Supplementary Materials: 2-(2-Phenylethyl)chromone Derivatives of Agarwood Originating from *Gyrinops salicifolia*

Hang Shao, Wen-Li Mei, Wen-Hua Dong, Cui-Juan Gai, Wei Li, Guo-Peng Zhu and Hao-Fu Dai

Contents

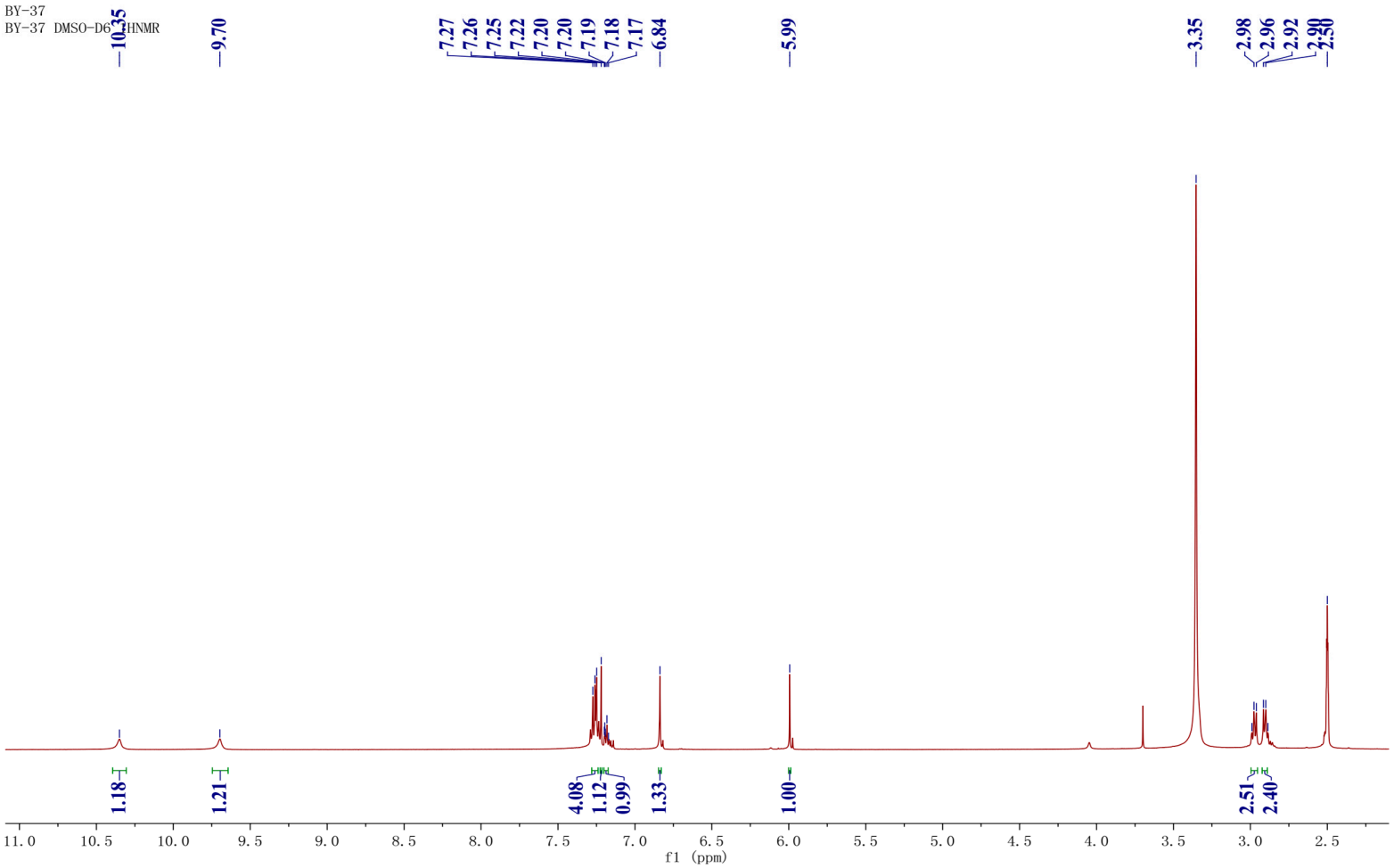


Figure S1. ^{1}H-NMR spectrum (500 MHz) of compound **1** in DMSO.

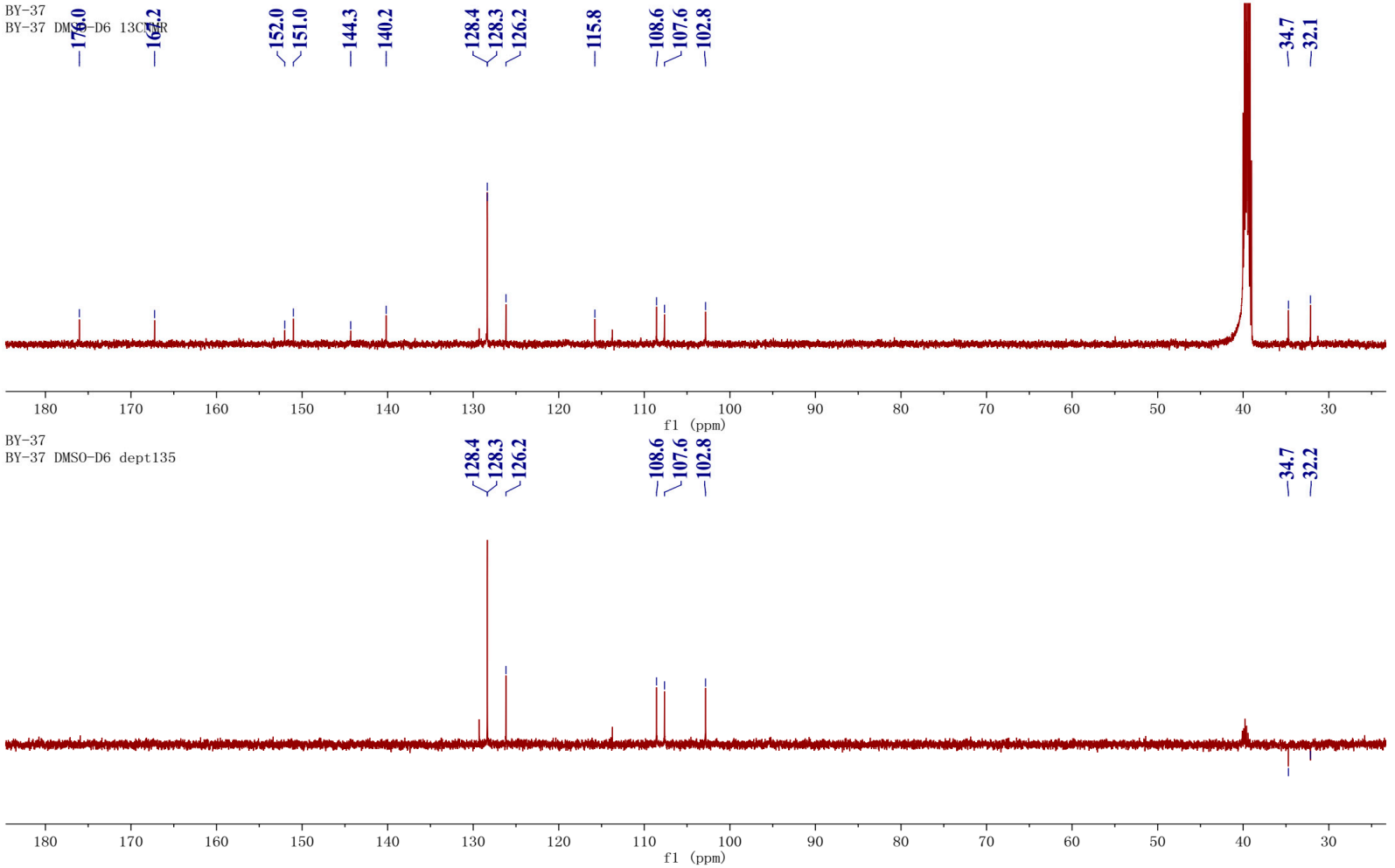


Figure S2. ^{13}C-NMR spectrum (125 MHz) of compound **1** in DMSO.

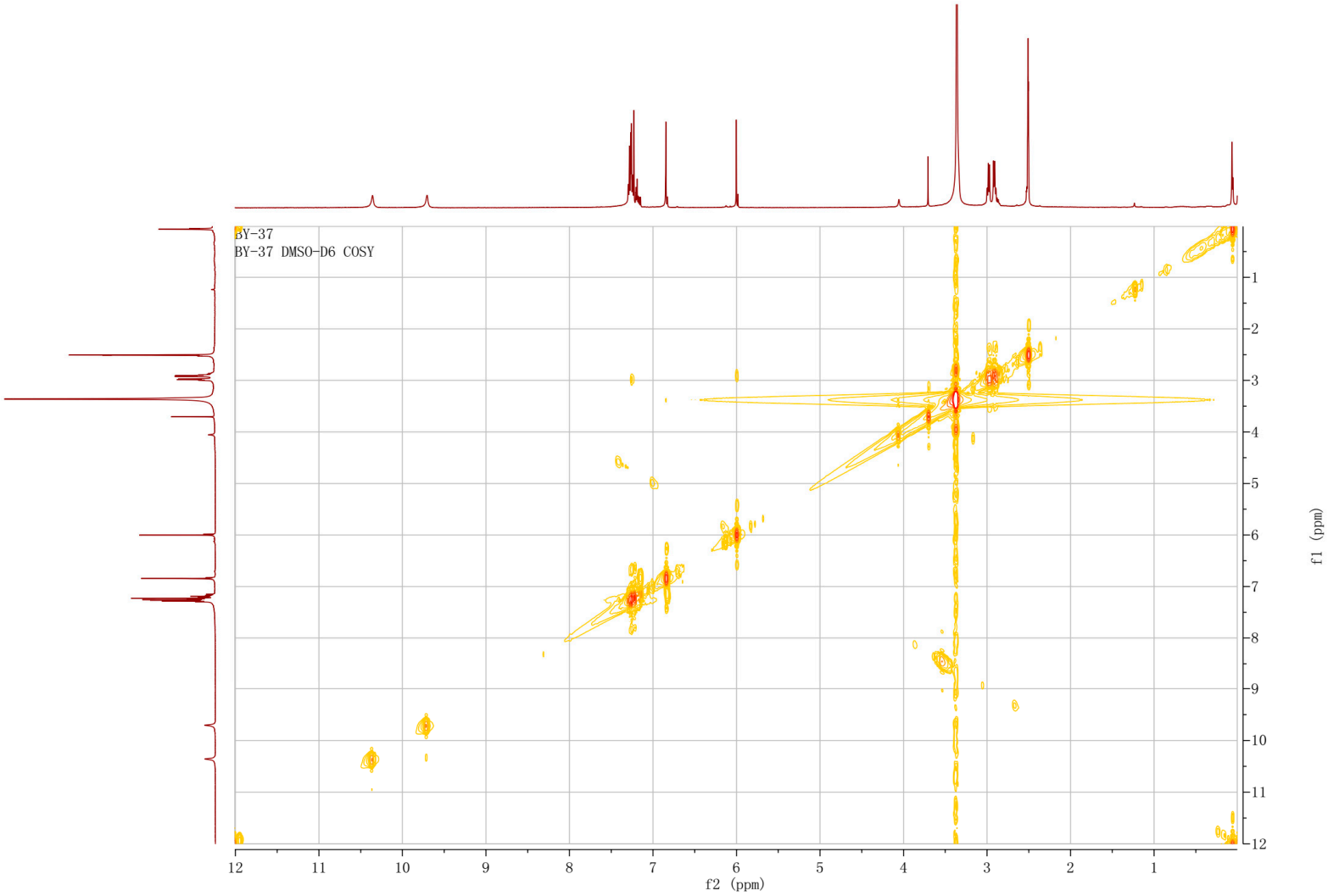


Figure S3. ^{1}H-^{1}H COSY spectrum (500 MHz) of compound **1** in DMSO.

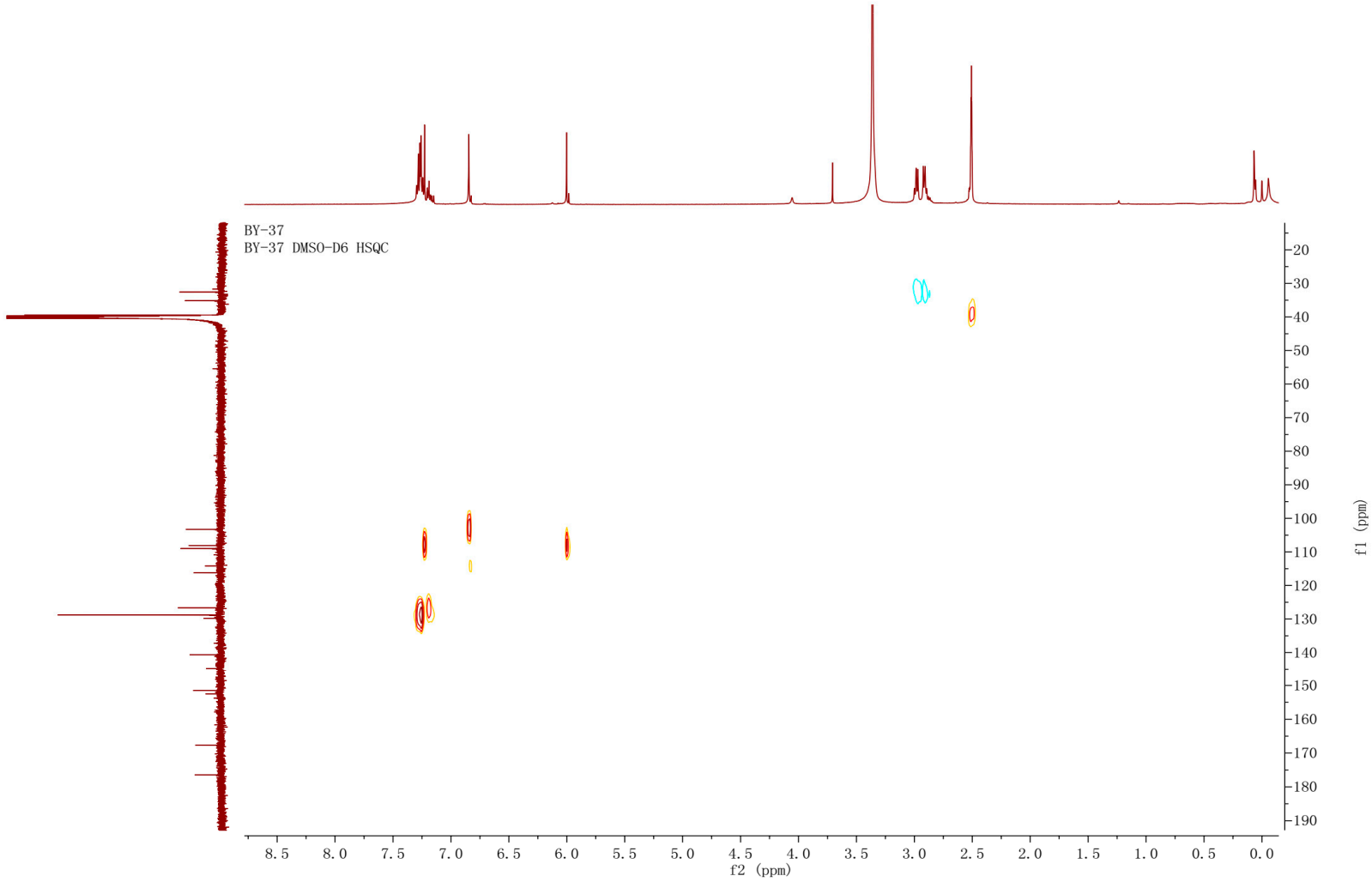


Figure S4. HSQC spectrum (500 MHz) of compound **1** in DMSO.

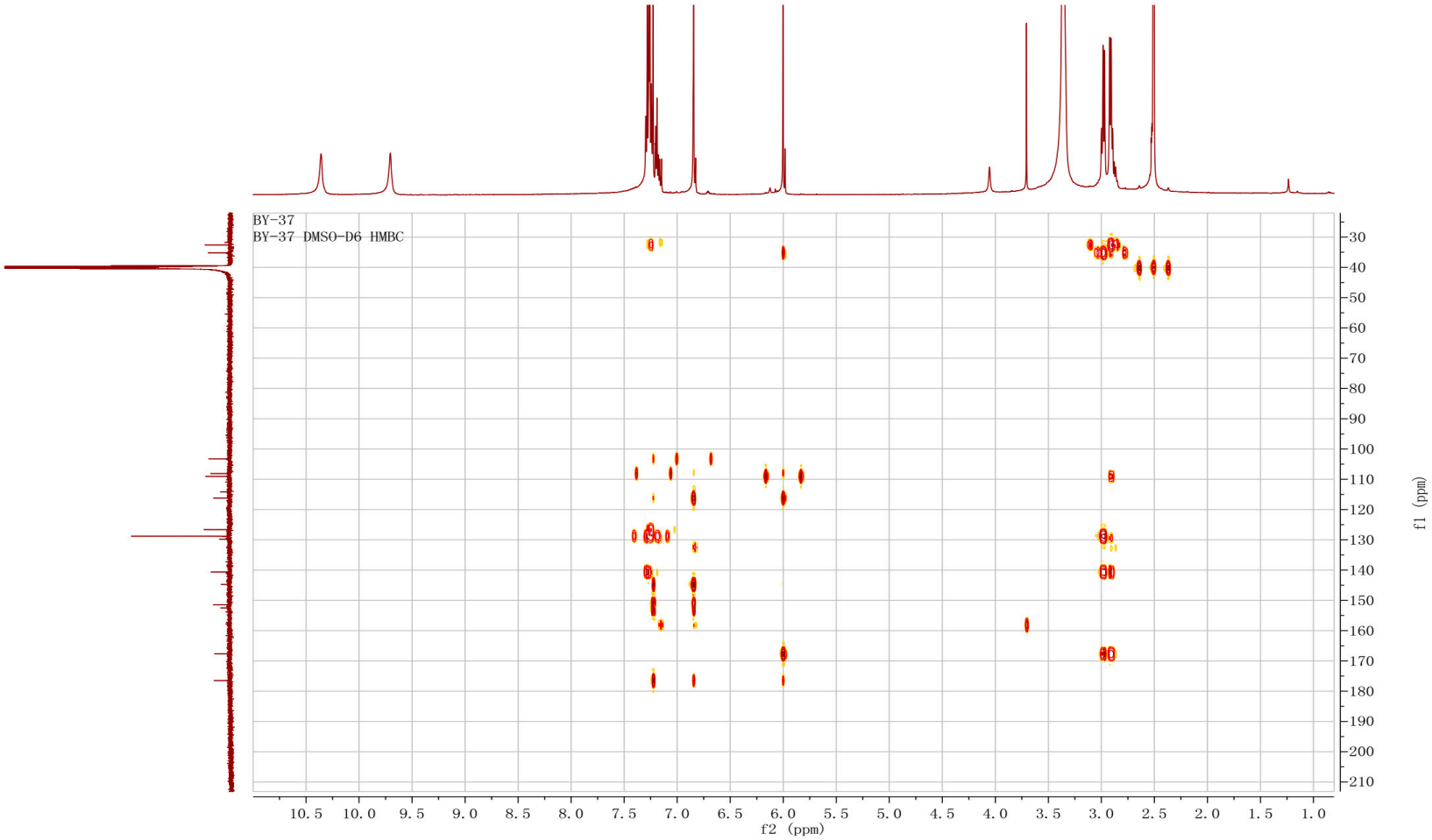


Figure S5. HMBC spectrum (500 MHz) of compound **1** in DMSO.

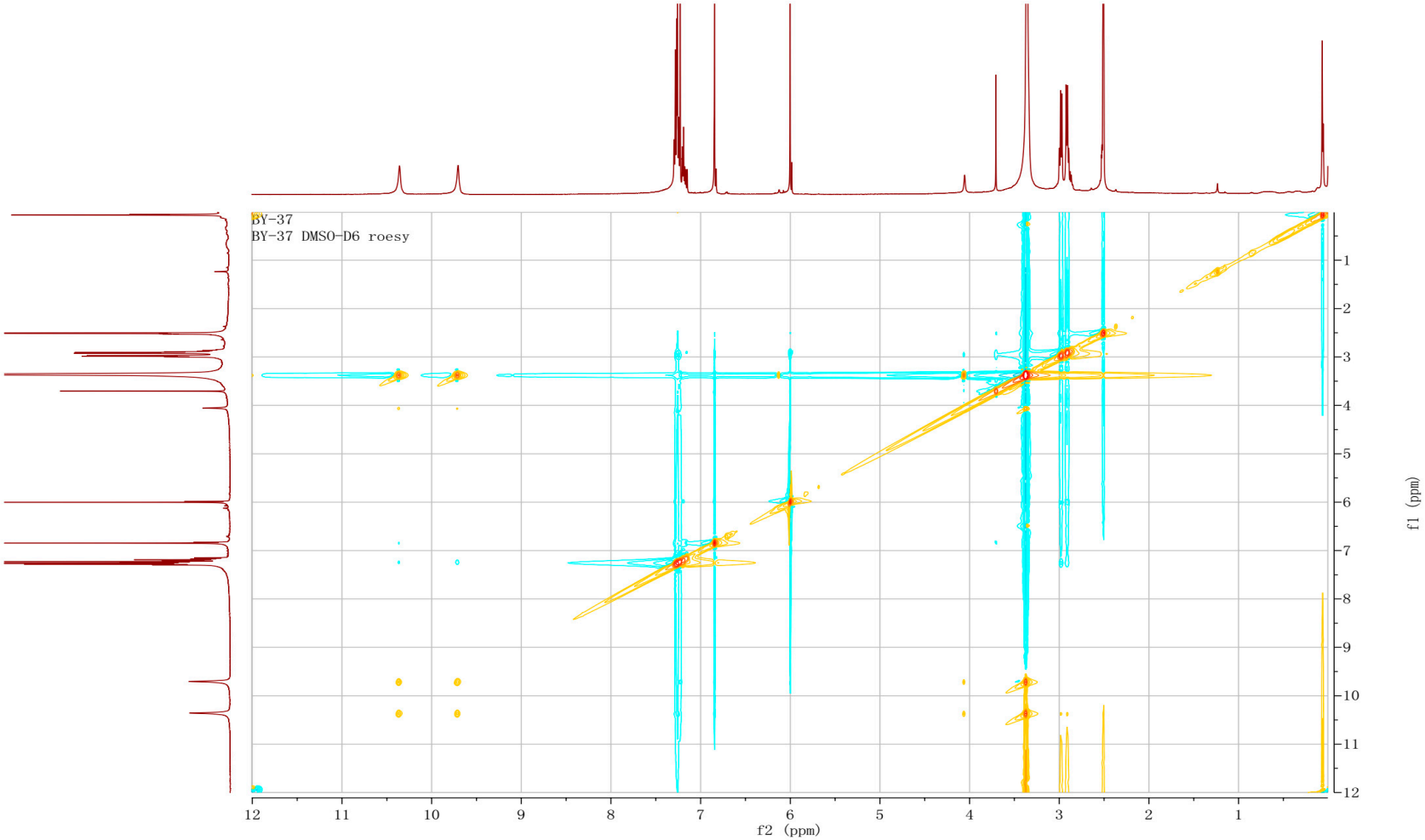


Figure S6. ROESY spectrum (400 MHz) of compound **1** in DMSO.

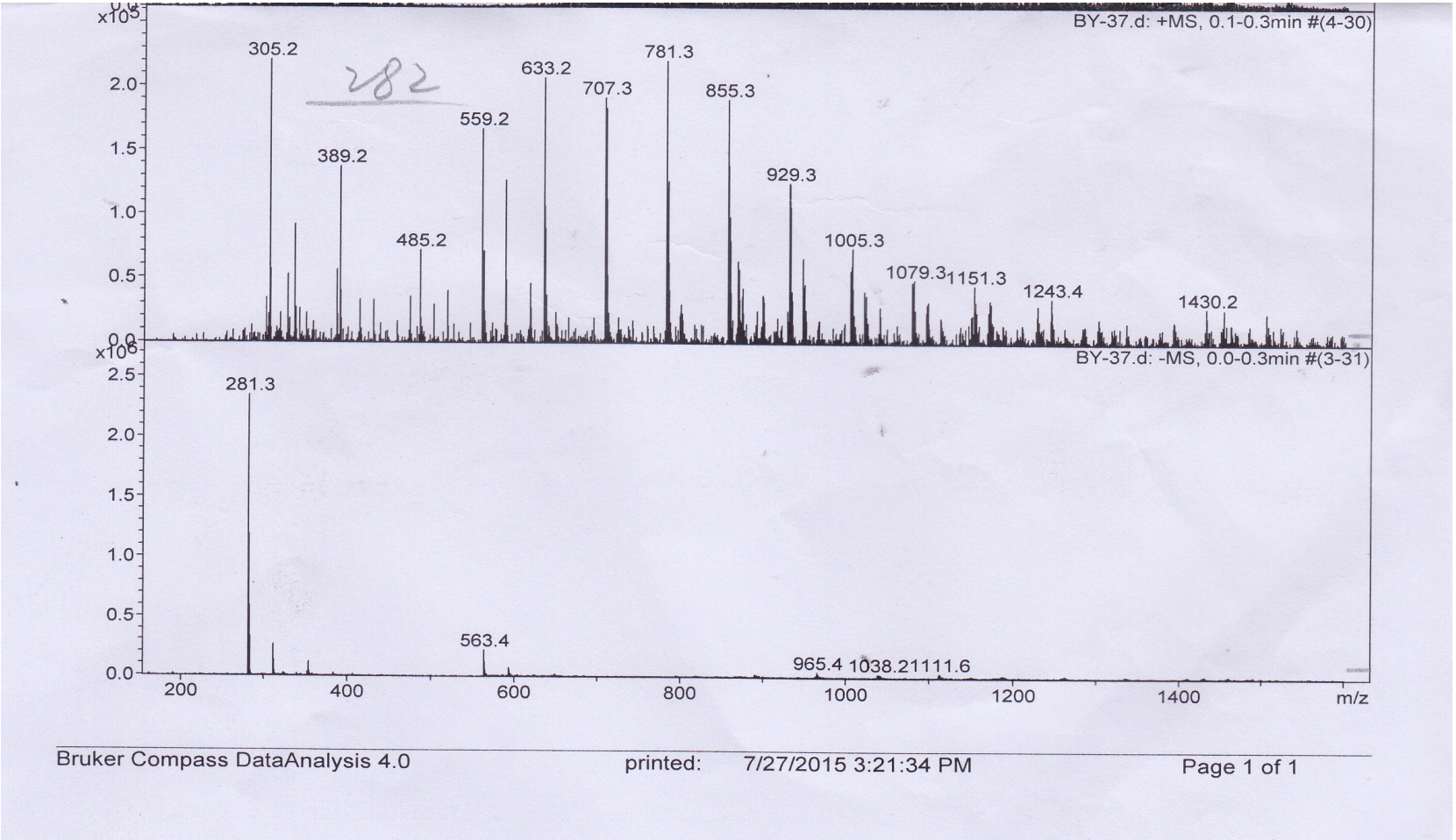


Figure S7. ESI(+)MS spectrum of compound **1**.

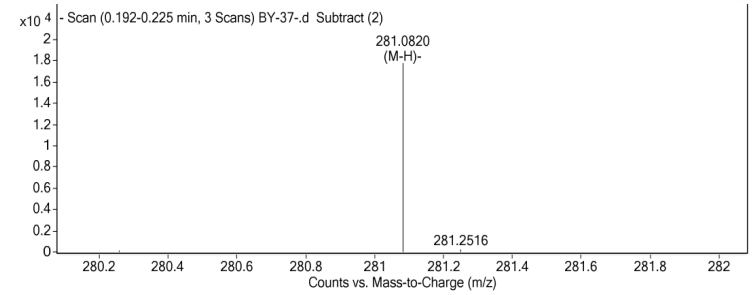
Qualitative Analysis Report

Data Filename	BY-37-.d	**Sample Name**	BY-37
Sample Type	Sample	**Position**	P1-C1
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU-ESI-i.m	**Acquired Time**	10/22/2015 3:18:42 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
281.082	1	17761.73	C17 H14 O4	(M-H)-
282.0851	1	3844.94	C17 H14 O4	(M-H)-
311.0921	1	4198.39		
395.0744	1	31143.69		
396.0783	1	6990.37		
397.0799	1	1059.28		
425.0846	1	10681.58		
426.0884	1	2398.21		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C17 H14 O4	282.0892	281.0819	281.0820	0.0	-0.1	11.0000

--- End Of Report ---

Figure S8. HRESI(+)MS spectrum of compound **1**.

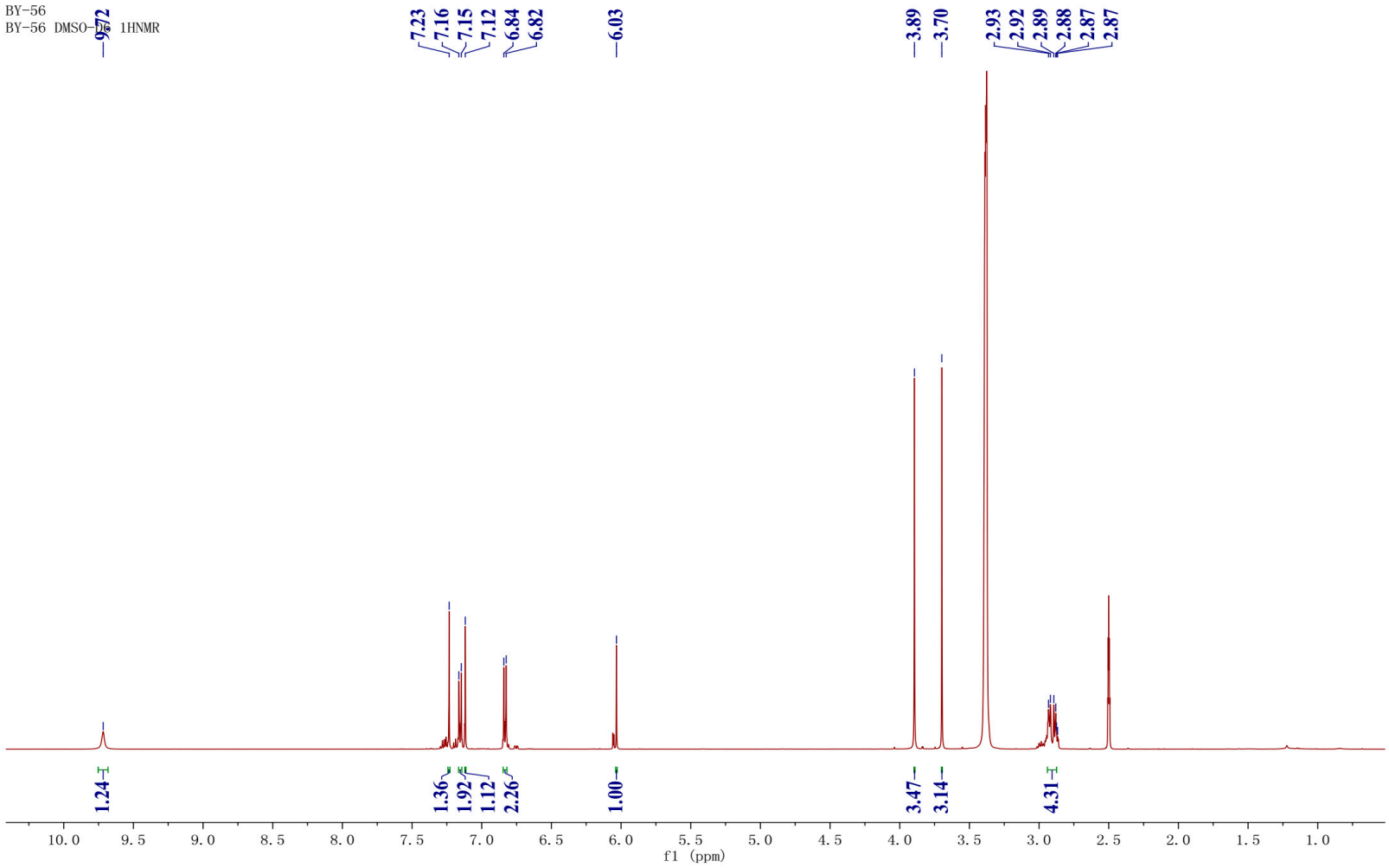


Figure S9. ^{1}H-NMR spectrum (500 MHz) of compound **2** in DMSO.

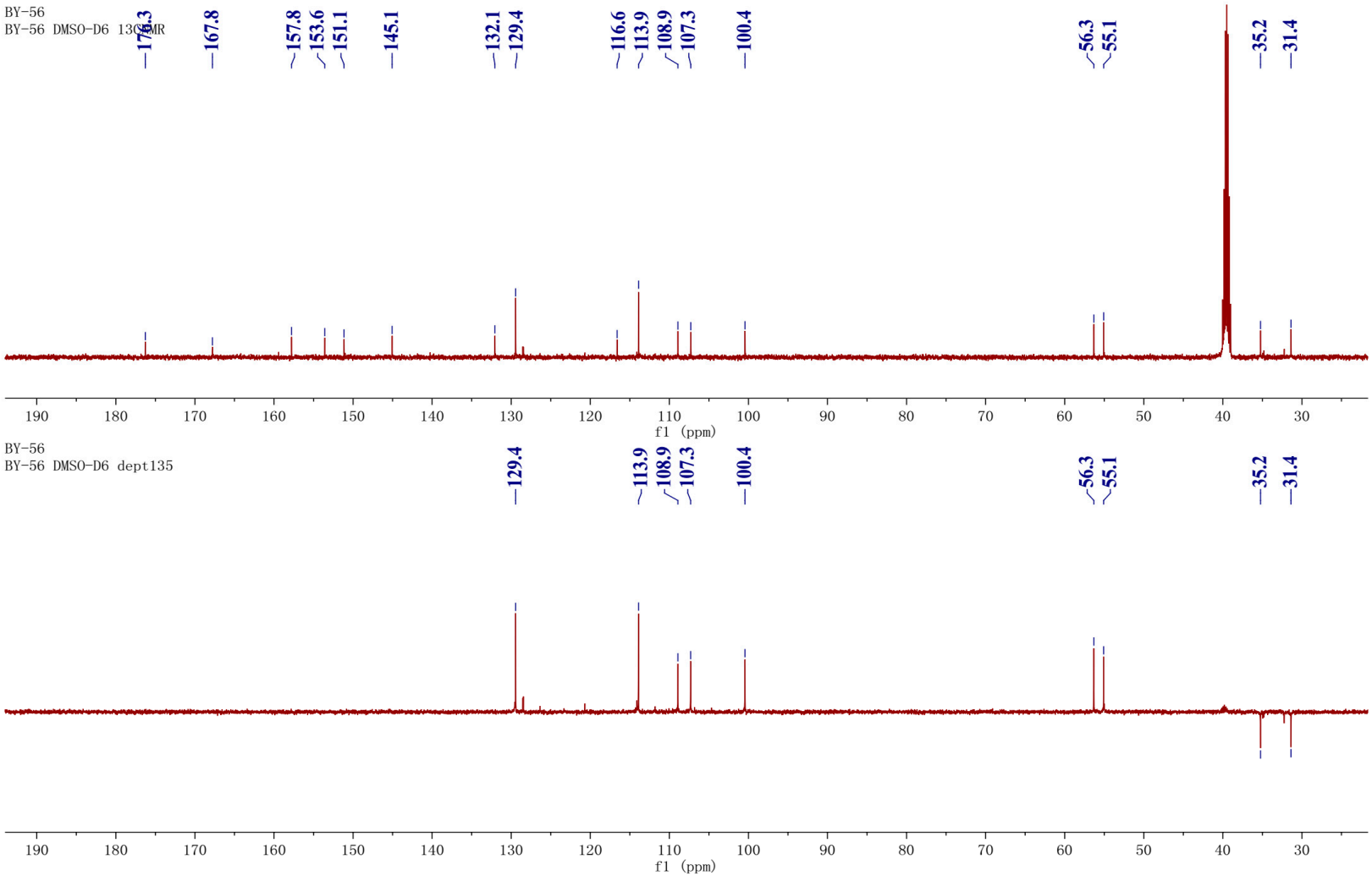


Figure S10. ^{13}C-NMR spectrum (125 MHz) of compound **2** in DMSO.

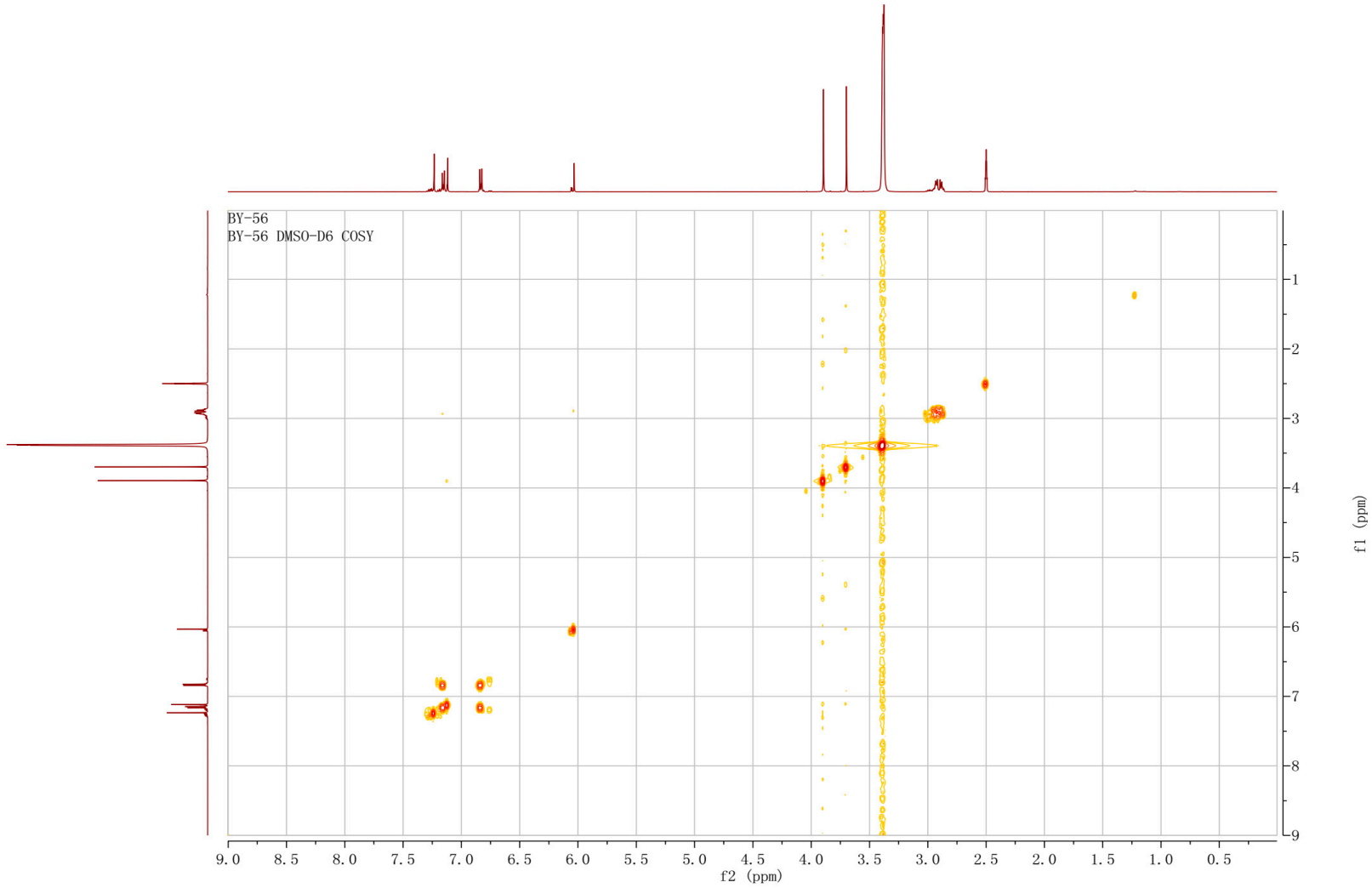


Figure S11. ^{1}H-^{1}H COSY spectrum (500 MHz) of compound **2** in DMSO.

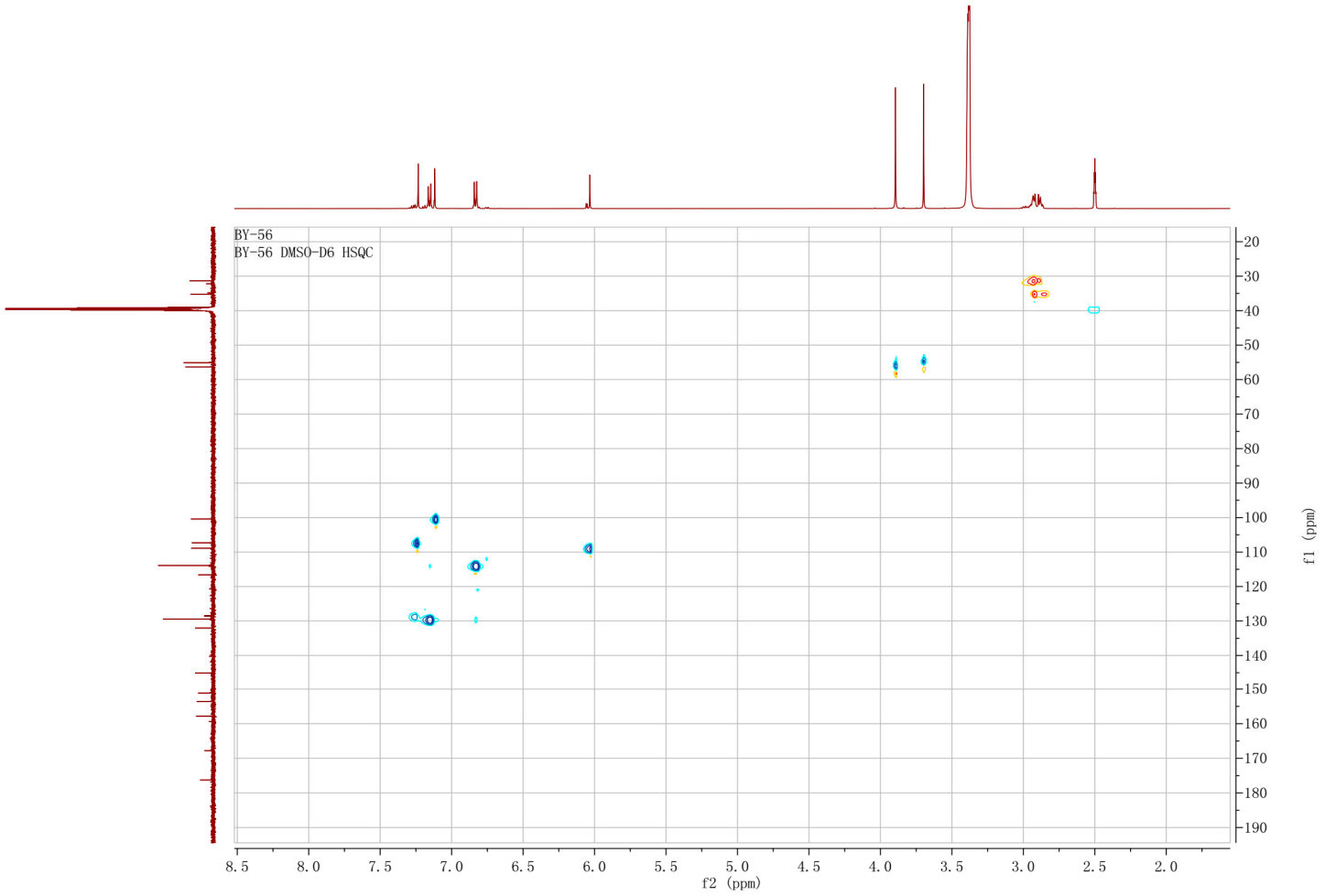


Figure S12. HSQC spectrum (500 MHz) of compound **2** in DMSO.

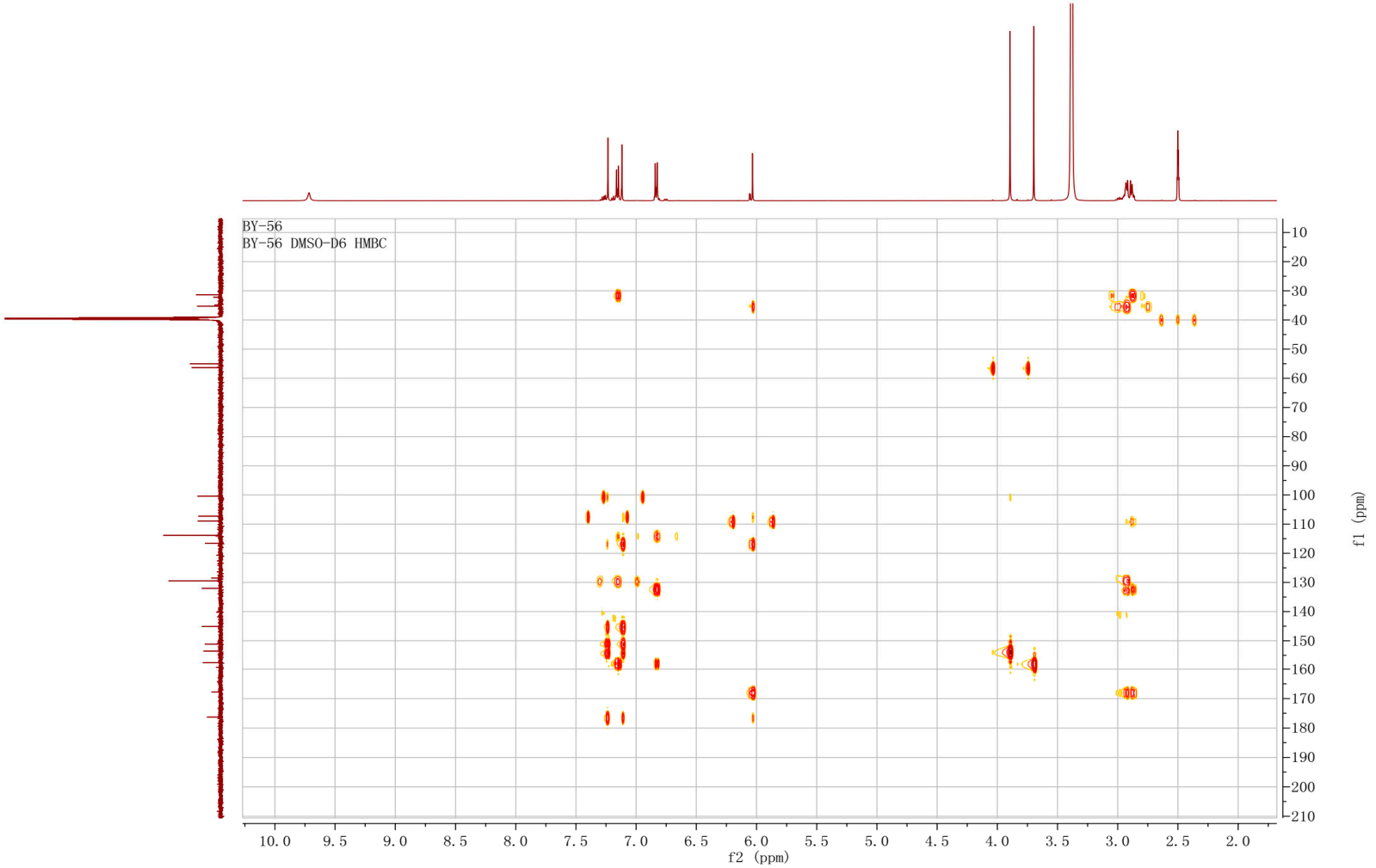


Figure S13. HMBC spectrum (500 MHz) of compound **2** in DMSO.

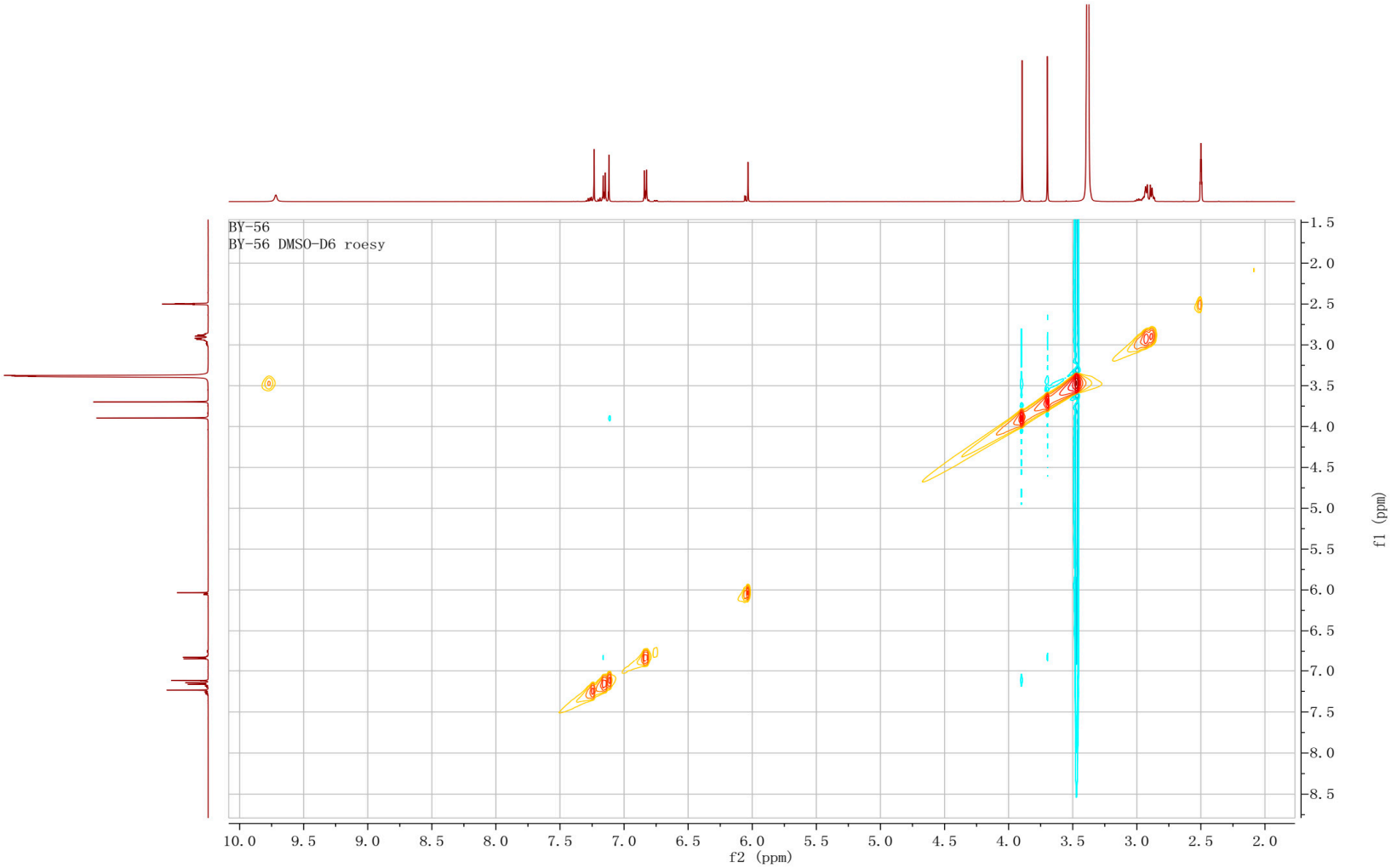


Figure S14. ROESY spectrum (400 MHz) of compound **2** in DMSO.

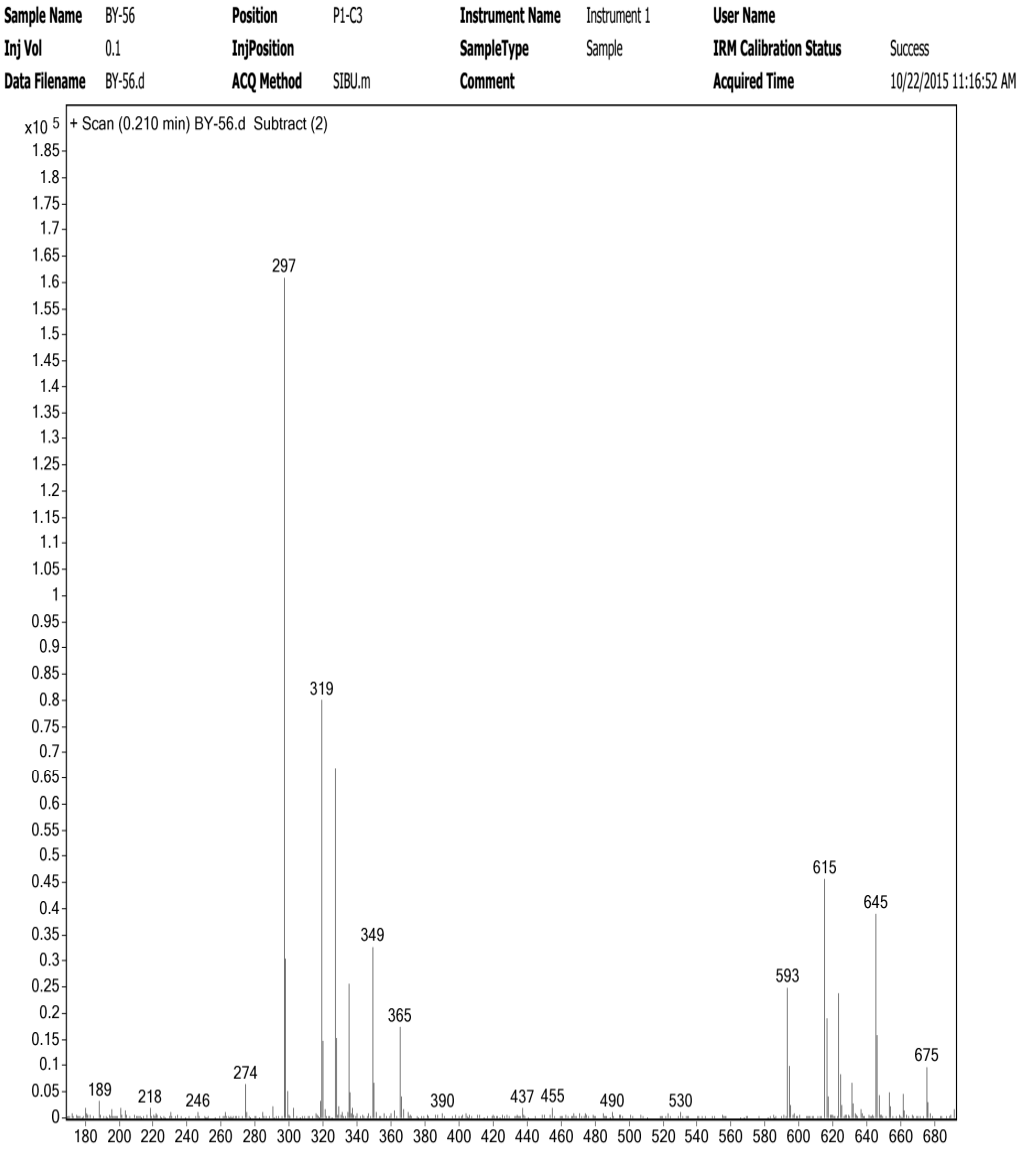


Figure S15. ESI(+)MS spectrum of compound **2**.

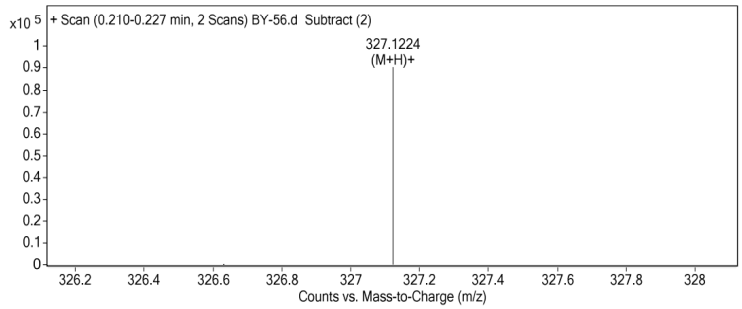
Qualitative Analysis Report

Data Filename	BY-56.d	**Sample Name**	BY-56
Sample Type	Sample	**Position**	P1-C3
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU.m	**Acquired Time**	10/22/2015 11:16:52 AM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	**Collision Energy**	**Ionization Mode**
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
297.1121	1	218337.25		
319.094	1	102590.45		
327.1224	1	90408.25	C19 H18 O5	(M+H)+
349.1047	1	43308.2		
593.2171	1	49472.85		
615.1992	1	108167.98		
623.2275	1	45127.51		
645.2098	1	93037.04		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	30

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C19 H18 O5	326.1154	327.1227	327.1224	0.3	1.0	11.0000

--- End Of Report ---

Figure S16. HRESI(+)MS spectrum of compound **2**.

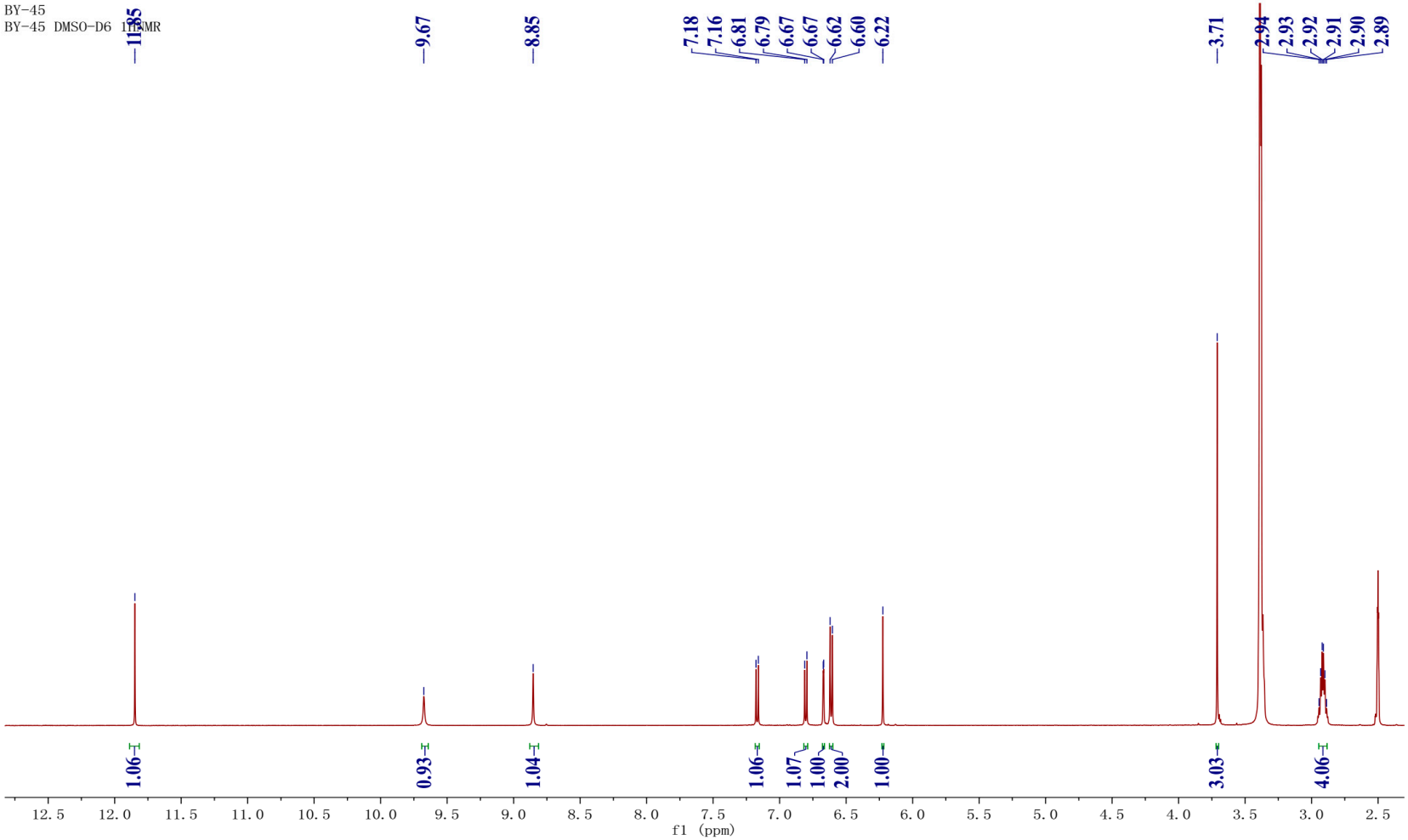


Figure S17. ^{1}H-NMR spectrum (500 MHz) of compound **3** in DMSO.

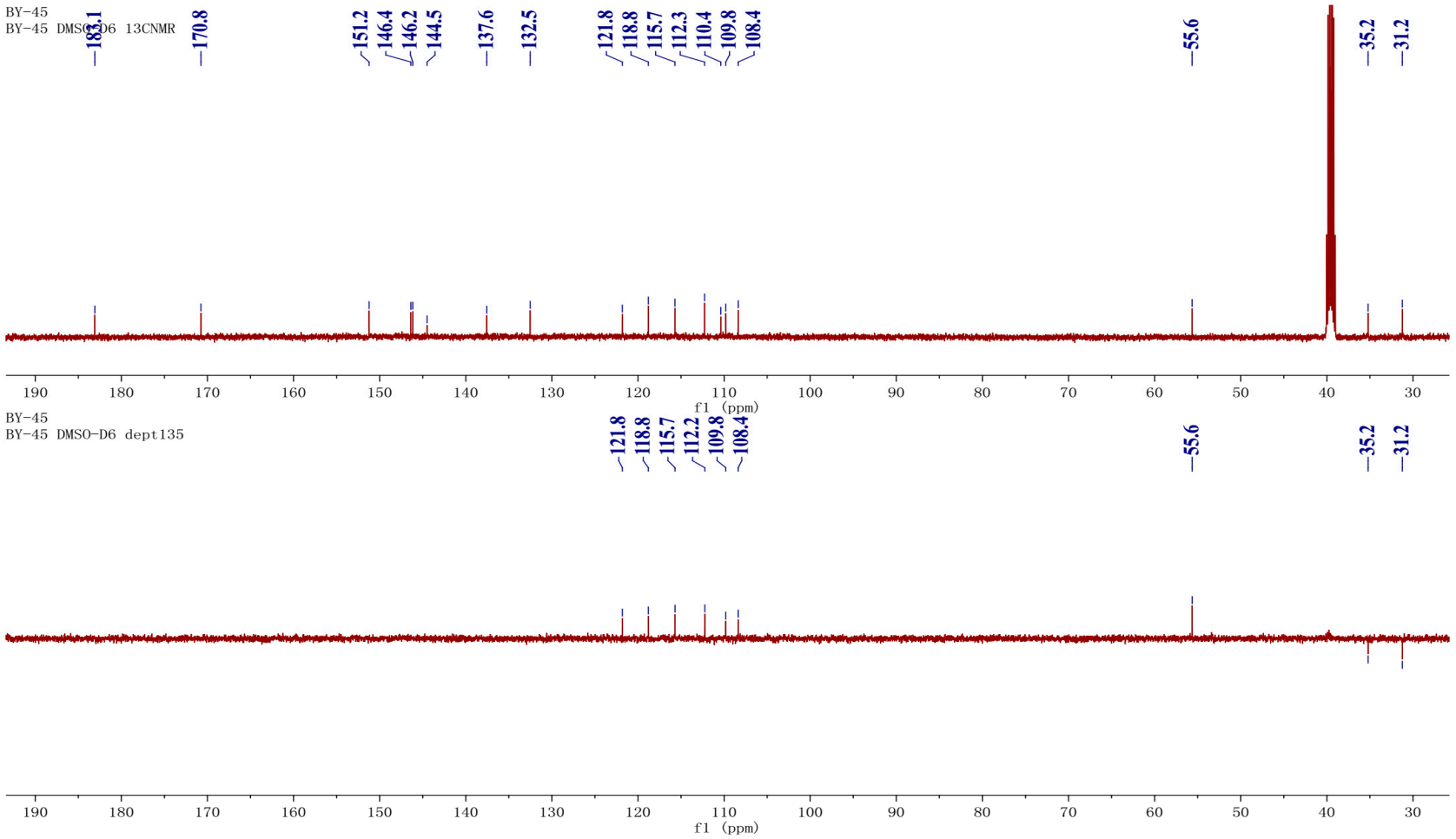


Figure S18. ^{13}C-NMR spectrum (125 MHz) of compound **3** in DMSO.

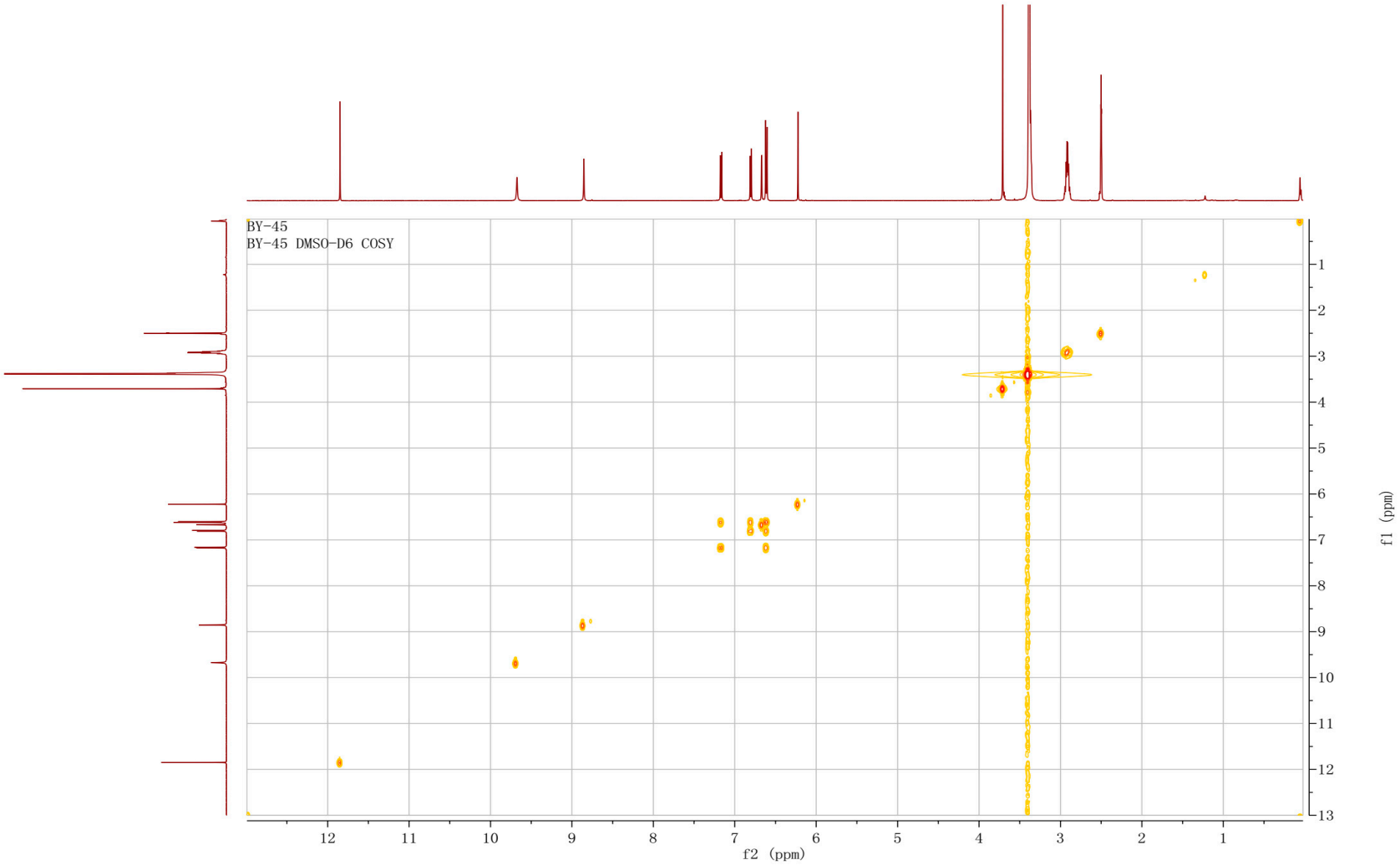


Figure S19. ^{1}H-^{1}H COSY spectrum (500 MHz) of compound **3** in DMSO.

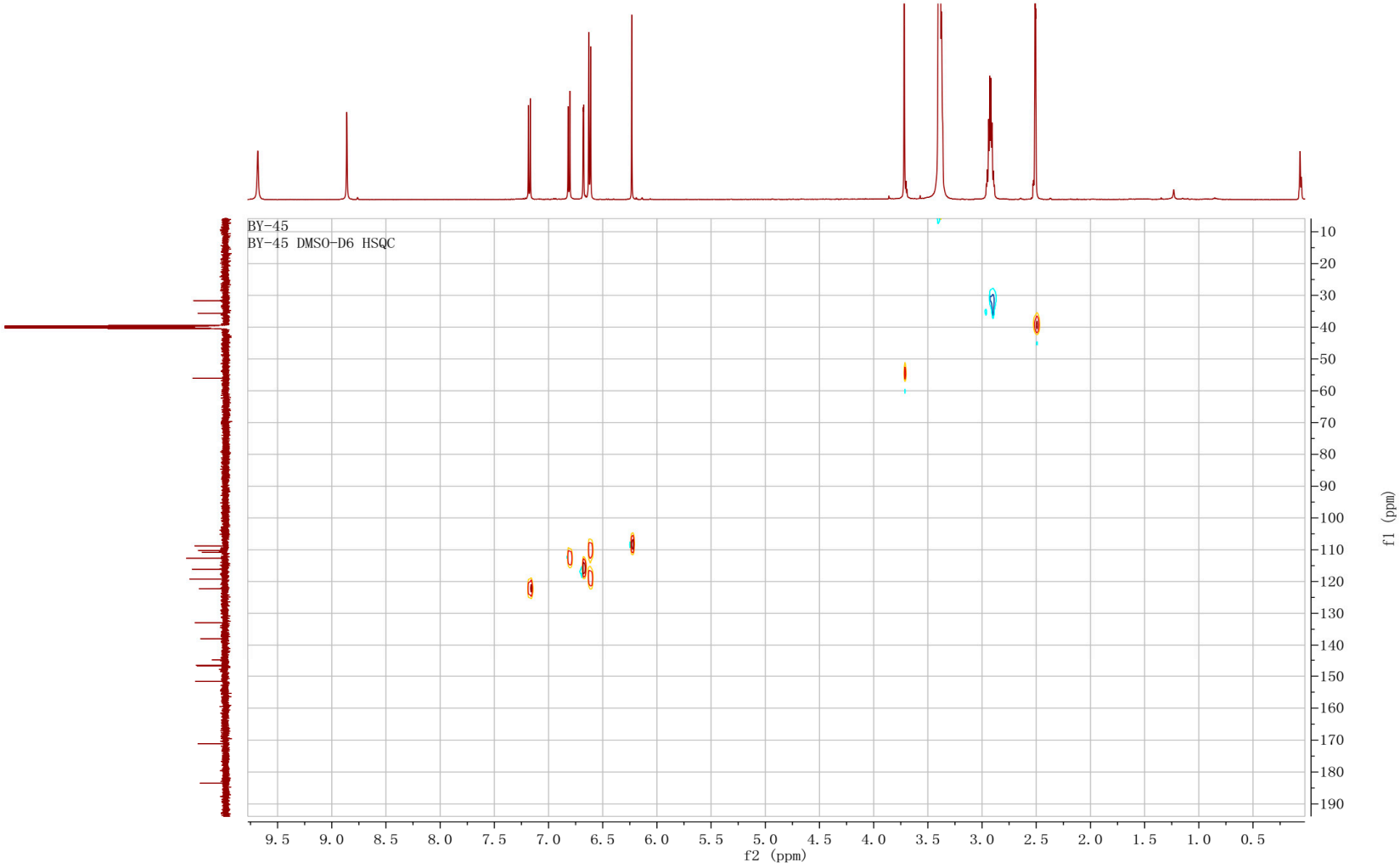


Figure S20. HSQC spectrum (500 MHz) of compound **3** in DMSO.

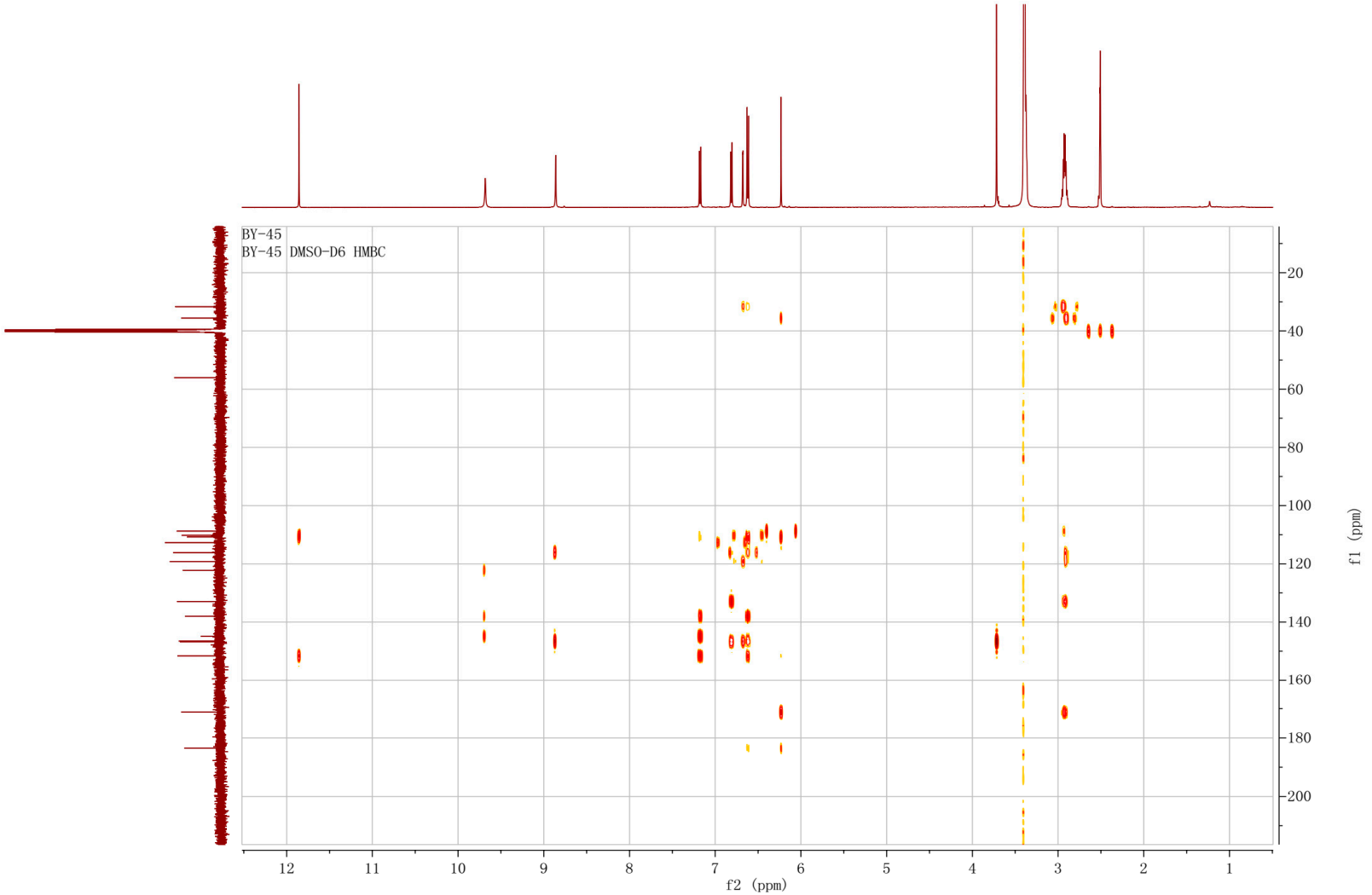


Figure S21. HMBC spectrum (500 MHz) of compound **3** in DMSO.

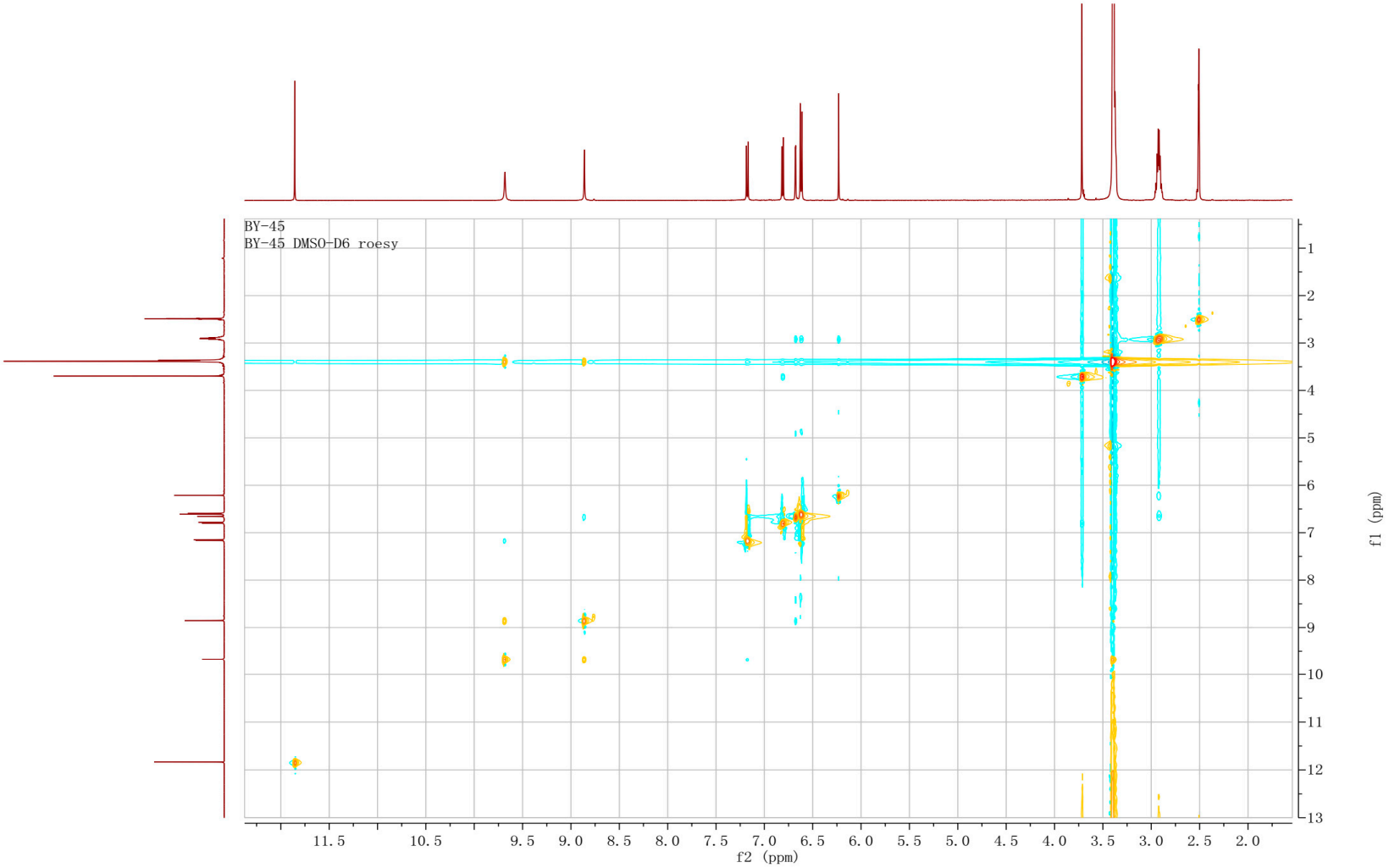


Figure S22. ROESY spectrum (400 MHz) of compound **3** in DMSO.

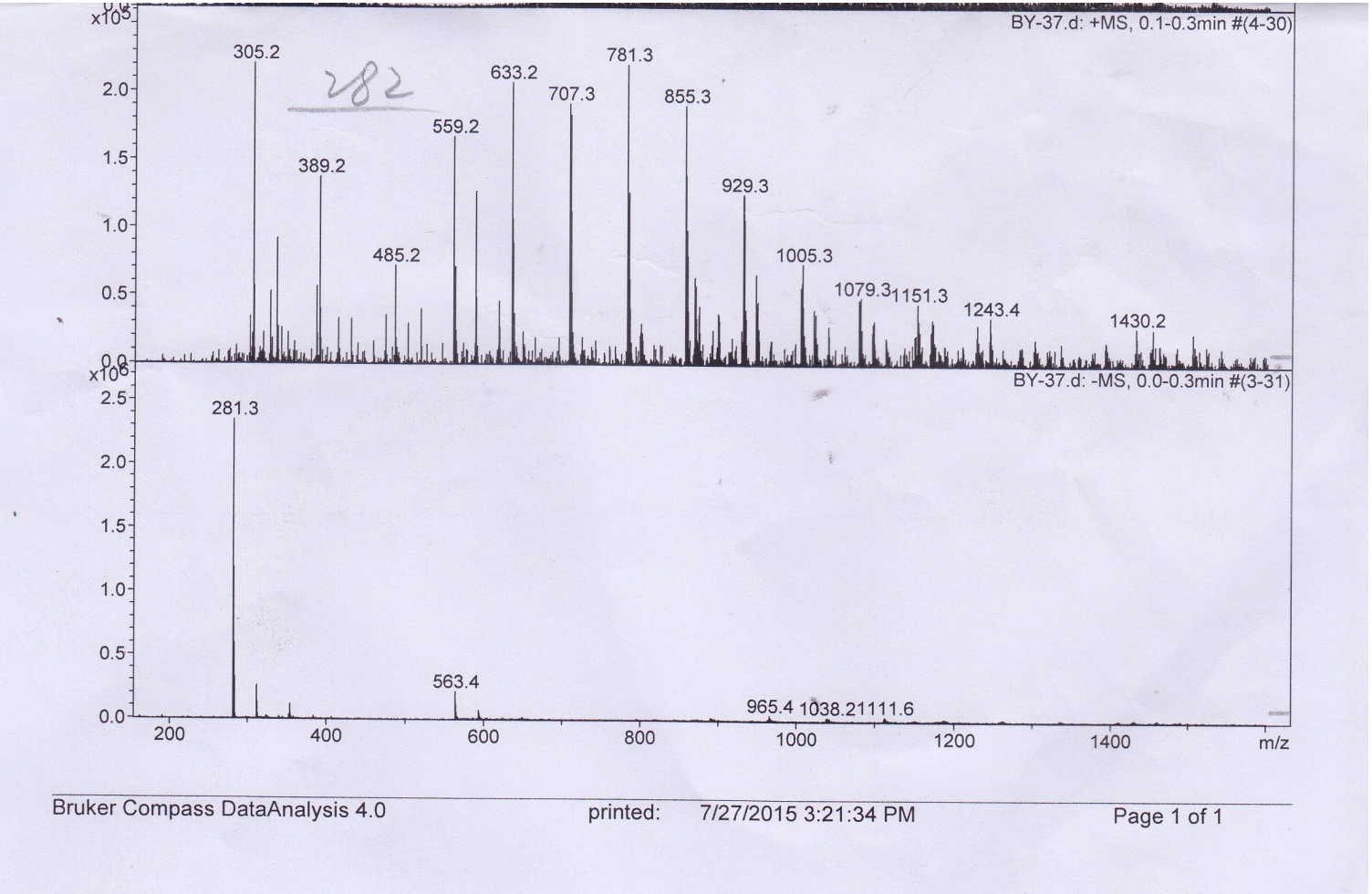


Figure S23. ESI(+)MS spectrum of compound **3**.

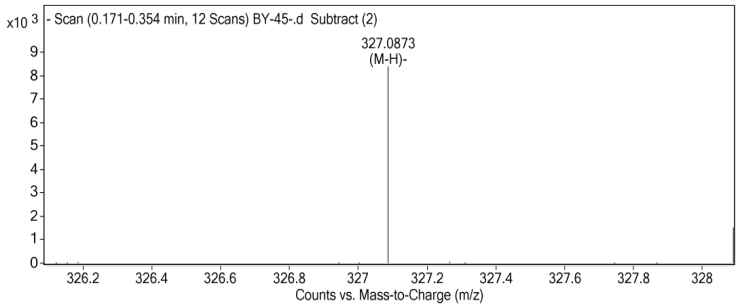
Qualitative Analysis Report

Data Filename	BY-45-.d	**Sample Name**	BY-45
Sample Type	Sample	**Position**	P1-C2
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU-ESI-i.m	**Acquired Time**	10/22/2015 3:20:12 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
89.0246		1365.38		
327.0873	1	8401.06	C18 H16 O6	(M-H)-
328.0908	1	1529.88	C18 H16 O6	(M-H)-
390.0831	1	1013.56		
411.0692	1	706.99		
441.08	1	19259.49		
442.0848	1	3664.01		
443.0859	1	724.34		

Formula Calculator Element Limits

Element	Min	Max
C	3	60
H	0	120
O	0	30
N	0	5

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C18 H16 O6	328.0947	327.0874	327.0873	-0.1	-0.3	11.0000

--- End Of Report ---

Figure S24. HRESI(+)MS spectrum of compound **3**.

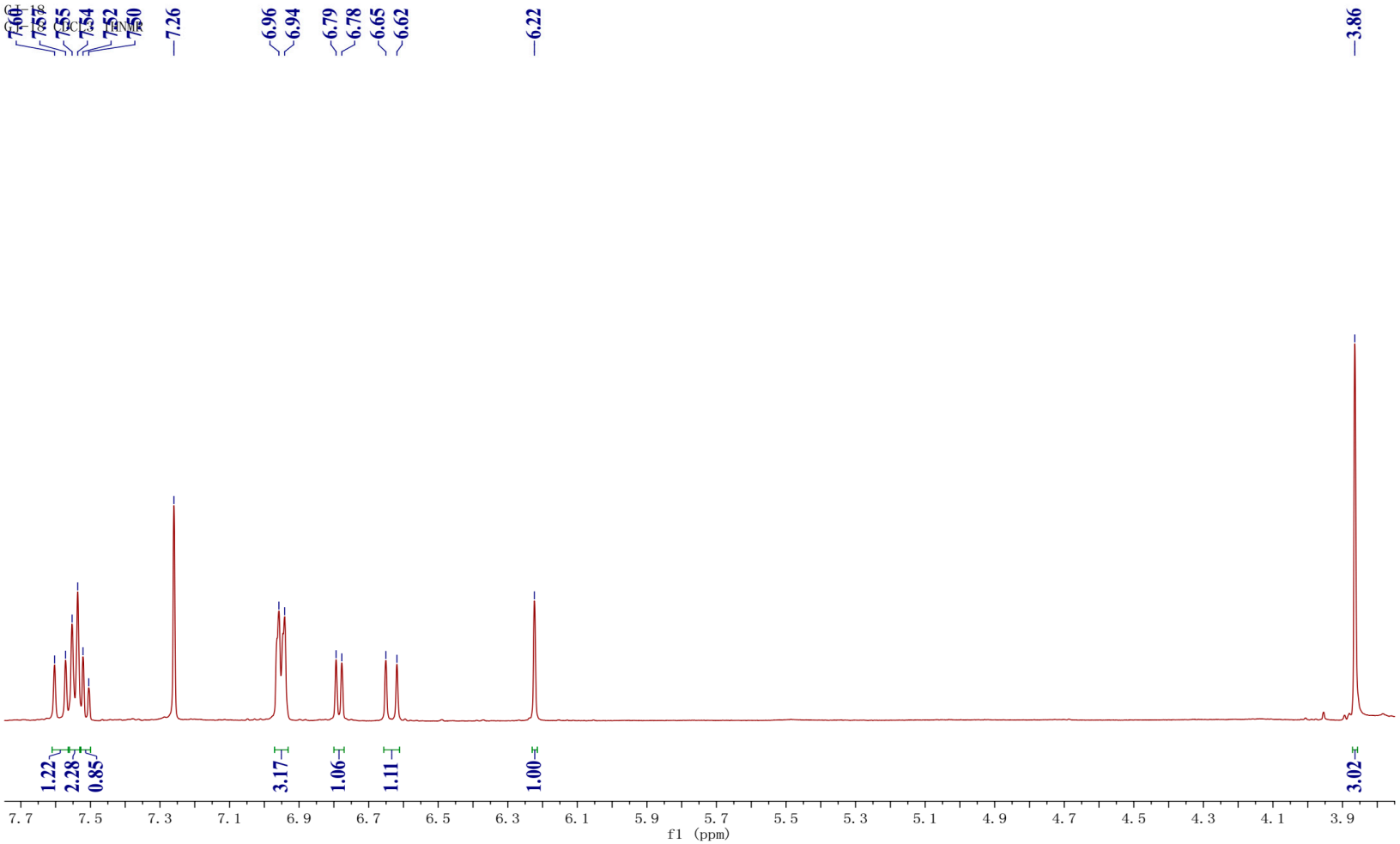


Figure S25. ^{1}H-NMR spectrum (500 MHz) of compound **4** in $CDCl_3$.

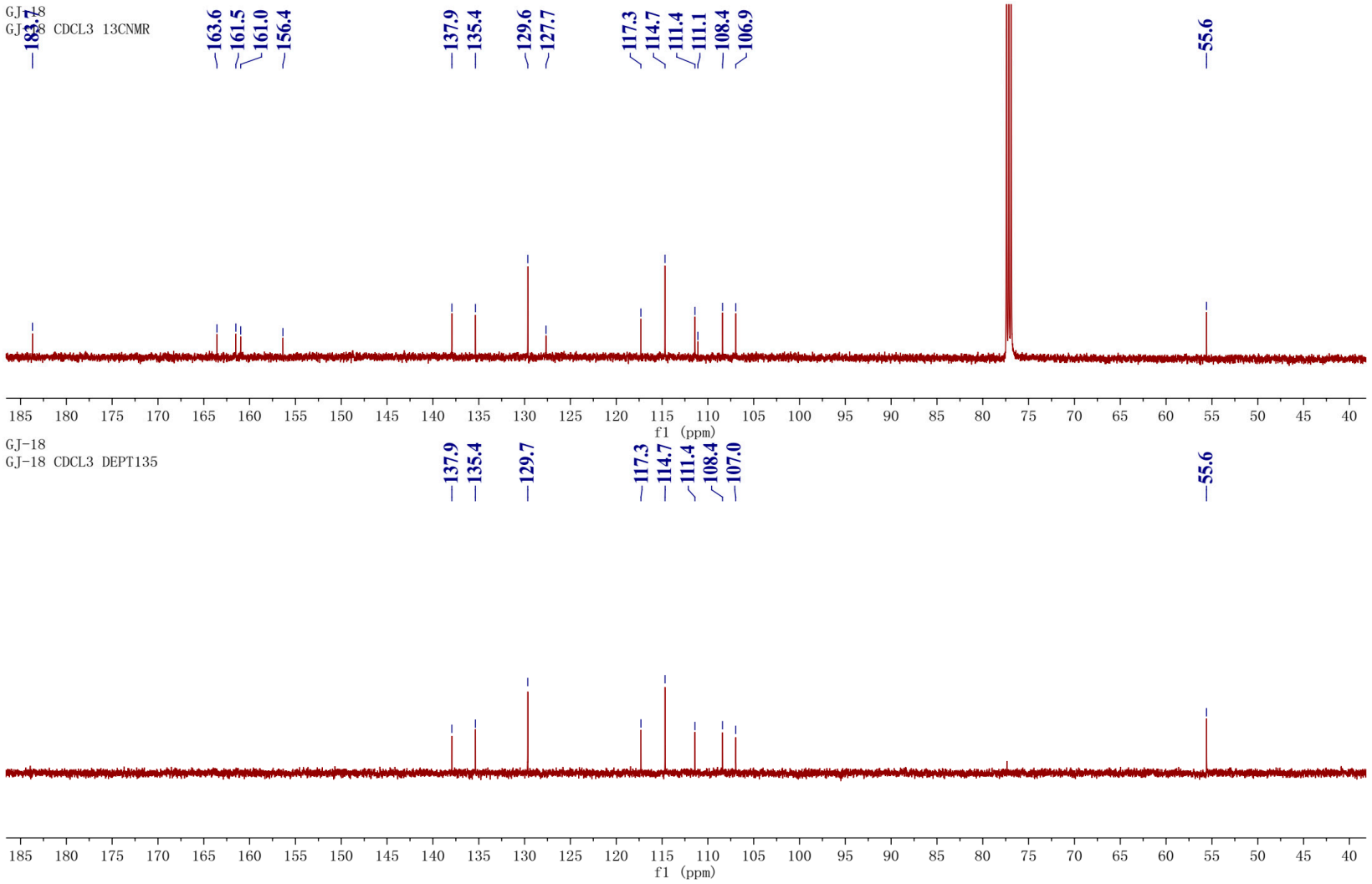


Figure S26. ^{13}C-NMR spectrum (125 MHz) of compound **4** in $CDCl_3$.

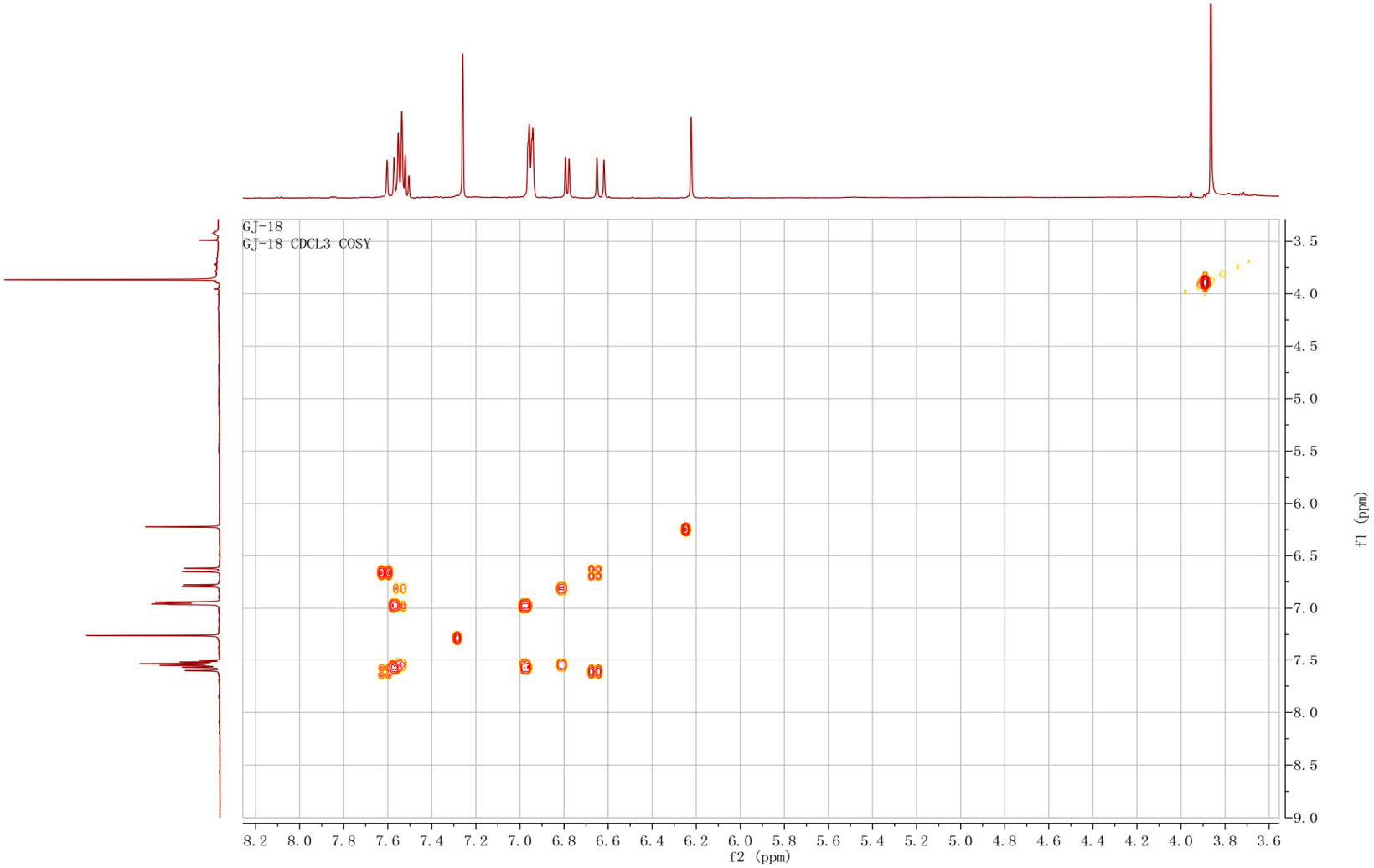


Figure S27. ^{1}H-^{1}H COSY spectrum (500 MHz) of compound **4** in $CDCl_3$.

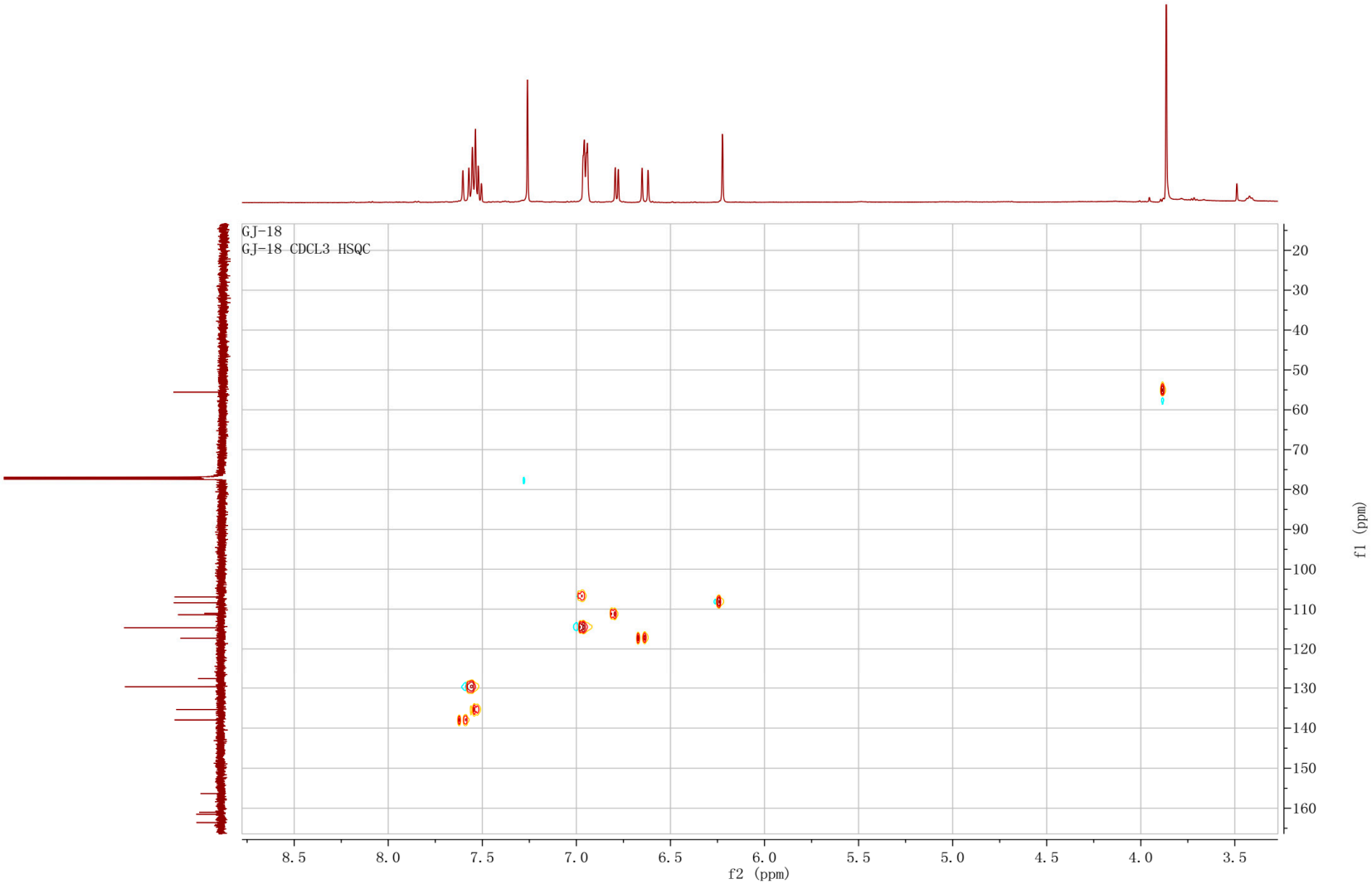


Figure S28. HSQC spectrum (500 MHz) of compound **4** in $CDCl_3$.

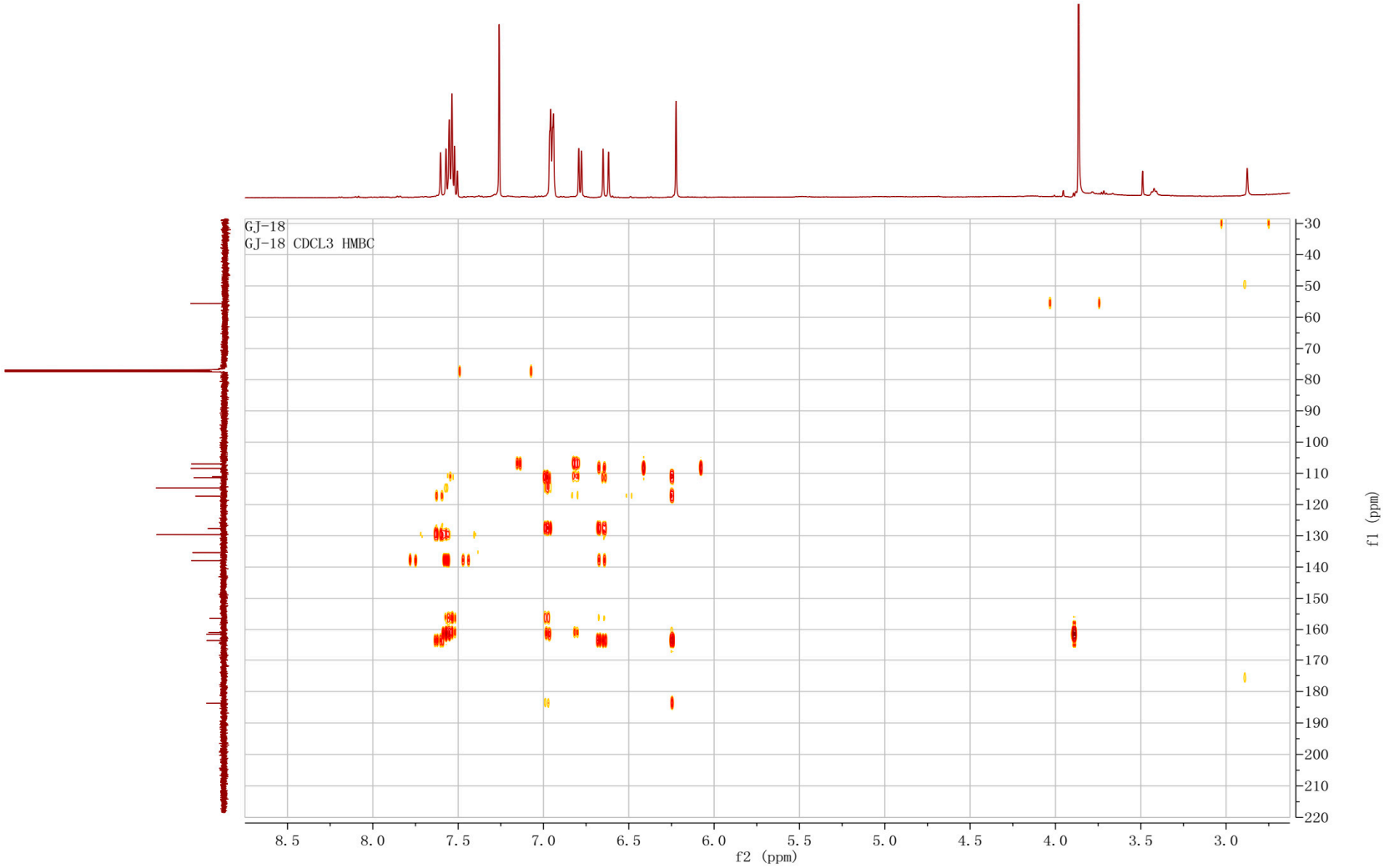


Figure S29. HMBC spectrum (500 MHz) of compound **4** in $CDCl_3$.

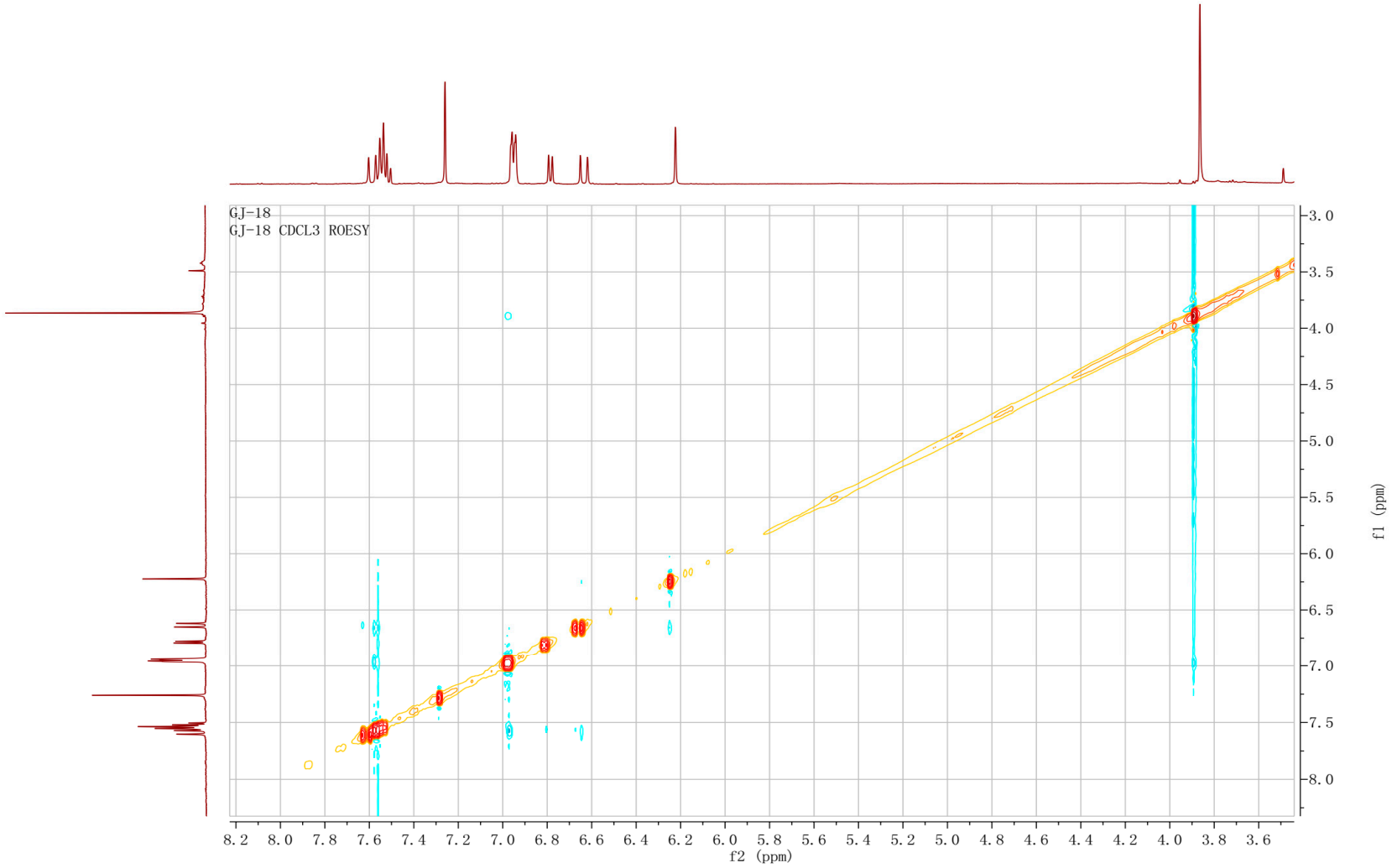


Figure S30. ROESY spectrum (400 MHz) of compound **4** in $CDCl_3$.

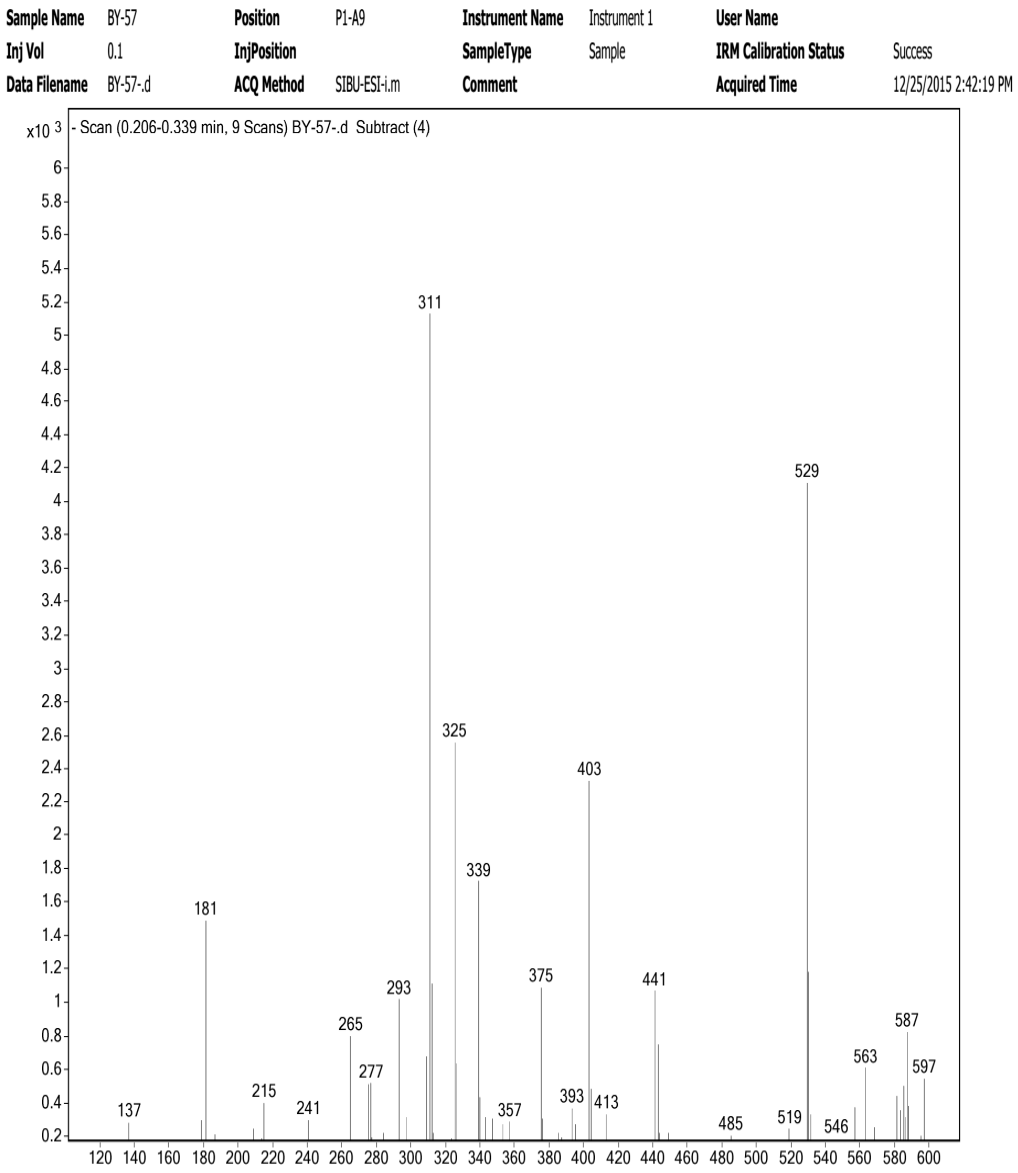


Figure S31. ESI(+)MS spectrum of compound **4**.

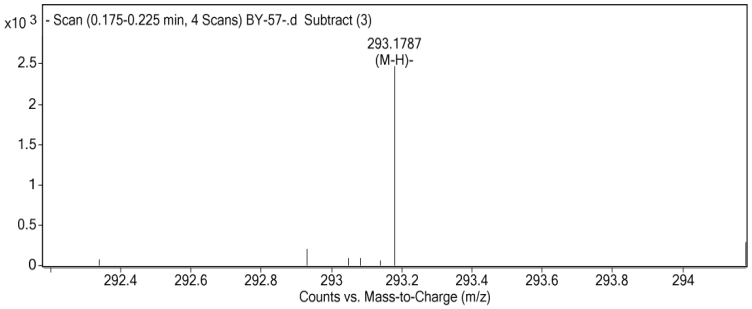
Qualitative Analysis Report

Data Filename	BY-57-.d	**Sample Name**	BY-57
Sample Type	Sample	**Position**	P1-A9
Instrument Name	Instrument 1	**User Name**	
Acq Method	SIBU-ESI-i.m	**Acquired Time**	12/25/2015 3:05:43 PM
IRM Calibration Status	Success	**DA Method**	ESI+.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125.2)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund
311.1687	1	5084.09
325.1844	1	6385.03
339.2001	1	4304.08
375.2752	1	4148.44
403.3066	1	6881.47
441.2495	1	3392.89
529.2812	1	12609.48
530.2839	1	4065.03

Formula Calculator Element Limits

Element	Min	Max
C	3	120
H	0	240
O	0	60
N	0	10

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C20 H24 N O	294.1858	293.1785	293.1787	0.0	-0.1	9.5000

--- End Of Report ---

Figure S32. HRESI(+)MS spectrum of compound **4**.