

Supporting Information

Rec. Nat. Prod. X:X (201X) XX-XX

Monoterpene Flavonoid from Aerial Parts of *Satureja khuzistanica*

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NMR data of compounds 2-6

Keshonin (2): ^1H NMR (500 MHz, DMSO) δ : 7.27 (1H, d, $J = 2.2$ Hz, H-2'), 7.68 (1H, dd, $J = 8.5, 2.2$ Hz, H-6'), 7.07 (1H, d, $J = 8.5$ Hz, H-5'), 6.79 (1H, s, H-3'''), 6.66 (1H, d, $J = 2.0$ Hz, H-8), 6.66 (1H, s, H-3), 6.53 (1H, s, H-6'''), 6.47 (1H, d, $J = 2.1$ Hz, H-6), 5.21 (1H, d, $J = 7.3$ Hz, H-1''), 3.98 (1H, d, $J = 9.6$ Hz, H-5''), 3.56 – 3.05 (3H, m, H-2'', H-3'', H-4''), 3.16 – 3.08 (1H, m, H-8'''), 2.04 (3H, s, H-7'''), 1.19 (3H, d, $J = 1.8$ Hz, H-9'''), 1.18 (3H, d, $J = 1.8$ Hz, H-10''').

Saturejin (3'-(2,5-dihydroxy-p-cymene) 5,7,4'-trihydroxy flavone) (3): ^1H NMR (500 MHz, DMSO) δ : 6.61 (1H, s, H-3), 6.16 (1H, d, $J = 2.0$, H-6), 6.30 (1H, d, $J = 2.0$, H-8), 7.20 (1H, d, $J = 2.2$, H-2'), 7.05 (1H, d, $J = 8.5$, H-5'), 7.64 (1H, dd, $J = 8.5, 2.2$, H-6'), 6.78 (1H, s, H-1''), 6.57 (1H, s, H-6''), 2.04 (3H, s, H-7''), 3.11 (1H, m, H-8''), 1.15 (1H, d, $J = 6.8$, H-9''), 1.15 (1H, d, $J = 6.8$, H-10'').

Ponciretin (4): ^1H NMR (500 MHz, DMSO) δ : 7.39 (2H, d, $J = 8.7$ Hz, H-2', H-6'), 6.93 (2H, d, $J = 8.7$ Hz, H-3', H-5'), 5.80 (2H, d, $J = 1.9$ Hz, H-6, H-8), 5.44 (1H, dd, $J = 12.4, 3.0$ Hz, H-2), 3.74 (3H, s, OMe), 3.17 (1H, dd, $J = 16.9, 12.3$ Hz, H-3ax), 2.67 (1H, dd, $J = 17.1, 3.2$ Hz, H-3eq).

5,6-dihydroxy-3',4',7-trimethoxyflavone (5): ^1H NMR (500 MHz, DMSO) δ 7.60 (1H, s, H-3), 7.59 (1H, s, H-8), 6.96 (2H, d, $J = 8.1$ Hz), 6.91 (1H, d, $J = 10.0$ Hz), 3.94 (3H, s, OMe), 3.91 (3H, s, OMe), 3.75 (3H, s, OMe).

5,6-dihydroxy-4',7-dimethoxyflavone (6): ^1H NMR (500 MHz, DMSO) δ : 7.95 (2H, d, $J = 8.8$ Hz, H-2', H-6'), 6.94 (2H, d, $J = 8.7$ Hz, H-3', H-5'), 6.90 (1H, s, H-3), 6.80 (1H, s, H-8), 3.94 (3H, s, OMe), 3.75 (3H, s, OMe).

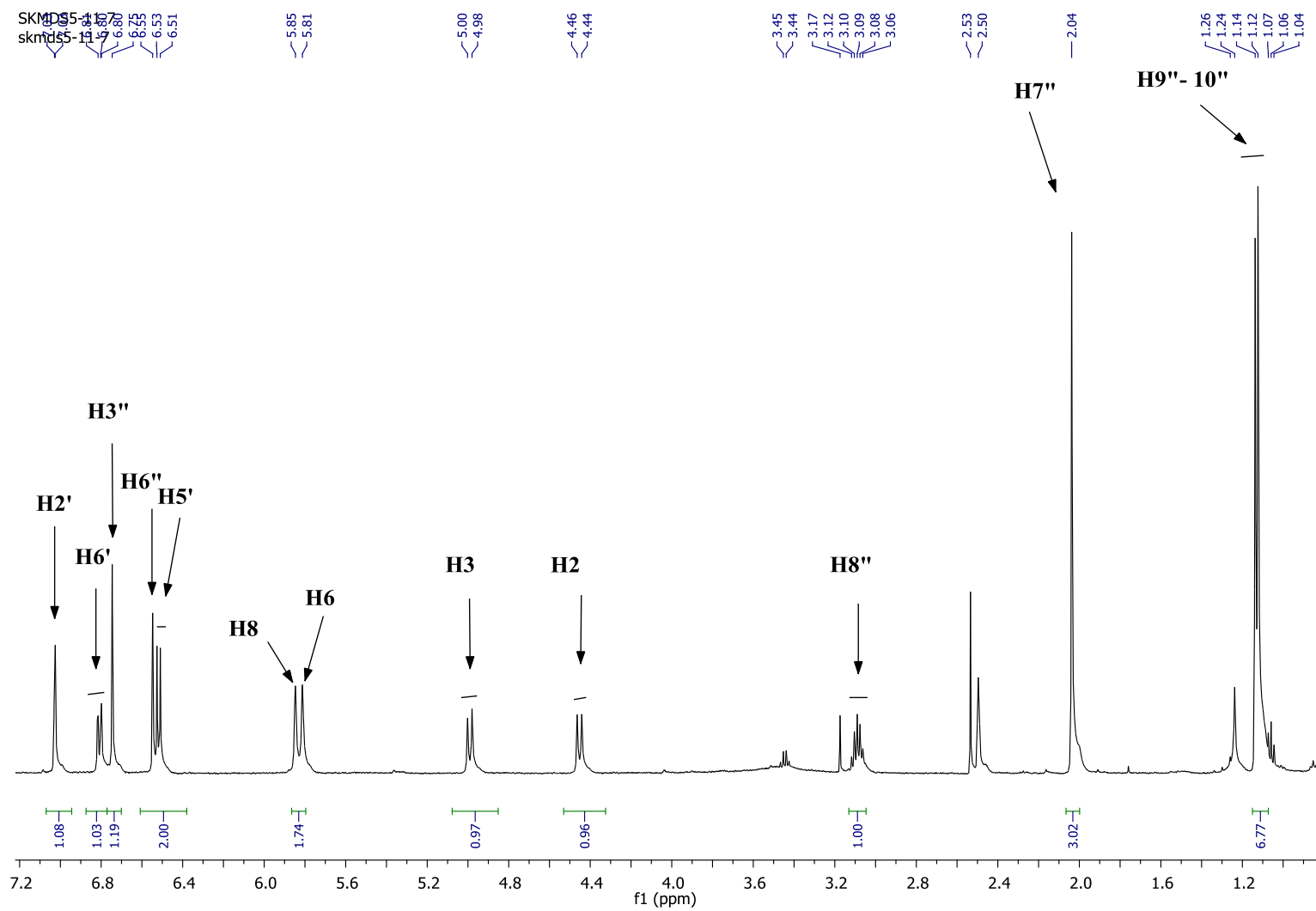


Figure S1: ^1H NMR (500 MHz, DMSO-d₆) spectrum of **1**

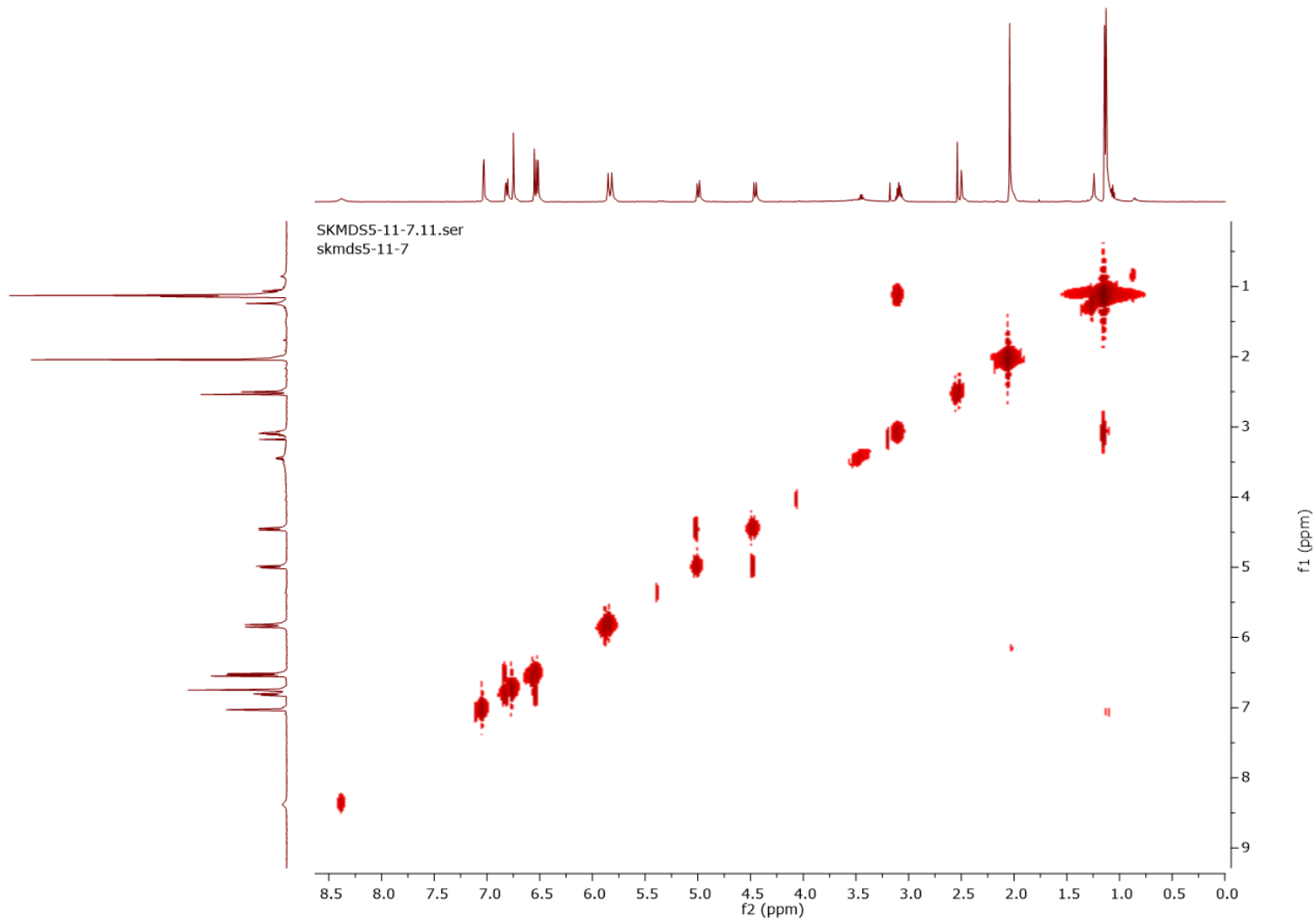


Figure S2: ^1H ^1H COSY (500 MHz, DMSO- d_6) spectrum of **1**

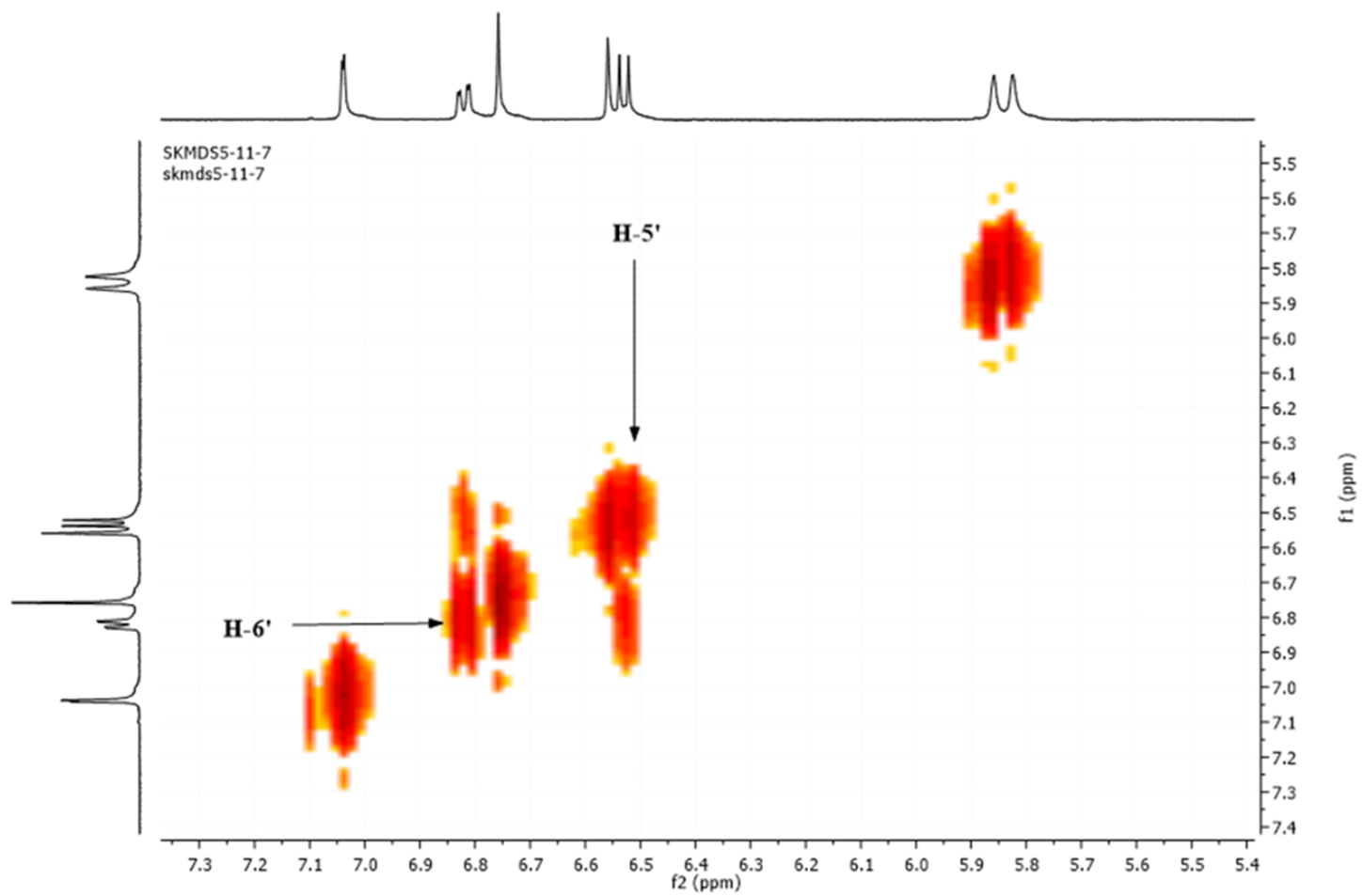


Figure S3: Expanded ^1H ^1H COSY (500 MHz, DMSO- d_6) spectrum of **1**

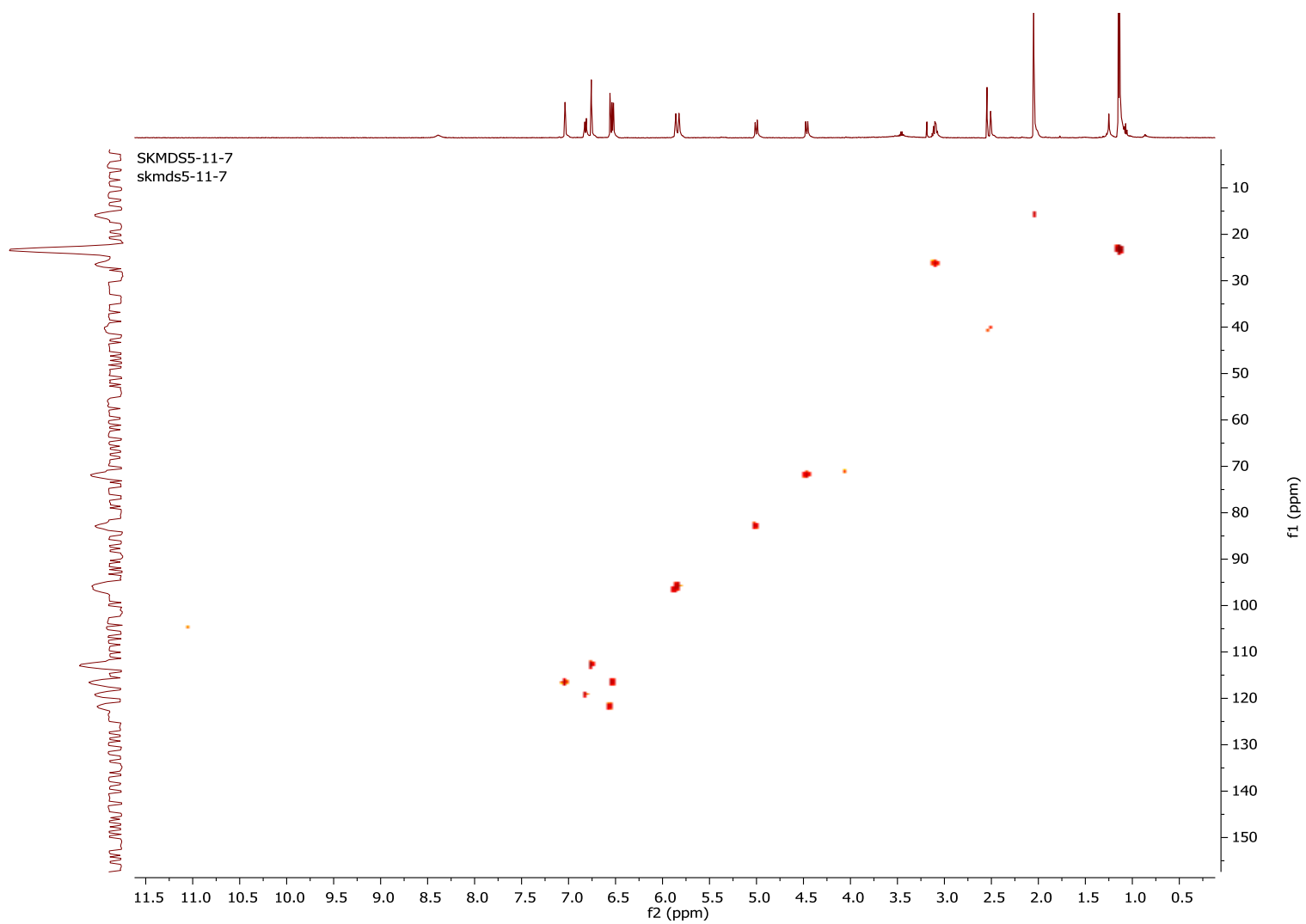


Figure S4: HSQC (500 MHz, DMSO-d₆) spectrum of **1**

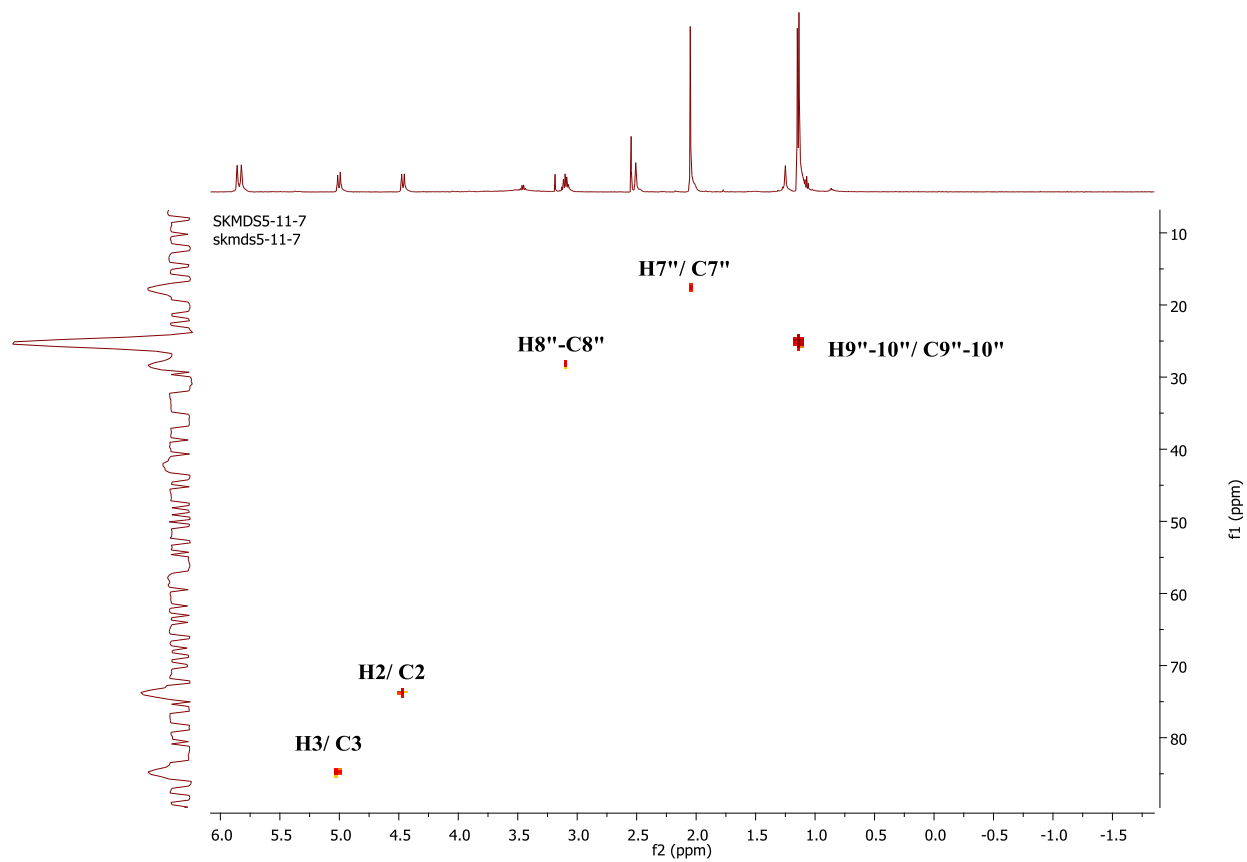


Figure S5: Expanded HSQC (500 MHz, DMSO-d₆) spectrum of **1**

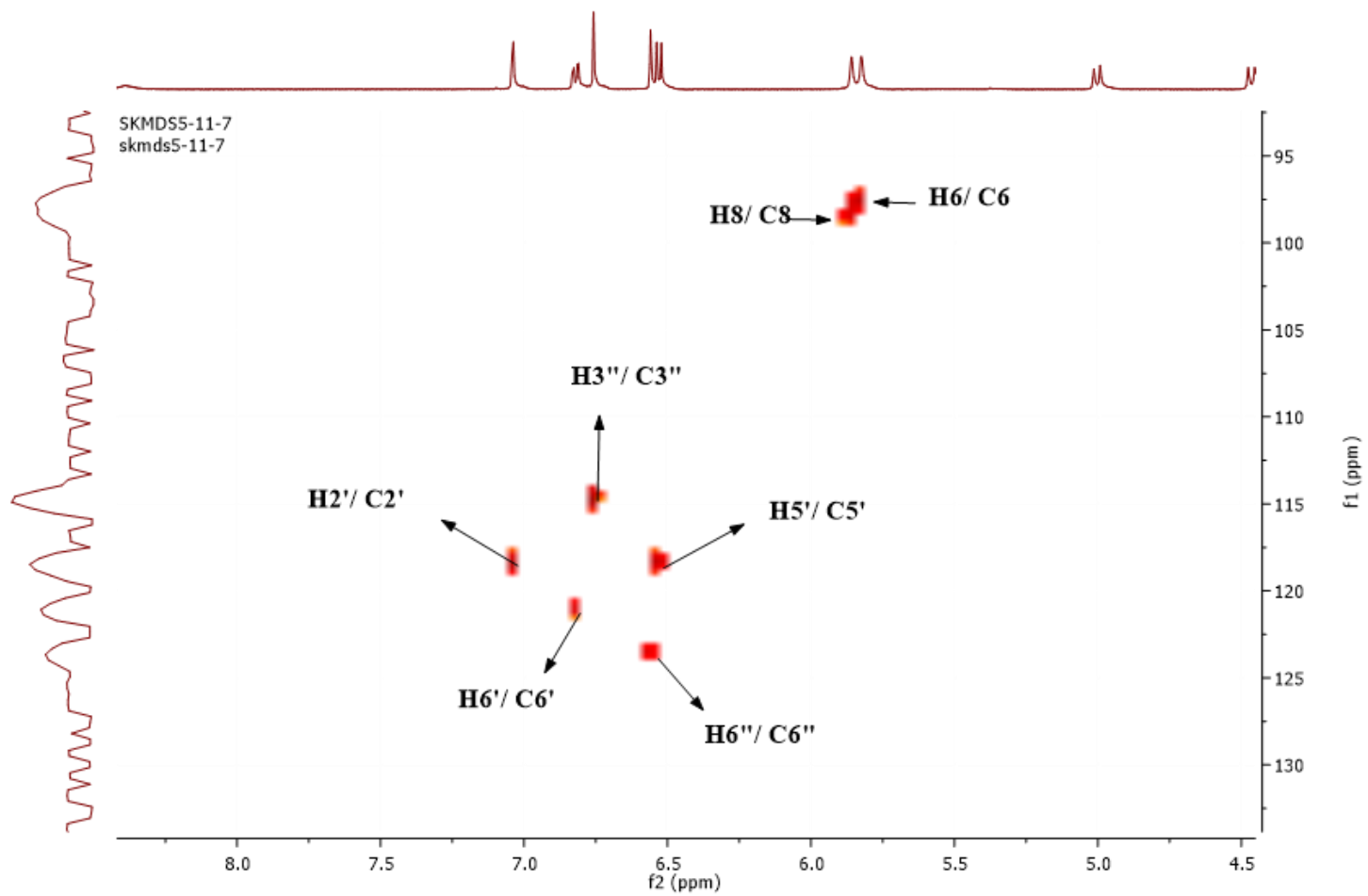


Figure S6: Expanded HSQC (500 MHz, DMSO-d₆) spectrum of **1**

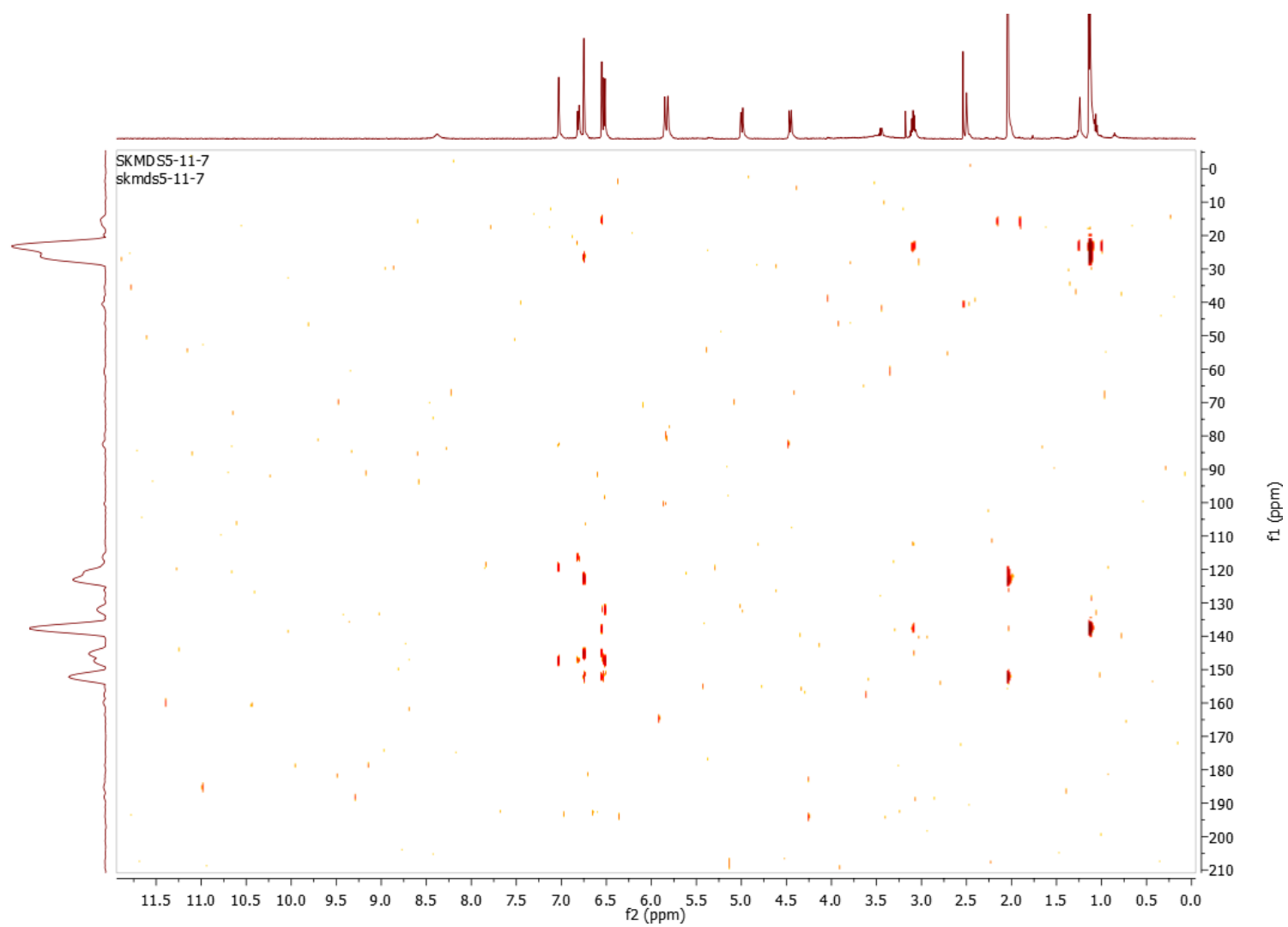


Figure S7: HMBC (500 MHz, DMSO-d₆) spectrum of **1**

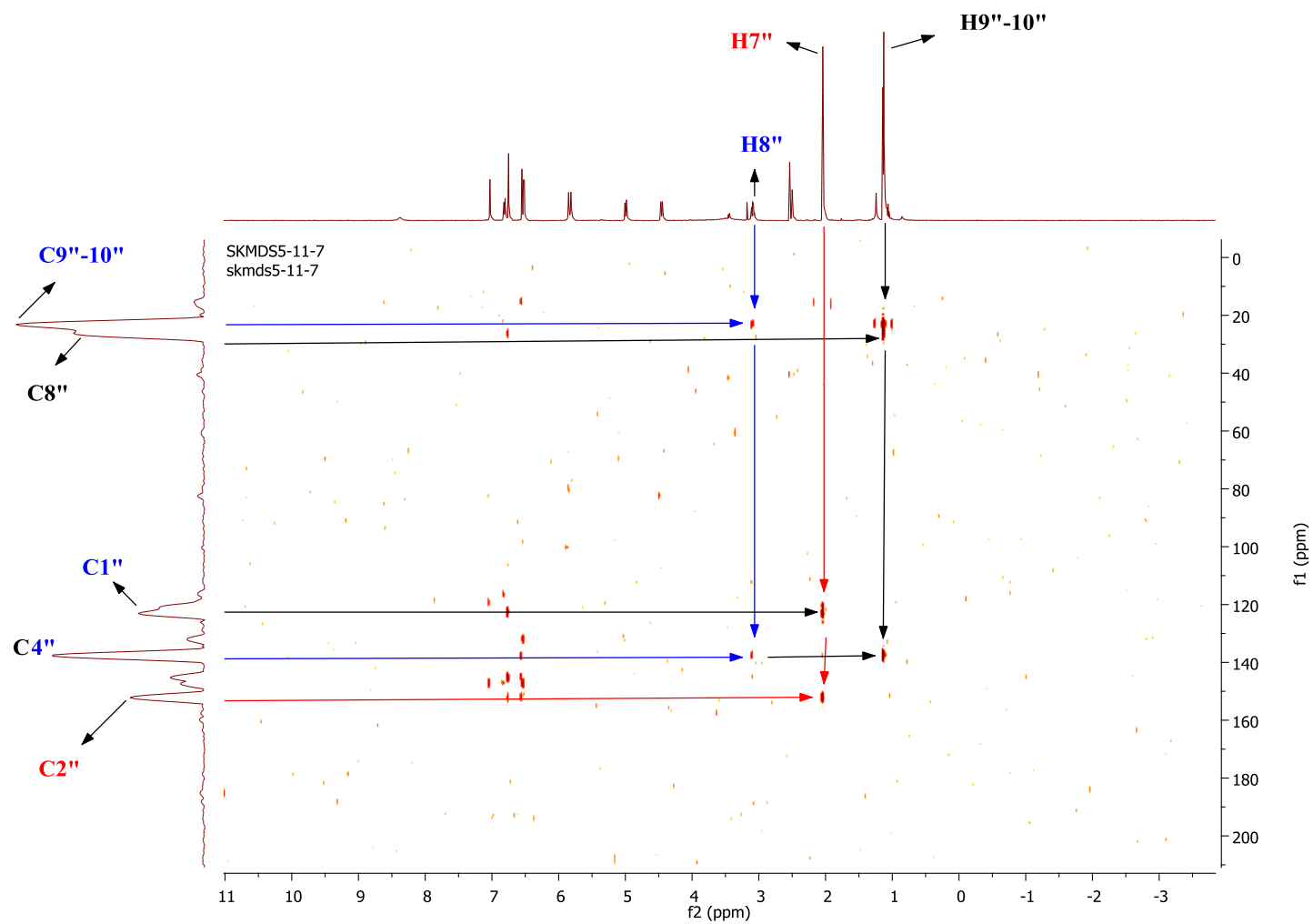


Figure S8: Expanded HMBC (500 MHz, DMSO-d₆) spectrum of **1**

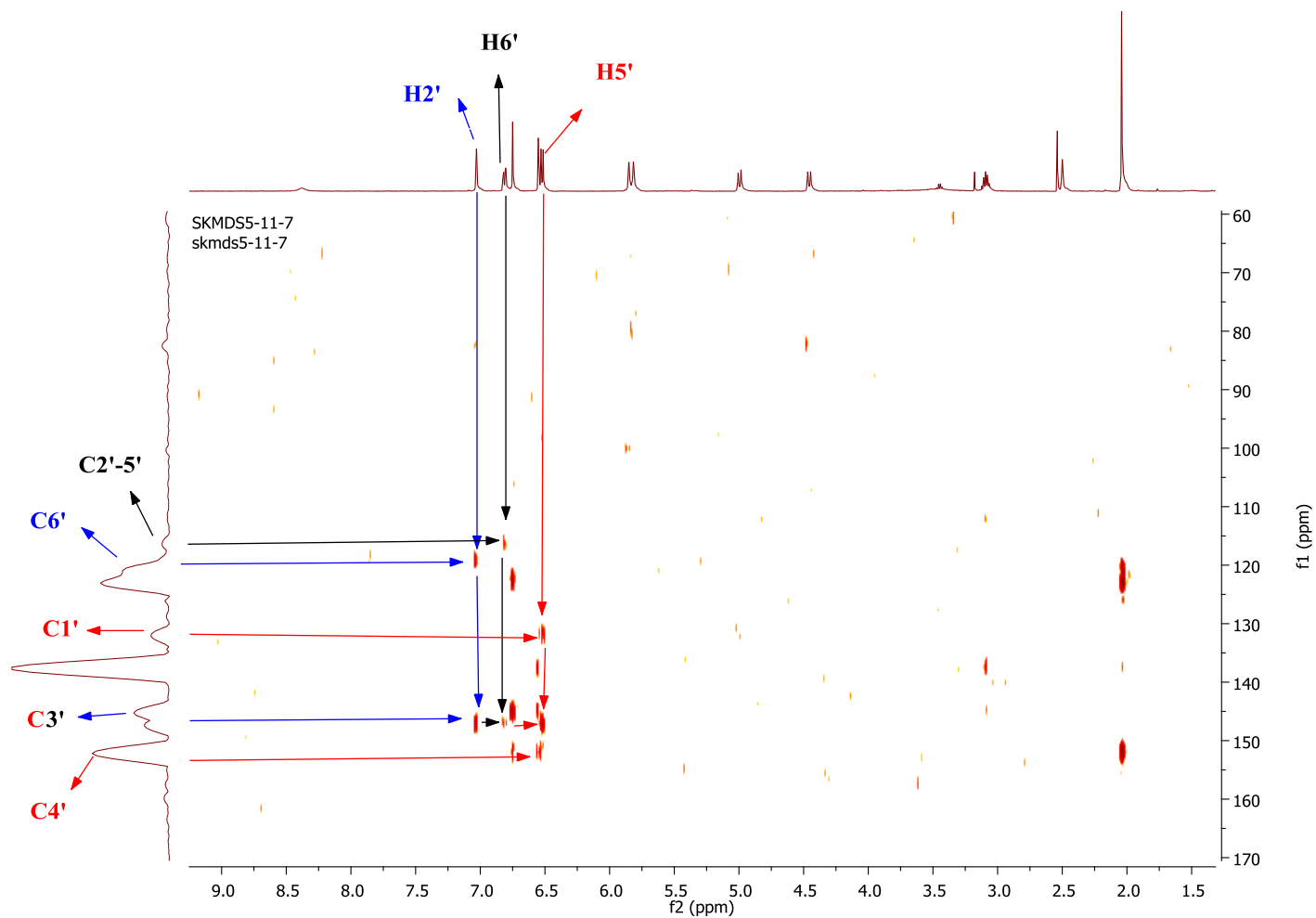


Figure S9: Expanded HMBC (500 MHz, DMSO-d₆) spectrum of **1**

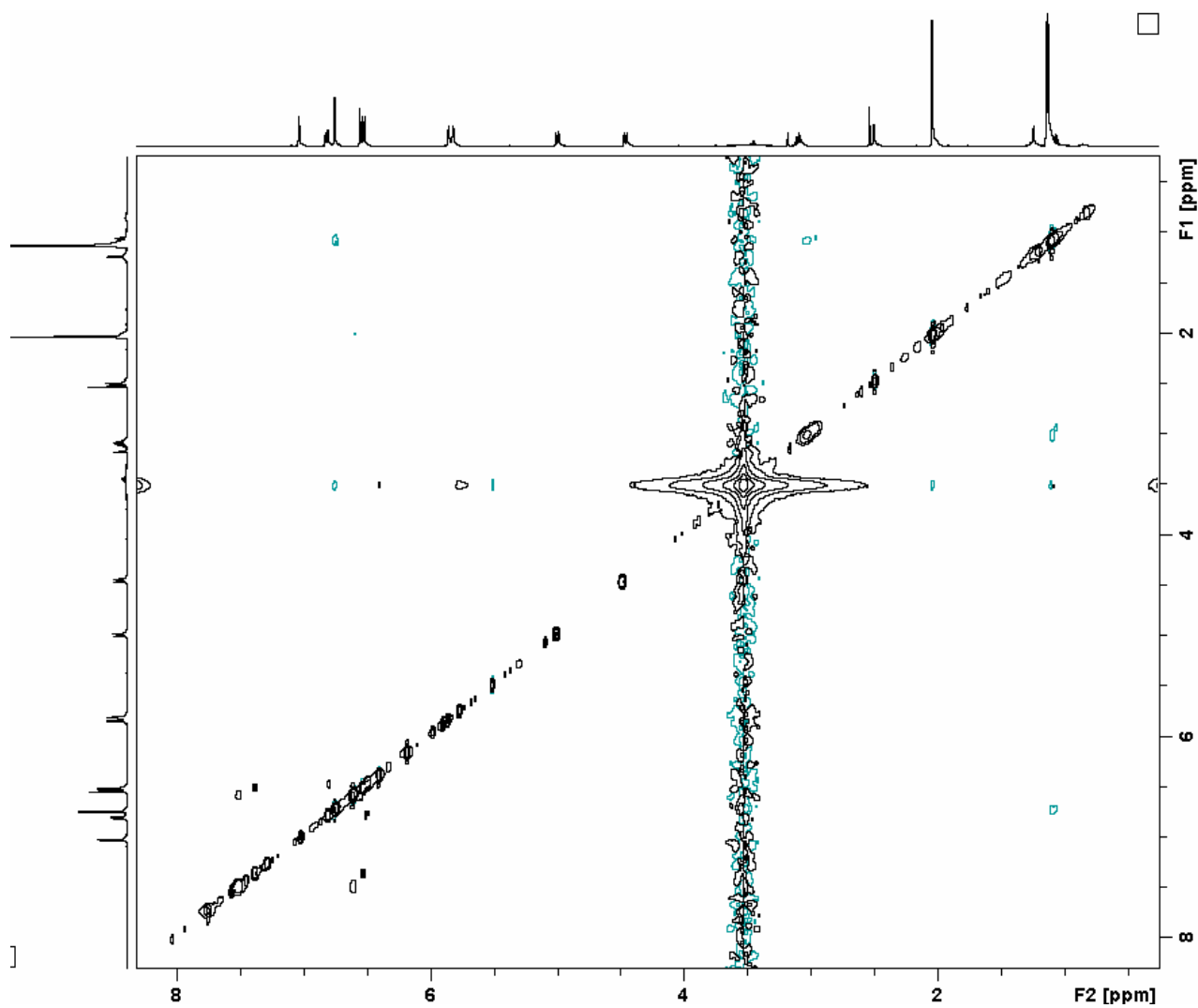


Figure S10: NOESY (500 MHz, DMSO-d₆) spectrum of compound **1**

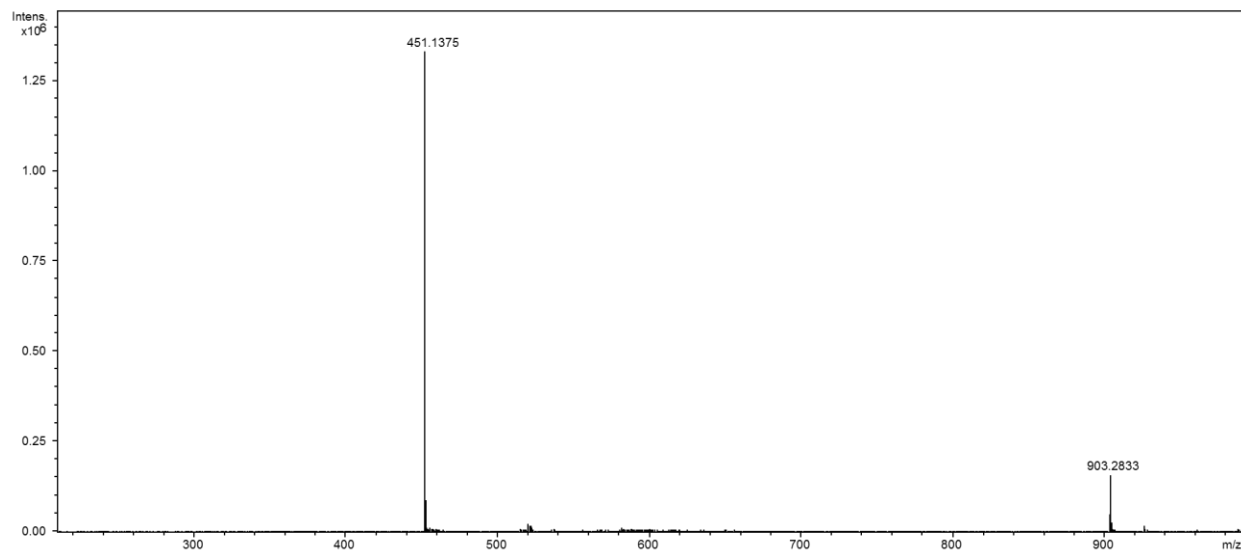


Figure S11: HR-ESIMS spectrum of **1**

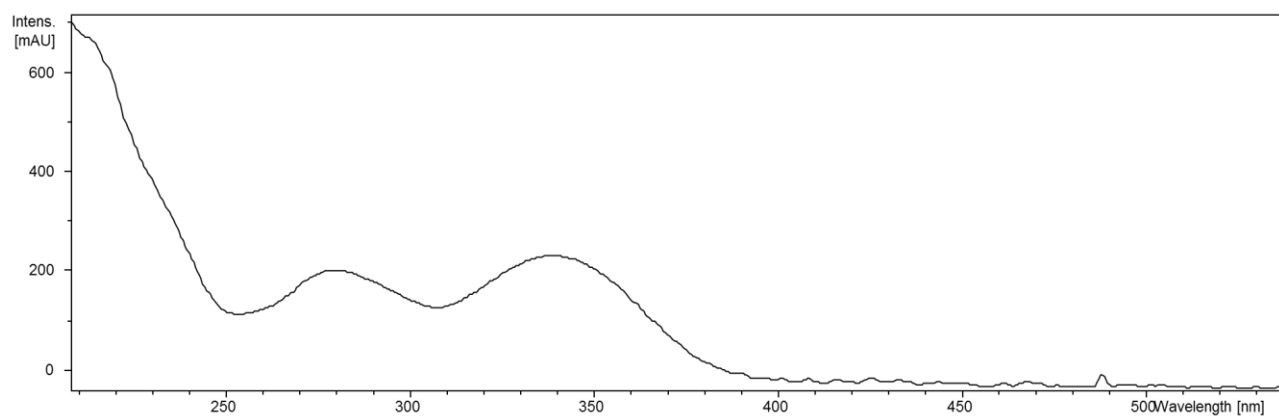


Figure S12: UV-Vis spectrum of compound **1**

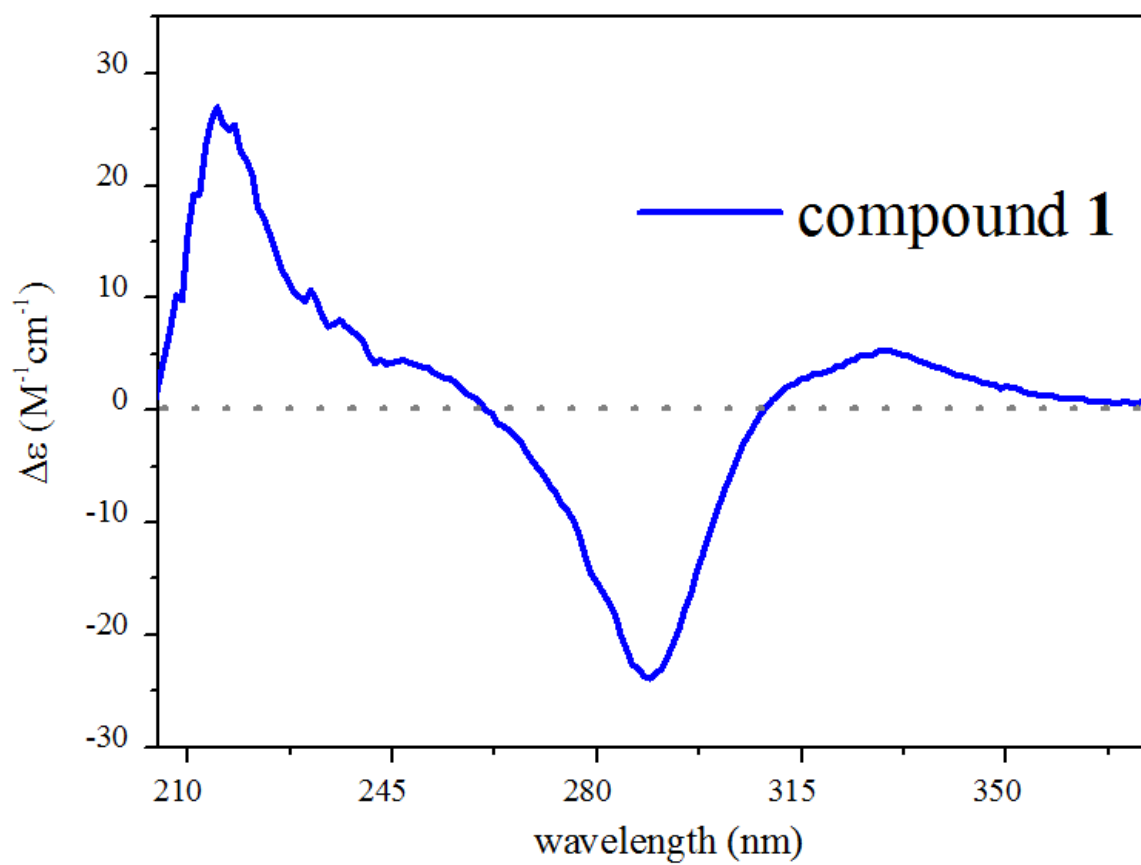


Figure S13: Experimental ECD spectrum of compound 1