BEILSTEIN JOURNAL OF ORGANIC CHEMISTRY

Supporting Information

for

New sesquiterpenoids from the South China Sea soft corals *Clavularia viridis* and *Lemnalia flava*

Qihao Wu, Yuan Gao, Meng-Meng Zhang, Li Sheng, Jia Li, Xu-Wen Li, Hong Wang and Yue-Wei Guo

Beilstein J. Org. Chem. **2019,** *15,* 695–702. doi:10.3762/bjoc.15.64

Spectral data of compounds 1–4 and 7

Contents

Figure S1: ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **1**.

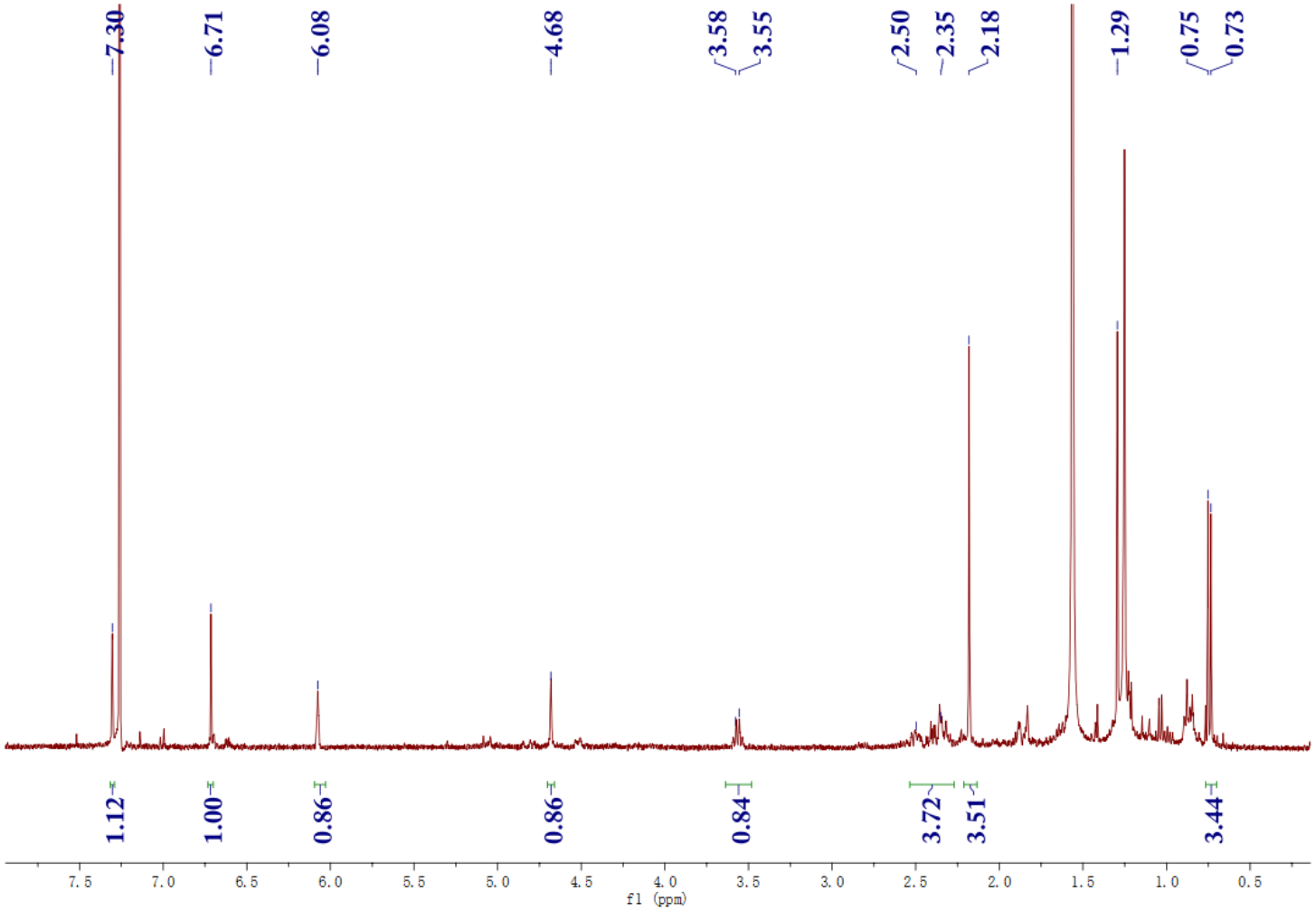


Figure S2: ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **1**.

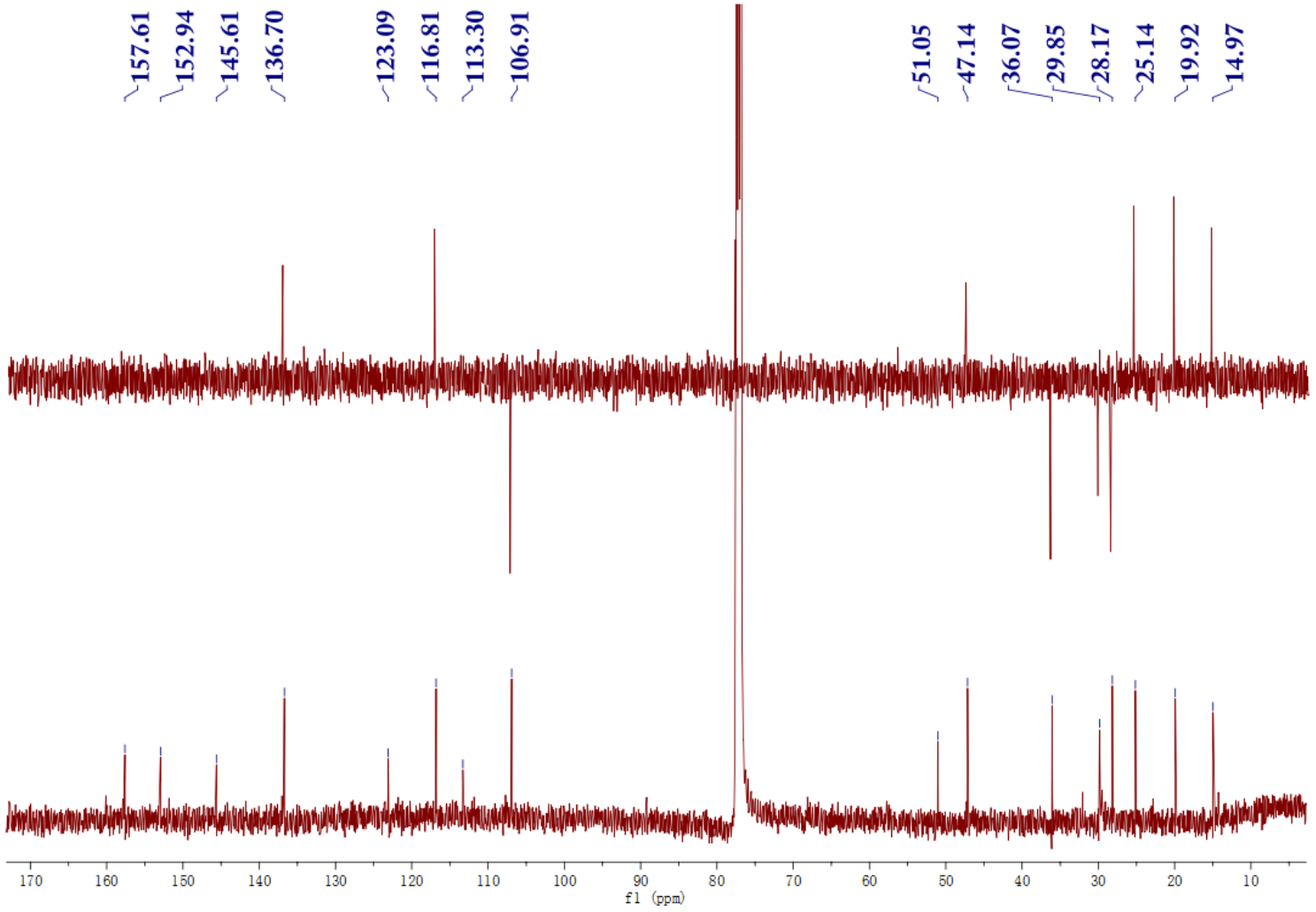


Figure S3: $^{1}H,^{1}H$ COSY spectrum (500 MHz, $CDCl_3$) of **1**.

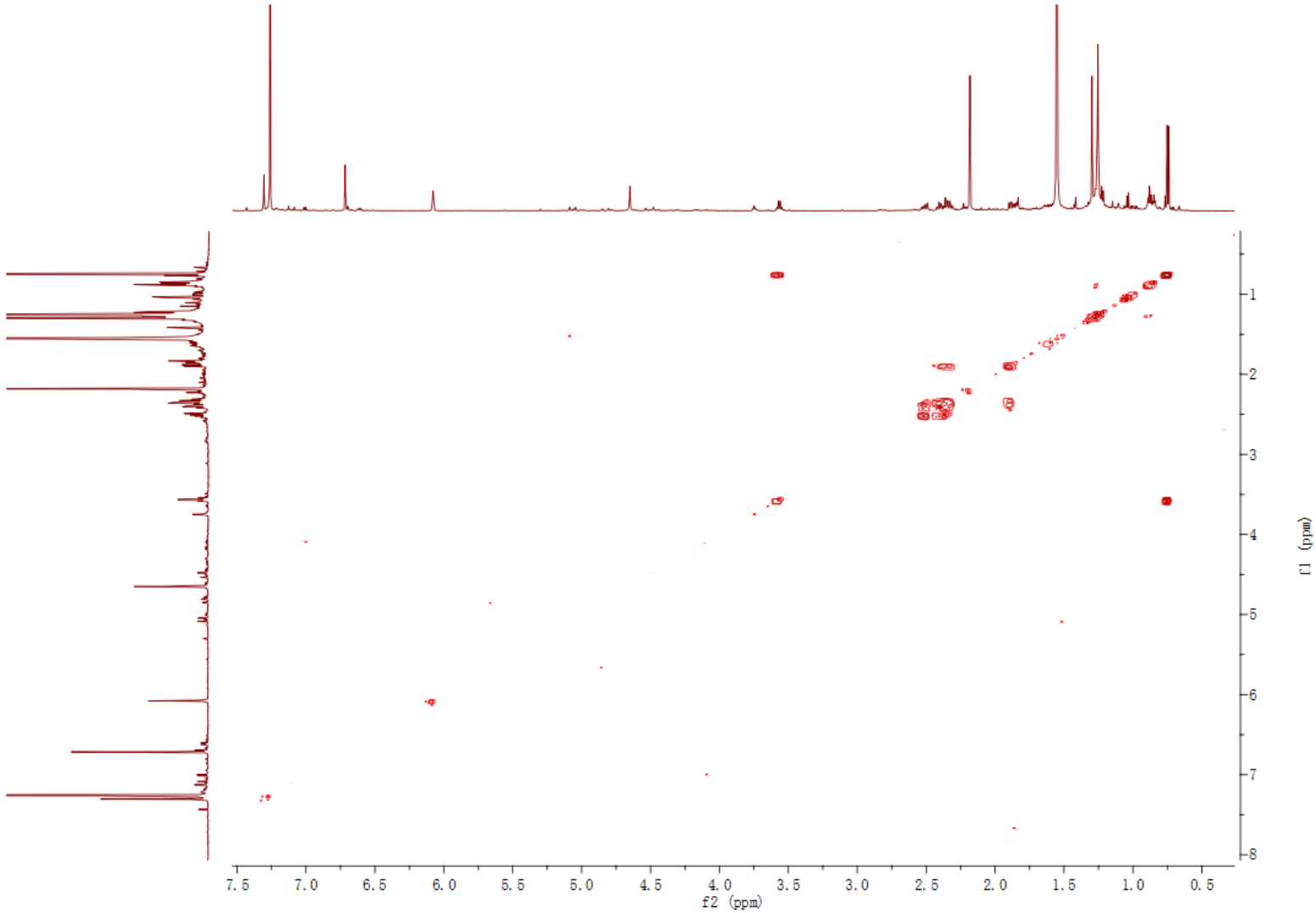


Figure S4: HMQC spectrum (500 MHz, $CDCl_3$) of **1**.

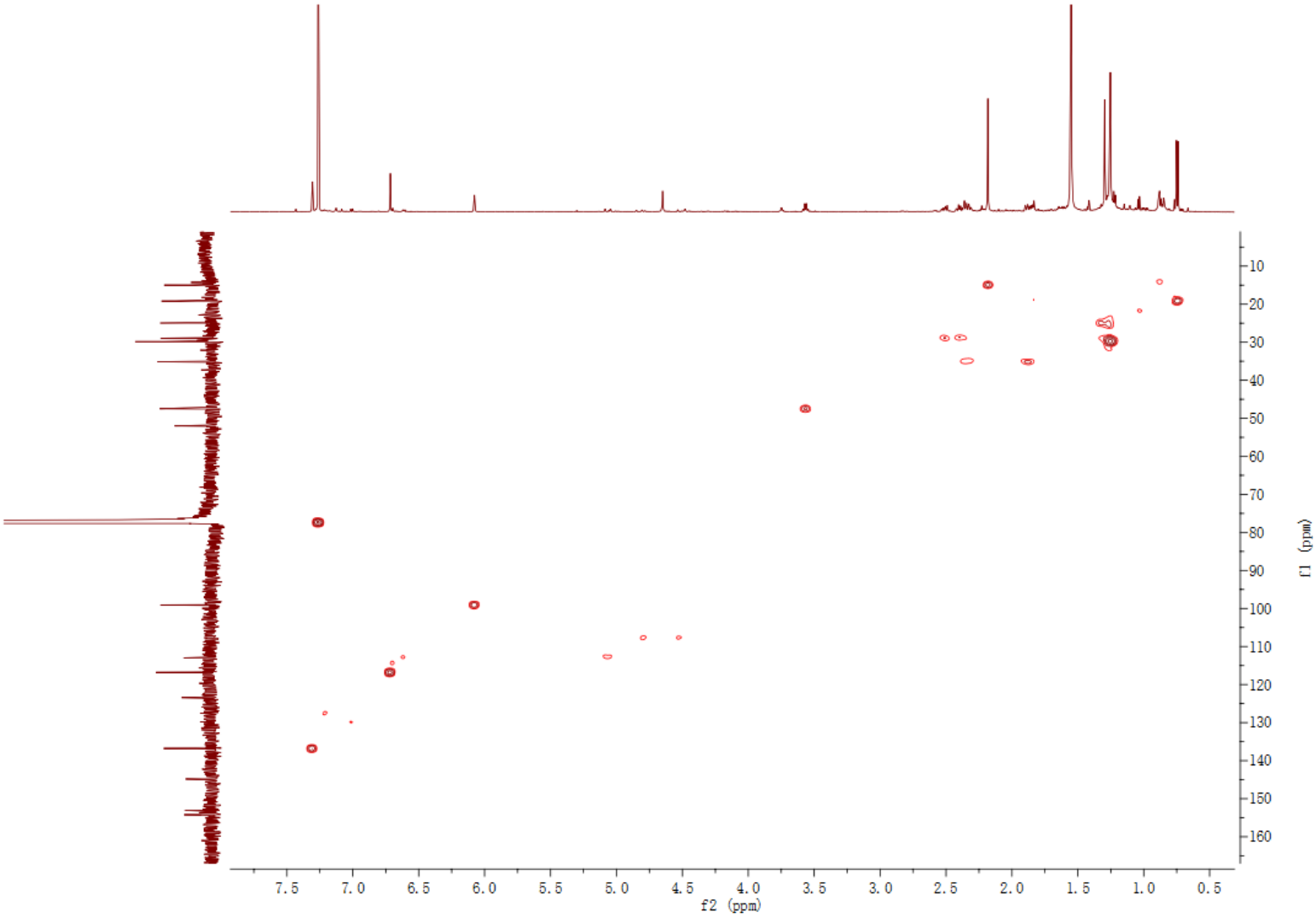


Figure S5: HMBC spectrum (500 MHz, $CDCl_3$) of **1**.

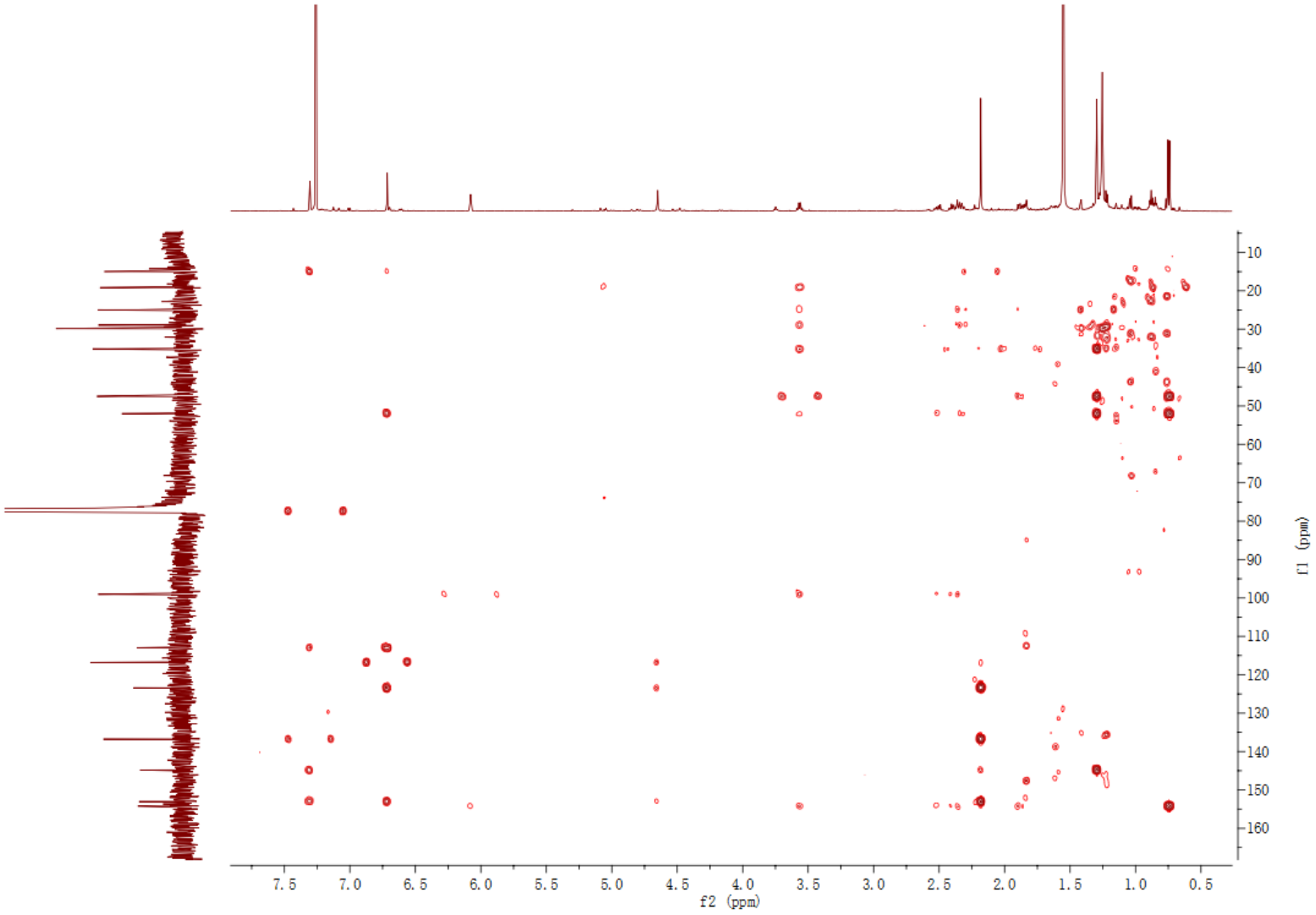


Figure S6: NOESY spectrum (500 MHz, $CDCl_3$) of **1**.

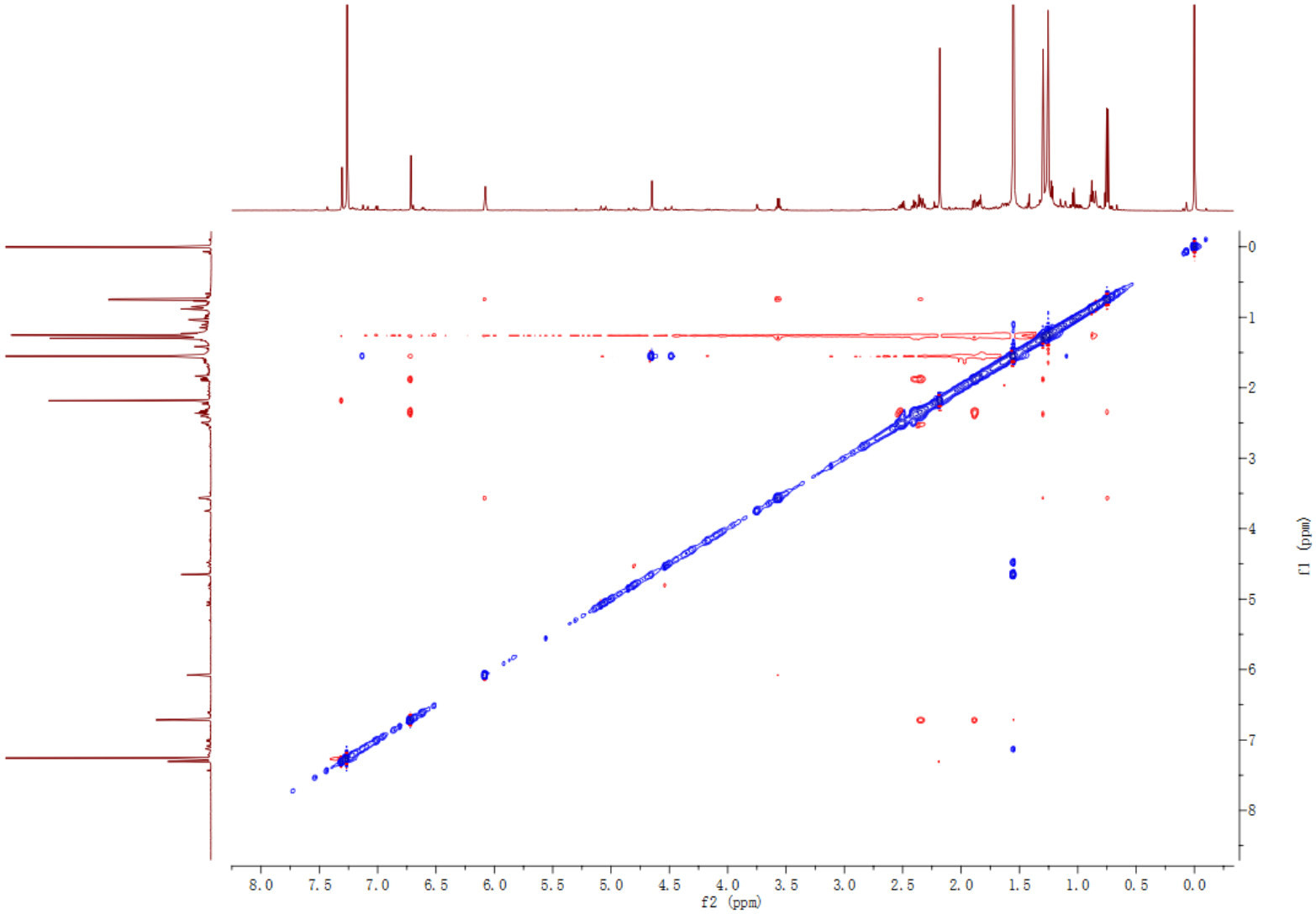


Figure S7: IR spectrum of **1**.

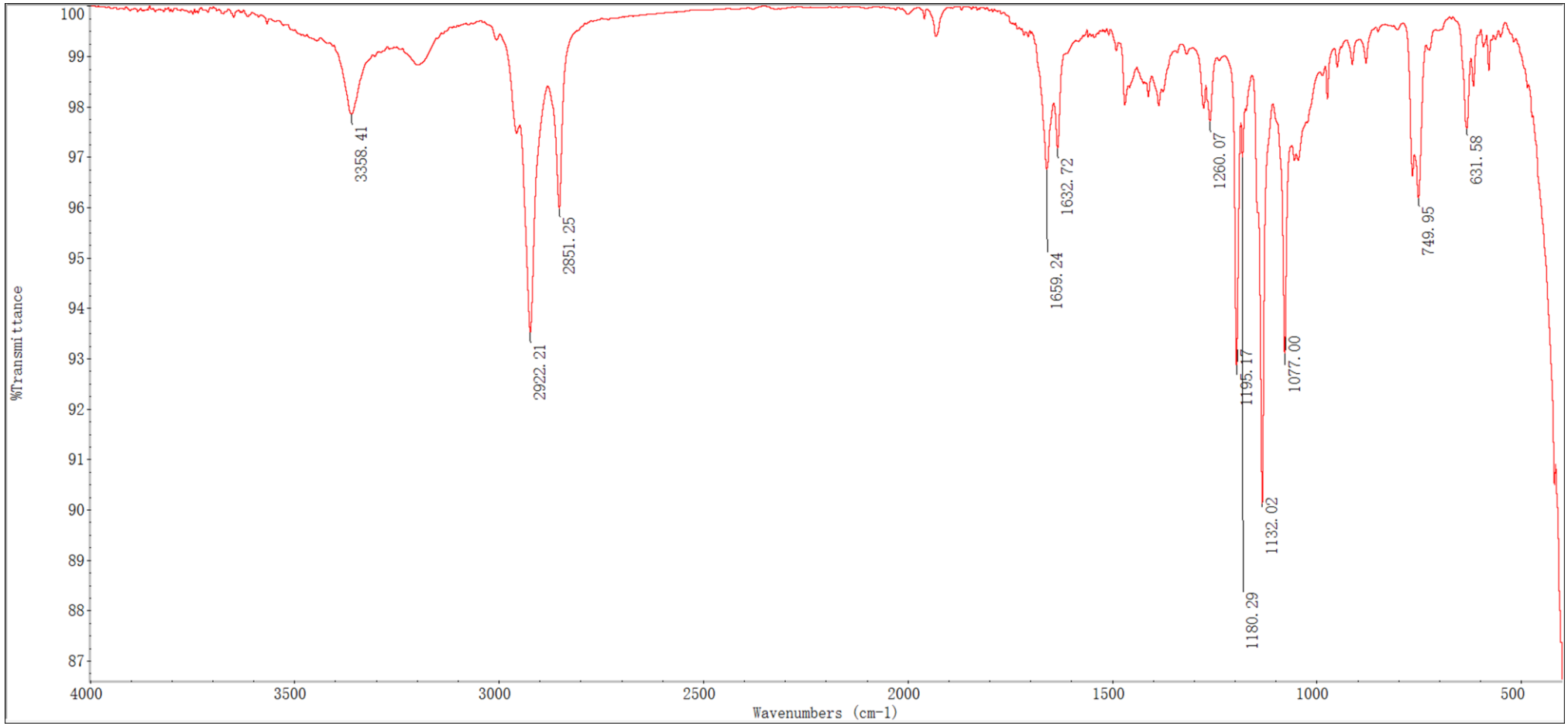


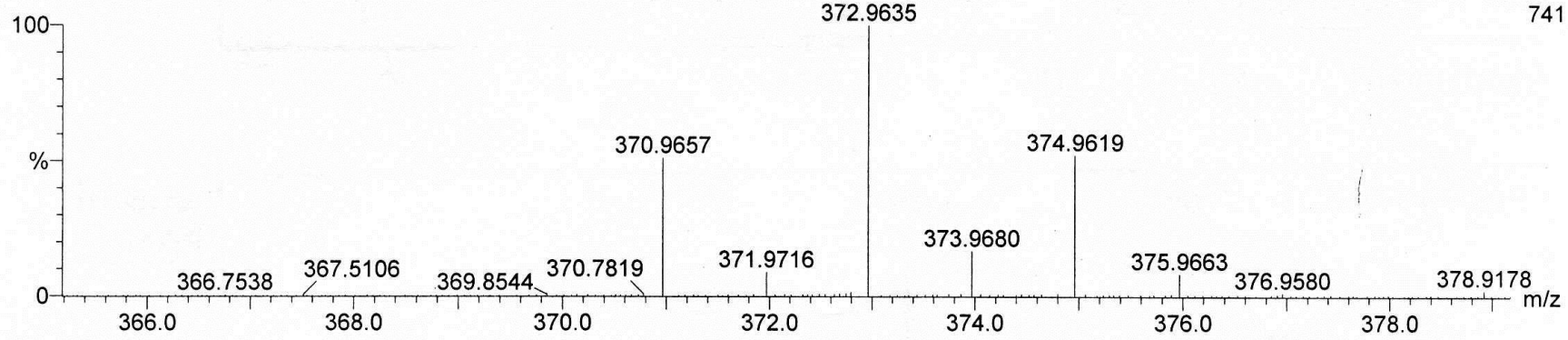
Figure S8: HR-ESIMS spectrum of **1**.

Elemental Composition Report **Page 1**

Multiple Mass Analysis: 3 mass(es) processed
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
19 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

SIMM-Mass Spec Q-Tof Ultima 30-Sep-2015
D4h2
151297-1 25 (0.479) AM (Cen,4, 80.00, Ht,9000.0,384.93,0.70); Sm (SG, 2x1.00); Cm (25:46) TOF MS ES-741



Minimum:	50.00				-1.5		
Maximum:	100.00		200.0	20.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
370.9657	51.04	370.9646	1.1	2.9	6.5	1	C15 H17 O Br2
372.9635	100.00	---					
374.9619	52.28	---					

Figure S9: ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **2**.

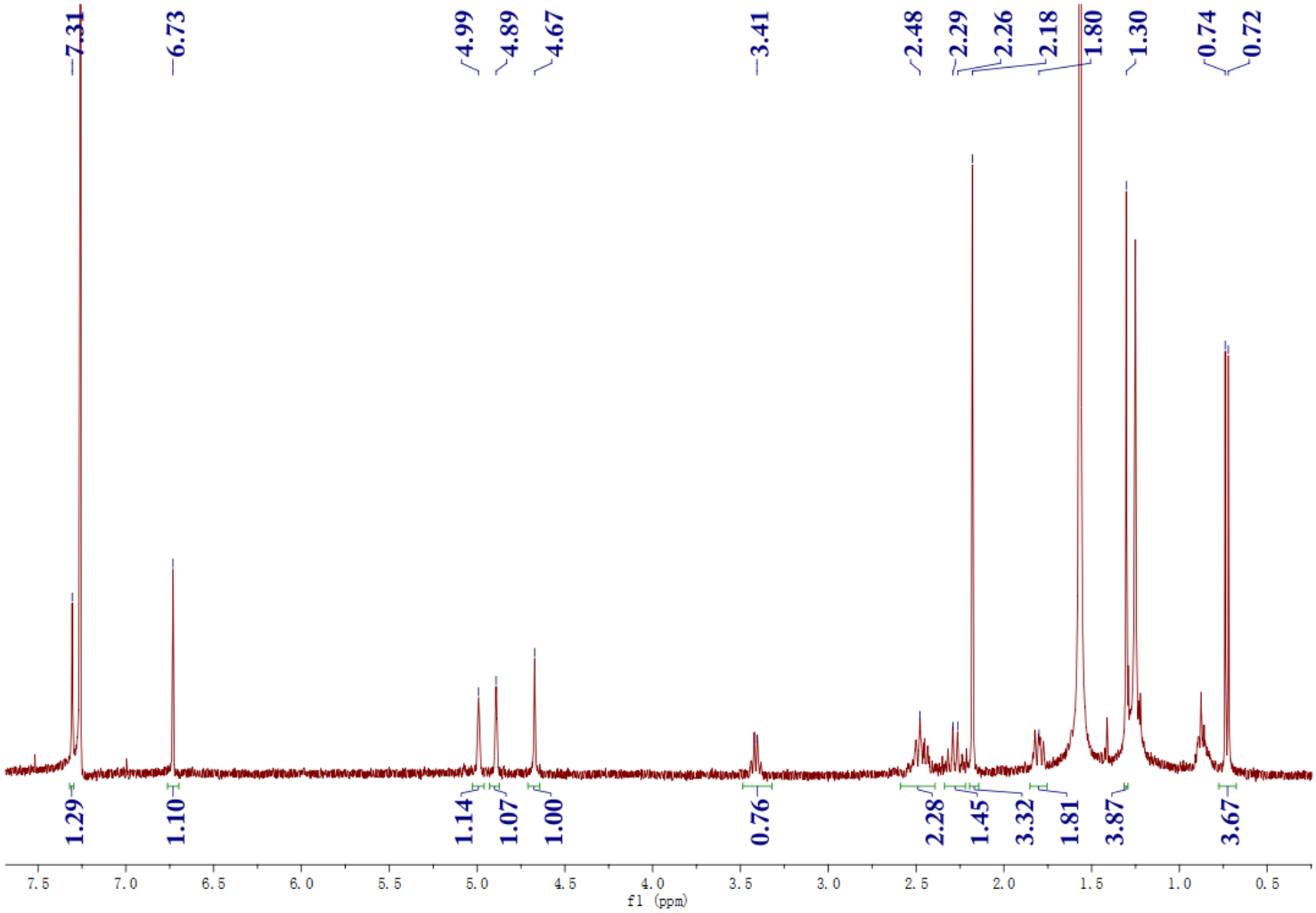


Figure S10: ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **2**.

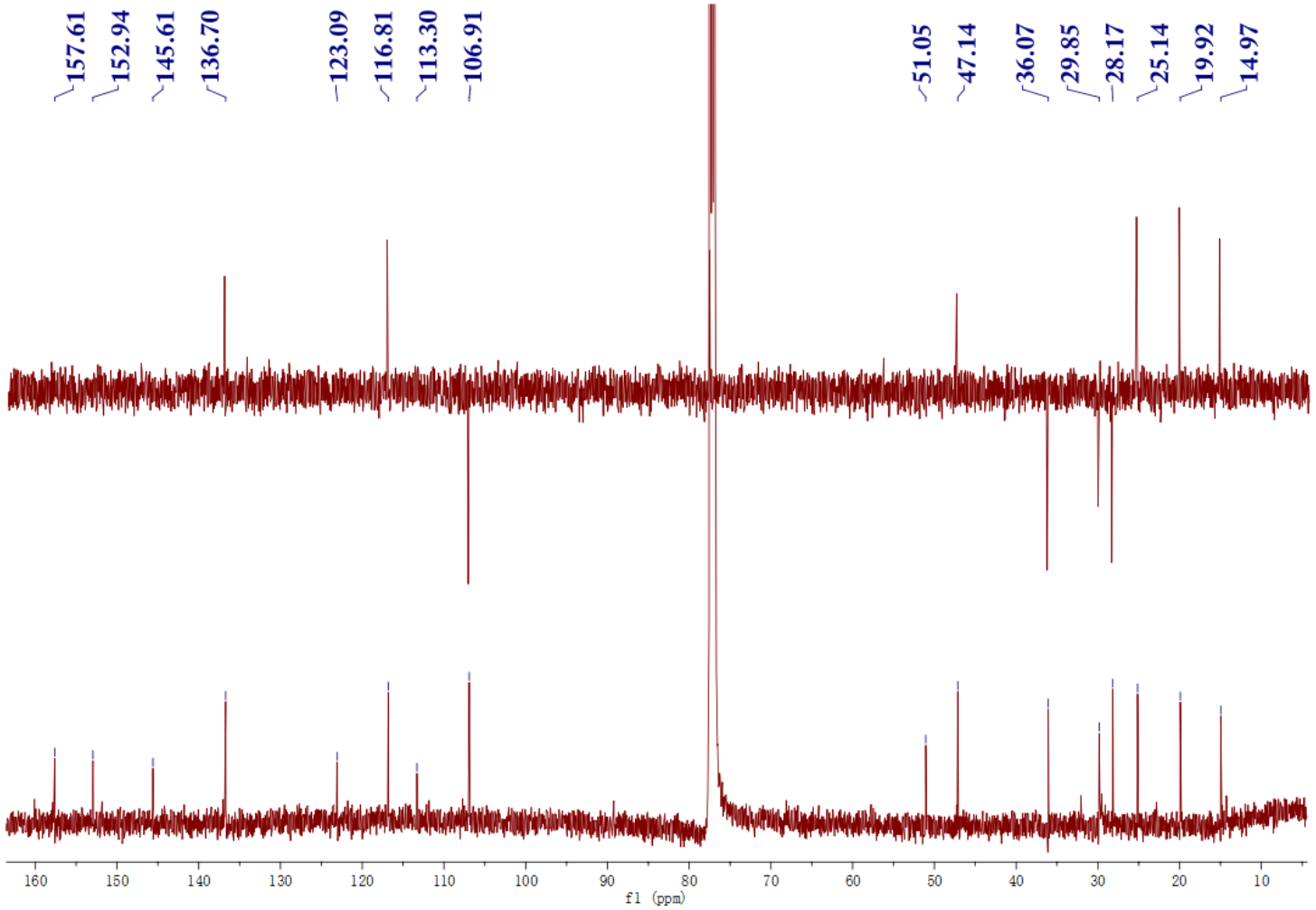


Figure S11: $^{1}H,^{1}H$ COSY spectrum (500 MHz, $CDCl_3$) of **2**.

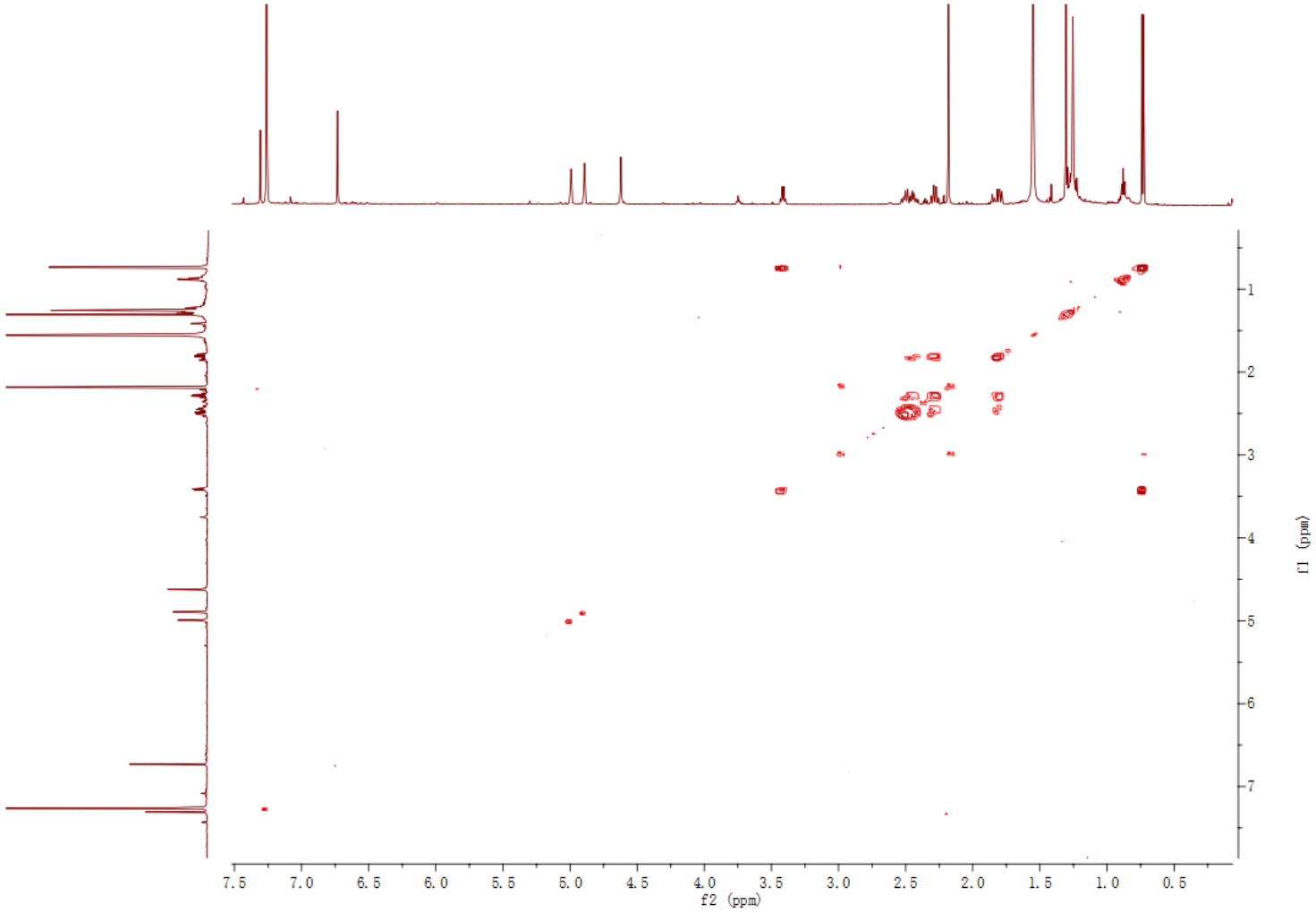


Figure S12: HMQC spectrum (500 MHz, $CDCl_3$) of **2**.

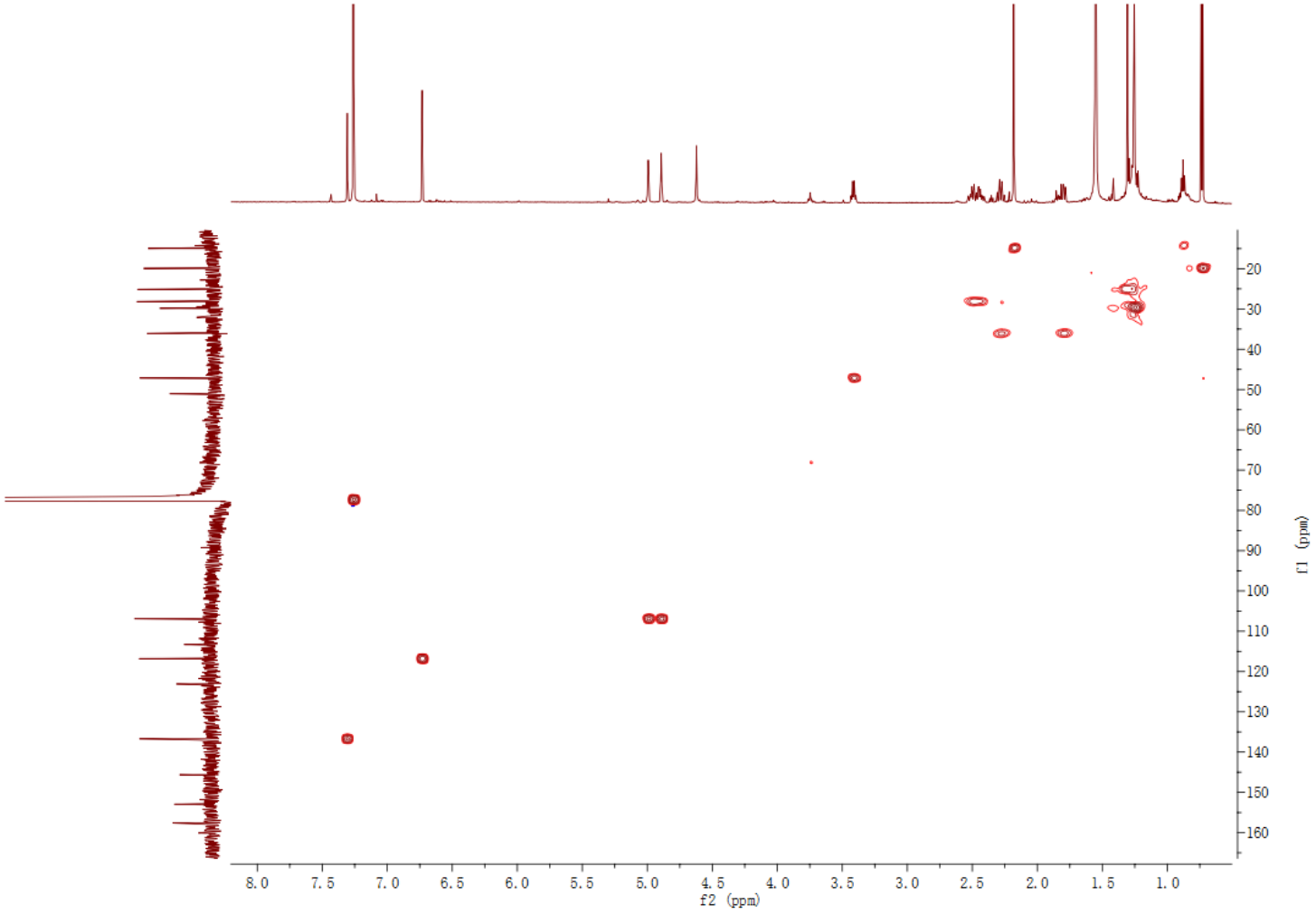


Figure S13: HMBC spectrum (500 MHz, $CDCl_3$) of **2**.

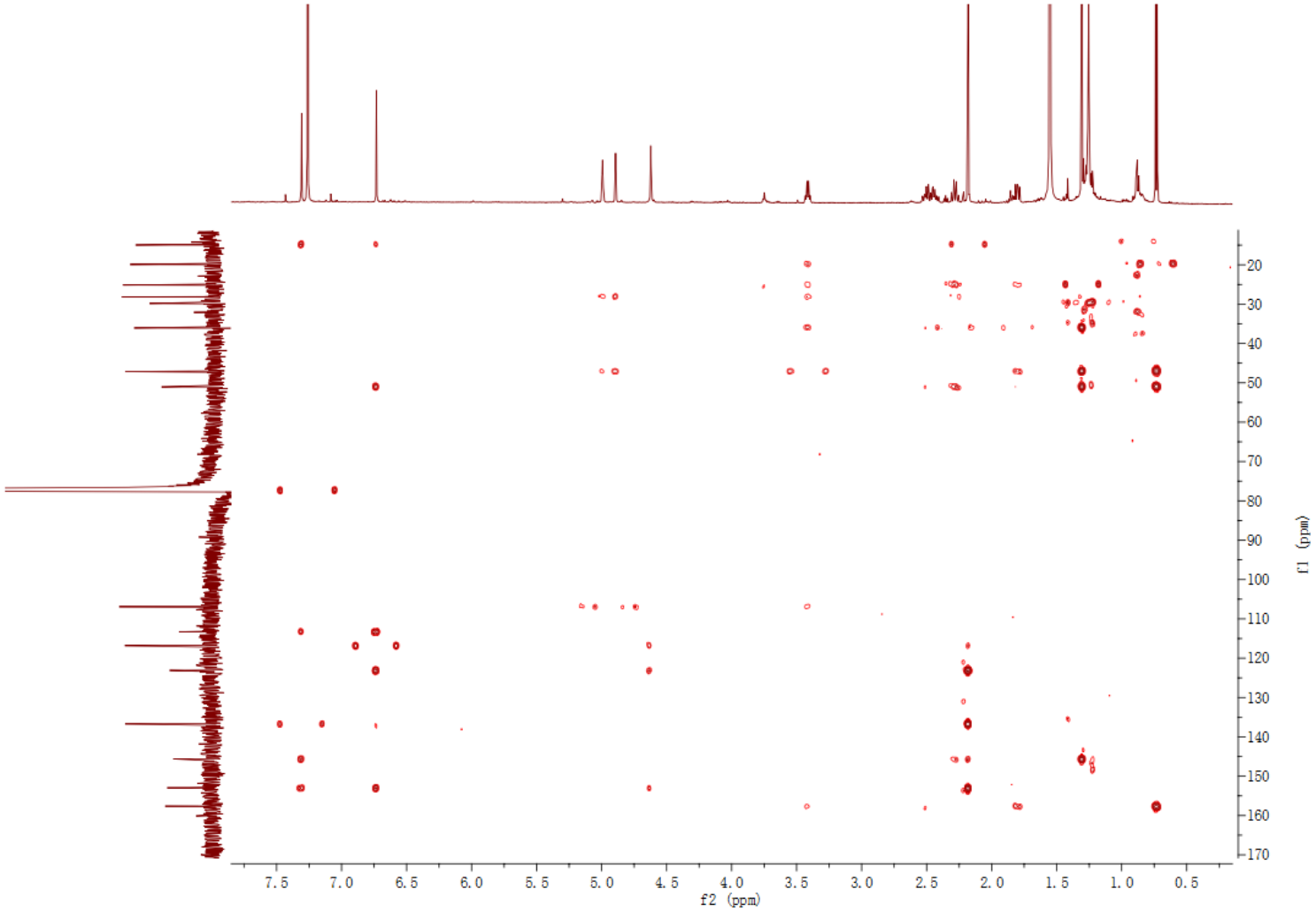


Figure S14: NOESY spectrum (500 MHz, $CDCl_3$) of **2**.

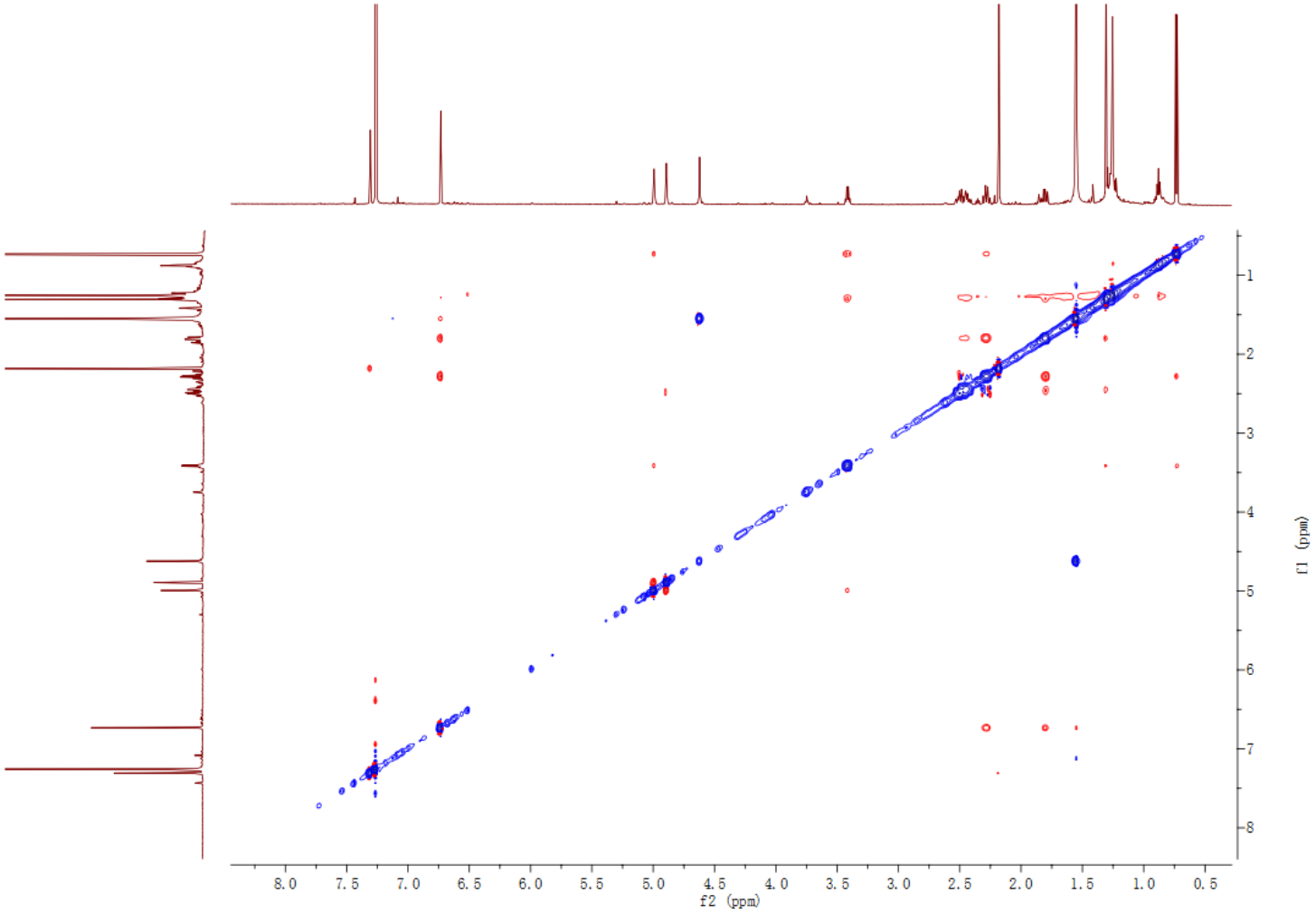


Figure S15: IR spectrum of **2**.

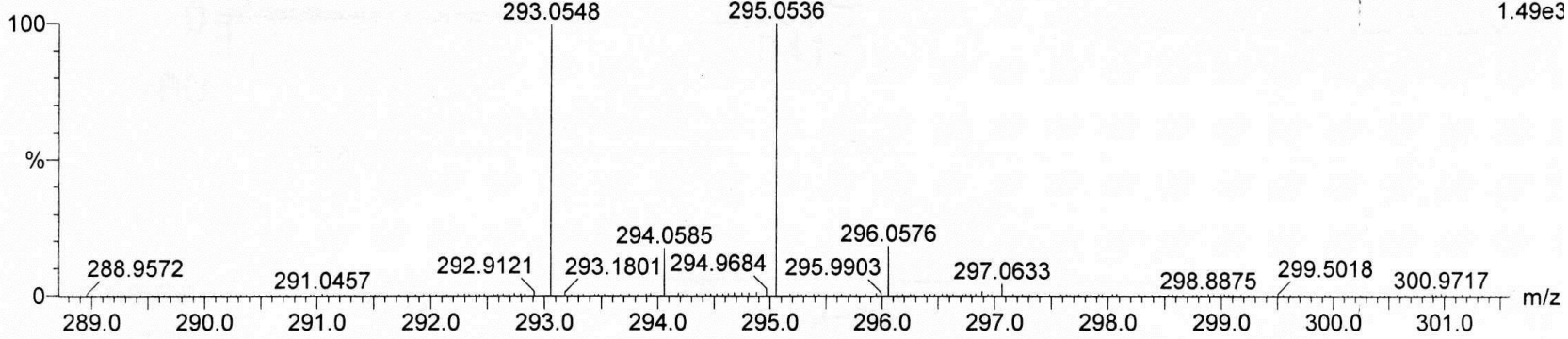
Figure S16: HR-ESIMS spectrum of **2**.

Elemental Composition Report **Page 1**

Multiple Mass Analysis: 2 mass(es) processed
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
9 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

SIMM-Mass Spec Q-Tof Ultima 30-Sep-201
D4g-2
151297-1 151 (2.855) AM (Cen,4, 80.00, Ht,9000.0,316.95,0.70); Sm (SG, 2x1.00); Cm (101:159) TOF MS ES-
1.49e3



Minimum:	50.00				-1.5		
Maximum:	100.00		200.0	20.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
293.0548	99.46	293.0541	0.7	2.4	6.5	1	C15 H18 O Br
295.0536	100.00	---					

Figure S17: ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **3**.

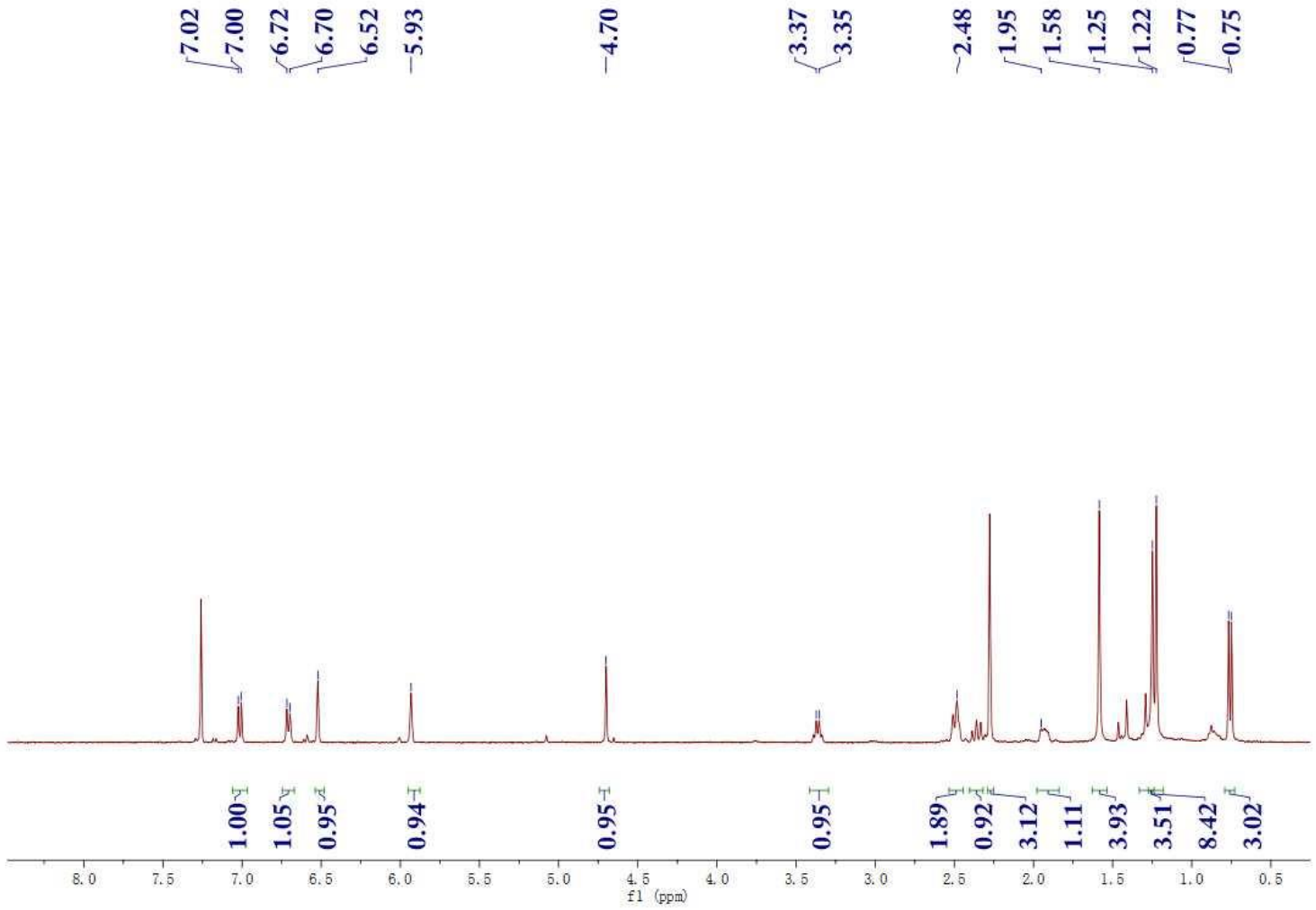


Figure S18: ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **3**.

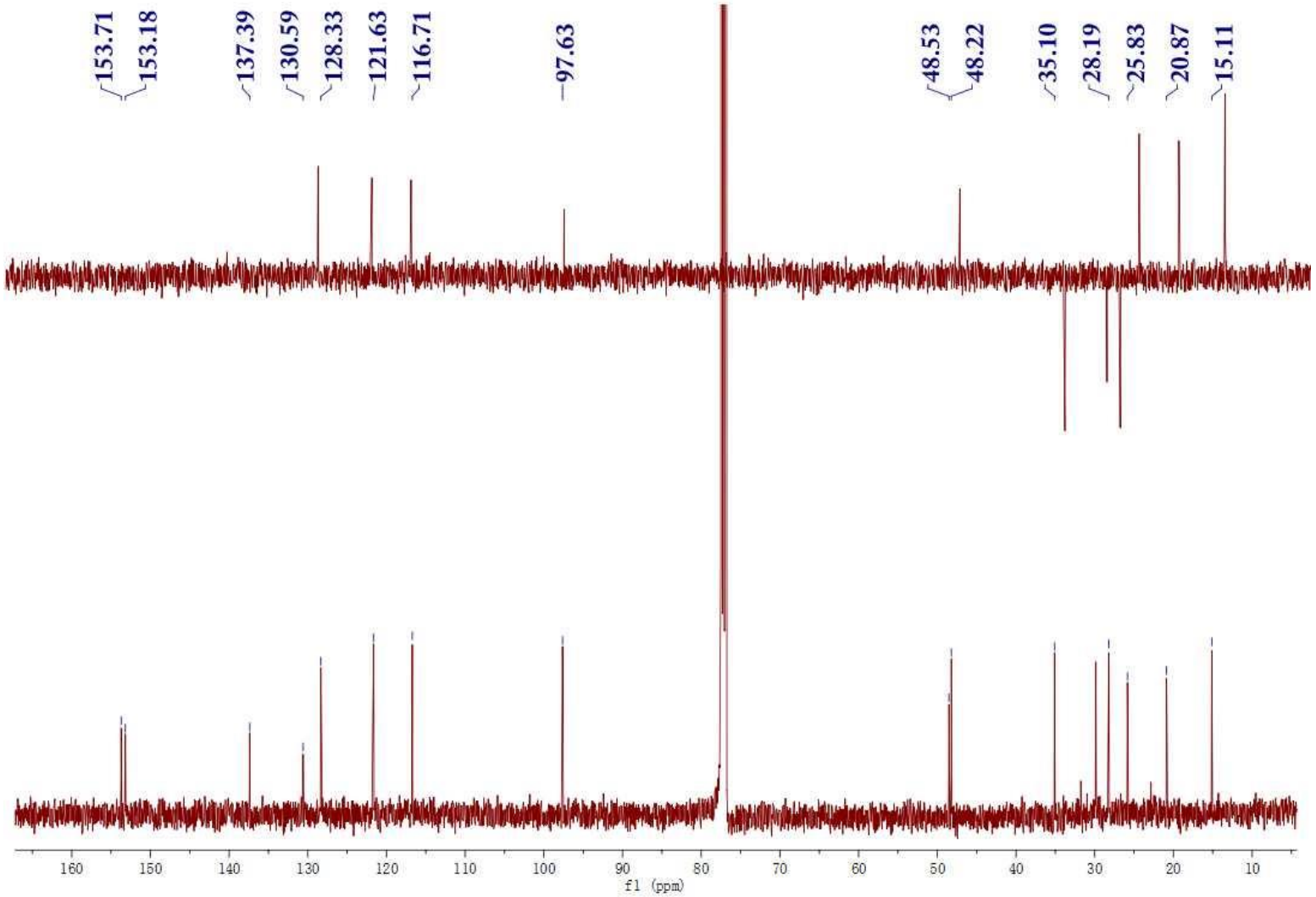


Figure S19: $^{1}H,^{1}H$ COSY spectrum (500 MHz, $CDCl_3$) of **3**.

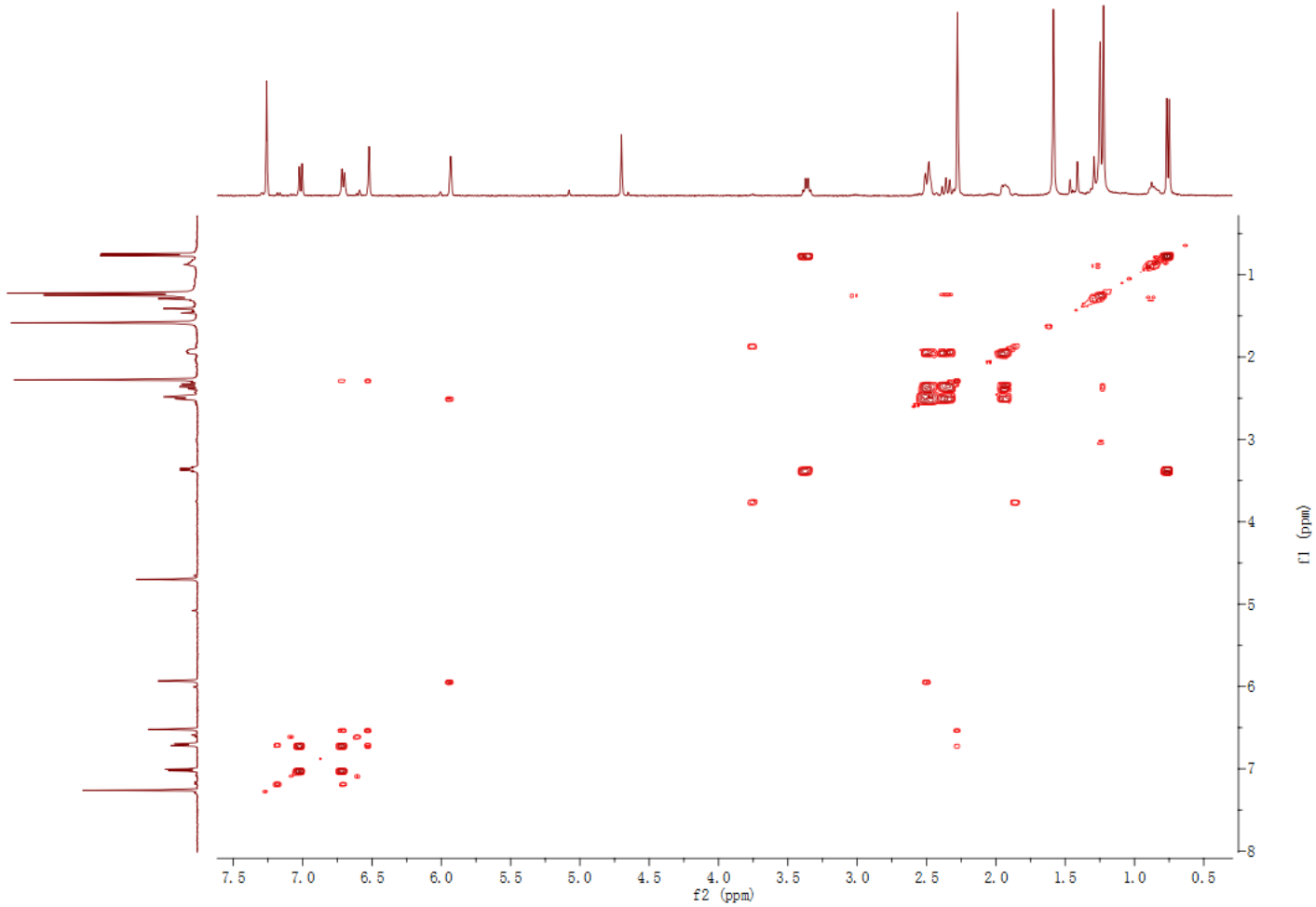


Figure S20: HMQC spectrum (500 MHz, $CDCl_3$) of **3**.

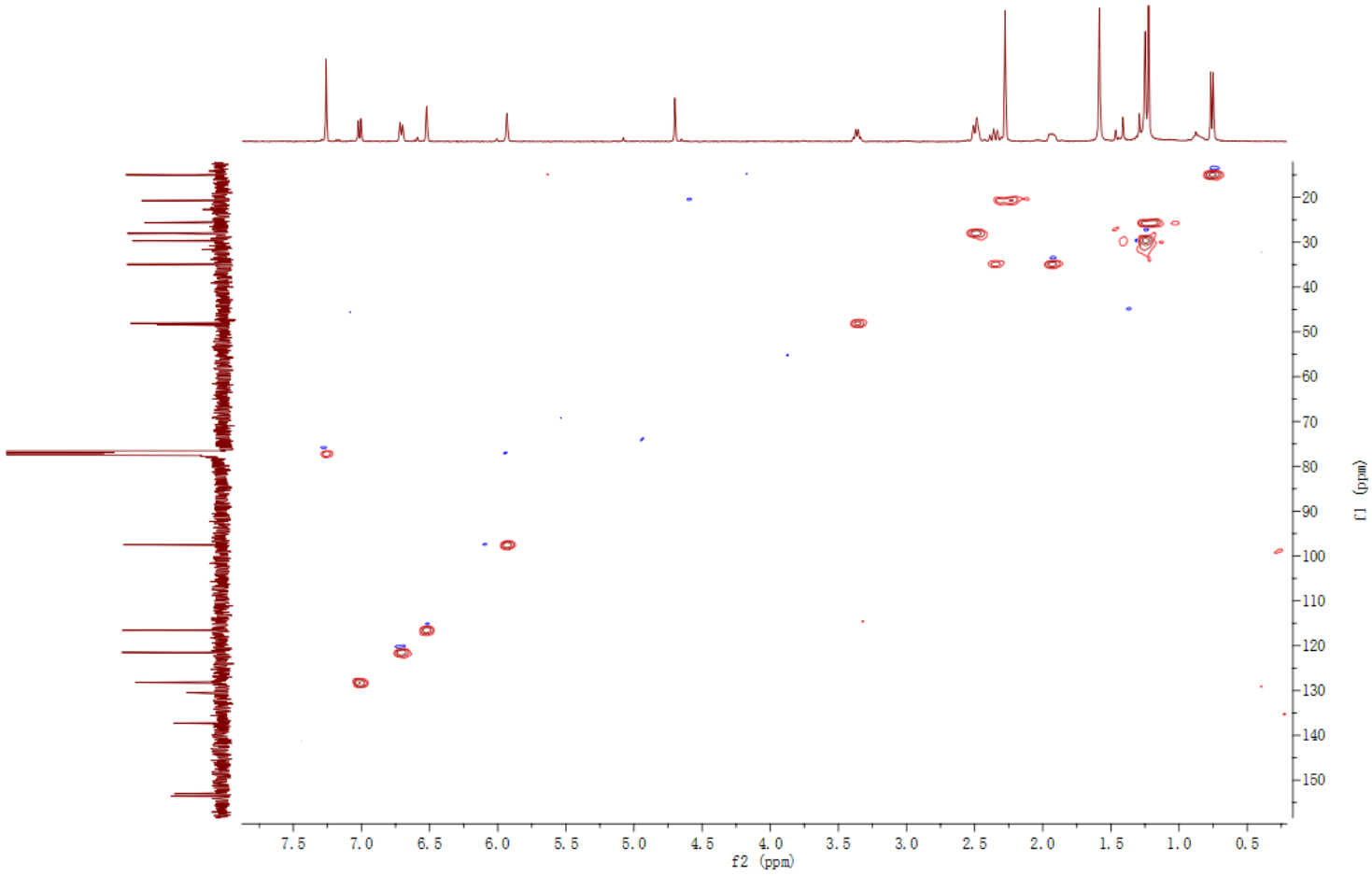


Figure S21: HMBC spectrum (500 MHz, $CDCl_3$) of **3**.

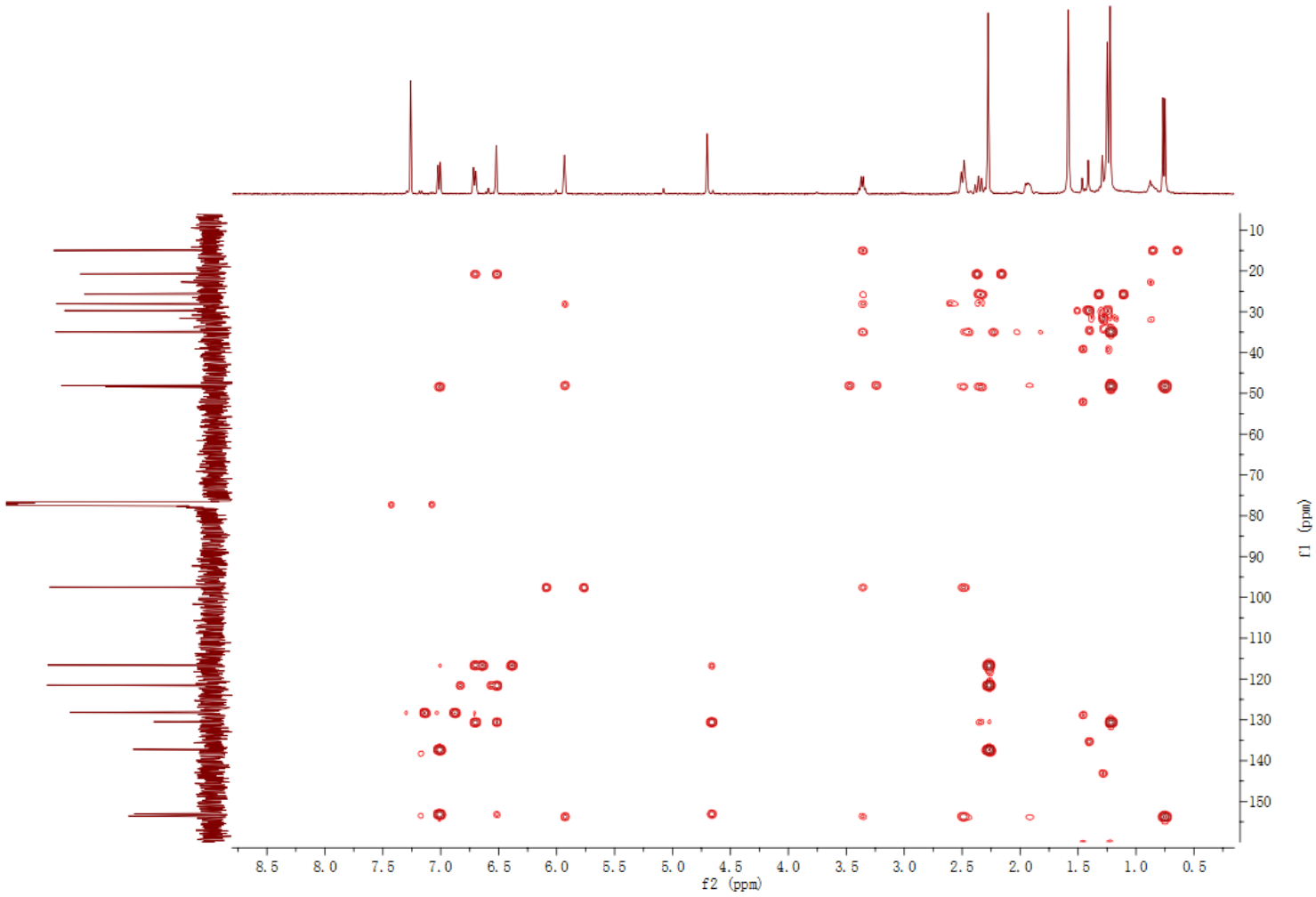


Figure S22: NOESY spectrum (500 MHz, $CDCl_3$) of **3**.

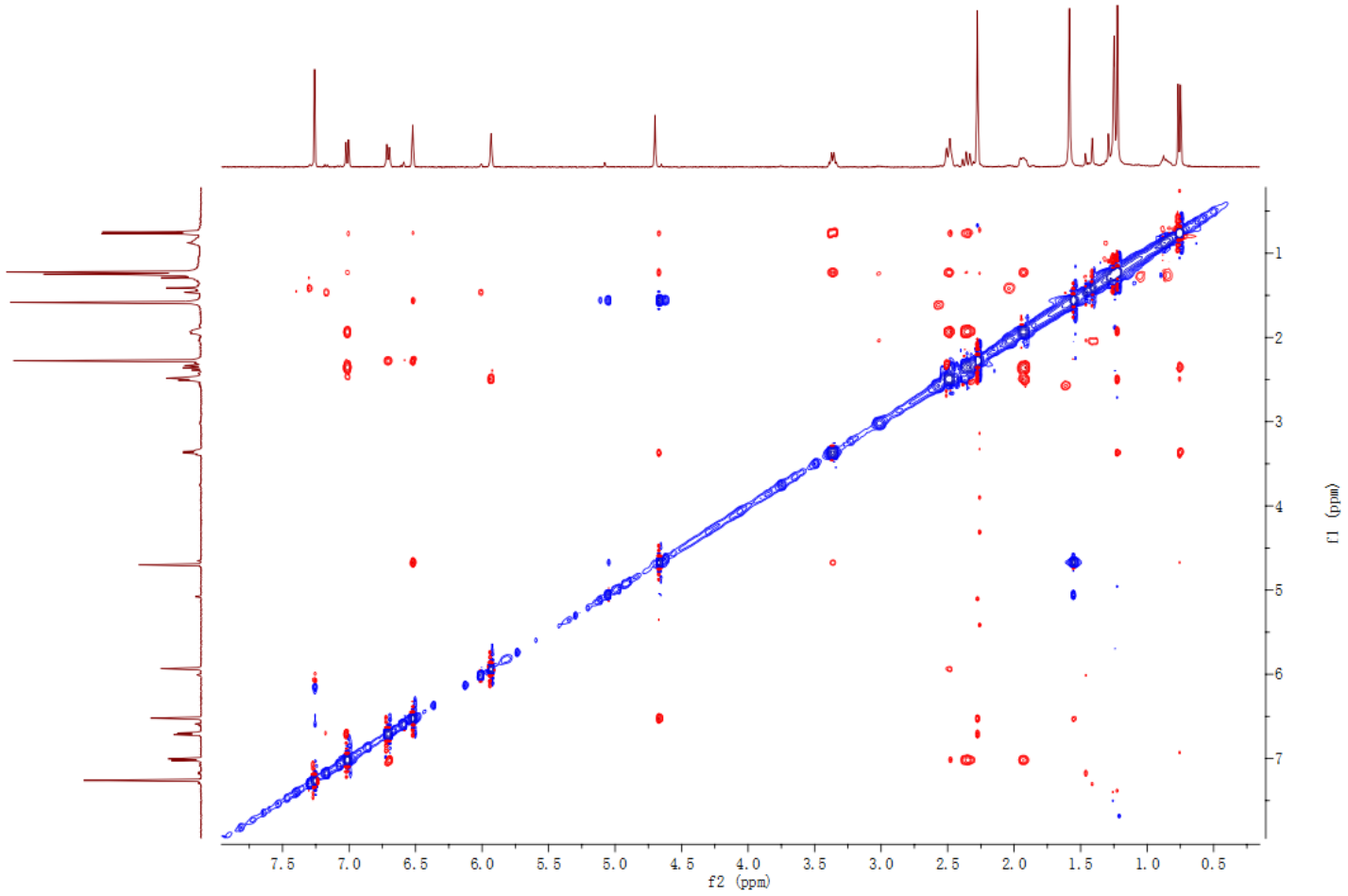


Figure S23: IR spectrum of **3**.

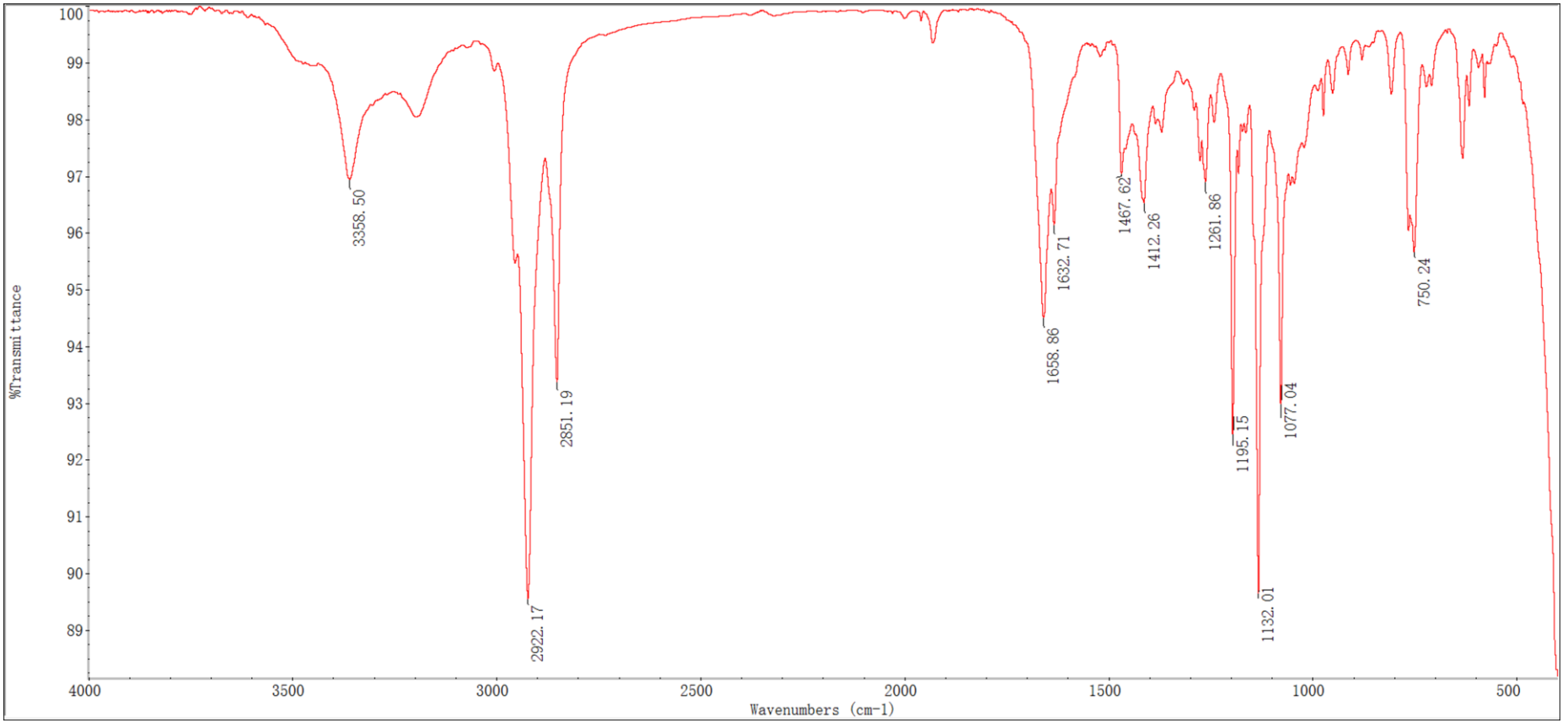


Figure S24: HR-EIMS spectrum of **3**.

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Samp:  c4a2                                                Start :   17:37:12      18
Comm:  Finnigan/MAT95/70eV/R:10000
Mode:  EI +VE +LMR  BSCAN (EXP) UP HR NRM                  Study :   S/N: PT200712-01-01
Oper:  SIMM.CAS      Client:  S/N: PT001263                Inlet :
Limt: (   0 )     .     .  .
    : ( 404 ) C16.H100.Br.O2
Peak:  1000.00  mmu    R+D:  -2.0 > 60.0
Data:  CMASS : converted
```

Mass	Intensity (4277)	%RA	%RIC	Delta (mmu)	R+D	Composition
55.06891 *	5569	2.60	0.03			
57.08490 *	5806	2.71	0.03			
67.06923 *	5450	2.55	0.03			
69.07027 *	6043	2.83	0.03	0.2	1.5	C5.H9
77.03876 *	10190	4.76	0.05	0.4	4.5	C6.H5
79.05401 *	6161	2.88	0.03	0.8	3.5	C6.H7
81.06935 *	8650	4.04	0.04	1.1	2.5	C6.H9
91.05108 *	13626	6.37	0.07			
92.99269 *	93137	43.55	0.45			
95.08308 *	4739	2.22	0.02	3.0	2.5	C7.H11
105.0727 *	11731	5.48	0.06	-2.3	4.5	C8.H9
107.0905 *	19670	9.20	0.10			
111.9990 *	28675	13.41	0.14			
115.0565 *	9361	4.38	0.05	-1.7	6.5	C9.H7
121.0658 *	100484	46.98	0.49	-0.4	4.5	C8.H9.O
122.0693 *	4384	2.05	0.02			
128.0619 *	5569	2.60	0.03	0.7	7.0	C10.H8
135.0821 *	24410	11.41	0.12	-1.1	4.5	C9.H11.O
145.0667 *	15522	7.26	0.08	-1.4	6.5	C10.H9.O
146.9841 *	4502	2.10	0.02			
147.0798 *	4384	2.05	0.02	1.2	5.5	C10.H11.O
149.0249 *	7583	3.55	0.04			
158.0730 *	4502	2.10	0.02	0.2	7.0	C11.H10.O
159.0809 *	38748	18.12	0.19	0.1	6.5	C11.H11.O
160.0870 *	9005	4.21	0.04	1.8	6.0	C11.H12.O
171.0823 *	4621	2.16	0.02	-1.3	7.5	C12.H11.O
173.0982 *	20144	9.42	0.10	-1.5	6.5	C12.H13.O
185.0952 *	15167	7.09	0.07	1.4	7.5	C13.H13.O
186.1021 *	6517	3.05	0.03	2.4	7.0	C13.H14.O
187.1103 *	8413	3.93	0.04	2.0	6.5	C13.H15.O
191.1435 *	8768	4.10	0.04	0.1	4.5	C13.H19.O
199.1113 *	17655	8.25	0.09	1.0	7.5	C14.H15.O
200.1184 *	14930	6.98	0.07	1.7	7.0	C14.H16.O
207.0335 *	14337	6.70	0.07			
214.1352 *	7228	3.38	0.04	0.5	7.0	C15.H18.O
215.1415 *	213884	100.00	1.04	2.1	6.5	C15.H19.O
216.1460 *	23225	10.86	0.11			
279.0407 *	8768	4.10	0.04	-2.2	6.5	C14.H16.Br.O
281.0369 *	11968	5.60	0.06			
294.0617 *	6754	3.16	0.03	0.2	6.0	C15.H19.Br.O
296.0594 *	7109	3.32	0.03			

Figure S25: ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **4**.

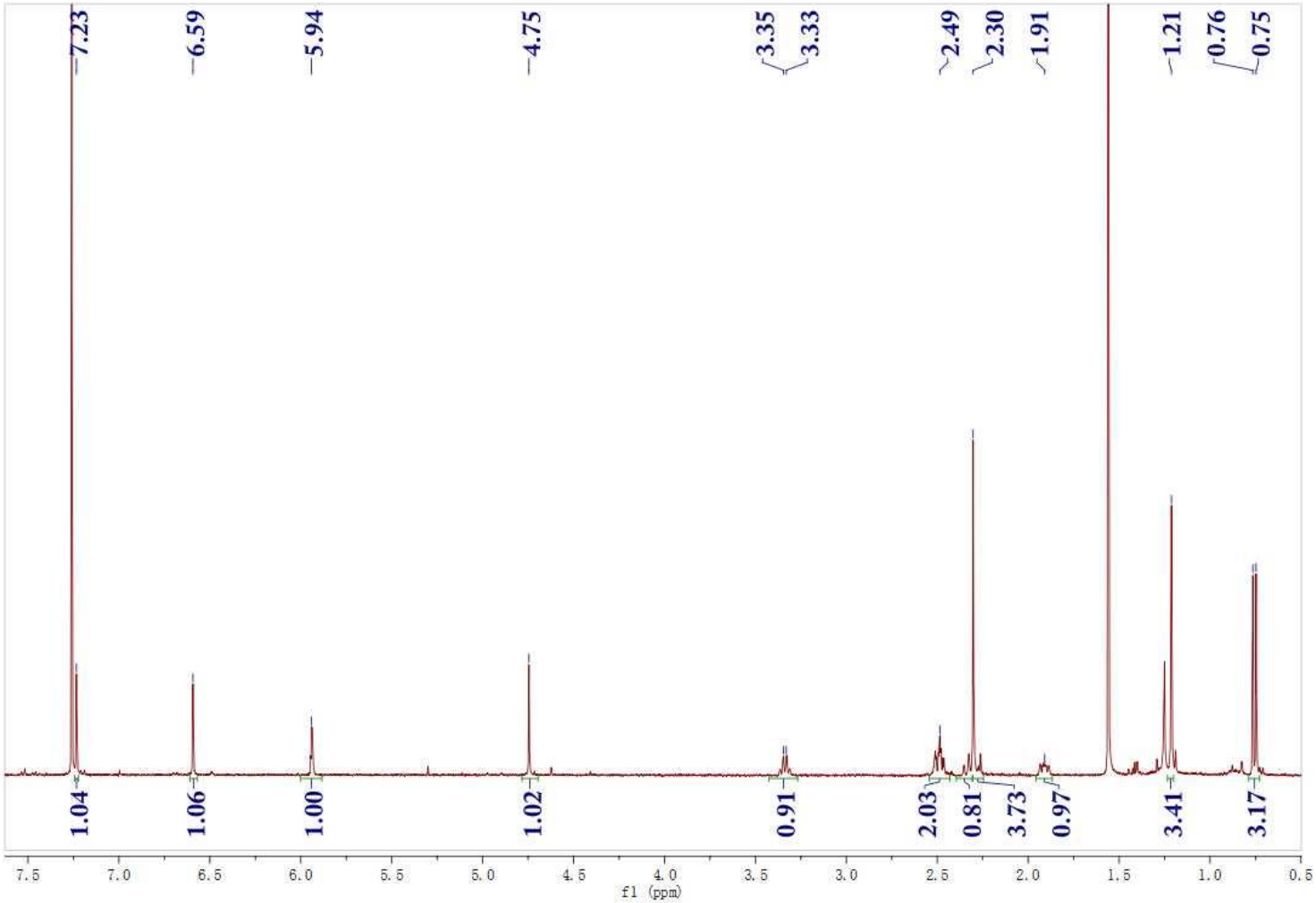


Figure S26: ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **4**.

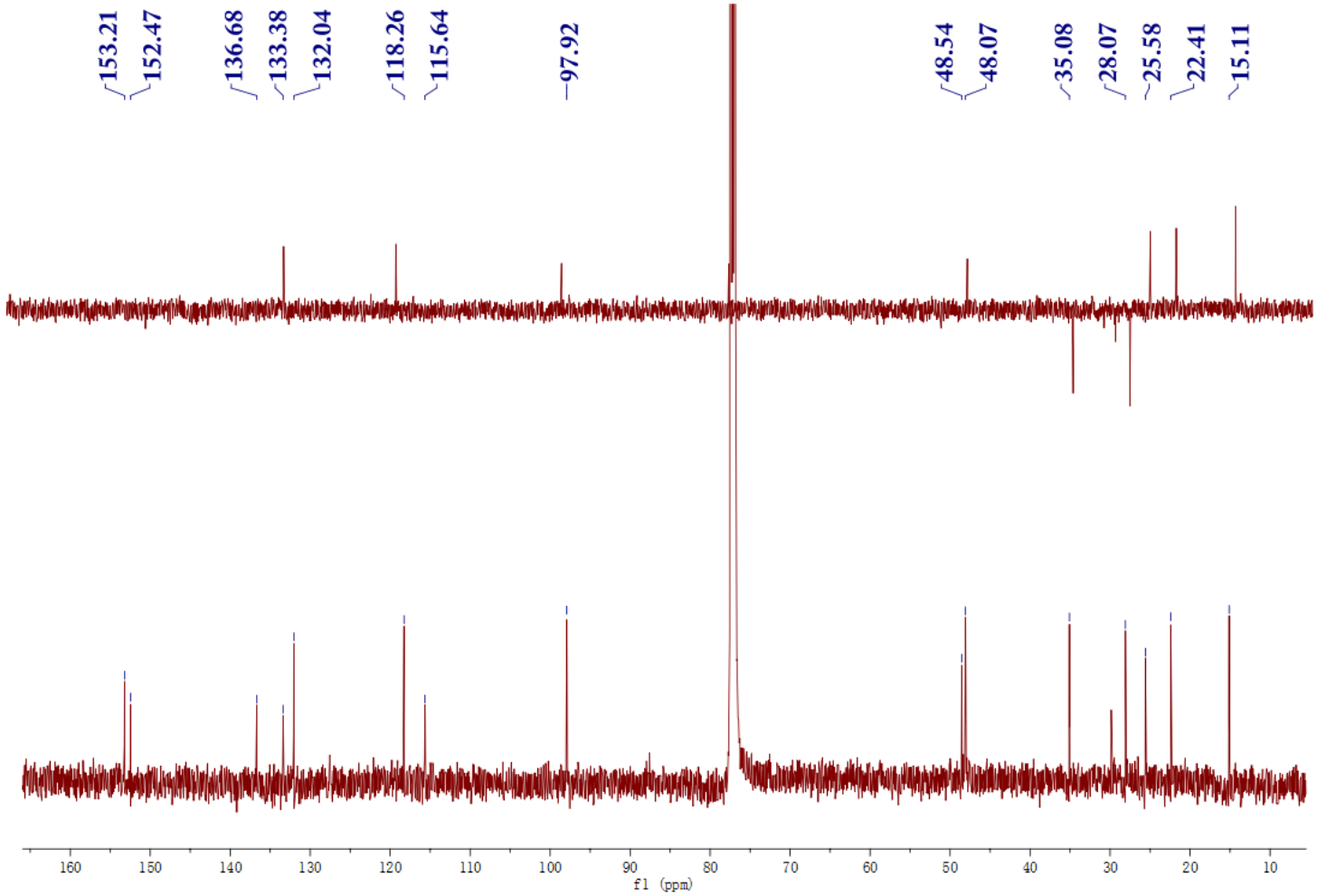


Figure S27: $^{1}H,^{1}H$ COSY spectrum (500 MHz, $CDCl_3$) of **4**.

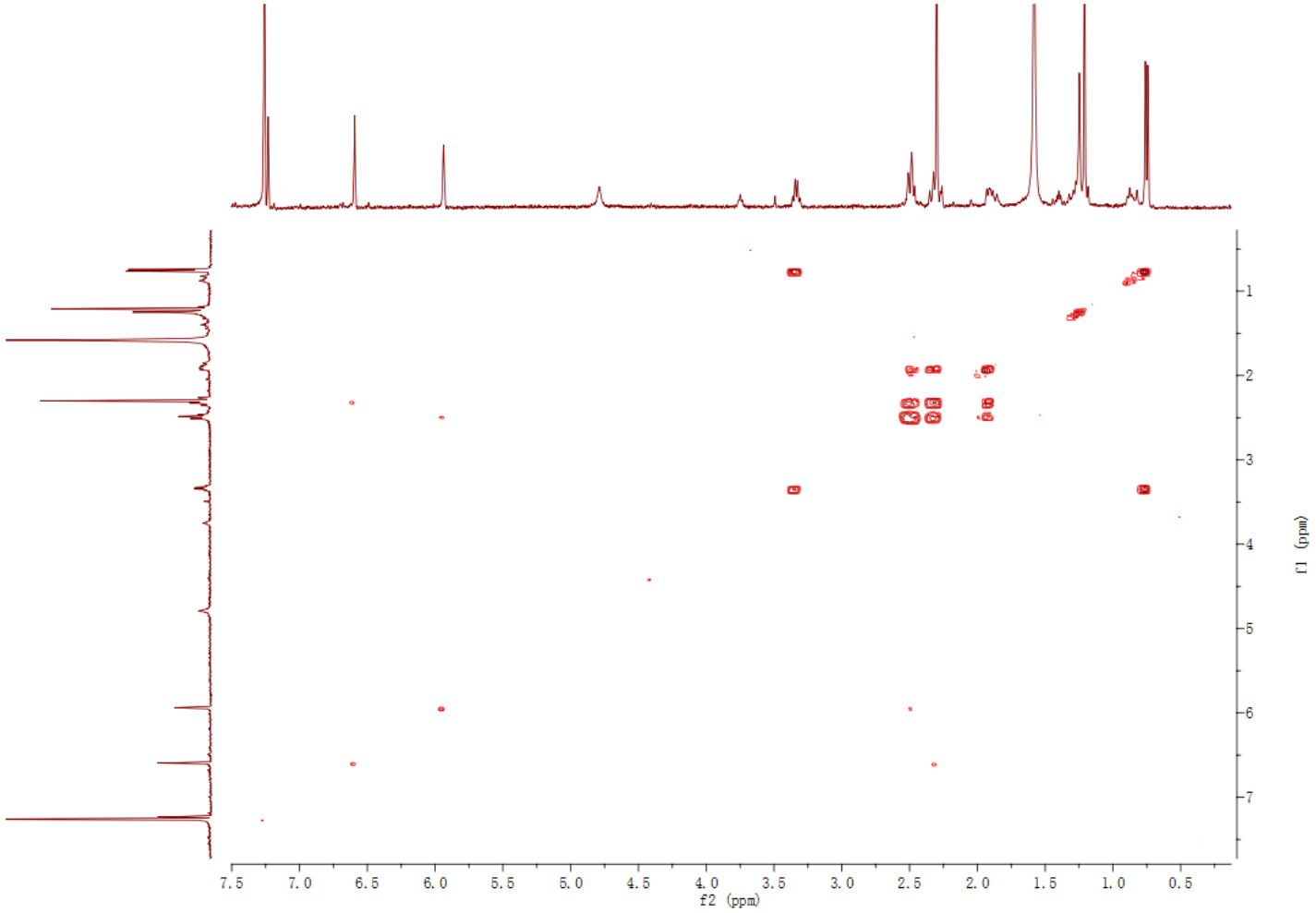


Figure S28: HMQC spectrum (500 MHz, $CDCl_3$) of **4**.

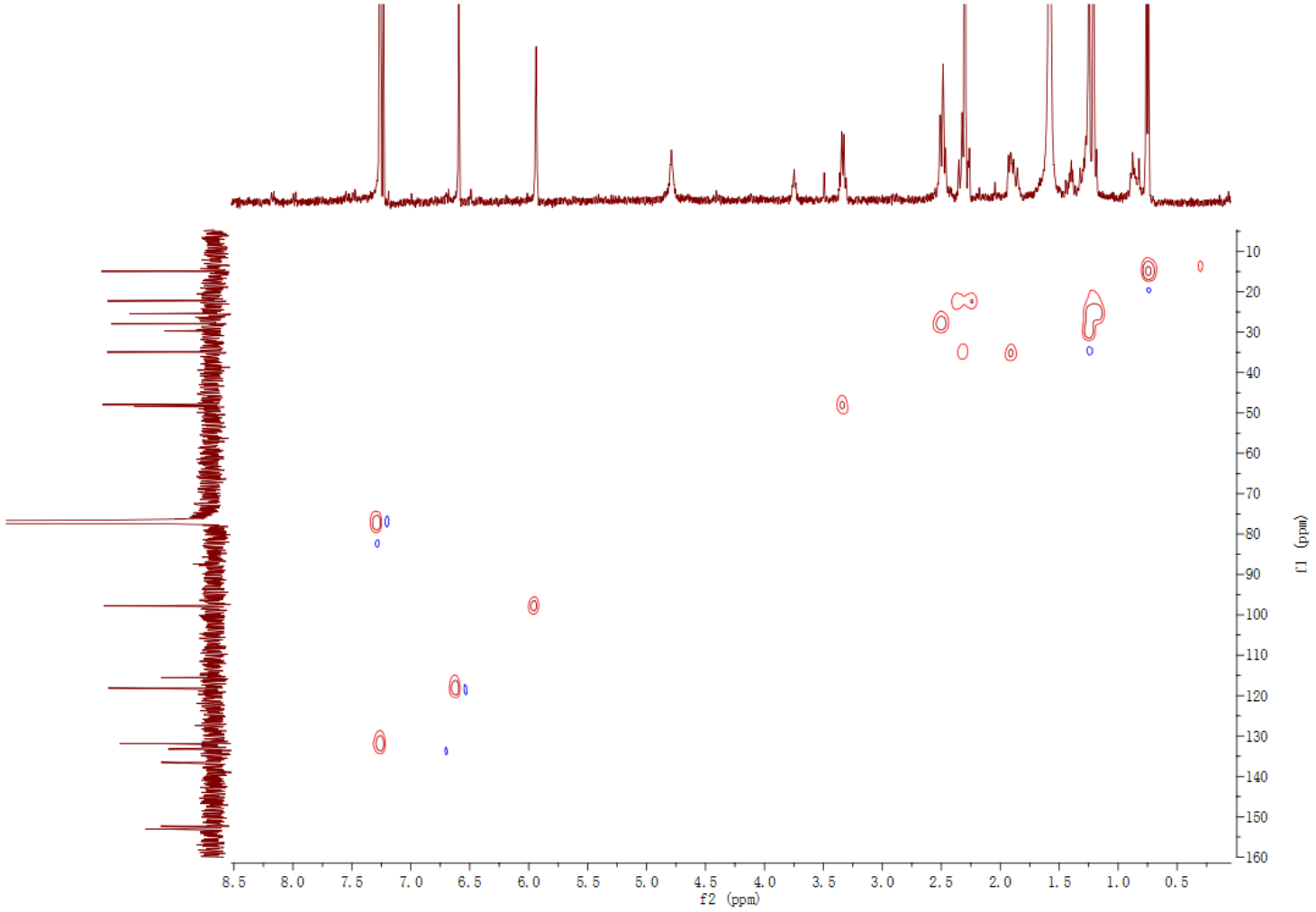


Figure S29: HMBC spectrum (500 MHz, $CDCl_3$) of **4**.

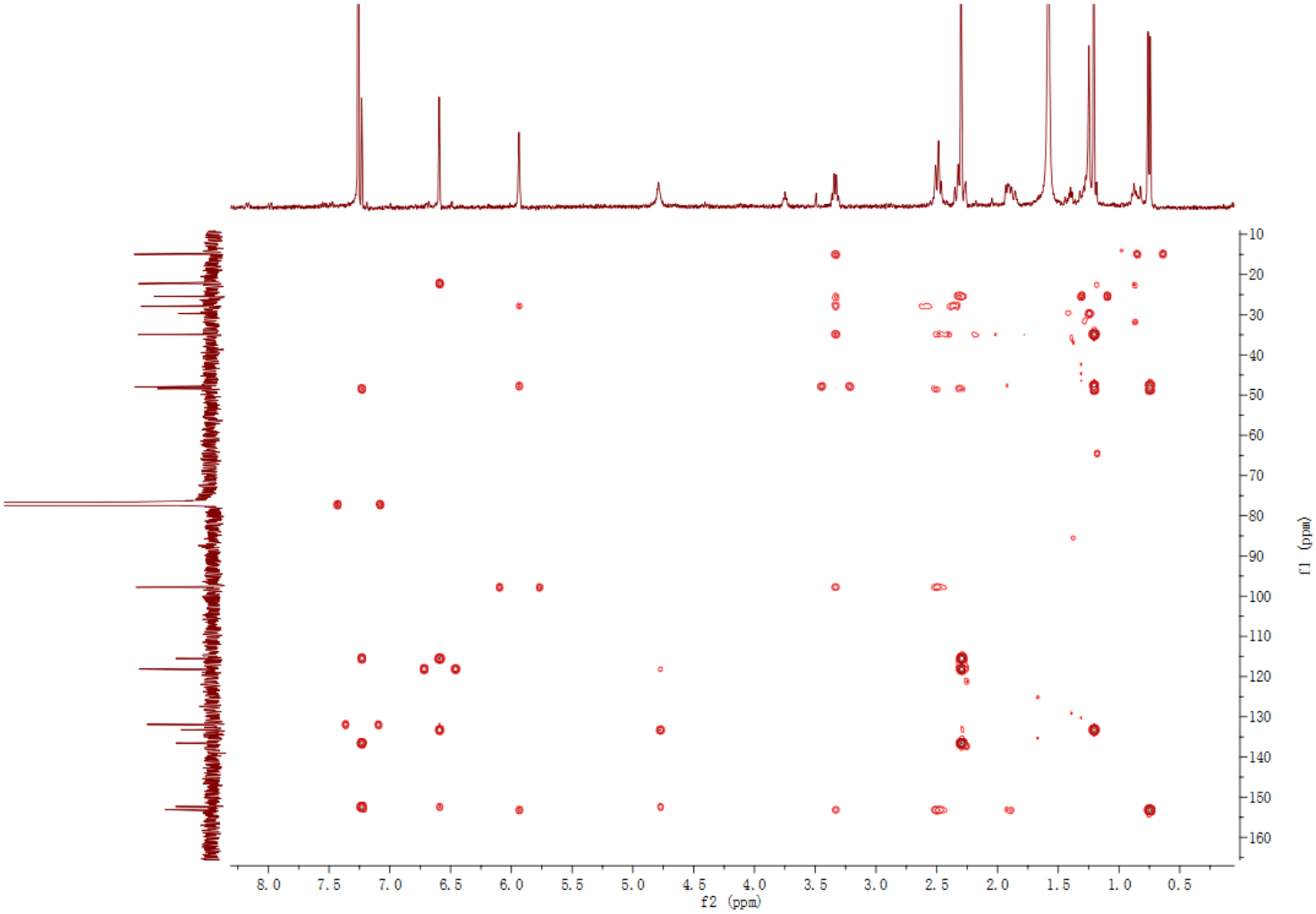


Figure S30: NOESY spectrum (500 MHz, $CDCl_3$) of **4**.

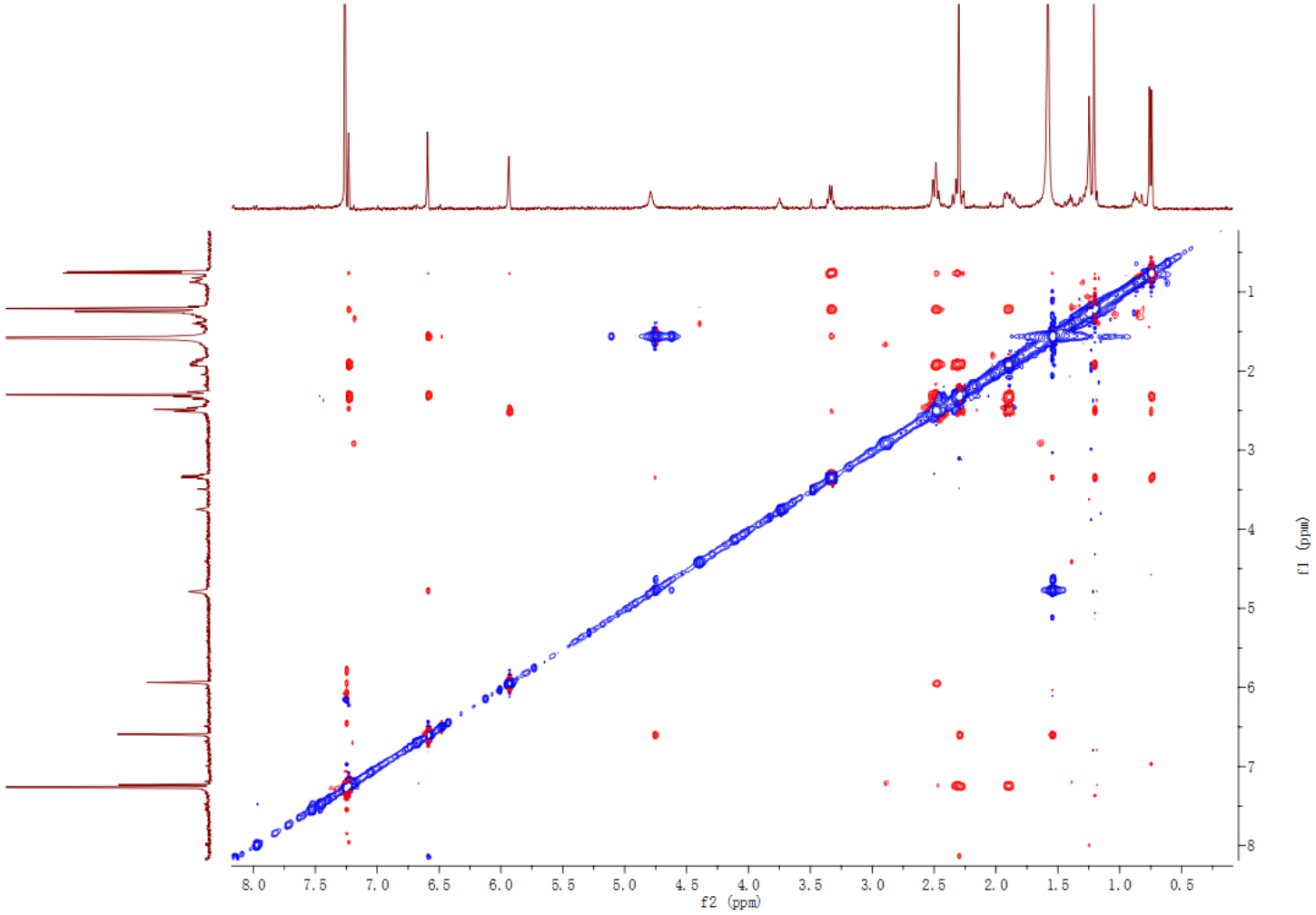


Figure S31: IR spectrum of **4**.

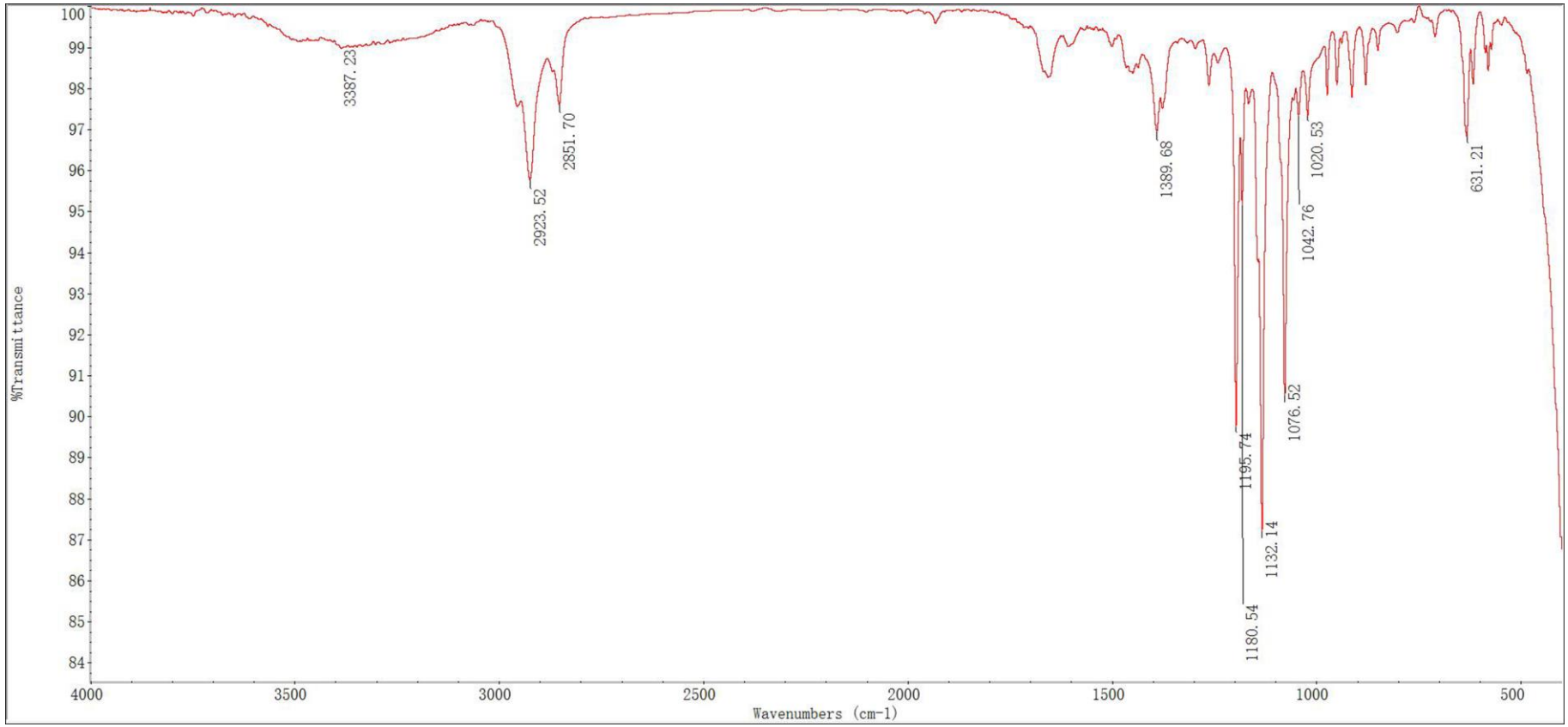


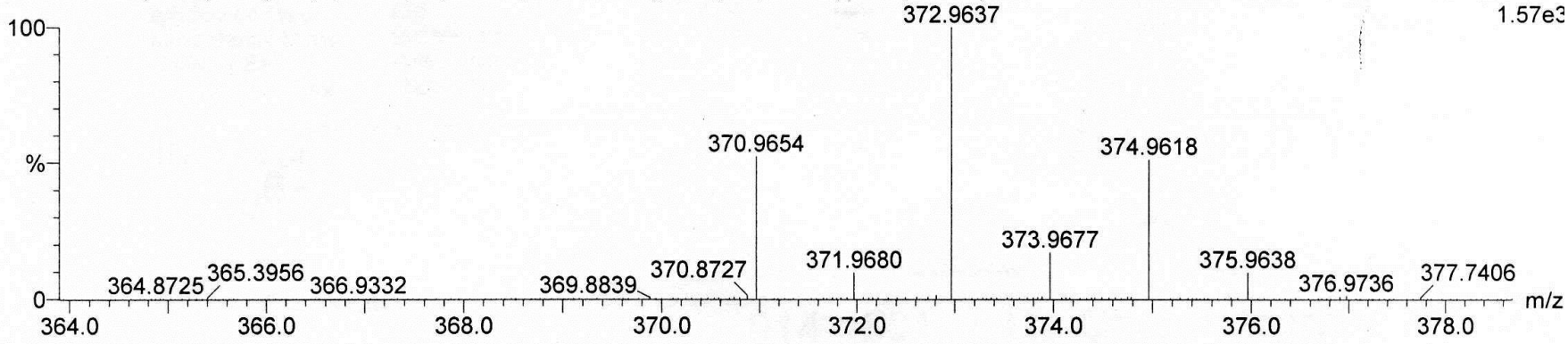
Figure S32: HR-ESIMS spectrum of **4**.

Elemental Composition Report

Multiple Mass Analysis: 3 mass(es) processed
Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
19 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

SIMM-Mass Spec Q-Tof Ultima 30-Sep-2015
D4d
151298-1 98 (1.858) AM (Cen,4, 80.00, Ht,9000.0,384.93,0.70); Sm (SG, 2x1.00); Cm (98:120) TOF MS ES-
1.57e3



Minimum:	50.00				-1.5		
Maximum:	100.00		200.0	20.0	50.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	Score	Formula
370.9654	52.30	370.9646	0.8	2.1	6.5	1	C15 H17 O Br2
372.9637	100.00	---					
374.9618	51.26	---					

Figure S33: ^{1}H NMR spectrum (500 MHz, $CDCl_3$) of **6**.

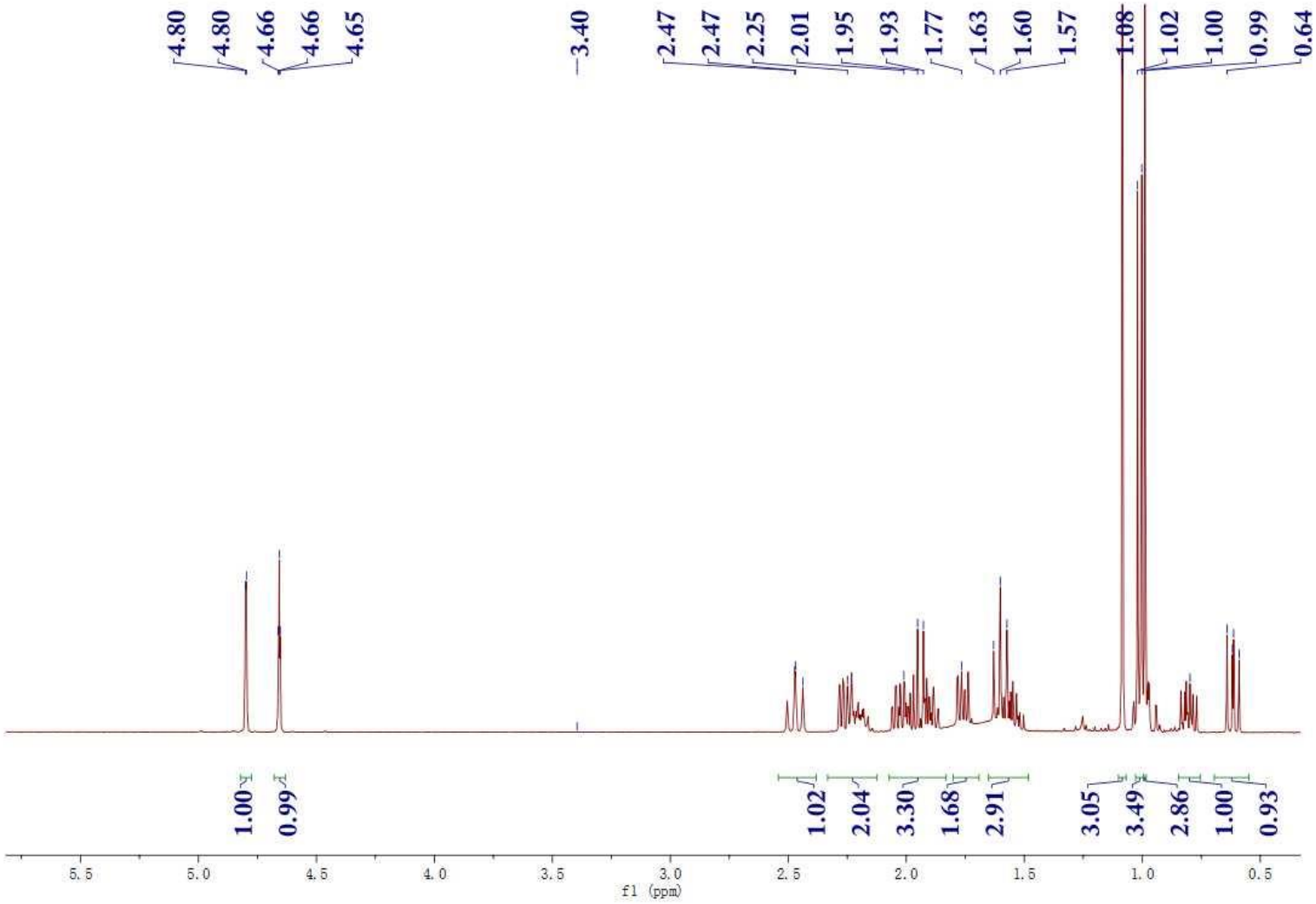


Figure S34: ^{13}C NMR spectrum (125 MHz, $CDCl_3$) of **6**.

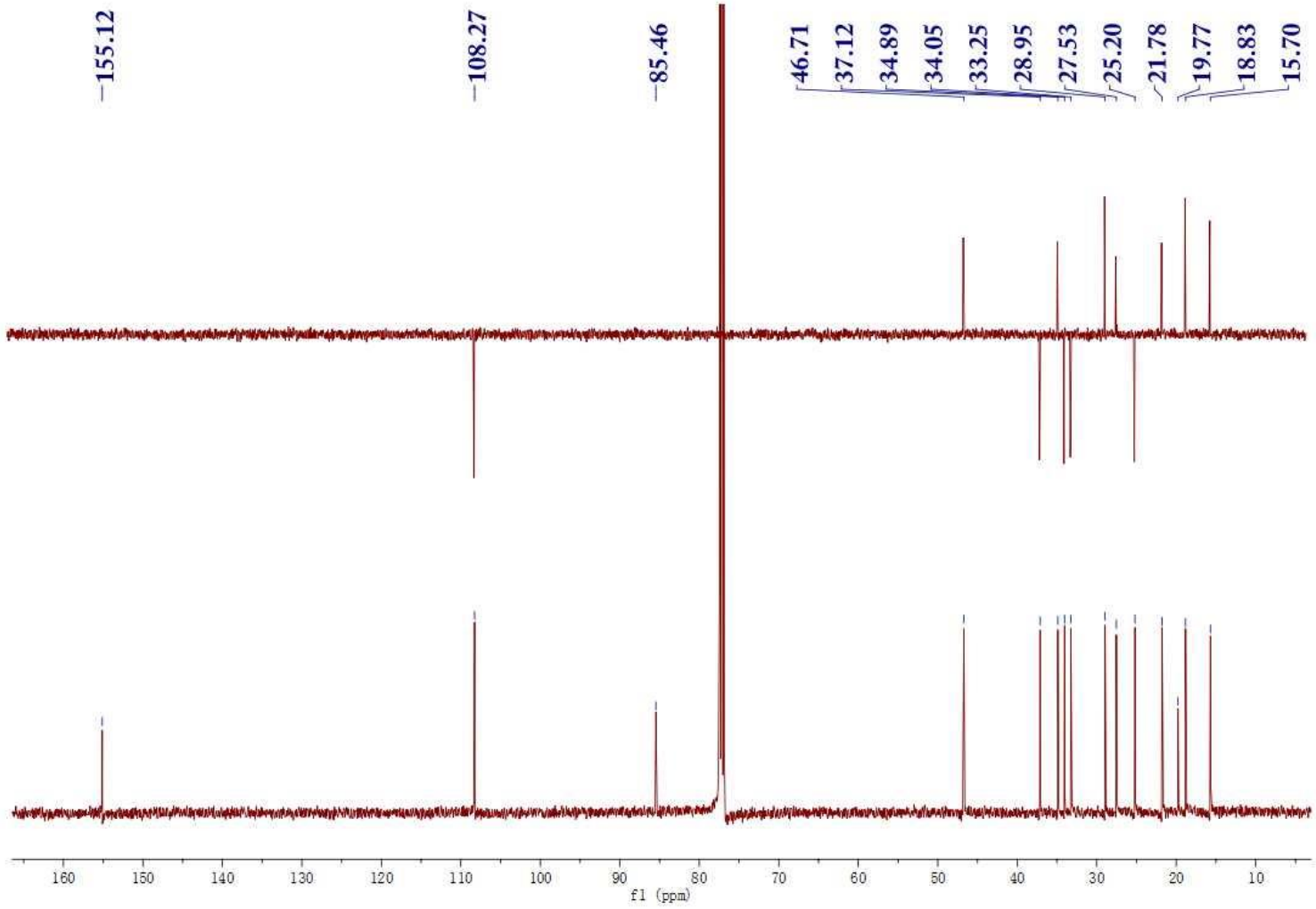


Figure S35: $^{1}H,^{1}H$ COSY spectrum (500 MHz, $CDCl_3$) of **6**.

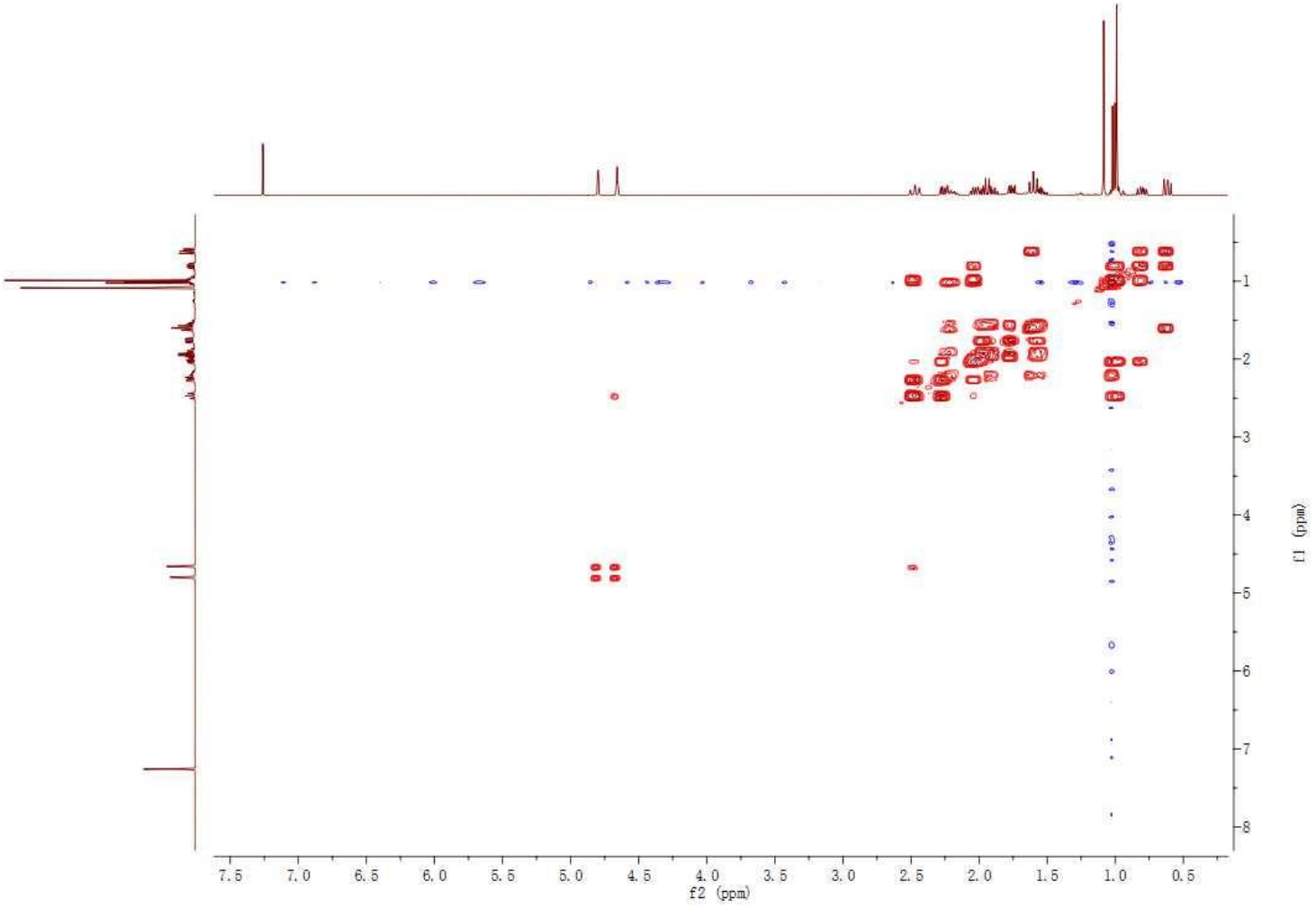


Figure S36: HMQC spectrum (500 MHz, $CDCl_3$) of **6**.

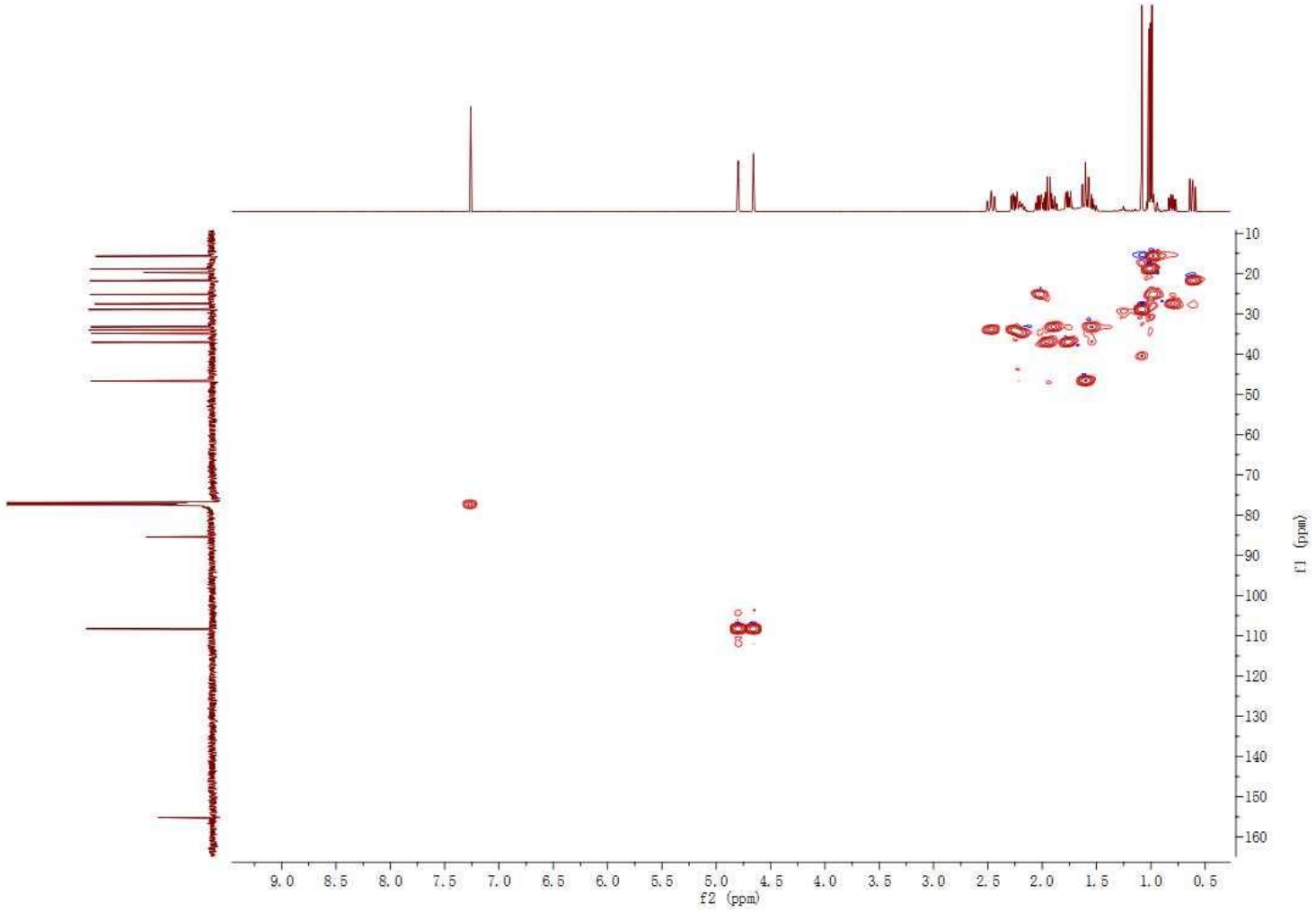


Figure S37: HMBC spectrum (500 MHz, $CDCl_3$) of **6**.

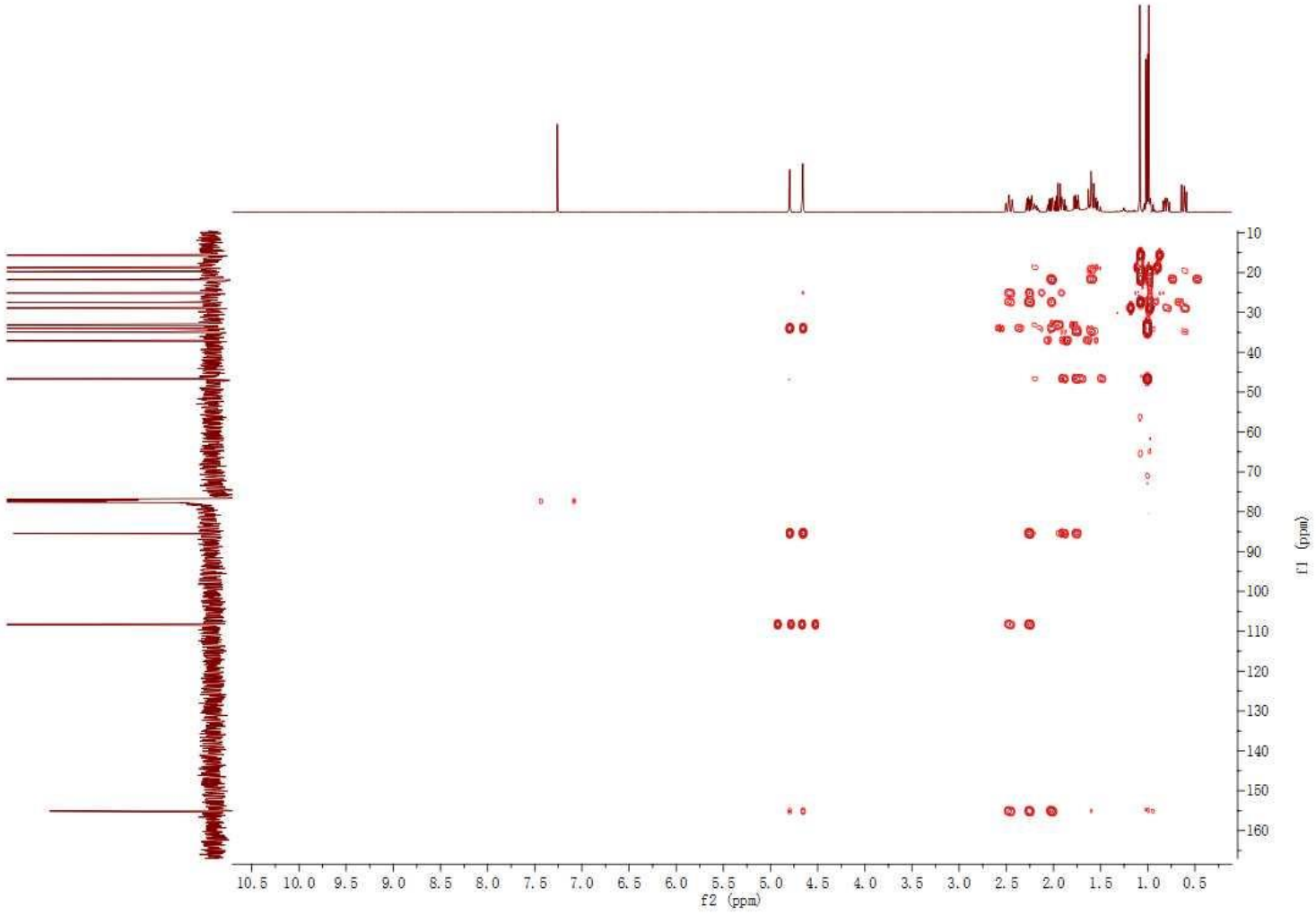


Figure S38: NOESY spectrum (500 MHz, $CDCl_3$) of **6**.

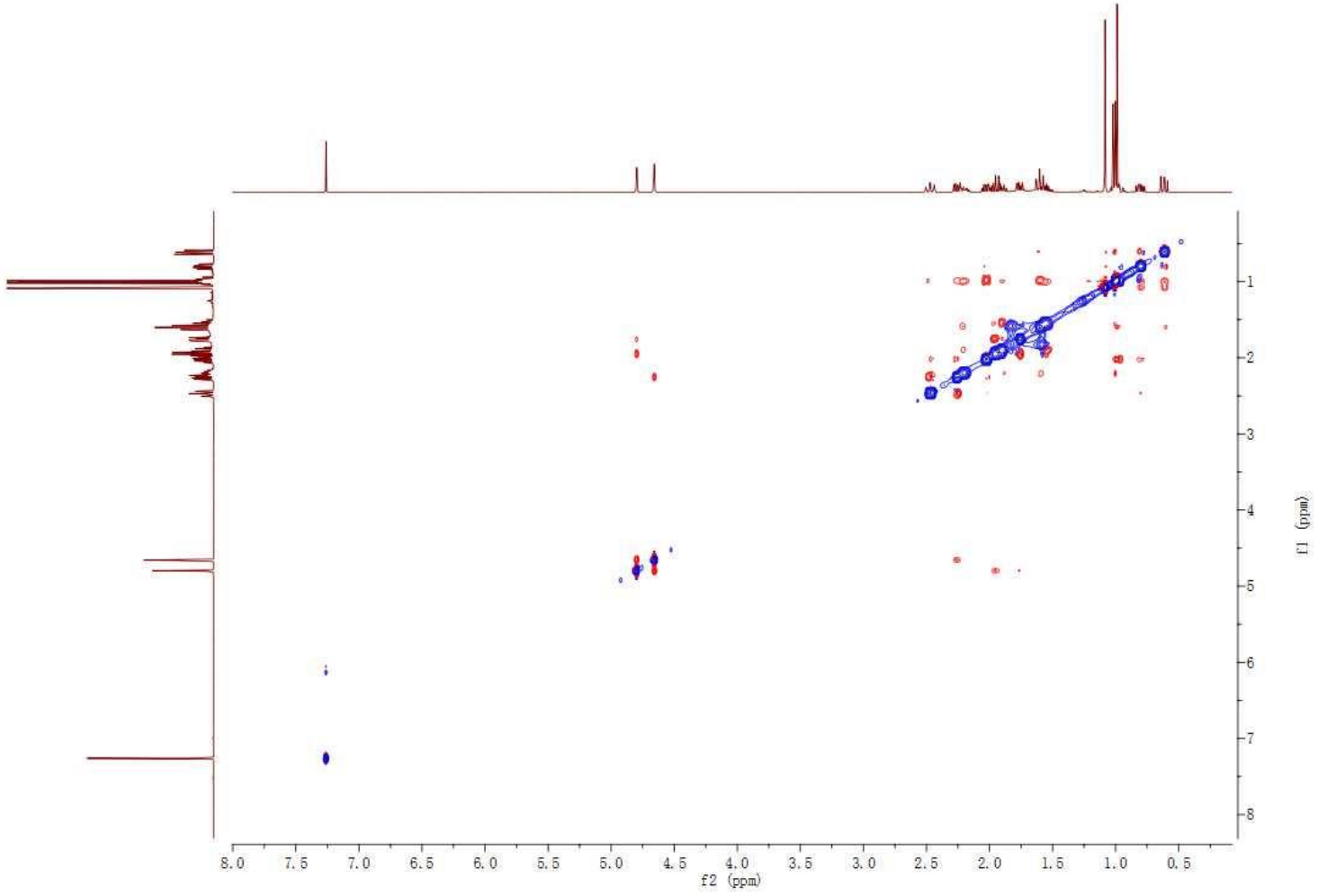


Figure S39: IR spectrum of **6**.

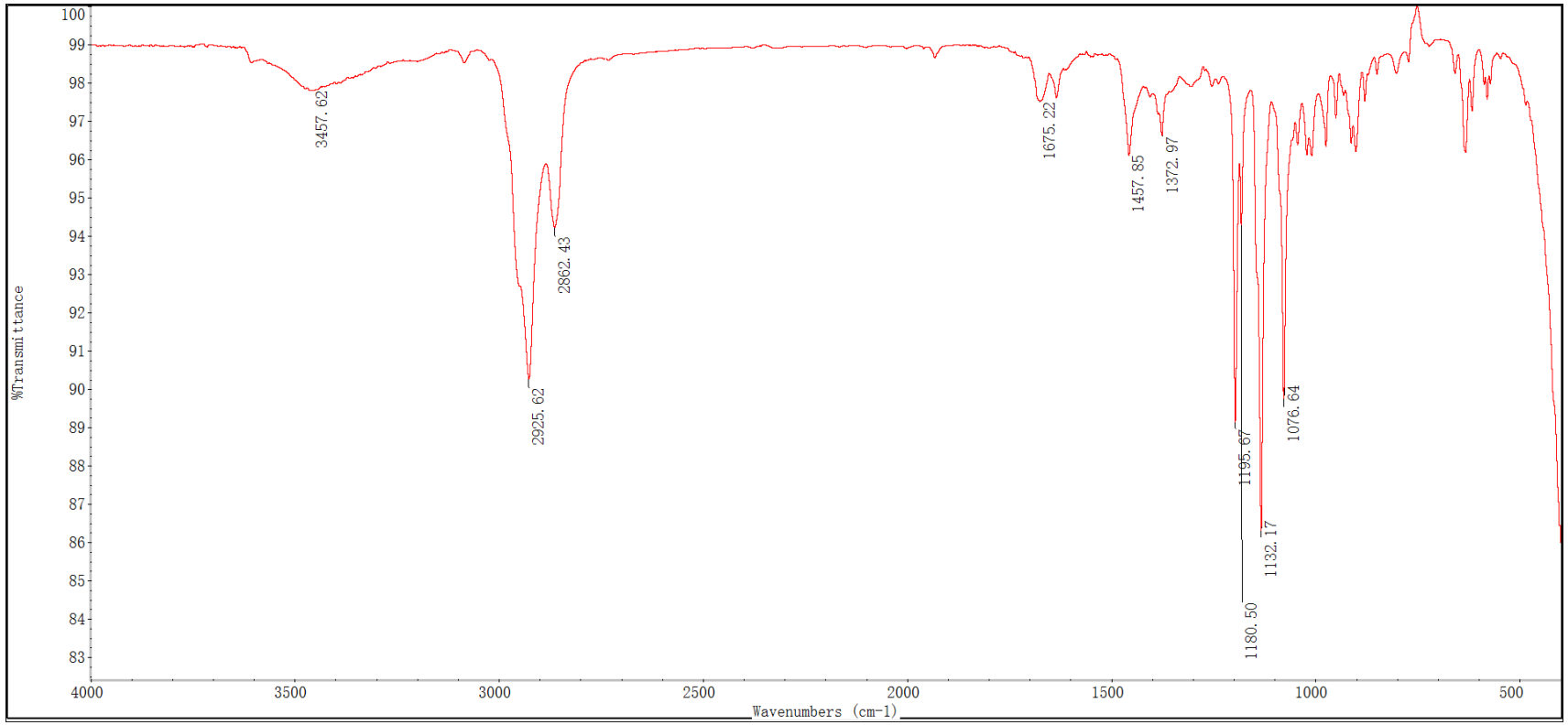


Figure S40: HR-EIMS spectrum of **6**.

LIST: h16377-c1 18-Sep-16 Elapse: 03:29.7 16
Samp: 21-F3b Start : 15:04:10 20
Comm: Finnigan/MAT95/70eV/R:10000
Mode: EI +VE +LMR BSCAN (EXP) UP HR NRM Study : S/N: PT200712-01-01
Oper: SIMM.CAS Client: S/N: PT001263 Inlet :
Limt: (0) . .
: (321) C17.H100.O
Peak: 1000.00 mmu R+D: -2.0 > 60.0
Data: CMASS : converted

	81092			(mmu)		
Mass	Intensity	%RA	%RIC	Delta	R+D	Composition
94.07697 *	114418	8.47	0.35	1.3	3.0	C7.H10
95.04998 *	168308	12.45	0.51	-0.3	3.5	C6.H7.O
95.08616 *	392362	29.03	1.20	-0.1	2.5	C7.H11
96.09313 *	165239	12.23	0.50	0.8	2.0	C7.H12
97.06499 *	94503	6.99	0.29	0.3	2.5	C6.H9.O
97.10086 *	98786	7.31	0.30	0.9	1.5	C7.H13
105.0674 *	786509	58.19	2.40			
106.0737 *	154461	11.43	0.47			
107.0463 *	84653	6.26	0.26			
107.0830 *	646823	47.86	1.97			
108.0891 *	131762	9.75	0.40			
109.0624 *	259600	19.21	0.79	3.0	3.5	C7.H9.O
109.0992 *	231620	17.14	0.71	2.6	2.5	C8.H13
115.0533 *	148393	10.98	0.45	1.5	6.5	C9.H7
117.0692 *	461027	34.11	1.40	1.3	5.5	C9.H9
118.0758 *	97430	7.21	0.30	2.5	5.0	C9.H10
119.0853 *	447680	33.12	1.36	0.8	4.5	C9.H11
120.0926 *	237830	17.60	0.72	1.3	4.0	C9.H12
121.0652 *	133832	9.90	0.41	0.2	4.5	C8.H9.O
121.1013 *	417915	30.92	1.27	0.5	3.5	C9.H13
122.0724 *	141684	10.48	0.43	0.8	4.0	C8.H10.O
122.1089 *	293219	21.70	0.89	0.7	3.0	C9.H14
123.0793 *	213847	15.82	0.65	1.7	3.5	C8.H11.O
123.1155 *	122269	9.05	0.37	1.8	2.5	C9.H15
125.0956 *	174232	12.89	0.53	1.1	2.5	C8.H13.O
128.0628 *	110492	8.18	0.34	-0.2	7.0	C10.H8
129.0699 *	141184	10.45	0.43	0.5	6.5	C10.H9
131.0864 *	642326	47.53	1.96	-0.3	5.5	C10.H11
132.0922 *	123483	9.14	0.38	1.7	5.0	C10.H12
133.1020 *	352676	26.09	1.07	-0.3	4.5	C10.H13
134.1082 *	147965	10.95	0.45	1.3	4.0	C10.H14
135.0805 *	132119	9.78	0.40	0.5	4.5	C9.H11.O
135.1166 *	214632	15.88	0.65	0.8	3.5	C10.H15
137.0962 *	134118	9.92	0.41	0.4	3.5	C9.H13.O
138.1038 *	135189	10.00	0.41	0.7	3.0	C9.H14.O
144.0939 *	88650	6.56	0.27	0.0	6.0	C11.H12
145.1017 *	654318	48.41	1.99	0.0	5.5	C11.H13
146.1076 *	205495	15.20	0.63	2.0	5.0	C11.H14
147.1169 *	270164	19.99	0.82	0.5	4.5	C11.H15
149.0965 *	252962	18.72	0.77	0.2	4.5	C10.H13.O
149.1327 *	110349	8.16	0.34	0.4	3.5	C11.H17
150.1034 *	206780	15.30	0.63	1.1	4.0	C10.H14.O
151.1124 *	343254	25.40	1.05	-0.1	3.5	C10.H15.O
159.1175 *	1351534	100.00	4.12	-0.2	5.5	C12.H15
160.1226 *	282655	20.91	0.86	2.6	5.0	C12.H16
161.1323 *	115488	8.54	0.35	0.7	4.5	C12.H17
162.1403 *	100142	7.41	0.31	0.5	4.0	C12.H18
163.1123 *	367665	27.20	1.12	0.0	4.5	C11.H15.O
164.1190 *	122198	9.04	0.37	1.1	4.0	C11.H16.O
173.1331 *	84582	6.26	0.26	0.0	5.5	C13.H17
177.1277 *	442540	32.74	1.35	0.2	4.5	C12.H17.O
178.1343 *	101927	7.54	0.31	1.5	4.0	C12.H18.O
187.1492 *	576802	42.68	1.76	-0.5	5.5	C14.H19
191.1438 *	132548	9.81	0.40	-0.2	4.5	C13.H19.O
202.1720 *	551748	40.82	1.68	0.2	5.0	C15.H22
205.1585 *	273661	20.25	0.83	0.7	4.5	C14.H21.O
220.1824 *	240756	17.81	0.73	0.3	4.0	C15.H24.O