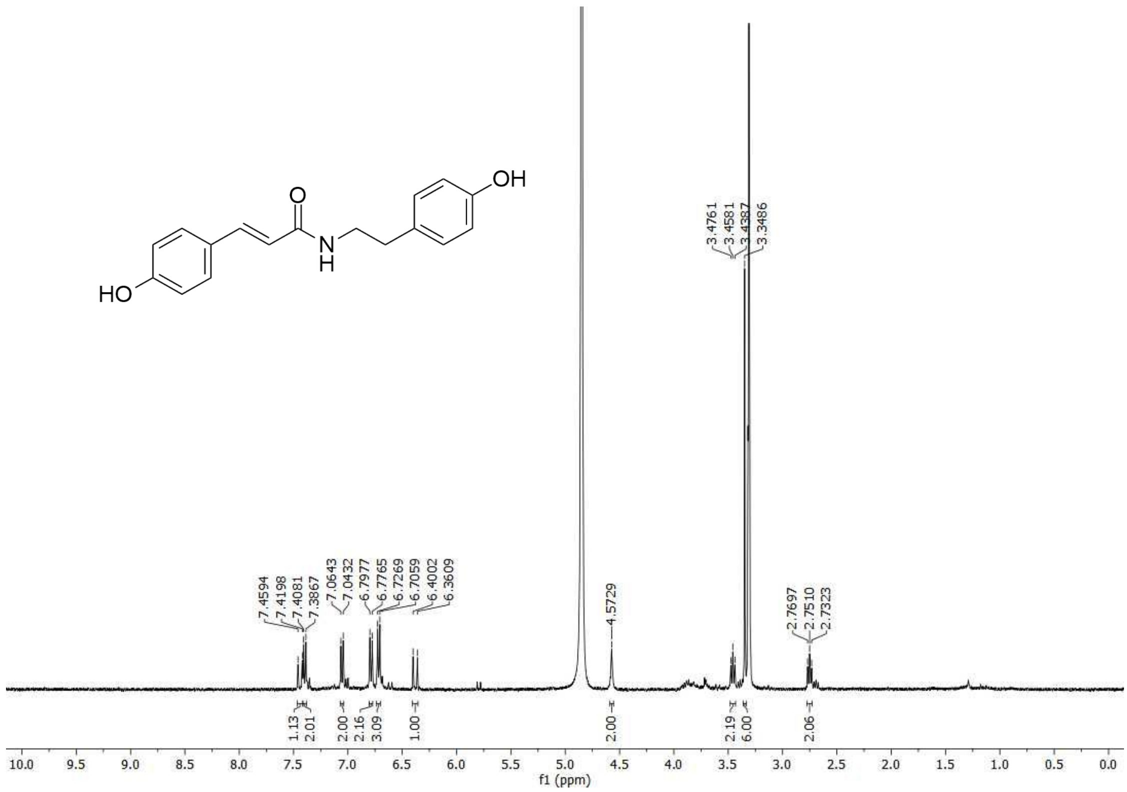

Figure S78. ^{1}H NMR spectrum of compound **10 (**400 MHz, MeOD).

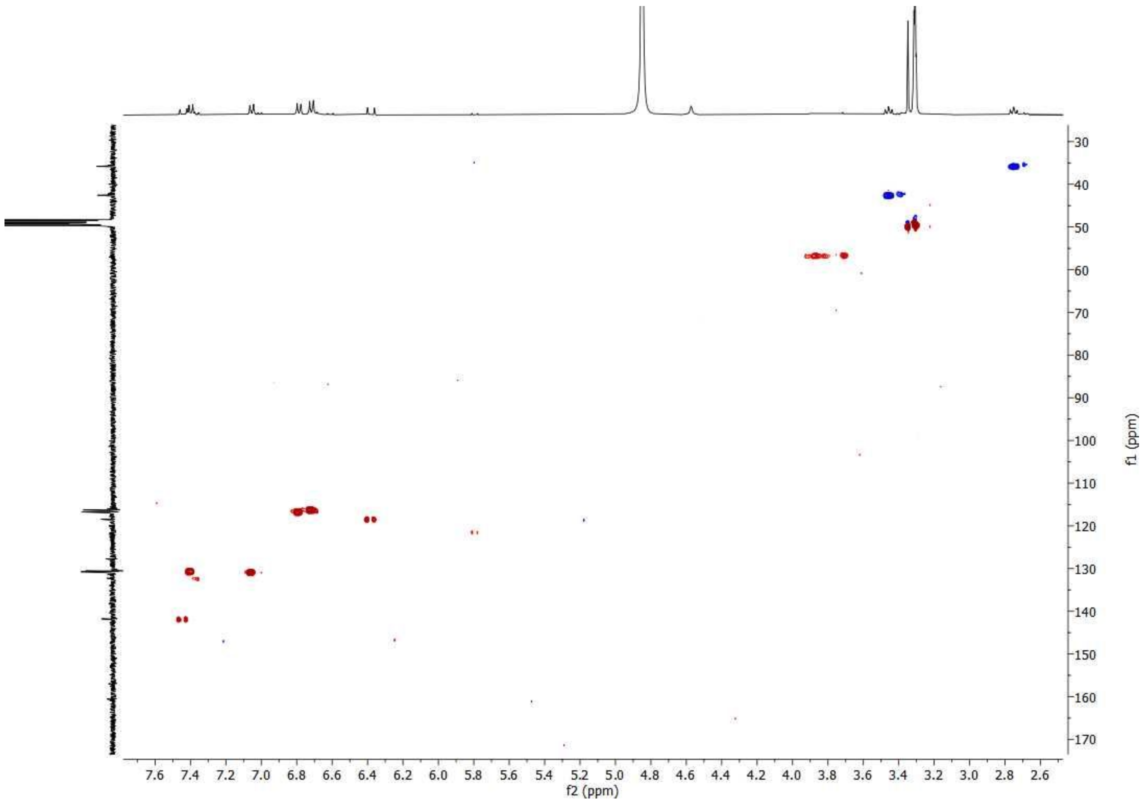

Figure S76. HSQC spectrum of compound **10 (**400/100 MHz, MeOD).

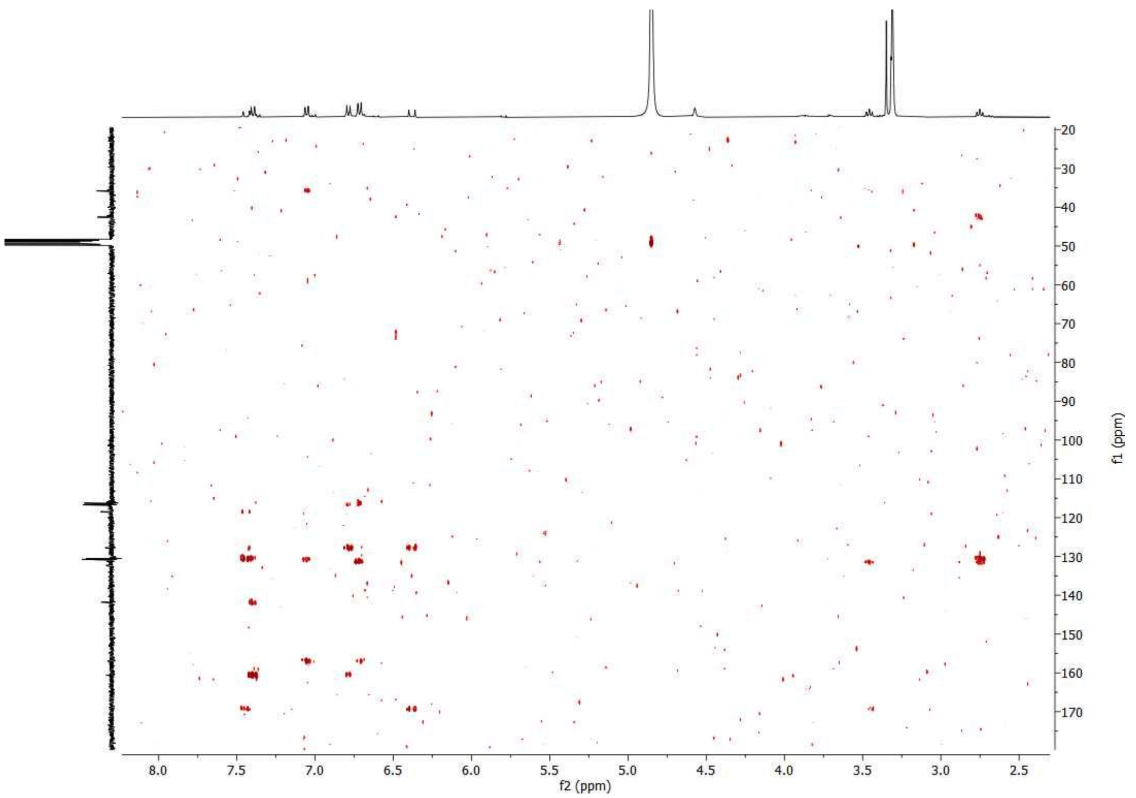

Figure S77. HMBC spectrum of compound **10 (**400/100 MHz, MeOD).

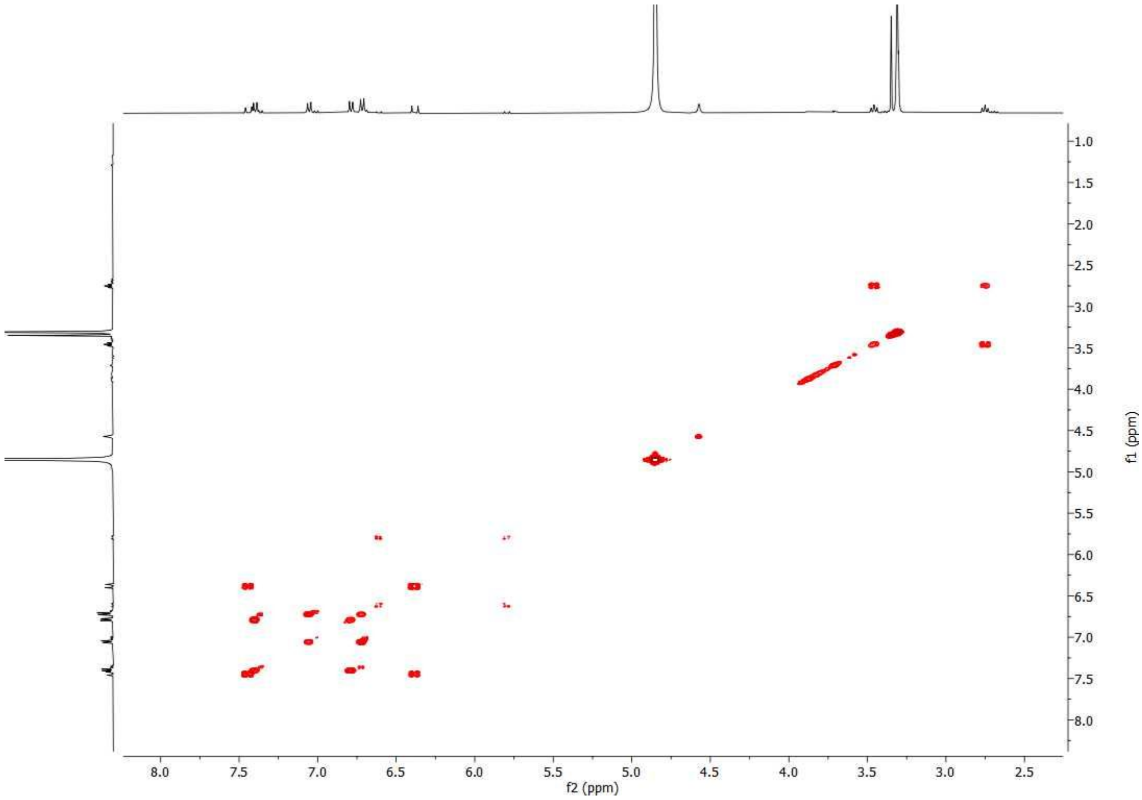

Figure S78. COSY spectrum of compound **10 (**400 MHz, MeOD).

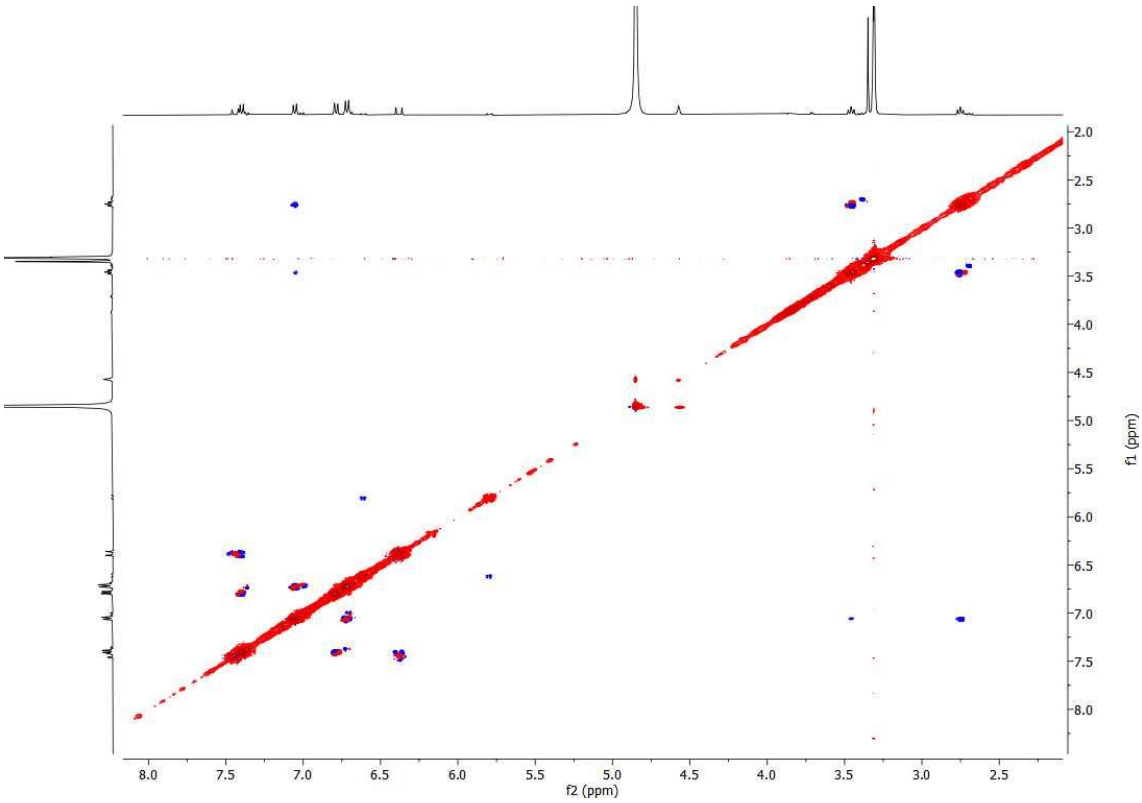

Figure S79. NOESY spectrum of compound **10 (**400 MHz, MeOD).

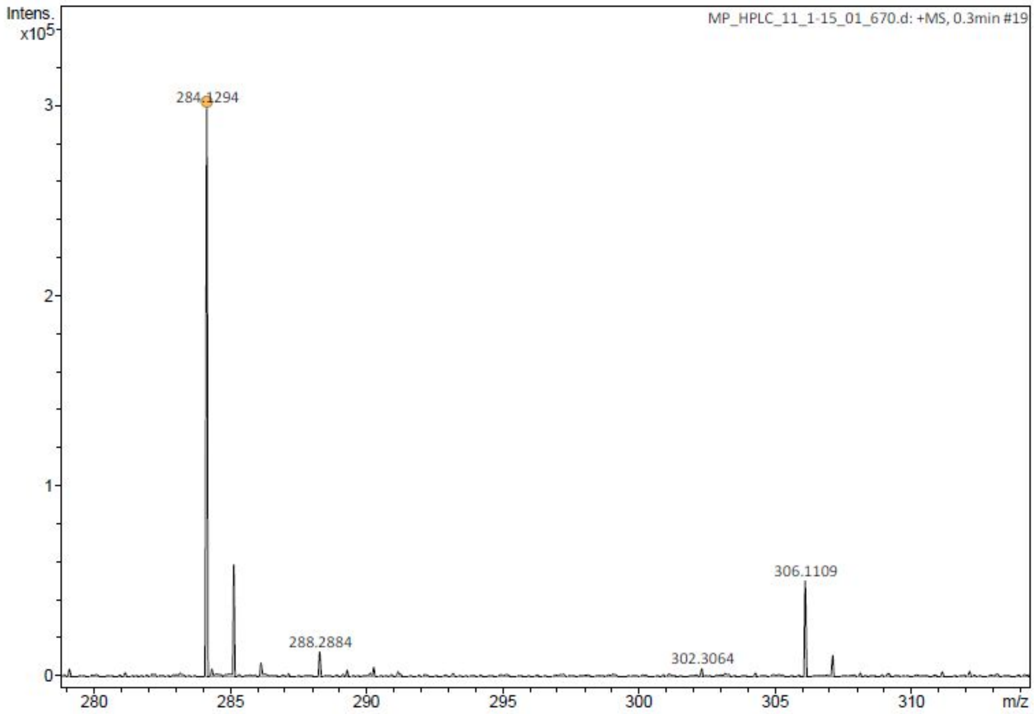

Figure S80. HRESIMS spectrum of compound **10** ([M + H]$^+$, positive mode).

11 Spectroscopic data for compounds 11,12

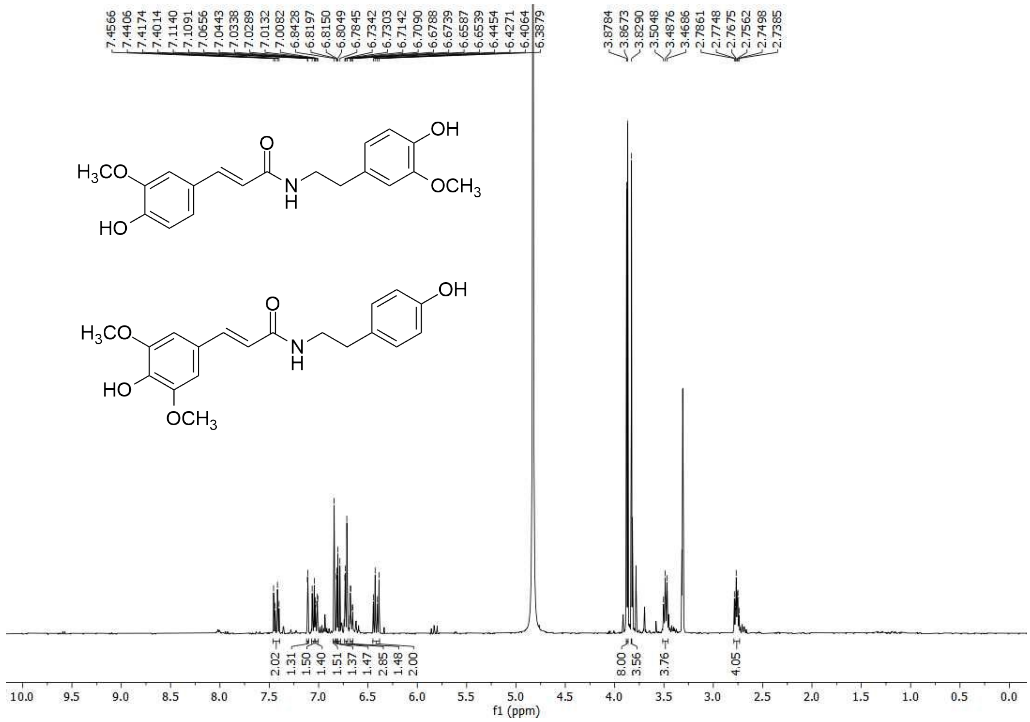

Figure S81. ^{1}H NMR spectrum of compound **11**, **12** (400 MHz, MeOD).

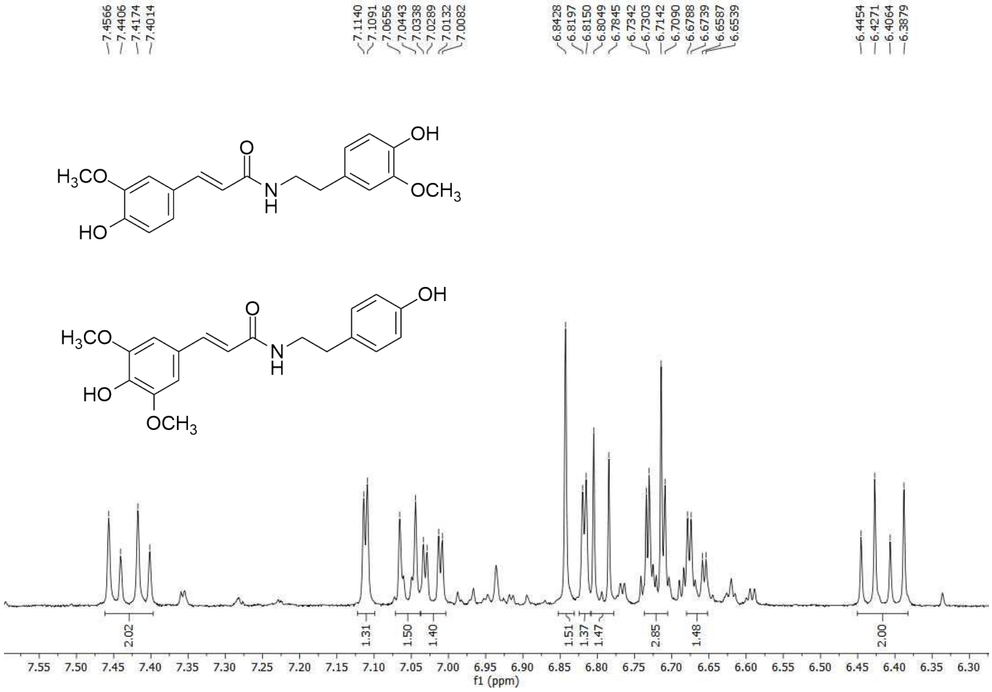

Figure S82. Amplification of the ^{1}H NMR spectrum of compound **11**, **12 (**400 MHz, MeOD).

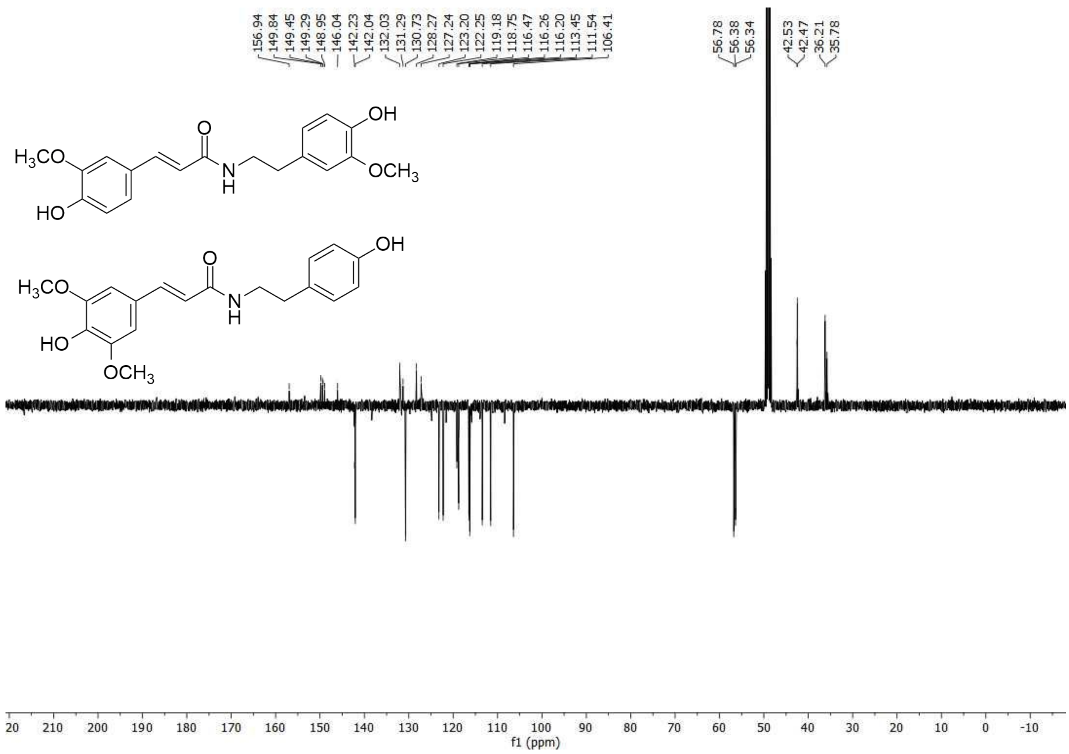

Figure S83. ^{13}C-APT NMR spectrum of compound **11**, **12** (100 MHz, MeOD).

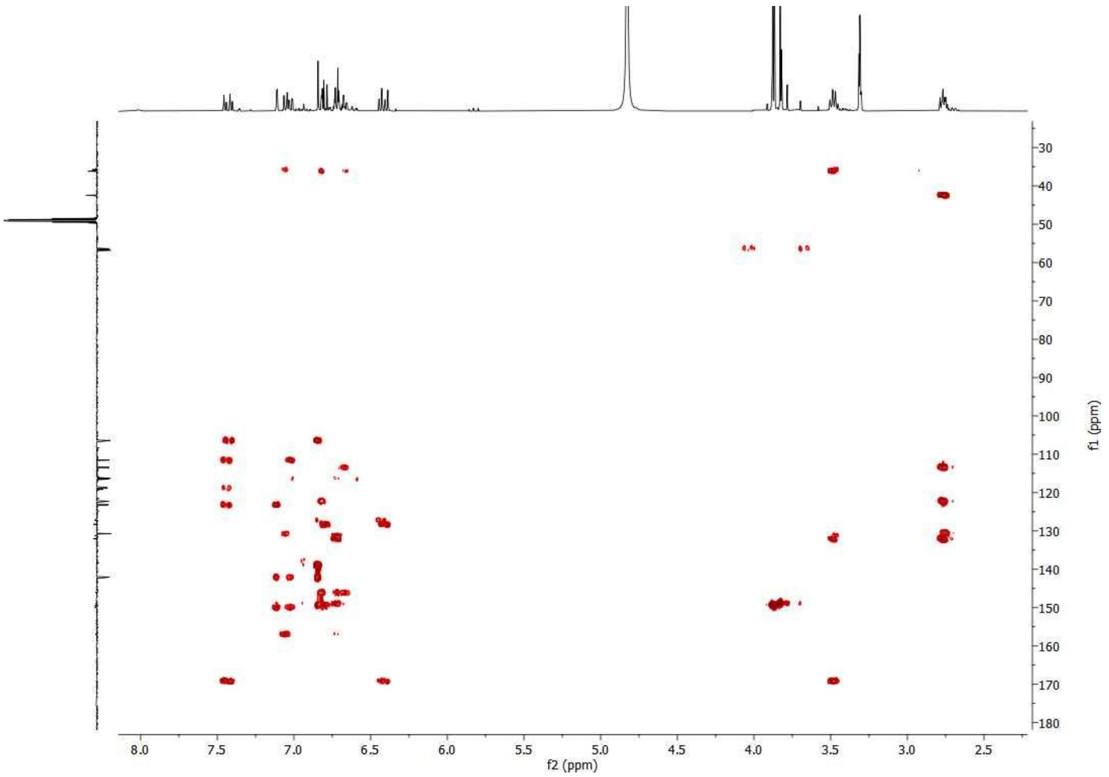

Figure S84. HMBC spectrum of compound **11**, **12** (400/100 MHz, MeOD).

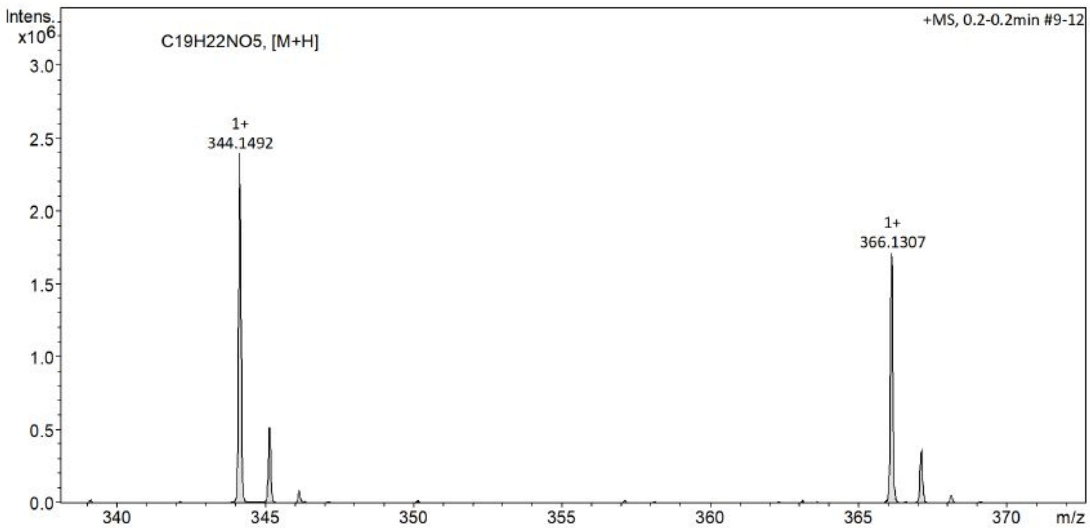

Figure S85. HRESIMS spectrum of compounds **11**, **12** ($[M + H]^+$, positive mode).

12 Spectroscopic data for compounds 13,14

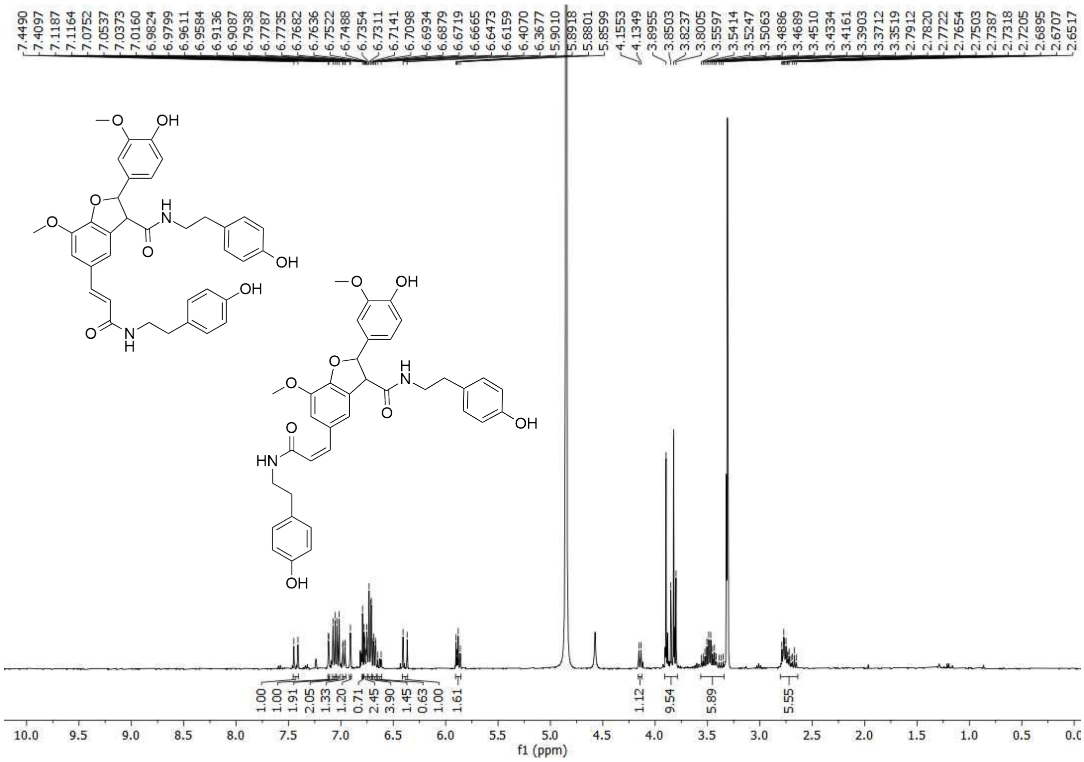

Figure S86. ^1H NMR spectrum of compounds **13**, **14 (**400 MHz, MeOD).

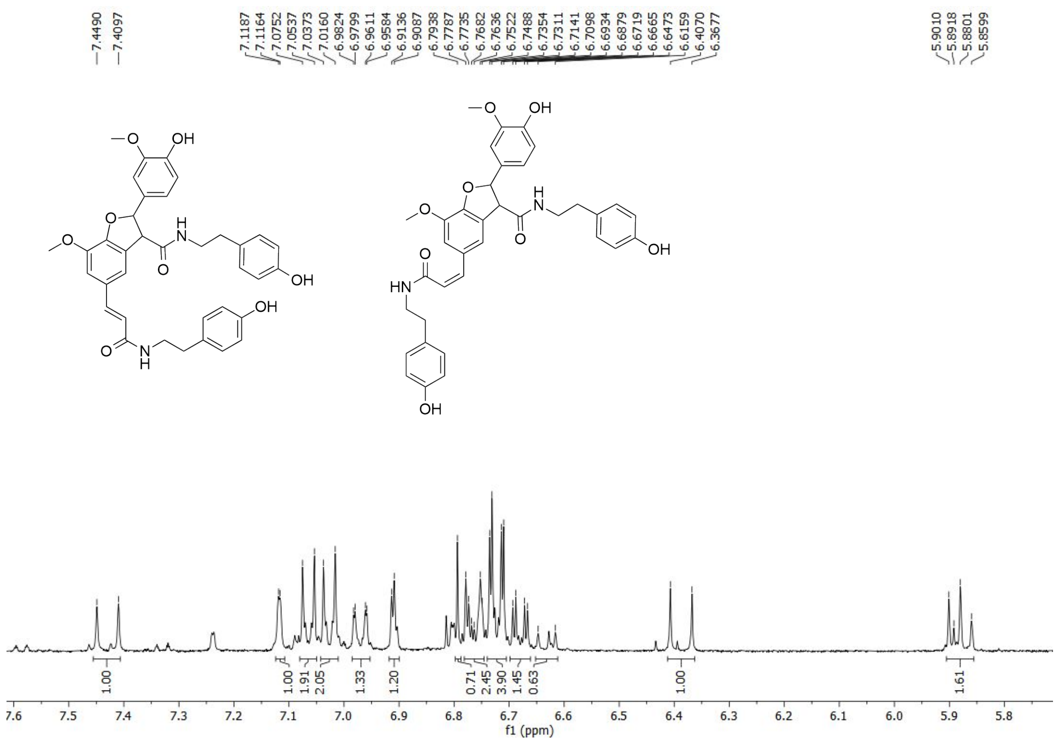

Figure S87. Amplification of the ^1H NMR spectrum of compounds **13**, **14 (**400 MHz, MeOD).

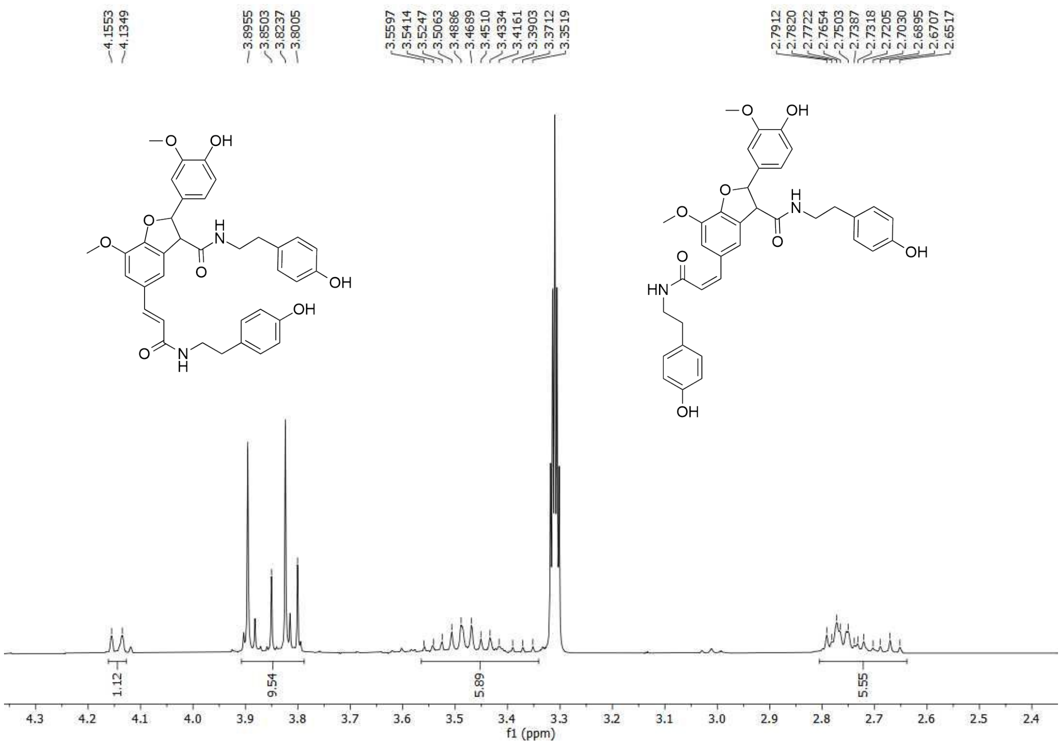

Figure S88. Amplification of the ^{1}H NMR spectrum of compounds **13**, **14** (400 MHz, MeOD).

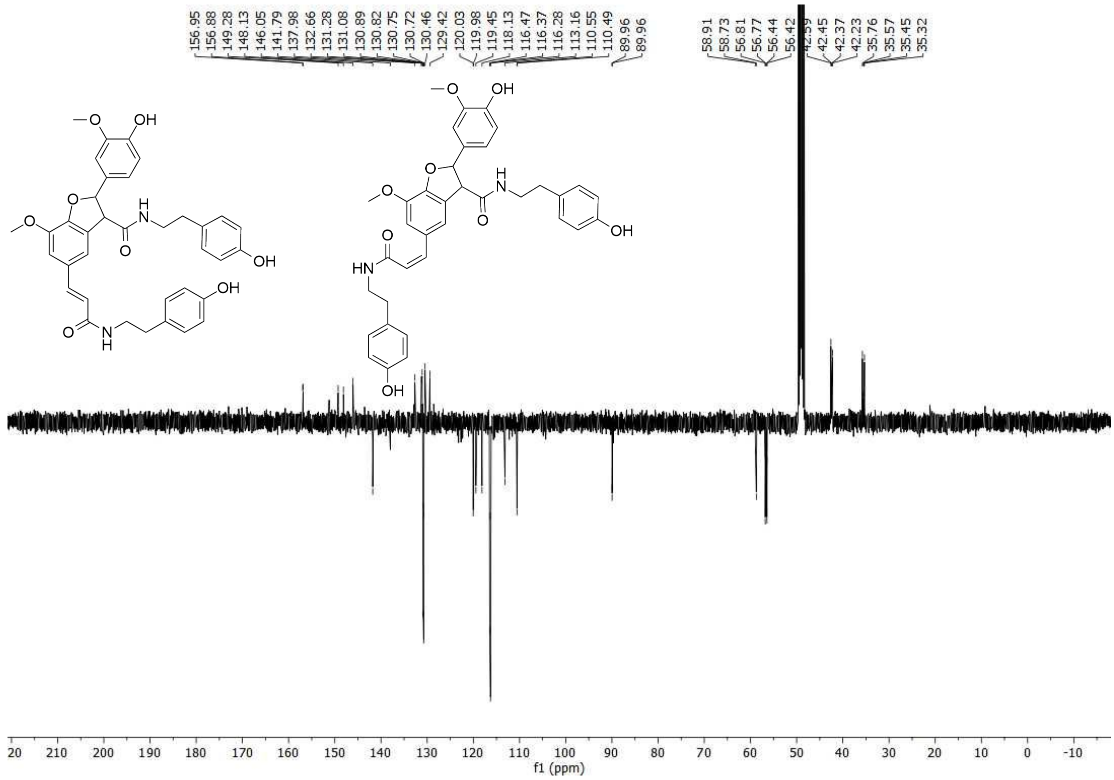

Figure S89. ^{13}C-APT NMR spectrum of compounds **13**, **14** (100 MHz, MeOD).

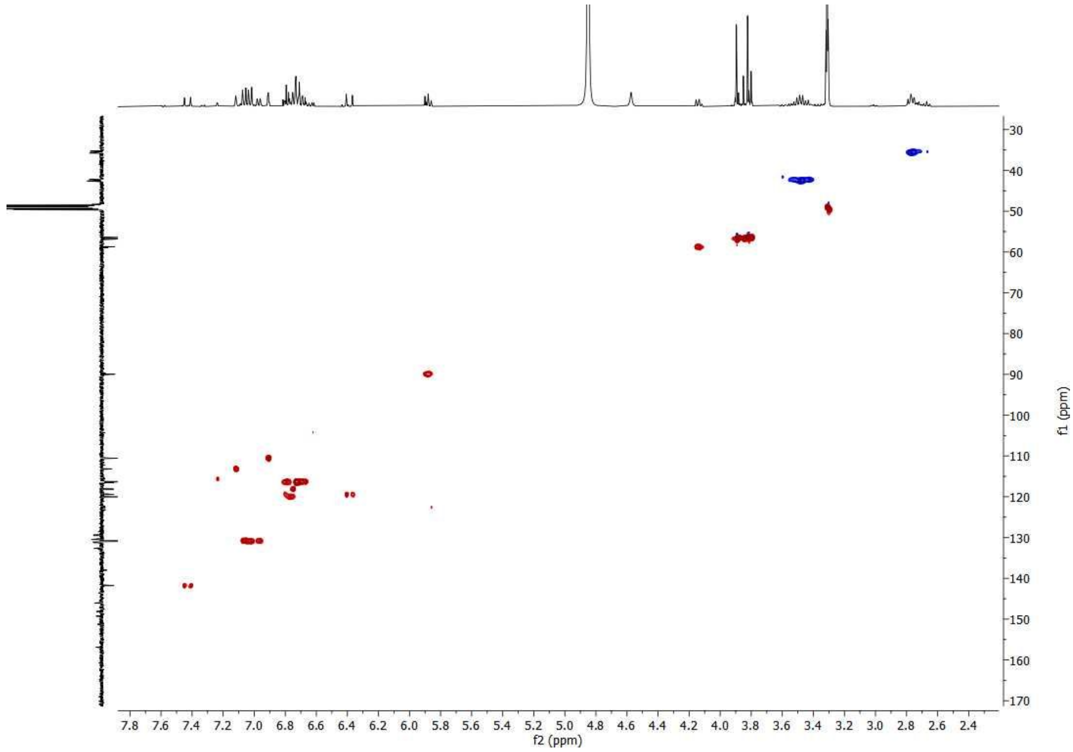

Figure S90. HSQC spectrum of compounds **13**, **14 (**400/100 MHz, MeOD).

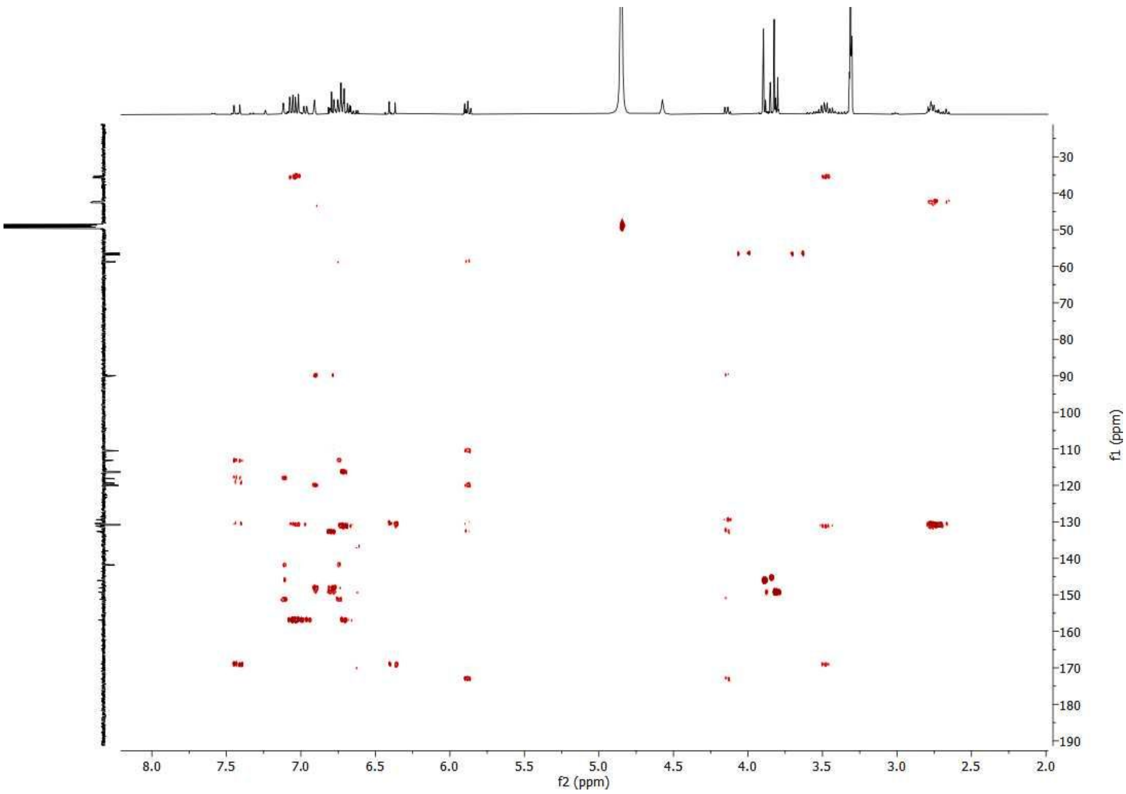

Figure S91. HMBC spectrum of compounds **13**, **14 (**400/100 MHz, MeOD).

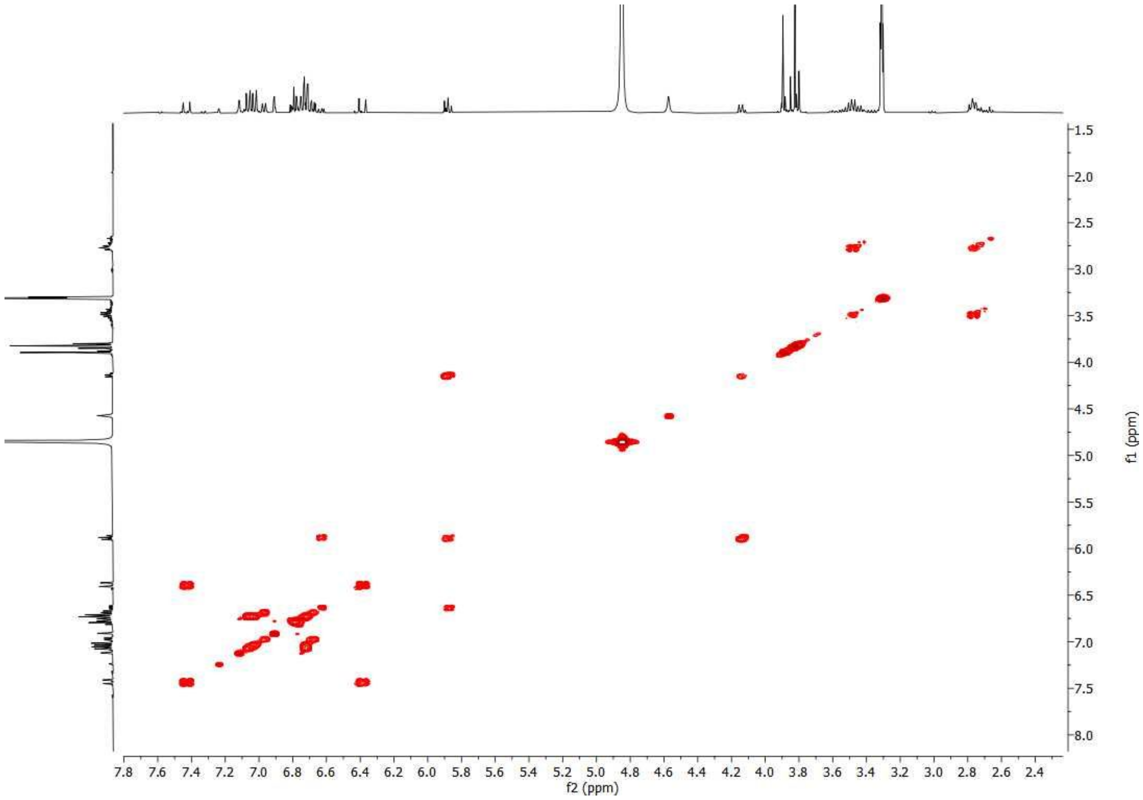

Figure S92. COSY spectrum of compounds **13**, **14 (**400 MHz, MeOD).

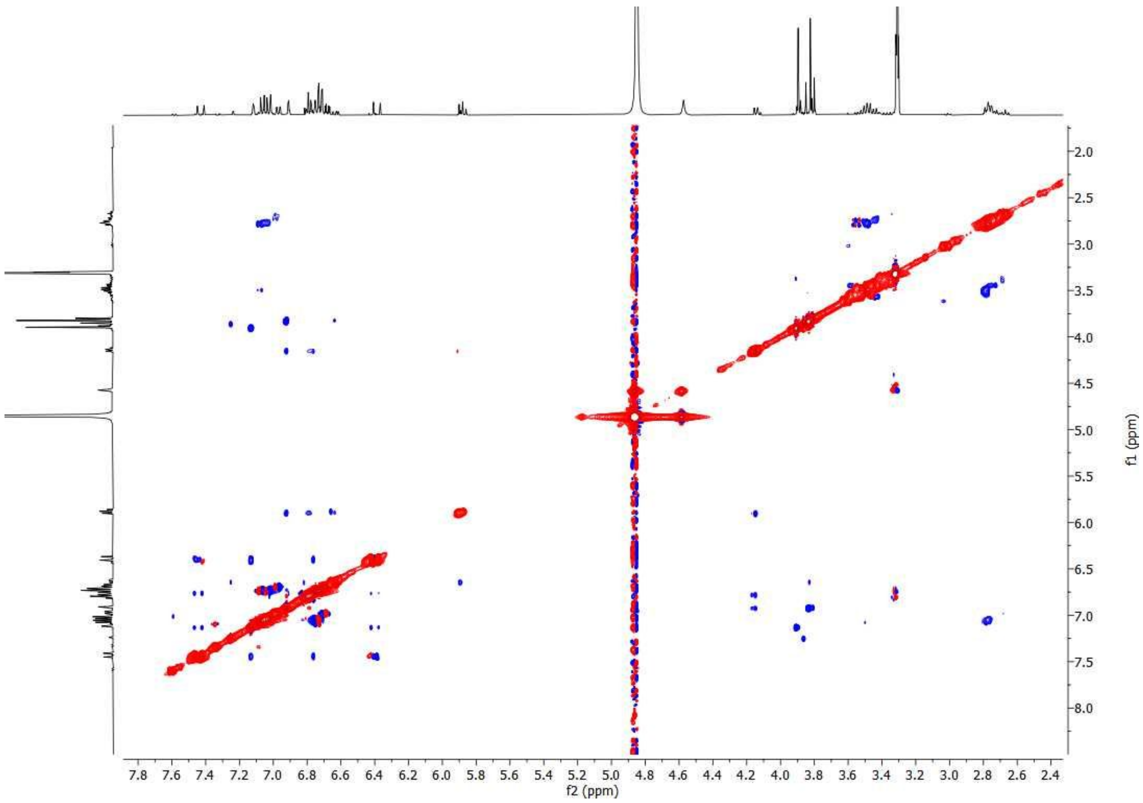

Figure S93. COSY spectrum of compounds **13**, **14 (**400 MHz, MeOD).

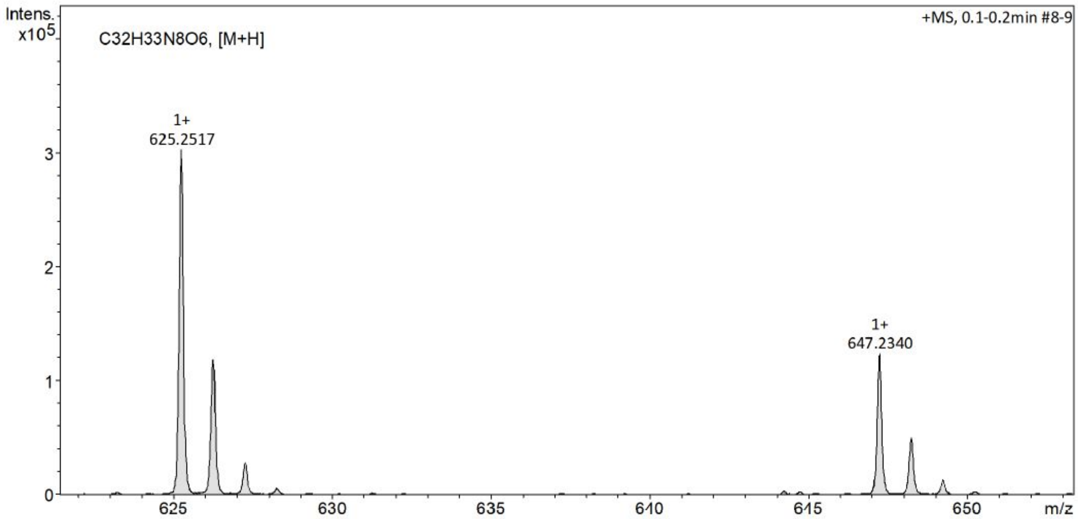

Figure S94. HRESIMS spectrum of compounds **13**, **14** ($[M + H]^+$, positive mode).

13 Spectroscopic data for compound 15

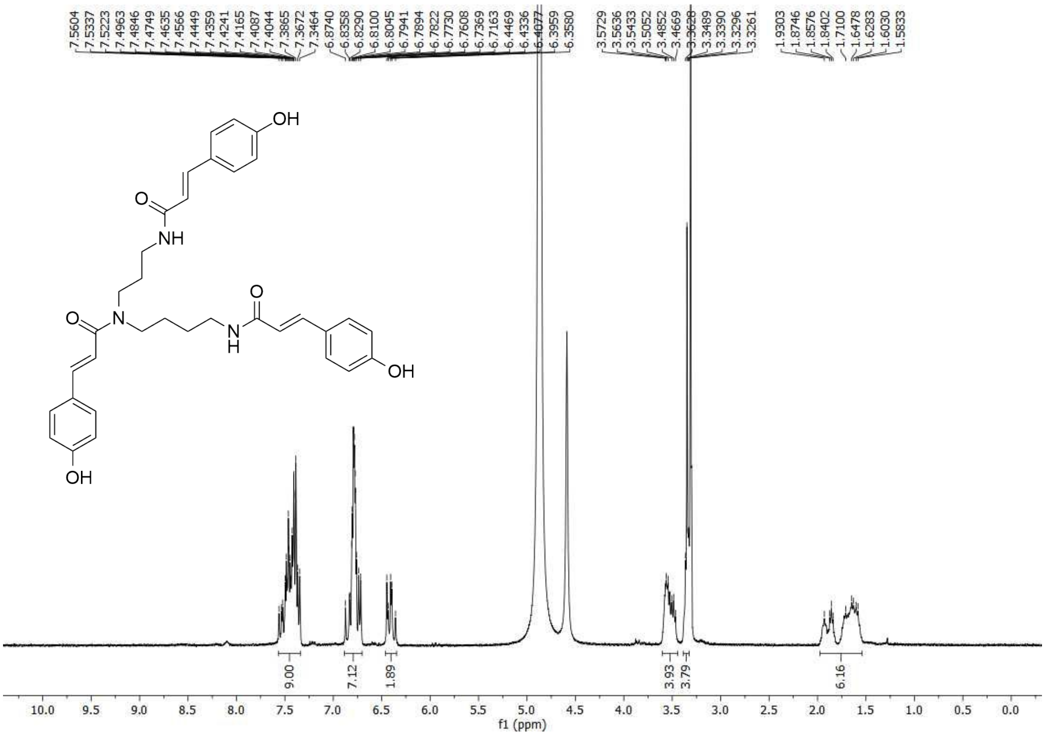

Figure S95. Amplification of the [1]H NMR spectrum of compound **15 (**400 MHz, MeOD).

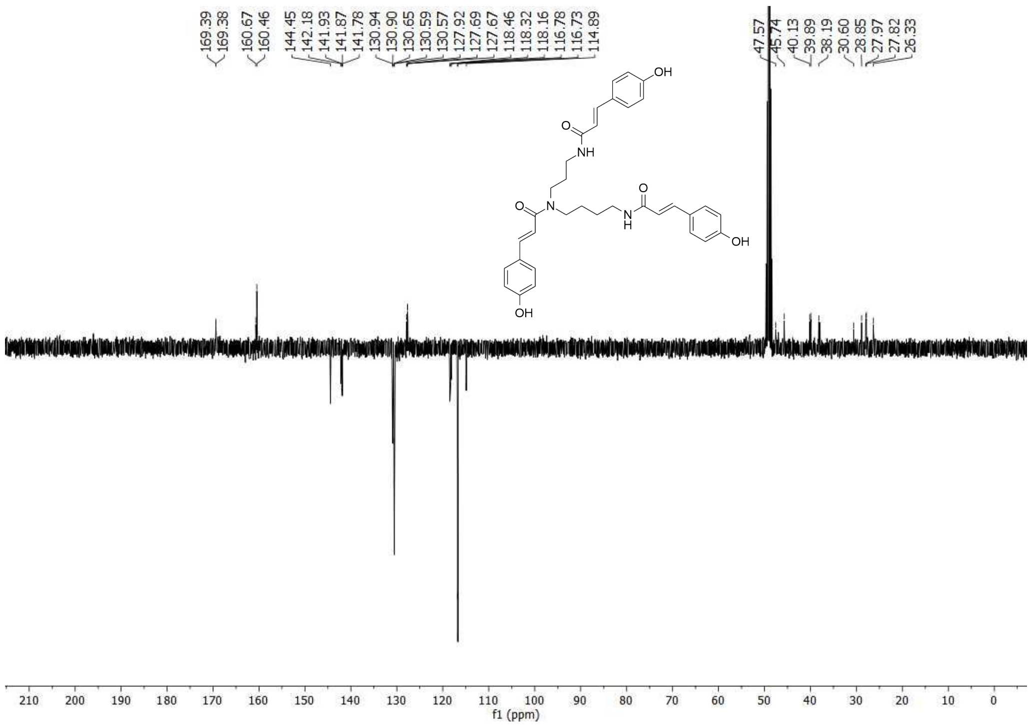

Figure S96. [13]C-APT NMR spectrum of compound **15** (100 MHz, MeOD).

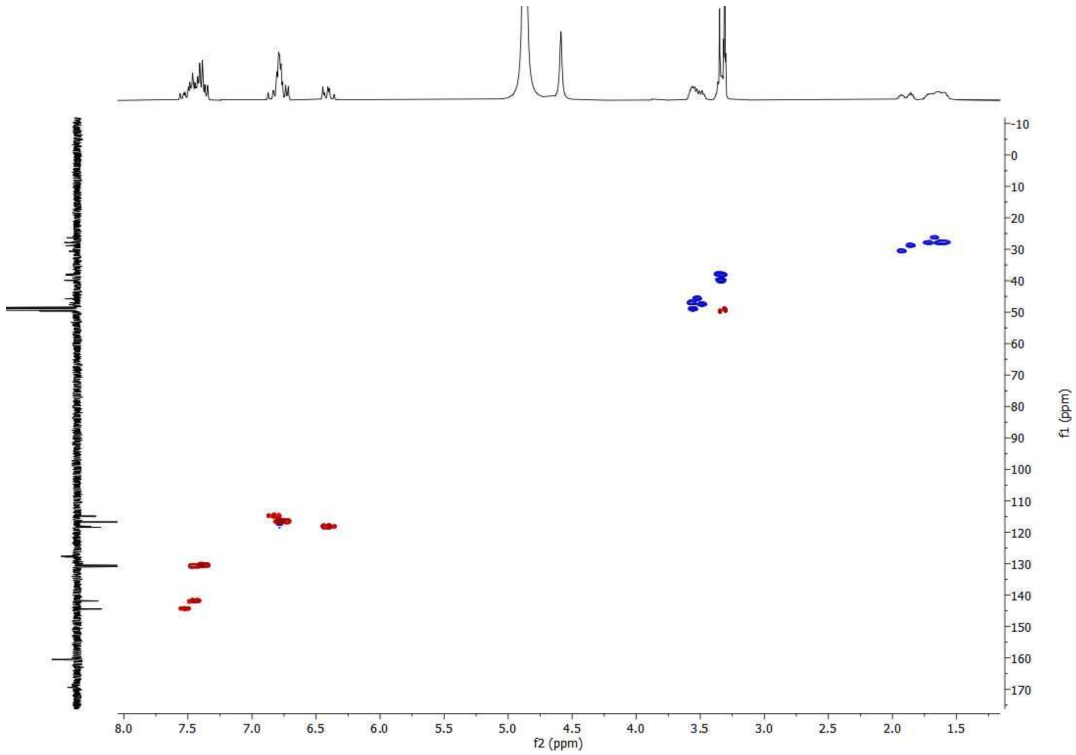

Figure S97. HSQC spectrum of compound **15 (**400/100 MHz, MeOD).

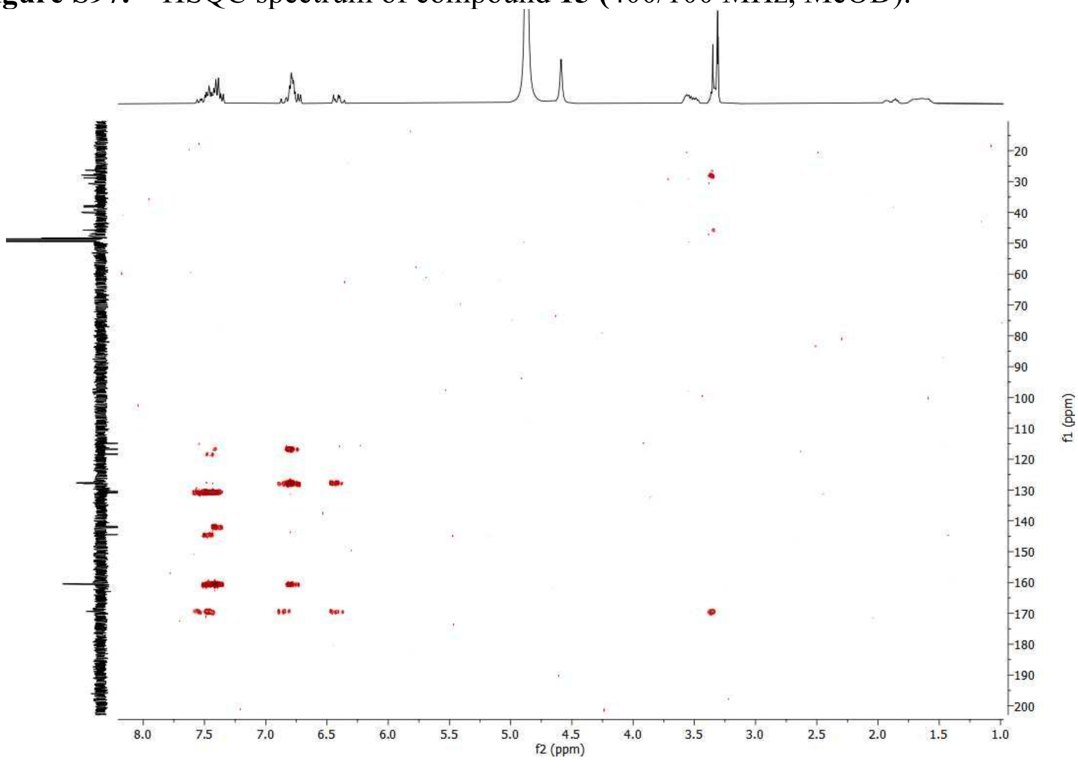

Figure S98. HMBC spectrum of compound **15 (**400/100 MHz, MeOD).

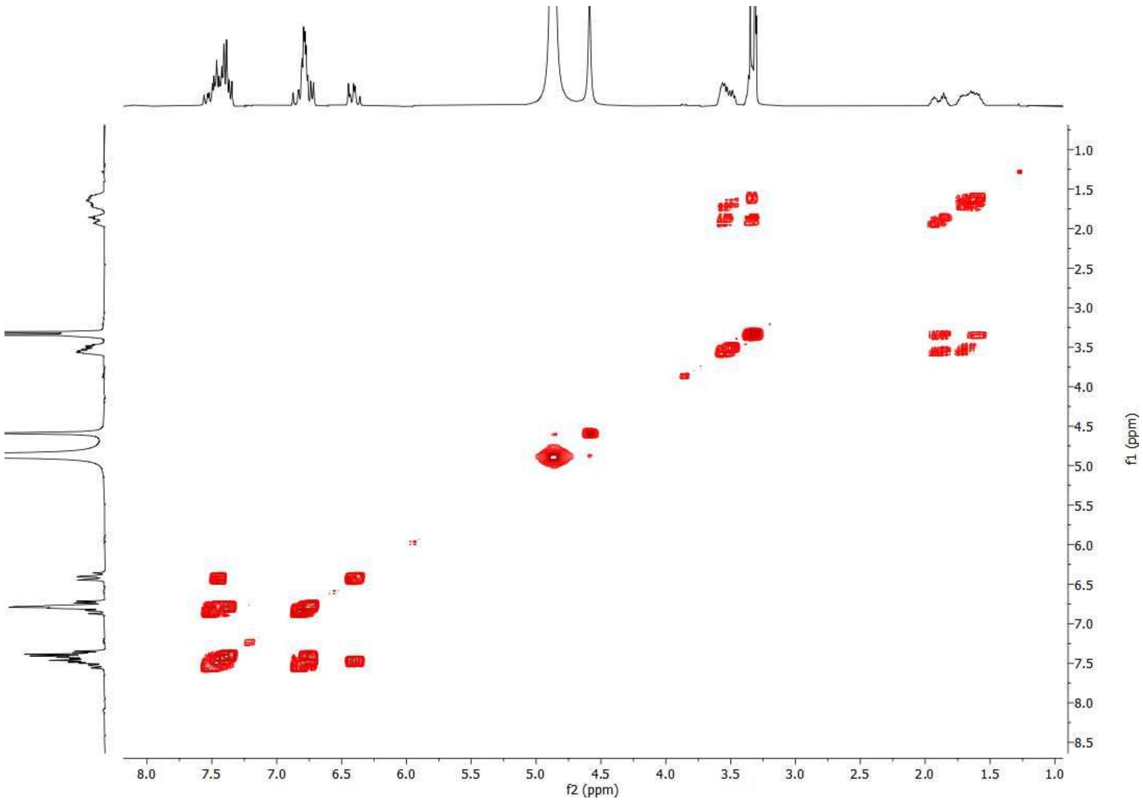

Figure S99. COSY spectrum of compound **15 (**400 MHz, MeOD).

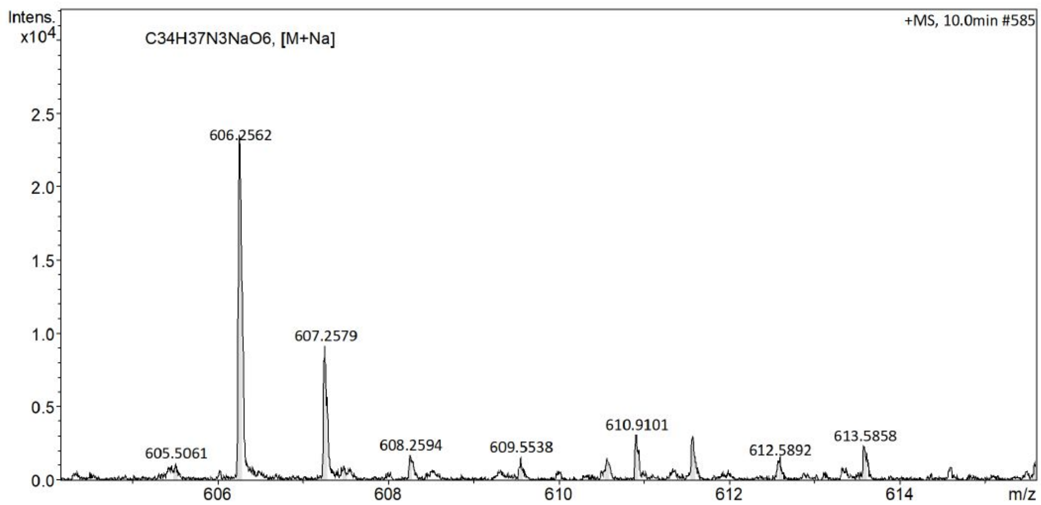

Figure S100. HRESIMS spectrum of compound **15** ($[M + Na]^+$, positive mode).

14 Quantum mechanical calculations for compound 1.

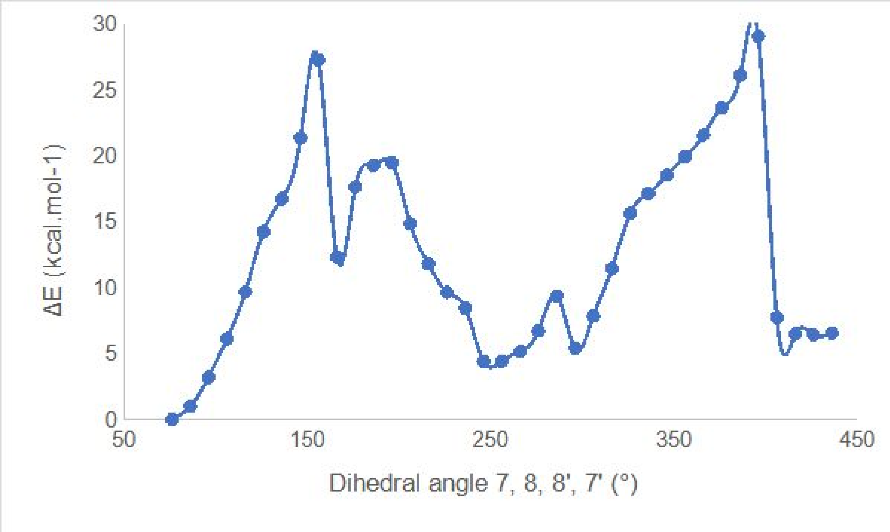

Figure S101. Calculated energy levels (in kcal.mol^{-1}) for the conformers of compound **1** as a function of rotation around the C7-C8-C8′-C7′ dihedral angle.

15 NMR calculation data for compound 1.

Table S1. DP4+ probabilities obtained by correlating the calculated ^{13}C and ^{1}H NMR chemical shifts of the 4 possible diastereoisomers of (a*S*)-compound **1** with the experimental NMR data of the isolated natural product.

	7″R*,7‴R*,8aS	***7″S*,7‴S*,8aS***	***7″R*,7‴S*,8aS***	***7″S*,7‴R*,8aS***
DP4+ Probabilities	0.00%	100.00%	0.00%	0.00%

Table S2. Calculated [GIAO-mPW1PW91/6-31G(d)-PCM//B3LYP/6-31G(d)] ^{1}H NMR chemical shifts (in ppm), obtained for 4 diastereoisomers of compound **1**, and experimental data of the isolated natural product.

Nuclei	δ_{calc} **[7″*R***,7‴*R***, 8a*S*]**	δ_{calc} **[7″*S***,7‴*S***, 8a*S*]**	δ_{calc} **[7″*R***,7‴*S***, 8a*S*]**	δ_{calc} **[7″*S***,7‴*R***, 8a*S*]**	δ_{exp}
2	8.45	6.13	6.70	6.65	6.87
6	7.62	6.99	6.37	6.66	6.87
7	8.06	6.53	7.71	6.44	7.82
2′	7.57	6.30	6.50	6.87	6.87
6′	7.41	6.65	7.17	8.06	6.87
7′	7.85	7.54	6.81	7.26	7.86
2″	8.23	7.84	7.21	7.52	6.94
3″	7.83	7.29	6.80	6.73	6.63
5″	7.39	6.59	6.30	6.93	6.63
6″	8.31	7.58	7.44	7.49	6.94
7″	6.03	4.98	5.08	5.29	4.54
8a″	4.35	4.05	2.98	3.95	3.40
8b″	5.58	3.35	4.42	2.68	3.40
2‴	8.50	7.22	7.36	7.59	7.03
3‴	7.86	6.95	6.88	6.82	6.69
5‴	7.67	6.67	6.75	6.81	6.69
6‴	8.49	7.29	7.85	7.24	7.03
7‴	6.13	4.85	5.08	4.87	4.38
8a‴	3.76	4.00	4.00	2.93	3.37
8b‴	4.91	3.02	2.70	4.36	3.37
3′,5′-OCH$_3$	4.92	3.84	3.99	3.94	3.75
3-OCH$_3$	4.87	3.78	3.86	4.03	3.75
5-OCH$_3$	4.86	3.94	3.79	3.65	3.75

Table S3. Calculated [GIAO-mPW1PW91/6-31G(d)-PCM//B3LYP/6-31G(d)] ^{13}C NMR chemical shifts (in ppm), obtained for 4 diastereoisomers of compound **1**, and experimental data of the isolated natural product.

Nuclei	δ_{calc} [7″*R**,7‴*R**, 8a*S*]	δ_{calc} [7″*S**,7‴*S**, 8a*S*]	δ_{calc} [7″*R**,7‴*S**, 8a*S*]	δ_{calc} [7″*S**,7‴*R**, 8a*S*]	δ_{exp}
1	119.5	115.6	118.3	116.3	126.7
2	104.1	103.5	109.6	114.1	108.8
3	139.1	136.1	134.1	134.3	139.0
4	134.3	128.5	131.5	132.5	149.2
5	137.9	136.7	137.9	137.7	139.0
6	111.1	98.7	101.2	97.5	108.8
7	136.6	130.5	134.2	123.1	142.3
8	125.4	122.1	126.0	125.9	127.4
9	166.2	160.9	163.3	160.1	168.2
1′	120.2	117.3	116.3	116.9	126.7
2′	104.0	99.6	113.7	107.5	108.9
3′	138.7	137.8	135.7	136.1	139.1
4′	132.5	130.1	132.9	131.8	149.2
5′	138.2	135.5	138.1	137.5	139.1
6′	107.6	108.6	100.5	100.4	108.9
7′	131.7	136.1	130.8	135.9	142.5
8′	130.5	124.1	123.1	123.3	127.6
9′	164.1	162.0	161.6	161.5	168.2
1″	125.5	126.6	124.9	123.0	134.2
2″	121.7	120.9	119.2	118.4	128.4
3″	109.5	107.6	105.5	105.5	116.0
4″	146.8	144.2	144.7	144.9	158.0
5″	108.9	104.7	104.9	105.9	116.0
6″	121.9	122.5	120.2	118.7	128.4
7″	75.9	70.4	71.7	68.8	73.0
8″	49.2	43.8	45.7	45.1	48.5
1‴	128.0	125.1	124.7	121.8	134.3
2‴	121.5	118.3	119.0	117.7	128.3
3‴	108.6	106.5	105.8	107.6	116.1
4‴	146.5	145.1	145.0	145.5	158.0
5‴	108.9	105.7	105.6	108.0	116.1
6‴	121.7	119.3	118.8	118.7	128.3
7‴	72.1	70.0	67.6	67.1	73.5
8‴	51.3	47.0	43.6	44.7	48.5

3′,5′-OCH$_3$	56.0	50.4	52.8	52.0	56.7
3-OCH$_3$	56.3	49.7	53.9	53.6	56.7
5-OCH$_3$	57.3	51.7	50.4	50.5	56.7

16 NMR calculation data for compound 2.

Table S4. DP4+ probabilities obtained by correlating the calculated ^{13}C and ^{1}H NMR chemical shifts of the 4 possible diastereoisomers of compound **2** with the experimental NMR data of the isolated natural product.

	7S*,7′S*,7″S*, 7‴R*,8S*,8′S*	***7S*,7′S*,7″R*, 7‴S*,8S*,8′S****	***7S*,7′S*,7″R*, 7‴R*,8S*,8′S****	***7S*,7′S*,7″S*, 7‴S*,8S*,8′S****
DP4+ Probabilities	0.00%	0.00%	100.00%	0.00%

Table S5. Calculated [GIAO-mPW1PW91/6-31G(d)-PCM//B3LYP/6-31G(d)] ^{1}H NMR chemical shifts (in ppm), obtained for 4 diastereoisomers of compound **2**, and experimental data of the isolated natural product.

Nuclei	δ_{calc} [7*S**,7′*S**,7″*S**, 7‴*R**,8*S**,8′*S**]	δ_{calc} [7*S**,7′*S**,7″*R**, 7‴*S**,8*S**,8′*S**]	δ_{calc} [7*S**,7′*S**,7″*R**, 7‴*R**,8*S**,8′*S**]	δ_{calc} [7*S**,7′*S**,7″*S**, 7‴*S**,8*S**,8′*S**]	δ_{exp}
2	6.00	5.88	6.39	6.71	6.73
6	6.98	7.00	7.08	6.96	6.73
7	5.46	5.52	5.20	6.18	5.27
8	1.62	1.20	2.81	3.16	3.38
2′	5.89	6.98	6.97	7.18	6.73
6′	6.98	6.00	6.84	6.82	6.73
7′	5.53	5.46	6.13	4.78	5.29
8′	1.17	1.63	3.55	2.23	3.38
2″	7.18	7.99	7.25	7.46	6.96
3″	6.18	7.04	7.02	6.96	6.66
5″	7.07	6.28	6.89	7.41	6.66
6″	7.52	7.20	7.79	7.91	6.96
7″	5.00	5.18	4.22	5.33	4.49
8a″	3.67	3.06	2.69	3.70	3.45
8b″	3.46	4.47	3.70	4.13	3.22
2‴	7.26	7.19	7.75	7.65	6.96
3‴	6.35	6.24	7.00	7.11	6.66
5‴	6.97	7.08	6.79	7.16	6.66
6‴	7.92	7.54	7.71	7.85	6.96
7‴	5.18	5.00	4.88	5.51	4.49
8a‴	4.47	3.67	4.54	3.24	3.45
8b‴	3.05	3.46	3.25	4.55	3.22
3′,5′-OCH$_3$	4.08	3.94	4.04	4.58	3.87
3-OCH$_3$	4.10	4.10	4.07	4.19	3.87
5-OCH$_3$	3.94	3.95	4.12	4.46	3.87

Table S6. Calculated [GIAO-mPW1PW91/6-31G(d)-PCM//B3LYP/6-31G(d)] ^{13}C NMR chemical shifts (in ppm), obtained for 4 diastereoisomers of compound **2**, and experimental data of the isolated natural product.

Nuclei	δ_{calc} [7*S**,7′*S**,7″*S**, 7‴*R**,8*S**,8′*S**]	δ_{calc} [7*S**,7′*S**,7″*R**, 7‴*S**,8*S**,8′*S**]	δ_{calc} [7*S**,7′*S**,7″*R**, 7‴*R**,8*S**,8′*S**]	δ_{calc} [7*S**,7′*S**,7″*S**, 7‴*S**,8*S**,8′*S**]	δ_{exp}
1	126.0	125.3	123.1	128.7	132.3
2	104.8	105.4	107.0	97.8	104.8
3	134.8	134.1	135.6	138.6	149.4
4	129.4	130.0	130.9	130.2	136.6
5	137.6	137.4	138.6	135.1	149.4
6	96.3	97.9	95.8	103.5	104.8
7	75.9	76.0	79.3	76.7	86.3
8	56.4	55.7	57.5	54.6	60.3
9	163.5	159.7	163.1	163.9	172.5
1′	125.4	126.0	124.7	122.7	132.3
2′	104.5	96.3	95.6	108.4	104.8
3′	134.3	137.6	138.1	136.6	149.4
4′	129.6	129.4	130.2	132.3	136.6
5′	137.4	134.8	136.3	138.4	149.4
6′	97.5	104.8	105.1	101.5	104.8
7′	76.0	75.9	77.9	80.2	86.3
8′	55.9	56.4	53.5	56.3	60.3
9′	159.7	163.5	158.6	162.5	172.5
1″	124.2	120.4	123.8	125.2	134.2
2″	118.9	119.1	119.6	119.3	128.5
3″	107.1	107.6	106.5	107.8	116.1
4″	145.8	146.1	145.4	145.8	158.0
5″	107.0	107.4	106.0	107.3	116.1
6″	118.7	119.3	119.5	119.5	128.5
7″	67.2	69.0	71.7	69.7	73.1
8″	46.1	40.5	47.5	48.1	48.1
1‴	120.4	124.1	124.7	121.1	134.2
2‴	119.3	118.9	121.0	119.6	128.5
3‴	107.4	107.3	106.7	107.5	116.1
4‴	146.1	145.9	145.2	146.6	158.0
5‴	107.6	107.0	106.2	108.5	116.1
6‴	119.1	118.8	120.6	120.7	128.5
7‴	69.0	67.2	68.1	69.6	73.1
8‴	40.4	46.1	39.8	44.7	48.1

3′,5′-OCH$_3$	52.3	52.3	52.1	54.1	56.8
3-OCH$_3$	54.2	54.2	53.4	52.1	56.8
5-OCH$_3$	50.4	50.6	51.1	55.6	56.8

17 NMR calculation data for compound 3.

Table S7. DP4+ probabilities obtained by correlating the calculated ^{13}C and ^{1}H NMR chemical shifts of both stereoisomers of compound **3** with the experimental NMR data of the isolated natural product.

	7S,7′S,7‴S,8S,8′S	***7R,7′R,7‴S,8R,8′R***
DP4+ Probabilities	100.00%	0.00%

Table S8. Calculated [GIAO-mPW1PW91/6-31G(d)-PCM//B3LYP/6-31G(d)] ^{1}H NMR chemical shifts (in ppm), obtained for both diastereoisomers of compound **3**, and experimental data of the isolated natural product.

Nuclei	δ_{calc} **[*7S,7′S,7‴S,8S,8′S*]**	δ_{calc} **[*7R,7′R,7‴S,8R,8′R*]**	δ_{exp}
2	6.49	6.25	6.71
6	7.13	6.89	6.71
7	5.55	5.34	5.26
8	2.22	0.87	3.35
2′	6.26	6.61	6.73
6′	7.09	6.58	6.73
7′	5.45	5.63	5.28
8′	1.76	1.38	3.40
2″	7.38	7.52	6.83
3″	6.53	6.92	6.63
5″	7.02	6.36	6.63
6″	7.24	6.99	6.83
7a″	2.87	2.64	2.59
7b″	2.40	3.02	2.53
8a″	2.80	3.77	3.37
8b″	4.28	3.00	3.18
2‴	7.60	7.12	6.95
3‴	7.22	6.26	6.66
5‴	6.72	6.82	6.66
6‴	7.49	7.81	6.95
7‴	5.15	5.13	4.46
8a‴	3.38	4.38	3.49
8b‴	3.89	3.05	3.18
3,5-OCH3	4.12	4.03	3.88
3′,5′-OCH3	4.07	4.00	3.86

Table S9. Calculated [GIAO-mPW1PW91/6-31G(d)-PCM//B3LYP/6-31G(d)] ^{13}C NMR chemical shifts (in ppm), obtained for both diastereoisomers of compound **3**, and experimental data of the isolated natural product.

Nuclei	δ_{calc} [7*S*,7′*S*,7‴*S*,8*S*,8′*S*]	δ_{calc} [7*R*,7′*R*,7‴*S*,8*R*,8′*R*]	δ_{exp}
1	123.2	126.3	131.0
2	103.7	98.7	104.7
3	136.0	135.7	149.5
4	129.2	127.7	136.7
5	138.2	136.8	149.5
6	95.2	97.9	104.7
7	78.3	79.1	86.4
8	58.4	58.4	60.6
9	159.1	160.1	172.1
1′	125.6	126.8	132.4
2′	105.3	101.1	104.9
3′	135.2	136.0	149.4
4′	129.8	129.3	136.7
5′	137.9	136.0	149.4
6′	96.8	100.6	104.9
7′	77.6	78.5	86.4
8′	56.2	56.6	60.3
9′	165.9	161.1	172.5
1″	120.3	121.0	130.8
2″	121.9	121.8	130.7
3″	108.2	106.7	116.2
4″	145.6	145.3	156.9
5″	106.9	107.3	116.2
6″	122.3	122.5	130.7
7″	32.5	31.1	35.7
8″	33.8	37.0	42.6
1‴	126.5	121.0	134.5
2‴	119.5	118.7	128.5
3‴	107.3	106.9	116.1
4‴	145.2	145.5	158.0
5‴	106.0	106.5	116.1
6‴	118.8	118.8	128.5
7‴	68.4	68.4	73.2
8‴	47.2	41.2	48.1
3,5-OCH3	51.2	70.9	56.8
3′,5′-OCH3	54.6	51.8	56.9

18 NMR calculation data for compound 4.

Table S10. DP4+ probabilities obtained by correlating the calculated [13]C and [1]H NMR chemical shifts of the 4 possible diastereoisomers of compound **4** with the experimental NMR data of the isolated natural product.

	7′S*,7″R*, 7‴R*,8′R*	***7′S*,7″S*, 7‴S*,8′R****	***7′S*,7″R*, 7‴S*,8′R****	***7′S*,7″S*, 7‴R*,8′R****
DP4+ Probabilities	0.00%	0.00%	100.00%	0.00%

Table S11. Calculated [GIAO-mPW1PW91/6-31G(d)-PCM//B3LYP/6-31G(d)] [1]H NMR chemical shifts (in ppm), obtained for 4 diastereoisomers of compound **4**, and experimental data of the isolated natural product.

Nuclei	δ_{calc} [7′*S**,7″*R**, 7‴*R**,8′*R**]	δ_{calc} [7′*S**,7″*S**, 7‴*S**,8′*R**]	δ_{calc} [7′*S**,7″*R**, 7‴*S**,8′*R**]	δ_{calc} [7′*S**,7″*S**, 7‴*R**,8′*R**]	δ_{exp}
2	6.59	6.53	6.84	6.57	6.77
7	7.02	6.76	7.47	7.37	7.33
2′	5.66	6.82	6.45	6.59	6.33
6′	6.49	7.07	6.22	5.95	6.33
7′	5.25	4.67	4.87	4.61	4.87
8′	3.60	3.87	3.37	2.59	3.72
2″	7.15	7.40	7.46	7.07	7.14
3″	6.80	6.91	6.66	6.25	6.72
5″	6.38	6.73	6.81	6.89	6.72
6″	7.13	7.62	7.39	7.24	7.14
7″	5.03	5.19	5.11	5.09	4.68
8a″	3.29	2.70	3.23	3.33	3.39
8b″	4.08	3.58	3.22	4.05	3.39
2‴	7.49	7.55	7.21	7.25	6.96
3‴	6.71	6.87	6.74	6.89	6.67
5‴	6.91	6.78	6.92	6.70	6.67
6‴	7.54	7.26	7.44	7.25	6.96
7‴	4.85	4.42	4.84	5.02	4.53
8a‴	3.51	3.66	3.38	4.06	3.34
8b‴	2.87	2.91	3.29	3.12	3.25
3′,5′-OCH_3	3.66	3.89	3.90	4.18	3.68
3-OCH_3	3.97	3.95	4.04	4.15	3.92
5-OCH_3	4.05	3.89	3.49	3.63	3.58

Table S12. Calculated [GIAO-mPW1PW91/6-31G(d)-PCM//B3LYP/6-31G(d)] ^{13}C NMR chemical shifts (in ppm), obtained for 4 diastereoisomers of compound **4**, and experimental data of the isolated natural product.

Nuclei	δ_{calc} [7''*R**,7'''*R**, 8a*S*]	δ_{calc} [7''*S**,7'''*S**, 8a*S*]	δ_{calc} [7''*R**,7'''*S**, 8a*S*]	δ_{calc} [7''*S**,7'''*R**, 8a*S*]	δ_{exp}
1	115.4	113.9	116.0	116.9	124.2
2	100.7	99.6	109.2	101.3	109.1
3	136.9	137.1	137.1	137.8	149.3
4	135.5	133.1	137.2	134.4	143.3
5	135.1	135.5	136.9	135.3	146.9
6	119.8	115.9	118.1	114.1	125.2
7	129.9	121.7	129.9	129.6	135.4
8	117.9	124.7	118.8	118.4	126.8
9	164.4	161.7	160.0	158.8	170.3
1′	126.9	129.0	126.9	125.2	135.3
2′	99.5	106.1	100.5	103.5	106.0
3′	136.5	135.7	136.6	136.3	149.0
4′	123.7	129.8	125.8	128.6	135.3
5′	137.6	137.7	137.0	137.3	149.0
6′	96.6	98.4	96.2	99.4	106.0
7′	36.4	36.0	38.0	37.7	41.4
8′	47.6	49.1	48.9	47.5	50.2
9′	163.6	165.2	162.3	166.7	174.3
1″	123.6	124.1	123.5	125.2	134.7
2″	117.5	119.3	119.6	118.2	128.4
3″	107.0	105.7	106.0	106.3	116.1
4″	145.5	144.9	145.5	145.1	158.0
5″	106.4	105.7	106.2	106.9	116.1
6″	118.3	118.4	119.6	117.8	128.4
7″	69.4	67.0	68.3	69.5	73.4
8″	47.2	47.1	48.1	46.7	48.4
1‴	125.7	124.2	123.1	125.1	134.3
2‴	119.2	118.9	119.0	118.9	128.4
3‴	105.4	106.6	106.9	106.5	116.1
4‴	144.9	145.5	145.8	144.4	157.9
5‴	105.8	105.7	107.4	105.7	116.1
6‴	119.4	120.8	119.5	118.7	128.4
7‴	71.7	70.6	69.1	69.3	72.8
8‴	49.7	43.6	44.1	46.4	48.0

3′,5′-OCH$_3$	50.6	51.3	50.2	51.1	56.7
3-OCH$_3$	50.5	50.2	52.1	51.1	56.8
5-OCH$_3$	53.6	53.0	54.9	53.4	60.8

19 NMR calculation data for compound 5.

Table S13. DP4+ probabilities obtained by correlating the calculated ^{13}C and ^{1}H NMR chemical shifts of both diastereoisomers of compound **5** with the experimental NMR data of the isolated natural product.

	7′S*,7′′′R*,8′R*	***7′S*,7′′′S*,8′R****
DP4+ Probabilities	0.00%	100.00%

Table S14. Calculated [GIAO-mPW1PW91/6-31G(d)-PCM//B3LYP/6-31G(d)] ^{1}H NMR chemical shifts (in ppm), obtained for both diastereoisomers of compound **5**, and experimental data of the isolated natural product.

Nuclei	δ_{calc} [7′*S*,7′′′*R*,8′*R*]	δ_{calc} [7′*S*,7′′′*S*,8′*R*]	δ_{exp}
2	6.41	6.62	6.76
7	6.20	6.88	7.27
7′	5.08	5.31	4.90
8′	3.28	3.44	3.72
2′,6′	6.04	6.24	6.33
2′′,6′′	7.06	7.17	6.94
3′′,5′′	6.65	6.67	6.66
7′′	2.82	2.22	2.68
8′′	3.46	3.70	3.38
2′′′,6′′′	7.39	7.52	6.98
3′′′,5′′′	6.53	6.85	6.67
7′′′	4.79	3.12	4.52
8a′′′	3.90	4.15	3.35
8b′′′	3.22	3.35	3.26
3′-OCH3	4.06	4.05	3.70
5′-OCH3	3.39	3.87	3.70
3-OCH3	4.05	4.24	3.92
5-OCH3	4.05	4.11	3.53

Table S15. Calculated [GIAO-mPW1PW91/6-31G(d)-PCM//B3LYP/6-31G(d)] ^{13}C NMRchemical shifts (in ppm), obtained for both diastereoisomers of compound **5**, and experimental data of the isolated natural product.

Nuclei	δ_{calc} [7′*S*,7‴*R*,8′*R*]	δ_{calc} [7′*S*,7‴*S*,8′*R*]	δ_{exp}
1	116.1	116.3	124.2
2	110.1	102.2	109.1
3	135.5	136.7	149.3
4	137.0	135.3	143.2
5	136.8	135.3	147.0
6	119.4	119.9	125.3
7	124.9	127.5	135.0
8	121.5	121.5	127.1
9	163.4	162.9	170.0
1′	126.2	127.9	135.2
2′,6′	100.3	98.6	106.1
3′,5′	136.7	137.3	149.0
4′	126.0	124.5	135.3
7′	36.0	37.9	41.4
8′	47.7	49.0	50.1
9′	159.5	158.9	174.2
1″	117.8	120.1	131.4
2″,6″	121.9	122.3	130.8
3″,5″	107.4	107.7	116.2
4″	145.6	145.8	156.8
7″	28.7	31.8	35.6
8″	36.9	40.8	42.8
1‴	123.3	125.9	134.4
2‴,6‴	119.2	121.3	128.4
3‴,5‴	106.3	123.8	116.0
4‴	145.0	145.6	157.9
7‴	68.7	70.8	72.8
8‴	41.6	43.1	47.9
3′-OCH$_3$	52.4	51.5	56.7
5′-OCH$_3$	49.8	51.6	56.7
3-OCH$_3$	52.9	52.1	56.8
5-OCH$_3$	55.5	54.7	60.8

20 Monte Carlo/MMFF force field calculations and Boltzmann population.

Table S16. Relative energy values (in $kcal.mol^{-1}$) and Boltzmann population of the conformers obtained from the Monte Carlo/MMFF force field calculations for each stereoisomer considered for compound **1**.

Conformers	**Relative energy values ($kcal.mol^{-1}$)**	**Boltzmann population (%)**
7''R*,7'''R*,8aS		
1	0.0000	8.5690
2	0.0209	8.2717
3	0.0209	8.2717
4	0.0209	8.2717
5	0.1650	6.4861
6	0.1650	6.4861
7	0.3273	4.9321
8	0.3273	4.9321
9	0.3459	4.7800
10	0.3459	4.7799
11	0.3615	4.6558
12	0.4595	3.9459
13	0.4945	3.7194
14	0.5574	3.3451
15	1.0433	1.4731
16	1.0433	1.4731
17	1.1197	1.2949
18	1.1429	1.2452
19	1.2035	1.1241
20	1.2035	1.1241
21	1.2553	1.0301
22	1.2553	1.0301
23	1.3343	0.9015
24	1.4165	0.7846
25	1.4165	0.7846
26	1.4191	0.7813
27	1.5008	0.6806
28	1.6659	0.5151
29	1.8394	0.3843
30	1.8853	0.3557
31	1.9914	0.2974
32	2.0386	0.2746
33	2.1857	0.2143
34	2.1909	0.2124
35	2.2144	0.2041
36	2.2621	0.1883
37	2.2718	0.1853
38	2.2718	0.1853
39	2.2820	0.1821
40	2.3211	0.1705
41	2.3881	0.1522
42	2.4206	0.1441
43	2.4947	0.1272
44	2.4947	0.1272
45	2.5237	0.1211
46	2.6646	0.0955

47	2.6761	0.0936
48	2.6783	0.0933
49	2.7046	0.0892
50	2.7251	0.0862
51	2.8813	0.0662
52	2.9062	0.0635
53	3.0604	0.0490
54	3.3676	0.0291
55	3.3801	0.0285
56	3.4850	0.0239
57	3.7031	0.0165
58	4.0012	0.0100
59	4.0098	0.0099
60	4.3094	0.0059
61	4.5103	0.0042
62	4.5104	0.0042
63	4.5996	0.0036
64	4.6958	0.0031
65	4.8275	0.0025
66	5.0226	0.0018
67	5.1306	0.0015
68	5.5265	0.0008
69	5.8014	0.0005
70	6.0228	0.0003
71	6.0292	0.0003
72	6.0784	0.0003
73	6.3552	0.0002
74	6.3930	0.0002
75	6.4049	0.0002
76	6.5492	0.0001
77	6.5593	0.0001
78	6.6731	0.0001
79	6.7380	0.0001
80	6.8455	0.0001
81	7.0074	0.0001
82	7.2899	0.0000
83	7.8838	0.0000
84	8.0769	0.0000
85	8.3550	0.0000
86	8.4226	0.0000
87	8.5591	0.0000
88	8.5966	0.0000
89	8.7835	0.0000
90	8.8769	0.0000
91	8.9235	0.0000
92	8.9418	0.0000
93	9.0179	0.0000
94	9.0651	0.0000
95	9.1651	0.0000
96	9.1950	0.0000
97	9.4030	0.0000
98	9.7442	0.0000
99	9.7557	0.0000
100	9.8814	0.0000
7''S*,7'''S*,8aS		
1	0.0000	0.5070
2	0.2357	0.3406
3	0.7660	0.1392

4	2.2771	0.0109
5	4.0911	0.0005
6	4.1949	0.0004
7	4.3348	0.0003
8	4.3611	0.0003
9	4.6933	0.0002
10	5.3188	0.0001
11	5.5829	0.0000
12	5.7793	0.0000
13	5.8108	0.0000
14	5.8557	0.0000
15	5.9016	0.0000
16	5.9063	0.0000
17	6.0269	0.0000
18	6.0399	0.0000
19	6.0619	0.0000
20	6.0686	0.0000
21	6.1820	0.0000
22	6.1903	0.0000
23	6.2597	0.0000
24	6.3062	0.0000
25	6.3076	0.0000
26	6.3247	0.0000
27	6.3474	0.0000
28	6.4593	0.0000
29	6.5036	0.0000
30	6.5567	0.0000
31	6.5767	0.0000
32	6.5838	0.0000
33	6.5841	0.0000
34	6.6344	0.0000
35	6.6880	0.0000
36	6.7029	0.0000
37	6.8126	0.0000
38	6.8721	0.0000
39	6.9561	0.0000
40	7.0296	0.0000
41	7.0479	0.0000
42	7.1392	0.0000
43	7.1733	0.0000
44	7.1765	0.0000
45	7.1773	0.0000
46	7.2686	0.0000
47	7.2988	0.0000
48	7.3906	0.0000
49	7.4024	0.0000
50	7.4029	0.0000
51	7.4817	0.0000
52	7.4869	0.0000
53	7.5580	0.0000
54	7.6024	0.0000
55	7.6347	0.0000
56	7.7017	0.0000
57	7.7797	0.0000
58	7.8838	0.0000
59	7.9804	0.0000
60	8.1489	0.0000
61	8.1489	0.0000

62	8.1589	0.0000
63	8.1803	0.0000
64	8.1906	0.0000
65	8.2355	0.0000
66	8.3627	0.0000
67	8.3654	0.0000
68	8.3905	0.0000
69	8.4071	0.0000
70	8.4459	0.0000
71	8.5094	0.0000
72	8.5094	0.0000
73	8.5302	0.0000
74	8.5506	0.0000
75	8.6679	0.0000
76	8.7056	0.0000
77	8.9559	0.0000
78	8.9661	0.0000
79	9.0165	0.0000
80	9.0853	0.0000
81	9.1243	0.0000
82	9.1441	0.0000
83	9.1766	0.0000
84	9.2273	0.0000
85	9.3385	0.0000
86	9.3644	0.0000
87	9.3947	0.0000
88	9.5655	0.0000
89	9.5848	0.0000
90	9.6017	0.0000
91	9.6368	0.0000
92	9.7162	0.0000
93	9.7164	0.0000
94	9.7294	0.0000
95	9.7823	0.0000
96	9.8809	0.0000
97	9.8945	0.0000
98	9.9546	0.0000
99	9.9939	0.0000
100	9.9939	0.0000
7''R*,7'''S*,8aS		
1	0.0000	0.4785
2	0.1715	0.3583
3	1.6139	0.0314
4	1.7959	0.0231
5	1.8344	0.0216
6	1.8980	0.0194
7	1.9399	0.0181
8	1.9676	0.0173
9	2.1054	0.0137
10	3.0161	0.0029
11	3.0593	0.0027
12	3.1241	0.0025
13	3.2690	0.0019
14	3.4246	0.0015
15	3.4477	0.0014
16	3.4625	0.0014
17	3.5293	0.0012
18	3.8456	0.0007

19	4.3533	0.0003
20	4.4129	0.0003
21	4.4263	0.0003
22	4.7272	0.0002
23	4.9532	0.0001
24	4.9620	0.0001
25	4.9773	0.0001
26	5.2757	0.0001
27	5.2757	0.0001
28	5.4126	0.0001
29	5.4212	0.0001
30	5.4848	0.0000
31	5.4930	0.0000
32	5.4996	0.0000
33	5.6077	0.0000
34	5.6176	0.0000
35	5.6402	0.0000
36	5.6469	0.0000
37	5.7228	0.0000
38	5.7945	0.0000
39	5.8213	0.0000
40	5.9035	0.0000
41	5.9721	0.0000
42	6.0904	0.0000
43	6.2142	0.0000
44	6.2142	0.0000
45	6.2203	0.0000
46	6.3783	0.0000
47	6.3860	0.0000
48	6.4346	0.0000
49	6.5282	0.0000
50	6.5282	0.0000
51	6.5282	0.0000
52	6.5916	0.0000
53	6.6627	0.0000
54	6.9334	0.0000
55	6.9741	0.0000
56	6.9881	0.0000
57	7.2907	0.0000
58	7.4147	0.0000
59	7.4428	0.0000
60	7.4781	0.0000
61	7.5432	0.0000
62	7.5432	0.0000
63	7.6305	0.0000
64	7.7574	0.0000
65	7.7961	0.0000
66	7.8515	0.0000
67	7.8831	0.0000
68	7.9897	0.0000
69	8.0404	0.0000
70	8.1427	0.0000
71	8.2598	0.0000
72	8.3844	0.0000
73	8.4197	0.0000
74	8.5094	0.0000
75	8.5094	0.0000
76	8.5569	0.0000

77	8.5899	0.0000
78	8.6345	0.0000
79	8.6769	0.0000
80	8.6930	0.0000
81	8.7489	0.0000
82	8.7876	0.0000
83	8.9889	0.0000
84	9.0014	0.0000
85	9.0038	0.0000
86	9.1194	0.0000
87	9.1366	0.0000
88	9.1779	0.0000
89	9.1903	0.0000
90	9.2469	0.0000
91	9.2483	0.0000
92	9.2871	0.0000
93	9.2872	0.0000
94	9.3736	0.0000
95	9.4640	0.0000
96	9.4946	0.0000
97	9.4946	0.0000
98	9.5000	0.0000
99	9.6790	0.0000
100	9.9669	0.0000
7''S*,7'''R*,8aS		
1	0.0000	0.2449
2	0.1320	0.1960
3	0.6308	0.0845
4	0.6780	0.0780
5	1.1641	0.0343
6	1.1641	0.0343
7	1.2035	0.0321
8	1.2035	0.0321
9	1.2244	0.0310
10	1.2244	0.0310
11	1.2612	0.0292
12	1.2612	0.0292
13	1.4257	0.0221
14	1.5012	0.0194
15	1.5012	0.0194
16	1.9860	0.0086
17	1.9860	0.0086
18	2.0108	0.0082
19	2.0108	0.0082
20	2.0156	0.0082
21	2.0156	0.0082
22	2.0670	0.0075
23	2.0670	0.0075
24	2.2002	0.0060
25	2.2307	0.0057
26	2.7248	0.0025
27	3.3742	0.0008
28	3.4393	0.0007
29	3.4739	0.0007
30	3.9859	0.0003
31	4.5069	0.0001
32	4.6936	0.0001
33	4.9698	0.0001

34	4.9833	0.0001
35	4.9833	0.0001
36	5.0324	0.0001
37	5.0547	0.0000
38	5.3279	0.0000
39	5.4244	0.0000
40	5.4981	0.0000
41	5.4988	0.0000
42	5.6296	0.0000
43	5.6988	0.0000
44	5.9575	0.0000
45	5.9883	0.0000
46	6.2254	0.0000
47	6.3318	0.0000
48	6.3478	0.0000
49	6.3580	0.0000
50	6.4715	0.0000
51	6.4715	0.0000
52	6.5614	0.0000
53	6.7668	0.0000
54	6.9544	0.0000
55	7.0048	0.0000
56	7.1901	0.0000
57	7.3691	0.0000
58	7.7395	0.0000
59	7.8269	0.0000
60	7.8836	0.0000
61	7.9716	0.0000
62	8.0099	0.0000
63	8.1025	0.0000
64	8.2941	0.0000
65	8.3668	0.0000
66	8.3787	0.0000
67	8.3787	0.0000
68	8.4182	0.0000
69	8.4803	0.0000
70	8.5165	0.0000
71	8.5900	0.0000
72	8.6343	0.0000
73	8.7250	0.0000
74	8.7255	0.0000
75	8.7345	0.0000
76	8.7733	0.0000
77	8.8228	0.0000
78	8.8833	0.0000
79	8.9197	0.0000
80	8.9387	0.0000
81	8.9454	0.0000
82	8.9504	0.0000
83	8.9840	0.0000
84	9.0548	0.0000
85	9.1032	0.0000
86	9.1089	0.0000
87	9.1437	0.0000
88	9.1440	0.0000
89	9.1511	0.0000
90	9.2641	0.0000
91	9.3626	0.0000

92	9.5135	0.0000
93	9.5521	0.0000
94	9.5809	0.0000
95	9.5944	0.0000
96	9.6309	0.0000
97	9.8343	0.0000
98	9.8570	0.0000
99	9.9638	0.0000
100	9.9709	0.0000

Table S17. Relative energy values (in kcal.mol^{-1}) and Boltzmann population of the conformers obtained from the Monte Carlo/MMFF force field calculations for each stereoisomer considered for compound **2**.

Conformers	Relative energy values (kcal.mol^{-1})	Boltzmann population (%)
	7S*,7′S*,7″S*,7‴R*,8S*,8′S*	
1	0.0000	33.0733
2	0.0000	33.0733
3	0.0000	33.0733
4	2.2981	0.6841
5	3.8945	0.0462
6	3.8945	0.0462
7	6.0466	0.0012
8	6.1484	0.0010
9	6.7018	0.0004
10	6.7018	0.0004
11	7.3384	0.0001
12	7.3420	0.0001
13	7.7160	0.0001
14	8.1906	0.0000
15	8.3709	0.0000
16	8.6442	0.0000
17	8.8499	0.0000
18	9.1383	0.0000
19	9.2595	0.0000
20	9.6297	0.0000
21	9.6824	0.0000
22	9.8625	0.0000
23	9.9175	0.0000
24	9.9527	0.0000
25	10.0108	0.0000
26	10.0780	0.0000
27	10.3156	0.0000
28	10.9182	0.0000
29	11.0984	0.0000
30	11.1585	0.0000
31	11.5216	0.0000
32	11.7046	0.0000
33	11.7425	0.0000
34	12.3711	0.0000
35	12.4805	0.0000
36	12.5573	0.0000
37	12.5825	0.0000
38	13.0508	0.0000
39	13.3534	0.0000
40	13.5627	0.0000
41	13.6613	0.0000
42	14.5160	0.0000
43	14.5310	0.0000
44	14.5759	0.0000
45	14.6425	0.0000
46	14.7525	0.0000
47	15.4807	0.0000
48	15.6262	0.0000
49	15.9843	0.0000

50	16.1476	0.0000
51	16.3640	0.0000
52	16.8362	0.0000
53	16.9262	0.0000
54	17.1464	0.0000
55	17.2401	0.0000
56	17.5103	0.0000
57	17.7214	0.0000
58	18.3201	0.0000
59	18.4538	0.0000
60	18.6685	0.0000
61	18.6686	0.0000
62	19.0129	0.0000
63	19.2383	0.0000
64	19.3026	0.0000
65	20.1032	0.0000
66	20.2629	0.0000
67	20.3339	0.0000
68	20.8890	0.0000
69	20.9855	0.0000
70	21.0685	0.0000
71	21.1572	0.0000
72	21.3028	0.0000
73	21.4586	0.0000
74	21.6990	0.0000
75	21.8724	0.0000
76	22.1640	0.0000
77	22.2880	0.0000
78	22.5256	0.0000
79	22.6523	0.0000
80	22.7300	0.0000
81	23.0933	0.0000
82	23.1548	0.0000
83	23.1925	0.0000
84	23.4465	0.0000
85	23.6105	0.0000
86	23.9486	0.0000
87	24.7109	0.0000
88	26.1529	0.0000
89	26.7070	0.0000
90	28.3617	0.0000
91	28.3682	0.0000
92	28.4097	0.0000
93	28.5713	0.0000
94	28.6873	0.0000
95	28.7357	0.0000
96	30.5853	0.0000
97	31.4692	0.0000
98	31.5103	0.0000
99	34.6216	0.0000
100	38.1970	0.0000
7S*,7′S*,7′′R*,7′′′S*,8S*,8′S*		
1	0.0000	99.2048
2	3.1036	0.5269
3	3.7332	0.1821
4	4.5128	0.0488
5	5.5730	0.0082
6	5.6671	0.0070

7	5.8661	0.0050
8	5.9651	0.0042
9	5.9878	0.0041
10	6.3251	0.0023
11	6.5329	0.0016
12	6.6221	0.0014
13	6.7507	0.0011
14	6.7719	0.0011
15	7.0083	0.0007
16	7.1128	0.0006
17	8.6949	0.0000
18	8.6986	0.0000
19	9.0675	0.0000
20	9.0748	0.0000
21	9.1269	0.0000
22	9.2703	0.0000
23	9.4095	0.0000
24	10.0989	0.0000
25	10.6310	0.0000
26	11.1979	0.0000
27	11.2705	0.0000
28	11.2706	0.0000
29	11.6894	0.0000
30	11.9173	0.0000
31	12.0665	0.0000
32	12.0665	0.0000
33	13.2429	0.0000
34	13.9489	0.0000
35	14.0532	0.0000
36	14.5127	0.0000
37	14.5500	0.0000
38	14.5500	0.0000
39	14.6209	0.0000
40	14.8192	0.0000
41	14.8228	0.0000
42	14.8479	0.0000
43	14.9307	0.0000
44	15.9085	0.0000
45	16.1337	0.0000
46	16.2588	0.0000
47	16.7345	0.0000
48	16.7938	0.0000
49	16.9281	0.0000
50	17.0139	0.0000
51	17.2849	0.0000
52	17.5994	0.0000
53	17.9474	0.0000
54	18.1482	0.0000
55	18.3550	0.0000
56	18.4008	0.0000
57	18.8640	0.0000
58	19.5154	0.0000
59	19.5587	0.0000
60	19.9580	0.0000
61	19.9585	0.0000
62	20.7516	0.0000
63	20.8207	0.0000
64	21.1796	0.0000

65	21.3844	0.0000
66	21.3973	0.0000
67	21.7080	0.0000
68	22.0108	0.0000
69	22.0898	0.0000
70	22.4763	0.0000
71	24.0812	0.0000
72	24.4194	0.0000
73	28.7728	0.0000
74	28.8256	0.0000
75	28.9203	0.0000
76	29.9774	0.0000
77	31.4242	0.0000
78	31.4361	0.0000
79	31.6444	0.0000
80	31.9760	0.0000
81	32.0791	0.0000
82	32.2635	0.0000
83	32.7862	0.0000
84	33.0537	0.0000
85	33.0681	0.0000
86	33.1837	0.0000
87	33.2172	0.0000
88	33.4049	0.0000
89	33.6821	0.0000
90	35.0170	0.0000
91	35.3334	0.0000
92	35.8367	0.0000
93	36.7811	0.0000
94	36.9757	0.0000
95	37.1403	0.0000
96	37.6950	0.0000
97	38.5137	0.0000
98	45.8392	0.0000
99	48.1850	0.0000
100	48.4624	0.0000
7S*,7′S*,7′′R*,7′′′R*,8S*,8′S*		
1	0.0000	17.2060
2	0.0000	17.2060
3	0.1854	12.5841
4	0.5260	7.0820
5	0.5260	7.0820
6	0.6418	5.8245
7	0.8343	4.2087
8	0.8343	4.2087
9	0.9364	3.5429
10	1.1342	2.5372
11	1.1342	2.5372
12	1.2482	2.0932
13	1.3044	1.9036
14	1.3122	1.8787
15	1.4268	1.5485
16	1.5093	1.3473
17	1.6752	1.0183
18	1.7109	0.9587
19	1.9086	0.6867
20	1.9582	0.6315
21	2.0098	0.5789

22	2.0208	0.5683
23	2.0896	0.5059
24	2.1861	0.4299
25	2.4009	0.2992
26	2.6647	0.1917
27	2.6791	0.1871
28	3.0750	0.0959
29	3.0913	0.0933
30	3.1356	0.0866
31	3.1735	0.0812
32	3.2582	0.0704
33	3.2582	0.0704
34	3.2862	0.0671
35	3.4086	0.0546
36	3.6292	0.0376
37	3.6591	0.0358
38	3.6726	0.0350
39	3.6772	0.0347
40	3.7223	0.0322
41	3.7263	0.0320
42	3.7506	0.0307
43	3.7851	0.0289
44	3.8065	0.0279
45	3.8228	0.0272
46	3.8469	0.0261
47	3.9025	0.0237
48	4.0025	0.0200
49	4.1504	0.0156
50	4.2431	0.0134
51	4.3138	0.0119
52	4.3801	0.0106
53	4.5164	0.0084
54	4.5222	0.0083
55	4.6074	0.0072
56	4.6558	0.0067
57	4.6720	0.0065
58	4.7008	0.0062
59	4.7136	0.0060
60	4.7777	0.0054
61	4.8986	0.0044
62	4.9426	0.0041
63	4.9434	0.0041
64	4.9434	0.0041
65	5.2115	0.0026
66	5.2377	0.0025
67	5.3140	0.0022
68	5.3351	0.0021
69	5.6559	0.0012
70	5.6842	0.0012
71	5.6842	0.0012
72	5.7859	0.0010
73	5.8367	0.0009
74	5.9189	0.0008
75	5.9307	0.0008
76	6.0950	0.0006
77	6.3718	0.0004
78	6.6375	0.0002
79	6.7636	0.0002

80	6.8120	0.0002
81	6.8535	0.0002
82	7.0124	0.0001
83	7.1298	0.0001
84	7.2250	0.0001
85	7.3355	0.0001
86	7.4099	0.0001
87	7.6127	0.0000
88	7.6418	0.0000
89	7.6704	0.0000
90	7.7269	0.0000
91	7.9015	0.0000
92	7.9193	0.0000
93	8.0118	0.0000
94	8.0827	0.0000
95	8.4418	0.0000
96	8.5330	0.0000
97	9.3188	0.0000
98	9.3838	0.0000
99	9.8595	0.0000
100	9.9848	0.0000
7S*,7′S*,7′′S*,7′′′S*,8S*,8′S*		
1	0.0000	34.0631
2	0.3462	18.9918
3	0.5899	12.5878
4	0.8730	7.8051
5	0.9178	7.2373
6	1.1296	5.0622
7	1.3614	3.4233
8	1.5178	2.6292
9	1.9374	1.2949
10	1.9535	1.2603
11	1.9535	1.2603
12	2.2358	0.7826
13	2.2796	0.7268
14	2.3001	0.7022
15	2.5982	0.4246
16	2.6188	0.4101
17	2.9096	0.2510
18	2.9248	0.2447
19	3.0450	0.1997
20	3.1567	0.1654
21	3.4223	0.1056
22	3.5775	0.0813
23	3.7401	0.0618
24	3.9252	0.0452
25	3.9507	0.0433
26	4.1727	0.0298
27	4.3700	0.0213
28	4.3701	0.0213
29	4.7690	0.0109
30	4.8707	0.0092
31	4.8707	0.0092
32	5.1156	0.0061
33	5.2038	0.0052
34	5.2759	0.0046
35	5.3476	0.0041
36	5.3476	0.0041

37	5.5131	0.0031
38	5.5853	0.0027
39	5.9041	0.0016
40	6.0998	0.0012
41	6.1286	0.0011
42	6.4258	0.0007
43	6.5823	0.0005
44	6.5901	0.0005
45	6.5968	0.0005
46	6.9547	0.0003
47	7.0770	0.0002
48	7.1739	0.0002
49	7.2017	0.0002
50	7.2479	0.0002
51	7.3289	0.0001
52	7.4301	0.0001
53	7.4332	0.0001
54	7.4417	0.0001
55	7.4699	0.0001
56	7.5034	0.0001
57	7.5038	0.0001
58	7.5473	0.0001
59	7.6497	0.0001
60	7.7486	0.0001
61	7.7859	0.0001
62	7.8215	0.0001
63	7.9647	0.0000
64	8.0631	0.0000
65	8.0674	0.0000
66	8.1469	0.0000
67	8.1719	0.0000
68	8.2715	0.0000
69	8.2827	0.0000
70	8.3292	0.0000
71	8.3300	0.0000
72	8.3441	0.0000
73	8.5853	0.0000
74	8.6069	0.0000
75	8.6689	0.0000
76	8.6708	0.0000
77	8.6882	0.0000
78	8.7274	0.0000
79	8.7383	0.0000
80	8.7771	0.0000
81	8.9583	0.0000
82	8.9877	0.0000
83	9.0802	0.0000
84	9.1610	0.0000
85	9.1669	0.0000
86	9.2127	0.0000
87	9.2951	0.0000
88	9.3543	0.0000
89	9.4714	0.0000
90	9.5032	0.0000
91	9.5395	0.0000
92	9.5966	0.0000
93	9.6446	0.0000
94	9.6781	0.0000

95	9.6820	0.0000
96	9.6861	0.0000
97	9.7356	0.0000
98	9.8756	0.0000
99	9.8835	0.0000
100	9.9630	0.0000

Table S18. Relative energy values (in kcal.mol^{-1}) and Boltzmann population of the conformers obtained from the Monte Carlo/MMFF force field calculations for each stereoisomer considered for compound **3**.

Conformers	Relative energy values (kcal.mol^{-1})	Boltzmann population (%)
	7S,7'S,7'''S,8S,8'S	
1	0.0000	93.4641
2	2.2101	2.2427
3	2.4292	1.5493
4	2.8251	0.7942
5	3.1619	0.4499
6	3.4406	0.2811
7	3.6901	0.1845
8	3.7061	0.1796
9	3.7072	0.1792
10	3.9564	0.1177
11	3.9727	0.1145
12	4.5663	0.0420
13	4.5741	0.0415
14	4.6040	0.0395
15	4.6548	0.0362
16	4.8089	0.0279
17	4.8336	0.0268
18	4.9080	0.0236
19	4.9686	0.0213
20	4.9790	0.0210
21	5.0257	0.0194
22	5.2863	0.0125
23	5.2863	0.0125
24	5.2866	0.0125
25	5.3062	0.0121
26	5.4056	0.0102
27	5.4706	0.0091
28	5.6186	0.0071
29	5.6413	0.0069
30	5.8325	0.0050
31	5.8753	0.0046
32	6.0275	0.0036
33	6.0587	0.0034
34	6.0655	0.0033
35	6.0755	0.0033
36	6.1881	0.0027
37	6.1968	0.0027
38	6.1968	0.0027
39	6.2145	0.0026
40	6.2145	0.0026
41	6.3200	0.0022
42	6.3352	0.0021
43	6.3408	0.0021
44	6.3889	0.0019
45	6.4329	0.0018
46	6.4903	0.0016
47	6.5436	0.0015
48	6.7385	0.0011
49	6.8499	0.0009

50	6.8988	0.0008
51	6.9080	0.0008
52	7.0848	0.0006
53	7.0849	0.0006
54	7.1077	0.0006
55	7.1822	0.0005
56	7.2074	0.0005
57	7.2097	0.0005
58	7.2909	0.0004
59	7.2909	0.0004
60	7.2950	0.0004
61	7.3903	0.0004
62	7.5238	0.0003
63	7.5238	0.0003
64	7.5512	0.0003
65	7.6174	0.0002
66	7.6566	0.0002
67	7.7521	0.0002
68	7.8356	0.0002
69	7.8804	0.0002
70	7.9416	0.0001
71	8.0022	0.0001
72	8.1363	0.0001
73	8.2153	0.0001
74	8.2622	0.0001
75	8.3024	0.0001
76	8.3795	0.0001
77	8.4228	0.0001
78	8.4647	0.0001
79	8.5500	0.0001
80	8.6197	0.0000
81	8.6278	0.0000
82	8.8834	0.0000
83	8.9886	0.0000
84	9.1247	0.0000
85	9.2238	0.0000
86	9.2462	0.0000
87	9.3258	0.0000
88	9.3299	0.0000
89	9.4397	0.0000
90	9.5381	0.0000
91	9.5383	0.0000
92	9.6322	0.0000
93	9.6512	0.0000
94	9.6924	0.0000
95	9.7235	0.0000
96	9.7302	0.0000
97	9.8046	0.0000
98	9.8853	0.0000
99	9.9679	0.0000
100	9.9747	0.0000
7R,7'R,7'''S,8R,8'R		
1	0.0000	45.6698
2	0.3853	23.8357
3	1.2617	5.4312
4	1.3594	4.6051
5	1.3594	4.6051
6	1.5808	3.1694

7	1.5808	3.1694
8	2.0553	1.4230
9	2.1040	1.3106
10	2.2164	1.0843
11	2.5184	0.6513
12	2.6302	0.5393
13	2.7112	0.4704
14	2.7350	0.4519
15	2.7398	0.4482
16	2.7922	0.4103
17	2.8275	0.3865
18	2.8275	0.3865
19	2.8427	0.3767
20	2.8427	0.3767
21	2.9988	0.2895
22	3.2842	0.1788
23	3.5732	0.1098
24	3.5812	0.1083
25	3.7437	0.0824
26	3.9931	0.0541
27	4.2081	0.0376
28	4.2501	0.0350
29	4.2562	0.0347
30	4.2562	0.0347
31	4.2719	0.0338
32	4.4534	0.0249
33	4.4673	0.0243
34	4.5087	0.0226
35	4.6836	0.0169
36	4.7168	0.0159
37	4.7275	0.0157
38	5.0125	0.0097
39	5.0192	0.0096
40	5.1081	0.0082
41	5.1387	0.0078
42	5.3062	0.0059
43	5.4626	0.0045
44	5.5313	0.0040
45	5.5313	0.0040
46	5.5471	0.0039
47	5.5975	0.0036
48	5.7320	0.0029
49	5.9323	0.0020
50	6.0895	0.0016
51	6.0929	0.0016
52	6.1755	0.0014
53	6.1854	0.0013
54	6.3700	0.0010
55	6.3862	0.0010
56	6.5408	0.0007
57	6.6489	0.0006
58	6.9507	0.0004
59	6.9740	0.0004
60	6.9951	0.0003
61	7.0454	0.0003
62	7.1378	0.0003
63	7.1663	0.0003
64	7.2179	0.0002

65	7.2517	0.0002
66	7.4042	0.0002
67	7.4079	0.0002
68	7.4919	0.0001
69	7.5502	0.0001
70	7.5502	0.0001
71	7.5675	0.0001
72	7.5675	0.0001
73	7.5675	0.0001
74	7.6641	0.0001
75	7.6828	0.0001
76	7.7473	0.0001
77	7.7473	0.0001
78	7.9727	0.0001
79	8.0519	0.0001
80	8.1326	0.0000
81	8.1663	0.0000
82	8.1826	0.0000
83	8.2414	0.0000
84	8.4790	0.0000
85	8.7227	0.0000
86	8.7690	0.0000
87	8.8022	0.0000
88	8.8107	0.0000
89	8.8768	0.0000
90	9.0088	0.0000
91	9.1232	0.0000
92	9.1565	0.0000
93	9.3744	0.0000
94	9.3814	0.0000
95	9.4500	0.0000
96	9.5003	0.0000
97	9.5575	0.0000
98	9.6430	0.0000
99	9.8197	0.0000
100	9.8594	0.0000

Table S19. Relative energy values (in kcal.mol^{-1}) and Boltzmann population of the conformers obtained from the Monte Carlo/MMFF force field calculations for each stereoisomer considered for compound **4**.

Conformers	Relative energy values (kcal.mol^{-1})	Boltzmann population (%)
	7′S*,7″R*,7‴R*,8′R*	
1	0.0000	24.8622
2	0.0109	24.4095
3	0.3115	14.6969
4	0.4198	12.2420
5	0.9989	4.6069
6	1.0647	4.1227
7	1.1904	3.3344
8	1.3652	2.4825
9	1.4071	2.3130
10	1.4150	2.2825
11	1.8529	1.0901
12	1.8868	1.0294
13	2.0824	0.7400
14	2.2984	0.5139
15	2.8728	0.1949
16	3.0202	0.1520
17	3.0584	0.1425
18	3.1862	0.1149
19	3.2599	0.1014
20	3.3441	0.0880
21	3.3920	0.0812
22	3.5290	0.0644
23	3.6000	0.0571
24	3.7820	0.0420
25	3.8571	0.0370
26	3.9192	0.0333
27	4.3471	0.0162
28	4.3752	0.0154
29	4.4399	0.0138
30	4.4818	0.0129
31	4.5525	0.0114
32	4.5763	0.0110
33	4.5884	0.0108
34	4.5971	0.0106
35	4.6440	0.0098
36	4.6731	0.0093
37	4.8513	0.0069
38	4.9302	0.0061
39	4.9598	0.0058
40	4.9921	0.0055
41	5.3387	0.0030
42	5.5421	0.0022
43	5.5995	0.0020
44	5.7484	0.0015
45	5.8858	0.0012
46	5.9637	0.0011
47	6.0079	0.0010
48	6.0634	0.0009
49	6.1413	0.0008

50	6.2065	0.0007
51	6.3531	0.0005
52	6.4410	0.0005
53	6.4437	0.0005
54	6.5028	0.0004
55	6.5073	0.0004
56	6.5279	0.0004
57	6.6079	0.0004
58	6.6727	0.0003
59	6.7552	0.0003
60	6.7994	0.0003
61	7.0076	0.0002
62	7.1417	0.0001
63	7.2206	0.0001
64	7.2346	0.0001
65	7.3881	0.0001
66	7.4542	0.0001
67	7.5734	0.0001
68	7.7071	0.0001
69	7.7086	0.0001
70	7.8340	0.0000
71	7.9632	0.0000
72	7.9636	0.0000
73	8.0311	0.0000
74	8.3795	0.0000
75	8.5033	0.0000
76	8.5120	0.0000
77	8.5628	0.0000
78	8.6727	0.0000
79	8.7387	0.0000
80	8.7426	0.0000
81	8.7742	0.0000
82	8.9077	0.0000
83	8.9327	0.0000
84	8.9377	0.0000
85	9.1200	0.0000
86	9.1363	0.0000
87	9.1550	0.0000
88	9.2015	0.0000
89	9.2037	0.0000
90	9.2052	0.0000
91	9.2936	0.0000
92	9.3931	0.0000
93	9.4454	0.0000
94	9.5483	0.0000
95	9.6348	0.0000
96	9.6994	0.0000
97	9.7597	0.0000
98	9.8769	0.0000
99	9.8842	0.0000
100	9.9142	0.0000
7′S*,7′′S*,7′′′S*,8′R*		
1	0.0000	56.0088
2	0.2614	36.0319
3	1.7922	2.7207
4	2.1548	1.4753
5	2.4012	0.9733
6	2.4365	0.9171

7	2.5959	0.7007
8	3.0530	0.3240
9	3.2102	0.2485
10	3.5725	0.1348
11	3.7663	0.0972
12	3.9754	0.0683
13	4.0267	0.0626
14	4.0858	0.0567
15	4.3970	0.0335
16	4.5998	0.0238
17	4.7650	0.0180
18	4.9199	0.0139
19	4.9510	0.0132
20	5.1189	0.0099
21	5.1955	0.0087
22	5.2143	0.0084
23	5.4465	0.0057
24	5.5200	0.0050
25	5.5806	0.0045
26	5.6504	0.0040
27	5.6768	0.0039
28	5.7312	0.0035
29	5.7637	0.0033
30	5.7747	0.0033
31	5.7949	0.0032
32	5.9811	0.0023
33	6.1064	0.0019
34	6.4036	0.0011
35	6.4637	0.0010
36	6.5122	0.0009
37	6.7455	0.0006
38	6.8541	0.0005
39	6.9215	0.0005
40	6.9450	0.0005
41	6.9644	0.0004
42	6.9940	0.0004
43	7.0324	0.0004
44	7.0576	0.0004
45	7.0947	0.0004
46	7.1803	0.0003
47	7.1985	0.0003
48	7.2113	0.0003
49	7.2321	0.0003
50	7.2550	0.0003
51	7.3784	0.0002
52	7.5479	0.0002
53	7.6693	0.0001
54	8.1248	0.0001
55	8.1672	0.0001
56	8.2146	0.0001
57	8.2449	0.0001
58	8.3623	0.0000
59	8.3803	0.0000
60	8.5087	0.0000
61	8.5188	0.0000
62	8.5240	0.0000
63	8.6031	0.0000
64	8.6288	0.0000

65	8.7202	0.0000
66	8.9103	0.0000
67	9.0109	0.0000
68	9.0827	0.0000
69	9.1258	0.0000
70	9.1506	0.0000
71	9.2411	0.0000
72	9.2795	0.0000
73	9.4952	0.0000
74	9.5413	0.0000
75	9.7095	0.0000
76	9.7196	0.0000
77	9.7741	0.0000
78	9.7983	0.0000
79	9.8566	0.0000
80	9.8613	0.0000
7'S*,7''R*,7'''S*,8'R*		
1	0.0000	64.3308
2	0.9094	13.8639
3	0.9644	12.6355
4	1.7393	3.4164
5	2.4308	1.0635
6	2.5702	0.8406
7	2.7034	0.6714
8	2.9460	0.4458
9	2.9685	0.4292
10	3.1754	0.3027
11	3.2117	0.2847
12	3.2629	0.2611
13	3.2630	0.2611
14	3.3421	0.2285
15	3.3566	0.2230
16	3.6683	0.1317
17	3.7594	0.1130
18	3.8860	0.0912
19	4.0840	0.0653
20	4.2149	0.0524
21	4.2903	0.0461
22	4.3299	0.0431
23	4.3570	0.0412
24	4.4171	0.0372
25	4.4822	0.0334
26	5.1807	0.0103
27	5.1991	0.0099
28	5.2811	0.0087
29	5.4376	0.0067
30	5.5235	0.0058
31	5.5872	0.0052
32	5.6240	0.0049
33	5.7164	0.0042
34	5.7211	0.0041
35	5.7646	0.0038
36	5.7964	0.0036
37	5.8313	0.0034
38	5.9685	0.0027
39	6.3097	0.0015
40	6.3959	0.0013
41	6.4290	0.0012

42	6.5043	0.0011
43	6.6171	0.0009
44	6.6307	0.0009
45	6.6495	0.0009
46	6.8270	0.0006
47	6.8736	0.0006
48	7.0394	0.0004
49	7.1326	0.0004
50	7.1758	0.0004
51	7.1788	0.0004
52	7.4115	0.0002
53	7.4502	0.0002
54	7.4569	0.0002
55	7.4781	0.0002
56	7.5029	0.0002
57	7.5170	0.0002
58	7.5430	0.0002
59	7.6001	0.0002
60	7.6111	0.0002
61	7.6305	0.0002
62	7.6903	0.0001
63	7.7841	0.0001
64	7.8527	0.0001
65	7.9054	0.0001
66	7.9282	0.0001
67	8.0711	0.0001
68	8.1066	0.0001
69	8.1156	0.0001
70	8.1639	0.0001
71	8.2136	0.0001
72	8.2169	0.0001
73	8.3008	0.0001
74	8.4011	0.0000
75	8.4253	0.0000
76	8.5681	0.0000
77	8.5939	0.0000
78	8.6055	0.0000
79	8.6981	0.0000
80	8.7472	0.0000
81	8.7772	0.0000
82	8.7919	0.0000
83	8.9574	0.0000
84	8.9646	0.0000
85	9.0368	0.0000
86	9.1555	0.0000
87	9.1973	0.0000
88	9.2466	0.0000
89	9.3435	0.0000
90	9.4750	0.0000
91	9.6051	0.0000
92	9.6169	0.0000
93	9.6331	0.0000
94	9.6886	0.0000
95	9.7468	0.0000
96	9.7896	0.0000
97	9.8717	0.0000
98	9.8973	0.0000
99	9.9292	0.0000

100	9.9508	0.0000
7′S*,7′′S*,7′′′R*,8′R*		
1	0.0000	57.8901
2	0.9767	11.1352
3	1.0667	9.5671
4	1.1819	7.8763
5	1.2315	7.2443
6	1.9992	1.9829
7	2.3408	1.1141
8	2.5656	0.7624
9	2.7902	0.5218
10	2.9697	0.3854
11	3.0053	0.3629
12	3.4159	0.1815
13	3.4842	0.1617
14	3.5163	0.1532
15	3.5769	0.1383
16	3.6983	0.1127
17	3.7353	0.1059
18	3.8656	0.0850
19	4.2523	0.0442
20	4.4831	0.0300
21	4.5659	0.0261
22	4.6265	0.0235
23	4.7267	0.0199
24	4.8916	0.0150
25	5.2289	0.0085
26	5.5190	0.0052
27	5.5634	0.0048
28	5.6094	0.0045
29	5.6509	0.0042
30	5.7216	0.0037
31	5.7950	0.0033
32	5.8390	0.0030
33	5.8407	0.0030
34	5.9290	0.0026
35	5.9401	0.0026
36	5.9962	0.0023
37	6.0051	0.0023
38	6.4700	0.0010
39	6.4908	0.0010
40	6.5136	0.0010
41	6.5886	0.0009
42	6.6839	0.0007
43	6.8322	0.0006
44	6.8809	0.0005
45	6.8996	0.0005
46	6.9425	0.0005
47	7.0989	0.0004
48	7.1627	0.0003
49	7.1987	0.0003
50	7.2185	0.0003
51	7.2973	0.0003
52	7.3556	0.0002
53	7.4198	0.0002
54	7.4930	0.0002
55	7.4950	0.0002
56	7.6026	0.0002

57	7.6716	0.0001
58	7.7197	0.0001
59	7.8214	0.0001
60	8.0874	0.0001
61	8.0932	0.0001
62	8.1500	0.0001
63	8.3858	0.0000
64	8.7093	0.0000
65	8.7144	0.0000
66	8.8055	0.0000
67	8.8058	0.0000
68	8.8721	0.0000
69	8.9009	0.0000
70	8.9061	0.0000
71	8.9288	0.0000
72	8.9609	0.0000
73	9.0619	0.0000
74	9.0775	0.0000
75	9.0848	0.0000
76	9.1418	0.0000
77	9.3026	0.0000
78	9.3843	0.0000
79	9.5775	0.0000
80	9.5917	0.0000
81	9.8066	0.0000
82	9.8473	0.0000
83	9.8604	0.0000
84	9.8795	0.0000
85	9.9233	0.0000
86	9.9261	0.0000
87	9.9705	0.0000
88	9.9786	0.0000
89	9.9795	0.0000
90	9.9829	0.0000

Table S20. Relative energy values (in kcal.mol^{-1}) and Boltzmann population of the conformers obtained from the Monte Carlo/MMFF force field calculations for each stereoisomer considered for compound **5**.

Conformers	Relative energy values (kcal.mol^{-1})	Boltzmann population (%)
	7′S*,7′′R*,8′R*	
1	0.0000	51.7000
2	0.4400	24.5000
3	1.0100	9.4000
4	1.4441	4.5177
5	1.7956	2.4962
6	1.8952	2.1097
7	2.2652	1.1300
8	2.5023	0.7573
9	2.5161	0.7399
10	2.6006	0.6415
11	2.6657	0.5748
12	3.0149	0.3189
13	3.1620	0.2487
14	3.2030	0.2321
15	3.3872	0.1701
16	3.7637	0.0901
17	3.8550	0.0772
18	3.8865	0.0732
19	4.2460	0.0399
20	4.2599	0.0390
21	4.2858	0.0373
22	4.3234	0.0350
23	4.5841	0.0226
24	4.8372	0.0147
25	4.9108	0.0130
26	4.9193	0.0128
27	4.9221	0.0128
28	4.9812	0.0115
29	5.0384	0.0105
30	5.0845	0.0097
31	5.1771	0.0083
32	5.1847	0.0082
33	5.3240	0.0065
34	5.3296	0.0064
35	5.4538	0.0052
36	5.5003	0.0048
37	5.8767	0.0025
38	5.9147	0.0024
39	6.0295	0.0020
40	6.0525	0.0019
41	6.1628	0.0016
42	6.2281	0.0014
43	6.3183	0.0012
44	6.4923	0.0009
45	6.5525	0.0008
46	6.6361	0.0007
47	6.6393	0.0007
48	6.6808	0.0007
49	6.7461	0.0006

50	6.7819	0.0006
51	6.7989	0.0005
52	6.8353	0.0005
53	6.8577	0.0005
54	6.9101	0.0004
55	6.9671	0.0004
56	7.0158	0.0004
57	7.1100	0.0003
58	7.2216	0.0003
59	7.3088	0.0002
60	7.3698	0.0002
61	7.5946	0.0001
62	7.6327	0.0001
63	7.6717	0.0001
64	7.7084	0.0001
65	7.7729	0.0001
66	8.0619	0.0001
67	8.0874	0.0001
68	8.1578	0.0001
69	8.2122	0.0000
70	8.2508	0.0000
71	8.2653	0.0000
72	8.3414	0.0000
73	8.3846	0.0000
74	8.3972	0.0000
75	8.4325	0.0000
76	8.4503	0.0000
77	8.4770	0.0000
78	8.6443	0.0000
79	8.6901	0.0000
80	8.6980	0.0000
81	8.6992	0.0000
82	8.7203	0.0000
83	8.8273	0.0000
84	8.9041	0.0000
85	9.0070	0.0000
86	9.0342	0.0000
87	9.1554	0.0000
88	9.1793	0.0000
89	9.2959	0.0000
90	9.3506	0.0000
91	9.3724	0.0000
92	9.4083	0.0000
93	9.4176	0.0000
94	9.4873	0.0000
95	9.5743	0.0000
96	9.6294	0.0000
97	9.6934	0.0000
98	9.8254	0.0000
99	9.8608	0.0000
100	9.9165	0.0000
7'S*,7'''S*,8'R*		
1	0.0000	25.3914
2	0.1490	19.7452
3	0.3329	14.4765
4	0.6771	8.0985
5	0.9235	5.3436
6	0.9785	4.8697

7	1.2449	3.1064
8	1.3005	2.8280
9	1.4830	2.0785
10	1.6045	1.6929
11	1.6115	1.6730
12	1.6601	1.5414
13	1.7253	1.3808
14	1.8126	1.1915
15	1.8733	1.0757
16	1.9674	0.9176
17	2.0426	0.8083
18	2.1373	0.6889
19	2.2582	0.5617
20	2.4768	0.3885
21	2.4811	0.3856
22	2.5751	0.3291
23	2.6042	0.3133
24	2.7118	0.2612
25	3.2046	0.1137
26	3.3556	0.0881
27	3.4066	0.0809
28	3.5774	0.0606
29	3.6280	0.0557
30	3.7681	0.0439
31	3.8684	0.0371
32	3.9034	0.0350
33	3.9081	0.0347
34	3.9391	0.0329
35	4.0815	0.0259
36	4.0818	0.0259
37	4.1263	0.0240
38	4.2032	0.0211
39	4.2056	0.0210
40	4.2793	0.0185
41	4.2871	0.0183
42	4.3805	0.0156
43	4.4862	0.0131
44	4.5280	0.0122
45	4.5424	0.0119
46	4.5538	0.0117
47	4.6212	0.0104
48	4.9883	0.0056
49	5.1727	0.0041
50	5.3095	0.0033
51	5.3838	0.0029
52	5.3993	0.0028
53	5.4604	0.0025
54	5.4629	0.0025
55	5.4718	0.0025
56	5.5877	0.0020
57	5.6744	0.0018
58	5.6938	0.0017
59	5.7442	0.0016
60	5.7977	0.0014
61	5.8084	0.0014
62	6.0730	0.0009
63	6.2302	0.0007
64	6.3006	0.0006

65	6.3565	0.0006
66	6.6612	0.0003
67	6.9510	0.0002
68	6.9699	0.0002
69	7.2123	0.0001
70	7.2404	0.0001
71	7.2980	0.0001
72	7.3075	0.0001
73	7.6532	0.0001
74	7.7004	0.0001
75	7.7029	0.0001
76	7.7462	0.0001
77	7.7614	0.0001
78	7.7825	0.0001
79	7.9328	0.0000
80	7.9440	0.0000
81	8.0832	0.0000
82	8.1518	0.0000
83	8.4283	0.0000
84	8.4395	0.0000
85	8.4572	0.0000
86	8.4659	0.0000
87	8.5106	0.0000
88	8.6083	0.0000
89	8.7127	0.0000
90	9.1970	0.0000
91	9.3264	0.0000
92	9.3273	0.0000
93	9.3463	0.0000
94	9.3766	0.0000
95	9.5612	0.0000
96	9.5912	0.0000
97	9.6797	0.0000
98	9.8304	0.0000
99	9.8584	0.0000
100	9.9324	0.0000

Table S21. Relative energy values (in kcal.mol^{-1}) and Boltzmann population of the conformers obtained from the Monte Carlo/MMFF force field calculations for each stereoisomer considered for compound **6**.

Conformers	Relative energy values (kcal.mol^{-1})	Boltzmann population (%)
	7′R	
1	0.0000	0.2690
2	0.0538	0.2456
3	0.4760	0.1205
4	0.6309	0.0927
5	0.8314	0.0661
6	1.0000	0.0497
7	1.5445	0.0198
8	1.6442	0.0168
9	1.6716	0.0160
10	1.6992	0.0153
11	1.7092	0.0150
12	1.8463	0.0119
13	1.8593	0.0117
14	2.1331	0.0073
15	2.1724	0.0069
16	2.1846	0.0067
17	2.3074	0.0055
18	2.5704	0.0035
19	2.5909	0.0034
20	2.6865	0.0029
21	3.0285	0.0016
22	3.0893	0.0015
23	3.2275	0.0012
24	3.2496	0.0011
25	3.2673	0.0011
26	3.3606	0.0009
27	3.4511	0.0008
28	3.4982	0.0007
29	3.5160	0.0007
30	3.5471	0.0007
31	3.6767	0.0005
32	3.7859	0.0005
33	4.0558	0.0003
34	4.0778	0.0003
35	4.3343	0.0002
36	4.3717	0.0002
37	4.4474	0.0001
38	4.4744	0.0001
39	4.5128	0.0001
40	4.5472	0.0001
41	4.5742	0.0001
42	4.6828	0.0001
43	4.7409	0.0001
44	5.0291	0.0001
45	5.0291	0.0001
46	5.0293	0.0001
47	5.0971	0.0000
48	5.1490	0.0000
49	5.1538	0.0000

50	5.4576	0.0000
51	5.5053	0.0000
52	5.5960	0.0000
53	5.7592	0.0000
54	5.7837	0.0000
55	5.8344	0.0000
56	6.0552	0.0000
57	6.1319	0.0000
58	6.1492	0.0000
59	6.3266	0.0000
60	6.4406	0.0000
61	6.4466	0.0000
62	6.4894	0.0000
63	6.5707	0.0000
64	6.7058	0.0000
65	6.8110	0.0000
66	6.9090	0.0000
67	7.1094	0.0000
68	7.2290	0.0000
69	7.3039	0.0000
70	7.3229	0.0000
71	7.3554	0.0000
72	7.4127	0.0000
73	7.4590	0.0000
74	7.5309	0.0000
75	7.6418	0.0000
76	7.7912	0.0000
77	7.8582	0.0000
78	7.9293	0.0000
79	7.9517	0.0000
80	8.0039	0.0000
81	8.0918	0.0000
82	8.1581	0.0000
83	8.1661	0.0000
84	8.2054	0.0000
85	8.2466	0.0000
86	8.2866	0.0000
87	8.3273	0.0000
88	8.3559	0.0000
89	8.5322	0.0000
90	8.6223	0.0000
91	8.7758	0.0000
92	8.8972	0.0000
93	9.2438	0.0000
94	9.4383	0.0000
95	9.6274	0.0000
96	9.6981	0.0000
97	9.7441	0.0000
98	9.7493	0.0000
99	9.8048	0.0000
100	9.9038	0.0000

Table S22. Boltzmann population of the conformers considered in the final simulated ECD spectra of compounds **1-6**.

Conformers	Boltzmann population (%)	Total population (%)
Compound 1		
1	36.60	100.00
2	34.83	
3	27.80	
4	0.77	
Compound 2		
1	52.35	99.47
2	28.93	
3	8.28	
4	7.22	
5	2.69	
Compound 3		
1	50.15	99.55
2	28.46	
3	14.26	
4	4.90	
5	1.78	
Compound 4		
1	29.29	99.91
2	19.25	
3	11.05	
4	10.68	
5	10.32	
6	9.17	
7	4.92	
8	3.38	
9	1.85	
Compound 5		
1	51.42	99.10
2	16.91	
3	8.66	
4	4.47	
5	4.33	
6	1.70	
7	1.56	
8	1.54	
9	1.44	
10	1.41	
11	1.29	
12	1.28	
13	1.02	
14	0.78	
15	0.66	
16	0.34	
17	0.29	
Compound 6		
1	9.21	99.97
2	7.38	
3	7.37	
4	7.36	
5	5.45	
6	5.27	

7	5.26	
8	4.78	
9	4.58	
10	4.56	
11	3.79	
12	3.73	
13	3.35	
14	3.33	
15	3.05	
16	2.72	
17	2.45	
18	2.43	
19	2.40	
20	2.24	
21	2.17	
22	1.96	
23	1.81	
24	1.37	
25	1.34	
26	0.16	
27	0.15	
28	0.11	
29	0.10	
30	0.09	