Supporting Information

Synthesis and anticancer activity of dimeric polyether ionophores

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Spectroscopic and spectrometric analysis of synthesized compounds

FT-IR and NMR analysis of propargyl and azide components

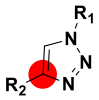
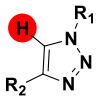
Table S1. The yields of the synthesis, and the analytical bands in the FT-IR spectra (wavenumbers in cm^{-1}) and signals in the ^{1}H and ^{13}C NMR spectra (δ in ppm) of propargyl and azide partners for the CuAAC reaction.

	No.	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**
	Yield (%)	54	60	51	65	51	60	15	88	90	70
FT-IR KBr tablet	***ν*(≡C–H)**	3313	3311	3315	3314	3311	3310	3297	3319	3314	-----
	***ν*(C≡C)**	2125	2130	2120	2128	2120	2129	2130	2128	2127	-----
	***ν*(N_3)**	-----	-----	-----	-----	-----	-----	-----	-----	-----	2098
^{1}H NMR in CD_2Cl_2	***δ*(≡C–H)**	2.32 (t, *J* = 2.5 Hz, 1H)	2.58[(a)] (t, *J* = 2.5 Hz, 1H)	signal overlapped	2.56 (t, *J* = 2.5 Hz, 1H)	2.22 (t, *J* = 2.5 Hz, 1H)	2.48 (t, *J* = 2.4 Hz, 1H)	2.51[(a)] (t, *J* = 2.4 Hz, 1H)	2.16 (t, *J* = 2.5 Hz, 1H)	2.05[(b)] (t, *J* = 2.5 Hz, 1H)	-----
^{13}C NMR in CD_2Cl_2	***δ*(C=O) amide/ester**	170.6	171.1[(a)]	175.7[(a)]	175.1	176.0	175.5	154.5[(a,c)]	175.2	173.9[(b)]	-----

[(a)] in $CDCl_3$; [(b)] in C_6D_6; [(c)] *δ*(C=O)carbonate in **10**

^{1}H and ^{13}C NMR analysis of newly synthesized compounds

Table S2. The yields of the synthesis, and the analytical signals in the ^{1}H and ^{13}C NMR spectra of novel dimeric polyether ionophores.

No.	**Yield (%)**	**Analytical NMR signals (ppm) in $CDCl_3$**					
		***δ*(C=O) carboxylate**	***δ*(C=O) amide/ester**	***δ*(H–N) amide**	***δ*(CH_2–O) ester**		
14	70	184.5	170.1	7.28–7.19 (m, 1H)	-----	144.5[(a)]	7.82 (s, 1H)
15	70	184.4	171.5	-----	5.41 (dd, *J* = 26.1, 12.6 Hz, 2H)	141.6[(a)]	7.68 (s, 1H)
16	63	184.3	175.7	7.15–7.06 (m, 1H)	-----	144.7	7.46 (s, 1H)
17	52	184.4	175.0	-----	5.24 (d, *J* = 12.8 Hz, 1H) 5.16 (d, *J* = 12.8 Hz, 1H)	142.4	7.63 (s, 1H)
18	56	184.6	176.1	6.23 (t, *J* = 5.5 Hz, 1H)	-----	144.4	7.48 (s, 1H)
19	81	184.5	175.7	-----	5.09 (dd, *J* = 25.8, 12.7 Hz, 2H)	142.5	7.58 (s, 1H)
20	37	184.5	155.0[(b)]	-----	5.23–5.15 (m, 2H)[(c)]	141.8	7.67 (s, 1H)
21	63	184.4	175.0	6.97 (t, *J* = 5.1 Hz, 1H)	-----	144.9	7.60 (s, 1H)
22	52	184.4	175.2	-----	5.50 (d, *J* = 12.8 Hz, 1H) 5.25 (d, *J* = 12.8 Hz, 1H)	142.3	7.66 (s, 1H)
23	32	173.5[(d)]	175.3	-----	5.43 (d, *J* = 12.8 Hz, 1H) second signal overlapped	142.9	7.55 (s, 1H)
24	31	173.4[(d)]	175.3	-----	5.50 (d, *J* = 12.9 Hz, 1H) second signal overlapped	142.9	7.62 (s, 1H)

[(a)] based on the ^{1}H-^{13}C HMBC spectrum; [(b)] *δ*(C=O)carbonate in **20**; [(c)] *δ*(CH_2–O)carbonate in **20**; [(d)] *δ*(C=O)ester after conjugation with hydroxamic acid in **23** and **24**

1) The NMR spectra of newly synthesized propargyl precursors

List of spectra

2) The NMR spectra of dimeric polyether ionophores

List of spectra

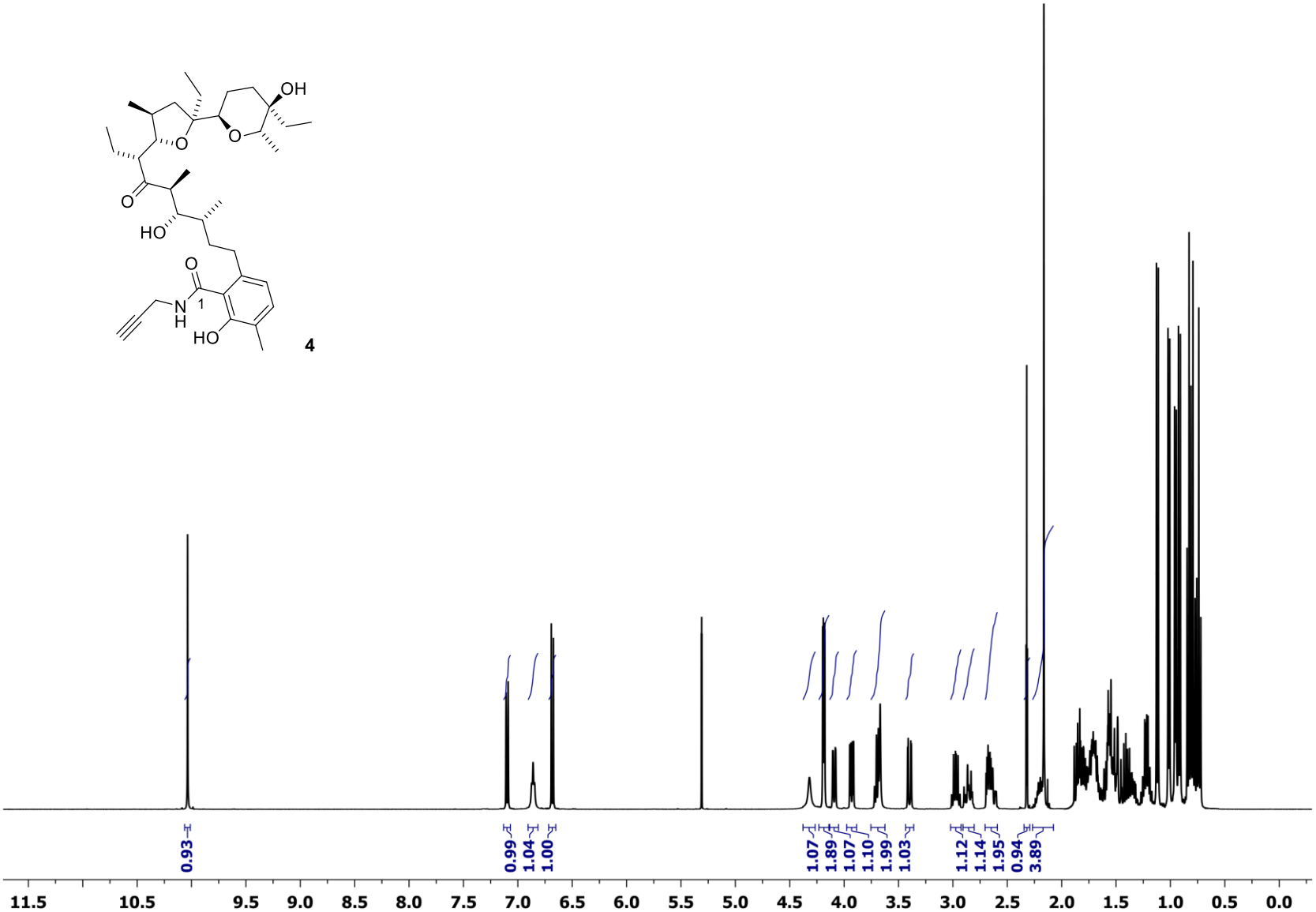


Figure S1. The ^{1}H NMR spectrum of **4** in dichloromethane-d_2.

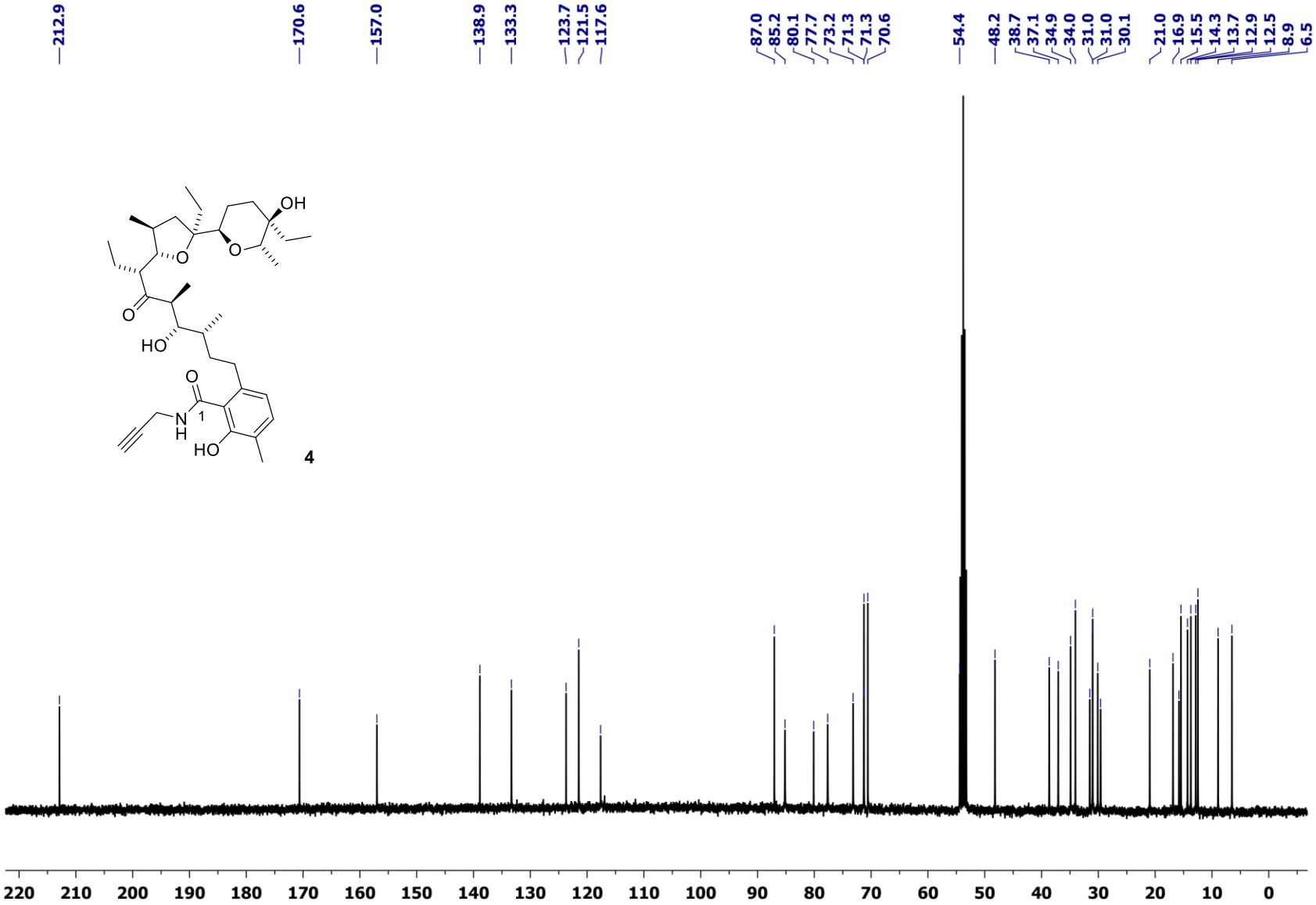


Figure S2. The ^{13}C NMR spectrum of **4** in dichloromethane-d_2.

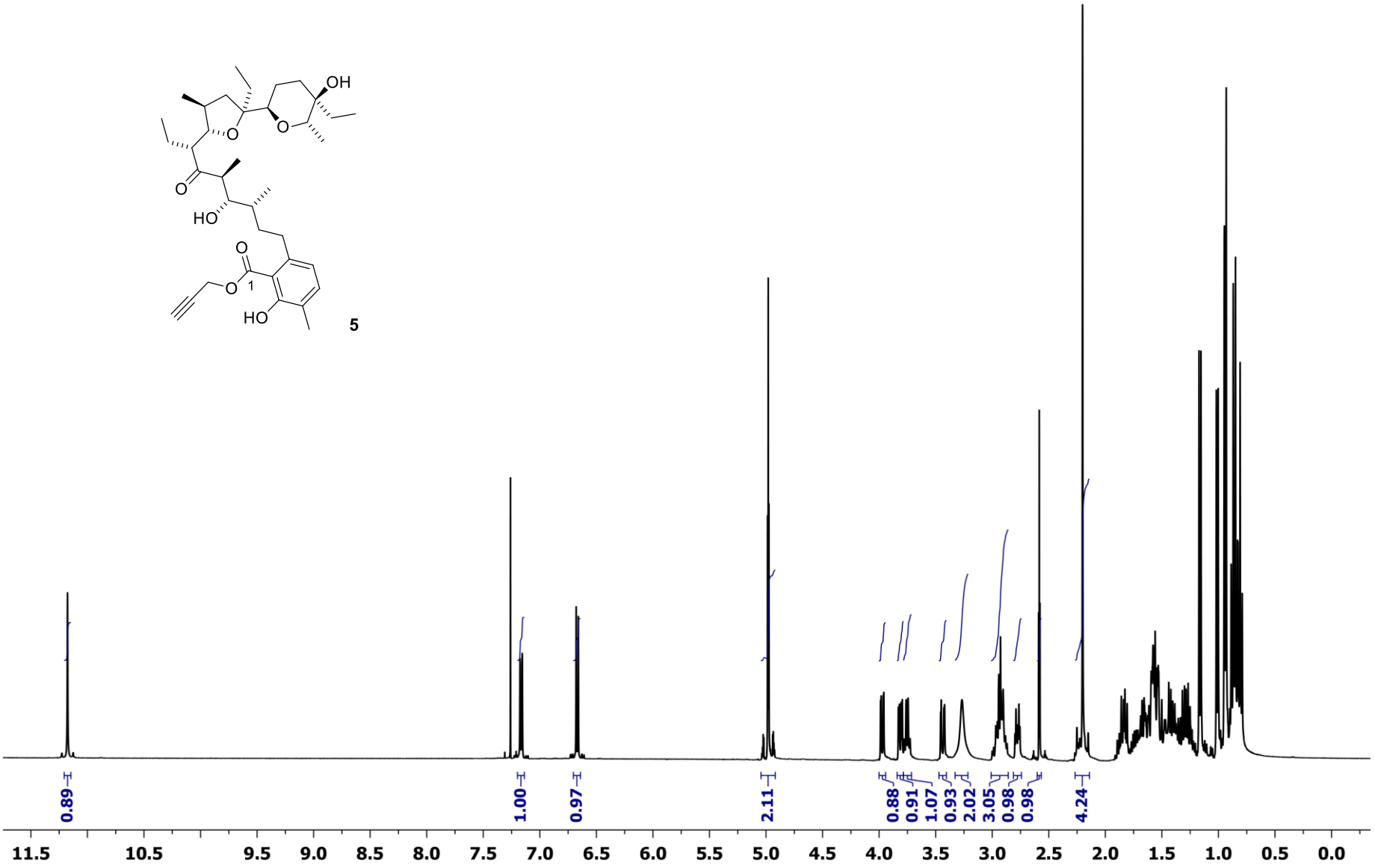


Figure S3. The ^{1}H NMR spectrum of **5** in chloroform-d.

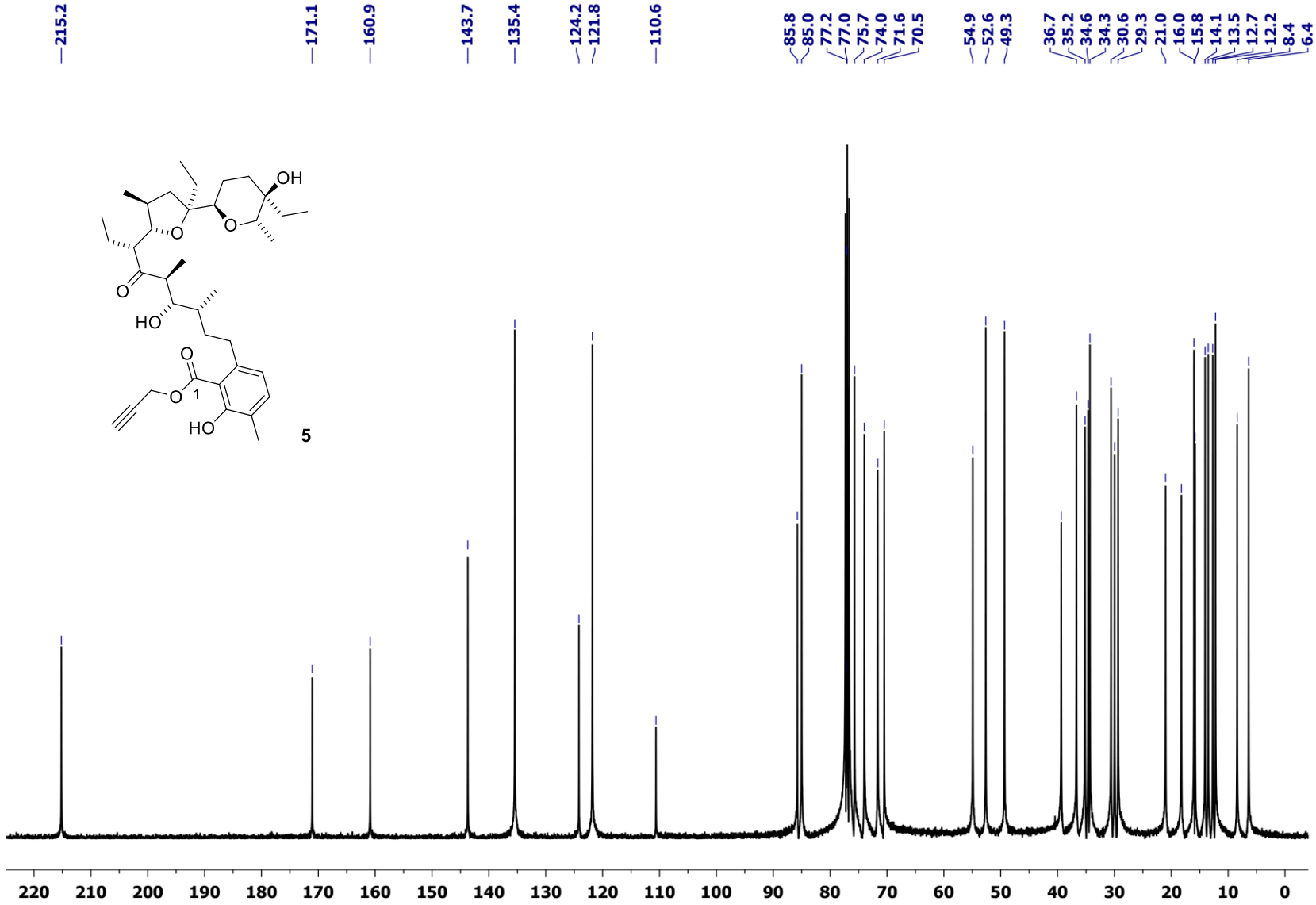


Figure S4. The ^{13}C NMR spectrum of **5** in chloroform-d.

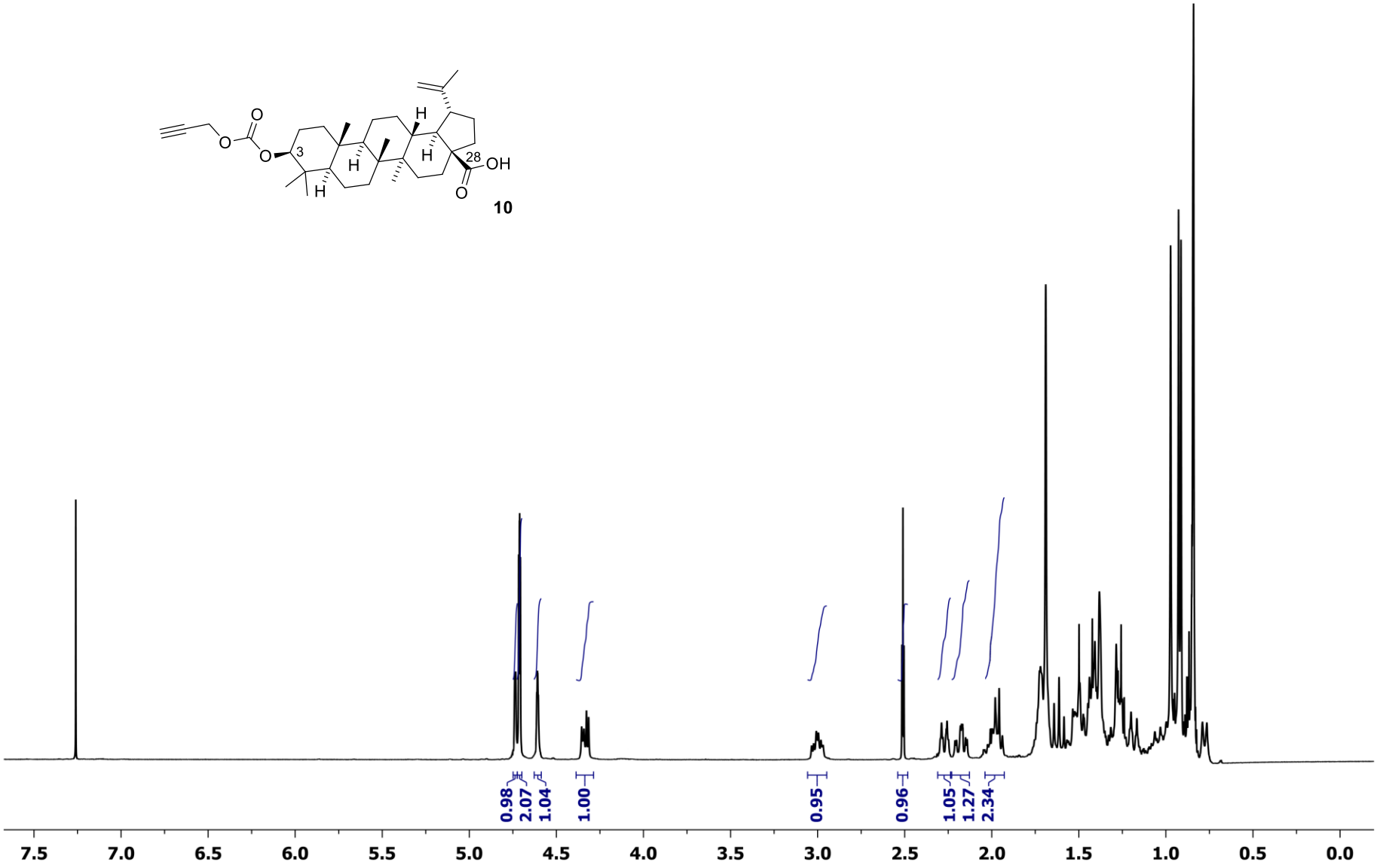


Figure S5. The ^{1}H NMR spectrum of **10** in chloroform-d.

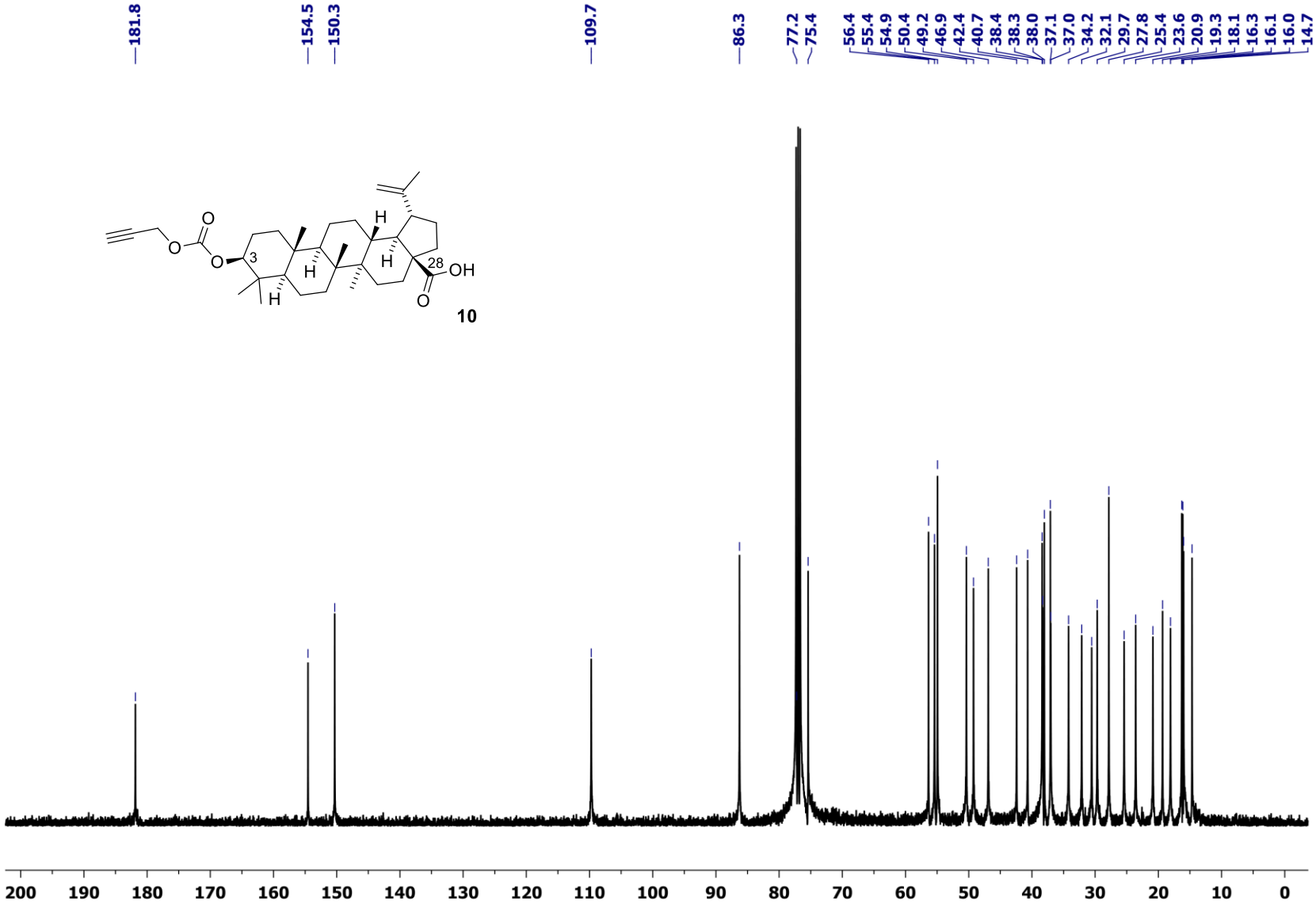


Figure S6. The ^{13}C NMR spectrum of **10** in chloroform-d.

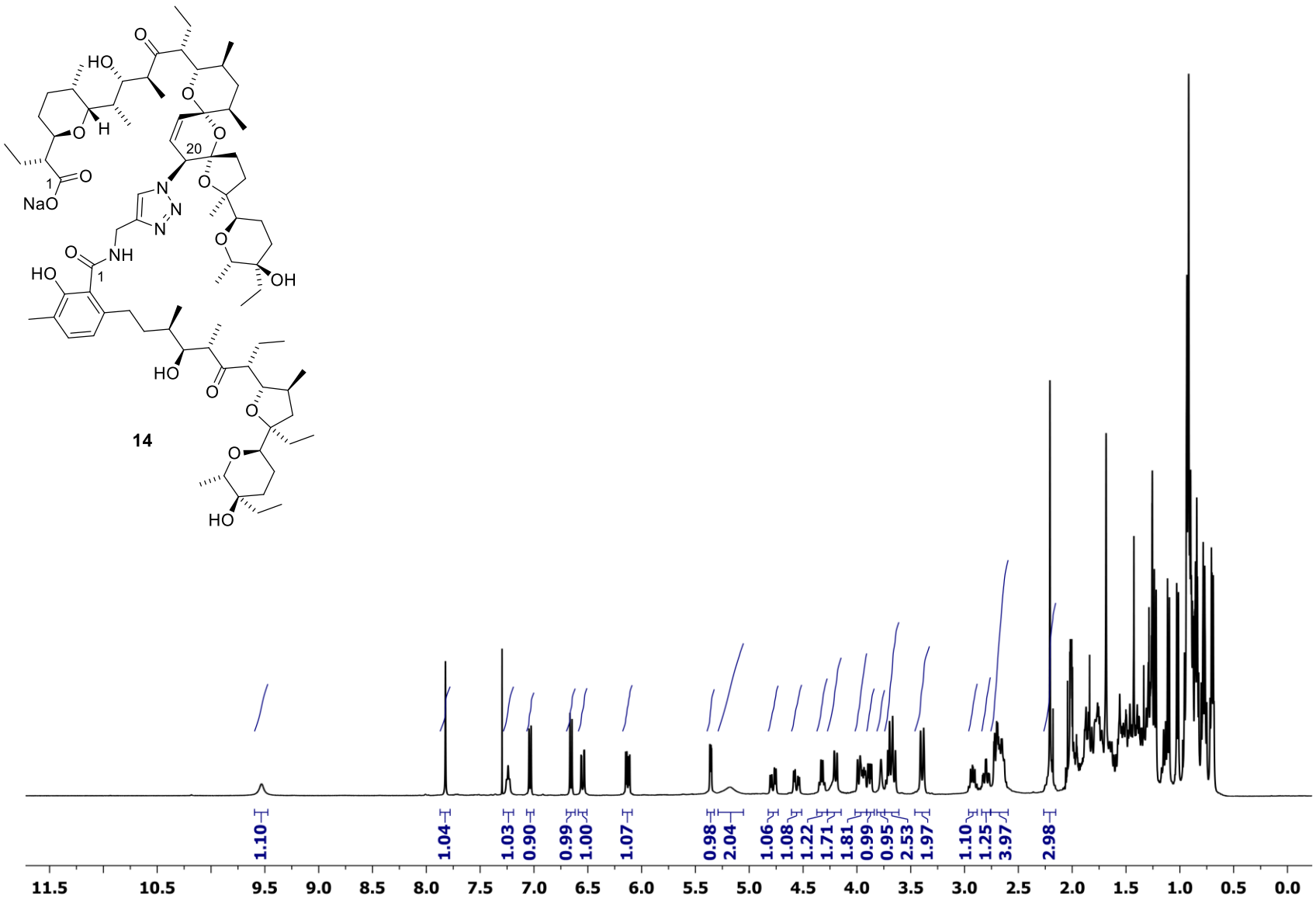


Figure S7. The ^{1}H NMR spectrum of **14** in chloroform-d.

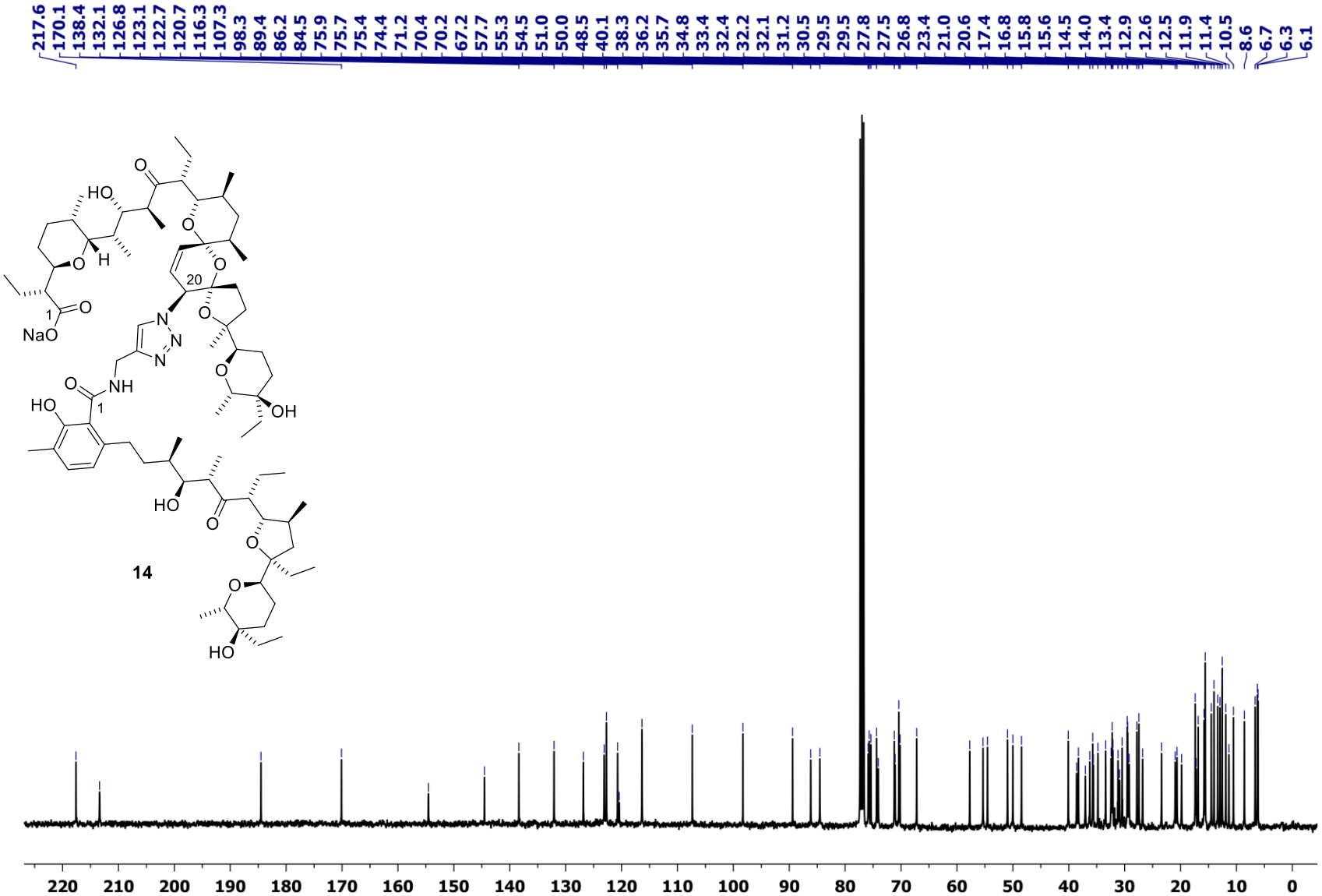


Figure S8. The ^{13}C NMR spectrum of **14** in chloroform-d.

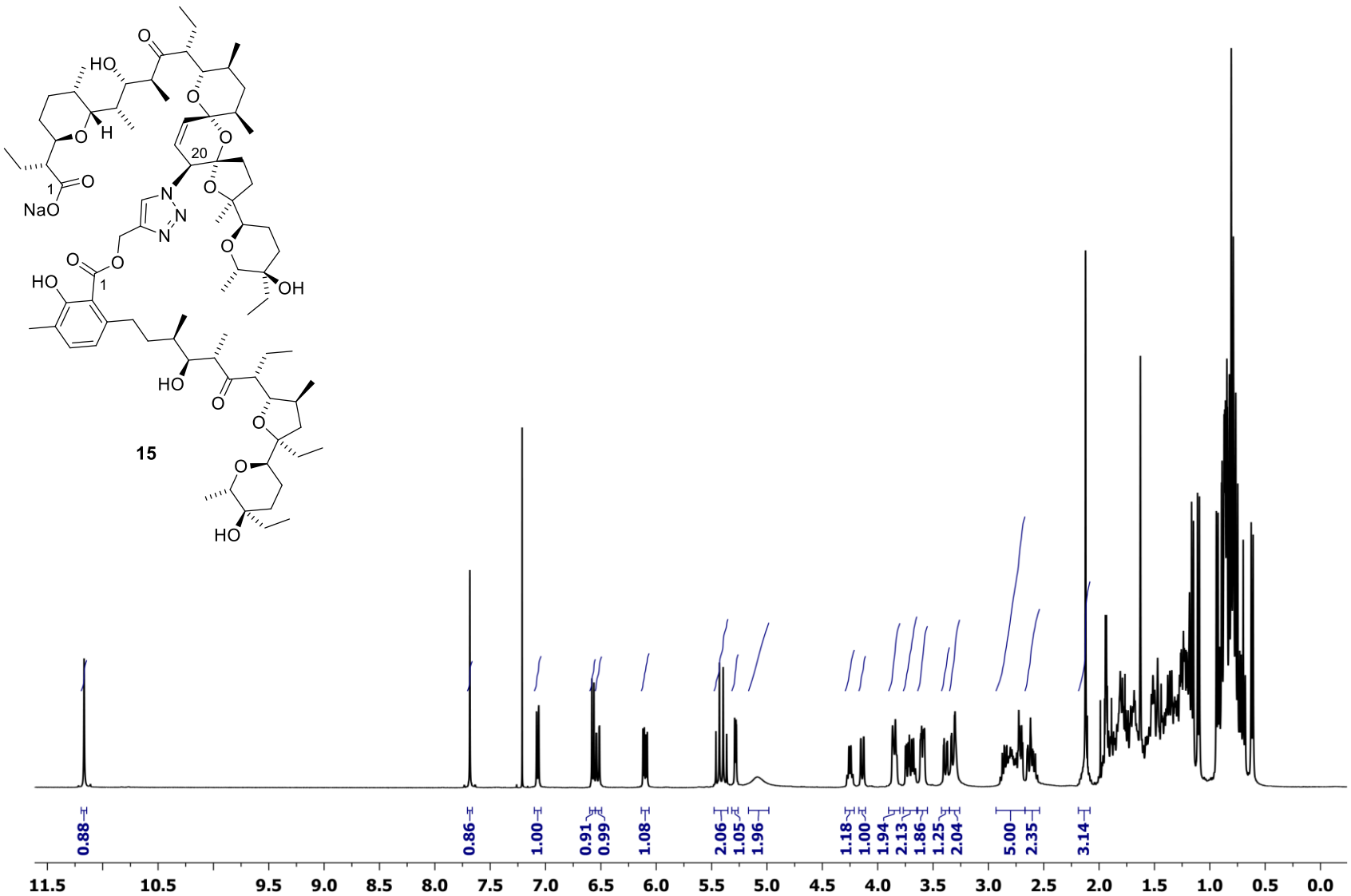


Figure S9. The ^{1}H NMR spectrum of **15** in chloroform-d.

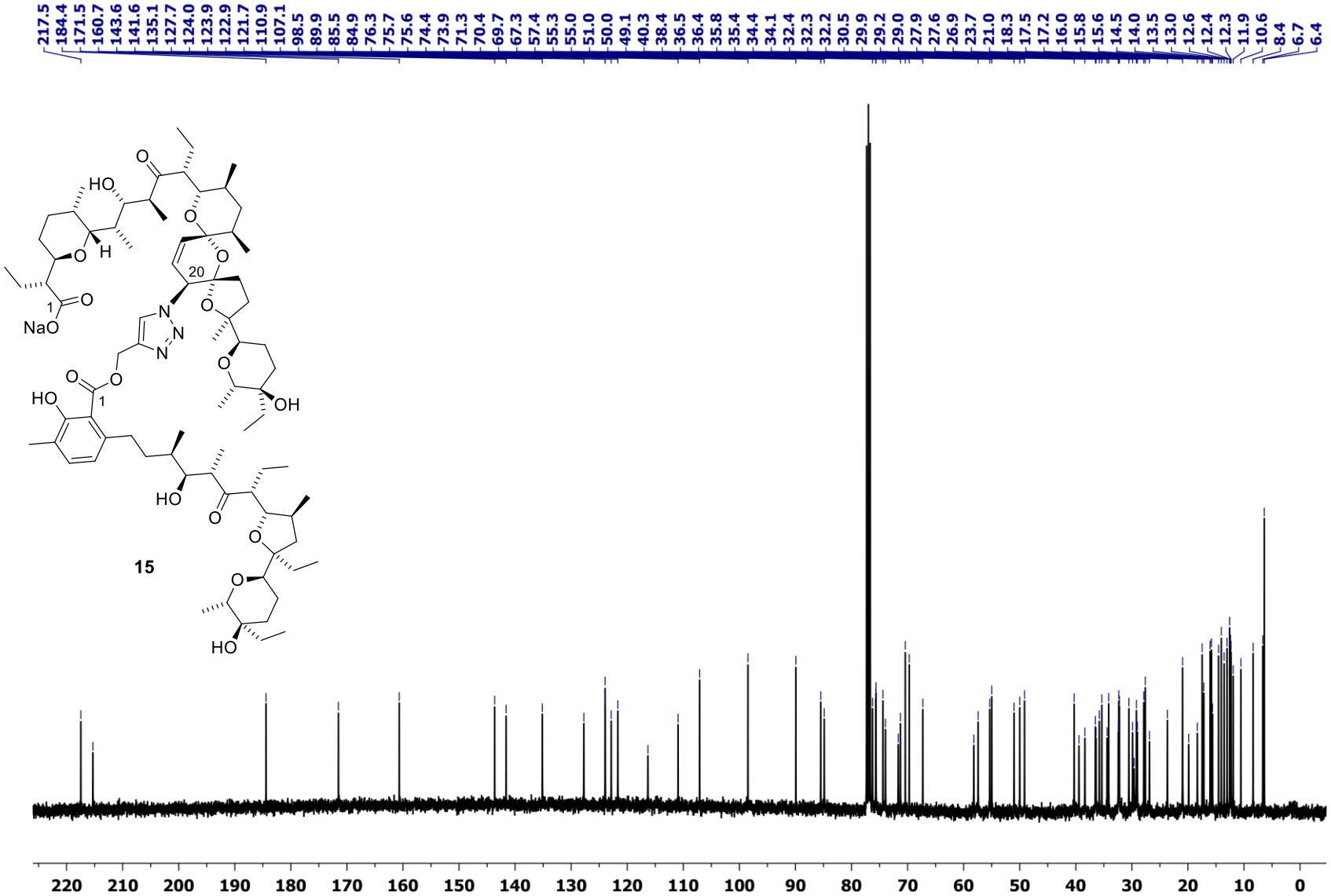


Figure S10. The ^{13}C NMR spectrum of **15** in chloroform-d.

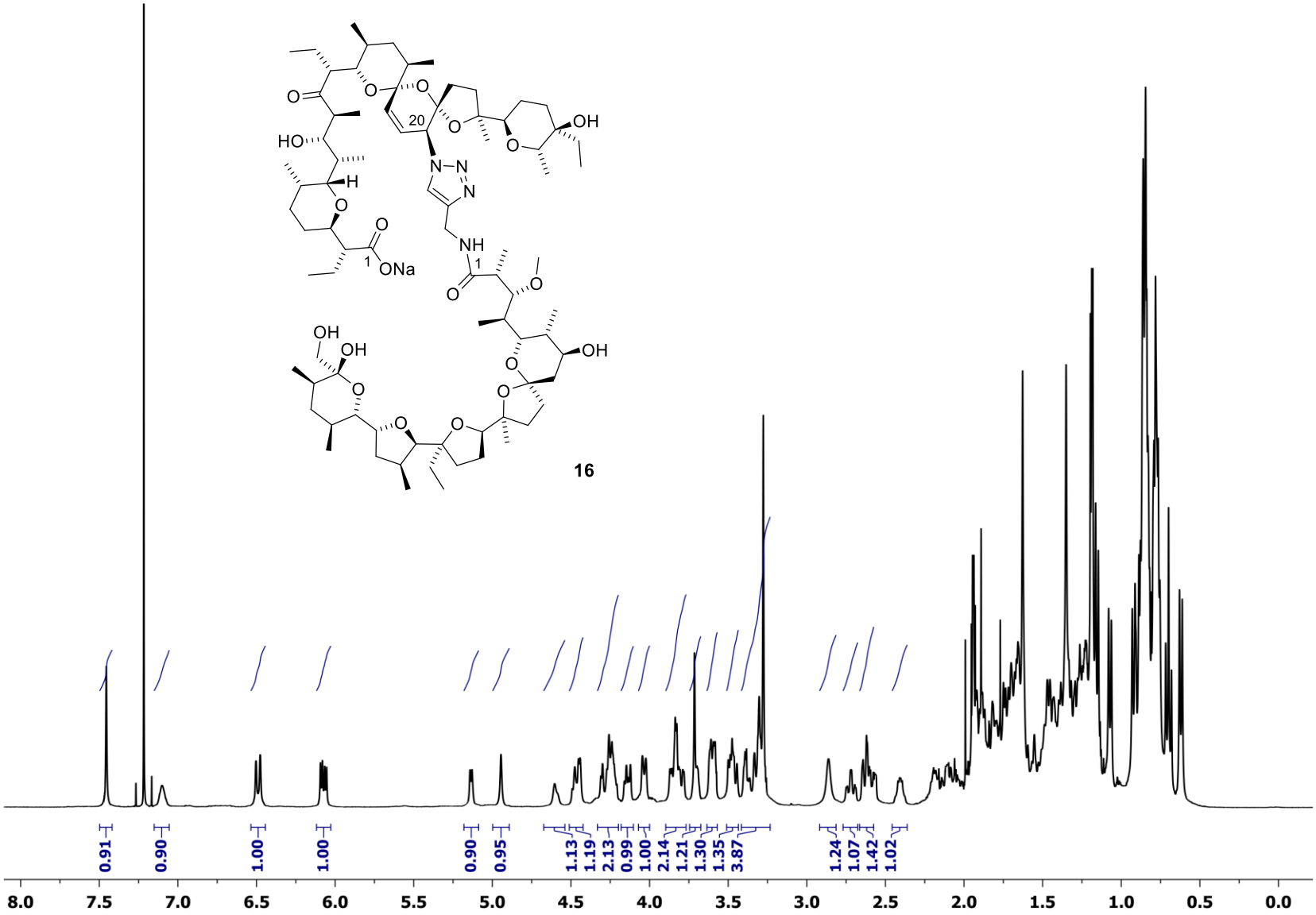


Figure S11. The ^{1}H NMR spectrum of **16** in chloroform-d.

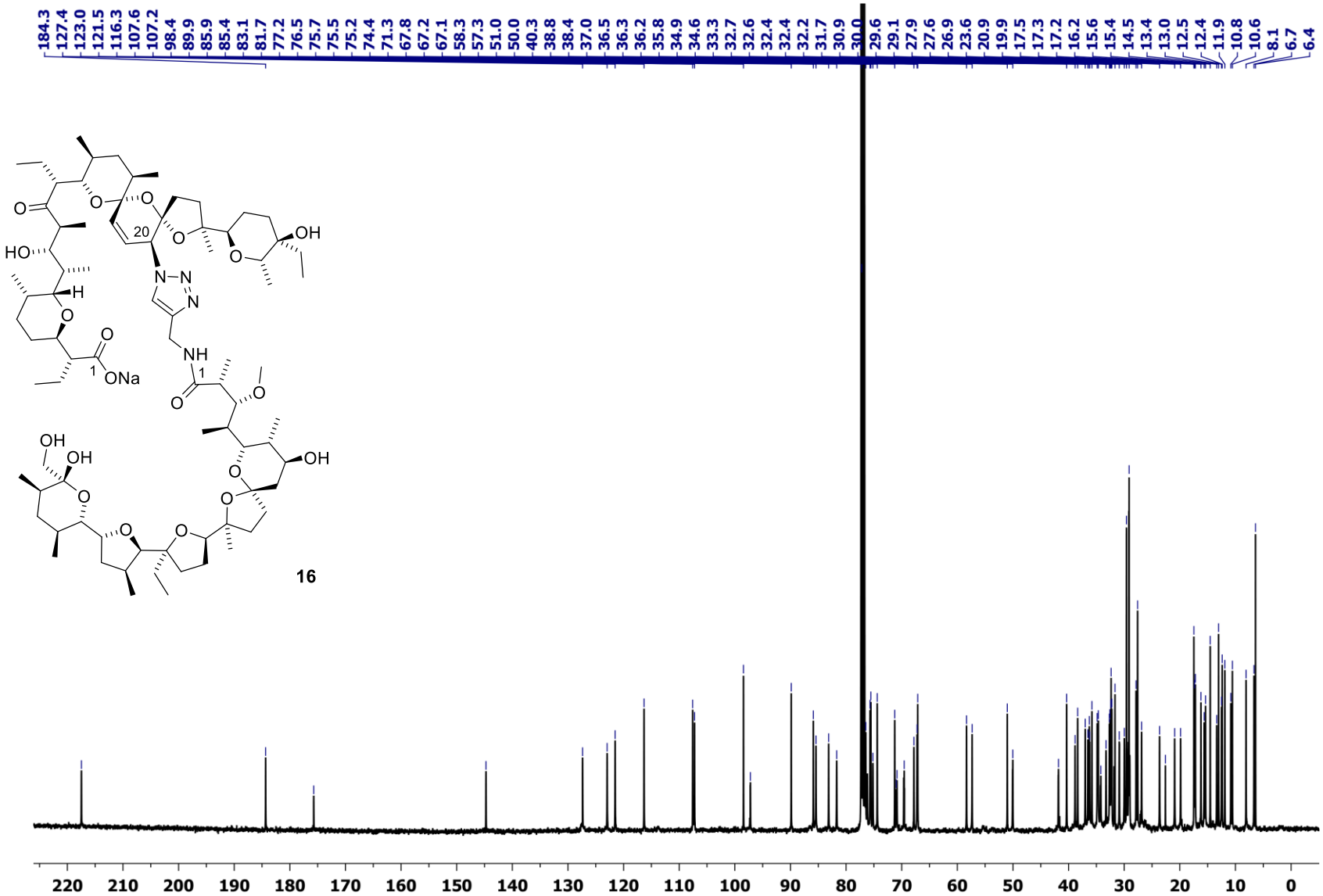


Figure S12. The ^{13}C NMR spectrum of **16** in chloroform-d.

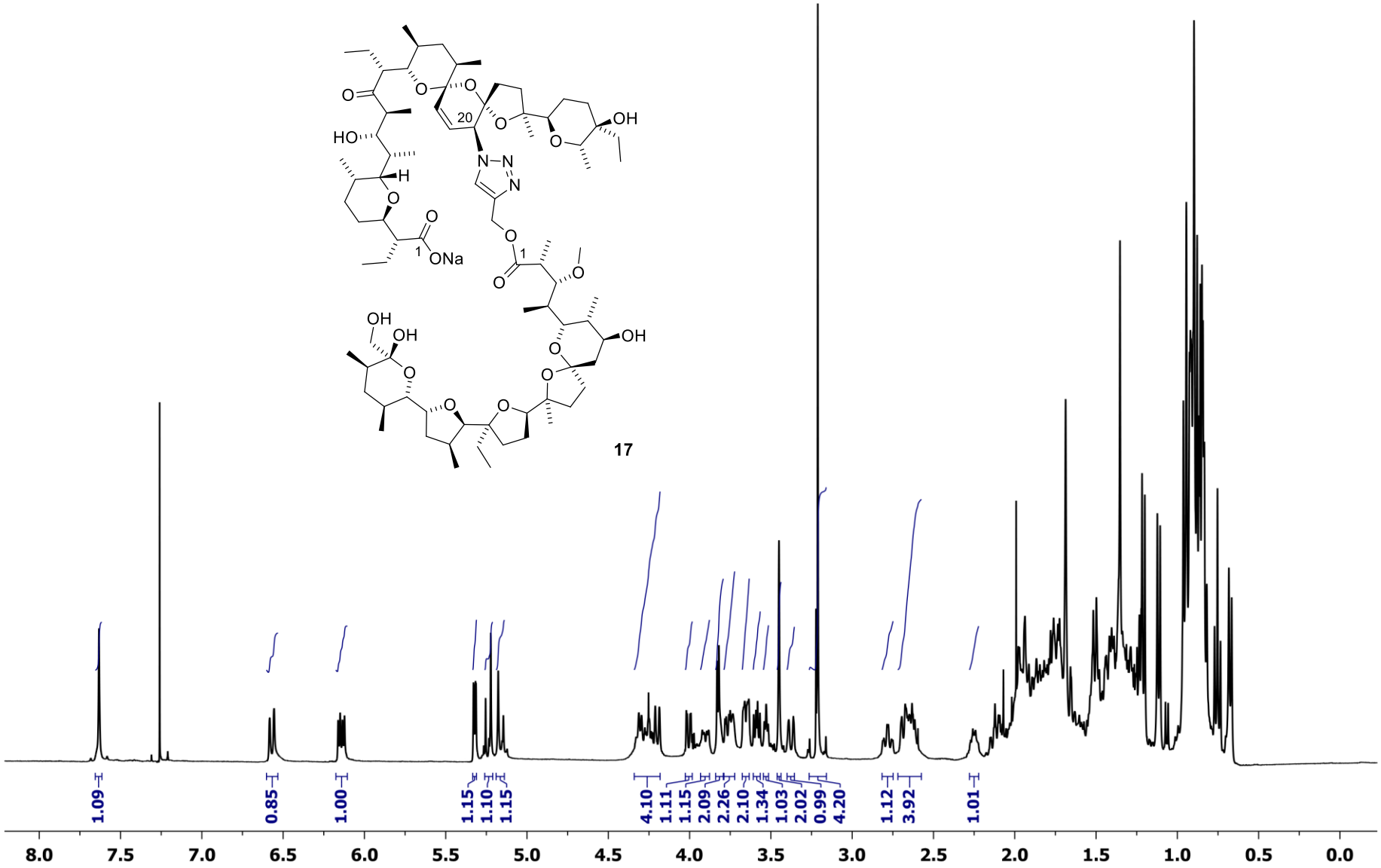


Figure S13. The ^{1}H NMR spectrum of **17** in chloroform-d.

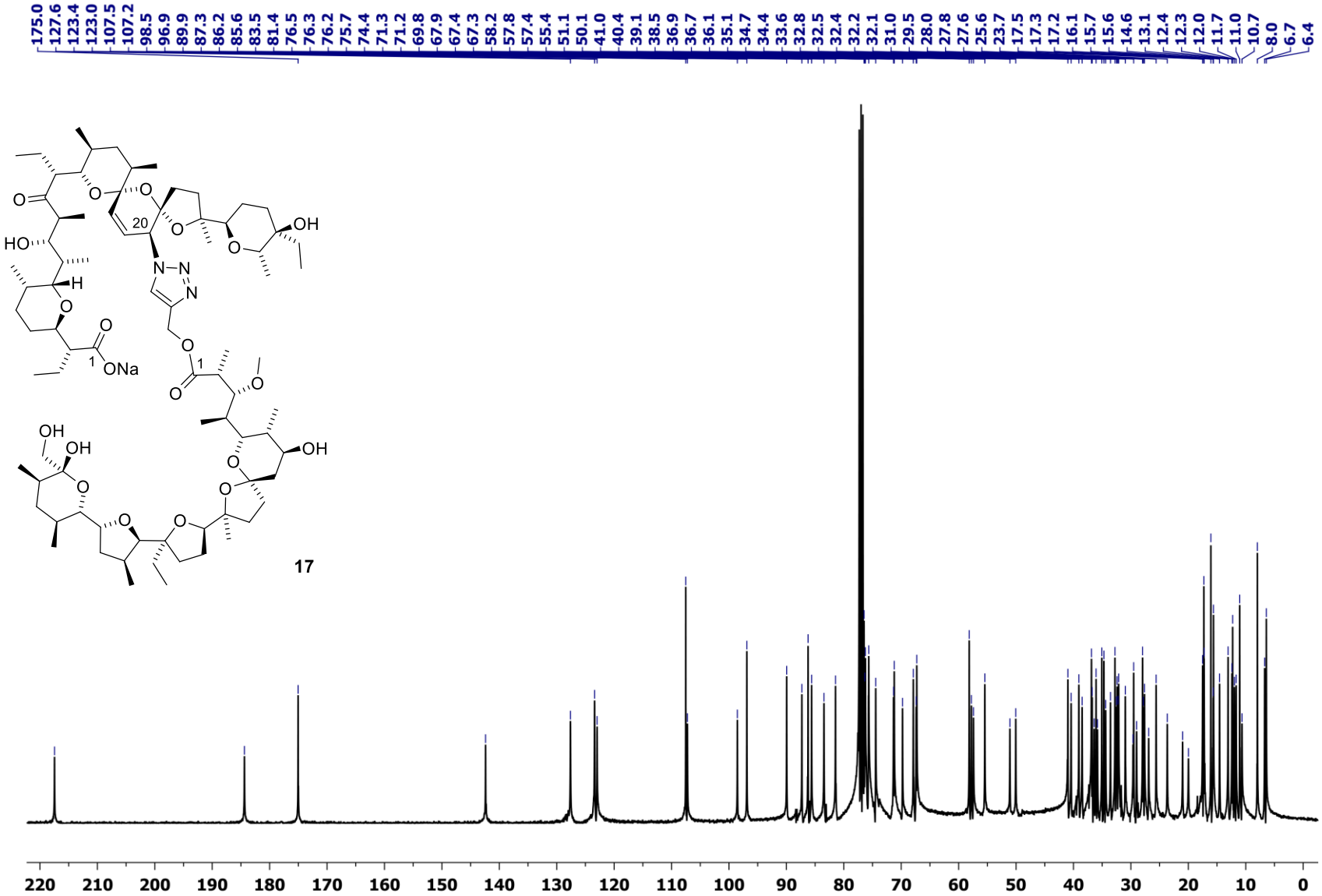


Figure S14. The ^{13}C NMR spectrum of **17** in chloroform-d.

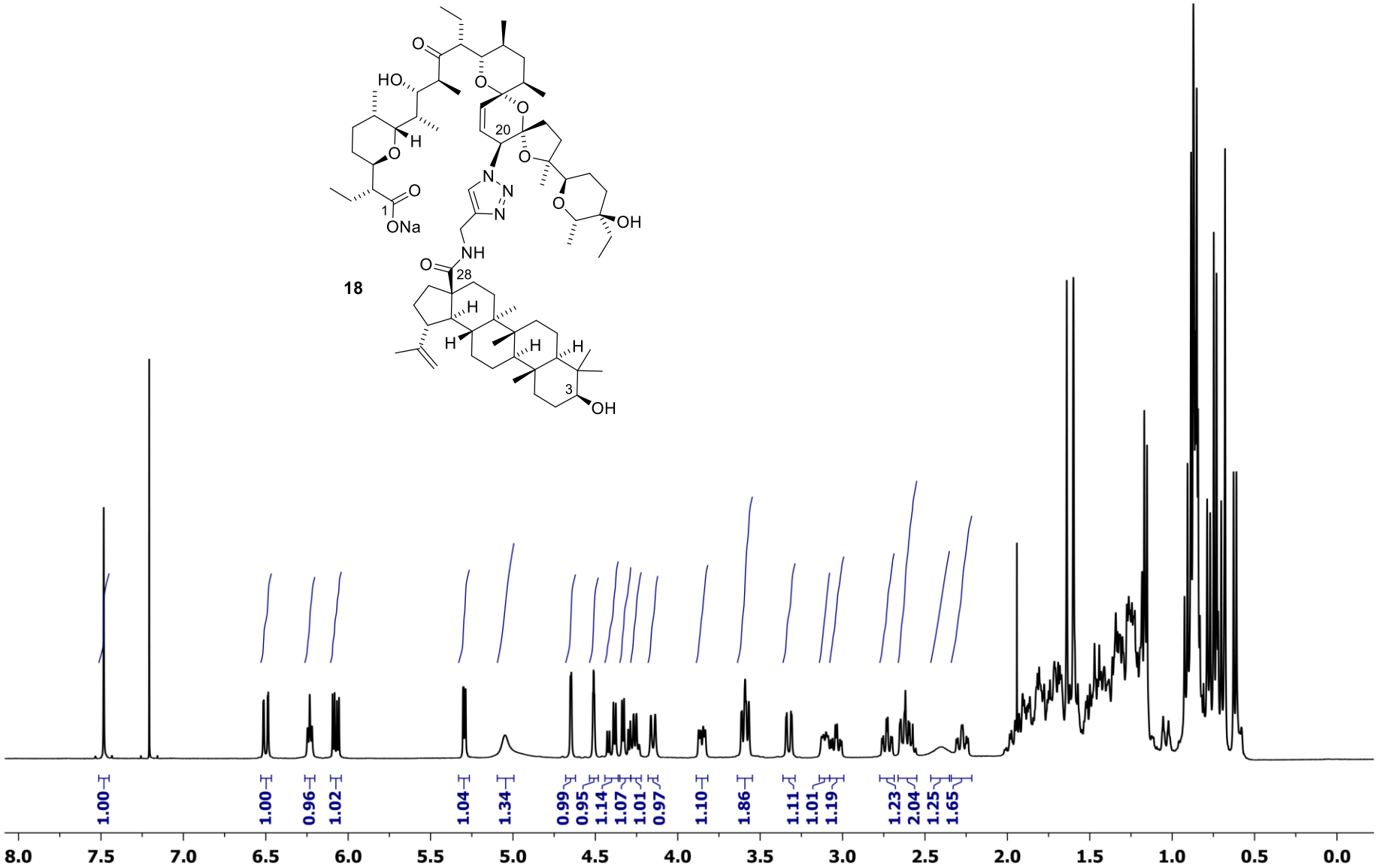


Figure S15. The ^{1}H NMR spectrum of **18** in chloroform-d.

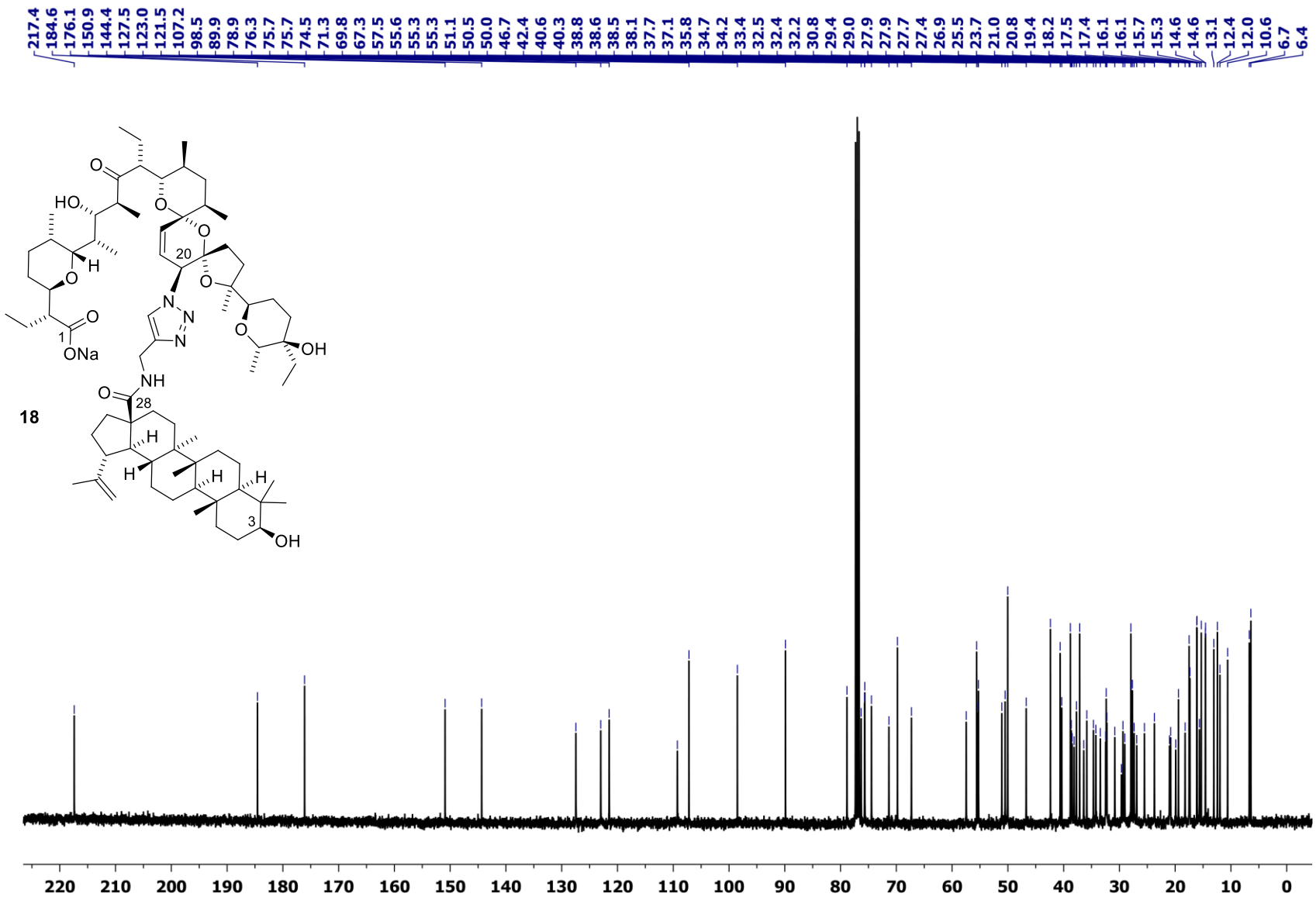


Figure S16. The ^{13}C NMR spectrum of **18** in chloroform-d.

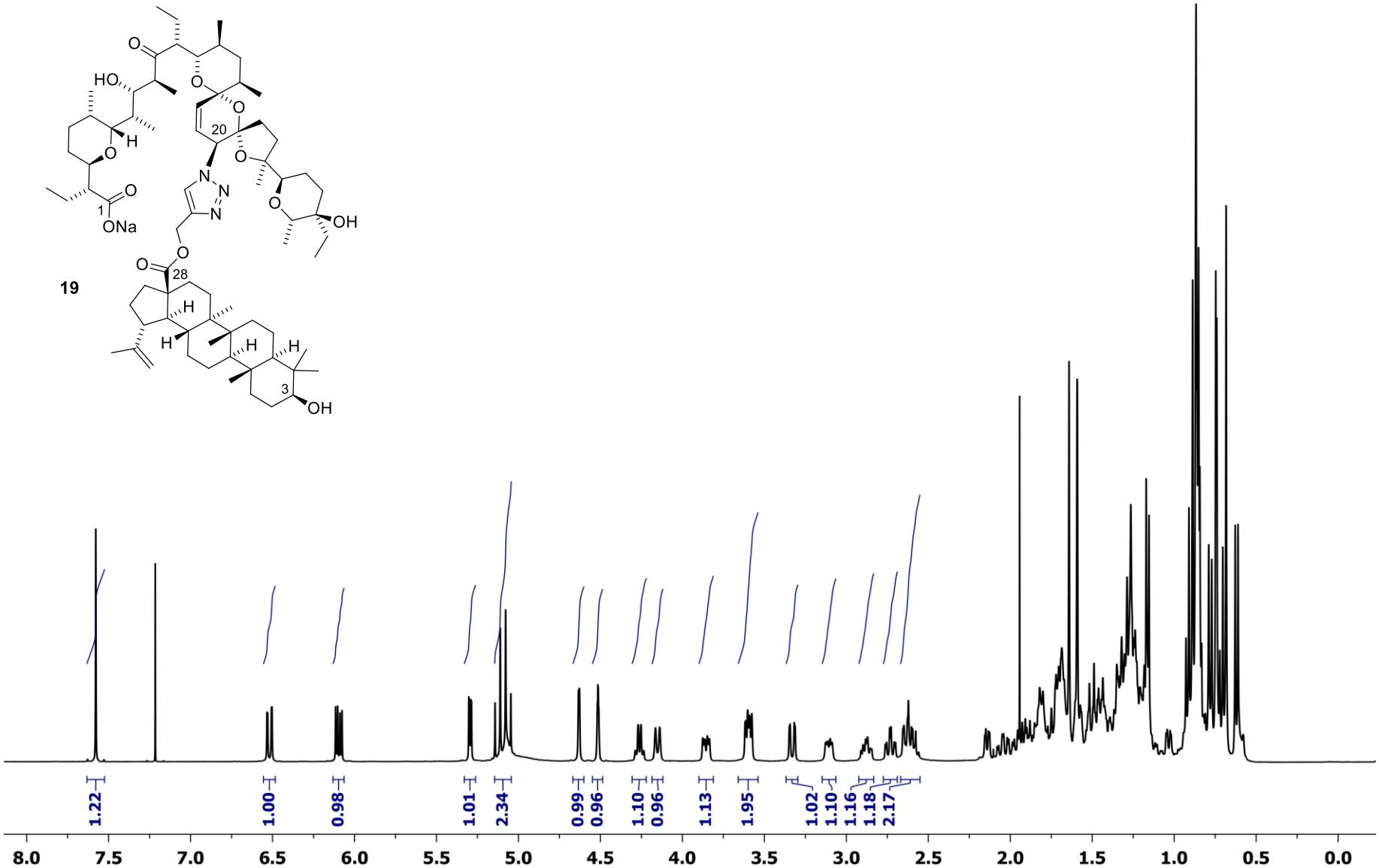


Figure S17. The ^{1}H NMR spectrum of **19** in chloroform-d.

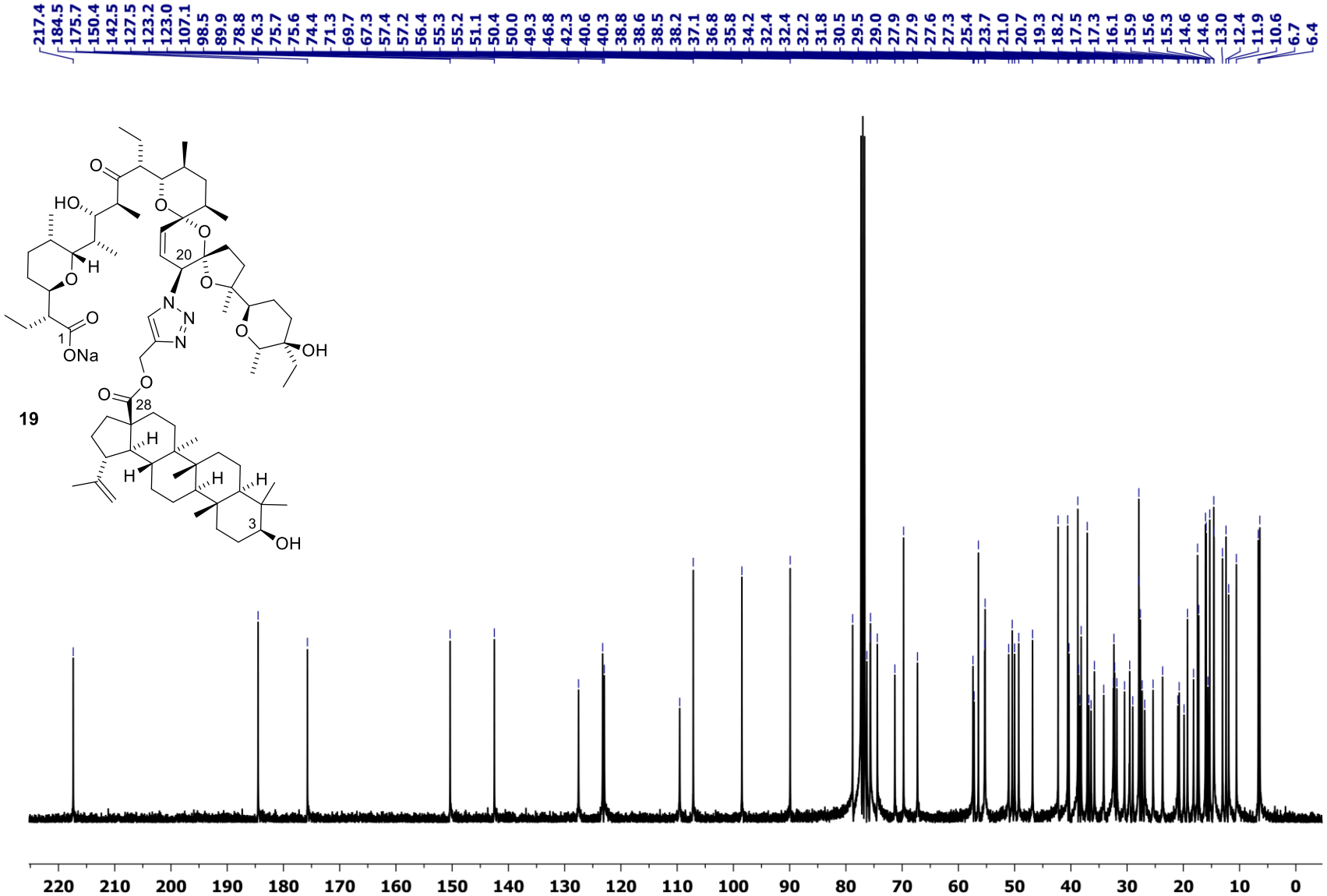


Figure S18. The ^{13}C NMR spectrum of **19** in chloroform-d.

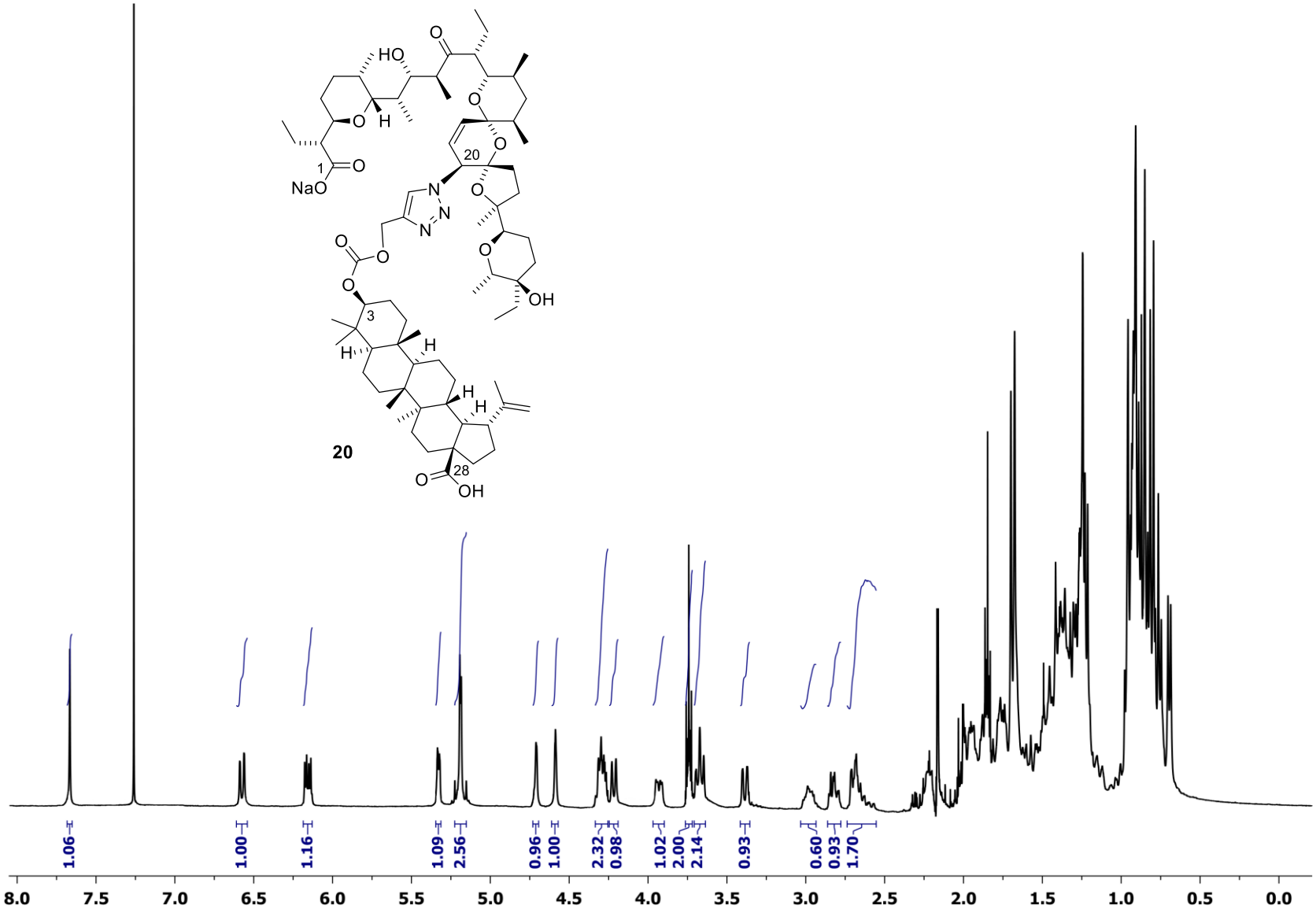


Figure S19. The ^{1}H NMR spectrum of **20** in chloroform-d.

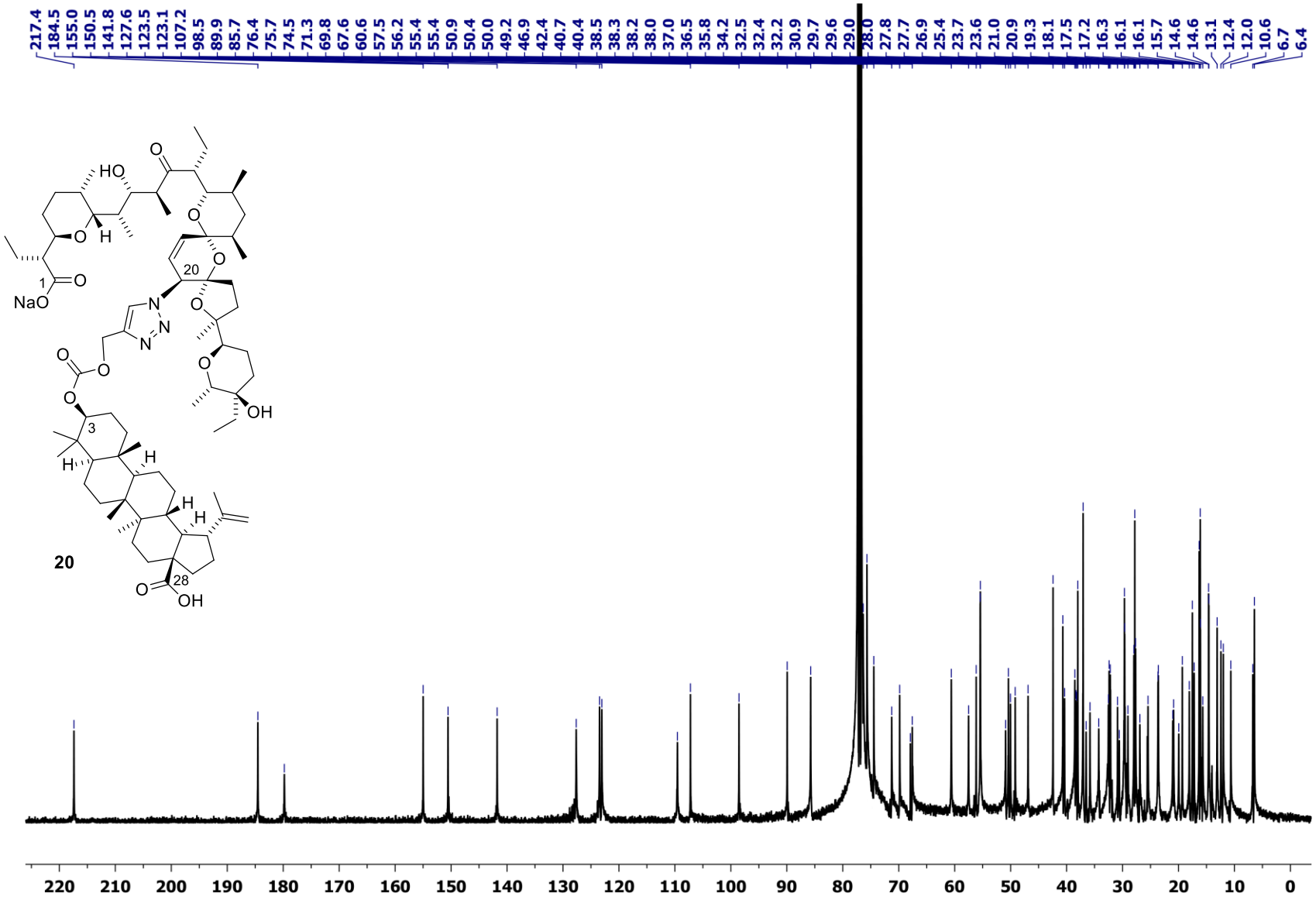


Figure S20. The ^{13}C NMR spectrum of **20** in chloroform-d.

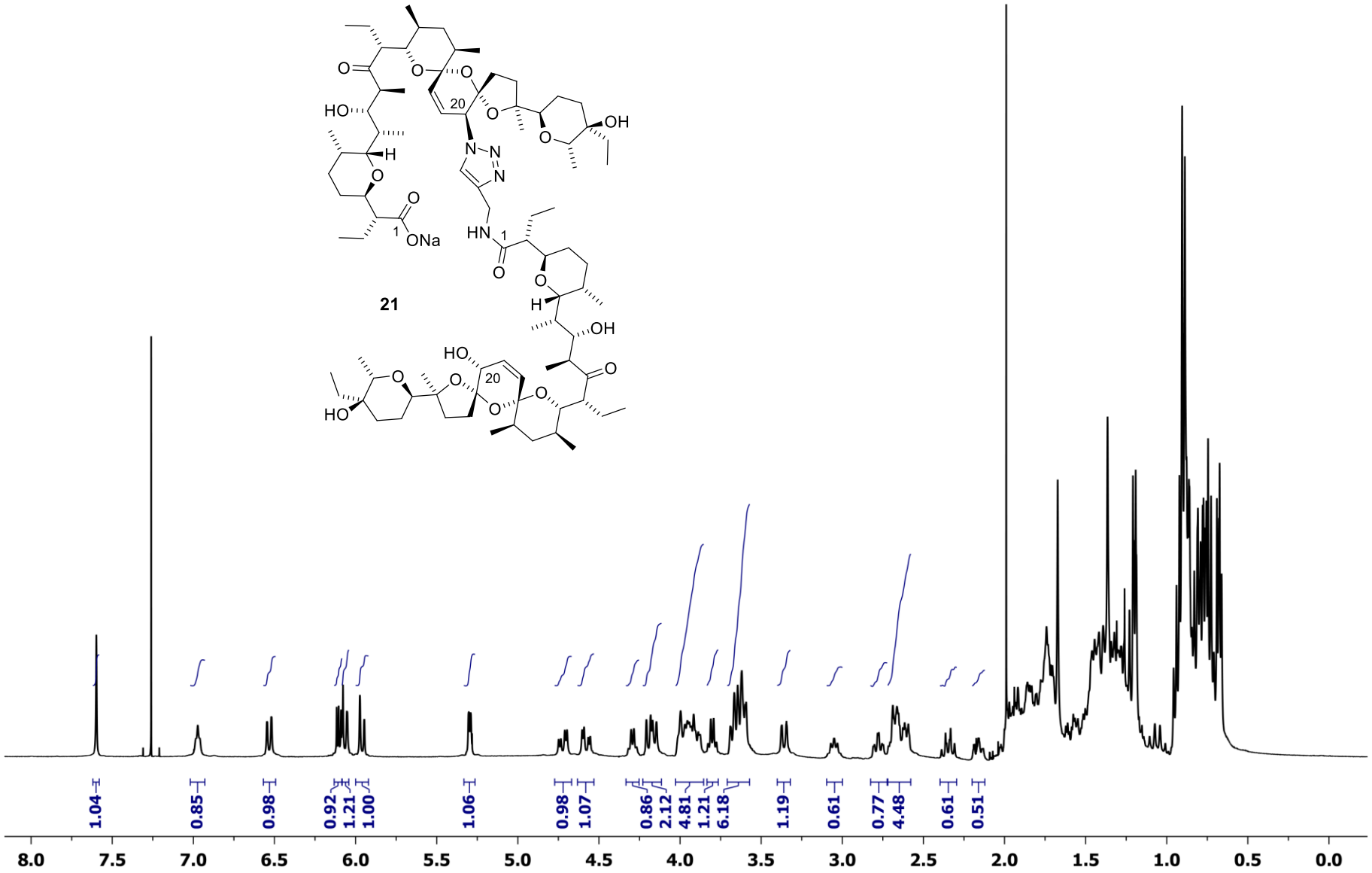


Figure S21. The ^{1}H NMR spectrum of **21** in chloroform-d.

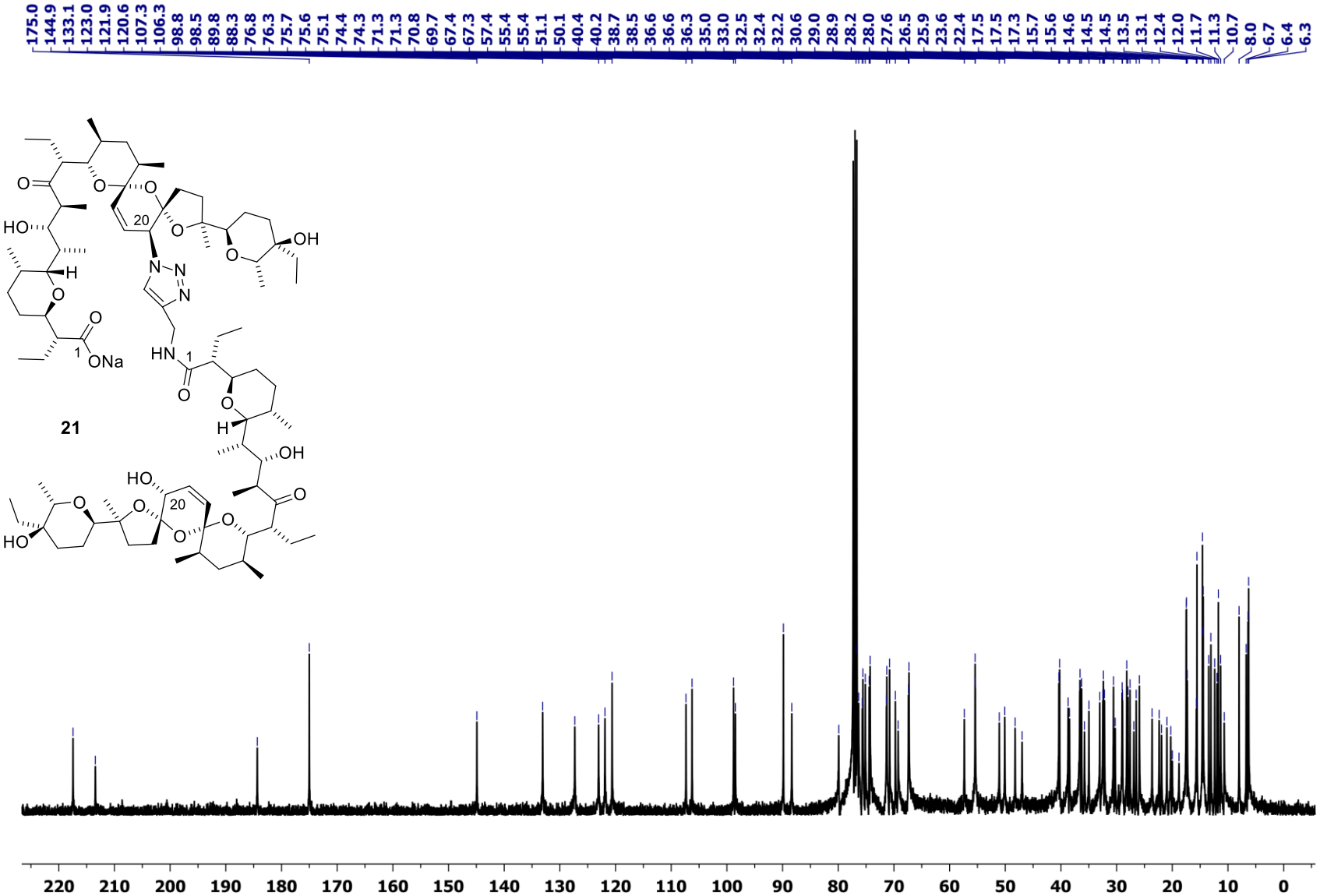


Figure S22. The ^{13}C NMR spectrum of **21** in chloroform-d.

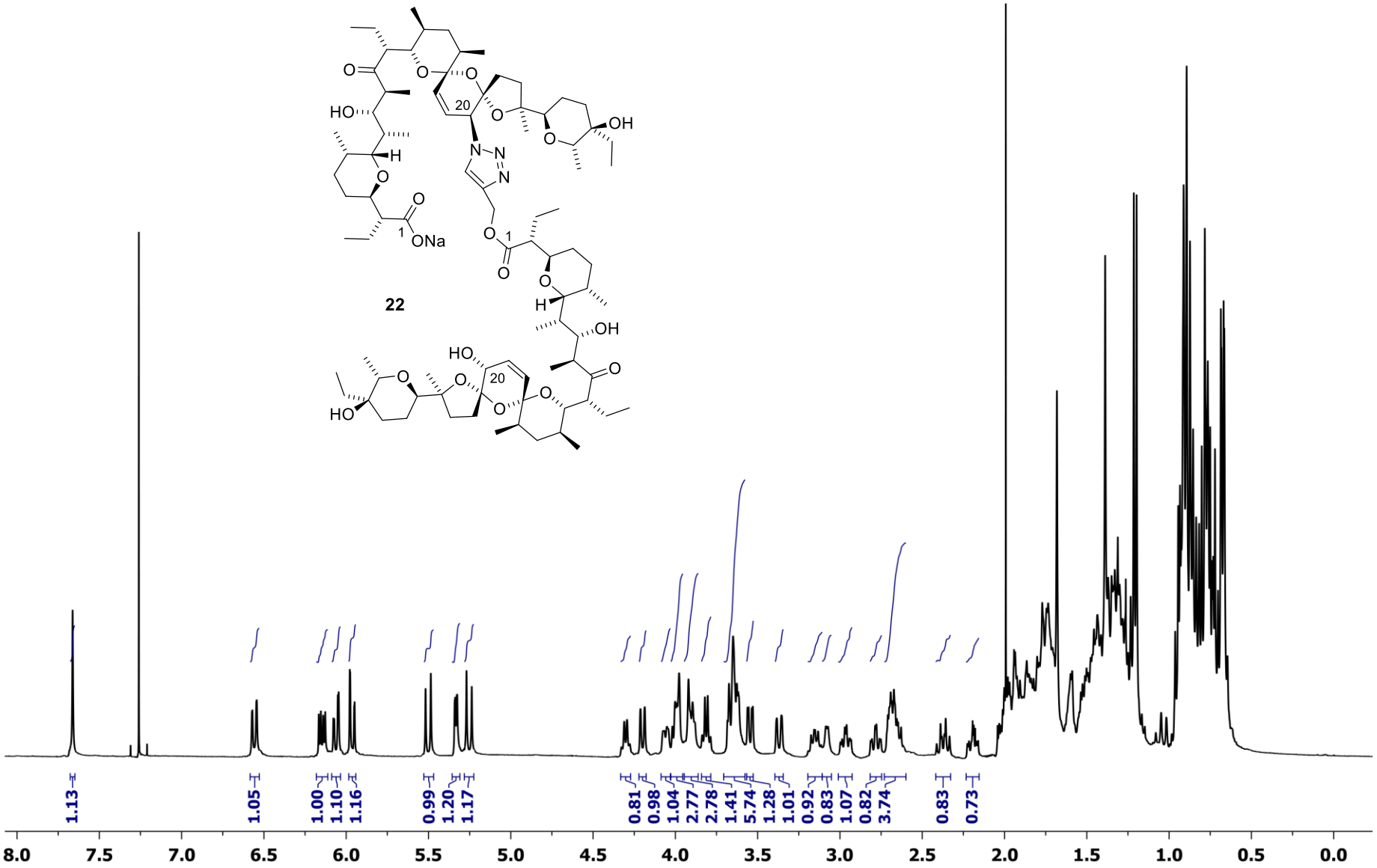


Figure S23. The ^{1}H NMR spectrum of **22** in chloroform-d.

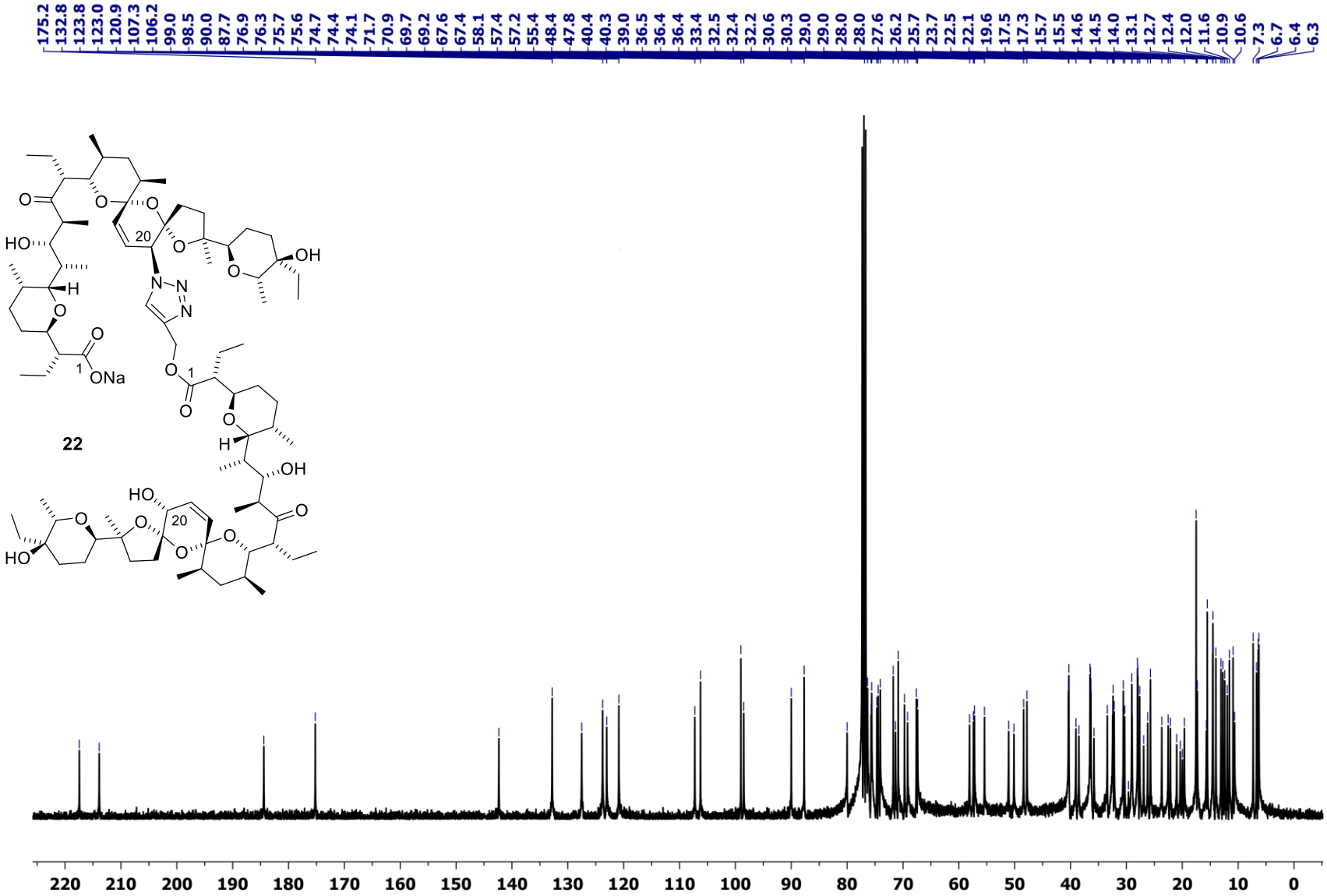


Figure S24. The ^{13}C NMR spectrum of **22** in chloroform-d.

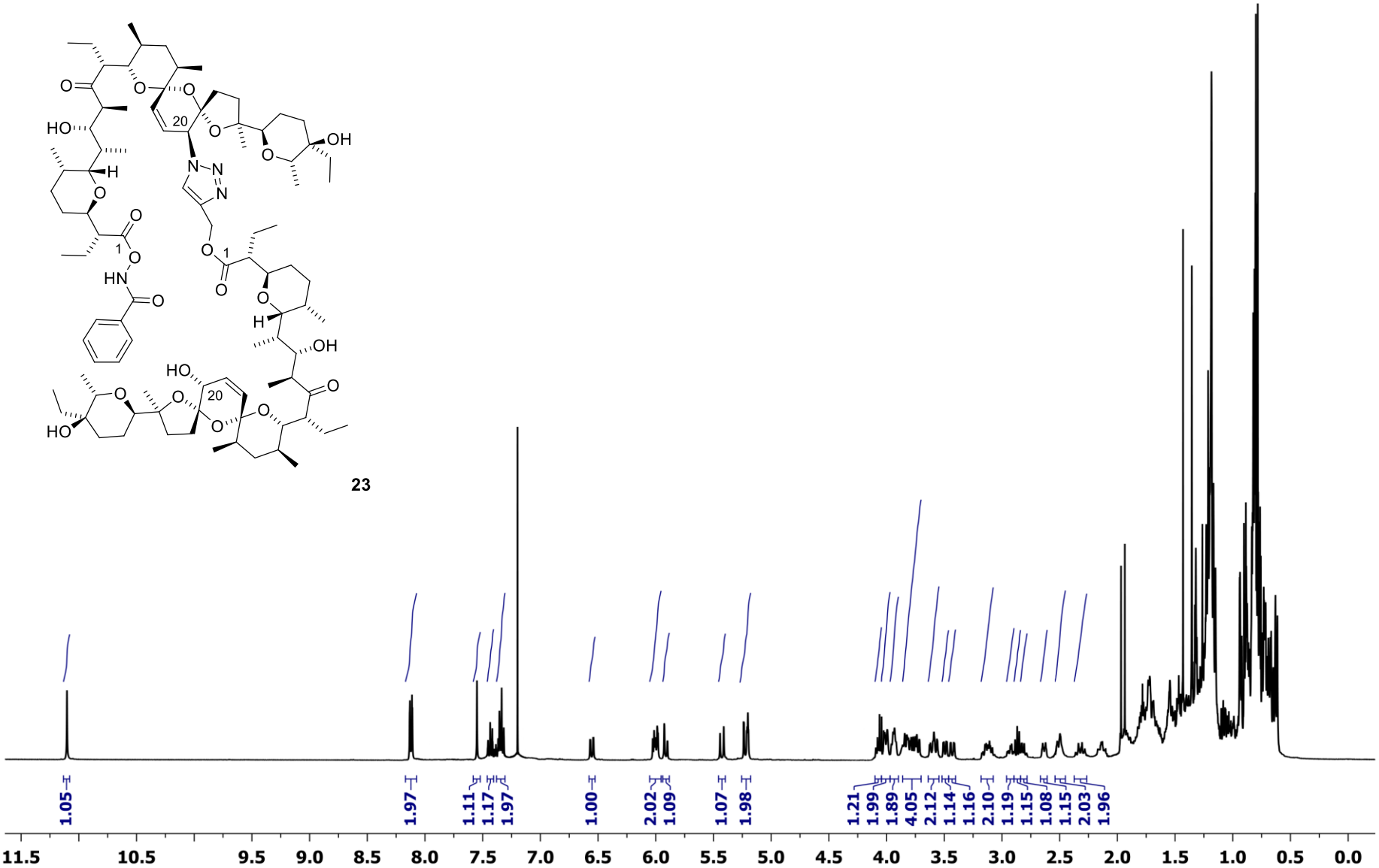


Figure S25. The ^{1}H NMR spectrum of **23** in chloroform-d.

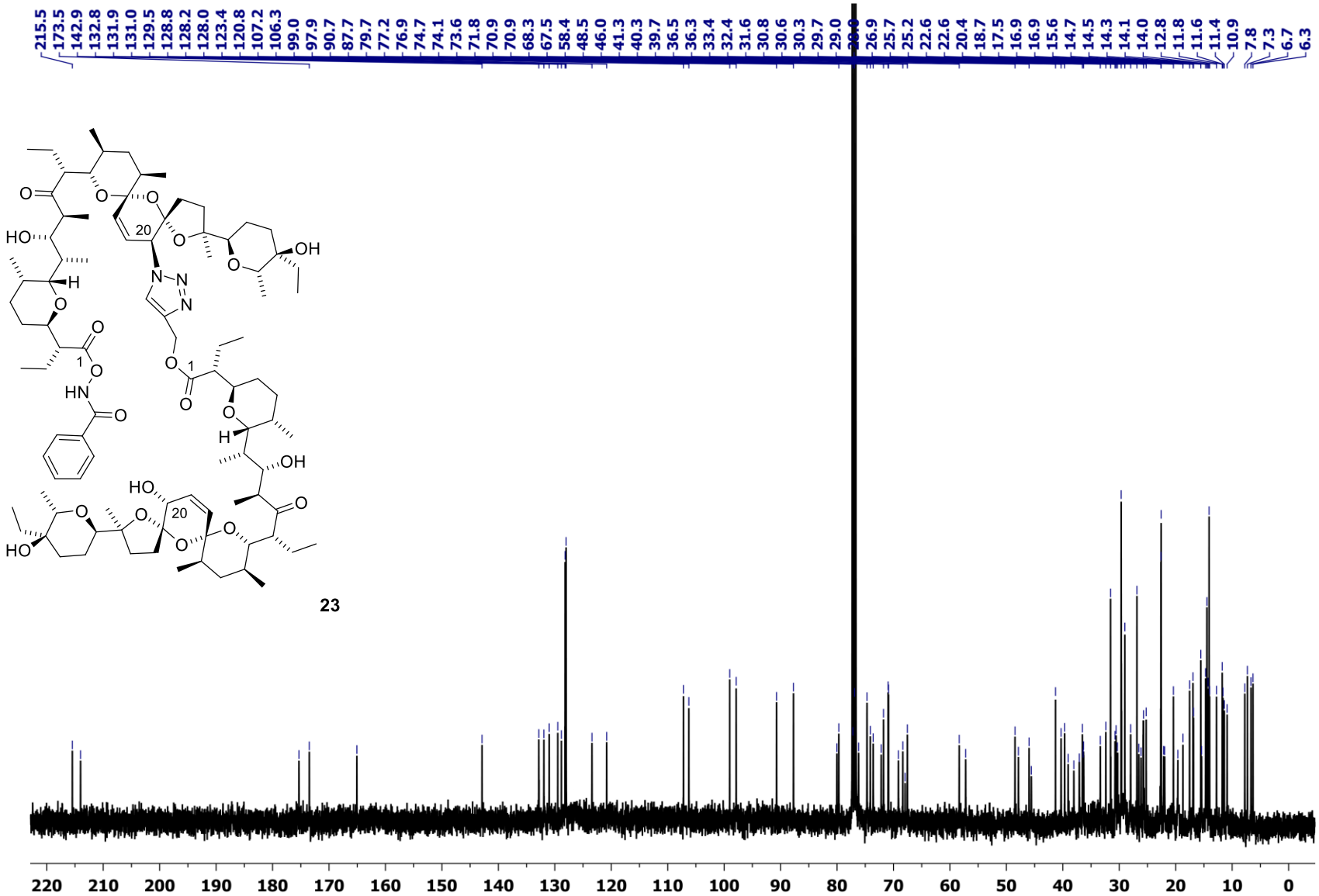


Figure S26. The ^{13}C NMR spectrum of **23** in chloroform-d.

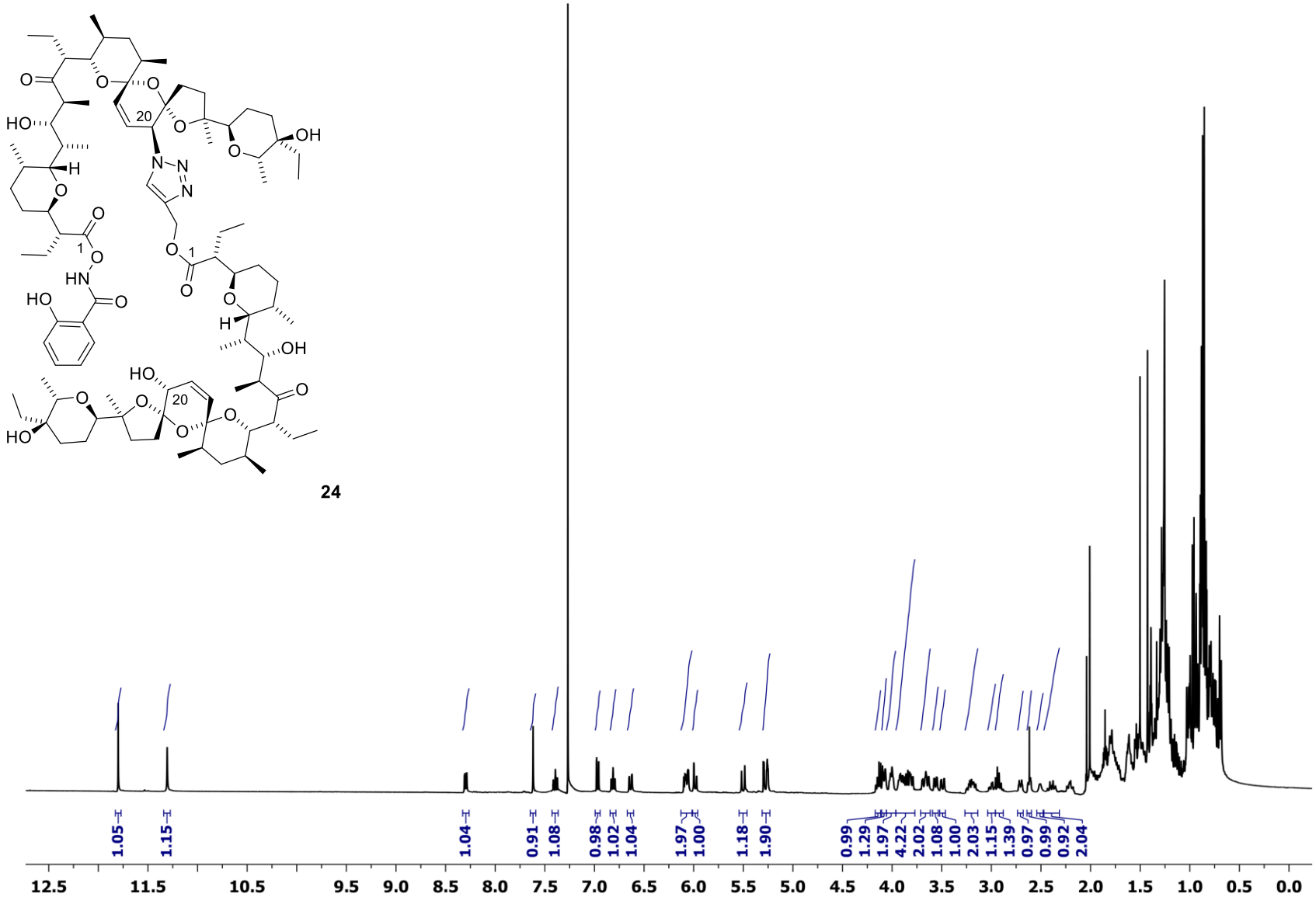


Figure S27. The ^{1}H NMR spectrum of **24** in chloroform-d.

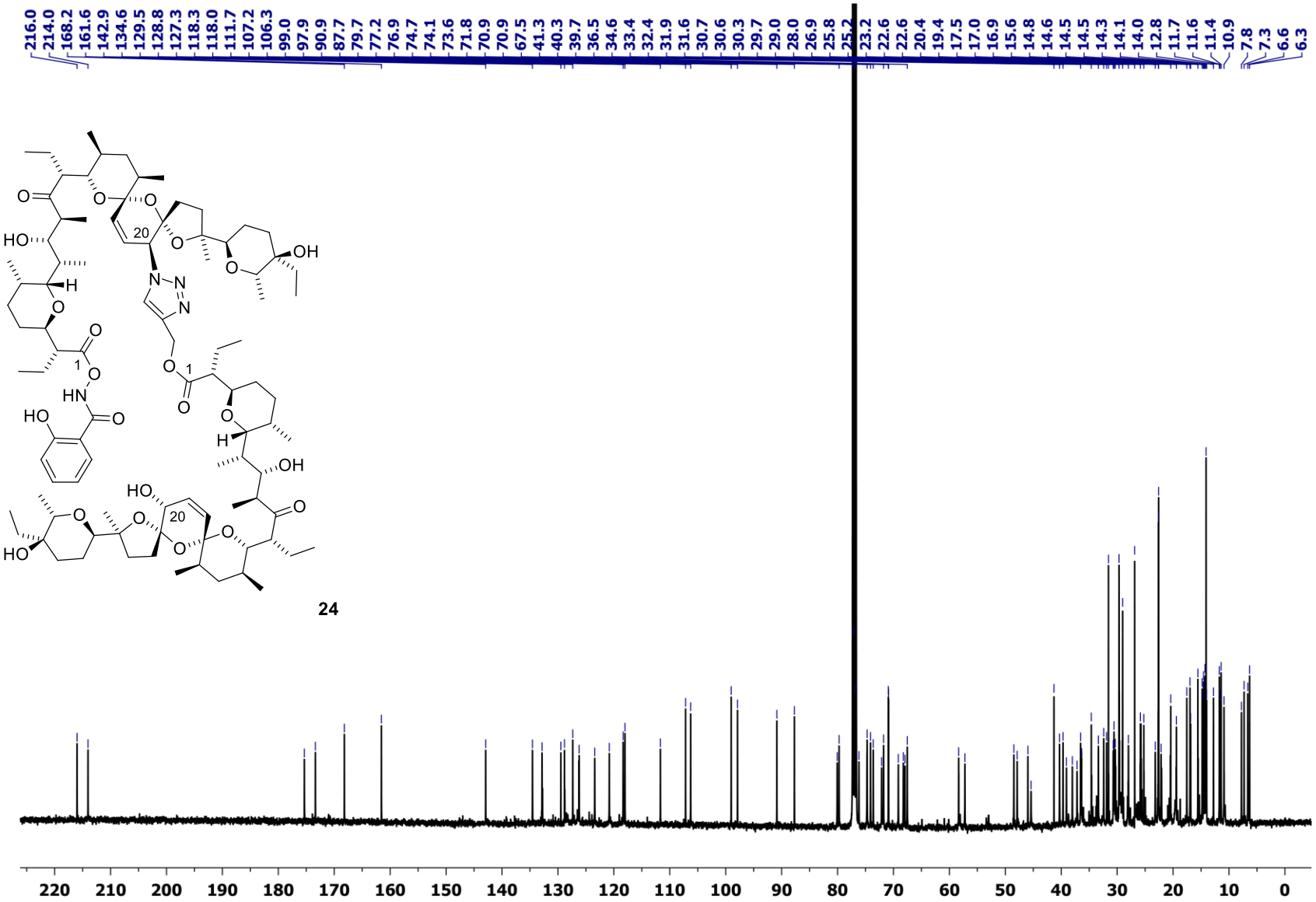


Figure S28. The ^{13}C NMR spectrum of **24** in chloroform-d.

ESI MS analysis of dimeric polyether ionophores

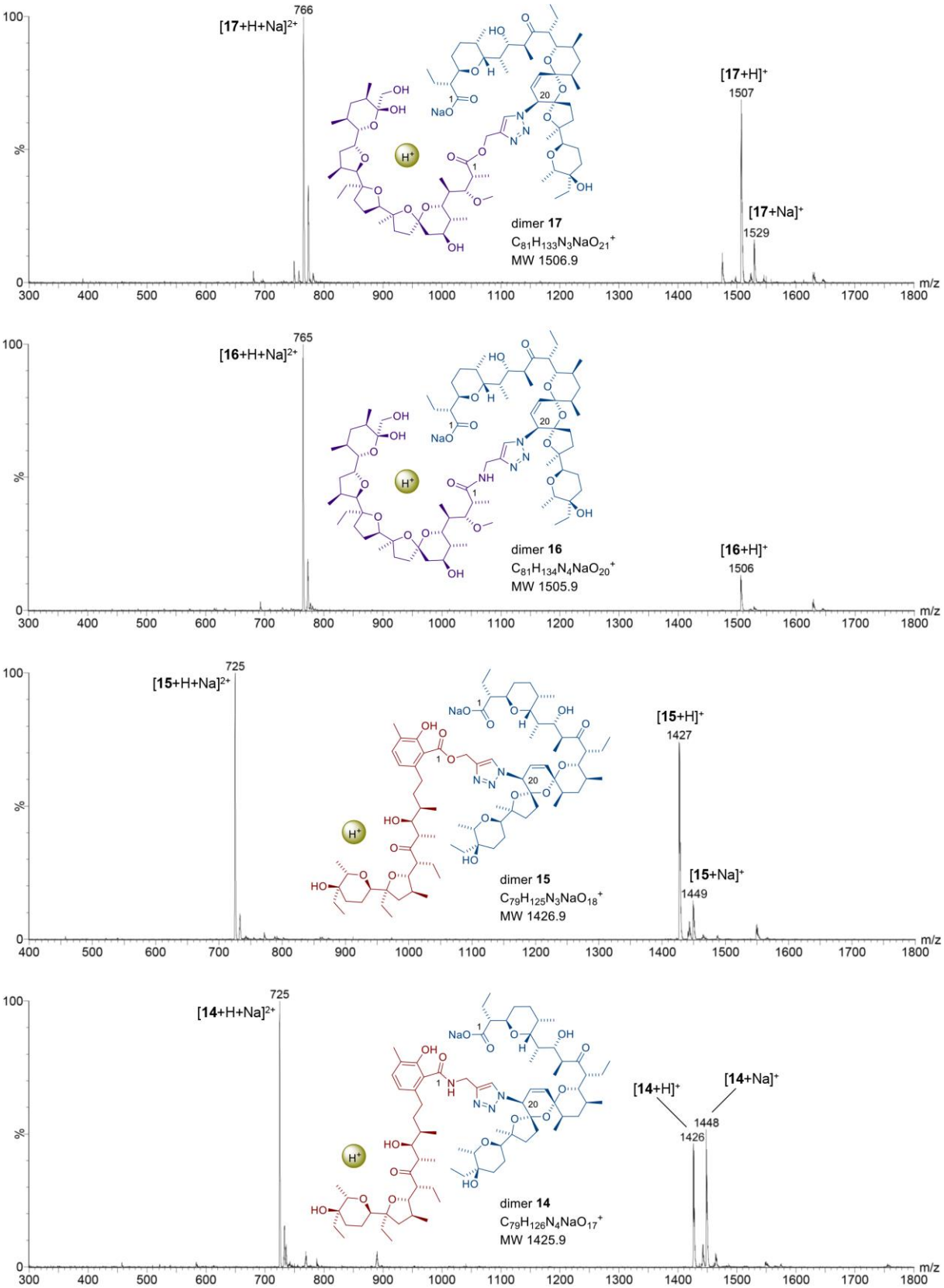


Figure S29. The ESI mass spectra of a mixture of **14**, **15**, **16** and **17** with $NaClO_4$ at cv = 30 V.

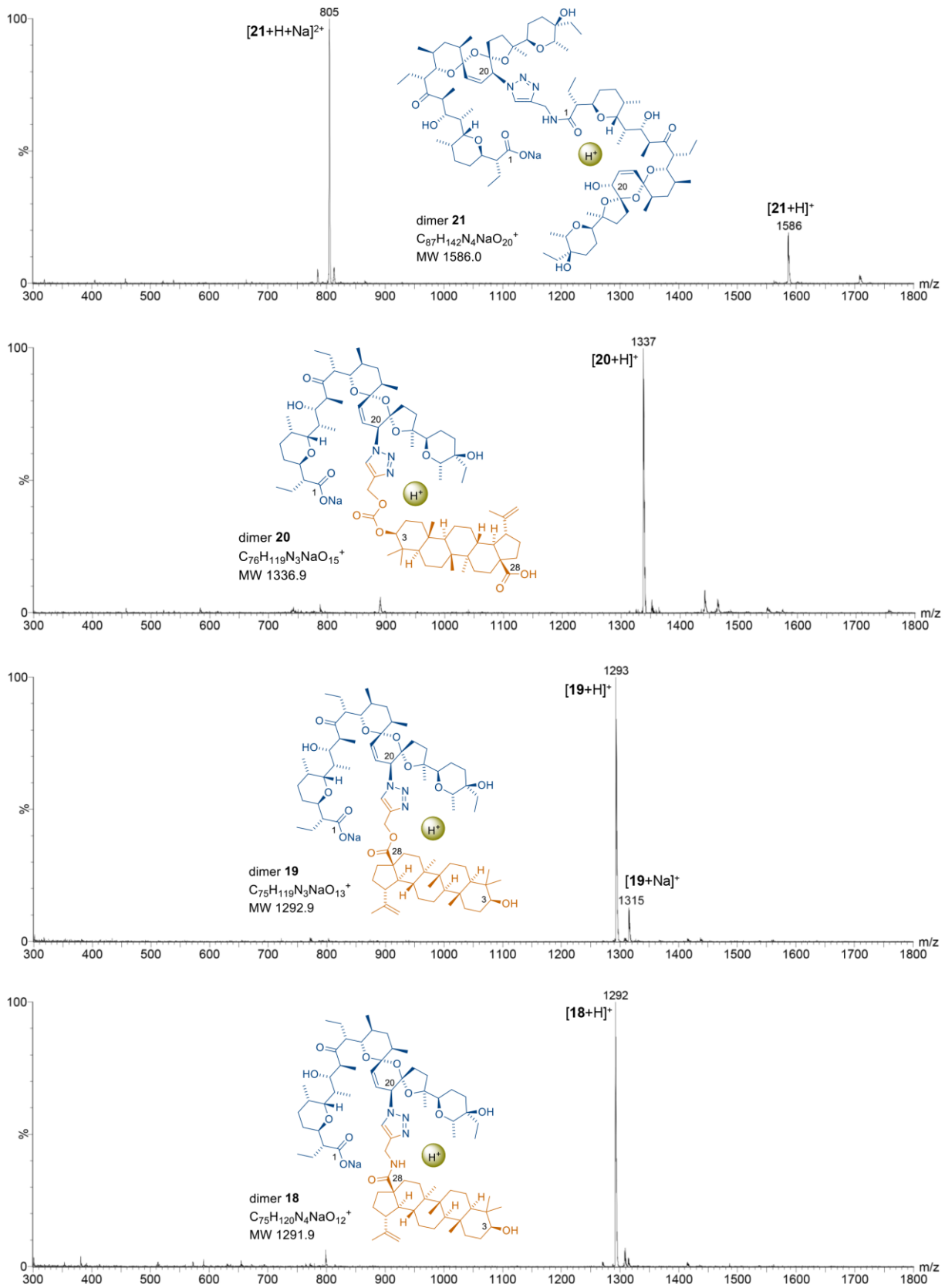


Figure S30. The ESI mass spectra of a mixture of **18**, **19**, **20** and **21** with $NaClO_4$ at cv = 30 V.

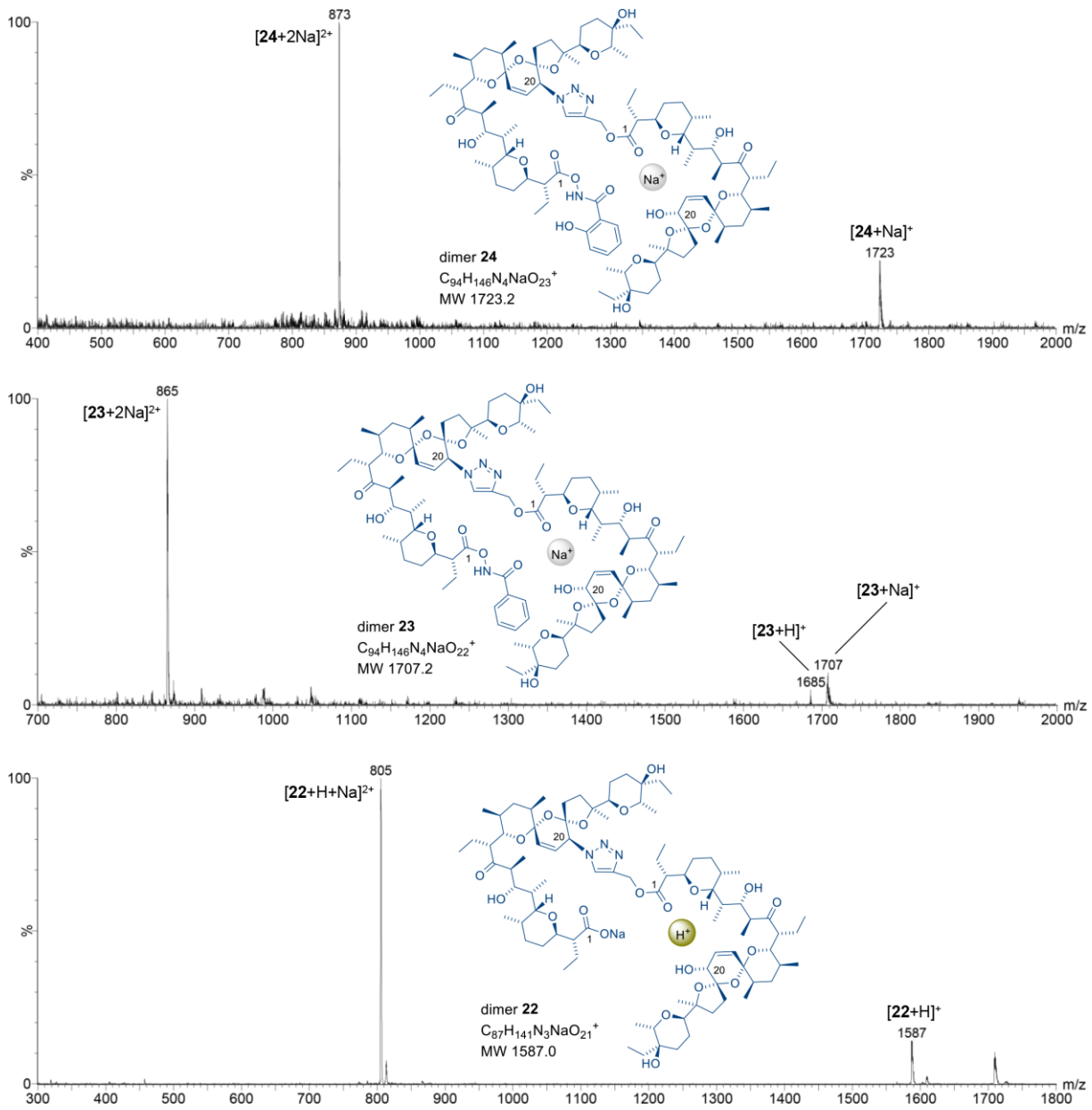


Figure S31. The ESI mass spectra of a mixture of **22**, **23**, and **24** with $NaClO_4$ at cv = 30 V.