Supporting Information

Toward the Synthesis of SB-203207: Construction of Four Contiguous Nitrogen-Containing Stereogenic Centers

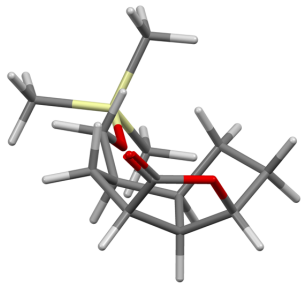
Ichiro Hayakawa,* Anna Nagayasu, and Akira Sakakura*

Division of Applied Chemistry, Graduate School of Natural Science and Technology, Okayama University, 3-1-1 Tsushima-naka, Kita-ku, Okayama 700-8530, Japan

E-mail address: ichiro.hayakawa@okayama-u.ac.jp, sakakura@okayama-u.ac.jp

Contents

Computed geometries and energies of tricyclic lactone 11



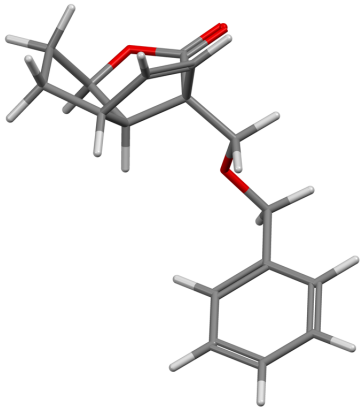
The DFT-optimized structure of tricyclic lactone **11** at B3LYP/6-31G* level (the TBDPS group was replaced by the TMS group).

C	1.837595	1.057372	2.118427
C	1.199513	0.670446	0.753785
C	0.282136	-0.523671	1.090610
C	-0.292337	-0.195363	2.486758
C	0.824304	0.626321	3.199770
C	1.861936	2.608193	2.182933
C	1.437138	3.087010	0.789173
C	0.512049	1.971426	0.272352
C	0.290968	1.931079	3.782819
O	0.874087	2.997808	3.167975
H	1.959984	0.380465	0.021745
H	2.827125	0.617941	2.266934
O	-0.547179	2.063159	4.638179
C	-0.782864	-0.854538	0.049820
O	-0.148921	-1.186628	-1.178621
Si	-0.939585	-1.765276	-2.543427
C	0.432070	-2.082666	-3.789341
C	-1.859583	-3.364463	-2.137953
C	-2.150938	-0.472113	-3.198138
H	0.924323	-1.411496	1.181643
H	-0.557317	-1.094986	3.050099
H	-1.210416	0.400371	2.407165
H	1.276282	0.049362	4.011990
H	2.813948	3.033471	2.513254
H	2.332678	3.155750	0.157479
H	0.974493	4.078058	0.822009
H	0.377370	1.995470	-0.813204
H	-0.482567	2.082407	0.723518
H	-1.396538	-1.695361	0.409150
H	-1.457378	0.004606	-0.088401
H	0.032102	-2.467664	-4.735235
H	0.985774	-1.162967	-4.010586
H	1.147486	-2.818125	-3.404520
H	-2.344131	-3.772236	-3.033918

H	-2.643421	-3.213458	-1.385886
H	-1.173316	-4.128754	-1.754887
H	-1.626302	0.446421	-3.486870
H	-2.681460	-0.844408	-4.083654
H	-2.909110	-0.202965	-2.452944

Computed total energy of **11**: –2688228.24 kJ/mol

Computed geometries and energies of cycloalkene 10



The DFT-optimized structure of cycloalkene **10** at B3LYP/6-31G* level).

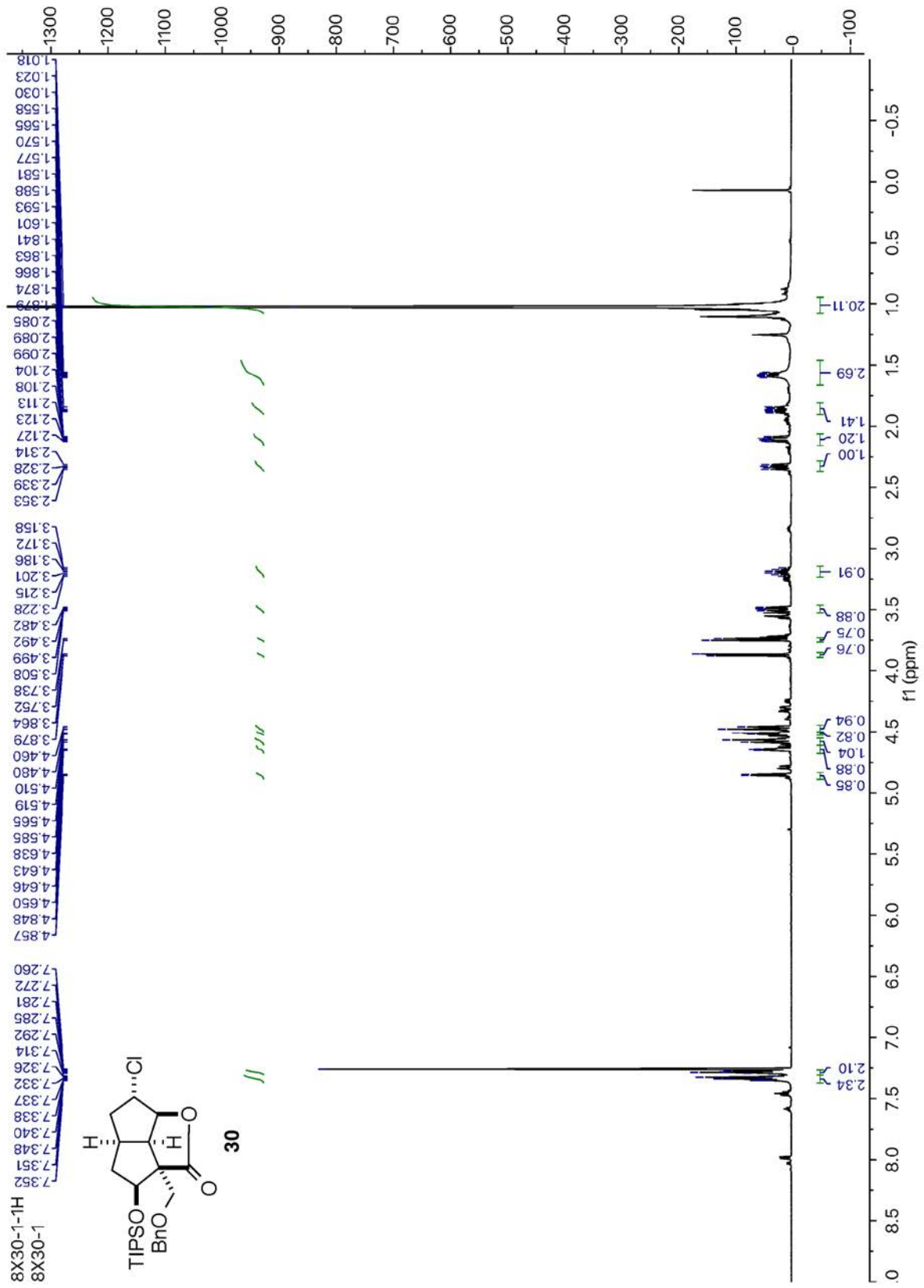
C	1.155131	1.199532	-0.213432
C	0.567474	2.522250	-0.787884
C	-0.201115	3.080837	0.390199
C	-0.213627	2.263452	1.446385
C	0.538646	0.969896	1.182599
C	2.655019	1.480915	0.084726
C	2.889675	2.979220	-0.189986
C	1.801026	3.360809	-1.208011
C	1.745394	0.854264	2.131056
O	2.895205	1.148157	1.469717
O	1.718591	0.582872	3.303995
H	-0.102124	2.359905	-1.642633
H	1.028076	0.334514	-0.865918
C	-0.352883	-0.263730	1.322706
O	0.413837	-1.402265	0.961071
C	-0.295871	-2.631083	1.073810
C	-1.315060	-2.840024	-0.031165
C	-2.644453	-3.163901	0.256248
C	-3.567038	-3.370523	-0.772873
C	-3.168078	-3.244304	-2.103373
C	-1.842360	-2.915113	-2.401144
C	-0.924175	-2.715478	-1.372072
H	-0.680404	4.056658	0.359494
H	-0.691268	2.458932	2.402205

H	3.324927	0.847249	-0.502544
H	3.903891	3.190004	-0.542849
H	2.748133	3.527091	0.748269
H	1.598646	4.437513	-1.227793
H	2.108647	3.071331	-2.221244
H	-0.690378	-0.349797	2.367225
H	-1.237904	-0.162173	0.677486
H	0.478141	-3.405725	1.030897
H	-0.782709	-2.701784	2.058509
H	-2.961050	-3.257043	1.293045
H	-4.596694	-3.623470	-0.533677
H	-3.884445	-3.402378	-2.905400
H	-1.525763	-2.818313	-3.436659
H	0.106942	-2.458294	-1.600985

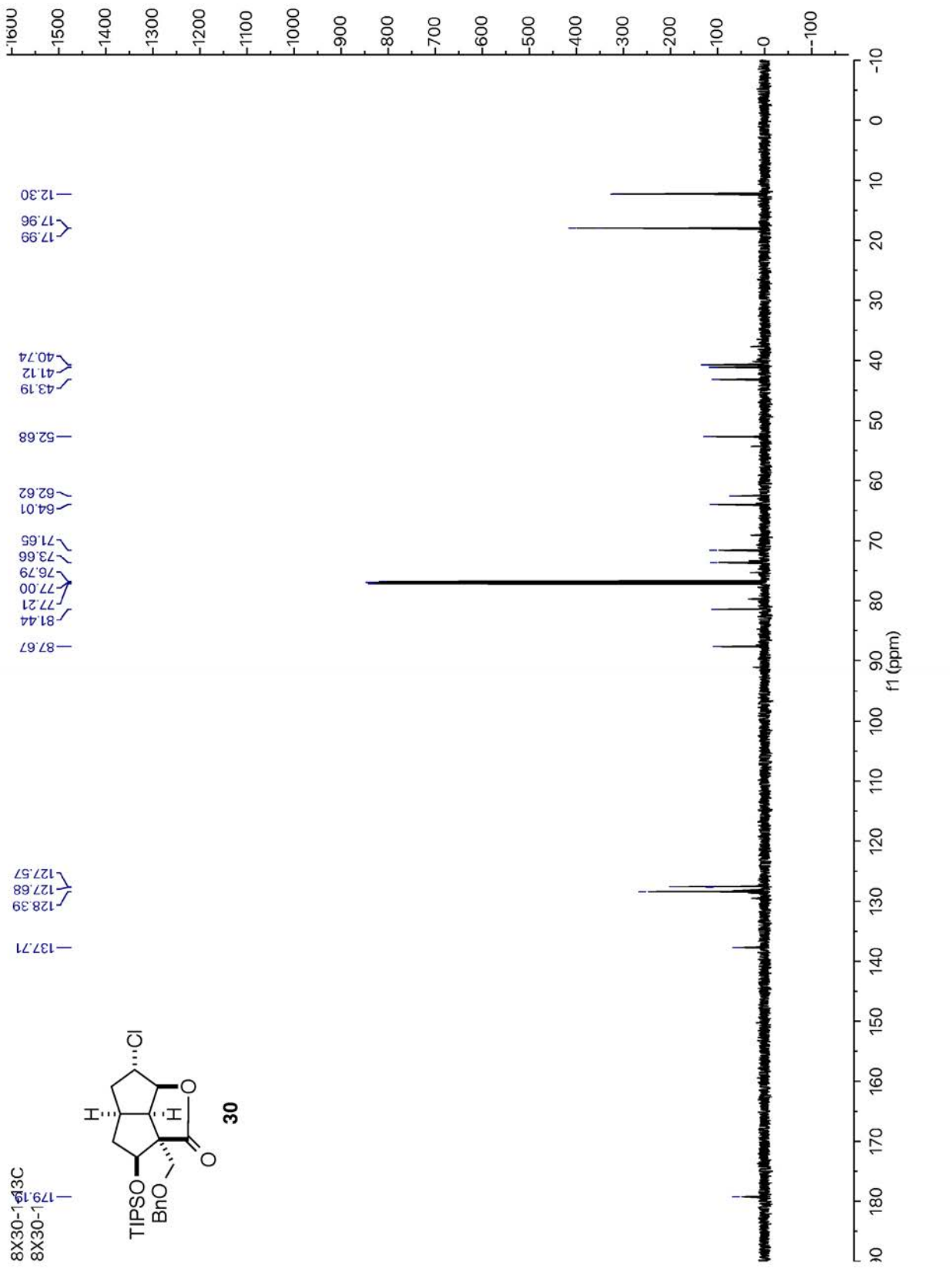
Computed total energy of **10**: –2321744.17 kJ/mol

Spectral data of chlorolactone 30

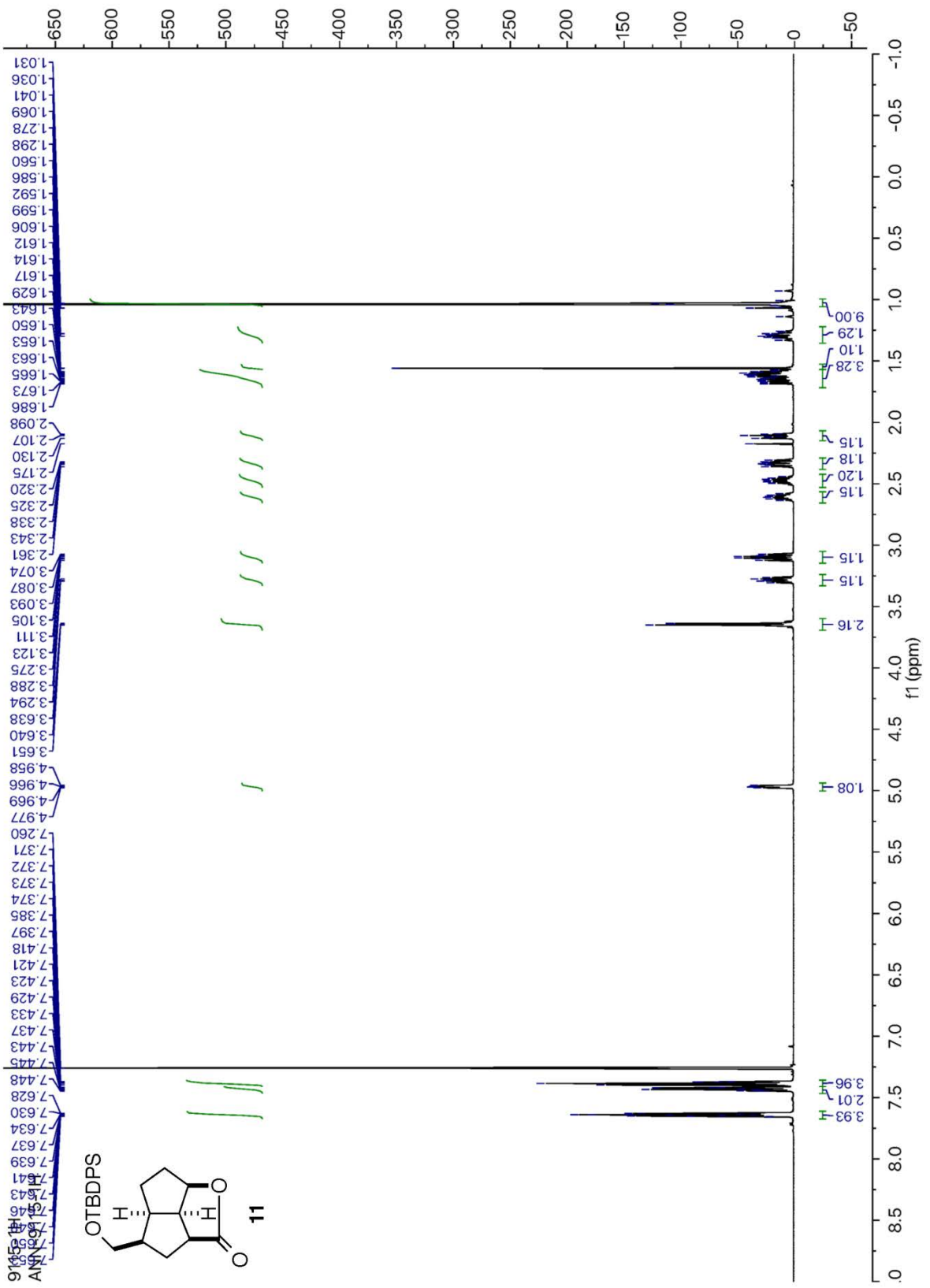
*(2a*S*,2a*^{1}*R*,3*S*,4a*S*,6*S*,6a*S*)-6a-((benzyloxy)methyl)-3-chloro-6-((triisopropylsilyl)oxy)octahydro-1*H*-pentaleno[1,6-*bc*]furan-1-one (**30**).* Colorless oil; IR (neat) 3530, 2893, 1775, 1728, 1454, 1354, 1261, 1227, 1202, 1155, 1084, 1015, 883, 820, 750, 683 cm^{-1}; ^1H NMR (600 MHz, $CDCl_3$) δ 7.37–7.31 (m, 2H), 7.30–7.27 (m, 3H), 4.85 (d, *J* = 5.4 Hz, 1H), 4.64 (dd, *J* = 4.2, 2.4 Hz, 1H), 4.58 (d, *J* = 12.0 Hz, 1H), 4.51 (d, *J* = 5.4 Hz, 1H), 4.47 (d, *J* = 12.0 Hz, 1H), 3.87, (d, *J* = 8.4 Hz, 1H), 3.75 (d, *J* = 8.4 Hz, 1H), 3.50 (dd, *J* = 9.6, 5.4 Hz, 1H), 3.19 (ddd, *J* = 16.2, 16.2, 7.8 Hz, 1H), 2.33 (dd, *J* = 15.0, 8.4 Hz, 1H), 2.11 (ddd, *J* = 13.8, 8.4, 2.4 Hz, 1H), 1.86 (ddd, *J* = 13.2, 8.4, 5.4 Hz, 1H), 1.58 (ddd, *J* = 12.0, 7.8, 4.8 Hz, 1H), 1.02 (m, 21H); $^{13}C\{^1H\}$ NMR (150 MHz, $CDCl_3$) δ 179.2, 137.7, 128.4 (2C), 127.7, 127.6 (2C), 87.7, 81.4, 73.7, 71.7, 64.0, 62.6, 52.7, 43.2, 41.1, 40.7, 17.99 (3C), 17.96 (3C), 12.3 (3C); HRMS (ESI) *m/z* 501.2194, calcd for $C_{26}H_{39}ClNaO_4Si$ $[M+Na]^+$ 501.2198.



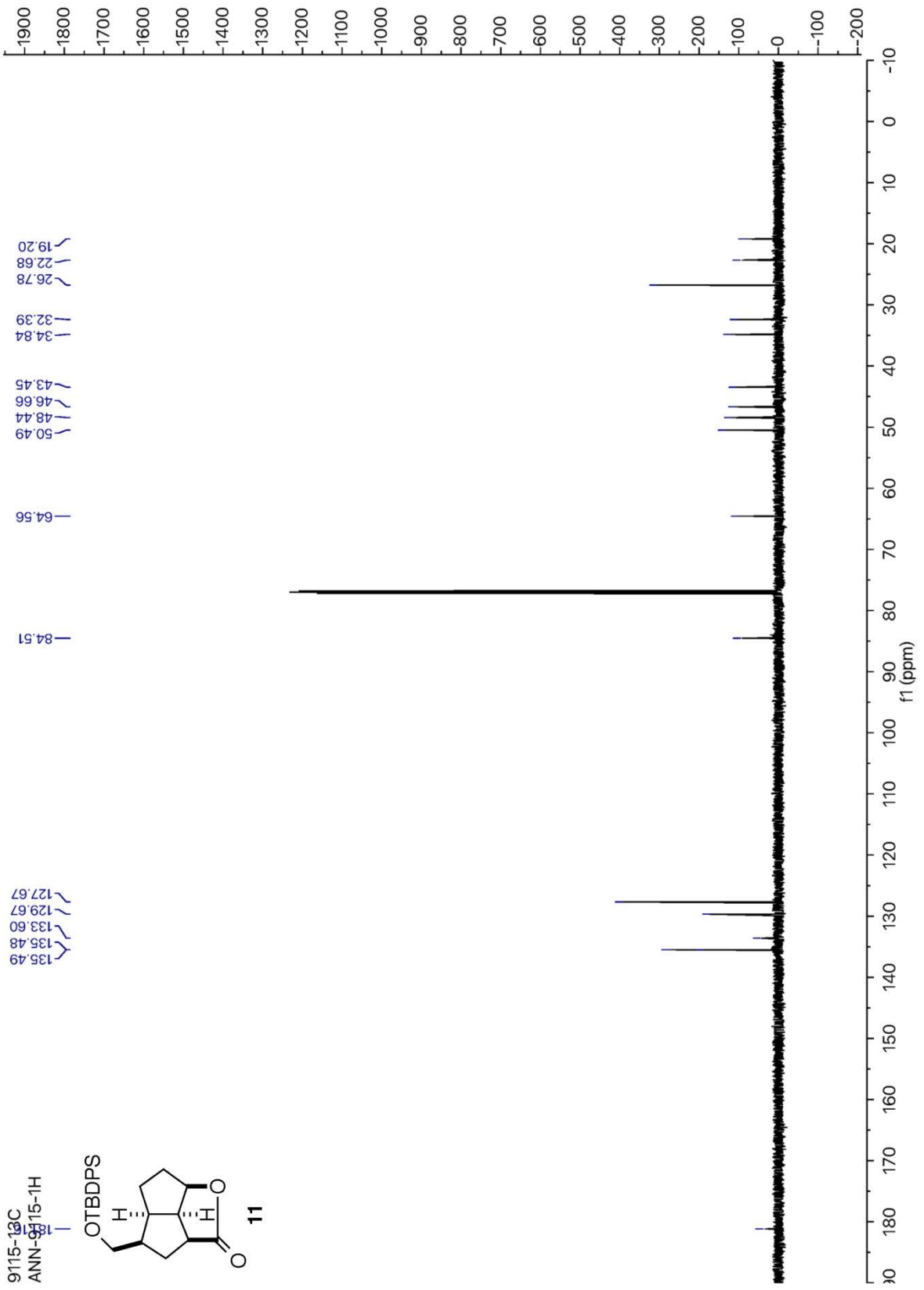
^{1}H NMR spectra of **30** (600 MHz, $CDCl_3$)



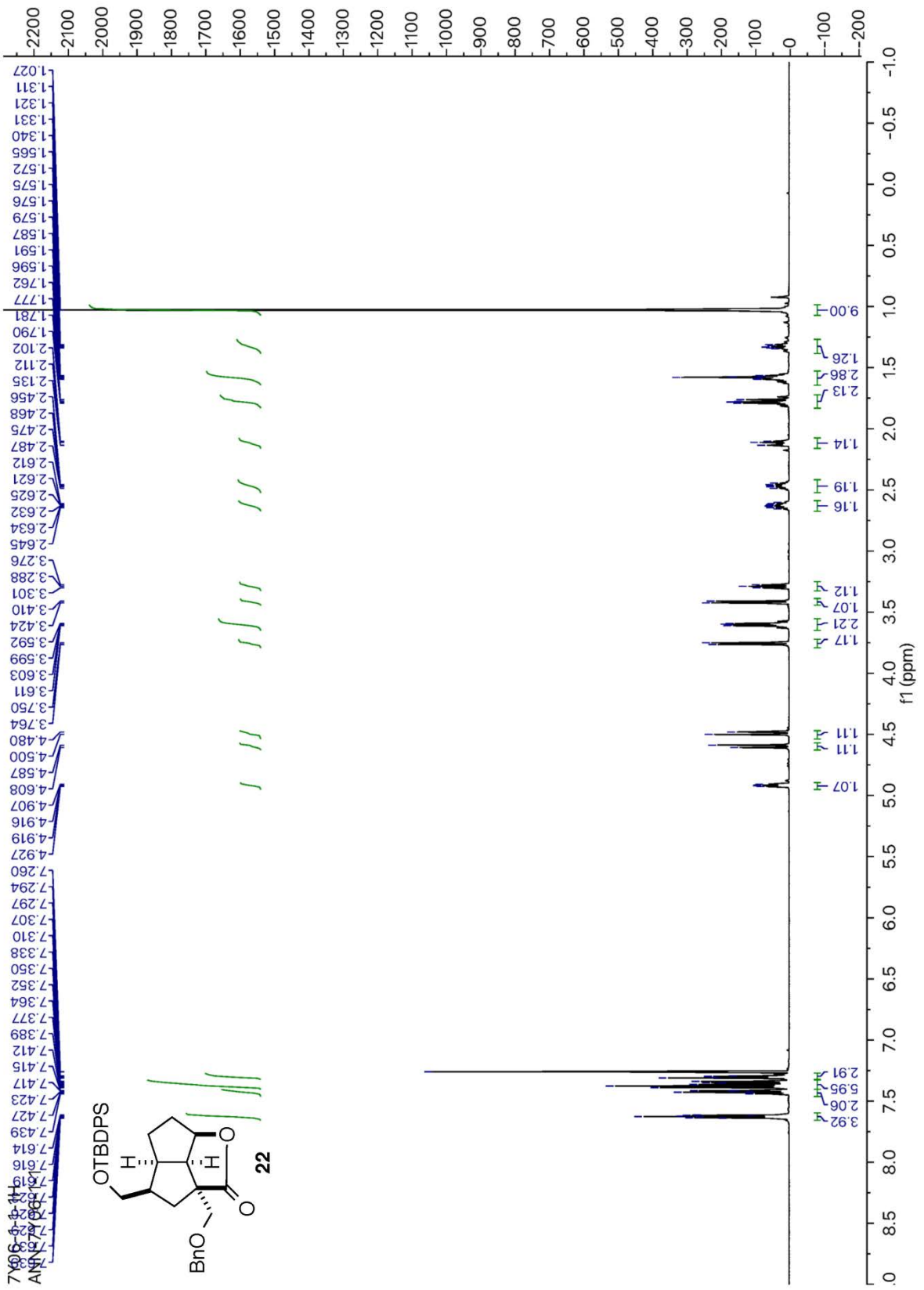
$^{13}C\{^{1}H\}$ NMR spectra of **30** (150 MHz, $CDCl_3$)



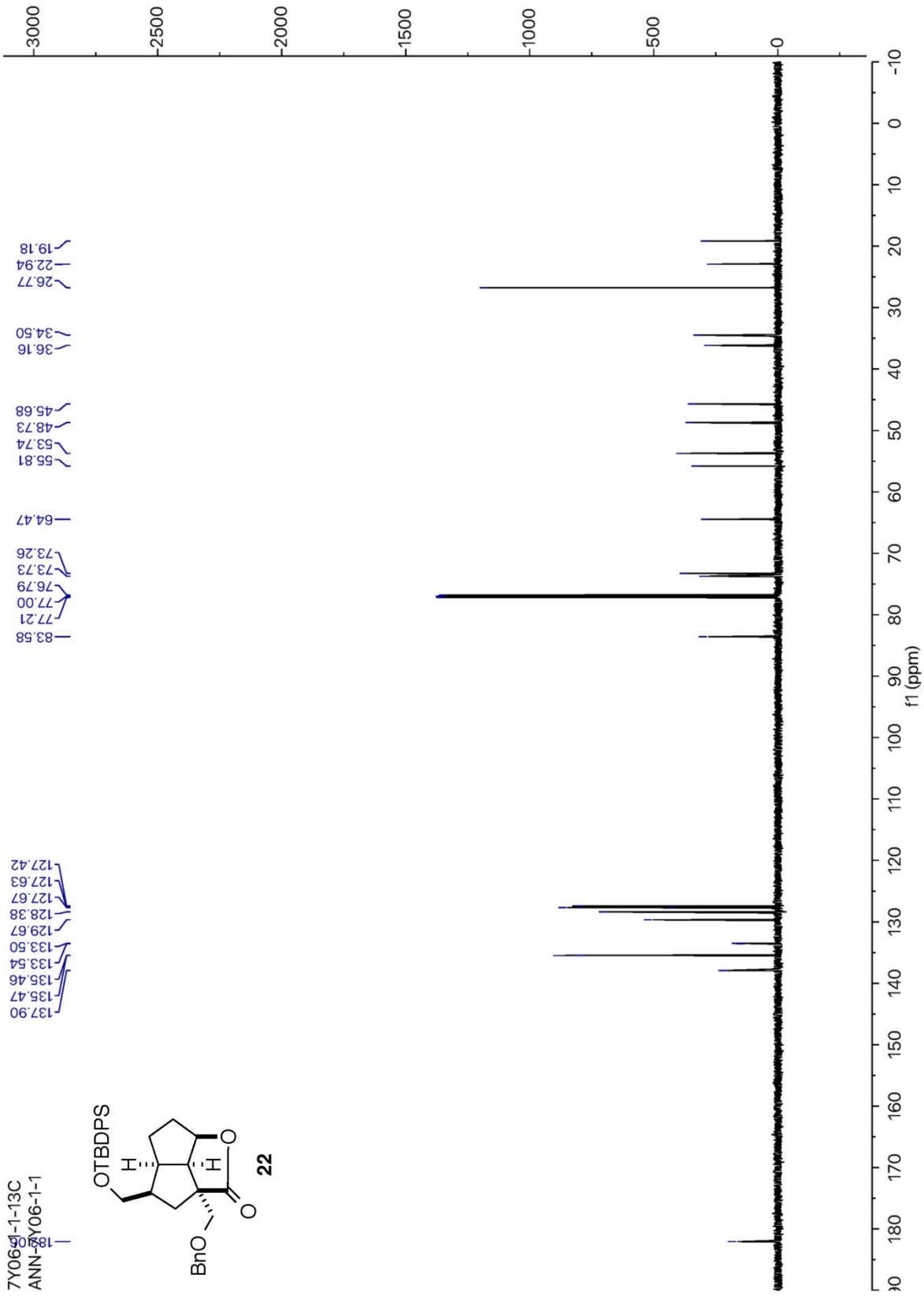
^{1}H NMR spectra of **11** (600 MHz, $CDCl_3$)



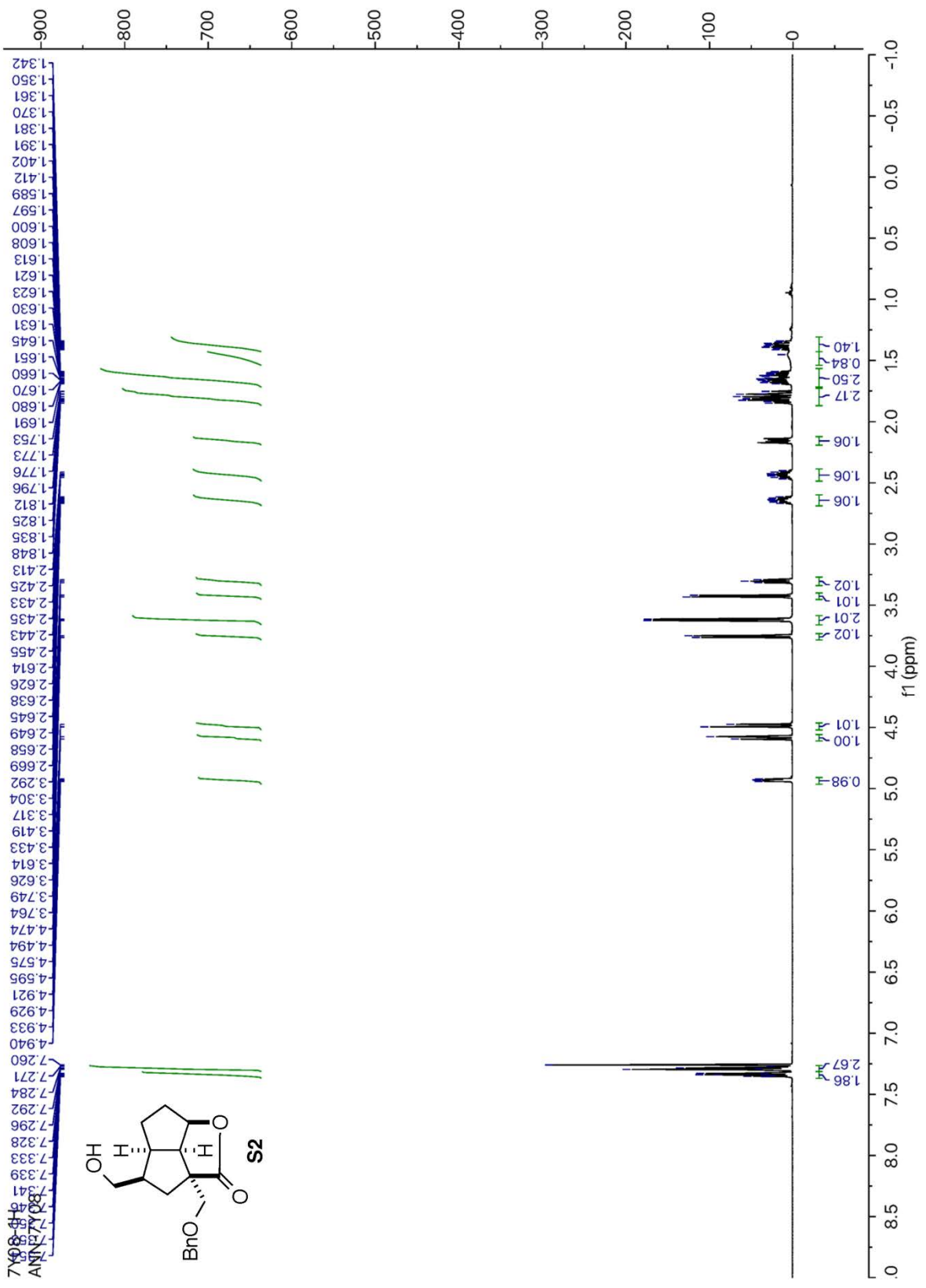
$^{13}C\{^{1}H\}$ NMR spectra of **11** (150 MHz, $CDCl_3$)



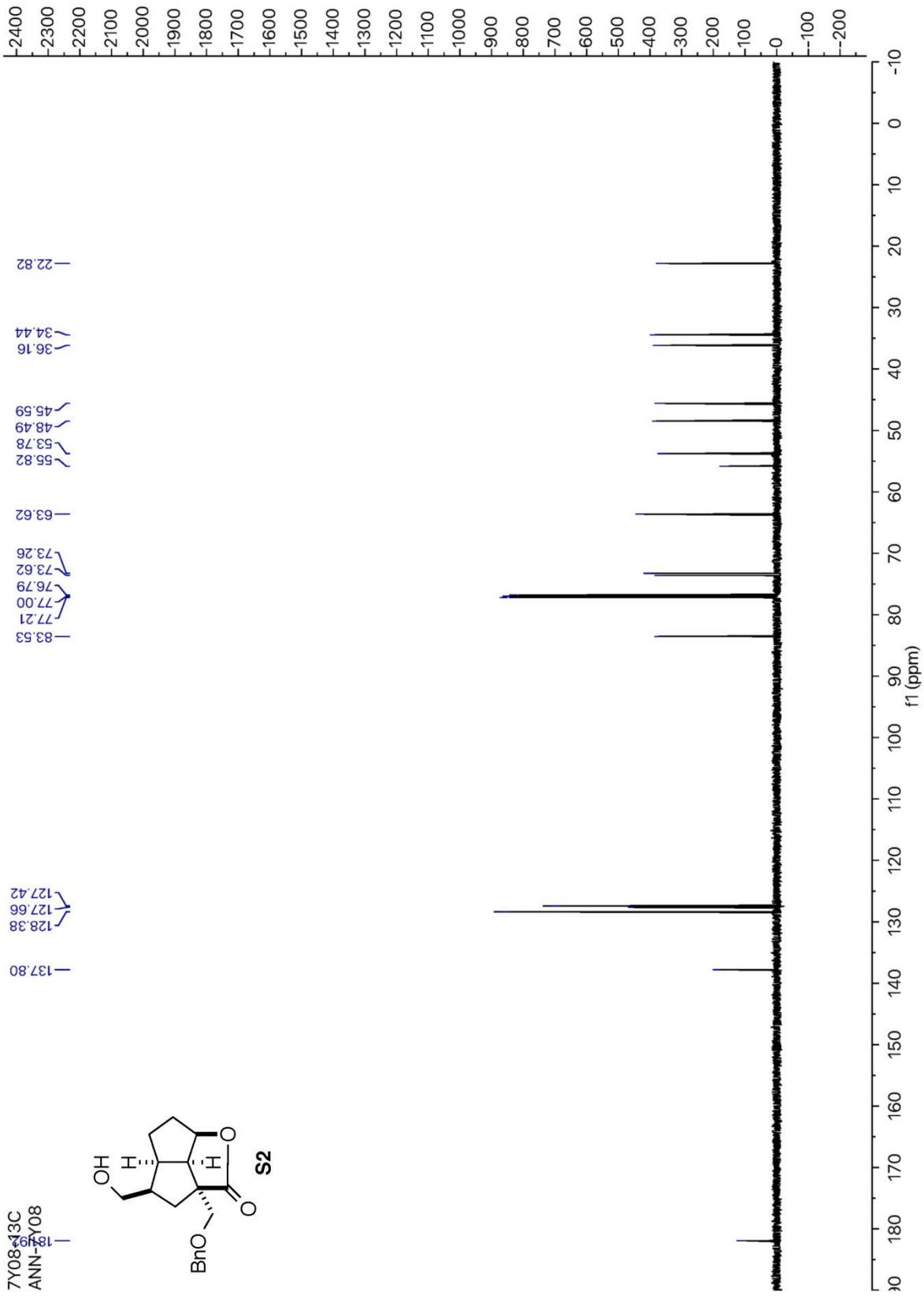
^{1}H NMR spectra of **22** (600 MHz, $CDCl_3$)



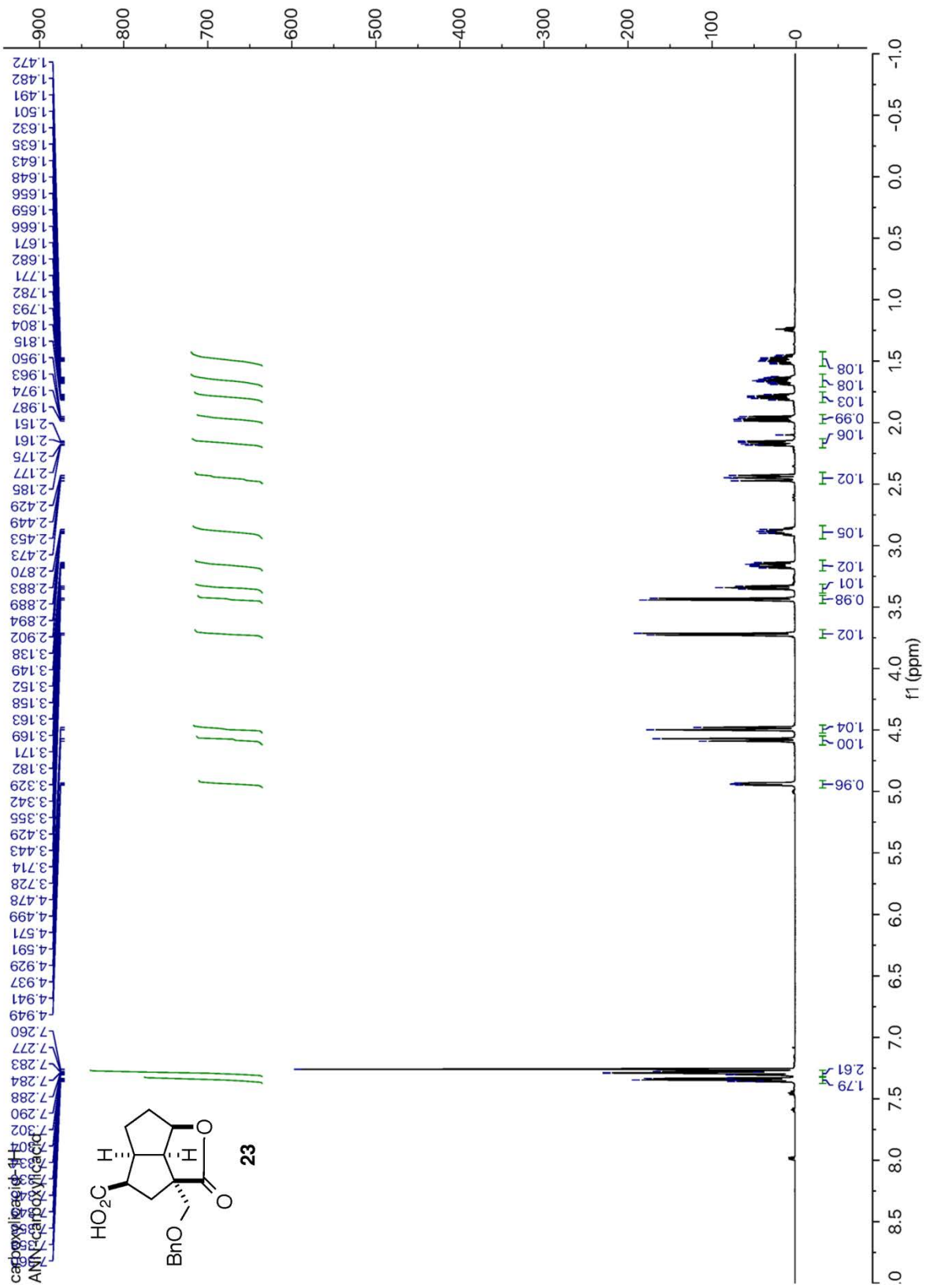
$^{13}C\{^{1}H\}$ NMR spectra of **22** (150 MHz, $CDCl_3$)



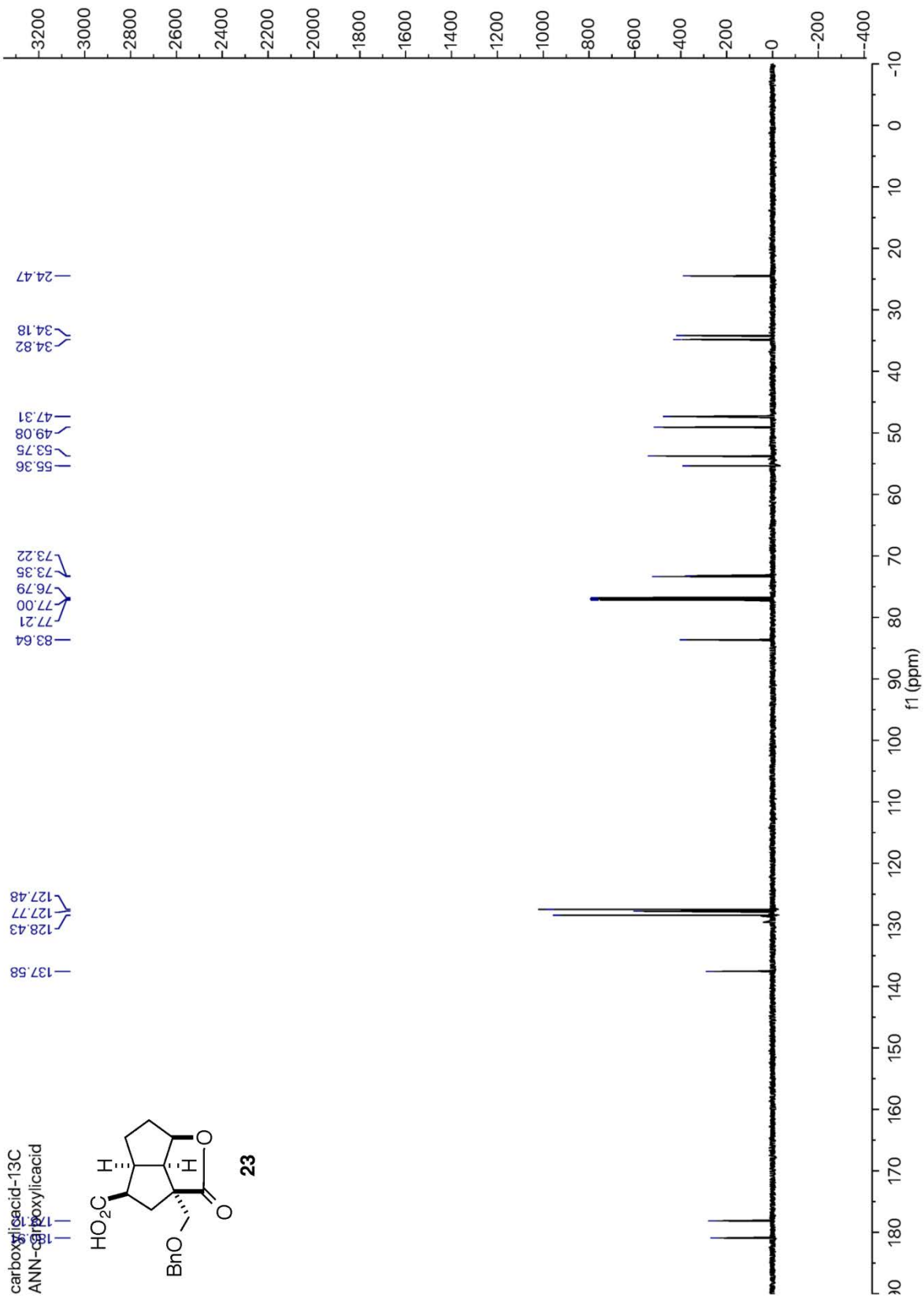
^{1}H NMR spectra of **S2** (600 MHz, $CDCl_3$)



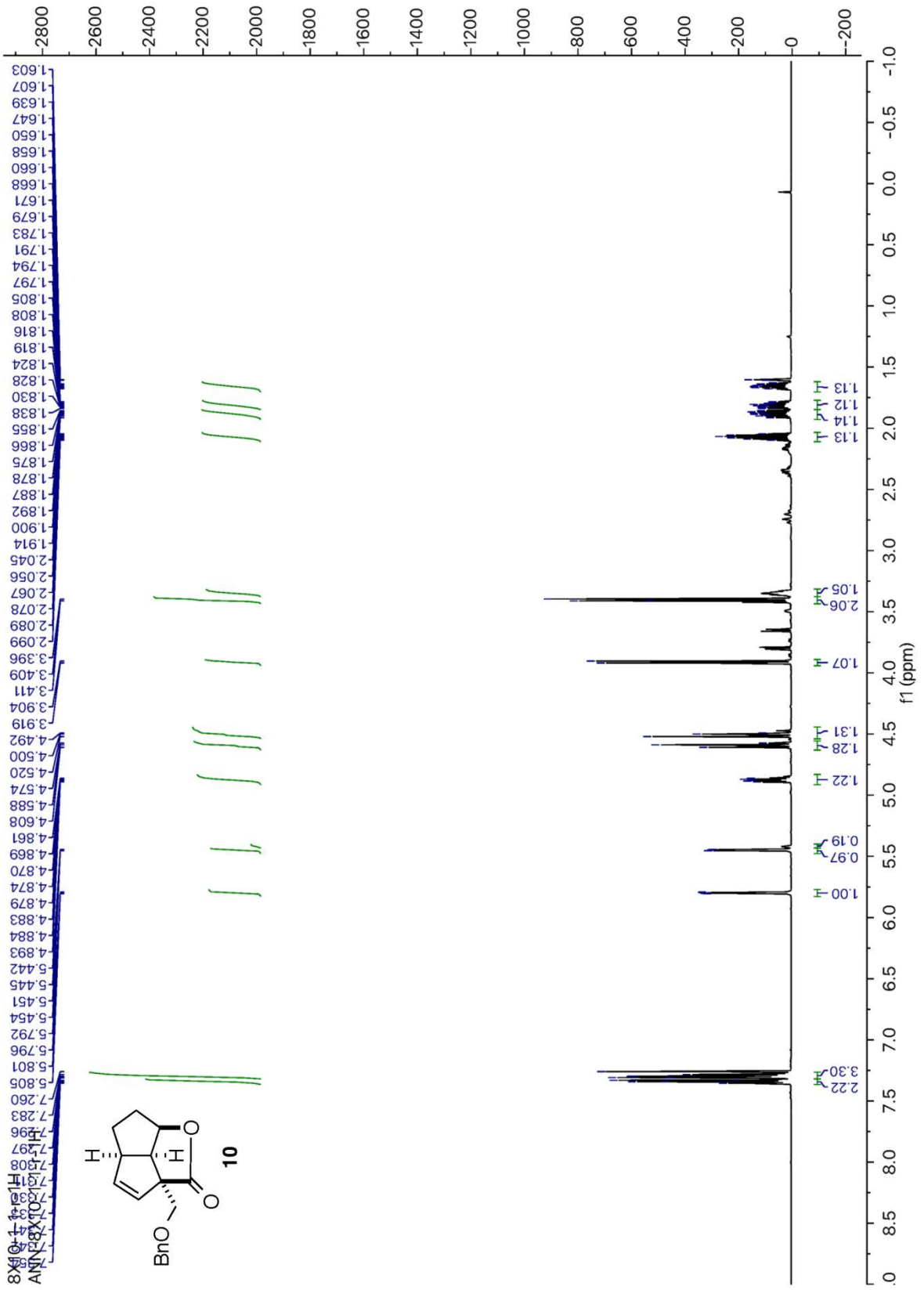
$^{13}C\{^{1}H\}$ NMR spectra of **S2** (150 MHz, $CDCl_3$)



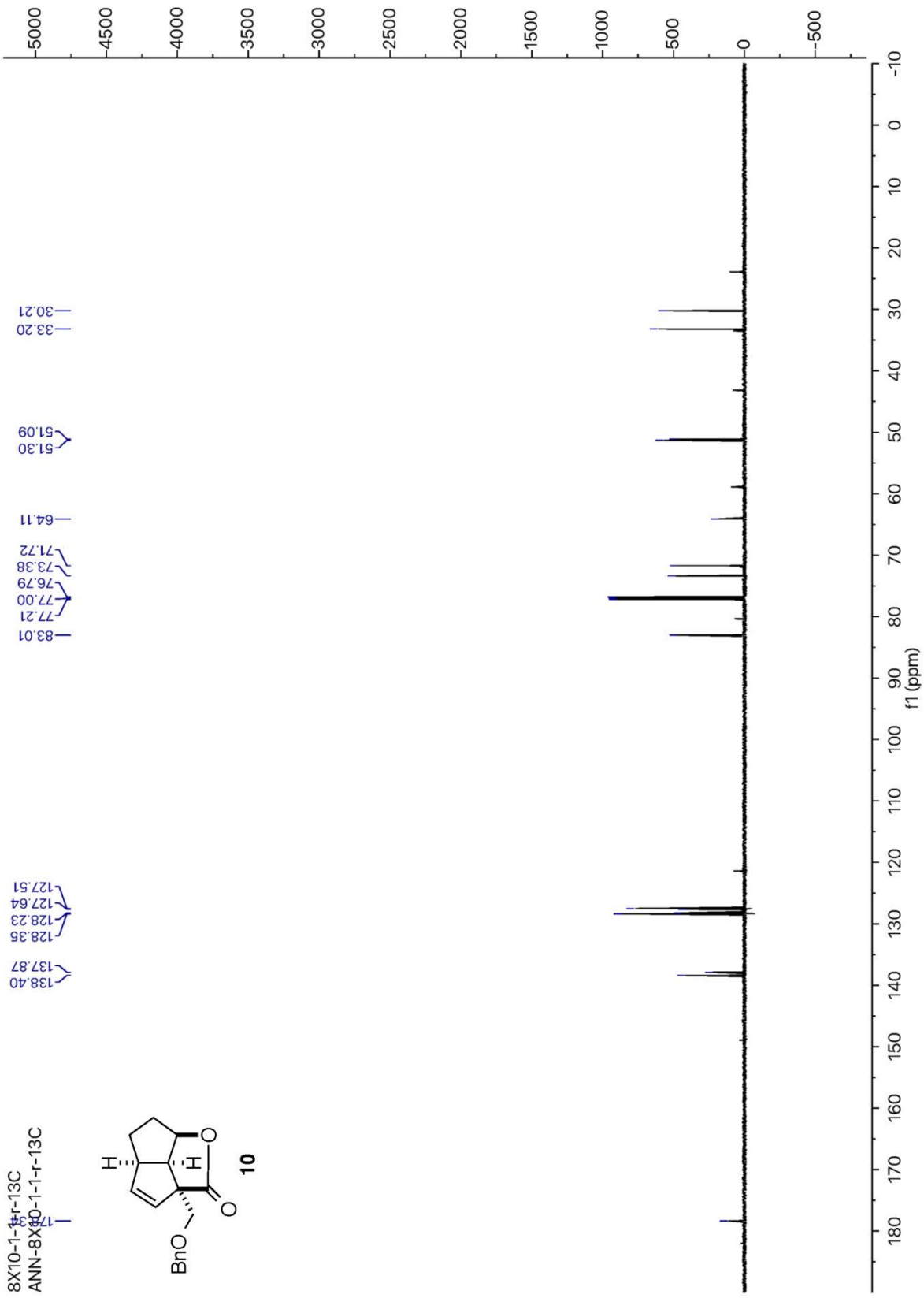
^{1}H NMR spectra of **23** (600 MHz, $CDCl_3$)



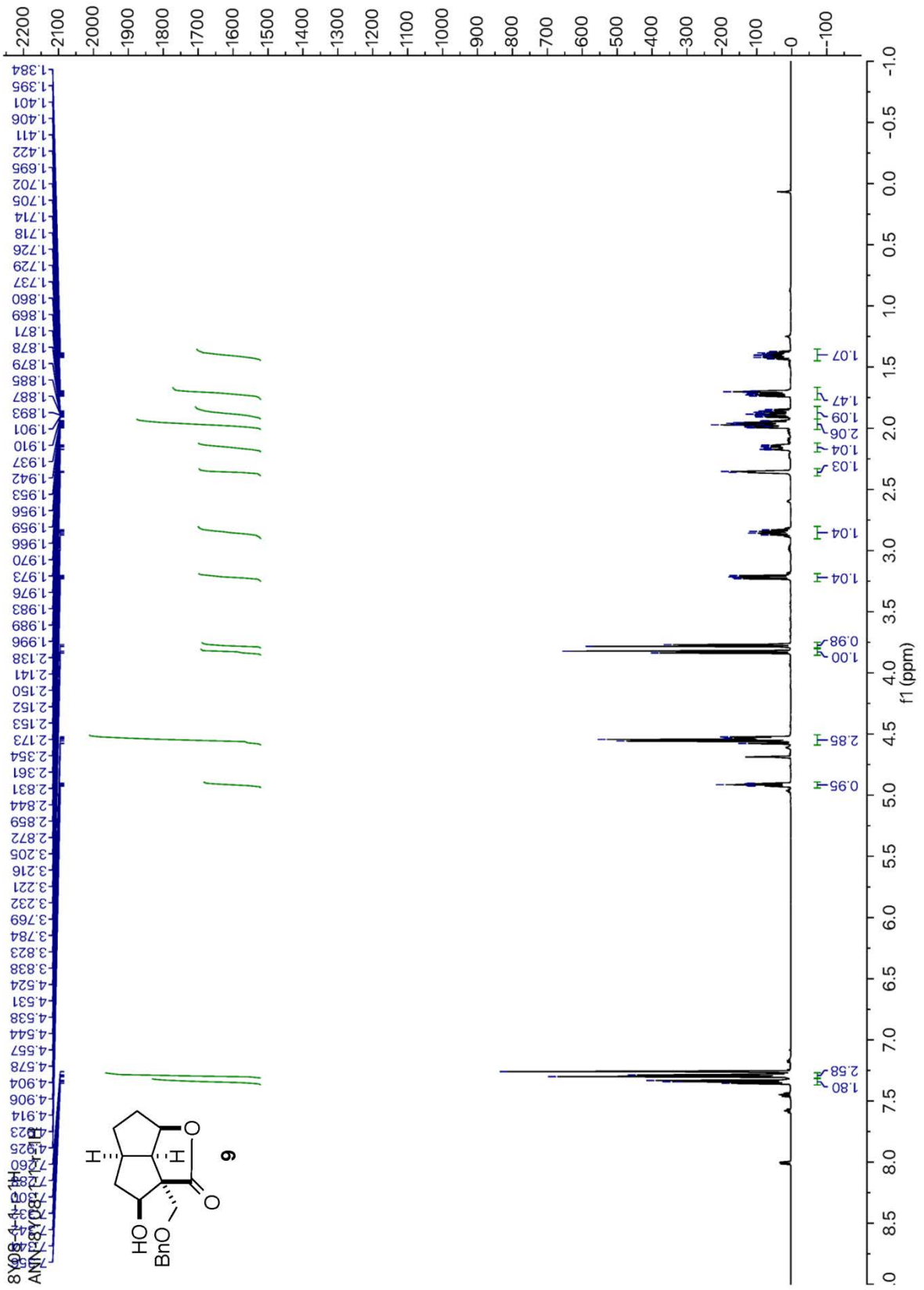
$^{13}C\{^{1}H\}$ NMR spectra of **23** (150 MHz, $CDCl_3$)



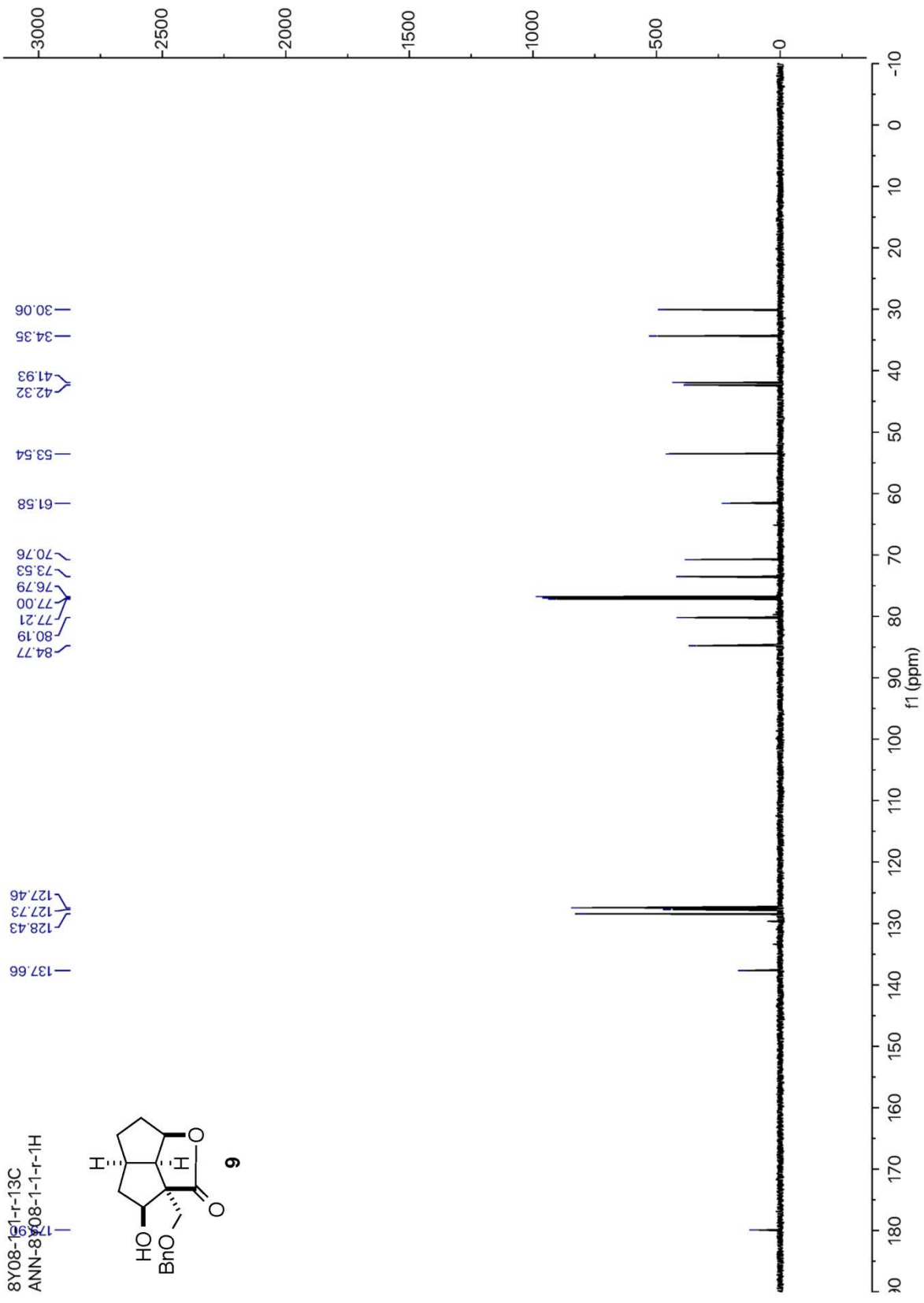
^{1}H NMR spectra of **10** (600 MHz, $CDCl_3$)



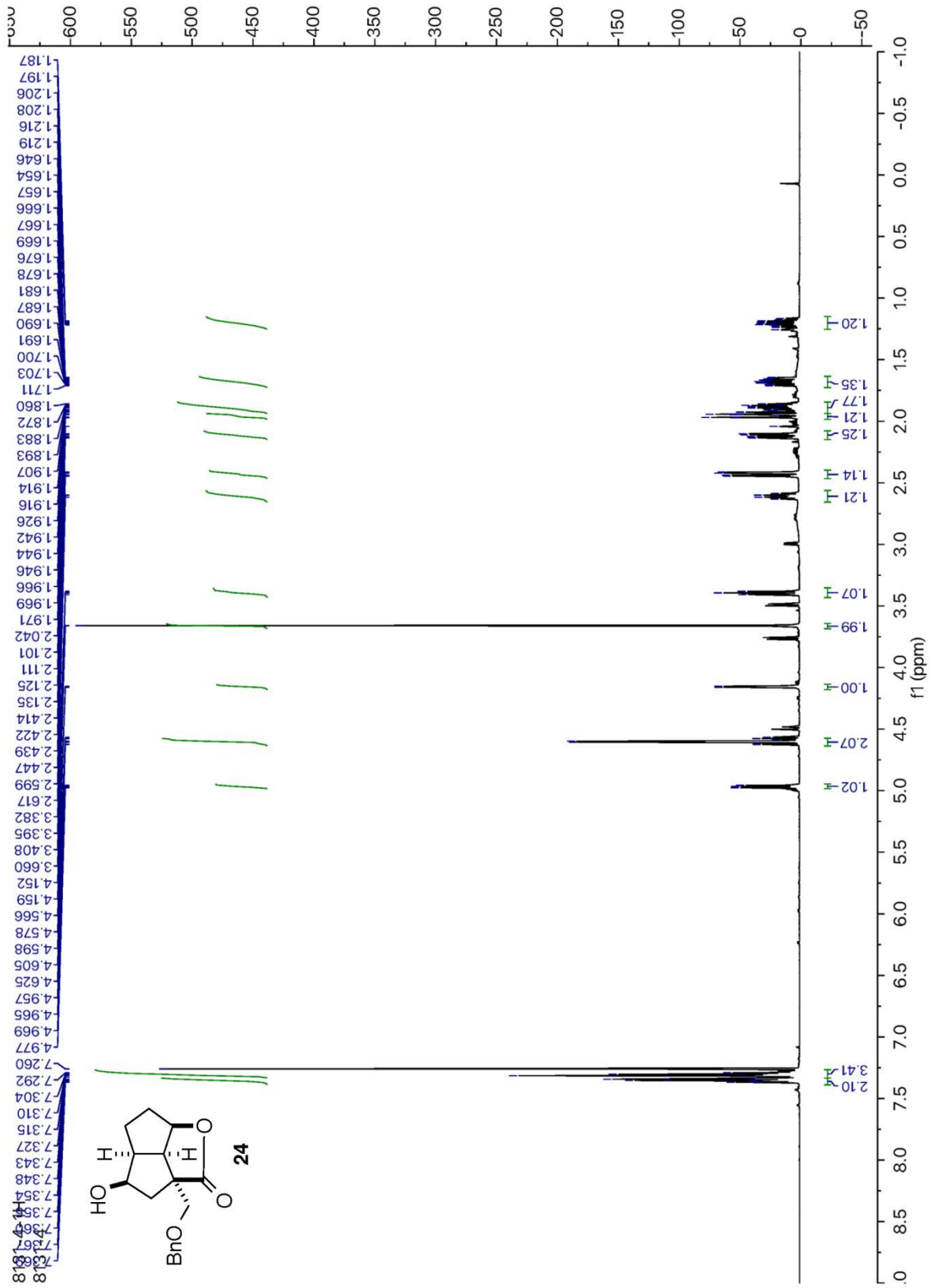
$^{13}C\{^{1}H\}$ NMR spectra of **10** (150 MHz, $CDCl_3$)



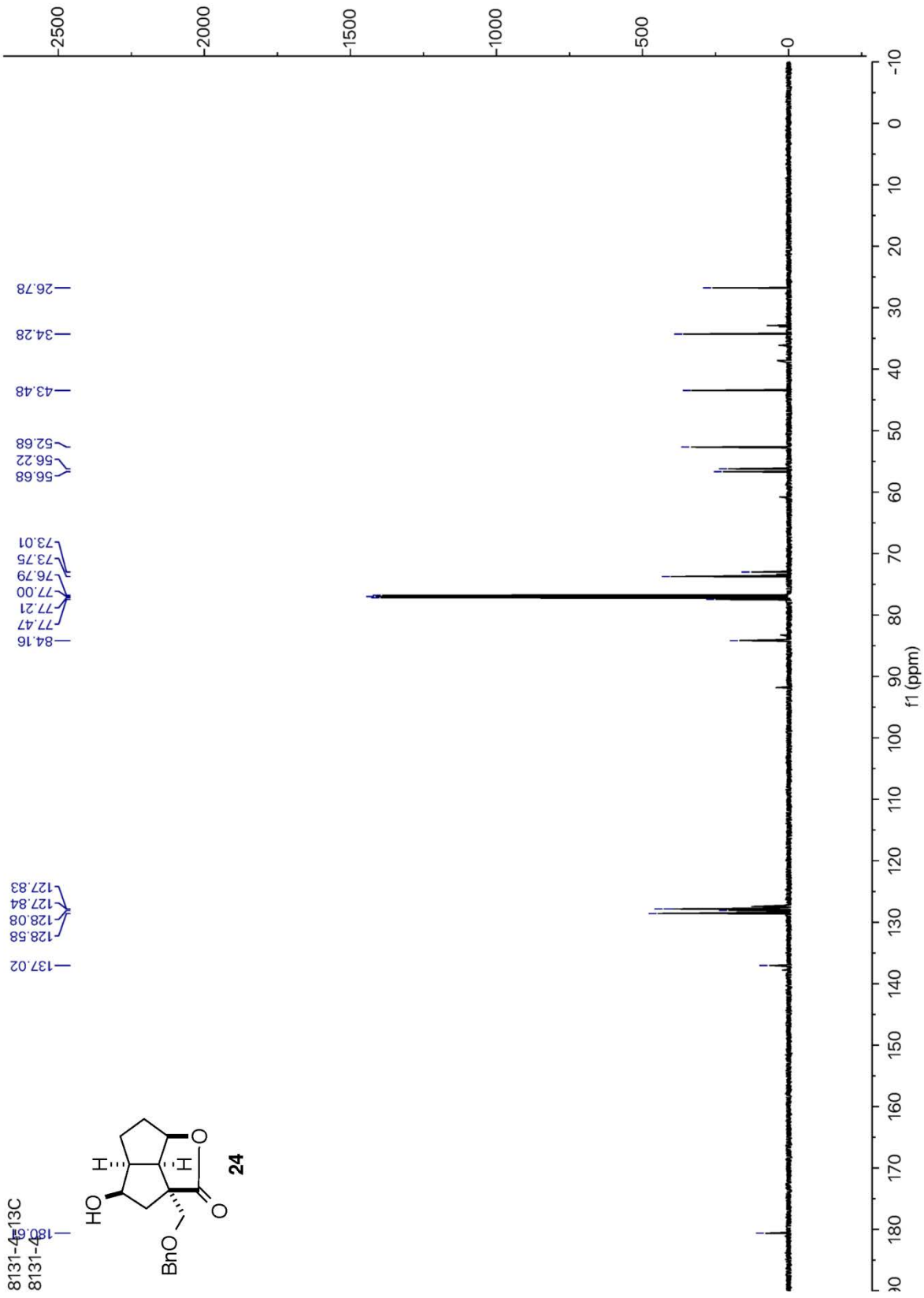
^{1}H NMR spectra of **9** (600 MHz, $CDCl_3$)



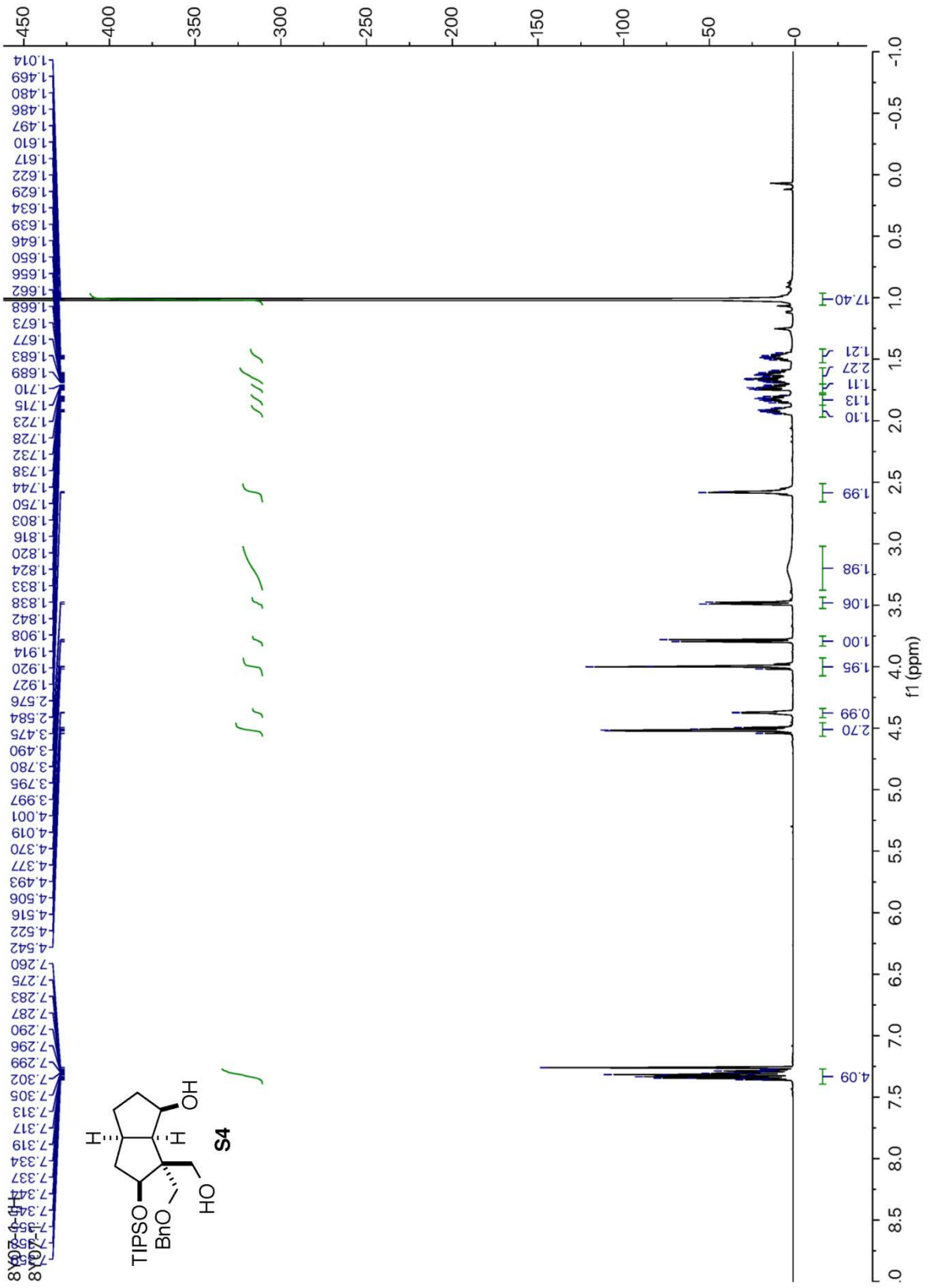
$^{13}C\{^{1}H\}$ NMR spectra of **9** (150 MHz, $CDCl_3$)



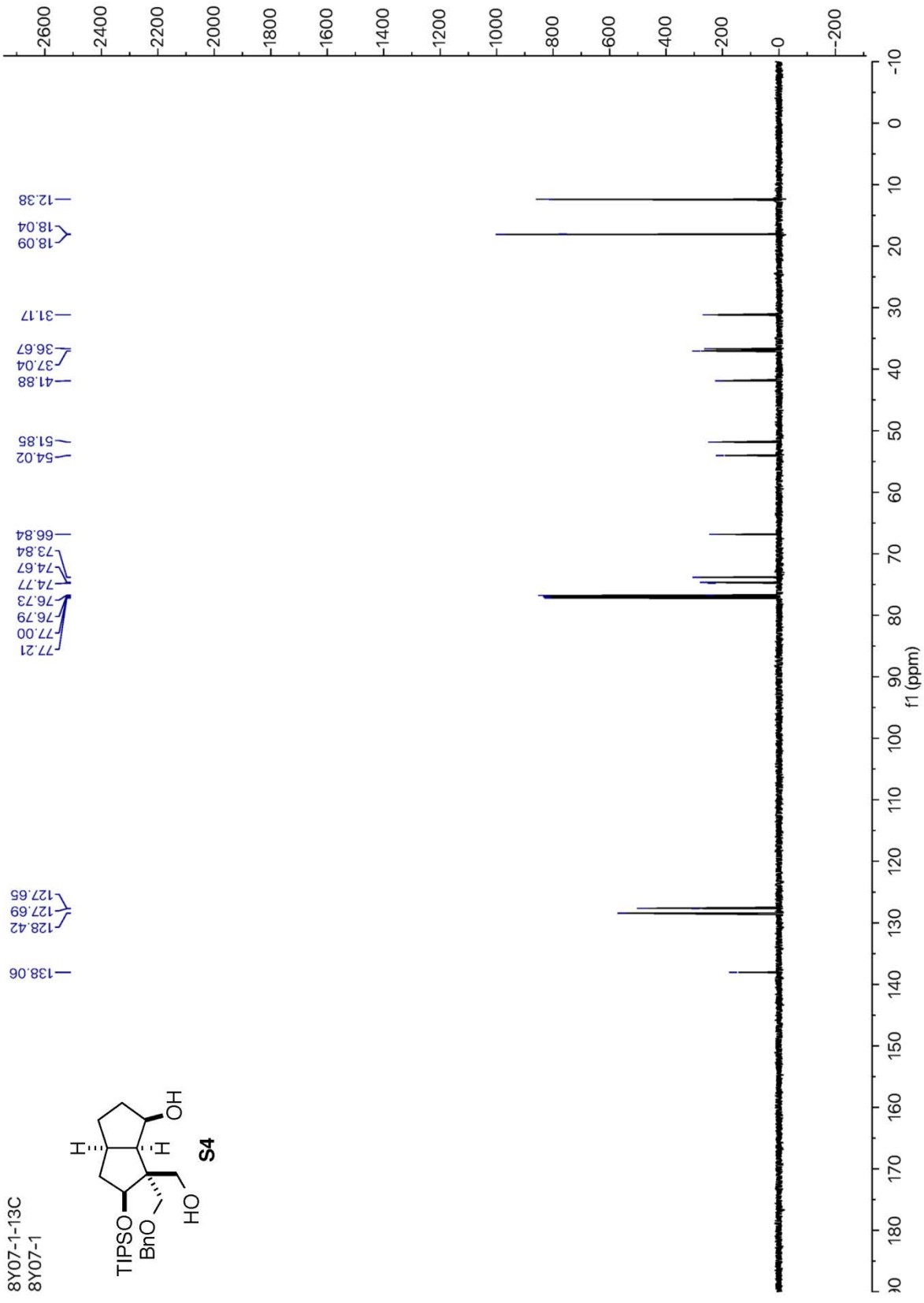
^{1}H NMR spectra of **24** (600 MHz, $CDCl_3$)



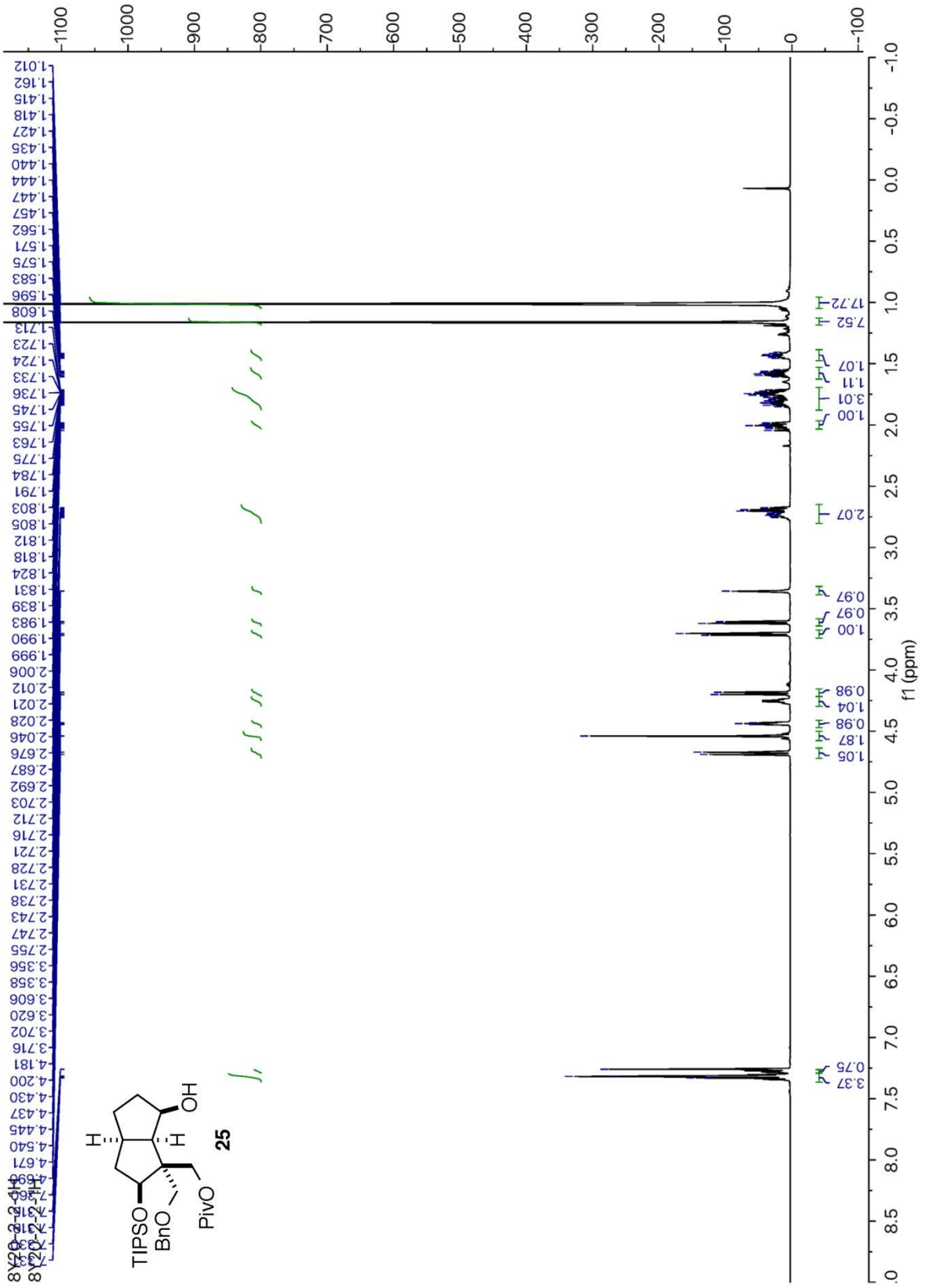
$^{13}C\{^{1}H\}$ NMR spectra of **24** (150 MHz, $CDCl_3$)



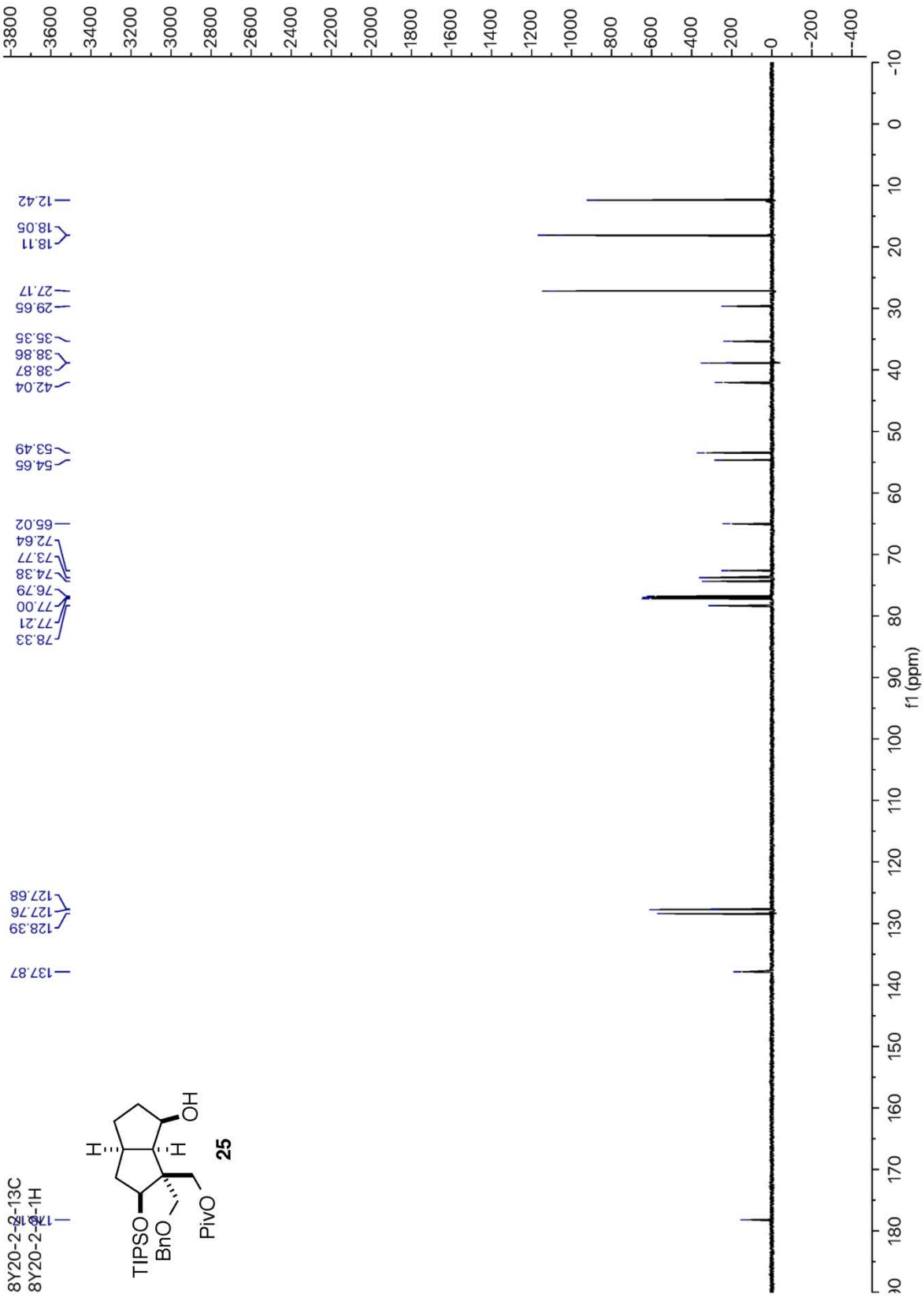
^{1}H NMR spectra of **S4** (600 MHz, $CDCl_3$)



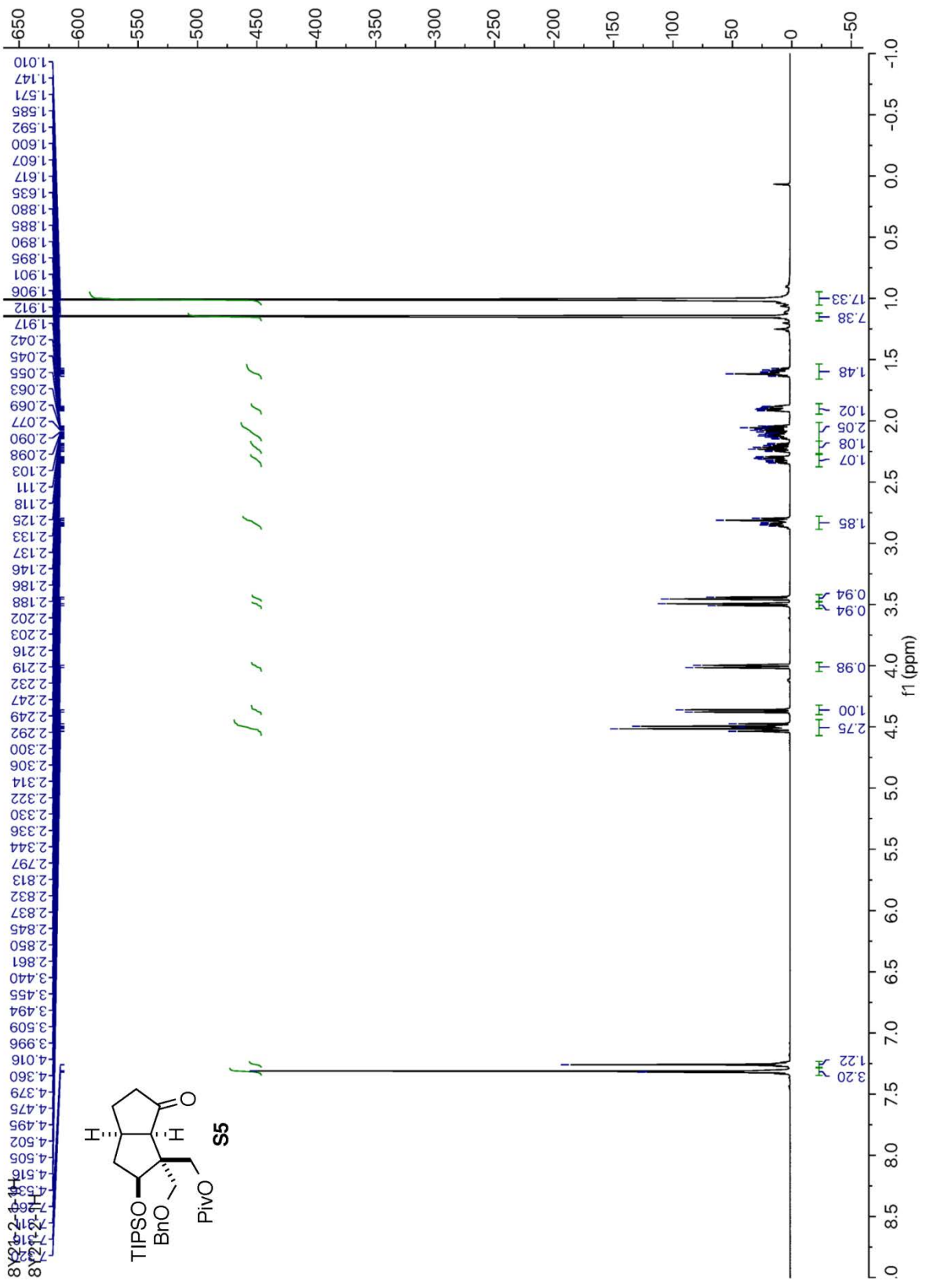
$^{13}C\{^{1}H\}$ NMR spectra of **S4** (150 MHz, $CDCl_3$)



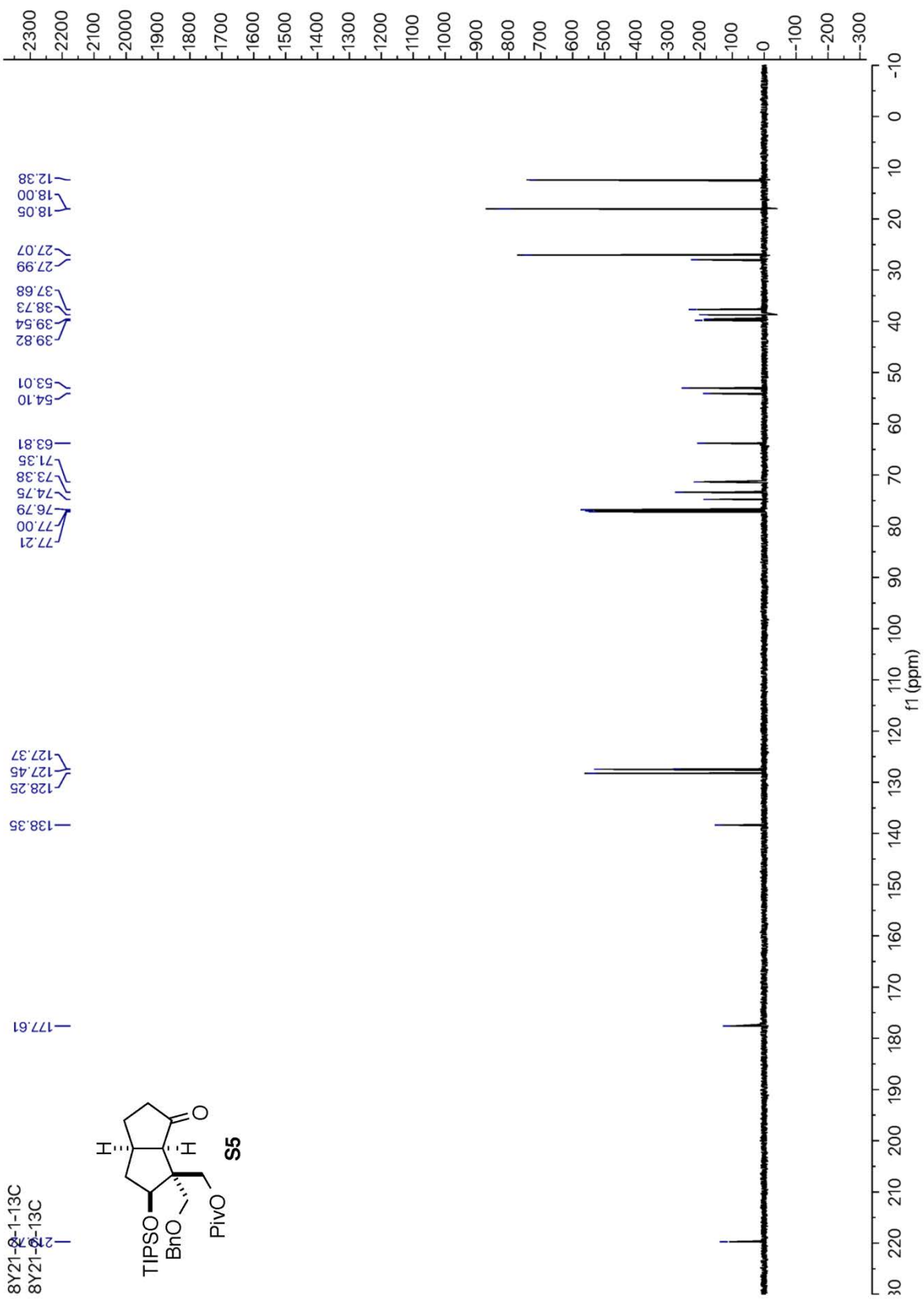
^{1}H NMR spectra of **25** (600 MHz, $CDCl_3$)



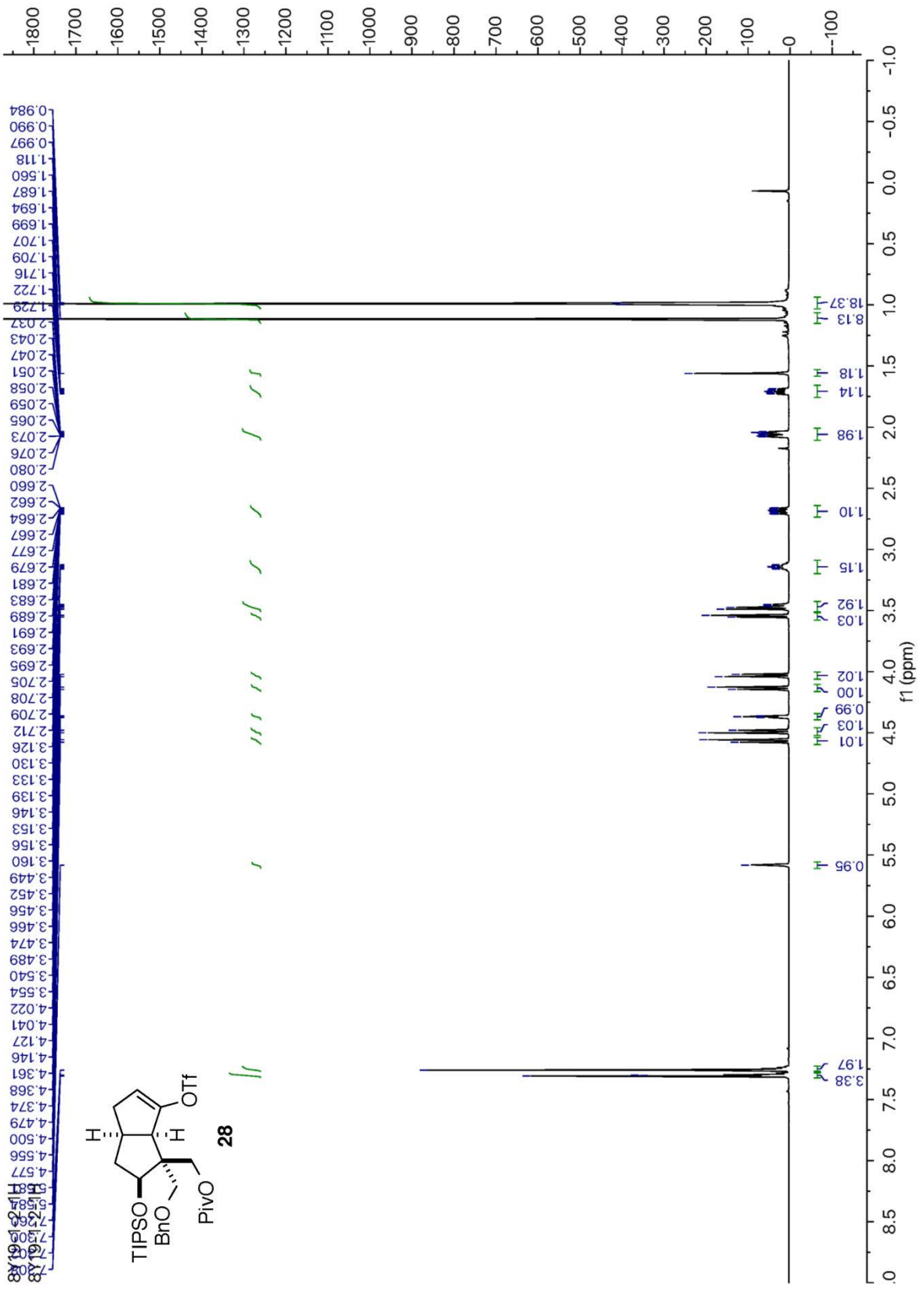
$^{13}C\{^{1}H\}$ NMR spectra of **25** (150 MHz, $CDCl_3$)



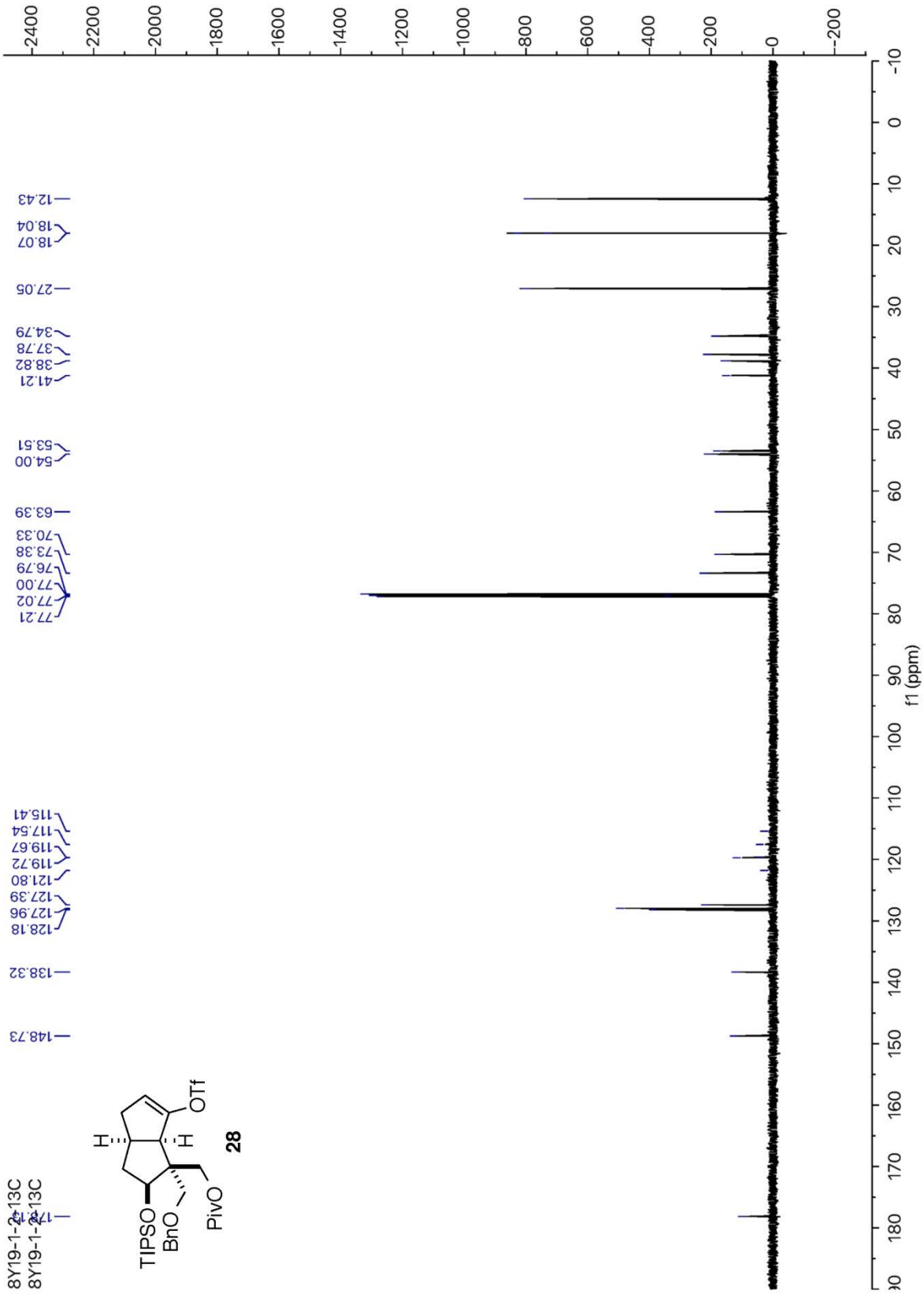
^{1}H NMR spectra of **S5** (600 MHz, $CDCl_3$)



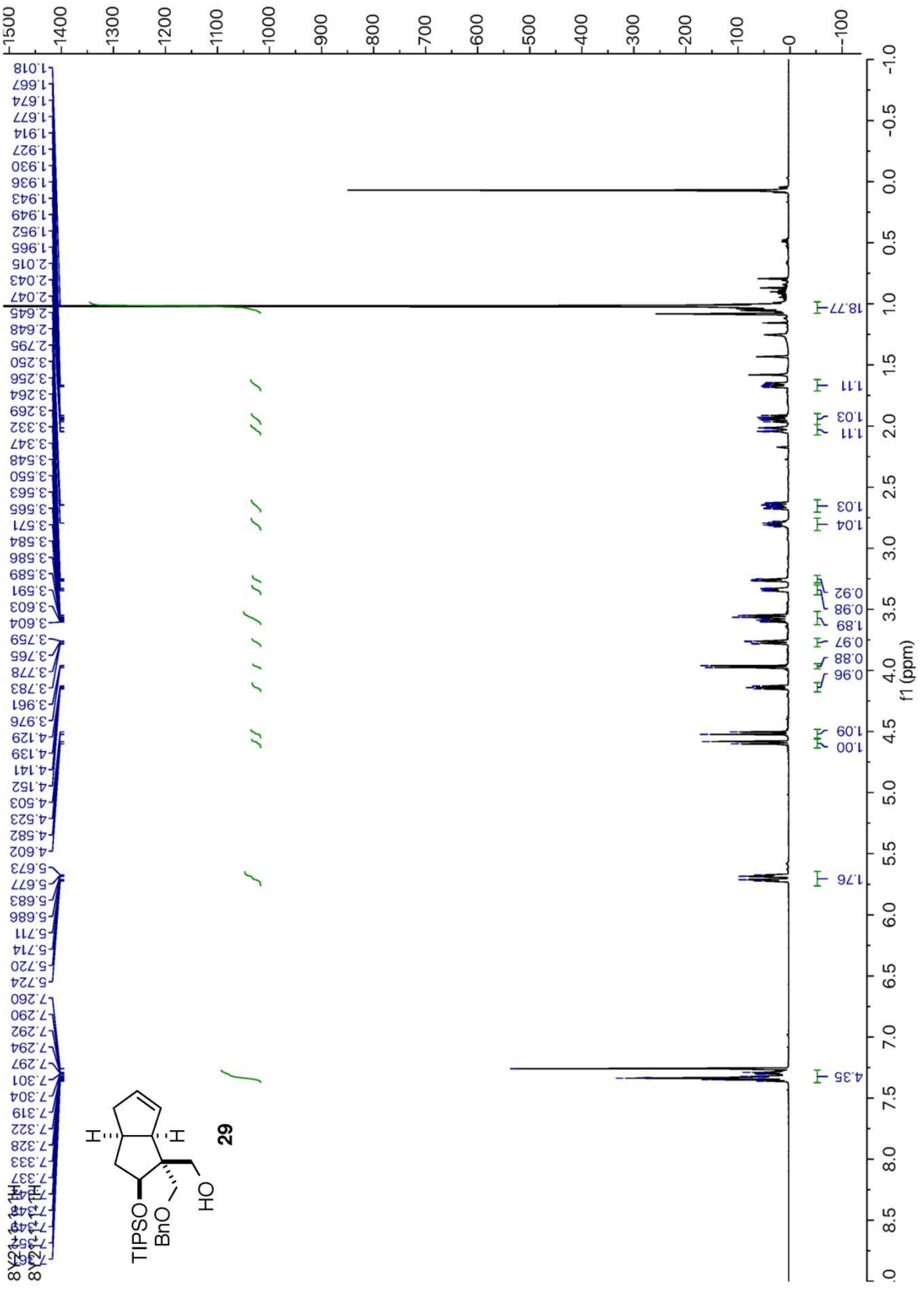
$^{13}C\{^{1}H\}$ NMR spectra of **S5** (150 MHz, $CDCl_3$)



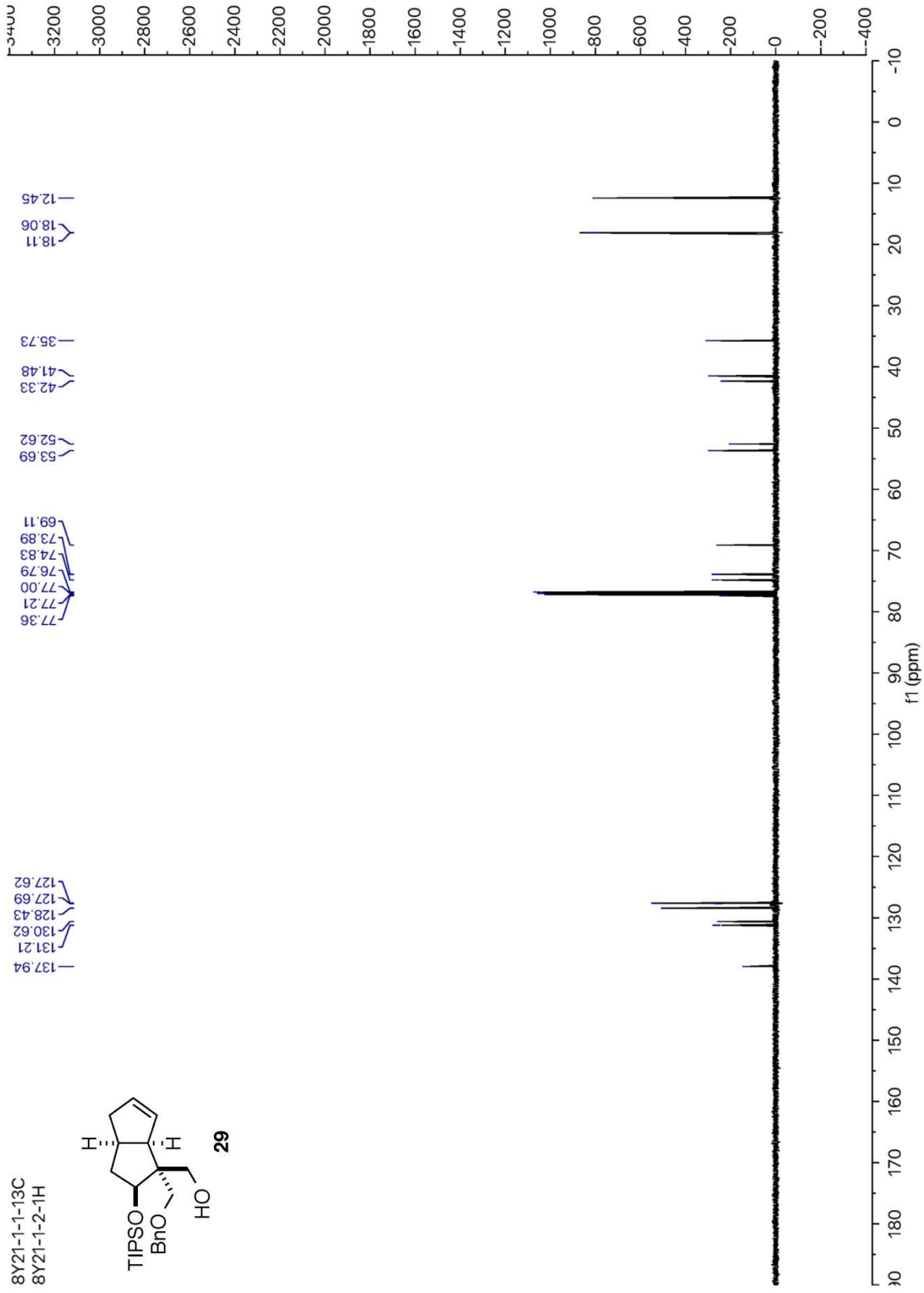
^{1}H NMR spectra of **28** (600 MHz, $CDCl_3$)



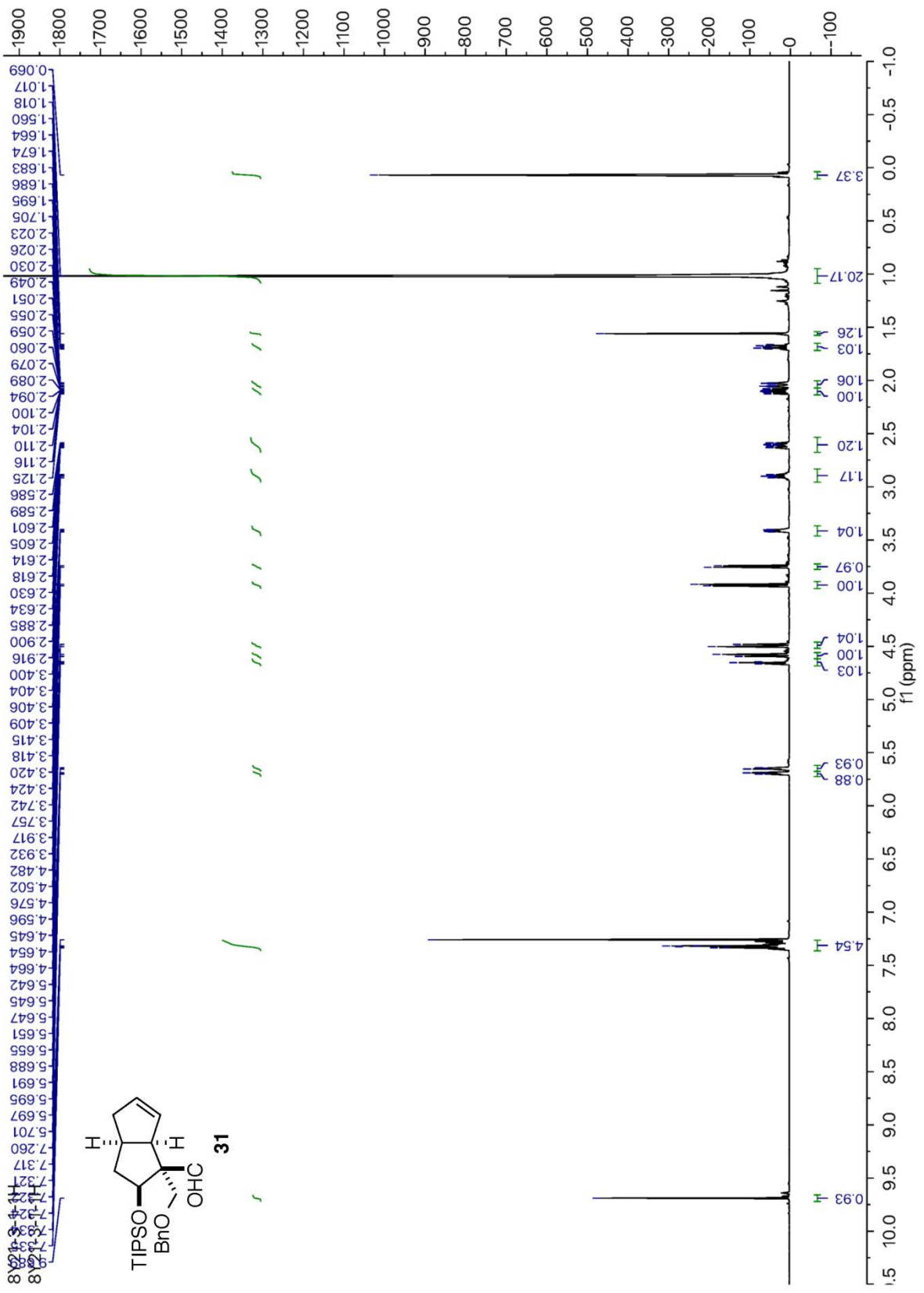
$^{13}C\{^{1}H\}$ NMR spectra of **28** (150 MHz, $CDCl_3$)



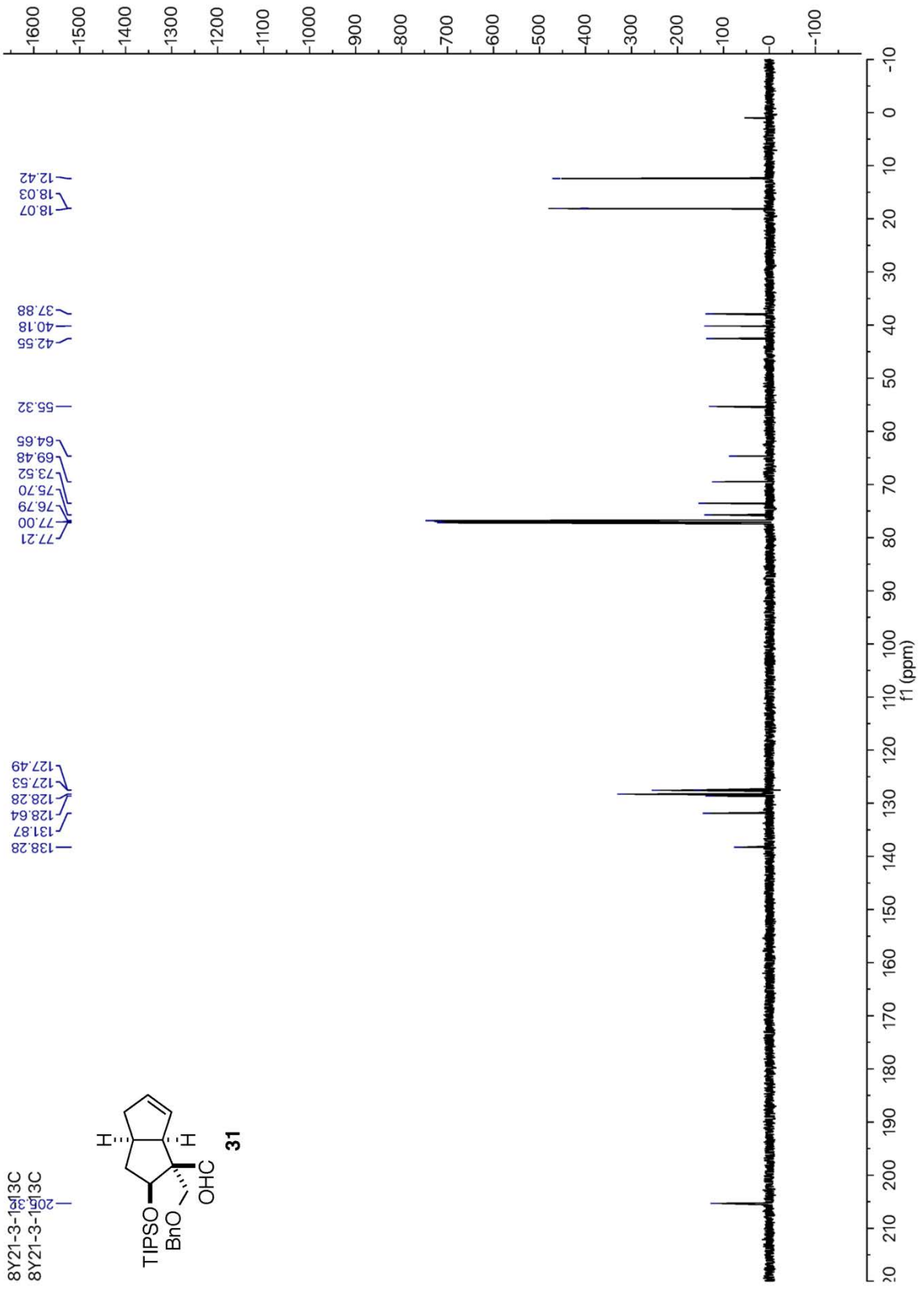
^{1}H NMR spectra of **29** (600 MHz, $CDCl_3$)



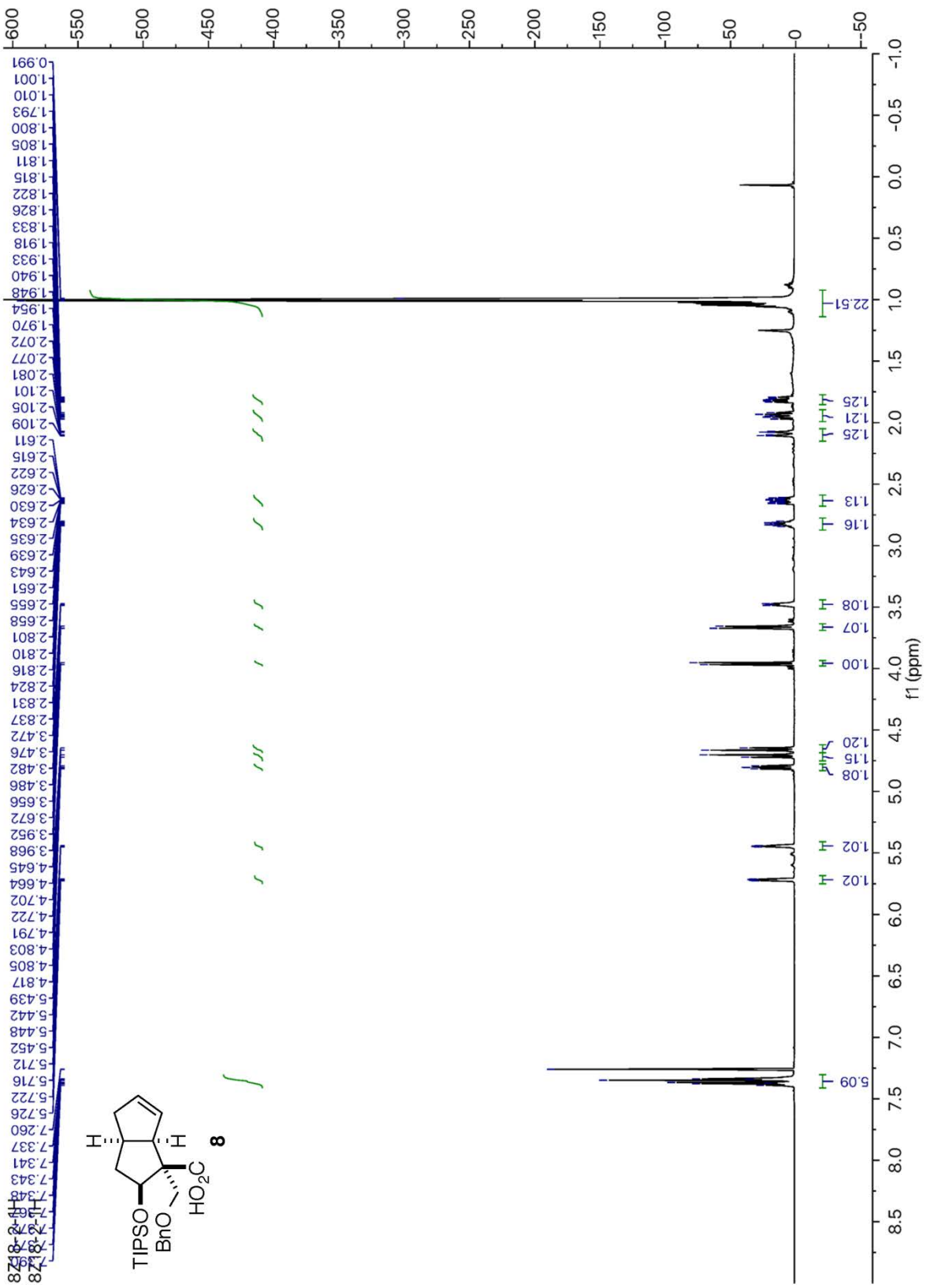
$^{13}C\{^{1}H\}$ NMR spectra of **29** (150 MHz, $CDCl_3$)



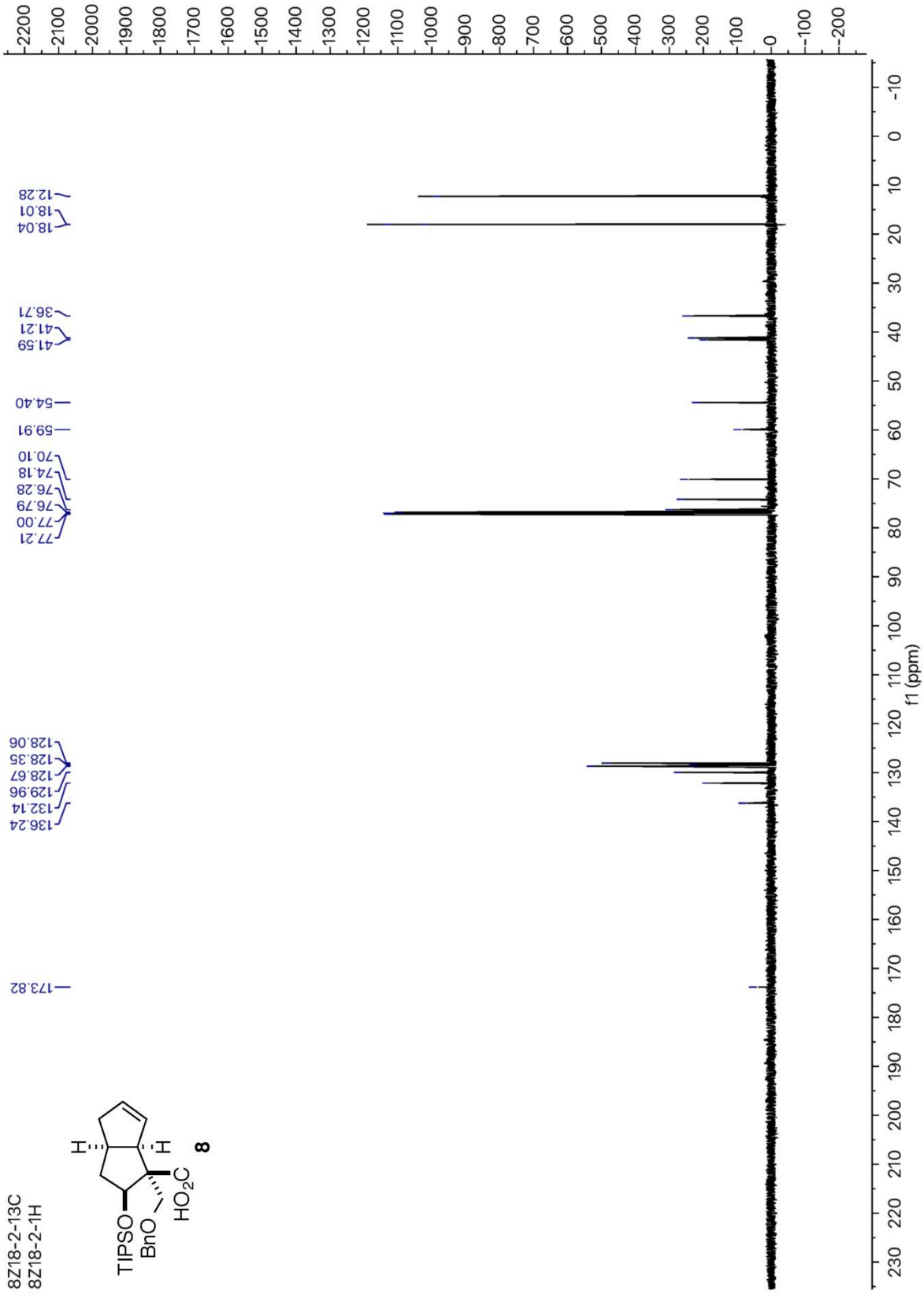
^{1}H NMR spectra of **31** (600 MHz, $CDCl_3$)



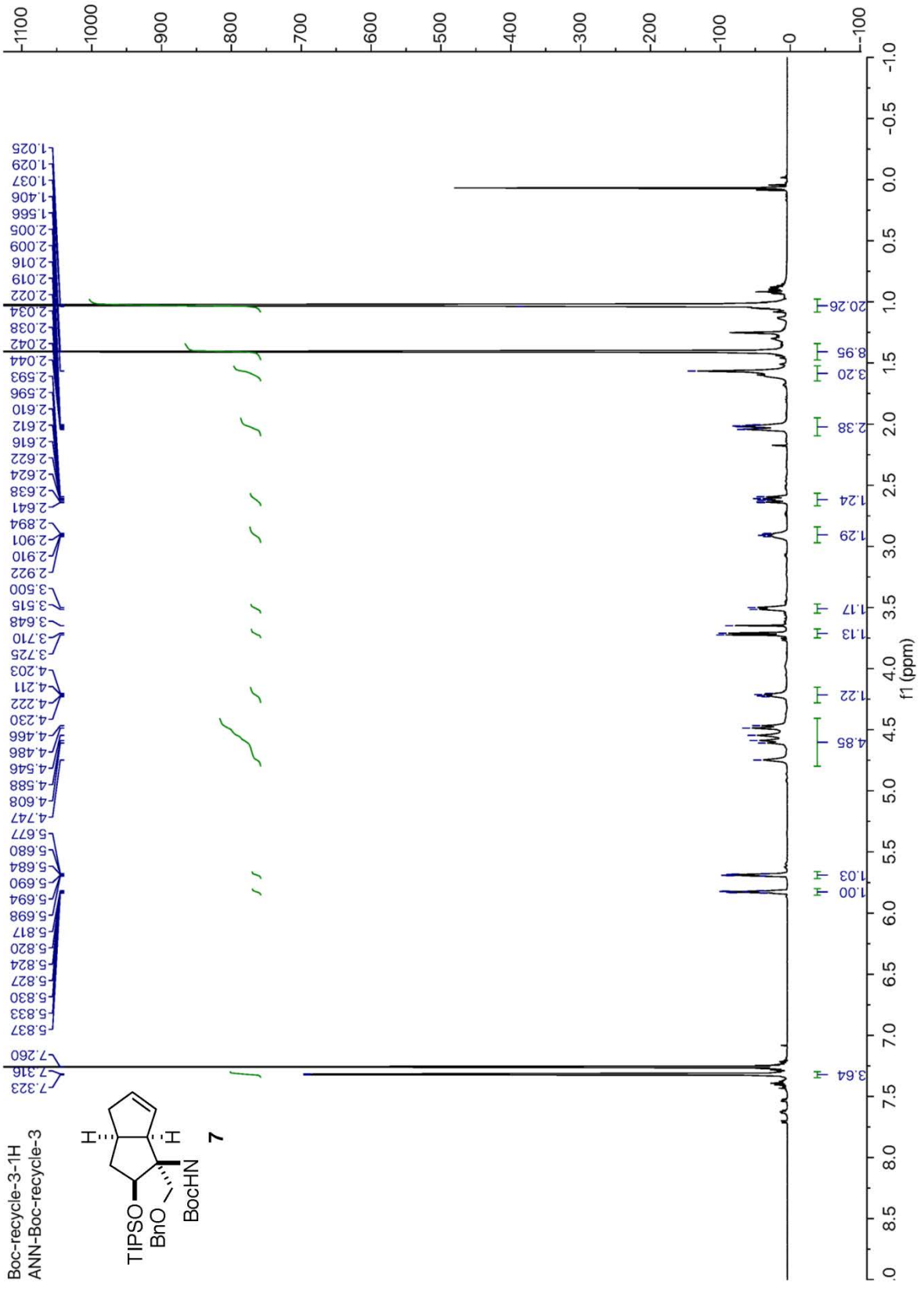
$^{13}C\{^{1}H\}$ NMR spectra of **31** (150 MHz, $CDCl_3$)



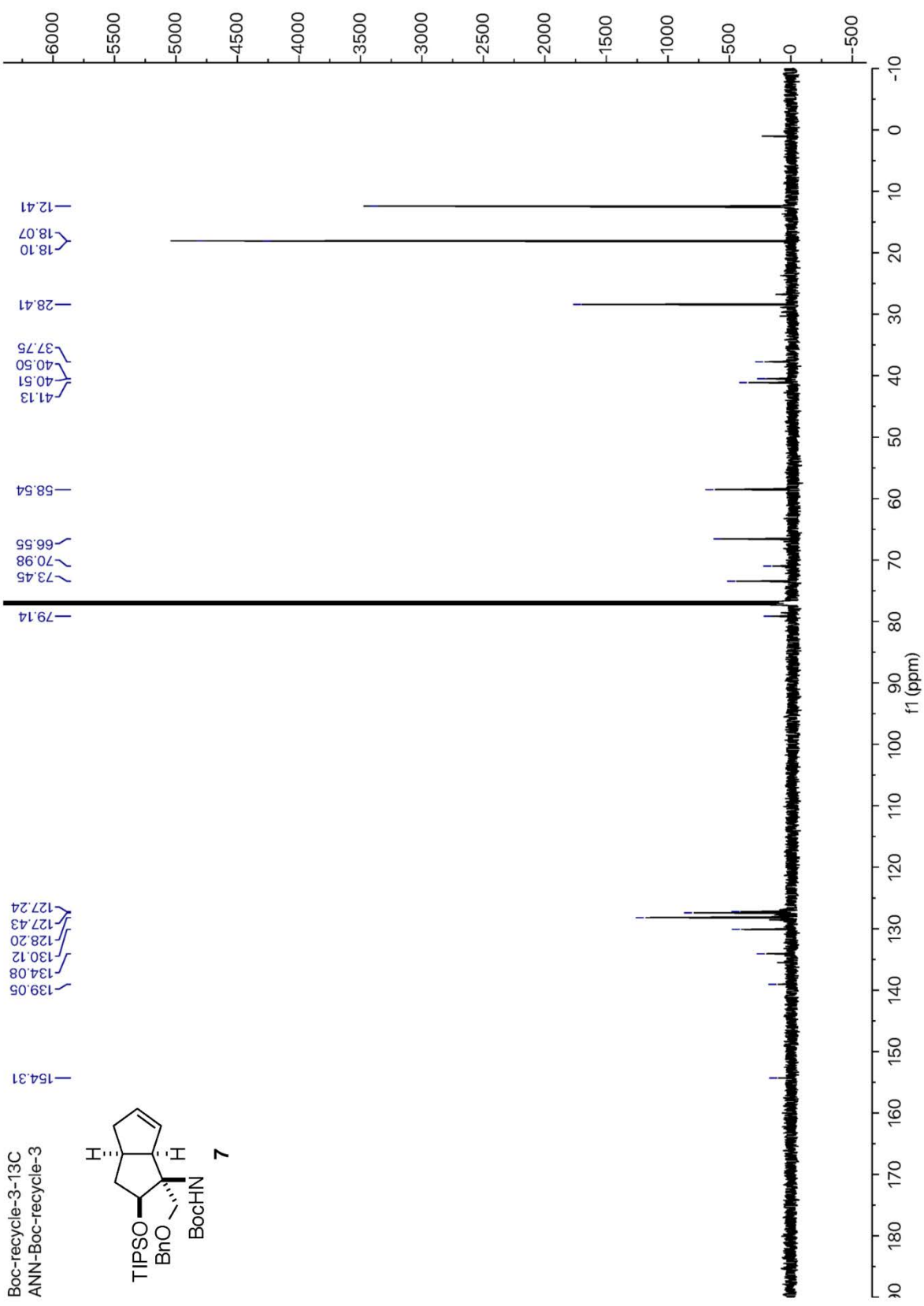
^{1}H NMR spectra of **8** (600 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR spectra of **8** (150 MHz, $CDCl_3$)



^{1}H NMR spectra of **7** (600 MHz, $CDCl_3$)



$^{13}C\{^{1}H\}$ NMR spectra of **7** (150 MHz, $CDCl_3$)