

Supplementary Material

**Using Quenching Kinetics and Thermodynamics of Amino-Fluorophores As
Empirical Tools for Predicting Boronic Acid Sensors Suitable for Use in
Physiological Conditions**

Nicholas McGregor,¹ Christophe Pardin,^{1,2} W.G. Skene^{*1}

¹Laboratoire de caractérisation photophysique des matériaux conjugués

Department of Chemistry, Pavillon JA Bombardier,

Université de Montréal, CP 6128, succ. Centre-ville,

Montreal, Quebec, Canada H3C 3J6

² Department of Chemistry, D'Iorio Hall,

University of Ottawa, 10 Marie Curie,

Ottawa, Ontario, Canada K1N 6N5

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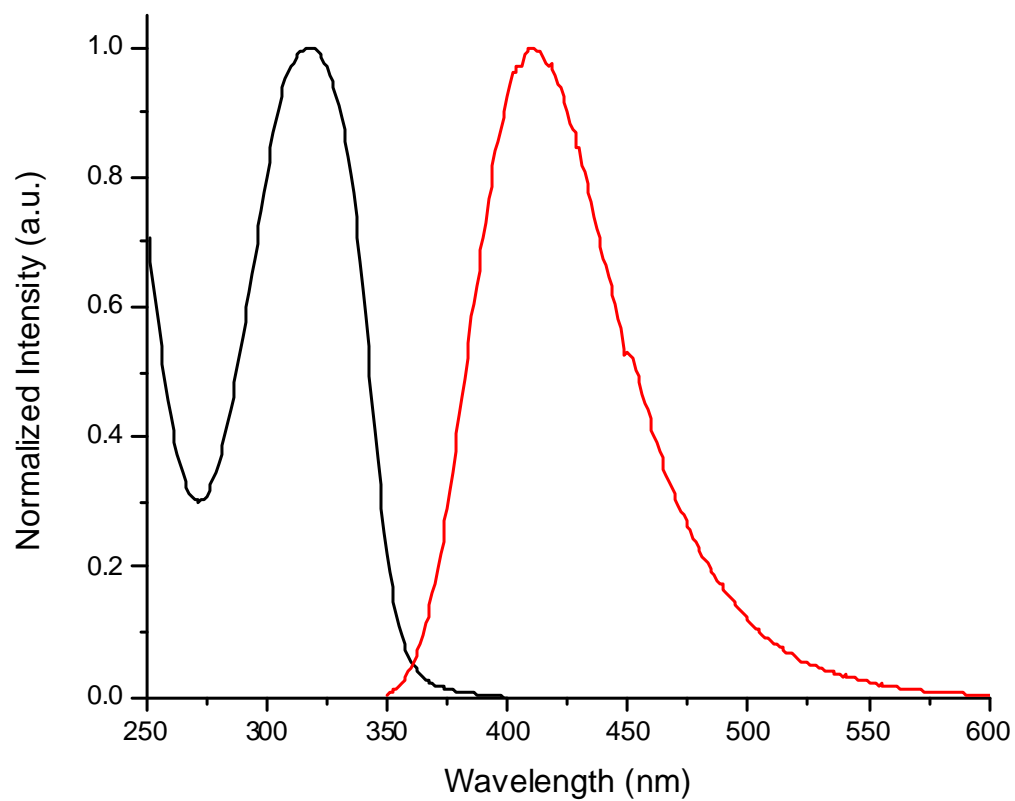


Figure 1: Normalized absorbance (black) and fluorescence (red) spectra of **1**.

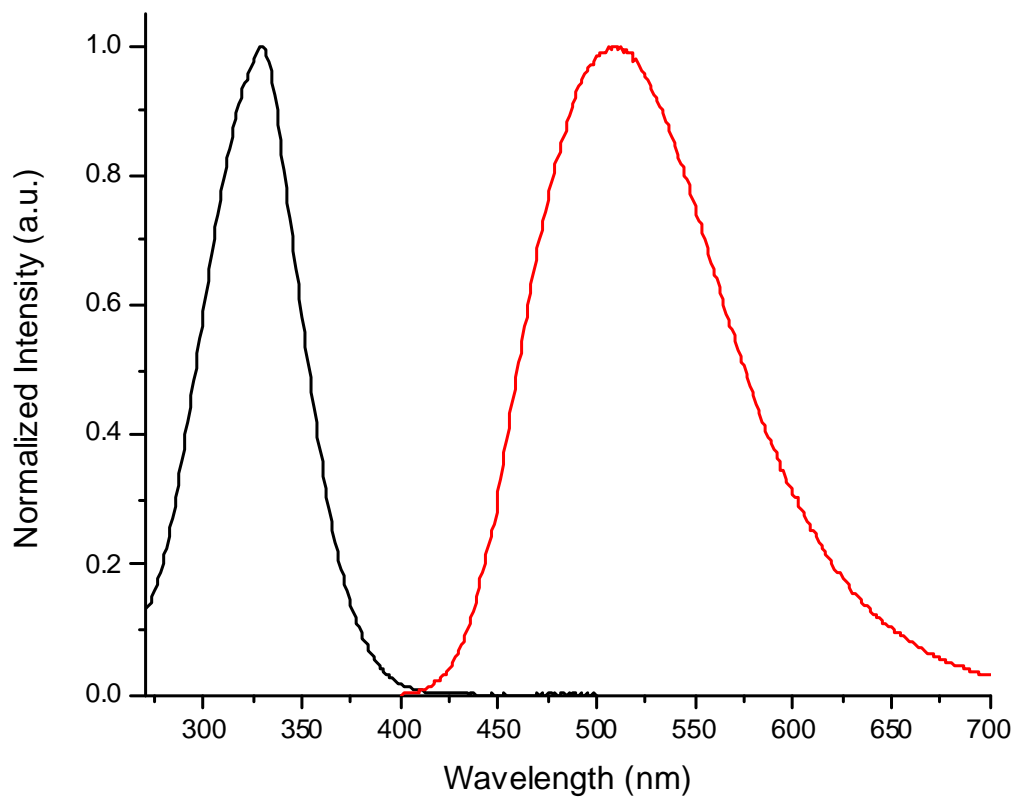


Figure 2: Normalized absorbance (black) and fluorescence (red) spectra of **2**.

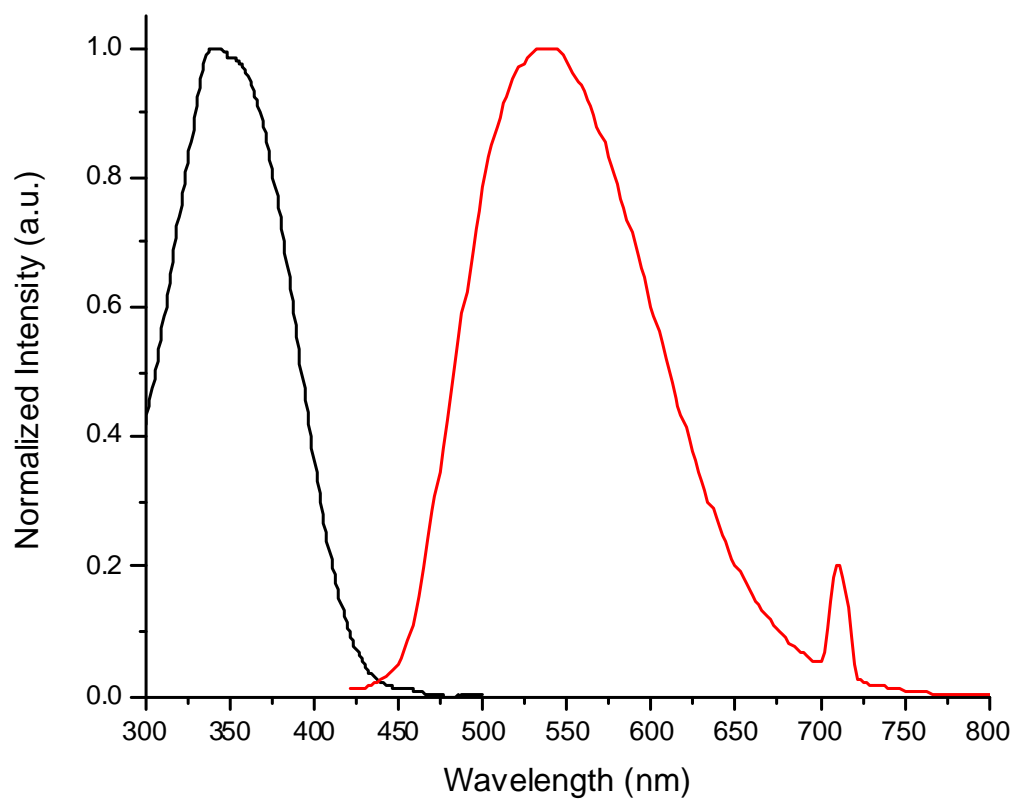


Figure 3: Normalized absorbance (black) and fluorescence (red) spectra of **3**.

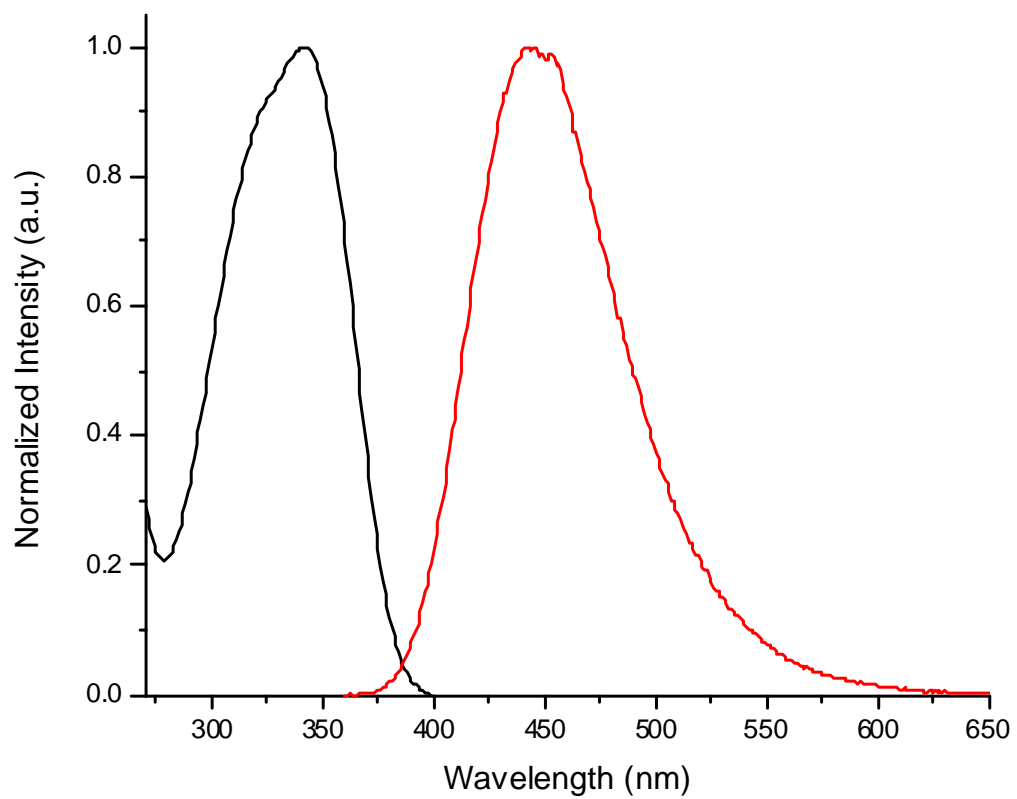


Figure 4: Normalized absorbance (black) and fluorescence (red) spectra of **4**.

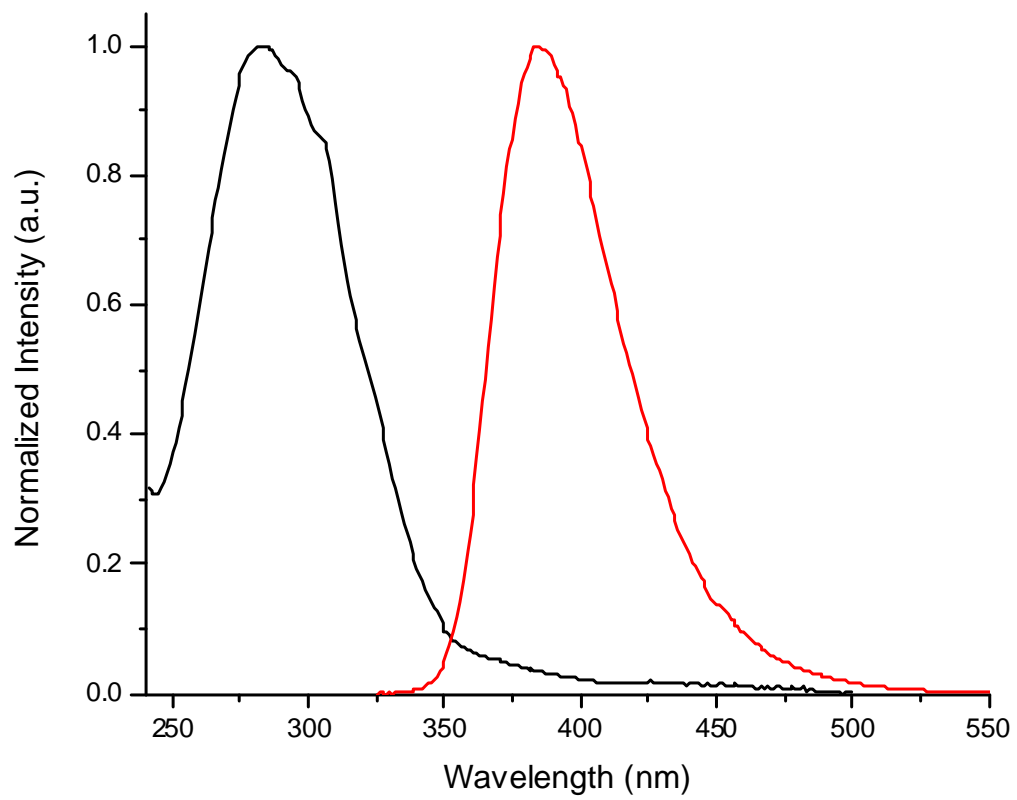


Figure 5: Normalized absorbance (black) and fluorescence (red) spectra of **5**.

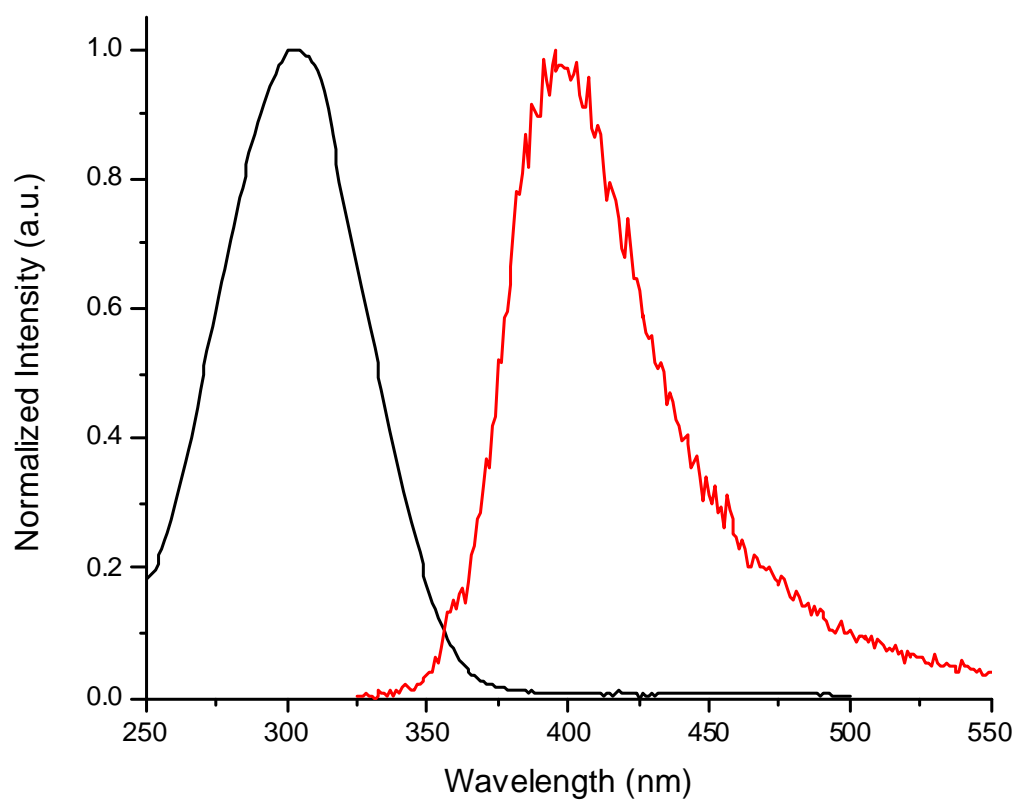


Figure 6: Normalized absorbance (black) and fluorescence (red) spectra of **6**.

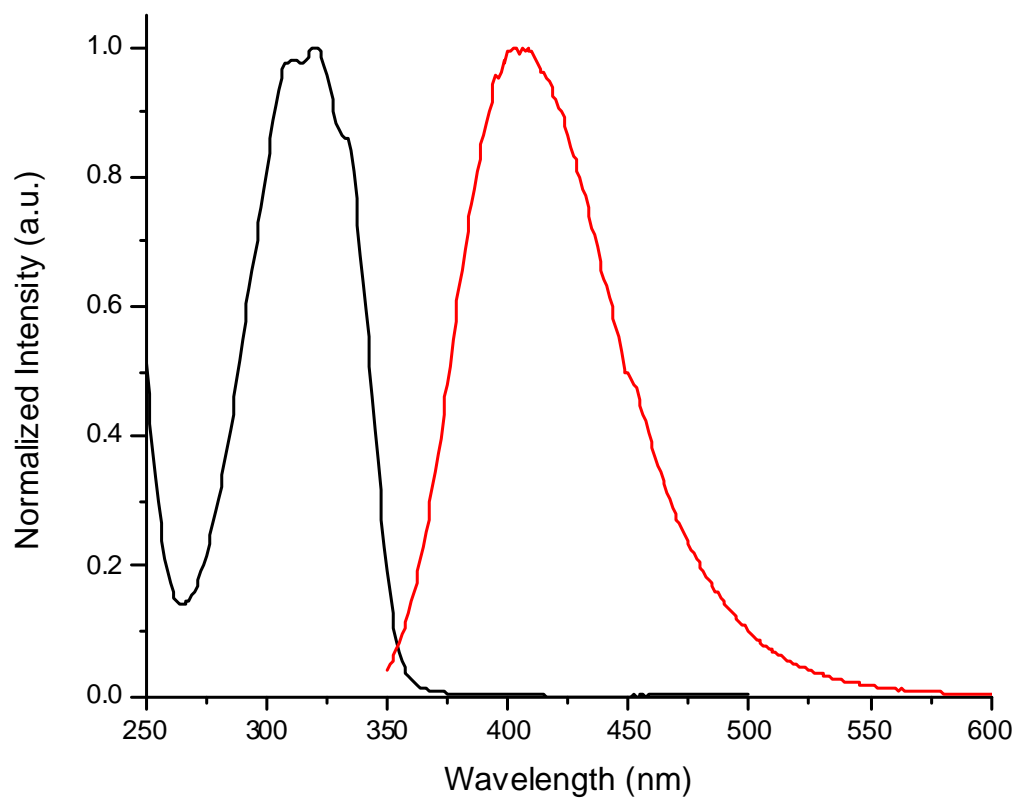


Figure 7: Normalized absorbance (black) and fluorescence (red) spectra of **11**.

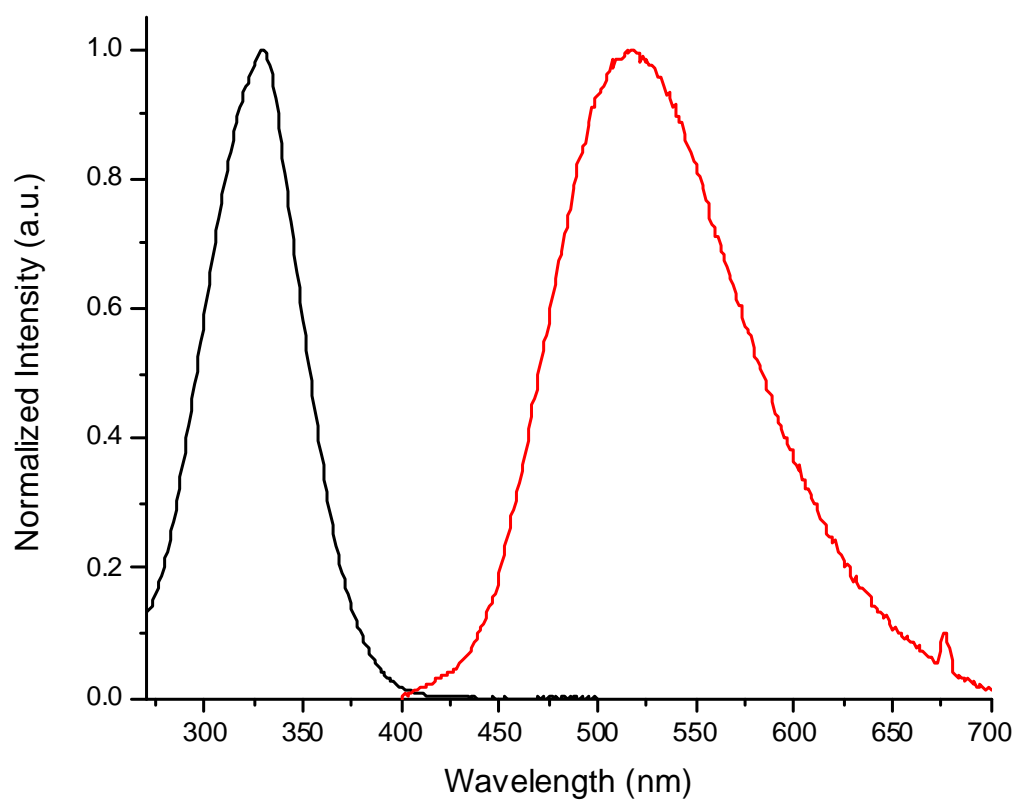


Figure 8: Normalized absorbance (black) and fluorescence (red) spectra of **12**.

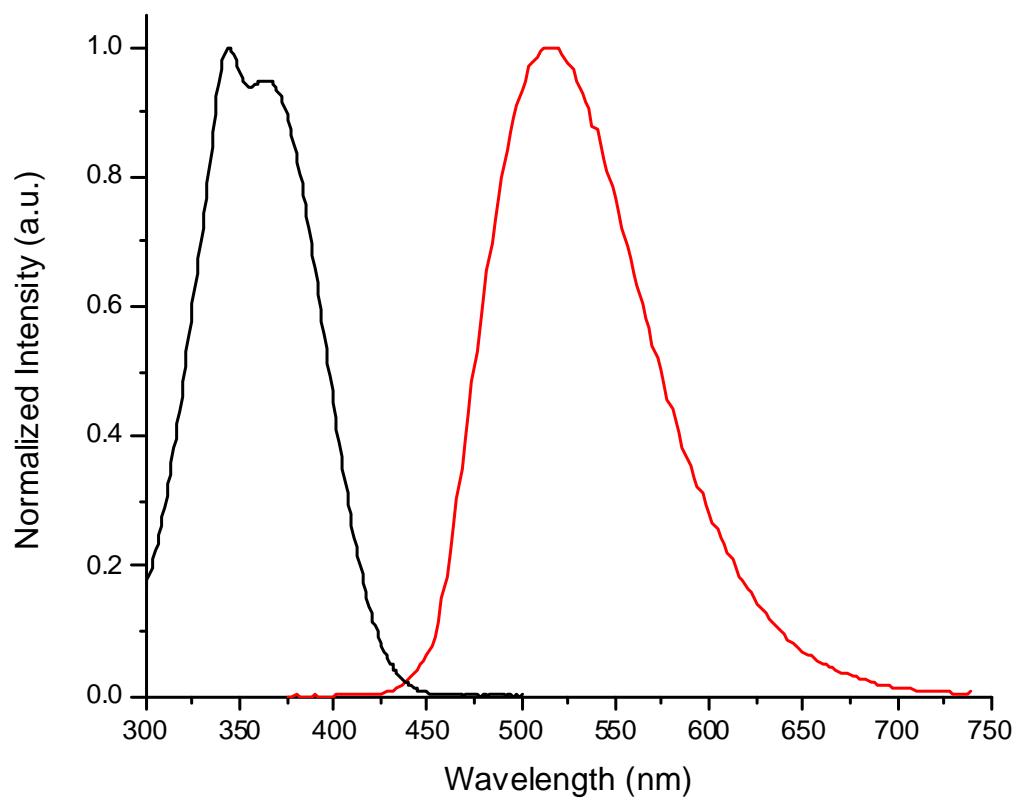


Figure 9: Normalized absorbance (black) and fluorescence (red) spectra of **13**.

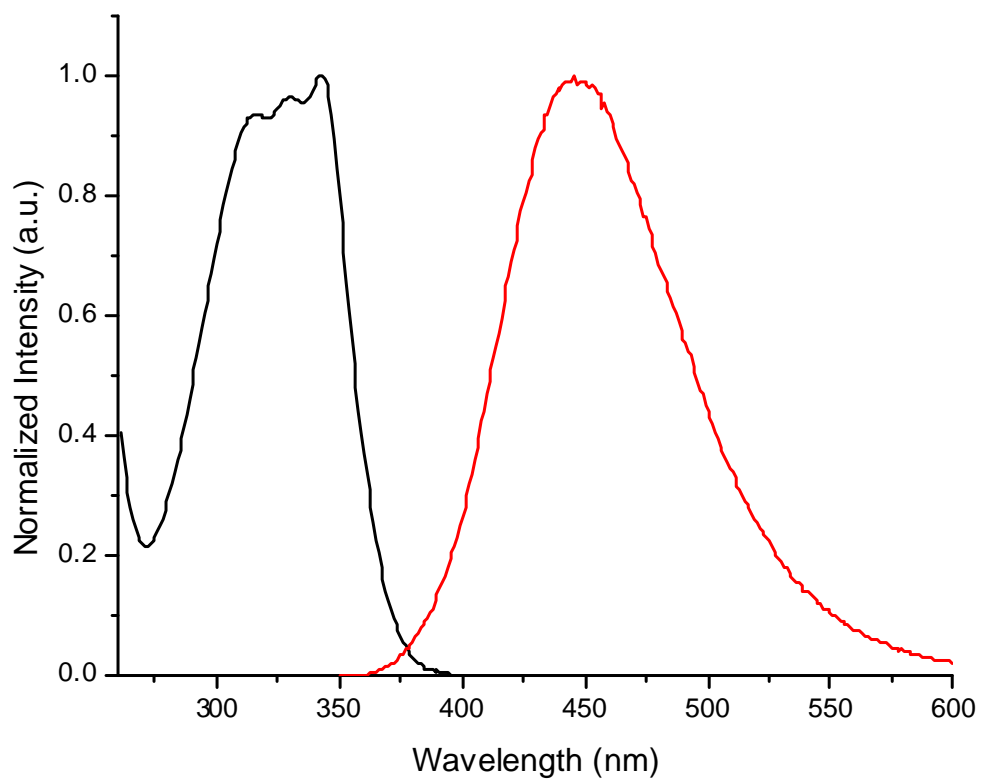


Figure 10: Normalized absorbance (black) and fluorescence (red) spectra of **14**.

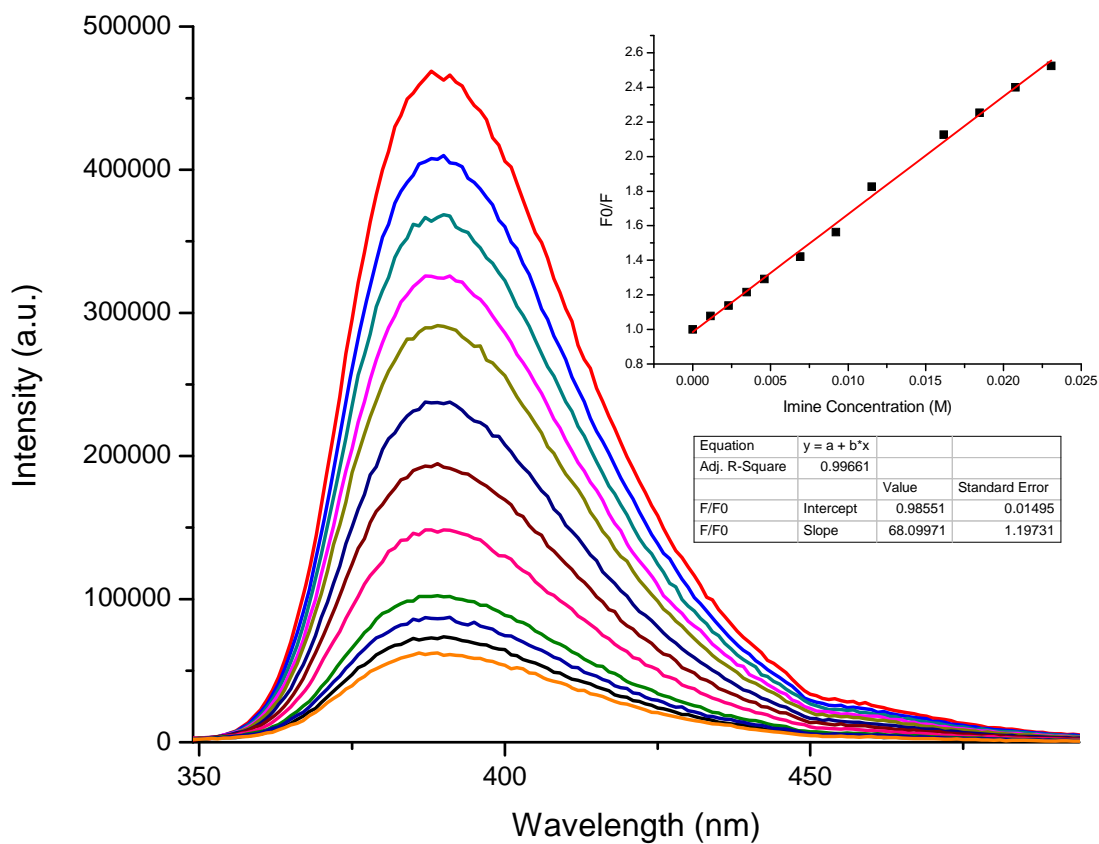


Figure 11: Fluorescence spectra of **21** with increasing concentrations of **10** in anhydrous acetonitrile. Inset: Stern-Volmer plot of Φ_0/Φ vs. [**10**] including linear fit and basic statistics showing diffusion limited fluorescence quenching of **21** with **10**.

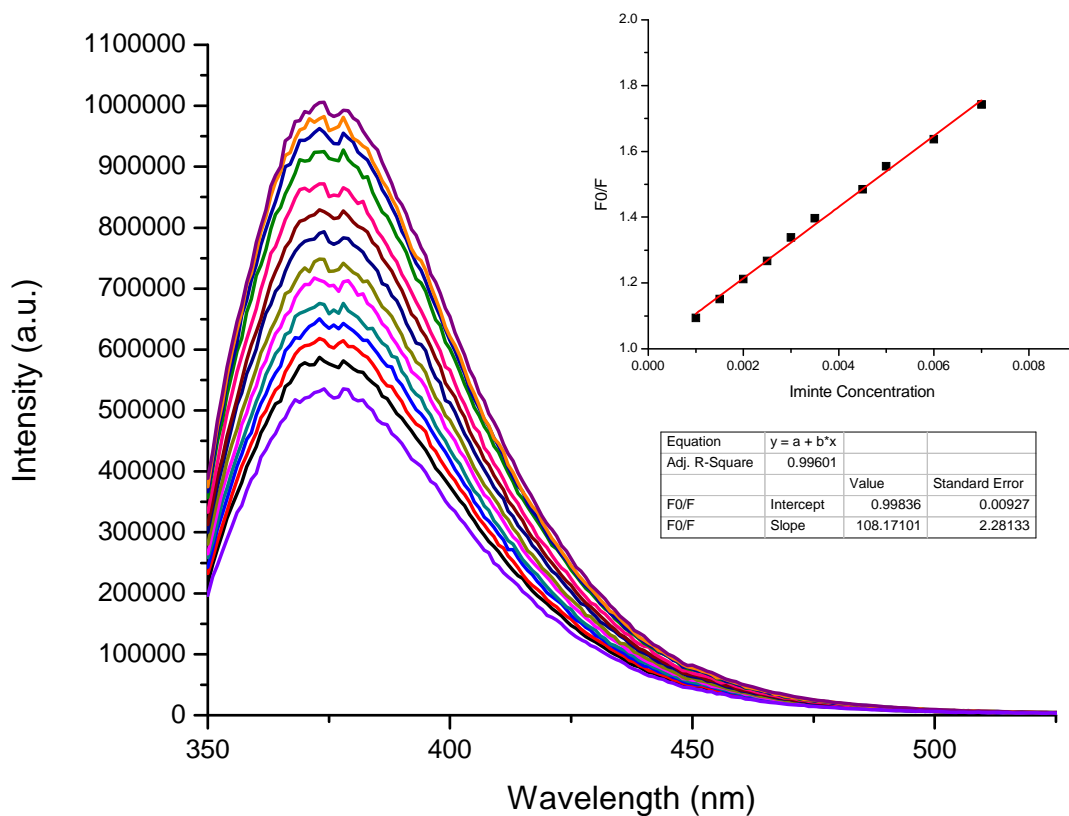


Figure 12: Fluorescence spectra of **11** with increasing concentrations of **10** in anhydrous acetonitrile. Inset: Stern-Volmer plot of Φ_0/Φ vs. [**10**] including linear fit and basic statistics showing the diffusion limited relationship between imine concentration and fluorescence quenching.

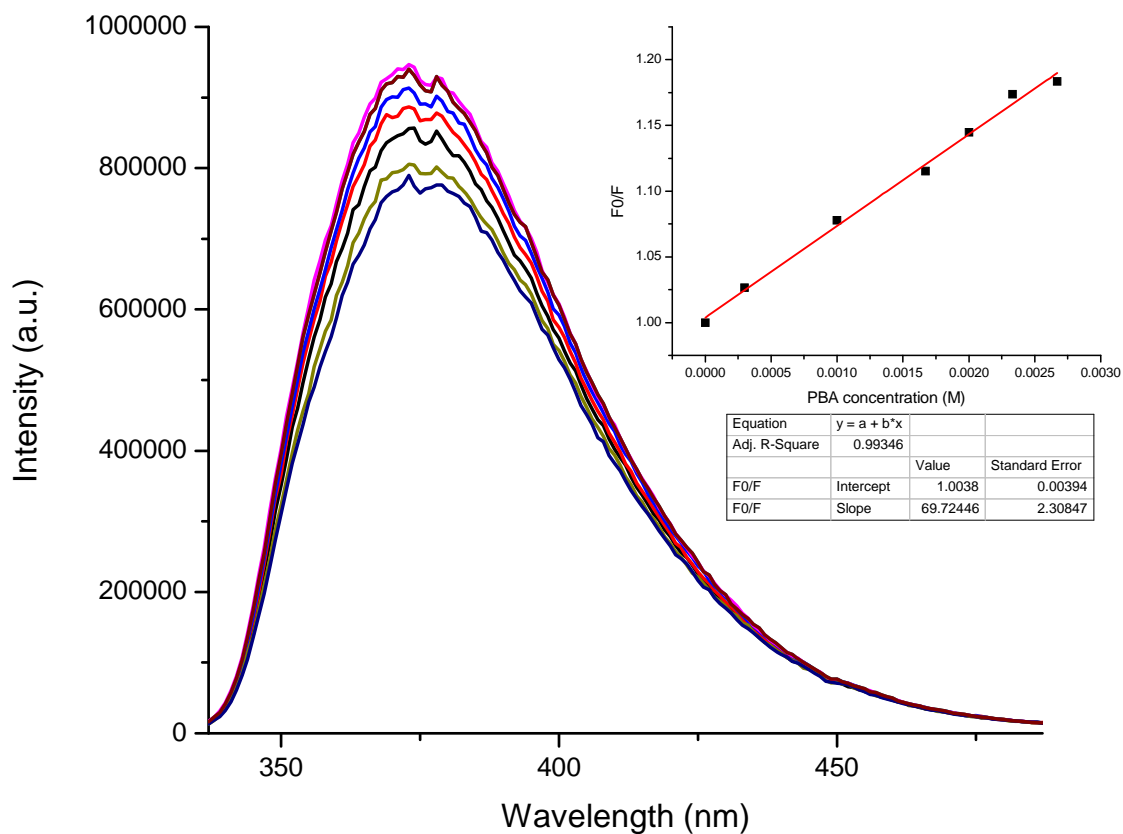


Figure 13: Fluorescence spectra of **11** with increasing concentrations of phenylboronic acid in anhydrous acetonitrile. Inset: Stern-Volmer plot of F_0/Φ vs. [phenylboronic acid] including linear fit and basic statistics showing the diffusion limited relationship between phenylboronic acid concentration and fluorescence quenching.

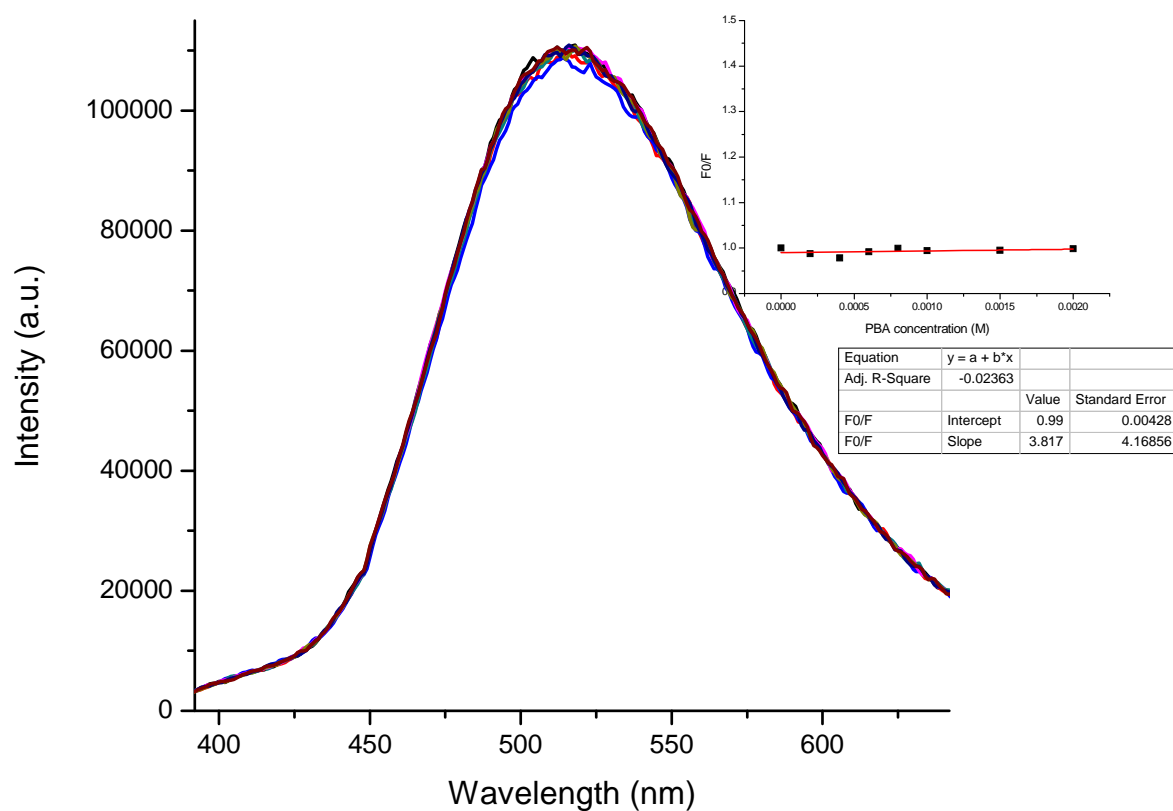


Figure 14: Fluorescence spectra of **12** with increasing concentrations of phenylboronic acid in pH 7.4 PBS. Inset: Stern-Volmer plot of Φ_0/Φ vs. [phenylboronic acid] including linear fit and basic statistics showing the lack of fluorescence quenching of **12** with phenylboronic acid.

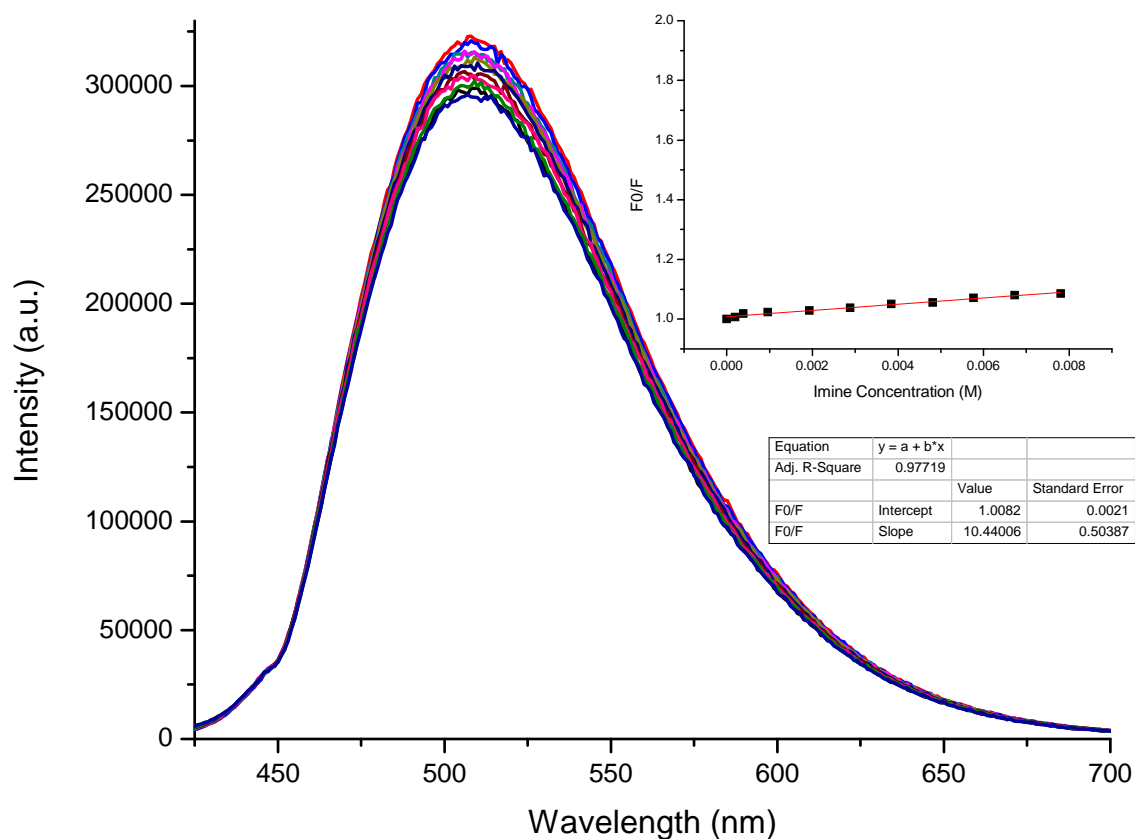


Figure 15: Fluorescence spectra of **13** with increasing concentrations of **10** in anhydrous acetonitrile. Inset: Stern-Volmer plot of Φ_0/Φ vs. $[10]$ including linear fit and basic statistics showing the lack of fluorescence quenching of **13** with **10**.

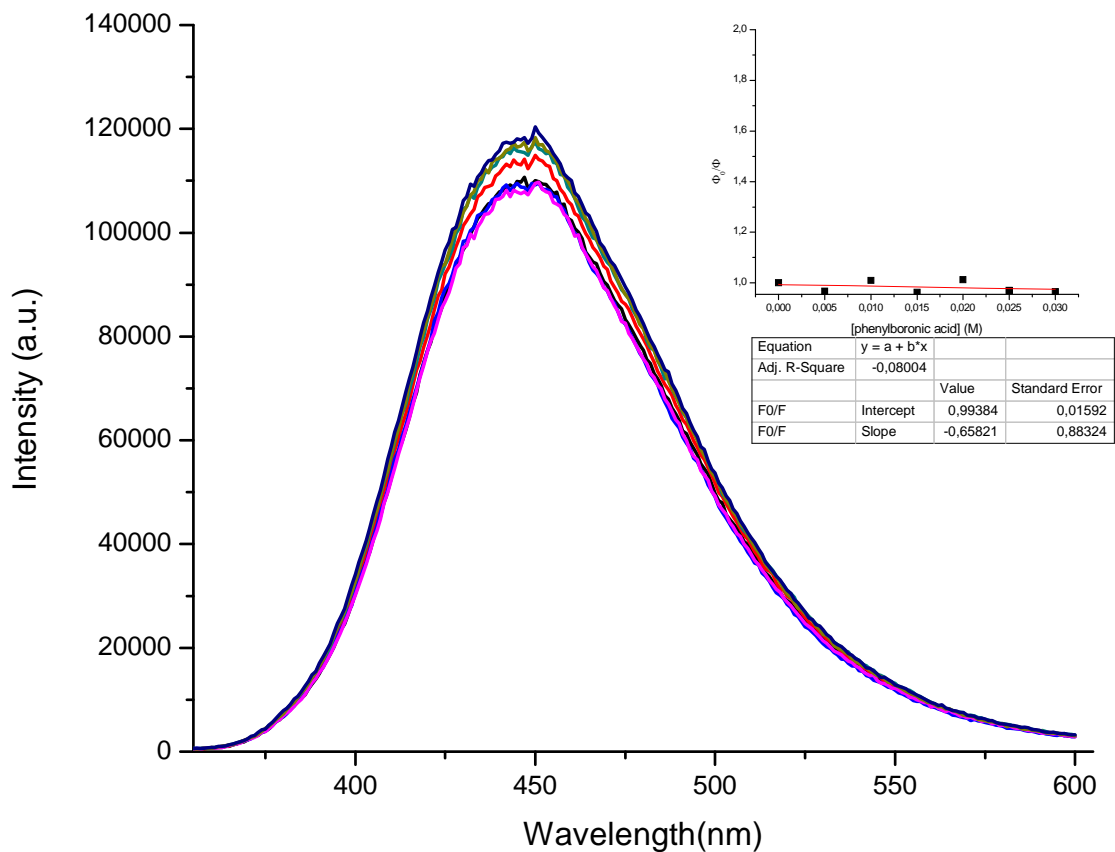


Figure 16: Fluorescence spectra of **14** with increasing concentrations of phenylboronic acid in pH 7.4 PBS. Inset: Stern-Volmer plot of Φ_0/Φ vs. [phenylboronic acid] including linear fit and basic statistics showing the lack of fluorescence quenching of **14** with phenylboronic acid.

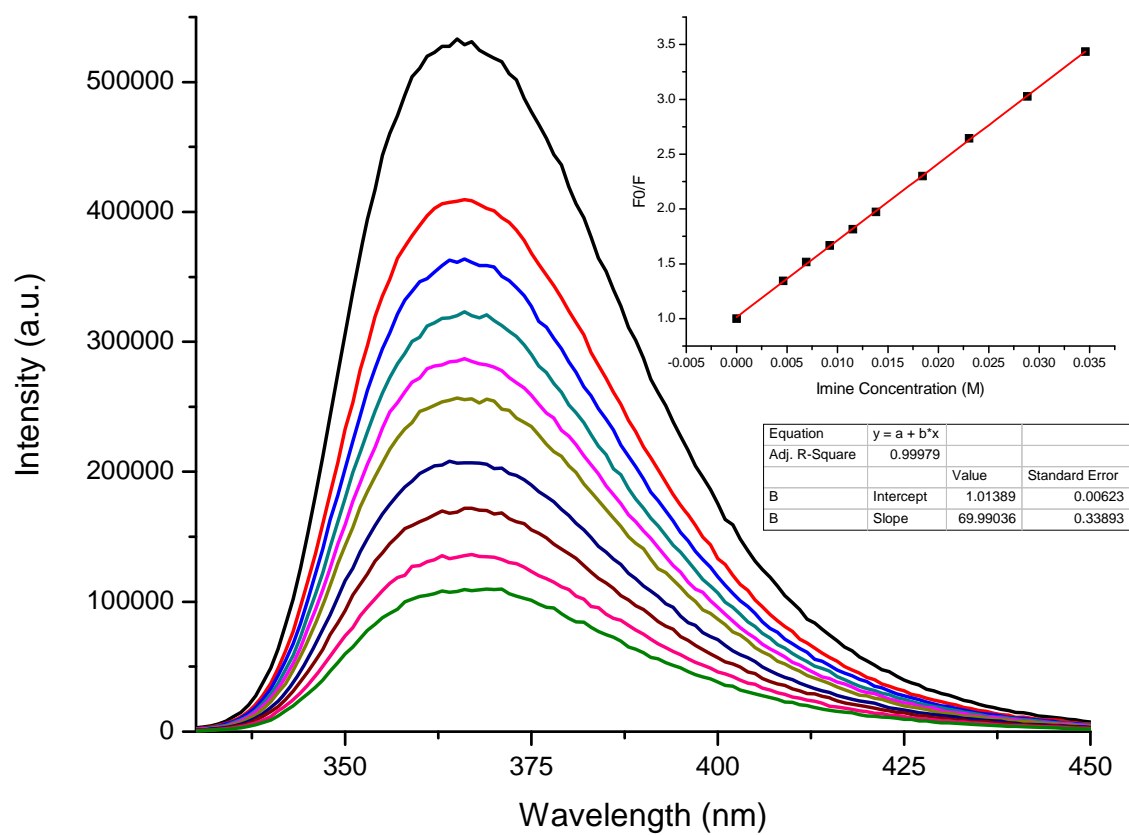


Figure 17: Fluorescence spectra of **20** with increasing concentrations of **10** in anhydrous acetonitrile. Inset: Stern-Volmer plot of Φ_0/Φ vs. [**10**] including linear fit and basic statistics showing diffusion limited fluorescence quenching of **20** with **10**.

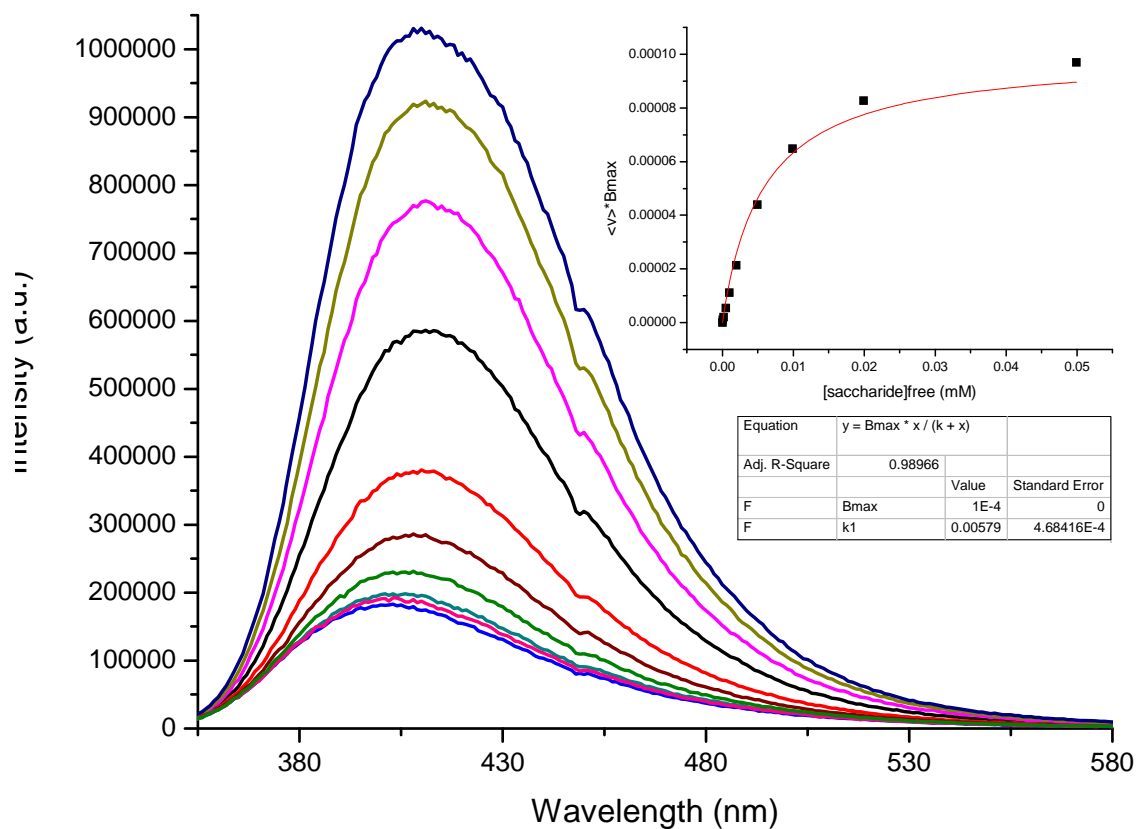


Figure 18: Fluorescence spectra of **1** in pH 7.4 PBS with added fructose demonstrating the fluorescence revival of **1** upon saccharide addition. Inset: Plot of [**1**:fructose] vs. [fructose] with a one-site binding fit overlaid and basic statistics used to determine the binding constant of **1** with fructose.

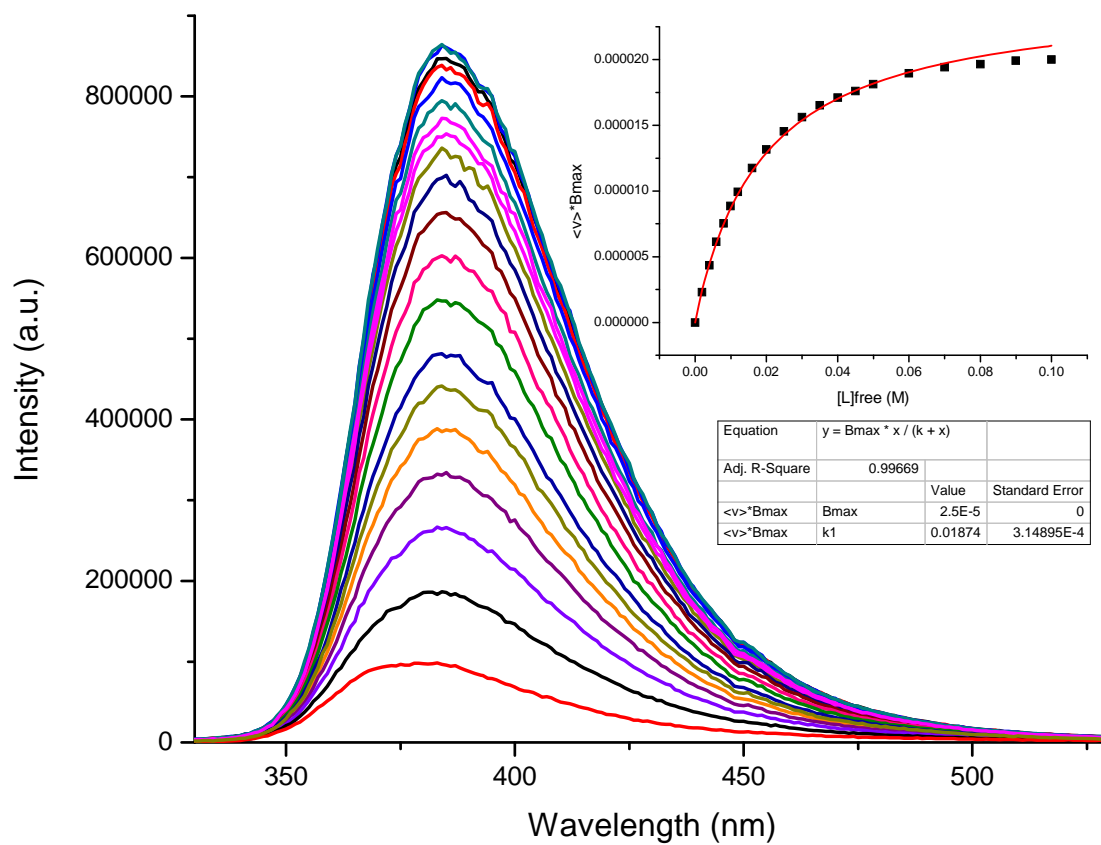


Figure 19: Fluorescence spectra of **5** in pH 7.4 PBS with added fructose demonstrating the fluorescence revival of **5** upon saccharide addition. Inset: Plot of [**5**:fructose] vs. [fructose] with a one-site binding fit overlaid and basic statistics used to determine the binding constant of **5** with fructose.

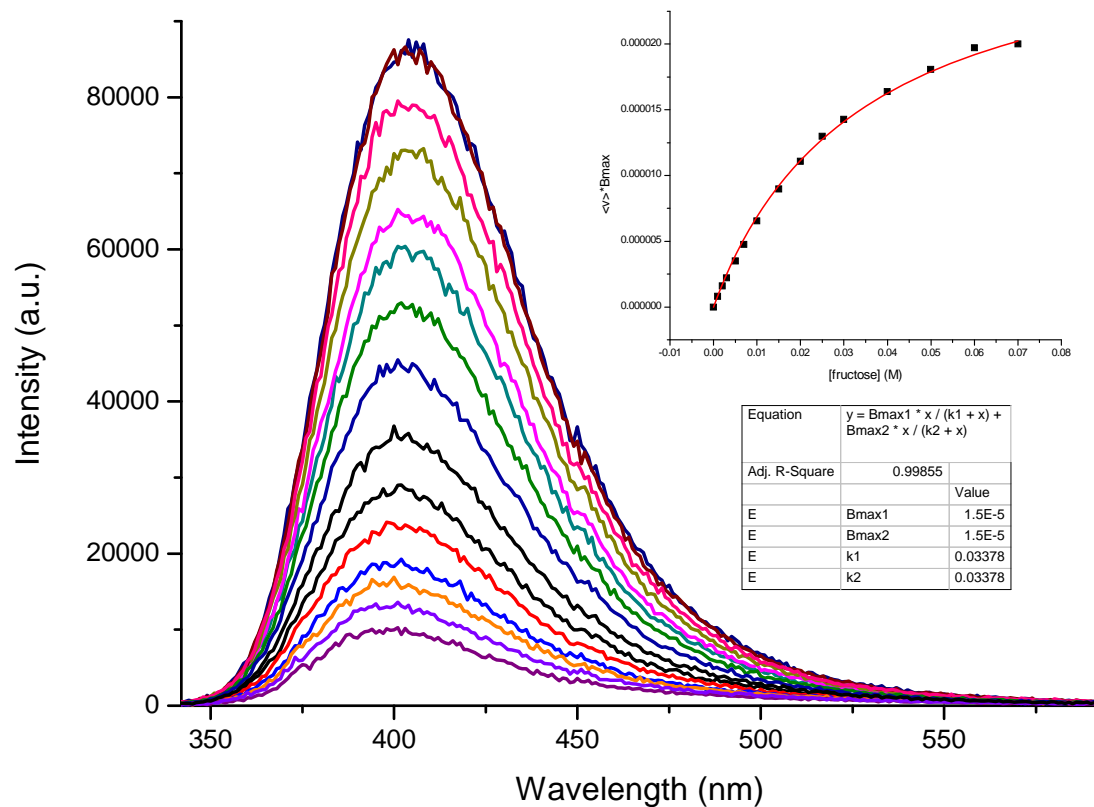


Figure 20: Fluorescence spectra of **6** in pH 7.4 PBS with added fructose demonstrating the fluorescence revival of **6** upon saccharide addition. Inset: Plot of [**6**:fructose] vs. [fructose] with a two-site binding fit overlaid and basic statistics used to determine the binding constant of **6** with fructose.

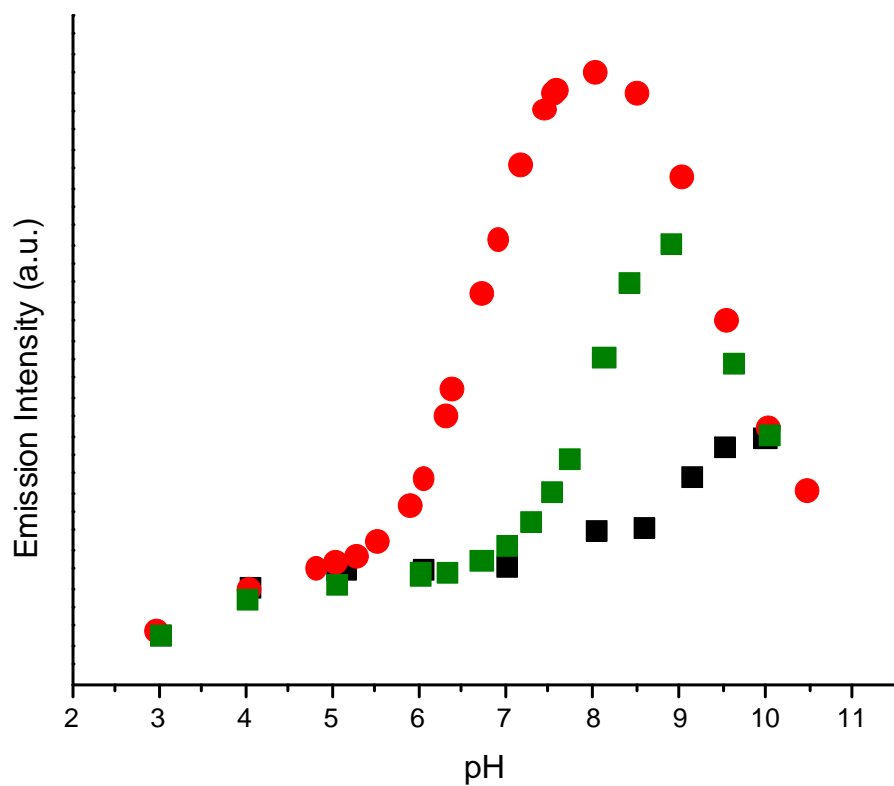


Figure 21: Fluorescence pH titrations of **1** without saccharide (■), with 100 mM glucose (■) and with 50 mM fructose (■) (~saturation) demonstrating the reduction of pKa of the boronic acid by formation of the boronic ester.

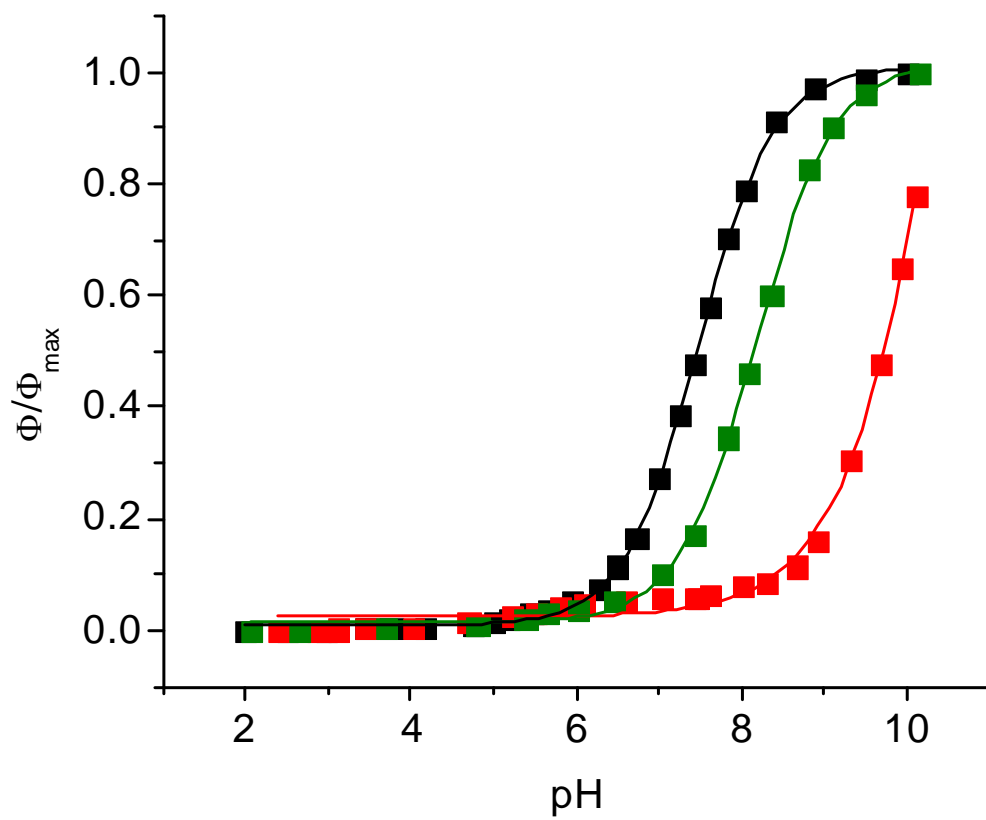


Figure 22: Fluorescence pH titrations of **1** without saccharide (■), with 10 mM fructose (■) and with 100 mM fructose (■) (~saturation) demonstrating the reduction of pKa of the boronic acid by formation of the boronic ester.

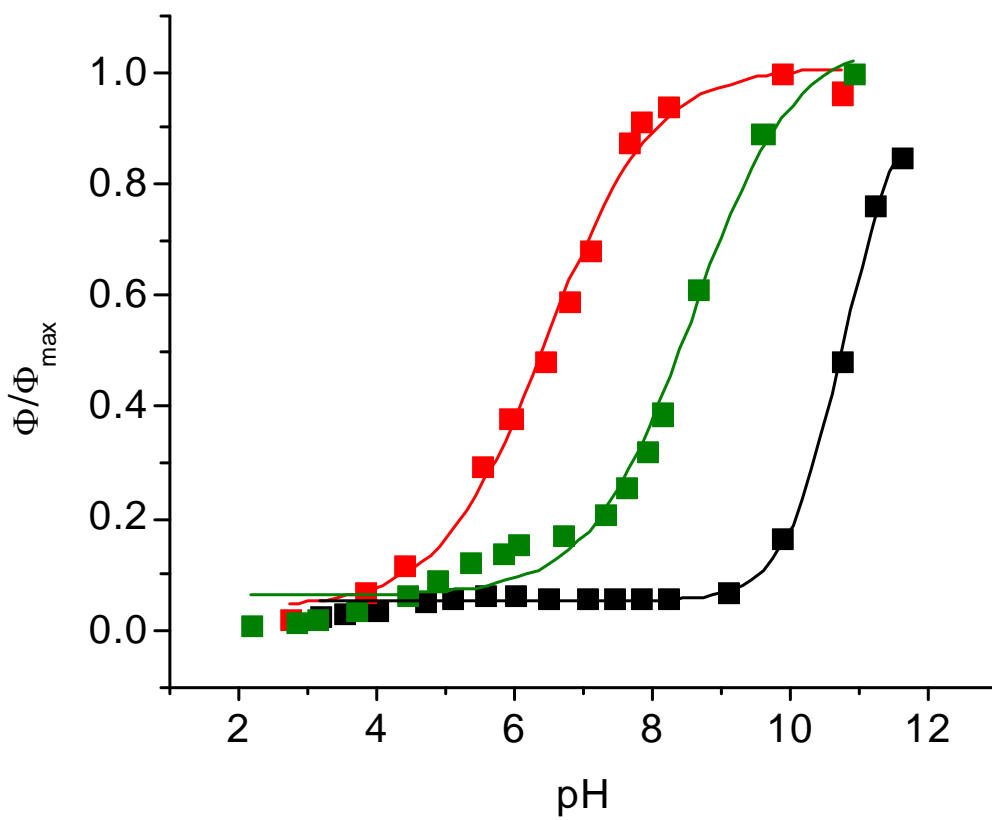


Figure 23: Fluorescence pH titrations of **1** without saccharide (■), with 10 mM fructose (■) and with 100 mM fructose (■) (~saturation) demonstrating the reduction of pKa of the boronic acid by formation of the boronic ester.

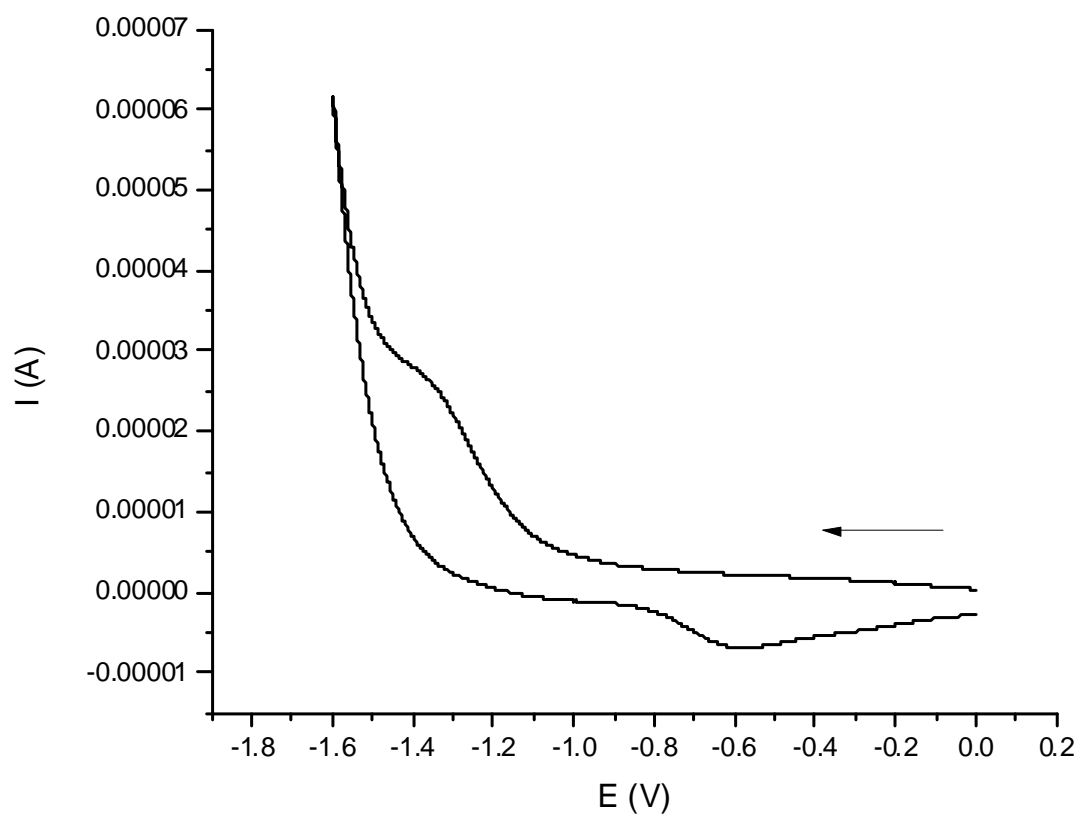


Figure 24: Cyclic voltammogram of the cathodic process of phenylboronic acid in anhydrous dimethylformamide.

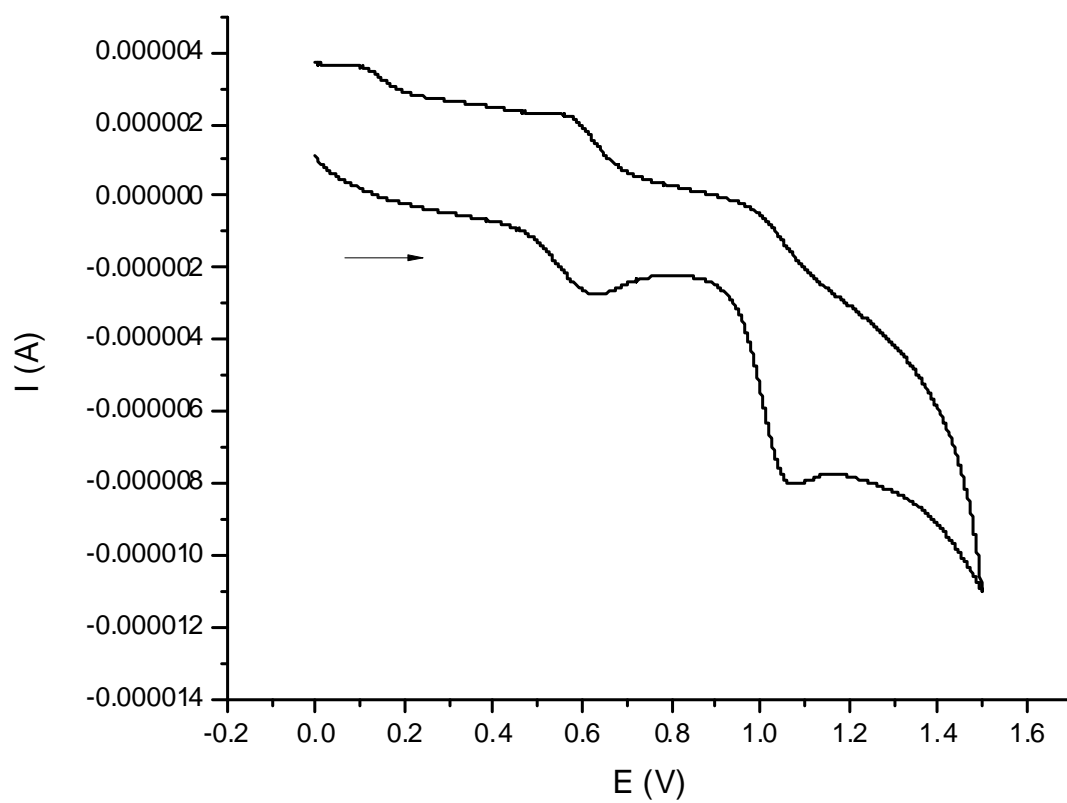


Figure 25: Cyclic voltammogram of the anodic process of **9** in anhydrous dimethylformamide.

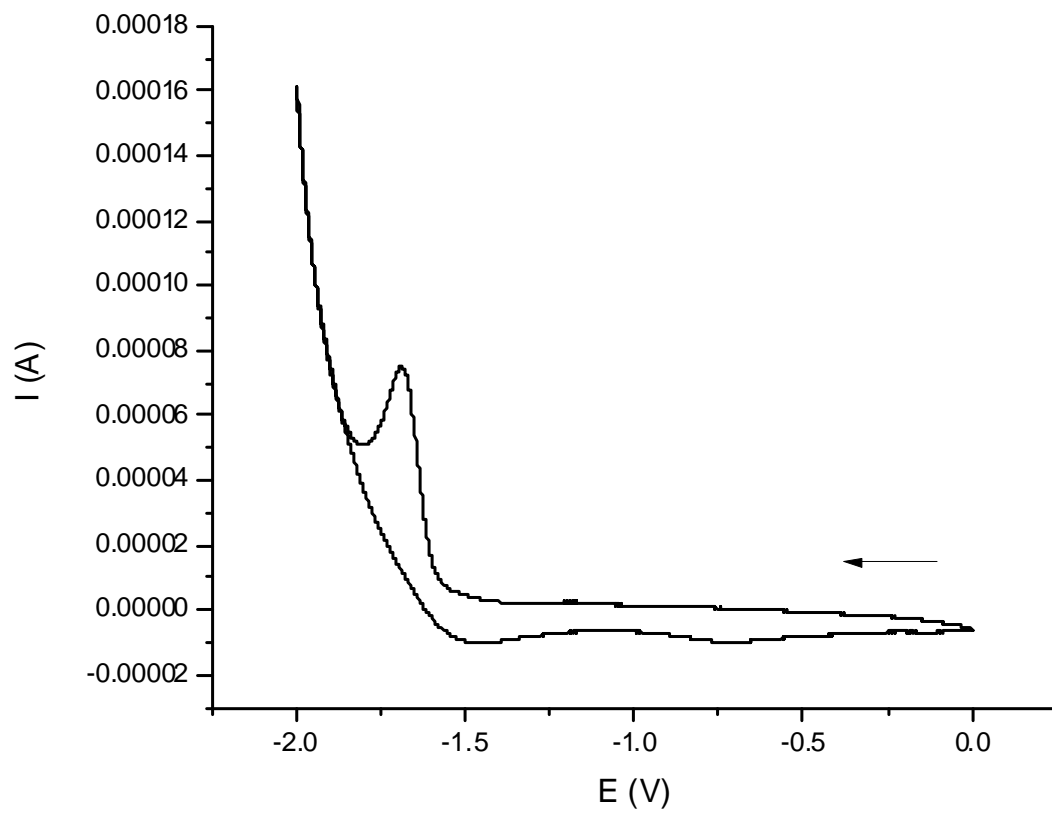


Figure 26: Cyclic voltammogram of the cathodic process of **10** in anhydrous dimethylformamide.

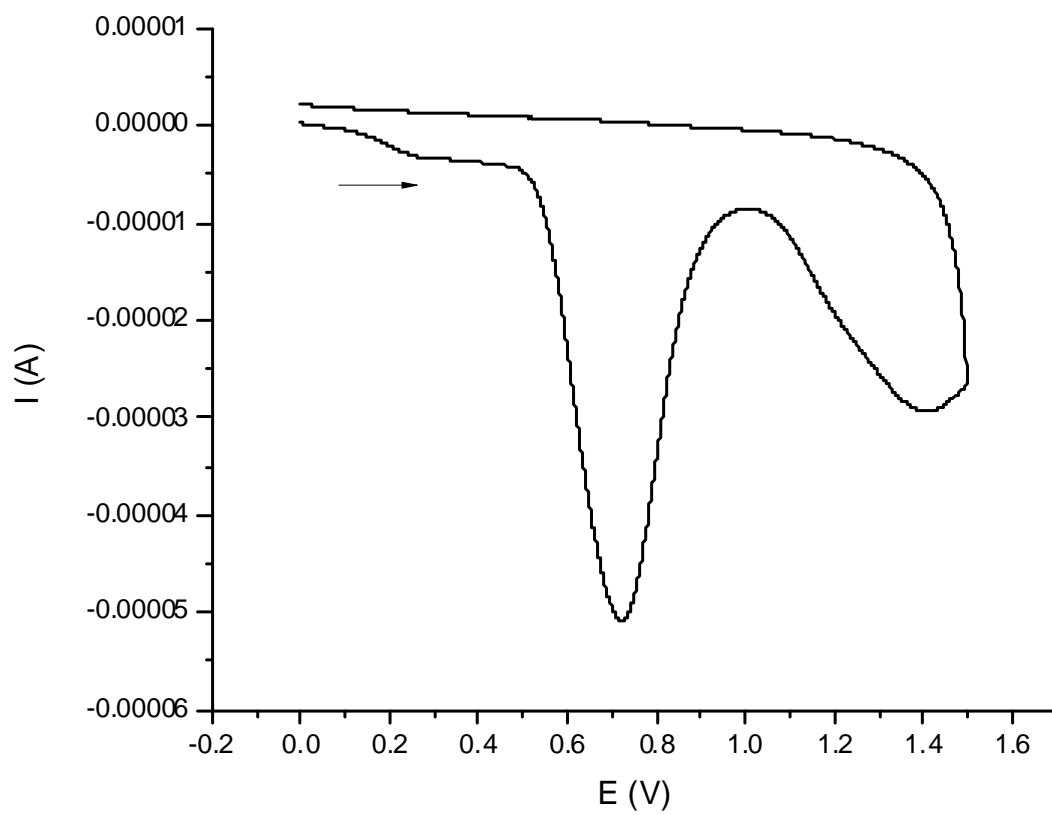


Figure 27: Cyclic voltammogram of the anodic process of **11** in anhydrous dimethylformamide.

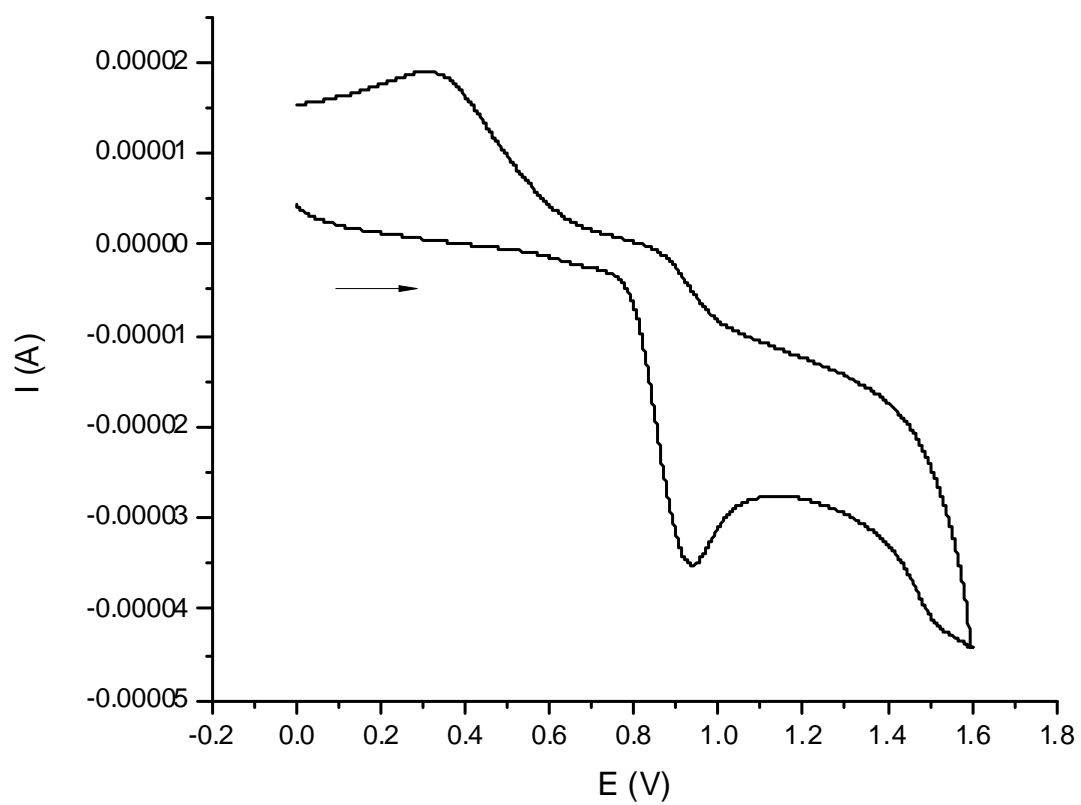


Figure 28: Cyclic voltammogram of the anodic process of **12** in anhydrous dimethylformamide.

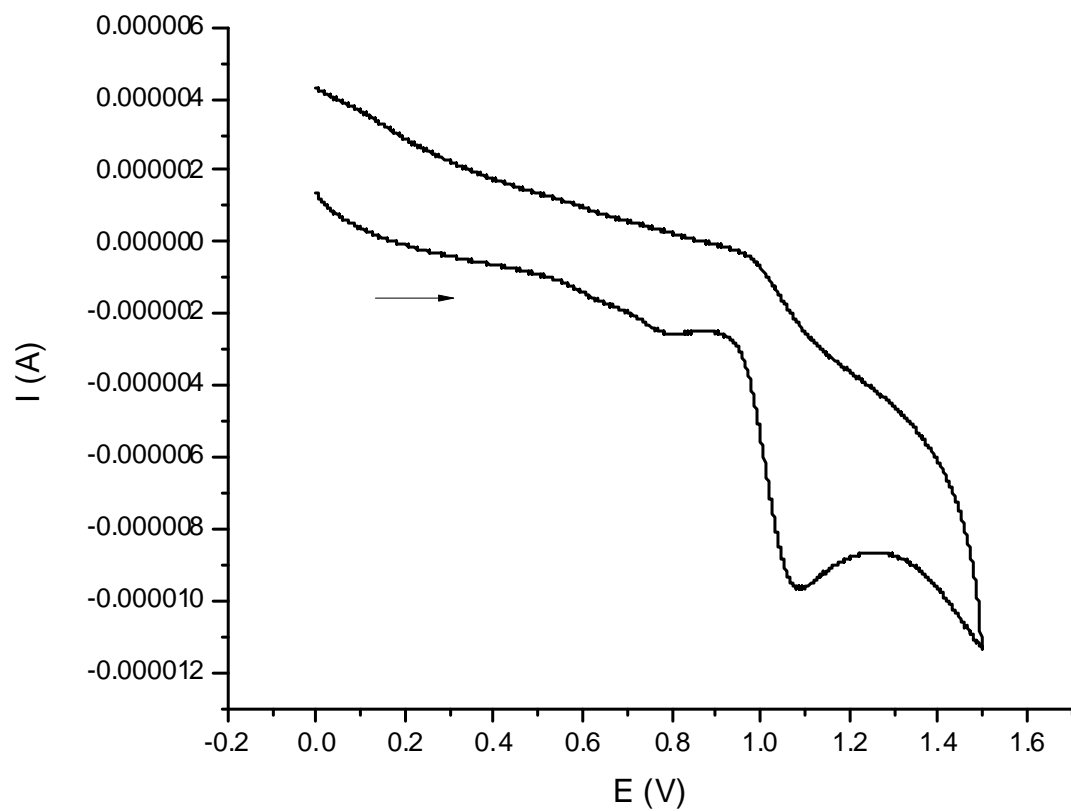


Figure 29: Cyclic voltammogram of the anodic process of **13** in anhydrous dimethylformamide.

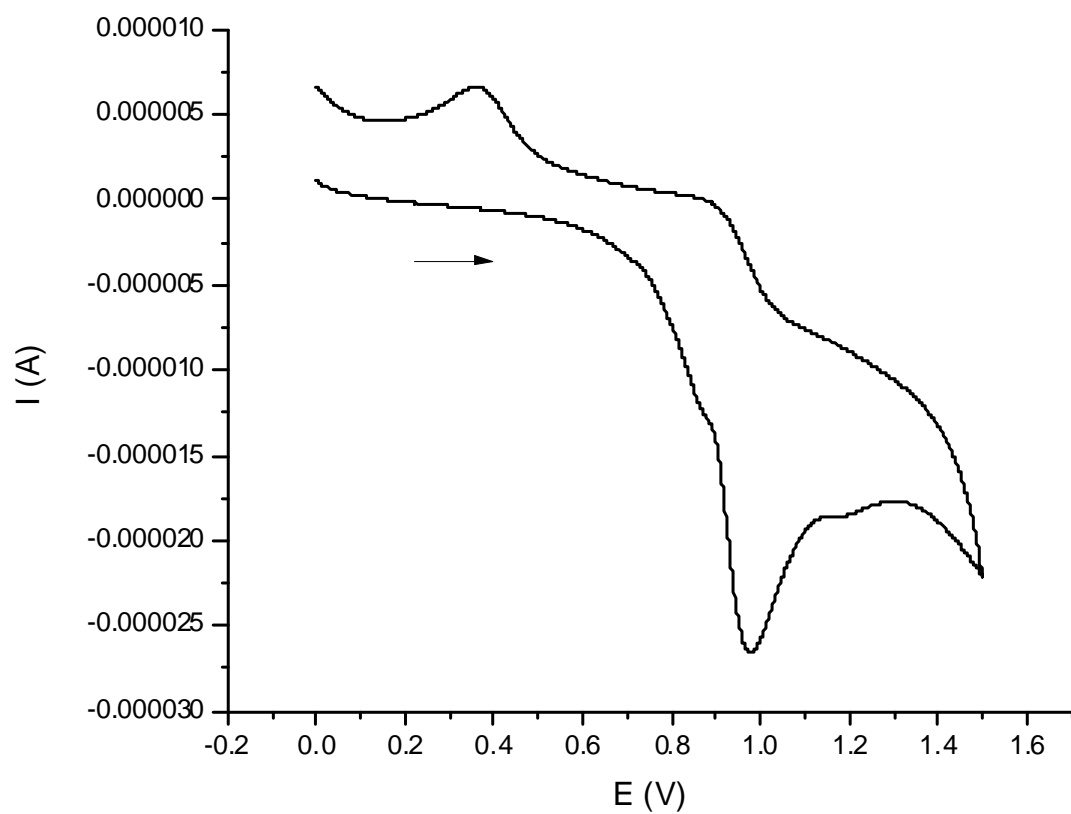


Figure 30: Cyclic voltammogram of the anodic process of **20** in anhydrous dimethylformamide.

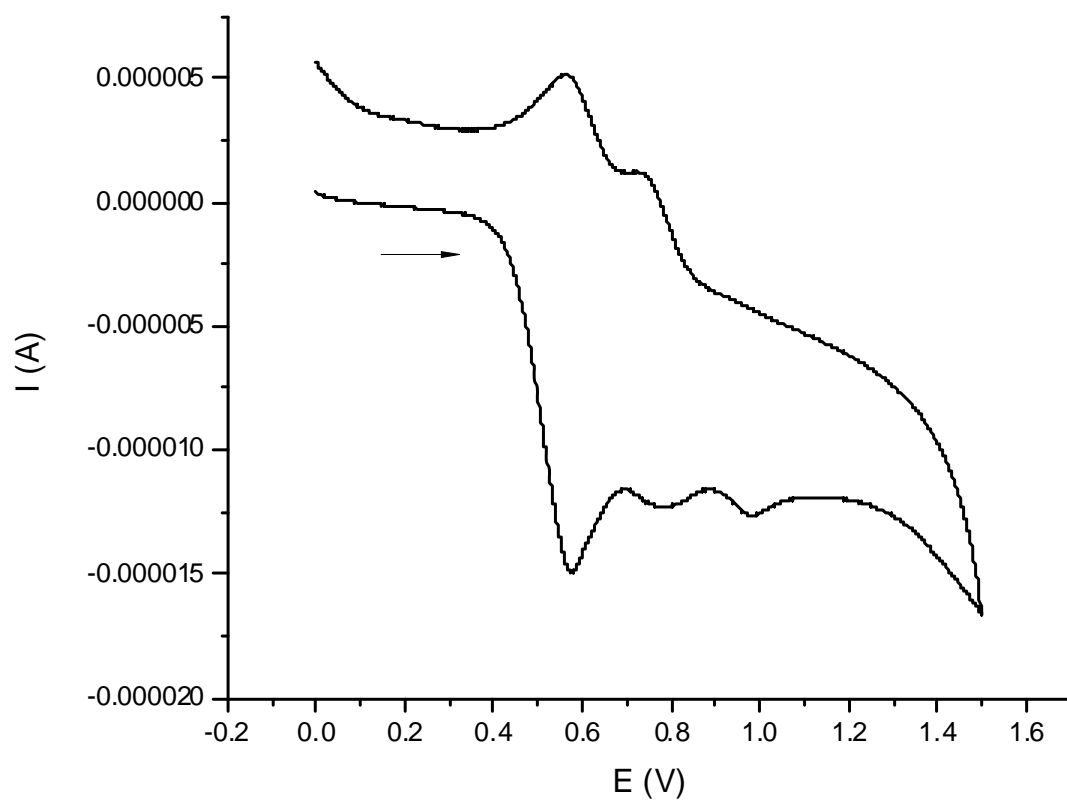


Figure 31: Cyclic voltammogram of the anodic process of **21** in anhydrous dimethylformamide.

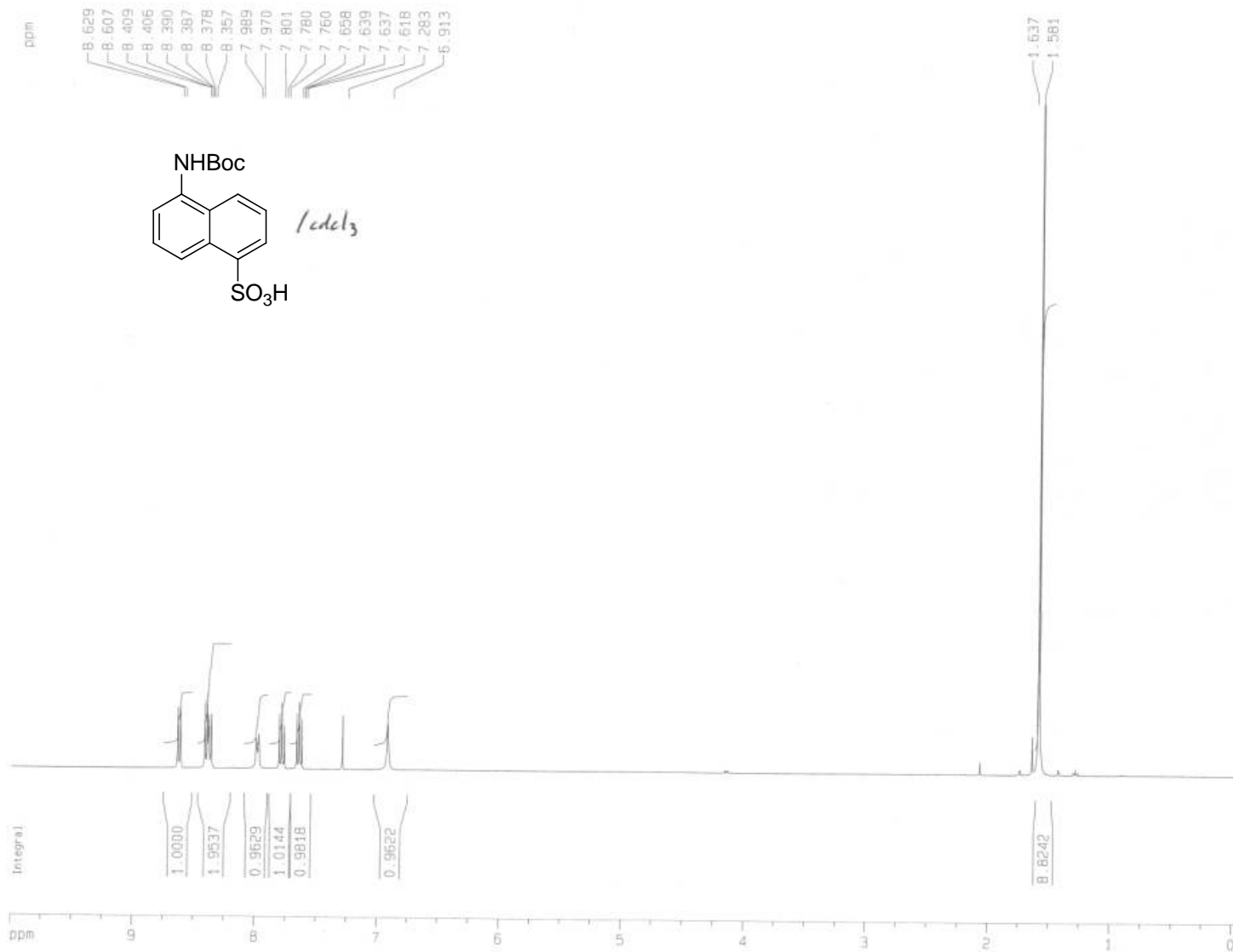


Figure 32: 1H NMR of N-Boc-5-aminonaphthalene-1-sulfonic acid in $CDCl_3$.

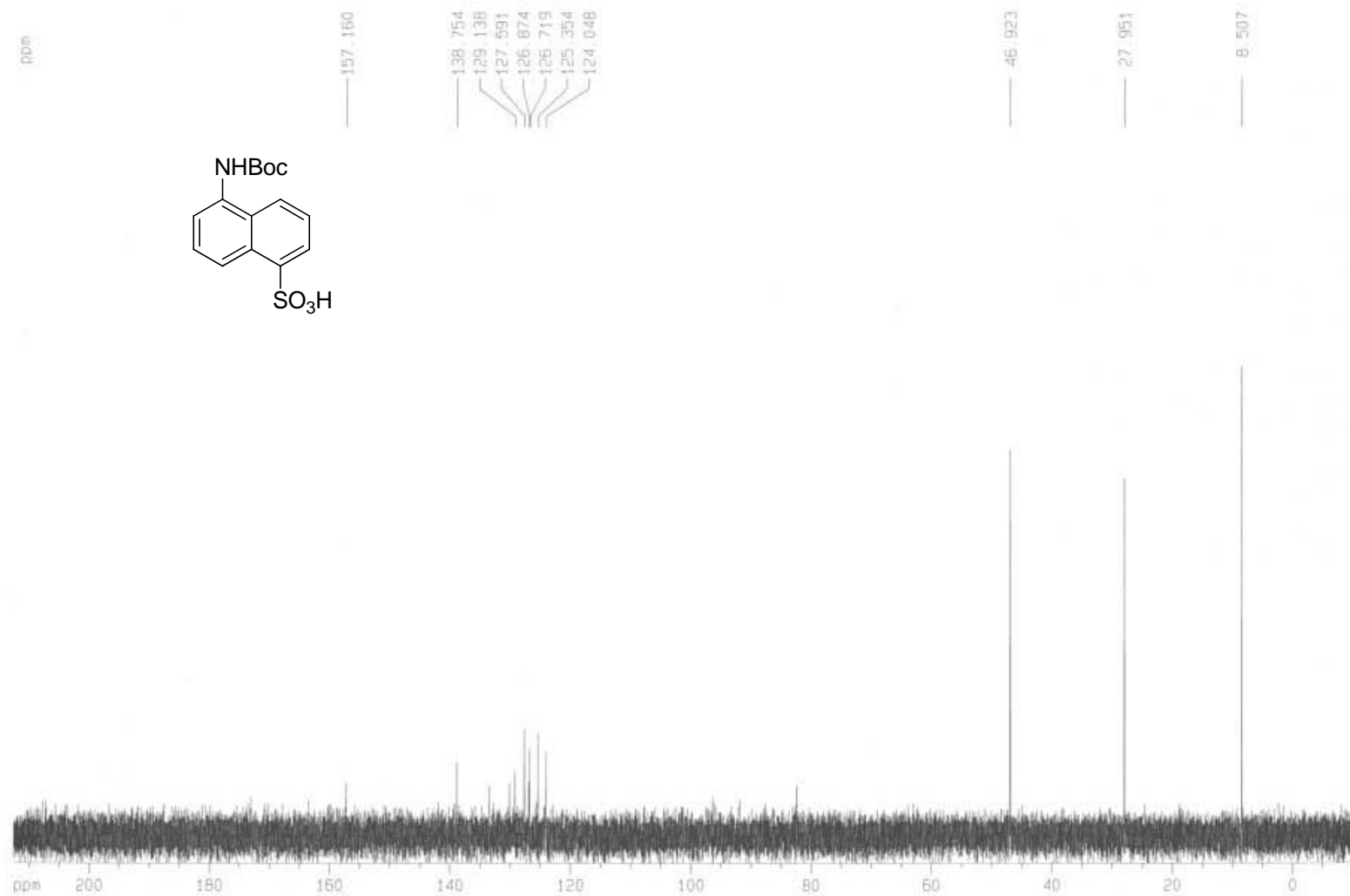


Figure 33: ^{13}C NMR of N-Boc-5-aminonaphthalene-1-sulfonic acid in CDCl_3 .

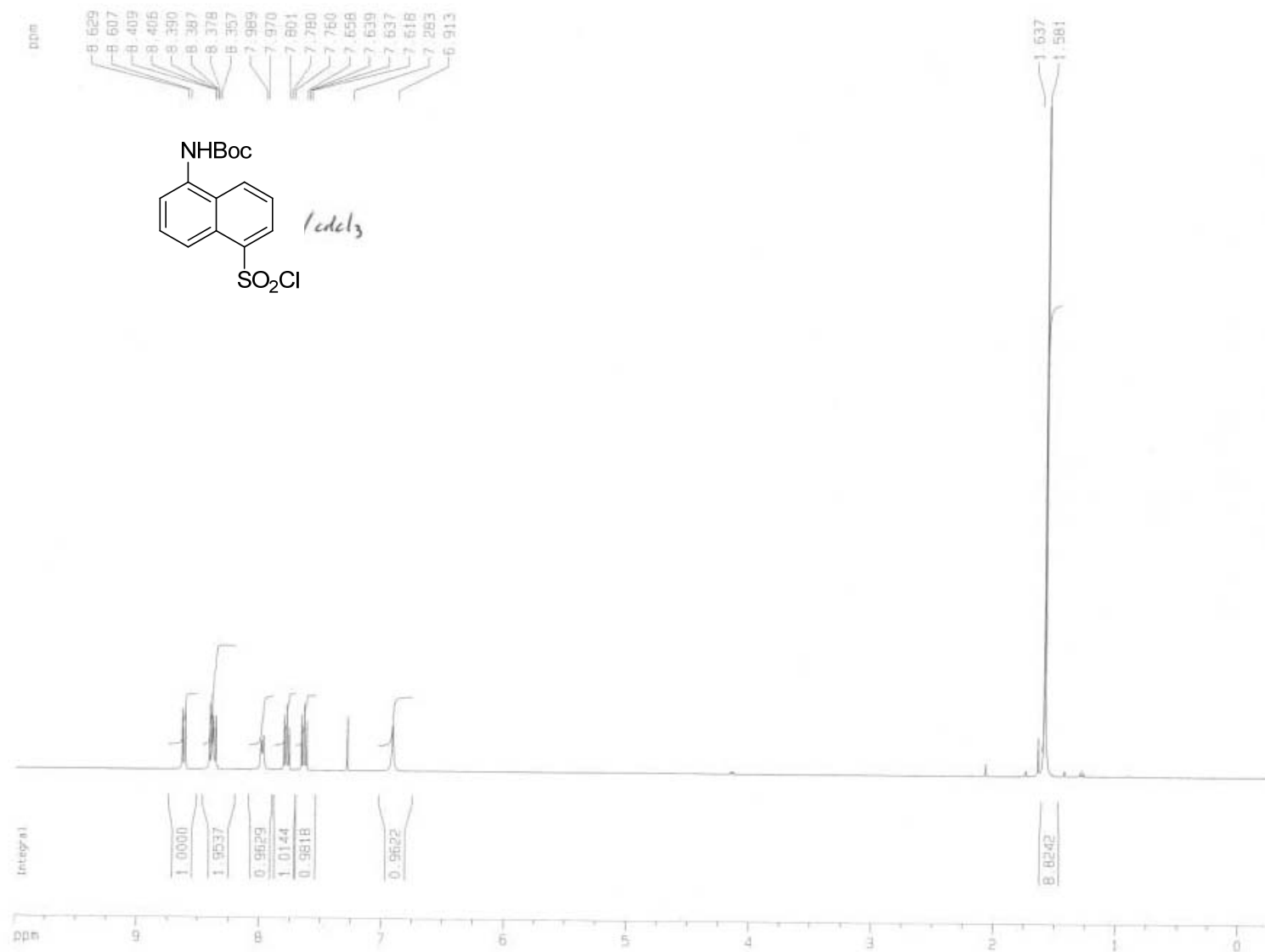


Figure 34: ¹H NMR of N-Boc-5-aminonaphthalene-1-sulfonyl chloride in CDCl₃.

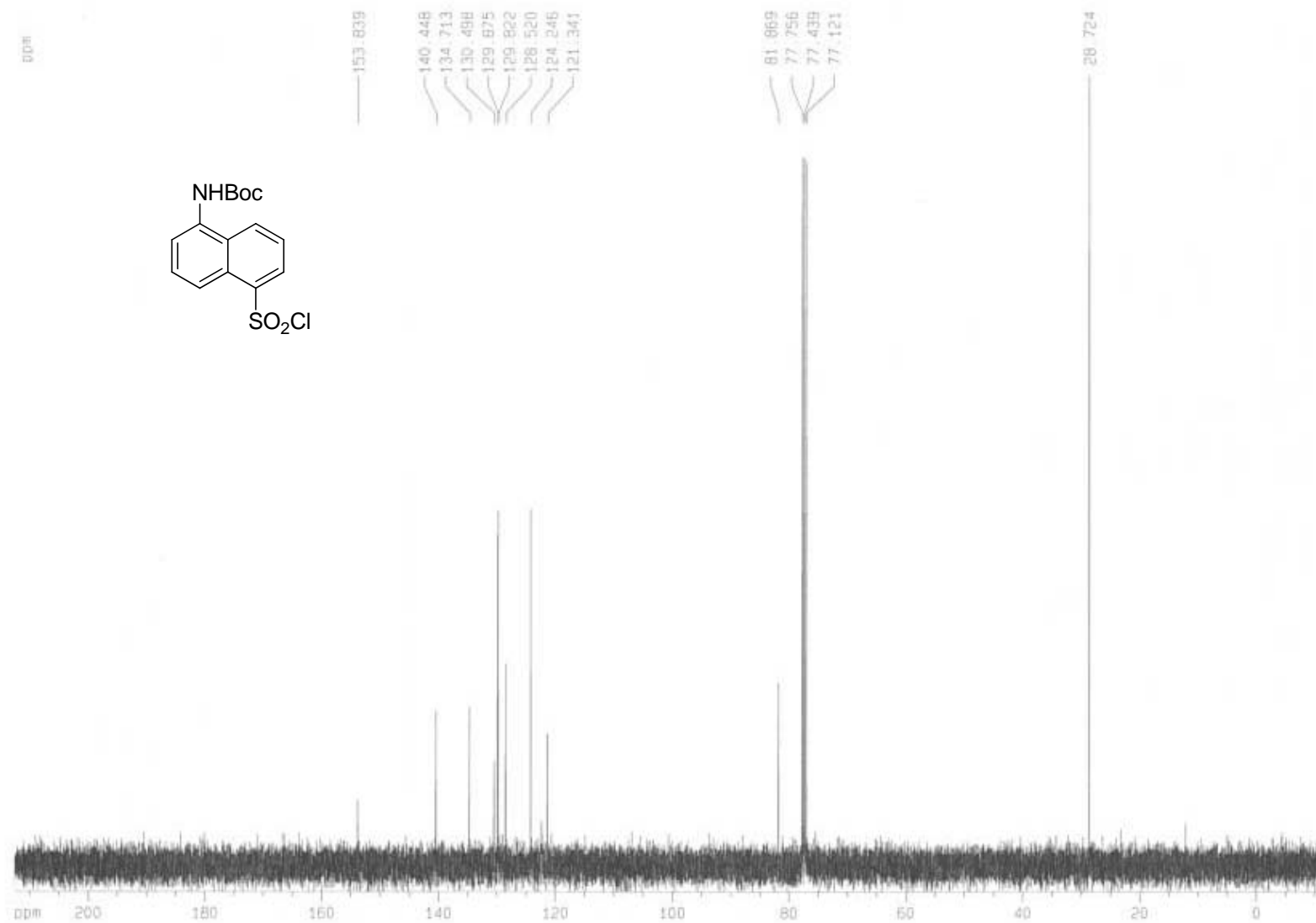


Figure 35: ^{13}C NMR of N-Boc-5-aminonaphthalene-1-sulfonyl chloride in CDCl_3 .

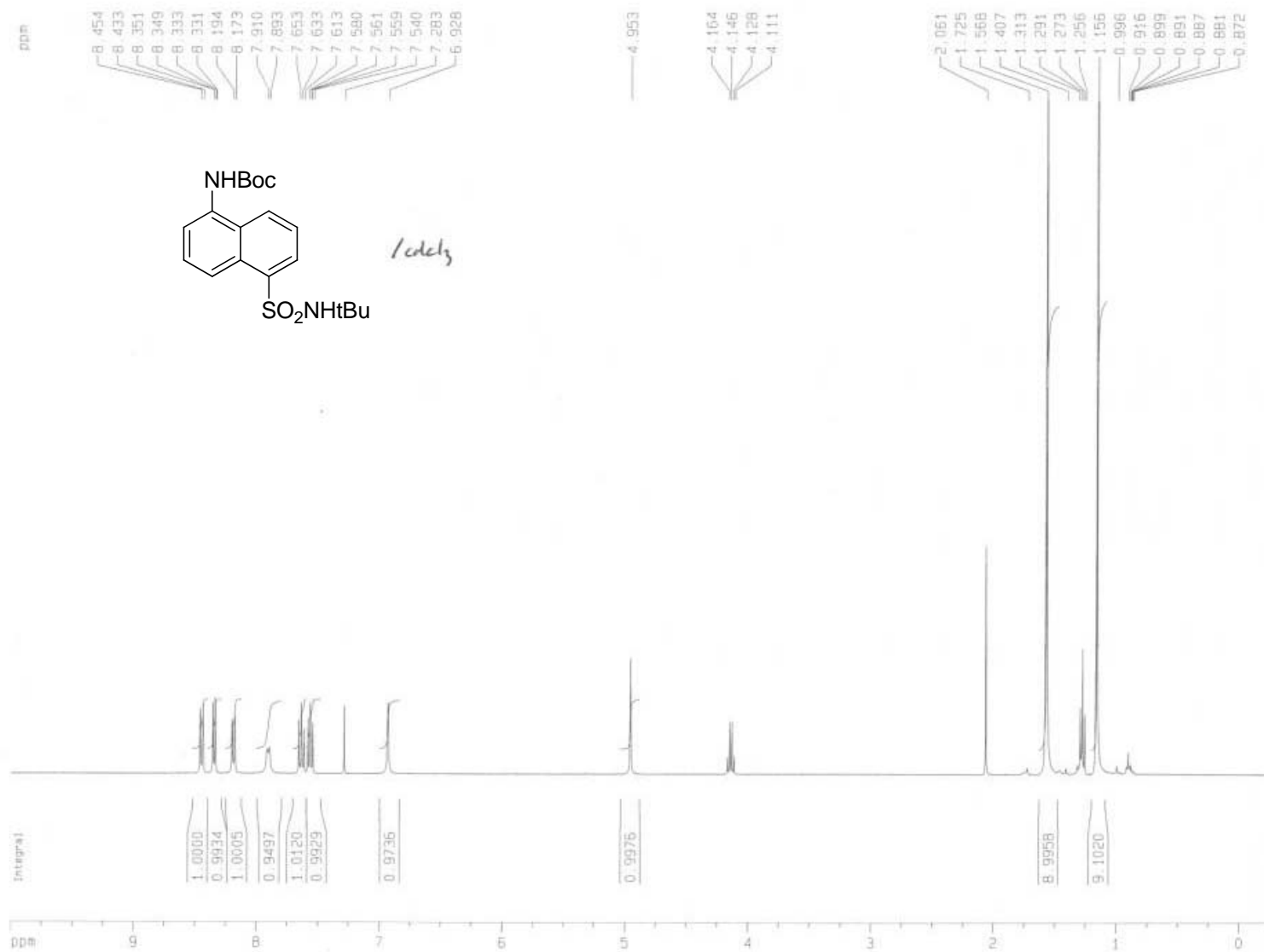


Figure 36: ¹H NMR of N-Boc-5-aminonaphthalene-1-*tert*-butylsulfonamide in CDCl₃.

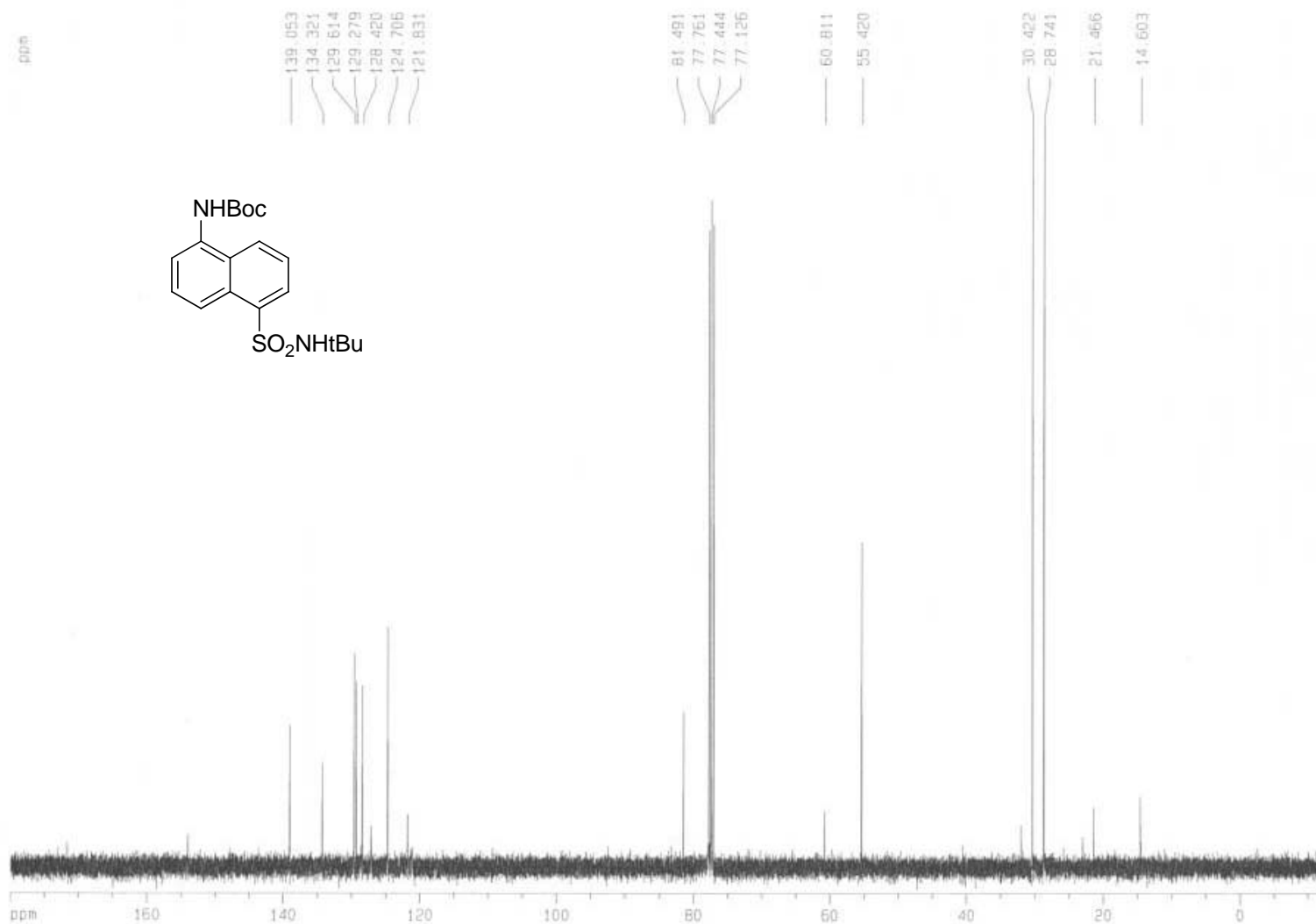


Figure 37: ^{13}C NMR of N-Boc-5-aminonaphthalene-1-*tert*-butylsulfonamide in CDCl_3 .

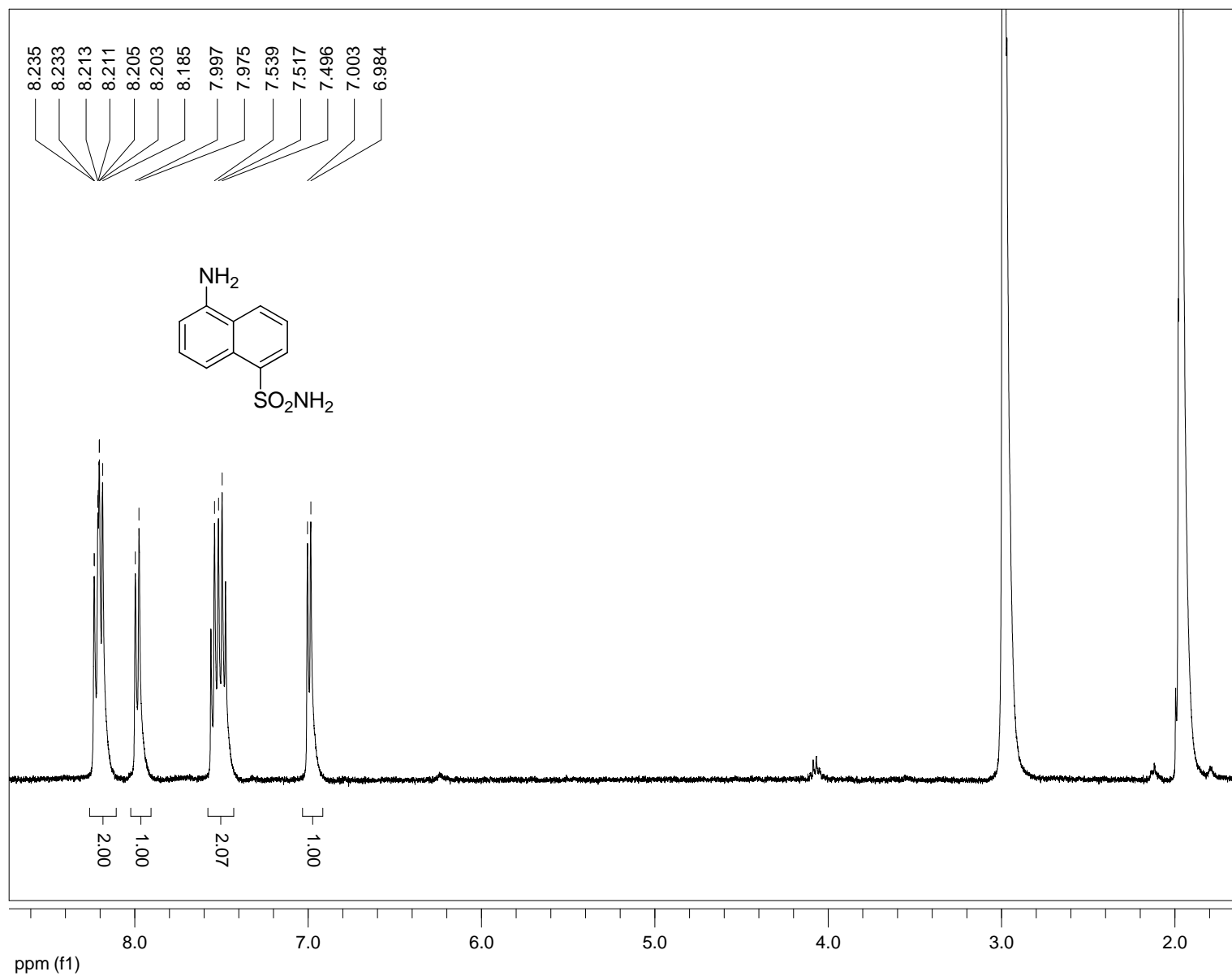


Figure 38: ^1H NMR of 5-aminonaphthalene-1-sulfonamide in 5% D_2O in CD_3CN .

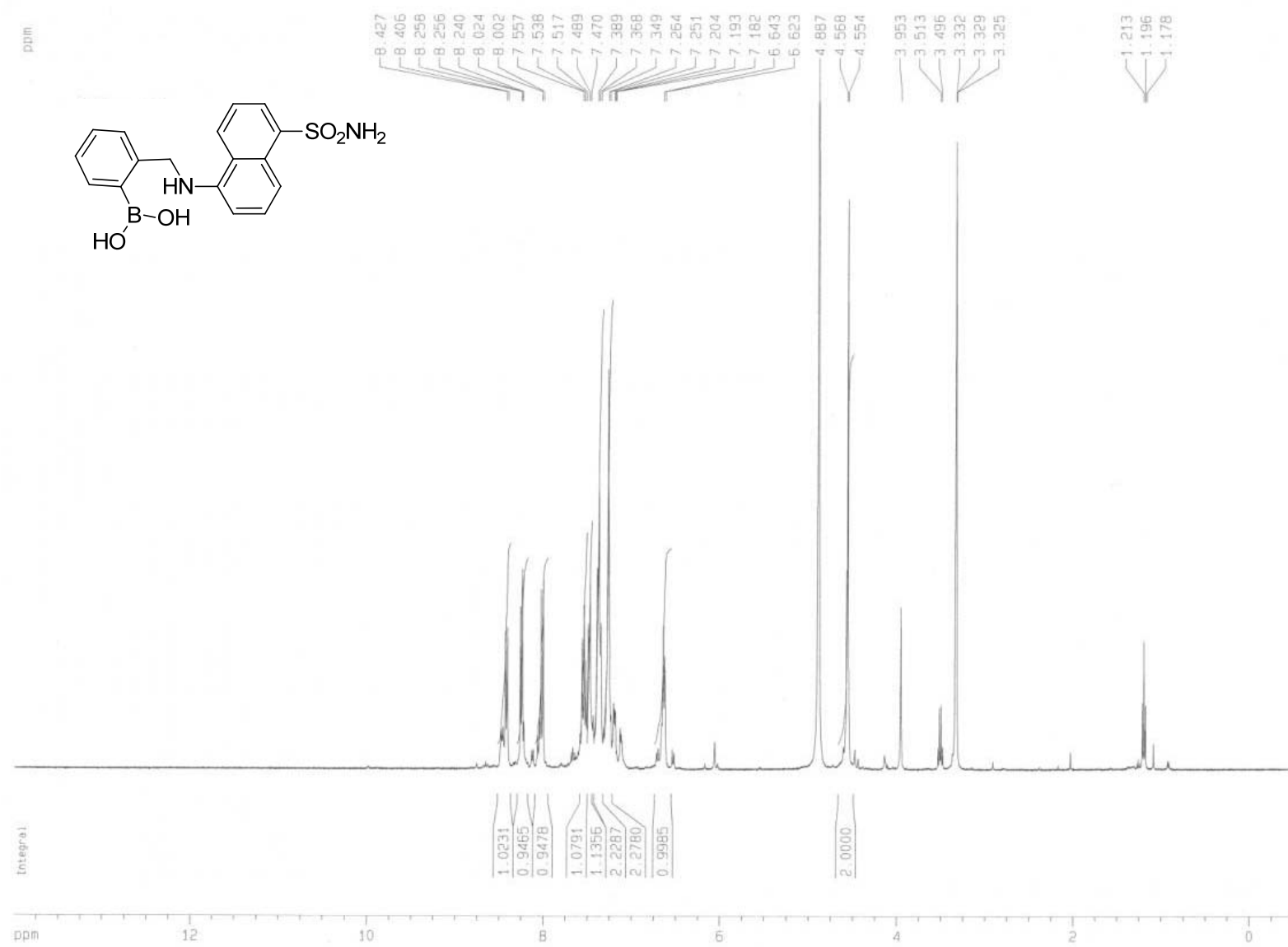


Figure 39: ¹H NMR of N-phenylborono-5-aminonaphthalene-1-sulfonamide in CD₃OD.

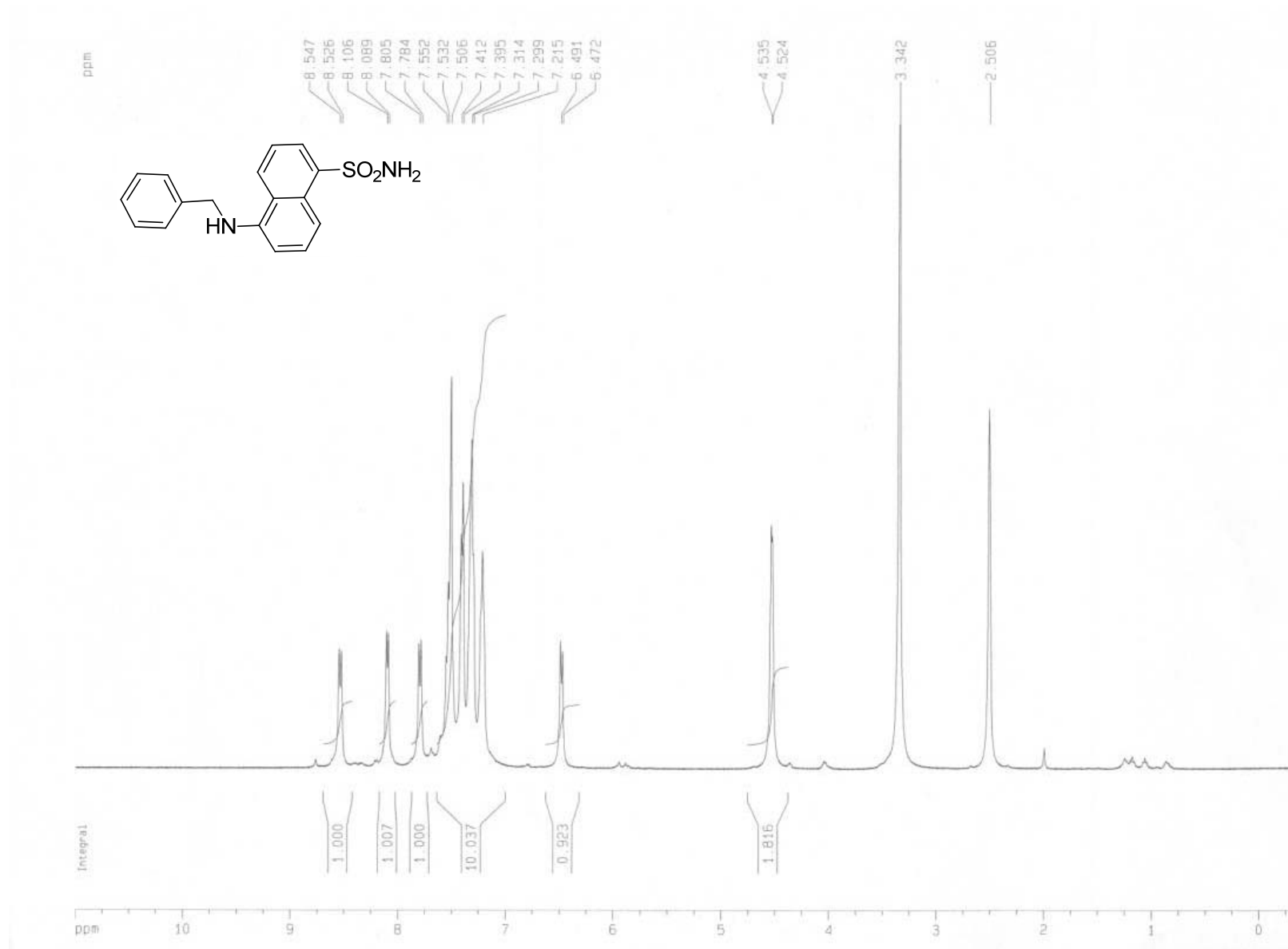


Figure 40: ¹H NMR of N-benzyl-5-aminonaphthalene-1-sulfonamide in D₆-DMSO.

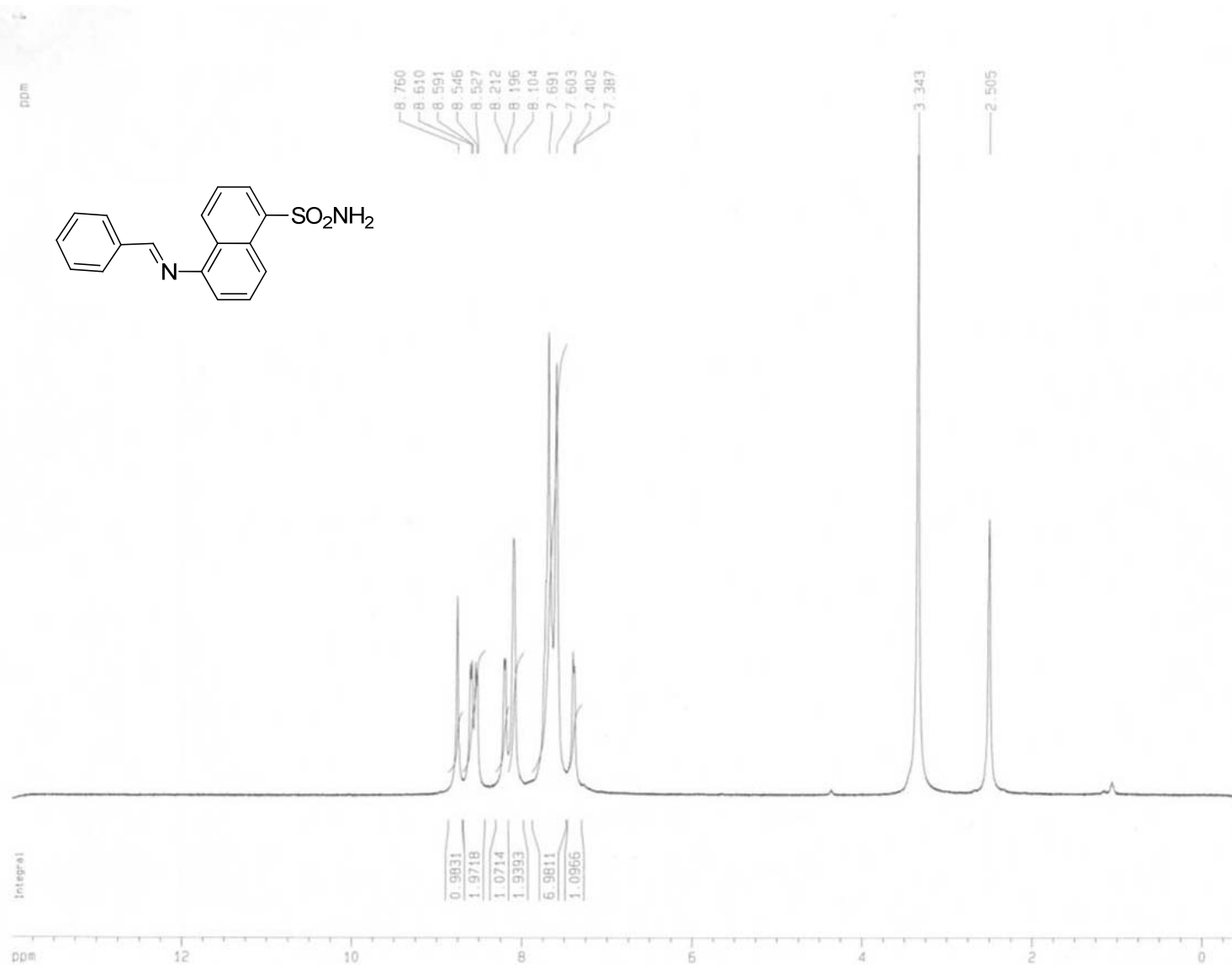


Figure 41: ¹H-NMR of N-benzylidene-5-aminonaphthalene-1-sulfonamide in D₆-DMSO.

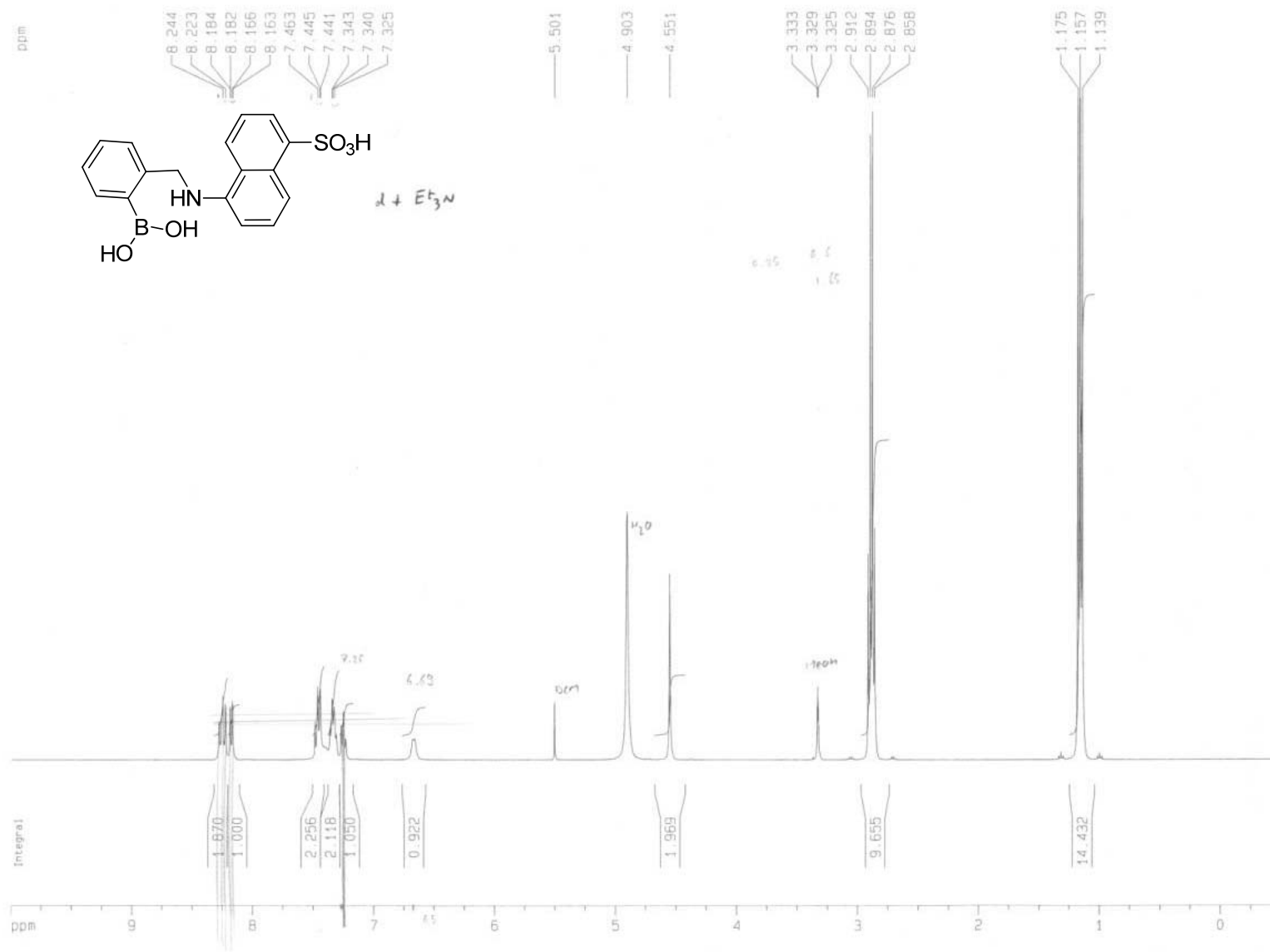


Figure 42: ¹H NMR of N-phenylborono-5-aminonaphthalene-1-sulfonic acid in CD₃OD+Et₃N.

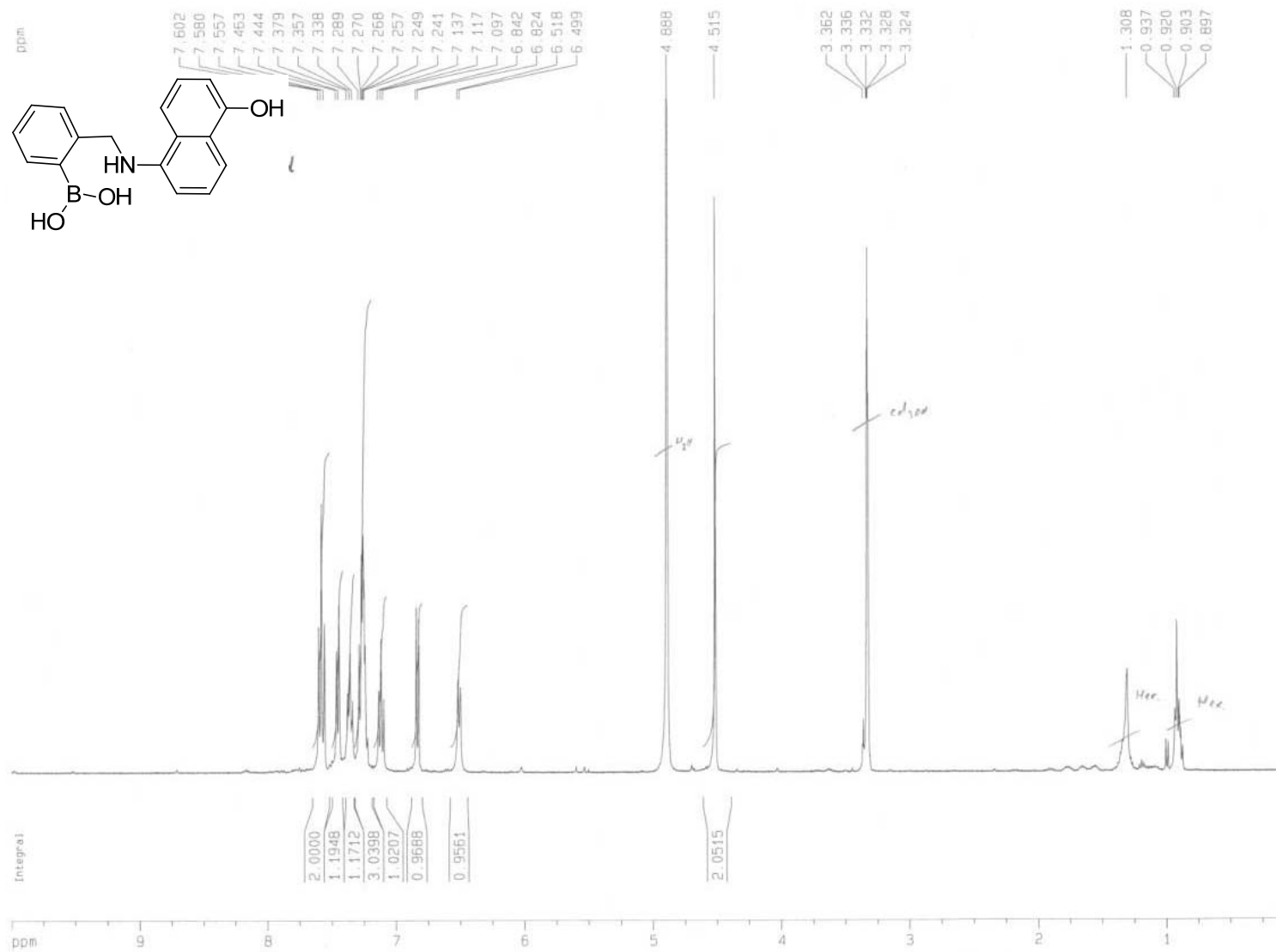


Figure 43: ^1H NMR of N-phenylborono-5-amino-1-naphthol in CD_3OD .

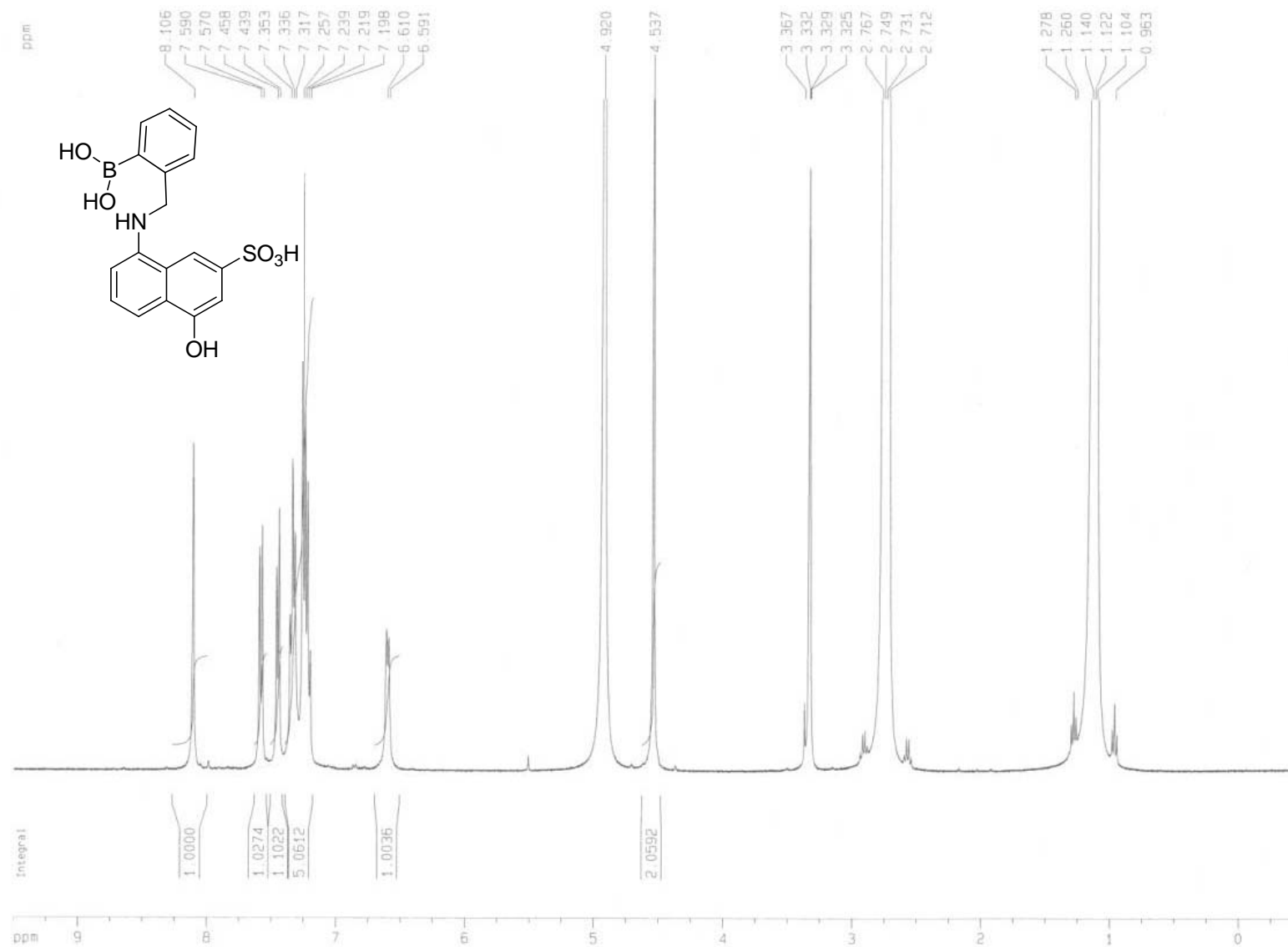


Figure 44: ¹H NMR of N-phenylborono-5-amino-1-naphthol-3-sulfonic acid in CD₃OD+Et₃N.

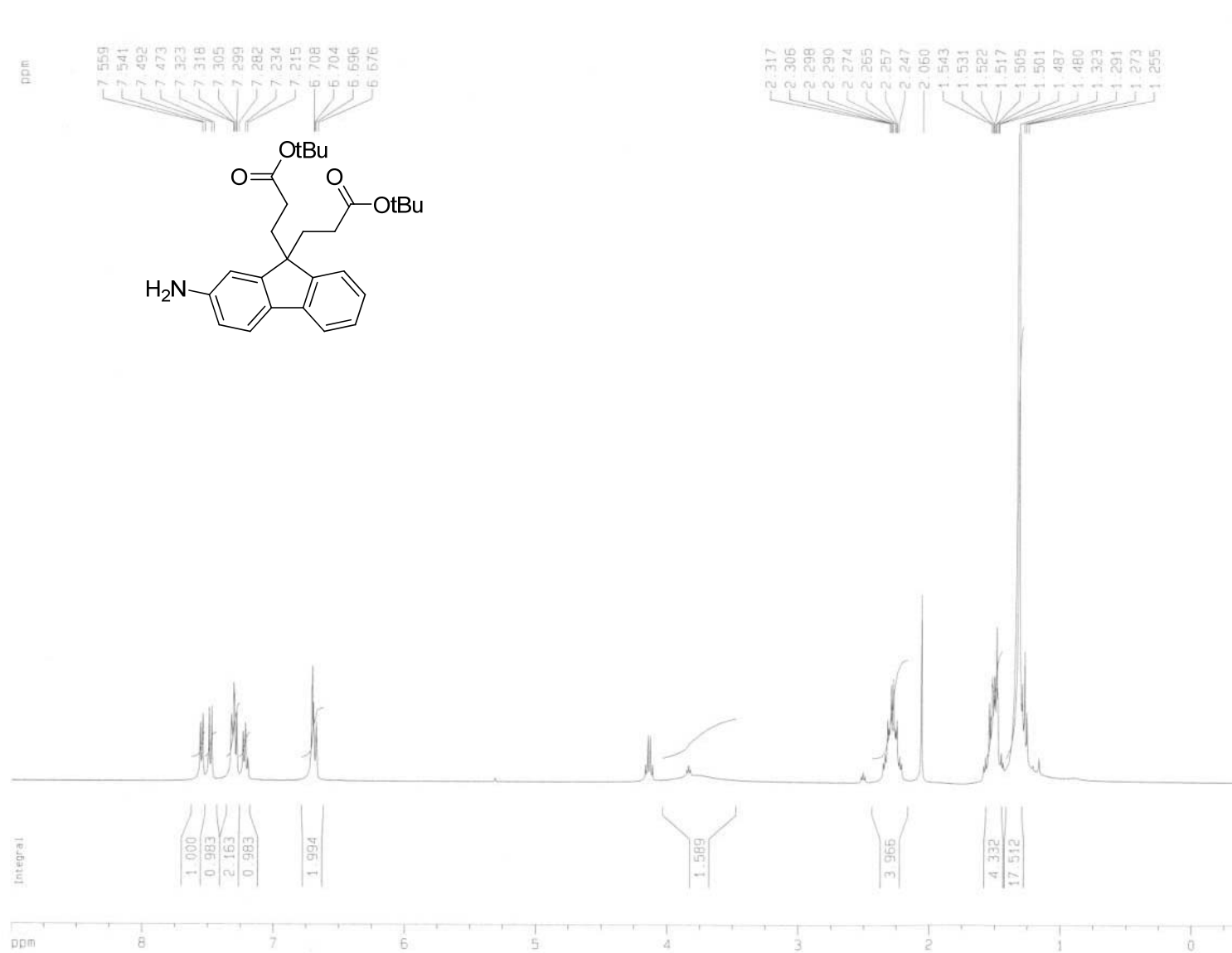


Figure 45: ¹H NMR of 'BuFluoHa in CDCl₃.

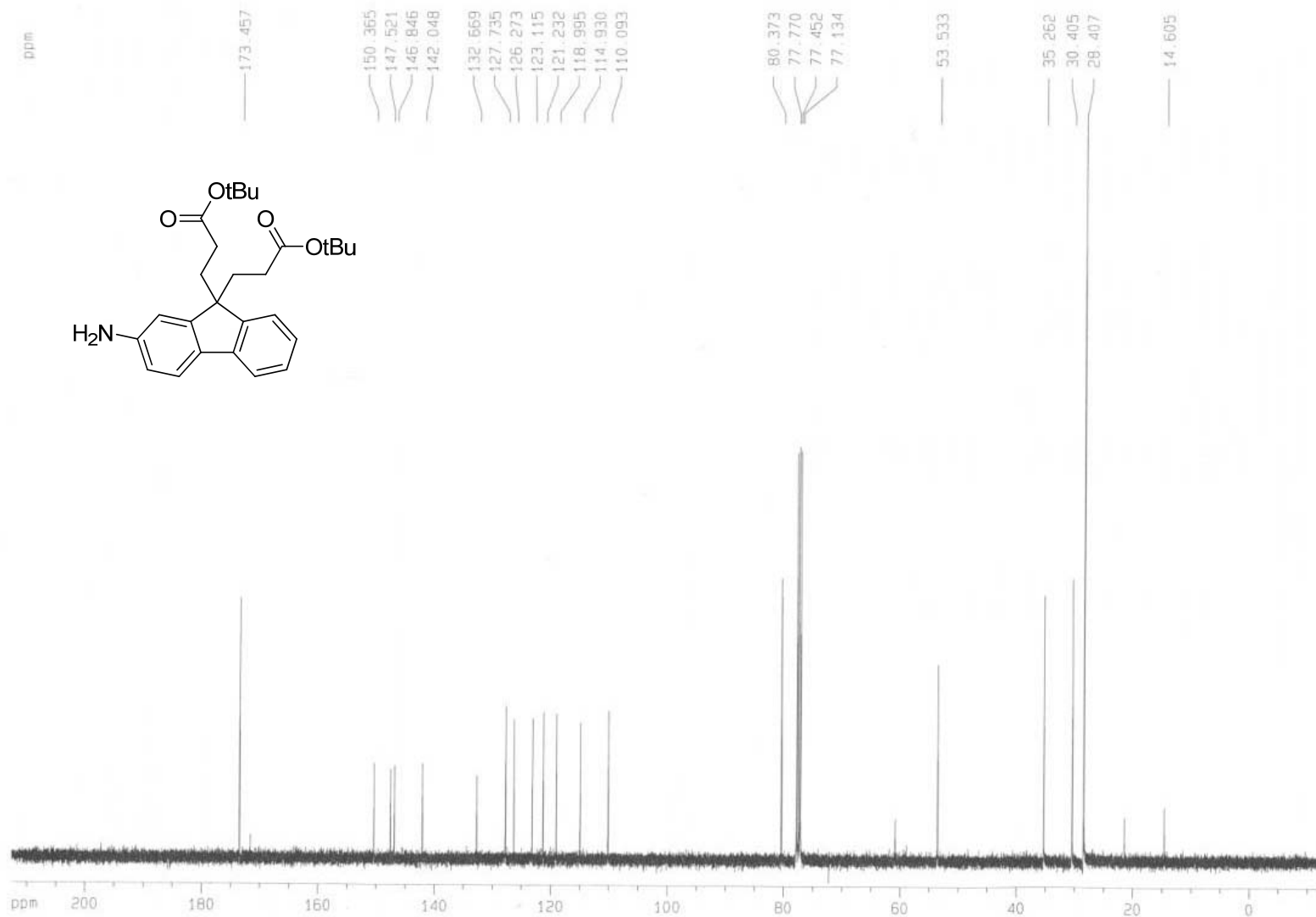


Figure 46: ¹³C NMR of 'BuFluoHa in CDCl₃.

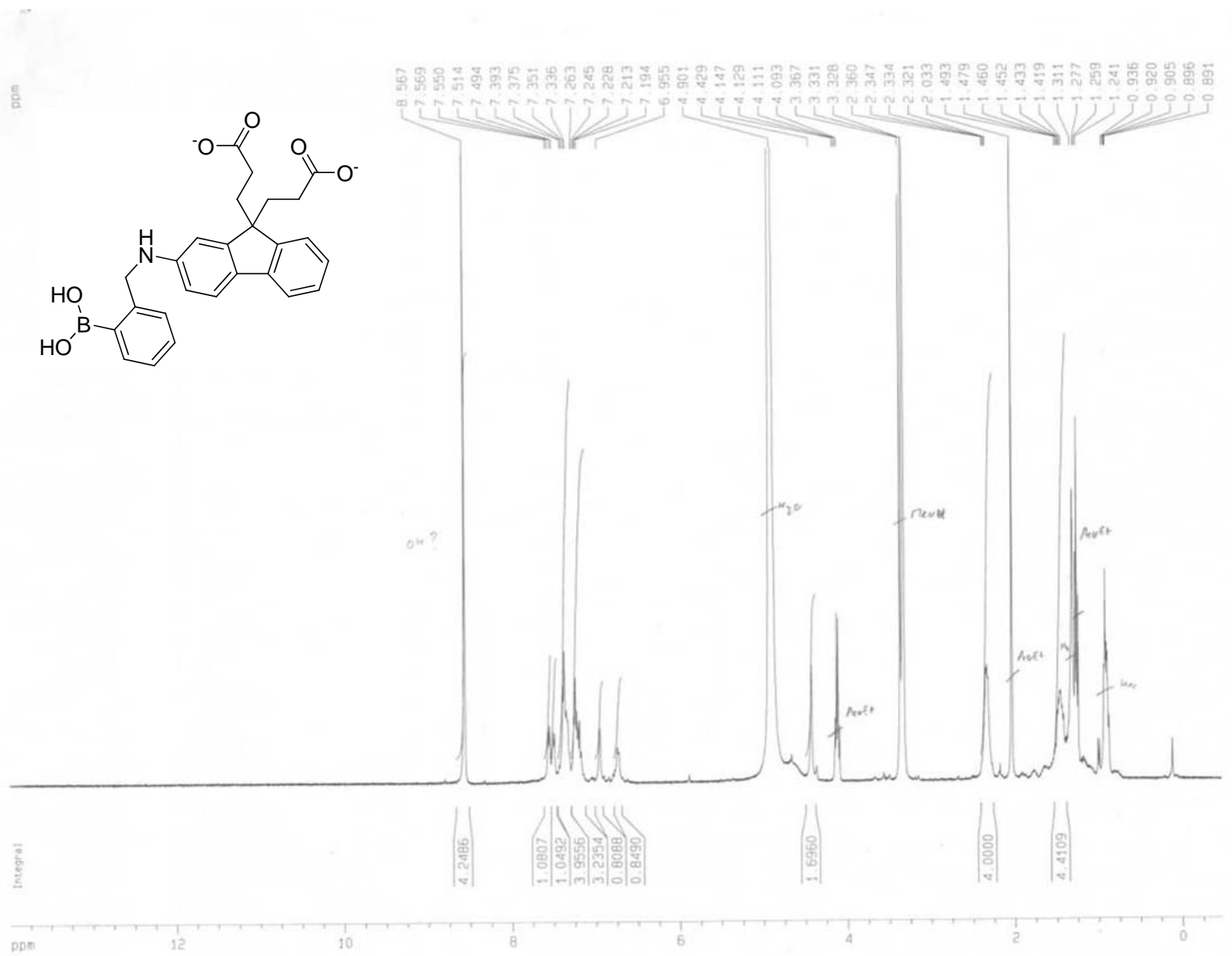


Figure 47: ¹H NMR of FluoHc in CD₃OD.



Figure 48: ¹H NMR of tBuFluoNH₂ in CDCl₃.

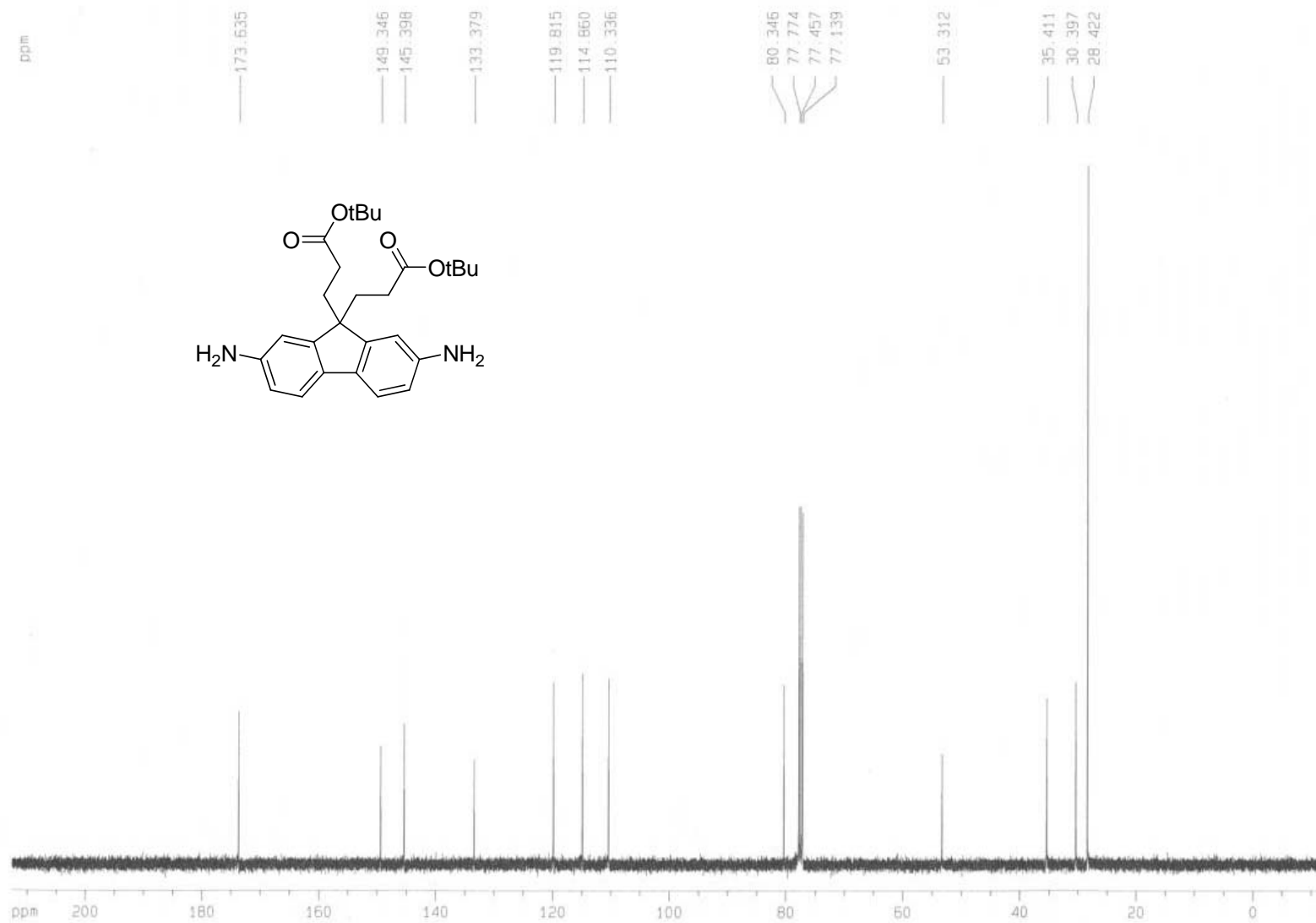


Figure 49: ^{13}C NMR of $t\text{BuFluoNH}_2\text{a}$ in CDCl_3 .

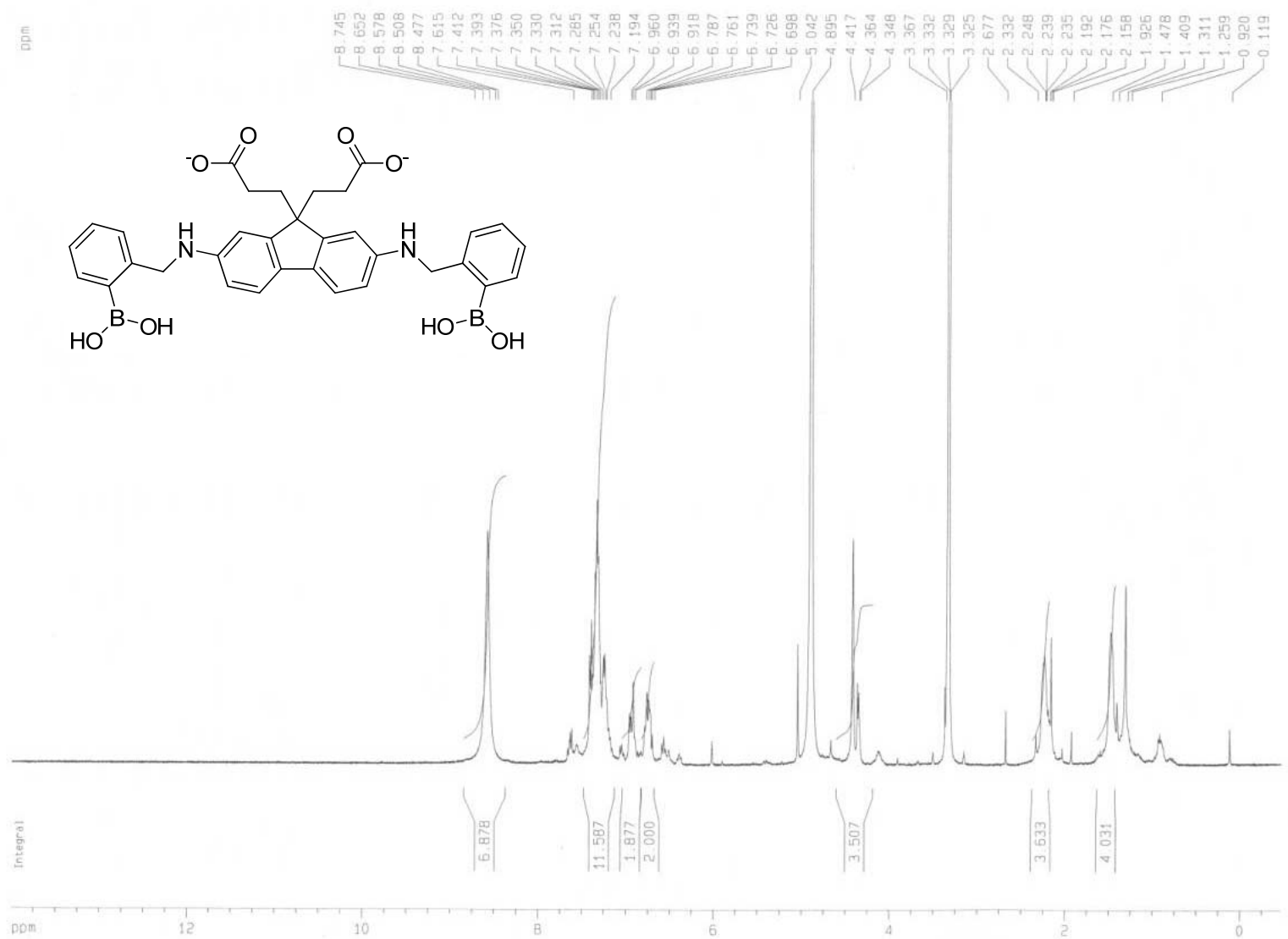


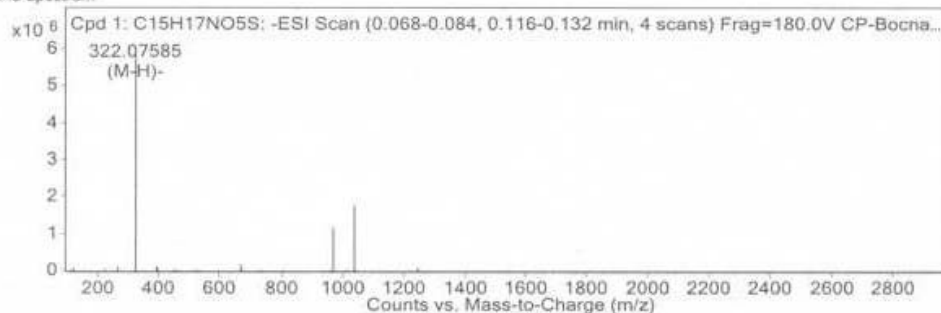
Figure 50: ¹H NMR of FluoNH₂c in CD₃OD.

Rapport d'analyse

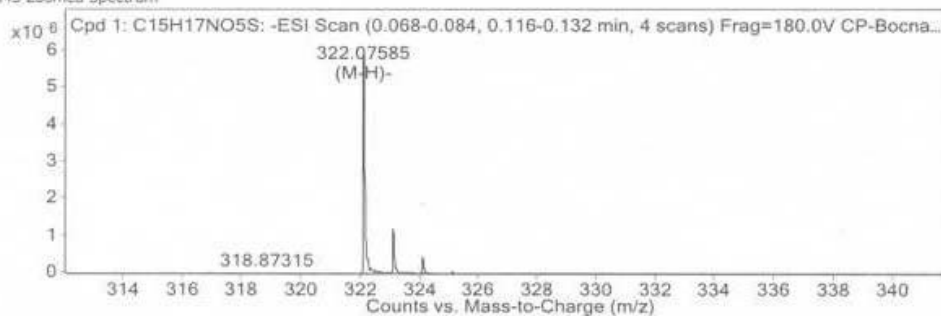
Data File CP-Bocnaphsulf_b.d **Sample Name** CP-Bocnaphsulf
Sample Type Sample **Position** P1-C6
Analysis Date 5/27/2010 1:56:05 PM **User Name** Marie-Christine
Acq Method ESI_NEG_DI.m **DA Method** ESI_NEG_DI.m

Comment

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M-H)-	C ₁₅ H ₁₆ N O ₅ S	6071560	322.07585	322.07547	1.19

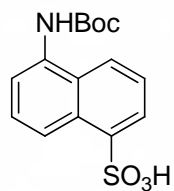


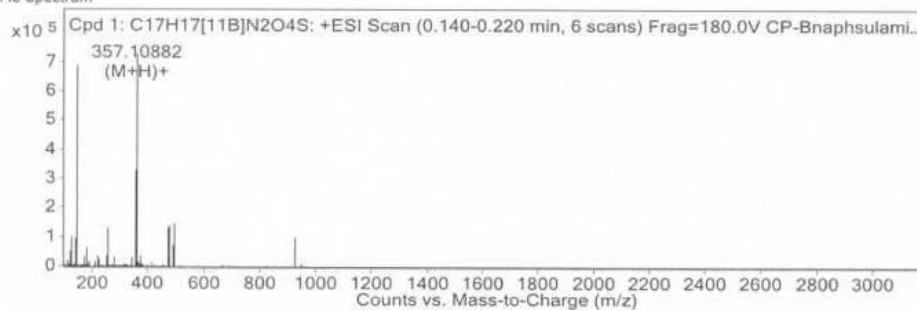
Figure 51: (-)ESI-HRMS analysis of N-Boc-5-aminonaphthalene-1-sulfonic acid.

Rapport d'analyse

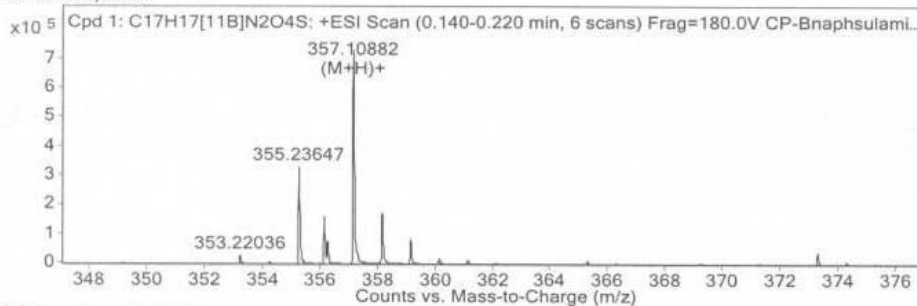
Data File CP-Bnaphsulamide.d **Sample Name** CP-Bnaphsulamide
Sample Type Sample **Position** P1-D1
Analysis Date 7/6/2010 12:24:35 PM **User Name** Marie-Christine
Acq Method ESI_POS_DI.m **DA Method** ESI_POS_DI.m

Comment

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M+H)+	C ₁₇ H ₁₈ [¹¹ B] N ₂ O ₄ S	734171	357.10882	357.10748	3.73

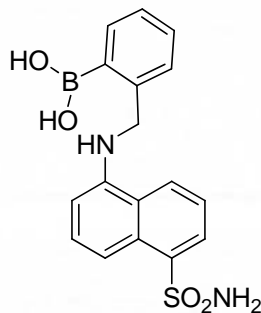
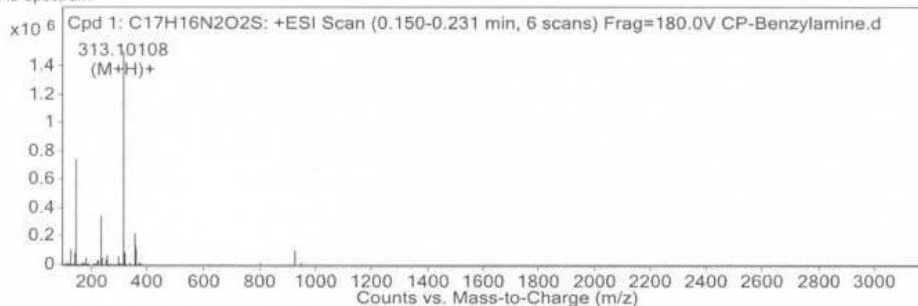


Figure 52: (+)ESI-HRMS of N-phenylborono-5-aminonaphthalene-1-sulfonamide.

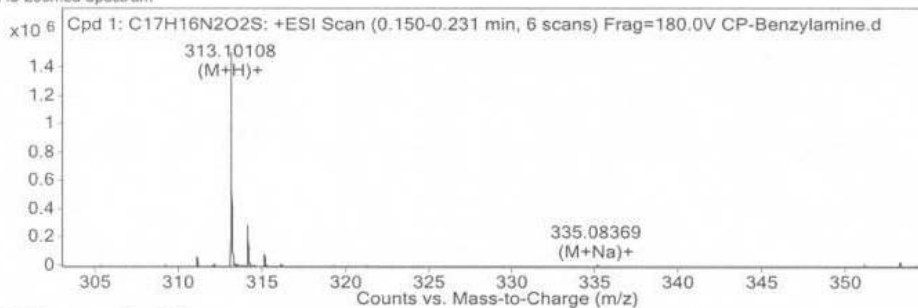
Rapport d'analyse

Data File CP-Benzylamine.d **Sample Name** CP-Benzylamine
Sample Type Sample **Position** P1-D4
Analysis Date 7/6/2010 12:29:44 PM **User Name** Marie-Christine
Acq Method ESI_POS_DI.m **DA Method** ESI_POS_DI.m
Comment

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M+H) ⁺	C ₁₇ H ₁₇ N ₂ O ₂ S	1503984	313.10108	313.10052	1.77
(M+Na) ⁺	C ₁₇ H ₁₆ N ₂ Na O ₂ S	16096	335.08369	335.08247	3.63

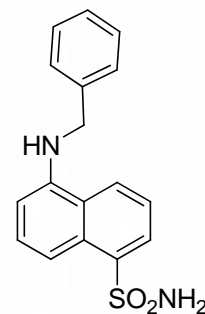


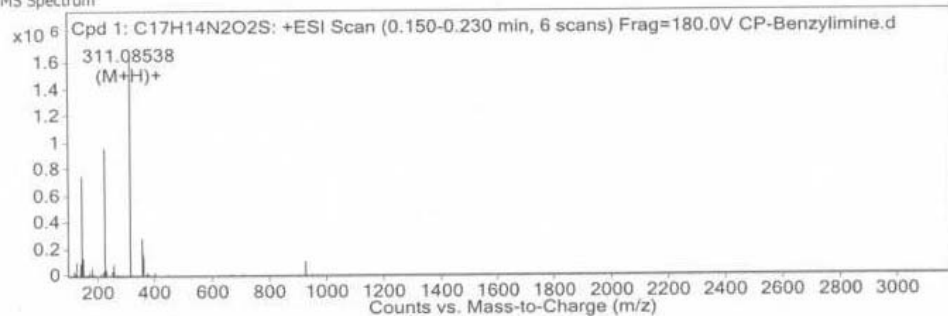
Figure 53: (+)ESI-HRMS of N-benzyl-5-aminonaphthalene-1-sulfonamide.

Rapport d'analyse

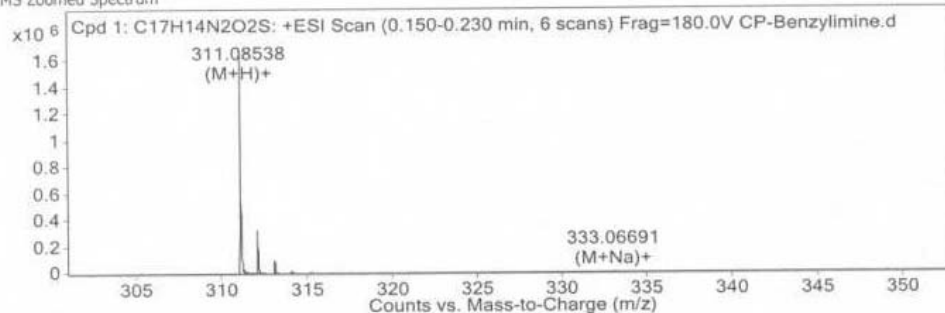
Data File CP-Benzylimine.d **Sample Name** CP-Benzylimine
Sample Type Sample **Position** P1-D3
Analysis Date 7/6/2010 12:28:01 PM **User Name** Marie-Christine
Acq Method ESI_POS_DI.m **DA Method** ESI_POS_DI.m

Comment

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M+H) ⁺	C ₁₇ H ₁₅ N ₂ O ₂ S	1653771	311.08538	311.08487	1.61
(M+Na) ⁺	C ₁₇ H ₁₄ N ₂ Na O ₂ S	11174	333.06691	333.06682	0.26

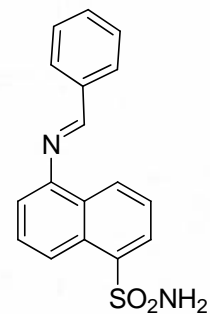
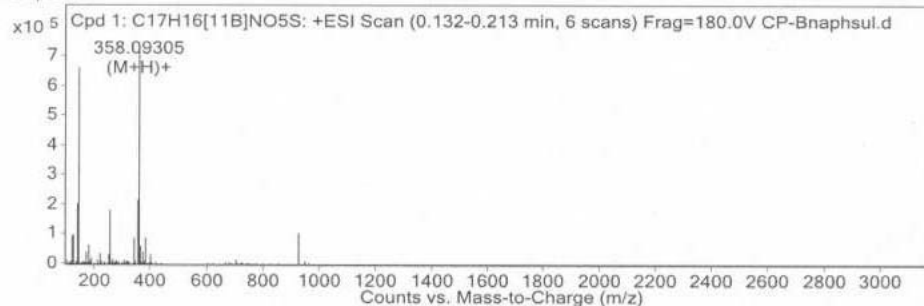


Figure 54: (+)ESI-HRMS of N-benzylidene-5-aminonaphthalene-1-sulfonamide.

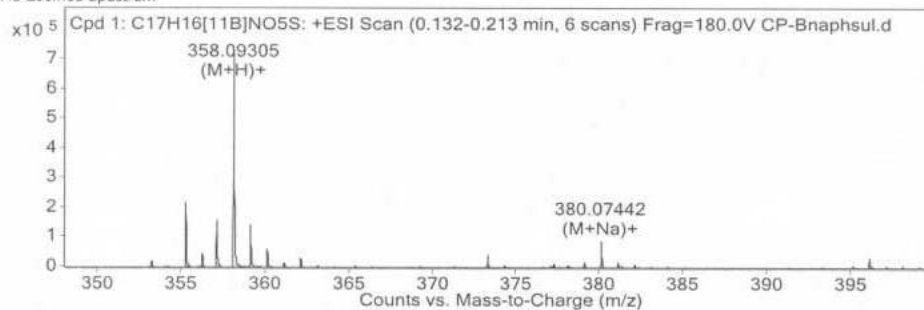
Rapport d'analyse

Data File CP-Bnaphsul.d **Sample Name** CP-Bnaphsul
Sample Type Sample **Position** P1-C9
Analysis Date 7/6/2010 12:22:53 PM **User Name** Marie-Christine
Acq Method ESI_POS_DI.m **DA Method** ESI_POS_DI.m
Comment

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M+H)+	C17 H17 [11B] N O5 S	725398	358.09305	358.0915	4.34
(M+Na)+	C17 H16 [11B] N Na O5 S	88567	380.07442	380.07344	2.57

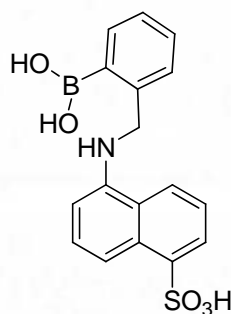


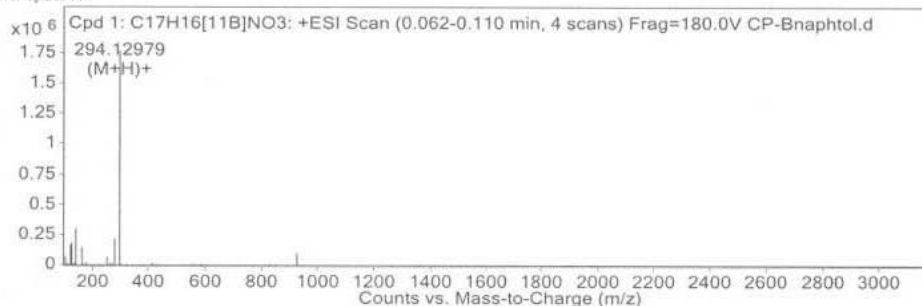
Figure 55: (+)ESI-HRMS of N-phenylborono-5-aminonaphthalene-1-sulfonic acid.

Rapport d'analyse

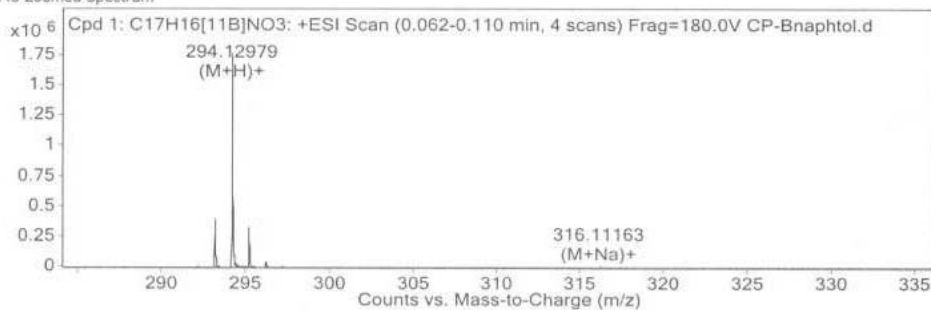
Data File	CP-Bnaphtol.d	Sample Name	CP-Bnaphtol
Sample Type	Sample	Position	P1-C5
Analysis Date	5/27/2010 1:44:39 PM	User Name	Marie-Christine
Acq Method	ESI_POS_DI.m	DA Method	ESI_POS_DI.m

Comment

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M+H) ⁺	C ₁₇ H ₁₇ [¹¹ B]N O ₃	1768149	294.12979	294.1296	0.63
(M+Na) ⁺	C ₁₇ H ₁₆ [¹¹ B]N Na O ₃	13160	316.11163	316.11154	0.27

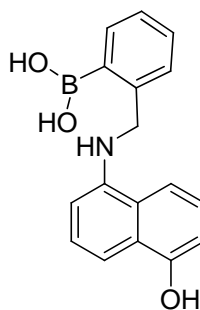
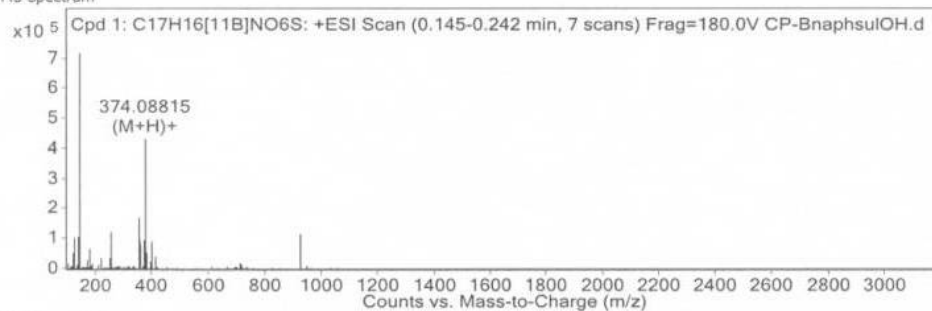


Figure S6: (+)ESI-HRMS of N-phenylborono-5-amino-1-naphthol.

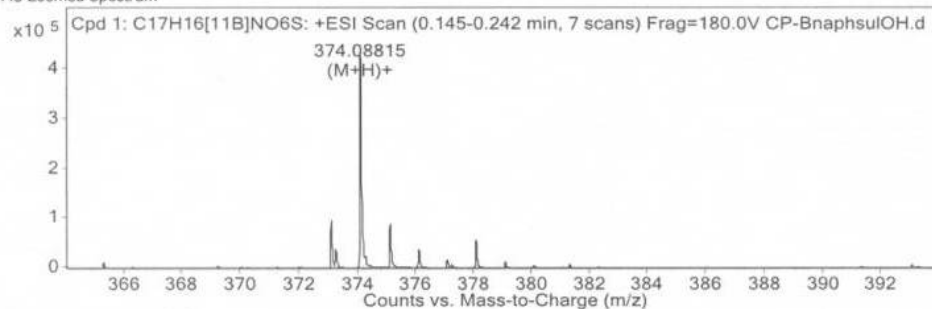
Rapport d'analyse

Data File CP-BnaphsulOH.d **Sample Name** CP-BnaphsulOH
Sample Type Sample **Position** P1-D2
Analysis Date 7/6/2010 12:26:19 PM **User Name** Marie-Christine
Acq Method ESI_POS_DI.m **DA Method** ESI_POS_DI.m
Comment

MS Spectrum

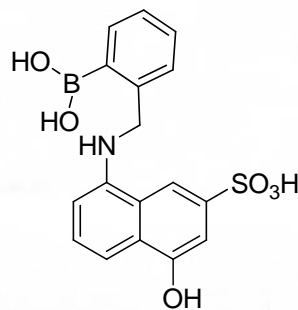


MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M+H)+	C17 H17 [11B] N O6 S	442257	374.08815	374.08641	4.64



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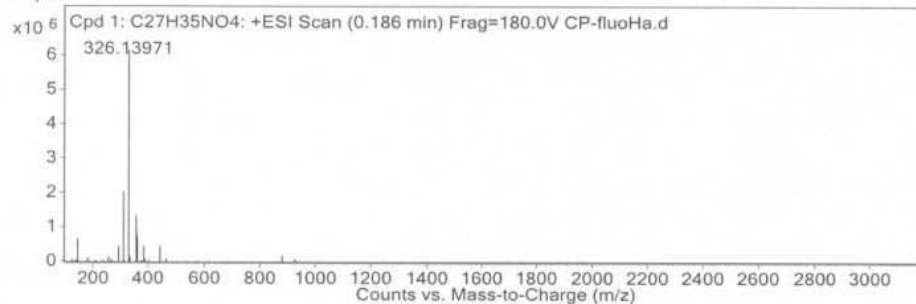
Page 1 of 1

Figure 57: (+)ESI-HRMS of N-phenylborono-5-amino-1-naphthol-3-sulfonic acid.

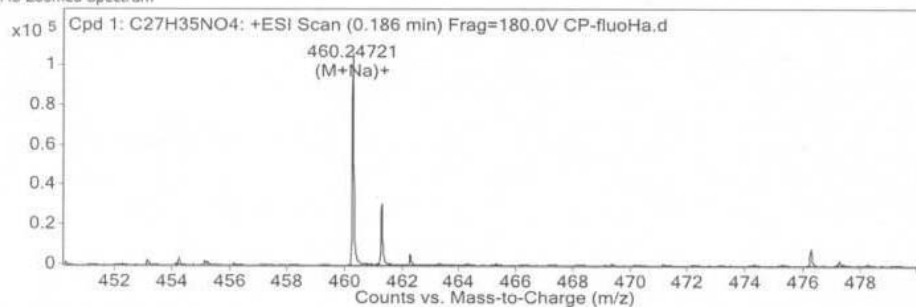
Rapport d'analyse

Data File CP-fluoHa.d **Sample Name** CP-fluoHa
Sample Type Sample **Position** P1-C5
Analysis Date 7/6/2010 12:15:57 PM **User Name** Marie-Christine
Acq Method ESI_POS_DI.m **DA Method** ESI_POS_DI.m
Comment

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M+Na)+	C27 H35 N Na O4	107045	460.24721	460.24583	3

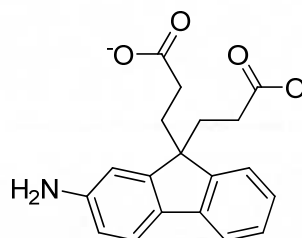


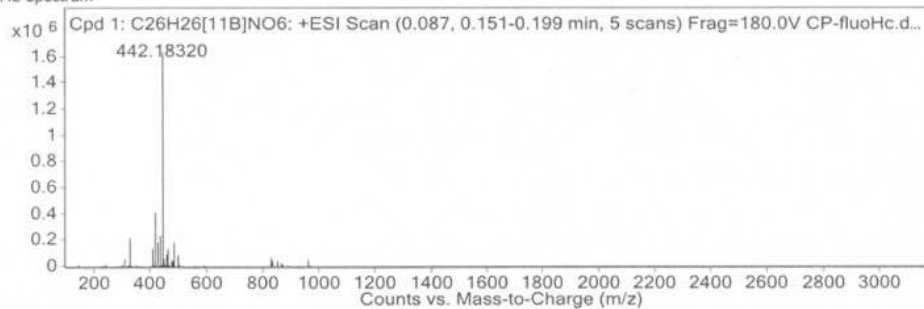
Figure 58: (+)ESI-HRMS of FluoHa.

Rapport d'analyse

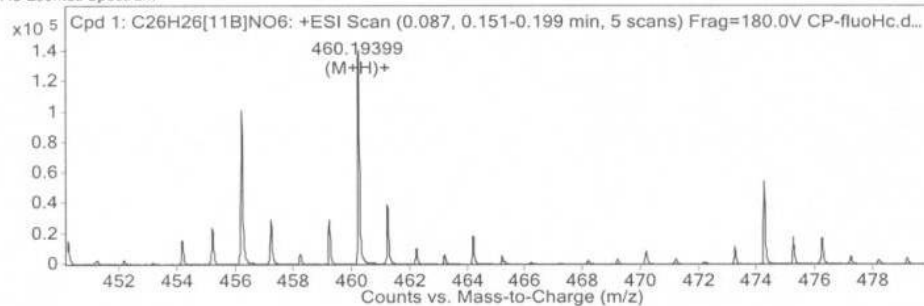
Data File CP-fluoHc.d **Sample Name** CP-fluoHc
Sample Type Sample **Position** P1-F6
Analysis Date 7/23/2010 11:34:48 AM **User Name** Marie-Christine
Acq Method ESI_POS_DI.m **DA Method** ESI_POS_DI.m

Comment

MS Spectrum

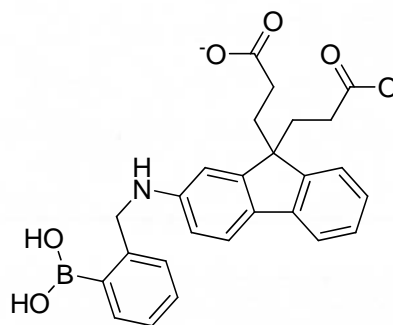


MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M+H)+	C26 H27 [11B] N O6	142073	460.19399	460.19259	3.02



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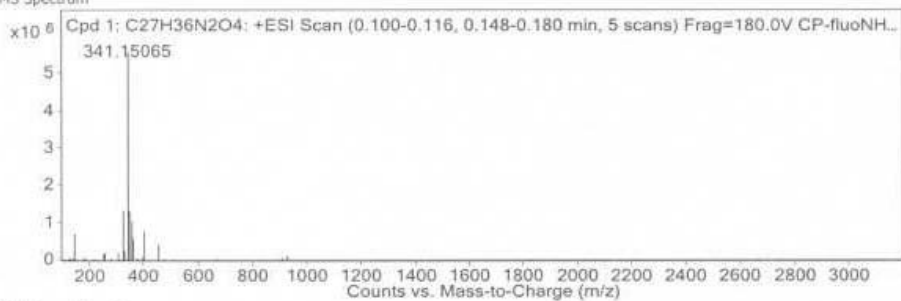
Figure 59: (+)ESI-HRMS of FluoHc.

Rapport d'analyse

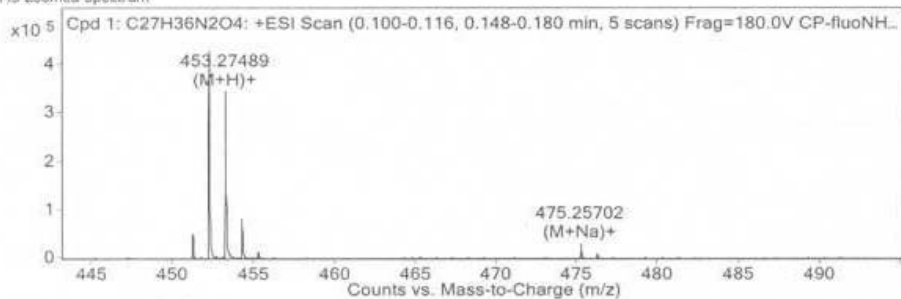
Data File	CP-fluoNH2a.d	Sample Name	CP-fluoNH2a
Sample Type	Sample	Position	P1-C6
Analysis Date	7/6/2010 12:17:41 PM	User Name	Marie-Christine
Acq Method	ESI_POS_DI.m	DA Method	ESI_POS_DI.m

Comment

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M+H)+	C27 H37 N2 O4	350549	453.27489	453.27478	0.24
(M+Na)+	C27 H36 N2 Na O4	29882	475.25702	475.25673	0.62

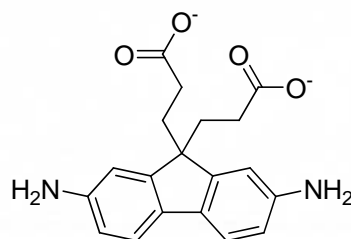
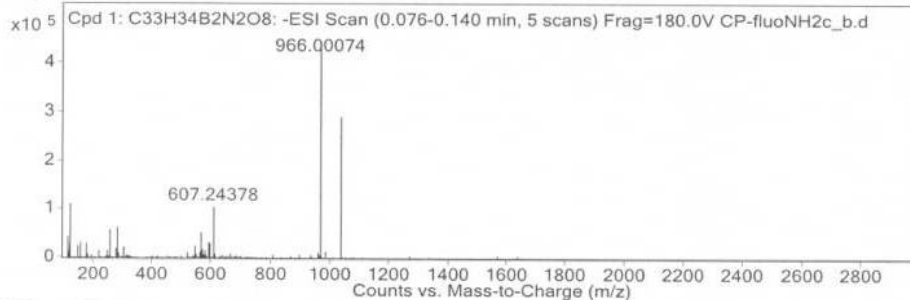


Figure 60: (+)ESI-HRMS of FluoNH2a.

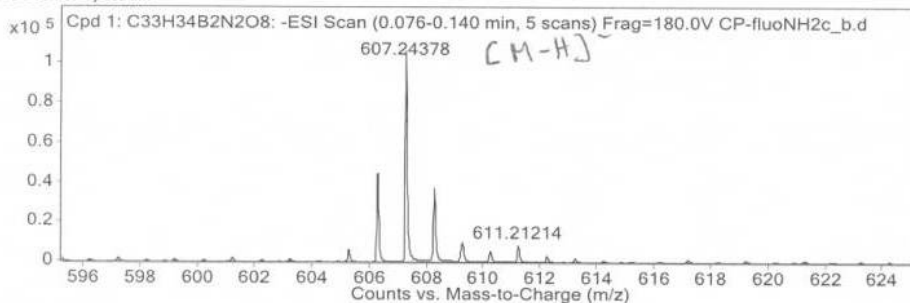
Rapport d'analyse

Data File CP-fluoNH2c_b.d **Sample Name** CP-fluoNH2c
Sample Type Sample **Position** P1-D2
Analysis Date 8/9/2010 12:10:06 PM **User Name** KV
Acq Method ESI_NEG_DI.m **DA Method** ESI_NEG_DI.m
Comment

MS Spectrum



MS Zoomed Spectrum



MS Spectrum Peak List

Ion	Ion Formula	Abund	Expe. m/z	Calc. m/z	Diff(ppm)
(M-H)-	C33 H33 B2 N2 O8	6461	605.2472	605.25011	-4.82

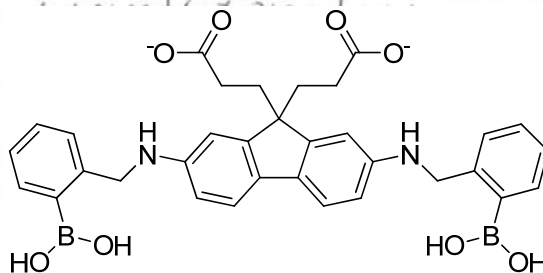


Figure 61: (-)ESI-HRMS of FluoHc.

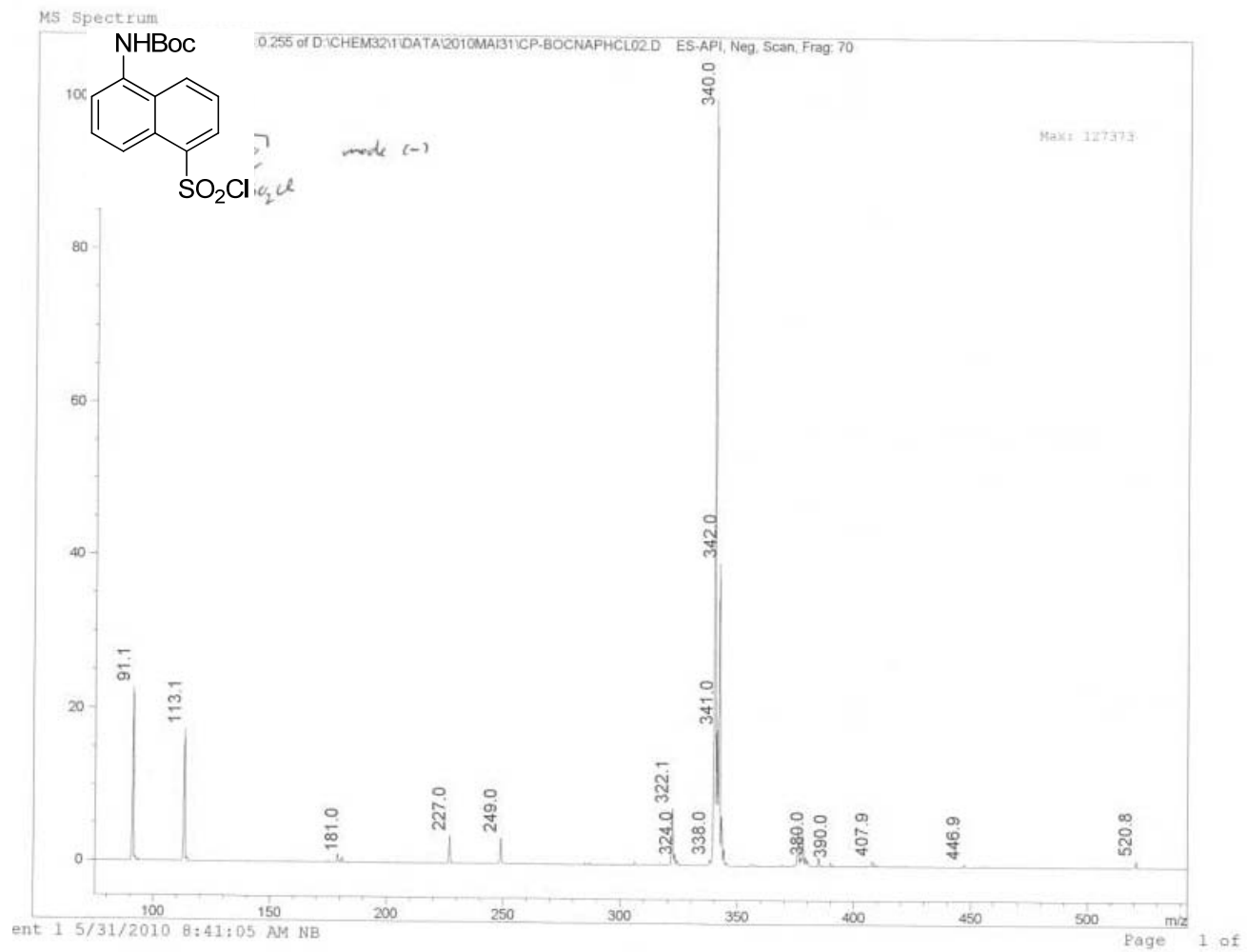


Figure 62: (-)ESI-MS N-Boc-5-aminonaphthalene-1-sulfonyl chloride.

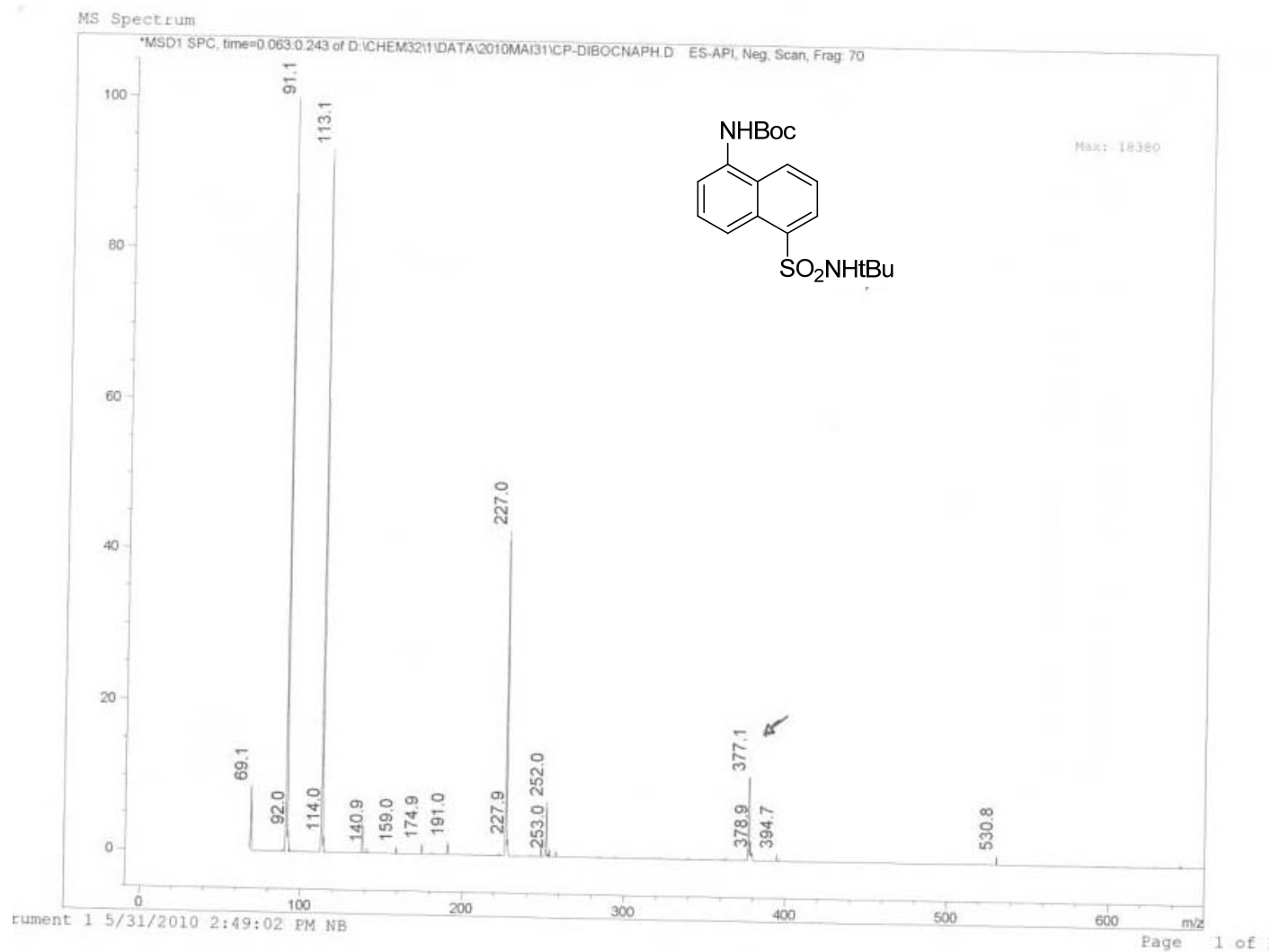


Figure 63: (-)ESI-MS of N-Boc-5-aminonaphthalene-1-*tert*-butylsulfonamide.

Print of window 80: MS Spectrum

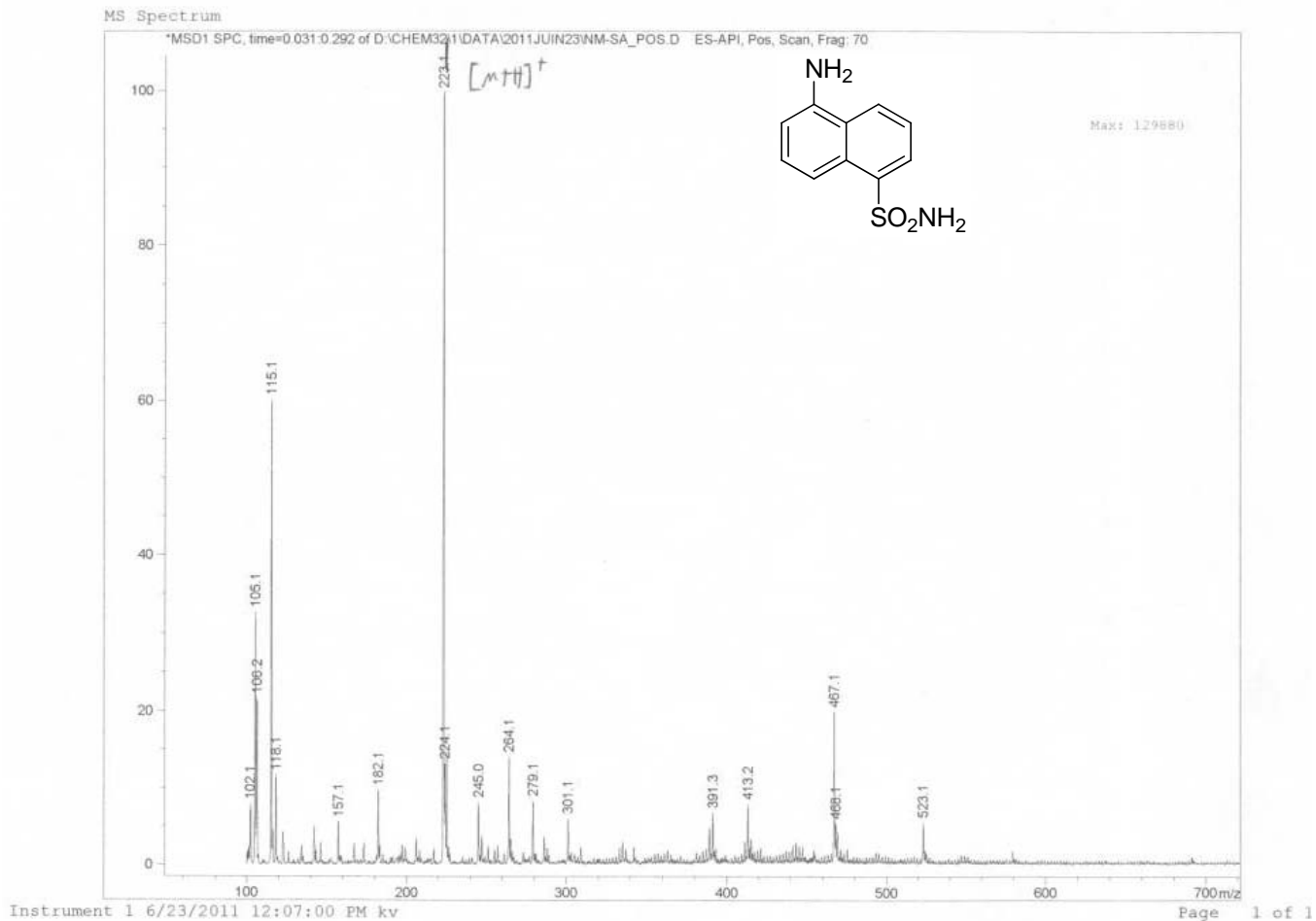


Figure 64: (-)ESI-MS of 5-aminonaphthalene-1-sulfonamide.

Print of window 80: MS Spectrum

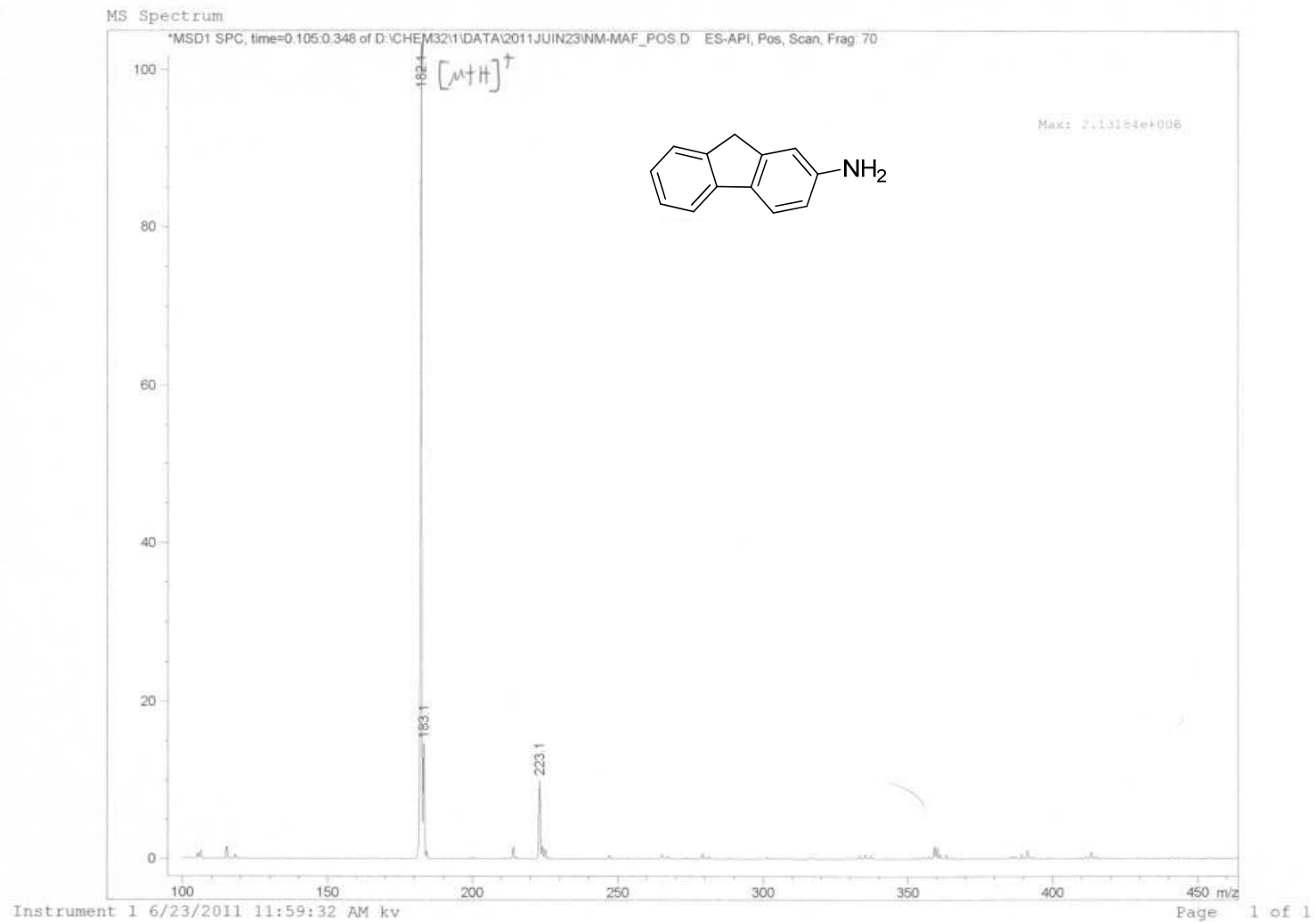


Figure 65: (+)ESI-MS of monoaminofluorene.

Print of window 80: MS Spectrum

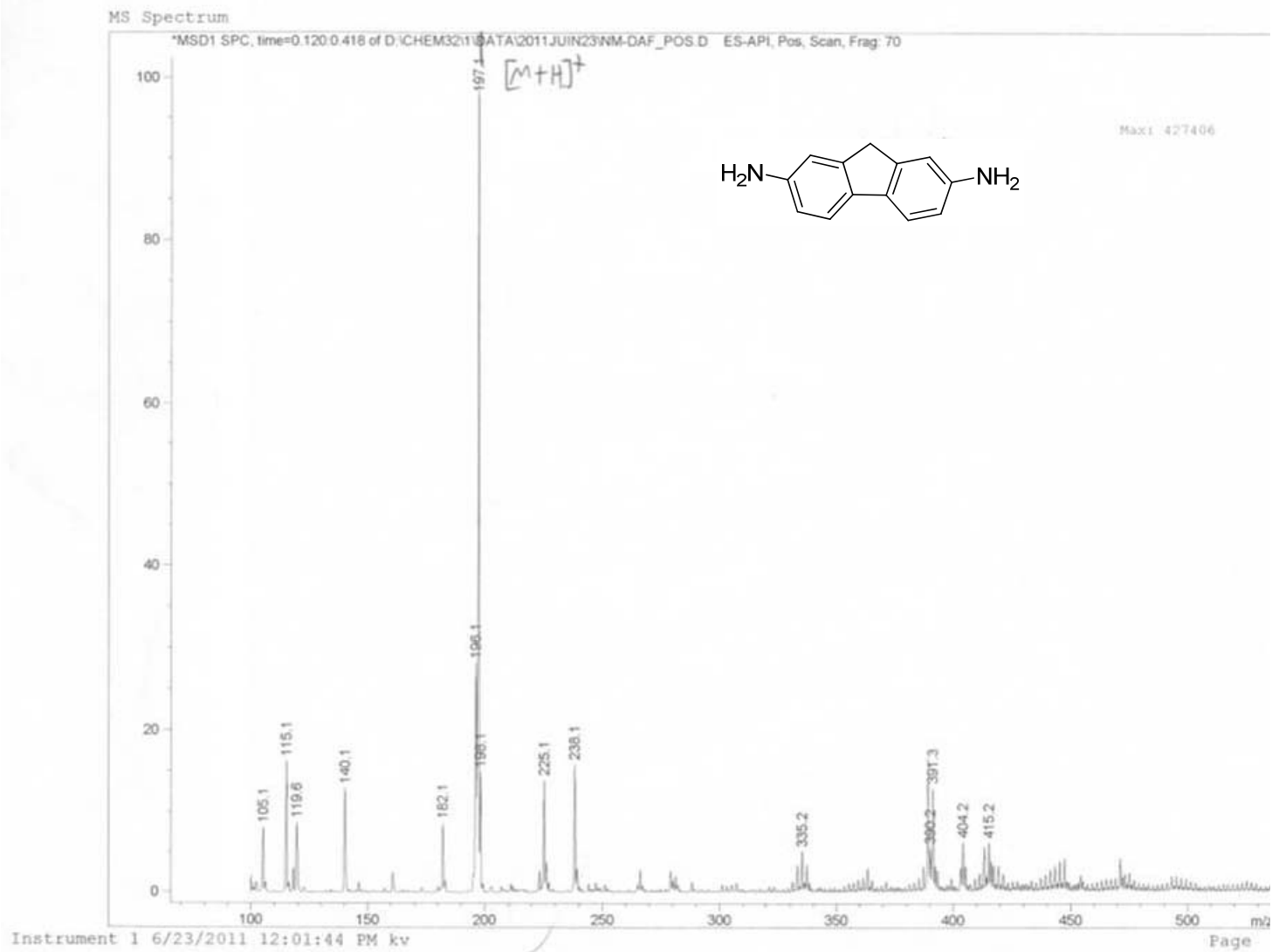


Figure 66: (+)ESI-MS of diaminofluorene.

rint of window 80: MS Spectrum

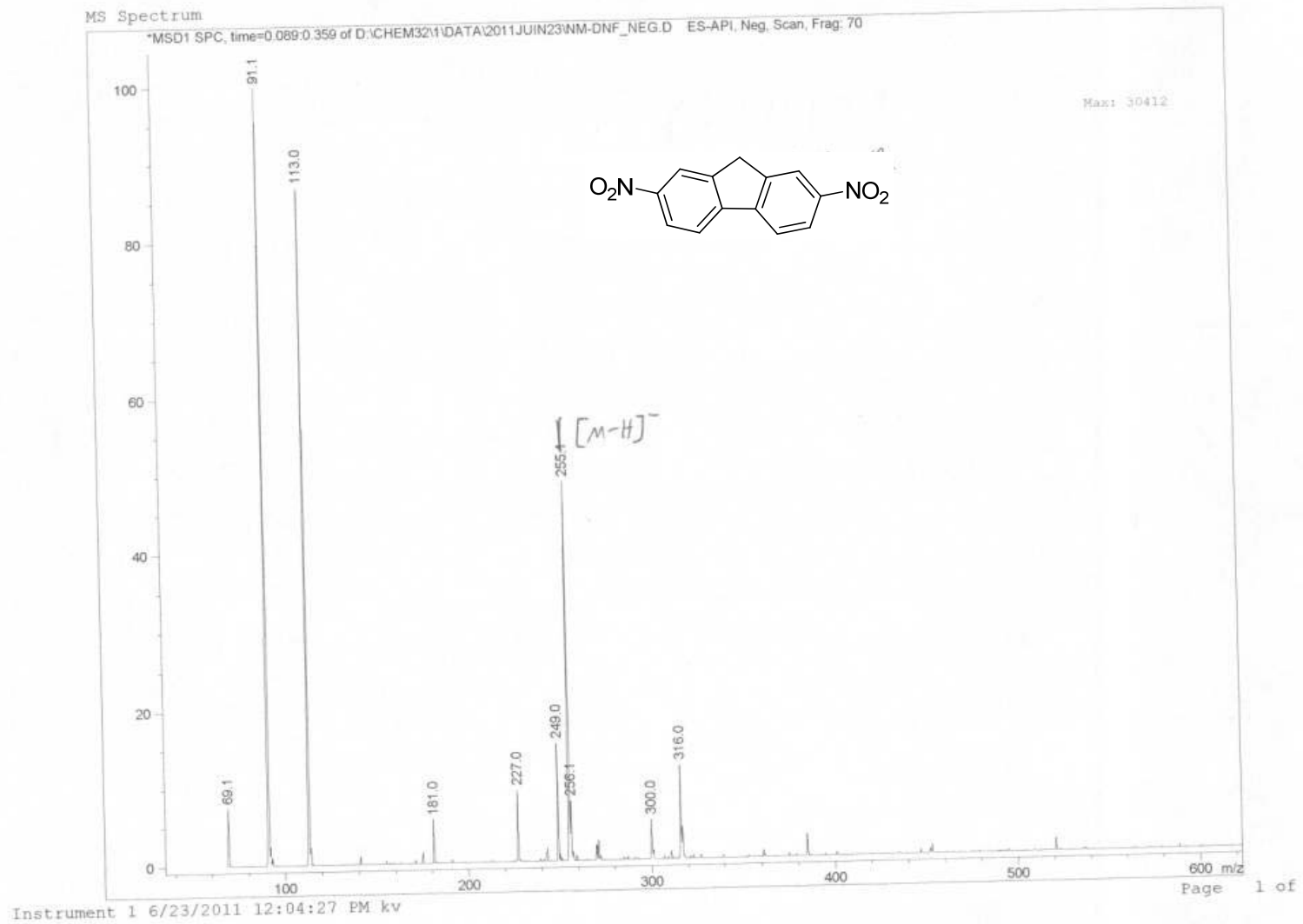


Figure 67: (-)ESI-MS of dinitrofluorene.