

Supplementary Materials

3'''-O-Foliamenthoyl-Rutin, a New Flavonoid Glycoside from the Roots of *Nymphoides peltata*

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Table S1. ¹H and ¹³C NMR Spectrum Data of Compounds **1-5**

Position	Compound 1		Compound 2		Compound 3		Compound 4		Compound 5	
	δ_c , type ^c	δ_H (J in Hz) ^b	δ_c , type ^c	δ_H (J in Hz) ^a	δ_c , type ^c	δ_H (J in Hz) ^a	δ_c , type ^c	δ_H (J in Hz) ^a	δ_c , type ^c	δ_H (J in Hz) ^a
2	145.9 C		156.6 C		156.8 C		156.8 C		159.1 C	
3	134.8 C		134.1 C		133.8 C		133.8 C		135.7 C	
4	174.9 C		177.2 C		177.9 C		177.8 C		179.8 C	
5	159.8 C		157.3 C		161.7 C		161.7 C		163.6 C	
6	102.1 CH	6.16 (d, 2.0)	100.6 CH	6.15 (d, 2.0)	99.2 CH	6.20 (d, 2.0)	99.2 CH	6.14 (d, 2.0)	101.1 CH	6.15 (d, 2.0)
7	163.0 C		161.6 C		164.8 C		164.7 C		166.7 C	
8	92.4 CH	6.38 (d, 2.0)	94.8 CH	6.34 (d, 2.0)	94.0 CH	6.40 (d, 2.0)	94.0 CH	6.34 (d, 2.0)	96.0 CH	6.34 (d, 2.0)
9	155.2 C		156.6 C		156.6 C		156.8 C		158.8 C	
10	97.3 C		102.4 C		104.4 C		104.5 C		106.3 C	
1'	121.0 C		121.5 C		122.1 C		122.1 C		123.5 C	
2'	114.7 CH	7.65 (d, 2.0)	115.9 CH	7.49 s	116.7 CH	7.61-7.53 (m)	116.6 CH	7.53 (s)	118.7 CH	7.49 (s)
3'	144.1 C		146.1 C		145.3 C		145.3 C		147.2 C	
4'	146.8 C		146.1 C		149.0 C		149.0 C		150.9 C	
5'	114.7 CH	6.86 (d, 8.5)	115.9 CH	6.80 (d, 8.0)	115.7 CH	6.84 (d, 9.0)	115.8 CH	6.81 (d, 9.0)	117.7 CH	6.80 (d, 8.0)
6'	119.1 CH	7.52 (dd, 8.5, 2.0)	121.5 CH	7.50 (d, 8.0)	121.6 CH	7.61-7.53 (m)	121.6 CH	7.54 (d, 2.0)	124.0 CH	7.51 (d, 2.0)
1''			102.2 CH	5.30 (d, 7.5)	101.4 CH	5.46 (d, 7.5)	101.3 CH	5.33 (d, 7.5)	103.6 CH	5.30 (d, 7.5)
2''			70.8 CH	4.90 (m)	74.6 CH	3.03 (m)	72.9 CH	2.92 (m)	76.5 CH	3.18 (m)
3''			71.0 CH	3.99 (m)	78.11 CH	3.21 (m)	77.4 CH	3.25 (m)	78.9 CH	3.17 (m)
4''			71.7 CH	3.52 (m)	70.4 CH	3.17 (m)	70.5 CH	3.04 (m)	72.4 CH	3.30 (m)
5''			70.6 CH	3.22 (m)	77.0 CH	3.04 (m)	76.8 CH	3.18 (m)	78.3 CH	3.20 (m)
6''			18.0 CH ₃	0.95 (d, 6.0)	61.5 CH ₂	3.58 (d, 11.5), 3.28 (overlap)	67.7 CH ₂	3.73 (d, 11.0), 3.41 (overlap)	69.4 CH ₂	3.66 (d, 10.0), 3.24 (overlap)
1'''							103.2 CH	3.91 (d, 6.5)	103.2 CH	4.34 (d, 1.5)
2'''							70.9 CH	3.10 (m)	70.7 CH	3.23 (m)
3'''							74.4 CH	3.19 (m)	74.3 CH	3.03 (m)
4'''							67.8 CH	3.36 (m)	72.9 CH	3.25 (m)
5'''							65.3 CH ₂	3.42 (overlap), 2.85 (dd, 12.0, 2.0)	72.8 CH	3.36 (m)
6'''									20.2 CH ₃	0.95 (d, 6.0)

^a Measured at 400 MHz in DMSO-*d*₆. ^b Measured at 500 MHz in DMSO-*d*₆. ^c Measured at 100 MHz in DMSO-*d*₆.

Figure S1. HR-ESI-MS data of 6

Compound Identification Results: Cpd 663: C37 H44 O18; 4.612

ID Techniques Applied: MFG

Best	Name	Formula	m/z	Mass	Species	Diff (ppm)	RT	Score
⊙		C37 H44 O18	777.2561	776.251	(M+H) ⁺ (M+Na) ⁺	-2.29	4.612	94.7
○		C44 H40 O13	777.2561	776.251	(M+H) ⁺ (M+Na) ⁺	5.23	4.612	76.14
○		C26 H48 O26	777.2561	776.2499	(M+H) ⁺	8.41	4.612	56.61

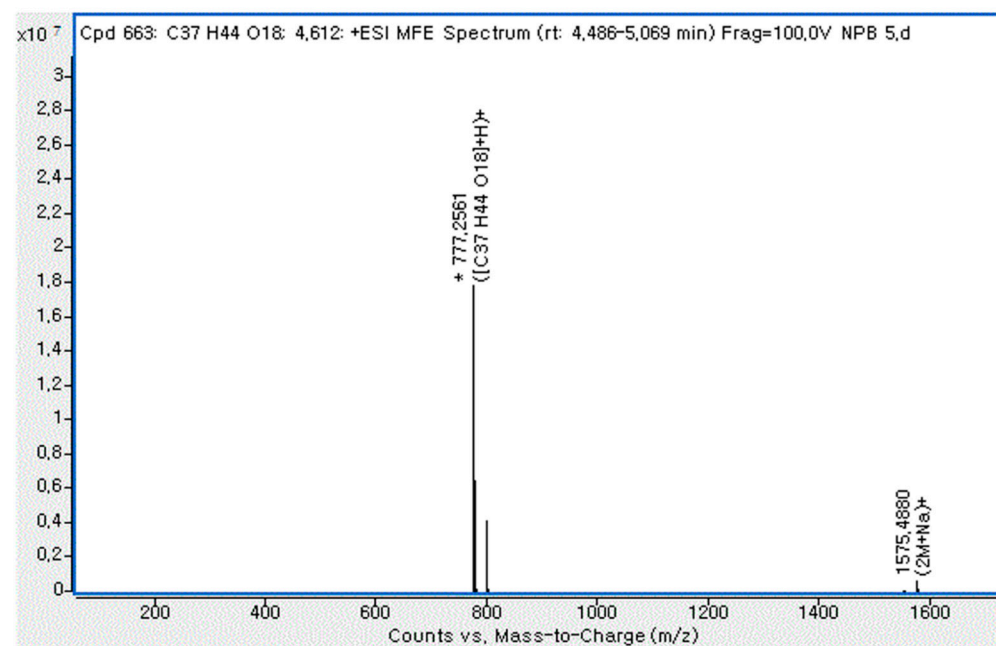


Figure S2. ^1H NMR spectrum of **6** in $\text{DMSO-}d_6$ (500 MHz)

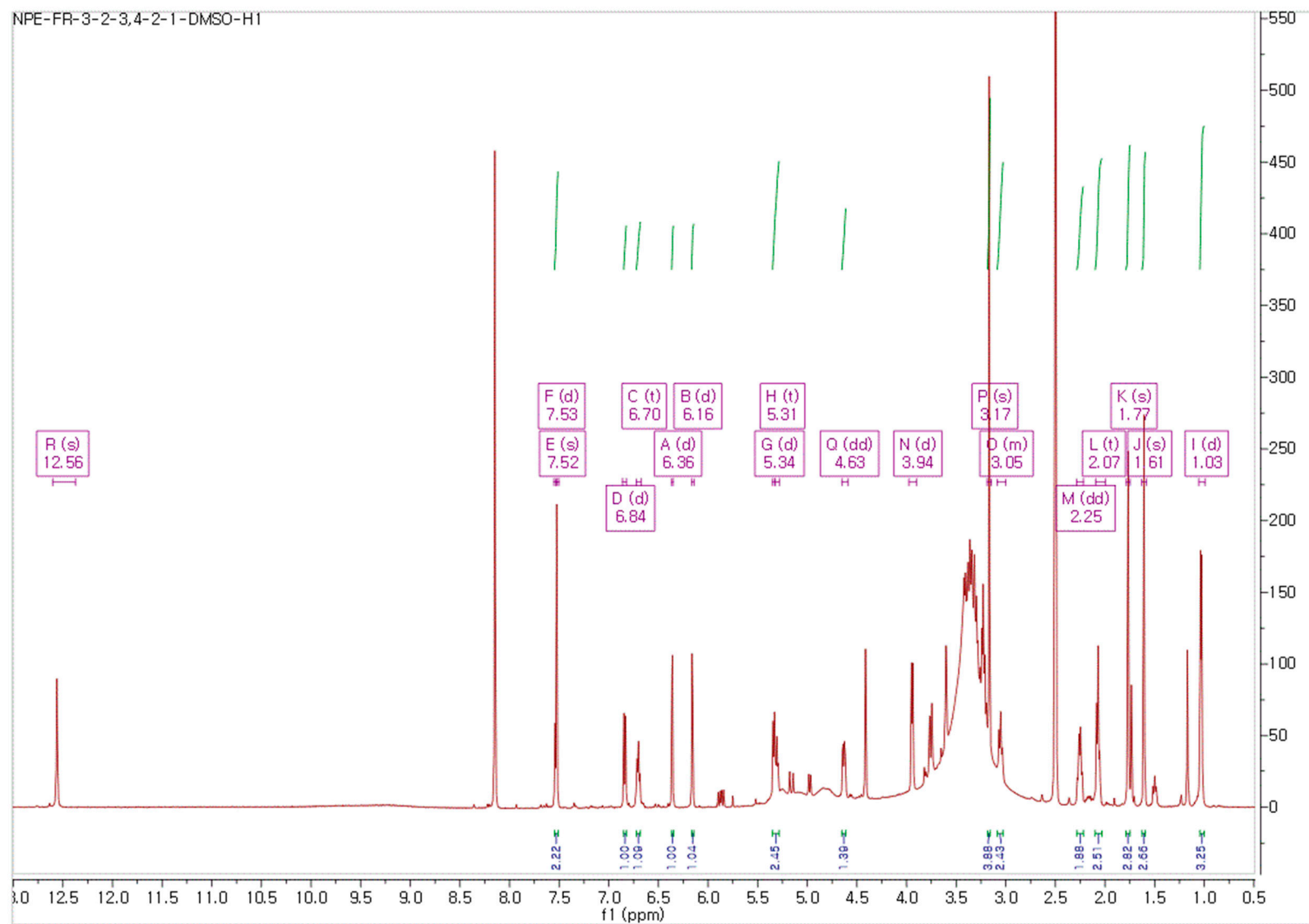


Figure S3. ^{13}C NMR spectrum of **6** in $\text{DMSO}-d_6$ (100 MHz)

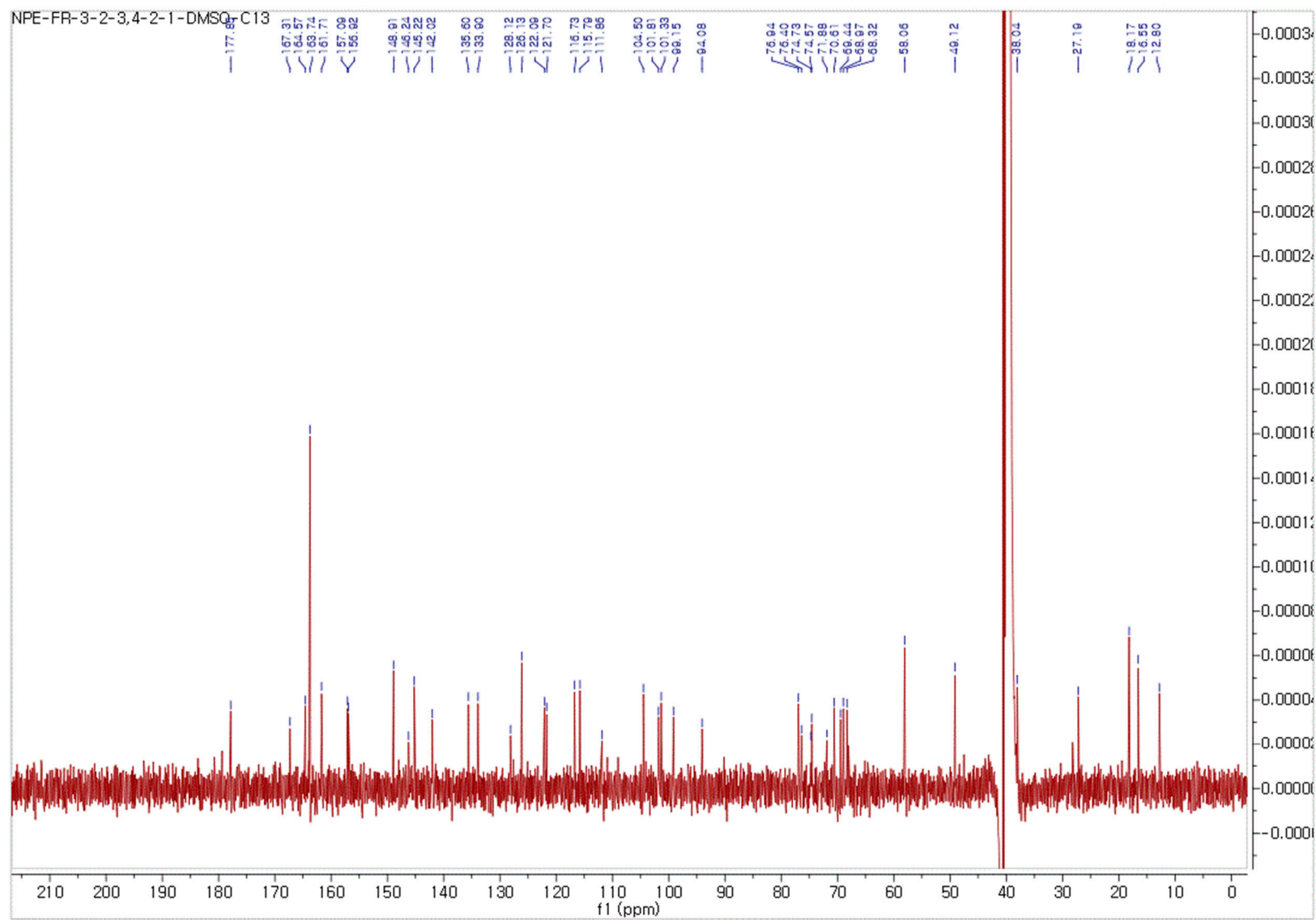


Figure S4. ^1H - ^1H COSY spectrum of **6** in $\text{DMSO-}d_6$

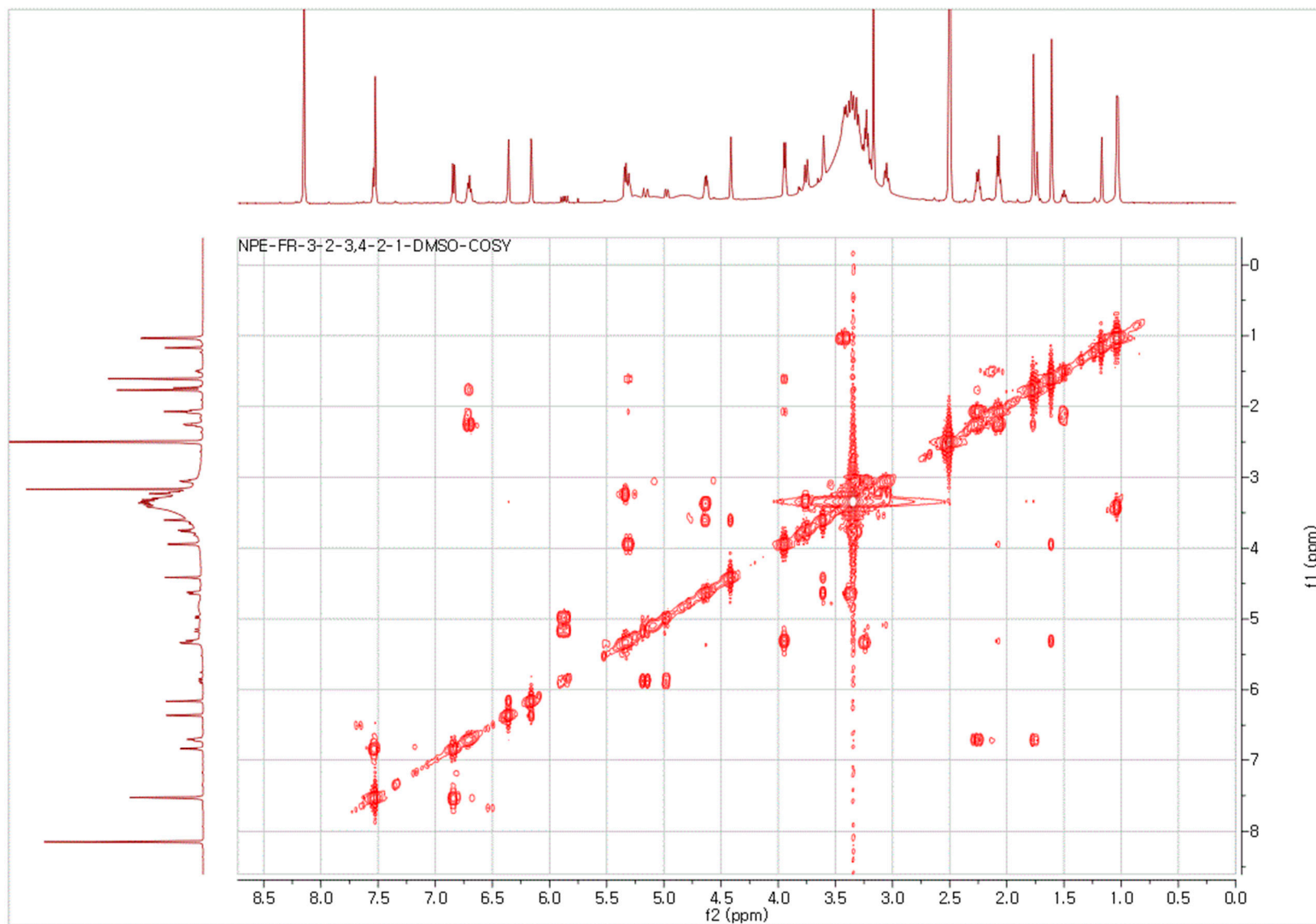


Figure S5. HSQC spectrum of **6** in DMSO- d_6

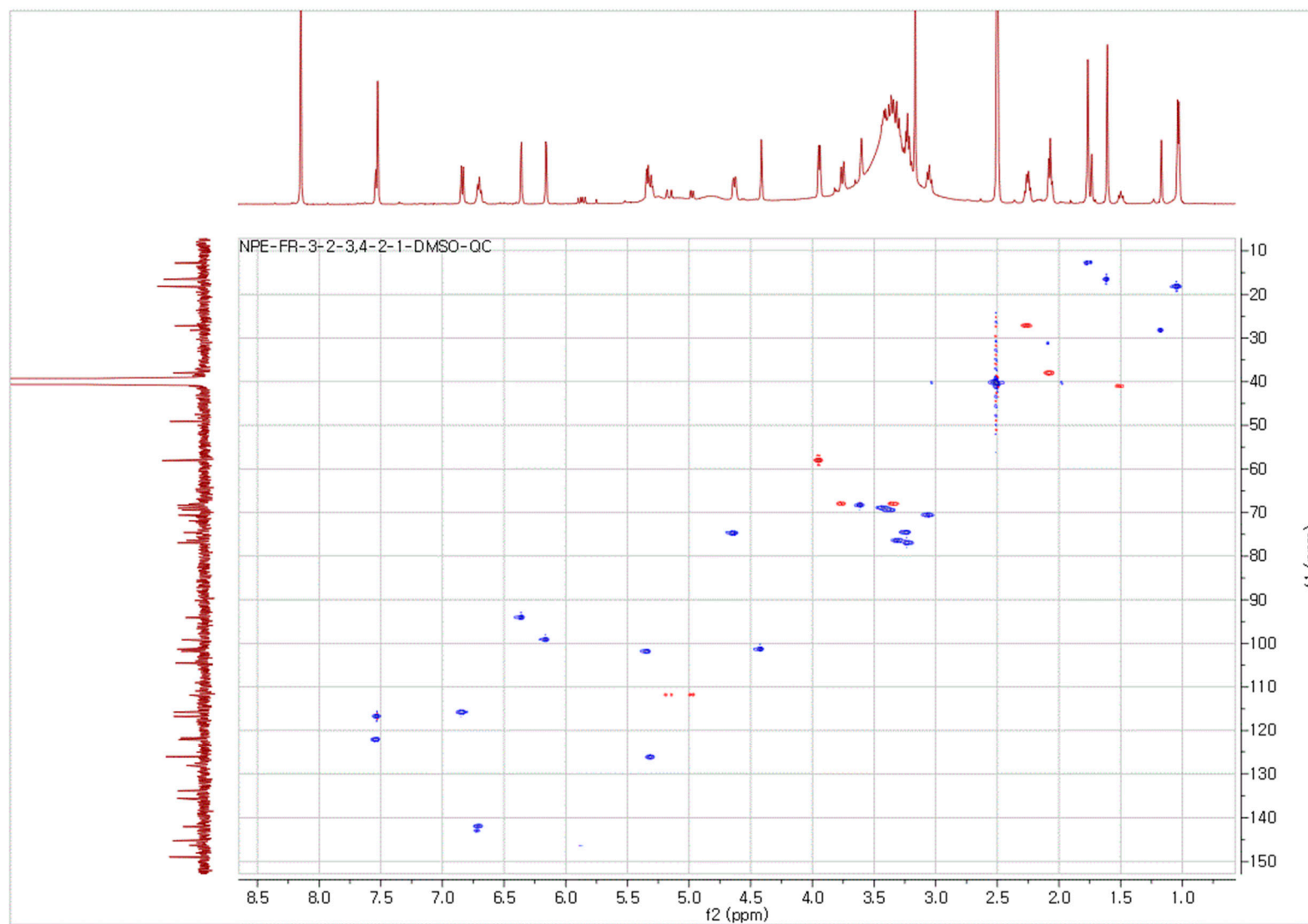


Figure S6. HMBC spectrum of **6** in DMSO- d_6

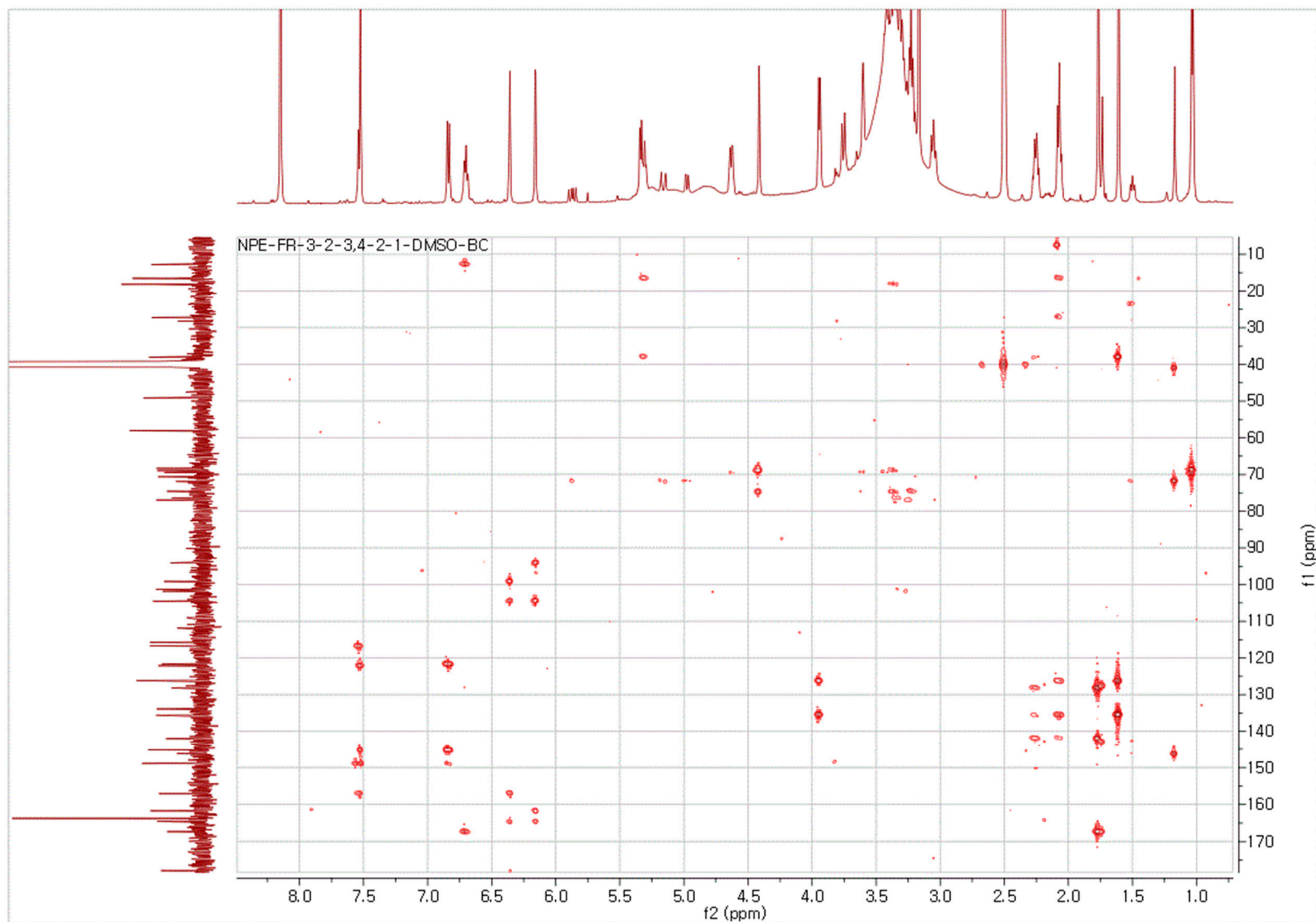


Figure S7. UV/PDA spectrum of **6**

