

Development of an enantioselective synthesis of (–)-euonyminol.

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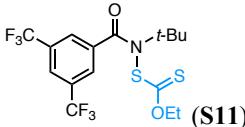
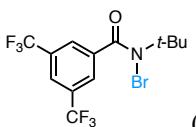
Supporting Information

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Complete set of reaction conditions described in Table 3.

Table S1. Attempted conditions aimed at the C8 oxidation of the acetonide 78

entry	conditions	result
1	Fe(<i>S,S</i> -PDP), H ₂ O ₂	oxidation of the methoxymethyl ether group
2	Fe(<i>R,R</i> -PDP), H ₂ O ₂	oxidation of the methoxymethyl ether group
3	DMDO	no reaction
4	TFDO	complex mixture
5	 (S11) blue LED	no reaction
6	 (S12) visible light	no reaction

Entry 1: A solution of (2*S,2'S*-(-)-[*N,N'*-bis(2-pyridylmethyl)]-2,2'-bipyrrolidinebis(acetonitrile)iron(II) hexafluoroantimonate (2.4 mg, 2.60 µmol, 0.25 equiv) in acetonitrile (150 µL) and a solution of aqueous hydrogen peroxide (50 wt% in H₂O, 3.60 µL, 51.2 µmol, 5.0 equiv) in acetonitrile (100 µL) were added via two syringe pumps over 1 h simultaneously to a solution of the lactone **78** (6.3 mg, 10.2 µmol, 1 equiv) and acetic acid (1.0 µL, 5.10 µmol, 0.50 equiv) in acetonitrile (200 µL) at 23 °C. The reaction was monitored by LC/MS analysis, which indicated oxidation of the methoxymethyl ether group and subsequent decomposition.

Entry 2: A solution of (2*R,2'R*-(-)-[*N,N'*-bis(2-pyridylmethyl)]-2,2'-bipyrrolidinebis(acetonitrile)iron(II) hexafluoroantimonate (2.7 mg, 2.90 µmol, 0.25 equiv) in acetonitrile (160 µL) and a solution of aqueous hydrogen peroxide (50 wt% in H₂O, 4.00 µL, 58.6 µmol, 5.0 equiv) in acetonitrile (110 µL) were added via two syringe pumps over 1 h simultaneously to a solution of the lactone **78** (7.2 mg, 11.7 µmol, 1 equiv) and acetic acid (1.0 µL, 5.90 µmol, 0.50 equiv) in acetonitrile (200 µL) at 23 °C. The reaction was monitored by LC/MS analysis, which indicated oxidation of the methoxymethyl ether group and subsequent decomposition.

Entry 3: A solution of dimethyldioxirane in acetone (~60 mM, 340 μ L, 20.3 μ mol, 2.50 equiv) was added to a solution of the lactone **78** (5.0 mg, 8.10 μ mol, 1 equiv) in acetone (200 μ L) at -78 °C. The reaction mixture was stirred for 30 min at -78 °C. The product mixture was then warmed to -40 °C over 30 min. The product mixture was then warmed to 0 °C over 30 min. The reaction was monitored by LC/MS analysis, which indicated no reaction.

Entry 4: A solution of methyl(trifluoromethyl)dioxirane in trifluoroacetone (~0.5 M, 50.0 μ L, 24.4 μ mol, 2.50 equiv) was added dropwise via a cold glass pipette to a solution of the lactone **101** (5.0 mg, 9.80 μ mol, 1 equiv) in dichloromethane (200 μ L) at -78 °C. The reaction mixture was stirred for 30 min at -78 °C. The product mixture was then warmed to -40 °C over 30 min. The product mixture was then warmed to 0 °C over 30 min. The reaction was monitored by LC/MS analysis, which indicated formation of a complex mixture of products.

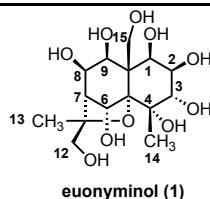
Entry 5: The xanthylamide **S11**^{17a} (4.7 mg, 10.7 μ mol, 1.10 equiv), the lactone **78** (6.0 mg, 9.80 μ mol, 1 equiv), and trifluorotoluene (200 μ L) were combined in a 1-dram vial in a nitrogen-filled glovebox. The reaction vial was sealed and the sealed reaction vial was removed from the glovebox. The reaction vial was suspended above a stir plate and next to a Kessil Blue LED light such that the LED lamp was 1.0 cm away from the reaction vial. The reaction vial, the Kessil Blue LED lamp, and the stir plate were covered with an aluminum foil. The covered reaction vial was irradiated and stirred for 24 h at 23 °C. The reaction was monitored by LC/MS analysis, which indicated no reaction.

Entry 6: The bromoamide **S12**^{17b} (3.5 mg, 8.90 μ mol, 1.10 equiv), the lactone **78** (5.0 mg, 8.10 μ mol, 1 equiv), and benzene (200 μ L) were combined in a 1-dram vial in a nitrogen-filled glovebox. The reaction vial was sealed and the sealed reaction vial was removed from the glovebox. The reaction vial was suspended above a stir plate and next to a 100 W tungsten lightbulb such that the light source was 1.0 cm away from the reaction vial. The reaction vial, the light source, and the stir plate were covered with an aluminum foil. The covered reaction vial was irradiated and stirred for 24 h at 23 °C. The reaction was monitored by LC/MS analysis, which indicated no reaction.

Comparison of ^1H NMR spectroscopic data of synthetic euonyminol (1**).**

Table S2. Comparison of synthetic ^1H NMR data of euonyminol (1**) from the White and Herzon laboratories.**

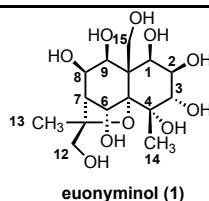
position	synthetic $(-)$ - 1 ¹ [500 MHz, D ₂ O]	synthetic (\pm) - 1 ² [D ₂ O]	abs ($\Delta\delta$)
	^1H [δ H (ppm), mult, J (Hz)]	^1H [δ H (ppm), mult, J (Hz)]	
H-1	4.33 (d, 3.5)	4.30 (m)	0.03
H-2	4.03 (t, 3.2)	4.00 (m)	0.03
H-3	3.66 (d, 2.9)	3.65 (d, 4)	0.01
H-6	5.22 (s)	5.10 (s)	0.02
H-7	2.39 (d, 4.0)	2.30 (s)	0.09
H-8	4.21 (dd, 5.3, 4.1)	4.30 (m)	0.09
H-9	4.37 (d, 5.4)	4.30 (m)	0.07
H-12 _a	3.92 (d, 11.4)	3.95 (m)	0.03
H-12 _b	3.73 (d, 11.4)	3.68 (d, 11)	0.05
H-13	1.44 (s)	1.36 (s)	0.08
H-14	1.74 (s)	1.58 (s)	0.16
H-15 _a	4.43 (d, 13.1)	4.30 (m)	0.13
H-15 _b	4.09 (d, 13.1)	4.09 (d, 11)	0.00



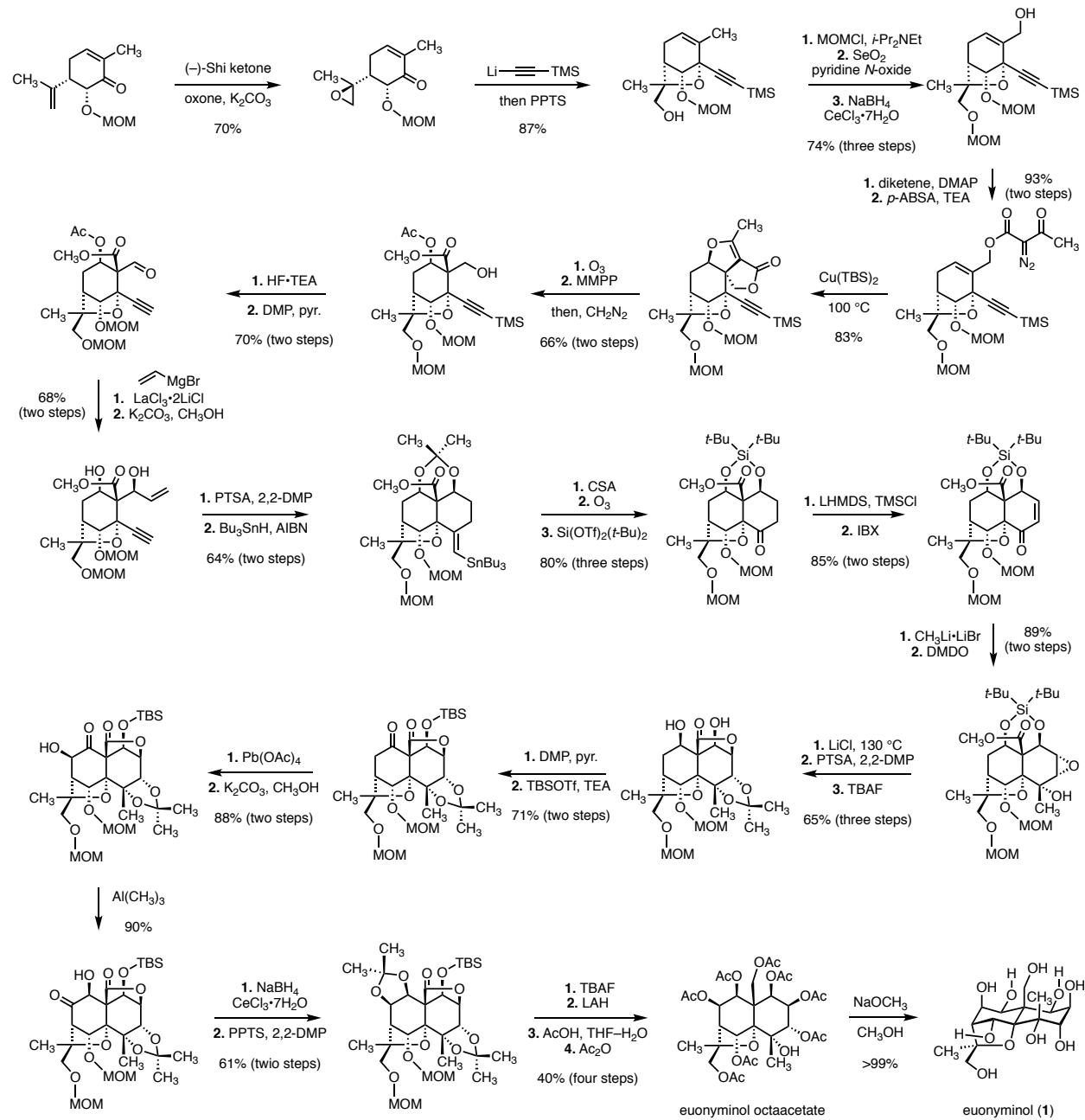
Comparison of ^{13}C NMR spectroscopic data of synthetic calculated euonyminol (1).

Table S3. Comparison of synthetic ^1H NMR data of euonyminol (1) from the White and Herzog laboratories.

position	synthetic (-)-3 [500 MHz, CD_3OD]	Calculated	abs(exp-calc)
	^{13}C [δ C (ppm)]	^{13}C [δ C (ppm)]	
C-1	74.97	77.9	2.93
C-2	75.81	75.4	0.41
C-3	79.32	77.7	1.62
C-4	73.36	73.3	0.06
C-5	94.50	95.5	1.00
C-6	74.97	73.7	1.27
C-7	53.92	50.1	3.82
C-8	70.98	71.2	0.22
C-9	76.86	79.3	2.44
C-10	54.96	50.4	4.56
C-11	85.92	87.9	1.98
C-12	68.89	73.2	4.31
C-13	18.89	21.8	2.91
C-14	25.85	26.6	0.75
C-15	59.60	65.1	5.50



Summary of the revised synthetic approach to euonyminol (1).



DFT Calculations.

*Radical cyclization calculations of **71**:*

Density functional theory calculations were performed by Gaussian 2016 software package, revision A.03.³ All geometry optimizations, including transition state optimizations, were achieved by (U)B3LYP functional⁴⁻⁵ with Def2SVP basis sets⁶ for tin element, and 6-31G(d) basis sets⁷⁻⁸ for hydrogen, carbon, and oxygen elements. Single point energy calculations were achieved by (U)B3LYP functional with Def2TZVP basis sets for tin element, and 6-311+G(2df,p) basis sets⁹⁻¹⁸ for hydrogen, carbon, and oxygen elements. Frequency calculations were performed with transition state optimizations for inspection purpose. All calculations were performed with D3 Grimme's empirical dispersion.¹⁹

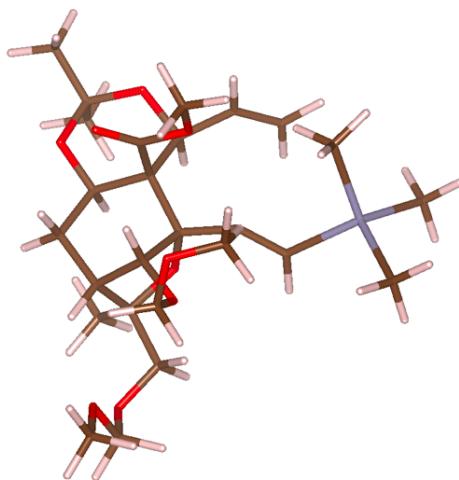
Table S4. Summary of energies for the optimized structures and transition states.

entry	compound/ transition state	absolute energy (Hartree)	relative energy (kcal/mol)	Imaginary Frequency Number
1	71	-1908.53049	0.00	Not Applicable
2	72	-1908.53797	-4.68	Not Applicable
3	73	-1908.54384	-8.38	Not Applicable
4	74	-1908.56517	-21.76	Not Applicable
5	TS-1	-1908.51710	8.41	1
6	TS-2	-1908.51604	9.07	1
7	TS-3	-1908.51107	12.19	1
8	75	-1908.52533	3.24	Not Applicable
9	76	-1908.53327	-1.74	Not Applicable
10	TS-4	-1908.51920	7.09	1
11	TS-5	-1908.50433	16.42	1
12	TS-6	-1908.52812	1.49	1
13	TS-7	-1908.52322	4.56	1

Cartesian coordinates for optimized structures and transition states:

Compound 71:

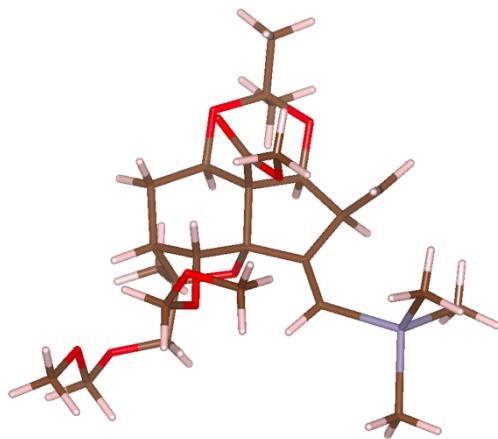
C	3.451900	-1.537600	-0.165500
C	4.447100	0.939600	-0.174300
C	4.187800	-0.406900	0.615200
C	5.598400	-1.008400	0.894800
C	6.595800	-0.017500	1.508400
C	6.590300	1.332900	0.745700
C	5.155700	1.883400	0.843500
O	5.445800	0.690400	-1.209800
C	6.757500	1.164400	-0.782100
C	7.829500	0.175600	-1.244600
C	7.000700	2.497900	-1.523600
O	8.299700	3.014500	-1.201700
C	8.345200	4.305600	-0.712700
O	7.991700	4.325600	0.662500
C	8.086000	5.621500	1.219500
C	3.266800	1.542400	-0.809600
C	2.902400	2.126800	-1.916800
O	5.517600	-2.170200	1.700300
O	3.443700	-2.692000	0.691200
C	4.702500	-3.197700	1.144700
C	4.365600	-4.121300	2.306000
C	5.430200	-3.933600	0.009800
H	7.326800	2.025900	1.157000
H	5.972100	-1.291300	-0.092300
Sn	0.832900	2.751900	-2.103800
C	-0.166800	2.065500	-0.295000
C	0.754200	4.930400	-2.246400
C	-0.040800	1.839700	-3.883700
C	3.454400	-0.102600	1.928800
O	2.255300	0.483900	1.703600
O	3.880900	-0.289300	3.046800
C	1.567300	0.937300	2.884100
H	4.037600	-1.716500	-1.078500
C	2.012100	-1.338500	-0.550800
H	7.591500	-0.472600	1.496800
H	6.327500	0.147300	2.555400
H	4.748300	1.763900	1.847500
H	7.727400	0.012800	-2.322900
H	8.816900	0.606000	-1.054500
H	7.771600	-0.795000	-0.750800
H	6.972200	2.292300	-2.601400
H	6.220100	3.215200	-1.276300
H	9.383200	4.652100	-0.834500



H	7.670200	4.981900	-1.271200
H	9.109400	6.024300	1.148000
H	7.812400	5.540500	2.274100
H	7.399700	6.331100	0.728100
H	3.609600	2.280600	-2.741100
H	5.283500	-4.544900	2.723500
H	3.858400	-3.537300	3.077700
H	3.711600	-4.930600	1.969500
H	5.664000	-3.274200	-0.830600
H	6.369100	-4.350100	0.386300
H	4.800100	-4.745900	-0.363800
H	-1.208800	1.798700	-0.493100
H	-0.140800	2.846800	0.470700
H	-0.282600	5.276000	-2.304700
H	1.290100	5.277200	-3.134900
H	0.030600	0.750600	-3.810900
H	-1.094500	2.119300	-3.980000
H	0.634200	1.369900	2.523300
H	2.172200	1.689200	3.398600
H	1.375400	0.101900	3.561900
C	1.589500	-1.248400	-1.810600
H	2.279900	-1.264400	-2.650700
H	0.535700	-1.128800	-2.048600
H	1.308500	-1.314900	0.275300
H	0.375500	1.190600	0.070400
H	1.223200	5.371300	-1.361200
H	0.492200	2.166500	-4.781600
O	5.001700	3.246400	0.470600
C	4.955600	4.127800	1.566700
O	3.812700	3.966600	2.364200
H	5.809300	3.979100	2.236900
H	4.993900	5.130700	1.118200
C	2.593100	4.166300	1.655200
H	1.795700	4.173000	2.402400
H	2.416100	3.362200	0.933300
H	2.595100	5.129600	1.121100

Compound 72:

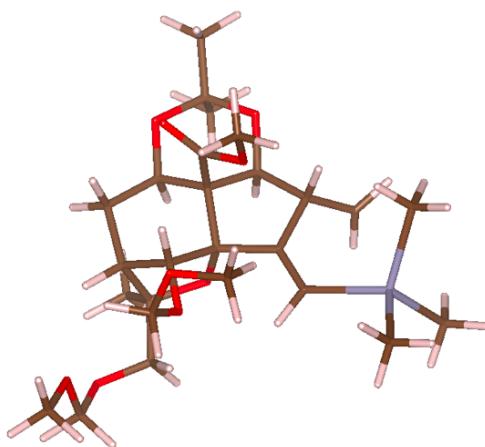
C	3.502900	-1.242800	-0.309700
C	4.392000	0.966900	-0.084700
C	4.305400	-0.385500	0.643200
C	5.655600	-1.055300	0.778800
C	6.641800	-0.090300	1.461800
C	6.537400	1.326900	0.781300
C	5.082900	1.885400	0.932800
O	5.331400	0.879800	-1.195800
C	6.667500	1.276400	-0.761100
C	7.717100	0.323400	-1.342300
C	6.927200	2.664100	-1.391200
O	8.251300	3.106900	-1.055600
C	8.354400	4.389400	-0.555900
O	7.939900	4.419700	0.802500
C	8.061900	5.708900	1.370300
C	2.985500	1.100800	-0.690000
C	2.455100	2.257400	-1.098000
O	5.444300	-2.326400	1.394600
O	3.231200	-2.470700	0.343600
C	4.454900	-3.159900	0.752900
C	4.004100	-4.130000	1.832100
C	5.071800	-3.866900	-0.459800
H	7.274000	2.005900	1.216500
H	6.012500	-1.226700	-0.238400
Sn	0.517200	2.578300	-2.002700
C	-0.984000	2.785500	-0.430200
C	0.662100	4.460400	-3.098900
C	-0.008200	0.956100	-3.359600
C	3.633900	-0.240200	2.027200
O	2.528000	0.535200	1.971700
O	4.047800	-0.683700	3.074600
C	1.905200	0.819700	3.233900
H	4.139700	-1.417000	-1.187300
C	2.346300	-0.315700	-0.828700
H	7.668700	-0.463100	1.386900
H	6.400400	-0.004700	2.524600
H	4.708100	1.723400	1.942700
H	7.562200	0.242500	-2.423700
H	8.712400	0.742000	-1.169300
H	7.690400	-0.682300	-0.923700
H	6.861100	2.558400	-2.481800
H	6.179600	3.378500	-1.054100
H	9.415800	4.672400	-0.629100
H	7.747200	5.110400	-1.136500
H	9.104400	6.066000	1.354400



H	7.730500	5.637600	2.408900
H	7.434300	6.449500	0.847200
H	3.066200	3.145400	-0.943200
H	4.857100	-4.714400	2.187900
H	3.592900	-3.555700	2.665200
H	3.239600	-4.804800	1.436700
H	5.410500	-3.159800	-1.222100
H	5.936400	-4.453200	-0.135800
H	4.333500	-4.533100	-0.915500
H	-0.625100	3.474200	0.341300
H	-1.173100	1.811000	0.028400
H	0.971200	5.267200	-2.426800
H	-0.304100	4.726200	-3.538700
H	-0.905300	1.211400	-3.931700
H	0.813100	0.770400	-4.058100
H	1.002500	1.380900	2.989300
H	2.576000	1.424100	3.851300
H	1.658800	-0.105400	3.760500
H	2.235700	-0.530700	-1.902200
C	1.004500	-0.503900	-0.206900
H	0.455800	-1.417900	-0.410700
H	0.632100	0.166100	0.554600
H	-1.923100	3.173900	-0.836400
H	1.399900	4.375500	-3.902400
H	-0.199000	0.045900	-2.785200
O	4.920400	3.269500	0.641300
C	4.993100	4.092000	1.784900
O	3.948800	3.876700	2.695800
H	5.917200	3.912300	2.343100
H	4.978700	5.117900	1.390600
C	2.653000	4.103300	2.147800
H	1.953300	4.082100	2.987000
H	2.382800	3.327500	1.423300
H	2.595200	5.087300	1.656600

Compound 73:

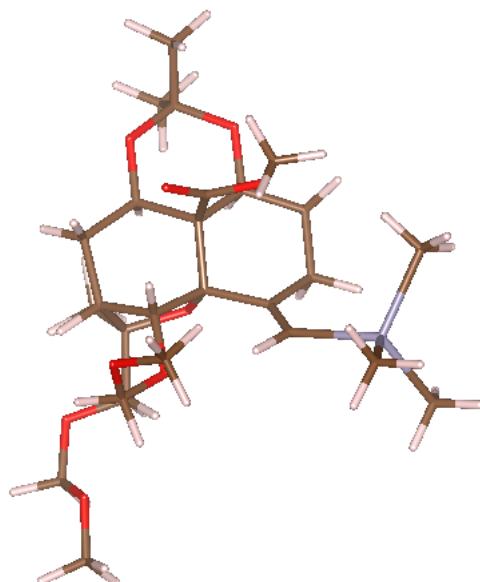
C	3.547900	-1.275800	-0.154800
C	4.499700	0.917000	-0.125600
C	4.360700	-0.356400	0.727700
C	5.689200	-1.039200	0.963400
C	6.686800	-0.035100	1.571300
C	6.628300	1.314300	0.760700
C	5.182500	1.914900	0.818600
O	5.462400	0.704900	-1.196800
C	6.795600	1.115300	-0.766200
C	7.836200	0.089200	-1.225900
C	7.103000	2.431200	-1.517000
O	8.427400	2.876700	-1.186200
C	8.545700	4.198900	-0.807600
O	8.091200	4.368000	0.527500
C	8.226400	5.703000	0.973500
C	3.110200	1.021500	-0.765800
C	2.614100	2.138500	-1.305200
O	5.424600	-2.236000	1.698900
O	3.242100	-2.434700	0.603600
C	4.441600	-3.107400	1.100000
C	3.946600	-3.978100	2.242900
C	5.076200	-3.923300	-0.032500
H	7.368800	2.016600	1.149900
H	6.064500	-1.322600	-0.021800
Sn	0.597200	2.415200	-2.031600
C	-0.769300	1.302300	-0.743500
C	0.216100	4.553800	-1.788600
C	0.351800	1.857800	-4.124100
C	3.661300	-0.059600	2.075600
O	2.494600	0.608800	1.915200
O	4.103000	-0.308100	3.175100
C	1.869700	1.054500	3.130400
H	4.173500	-1.536700	-1.019600
C	2.403600	-0.373000	-0.711600
H	7.705700	-0.435600	1.547600
H	6.431500	0.154200	2.616400
H	4.776100	1.857900	1.828200
H	7.710900	-0.085900	-2.299900
H	8.836900	0.497700	-1.060000
H	7.769600	-0.873400	-0.719700
H	7.063700	2.224100	-2.594300
H	6.363200	3.189000	-1.269900
H	9.615300	4.451400	-0.873200
H	7.973600	4.873400	-1.473600
H	9.276900	6.035500	0.957000



H	7.862300	5.738500	2.003000
H	7.632300	6.402600	0.362300
H	3.249400	3.021600	-1.259200
H	4.779600	-4.543800	2.668900
H	3.523300	-3.331600	3.015200
H	3.180600	-4.671300	1.884000
H	5.440900	-3.289400	-0.845400
H	5.924700	-4.490400	0.360800
H	4.338300	-4.616400	-0.446500
H	-0.811100	0.253600	-1.048400
H	-1.777000	1.726200	-0.789400
H	-0.809100	4.804800	-2.077700
H	0.904600	5.135900	-2.409200
H	0.519400	0.783400	-4.235700
H	-0.657900	2.100400	-4.469300
H	0.940800	1.532800	2.817100
H	2.519100	1.771200	3.641500
H	1.668100	0.209900	3.793700
C	1.866100	-0.823700	-2.024100
H	2.452200	-0.677400	-2.926500
H	0.999400	-1.474800	-2.076100
H	1.599000	-0.343200	0.028200
H	-0.411700	1.351400	0.289900
H	0.363200	4.843100	-0.742900
H	1.075000	2.395100	-4.744700
O	5.058100	3.266400	0.389900
C	5.106100	4.195400	1.450200
O	4.029200	4.082700	2.341700
H	6.008400	4.059200	2.054600
H	5.120500	5.178000	0.958000
C	2.755000	4.265200	1.730200
H	2.028400	4.339800	2.543100
H	2.497900	3.420600	1.081800
H	2.726100	5.191600	1.135500

Compound 74:

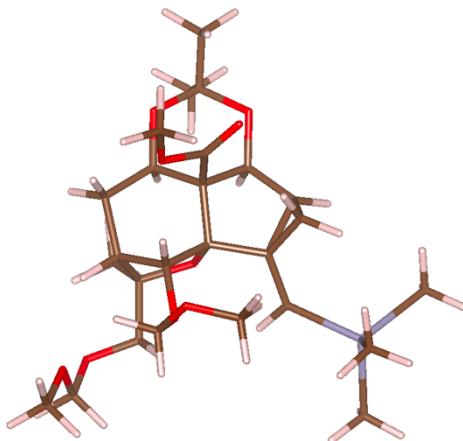
C	0.110000	-2.794800	-0.956400
C	0.532200	-0.986400	0.859400
C	-0.442100	-2.105200	0.326400
C	-0.501600	-3.271400	1.332700
C	-0.661600	-2.847100	2.790100
C	0.318900	-1.679900	3.101900
C	-0.070600	-0.488900	2.196600
O	1.774800	-1.650300	1.234800
C	1.788000	-1.923300	2.665300
C	2.363000	-3.316500	2.936700
C	2.762000	-0.897700	3.281500
O	2.680300	-1.008400	4.709300
C	3.384700	-0.031500	5.391200
O	2.729300	1.214400	5.243700
C	3.453700	2.287700	5.809200
C	0.795300	-0.024700	-0.294300
C	0.399900	1.254800	-0.302100
O	-1.492000	-4.194600	0.892200
O	-0.871800	-3.740700	-1.377000
C	-1.224500	-4.743600	-0.407900
C	-2.554500	-5.307300	-0.884900
C	-0.136000	-5.823600	-0.331700
H	0.267100	-1.433000	4.163300
H	0.474000	-3.753700	1.254400
Sn	0.318100	2.563100	-2.017300
C	-0.563200	1.447600	-3.676700
C	-0.994200	4.202600	-1.425300
C	2.282400	3.326000	-2.582300
C	-1.844100	-1.527500	0.087500
O	-2.004100	-1.012000	-1.146500
O	-2.725600	-1.485600	0.922600
C	-3.285700	-0.416200	-1.399000
H	1.030900	-3.310200	-0.634000
C	0.500200	-1.830300	-2.011500
C	1.402600	-0.734800	-1.512400
H	-0.466800	-3.706000	3.442100
H	-1.686700	-2.515200	2.971600
H	-1.152700	-0.385000	2.144300
H	3.299200	-3.431100	2.379800
H	2.585200	-3.402600	4.004700
H	1.701400	-4.137400	2.658600
H	3.784700	-1.134700	2.949000
H	2.504600	0.108500	2.959200
H	3.402900	-0.334300	6.449400
H	4.425600	0.053100	5.019100



H	3.600500	2.158700	6.894100
H	2.868000	3.194200	5.638900
H	4.443000	2.408500	5.337900
H	-0.007200	1.661900	0.617400
H	-2.899200	-6.085400	-0.198300
H	-3.291700	-4.500900	-0.908100
H	-2.447200	-5.728400	-1.888300
H	0.827700	-5.422300	-0.006800
H	-0.438800	-6.599000	0.377900
H	0.002700	-6.272600	-1.319400
H	-1.035400	0.549000	-3.270900
H	0.206400	1.145700	-4.393600
H	-0.572900	4.734300	-0.566400
H	-1.976800	3.810900	-1.143400
H	2.729600	3.874100	-1.748000
H	2.942800	2.494800	-2.847400
H	-3.242000	-0.056100	-2.427100
H	-3.464100	0.412200	-0.707100
H	-4.082100	-1.155800	-1.279700
H	2.366000	-1.162500	-1.192000
H	1.619400	-0.012900	-2.304600
H	-0.108400	-1.710300	-2.898700
H	-1.314500	2.046500	-4.200100
H	-1.126000	4.914800	-2.245400
H	2.200200	3.997800	-3.442300
O	0.483200	0.768300	2.583100
C	-0.044200	1.309600	3.779800
O	-1.438300	1.442100	3.773900
H	0.196900	0.687000	4.645300
H	0.459600	2.280700	3.876800
C	-1.938000	2.326000	2.781100
H	-2.988200	2.508900	3.021700
H	-1.874300	1.890600	1.775000
H	-1.393500	3.283300	2.783000

Compound 75:

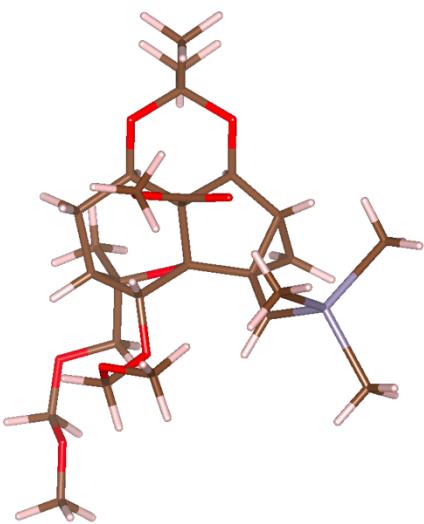
C -1.031600 -2.529000 -2.095700
C -0.746300 -1.080300 -0.224200
C -1.671400 -2.201500 -0.755900
C -1.553300 -3.456100 0.091600
C -1.745400 -3.146800 1.590200
C -0.903100 -1.872400 1.974800
C -1.328000 -0.630500 1.114200
O 0.536300 -1.687600 0.135900
C 0.580300 -2.010700 1.553700
C 1.242200 -3.379200 1.756100
C 1.519700 -0.975300 2.218300
O 1.632900 -1.243900 3.623800
C 1.353100 -0.191200 4.472600
O -0.051000 -0.016400 4.596300
C -0.382600 1.019200 5.499800
O -0.767800 0.607500 1.546700
C -1.666300 1.408900 2.273300
O -2.732500 1.884800 1.496600
C -2.310700 2.685600 0.396600
C -0.430100 -0.205400 -1.457400
C 0.739400 0.663500 -1.380500
O -2.437200 -4.399100 -0.533200
O -1.812100 -3.528600 -2.747400
H -1.414200 -3.997000 2.196300
H -2.795700 -2.972100 1.820800
H -0.999900 -1.668900 3.043000
H -2.406600 -0.516700 1.067000
H -0.534100 -3.818900 -0.028500
H 1.443100 0.411700 -0.592000
H -2.122800 0.850600 3.097900
H -1.053700 2.233300 2.666500
H -3.216500 3.022700 -0.113000
H -1.683700 2.118300 -0.299700
H -1.743800 3.565400 0.740800
H -1.473000 1.074900 5.541300
H 0.001600 0.817300 6.512900
H 0.010000 1.995000 5.168900
H 1.806800 0.754900 4.120100
H 1.783000 -0.453300 5.451900
H 2.514800 -1.088900 1.768700
H 1.159100 0.034300 2.040700
H 1.430100 -3.528200 2.823100
H 2.205200 -3.386000 1.234300
H 0.659300 -4.223400 1.389100
C -3.191100 -1.903800 -0.940200



O	-3.856500	-1.788800	0.234000
O	-3.778200	-1.820200	-1.995100
C	-5.277000	-1.604100	0.118000
H	-5.500700	-0.694800	-0.445800
H	-5.641800	-1.523100	1.142300
H	-5.728400	-2.460300	-0.390000
H	-0.039900	-2.950000	-1.880200
C	-0.718100	-1.171800	-2.719700
C	-1.534500	0.053800	-2.466700
C	-3.324700	-5.315100	-2.515400
C	-0.869100	-5.636600	-1.950900
Sn	1.198200	2.340700	-2.630100
C	-0.344200	3.877300	-2.412000
C	3.128000	3.124700	-1.989600
C	1.276500	1.743000	-4.731400
H	-1.329300	3.457200	-2.637100
H	-0.155800	4.712700	-3.093400
H	3.400700	4.005500	-2.578600
H	3.905200	2.365100	-2.116300
H	0.323300	1.300000	-5.036600
H	1.478300	2.608900	-5.369600
H	2.068100	1.003200	-4.882800
H	3.086900	3.409600	-0.933900
H	-0.353500	4.255400	-1.385400
H	0.000200	-1.144500	-3.533500
H	-1.331100	0.882700	-3.140600
H	-2.577900	-0.005500	-2.197300
C	-2.075000	-4.689800	-1.917800
H	-3.143100	-5.582900	-3.559800
H	-3.605200	-6.210300	-1.953000
H	-4.135100	-4.583900	-2.472300
H	0.035700	-5.171500	-1.550100
H	-1.085400	-6.531400	-1.359900
H	-0.666100	-5.927000	-2.985600

Compound 76:

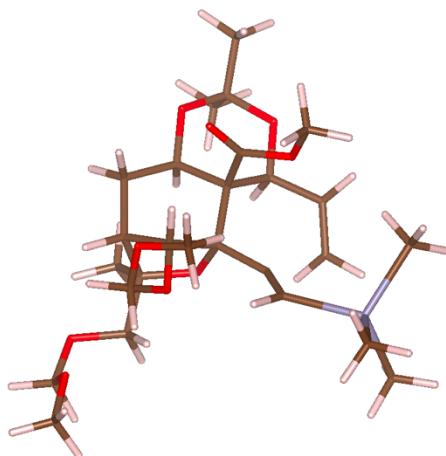
C	-0.509000	-2.404200	-1.972700
C	-0.083100	-1.171800	0.047900
C	-1.200100	-1.927000	-0.709200
C	-1.697600	-3.154400	0.014600
C	-2.041000	-2.848900	1.482500
C	-0.908800	-1.948700	2.097900
C	-0.777000	-0.608400	1.297100
O	0.872500	-2.135400	0.566000
C	0.518600	-2.529000	1.920100
C	0.680500	-4.042800	2.092600
C	1.550700	-1.858400	2.850700
O	1.153500	-2.110700	4.206300
C	1.820300	-1.338800	5.141300
O	1.362000	-0.001100	5.062700
C	2.089200	0.880100	5.894400
O	-0.009200	0.408400	1.931800
C	-0.677300	1.071900	2.989500
O	-1.892100	1.655000	2.604700
C	-1.756700	2.656200	1.603100
C	0.541000	-0.342800	-1.124300
C	0.496900	1.122200	-1.050300
O	-2.720900	-3.712600	-0.823300
O	-1.512200	-2.964000	-2.815800
H	-2.127700	-3.777000	2.058100
H	-2.994400	-2.324700	1.556900
H	-1.126500	-1.774400	3.153500
H	-1.760100	-0.197200	1.076400
H	-0.858500	-3.852300	0.030100
H	0.738200	1.523600	-0.067600
H	-0.915500	0.387100	3.808000
H	0.045800	1.822500	3.335300
H	-2.741100	3.115300	1.481700
H	-1.433600	2.230100	0.646200
H	-1.032600	3.429300	1.905200
H	1.662000	1.876400	5.755700
H	2.006700	0.604000	6.958400
H	3.157900	0.909800	5.625800
H	2.916800	-1.362800	4.982300
H	1.589400	-1.766500	6.128900
H	2.539400	-2.305400	2.665200
H	1.596900	-0.789900	2.656800
H	0.612100	-4.287800	3.156700
H	1.674300	-4.334700	1.736500
H	-0.056200	-4.639600	1.555000
C	-2.336800	-0.959700	-1.134300



O -3.397700 -0.991300 -0.300500
O -2.306500 -0.217100 -2.092700
C -4.469300 -0.091600 -0.625800
H -4.129200 0.946200 -0.564600
H -5.244600 -0.285900 0.115600
H -4.838900 -0.287100 -1.635800
H 0.212400 -3.186000 -1.700800
C 0.279800 -1.161800 -2.414100
H -0.013100 -0.660400 -3.326600
C 1.677200 -1.052100 -1.891000
H 2.143100 -1.910900 -1.416300
H 2.364100 -0.390900 -2.413300
Sn -0.126600 2.525100 -2.552800
C -0.007600 1.720900 -4.576000
C -2.187500 3.152000 -2.185100
C 1.173400 4.273900 -2.368400
H 0.938600 1.196000 -4.737100
H -0.083000 2.534700 -5.304000
H -2.519200 3.847000 -2.963000
H -2.279500 3.644800 -1.212600
H 2.202900 4.015900 -2.634100
H 0.831400 5.076400 -3.029700
H 1.164100 4.645400 -1.338600
H -2.814700 2.258100 -2.202700
H -0.834600 1.024400 -4.740000
C -2.268400 -4.023300 -2.166700
C -1.455900 -5.324100 -2.164600
C -3.543000 -4.142300 -2.986600
H -0.536400 -5.240800 -1.579400
H -1.180300 -5.583900 -3.190700
H -2.058800 -6.130300 -1.736800
H -3.299200 -4.380900 -4.025300
H -4.074700 -3.188000 -2.955300
H -4.184300 -4.925400 -2.572900

Transition state **TS-1**:

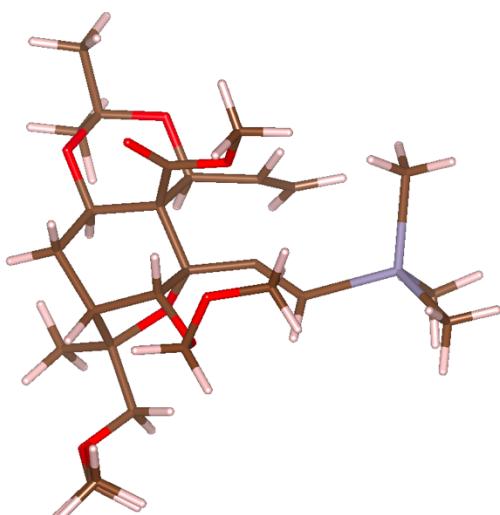
C	0.030700	-2.778600	-0.999200
C	0.487500	-0.947800	0.873200
C	-0.449700	-2.104500	0.330400
C	-0.383800	-3.300700	1.319500
C	-0.469400	-2.945300	2.801900
C	0.446500	-1.732100	3.108300
C	-0.092500	-0.557200	2.270300
O	1.783500	-1.548400	1.158400
C	1.898700	-1.856500	2.577000
C	2.582500	-3.213200	2.762400
C	2.826200	-0.779800	3.174900
O	2.912900	-1.002500	4.589800
C	3.381900	0.084400	5.305800
O	2.379300	1.083500	5.357200
C	2.825700	2.282000	5.957800
C	0.661100	0.149700	-0.121100
C	0.458900	1.447400	-0.160000
O	-1.354900	-4.270500	0.952400
O	-0.957400	-3.754100	-1.338400
C	-1.183300	-4.789100	-0.370700
C	-2.526500	-5.399500	-0.741900
C	-0.048300	-5.822400	-0.411600
H	0.448000	-1.518500	4.179500
H	0.608500	-3.727000	1.159600
Sn	0.520300	2.627400	-1.977500
C	-0.826800	1.664300	-3.401500
C	-0.200900	4.624100	-1.468200
C	2.544500	2.747900	-2.783200
C	-1.884600	-1.587700	0.190500
O	-2.072600	-0.899200	-0.953300
O	-2.760300	-1.715500	1.021700
C	-3.377500	-0.323500	-1.117600
H	0.989500	-3.258100	-0.758100
C	0.268800	-1.839600	-2.131400
C	1.338700	-1.005200	-2.034200
H	-0.179900	-3.821100	3.393100
H	-1.502000	-2.696400	3.060600
H	-1.181300	-0.552000	2.264000
H	3.509000	-3.229500	2.178400
H	2.839500	-3.340700	3.818000
H	1.972700	-4.062300	2.452000
H	3.824000	-0.879800	2.721800
H	2.431800	0.212500	2.965700
H	3.613900	-0.278600	6.318700
H	4.300400	0.506900	4.852300



H	3.136900	2.127600	7.003800
H	1.985200	2.980300	5.940900
H	3.670400	2.727300	5.406800
H	0.174300	1.972700	0.755300
H	-2.777300	-6.203600	-0.044500
H	-3.293600	-4.623600	-0.680700
H	-2.492000	-5.798100	-1.759600
H	0.920900	-5.386400	-0.154600
H	-0.259200	-6.625400	0.300500
H	0.027900	-6.243600	-1.418200
H	-1.073500	0.675900	-3.006100
H	-0.358700	1.553400	-4.384000
H	0.461000	5.092400	-0.733300
H	-1.207500	4.563200	-1.042500
H	3.186400	3.310000	-2.098600
H	2.963000	1.745100	-2.907500
H	-3.342600	0.207000	-2.069500
H	-3.594900	0.367200	-0.297600
H	-4.141700	-1.105300	-1.134600
H	2.188000	-1.256400	-1.405000
H	1.507900	-0.226300	-2.770900
H	-0.534900	-1.676400	-2.839500
H	-1.745900	2.247700	-3.513500
H	-0.237900	5.259500	-2.358400
H	2.539400	3.251300	-3.755000
O	0.354600	0.732000	2.676400
C	-0.291000	1.235200	3.830400
O	-1.684100	1.312400	3.707500
H	-0.099800	0.608400	4.705700
H	0.161800	2.225300	3.978500
C	-2.130800	2.162300	2.660700
H	-3.210200	2.275400	2.787400
H	-1.926500	1.733100	1.671100
H	-1.653200	3.153600	2.716200

Transition state **TS-2**:

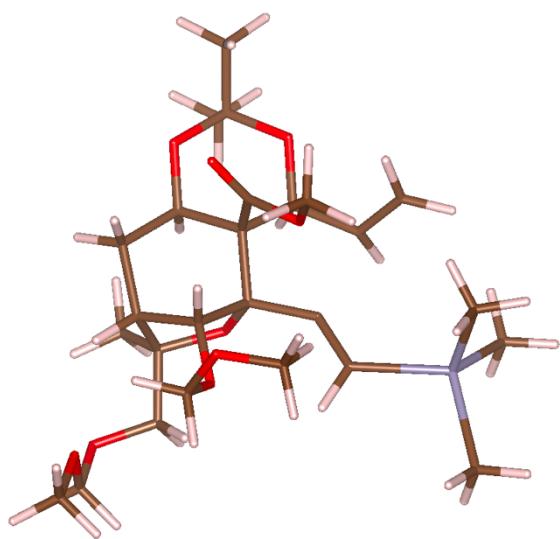
C	3.508600	-1.329100	-0.185300
C	4.495200	0.941100	-0.149800
C	4.295100	-0.351900	0.680300
C	5.642400	-1.020200	0.945700
C	6.645400	-0.030800	1.560200
C	6.627300	1.314400	0.758400
C	5.192600	1.916500	0.823100
O	5.469200	0.704700	-1.204500
C	6.798900	1.116600	-0.767500
C	7.837200	0.085600	-1.220100
C	7.111000	2.432600	-1.515000
O	8.438500	2.868900	-1.184500
C	8.567200	4.192200	-0.813300
O	8.110800	4.371800	0.519600
C	8.253200	5.708400	0.958500
C	3.177000	1.237100	-0.795200
C	2.635300	2.324400	-1.299300
O	5.425800	-2.203900	1.705200
O	3.286200	-2.495700	0.612900
C	4.493700	-3.122000	1.109600
C	4.029500	-4.009600	2.253600
C	5.168700	-3.919600	-0.014400
H	7.374800	2.006300	1.153700
H	6.022500	-1.308500	-0.036600
Sn	0.599700	2.505500	-2.011400
C	-0.692900	1.381100	-0.658800
C	0.125400	4.631200	-1.855900
C	0.389000	1.839300	-4.076100
C	3.574600	-0.049700	2.011600
O	2.399300	0.597200	1.825000
O	4.003600	-0.279200	3.120300
C	1.742300	1.028300	3.028800
H	4.143800	-1.568600	-1.050200
C	2.240600	-0.713400	-0.740000
H	7.652000	-0.461800	1.551100
H	6.379000	0.158300	2.603000
H	4.779700	1.842100	1.829300
H	7.722800	-0.085300	-2.295900
H	8.839000	0.485700	-1.041200
H	7.755300	-0.877600	-0.716900
H	7.067600	2.229600	-2.592900
H	6.375800	3.193700	-1.262900
H	9.639000	4.435200	-0.877900
H	8.002400	4.867700	-1.484500
H	9.306000	6.033800	0.944000



H	7.885700	5.752100	1.986500
H	7.666000	6.408500	0.341200
H	3.225200	3.244600	-1.252600
H	4.883600	-4.537000	2.687600
H	3.573300	-3.378600	3.020000
H	3.296600	-4.737000	1.893500
H	5.505700	-3.278100	-0.833300
H	6.040900	-4.445500	0.384800
H	4.462900	-4.648400	-0.423200
H	-0.785000	0.339300	-0.977200
H	-1.691400	1.826700	-0.619000
H	-0.910900	4.820900	-2.152000
H	0.784900	5.216700	-2.504000
H	0.822700	0.841900	-4.184100
H	-0.666600	1.804100	-4.362700
H	0.822200	1.511600	2.697700
H	2.378100	1.735600	3.569100
H	1.521900	0.174900	3.674800
C	1.797300	-1.096200	-2.002400
H	2.473400	-1.547000	-2.724200
H	0.789600	-0.879900	-2.341800
H	1.490700	-0.441600	-0.004900
H	-0.253600	1.399900	0.343100
H	0.260000	4.971600	-0.824200
H	0.913800	2.526400	-4.746200
O	5.070100	3.272400	0.412200
C	5.151000	4.188700	1.482800
O	4.093600	4.076700	2.396100
H	6.065100	4.036000	2.064600
H	5.165400	5.176500	1.000900
C	2.808700	4.292800	1.819800
H	2.102700	4.359800	2.651300
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Transition state **TS-3**:

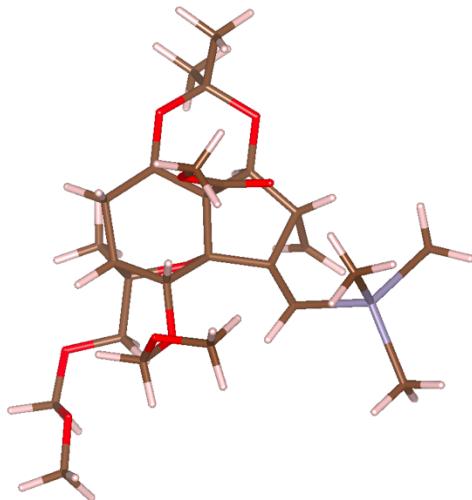
C	3.478900	-1.302100	-0.360400
C	4.420800	0.982000	-0.151900
C	4.236400	-0.366200	0.582500
C	5.591300	-1.032500	0.815700
C	6.569300	-0.072100	1.509400
C	6.541500	1.322700	0.797400
C	5.098800	1.898400	0.890400
O	5.406100	0.835900	-1.214200
C	6.727700	1.231200	-0.737100
C	7.783600	0.247100	-1.249800
C	7.029500	2.599200	-1.389600
O	8.347700	3.029100	-1.016500
C	8.454800	4.325400	-0.554100
O	7.984100	4.406800	0.783400
C	8.101900	5.712400	1.313600
C	3.100400	1.306000	-0.784000
C	2.560900	2.419200	-1.231400
O	5.391700	-2.269100	1.488400
O	3.258600	-2.513100	0.364700
C	4.467000	-3.156800	0.838000
C	3.998700	-4.106800	1.928900
C	5.156500	-3.886900	-0.322300
H	7.276300	1.996200	1.244500
H	5.985800	-1.244200	-0.180500
Sn	0.524700	2.640000	-1.929000
C	-0.757000	2.453100	-0.172000
C	0.351100	4.648500	-2.763800
C	0.023500	1.167300	-3.456800
C	3.495300	-0.163100	1.921600
O	2.388800	0.598000	1.771400
O	3.858300	-0.558500	3.007200
C	1.700800	0.937700	2.985500
H	4.149100	-1.482500	-1.211700
C	2.223500	-0.662100	-0.940600
H	7.582300	-0.487300	1.490600
H	6.282900	0.044500	2.558300
H	4.680500	1.751500	1.886300
H	7.675700	0.143600	-2.334900
H	8.778200	0.650700	-1.041200
H	7.716200	-0.747600	-0.809500
H	6.999200	2.469800	-2.479200
H	6.281600	3.331700	-1.093800
H	9.523600	4.586500	-0.591400
H	7.886500	5.037900	-1.182900
H	9.149500	6.053700	1.331700



H	7.724600	5.680300	2.338500
H	7.509200	6.444000	0.739700
H	3.153300	3.334800	-1.141100
H	4.852500	-4.651300	2.341600
H	3.532800	-3.518800	2.723000
H	3.273800	-4.818600	1.524000
H	5.500800	-3.197600	-1.098500
H	6.026500	-4.431300	0.056200
H	4.459000	-4.594000	-0.780500
H	-0.635100	3.332400	0.468600
H	-0.452000	1.562900	0.384600
H	0.646600	5.394000	-2.018900
H	-0.680200	4.851900	-3.068000
H	-1.009000	1.308300	-3.791300
H	0.689900	1.288000	-4.315800
H	0.821200	1.499000	2.668400
H	2.344800	1.554100	3.619500
H	1.412200	0.036200	3.531900
H	2.220200	-0.601400	-2.027300
C	0.981600	-0.830400	-0.337200
H	0.063300	-0.604500	-0.868900
H	0.892600	-1.159500	0.690300
H	-1.811900	2.362600	-0.448200
H	0.999900	4.753800	-3.638600
H	0.131200	0.150700	-3.070700
O	4.960700	3.276900	0.570100
C	5.019900	4.120600	1.699900
O	3.949900	3.942500	2.587400
H	5.926600	3.935000	2.283900
H	5.035100	5.138300	1.285100
C	2.673300	4.196400	2.007000
H	1.953000	4.196200	2.828800
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Transition state **TS-4**:

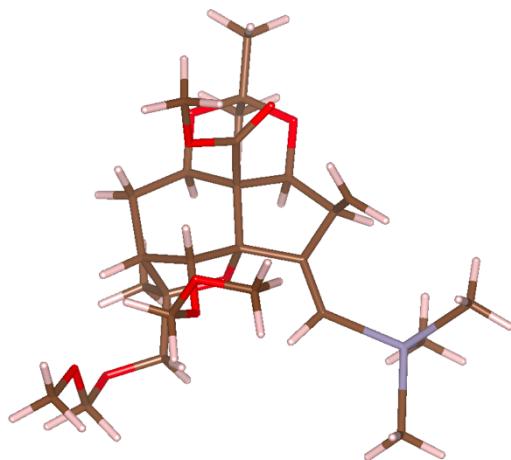
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C	-0.150900	-1.136800	0.054300
C	-1.283300	-1.925100	-0.649200
C	-1.689500	-3.184300	0.076000
C	-1.949900	-2.923500	1.569300
C	-0.812400	-1.993900	2.130400
C	-0.795300	-0.633800	1.354000
O	0.881700	-2.062300	0.483200
C	0.623800	-2.508000	1.846200
C	0.862400	-4.016600	1.963200
C	1.676800	-1.813100	2.733800
O	1.426900	-2.187700	4.097000
C	1.945100	-1.309100	5.031300
O	1.162300	-0.128400	5.052500
C	1.703100	0.876400	5.886300
O	-0.056900	0.416100	1.968500
C	-0.763300	1.091000	2.993500
O	-1.979600	1.644000	2.570600
C	-1.852000	2.616500	1.538900
C	0.296600	-0.253600	-1.131900
C	0.436700	1.122300	-1.034700
O	-2.740400	-3.762100	-0.713200
O	-1.670900	-2.933300	-2.755900
H	-1.965900	-3.866600	2.126400
H	-2.915100	-2.436200	1.715900
H	-0.960900	-1.848100	3.202800
H	-1.809300	-0.274200	1.193900
H	-0.826700	-3.850600	0.024700
H	0.576800	1.505600	-0.027400
H	-1.009900	0.417700	3.819300
H	-0.062800	1.864100	3.337900
H	-2.829100	3.095800	1.437500
H	-1.570100	2.160100	0.582800
H	-1.101500	3.379700	1.798300
H	1.033300	1.737800	5.824300
H	1.764500	0.550300	6.937300
H	2.709900	1.183300	5.558700
H	2.998600	-1.048600	4.808800
H	1.897700	-1.817400	6.006400
H	2.676700	-2.159300	2.433100
H	1.615800	-0.734000	2.613900
H	0.851900	-4.299200	3.019800
H	1.851800	-4.250800	1.555800
H	0.130400	-4.628900	1.436800
C	-2.472700	-0.992800	-0.994800



O -3.485500 -1.065900 -0.105800
O -2.510700 -0.237300 -1.942600
C -4.588200 -0.179400 -0.357000
H -4.254300 0.861900 -0.330700
H -5.304100 -0.375000 0.441400
H -5.029400 -0.387500 -1.335300
H 0.108100 -3.123000 -1.729600
C 0.113600 -1.087200 -2.405200
H -0.295400 -0.582600 -3.276700
C 1.586500 -1.172800 -2.269300
H 2.052000 -1.983800 -1.723700
H 2.220500 -0.430700 -2.738800
Sn 0.087900 2.572100 -2.582200
C 0.438900 1.772500 -4.583100
C -2.002400 3.182000 -2.399300
C 1.390100 4.290000 -2.228400
H 1.317700 1.121100 -4.593800
H 0.602900 2.590800 -5.291100
H -2.309300 3.809500 -3.241800
H -2.153500 3.742400 -1.470900
H 2.438800 4.007700 -2.361800
H 1.154300 5.100800 -2.924700
H 1.257800 4.660100 -1.206700
H -2.613300 2.275800 -2.374700
H -0.430000 1.195400 -4.912500
C -2.357100 -4.029600 -2.088000
C -1.506100 -5.303300 -2.161800
C -3.672600 -4.171100 -2.836000
H -0.556800 -5.202600 -1.629300
H -1.283300 -5.533100 -3.207600
H -2.057700 -6.136900 -1.717600
H -3.482200 -4.379300 -3.892300
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Transition state **TS-5**:

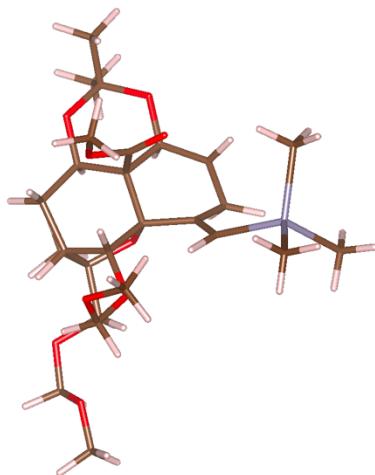
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C	-1.787100	-2.005900	-0.737000
C	-1.564700	-3.333000	-0.034000
C	-1.676800	-3.179500	1.496600
C	-0.850200	-1.917800	1.957000
C	-1.364600	-0.610000	1.252300
O	0.467900	-1.500900	0.067300
C	0.607100	-1.964900	1.438500
C	1.318700	-3.324100	1.461400
C	1.556200	-0.970800	2.149500
O	1.777200	-1.392200	3.504600
C	1.557400	-0.442300	4.481500
O	0.164200	-0.287700	4.713300
C	-0.105400	0.644900	5.741200
O	-0.819300	0.601900	1.773200
C	-1.678700	1.257600	2.676300
O	-2.863900	1.713600	2.084300
C	-2.649200	2.622300	1.007600
C	-0.599100	0.025800	-1.348600
C	0.227300	1.133100	-1.229000
O	-2.445800	-4.248100	-0.702600
O	-1.980400	-3.130800	-2.850900
H	-1.283900	-4.071300	1.996400
H	-2.716400	-3.066000	1.802500
H	-0.887200	-1.824600	3.044500
H	-2.445100	-0.530200	1.287700
H	-0.540900	-3.632600	-0.249500
H	0.418500	1.453400	-0.207100
H	-1.987900	0.588700	3.486100
H	-1.079900	2.088700	3.076700
H	-3.635100	2.983300	0.704700
H	-2.157200	2.135300	0.157600
H	-2.034500	3.478700	1.327700
H	-1.190600	0.692500	5.858500
H	0.342200	0.337700	6.700300
H	0.268700	1.651700	5.491500
H	1.990400	0.539500	4.208900
H	2.048500	-0.810300	5.395800
H	2.518500	-0.989200	1.621900
H	1.148500	0.035700	2.115800
H	1.572300	-3.576000	2.494900
H	2.249700	-3.243400	0.890100
H	0.740900	-4.146100	1.039900
C	-3.327100	-1.767300	-0.779000



O -3.894500 -1.701500 0.448900
O -4.013500 -1.709300 -1.775000
C -5.326700 -1.579300 0.459000
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H -5.782900 -2.448800 -0.021300
H -0.195100 -2.547700 -2.013400
C -0.987200 -0.725200 -2.639700
C -2.070600 0.280700 -2.652500
C -3.415800 -4.992500 -2.718000
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H 0.542400 3.733600 -4.910500
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H 3.146300 3.271800 -1.043700
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H 3.247700 1.292600 -4.546000
H 3.285400 0.265300 -3.091700
H 1.812100 4.422400 -1.277600
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H -0.264700 -0.661400 -3.457800
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C -2.156600 -4.380500 -2.127900
H -3.287300 -5.141400 -3.793600
H -3.627800 -5.953200 -2.240100
H -4.247600 -4.305000 -2.550500
H -0.010500 -4.798600 -1.934100
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H -0.770300 -5.443900 -3.393700

Transition state **TS-6**:

C	-0.516000	-2.396600	-2.004700
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C	-1.254700	-1.970200	-0.738100
C	-1.609400	-3.248400	-0.004000
C	-1.977500	-2.998700	1.465500
C	-0.952600	-1.987900	2.089000
C	-0.993600	-0.639000	1.302900
O	0.822900	-1.957900	0.539300
C	0.531700	-2.391500	1.894900
C	0.871800	-3.875400	2.063300
C	1.485200	-1.599800	2.814200
O	1.108900	-1.861500	4.173700
C	1.788400	-1.093600	5.103600
O	1.347000	0.248700	5.021400
C	2.084800	1.122800	5.851300
O	-0.355900	0.467800	1.930200
C	-1.016200	0.959300	3.081100
O	-2.355100	1.311700	2.858300
C	-2.536500	2.380800	1.940500
C	0.323900	-0.137200	-1.035300
C	-0.053800	1.223500	-1.038200
O	-2.571100	-3.924800	-0.823400
O	-1.451400	-3.094300	-2.823500
H	-1.960900	-3.939600	2.026500
H	-2.983000	-2.583800	1.547900
H	-1.184800	-1.855500	3.147000
H	-2.023300	-0.359000	1.091300
H	-0.695300	-3.845200	0.004400
H	-0.708600	1.530600	-0.229700
H	-1.029400	0.219300	3.885700
H	-0.412700	1.823400	3.388500
H	-3.568200	2.724100	2.055200
H	-2.380300	2.061400	0.901600
H	-1.852300	3.216300	2.152600
H	1.670300	2.123900	5.710100
H	1.998700	0.849800	6.915800
H	3.153800	1.138400	5.582700
H	2.884000	-1.132400	4.939200
H	1.556400	-1.515800	6.093400
H	2.515900	-1.947100	2.641300
H	1.425500	-0.536300	2.596600
H	0.847500	-4.124700	3.128500
H	1.887200	-4.051300	1.692400
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C	-2.498400	-1.152800	-1.177100



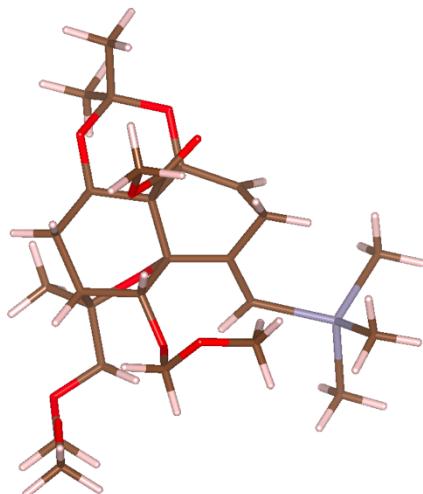
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H -5.419100 -0.712200 0.148000
H -5.095700 -0.849200 -1.615000
H 0.292500 -3.079800 -1.705600
C 0.119400 -1.135700 -2.542700
H -0.319800 -0.610200 -3.377100
C 1.400400 -0.722100 -1.925900
H 2.020000 -1.497000 -1.475700
H 1.989300 0.020200 -2.464400
Sn 0.178000 2.677900 -2.592400
C -0.857600 1.970500 -4.382500
C -0.776200 4.485800 -1.829700
C 2.272700 3.080300 -3.071700
H -0.187300 1.360500 -4.996400
H -1.215700 2.810100 -4.986200
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H -0.258400 4.838300 -0.932400
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H 2.828100 3.327900 -2.162300
H -1.818700 4.274500 -1.570800
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C -2.087200 -4.215000 -2.157500
C -1.137200 -5.419400 -2.130100
C -3.339100 -4.489400 -2.975500
H -0.228900 -5.221300 -1.554800
H -0.840000 -5.672300 -3.151800
H -1.645800 -6.276300 -1.678900
H -3.068100 -4.722700 -4.008700
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Transition state **TS-7**:

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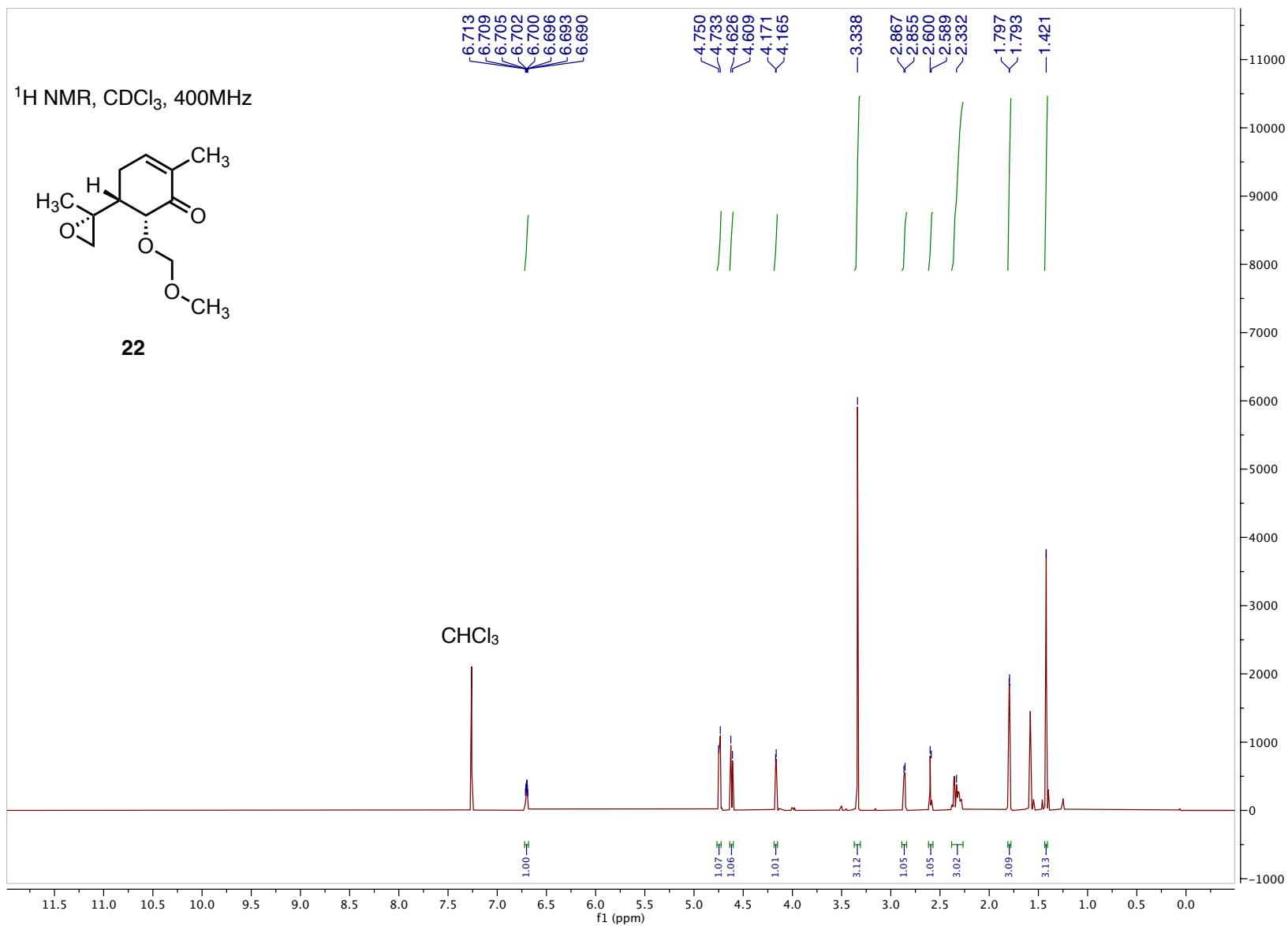
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C -1.554100 -3.440100 0.079400
C -1.734300 -3.140000 1.579600
C -0.890700 -1.872500 1.968400
C -1.329400 -0.633100 1.119300
O 0.534100 -1.674800 0.117700
C 0.589100 -2.003700 1.534100
C 1.256100 -3.371100 1.724900
C 1.529200 -0.967300 2.195900
O 1.653800 -1.240300 3.599600
C 1.371600 -0.193200 4.454600
O -0.032900 -0.031800 4.591400
C -0.366100 0.997600 5.501200
O -0.777600 0.605500 1.558500
C -1.680700 1.397900 2.289000
O -2.746300 1.876800 1.513300
C -2.325000 2.699300 0.428900
C -0.451100 -0.109500 -1.398600
C 0.709200 0.694600 -1.341700
O -2.444300 -4.389800 -0.519400
O -1.851300 -3.552100 -2.740500
H -1.401800 -3.997700 2.174100
H -2.783500 -2.966700 1.817100
H -0.979300 -1.674800 3.038400
H -2.409200 -0.527900 1.076200
H -0.535700 -3.802300 -0.050200
H 1.416000 0.441500 -0.556700
H -2.137800 0.831500 3.107800
H -1.071900 2.220800 2.690900
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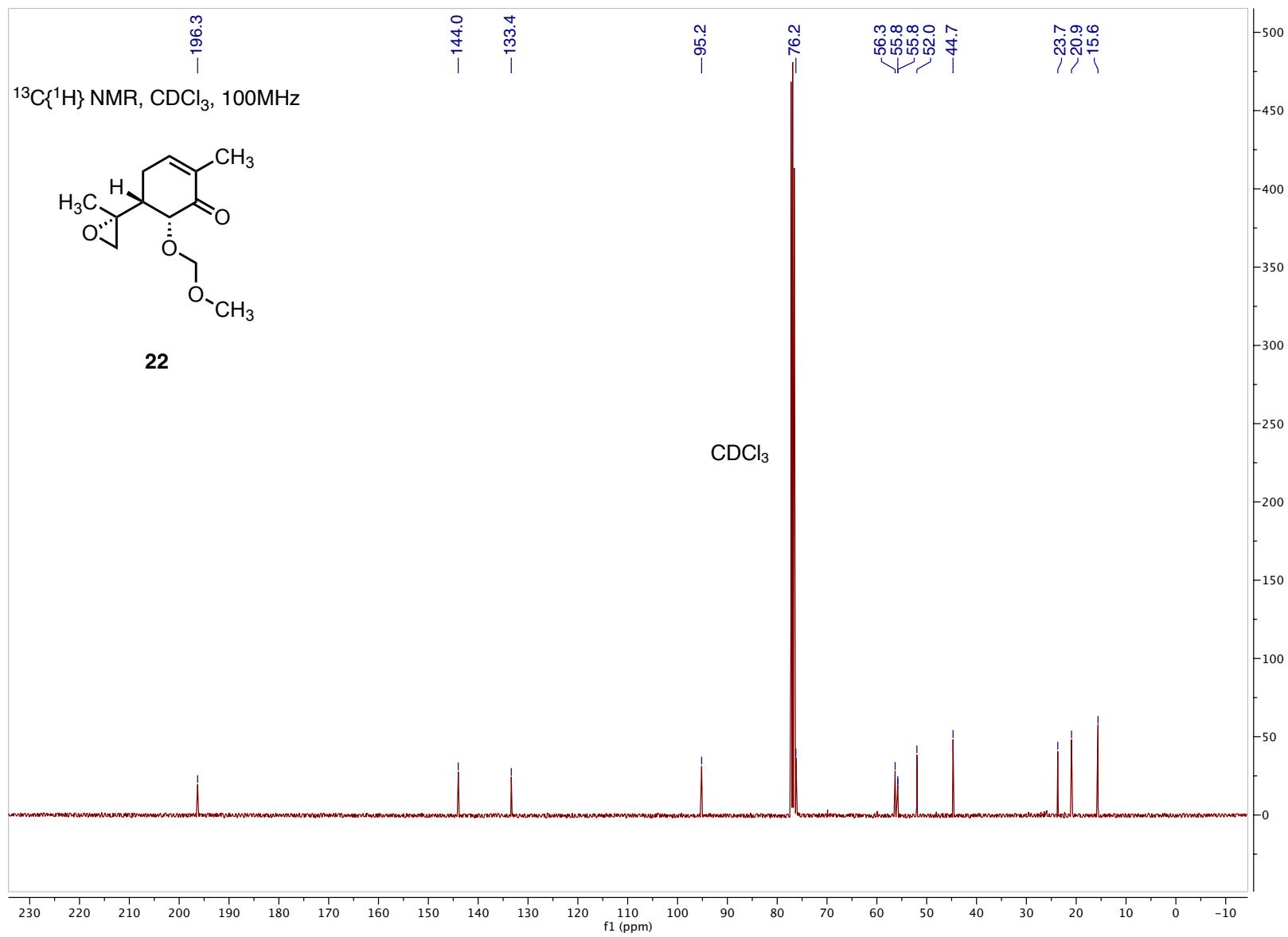
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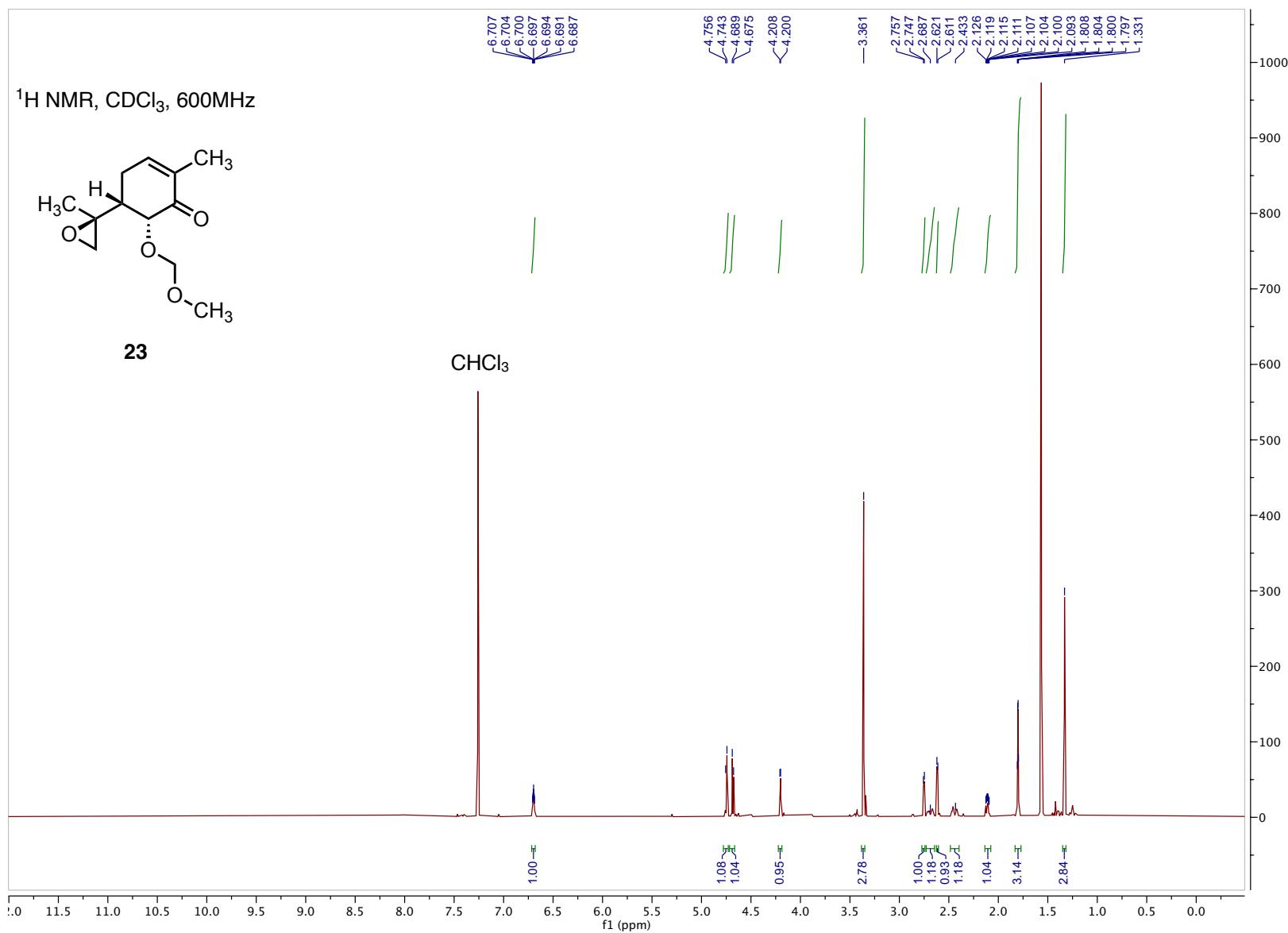


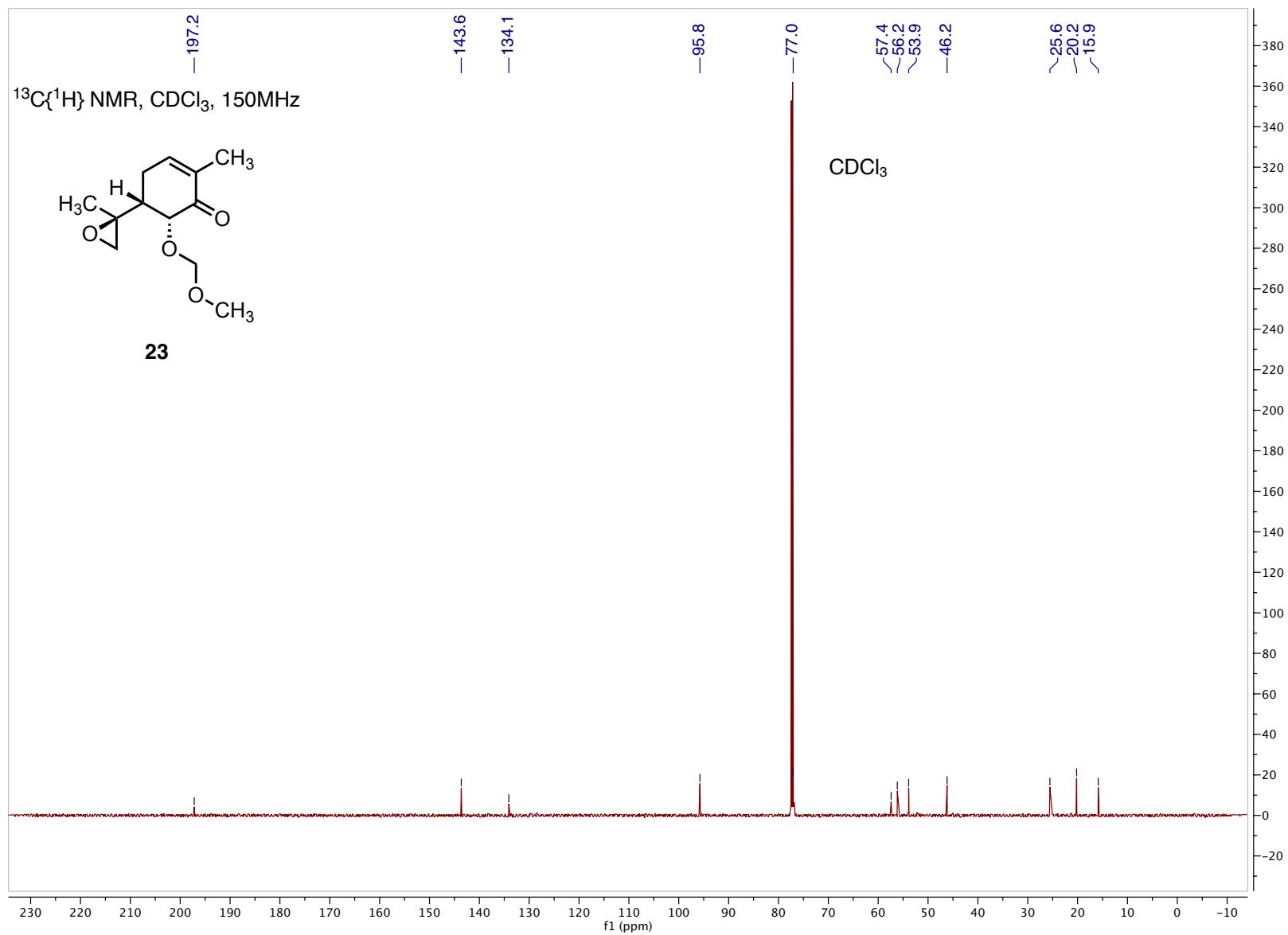
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H	-5.645300	-1.543700	1.134600
H	-5.733000	-2.439800	-0.421900
H	-0.059300	-2.949700	-1.919000
C	-0.795200	-1.222500	-2.829900
C	-1.493600	0.043000	-2.478500
C	-3.345000	-5.346300	-2.475100
C	-0.883300	-5.644700	-1.930600
Sn	1.200100	2.347100	-2.615700
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C	3.105500	3.156500	-1.934900
C	1.348300	1.711600	-4.701900
H	-1.334600	3.442100	-2.718000
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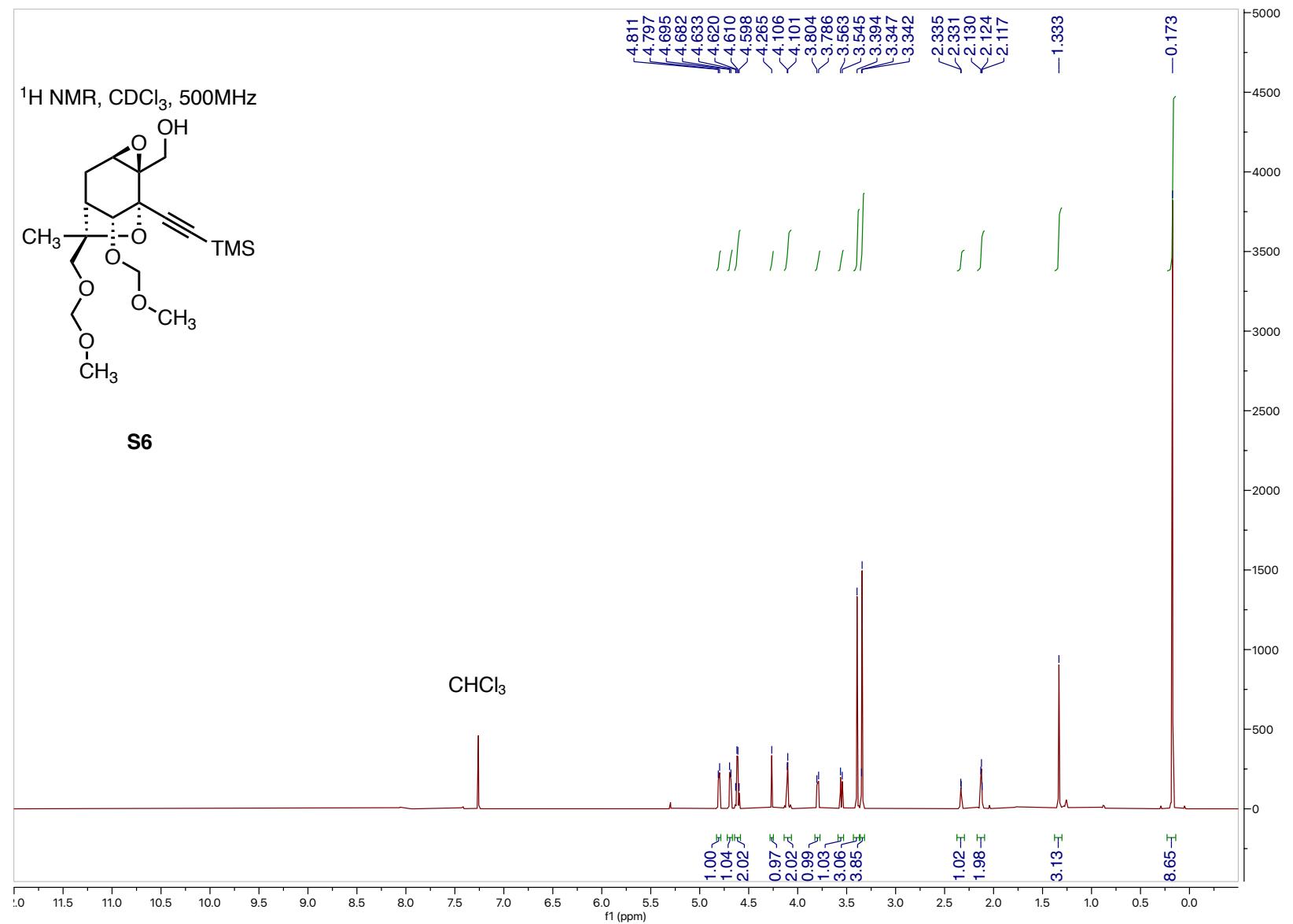
Catalog of nuclear magnetic resonance spectra.

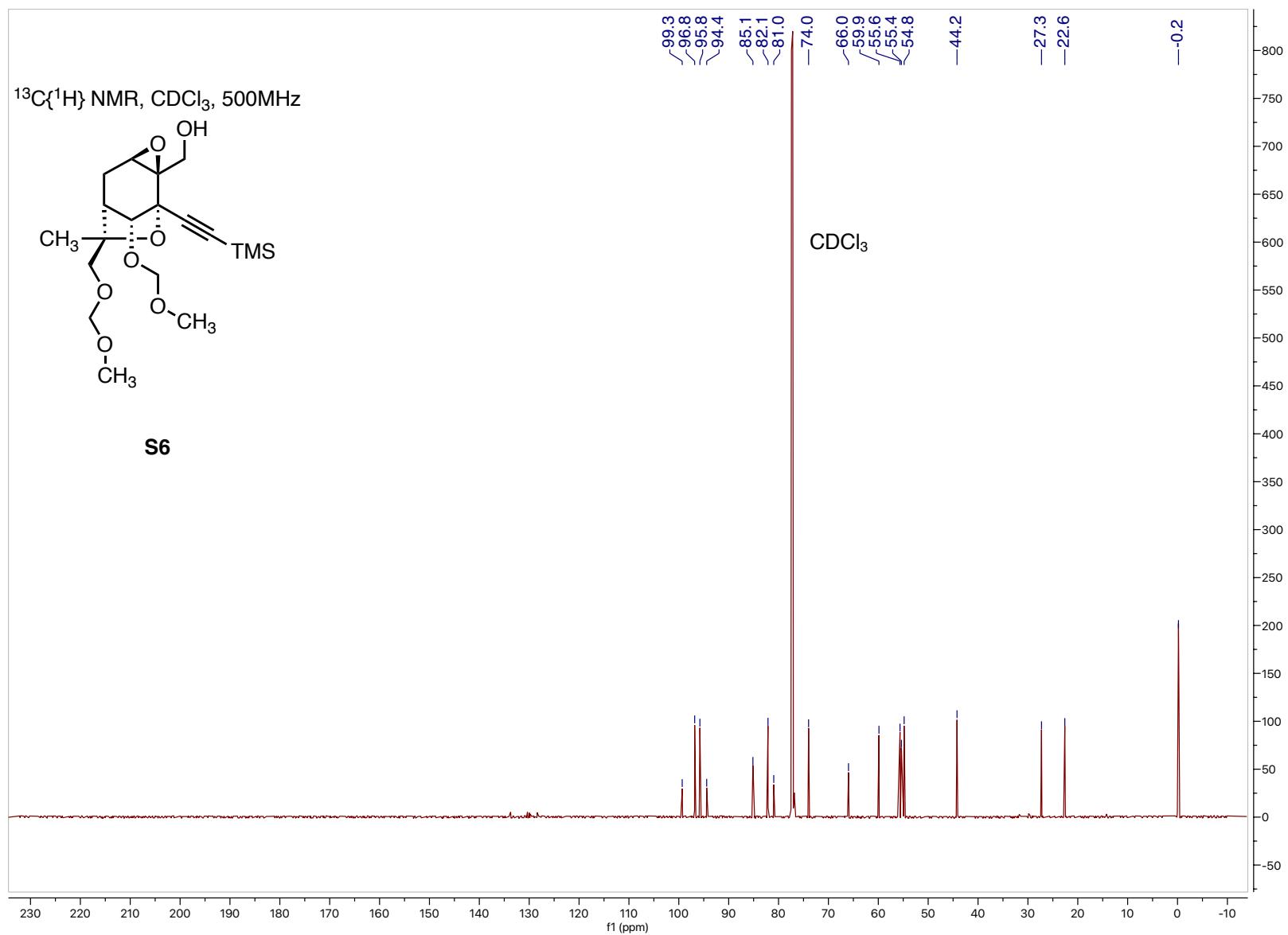


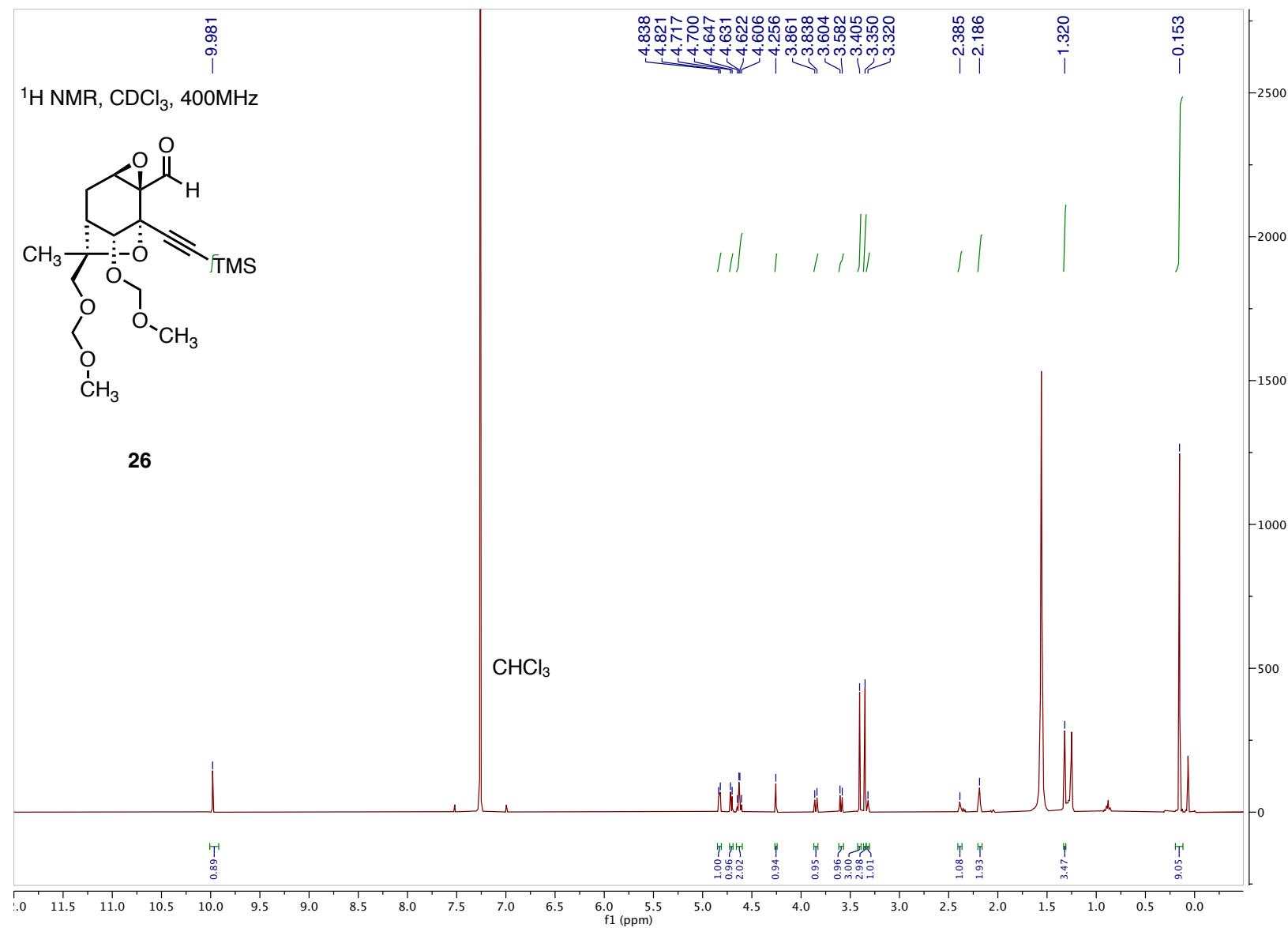


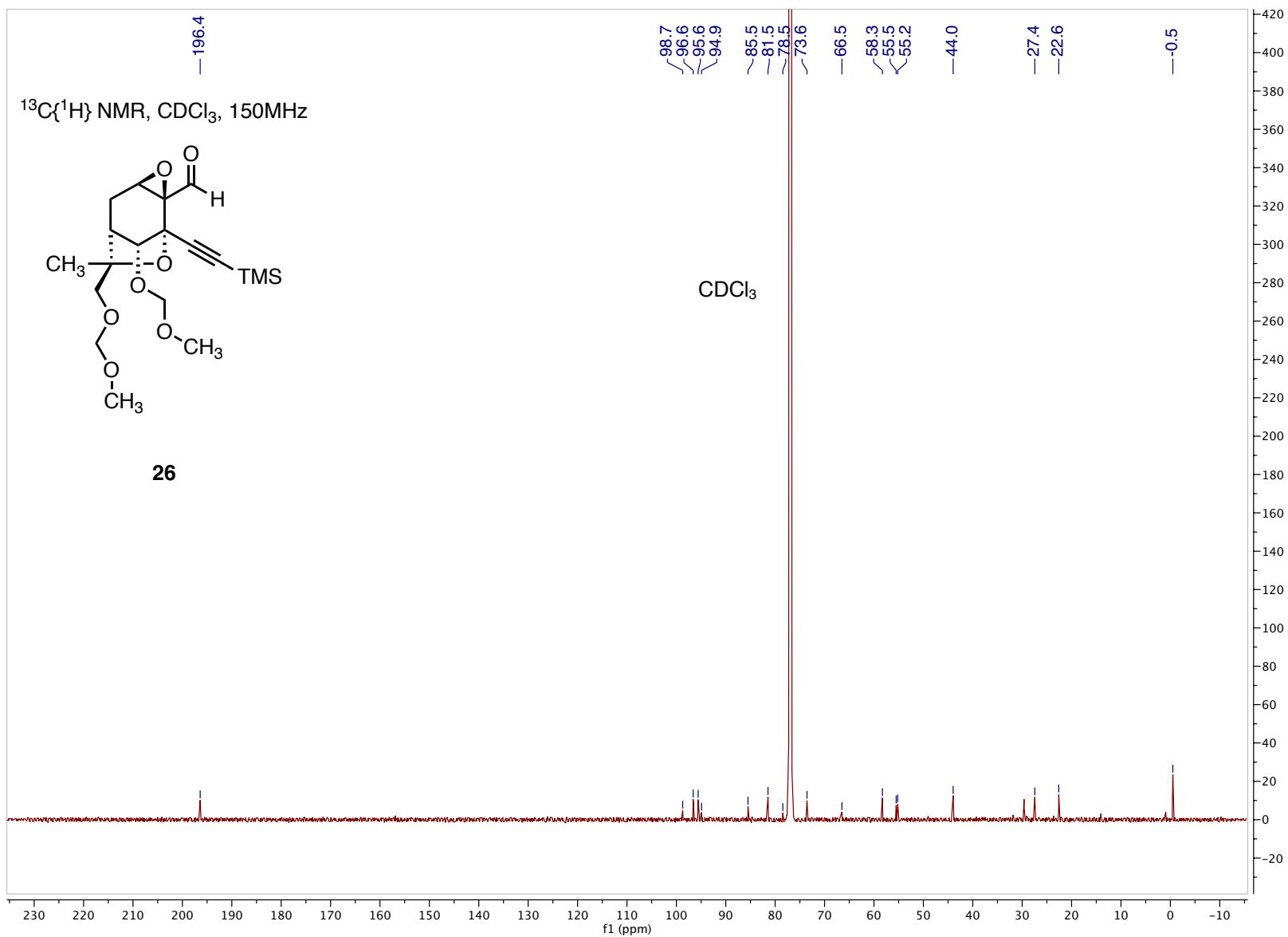


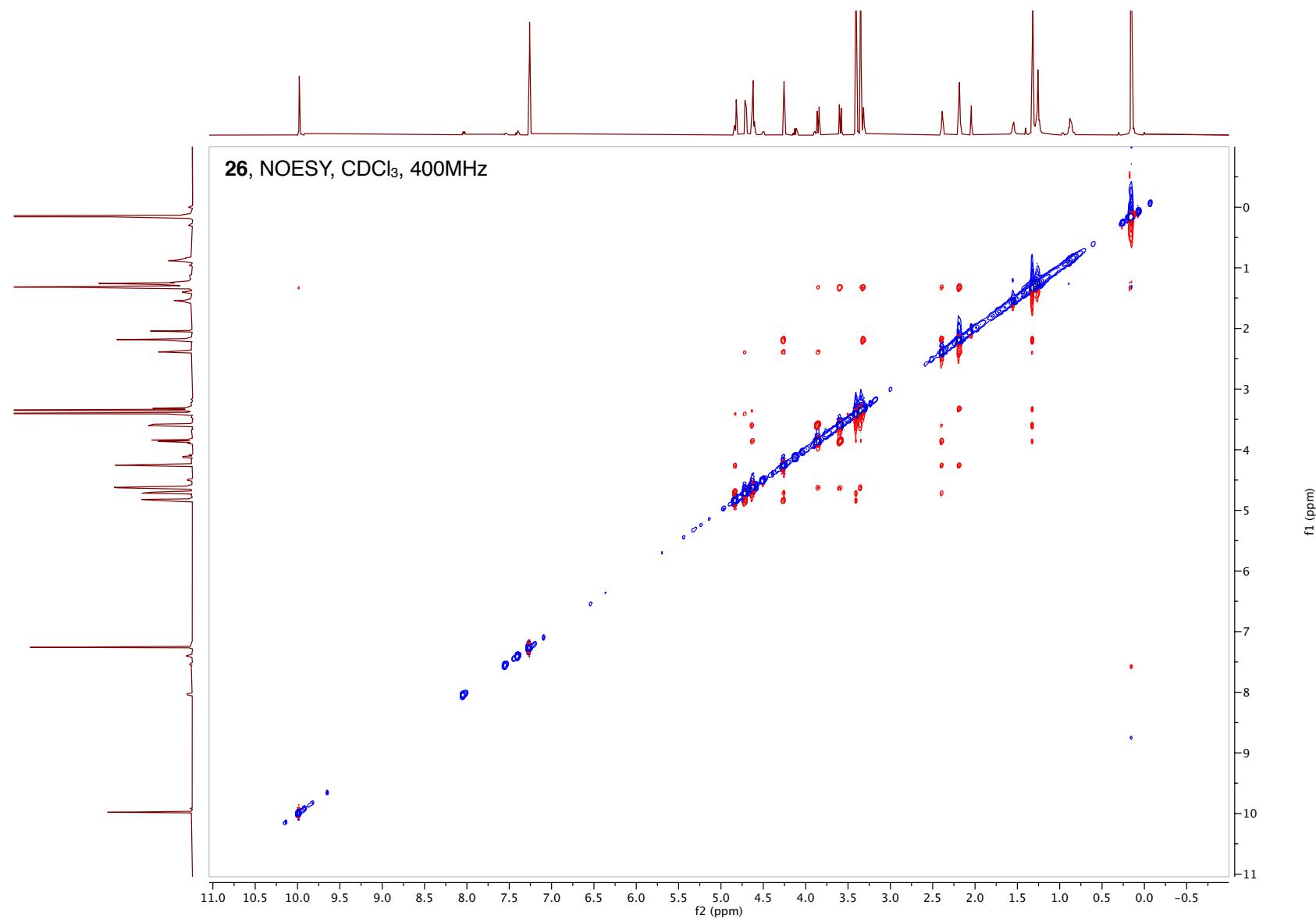


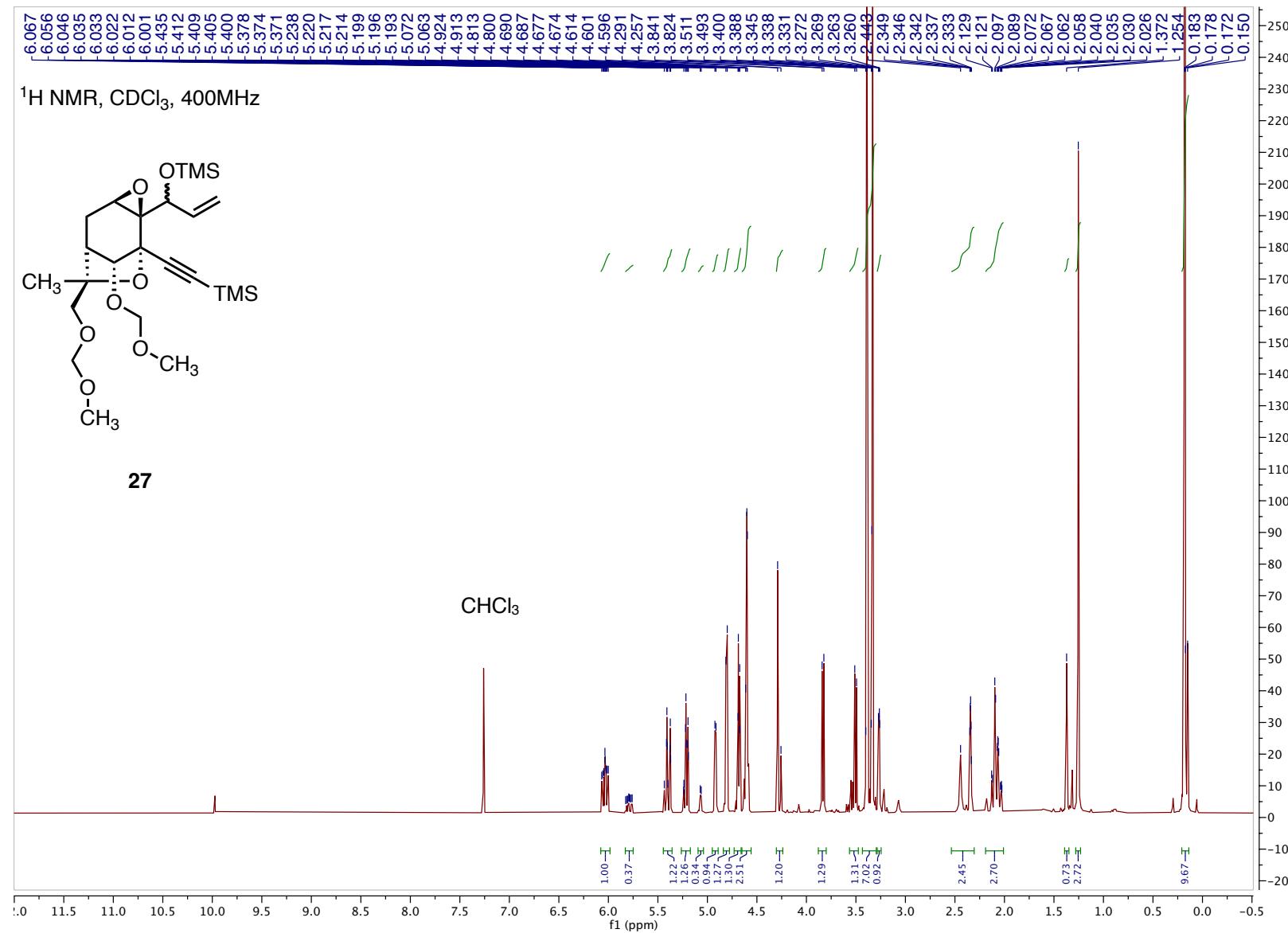


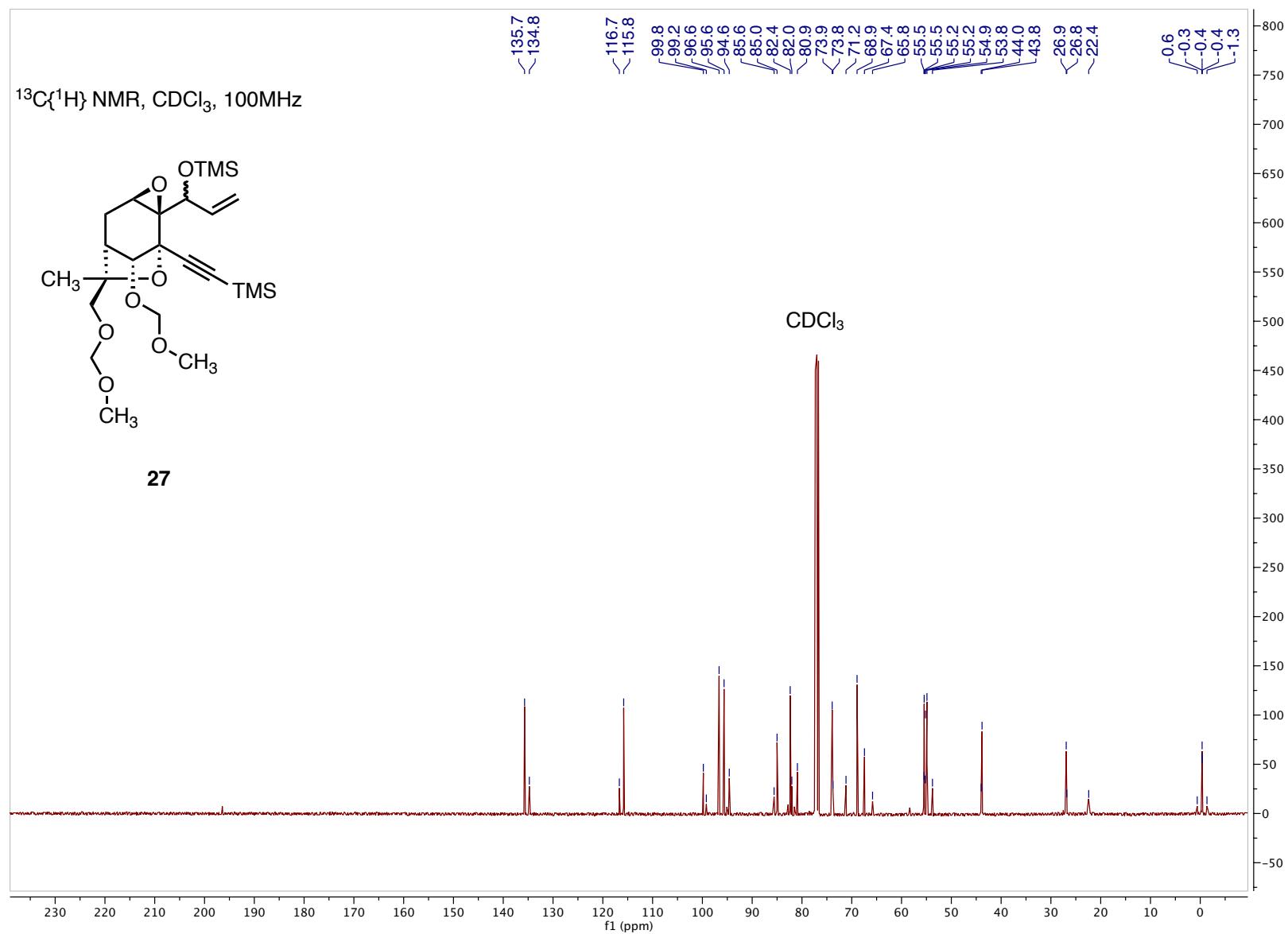


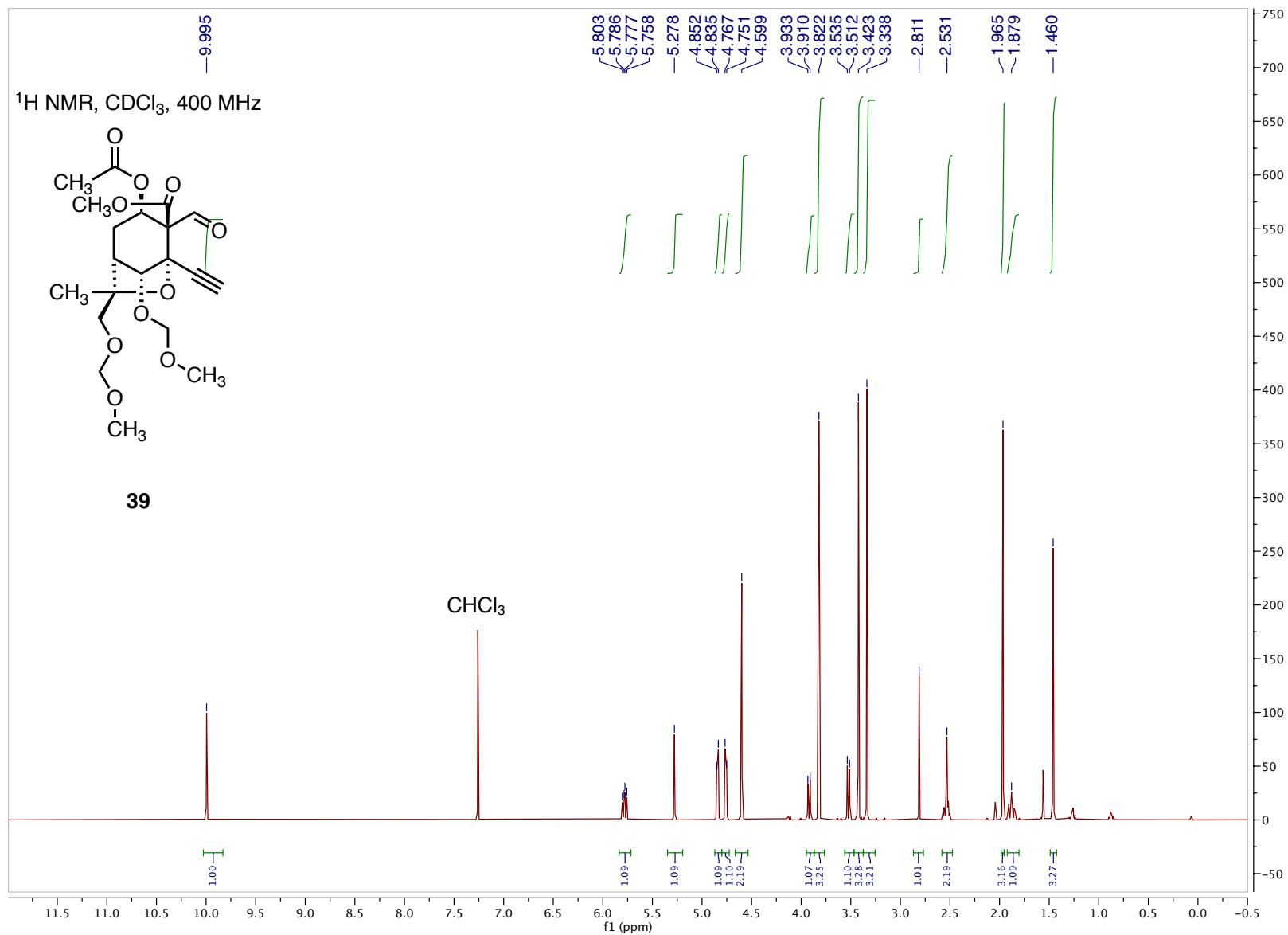


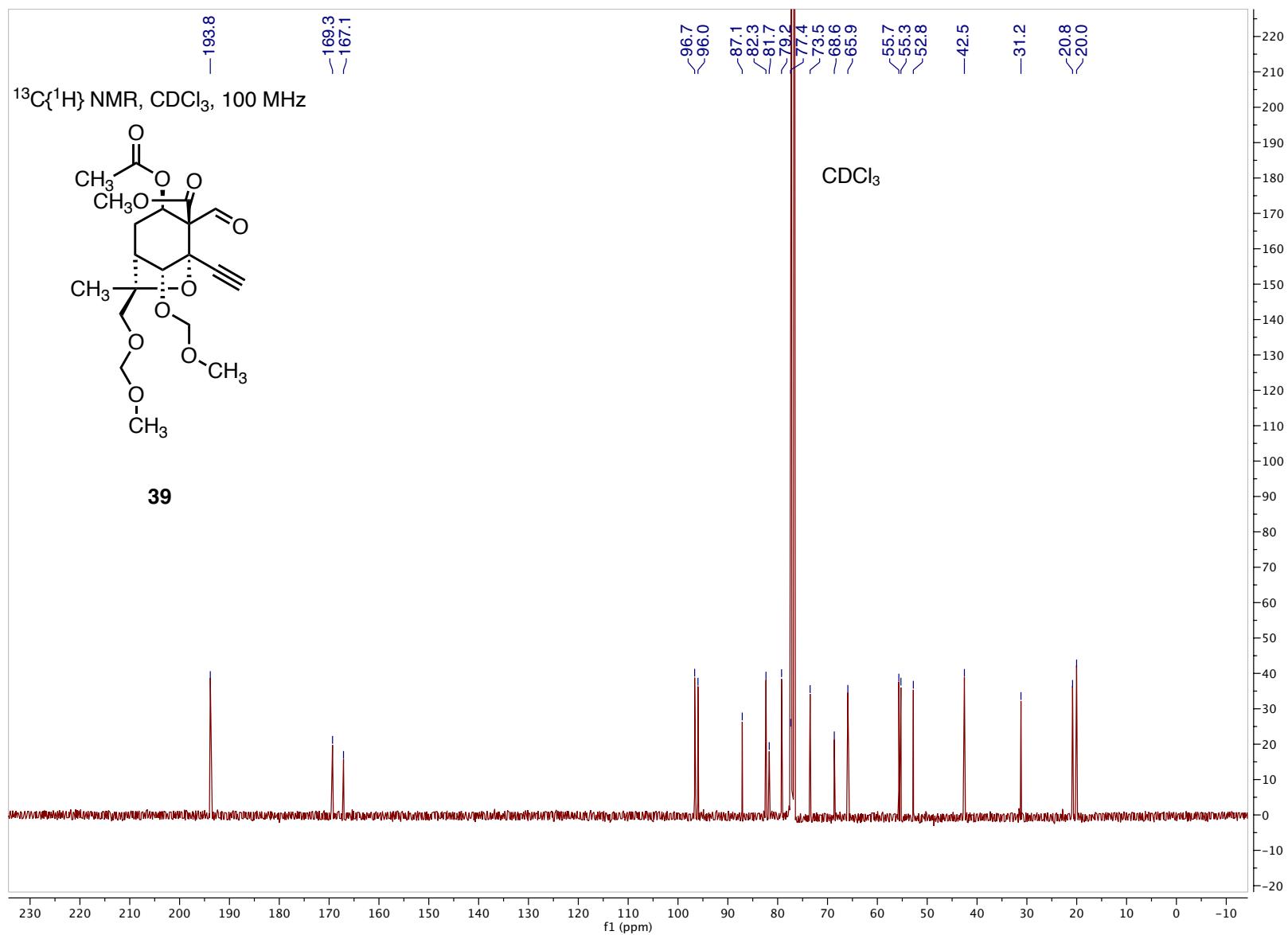


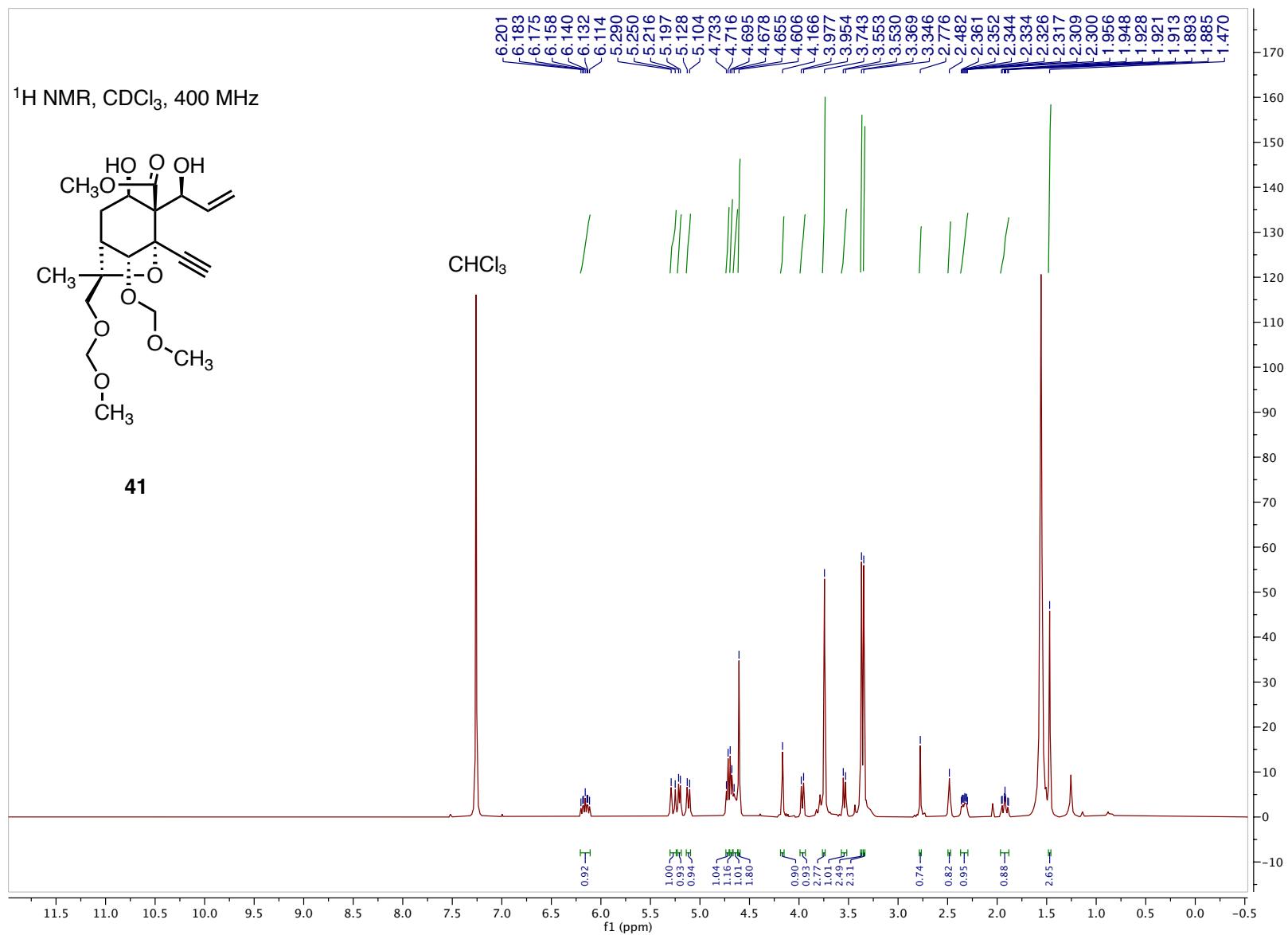


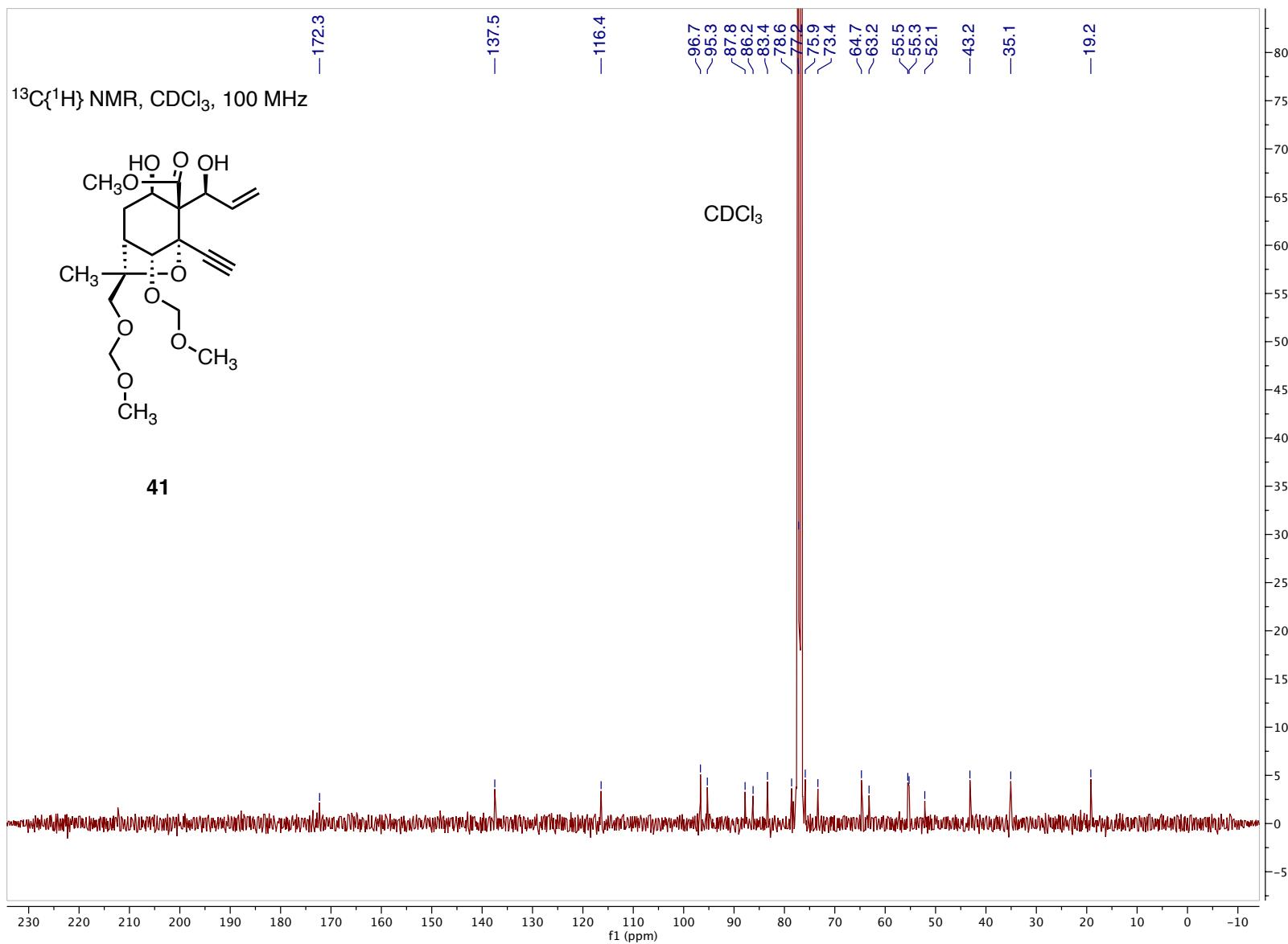


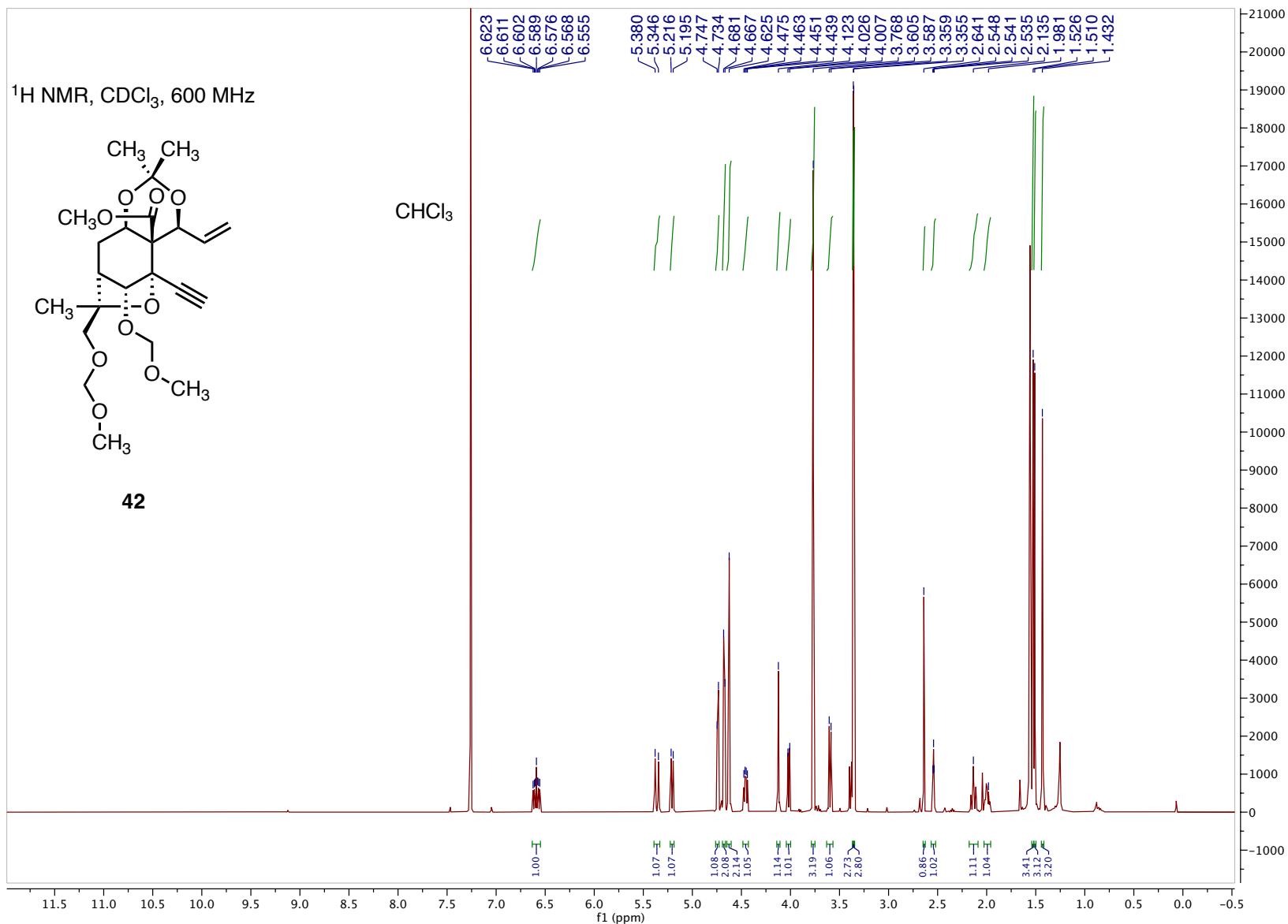


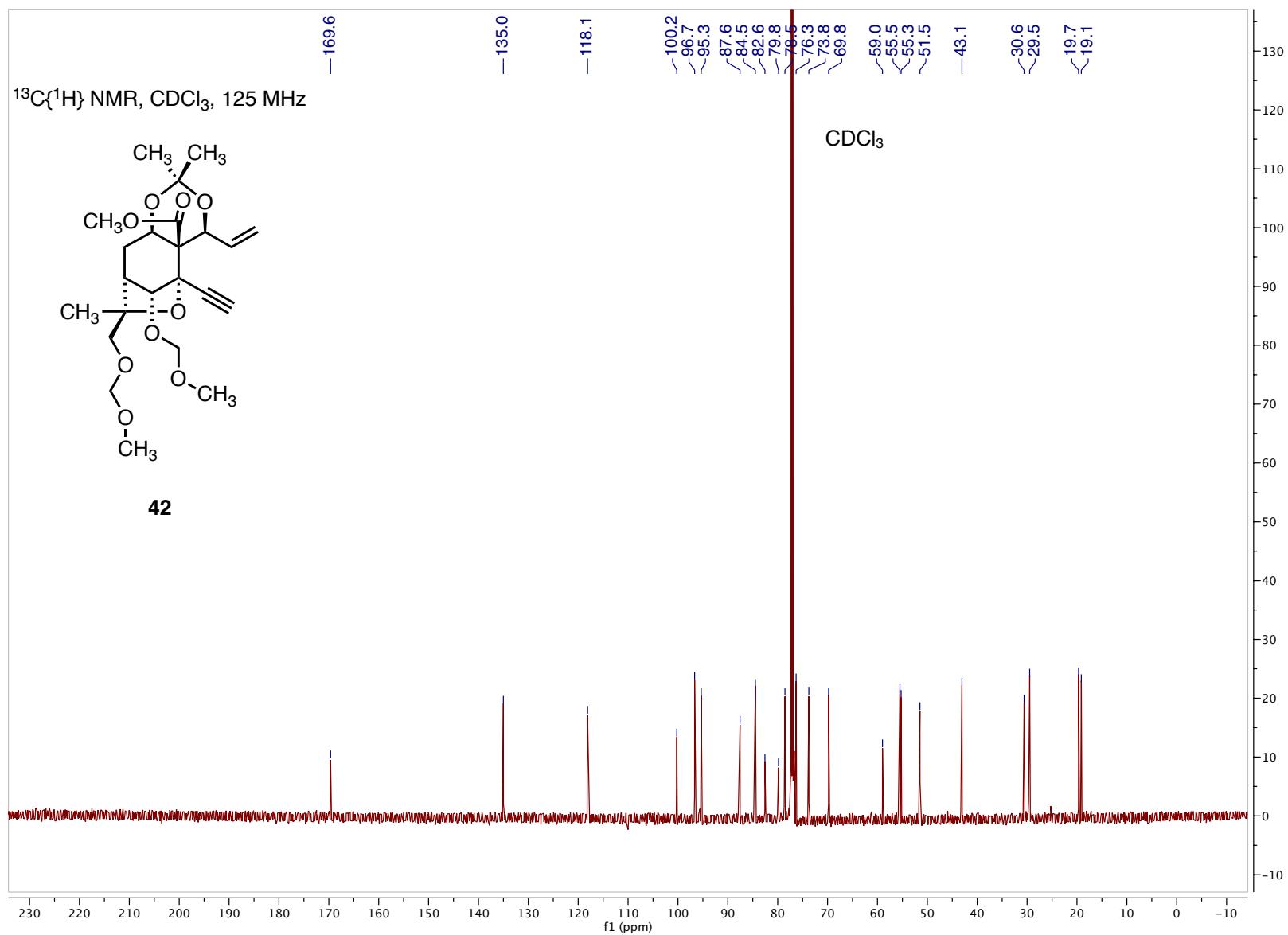


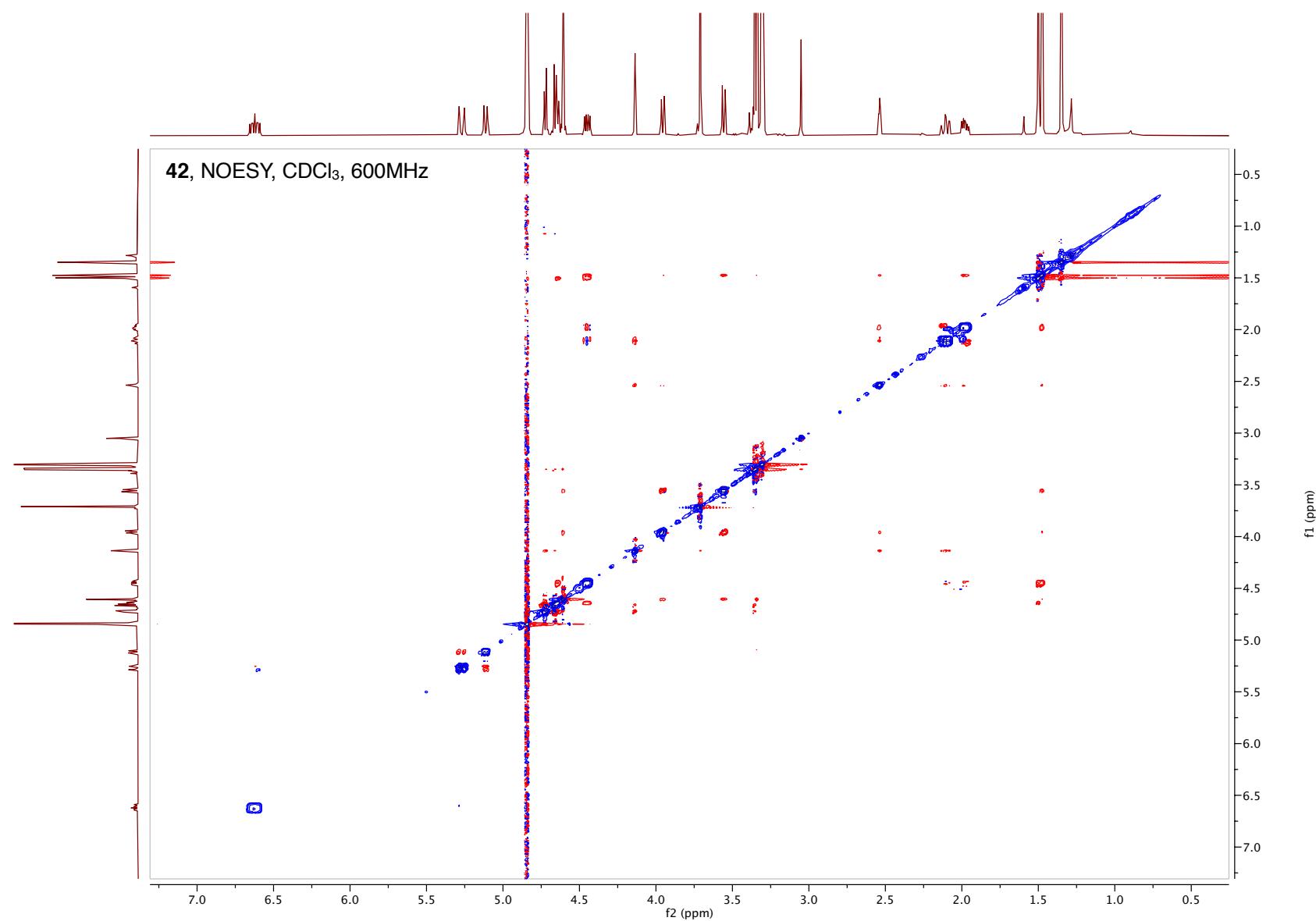


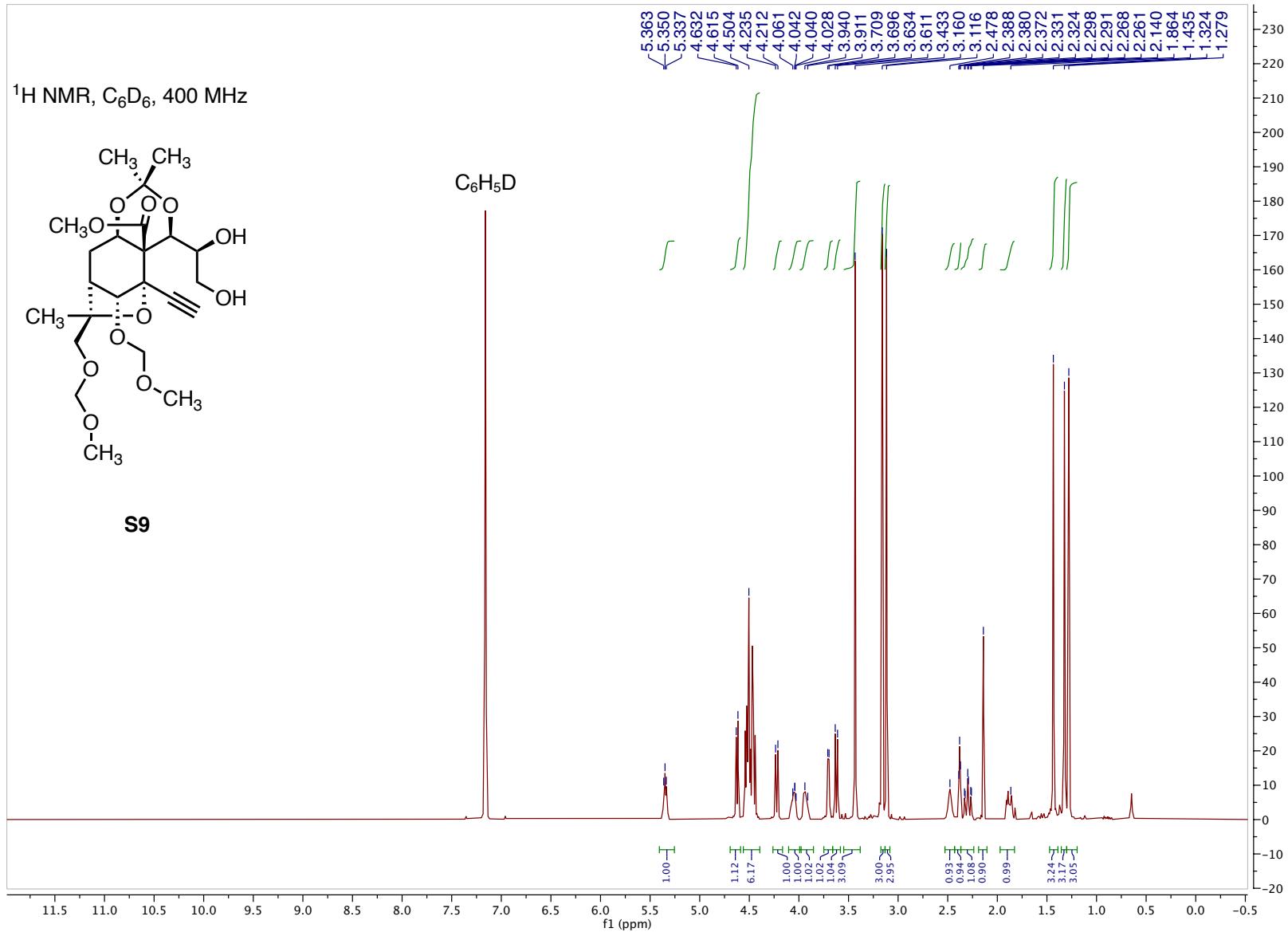


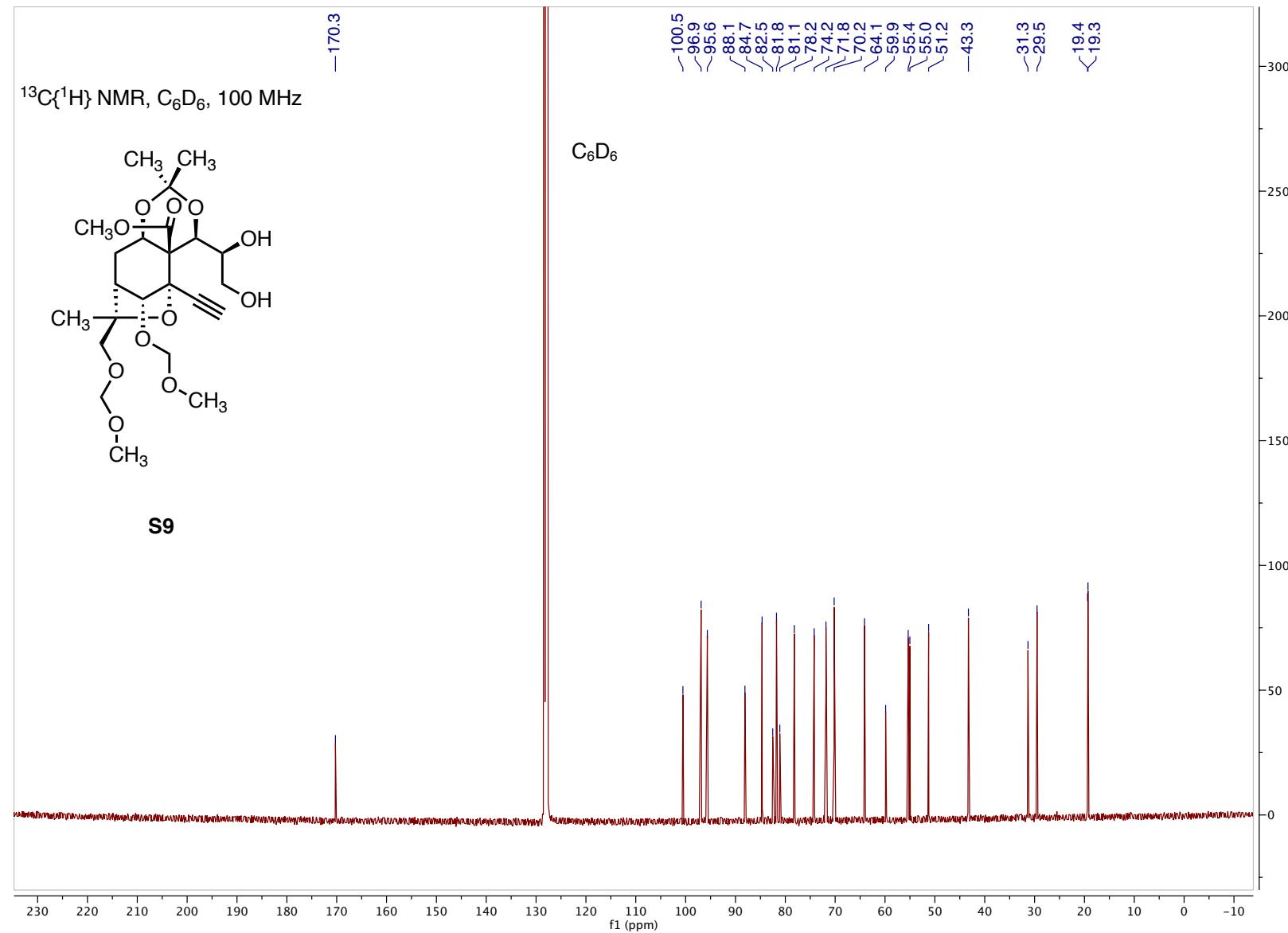


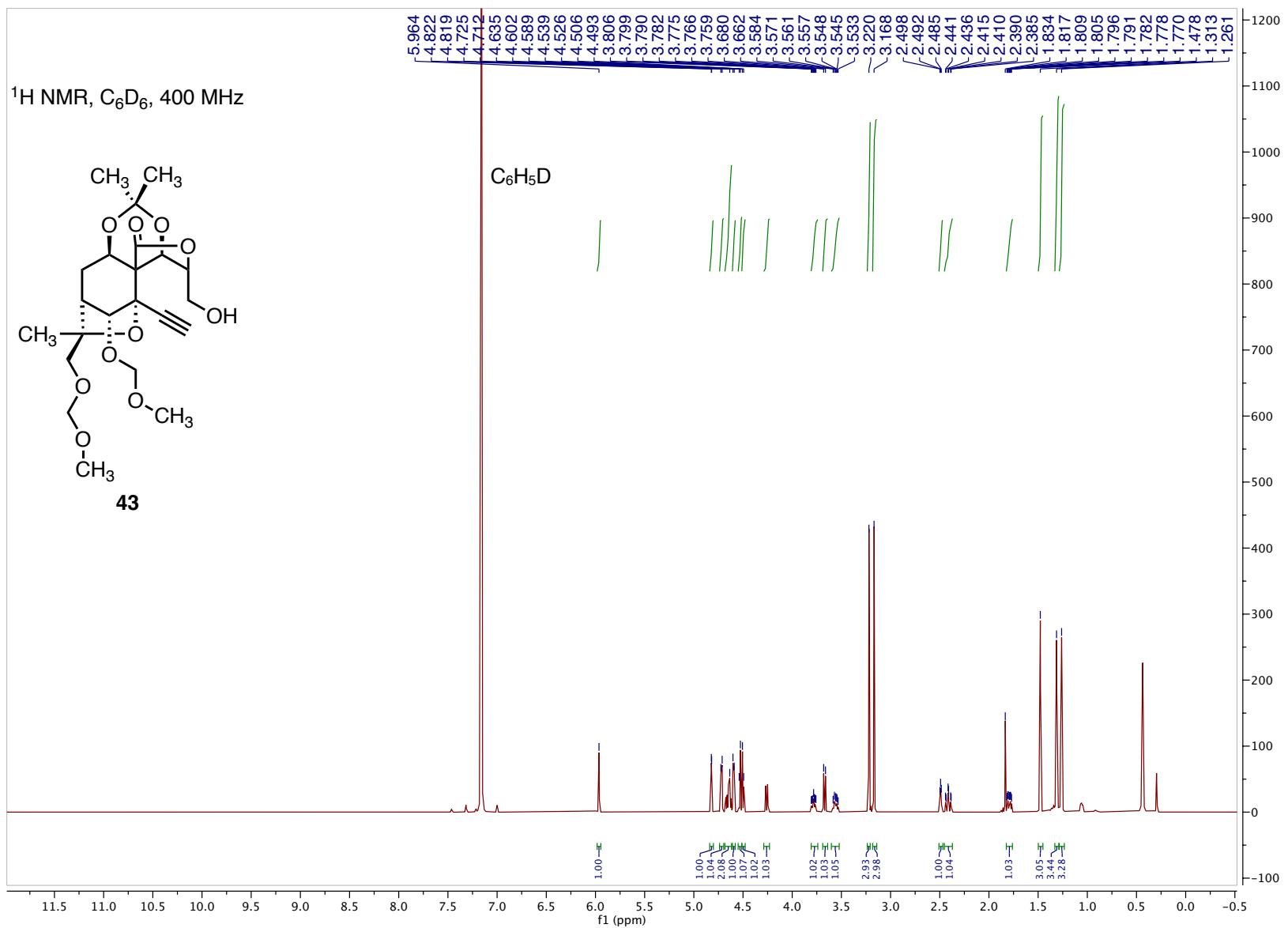


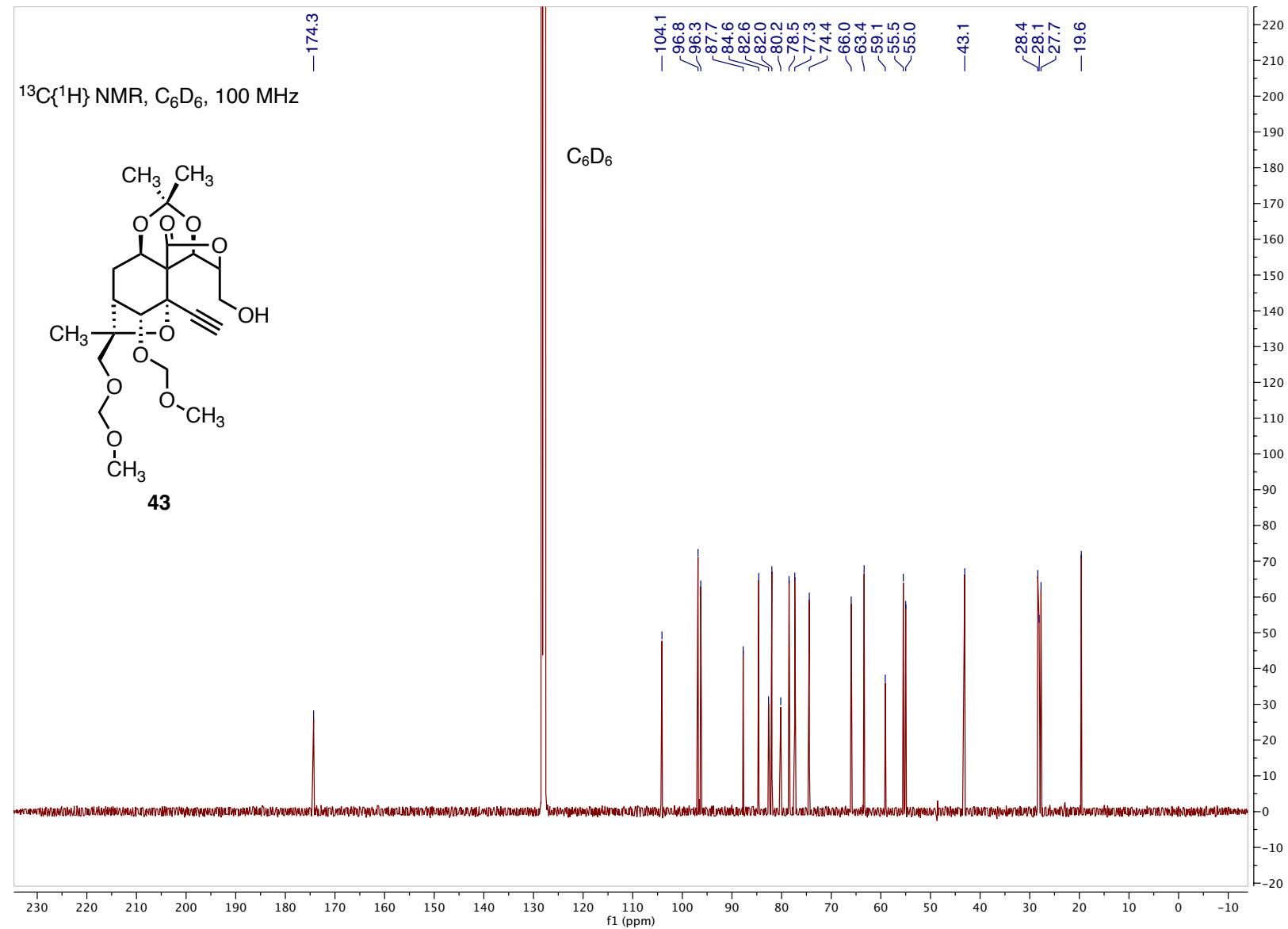


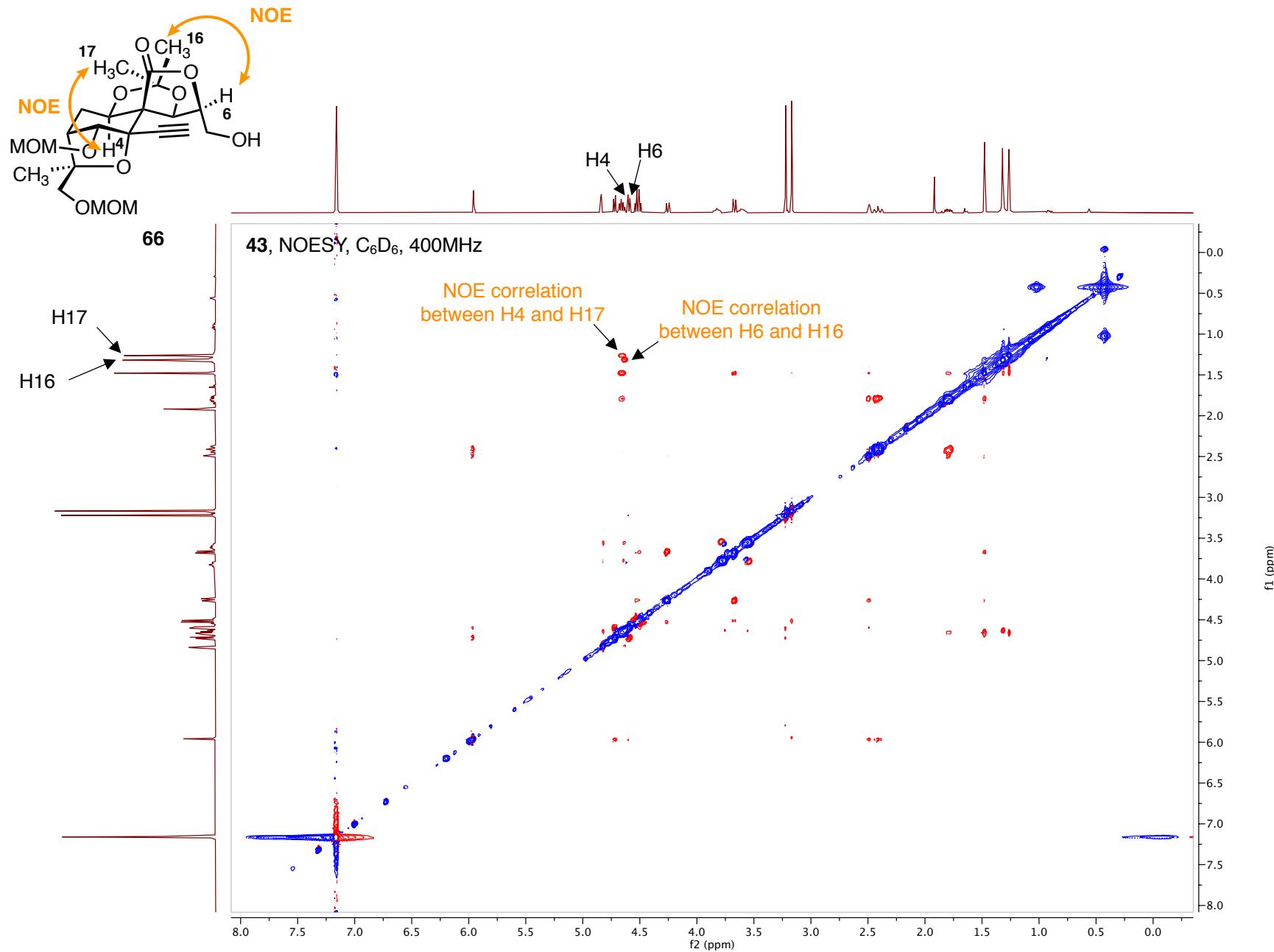


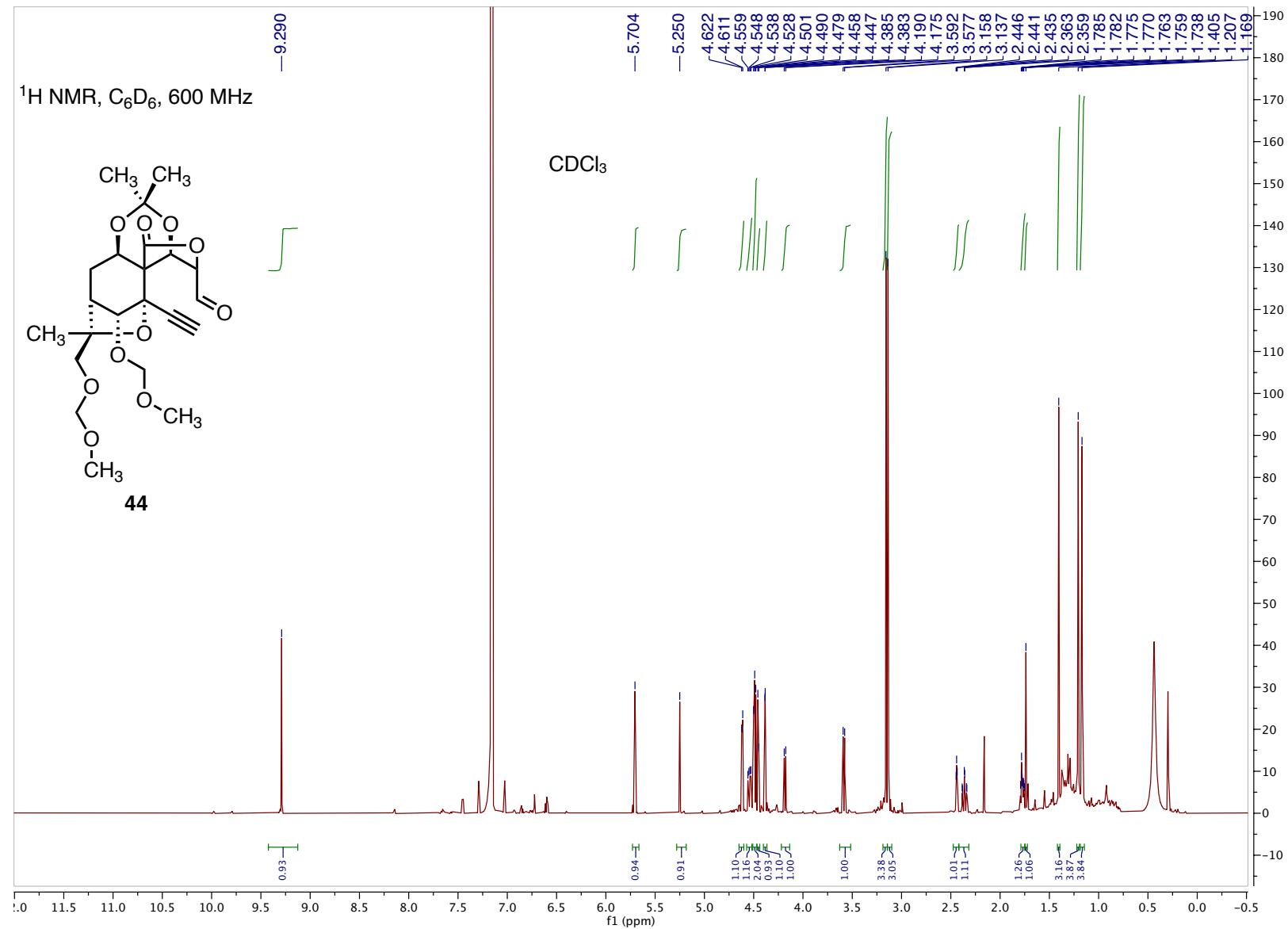


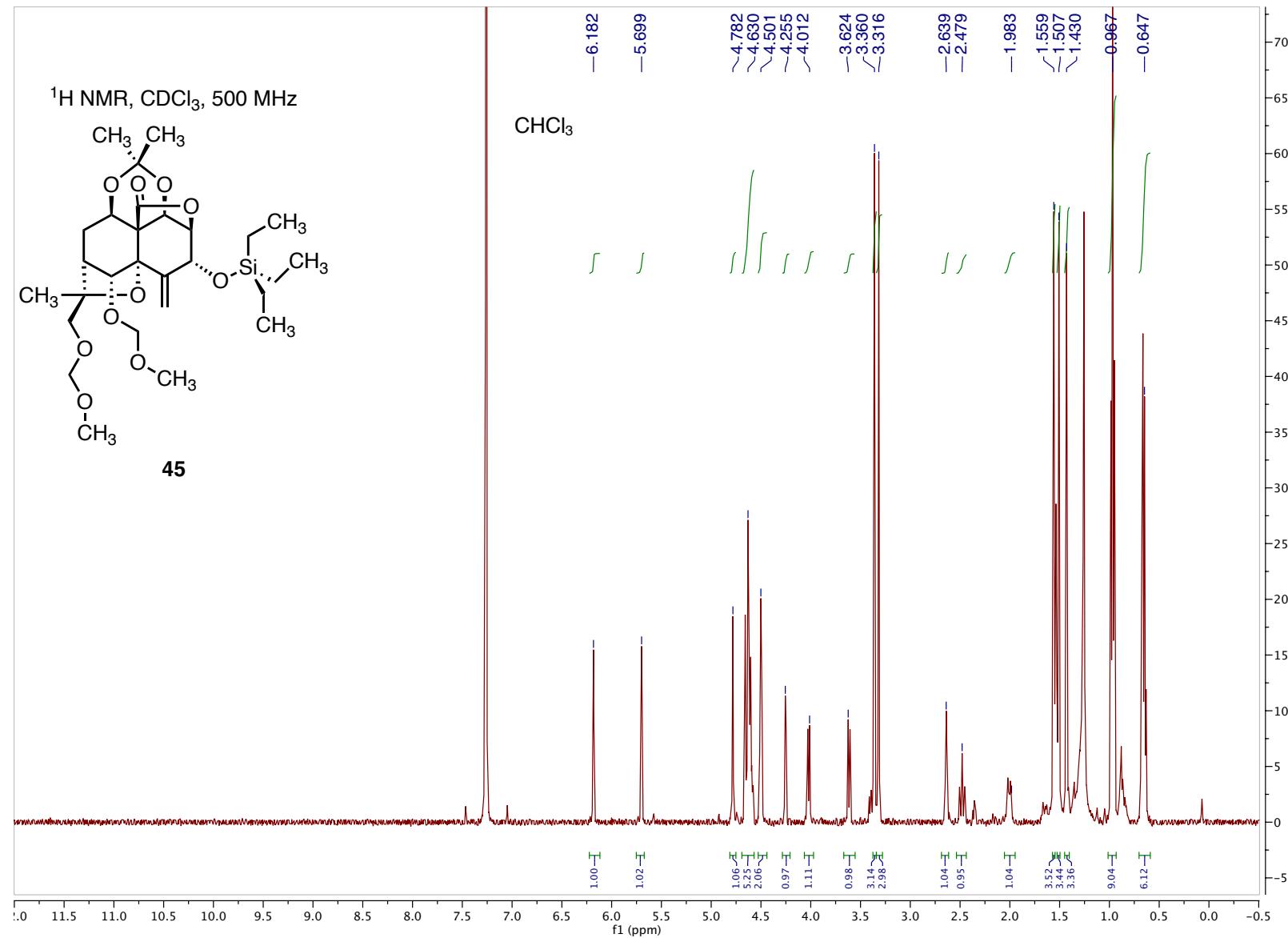


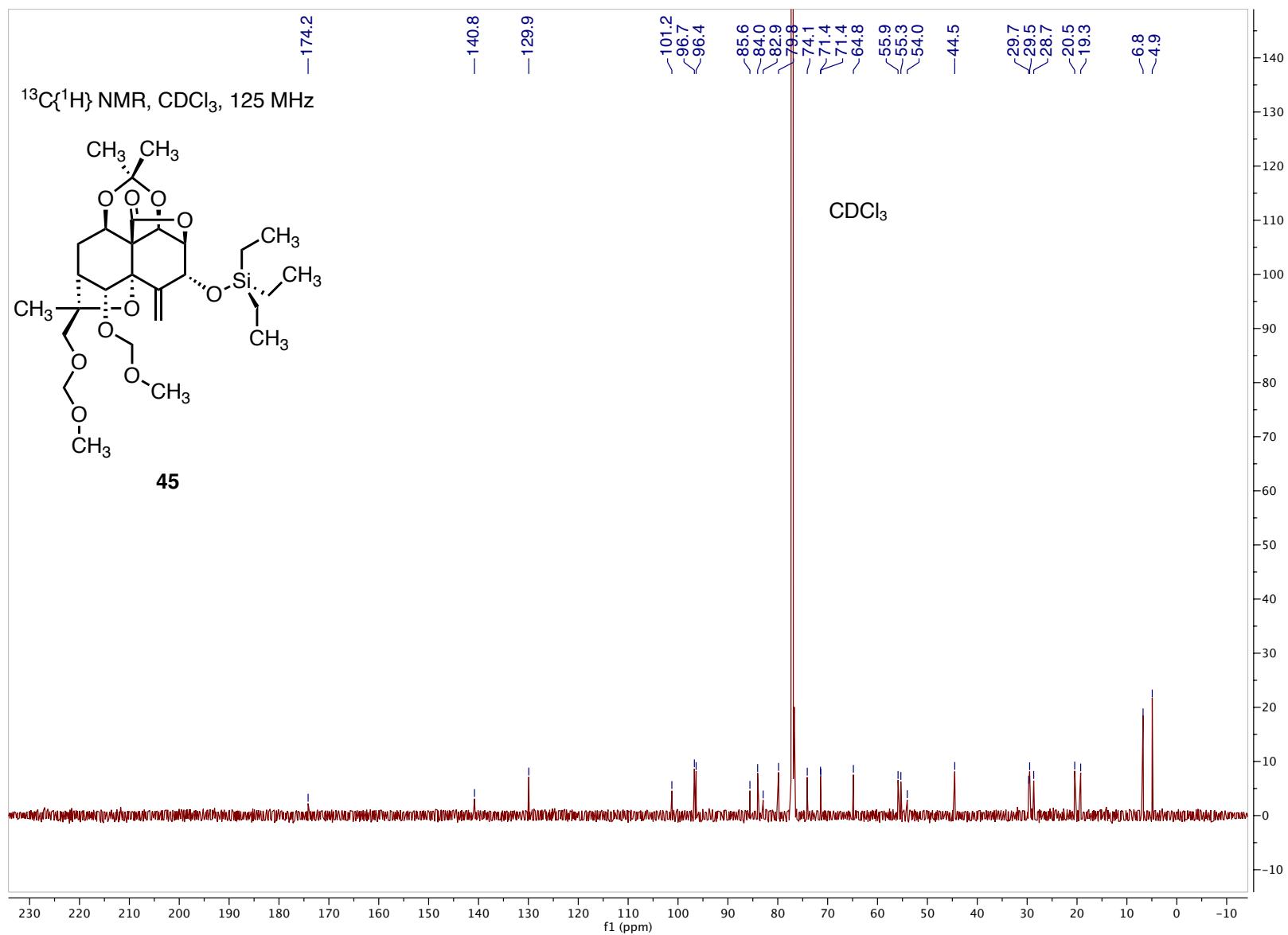


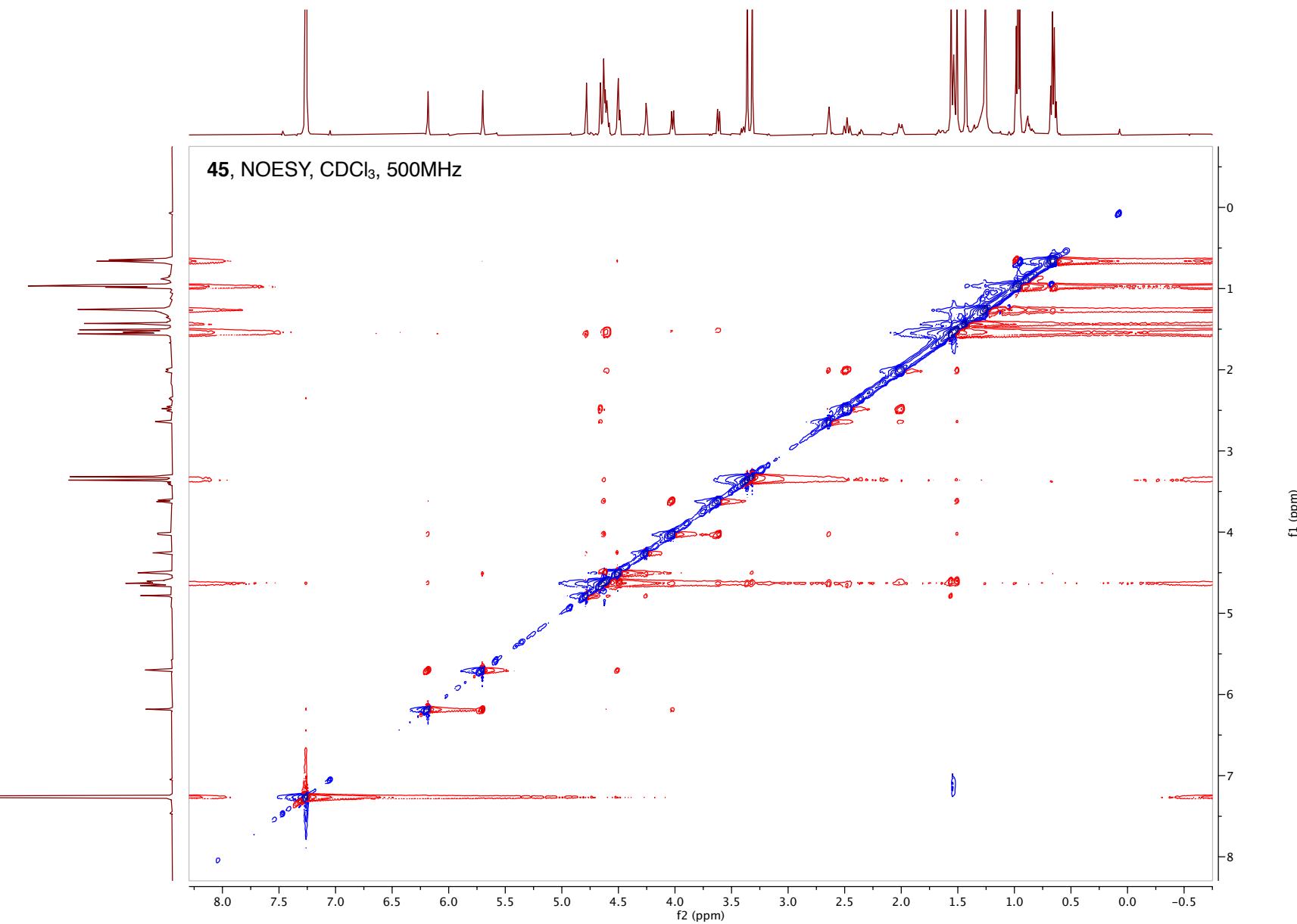


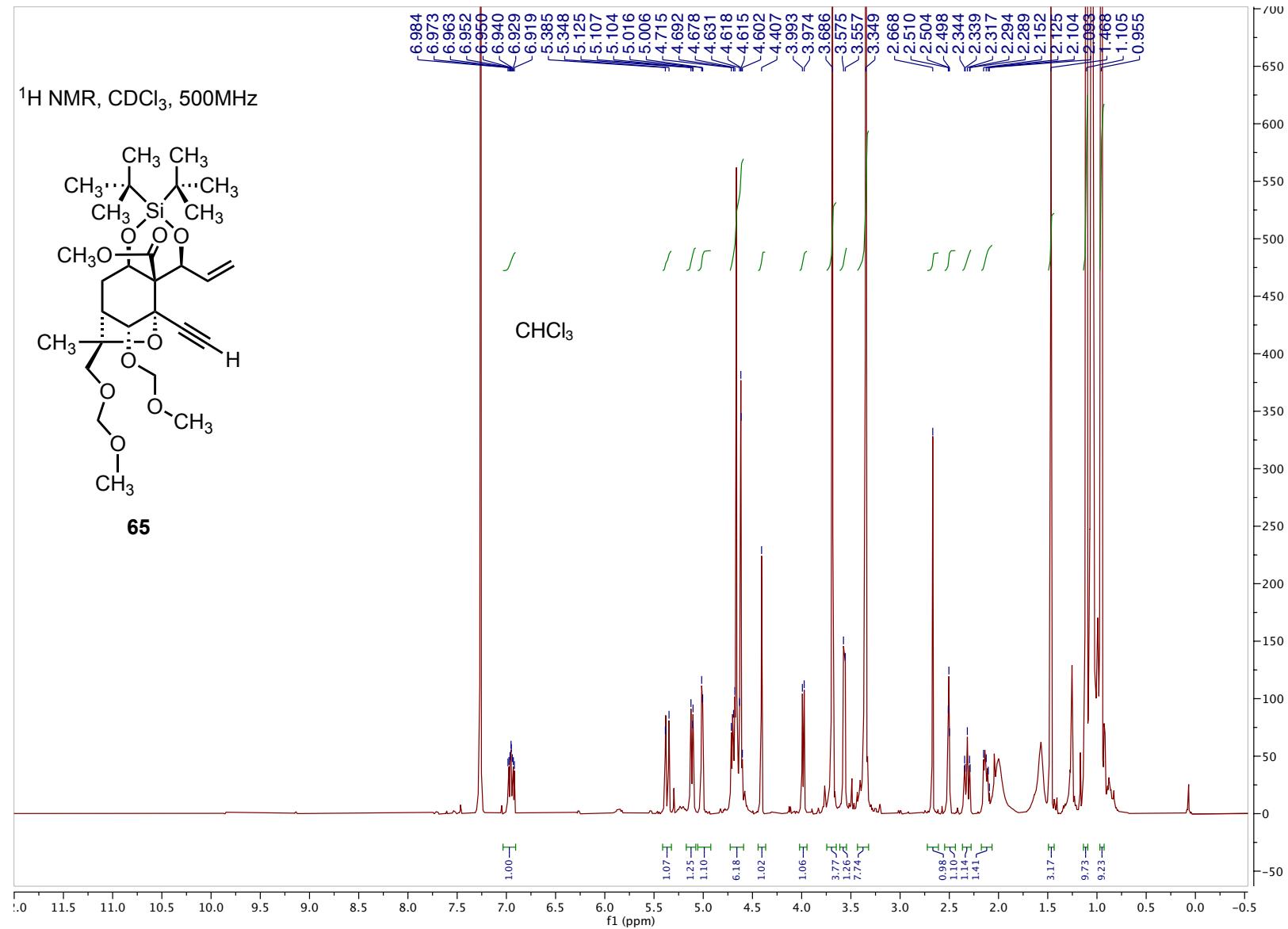


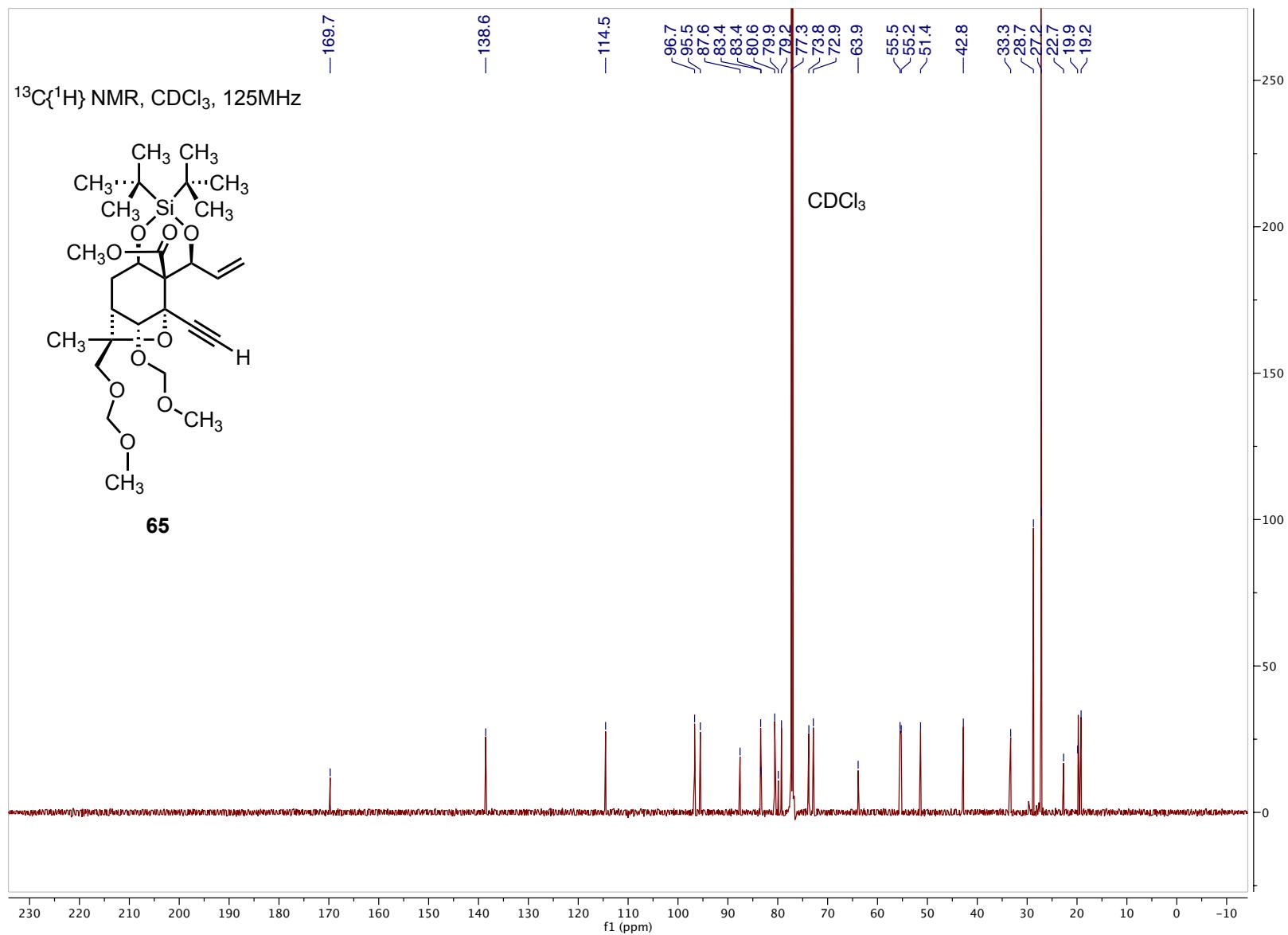


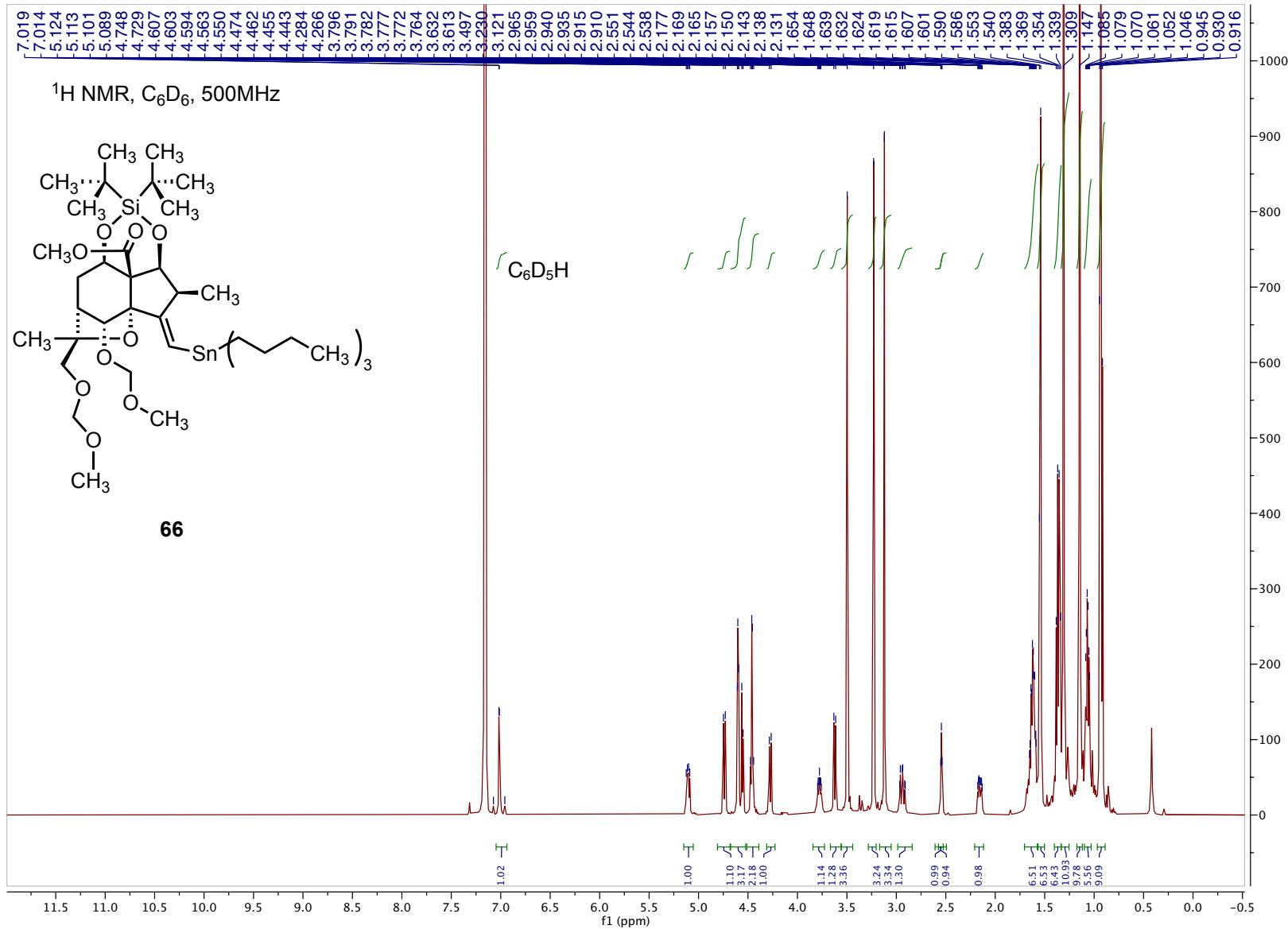


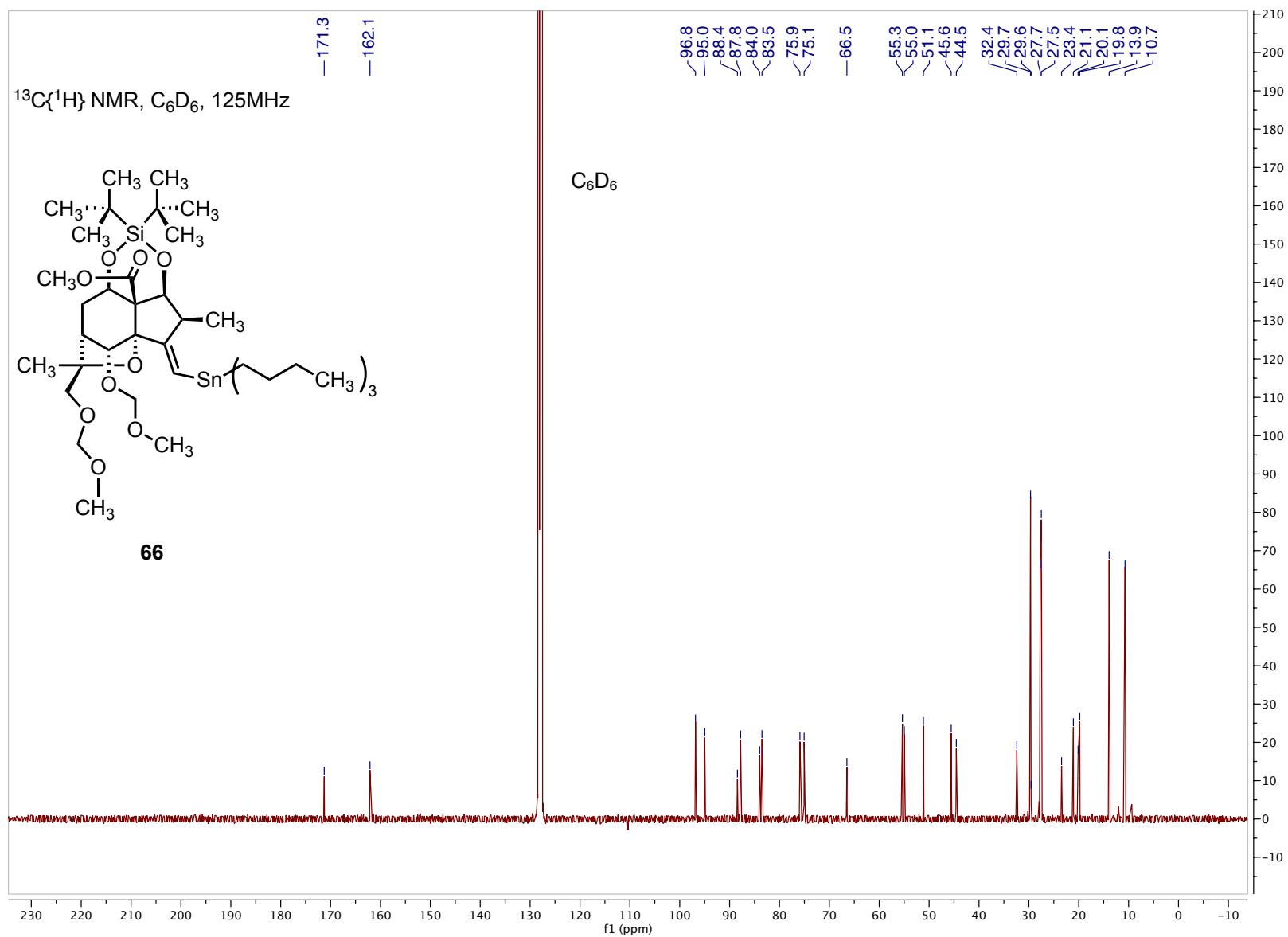


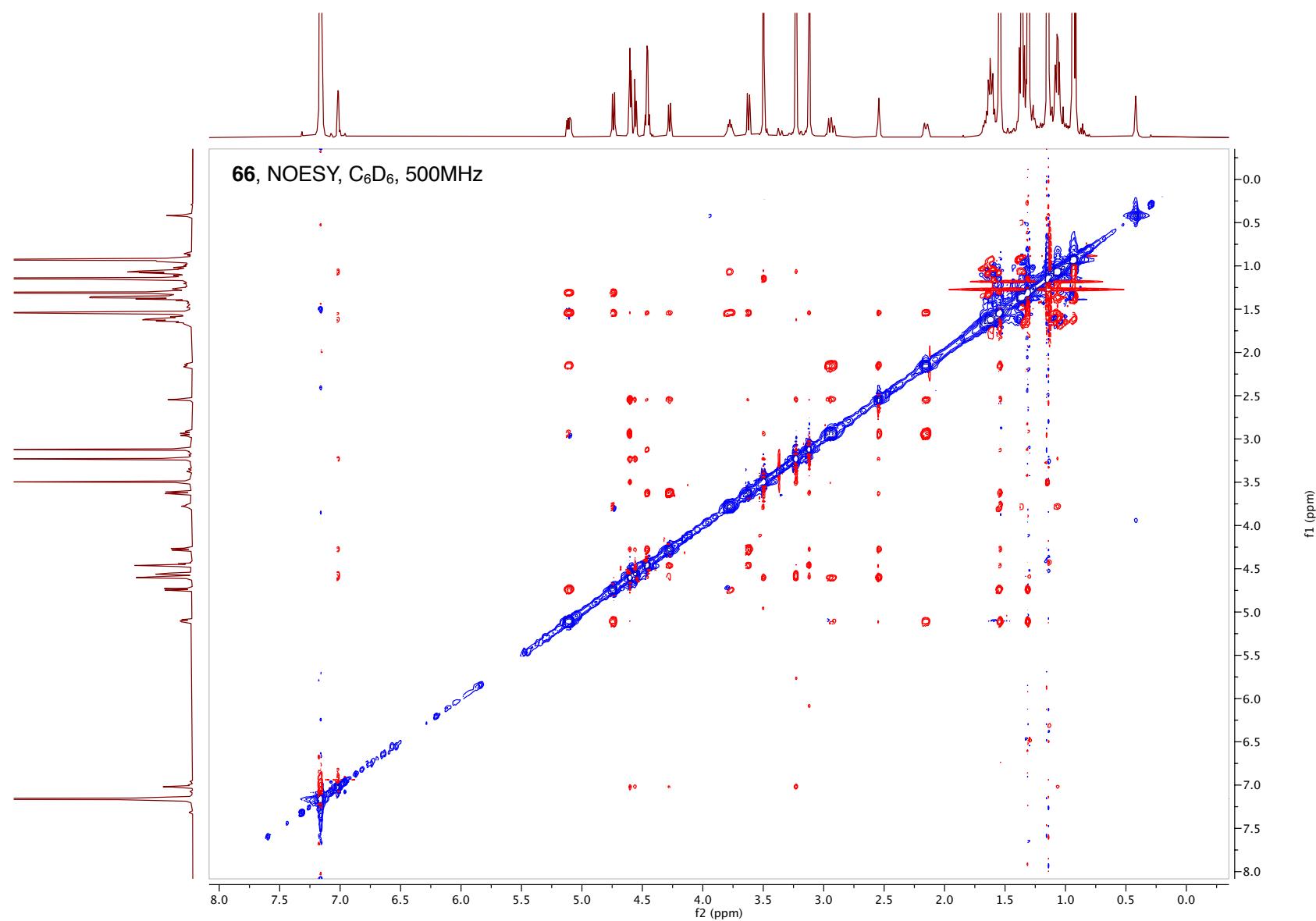


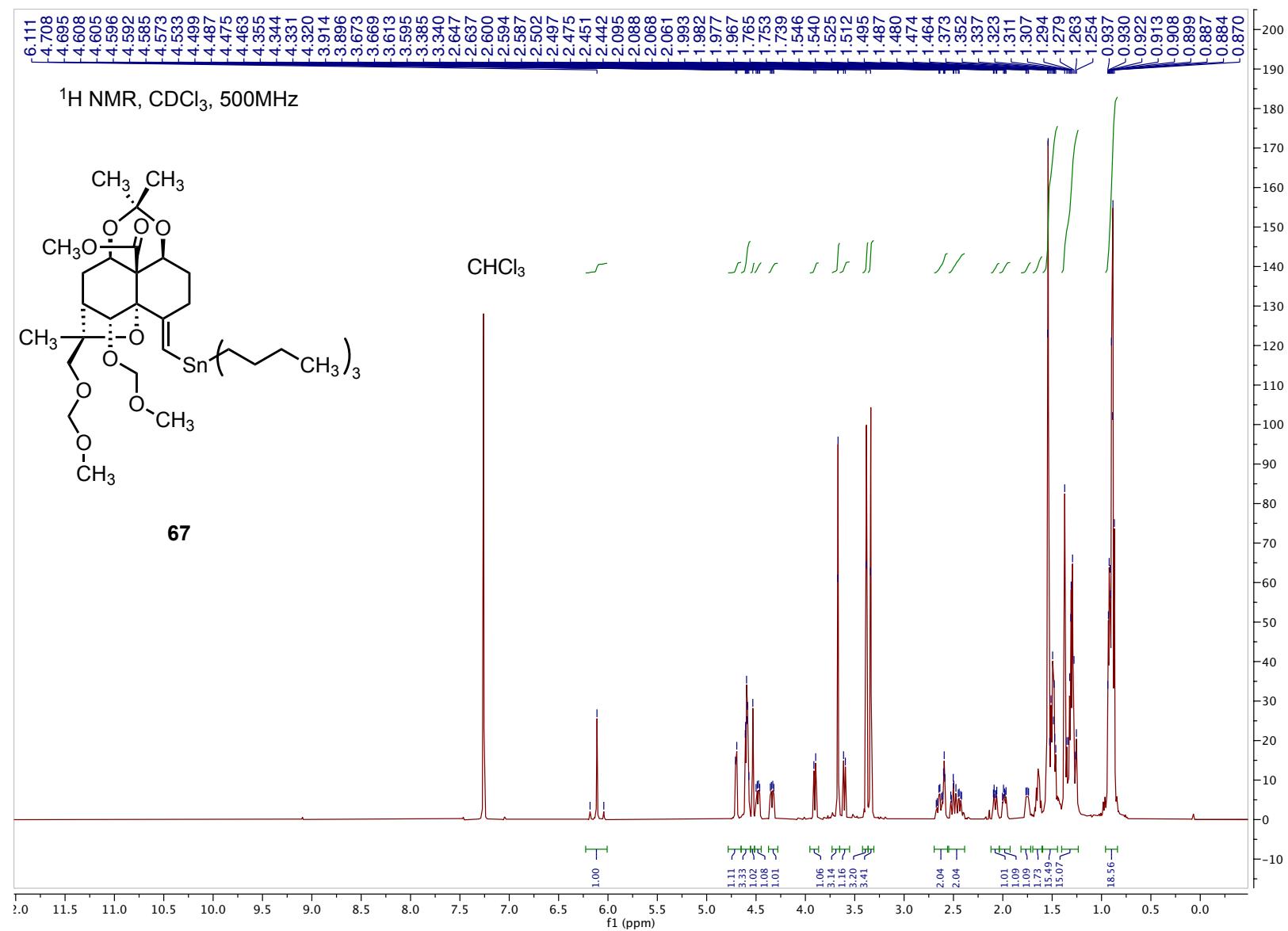


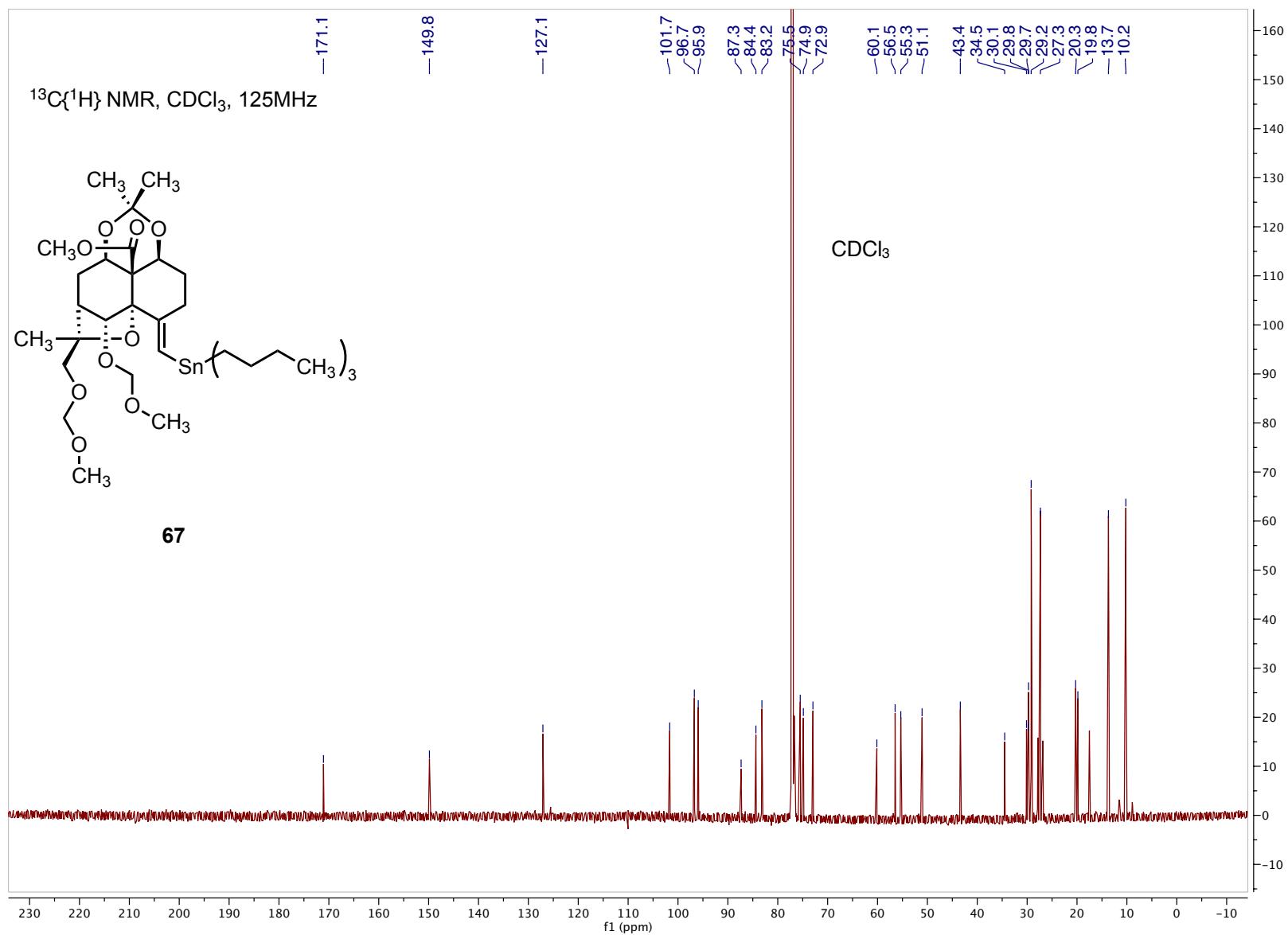


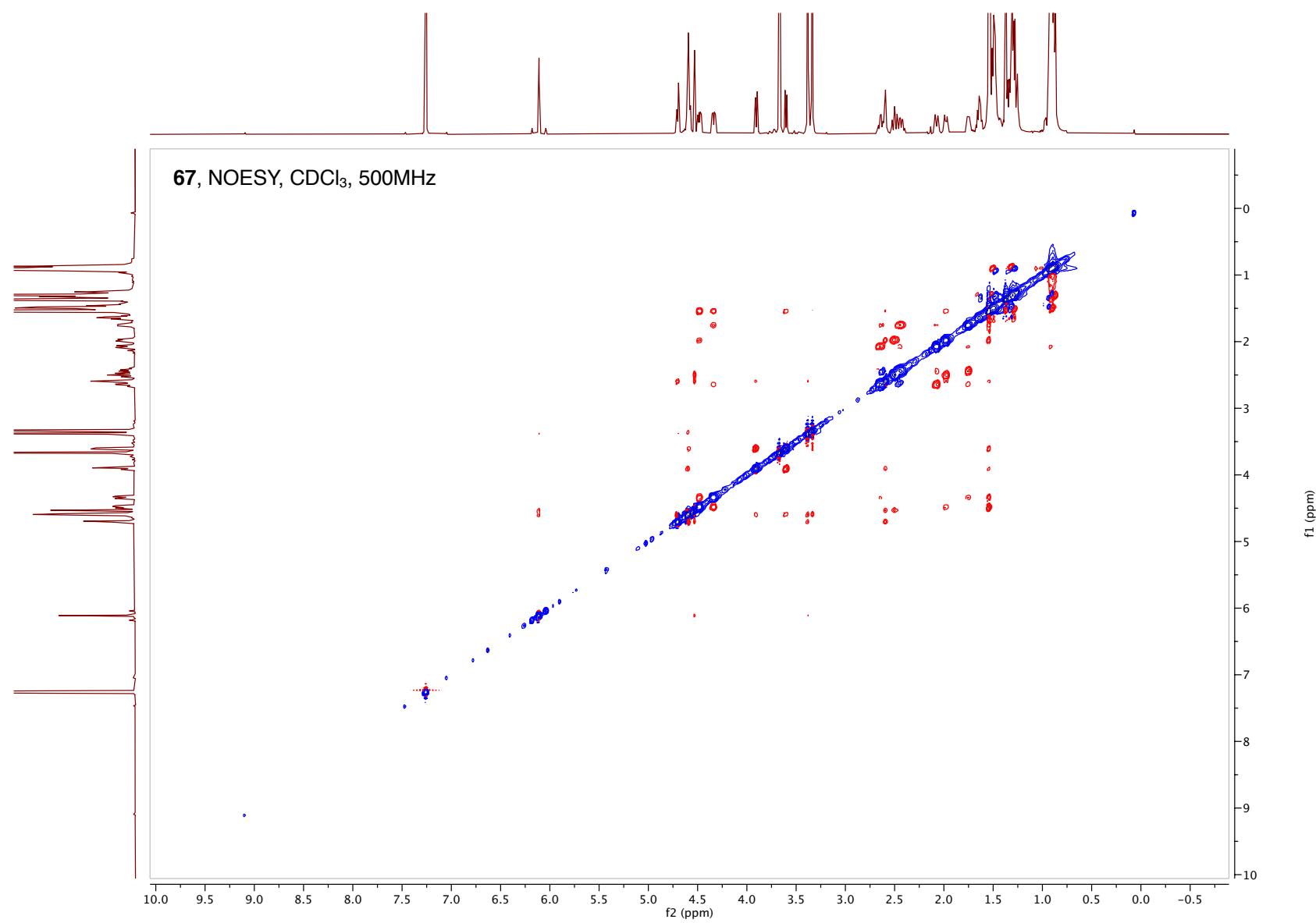


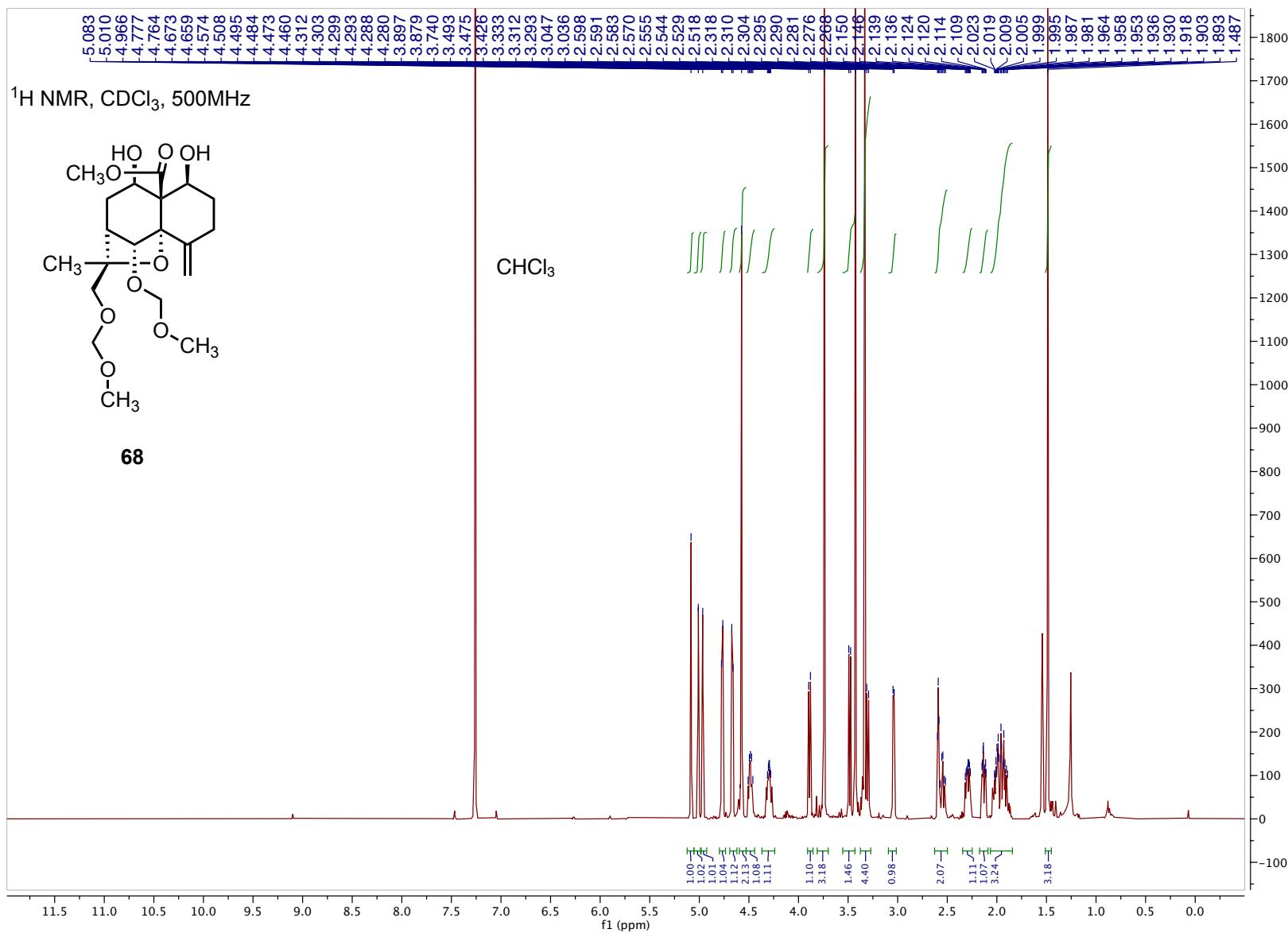


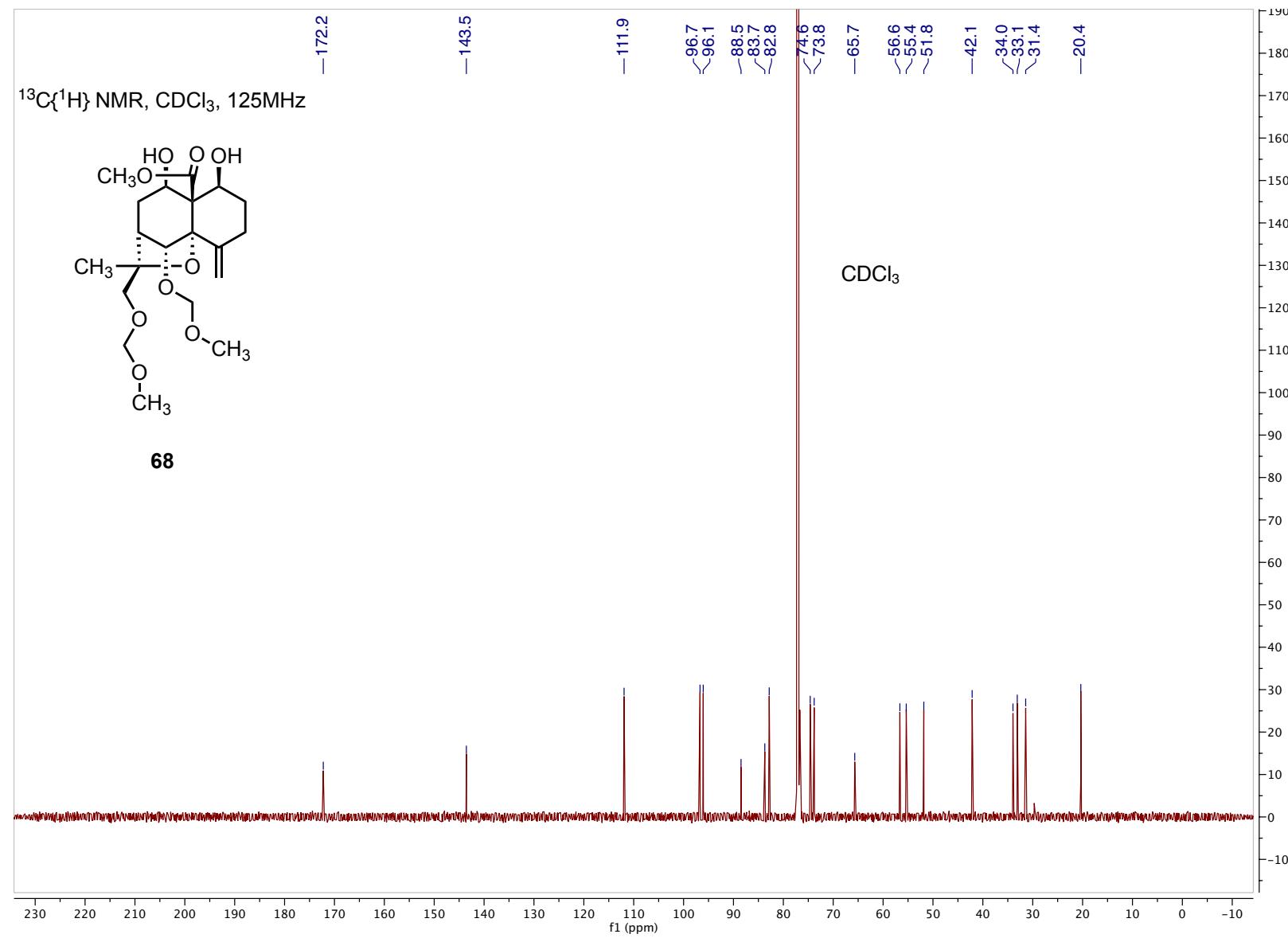


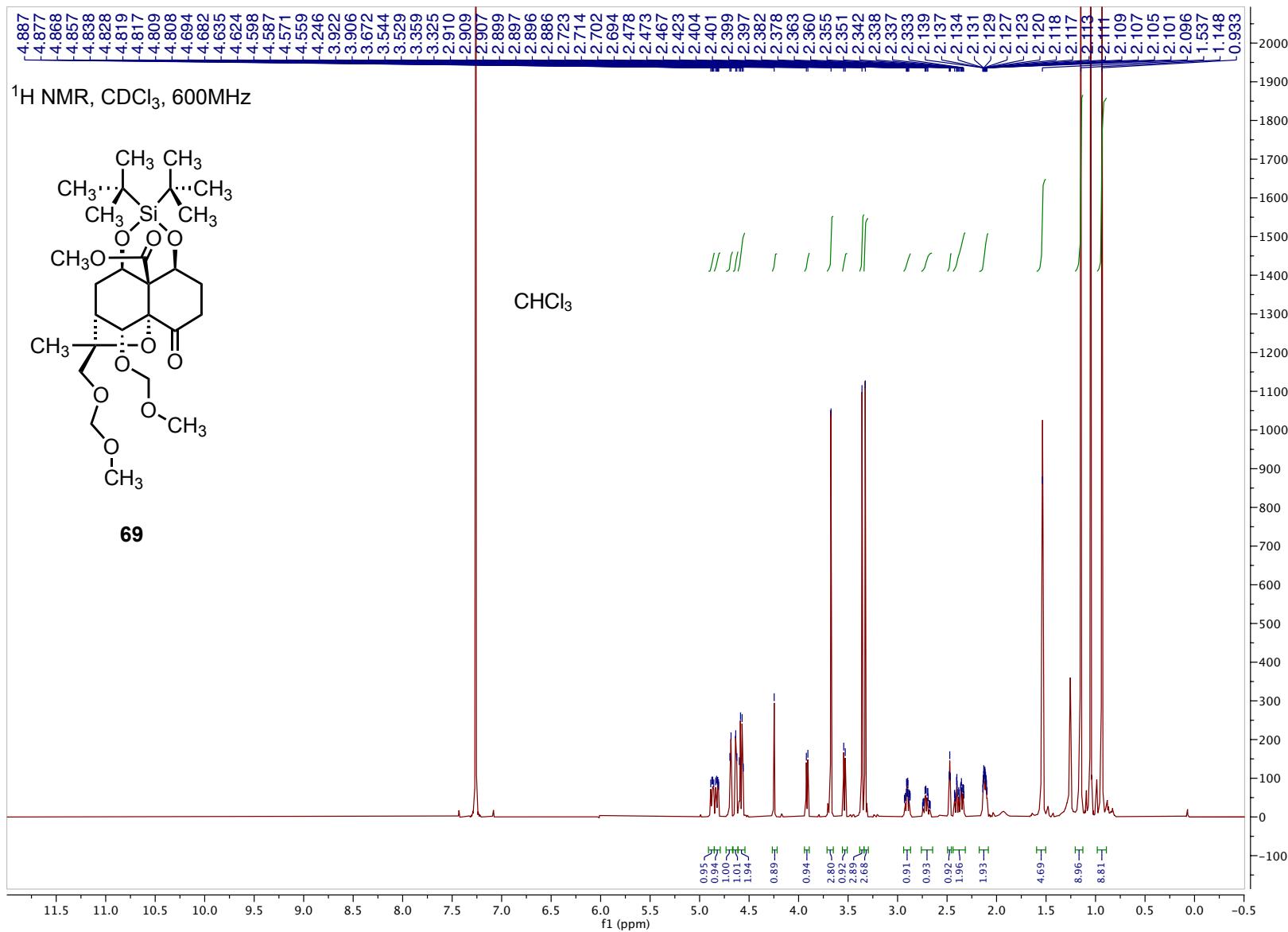


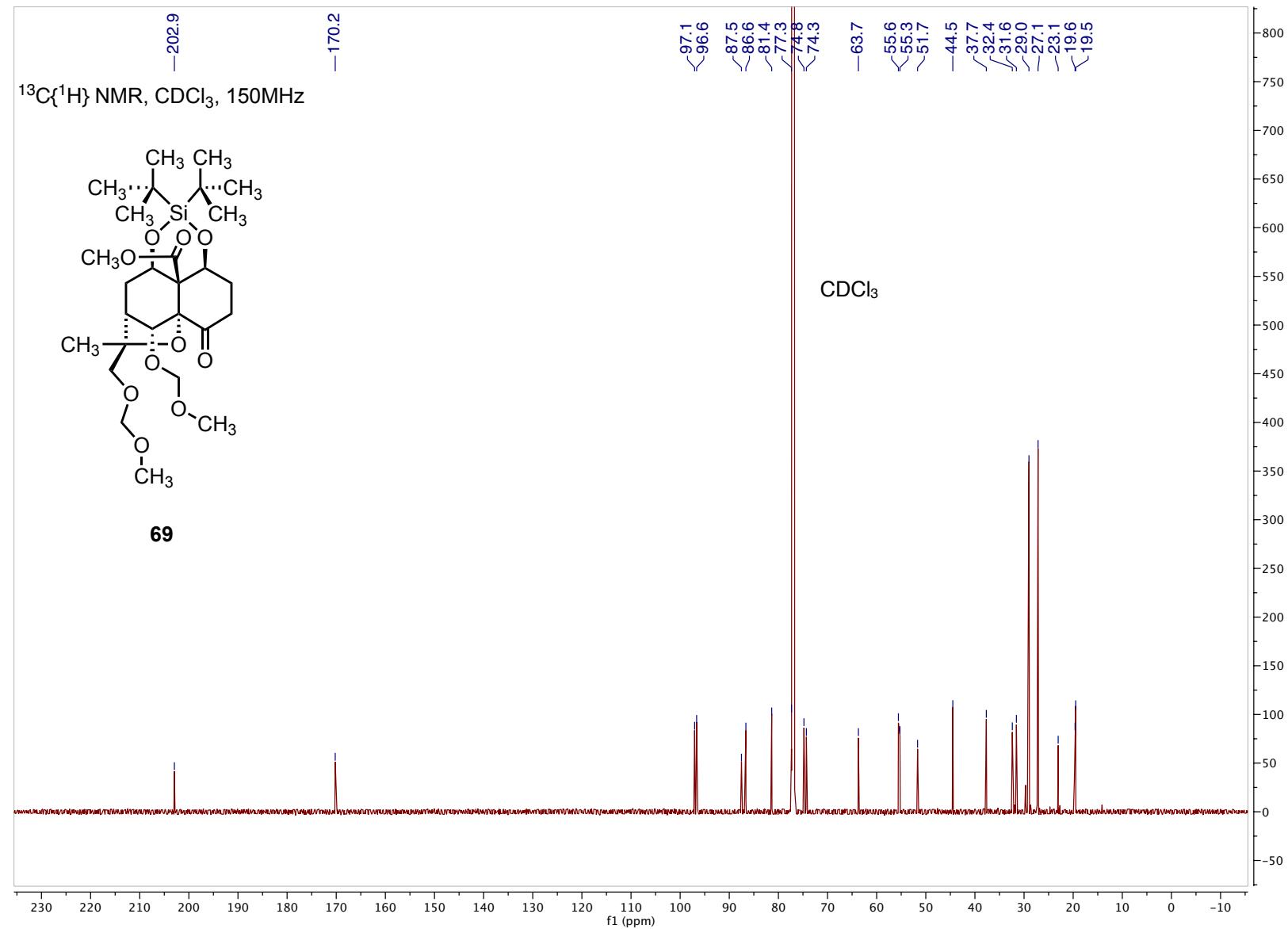


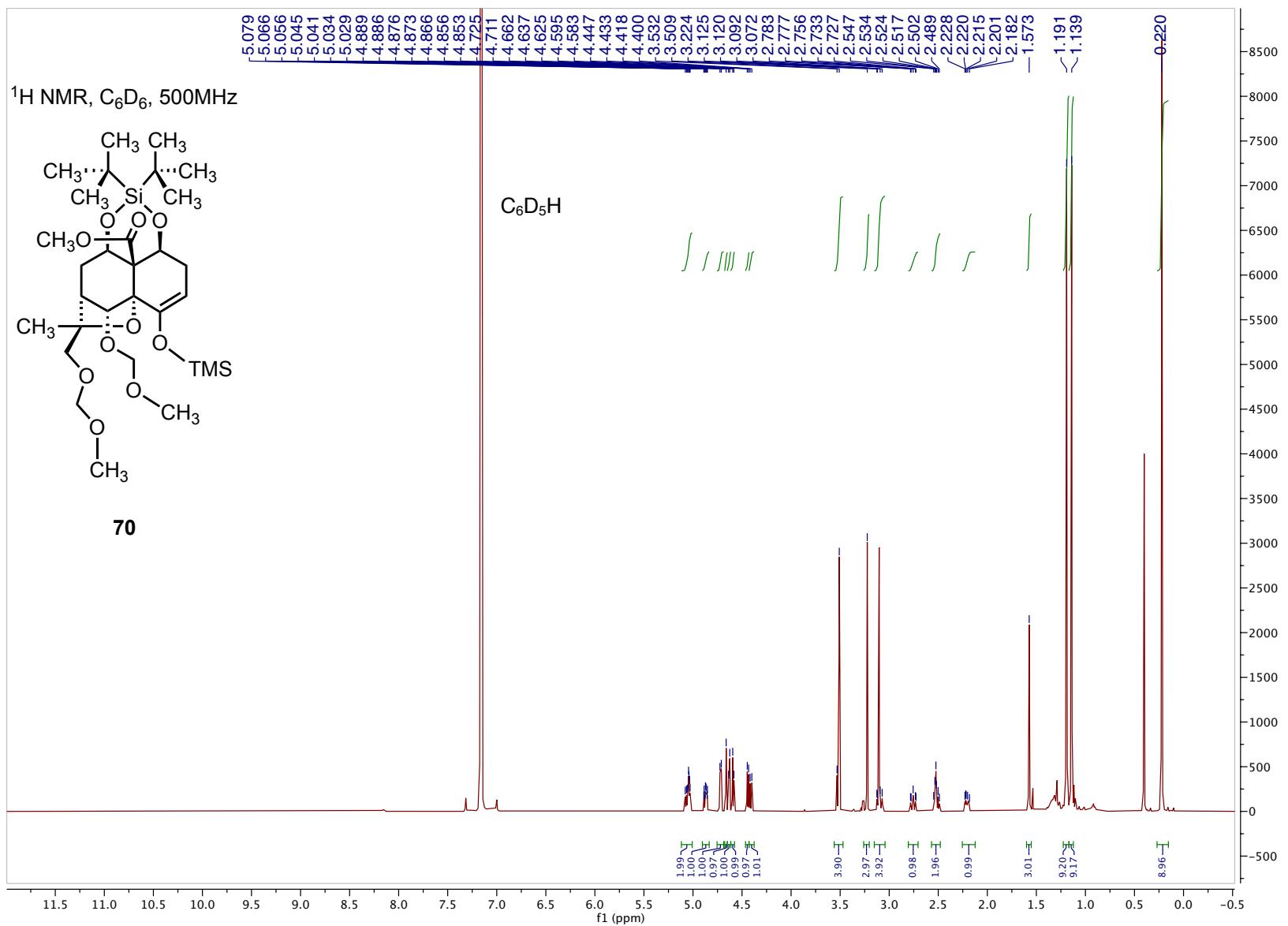


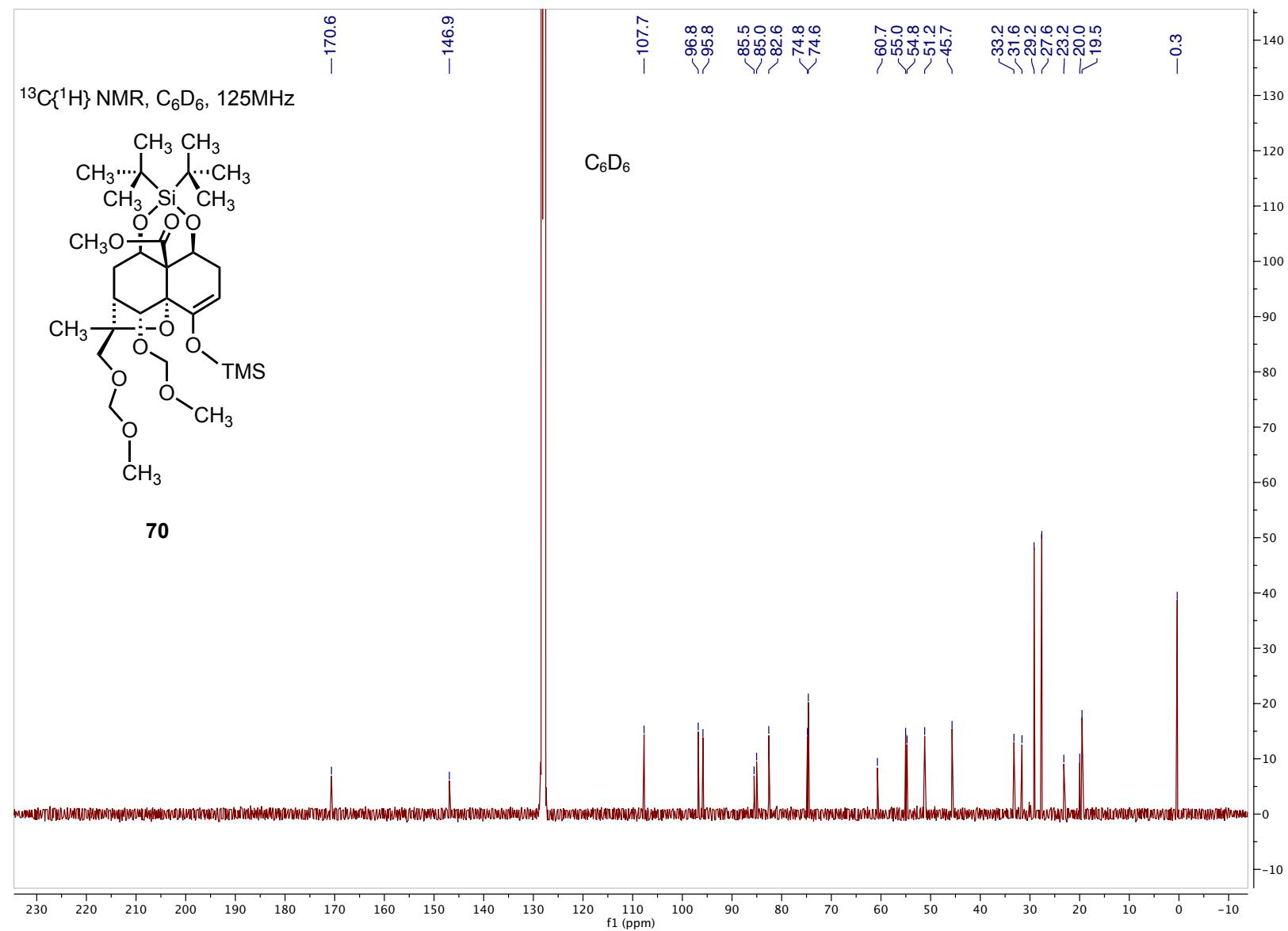


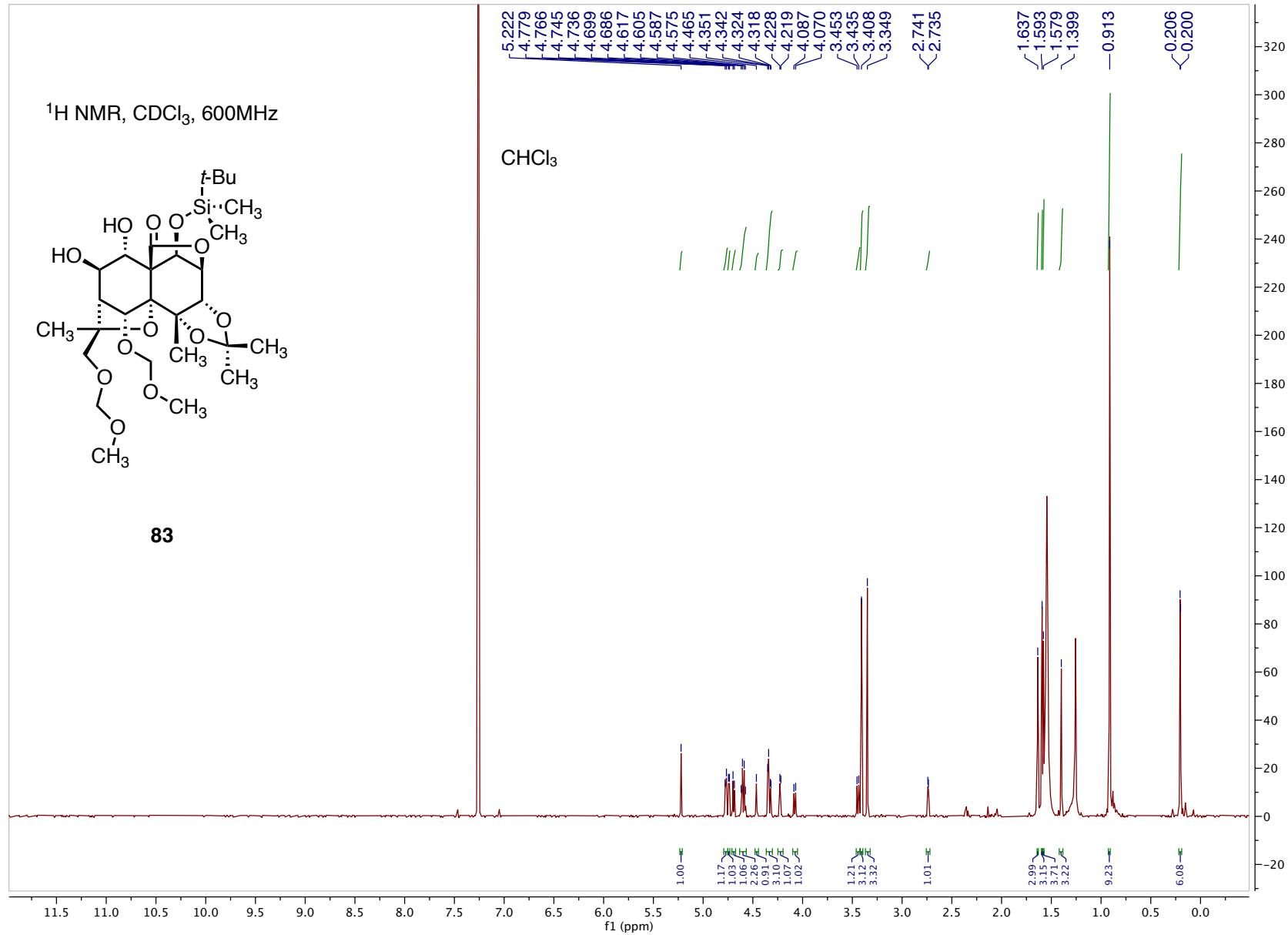


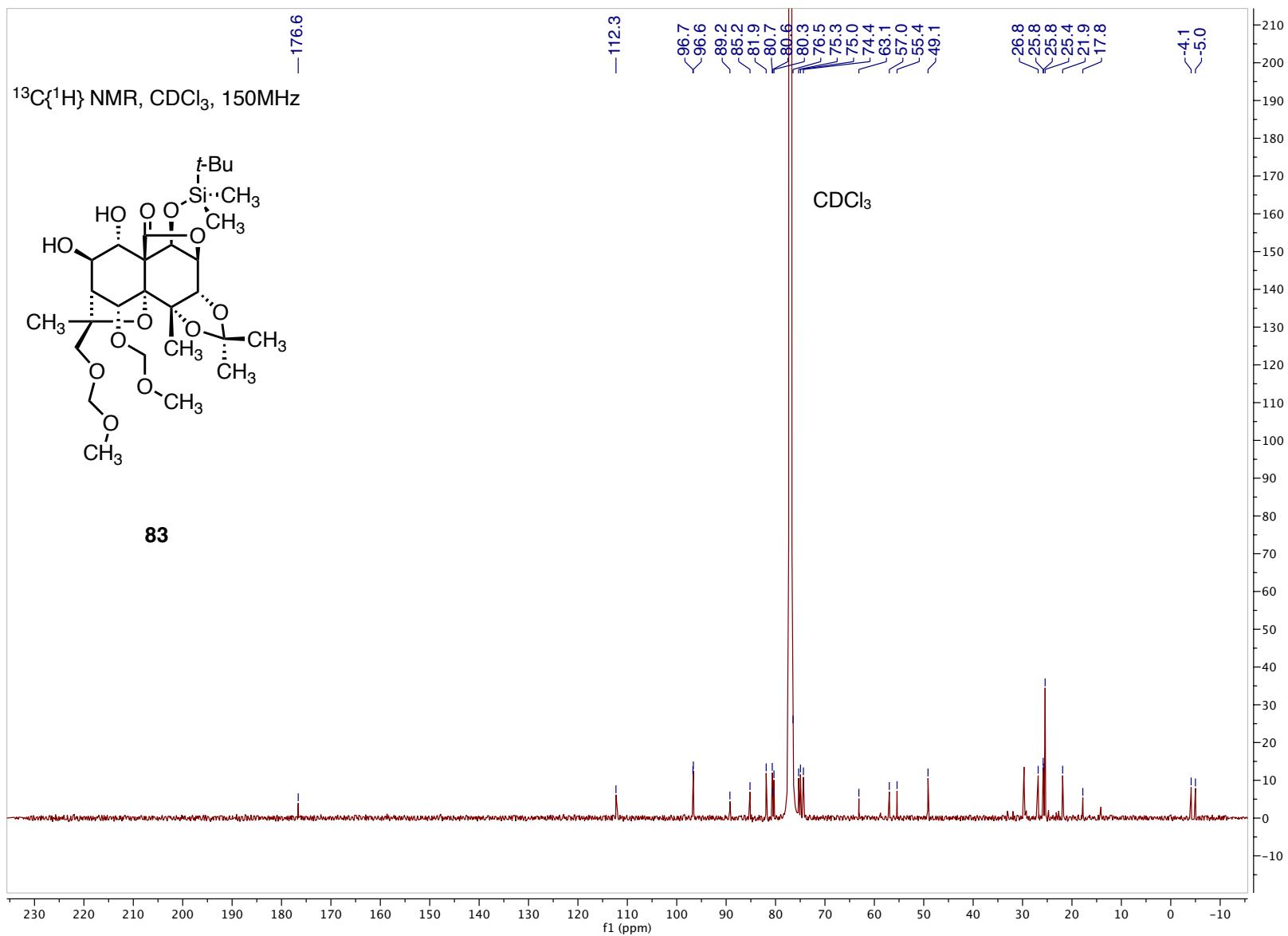


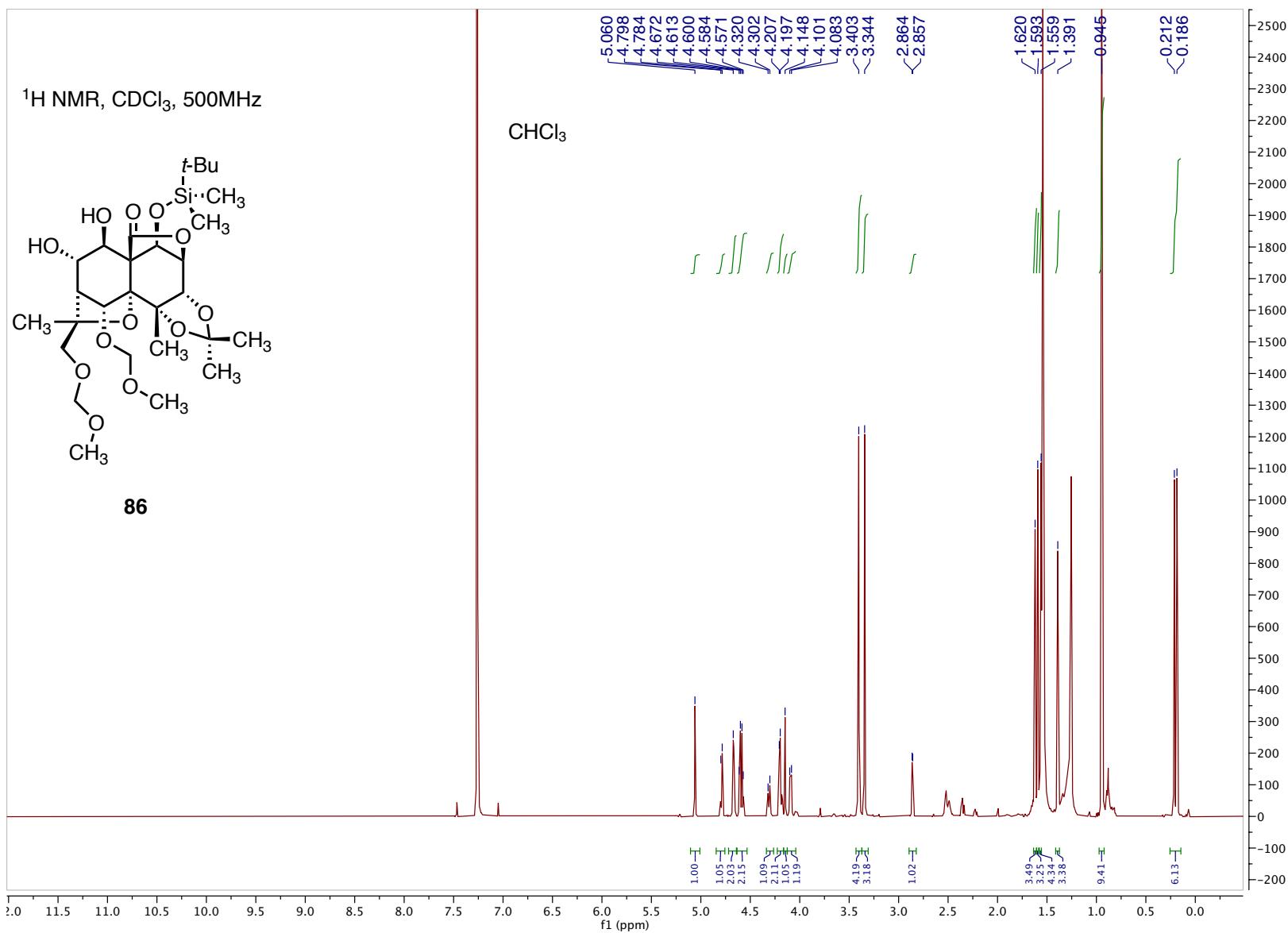


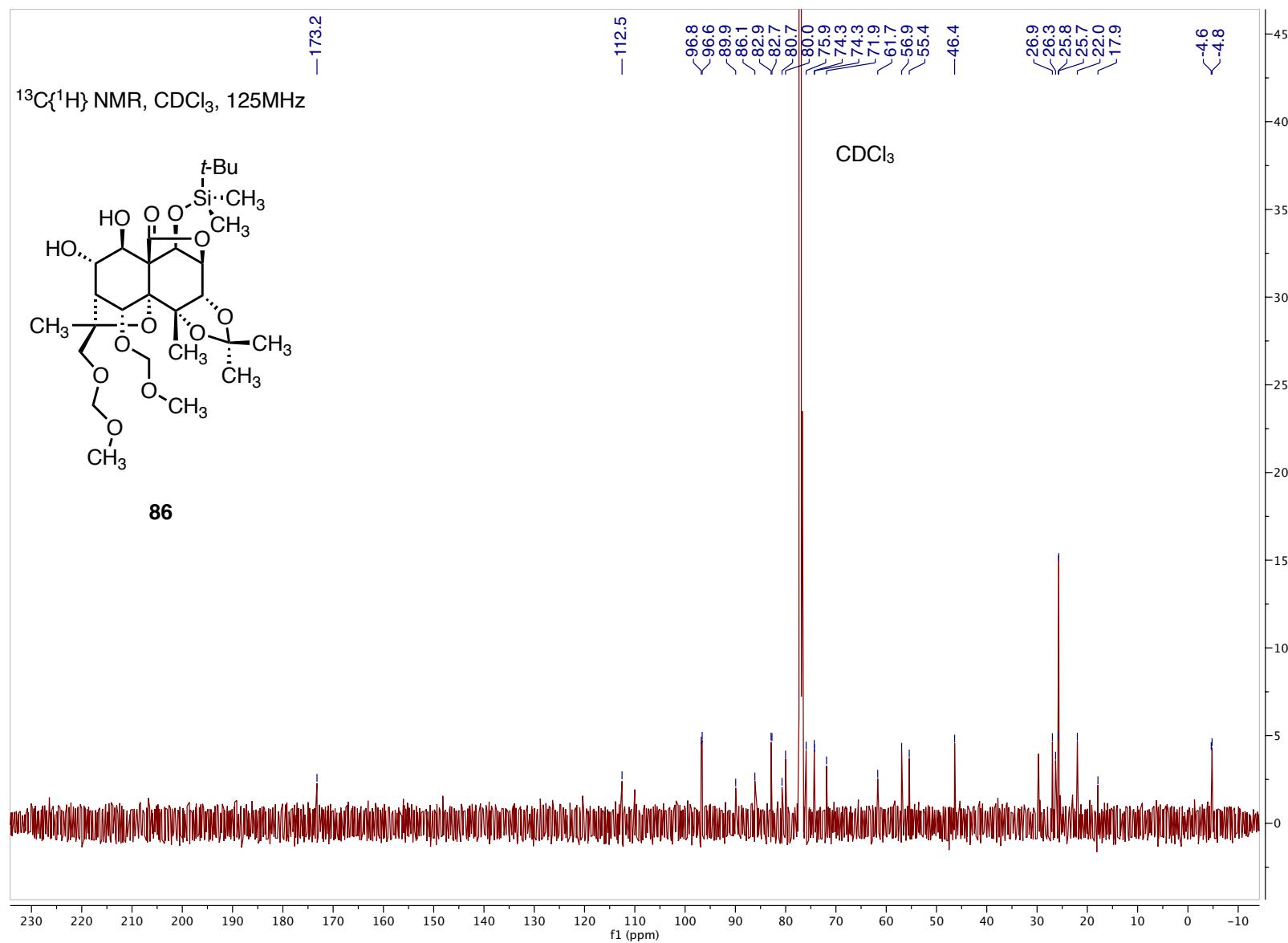


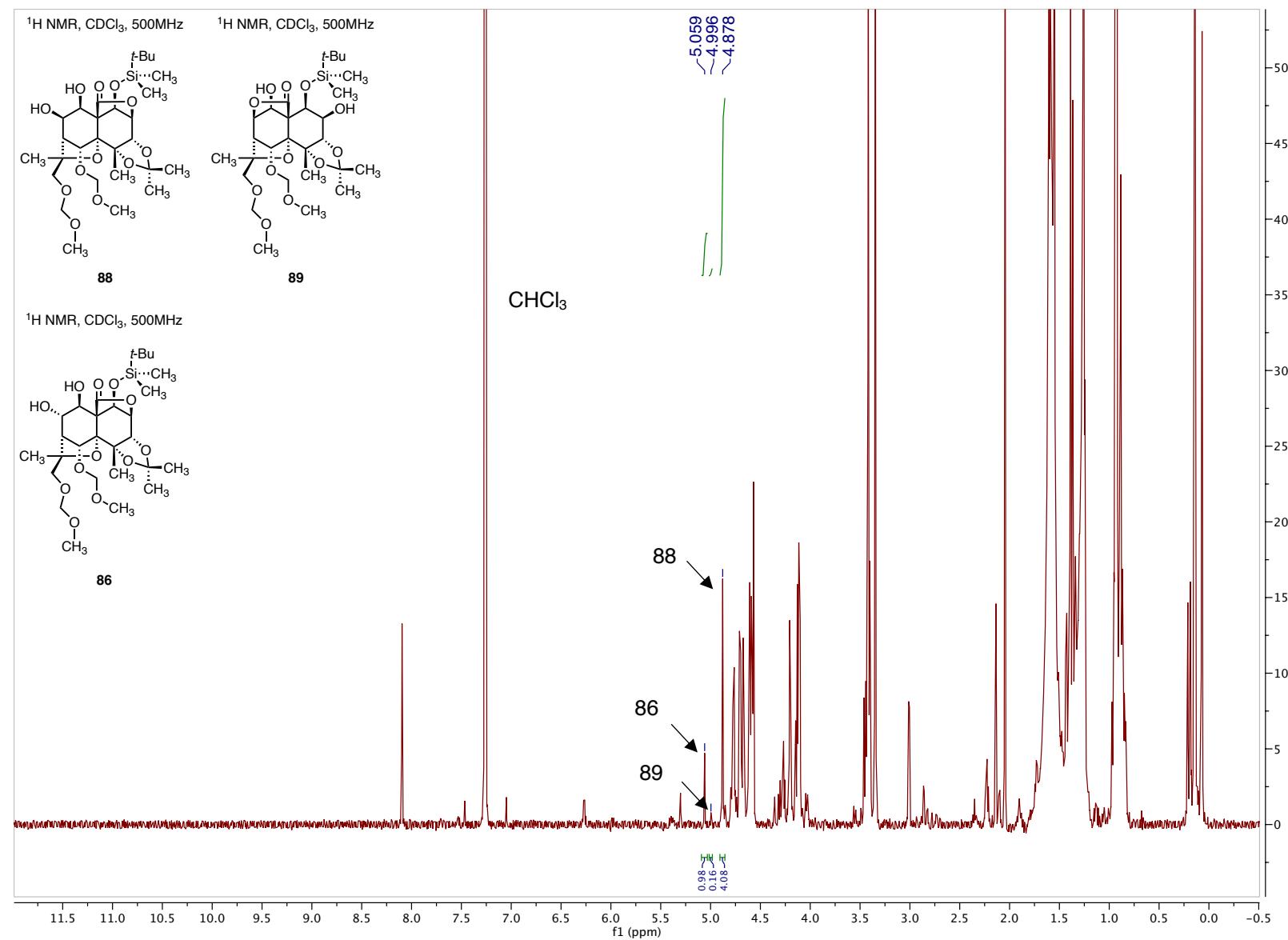


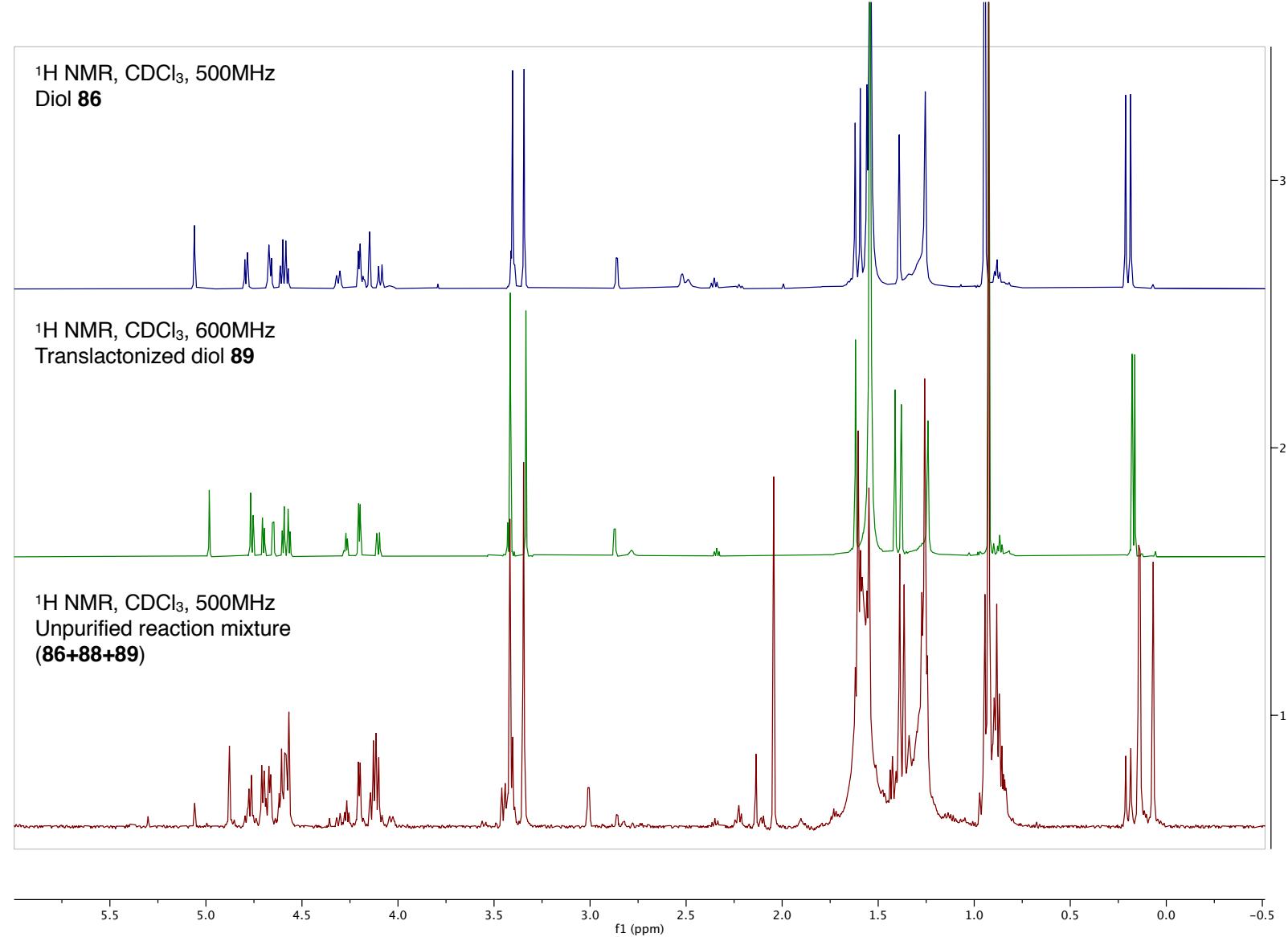


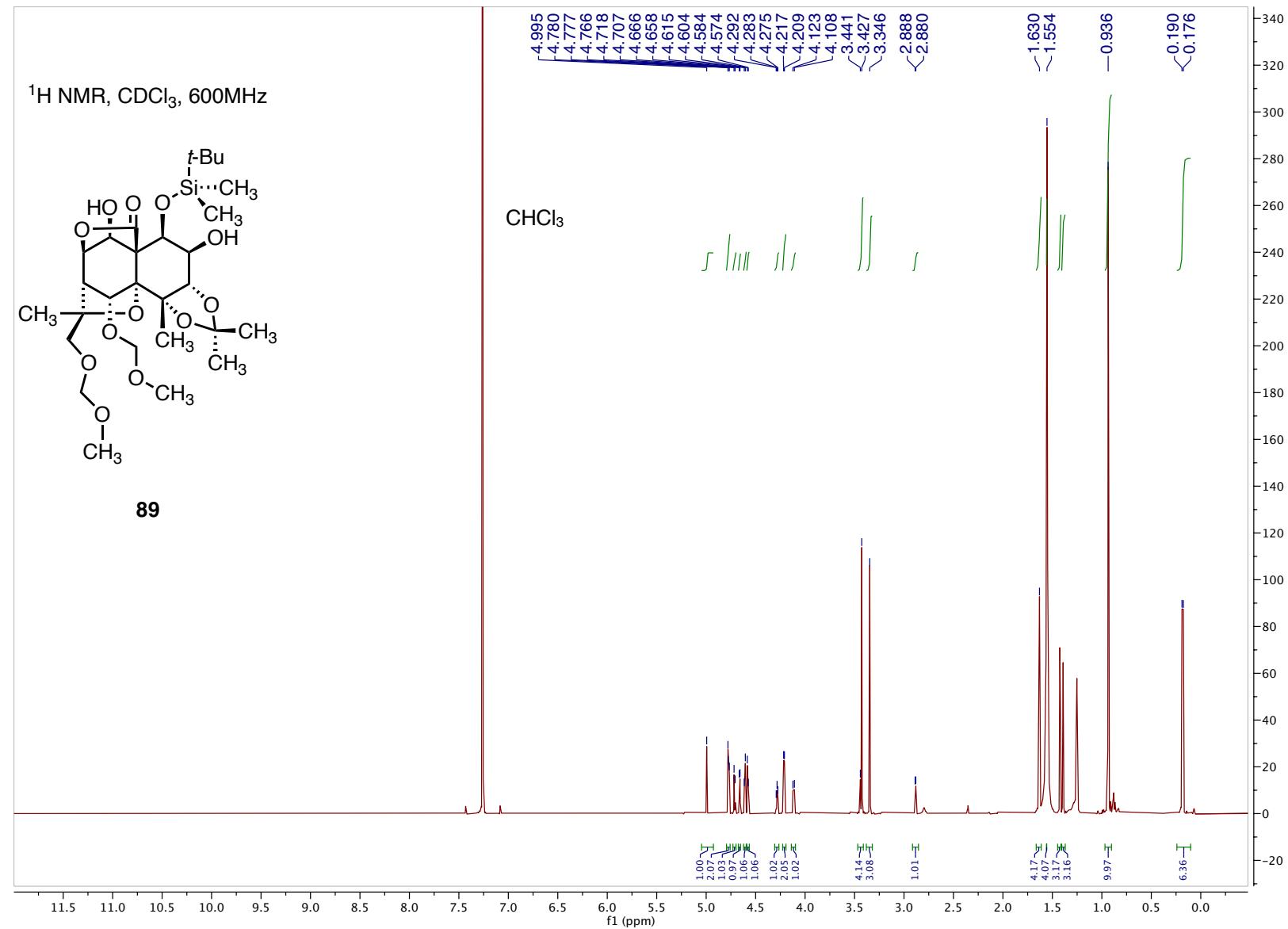


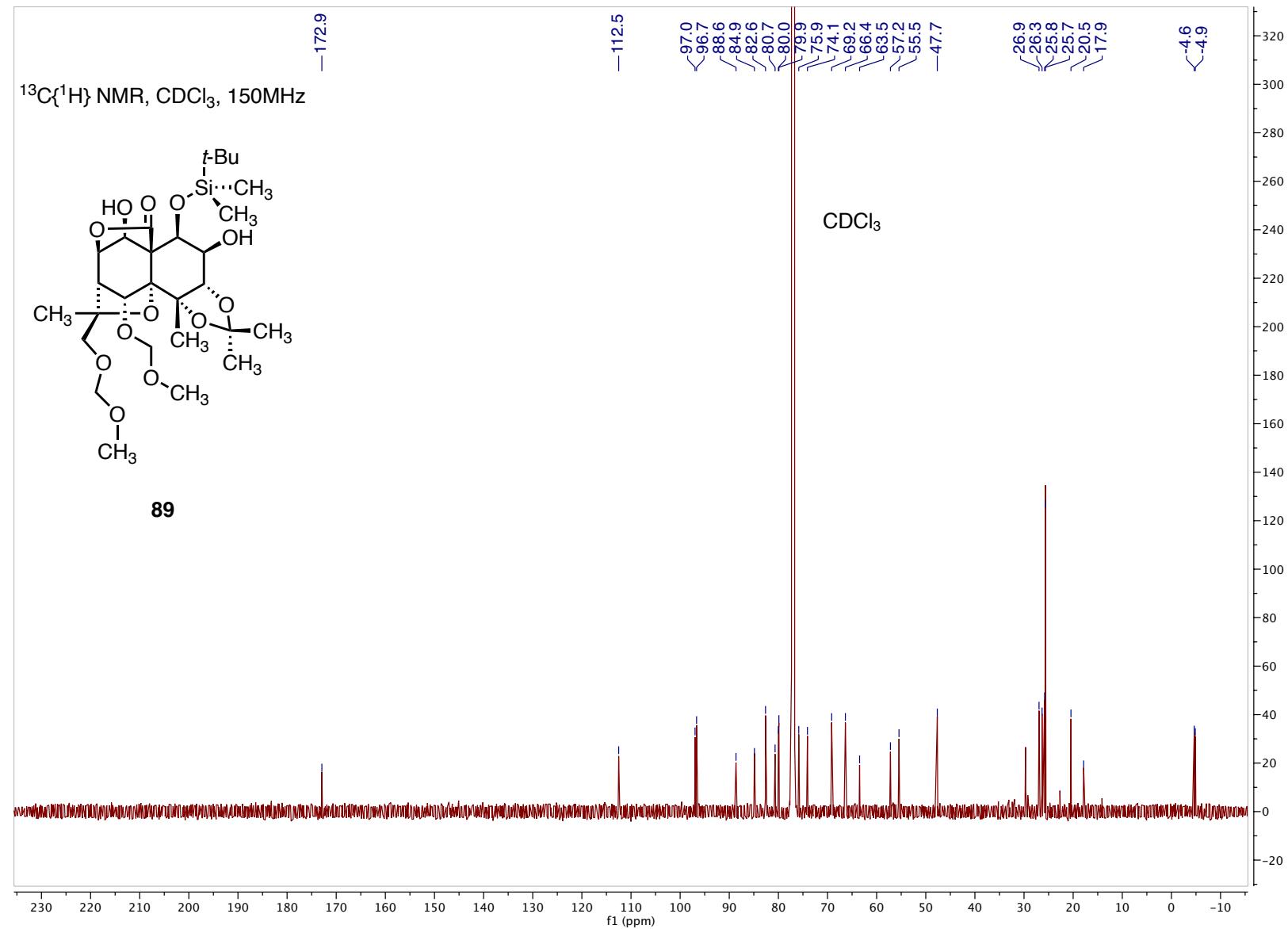












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