# Supporting Information

# Brominated Boron Dipyrrins: Synthesis, Structure, Spectral and Electrochemical Properties

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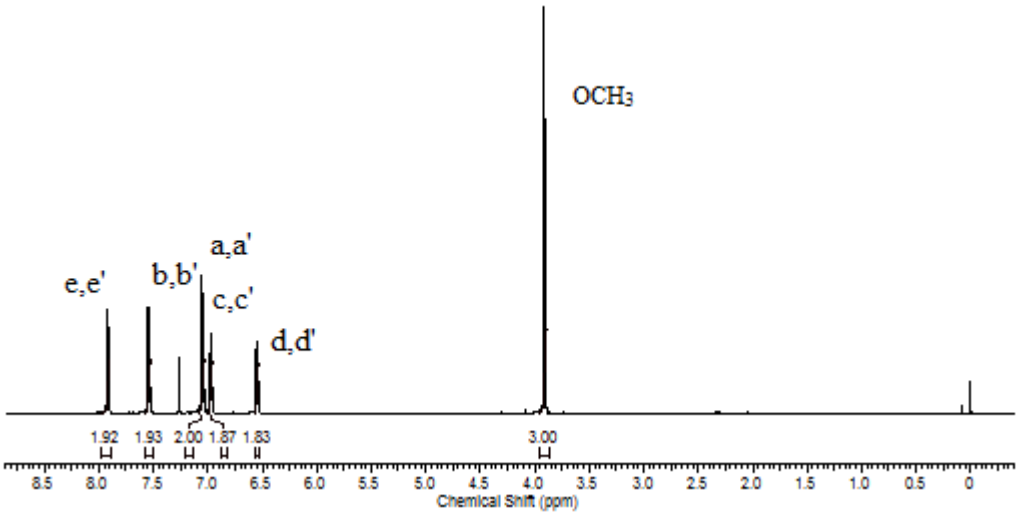



**Figure 1:** $^{1}$H NMR spetrum of compound **8** recorded in $CDCl_3$.

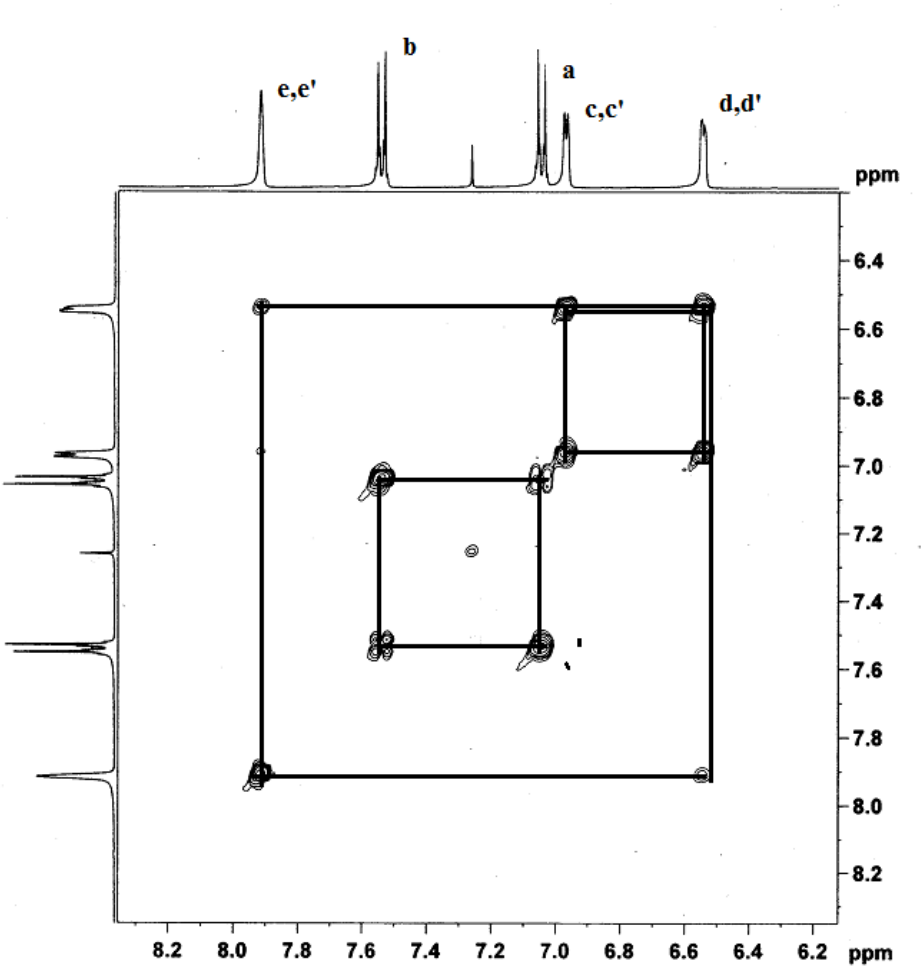
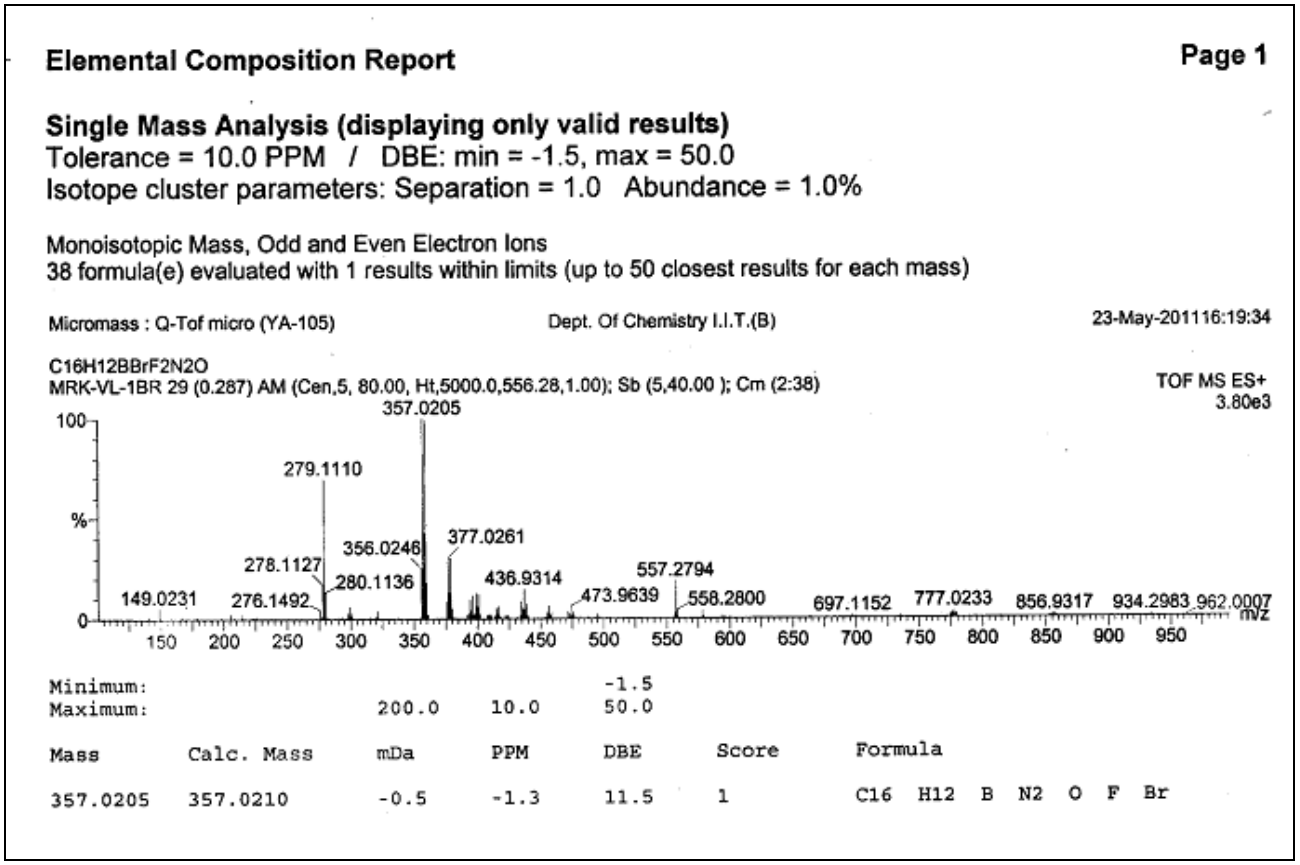



**Figure 2:** $^{1}$H-$^{1}$H correlation spectrum of comppound **8** recorded in $CDCl_3$.



**Elemental Composition Report** Page 1

**Single Mass Analysis (displaying only valid results)**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
38 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 23-May-201116:19:34

C16H12BBrF2N2O
MRK-VL-1BR 29 (0.287) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sb (5,40.00 ); Cm (2:38) TOF MS ES+ 3.80e3



| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 357.0205 | 357.0210 | -0.5 | -1.3 | 11.5 | 1 | C16 H12 B N2 O F Br |

**Figure 3:** HRMS mass spectrum of compound **1**.

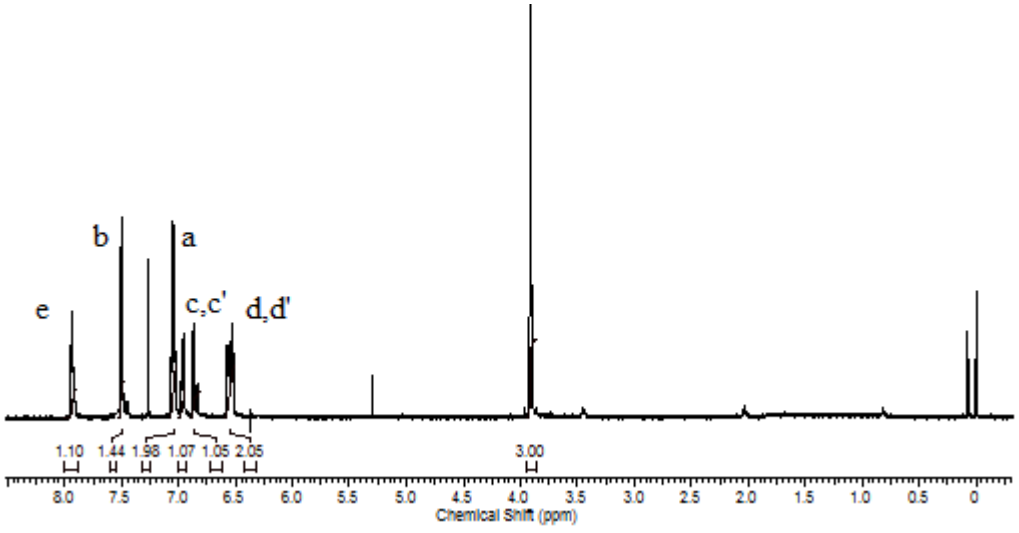




**Figure 4:** $^{1}$H NMR spectrum of compound **1** recorded in $CDCl_3$ ($\delta$ in ppm).

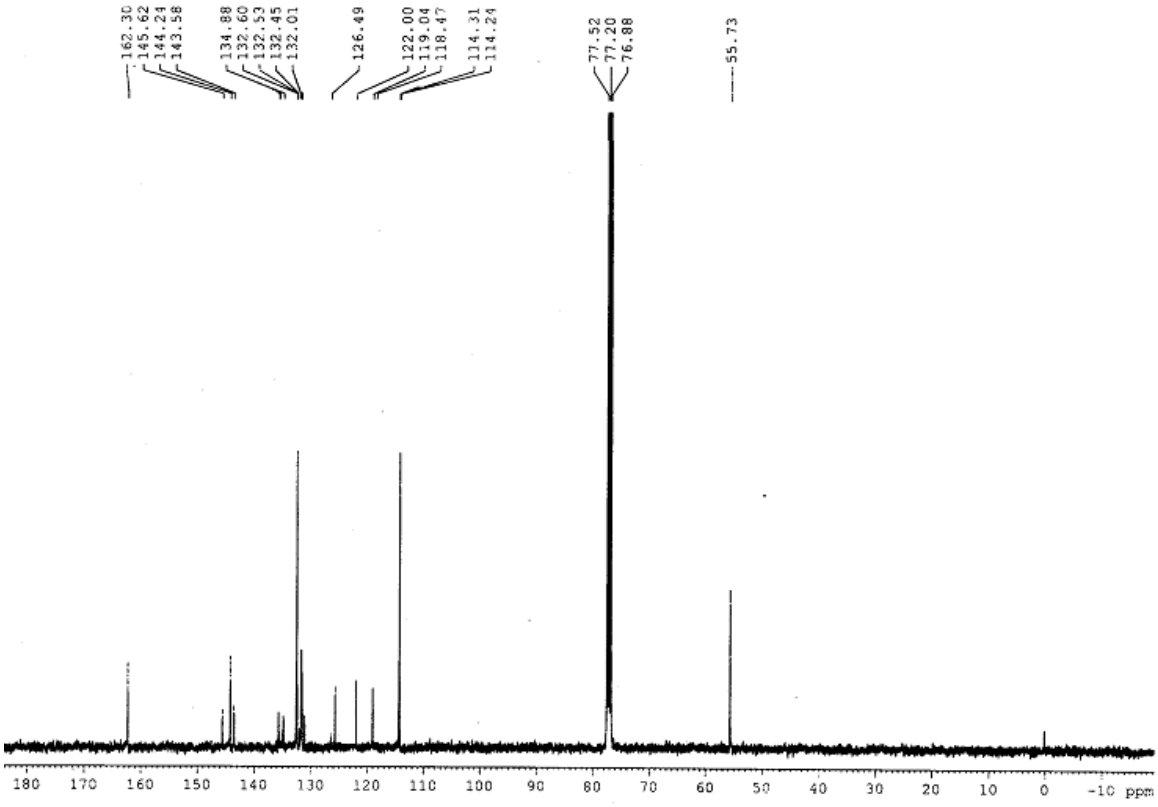



**Figure 5:** $^{13}C$ NMR spectrum of compound **1** recorded in $CDCl_3$ (δ in ppm).

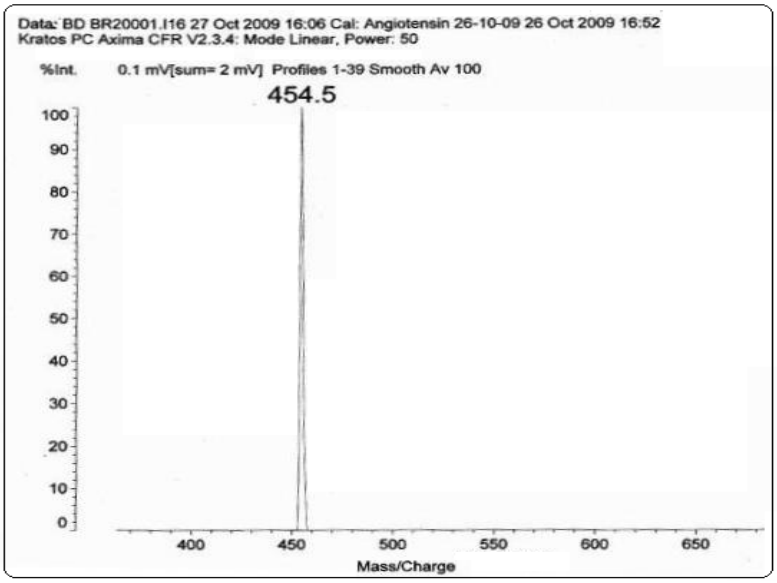



**Figure 6:** MALDI-TOF mass spectrum for compound **2**.

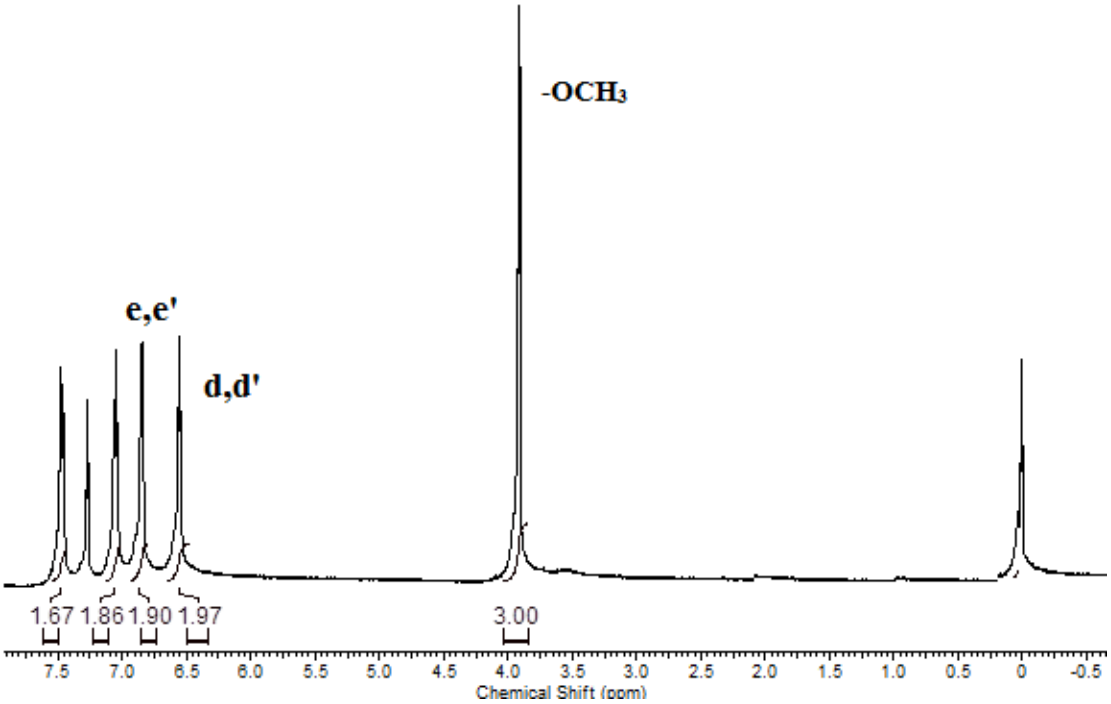



**Figure 7:** $^{1}$H NMR spectrum of compound **2** recorded in $CDCl_3$ (δ in ppm).

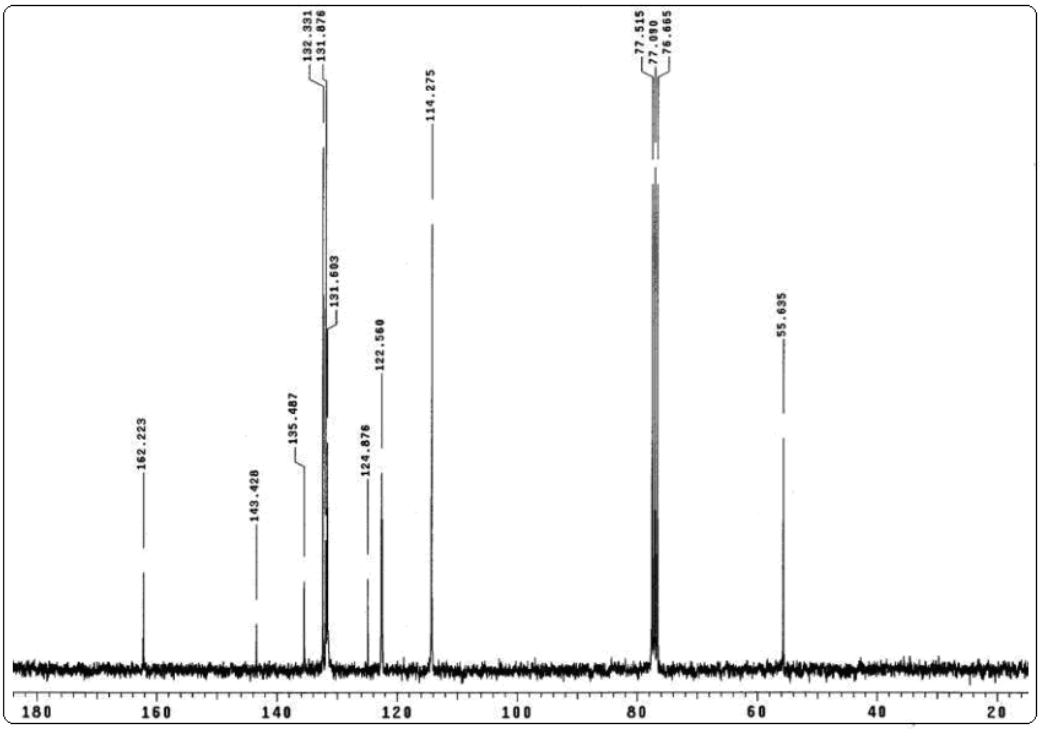



**Figure 8:** $^{13}C$ NMR spectrum of compound **2** recorded in $CDCl_3$ (δ in ppm).

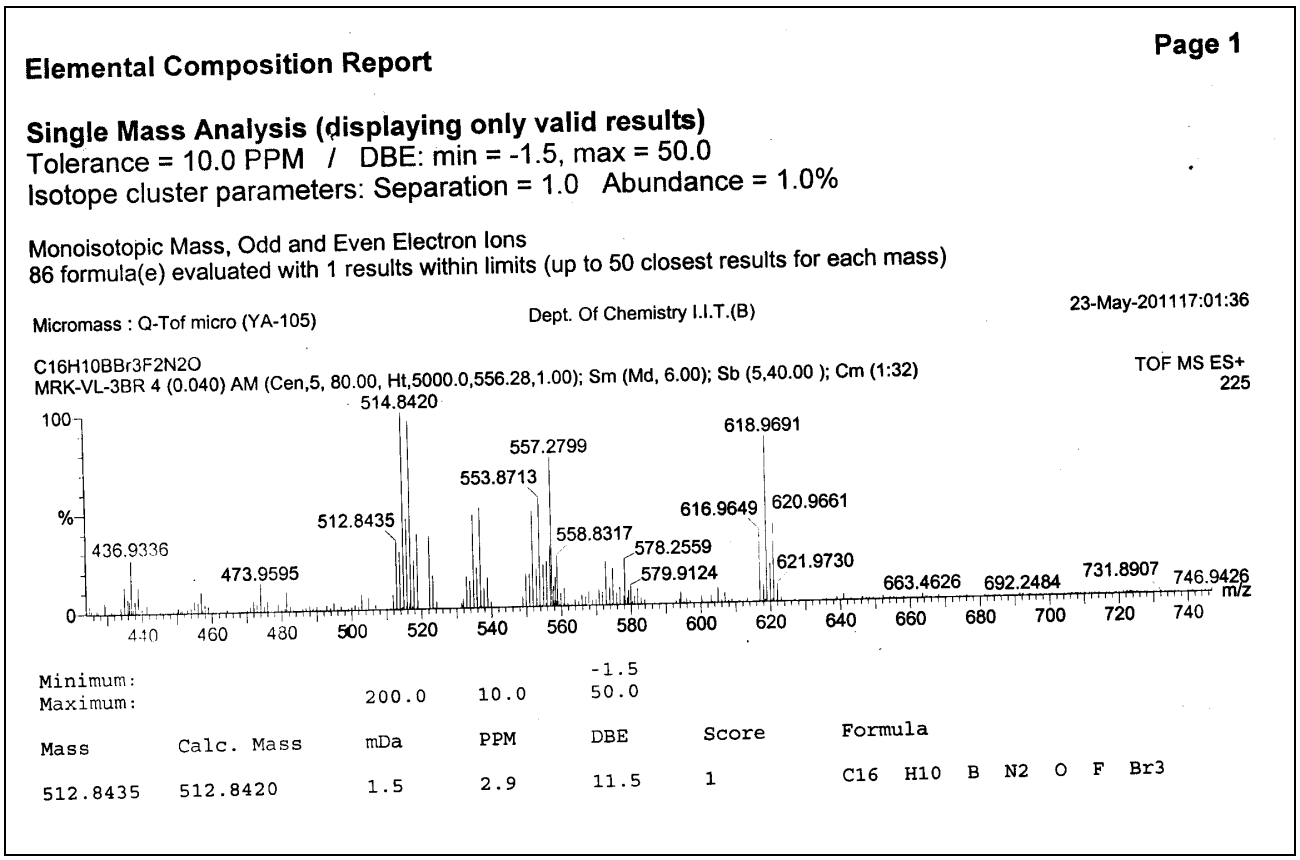



**Figure 9:** HR-MS mass spectrum of compound **3**.

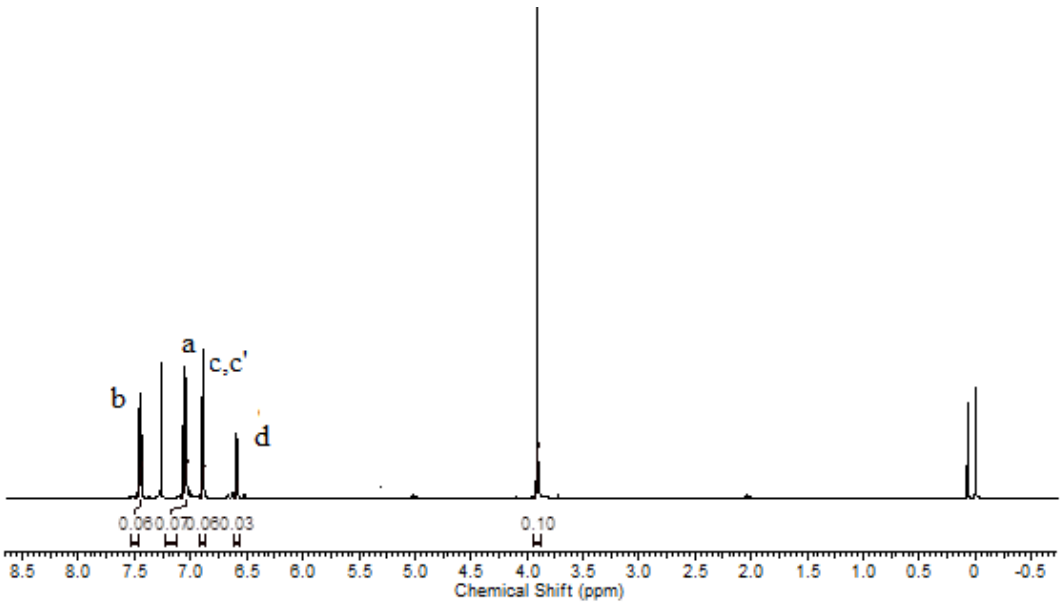



**Figure 10:** $^{1}$H-NMR spectrum of compound **3** recorded in $CDCl_3$ ($\delta$ in ppm).

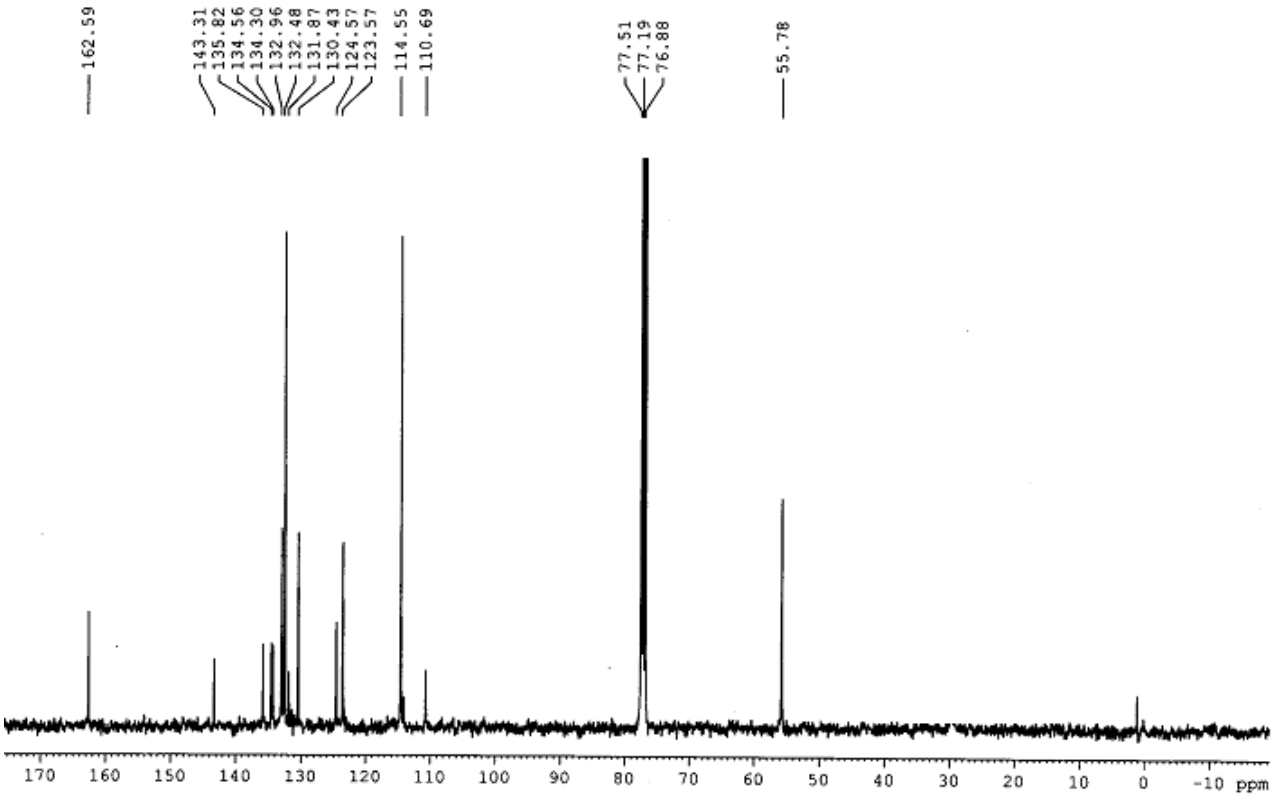



**Figure 11:** $^{13}C$ NMR spectrum of compound **3** recorded in $CDCl_3$ (δ in ppm).

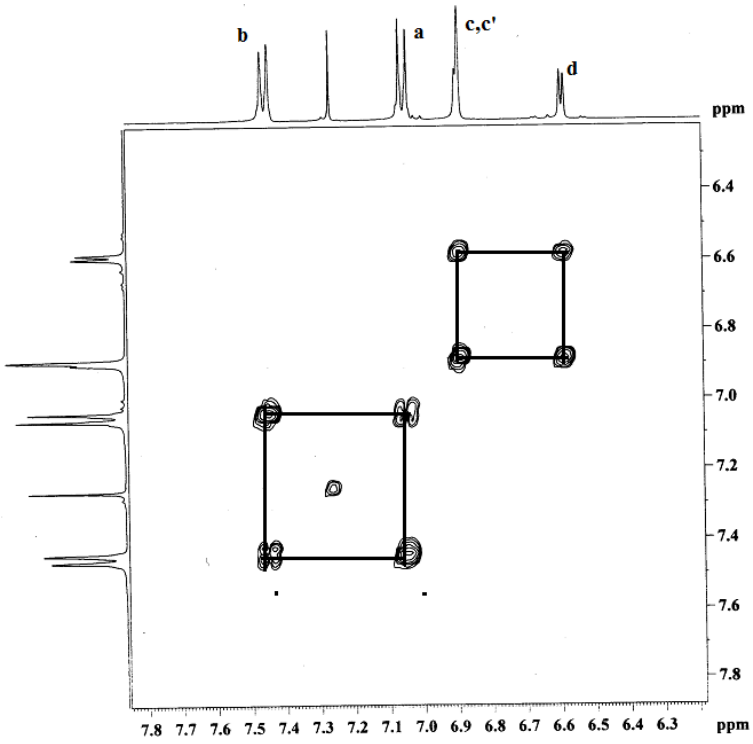



**Figure 12:** $^{1}H$-$^{1}H$ correlation spectrum of compound **3** recorded in $CDCl_3$(δ in ppm).

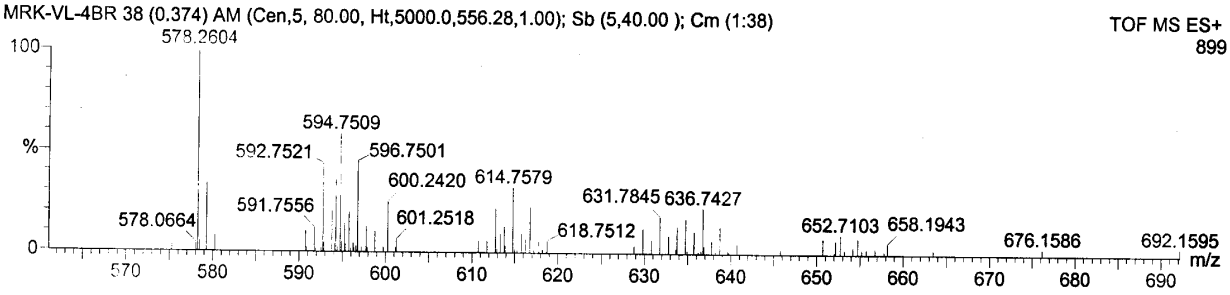
**Elemental Composition Report** Page 1

**Single Mass Analysis (displaying only valid results)**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
110 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 23-May-201116:00:31

C16H9BBr4F2N2O
MRK-VL-4BR 38 (0.374) AM (Cen,5, 80.00, Ht,5000.0,556.28,1.00); Sb (5,40.00 ); Cm (1:38) TOF MS ES+
899




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 590.7523 | 590.7525 | -0.2 | -0.4 | 11.5 | 1 | C16 H9 B N2 O F Br4 |

**Figure 13:** HRMS mass spectrum of compound **4**.

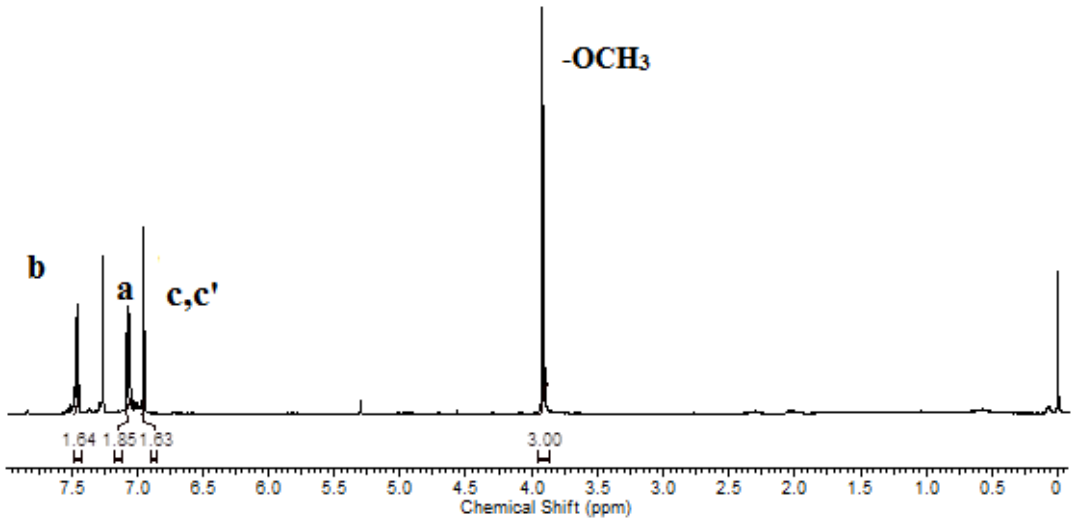



**Figure 14:** $^{1}H$ NMR spectrum of compound **4** recorded in $CDCl_3$ ($\delta$ in ppm).

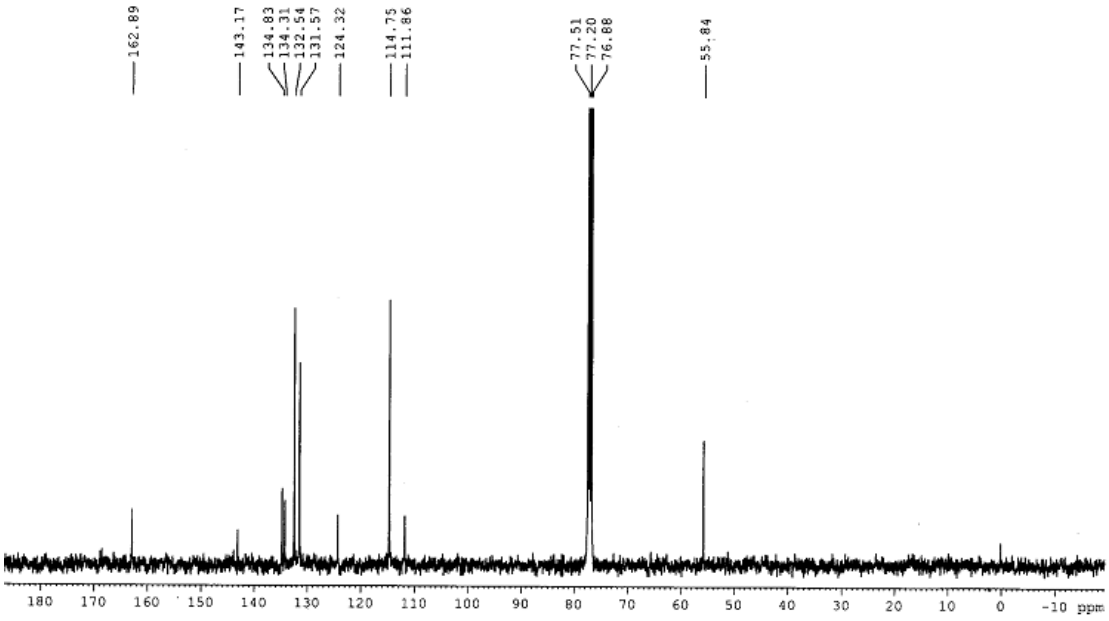



**Figure 15:** $^{13}C$ NMR spectrum of compound **4** recorded in $CDCl_3$(δ in ppm).

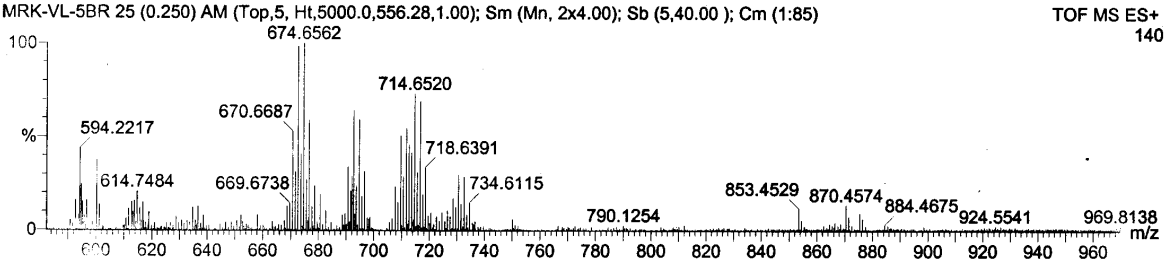
**Elemental Composition Report** **Page 1**

**Single Mass Analysis (displaying only valid results)**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
134 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 24-May-201110:24:15

C16H8BBr5F2N2O
MRK-VL-5BR 25 (0.250) AM (Top,5, Ht,5000.0,556.28,1.00); Sm (Mn, 2x4.00); Sb (5,40.00 ); Cm (1:85) TOF MS ES+
140




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 668.6657 | 668.6631 | 2.7 | 4.0 | 11.5 | 1 | C16 H8 B N2 O F Br5 |

**Figure 16:** HRMS mass spectrum of compound **5**.

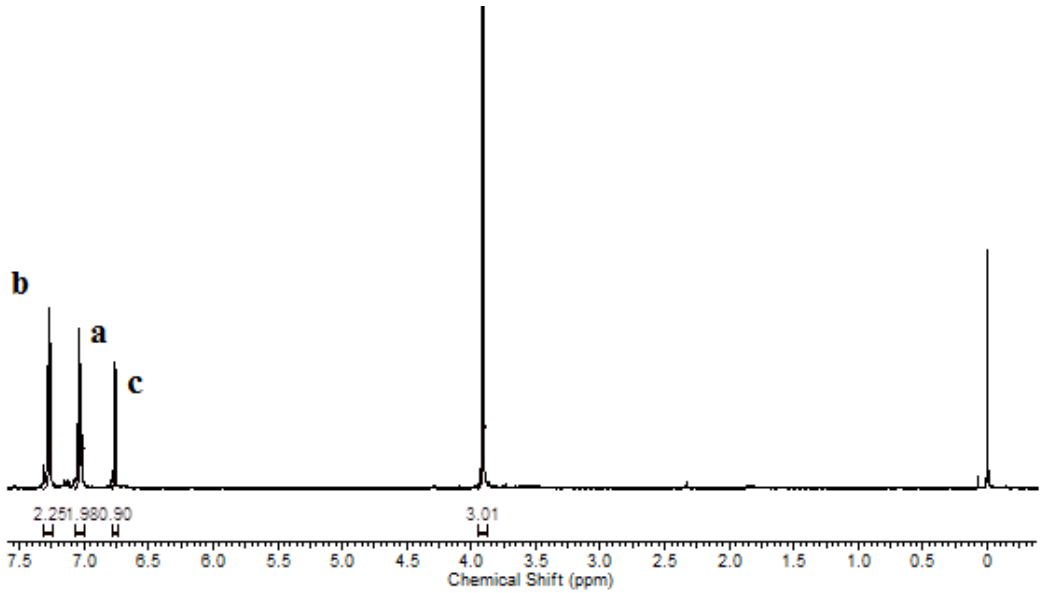



**Figure 17:** $^{1}$H NMR spectrum of compound **5** recorded in $CDCl_3$ (δ in ppm).

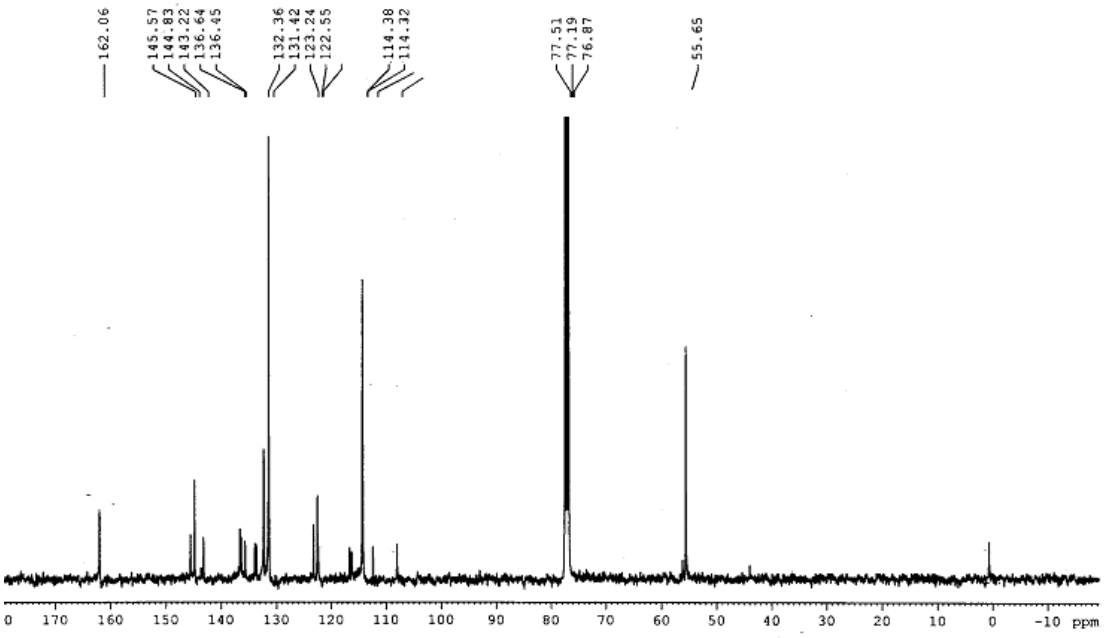



**Figure 18:** $^{13}C$ NMR spectrum of compound **5** recorded in $CDCl_3$ ($\delta$ in ppm).

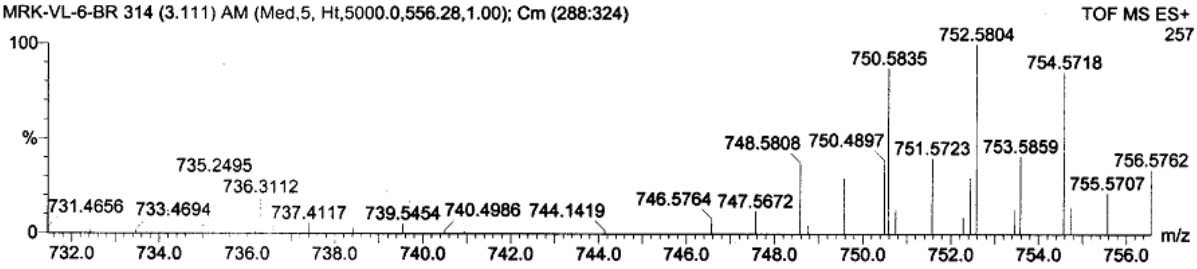
**Elemental Composition Report**

**Single Mass Analysis (displaying only valid results)**
Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
158 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Micromass : Q-Tof micro (YA-105) Dept. Of Chemistry I.I.T.(B) 27-Apr-201114:35:43

C16H7BBr6F2N2O
MRK-VL-6-BR 314 (3.111) AM (Med,5, Ht,5000.0,556.28,1.00); Cm (288:324) TOF MS ES+




| | | | | | | |
|---|---|---|---|---|---|---|
| Minimum: | | | | -1.5 | | |
| Maximum: | | 200.0 | 10.0 | 50.0 | | |
| Mass | Calc. Mass | mDa | PPM | DBE | Score | Formula |
| 746.5764 | 746.5736 | 2.9 | 3.8 | 11.5 | 1 | C16 H7 B N2 O F Br6 |

**Figure 19:** HRMS mass spectrum of compound **6.**

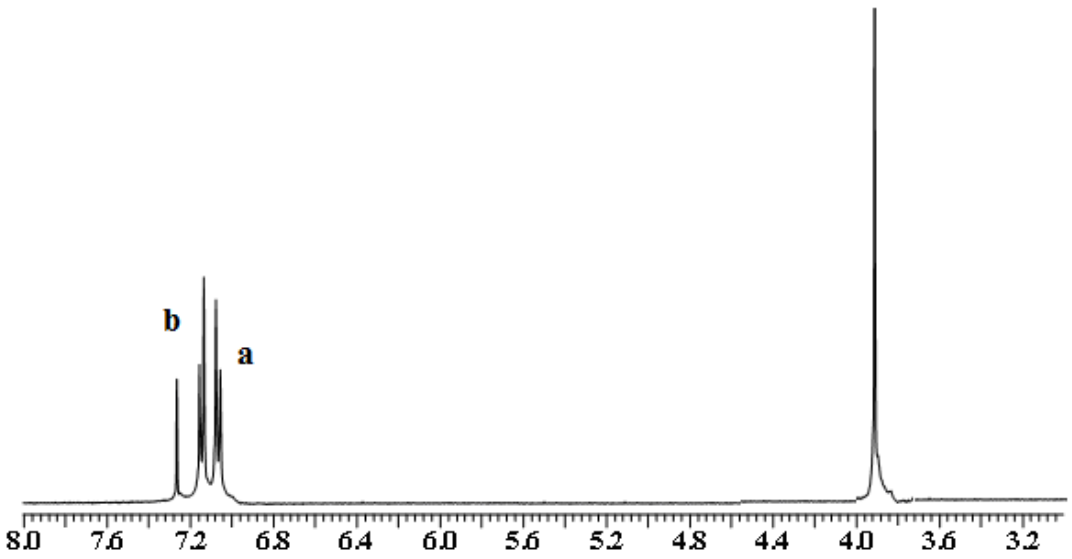



**Figure 20:** $^{1}$H NMR spectrum of compound **6** recorded in $CDCl_3$ (δ in ppm).

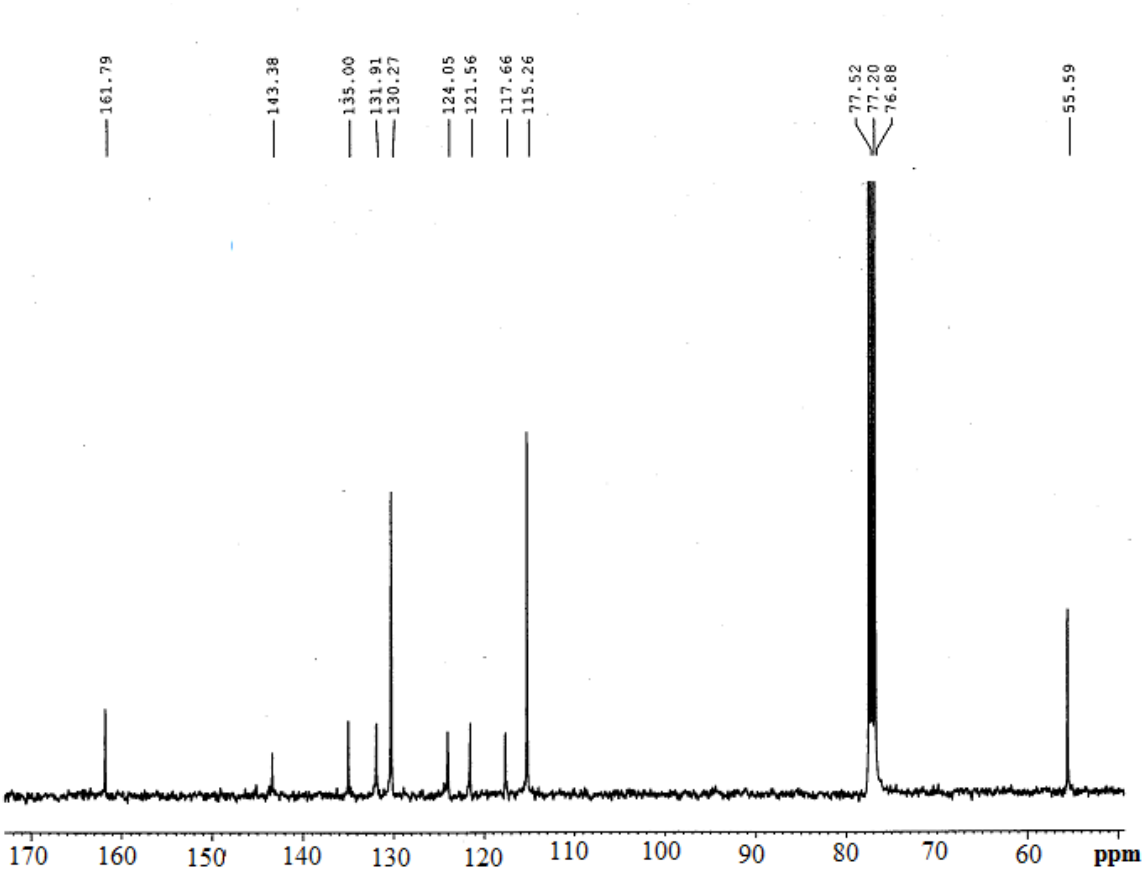



**Figure 21:** $^{13}C$ NMR spectrum of compound **6** recorded in $CDCl_3$ (δ in ppm).

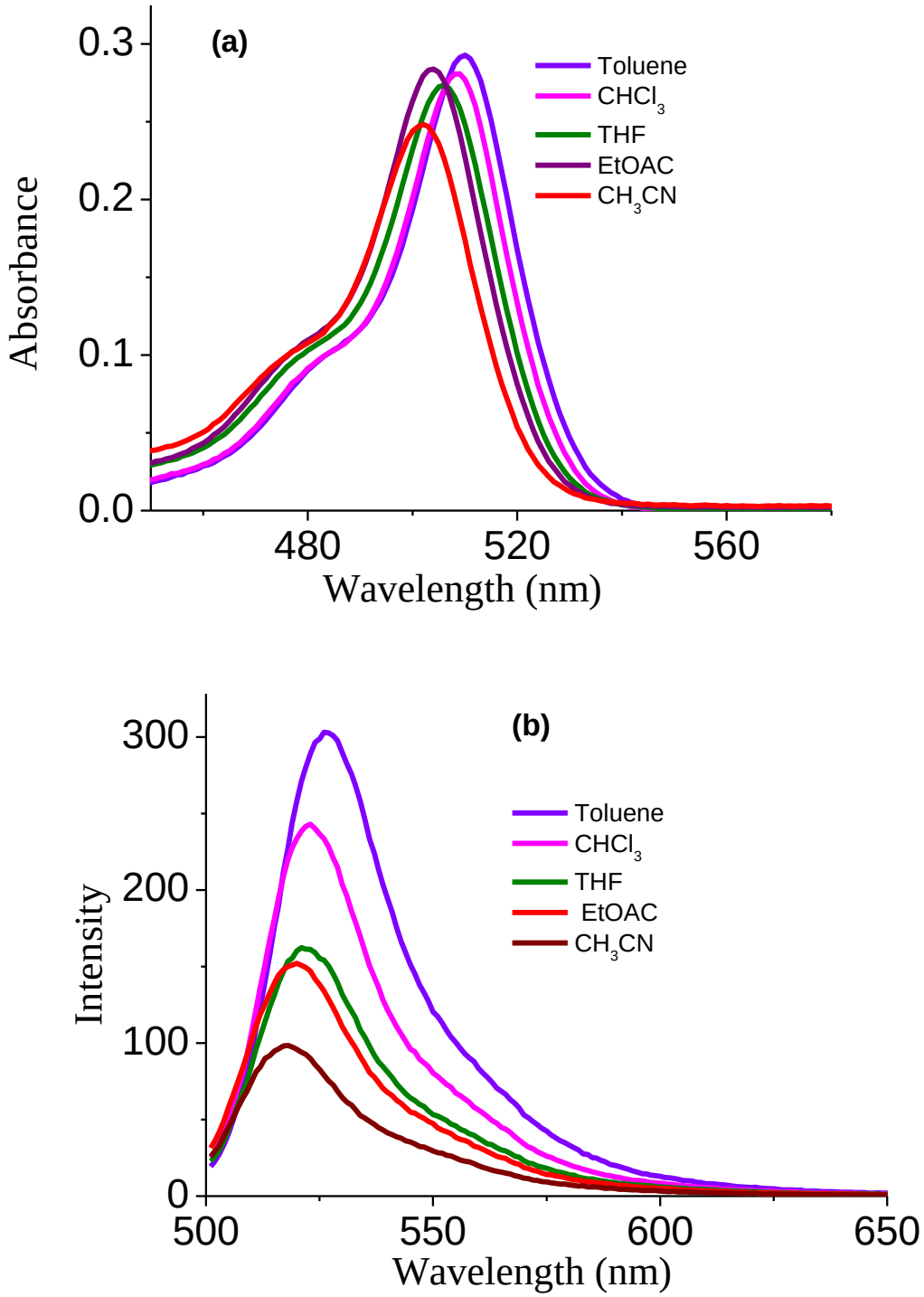



**Figure 22:** (a) Comparison of absorption spectra (b) Comparison of fluorescence emission spectra ($\lambda_{ex}$= 488 nm) of **1** recorded in five different solvents. The concentration used was $1x10^{-6}$.

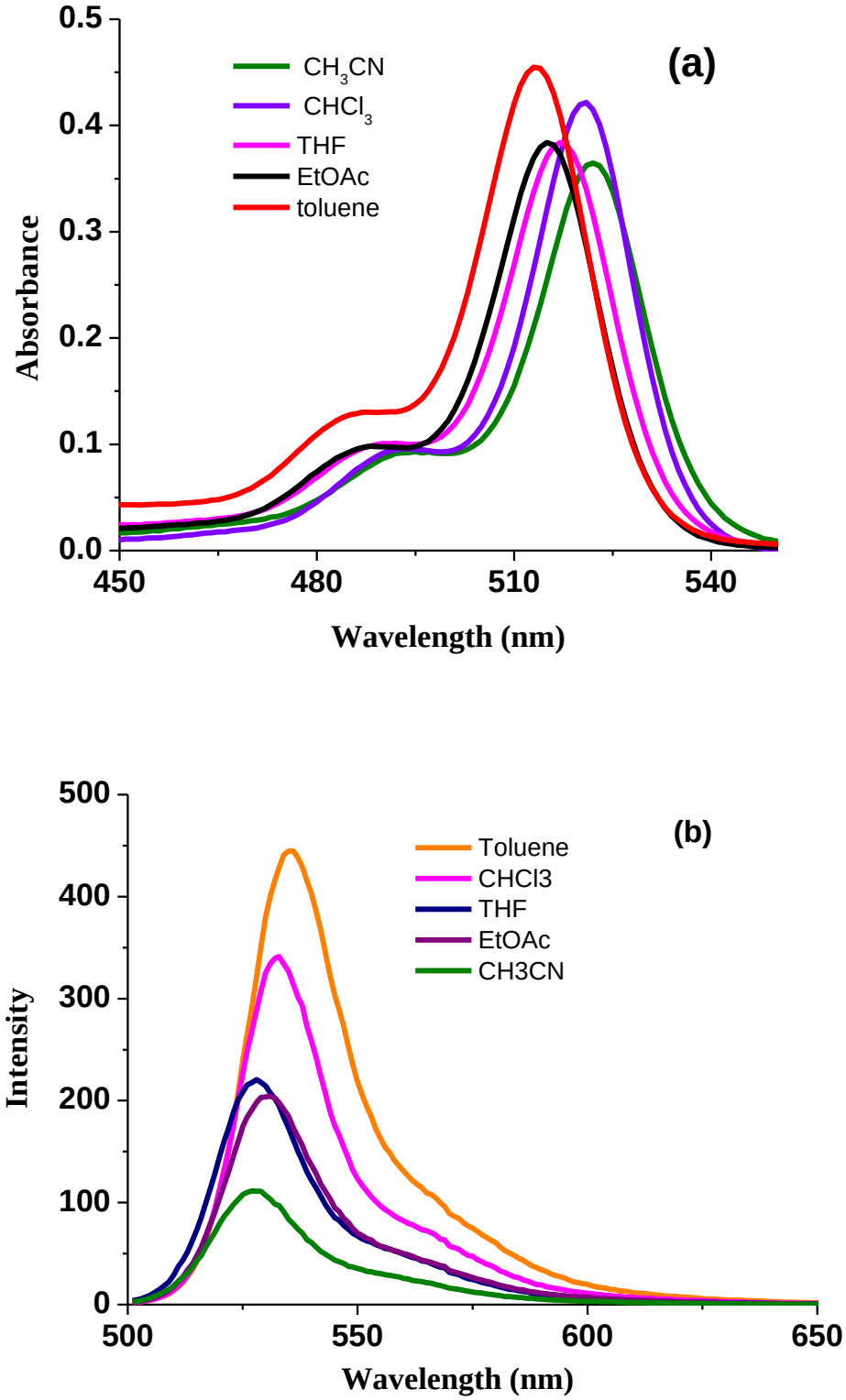



**Figure 23:** (a) Comparison of absorption spectra (b) Comparison of fluorescence emission spectra ($\lambda_{ex}$= 488 nm) of **2** recorded in five different solvents. The concentration used was $1x10^{-6}$ M.

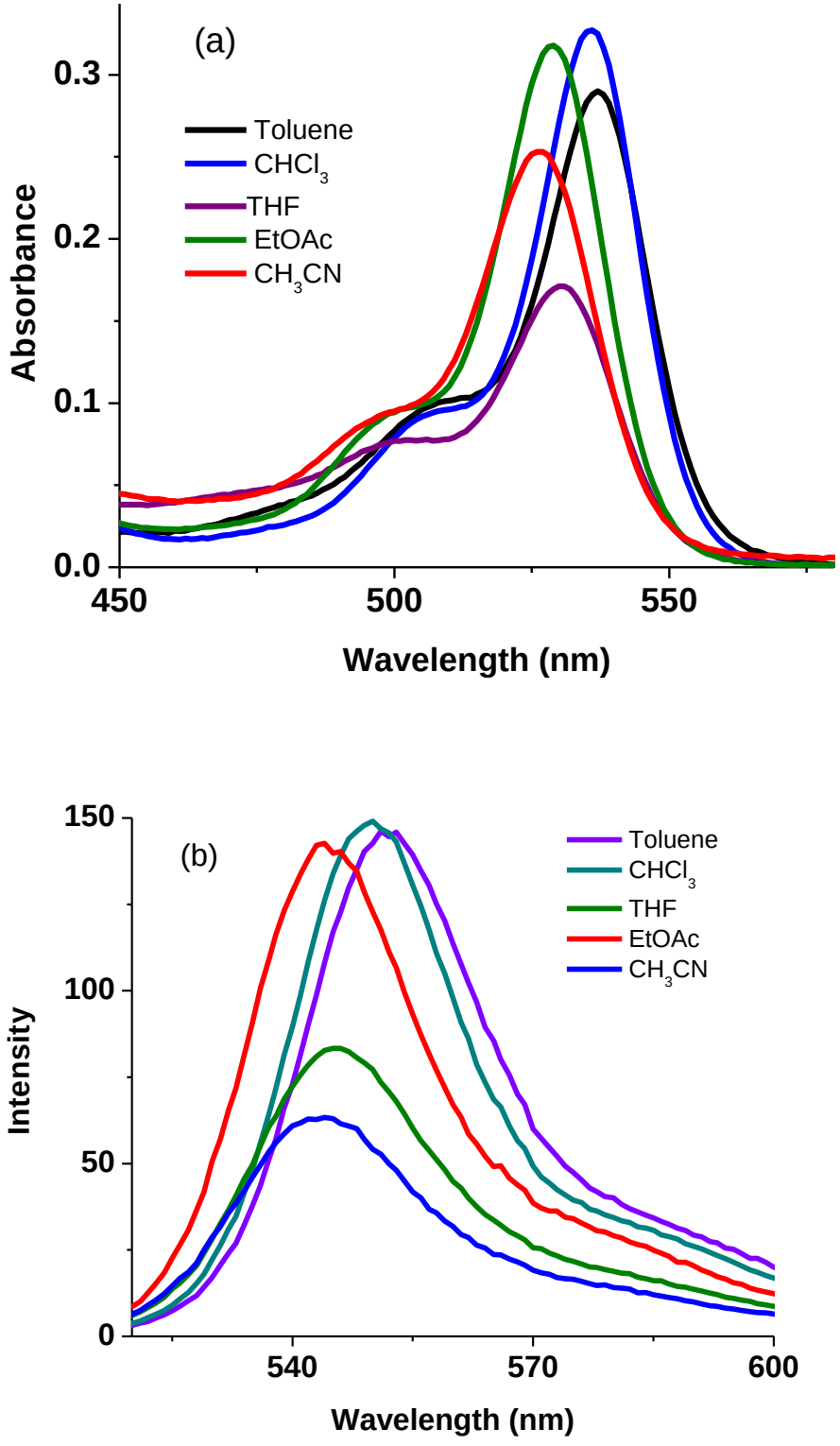



**Figure 24:** (a) Comparison of absorption spectra (b) Comparison of fluorescence emission spectra ($\lambda_{ex}$= 488 nm) of **3** recorded in five different solvents. The concentration used was $1x10^{-6}$ M.

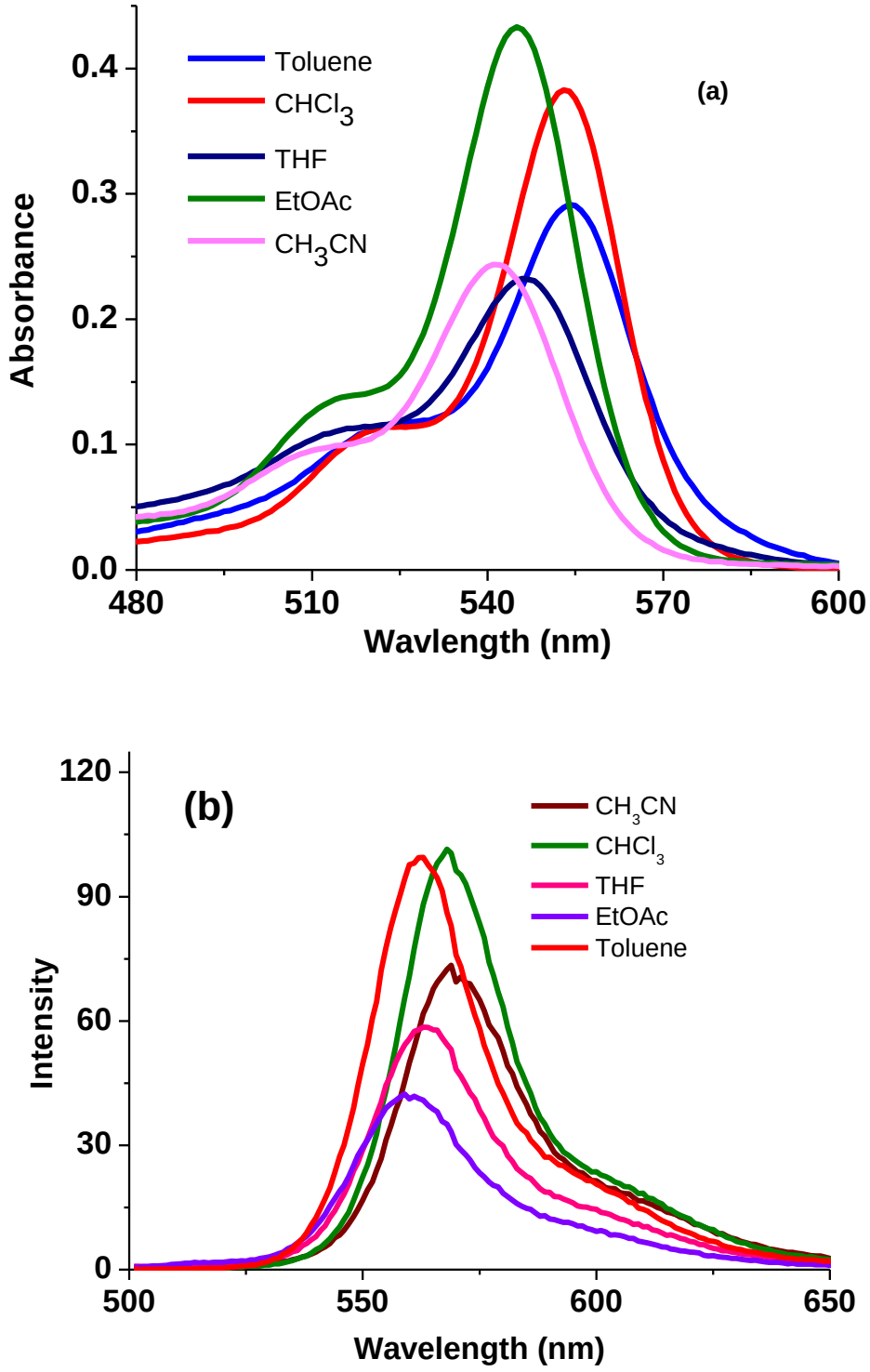



**Figure 25:** (a) Comparison of absorption spectra (b) Comparison of fluorescence emission spectra ($\lambda_{ex}$= 488 nm) of **4** recorded in five different solvents. The concentration used was $1x10^{-6}$ M.

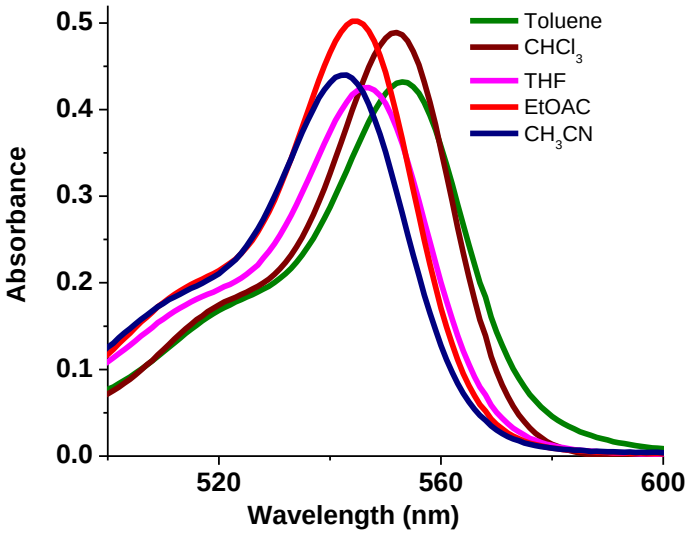



**Figure 26:** Comparison of absorption spectra of **5** recorded in five different solvents. The concentration used was $1x10^{-6}$ M.

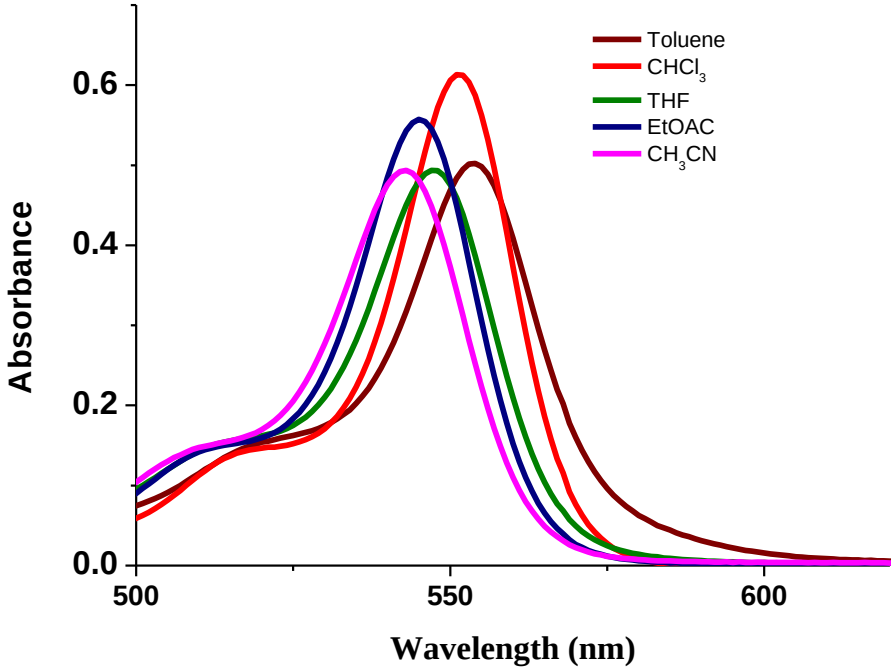



**Figure 27:** Comparison of absorption spectra of **6** recorded in five different solvents. The concentration used was $1x10^{-6}$ M.

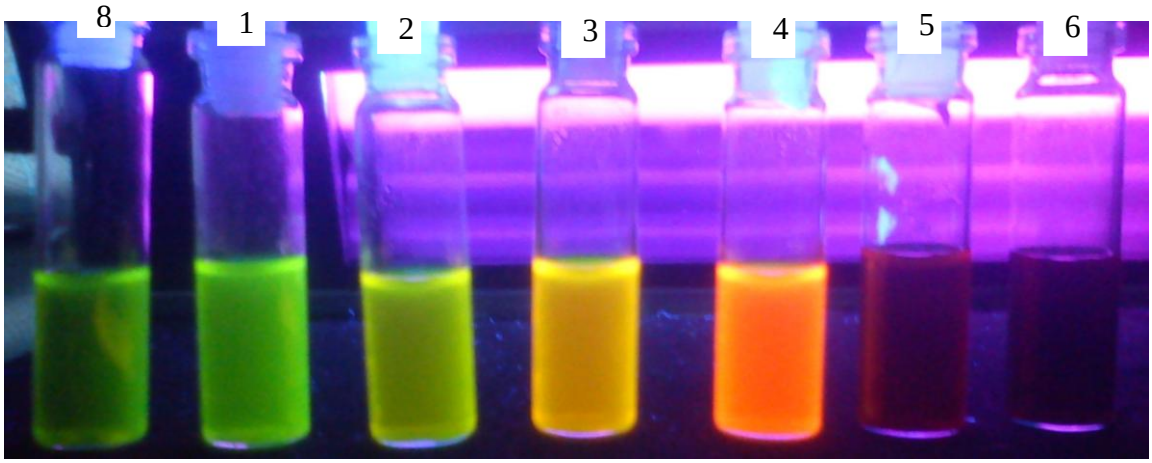



**Figure 28:** Compounds **1-6** in solution state under UV lamp.

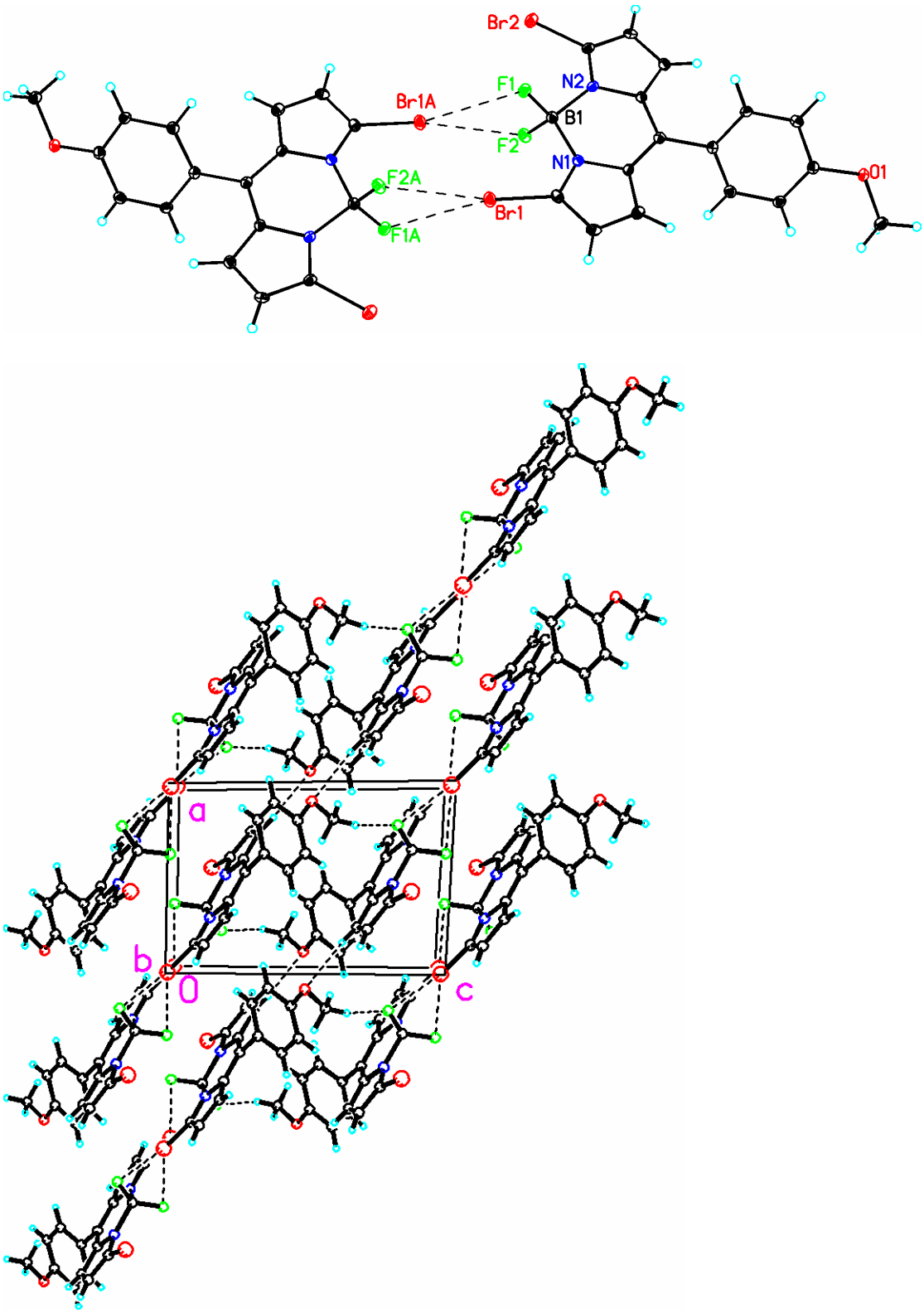



**Figure 29:** ORTEP diagram for the intermolecular interactions in compound **2**.

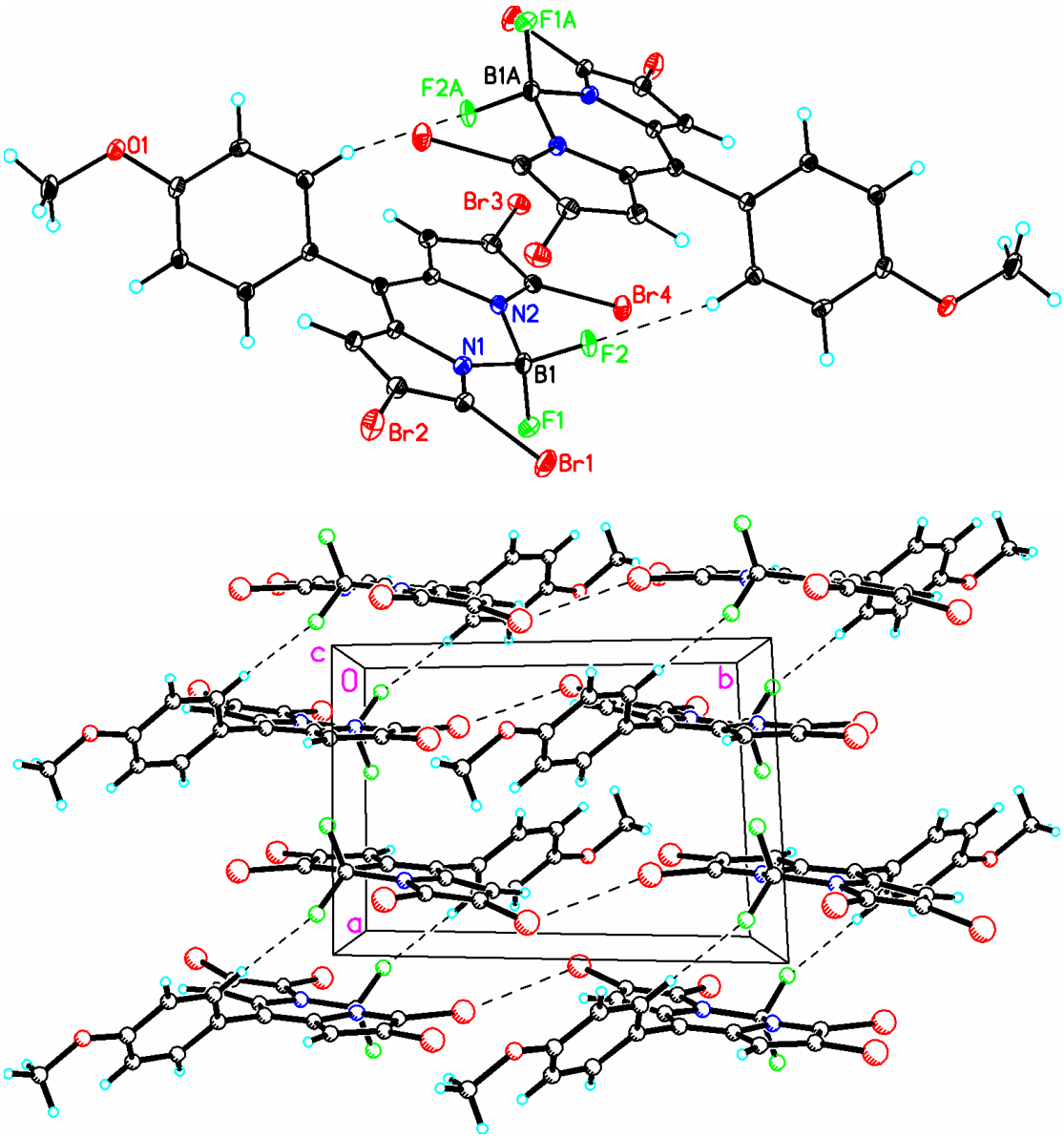



**Figure 30:** ORTEP diagram for the intermolecular interactions in compound **4**.

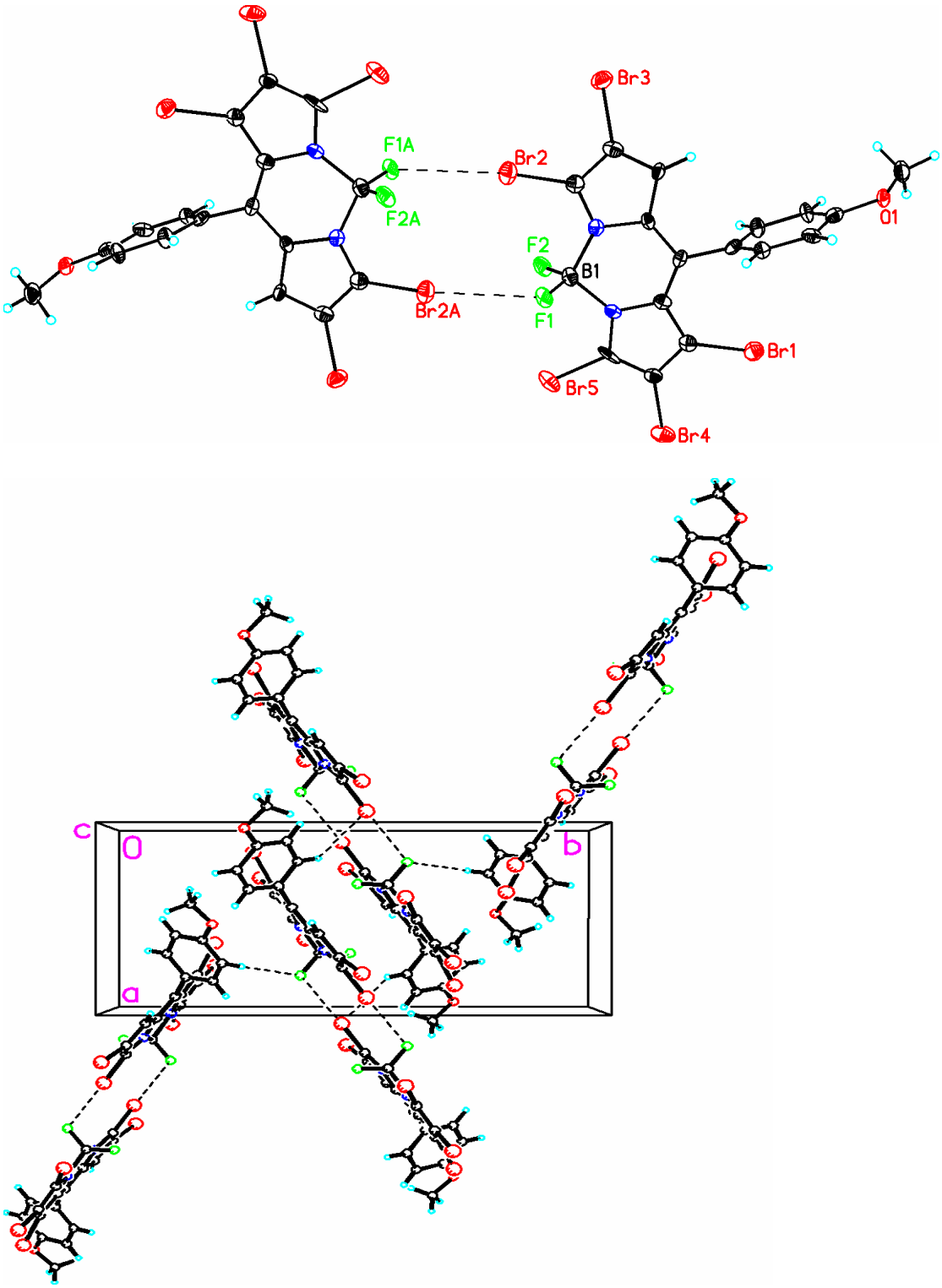



**Figure 31:** ORTEP diagram for the intermolecular interactions in compound **5**.