

Supporting Information

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Bromophenols from the Marine Red Alga *Symphyclocladia latiuscula* and Their Radical Scavenging Activity

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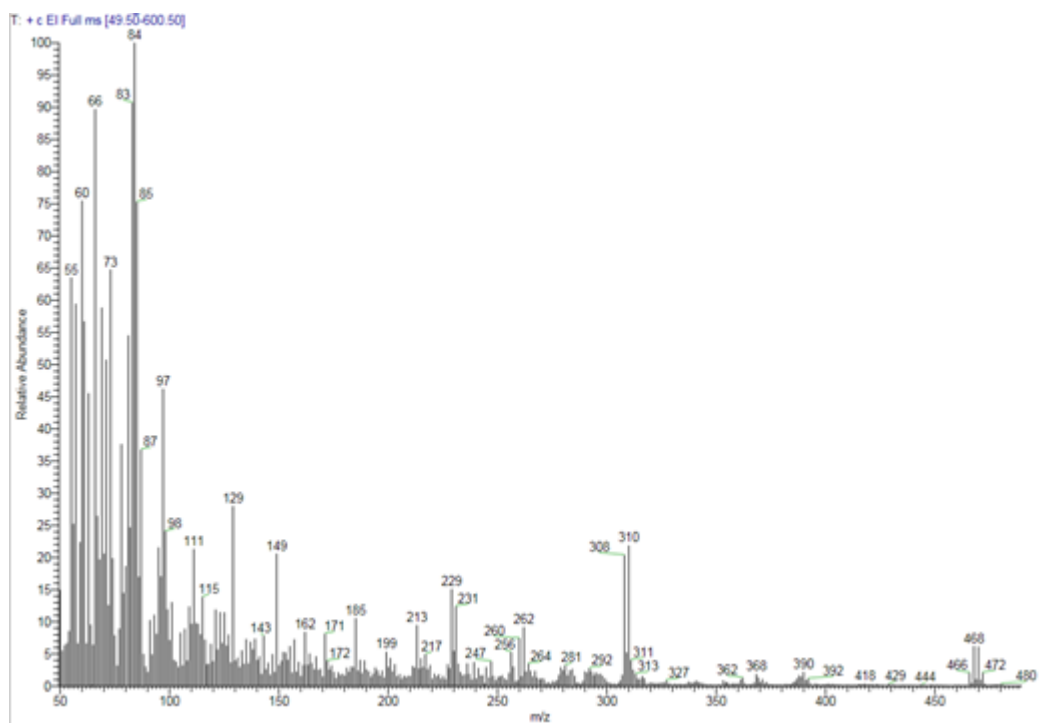


Figure S1: EIMS spectrum of 1

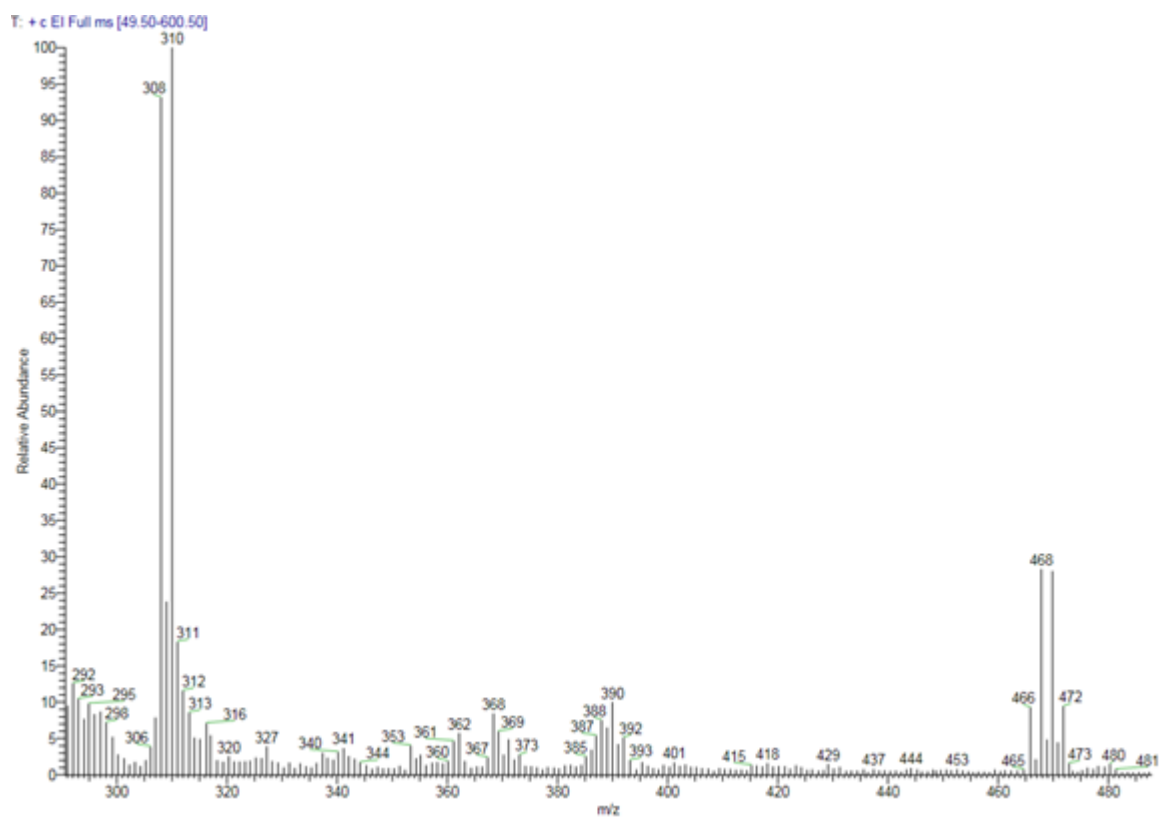


Figure S2: Enlarged EIMS spectrum of **1**

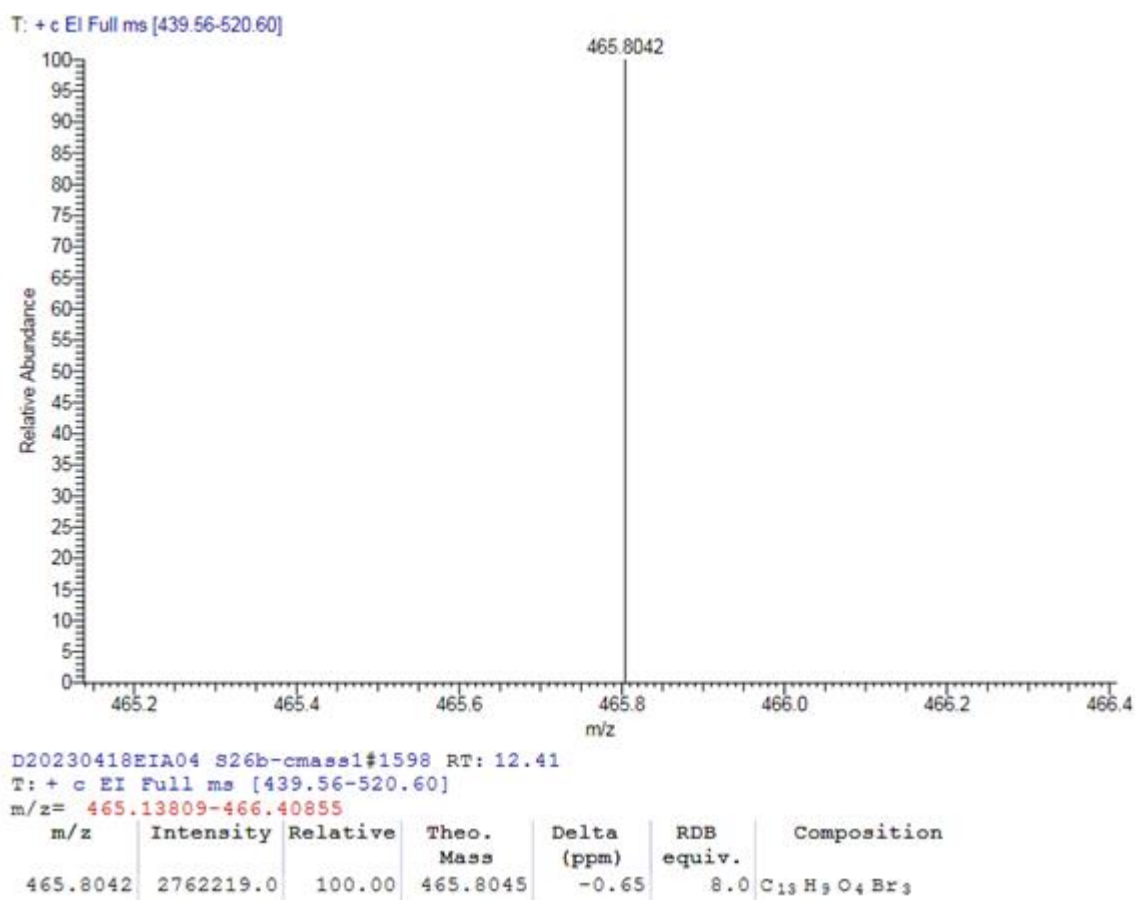


Figure S3: HR-EI-MS spectrum of **1**

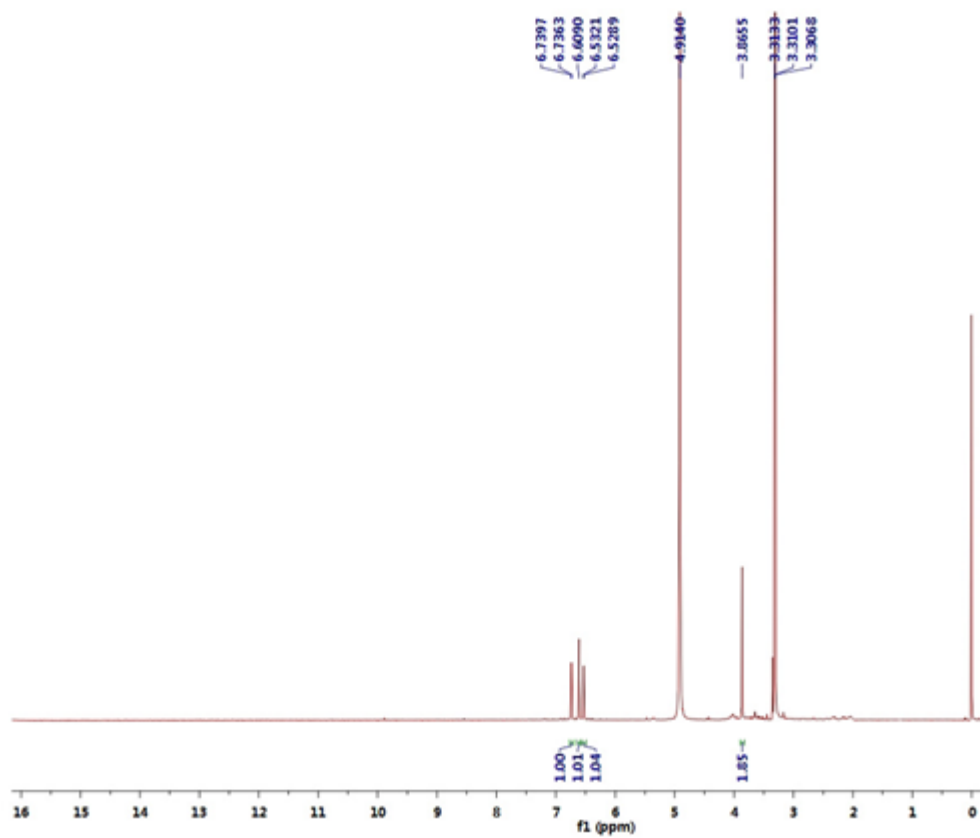


Figure S4: $^1\text{H-NMR}$ (500 MHz, MeOD) spectrum of **1**

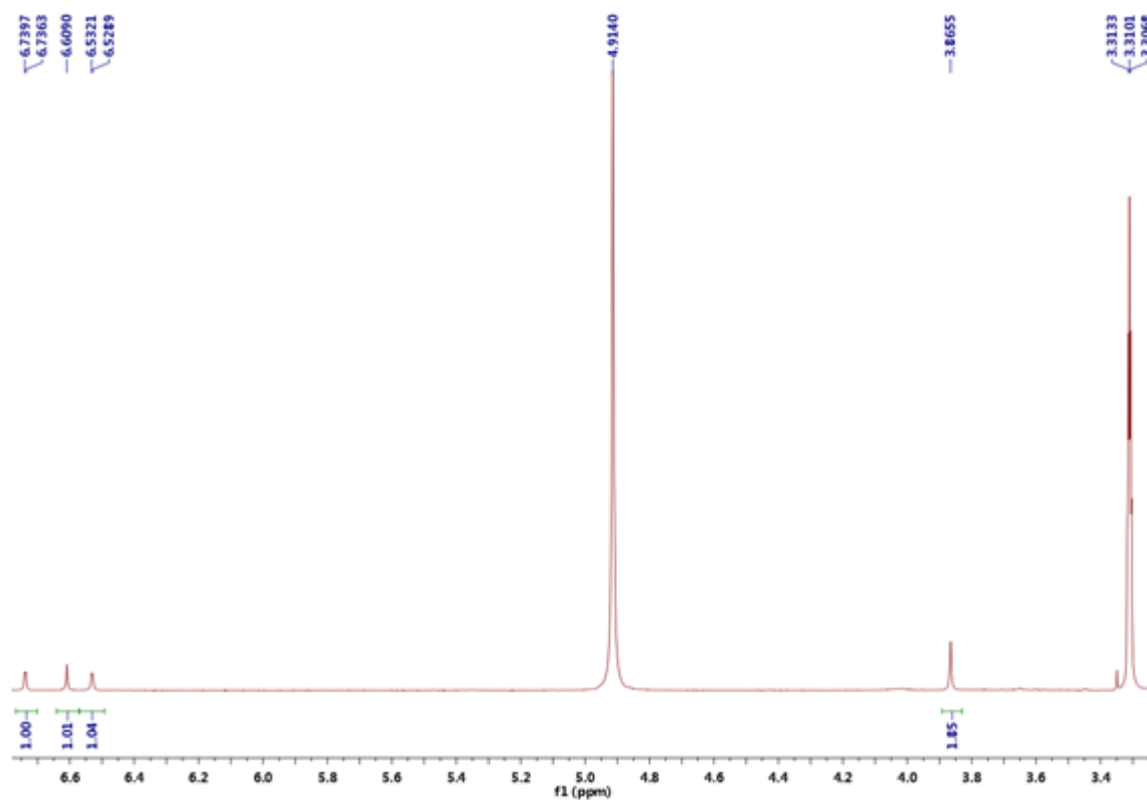


Figure S5: Enlarged $^1\text{H-NMR}$ (500 MHz, MeOD) spectrum of **1**

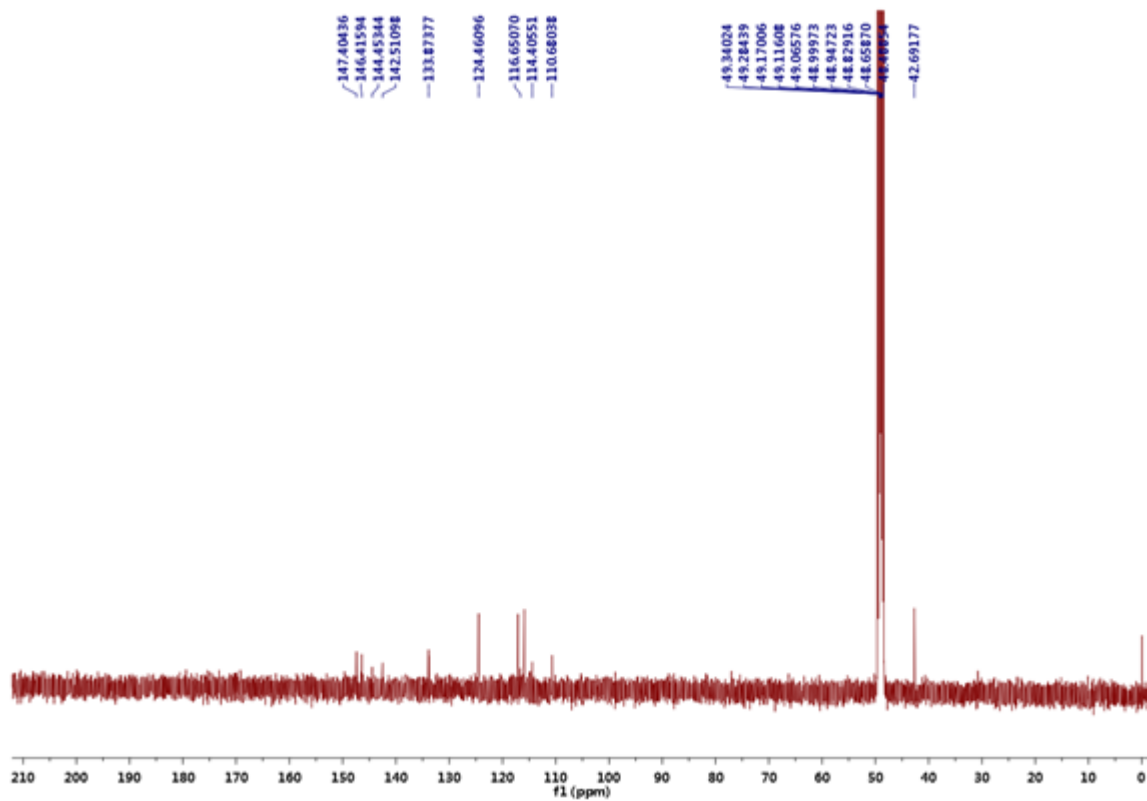


Figure S6: ^{13}C -NMR (125 MHz, MeOD) spectrum of **1**

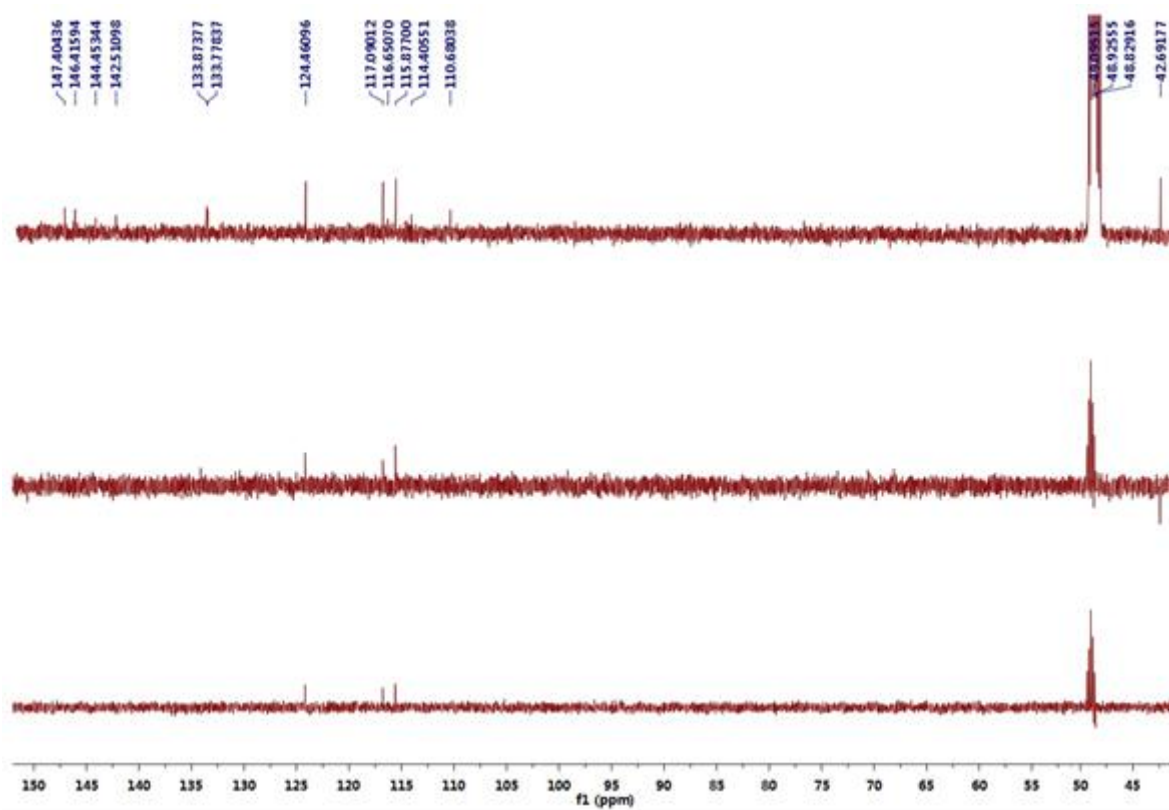


Figure S7: ^{13}C -NMR and DEPT (125 MHz, MeOD) spectra of **1**

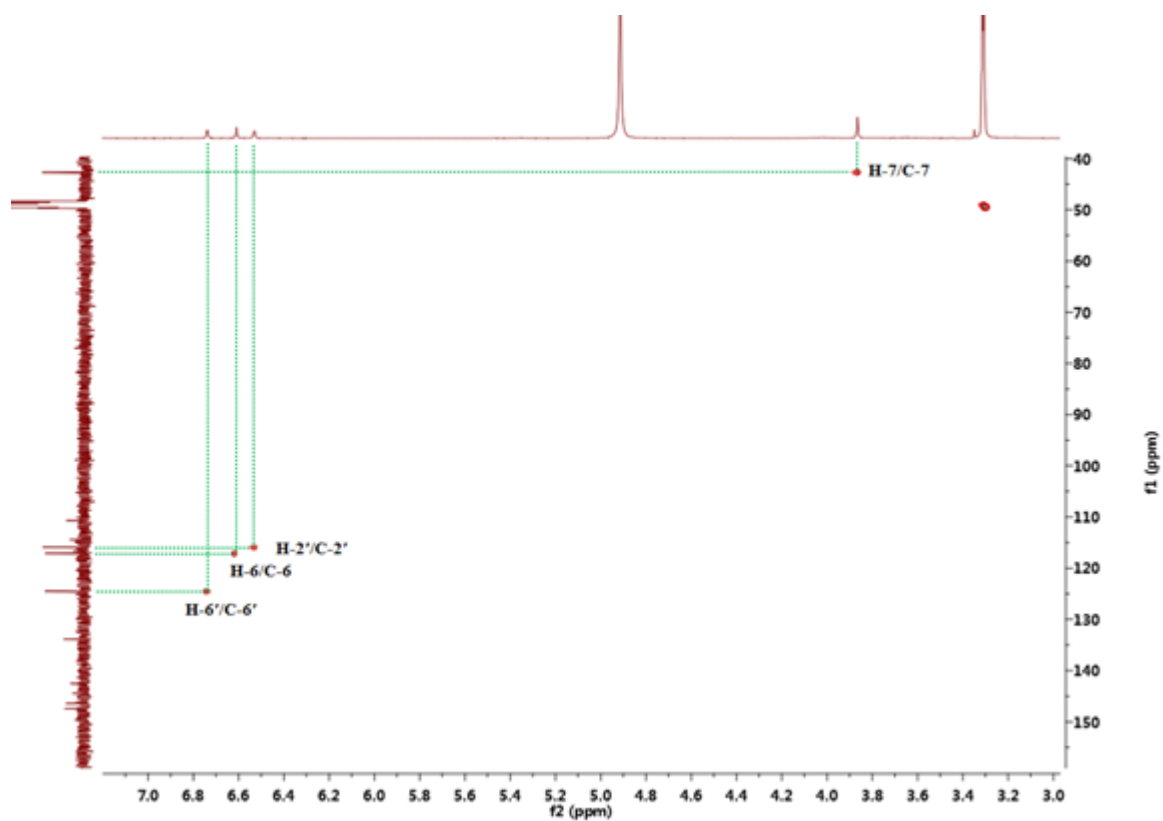


Figure S8: HSQC spectrum of **1**

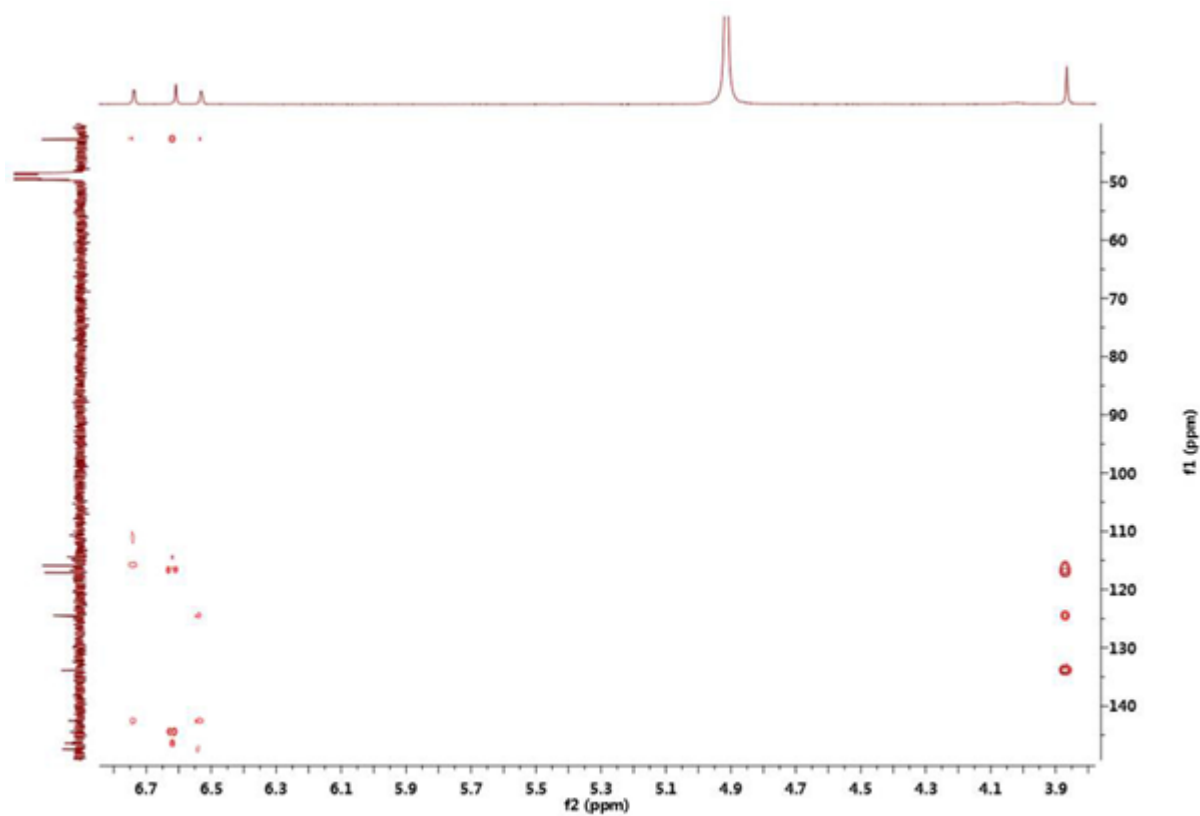


Figure S9: HMBC spectrum of **1**

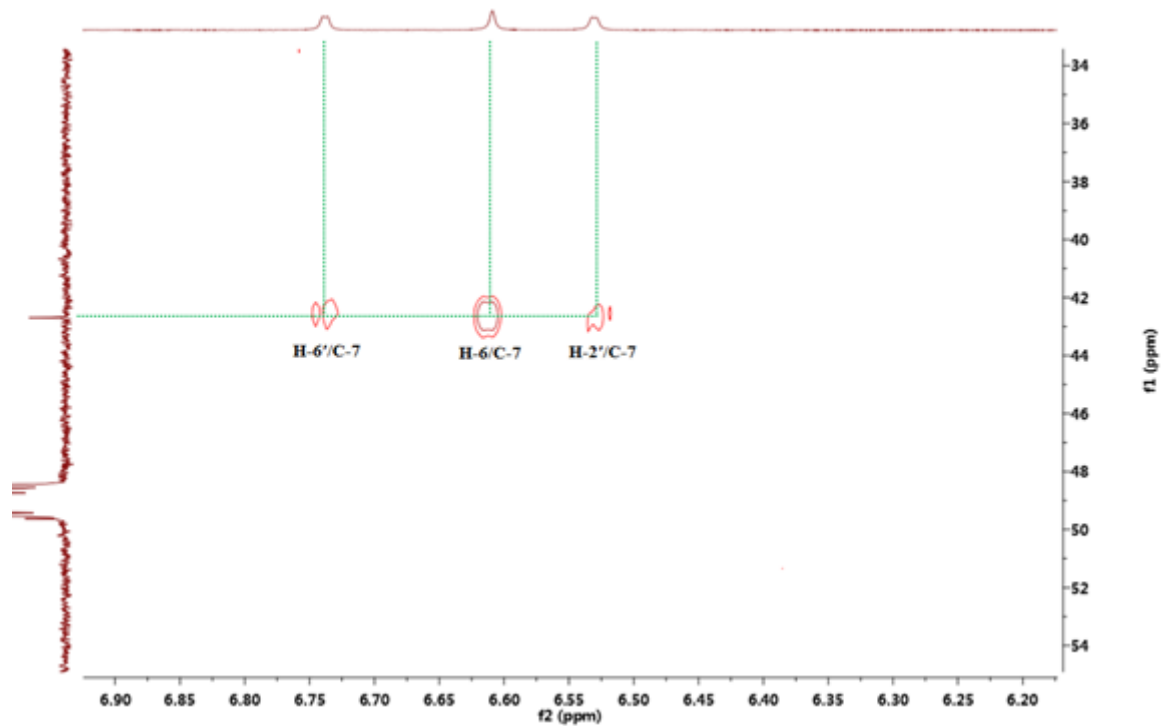


Figure S10: Enlarged HMBC spectrum of **1**

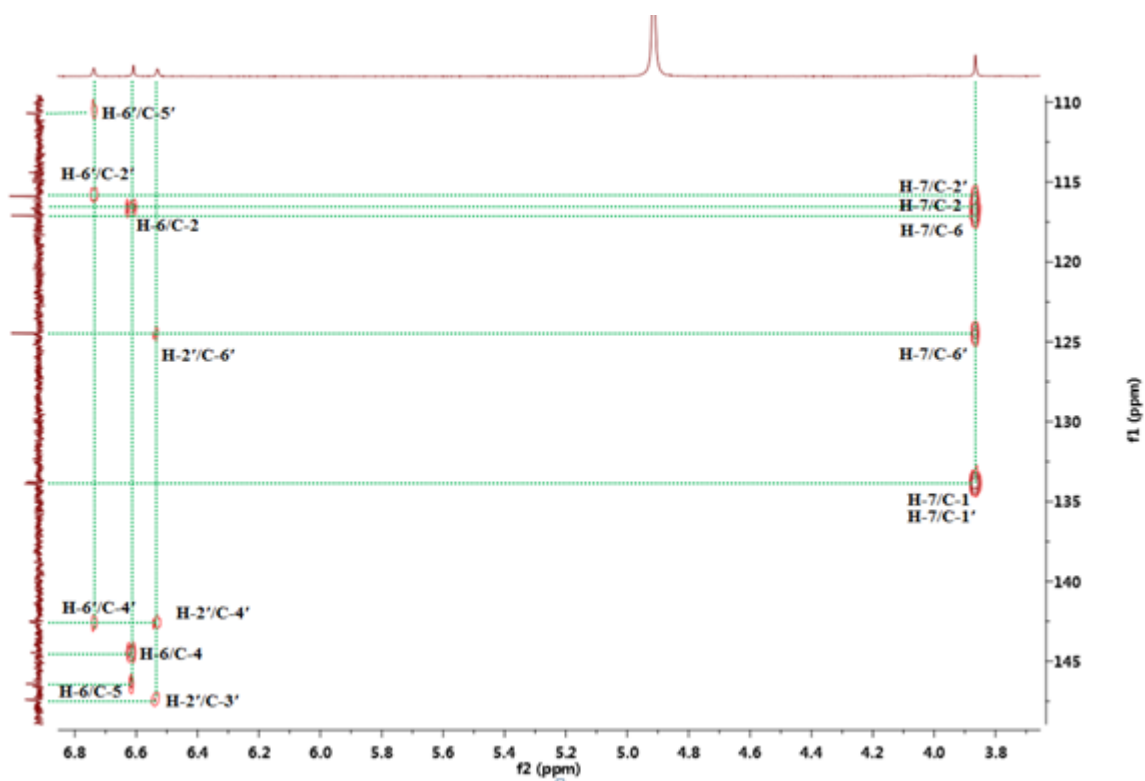


Figure S11: Enlarged HMBC spectrum of **1**

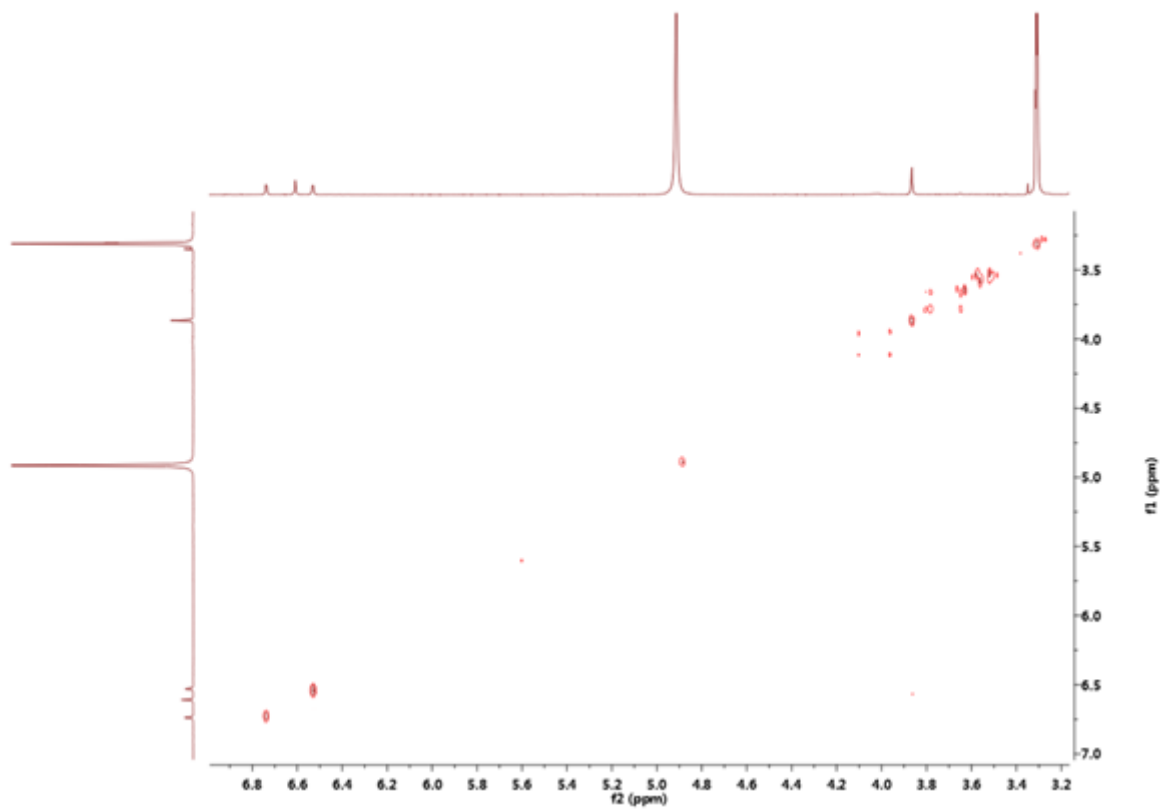


Figure S12: ^1H - ^1H COSY spectrum of **1**

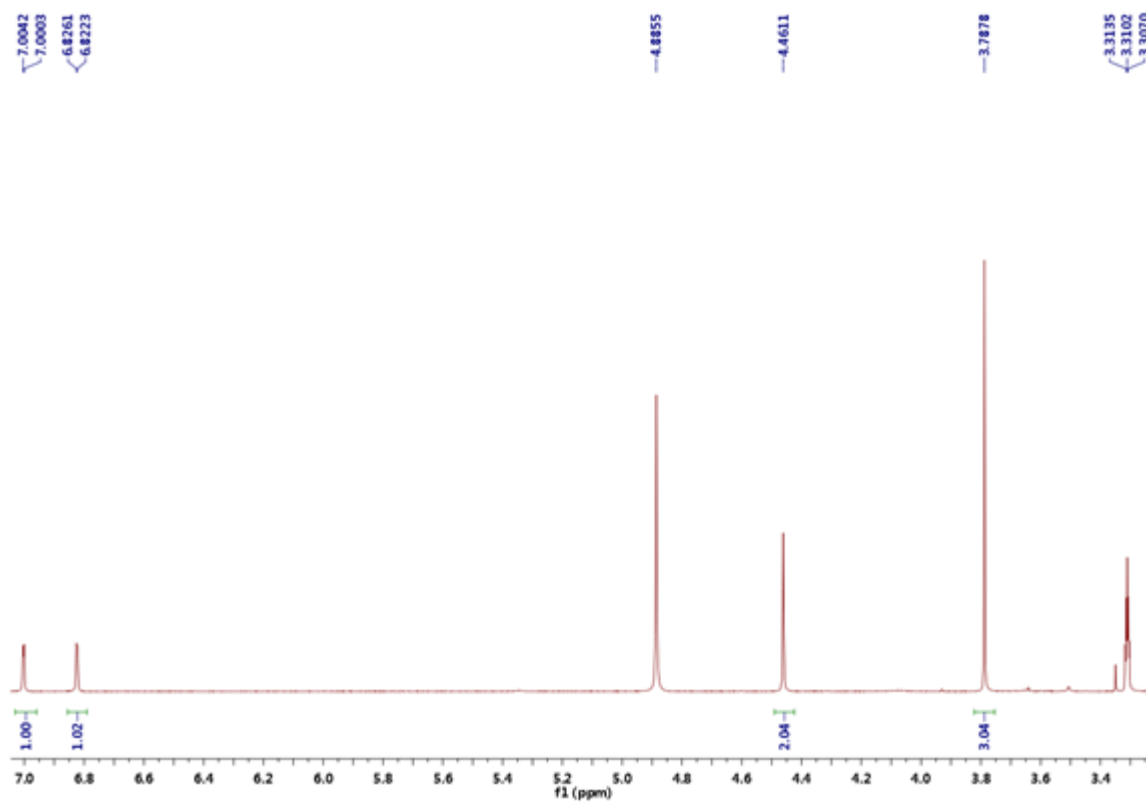


Figure S13: ¹H-NMR (500 MHz, MeOD) spectrum of **2**

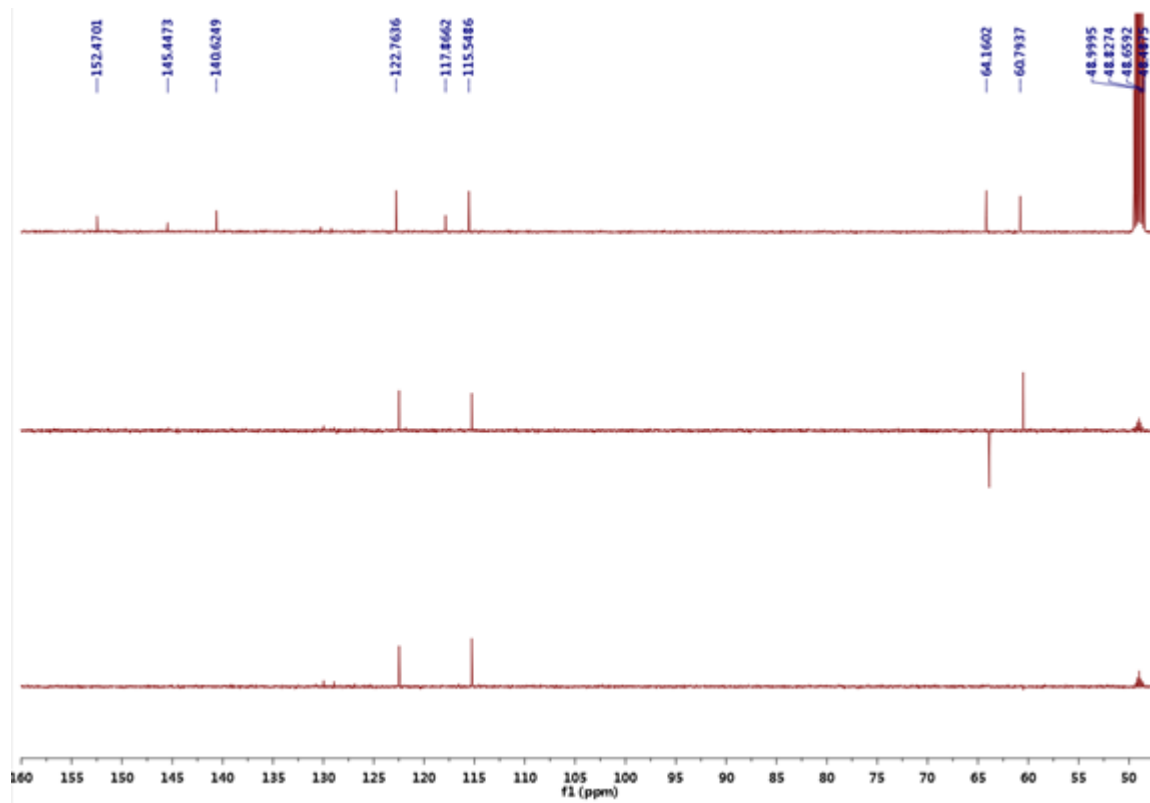


Figure S14: ^{13}C -NMR and DEPT (125 MHz, MeOD) spectra of 2

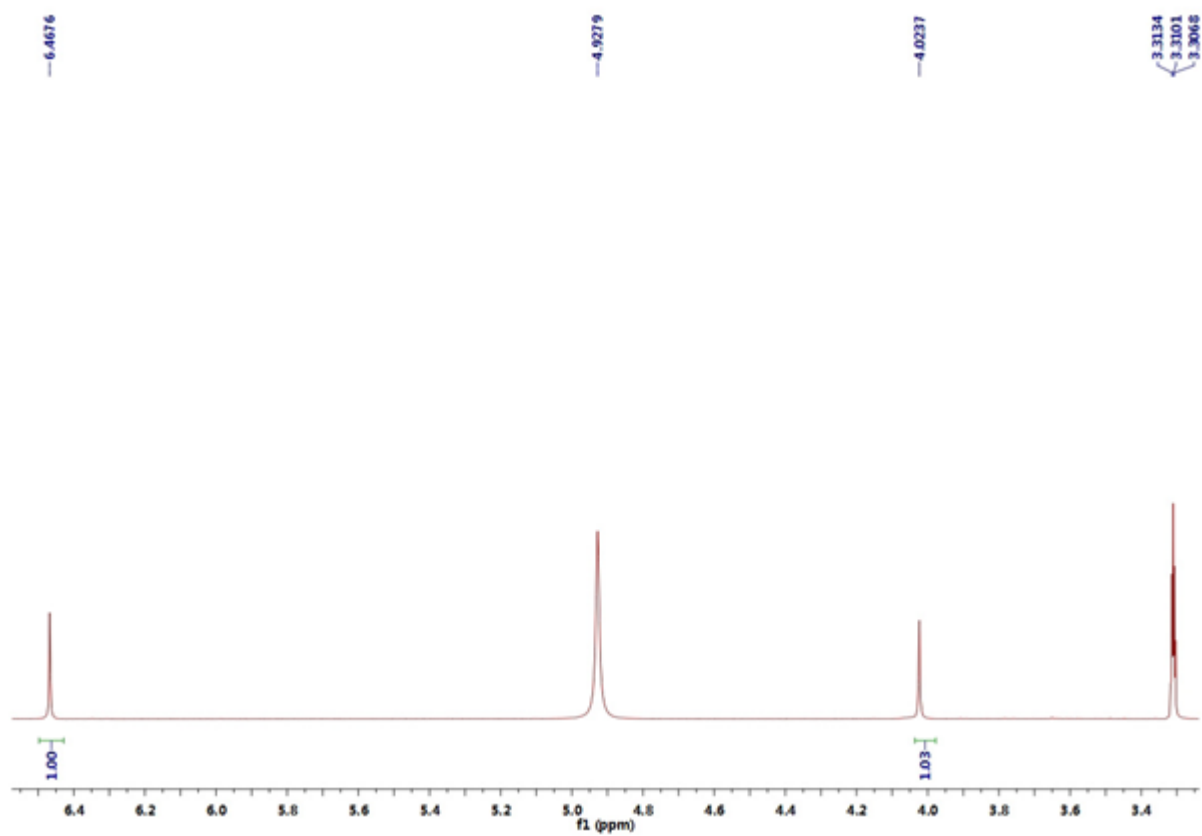


Figure S15: $^1\text{H-NMR}$ (500 MHz, MeOD) spectrum of **3**

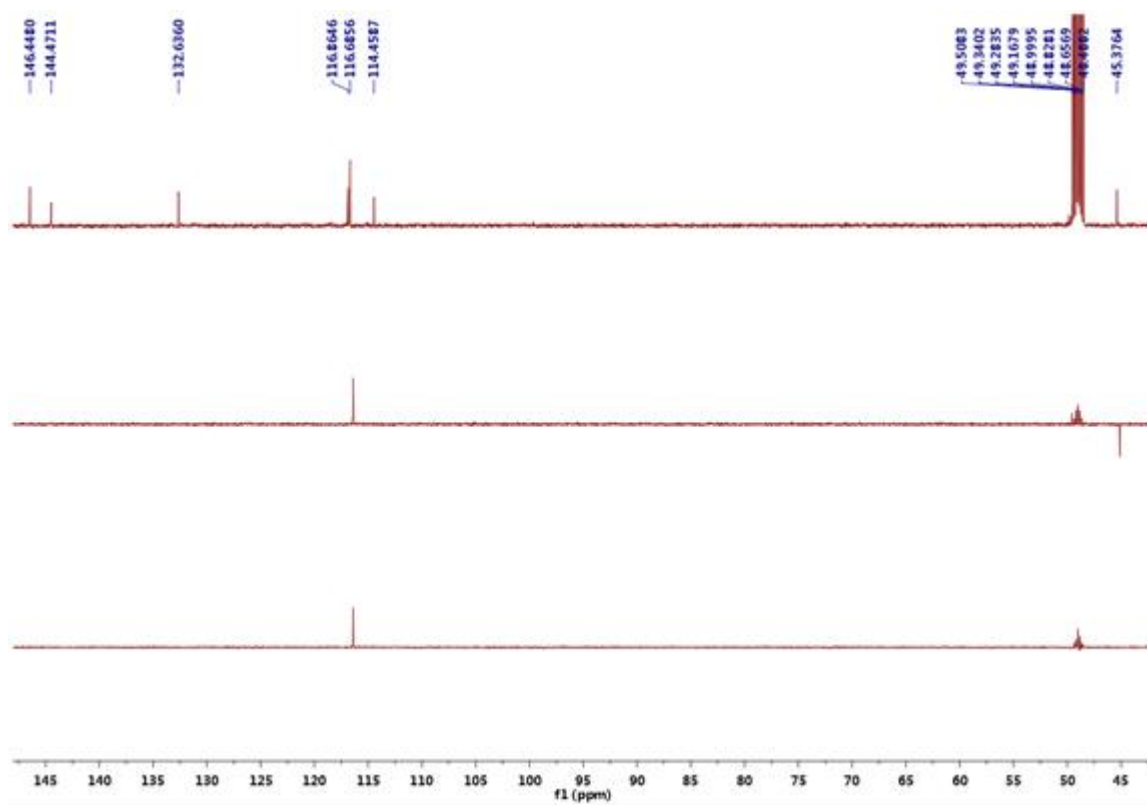


Figure S16: ^{13}C -NMR and DEPT (125 MHz, MeOD) spectra of **3**

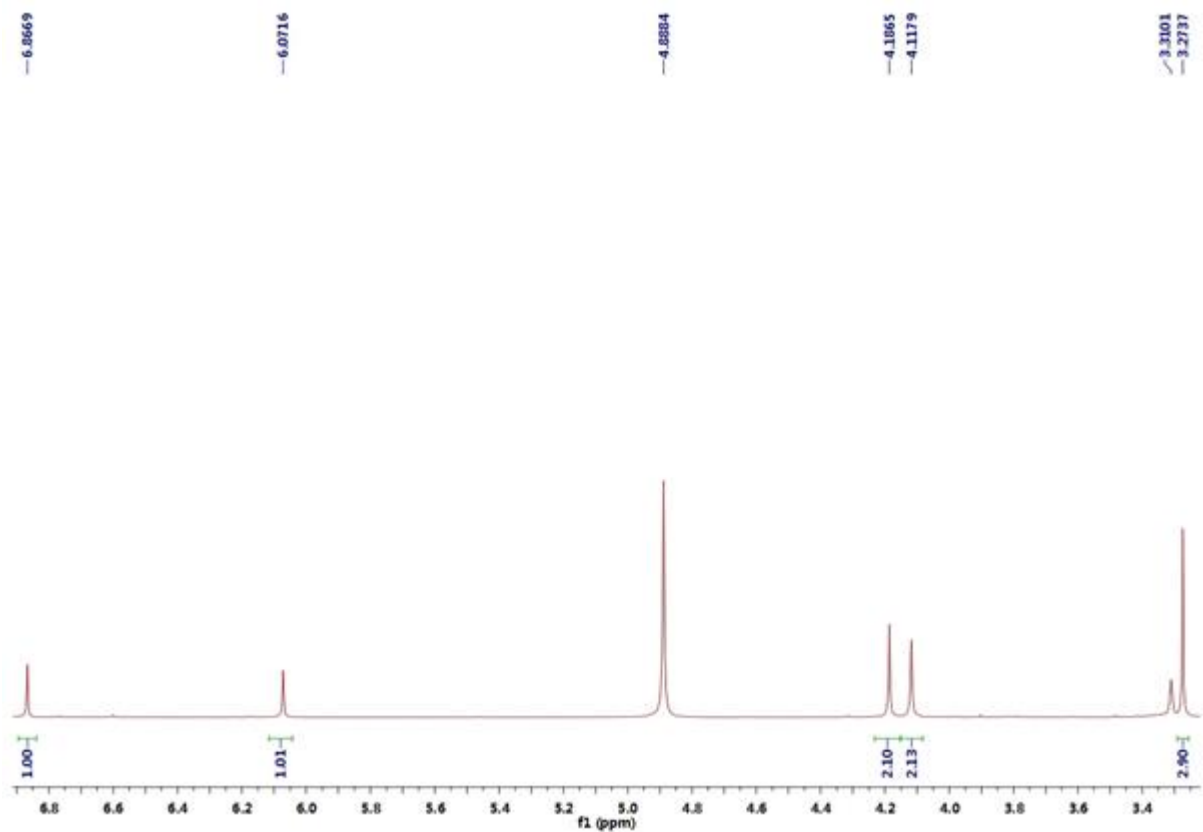


Figure S17: ^1H -NMR (500 MHz, MeOD) spectrum of **4**

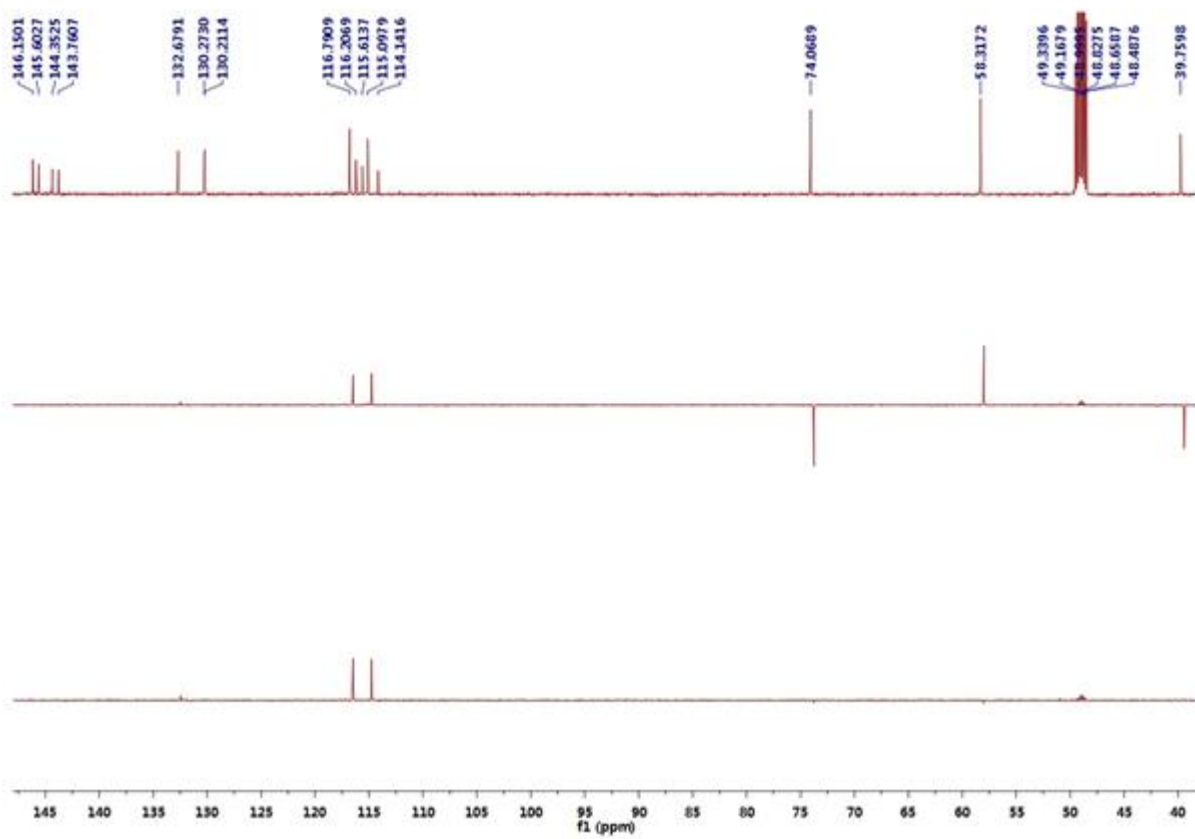


Figure S18: ^{13}C -NMR and DEPT (125 MHz, MeOD) spectra of **4**

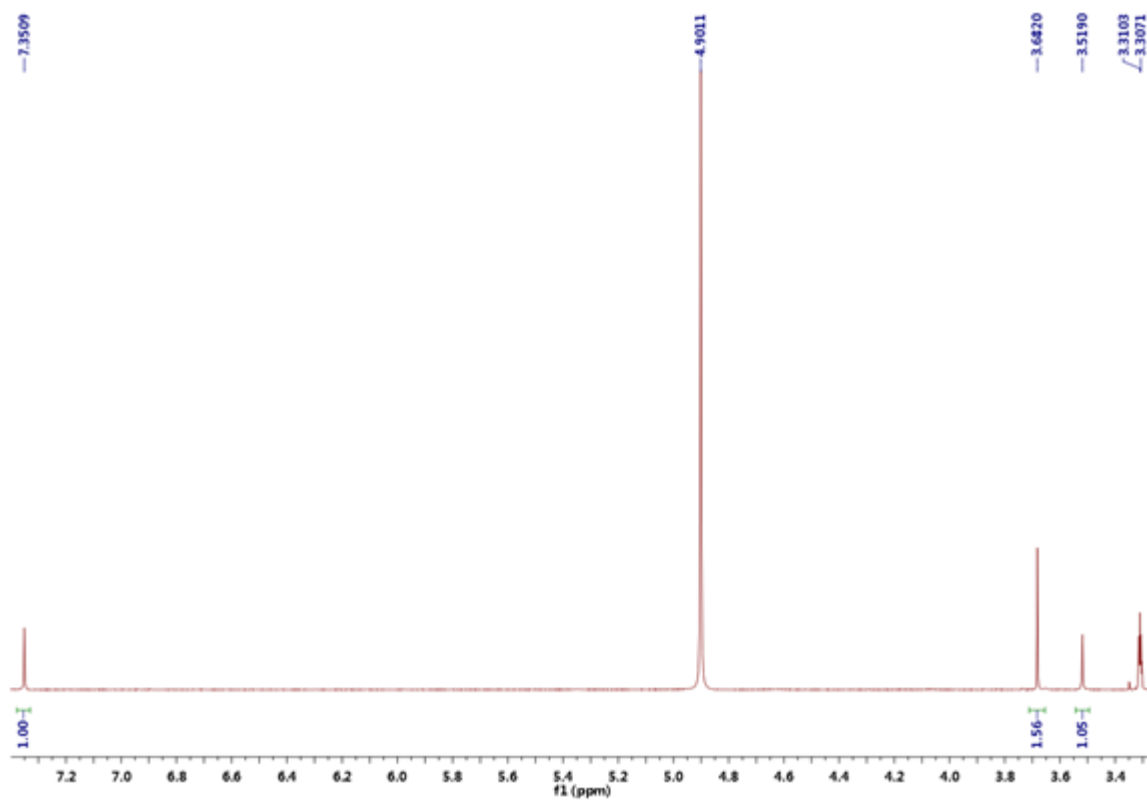


Figure S19: ¹H-NMR (500 MHz, MeOD) spectrum of **5**

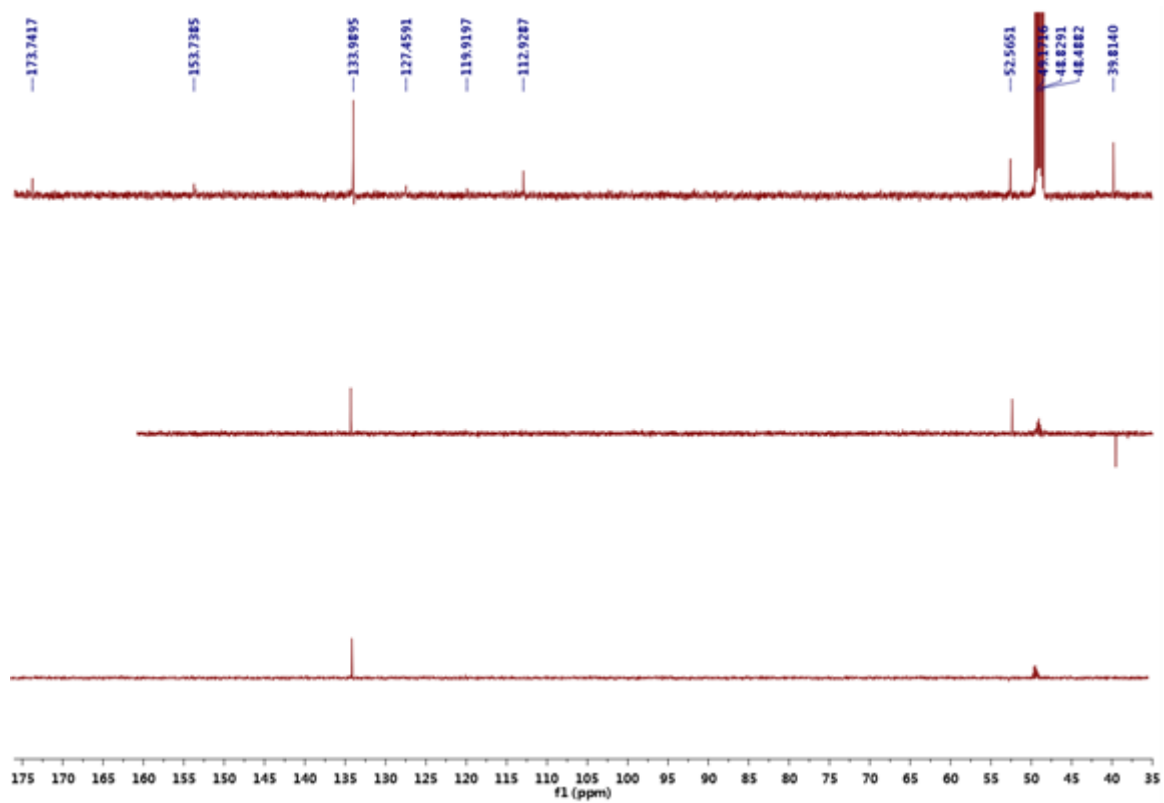


Figure S20: ^{13}C -NMR and DEPT (125 MHz, MeOD) spectra of **5**

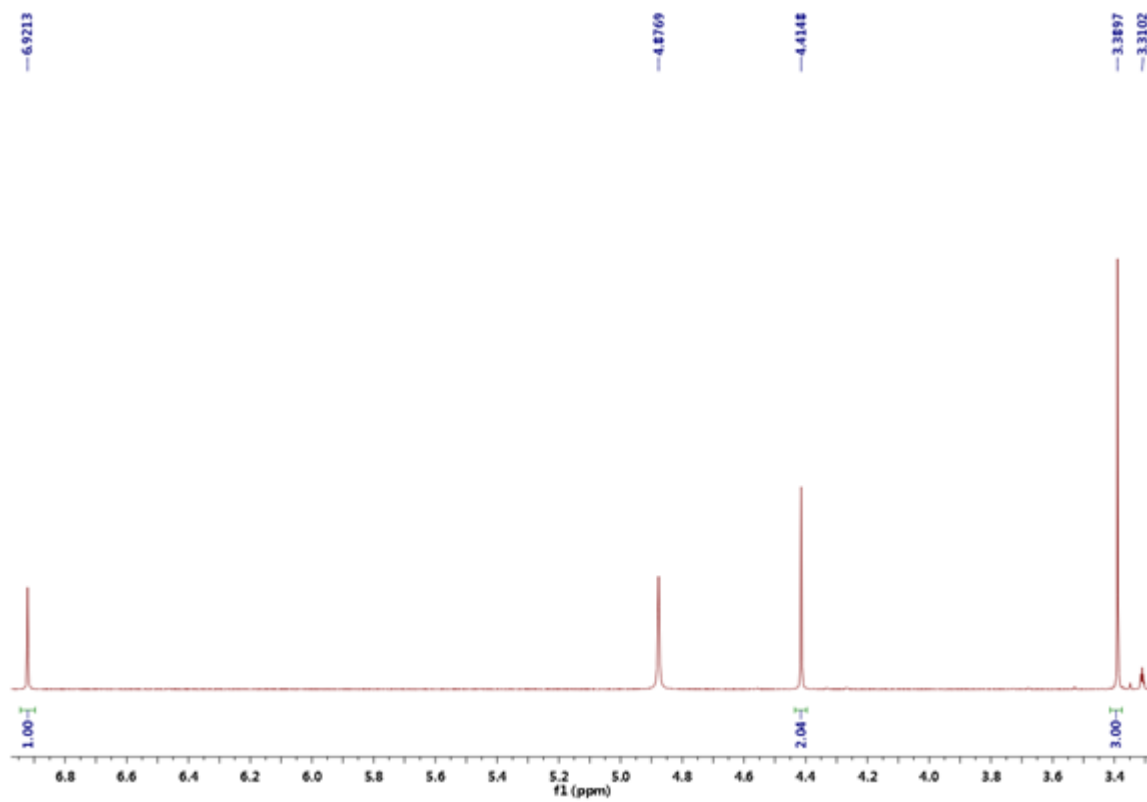


Figure S21: ¹H-NMR (500 MHz, MeOD) spectrum of **6**

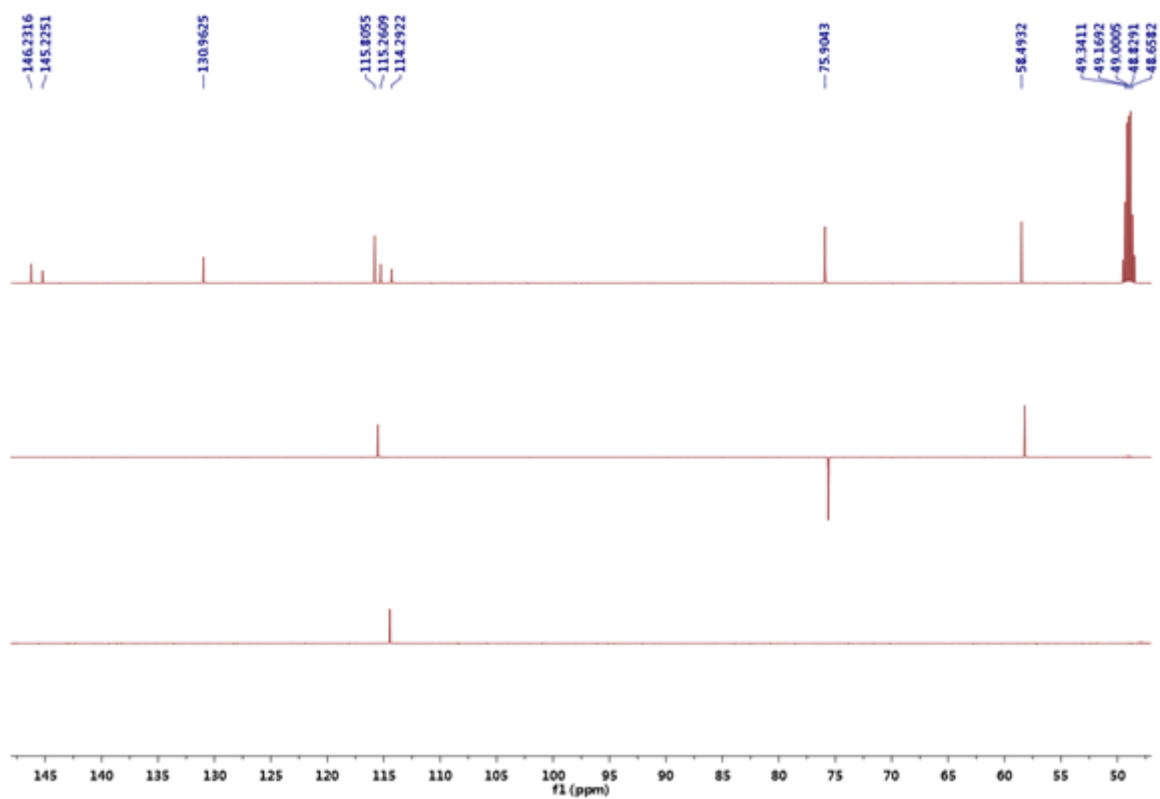


Figure S22: ^{13}C -NMR and DEPT (125 MHz, MeOD) spectra of **6**

S1: ¹H- and ¹³C-NMR data of **2-6**

2-Methoxy-3-bromo-5-hydroxymethylphenol (2): ¹H NMR (MeOD, 500 MHz) δ 7.00 (1H, d, $J = 1.9$), 6.82 (1H, d, $J = 1.9$), 4.46 (2H, s), 3.79 (3H, s); ¹³C NMR (MeOD, 125 MHz) δ 152.5 (C), 145.4 (C), 140.6 (C), 122.8 (CH), 117.9 (C), 115.5 (CH), 64.2 (CH₂), 60.8 (CH₃).

5-(2,3-Dihydroxybenzyl)-3,4-dibromobenzene-1,2-diol (3): ¹H NMR (MeOD, 500 MHz) δ 6.47 (2H, s), 4.02 (2H, s); ¹³C NMR (MeOD, 125 MHz) δ 146.4 (C), 144.5 (C), 132.6 (C), 116.9 (C), 116.7 (CH), 114.5 (CH), 45.4 (CH₂).

5-(2-bromo-3,4-dihydroxy-6-(methoxymethyl)benzyl)-3,4-dibromobenzene-1,2-diol (4): ¹H NMR (MeOD, 500 MHz) δ 6.87 (1H, s), 6.07 (H, s), 4.19 (2H, s), 4.12 (2H, s), 3.27 (3H, s); ¹³C NMR (MeOD, 125 MHz) δ 146.2 (C), 145.6 (C), 144.4 (C), 143.8 (C), 132.7 (C), 130.3 (C), 130.2 (C), 116.8 (CH), 116.2 (C), 115.6 (C), 115.1 (CH), 114.1 (C), 74.1 (CH₂), 58.3 (CH₃), 39.8 (CH₂).

Methyl 2-(3,5-dibromo-4-hydroxybenzyl)acetate (5): ¹H NMR (MeOD, 500 MHz) δ 7.35 (2H, s), 3.68 (3H, s), 3.52 (2H, s); ¹³C NMR (MeOD, 125 MHz) δ 173.7 (C), 153.7 (C), 134.0 (CH), 134.0 (CH), 127.5 (C), 119.9 (C), 112.9 (C), 52.7 (CH₃), 39.8 (CH₂).

3,4-Dibromo-5-(methoxymethyl)benzene-1,2-diol (6): ¹H NMR (MeOD, 500 MHz) δ 6.92 (1H, s), 4.41 (2H, s), 3.39 (3H, s); ¹³C NMR (MeOD, 125 MHz) δ 146.2 (C), 145.2 (C), 131.0 (C), 115.8 (CH), 115.3 (C), 114.3 (C), 75.9 (CH₂), 58.5 (CH₃).

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Reaction Role

Product (12)

15 Results Sort: Relevance View: Partial

1

65487-76-5

C₁₃H₈Br₄O₄
4,4'-Methylenebis[5,6-dibromo-1,2-benzenediol]

42 References 31 Reactions 5 Suppliers

2

852547-27-4

C₁₃H₇Br₅O₄
3,4,6-Tribromo-5-[(2,5-dibromo-3,4-dihydroxyphenyl)methyl]-1,2-benzenediol

6 References 6 Reactions 0 Suppliers

3

1130428-33-9

C₁₃H₇Br₅O₄
3,4,6-Tribromo-5-[(2,3-dibromo-4,5-dihydroxyphenyl)methyl]-1,2-benzenediol

5 References 17 Reactions 1 Supplier

4

852547-26-3

6 References 6 Reactions 0 Suppliers

5

1251090-69-3

5 References 17 Reactions 1 Supplier

6

1251090-70-6

5 References 17 Reactions 1 Supplier

1	133.8 ^a , C	132.0, C	130.5, C	131.0, C
2	116.7, C	116.4, C	112.1, C	116.3, C
3	114.4, C	113.6, C	144.4, C	114.4 ^c , C
4	144.5 ^b , C	143.8, C	142.4, C	144.0, C
5	146.4 ^b , C	145.4, C	109.5, C	146.3, C
6	117.1, CH	116.5, CH	121.9, CH	116.3, CH
	6.61, s	6.58, s	6.25, s	6.04, s
7	42.7, CH ₂	44.5, CH ₂	44.6, CH ₂	46.6, CH ₂
	3.87, s	4.04, s	4.42, d (0.8)	4.37, s
1'	133.9 ^a , C	132.0, C	131.0, C	131.9, C
2'	115.9, CH	116.5, CH	113.9, C	114.3 ^c , C
	6.53, d (1.6)	6.58, s		
3'	147.4, C	145.4, C	113.9, C	114.5 ^c , C
4'	142.5, C	143.8, C	144.7, C	145.5, C
5'	110.7, C	113.6, C	144.0, C	145.2, C
6'	124.5, CH	116.4, C	118.1, C	118.4, C
	6.74, d (1.7)			

^{a,b,c}Data are interchangeable

Figure S23: SciFinder search results of **1** and the NMR data of compounds