

Supporting Information

for

Bioactive selaginellins from *Selaginella tamariscina* (Beauv.) Spring

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Spectroscopic data and other relevant information for compounds 1–4.

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Figure S1: ^1H NMR (400 MHz, CD_3COCD_3) of compound **1**

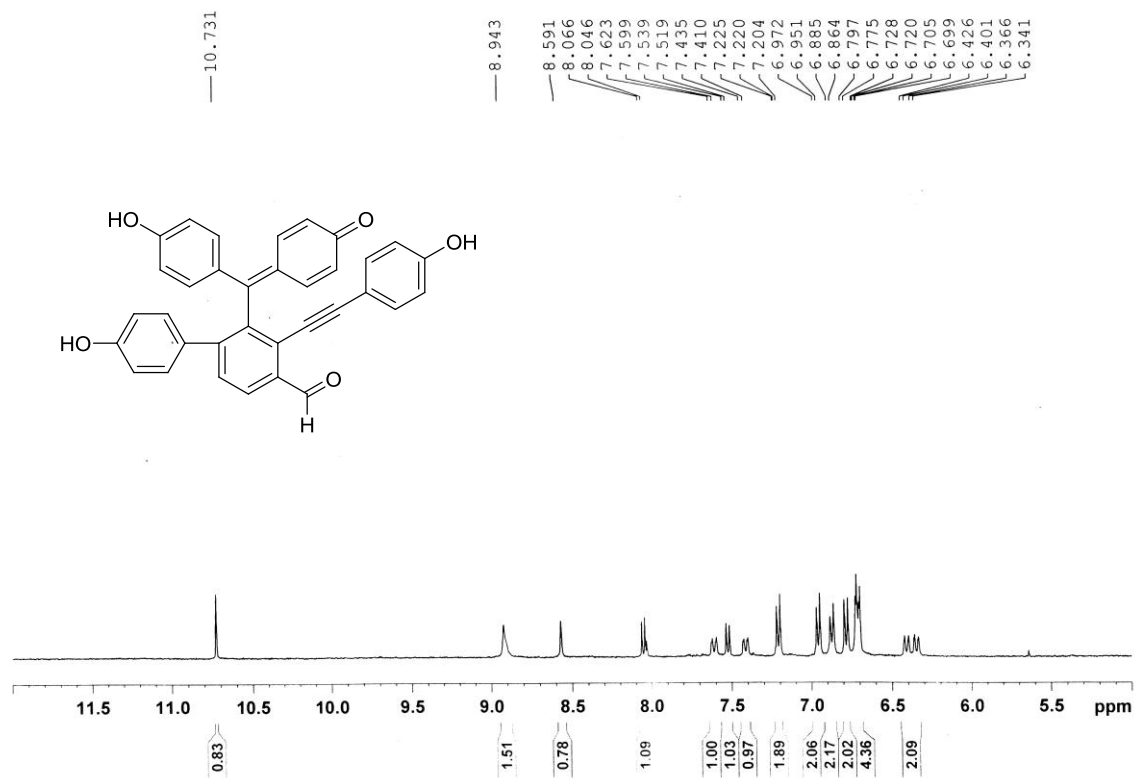


Figure S2: ^{13}C NMR (100 MHz, CD_3COCD_3) of compound **1**

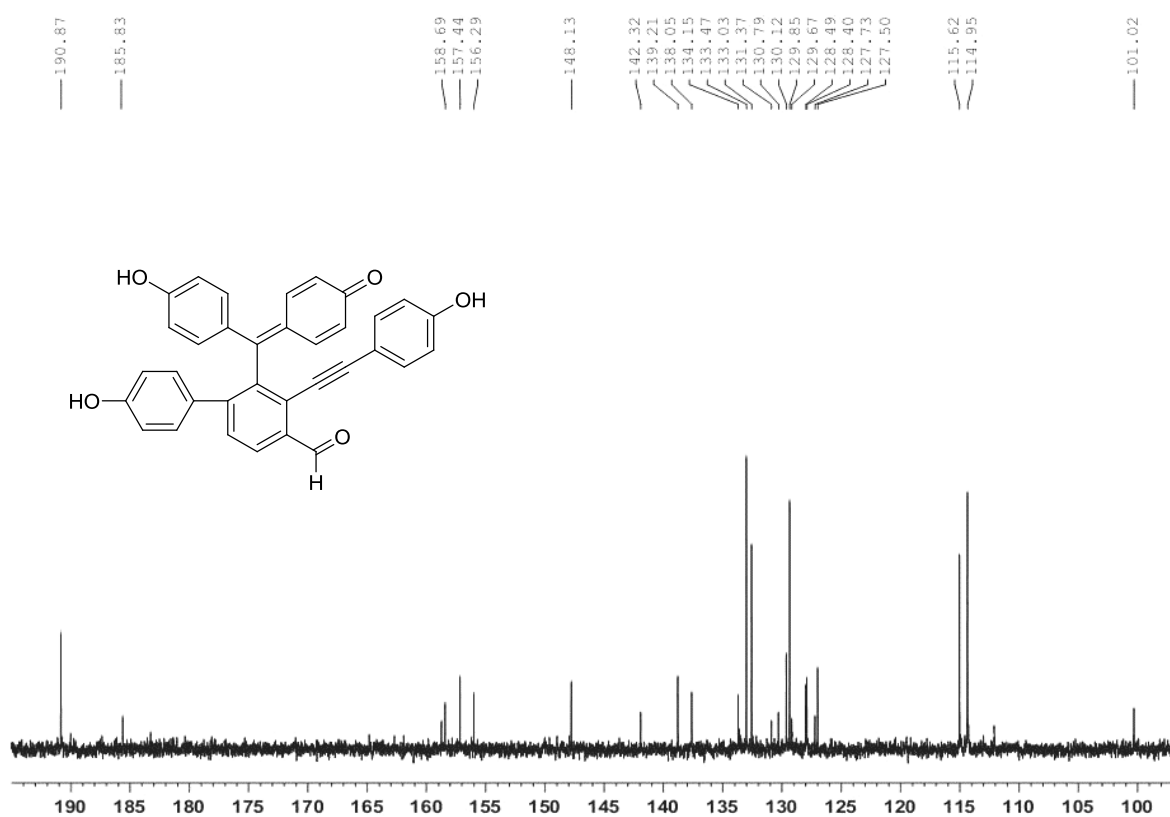
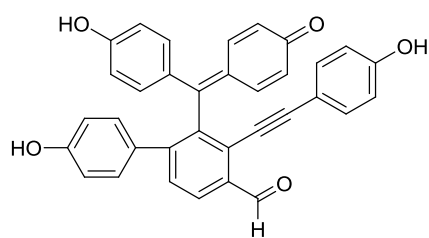


Figure S3: ^1H - ^1H COSY of compound **1**



Selaginellin O

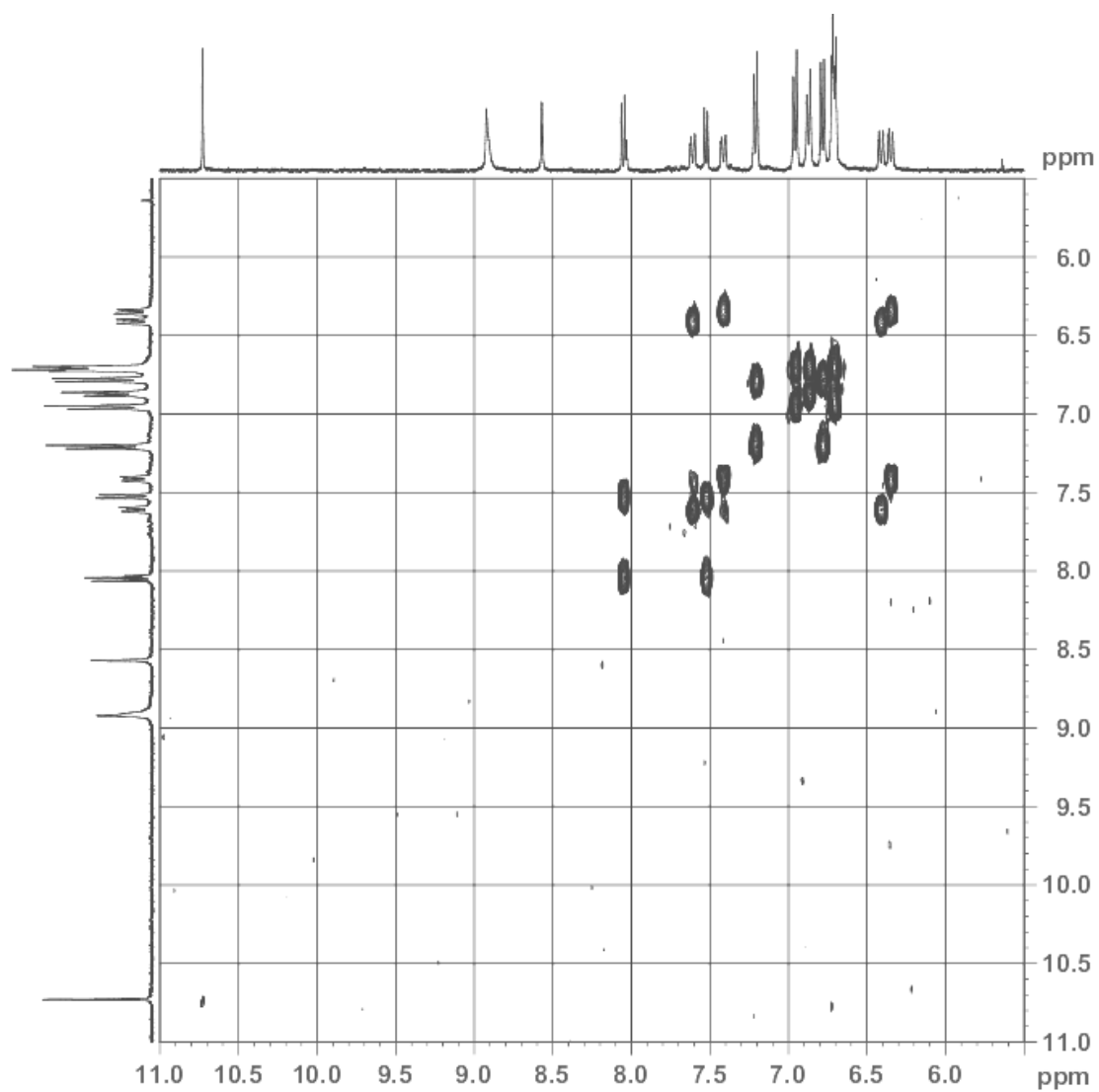
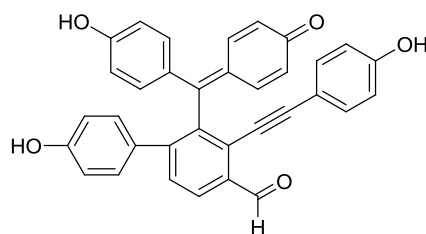


Figure S4: HMQC of compound **1**



Selaginellin O

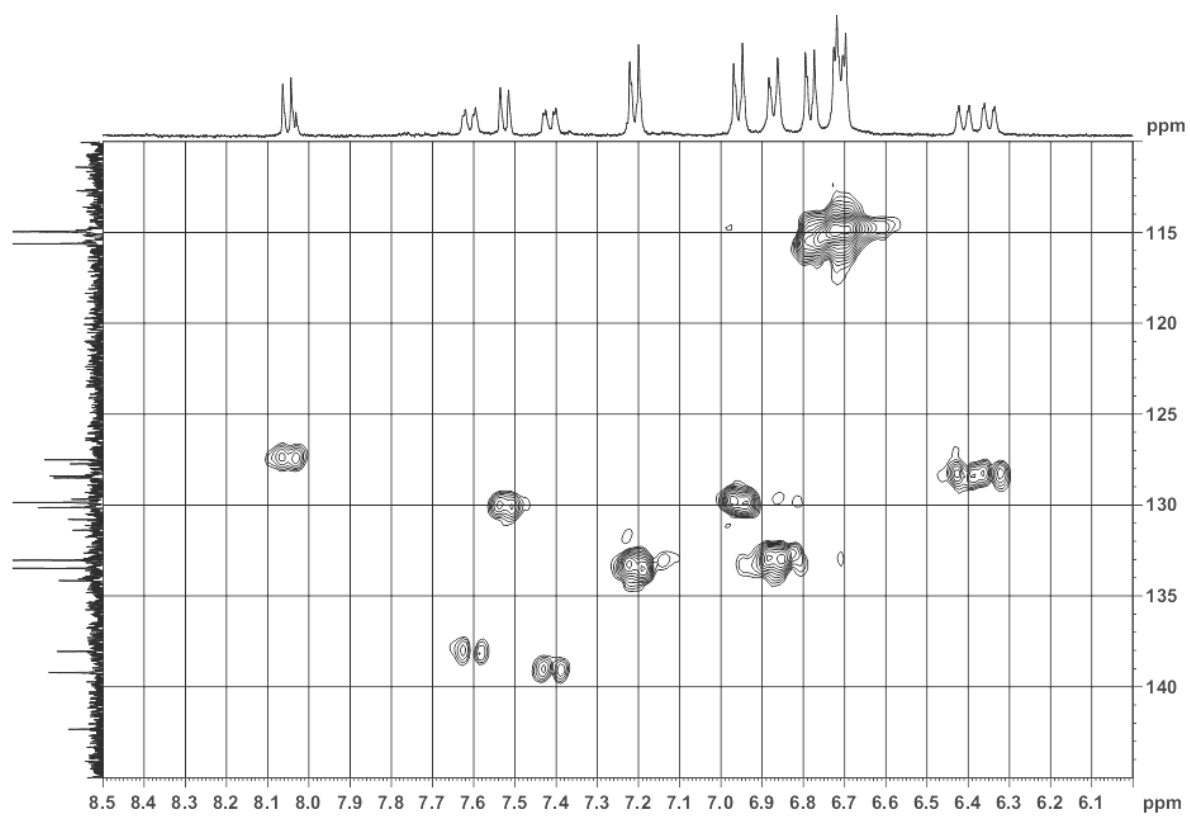
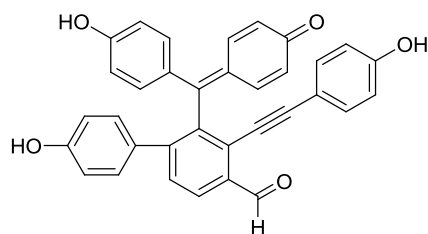
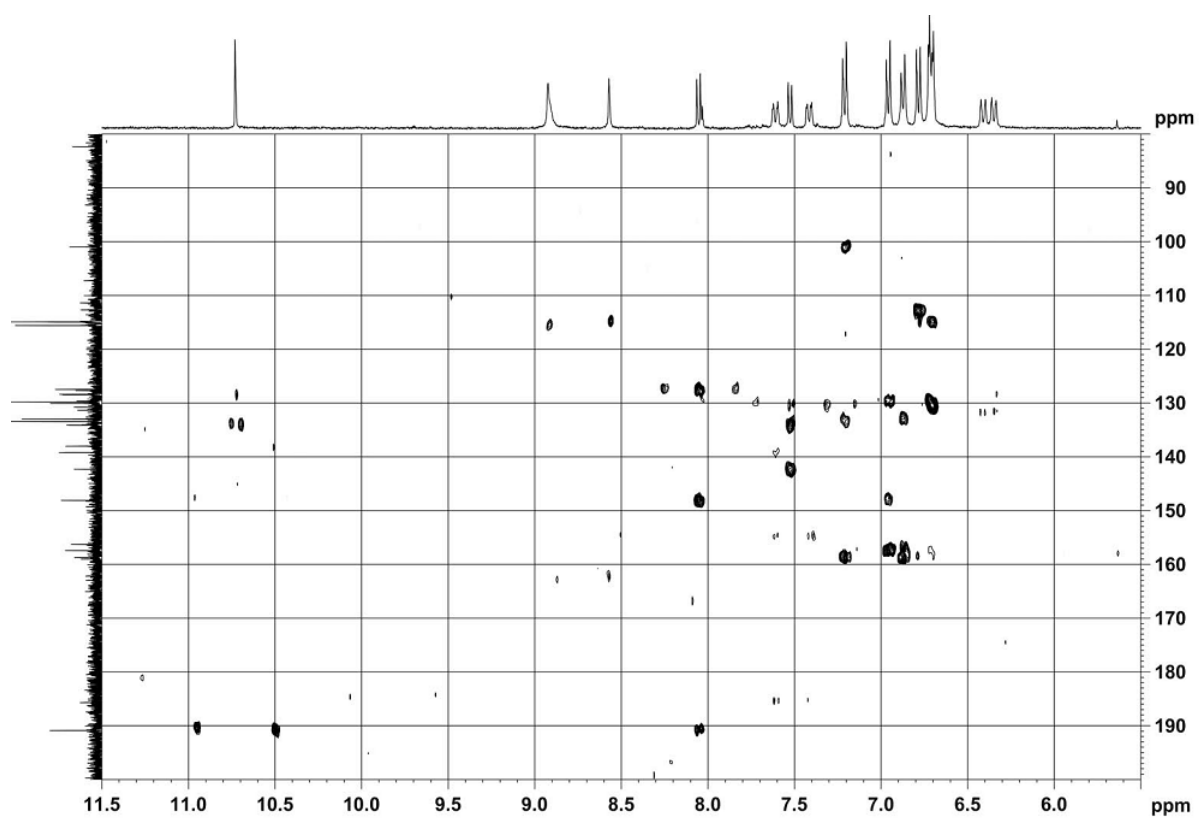


Figure S5: HMBC of compound **1**



Selaginellin O

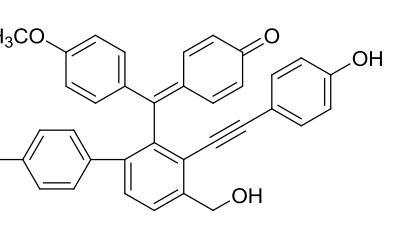


Chemical structure of Selaginellin M is shown above the ¹H NMR spectrum. The structure is a complex polycyclic molecule featuring a central benzene ring substituted with a 4-methoxyphenyl group, a 4-hydroxyphenyl group, and a 4-hydroxyphenyl group connected via an ethynyl bridge. The central ring also has a hydroxymethyl group and a side chain containing a ketone and a double bond.

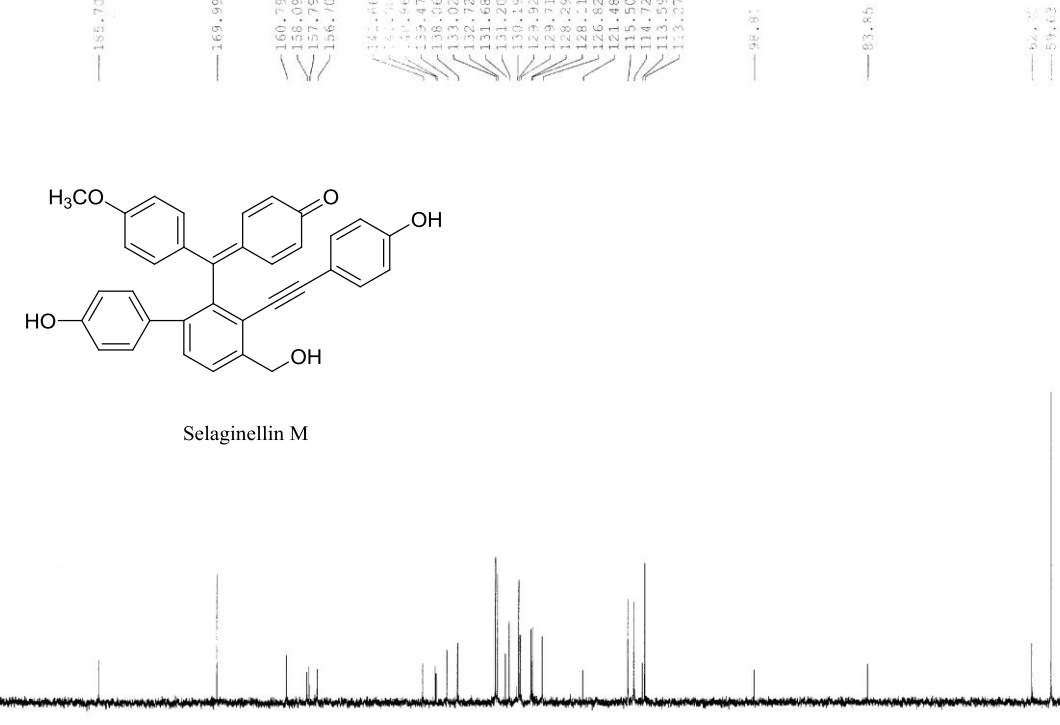
¹H NMR spectrum (CDCl₃) of Selaginellin M is displayed below the structure. The spectrum shows peaks in the aromatic region (6.3–8.4 ppm) and a small peak in the aliphatic region (3.7 ppm). Integration values are provided below the baseline.

Chemical Shift (ppm)	Integration
8.363	0.74
8.309	0.77
7.789	1.00
7.537	1.13
7.512	1.02
7.391	1.11
7.371	2.21
7.355	4.88
7.348	4.55
7.330	2.14
7.324	2.15
7.130	
7.123	
7.118	
7.107	
7.102	
7.095	
6.930	
6.925	
6.913	
6.908	
6.901	
6.895	
6.890	
6.879	
6.874	
6.867	
6.822	
6.816	
6.810	
6.798	
6.793	
6.776	
6.769	
6.764	
6.753	
6.741	
6.715	
6.679	
6.672	
6.667	
6.655	
6.650	
6.381	
6.376	
6.356	
6.351	
6.338	
6.334	
6.314	
6.309	
5.023	
5.009	
3.787	2.99

Selaginellin M

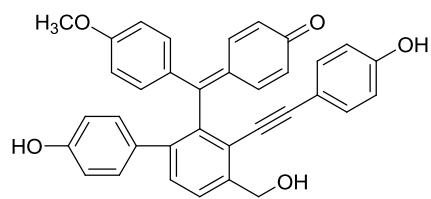
COc1ccc(cc1)/C(=C2/C(=C3C(=C2)C(=CC3)C(=O)C4=CC=C(C=C4)O)C#CC5=CC=C(C=C5)O)C6=CC=C(C=C6)O


The chemical structure of Selaginellin M is a complex polycyclic molecule. It features a central benzene ring substituted with a 4-methoxyphenyl group, a 4-hydroxyphenyl group, and a 4-hydroxy-2-(4-hydroxyphenyl)-2-propynyl group. A cyclohexenone ring is fused to the central benzene ring.



The ¹³C NMR spectrum of Selaginellin M shows 25 distinct peaks. The x-axis represents the chemical shift in ppm, ranging from 190 to 50. The peaks are labeled with their corresponding chemical shift values: 185.70, 169.99, 160.79, 156.09, 157.79, 156.70, 145.66, 145.22, 143.97, 138.47, 138.06, 135.02, 132.72, 131.68, 131.20, 130.49, 129.32, 129.11, 128.29, 126.82, 126.81, 121.48, 115.50, 114.72, 113.59, 113.37, 98.81, 83.85, 62.35, 59.62, and 54.81.

Figure S8: ^1H - ^1H COSY of compound **2**



Selaginellin M

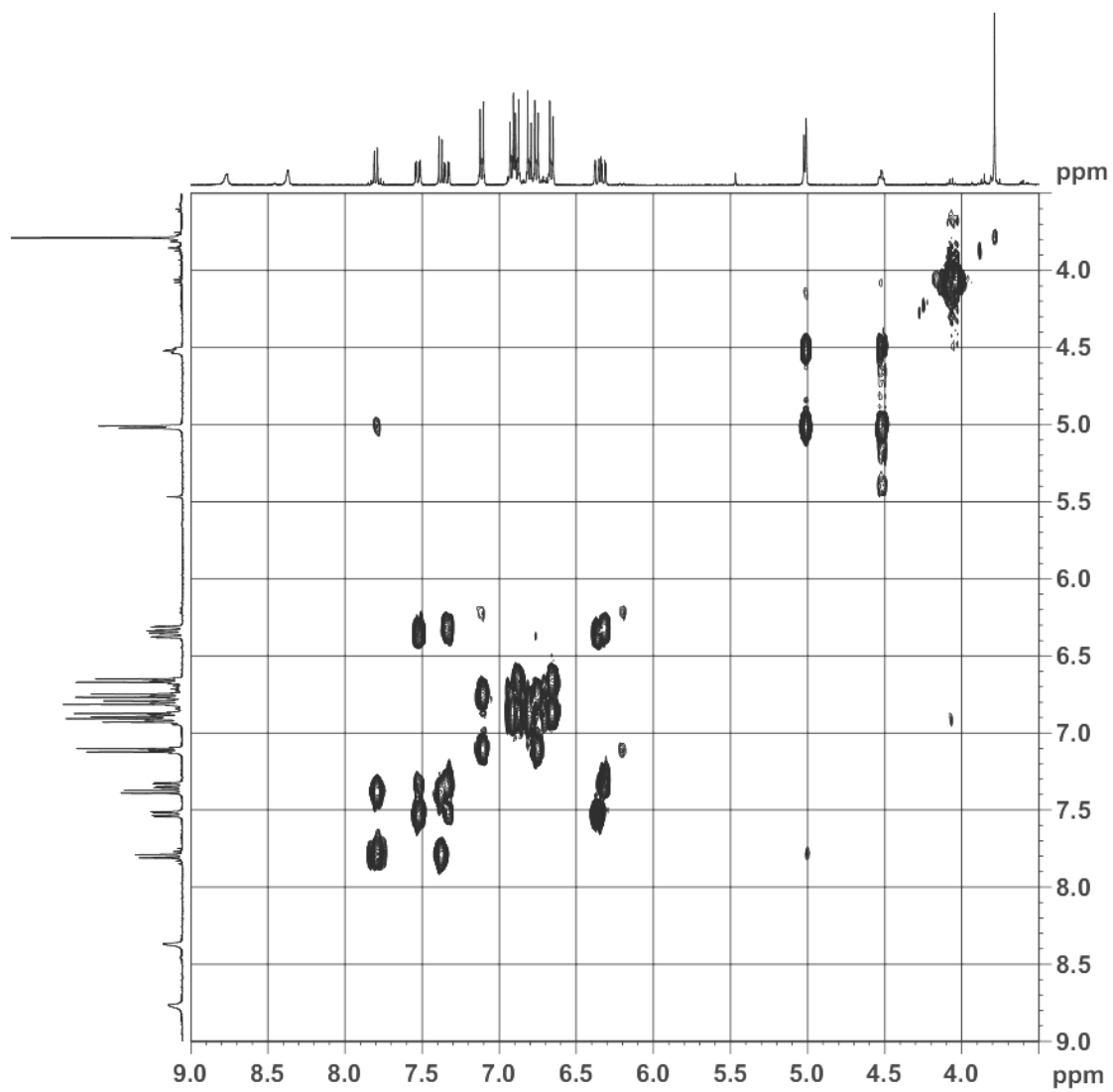


Figure S9: HMQC of compound **2**

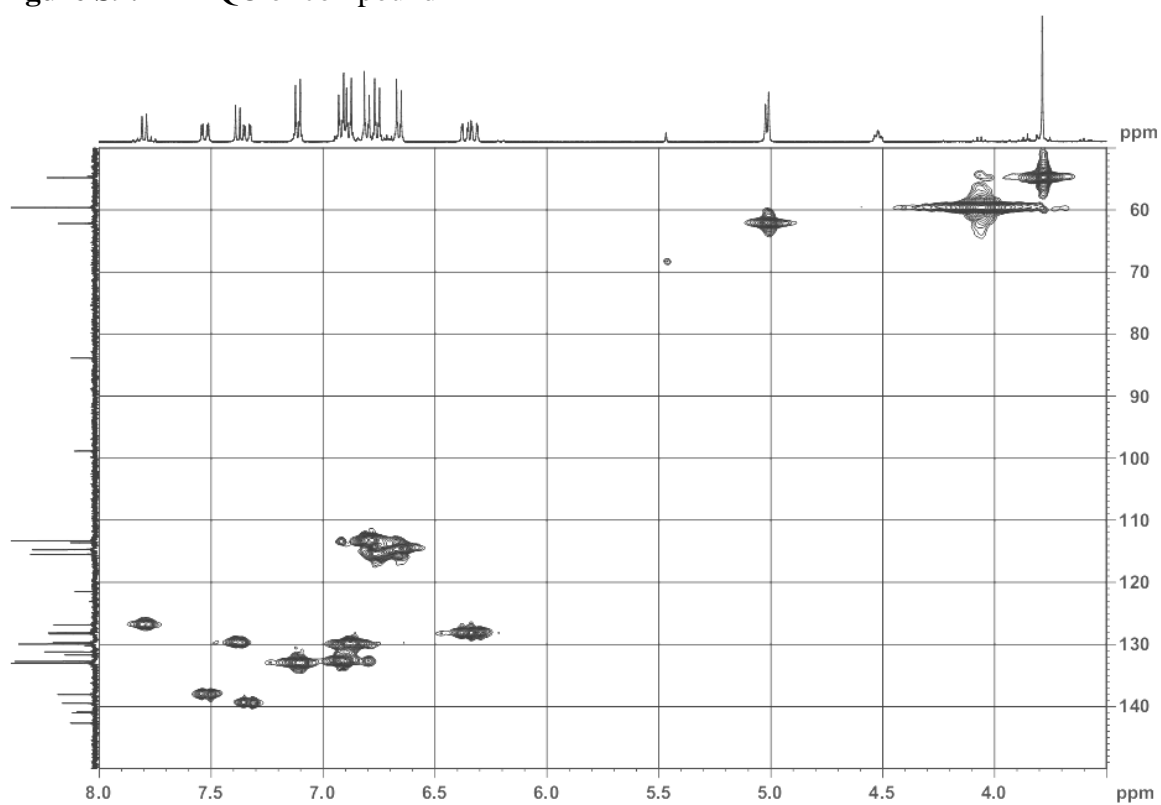


Figure S10: HMBC of compound **2**

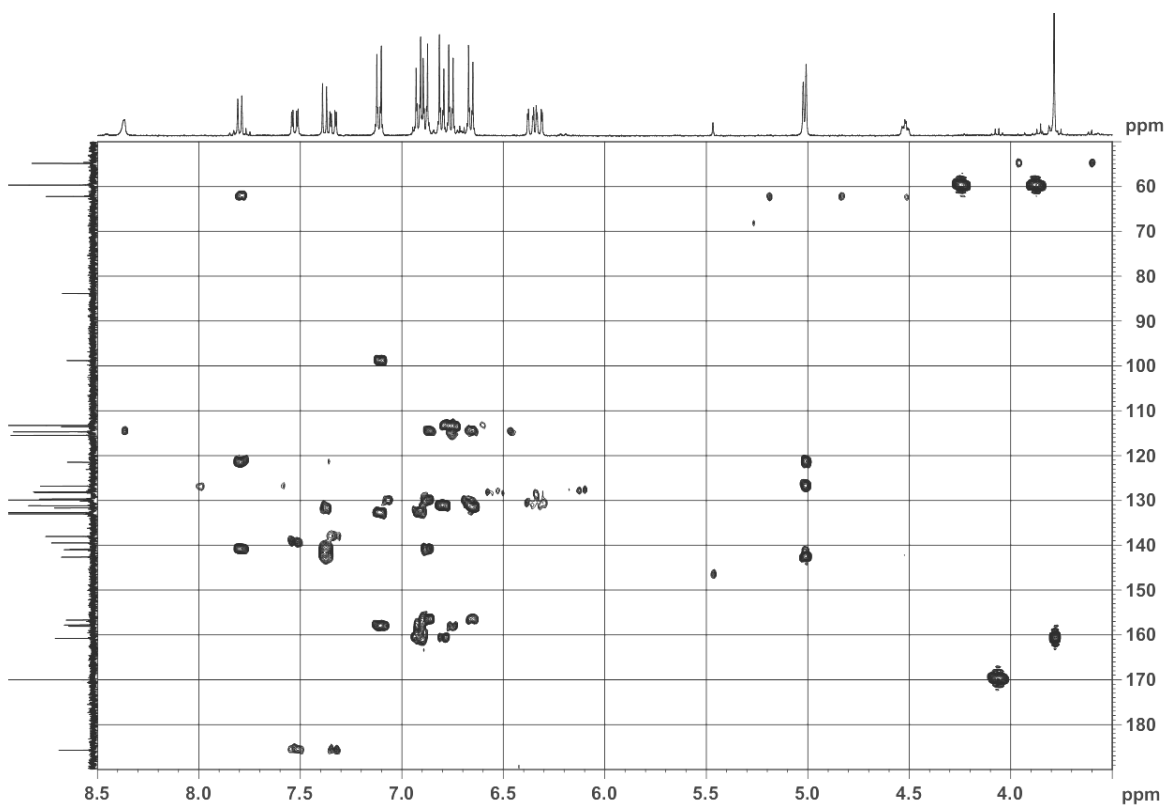


Figure S11: ^1H NMR (400 MHz, CD_3COCD_3) of compound **3**

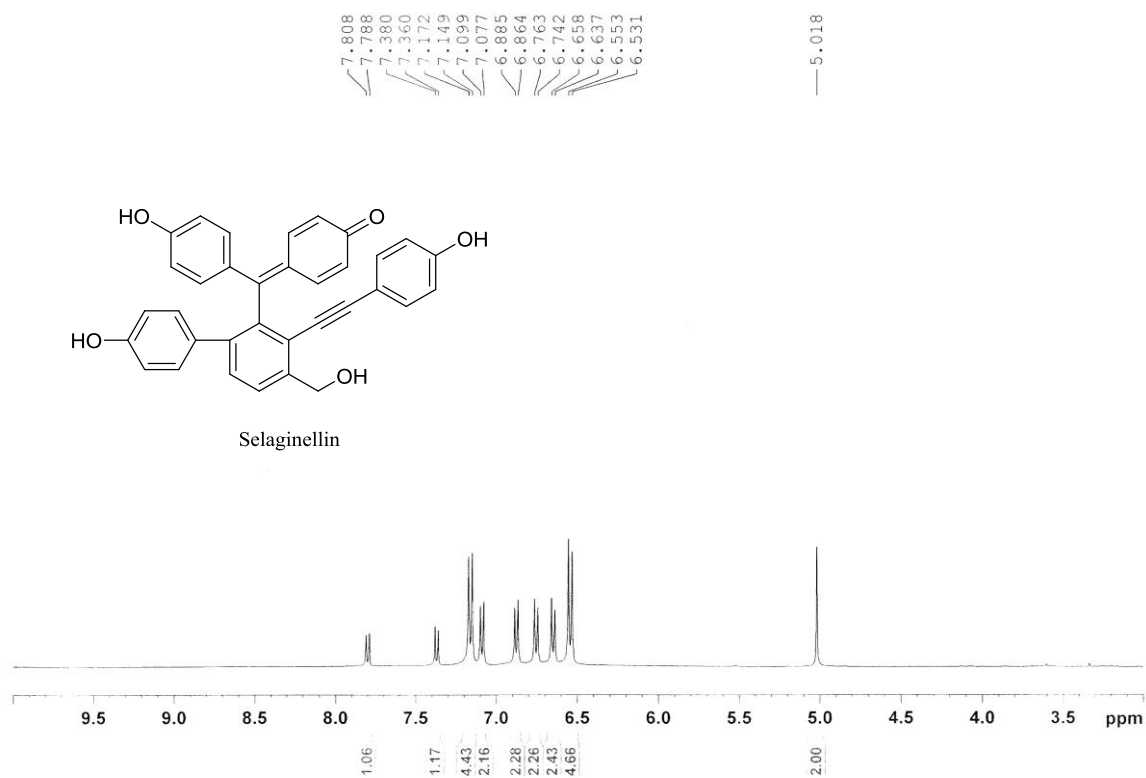


Figure S12: ^{13}C NMR (100 MHz, CD_3COCD_3) of compound **3**

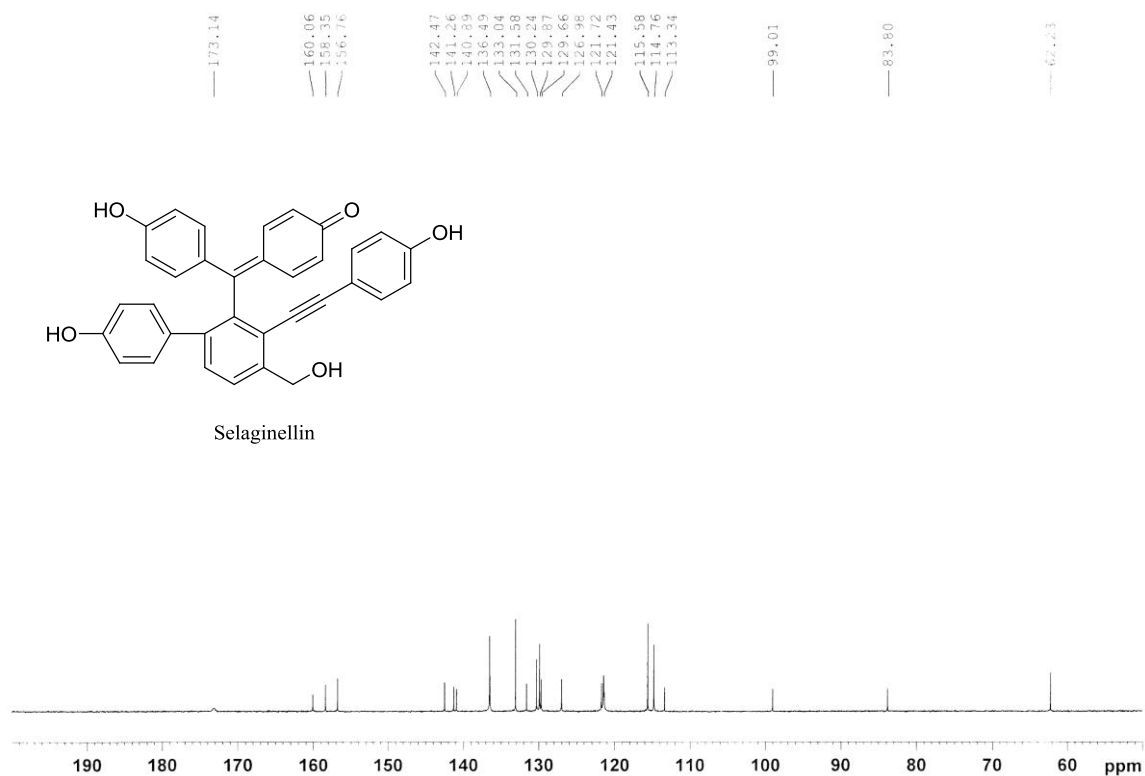


Figure S13: ^1H - ^1H COSY of compound **3**

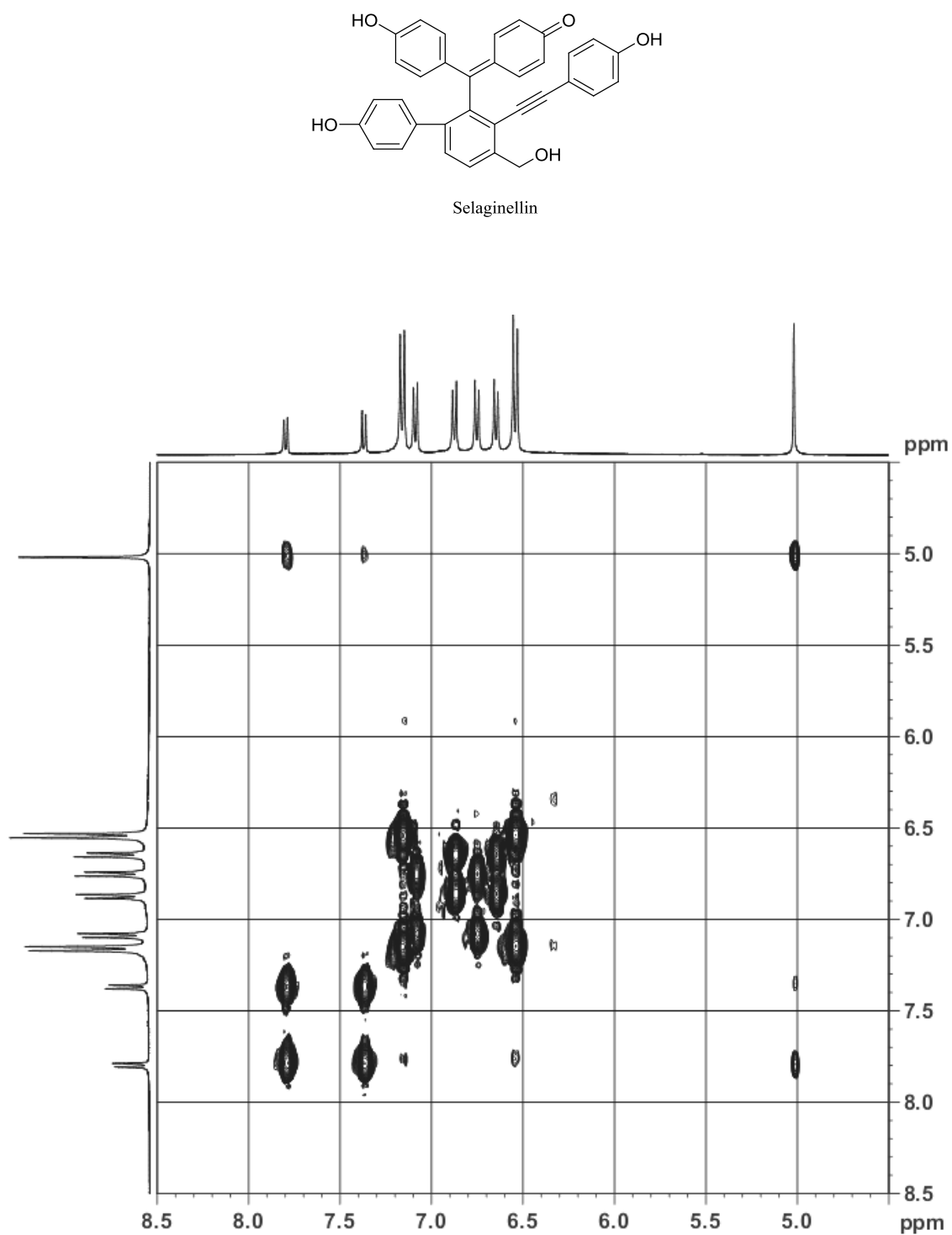


Figure S14: HMQC of compound **3**

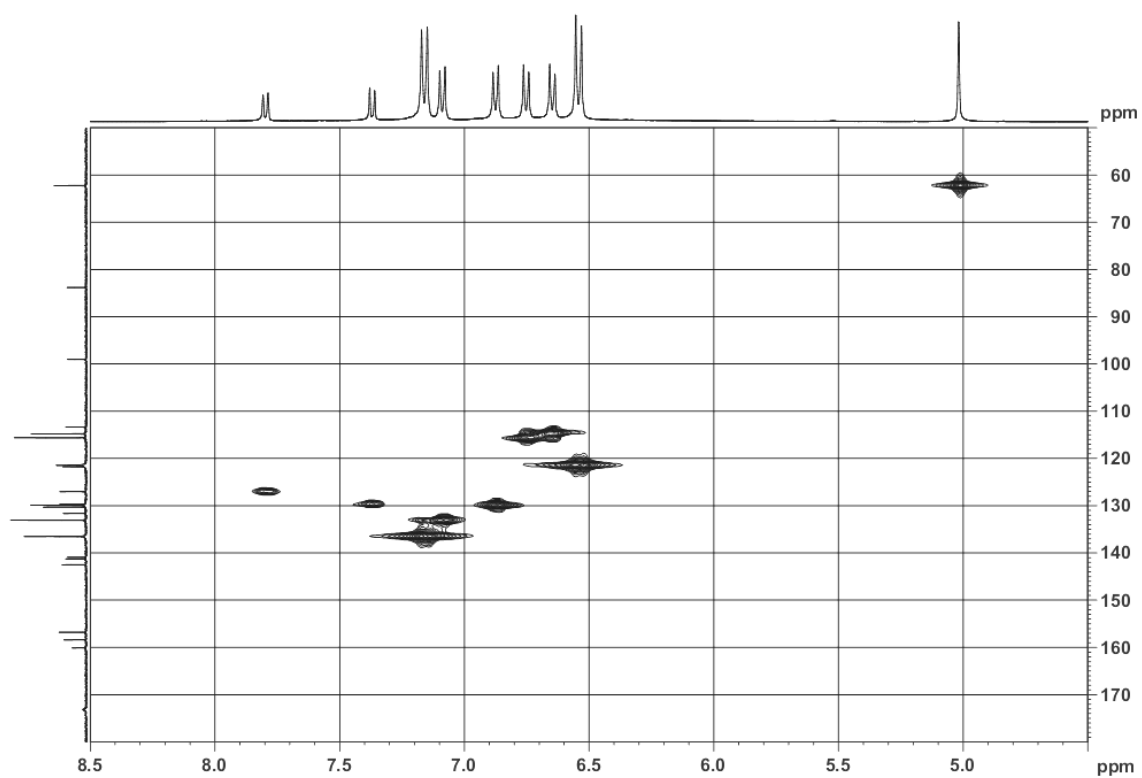


Figure S15: HMBC of compound **3**

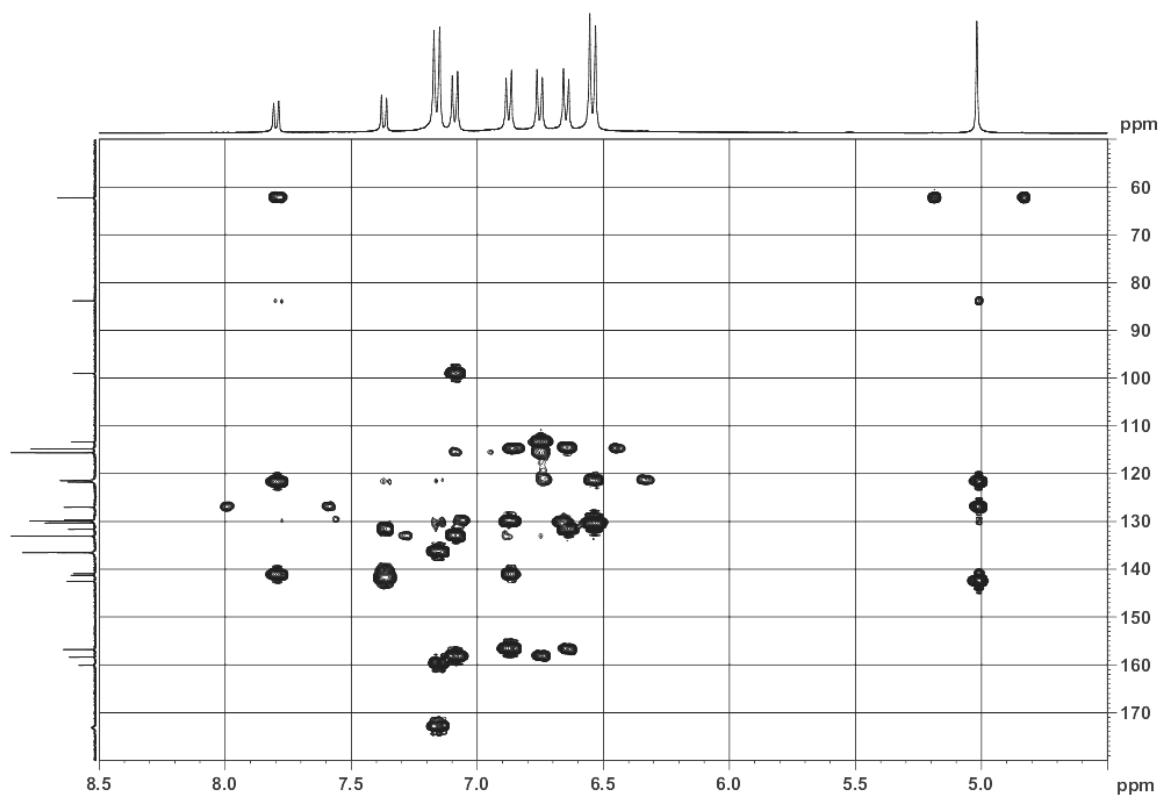


Figure S16: ^1H NMR (400 MHz, CD_3COCD_3) of compound **4**

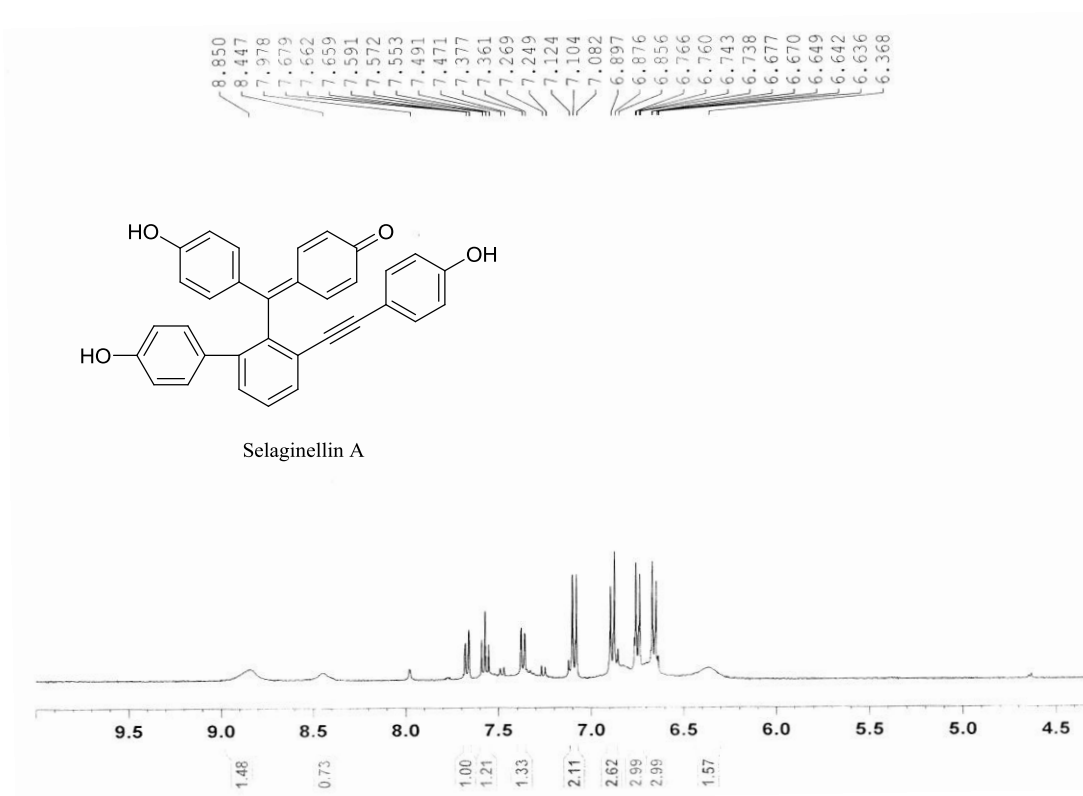


Figure S17: ^{13}C NMR (100 MHz, CD_3COCD_3) of compound **4**

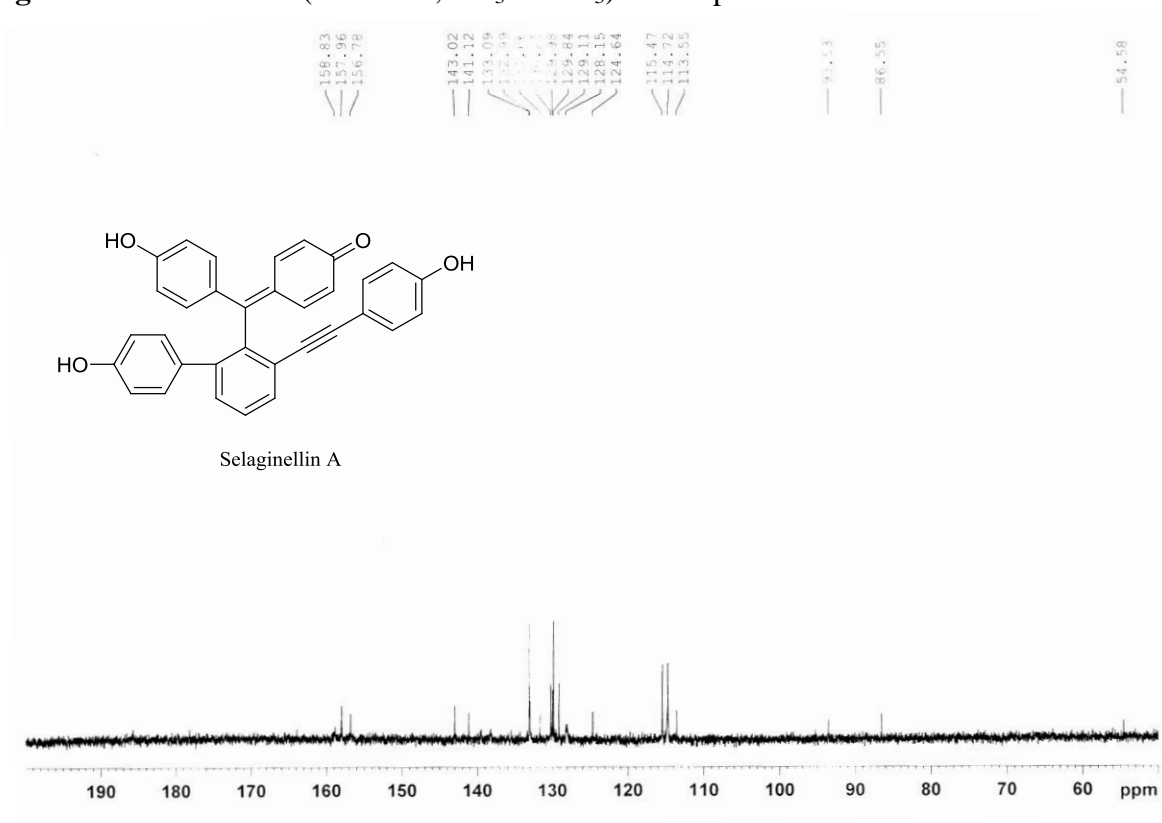
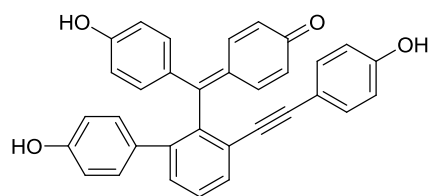


Figure S18: ^1H - ^1H COSY of compound **4**



Selaginellin A

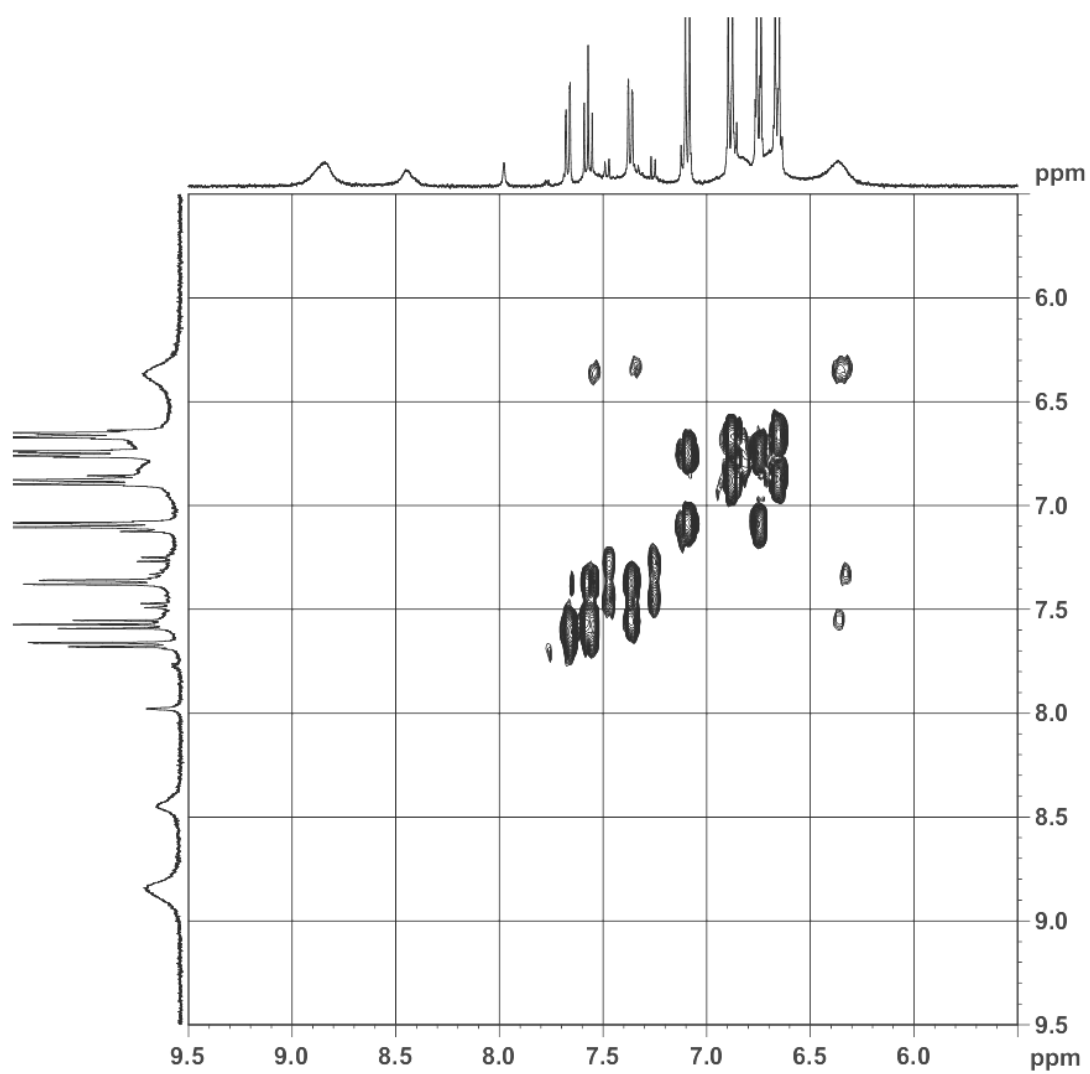


Figure S19: HMQC of compound **4**

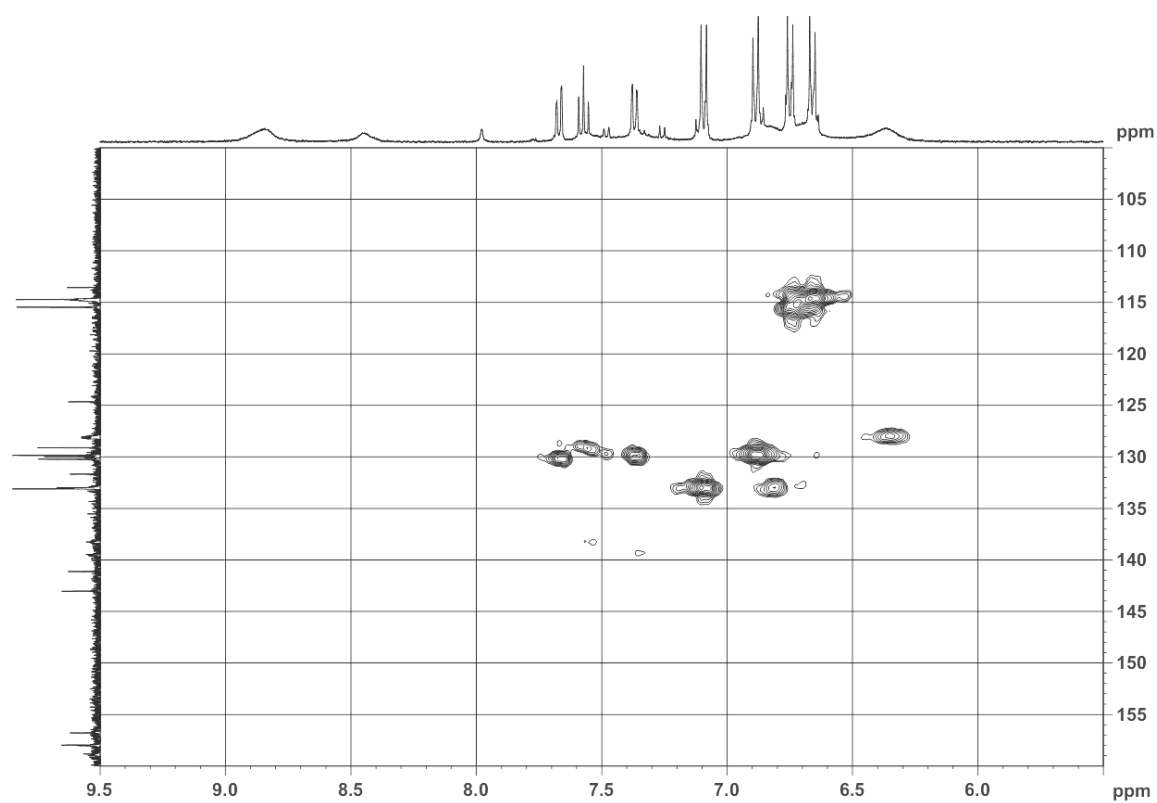


Figure S20: HMBC of compound **4**

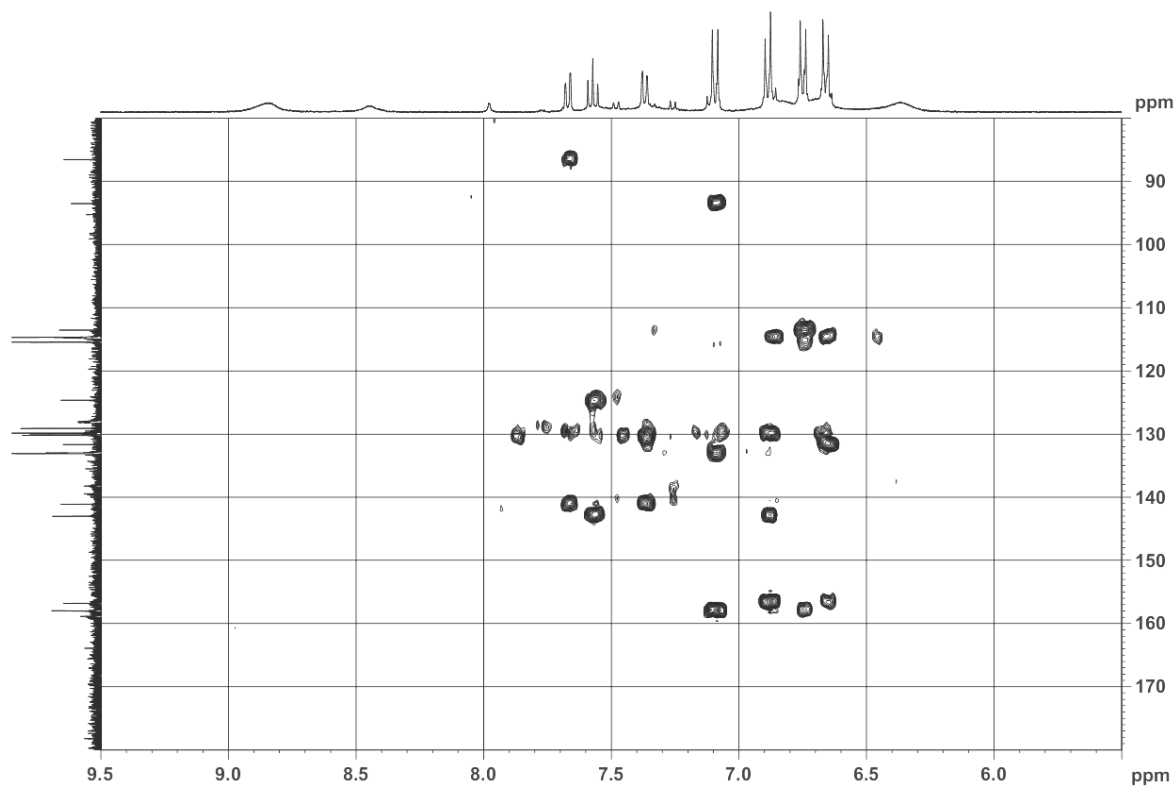


Table S1: Cytotoxic activity of compounds **1–3** evaluated with MTT assay.

Compounds	IC ₅₀ (μM ± SD) ^a
1	26.4 ± 0.80
2	28.5 ± 0.64
3	33.1 ± 1.21
Cisplatin ^b	15.4 ± 1.10

^aThe values represent means ± SD of three independent experiments^bPositive control**Table S2:** Antioxidant activity of compounds **1–3** evaluated with ABTS and FRAP assays^a

Compounds	ABTS assay	FRAP assay
	IC ₅₀ (μM ± SD)	Fe ^{II} (μmol/μmol ± SD)
1	2.94 ± 0.014	1.10 ± 0.058
2	3.02 ± 0.029	1.05 ± 0.056
3	3.07 ± 0.012	0.94 ± 0.050
Trolox ^b	5.23 ± 0.019	0.87 ± 0.043

^aValues are mean ± SD of three separated experiments.^bReference compound.