Biscembranoids and cembranoids from the South China Sea Soft Coral *Sarcophyton elegans*

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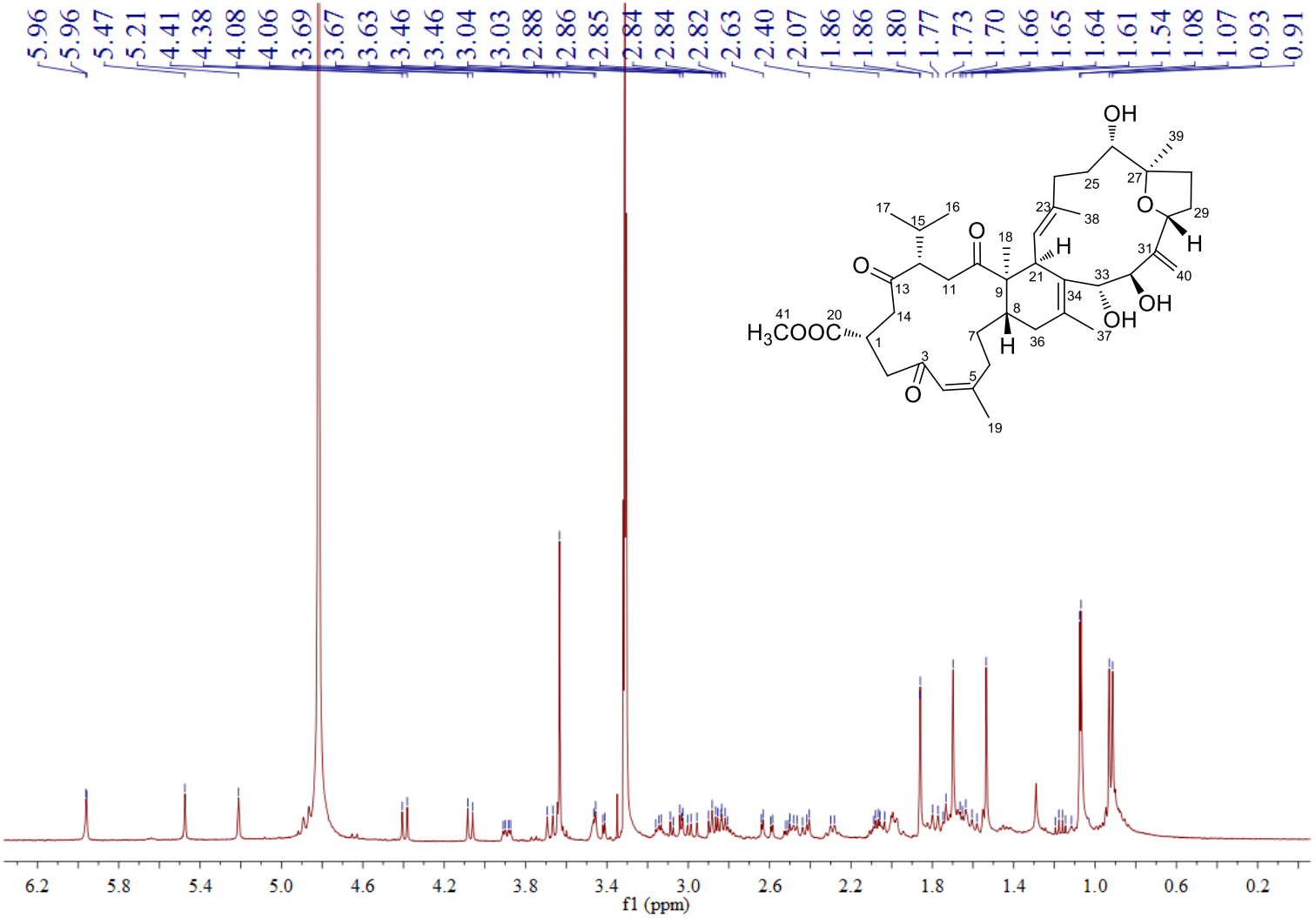
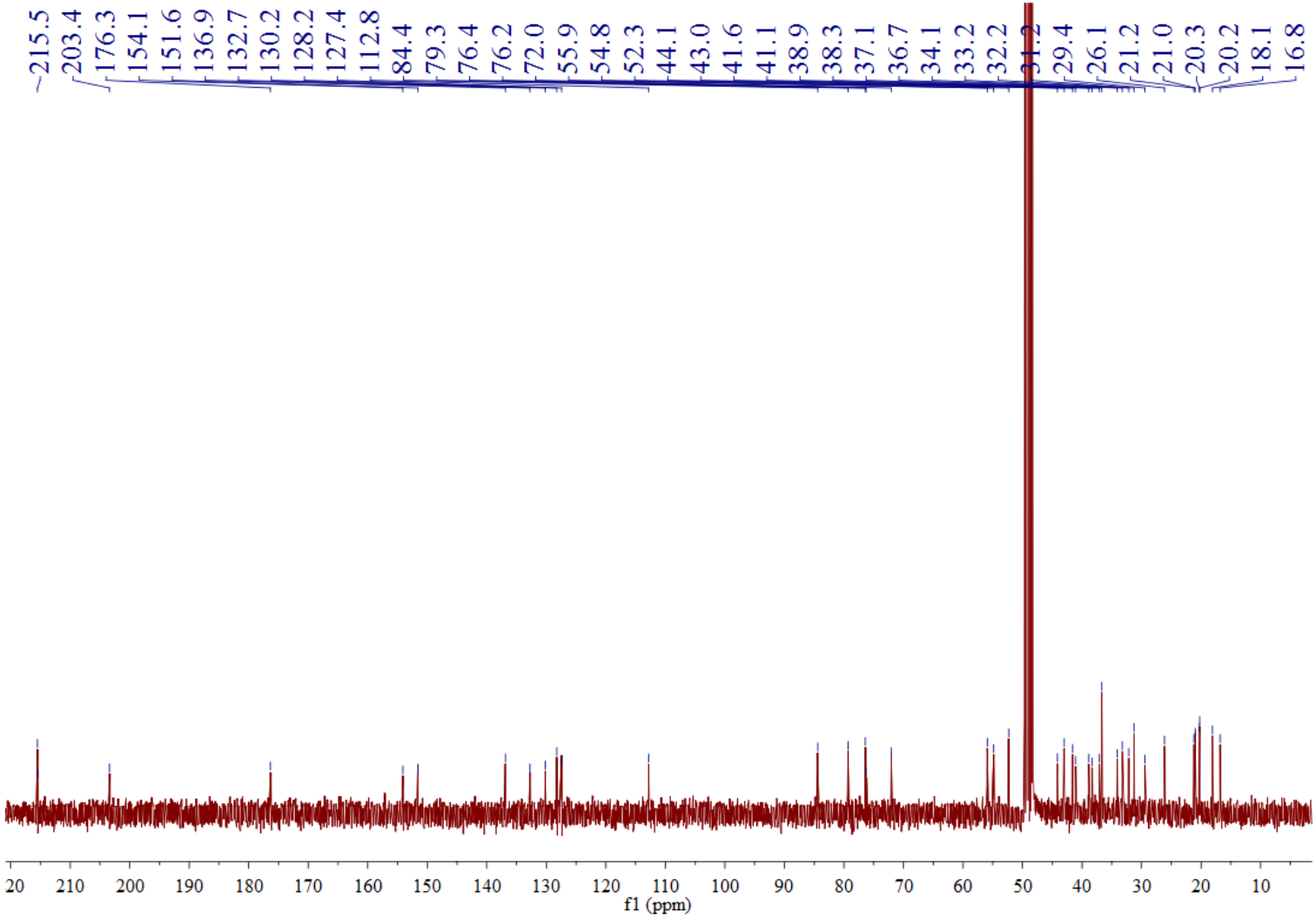
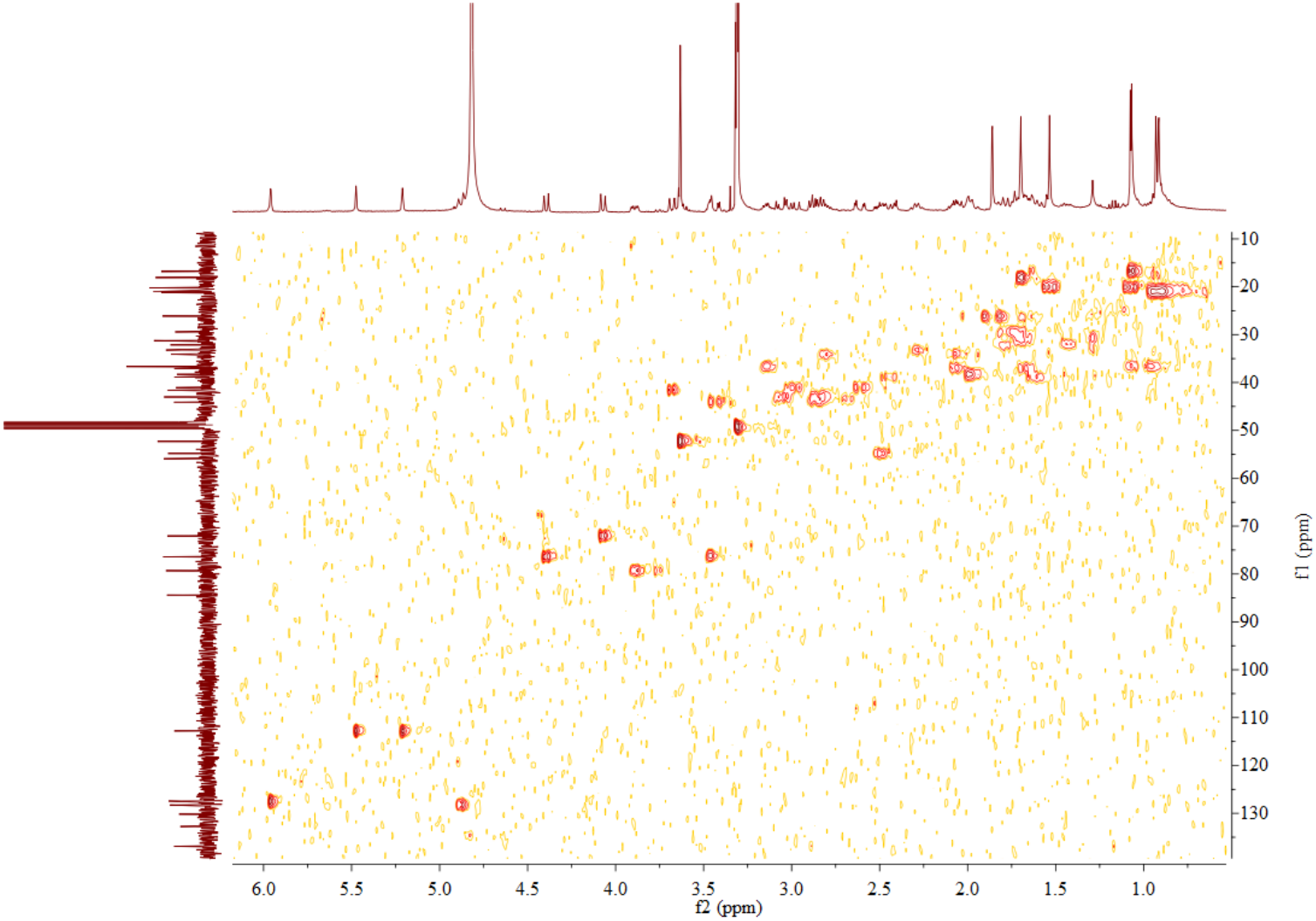


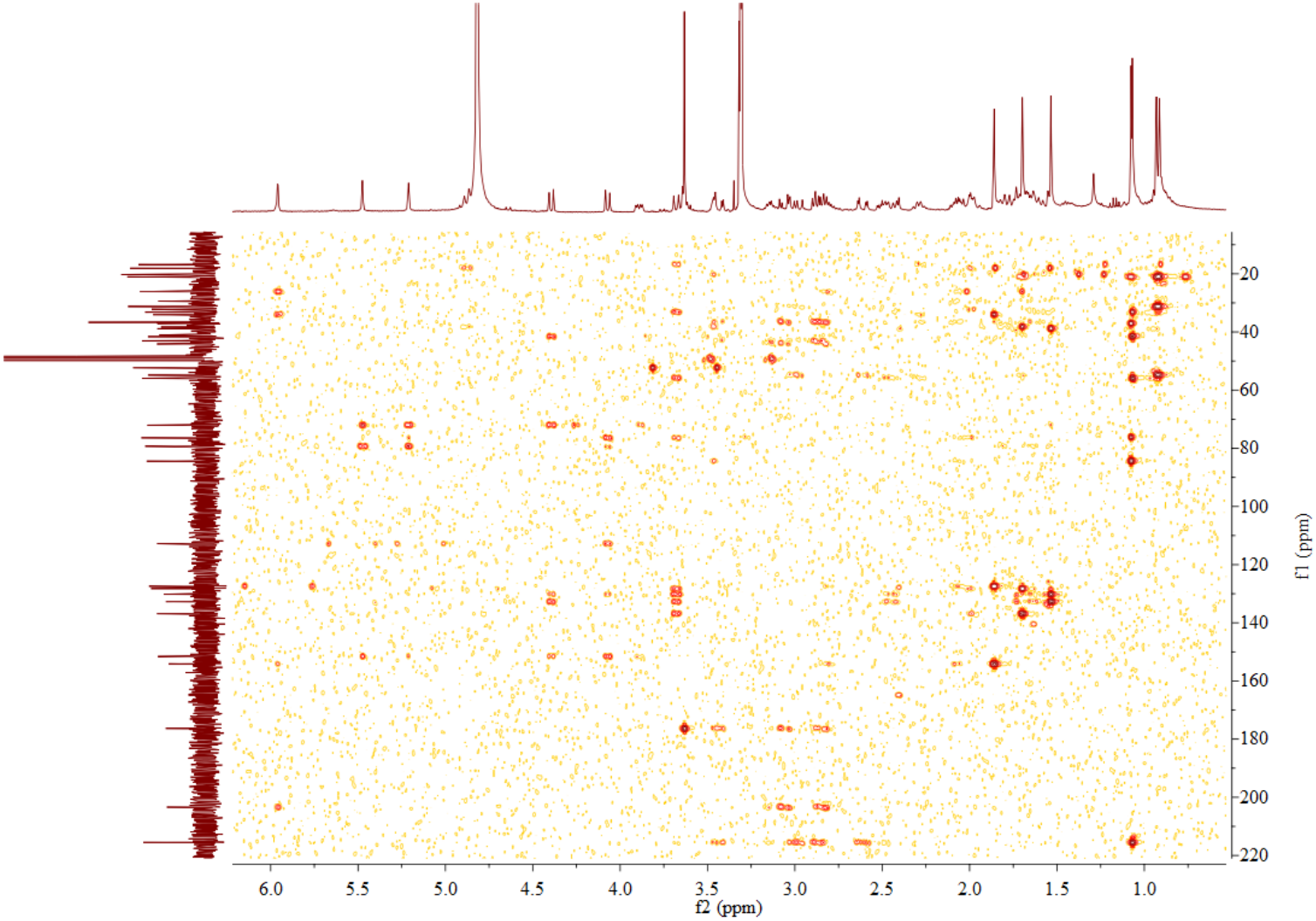
S2 ^{13}C NMR spectrum of **1** in Methanol-d_4



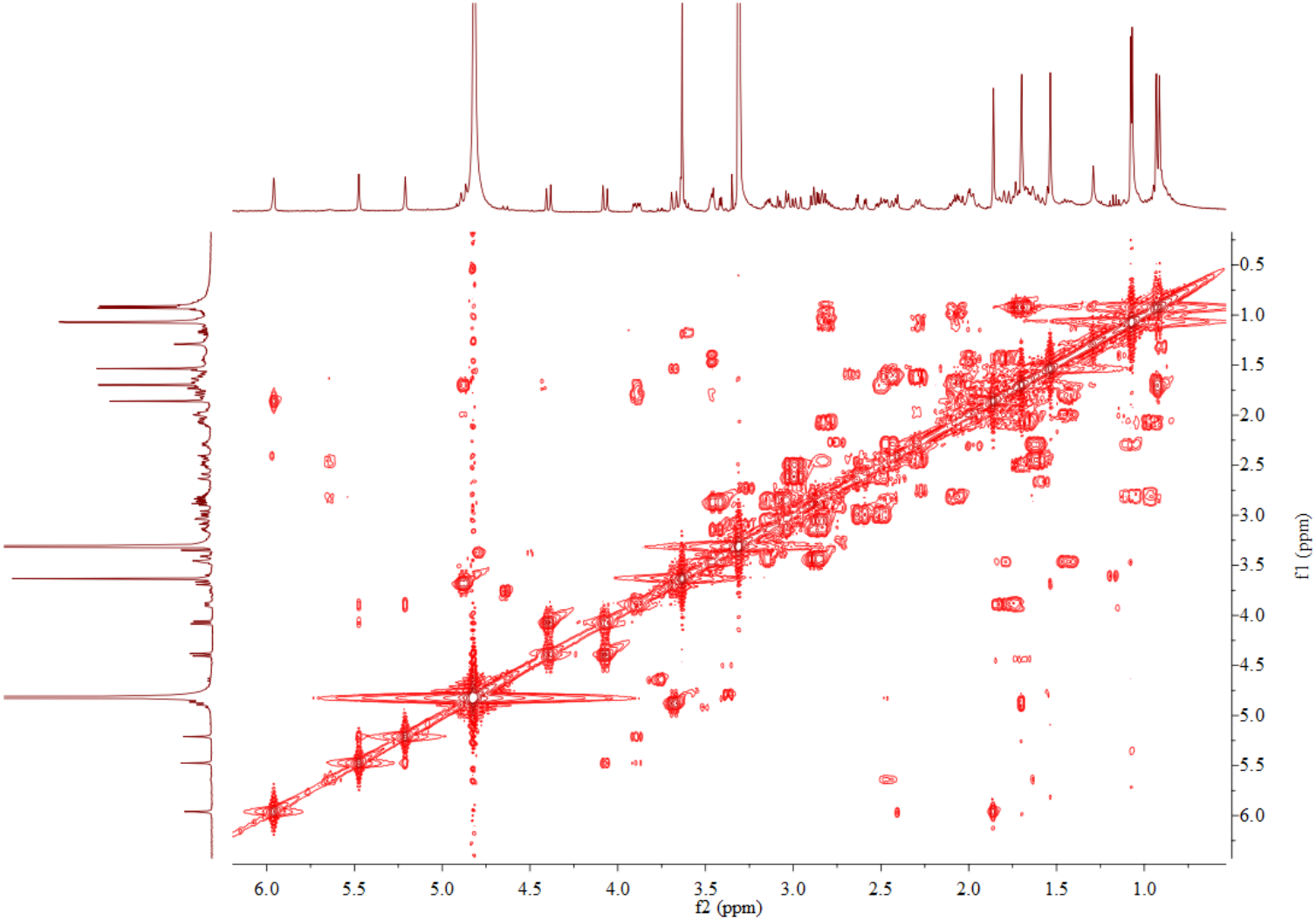
S3 HSQC spectrum of **1** in Methanol-d_4



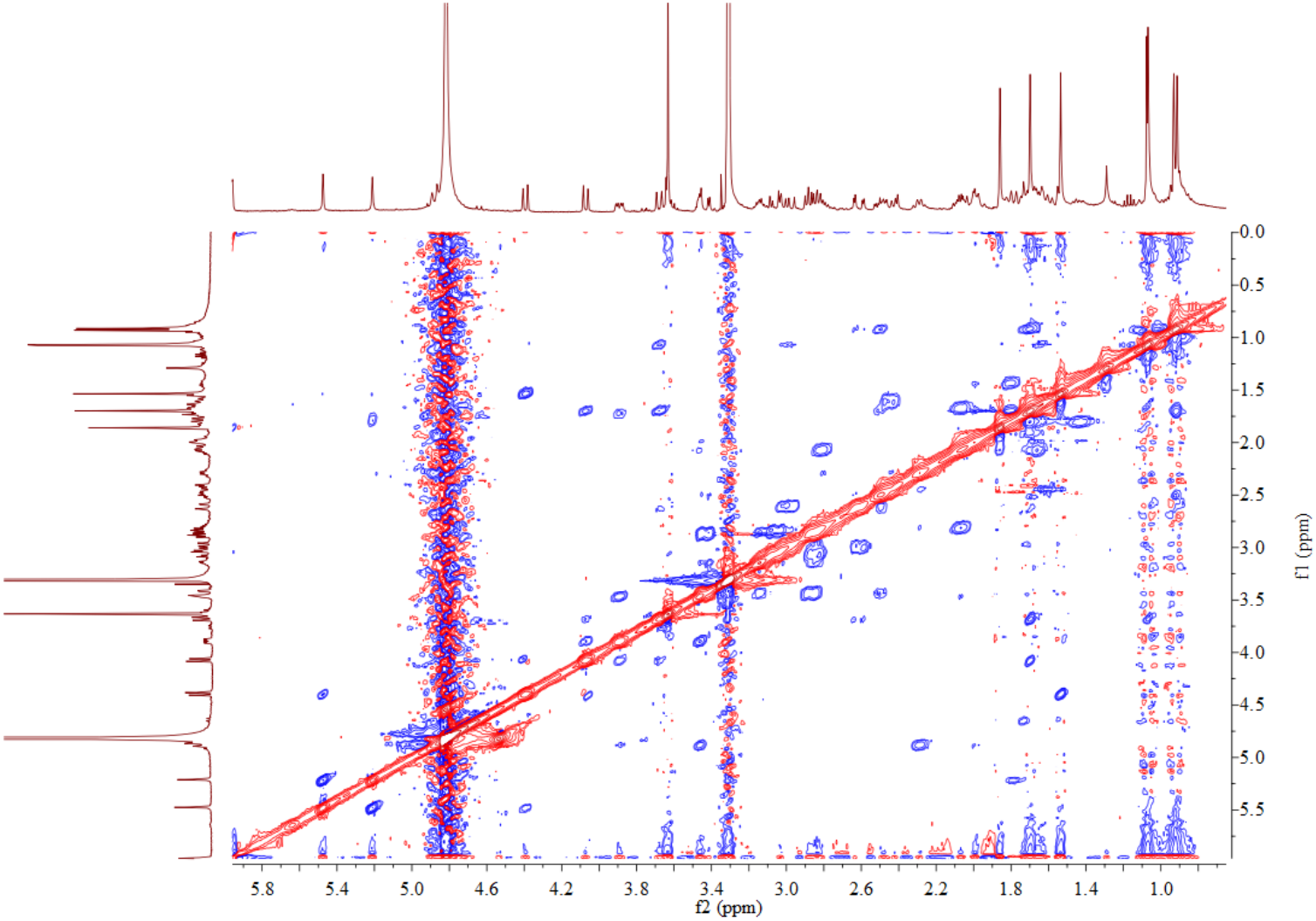
S4 HMBC spectrum of **1** in Methanol-d_4



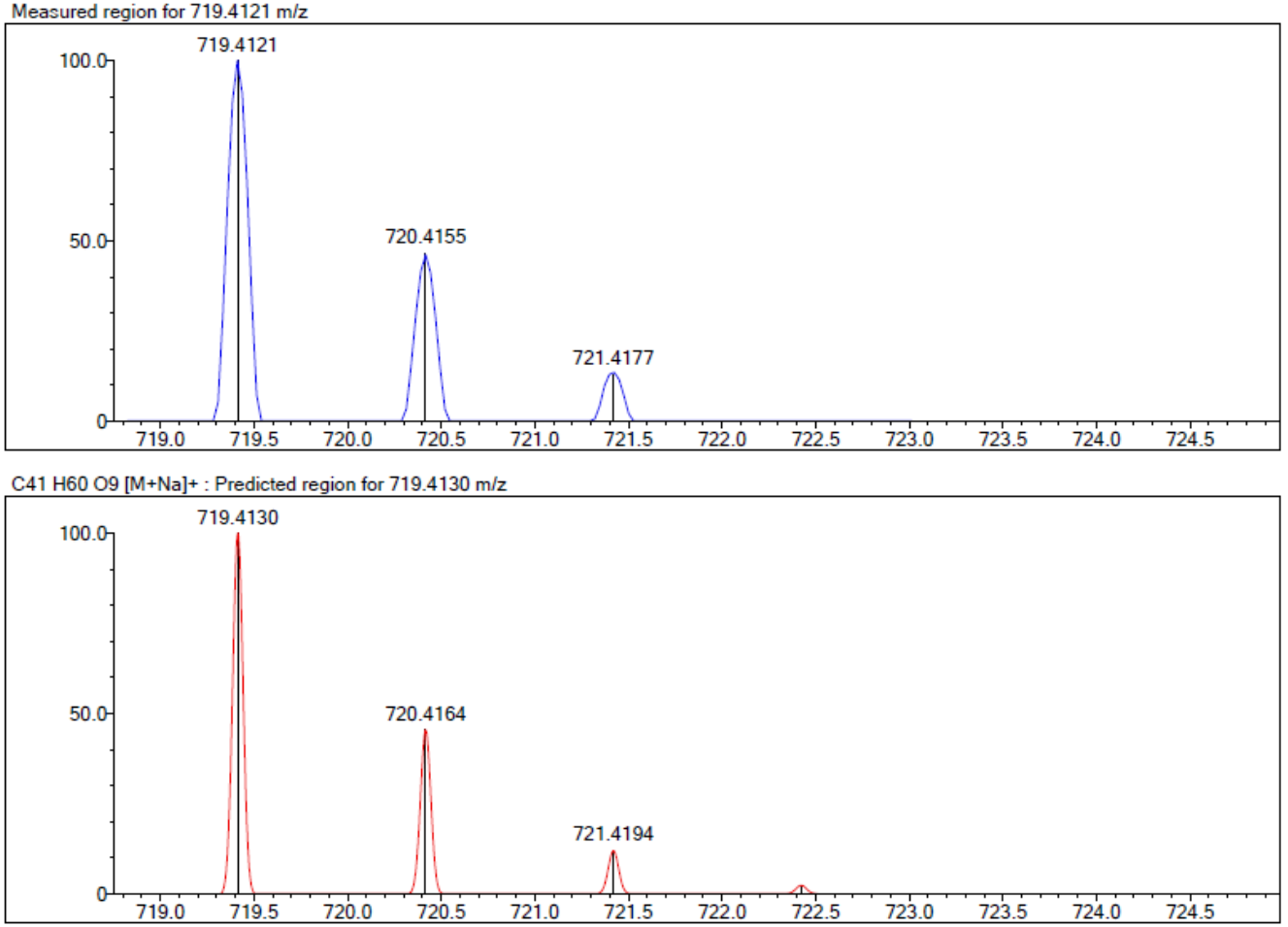
S5 $^{1}H–^{1}H$ COSY spectrum of **1** in Methanol-d_4



S6 NOESY spectrum of **1** in Methanol-d_4

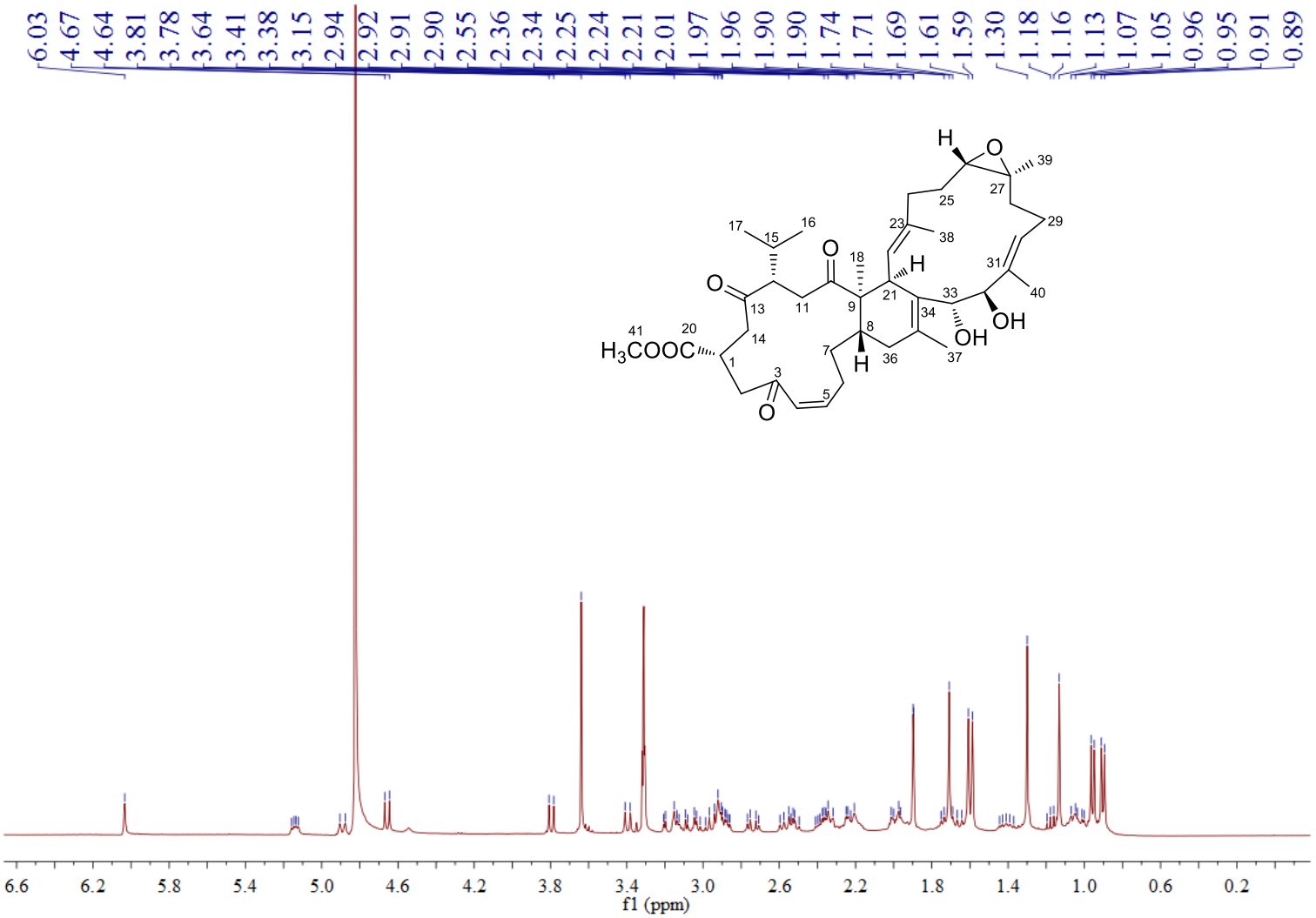


S7 HRESIMS spectrum of **1**

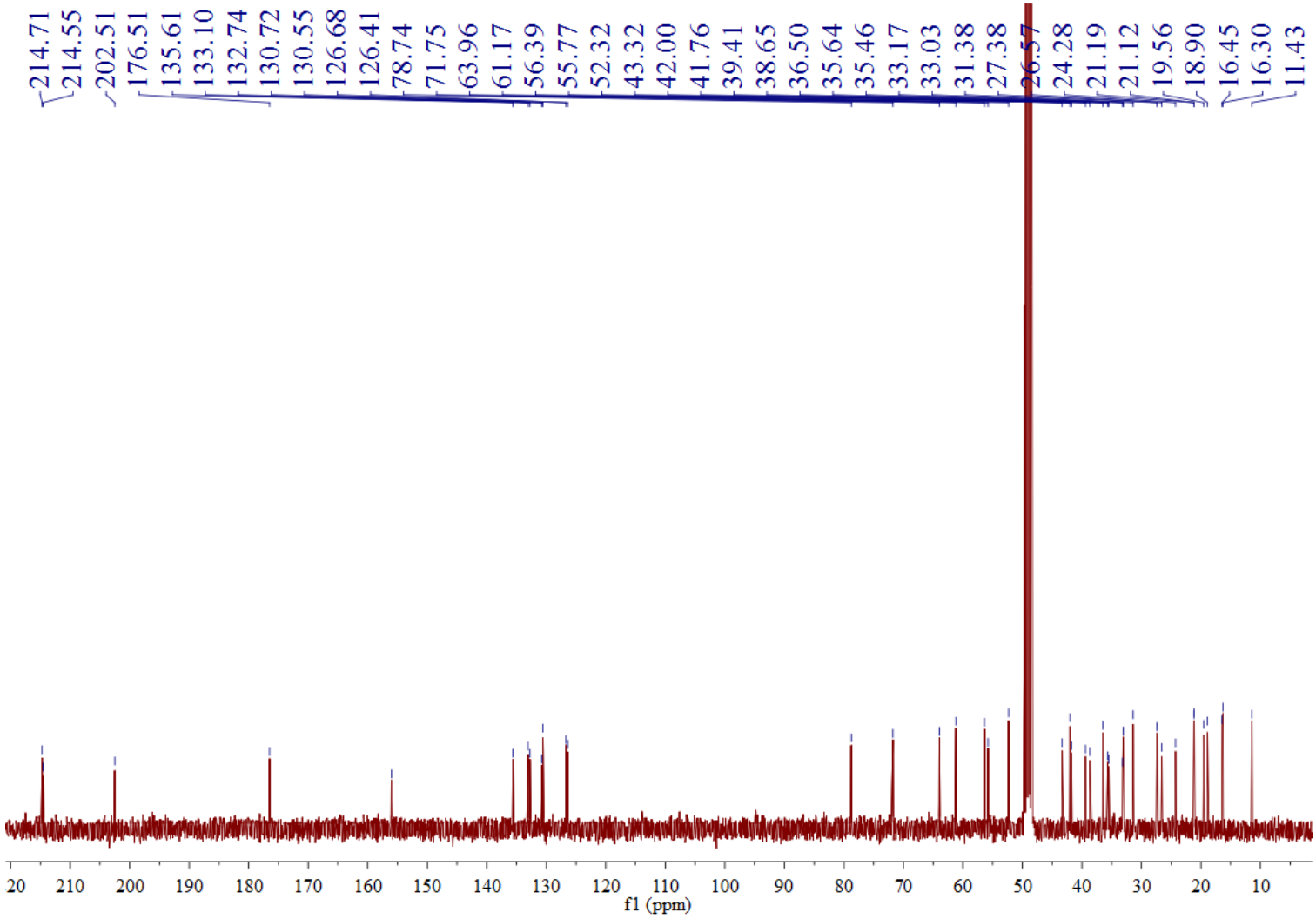


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	99.38	C41 H60 O9	[M+Na]+	719.4121	719.4130	-0.9	-1.25	100.00	12.0

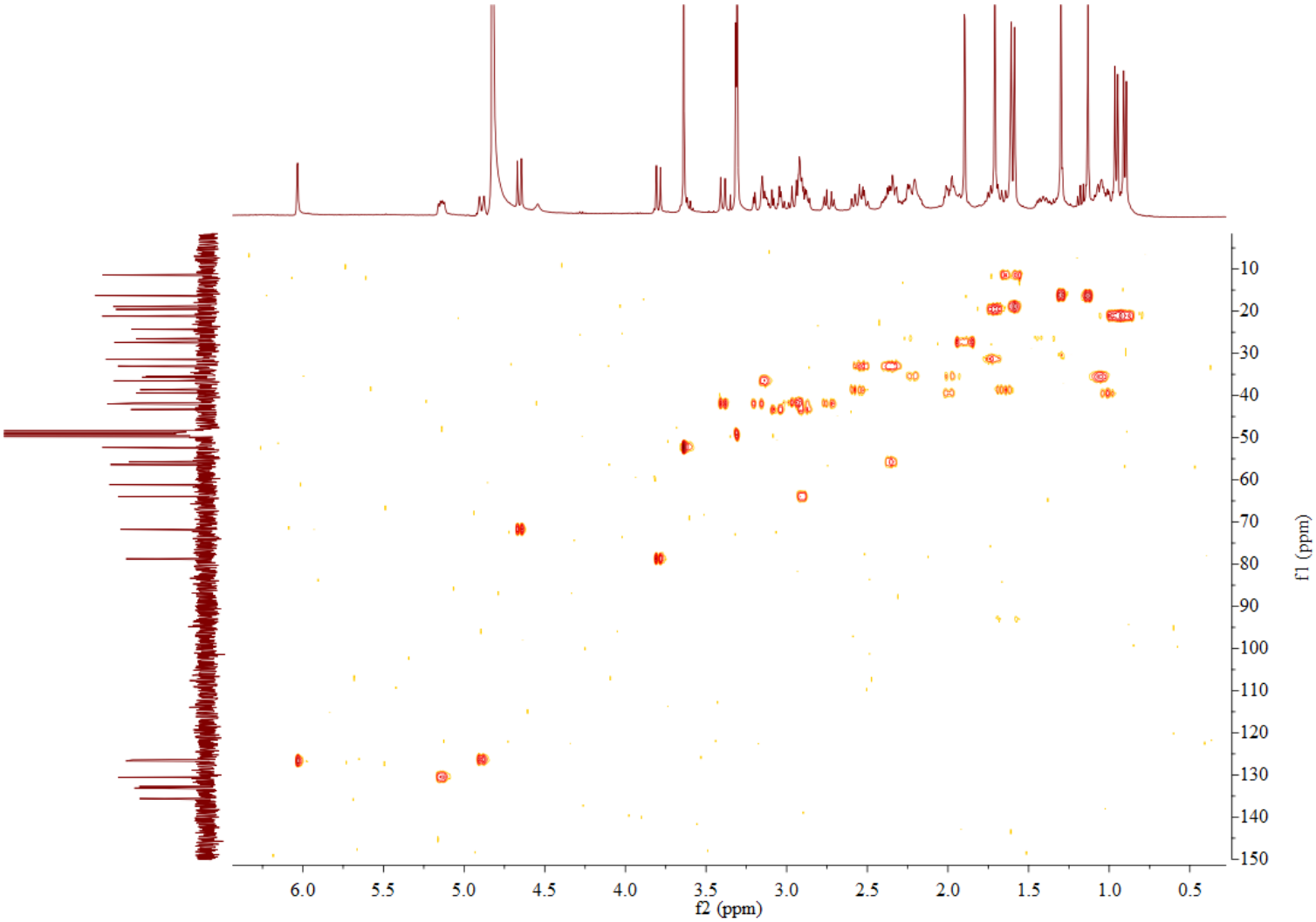
S8 ^{1}H NMR spectrum of **2** in Methanol-d_4



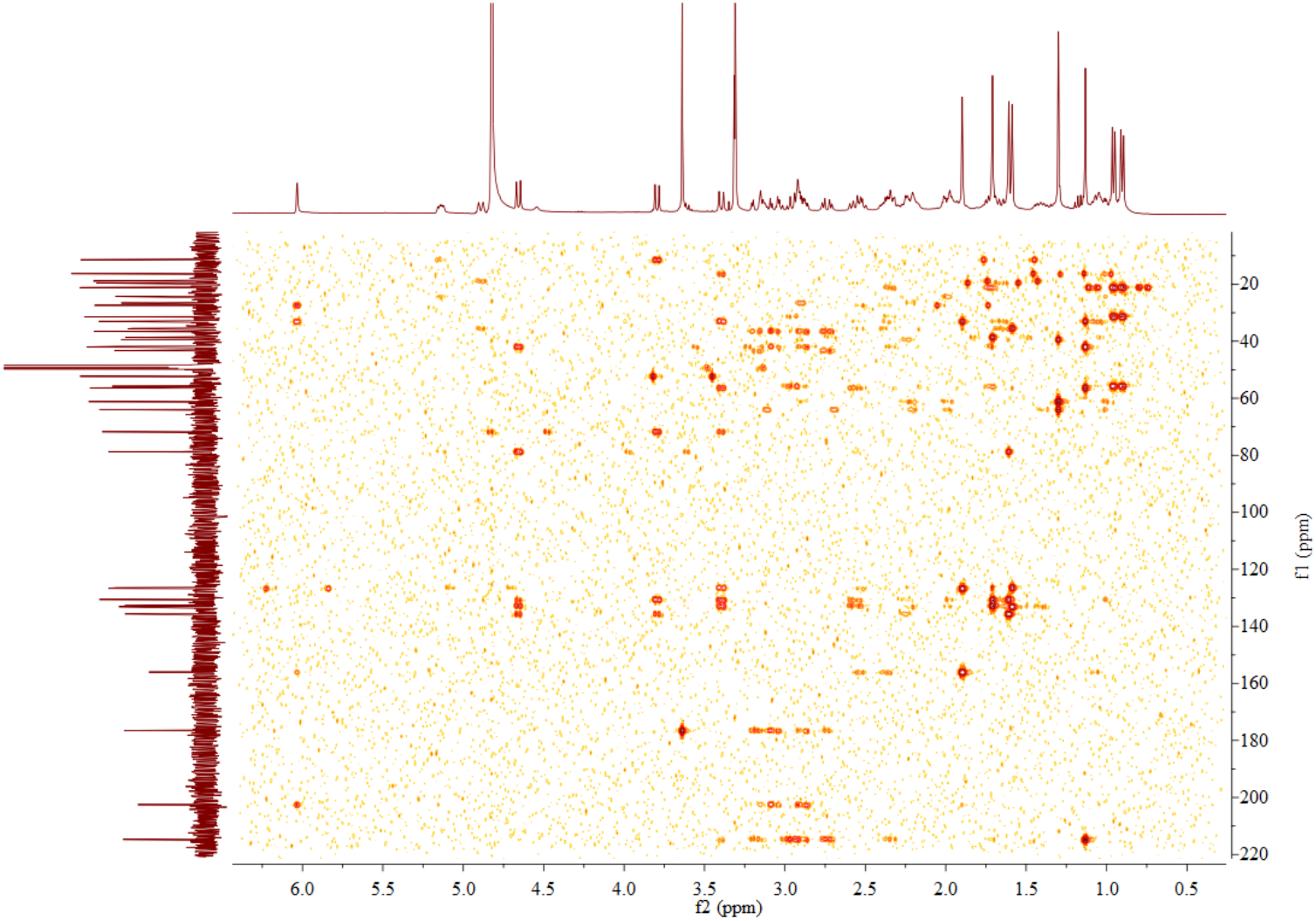
S9 ^{13}C NMR spectrum of **2** in Methanol-d_4



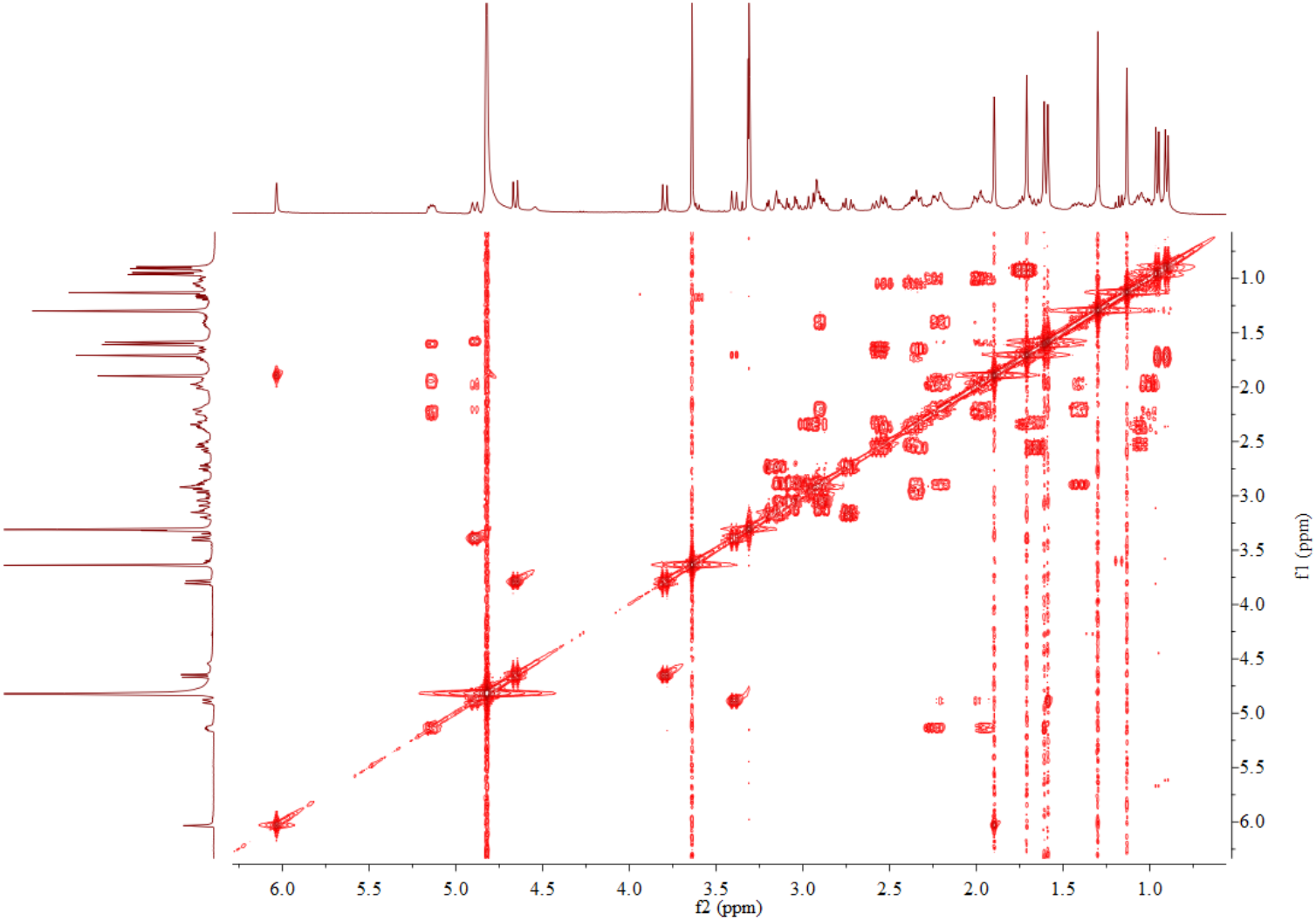
S10 HSQC spectrum of **2** in Methanol-d_4



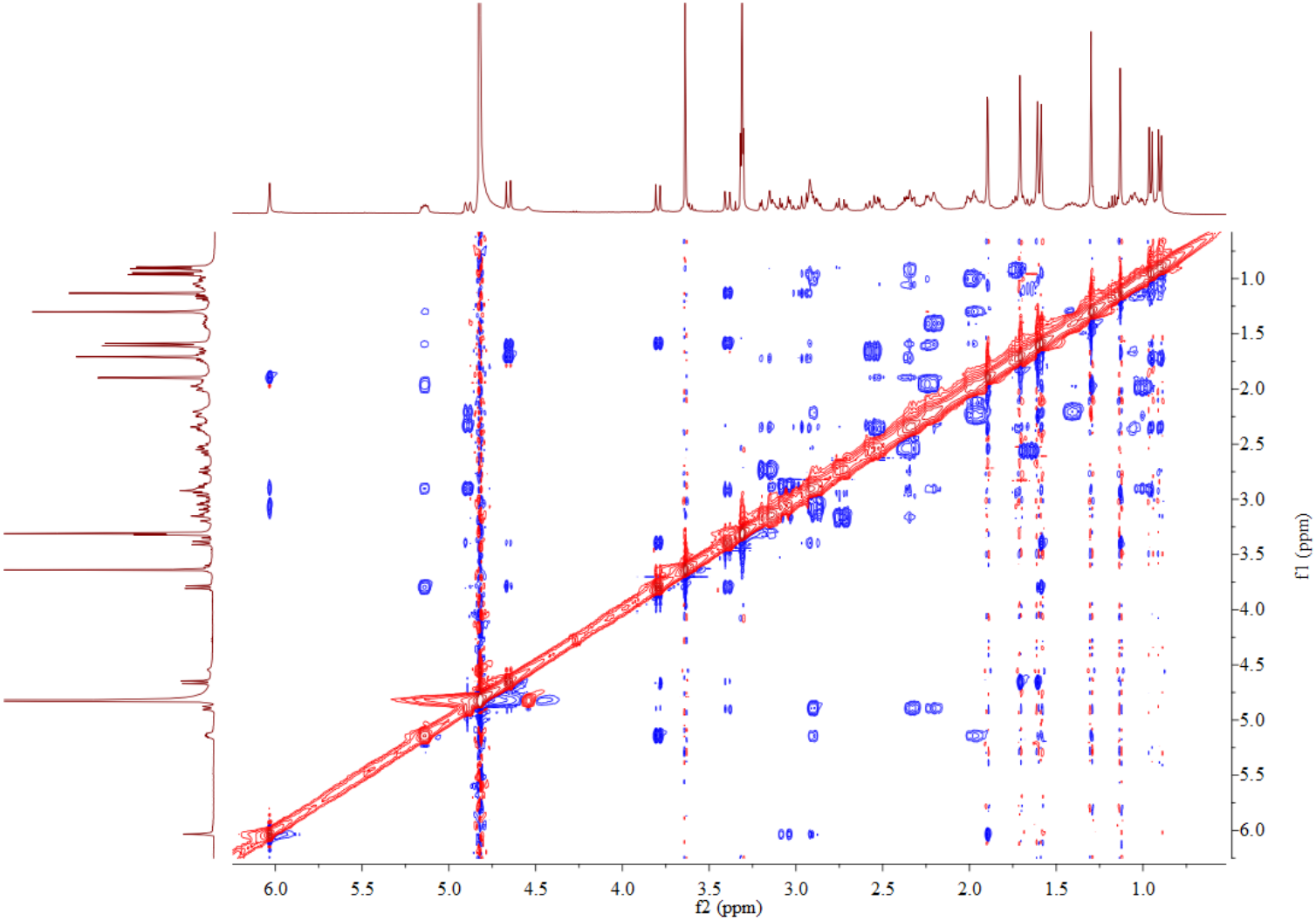
S11 HMBC spectrum of **2** in Methanol-d_4



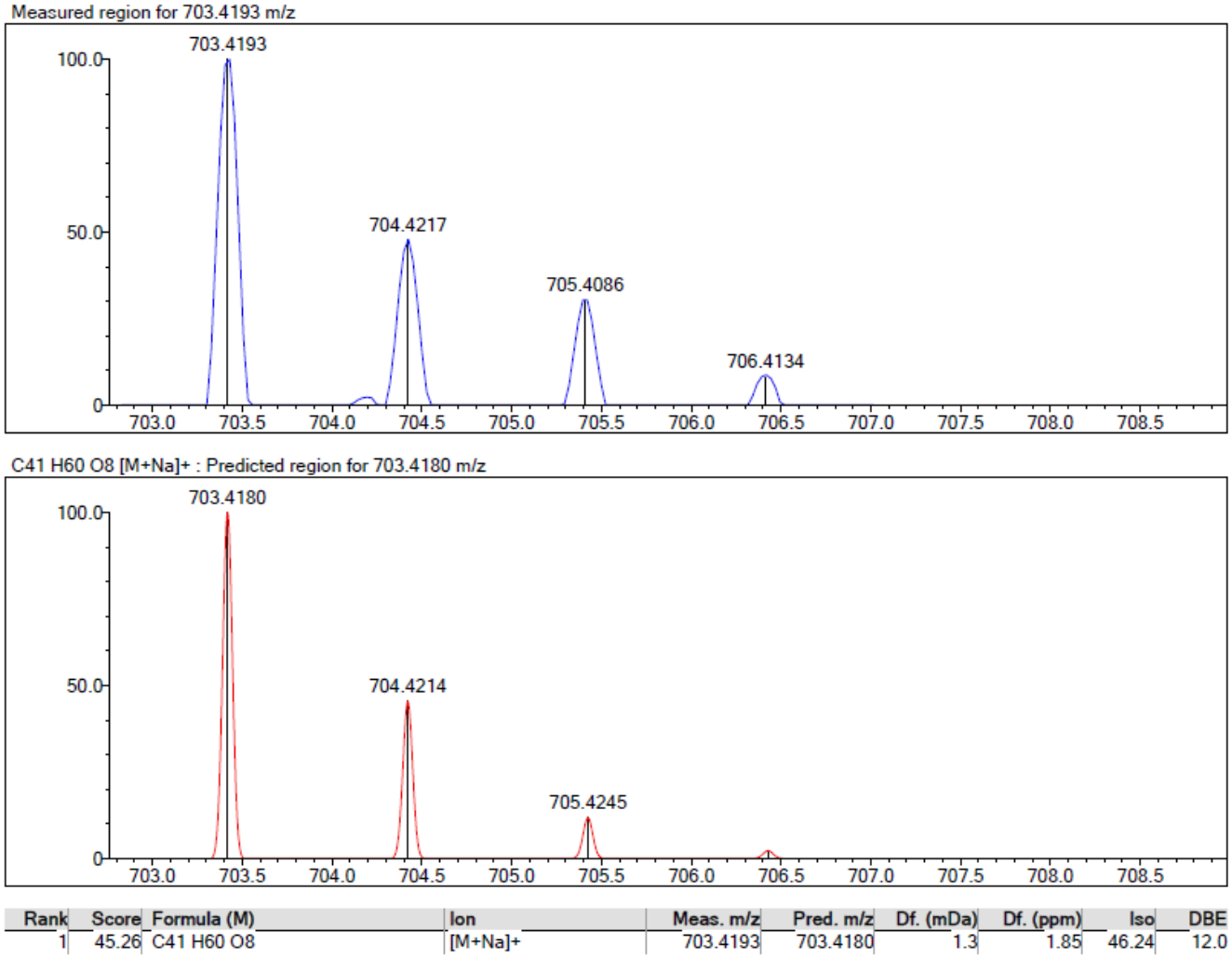
S12 $^{1}H–^{1}H$ COSY spectrum of **2** in Methanol-d_4



S13 NOESY spectrum of **2** in Methanol-d_4

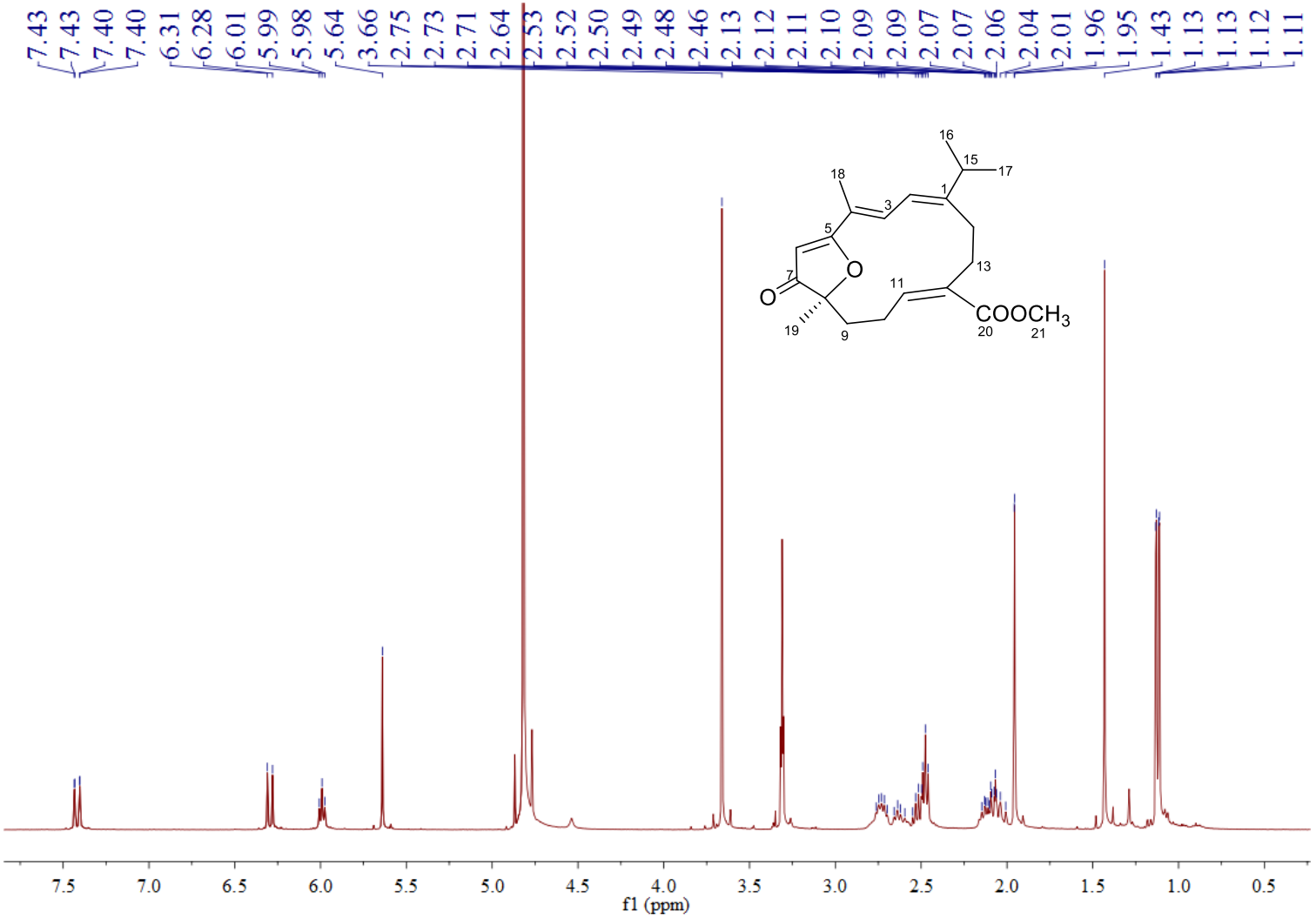


S14 HRESIMS spectrum of **2**

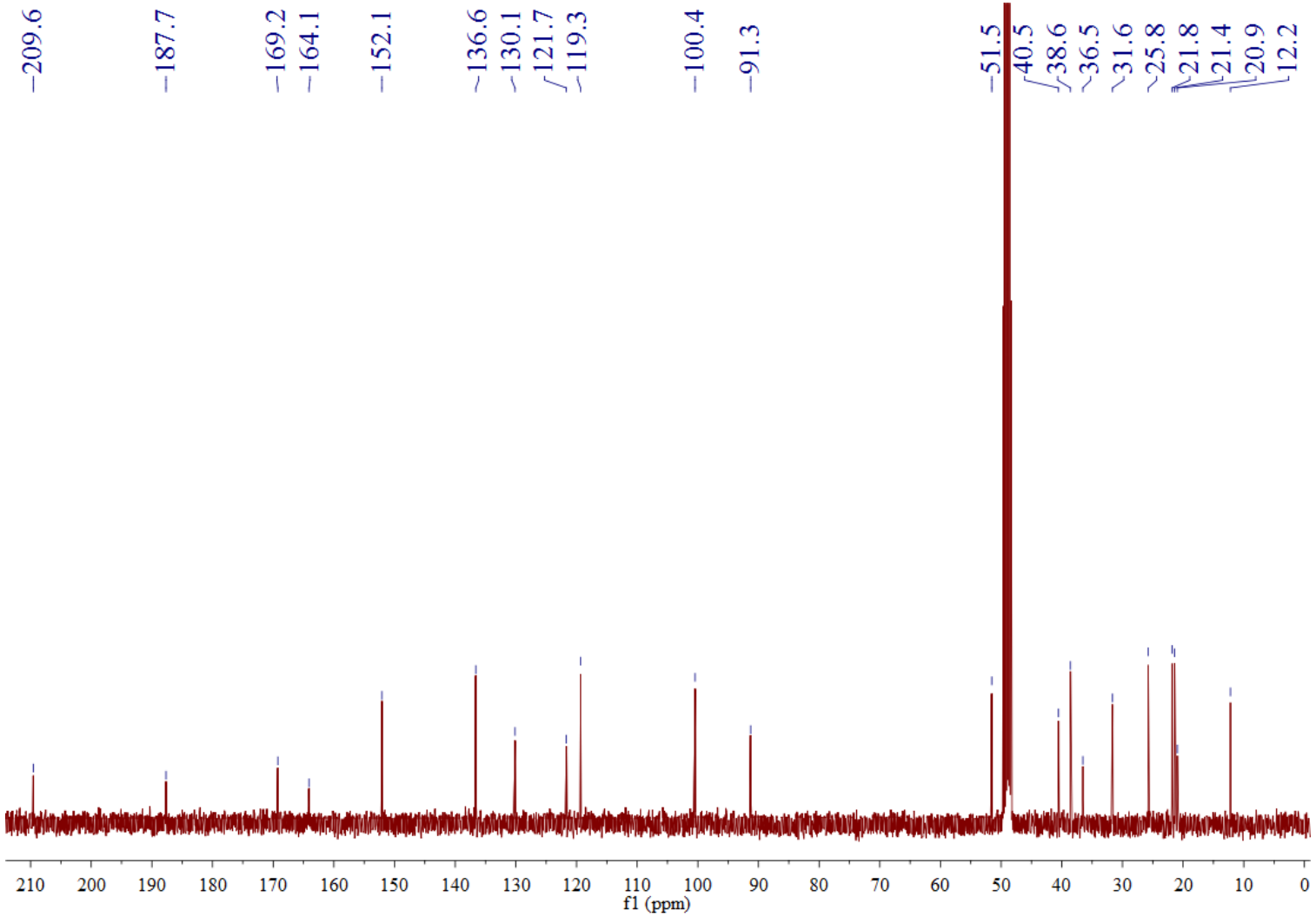


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	45.26	C41 H60 O8	[M+Na]+	703.4193	703.4180	1.3	1.85	46.24	12.0

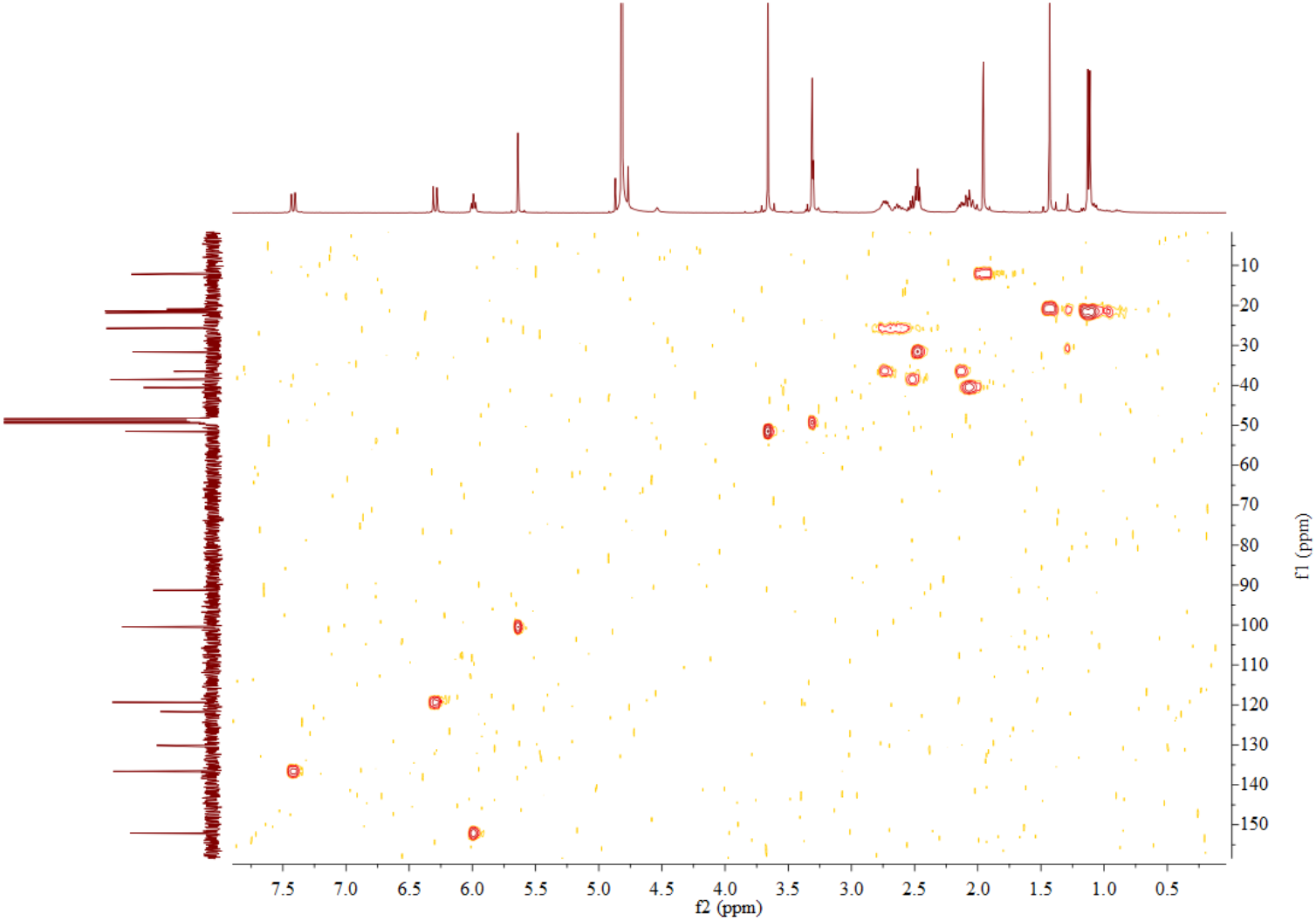
S15 ^{1}H NMR spectrum of **3** in Methanol-d_4



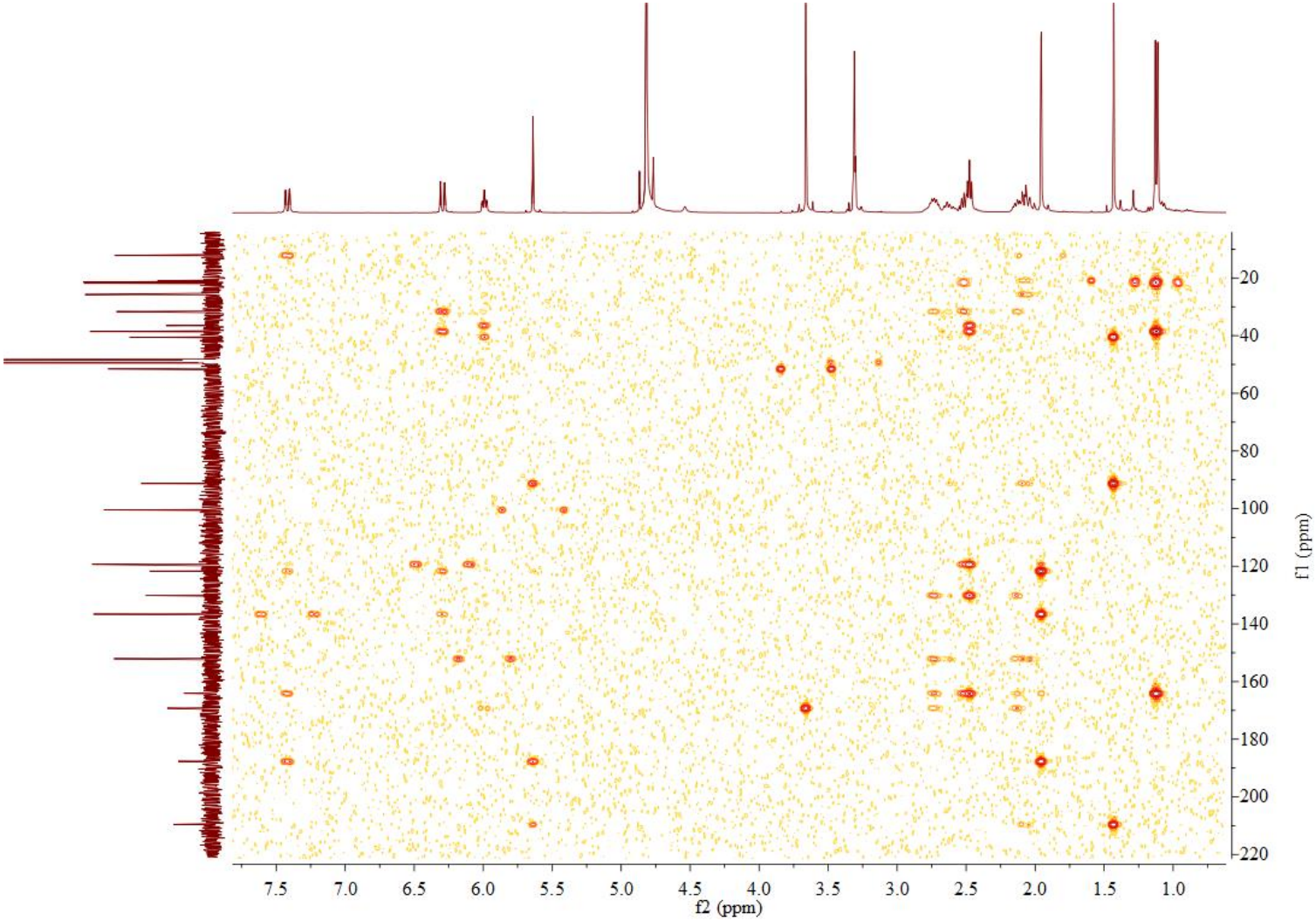
S16 ^{13}C NMR spectrum of **3** in Methanol-d_4



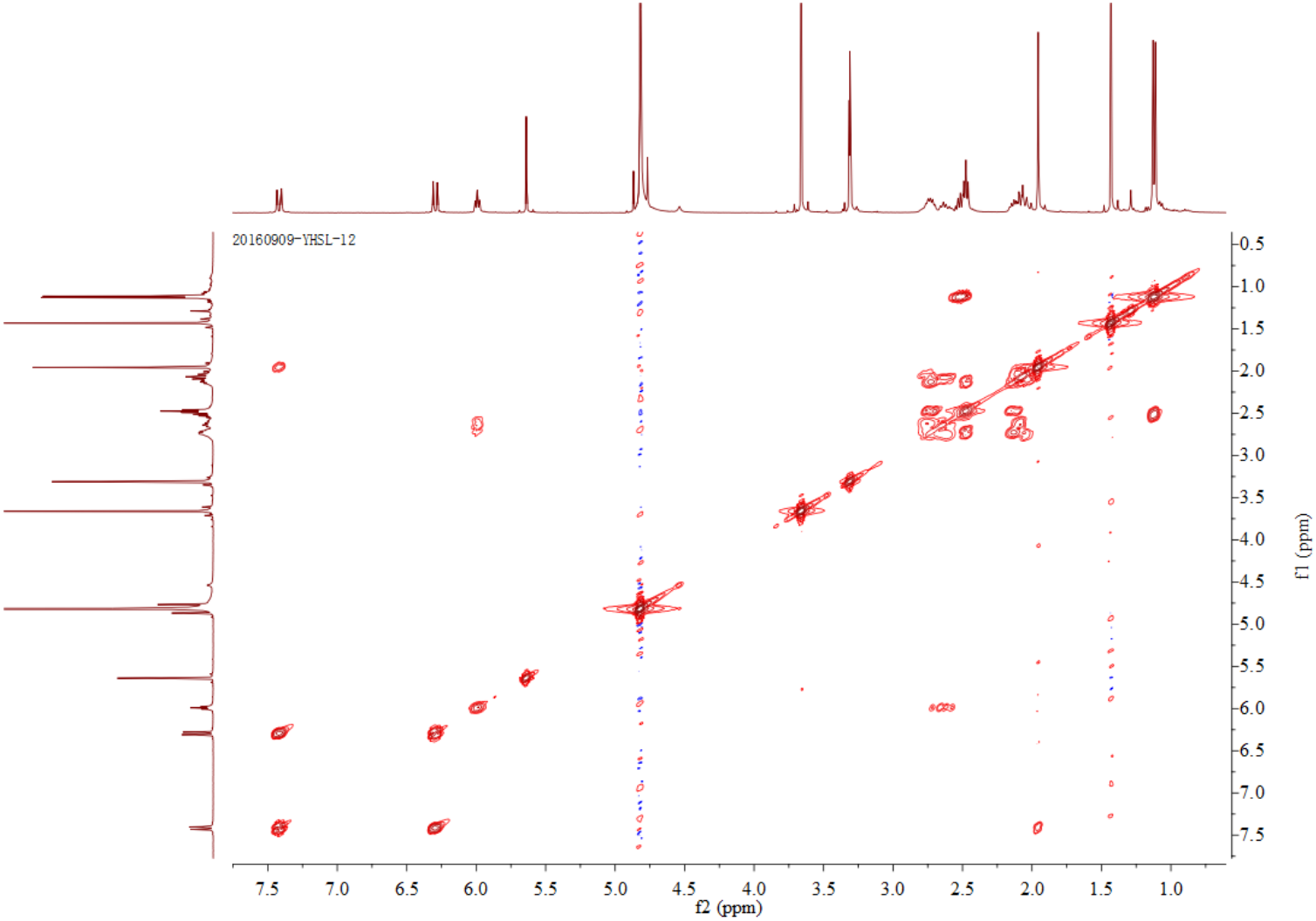
S17 HSQC spectrum of **3** in Methanol-d_4



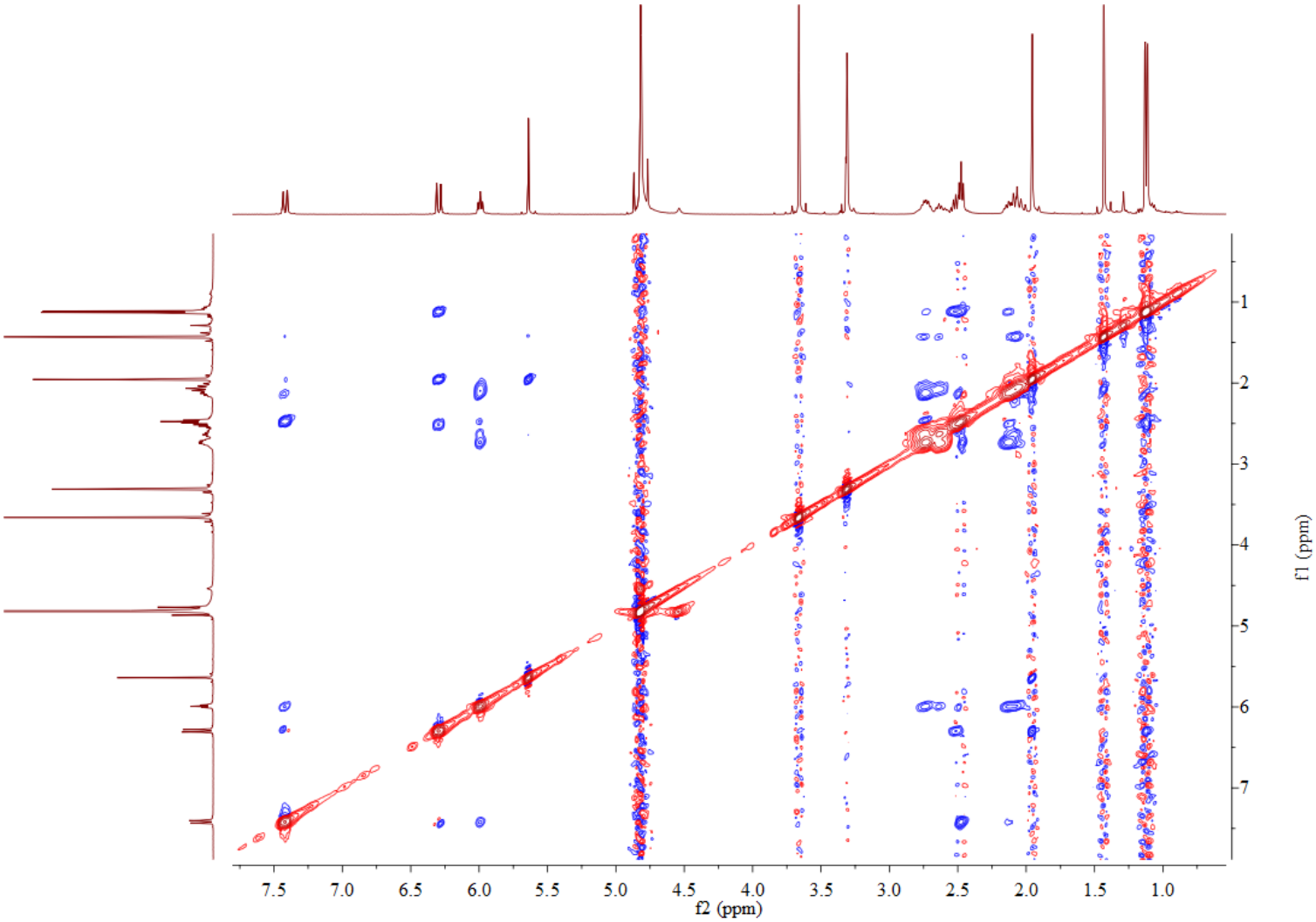
S18 HMBC spectrum of **3** in Methanol-d_4



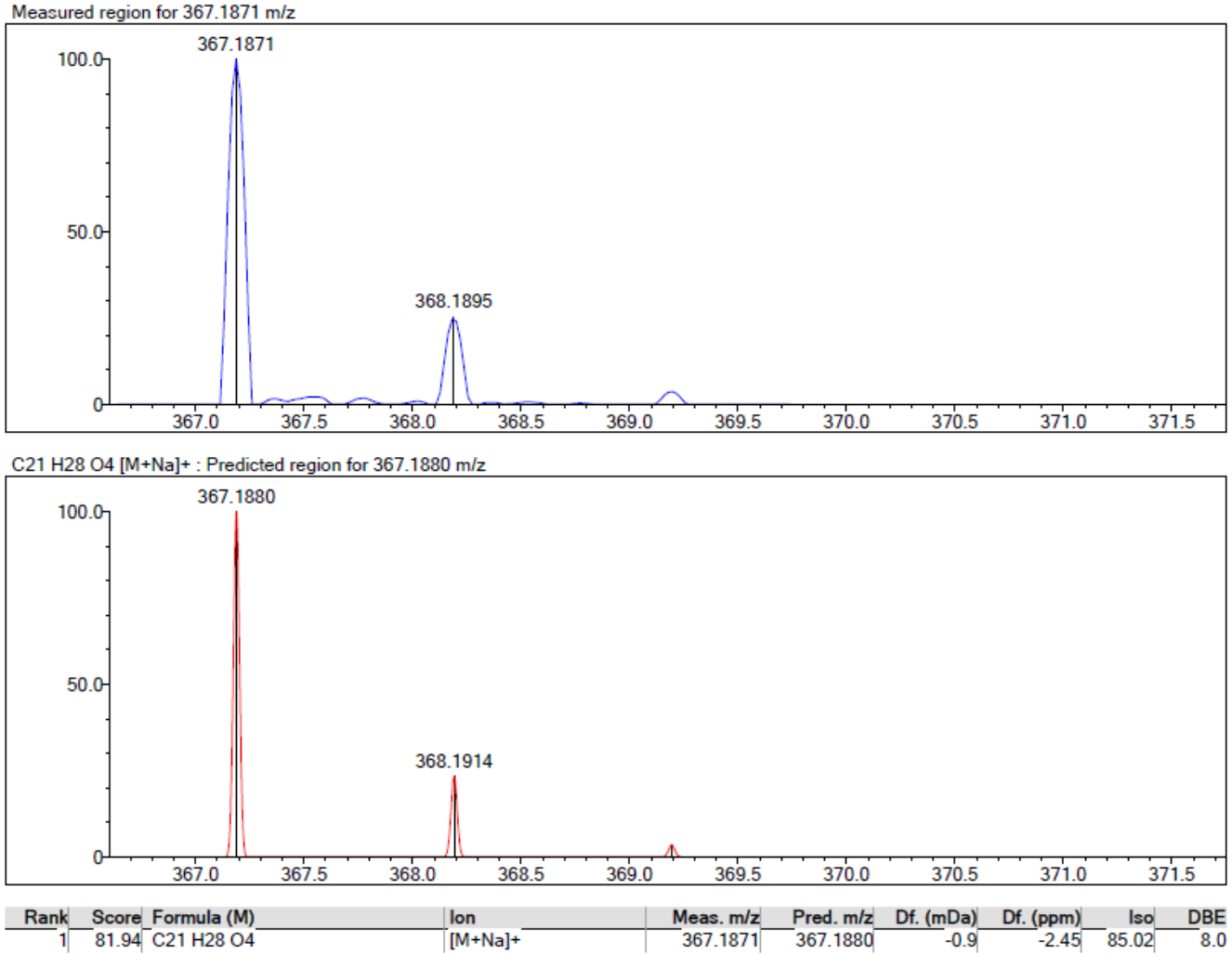
S19 $^{1}H–^{1}H$ COSY spectrum of **3** in Methanol-d_4



S20 NOESY spectrum of **3** in Methanol-d_4

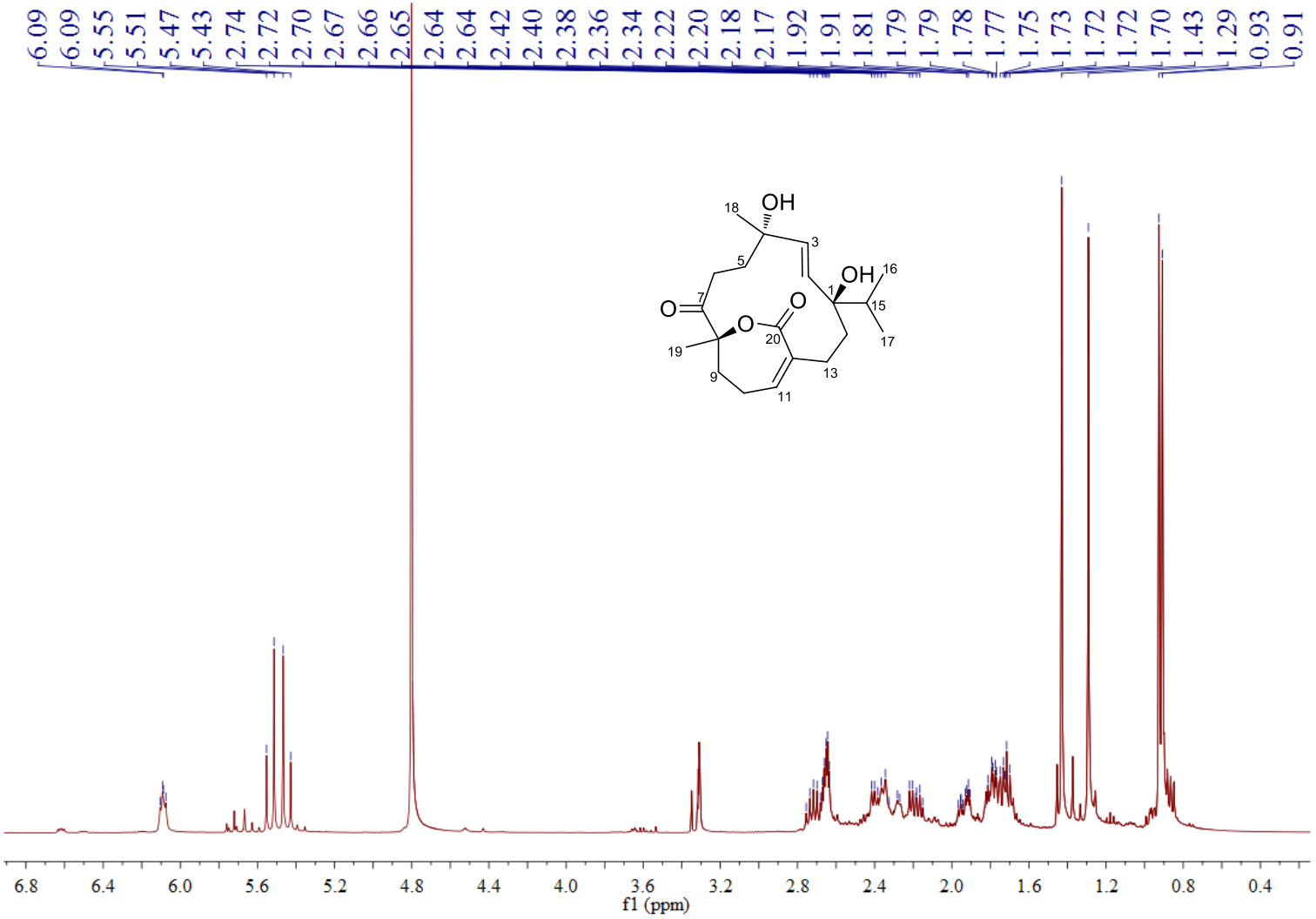


S21 HRESIMS spectrum of **3**

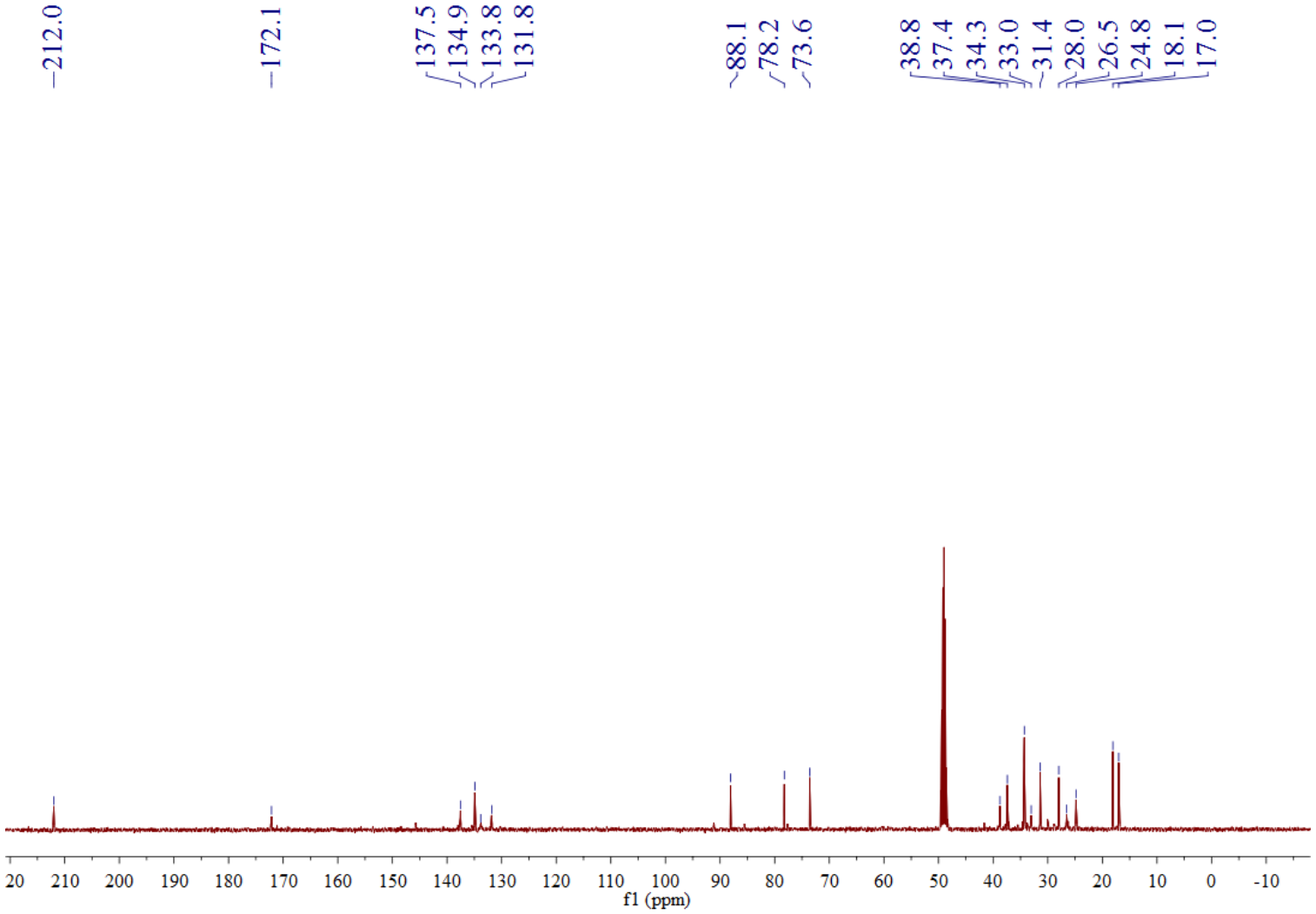


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	81.94	C21 H28 O4	[M+Na]+	367.1871	367.1880	-0.9	-2.45	85.02	8.0

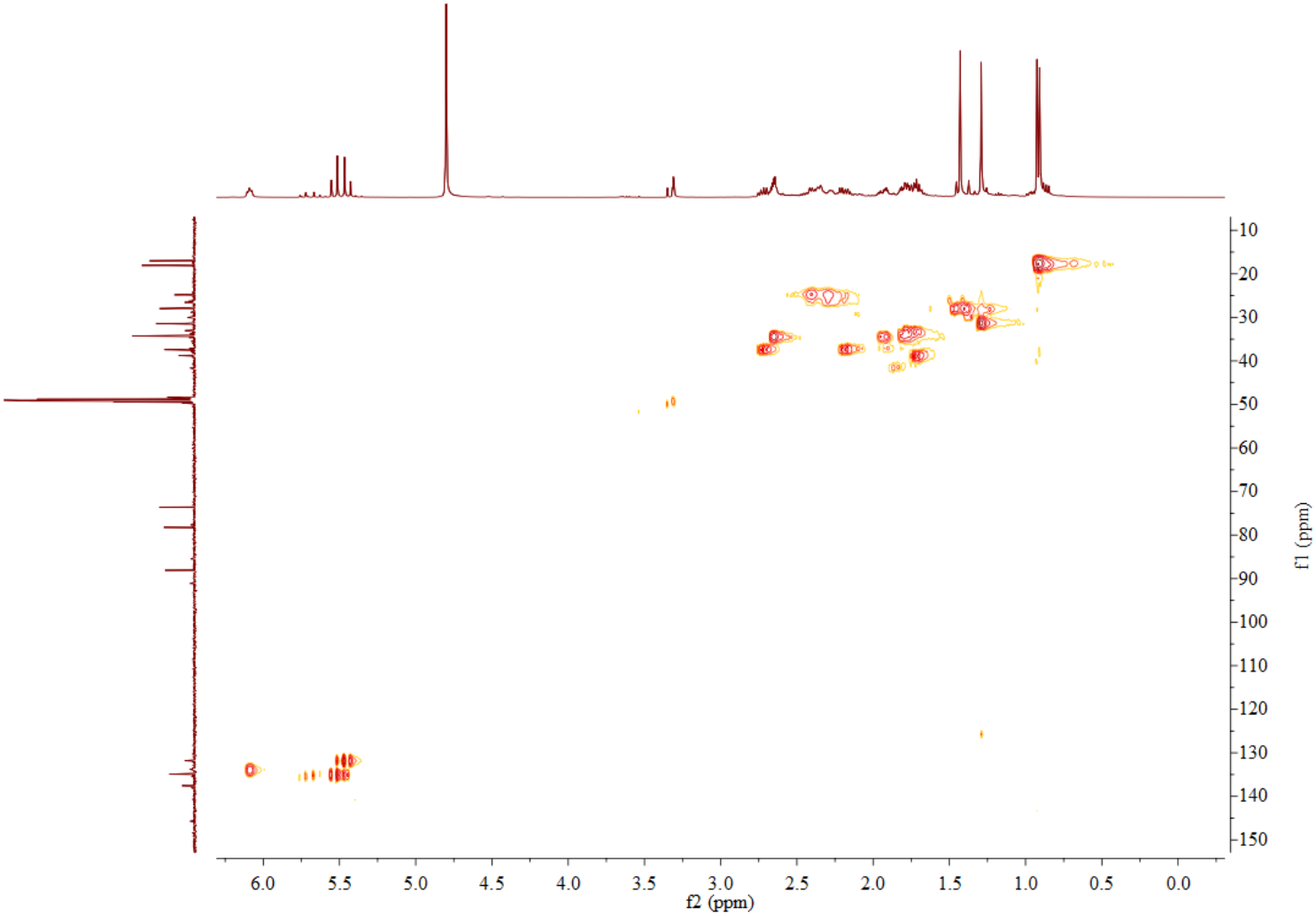
S22 ^{1}H NMR spectrum of **4** in Methanol-d_4



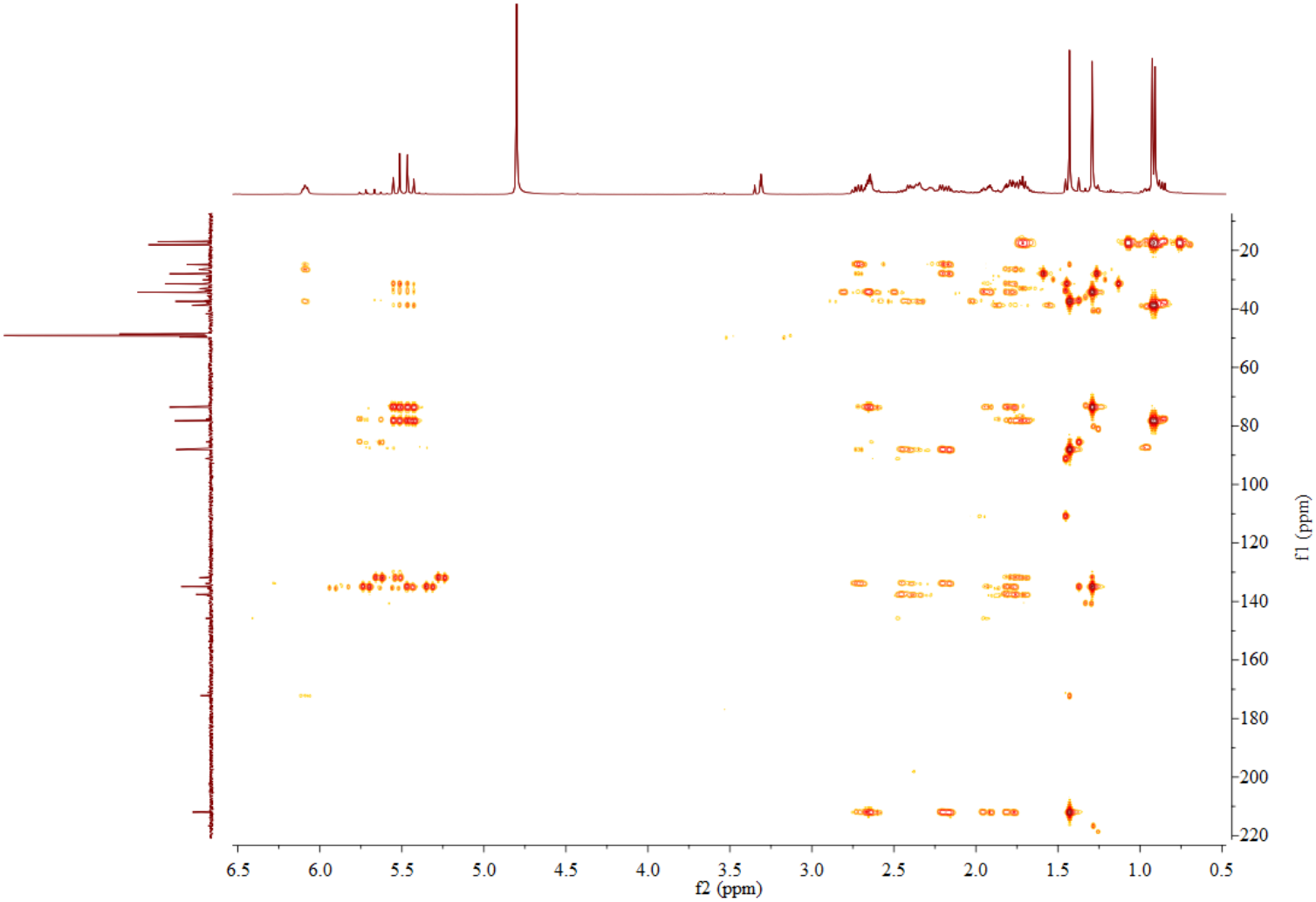
S23 ^{13}C NMR spectrum of **4** in Methanol-d_4



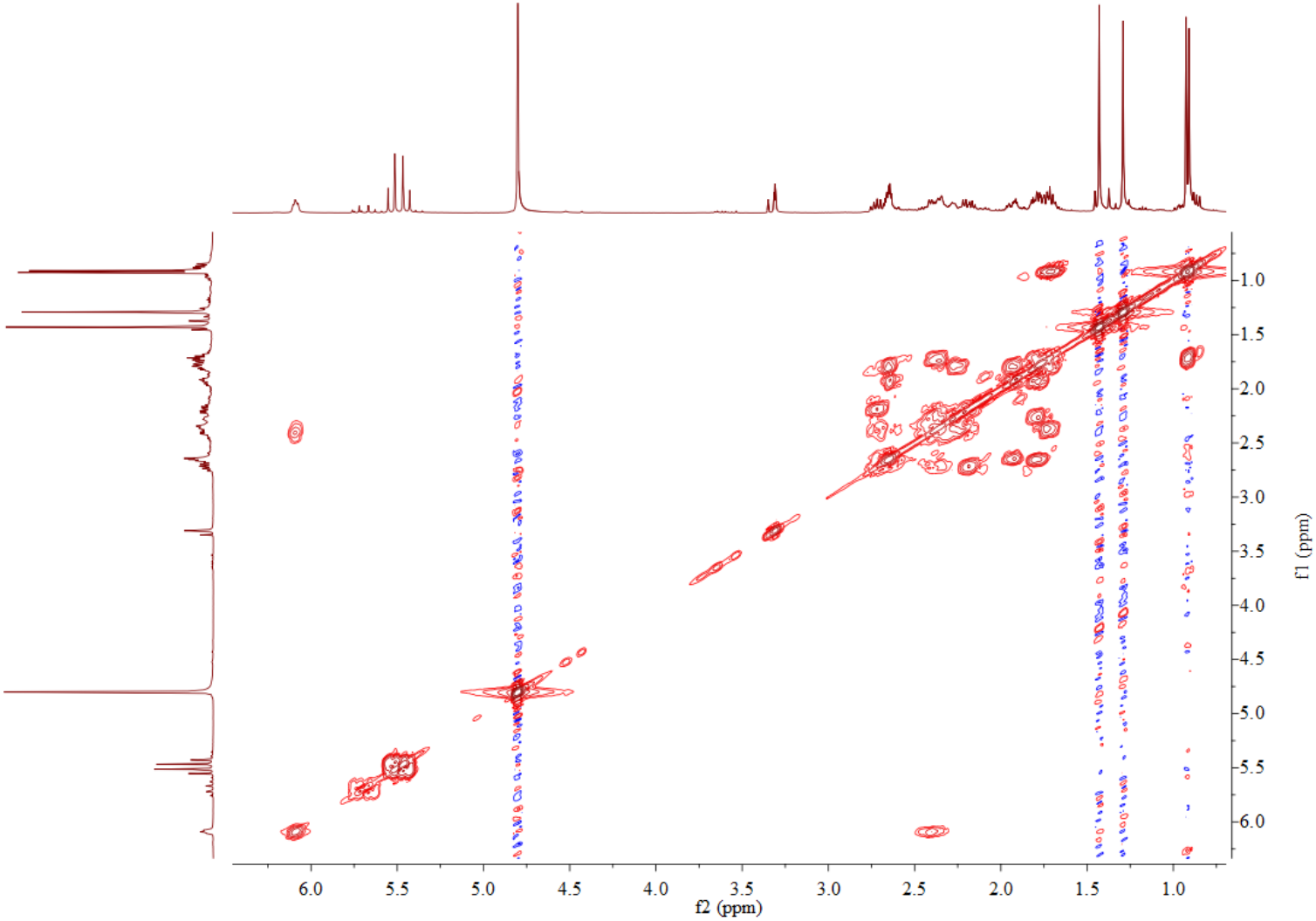
S24 HSQC spectrum of **4** in Methanol-d_4



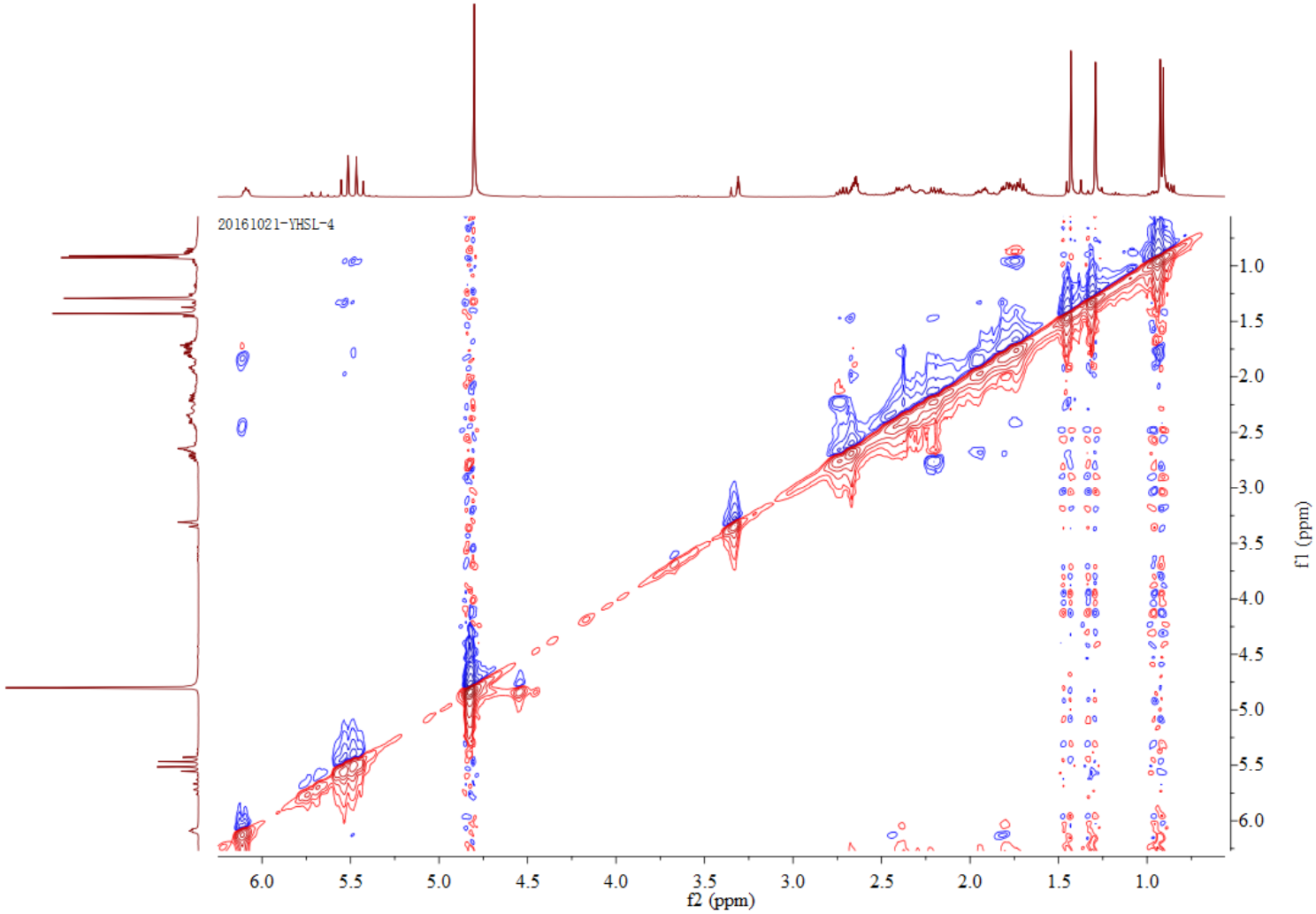
S25 HMBC spectrum of **4** in Methanol-d_4



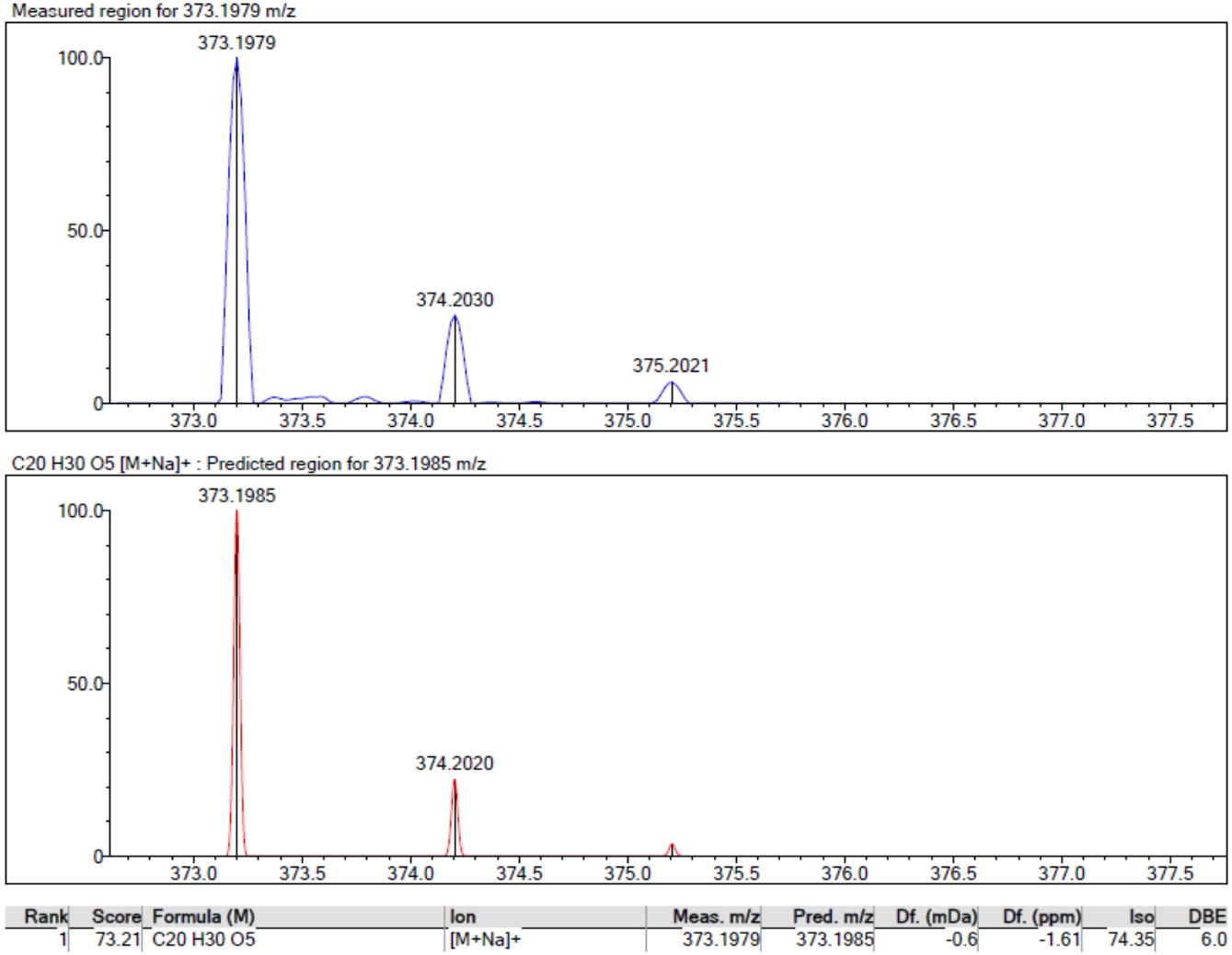
S26 ^{1}H–^{1}H COSY spectrum of **4** in Methanol-d_4



S27 NOESY spectrum of **4** in Methanol-d_4

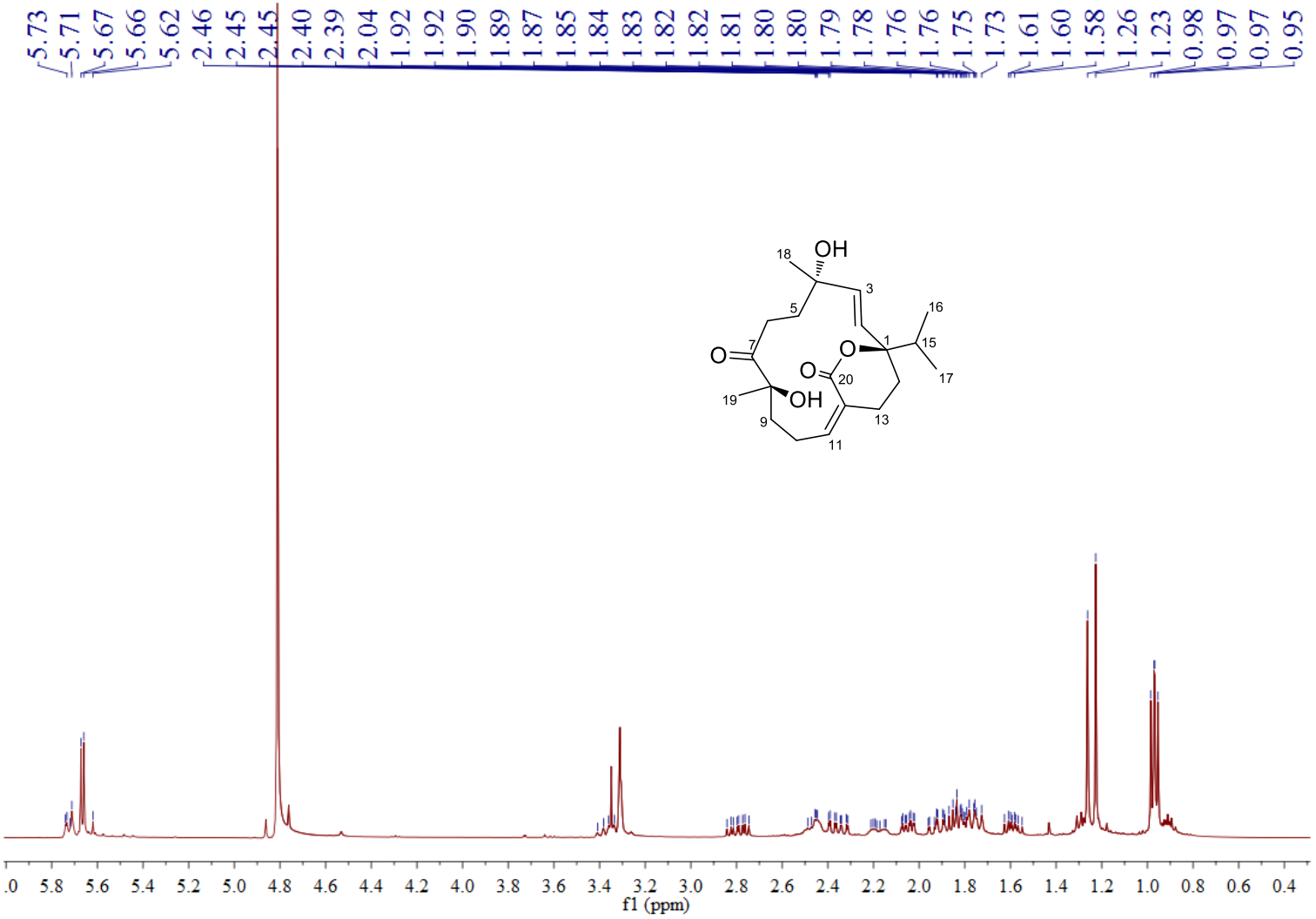


S28 HRESIMS spectrum of **4**

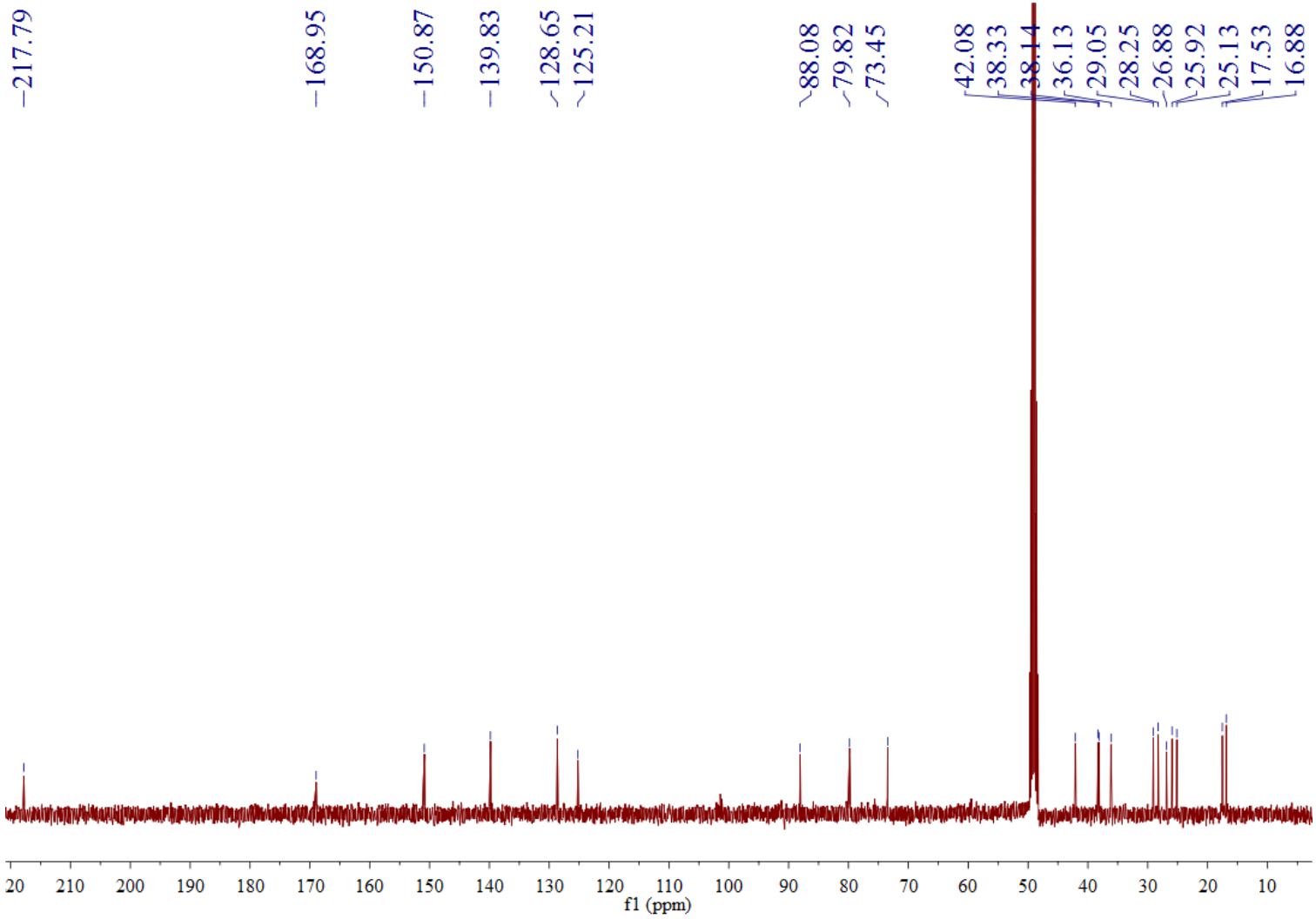


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	73.21	C20 H30 O5	[M+Na]+	373.1979	373.1985	-0.6	-1.61	74.35	6.0

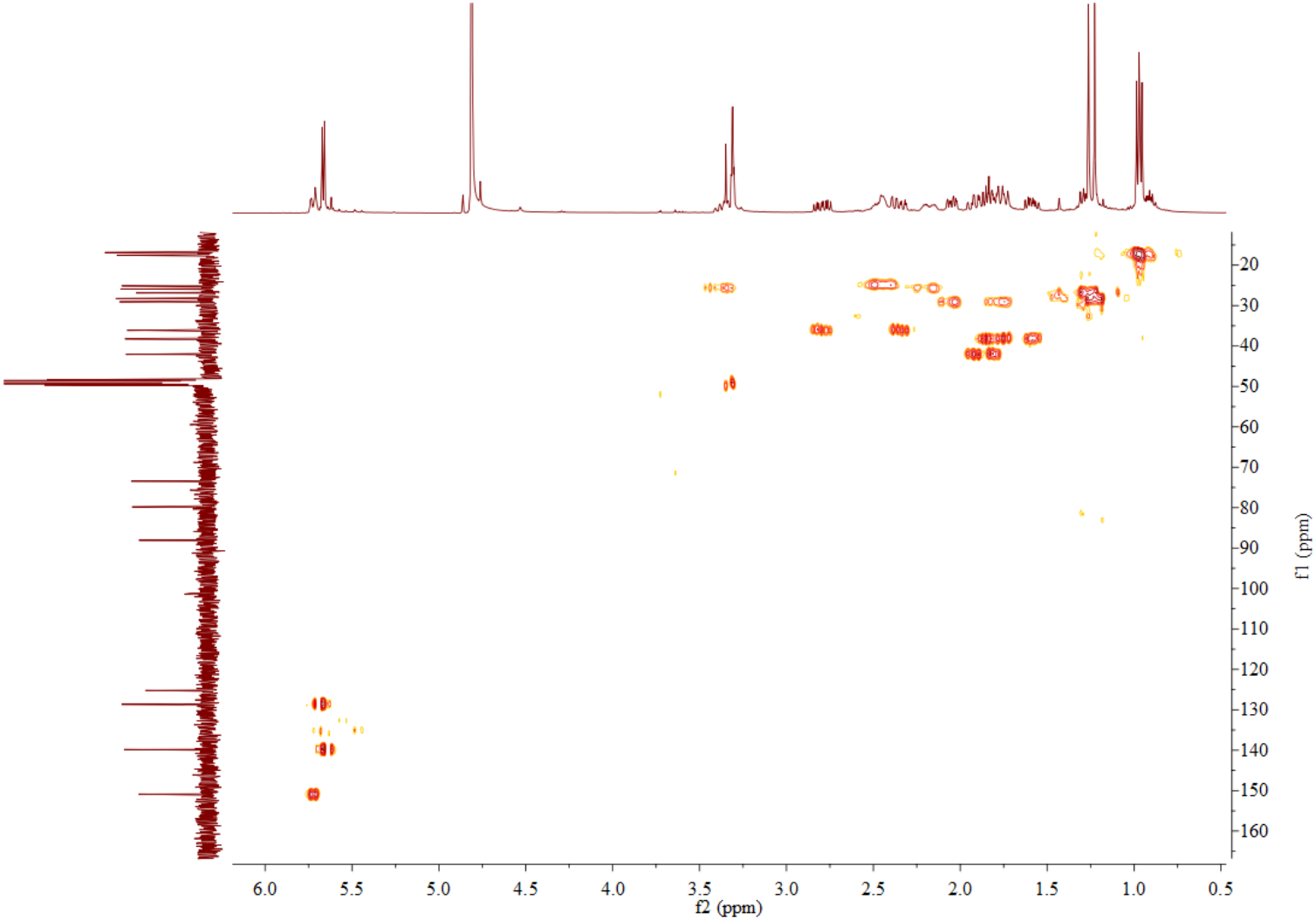
S29 ^{1}H NMR spectrum of **5** in Methanol-d_4



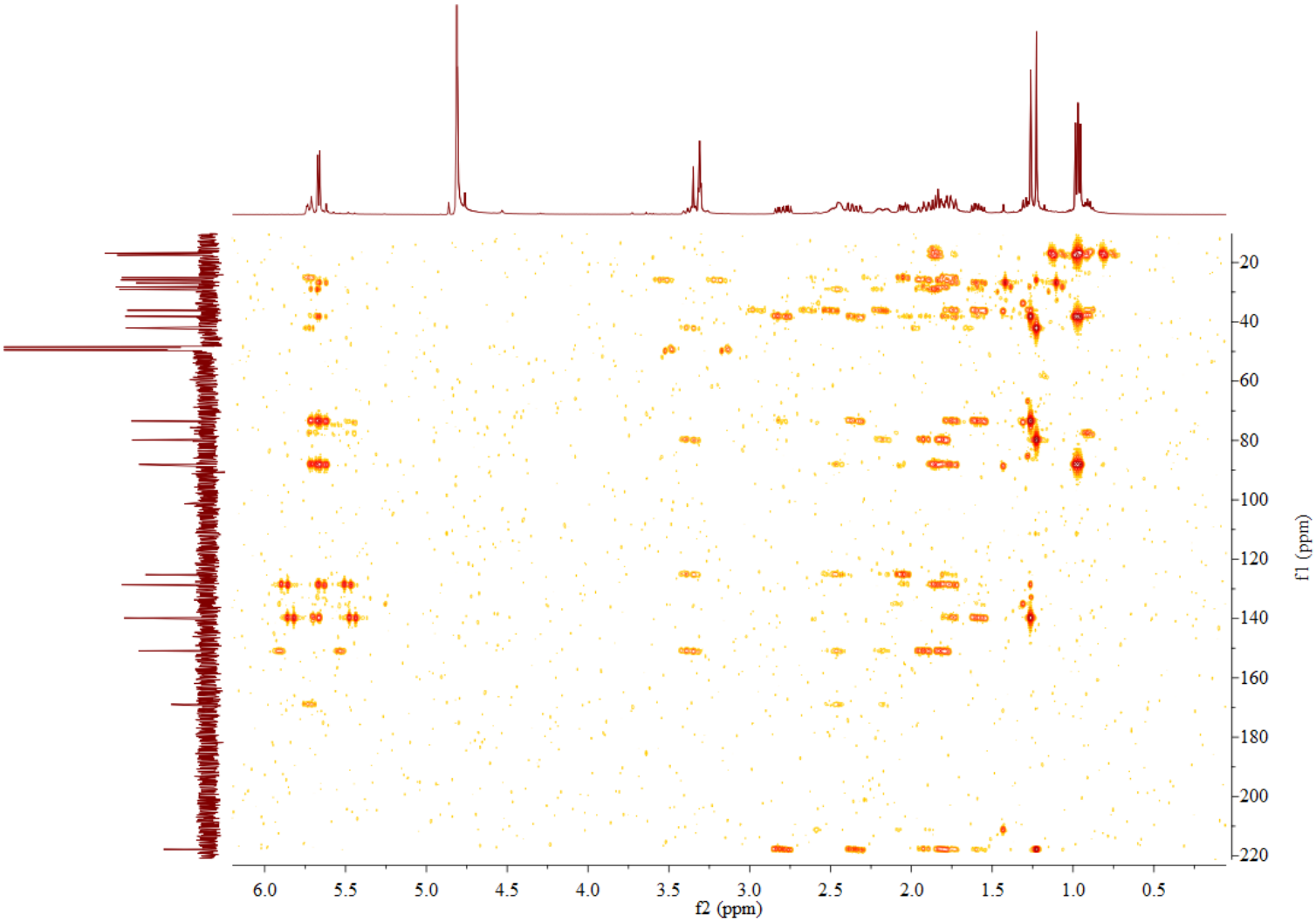
S30 ^{13}C NMR spectrum of **5** in Methanol-d_4



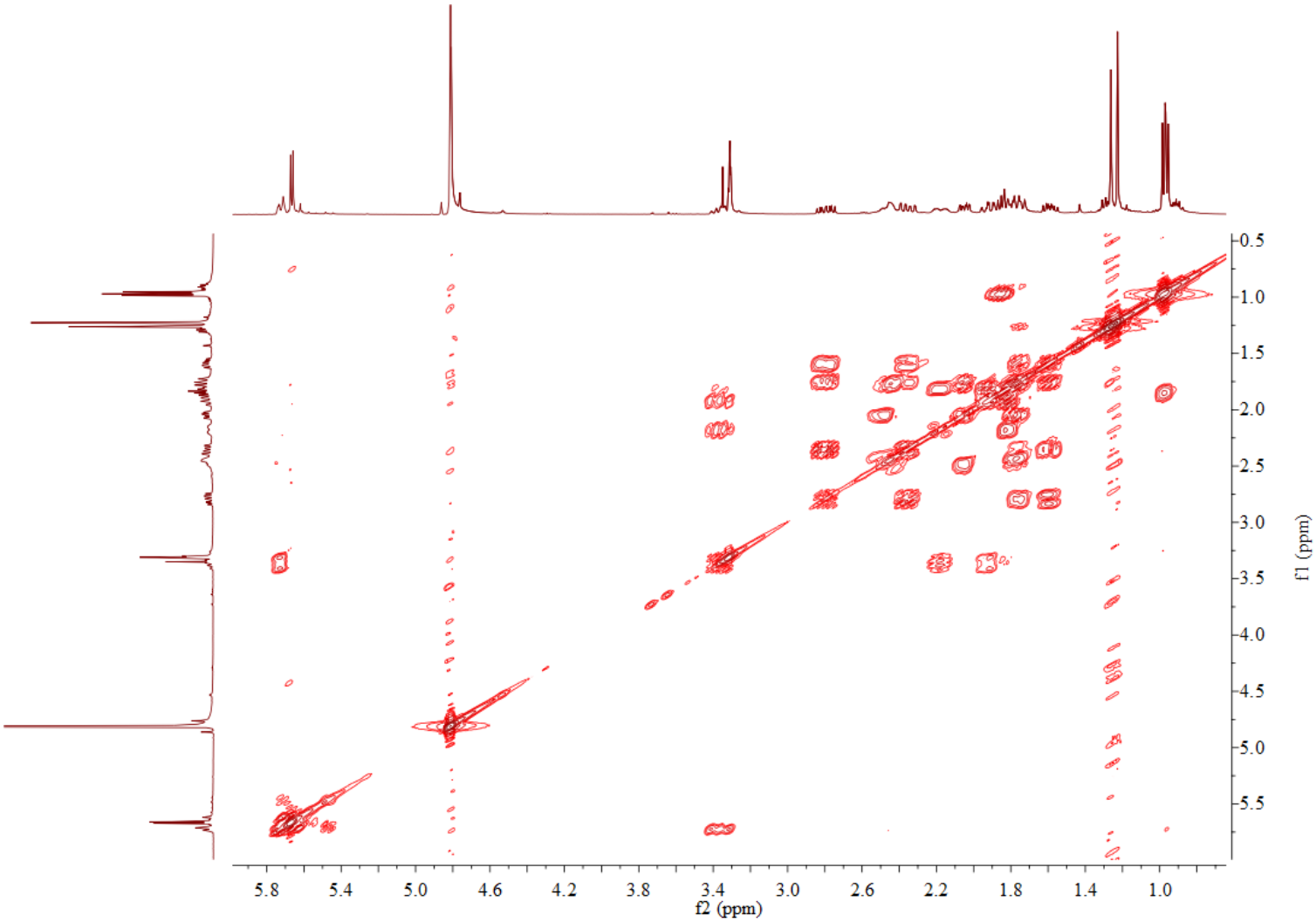
S31 HSQC spectrum of **5** in Methanol-d_4



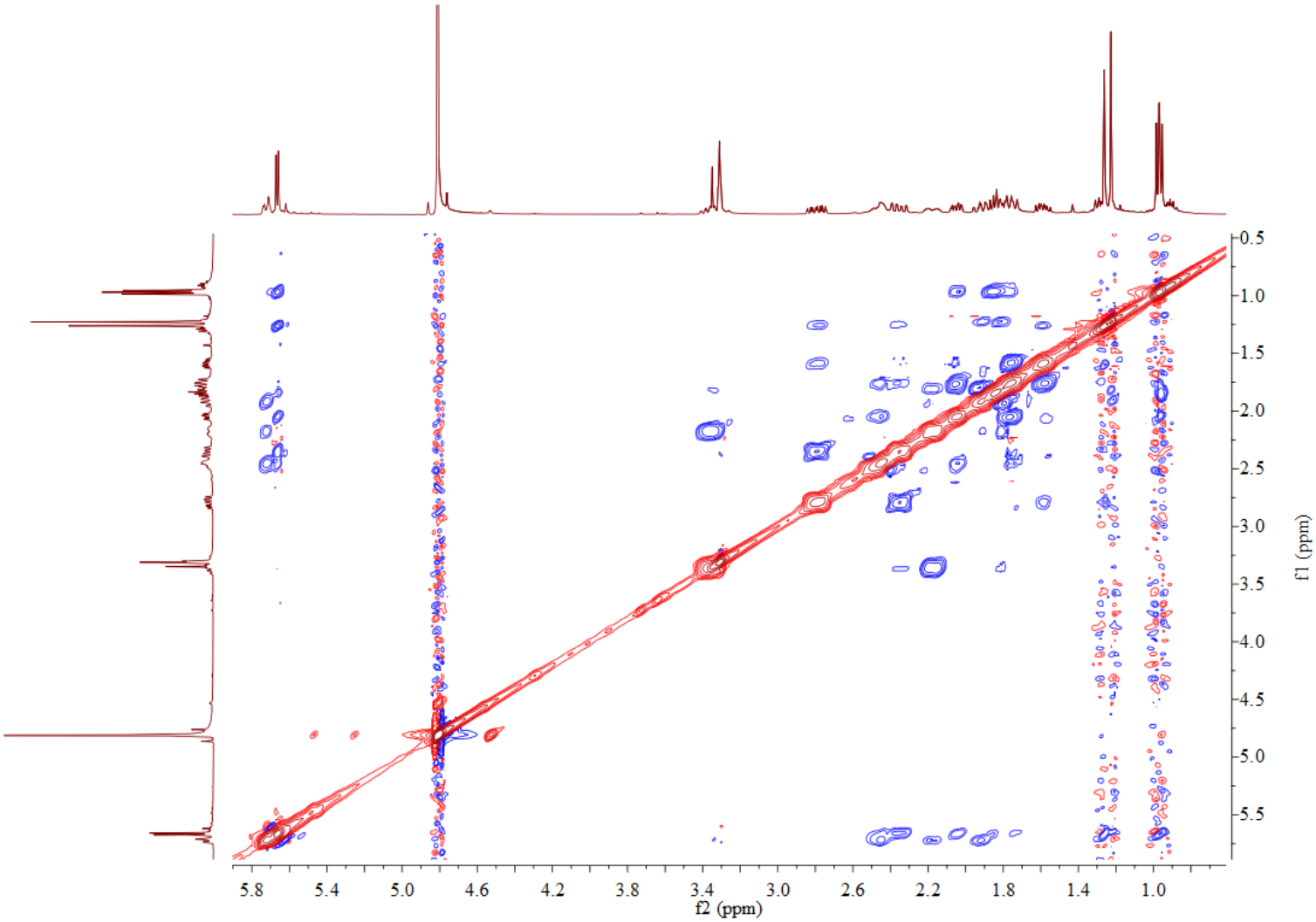
S32 HMBC spectrum of **5** in Methanol-d_4



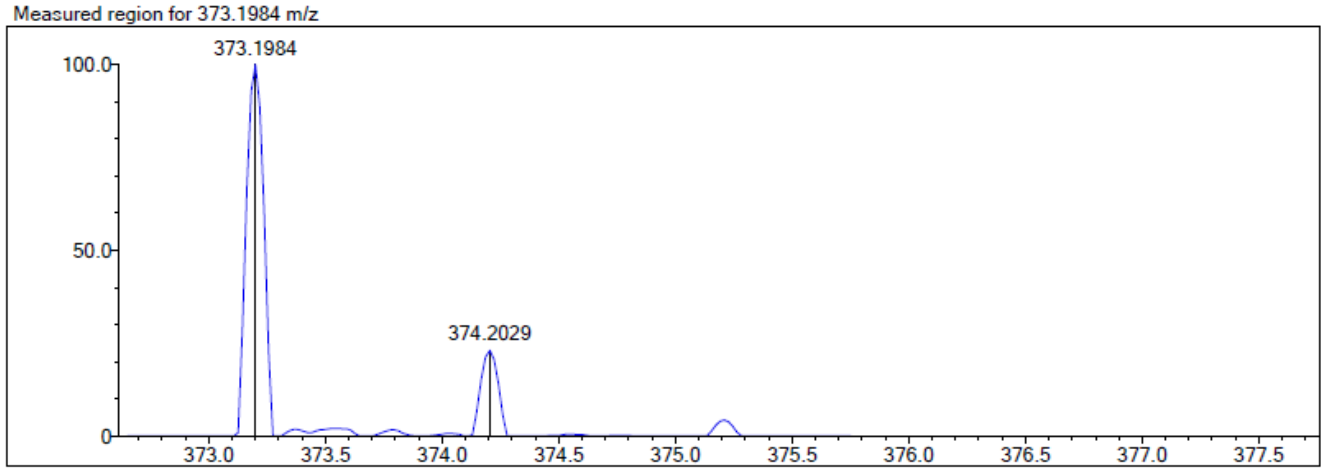
S33 $^{1}H–^{1}H$ COSY spectrum of **5** in Methanol-d_4

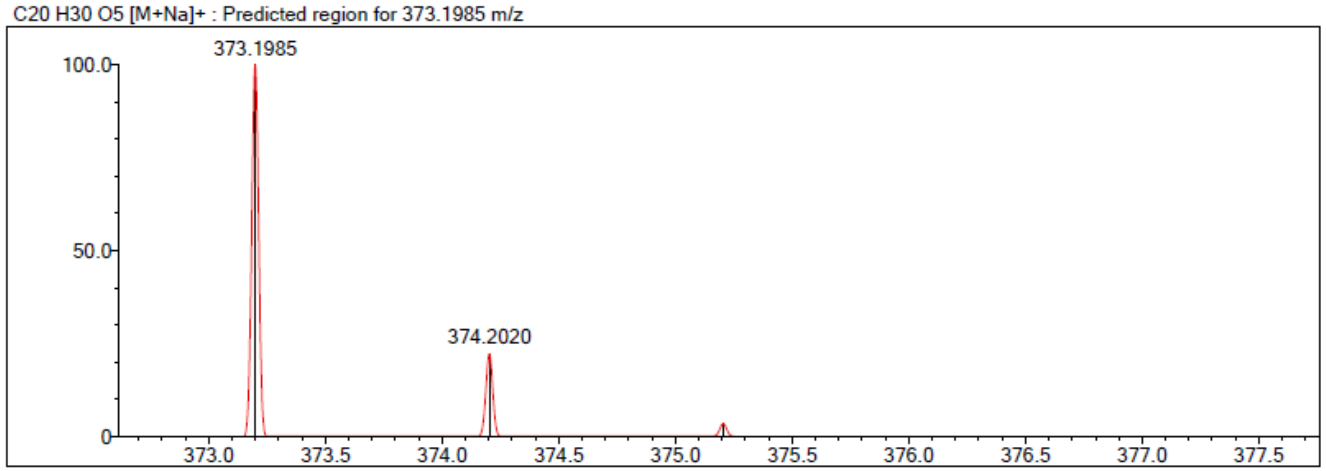


S34 NOESY spectrum of **5** in Methanol-d_4



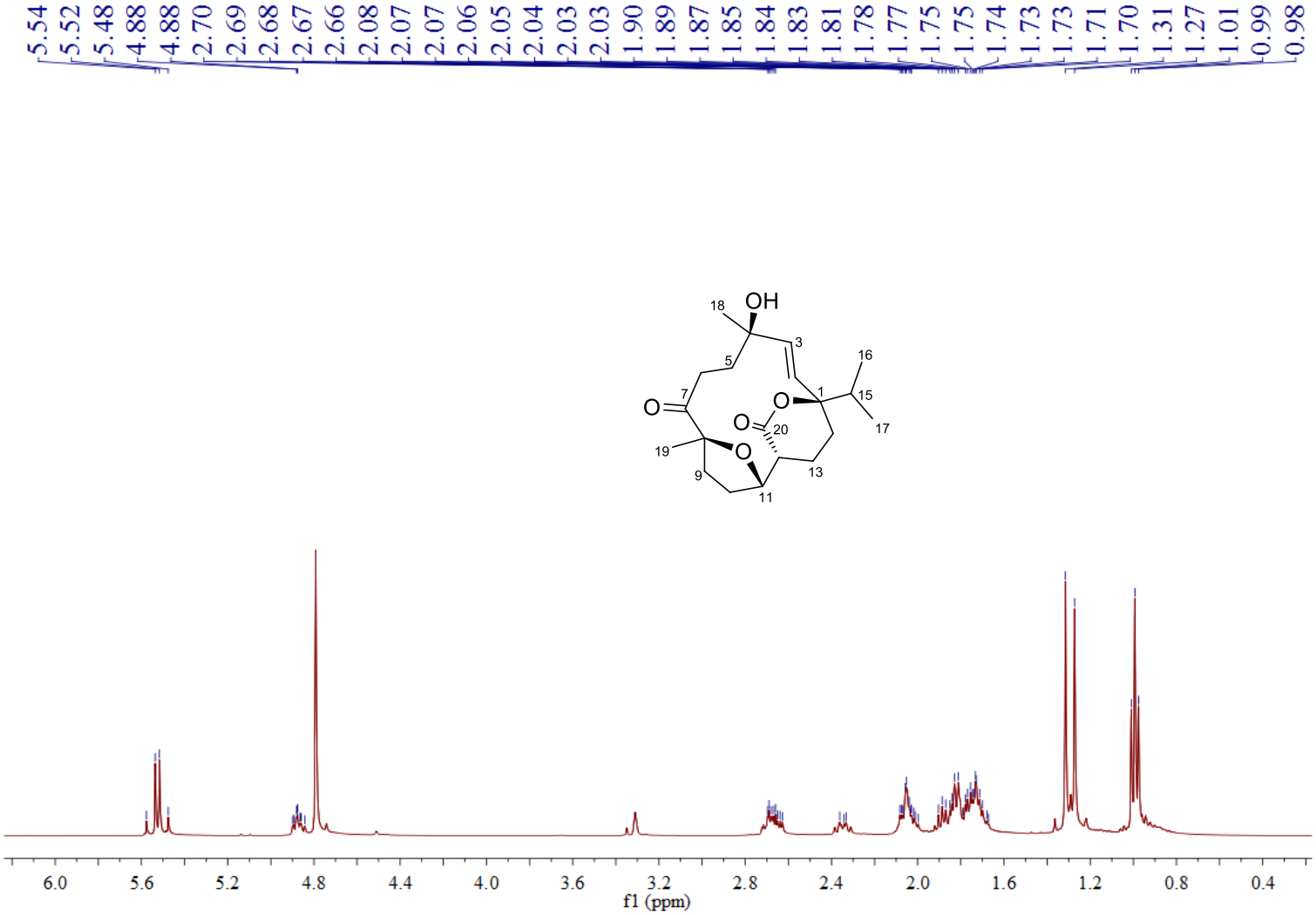
S35 HRESIMS spectrum of **5**



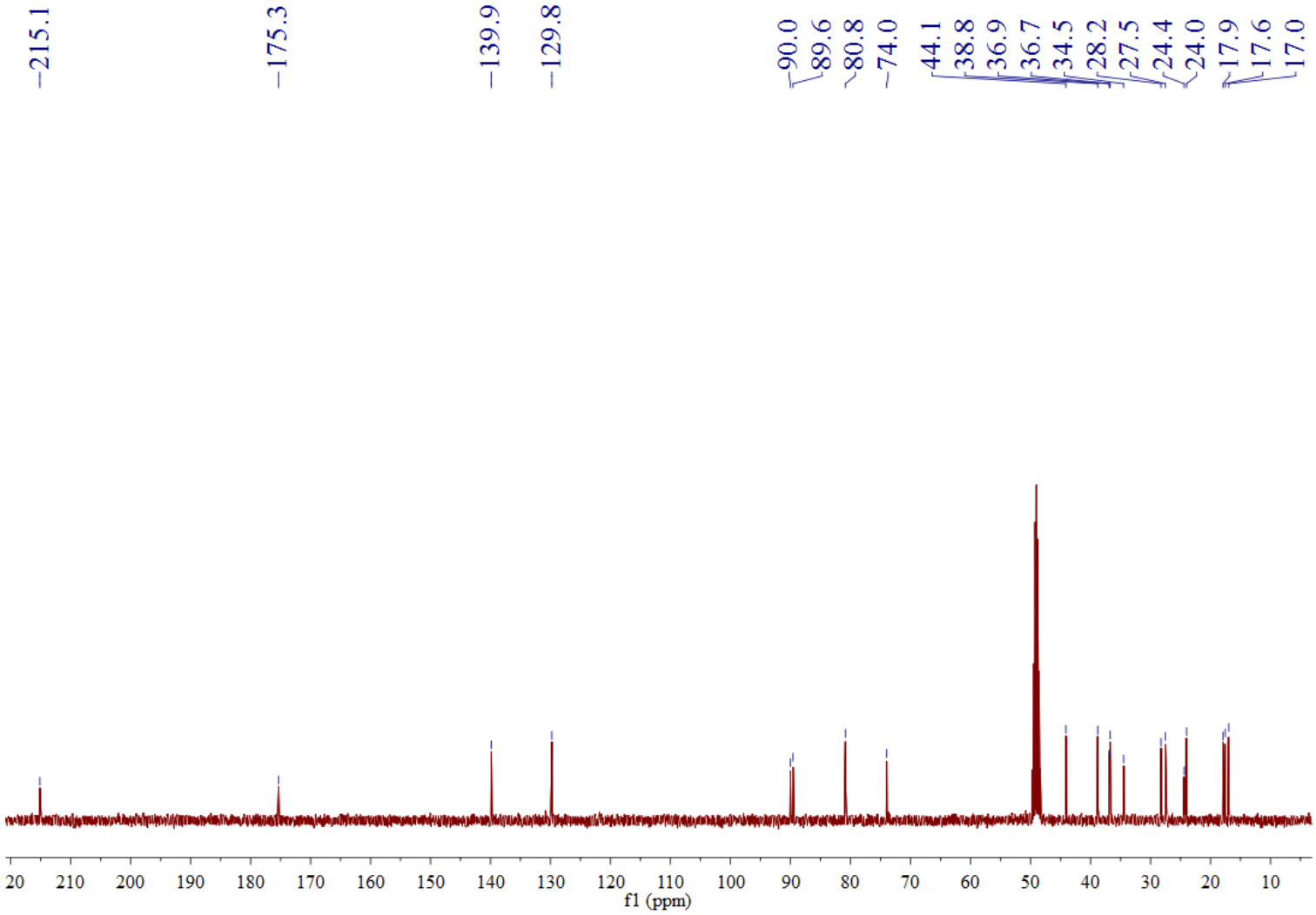


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	87.48	C20 H30 O5	[M+Na]+	373.1984	373.1985	-0.1	-0.27	87.48	6.0

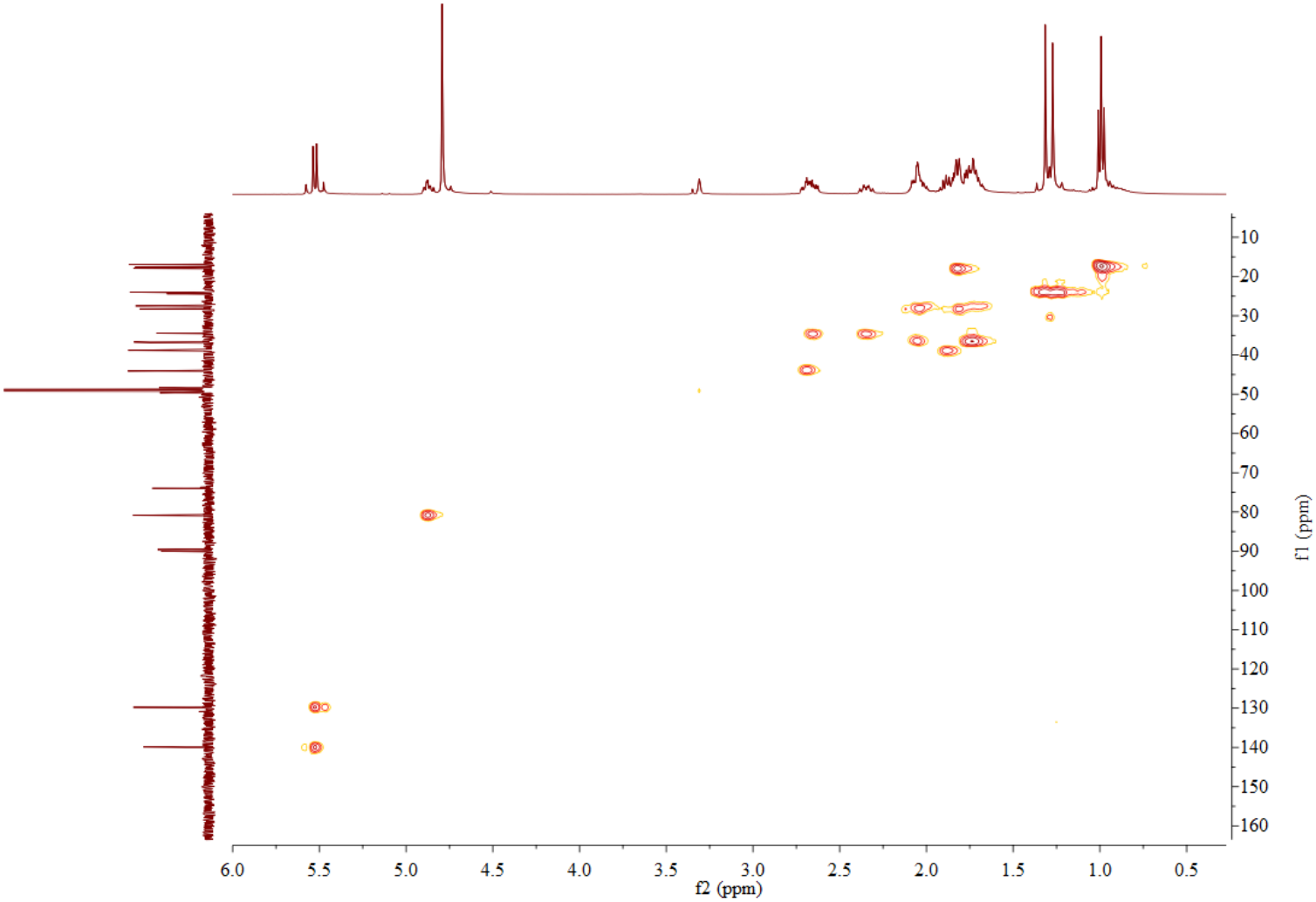
S36 ^{1}H NMR spectrum of **6** in Methanol-d_4



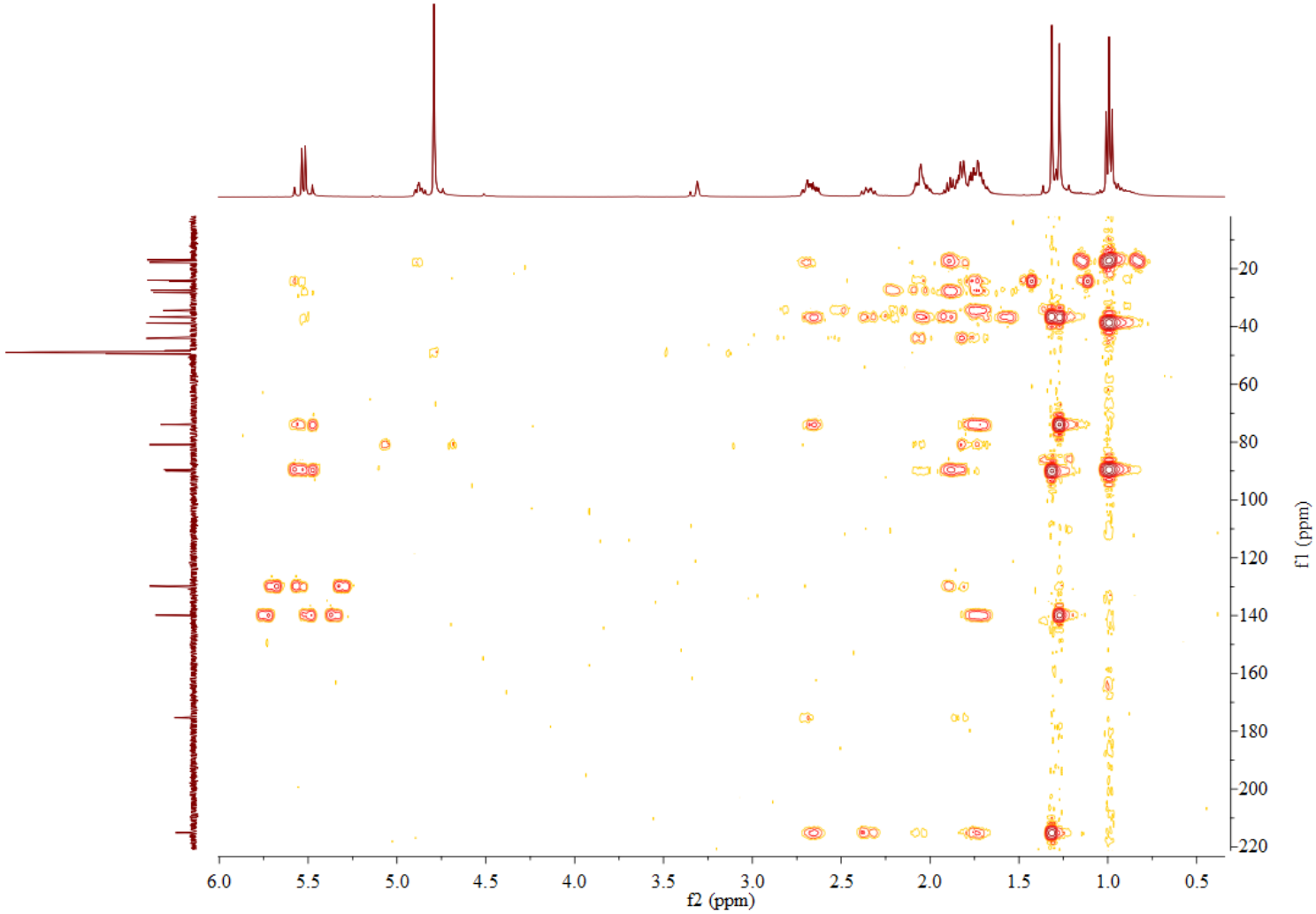
S37 ^{13}C NMR spectrum of **6** in Methanol-d_4



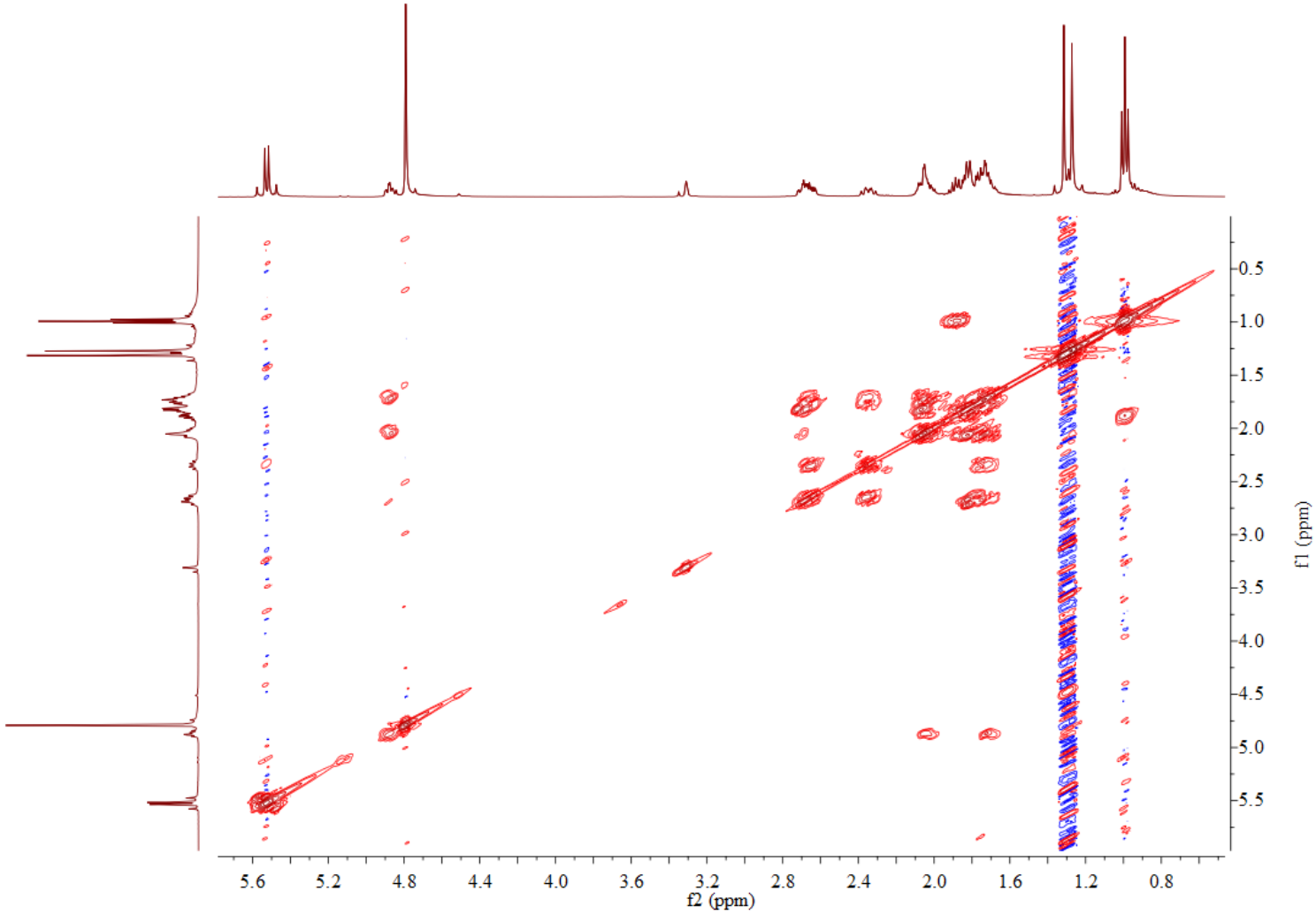
S38 HSQC spectrum of **6** in Methanol-d_4



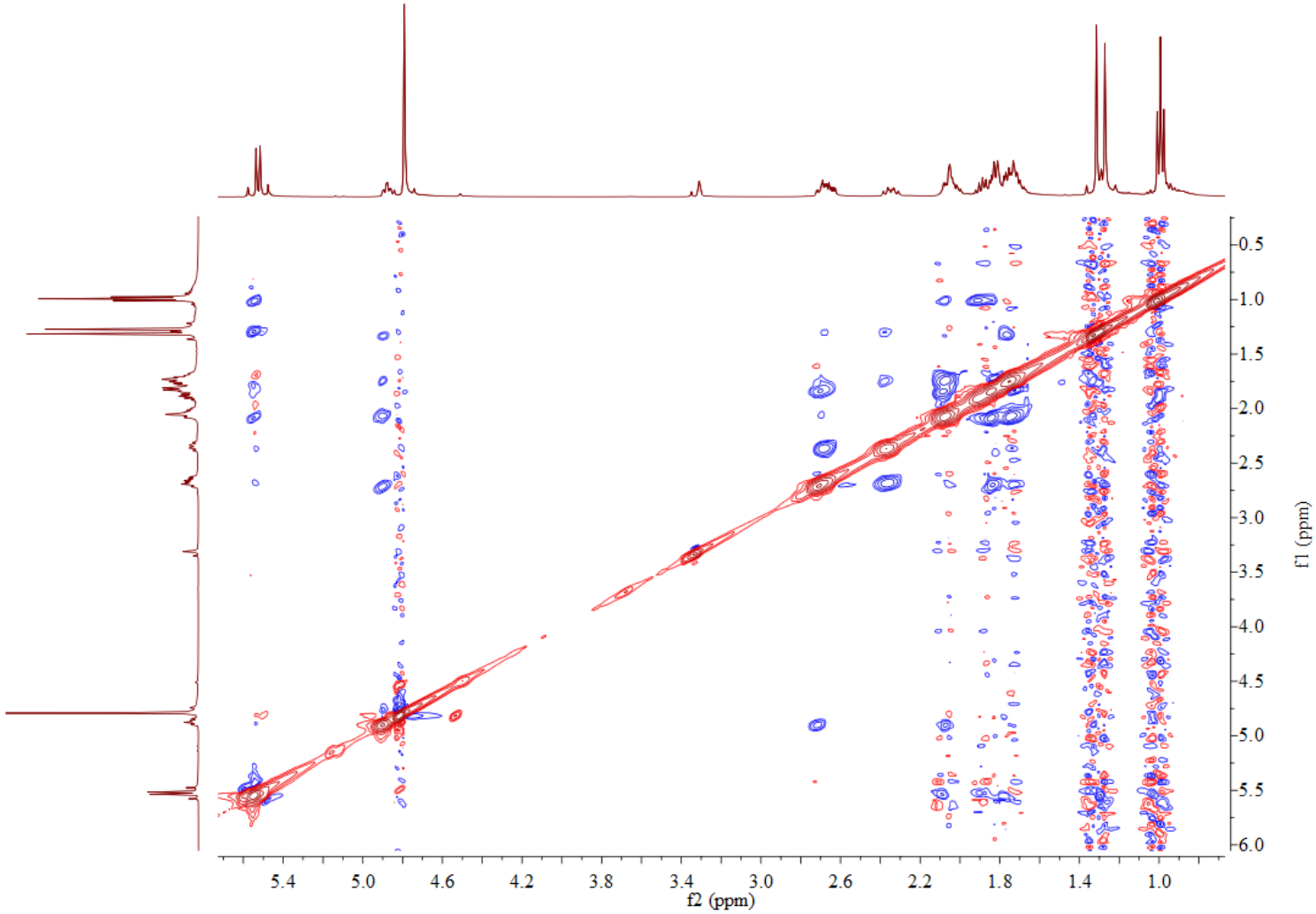
S39 HMBC spectrum of **6** in Methanol-d_4



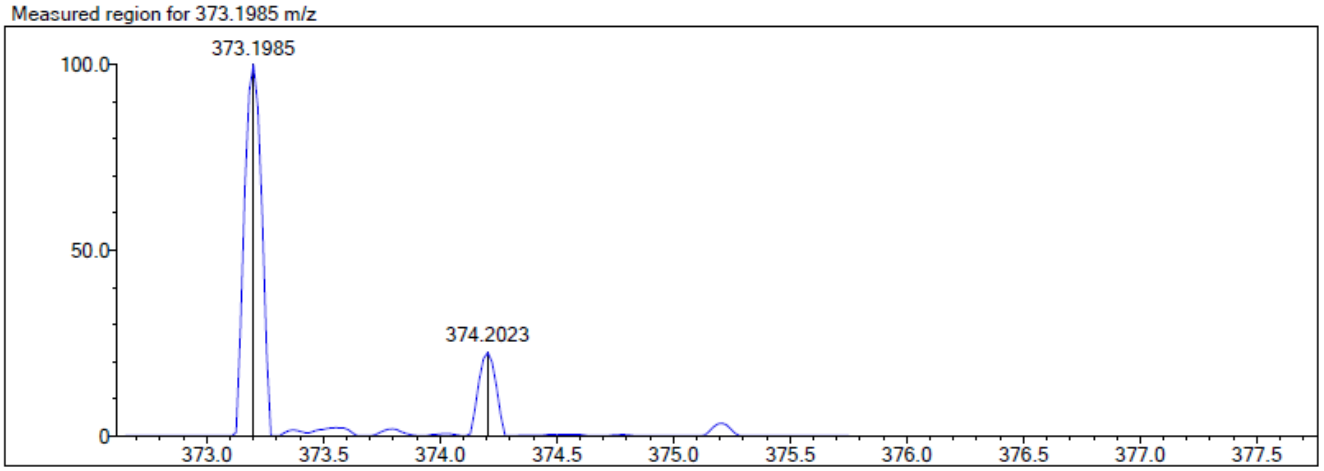
S40 $^{1}H–^{1}H$ COSY spectrum of **6** in Methanol-d_4

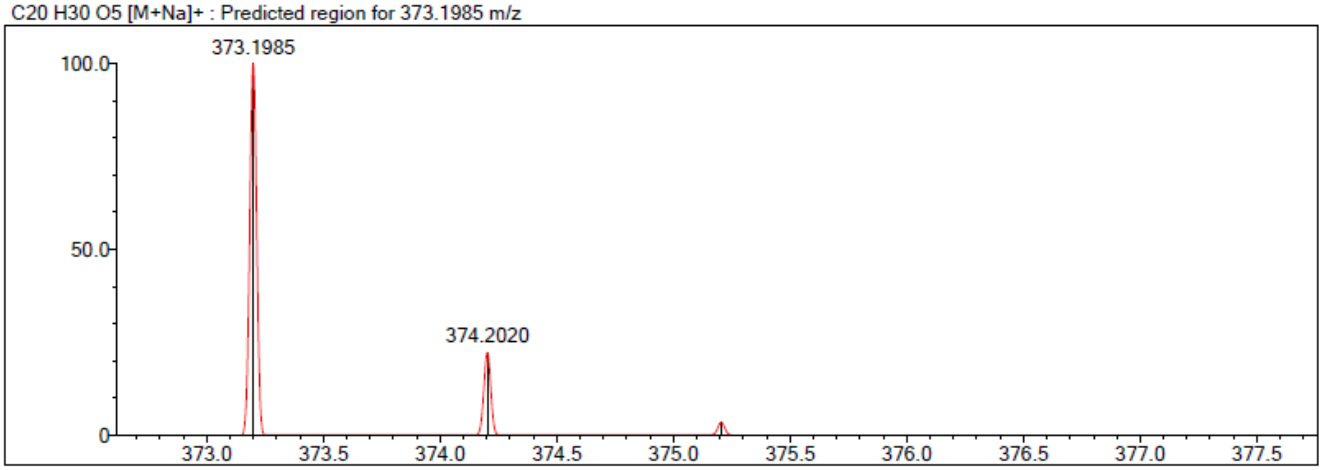


S41 NOESY spectrum of **6** in Methanol-d_4



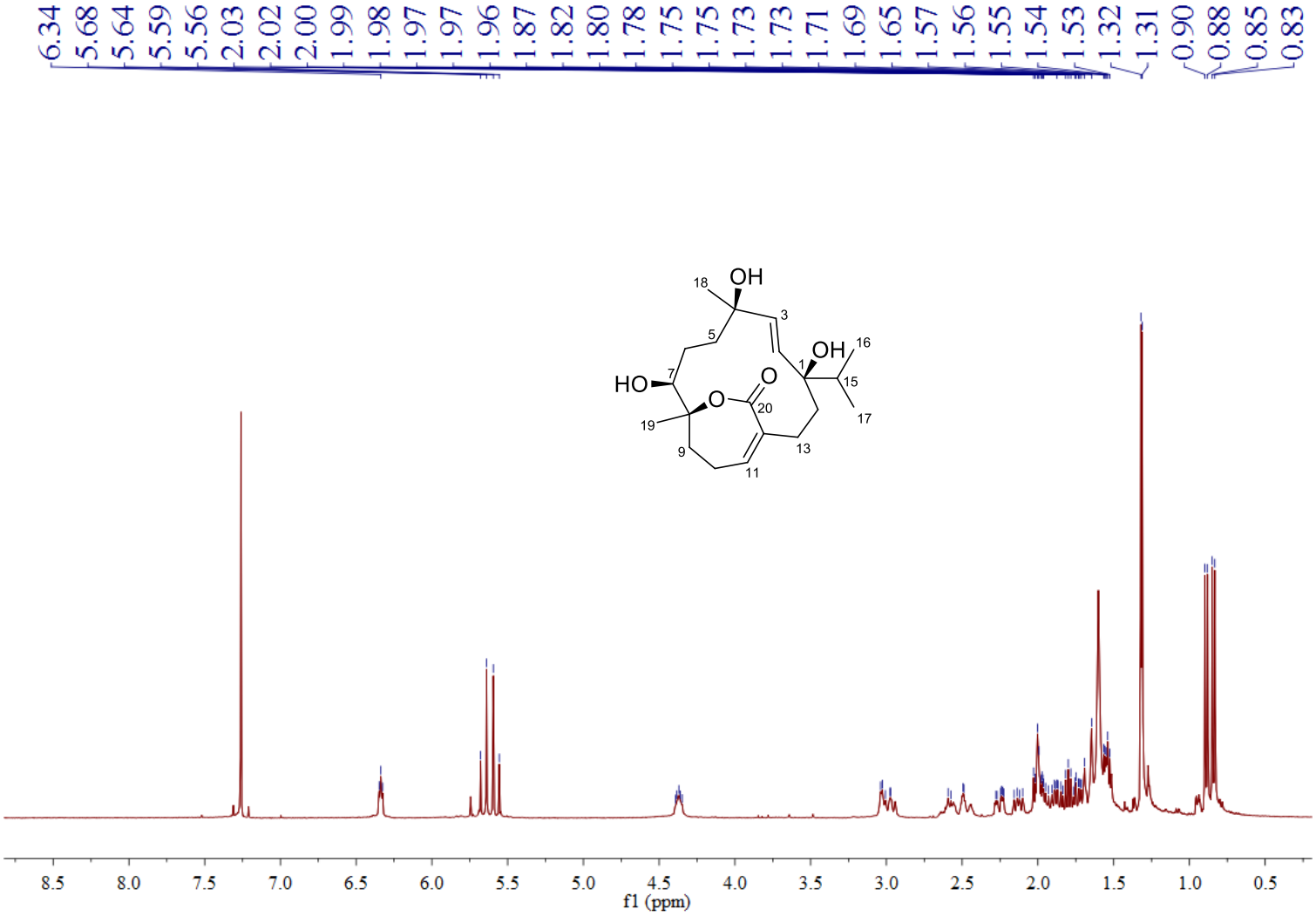
S42 HRESIMS spectrum of **6**



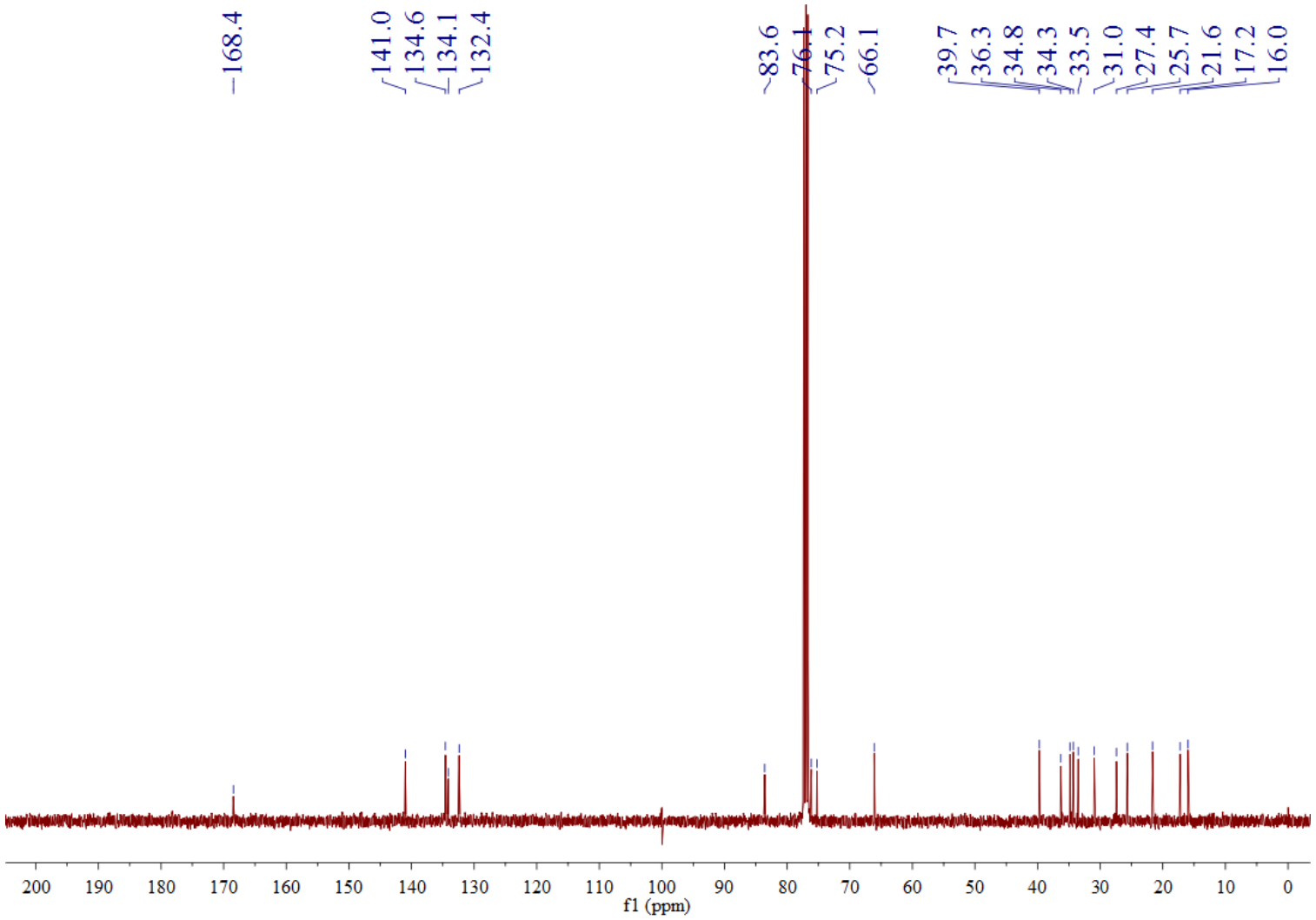


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	88.02	C20 H30 O5	[M+Na]+	373.1985	373.1985	-0.0	0.00	88.02	6.0

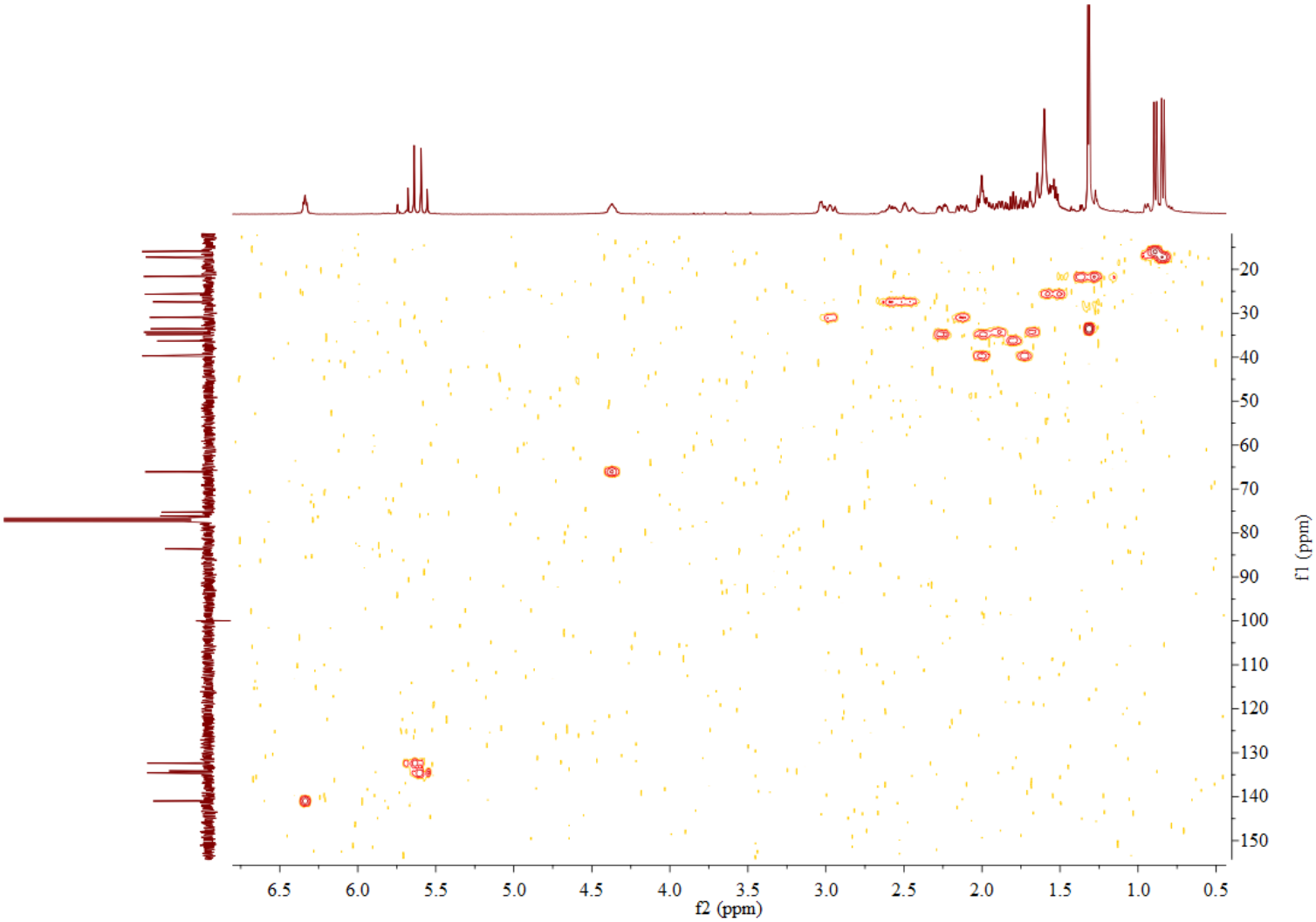
S43 ^{1}H NMR spectrum of **7** in $CDCl_3$



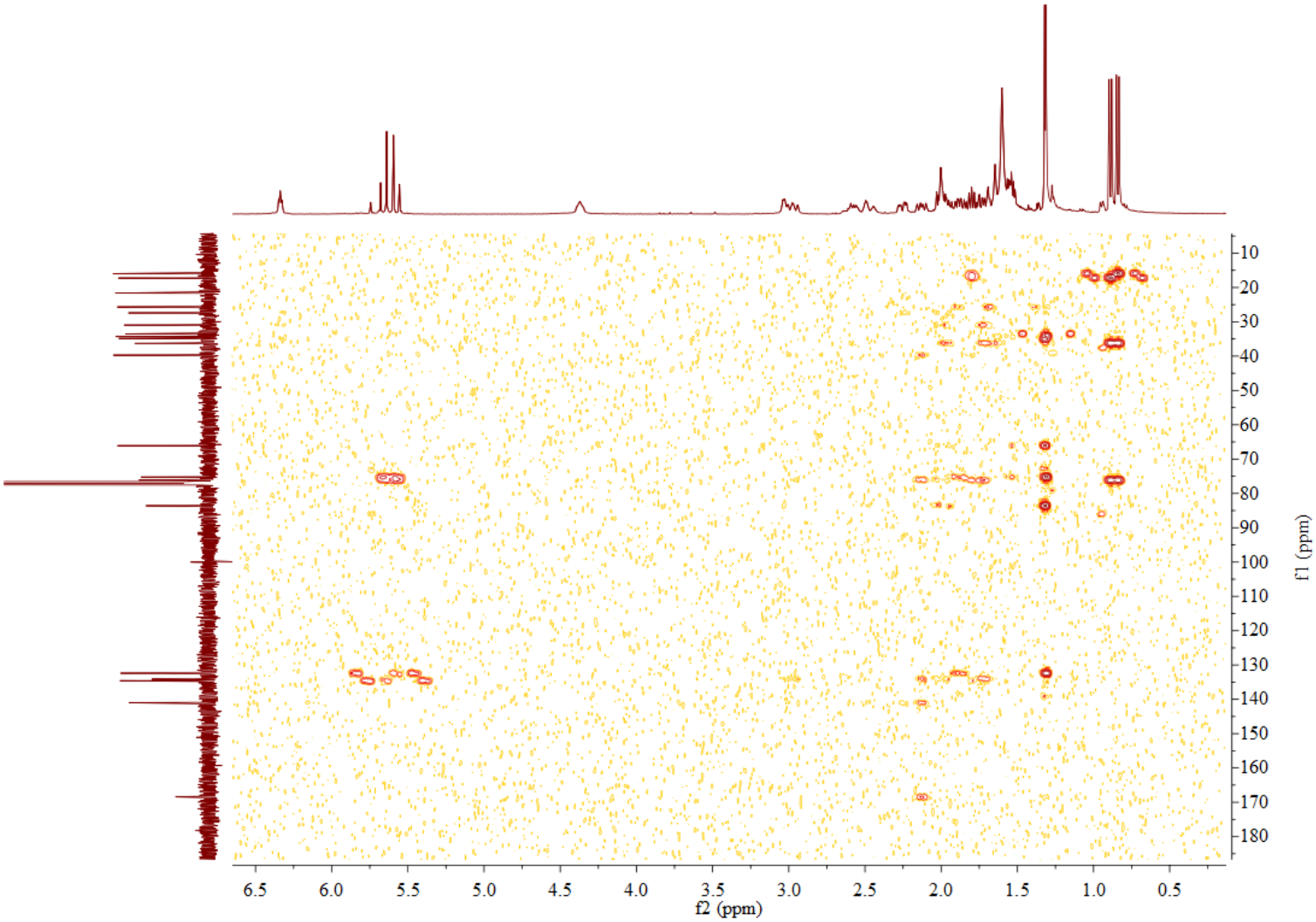
S44 ^{13}C NMR spectrum of **7** in $CDCl_3$



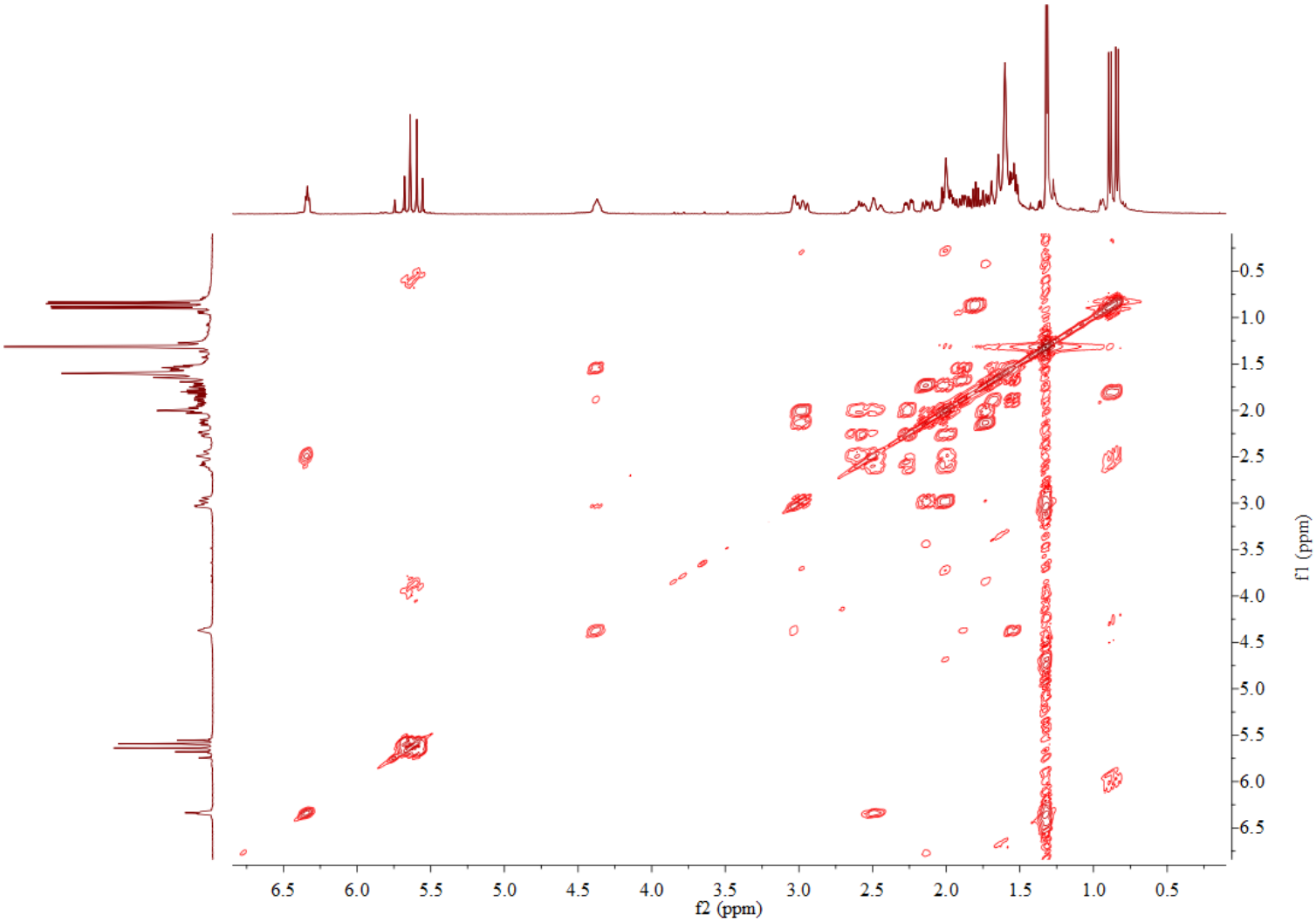
S45 HSQC spectrum of **7** in $CDCl_3$



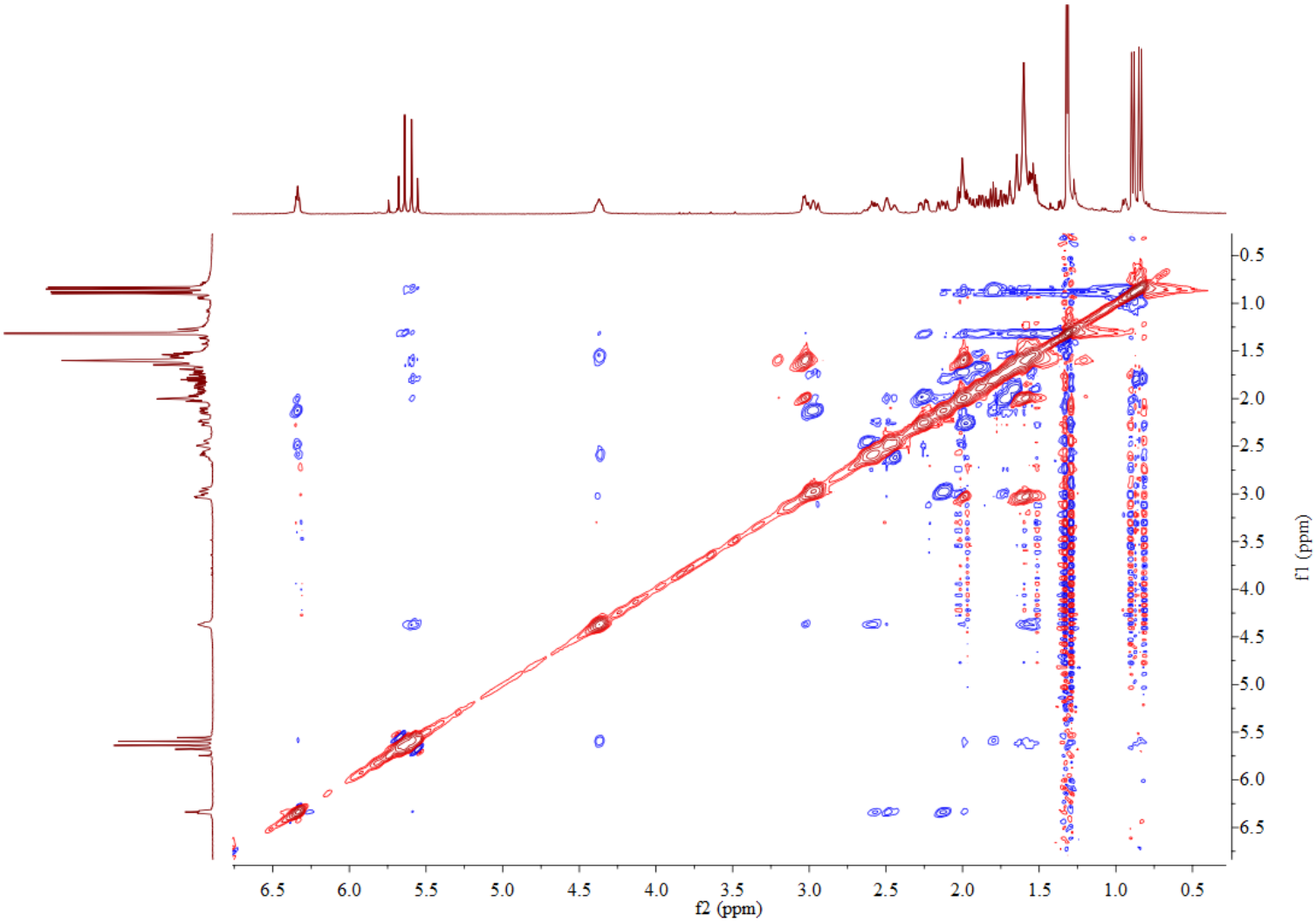
S46 HMBC spectrum of **7** in $CDCl_3$



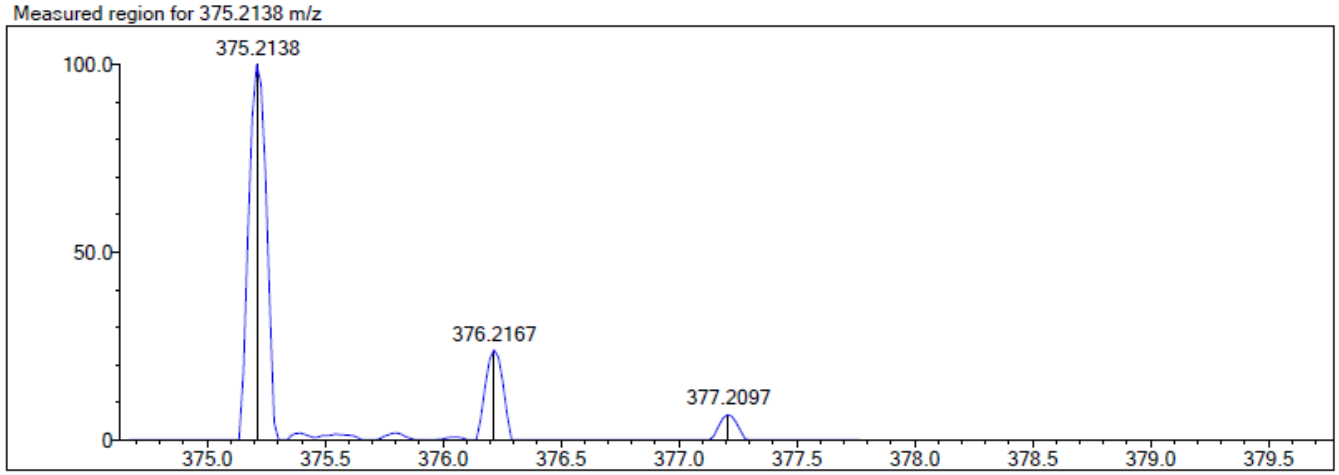
S47 $^{1}H–^{1}H$ COSY spectrum of **7** in $CDCl_3$

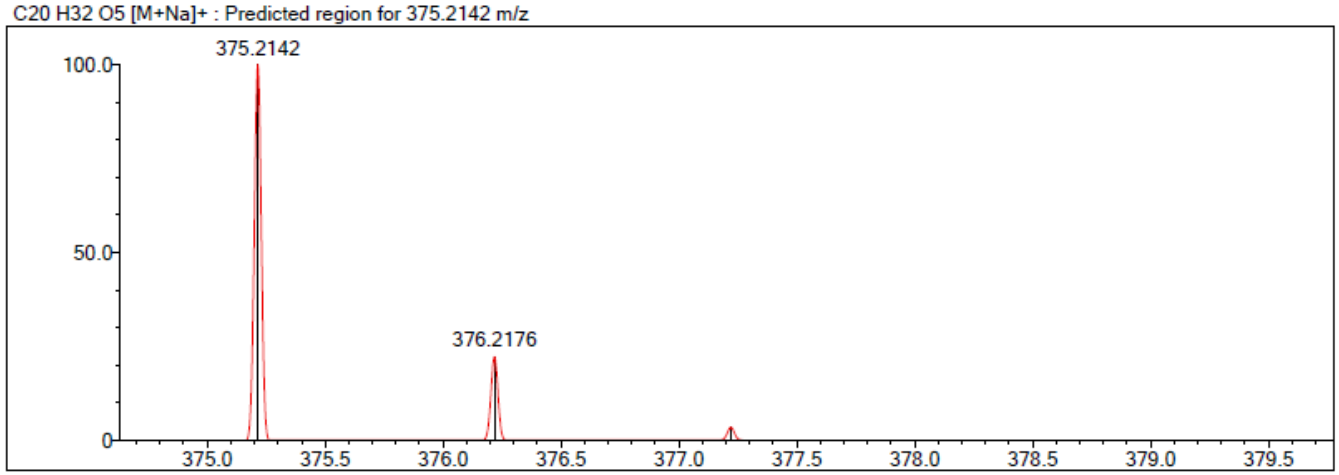


S48 NOESY spectrum of **7** in $CDCl_3$



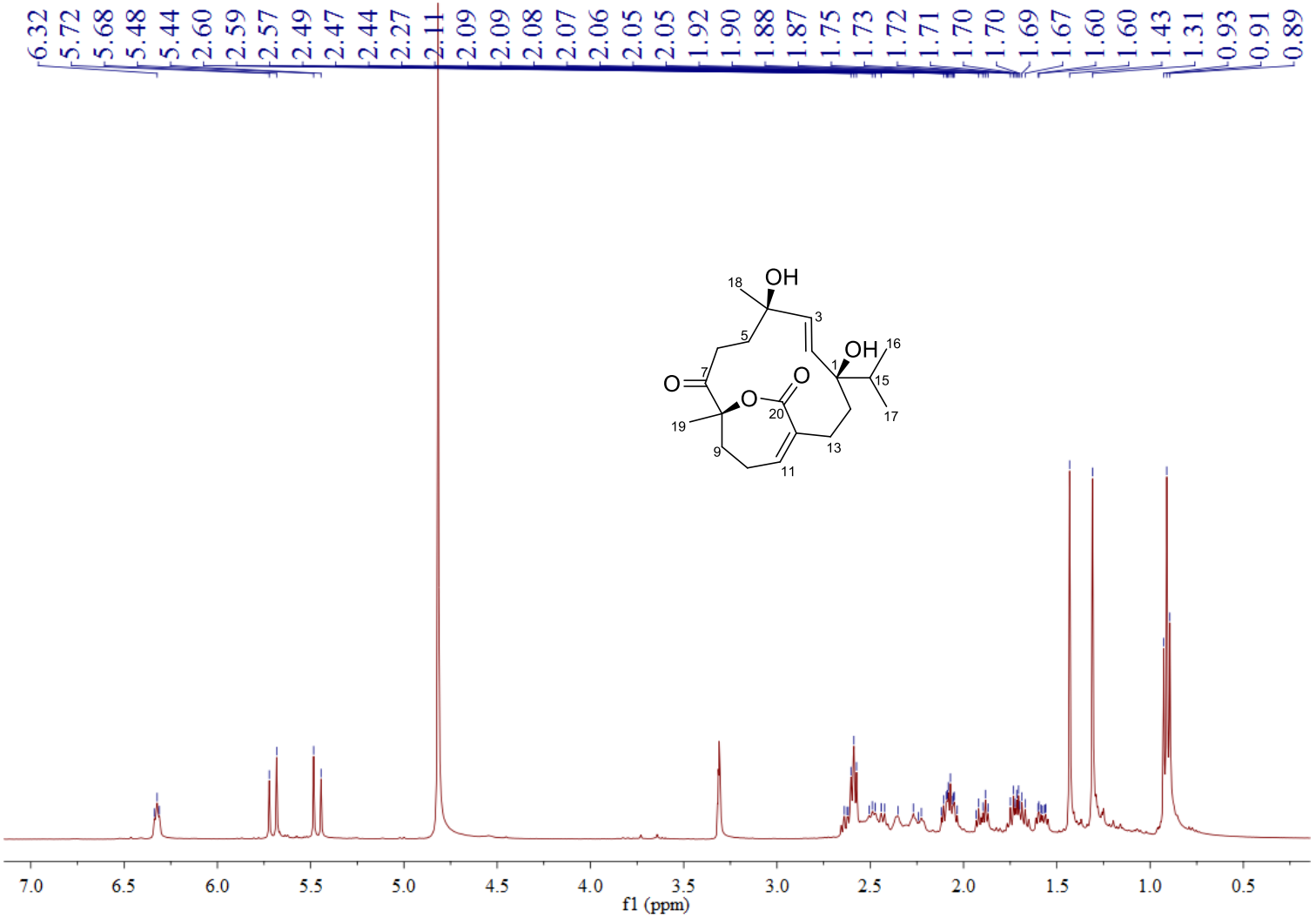
S49 HRESIMS spectrum of **7**



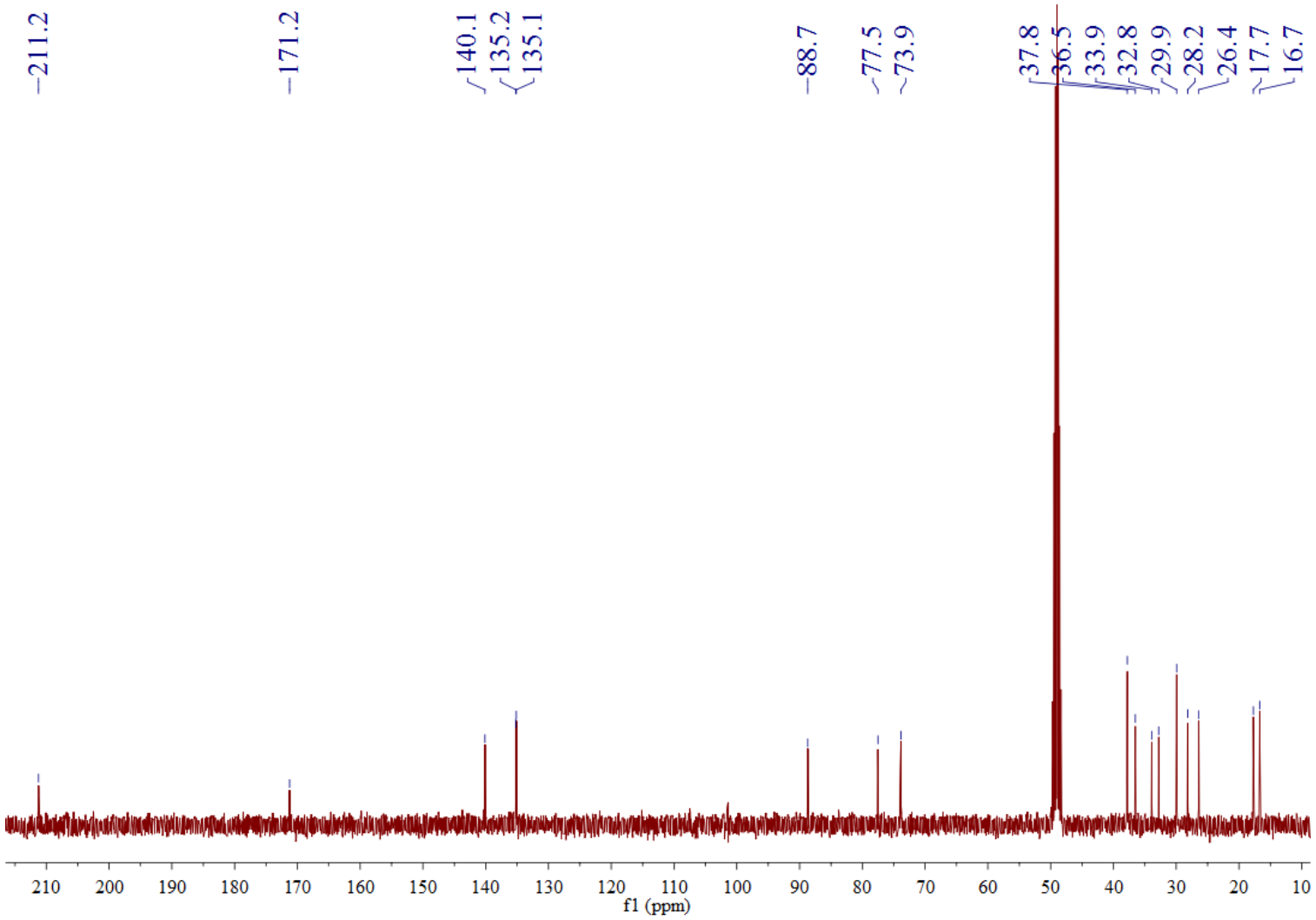


Rank	Score	Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	Iso	DBE
1	67.27	C20 H32 O5	[M+Na]+	375.2138	375.2142	-0.4	-1.07	67.38	5.0

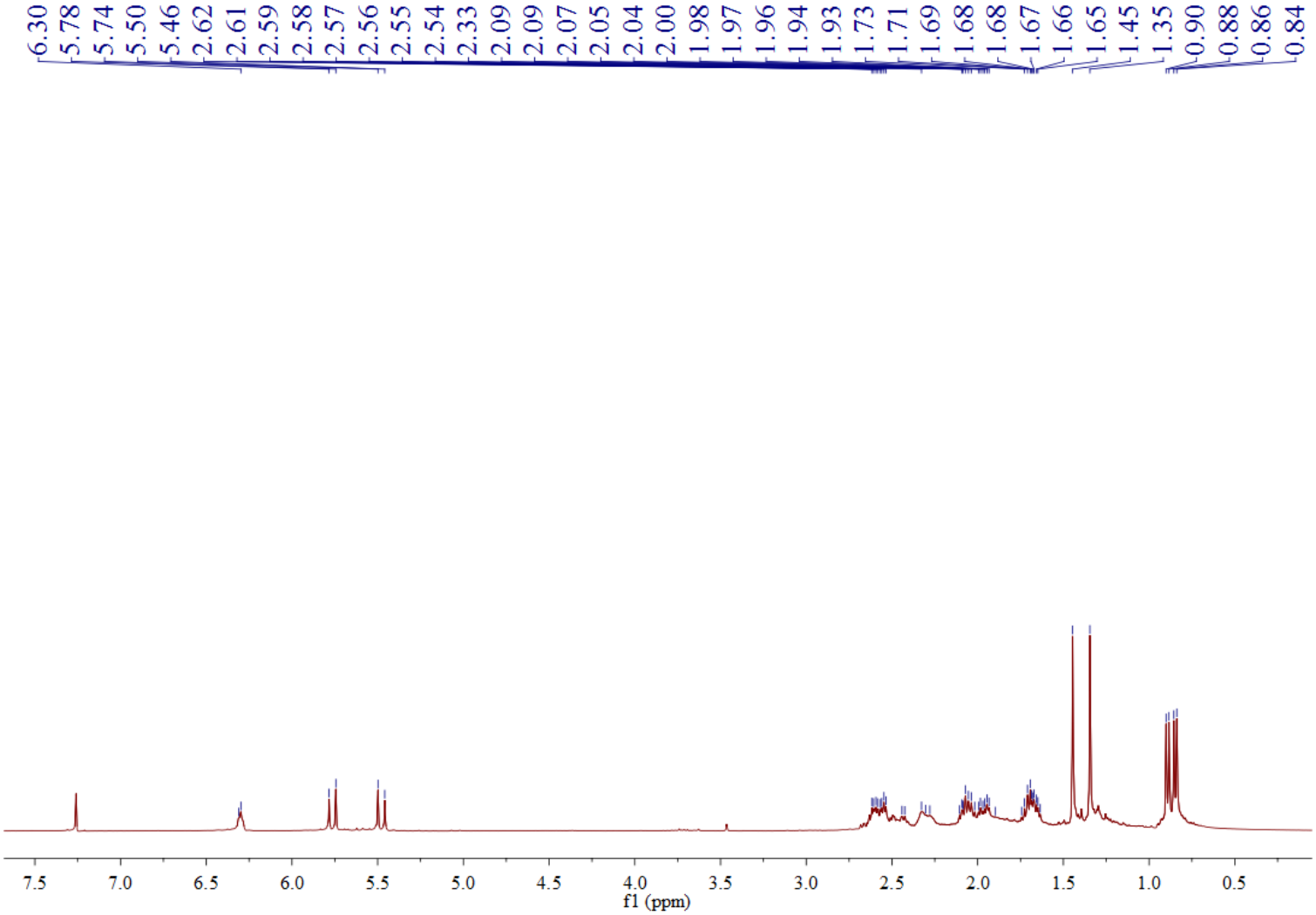
S50 ^{1}H NMR spectrum of **8** in Methanol-d_4



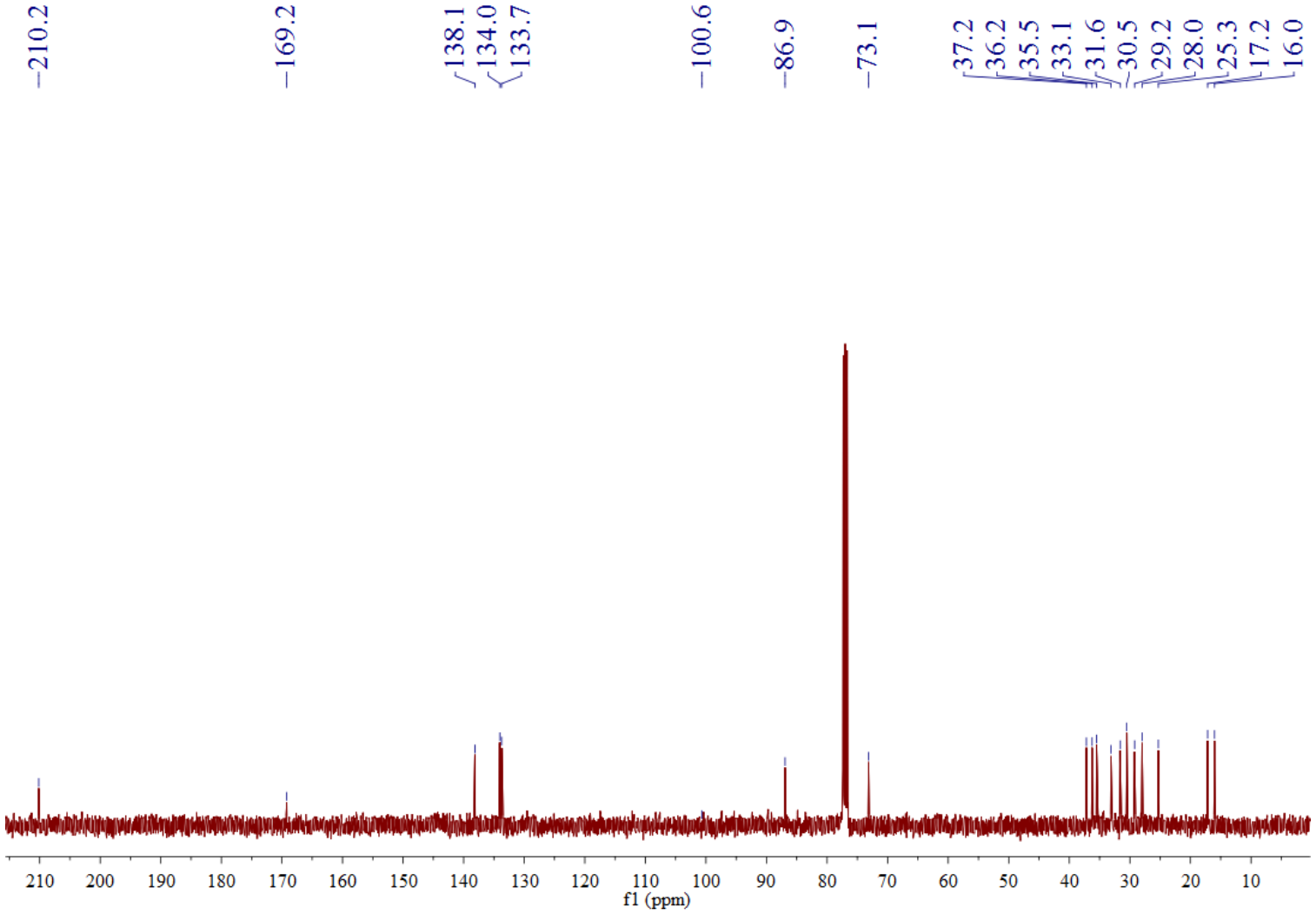
S51 ^{13}C NMR spectrum of **8** in Methanol-d_4



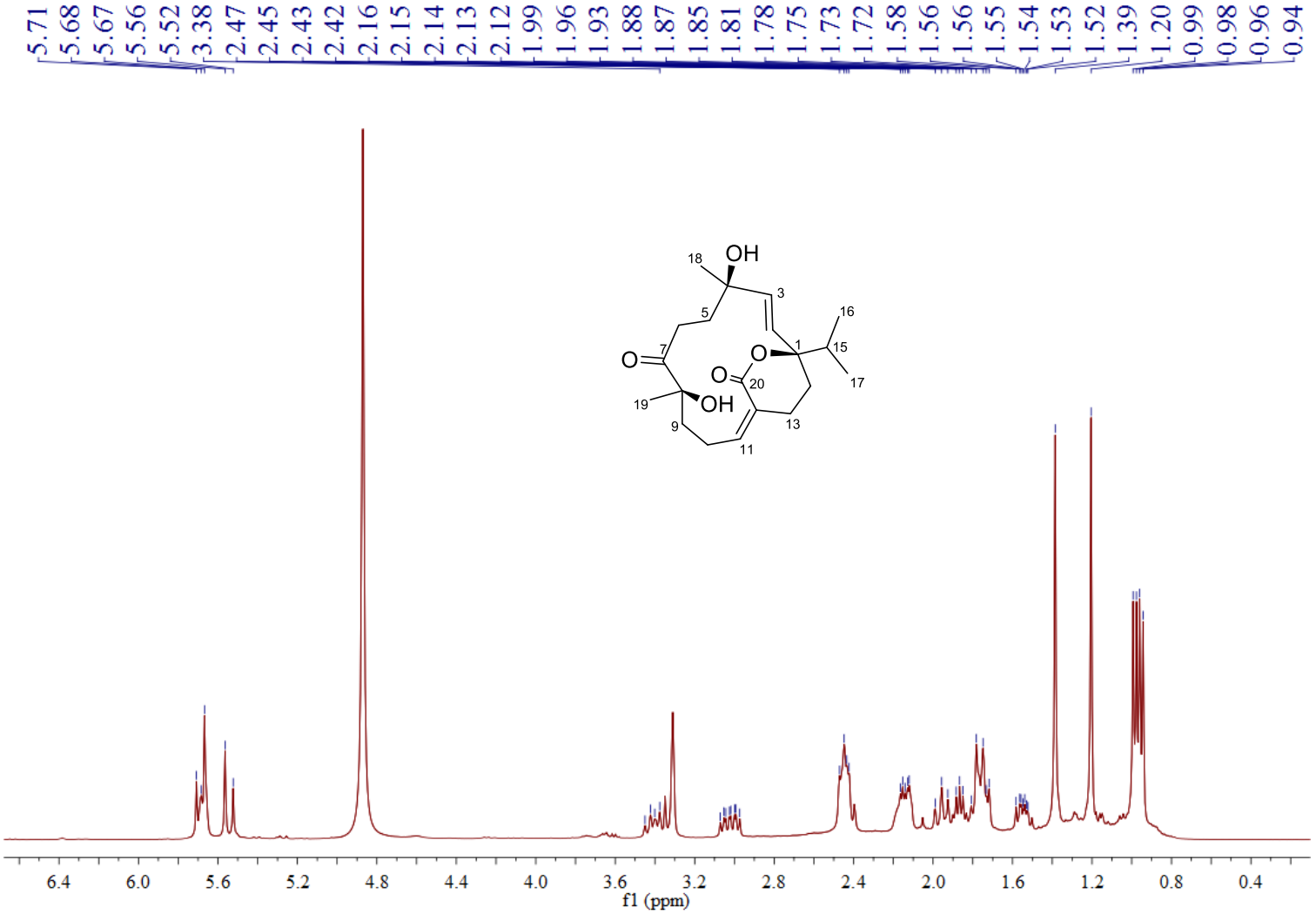
S52 ^{1}H NMR spectrum of **8** in $CDCl_3$



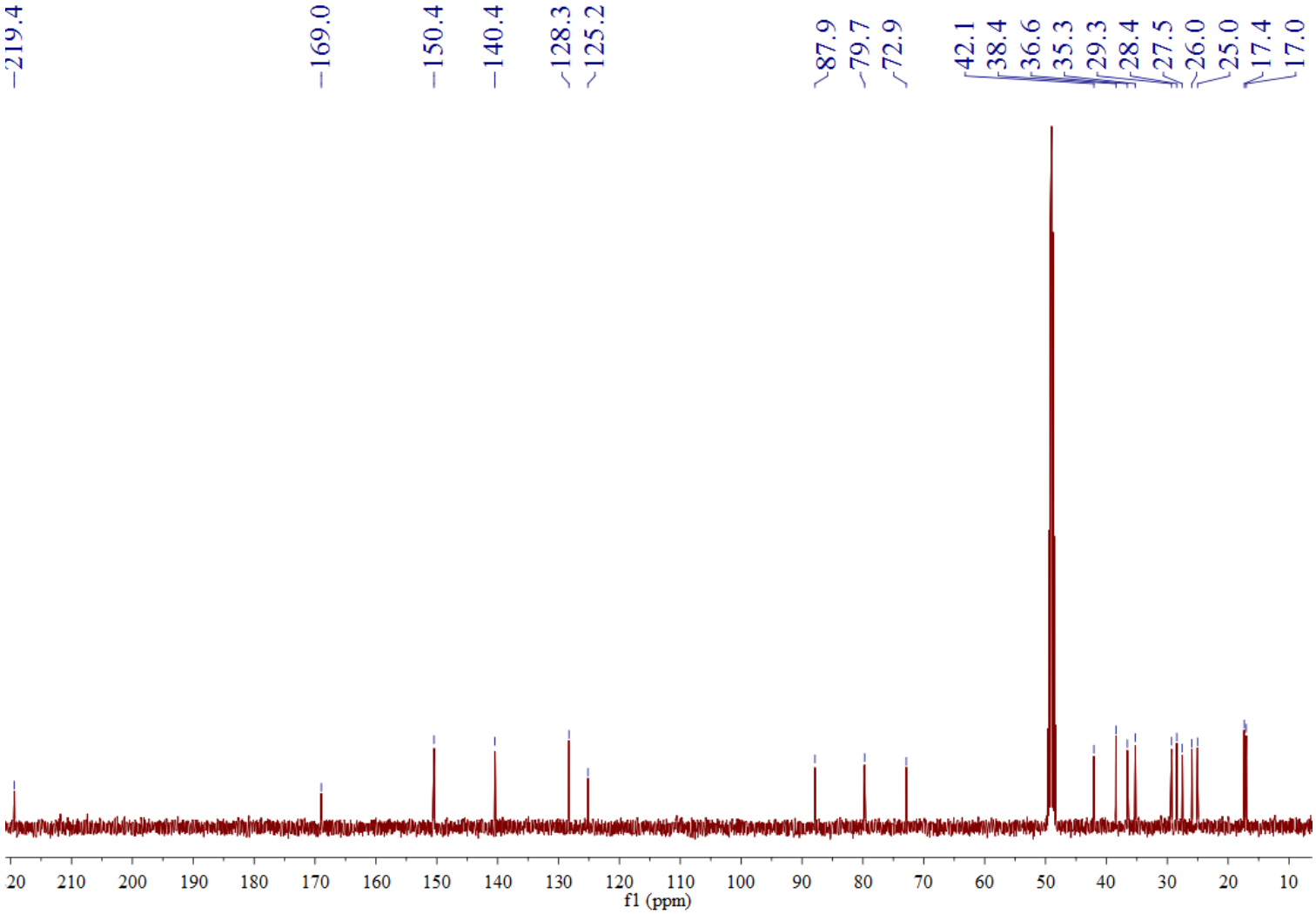
S53 ^{13}C NMR spectrum of **8** in $CDCl_3$



S54 ^{1}H NMR spectrum of **9** in Methanol-d_4



S55 ^{13}C NMR spectrum of **9** in Methanol-d_4



S56 Selected NOESY ( ) correlations of **2**.