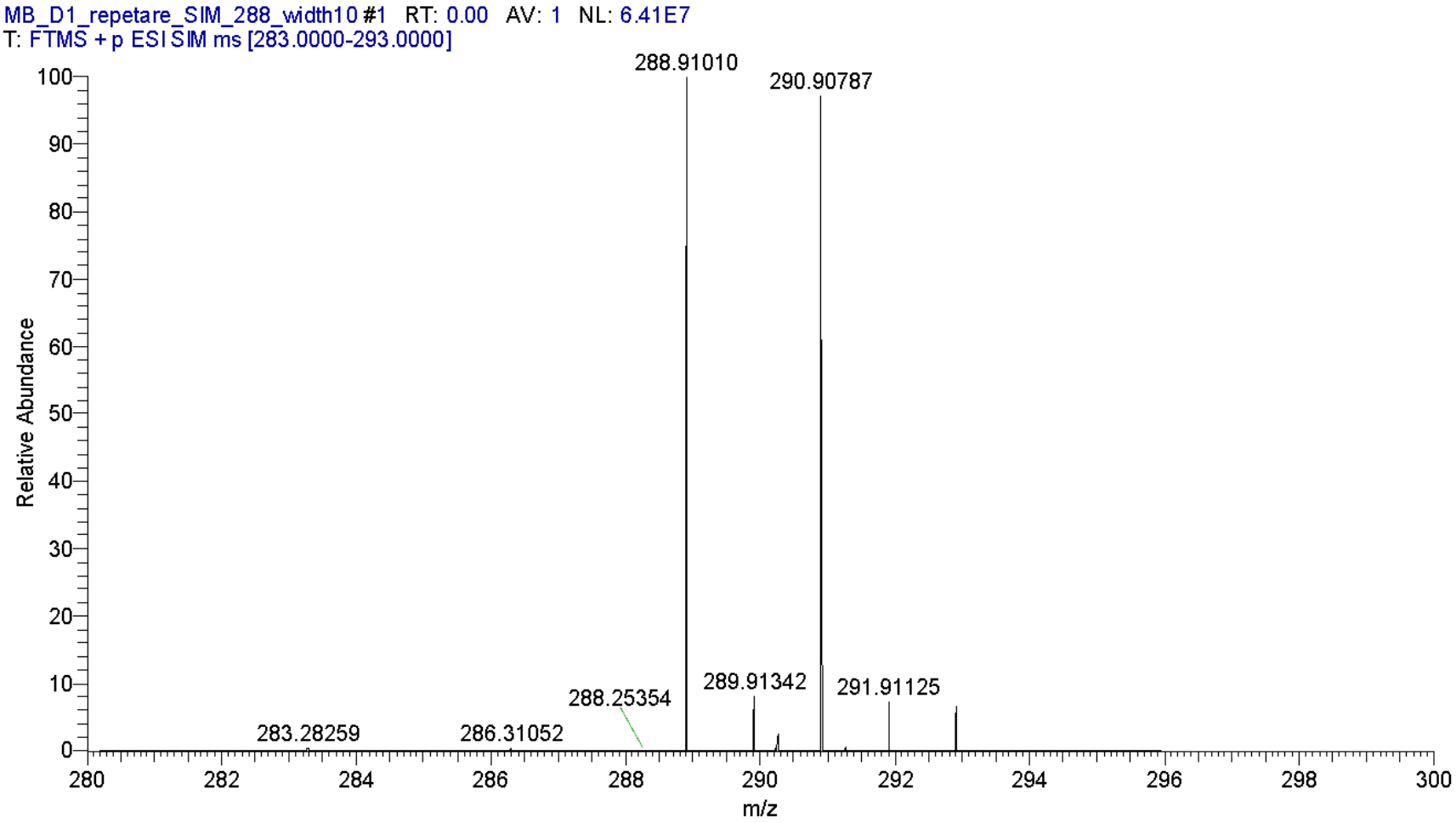


Figure S1. ESI-HR-MS spectrum of **MB-D1**

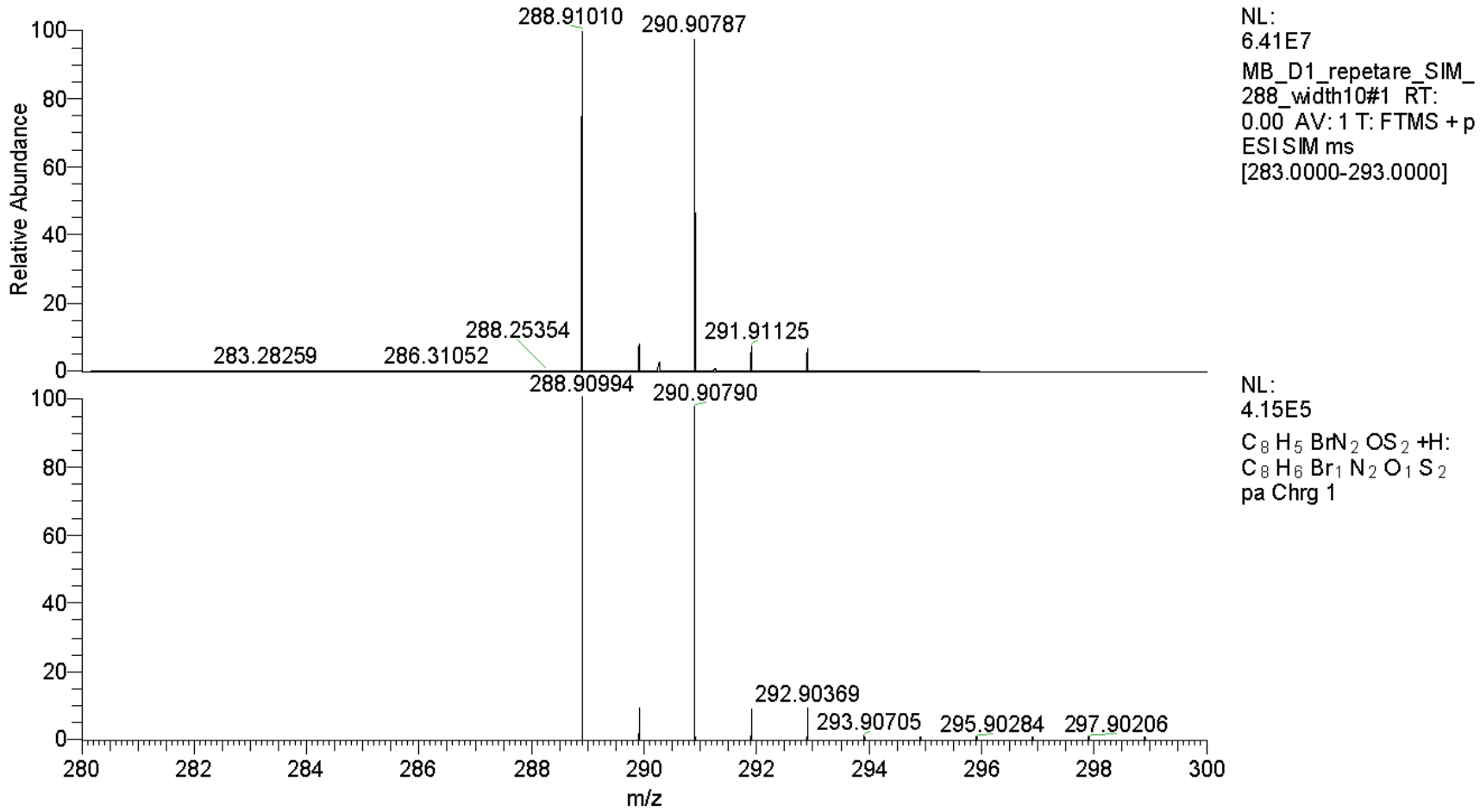


Figure S2. Mass analysis of **MB-D1**: ESI-HR-MS experimental spectrum (top); isotope simulation for predicted compound (bottom)

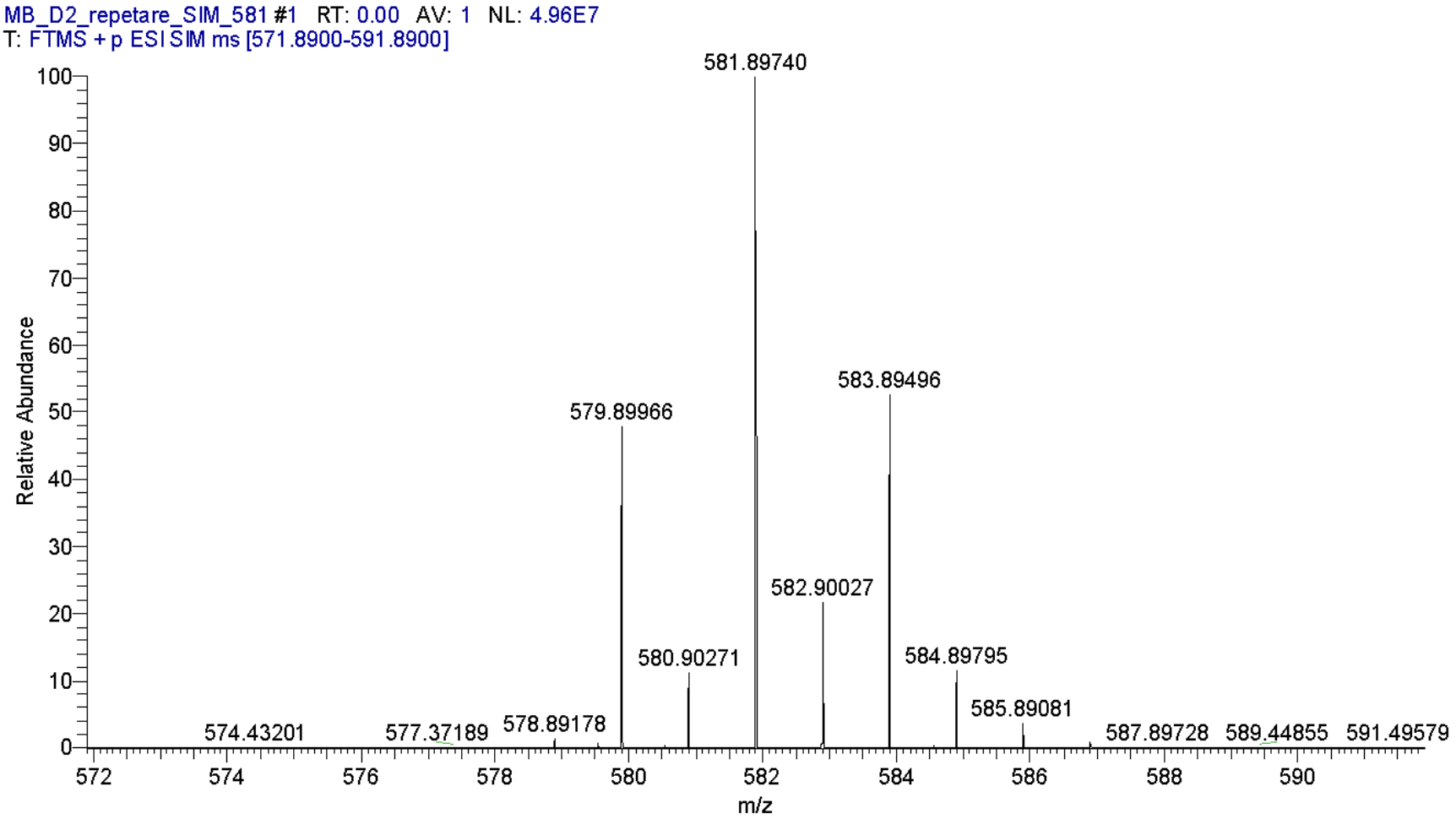


Figure S3. ESI-HR-MS spectrum of **MB-D2**

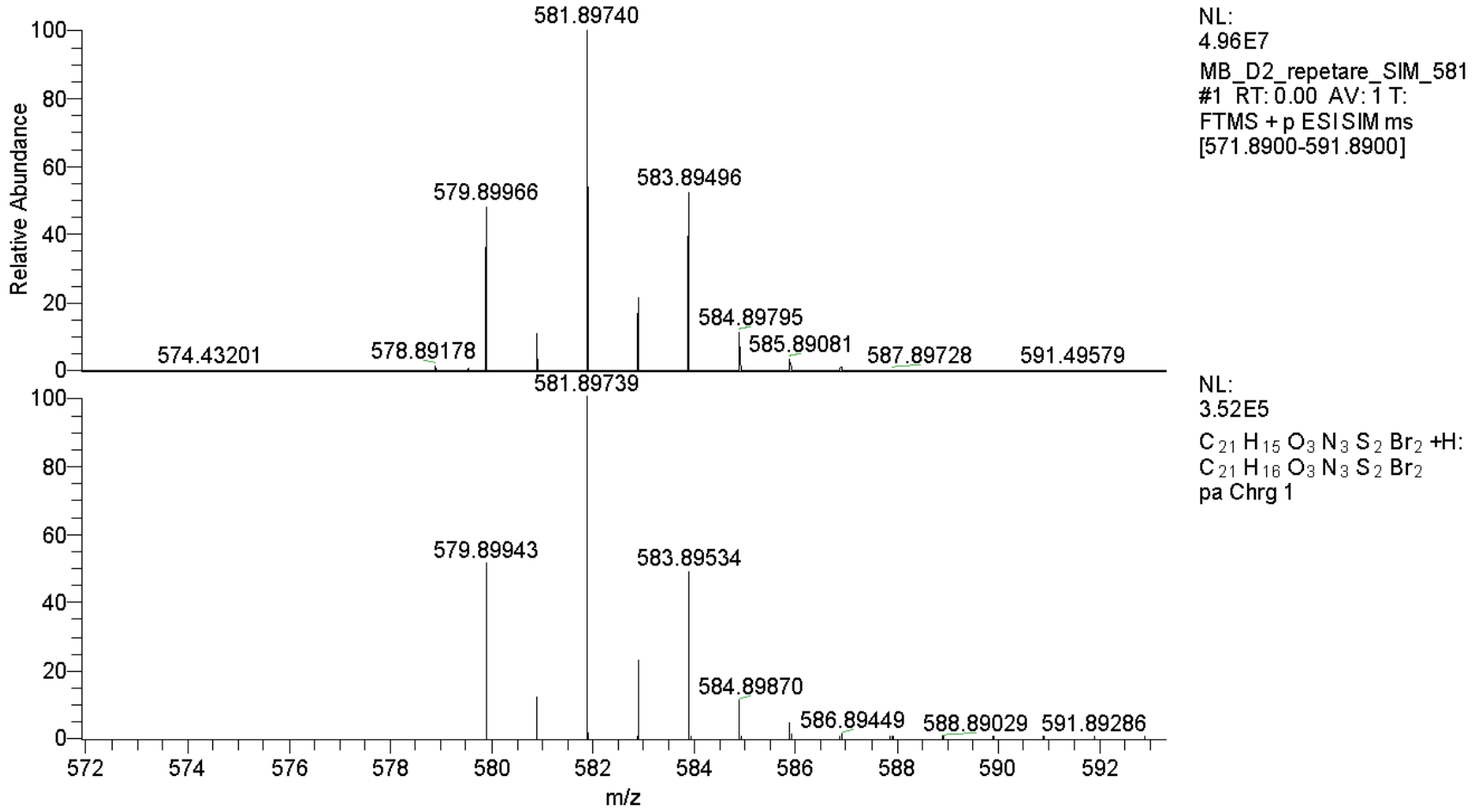


Figure S4. Mass analysis of **MB-D2**: ESI-HR-MS experimental spectrum (top); isotope simulation for predicted compound (bottom)

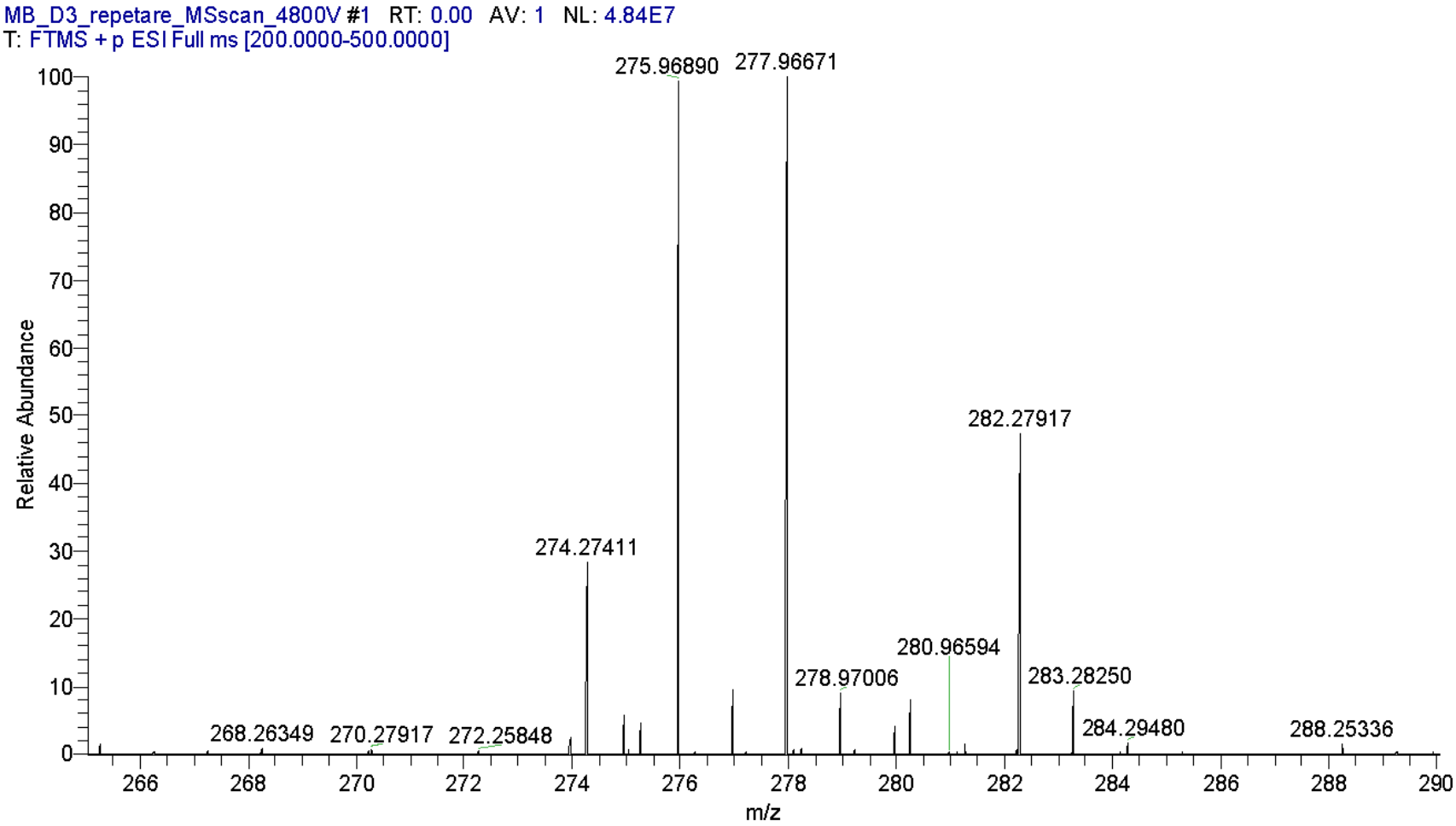


Figure S5. ESI-HR-MS spectrum of **MB-D3**

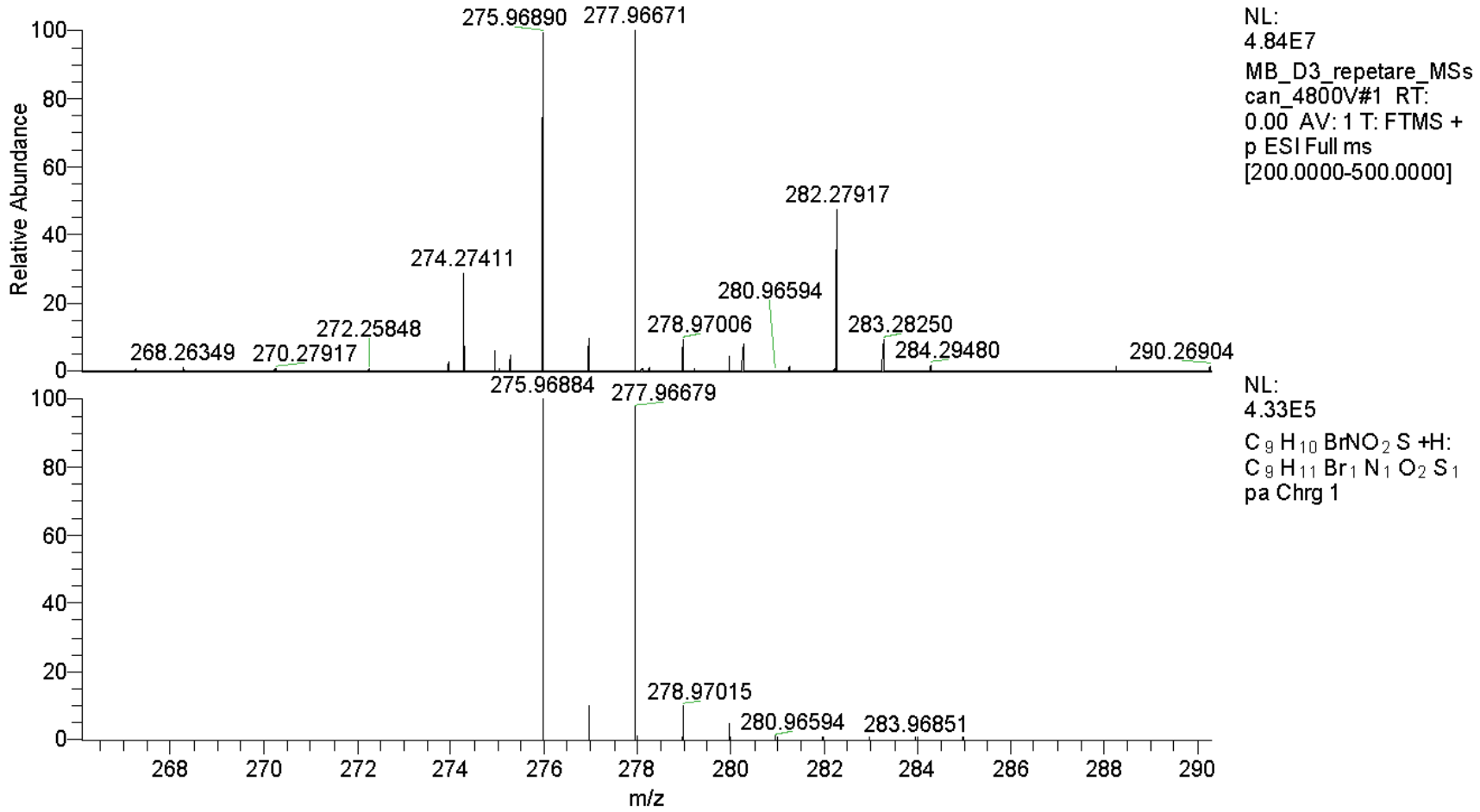


Figure S6. Mass analysis of **MB-D3**: ESI-HR-MS experimental spectrum (top); isotope simulation for predicted compound (bottom)

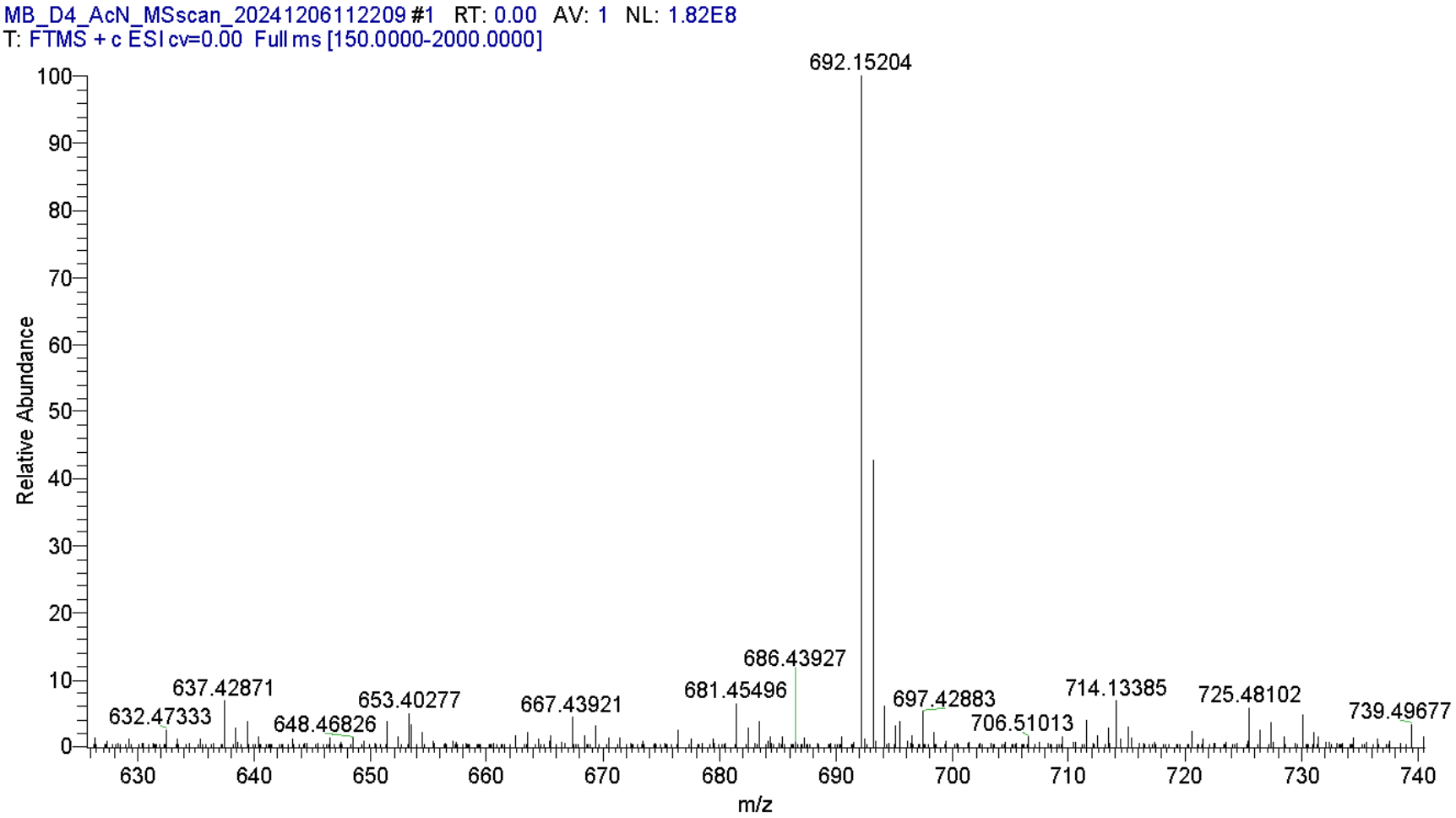


Figure S7. ESI-HR-MS spectrum of **MB-D4**

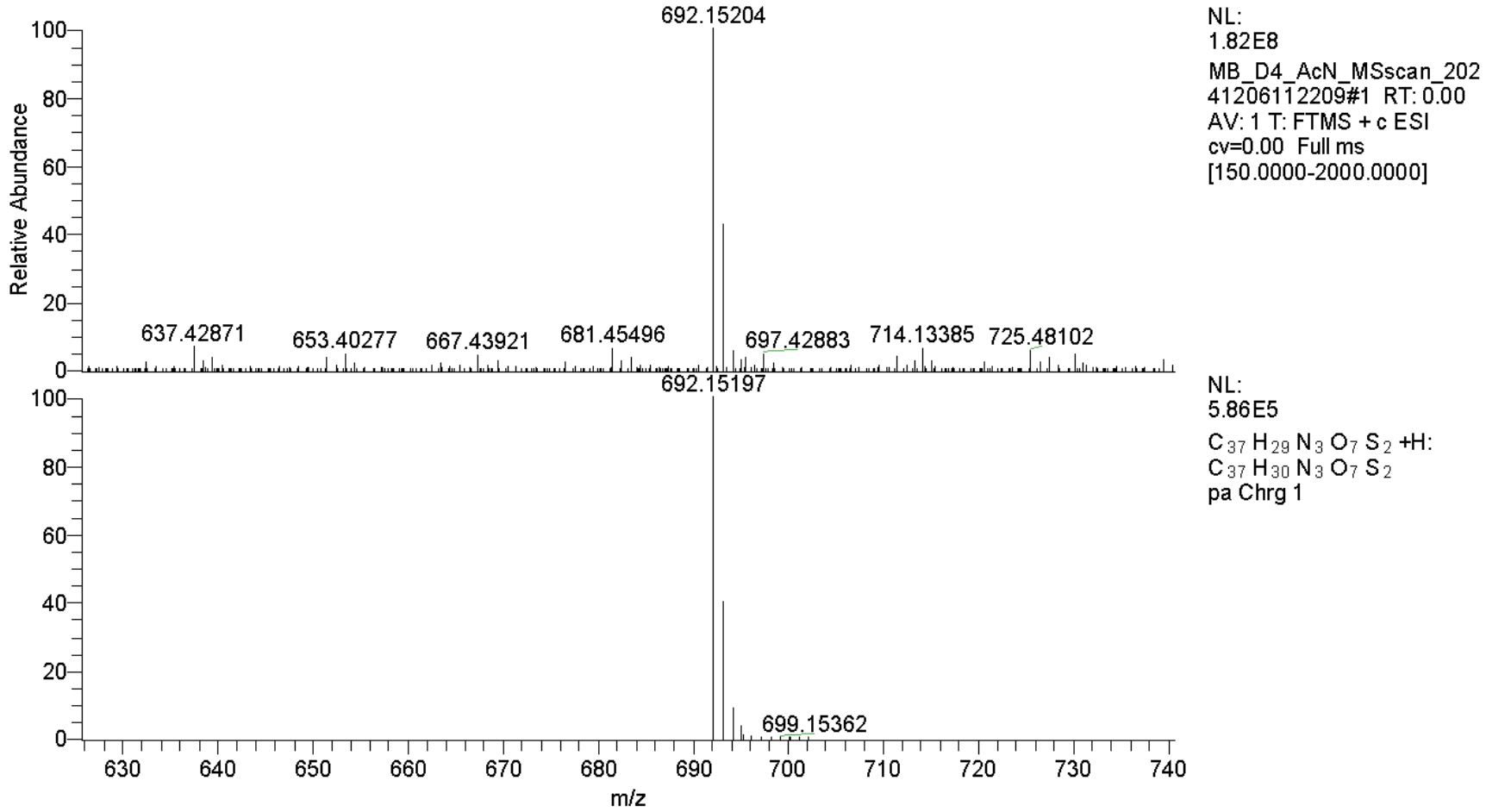


Figure S8. Mass analysis of **MB-D4**: ESI-HR-MS experimental spectrum (top); isotope simulation for predicted compound (bottom)

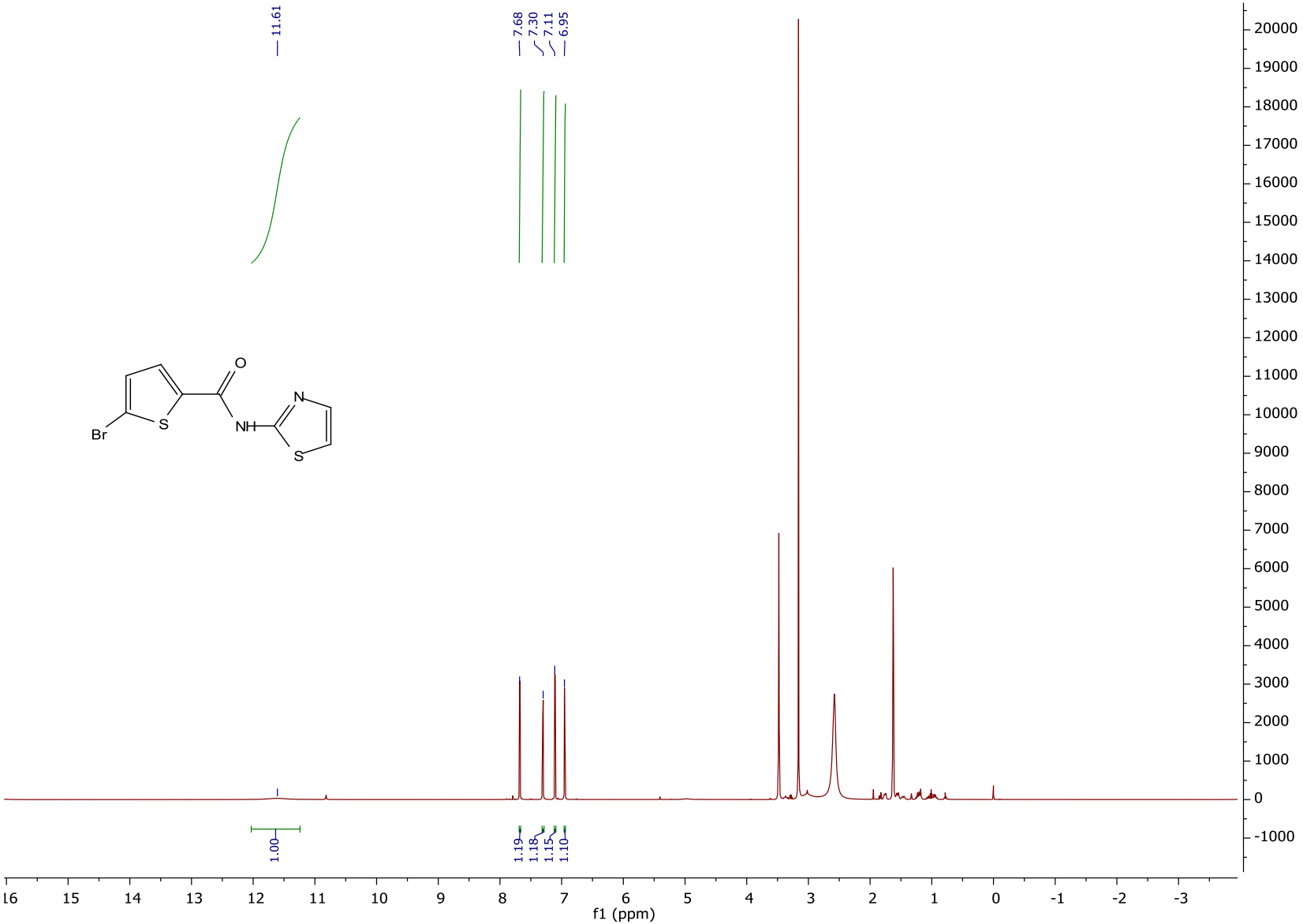


Figure S9. [1]H-NMR spectrum of **MB-D1** in THF-*d8*, (500 MHz), 298K

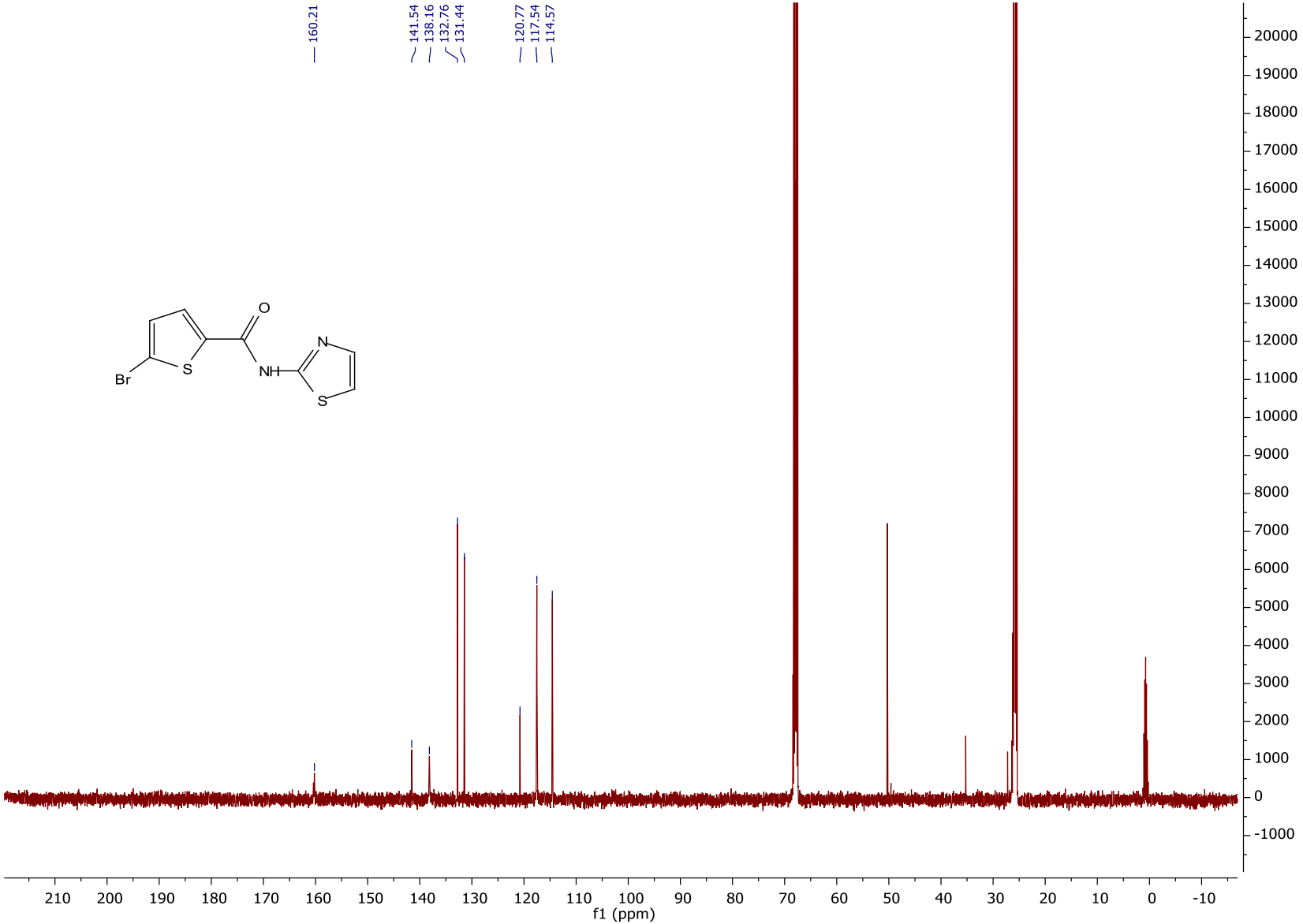


Figure S10. ^{13}C-NMR spectrum of **MB-D1** in THF-*d8*, (125 MHz), 298K

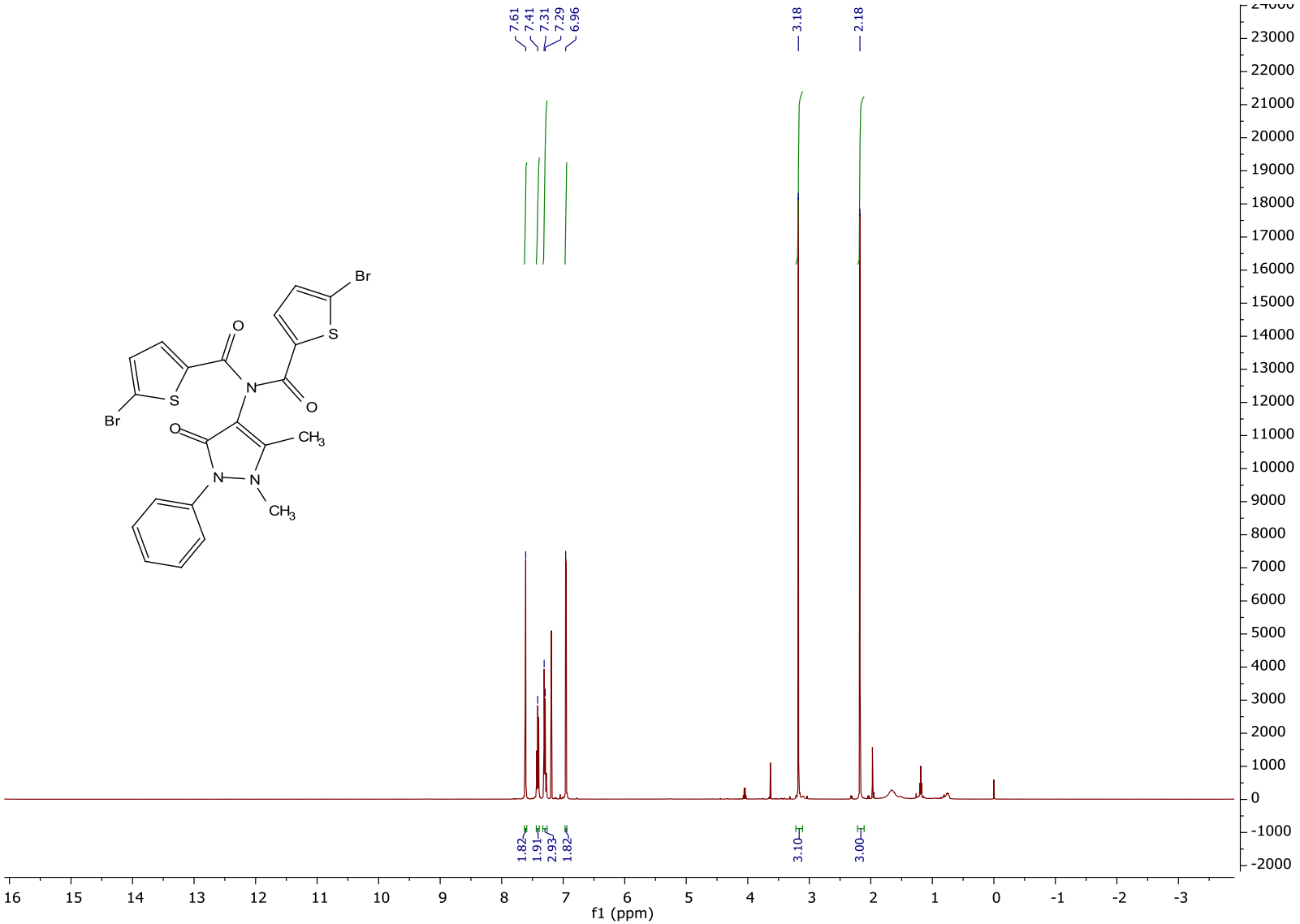


Figure S11. ^{1}H-NMR spectrum of **MB-D2** in $CDCl_3$, (500 MHz), 298K

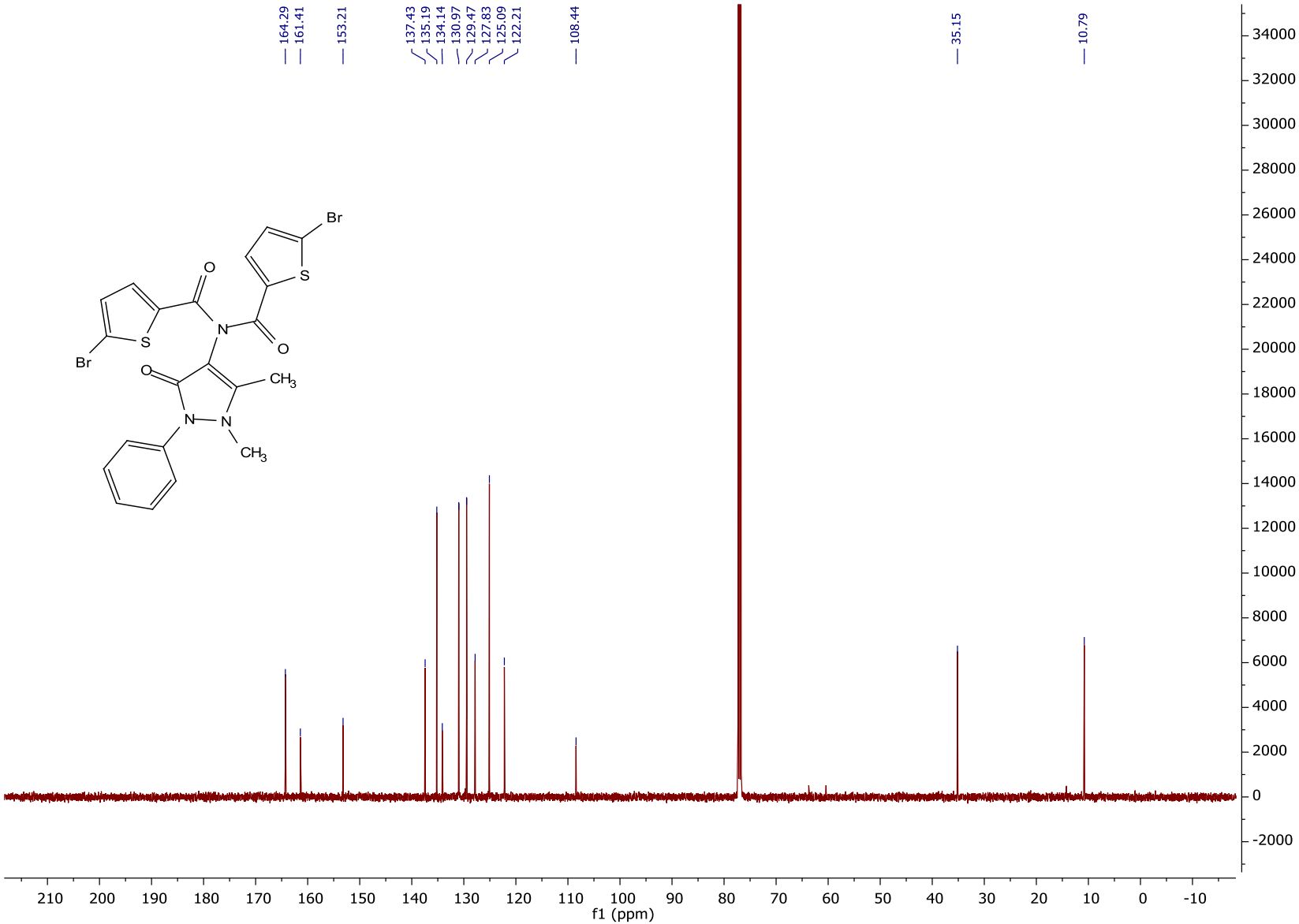


Figure S12. ^{13}C-NMR spectrum of **MB-D2** in $CDCl_3$, (125 MHz), 298K

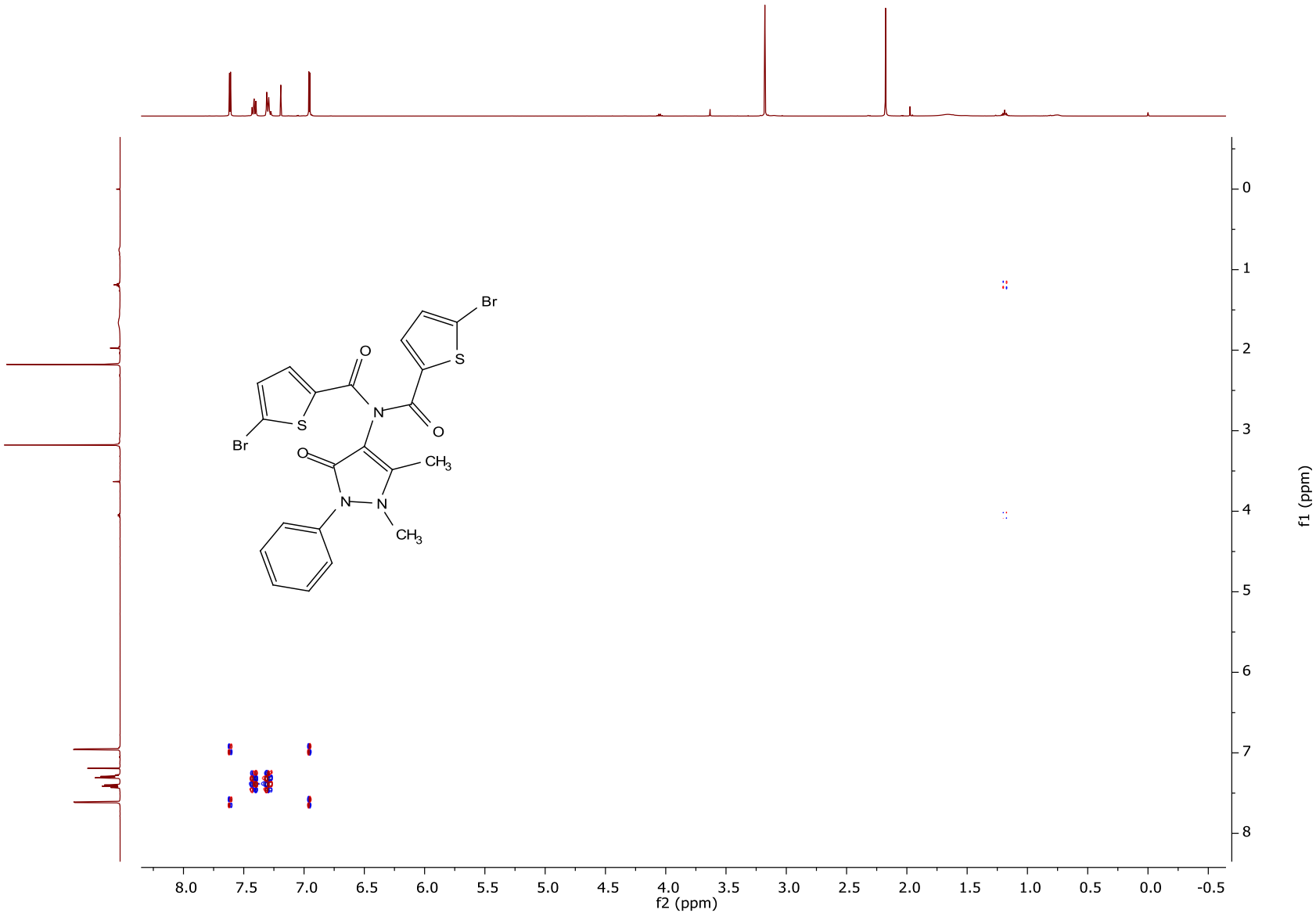


Figure S13. ^{1}H-^{1}H-COSY of **MB-D2** in $CDCl_3$, (125 MHz), 298K

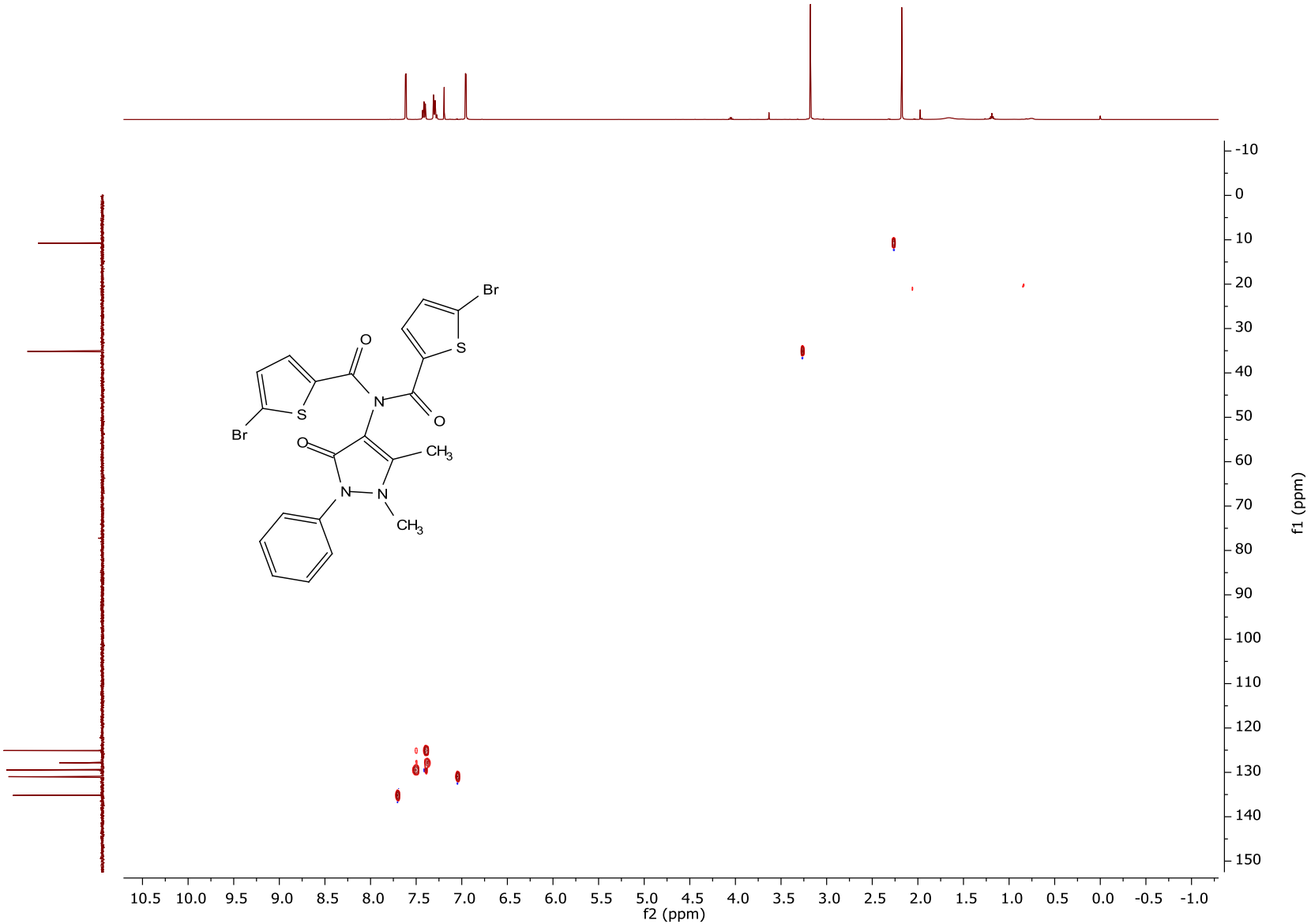


Figure S14. ^{1}H-^{13}C-HSQC of **MB-D2** in $CDCl_3$, (125 MHz), 298K

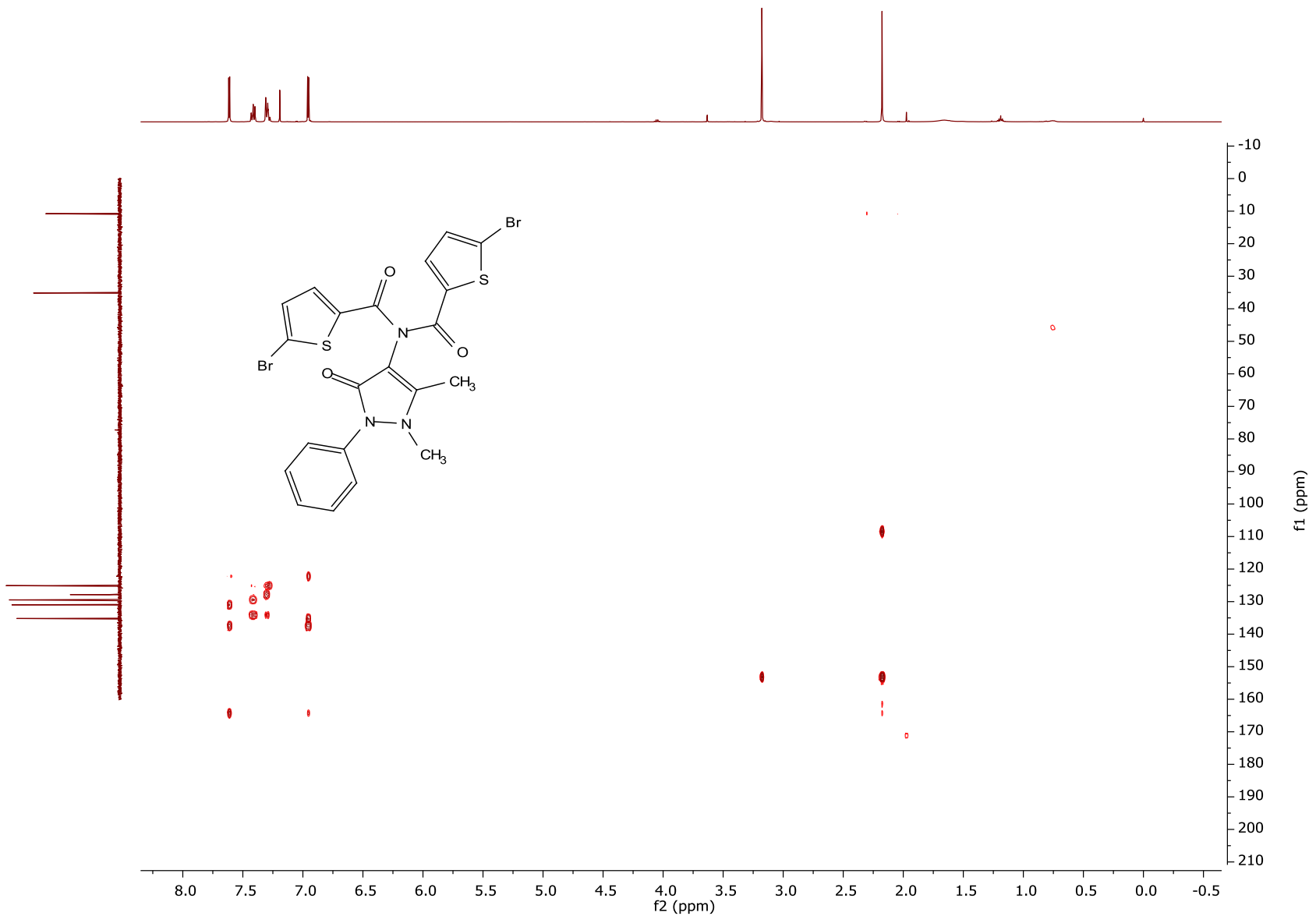


Figure S15. ^{1}H-^{13}C-HMBC of **MB-D2** in $CDCl_3$, (125 MHz), 298K

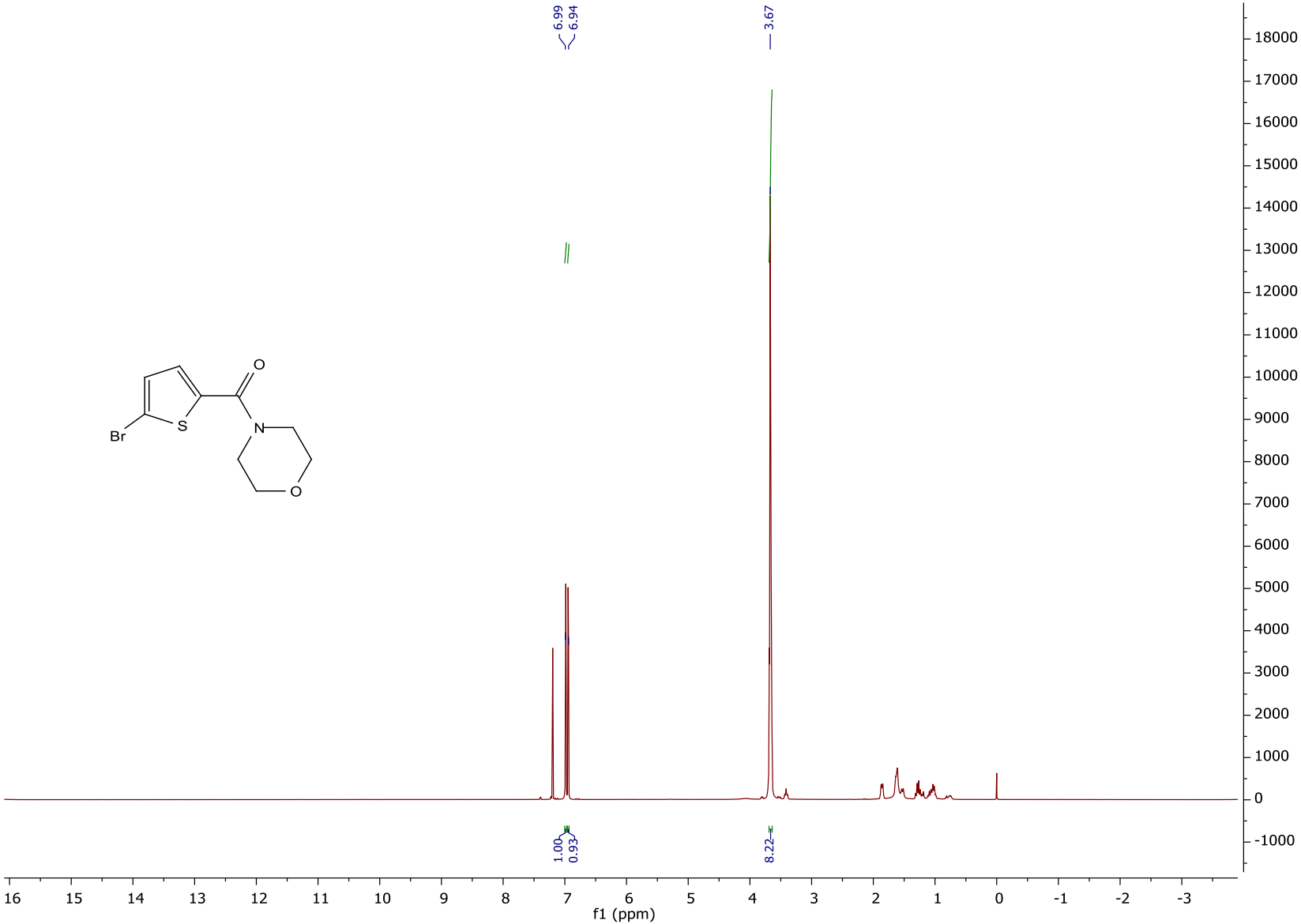


Figure S16. ^{1}H-NMR spectrum of **MB-D3** in $CDCl_3$, (500 MHz), 298K

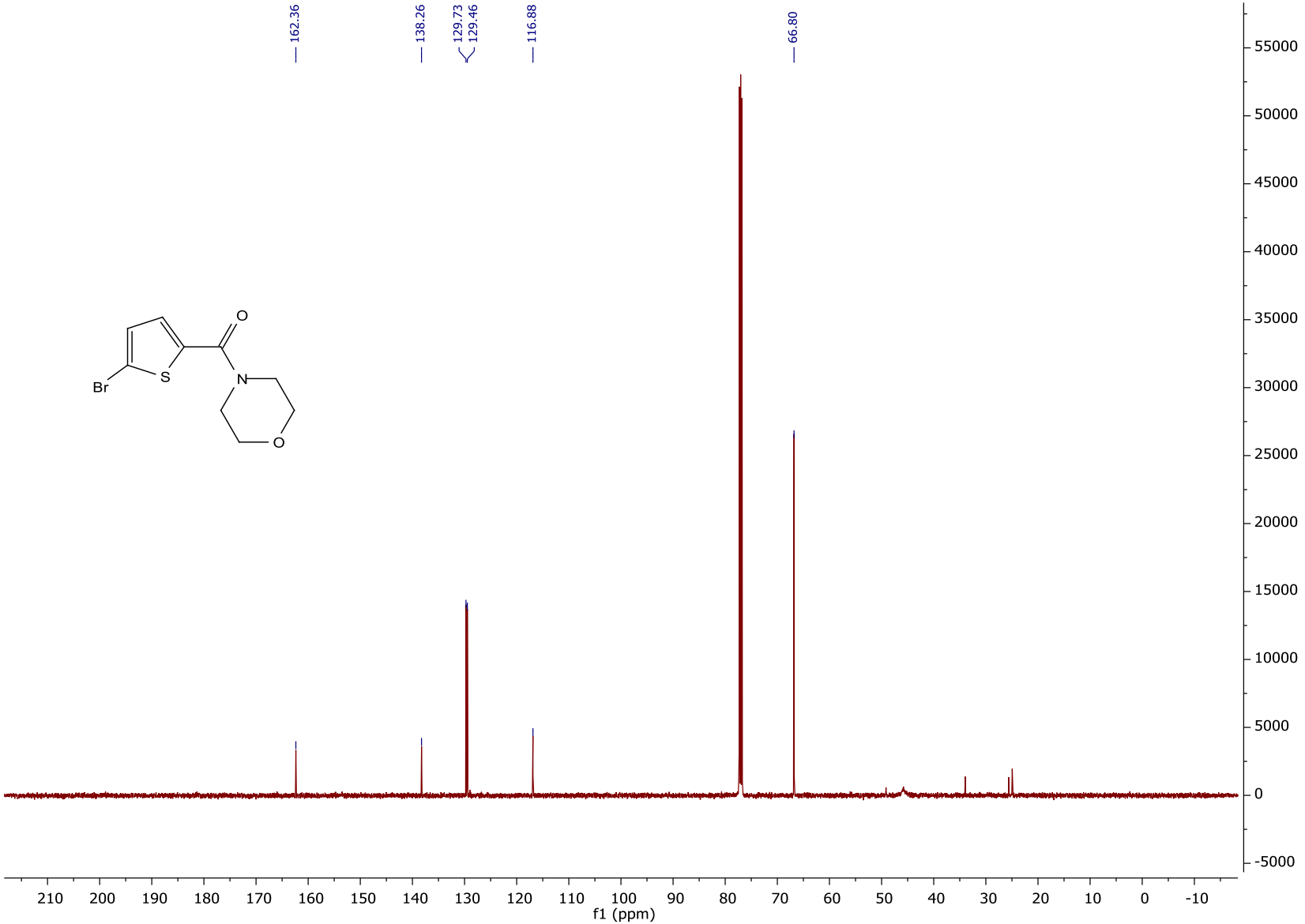


Figure S17. ^{13}C-NMR of **MB-D3** in $CDCl_3$, (125 MHz), 298K

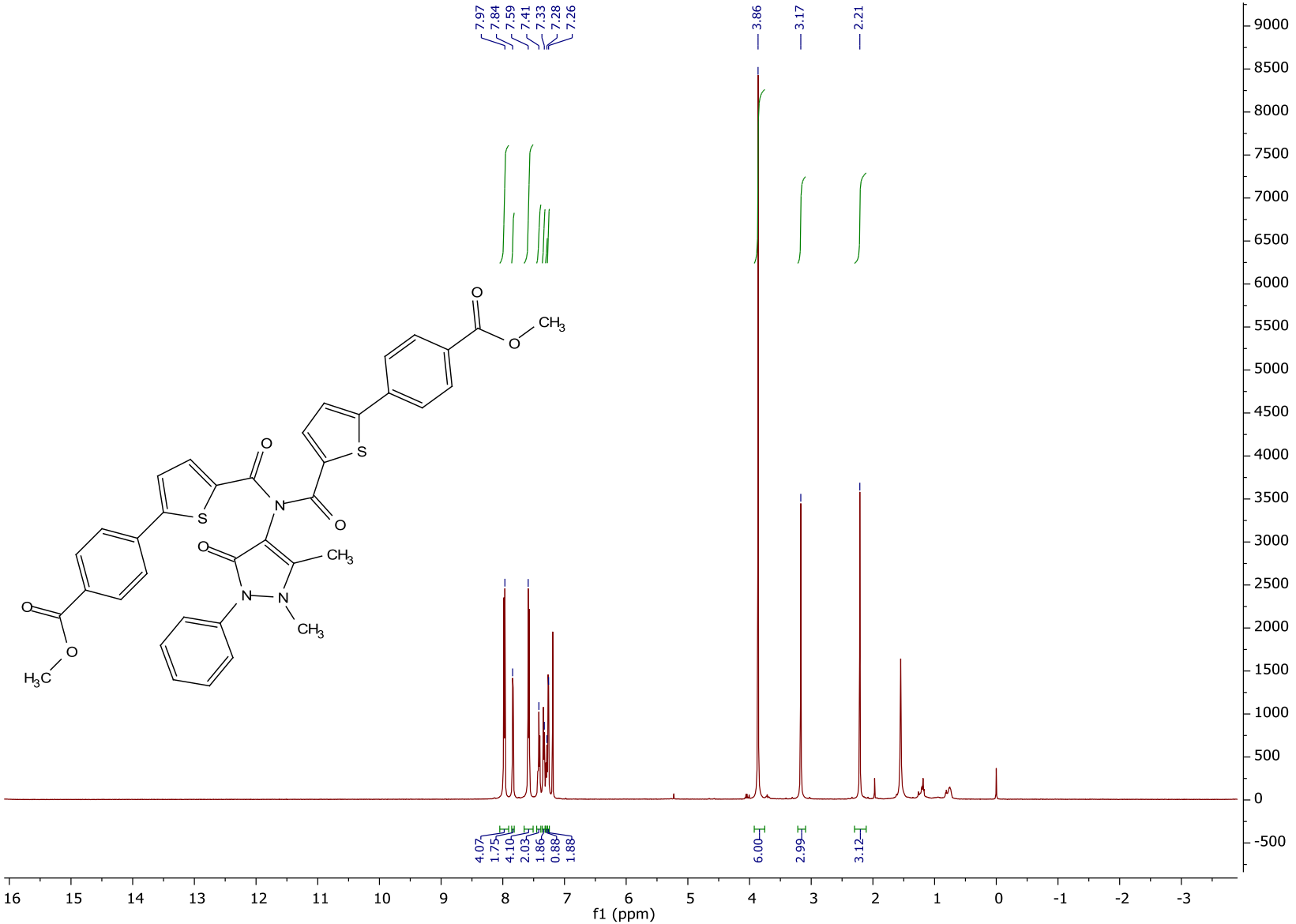


Figure S18. ^{1}H-NMR spectrum of **MB-D4** in $CDCl_3$, (500 MHz), 298K

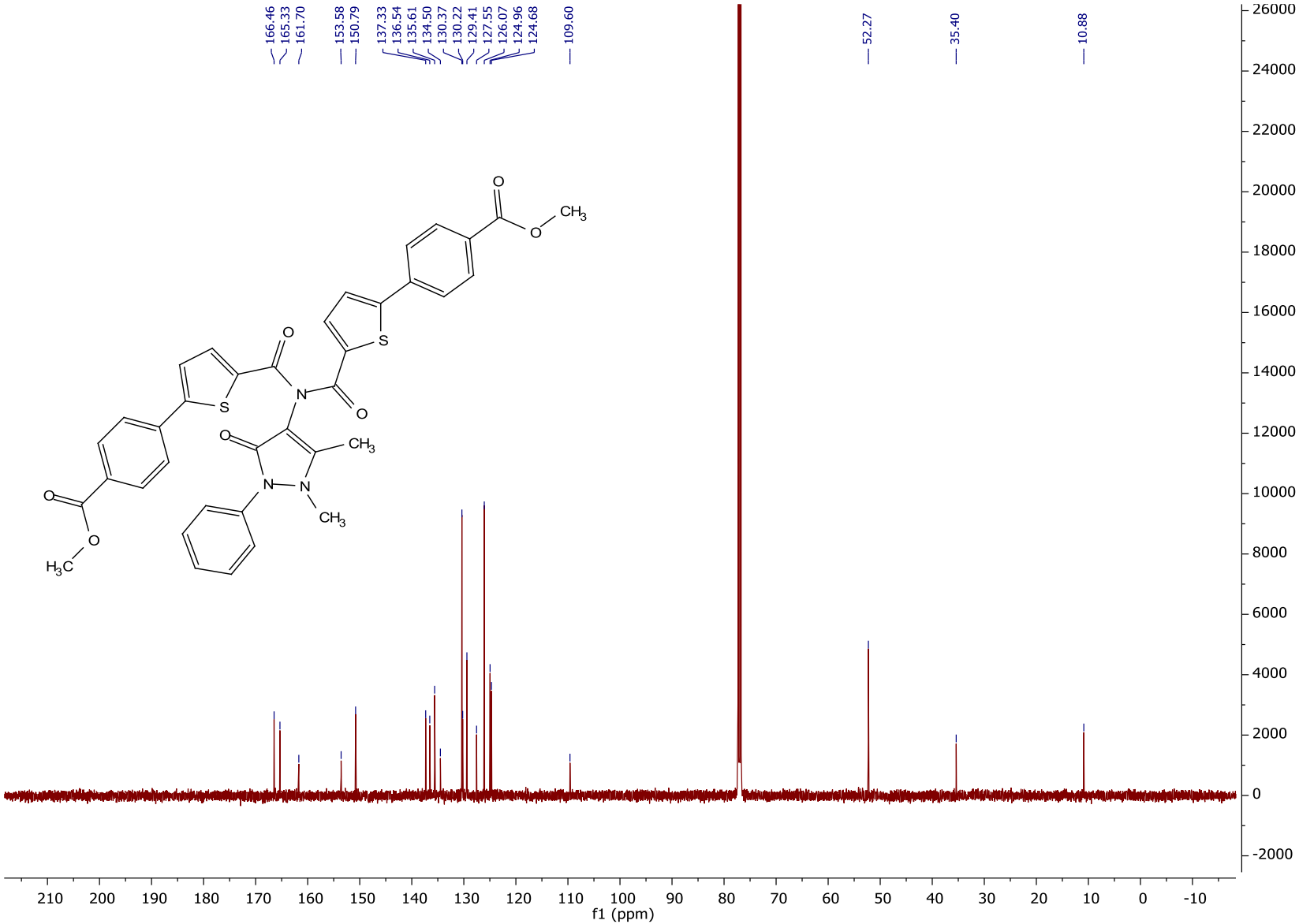


Figure S19. ^{13}C-NMR of **MB-D4** in $CDCl_3$, (125 MHz), 298K

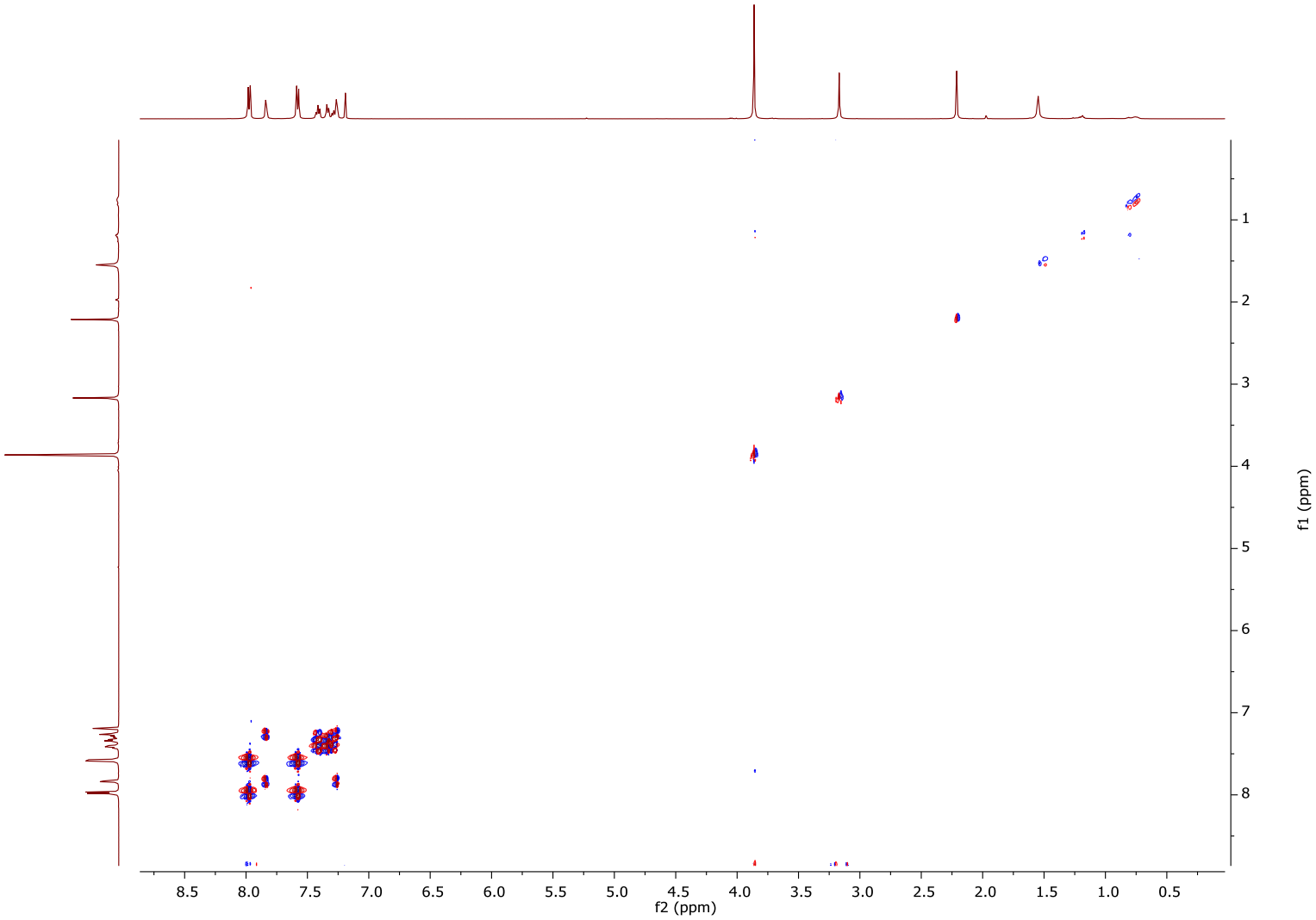


Figure S20. ^{1}H-^{1}H-COSY of **MB-D4** in $CDCl_3$, (125 MHz), 298K

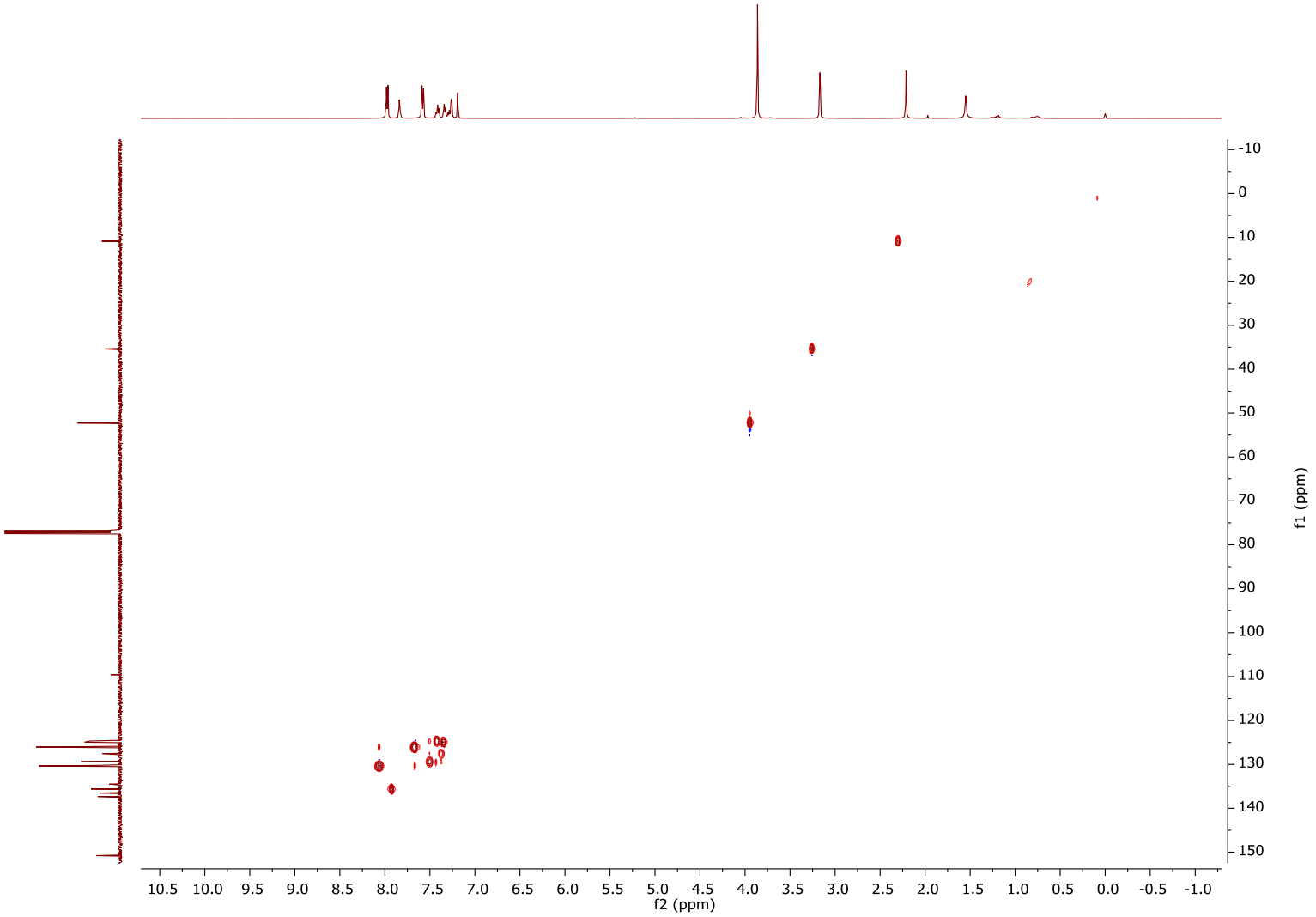


Figure S21. ^{1}H-^{13}C-HSQC of **MB-D4** in $CDCl_3$, (125 MHz), 298K

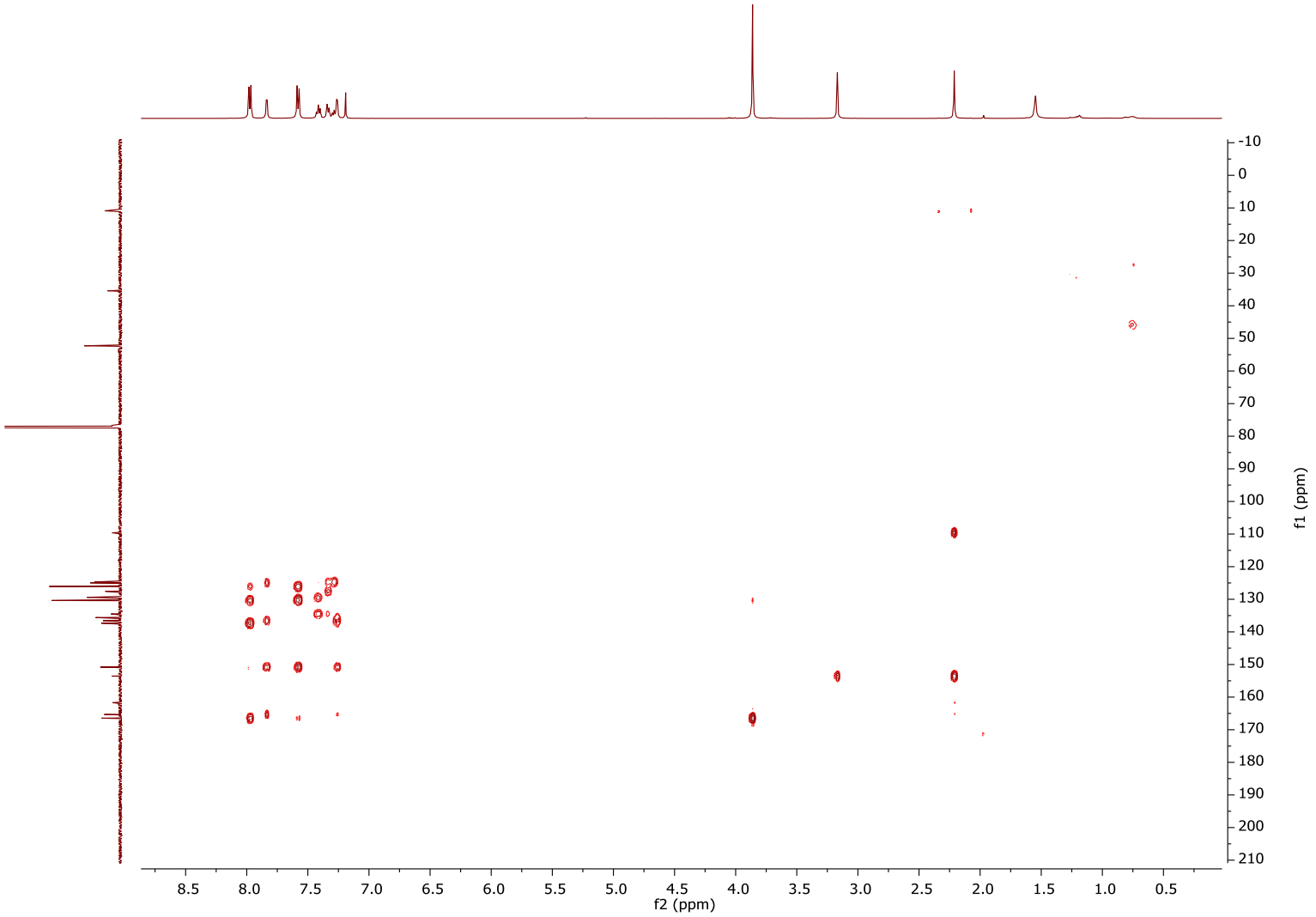
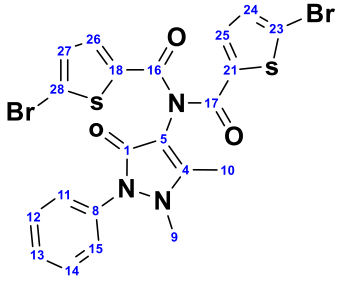


Figure S22. ^{1}H-^{13}C-HMBC of **MB-D4** in $CDCl_3$, (125 MHz), 298K

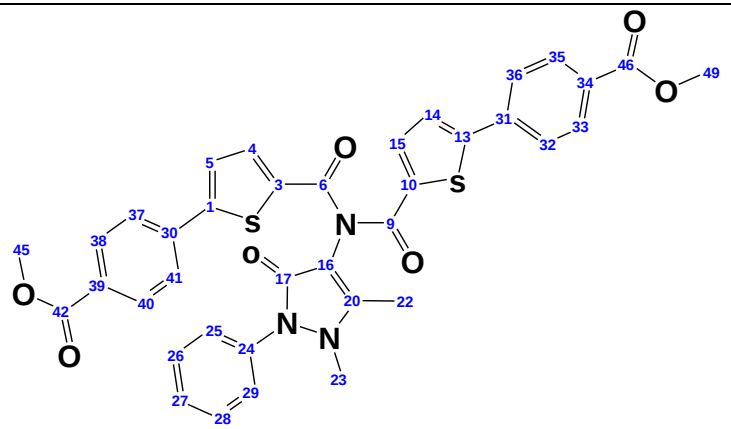
Table S1. MS source and acquisition parameters in positive mode

Source parameters	**Values**
Ionization mode	Positive electrospray ionization
Spray voltage	3500 - 4800 V
Sheath gas flow rate	5 Arb
Auxiliary gas flow rate	2 Arb
Sweep gas flow rate	0 Arb
Ion transfer tube temperature	300℃
Vaporizer temperature	20℃
Acquisition parameters	**Values**
Detector type	Orbitrap
Orbitrap resolution	120000
Scan range	150-1000 m/z
AGC target	100 %
Injection time	100 ms
Syringe flow	5 μl/min

Tabel S2. 1D and 2D -NMR full peak assignment of **MB-D2**

			
Position	**^{1}H δ/ppm (J/Hz)**	**^{13}C δ/ppm**	**HMBC**
25;26	7.61 (d, J = 4.1 Hz, 2H)	135.2	H24, H27
12;14	7.41 (m, 2H)	129.5	H12, H14
11;15	7.31 (d, J = 2.2 Hz, 2H)	125.1	H12, H13, H14
13	7.29 (m, 1H)	127.8	H11, H15
24;27	6.96 (d, J = 4.1 Hz, 2H)	131.0	H25, H26
9	3.18 (s, 3H)	35.2	-
10	2.18 (s, 3H)	10.8	-
16;17	-	164.3	H10, H24, H25, H26, H27
1	-	161.4	H10
4	-	153.2	H9, H10
18;21	-	137.4	H24, H25, H26, H27
8	-	134.1	H12, H14
23;28	-	122.2	H24, H25, H26, H27
5	-	108.44	H10

Tabel S3. 1D and 2D -NMR full peak assignment of **MB-D4**



Position	^{1}H δ/ppm (J/Hz)	^{13}C δ/ppm	HMBC
35;33;40;38	7.97 (m, 4H)	130.4	H35, H33, H40, H38, H41, H37, H36, H32
4;15	7.84 (d, J= 4.0 Hz, 2H)	135.6	H5, H14
36;32;41;37	7.59 (d, J = 8.4 Hz, 4H)	126.1	H33, H35, H40, H38, H36, H32, H41, H37
26;28	7.41 (t, J = 7.6 Hz, 2H)	129.4	H26, H28, H32, H33, H35, H36, H37, H38, H40, H41
25;29	7.33 (d, J = 7.8 Hz, 2H)	124.7	H4, H15, H5, H14, H25, H27, H29
27	7.28 (d, J = 7.4 Hz, 1H)	127.6	H25,H29
5;14	7.26 (d, J = 4.1 Hz, 2H)	125.0	H4, H15, H25, H27, H29
45;49	3.86 (s, 6H)	52.3	-
23	3.17 (s, 3H)	35.4	-
22	2.21 (s, 3H)	10.9	-
42;46	-	166.5	H49, H45, H40, H38, H35, H33, H41, H37, H36, H32

6;9	-	165.3	H4, H15
17	-	161.7	-
20	-	153.6	H23
1;13	-	150.8	H4, H5, H14, H15, H32, H36, H37, H41
30;31	-	137.3	H4, H5, H14, H15, H33, H35, H38, H40
3;10	-	136.5	H4, H5, H14, H15
4;15	-	135.6	H5, H14
24	-	134.5	H26, H28
35;33;40;38	-	130.4	H35, H33, H40, H38, H41, H37, H36, H32
34;39	-	130.2	H32, H33, H35, H36, H37, H38, H40, H41
16	-	109.6	H22