

## **Supporting Information**

# Synthesis, characterization, DNA binding, anticancer and molecular docking studies of novel imidazolium-based ionic liquids with fluorinated phenylacetamide tethers

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## Characterization of imidazolium IL halides 4a-f

3-(2-((4-Fluorophenyl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium iodide (**4a**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 5.22 (s, 2H, NCH<sub>2</sub>), 7.20 (t, *J* = 8.0 Hz, 2H, Ar-H), 7.59-7.62 (m, 2H, Ar-H), 7.76 (d, *J* = 8.0 Hz, 2H, Ar-H), 9.12 (s, 1H, Ar-H), 10.59 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.34 (NCH<sub>3</sub>); 51.54 (NCH<sub>2</sub>); 115.99, 121.36, 123.26, 124.55, 135.64, 138.14, 157.73, 159.95 (Ar-C); 164.38 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -118.56 to -118.48 (m, 1F, Ar-F). MS (ES) *m/z* = 361.0211 [M<sup>+</sup>].

3-(2-((4-Fluorophenyl)amino)-2-oxoethyl)-1,2-dimethyl-1H-imidazol-3-ium iodide (**4b**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.59 (s, 3H, NCH<sub>3</sub>), 5.20 (s, 2H, NCH<sub>2</sub>), 7.19 (t, *J* = 8.0 Hz, 2H, Ar-H), 7.61-7.64 (m, 2H, Ar-H), 7.70 (d, *J* = 12.0 Hz, 2H, Ar-H), 10.77 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.71 (CH<sub>3</sub>); 35.40 (NCH<sub>3</sub>); 50.54 (NCH<sub>2</sub>); 116.33, 121.34, 123.00, 135.29, 146.36, 157.43, 159.95 (Ar-C); 163.75 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -118.55 to -118.48 (m, 1F, Ar-F). MS (ES) *m/z* = 375.0170 [M<sup>+</sup>].

3-(2-((2-Fluorophenyl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium chloride (**4c**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 4.64 (s, 2H, NCH<sub>2</sub>), 7.18-7.32 (m, 4H, Ar-H), 7.85-7.93 (m, 2H, Ar-H), 9.32 (s, 1H, Ar-H), 10.60 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.34 (NCH<sub>3</sub>); 51.54 (NCH<sub>2</sub>); 115.99, 121.36, 123.26, 124.55, 135.64, 138.14, 157.73, 159.95 (Ar-C); 164.38 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -124.75 to -124.69 (m, 1F, Ar-F). MS (ES) *m/z* = 269.0834 [M<sup>+</sup>].

3-(2-((2-Fluorophenyl)amino)-2-oxoethyl)-1,2-dimethyl-1H-imidazol-3-ium chloride (**4d**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.58 (s, 3H, NCH<sub>3</sub>), 5.25 (s, 2H, NCH<sub>2</sub>), 7.20-7.32 (m, 4H, Ar-H), 7.70 (d, *J* = 12.0 Hz, 1H, Ar-H), 7.90 (s, 1H, Ar-H), 10.39 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.95 (CH<sub>3</sub>); 35.40 (NCH<sub>3</sub>); 50.68 (NCH<sub>2</sub>); 116.07, 116.26, 122.59, 122.82, 124.26, 125.01, 125.04, 125.69, 125.80, 126.35, 126.42, 146.32, 152.72, 155.16 (Ar-C); 164.59 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -124.75 to -124.69 (m, 1F, Ar-F). MS (ES) *m/z* = 283.0790 [M<sup>+</sup>].

1-Methyl-3-(2-oxo-2-((2,4,5-trifluorophenyl) amino)ethyl)-1H-imidazol-3-ium iodide (**4e**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 5.29 (s, 2H, NCH<sub>2</sub>), 7.69-7.74 (m, 3H, Ar-H), 7.97-8.04 (m, 1H, Ar-H), 9.11 (s, 1H, Ar-H), 10.61 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.40 (NCH<sub>3</sub>); 51.56 (NCH<sub>2</sub>); 106.43, 106.68, 106.90, 111.82, 112.06, 122.65, 123.58, 124.40, 138.34, 144.57, 147.00 (Ar-C); 164.99 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -141.54 to -141.38, -139.10 to -138.98, -125.91 to -125.82 (3m, 3F, Ar-F). MS (ES) *m/z* = 396.9802 [M<sup>+</sup>].

1,2-Dimethyl-3-(2-oxo-2-((2,4,5-trifluorophenyl) amino)ethyl)-1H-imidazol-3-ium iodide (**4f**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.57 (s, 3H, NCH<sub>3</sub>), 5.25 (s, 2H, NCH<sub>2</sub>), 7.66-7.75 (m, 3H, Ar-H), 7.97-8.05 (m, 1H, Ar-H), 10.62 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.94 (CH<sub>3</sub>); 35.41 (NCH<sub>3</sub>); 50.63 (NCH<sub>2</sub>); 106.38, 106.61, 106.86, 111.98, 112.24, 122.60, 122.81, 146.38 (Ar-C); 164.99 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -141.63 to -141.46, -139.01 to -138.90, -125.77 to -125.66 (3m, 3F, Ar-F). MS (ES) *m/z* = 411.0126 [M<sup>+</sup>].

## Characterization of imidazolium ILs tethering fluorinated counter anion 5a-r

3-(2-((4-Fluorophenyl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium hexafluorophosphate (**5a**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 5.22 (s, 2H, NCH<sub>2</sub>), 7.20 (t, *J* = 8.0 Hz, 2H, Ar-H), 7.59-7.62 (m, 2H, Ar-H), 7.76 (d, *J* = 8.0 Hz, 2H, Ar-H), 9.12 (s, 1H, Ar-H), 10.59 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.34 (NCH<sub>3</sub>); 51.54 (NCH<sub>2</sub>); 115.99, 121.36, 123.26, 124.55, 135.64, 138.14, 157.73, 159.95 (Ar-C); 164.38 (C=O). <sup>31</sup>P NMR (162 MHz, DMSO-*d*<sub>6</sub>): δ<sub>P</sub> = -157.40 to -131.05 (sept, 1P, PF<sub>6</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -69.16 (d, 6F, PF<sub>6</sub>); -118.42 to -118.35 (m, 1F, Ar-F). MS (ES) *m/z* = 379.0554 [M<sup>+</sup>].

3-(2-((4-Fluorophenyl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium tetrafluoroborate (**5b**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 5.22 (s, 2H, NCH<sub>2</sub>), 7.20 (t, *J* = 8.0 Hz, 2H, Ar-H), 7.59-7.62 (m, 2H, Ar-H), 7.76 (d, *J* = 8.0 Hz, 2H, Ar-H), 9.12 (s, 1H, Ar-H), 10.59 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.34 (NCH<sub>3</sub>); 51.54 (NCH<sub>2</sub>); 115.99, 121.36, 123.26, 124.55, 135.64, 138.14, 157.73, 159.95 (Ar-C); 164.38 (C=O). <sup>11</sup>B NMR (128 MHz, DMSO-*d*<sub>6</sub>): δ<sub>B</sub> = -1.32 to -1.31 (m, 1B, BF<sub>4</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -118.43 to -118.35 (m, 1F, Ar-F); -148.19, -148.14 (2d, 4F, BF<sub>4</sub>). MS (ES) *m/z* = 321.1298 [M<sup>+</sup>].

3-(2-((4-Fluorophenyl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium trifluoroacetate (**5c**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 5.22 (s, 2H, NCH<sub>2</sub>), 7.20 (t, *J* = 8.0 Hz, 2H, Ar-H), 7.59-7.62 (m, 2H, Ar-H), 7.76 (d, *J* = 8.0 Hz, 2H, Ar-H), 9.12 (s, 1H, Ar-H), 10.59 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.34 (NCH<sub>3</sub>); 51.54 (NCH<sub>2</sub>); 115.99, 121.36, 123.26, 124.55, 135.64, 138.14, 157.73, 159.95 (Ar-C); 164.38 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -73.67 (s, 3F, CF<sub>3</sub>); -118.43 to -118.35 (m, 1F, Ar-F). MS (ES) *m/z* = 347.0728 [M<sup>+</sup>].

3-(2-((4-Fluorophenyl)amino)-2-oxoethyl)-1,2-dimethyl-1H-imidazol-3-ium hexafluorophosphate (**5d**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.59 (s, 3H, NCH<sub>3</sub>), 5.20 (s, 2H, NCH<sub>2</sub>), 7.19 (t, *J* = 8.0 Hz, 2H, Ar-H), 7.61-7.64 (m, 2H, Ar-H), 7.70 (d, *J* = 12.0 Hz, 2H, Ar-H), 10.77 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.71 (CH<sub>3</sub>); 35.40 (NCH<sub>3</sub>); 50.54 (NCH<sub>2</sub>); 116.33, 121.34, 123.00, 135.29, 146.36, 157.43, 159.95 (Ar-C); 163.75 (C=O). <sup>31</sup>P NMR (162 MHz, DMSO-*d*<sub>6</sub>) δ<sub>P</sub> = -157.40 to -131.05 (sept, 1P, PF<sub>6</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -69.18 (d, 6F, PF<sub>6</sub>); -118.40 to -118.33 (m, 1F, Ar-F). MS (ES) *m/z* = 393.0878 [M<sup>+</sup>].

3-(2-((4-Fluorophenyl)amino)-2-oxoethyl)-1,2-dimethyl-1H-imidazol-3-ium tetrafluoroborate (**5e**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.57 (s, 3H, NCH<sub>3</sub>), 5.16 (s, 2H, NCH<sub>2</sub>), 7.19 (t, *J* = 8.0 Hz, 2H, Ar-H), 7.58-7.66 (m, 4H, Ar-H), 10.58 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.71 (CH<sub>3</sub>); 35.40 (NCH<sub>3</sub>); 50.54 (NCH<sub>2</sub>); 116.33, 121.34, 123.00, 135.29, 146.36, 157.43, 159.95 (Ar-C); 163.75 (C=O). <sup>11</sup>B NMR (128 MHz, DMSO-*d*<sub>6</sub>): δ<sub>B</sub> = -1.32 to -1.31 (m, 1B, BF<sub>4</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -118.40 to -118.33 (m, 1F, Ar-F); -148.19, -148.14 (2d, 4F, BF<sub>4</sub>). MS (ES) *m/z* = 335.1487 [M<sup>+</sup>].

3-(2-((4-Fluorophenyl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium trifluoroacetate (**5f**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.57 (s, 3H, NCH<sub>3</sub>), 5.16 (s, 2H, NCH<sub>2</sub>), 7.19 (t, *J* = 8.0 Hz, 2H, Ar-H), 7.58-7.66 (m, 4H, Ar-H), 10.58 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.71 (CH<sub>3</sub>); 35.40 (NCH<sub>3</sub>); 50.54 (NCH<sub>2</sub>); 116.33, 121.34, 123.00, 135.29, 146.36, 157.43, 159.95 (Ar-C); 163.75 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -73.56 (s, 3F, CF<sub>3</sub>); -118.38 to -118.31 (m, 1F, Ar-F). MS (ES) *m/z* = 361.1456 [M<sup>+</sup>].

3-(2-((2-Fluorophenyl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium hexafluorophosphate (**5g**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 4.64 (s, 2H, NCH<sub>2</sub>), 3.83 (s, 1H, Ar-H), 7.18-7.32 (m, 4H, Ar-H), 7.85-7.93 (m, 2H, Ar-H), 9.32 (s, 1H, Ar-H), 10.60 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.34 (NCH<sub>3</sub>); 51.54 (NCH<sub>2</sub>); 115.99, 121.36, 123.26, 124.55, 135.64, 138.14, 157.73, 159.95 (Ar-C); 164.38 (C=O). <sup>31</sup>P NMR (162 MHz, DMSO-*d*<sub>6</sub>) δ<sub>P</sub> = -157.39 to -131.04 (sept, 1P, PF<sub>6</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -69.18 (d, 6F, PF<sub>6</sub>); -124.74 to -124.68 (m, 1F, Ar-F). MS (ES) *m/z* = 379.0634 [M<sup>+</sup>].

3-(2-((2-Fluorophenyl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium tetrafluoroborate (**5h**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 4.64 (s, 2H, NCH<sub>2</sub>), 7.18-7.32 (m, 4H, Ar-H), 7.85-7.93 (m, 2H, Ar-H), 9.32 (s, 1H, Ar-H), 10.60 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.34 (NCH<sub>3</sub>); 51.54 (NCH<sub>2</sub>); 115.99, 121.36, 123.26, 124.55, 135.64, 138.14, 157.73, 159.95 (Ar-C); 164.38 (C=O). <sup>11</sup>B NMR (128 MHz, DMSO-*d*<sub>6</sub>): δ<sub>B</sub> = -1.30 to -1.29 (m, 1B, BF<sub>4</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -124.69 to -124.63 (m, 1F, Ar-F); -148.23, -148.18 (2d, 4F, BF<sub>4</sub>). MS (ES) *m/z* = 321.1301 [M<sup>+</sup>].

3-(2-((2-Fluorophenyl)amino)-2-oxoethyl)-1-methyl-1H-imidazol-3-ium trifluoroacetate (**5i**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 4.64 (s, 2H, NCH<sub>2</sub>), 7.18-7.32 (m, 4H, Ar-H), 7.85-7.93 (m, 2H, Ar-H), 9.32 (s, 1H, Ar-H), 10.60 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.34 (NCH<sub>3</sub>); 51.54 (NCH<sub>2</sub>); 115.99, 121.36, 123.26, 124.55, 135.64, 138.14, 157.73, 159.95 (Ar-C); 164.38 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -73.52 (s, 3F, CF<sub>3</sub>); -124.69 to -124.63 (m, 1F, Ar-F). MS (ES) *m/z* = 347.0874 [M<sup>+</sup>].

3-(2-((2-Fluorophenyl)amino)-2-oxoethyl)-1,2-dimethyl-1H-imidazol-3-ium hexafluorophosphate (**5j**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.58 (s, 3H, NCH<sub>3</sub>), 5.25 (s, 2H, NCH<sub>2</sub>), 7.20-7.32 (m, 3H, Ar-H), 7.70 (d, *J* = 12.0 Hz, 1H, Ar-H), 7.90 (s, 1H, Ar-H), 10.39 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.95 (CH<sub>3</sub>); 35.40 (NCH<sub>3</sub>); 50.68 (NCH<sub>2</sub>); 116.07, 116.26, 122.59, 122.82, 124.26, 125.01, 125.04, 125.69, 125.80, 126.35, 126.42, 146.32, 152.72, 155.16 (Ar-C); 164.59 (C=O). <sup>31</sup>P NMR (162 MHz, DMSO-*d*<sub>6</sub>) δ<sub>P</sub> = -157.43 to -131.07 (sept, 1P, PF<sub>6</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -69.16 (d, 6F, PF<sub>6</sub>); -124.32 to -124.25 (m, 1F, Ar-F). MS (ES) *m/z* = 393.0823 [M<sup>+</sup>].

3-(2-((2-Fluorophenyl)amino)-2-oxoethyl)-1,2-dimethyl-1H-imidazol-3-ium tetrafluoroborate (**5k**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.58 (s, 3H, NCH<sub>3</sub>), 5.25 (s, 2H, NCH<sub>2</sub>), 7.20-7.32 (m, 3H, Ar-H), 7.70 (d, *J* = 12.0 Hz, 1H, Ar-H), 7.90 (s, 1H, Ar-H), 10.39 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.95 (CH<sub>3</sub>); 35.40 (NCH<sub>3</sub>); 50.68 (NCH<sub>2</sub>); 116.07, 116.26, 122.59, 122.82, 124.26, 125.01, 125.04, 125.69, 125.80, 126.35, 126.42, 146.32, 152.72, 155.16 (Ar-C); 164.59 (C=O). <sup>11</sup>B NMR (128 MHz, DMSO-*d*<sub>6</sub>): δ<sub>B</sub> = -1.30 to -1.29 (m, 1B, BF<sub>4</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -124.33 to -124.20 (m, 1F, Ar-F); -148.19, -148.14 (2d, 4F, BF<sub>4</sub>). MS (ES) *m/z* = 335.1071 [M<sup>+</sup>].

3-(2-((2-Fluorophenyl)amino)-2-oxoethyl)-1,2-dimethyl-1H-imidazol-3-ium trifluoroacetate (**5l**). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.58 (s, 3H, NCH<sub>3</sub>), 5.25 (s, 2H, NCH<sub>2</sub>), 7.20-7.32 (m, 3H, Ar-H), 7.70 (d, *J* = 12.0 Hz, 1H, Ar-H), 7.90 (s, 1H, Ar-H), 10.39 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.95 (CH<sub>3</sub>); 35.40 (NCH<sub>3</sub>); 50.68 (NCH<sub>2</sub>); 116.07, 116.26, 122.59, 122.82, 124.26, 125.01, 125.04, 125.69, 125.80, 126.35, 126.42, 146.32, 152.72, 155.16 (Ar-C); 164.59 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -73.52 (s, 3F, CF<sub>3</sub>); -124.32 to -124.26 (m, 1F, Ar-F). MS (ES) *m/z* = 361.0920 [M<sup>+</sup>].

*1-Methyl-3-(2-oxo-2-((2,4,5-trifluorophenyl) amino)ethyl)-1H-imidazol-3-ium hexafluoro-phosphate (5m)*. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 5.29 (s, 2H, NCH<sub>2</sub>), 7.69-7.74 (m, 3H, Ar-H), 7.97-8.04 (m, 1H, Ar-H), 9.11 (s, 1H, Ar-H), 10.61 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.40 (NCH<sub>3</sub>); 51.56 (NCH<sub>2</sub>); 106.43, 106.68, 106.90, 111.82, 112.06, 122.65, 123.58, 124.40, 138.34, 144.57, 147.00 (Ar-C); 164.99 (C=O). <sup>31</sup>P NMR (162 MHz, DMSO-*d*<sub>6</sub>) δ<sub>P</sub> = -157.40 to -131.05 (sept, 1P, PF<sub>6</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -69.18 (d, 6F, PF<sub>6</sub>); -141.50 to -141.41, -139.01 to -138.89, -125.88 to -125.79 (3m, 3F, Ar-F). MS (ES) *m/z* = 415.0500 [M<sup>+</sup>].

*1-Methyl-3-(2-oxo-2-((2,4,5-trifluorophenyl) amino)ethyl)-1H-imidazol-3-ium tetrafluoroborate (5n)*. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 5.29 (s, 2H, NCH<sub>2</sub>), 7.69-7.74 (m, 3H, Ar-H), 7.97-8.04 (m, 1H, Ar-H), 9.11 (s, 1H, Ar-H), 10.61 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.40 (NCH<sub>3</sub>); 51.56 (NCH<sub>2</sub>); 106.43, 106.68, 106.90, 111.82, 112.06, 122.65, 123.58, 124.40, 138.34, 144.57, 147.00 (Ar-C); 164.99 (C=O). <sup>11</sup>B NMR (128 MHz, DMSO-*d*<sub>6</sub>): δ<sub>B</sub> = -1.31 to -130 (m, 1B, BF<sub>4</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -141.54 to -141.38, -139.00 to -138.88, -125.86 to -125.77 (3m, 3F, Ar-F); -148.21, -148.15 (2d, 4F, BF<sub>4</sub>). MS (ES) *m/z* = 357.0729 [M<sup>+</sup>].

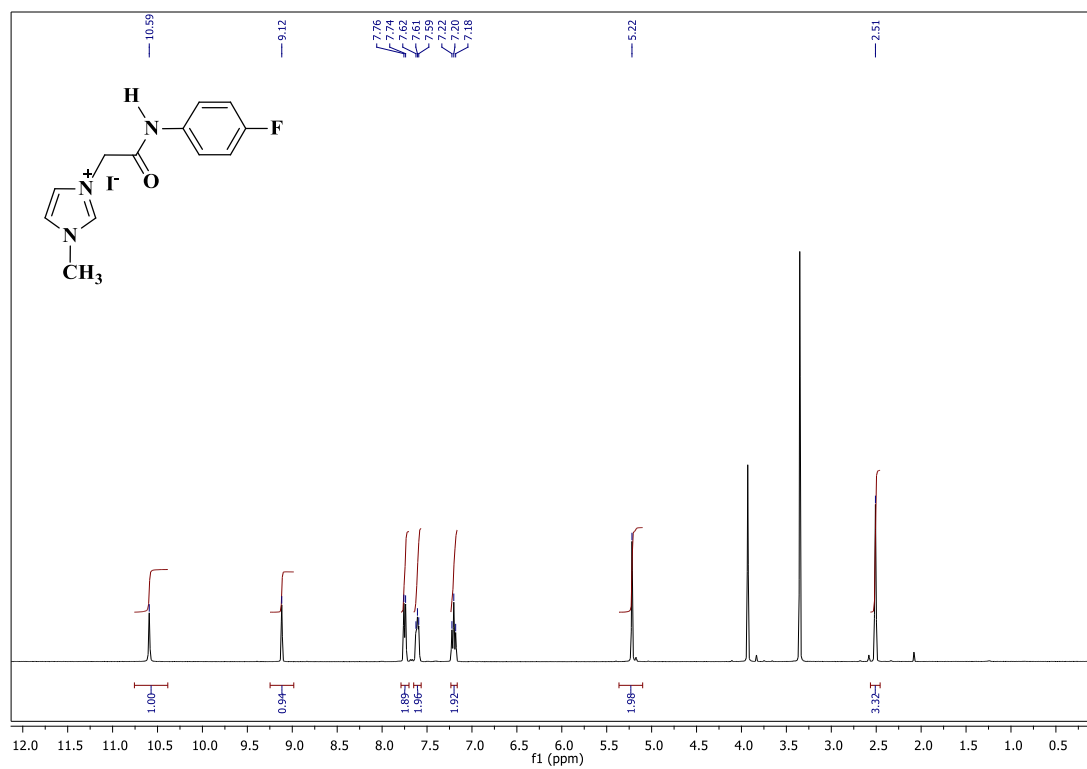
*1-Methyl-3-(2-oxo-2-((2,4,5-trifluorophenyl) amino)ethyl)-1H-imidazol-3-ium trifluoroacetate (5o)*. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, NCH<sub>3</sub>), 5.29 (s, 2H, NCH<sub>2</sub>), 7.69-7.74 (m, 3H, Ar-H), 7.97-8.04 (m, 1H, Ar-H), 9.11 (s, 1H, Ar-H), 10.61 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 36.40 (NCH<sub>3</sub>); 51.56 (NCH<sub>2</sub>); 106.43, 106.68, 106.90, 111.82, 112.06, 122.65, 123.58, 124.40, 138.34, 144.57, 147.00 (Ar-C); 164.99 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -73.57 (s, 3F, CF<sub>3</sub>); -141.54 to -141.38, -139.01 to -138.89, -125.85 to -125.76 (3m, 3F, Ar-F). MS (ES) *m/z* = 383.0520 [M<sup>+</sup>].

*1,2-Dimethyl-3-(2-oxo-2-((2,4,5-trifluorophenyl) amino)ethyl)-1H-imidazol-3-ium hexafluorophosphate (5p)*. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.57 (s, 3H, NCH<sub>3</sub>), 5.25 (s, 2H, NCH<sub>2</sub>), 7.66-7.75 (m, 3H, Ar-H), 7.97-8.05 (m, 1H, Ar-H), 10.62 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.94 (CH<sub>3</sub>); 35.41 (NCH<sub>3</sub>); 50.63 (NCH<sub>2</sub>); 106.38, 106.61, 106.86, 111.98, 112.24, 122.60, 122.81, 146.38 (Ar-C); 164.99 (C=O). <sup>31</sup>P NMR (162 MHz, DMSO-*d*<sub>6</sub>) δ<sub>P</sub> = -157.40 to -131.05 (sept, 1P, PF<sub>6</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -69.18 (d, 6F, PF<sub>6</sub>); -141.60 to -141.50, -138.93 to -138.81, -125.75 to -125.66 (3m, 3F, Ar-F). MS (ES) *m/z* = 429.0535 [M<sup>+</sup>].

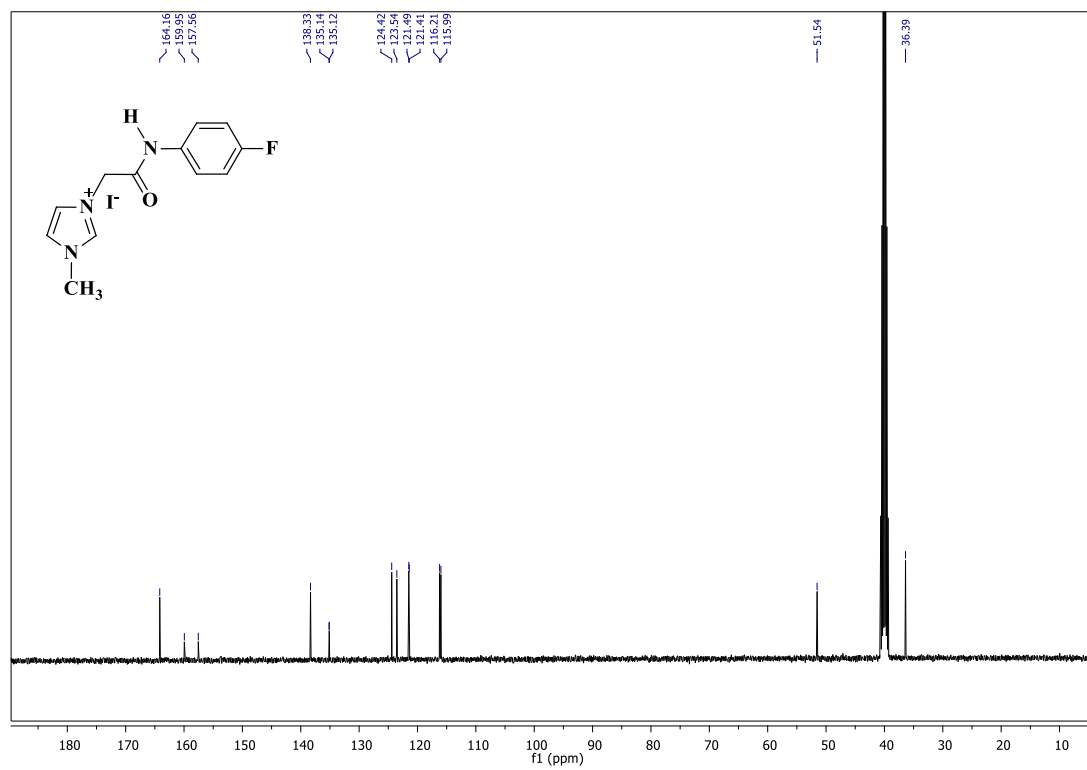
*1,2-Dimethyl-3-(2-oxo-2-((2,4,5-trifluorophenyl) amino)ethyl)-1H-imidazol-3-ium tetrafluoroborate (5q)*. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.57 (s, 3H, NCH<sub>3</sub>), 5.25 (s, 2H, NCH<sub>2</sub>), 7.66-7.75 (m, 3H, Ar-H), 7.97-8.05 (m, 1H, Ar-H), 10.62 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.94 (CH<sub>3</sub>); 35.41 (NCH<sub>3</sub>); 50.63 (NCH<sub>2</sub>); 106.38, 106.61, 106.86, 111.98, 112.24, 122.60, 122.81, 146.38 (Ar-C); 164.99 (C=O). <sup>11</sup>B NMR (128 MHz, DMSO-*d*<sub>6</sub>): δ<sub>B</sub> = -1.32 to -1.31 (m, 1B, BF<sub>4</sub>). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -141.60 to -141.47, -138.92 to -138.80, -125.73 to -125.64 (3m, 3F, Ar-F); -148.23, -148.17 (2d, 4F, BF<sub>4</sub>). MS (ES) *m/z* = 429.0546 [M<sup>+</sup>].

*1,2-Dimethyl-3-(2-oxo-2-((2,4,5-trifluorophenyl) amino)ethyl)-1H-imidazol-3-ium trifluoroacetate (5r)*. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ<sub>H</sub> = 2.51 (s, 3H, CH<sub>3</sub>), 2.57 (s, 3H, NCH<sub>3</sub>), 5.25 (s, 2H, NCH<sub>2</sub>), 7.66-7.75 (m, 3H, Ar-H), 7.97-8.05 (m, 1H, Ar-H), 10.62 (s, 1H, NHCO). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ<sub>C</sub> = 9.94 (CH<sub>3</sub>); 35.41 (NCH<sub>3</sub>); 50.63 (NCH<sub>2</sub>); 106.38, 106.61, 106.86, 111.98, 112.24, 122.60, 122.81, 146.38 (Ar-C); 164.99 (C=O). <sup>19</sup>F NMR (377 MHz, DMSO-*d*<sub>6</sub>): δ<sub>F</sub> = -73.57 (s, 3F, CF<sub>3</sub>); -141.60 to -141.51, -138.93 to -138.82, -125.69 to -125.61 (3m, 3F, Ar-F). MS (ES) *m/z* = 397.0845 [M<sup>+</sup>].

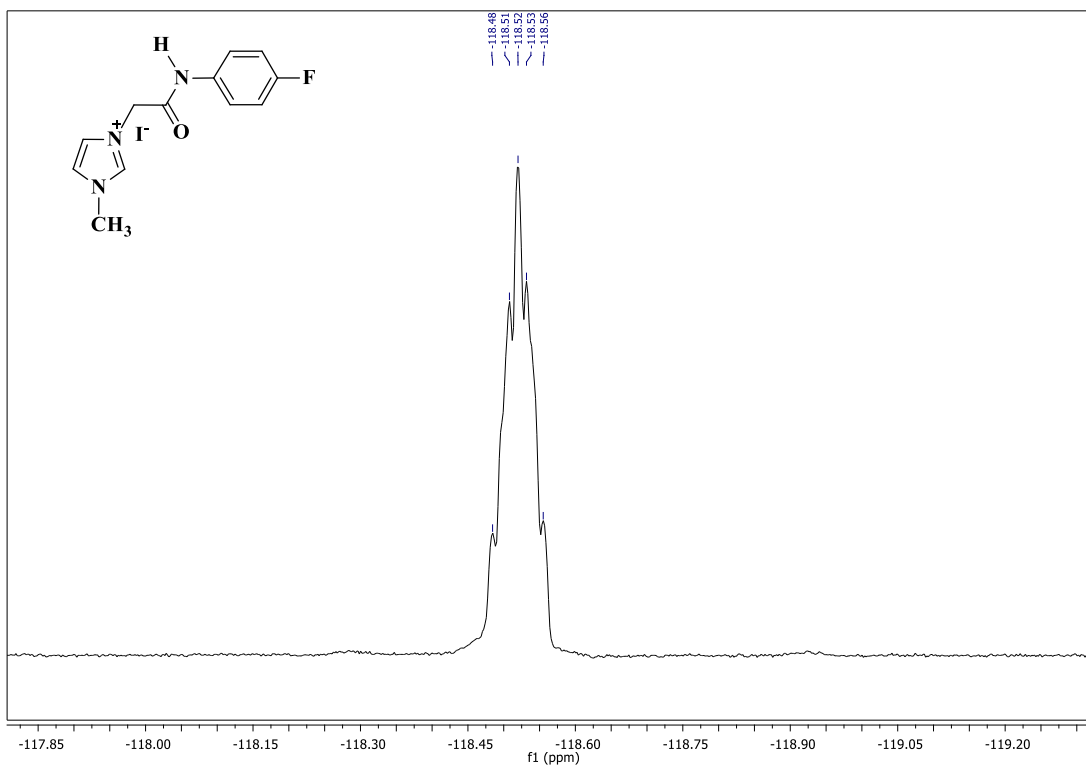
**<sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F-NMR and MS Spectra of Compounds 4a-f**



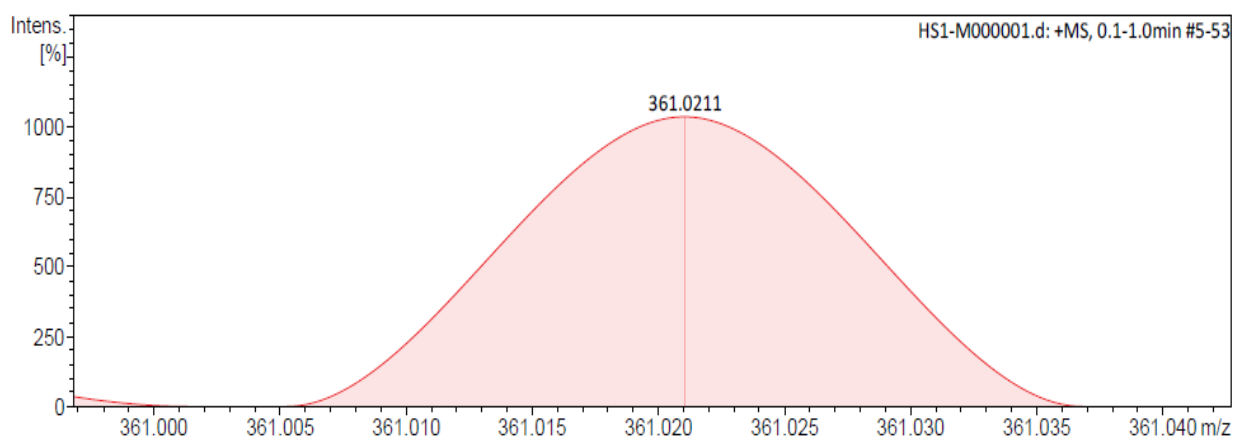
**Figure S1: <sup>1</sup>H NMR of compound 4a**



**Figure S2: <sup>13</sup>C NMR of compound 4a**



**Figure S3:**  $^{19}\text{F}$  NMR of compound **4a**



**Figure S4:** HRMS (ESI) of compound **4a**

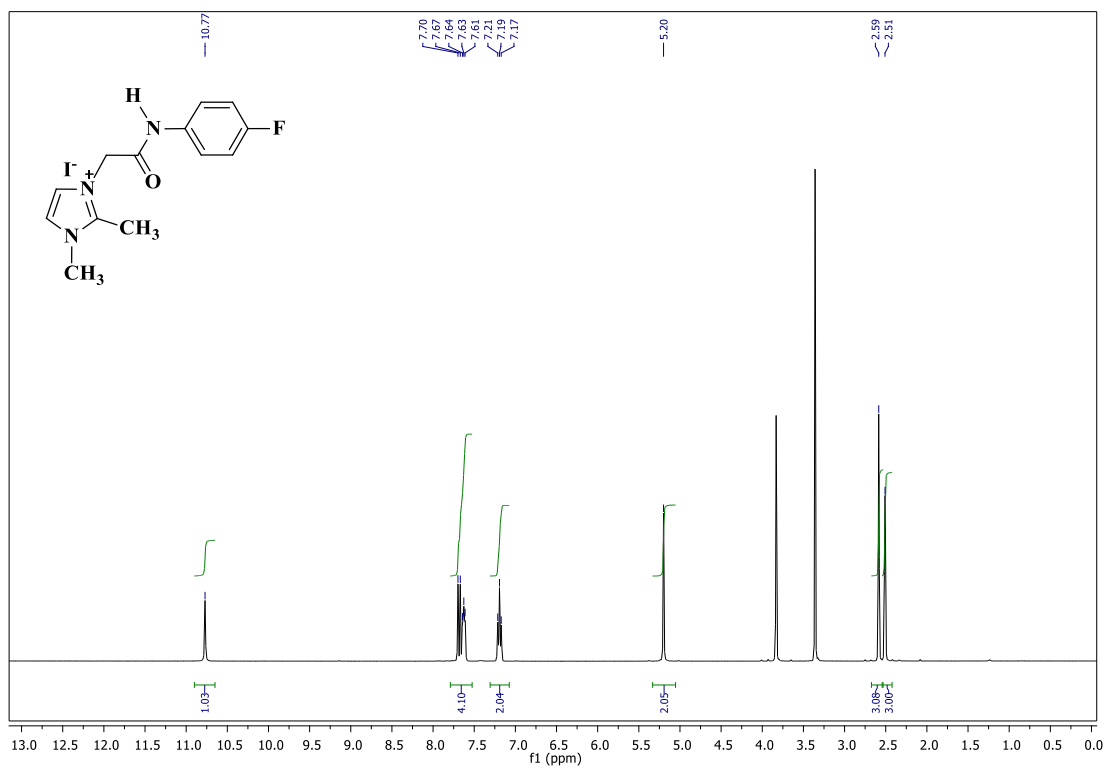


Figure S5: <sup>1</sup>H NMR of compound 4b

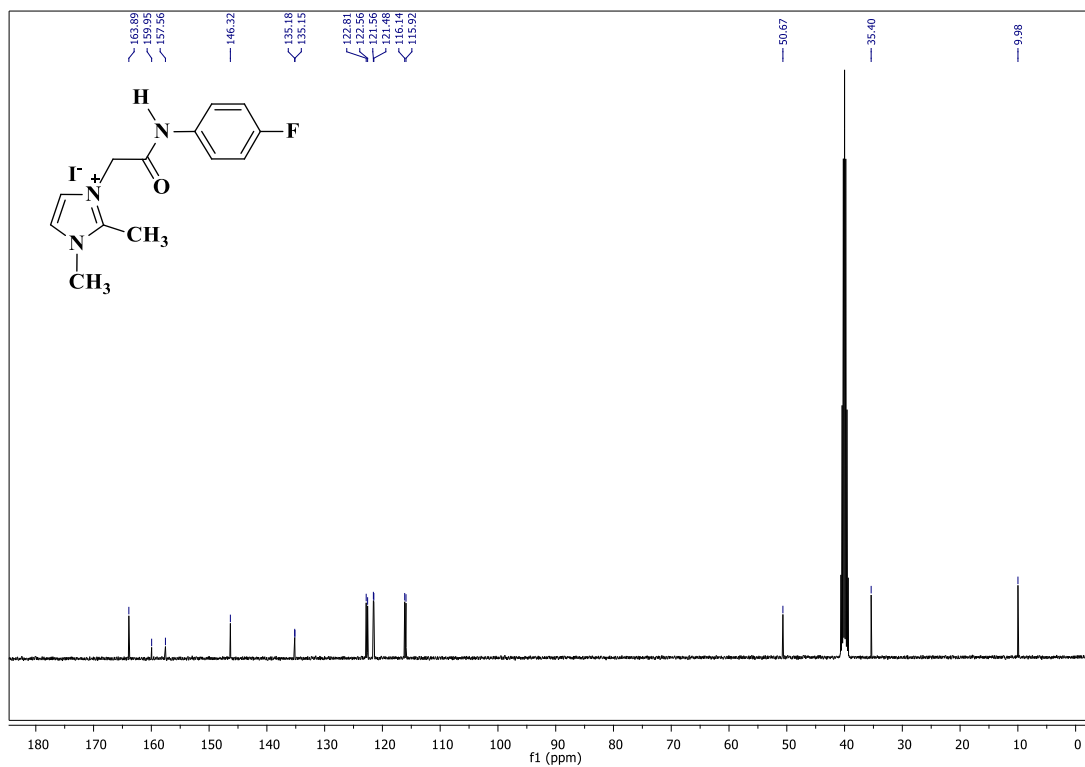
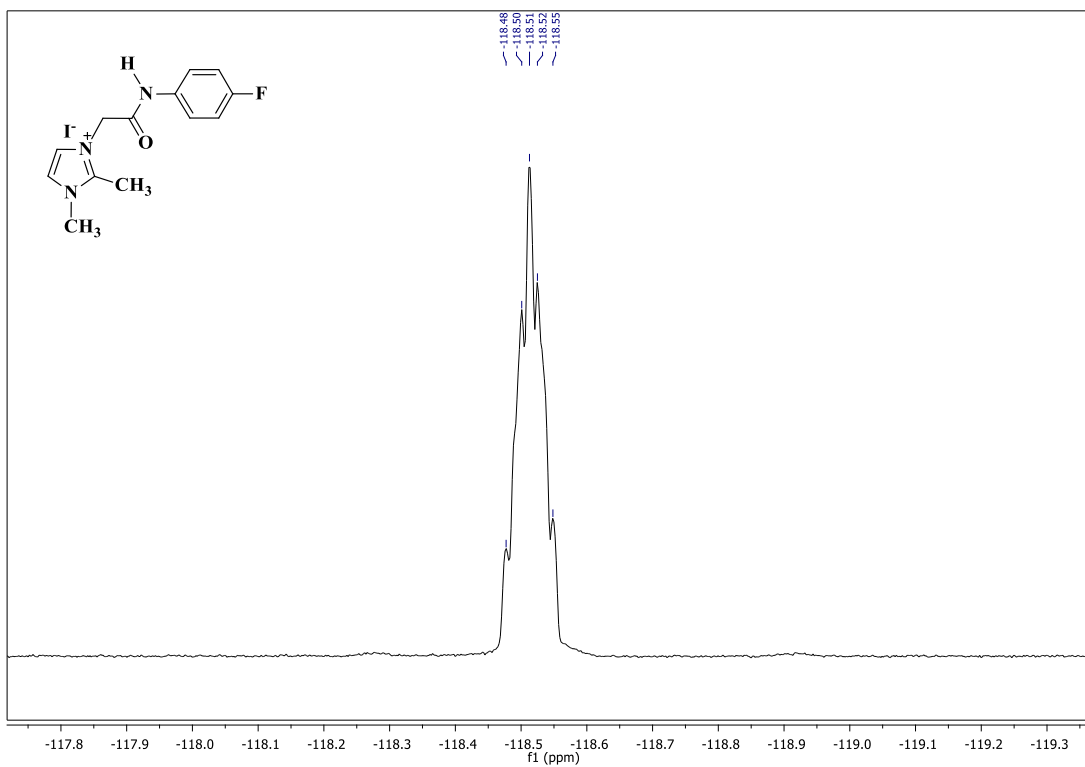
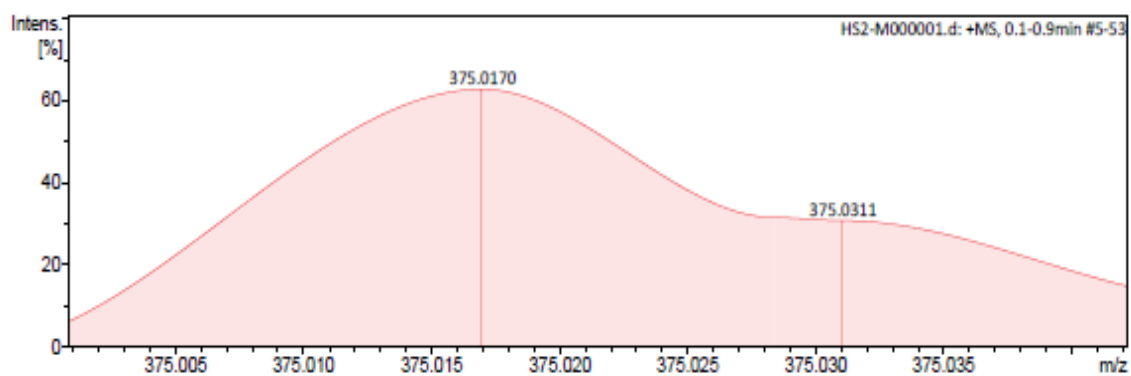


Figure S6: <sup>13</sup>C NMR of compound 4b





**Figure S7:**  $^{19}\text{F}$  NMR of compound **4b**



**Figure S8:** HRMS (ESI) of compound **4b**

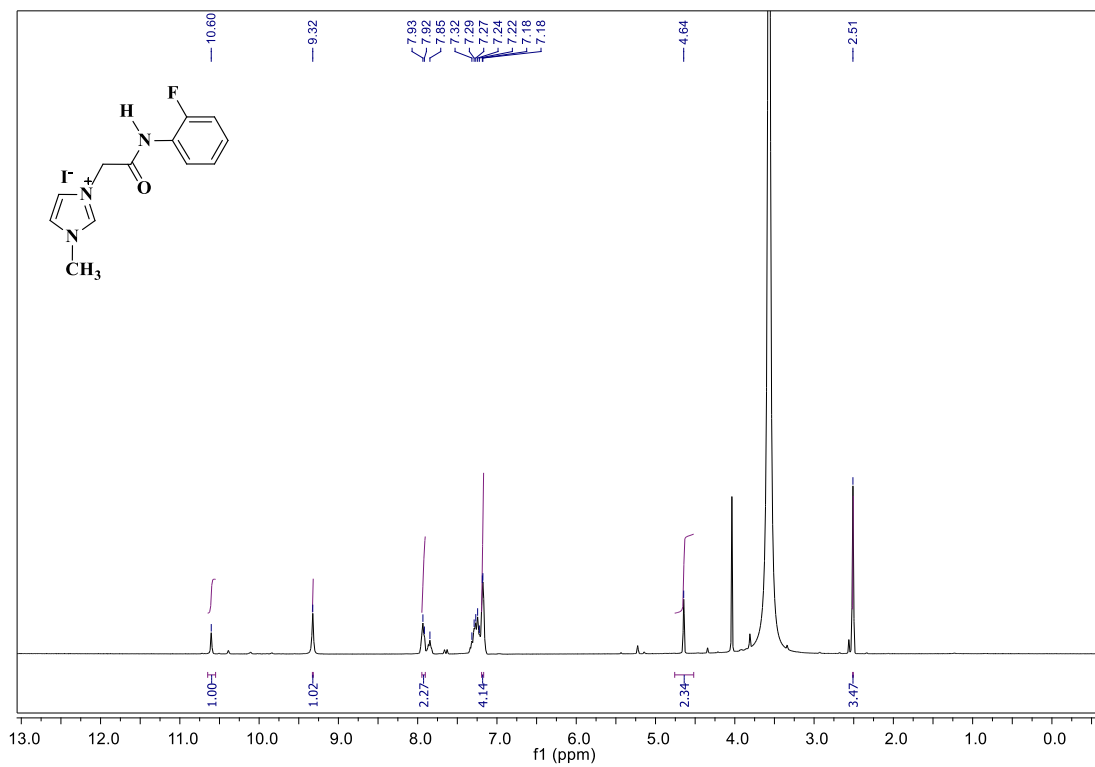


Figure S9: <sup>1</sup>H NMR compound 4c

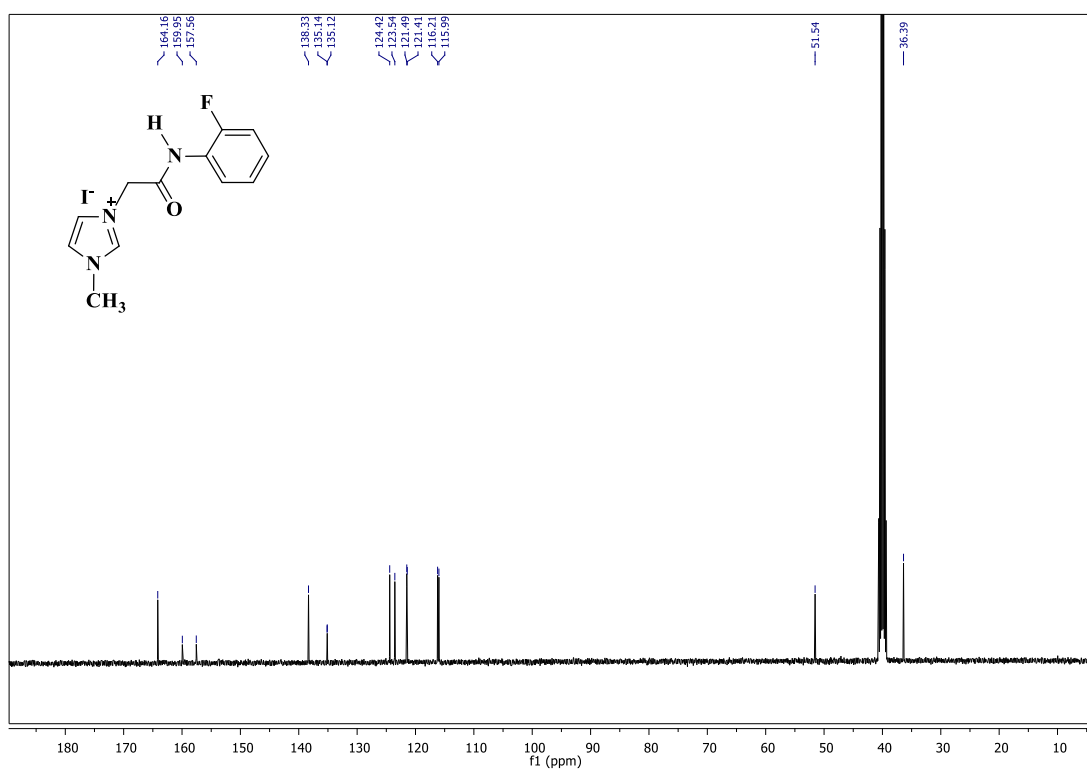
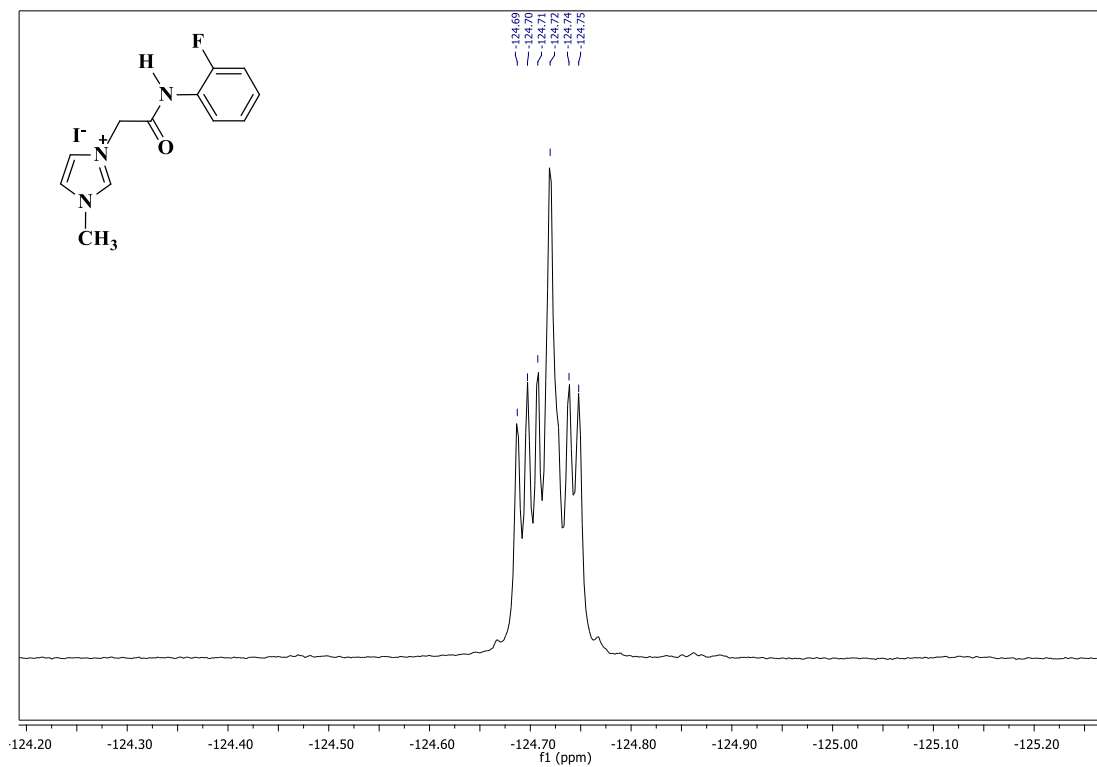
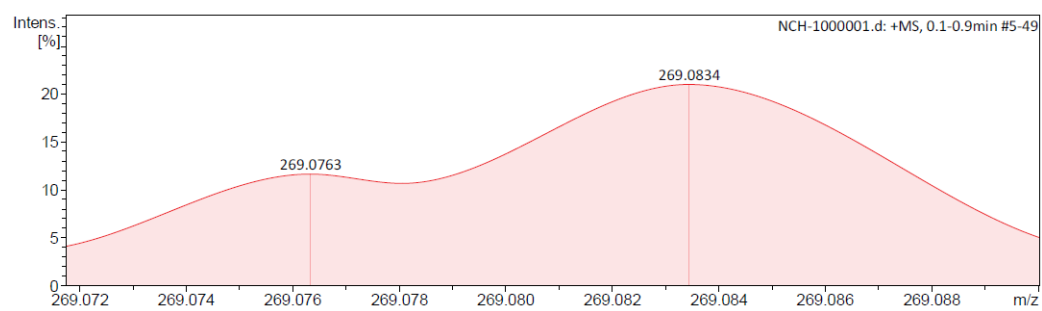


Figure S10: <sup>13</sup>C NMR compound 4c



**Figure S11:**  $^{19}\text{F}$  NMR compound **4c**



**Figure S12:** HRMS (ESI) of compound **4c**

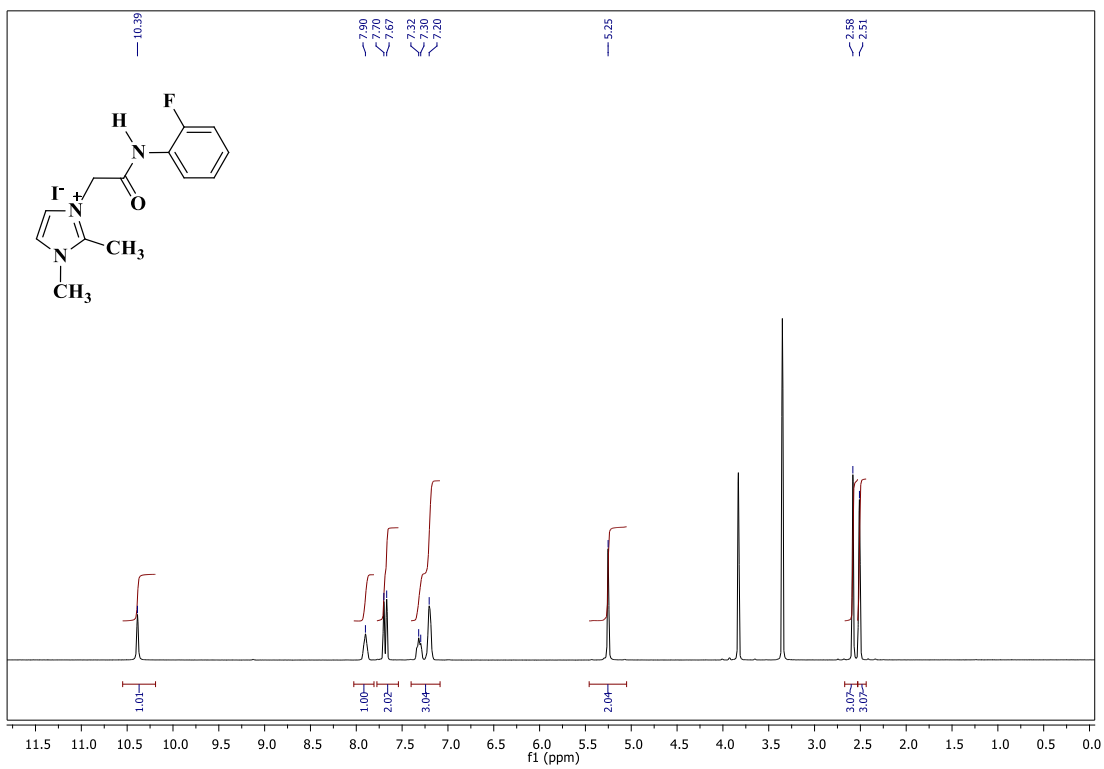


Figure S13: <sup>1</sup>H NMR compound 4d

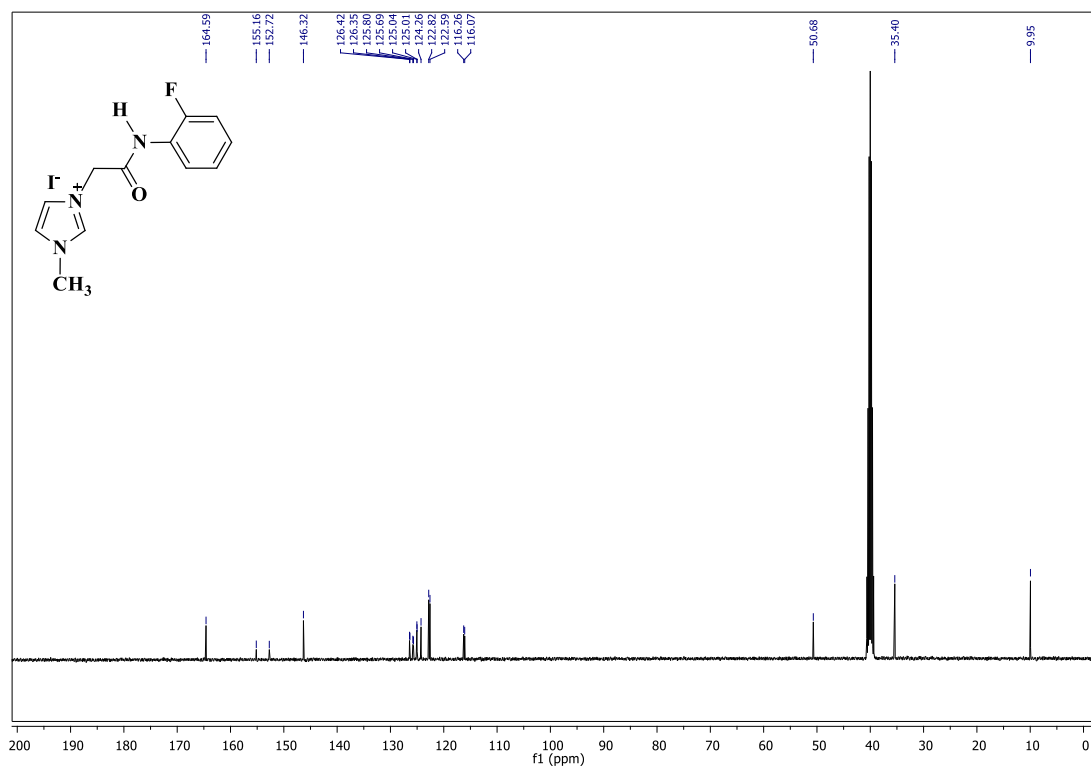
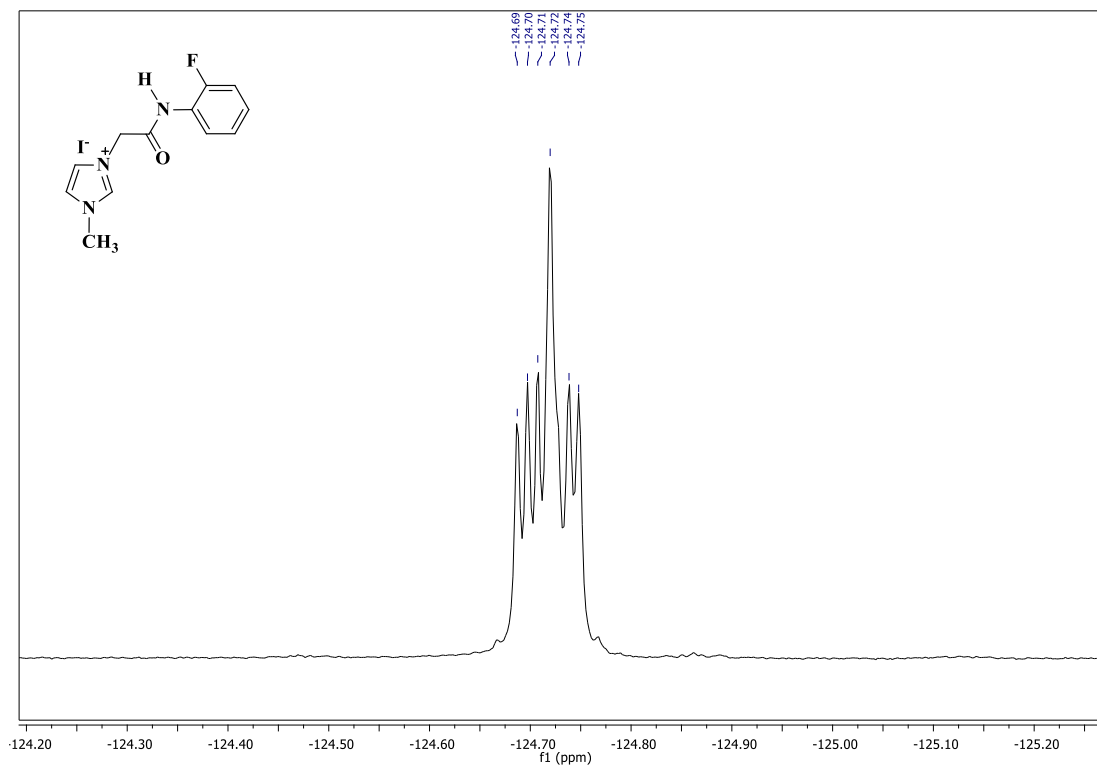
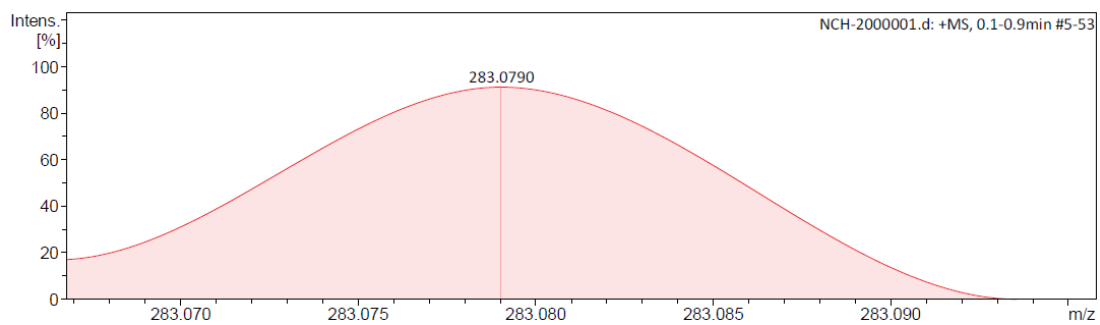


Figure S14: <sup>13</sup>C NMR compound 4d



**Figure S15:**  $^{19}\text{F}$  NMR compound **4d**



**Figure S16:** HRMS (ESI) of compound **4d**

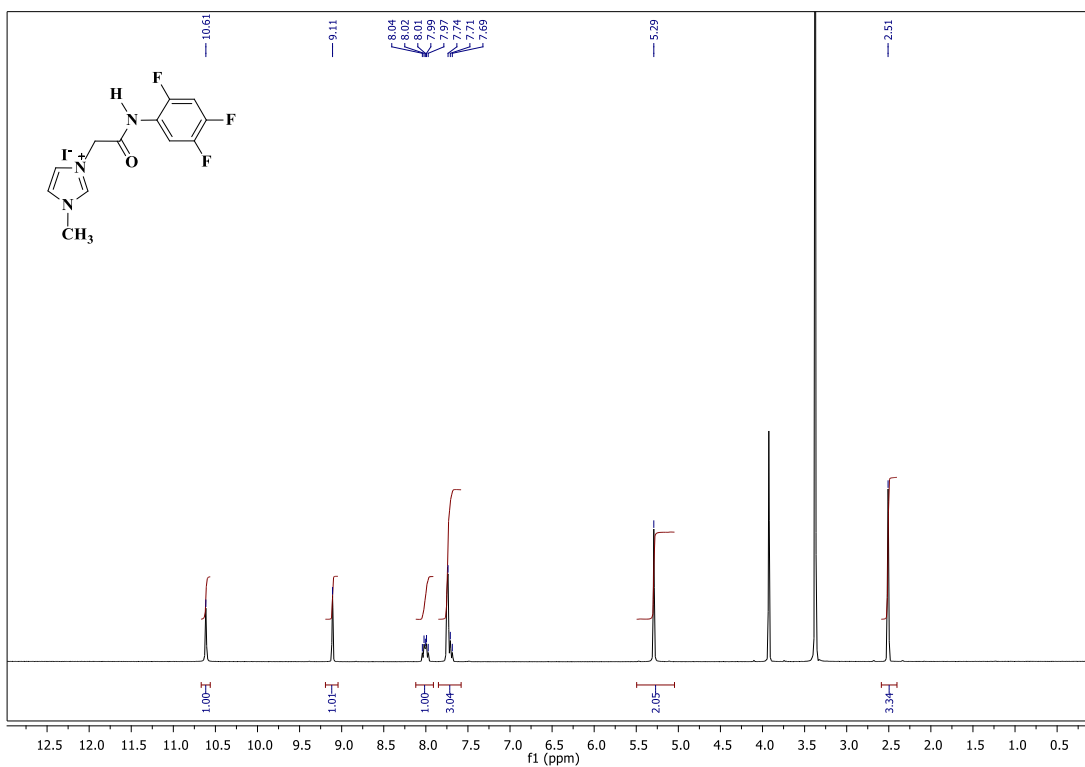


Figure S17:  $^1\text{H NMR}$  of compound 4e

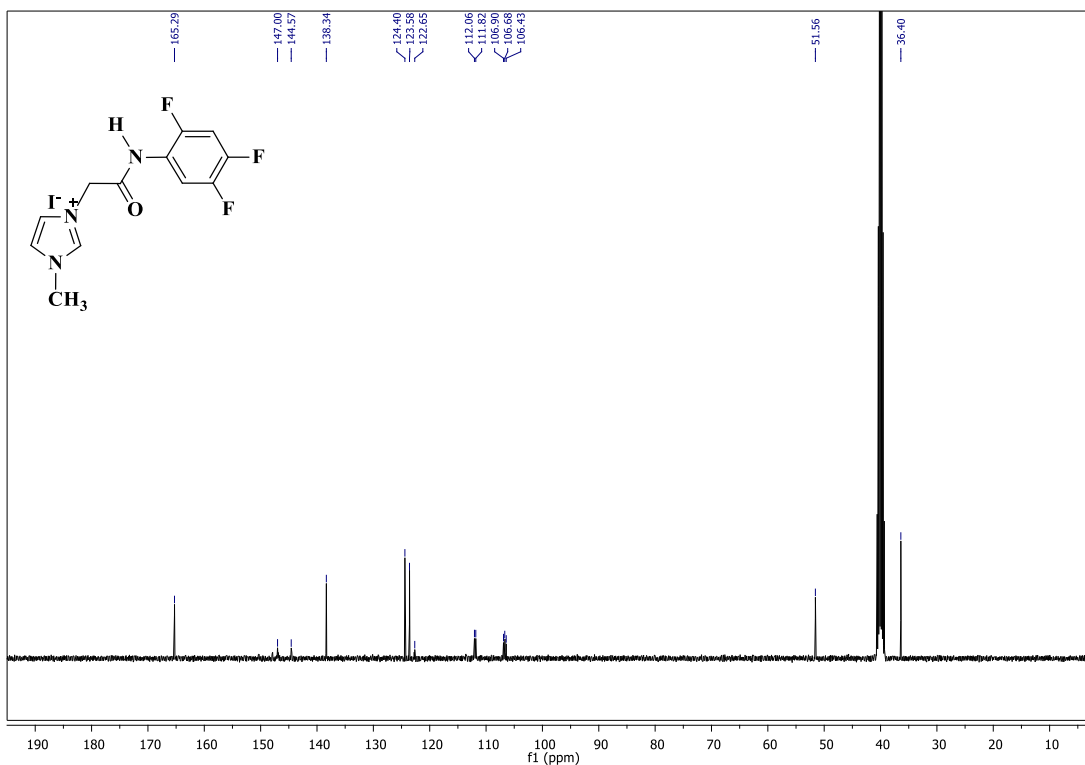


Figure S18:  $^{13}\text{C NMR}$  of compound 4e

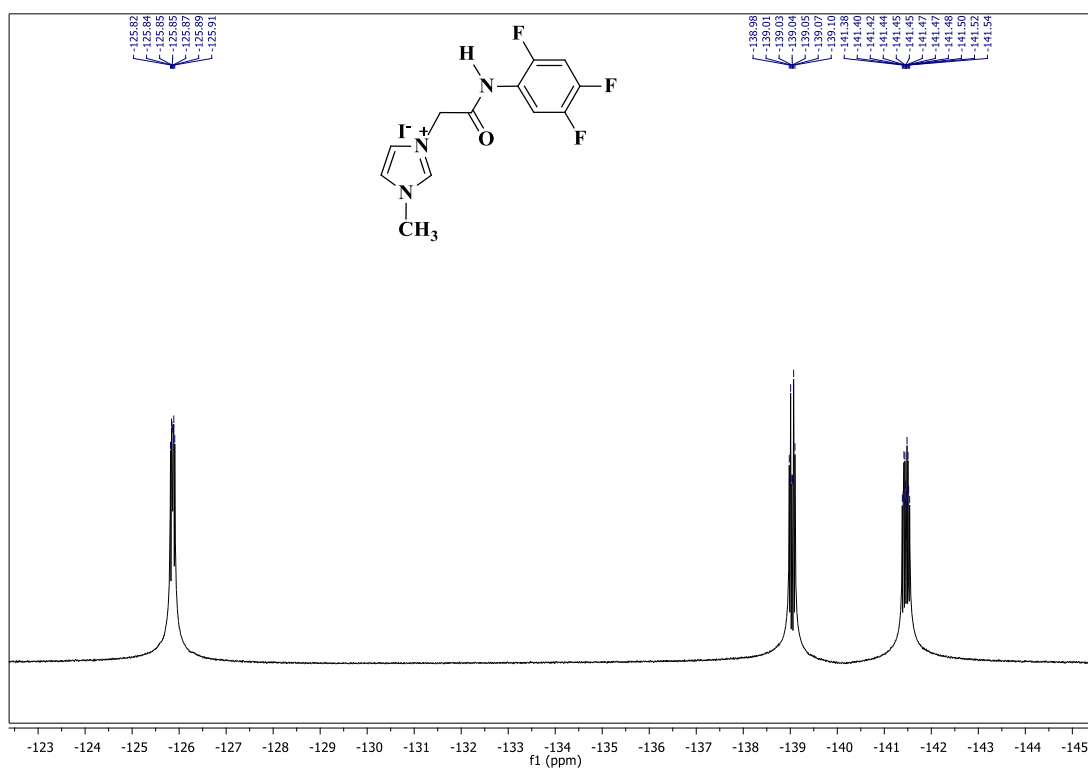


Figure S19:  $^{19}\text{F}$  NMR of compound 4e

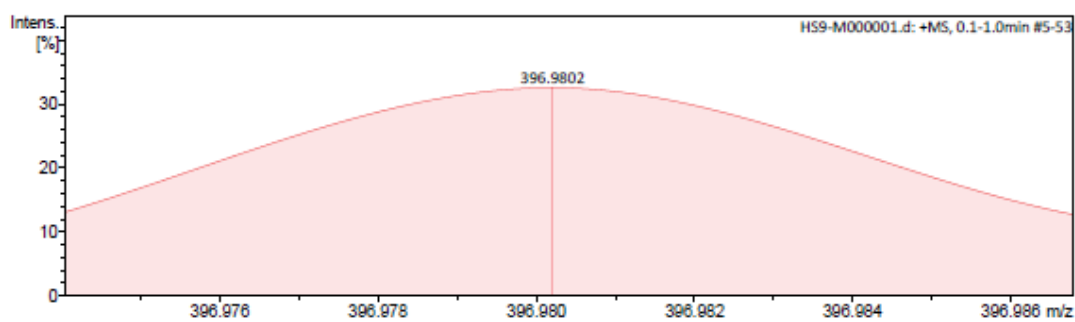


Figure S20: HRMS (ESI) of compound 4e

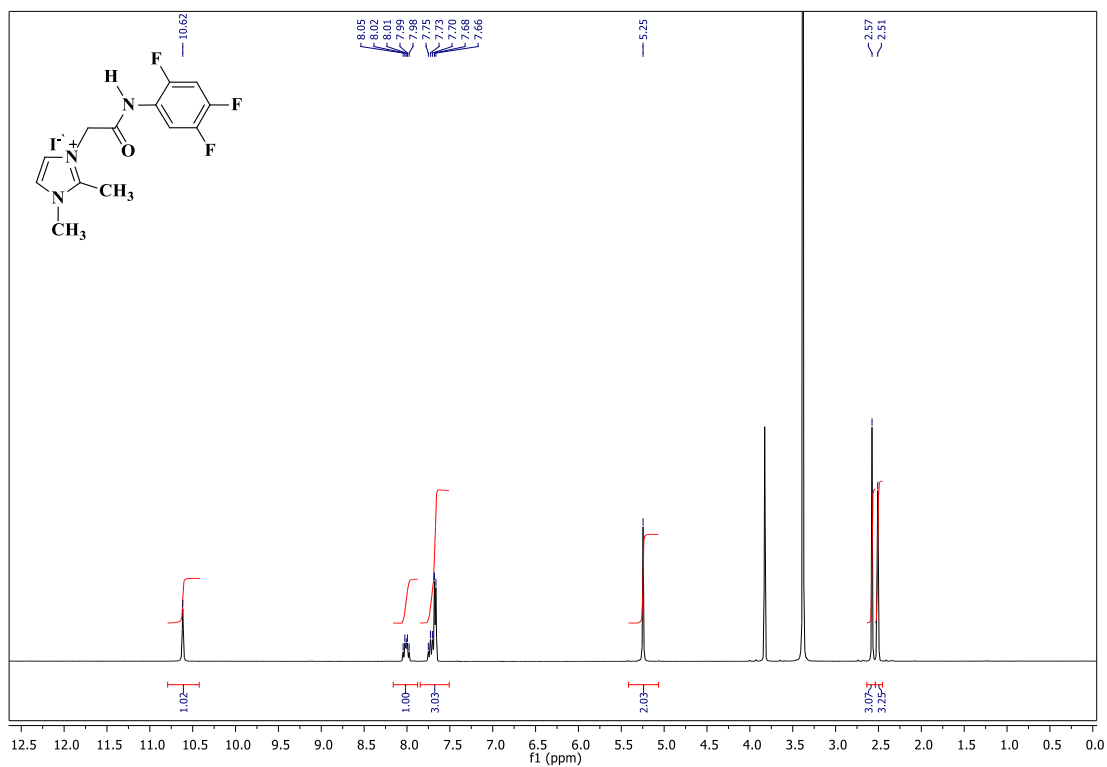


Figure S21: <sup>1</sup>H NMR of compound 4f

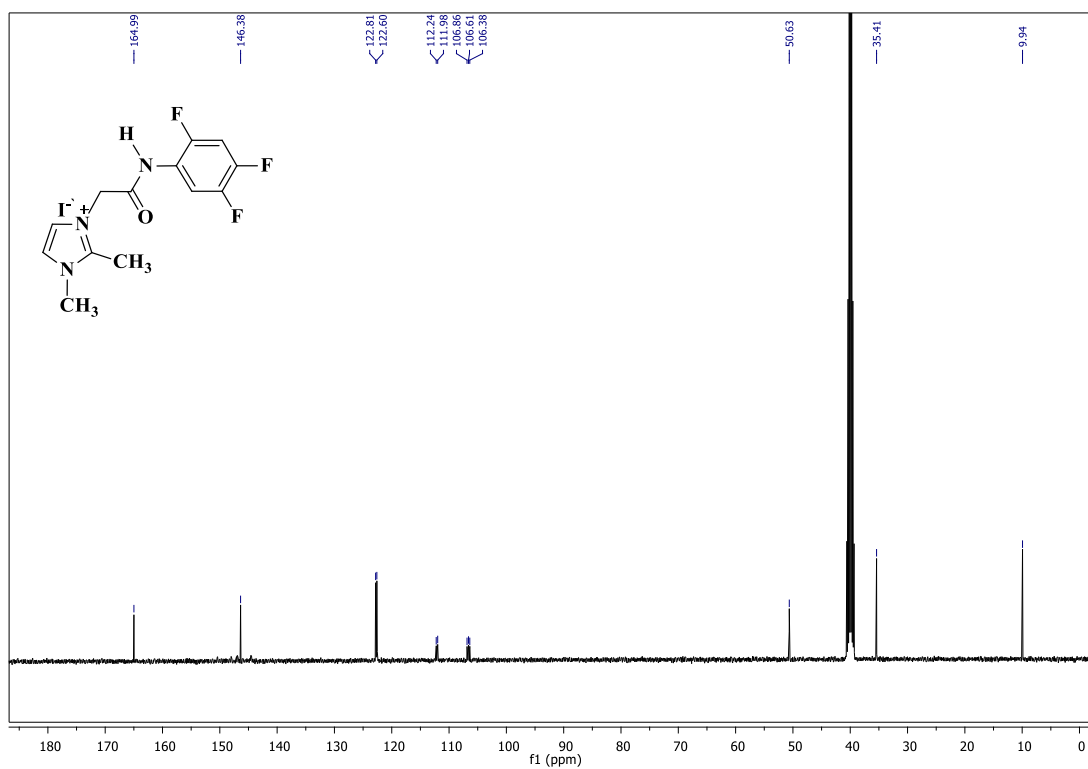
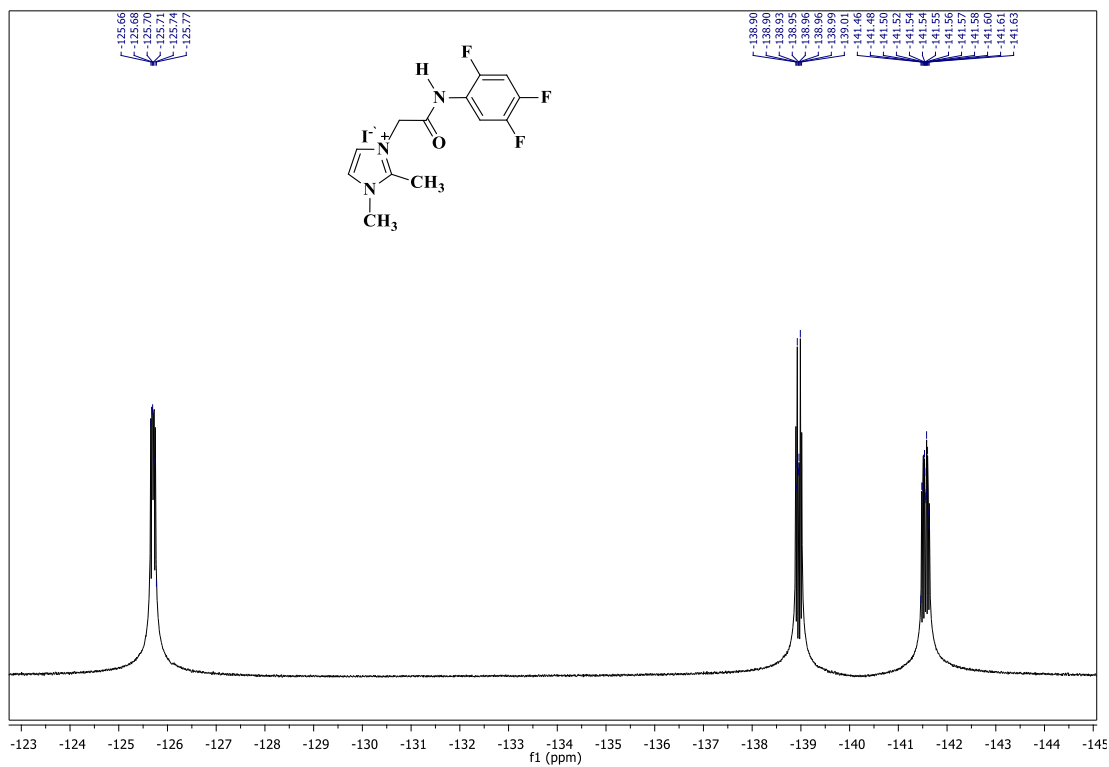
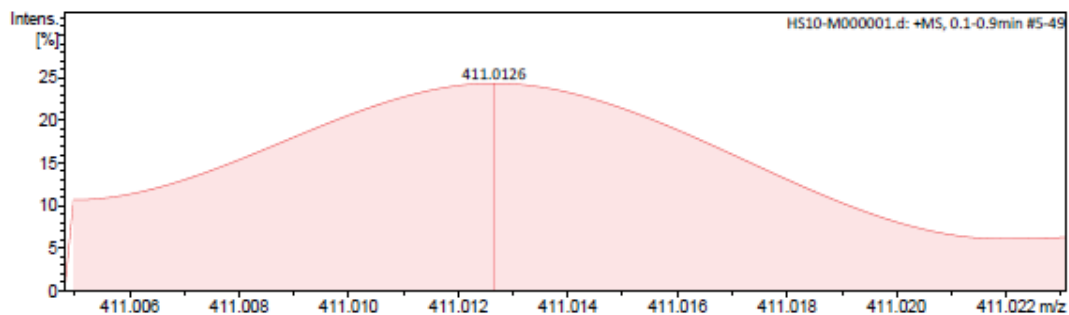


Figure S22: <sup>13</sup>C NMR of compound 4f





**Figure S23:** <sup>19</sup>F NMR of compound **4f**



**Figure S24:** HRMS (ESI) of compound **4f**

$^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{19}\text{F}$ ,  $^{11}\text{B}$ ,  $^{31}\text{P}$ -NMR and MS Spectra of Compounds 5a-r

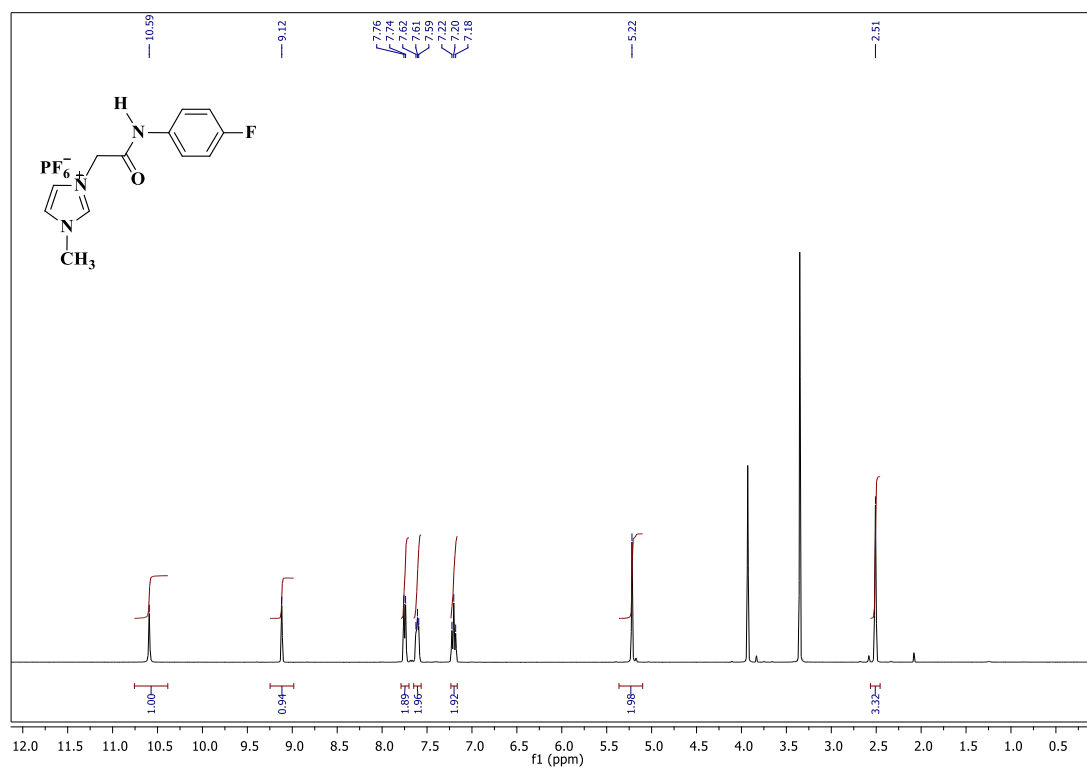


Figure S25:  $^1\text{H}$  NMR of compound 5a

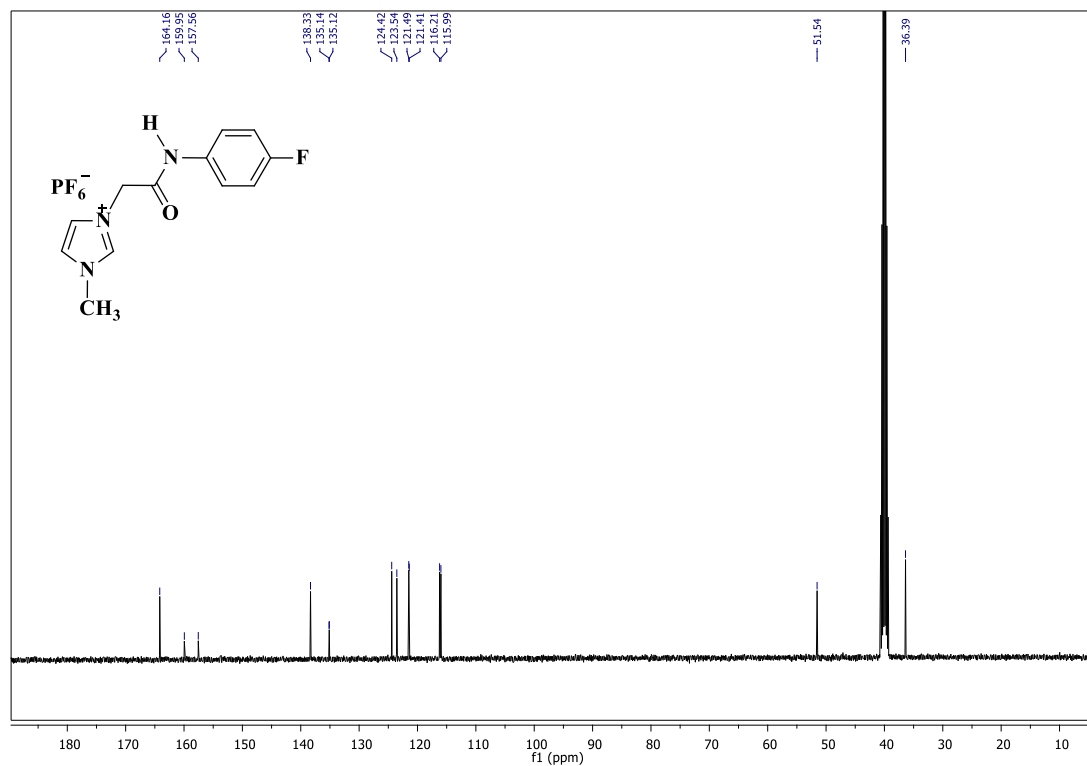
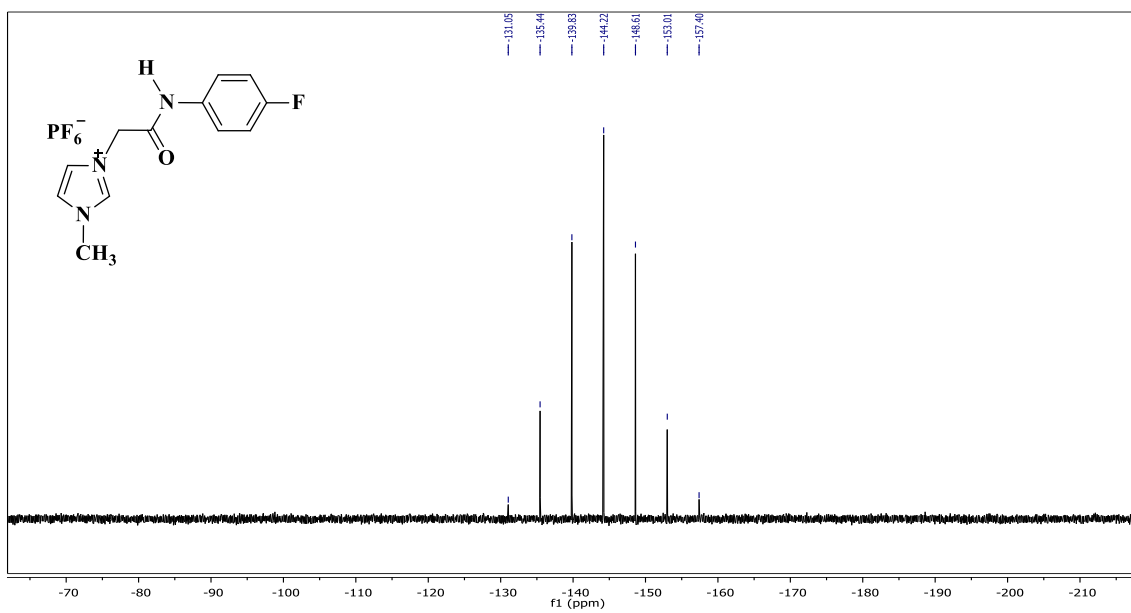
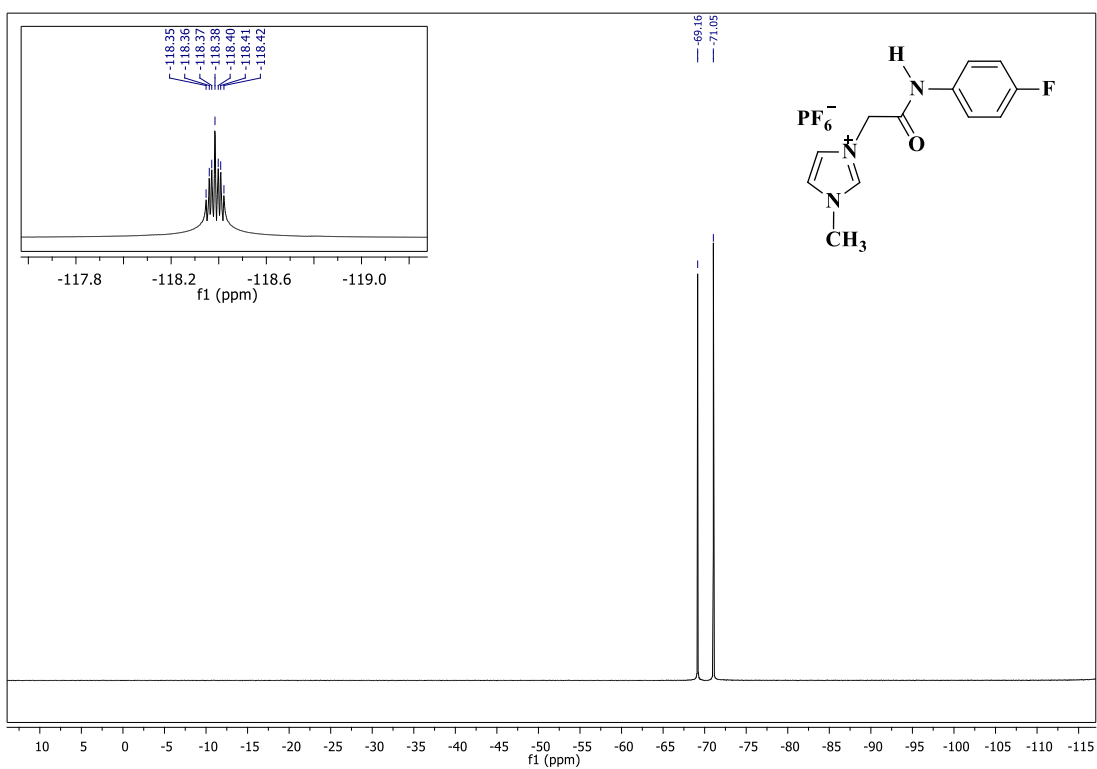


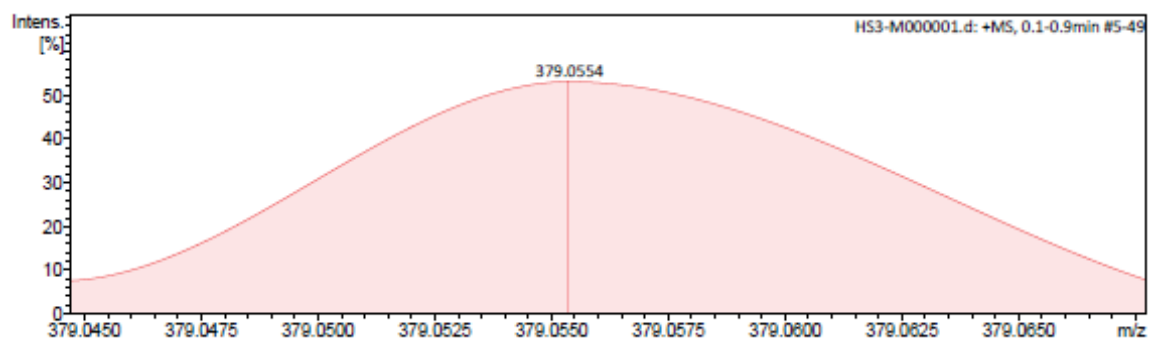
Figure S26:  $^{13}\text{C}$  NMR of compound 5a



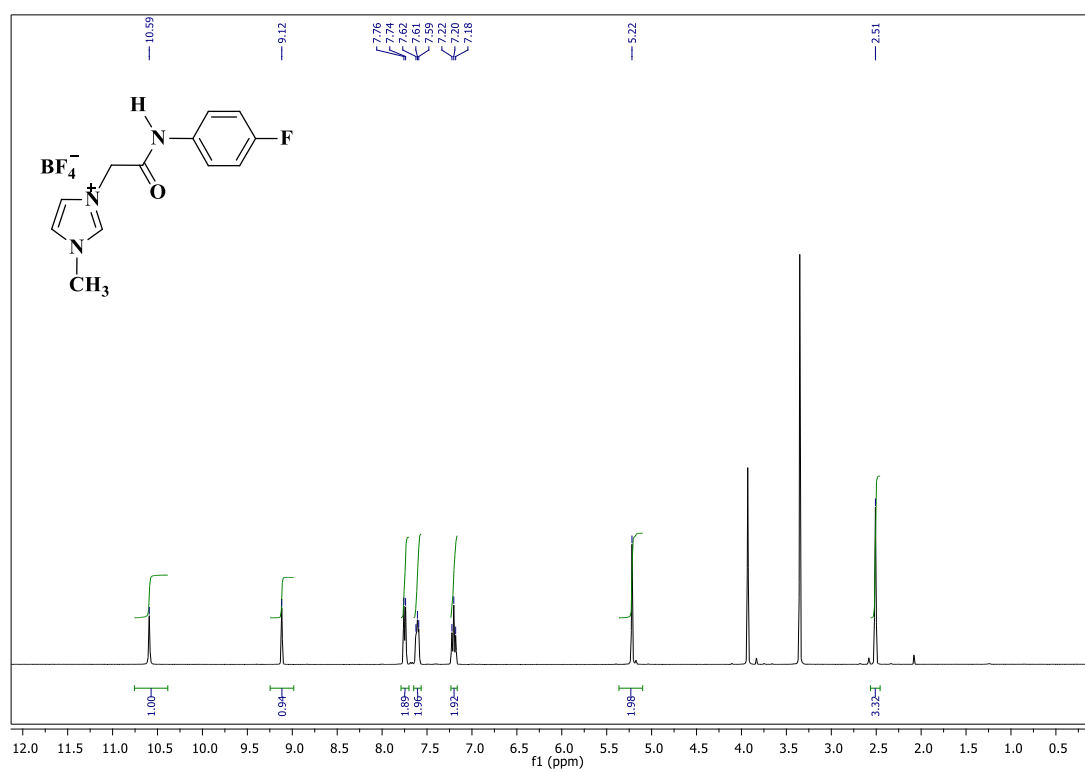
**Figure S27:**  $^{31}\text{P}$  NMR of compound **5a**



**Figure S28:**  $^{19}\text{F}$  NMR of compound **5a**



**Figure S29:** HRMS (ESI) of compound **5a**



**Figure S30:** <sup>1</sup>H NMR of compound **5b**

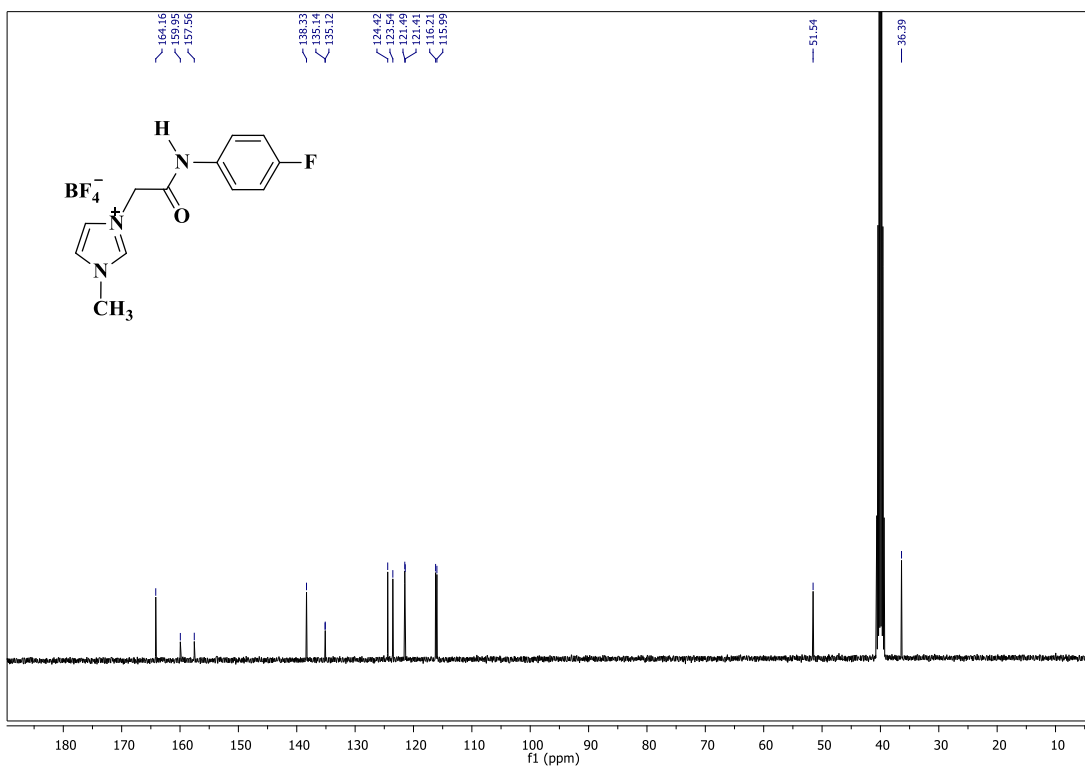


Figure S31:  $^{13}\text{C}$  NMR of compound **5b**

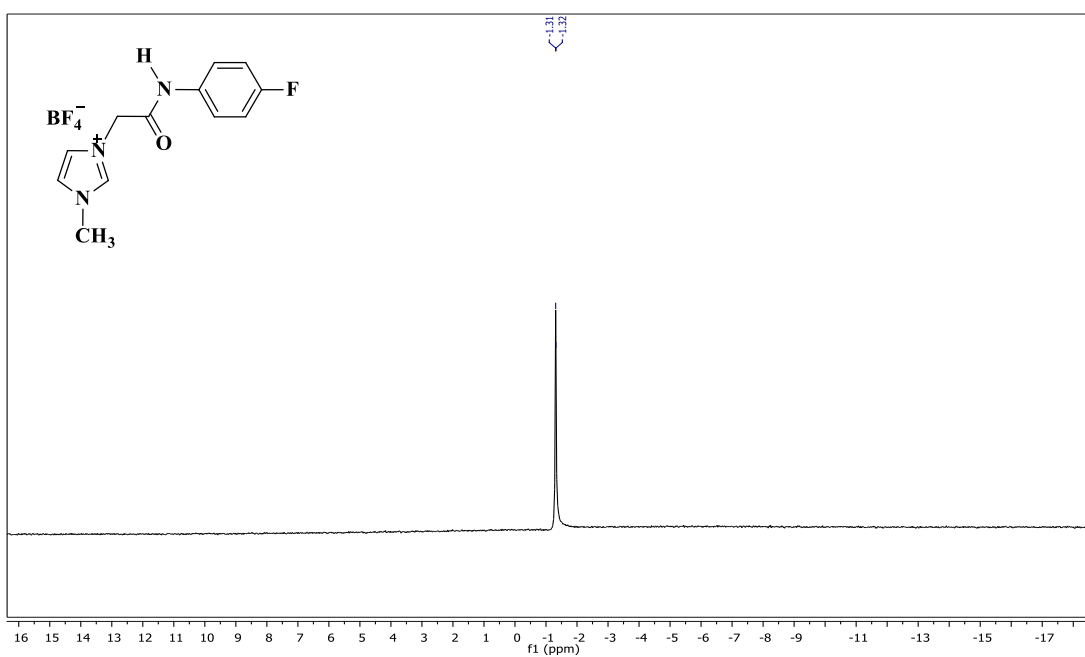
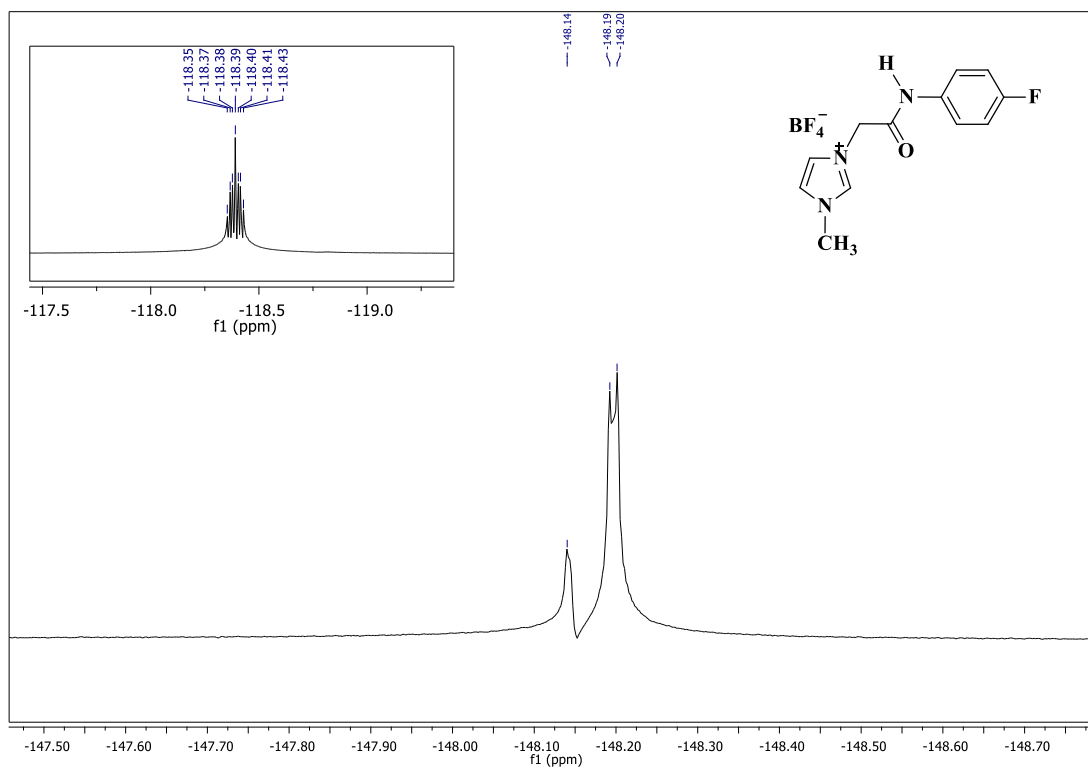
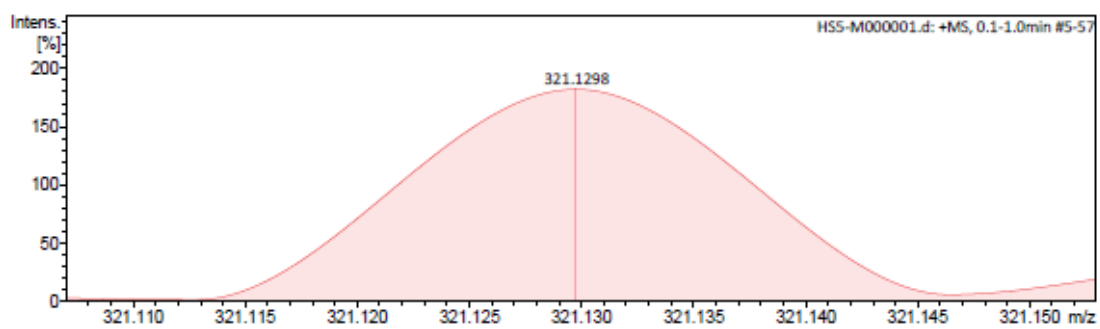


Figure S32:  $^{11}\text{B}$  NMR of compound **5b**.



**Figure S33:**  $^{19}\text{F}$  NMR of compound **5b**



**Figure S34:** HRMS (ESI) of compound **5b**

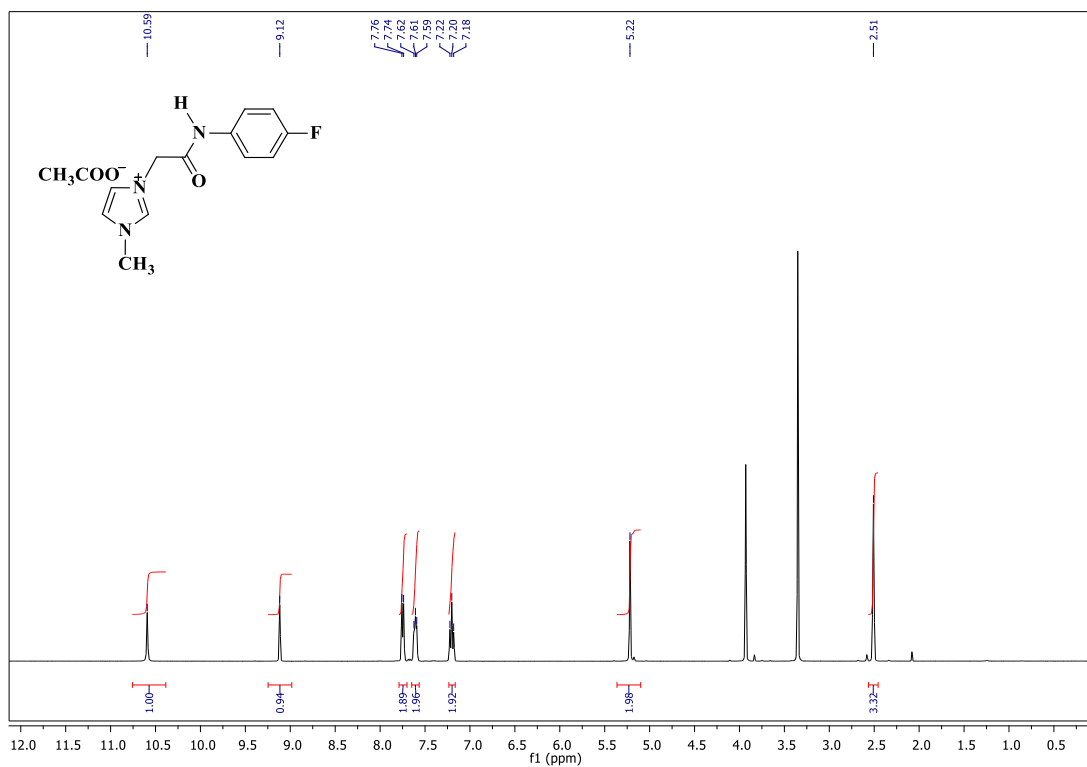


Figure S35: <sup>1</sup>H NMR of compound **5c**

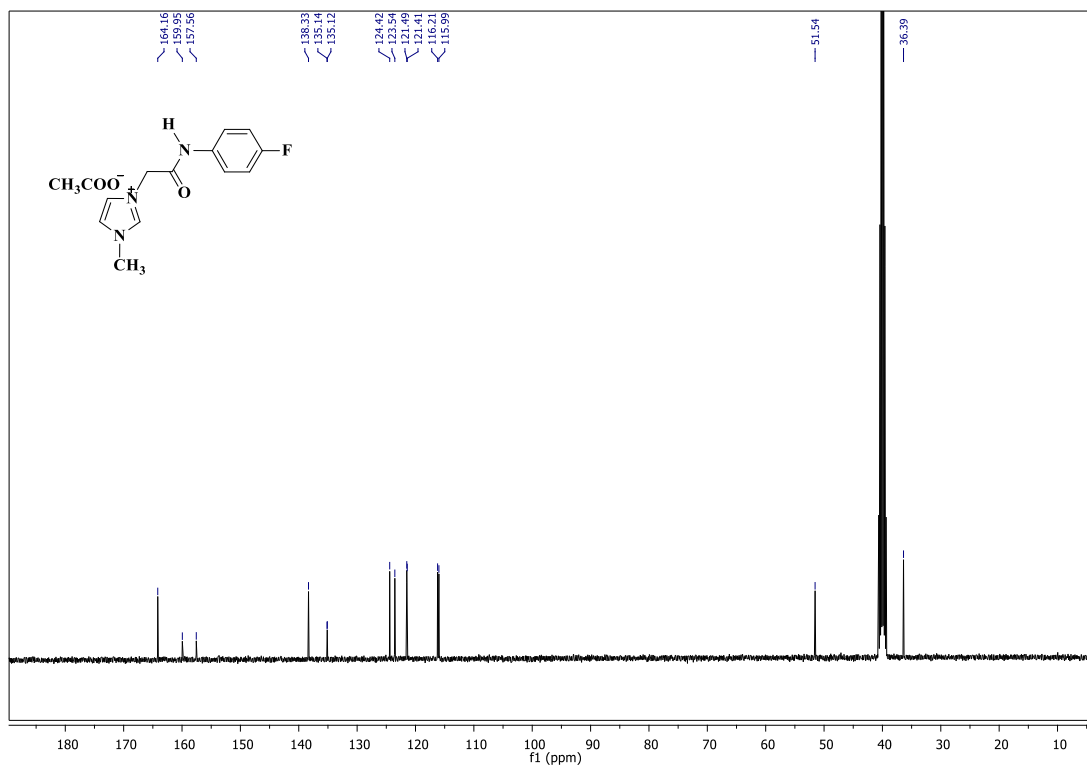
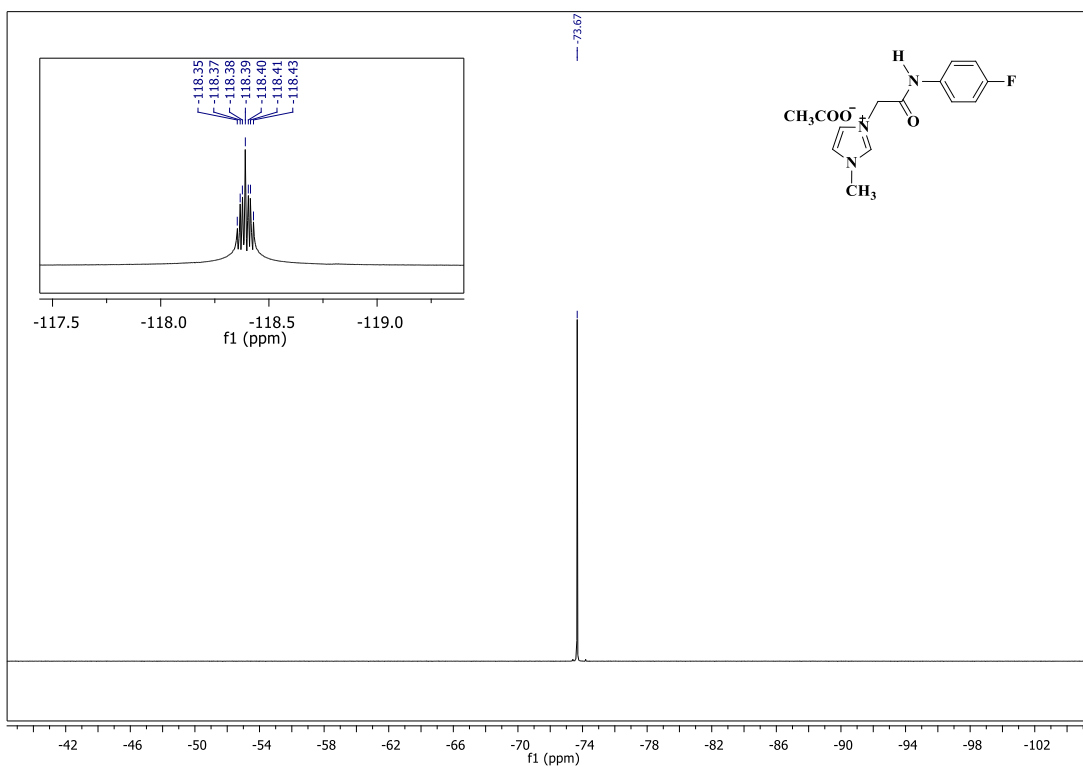
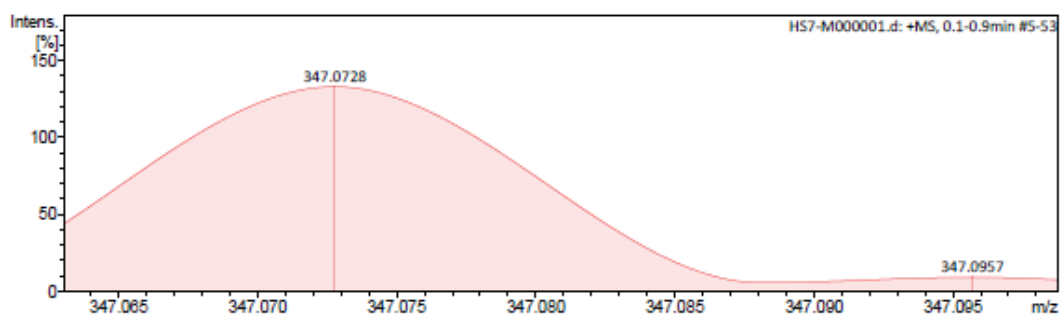


Figure S36: <sup>13</sup>C NMR of compound **5c**

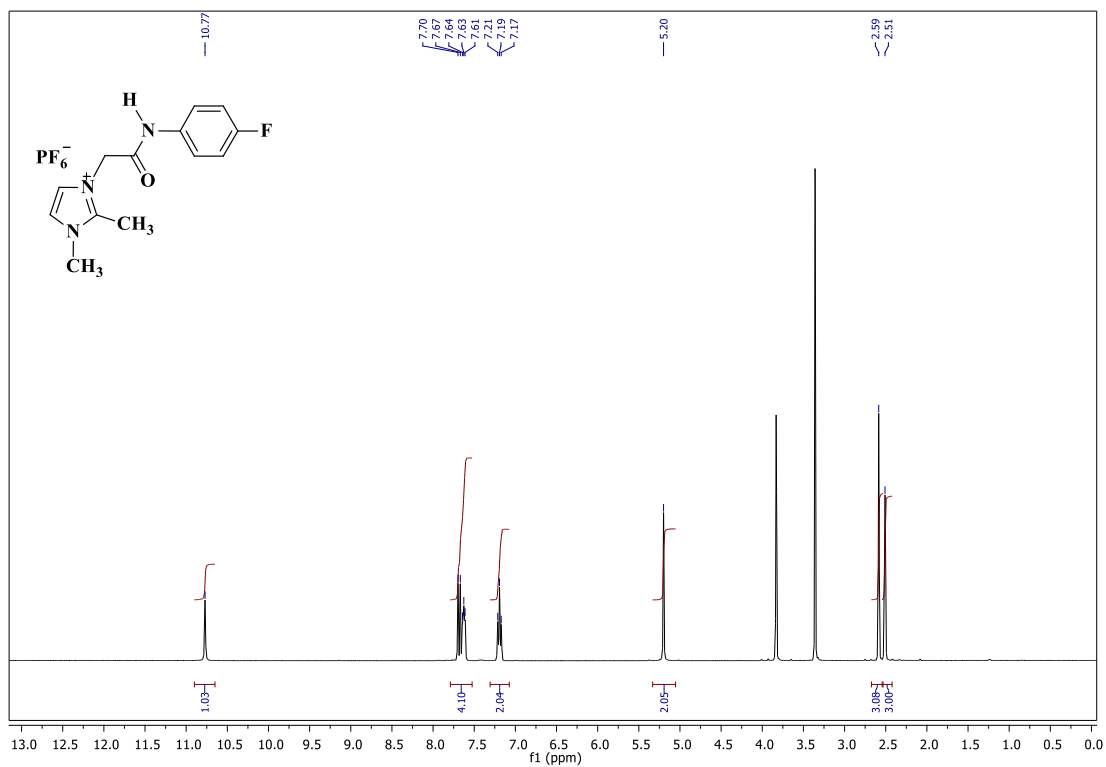


**Figure S37:**  $^{19}\text{F}$  NMR of compound **5c**

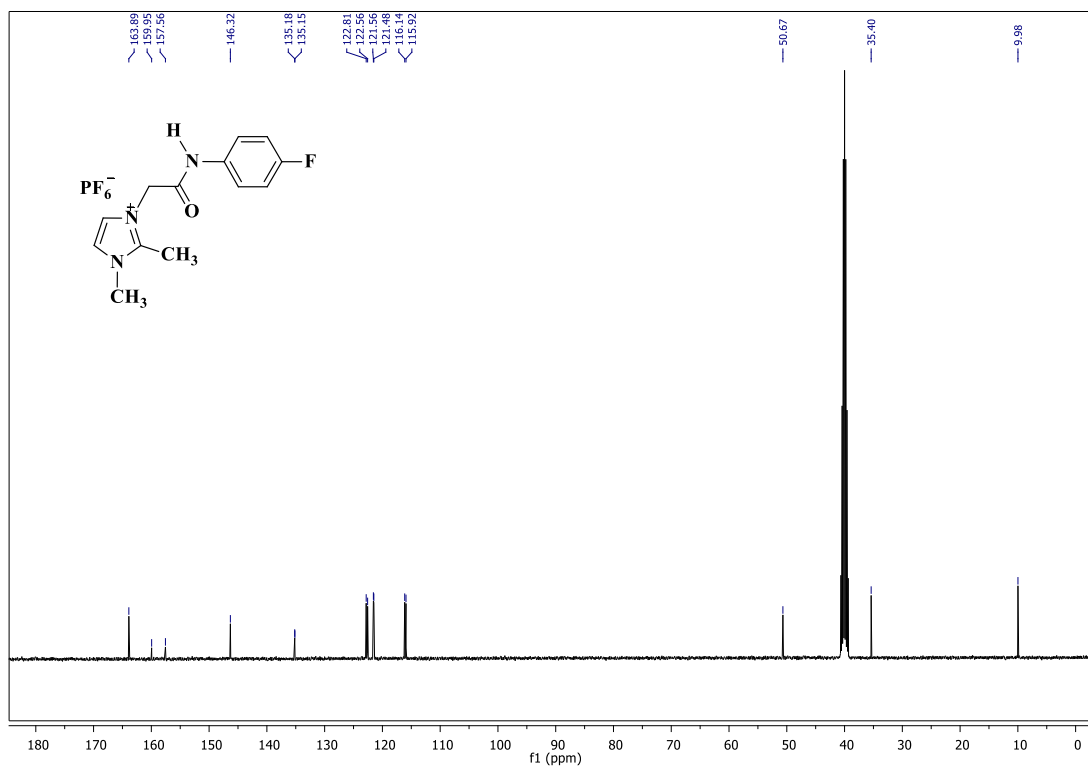


**Figure S38:** HRMS (ESI) of compound **5c**

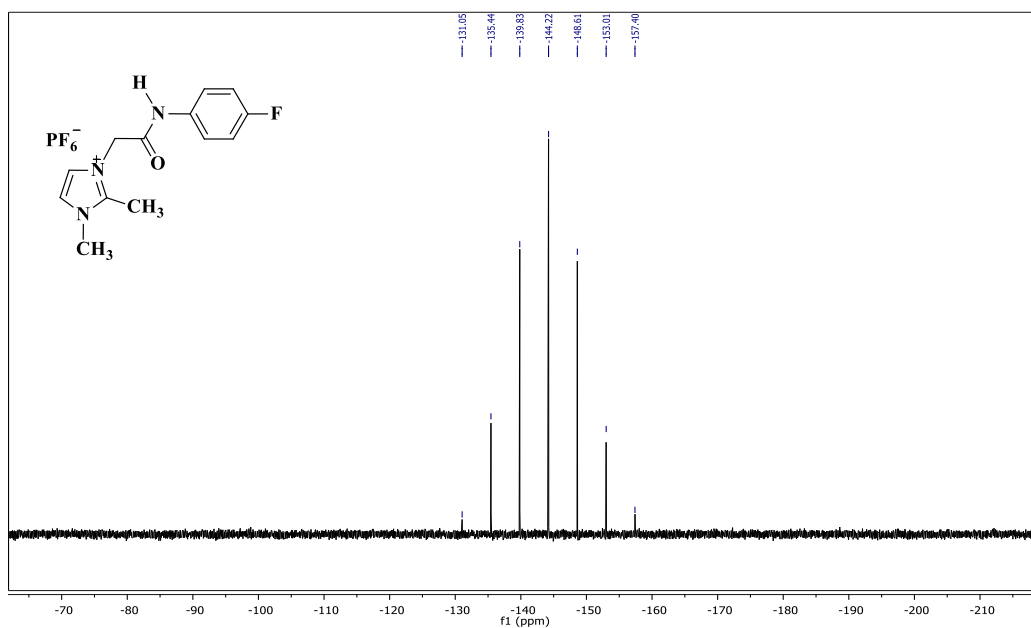




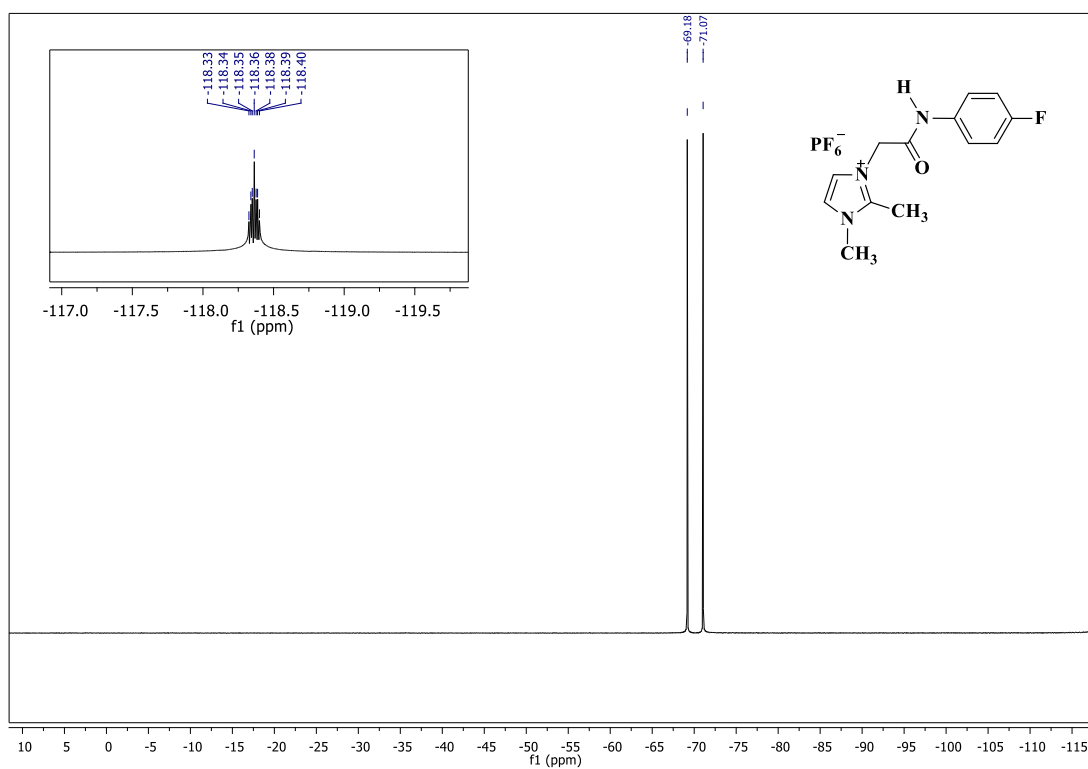
**Figure S39:** <sup>1</sup>H NMR of compound **5d**



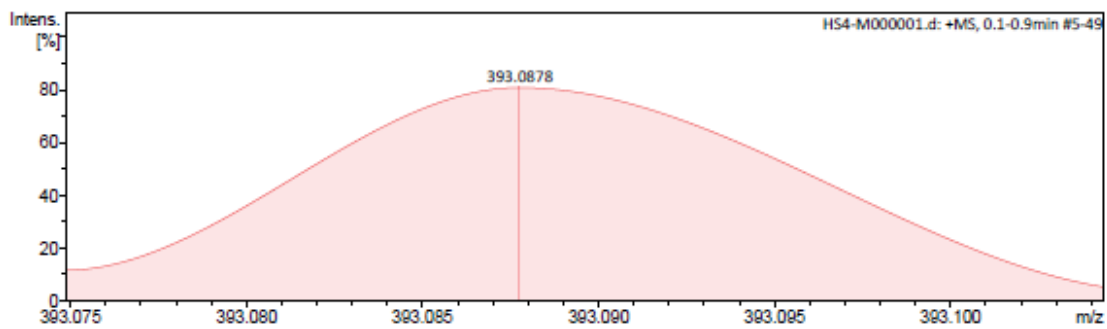
**Figure S40:** <sup>13</sup>C NMR of compound **5d**  
S25



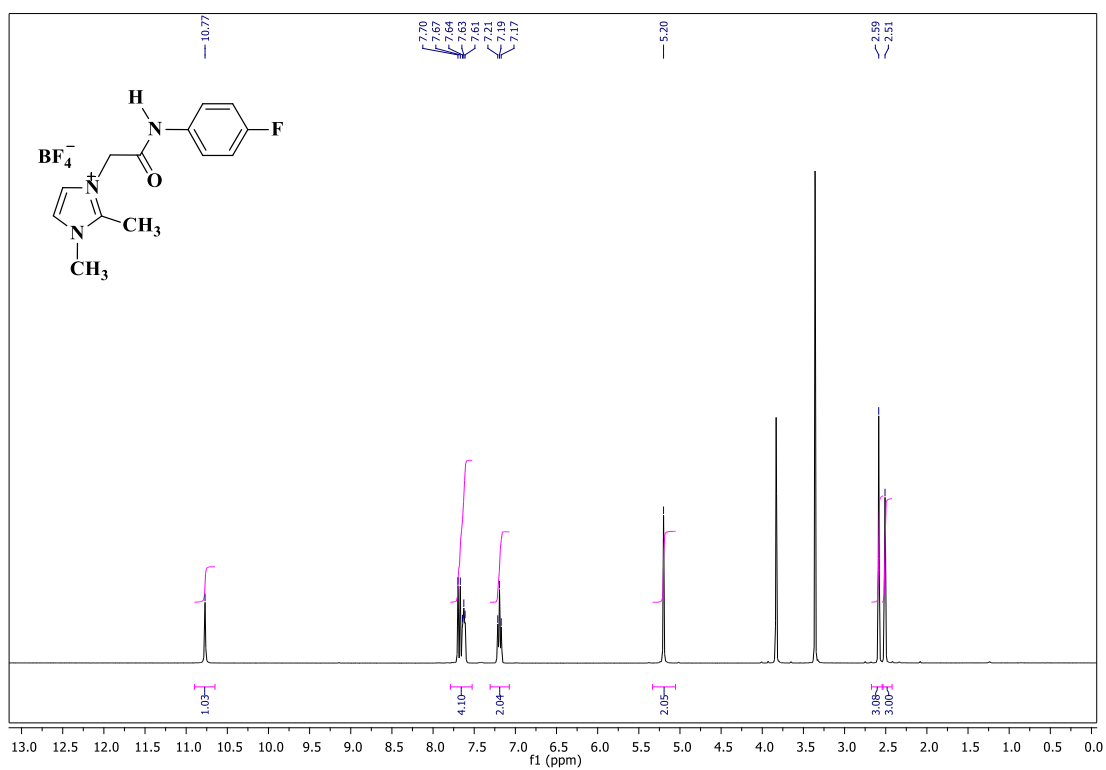
**Figure S41:**  $^{31}\text{P}$  NMR of compound **5d**



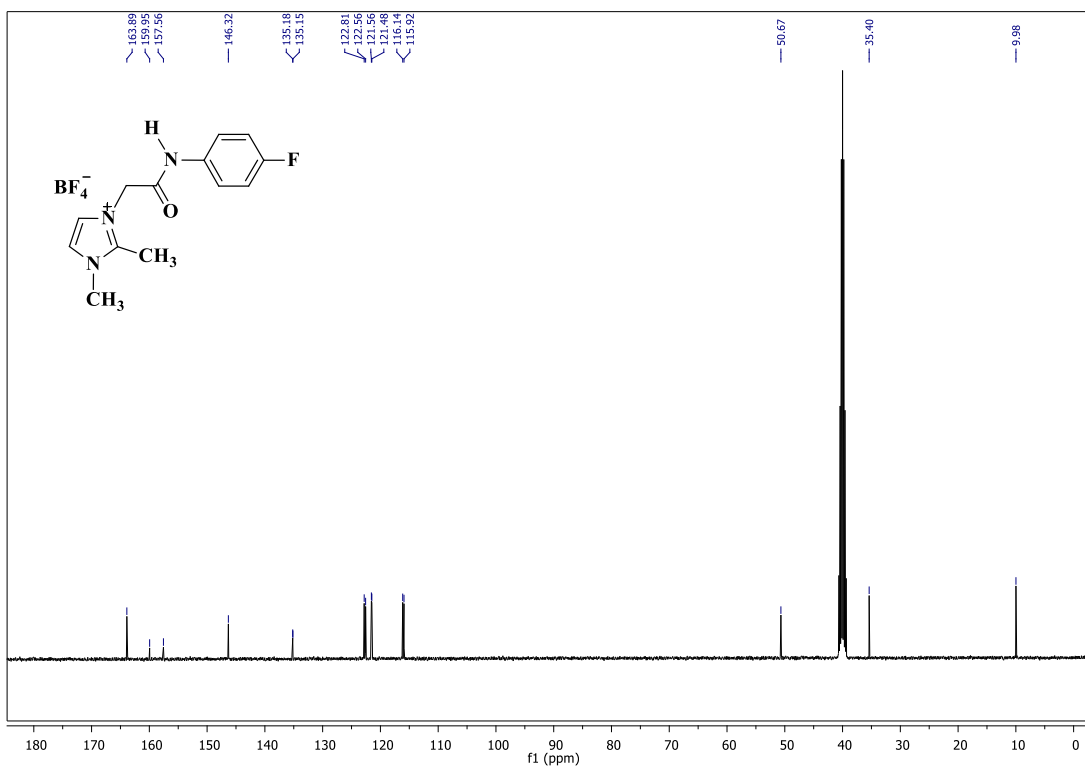
**Figure S42:**  $^{19}\text{F}$  NMR of compound **5d**



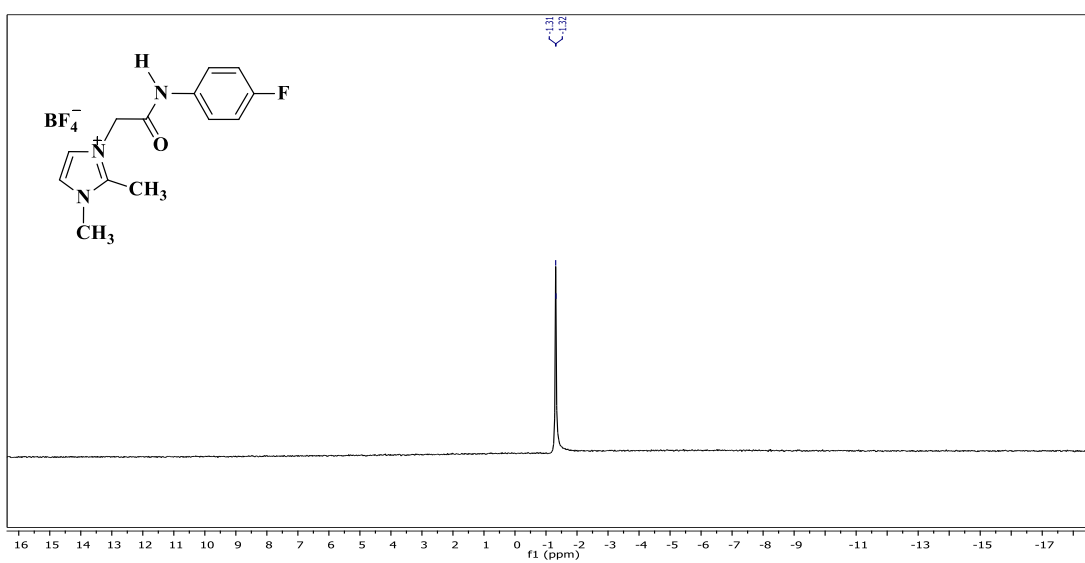
**Figure S43:** HRMS (ESI) of compound **5d**



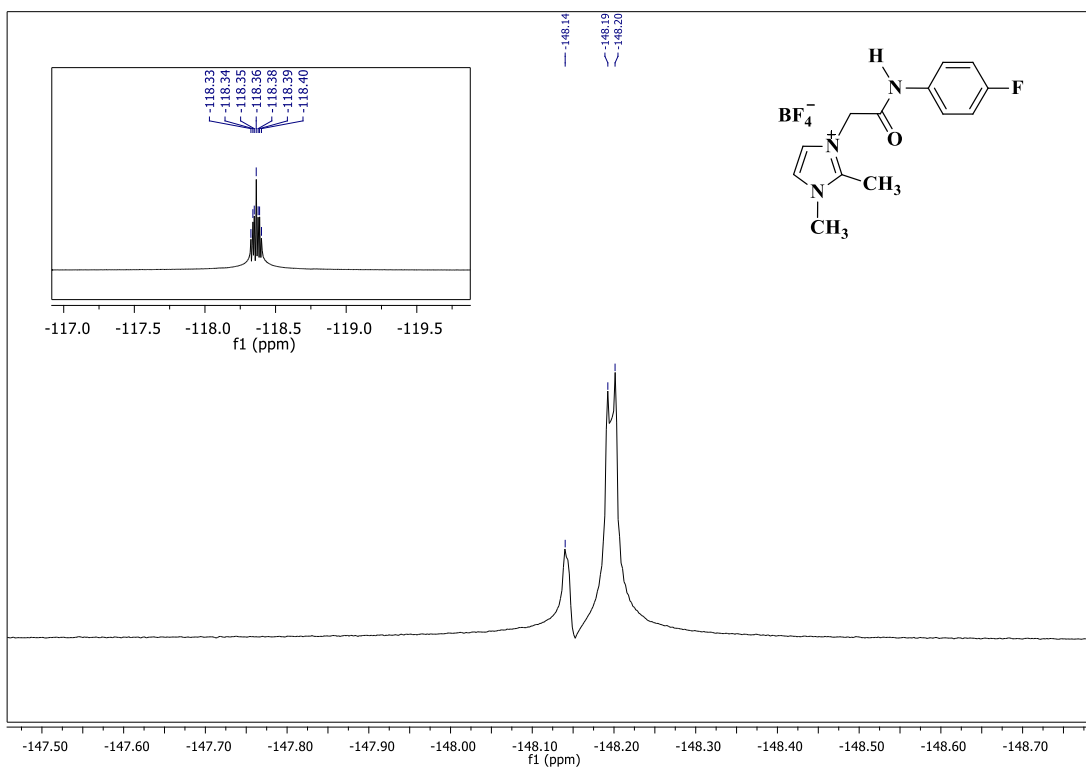
**Figure S44:** <sup>1</sup>H NMR of compound **5e**



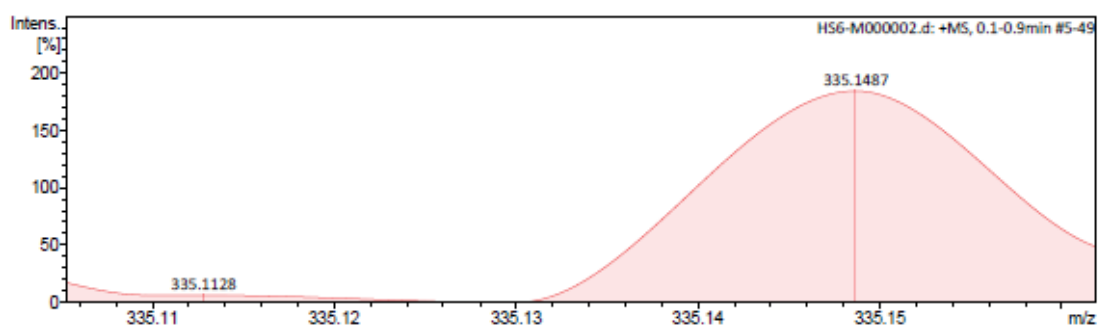
**Figure S45:**  $^{13}\text{C}$  NMR of compound **5e**



**Figure S46:**  $^{11}\text{B}$  NMR of compound **5e**



**Figure S47:**  $^{19}\text{F}$  NMR of compound **5e**



**Figure S48:** HRMS (ESI) of compound **5e**

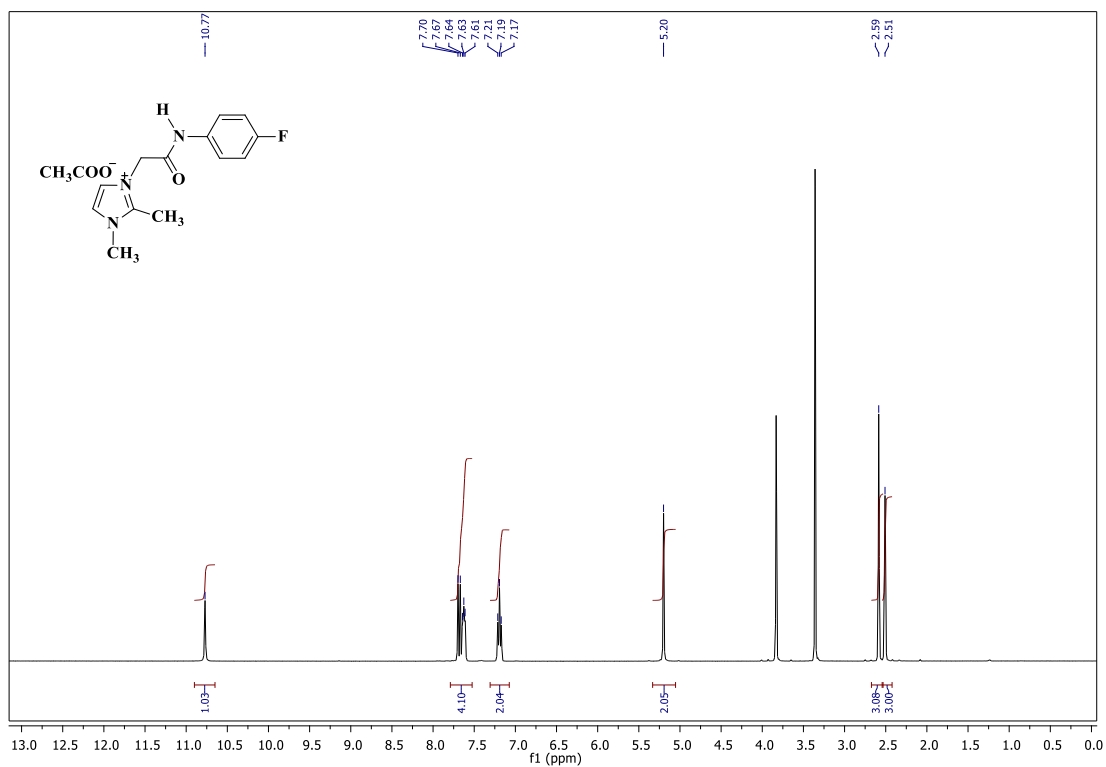


Figure S49: <sup>1</sup>H NMR of compound **5f**

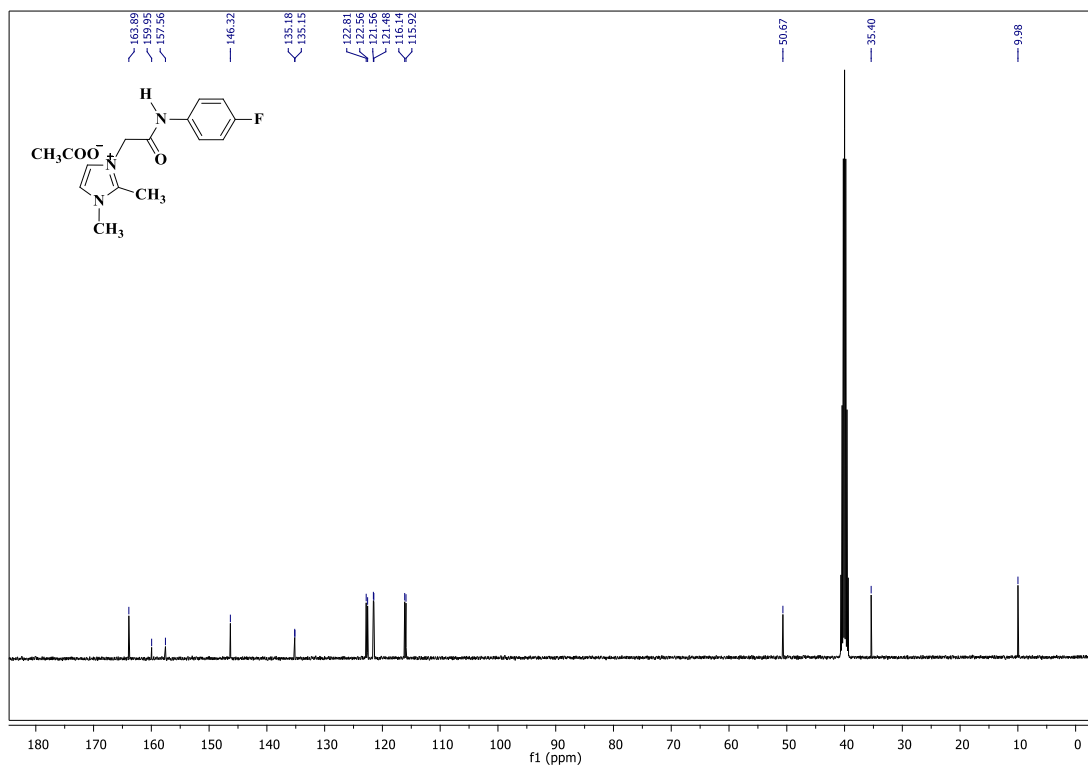


Figure S50: <sup>13</sup>C NMR of compound **5f**

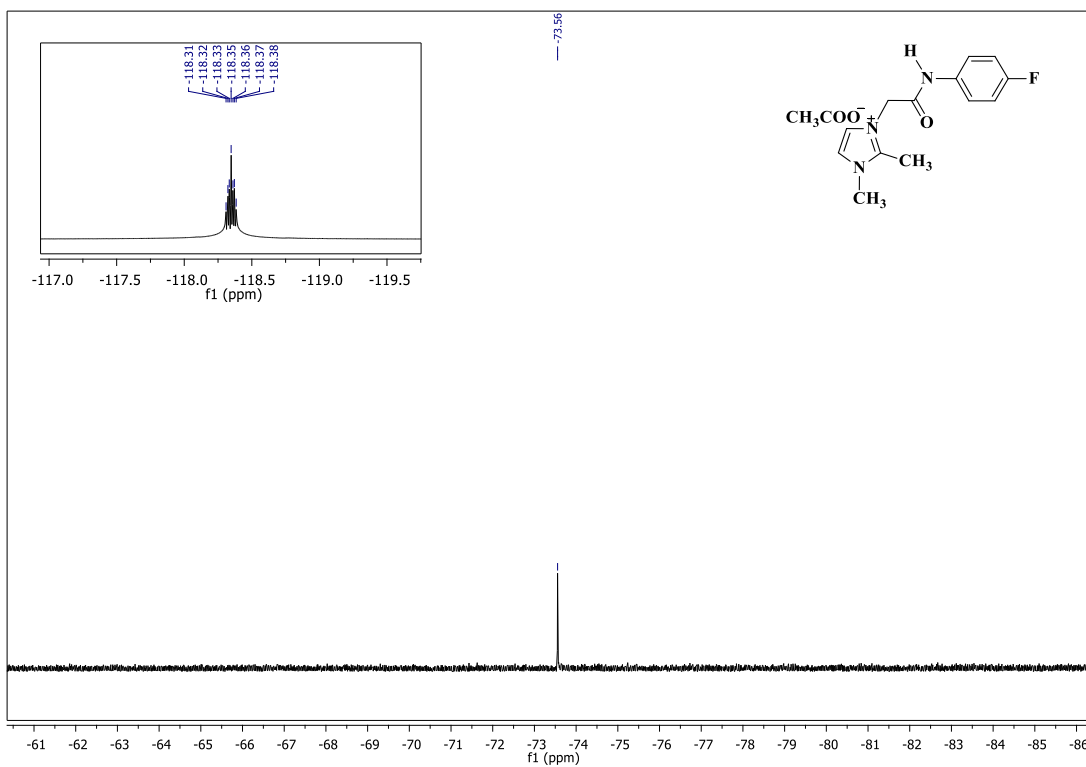


Figure S51:  $^{19}\text{F}$  NMR of compound **5f**

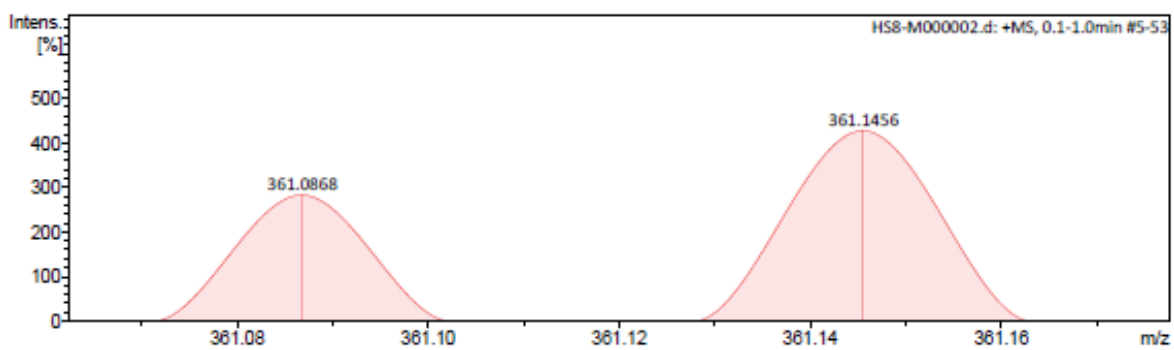


Figure S52: HRMS (ESI) of compound **5f**

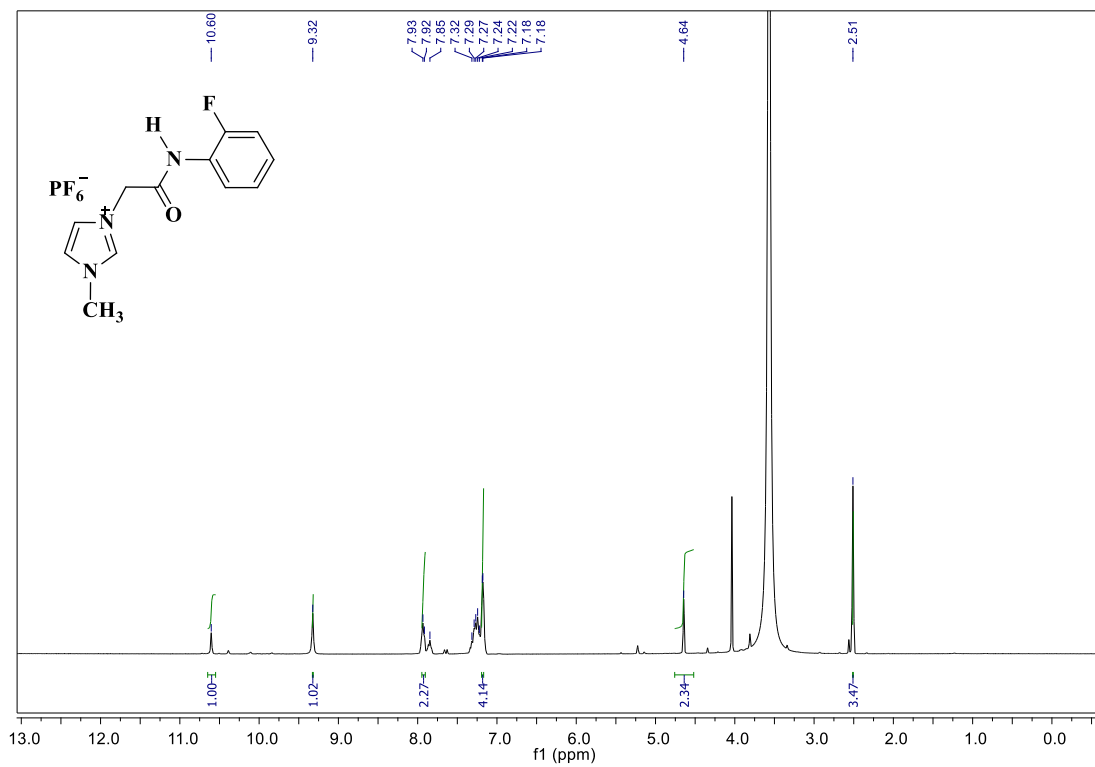


Figure S53:  $^1\text{H}$  NMR compound **5g**

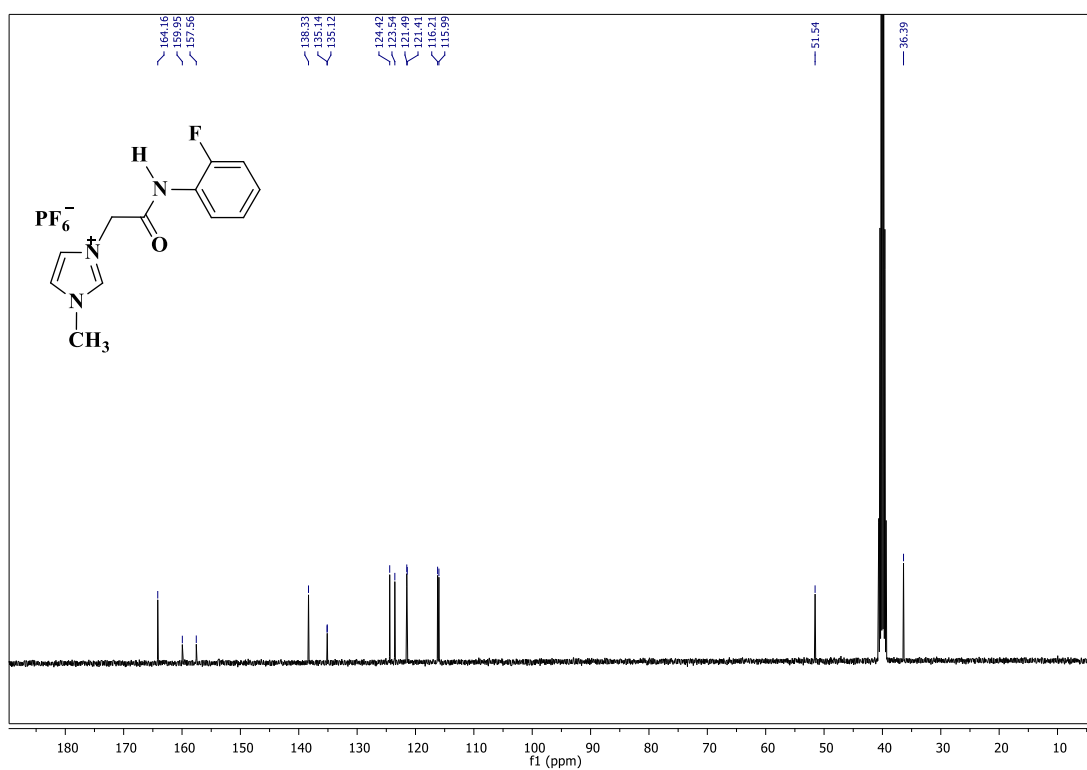
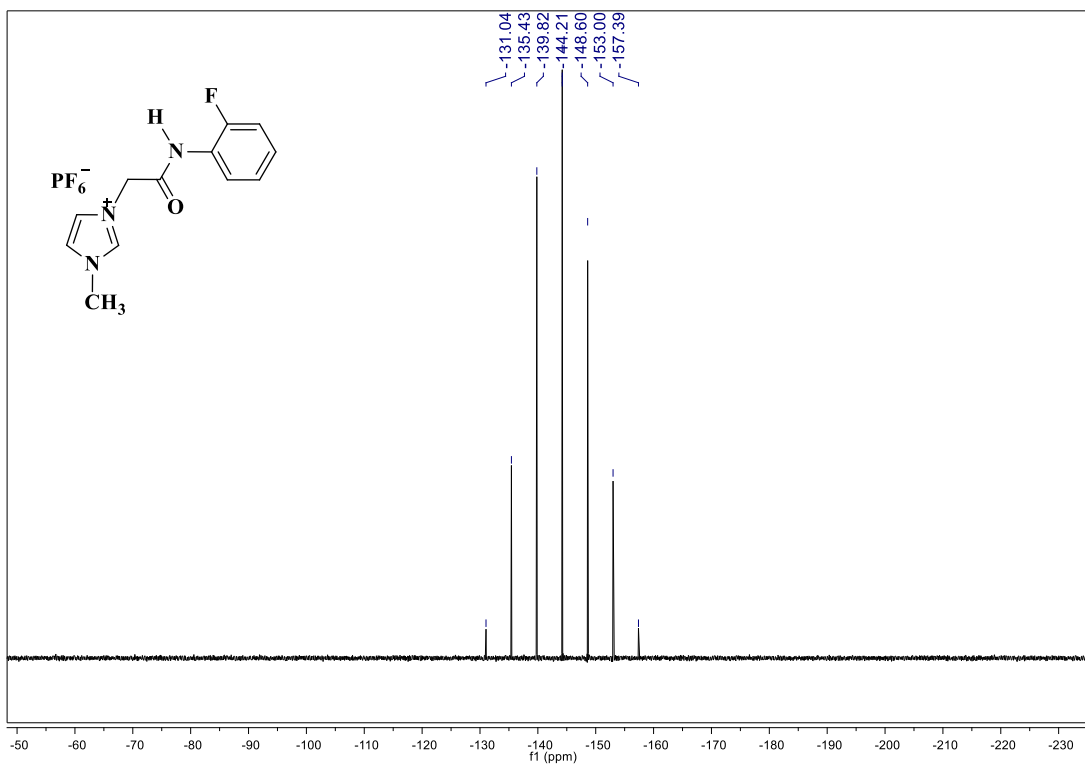
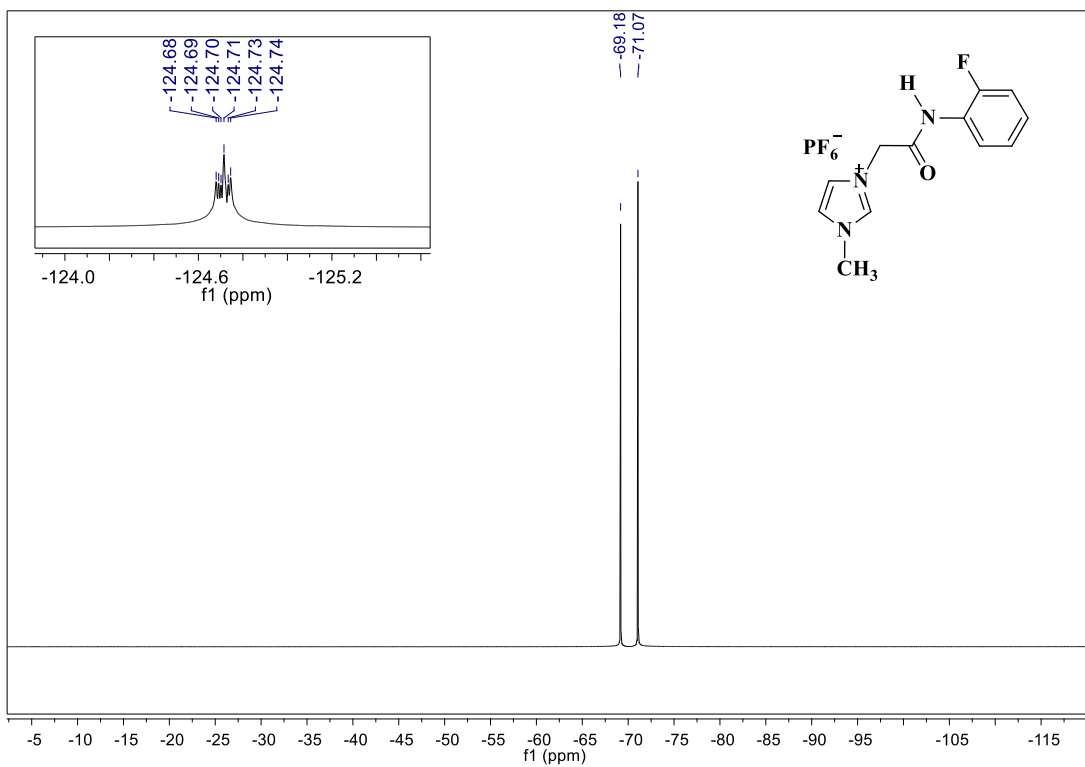


Figure S54:  $^{13}\text{C}$  NMR compound **5g**

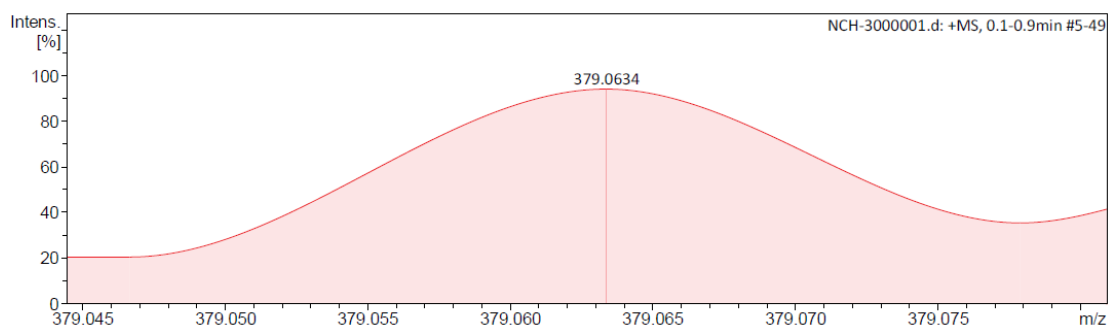




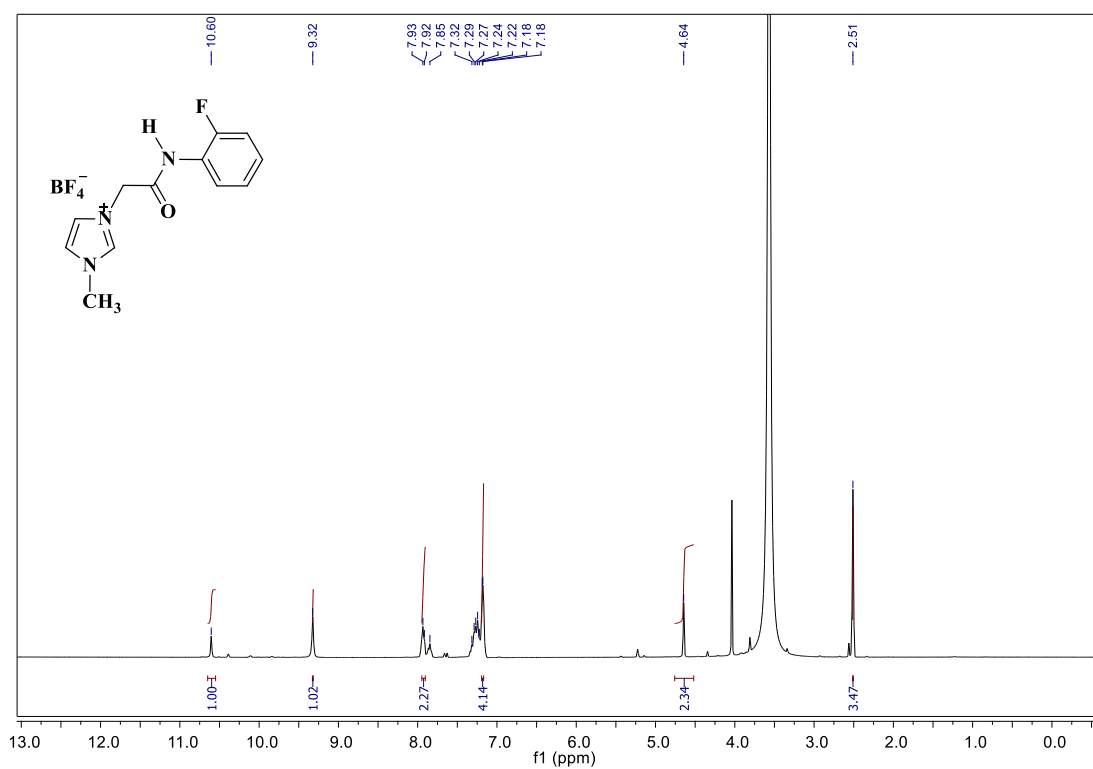
**Figure S55:  $^{31}\text{P}$  NMR compound 5g**



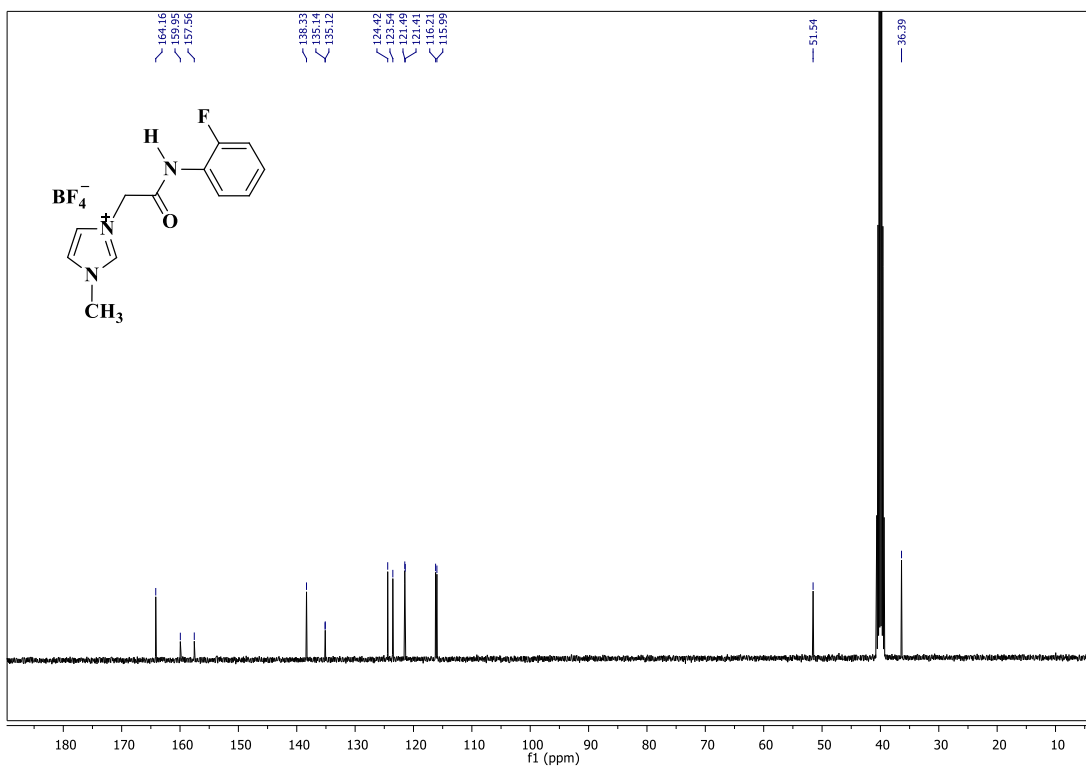
**Figure S56:  $^{19}\text{F}$  NMR of compound 5g**



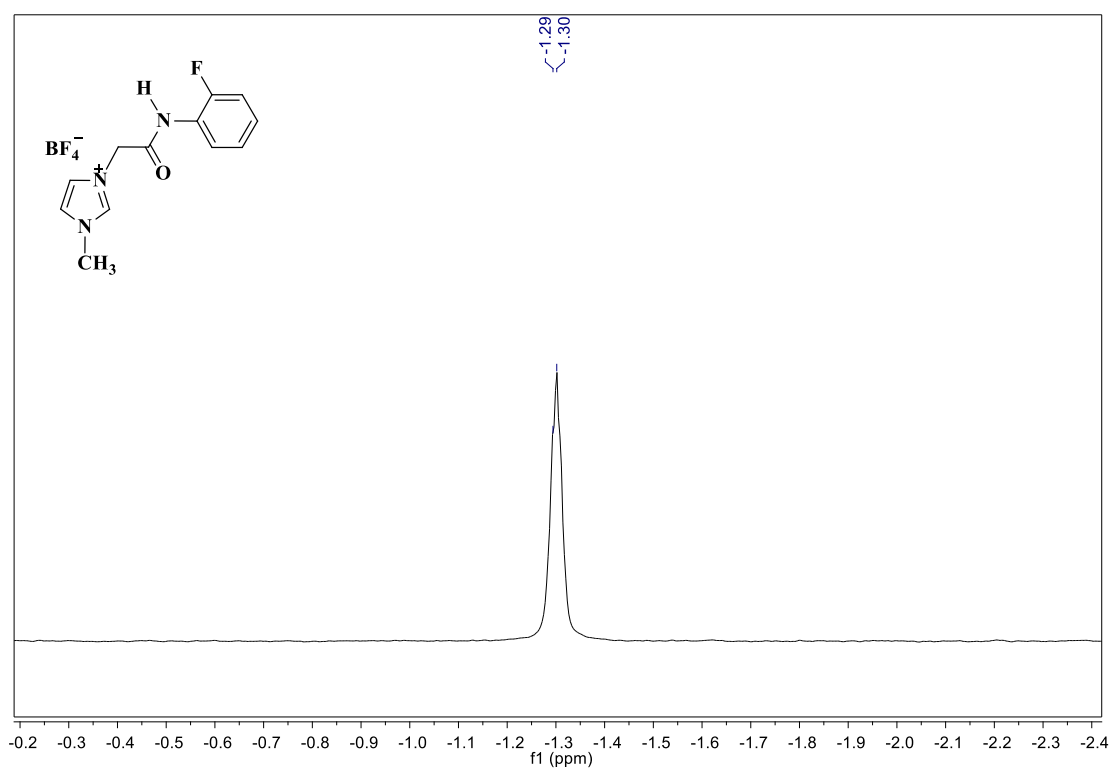
**Figure S57:** HRMS (ESI) of compound **5g**



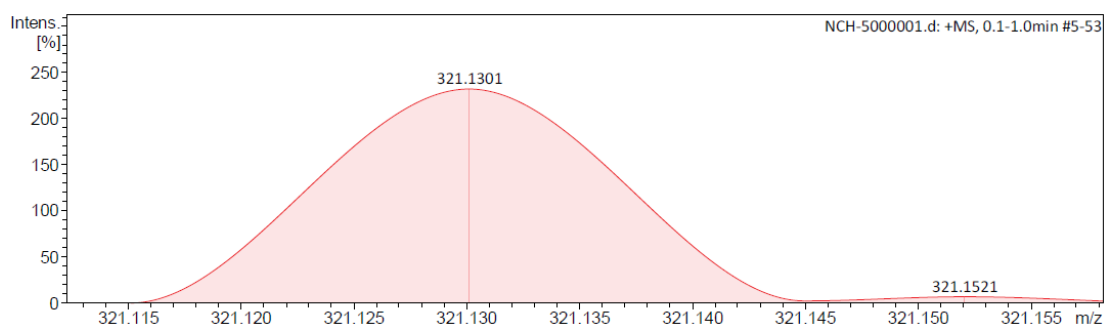
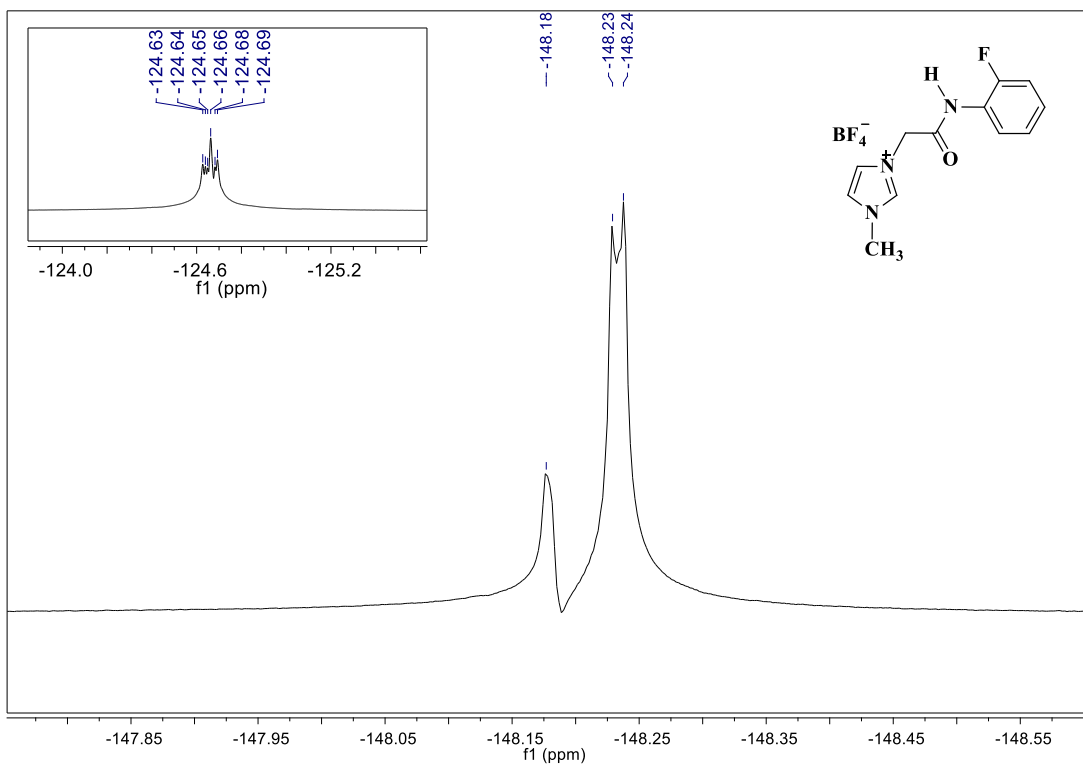
**Figure S58:**  $^1\text{H}$  NMR compound **5h**



**Figure S59:**  $^{13}\text{C}$  NMR compound **5h**



**Figure S60:**  $^{11}\text{B}$  NMR compound **5h**



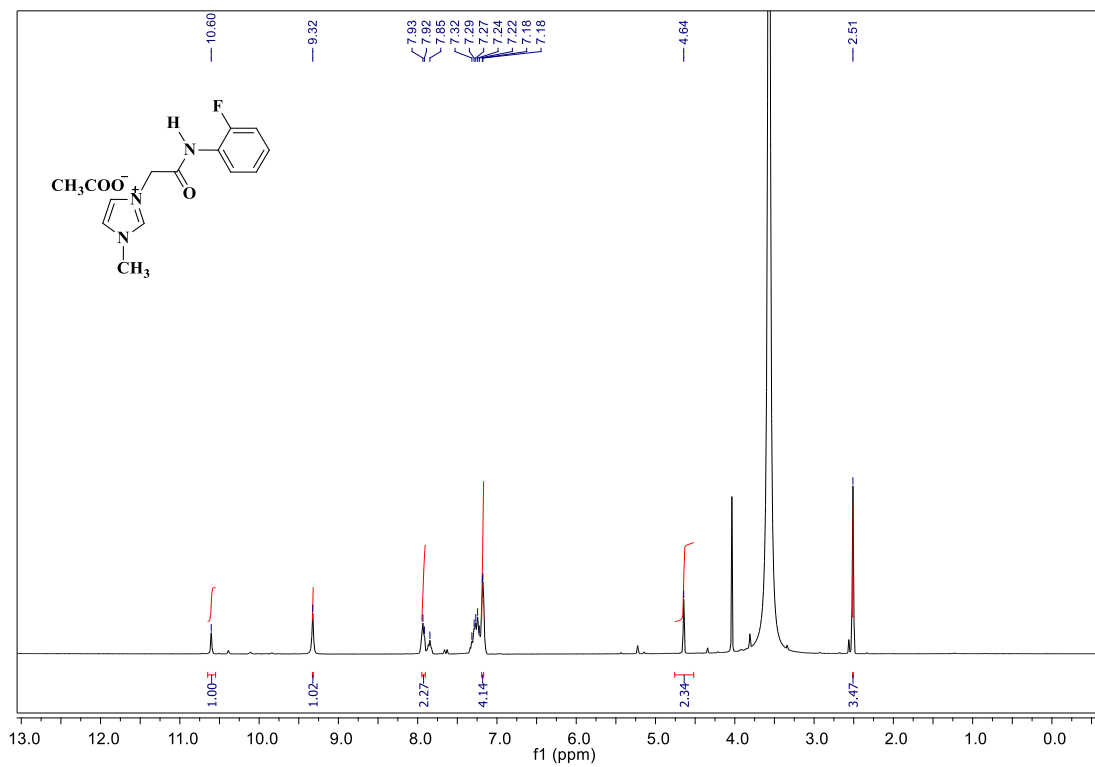


Figure S63: <sup>1</sup>H NMR compound 5i

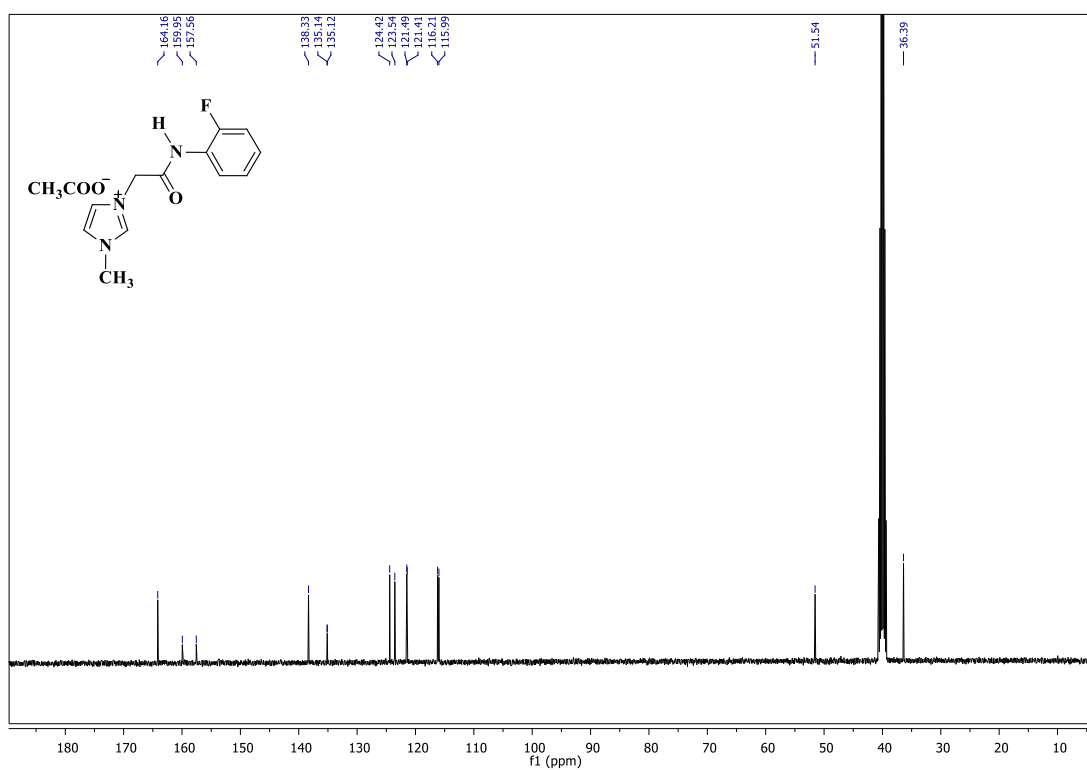
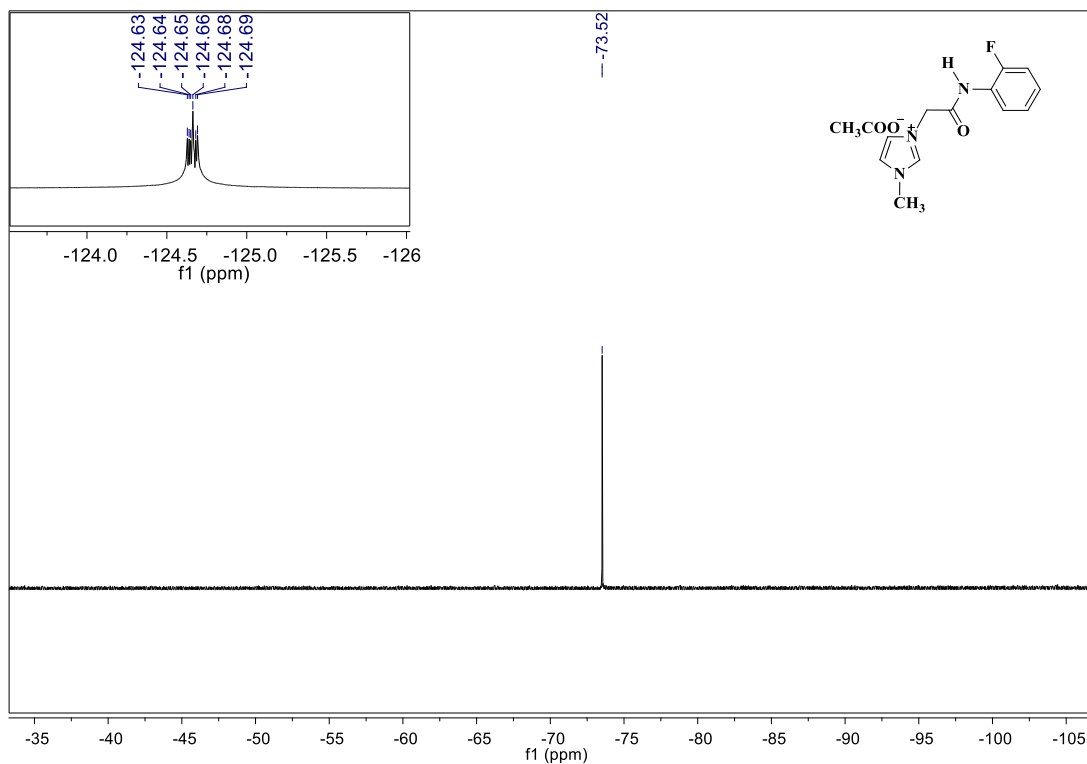
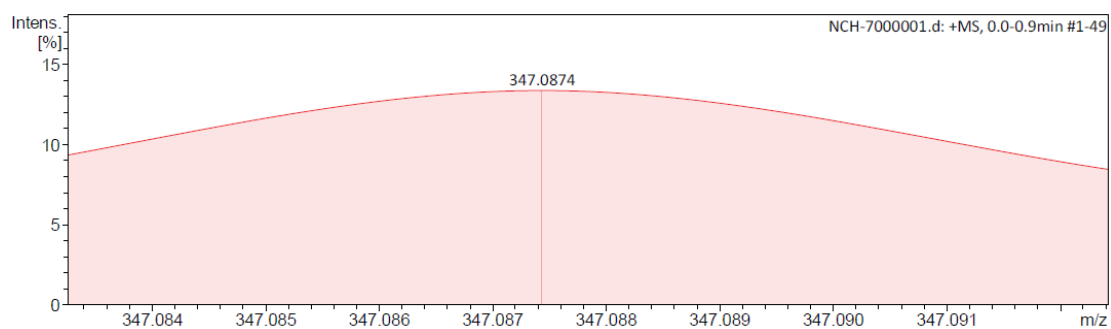


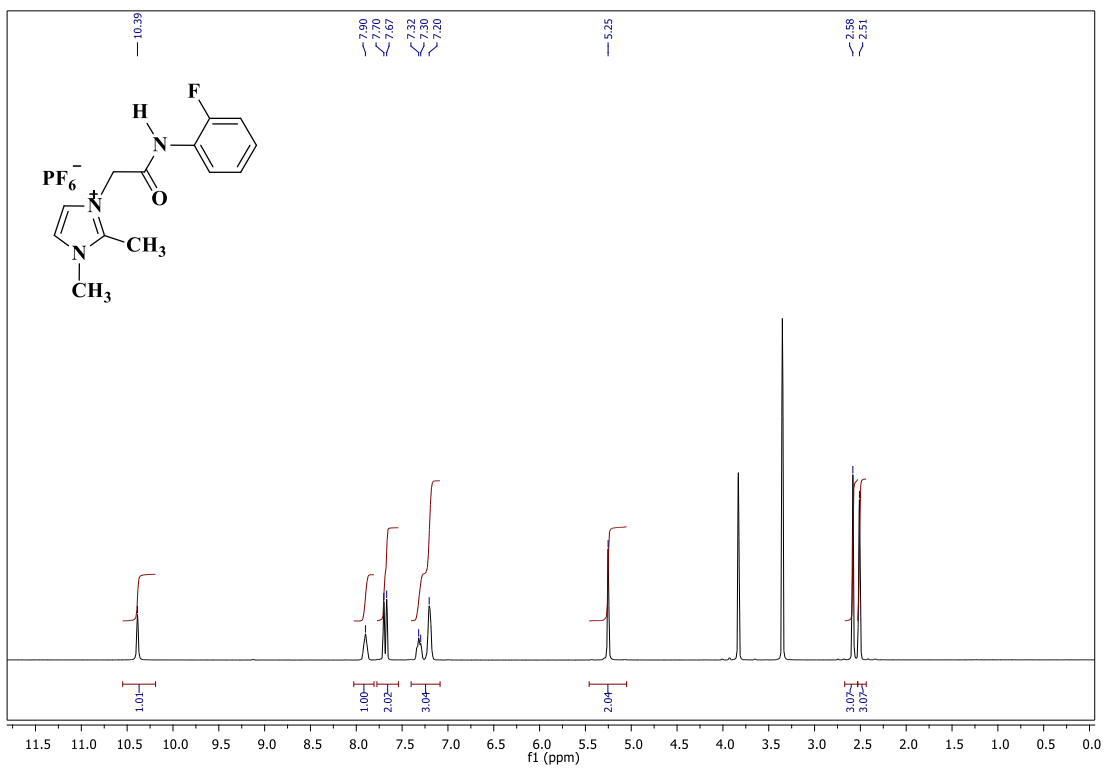
Figure S64: <sup>13</sup>C NMR compound 5i



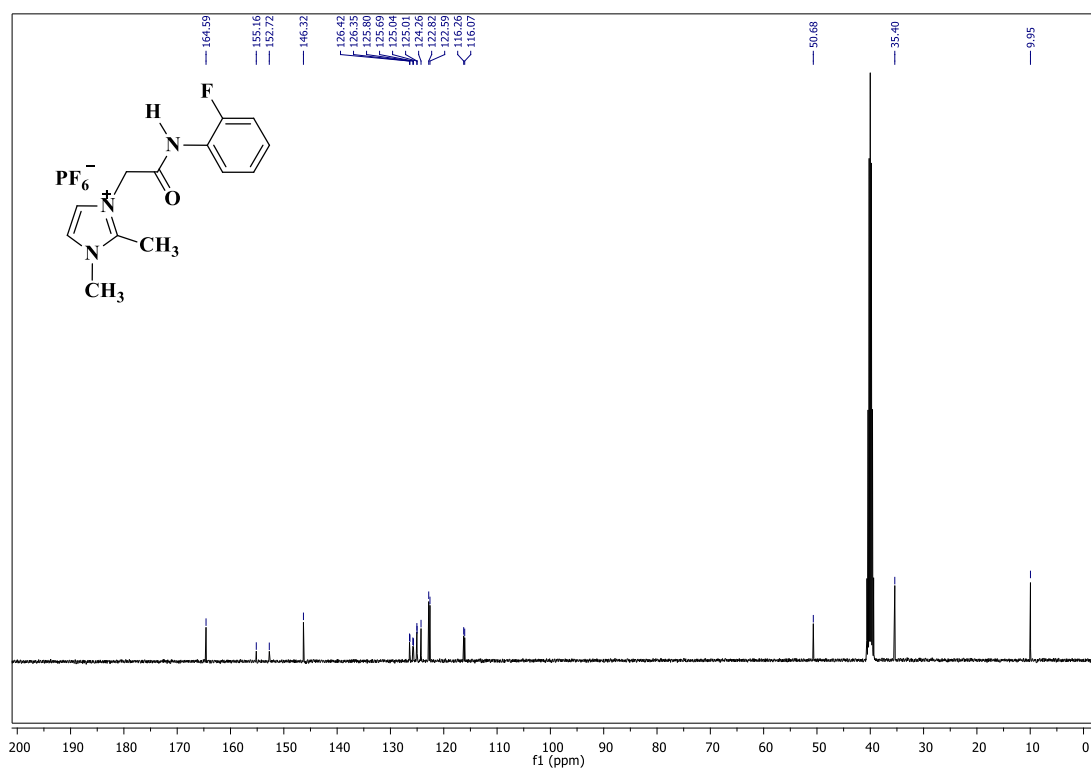
**Figure S65:**  $^{19}\text{F}$  NMR of compound **5i**



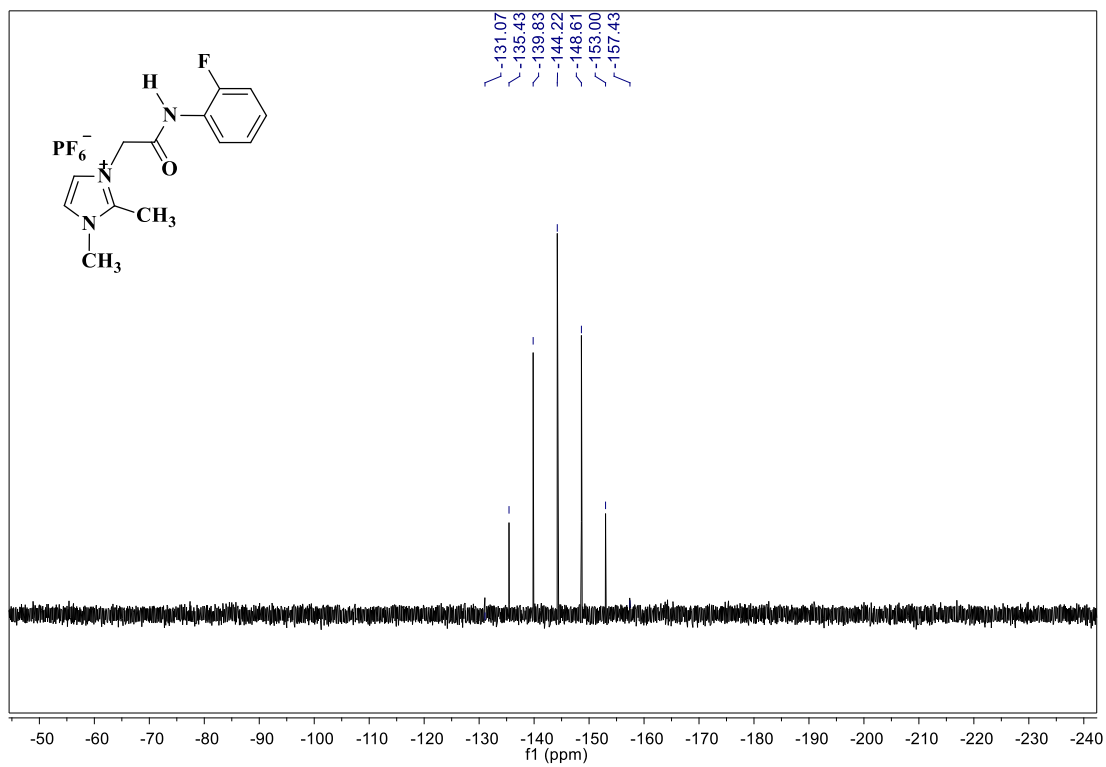
**Figure S66:** HRMS (ESI) of compound **5i**



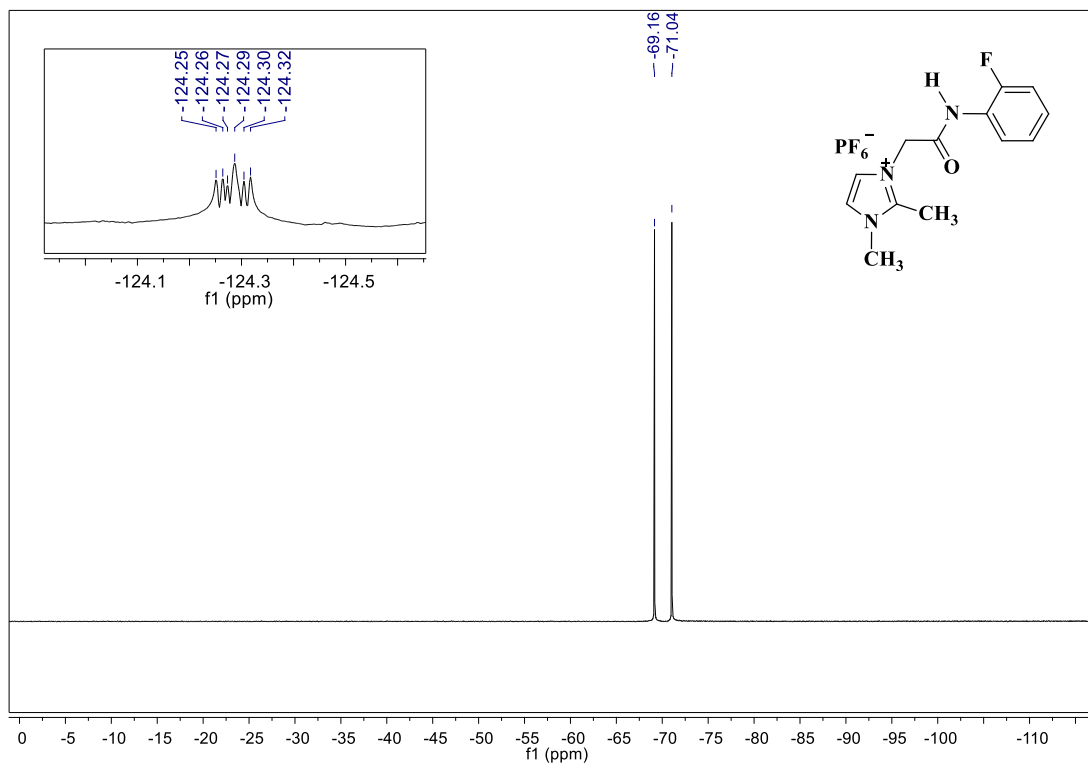
**Figure S67:** <sup>1</sup>H NMR compound **5j**



**Figure S68:** <sup>13</sup>C NMR compound **5j**

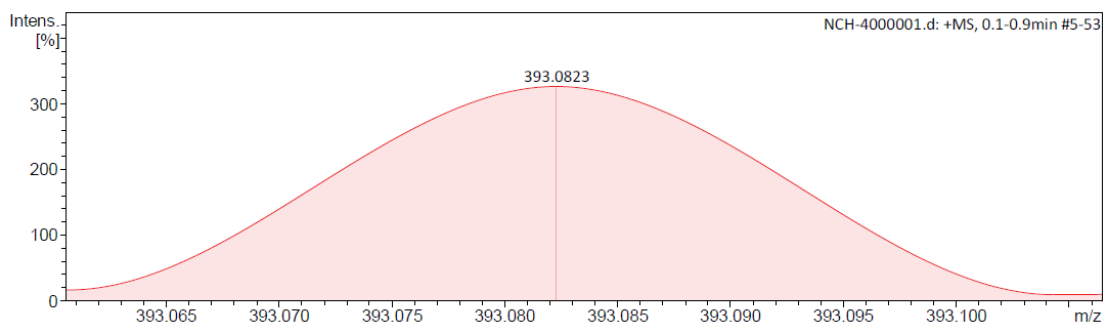


**Figure S69:** <sup>31</sup>P NMR compound **5j**

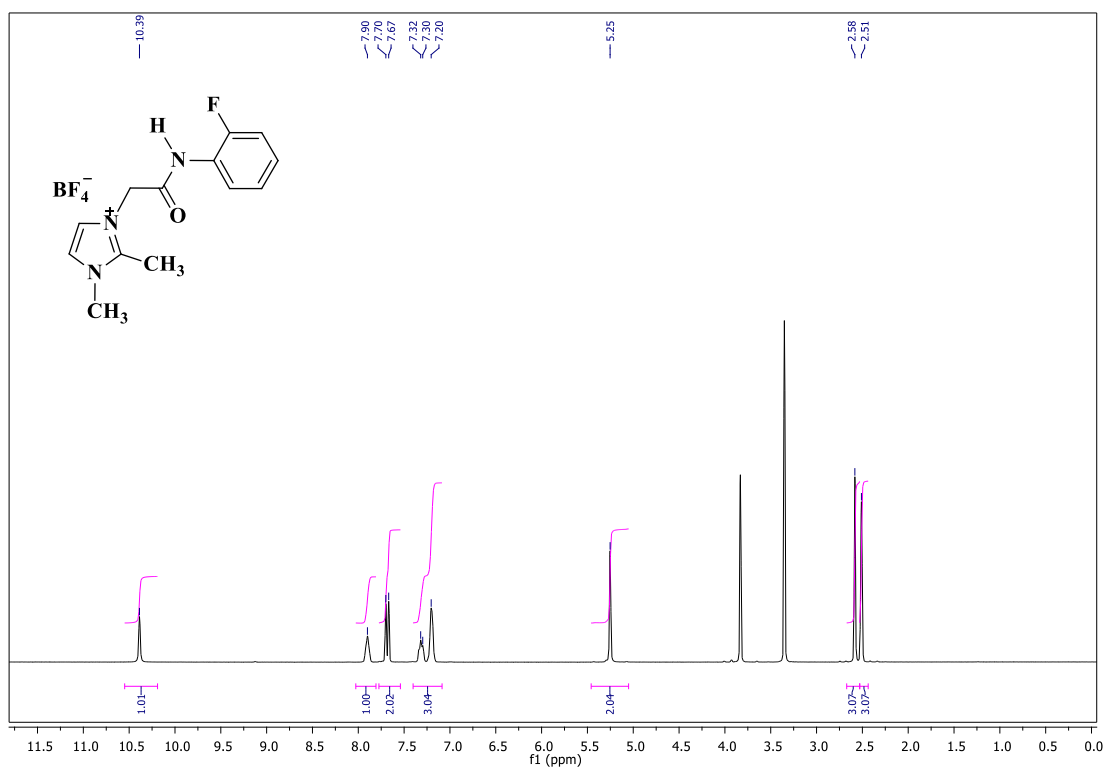


**Figure S70:** <sup>19</sup>F NMR of compound **5j**

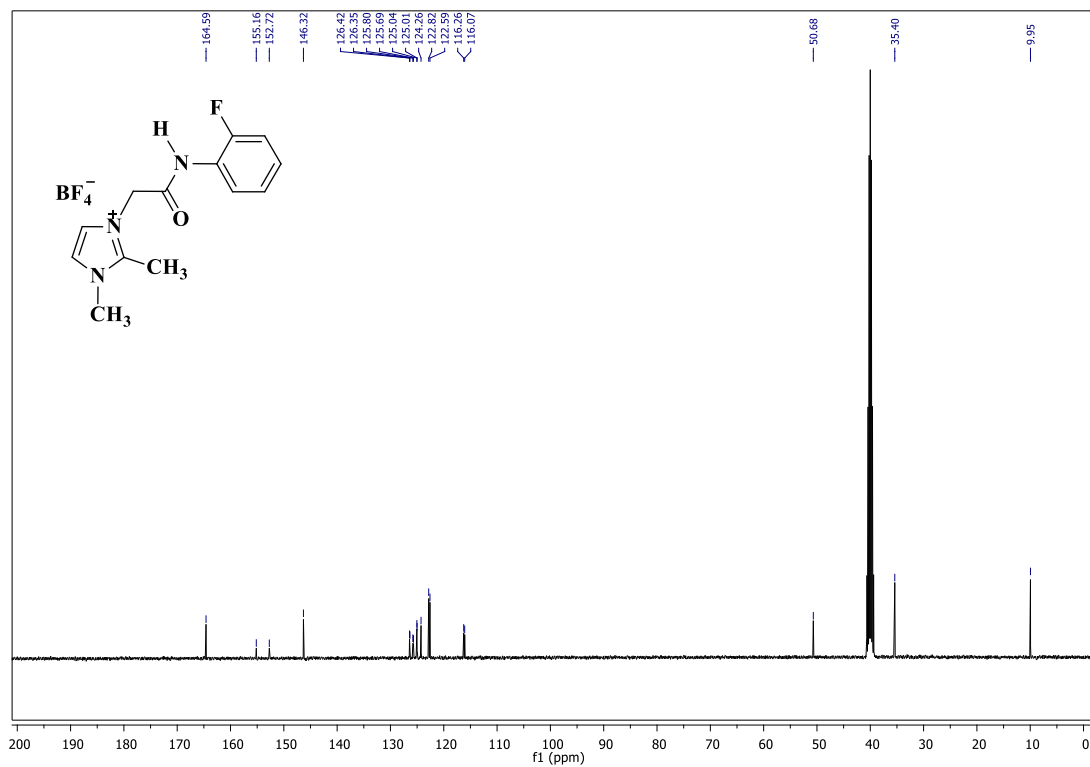




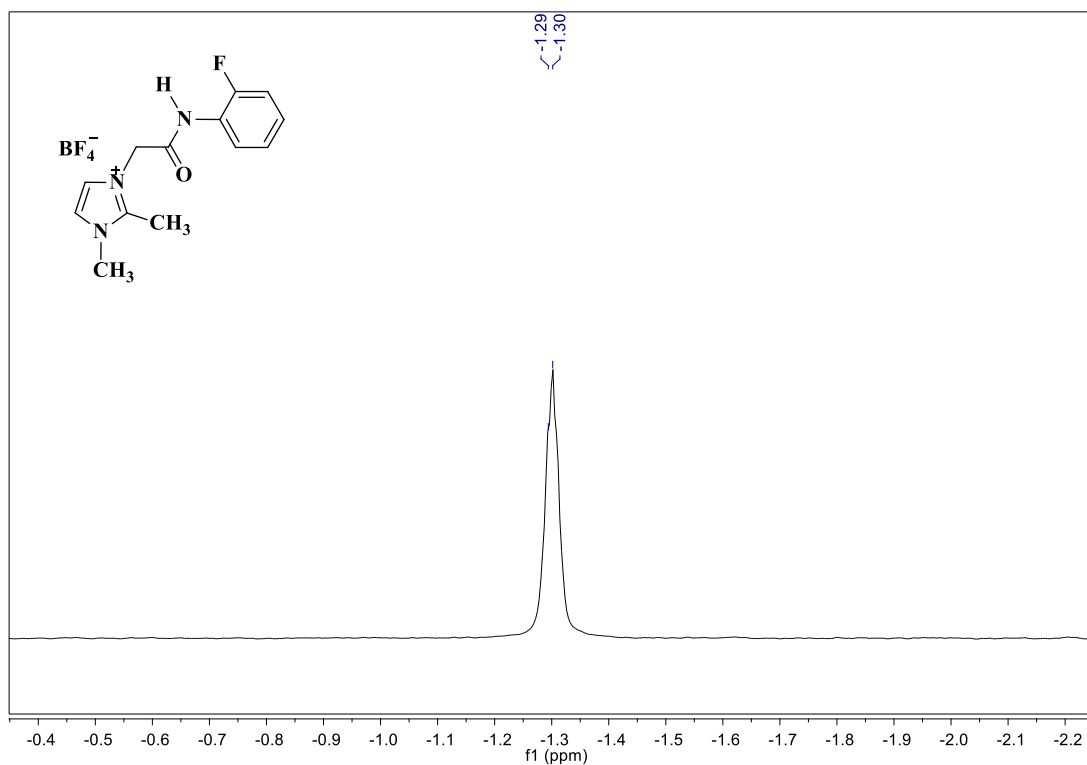
**Figure S71: HRMS (ESI) of compound 5j**



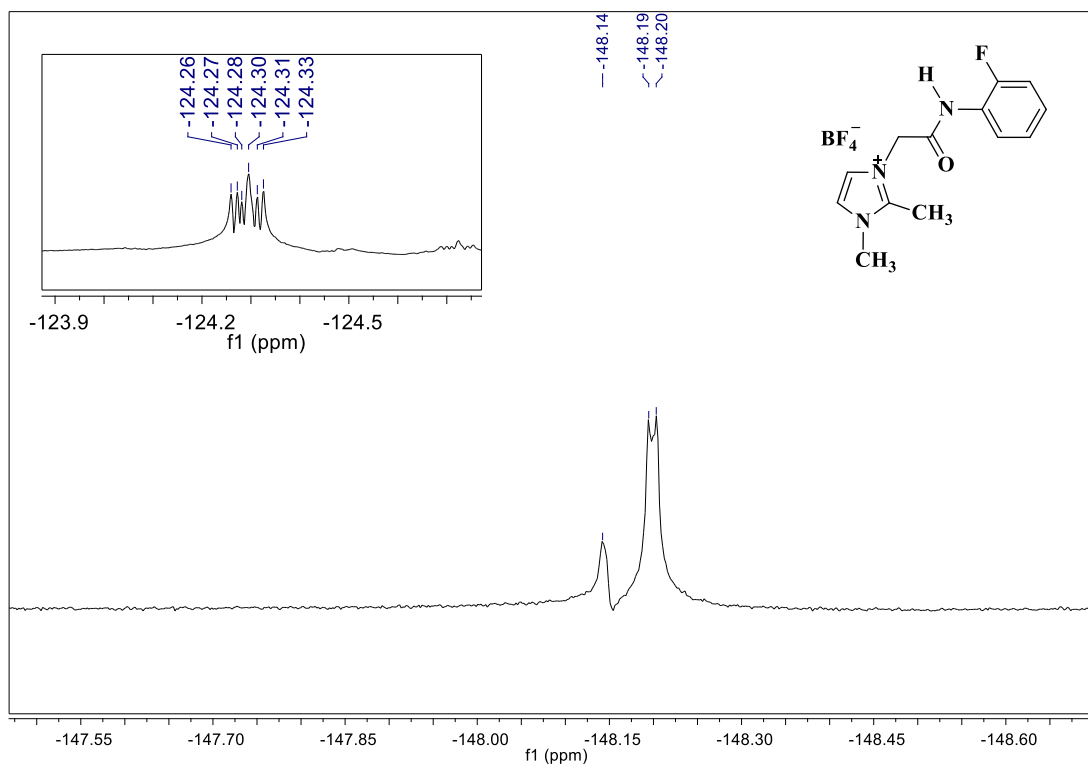
**Figure S72: <sup>1</sup>H NMR compound 5k**



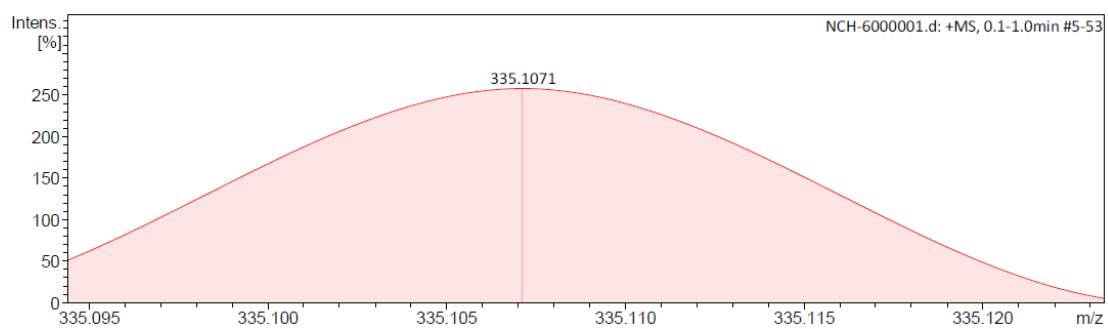
**Figure S73:**  $^{13}\text{C}$  NMR compound **5k**



**Figure S74:**  $^{11}\text{B}$  NMR compound **5k**



**Figure S75:**  $^{19}\text{F}$  NMR of compound **5k**



**Figure S76:** HRMS (ESI) of compound **5k**

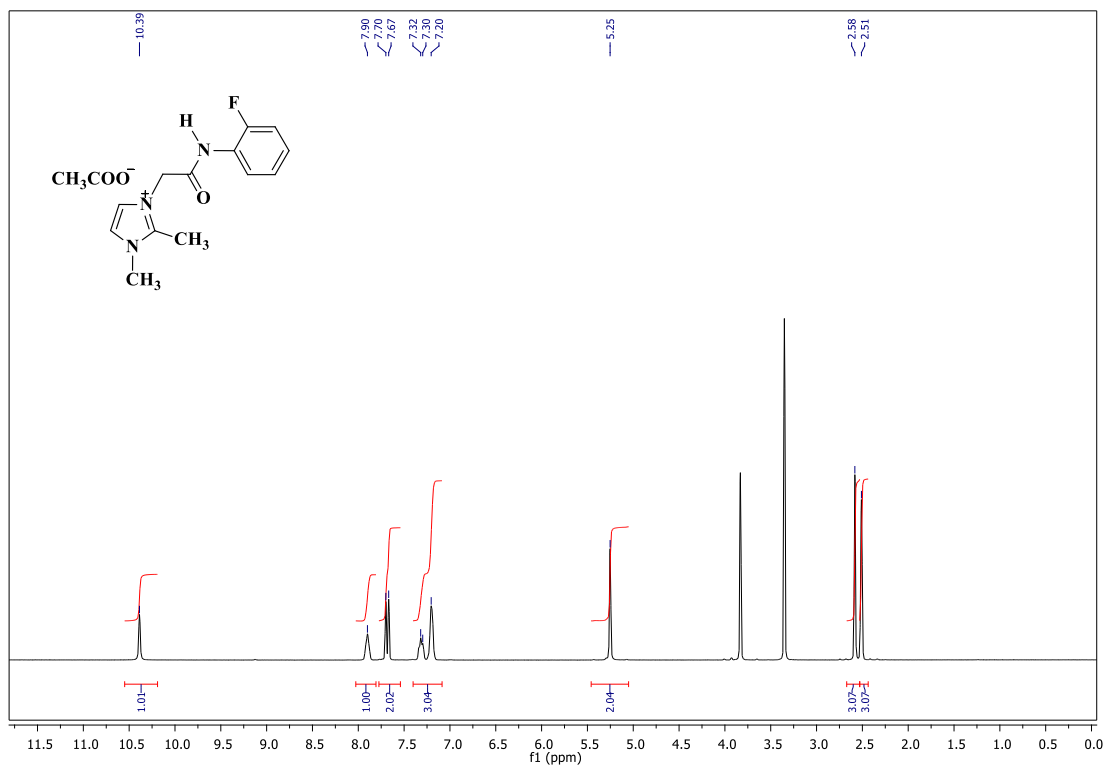


Figure S77: <sup>1</sup>H NMR compound 5l

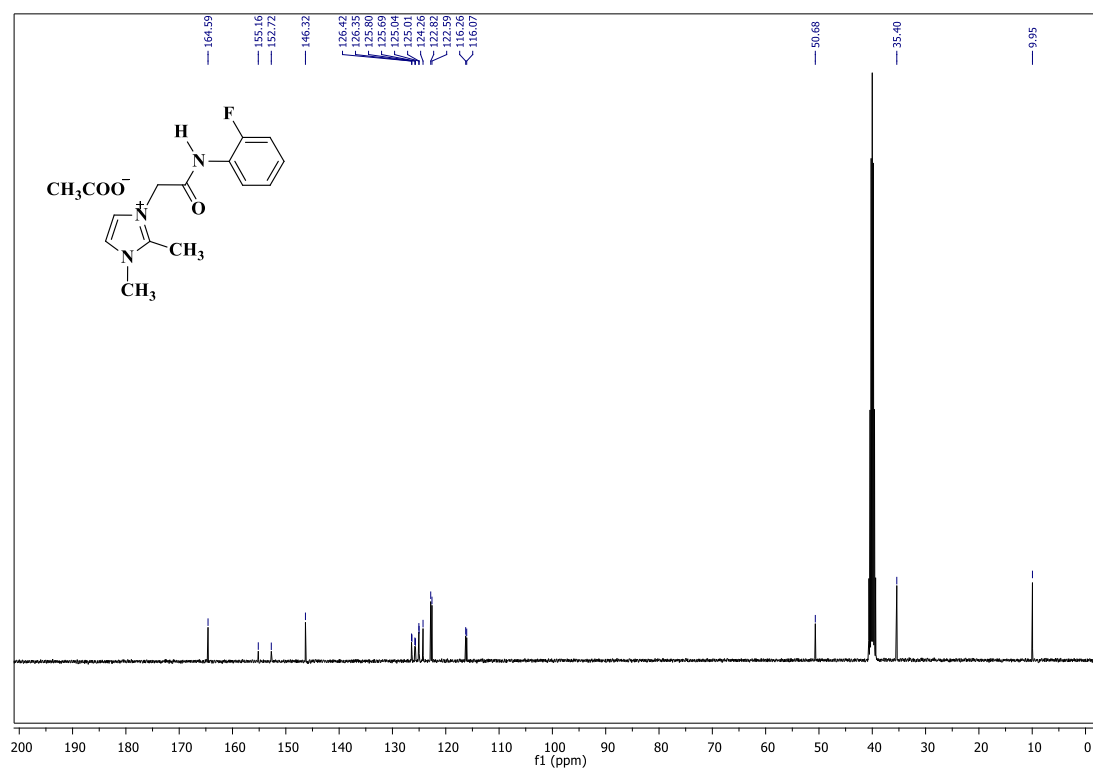
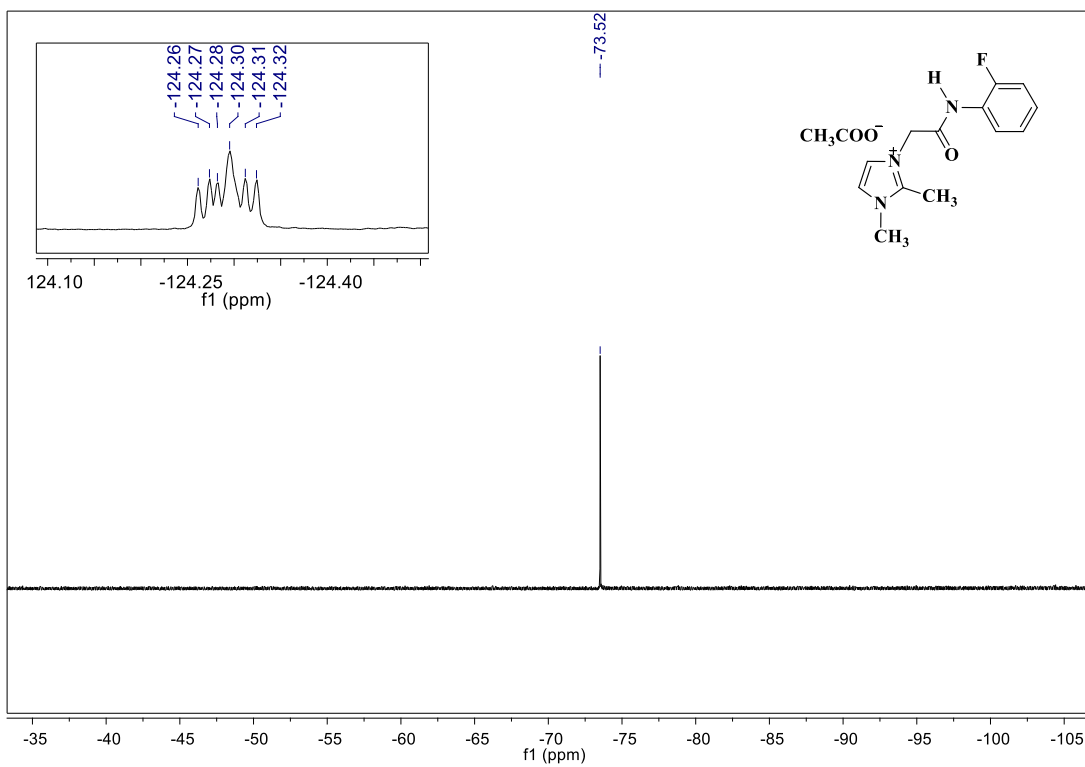
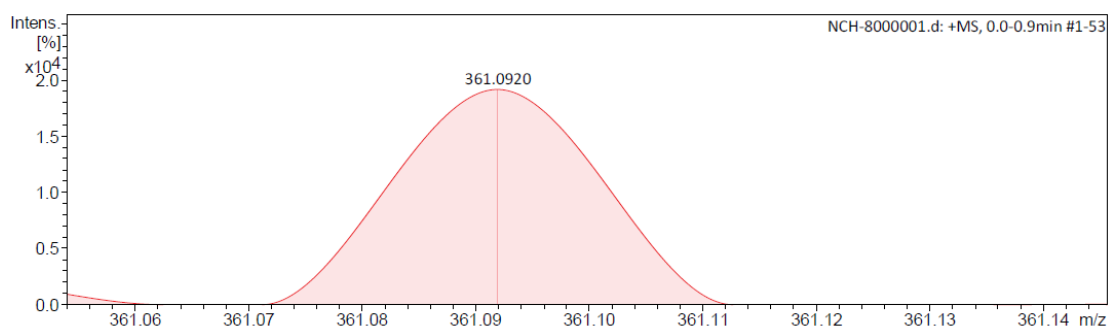


Figure S78: <sup>13</sup>C NMR compound 5l



**Figure S79:**  $^{19}\text{F}$  NMR of compound **51**



**Figure S80:** HRMS (ESI) of compound **51**

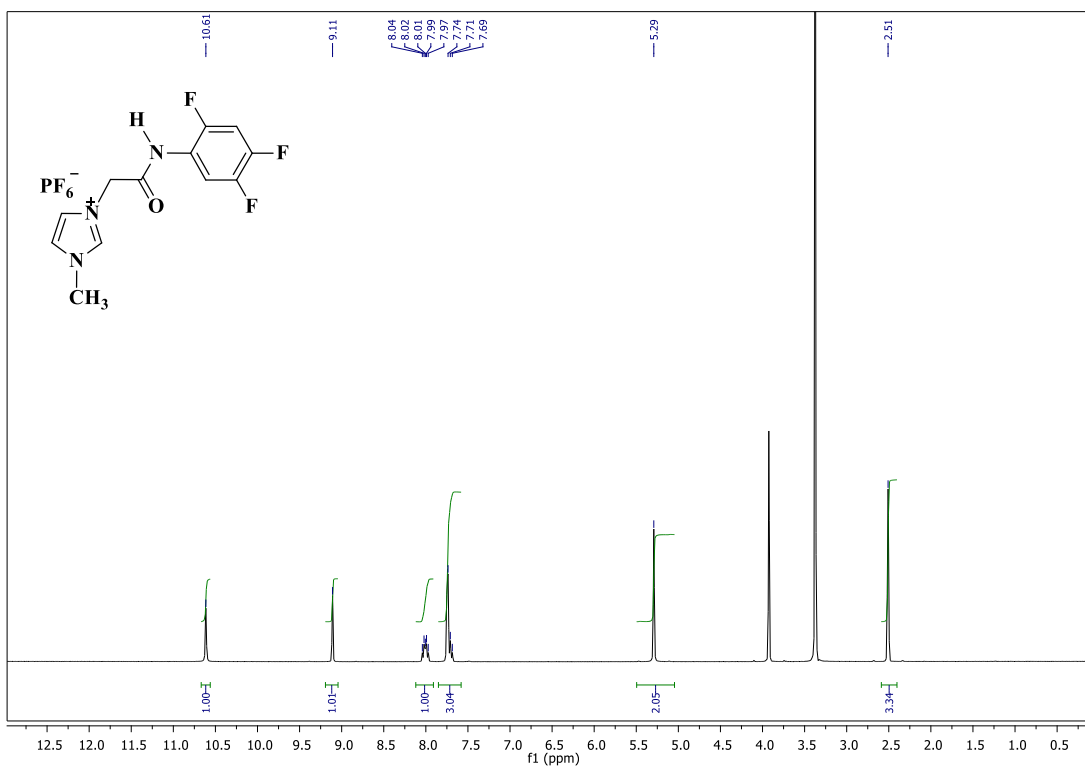


Figure S81: <sup>1</sup>H NMR of compound **5m**

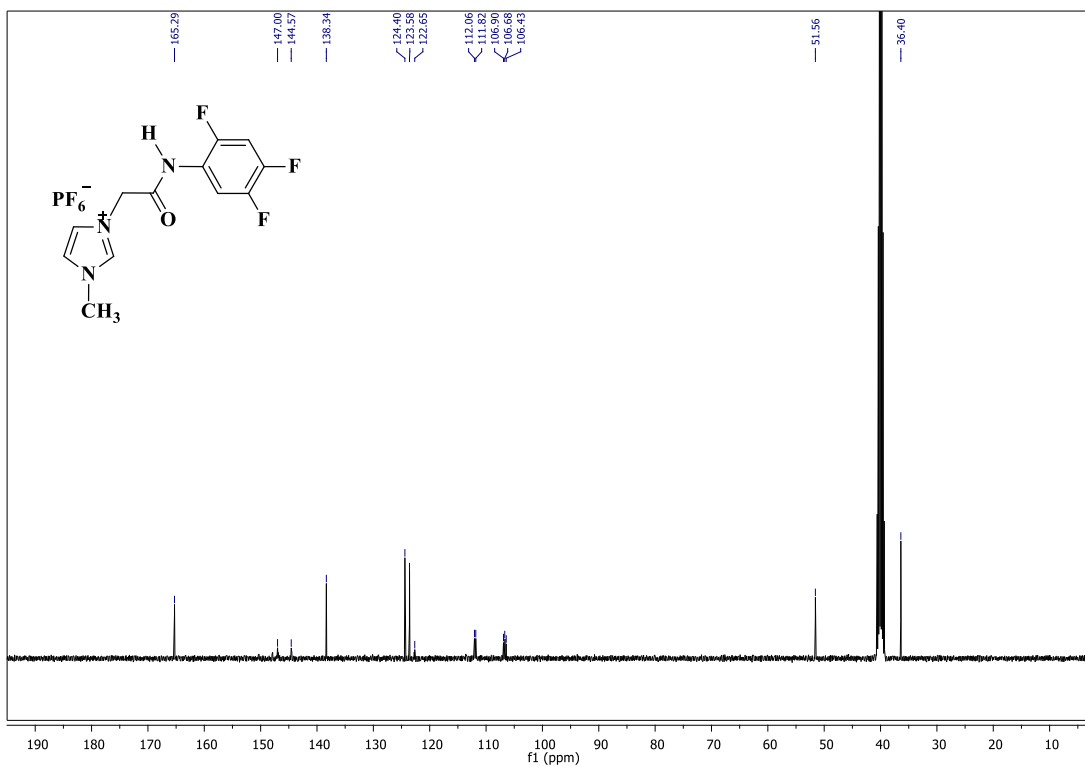


Figure S82: <sup>13</sup>C NMR of compound **5m**

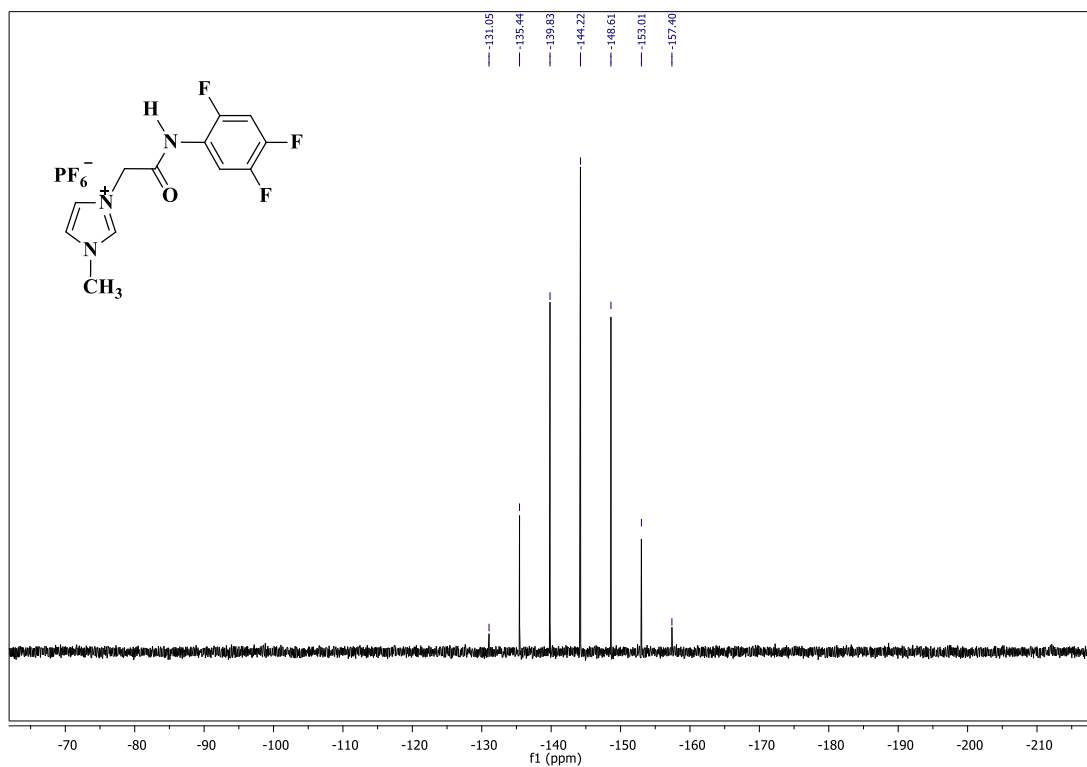


Figure S83: <sup>31</sup>P NMR of compound **5m**

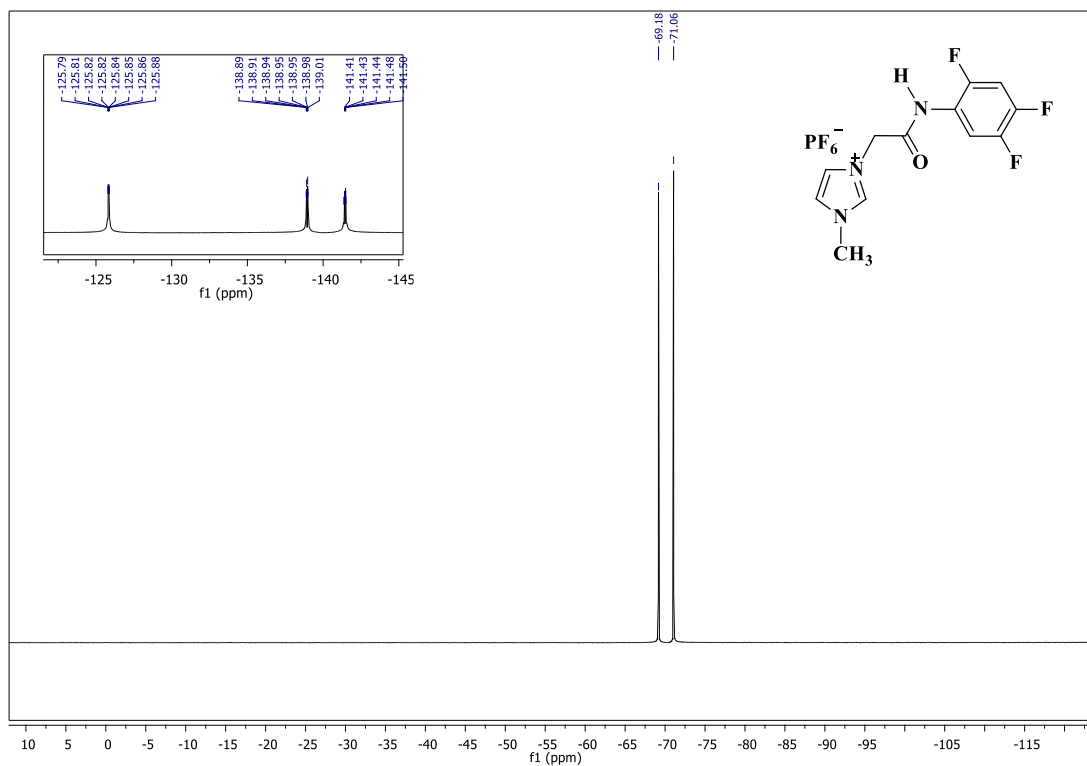
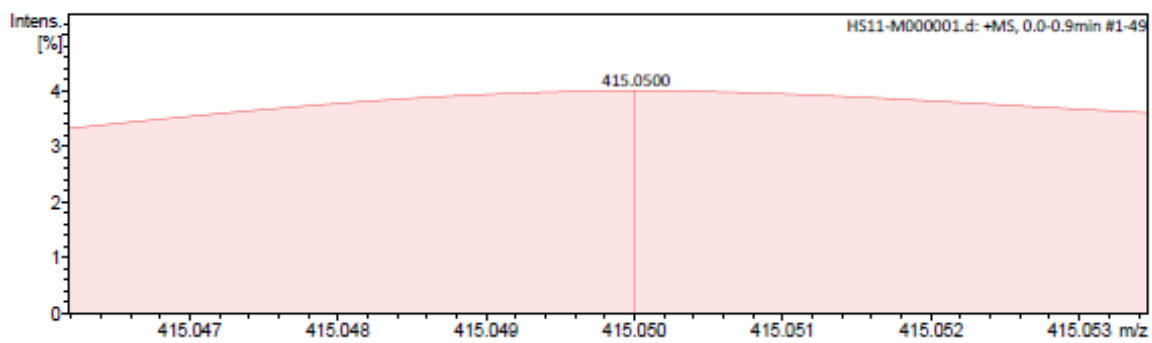
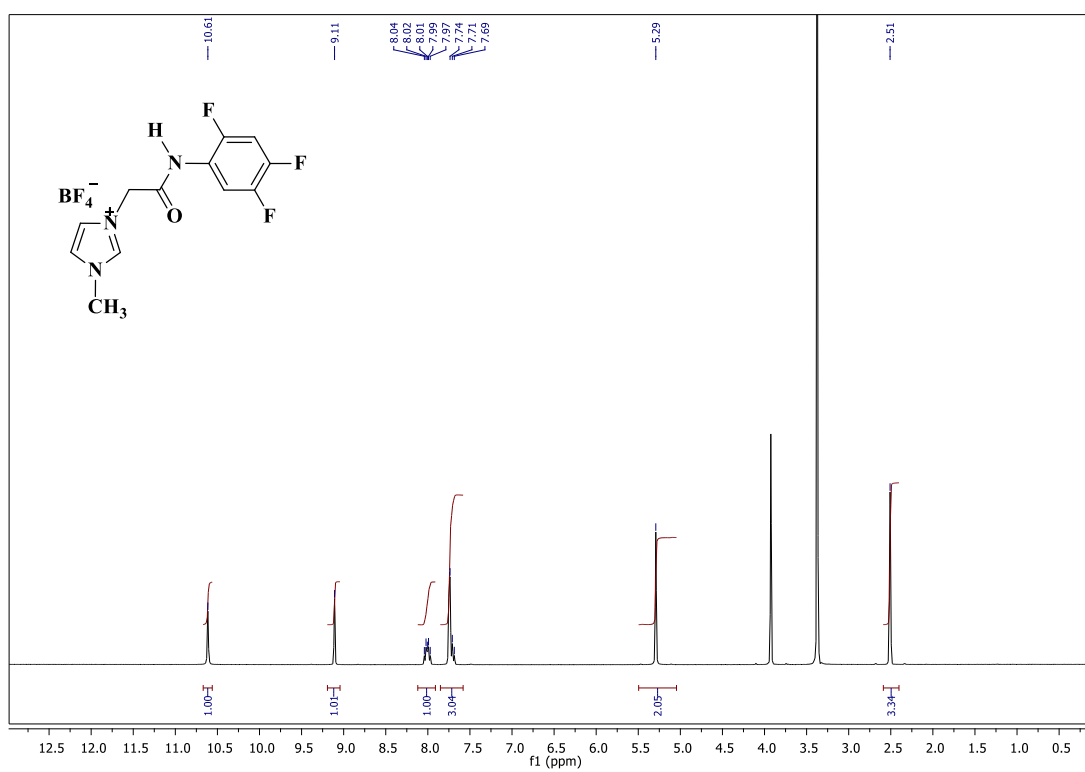


Figure S84: <sup>19</sup>F NMR of compound **5m**



**Figure S85:** HRMS (ESI) of compound **5m**



**Figure S86:** <sup>1</sup>H NMR of compound **5m**



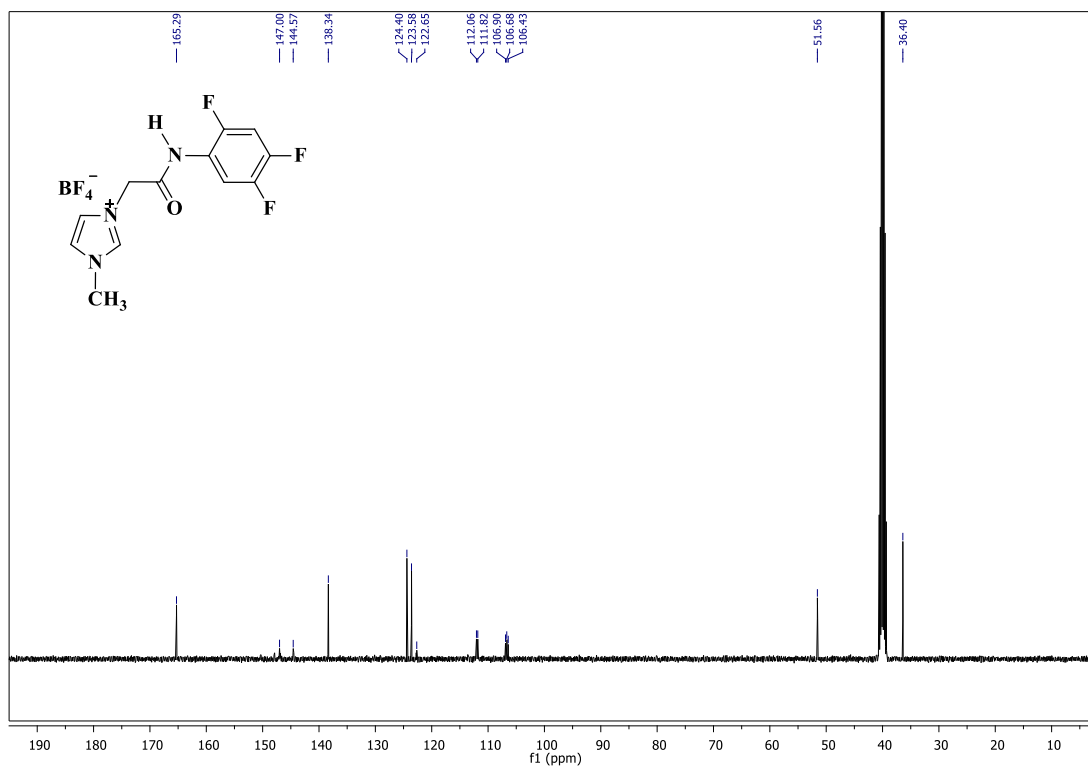


Figure S87:  $^{13}\text{C}$  NMR of compound 5n

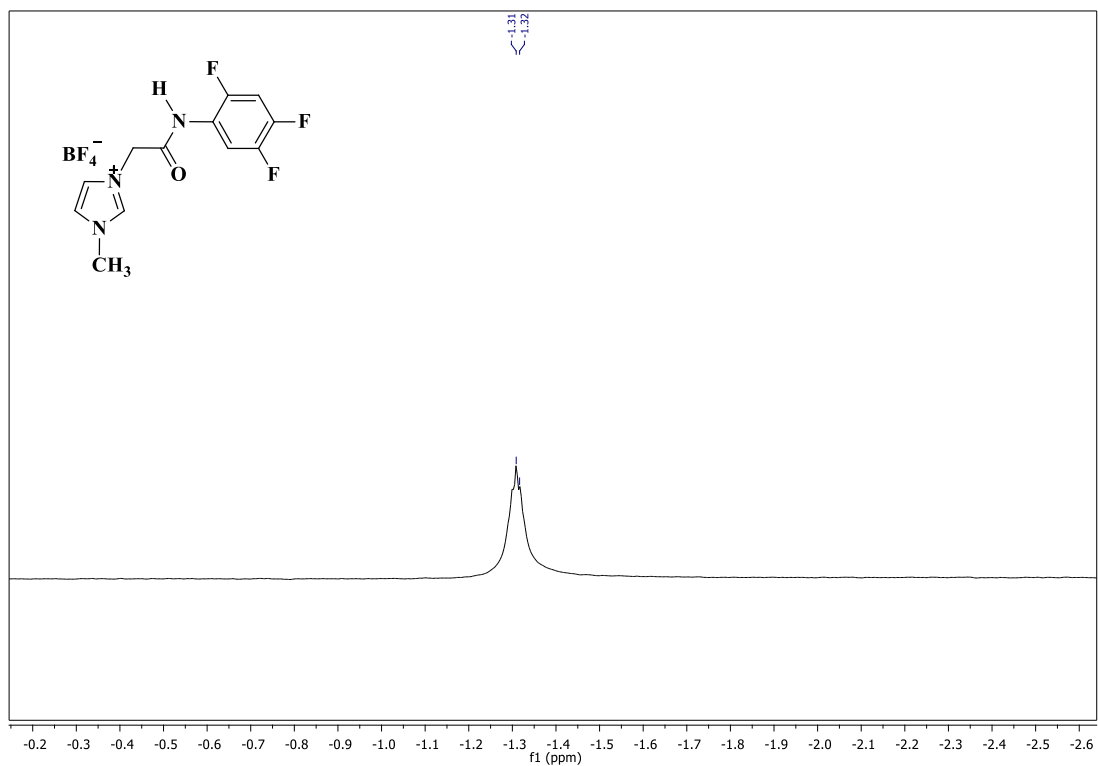
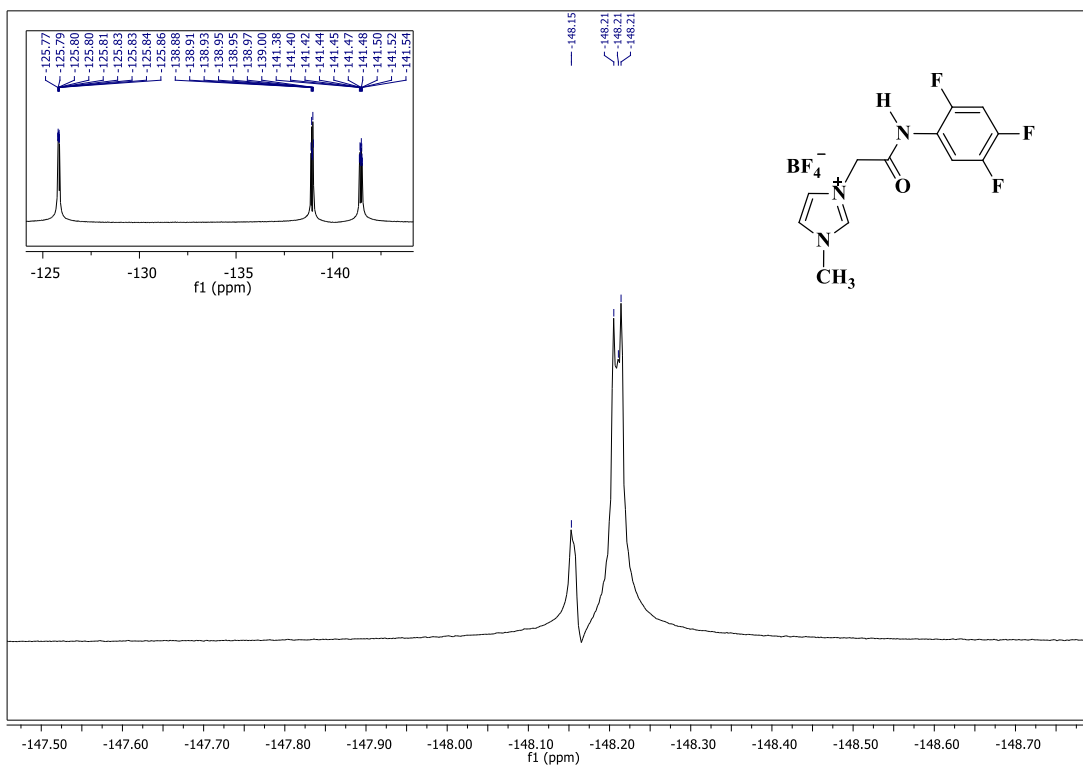
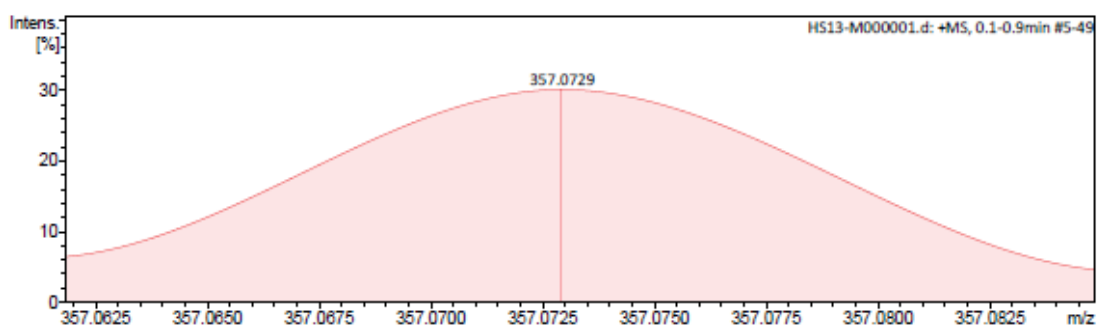


Figure S88:  $^{11}\text{B}$  NMR of compound 5n



**Figure S89:**  $^{19}\text{F}$  NMR of compound **5n**



**Figure S90:** HRMS (ESI) of compound **5n**

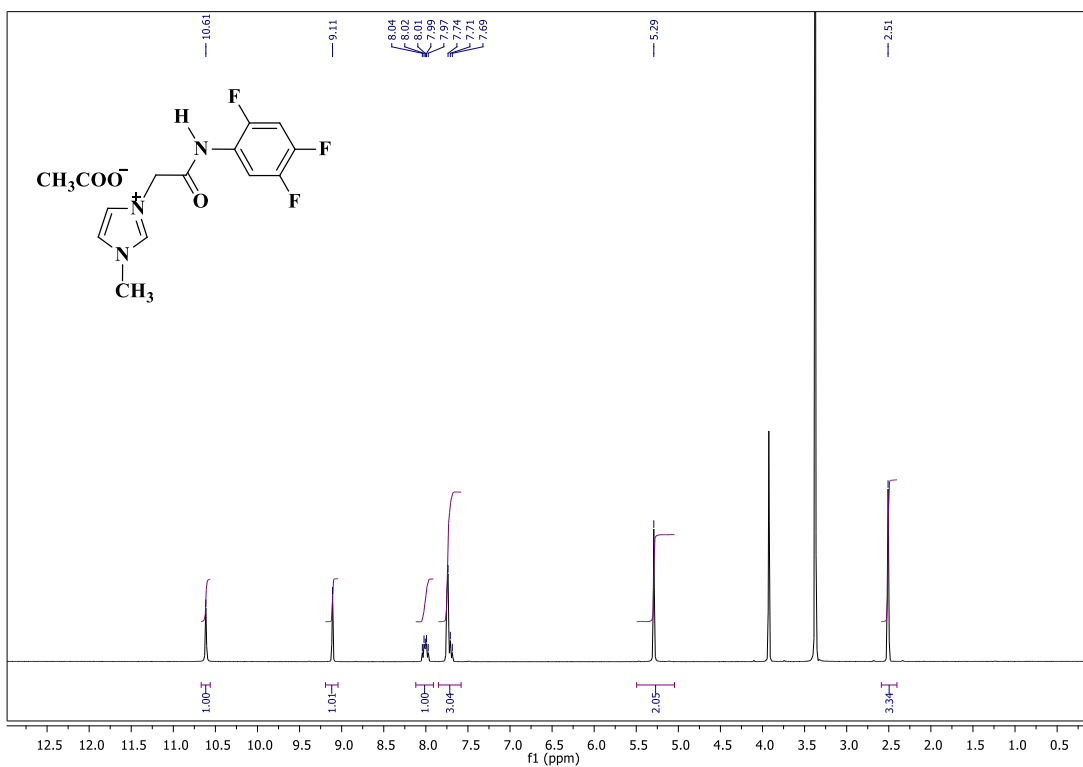


Figure S91:  $^1\text{H NMR}$  of compound **5o**

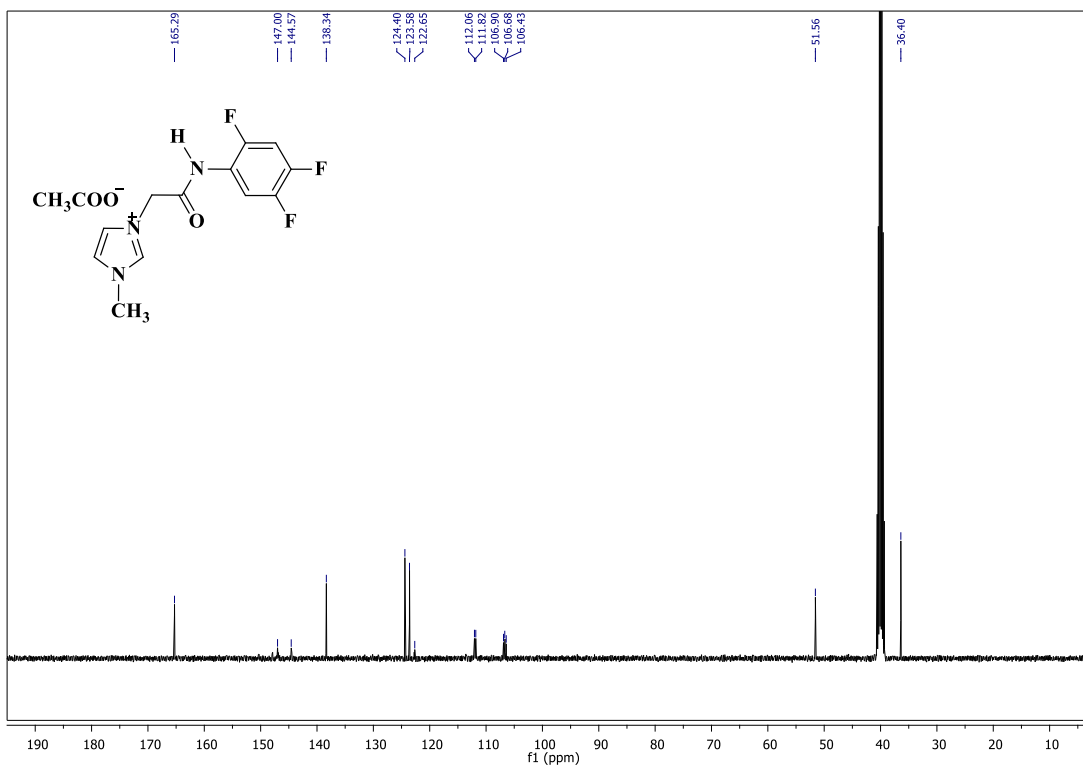
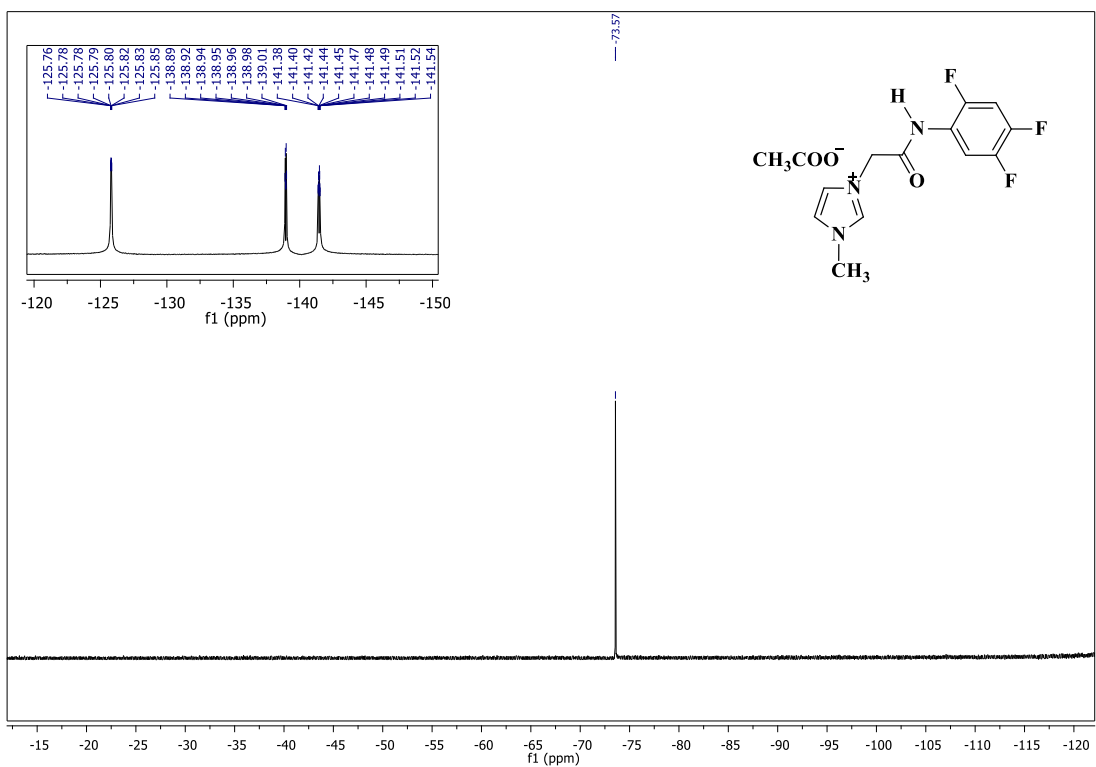
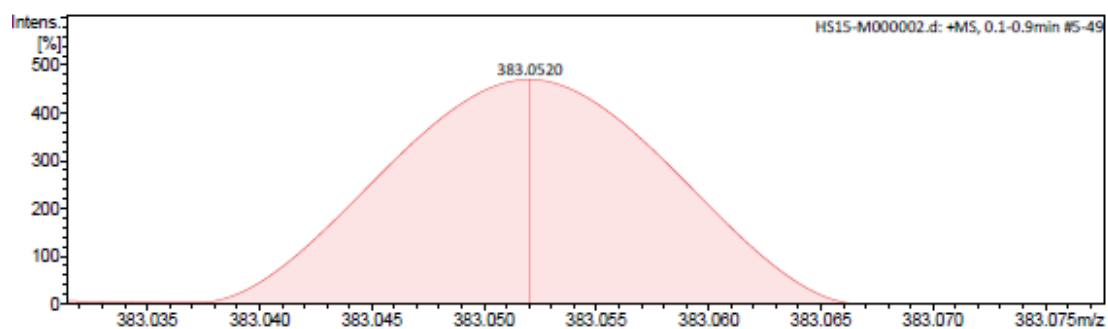


Figure S92:  $^{13}\text{C NMR}$  of compound **5o**



**Figure S93:**  $^{19}\text{F}$  NMR of compound **5o**



**Figure S94:** HRMS (ESI) of compound **5o**

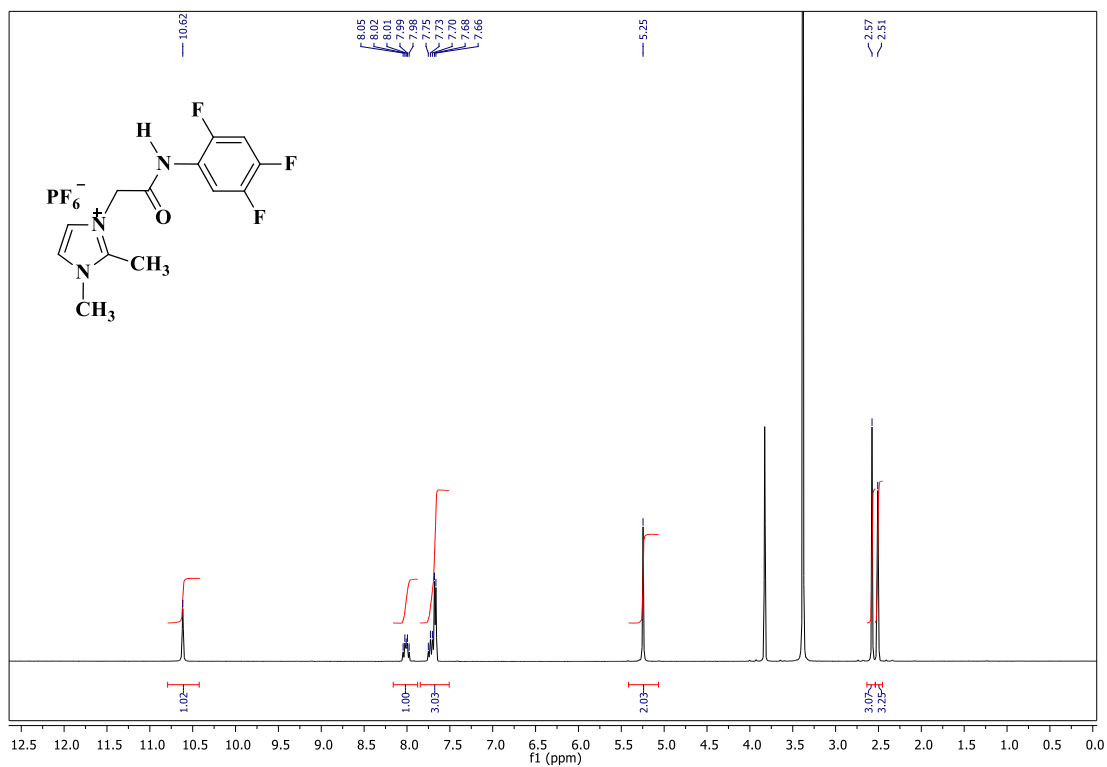


Figure S95: <sup>1</sup>H NMR of compound 5p

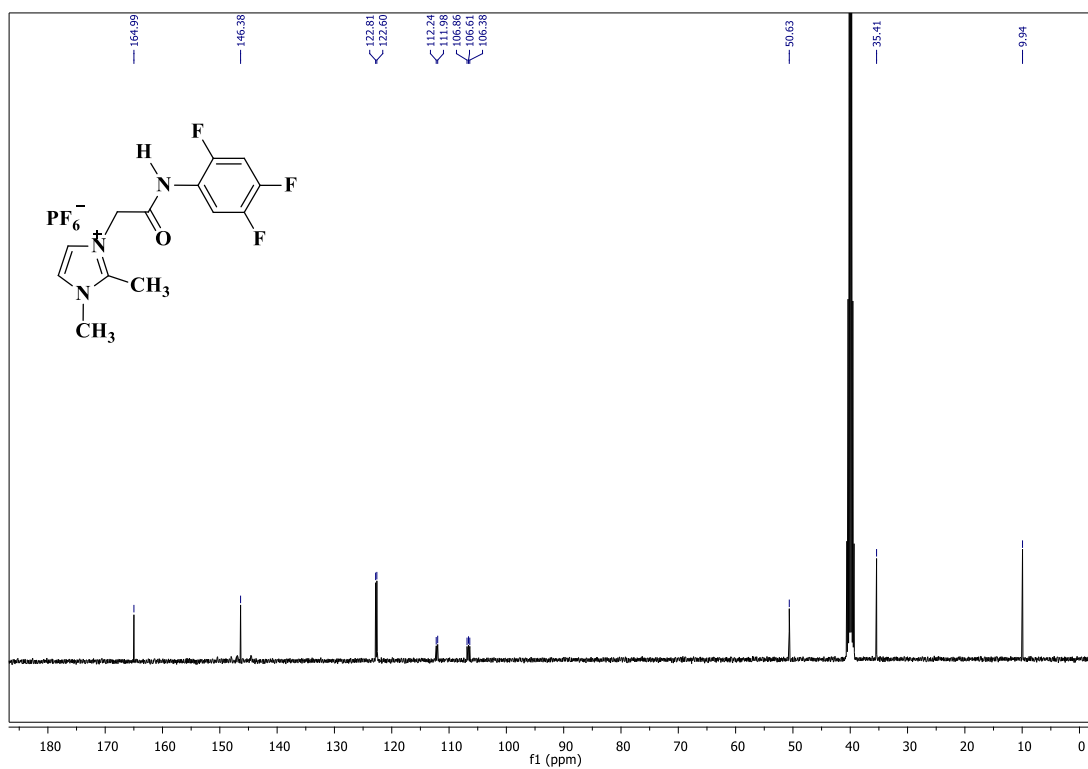


Figure S96: <sup>13</sup>C NMR of compound 5p

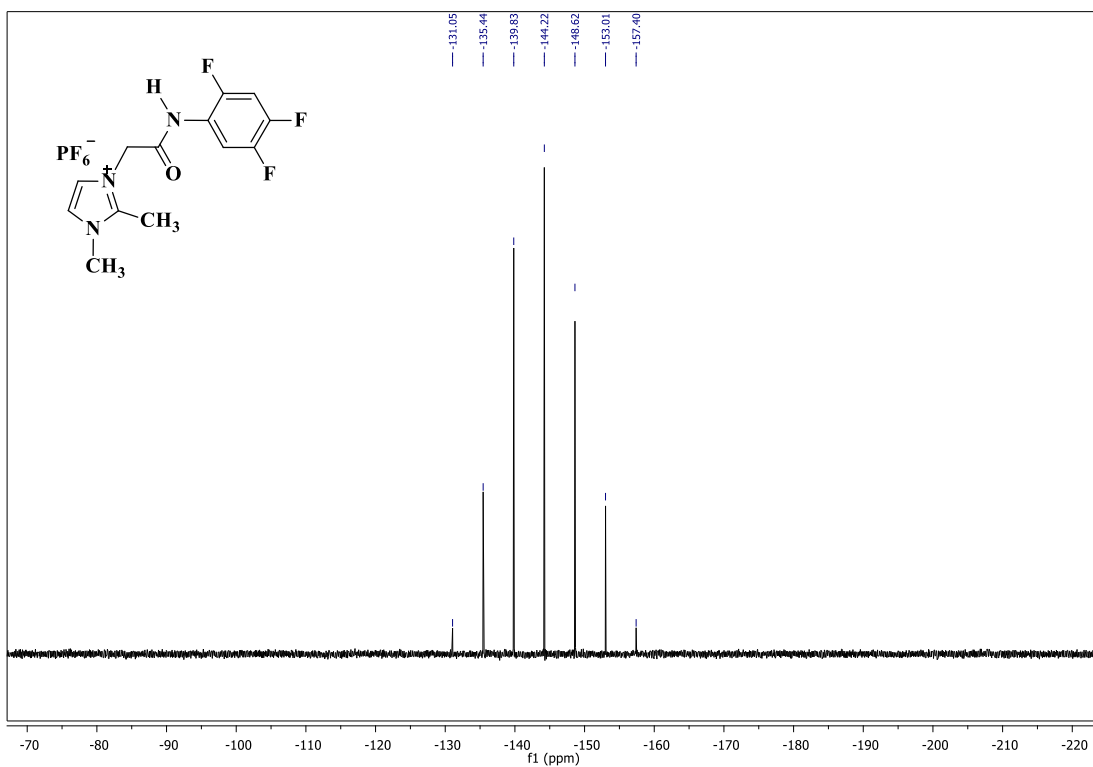


Figure S97:  $^{31}\text{P}$  NMR of compound 5p

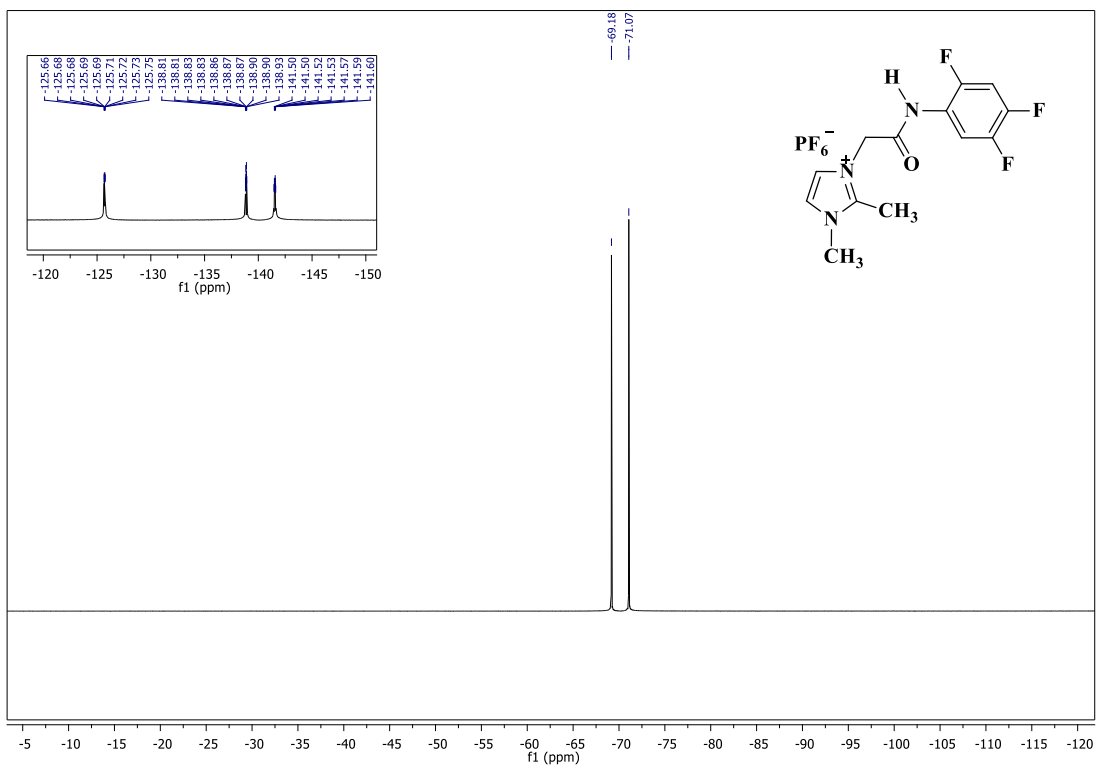
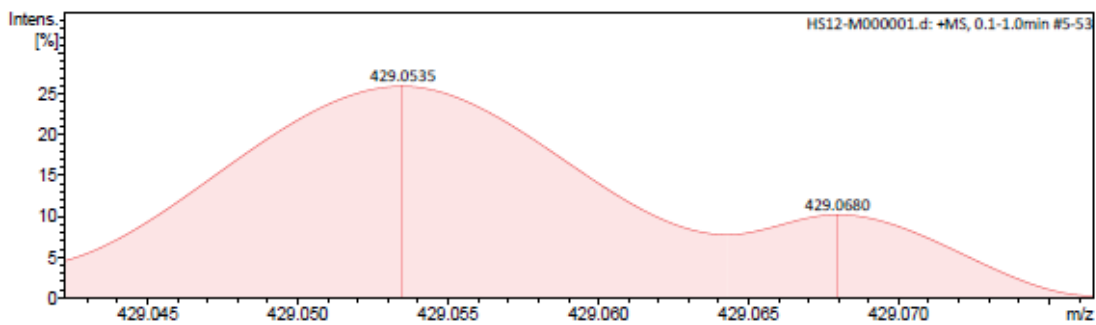
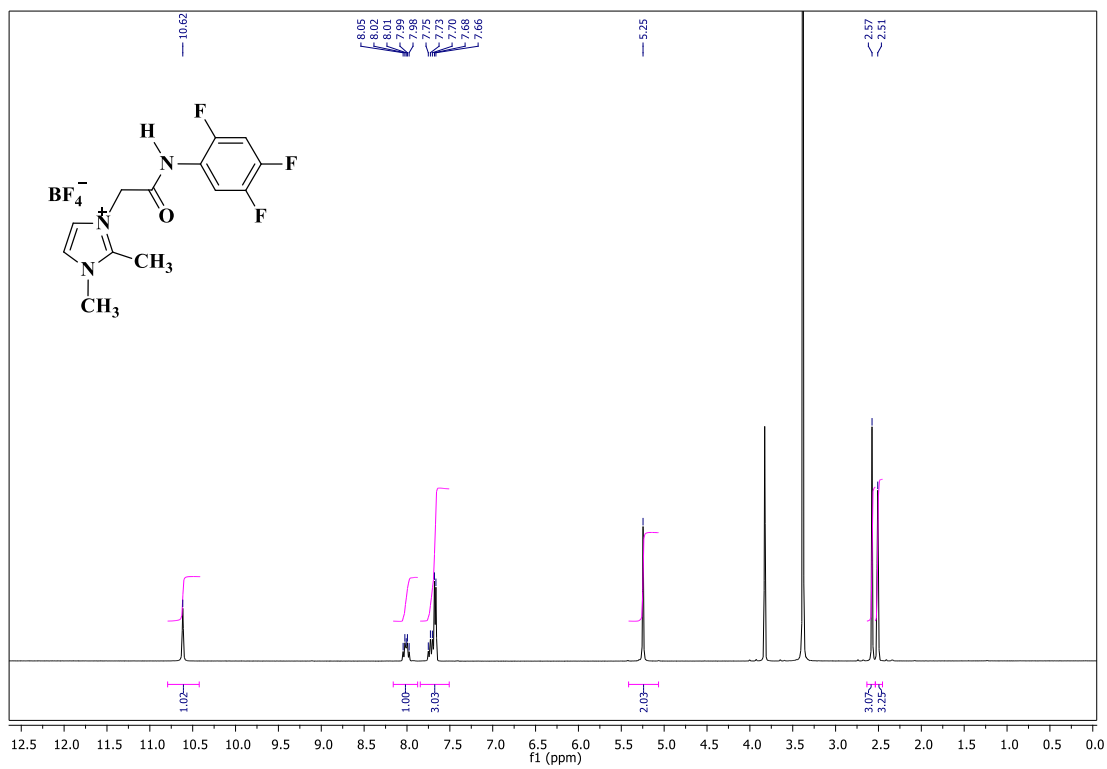


Figure S98:  $^{19}\text{F}$  NMR of compound 5p



**Figure S99:** HRMS (ESI) of compound **5p**



**Figure S100:**  $^1\text{H}$  NMR of compound **5q**

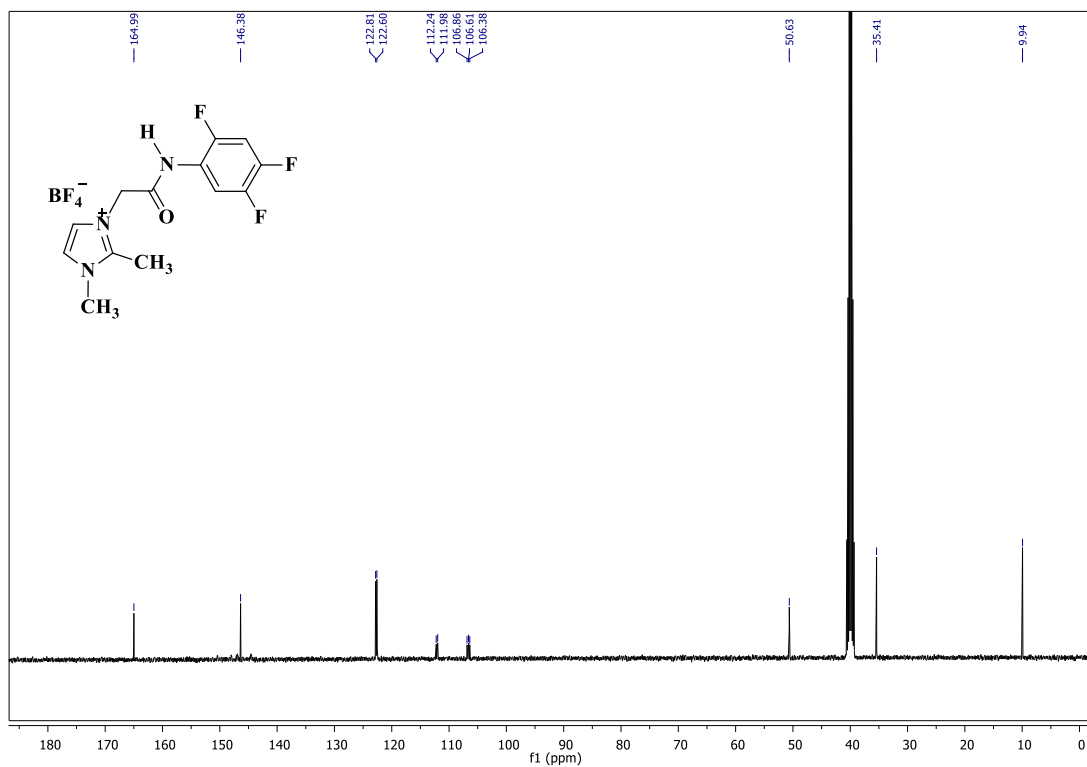


Figure S101:  $^{13}\text{C}$  NMR of compound 5q

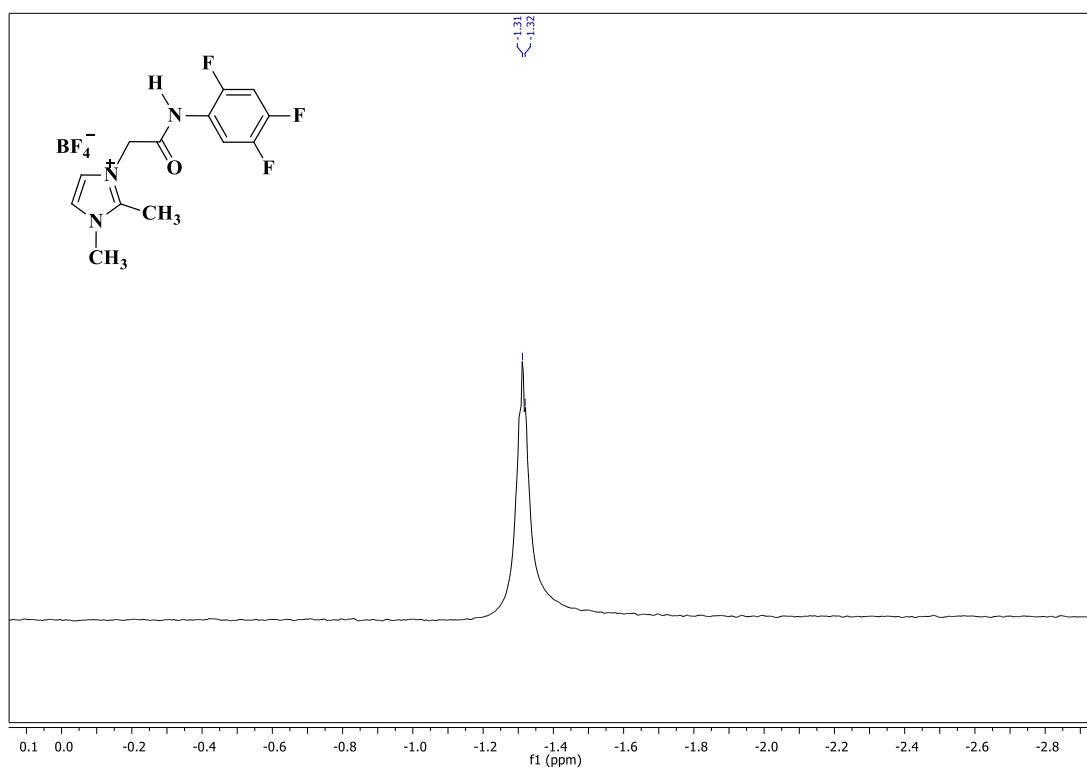
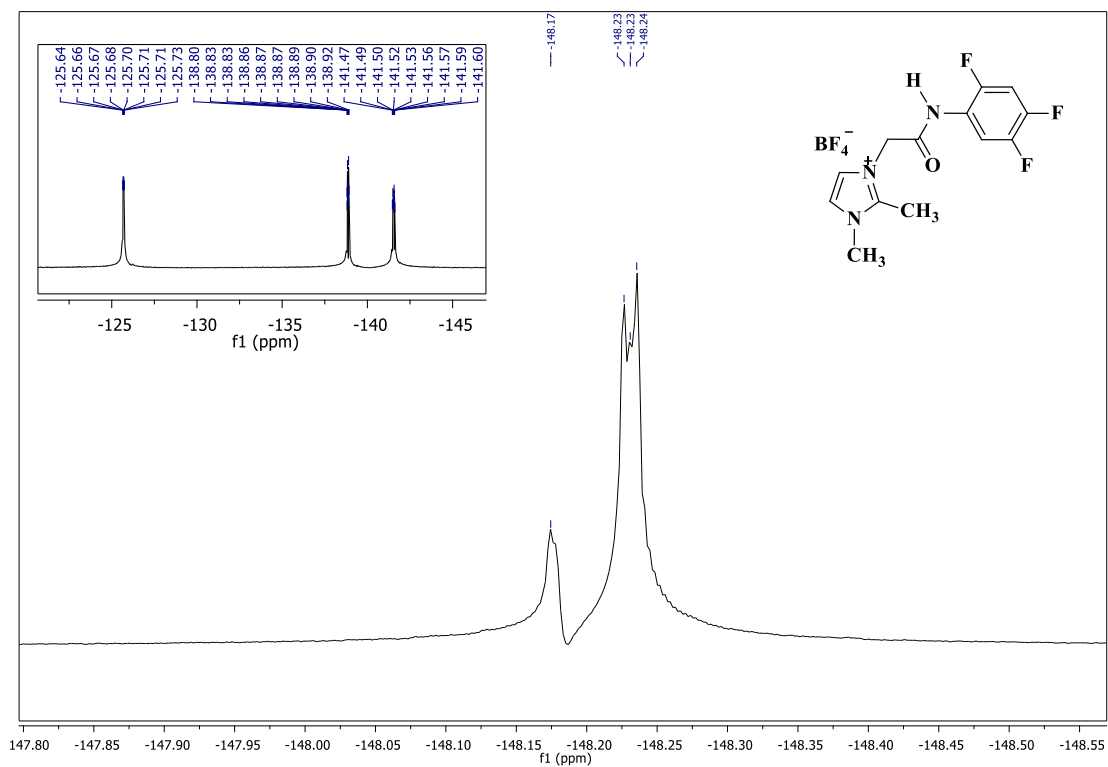
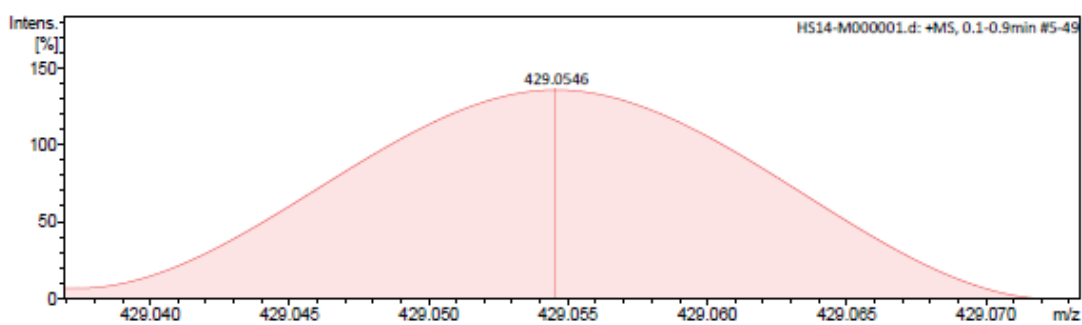


Figure S102:  $^{11}\text{B}$  NMR of compound 5q





**Figure S103:**  $^{19}\text{F}$  NMR of compound **5q**



**Figure S104:** HRMS (ESI) of compound **5q**

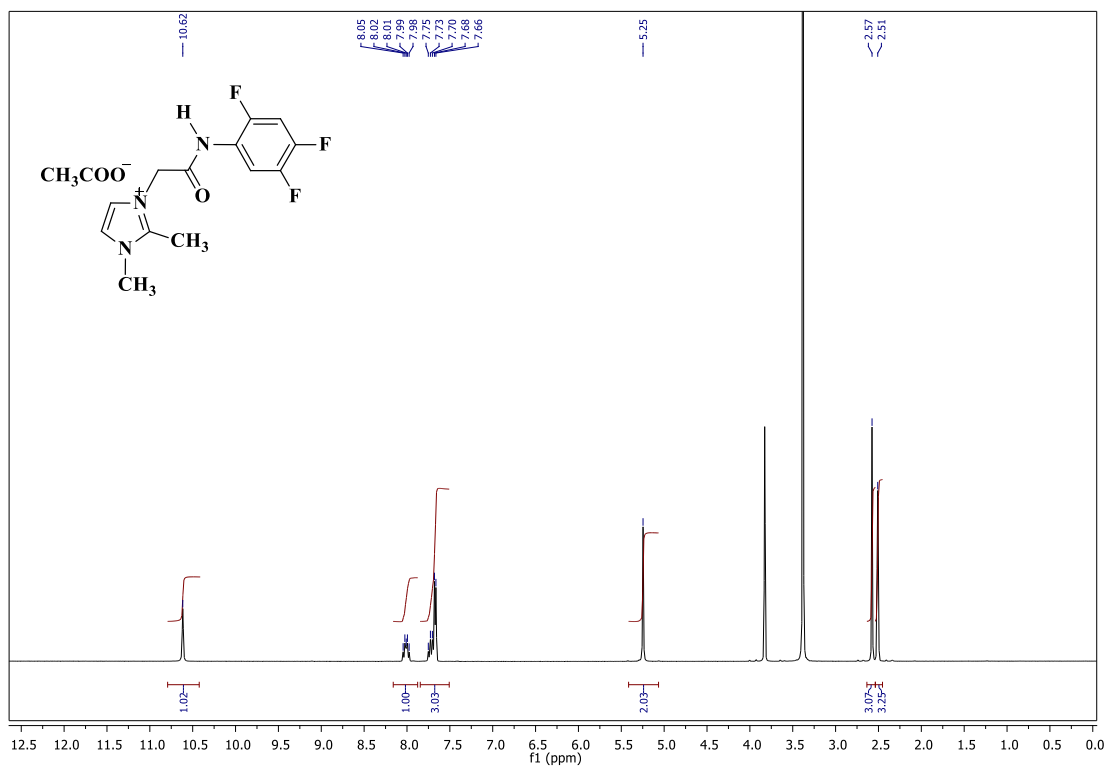


Figure S105:  $^1\text{H}$  NMR of compound 5r

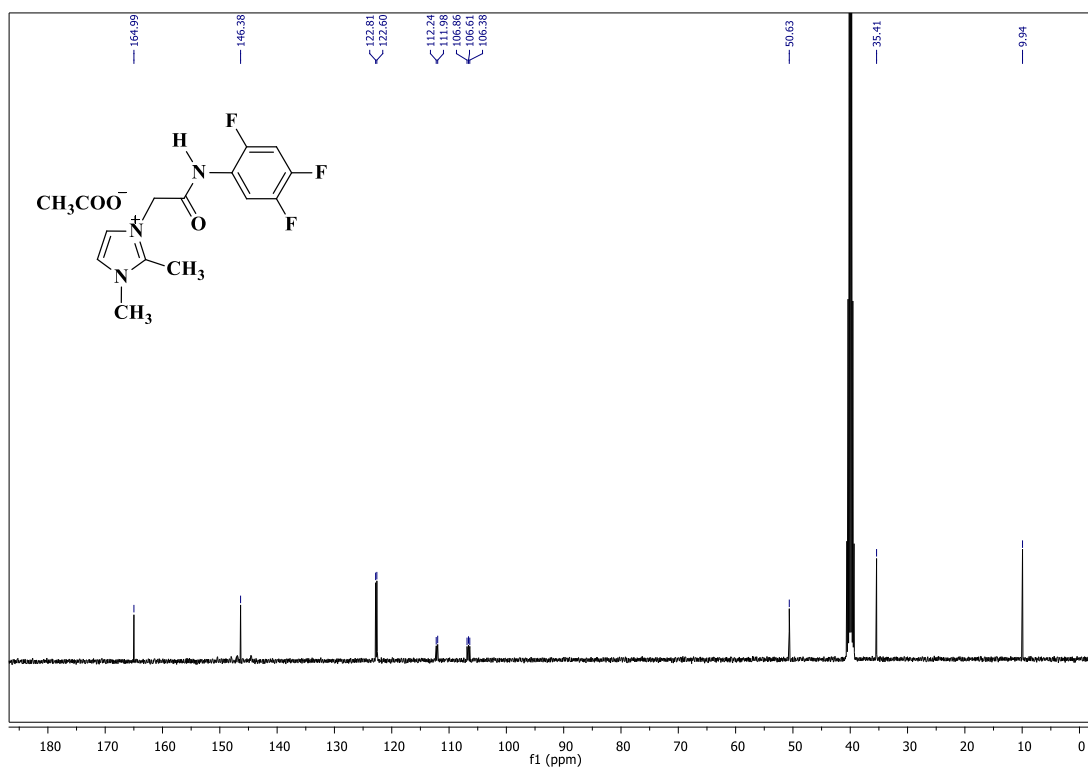
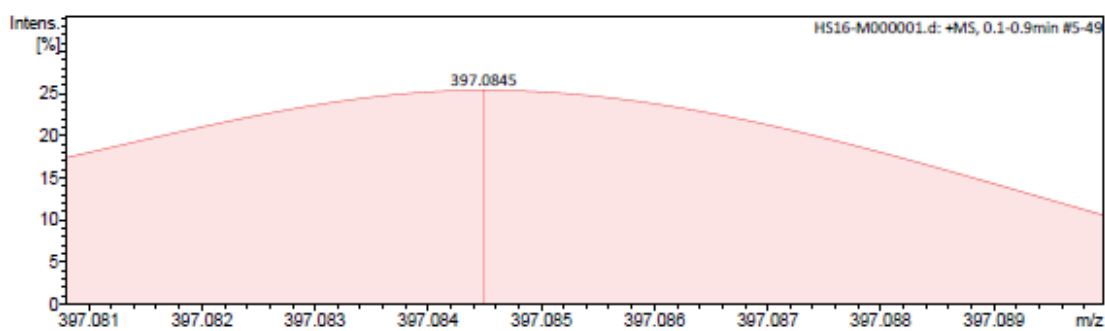
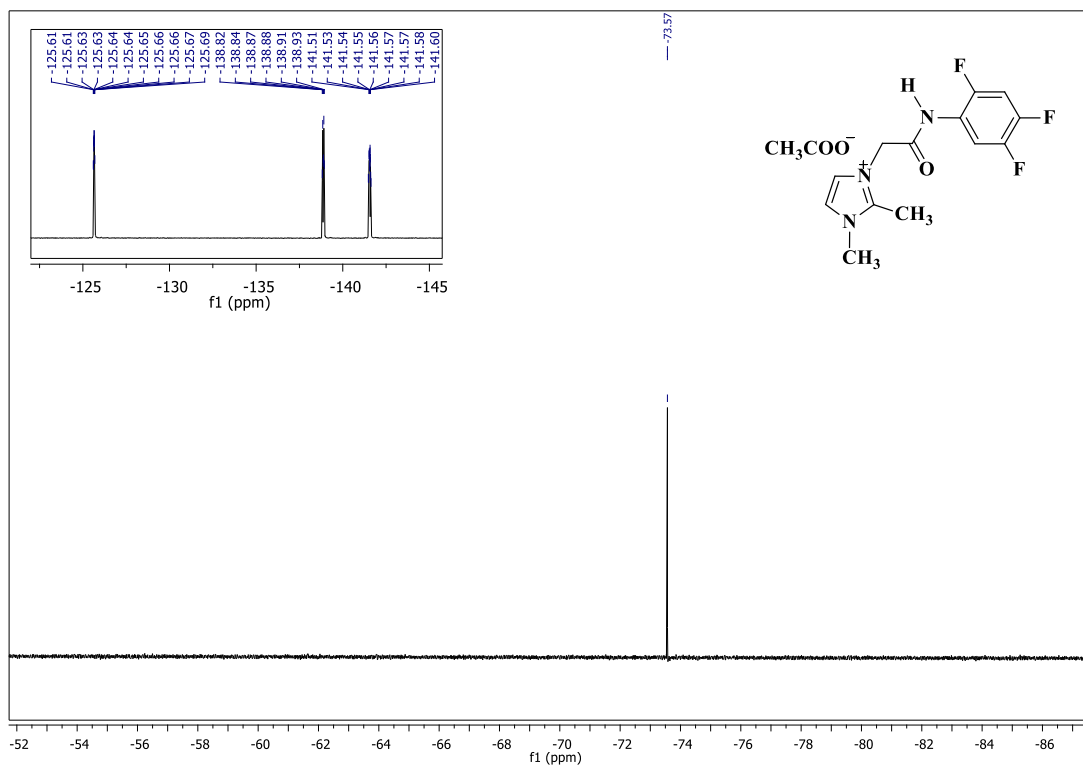


Figure S106:  $^{13}\text{C}$  NMR of compound 5r



## DNA Binding Study of Compound 4b-f and 5a-r

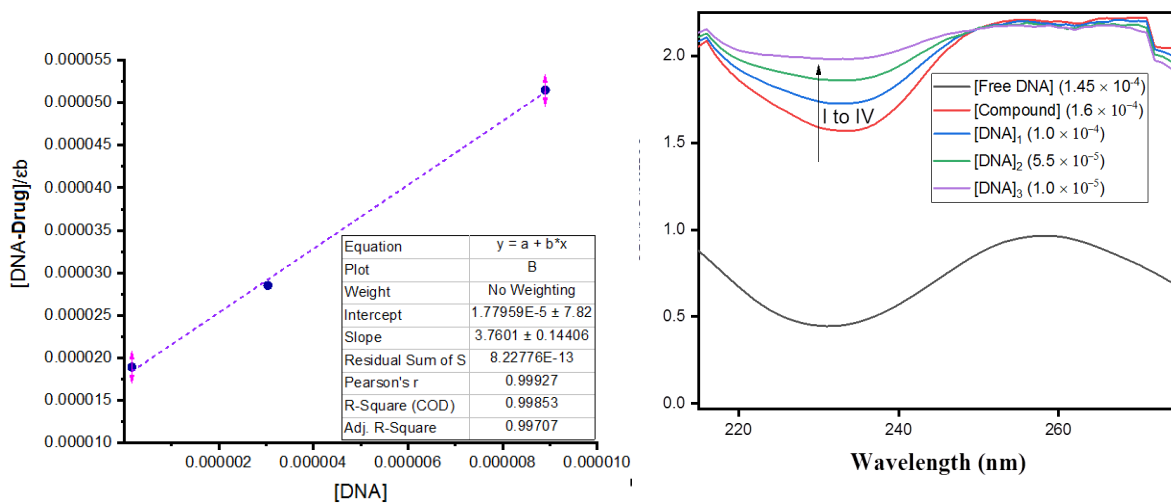


Figure S109: DNA binding study of compound 4b

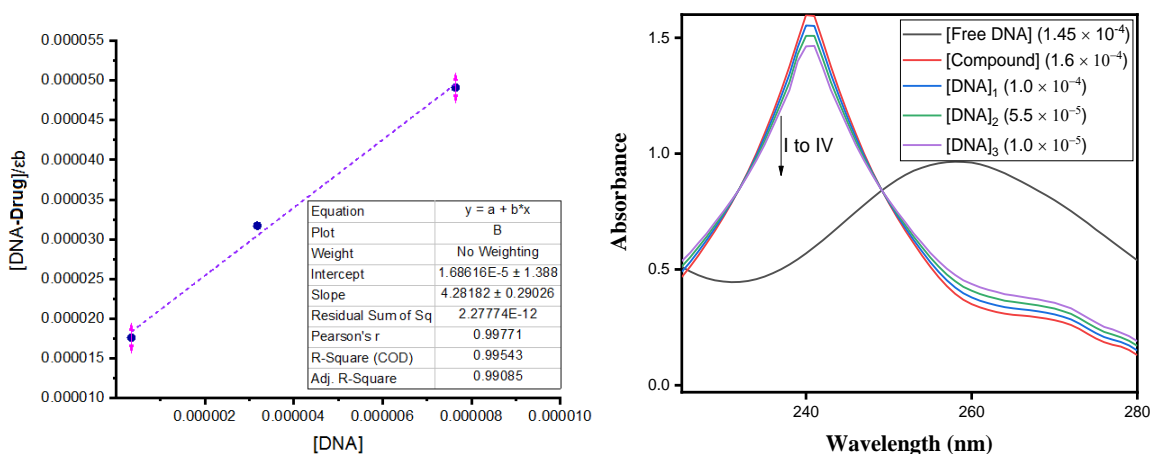


Figure S110: DNA binding study of compound 4c

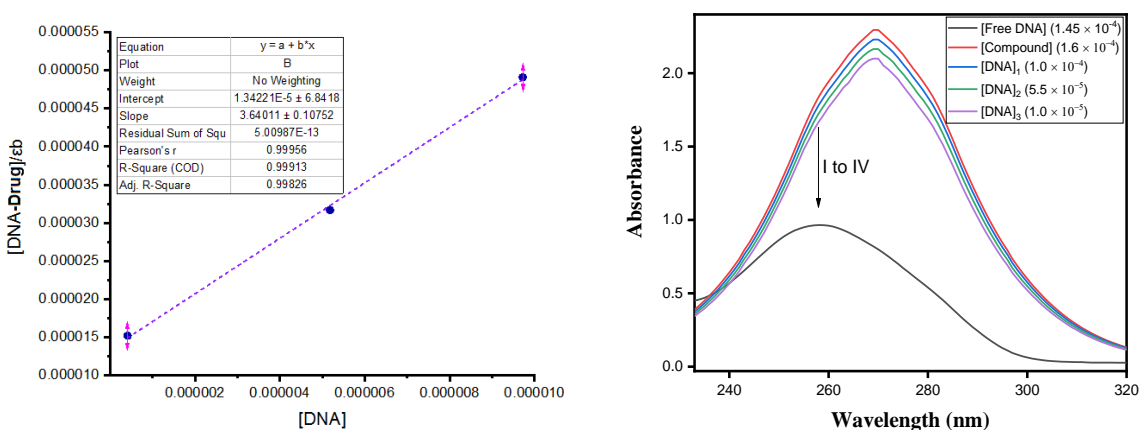
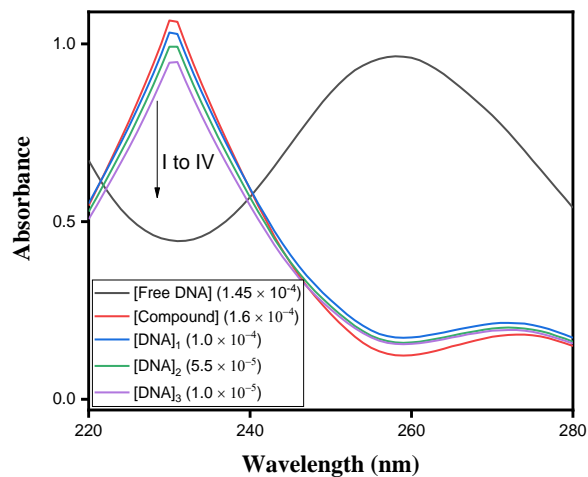
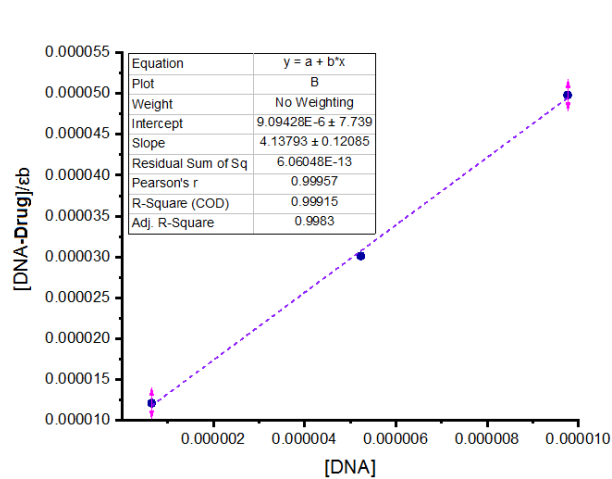
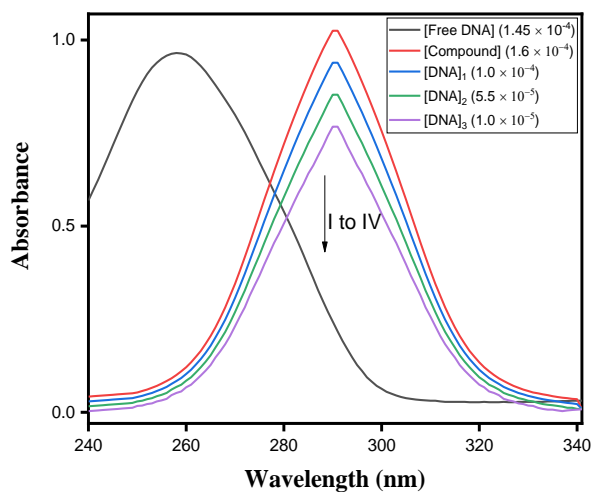
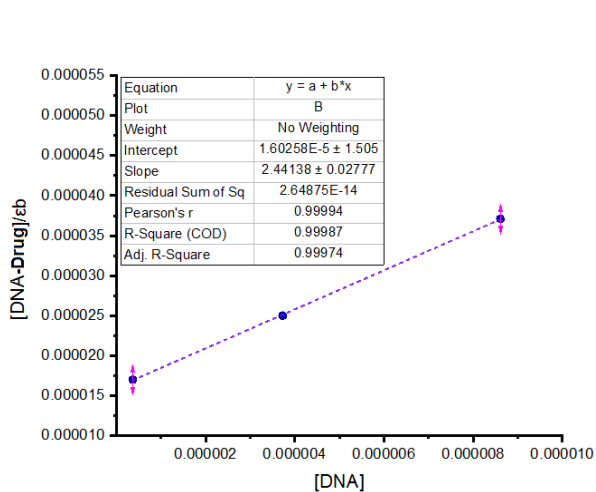


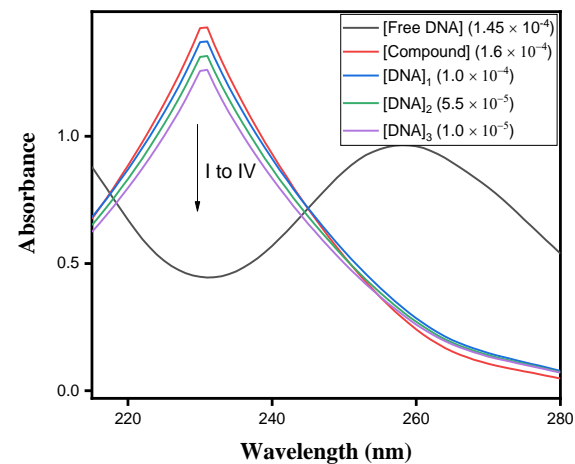
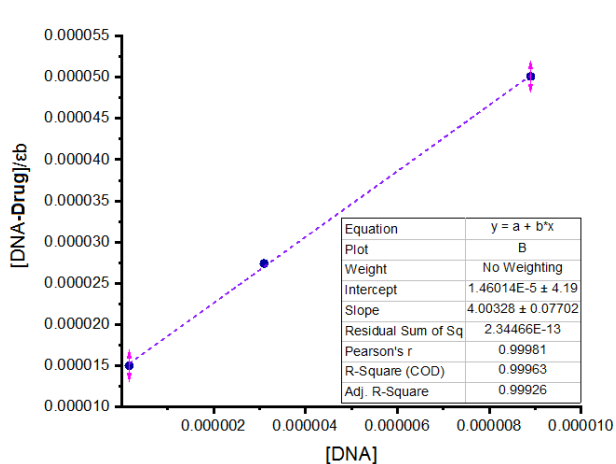
Figure S111: DNA binding study of compound 4d



**Figure S112: DNA binding study of compound 4e**



**Figure S113: DNA binding study of compound 4f**



**Figure S114: DNA binding study of compound 5a**

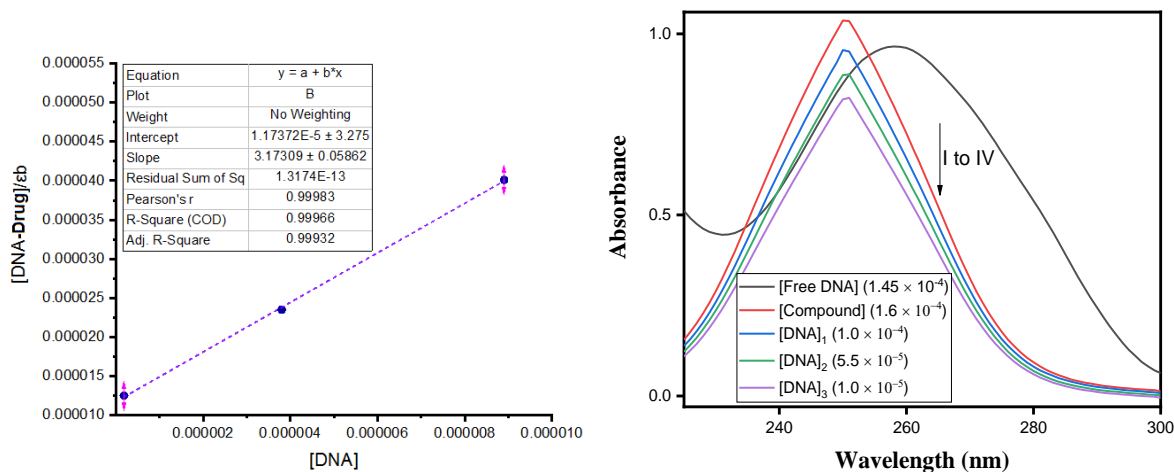


Figure S115: DNA binding study of compound 5b

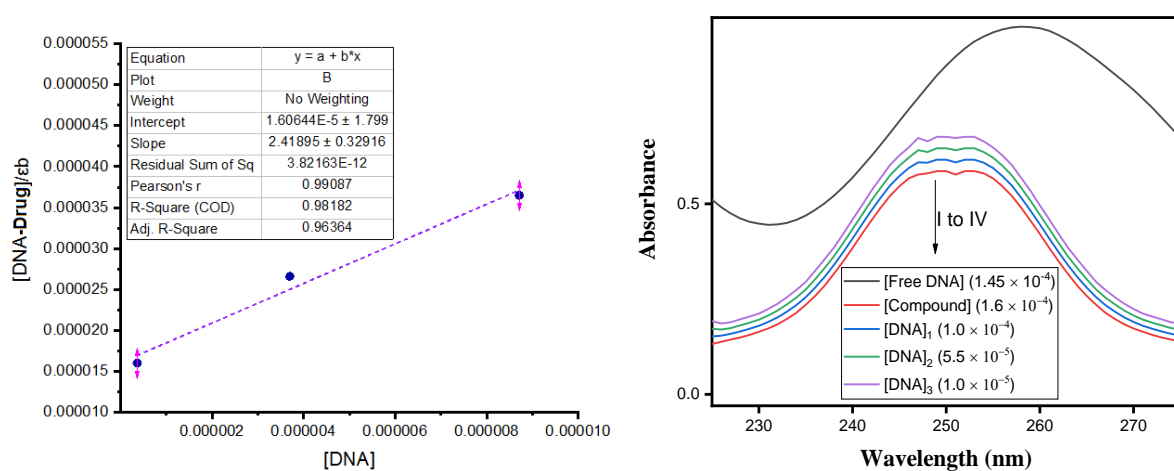


Figure S116: DNA binding study of compound 5c

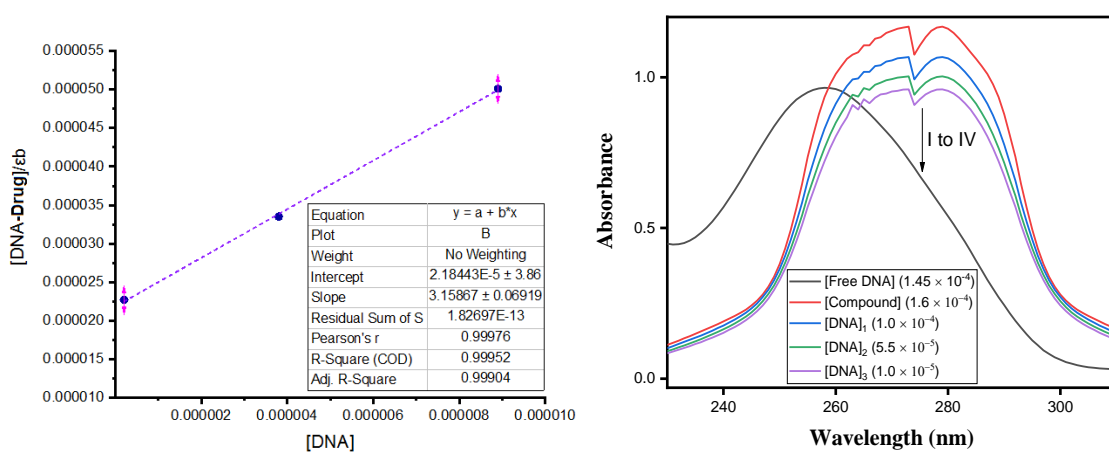


Figure S117: DNA binding study of compound 5d

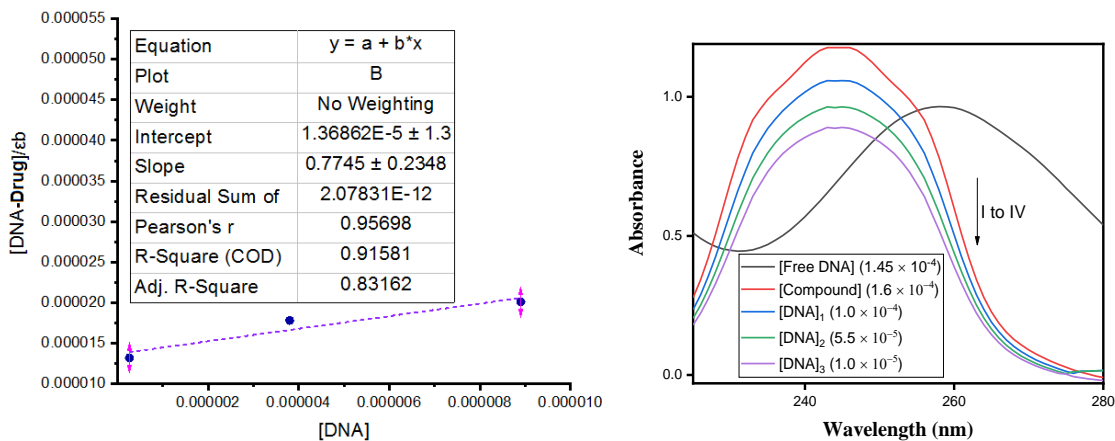


Figure S118: DNA binding study of compound 5e

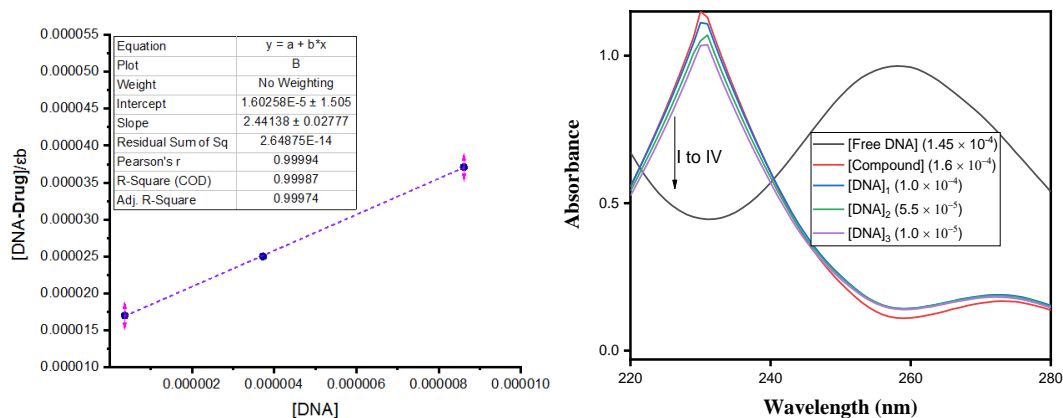


Figure S119: DNA binding study of compound 5f

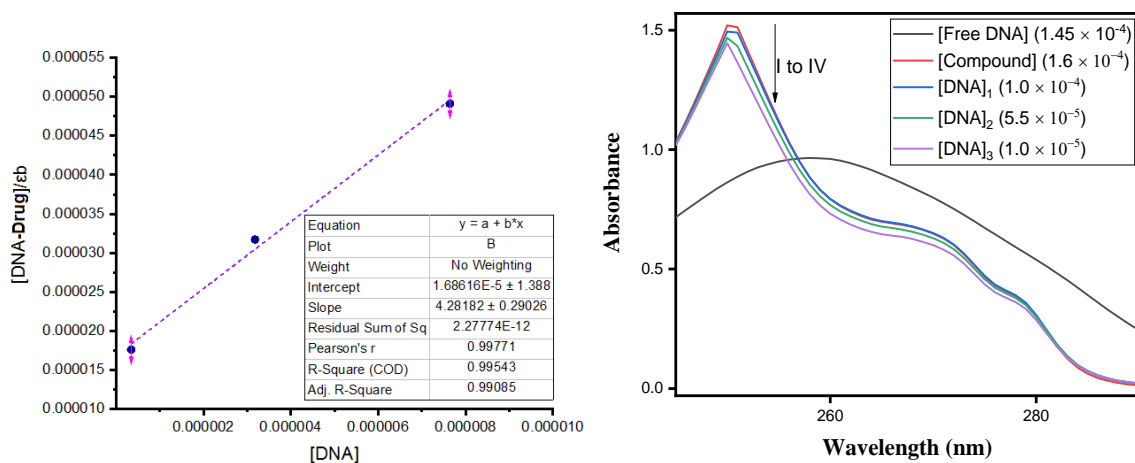
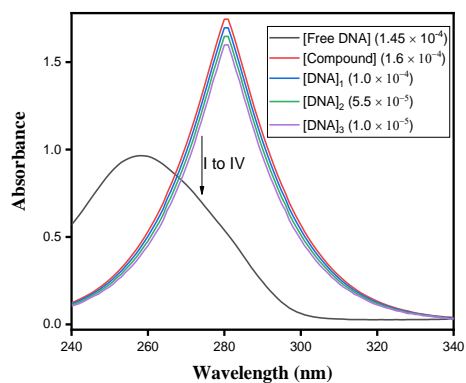
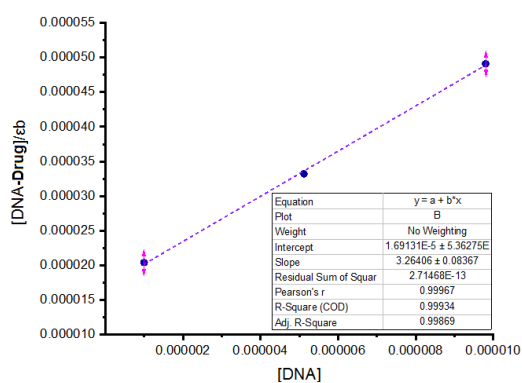
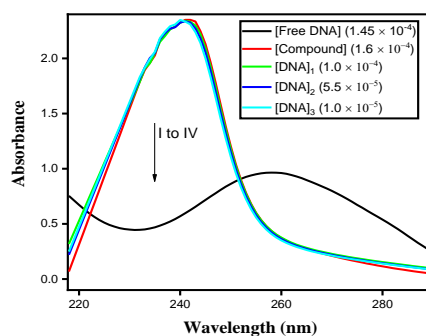
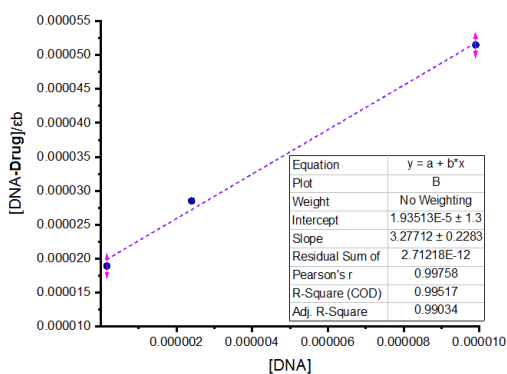


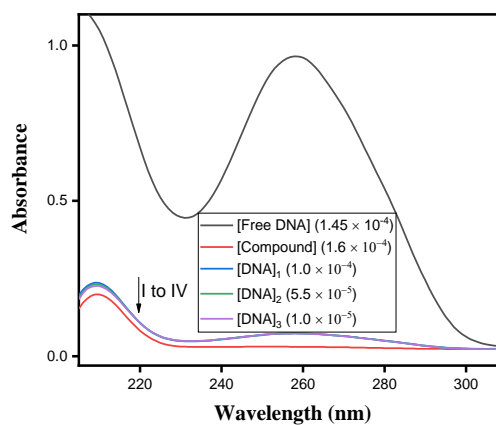
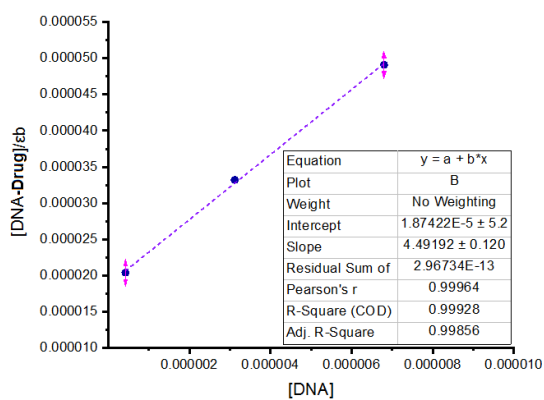
Figure S120: DNA binding study of compound 5g



**Figure S121: DNA binding study of compound 5h**

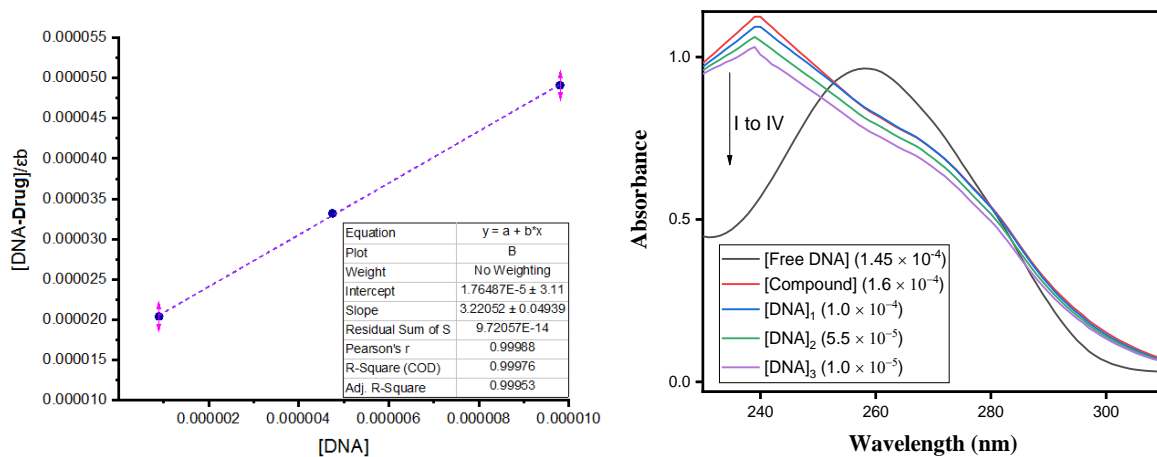


**Figure S122: DNA binding study of compound 5i**

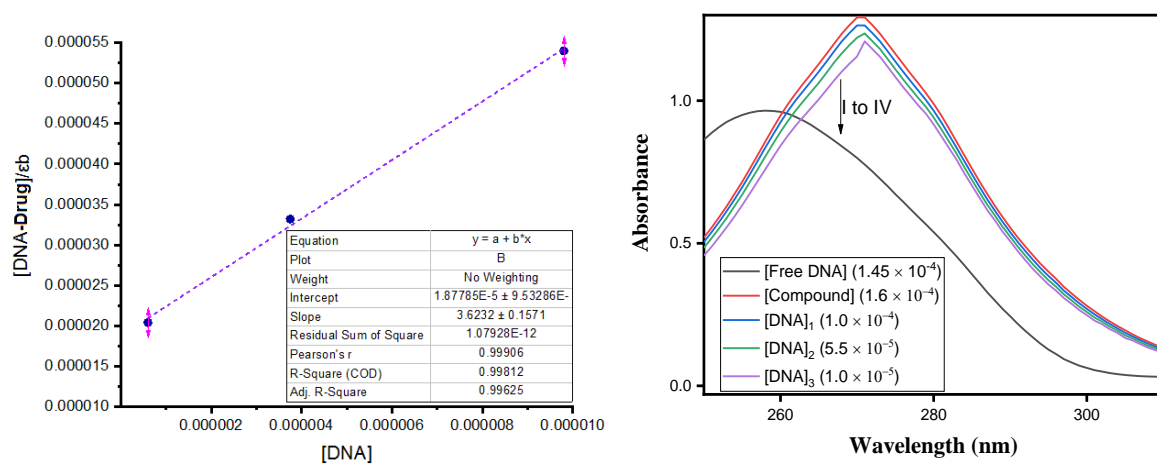


**Figure S123: DNA binding study of compound 5j**

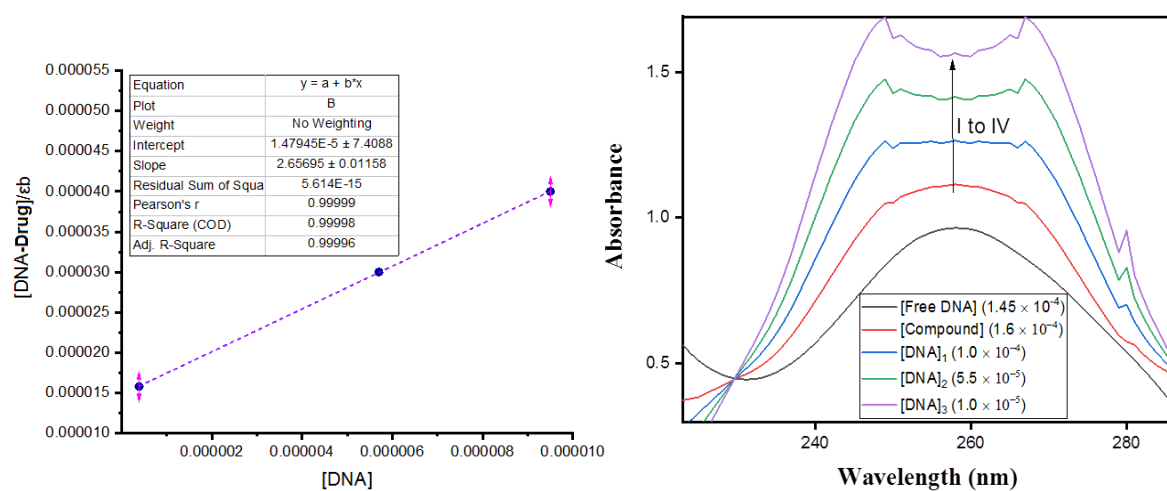




**Figure S124:** DNA binding study of compound **5k**



**Figure S125:** DNA binding study of compound **5l**



**Figure S126:** DNA binding study of compound **5m**

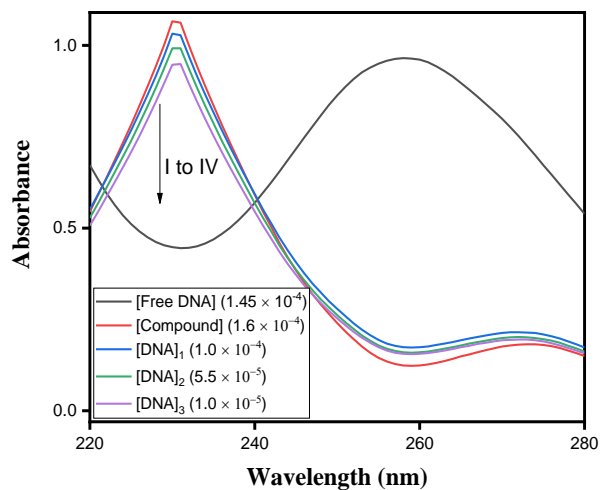
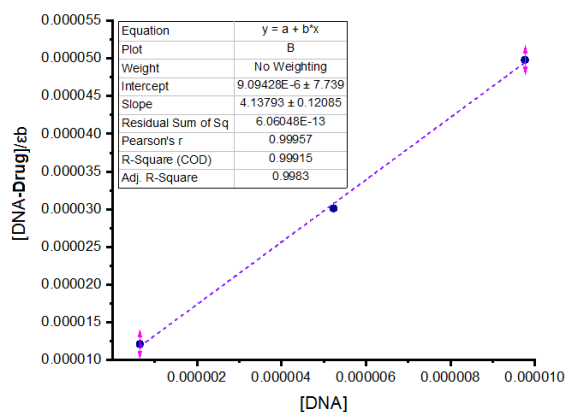


Figure S127: DNA binding study of compound 5n

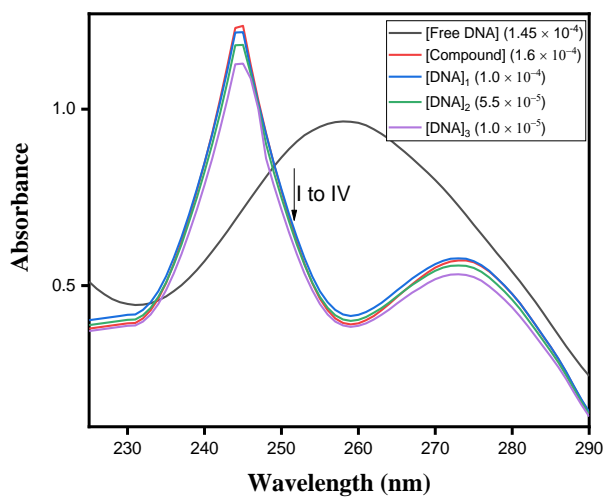
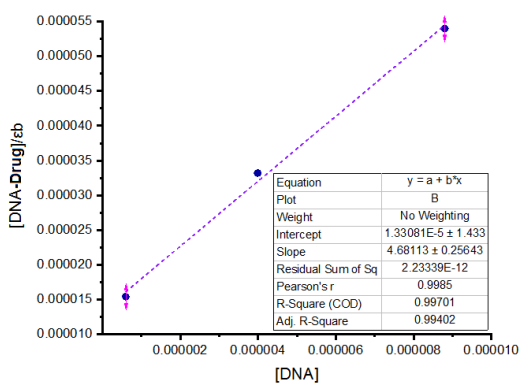


Figure S128: DNA binding study of compound 5o

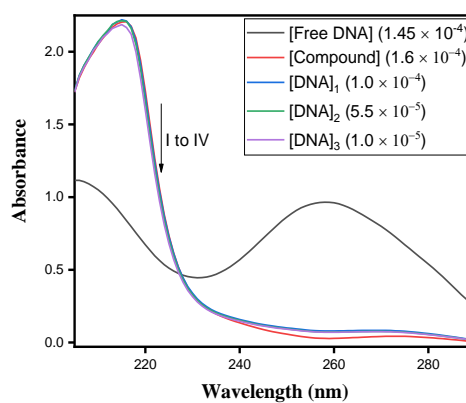
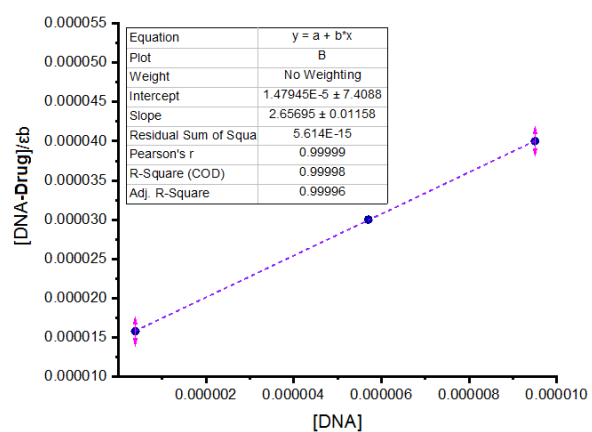


Figure S129: DNA binding study of compound 5p

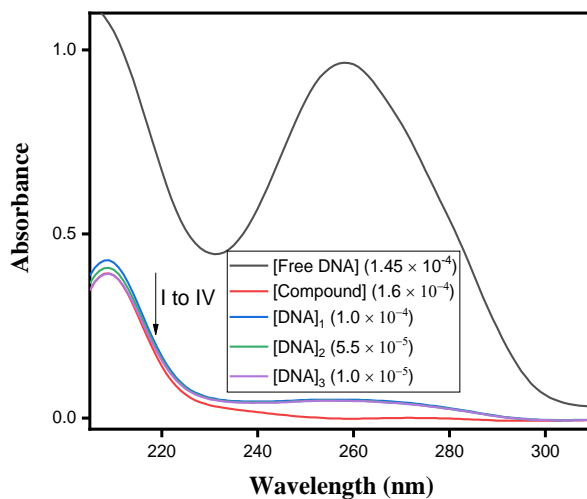
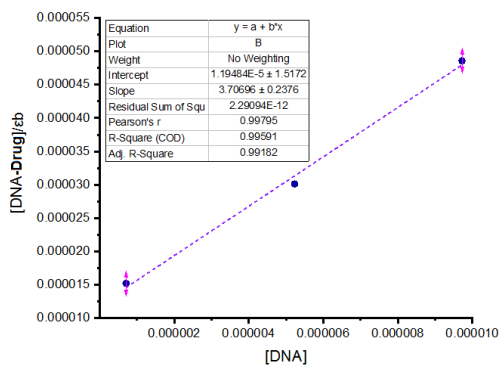


Figure S130: DNA binding study of compound 5q

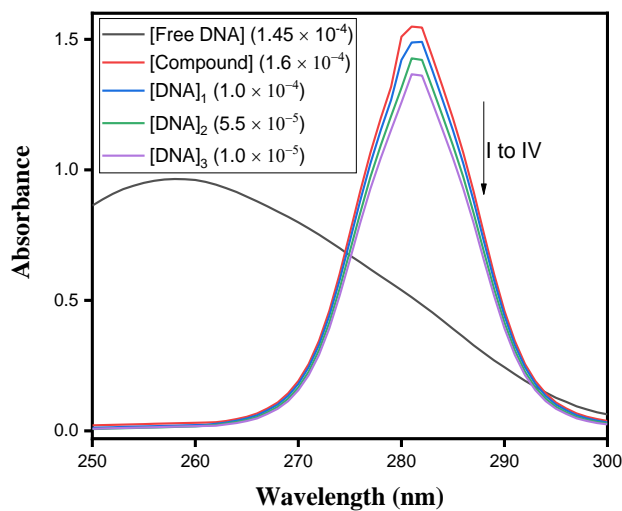
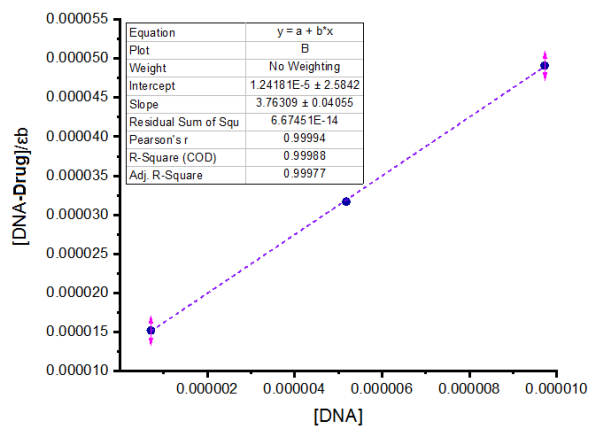
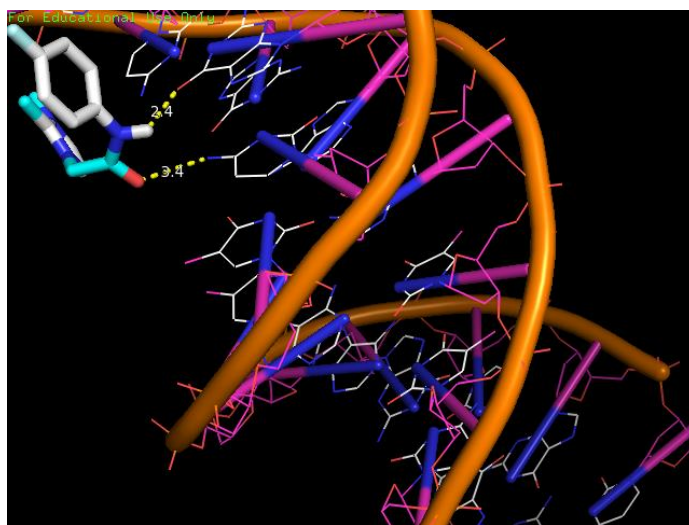
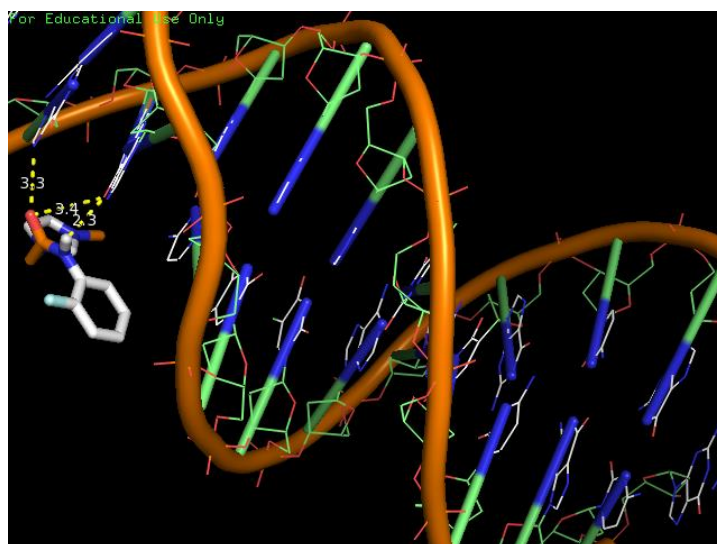


Figure S131: DNA binding study of compound 5q

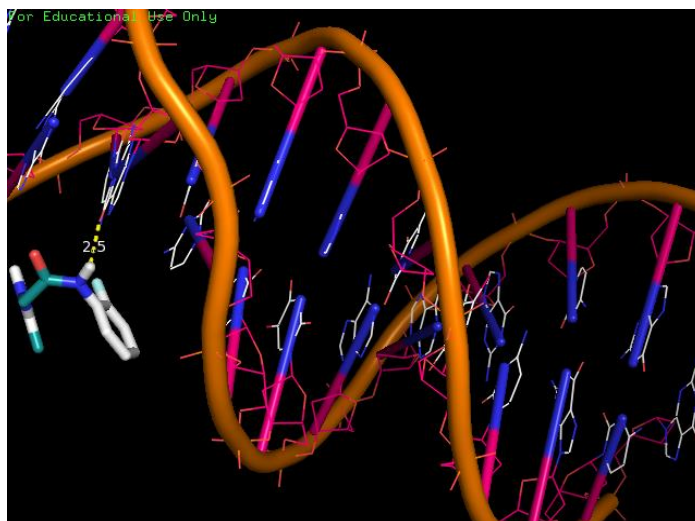
### *Docking Model of Compound 4b-f*



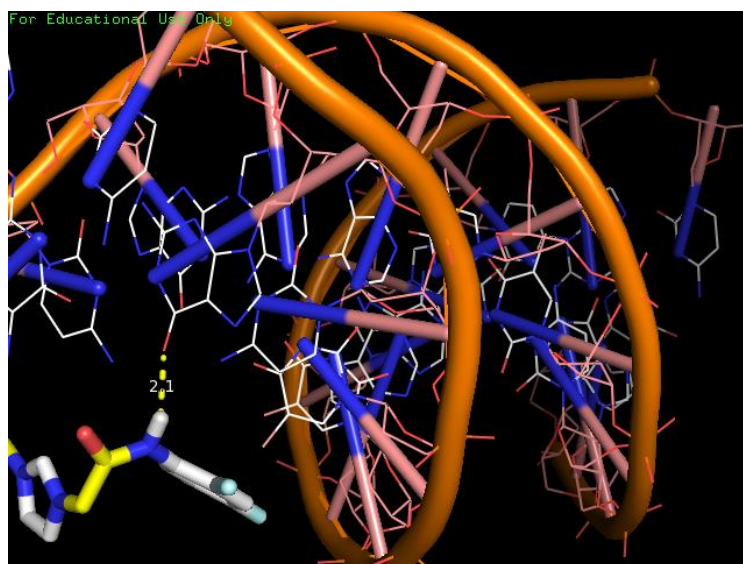
**Figure S132:** Docking model of compound **4b** with DNA



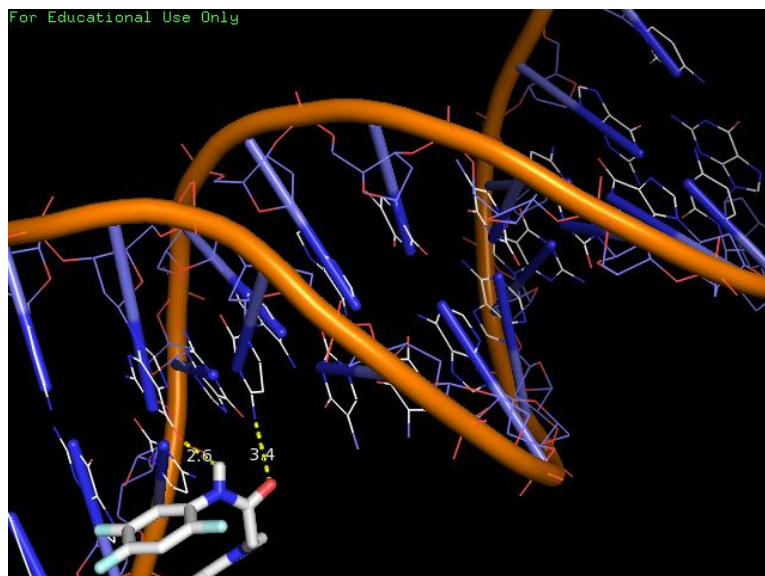
**Figure S133:** Docking model of compound **4c** with DNA



**Figure S134:** Docking model of compound **4d** with DNA



**Figure S135:** Docking model of compound **4e** with DNA



**Figure S136:** Docking model of compound 4f with DNA