

# Exploring the Chemical Diversity of Algerian Plants: Three New Pentacyclic

## Triterpenoids from *Launaea acanthoclada* roots

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S1. <sup>1</sup>H NMR spectrum of acantholupenone (**1**) (600 MHz, CDCl<sub>3</sub>).

S2. <sup>13</sup>C NMR spectrum of acantholupenone (**1**) (150 MHz, CDCl<sub>3</sub>).

S3. COSY spectrum of acantholupenone (**1**) (600 MHz, CDCl<sub>3</sub>).

S4. HSQC spectrum of acantholupenone (**1**) (600 MHz, CDCl<sub>3</sub>).

S5. HMBC spectrum of acantholupenone (**1**) (600 MHz, CDCl<sub>3</sub>).

S6. TOCSY spectrum of acantholupenone (**1**) (400 MHz, CDCl<sub>3</sub>).

S7. <sup>1</sup>H NMR spectrum of acantholupenone (**1**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).

S8. COSY spectrum of acantholupenone (**1**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).

S9. edHSQC spectrum of acantholupenone (**1**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).

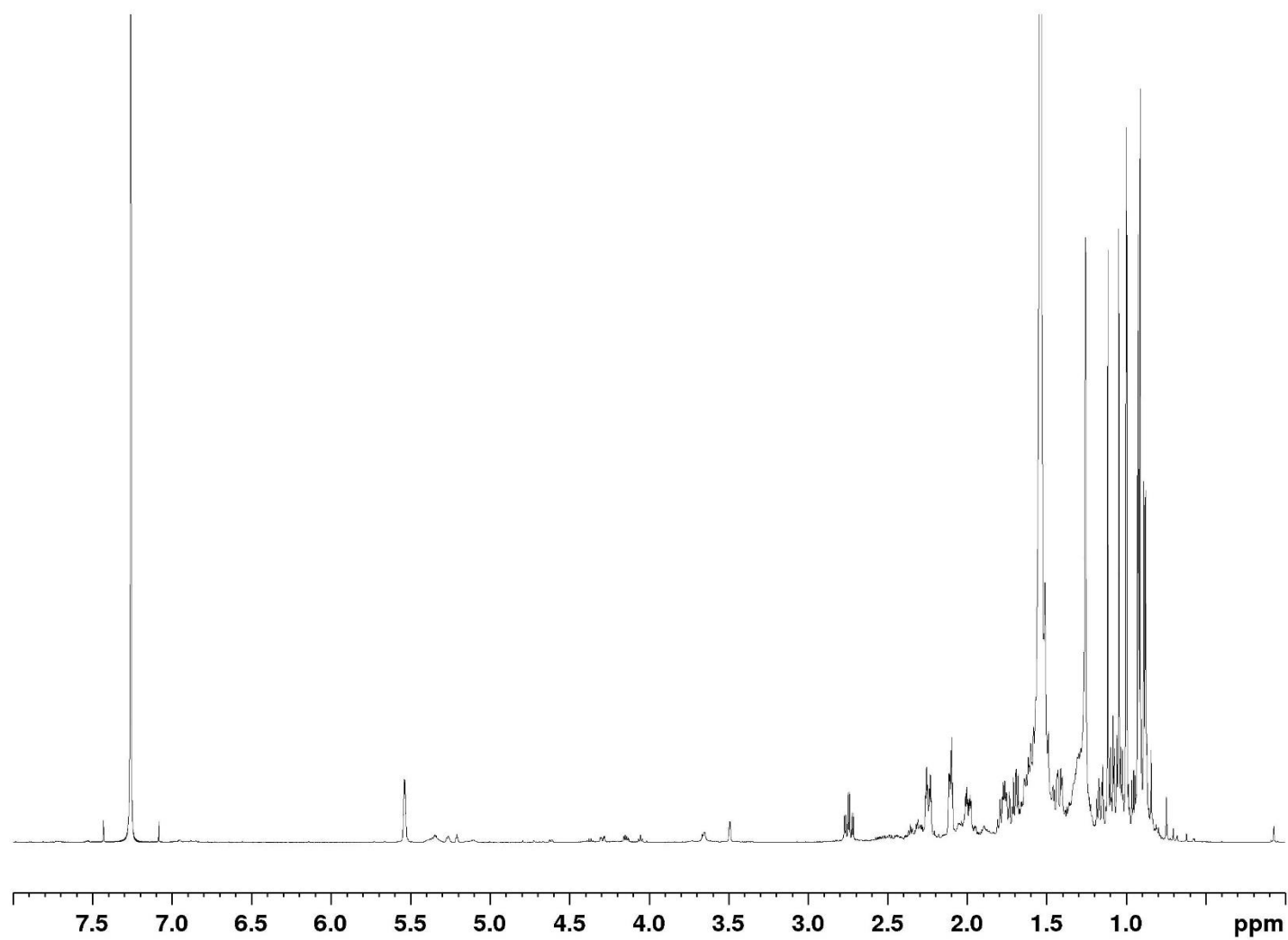
S10. HMBC spectrum of acantholupenone (**1**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).

S11. NOESY spectrum of acantholupenone (**1**) (400 MHz, C<sub>5</sub>D<sub>5</sub>N).

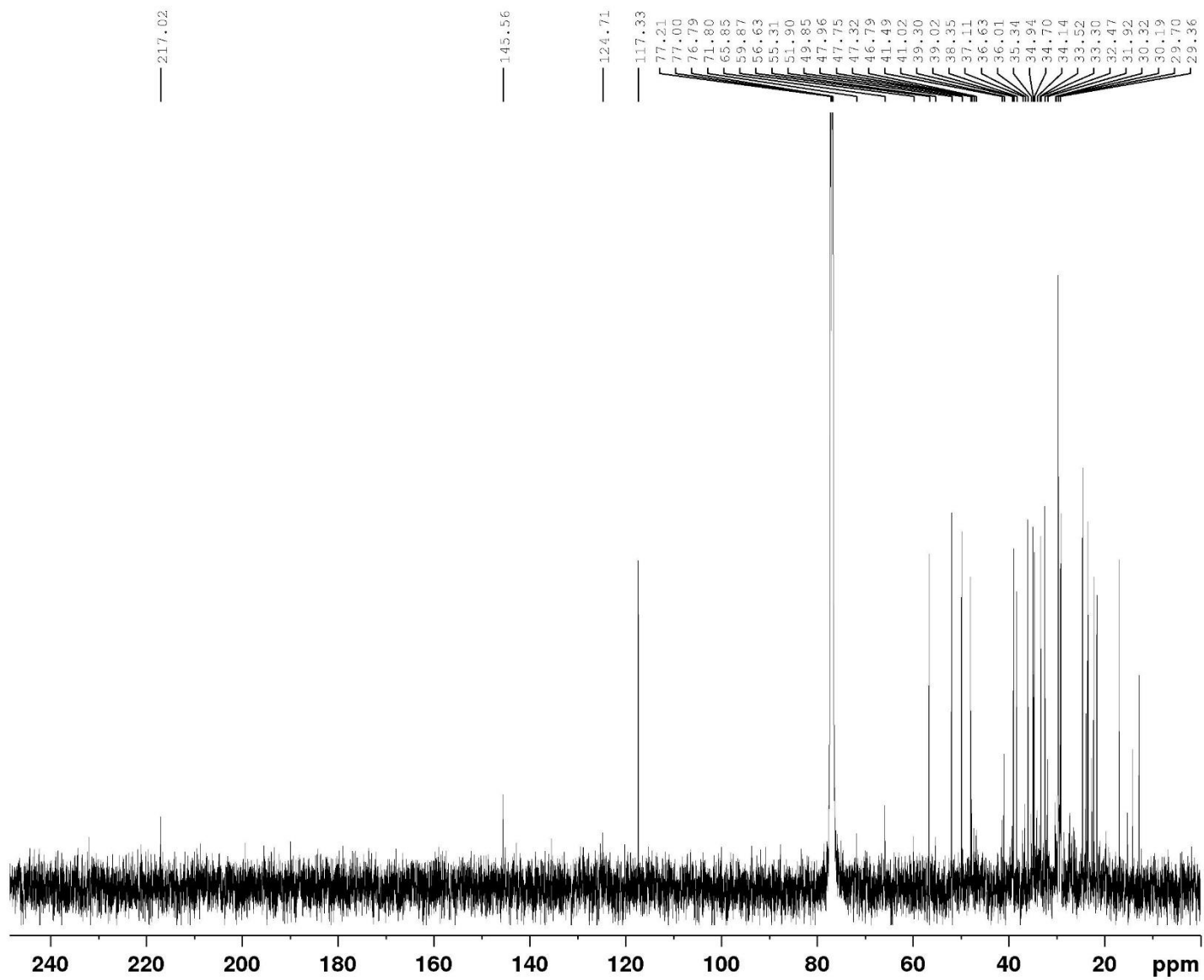
S12. HRESIMS spectrum of acantholupenone (**1**).

S13. <sup>1</sup>H NMR spectrum of acanthobauerendione (**2**) (600 MHz, CDCl<sub>3</sub>).

- S14.  $^{13}\text{C}$  NMR spectrum of acanthobauerendione (**2**) (150 MHz,  $\text{CDCl}_3$ ).
- S15. COSY spectrum of acanthobauerendione (**2**) (600 MHz,  $\text{CDCl}_3$ ).
- S16. edHSQC spectrum of acanthobauerendione (**2**) (400 MHz,  $\text{CDCl}_3$ ).
- S17. HMBC spectrum of acanthobauerendione (**2**) (600 MHz,  $\text{CDCl}_3$ ).
- S18. TOCSY spectrum of acanthobauerendione (**2**) (600 MHz,  $\text{CDCl}_3$ ).
- S19.  $^1\text{H}$  NMR spectrum of acanthobauerendione (**2**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S20.  $^{13}\text{C}$  NMR spectrum of acanthobauerendione (**2**) (150 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S21. COSY spectrum of acanthobauerendione (**2**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S22. edHSQC spectrum of acanthobauerendione (**2**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S23. HMBC spectrum of acanthobauerendione (**2**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S24. NOESY spectrum of acanthobauerendione (**2**) (400 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S25. HRESIMS spectrum of acanthobauerendione (**2**).
- S26.  $^1\text{H}$  NMR spectrum of acanthobauerenone (**3**) (600 MHz,  $\text{CDCl}_3$ ).
- S27.  $^{13}\text{C}$  NMR spectrum of acanthobauerenone (**3**) (150 MHz,  $\text{CDCl}_3$ ).
- S28. COSY spectrum of acanthobauerenone (**3**) (600 MHz,  $\text{CDCl}_3$ ).
- S29. edHSQC spectrum of acanthobauerenone (**3**) (600 MHz,  $\text{CDCl}_3$ ).
- S30. HMBC spectrum of acanthobauerenone (**3**) (600 MHz,  $\text{CDCl}_3$ ).
- S31.  $^1\text{H}$  NMR spectrum of acanthobauerenone (**3**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S32.  $^{13}\text{C}$  NMR spectrum of acanthobauerenone (**3**) (150 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S33. COSY spectrum of acanthobauerenone (**3**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S34. edHSQC spectrum of acanthobauerenone (**3**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S35. HMBC spectrum of acanthobauerenone (**3**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S36. TOCSY spectrum of acanthobauerenone (**3**) (400 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S37. NOESY spectrum of acanthobauerenone (**3**) (400 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).
- S38. HRESIMS spectrum of acanthobauerenone (**3**).
- S39. NMR data in  $\text{C}_5\text{D}_5\text{N}$  of acantholupenone (**1**) acanthobauerendione (**2**),  
and acanthobauerenone (**3**).

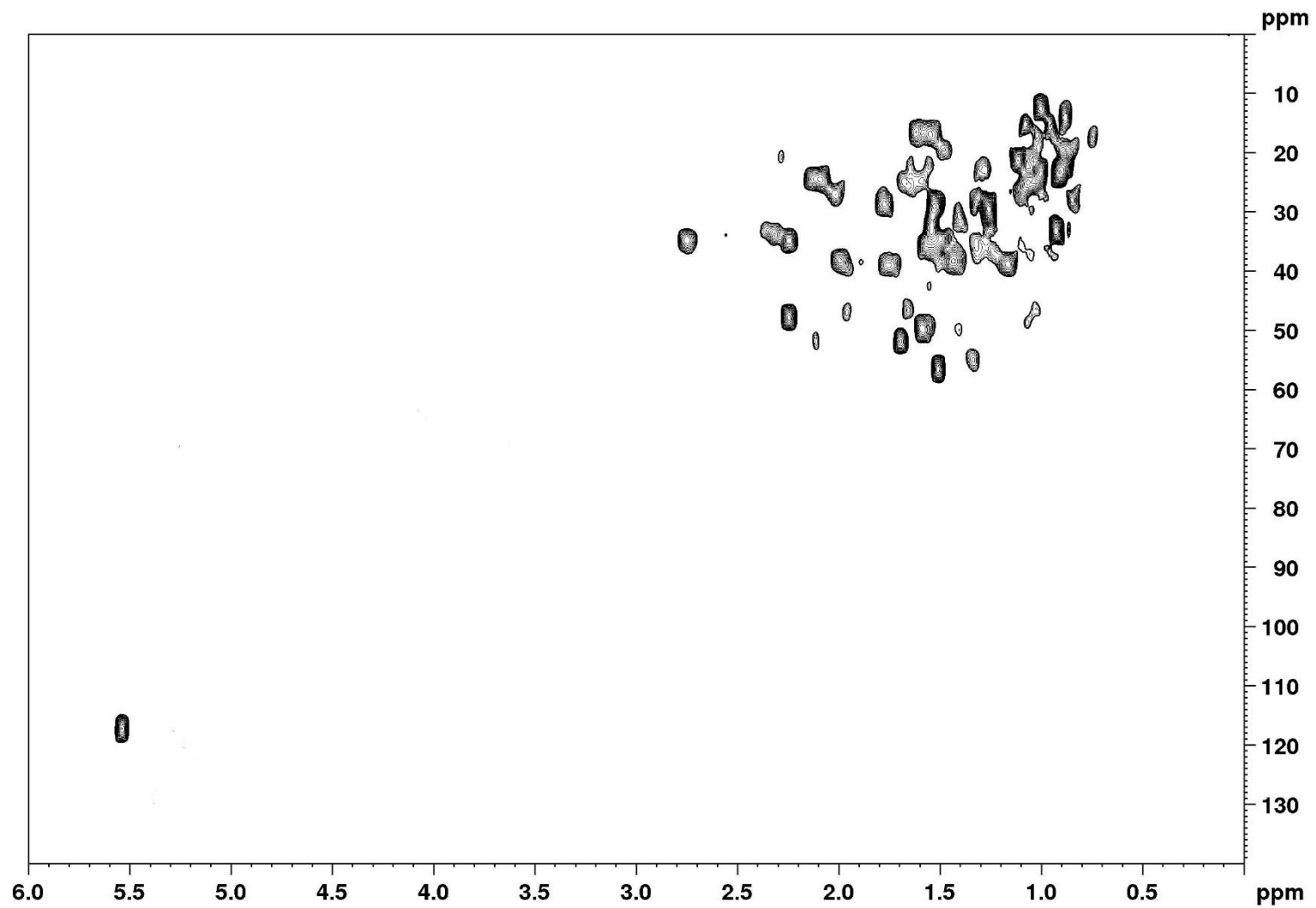


$^1\text{H}$  NMR spectrum of acantholupenone (**1**) (600 MHz,  $\text{CDCl}_3$ )

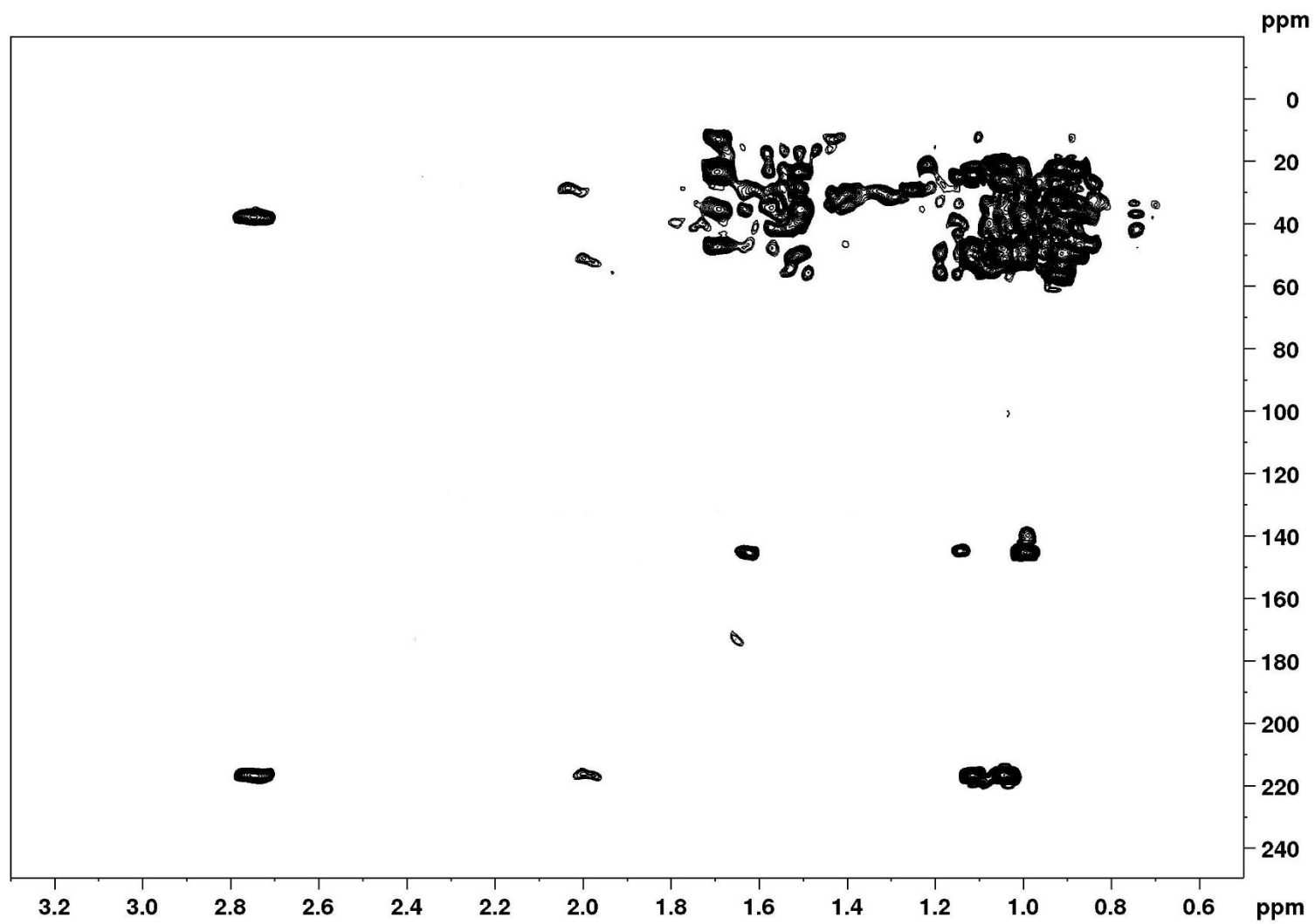


$^{13}\text{C}$  NMR spectrum of acantholupenone (**1**) (150 MHz,  $\text{CDCl}_3$ ).

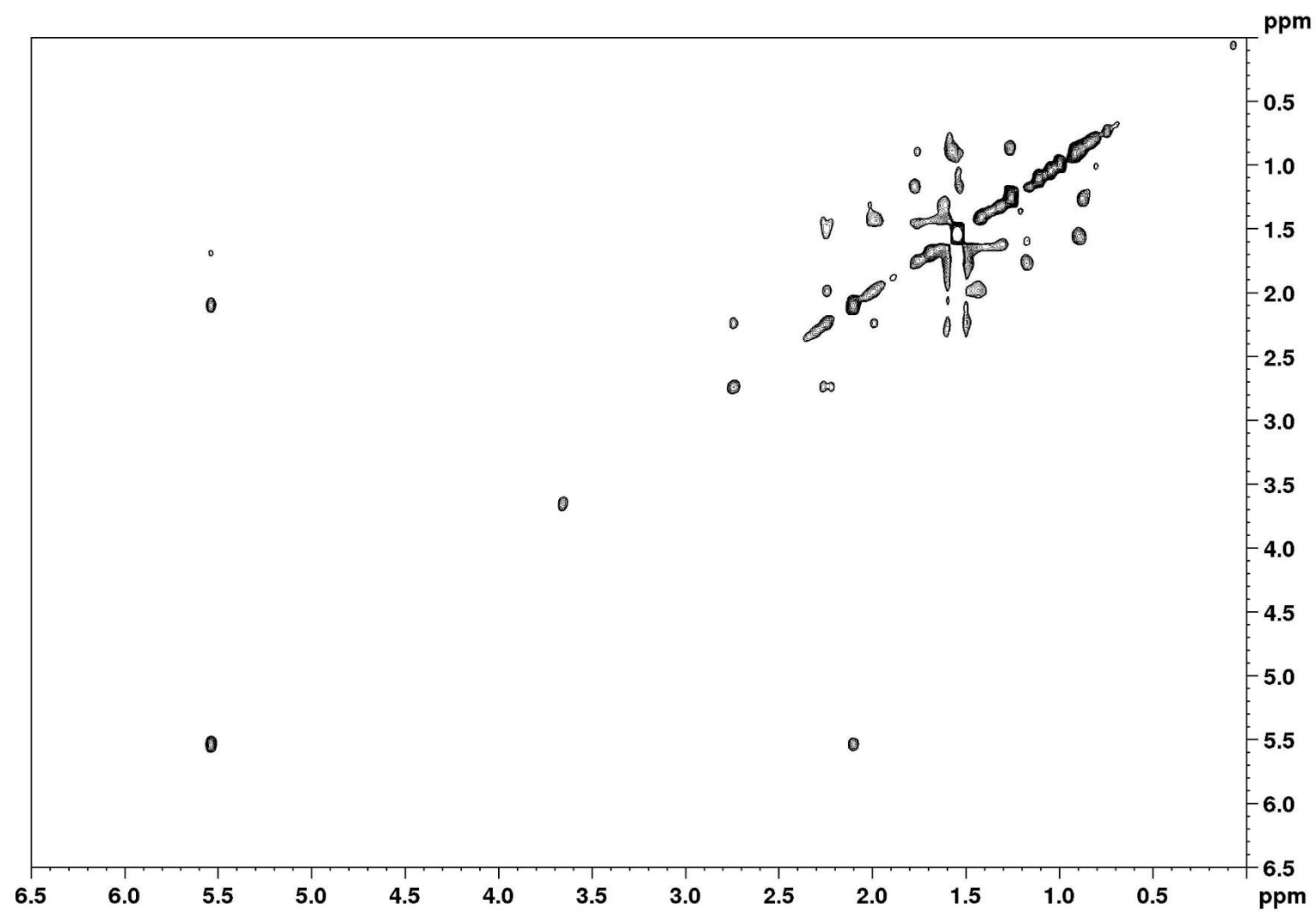




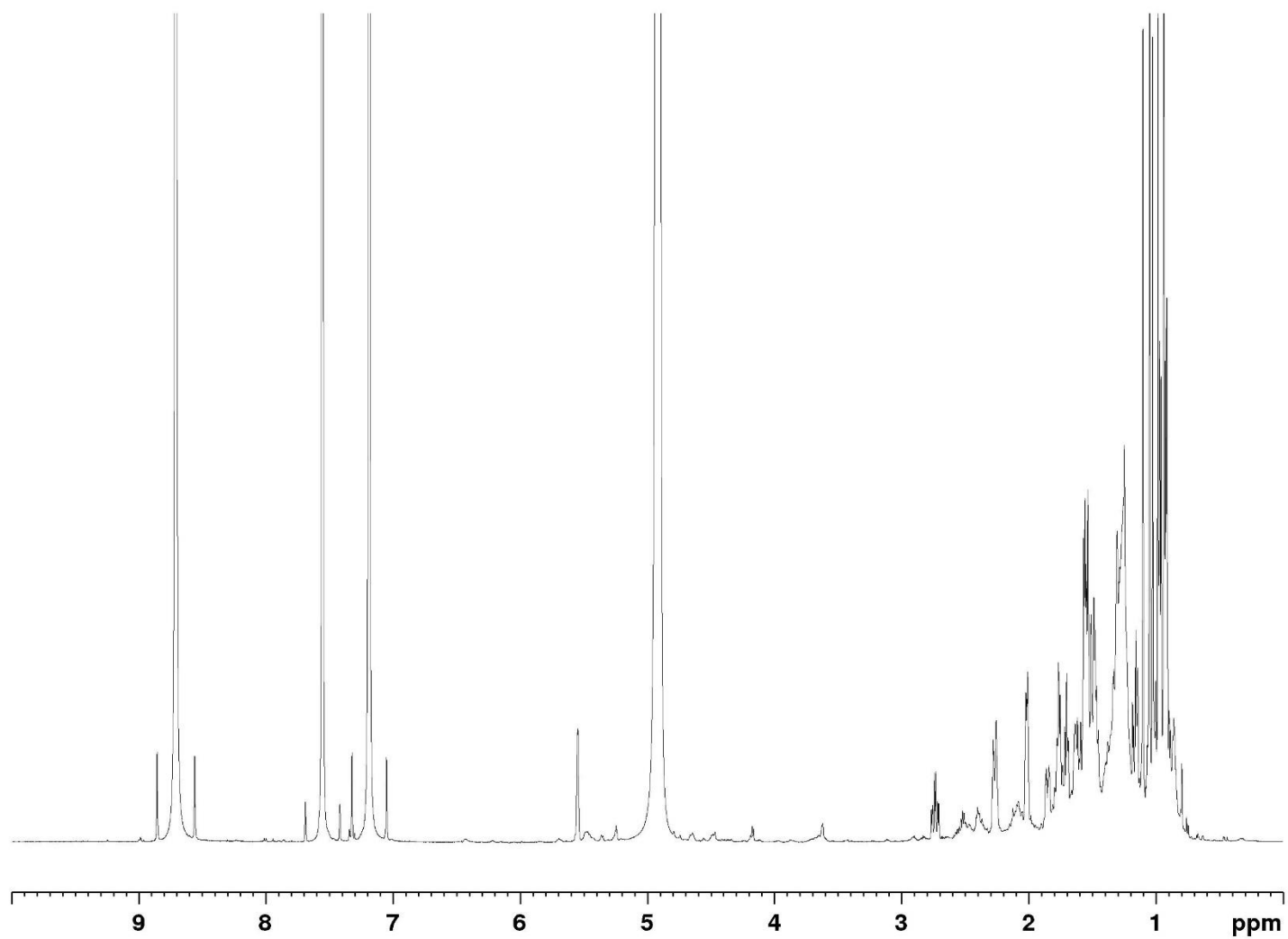
HSQC spectrum of acantholupenone (**1**) (600 MHz,  $\text{CDCl}_3$ ).



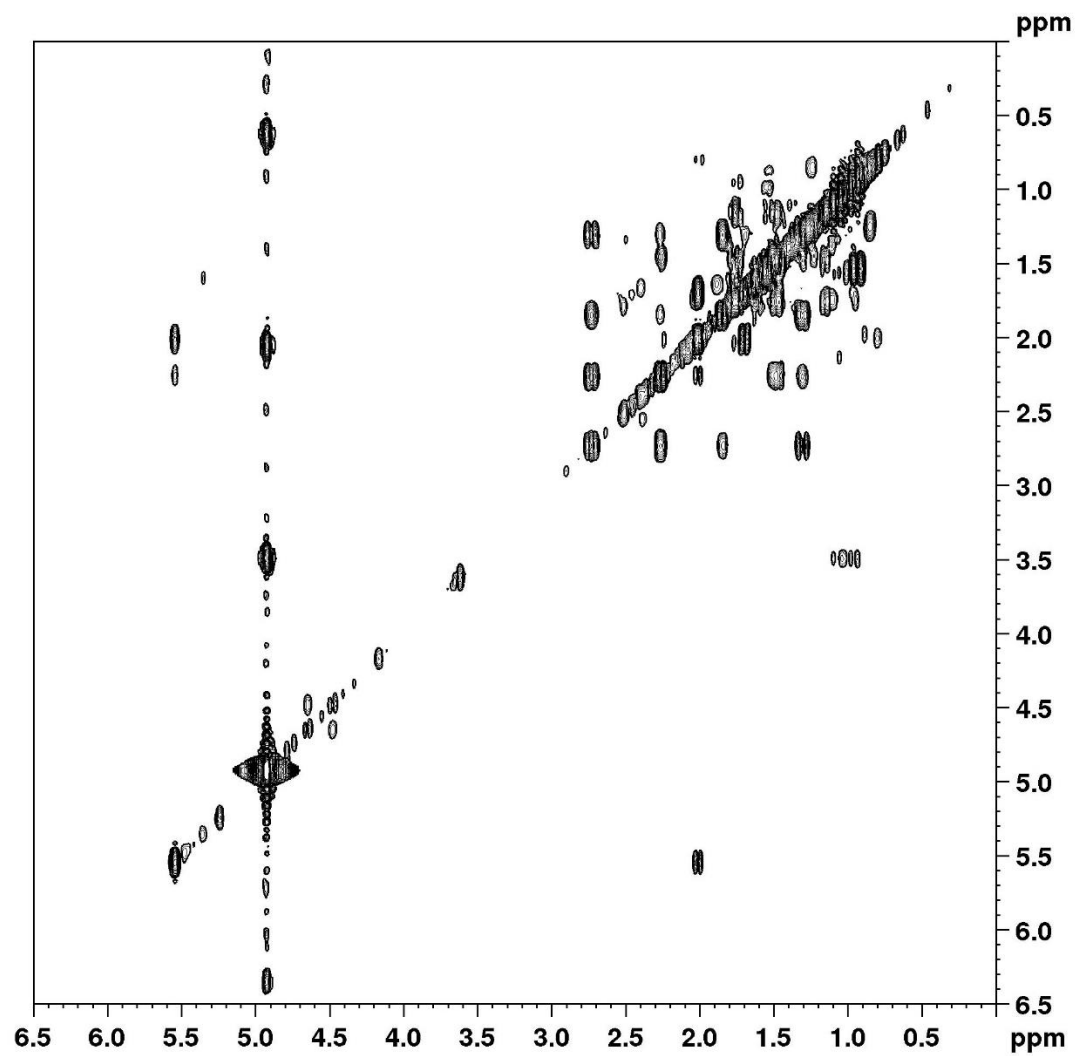
HMBC spectrum of acantholupenone (**1**) (600 MHz, CDCl<sub>3</sub>).



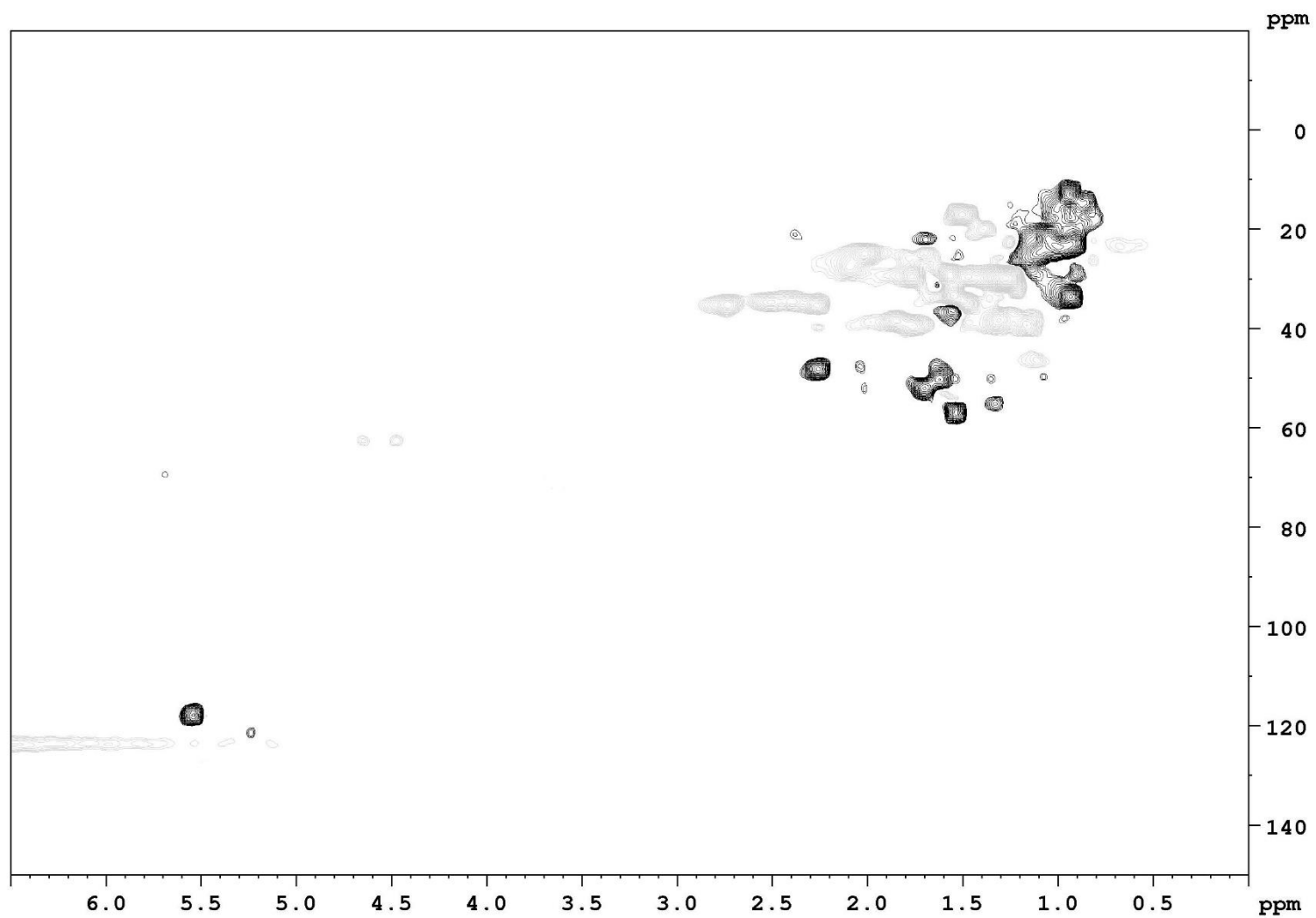




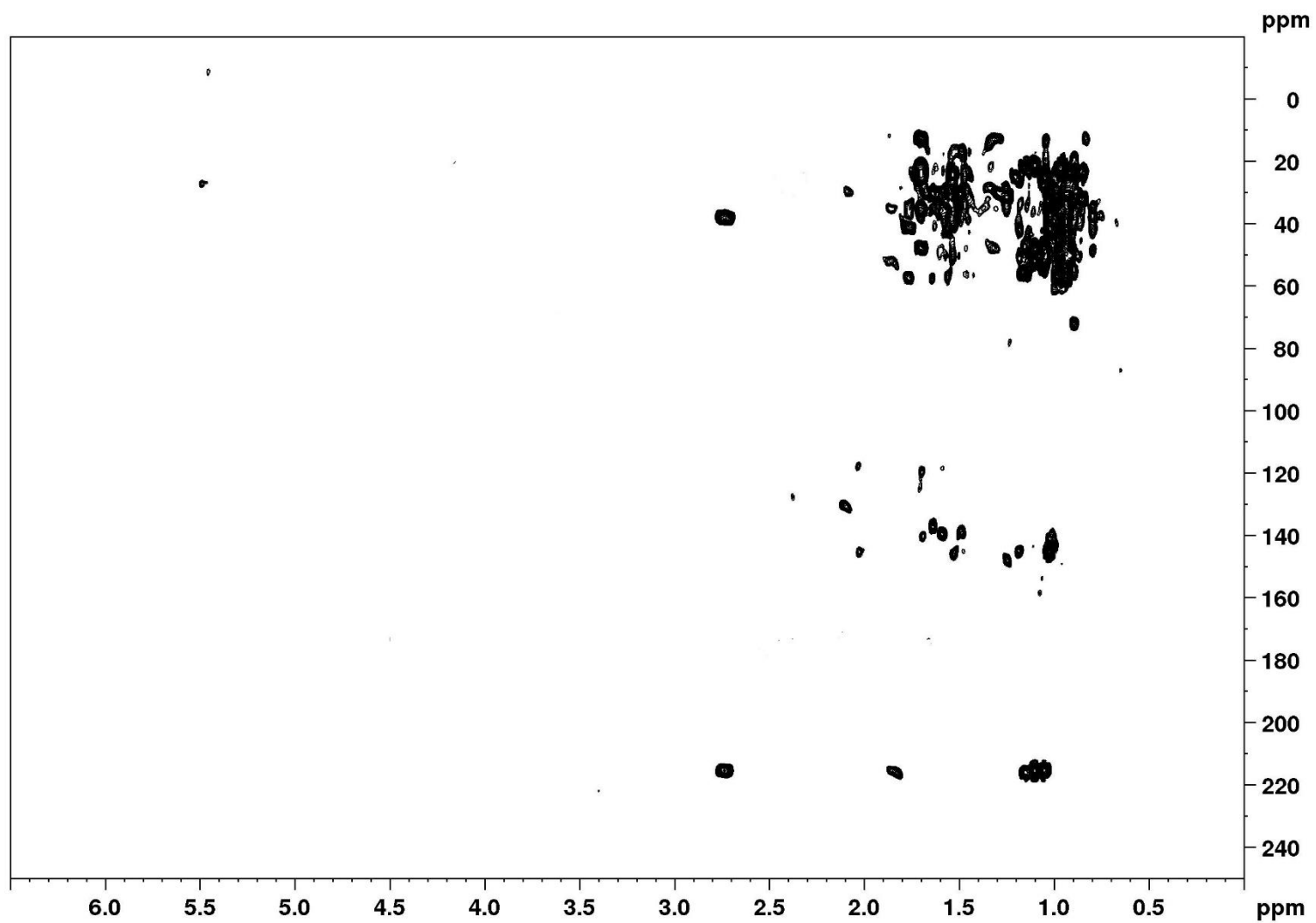
$^1\text{H}$  NMR spectrum of acantholupenone (**1**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).



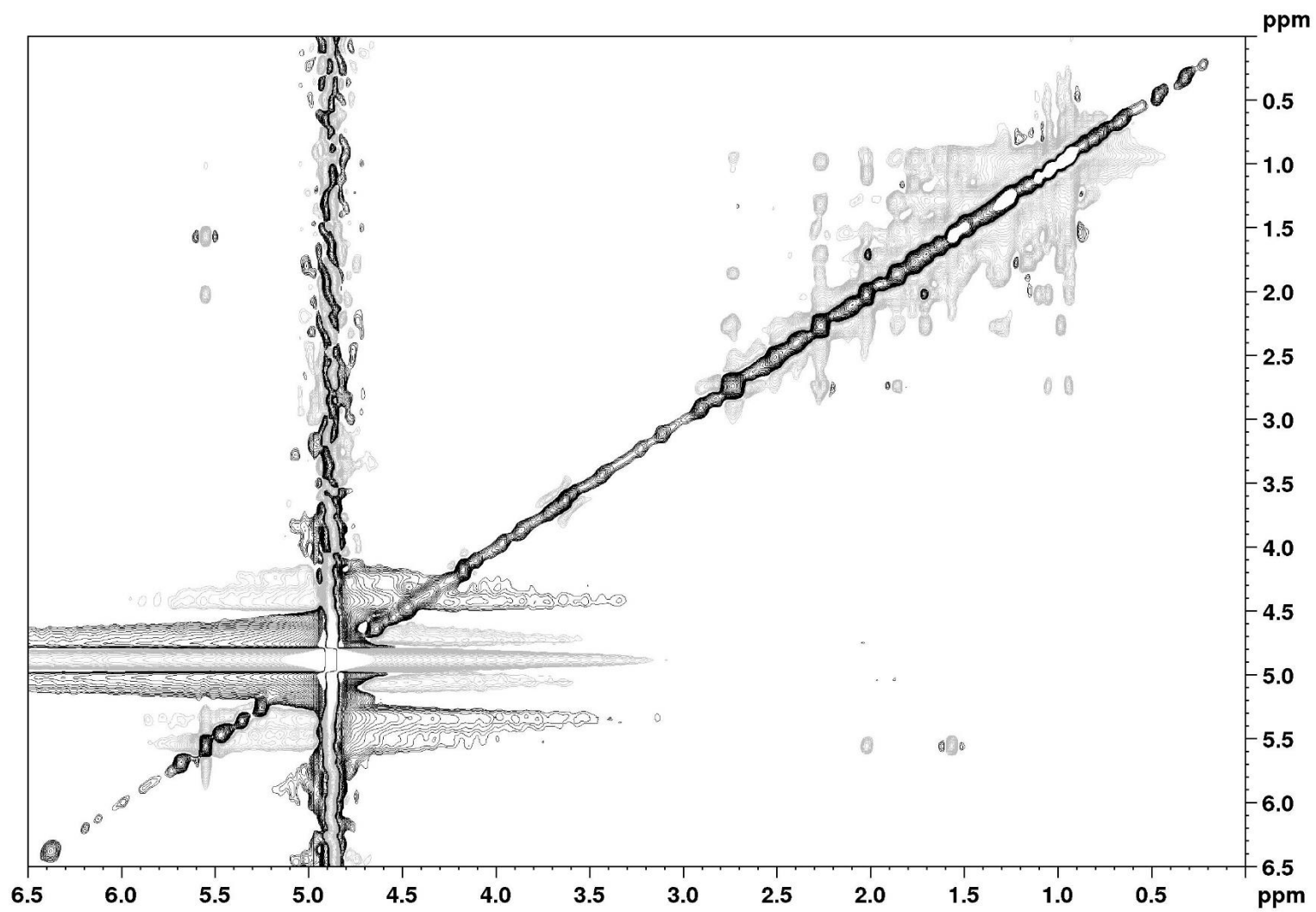
COSY spectrum of acantholupenone (**1**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).



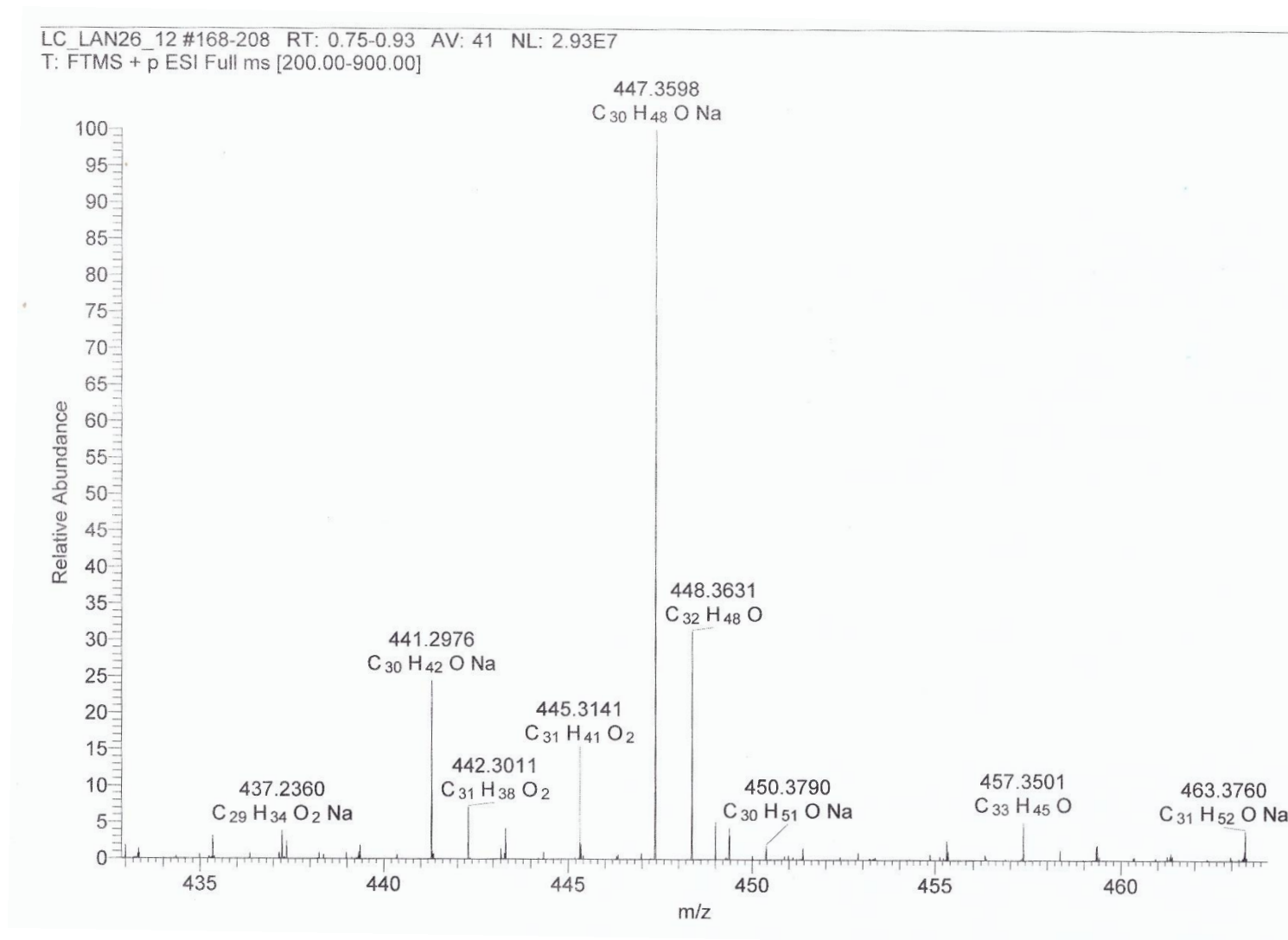
edHSQC spectrum of acantholupenone (**1**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).

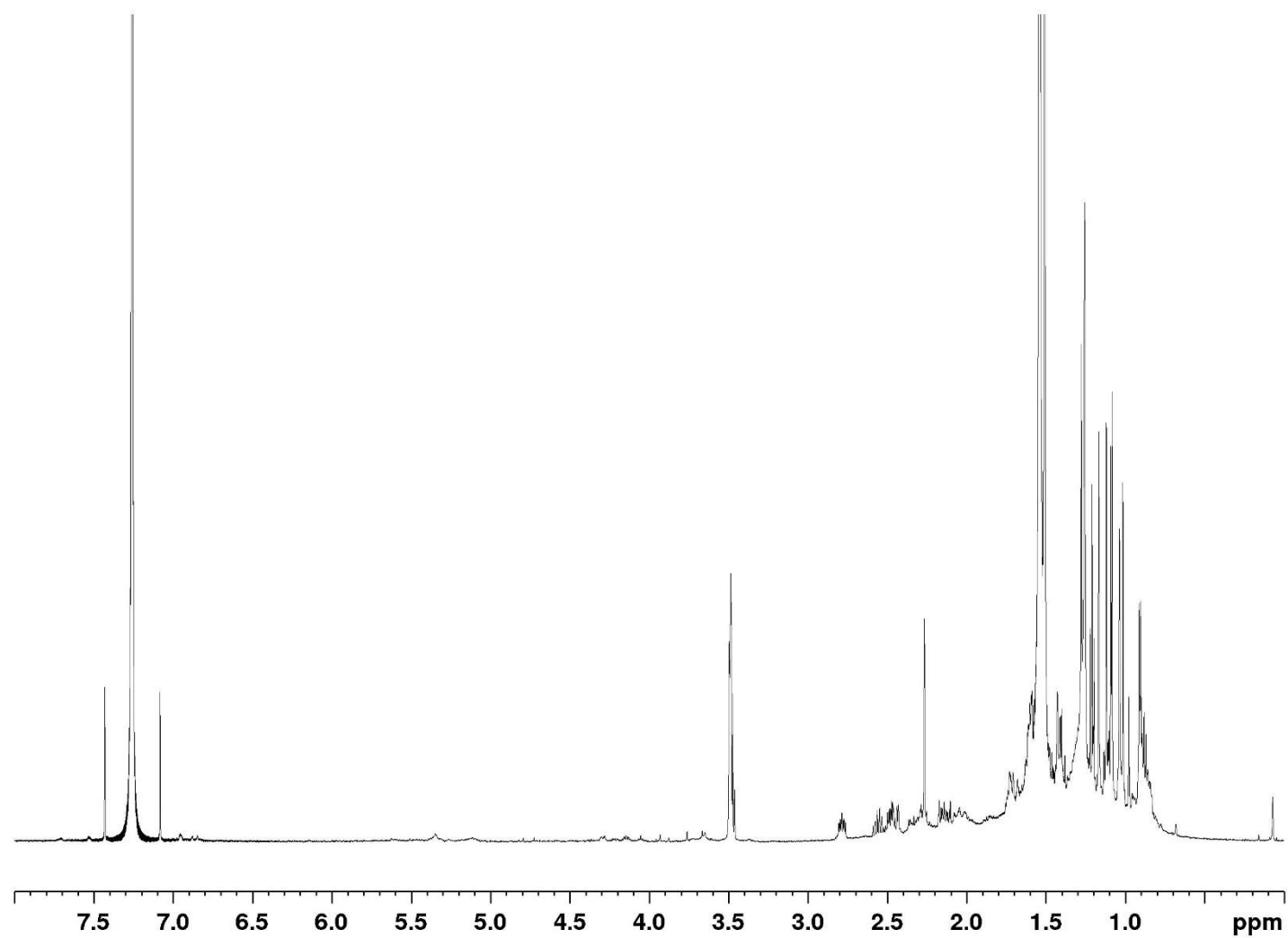


HMBC spectrum of acantholupenone (**1**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).

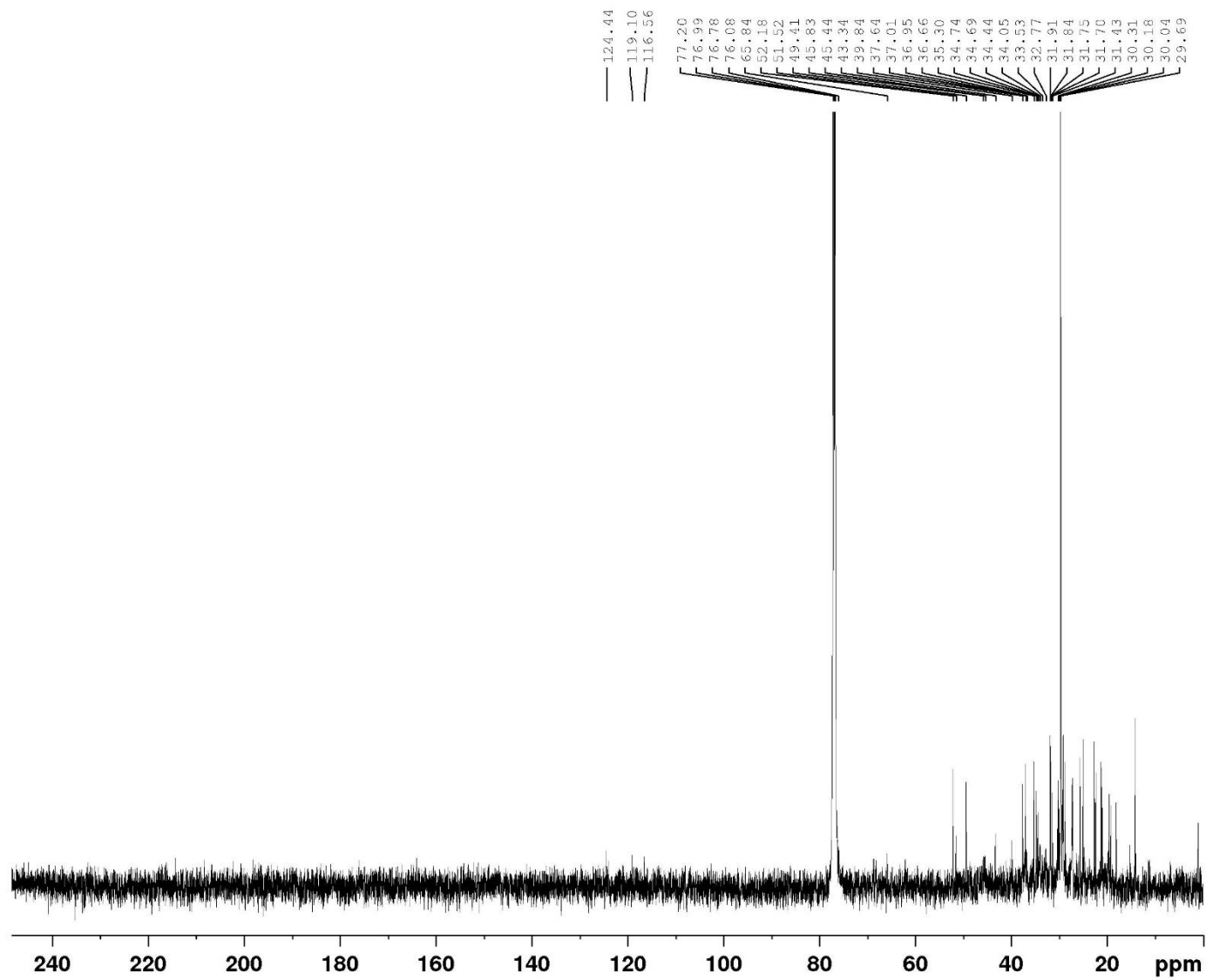


NOESY spectrum of acantholupenone (**1**) (400 MHz, C<sub>5</sub>D<sub>5</sub>N).

HRESIMS spectrum of acantholupenone (**1**).

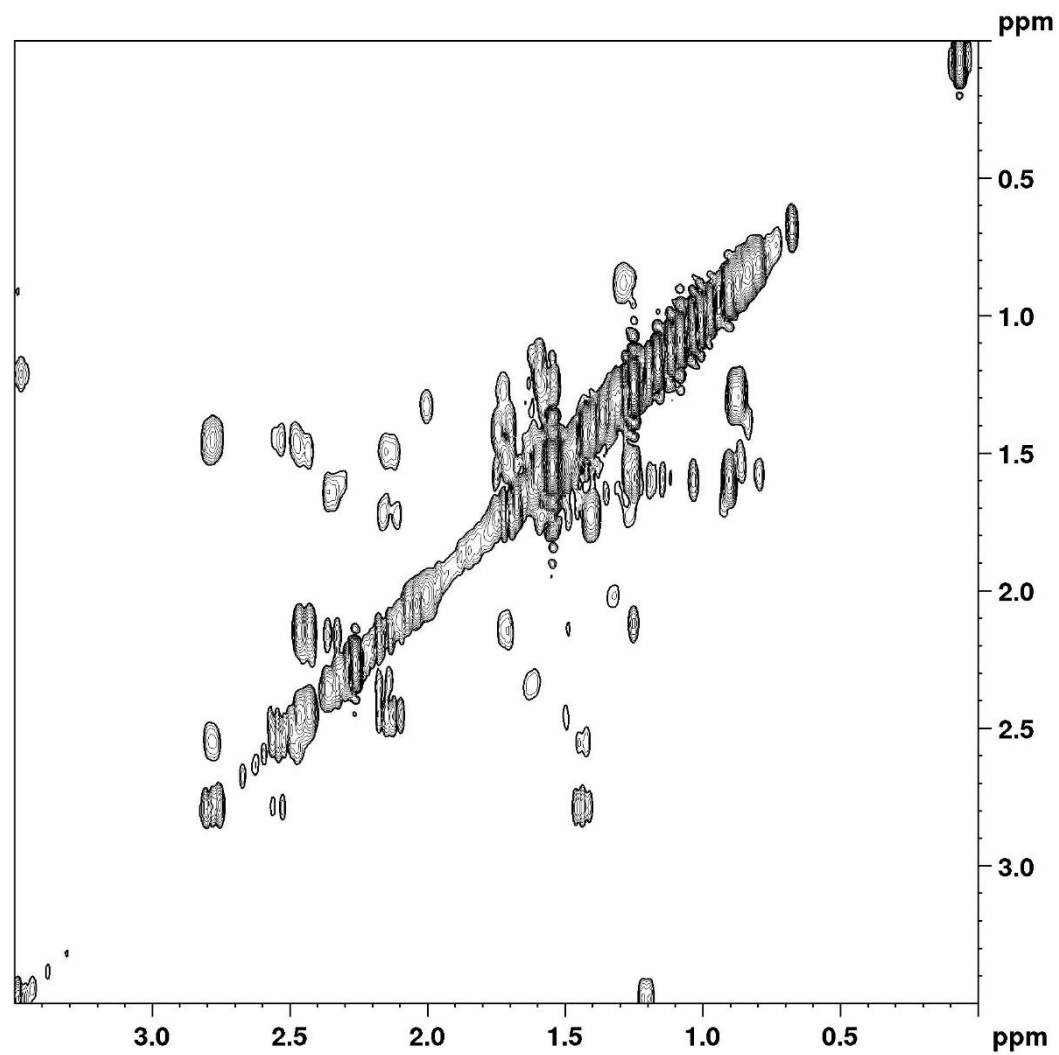


$^1\text{H}$  NMR spectrum of acanthobauerendione (**2**) (600 MHz,  $\text{CDCl}_3$ ).

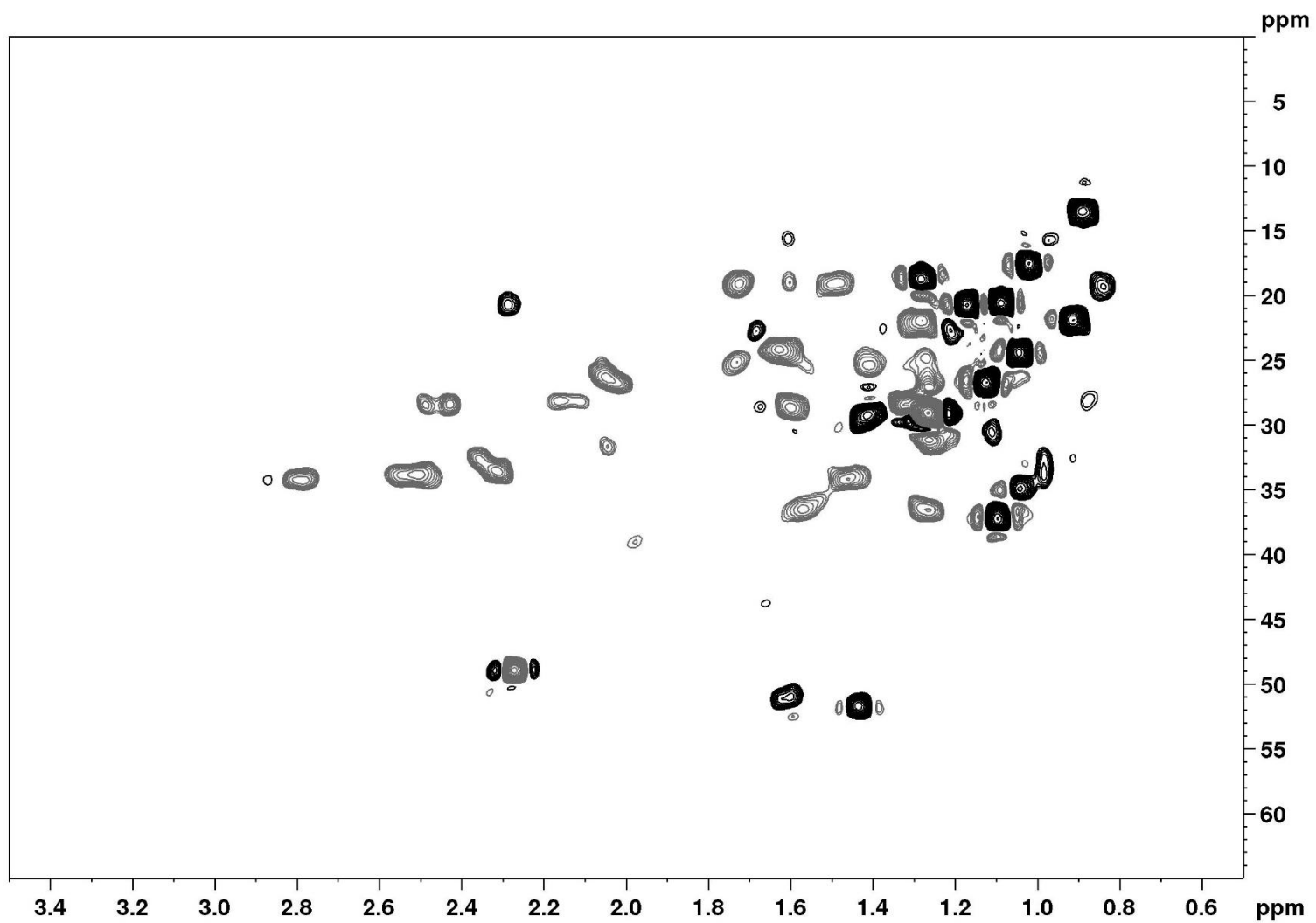


$^{13}\text{C}$  NMR spectrum of acanthobauerendione (**2**) (150 MHz,  $\text{CDCl}_3$ ).

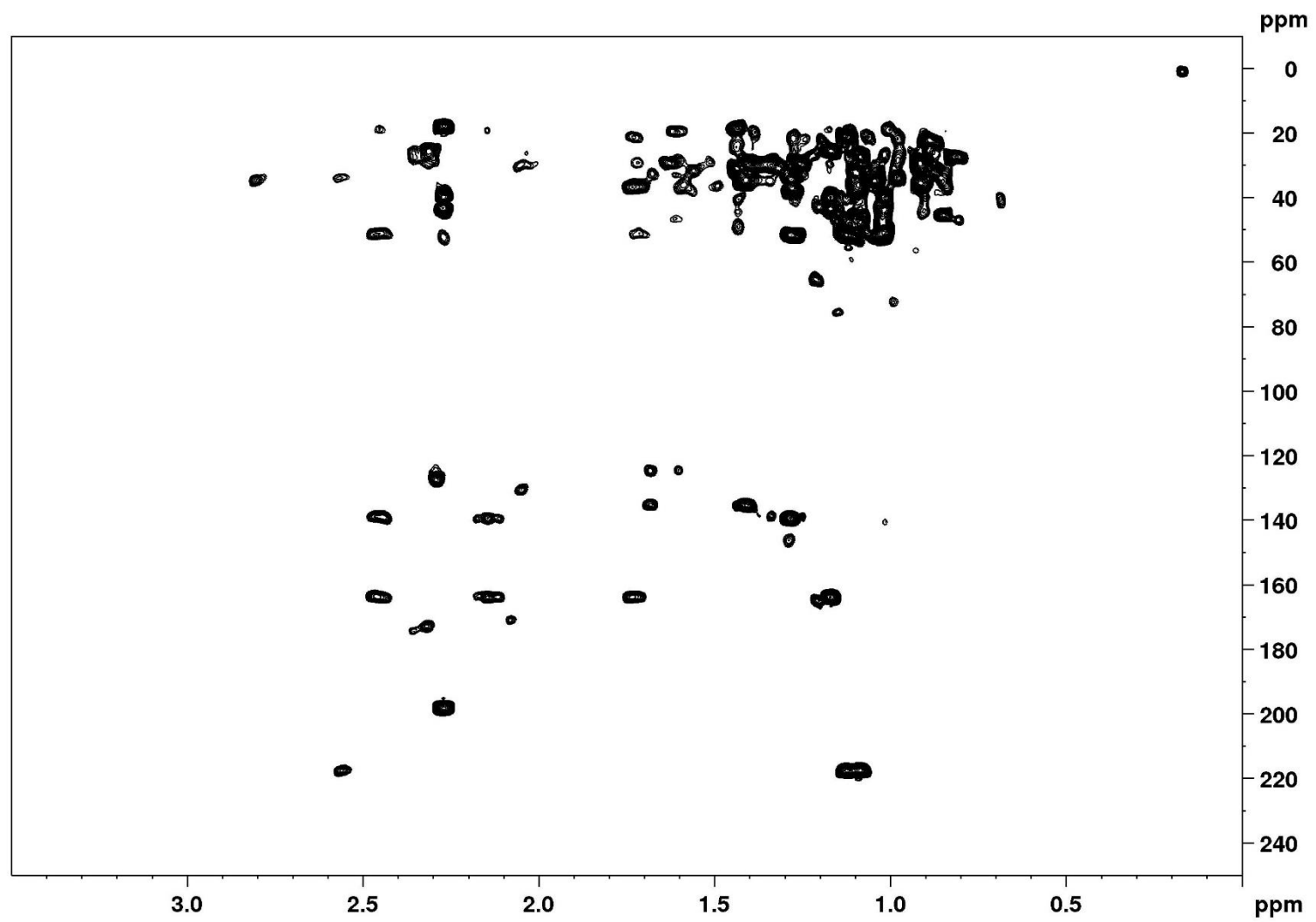




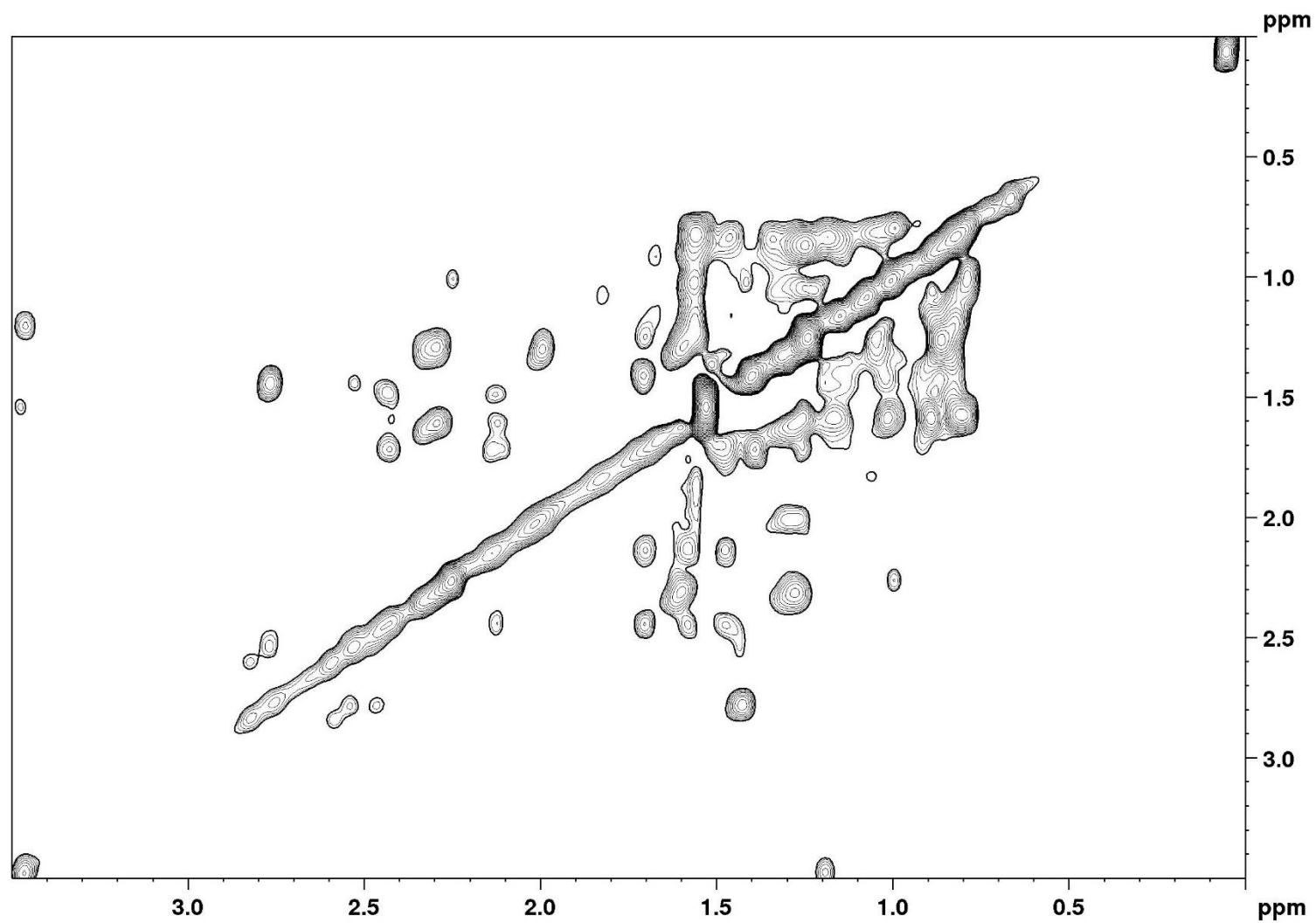
COSY spectrum of acanthobauerendione (**2**) (600 MHz, CDCl<sub>3</sub>).



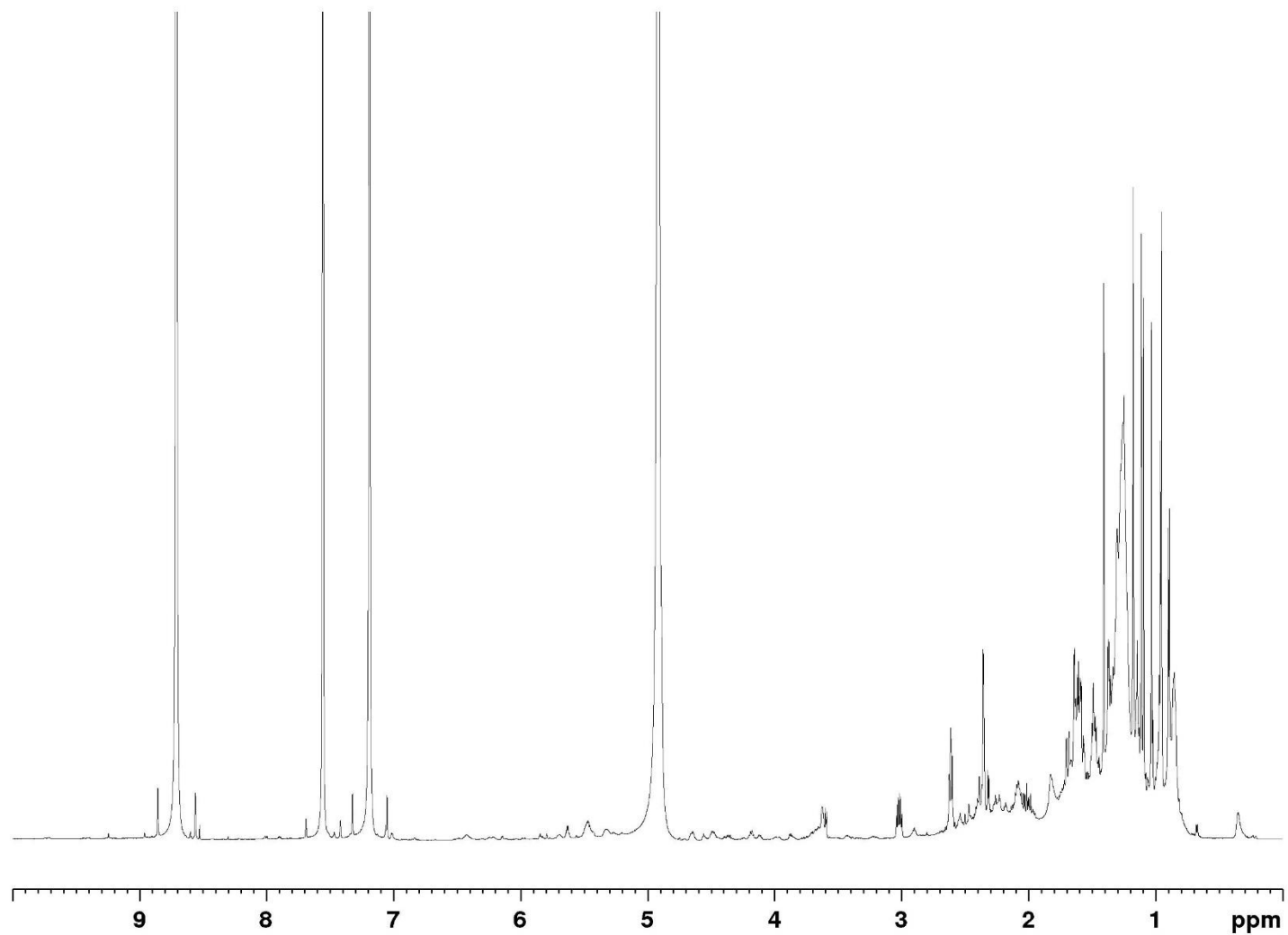
edHSQC spectrum of acanthobauerendione (**2**) (400 MHz, CDCl<sub>3</sub>).



HMBC spectrum of acanthobauerendione (**2**) (600 MHz, CDCl<sub>3</sub>).

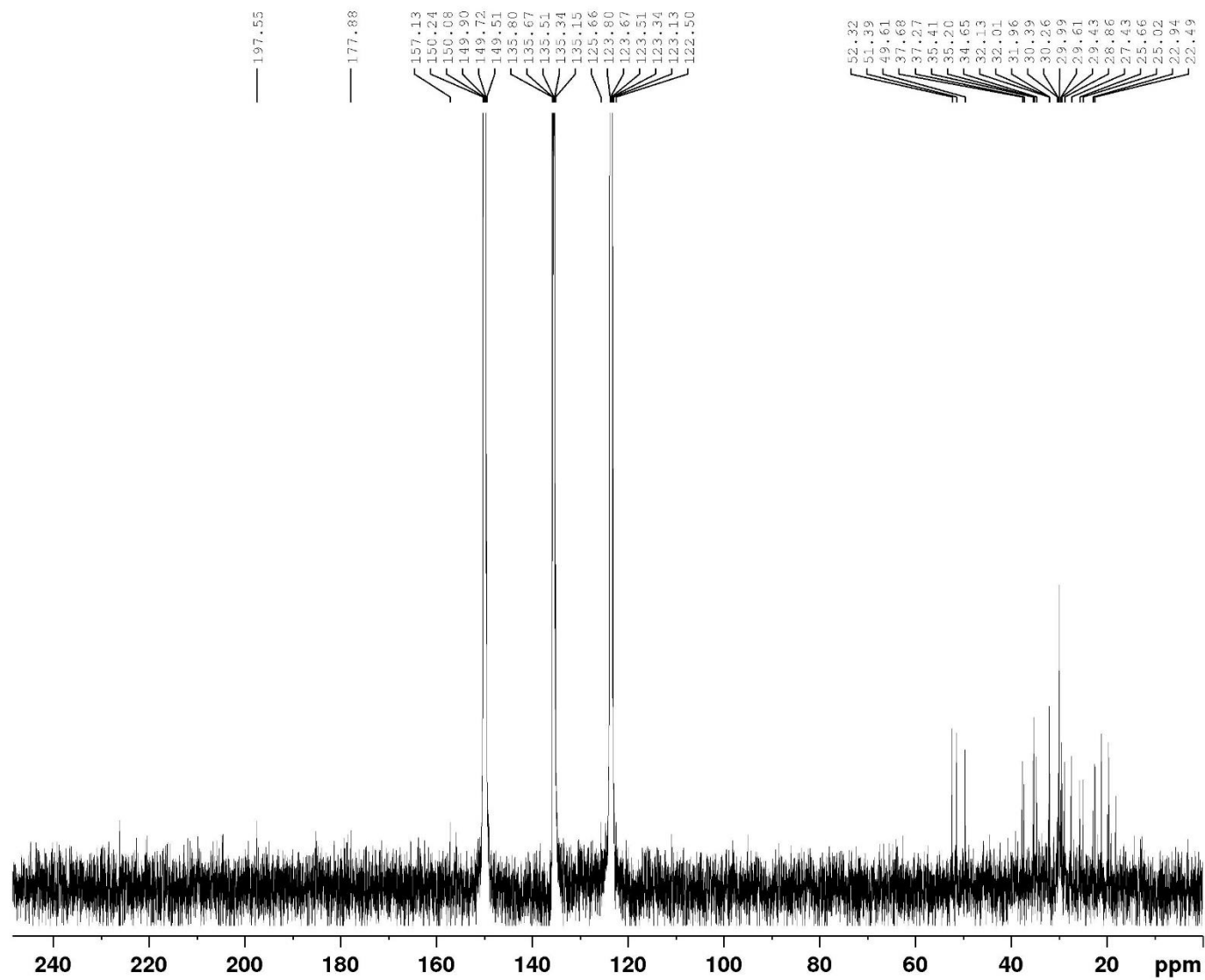


TOCSY spectrum of acanthobauerendione (**2**) (600 MHz, CDCl<sub>3</sub>).

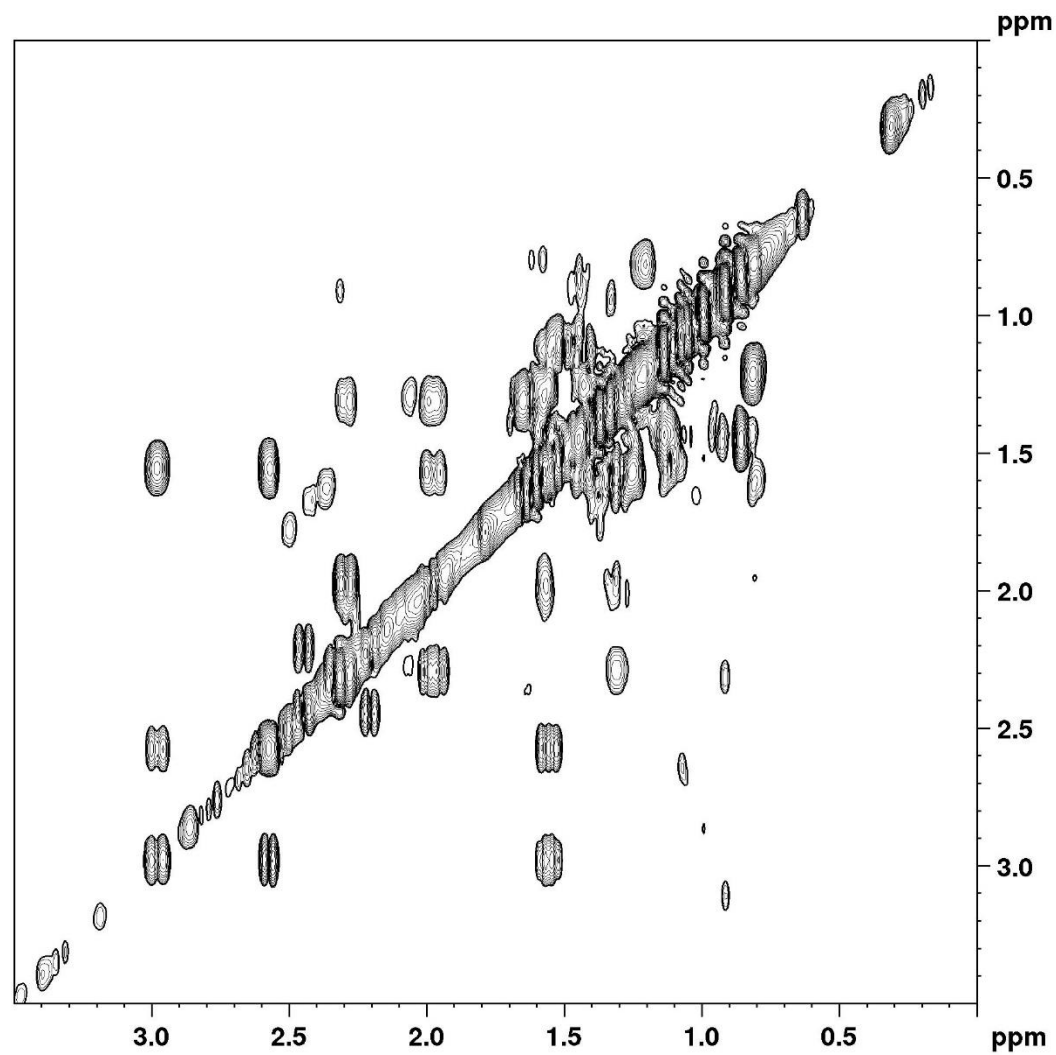


$^1\text{H}$  NMR spectrum of acanthobauerendione (**2**) (600 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).

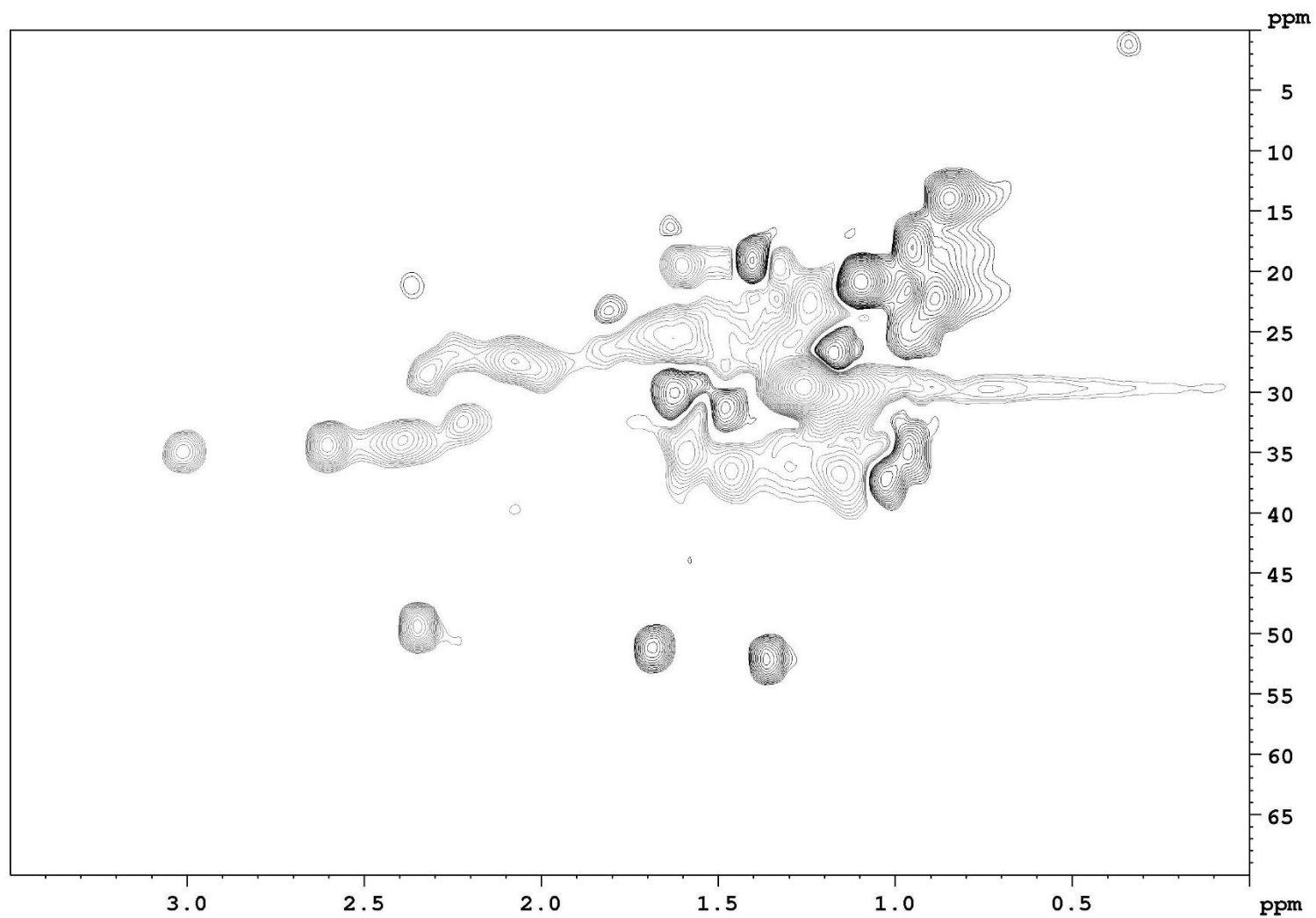
S20



$^{13}\text{C}$  NMR spectrum of acanthobauerendione (**2**) (150 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).

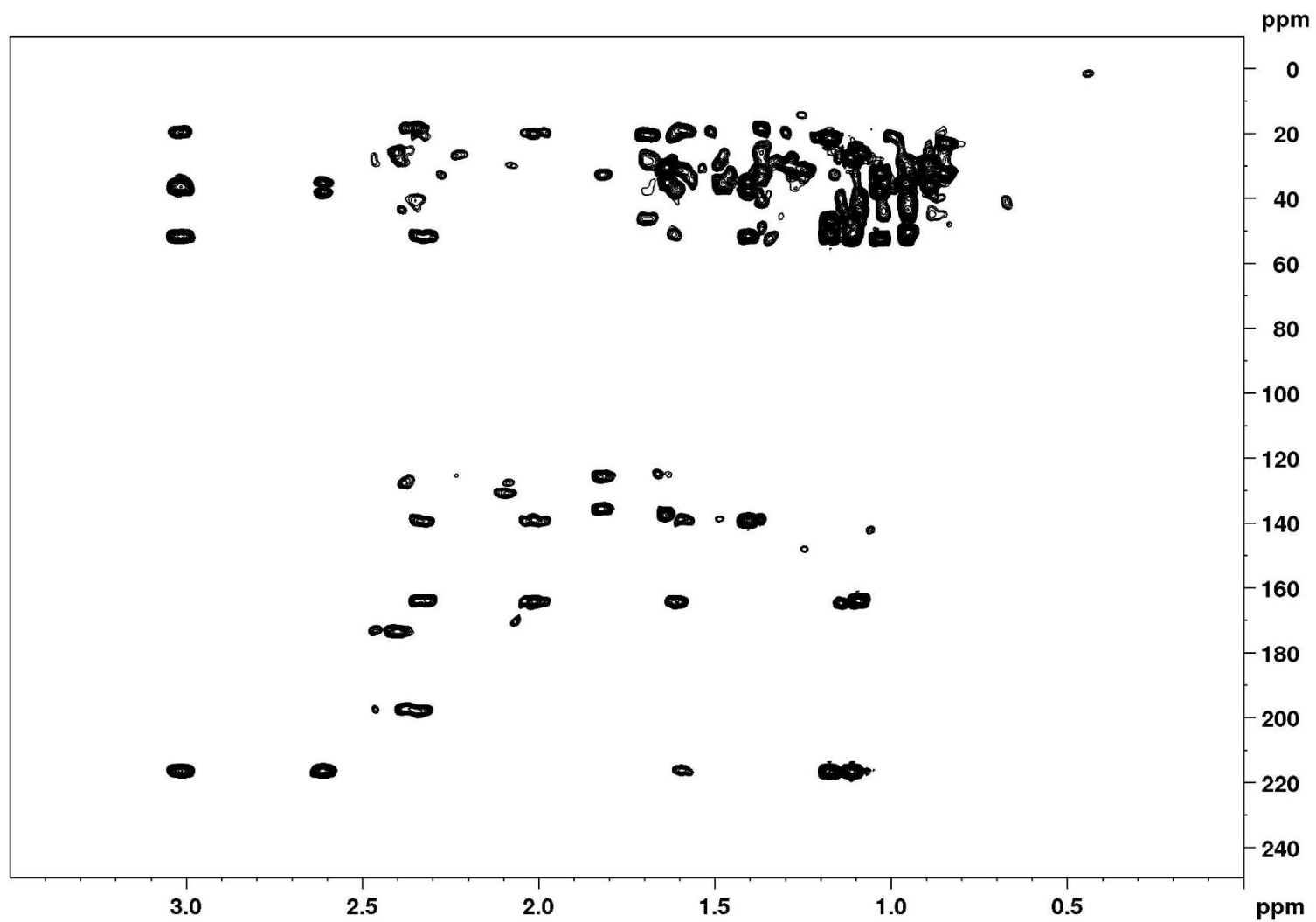


COSY spectrum of acanthobauerendione (**2**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).

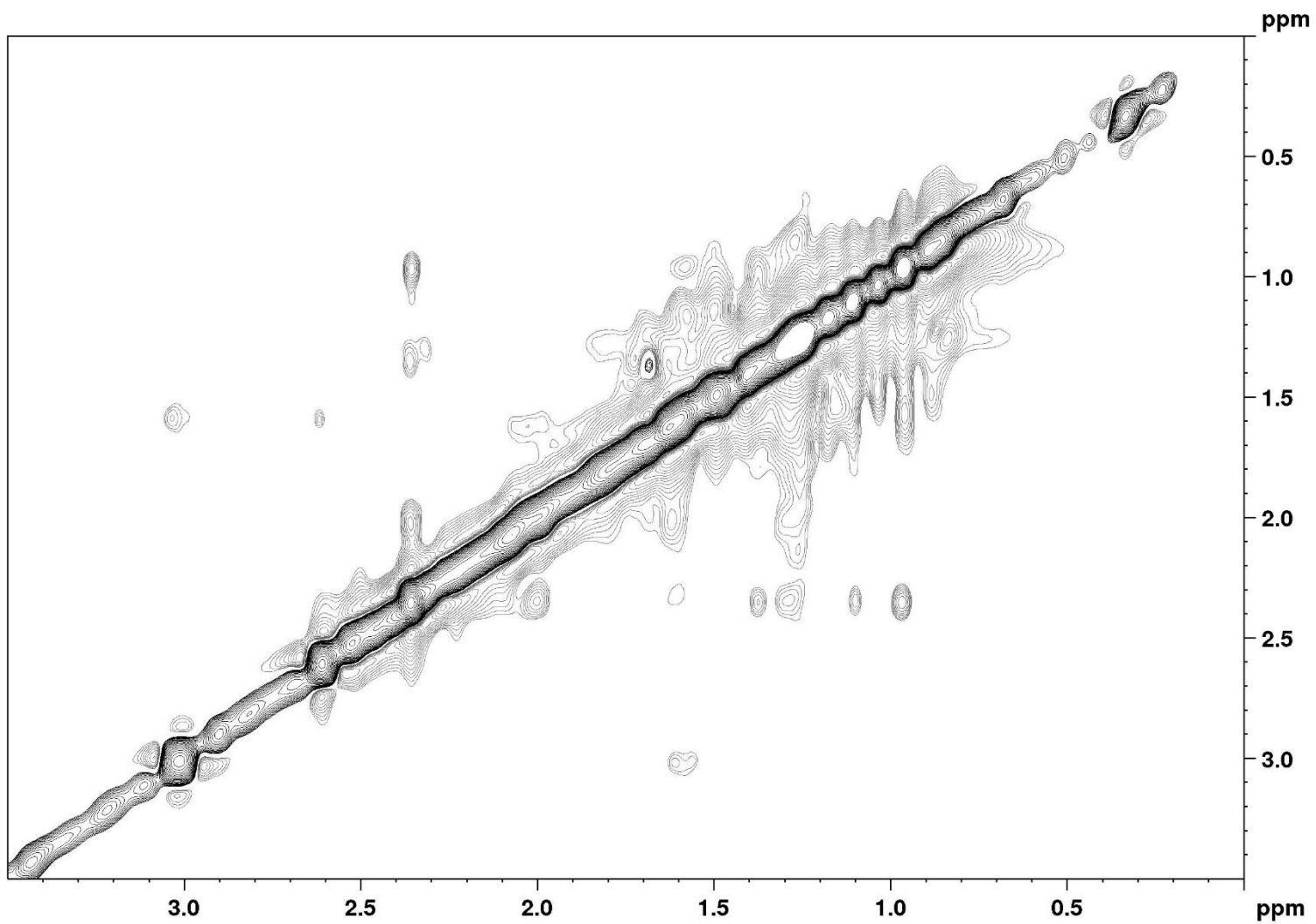


edHSQC spectrum of acanthobauerendione (**2**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).



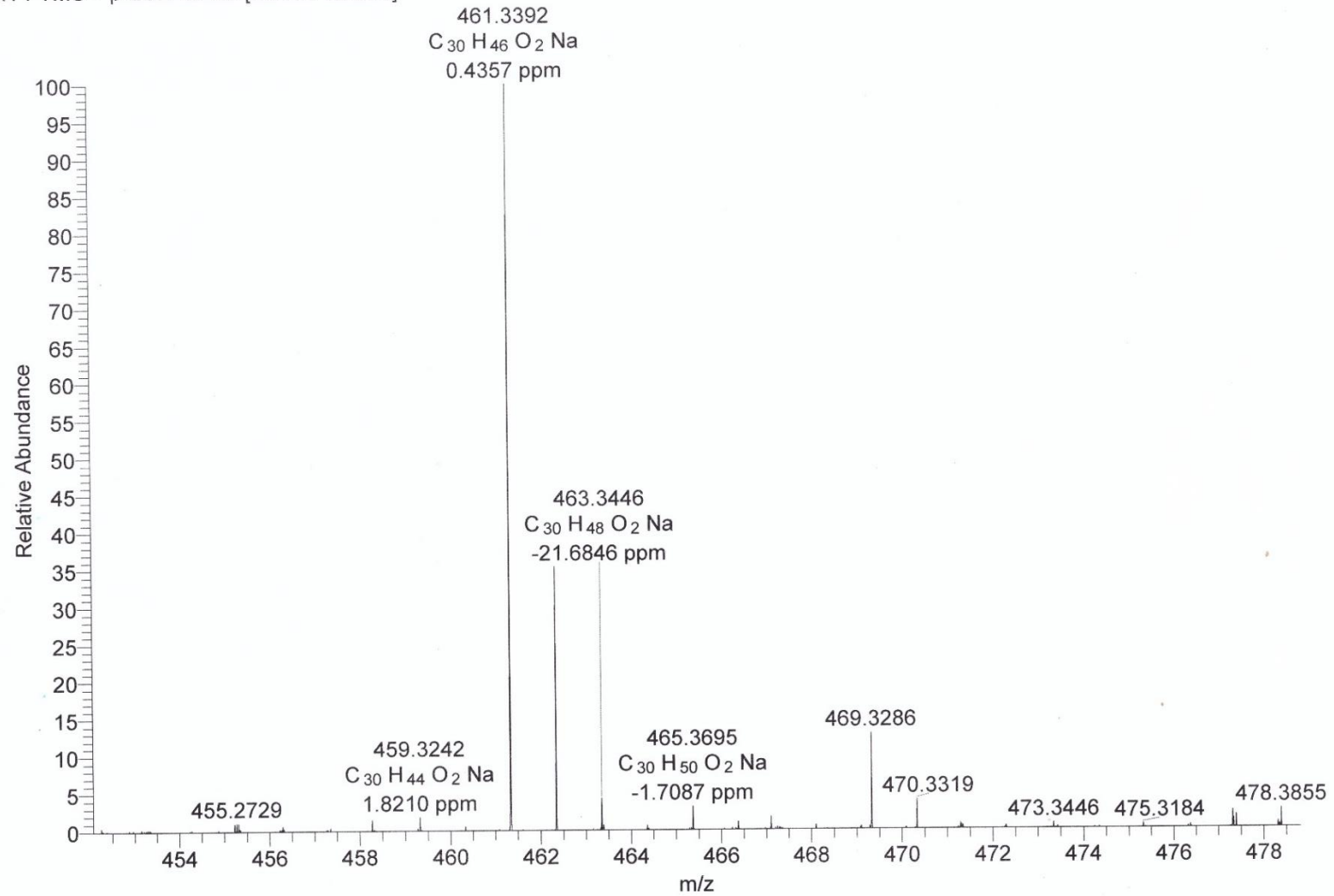


HMBC spectrum of acanthobauerendione (**2**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).

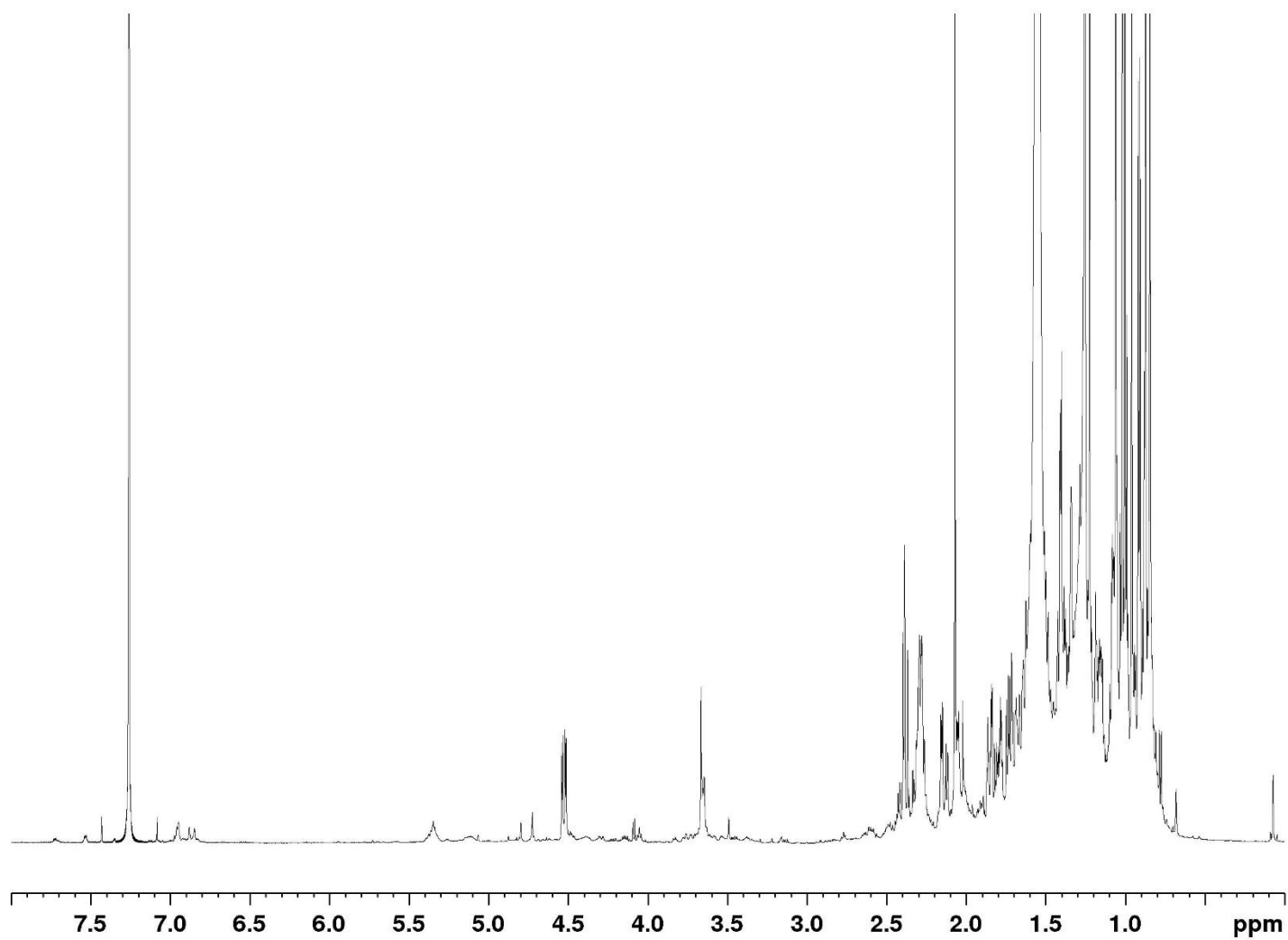


NOESY spectrum of acanthobauerendione (**2**) (400 MHz, C<sub>5</sub>D<sub>5</sub>N)

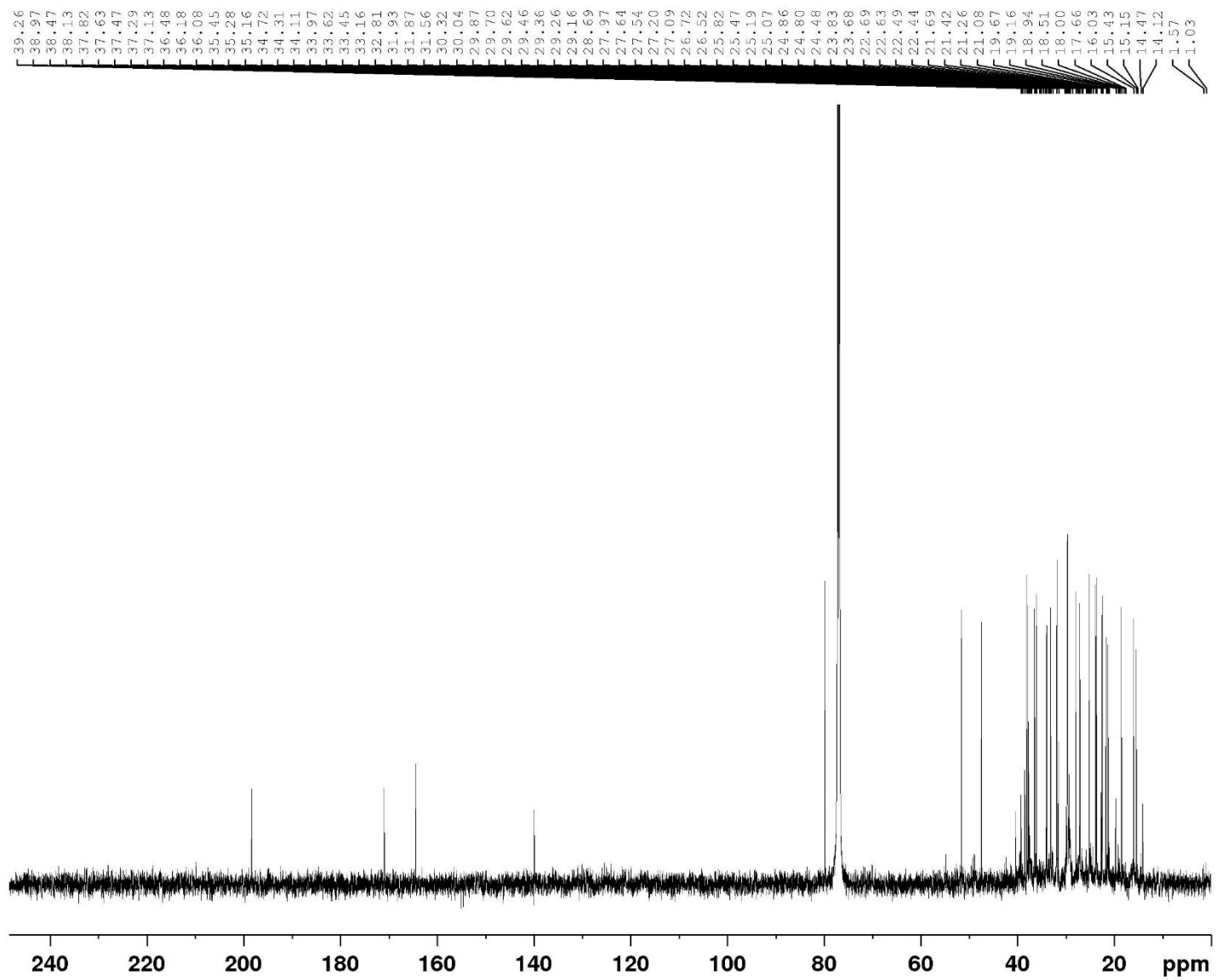
LC\_LAn12\_2 #1 RT: 0.00 AV: 1 NL: 3.00E7  
T: FTMS +p ESI Full ms [300.00-500.00]



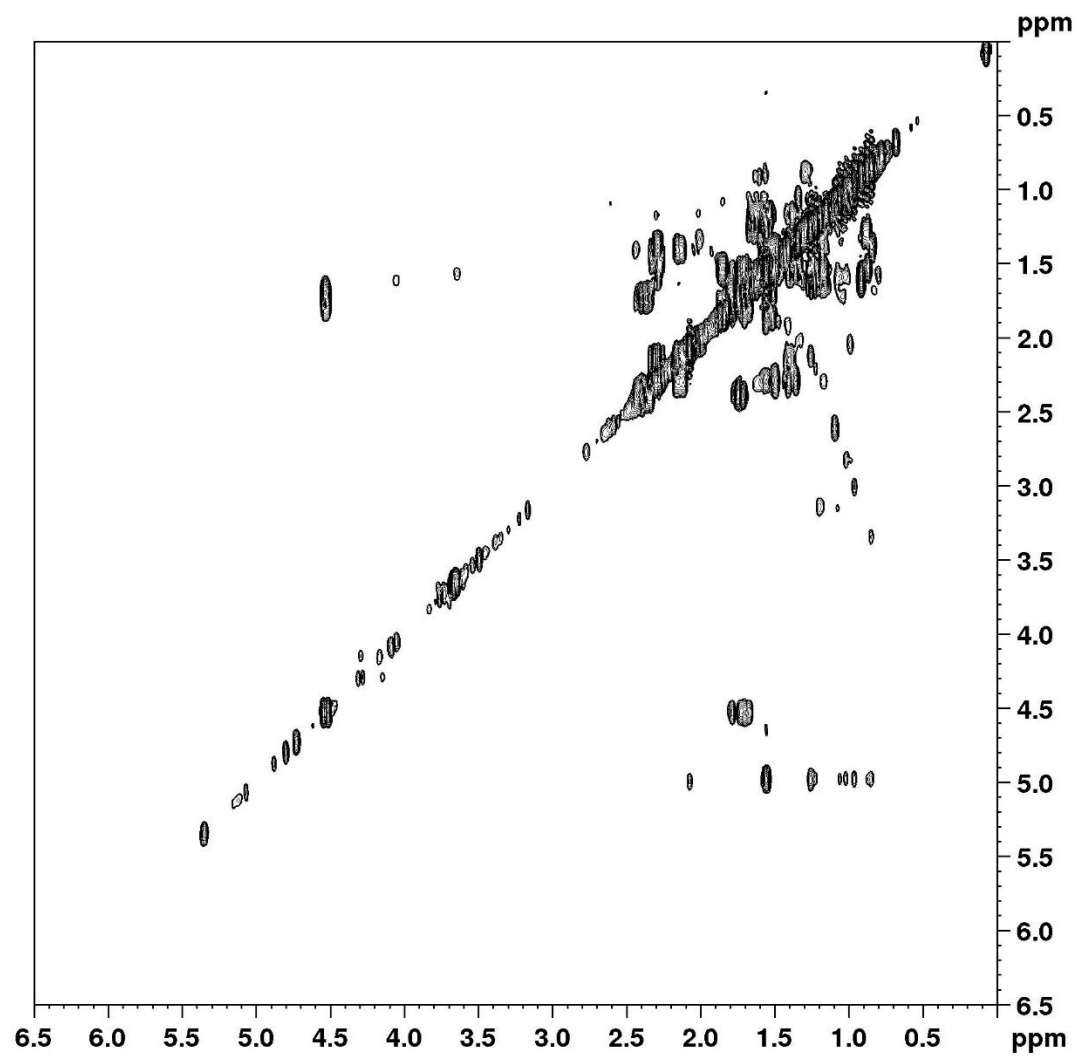
HRESIMS spectrum of acanthobauerendione (2).



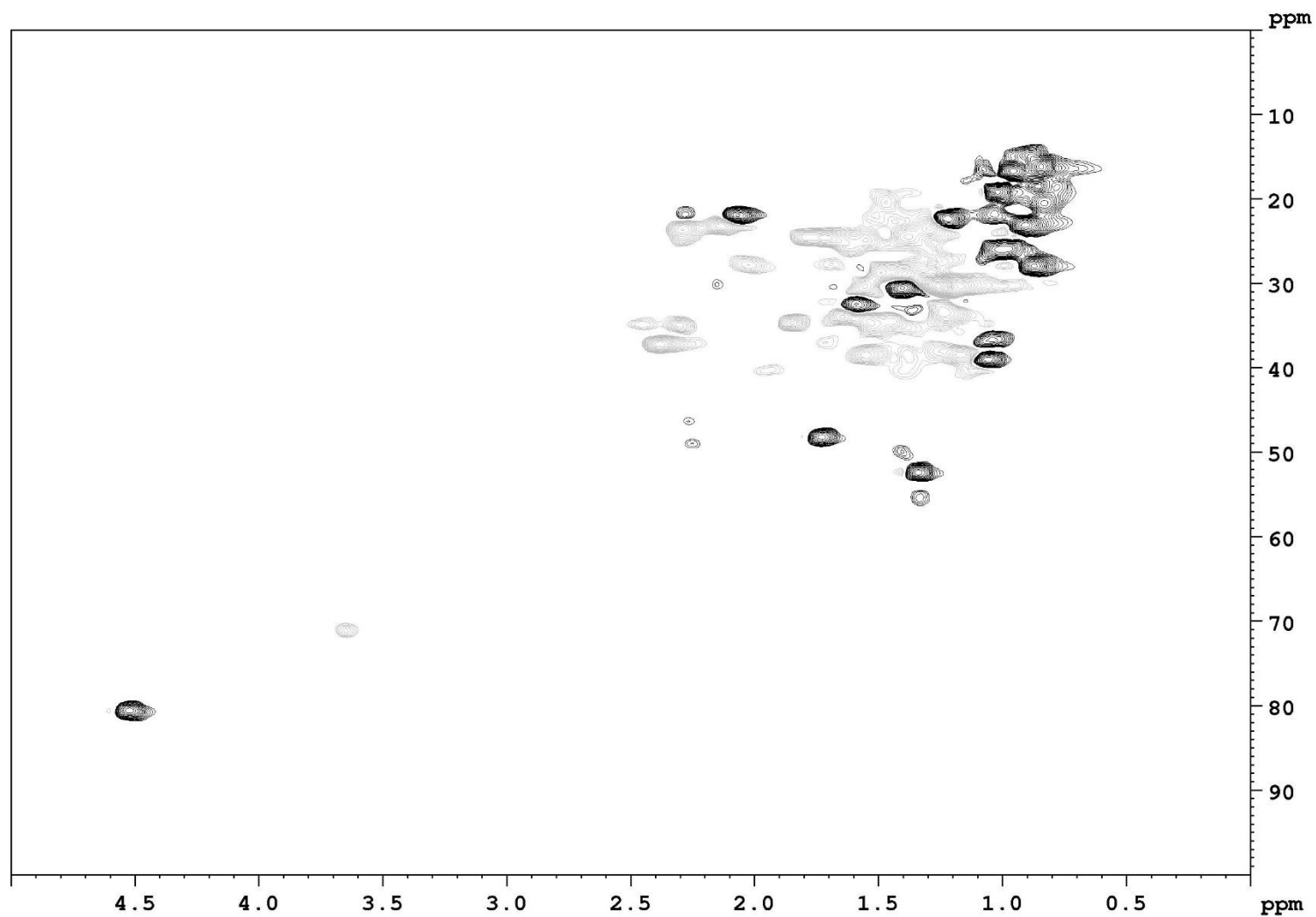
$^1\text{H}$  NMR spectrum of acanthobauerenone (**3**) (600 MHz,  $\text{CDCl}_3$ ).



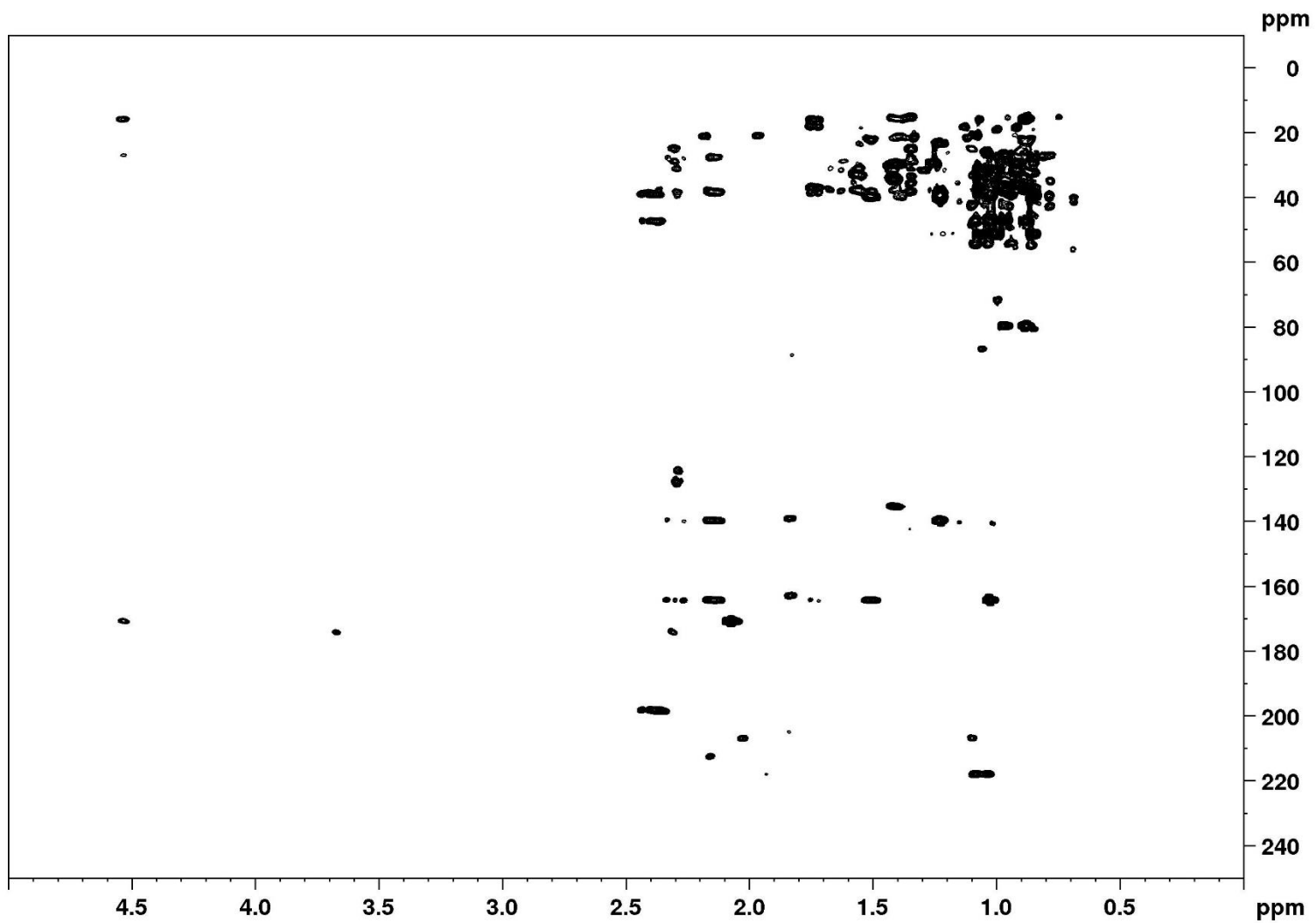
$^{13}\text{C}$  NMR spectrum of acanthobauerenone (**3**) (150 MHz,  $\text{CDCl}_3$ ).



COSY spectrum of acanthobauerenone (**3**) (600 MHz, CDCl<sub>3</sub>).

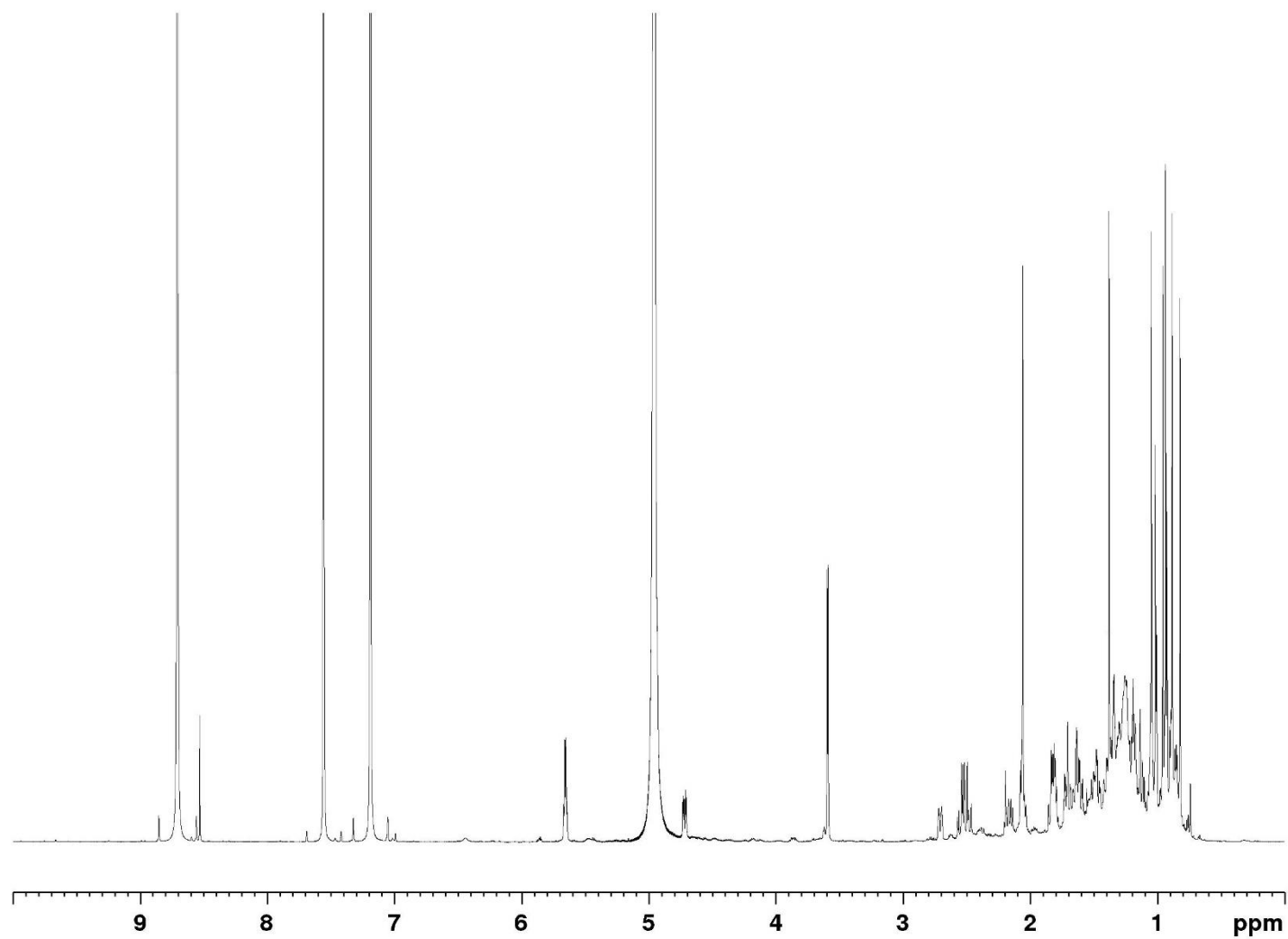


edHSQC spectrum of acanthobauerenone (**3**) (600 MHz, CDCl<sub>3</sub>).



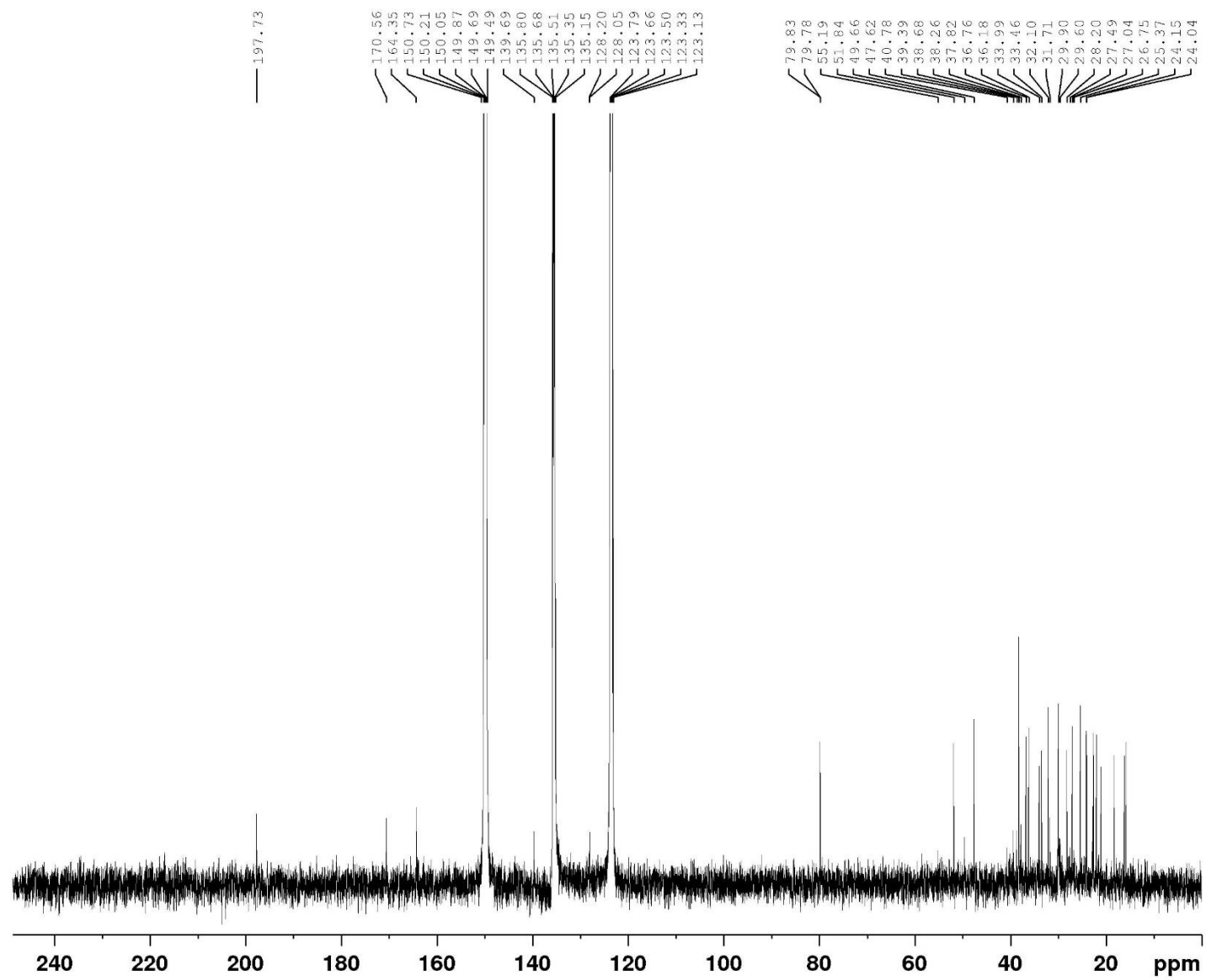
HMBC spectrum of acanthobauerenone (**3**) (600 MHz, CDCl<sub>3</sub>).



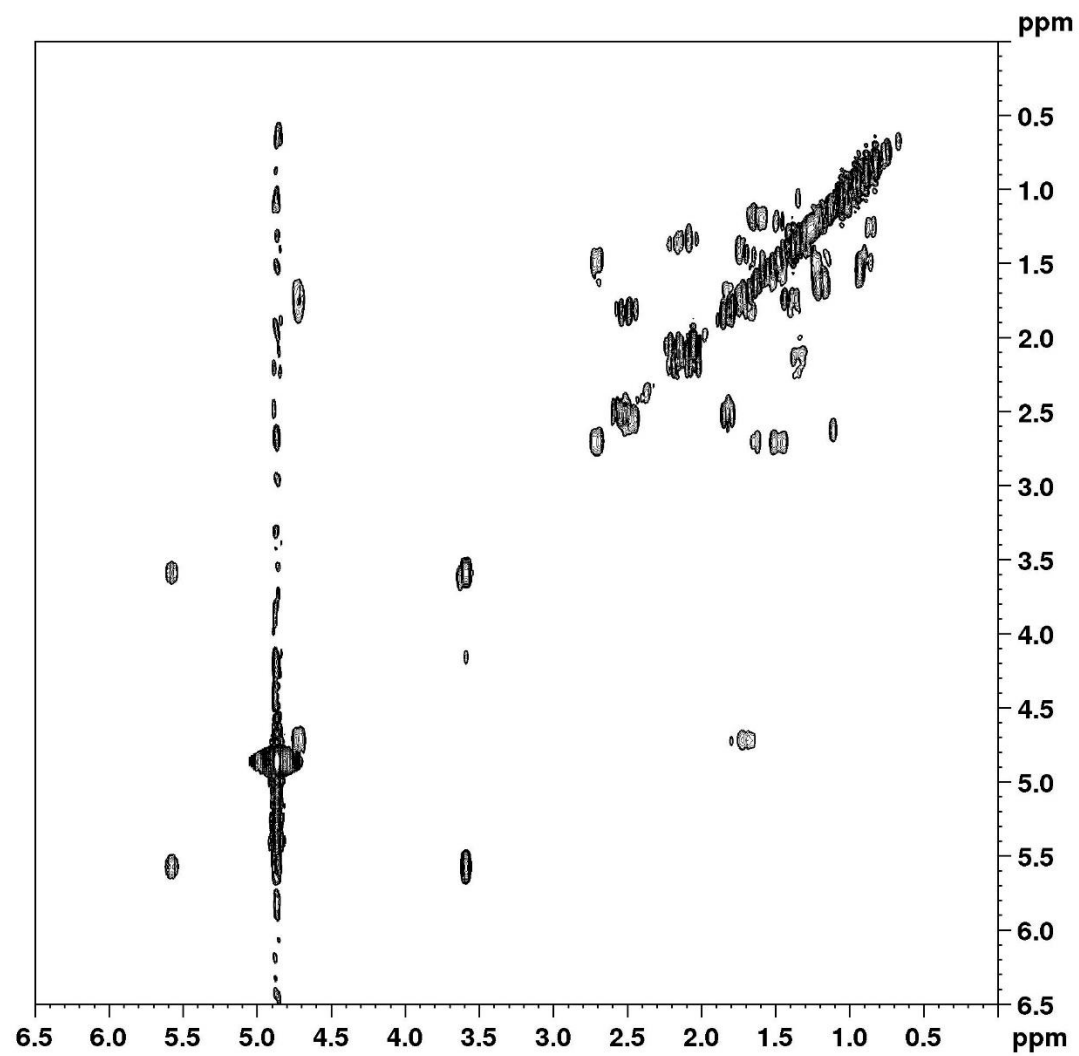


<sup>1</sup>H NMR spectrum of acanthobauerenone (**3**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).

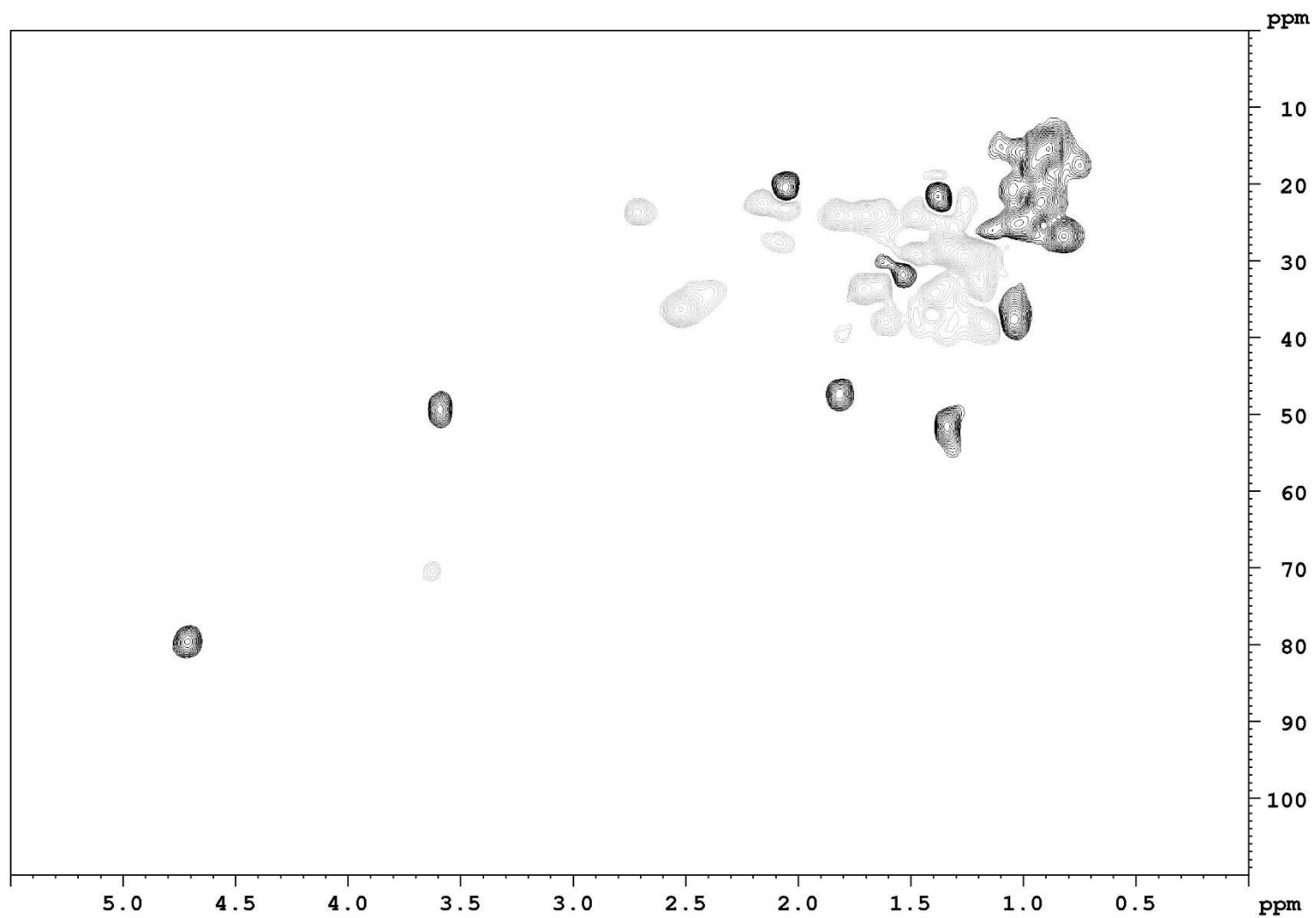
S32



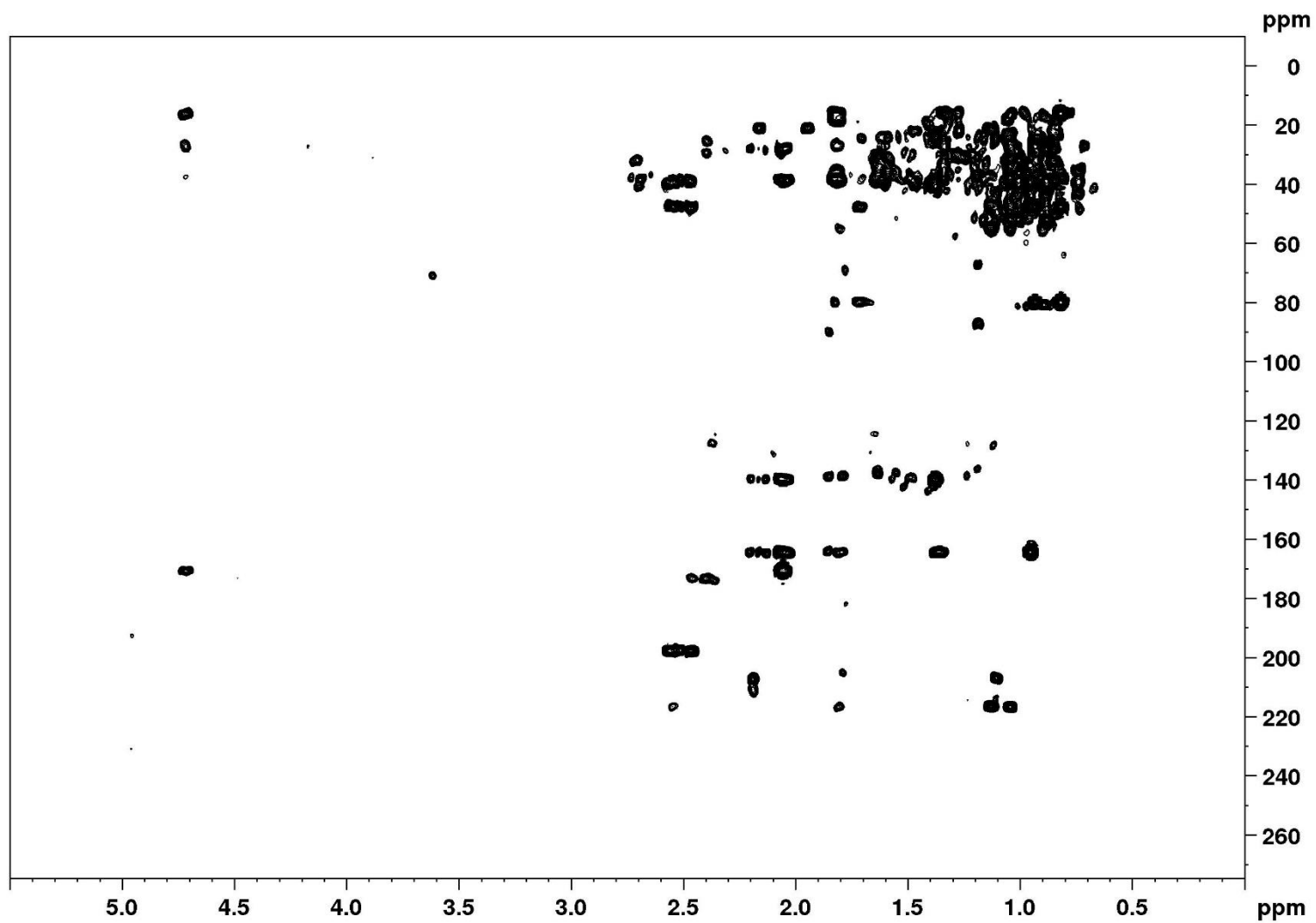
$^{13}\text{C}$  NMR spectrum of acanthobauerenone (3) (150 MHz,  $\text{C}_5\text{D}_5\text{N}$ ).



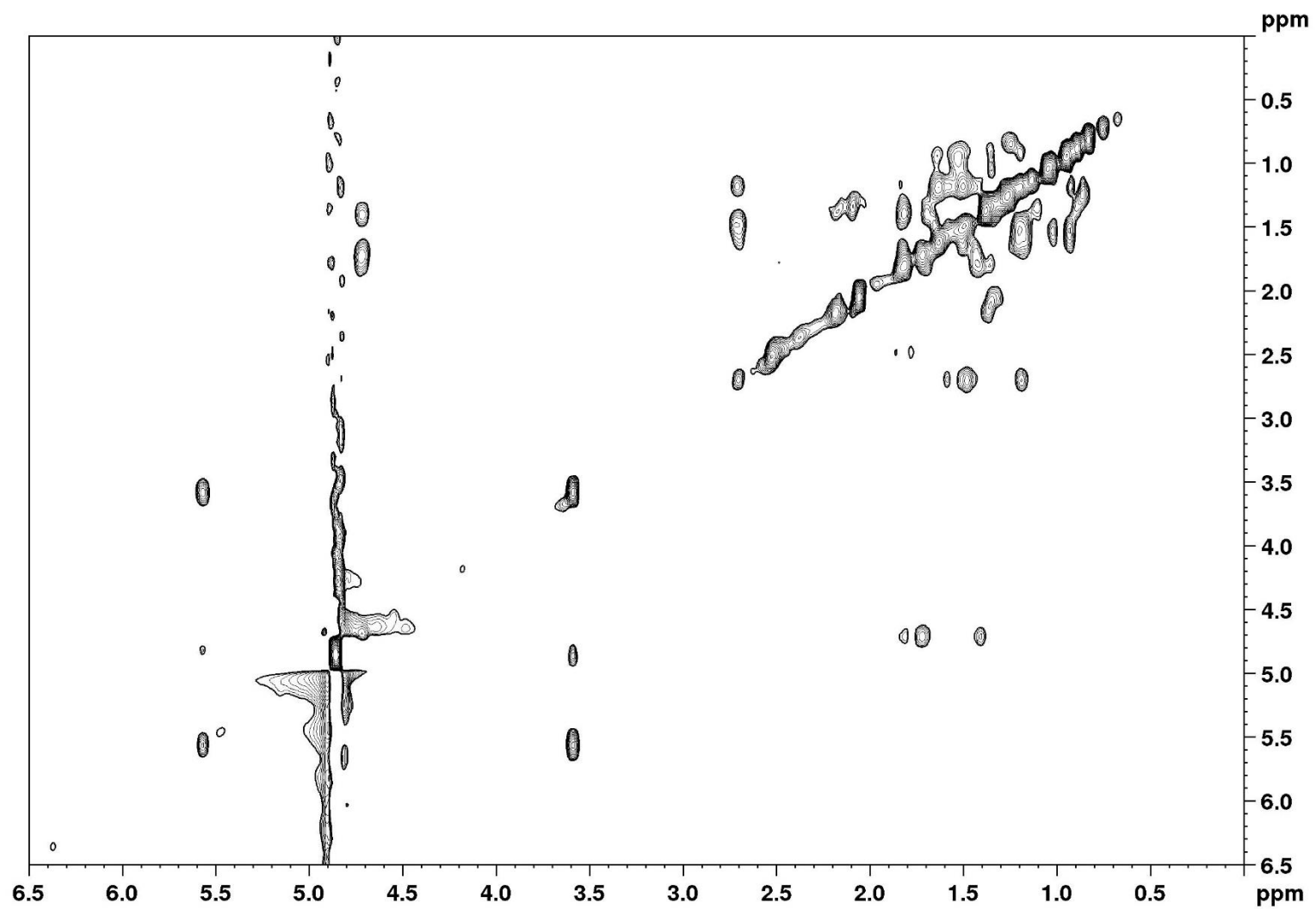
COSY spectrum of acanthobauerenone (**3**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).



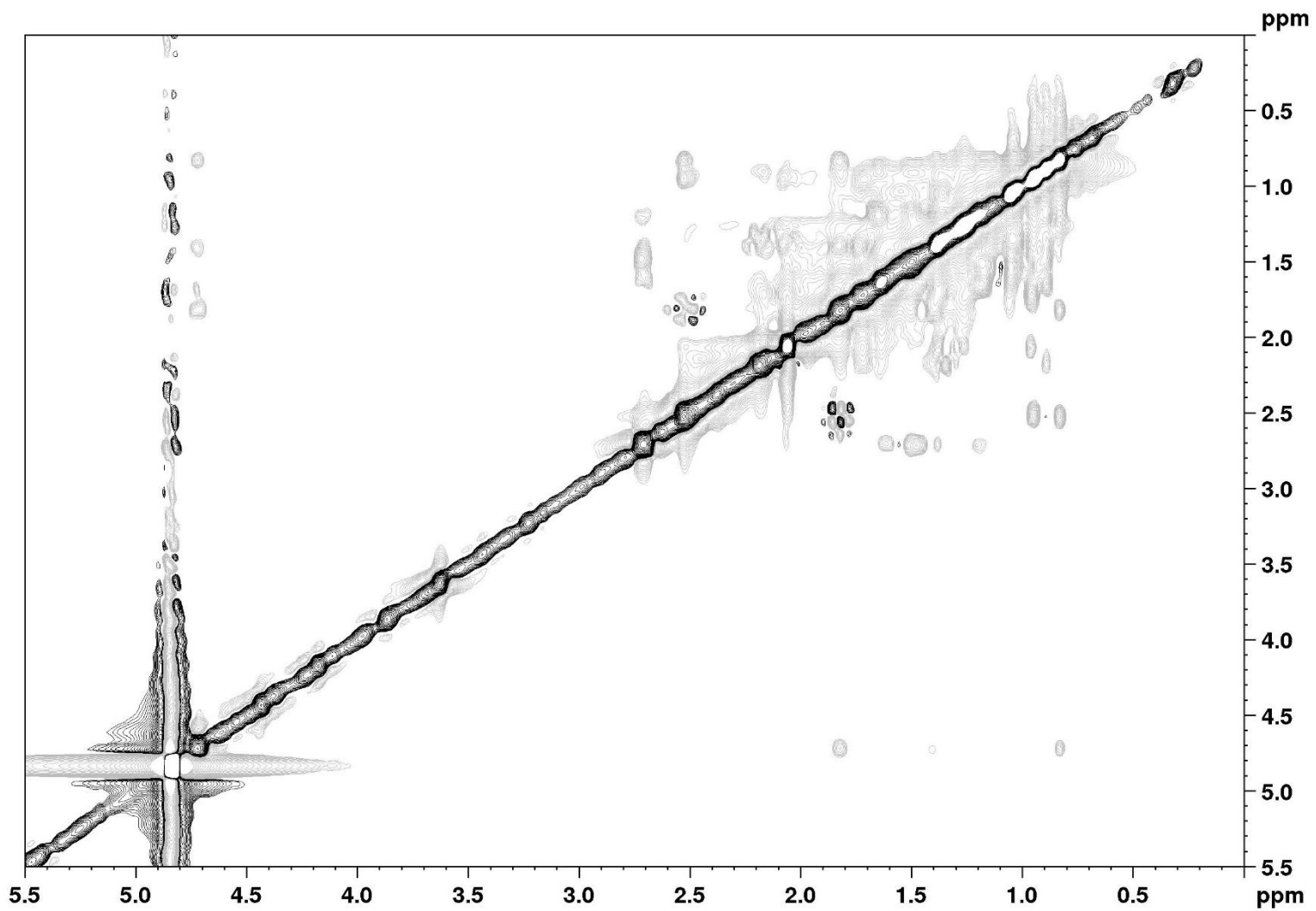
edHSQC spectrum of acanthobauerenone (**3**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).



HMBC spectrum of acanthobauerenone (**3**) (600 MHz, C<sub>5</sub>D<sub>5</sub>N).

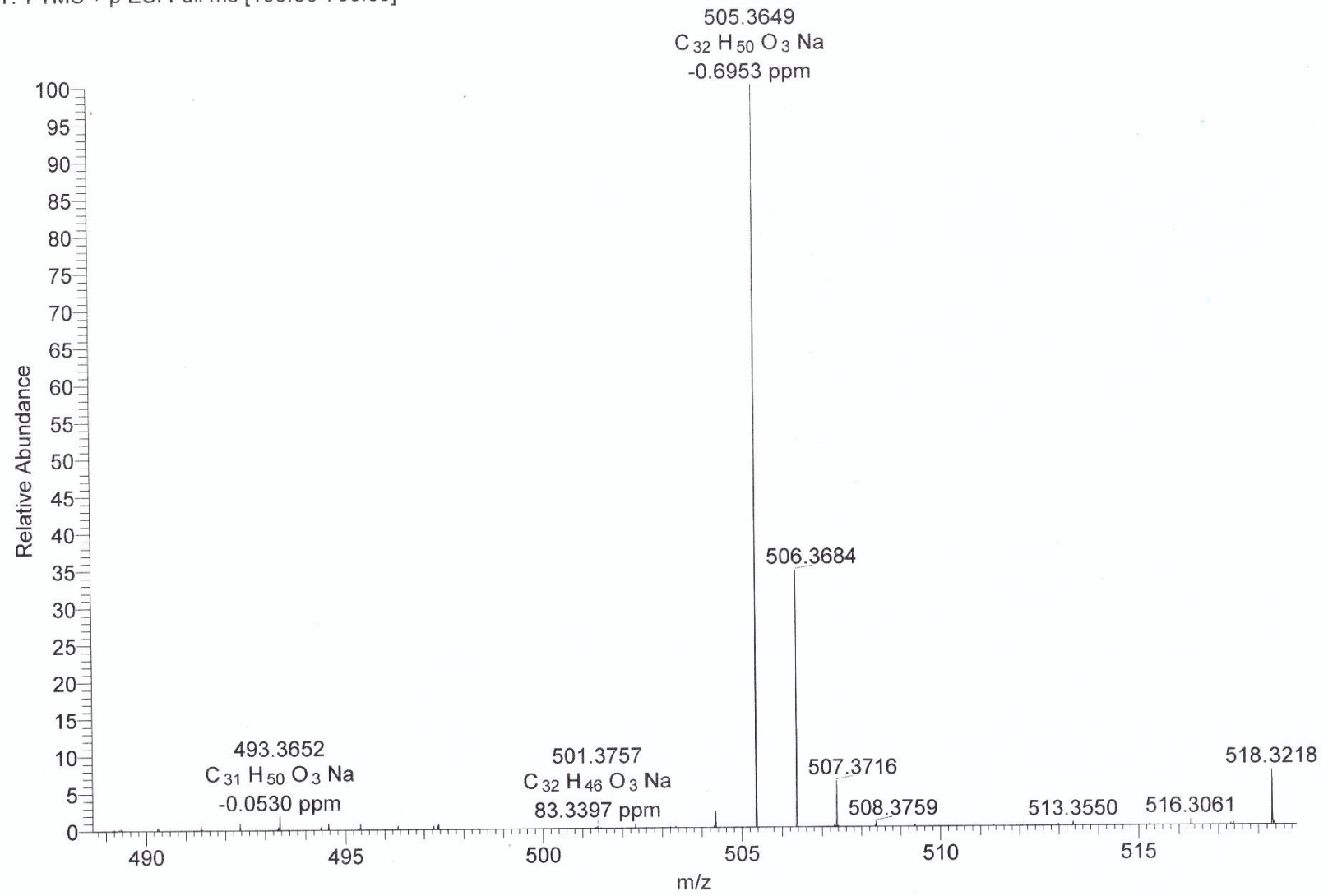


TOCSY spectrum of acanthobauerenone (**3**) (400 MHz, C<sub>5</sub>D<sub>5</sub>N).



NOESY spectrum of acanthobauerenone (**3**) (400 MHz, C<sub>5</sub>D<sub>5</sub>N).

LC\_LAn12\_5 #83-113 RT: 0.37-0.50 AV: 31 NL: 7.79E7  
T: FTMS + p ESI Full ms [100.00-700.00]



HRESIMS spectrum of acanthobauerenone (3).



Position	1		2		3	
	<sup>13</sup> C	<sup>1</sup> H (J, Hz)	<sup>13</sup> C	<sup>1</sup> H (J, Hz)	<sup>13</sup> C	<sup>1</sup> H (J, Hz)
1a	38.4, CH <sub>2</sub>	1.84, ddd (12.6, 4.3, 3.6)	35.1, CH <sub>2</sub>	3.01, dt (13.0, 6.8)	33.5, CH <sub>2</sub>	1.70, m
1b		1.33, m		1.60, m		1.39, m
2a	35.4, CH <sub>2</sub>	2.74, ddd (14.6, 14.6, 5.6)	34.3, CH <sub>2</sub>	2.61, m	24.0, CH <sub>2</sub>	1.80, m
2b		2.27, m		2.39, m		1.71, m
3	215.7, C		217.0, C		79.8, CH	4.72, dd (11.5, 4.2)
4	48.0, C		47.0, C		37.8, C	
5	51.8, CH	1.71, m	51.3, CH	1.68, dd (13.0, 2.0)	47.5, CH	1.82, dd (13.0, 5.9)
6a	24.7, CH <sub>2</sub>	2.01 m	19.4, CH <sub>2</sub>	1.60, m	36.2, CH <sub>2</sub>	2.55, dd (18.7, 5.9)
6b				1.34, m		2.49, dd (18.7, 13.0)
7a	117.8, CH	5.55 brd (2.7)	28.4, CH <sub>2</sub>	2.33, m	197.7, C	
7b				2.01, ddd (12.3, 11.7, 7.5)		
8	145.6, C		164.4, C		139.6, C	
9	48.2, CH	2.26, m	139.4, C		164.3, C	
10	34.2, C		36.5, C		39.4, C	
11a	17.1, CH <sub>2</sub>	1.50, m	197.8, C		22.5, CH <sub>2</sub>	2.16, m
11b						2.06, m
12a	30.0, CH <sub>2</sub>	1.76, m	49.6, CH <sub>2</sub>	2.35, ABq (18.7)	28.2, CH <sub>2</sub>	1.34, m
12b						
13	37.2, C		40.7, C		38.7, C	
14	41.5, C		43.4, C		40.7, C	
15a	29.1, CH <sub>2</sub>	1.56, m	25.9, CH <sub>2</sub>	1.62, m	23.7, CH <sub>2</sub>	2.70, ddd (13.0, 4.3, 2.5)
15b				1.28, m		1.49, ddd (14.0, 12.0, 4.3)
16a	34.6, CH <sub>2</sub>	1.54, m	37.4, CH <sub>2</sub>	1.46, m	36.7, CH <sub>2</sub>	1.60, ddd (14.5, 13.8, 4.3)
16b				1.15, m		1.18, m
17	40.0, C		32.2, C		31.5, C	
18	57.1, CH	1.53, m	52.3, CH	1.36, m	51.6, CH	1.34, m
19	50.3, CH	1.62, m	35.0, CH	0.96, m	34.0, CH	1.04, m
20	36.5, CH	1.53, m	31.6, CH	1.48, m	31.7, CH	1.53, m
21a	29.3, CH <sub>2</sub>	1.47, m	29.3, CH <sub>2</sub>	1.10, m	28.2, CH <sub>2</sub>	1.80, m
21b						1.41, m
22a	39.3, CH <sub>2</sub>	1.74, m	32.0, CH <sub>2</sub>	1.56, m	32.1, CH <sub>2</sub>	1.64, m
22b		1.14, m		1.20, m		1.19, m
23	24.5, CH <sub>3</sub>	1.10, s	26.8, CH <sub>3</sub>	1.17, s	27.0, CH <sub>3</sub>	0.83, s
24	21.7, CH <sub>3</sub>	1.05, s	21.0, CH <sub>3</sub>	1.11, s	16.1, CH <sub>3</sub>	0.93, s
25	13.1, CH <sub>3</sub>	0.93, s	19.5, CH <sub>3</sub>	1.40, s	18.3, CH <sub>3</sub>	0.95, s
26	23.2, CH <sub>3</sub>	1.02, s	21.0, CH <sub>3</sub>	1.09, s	21.0, CH <sub>3</sub>	1.37, s
27	23.3, CH <sub>3</sub>	0.98, s	18.2, CH <sub>3</sub>	0.95, s	15.7, CH <sub>3</sub>	0.88, s
28	33.6, CH <sub>3</sub>	0.93, s	37.3, CH <sub>3</sub>	1.03, s	38.9, CH <sub>3</sub>	1.04, s
29	22.3, CH <sub>3</sub>	0.92, d (6.2)	24.8, CH <sub>3</sub>	0.96, d, overlap	25.3, CH <sub>3</sub>	1.00, d (6.4)
30	23.8, CH <sub>3</sub>	0.96, d (6.2)	22.5, CH <sub>3</sub>	0.89, d (5.8)	22.0, CH <sub>3</sub>	0.92, brs
Ac-CO					170.5, C	
Ac-CH <sub>3</sub>					20.7, CH <sub>3</sub>	2.05, s

NMR data in C<sub>5</sub>D<sub>5</sub>N of acantholupenone (1) acanthobauerendione (2), and acanthobauerenone (3).