

Figure S1:  $^1\text{H}$  NMR of compound 1 ( $\text{CDCl}_3$ )

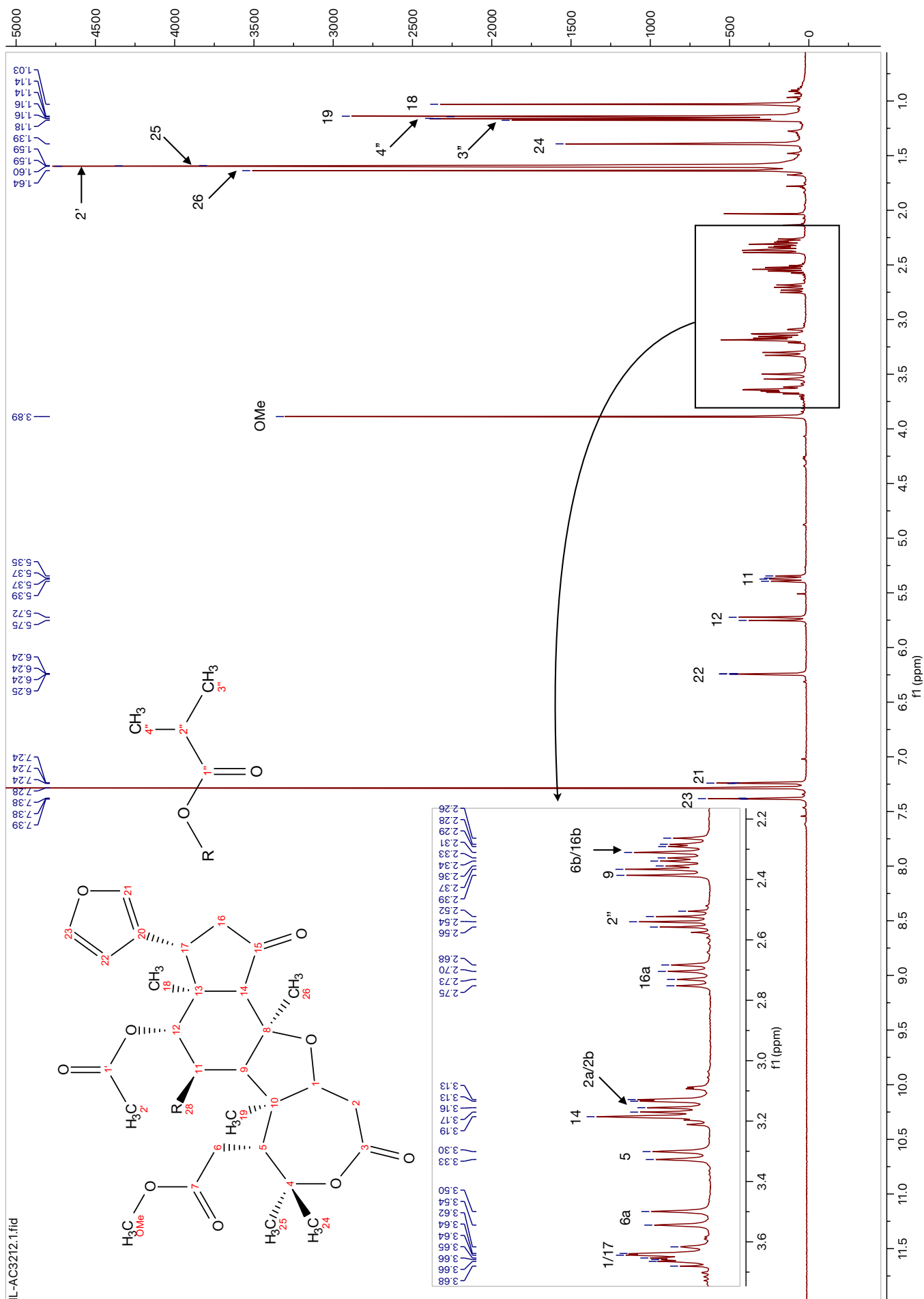


Figure S2:  $^{13}\text{C}$  NMR of compound 1 ( $\text{CDCl}_3$ )

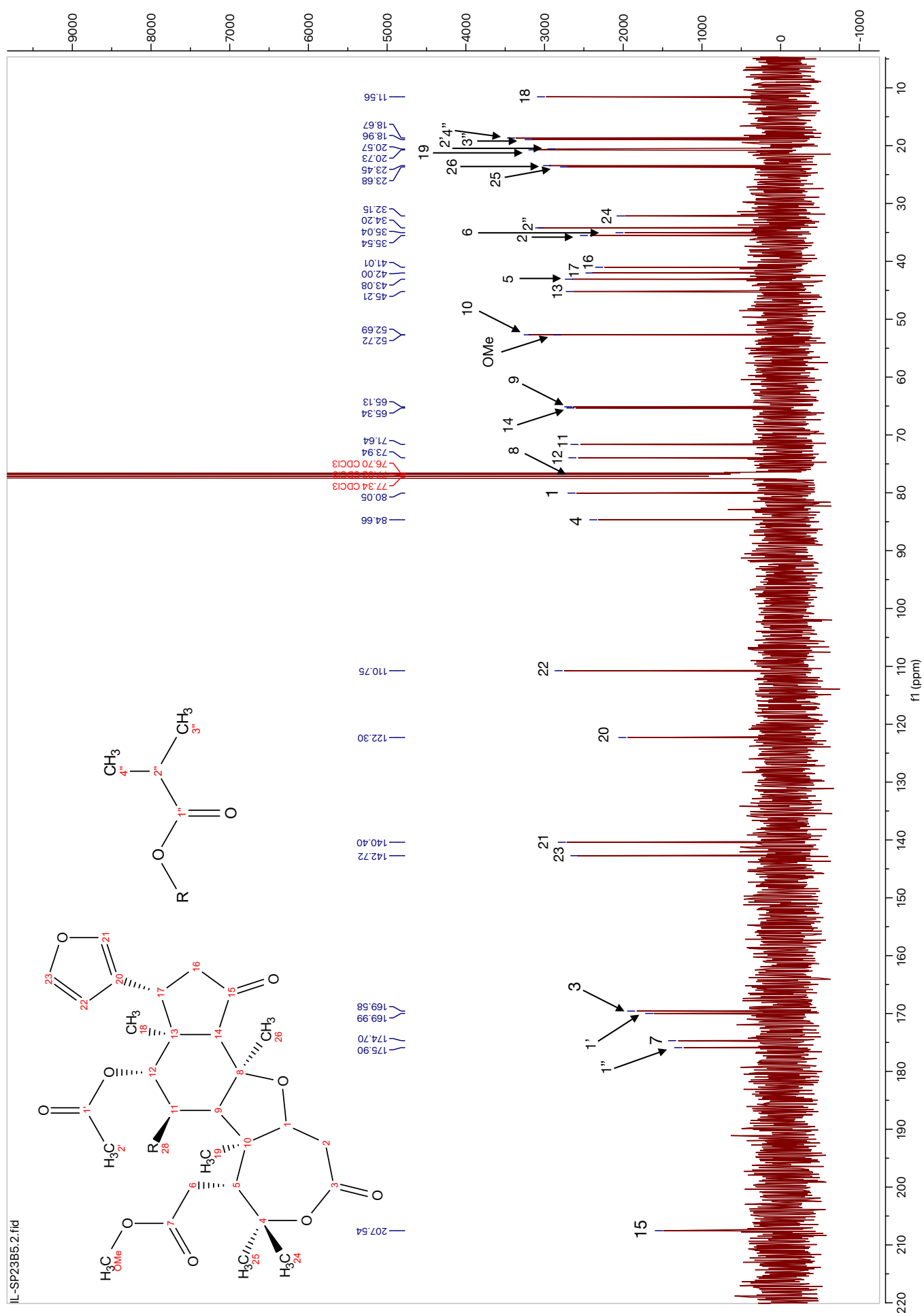


Figure S3: COSY experiment of compound 1 (CDCl<sub>3</sub>)

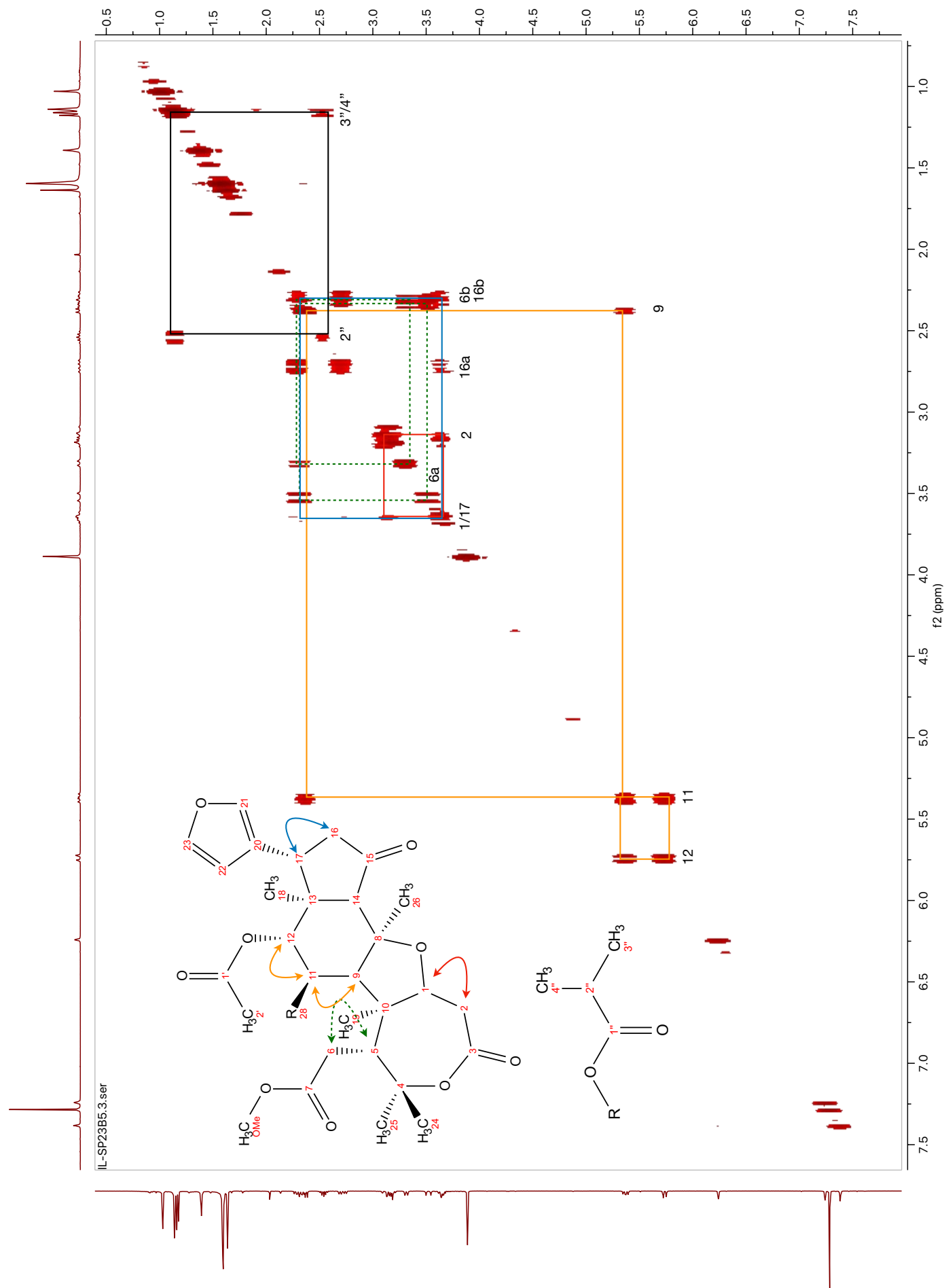


Figure S4: HMQC experiment of compound 1 ( $\text{CDCl}_3$ )<sub>3</sub>

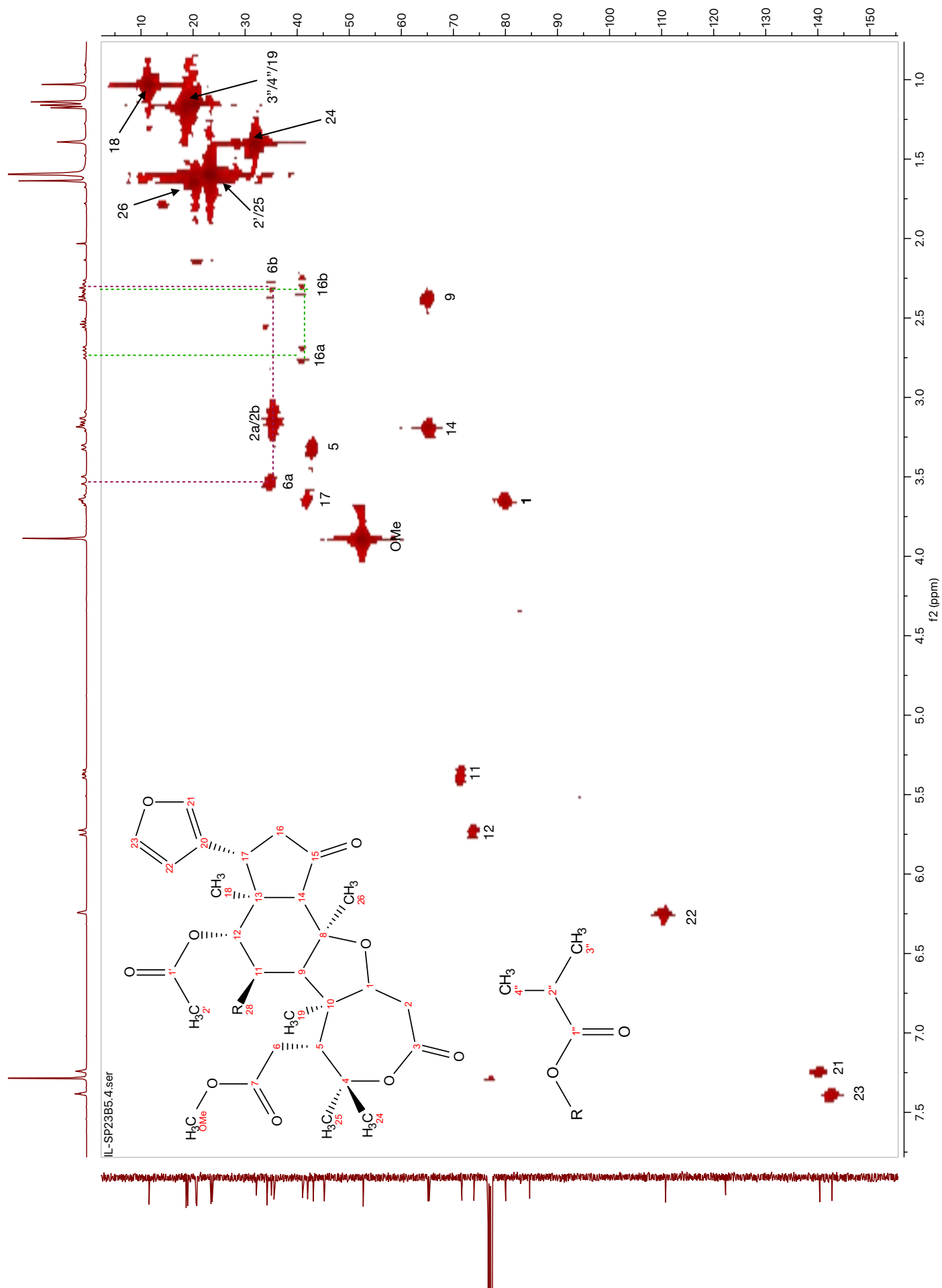




Figure S5: HMBC experiment of compound 1 (CDCl<sub>3</sub>)

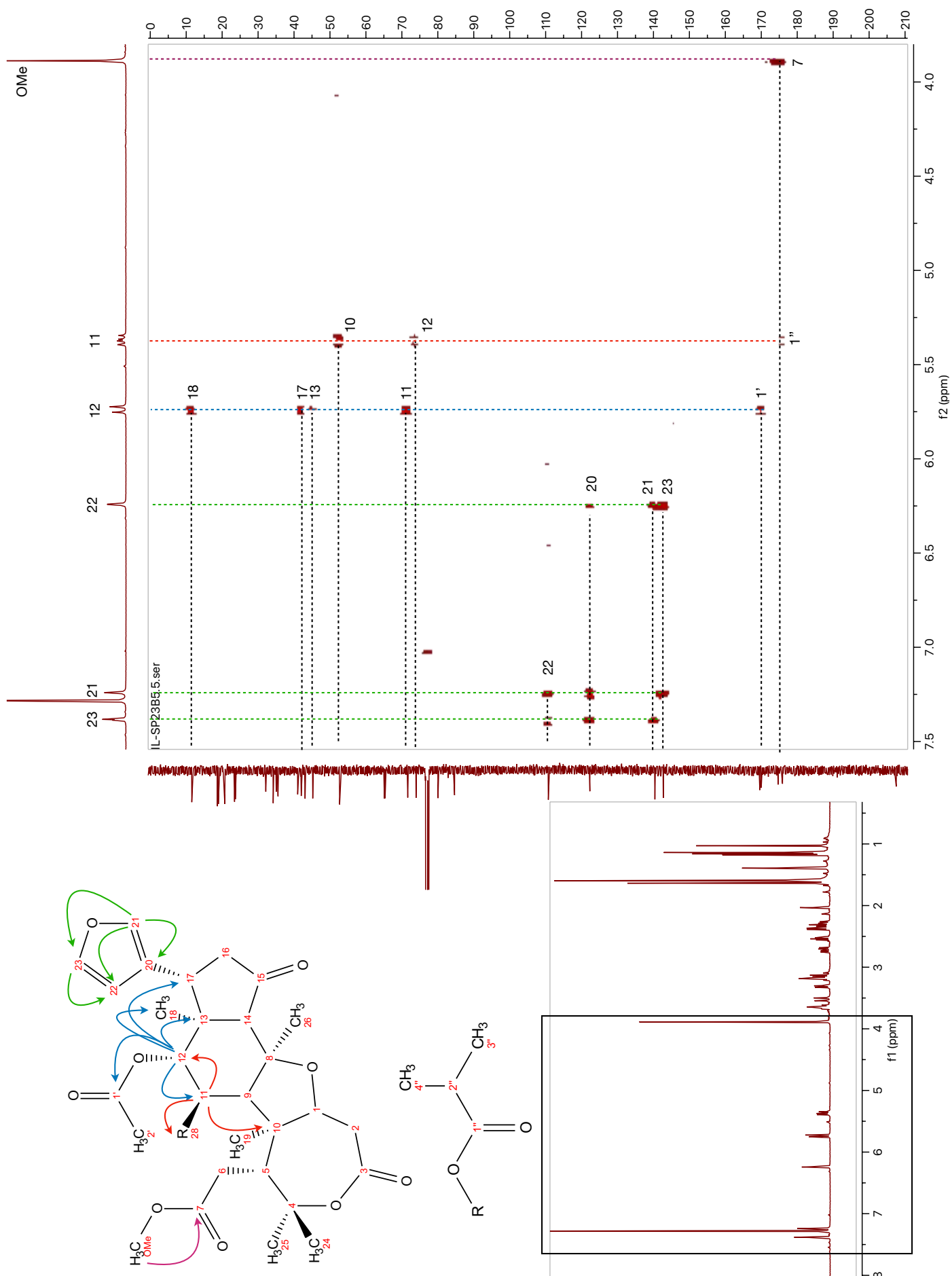


Figure S6: HMBC experiment of compound 1 (CDCl<sub>3</sub>)

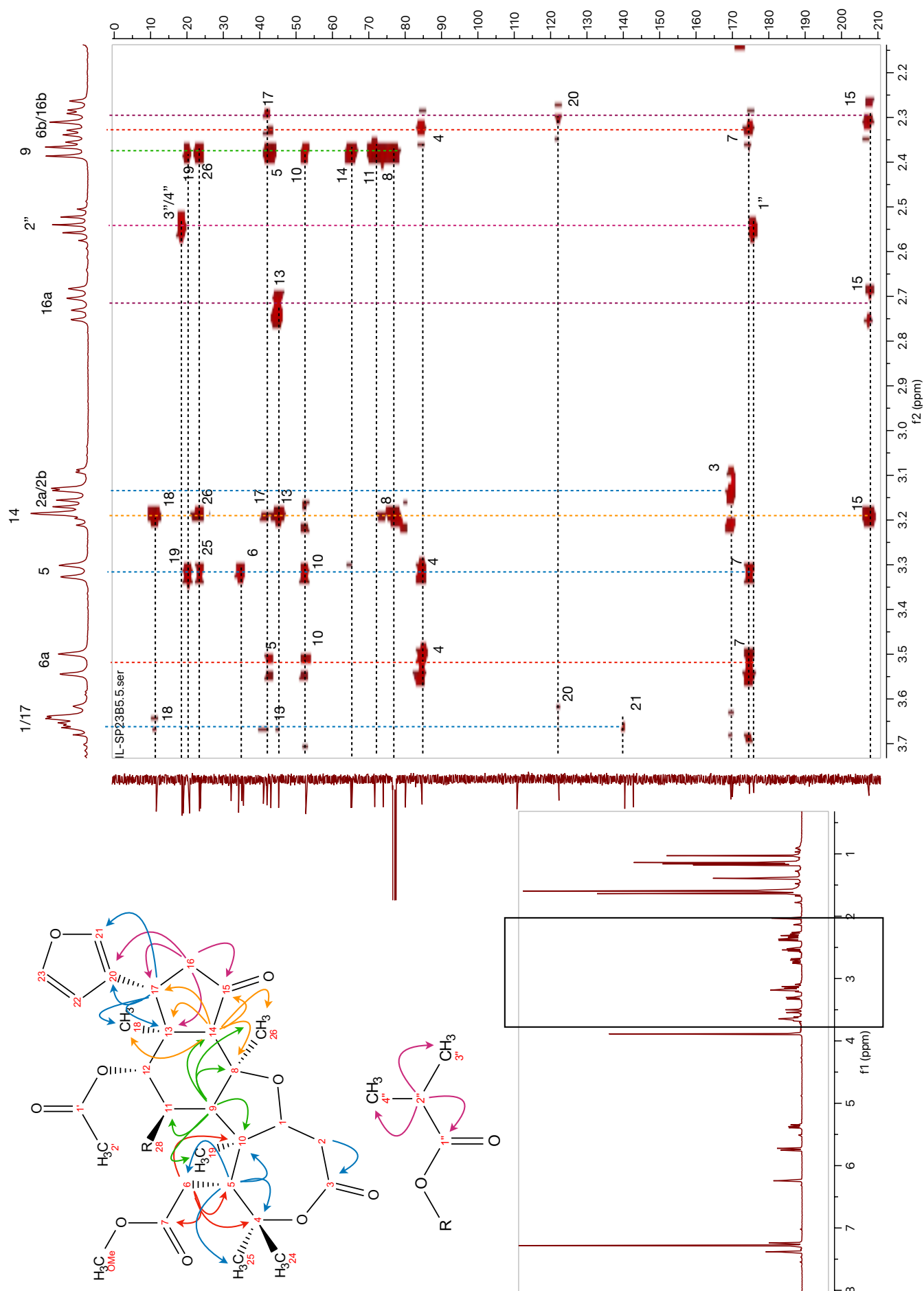


Figure S7: HMBC experiment of compound 1 (CDCl<sub>3</sub>)

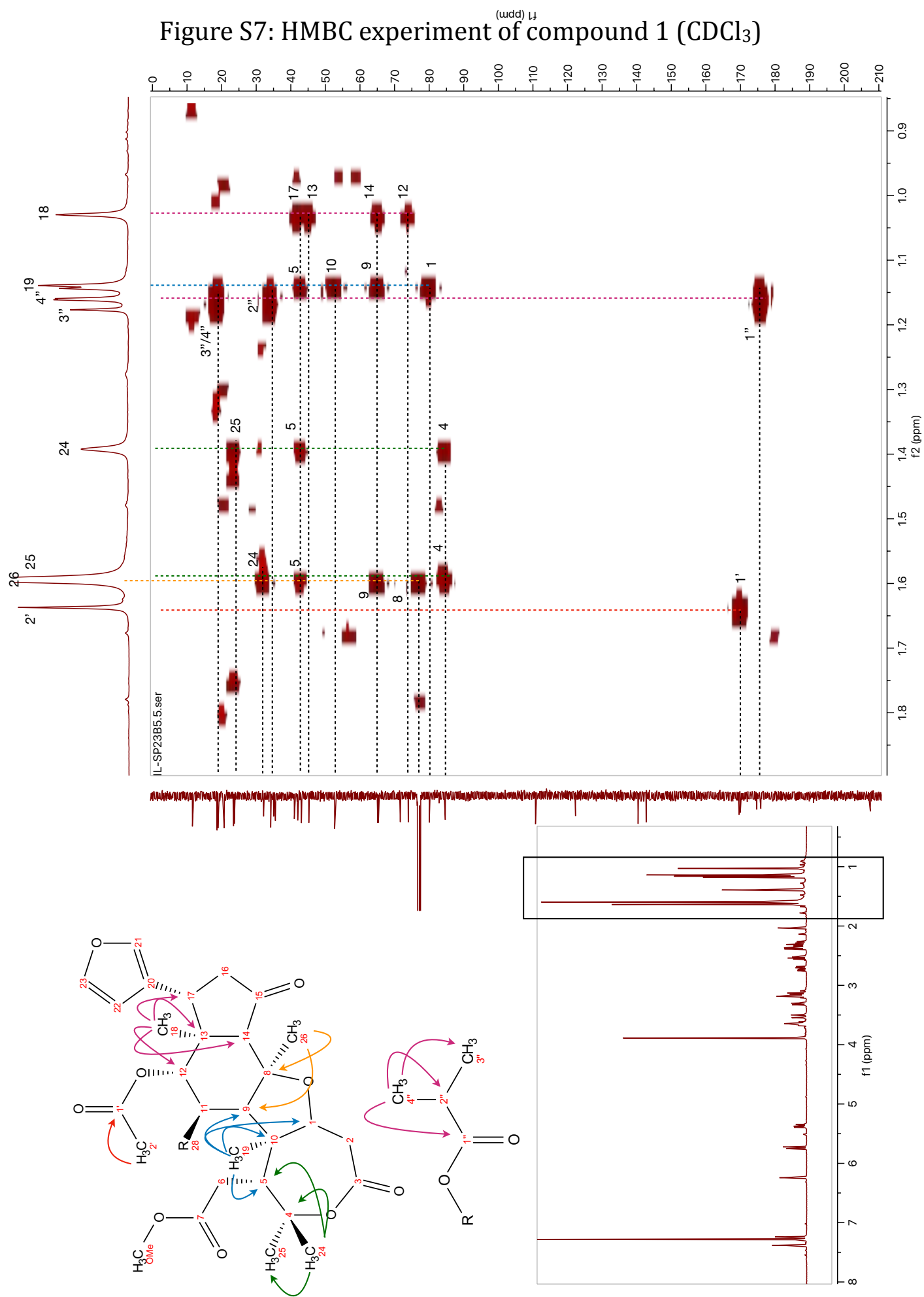


Figure S8: NOESY experiment of compound 1 ( $\text{CDCl}_3$ )

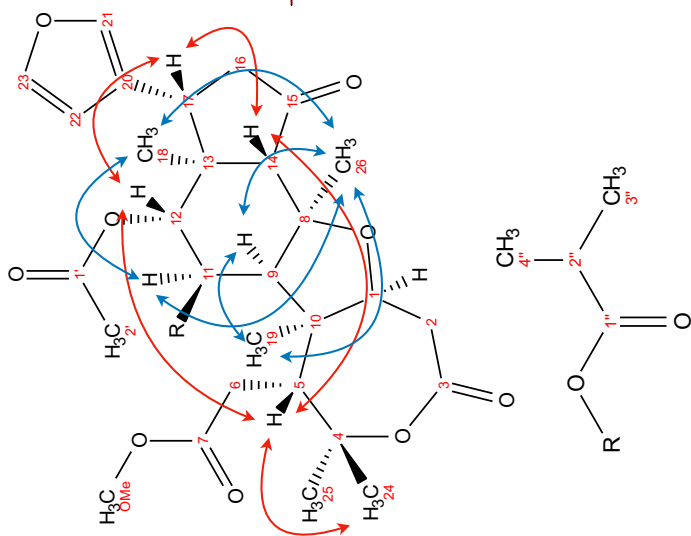
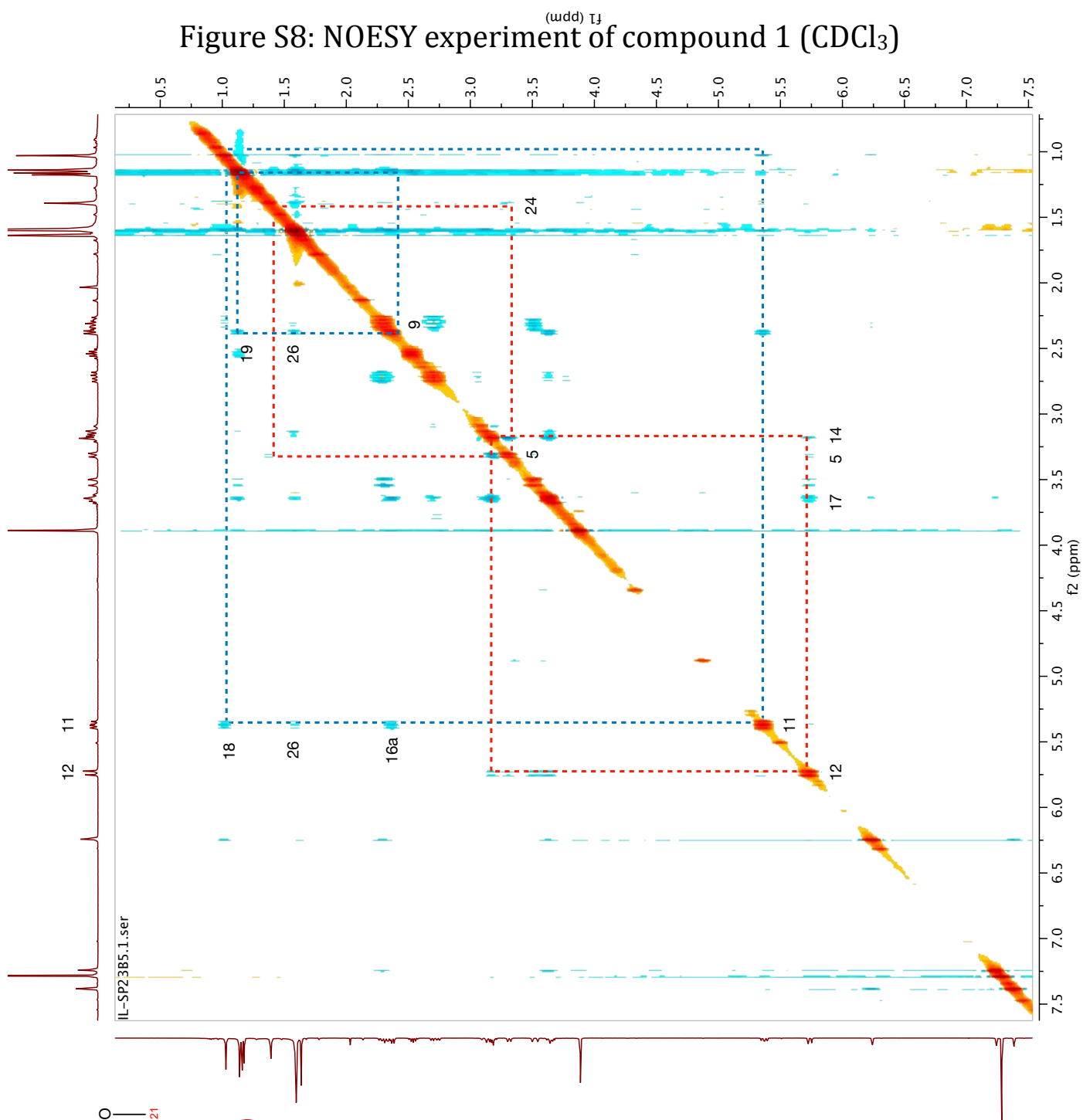


Figure S9: HRMS and IR spectra of compound 1

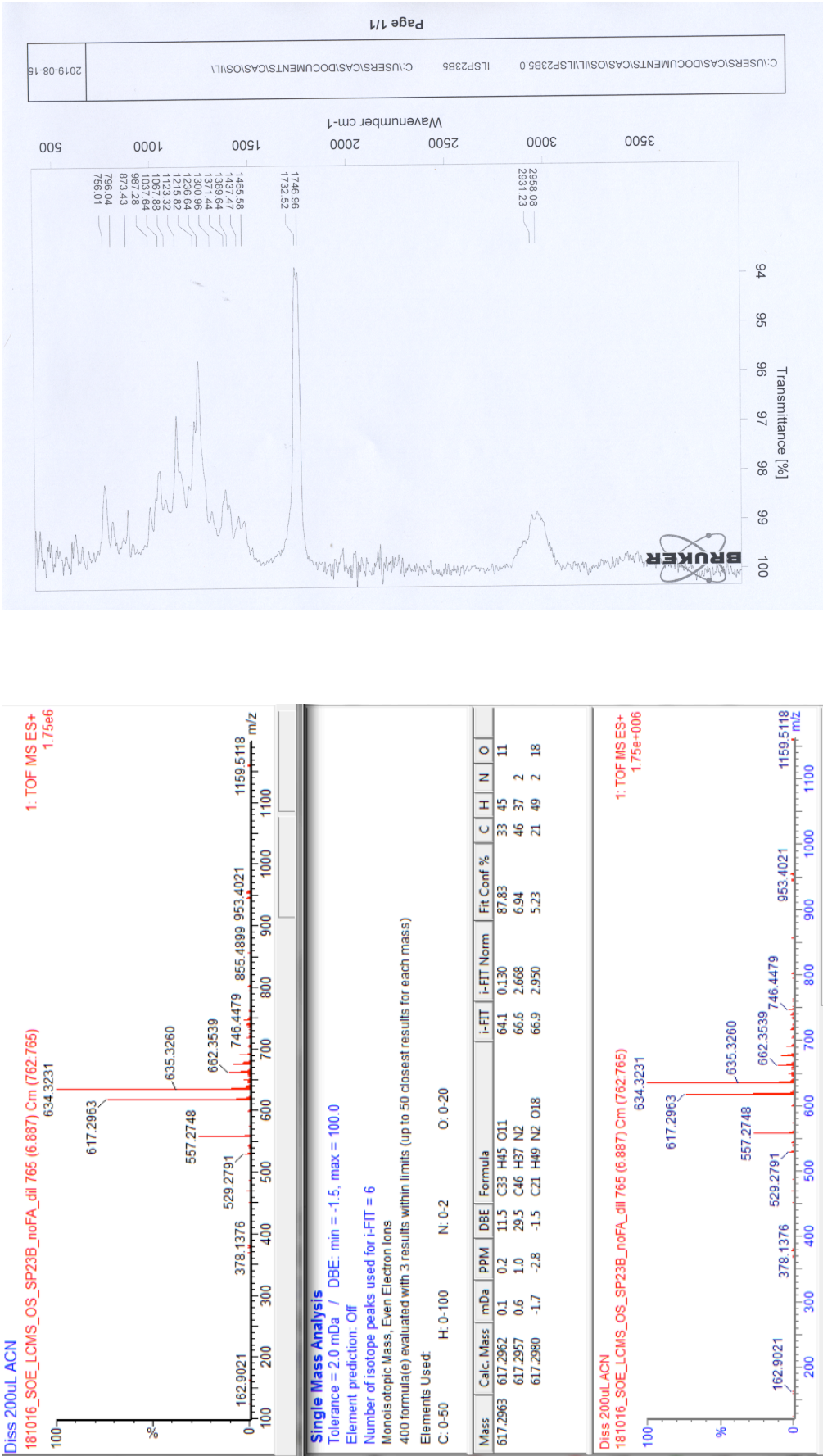


Figure S10:  $^1\text{H}$  NMR of compound 2 ( $\text{CDCl}_3$ )

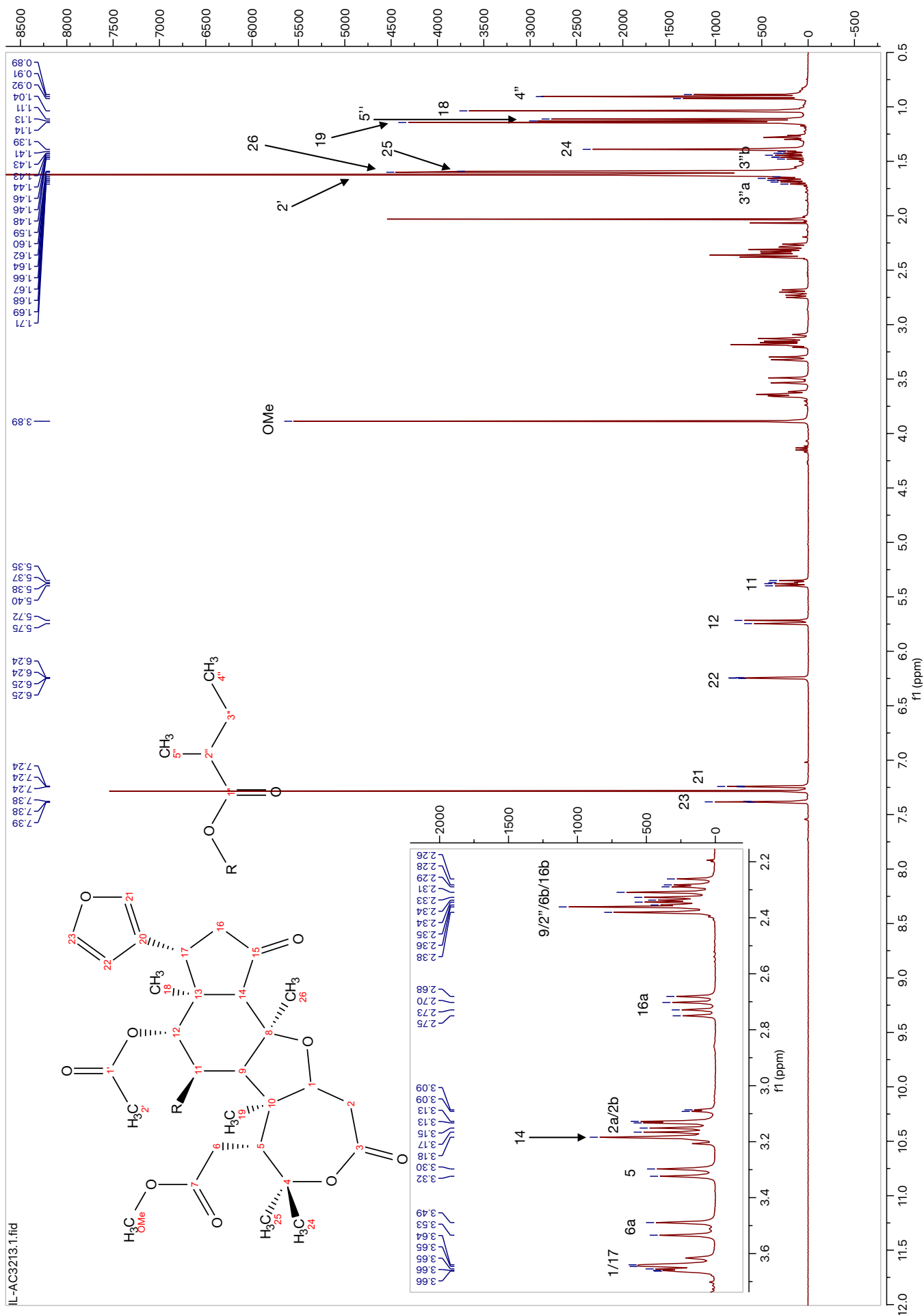


Figure S11:  $^{13}\text{C}$  NMR of compound 2 ( $\text{CDCl}_3$ )

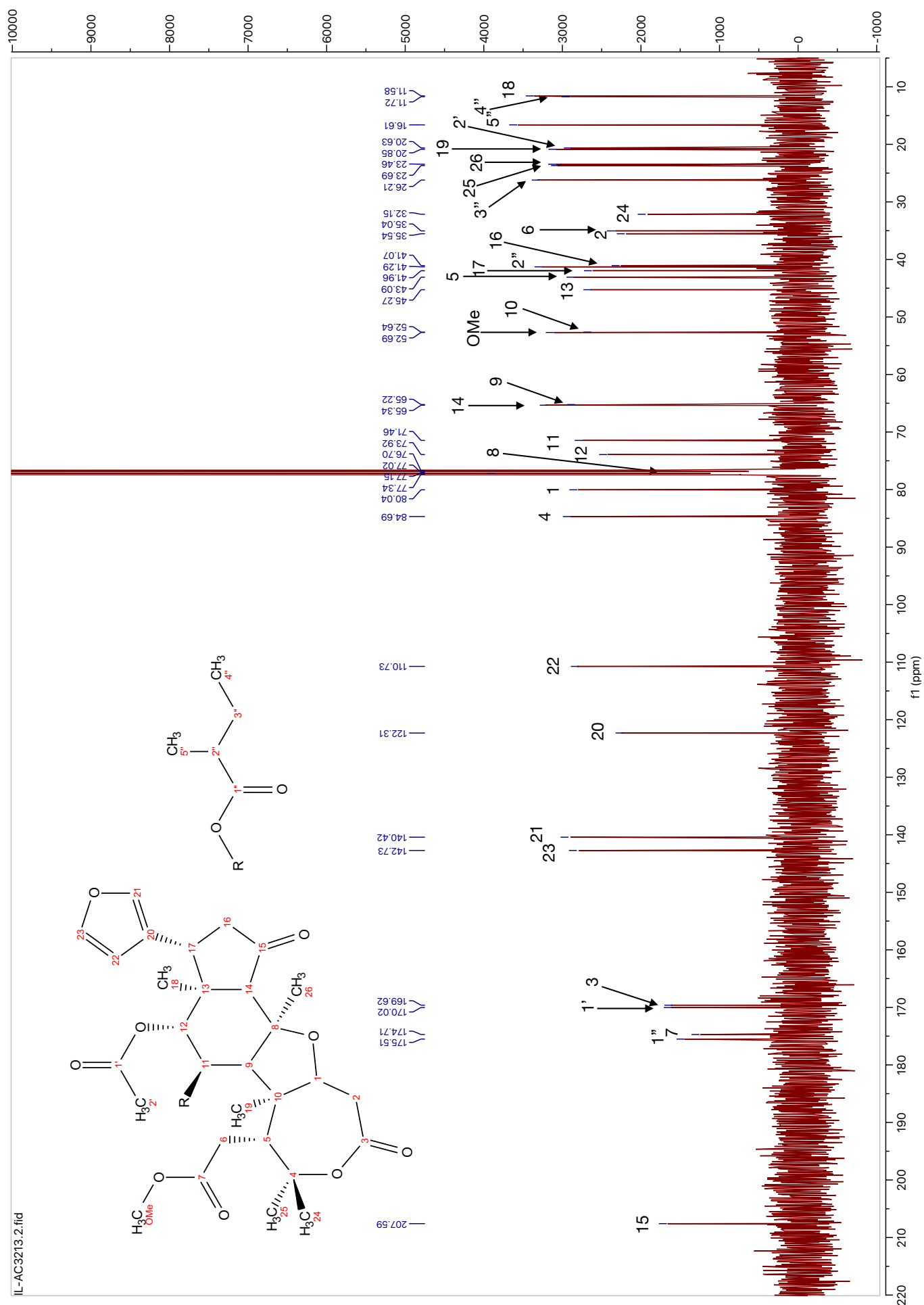


Figure S12:  $^{13}\text{C}$  NMR and DEPT135 of compound 2 ( $\text{CDCl}_3$ )

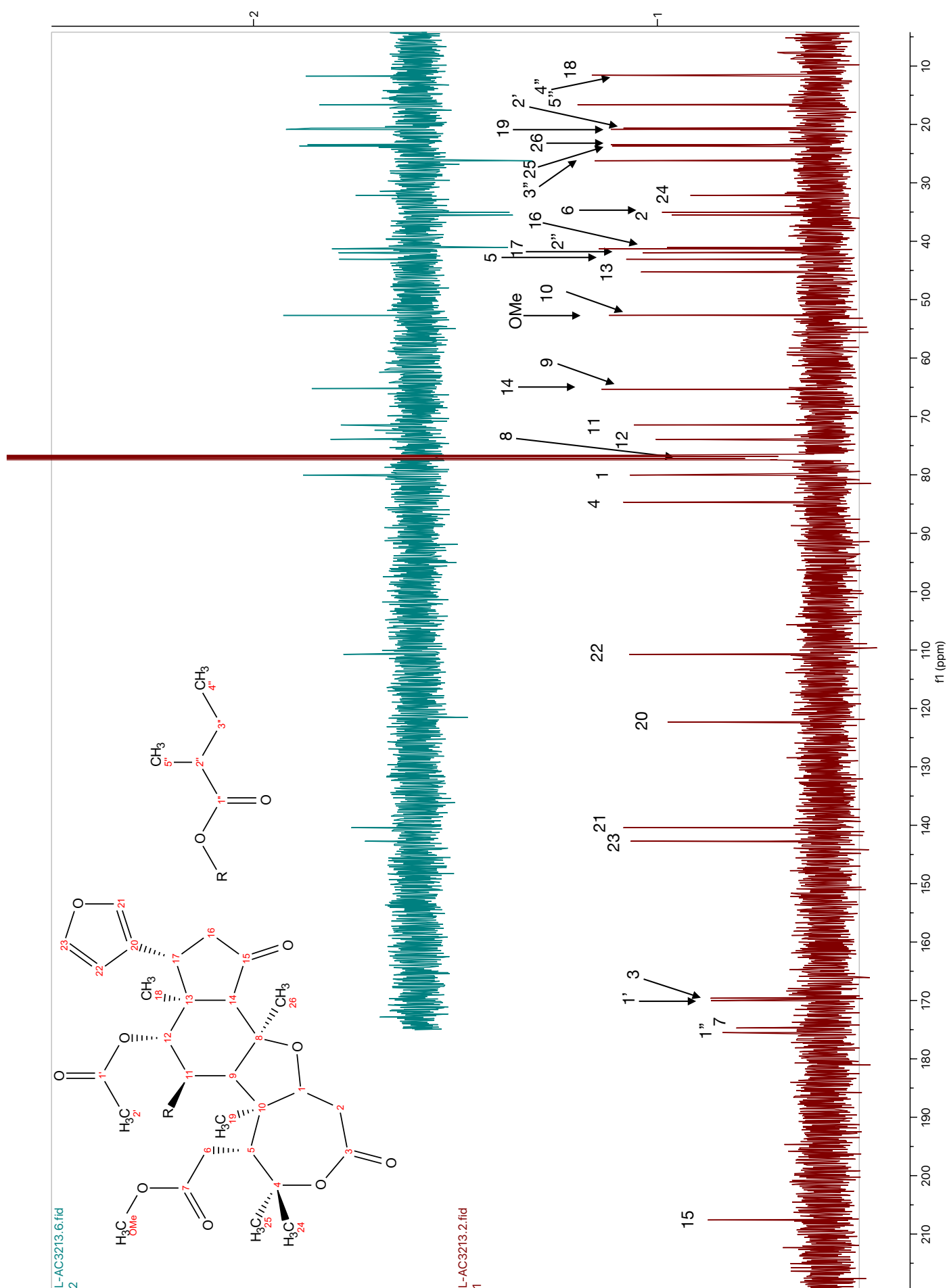




Figure S13: COSY experiment of compound 2 (CDCl<sub>3</sub>)

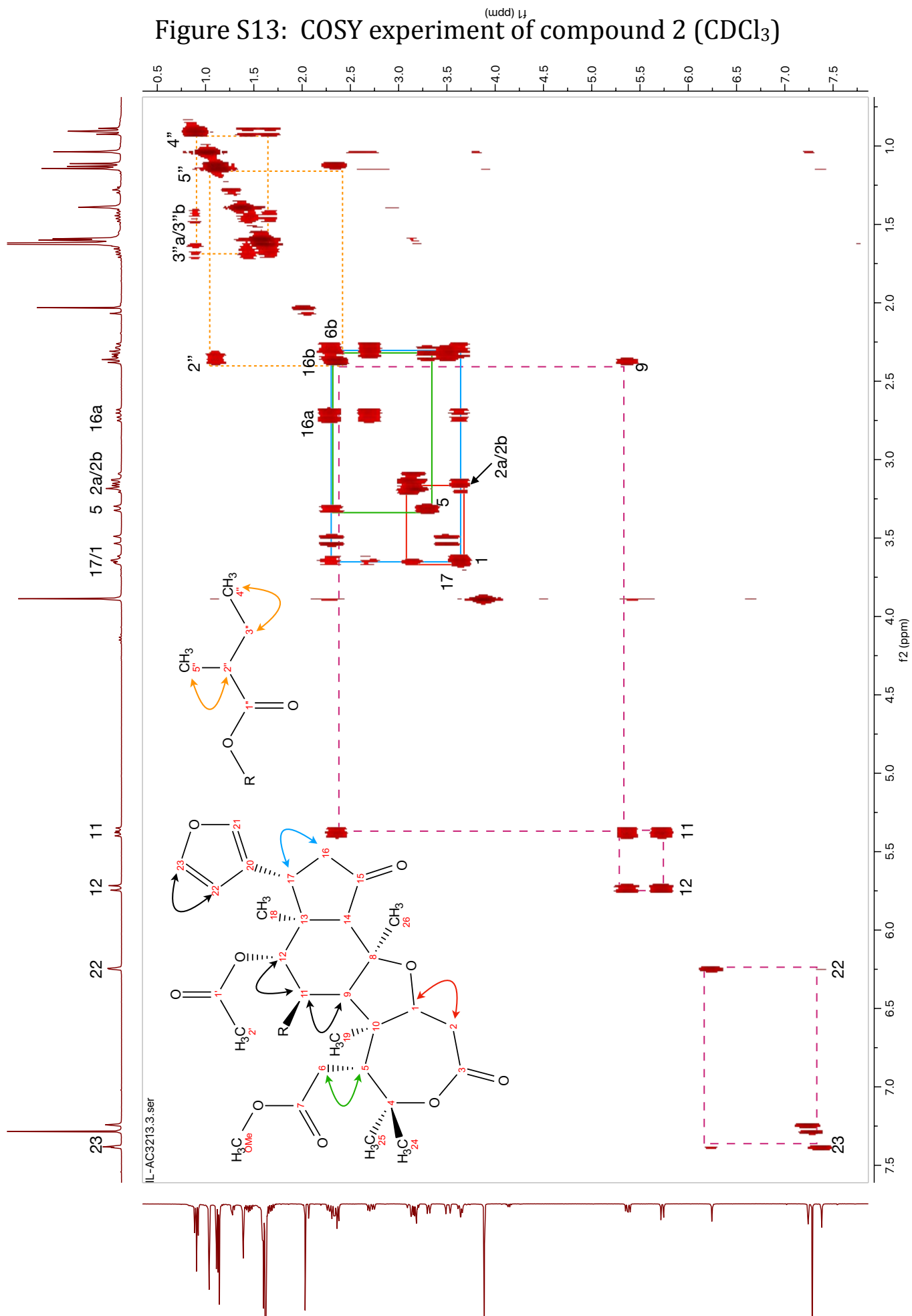


Figure S14: HMQC experiment of compound 2 (CDCl<sub>3</sub>)

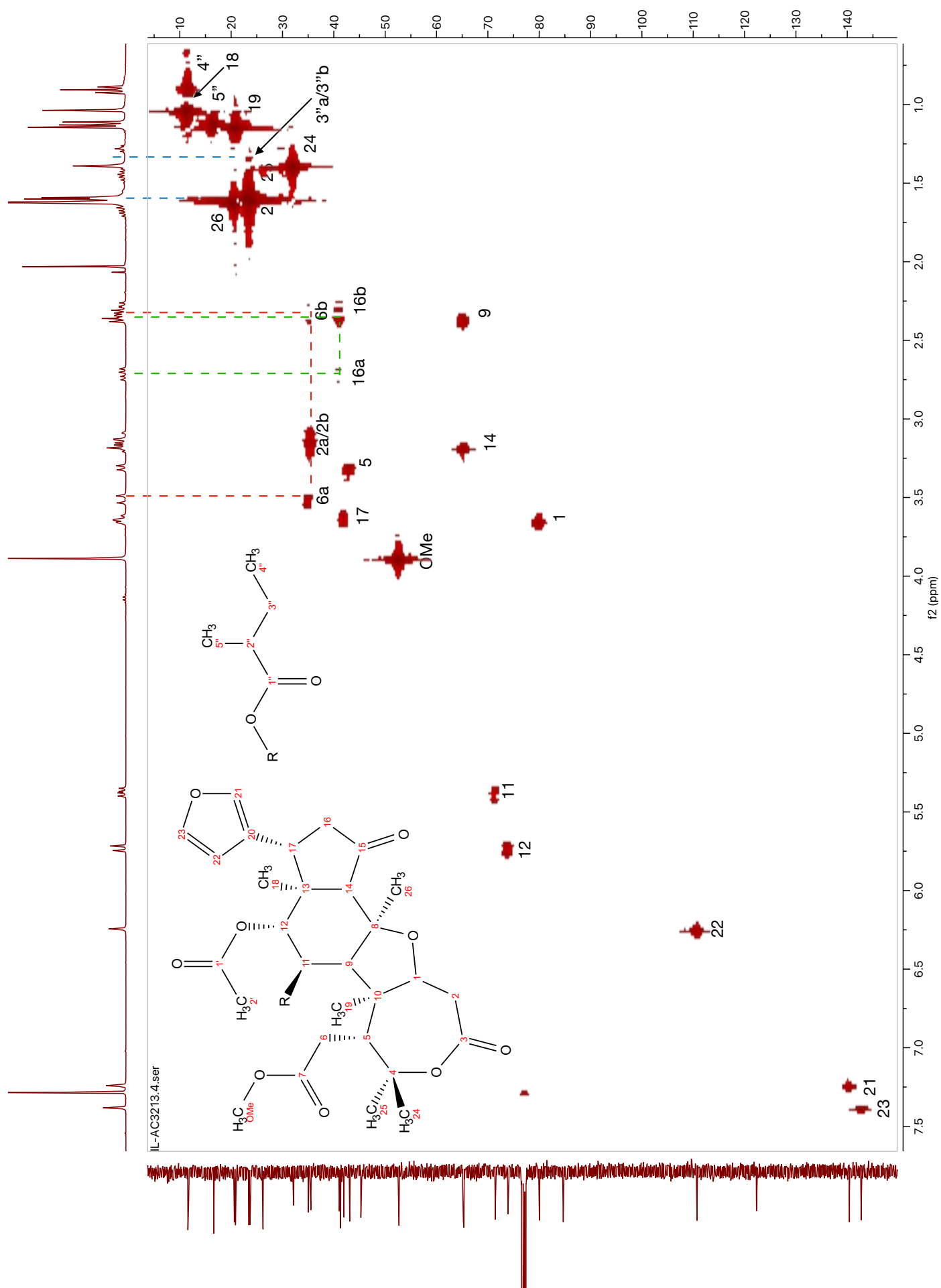


Figure S15: HMBC experiment of compound 2 (CDCl<sub>3</sub>)

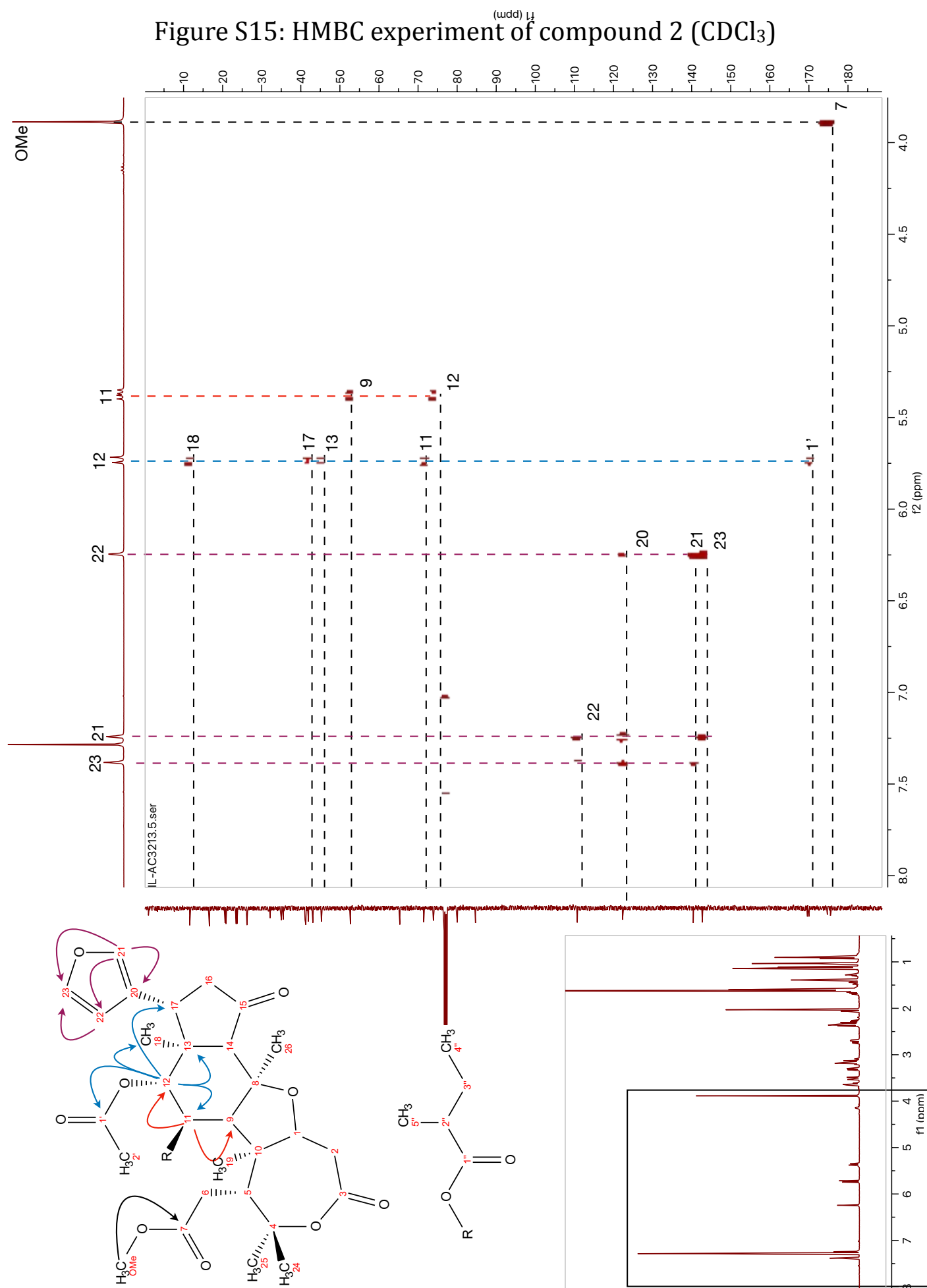


Figure S16: HMBC experiment of compound 2 (CDCl<sub>3</sub>)

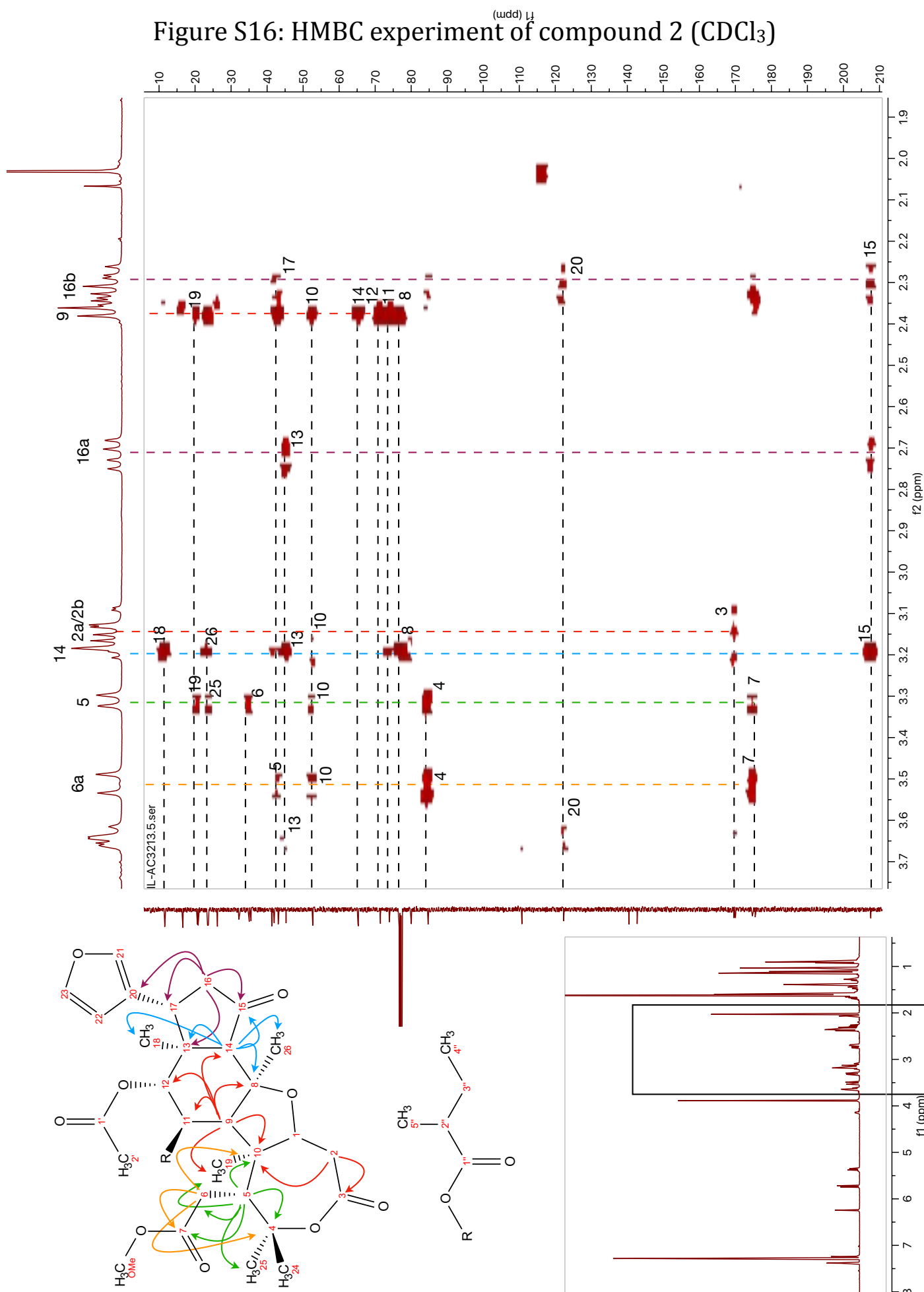


Figure S17: HMBC experiment of compound 2 (CDCl<sub>3</sub>)

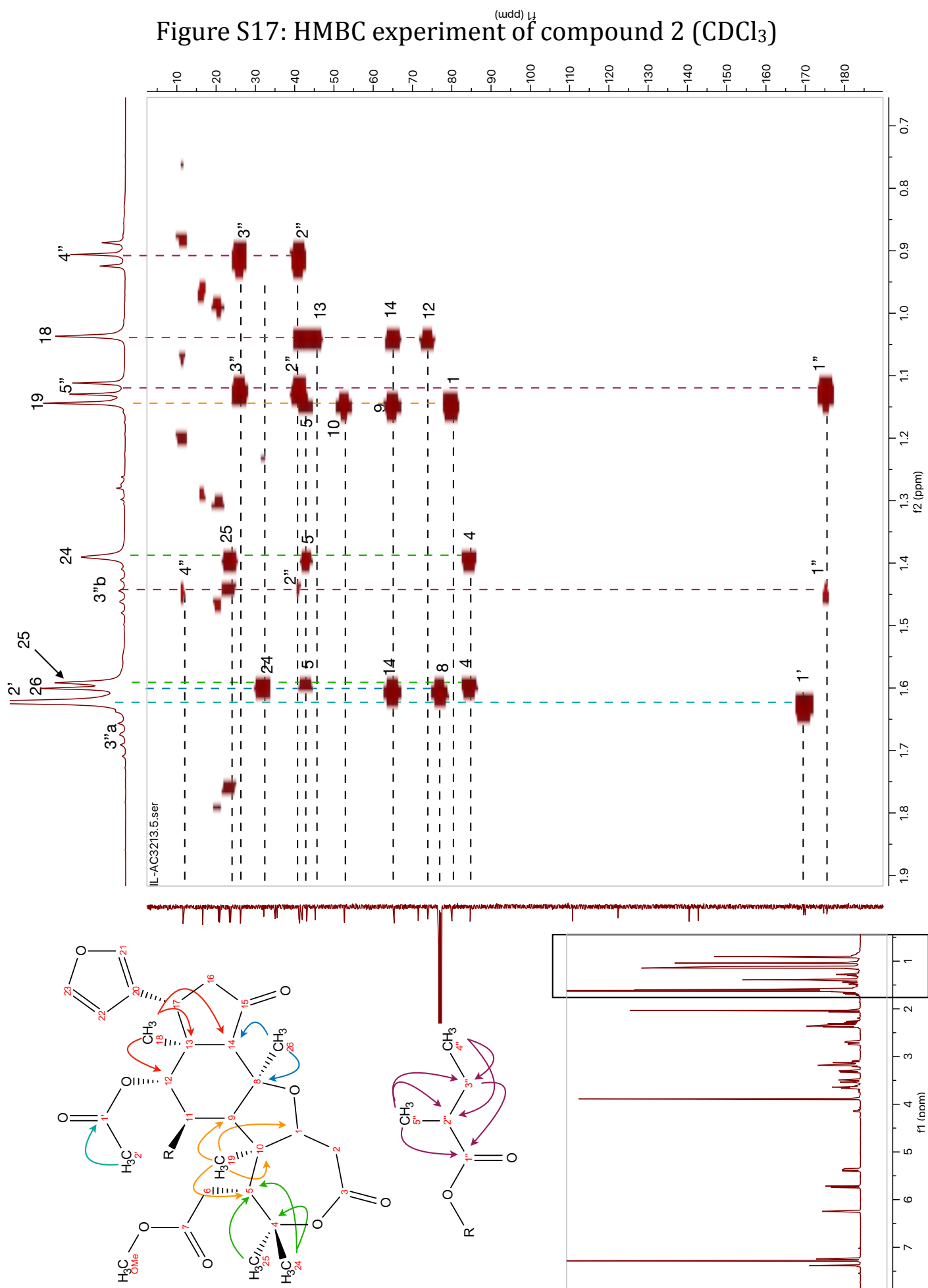
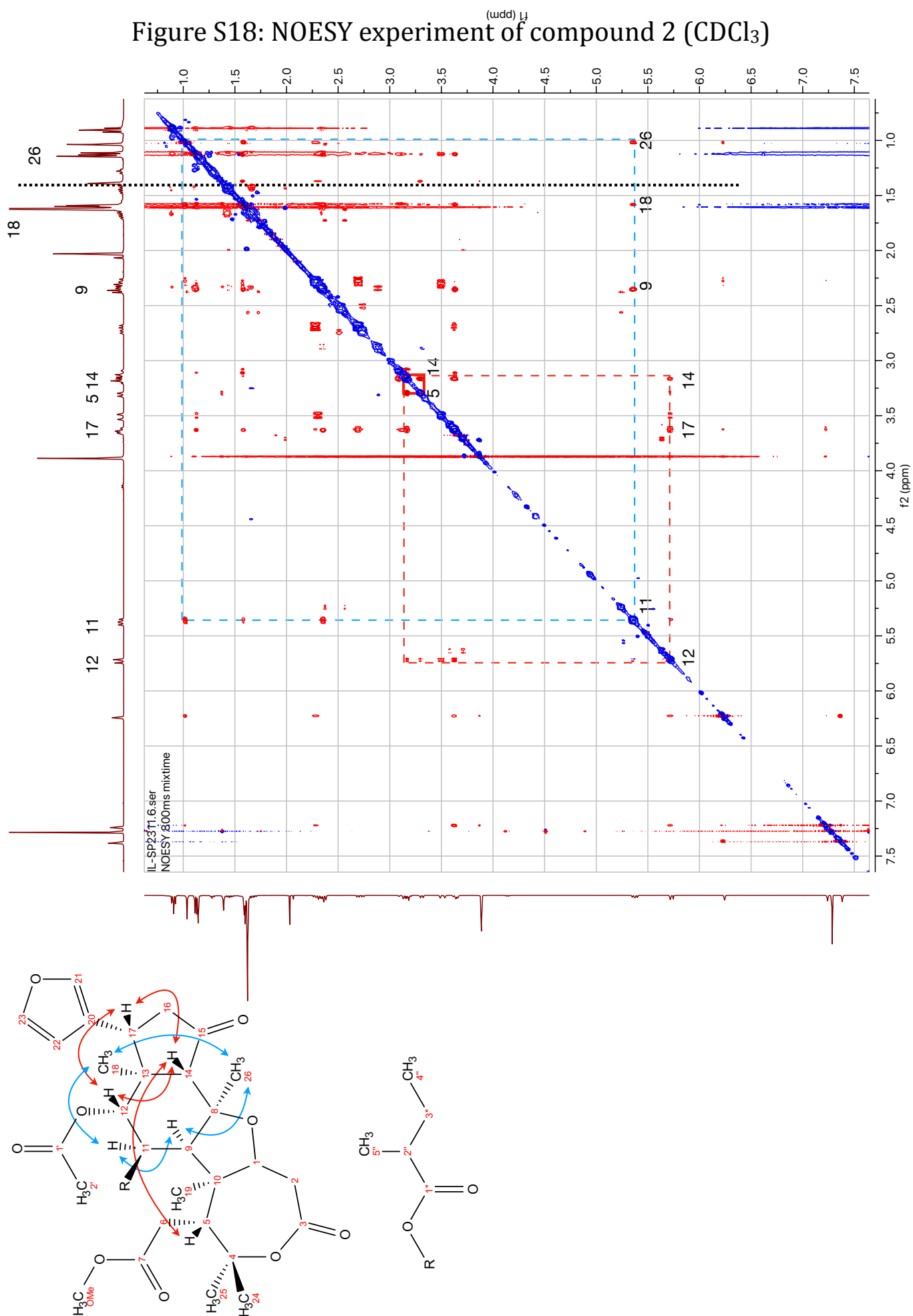


Figure S18: NOESY experiment of compound 2 (CDCl<sub>3</sub>)



97.0 97.5 98.0 98.5 99.0 99.5 100.0

Transmittance [%]

3500 3000 2500 2000 1500 1000 500

Wave number cm<sup>-1</sup>

409.25

1734.33

2956.74  
2930.62  
2920.23

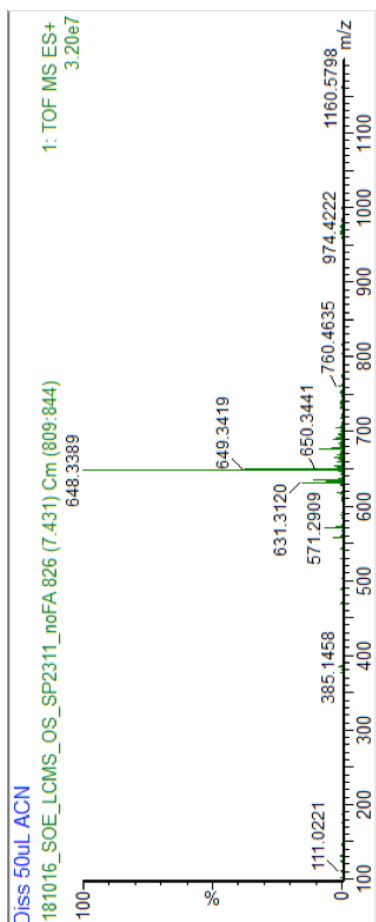
1457.96  
1434.26  
1371.84  
1303.03  
1237.01  
1212.00  
1184.36  
1124.16  
1079.67  
1067.40  
1031.57  
920.89  
874.09  
854.83  
796.70  
756.59

BRUKER

Page 1/1

C:\USERS\CA\DOCUMENTS\CA\SIO\IL\LA\CA3213\0 ILAC3213 C:\USERS\CA\DOCUMENTS\CA\SIO\IL\

2019-08-15



**Single Mass Analysis**  
Tolerance = 2.0 mDa / DBE: min = -1.5, max = 100.0  
Element prediction: Off  
Number of isotope peaks used for i-FIT = 6  
Monoisotopic Mass, Even Electron Ions  
8174 formulae (evaluated with 4 results within limits (up to 50 closest results for each mass))

C: 0-50	H: 0-100	N: 0-2	O: 0-20	S: 0-1
---------	----------	--------	---------	--------

Mass	Calc. Mass	mDa	PPM	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Si
631.3120	631.3118	0.2	0.3	11.5	C34 H47 O11	74.5	3.531	2.93	34	47		11	
	631.3113	0.7	1.1	29.5	C47 H39 N2	71.0	0.033	96.76	47	39	2		
	631.3110	1.0	1.6	2.5	H51 N2 O14 Si	81.9	10.977	0.00	25	51	2	14	1
	631.3137	-1.7	-2.7	-1.5	C22 H51 N2 O18	76.7	5.761	0.31	22	51	2	18	

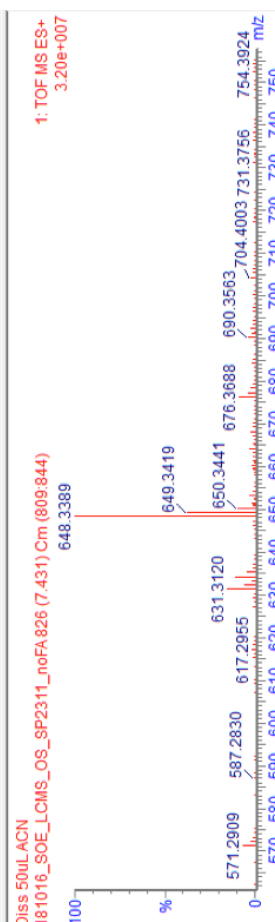


Figure S20:  $^1\text{H}$  NMR of compound 3 ( $\text{CDCl}_3$ )

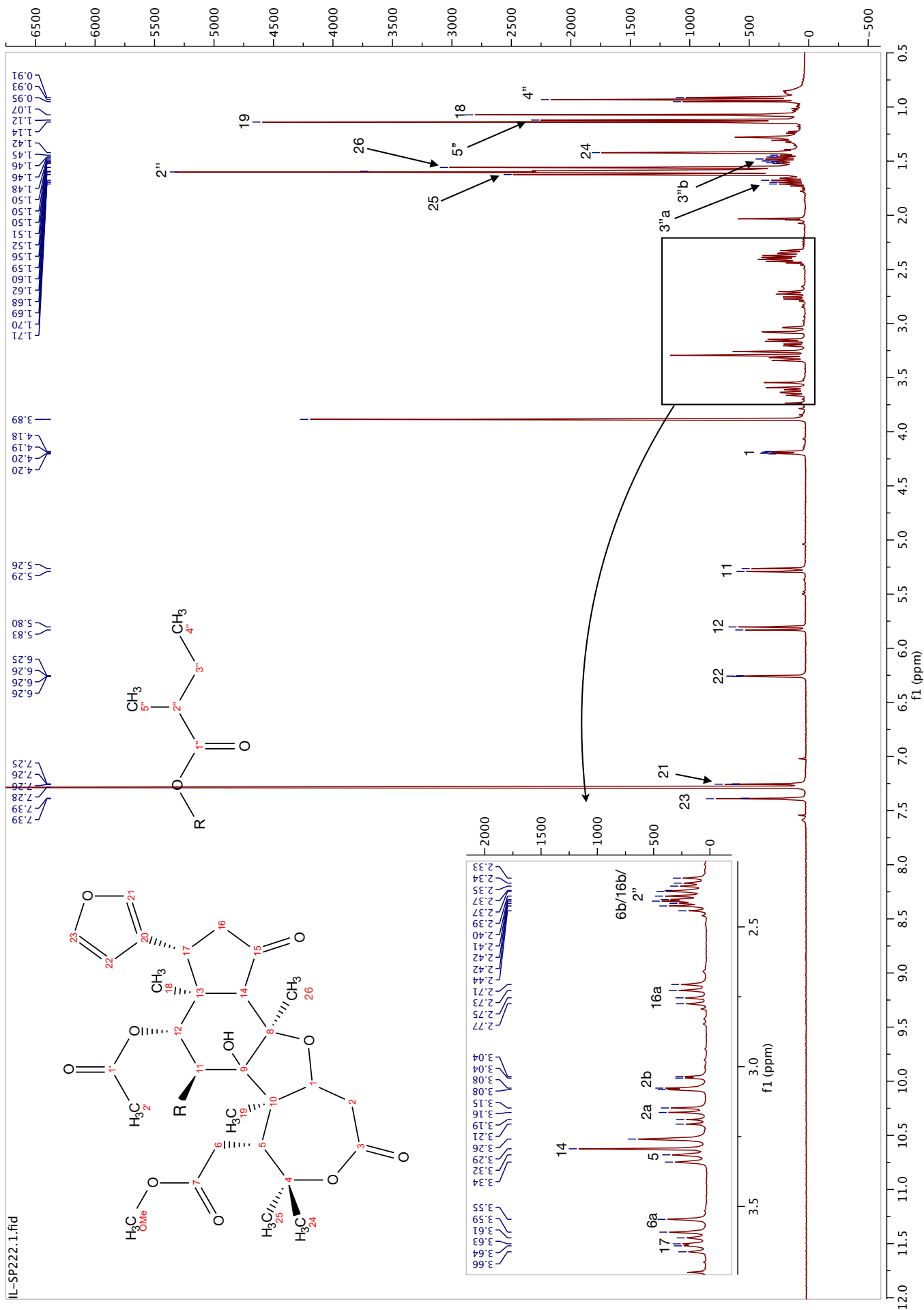




Figure S21:  $^{13}\text{C}$  NMR of compound 3 ( $\text{CDCl}_3$ )

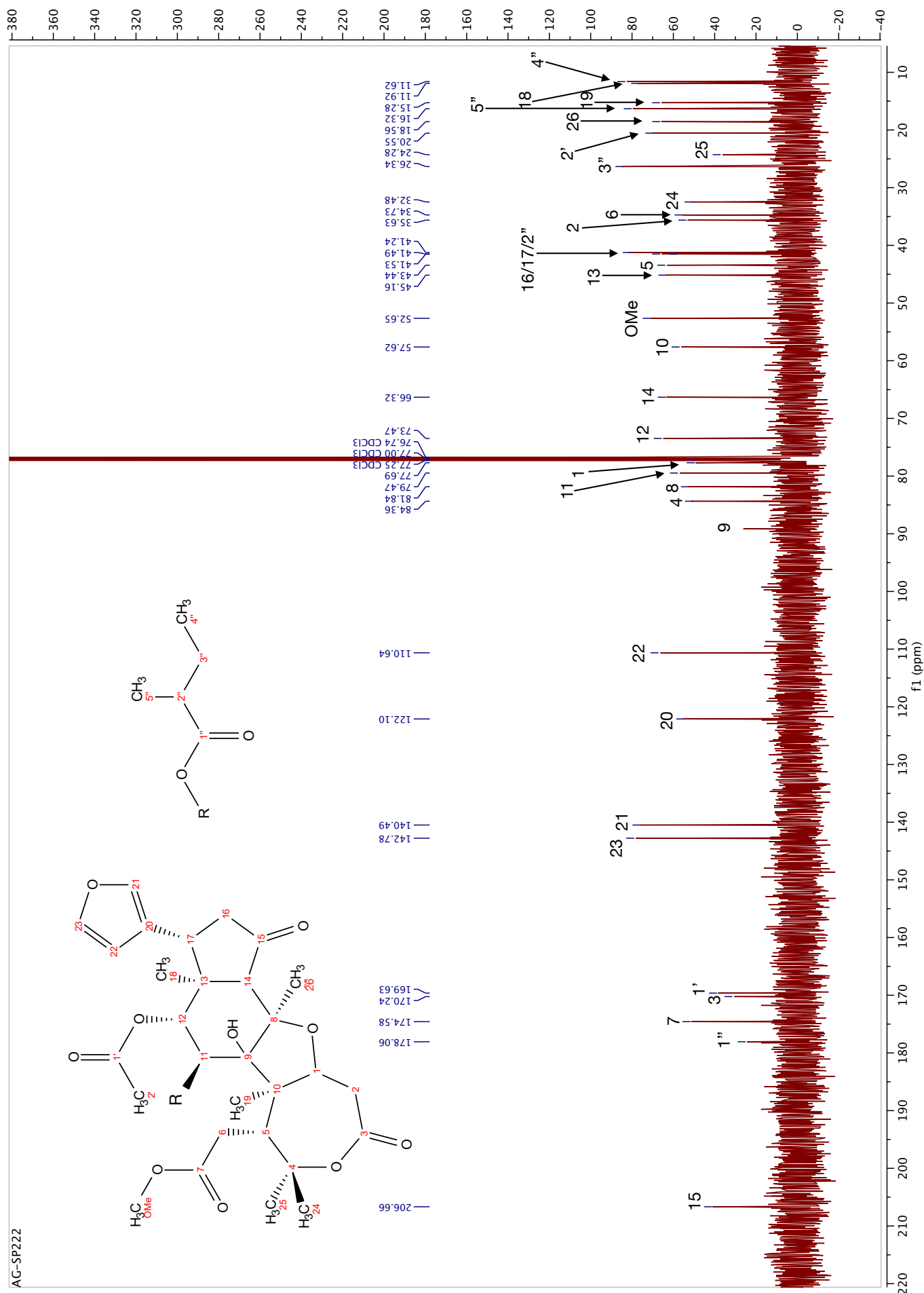


Figure S22: COSY experiment of compound 3 ( $\text{CDCl}_3$ )

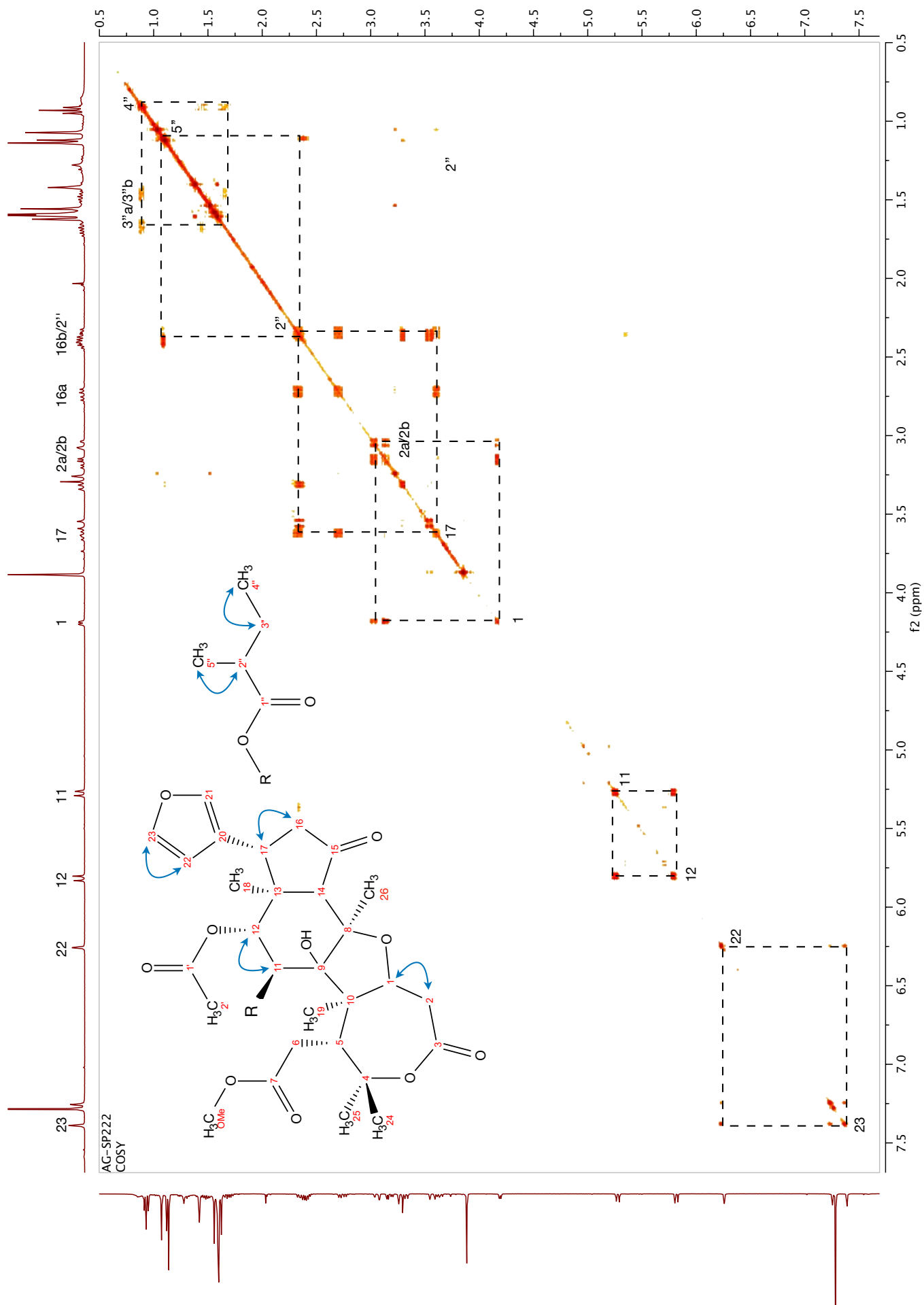


Figure S23: HMQC experiment of compound 3 (CDCl<sub>3</sub>)

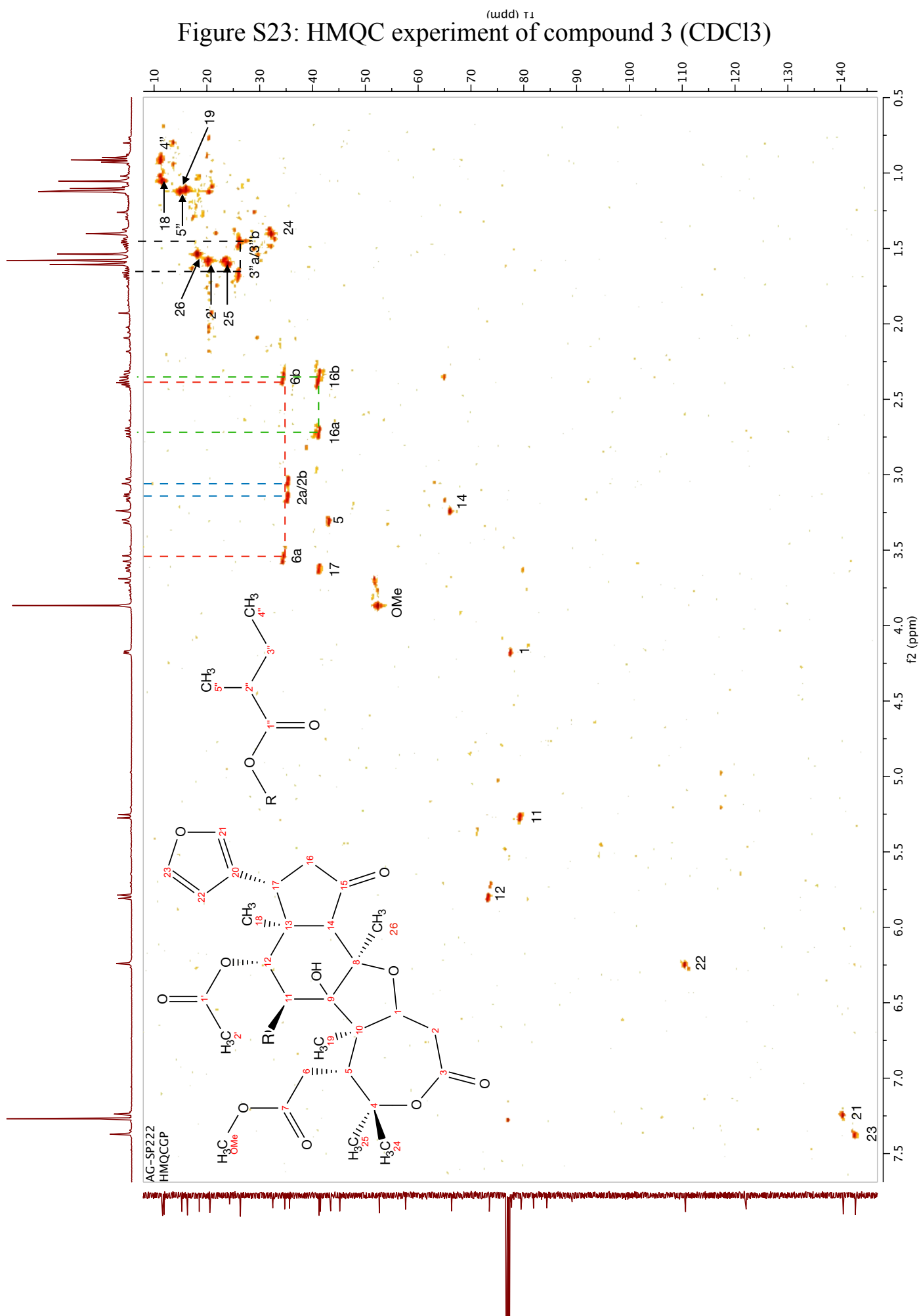
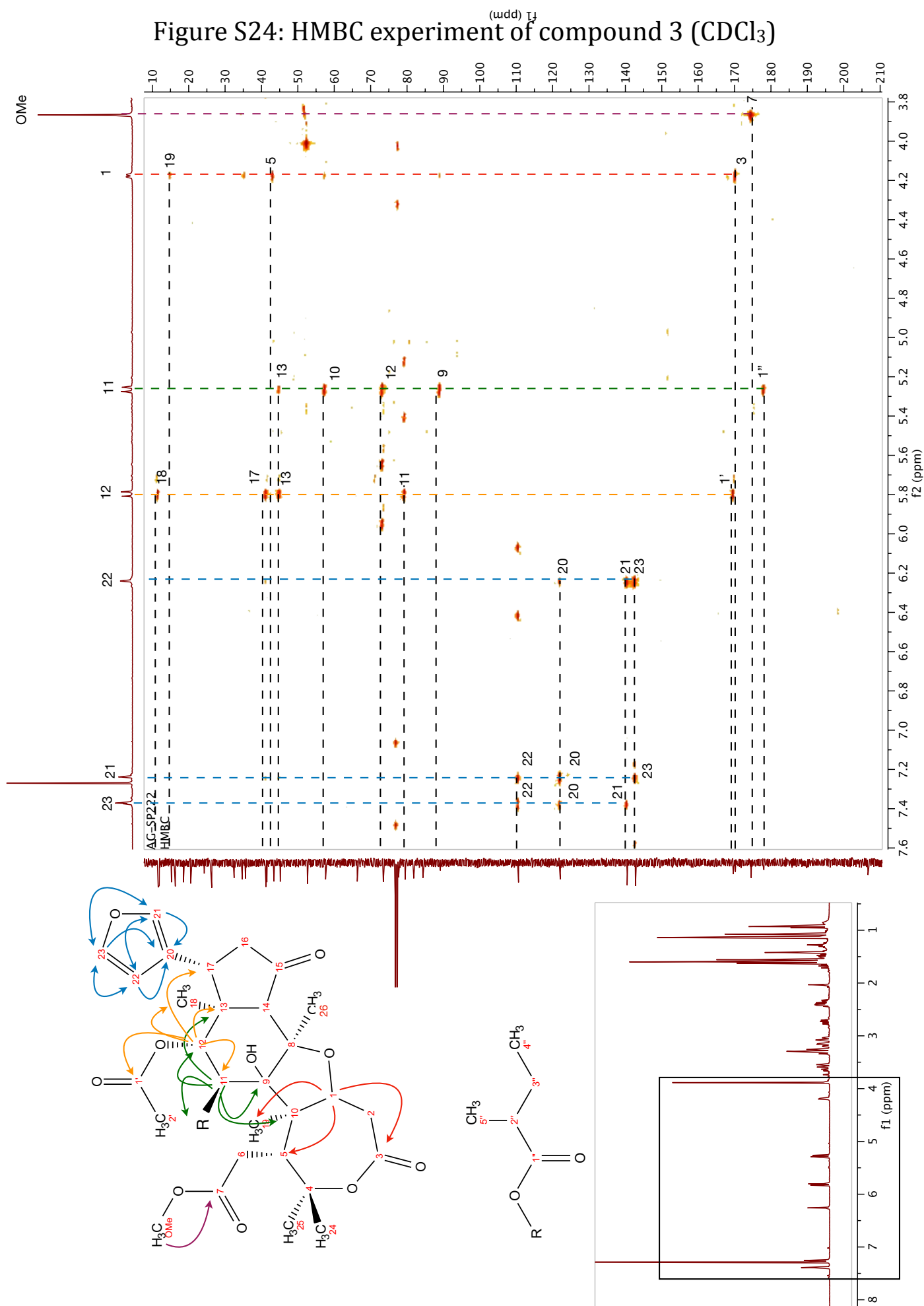


Figure S24: HMBC experiment of compound 3 (CDCl<sub>3</sub>)



(wdd) 14

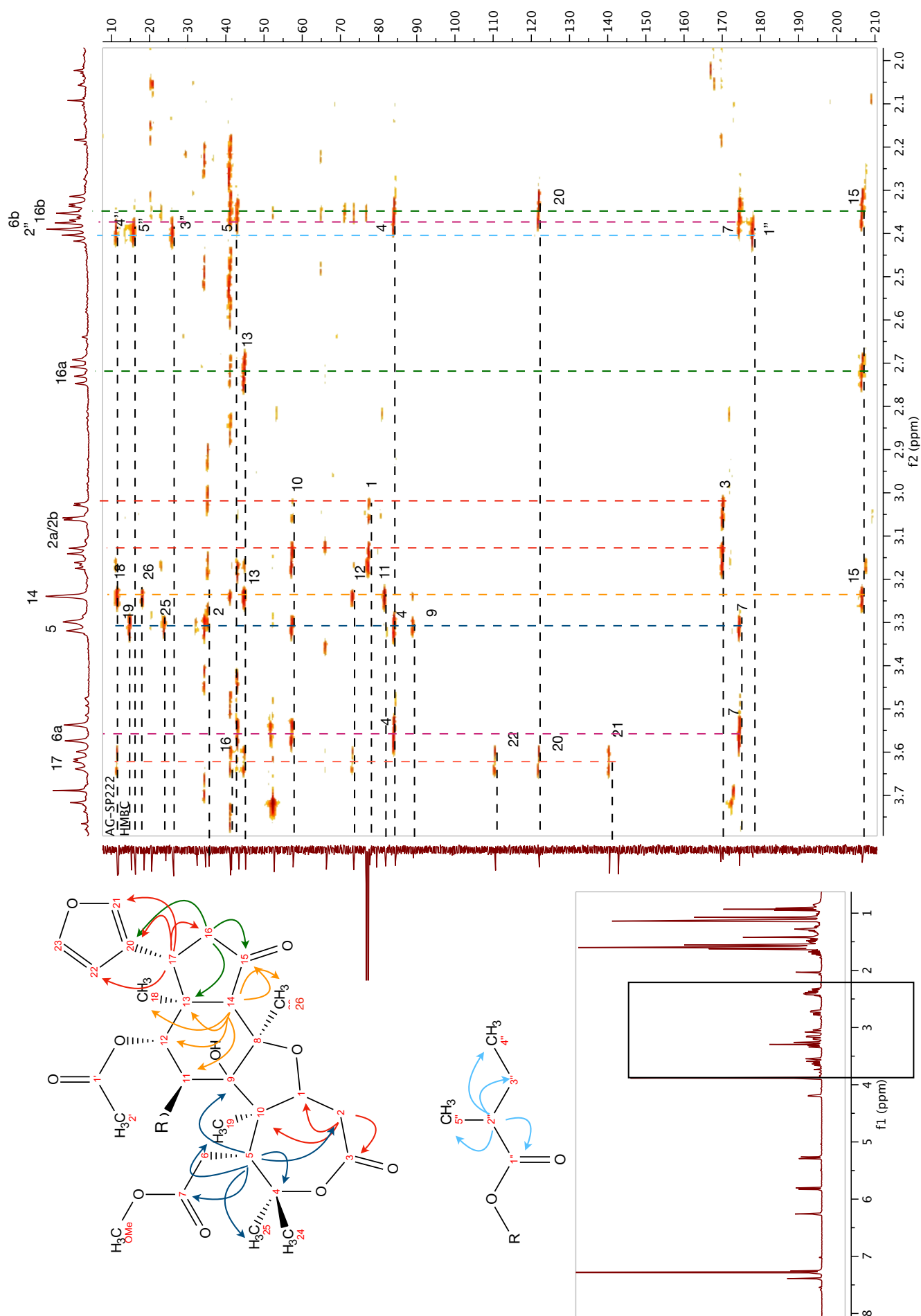


Figure S26: HMBC experiment of compound 3 (CDCl<sub>3</sub>)

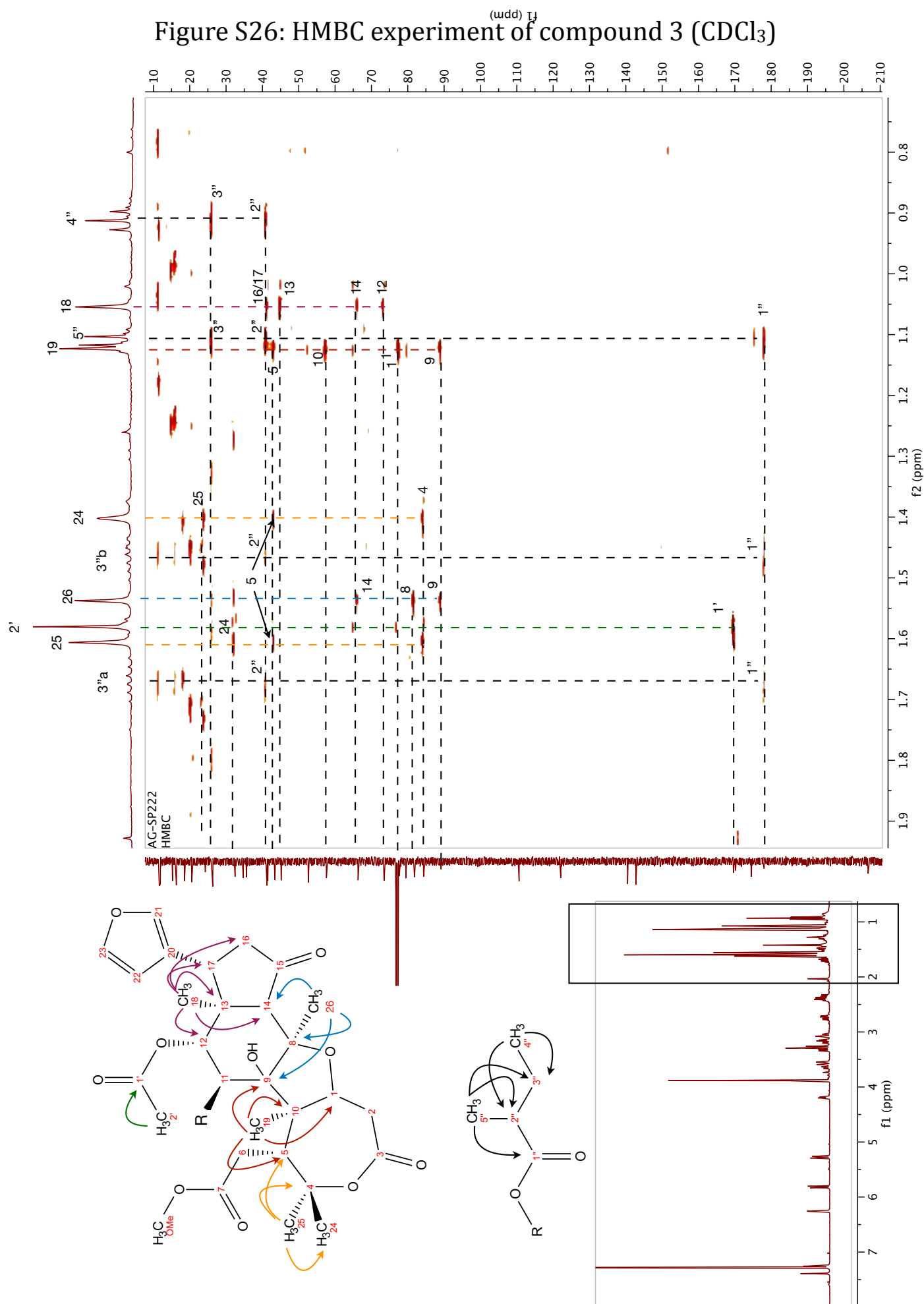


Figure S27: NOESY experiment of compound 3 (CDCl<sub>3</sub>)

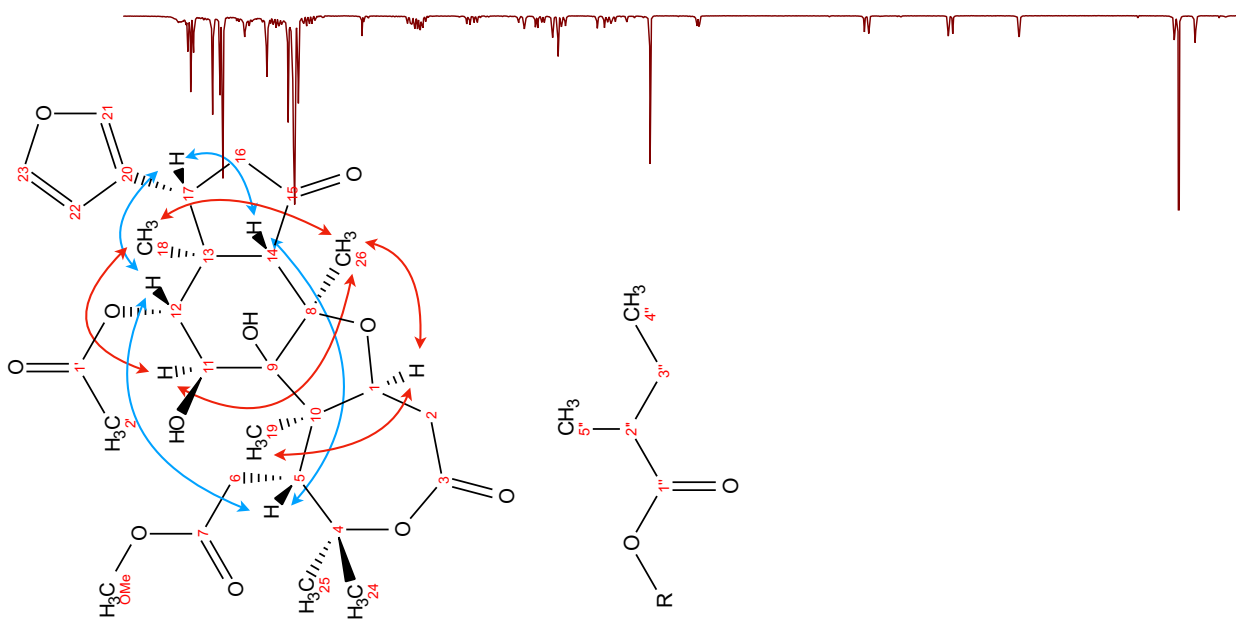
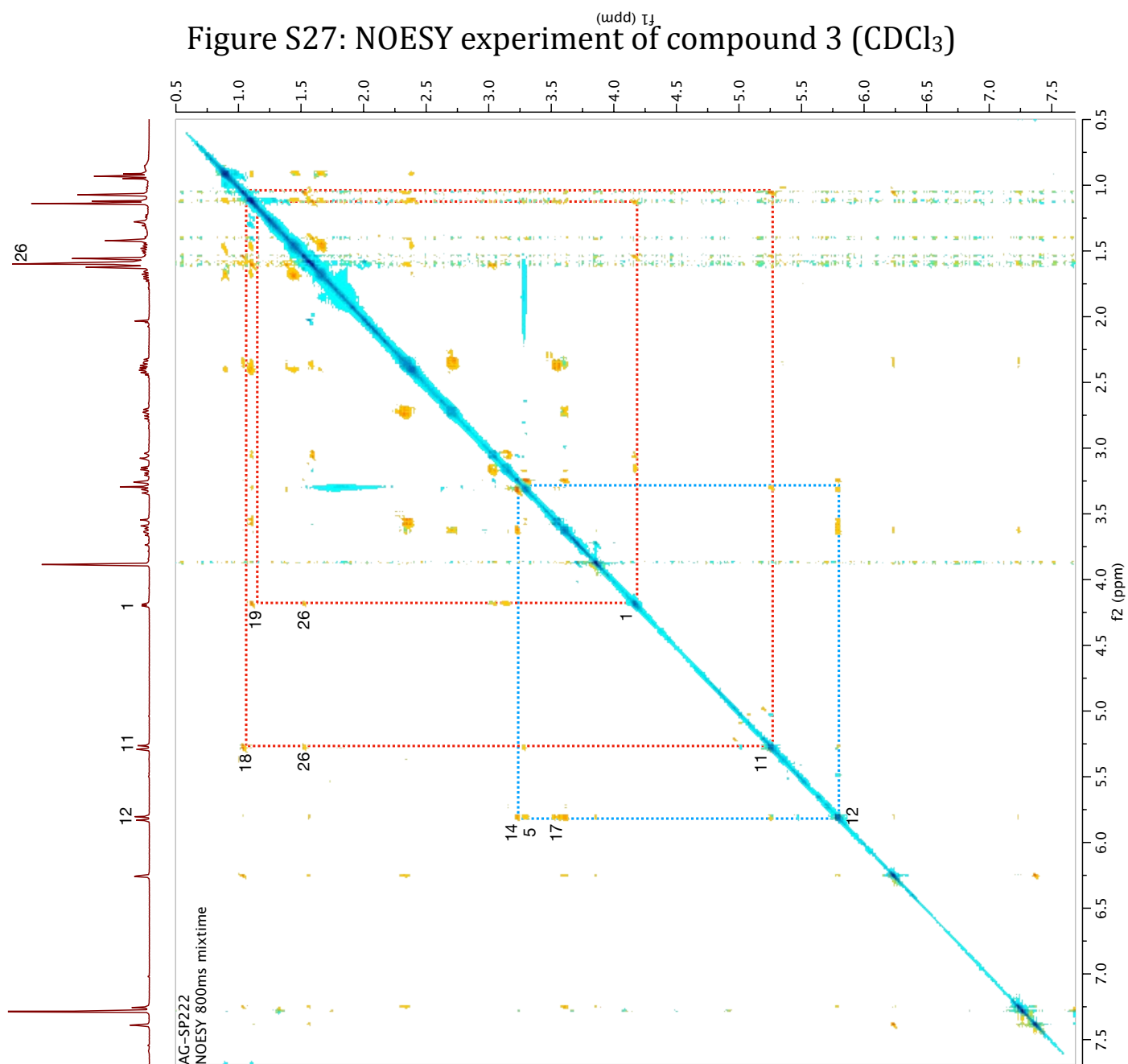
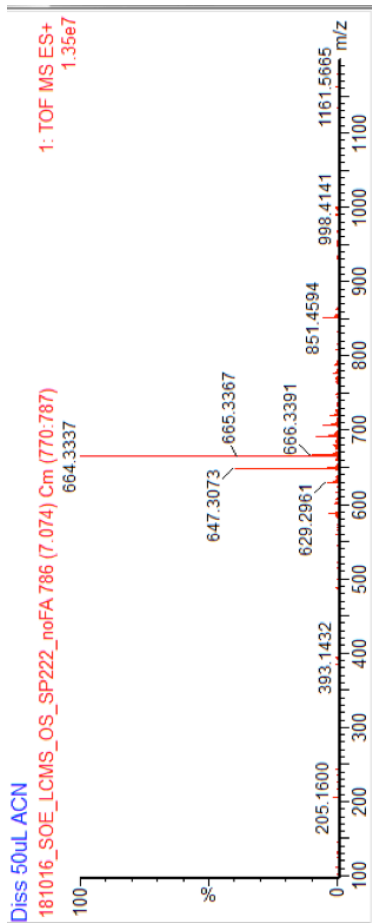
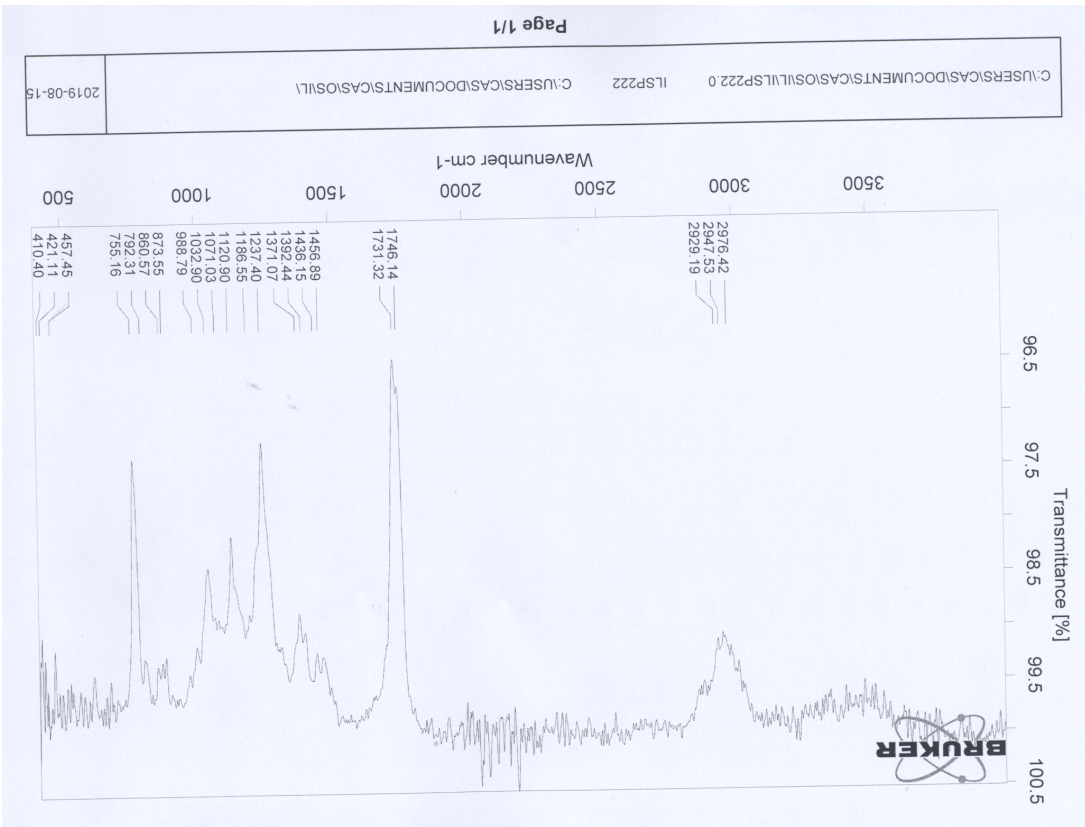


Figure S28: HRMS and IR of compound 3



#### Single Mass Analysis

Tolerance = 2.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 6

Monoisotopic Mass, Even Electron Ions

830 formulae evaluated with 4 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-50 H: 0-100 N: 0-2 O: 0-20 Si: 0-1

Mass	Calc. Mass	mDa	DBE	Formula	i-FIT	i-FIT Norm	Fit Conf %	C	H	N	O	Si
647.3073	647.3068	0.5	0.8	C <sub>34</sub> H <sub>47</sub> O <sub>12</sub>	114.8	0.038	96.32	34	47		12	
647.3062	647.3062	1.1	1.7	C <sub>47</sub> H <sub>59</sub> N <sub>2</sub> O	118.1	3.334	3.57	47	39	2	1	
647.3086	647.3086	-1.3	-2.0	C <sub>22</sub> H <sub>51</sub> N <sub>2</sub> O <sub>19</sub>	121.7	6.877	0.10	22	51	2	19	
647.3059	647.3059	1.4	2.2	C <sub>25</sub> H <sub>51</sub> N <sub>2</sub> O <sub>15</sub> Si	123.8	9.010	0.01	25	51	2	15	1

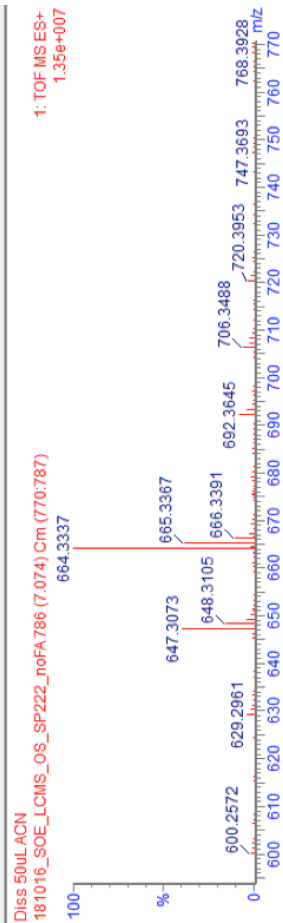




Figure S29:  $^1\text{H}$  NMR of compound 4 ( $\text{CDCl}_3$ )

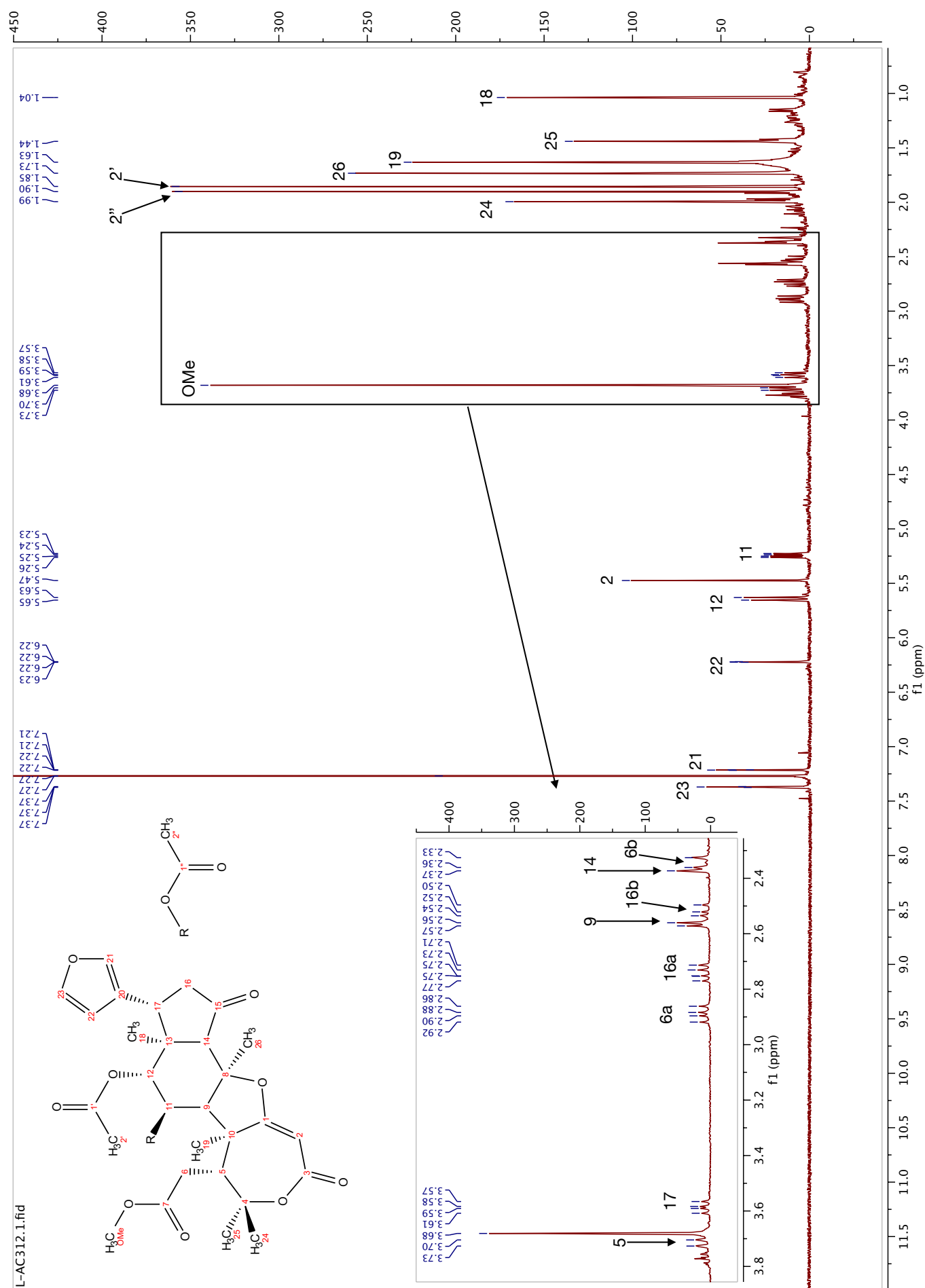


Figure S30:  $^{13}\text{C}$  NMR of compound 4 ( $\text{CDCl}_3$ )

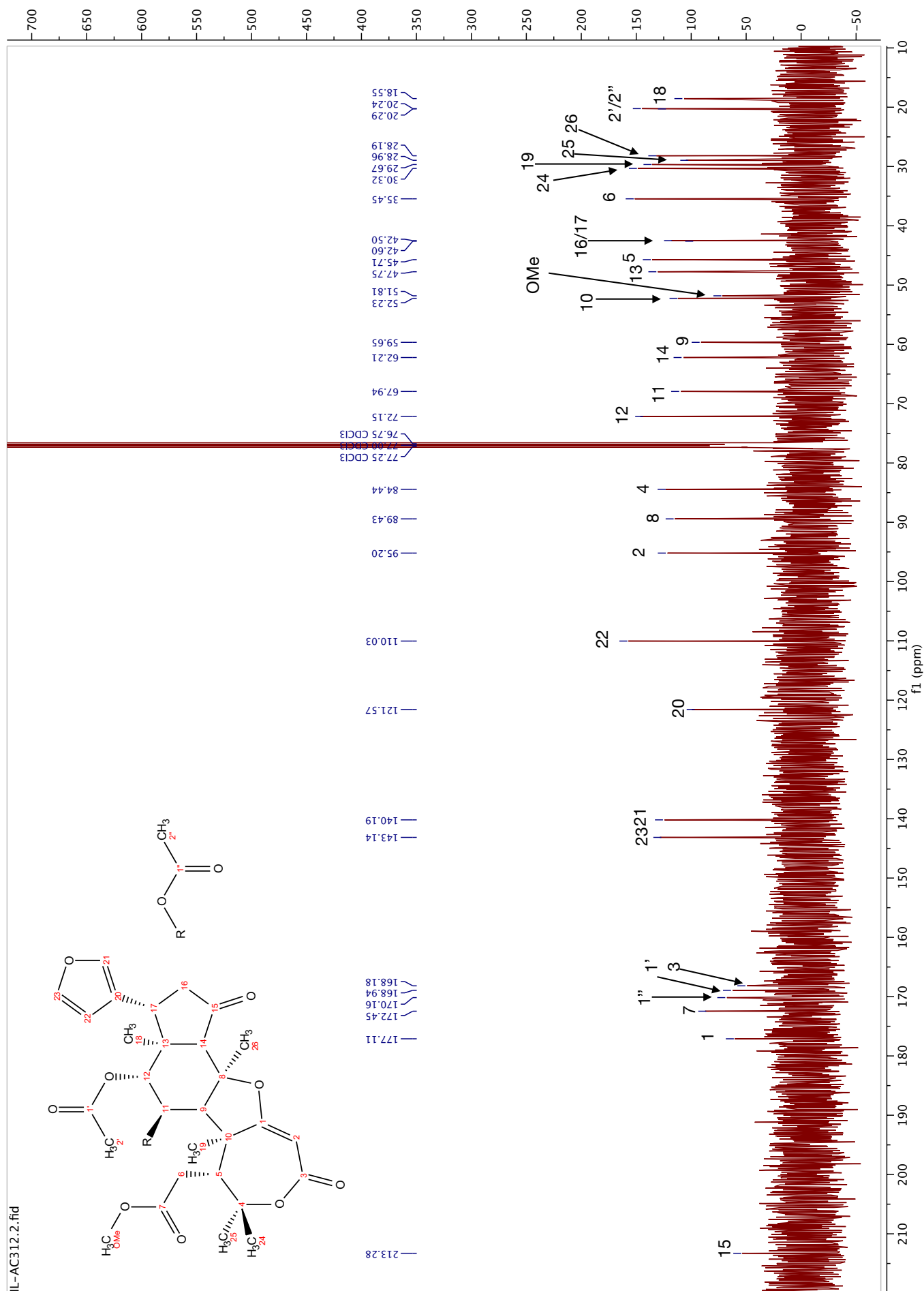
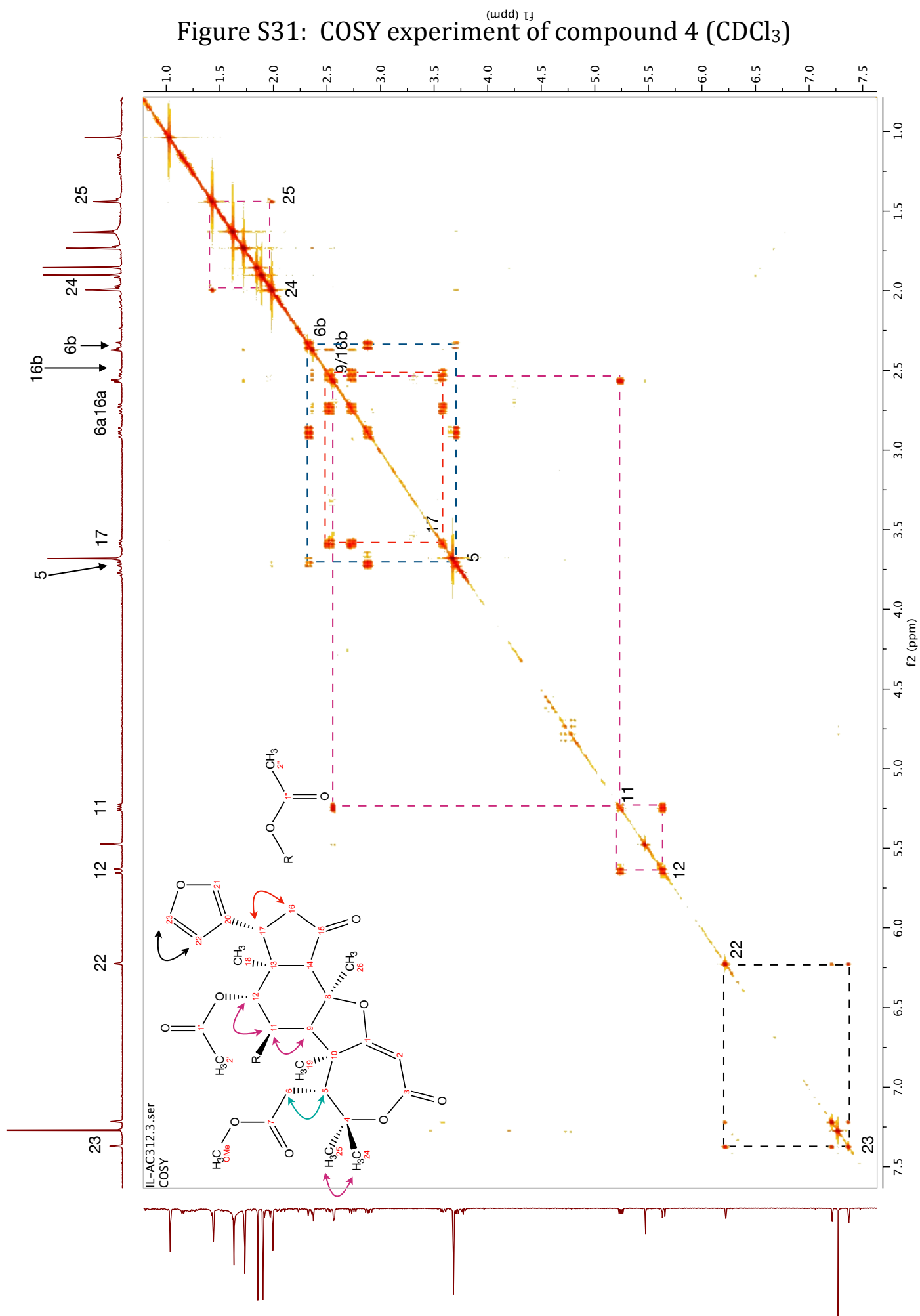


Figure S31: COSY experiment of compound 4 (CDCl<sub>3</sub>)



(add) τ

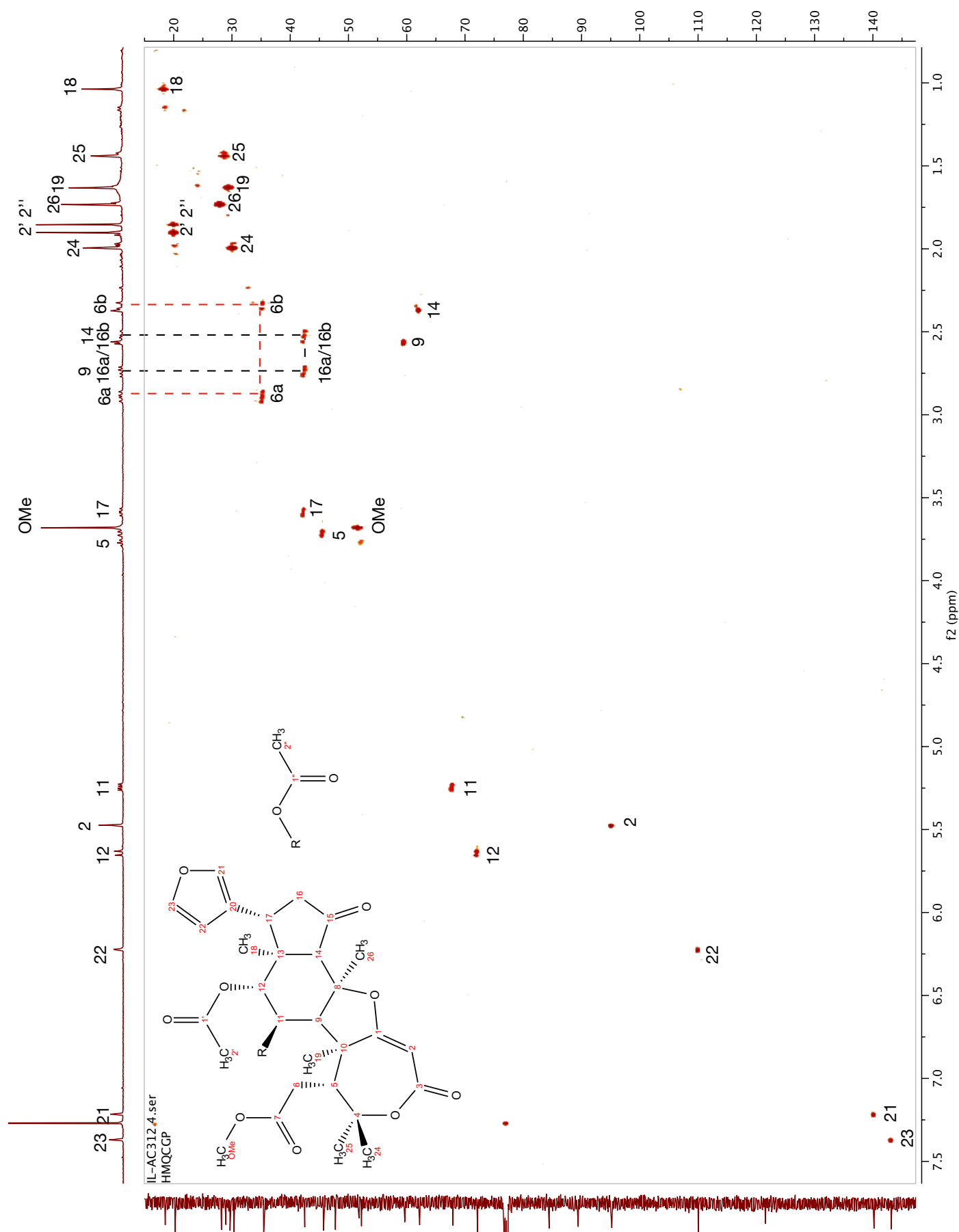


Figure S33: HMBC experiment of compound 4 (CDCl<sub>3</sub>)

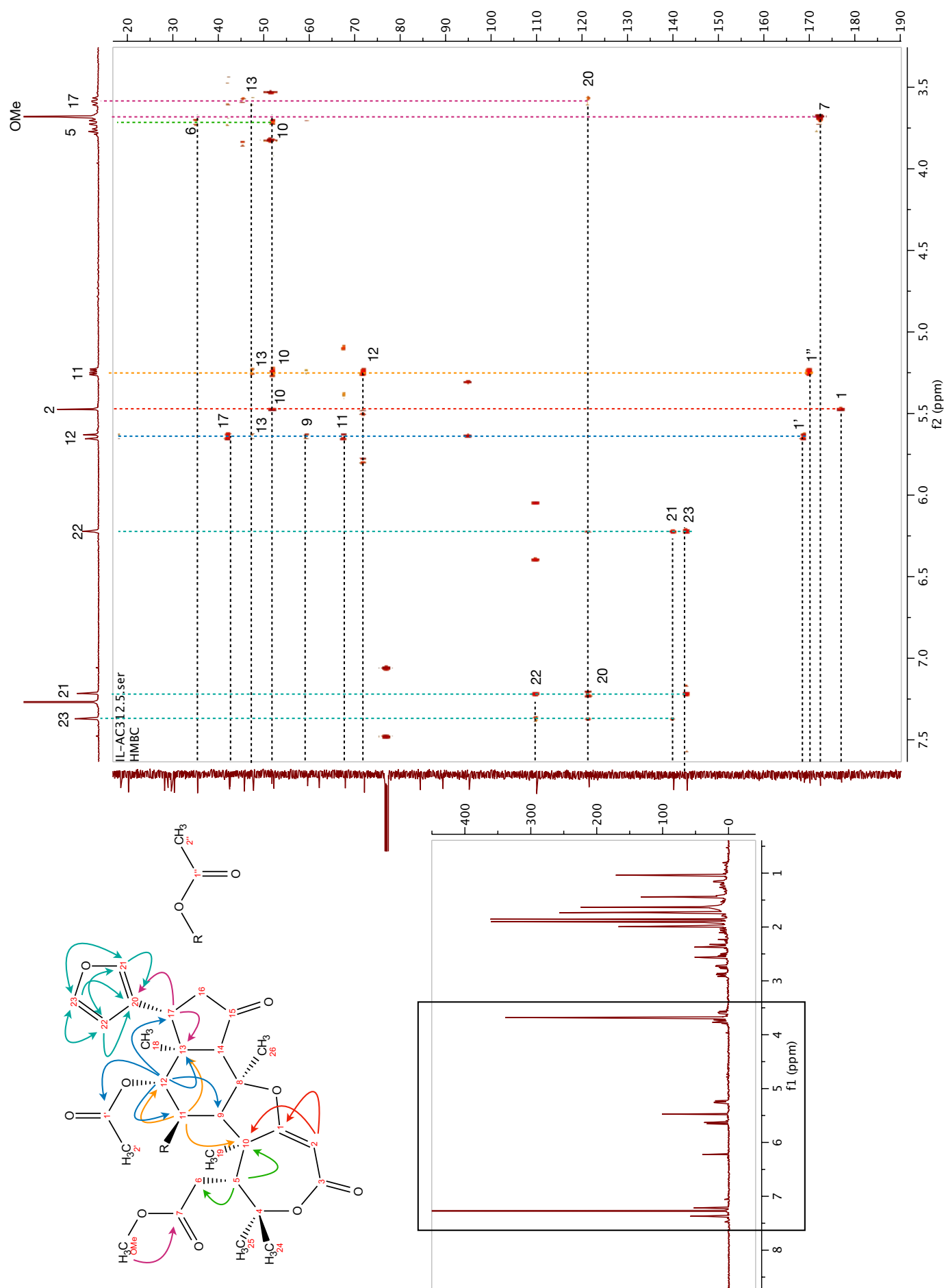
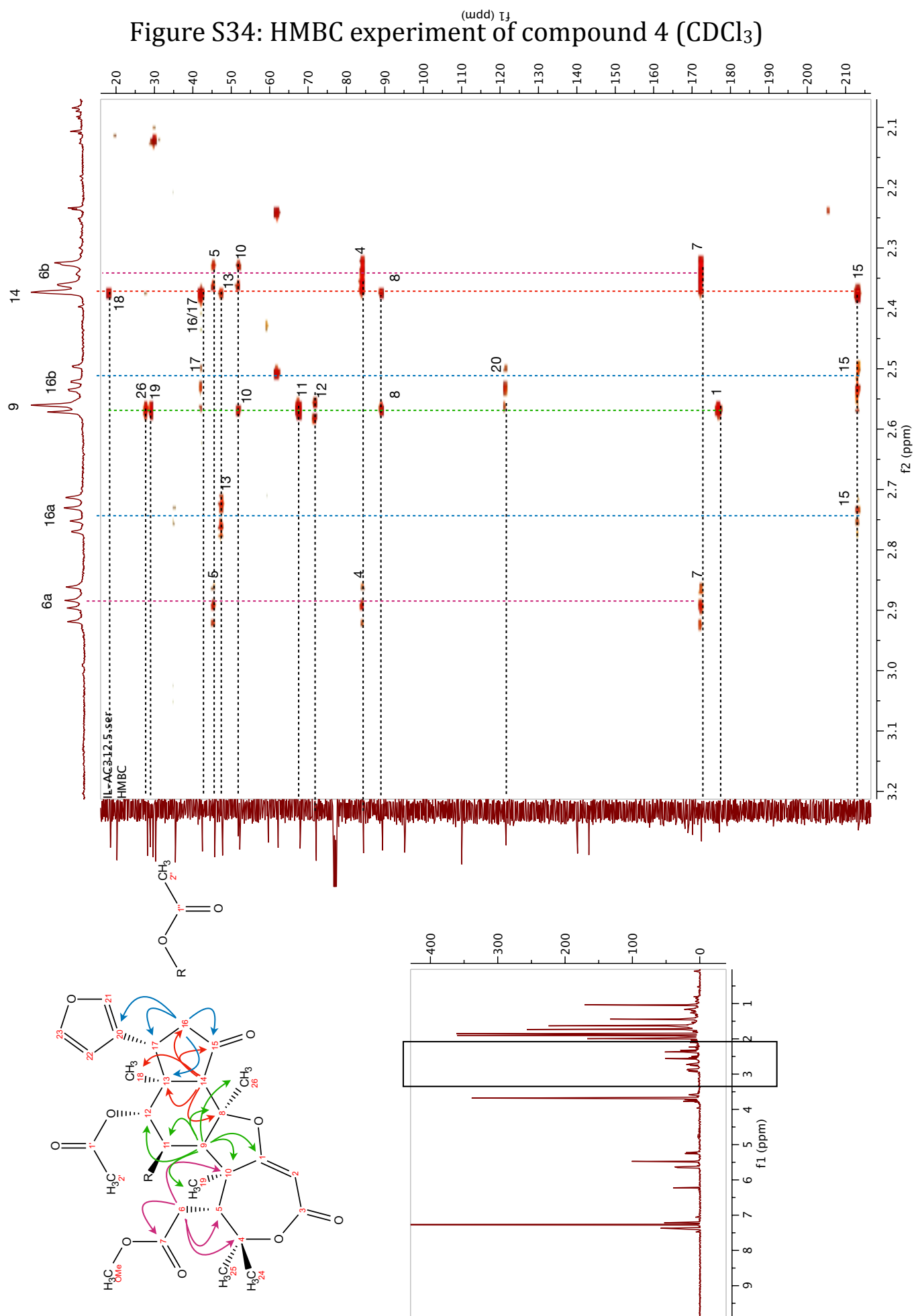


Figure S34: HMBC experiment of compound 4 (CDCl<sub>3</sub>)



(wdd) 1f

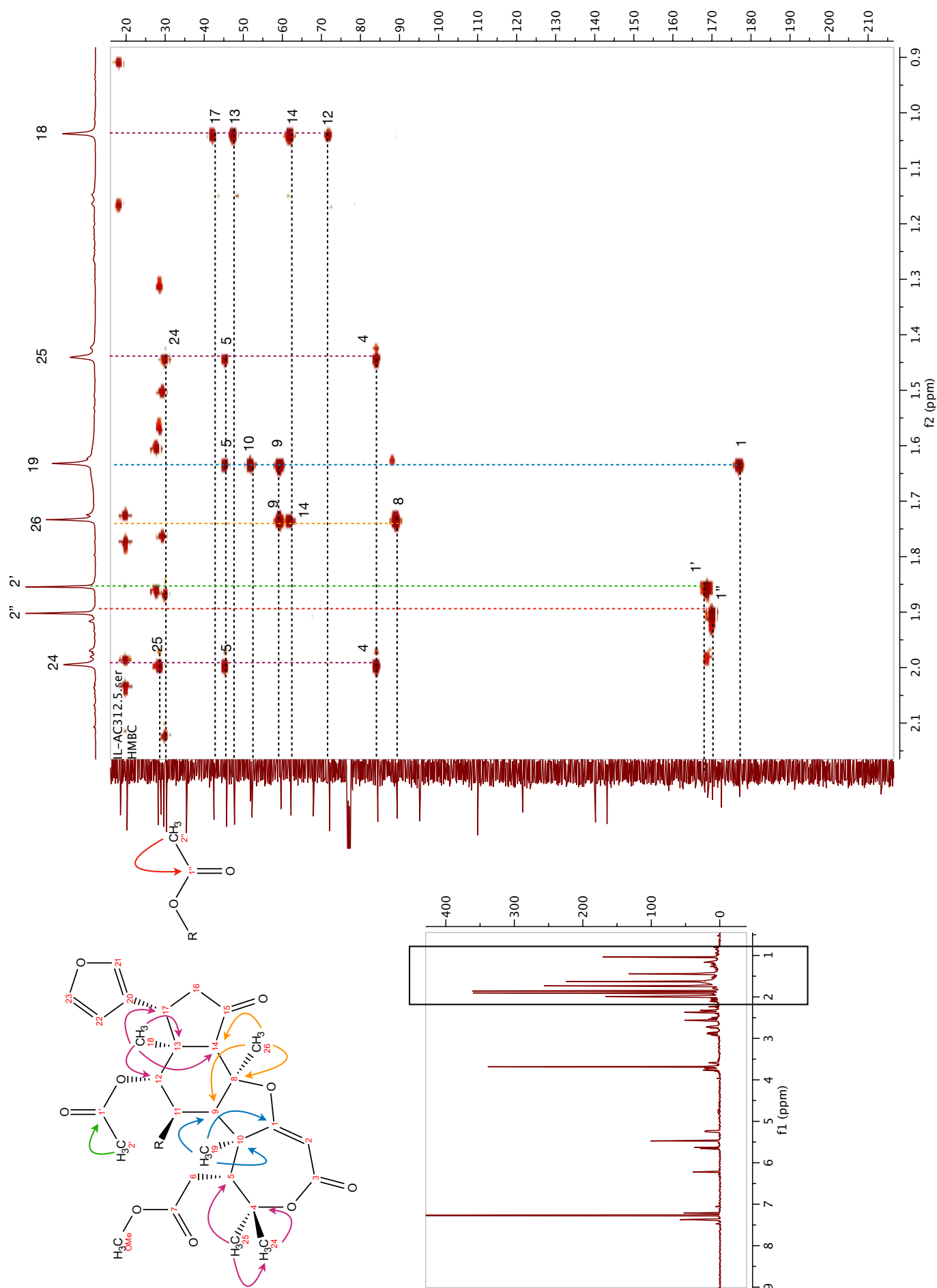


Figure S36: HRMS and IR spectra of compound 4

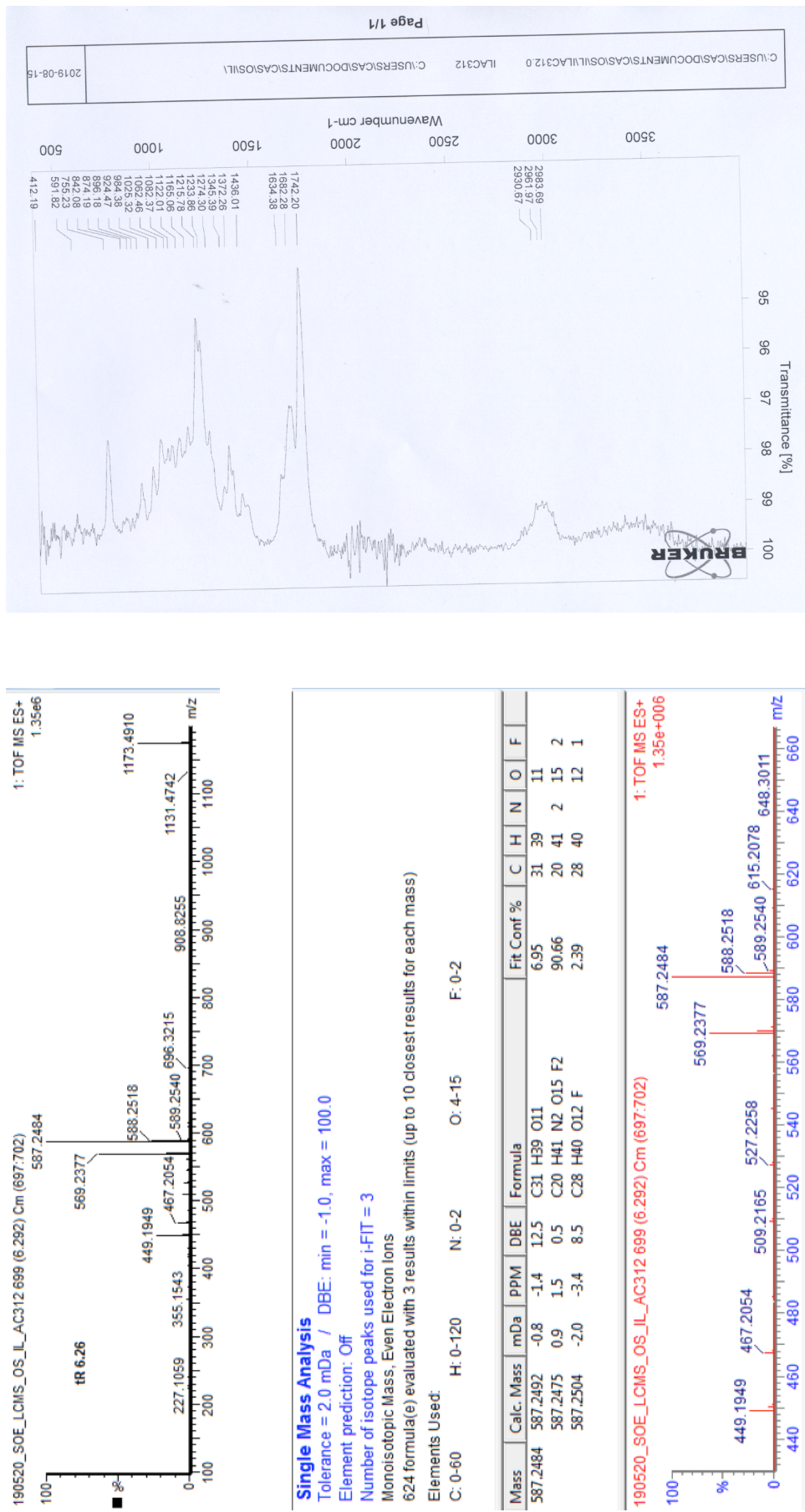




Figure S37:  $^1\text{H}$  NMR of compound 5 ( $\text{CDCl}_3$ )

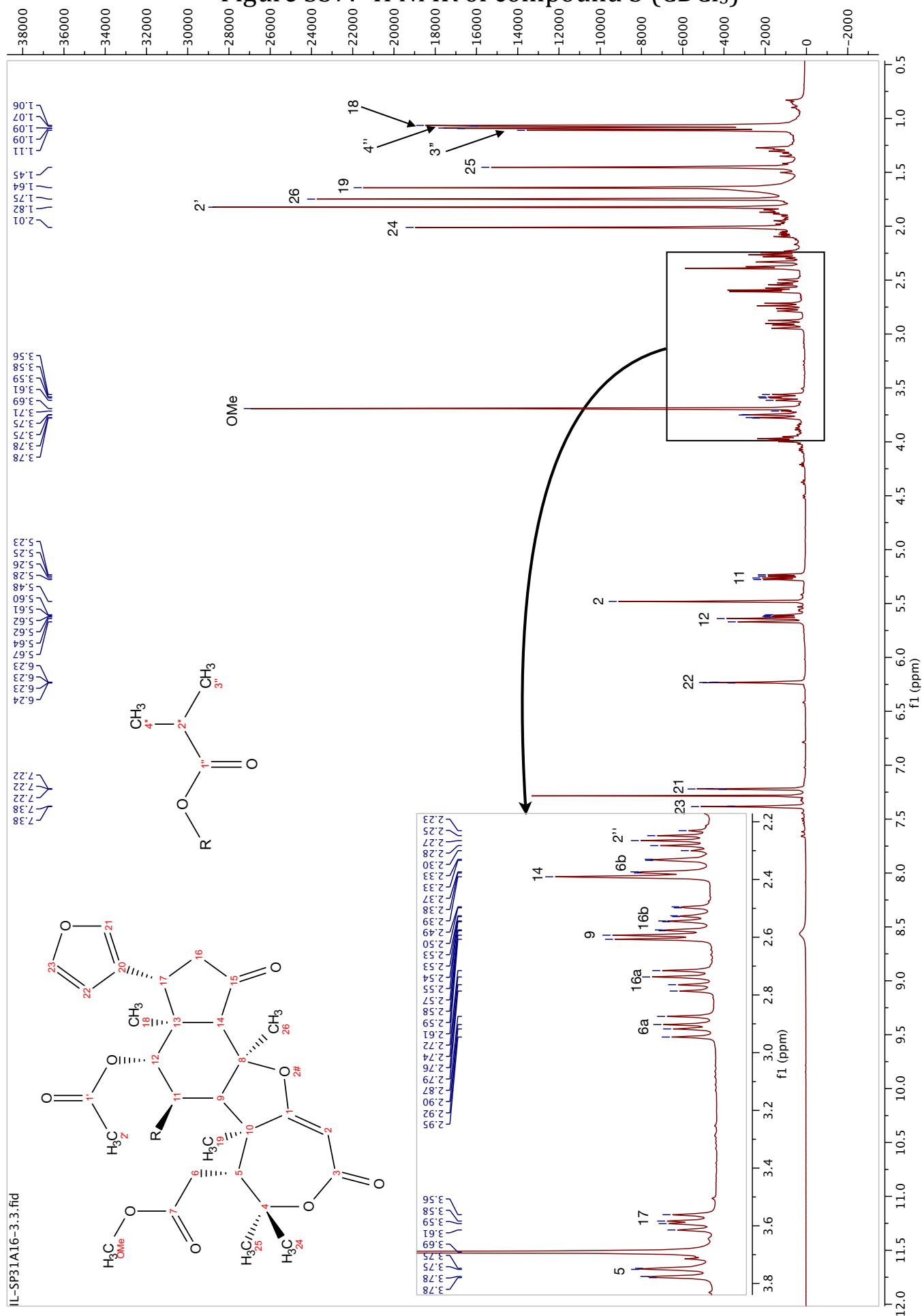


Figure S38:  $^{13}\text{C}$  NMR of compound 5 ( $\text{CDCl}_3$ )

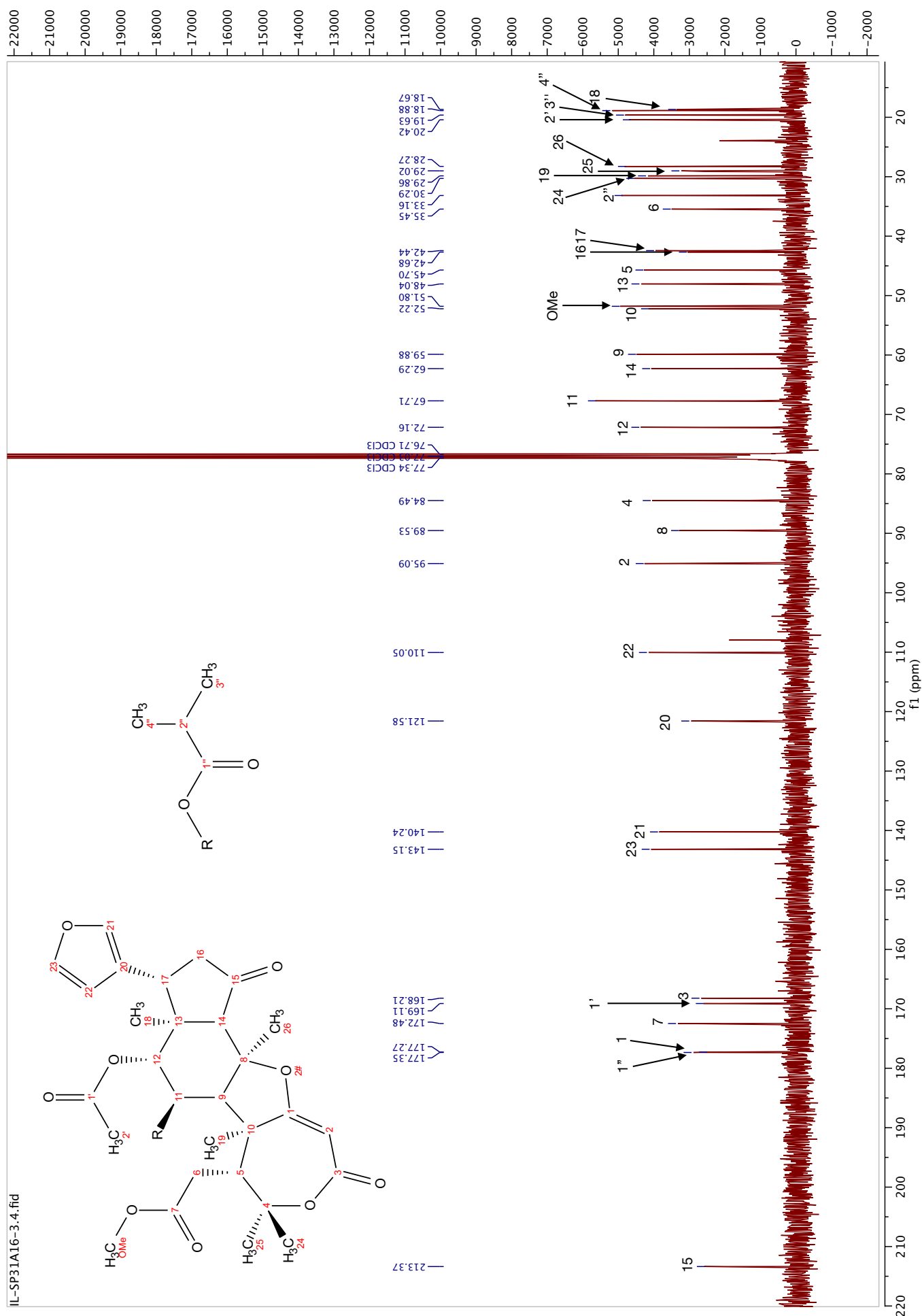


Figure S39:  $^{13}\text{C}$  and DEPT135 spectra of compound 5 ( $\text{CDCl}_3$ )

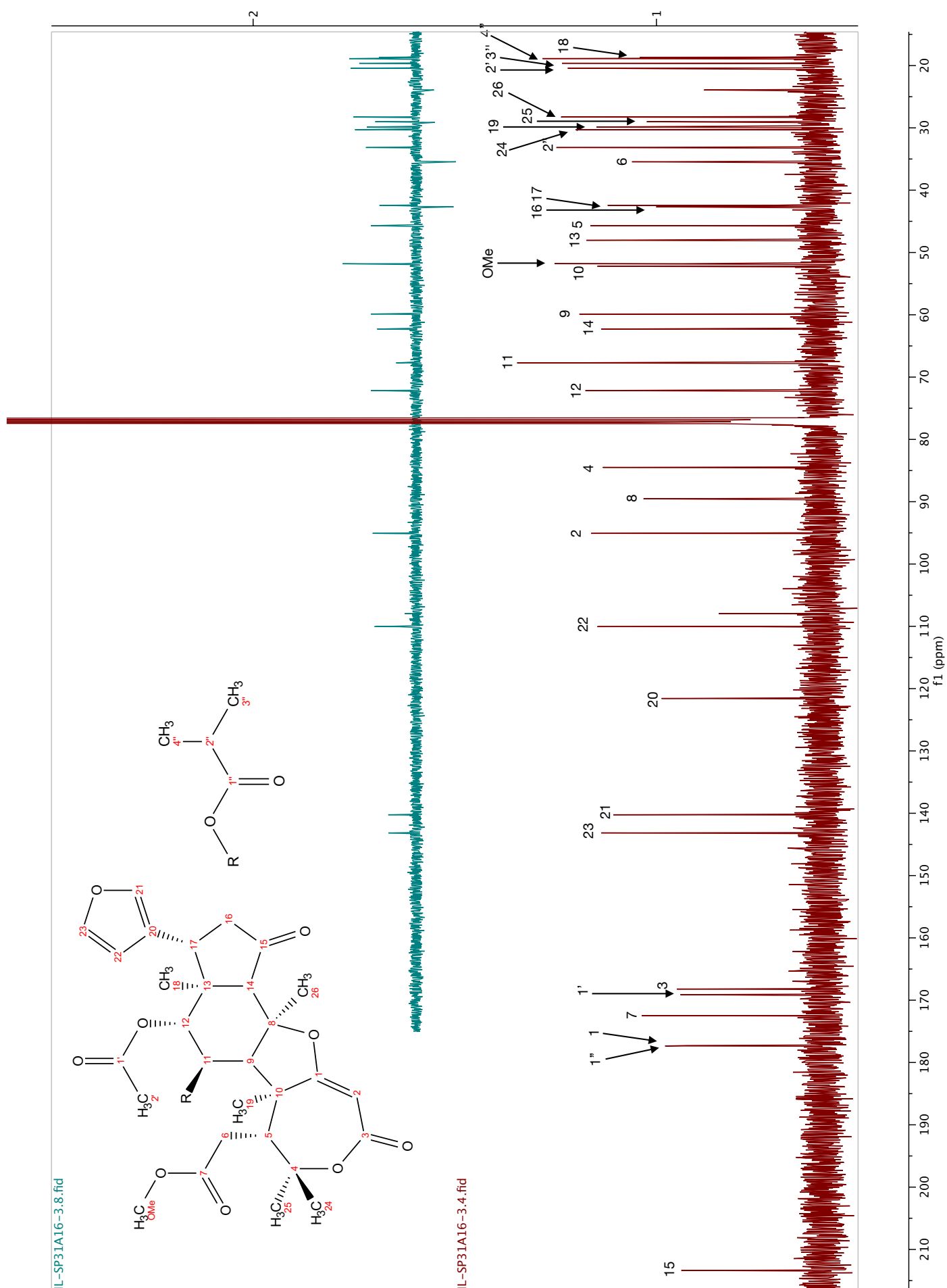


Figure S40: COSY experiment of compound 5 (CDCl<sub>3</sub>)

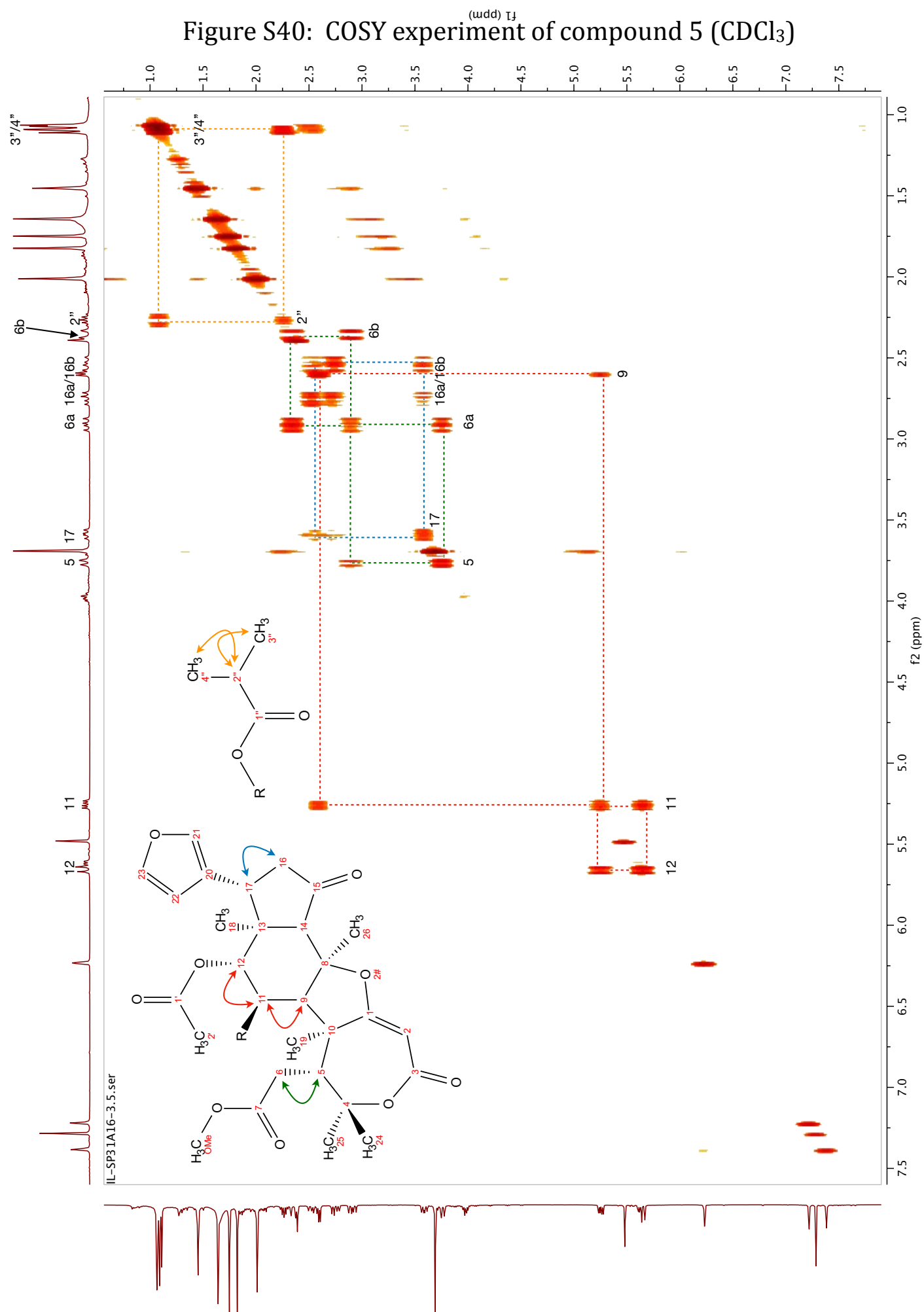


Figure S41: HMQC experiment of compound 5 (CDCl<sub>3</sub>)

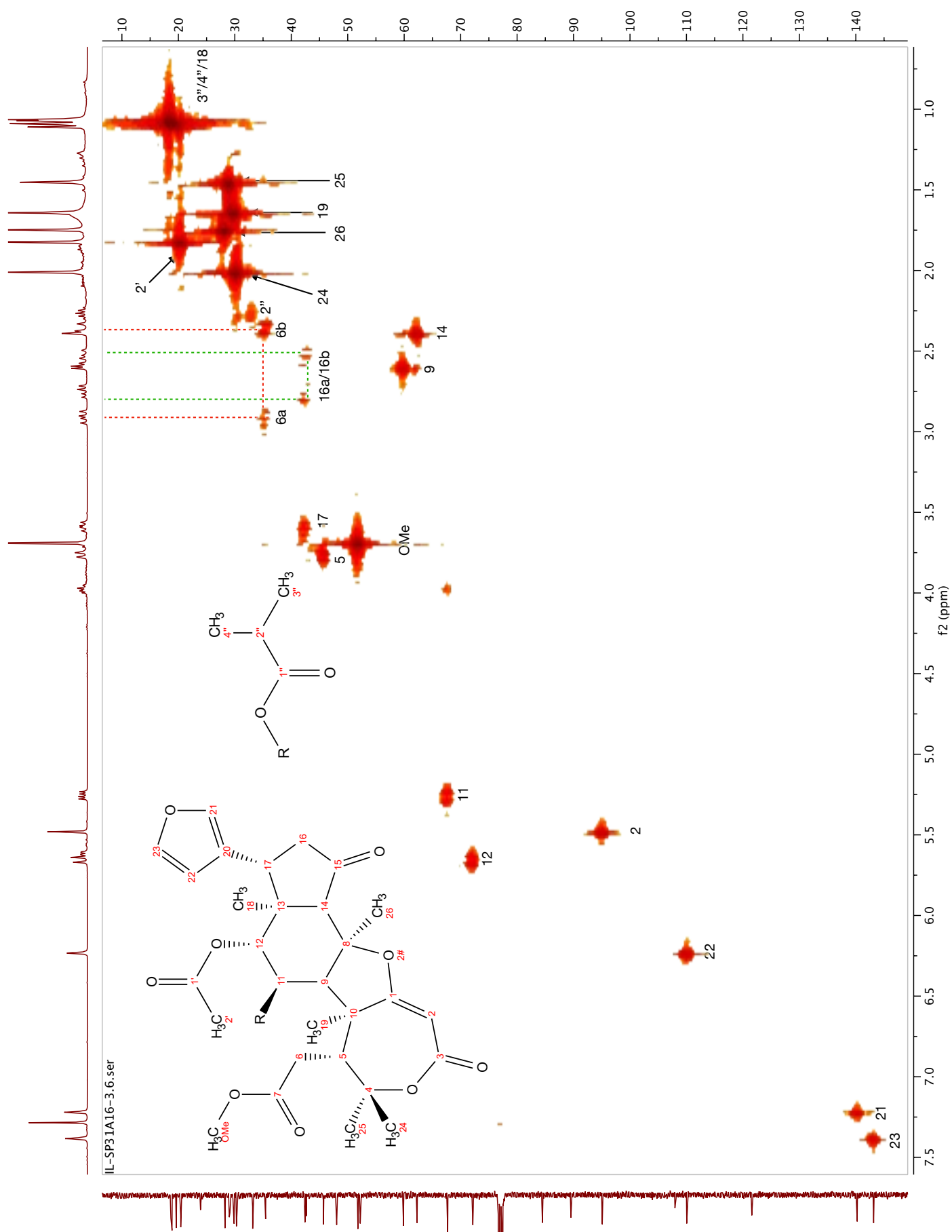


Figure S42: HMBC experiment of compound 5 (CDCl<sub>3</sub>)

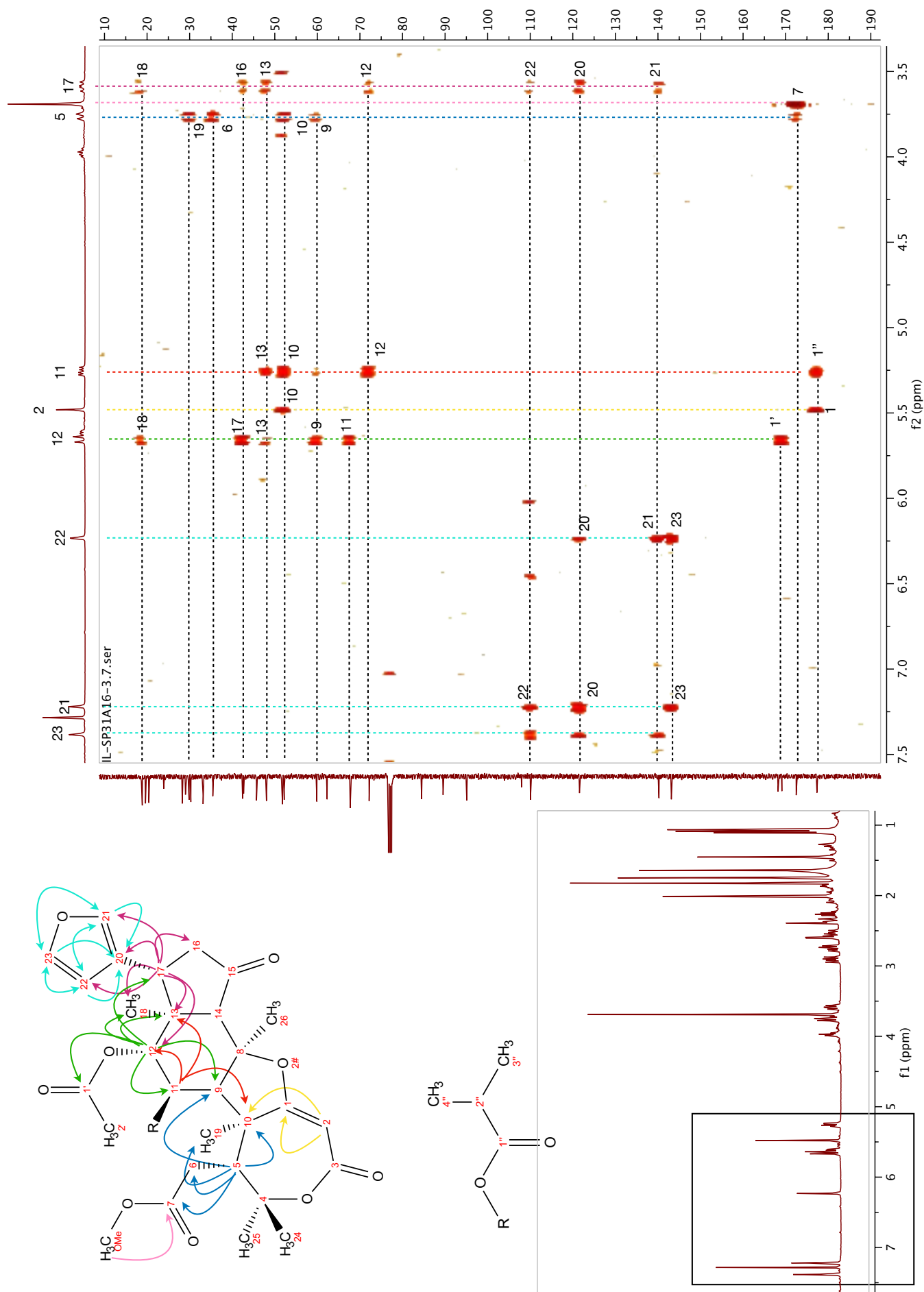
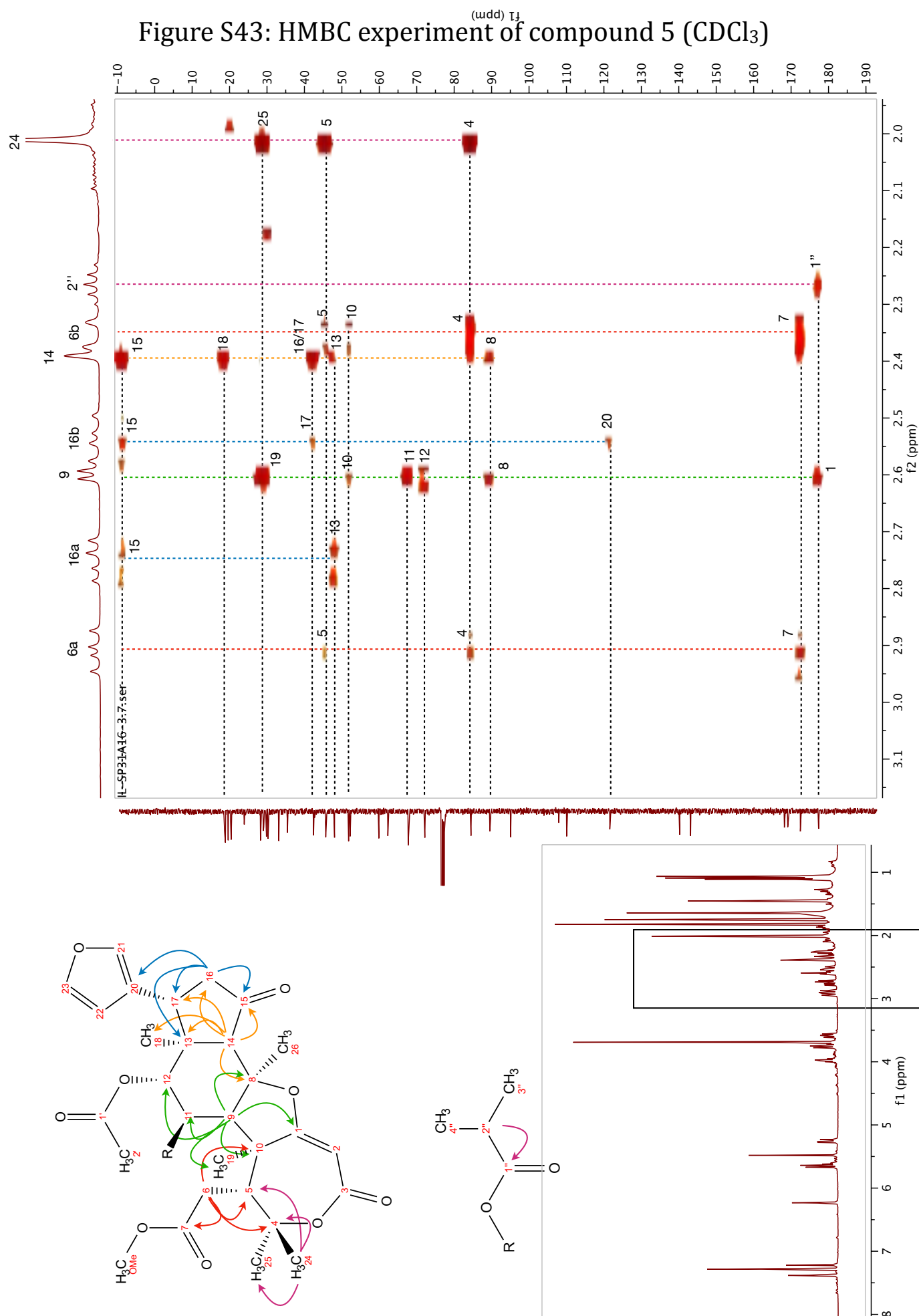


Figure S43: HMBC experiment of compound 5 (CDCl<sub>3</sub>)



(wdd) 14

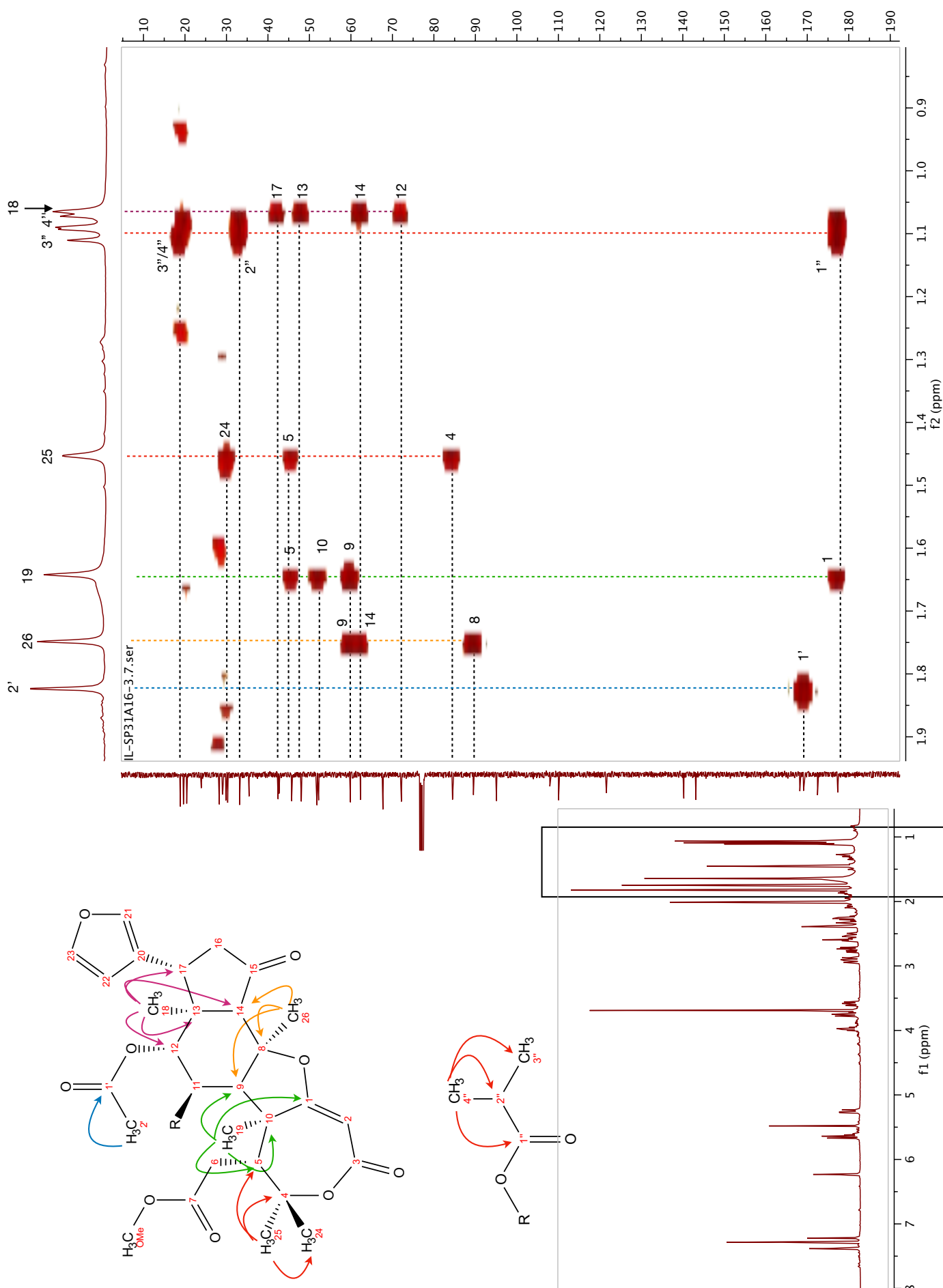




Figure S45: NOESY experiment of compound 5 (CDCl<sub>3</sub>)

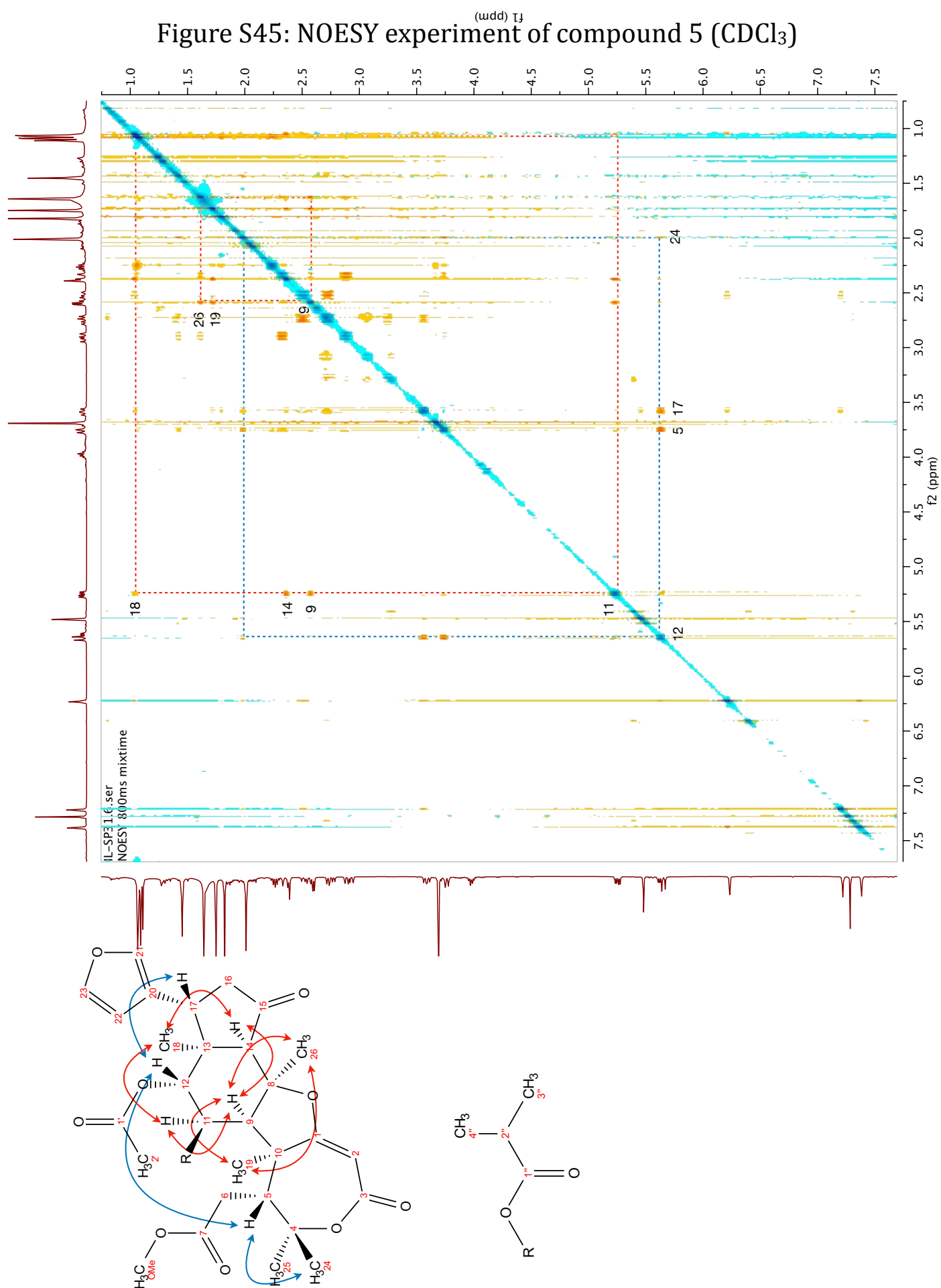


Figure S46: HRMS and IR spectra of compound 5

