

Polyacetylenes from the roots of *Swietenia macrophylla* King

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CR-5
CR-5 CDCl₃ 1HNMR

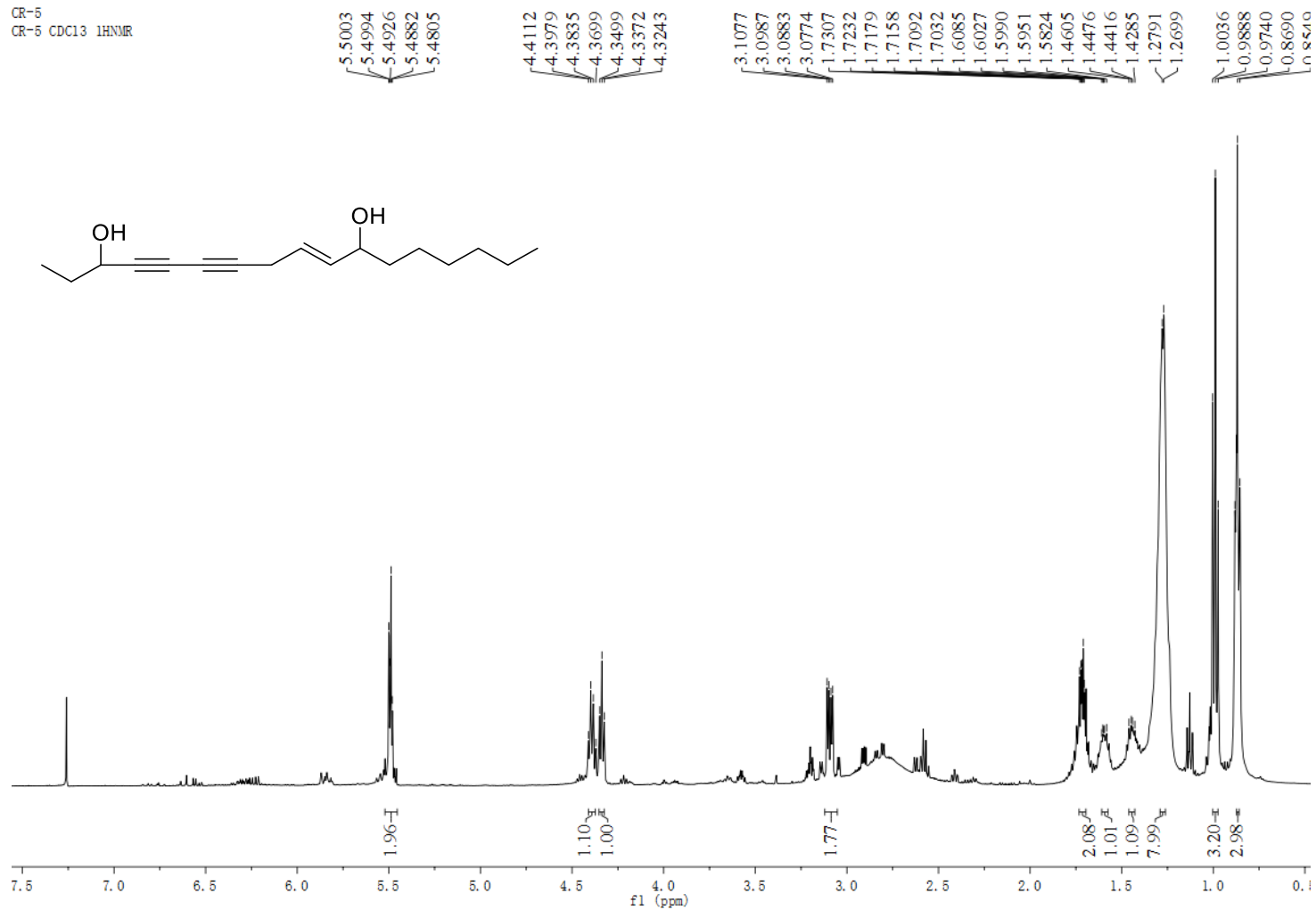


Figure S1. ¹H NMR spectrum (500 MHz) of compound 1 in CDCl₃.

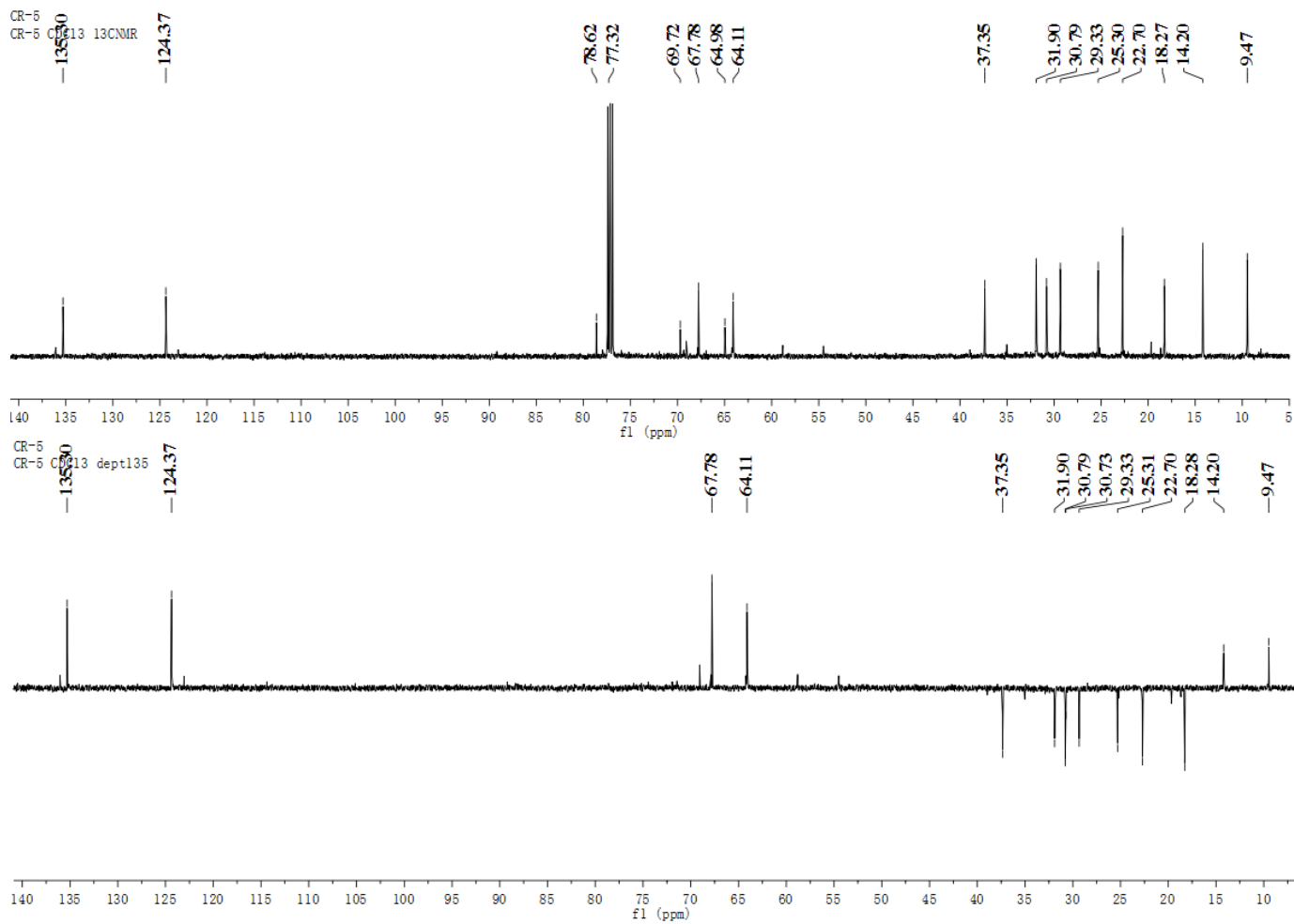


Figure S2. ^{13}C NMR spectrum (125 MHz) of compound **1** in CDCl_3 .

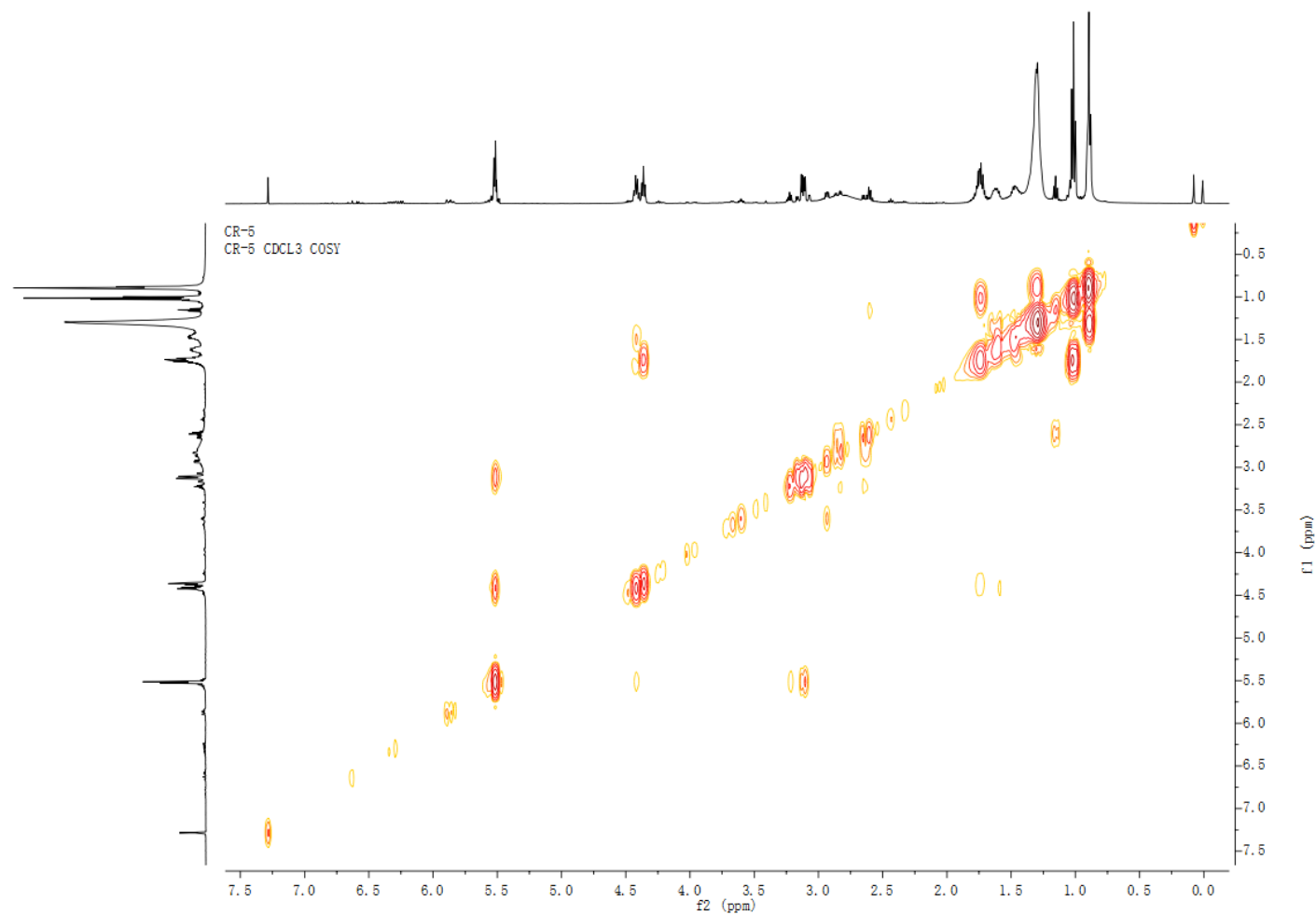


Figure S3. ^1H - ^1H COSY spectrum of compound **1** in CDCl_3 .

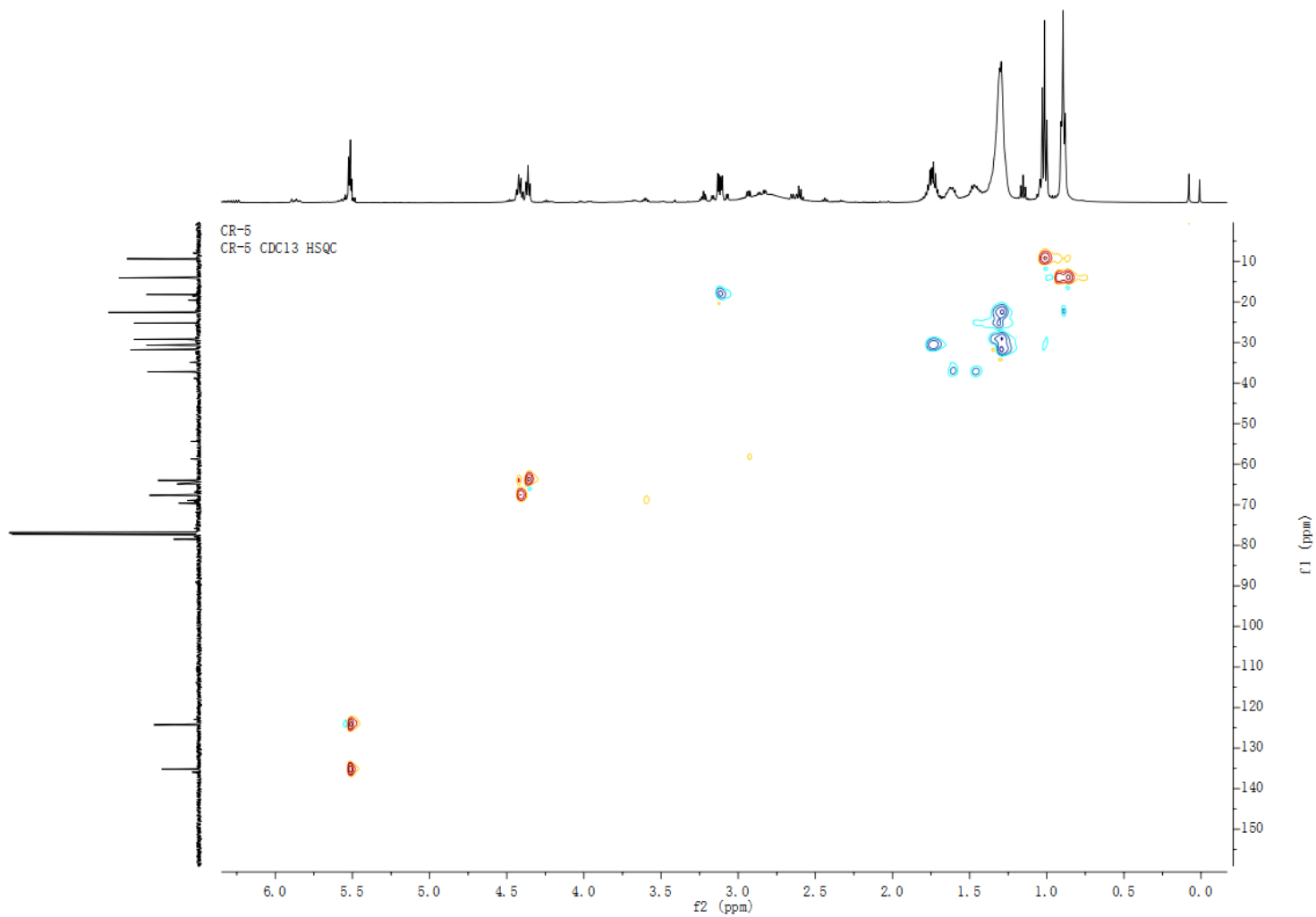


Figure S4. HSQC spectrum of compound **1** in CDCl₃.

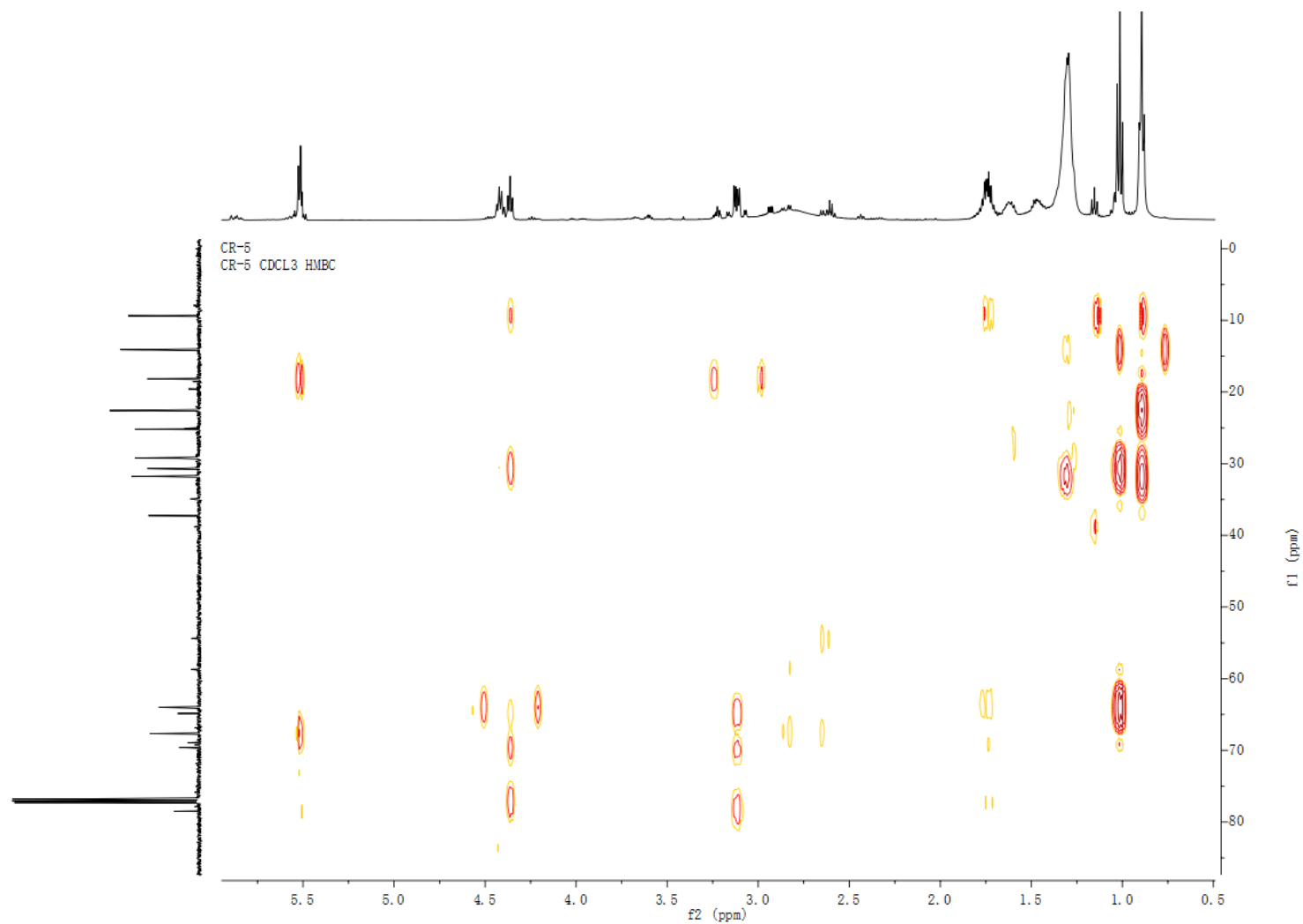


Figure S5. HMBC spectrum of compound **1** in CDCl₃.

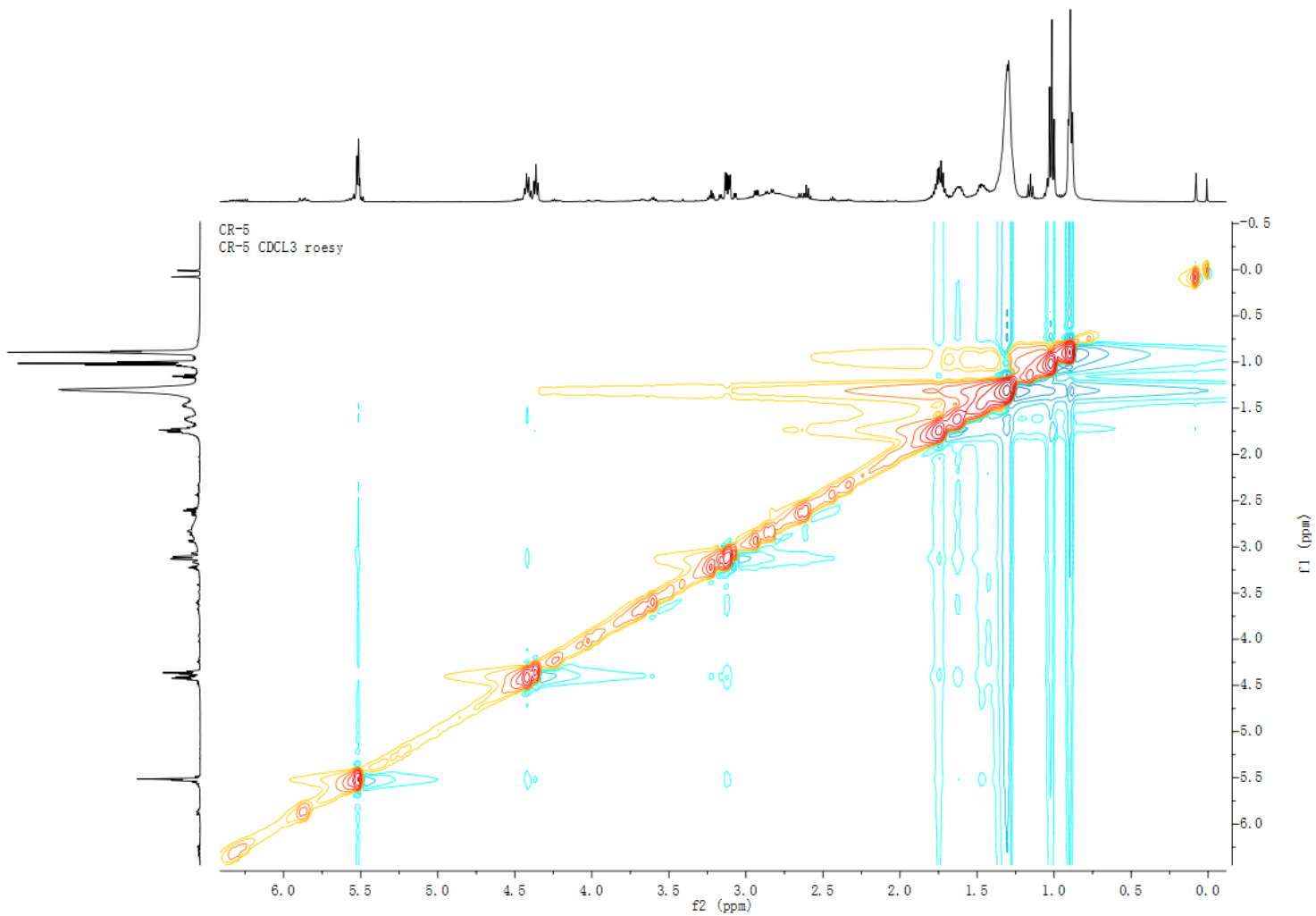


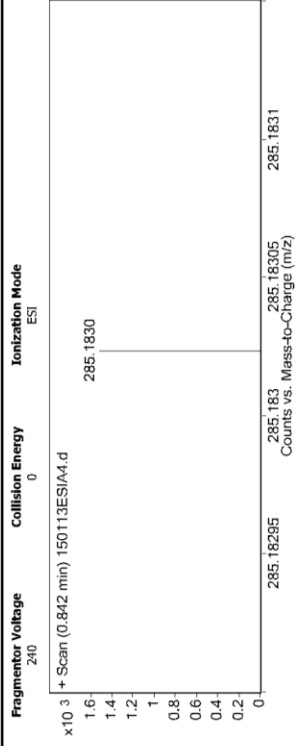
Figure S6. ROESY spectrum of compound **1** in CDCl₃.

Qualitative Analysis Report

Data Filename 150113ESI(A4).d Sample Type Sample Instrument Name Agilent G6230 TOF MS Acq Method ESI.m IRM Calibration Status Success Comment	Sample Name CR-5 Position KIB User Name KIB Acquired Time 1/12/2015 1:50:27 PM DA Method ESI.m
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Sample Group 6200 series TOF/6500 series
Acquisition SW Q-TOF B.05.01 (B5125.2)
Version Info.

User Spectra



Peak List	m/z	z	Abund
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	193.0494	1	2694.31
	274.2738	1	3758.84
	318.3002	1	4489.7
	512.5038	1	2579.33
	540.5347	1	3205.15
	922.0098	1	3292.58
	923.0125	1	5390.13
	1821.9496	1	3029.58

Formula Calculator Element Limits	
Element	Min Max
C	0 200
H	0 400
O	0 8
Na	1 1

Formula Calculator Results			
Formula	CalculatedMass	Mz	DBE
C17 H26 Na O2	285.1831	285.1830	4.5
		Diff. (mba)	0.2
		Diff. (ppm)	0.0

--- End Of Report ---

Figure S7. HRESI(+)-MS spectrum of compound 1.

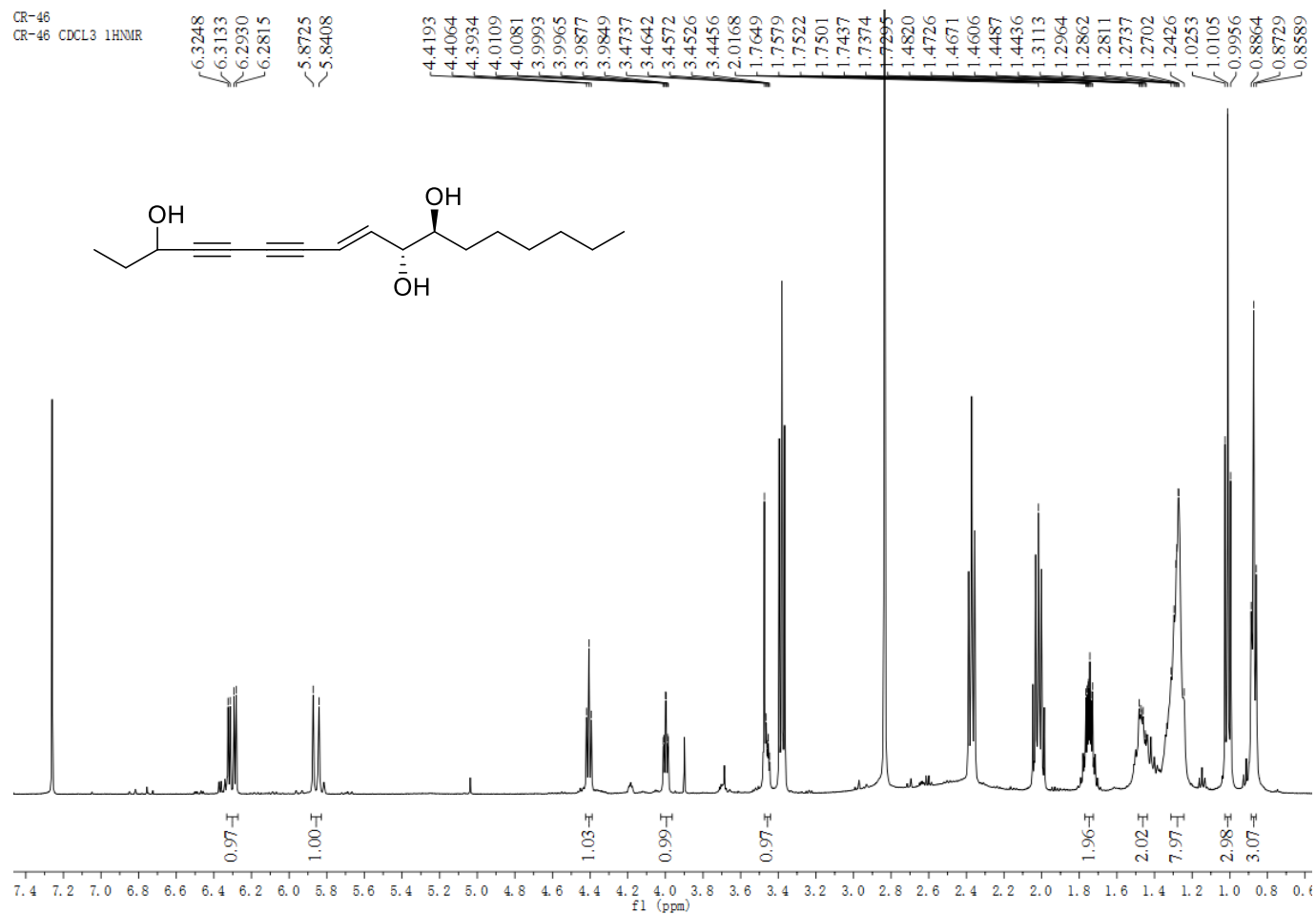


Figure S8. ¹H NMR spectrum (500 MHz) of compound **2** in CDCl₃.

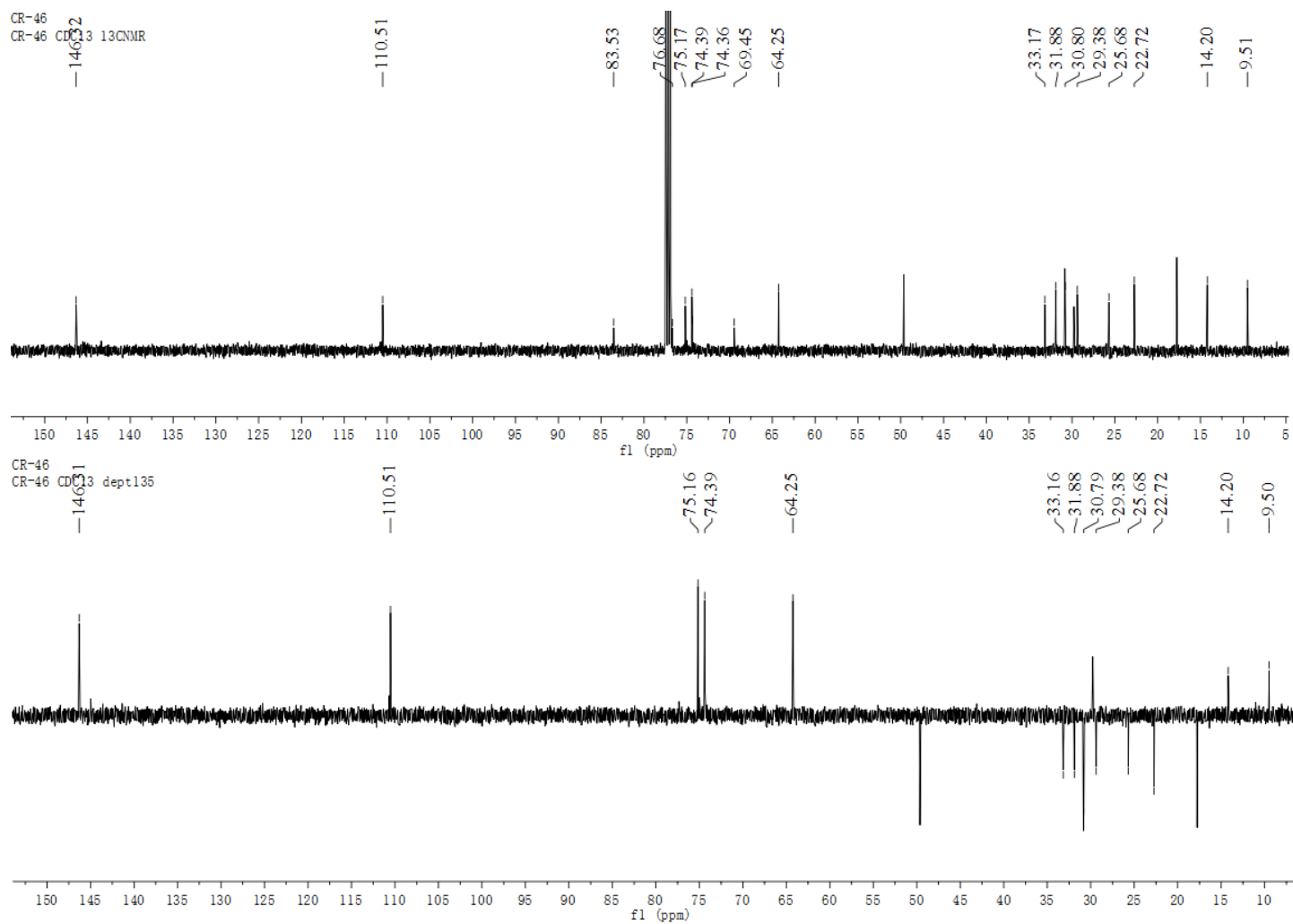


Figure S9. ¹³C NMR spectrum (125 MHz) of compound **2** in CDCl₃.

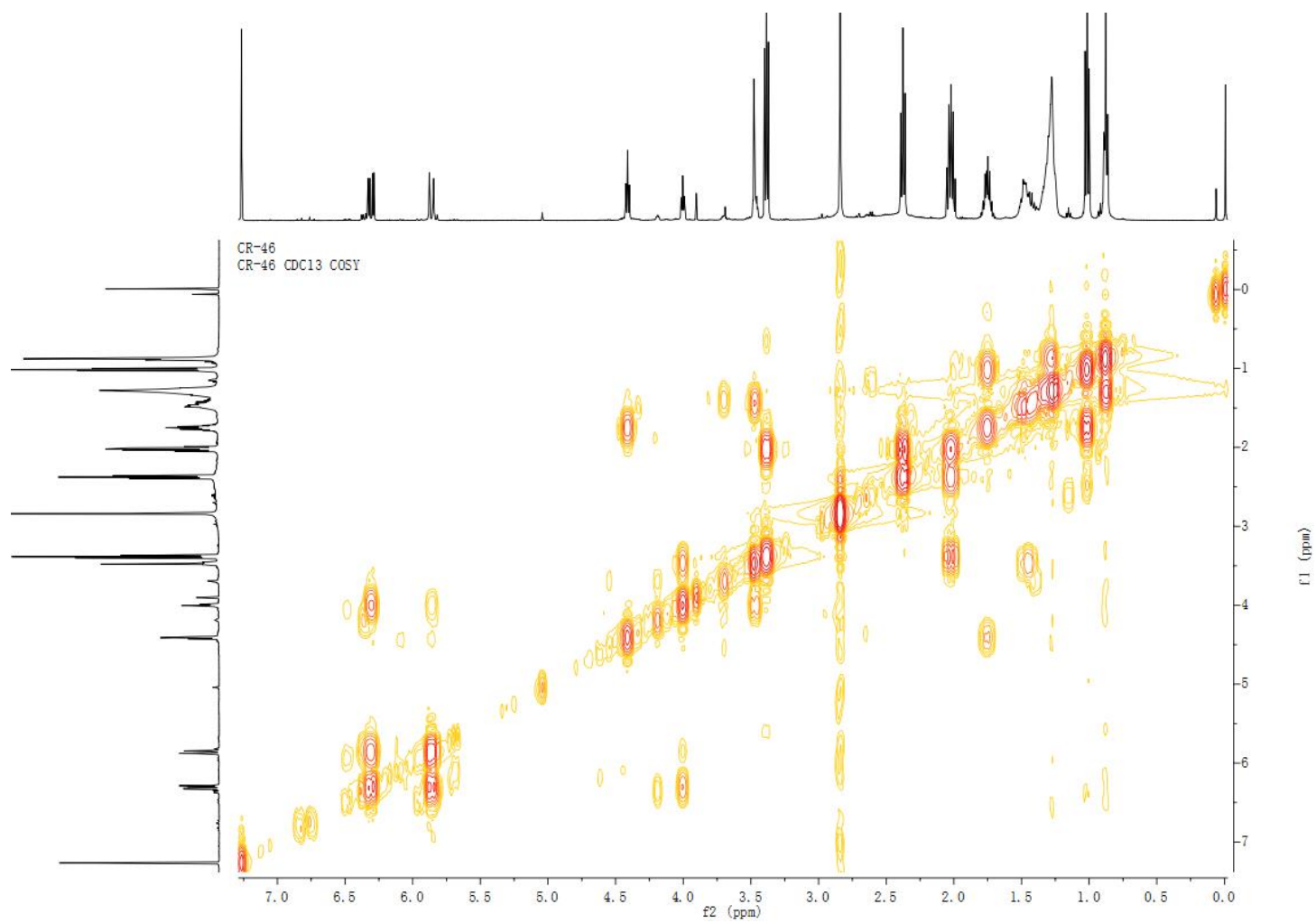


Figure S10. ^1H - ^1H COSY spectrum of compound **2** in CDCl_3 .

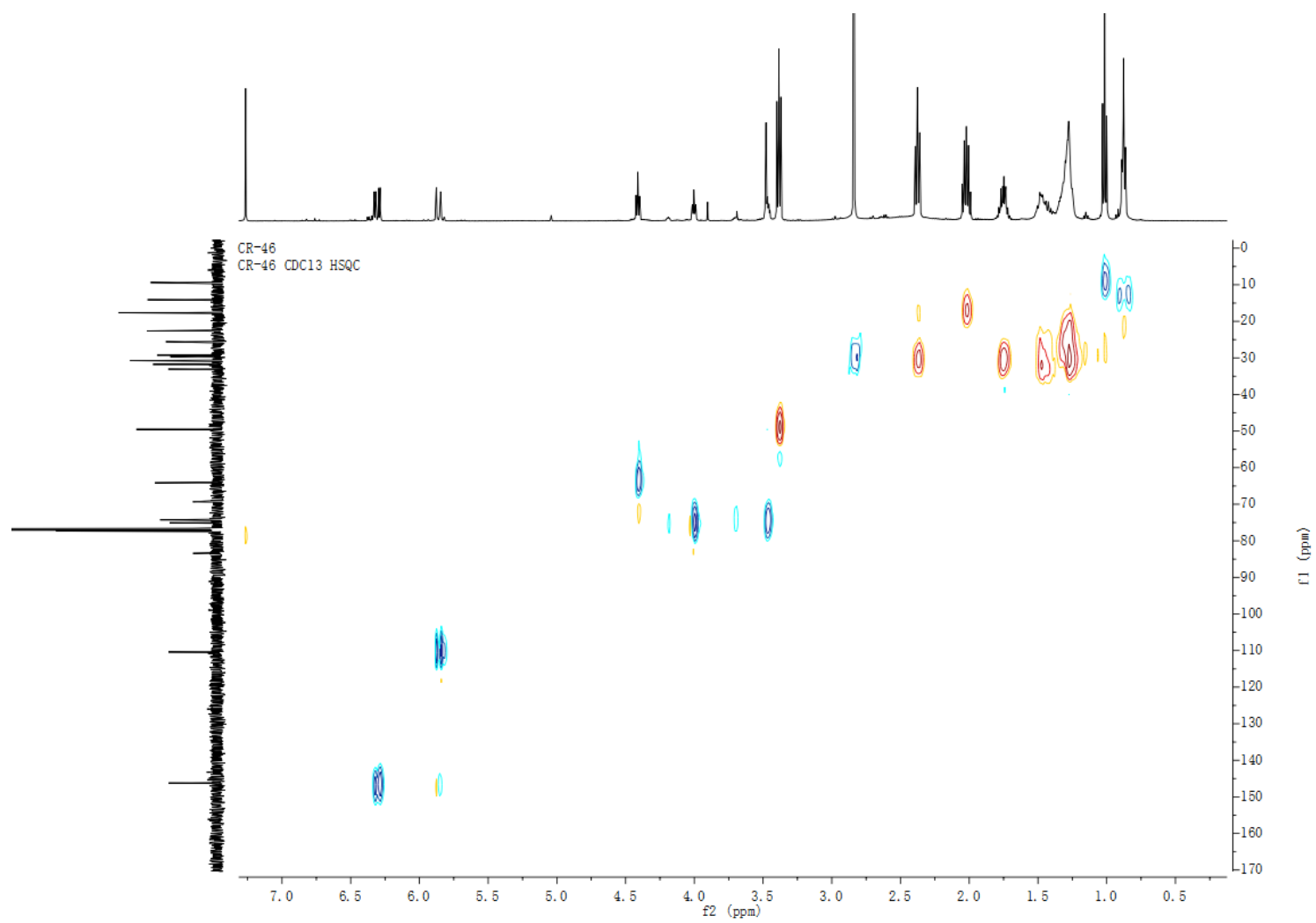


Figure S11. HSQC spectrum of compound **2** in CDCl₃.

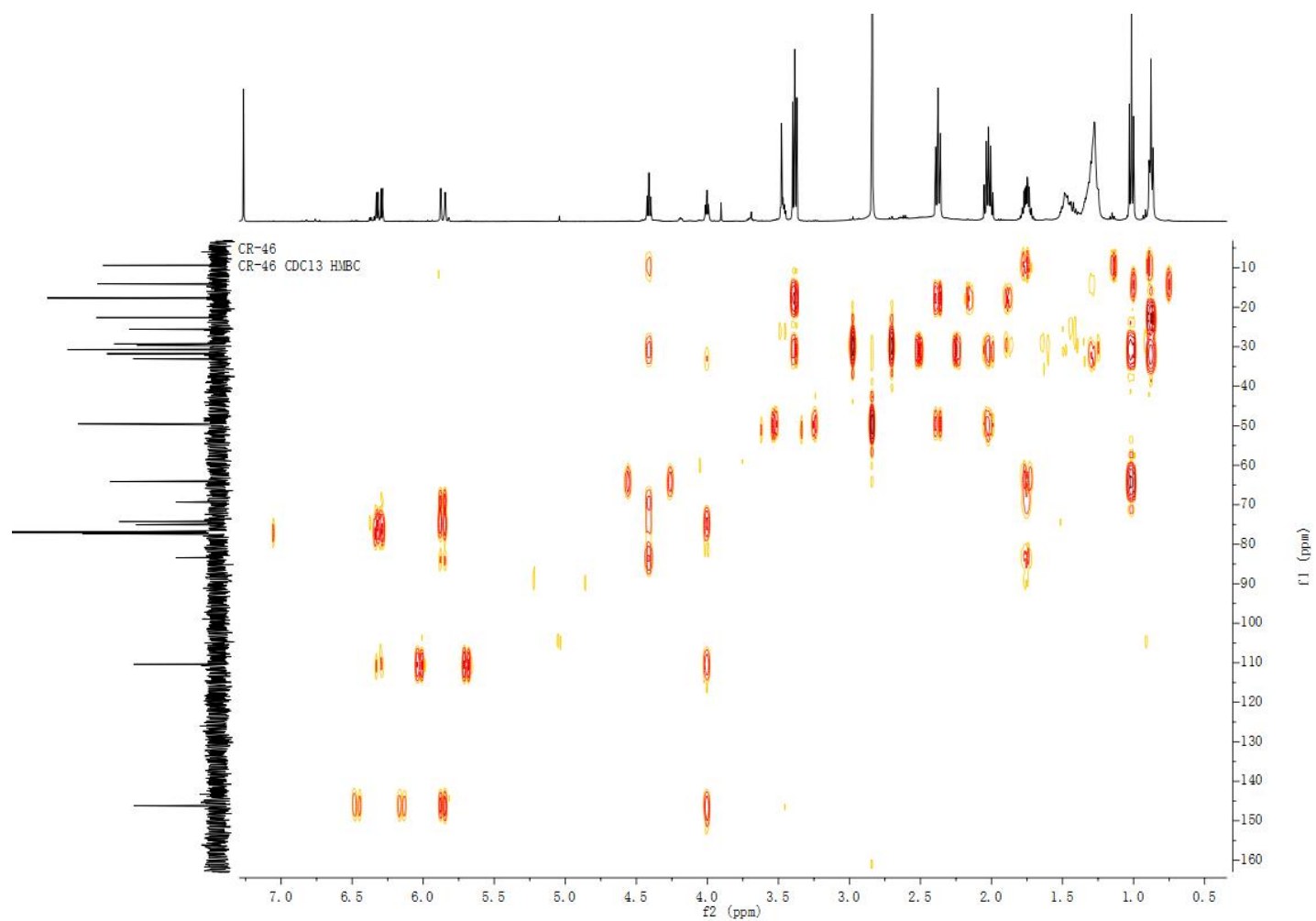


Figure S12. HMBC spectrum of compound 2 in CDCl₃.

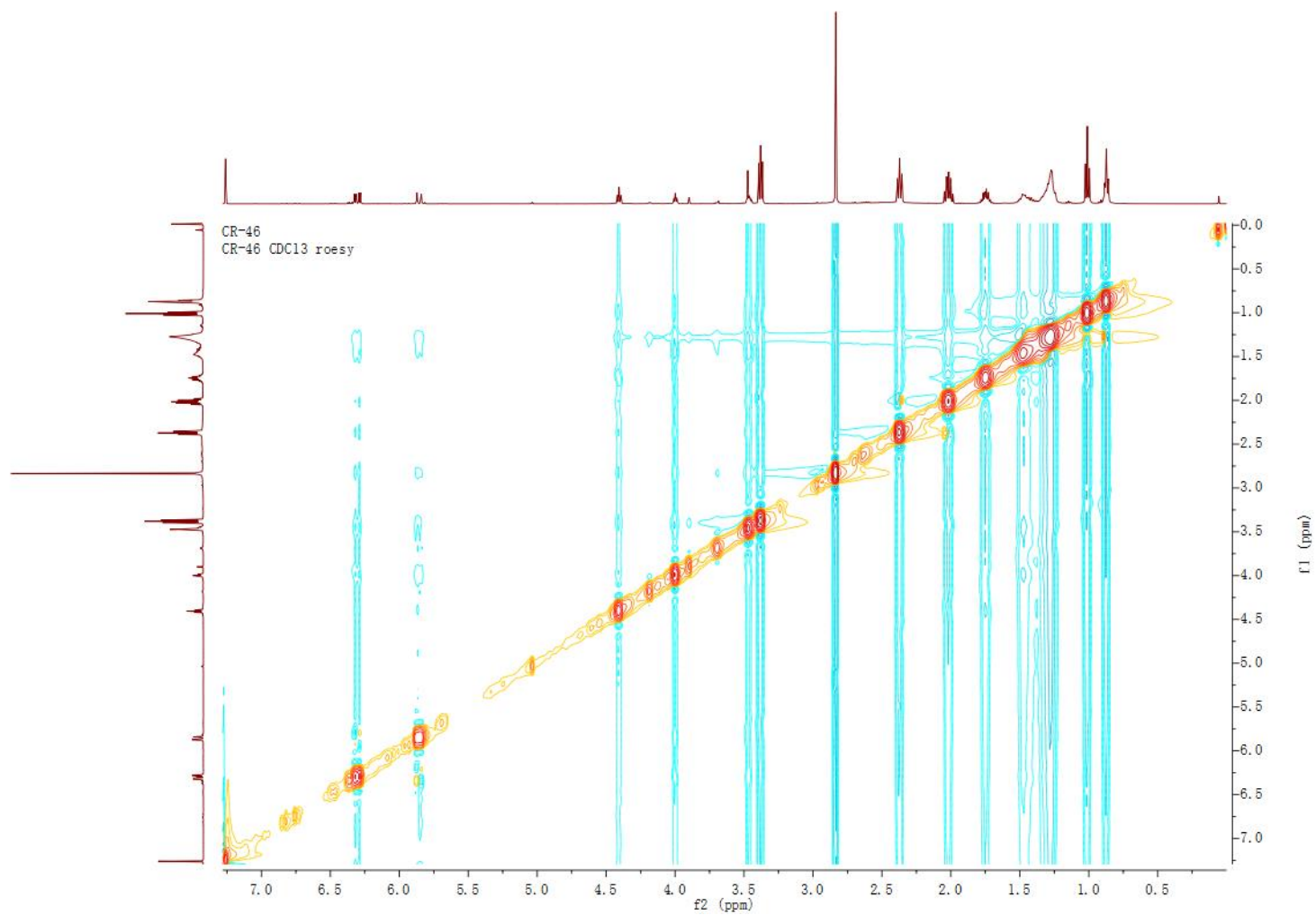
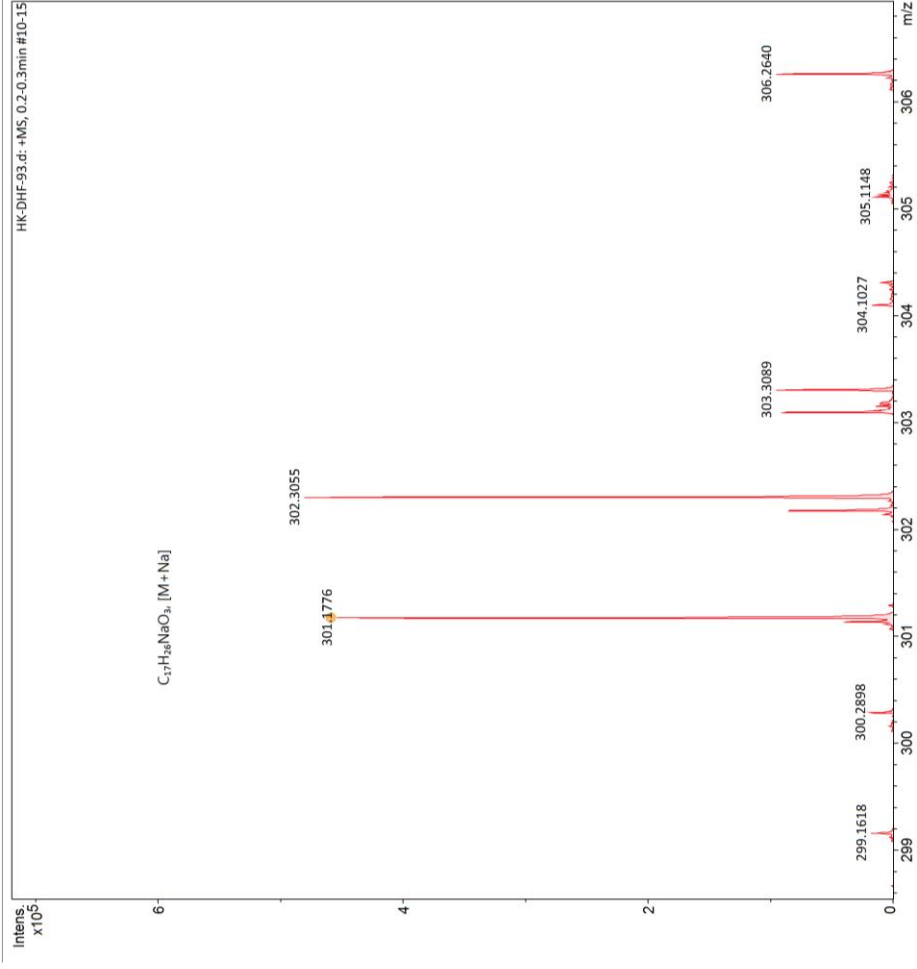


Figure S13. ROESY spectrum of compound **2** in CDCl₃.

Display Report

Analysis Info
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 Analysis Name D:\Data\bb\HK-DHF-93.d
 Method DirectInfusion - MS - positive.m
 Sample Name HK-DHF-93
 Comment

Acquisition Parameter
 Source Type ESI
 Focus Not active
 Scan Begin 50 m/z
 Scan End 1300 m/z
 Ion Polarity Positive
 Set Capillary 4500 V
 Set End Plate Offset -500 V
 Set Charging Voltage 2000 V
 Set Corona 0 nA
 Set Nebulizer 0.4 Bar
 Set Dry Heater 180 °C
 Set Dry Gas 4.0 l/min
 Set Divert Valve Waste
 Set APCI Heater 0 °C



Sum Formula	Ion Formula	Meas. m/z	m/z	err [ppm]
C ₁₇ H ₂₆ O ₃	C ₁₇ H ₂₆ NaO ₃	301.1780	301.1776	1.3

Figure S14. HRESI(+)-MS spectrum of compound **2**.

CR-30
CR-30 CDCl₃ 1HNMR

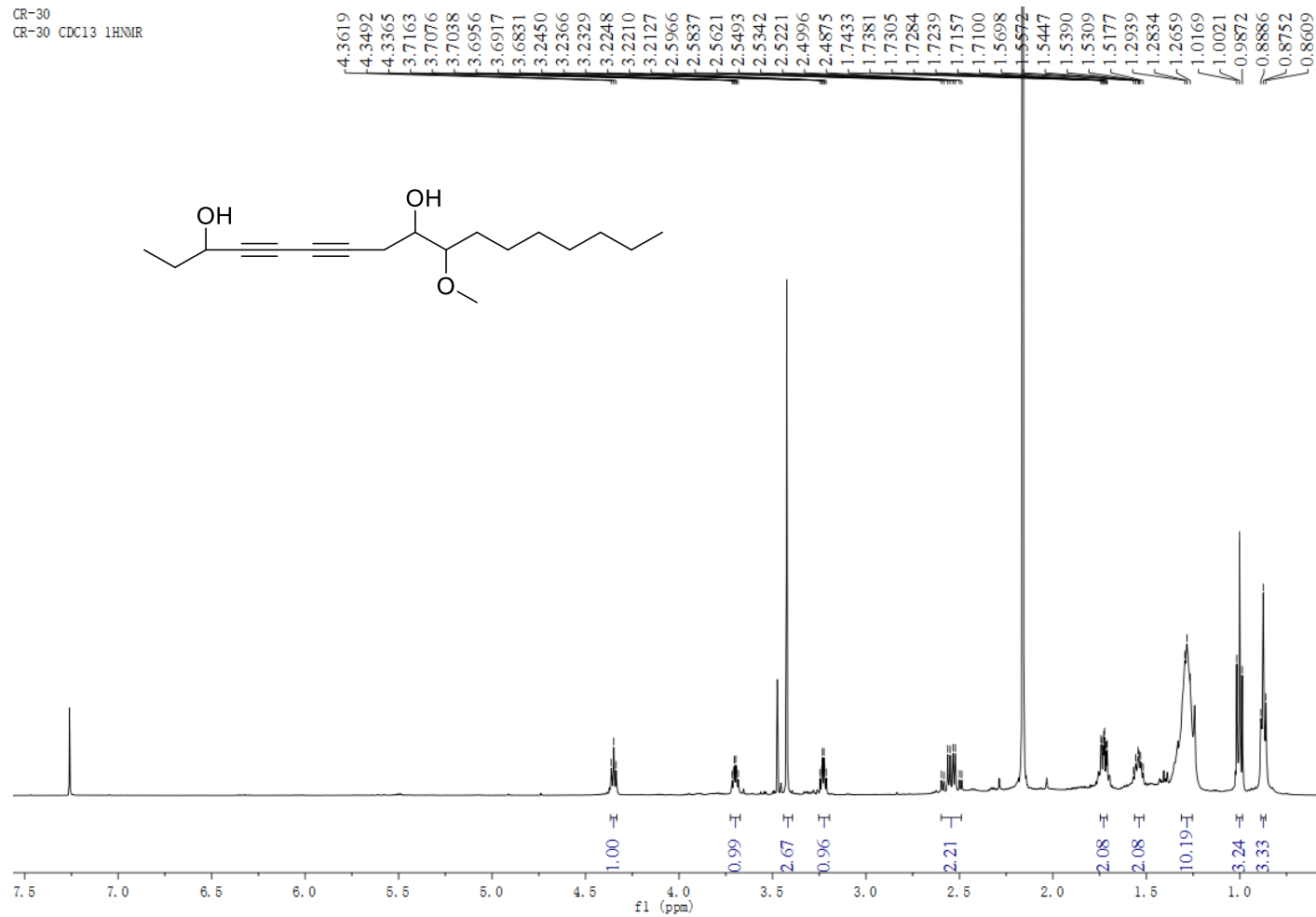


Figure S15. ¹H NMR spectrum (500 MHz) of compound **3** in CDCl₃.

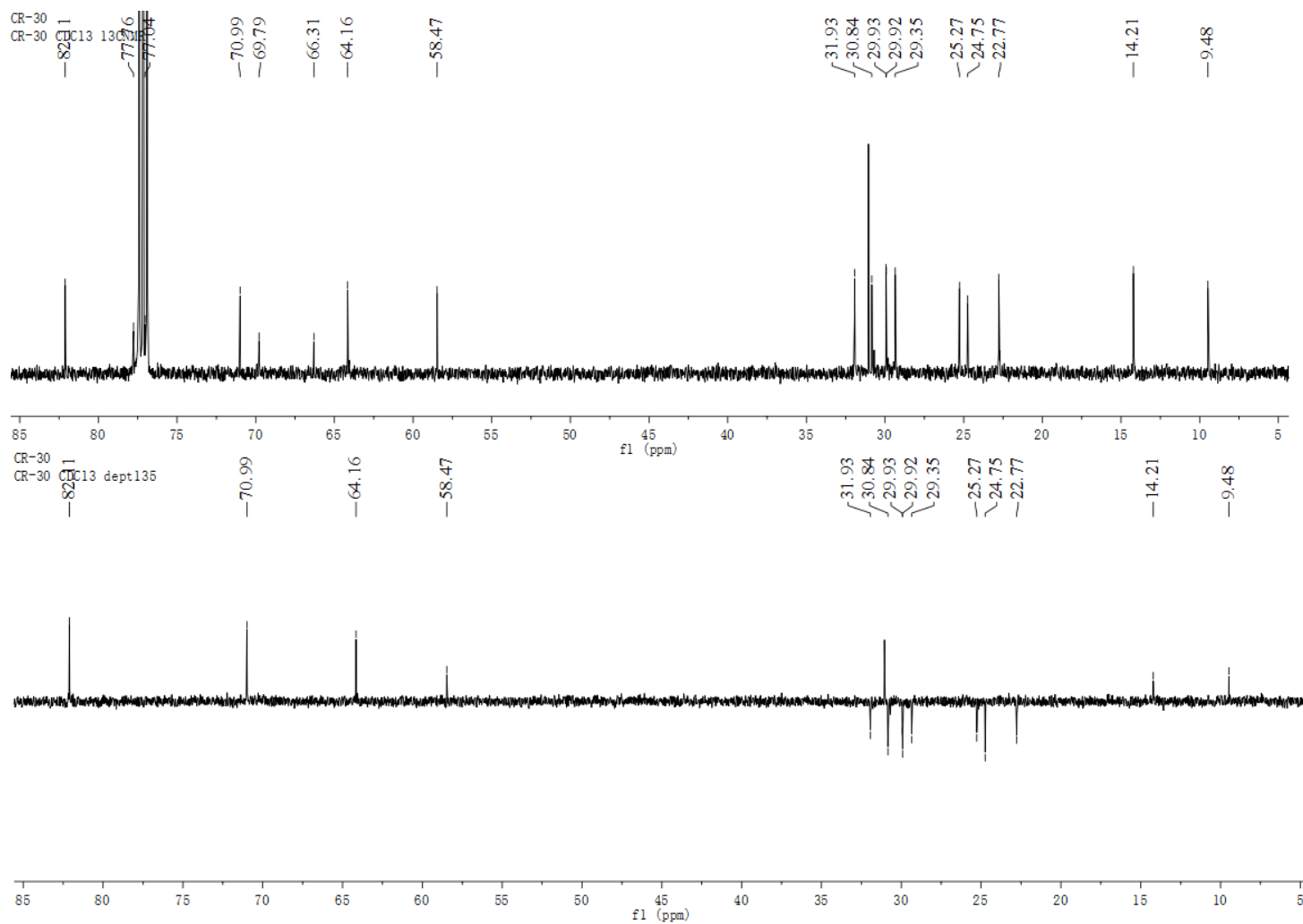


Figure S16. ^{13}C NMR spectrum (125 MHz) of compound **3** in CDCl_3 .

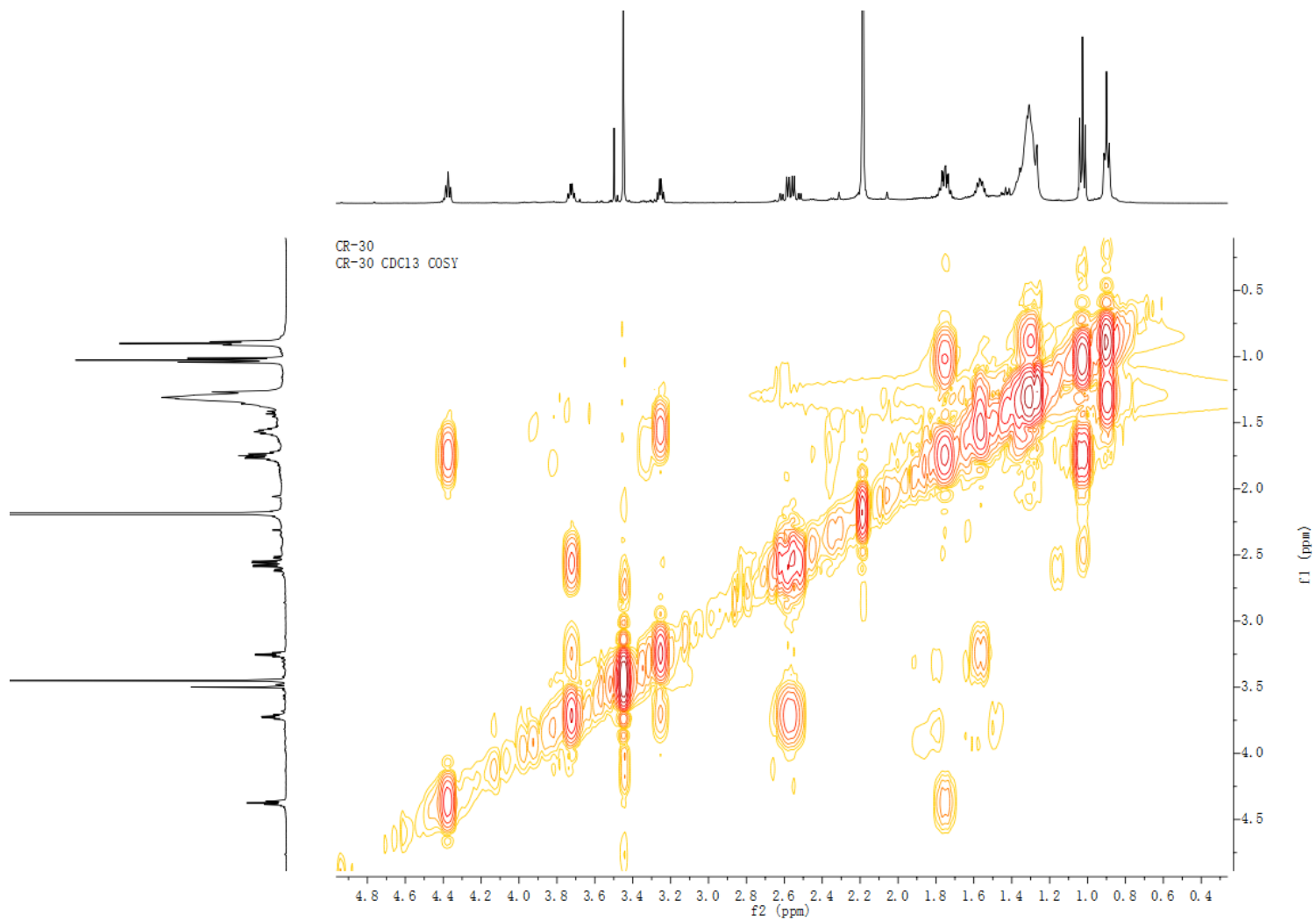


Figure S17. ^1H - ^1H COSY spectrum of compound **3** in CDCl_3 .

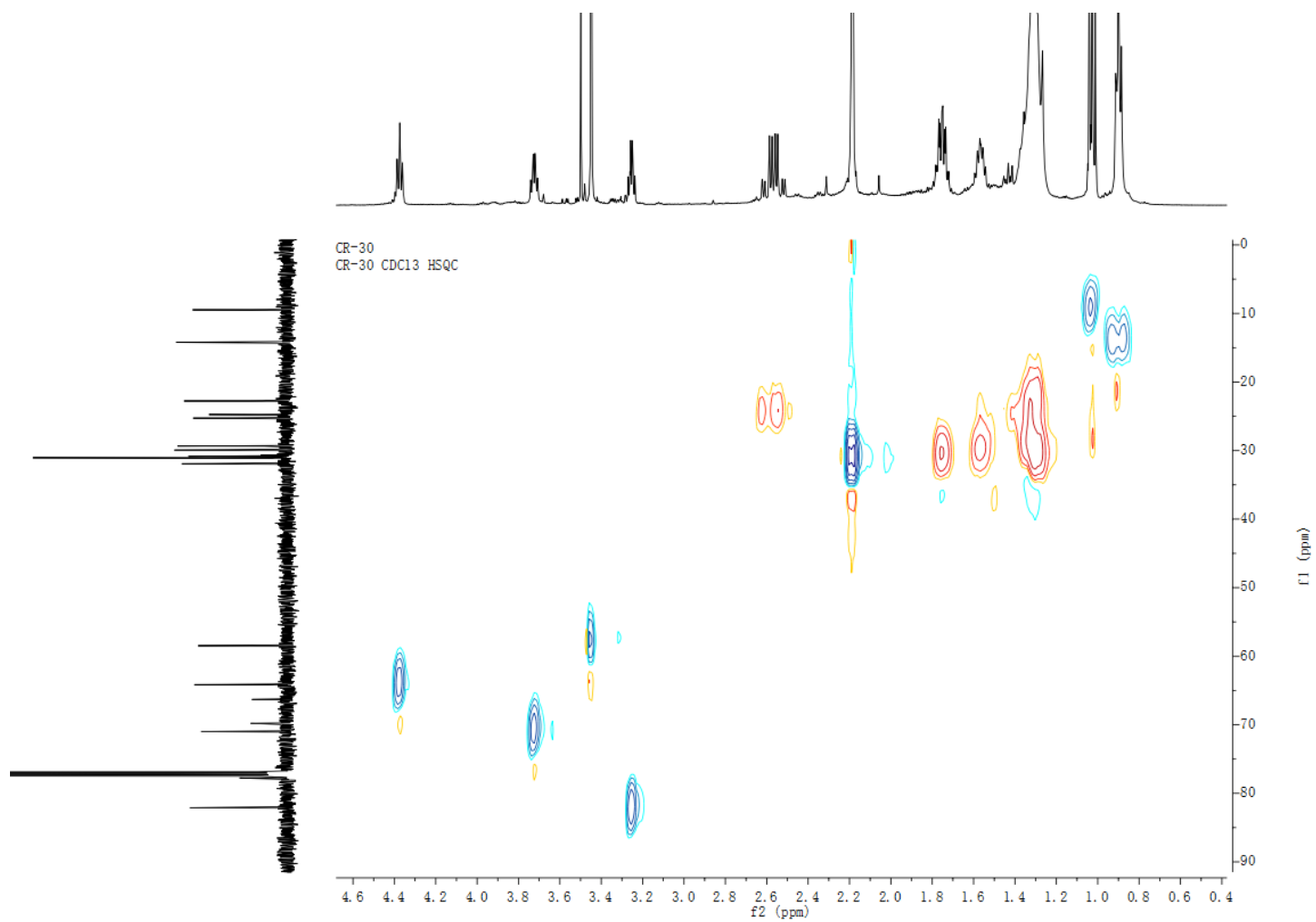


Figure S18. HSQC spectrum of compound **3** in CDCl₃.

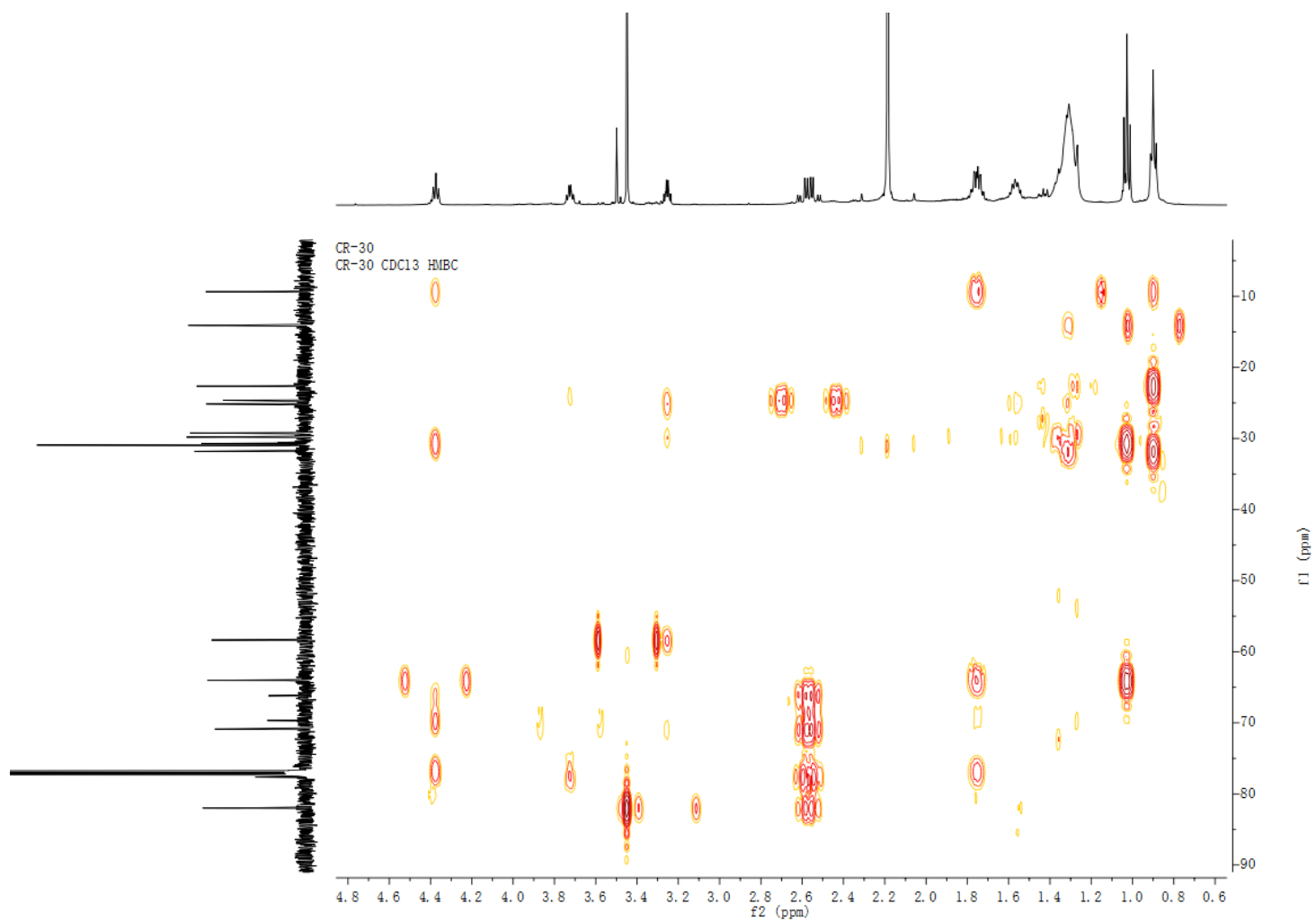


Figure S19. HMBC spectrum of compound **3** in CDCl₃.

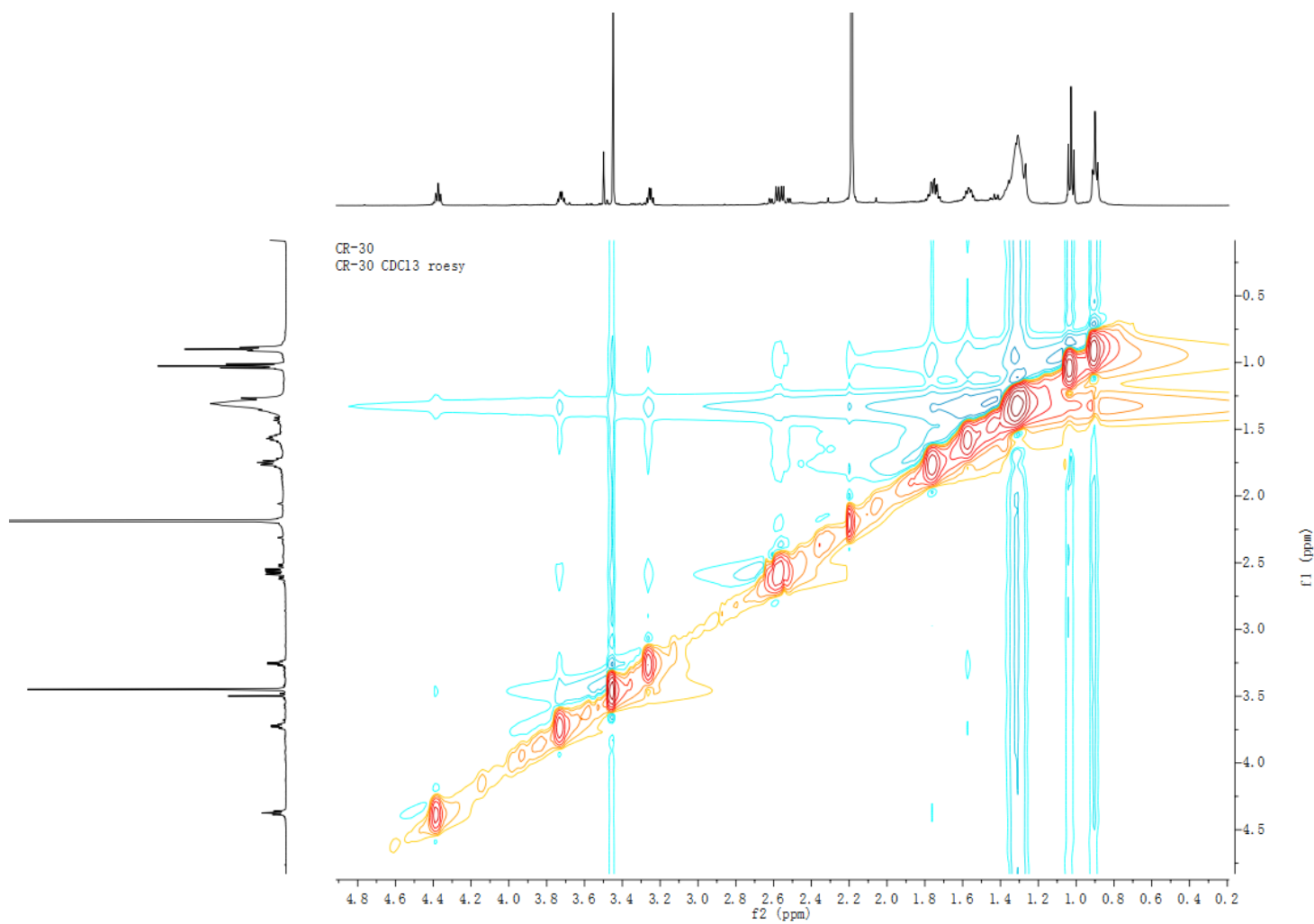
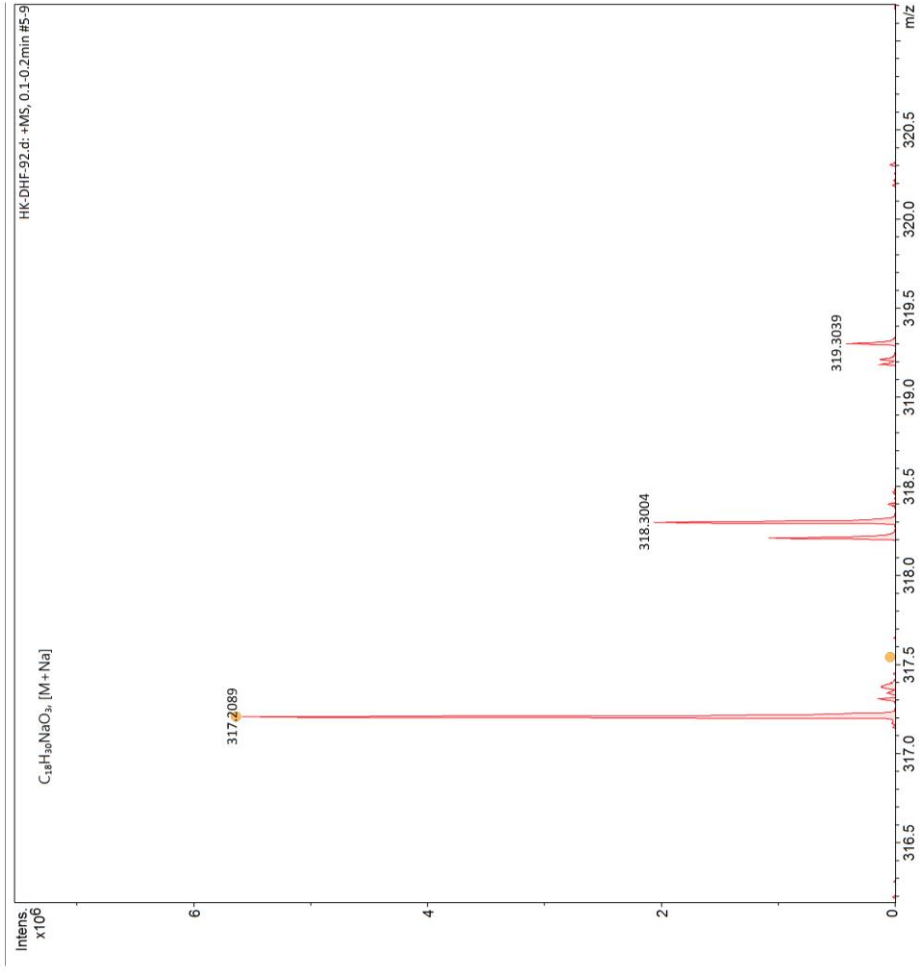


Figure S20. ROESY spectrum of compound **3** in CDCl₃.

Display Report

Analysis Info	Acquisition Date	5/28/2018 11:42:07 AM
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Sample Name	HK-DHF-92	
Comment		
Acquisition Parameter	Operator	Demo User
Source Type	Instrument	maxis II ETD
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Not active		
Focus		
50 m/z		
Scan Begin		
Scan End		
1300 m/z		
Ion Polarity	Set Nebulizer	0.4 Bar
Positive	Set Dry Heater	180 °C
4500 V	Set Dry Gas	4.0 l/min
-500 V	Set Divert Valve	Waste
Set End Plate Offset	Set APCI Heater	0 °C
2000 V		
Set Charging Voltage		
0 nA		
Set Corona		



Sum Formula	Ion Formula	Meas. m/z	m/z	err	[ppm]
C ₁₈ H ₃₀ O ₃	C ₁₈ H ₃₀ NaO ₃	317.2093	317.2089	1.3	

Figure S21. HRESI(+)-MS spectrum of compound 3.

CR-17
CR-17 CDCl₃ 1H NMR

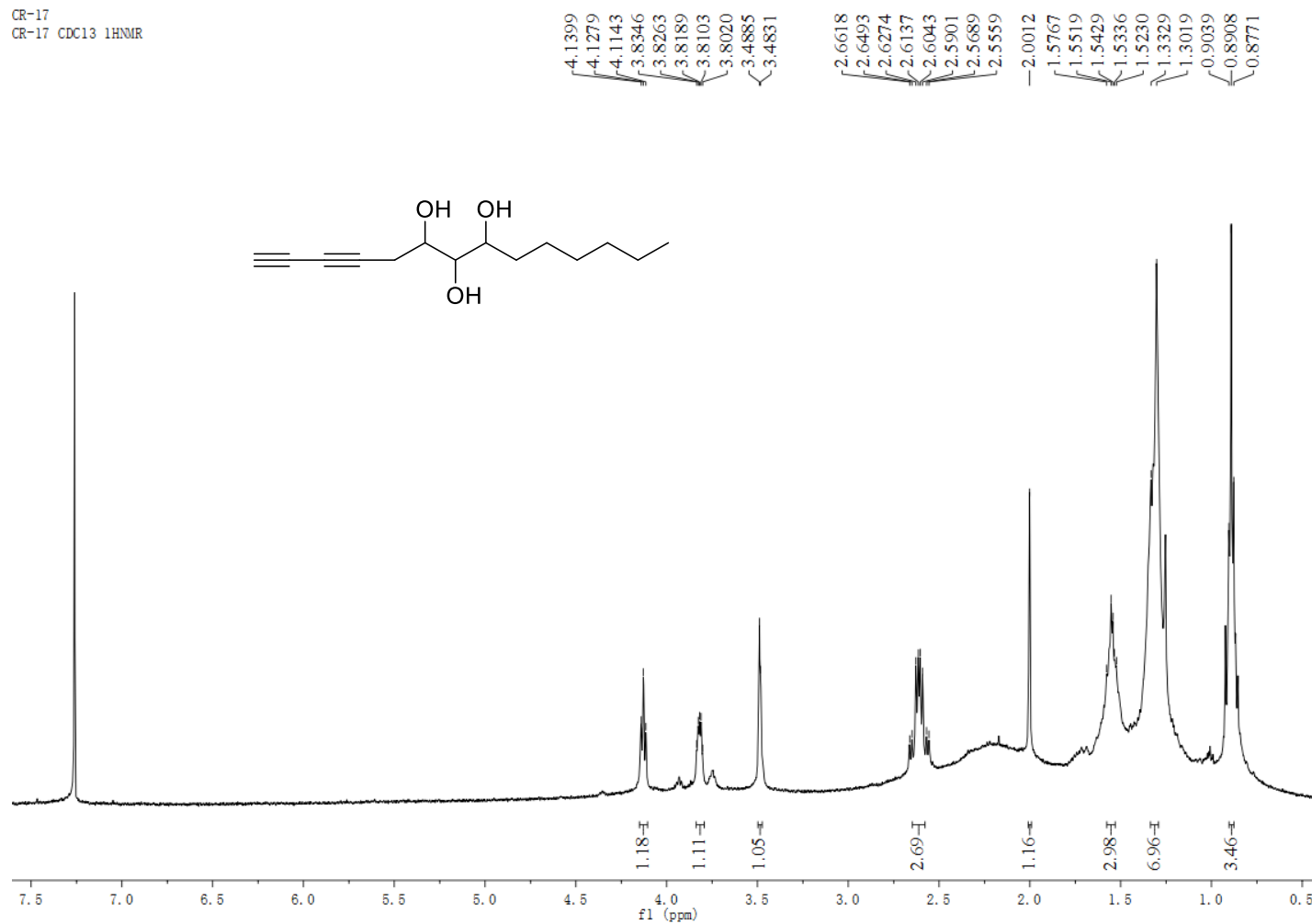


Figure S22. ¹H NMR spectrum (500 MHz) of compound 4 in CDCl₃.

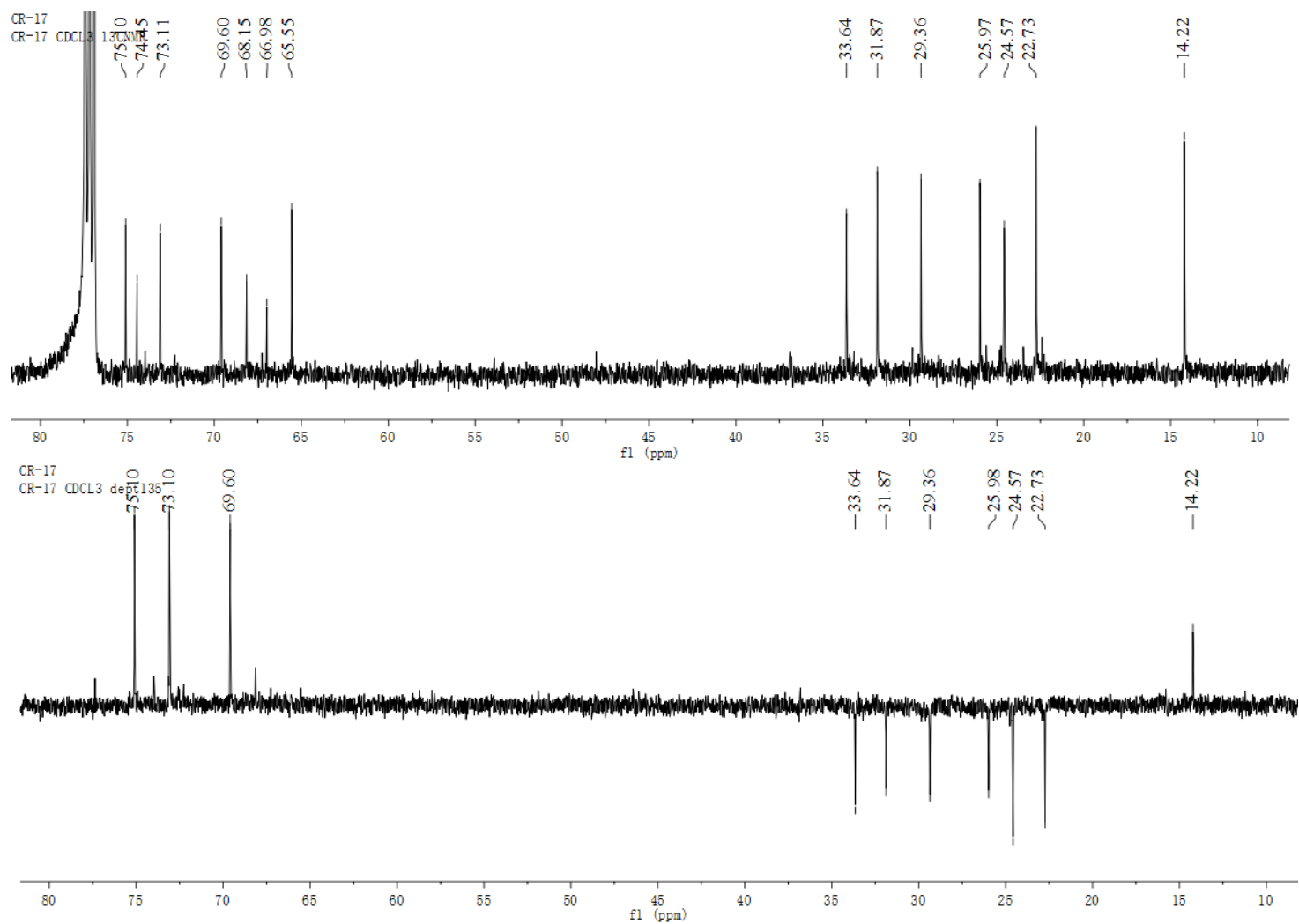


Figure S23. ¹³C NMR spectrum (125 MHz) of compound **4** in CDCl₃.

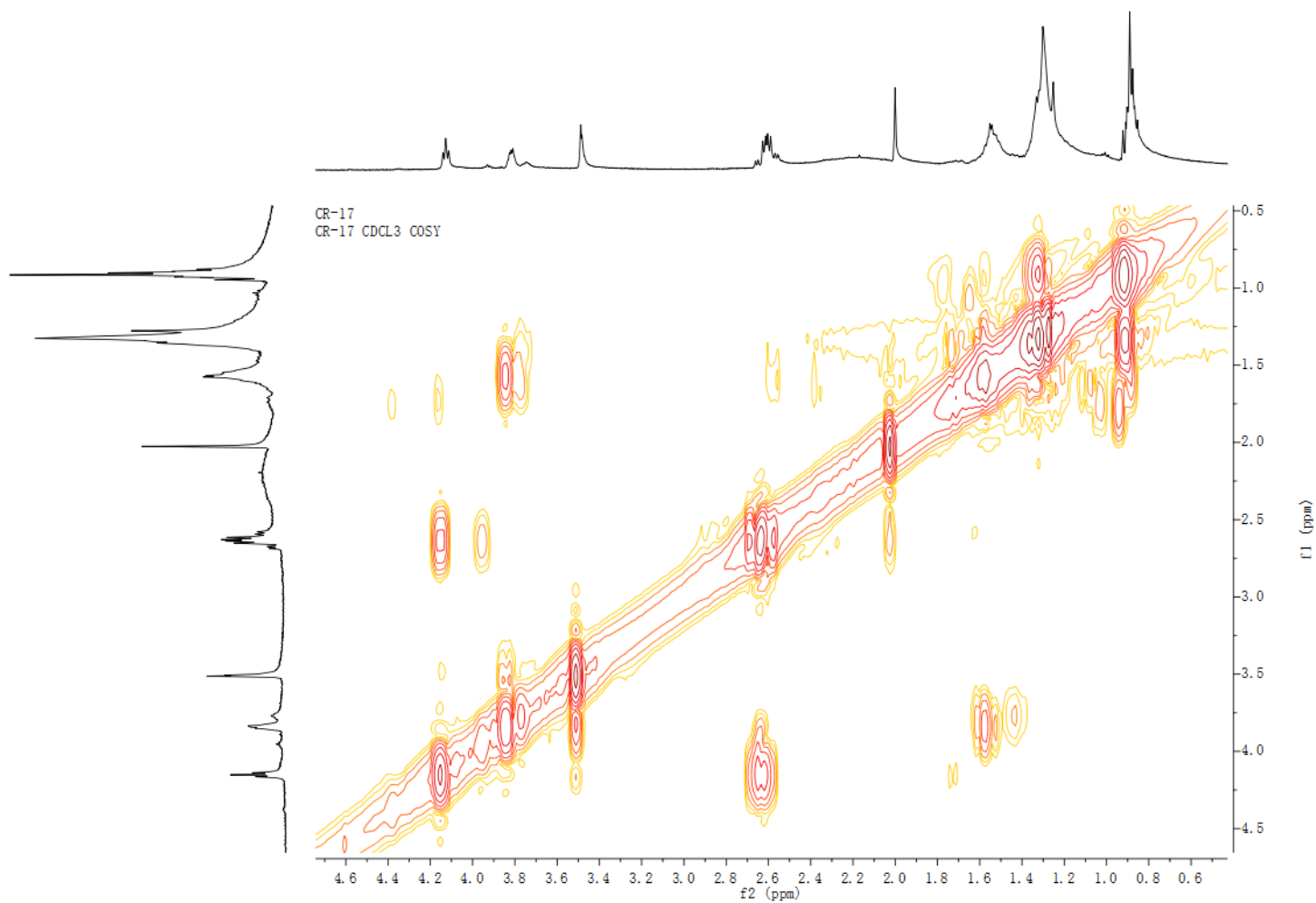


Figure S24. ^1H - ^1H COSY spectrum of compound **4** in CDCl_3 .

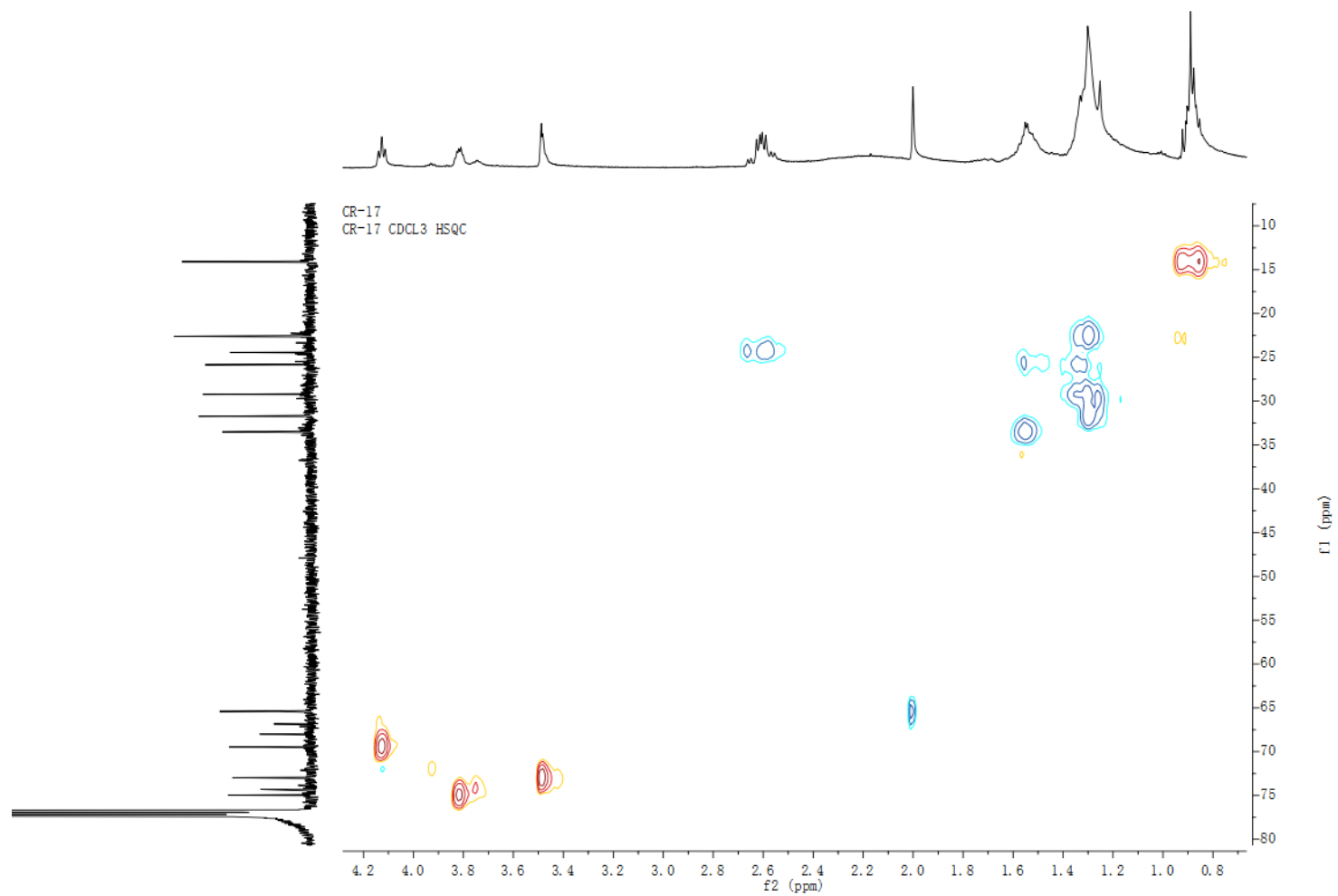


Figure S25. HSQC spectrum of compound **4** in CDCl₃.

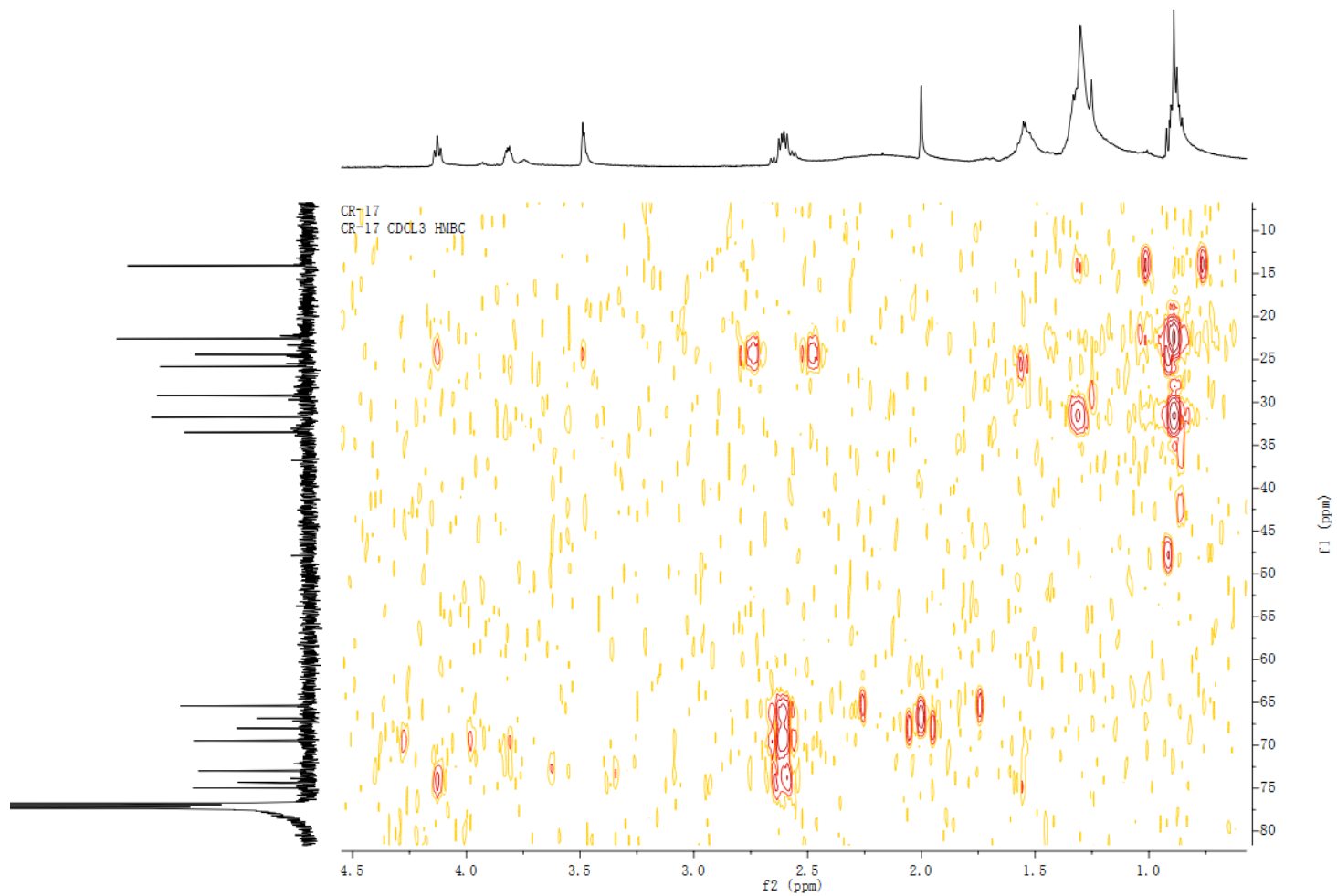


Figure S26. HMBC spectrum of compound **4** in CDCl₃.

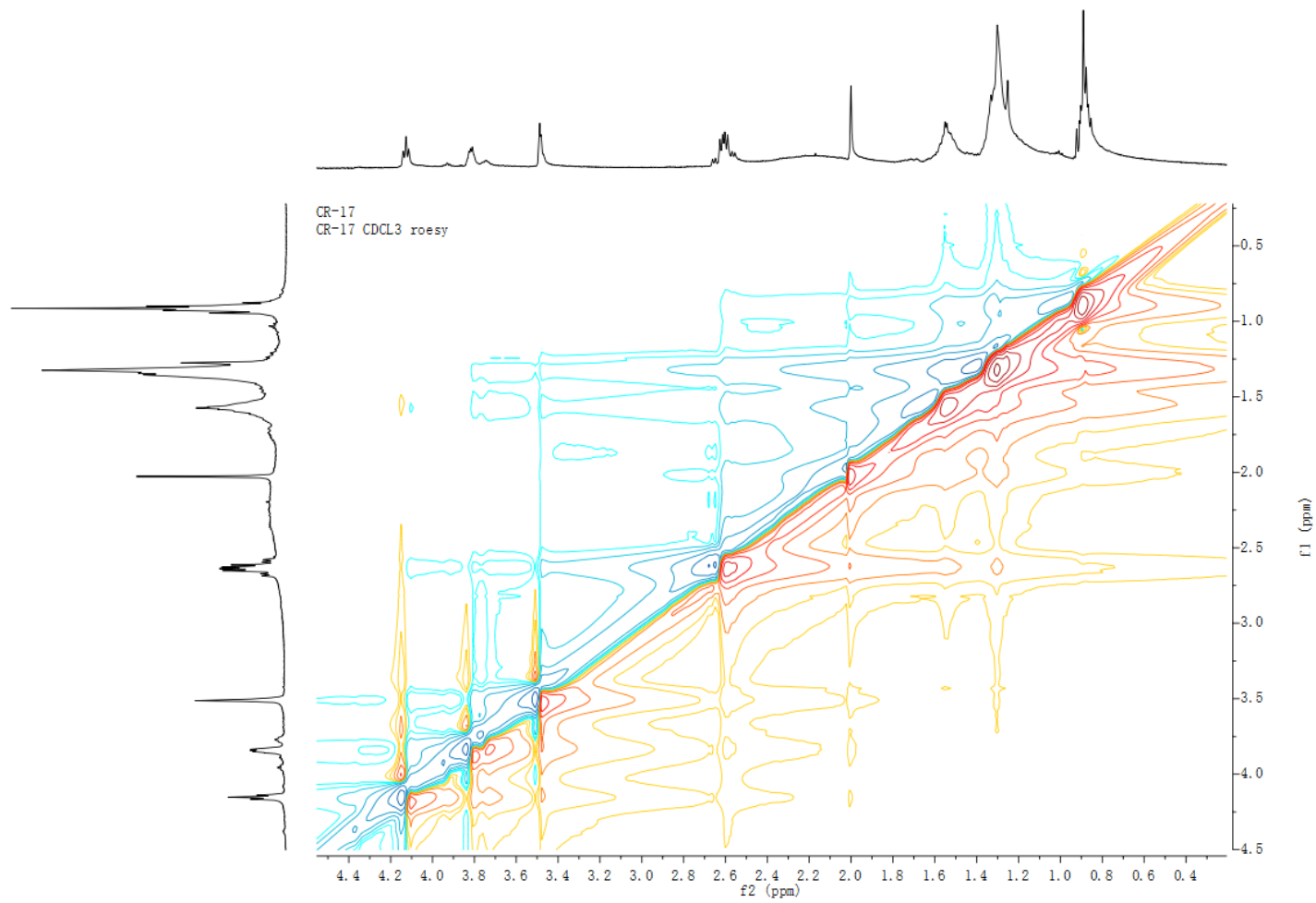
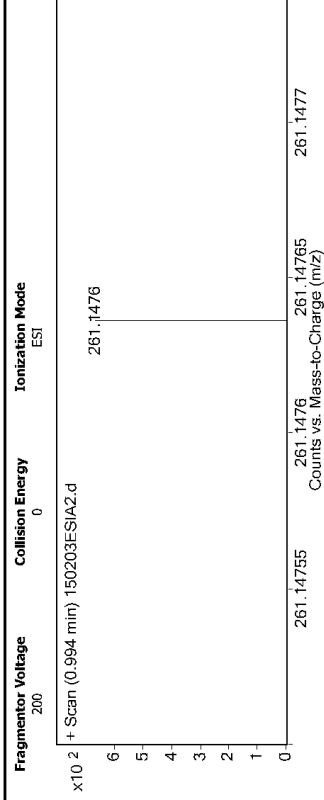


Figure S27. ROESY spectrum of compound **4** in CDCl₃.

Qualitative Analysis Report

Data Filename 150203ESI2.d	Sample Name CR-17	
Sample Type Sample	Position	
Instrument Name Agilent G6230 TOF MS	User Name KIB	
Acq Method ESL.m	Acquired Time 2/3/2015 11:07:25 AM	
IRM Calibration Status Success	DA Method ESL.m	
Comment		
Sample Group Info.		
Acquisition SW 6200 series TOF/6500 series		
Version Q-TOF B.05.01 (B5125.2)		

User Spectra



Peak List

m/z	z	Abund
121.0509	1	219630.8
122.0528	1	12863.49
135.0662		6055.44
274.2737	1	10609.1
318.2994	1	8079.25
922.0098	1	324422.59
923.0119	1	54759.75
924.0141	1	6479.02
1821.9503	1	17132.29
1941.9912	1	7572.69

Formula Calculator Element Limits

Element	Min	Max
C	0	200
H	0	400
O	0	5
Na	1	1

Formula Calculator Results

Formula	CalculatedMass	CalculatedMz	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C14 H22 Na O3	261.1467	261.1461	261.1476	-1.5	-5.8	3.5000

--- End Of Report ---

Figure S28. HRESI(+)MS spectrum of compound **4**.

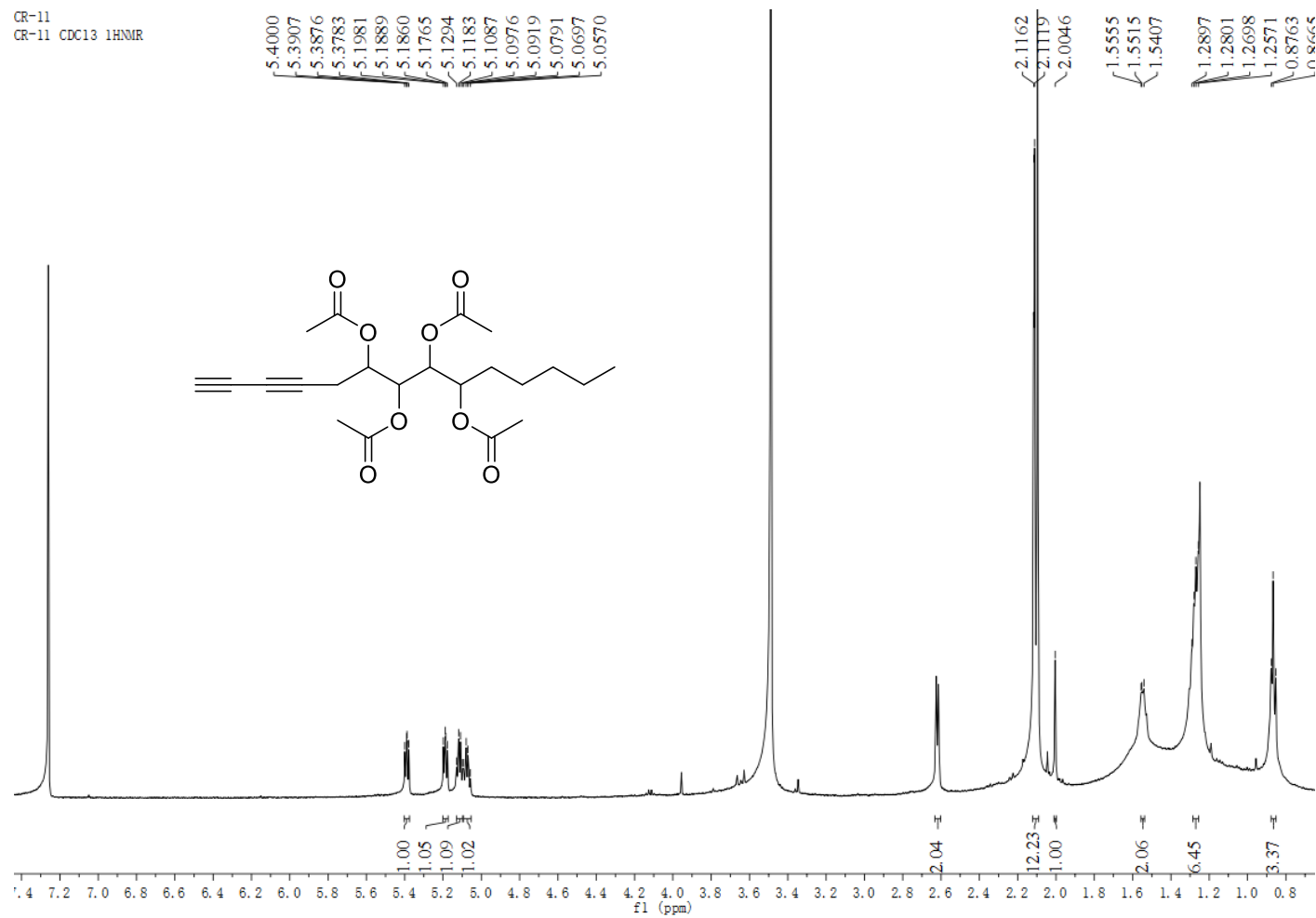


Figure S29. ¹H NMR spectrum (500 MHz) of compound **5** in CDCl₃.

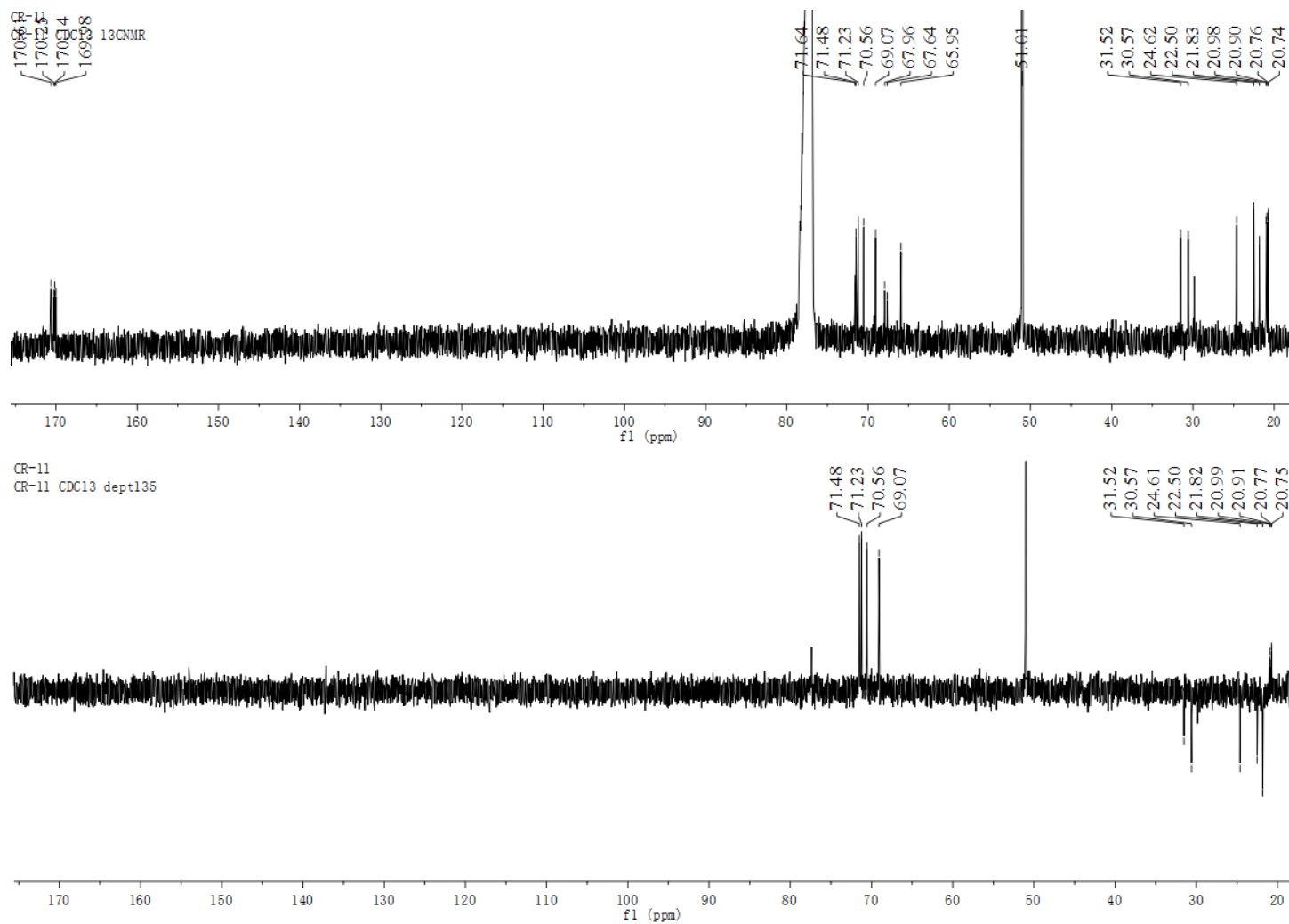


Figure S30. ¹³C NMR spectrum (125 MHz) of compound **5** in CDCl₃.

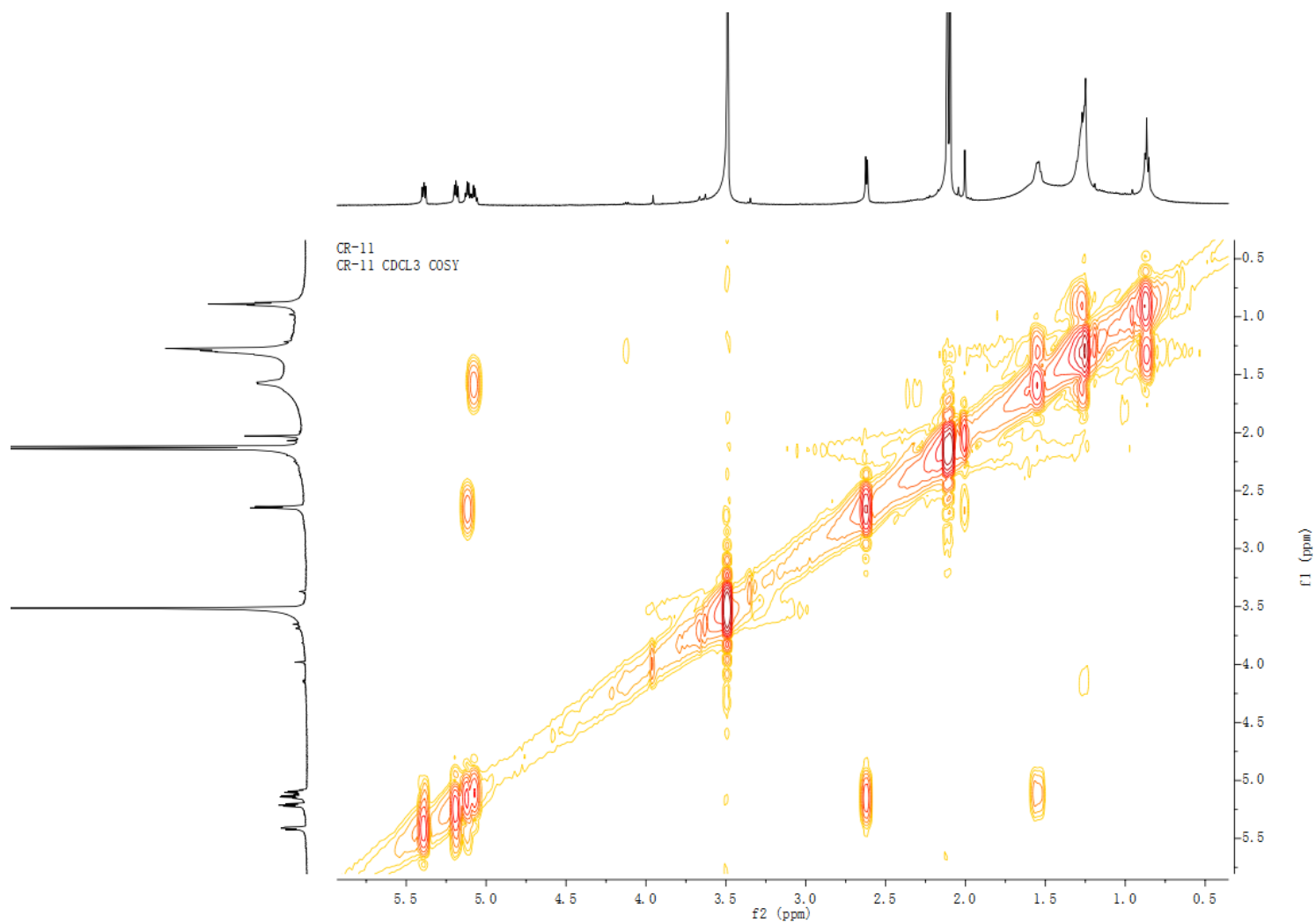


Figure S31. ^1H - ^1H COSY spectrum of compound **5** in CDCl_3 .

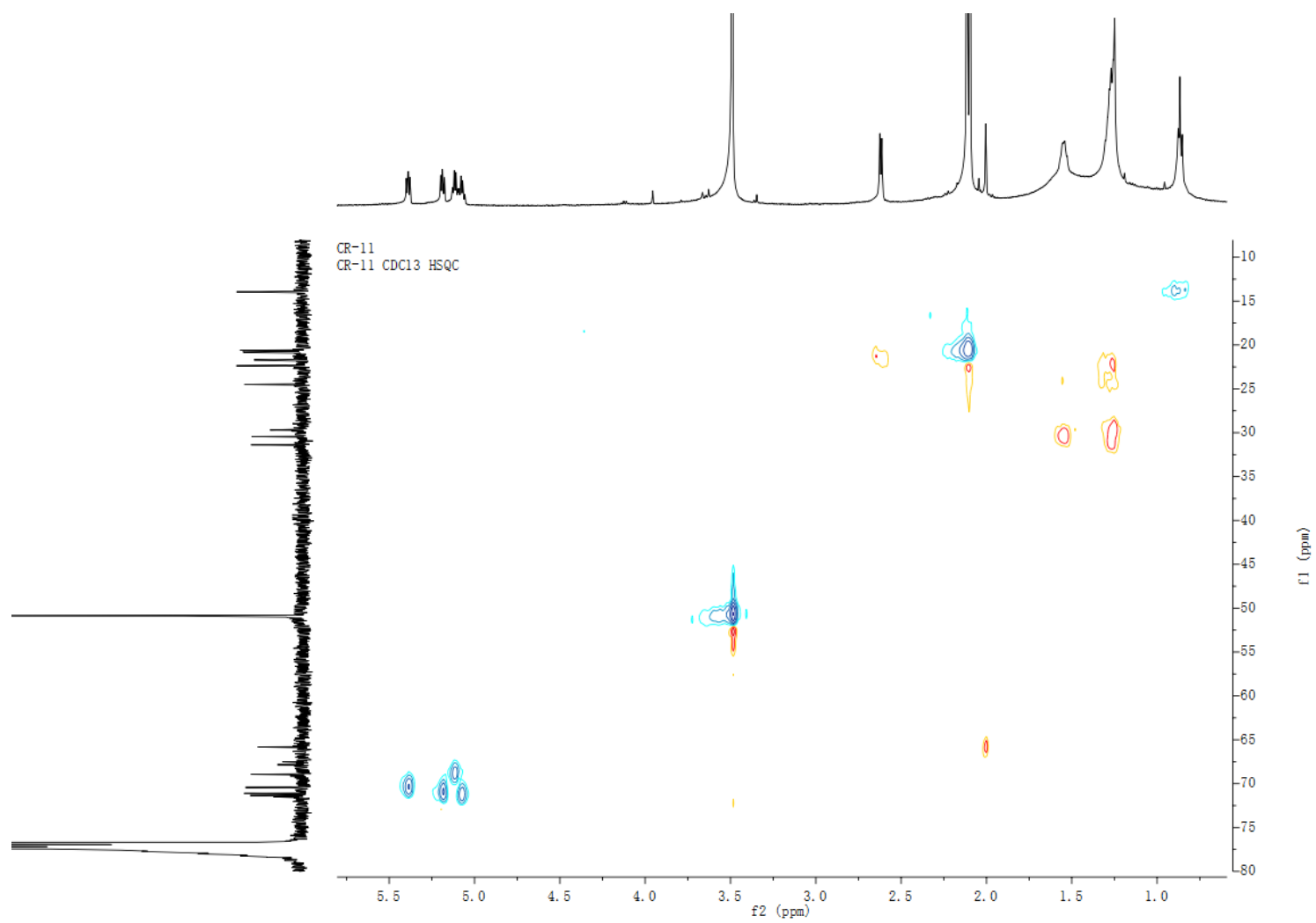


Figure S32. HSQC spectrum of compound **5** in CDCl₃.

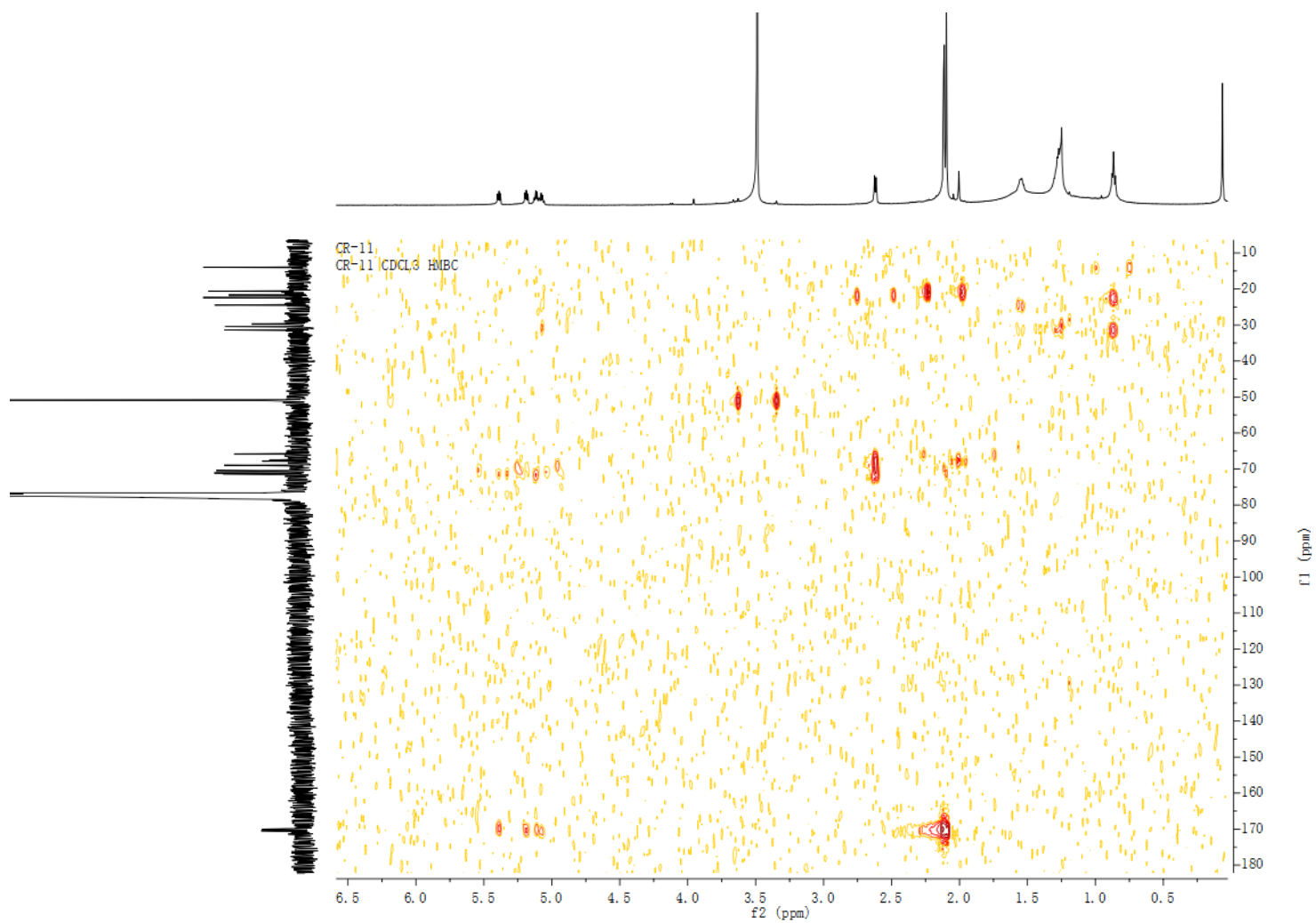


Figure S33. HMBC spectrum of compound **5** in CDCl₃.

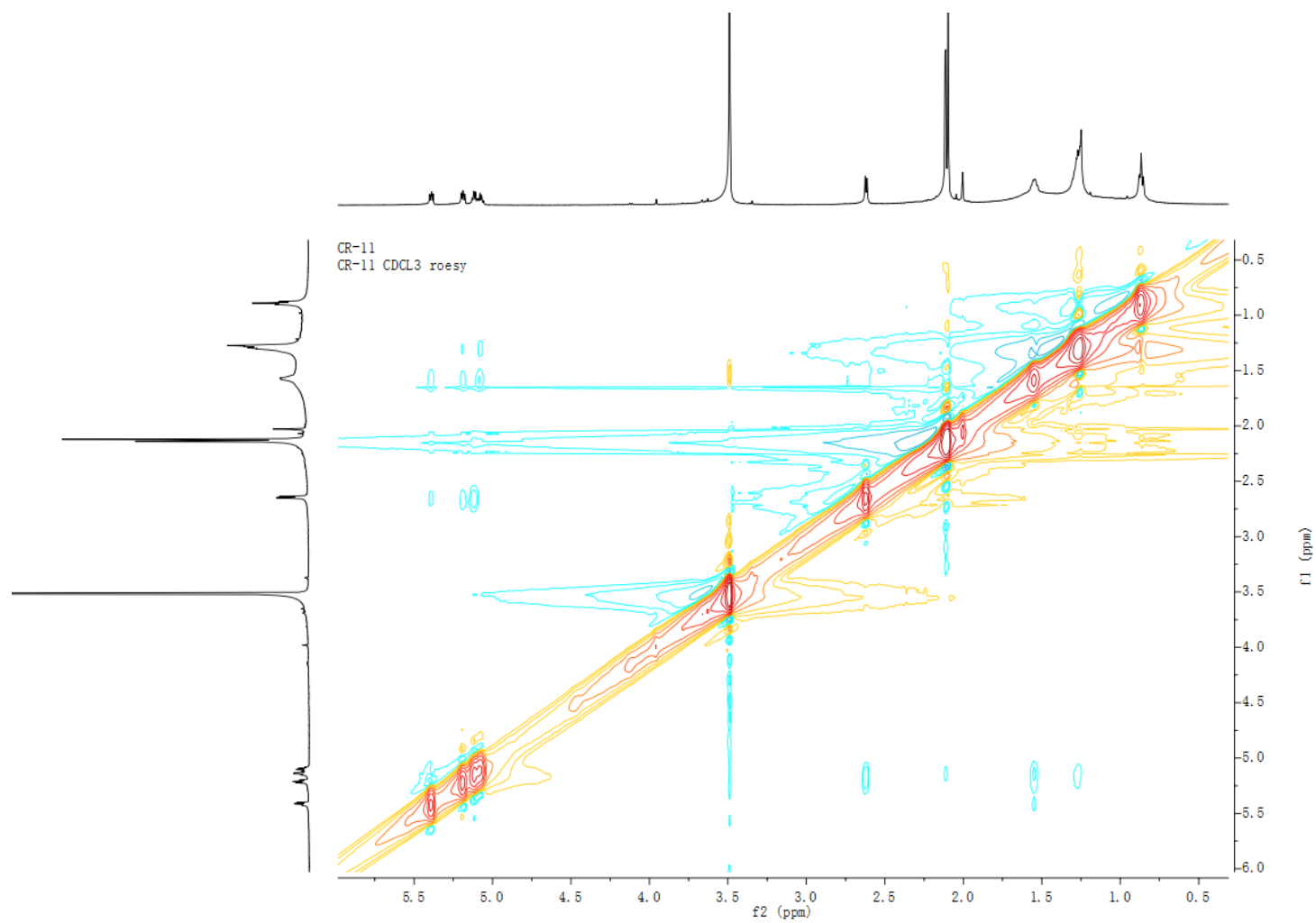


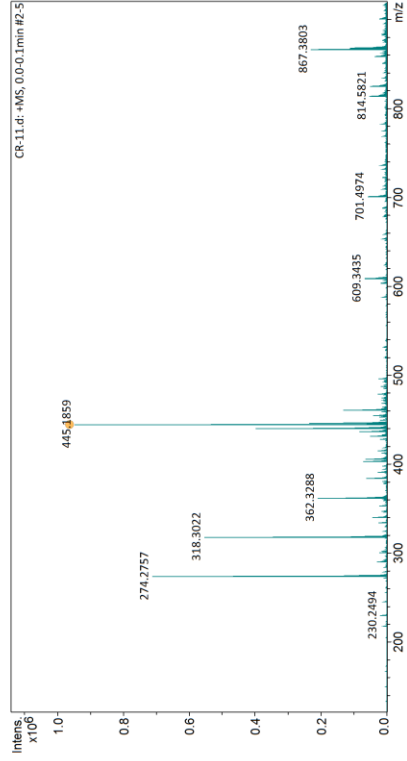
Figure S34. ROESY spectrum of compound **5** in CDCl₃.

Mass Spectrum SmartFormula Report

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 Method DirectInfusion - MS - positive.m
 Sample Name CR-11
 Operator Demo User
 Instrument compact
 Comment 8255754.20156

Acquisition Parameter

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Scan Begin	50 m/z	Set Capillary Offset	0 m/z
Scan End	1300 m/z	Set Entrance Voltage	2000 V
		Set Corona	0 nA
		Set Nebulizer	0.4 Bar
		Set Dry Heater	180 °C
		Set Dry Gas Flow	4 l/min
		Set Dry Gas Source	Source
		Set APCI Heats	0 °C
		Set APCI Heater	0 °C



Sum Formula	Ion Formula	Meas. m/z	m/z	err [mDa]	err [ppm]
C22H30O8	C22H30NO8	445.1859	445.1833	-2.6	-5.9

Figure S35. HRESI(+)-MS spectrum of compound 5.