

Supporting Information

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Dihydropyridinone Alkaloid Artifacts from *Curcuma longa* and their Anti-Migration Activity Against HepG2 cells

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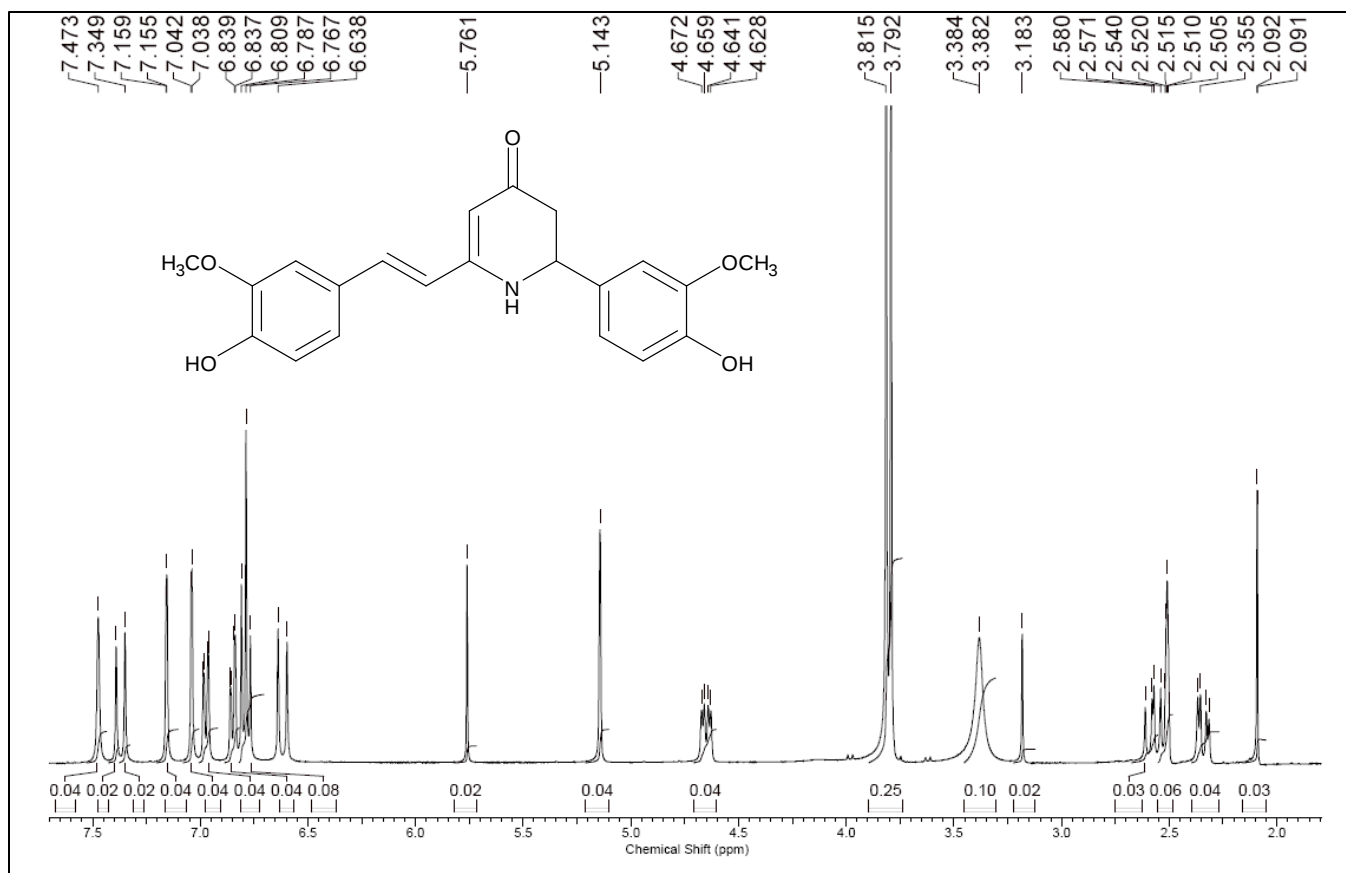


Figure 1S: ¹H-NMR spectrum (DMSO-d₆, at 400 MHz) of compound 1.

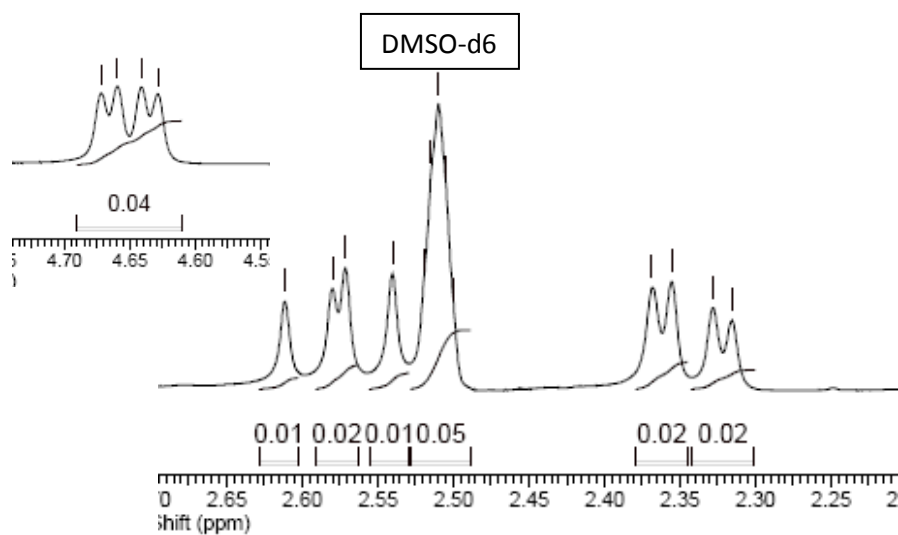


Figure 2S: Expansions of ¹H-NMR spectrum (400 MHz, DMSO-d₆) of compound 1.

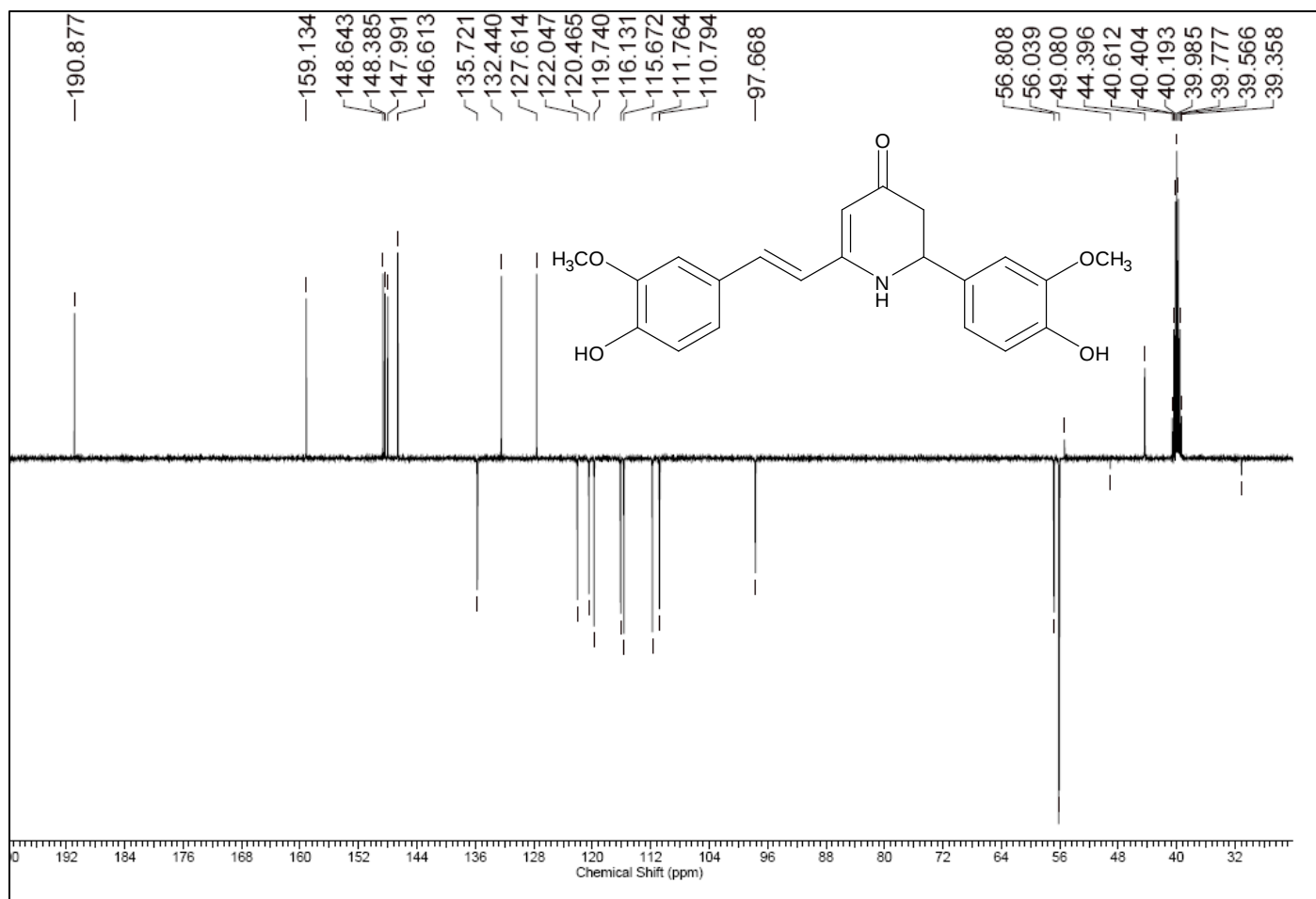


Figure 3S: APT spectrum (100 MHz, DMSO-d₆) of compound **1**.

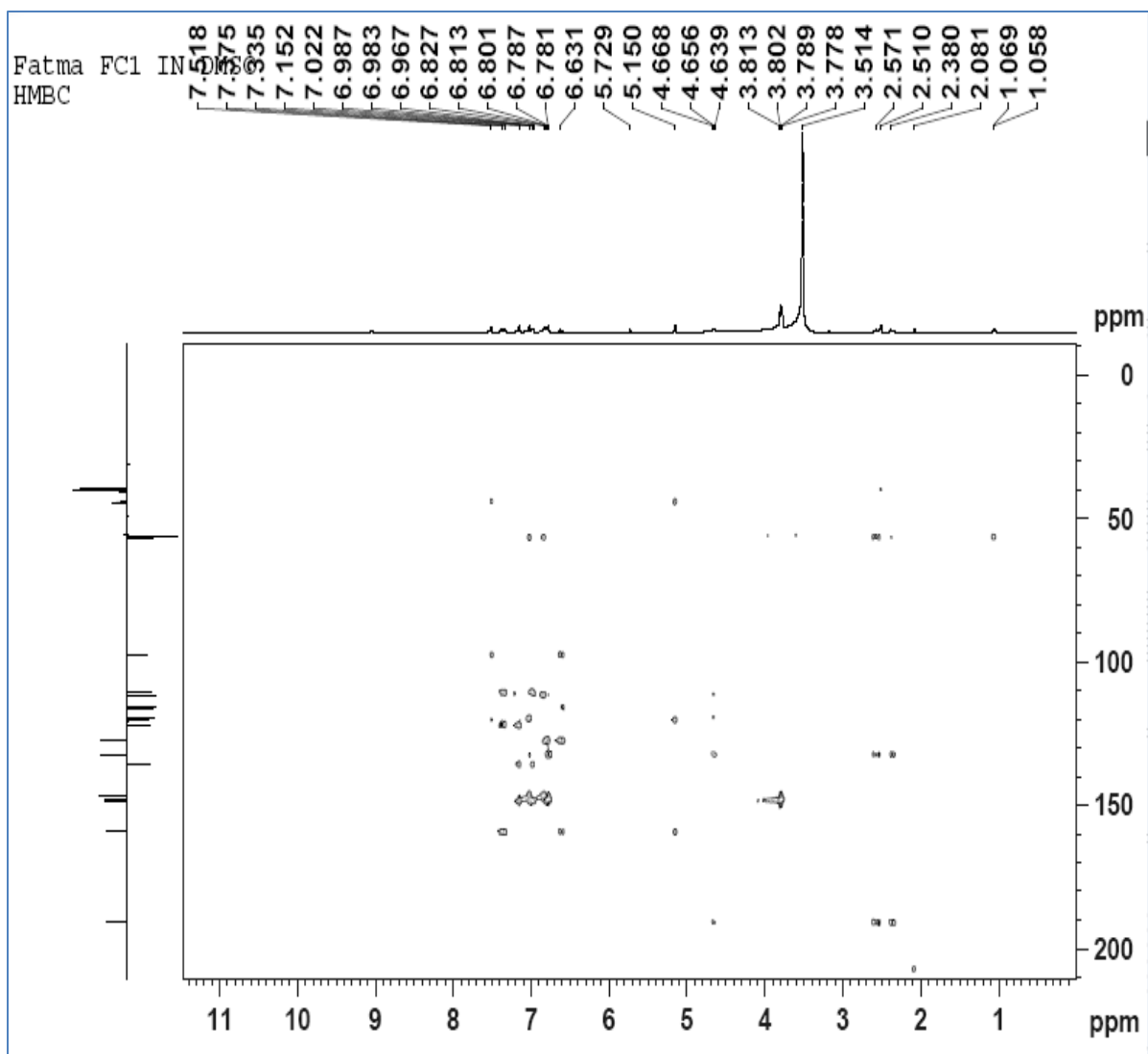
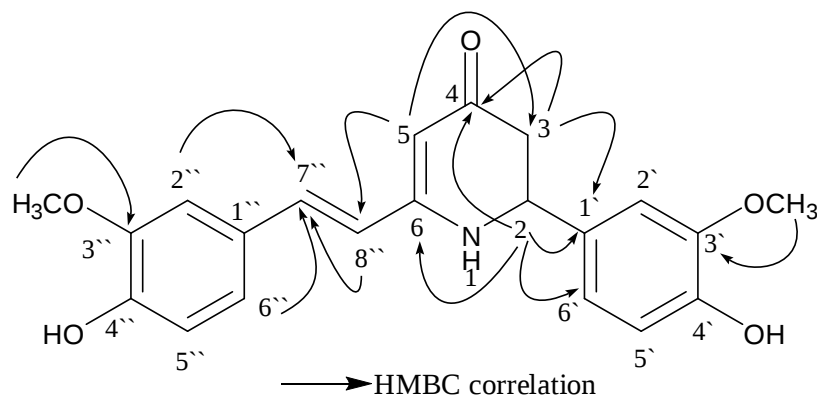


Figure 4S: HMBC spectrum (400 MHz, DMSO-d₆) of compound **1**.



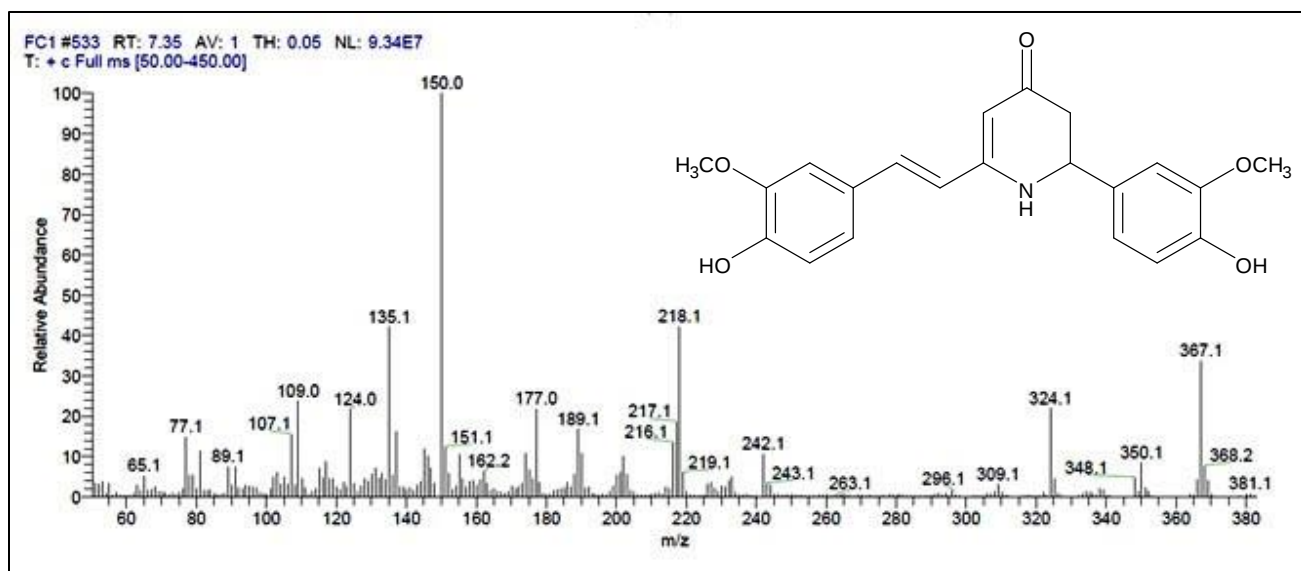


Figure 5S (a): EIMS spectrum of compound 1.

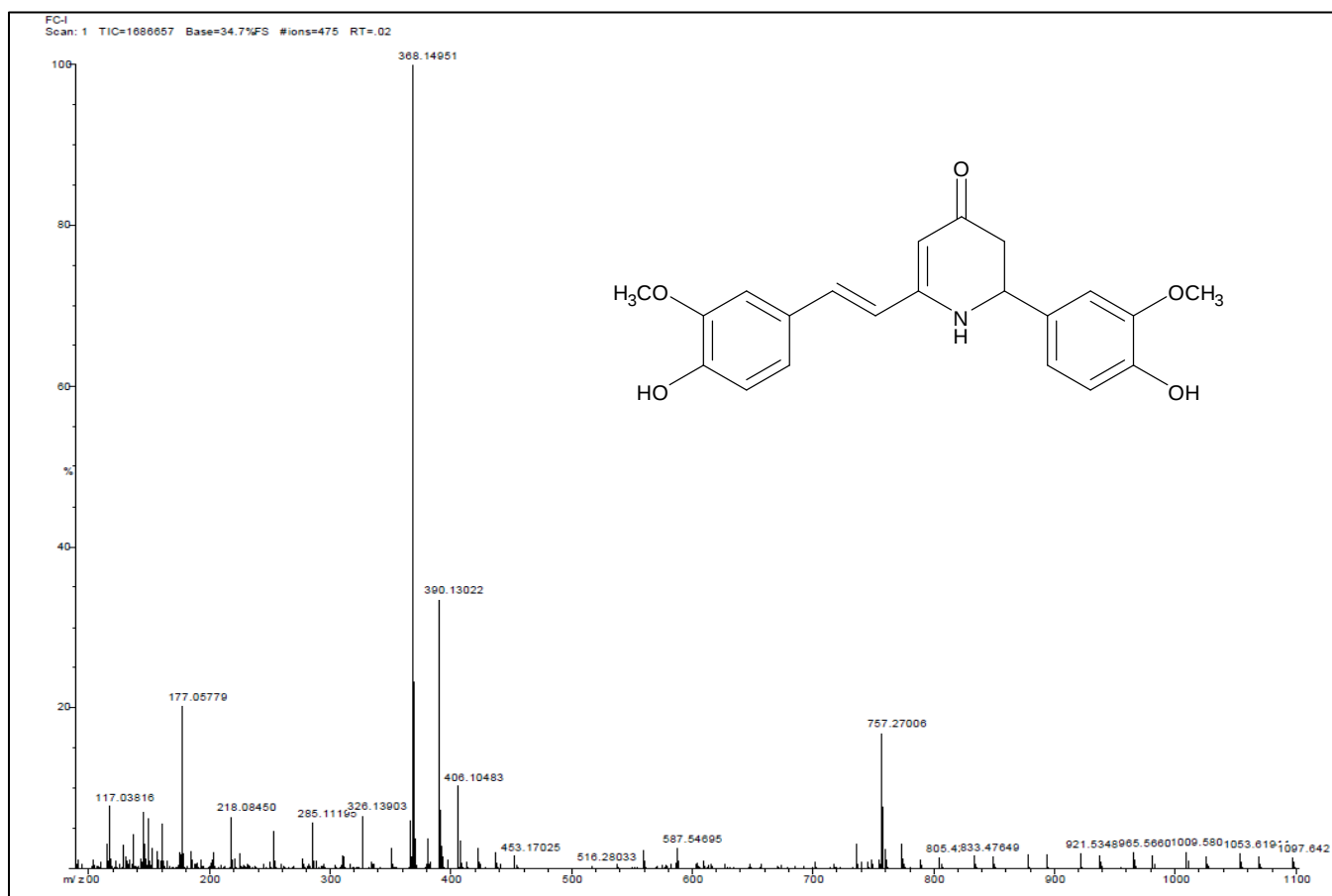


Figure 5S (b): HRESIMS spectrum of compound 1.

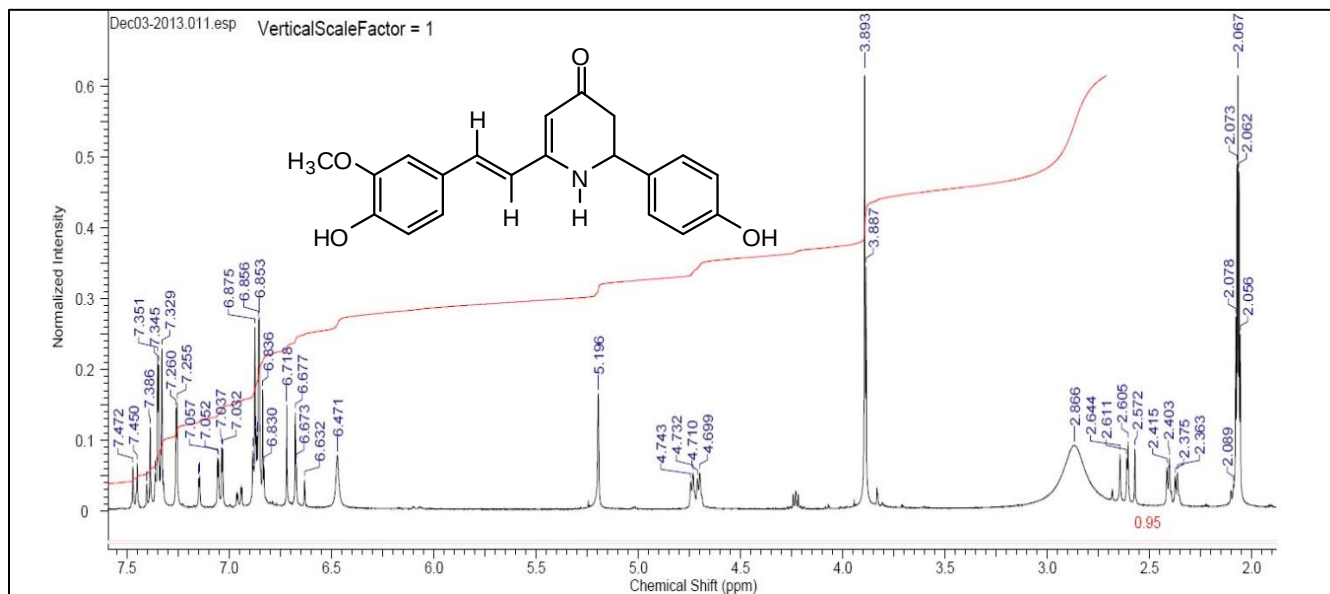


Figure 6S: ^1H -NMR spectrum (400 MHz, Acetone- d_6) of compound 2.

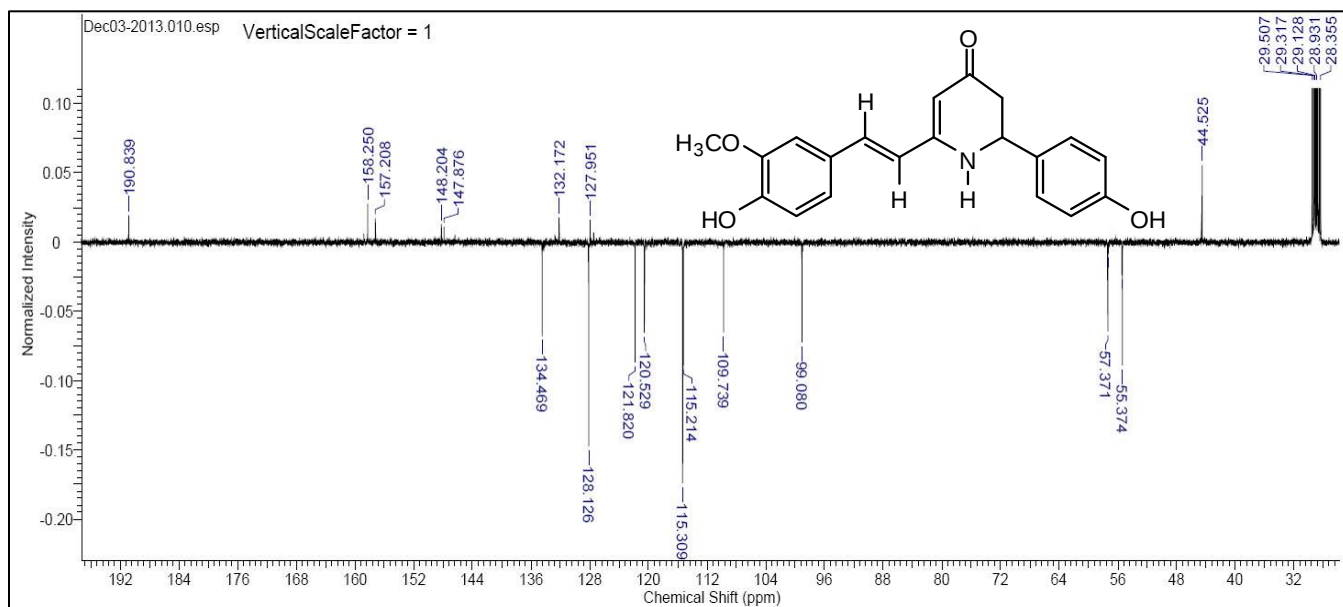


Figure 7S: APT spectrum (100 MHz, Acetone- d_6) of compound 2.

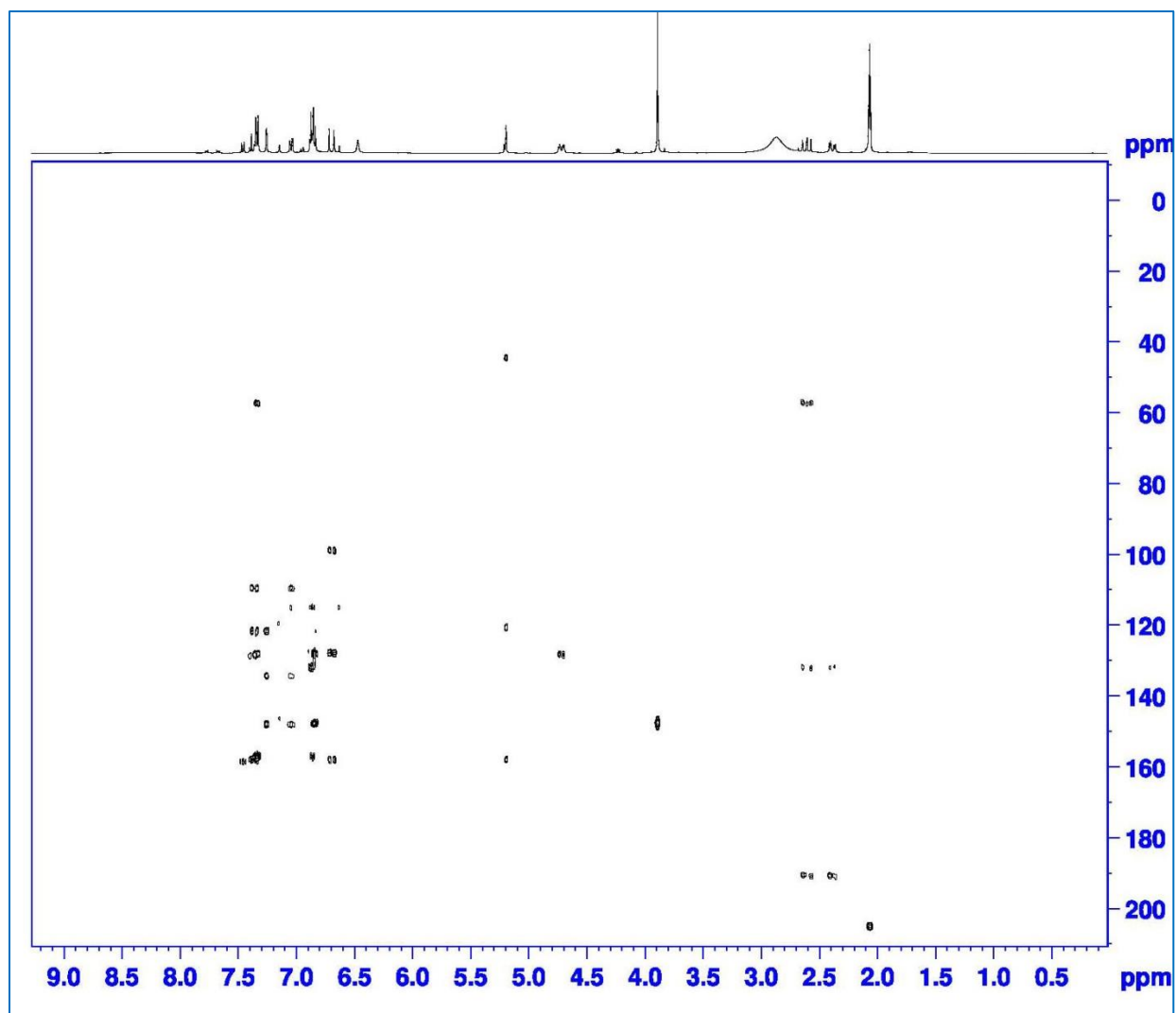
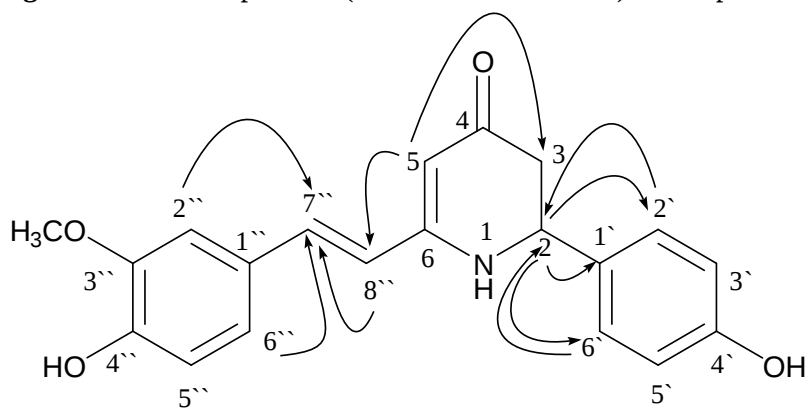


Figure 8S: HMBC spectrum (400 MHz, Acetone-d₆) of compound 2.



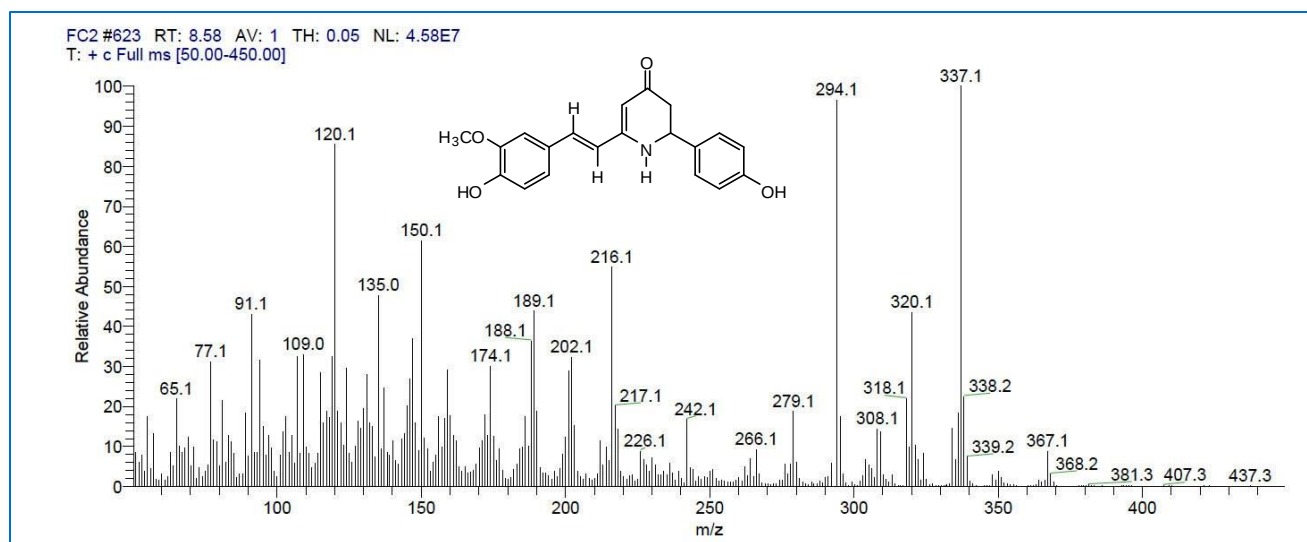


Figure 9S (a): EIMS spectrum of compound 2.

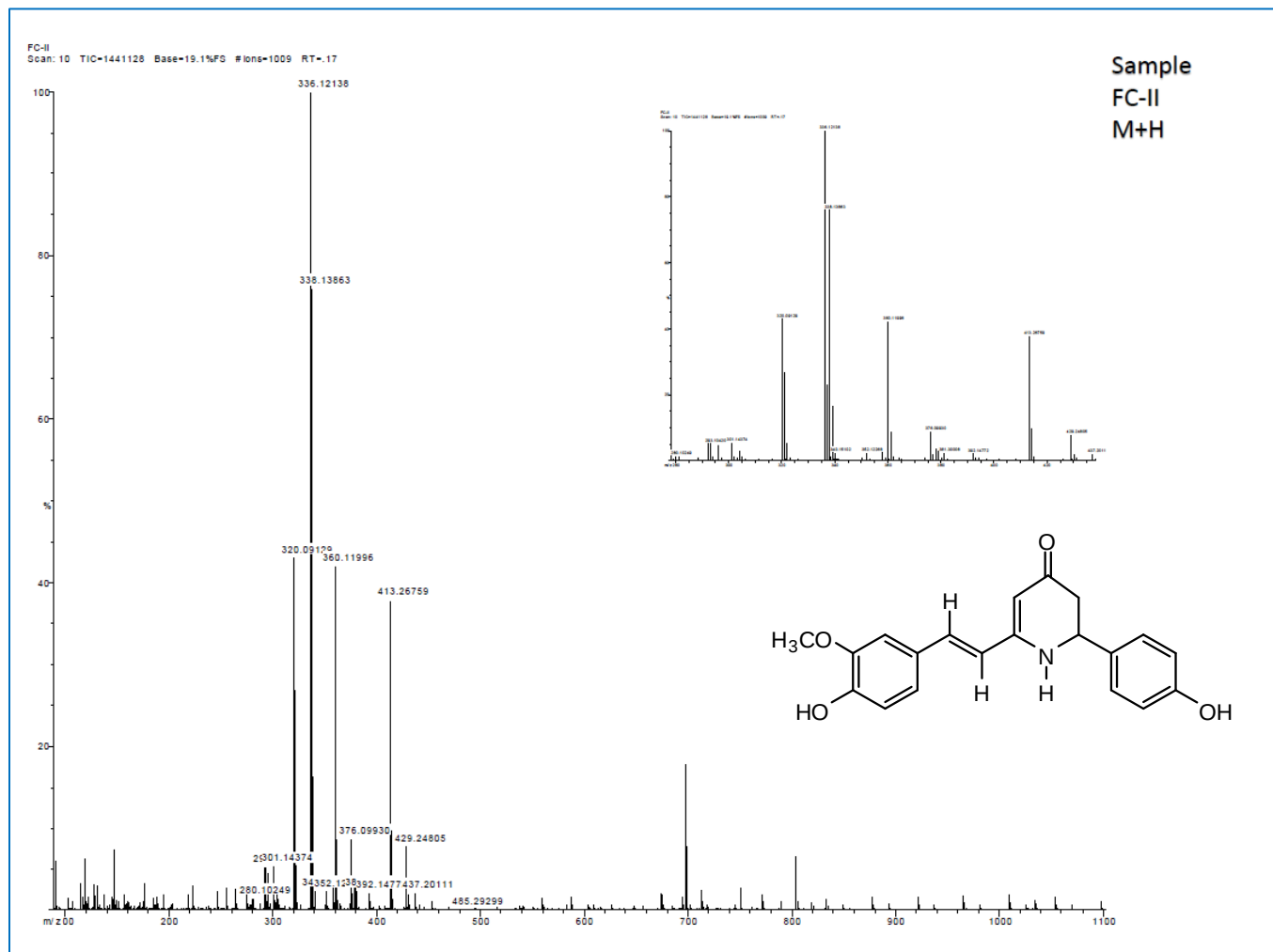


Figure 9S (b): HRESIMS spectrum of compound 2.

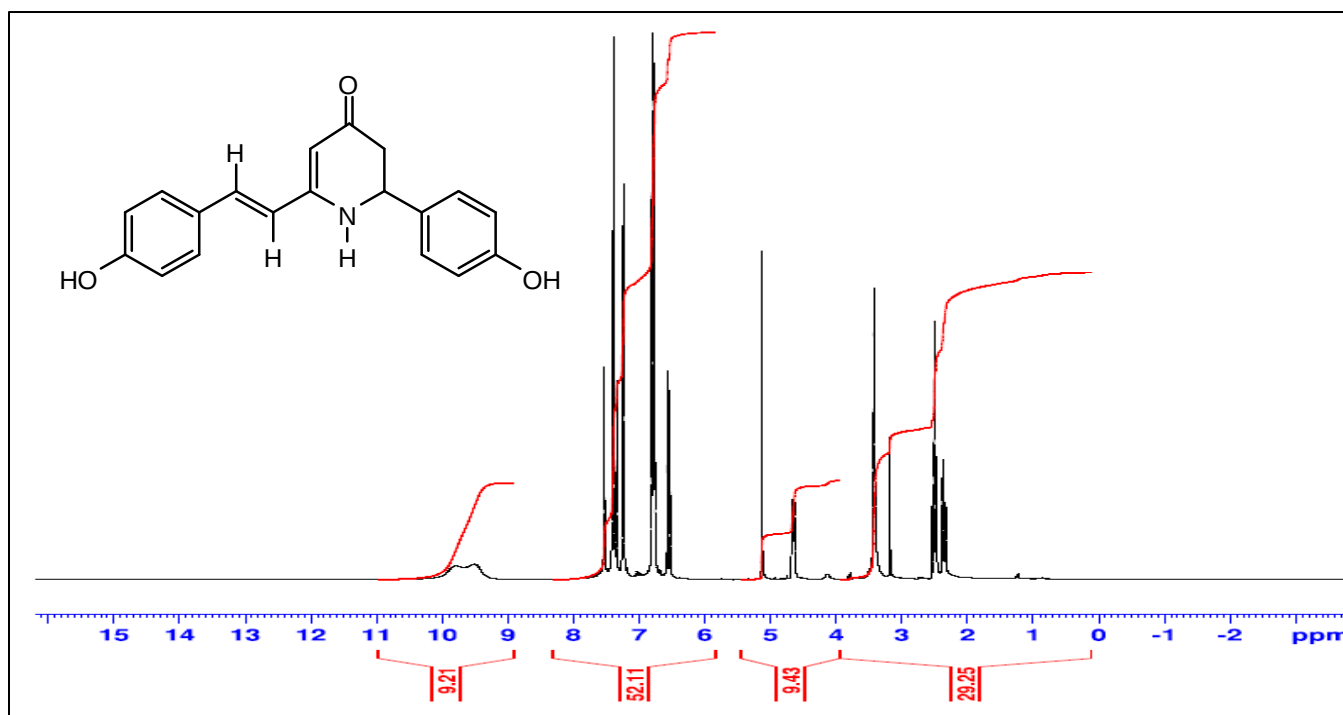


Figure 10S: ¹H-NMR spectrum (400 MHz, DMSO -d₆) of compound 3.

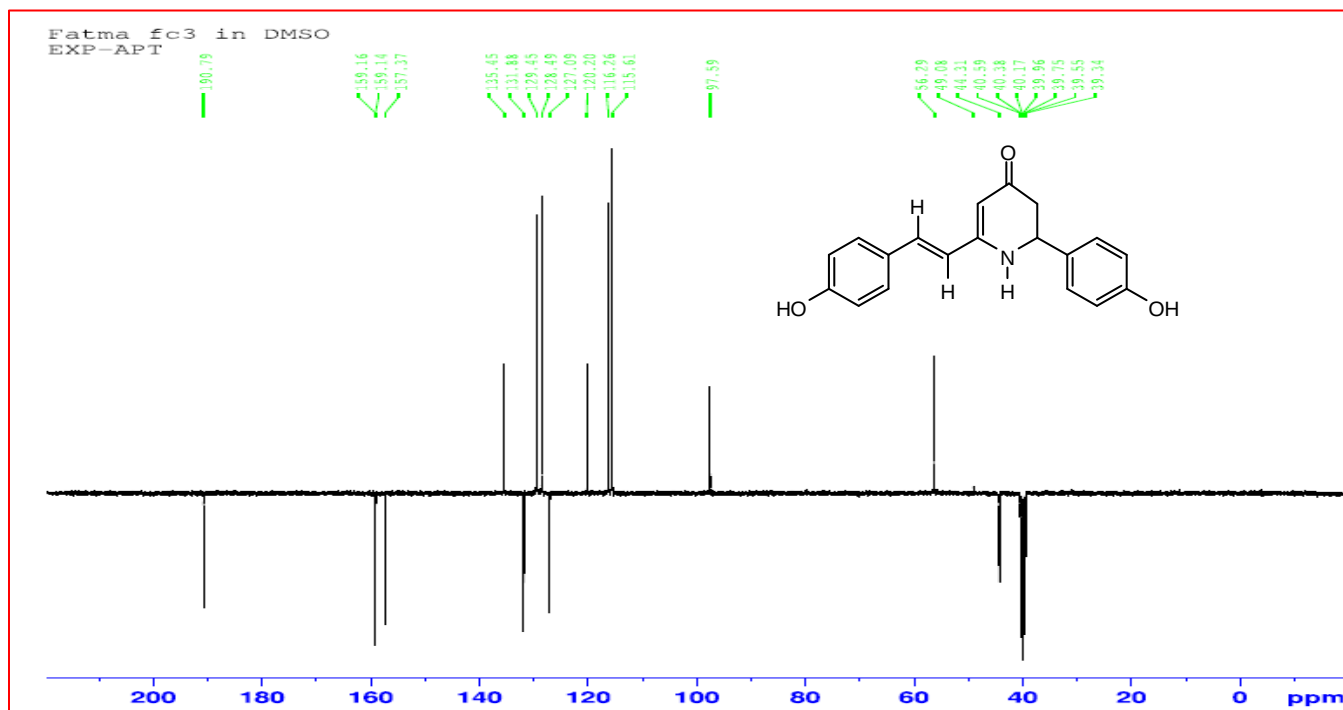


Figure 11S: APT spectrum (100 MHz, DMSO -d₆) of compound 3.

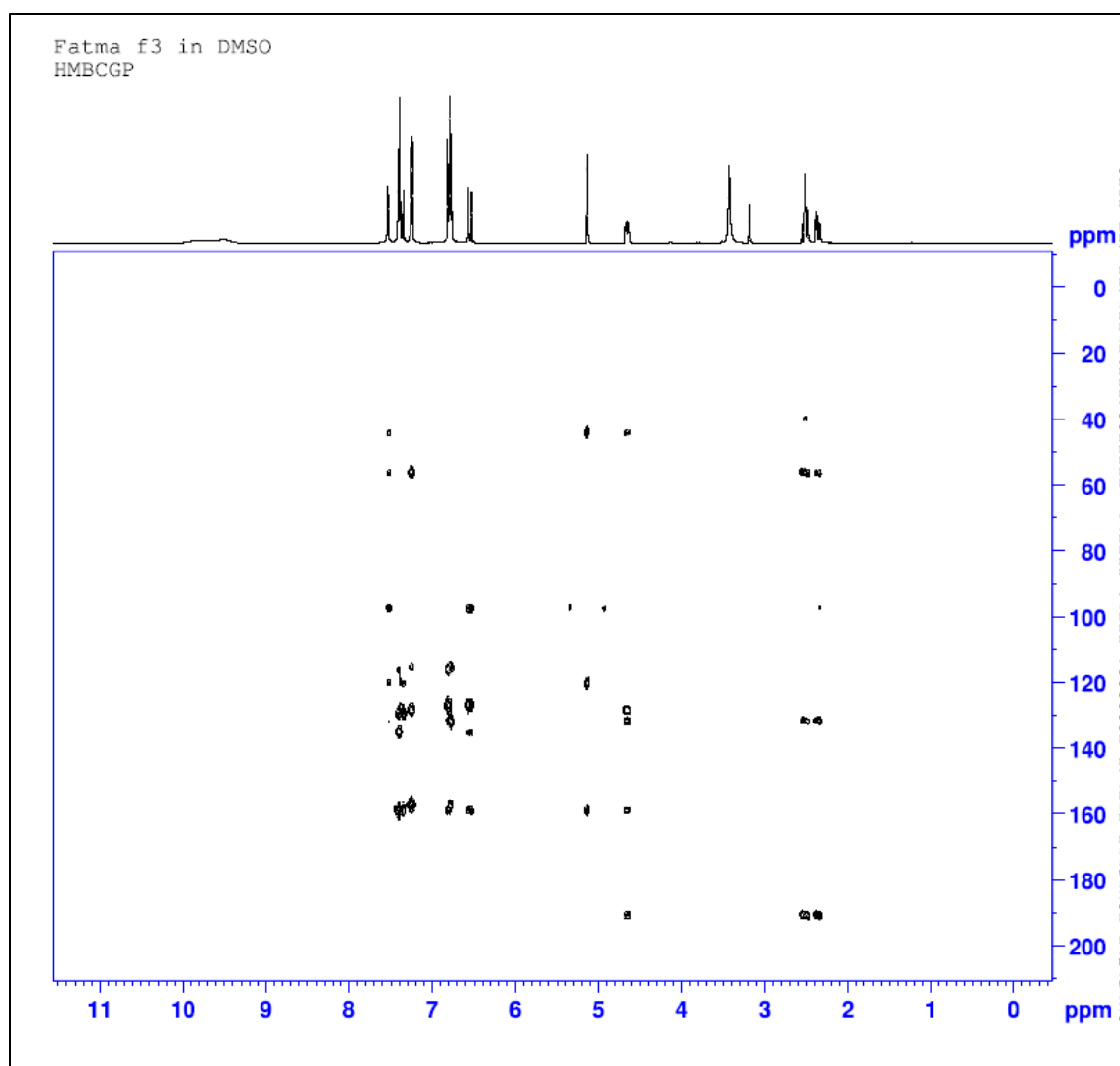
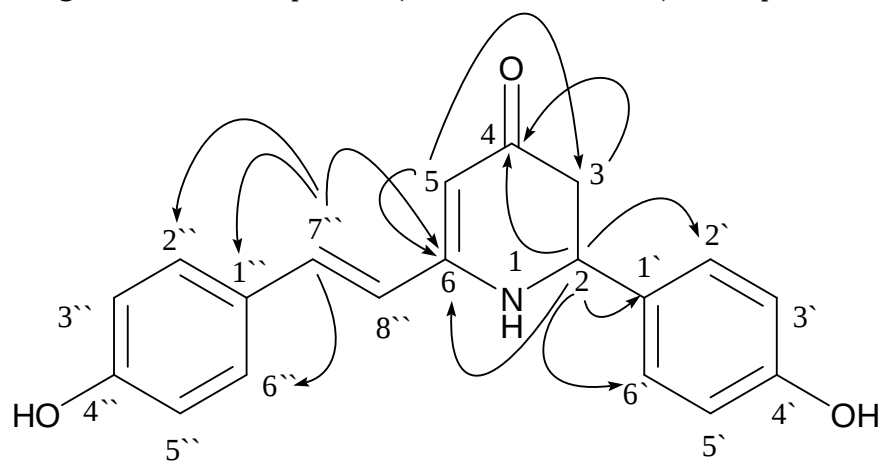


Figure 12S: HMBC spectrum (400 MHz, DMSO -d6) of compound 3.



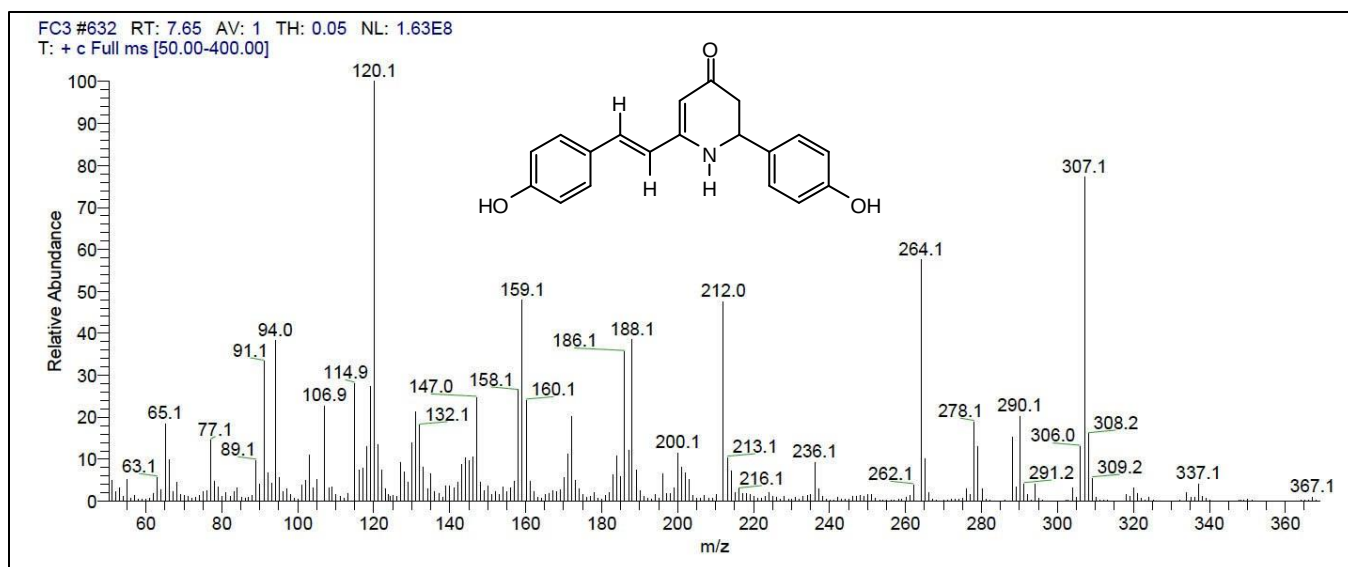


Figure 13S (a): EIMS spectrum of compound 3.

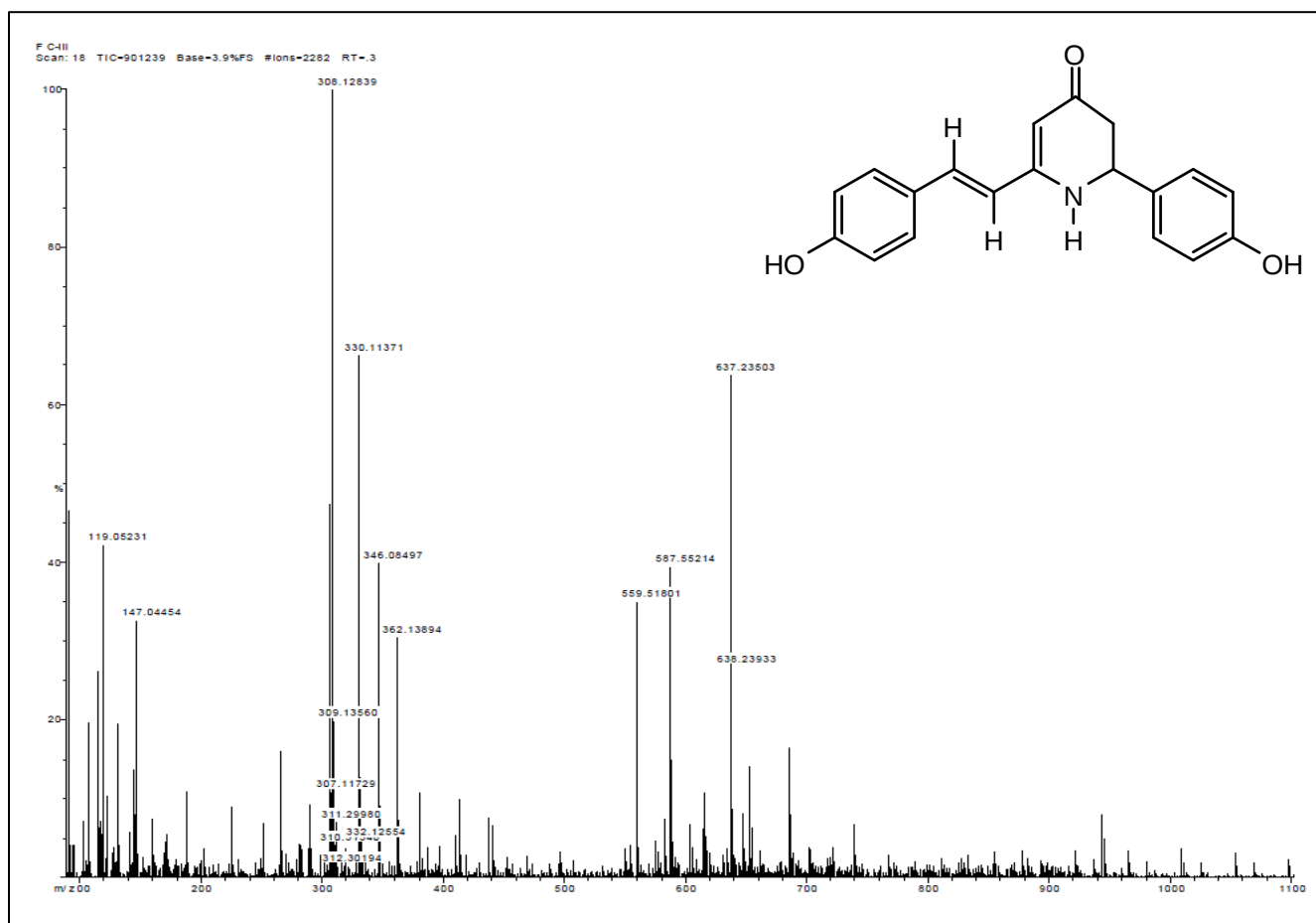


Figure 13S (b): HREIMS spectrum of compound 3.

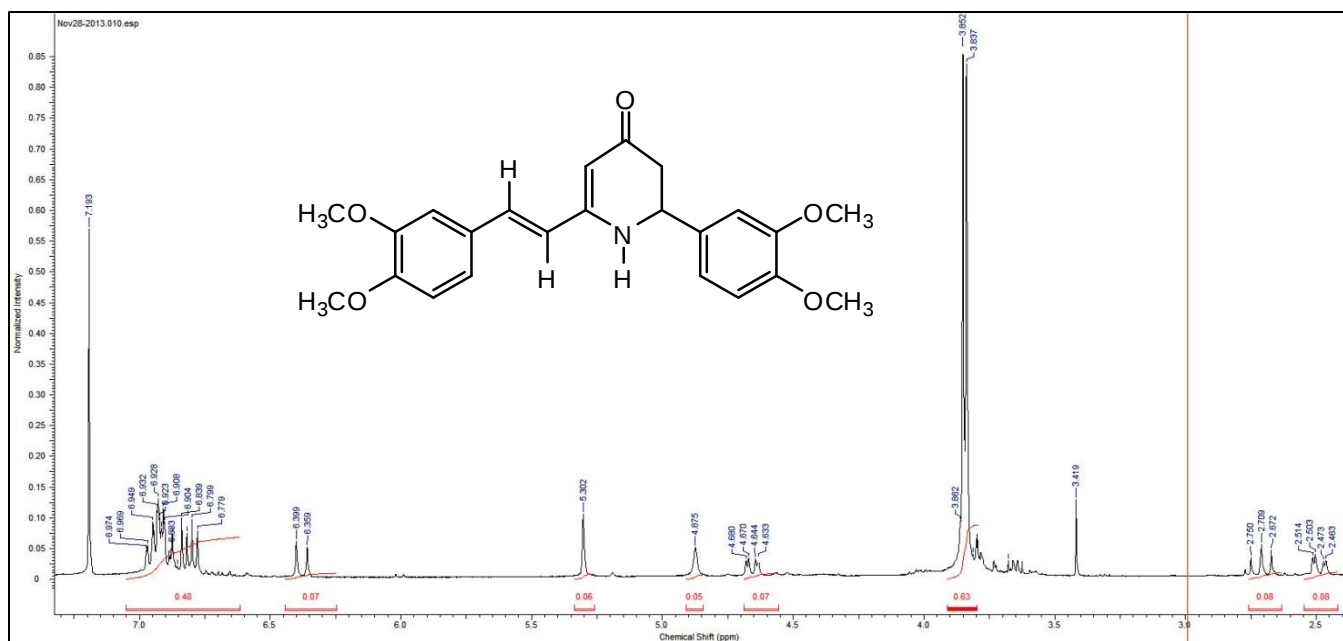


Figure 14S: ^1H -NMR spectrum (400 MHz, CDCl_3) of compound 4.

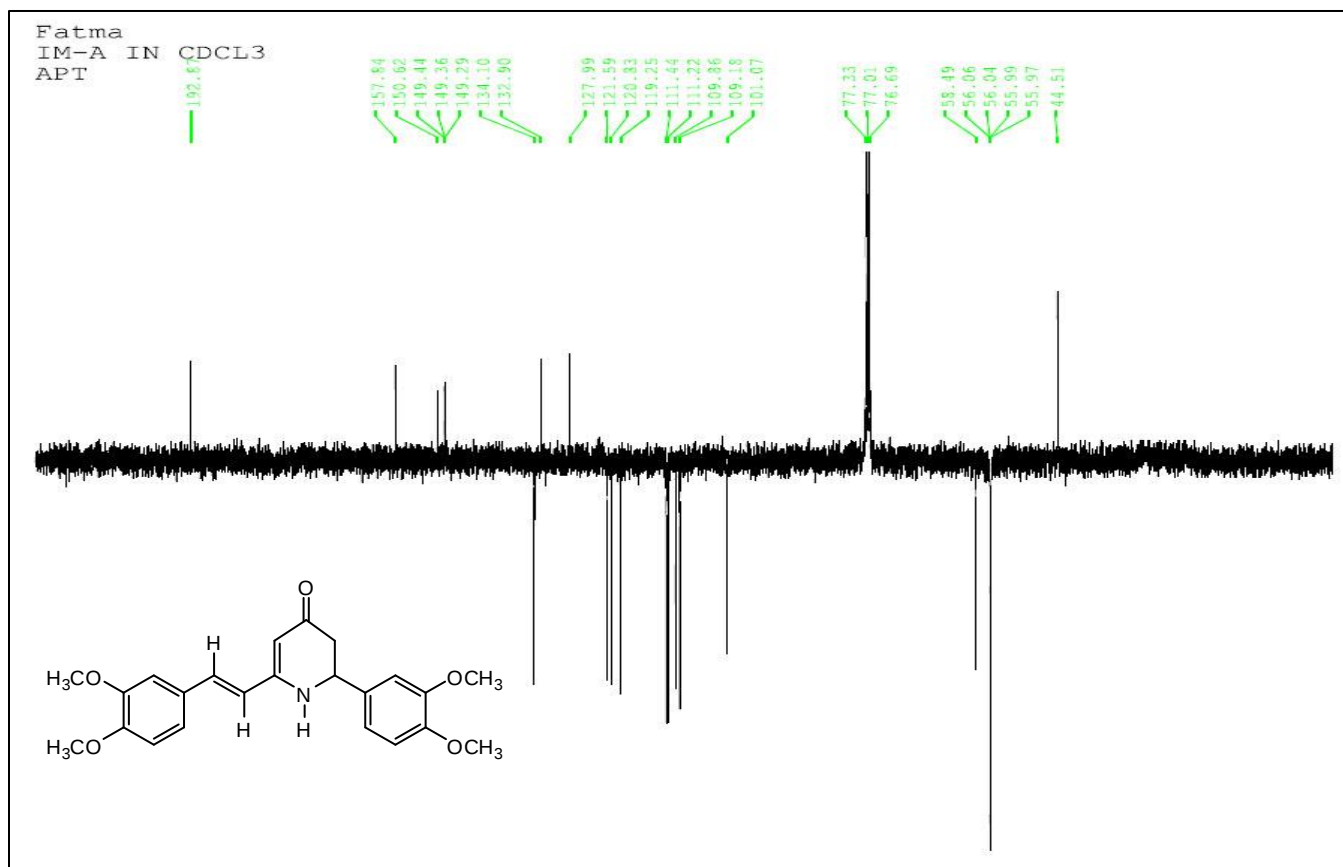


Figure 15S: APT spectrum (100 MHz, CDCl_3) of compound 4.

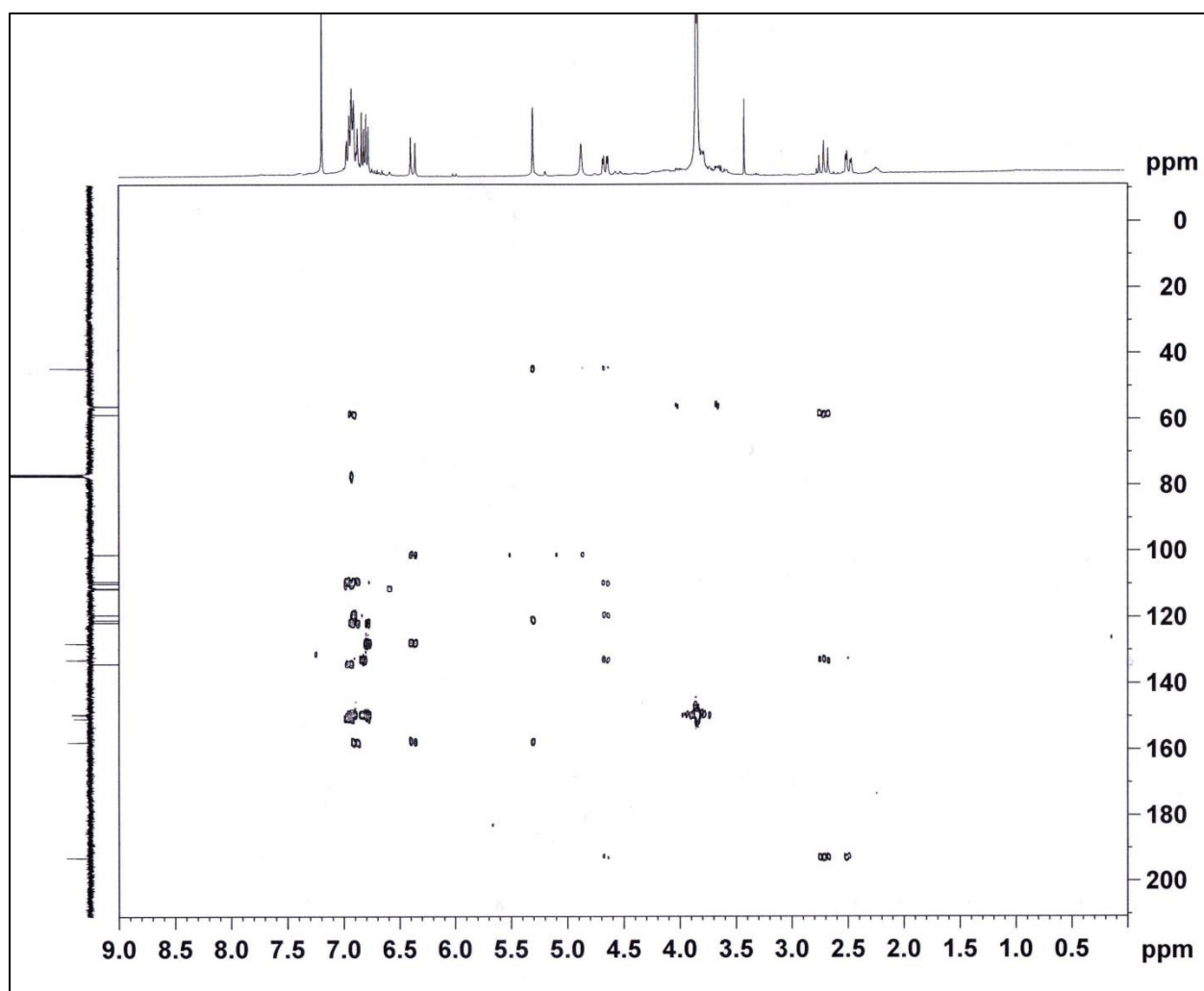
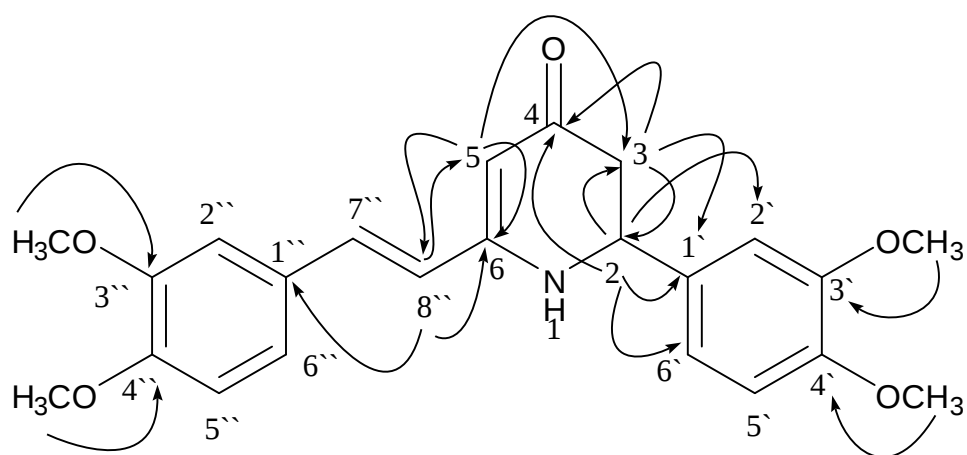


Figure 16S: HMBC spectrum (400 MHz, CDCl_3) of compound **4**.



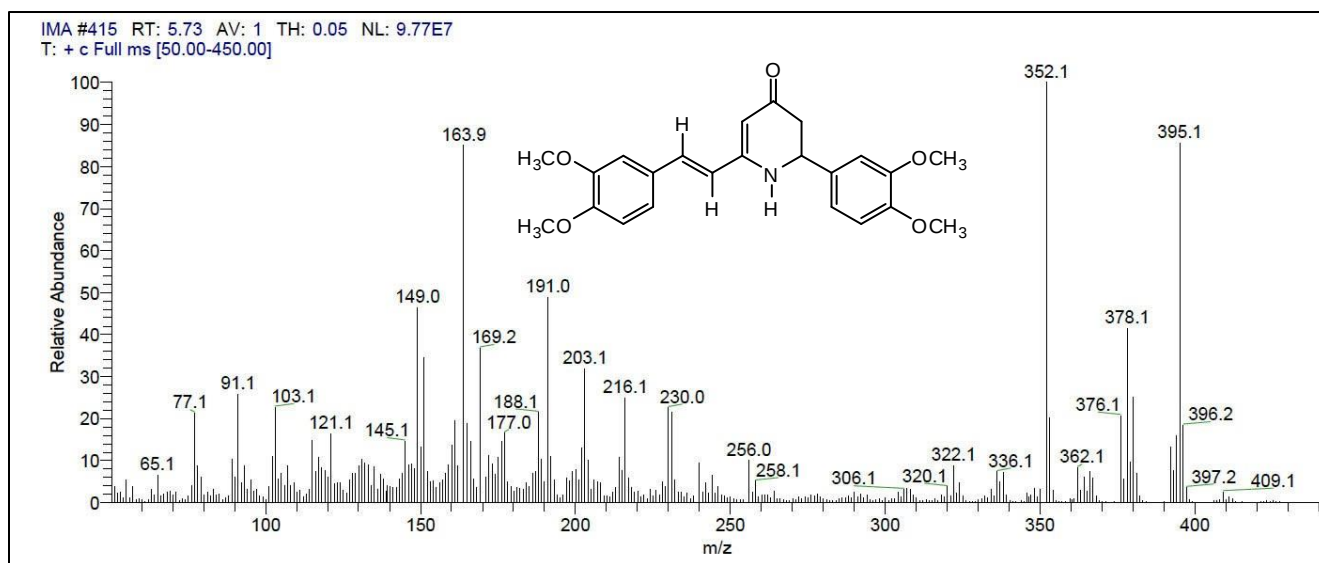


Figure 17S (a): EIMS spectrum of compound 4.

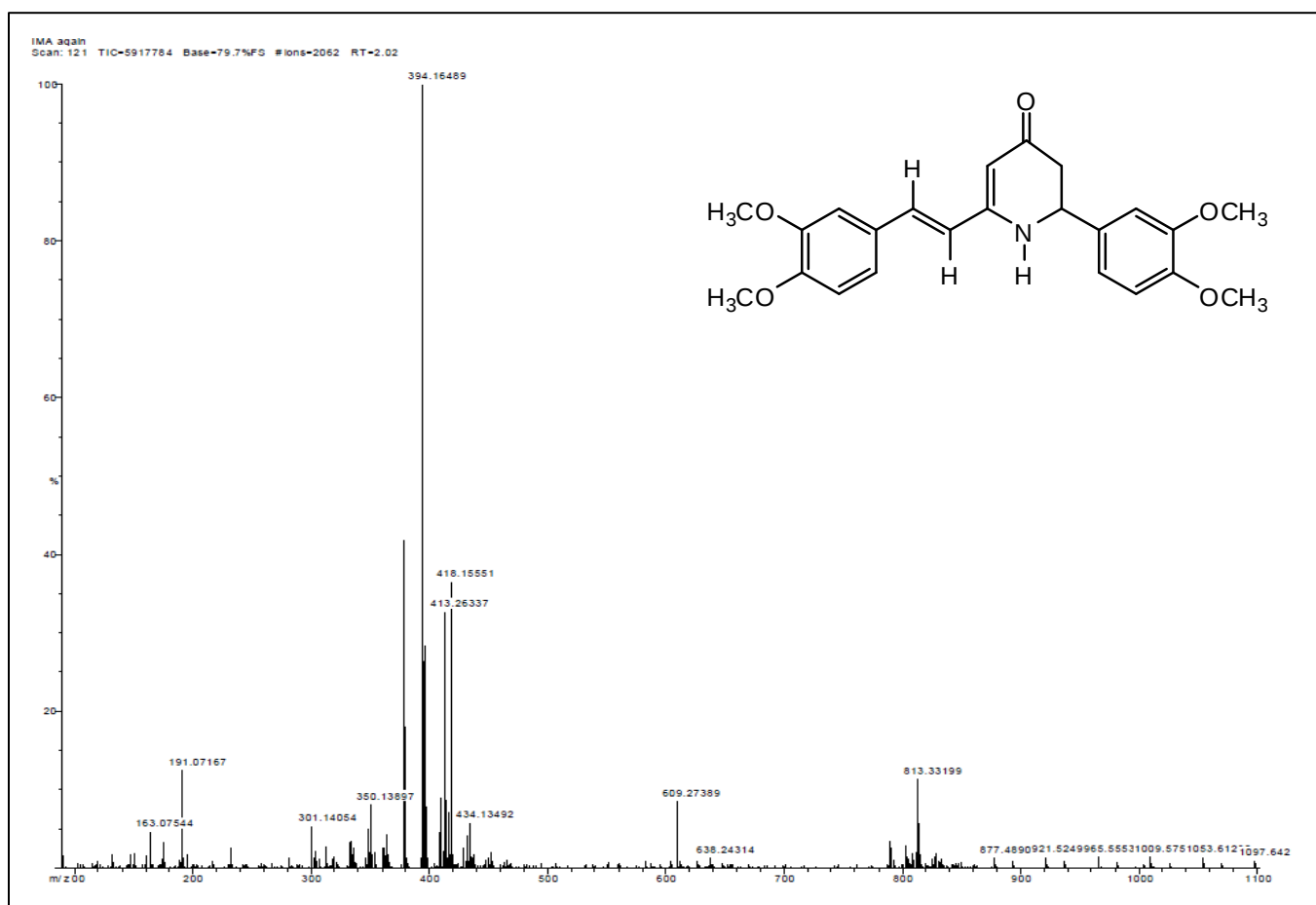


Figure 17S (b): HRESIMS spectrum of compound 4.

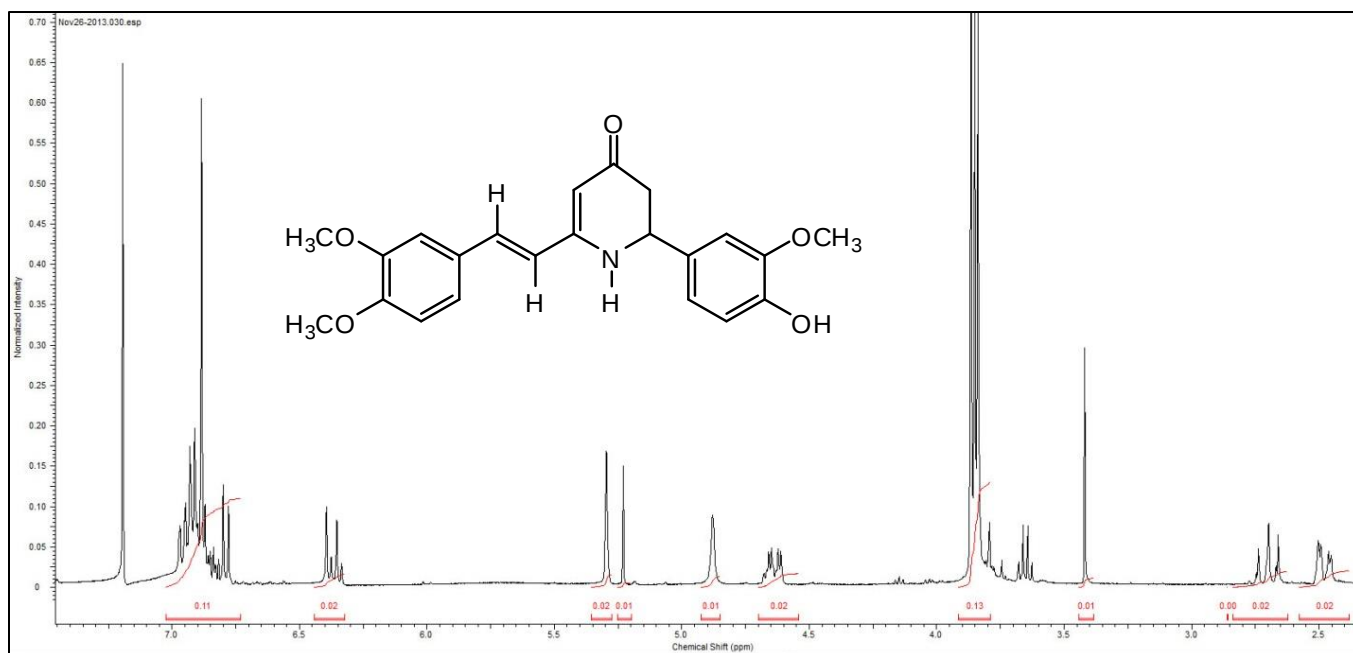


Figure 18S: ¹H-NMR spectrum (400 MHz, CDCl₃) of compound 5.

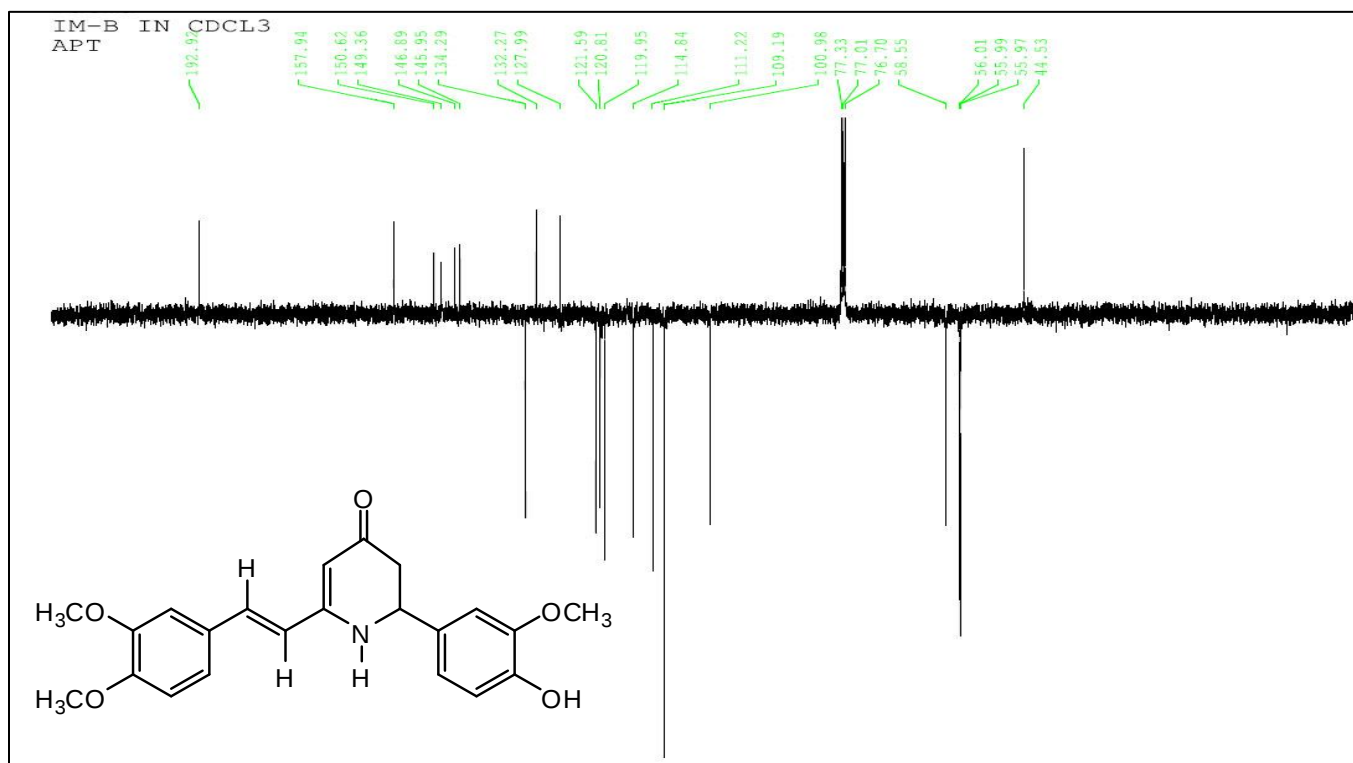


Figure 19S: APT spectrum (100 MHz, CDCl₃) of compound 5.

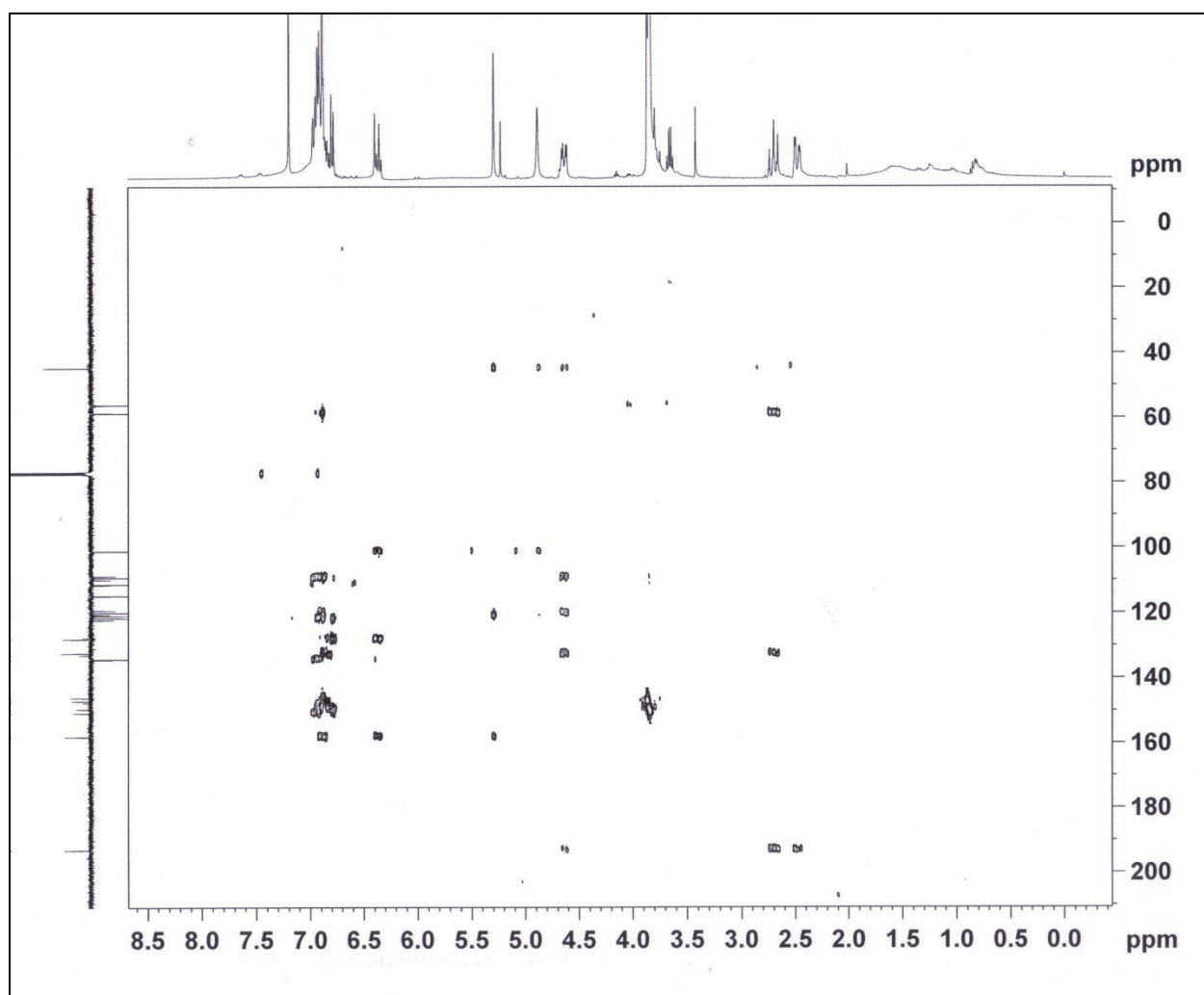
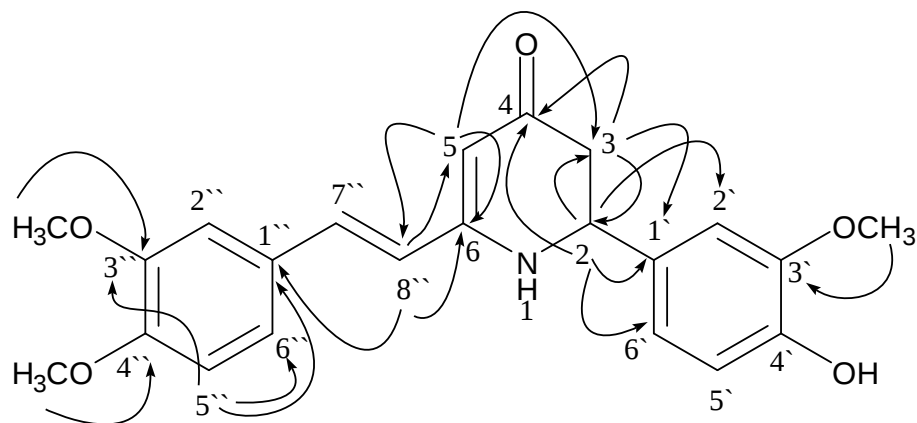


Figure 20S: HMBC spectrum (400 MHz, CDCl_3) of compound 5.



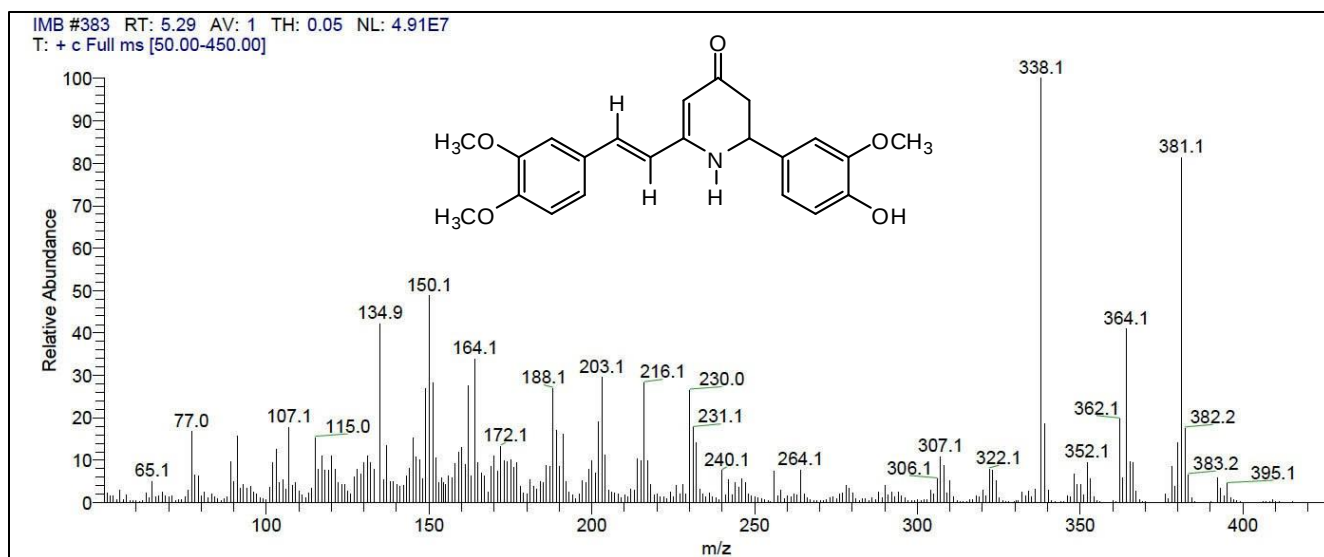
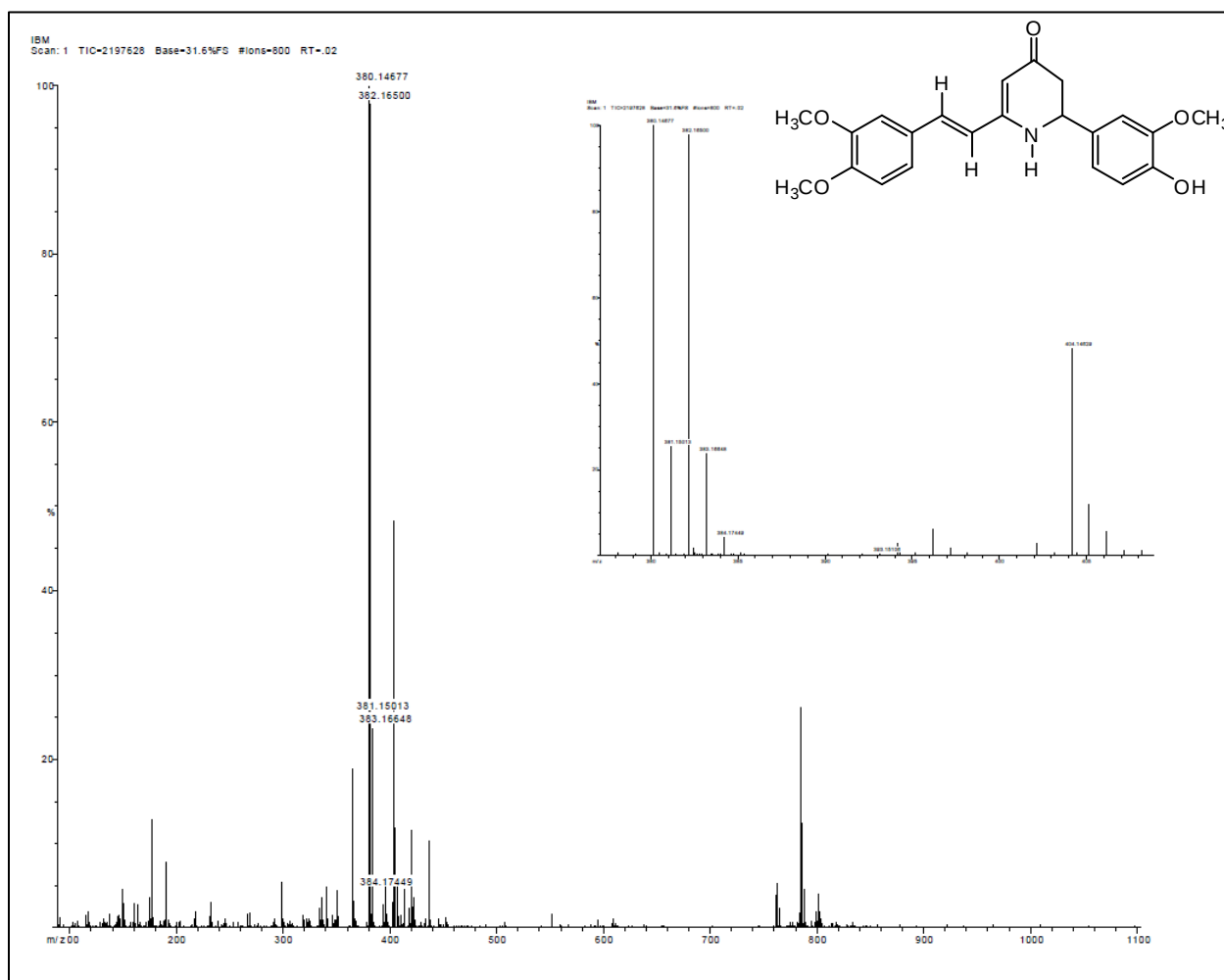


Figure 21S (a): EIMS spectrum of compound 5.



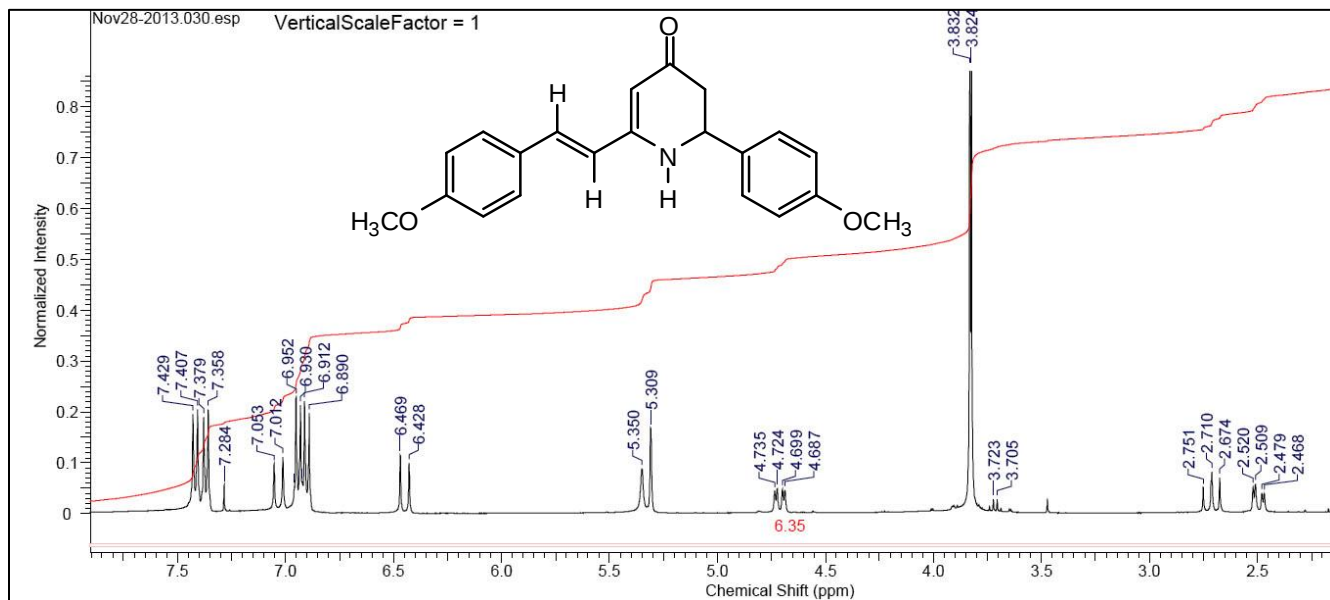


Figure 22S: ^1H -NMR spectrum (400 MHz, CDCl_3) of compound **6**.

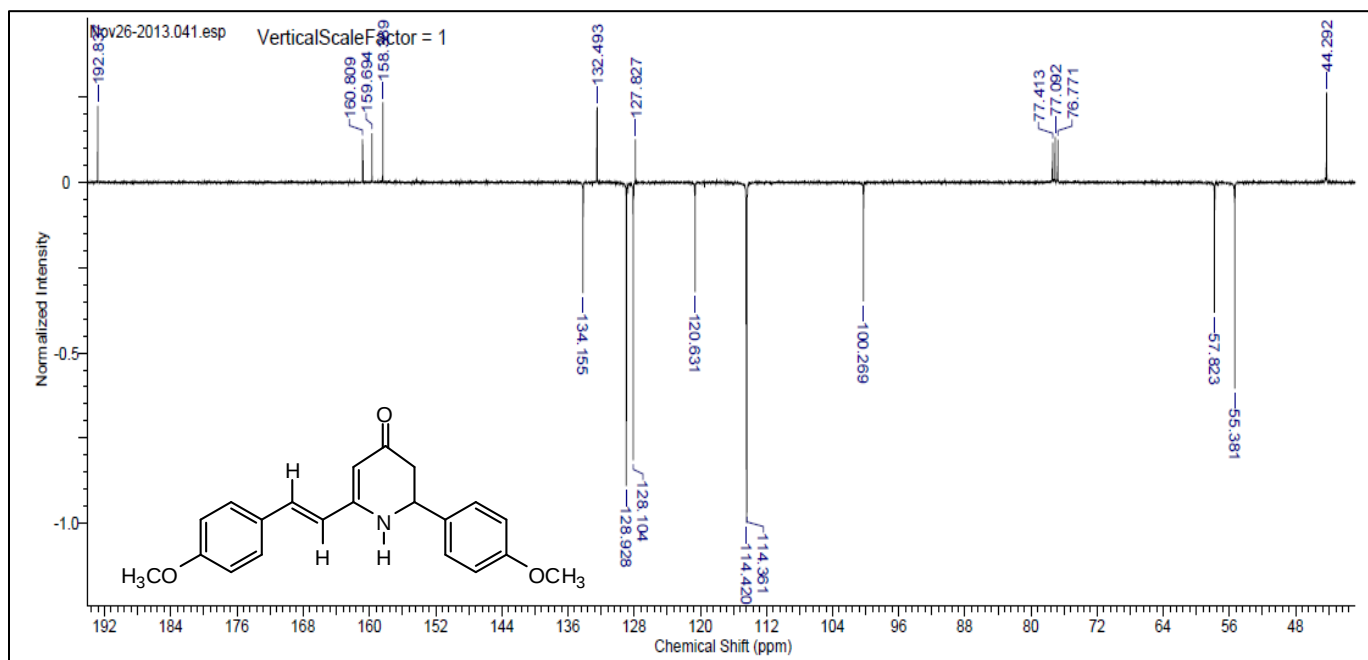


Figure 23S: APT spectrum (100 MHz, CDCl_3) of compound **6**.

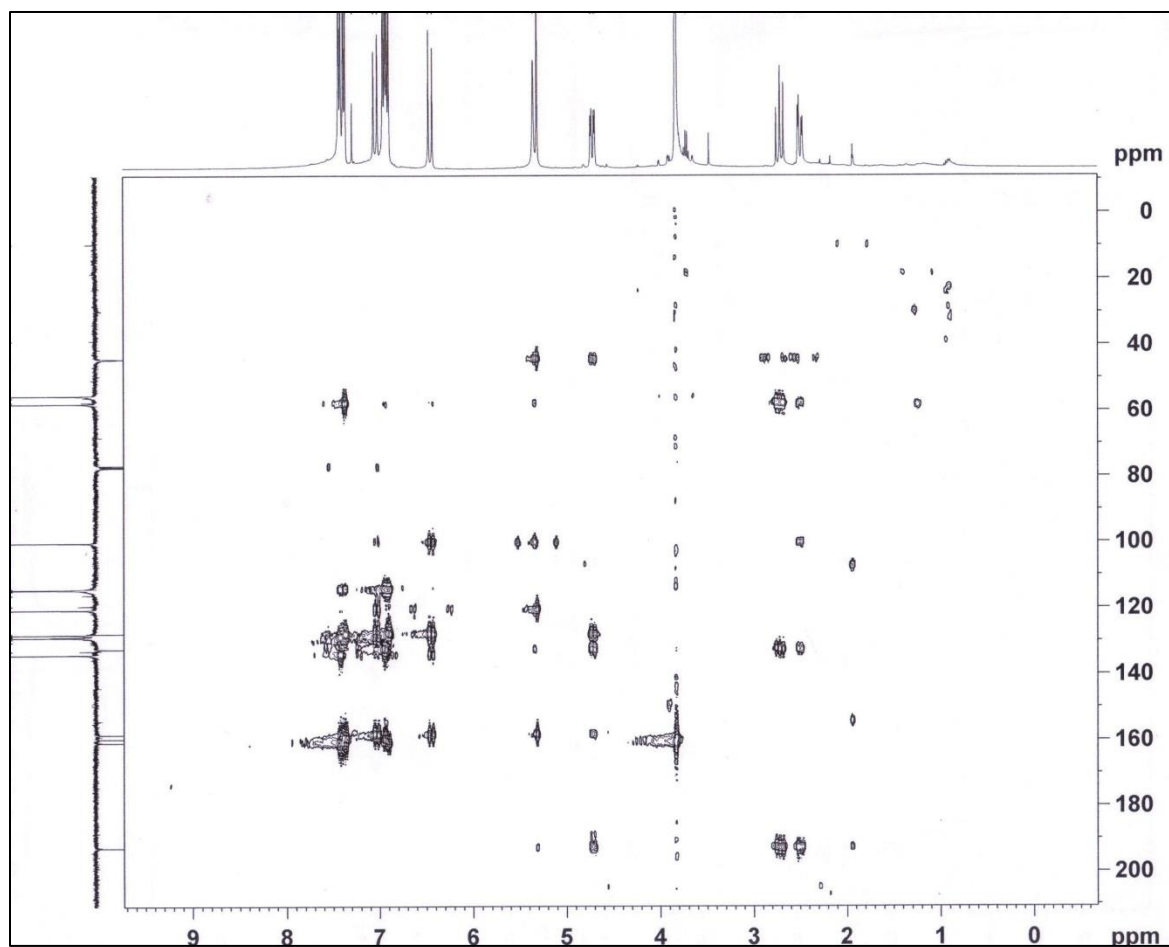
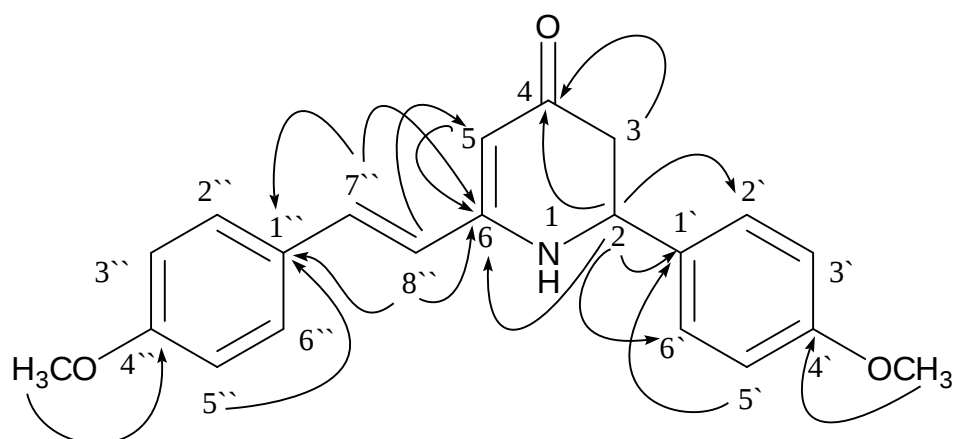


Figure 24S: HMBC spectrum (400 MHz, CDCl_3) of compound **6**.



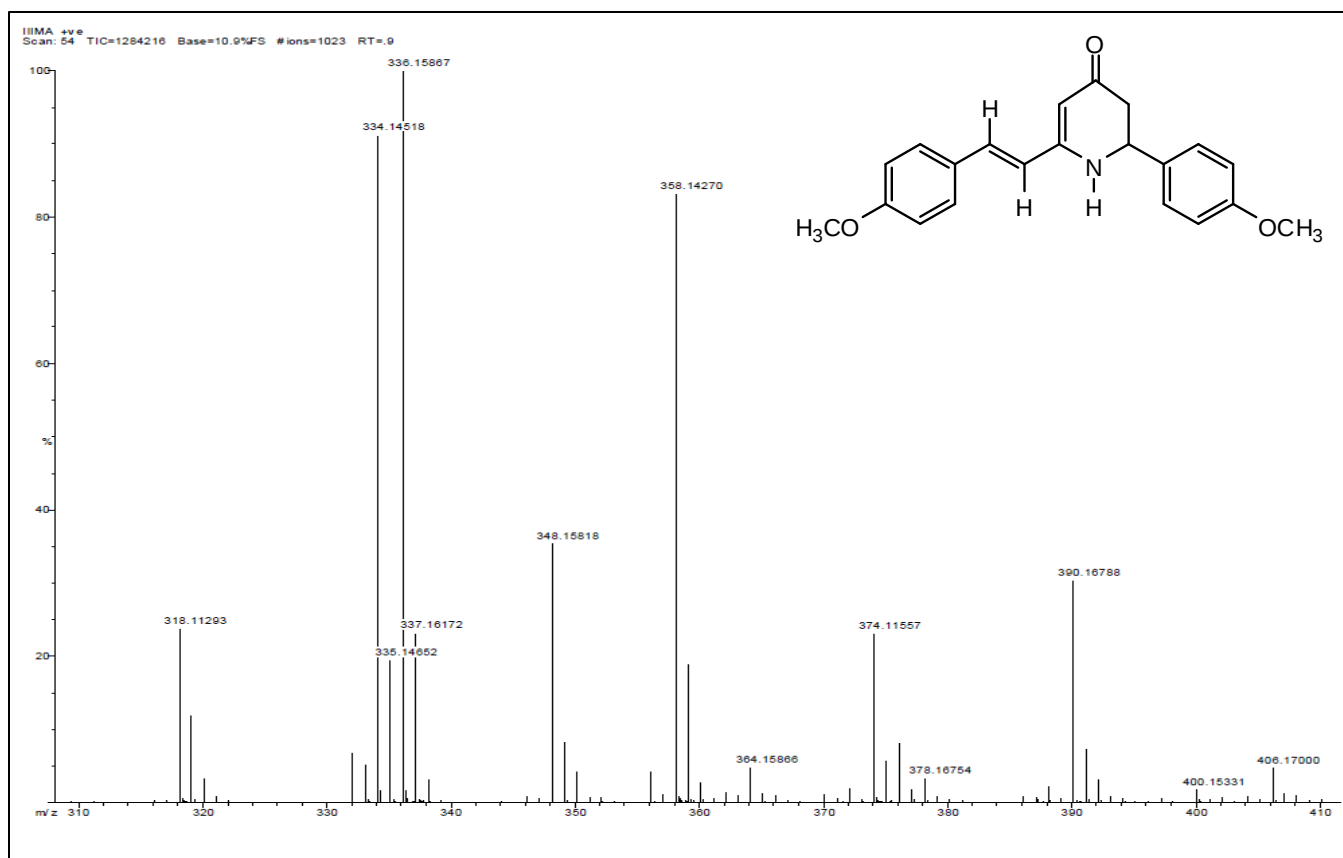


Figure 25S: HRESIM spectrum of compound 6.

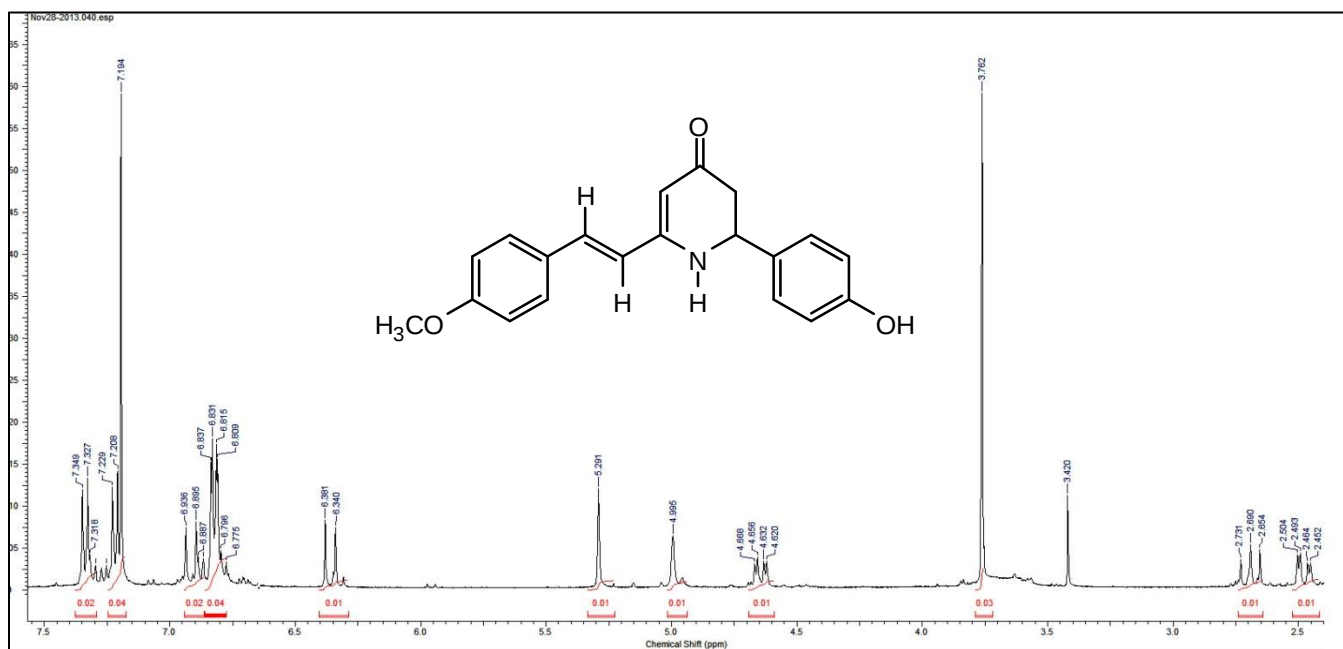


Figure 26S: ¹H-NMR spectrum (400 MHz, CDCl₃) of compound 7.

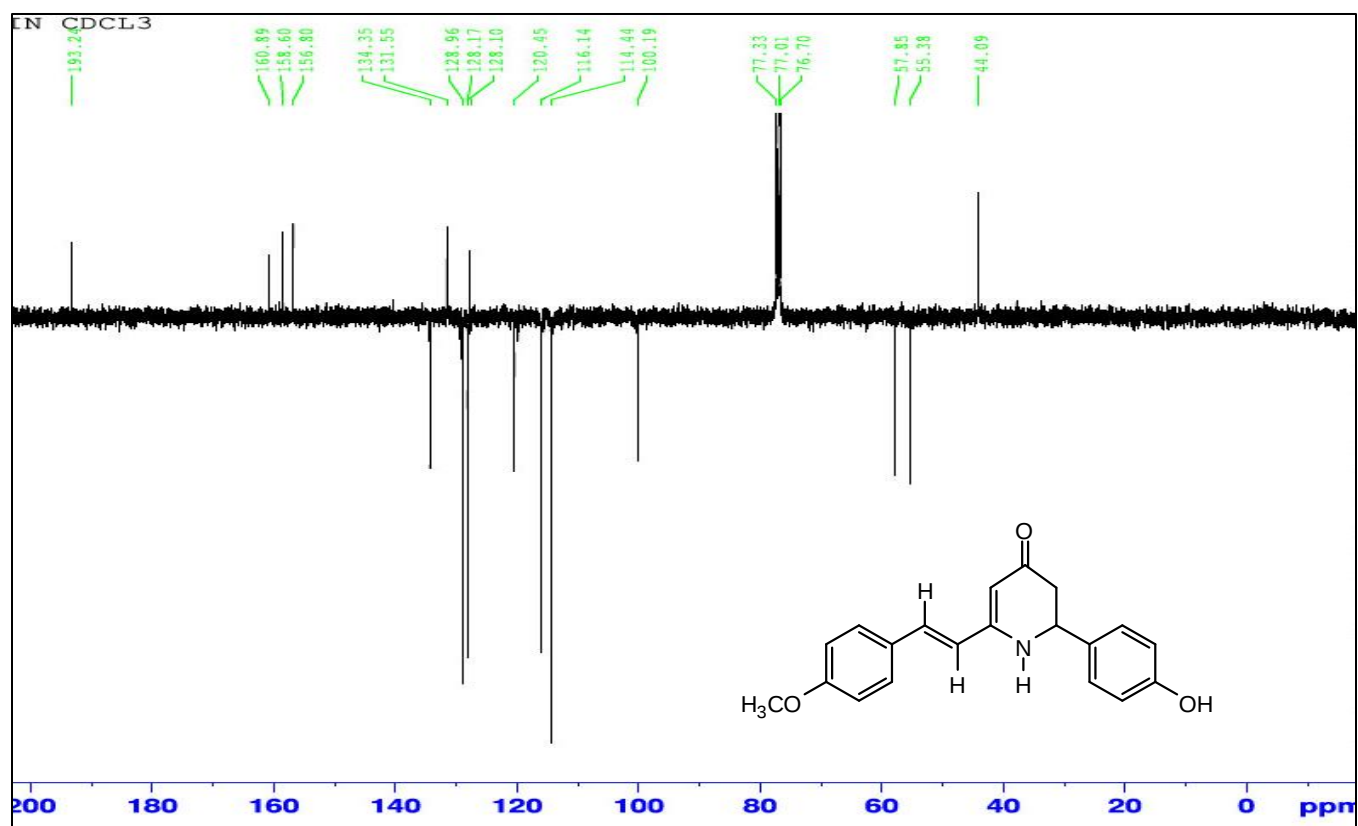


Figure 27S: APT spectrum (100 MHz, CDCl₃) of compound 7.

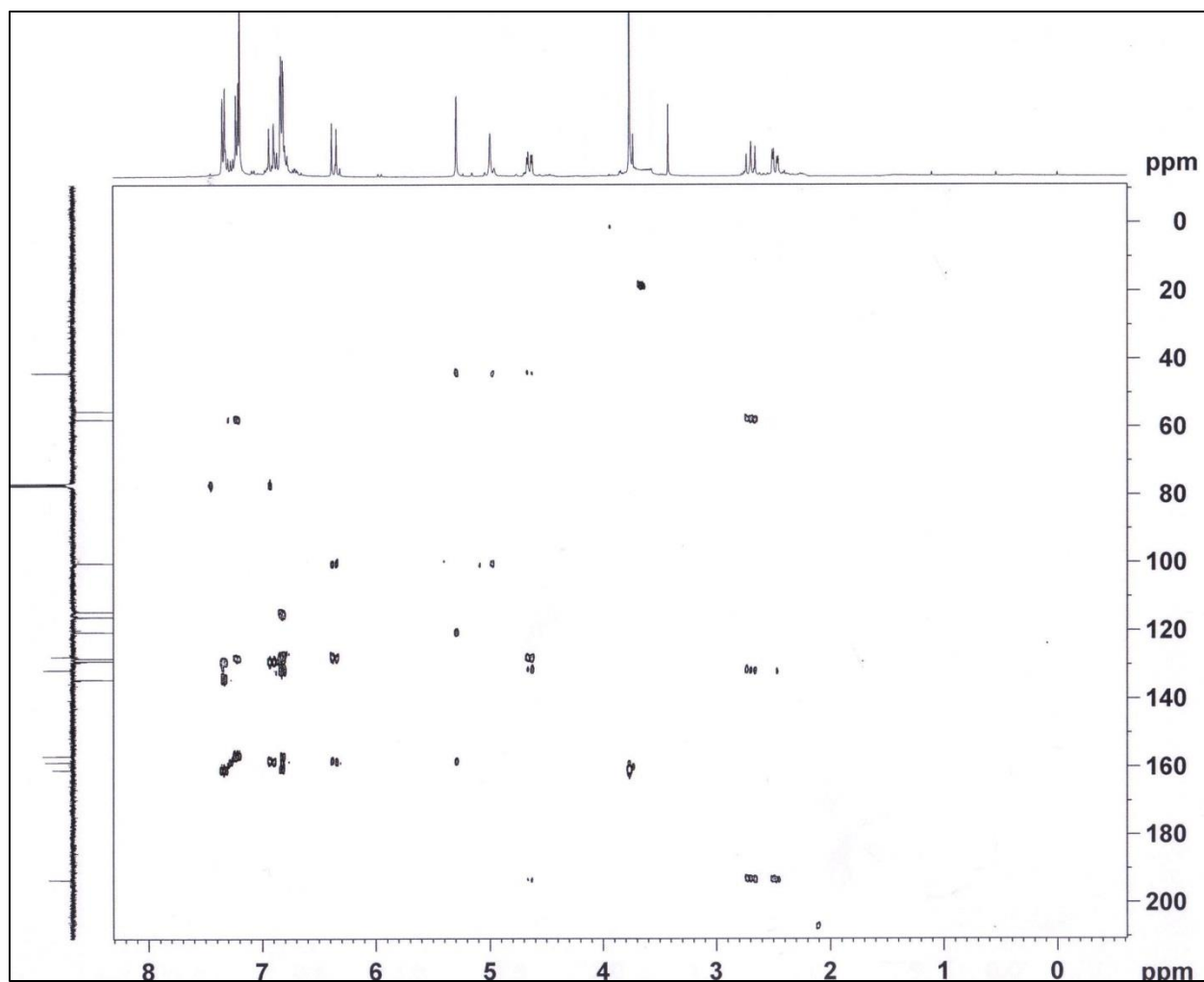
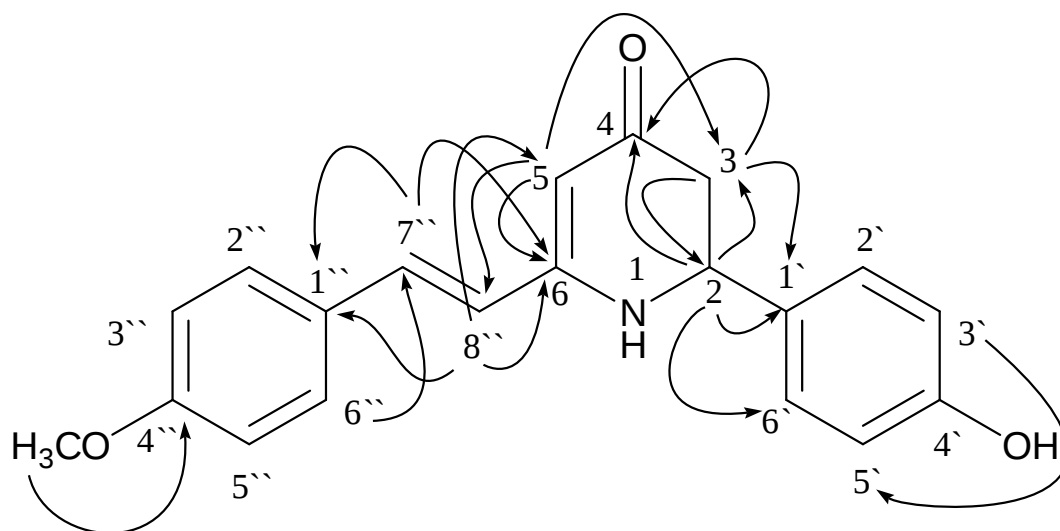


Figure 28S: HMBC spectrum (400 MHz, CDCl_3) of compound 7.



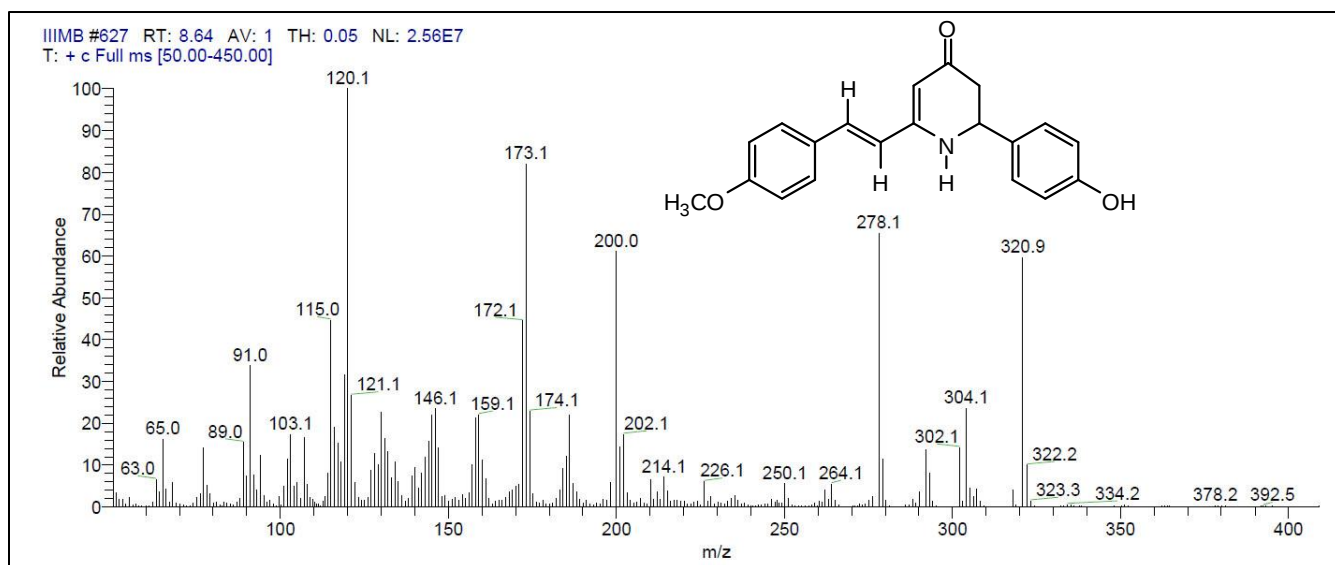


Figure 29S (a): EIMS spectrum of compound 7.

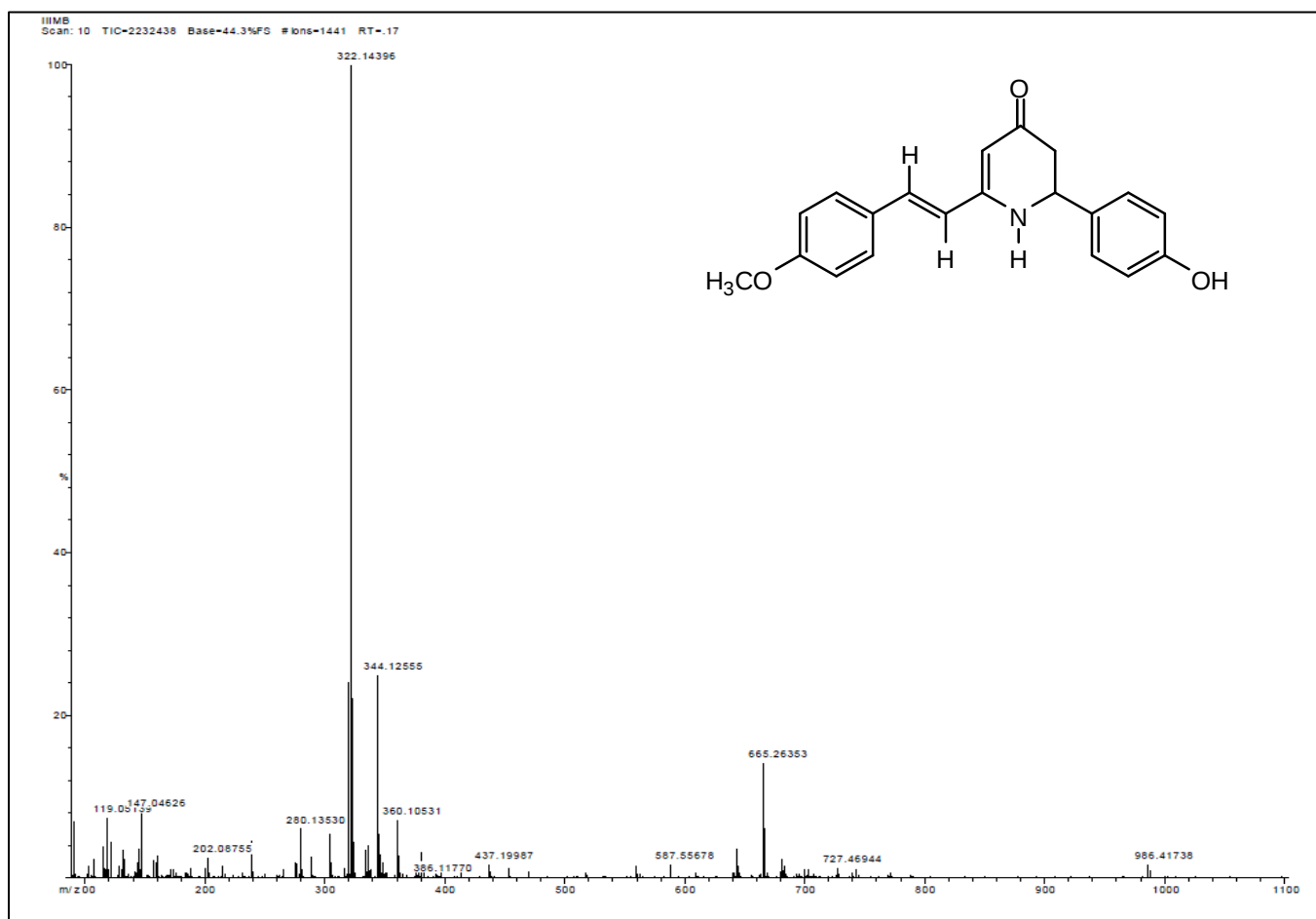


Figure 29S (b): HRESIMS spectrum of compound 7.

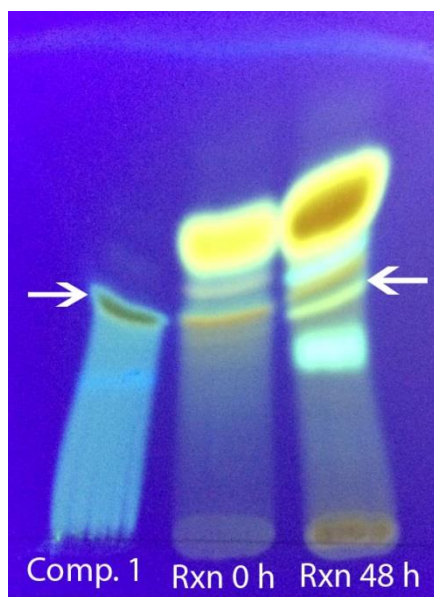


Figure 30S: Thin layer chromatogram [CDCl_3 - MeOH, 9: 1] showing production of compound **1** from curcumin I after 48 h treatment with NH_4OH -MeOH (1:4 v/v), visualized under UV light λ_{254} .

Physicochemical properties of compounds 1, 3, 4 and 6

Compound 1: Yellow amorphous powder, m.p. 200-204 °C, IR_{v_{max}} (KBr): 3348, 3002, 2924, 2840, 2812, 1636, 1603, 1558, 1512, 1467, 1428, 1288, 1161, 1030, 962 and 805 cm⁻¹, HRESIMS at m/z 368.14951 (M+H)⁺, {Calcd. for C₂₁H₂₁NO₅ 368.14980}, 390.13022 (M+Na)⁺, {Calcd. 390.13174} and 757.27006 (2M+Na)⁺, {Calcd. 757.27372}. EIMS fragmentation pattern is outlined in figure 3.

Compound 3: Yellow plates, m.p. 210-215 °C, IR_{v_{max}} (KBr) 3273, 3084, 3017, 2948, 1636, 1602, 1560, 1485, 1438, 1405, 1319, 1276, 1227, 1193, 1168, 1105, 1037, 967 and 918 cm⁻¹ and HRESIMS at m/z 308.12839 (M+H)⁺, {Calcd. for C₁₉H₁₇NO₃ 308.12867}, 330.11371(M+Na)⁺, {Calcd. 330.11061} and 637.23503 (2M+Na)⁺, {Calcd. 637.23146}.

Compound 4: Yellow amorphous powder, m.p. 137-142 °C, IR_{v_{max}} (KBr) 3444, 2959, 2923, 2853, 1649, 1617, 1595, 1575, 1559, 1514, 1458, 1422, 1399, 1265, 1142, 1098, 1028 and 905 cm⁻¹ and HRESIMS at m/z 394.16489 (M-H)⁻, {Calcd for C₂₃H₂₅NO₅. 394.16545}, 418.15551 (M+Na)⁺, {Calcd. 418.16304} and 813.33199 (2M+Na)⁺, {Calcd. 813.33632}.

Compound 6: Yellow amorphous powder, m.p. 165-170 °C, IR_{v_{max}} (KBr) 3259, 3075, 2959, 2929, 2837, 1644, 1595, 1565, 1507, 1405, 1279, 1253, 1175, 1121, 1028, 971, 919 and 827 cm⁻¹. HRESIMS at m/z 336.15867 (M+H)⁺, {Calcd. for C₂₁H₂₁NO₃ 336.15997}, 334.14518 (M-H)⁻ {Calcd. 334.14432} and 358.14270 (M+Na)⁺, {Calcd. 358.14191}.

Table S1: ^1H -NMR of compounds **1**, **3**, **4** and **6** (at 400 MHz, ^a in DMSO-d₆, ^b in CDCl₃, * Overlapped signal, δ in ppm, J in Hz).

Position (H)	1^a	3^a	4^b	6^b
2	4.63, 1H, dd (12.4, 5.2)	4.64, 1H, dd (11.6, 5.3)	4.63, 1H, dd (16.0, 4.0)	4.69, 1H, dd (14.4, 4.4)
3 _{eq.}	2.32, 1H, dd (16.4, 5.2)	2.33, 1H, dd (15.9, 5.2)	2.46, 1H, dd (16.0, 4.0)	2.47, 1H, dd (16.4, 4.4)
3 _{ax.}	2.54, 1H, dd (16.0, 12.4)	2.48, 1H, dd (15.8, 11.9)	2.67, 1H, dd (16.0, 16.0)	2.67, 1H, dd (16.4, 14.4)
4	---	---	---	---
5	5.14, 1H, s	5.14, 1H, s	5.30, 1H, s	5.31, 1H, s
6	---	---	---	---
1 [`]	---	---	---	---
2 [`]	7.04, brs	6.77, 2H, d (8.7)	6.90, 1H*	7.36, 2H, d (8.4)
3 [`]	---	7.24, 2H, d (8.5)	---	6.89, 2H, d (8.8)
4 [`]	---	---	---	---
5 [`]	6.77, 1H, d (8.0)	7.24, 2H, d (8.5)	6.78, 1H, d (8.0)	6.89, 2H, d (8.8)
6 [`]	6.84, 1H, dd (7.6, 1.6)	6.77, 2H, d (8.7)	6.88, 1H, dd (8.0, 2.0)	7.36, 2H, d (8.4)
1 ^{``}	---	---	---	---
2 ^{``}	7.15, brs	6.79, 2H, d (8.7)	6.92, 1H*	7.41, 2H, d (8.8)
3 ^{``}	---	7.39, 2H, d (8.6)	---	6.93, 2H, d (8.8)
4 ^{``}	---	---	---	---
5 ^{``}	6.81, 1H, d (8.8)	7.39, 2H, d (8.6)	6.82, 1H, d (8.0)	6.93, 2H, d (8.8)
6 ^{``}	6.96, 1H, dd (8.0, 2.0)	6.79, 2H, d (8.7)	6.95, 1H, dd (8.0, 2.0)	7.41, 2H, d (8.8)
7 ^{``}	7.35, 1H, d (16.4)	7.35, 1H, d (16.6)	6.87, 1H, d, (16.0)	7.01, d (16.4)
8 ^{``}	6.60, 1H, d (16.4)	6.53, 1H, d (16.4)	6.36, 1H, d (16.0)	6.43, 1H, d (16.4)
-NH-	7.47, brs	7.54, brs.	4.87, brs	5.35, brs
-OCH ₃	3.82, 3H, s	---	3.84, 3H, s	3.82, 3H, s
-OCH ₃	3.79, 3H, s	---	3.84, 3H, s	3.83, 3H, s
-OCH ₃	---	---	3.85, 3H, s	---
-OCH ₃	---	---	3.85, 3H, s	---
-OH	9.10, brs	9.50, brs.	---	---
-OH	9.40, brs	9.80, brs.	---	---

Table S2: APT data of compounds **1**, **3**, **4** and **6** (at 100 MHz, ^a in DMSO-d₆, ^b in CDCl₃, δ in ppm).

Position (C)	1 ^a	3 ^a	4 ^b	6 ^b
2	56.8 (CH)	56.3 (CH)	58.5 (CH)	57.8, (CH)
3	44.4 (CH ₂)	44.3 (CH ₂)	44.5 (CH ₂)	44.3 (q)
4	190.9 (q)	190.8 (q)	192.9 (q)	192.8 (q)
5	97.7 (CH)	97.6 (CH)	101.2 (CH)	100.3 (CH)
6	159.1 (q)	159.2 (q)	157.8 (q)	158.4 (q)
1`	132.4 (q)	131.9 (q)	132.9 (q)	132.5 (q)
2`	110.8 (CH)	128.5 (CH)	109.9 (CH)	128.1 (CH)
3`	148.0 (q)	115.6 (CH)	149.4 (q)	114.4 (CH)
4`	146.6 (q)	159.1 (q)	149.3 (q)	159.7 (q)
5`	115.7 (CH)	115.6 (CH)	111.2 (CH)	114.4 (CH)
6`	119.7 (CH)	128.5 (CH)	119.3 (CH)	128.1 (CH)
1``	127.6 (q)	127.1 (q)	128.0 (q)	127.8 (q)
2``	111.9 (CH)	129.4 (CH)	111.9 (CH)	128.9 (CH)
3``	148.6 (q)	116.3 (CH)	150.6 (q)	114.4 (CH)
4``	148.3 (q)	157.4 (q)	149.4 (q)	160.8 (q)
5``	116.1 (CH)	116.3 (CH)	111.4 (CH)	114.4 (CH)
6``	122.0 (CH)	129.4 (CH)	121.6 (CH)	128.9 (CH)
7``	135.7 (CH)	135.5 (CH)	134.1 (CH)	134.2 (CH)
8``	120.5 (CH)	120.2 (CH)	120.8 (CH)	120.6 (CH)
-OCH ₃	56.0 (CH ₃)	---	56.0 (CH ₃)	55.4 (CH ₃)
-OCH ₃	56.1 (CH ₃)	---	56.0 (CH ₃)	55.4 (CH ₃)
-OCH ₃	---	---	56.0 (CH ₃)	---
-OCH ₃	---	---	56.1 (CH ₃)	---