



Supporting Information

Selenocystine Peptides Performance in 5-endo-dig Reactions

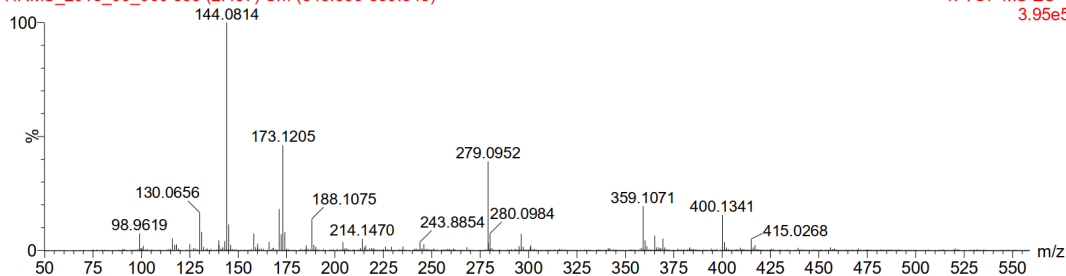
Sindija Lapcinska and Pavel Arsenyan*

ejoc201901548-sup-0001-SupMat.pdf

***N*-(2-(hex-1-yn-1-yl)phenyl)-4-nitrobenzenesulfonamide (5d).**

HRMS_2018_09_060 853 (2.437) Cm (848:853-839:843)

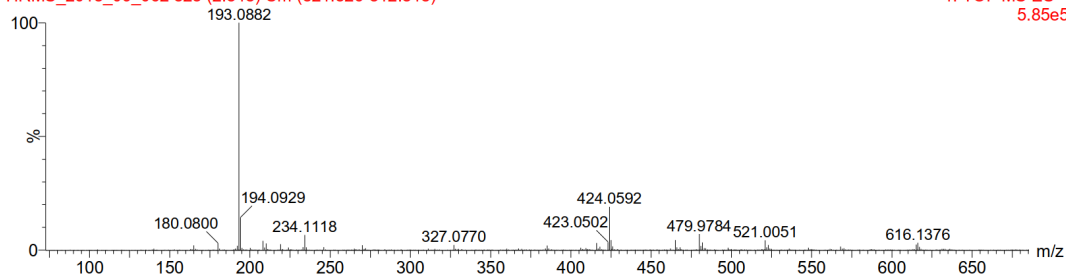
1: TOF MS ES+
3.95e5



2,4-Dinitro-*N*-(2-(phenylethynyl)phenyl)benzenesulfonamide (5e).

HRMS_2018_09_062 823 (2.348) Cm (821:826-812:818)

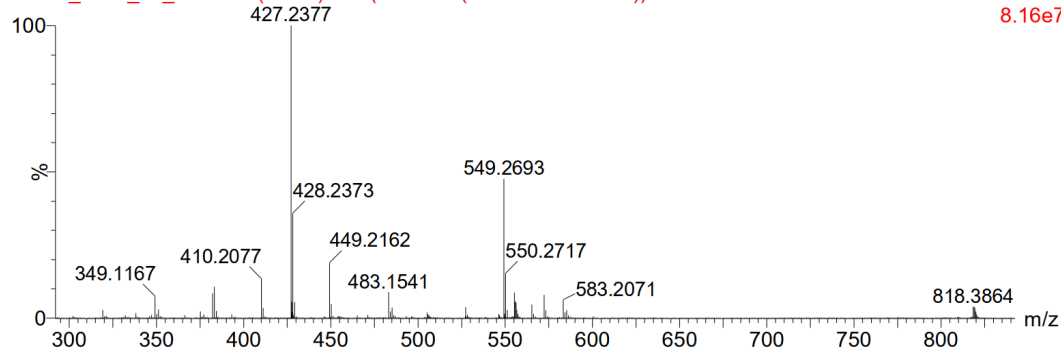
1: TOF MS ES+
5.85e5



Benzyl *tert*-butyl ((*S*)-6-(((*S*)-1-amino-1-oxo-3-phenylpropan-2-yl)amino)-6-oxohexane-1,5-diyl)dicarbamate (9).

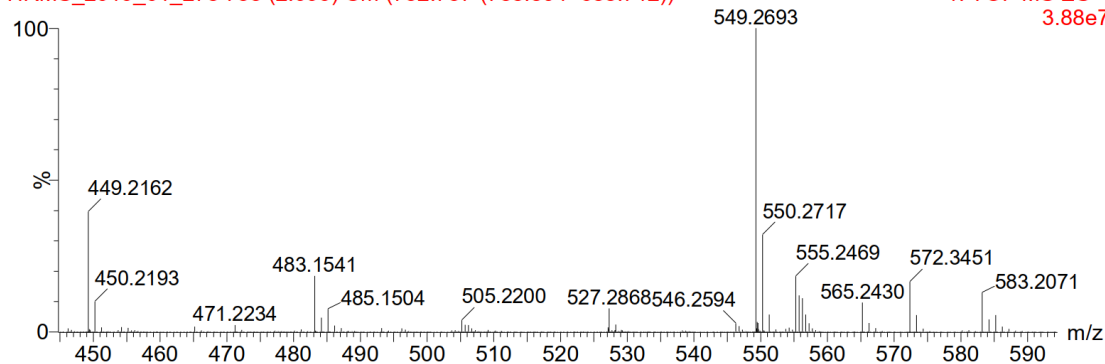
HRMS_2019_01_278 733 (2.096) Cm (732:757-(783:804+688:712))

1: TOF MS ES+
8.16e7



HRMS_2019_01_278 733 (2.096) Cm (732:757-(783:804+688:712))

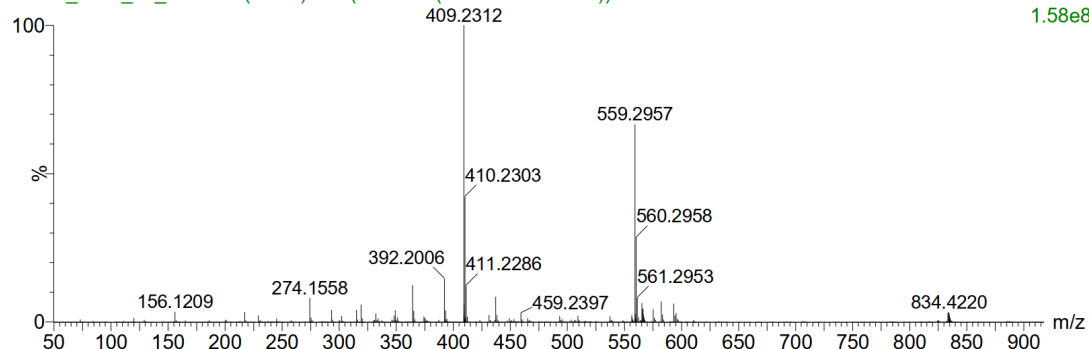
1: TOF MS ES+
3.88e7



Tert-butyl (2-(trimethylsilyl)ethyl) ((S)-6-(((S)-1-amino-1-oxo-3-phenylpropan-2-yl)amino)-6-oxohexane-1,5-diyl)dicarbamate (10).

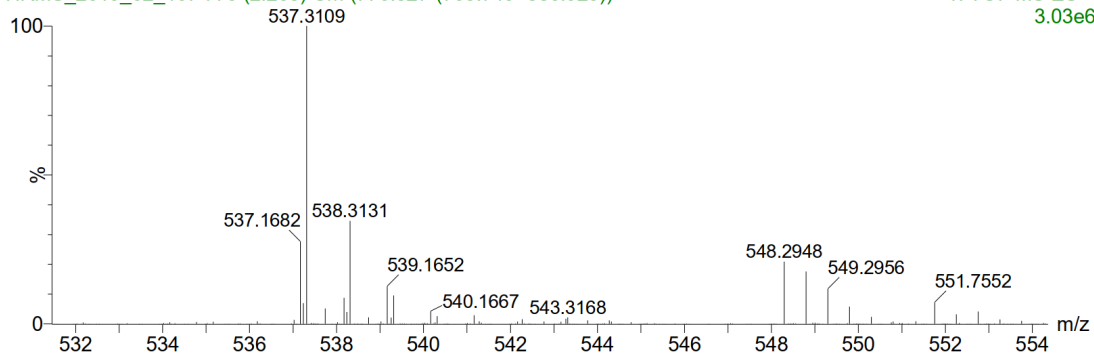
HRMS_2019_02_107 770 (2.203) Cm (770:827-(703:749+886:929))

1: TOF MS ES+
1.58e8



HRMS_2019_02_107 770 (2.203) Cm (770:827-(703:749+886:929))

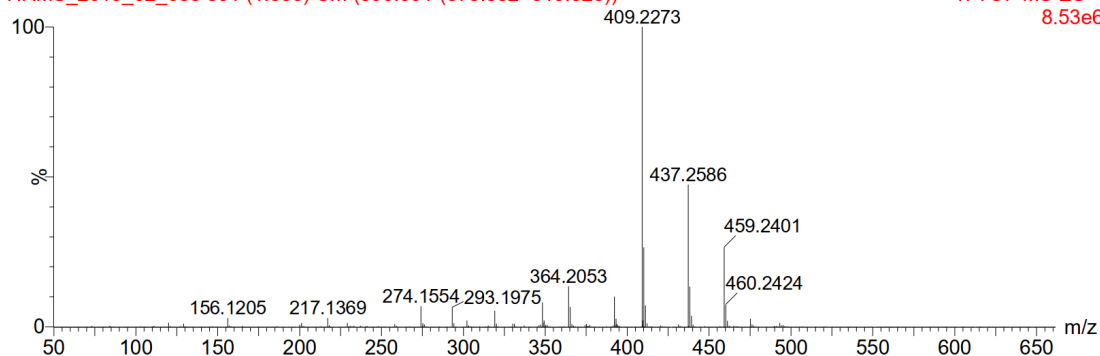
1: TOF MS ES+
3.03e6



(12S,15S)-16-amino-15-benzyl-2,2-dimethyl-6,13,16-trioxo-5-oxa-7,14-diaza-2-silahexadecan-12-aminium 4-methylbenzenesulfonate (11).

HRMS_2019_02_088 591 (1.696) Cm (590:601-(575:582+619:626))

1: TOF MS ES+
8.53e6

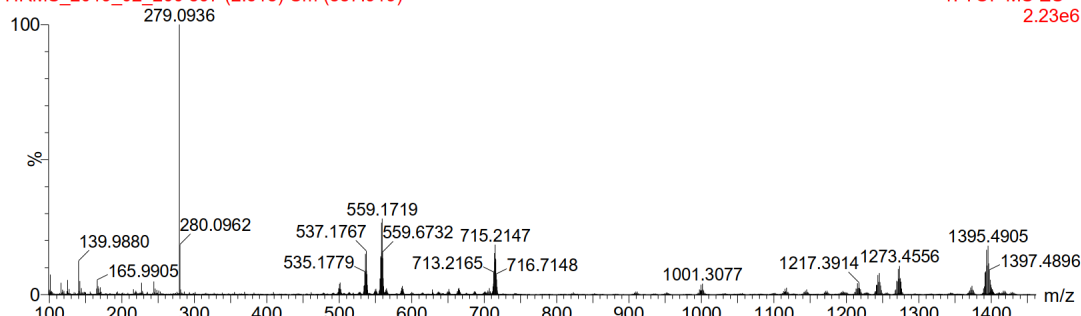


Di-tert-butyl (2-(trimethylsilyl)ethyl) ((12S,15R,20R,23S)-23-(((S)-1-amino-1-oxo-3-phenylpropan-2-yl)carbamoyl)-12-(((S)-1-amino-1-oxo-3-phenylpropan-2-yl)carbamoyl)-

2,2-dimethyl-6,14,21-trioxo-5-oxa-17,18-diselena-7,13,22-triaza-2-silaheptacosane-15,20,27-triyl)tricarbamate (3d).

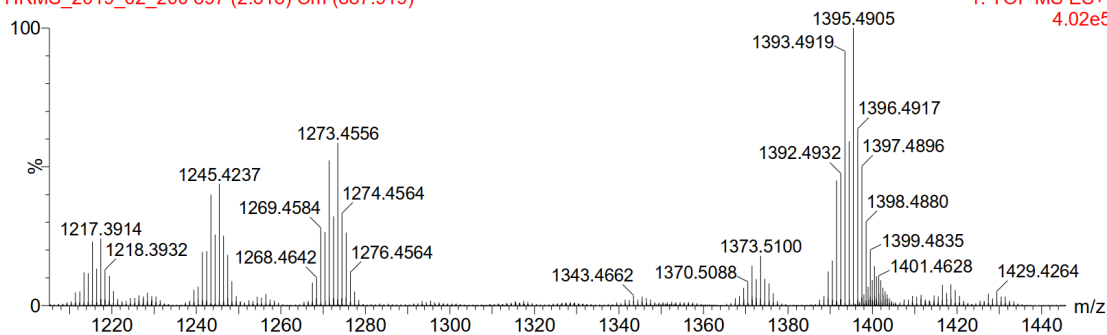
HRMS_2019_02_200 897 (2.518) Cm (887:919)

1: TOF MS ES+
2.23e6



HRMS_2019_02_200 897 (2.518) Cm (887:919)

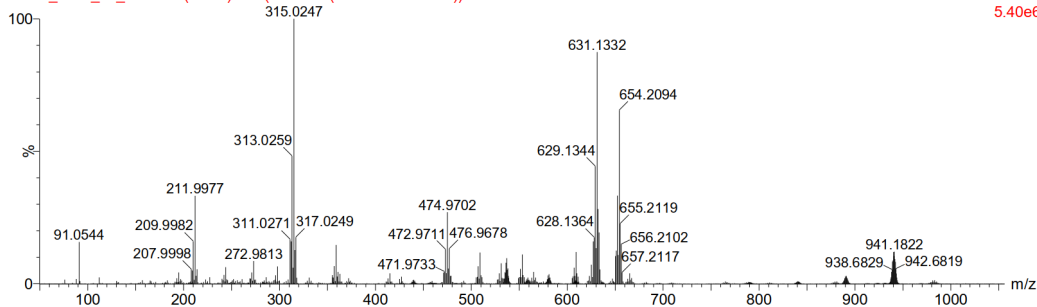
1: TOF MS ES+
4.02e5



Benzyl (R)-(2-((tert-butoxycarbonyl)amino)-3-((2-phenylbenzofuran-3-yl)selenanyl)propanoyl)glycinate (4a).

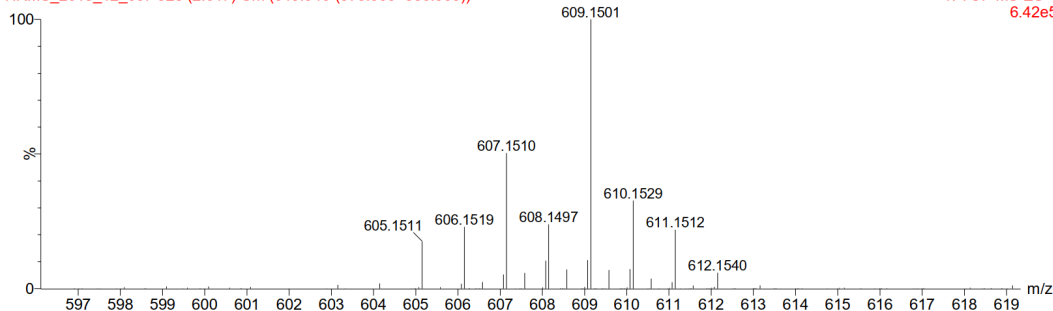
HRMS_2018_12_097 928 (2.647) Cm (919:946-(973:999+885:909))

1: TOF MS ES+
5.40e6



HRMS_2018_12_097 928 (2.647) Cm (919:946-(973:999+885:909))

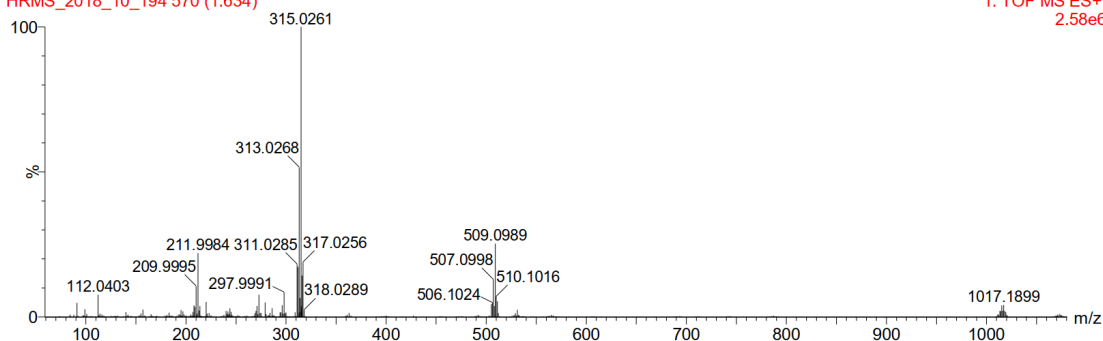
1: TOF MS ES+
6.42e5



(R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-1-oxo-3-((2-phenylbenzofuran-3-yl)selanyl)propan-2-aminium 2,2,2-trifluoroacetate (4b).

HRMS_2018_10_194 570 (1.634)

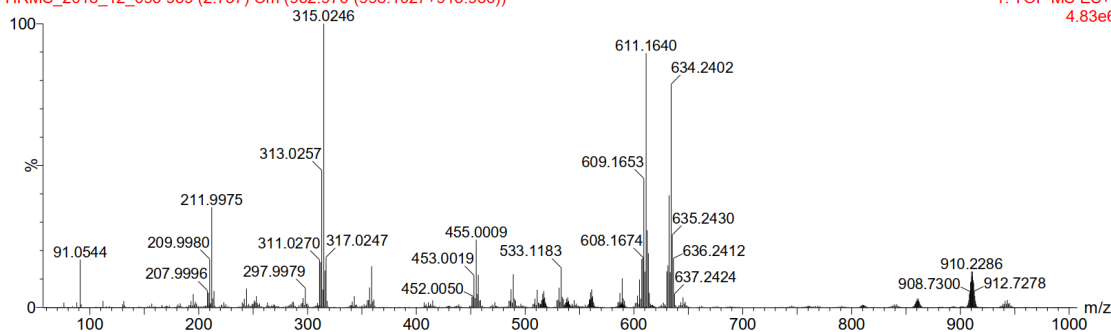
1: TOF MS ES+
2.58e6



Benzyl (R)-(2-amino-3-((2-butylbenzofuran-3-yl)selanyl)propanoyl)glycinate (4c).

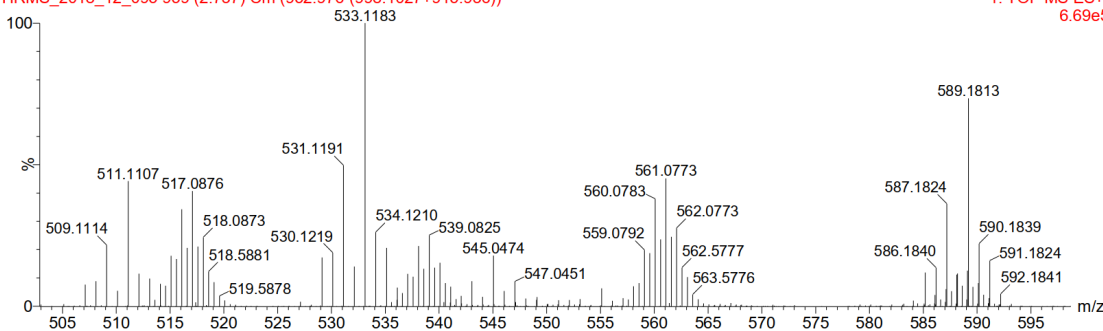
HRMS_2018_12_095 959 (2.737) Cm (952:976-(998:1027+915:936))

1: TOF MS ES+
4.83e6



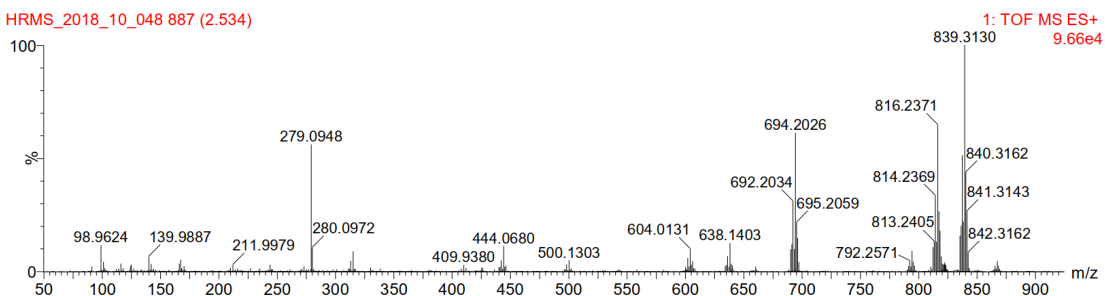
HRMS_2018_12_095 959 (2.737) Cm (952:976-(998:1027+915:936))

1: TOF MS ES+
6.69e5



Tert-butyl N⁵-((R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-1-oxo-3-((2-phenylbenzofuran-3-yl)selanyl)propan-2-yl)-N²-(tert-butoxycarbonyl)-L-glutamate (4d).

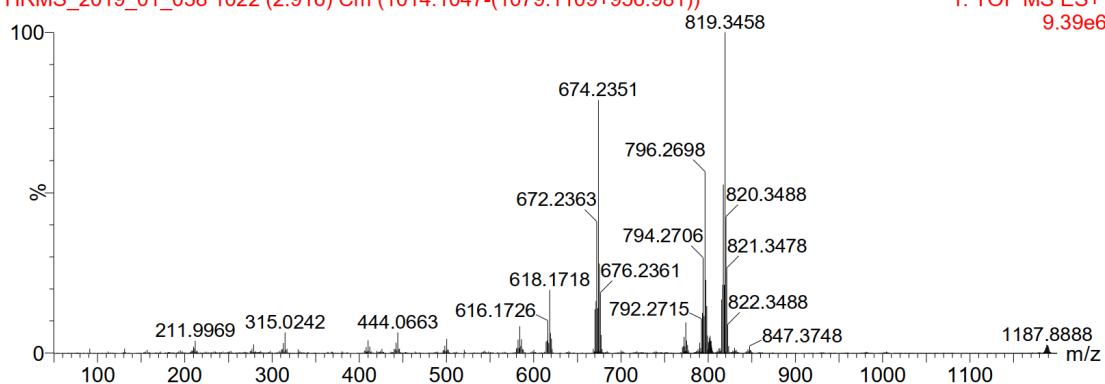
HRMS_2018_10_048 887 (2.534)



***Tert*-butyl N^5 -((*R*)-1-((2-(benzyloxy)-2-oxoethyl)amino)-3-((2-butylbenzofuran-3-yl)selanyl)-1-oxopropan-2-yl)- N^2 -(*tert*-butoxycarbonyl)-L-glutamate (4e).**

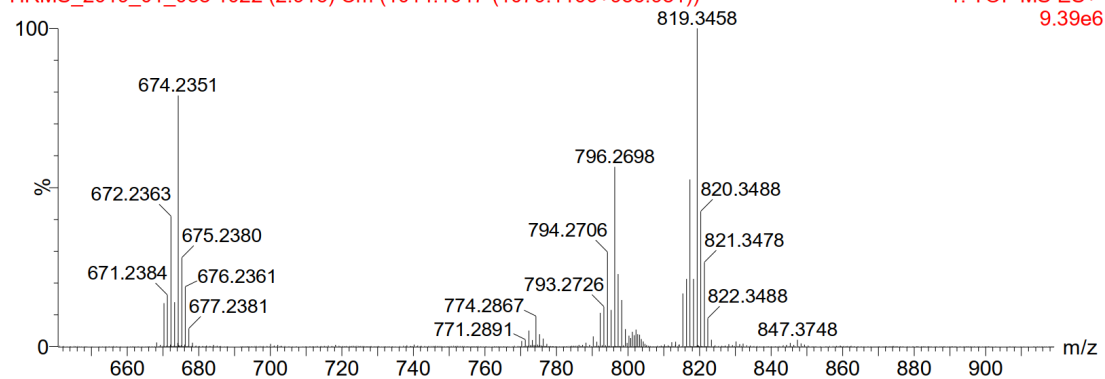
HRMS_2019_01_038 1022 (2.916) Cm (1014:1047-(1079:1109+956:981))

1: TOF MS ES+
9.39e6



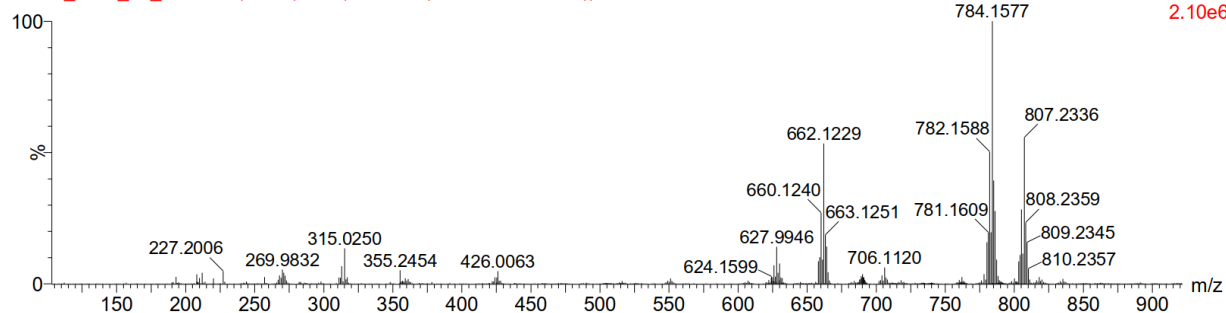
HRMS_2019_01_038 1022 (2.916) Cm (1014:1047-(1079:1109+956:981))

1: TOF MS ES+
9.39e6

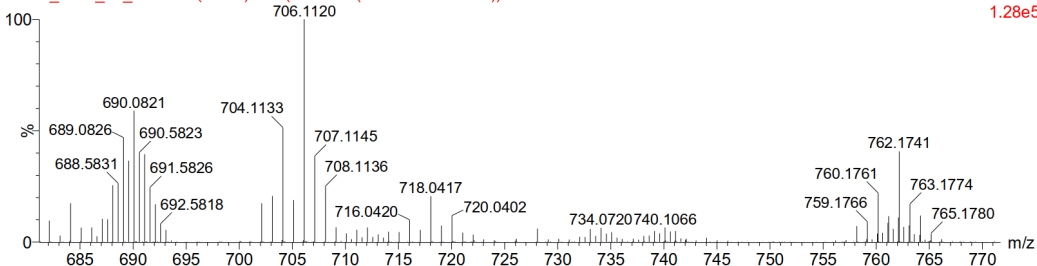


Benzyl (R)-2-((*tert*-butoxycarbonyl)amino)-3-((2-phenyl-1-tosyl-1*H*-indol-3-yl)selanyl)propanoyl)glycinate (6a).

HRMS_2018_09_044 916 (2.614) Cm (909:934-(859:892+953:983))

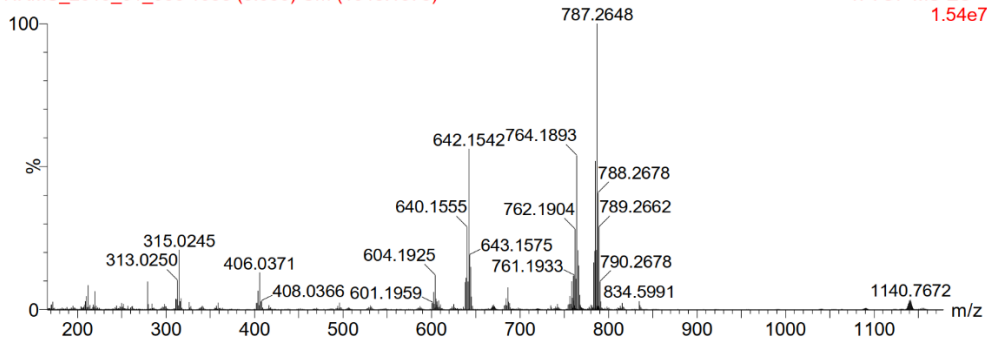


HRMS_2018_09_044 916 (2.614) Cm (909:934-(859:892+953:983))

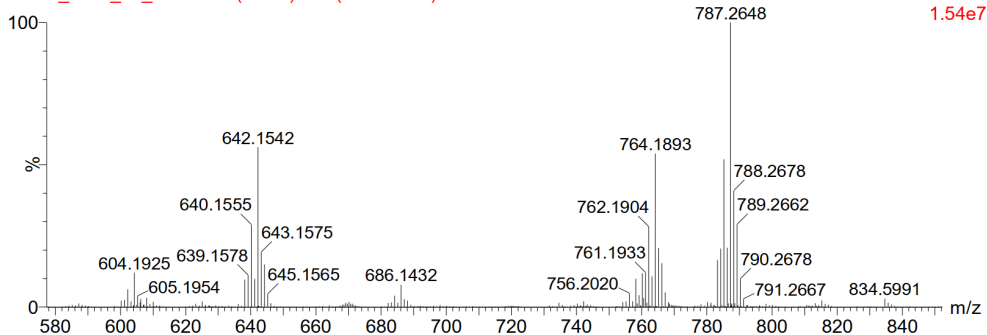


Benzyl (R)-(2-((tert-butoxycarbonyl)amino)-3-((2-butyl-1-tosyl-1H-indol-3-yl)selenanyl)propanoyl)glycinate (6b).

HRMS_2019_01_036 1053 (3.000) Cm (1048:1075)



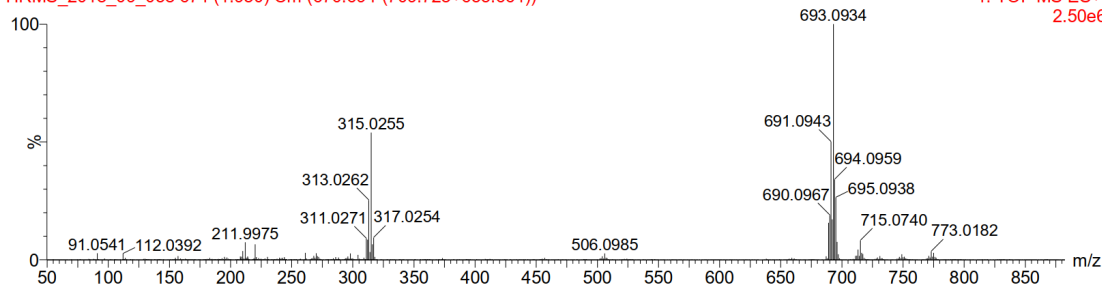
HRMS_2019_01_036 1053 (3.000) Cm (1048:1075)



(R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-3-((1-((4-nitrophenyl)sulfonyl)-2-phenyl-1H-indol-3-yl)selanyl)-1-oxopropan-2-aminium 2,2,2-trifluoroacetate (6c).

HRMS_2018_09_058 674 (1.930) Cm (670:694-(709:723+655:664))

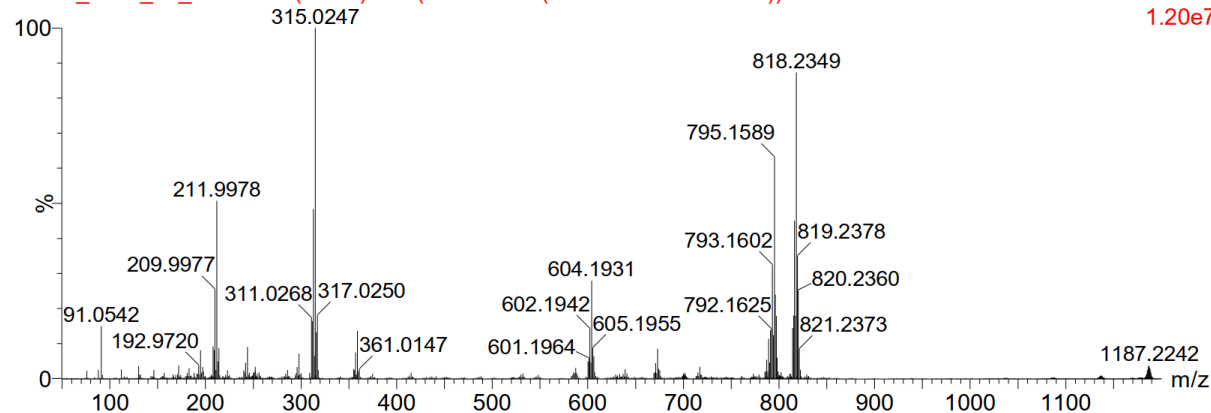
1: TOF MS ES+
2.50e6



Benzyl (R)-2-((tert-butoxycarbonyl)amino)-3-((2-butyl-1-((4-nitrophenyl)sulfonyl)-1H-indol-3-yl)selanyl)propanoyl)glycinate (6d).

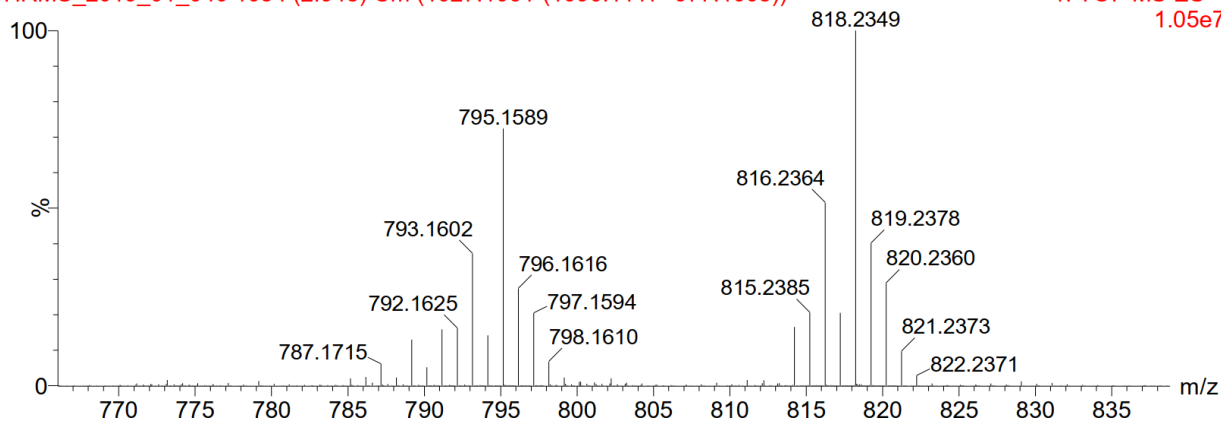
HRMS_2019_01_040 1034 (2.948) Cm (1027:1061-(1090:1117+977:1003))

1: TOF MS ES+
1.20e7



HRMS_2019_01_040 1034 (2.948) Cm (1027:1061-(1090:1117+977:1003))

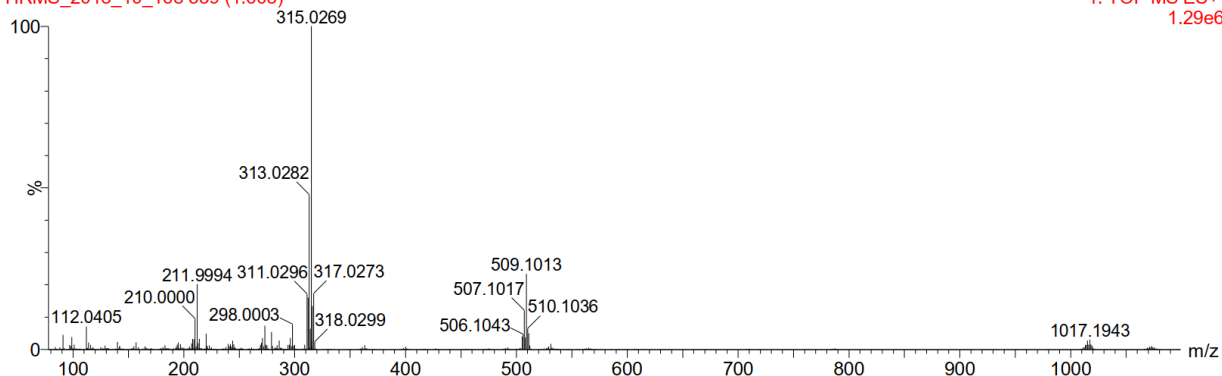
1: TOF MS ES+
1.05e7



(R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-1-oxo-3-((2-phenyl-1H-indol-3-yl)selanyl)propan-2-aminium 2,2,2-trifluoroacetate (6f).

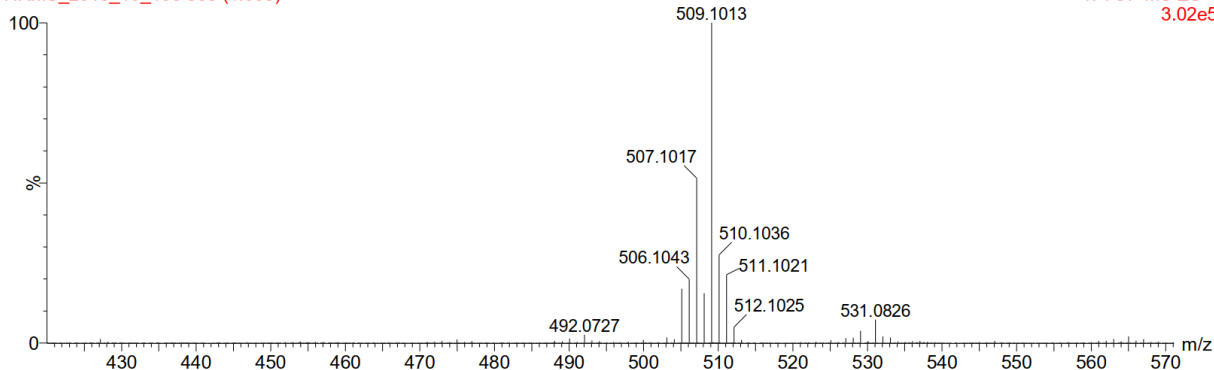
HRMS_2018_10_168 559 (1.603)

1: TOF MS ES+
1.29e6



HRMS_2018_10_168 559 (1.603)

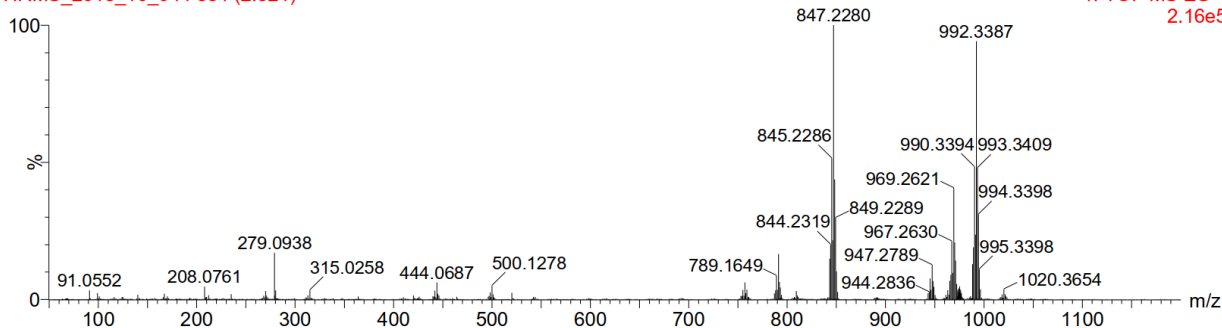
1: TOF MS ES+
3.02e5



Tert-butyl N⁵-((R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-1-oxo-3-((2-phenyl-1-tosyl-1H-indol-3-yl)selanyl)propan-2-yl)-N²-(tert-butoxycarbonyl)-L-glutamate (6j).

HRMS_2018_10_044 884 (2.521)

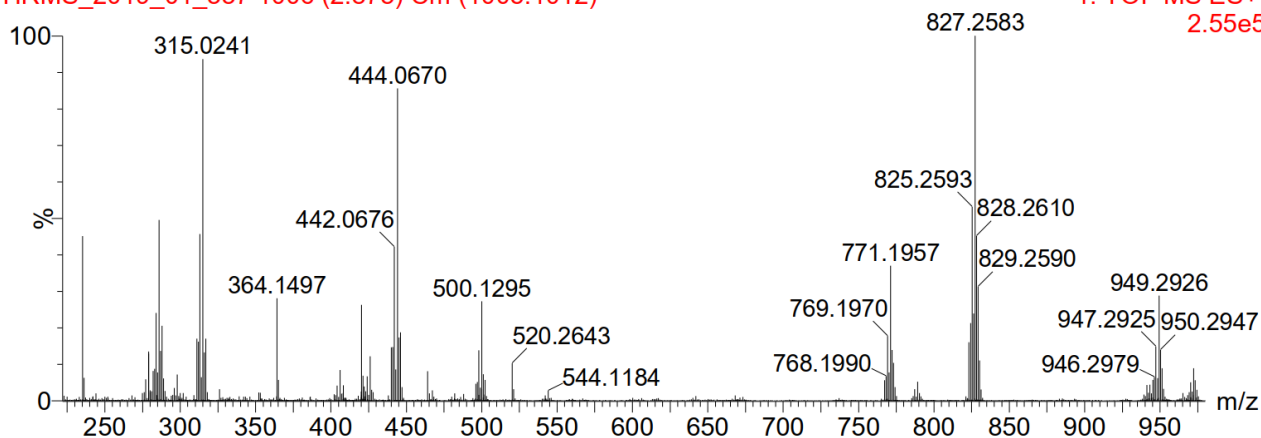
1: TOF MS ES+
2.16e5



Tert-butyl N⁵-((R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-3-((2-butyl-1-tosyl-1H-indol-3-yl)selanyl)-1-oxopropan-2-yl)-N²-(tert-butoxycarbonyl)-L-glutamate (6k).

HRMS_2019_01_337 1006 (2.873) Cm (1005:1012)

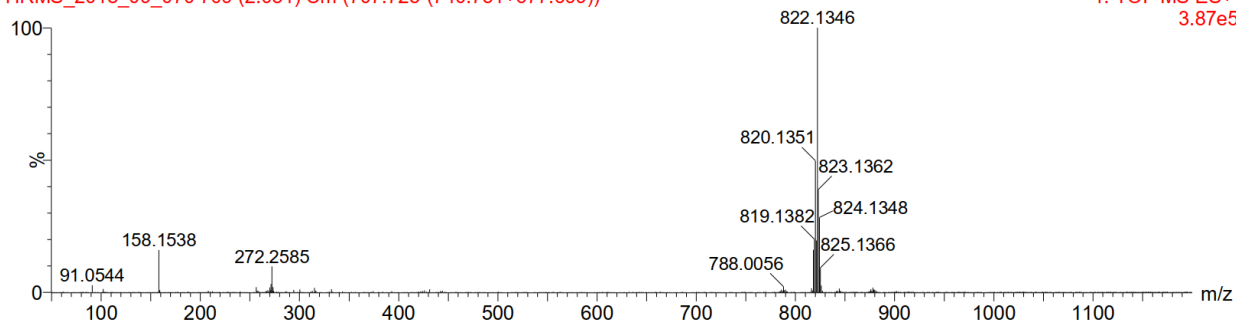
1: TOF MS ES+
2.55e5



(S)-4-(((R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-3-((1-((4-nitrophenyl)sulfonyl)-2-phenyl-1H-indol-3-yl)selanyl)-1-oxopropan-2-yl)amino)-1-carboxy-4-oxobutan-1-aminium 2,2,2-trifluoroacetate (6l).

HRMS_2018_09_070 709 (2.031) Cm (707:725-(740:751+677:699))

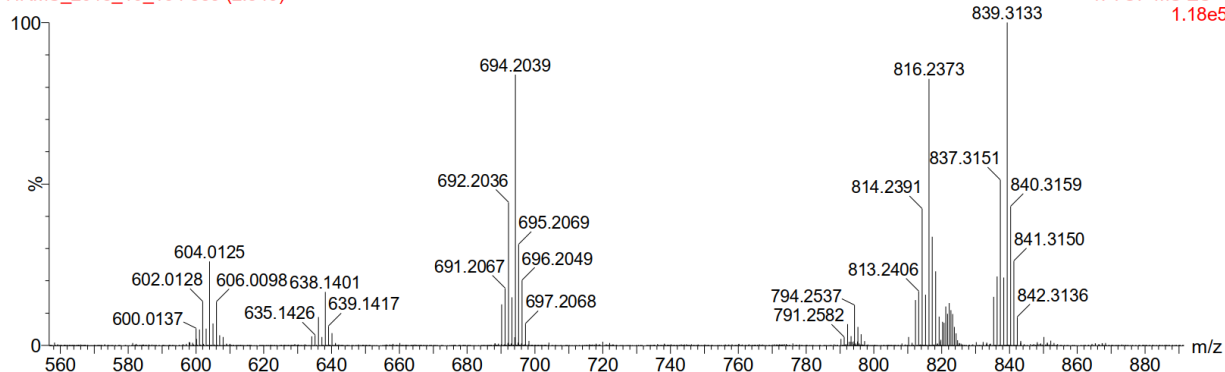
1: TOF MS ES+
3.87e5



Tert-butyl N⁵-((R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-1-oxo-3-((2-phenyl-1H-indol-3-yl)selanyl)propan-2-yl)-N²-(tert-butoxycarbonyl)-L-glutamate (6m).

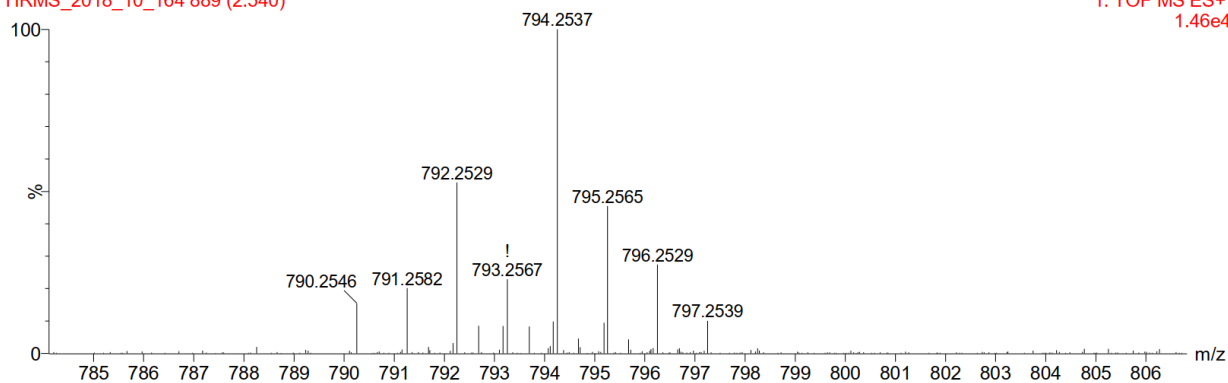
HRMS_2018_10_164 889 (2.540)

1: TOF MS ES+
1.18e5



HRMS_2018_10_164 889 (2.540)

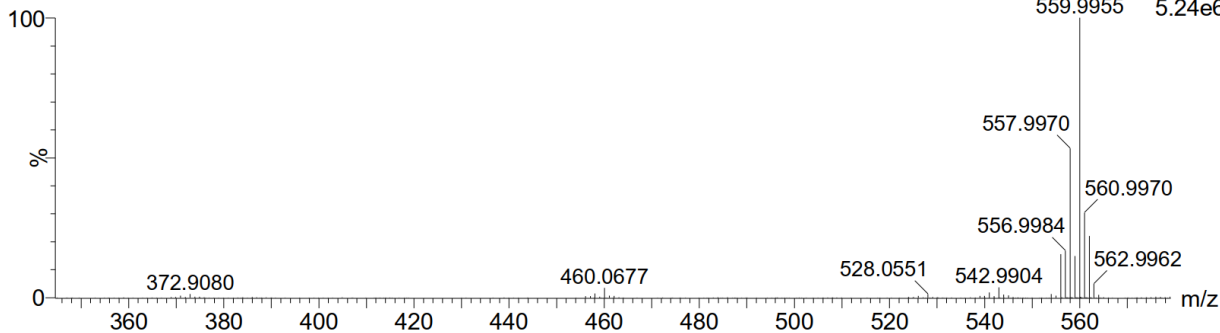
1: TOF MS ES+
1.46e4



(R)-2-((tert-butoxycarbonyl)amino)-3-((2-phenylbenzofuran-3-yl)selanyl)propanoic acid (4f).

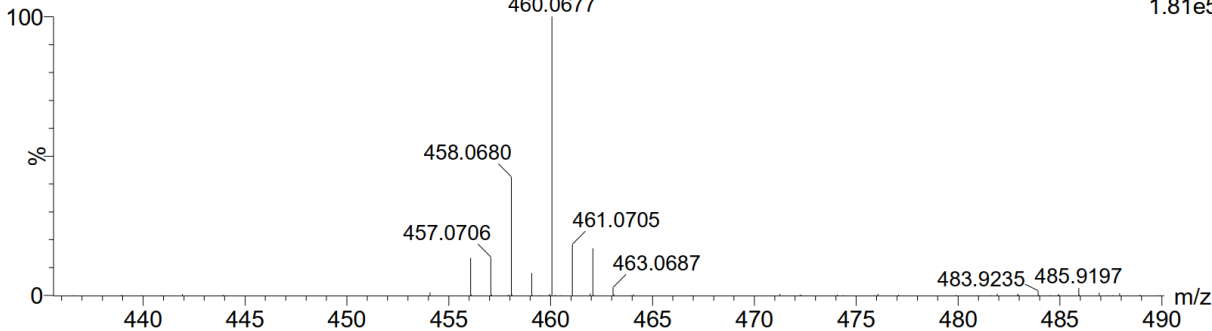
HRMS_2019_12_203 866 (2.433) Cm (866:881-(831:846+946:965))

1: TOF MS ES-
5.24e6



HRMS_2019_12_203 866 (2.433) Cm (866:881-(831:846+946:965))

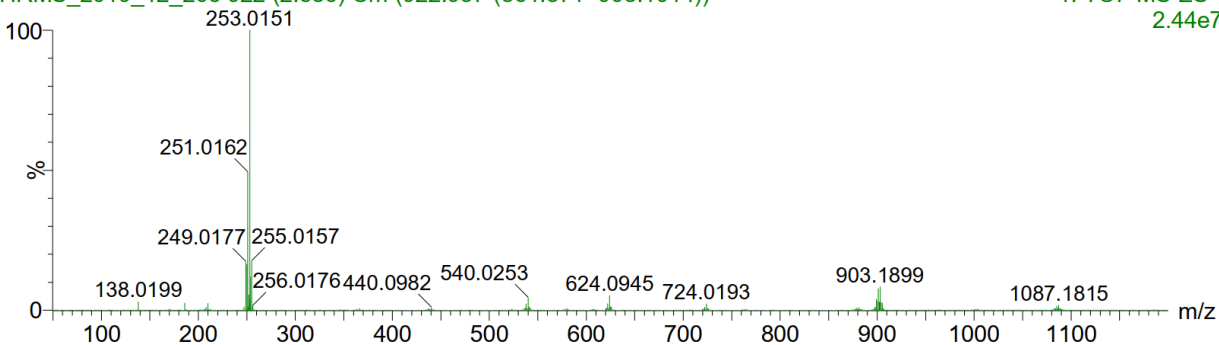
1: TOF MS ES-
1.81e5



(R)-2-((tert-butoxycarbonyl)amino)-3-((2-butylbenzofuran-3-yl)selanyl)propanoic acid (4g).

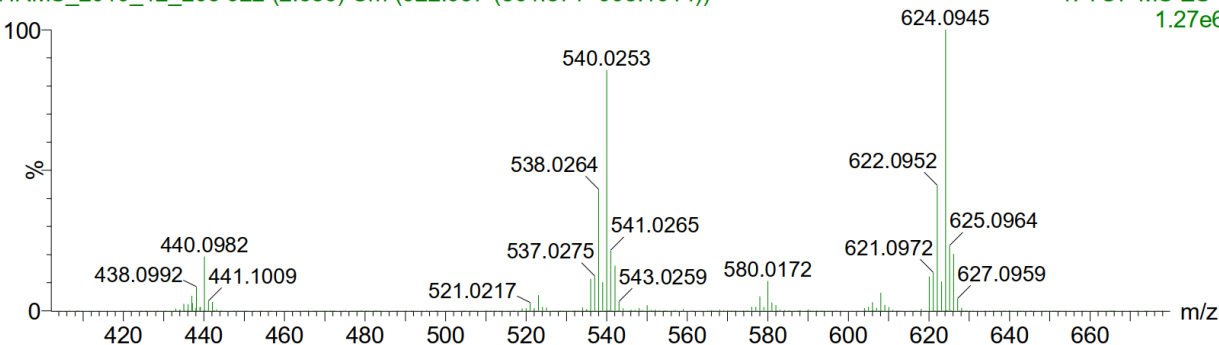
HRMS_2019_12_205 922 (2.586) Cm (922:937-(861:871+998:1014))

1: TOF MS ES-
2.44e7



HRMS_2019_12_205 922 (2.586) Cm (922:937-(861:871+998:1014))

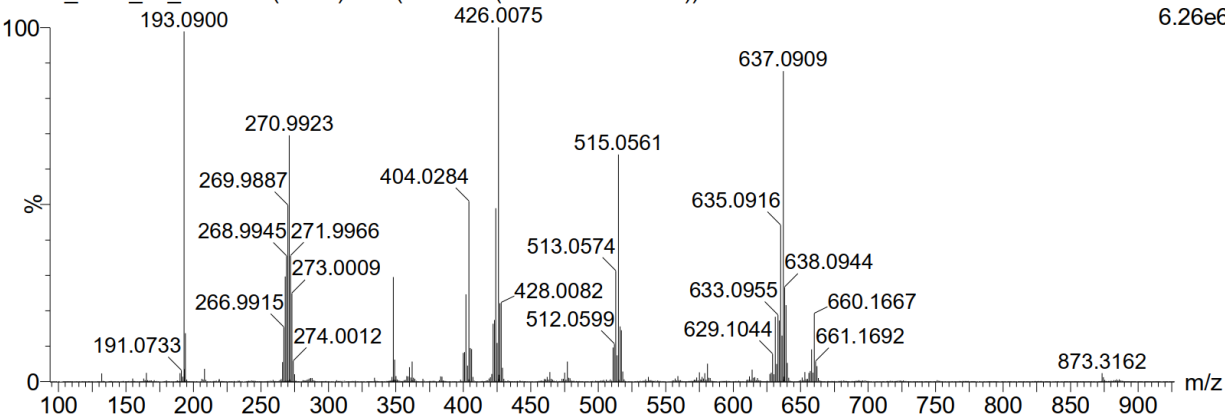
1: TOF MS ES-
1.27e6



(R)-2-((*tert*-butoxycarbonyl)amino)-3-((2-phenyl-1-tosyl-1*H*-indol-3-yl)selanyl)propanoic acid (6n).

HRMS_2019_12_046 850 (2.428) Cm (848:853-(829:837+876:879))

1: TOF MS ES+
6.26e6

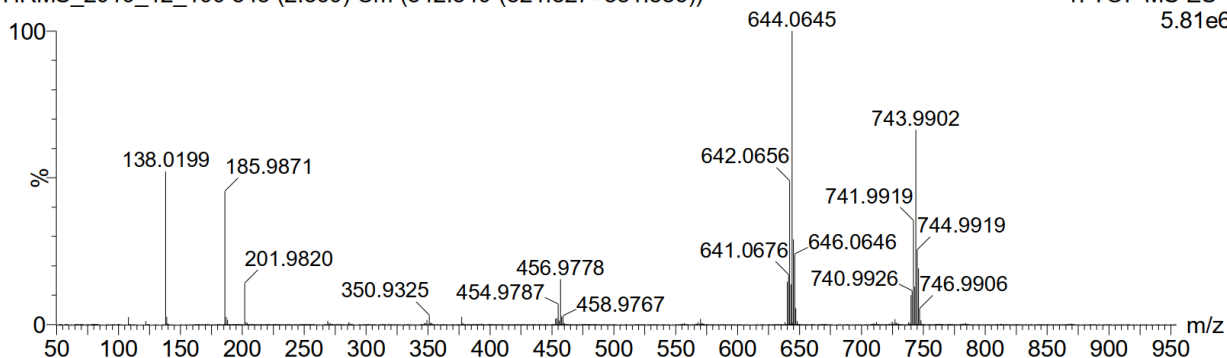


(R)-2-((*tert*-butoxycarbonyl)amino)-3-((1-((4-nitrophenyl)sulfonyl)-2-phenyl-1*H*-indol-3-yl)selanyl)propanoic acid

(6o).

HRMS_2019_12_199 843 (2.369) Cm (842:849-(821:827+881:886))

1: TOF MS ES-
5.81e6

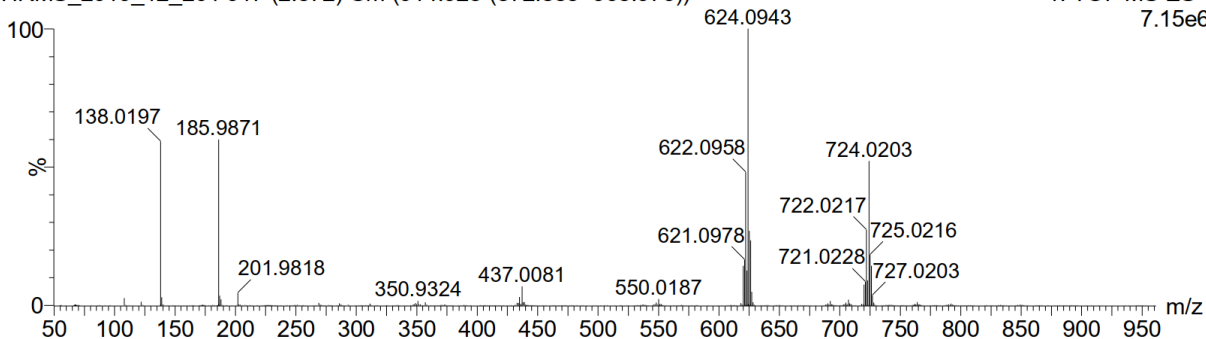


(R)-2-((*tert*-butoxycarbonyl)amino)-3-((2-butyl-1-((4-nitrophenyl)sulfonyl)-1*H*-indol-3-yl)selanyl)propanoic acid

(6p).

HRMS_2019_12_201 917 (2.572) Cm (914:923-(872:885+963:976))

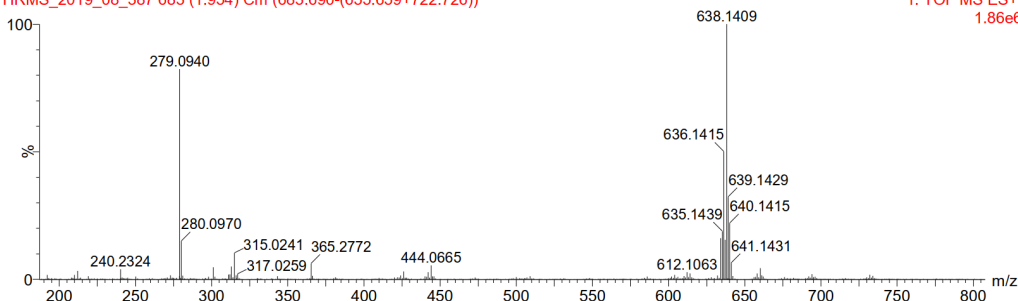
1: TOF MS ES-
7.15e6



(S)-4-(((R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-1-oxo-3-((2-phenylbenzofuran-3-yl)selanyl)propan-2-yl)amino)-1-carboxy-4-oxobutan-1-aminium chloride (4i).

HRMS_2019_08_387 683 (1.954) Cm (683:690-(655:659+722:726))

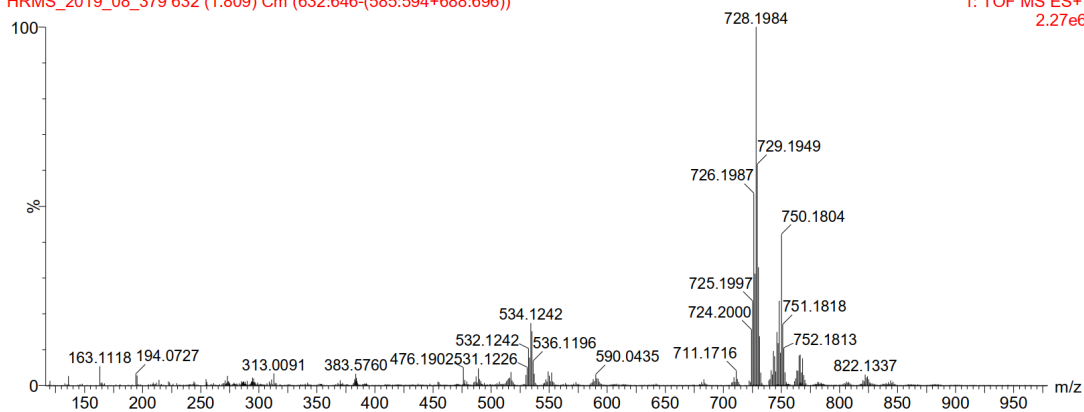
1: TOF MS ES+
1.86e6



3-((2-phenylbenzofuran-3-yl)selanyl)propan-2-yl)amino)-3-(4-hydroxyphenyl)-1-oxopropan-2-aminium chloride (4j).

HRMS_2019_08_379 632 (1.809) Cm (632:646-(585:594+688:696))

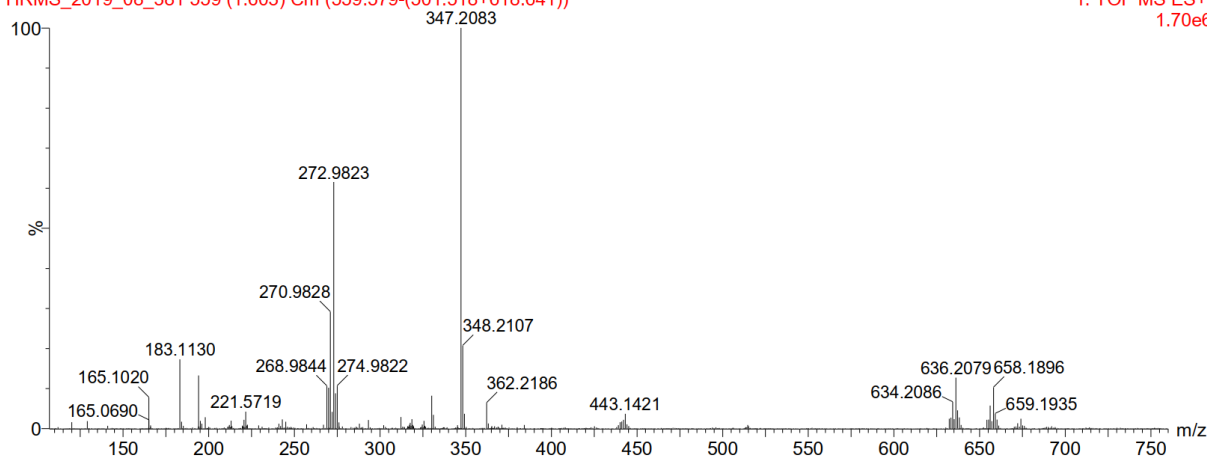
1: TOF MS ES+
2.27e6



(S)-6-(((S)-1-amino-1-oxo-3-phenylpropan-2-yl)amino)-5-((R)-2-ammonio-3-((2-phenylbenzofuran-3-yl)selanyl)propanamido)-6-oxohexan-1-aminium dichloride (4k).

HRMS_2019_08_381 559 (1.603) Cm (559:579-(501:518+618:641))

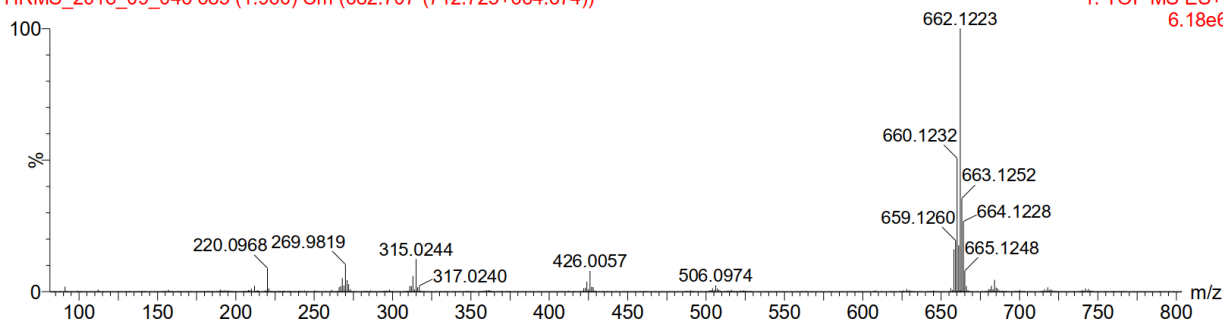
1: TOF MS ES+
1.70e6



(R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-1-oxo-3-((2-phenyl-1-tosyl-1H-indol-3-yl)selanyl)propan-2-aminium chloride (6r).

HRMS_2018_09_046 685 (1.960) Cm (682:707-(712:725+664:674))

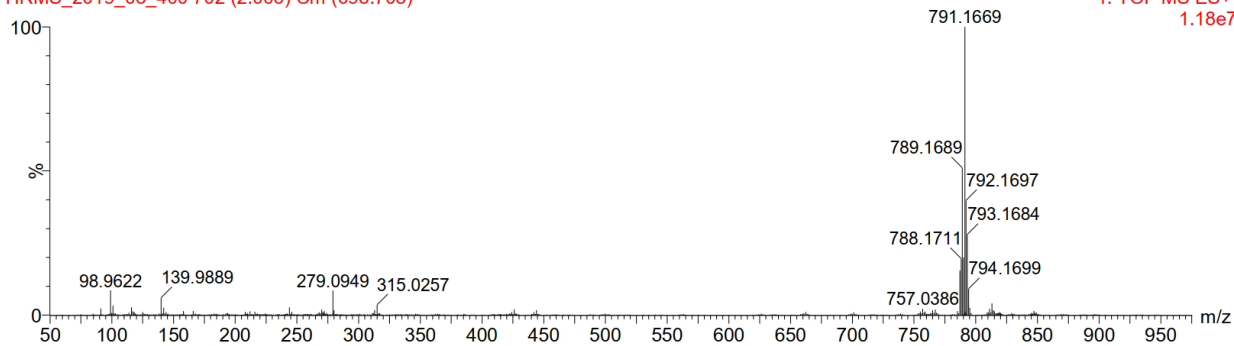
1: TOF MS ES+
6.18e6



(S)-4-(((R)-1-((2-(benzyloxy)-2-oxoethyl)amino)-1-oxo-3-((2-phenyl-1-tosyl-1H-indol-3-yl)selanyl)propan-2-yl)amino)-1-carboxy-4-oxobutan-1-aminium chloride (6s).

HRMS_2019_08_400 702 (2.006) Cm (698:708)

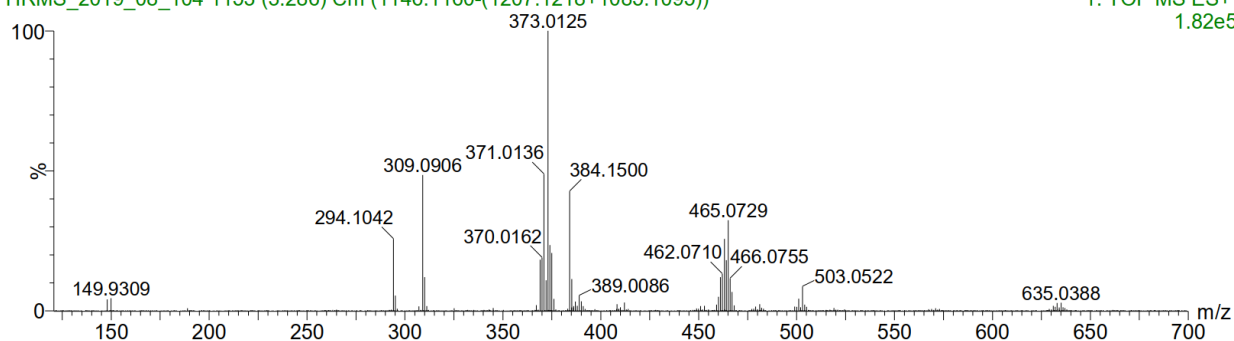
1: TOF MS ES+
1.18e7



11-(benzylselanyl)-6-phenylindeno[1,2-c]chromene (8a).

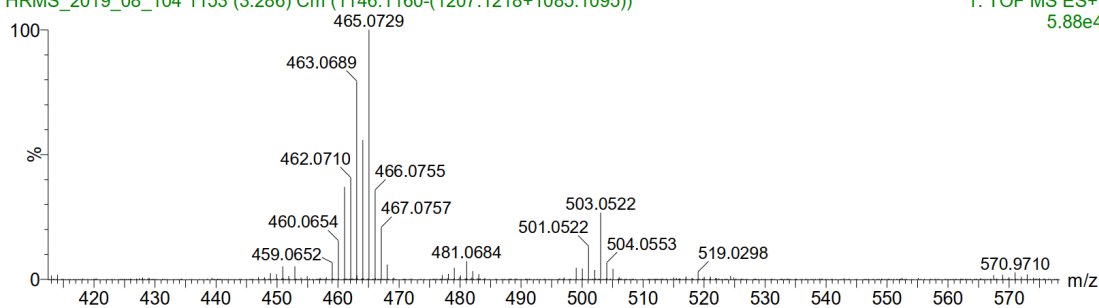
HRMS_2019_08_104 1153 (3.286) Cm (1146:1160-(1207:1218+1085:1095))

1: TOF MS ES+
1.82e5



HRMS_2019_08_104 1153 (3.286) Cm (1146:1160-(1207:1218+1085:1095))

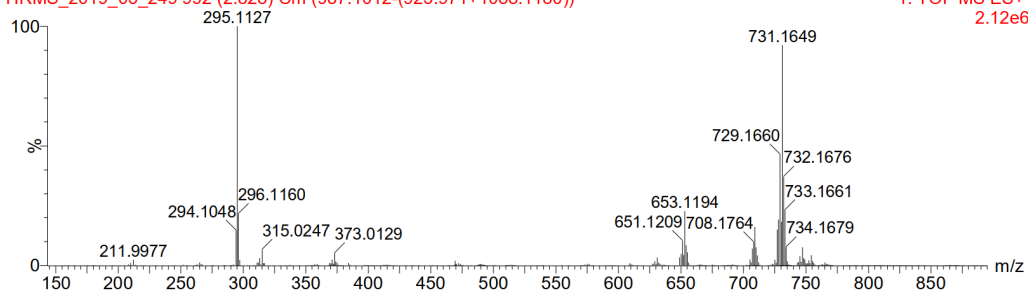
1: TOF MS ES+
5.88e4



(R)-benzyl 2-(2-((tert-butoxycarbonyl)amino)-3-((6-phenylindeno[1,2-c]chromen-11-yl)selanyl)propanamido)acetate (8b).

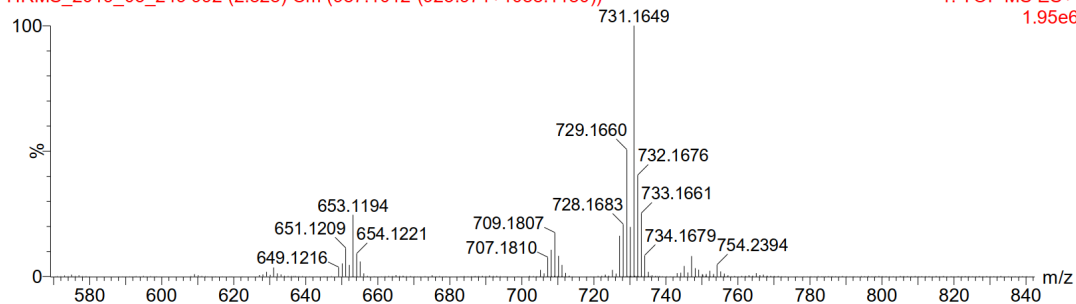
HRMS_2019_05_249 992 (2.828) Cm (987:1012-(923:971+1088:1180))

1: TOF MS ES+
2.12e6



HRMS_2019_05_249 992 (2.828) Cm (987:1012-(923:971+1088:1180))

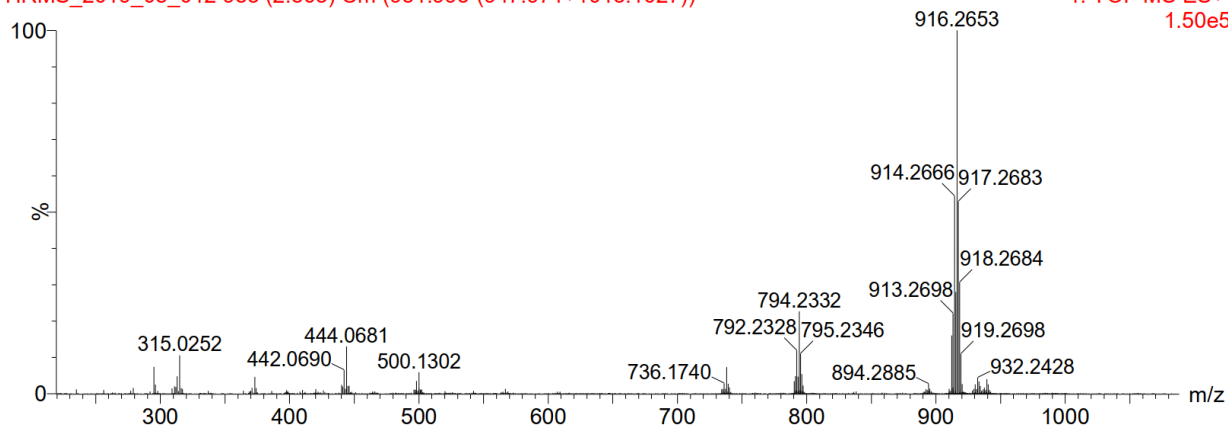
1: TOF MS ES+
1.95e6

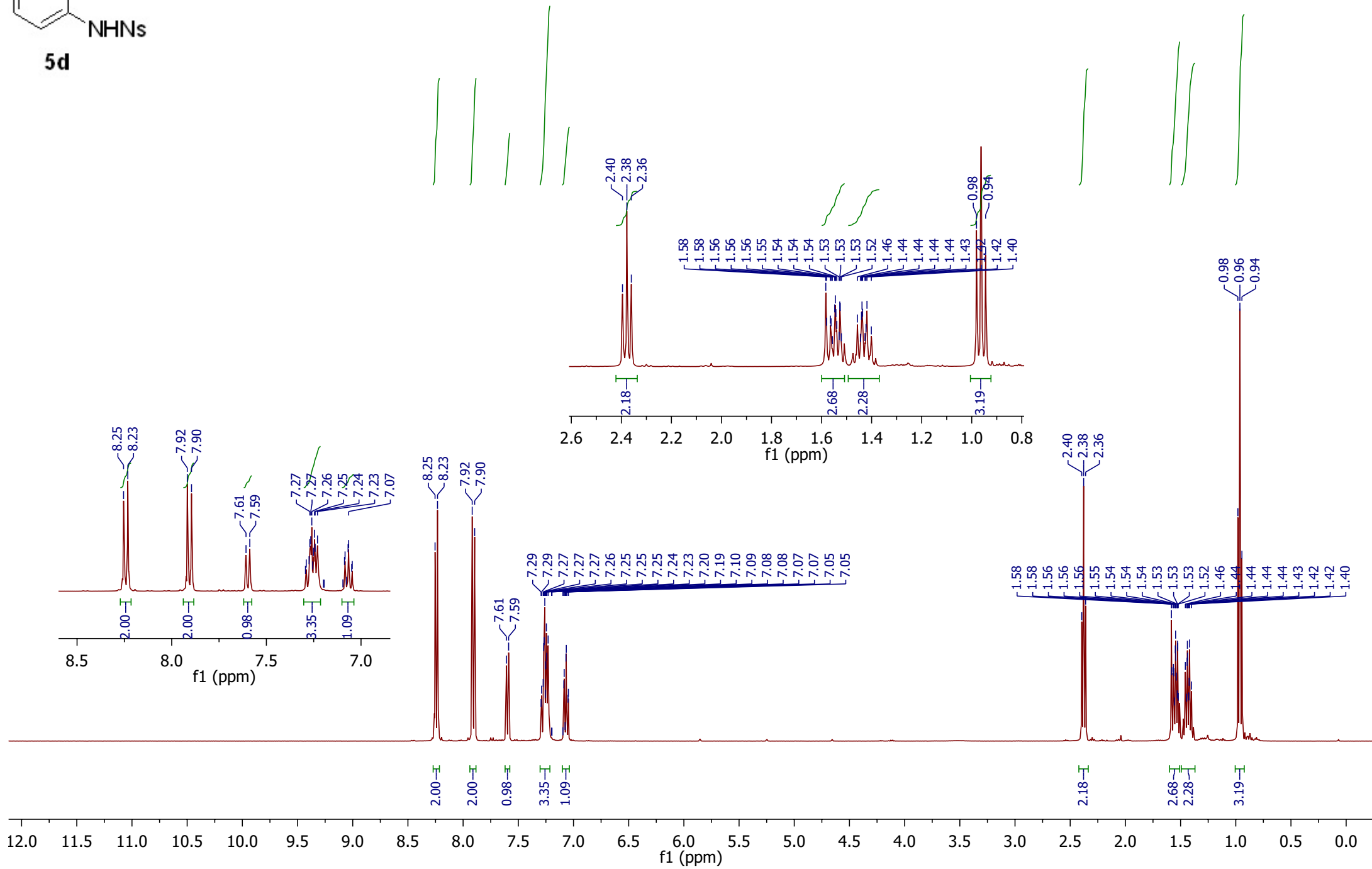
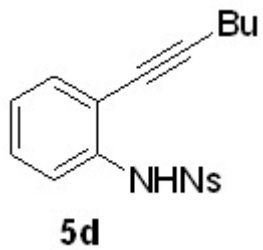


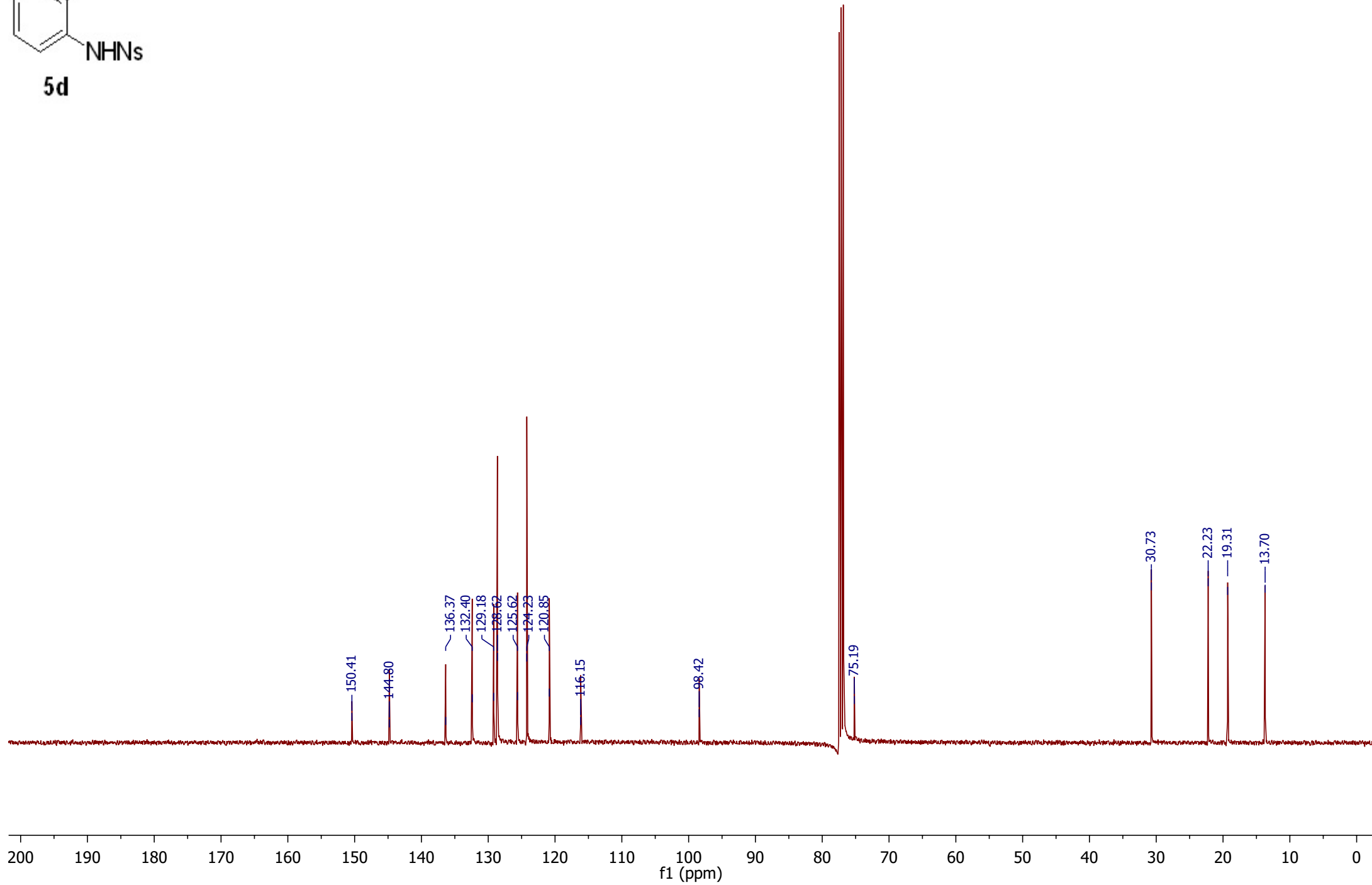
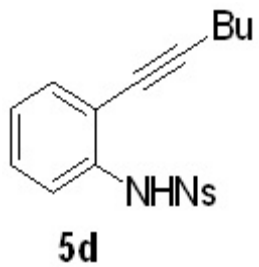
(6*S*,11*R*)-benzyl 6-(*tert*-butoxycarbonyl)-2,2-dimethyl-4,9,12-trioxo-11-(((6-phenylindeno[1,2-*c*]chromen-11-yl)selanyl)methyl)-3-oxa-5,10,13-triazapentadecan-15-oate (8c).

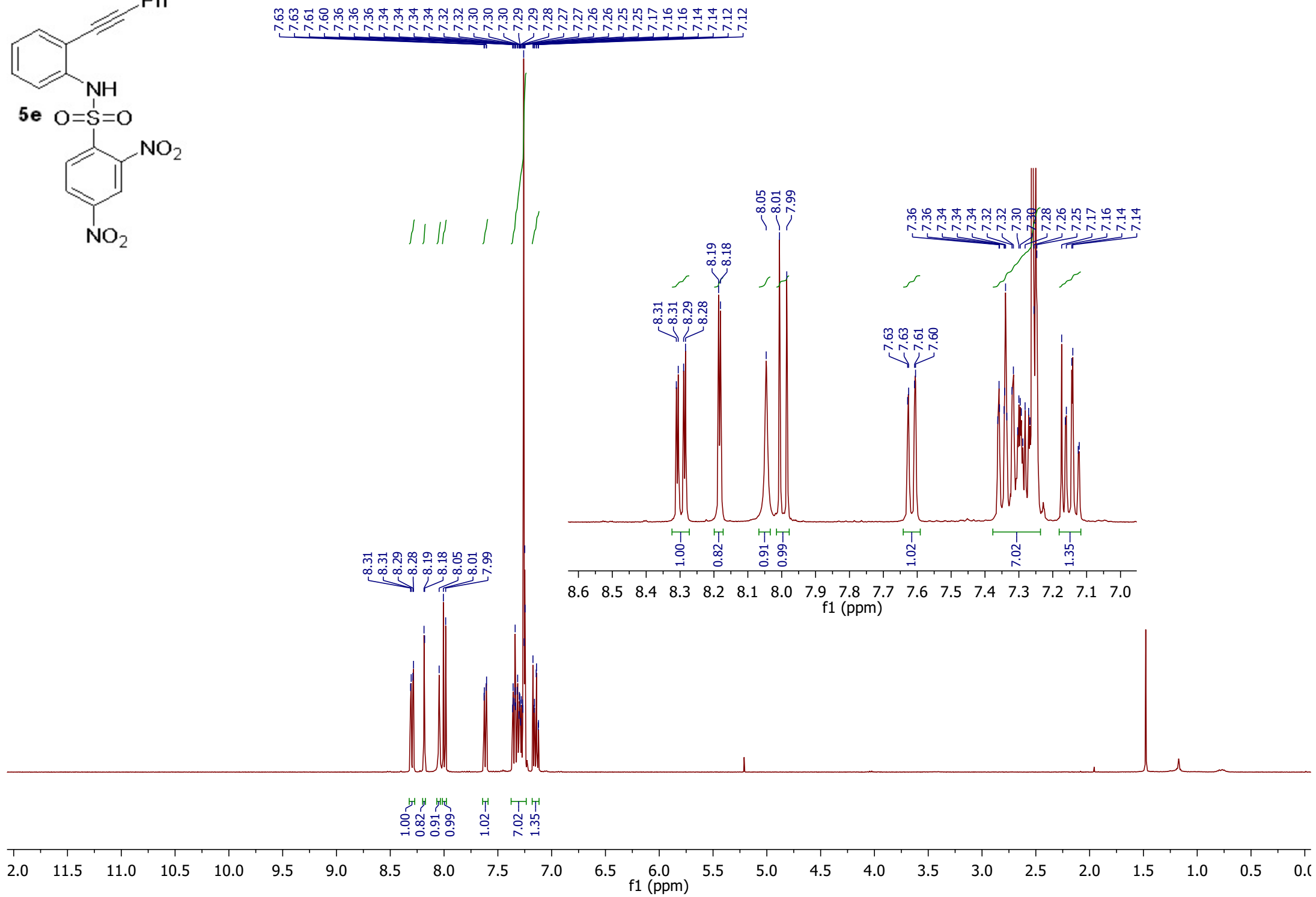
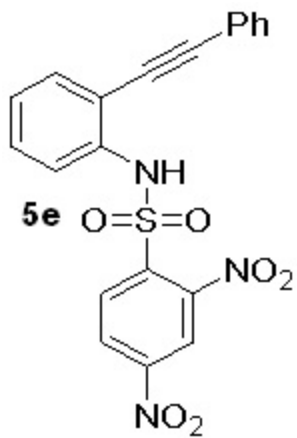
HRMS_2019_08_012 983 (2.803) Cm (981:995-(947:971+1013:1027))

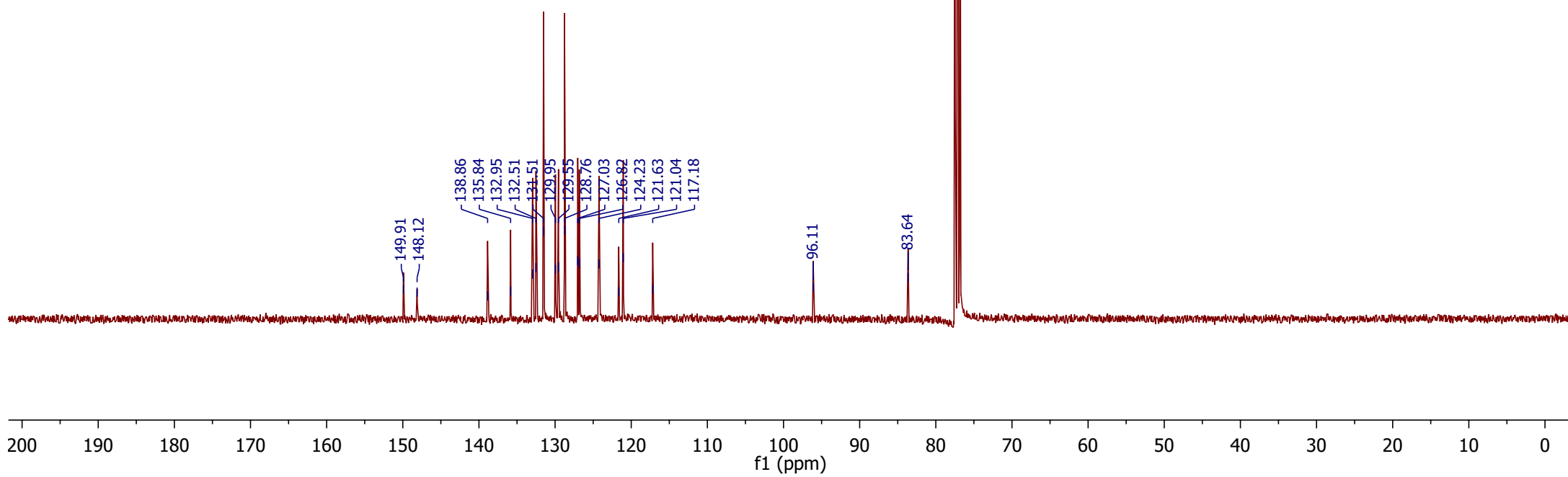
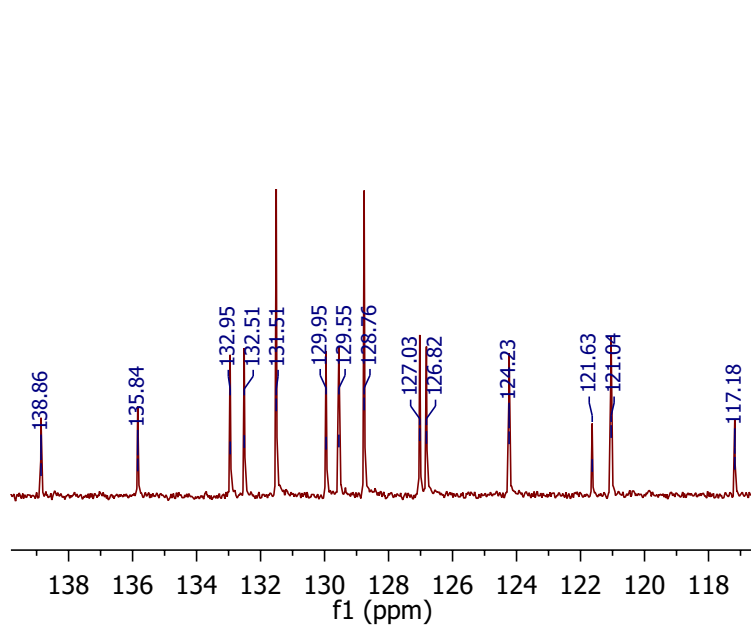
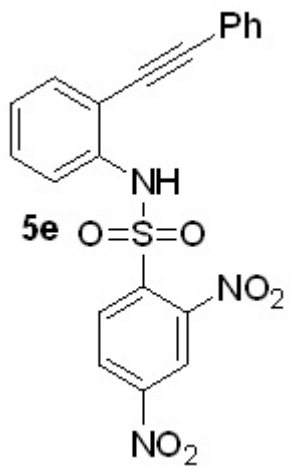
1: TOF MS ES+
1.50e5

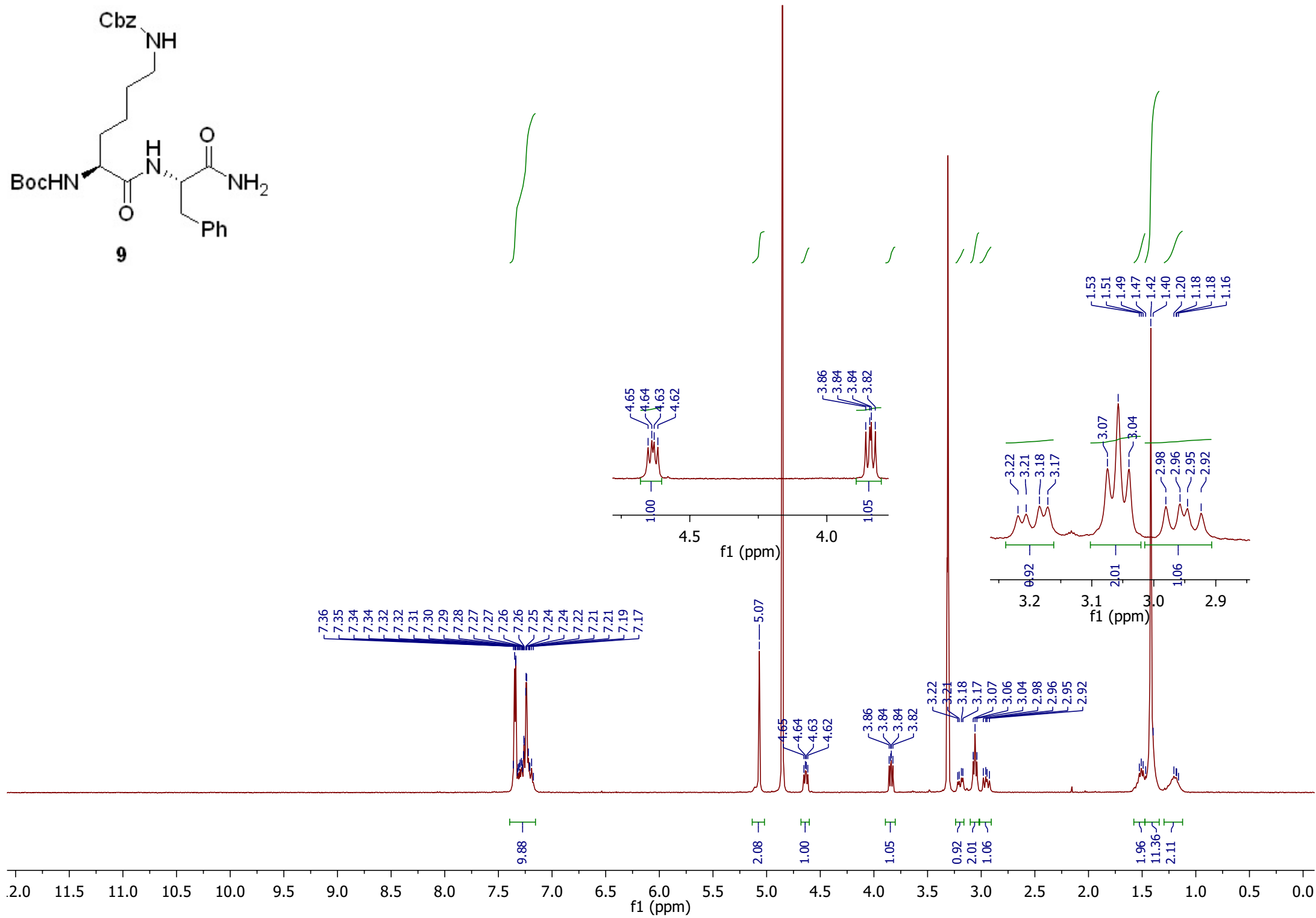
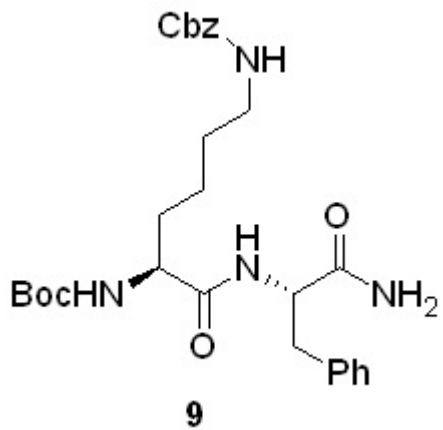


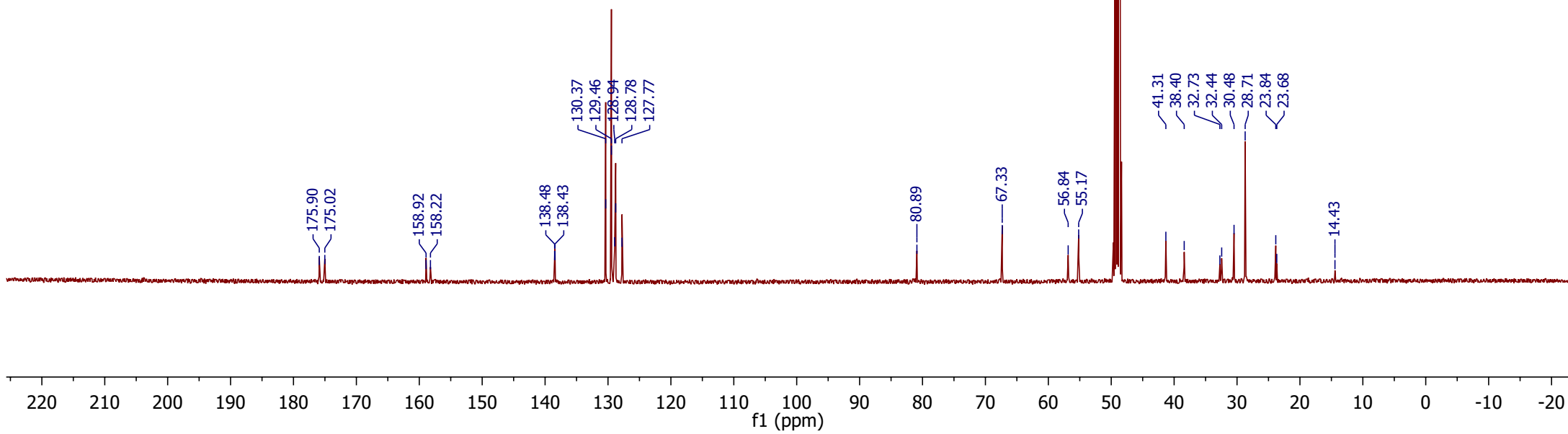
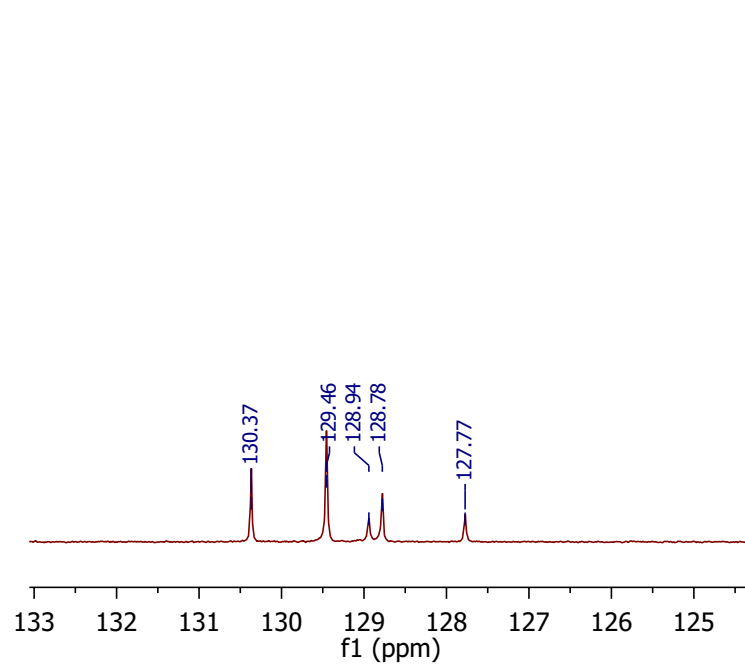
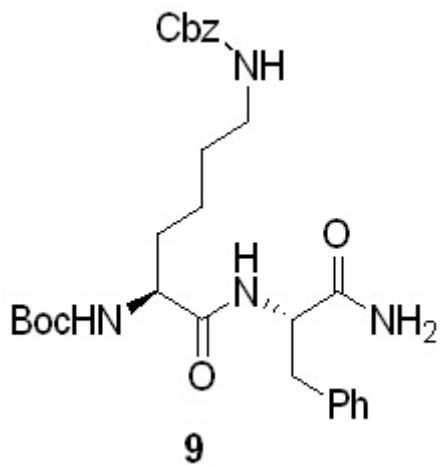


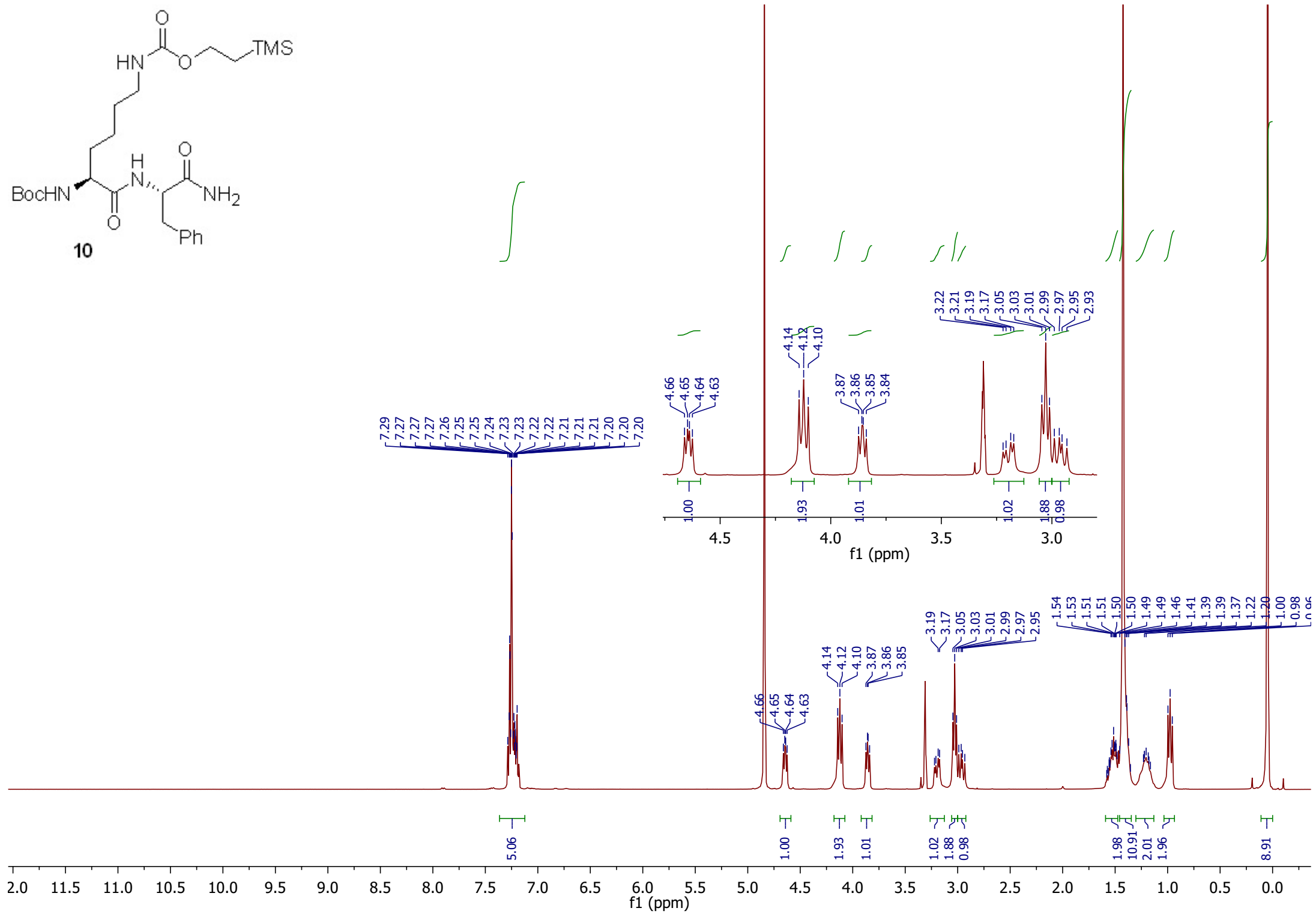
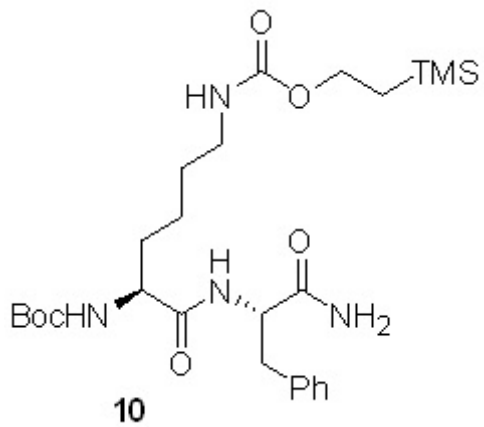


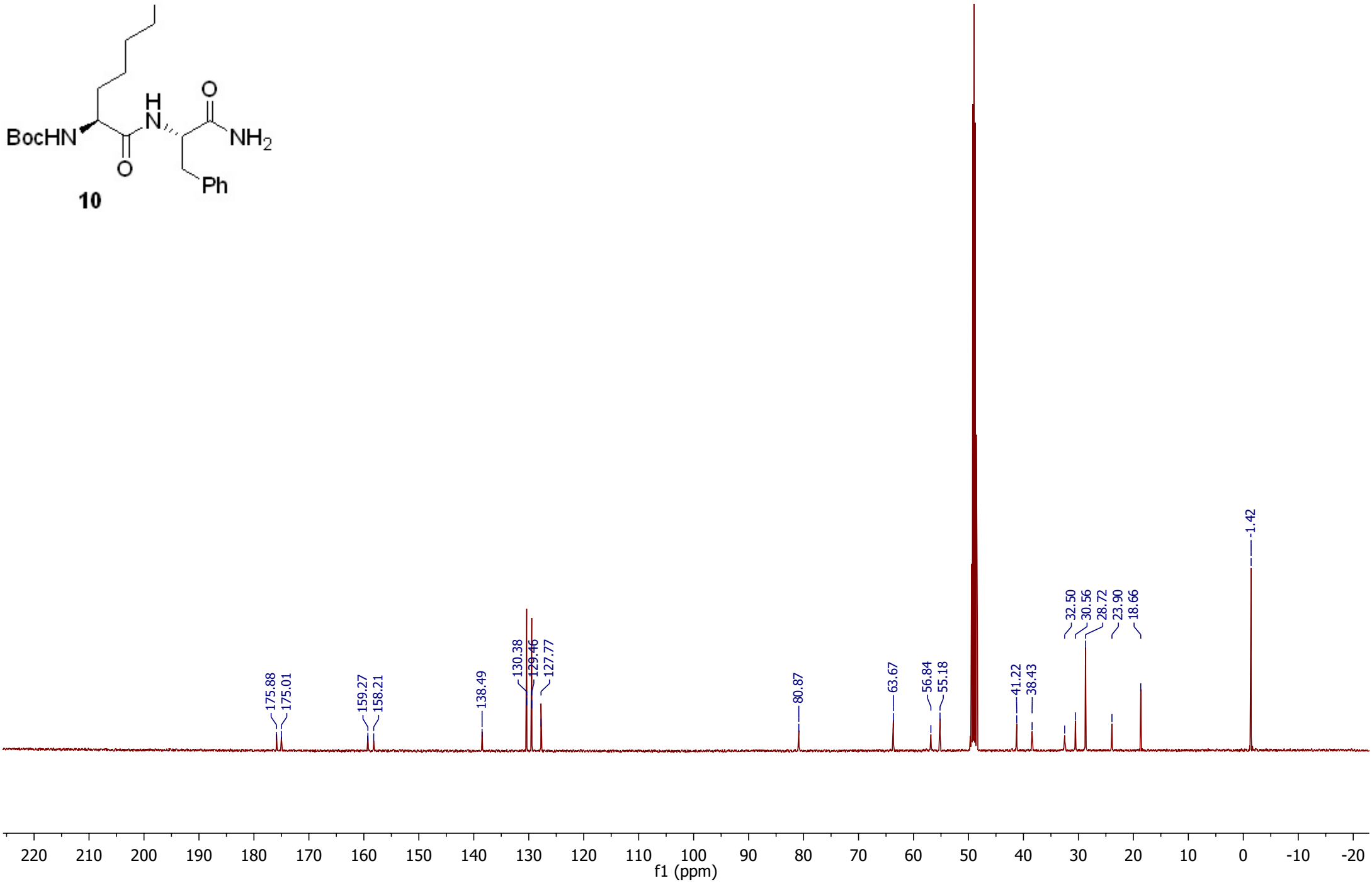
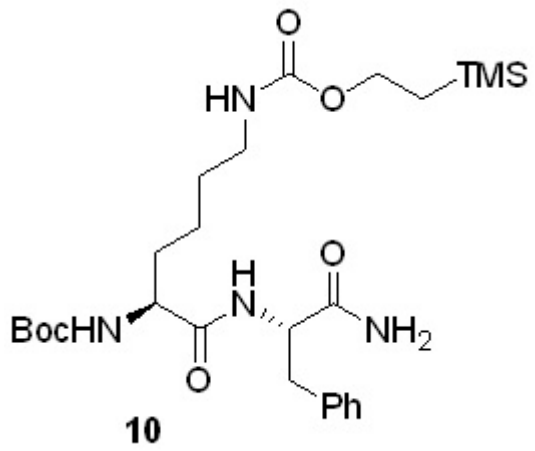


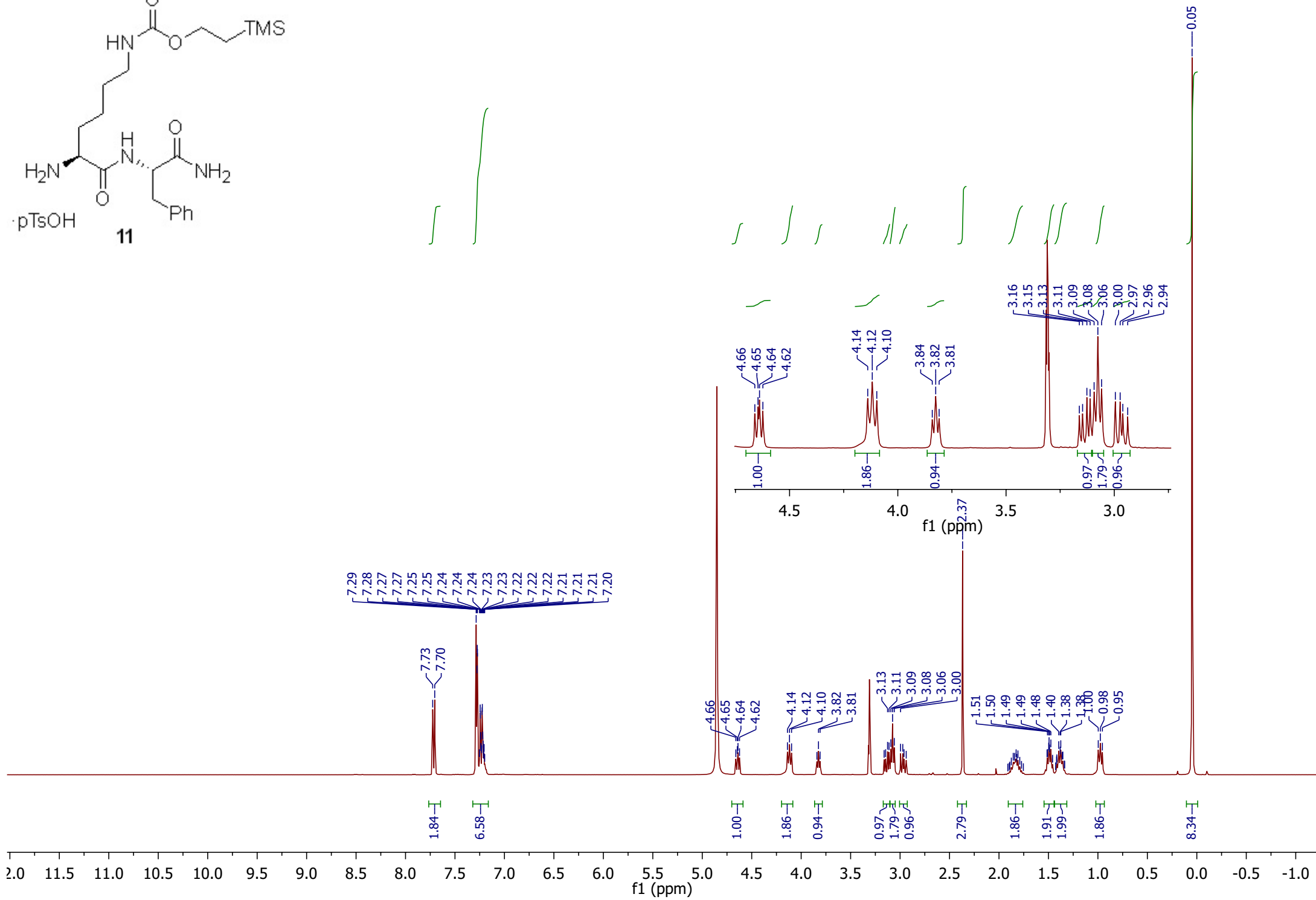
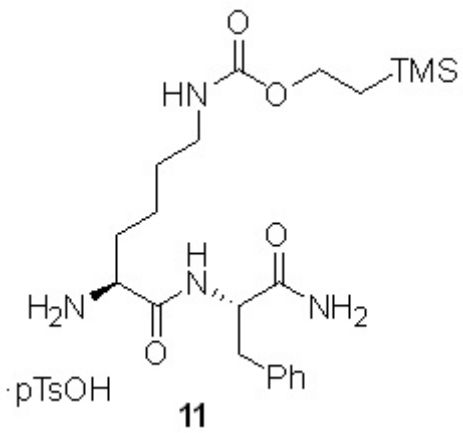


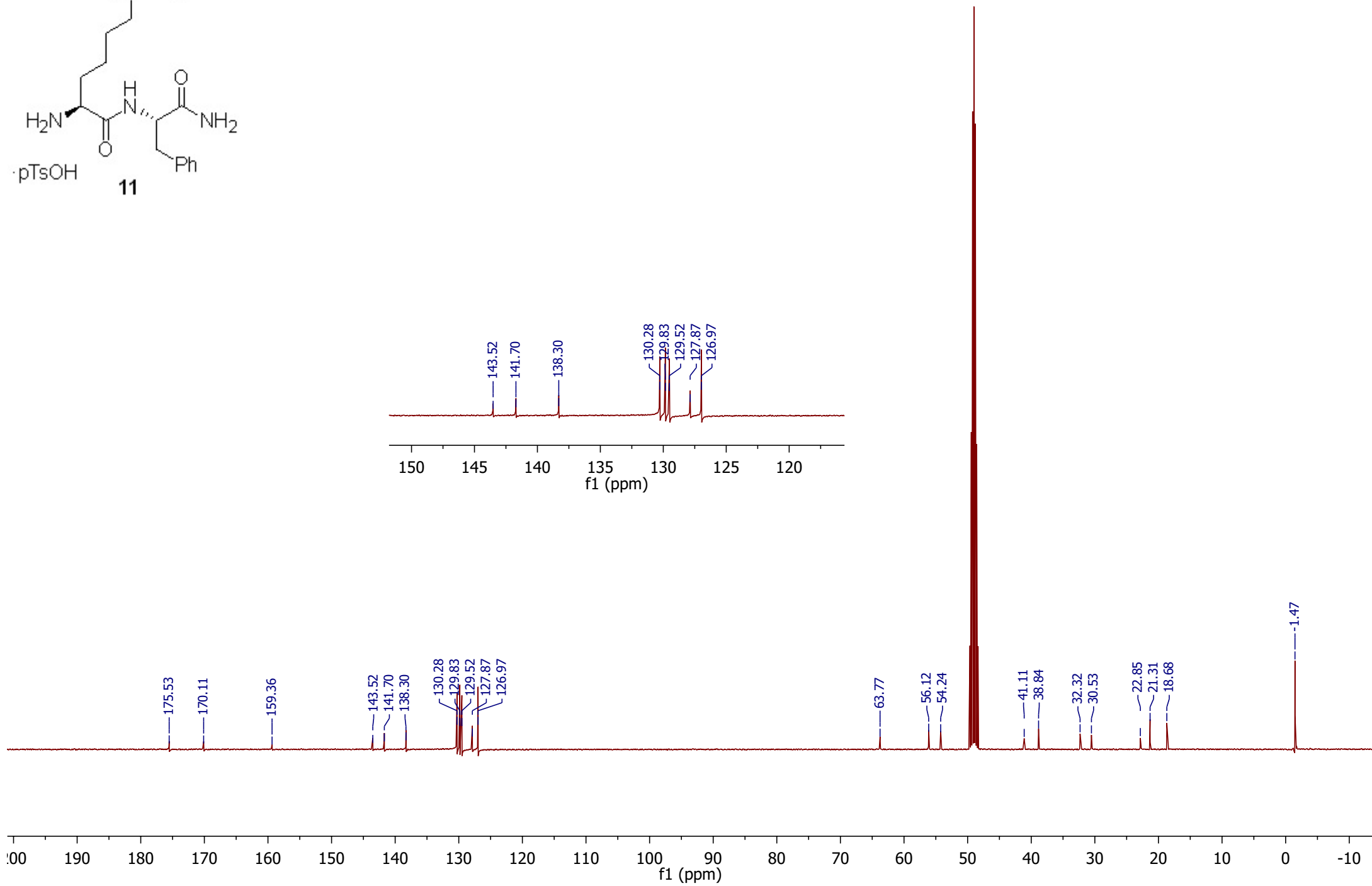
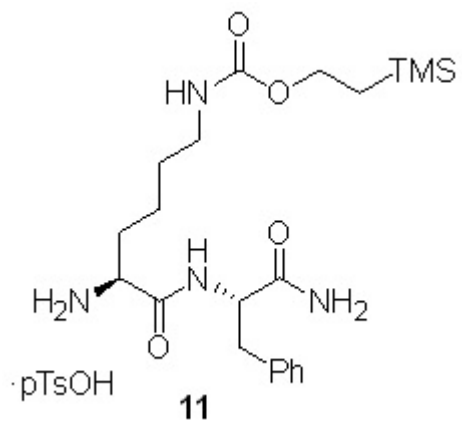


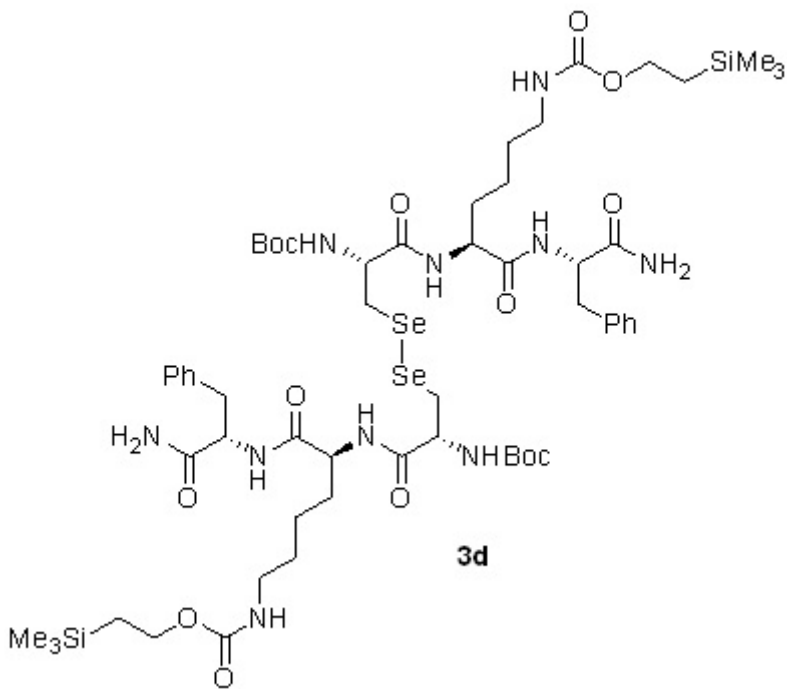




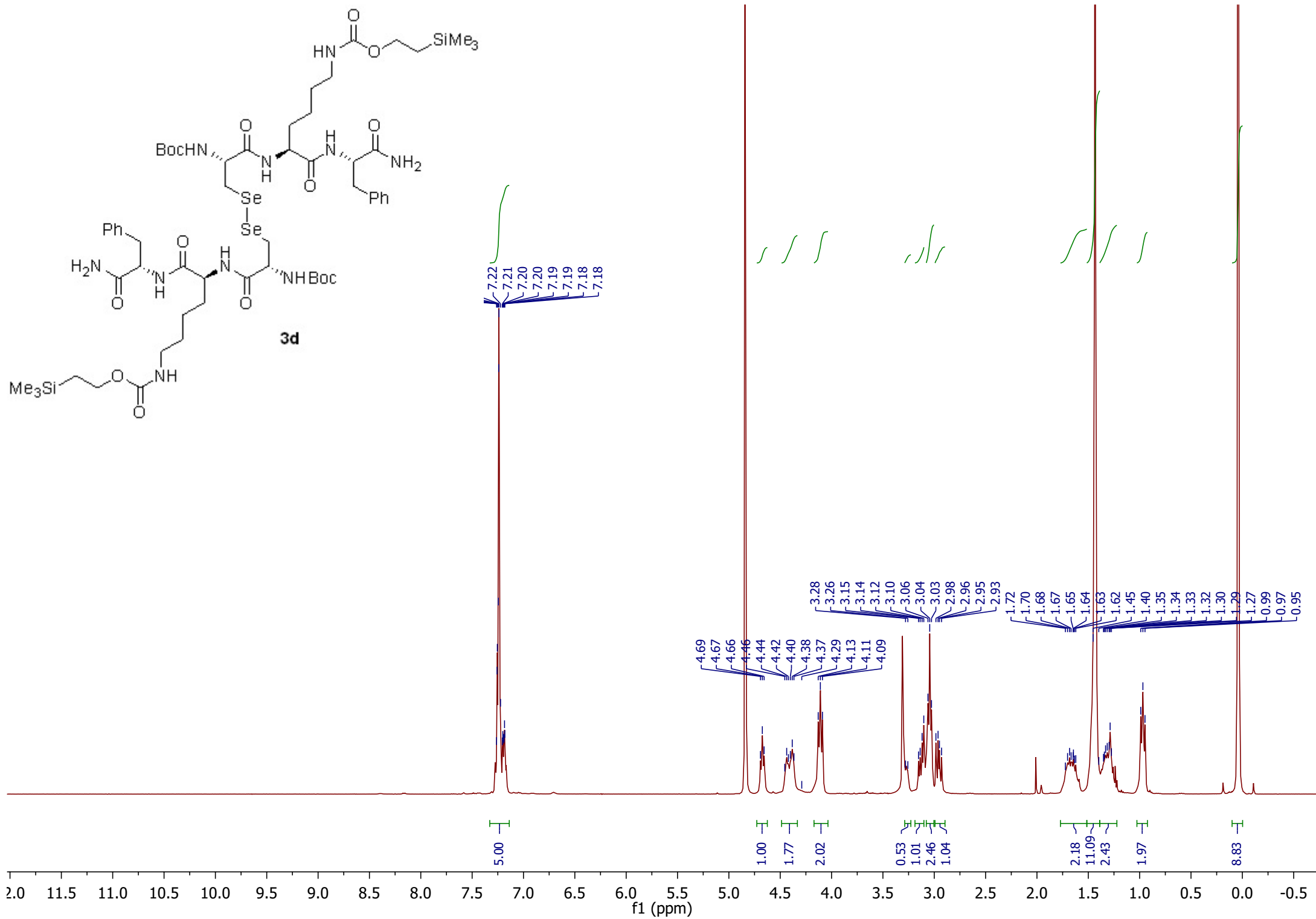


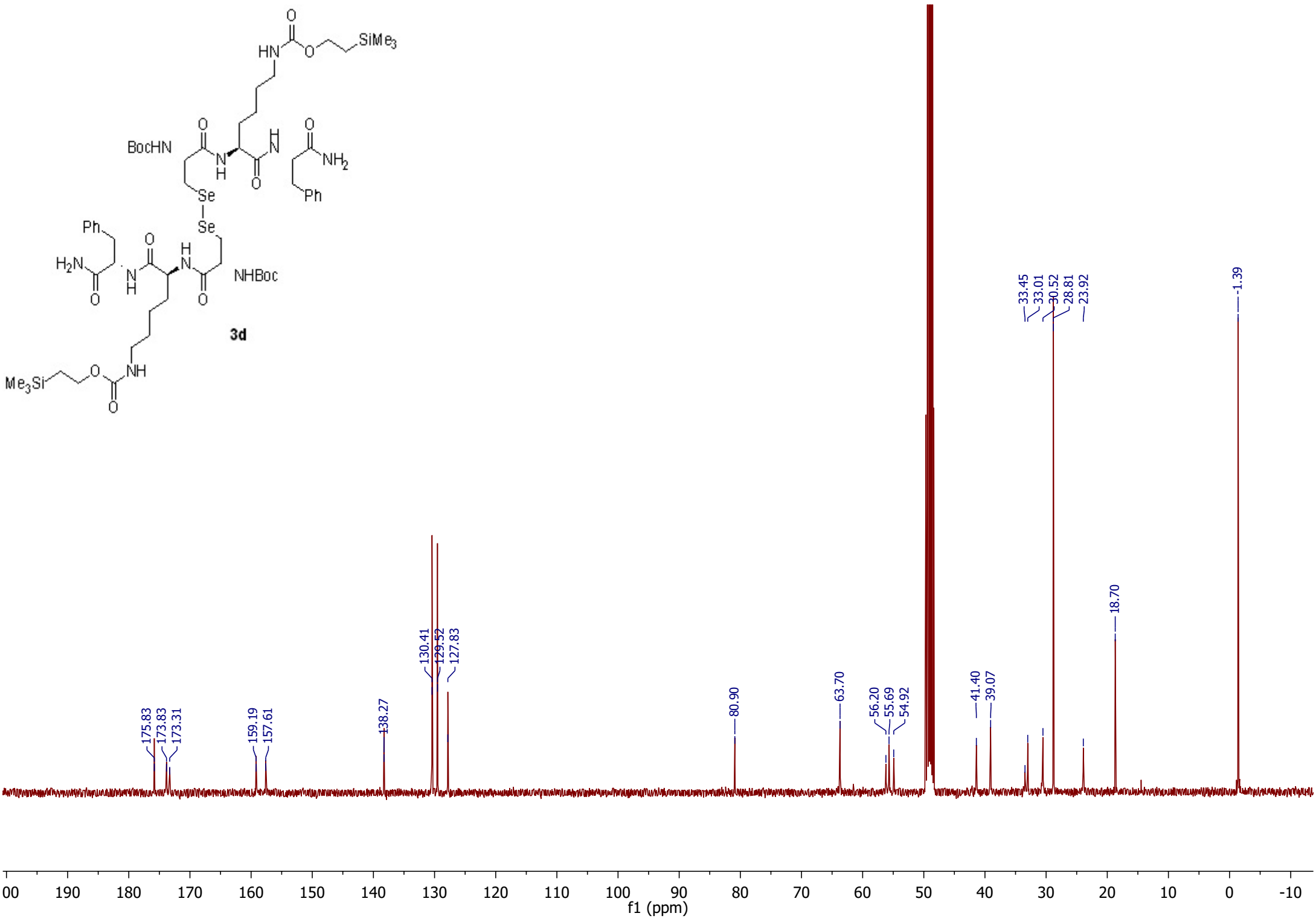
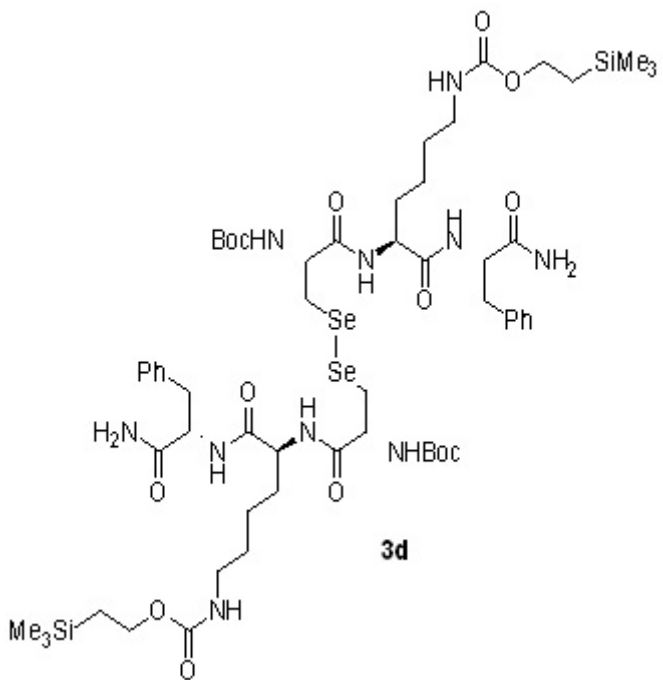


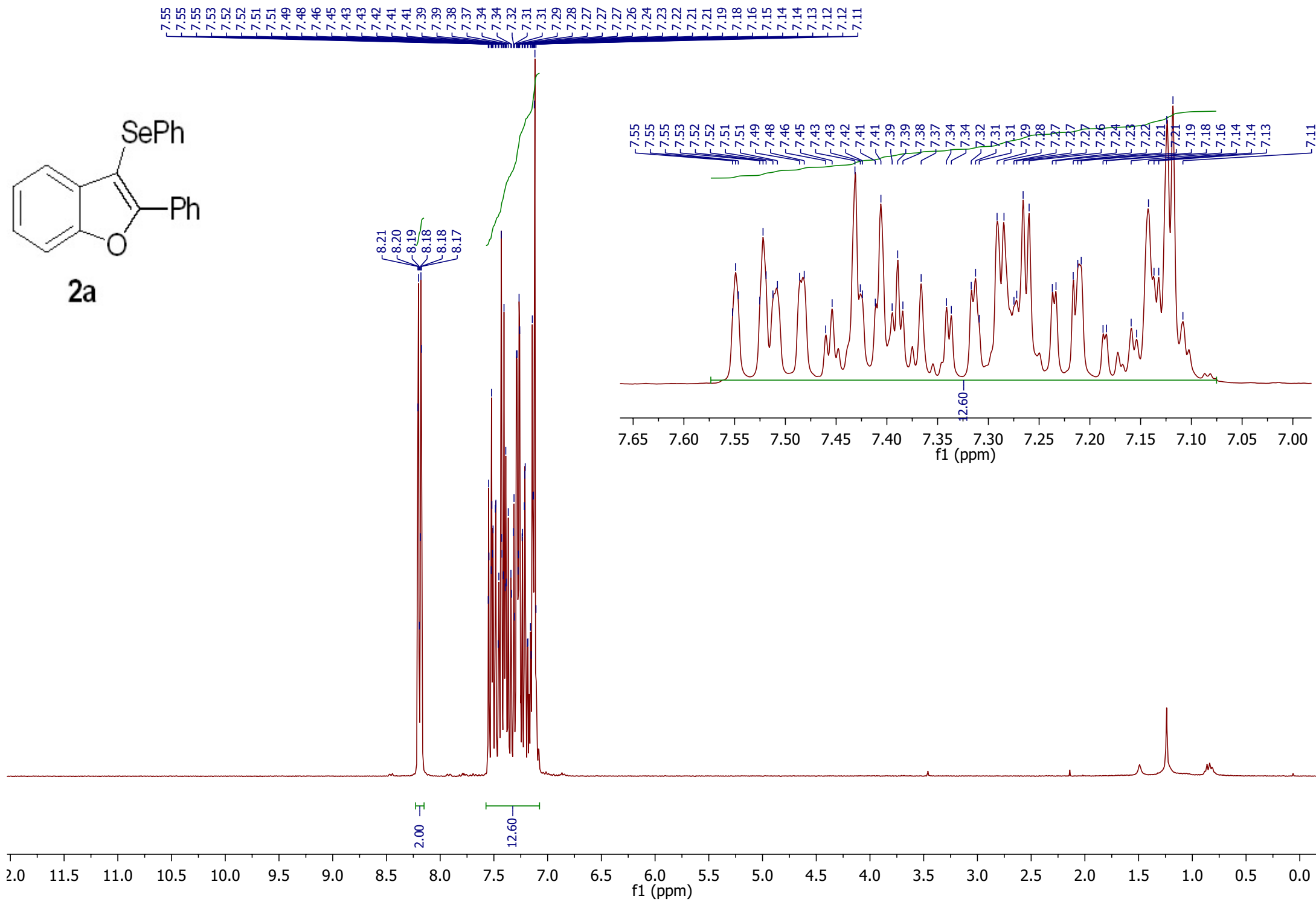
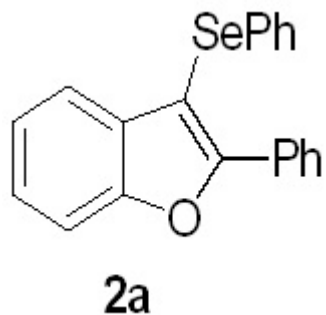




3d

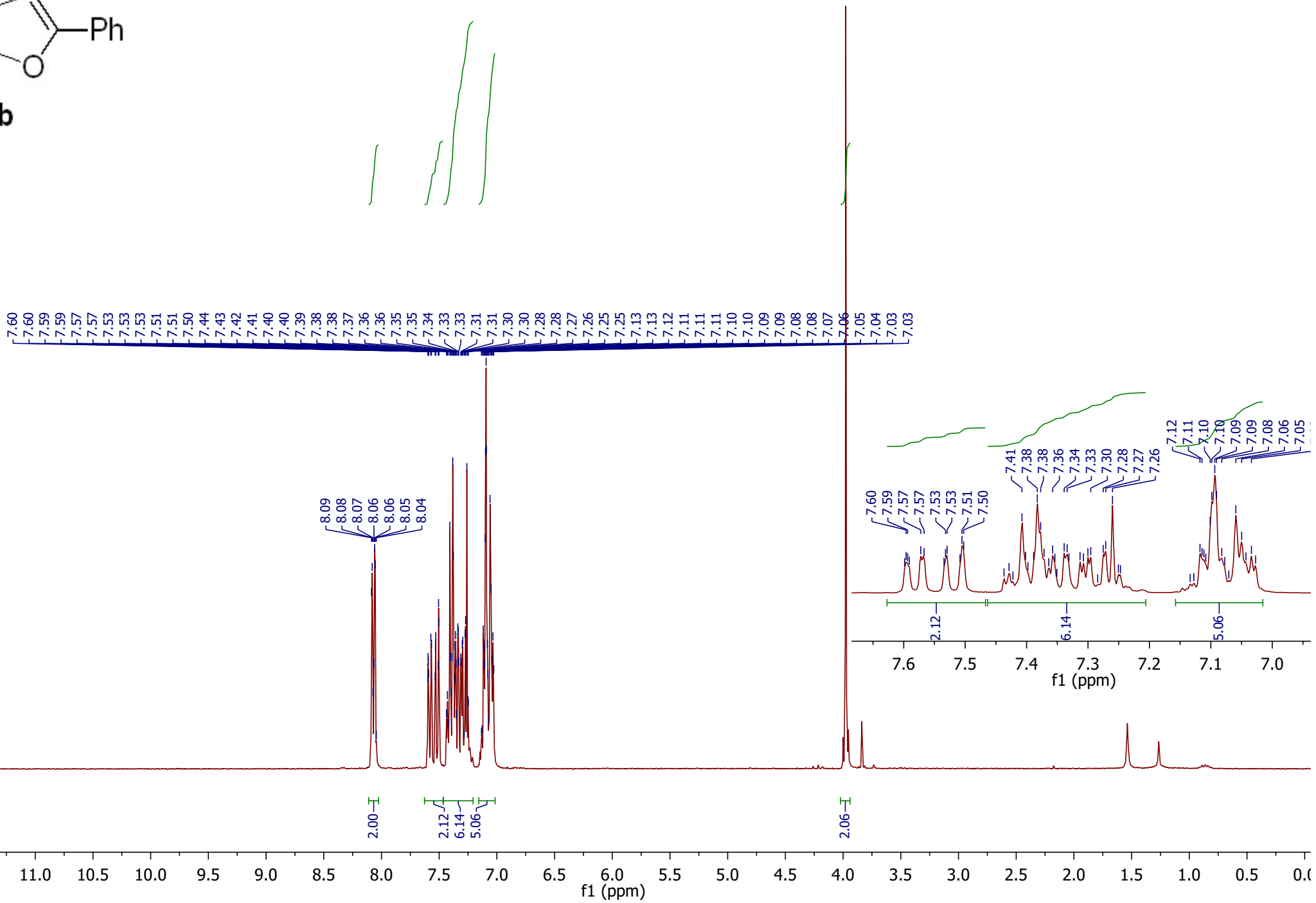


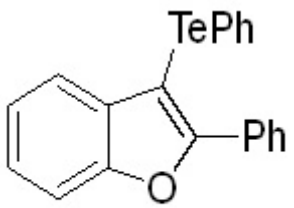




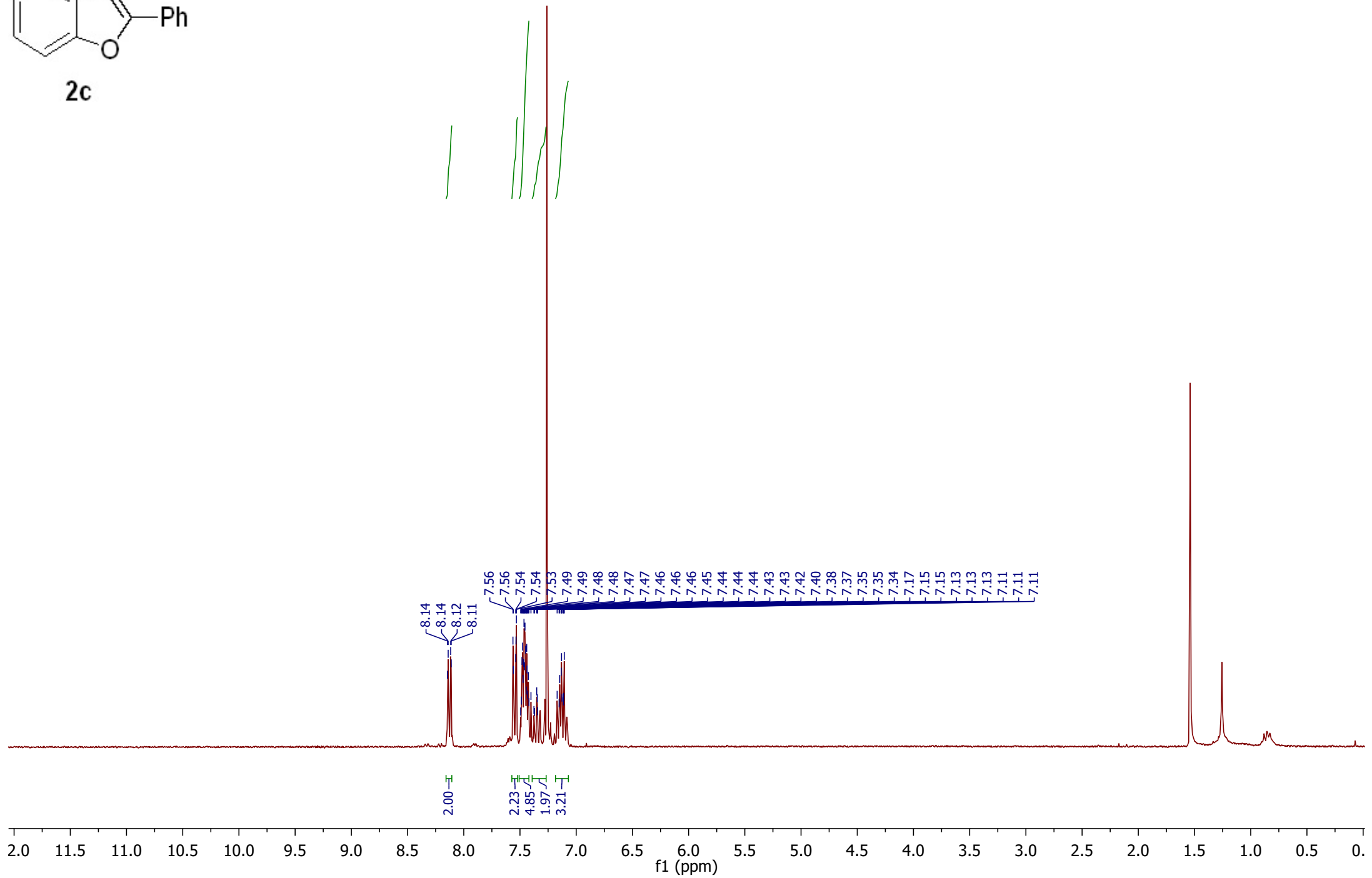


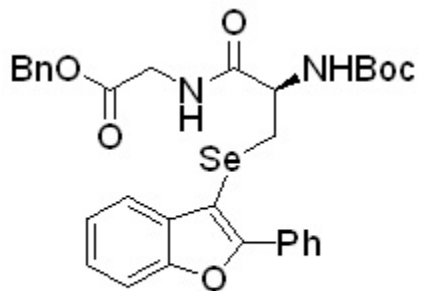
2b



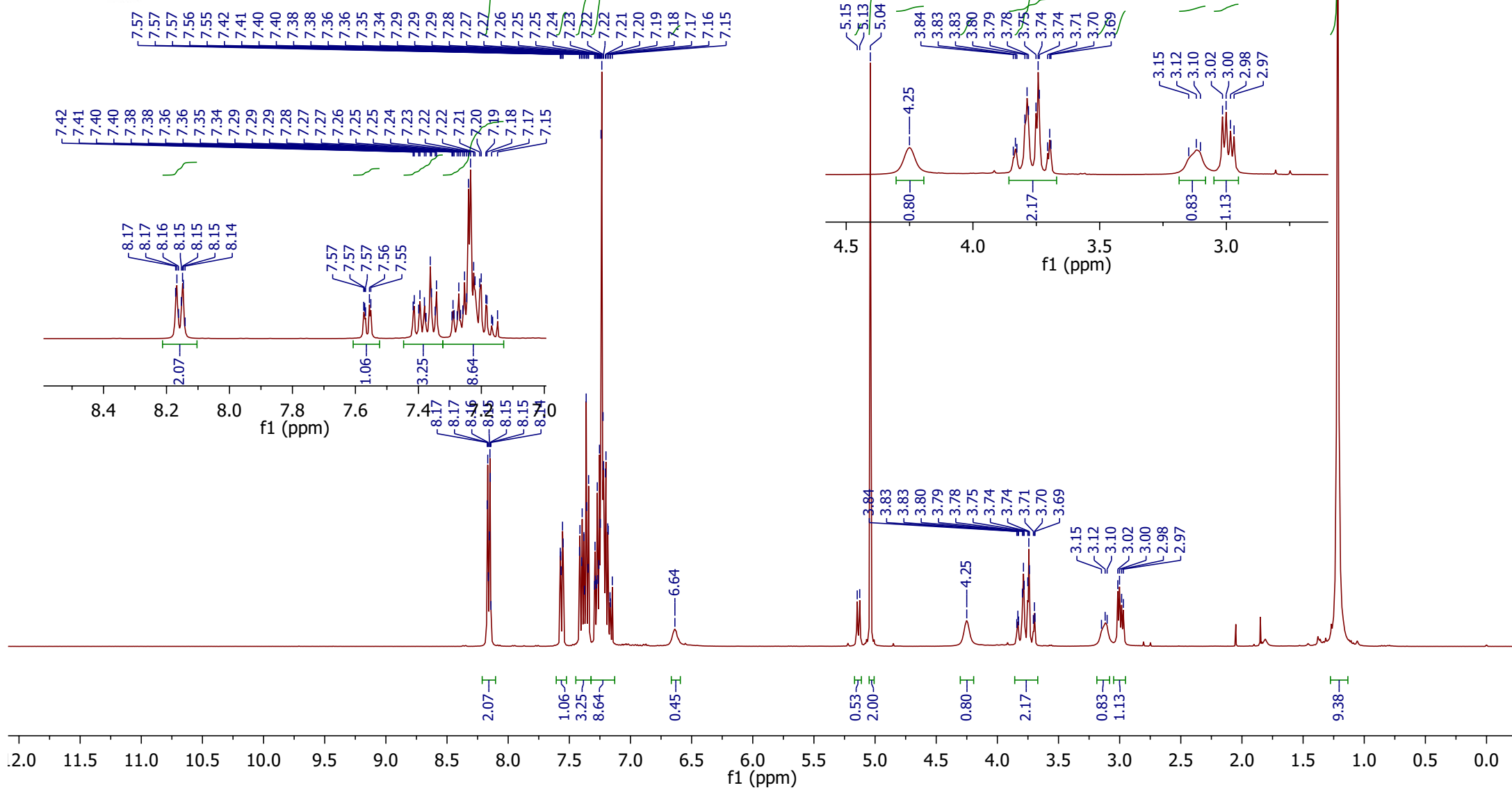


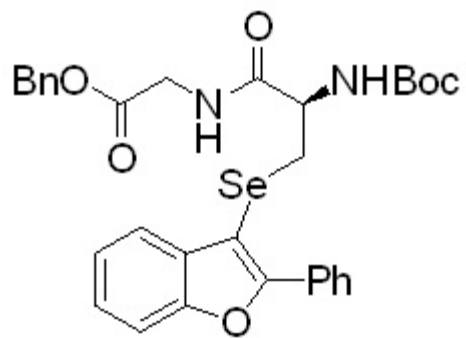
2c



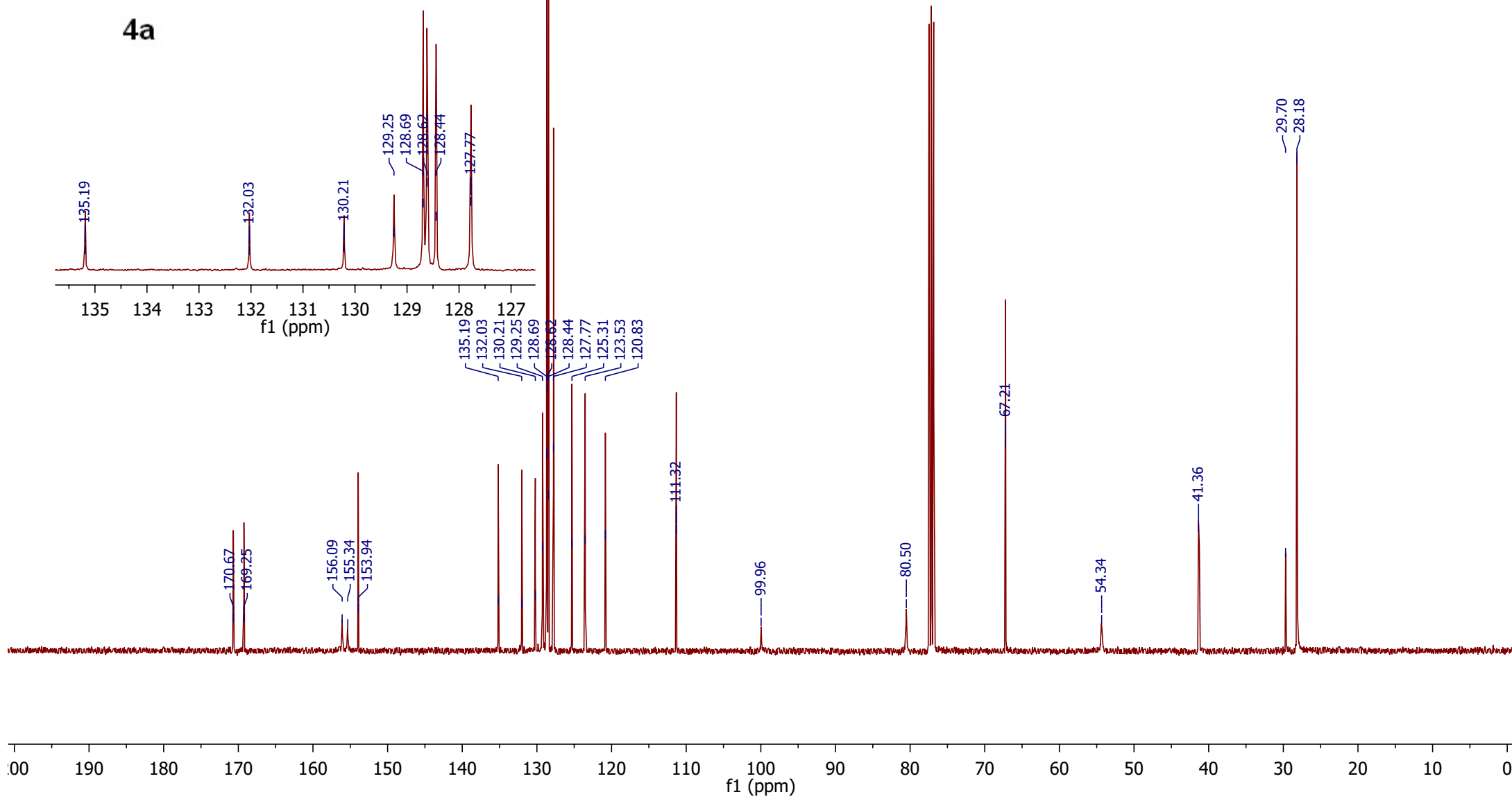


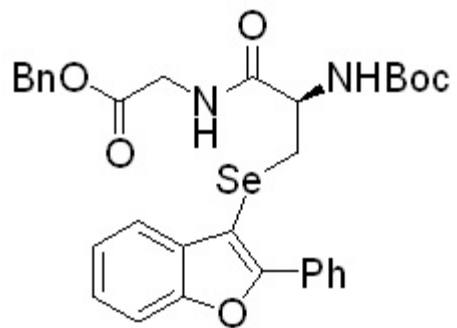
4a



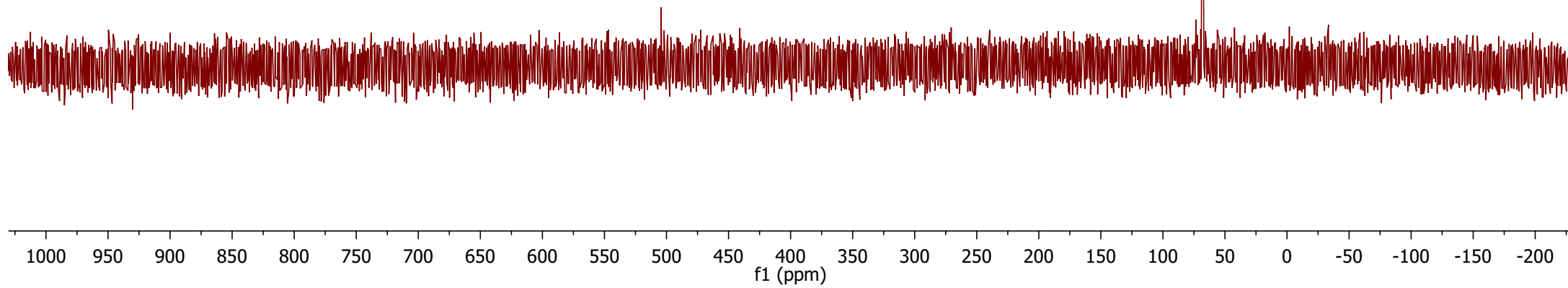
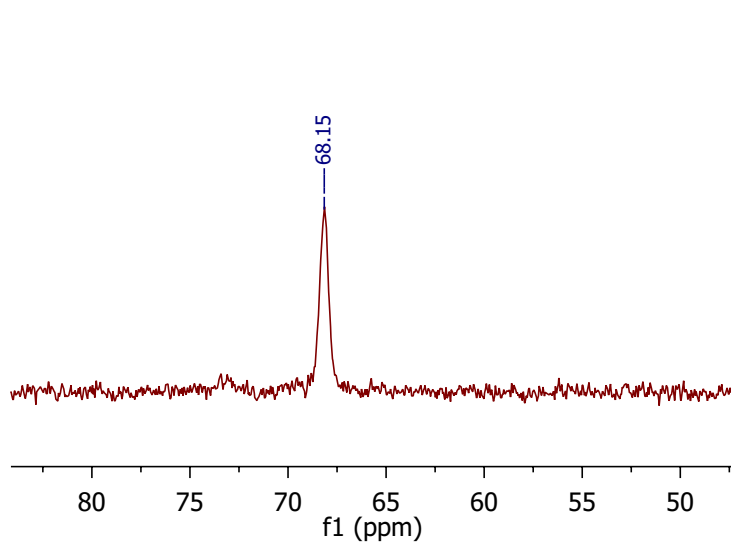


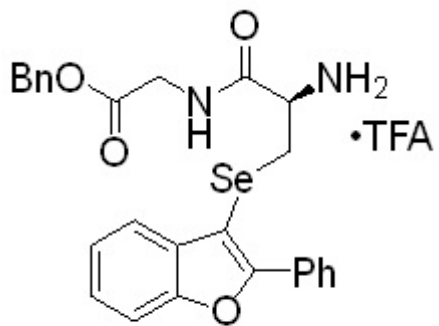
4a



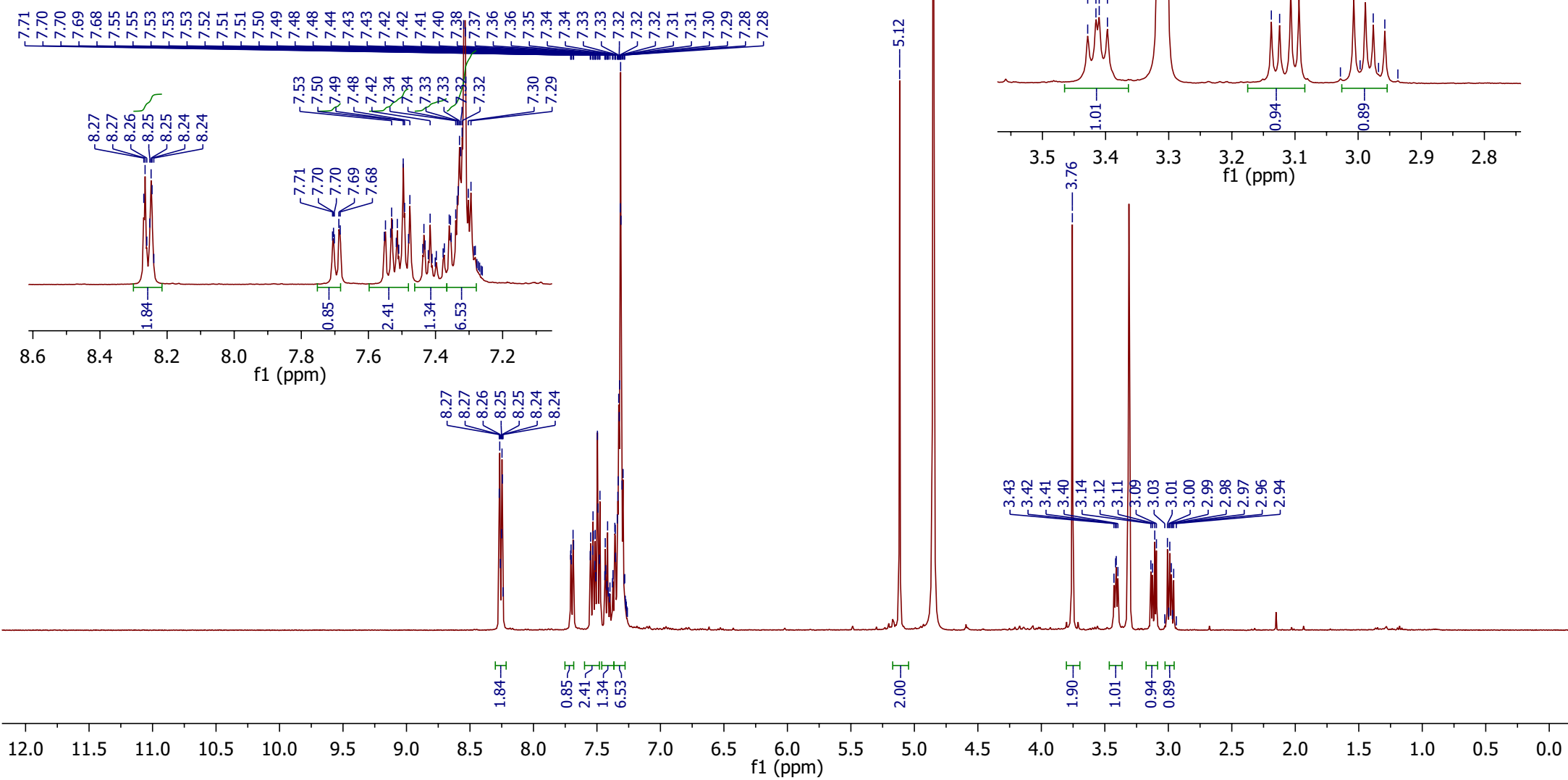


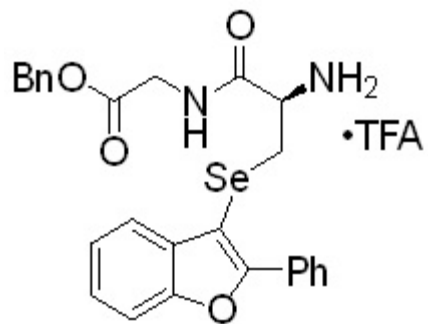
4a



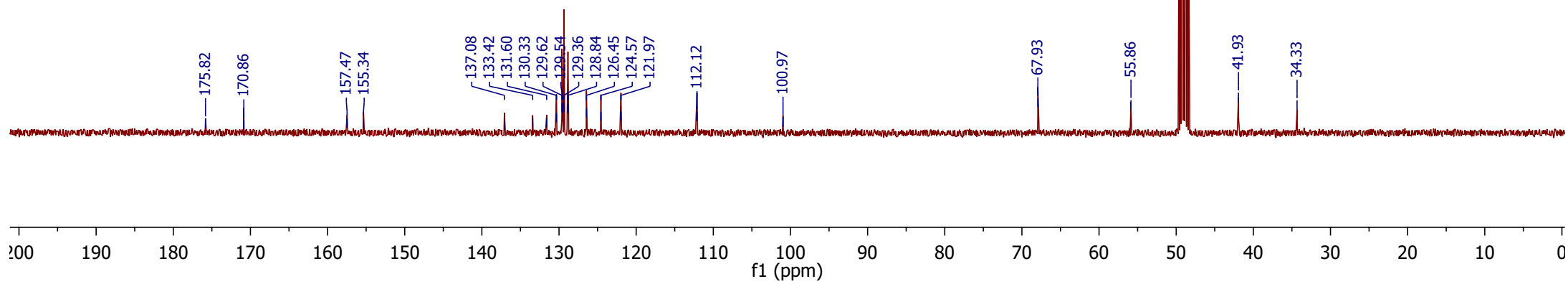
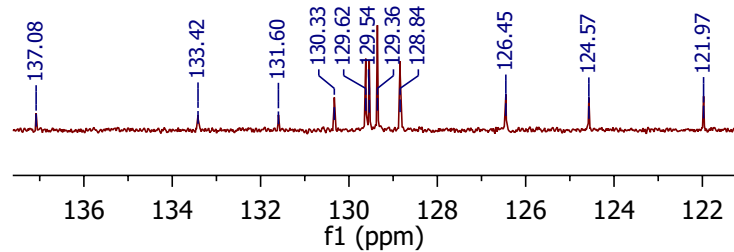


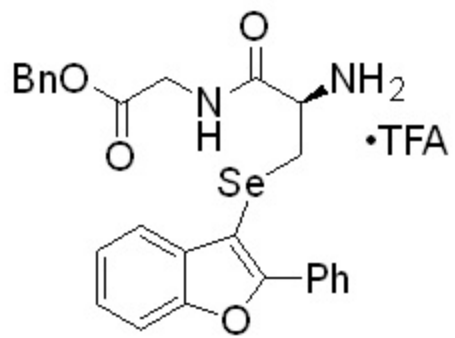
4b



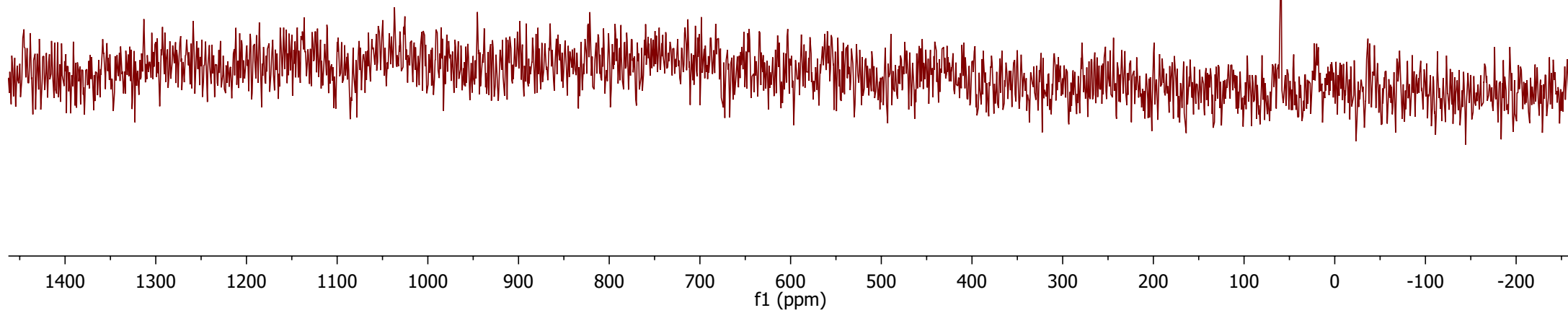
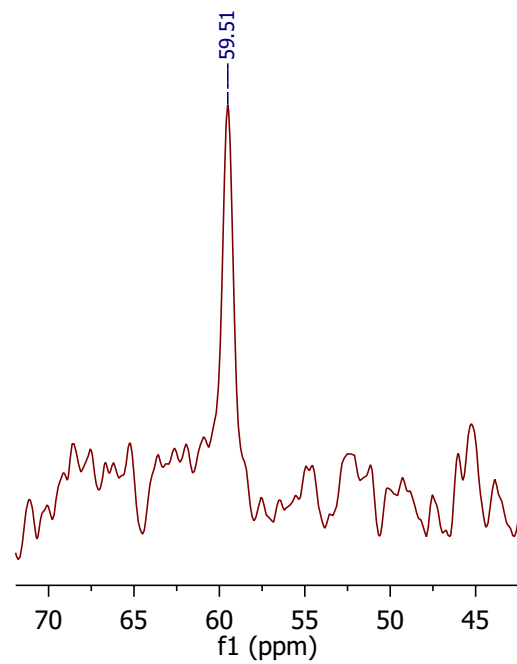


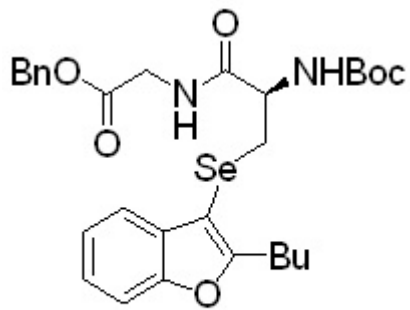
4b



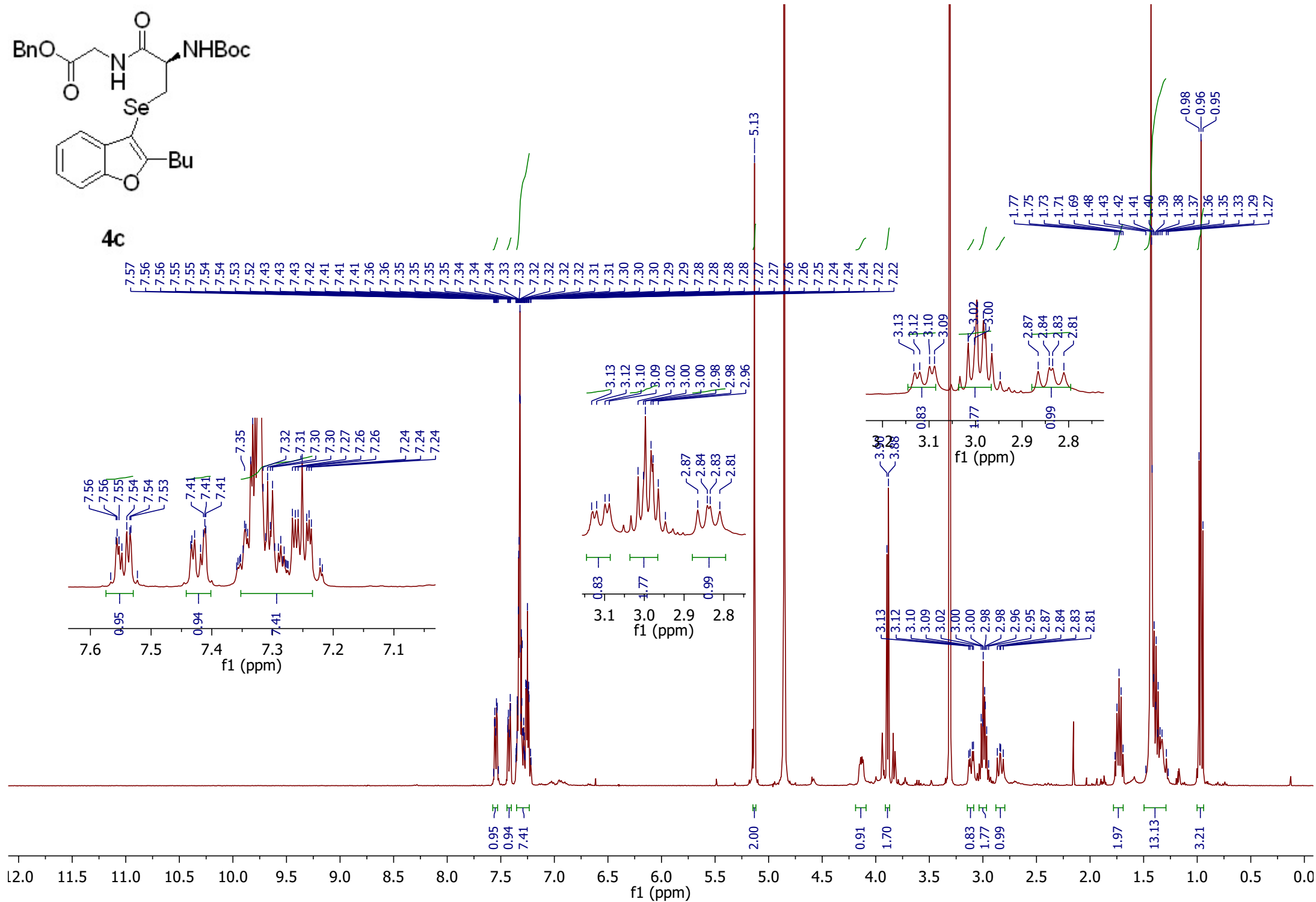


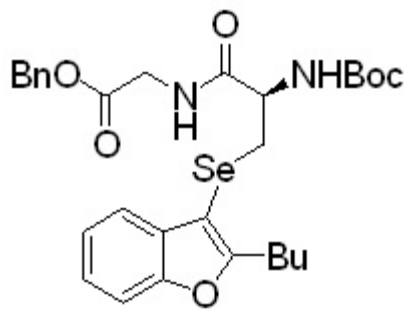
4b



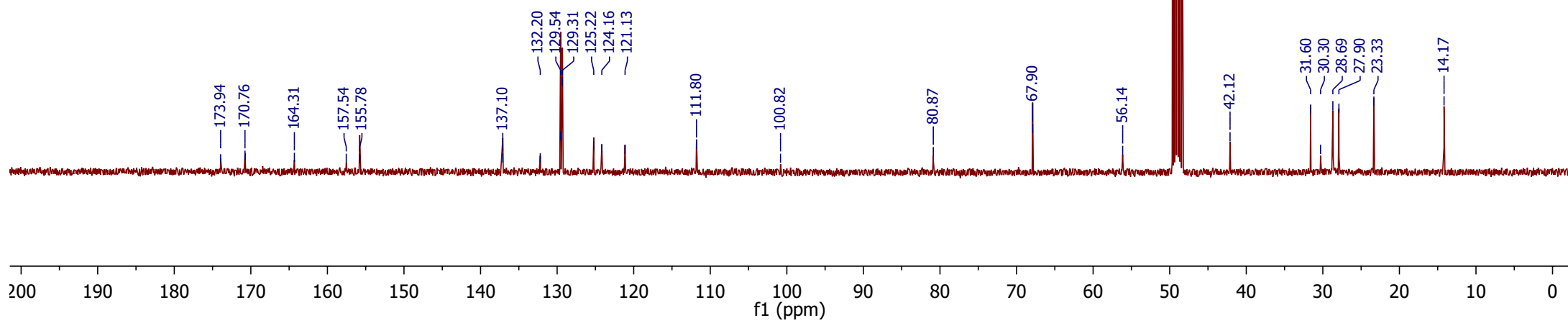
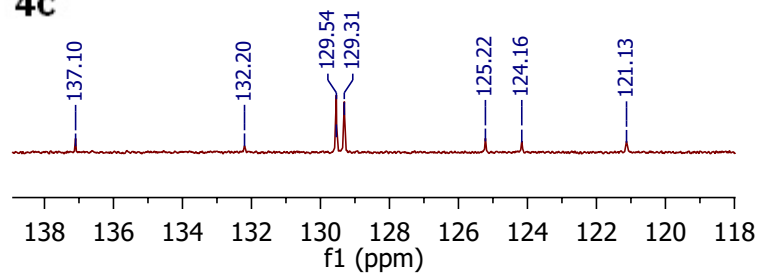


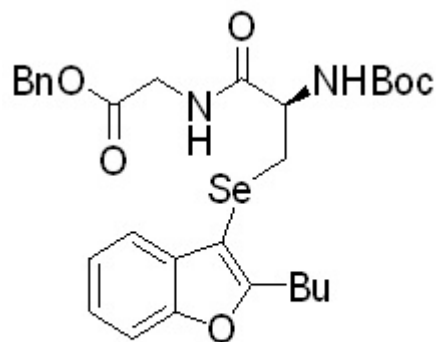
4c



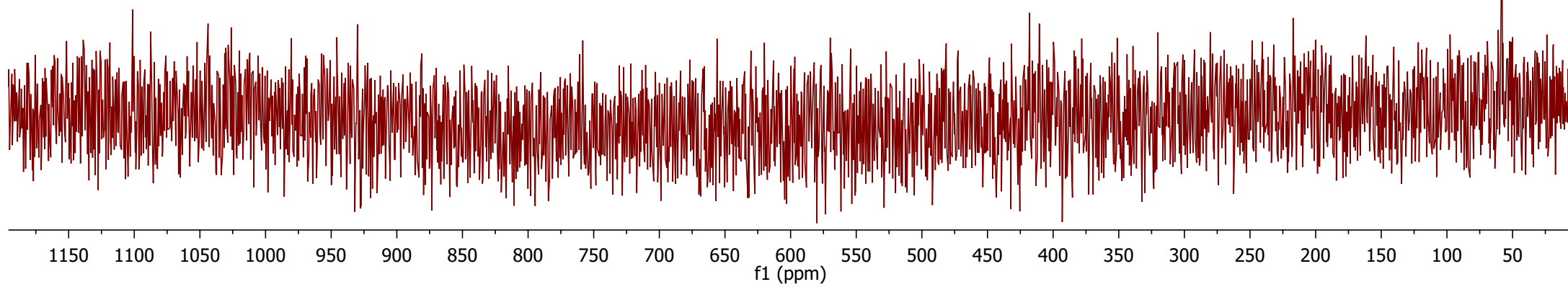
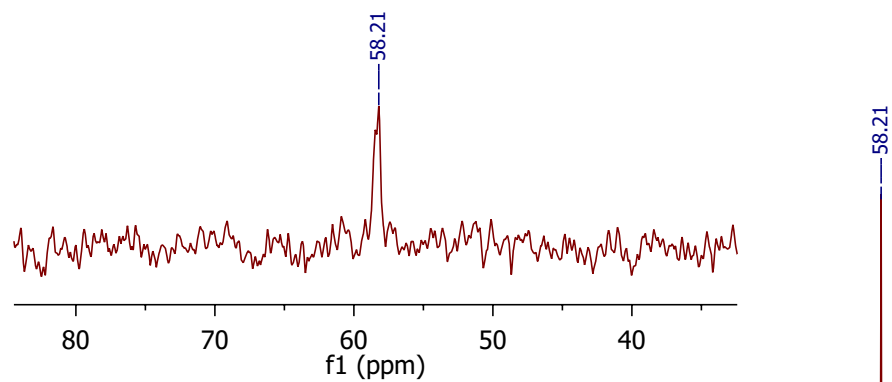


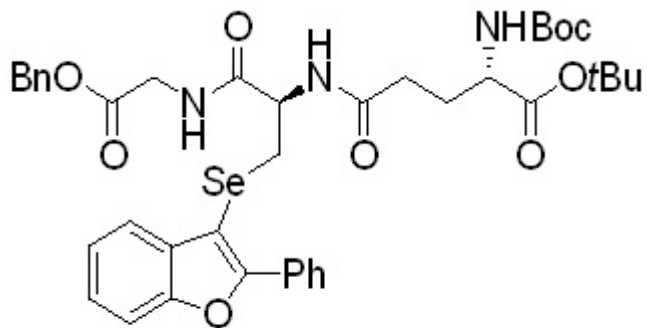
4c



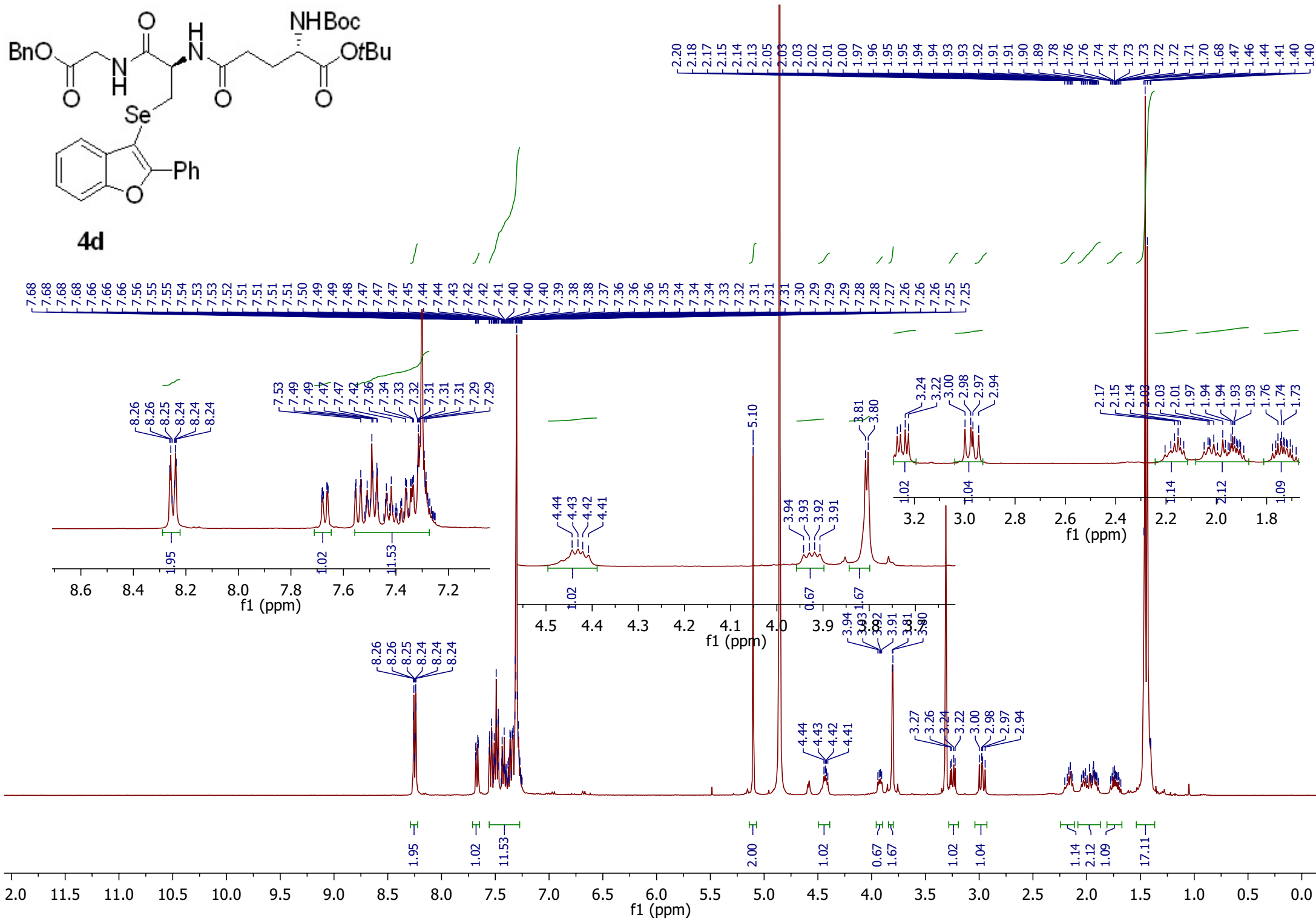


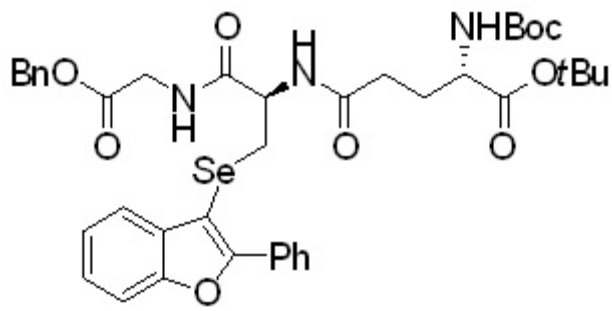
4c



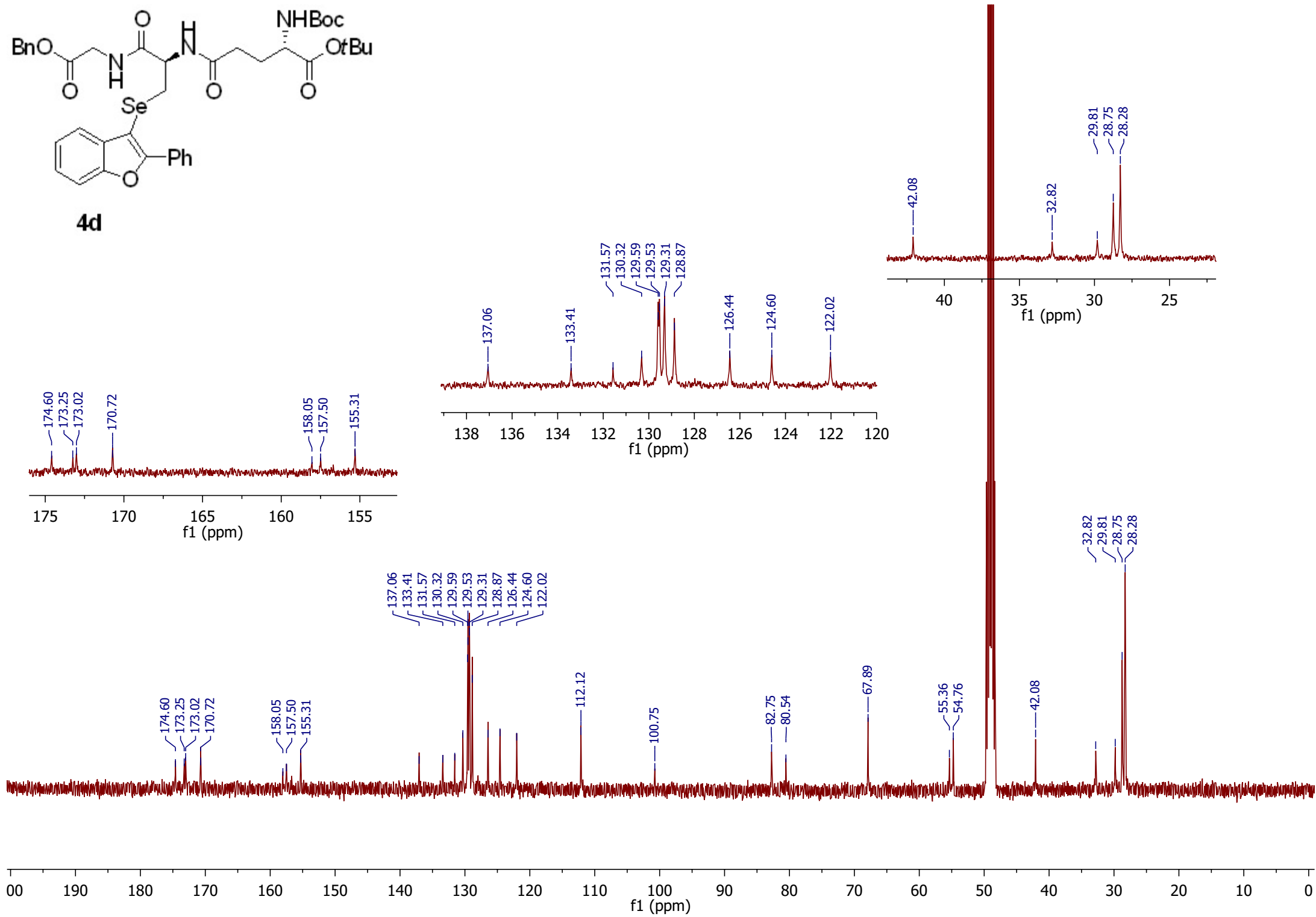


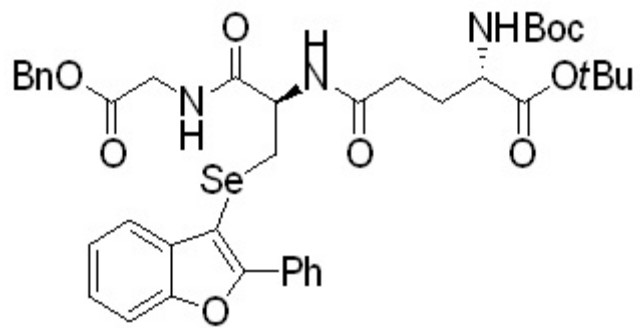
4d



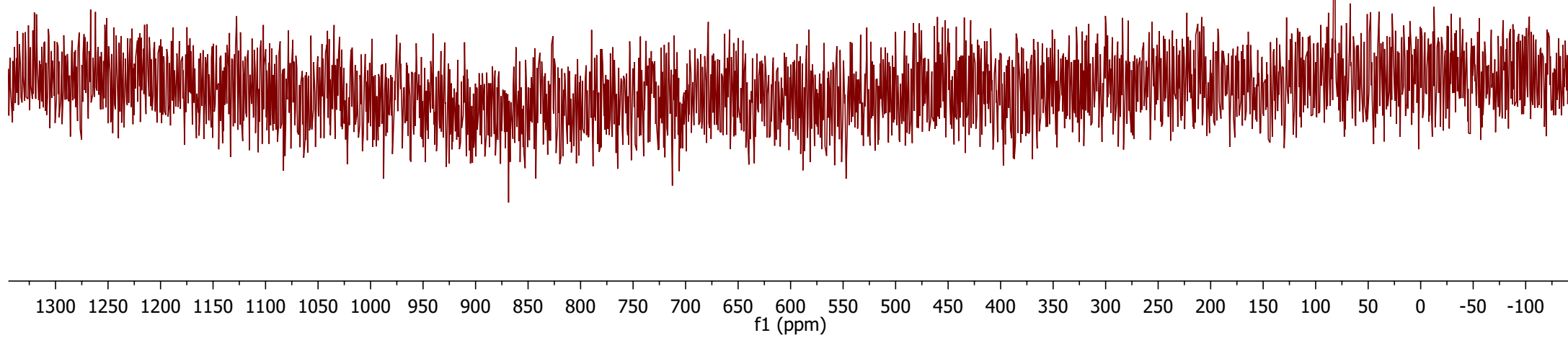
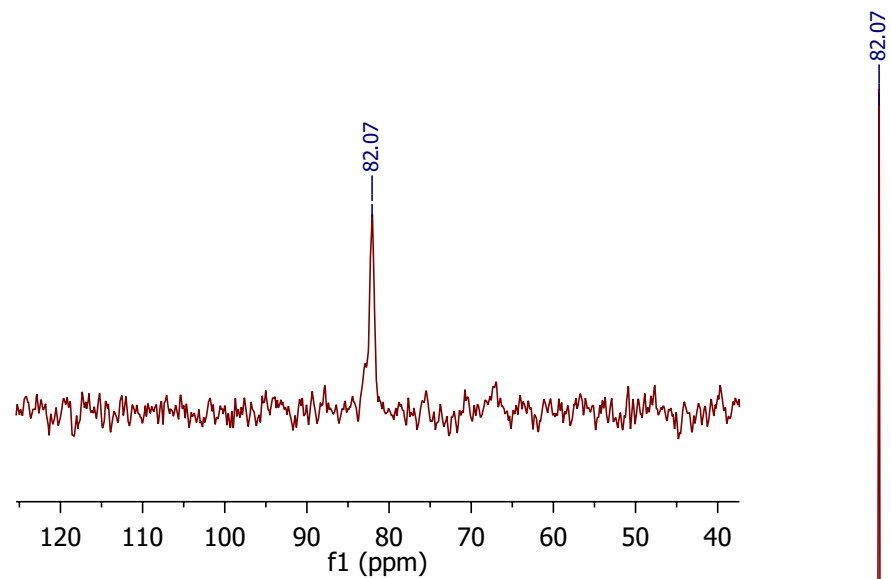


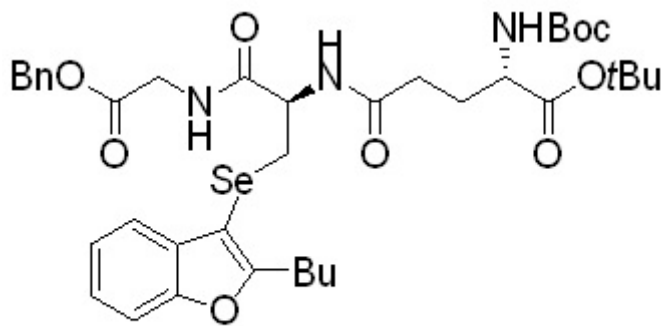
4d



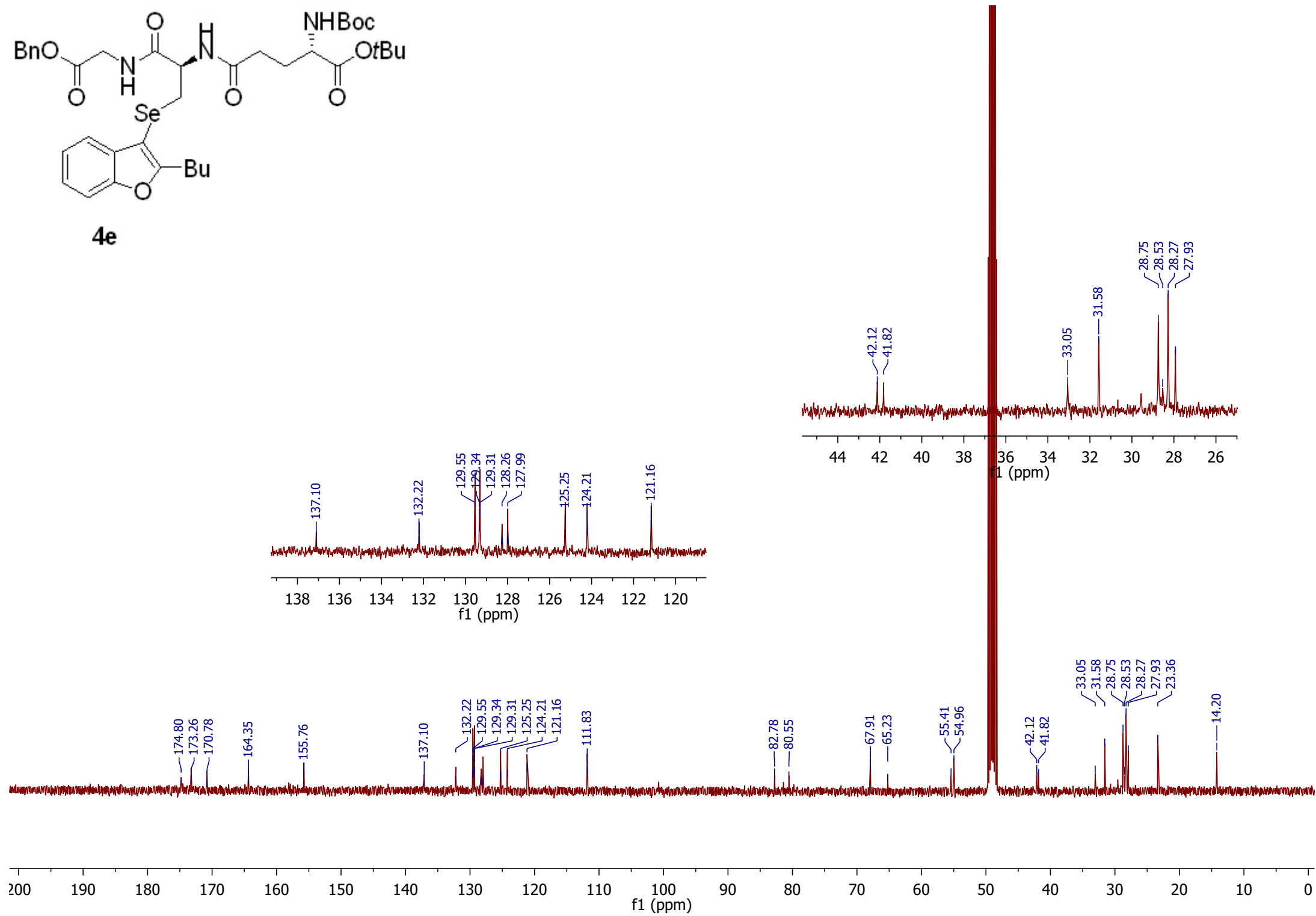


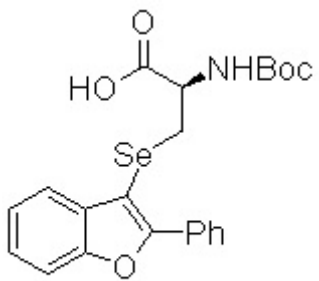
4d



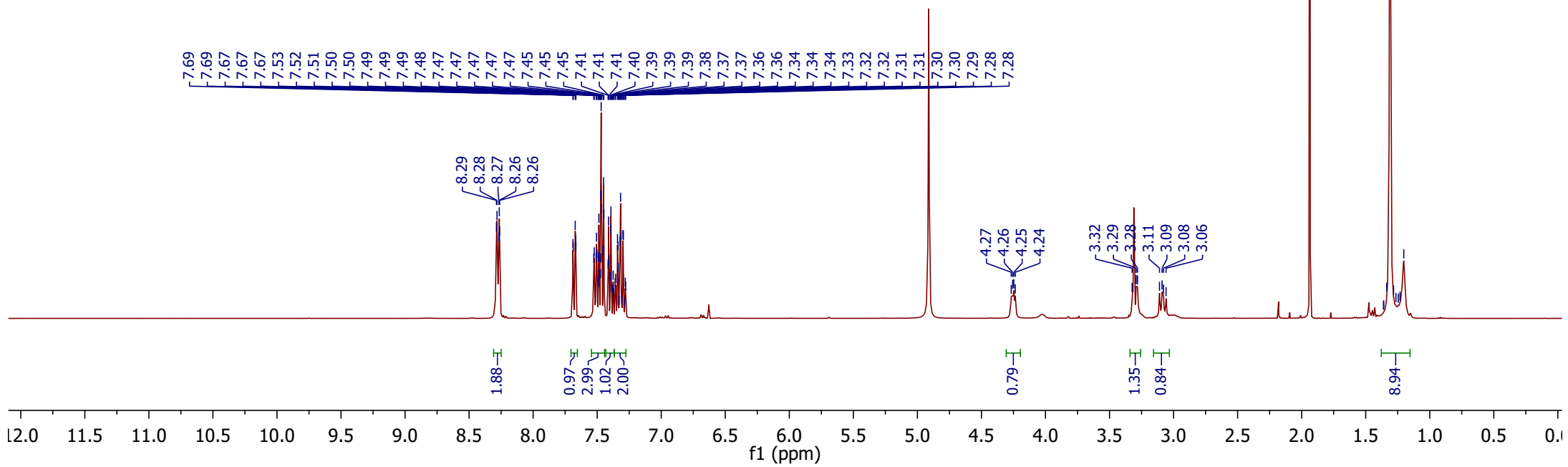
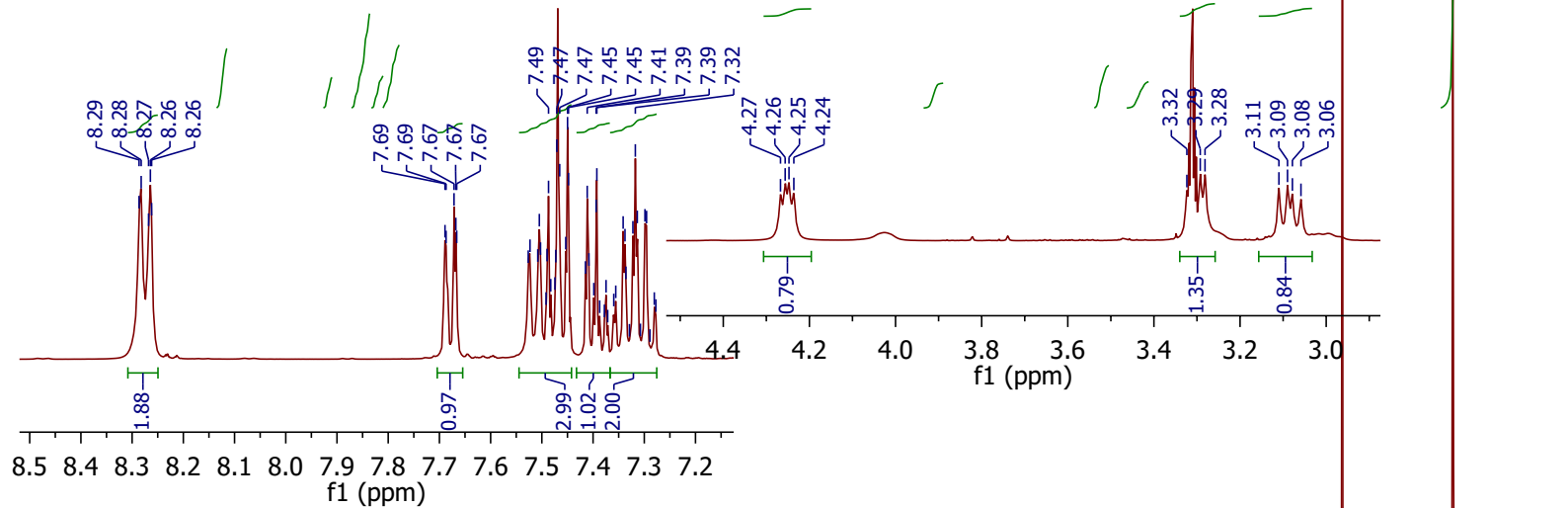


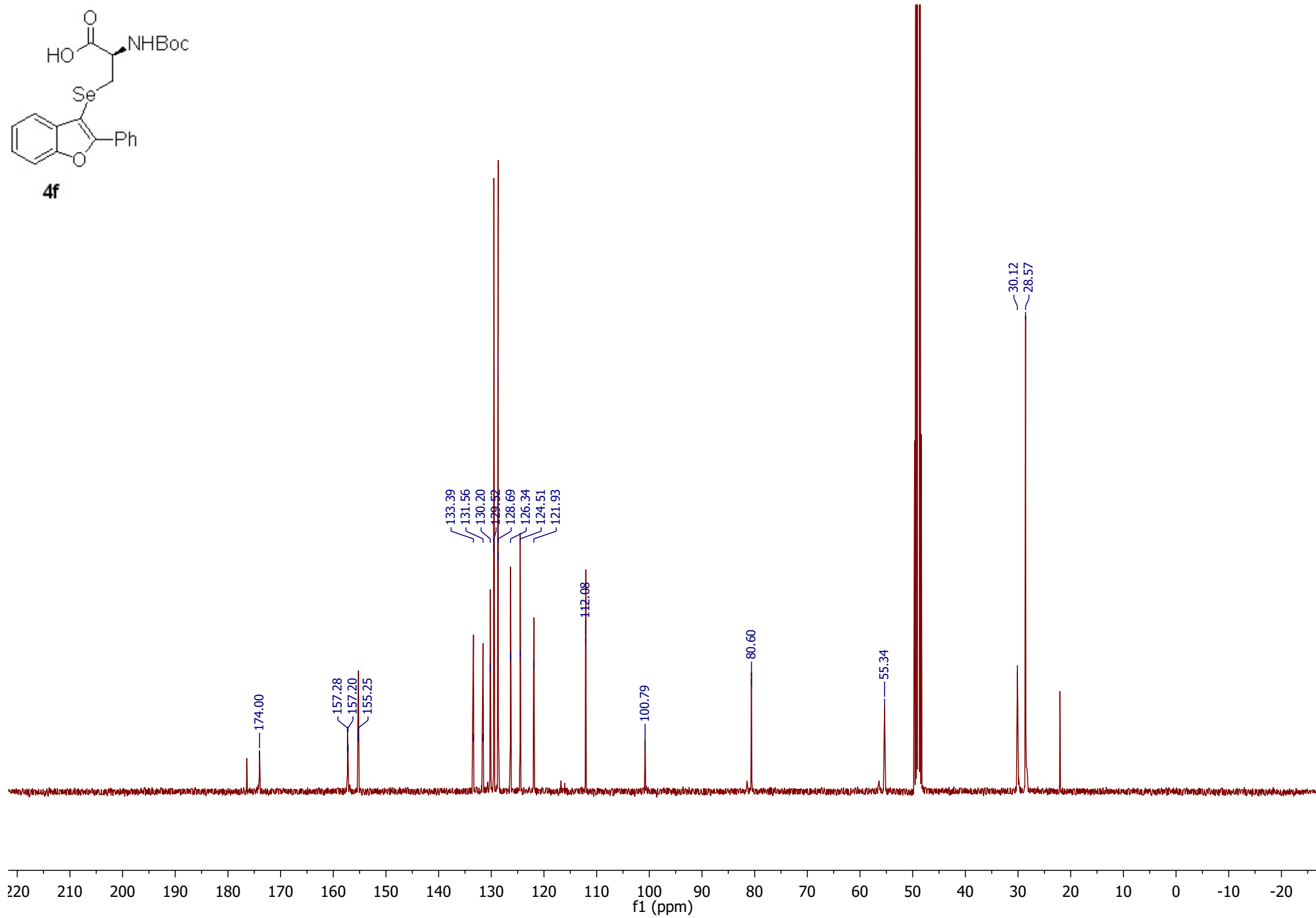
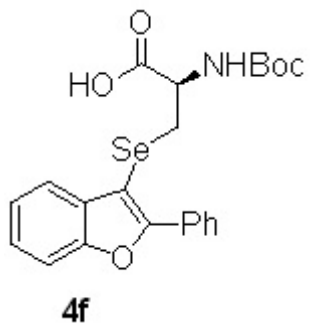
4e

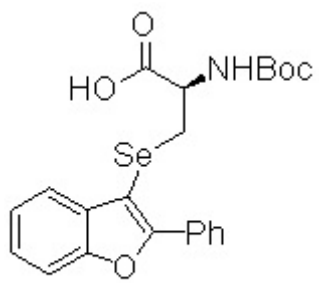




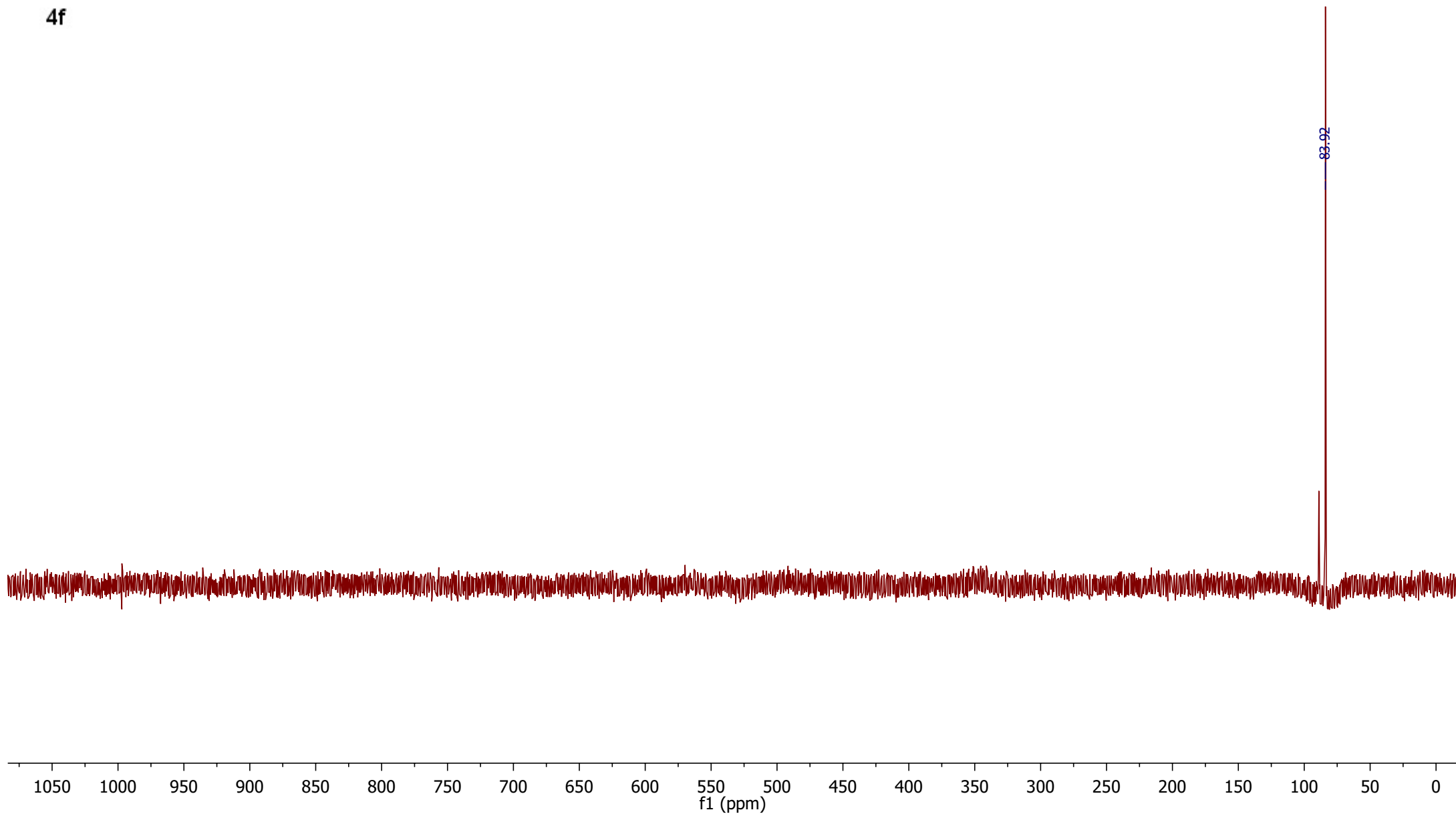
4f

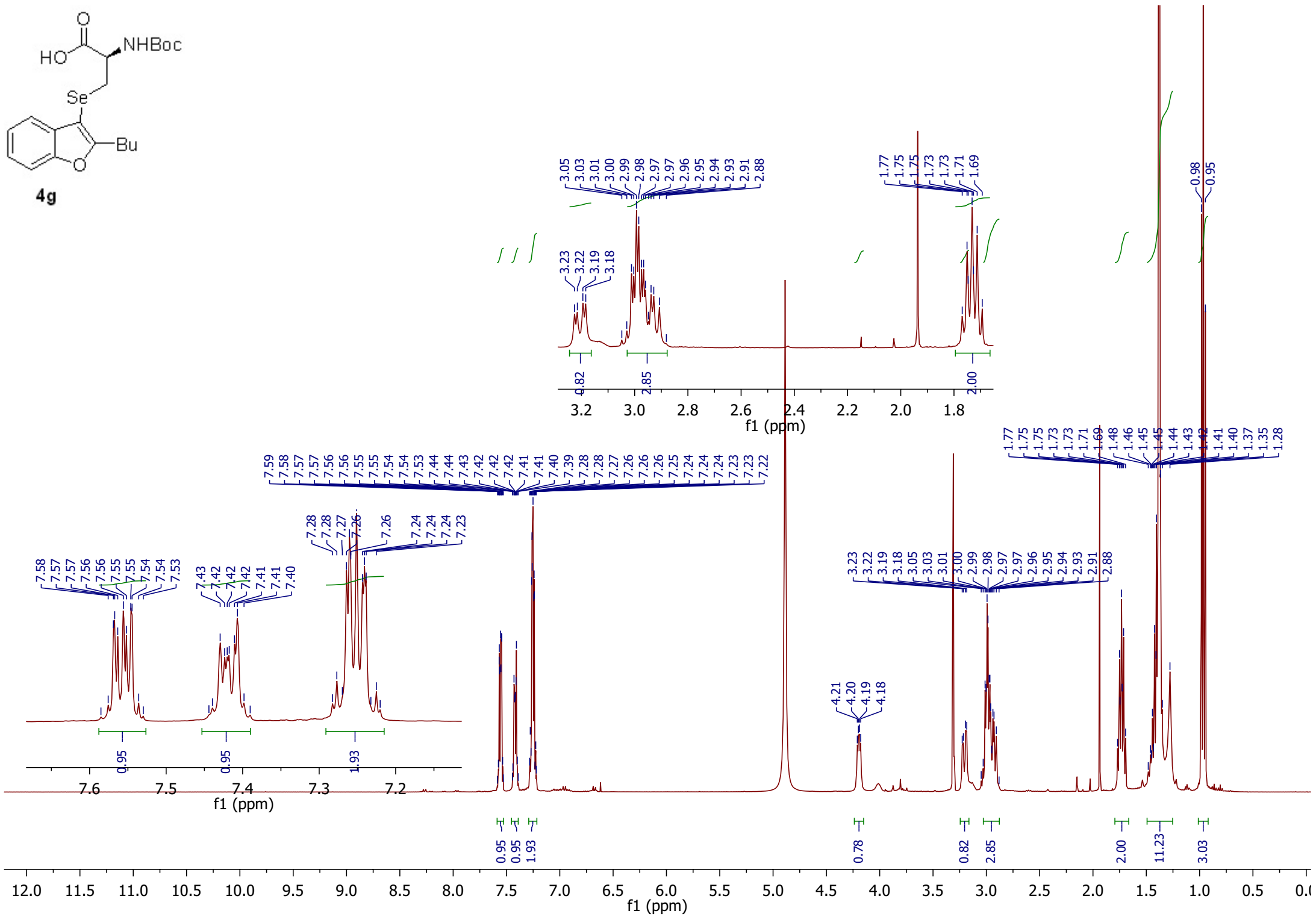
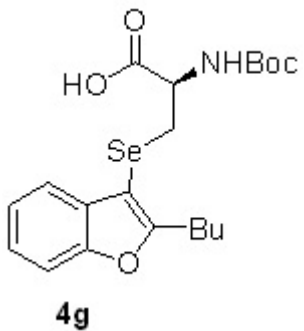


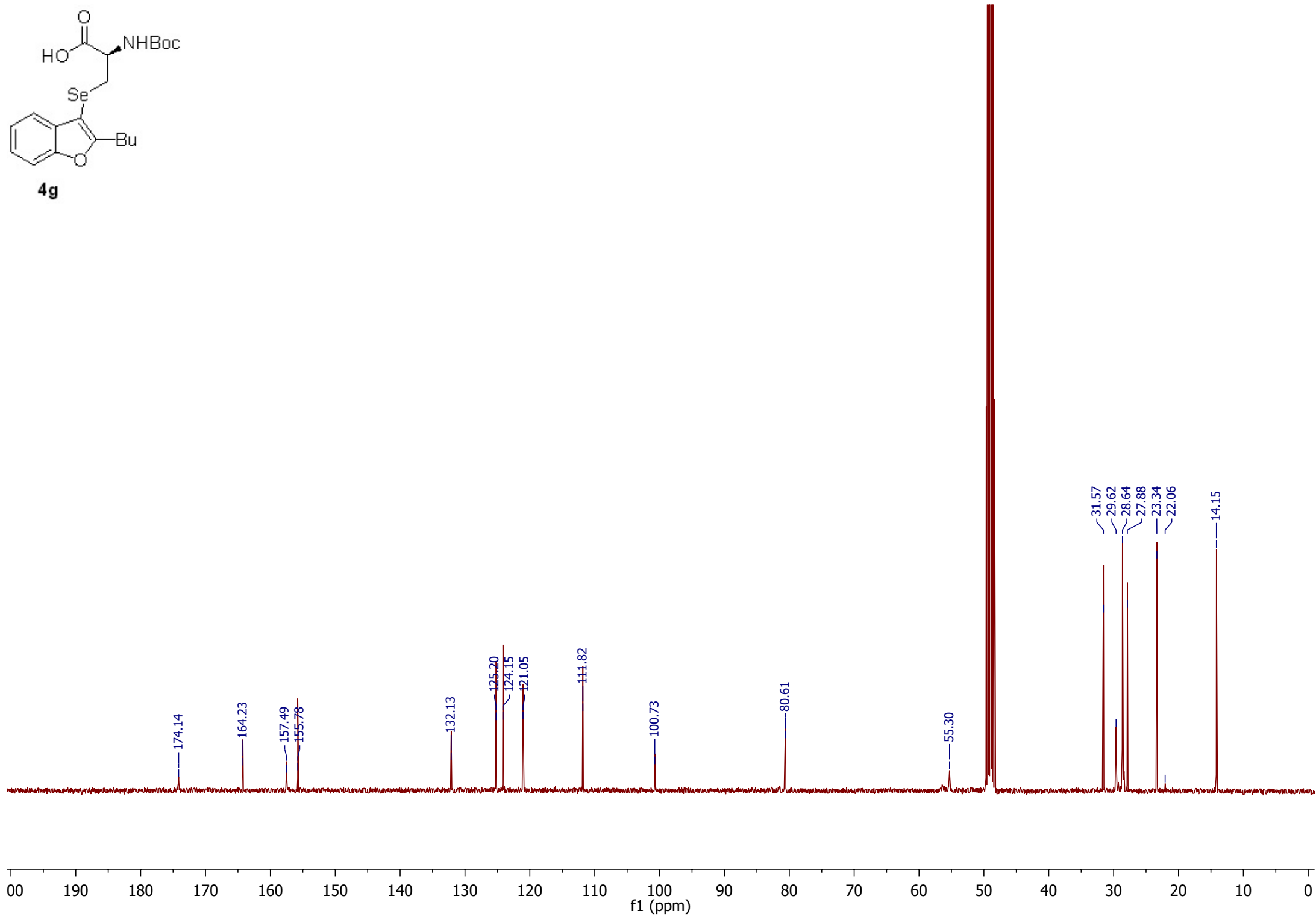
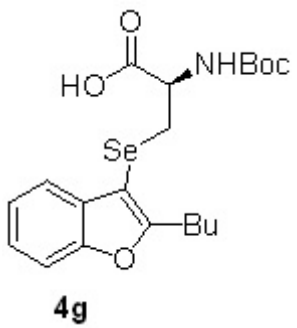


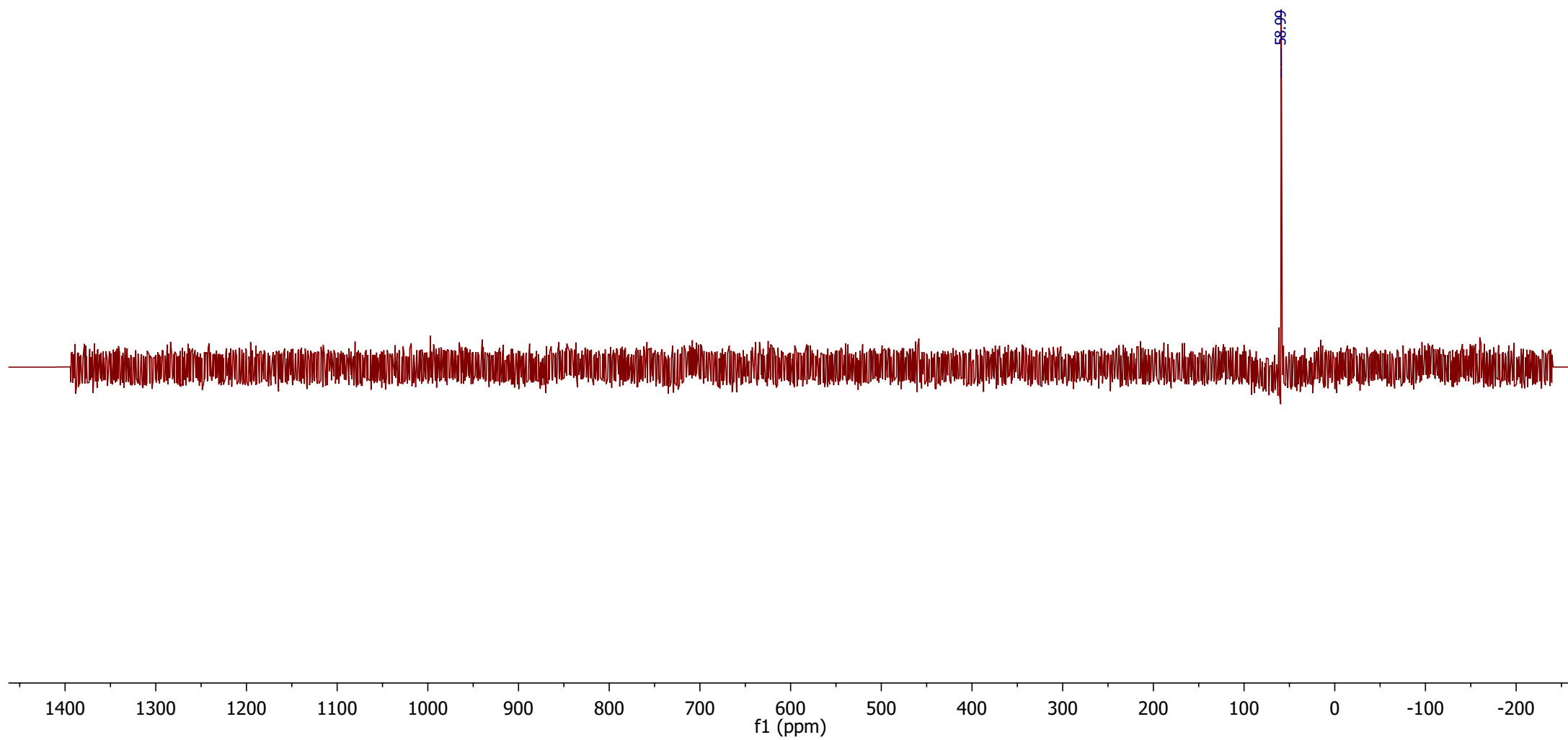
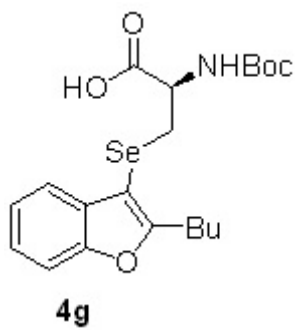


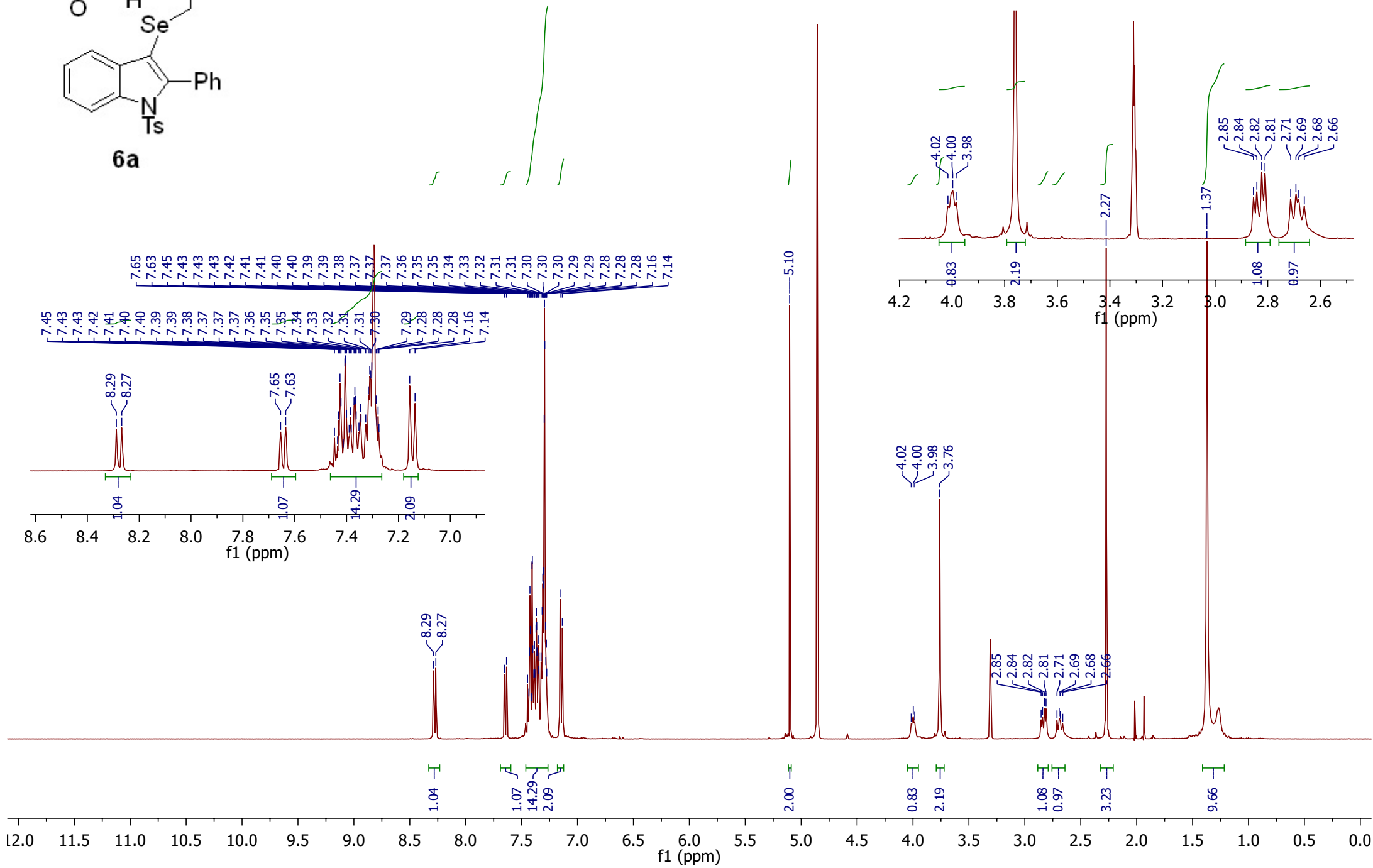
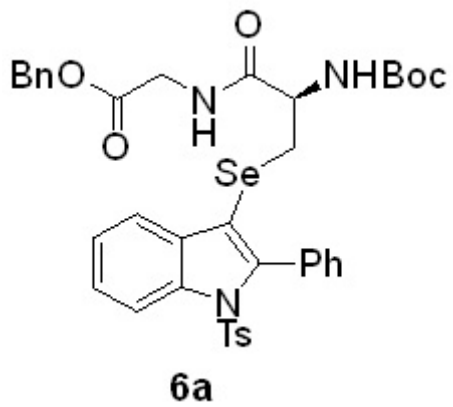
4f

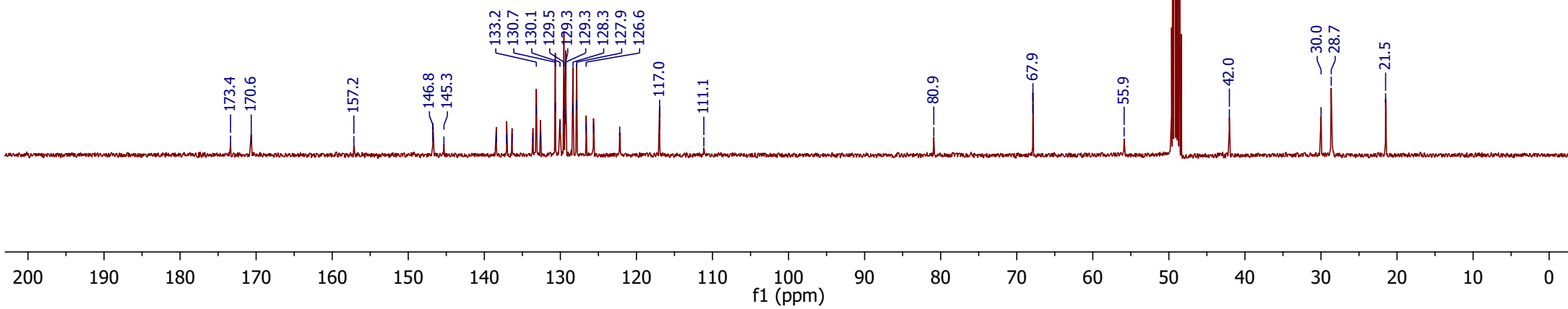
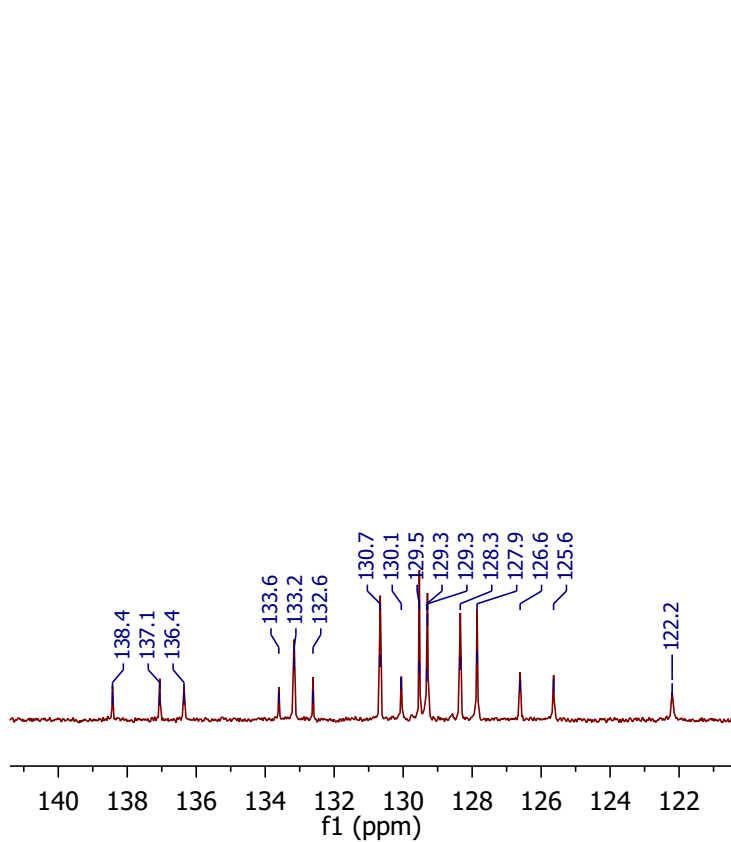
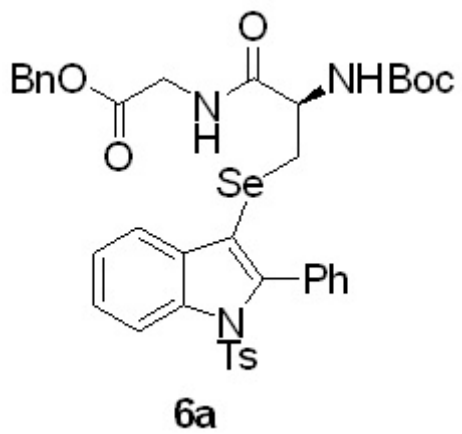


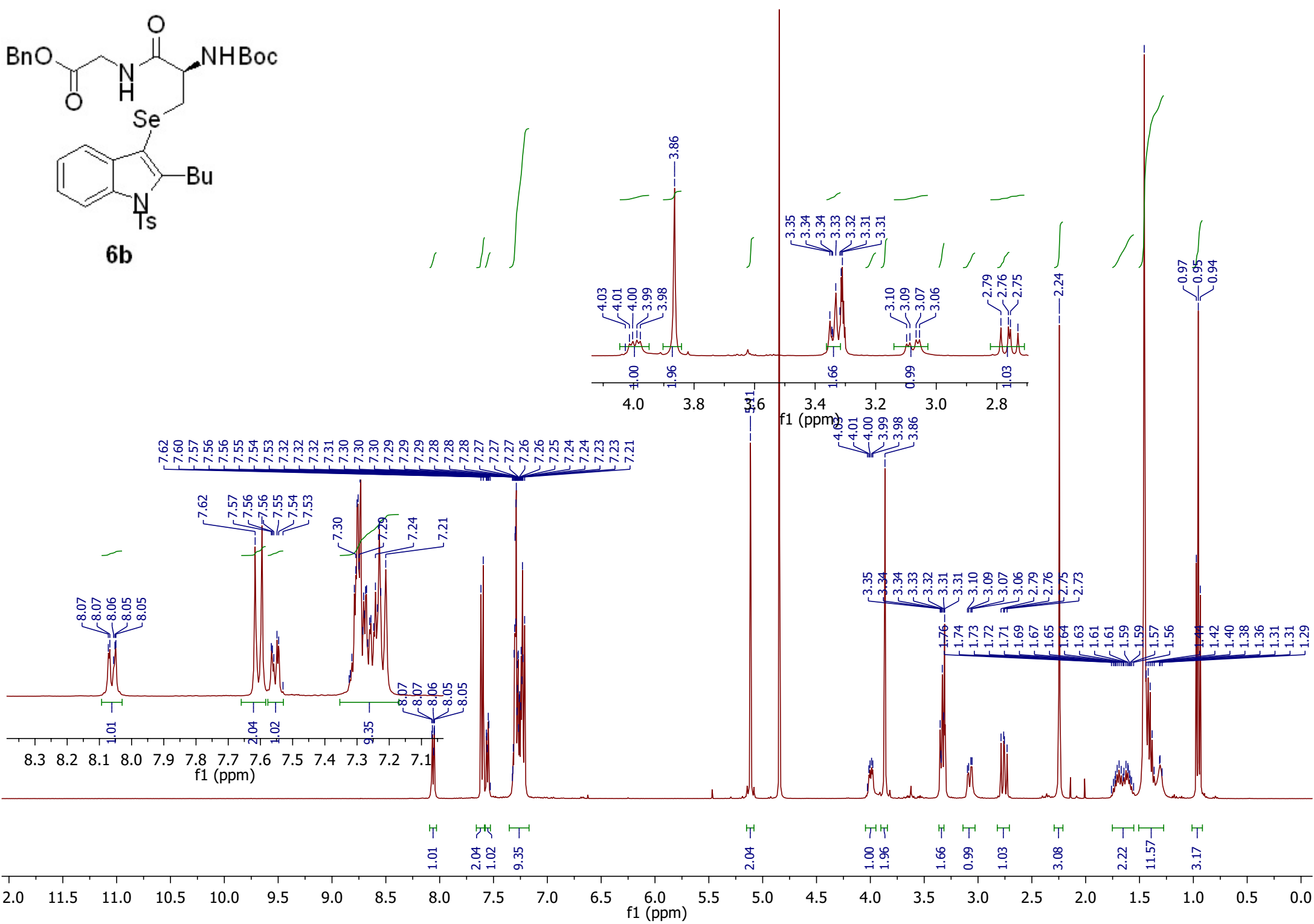
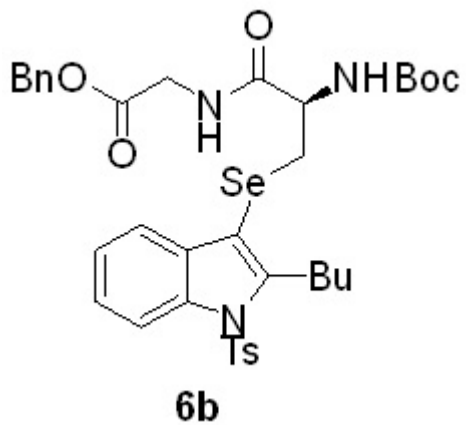


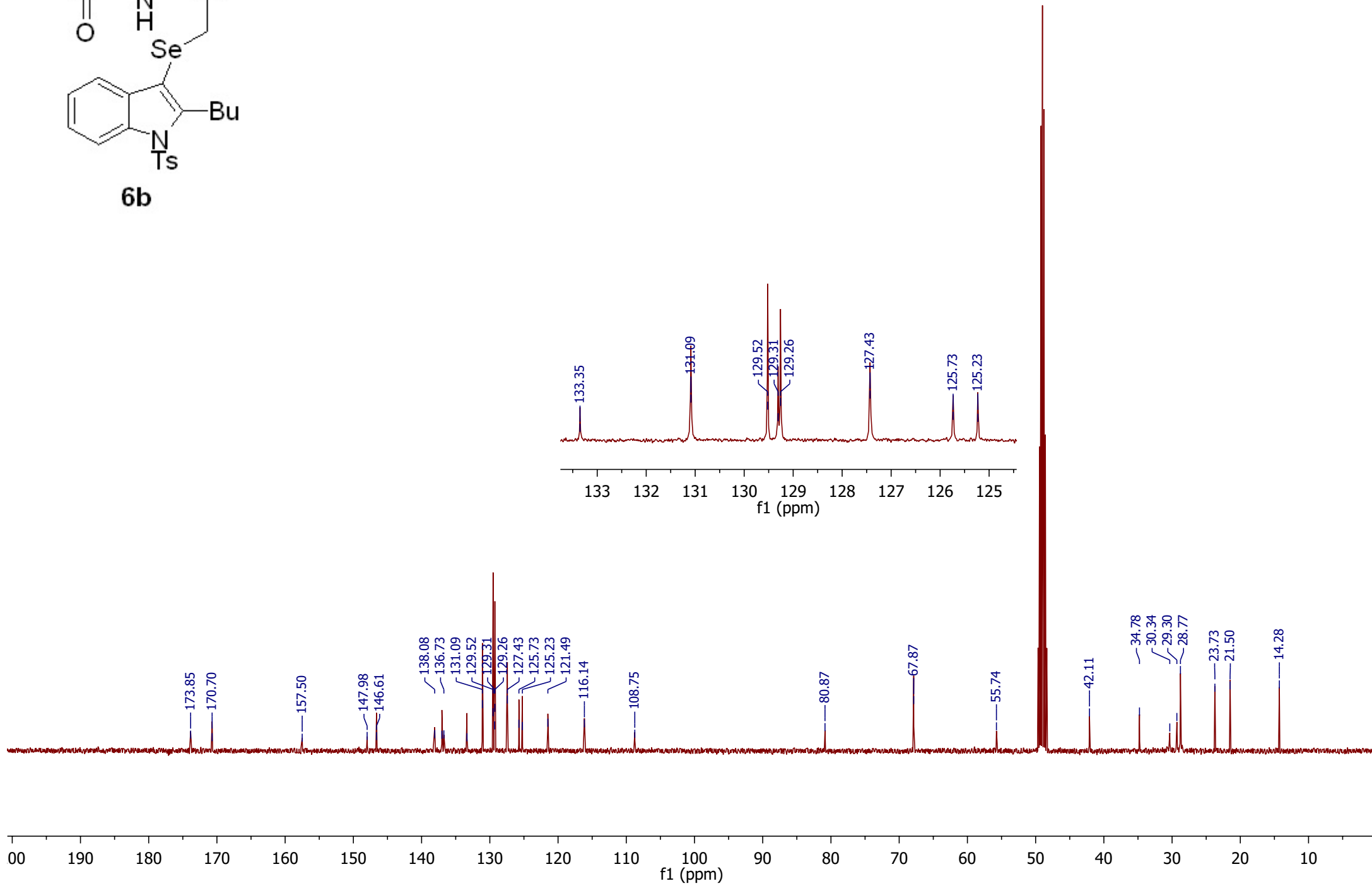
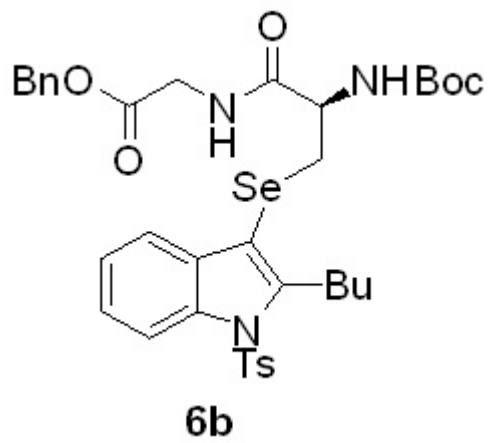


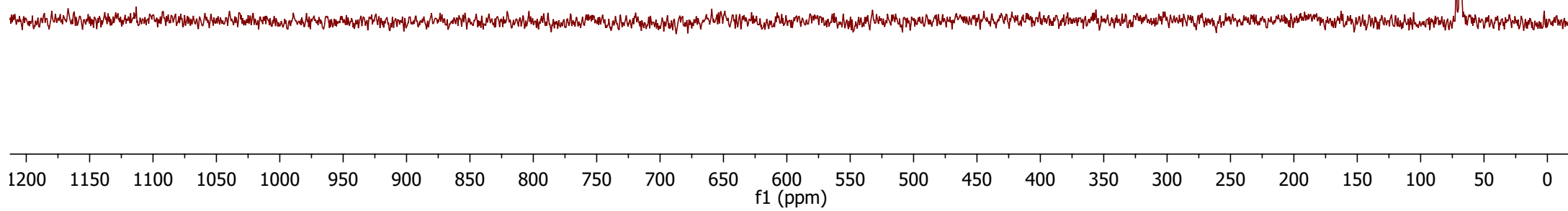
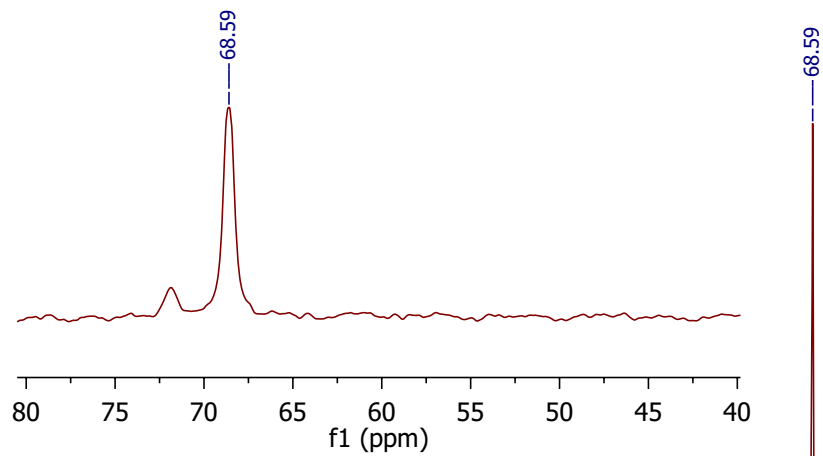
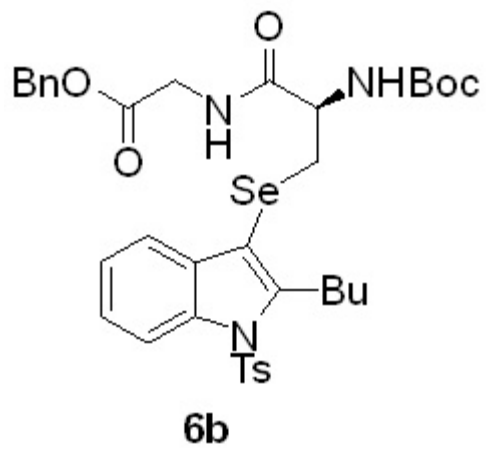


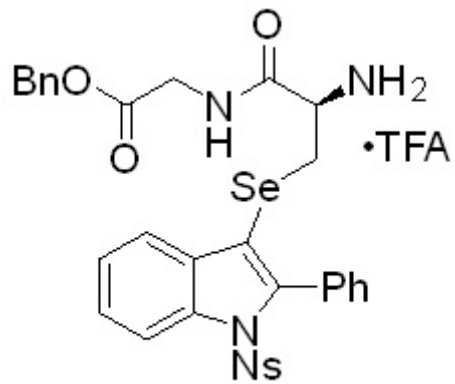




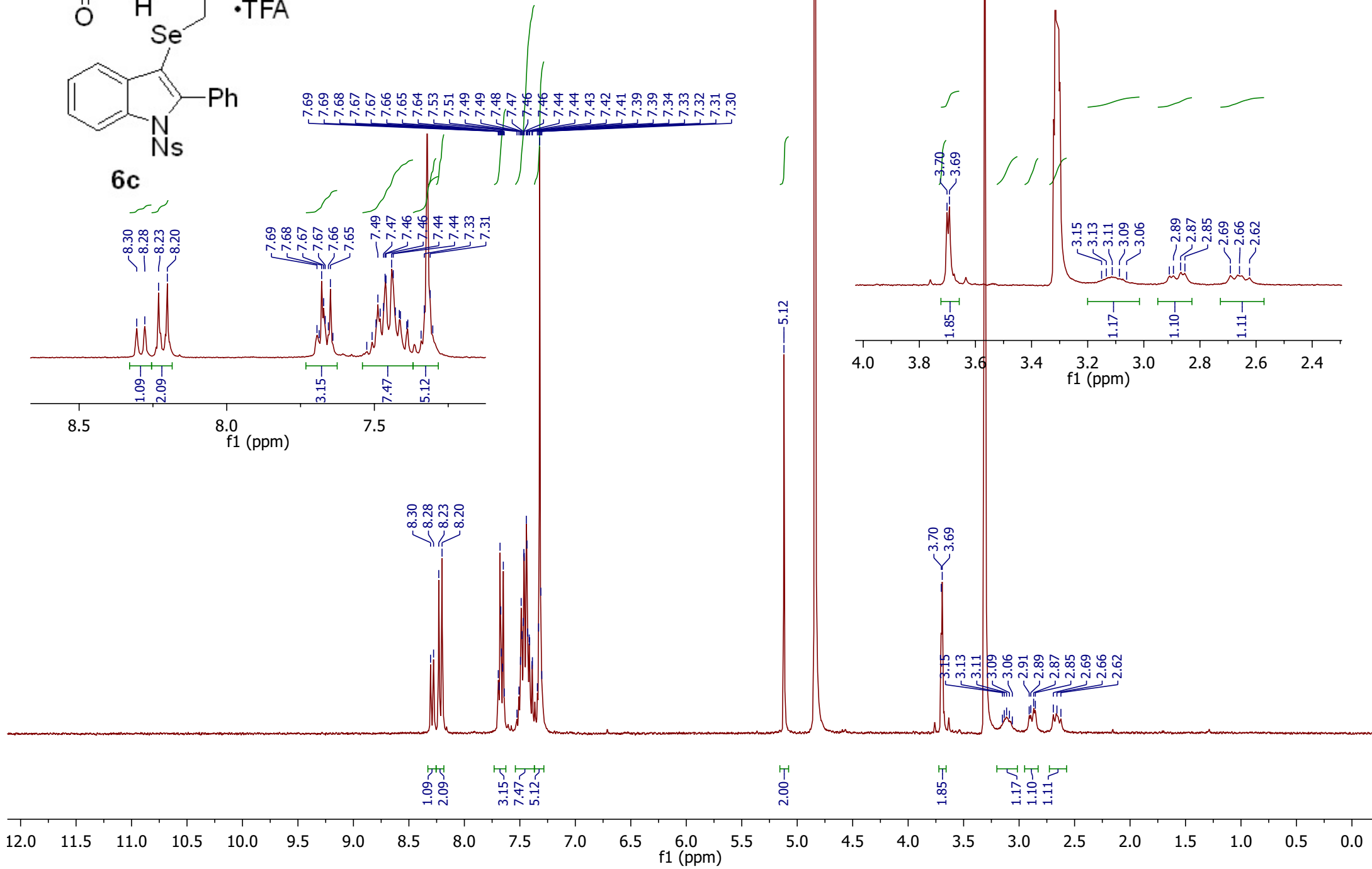


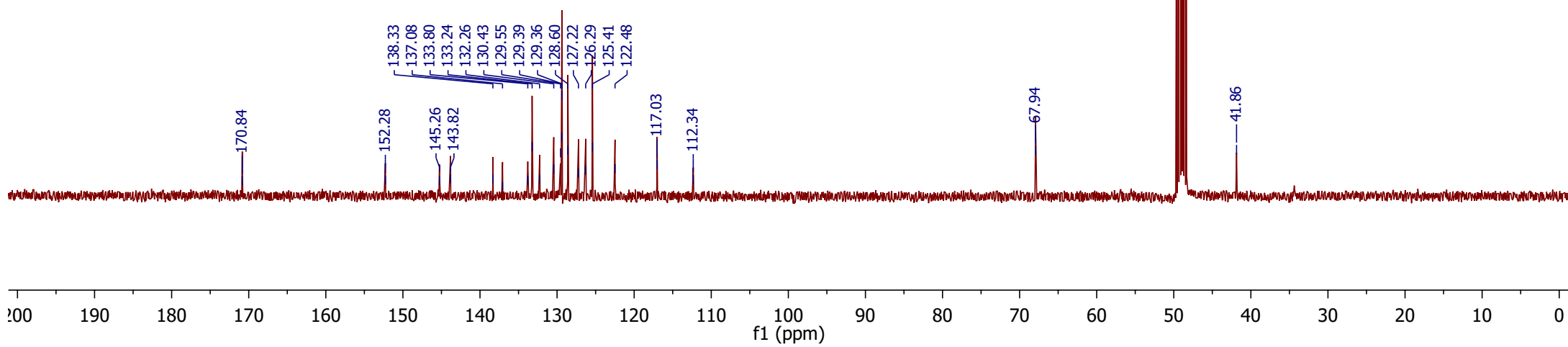
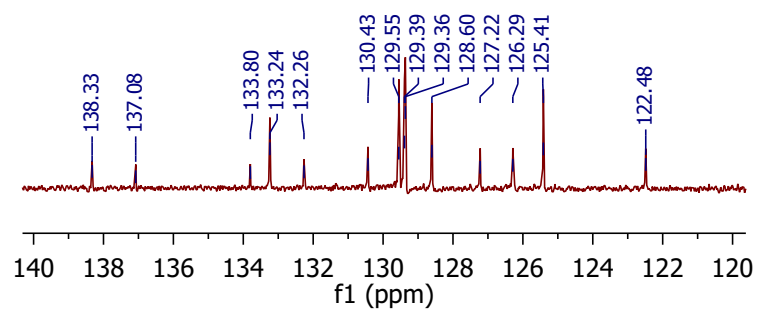
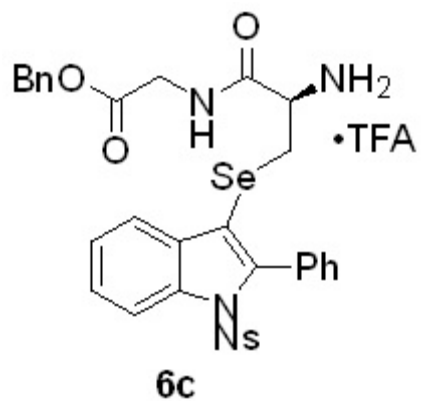


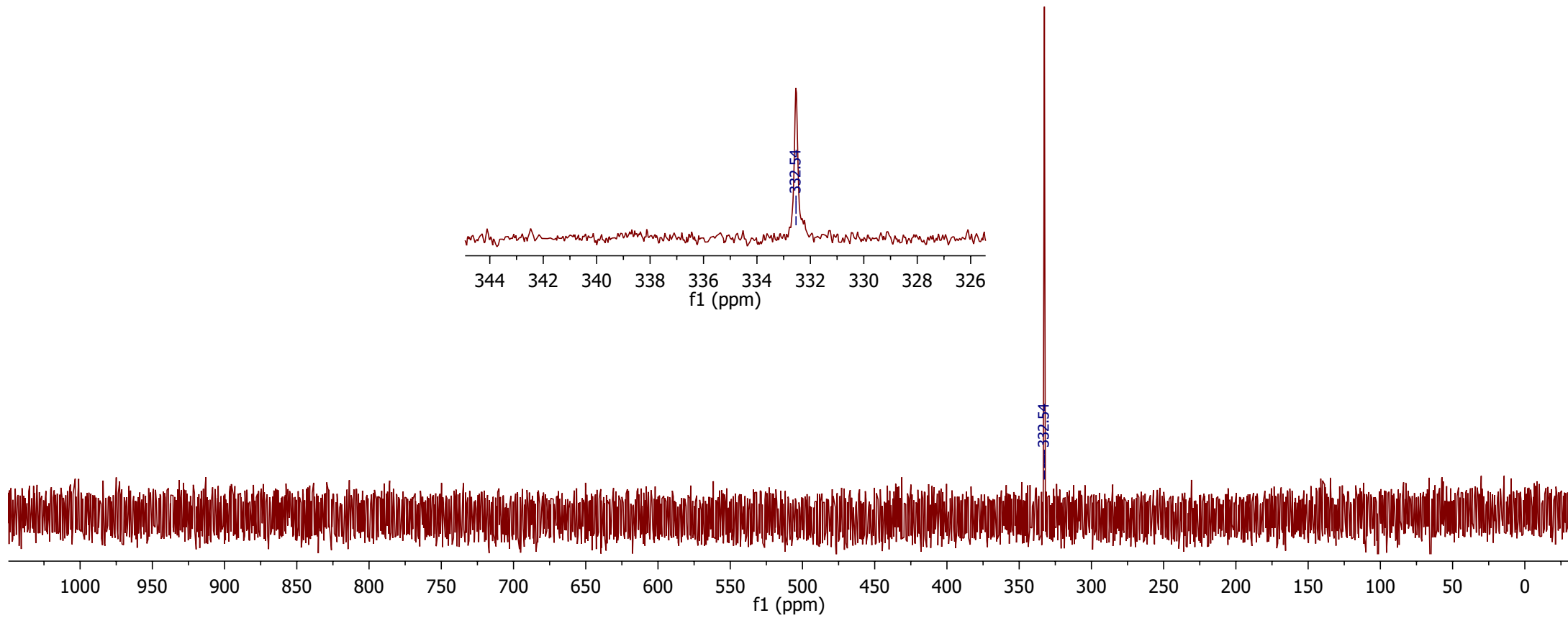
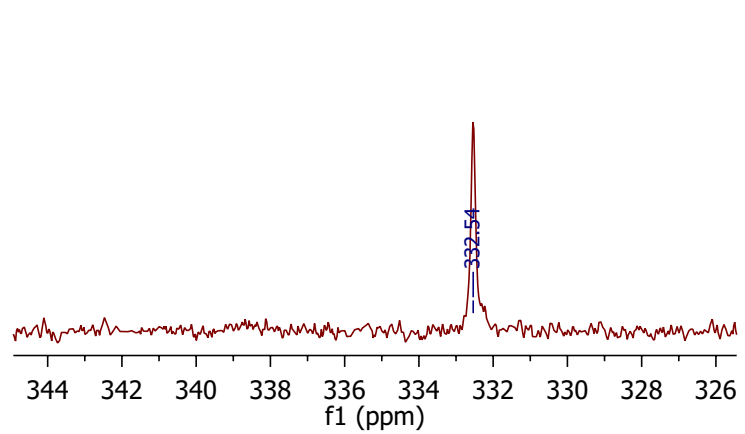
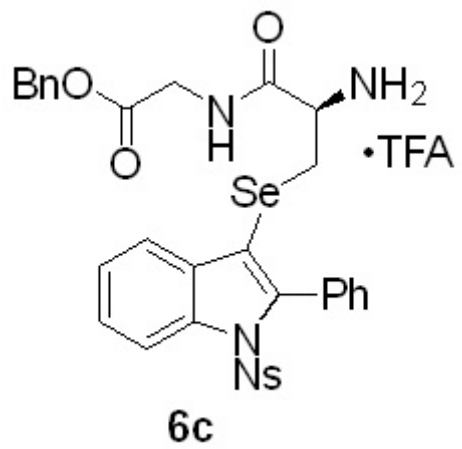


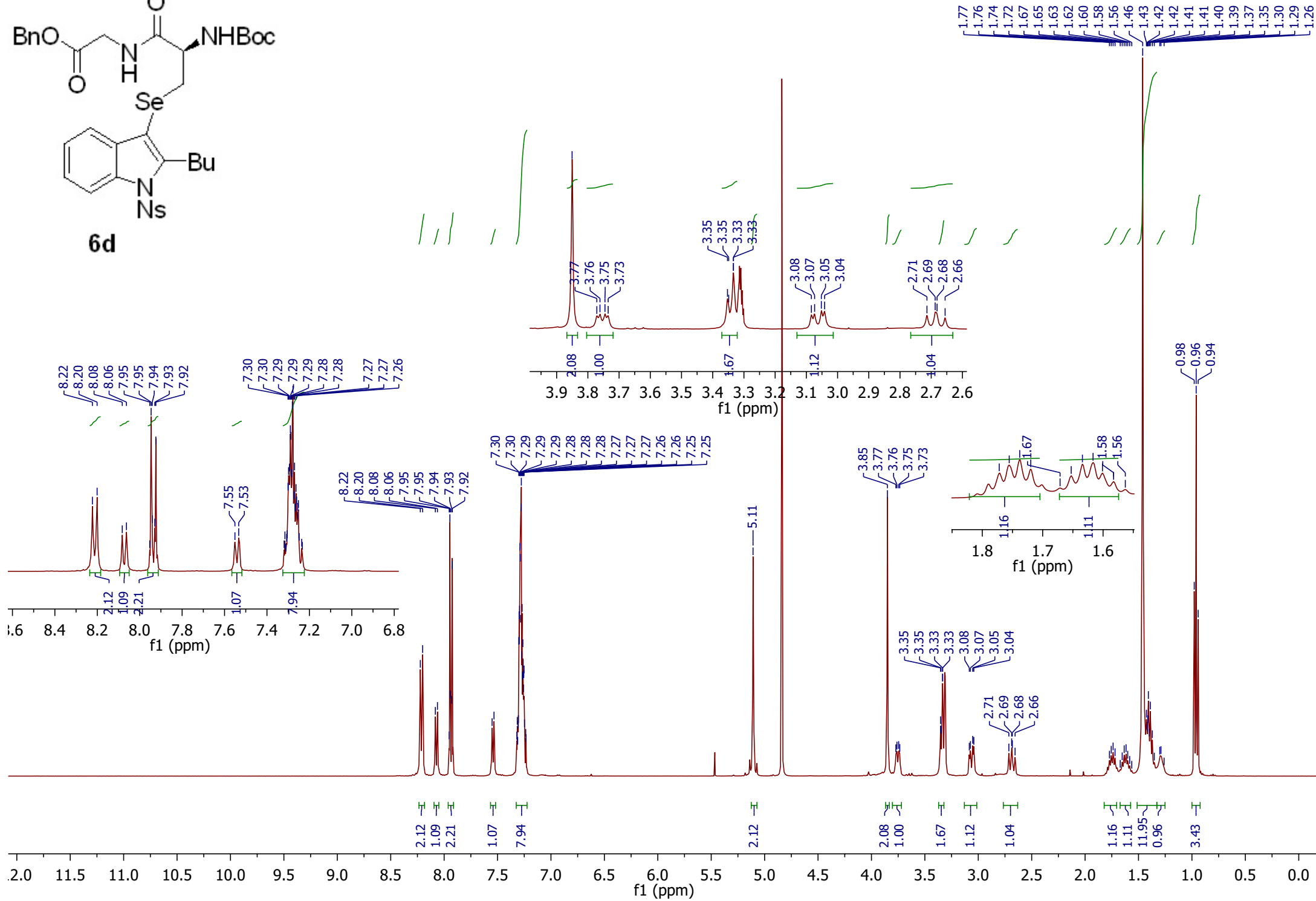
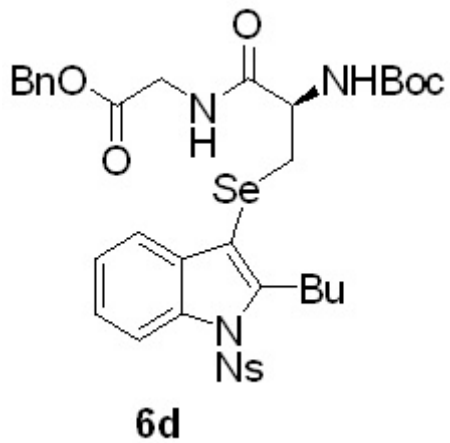


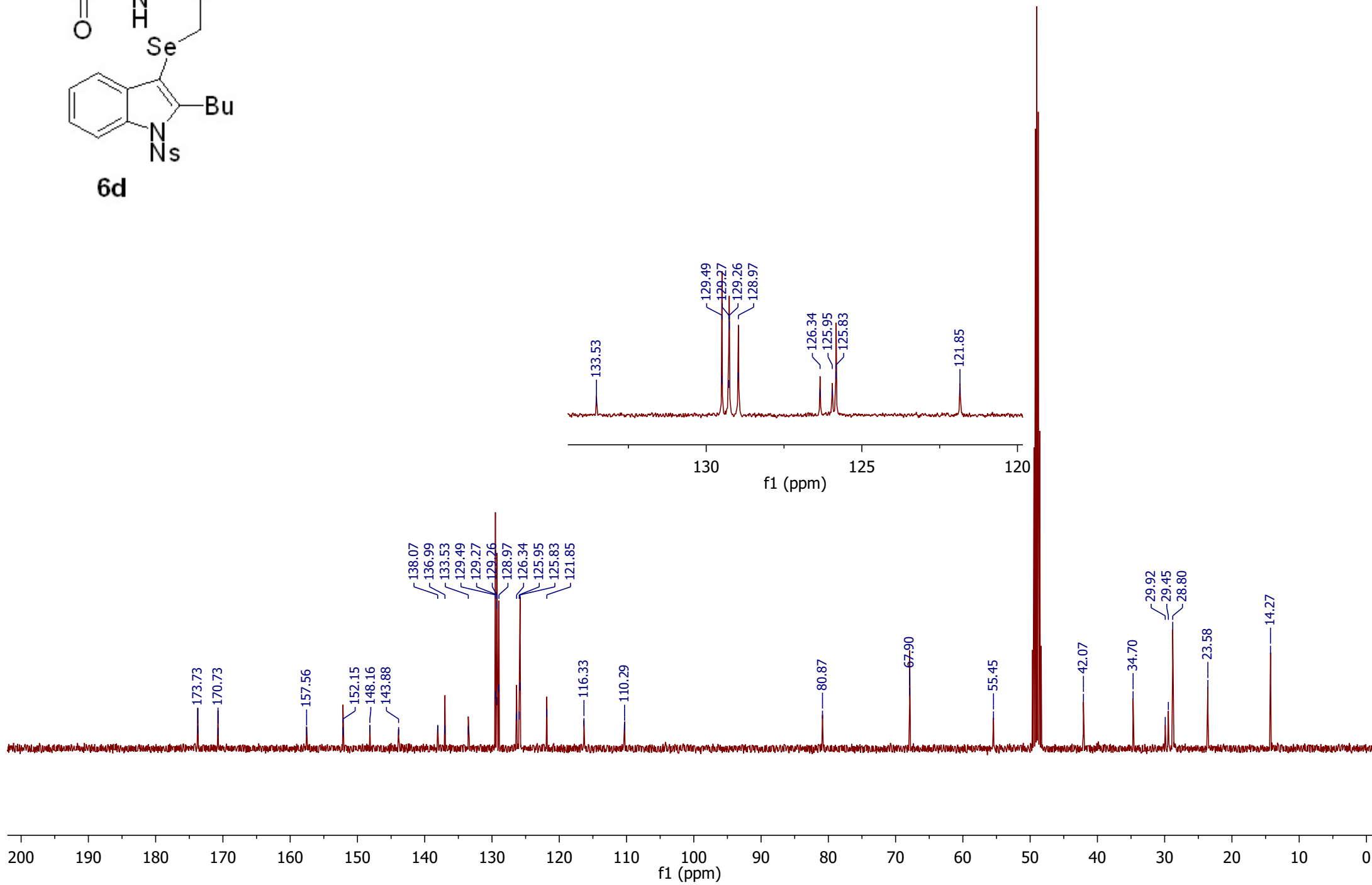
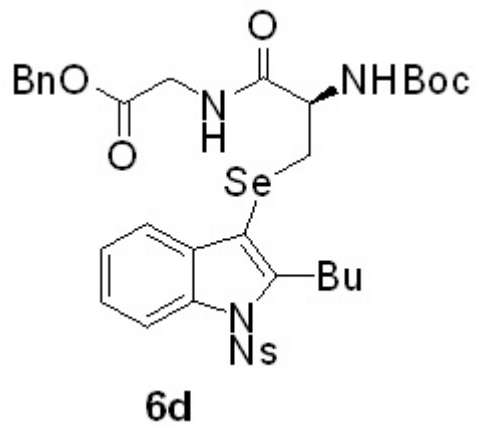
6c

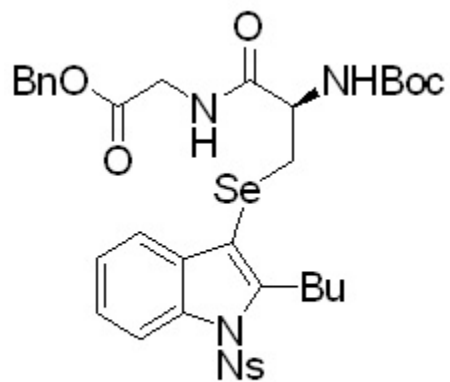




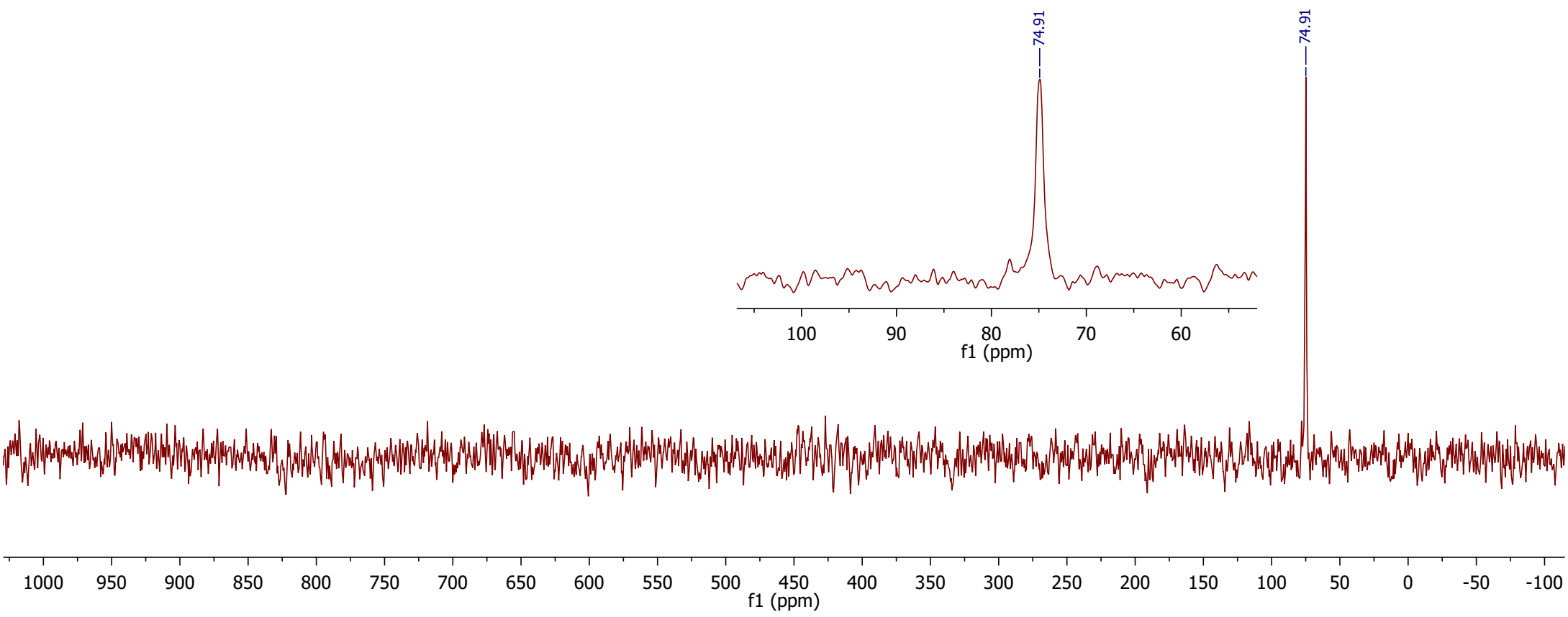


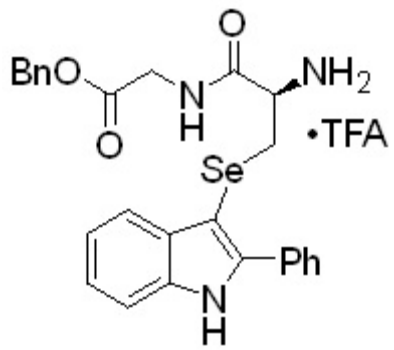




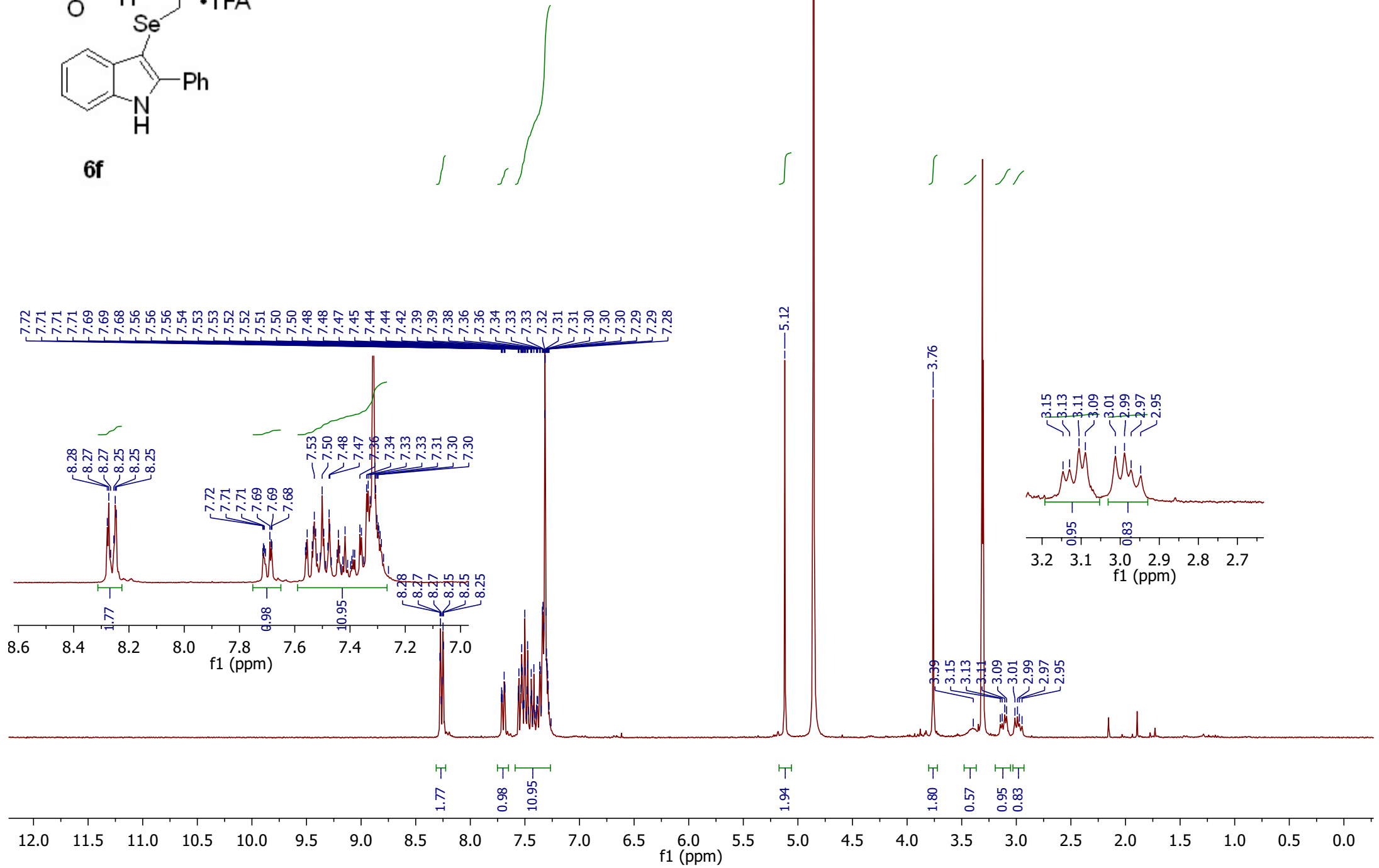


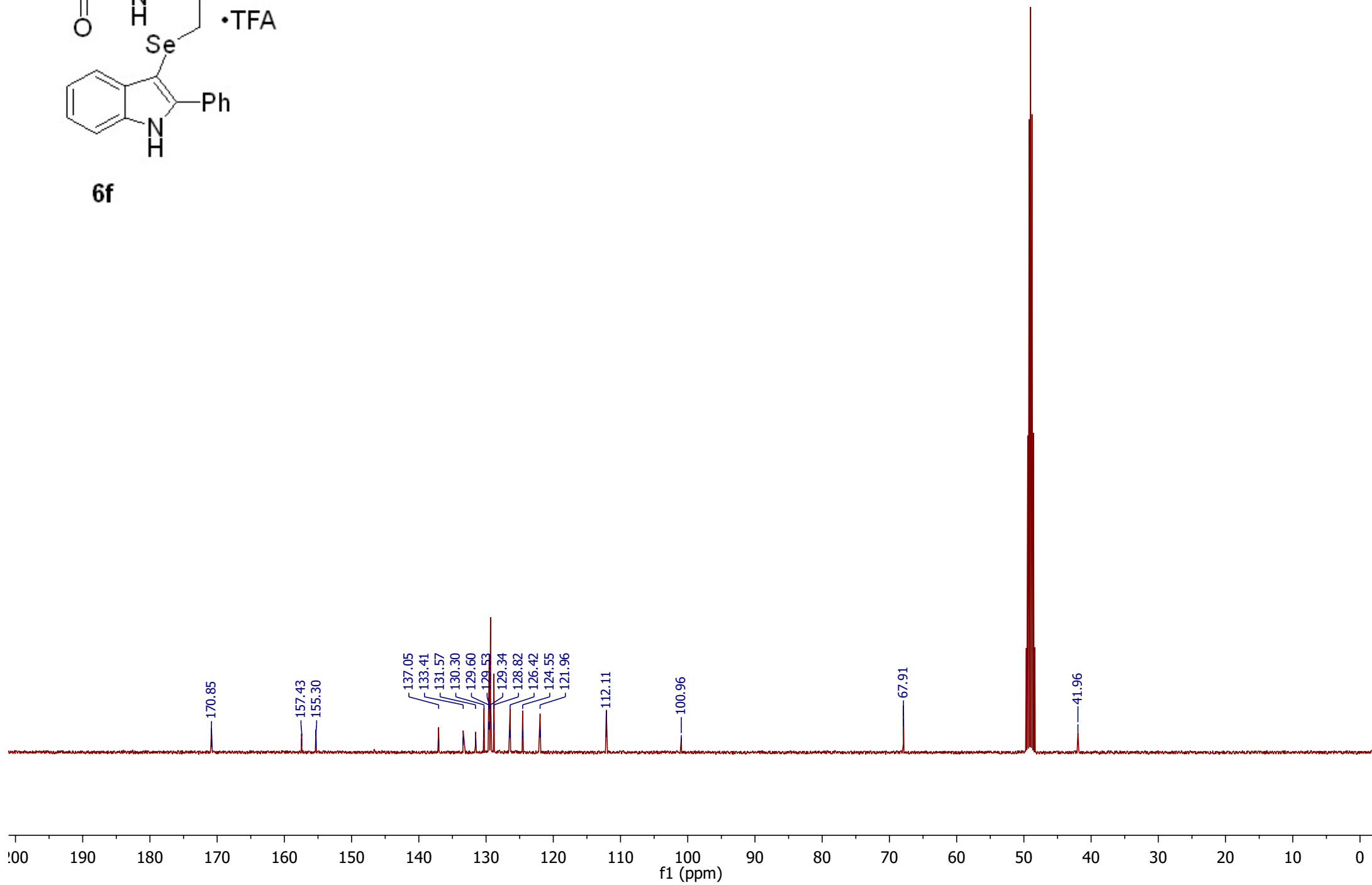
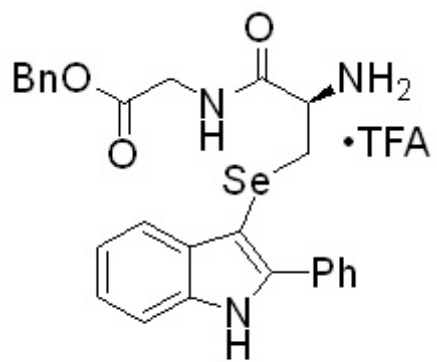
6d

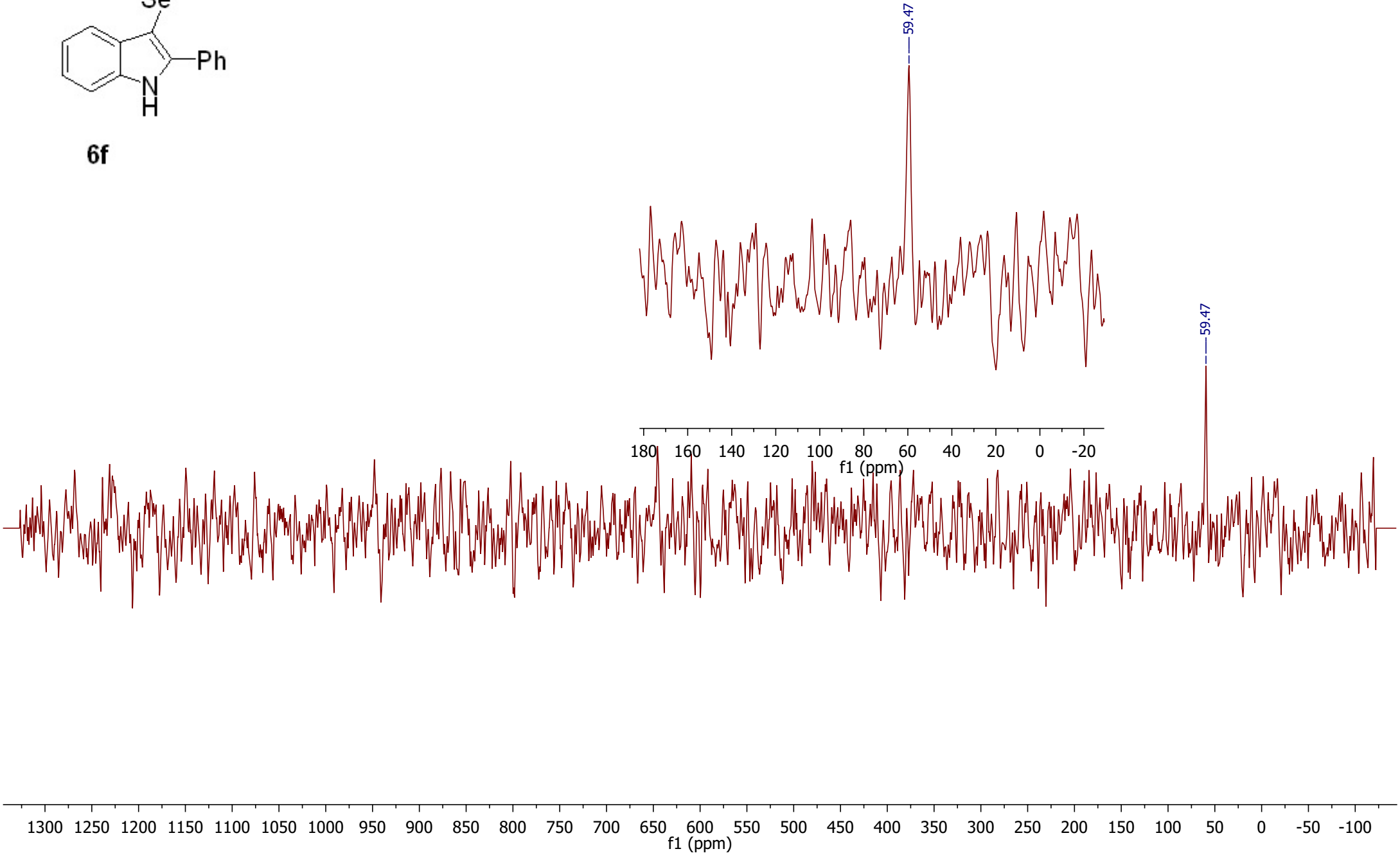
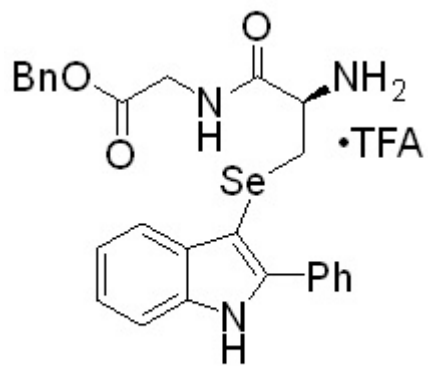


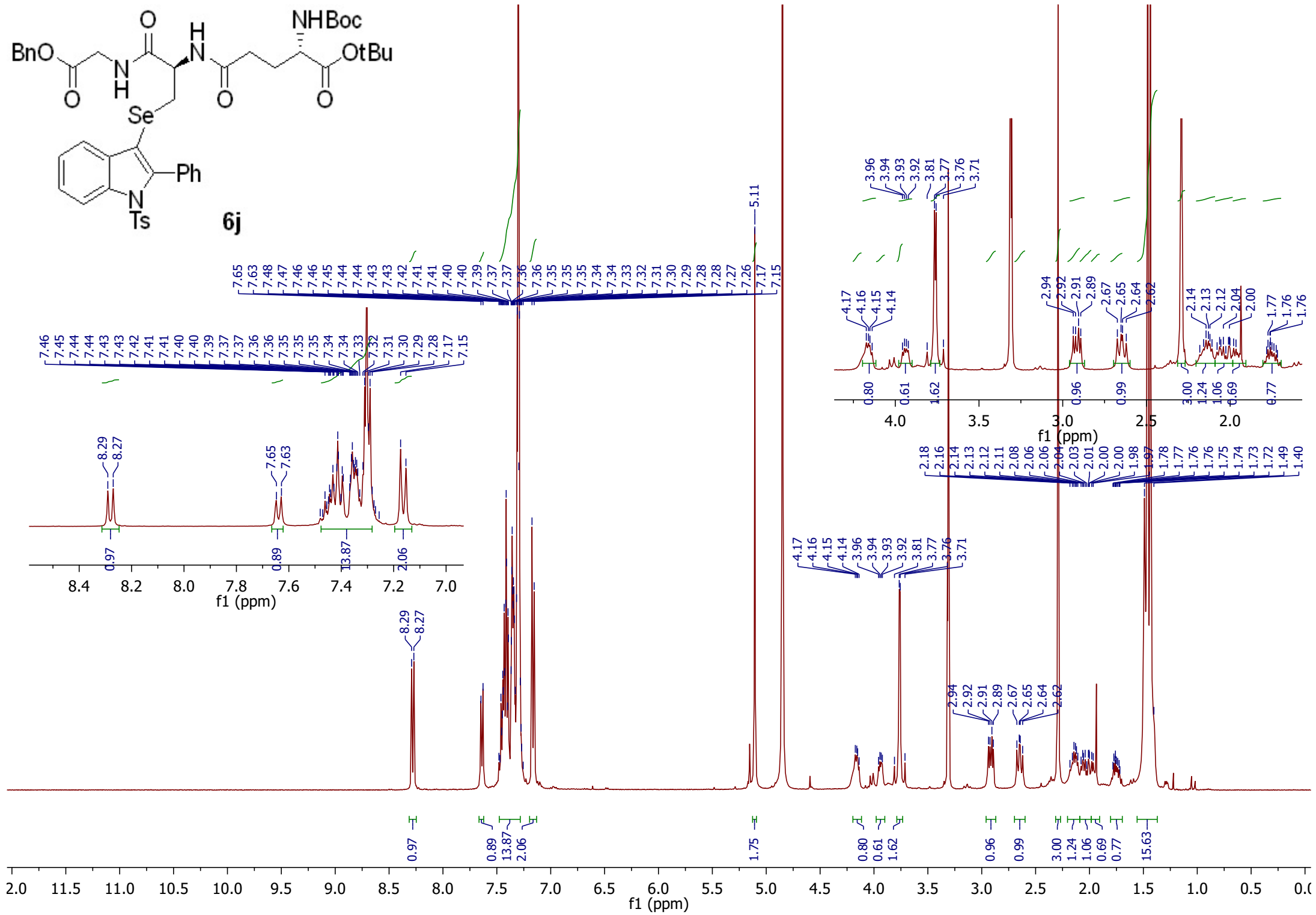
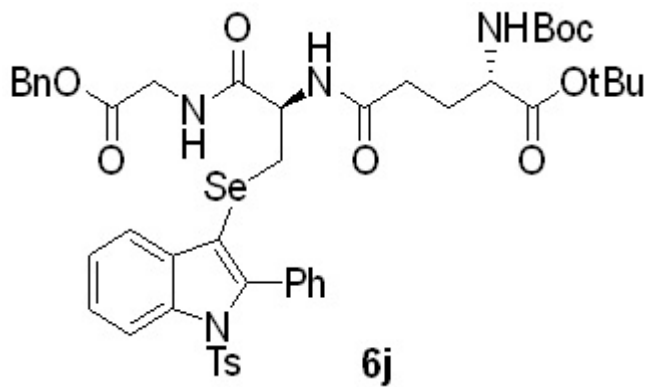


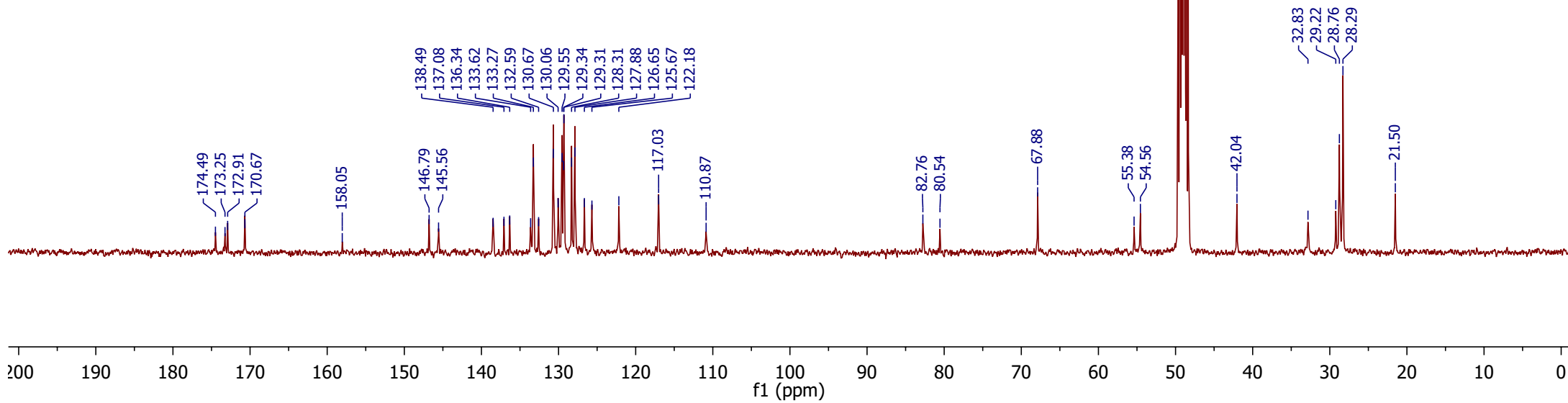
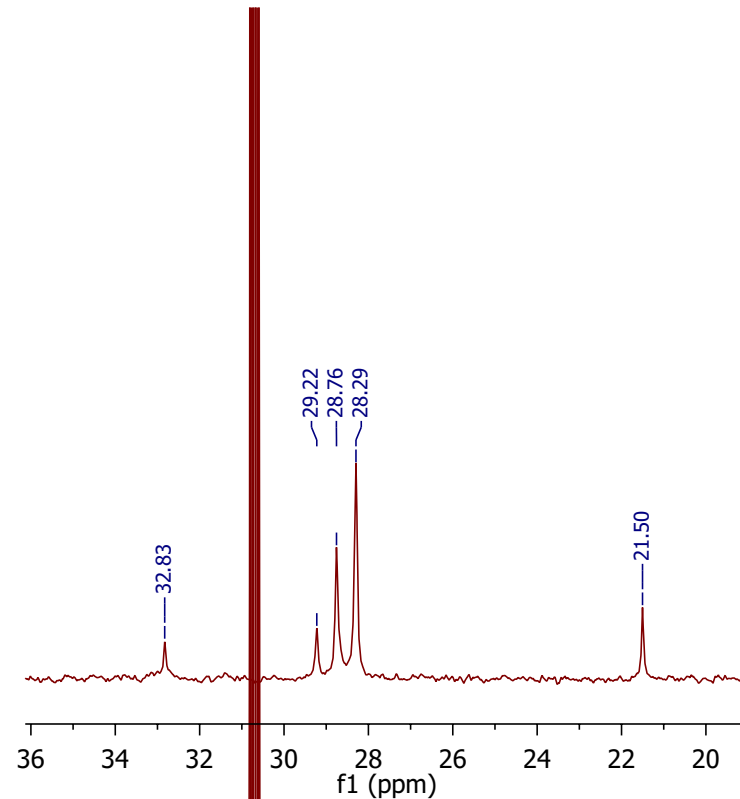
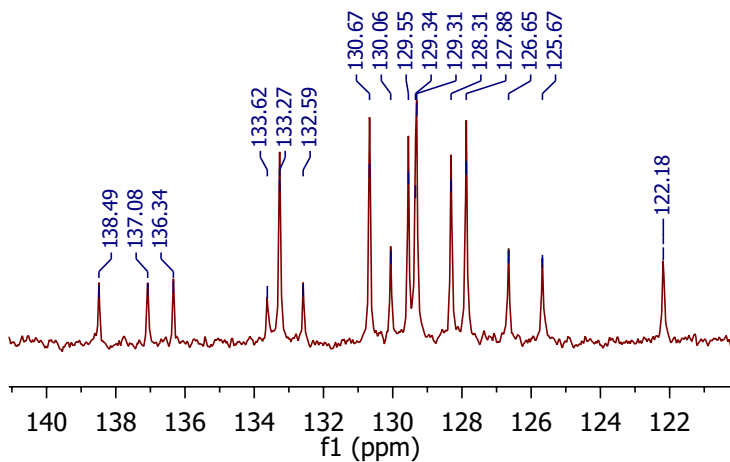
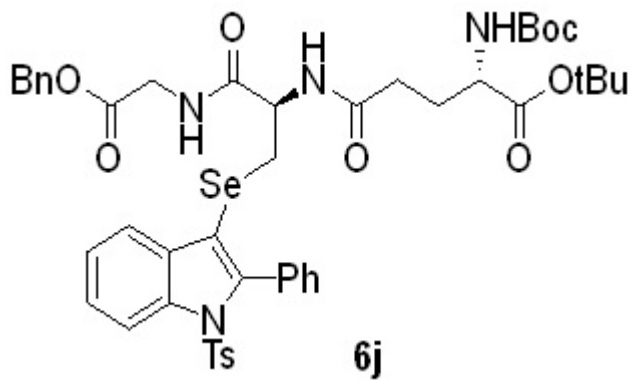
6f

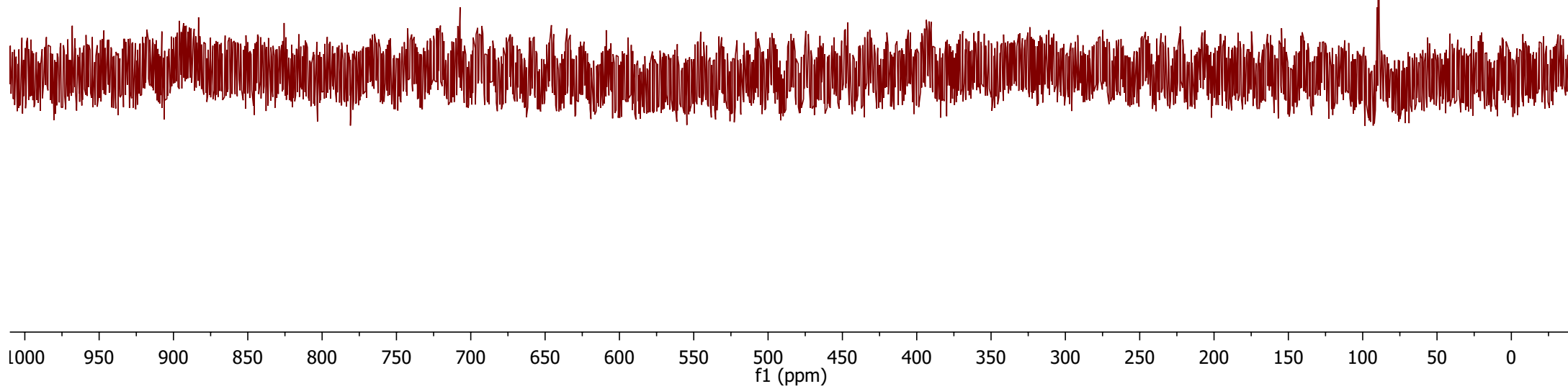
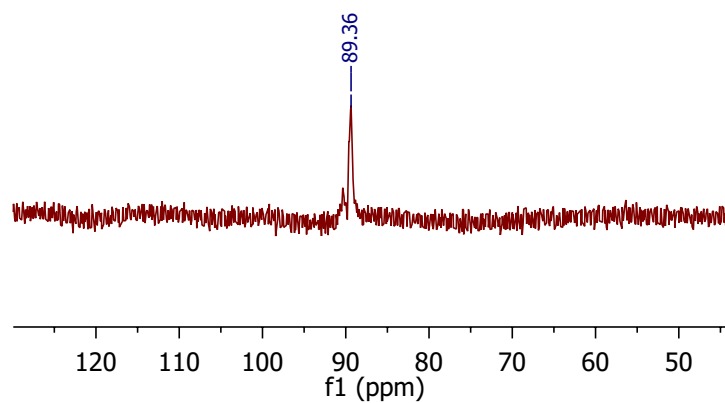
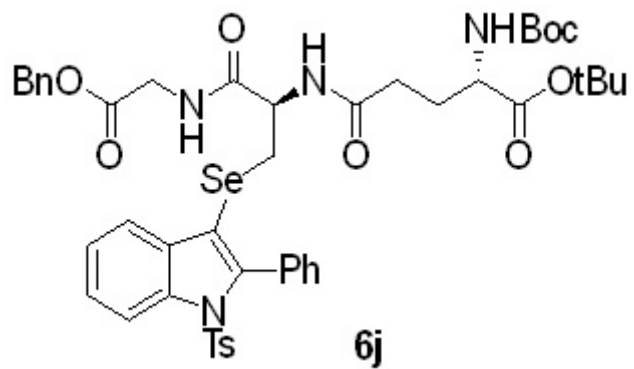


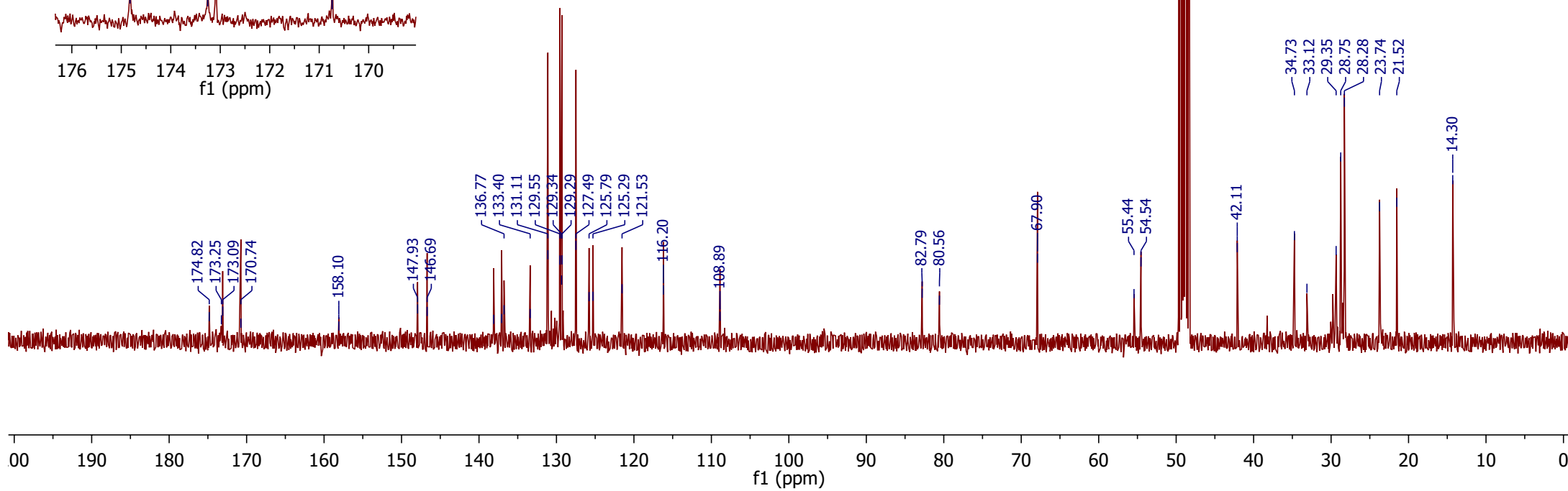
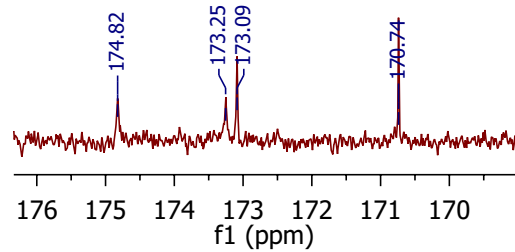
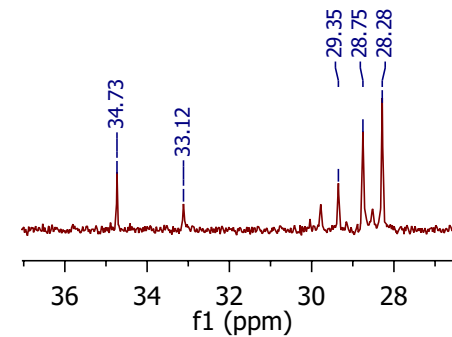
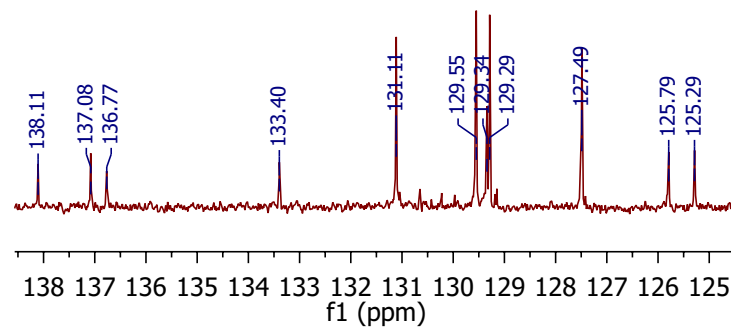
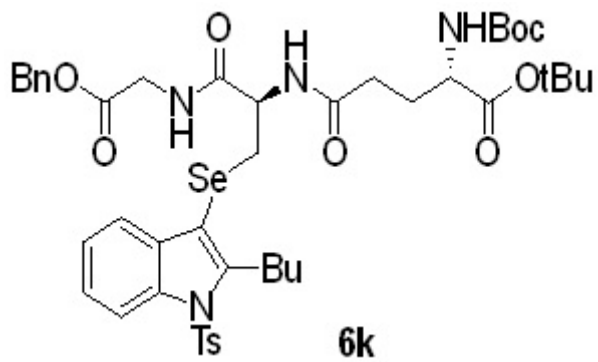


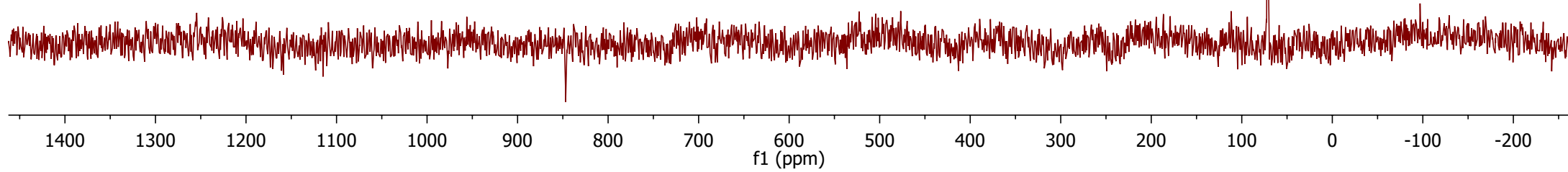
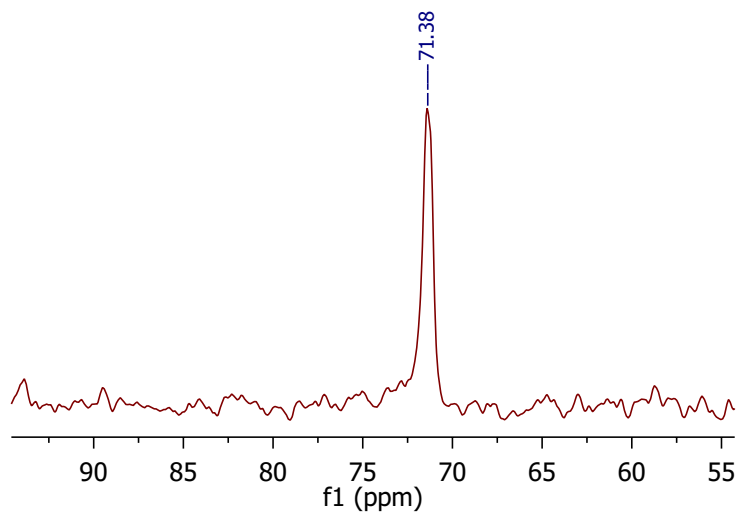
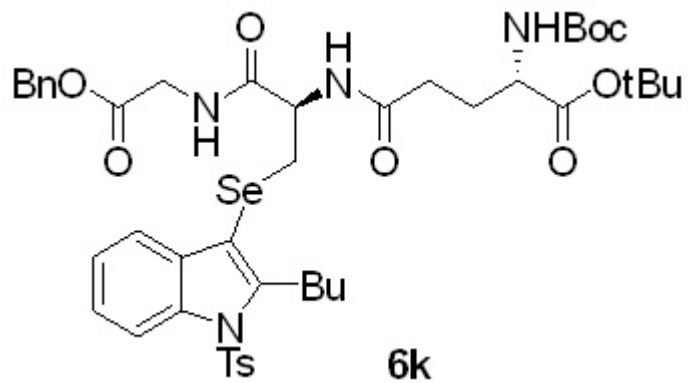


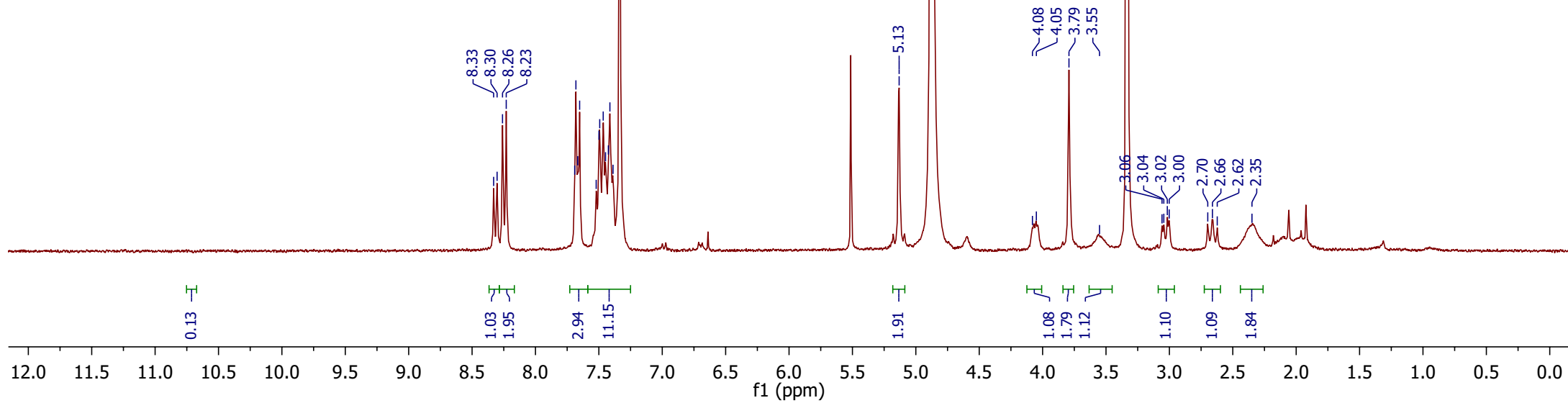
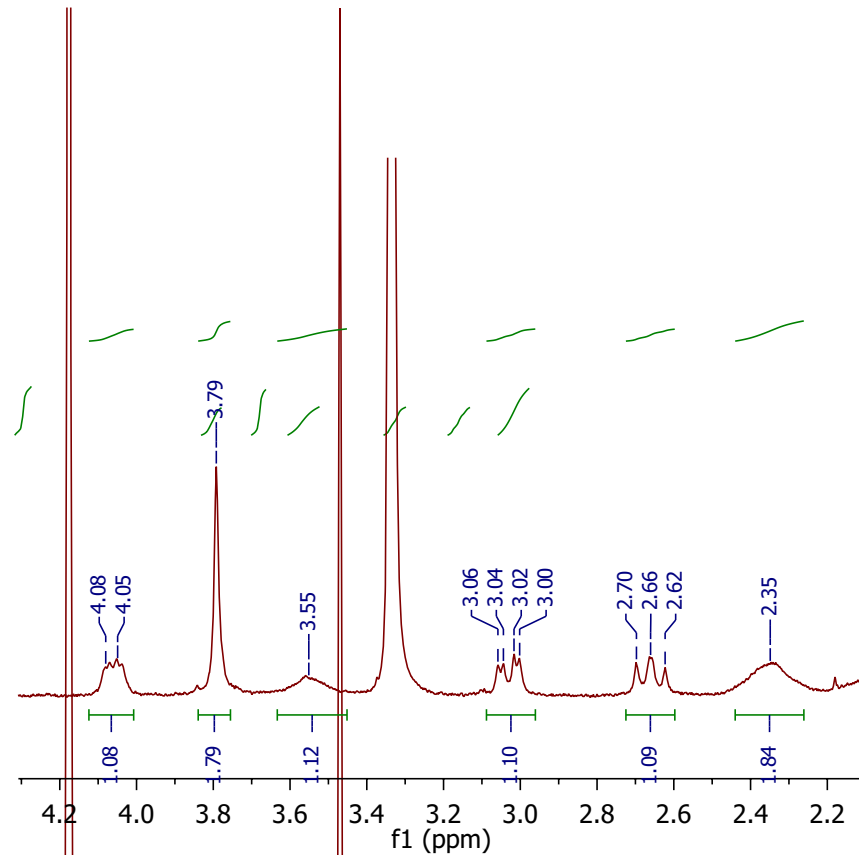
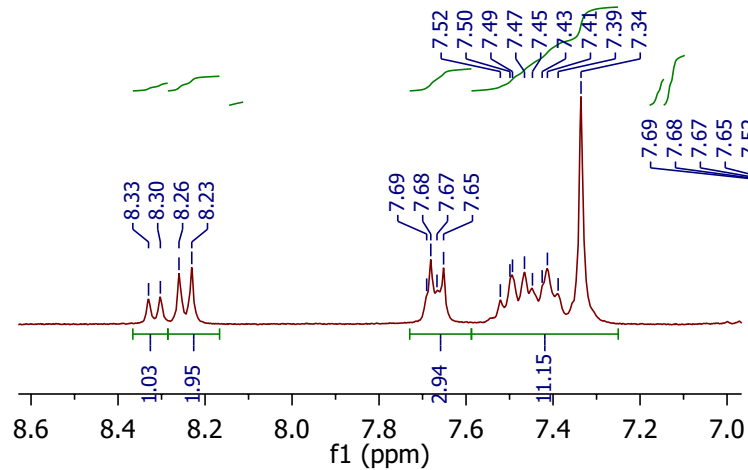
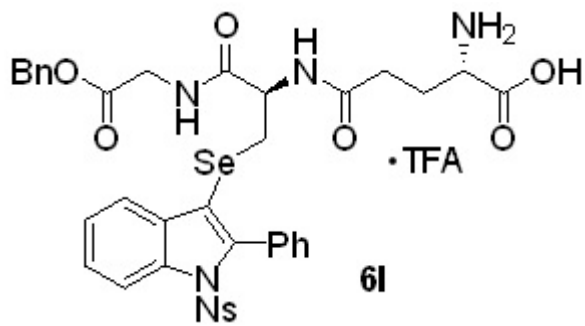


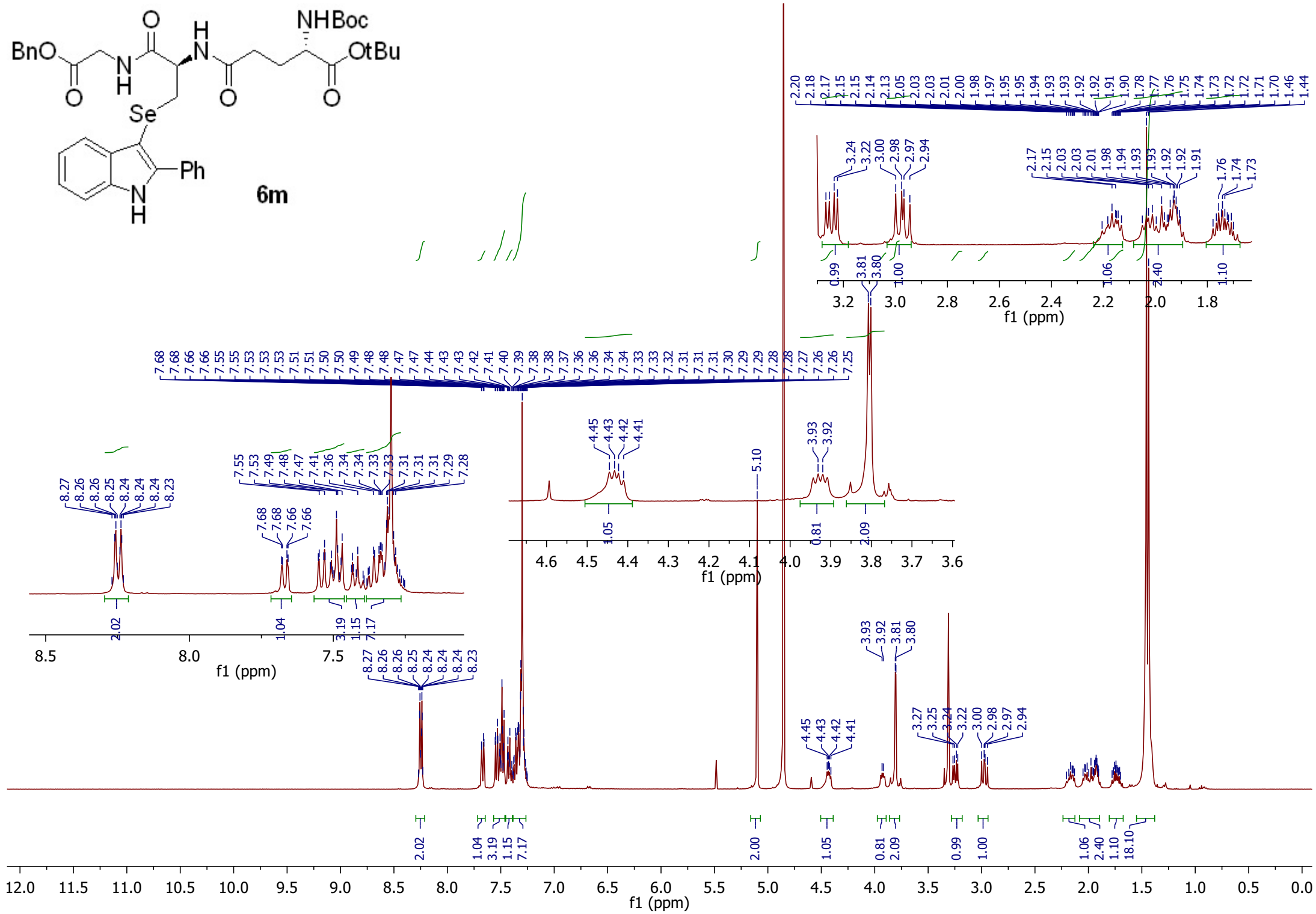
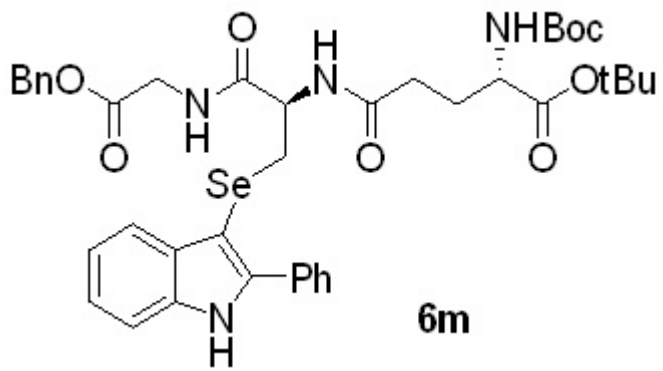


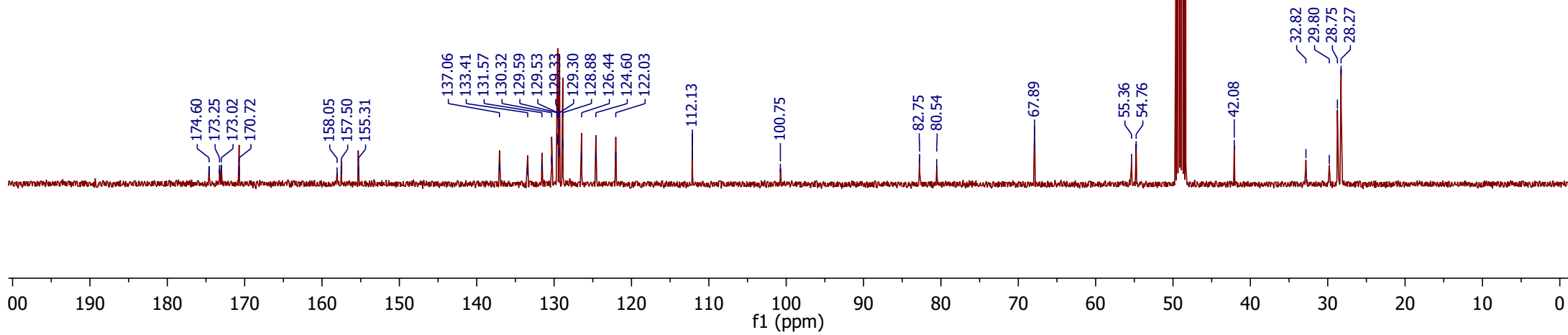
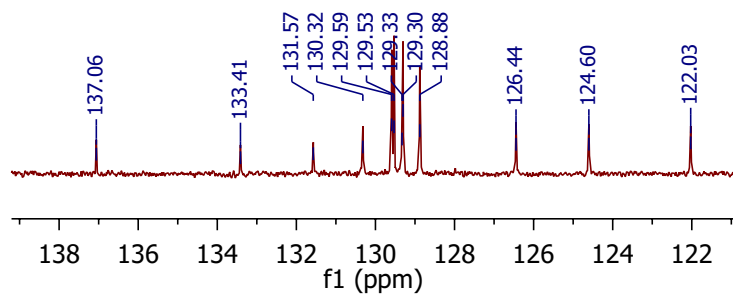
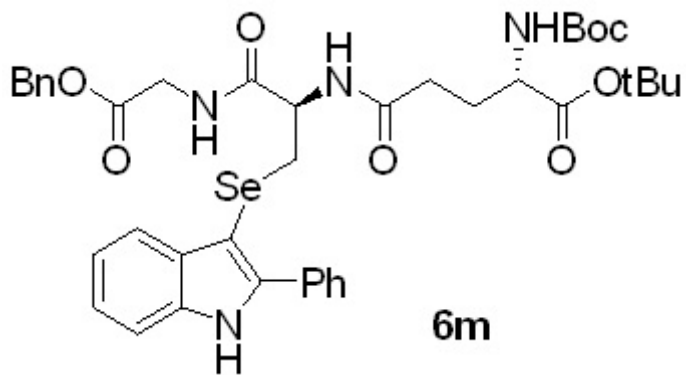


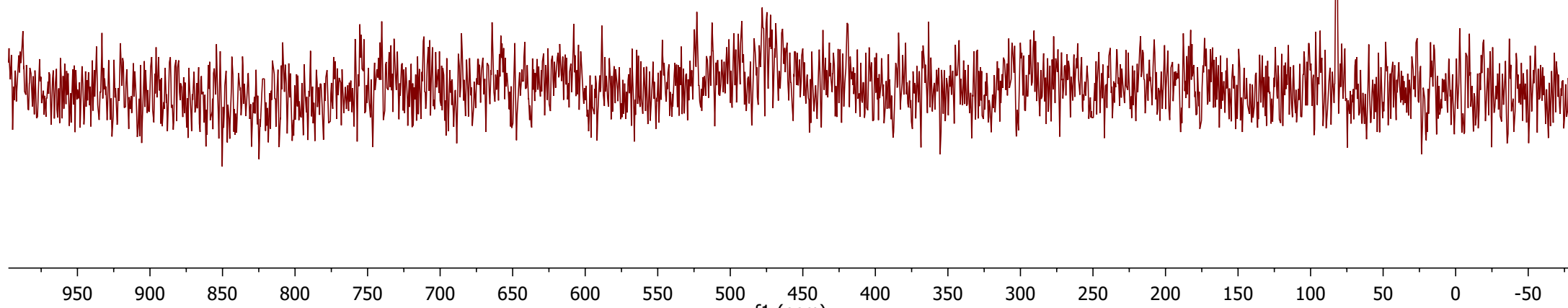
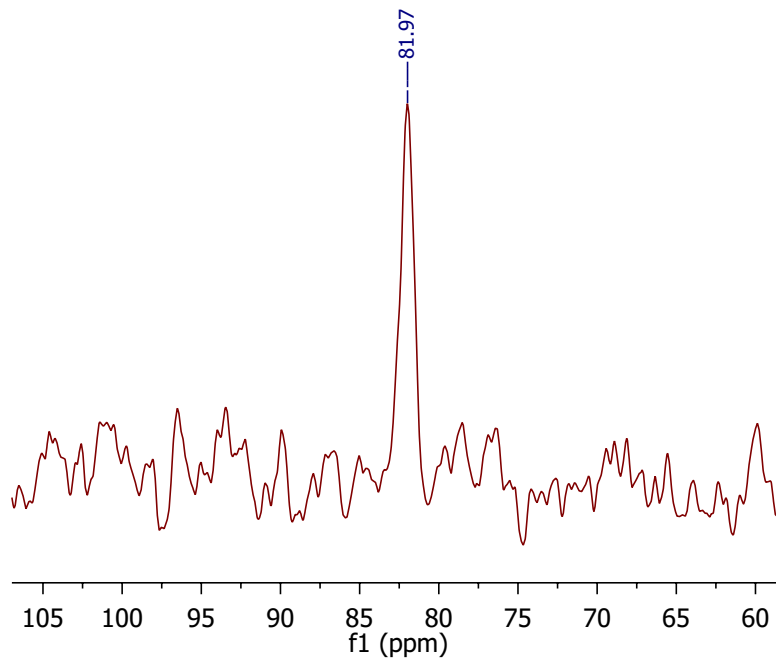
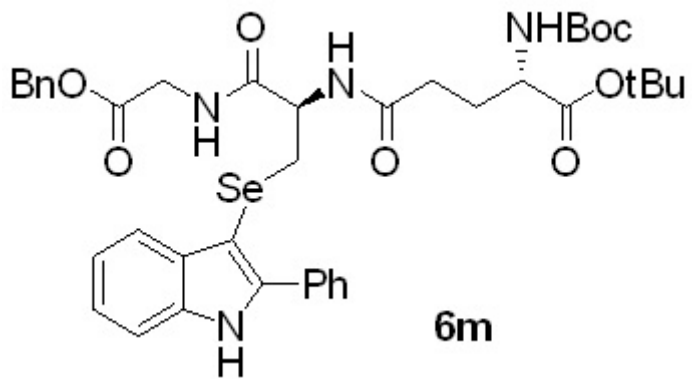


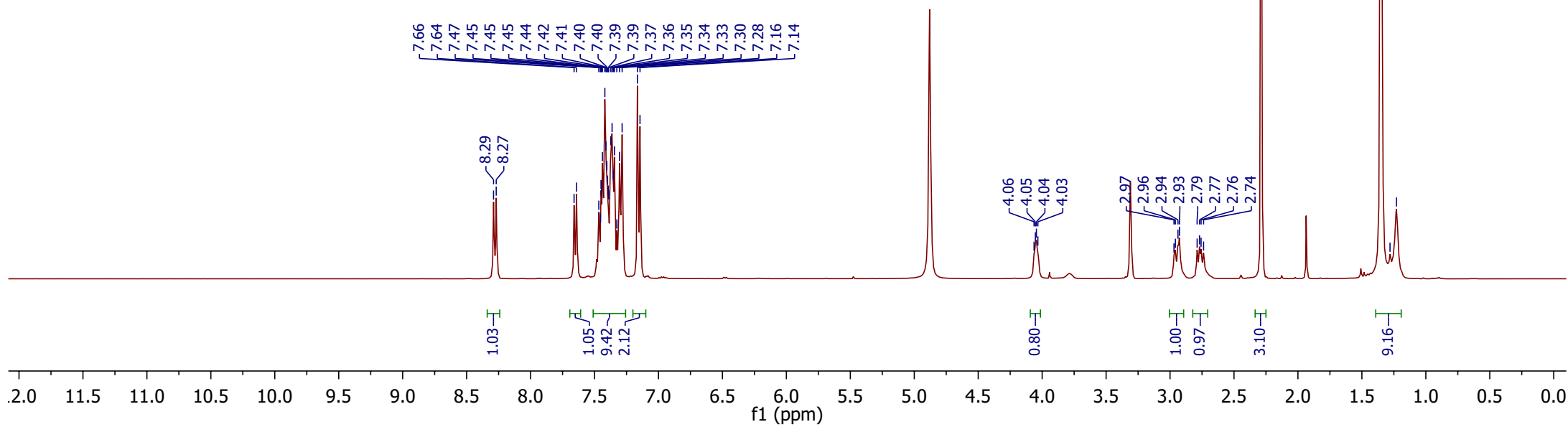
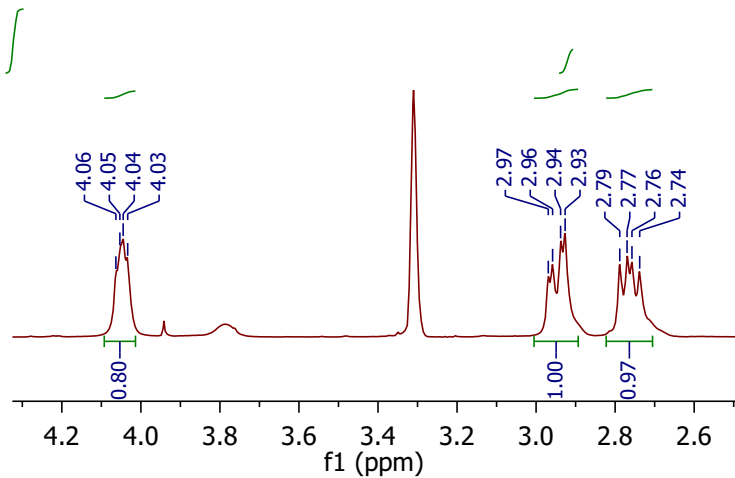
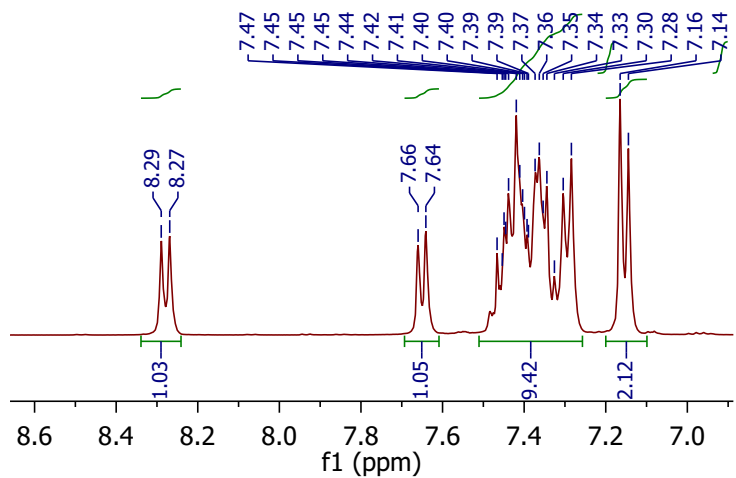
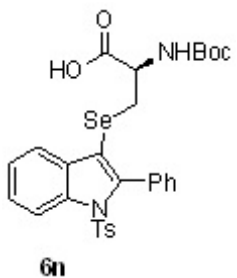


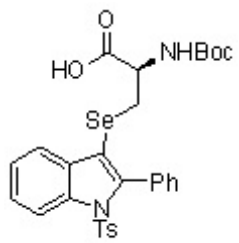




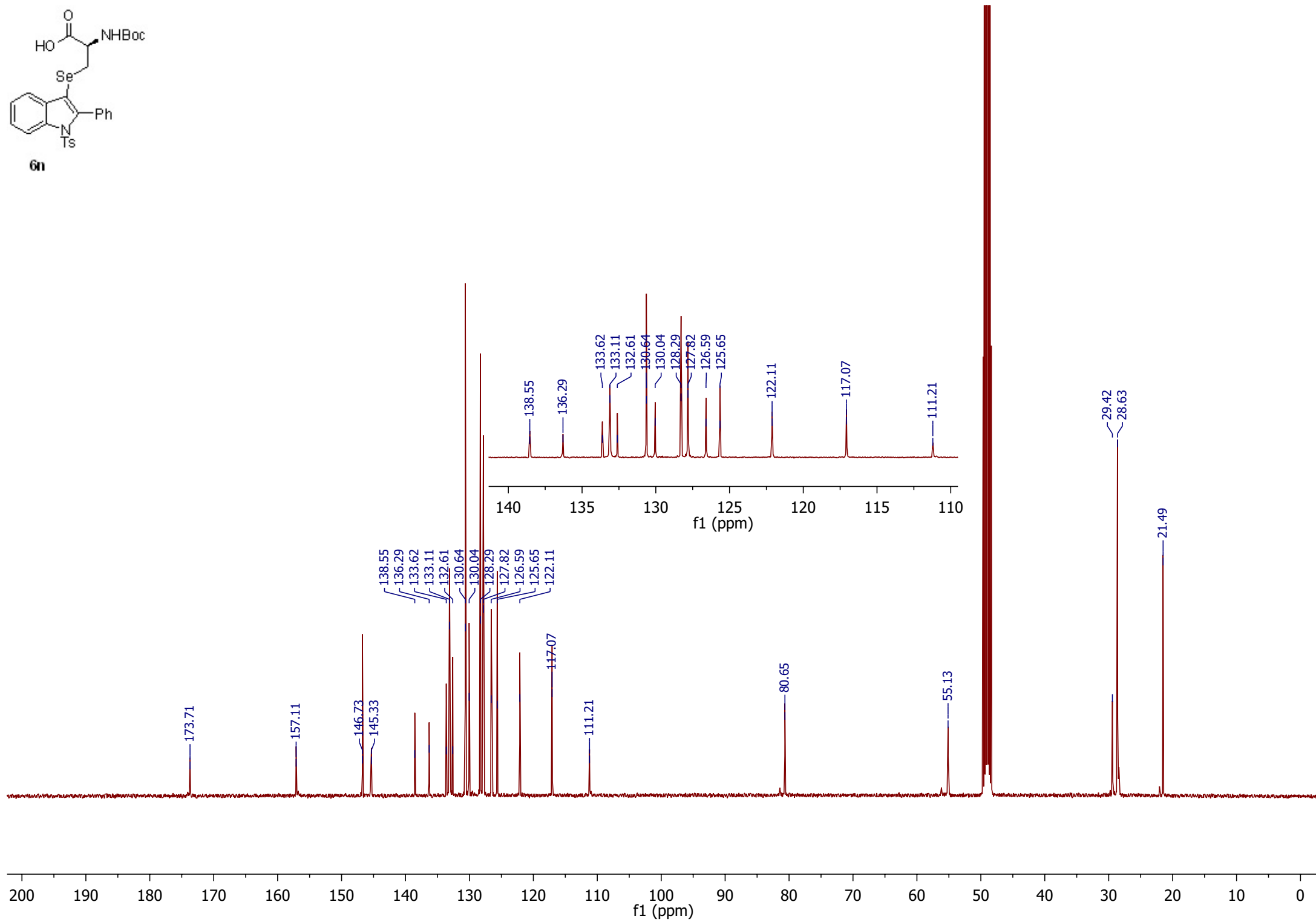


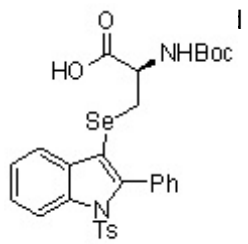




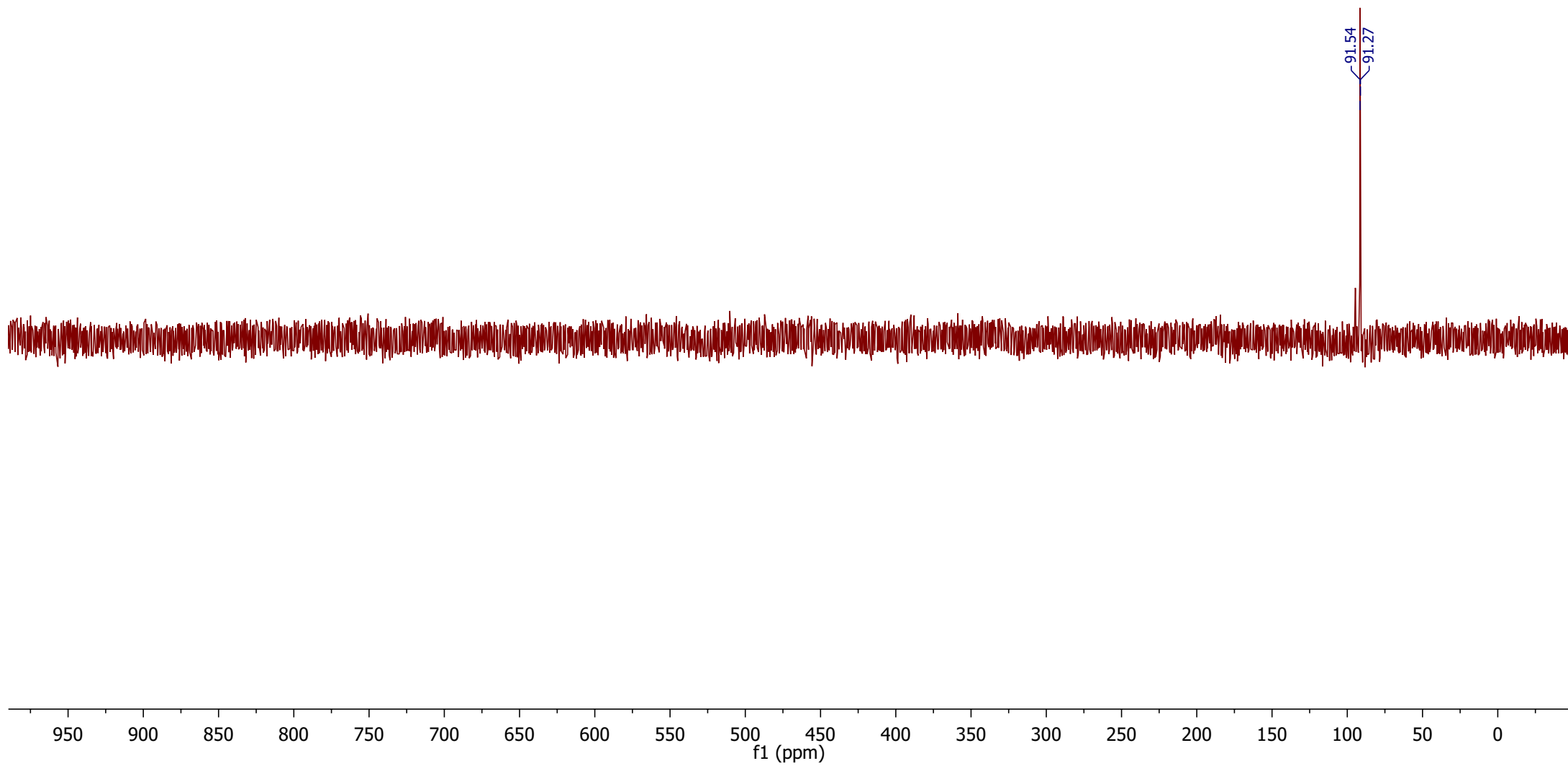


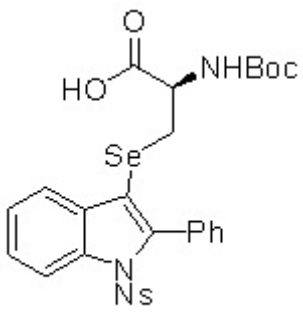
6h



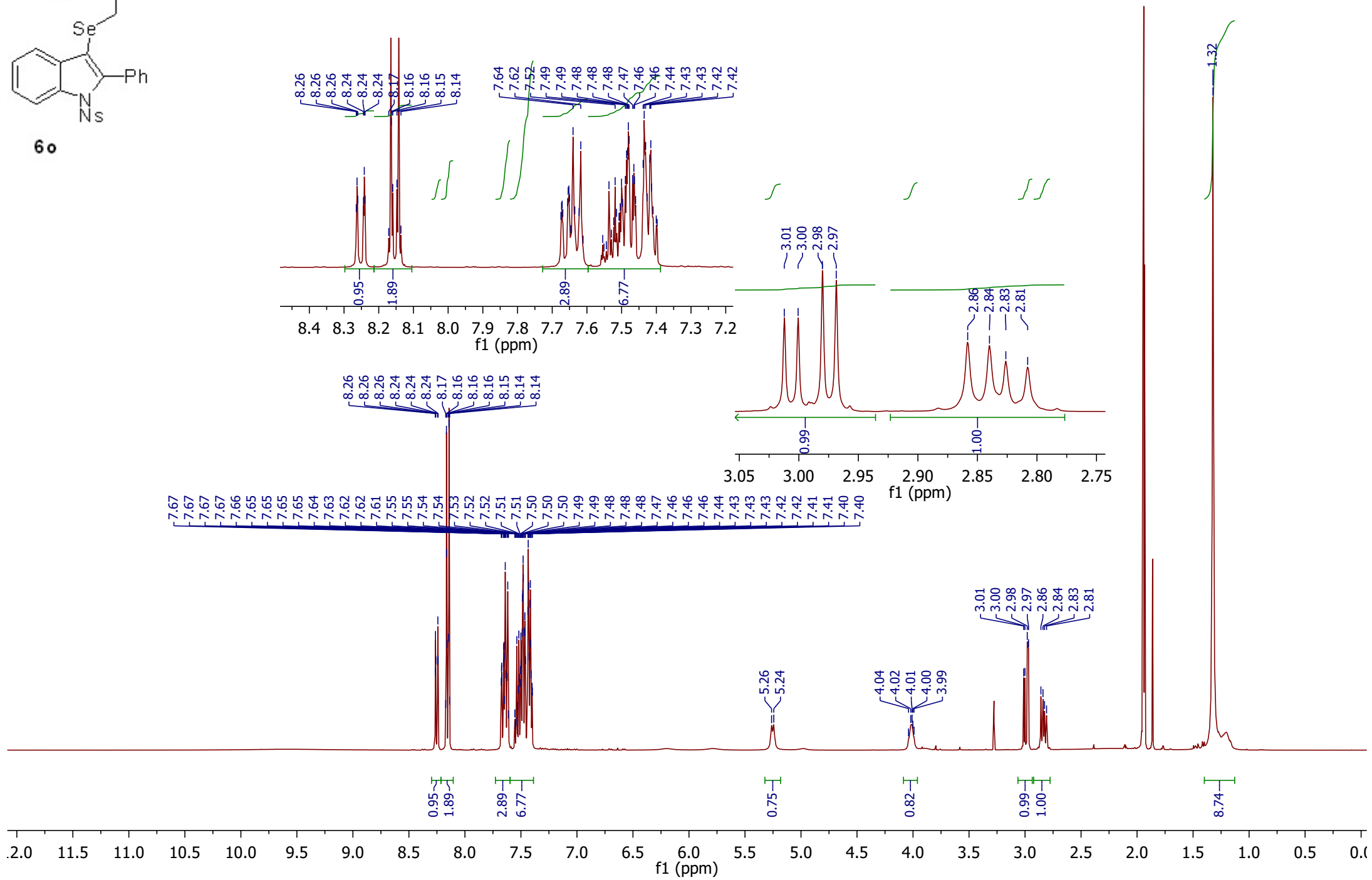


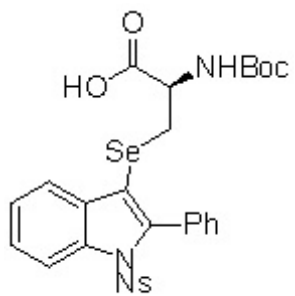
6h



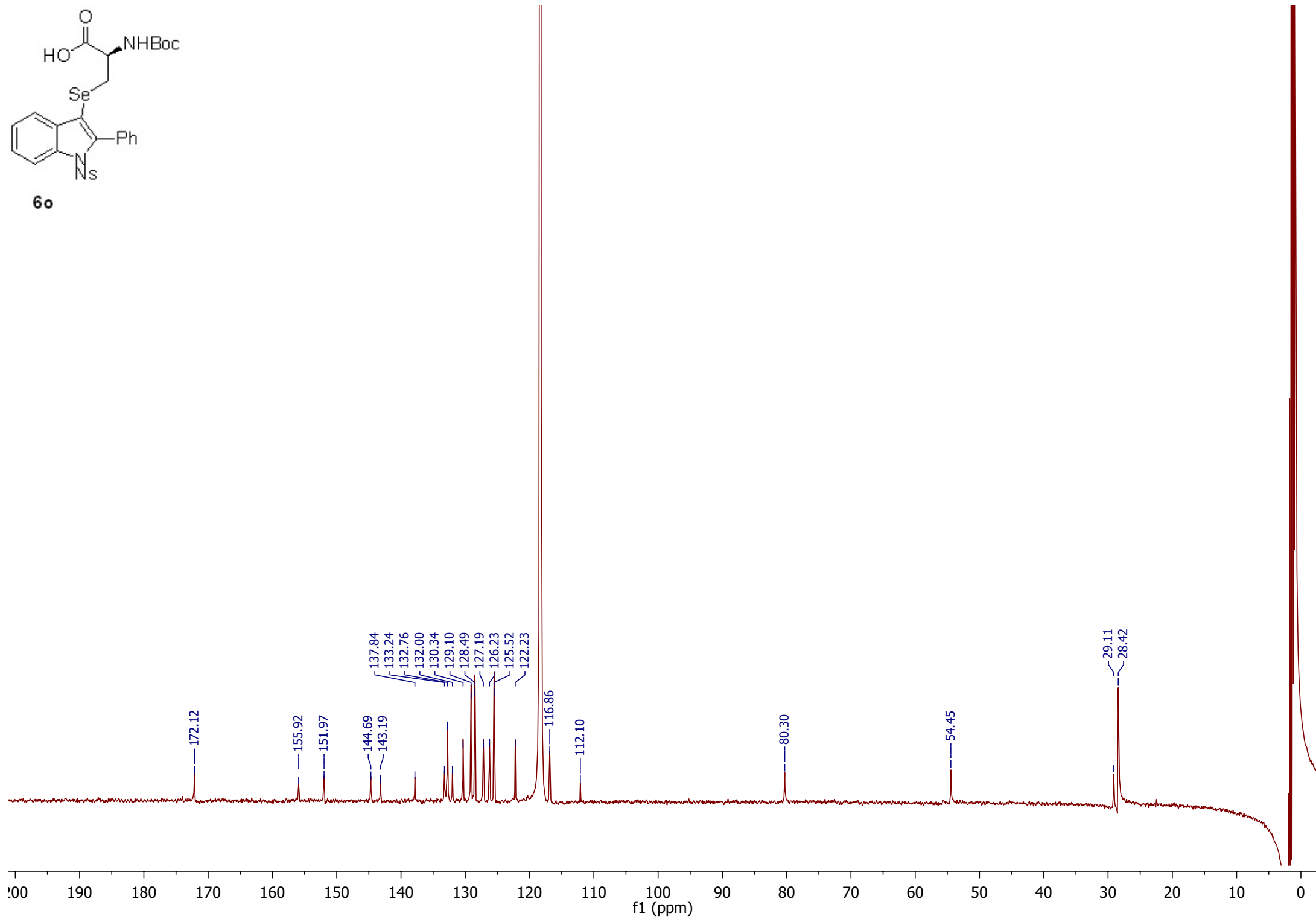


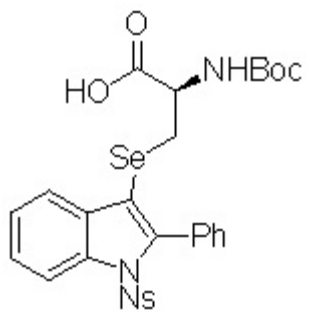
6o



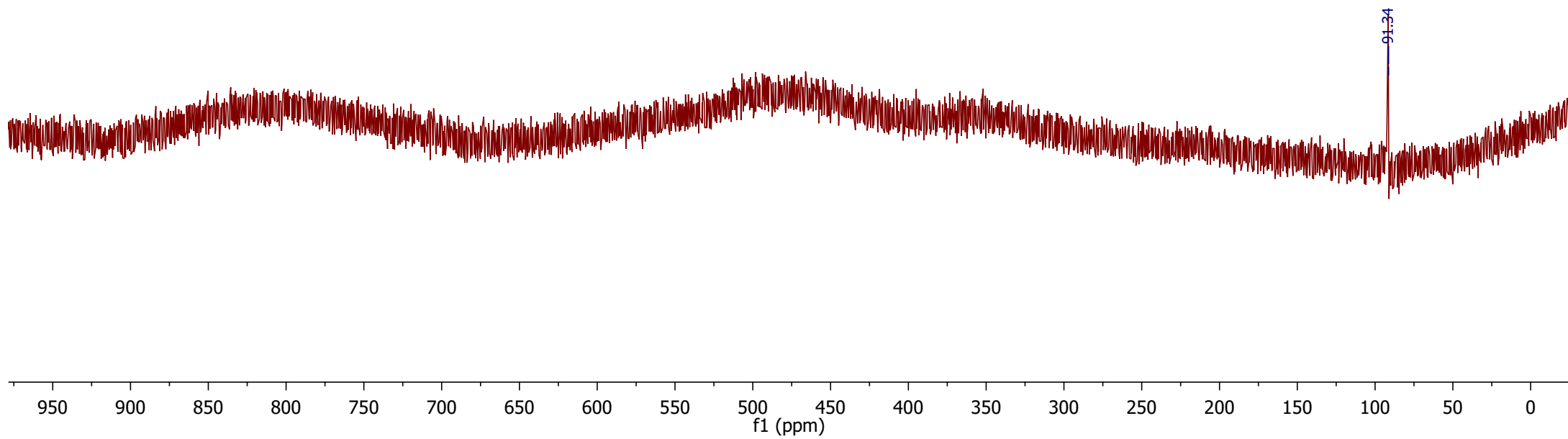


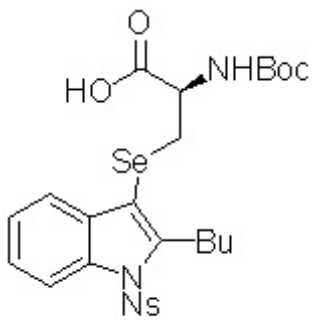
6o



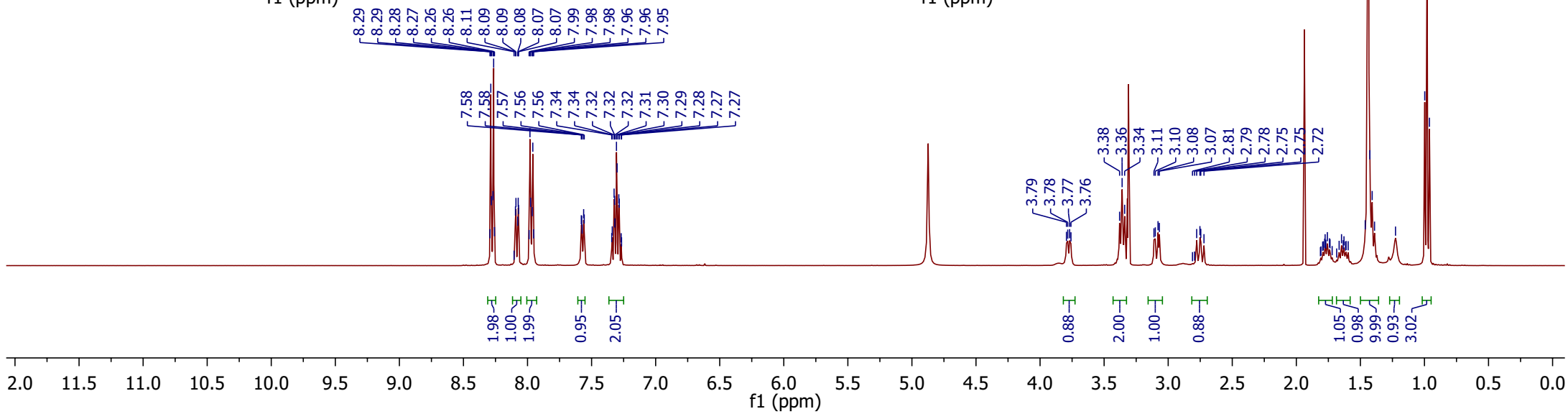
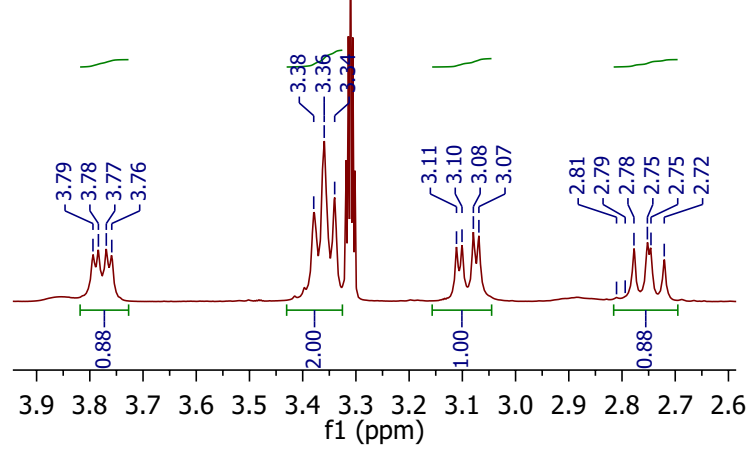
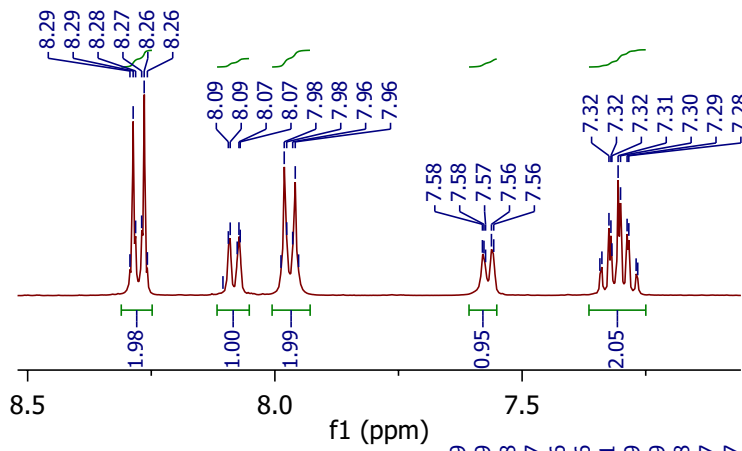


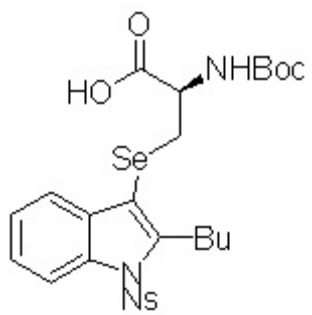
6o



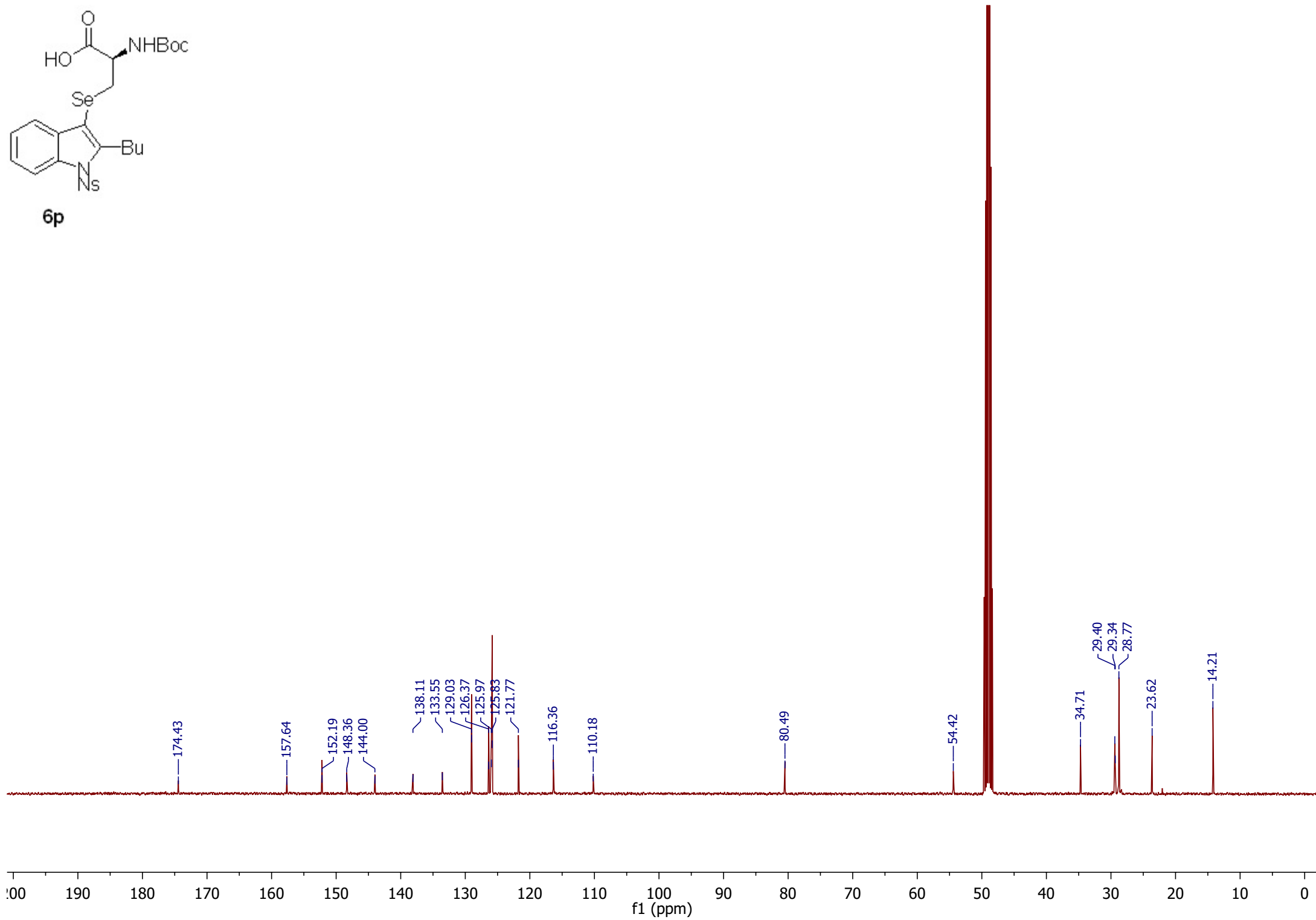


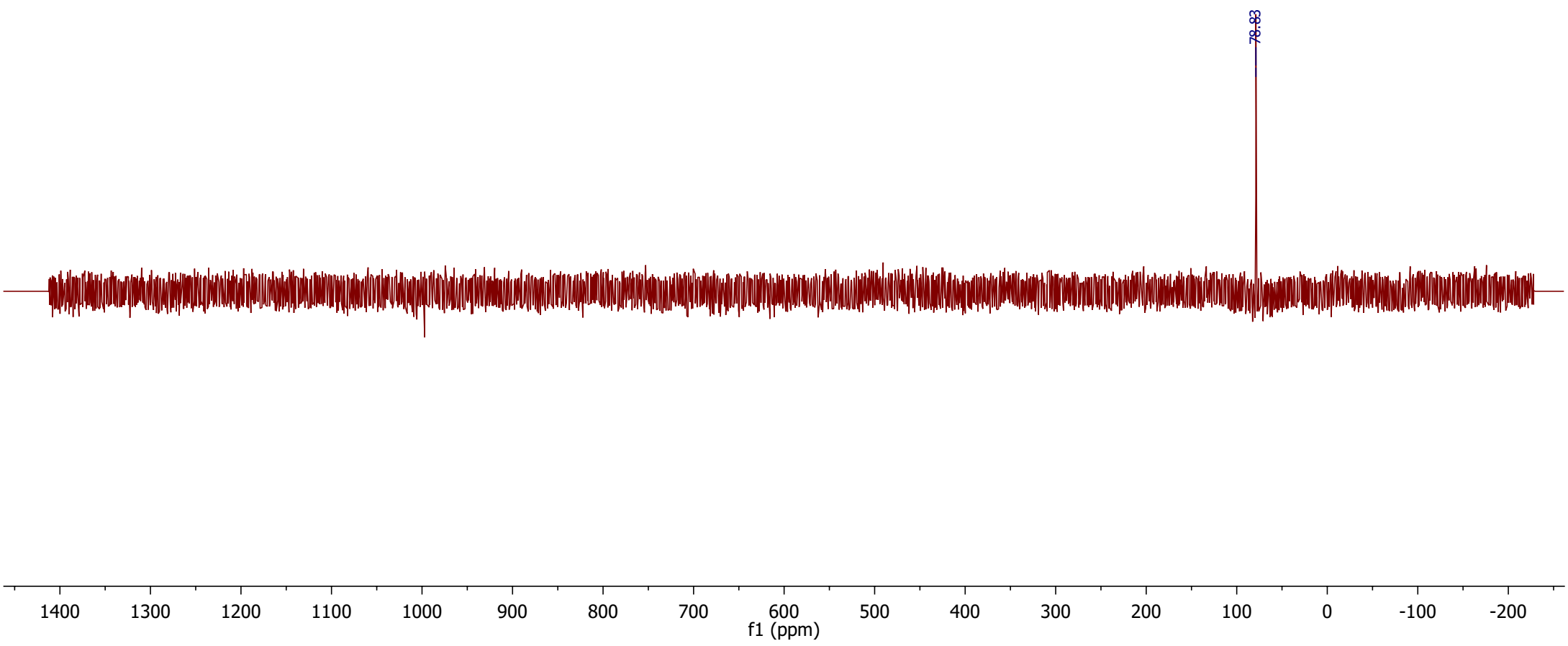
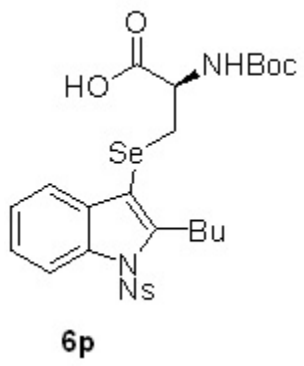
6p

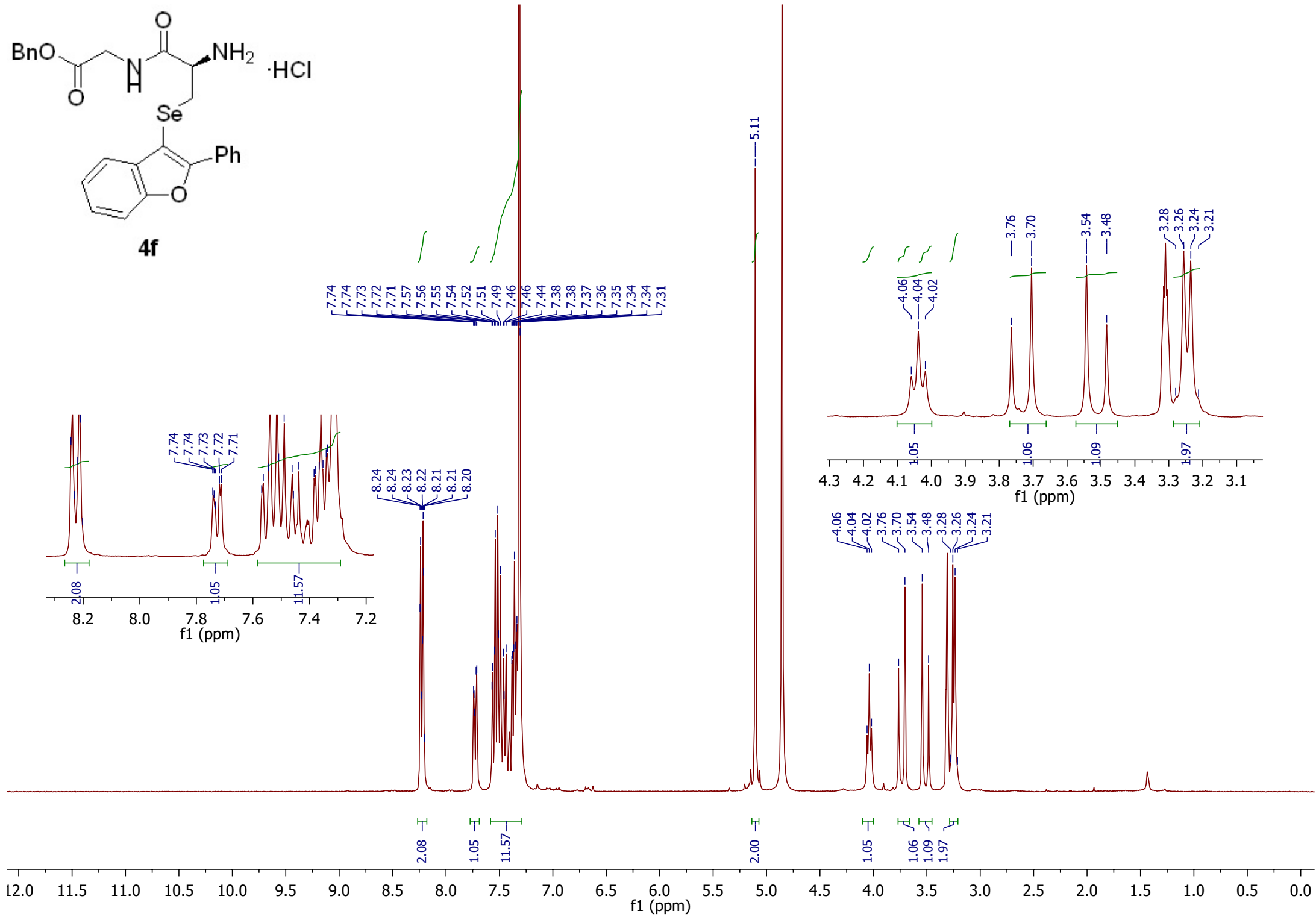
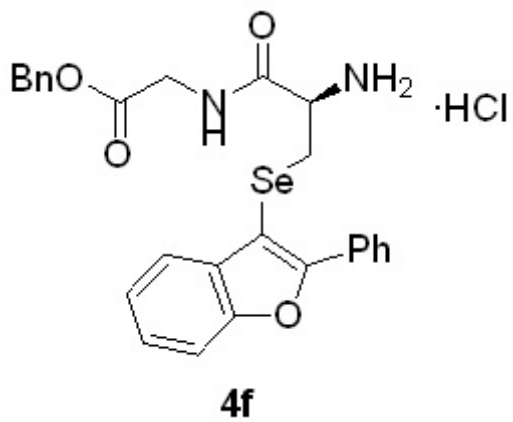


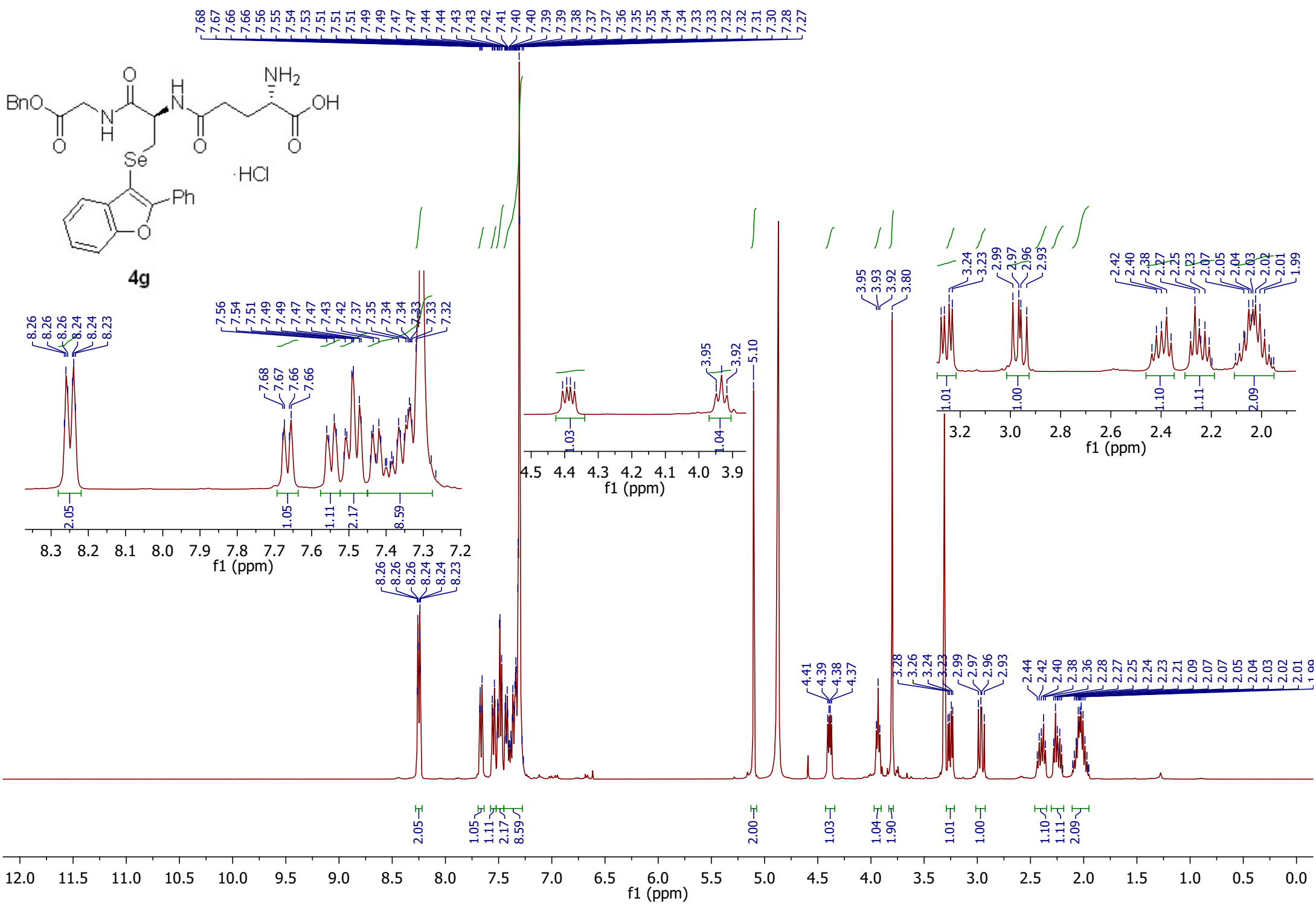


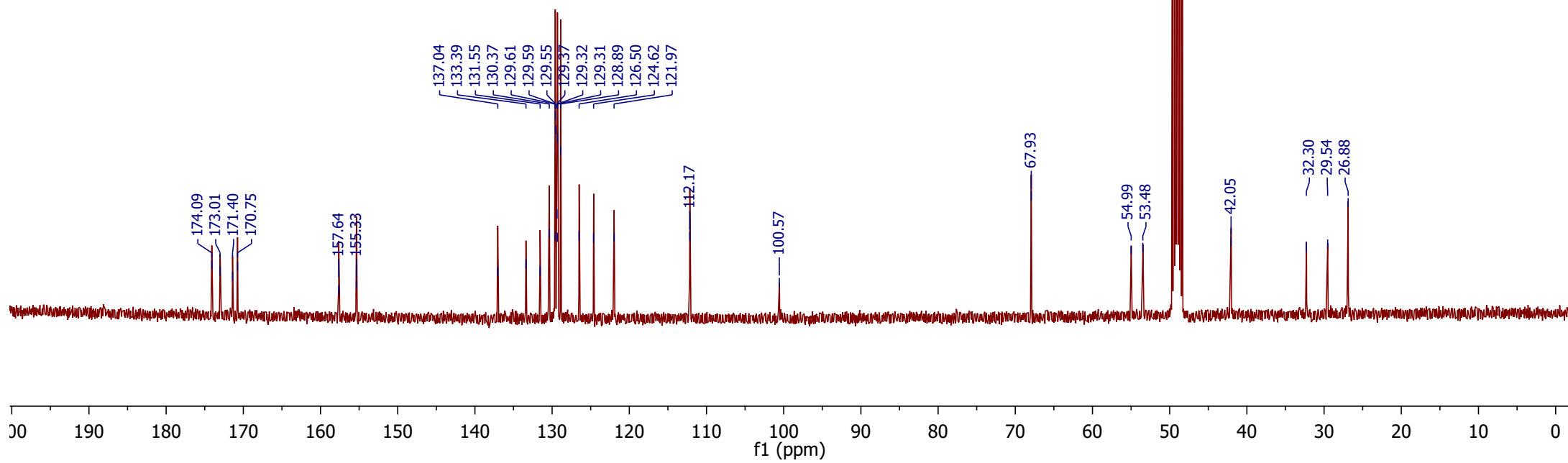
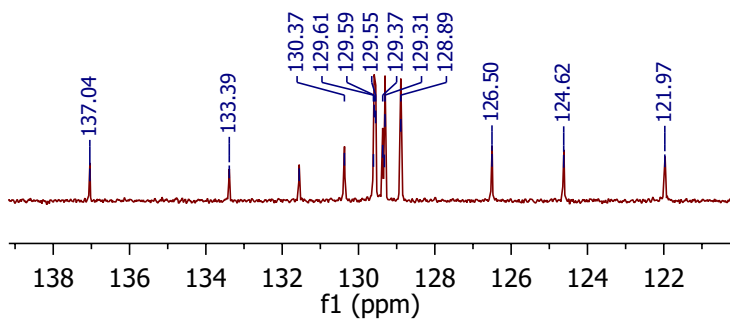
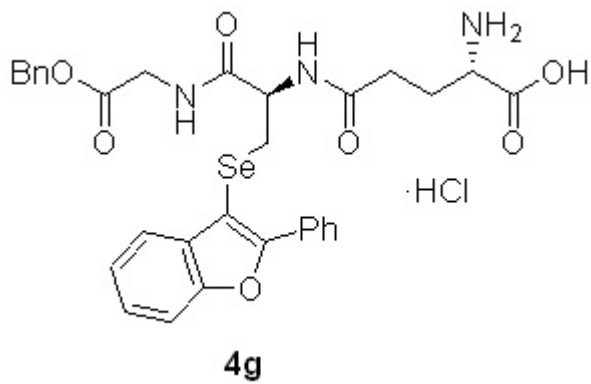
6p

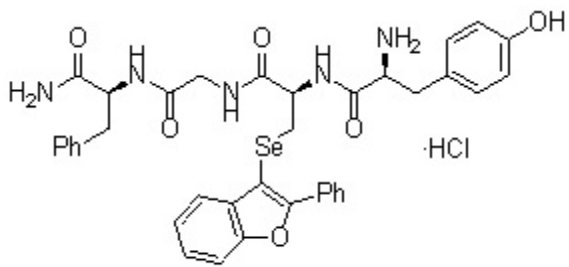




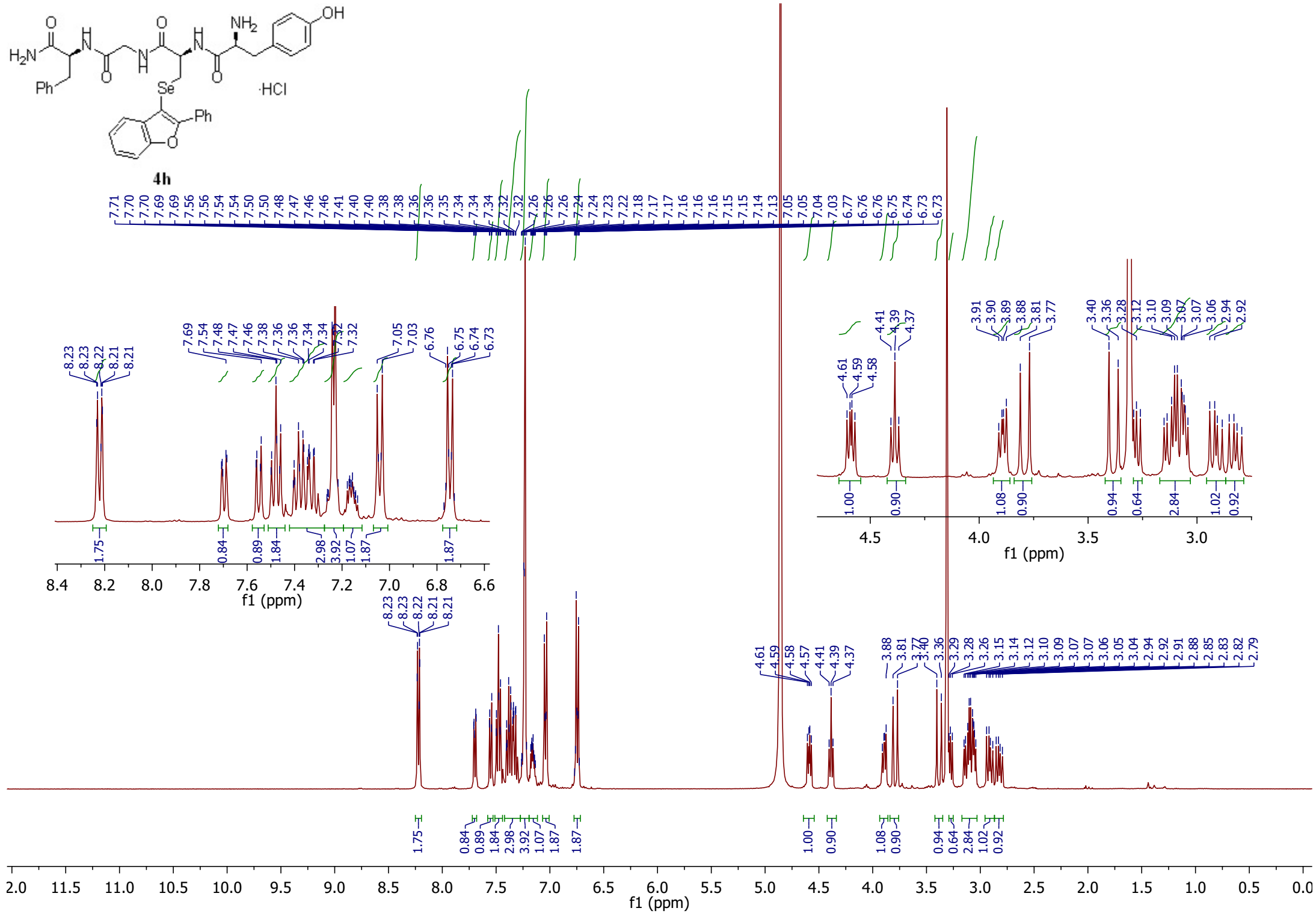


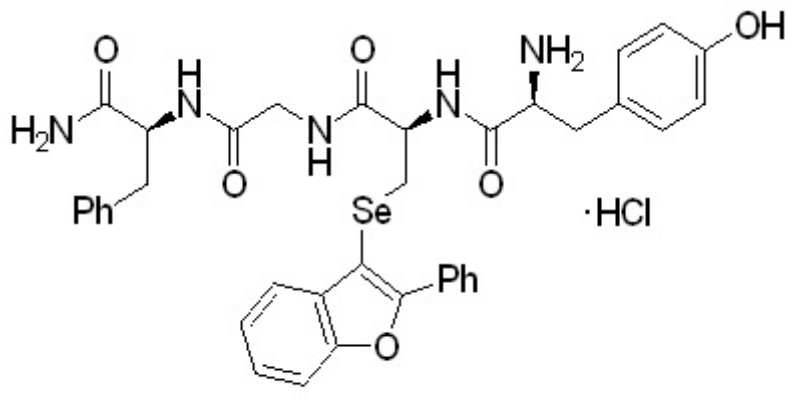




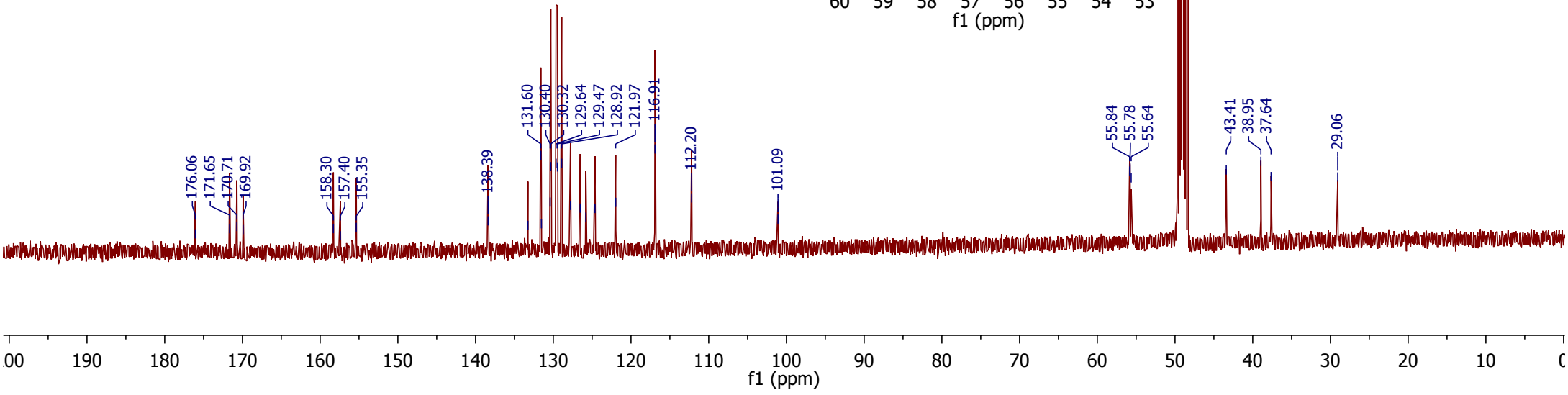
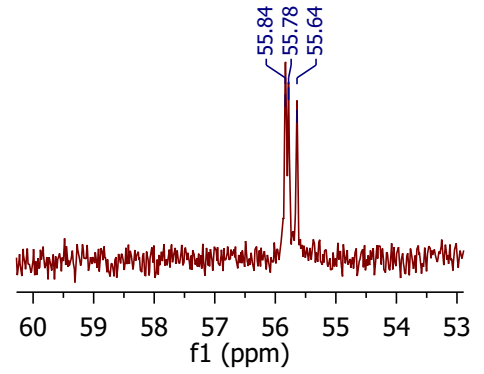
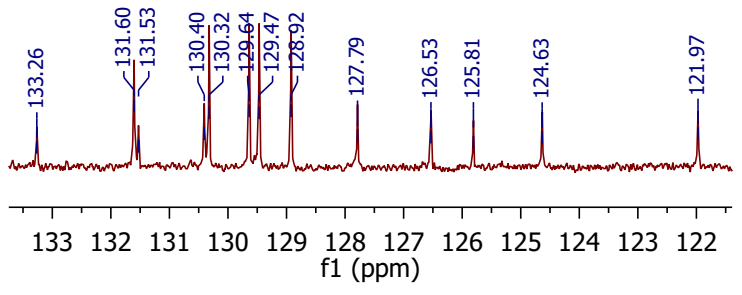


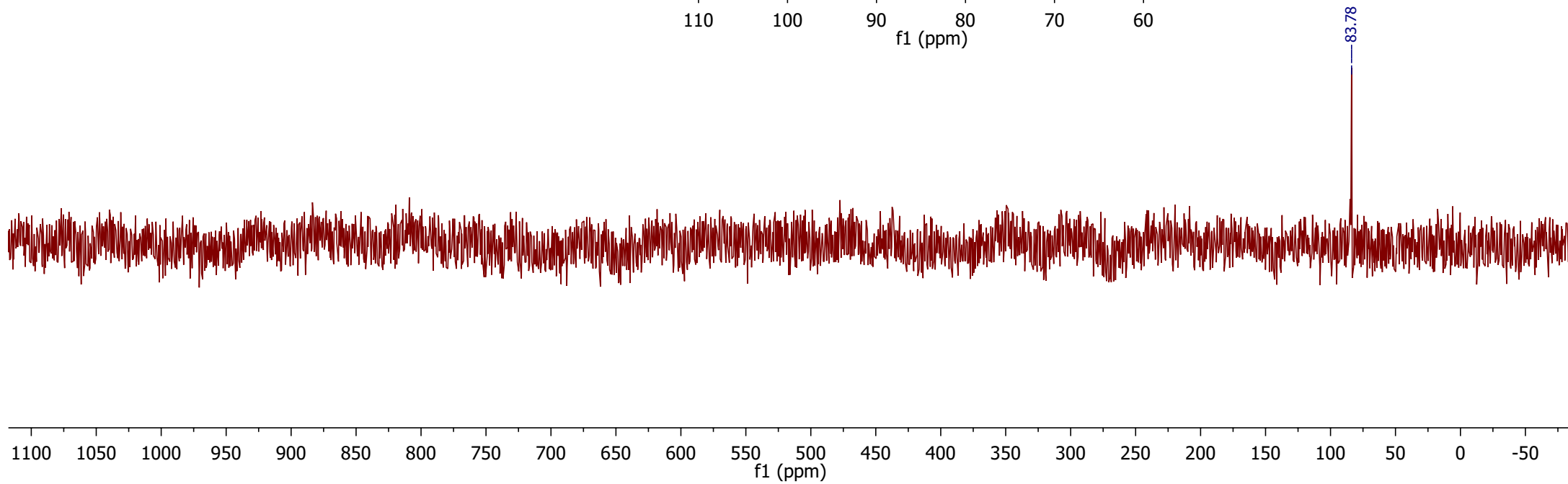
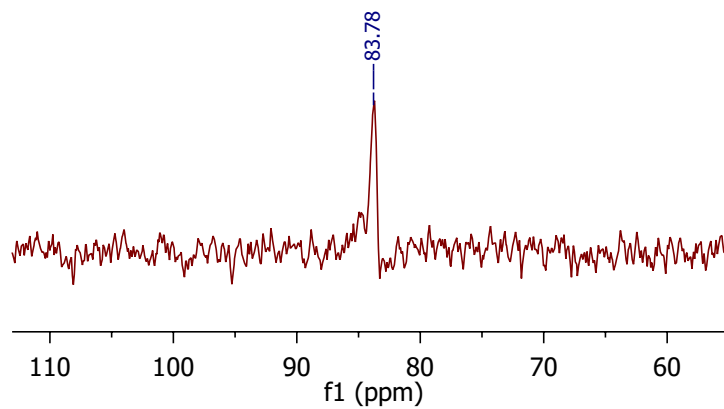
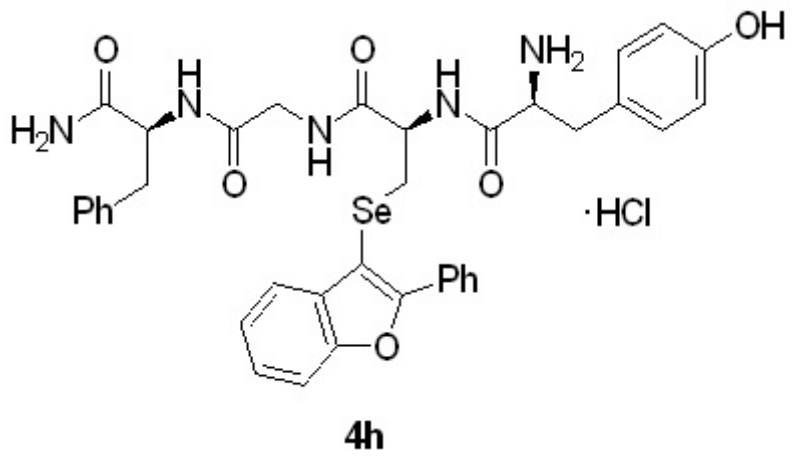
4h

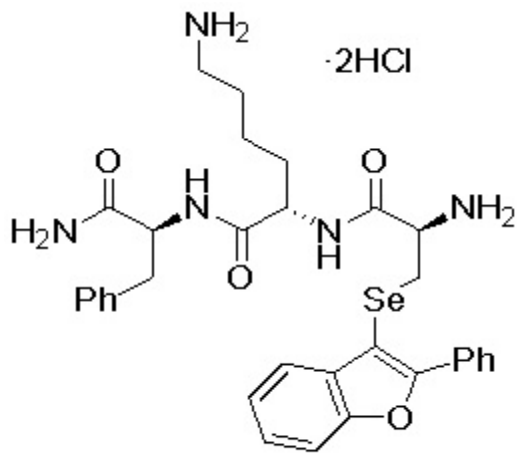




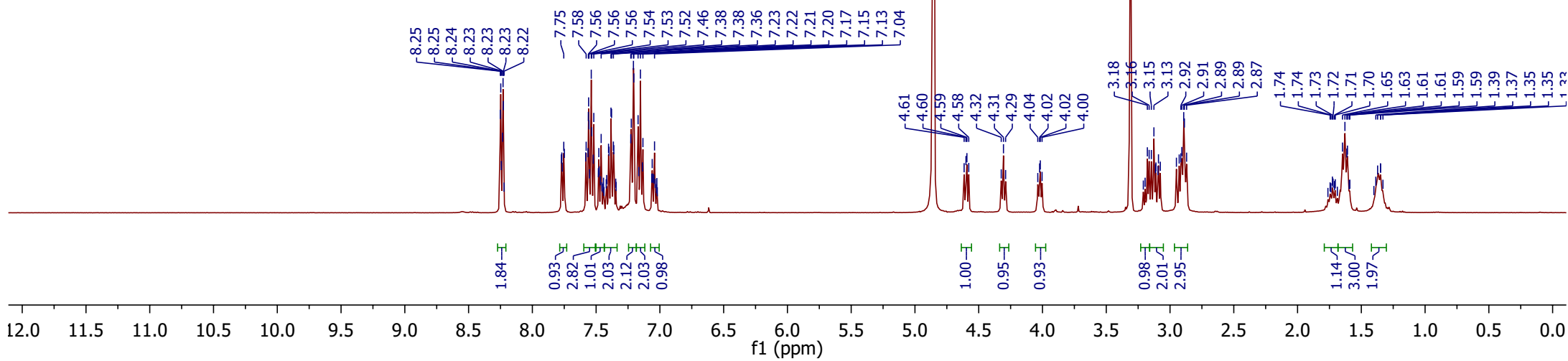
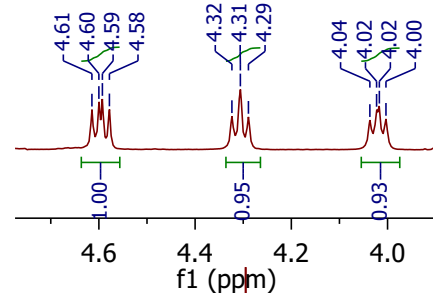
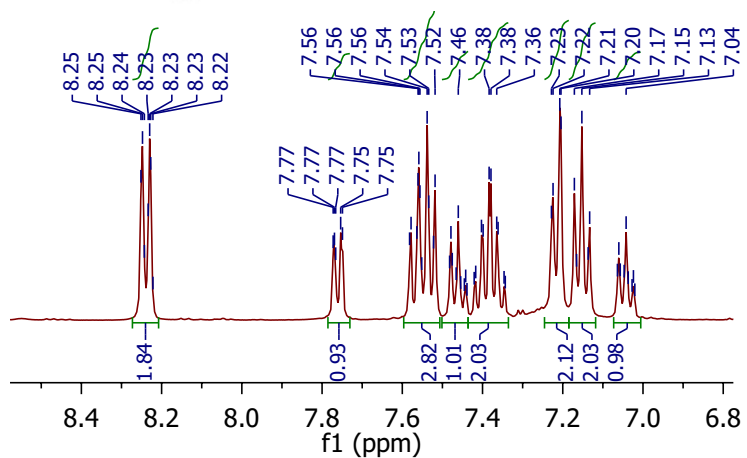
4h

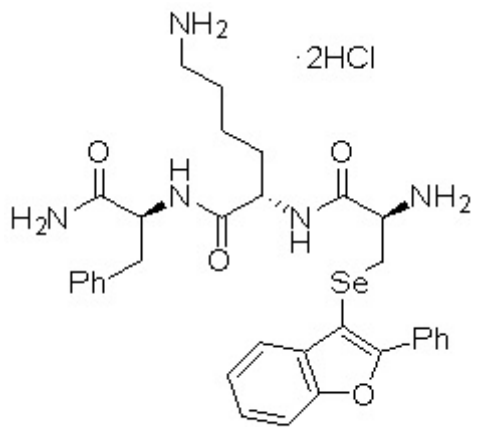




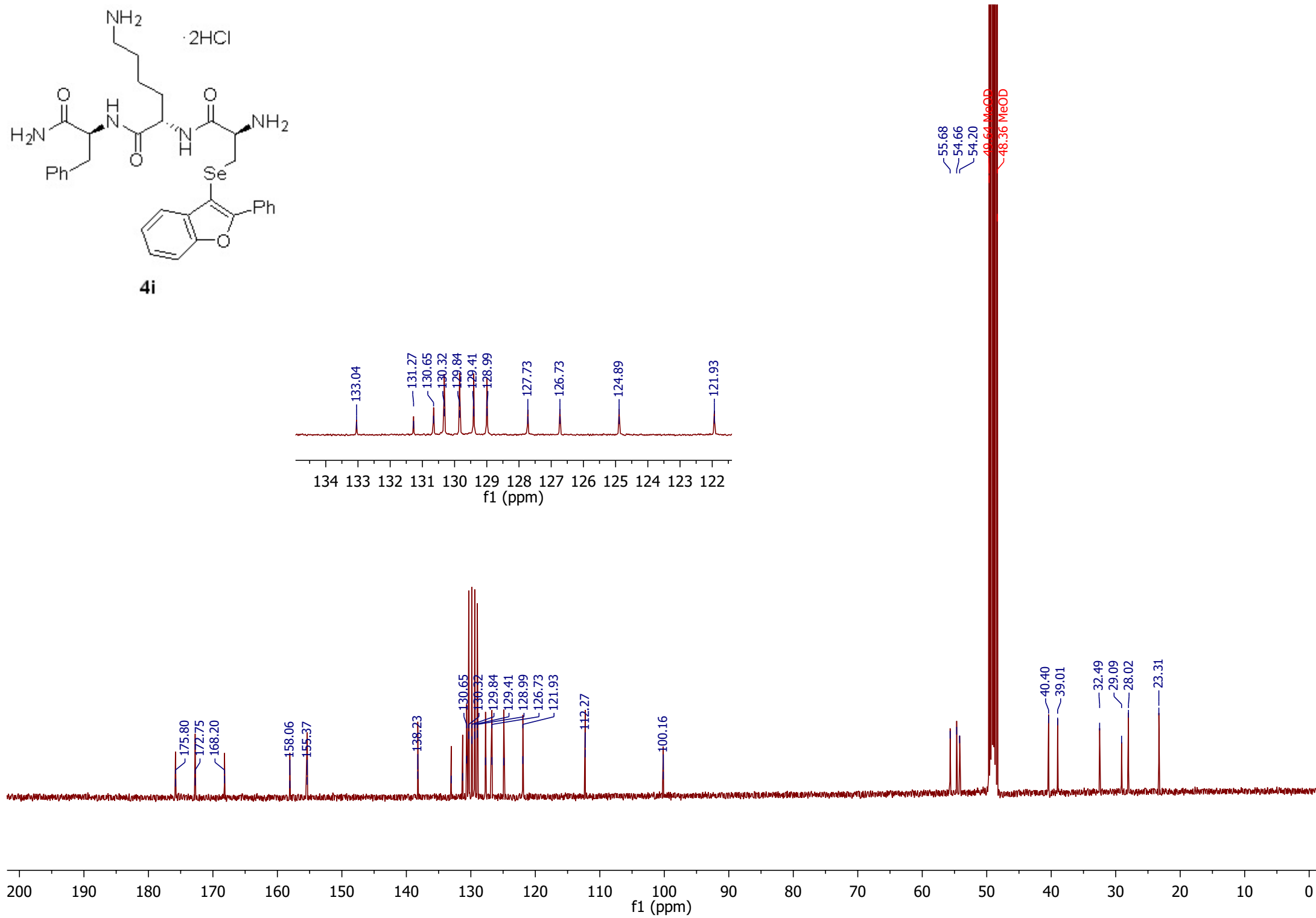


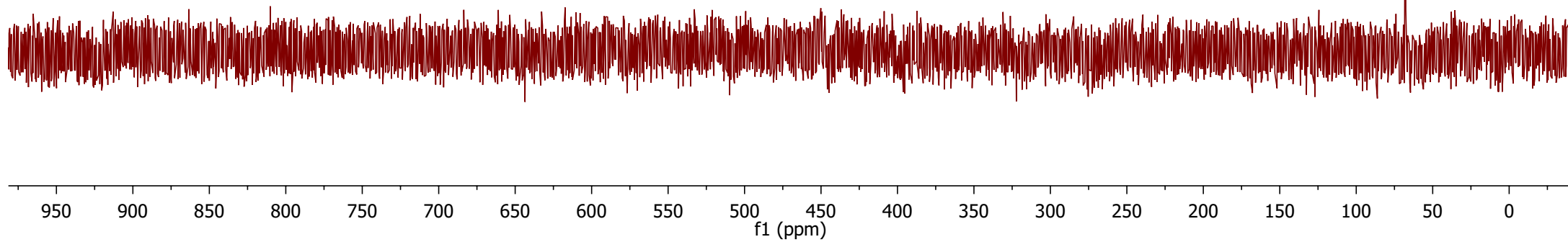
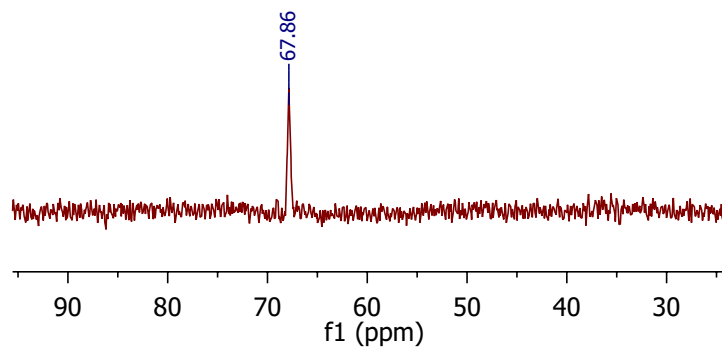
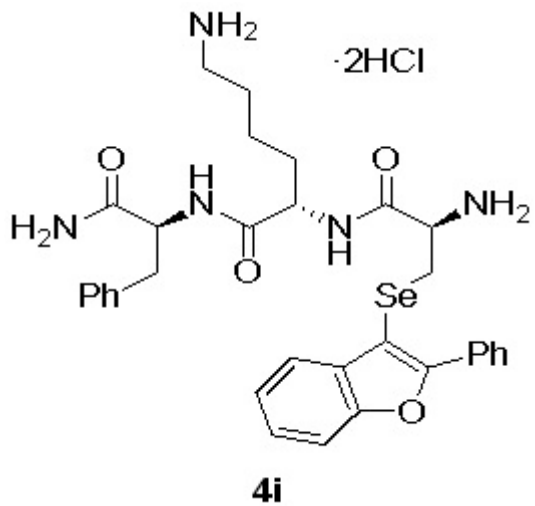
4i

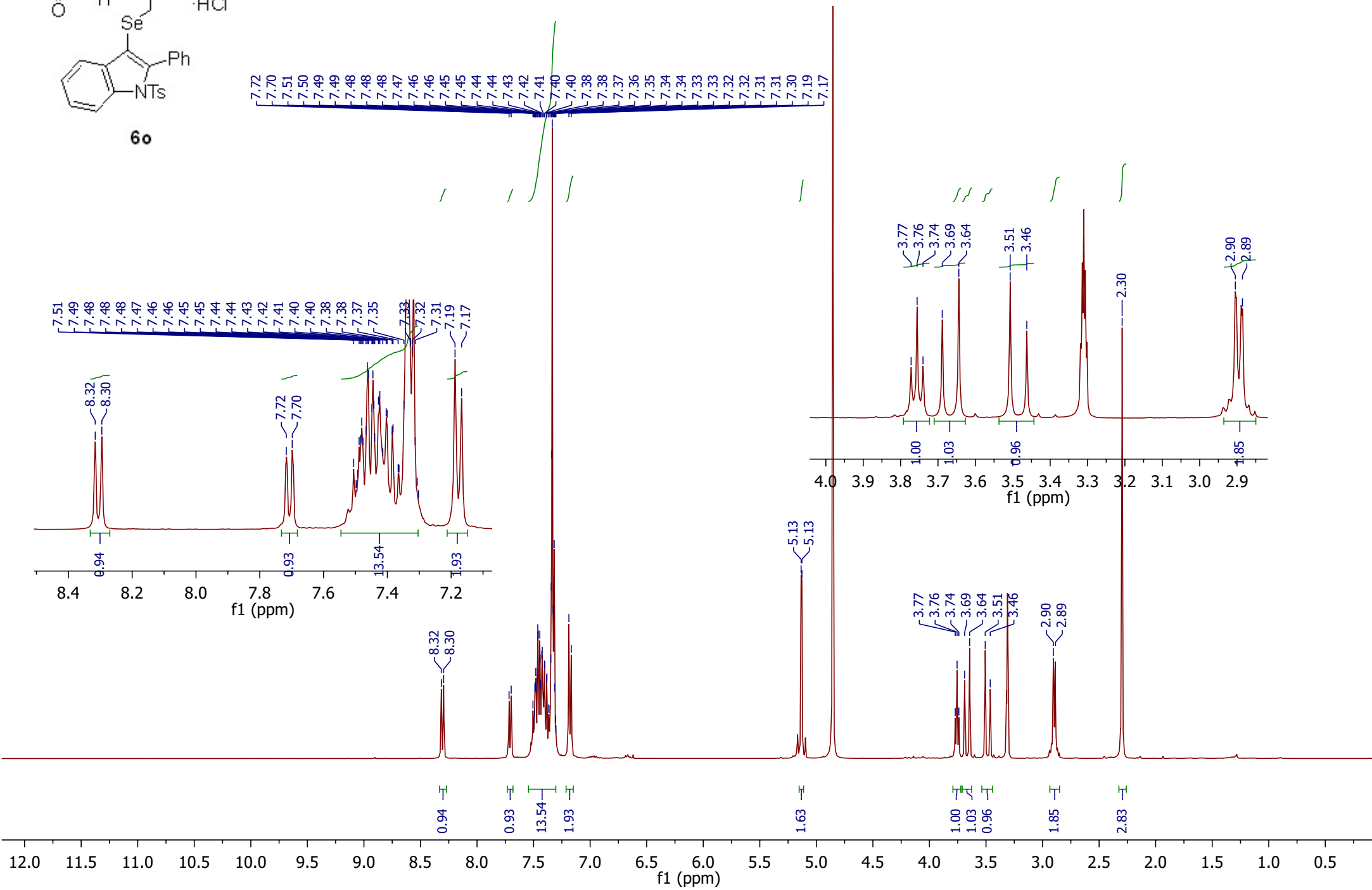
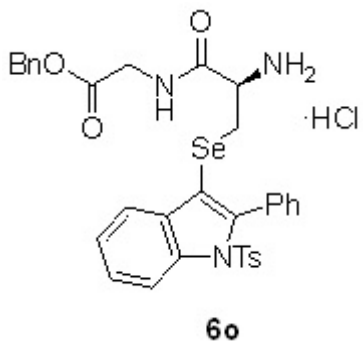


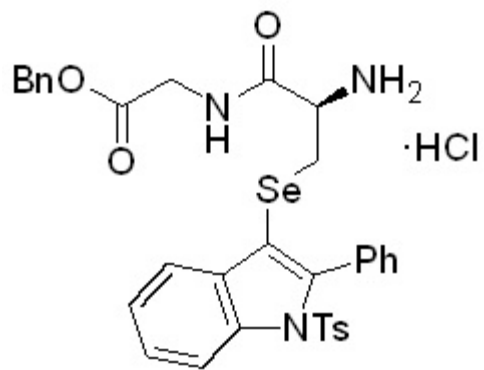


4i

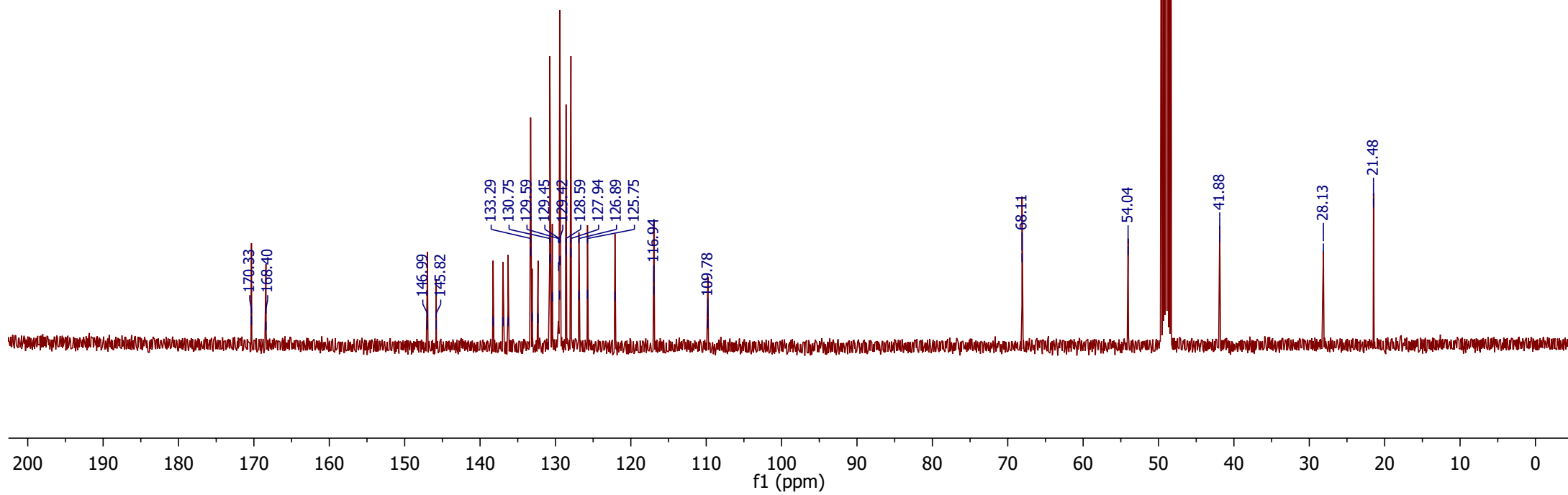
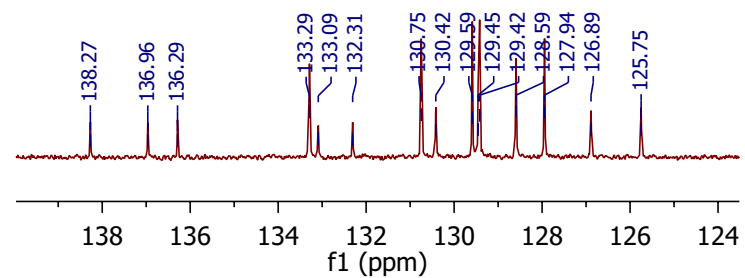


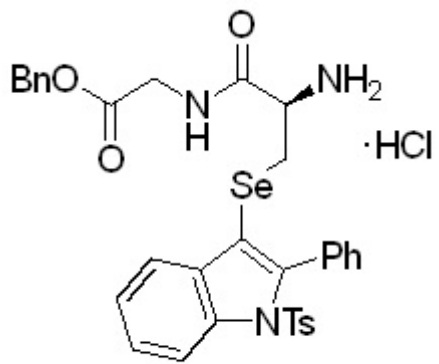




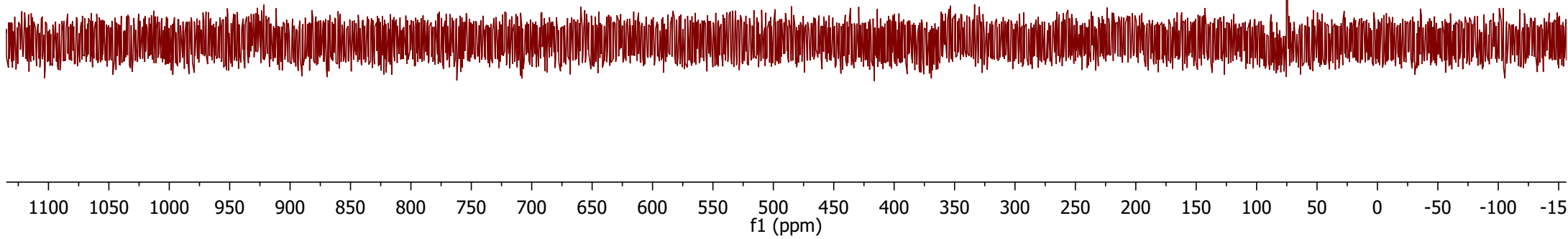
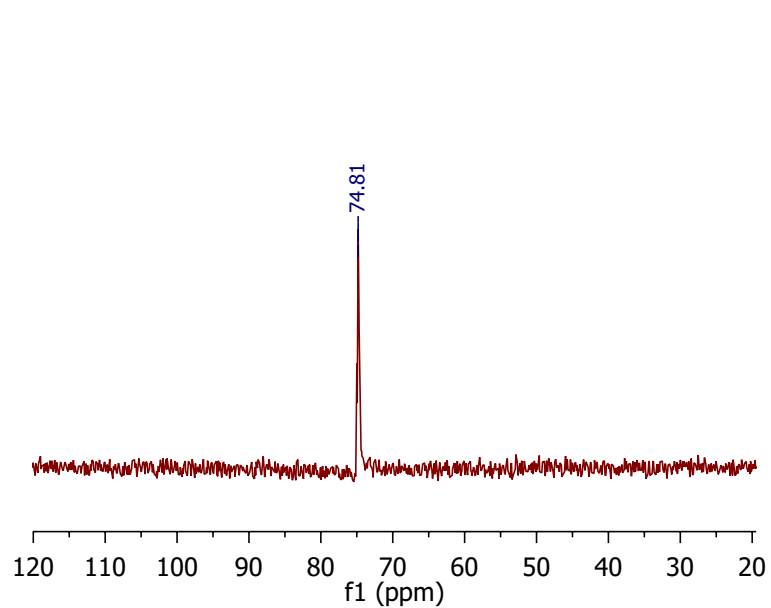


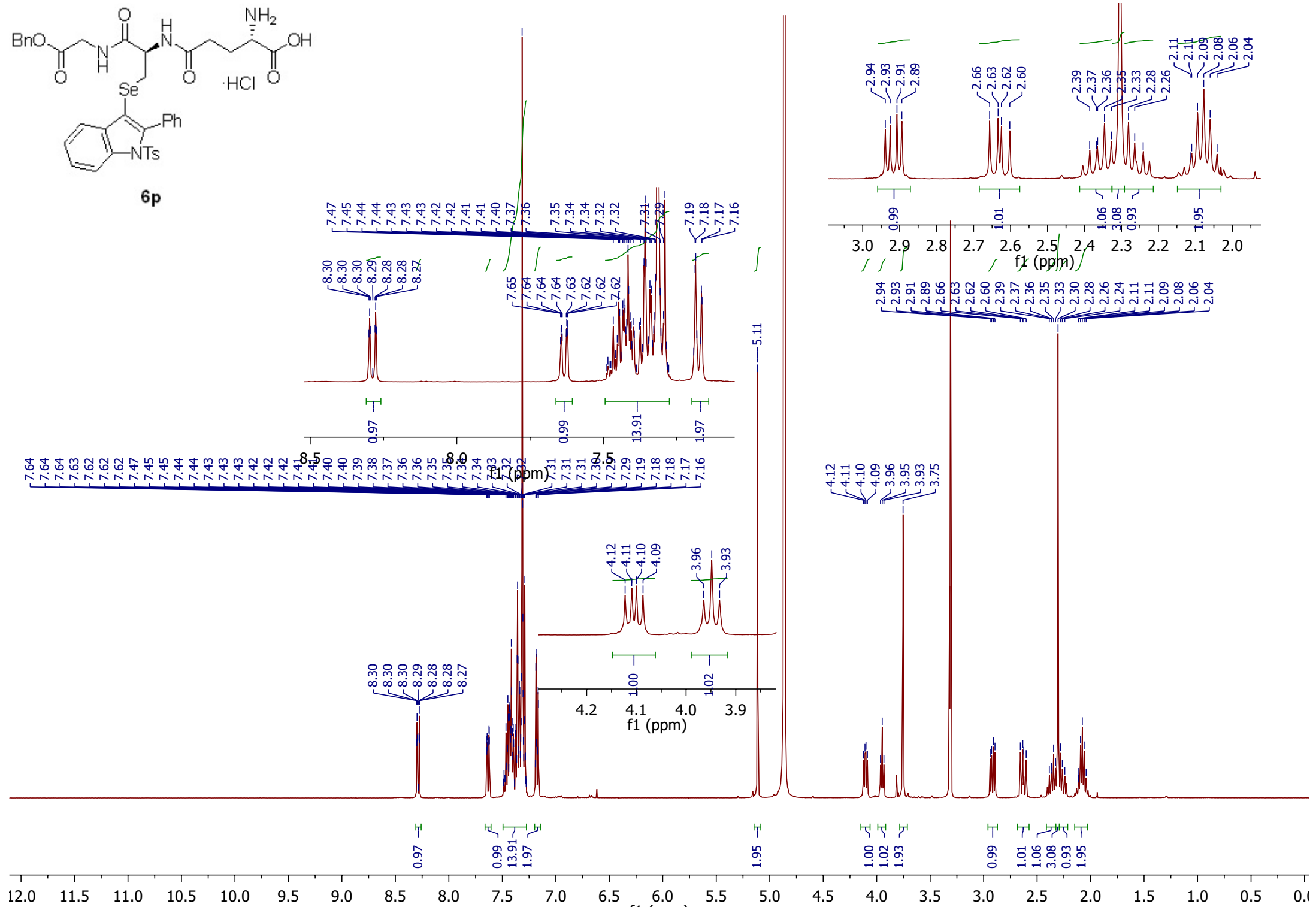
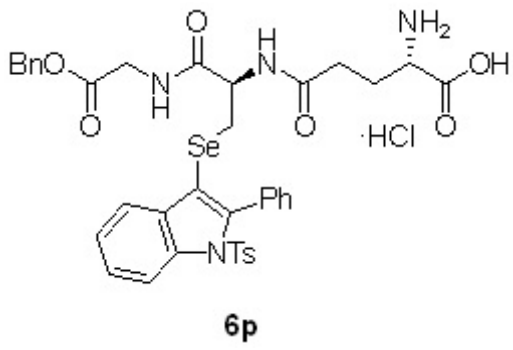
60

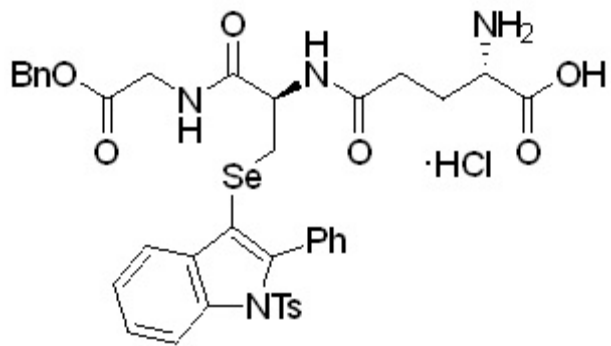




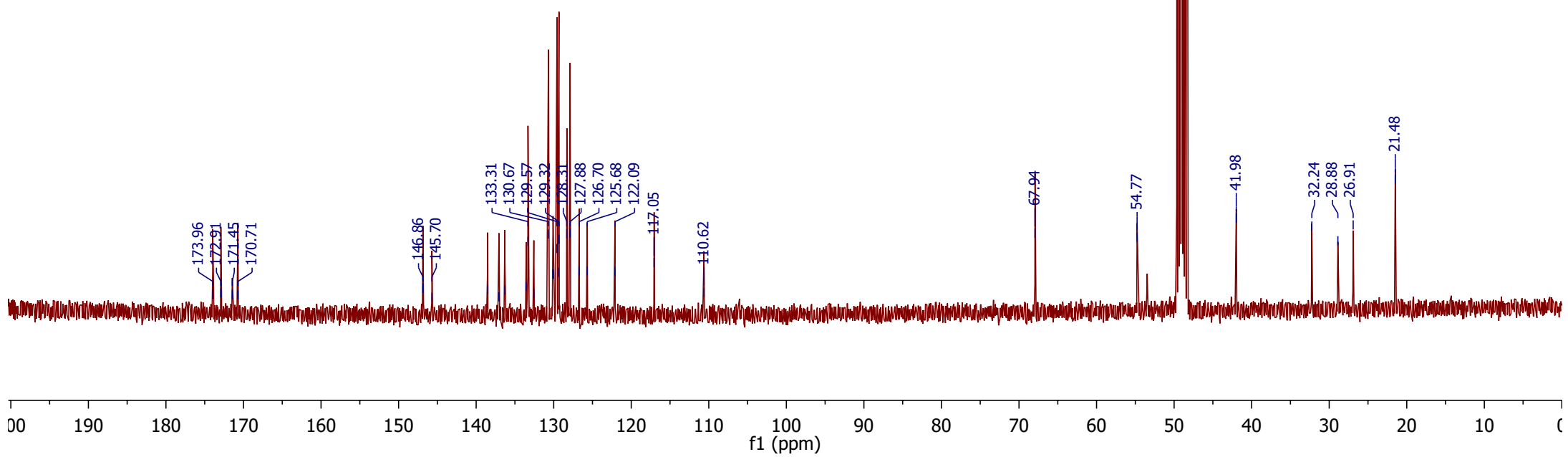
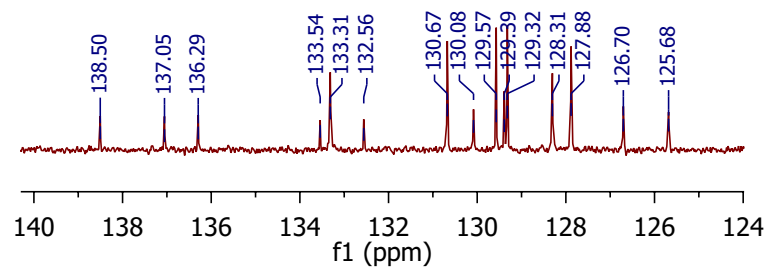
6o

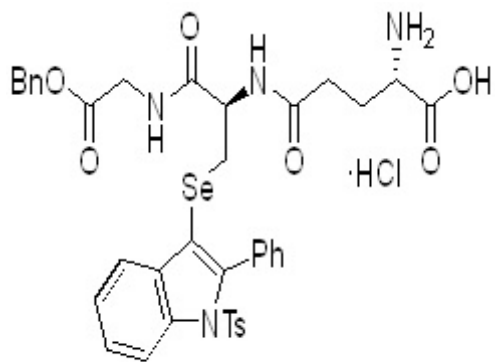




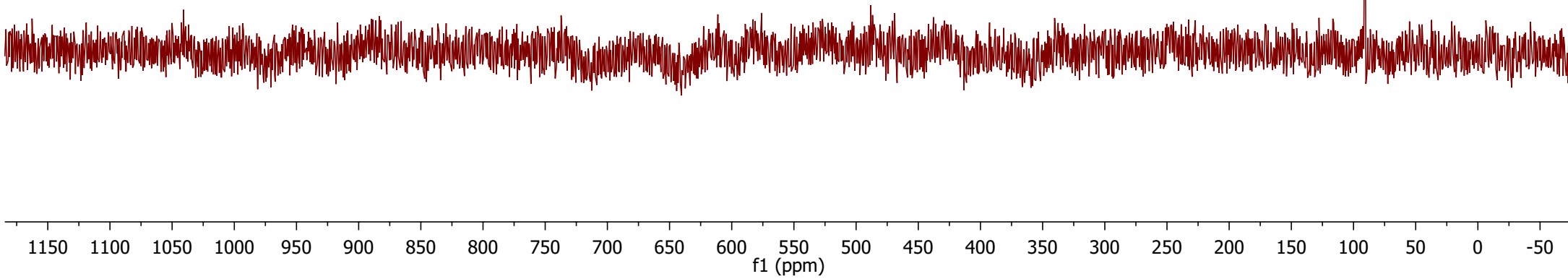
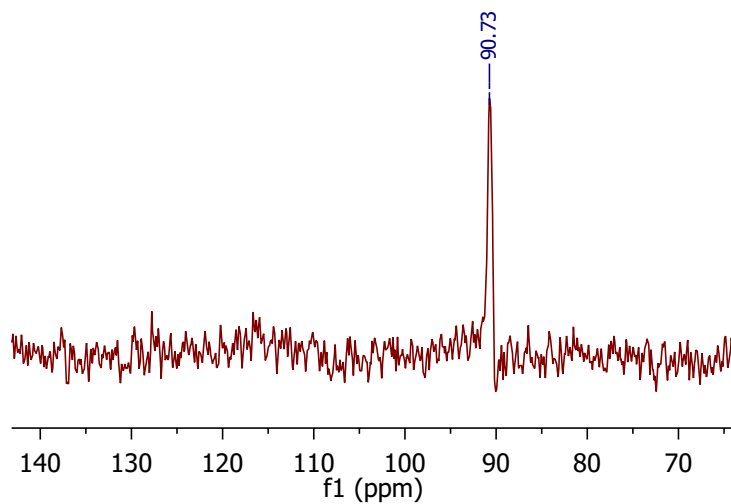


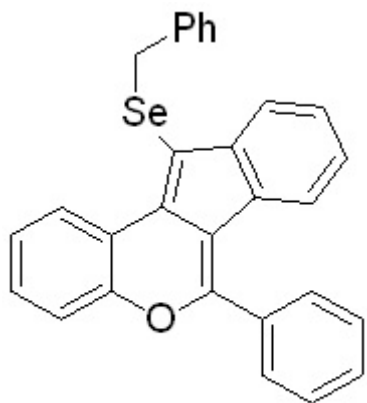
6p



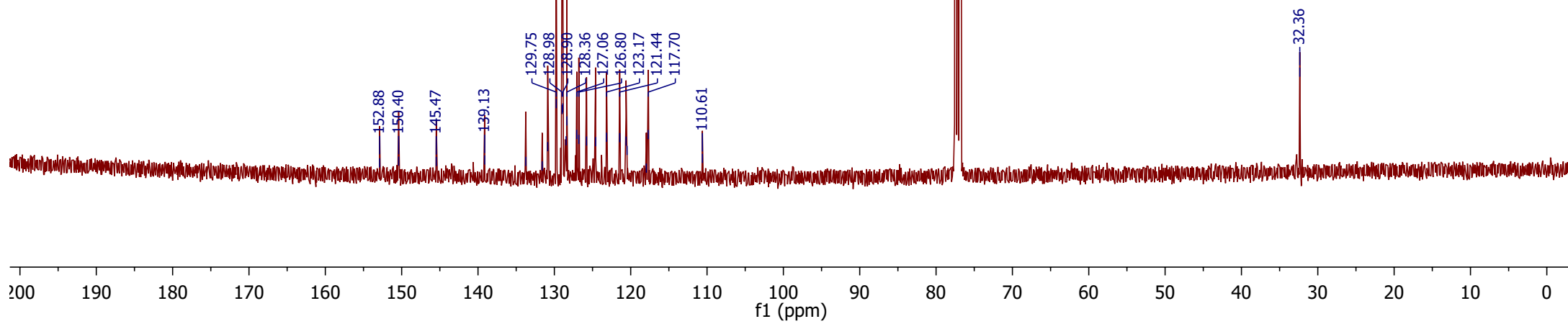
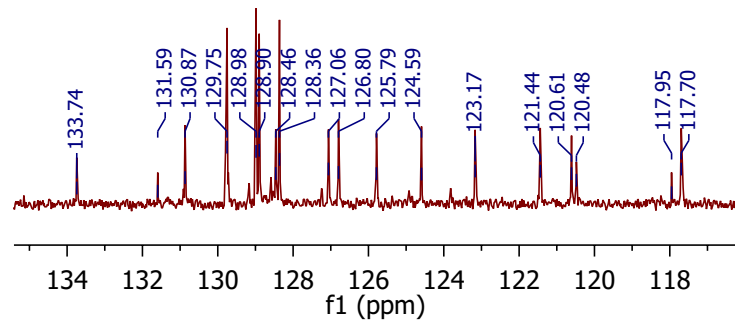


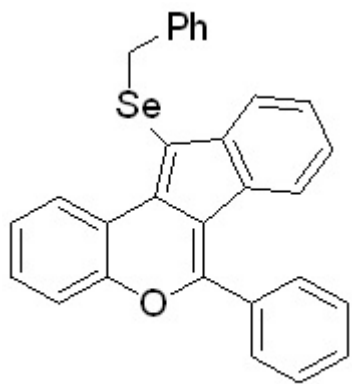
6p





8a





8a

