

## Supplementary Information

### Development of Unsymmetrical Boron Complexes Bearing (Iso)quinolyphenol Ligand and Their Halogenated Derivatives; Crystal Polymorphism for White-Light-Emitting Properties

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## Experimental section

### General

#### Measurement

$^1\text{H}$ ,  $^{13}\text{C}\{^1\text{H}\}$ ,  $^{11}\text{B}$ , and  $^{19}\text{F}$  NMR spectra were recorded in  $\text{CDCl}_3$  using JEOL ECA-500 and JEOL ECZ-400. High resolution mass spectra (HRMS) were measured with a positive mode by a Bruker micrOTOF II spectrometer; time of flight technique, electrospray ionization (ESI). UV-vis absorption spectra were recorded on a JASCO spectrophotometer V-750. Fluorescence emission spectra were recorded on a JASCO fluorescence spectrophotometer FP-8550. Absolute Fluorescence quantum yield ( $\Phi$ ) were measured by Labsphere 4P-GPS-040-SF with using SHIMADZU RF-5300 as a excited light source and JASCO MV-3600 as a spectrometer. PXRD measurement was carried out by  $\theta$ -2 $\theta$ XRD using  $\text{Cu K}\alpha$  radiation (Rigaku SmartLab). A sub-nanosecond time-resolved fluorescence system employing the time-correlated single-photon-counting method was built based on an inverted optical microscope (IX73, Olympus Corp., Tokyo, Japan). A pulsed 405-nm laser (FOLS-12/405, CRAFT CENTER SAWAKI Inc., Hamamatsu, Japan) was used as the excitation source to irradiate samples. The generated fluorescence was detected with a photon-counting detector (SPD-050-CTD, Micro Photon Device) attached to a spectrometer (H-20, JOBIN YVON S.A.S.) using an optical fiber. The generated signal was analyzed using a photon-counting board (TimeHarp 260 PICO; PicoQuant GmbH). The time resolution of the measurements was 500 ps. Differential scanning calorimetry (DSC) measurement were performed using a DSC-Q2000 (TA Instruments, Japan) at a heating rate of 10 or 5  $^\circ\text{C min}^{-1}$ .

#### Computational details

DFT calculations were carried out to investigate the frontier orbitals. In addition, the HOMO-LUMO transition energies ( $\Delta E$ ), their oscillator strength ( $f$ ), and the energy levels of single ( $S_n$ ) and triplet ( $T_n$ ) excited states were estimated by TD-DFT calculations of the frontier orbital energies and the electron transition energies employed B3LYP/6-31G+(d,p) set combination by using Gaussian 16 program package. We confirmed from the vibrational analyses that each optimized geometry corresponds to a local minimum that has only real frequencies.

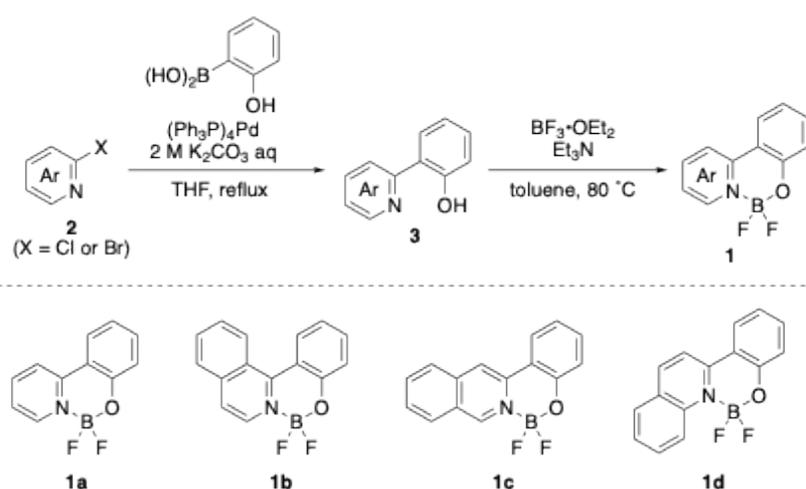
#### X-ray Crystallographic Data for Single Crystalline Products; for 1d, 1d-P5Cl(LB2), 1d-P5Cl(Y), 1d-P5F(Y), and 1d-P6Cl

The single crystal was mounted on a LithoLoops. Intensity data were collected at 100 K on a Rigaku XtaLAB Synergy-S (Dualflex; HyPix) with graphite monochromated  $\text{Cu K}\alpha$  radiation

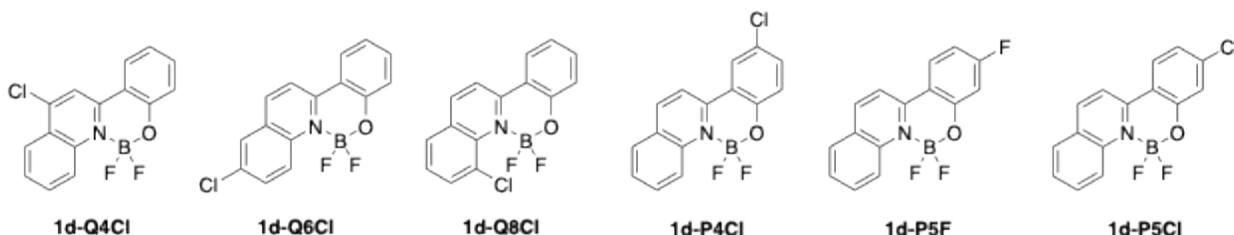
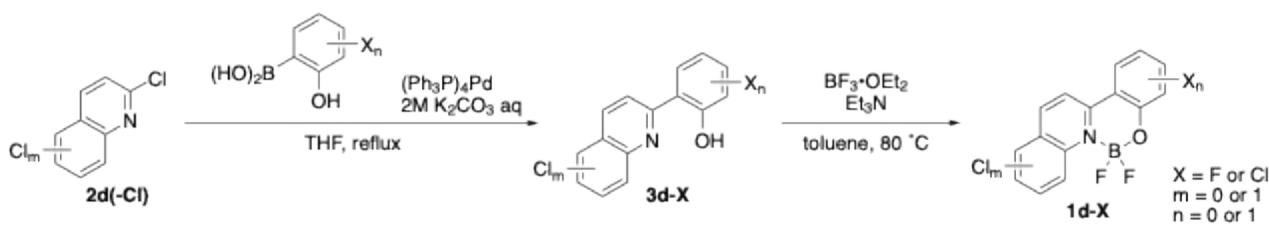
( $\lambda=1.54184 \text{ \AA}$ ). Data were processed using the CrysAlisPro. An analytical numeric absorption correction was applied. The data were corrected for Lorentz and polarization effects. The structure was solved by the ShelXT and expanded using Fourier techniques. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement on F2 was based on observed reflections and variable parameters. All calculations were performed using the Olex2 crystallographic software package except for refinement, which was performed using, SHELXL2018/3 or 2019/3 respectively.

### X-ray Crystallographic Data for Single Crystalline Products; for 1d-P5Cl(LB1) and 1d-P5F(LB)

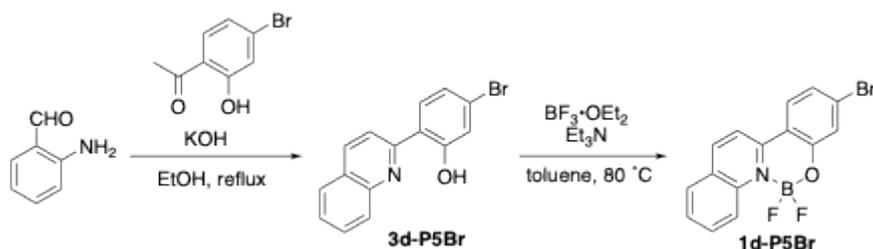
The single crystal was mounted on a glass fiber. Intensity data were collected at 100 K on a Rigaku XtaLAB mini with graphite monochromated Mo K $\alpha$  radiation. Readout was performed in the 0.073 mm pixel mode. The data were collected to a maximum  $2\theta$  value of  $55.0^\circ$ . Data were processed using the CrysAlisPro. An analytical numeric absorption correction was applied. The data were corrected for Lorentz and polarization effects. The structure was solved by the ShelXT and expanded using Fourier techniques. Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement on F2 was based on observed reflections and variable parameters. All calculations were performed using the Olex2 crystallographic software package except for refinement, which was performed using, SHELXL2016 respectively.



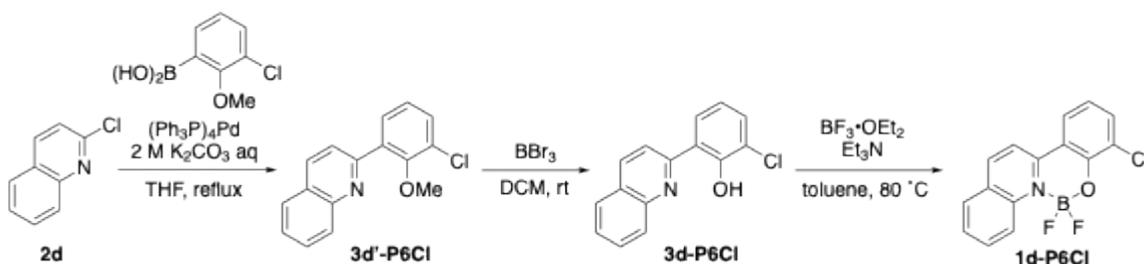
**Scheme S1.** Synthesis of 1a-d



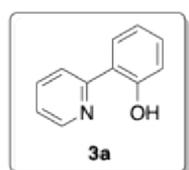
**Scheme S2.** Synthesis of **1d-Q4Cl**, **1d-Q6Cl**, **1d-Q8Cl**, **1d-P4Cl**, **1d-P5F**, and **1d-P5Cl**.



**Scheme S3.** Synthesis of **1d-P5Br**.<sup>[S1]</sup>



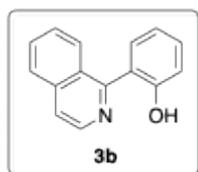
**Scheme S4.** Synthesis of **1d-P6Cl**.



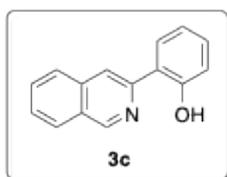
**2-(Pyridin-2-yl)phenol (3a)**<sup>[S2]</sup>: To a solution of **2a** (102 mg, 0.899 mmol), 2-hydroxyphenylboronic acid (199 mg, 1.44 mmol) and (Ph<sub>3</sub>P)<sub>4</sub>Pd (30 mg, 26 μmol) in THF (7.0 mL), 2M K<sub>2</sub>CO<sub>3</sub> aq (1.3 mL) was added at room temperature. The reaction mixture was stirred and refluxed under N<sub>2</sub>. After 15 h, the mixture was cooled down to room temperature, and H<sub>2</sub>O was added. The aqueous layer was extracted with CHCl<sub>3</sub> and dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation, the crude product was purified by silica gel column chromatography (Wakogel C-200, hexane/EtOAc = 20/1) to give **3a** (120 mg, 0.703 mmol) in 78% as a white solid; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 14.36 (s, 1H), 8.52 (dd, *J* = 5.0, 1.0 Hz,

1H), 7.93 (d,  $J = 8.0$  Hz, 1H), 7.86-7.82 (m, 1H), 7.81 (dd,  $J = 8.0, 1.5$  Hz, 1H), 7.33-7.29 (m, 1H), 7.25-7.24 (m, 1H), 7.03 (dd,  $J = 8.5, 1.5$  Hz, 1H), 6.93-6.90 (m, 1H).

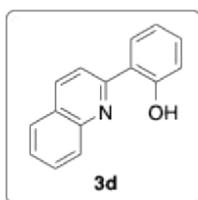
In a similar manner, **3b**, **3c**, **3d**, **3d-Q4Cl**, **3d-Q6Cl**, **3d-Q8Cl**, **3d-P4Cl**, **3d-P5F**, and **3d-P5Cl** were prepared from the corresponding (iso)quinoline derivatives **2**.



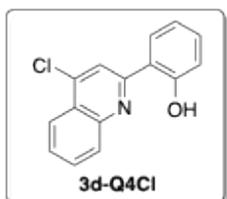
**2-(Isoquinolin-1-yl)phenol (3b)**<sup>[S3]</sup>: Title compound (229 mg, 1.03 mmol) was obtained in 85% yield as a white solid from 1-chloroisoquinoline (197 mg, 1.20 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  12.04 (brs, 1H), 8.48-8.46 (m, 2H), 7.90 (d,  $J = 8.5$  Hz, 1H), 7.76-7.73 (m, 2H), 7.65-7.61 (m, 2H), 7.40-7.37 (m, 1H), 7.18 (dd,  $J = 8.0, 1.0$  Hz, 1H), 7.03-7.00 (m, 1H).



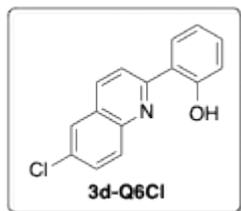
**2-(Isoquinolin-3-yl)phenol (3c)**<sup>[S2]</sup>: Title compound (194 mg, 0.877 mmol) was obtained in 95% yield as a pale orange solid from 3-bromoisoquinoline (191 mg, 0.918 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  14.04 (s, 1H), 9.21 (s, 1H), 8.25 (s, 1H), 8.02 (d,  $J = 8.5$  Hz, 1H), 7.94 (d,  $J = 8.0$  Hz, 1H), 7.91 (d,  $J = 8.0$  Hz, 1H), 7.77-7.73 (m, 1H), 7.63-7.60 (m, 1H), 7.33-7.30 (m, 1H), 7.06 (d,  $J = 8.5$  Hz, 1H), 6.98-6.95 (m, 1H).



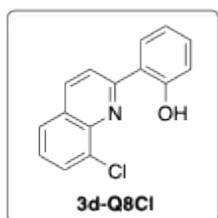
**2-(Quinolin-2-yl)phenol (3d)**<sup>[S4]</sup>: Title compound (244 mg, 1.10 mmol) was obtained in 91% yield as a yellow solid from 2-chloroquinoline (197 mg, 1.20 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  15.25 (s, 1H), 8.28 (d,  $J = 8.5$  Hz, 1H), 8.06 (d,  $J = 8.5$  Hz, 1H), 8.04 (d,  $J = 5.5$  Hz, 1H), 7.96 (dd,  $J = 8.0, 1.5$  Hz, 1H), 7.83 (dd,  $J = 7.5, 1.5$  Hz, 1H), 7.76-7.73 (m, 1H), 7.57-7.54 (m, 1H), 7.39-7.35 (m, 1H), 7.10 (dd,  $J = 7.5, 1.5$  Hz, 1H), 6.98-6.95 (m, 1H).



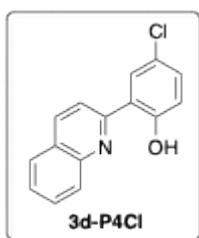
**2-(4-Chloroquinolin-2-yl)phenol (3d-Q4Cl)**<sup>[S5]</sup>: Title compound (78 mg, 0.305 mmol) was obtained in 30% yield as a yellow solid from 2,4-dichloroquinoline (202 mg, 1.01 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>)  $\delta$  14.76 (s, 1H), 8.24 (d,  $J = 9.0$  Hz, 1H), 8.14 (s, 1H), 8.06 (d,  $J = 8.5$  Hz, 1H), 7.89 (dd,  $J = 8.0, 1.0$  Hz, 1H), 7.82-7.79 (m, 1H), 7.67-7.64 (m, 1H), 7.40-7.37 (m, 1H), 7.09 (d,  $J = 8.5$  Hz, 1H), 6.99-6.96 (m, 1H).



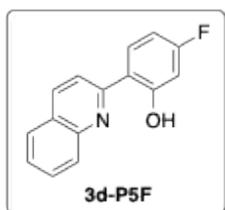
**2-(6-Chloroquinolin-2-yl)phenol (3d-Q6Cl)**<sup>[S4]</sup>: Title compound (208 mg, 0.811 mmol) was obtained in 81% yield as a yellow solid from 2,6-dichloroquinoline (200 mg, 1.00 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 14.83 (brs, 1H), 8.19 (d, *J* = 9.0 Hz, 1H), 8.07 (d, *J* = 9.0 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 7.94 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.82 (d, *J* = 2.0 Hz, 1H), 7.68 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.40-7.36 (m, 1H), 7.09 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.00-6.96 (m, 1H).



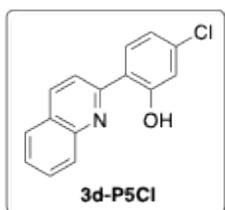
**2-(8-Chloroquinolin-2-yl)phenol (3d-Q8Cl)**<sup>[S6]</sup>: Title compound (164 mg, 0.641 mmol) was obtained in 66% yield as a yellow solid from 2,8-dichloroquinoline (192 mg, 0.967 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 14.85 (s, 1H), 8.68 (d, *J* = 9.0 Hz, 1H), 8.15 (d, *J* = 9.5 Hz, 1H), 7.99-7.96 (m, 2H), 7.68-7.61 (m, 2H), 7.41-7.38 (m, 1H), 7.10 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.01-6.97 (m, 1H).



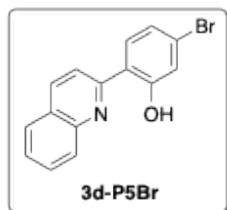
**4-Chloro-2-(quinolin-2-yl)phenol (3d-P4Cl)**<sup>[S7]</sup>: Title compound (238 mg, 0.934 mmol) was obtained in 74% yield as a yellow solid from 2-chloroquinoline (205 mg, 1.25 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 15.23 (brs, 1H), 8.32 (d, *J* = 9.0 Hz, 1H), 8.05 (d, *J* = 8.5 Hz, 1H), 8.00 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 2.5 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.79-7.75 (m, 1H), 7.60-7.57 (m, 1H), 7.31 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.04 (d, *J* = 9.0 Hz, 1H).



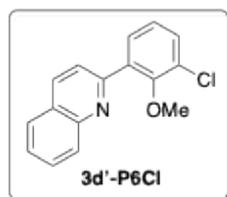
**5-Fluoro-2-(quinolin-2-yl)phenol (3d-P5F)**<sup>[S7]</sup>: Title compound (297 mg, 1.24 mmol) was obtained in 97% yield as a yellow solid from 2-chloroquinoline (207 mg, 1.27 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 15.75 (s, 1H), 8.28 (d, *J* = 8.5 Hz, 1H), 8.02 (d, *J* = 9.0 Hz, 1H), 7.96 (d, *J* = 8.5 Hz, 1H), 7.92 (dd, *J* = 8.5, 6.5 Hz, 1H), 7.83 (d, *J* = 8.5 Hz, 1H), 7.77-7.74 (m, 1H), 7.58-7.54 (m, 1H), 6.78 (dd, *J* = 10.5, 2.5 Hz, 1H), 6.70-6.66 (m, 1H).



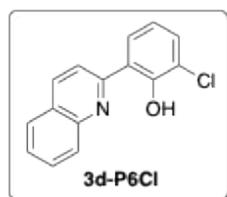
**5-Chloro-2-(quinolin-2-yl)phenol (3d-P5Cl)**<sup>[S7]</sup>: Title compound (276 mg, 1.08 mmol) was obtained in 86% yield as a yellow solid from 2-chloroquinoline (205 mg, 1.25 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 15.57 (brs, 1H), 8.29 (d, *J* = 9.0 Hz, 1H), 8.03 (d, *J* = 9.0 Hz, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 7.87 (d, *J* = 9.0 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.78-7.74 (m, 1H), 7.59-7.56 (m, 1H), 7.10 (d, *J* = 2.5 Hz, 1H), 6.93 (dd, *J* = 8.0, 2.5 Hz, 1H).



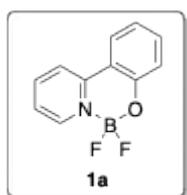
**5-Bromo-2-(quinolin-2-yl)phenol (3d-P5Br)**<sup>[S4]</sup>: To a solution of 2-aminobenzaldehyde (192 mg, 1.58 mmol) and 2-acetyl-5-bromophenol (346 mg, 1.61 mmol) in EtOH (15 mL), sat. solution of KOH in EtOH (2.8 mL) was added at room temperature under N<sub>2</sub>. The reaction mixture was stirred and refluxed under N<sub>2</sub>. After 18 h, the mixture was cooled down to room temperature, and sat. NH<sub>4</sub>Cl aq was added. Filtration and washing with H<sub>2</sub>O gave **3d-5PBr** (325 mg, 1.08 mmol) in 68% as a yellow solid; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>) δ 15.57 (s, 1H), 8.29 (d, *J* = 8.8 Hz, 1H), 8.04 (d, *J* = 8.8 Hz, 1H), 7.99 (d, *J* = 9.2 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.4 Hz, 1H), 7.78-7.74 (m, 1H), 7.60-7.56 (m, 1H), 7.27 (d, *J* = 2.0 Hz, 1H), 7.09 (dd, *J* = 8.4, 2.0 Hz, 1H).



**6-Chloro-2-(quinolin-2-yl)anisole (3d'-P6Cl)**: To a solution of **2d** (211 mg, 1.29 mmol), 3-chloro-2-methoxyphenylboronic acid (342 mg, 1.84 mmol) and (Ph<sub>3</sub>P)<sub>4</sub>Pd (43 mg, 37 μmol) in THF (8.5 mL), 2M K<sub>2</sub>CO<sub>3</sub> aq (1.8 mL) was added at room temperature. The reaction mixture was stirred and refluxed under N<sub>2</sub>. After 15 h, the mixture was cooled down to room temperature, and H<sub>2</sub>O was added. The aqueous layer was extracted with CHCl<sub>3</sub> and dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation, the crude product was purified by silica gel column chromatography (Wakogel C-200, hexane/EtOAc = 30/1) to give a corresponding anisole compound **3d'-P6Cl** (328 mg, 1.22 mmol) in 94% as a colorless oil; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.17 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.91 (d, *J* = 8.5 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.76 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.72-7.68 (m, 1H), 7.53-7.49 (m, 1H), 7.45 (d, *J* = 7.5 Hz, 1H), 7.18-7.15 (m, 1H), 3.60 (s, 3H); <sup>13</sup>C{<sup>1</sup>H} NMR (126 MHz, CDCl<sub>3</sub>) δ 155.9, 154.2, 148.2, 136.0, 135.9, 131.0, 130.1, 129.6, 129.5, 128.4, 127.5, 127.1, 126.6, 125.2, 122.5, 61.4; HRMS (ESI-TOF) found: *m/z* 270.0672, calcd. for C<sub>16</sub>H<sub>13</sub>ClNO [M+H<sup>+</sup>] 270.0680.

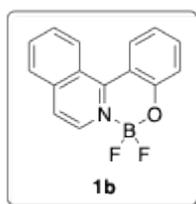


**6-Chloro-2-(quinolin-2-yl)phenol (3d-P6Cl)**<sup>[S4]</sup>: To a solution of **3d'-P6Cl** (310 mg, 1.15 mmol) in DCM (9.0 mL), BBr<sub>3</sub> (1.0 M DCM solution, 1.6 mL, 1.6 mmol) was added at room temperature under N<sub>2</sub>. After 15 h, H<sub>2</sub>O was added. The aqueous layer was extracted with CHCl<sub>3</sub> and dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation, the crude product was purified by reprecipitation (from MeOH/H<sub>2</sub>O) to give **3d-P6Cl** (263 mg, 1.03 mmol) in 79% as a yellow solid; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 16.51 (brs, 1H), 8.32 (d, *J* = 8.5 Hz, 1H), 8.07-8.04 (m, 2H), 7.89 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.80-7.76 (m, 1H), 7.61-7.58 (m, 1H), 7.48 (dd, *J* = 7.5, 1.5 Hz, 1H), 6.93-6.89 (m, 1H).

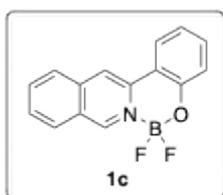


**Difluoro[2-(pyridin-2-yl)-phenolyl]borane (1a)**<sup>[S8]</sup>: To a solution of **3a** (121 mg, 0.703 mmol) and Et<sub>3</sub>N (300 μL, 2.14 mmol) in toluene (6.0 mL), BF<sub>3</sub>•OEt<sub>2</sub> (450 μL, 3.58 mmol) was added at room temperature. The reaction mixture was stirred at 80 °C. After 18 h, the mixture was cooled down to room temperature, and aq. sat. NaHCO<sub>3</sub> was added. The aqueous layer was extracted with CHCl<sub>3</sub> and dried over Na<sub>2</sub>SO<sub>4</sub>. After evaporation, the crude product was washed with MeOH and purified by reprecipitation (from DCM/hexane) to give **1a** (115 mg, 0.525 mmol) in 74% as a white solid; <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.72 (d, *J* = 5.5 Hz, 1H), 8.21-8.18 (m, 1H), 8.13 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.61-7.58 (m, 1H), 7.52-7.49 (m, 1H), 7.20 (d, *J* = 8.5 Hz, 1H), 7.08-7.05 (m, 1H).

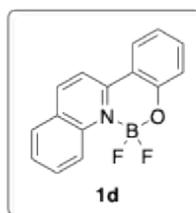
In a similar manner, **1b**, **1c**, and **1d** were prepared from the corresponding (iso)quinolinyl phenol derivatives **3**.



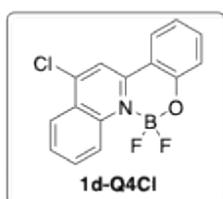
**Difluoro[2-(isoquinolin-1-yl)-phenolyl]borane (1b)**<sup>[S8]</sup>: Title compound (123 mg, 0.458 mmol) was obtained in 49% yield as a pale yellow solid from **3b** (205 mg, 0.924 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.72 (d, *J* = 8.5 Hz, 1H), 8.53 (d, *J* = 6.0 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 8.00-7.95 (m, 2H), 7.88 (d, *J* = 7.0 Hz, 1H), 7.84-7.81 (m, 1H), 7.60-7.57 (m, 1H), 7.34 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.17-7.13 (m, 1H).



**Difluoro[2-(isoquinolin-3-yl)-phenolyl]borane (1c)**<sup>[S8]</sup>: Title compound (122 mg, 0.455 mmol) was obtained in 54% yield as a pale yellow solid from **3c** (184 mg, 0.831 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 9.50 (s, 1H), 8.44 (s, 1H), 8.19 (d, *J* = 8.0, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 8.00-7.95 (m, 2H), 7.80-7.77 (m, 1H), 7.49-7.45 (m, 1H), 7.22 (d, *J* = 8.5 Hz, 1H), 7.11-7.08 (m, 1H).



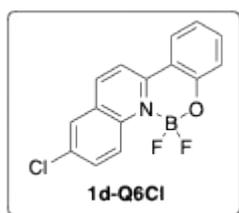
**Difluoro[2-(quinolin-2-yl)-phenolyl]borane (1d)**<sup>[S8]</sup>: Title compound (112 mg, 0.418 mmol) was obtained in 41% yield as a yellow solid from **3d** (224 mg, 1.01 mmol); <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>) δ 8.98 (d, *J* = 10.0 Hz, 1H), 8.53 (d, *J* = 8.5 Hz, 1H), 8.19 (d, *J* = 9.0 Hz, 1H), 7.95-7.90 (m, 3H), 7.72-7.69 (m, 1H), 7.57-7.54 (m, 1H), 7.22 (dd, *J* = 8.5, 1.0 Hz, 1H), 7.09-7.06 (m, 1H).



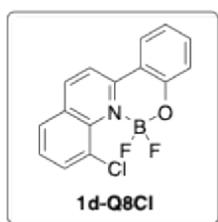
**Difluoro[2-(4-chloroquinolin-2-yl)-phenolyl]borane (1d-Q4Cl)**: To a solution of **3d-Q4Cl** (141 mg, 0.554 mmol) and Et<sub>3</sub>N (140 μL, 0.998 mmol) in

toluene (4.5 mL),  $\text{BF}_3 \cdot \text{OEt}_2$  (200  $\mu\text{L}$ , 1.59 mmol) was added at room temperature. The reaction mixture was stirred at 80 °C. After 18 h, the mixture was cooled down to room temperature, and the solvent was removed under reduced pressure. The crude product was washed with MeOH and purified by reprecipitation (from DCM/hexane) to give **1d-Q4Cl** (39 mg, 0.130 mmol) in 23% as a yellow solid;  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.00 (d,  $J$  = 9.0 Hz, 1H), 8.35 (dd,  $J$  = 8.0, 1.5 Hz, 1H), 8.27 (s, 1H), 7.99-7.95 (m, 1H), 7.89 (dd,  $J$  = 8.5, 1.5 Hz, 1H), 7.81-7.77 (m, 1H), 7.59-7.55 (m, 1H), 7.21 (dd,  $J$  = 8.5, 1.0 Hz, 1H), 7.10-7.06 (m, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.7, 152.8, 149.7, 141.4, 136.3, 134.0, 129.0, 126.8, 125.9, 125.4 (t,  $J$  = 9.6 Hz), 125.1, 120.8, 120.6, 117.6, 115.3;  $^{11}\text{B}$  NMR (160 MHz,  $\text{CDCl}_3$ )  $\delta$  0.53 (t,  $J$  = 17.0 Hz);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -131.8 - -131.9 (m). HRMS (ESI-TOF) found:  $m/z$  304.0515, calcd. for  $\text{C}_{15}\text{H}_9\text{ClBF}_2\text{NO}$  [ $\text{M}+\text{H}^+$ ] 304.0509.

In a similar manner, **1d-Q6Cl**, **1d-Q8Cl**, **1d-P4Cl**, **1d-P5F**, **1d-P5Cl**, **1d-P5Br**, and **1d-P6Cl** were prepared from the corresponding (iso)quinolinyl phenol derivatives **3**.

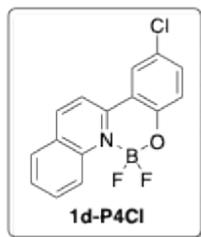


**Difluoro[2-(6-chloroquinolin-2-yl)-phenolyl]borane (1d-Q6Cl):** Title compound (72 mg, 0.238 mmol) was obtained in 38% yield as a yellow solid from **3d-Q6Cl** (159 mg, 0.621 mmol);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  8.92 (d,  $J$  = 9.5 Hz, 1H), 8.43 (d,  $J$  = 9.5 Hz, 1H), 8.21 (d,  $J$  = 8.5 Hz, 1H), 7.92-7.90 (m, 2H), 7.83 (dd,  $J$  = 10.0, 2.5 Hz, 1H), 7.58-7.55 (m, 1H), 7.21 (d,  $J$  = 8.5 Hz, 1H), 7.09-7.06 (m, 1H);  $^{13}\text{C}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.5, 153.1, 141.8, 138.8, 136.2, 134.4, 133.7, 128.5, 127.1, 126.9, 126.7 (t,  $J$  = 9.7 Hz), 120.8, 120.6, 118.4, 115.8;  $^{11}\text{B}$  NMR (160 MHz,  $\text{CDCl}_3$ )  $\delta$  0.54 (t,  $J$  = 15.4 Hz);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -131.8 (q,  $J$  = 15.4 Hz); HRMS (ESI-TOF) found:  $m/z$  304.0506, calcd. for  $\text{C}_{15}\text{H}_9\text{ClBF}_2\text{NO}$  [ $\text{M}+\text{H}^+$ ] 304.0509.

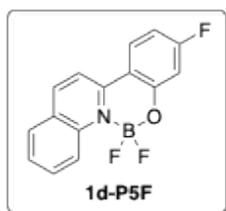


**Difluoro[2-(8-chloroquinolin-2-yl)-phenolyl]borane (1d-Q8Cl):** Title compound (154 mg, 0.510 mmol) was obtained in 91% yield as a yellow solid from **3d-Q8Cl** (143 mg, 0.558 mmol);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.00 (d,  $J$  = 8.5 Hz, 1H), 8.92 (d,  $J$  = 9.0 Hz, 1H), 8.28 (d,  $J$  = 10.0 Hz, 1H), 7.95 (dd,  $J$  = 8.0, 1.5 Hz, 1H), 7.84-7.80 (m, 1H), 7.78-7.61 (m, 1H), 7.59-7.56 (m, 1H), 7.22 (dd,  $J$  = 8.0, 1.5 Hz, 1H), 7.10-7.07 (m, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  156.7, 153.6, 141.5, 139.4, 136.3, 132.7, 132.5, 128.4, 127.1, 125.8, 124.0 (t,  $J$  = 9.7 Hz), 120.8, 120.6, 118.2, 115.8;  $^{11}\text{B}$  NMR (160 MHz,  $\text{CDCl}_3$ )  $\delta$  0.59 (t,  $J$  = 16.8 Hz);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -131.5

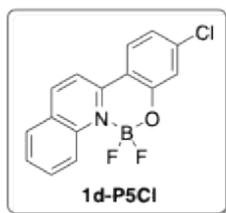
(q,  $J = 16.8$  Hz); HRMS (ESI-TOF) found:  $m/z$  304.0505, calcd. for  $C_{15}H_9ClBF_2NO$   $[M+H^+]$  304.0509.



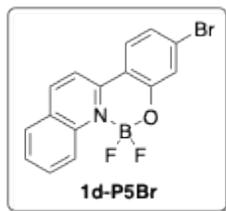
**Difluoro[4-chloro-2-(quinolin-2-yl)-phenoly]borane (1d-P4Cl):** Title compound (211 mg, 0.696 mmol) was obtained in 97% yield as a pale yellow solid from **3d-P4Cl** (183 mg, 0.717 mmol);  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  8.98 (d,  $J = 9.5$  Hz, 1H), 8.58 (d,  $J = 9.0$  Hz, 1H), 8.14 (d,  $J = 9.0$  Hz, 1H), 7.97-7.93 (m, 2H), 7.91 (d,  $J = 3.0$  Hz, 1H), 7.76-7.73 (m, 1H), 7.49 (dd,  $J = 9.0, 3.0$  Hz, 1H), 7.17 (d,  $J = 8.5$  Hz, 1H);  $^{13}C\{^1H\}$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  155.1, 151.7, 143.4, 140.6, 135.6, 133.5, 128.6, 128.1, 126.2, 125.5, 125.1 (t,  $J = 9.6$  Hz), 122.0, 117.1.  $^{11}B$  NMR (160 MHz,  $CDCl_3$ )  $\delta$  0.59 (t,  $J = 15.4$  Hz);  $^{19}F$  NMR (471 MHz,  $CDCl_3$ )  $\delta$  -132.1 (q,  $J = 15.4$  Hz); HRMS (ESI-TOF) found:  $m/z$  304.0512, calcd. for  $C_{15}H_9ClBF_2NO$   $[M+H^+]$  304.0509.



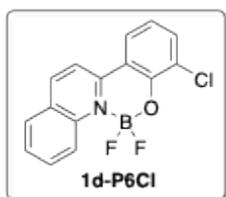
**Difluoro[5-fluoro-2-(quinolin-2-yl)-phenoly]borane (1d-P5F):** Title compound (176 mg, 0.615 mmol) was obtained in 75% yield as a pale yellow solid from **3d-P5F** (196 mg, 0.819 mmol);  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  8.93 (d,  $J = 9.5$  Hz, 1H), 8.51 (d,  $J = 9.0$  Hz, 1H), 8.09 (d,  $J = 9.5$  Hz, 1H), 7.94-7.90 (m, 3H), 7.71-7.68 (m, 1H), 6.89 (dd,  $J = 9.5, 2.5$  Hz, 1H), 6.81-6.77 (m, 1H);  $^{13}C\{^1H\}$  NMR (126 MHz,  $CDCl_3$ )  $\delta$  167.6 (d,  $J = 257.2$  Hz), 158.6 (d,  $J = 14.5$  Hz), 152.2, 143.1, 140.3, 133.3, 129.0 (d,  $J = 12.1$  Hz), 128.6, 128.2, 127.6, 124.8 (t,  $J = 9.6$  Hz), 117.0, 112.9, 109.1 (d,  $J = 24.0$  Hz), 106.9 (d,  $J = 24.0$  Hz);  $^{11}B$  NMR (160 MHz,  $CDCl_3$ )  $\delta$  0.51 (t,  $J = 16.8$  Hz);  $^{19}F$  NMR (471 MHz,  $CDCl_3$ )  $\delta$  -101.5 (s), -132.1 (q,  $J = 16.8$  Hz). HRMS (ESI-TOF) found:  $m/z$  288.0806, calcd. for  $C_{15}H_9BF_3NO$   $[M+H^+]$  288.0805.



**Difluoro[5-chloro-2-(quinolin-2-yl)-phenoly]borane (1d-P5Cl):** Title compound (116 mg, 0.384 mmol) was obtained in 66% yield as a pale yellow solid from **3d-P5Cl** (148 mg, 0.580 mmol);  $^1H$  NMR (500 MHz,  $CDCl_3$ )  $\delta$  8.94 (d,  $J = 9.5$  Hz, 1H), 8.53 (d,  $J = 9.0$  Hz, 1H), 8.12 (d,  $J = 9.5$  Hz, 1H), 7.94-7.91 (m, 2H), 7.84 (d,  $J = 8.5$  Hz, 1H), 7.73-7.70 (m, 1H), 7.22 (d,  $J = 2.5$  Hz, 1H), 7.03 (dd,  $J = 8.5, 2.5$  Hz, 1H);  $^{13}C\{^1H\}$  NMR (126 MHz,  $CDCl_3$ , 50 °C)  $\delta$  157.3, 152.2, 143.1, 141.7, 140.6, 133.3, 128.6, 128.4, 127.9, 127.8, 125.1 (t,  $J = 9.6$  Hz), 121.3, 120.5, 117.0, 114.9;  $^{11}B$  NMR (160 MHz,  $CDCl_3$ )  $\delta$  0.51 (t,  $J = 16.8$  Hz);  $^{19}F$  NMR (471 MHz,  $CDCl_3$ )  $\delta$  -132.1 (q,  $J = 16.8$  Hz). HRMS (ESI-TOF) found:  $m/z$  304.0510, calcd. for  $C_{15}H_9ClBF_2NO$   $[M+H^+]$  304.0509.



**Difluoro[5-bromo-2-(quinolin-2-yl)-phenolyl]borane (1d-P5Br):** Title compound (84 mg, 0.241 mmol) was obtained in 68% yield as a pale yellow solid from **3d-P5Br** (105 mg, 0.350 mmol);  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )  $\delta$  8.93 (d,  $J = 9.6$  Hz, 1H), 8.53 (d,  $J = 8.8$  Hz, 1H), 8.10 (d,  $J = 9.2$  Hz, 1H), 7.95-7.91 (m, 2H), 7.75 (d,  $J = 8.8$  Hz, 1H), 7.73-7.69 (m, 1H), 7.38 (d,  $J = 2.0$  Hz, 1H), 7.16 (dd,  $J = 8.4, 2.0$  Hz, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (100 MHz,  $\text{CDCl}_3$ , 50 °C)  $\delta$  157.0, 152.2, 143.2, 140.6, 133.3, 130.1, 128.6, 128.4, 127.9, 127.8, 125.0 (t,  $J = 9.1$  Hz), 124.1, 123.6, 117.0, 115.3.  $^{11}\text{B}$  NMR (128 MHz,  $\text{CDCl}_3$ )  $\delta$  0.64 (t,  $J = 16.6$  Hz);  $^{19}\text{F}$  NMR (376 MHz,  $\text{CDCl}_3$ )  $\delta$  -132.0 (q,  $J = 16.6$  Hz). HRMS (ESI-TOF) found:  $m/z$  348.0007, calcd. for  $\text{C}_{15}\text{H}_9\text{BrBF}_2\text{NO}$  [ $\text{M}+\text{H}^+$ ] 348.0004.



**Difluoro[6-chloro-2-(quinolin-2-yl)-phenolyl]borane (1d-P6Cl):** Title compound (103 mg, 0.340 mmol) was obtained in 44% yield as a pale yellow solid from **3d-P6Cl** (195 mg, 0.761 mmol);  $^1\text{H}$  NMR (500 MHz,  $\text{CDCl}_3$ )  $\delta$  9.00 (d,  $J = 9.0$  Hz, 1H), 8.57 (d,  $J = 9.0$  Hz, 1H), 8.18 (d,  $J = 9.0$  Hz, 1H), 7.96-7.94 (m, 2H), 7.85 (dd,  $J = 8.0, 1.5$  Hz, 1H), 7.75-7.72 (m, 1H), 7.64 (dd,  $J = 8.0, 1.5$  Hz, 1H), 7.03-7.00 (m, 1H);  $^{13}\text{C}\{^1\text{H}\}$  NMR (126 MHz,  $\text{CDCl}_3$ )  $\delta$  152.4, 152.3, 143.3, 140.5, 135.4, 133.5, 128.60, 128.57, 128.0, 125.4, 125.15, 125.11 (t,  $J = 8.4$  Hz), 120.5, 117.5, 117.4.  $^{11}\text{B}$  NMR (160 MHz,  $\text{CDCl}_3$ )  $\delta$  0.64 (t,  $J = 17.0$  Hz);  $^{19}\text{F}$  NMR (471 MHz,  $\text{CDCl}_3$ )  $\delta$  -132.2 (q,  $J = 17.0$  Hz). HRMS (ESI-TOF) found:  $m/z$  304.0514, calcd. for  $\text{C}_{15}\text{H}_9\text{ClBF}_2\text{NO}$  [ $\text{M}+\text{H}^+$ ] 304.0509.

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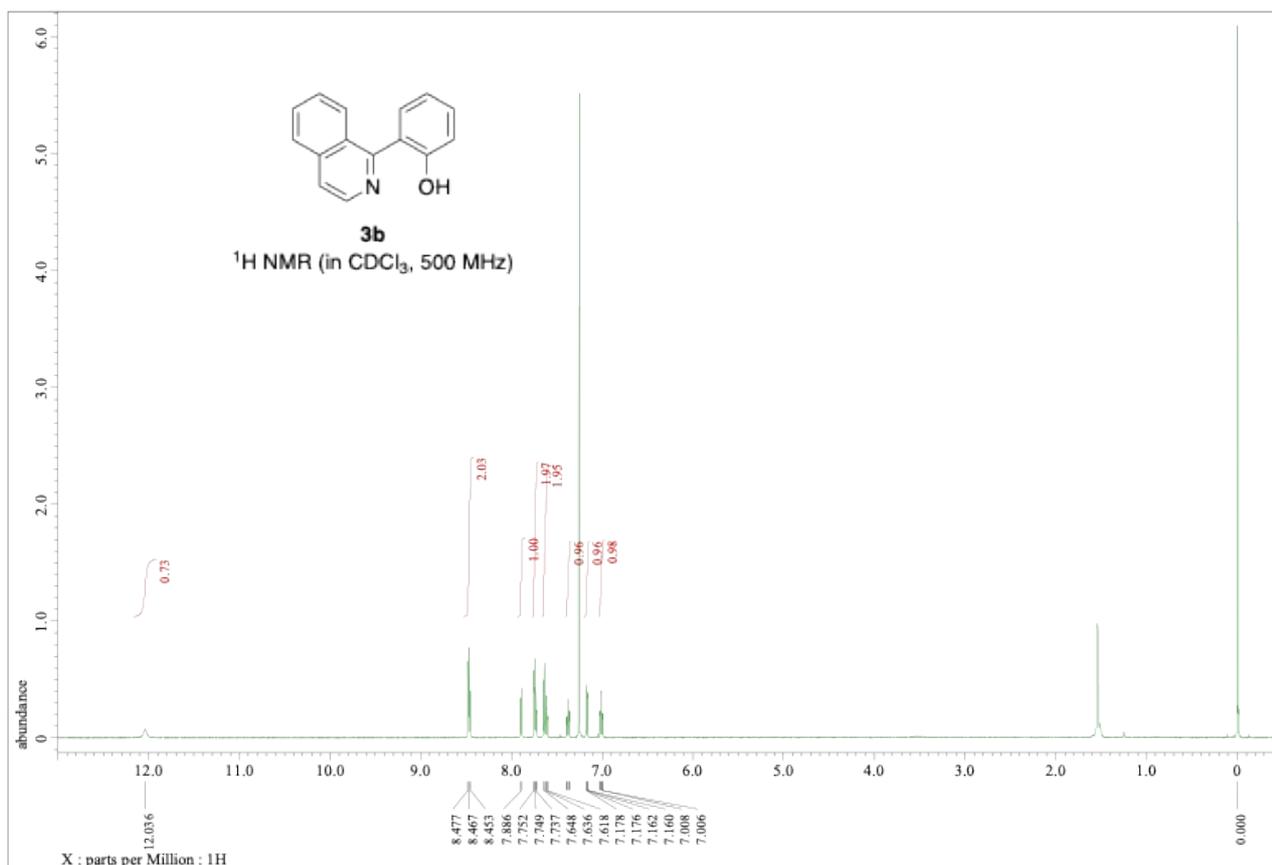
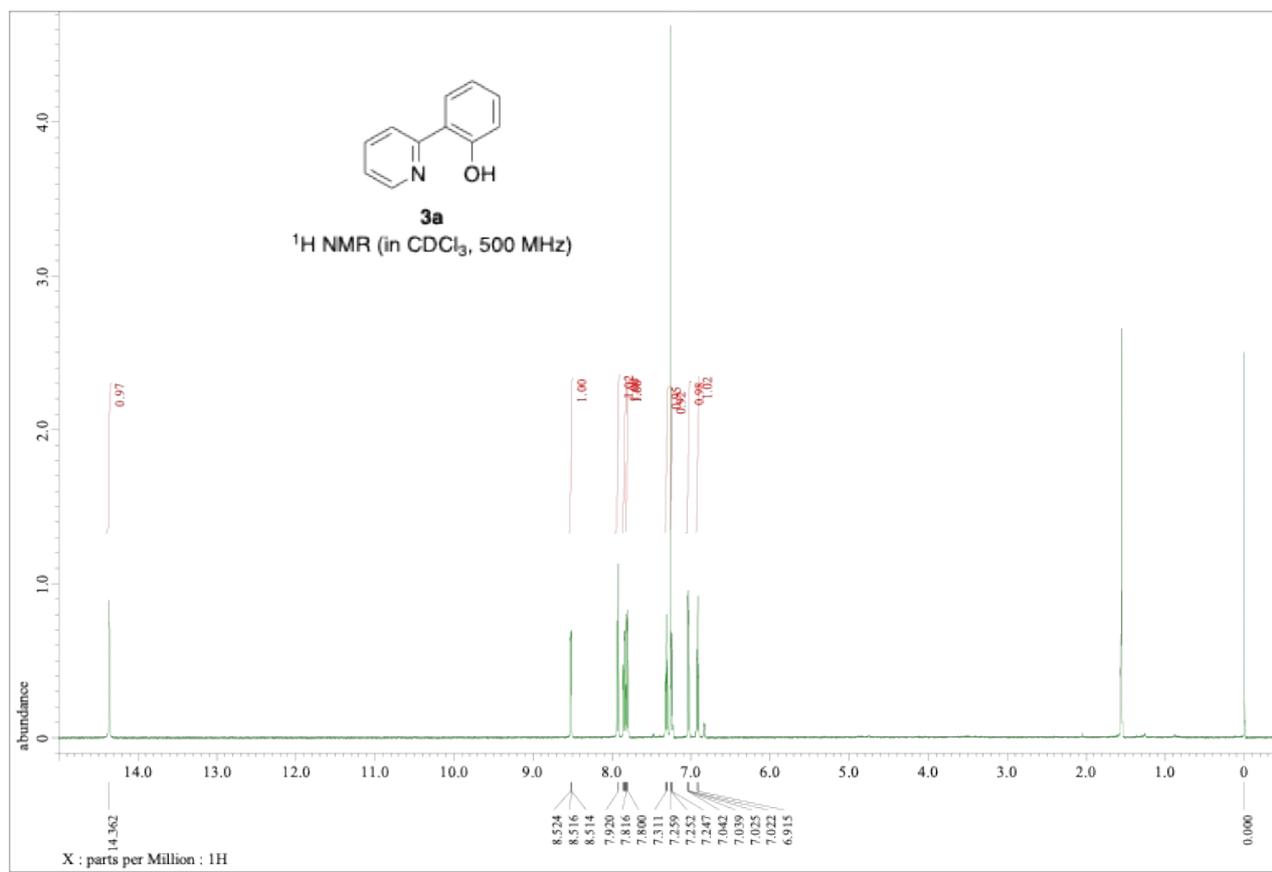
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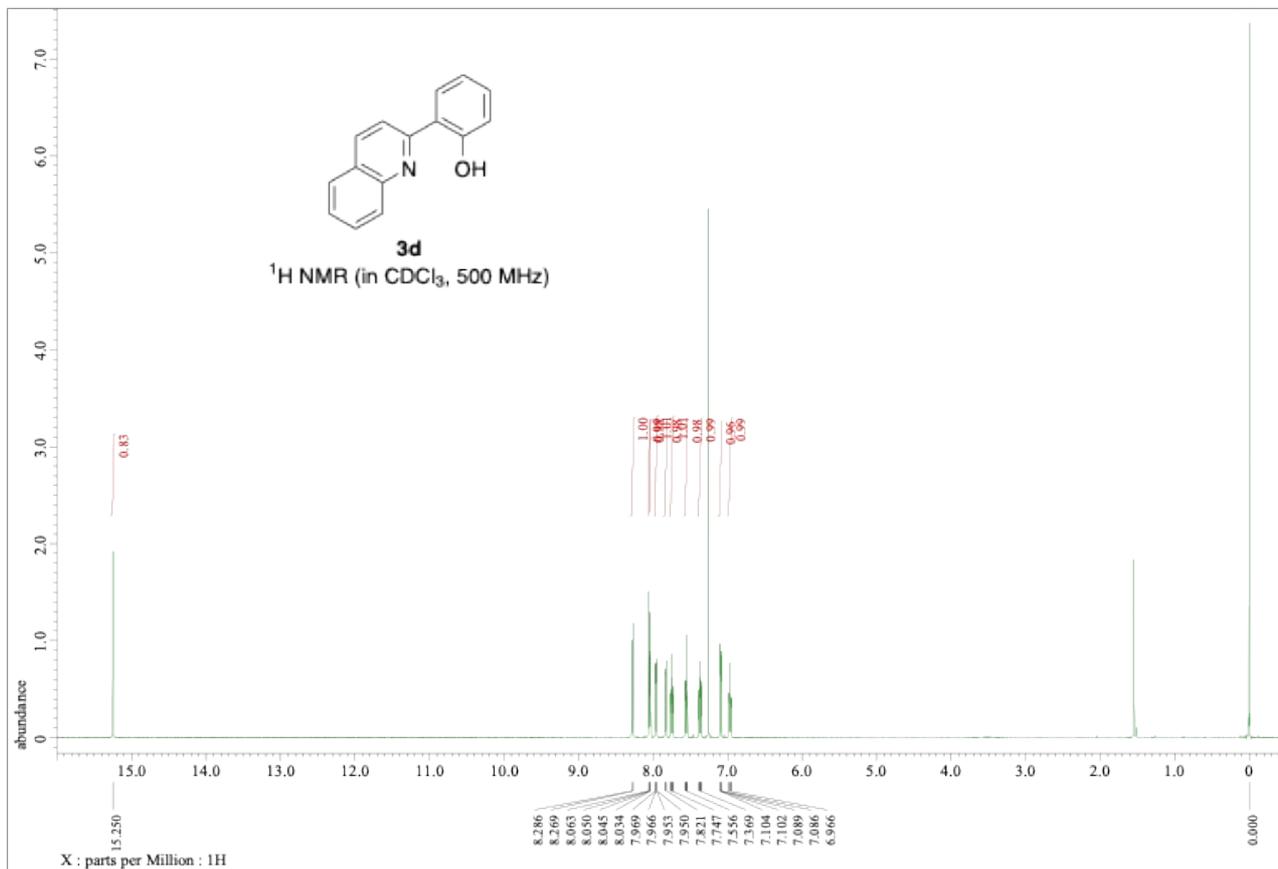
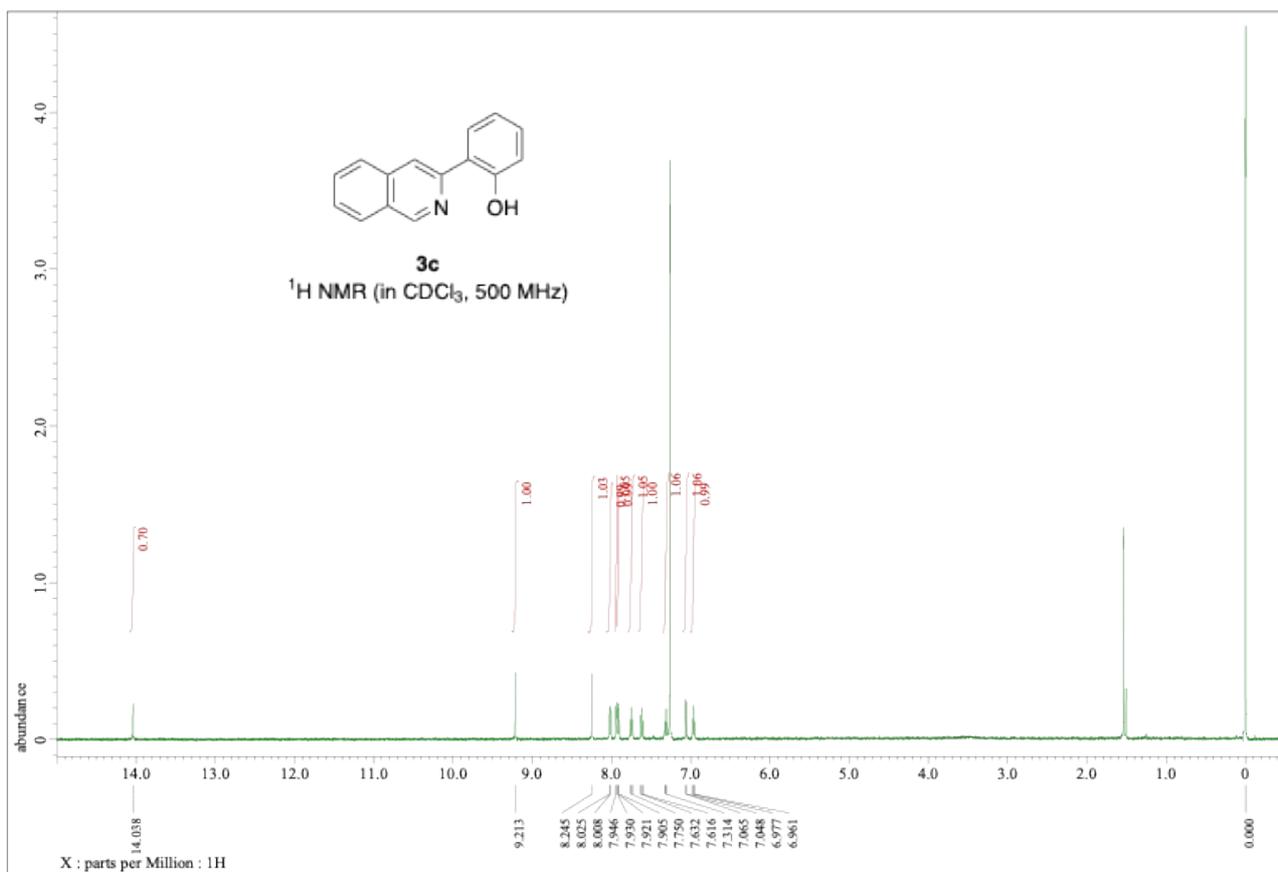
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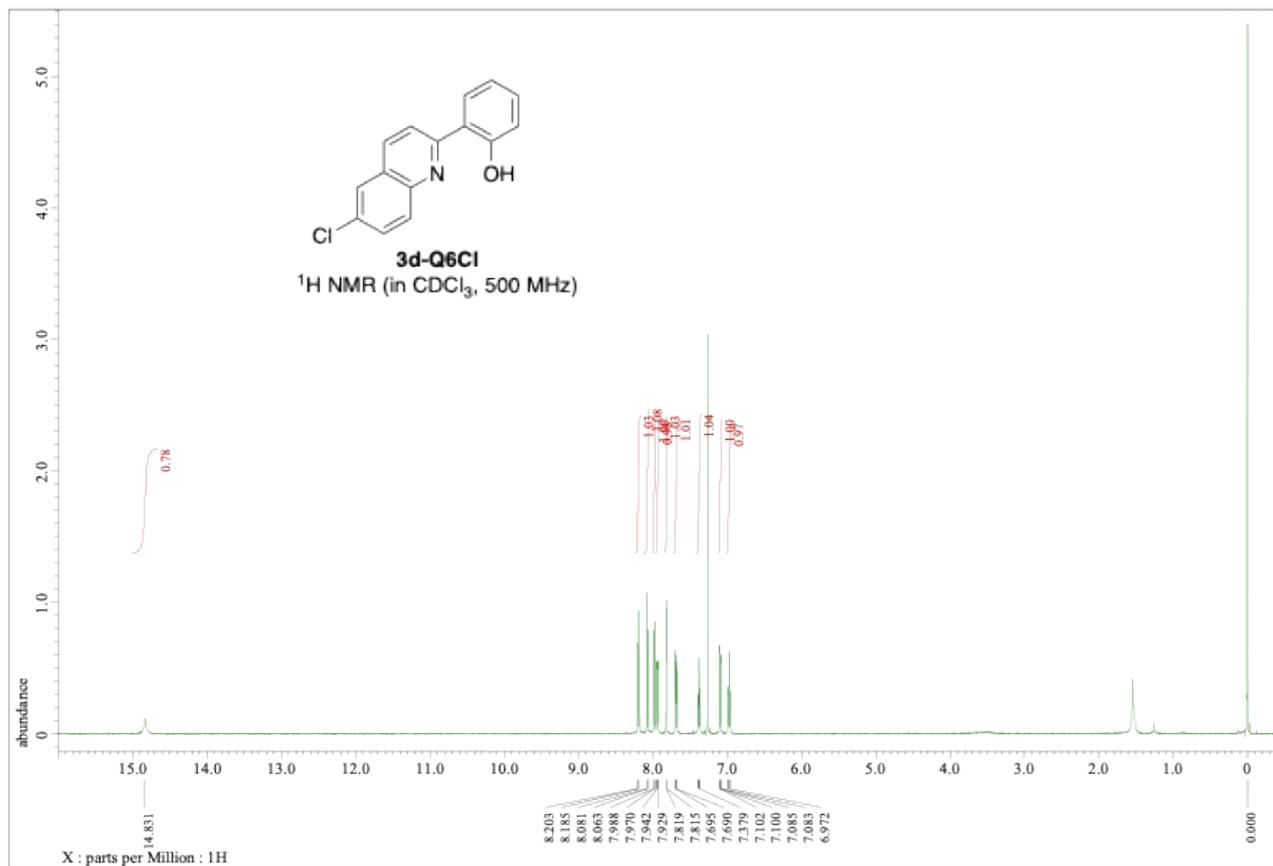
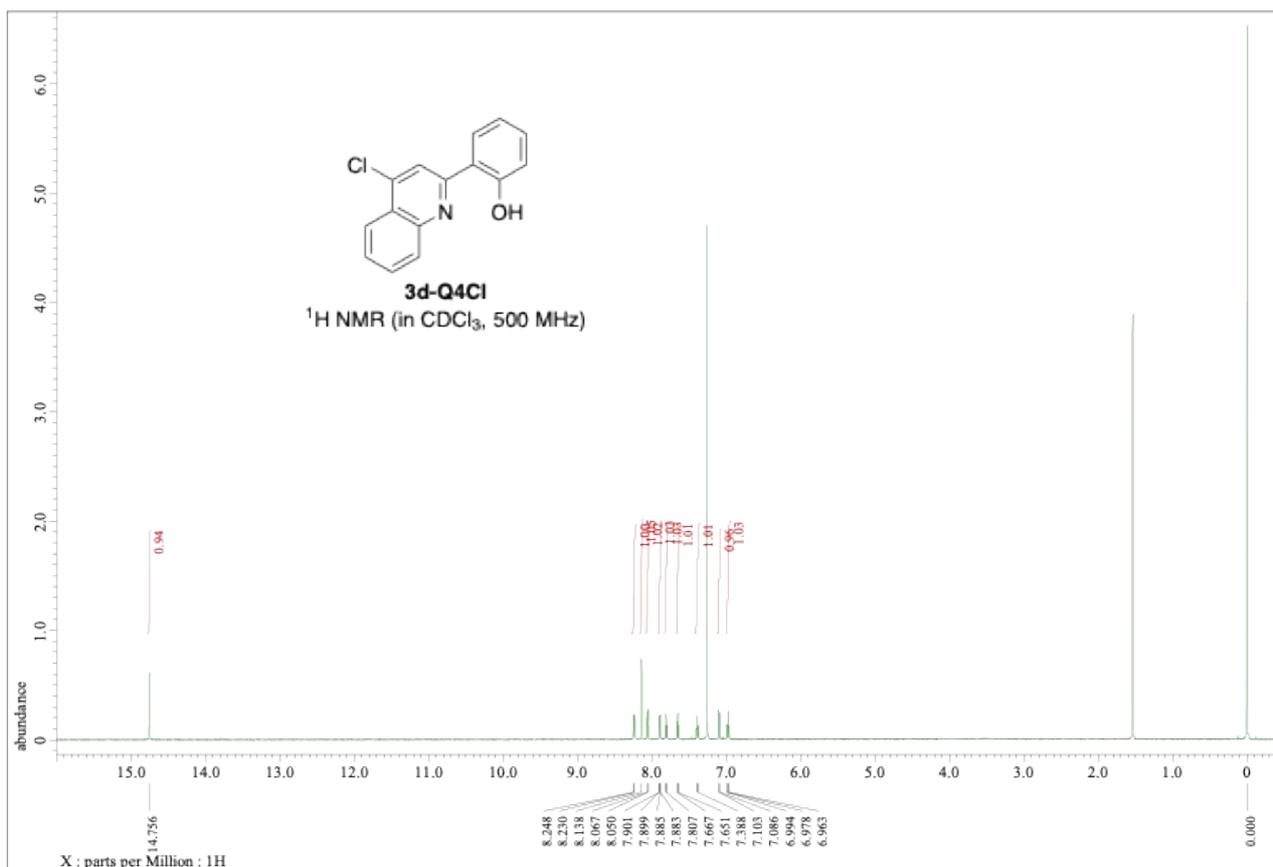
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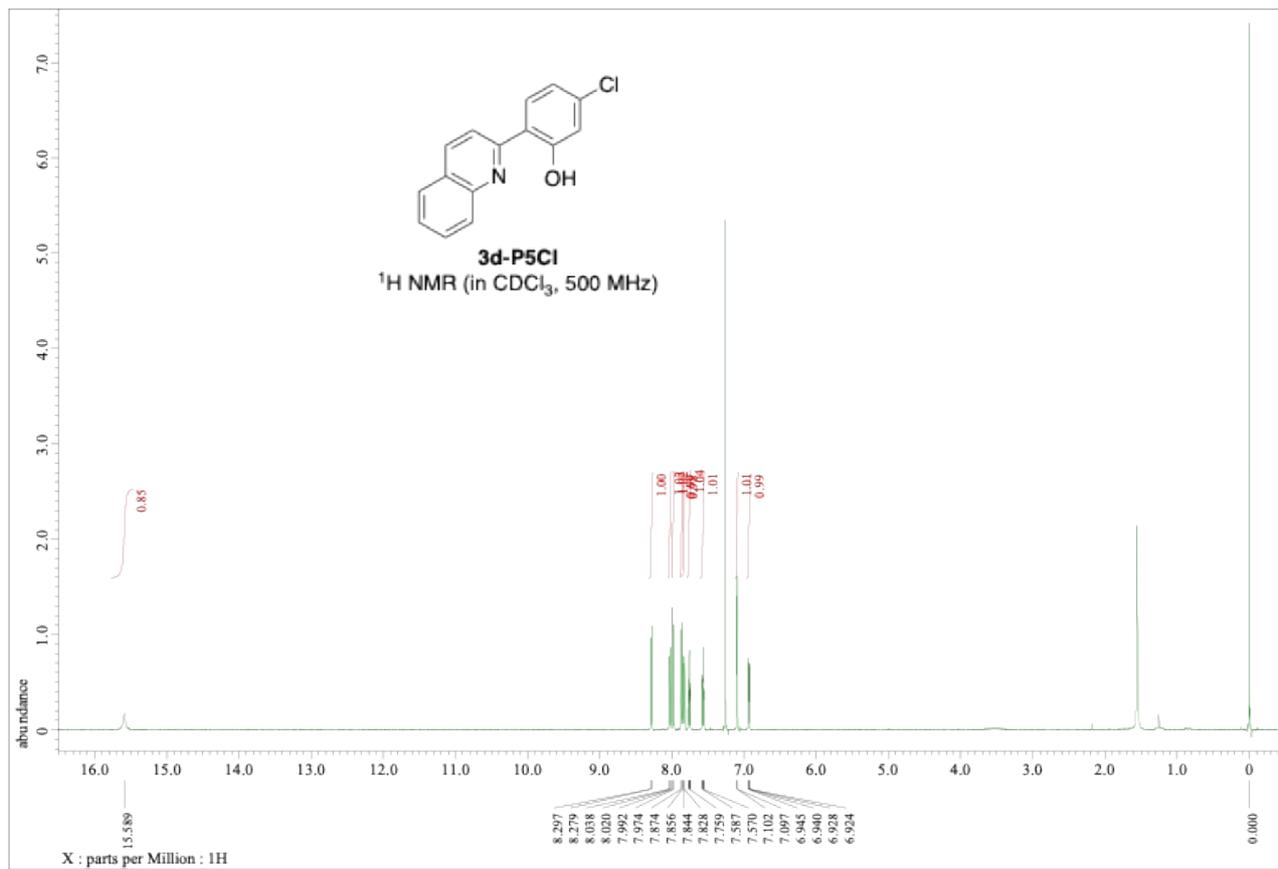
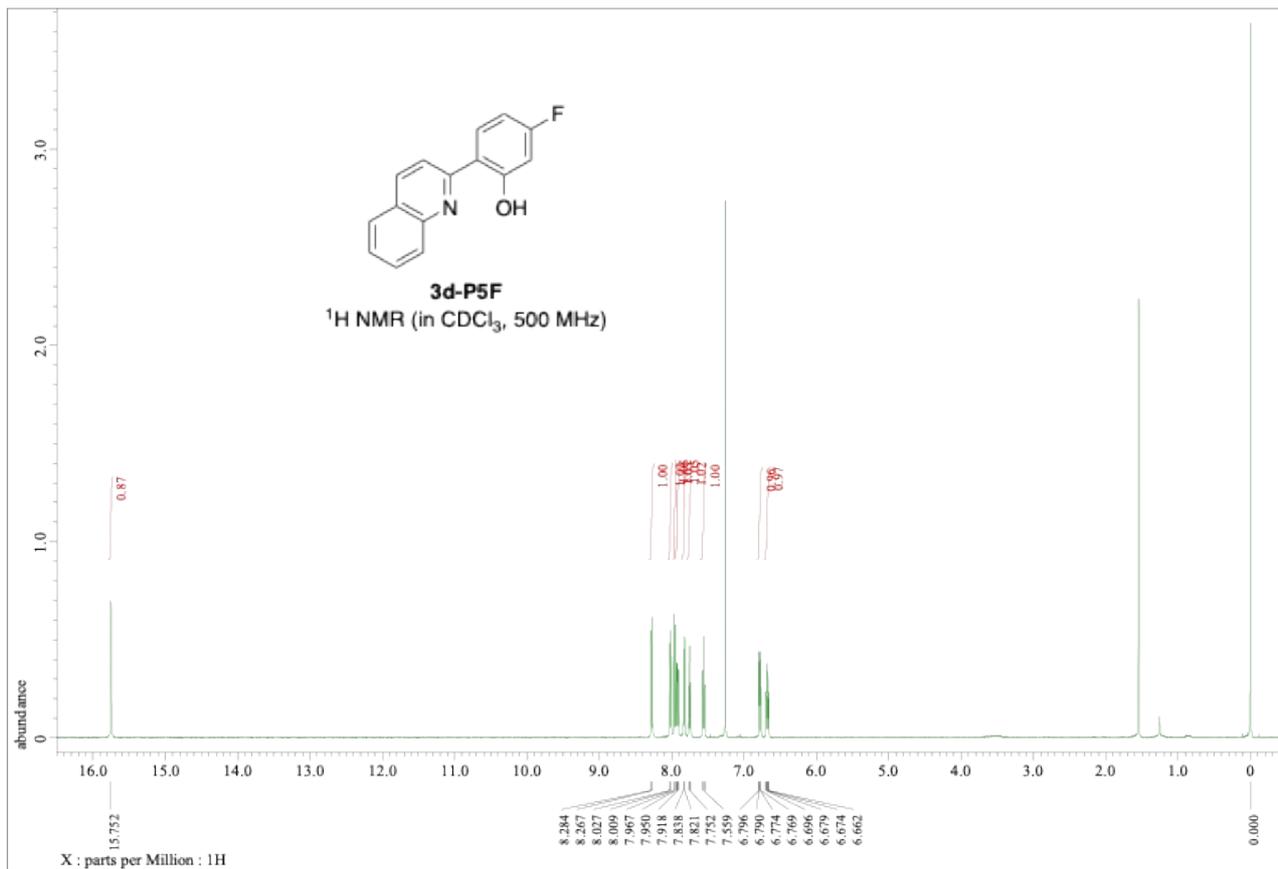
$^1\text{H}$ ,  $^{13}\text{C}\{^1\text{H}\}$ ,  $^{11}\text{B}$ ,  $^{19}\text{F}$  NMR Data of all Compounds

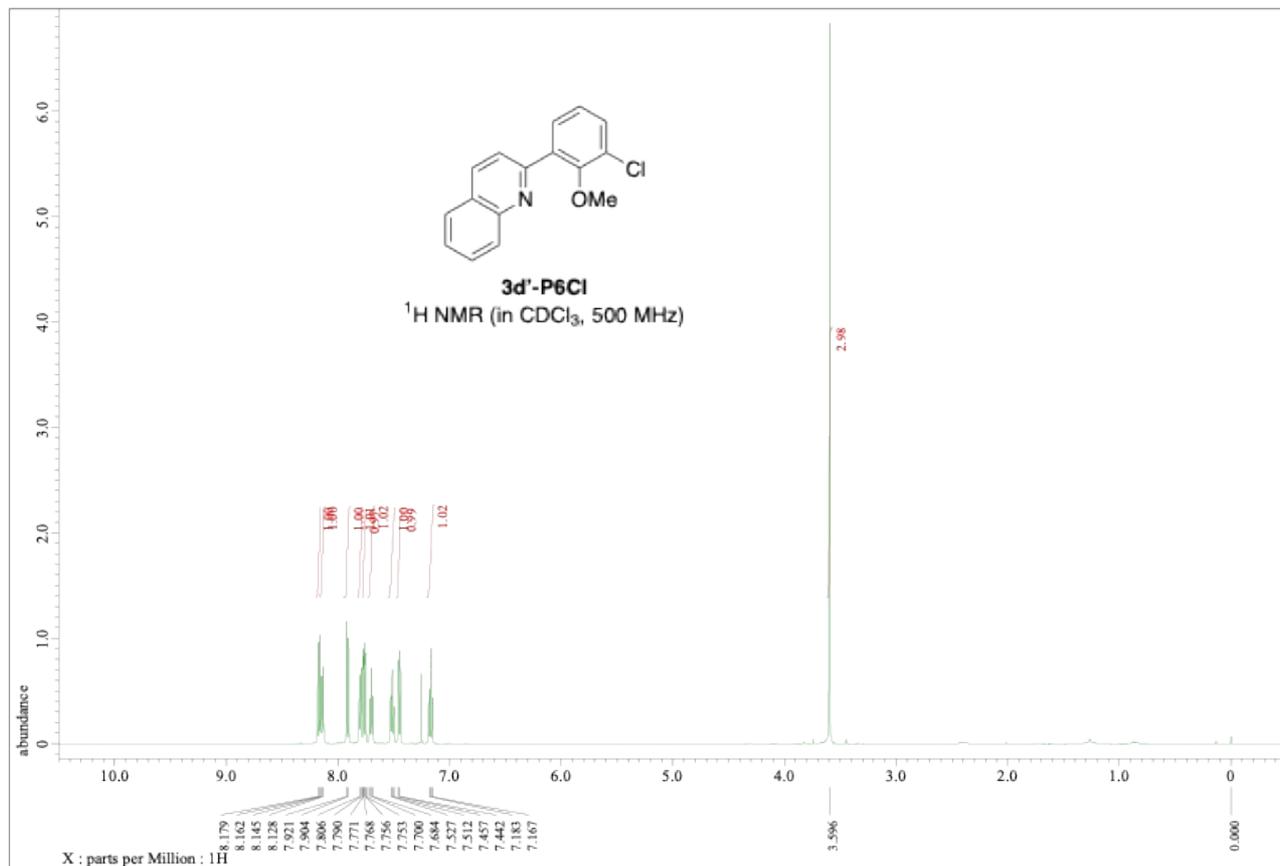
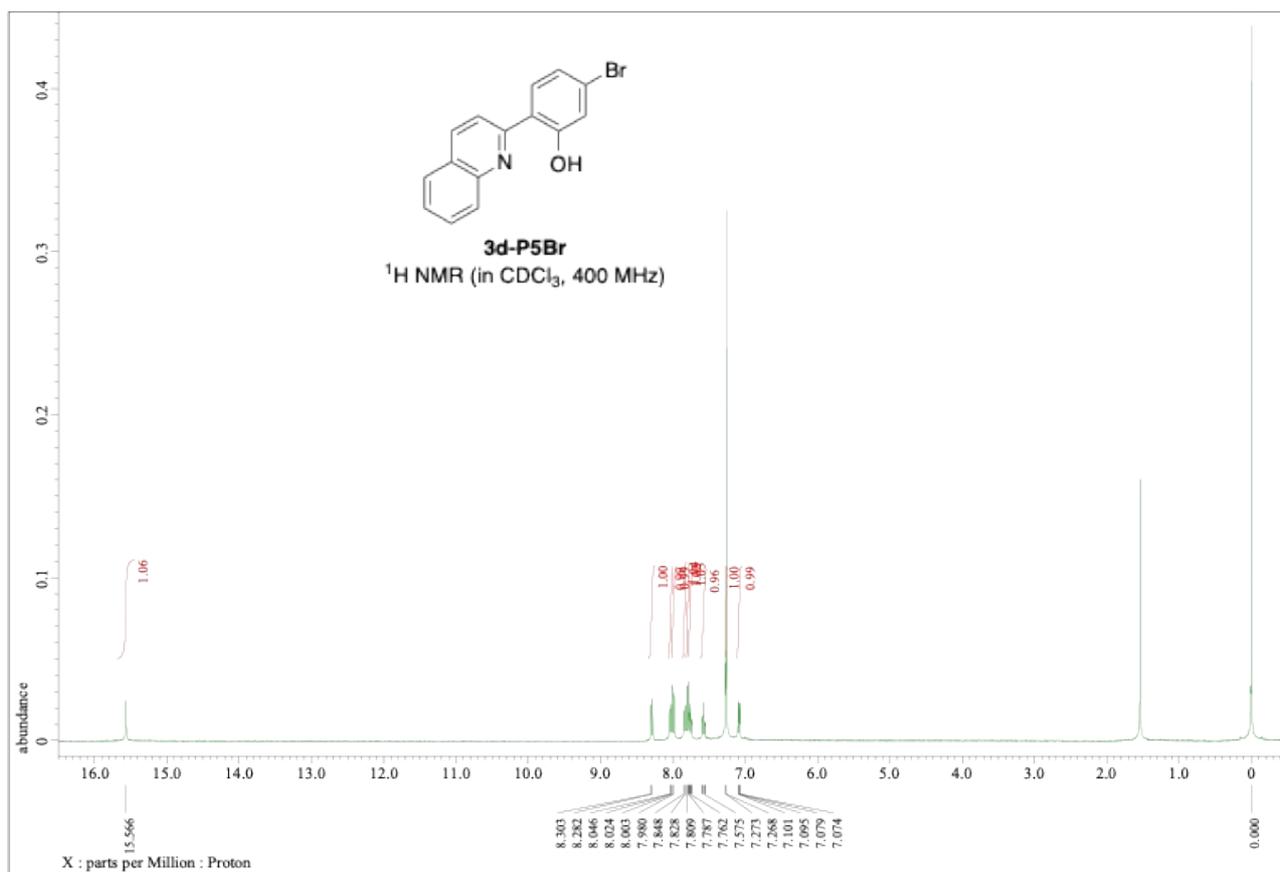


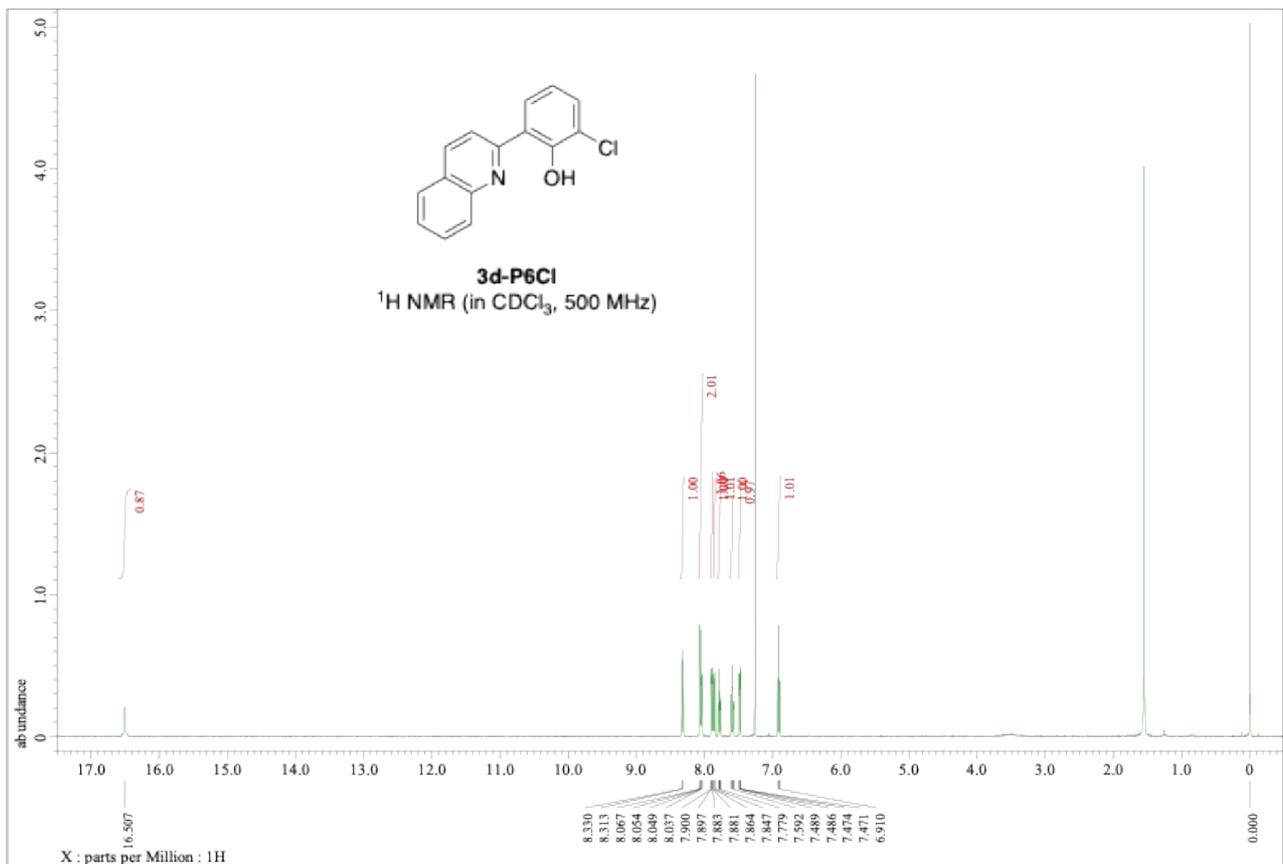
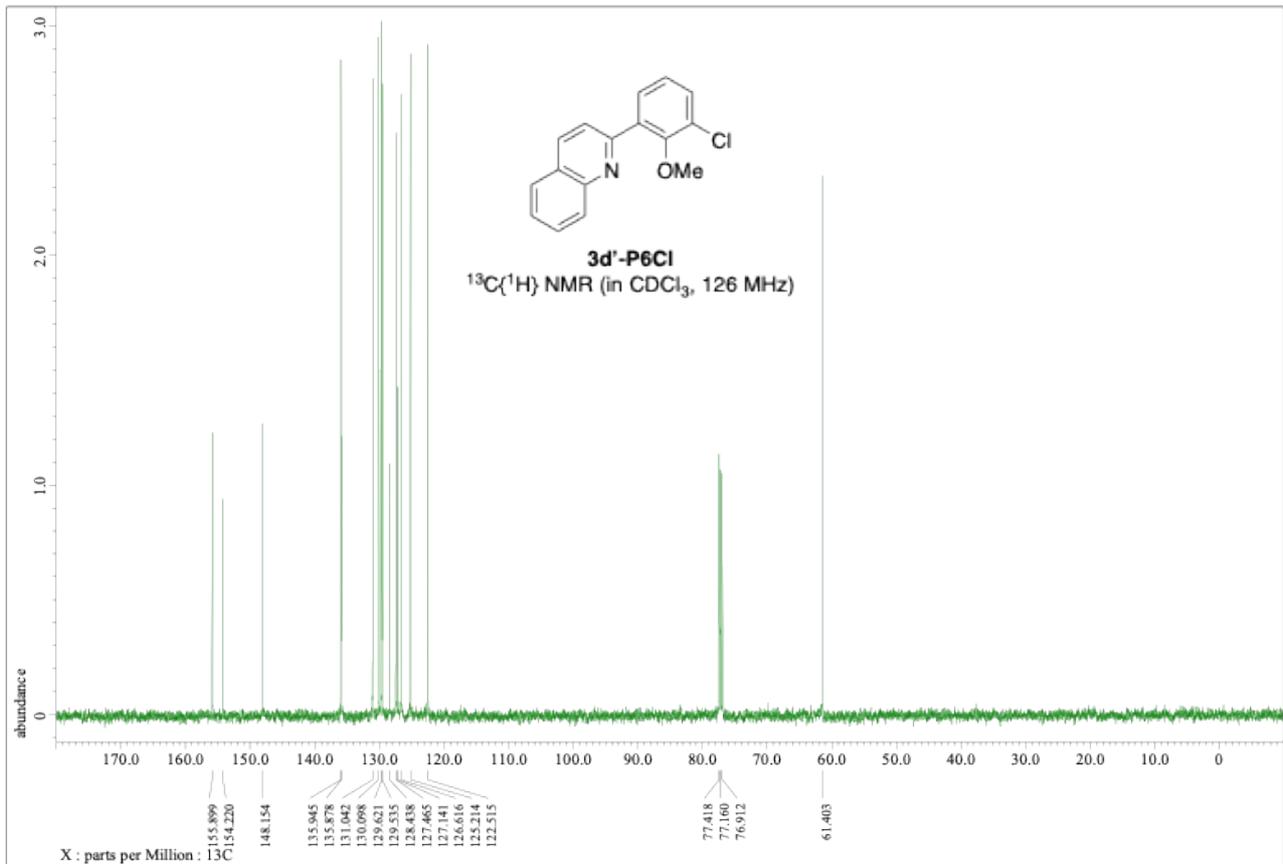


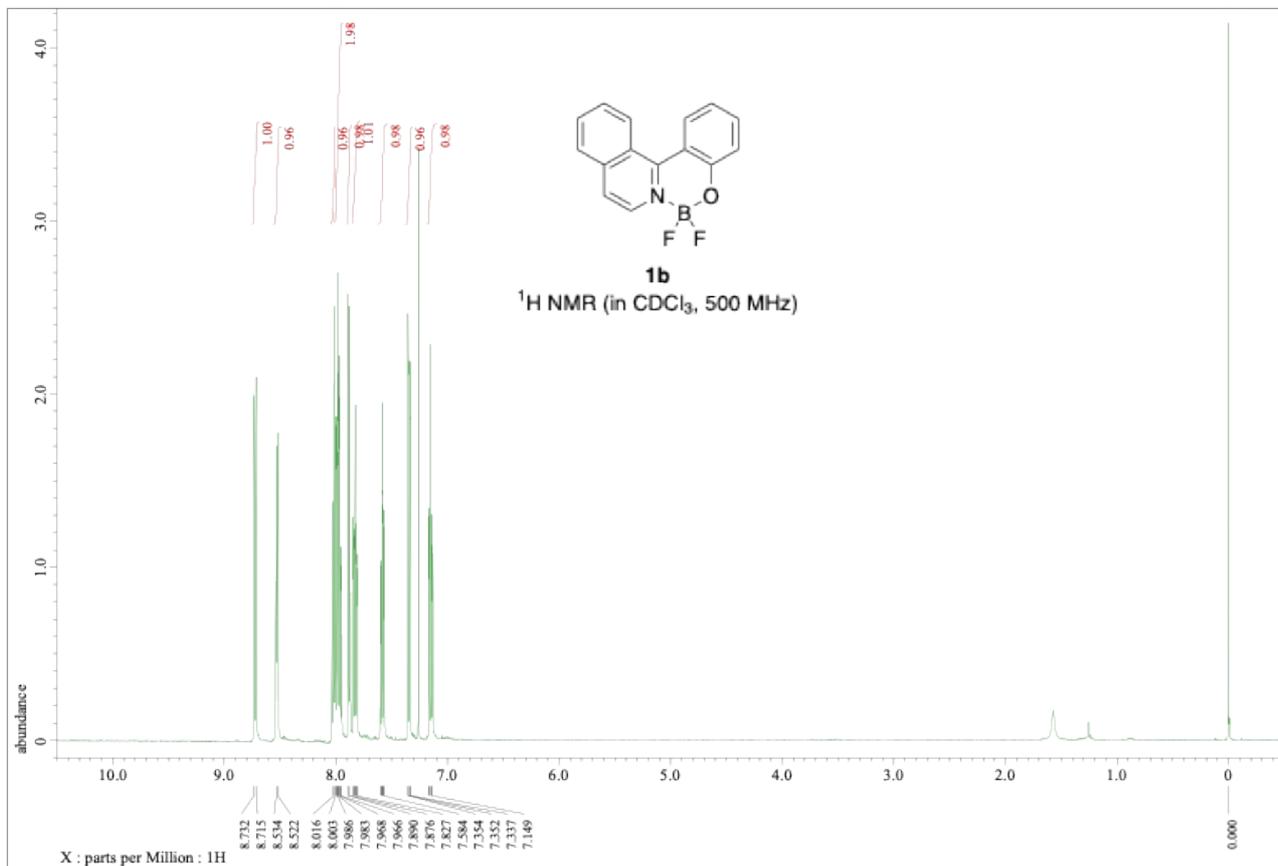
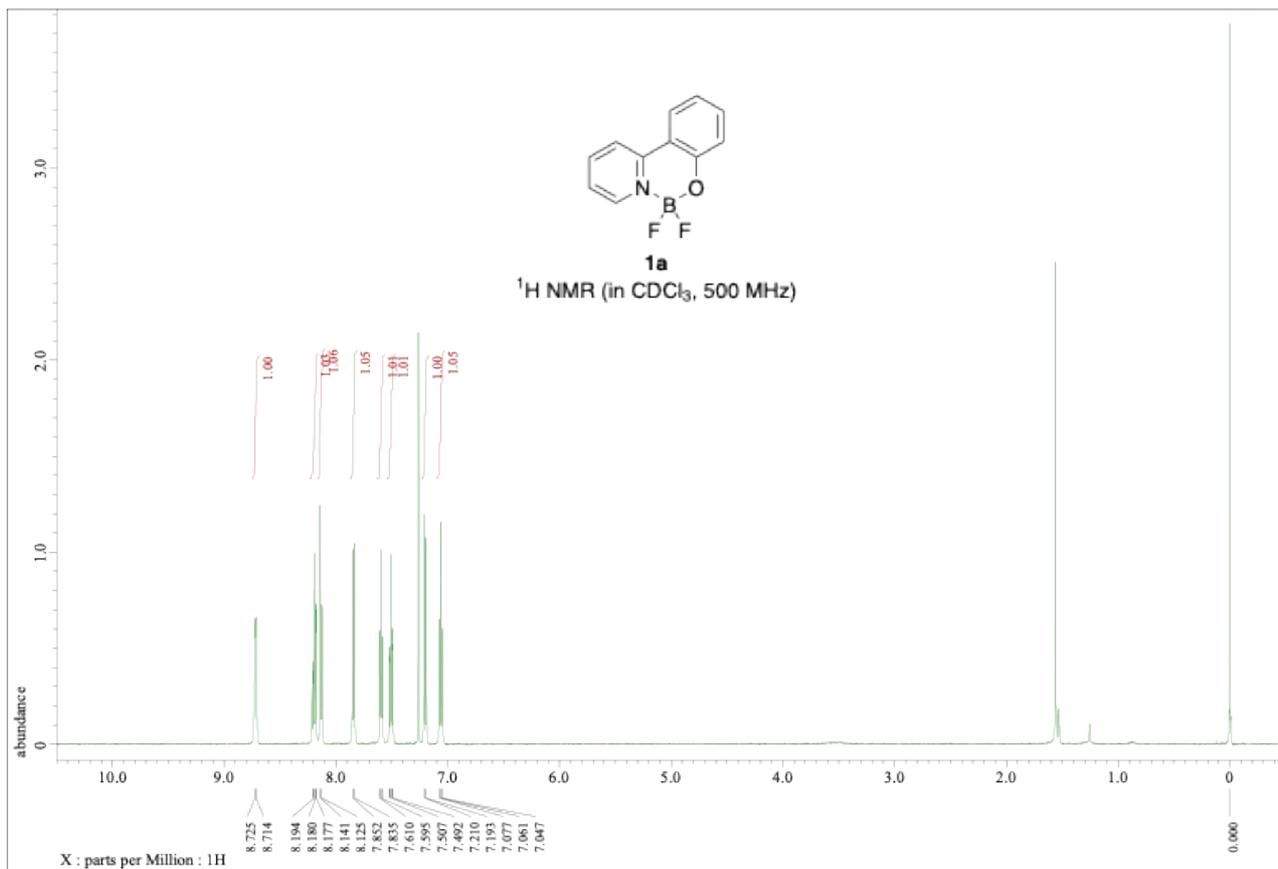


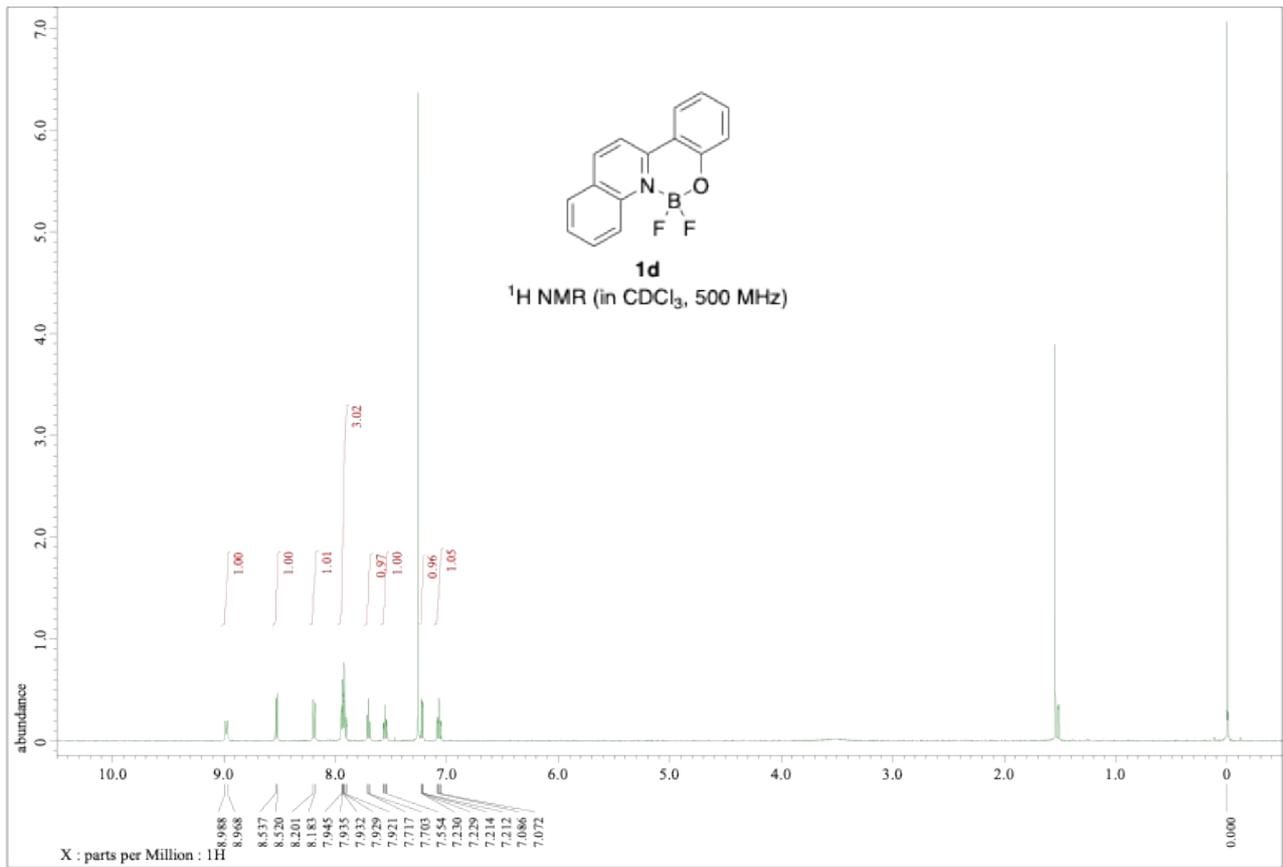
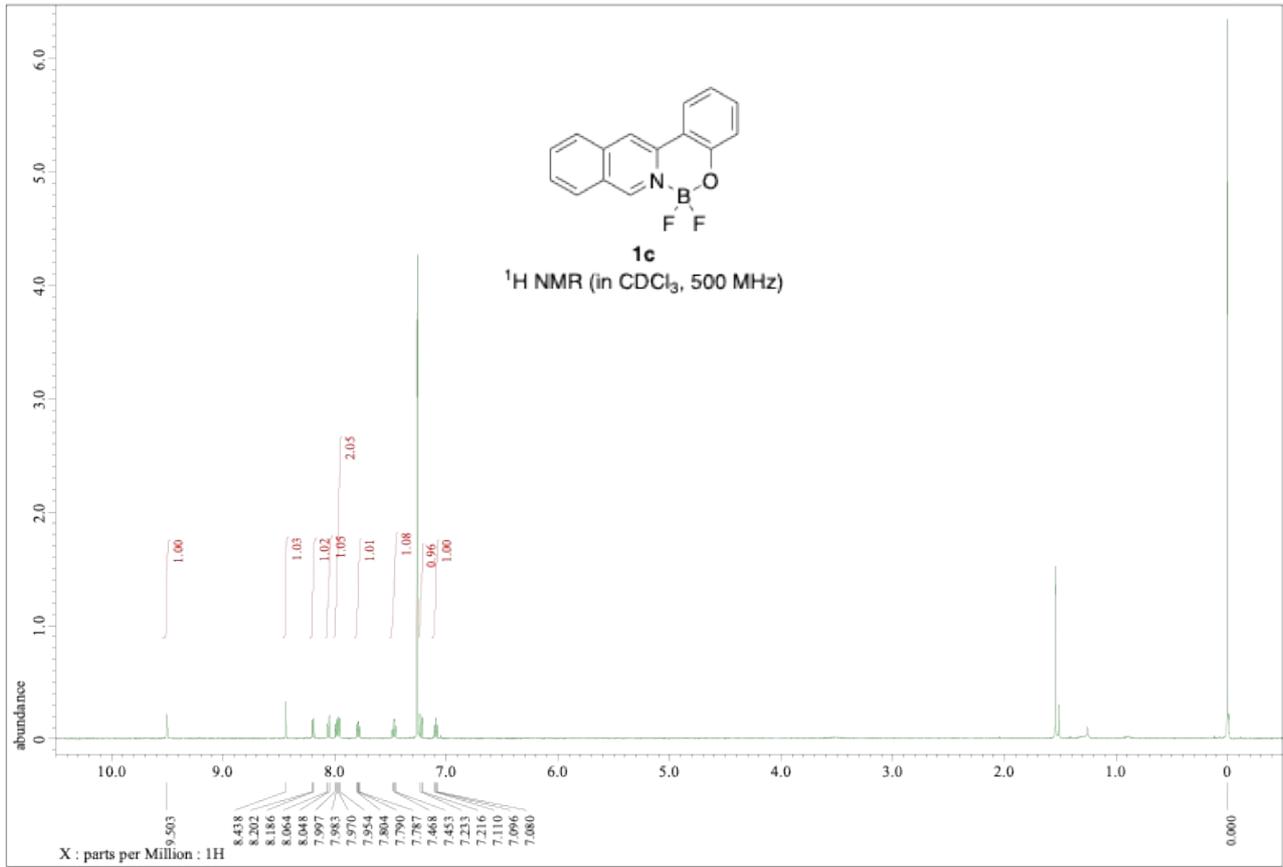


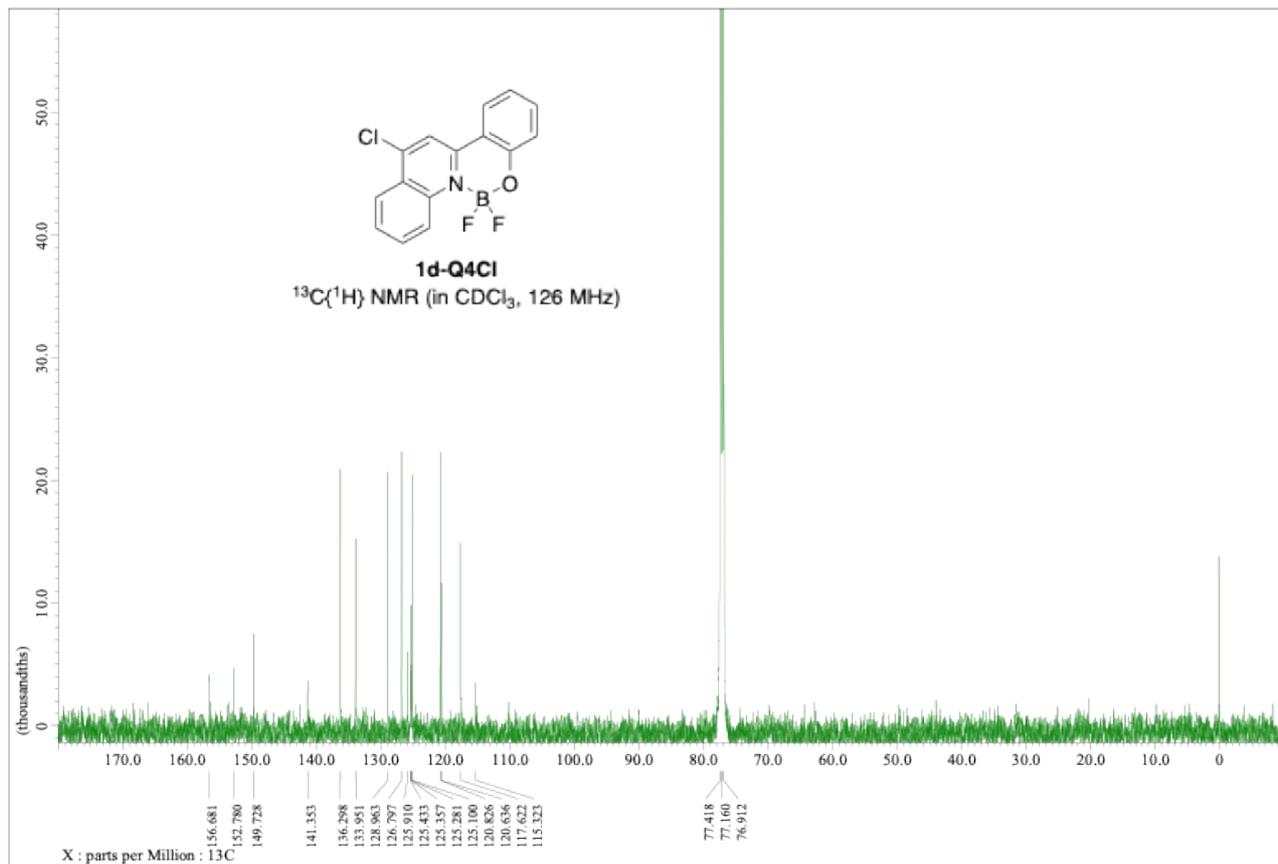
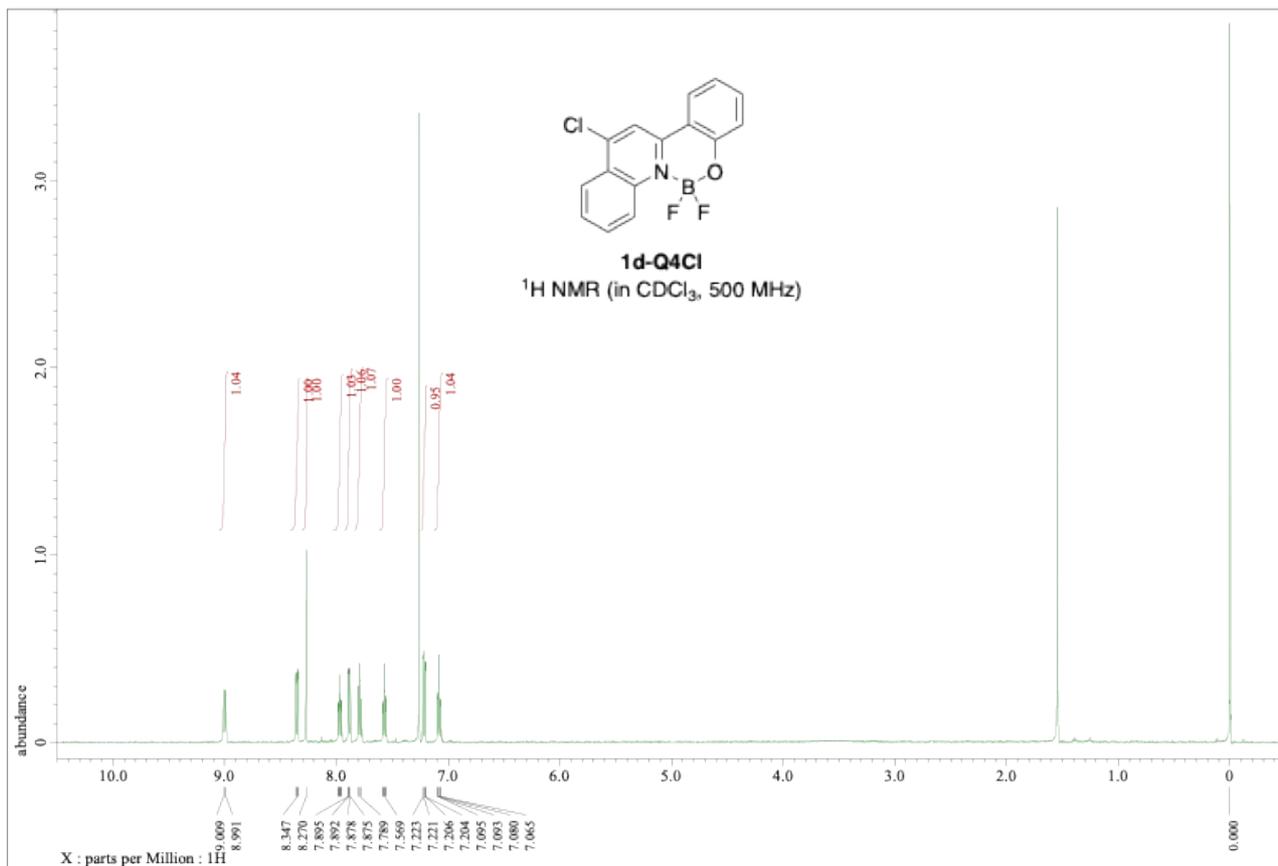


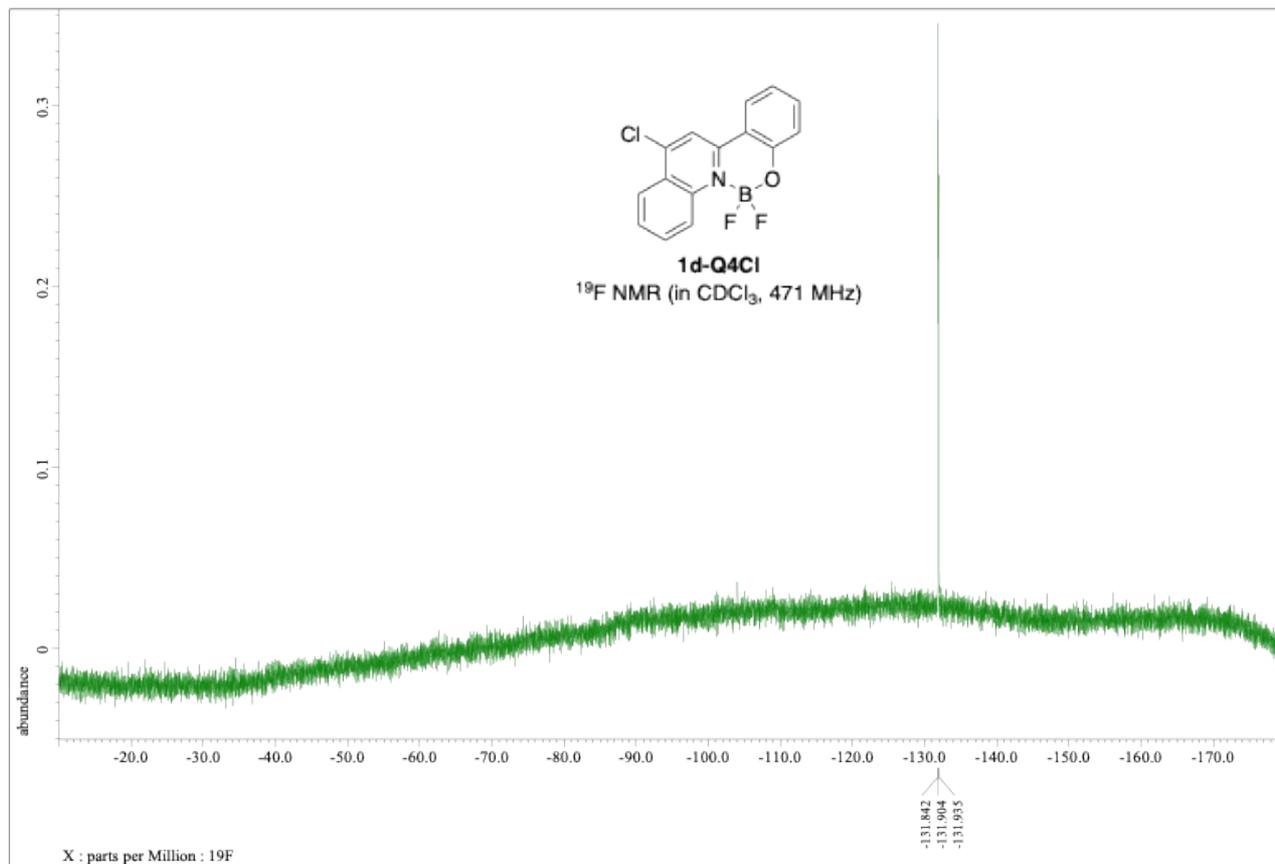
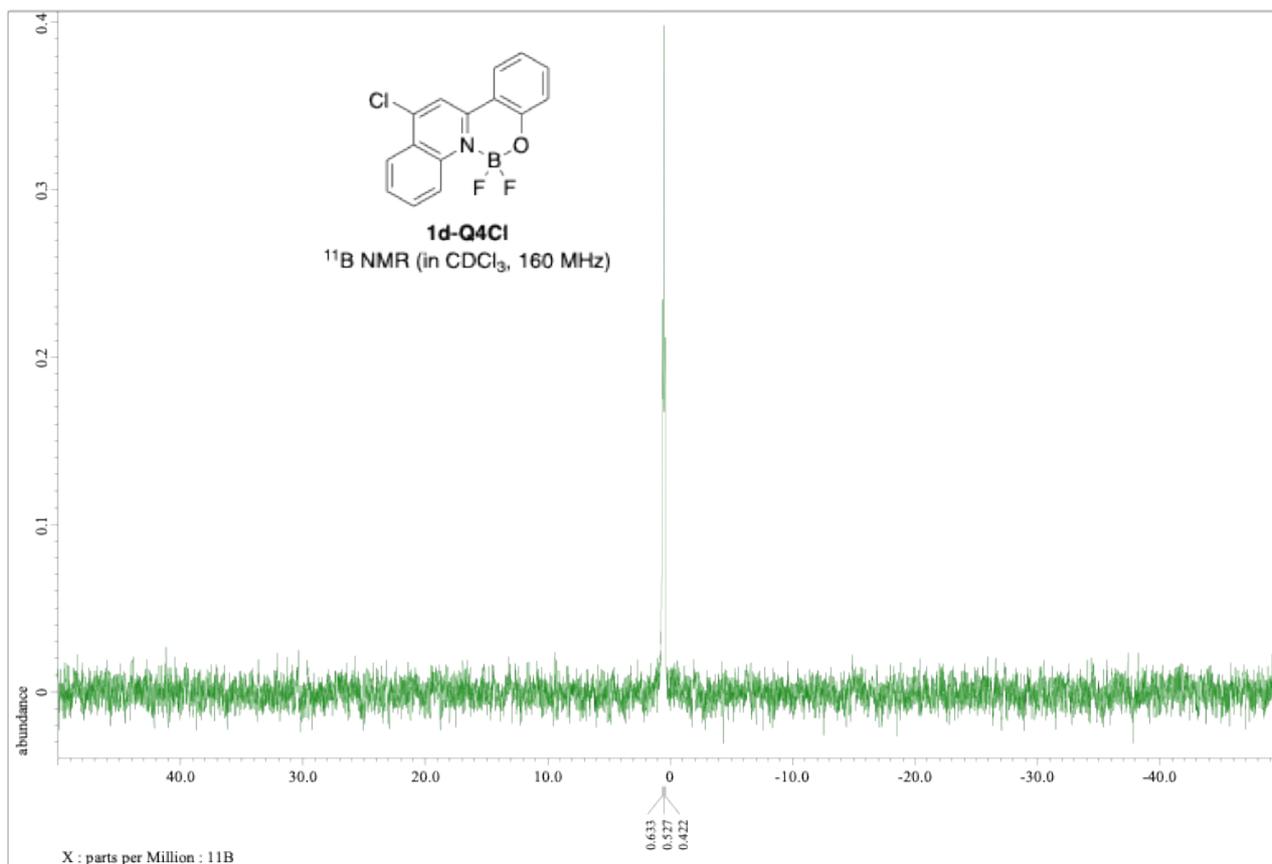


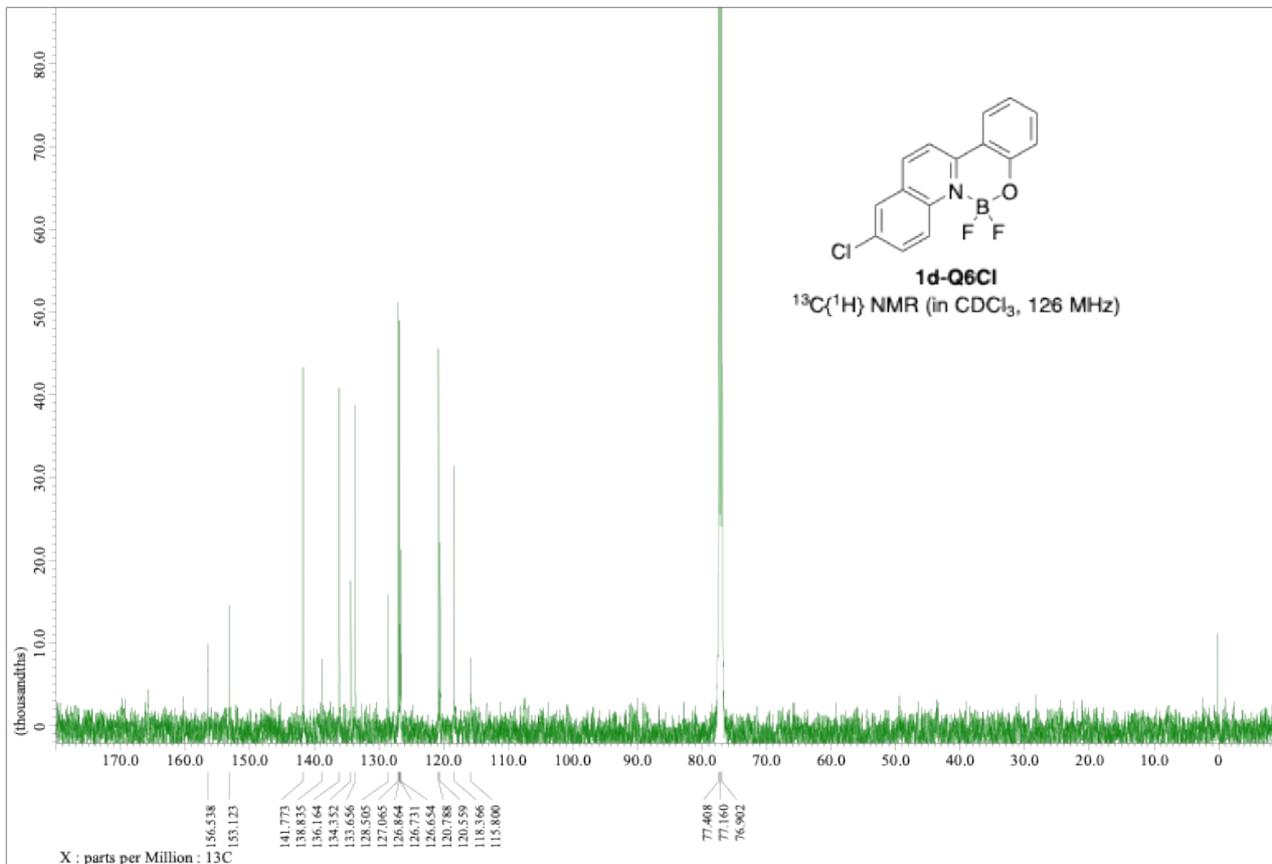
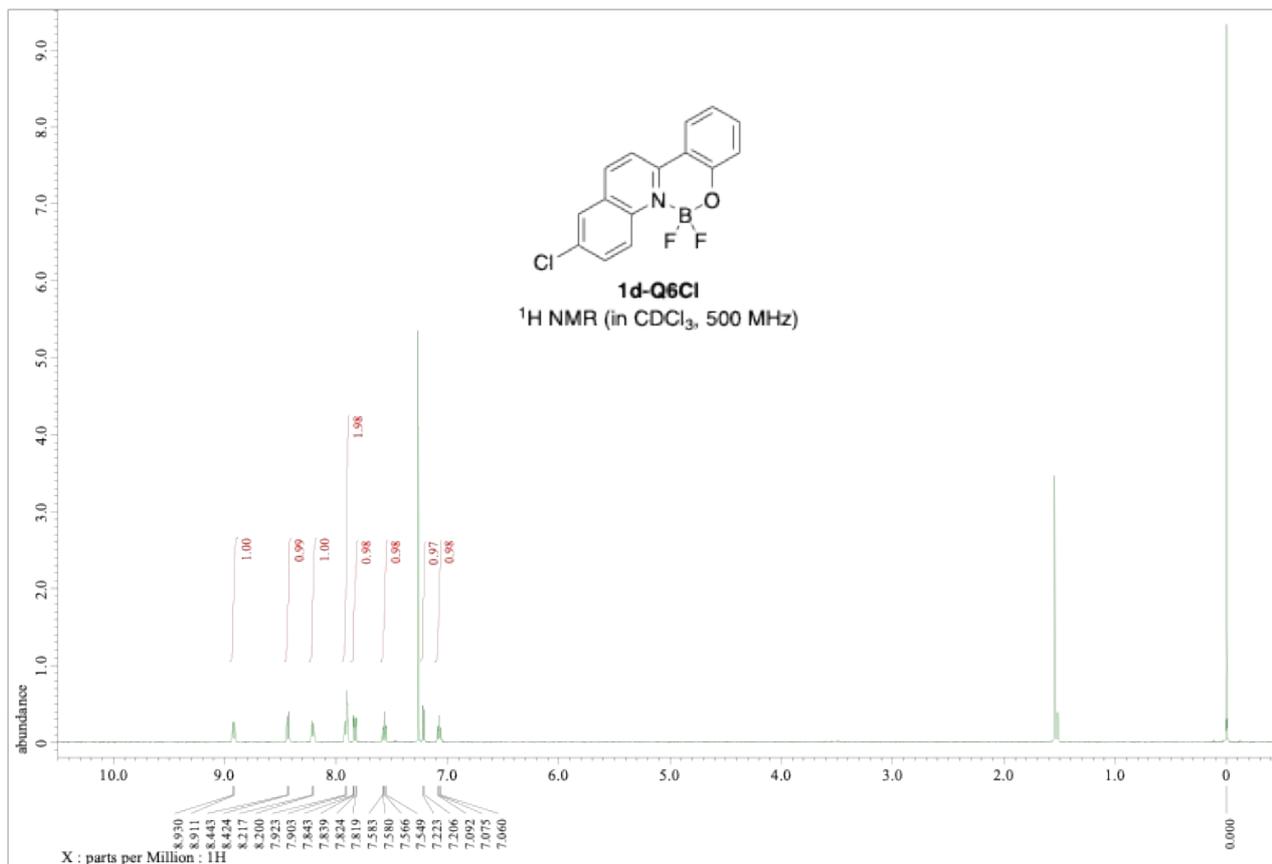


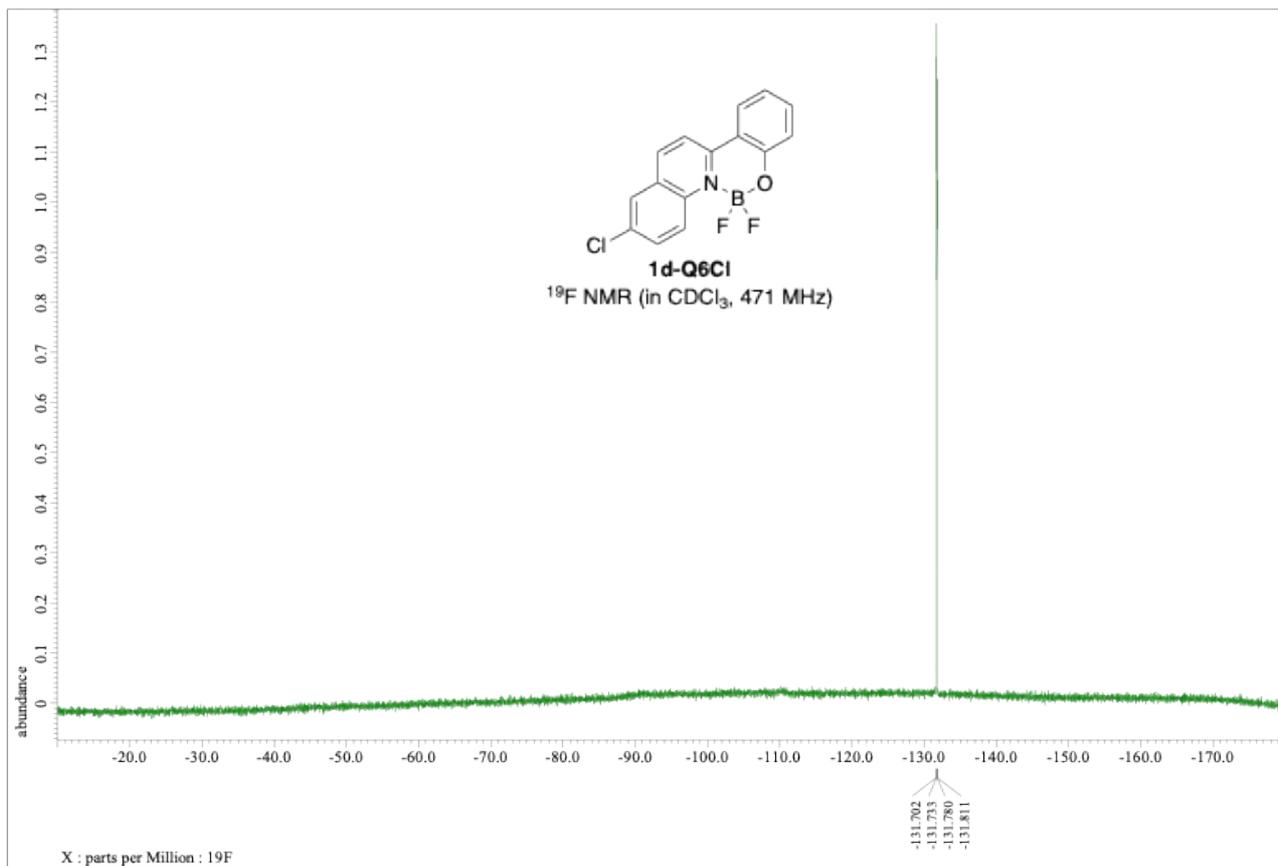
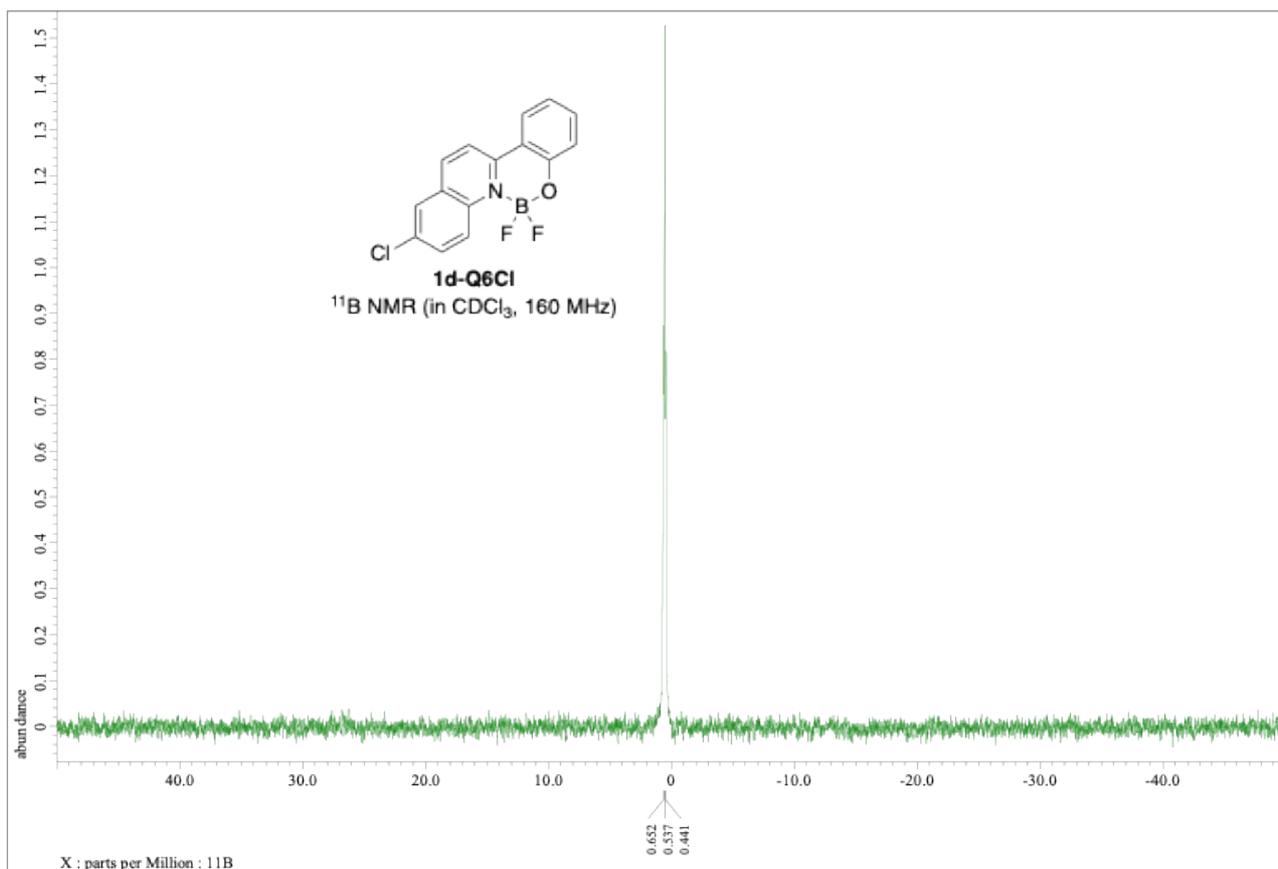


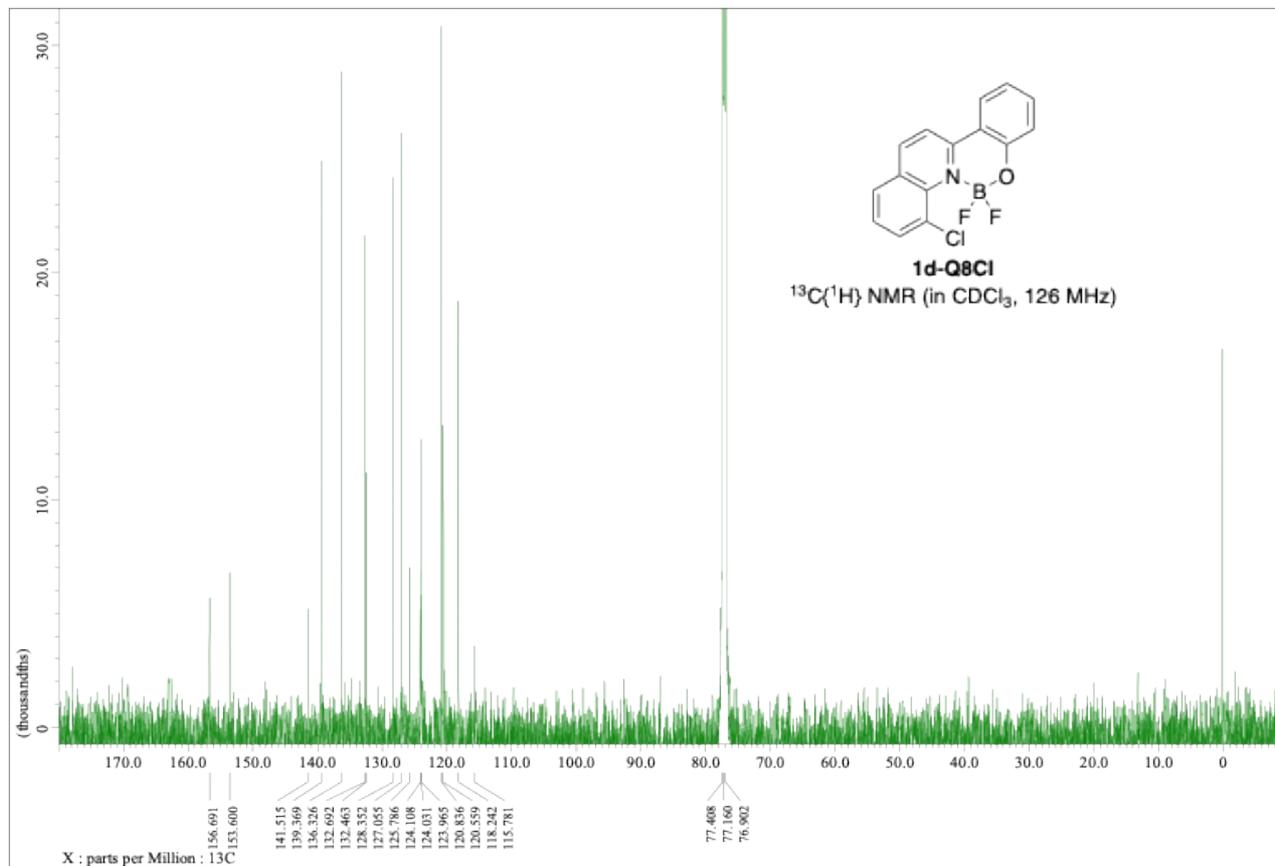
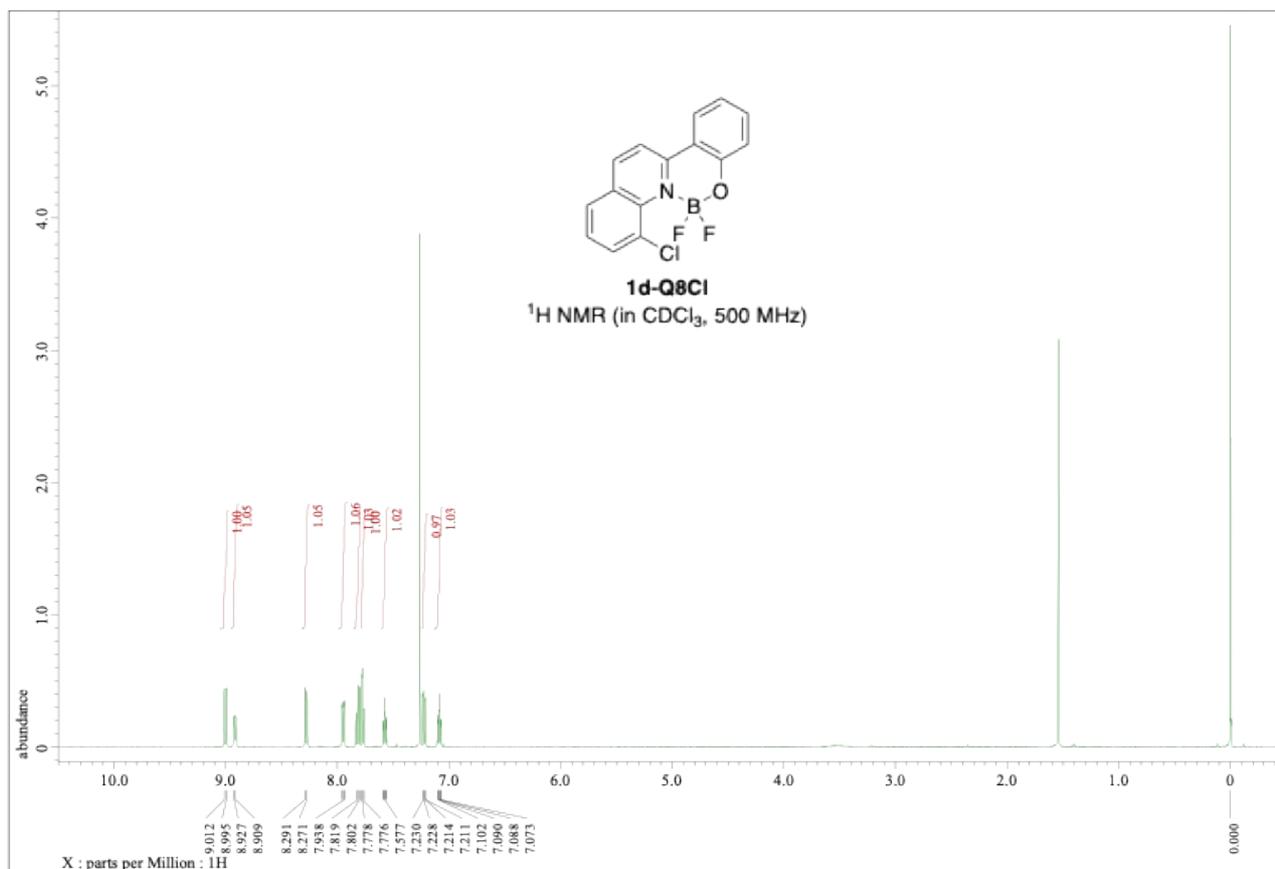


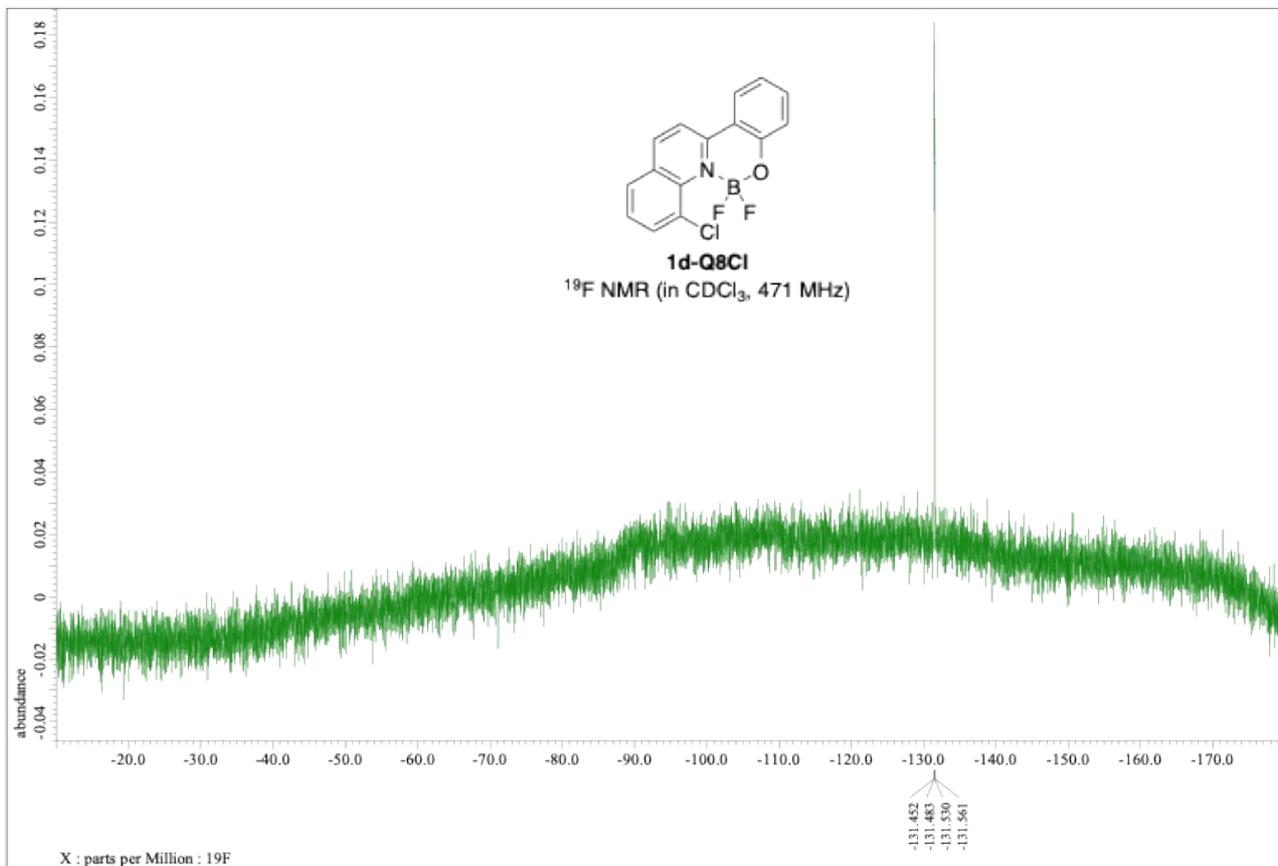
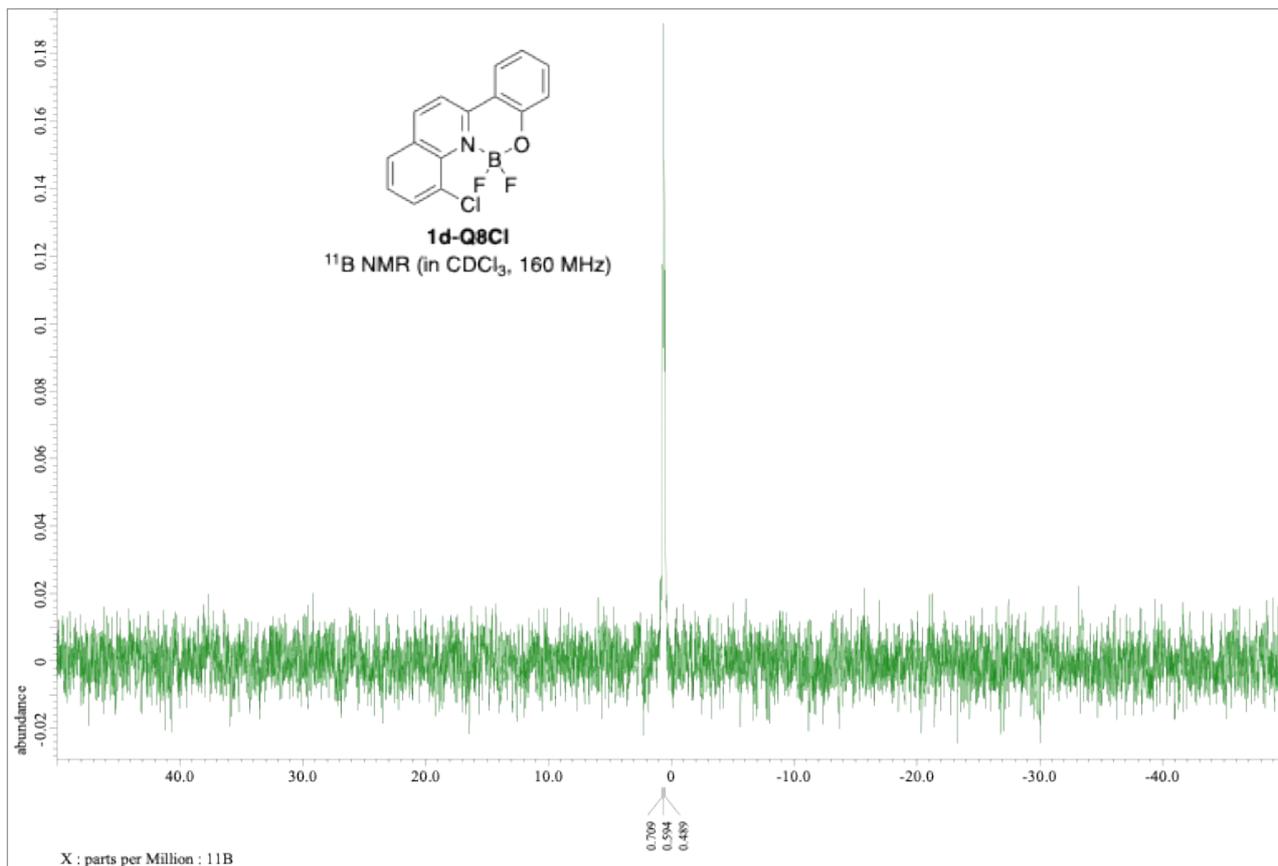


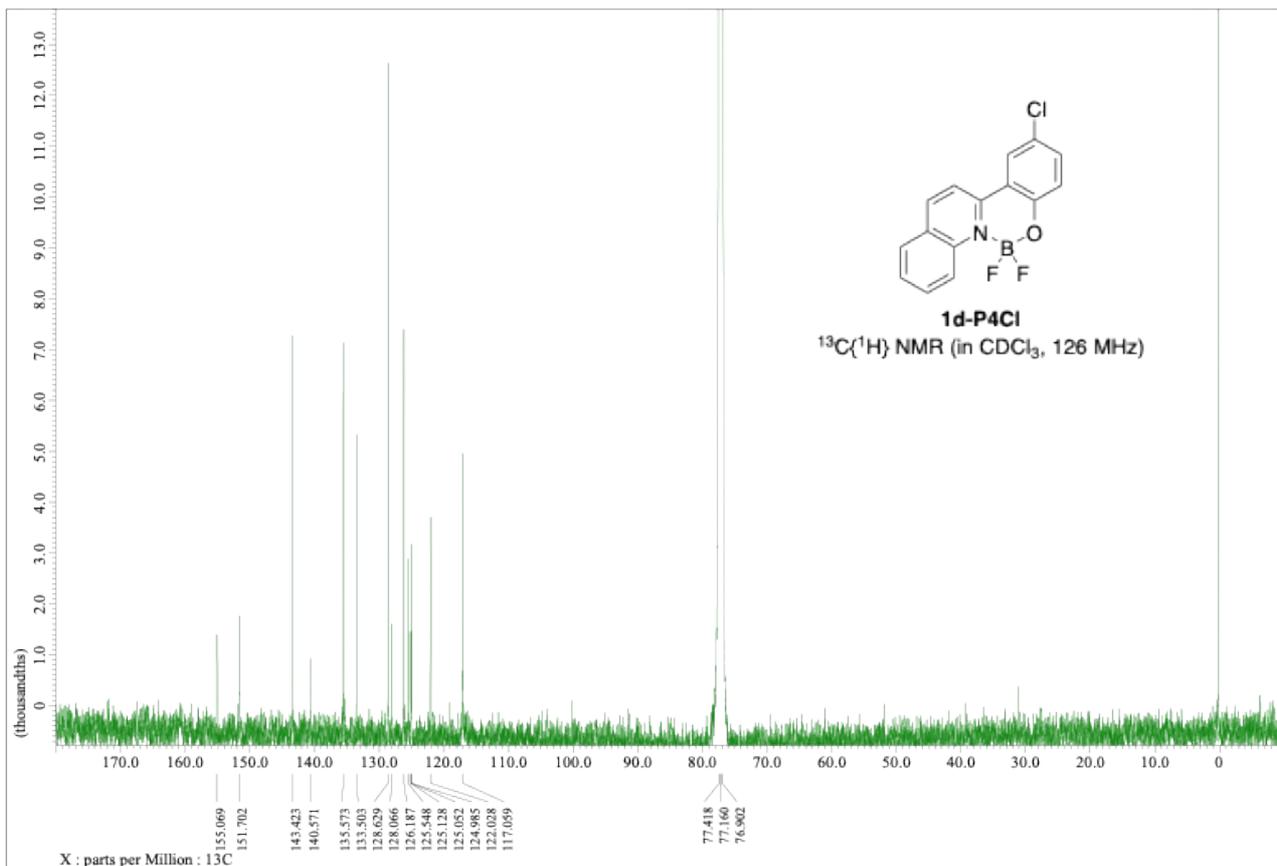
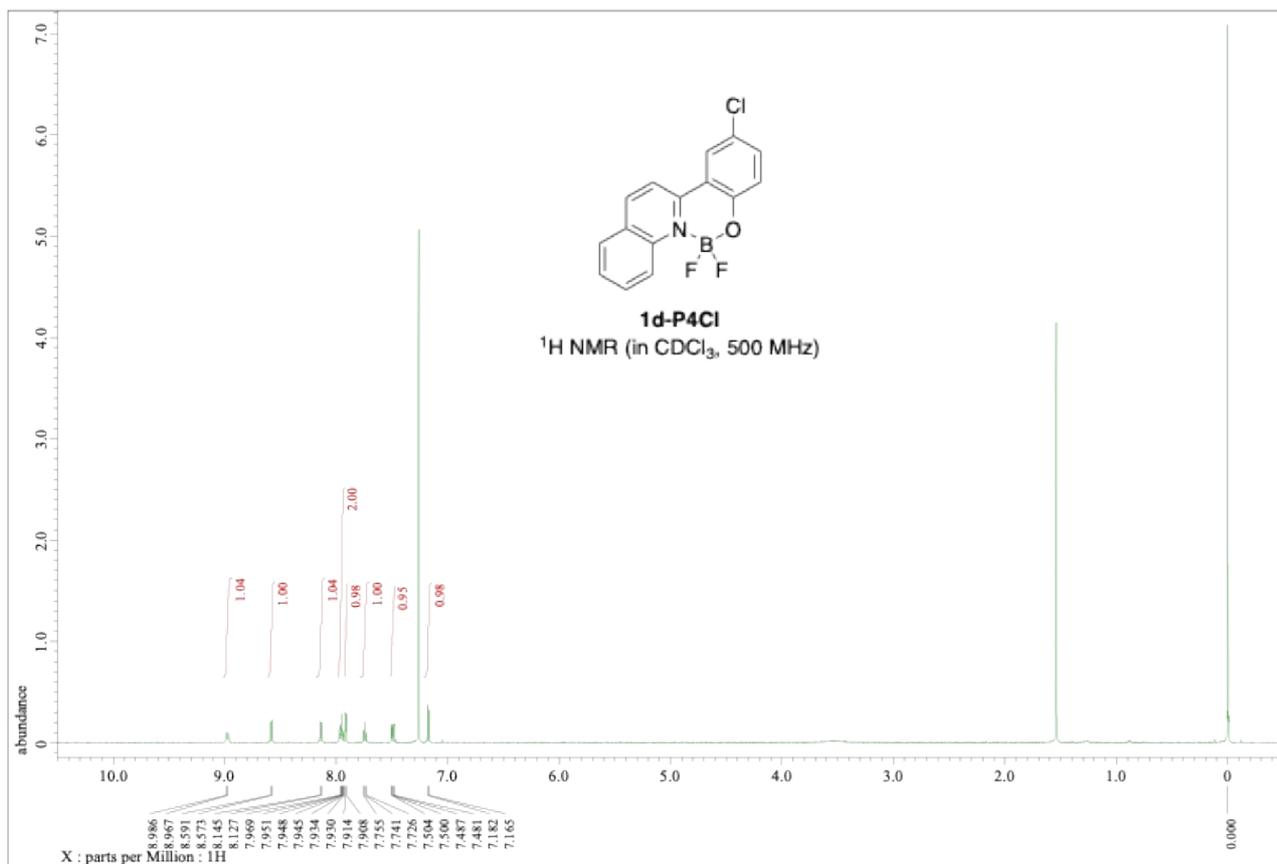


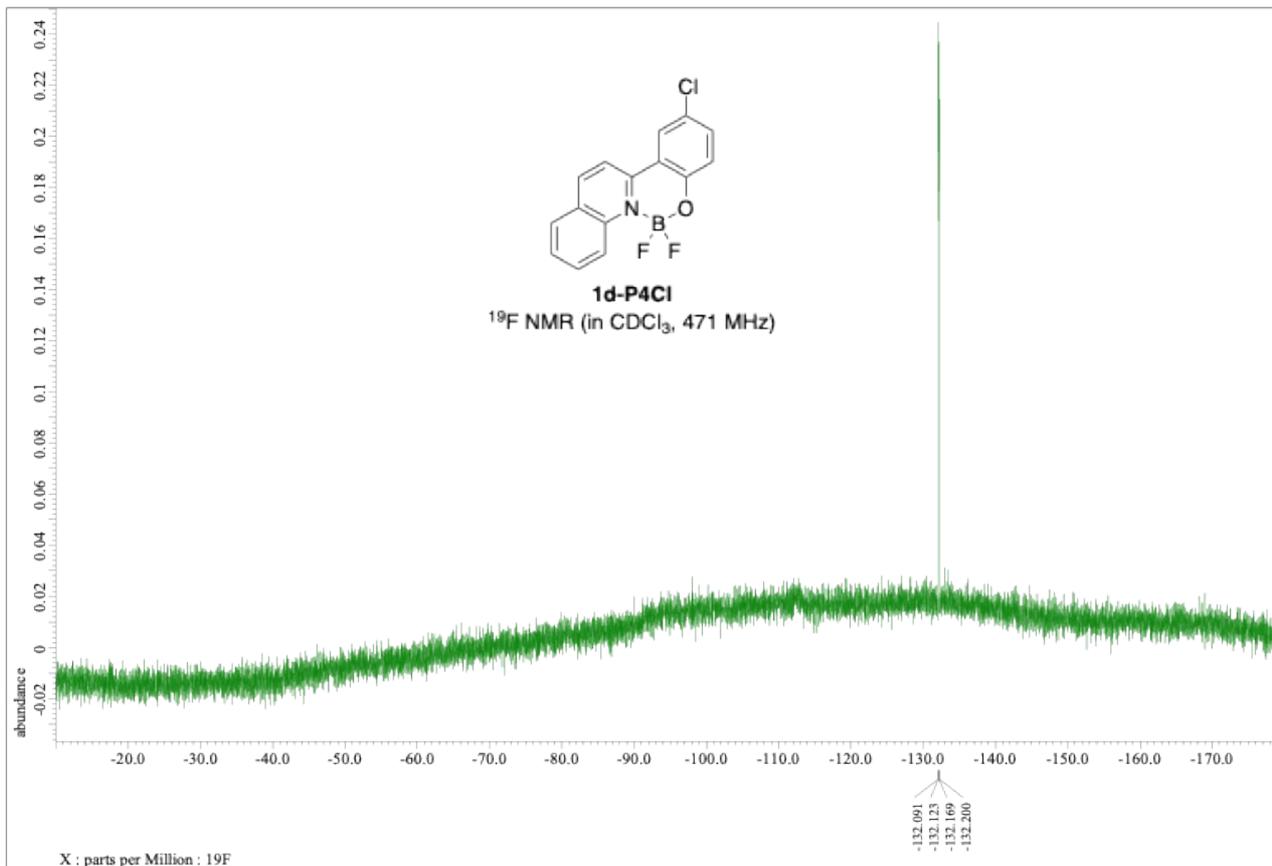
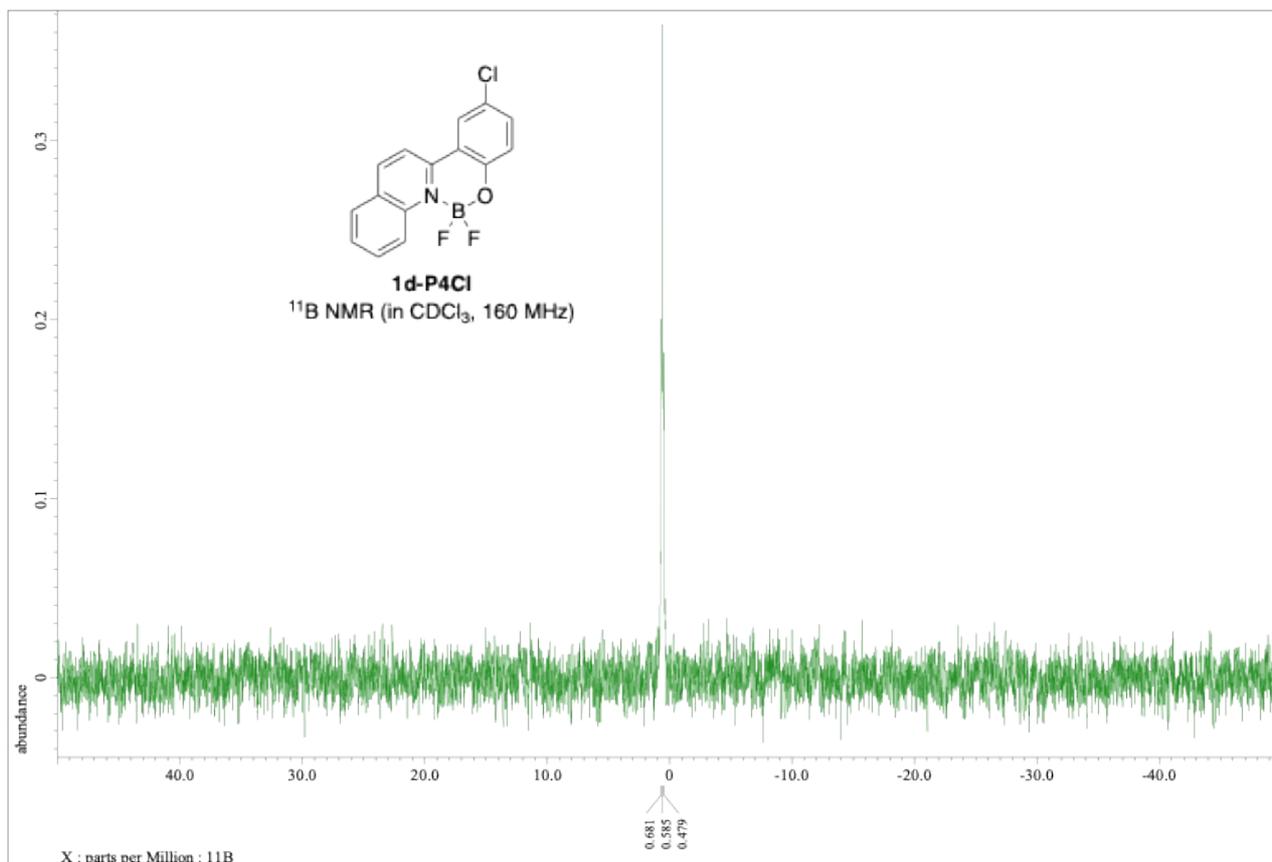


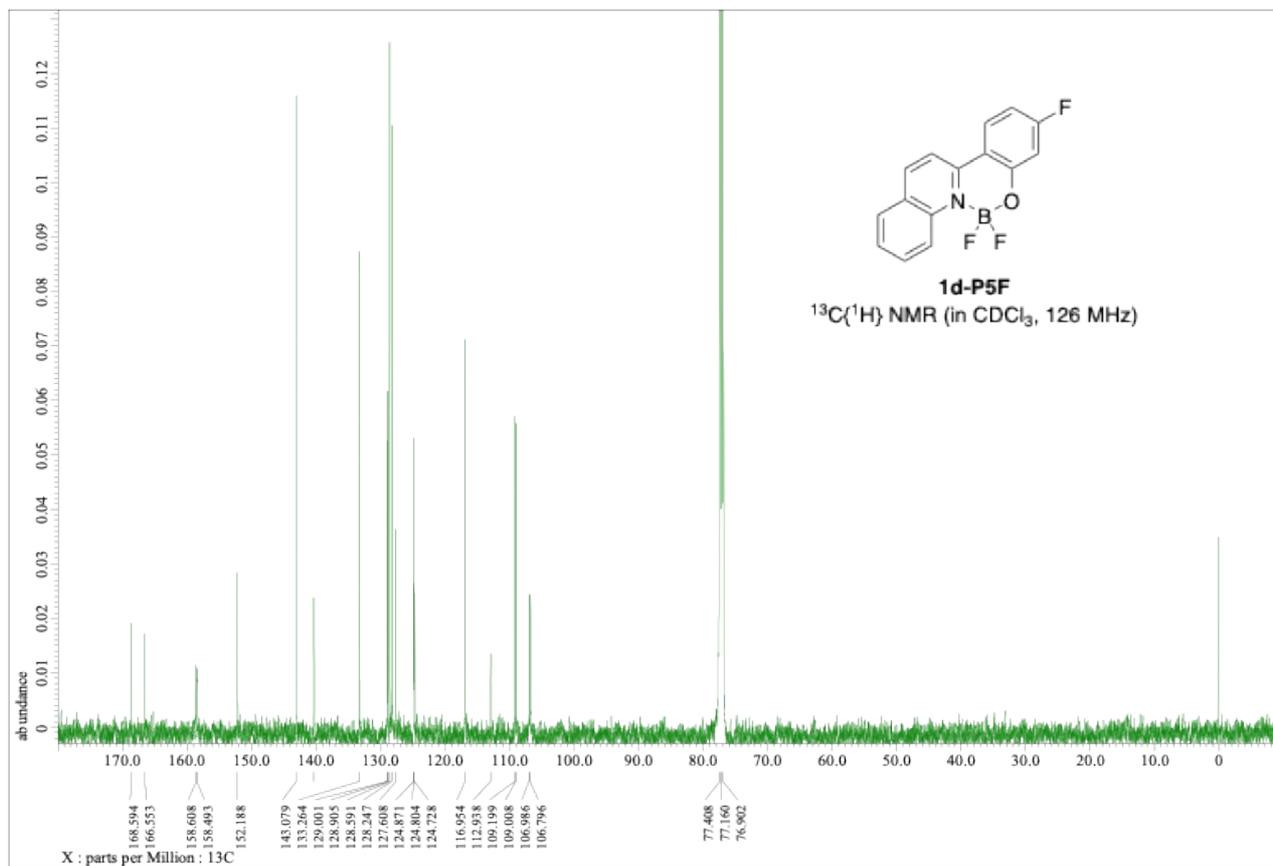
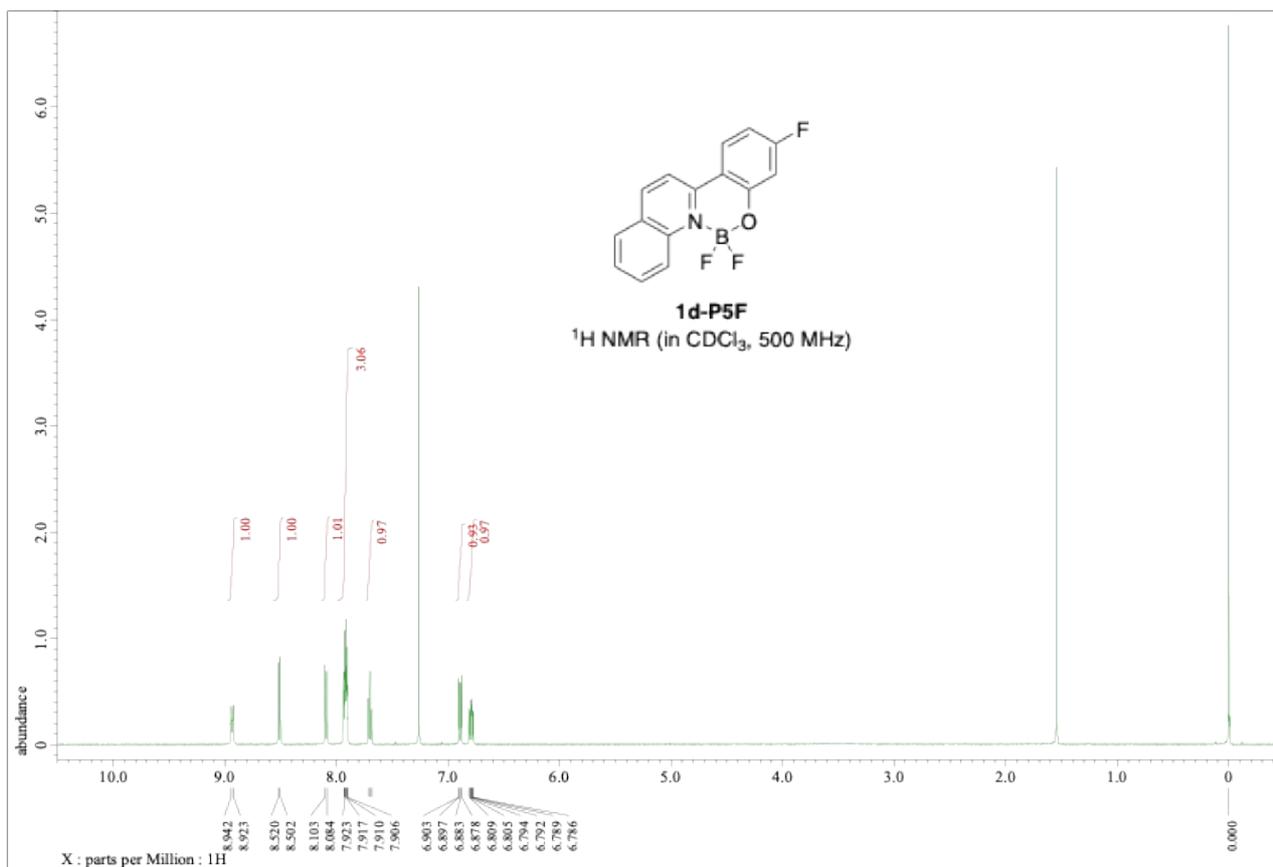


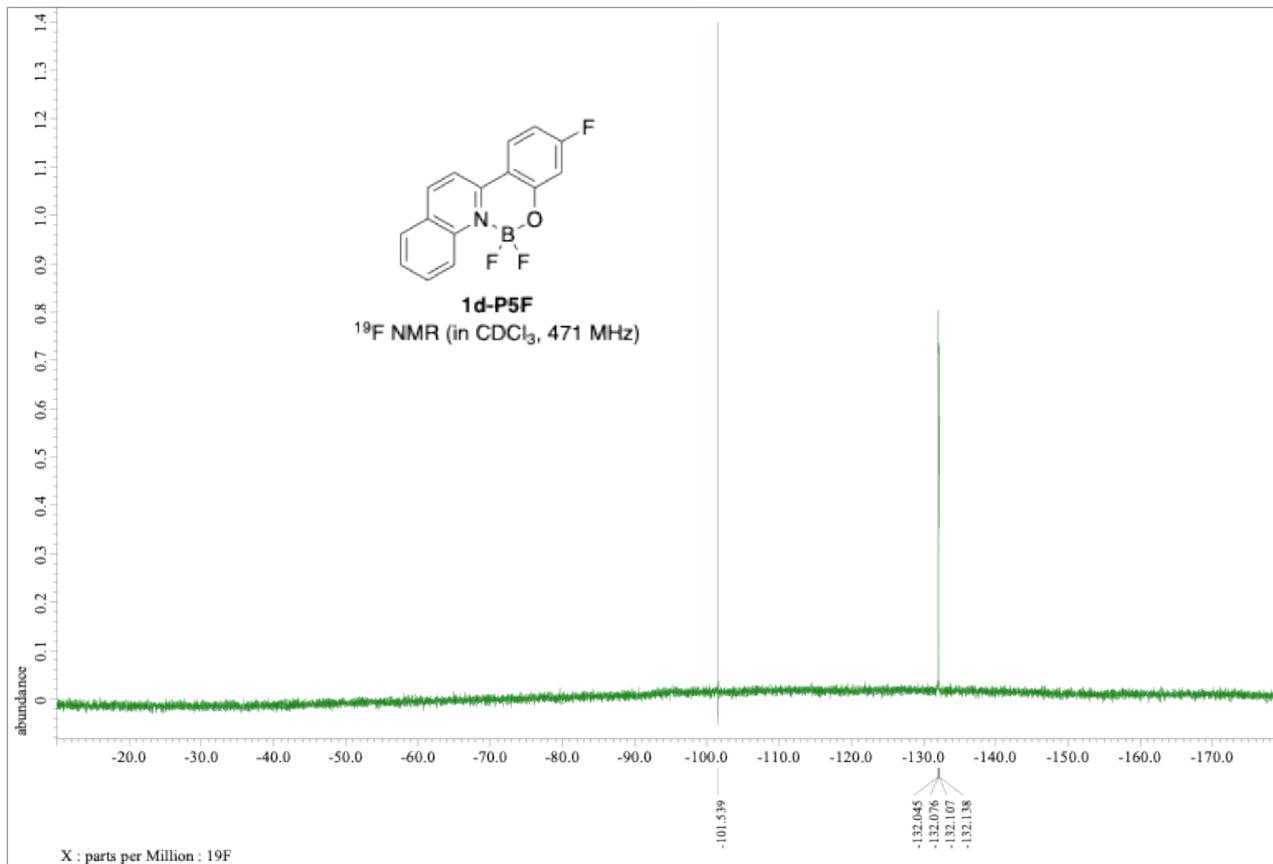
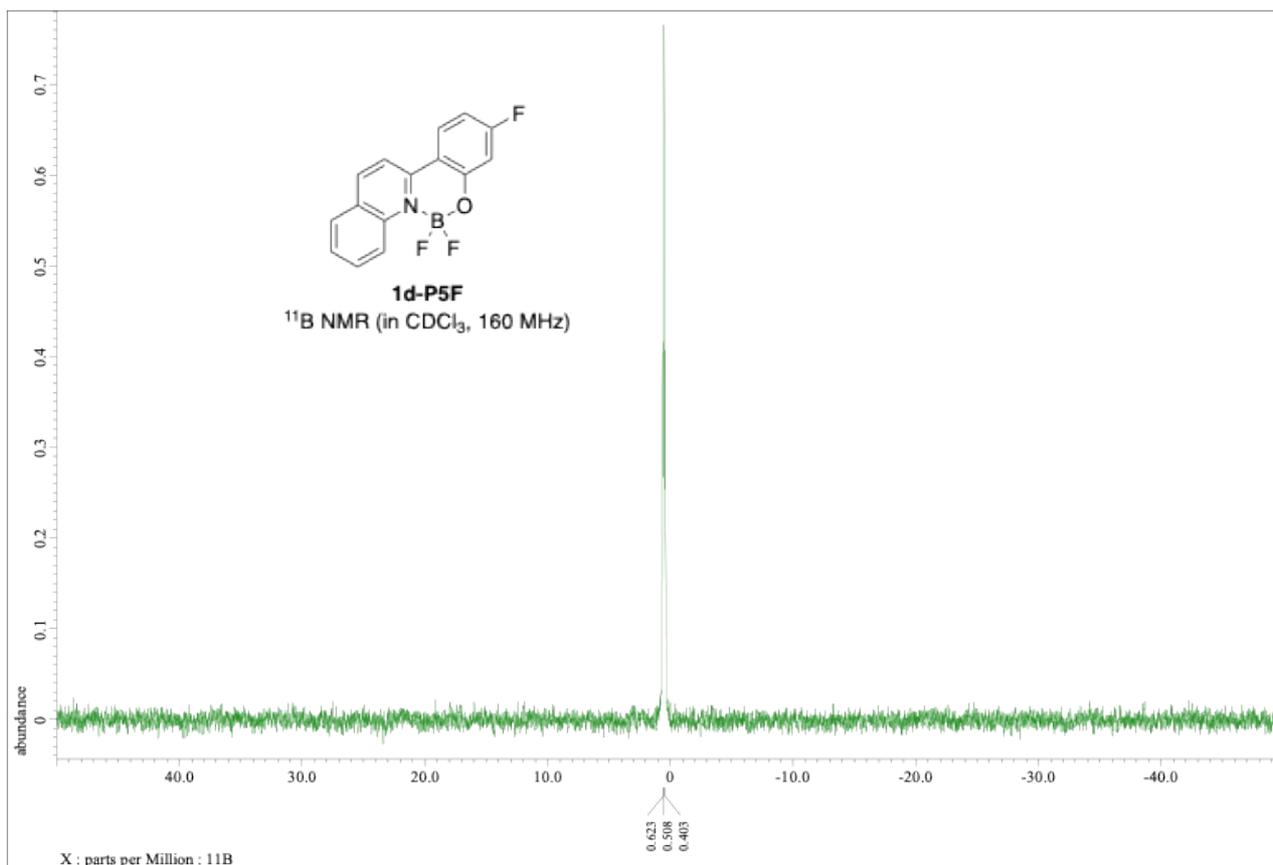


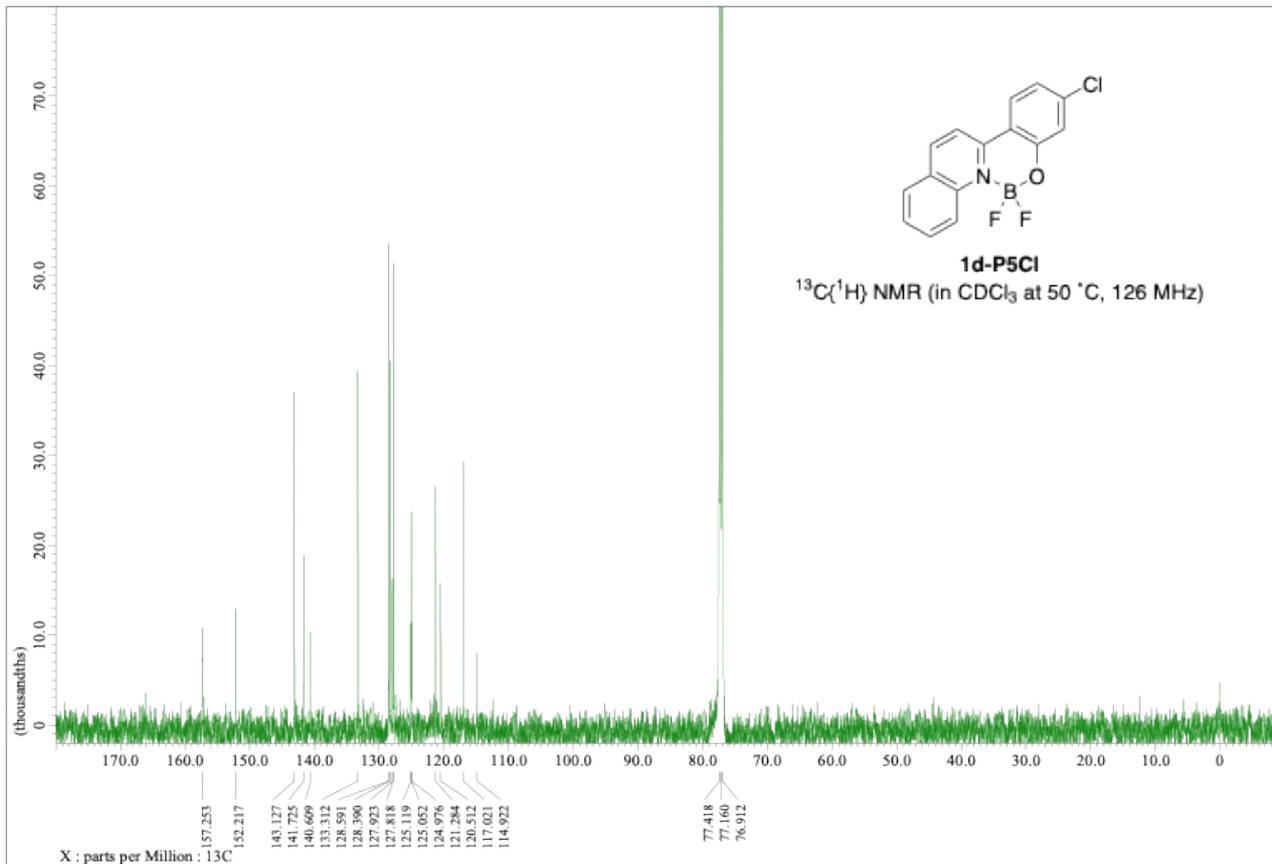
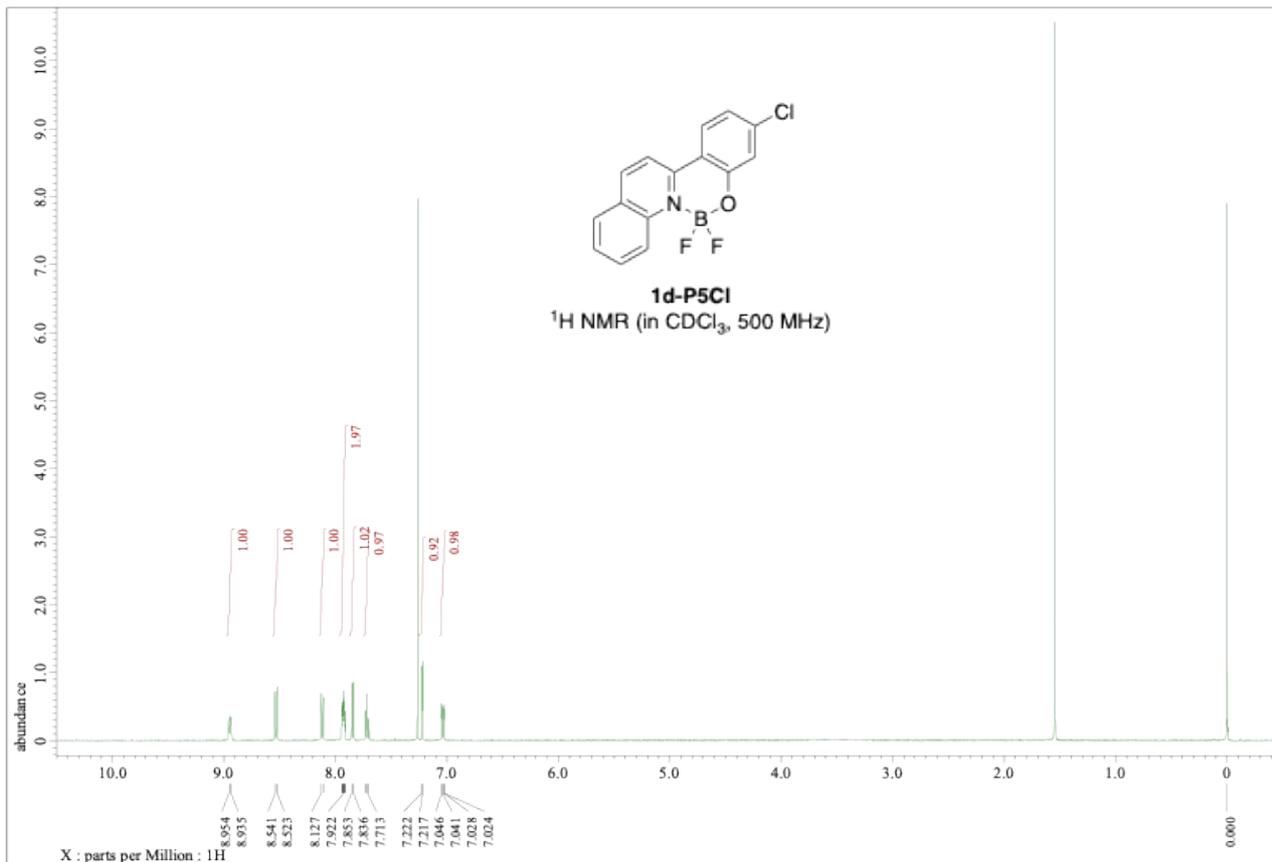


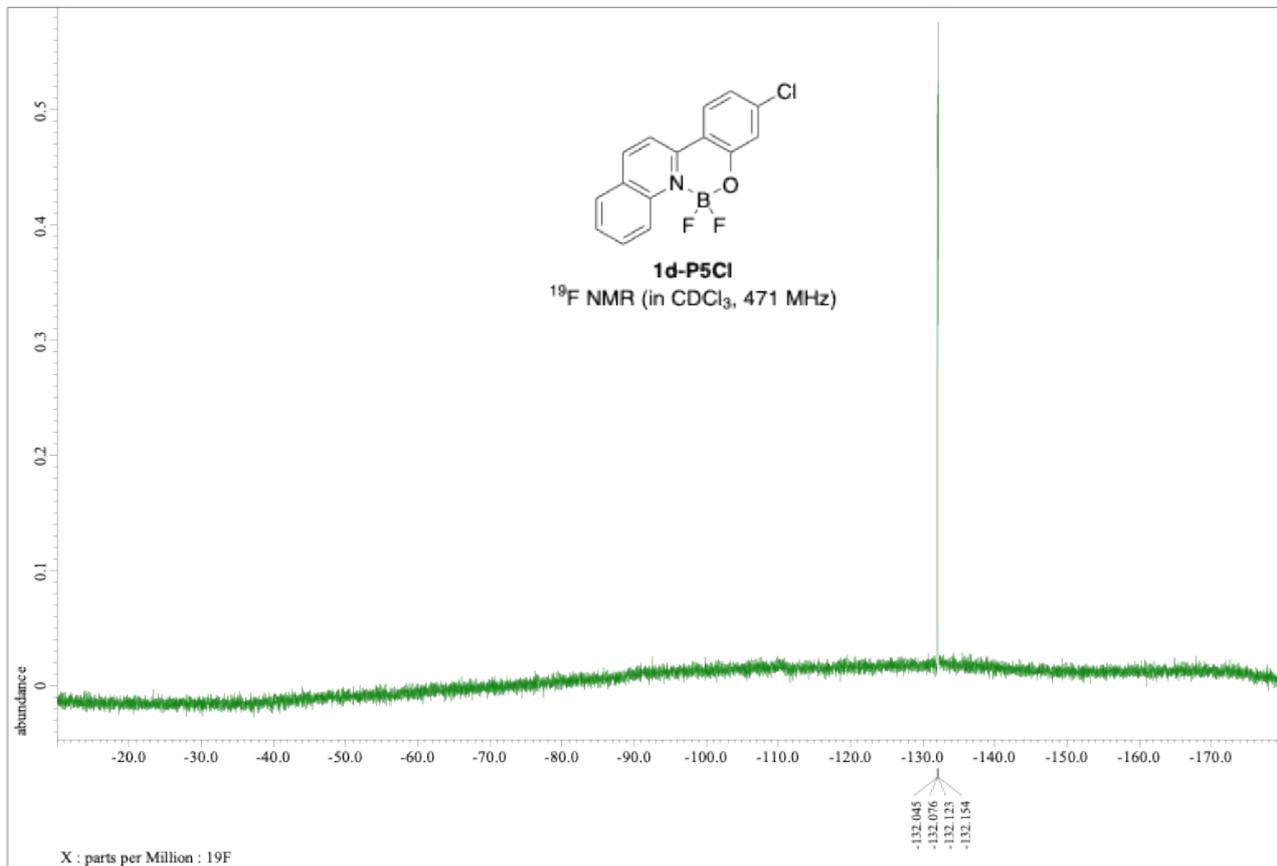
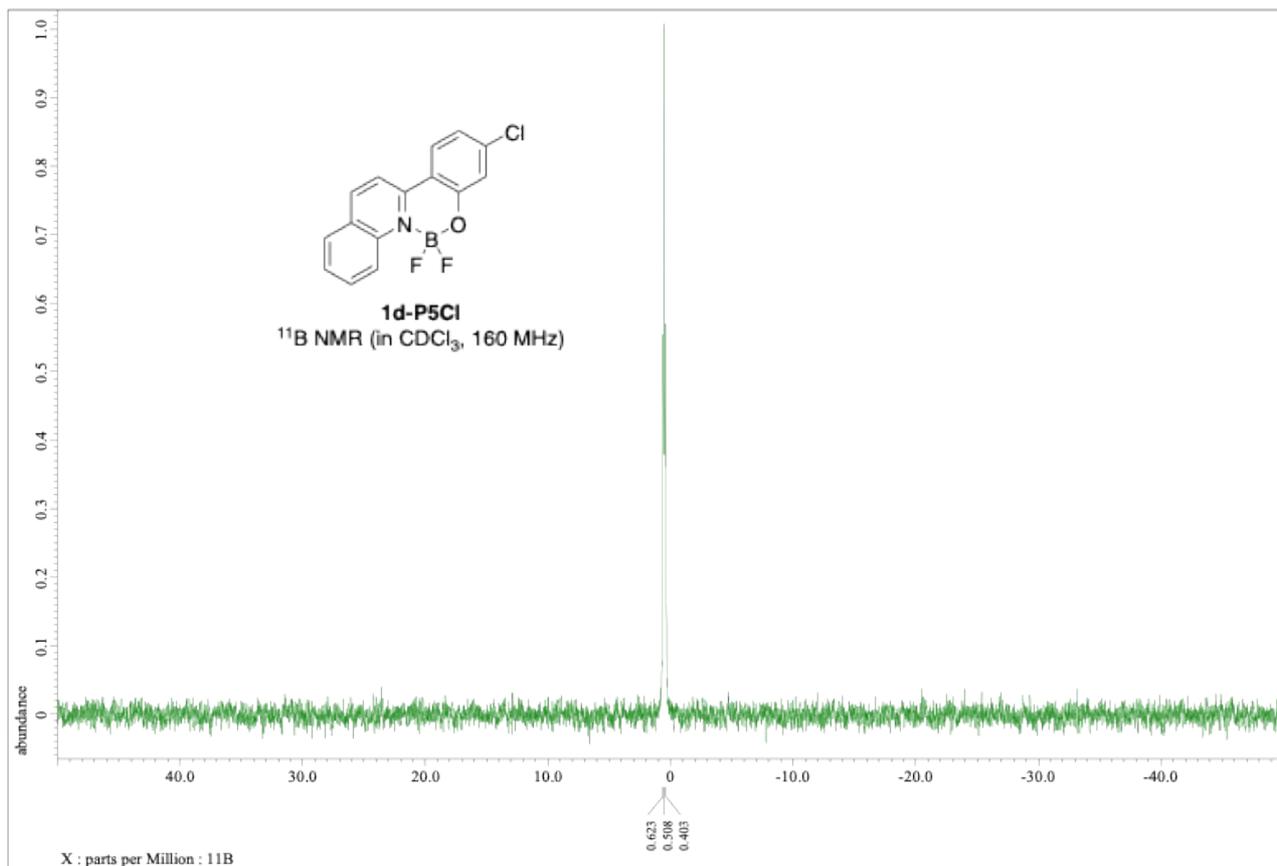


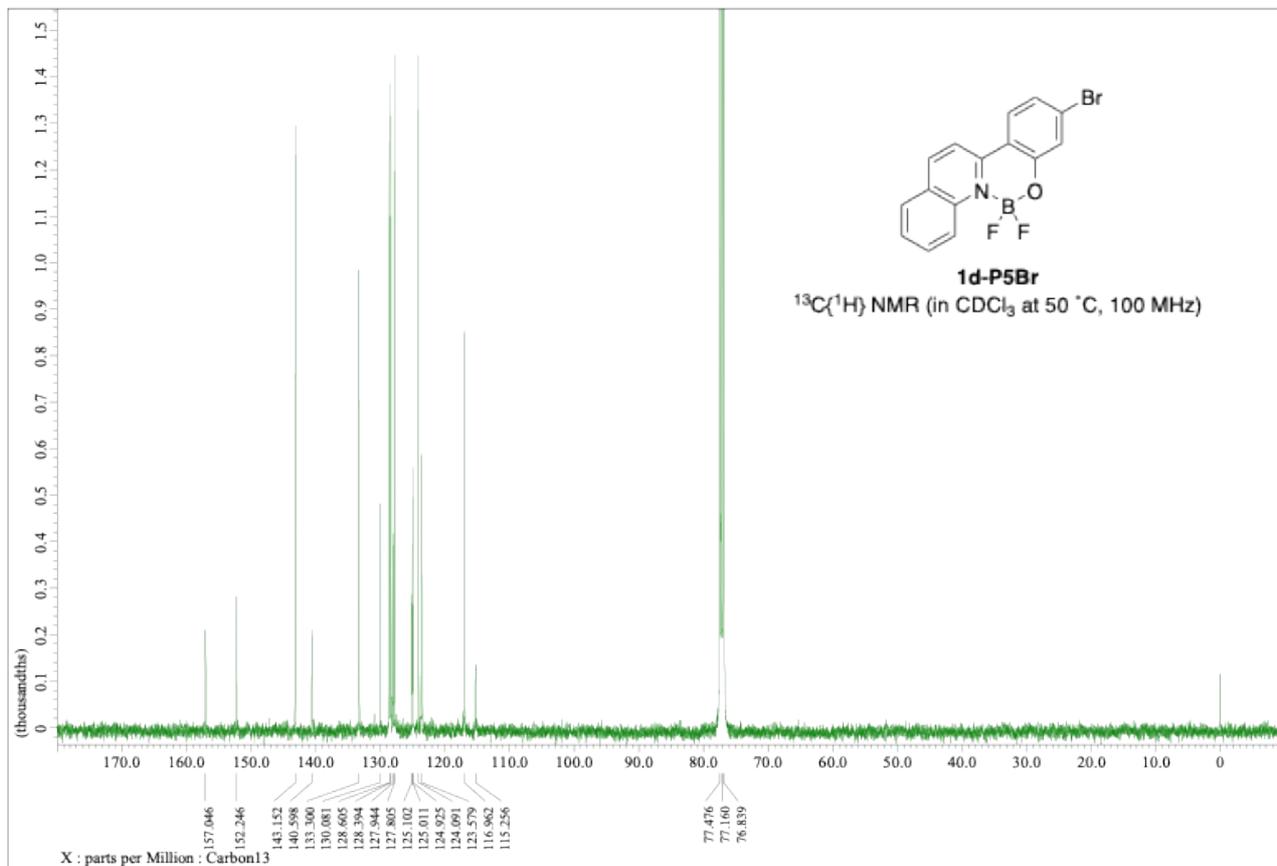
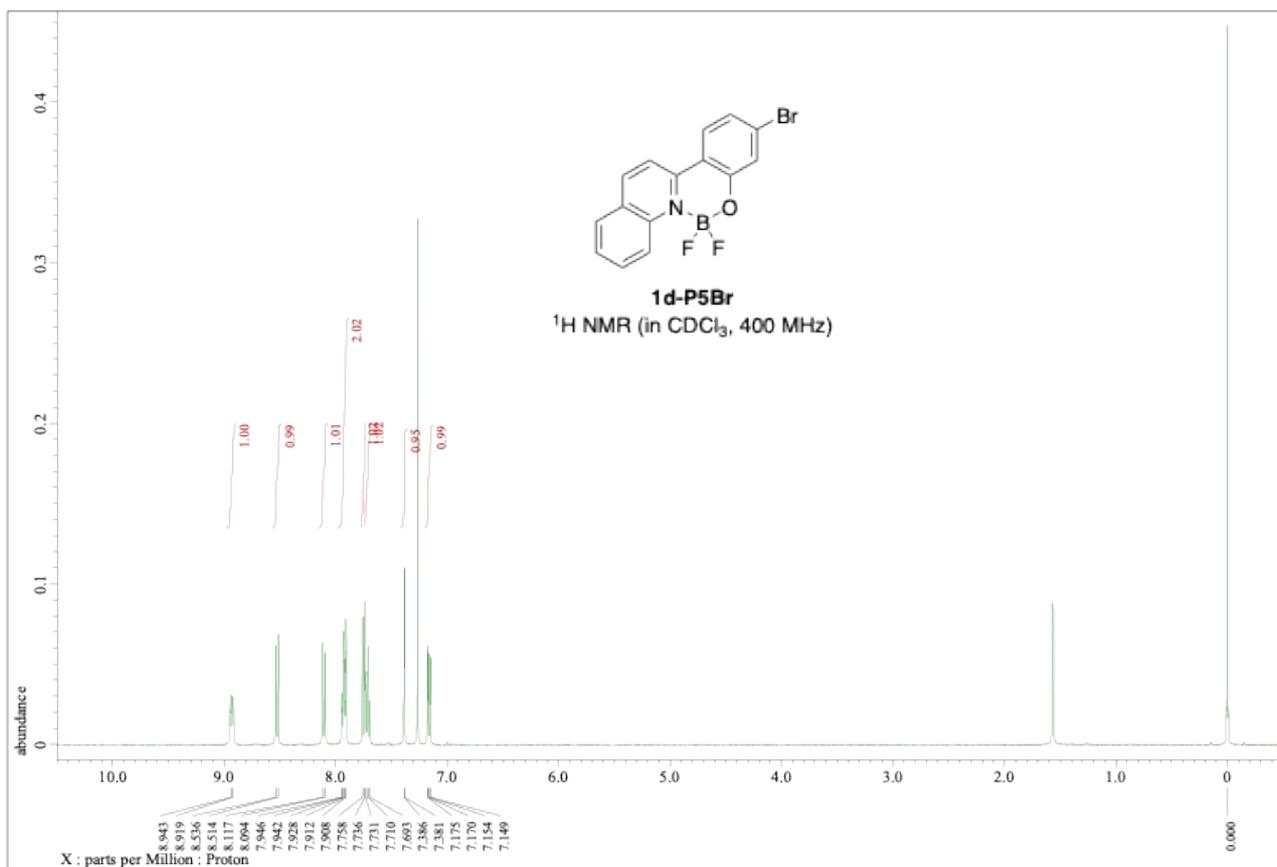


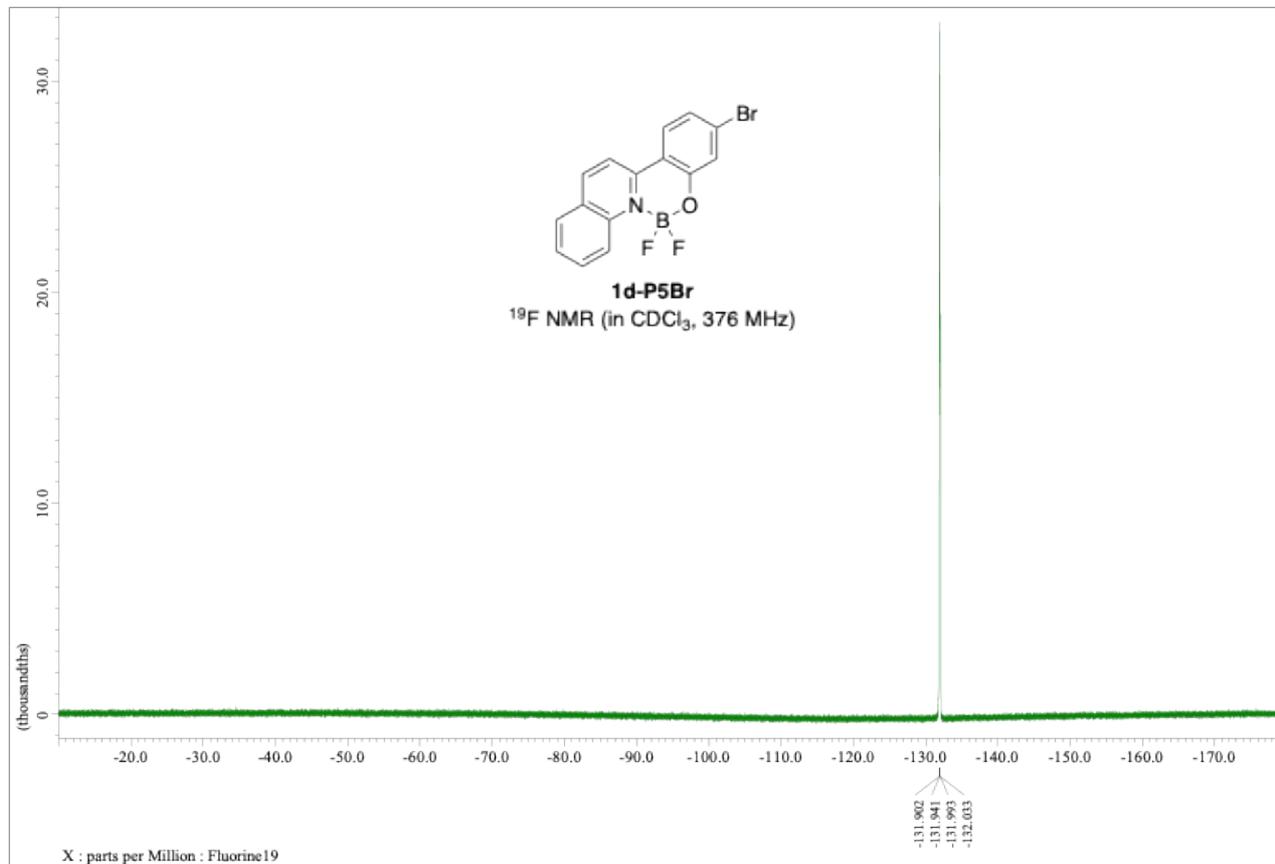
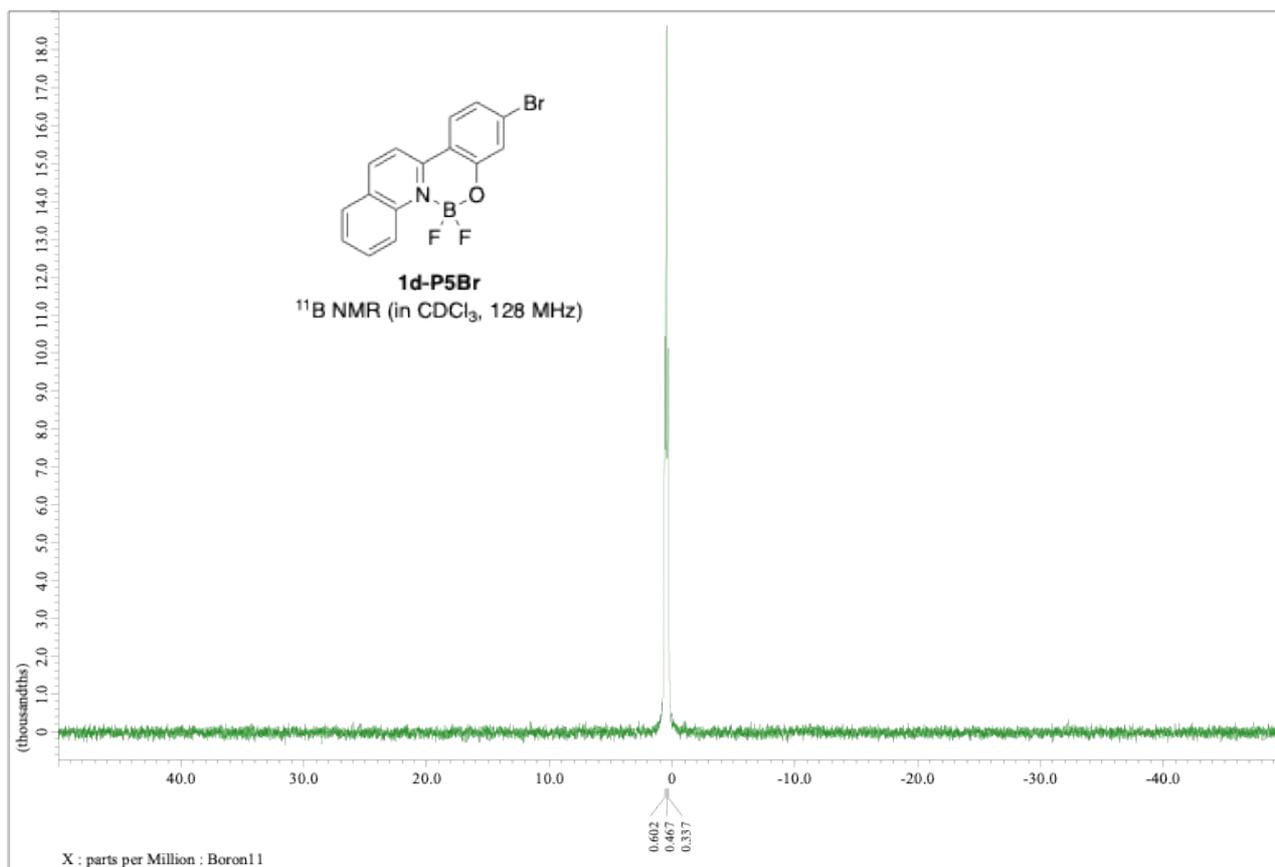


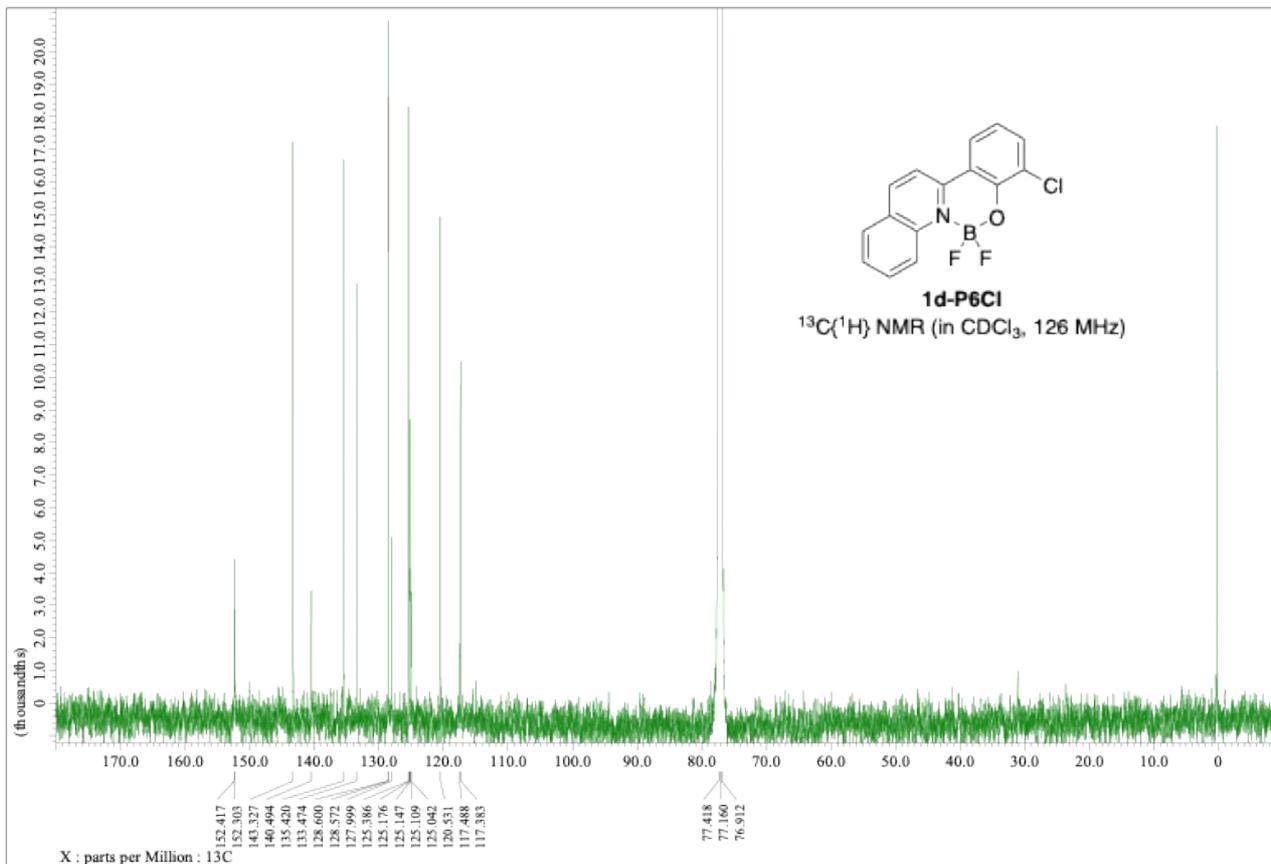
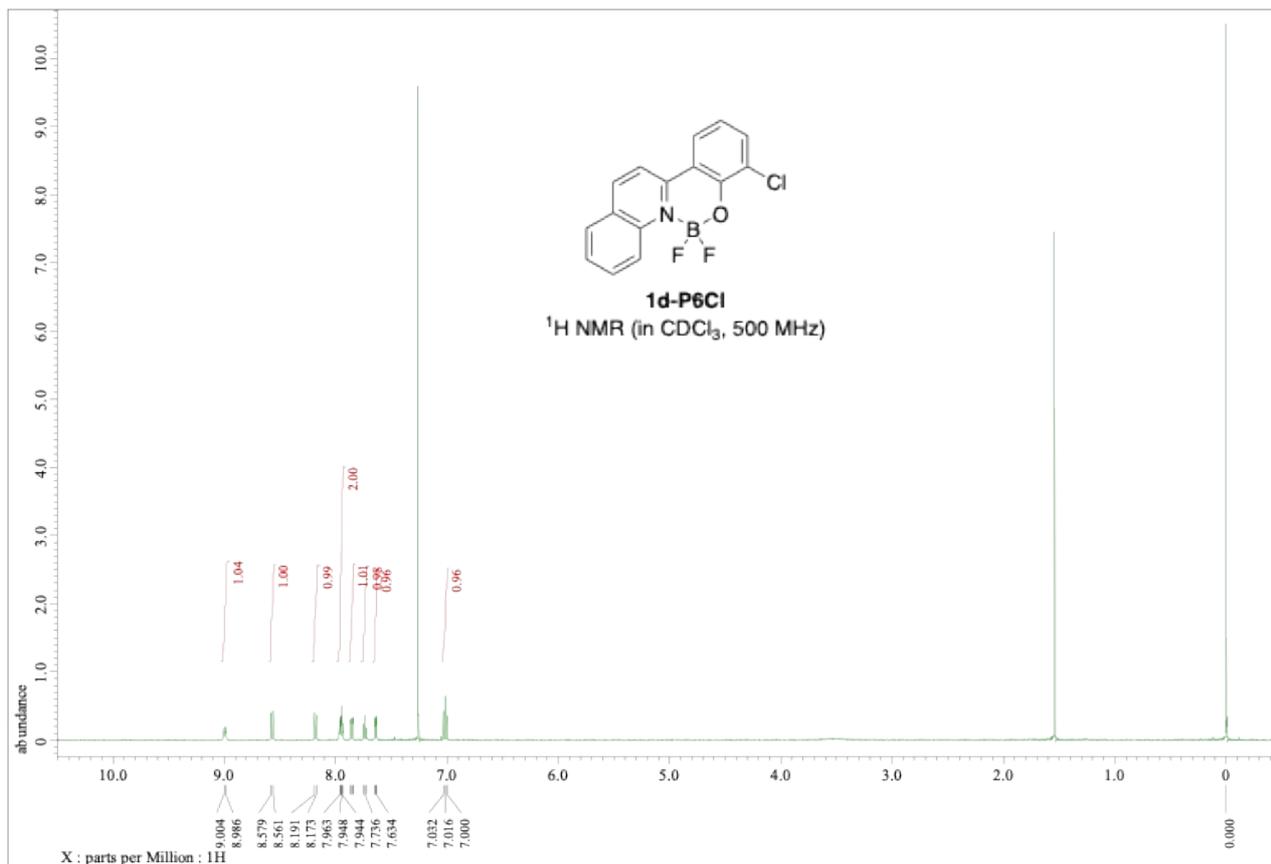


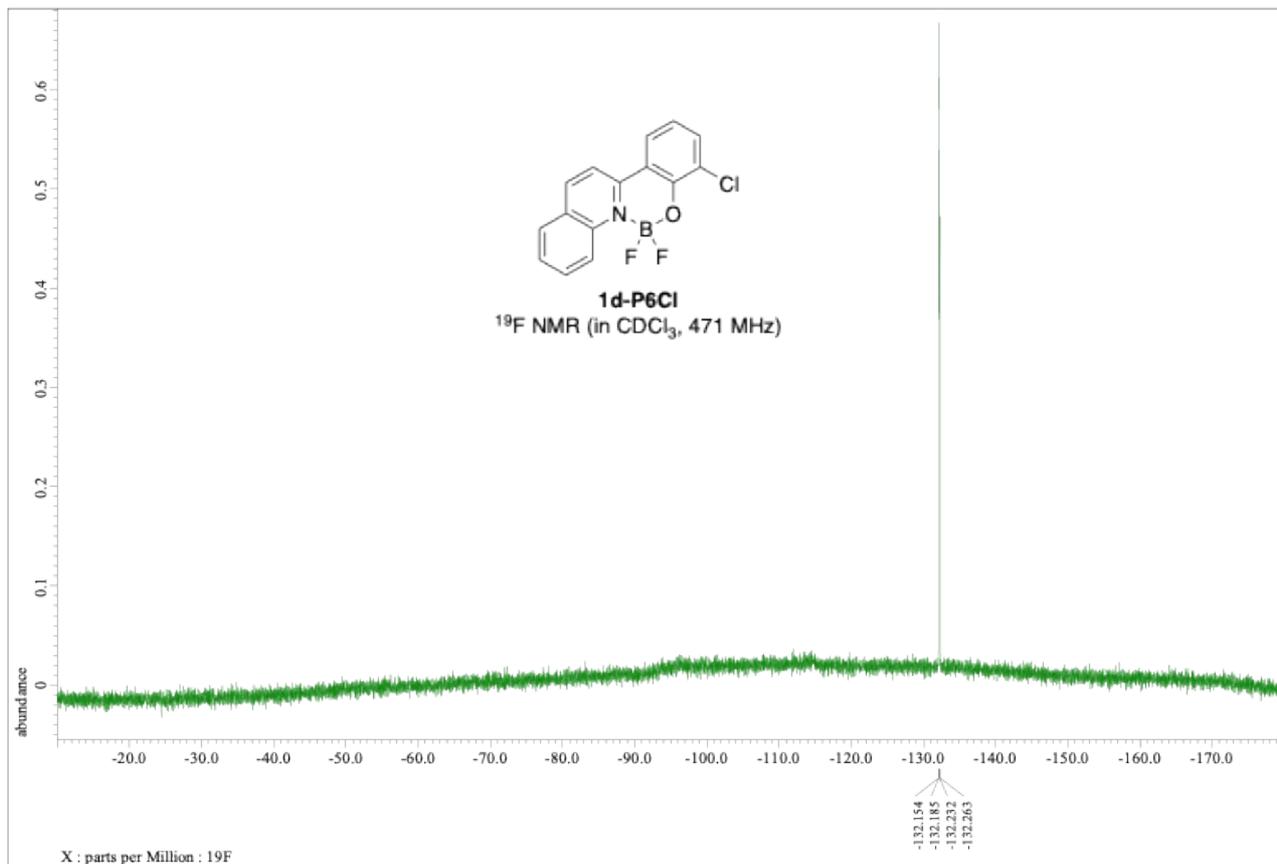
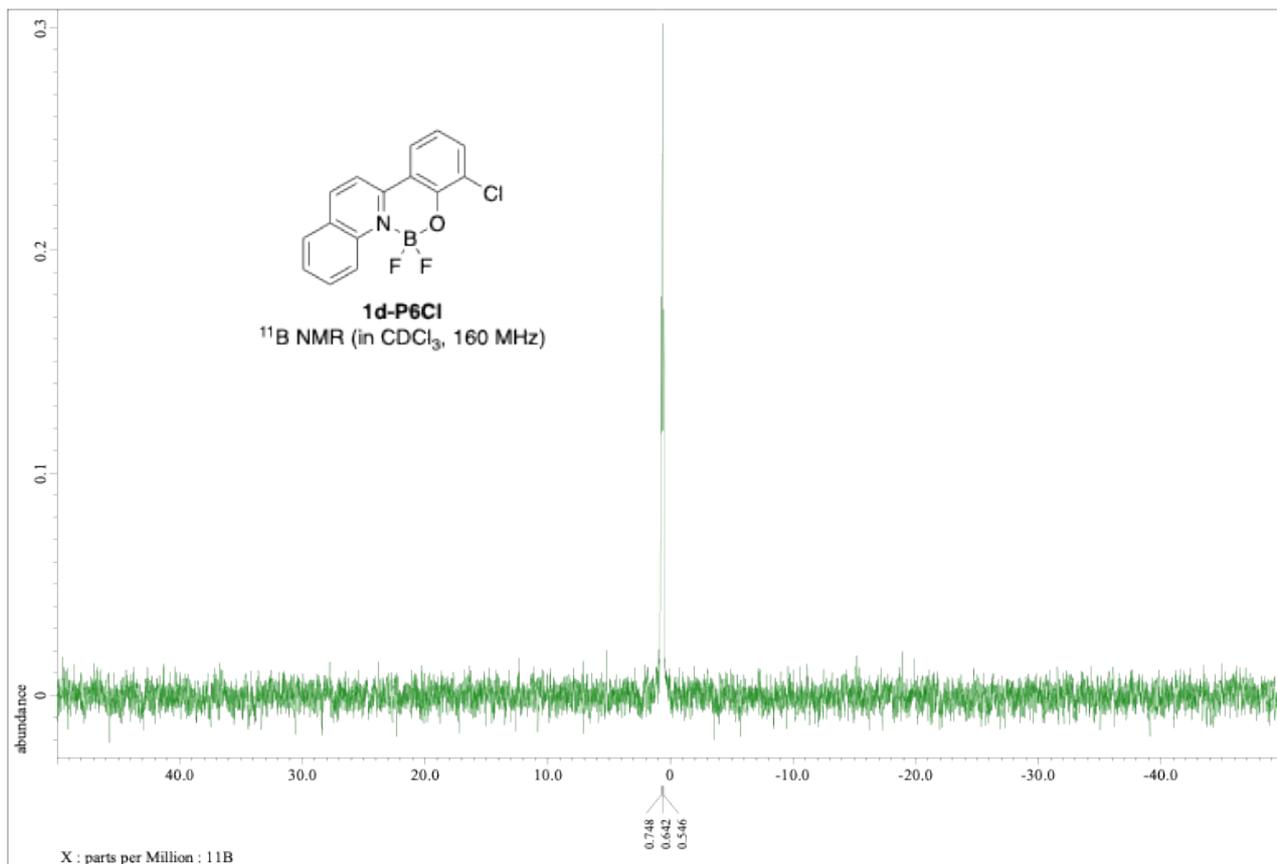




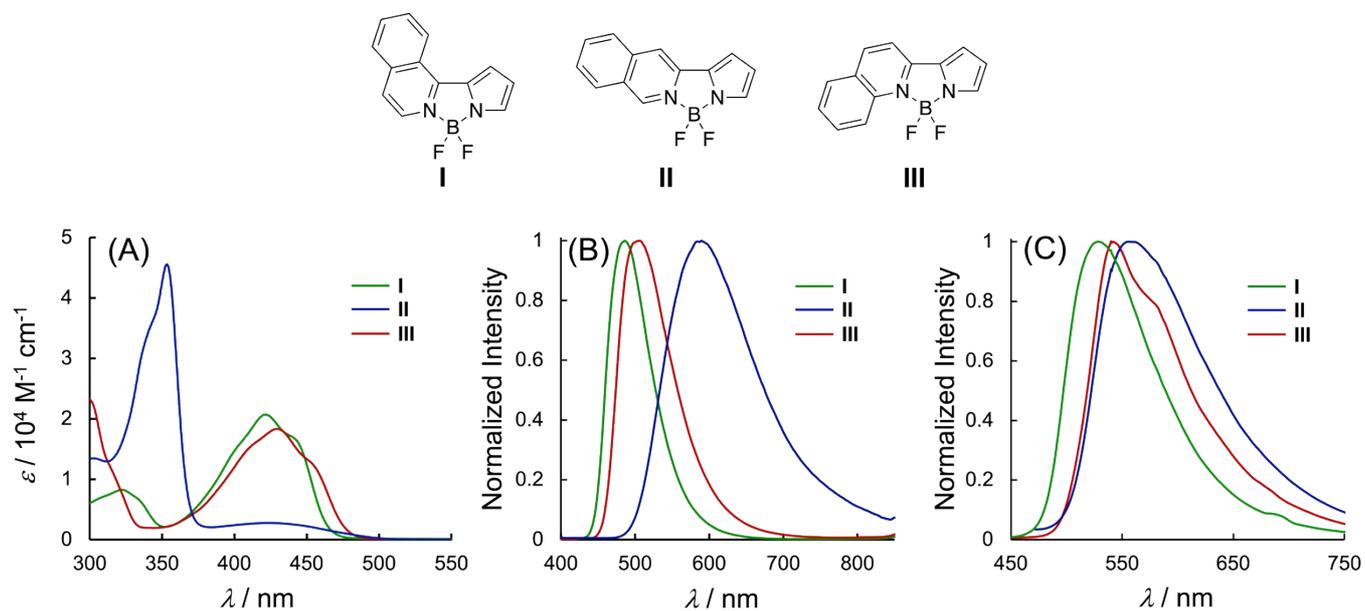








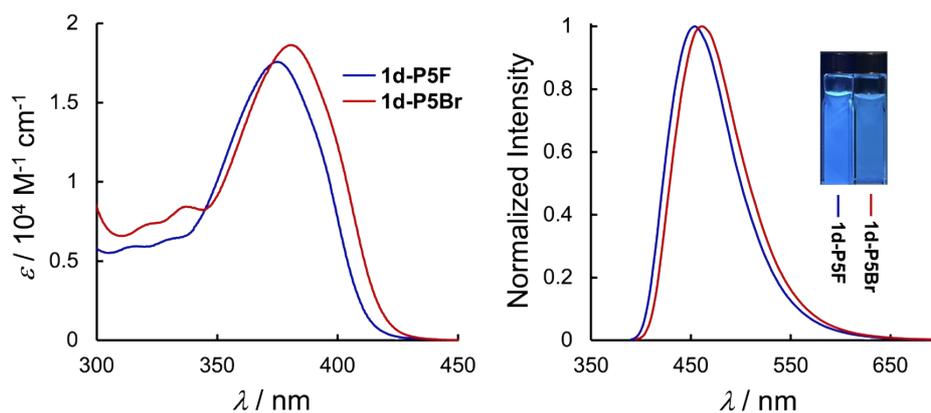
## Fluorescence emission properties



**Figure S1.** (A) UV-Vis spectra of I, II, and III in toluene; fluorescence emission spectra of I, II, and III in (B) toluene and (C) solid state.

**Table S1.** Optical properties of I, II, and III.

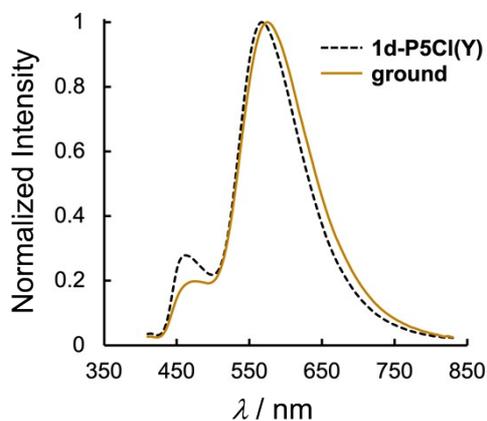
	in toluene				solid	
	$\lambda_{\text{max}}^{\text{abs}}/\text{nm}$ ( $\epsilon/\text{mol}^{-1} \text{ dm}^3 \text{ cm}^{-1}$ )	$\lambda^{\text{em}}/\text{nm}$	$\Delta/\text{cm}^{-1}$ (nm)	$\Phi_{\text{F}}$	$\lambda^{\text{em}}/\text{nm}$	$\Phi_{\text{F}}$
I	422 (20700)	486	3120 (64)	0.88	529	0.34
II	422 (2800)	590	6750 (168)	0.02	556	0.07
III	430 (18300)	507	3530 (77)	0.73	542	0.23



**Figure S2.** (A) UV-Vis spectra of **1d-P5F** and **1d-P5Br** in toluene; (B) fluorescence emission spectra of **1d-P5F** and **1d-P5Br** in toluene.

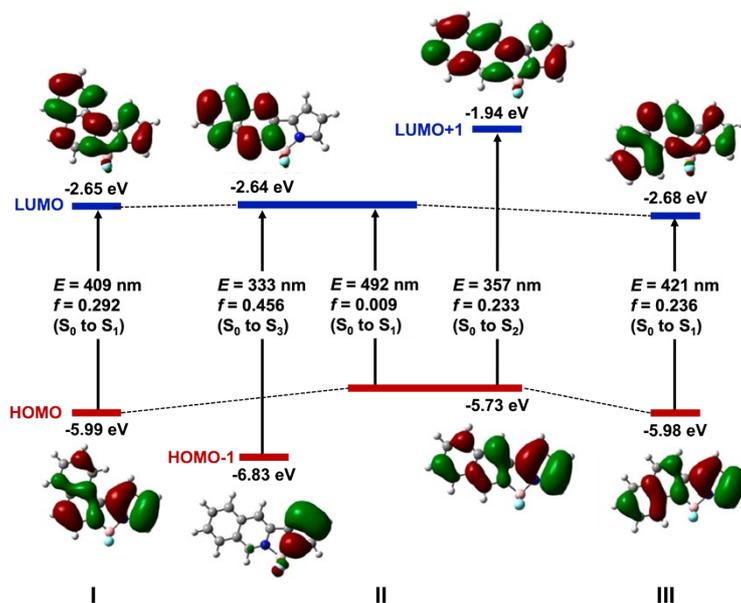
**Table S2.** Optical properties of **1d-P5F** and **1d-P5Br** in toluene.

	$\lambda_{\max}^{\text{abs}}/\text{nm}$ ( $\epsilon/\text{mol}^{-1} \text{ dm}^3 \text{ cm}^{-1}$ )	$\lambda^{\text{em}}/\text{nm}$	$\Delta/\text{cm}^{-1}$ (nm)	$\Phi_{\text{F}}$
<b>1-P5F</b>	375 (17600)	454	4640 (79)	0.38
<b>1-P5Br</b>	381 (18600)	461	4550 (80)	0.12

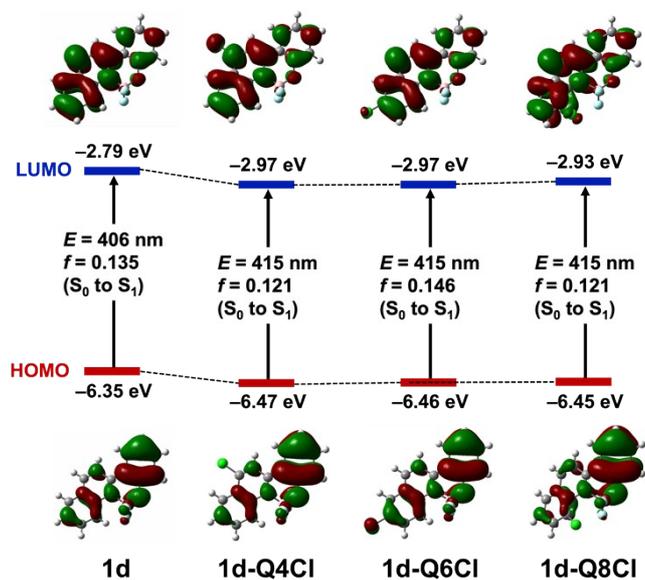


**Figure S3.** Fluorescence emission spectra of **1d-P5Cl(Y)** before and after grinding.

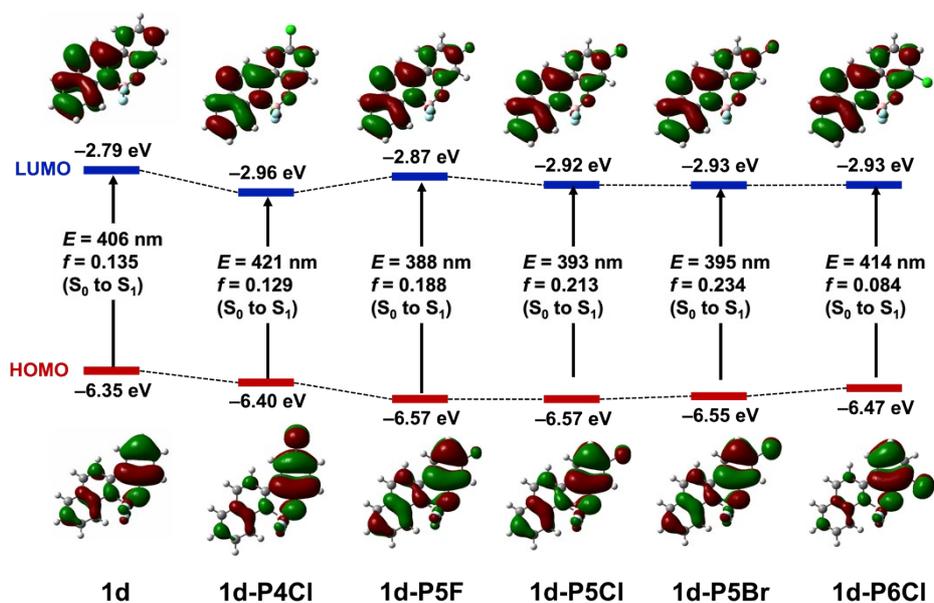
## Calculation studies



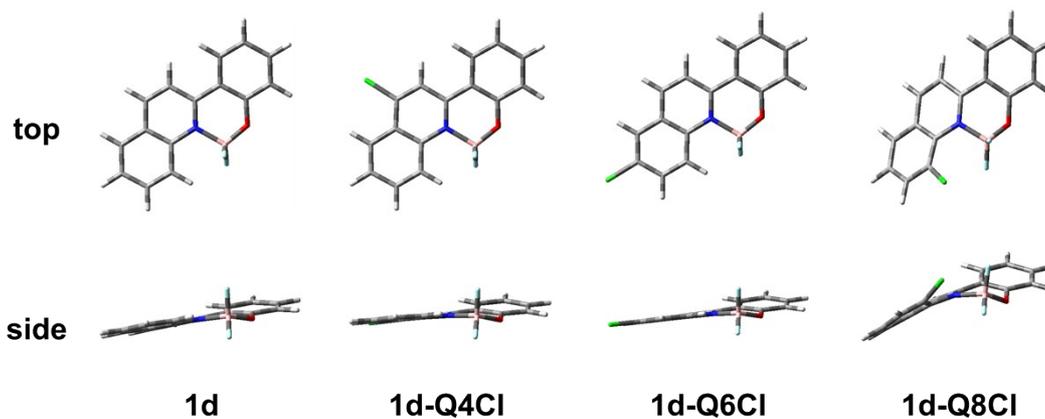
**Figure S4.** Molecular orbital energy diagrams of **I**, **II**, and **III** by TD-DFT calculations.



**Figure S5.** Molecular orbital energy diagrams of **1d**, **1d-Q4Cl**, **1d-Q6Cl**, and **1d-Q8Cl** by TD-DFT calculations.

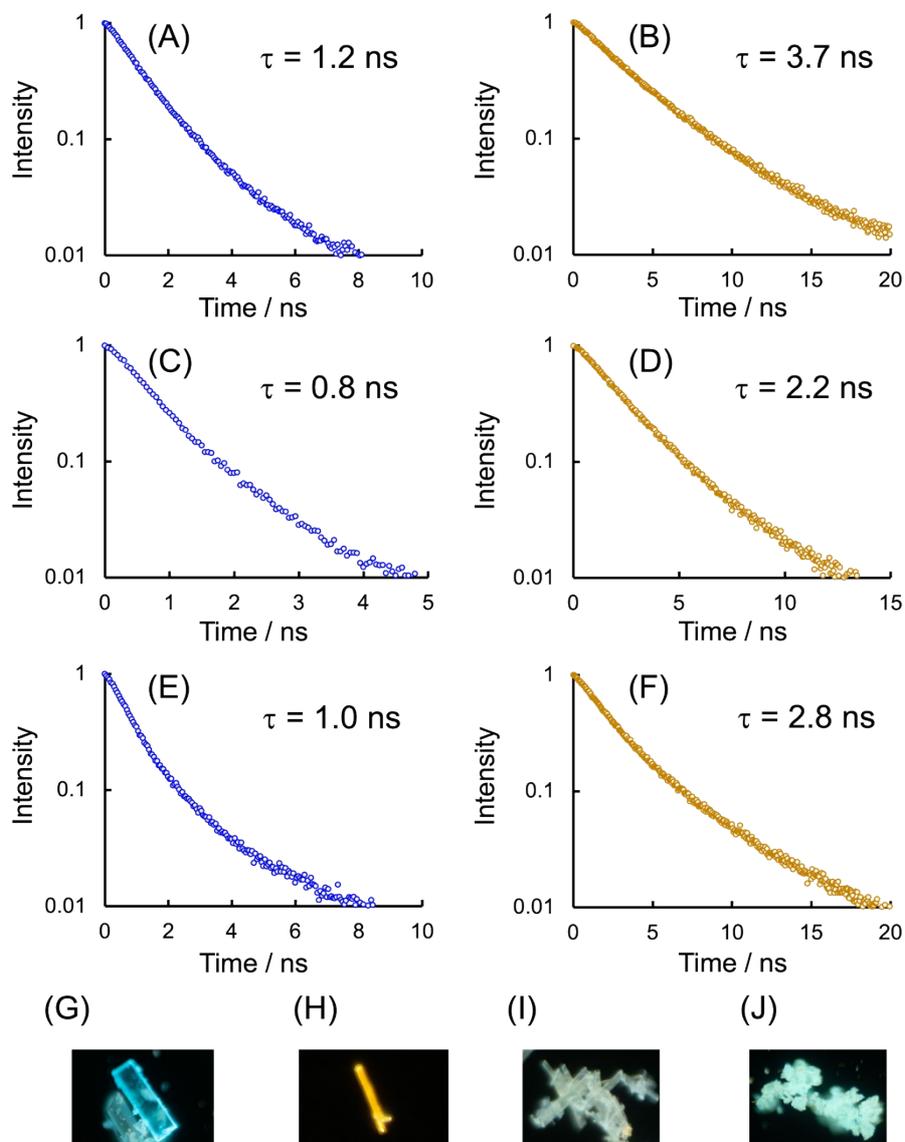


**Figure S6.** Molecular orbital energy diagrams of **1d**, **1d-P4Cl**, **1d-P5F**, **1d-P5Cl**, **1d-P5Br**, and **1d-P6Cl** by TD-DFT calculations.



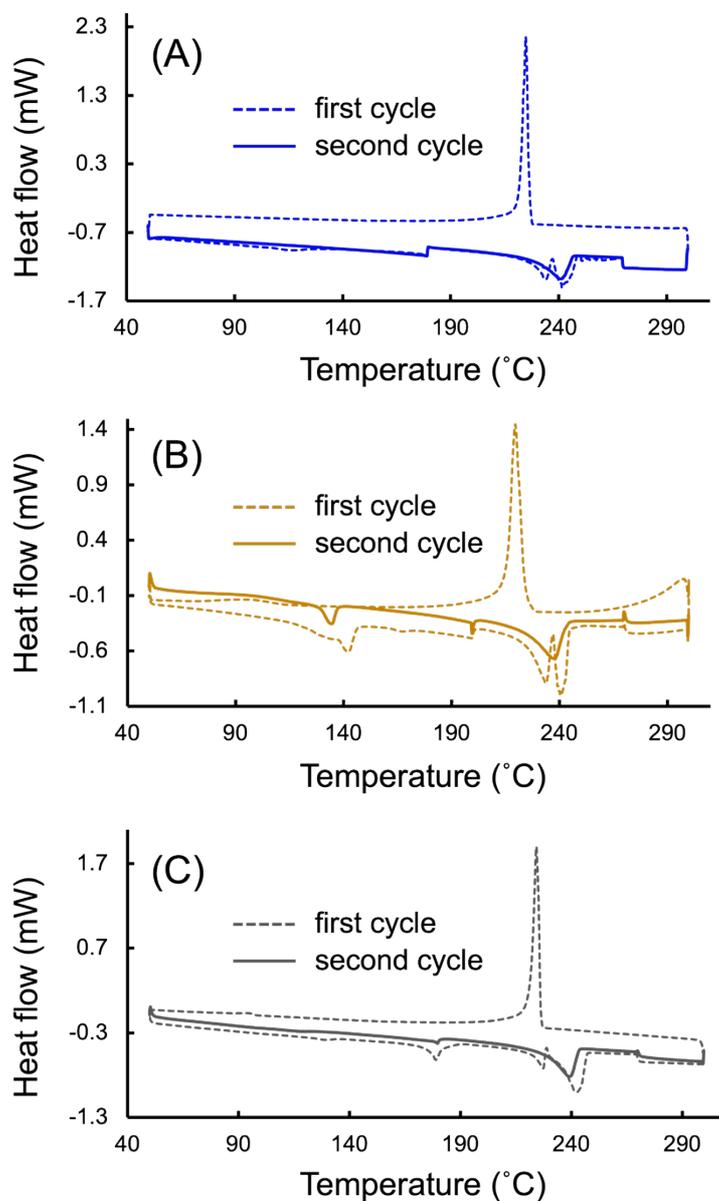
**Figure S7.** Optimized structure of **1d**, **1d-Q4Cl**, **1d-Q6Cl**, and **1d-Q8Cl** by DFT calculation.

## Fluorescence lifetime



**Figure S8.** Time domain data and estimated  $\tau$ -values obtained from (A) **1d-P5CI(LB)** ( $\lambda^{\text{em}} = 450$  nm), (B) **1d-P5CI(Y)** ( $\lambda^{\text{em}} = 570$  nm), (C) **1d-P5CI(b)** ( $\lambda^{\text{em}} = 450$  nm), (D) **1d-P5CI(b)** ( $\lambda^{\text{em}} = 570$  nm), (E) **1d-P5CI(G1)** ( $\lambda^{\text{em}} = 450$  nm), and (F) **1d-P5CI(G1)** ( $\lambda^{\text{em}} = 570$  nm) upon excitation with a pulsed 405-nm laser. Fluorescence microscope images of (G) **1d-P5CI(LB)**, (H) **1d-P5CI(Y)**, (I) **1d-P5CI(b)**, and (J) **1d-P5CI(G1)** upon excitation by mercury lamp with a  $400 \pm 25$  nm bandpass filter.

## Differential scanning calorimetry



**Figure S9.** DSC traces of (A) **1d-P5Cl(LB)**, (B) **1d-P5Cl(Y)**, and (C) **1d-P5Cl(G2)** in N<sub>2</sub> flow. (A) and (C) Heating rates were 5 °C/min (180 to 270 °C) and 10 °C/min (other ranges). (B) Heating rates were 5 °C/min (200 to 270 °C) and 10 °C/min (other ranges)

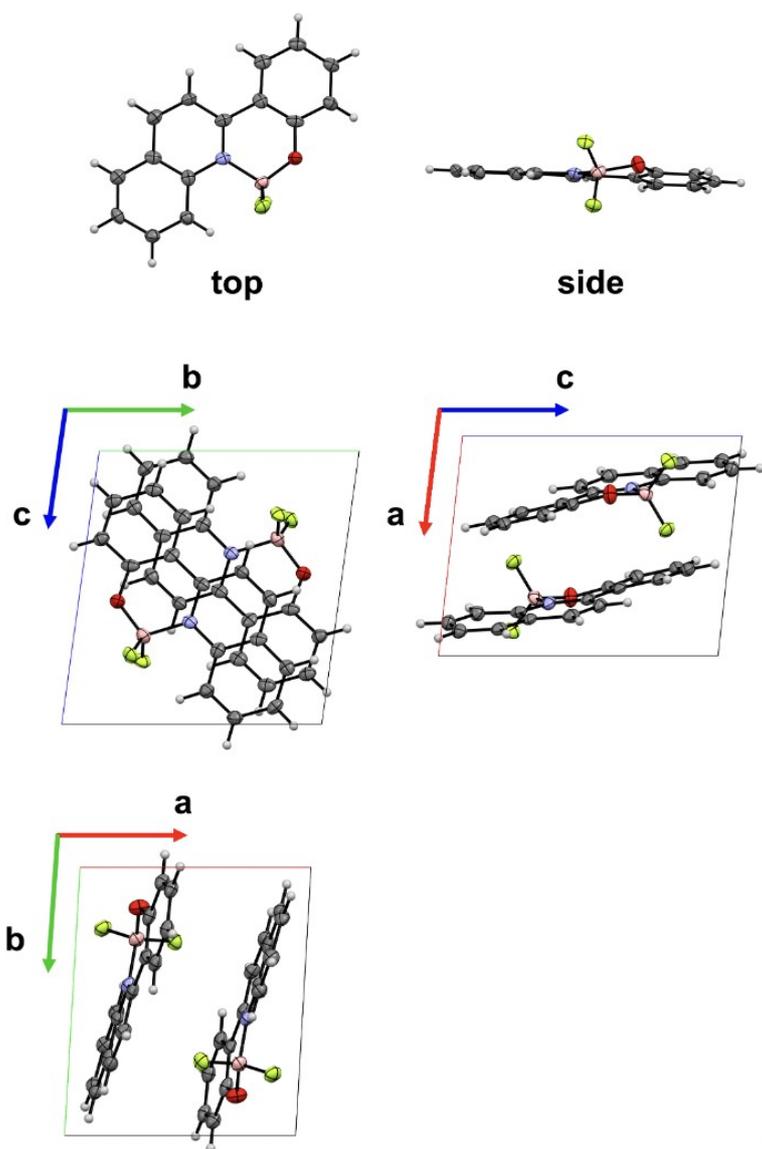
## X-ray crystal structure analysis

**Table S3.** Crystallographic data of **1d**.

Crystal data		Data collection	
Empirical formula	C <sub>15</sub> H <sub>10</sub> BF <sub>2</sub> NO	Temperature, K	100
Formula weight	269.05	2 $\theta$ <sub>max</sub> , deg	153.1
Crystal Dimension, mm <sup>3</sup>	0.11×0.04×0.03	T <sub>min</sub> /T <sub>max</sub>	0.813/1.000
Crystal system	triclinic	Refinement	
Space group	P –1	No. of observed data	2227
a, Å	7.3067(2)	No. of parameters	181
b, Å	8.5961(6)	R1 <sup>a</sup> , wR2 <sup>b</sup>	0.0718, 0.2178
c, Å	9.2256(5)	Goodness of fit indicator	1.098
$\alpha$ , deg	97.453(5)		
$\beta$ , deg	95.821(3)		
$\gamma$ , deg	92.451(4)		
Volume, Å <sup>3</sup>	570.67(5)		
D <sub>calc.</sub> , g cm <sup>-3</sup>	1.566		
Z	2		
F(000)	276.0		

<sup>a</sup> R1 =  $\sum | |F_o| - |F_c| | / \sum |F_o|$ , <sup>b</sup> wR2 =  $[\sum w (F_o^2 - F_c^2)^2 / \sum w (F_o^2)^2]^{1/2}$ , w =  $[\delta^2(F_o^2)]^{-1}$

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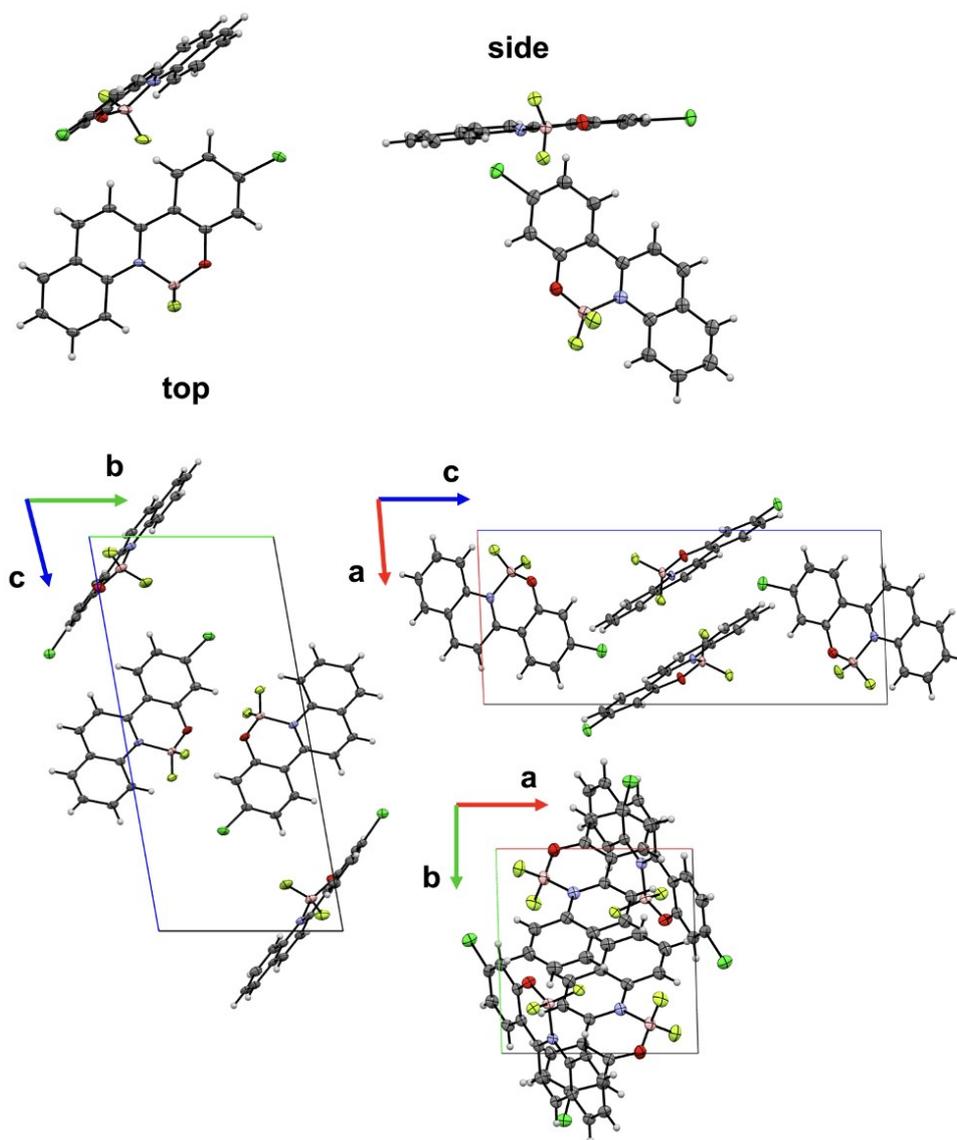
**Figure S10.** ORTEP drawing of **1d**.

**Table S4.** Crystallographic data of **1d-P5Cl(LB1)**.

Crystal data		Data collection	
Empirical formula	C <sub>15</sub> H <sub>9</sub> BClF <sub>2</sub> NO	Temperature, K	100
Formula weight	303.49	2 $\theta$ <sub>max</sub> , deg	52.7
Crystal Dimension, mm <sup>3</sup>	0.34×0.22×0.11	T <sub>min</sub> /T <sub>max</sub>	0.986/0.995
Crystal system	triclinic	Refinement	
Space group	P –1	No. of observed data	5186
a, Å	8.0402(4)	No. of parameters	379
b, Å	8.5609(2)	R1 <sup>a</sup> , wR2 <sup>b</sup>	0.0581, 0.1719
c, Å	18.7514(10)	Goodness of fit indicator	1.075
$\alpha$ , deg	79.984(4)		
$\beta$ , deg	87.560(4)		
$\gamma$ , deg	88.010(4)		
Volume, Å <sup>3</sup>	1269.37(11)		
D <sub>calc</sub> , g cm <sup>-3</sup>	1.588		
Z	4		
F(000)	616.0		

<sup>a</sup> R1 =  $\sum | |Fo| - |Fc| | / \sum | |Fo|$ , <sup>b</sup> wR2 =  $[\sum w (Fo^2 - Fc^2)^2 / \sum w (Fo^2)^2]^{1/2}$ , w =  $[\delta^2(Fo^2)]^{-1}$

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**Figure S11.** ORTEP drawing of **1d-P5Cl(LB1)**.

**Table S5.** Crystallographic data of **1d-P5Cl(LB2)**.

Crystal data		Data collection	
Empirical formula	C <sub>15</sub> H <sub>9</sub> BClF <sub>2</sub> NO	Temperature, K	100
Formula weight	303.49	2 $\theta$ <sub>max</sub> , deg	153.8
Crystal Dimension, mm <sup>3</sup>	0.22×0.06×0.04	T <sub>min</sub> /T <sub>max</sub>	0.798/1.000
Crystal system	monoclinic	Refinement	
Space group	C 1 2/c 1	No. of observed data	1239
a, Å	15.7169(13)	No. of parameters	186
b, Å	7.4273(4)	R1 <sup>a</sup> , wR2 <sup>b</sup>	0.0540, 0.1282
c, Å	10.7772(10)	Goodness of fit indicator	1.116
$\alpha$ , deg	90		
$\beta$ , deg	94.246(8)		
$\gamma$ , deg	90		
Volume, Å <sup>3</sup>	1254.61(17)		
D <sub>calc</sub> , g cm <sup>-3</sup>	1.607		
Z	4		
F(000)	616.0		

<sup>a</sup> R1 =  $\sum ||F_o| - |F_c|| / \sum |F_o|$ , <sup>b</sup> wR2 =  $[\sum w (F_o^2 - F_c^2)^2 / \sum w (F_o^2)^2]^{1/2}$ , w =  $[\delta^2(F_o^2)]^{-1}$

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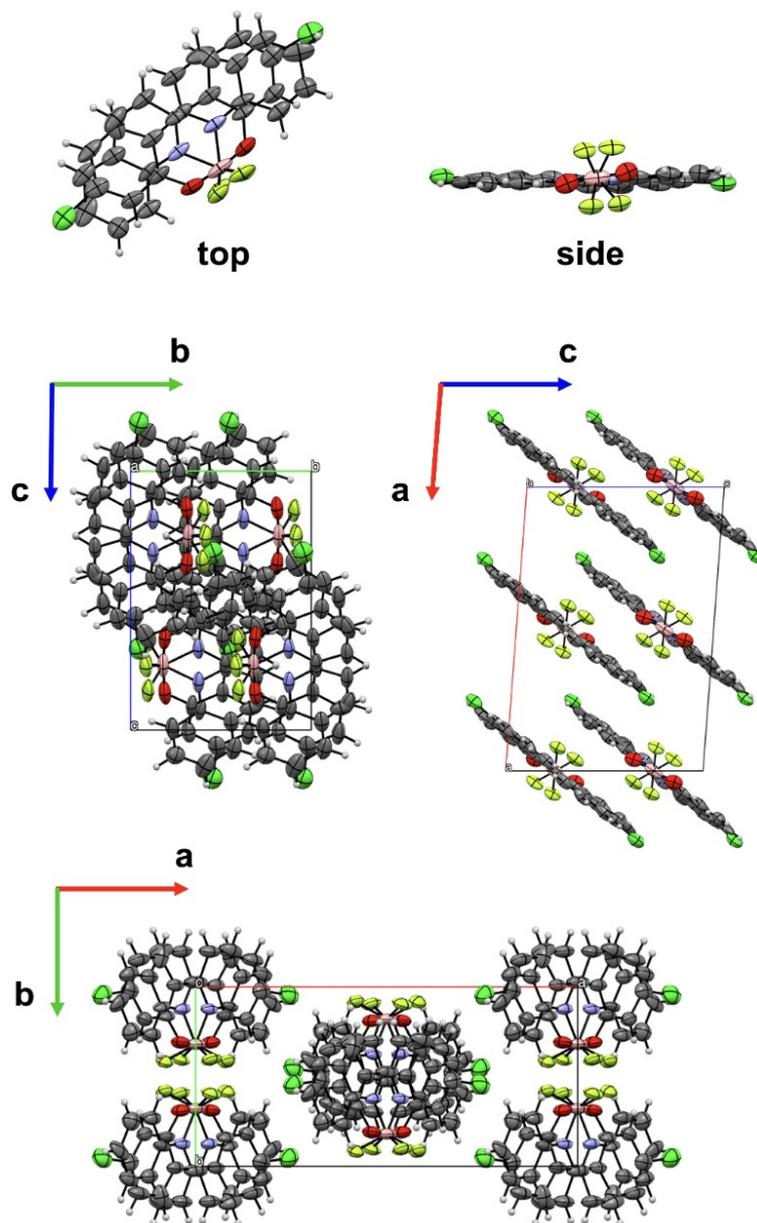


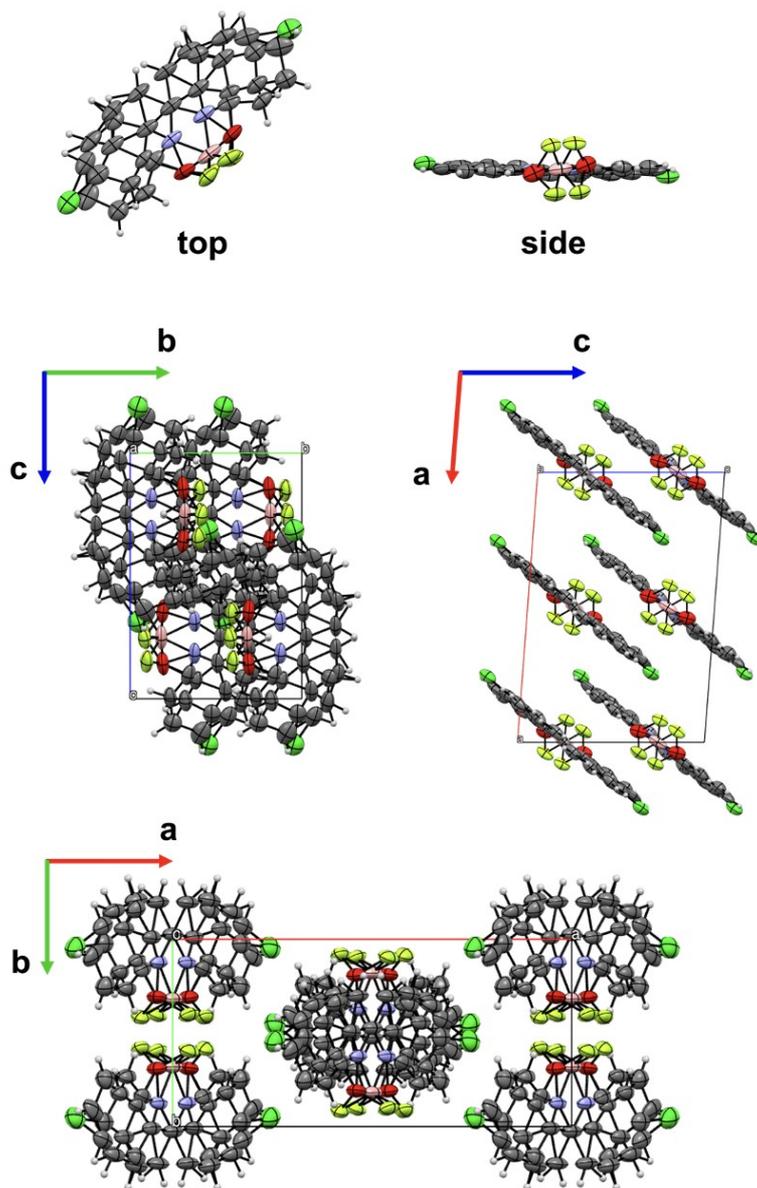
Figure S12. ORTEP drawing of 1d-P5Cl(LB2).

**Table S6.** Crystallographic data of **1d-P5Cl(Y)**.

Crystal data		Data collection	
Empirical formula	C <sub>15</sub> H <sub>9</sub> BClF <sub>2</sub> NO	Temperature, K	100
Formula weight	303.49	2 $\theta$ <sub>max</sub> , deg	153.1
Crystal Dimension, mm <sup>3</sup>	0.38×0.11×0.05	T <sub>min</sub> /T <sub>max</sub>	0.694/1.000
Crystal system	monoclinic	Refinement	
Space group	C 1 2/c 1	No. of observed data	1228
a, Å	15.7404(11)	No. of parameters	182
b, Å	7.4307(6)	R1 <sup>a</sup> , wR2 <sup>b</sup>	0.0501, 0.1311
c, Å	10.7770(9)	Goodness of fit indicator	1.061
$\alpha$ , deg	90		
$\beta$ , deg	94.249(7)		
$\gamma$ , deg	90		
Volume, Å <sup>3</sup>	1257.04(17)		
D <sub>calc</sub> , g cm <sup>-3</sup>	1.604		
Z	4		
F(000)	616.0		

<sup>a</sup> R1 =  $\sum | |Fo| - |Fc| | / \sum | |Fo|$ , <sup>b</sup> wR2 =  $[\sum w (Fo^2 - Fc^2)^2 / \sum w (Fo^2)^2]^{1/2}$ , w =  $[\delta^2(Fo^2)]^{-1}$

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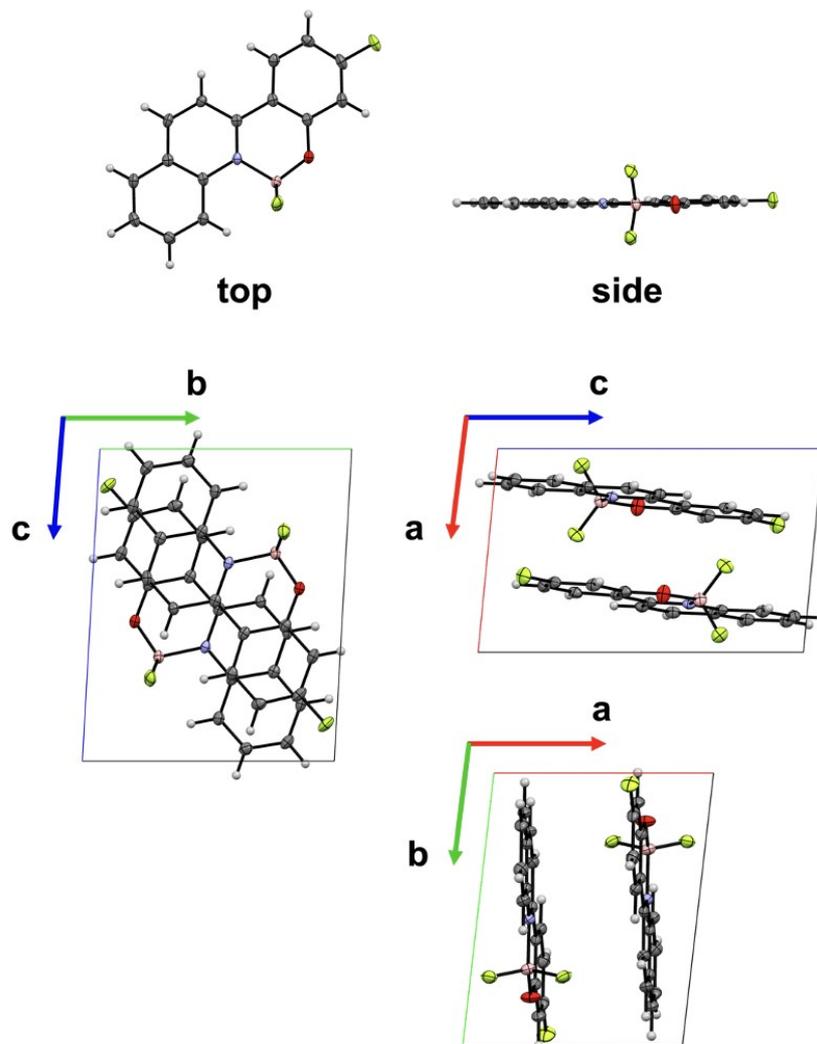
**Figure S13.** ORTEP drawing of **1d-P5Cl(Y)**.

**Table S7.** Crystallographic data of **1d-P5F(LB)**.

Crystal data		Data collection	
Empirical formula	C <sub>15</sub> H <sub>9</sub> BF <sub>3</sub> NO	Temperature, K	100
Formula weight	287.04	2 $\theta$ <sub>max</sub> , deg	52.7
Crystal Dimension, mm <sup>3</sup>	0.53×0.39×0.16	T <sub>min</sub> /T <sub>max</sub>	0.957/0.983
Crystal system	triclinic	Refinement	
Space group	P –1	No. of observed data	2466
a, Å	6.7696(4)	No. of parameters	190
b, Å	8.4846(6)	R1 <sup>a</sup> , wR2 <sup>b</sup>	0.0404, 0.1228
c, Å	10.5970(8)	Goodness of fit indicator	1.022
$\alpha$ , deg	92.590(6)		
$\beta$ , deg	95.124(6)		
$\gamma$ , deg	96.214(5)		
Volume, Å <sup>3</sup>	601.74(7)		
D <sub>calc</sub> , g cm <sup>-3</sup>	1.584		
Z	2		
F(000)	292.0		

<sup>a</sup> R1 =  $\sum | |Fo| - |Fc| | / \sum | |Fo|$ , <sup>b</sup> wR2 =  $[\sum w (Fo^2 - Fc^2)^2 / \sum w (Fo^2)^2]^{1/2}$ , w =  $[\delta^2(Fo^2)]^{-1}$

CCDC # 2498039



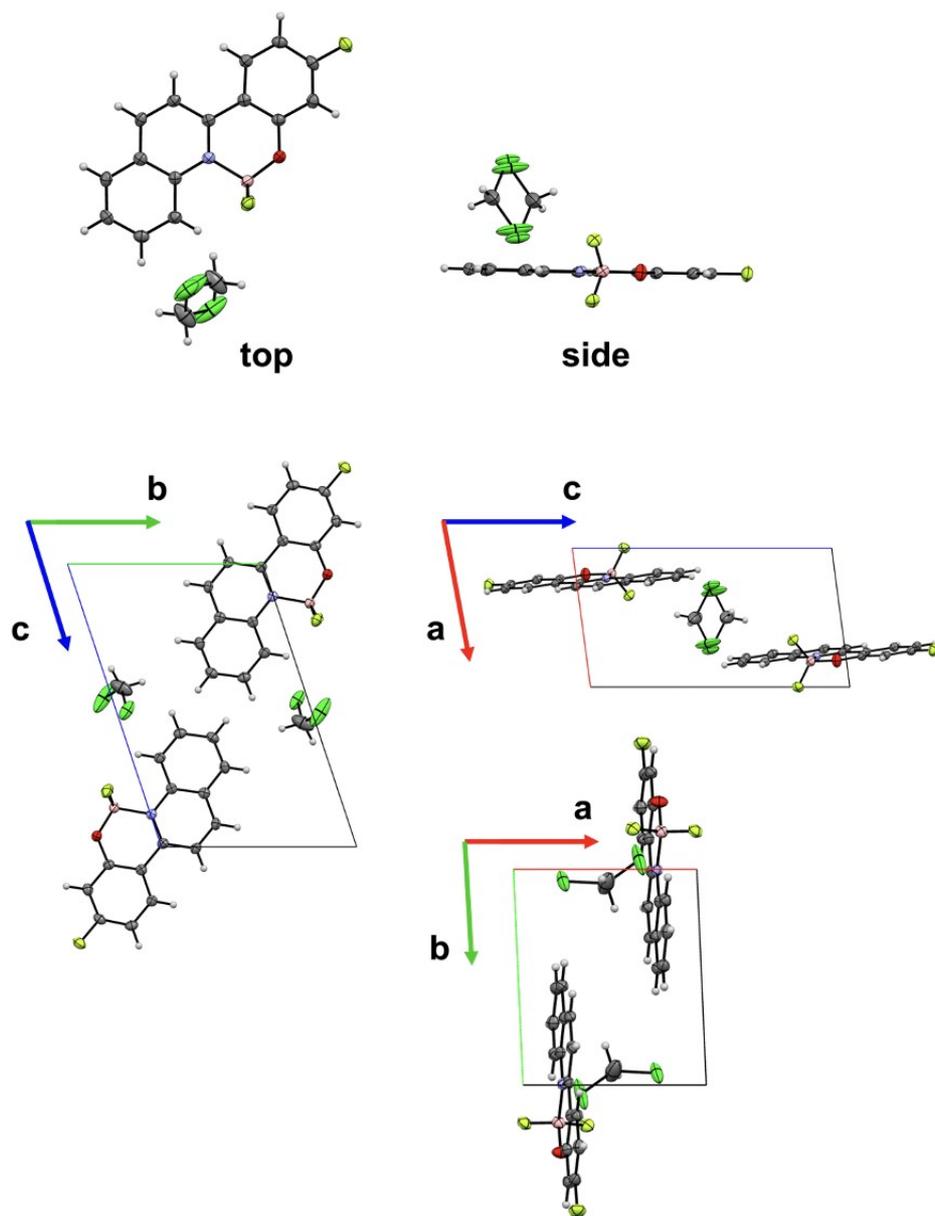
**Figure S14.** ORTEP drawing of 1d-P5F(LB).

**Table S8.** Crystallographic data of **1d-P5F(Y)**.

Crystal data		Data collection	
Empirical formula	C <sub>15.5</sub> H <sub>9</sub> BClF <sub>3</sub> NO	Temperature, K	293
Formula weight	328.50	2 $\theta_{\max}$ , deg	153.7
Crystal Dimension, mm <sup>3</sup>	0.21×0.07×0.03	T <sub>min</sub> /T <sub>max</sub>	0.696/1.000
Crystal system	triclinic	Refinement	
Space group	P –1	No. of observed data	2678
a, Å	6.7344(2)	No. of parameters	217
b, Å	8.3673(3)	R1 <sup>a</sup> , wR2 <sup>b</sup>	0.0514, 0.1469
c, Å	12.9637(5)	Goodness of fit indicator	1.041
$\alpha$ , deg	71.272(3)		
$\beta$ , deg	81.388(3)		
$\gamma$ , deg	84.912(3)		
Volume, Å <sup>3</sup>	683.36(4)		
D <sub>calc</sub> , g cm <sup>-3</sup>	1.596		
Z	2		
F(000)	332.0		

<sup>a</sup> R1 =  $\sum ||F_o| - |F_c|| / \sum |F_o|$ , <sup>b</sup> wR2 =  $[\sum w (F_o^2 - F_c^2)^2 / \sum w (F_o^2)^2]^{1/2}$ , w =  $[\delta^2(F_o^2)]^{-1}$

CCDC # 2498040



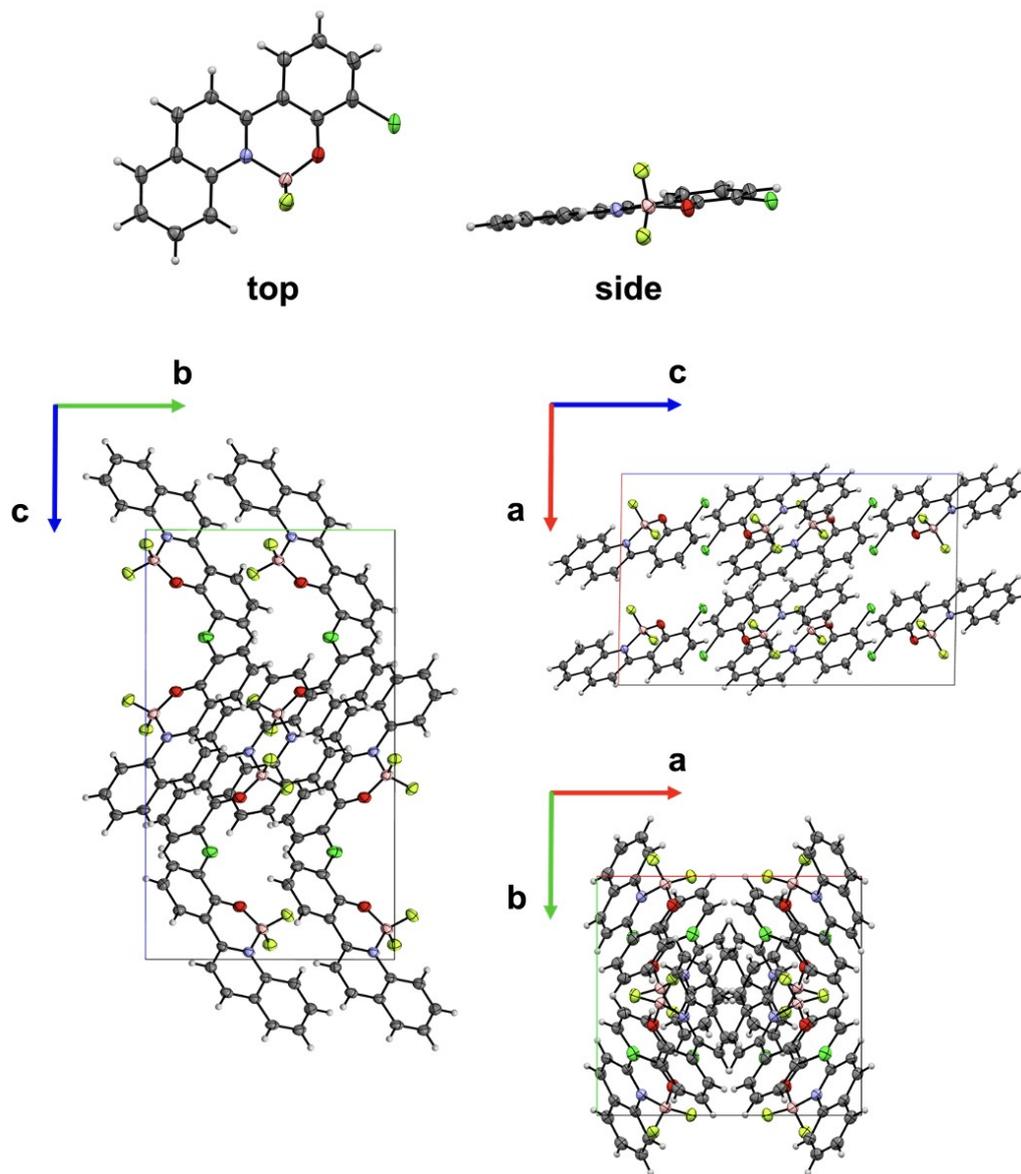
**Figure S15.** ORTEP drawing of 1d-P5F(Y).

**Table S9.** Crystallographic data of **1d-P6Cl**.

Crystal data		Data collection	
Empirical formula	C <sub>15</sub> H <sub>9</sub> BClF <sub>2</sub> NO	Temperature, K	100
Formula weight	303.49	2 $\theta$ <sub>max</sub> , deg	153.2
Crystal Dimension, mm <sup>3</sup>	0.09×0.08×0.07	T <sub>min</sub> /T <sub>max</sub>	0.491/1.000
Crystal system	monoclinic	Refinement	
Space group	C 1 2/c 1	No. of observed data	2470
a, Å	12.0315(4)	No. of parameters	190
b, Å	10.9383(4)	R1 <sup>a</sup> , wR2 <sup>b</sup>	0.0548, 0.1548
c, Å	18.9864(6)	Goodness of fit indicator	1.072
$\alpha$ , deg	90		
$\beta$ , deg	90.954(3)		
$\gamma$ , deg	90		
Volume, Å <sup>3</sup>	2498.34(15)		
D <sub>calc</sub> , g cm <sup>-3</sup>	1.614		
Z	8		
F(000)	1232.0		

<sup>a</sup> R1 =  $\sum ||F_o| - |F_c|| / \sum |F_o|$ , <sup>b</sup> wR2 =  $[\sum w (F_o^2 - F_c^2)^2 / \sum w (F_o^2)^2]^{1/2}$ , w =  $[\delta^2(F_o^2)]^{-1}$

CCDC # 2498041



**Figure S16.** ORTEP drawing of **1d-P6Cl**.

## Cartesian coordinates in the structures optimized by DFT calculations

**1a** ( $S_0$ ):  $E(\text{B3LYP}) = -778.752426$  Hartree

Row	Symbol	X	Y	Z
1	C	-2.6550201	-0.0326252	-0.1126153
2	C	-3.252949	1.2129536	-0.1470694
3	C	-2.4251098	2.3429006	-0.1094809
4	C	-1.0499635	2.1850374	-0.0457045
5	C	-0.4816338	0.8963853	-0.0006871
6	N	-1.3155707	-0.1804804	-0.0359143
7	H	-2.854204	3.3397288	-0.1432487
8	H	-3.2171295	-0.9579434	-0.1453921
9	H	-4.3317385	1.2959341	-0.2048429
10	H	-0.4039385	3.0529929	-0.051827
11	C	0.9575748	0.6445397	0.0285531
12	C	1.4371149	-0.6582654	-0.268139
13	C	1.8965168	1.6700706	0.2750696
14	C	2.8202503	-0.8864379	-0.3705102
15	C	3.2598071	1.429863	0.2004702
16	H	1.5528275	2.6634717	0.5438571
17	C	3.7185838	0.1447264	-0.1372808
18	H	3.1525421	-1.8890872	-0.6170417
19	H	3.9649927	2.2288422	0.4043999
20	H	4.7853309	-0.0488882	-0.2036107
21	O	0.6031024	-1.6773635	-0.4997219
22	B	-0.7104015	-1.6836845	0.1091499
23	F	-1.5630368	-2.5401733	-0.5613219
24	F	-0.6662441	-1.9352986	1.4774884

**1b** ( $S_0$ ):  $E(\text{B3LYP}) = -932.396388$  Hartree

Row	Symbol	X	Y	Z
1	C	-0.8824568	-2.3267543	0.1463551
2	C	-2.2049806	-2.0066899	0.2363393
3	C	-2.6008606	-0.647079	0.1198825

4	C	-1.5875457	0.3538083	-0.0348737
5	C	-0.2038058	-0.0508141	0.0537215
6	N	0.0871825	-1.3667957	0.0610966
7	H	-0.5153978	-3.3446028	0.1478601
8	H	-2.9488418	-2.7880391	0.3472758
9	C	0.9351524	0.869154	0.0941104
10	C	2.1882198	0.4102205	-0.3994154
11	C	0.8665865	2.1799926	0.6187901
12	C	3.265987	1.3025799	-0.5155867
13	C	1.9551729	3.0379701	0.5554669
14	H	-0.0350104	2.5082792	1.1220602
15	C	3.147289	2.6041516	-0.0478665
16	H	4.1935561	0.9276581	-0.9345903
17	H	1.886079	4.0335769	0.9814611
18	H	3.9969194	3.2775507	-0.1151082
19	O	2.3550618	-0.8613954	-0.7765416
20	B	1.6307608	-1.8718758	-0.0263256
21	F	1.630001	-3.0768603	-0.7029956
22	F	2.0809584	-1.9944293	1.2843566
23	C	-4.3326342	1.0370654	-0.142022
24	H	-5.3820326	1.3146456	-0.1702809
25	C	-3.3397886	2.012035	-0.39111
26	H	-3.631725	3.0273714	-0.6406003
27	C	-2.0013081	1.6803678	-0.3396974
28	H	-1.261476	2.4320126	-0.5776846
29	C	-3.9686903	-0.2709772	0.0936849
30	H	-4.7233031	-1.0389194	0.2369681

**1c** (S<sub>0</sub>):  $E(\text{B3LYP}) = -932.402271$  Hartree

Row	Symbol	X	Y	Z
1	C	1.3999645	1.2832603	-0.0400397
2	C	2.4917796	0.3978743	-0.0463859
3	C	2.2040972	-1.0037521	-0.011772
4	C	0.8519282	-1.405551	0.0175511

5	C	-0.1796455	-0.4781185	0.0371025
6	N	0.139989	0.8679789	0.0056896
7	H	1.5371585	2.3588679	-0.0725794
8	H	0.6195973	-2.4633535	0.0019462
9	C	-1.6036523	-0.8260222	0.0343199
10	C	-2.5614614	0.1615972	-0.3086224
11	C	-2.0541282	-2.1356055	0.3015987
12	C	-3.9148229	-0.1910408	-0.4364505
13	C	-3.3963578	-2.4722342	0.1972887
14	H	-1.3440793	-2.8961385	0.6101643
15	C	-4.3269619	-1.4932436	-0.1871408
16	H	-4.6174573	0.5862021	-0.7173053
17	H	-3.7216522	-3.4839074	0.4169103
18	H	-5.3787409	-1.7495232	-0.2759159
19	O	-2.2047198	1.4308393	-0.5589841
20	B	-1.0492429	1.9809411	0.1092096
21	F	-0.5981375	3.1218629	-0.5293708
22	F	-1.2500387	2.1759626	1.4732316
23	C	4.5885641	-1.4560544	-0.0628319
24	H	5.4136066	-2.1622132	-0.0701304
25	C	4.8686032	-0.0619684	-0.0940584
26	H	5.8993026	0.2764838	-0.1244973
27	C	3.2930795	-1.9206788	-0.0241904
28	H	3.0879021	-2.9869617	-0.0010703
29	C	3.8394437	0.8506731	-0.0871055
30	H	4.0394178	1.9180282	-0.1118515

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**1d** ( $S_0$ ):  $E(\text{B3LYP}) = -932.400342$  Hartree

Row	Symbol	X	Y	Z
1	C	-1.798002	0.0045265	0.0027082
2	C	-2.3519324	1.3156183	-0.0876191
3	C	-1.456712	2.4108318	-0.188494
4	C	-0.1078792	2.2022897	-0.1566862
5	C	0.4220769	0.8822032	-0.0531378

6	N	-0.41679	-0.1766242	-0.0308361
7	H	-1.8563346	3.4169672	-0.2832192
8	H	0.5718523	3.0384852	-0.2364172
9	C	1.8652455	0.6646013	0.0123951
10	C	2.3814345	-0.642433	-0.1645851
11	C	2.78071	1.720957	0.2331503
12	C	3.7719478	-0.8592684	-0.1688592
13	C	4.147942	1.4984463	0.2505461
14	H	2.4180058	2.7257821	0.4166289
15	C	4.6424846	0.1989903	0.0372052
16	H	4.1270537	-1.8720493	-0.3255585
17	H	4.8297144	2.3225112	0.4328842
18	H	5.7137296	0.0193614	0.0437616
19	O	1.5801869	-1.6787207	-0.3768651
20	B	0.1761864	-1.7011194	-0.028426
21	F	-0.5031281	-2.4328083	-0.991932
22	F	-0.0379207	-2.1977768	1.2557414
23	C	-4.5980718	0.412383	0.0721438
24	H	-5.6744227	0.5501856	0.0960892
25	C	-4.0465444	-0.8825867	0.1900402
26	H	-4.7057601	-1.7364003	0.3131985
27	C	-3.7573466	1.4956735	-0.0621918
28	H	-4.1534925	2.5041807	-0.1416853
29	C	-2.6815213	-1.0935184	0.155604
30	H	-2.2887922	-2.0943124	0.249619

**1d-Q4CI** ( $S_0$ ):  $E(\text{B3LYP}) = -1391.991591$  Hartree

Row	Symbol	X	Y	Z
1	C	-1.4571767	-0.7439931	0.0348531
2	C	-2.2961857	0.4138354	-0.005345
3	C	-1.6377148	1.6752815	-0.0749036
4	C	-0.2751792	1.7614849	-0.0566999
5	C	0.5211542	0.5839548	-0.0029276
6	N	-0.0708624	-0.6288537	-0.0159669

7	H	0.201016	2.7286116	-0.1131869
8	C	1.9768724	0.6845899	0.0483973
9	C	2.7602548	-0.4728039	-0.1818401
10	C	2.6443004	1.9056334	0.3067695
11	C	4.1645709	-0.3833346	-0.1993641
12	C	4.0270446	1.9829995	0.3108558
13	H	2.0759481	2.8008988	0.5316527
14	C	4.7878369	0.8297646	0.0450855
15	H	4.7283096	-1.2885209	-0.3971555
16	H	4.517042	2.9273977	0.5229217
17	H	5.8725353	0.8861252	0.0409908
18	O	2.1987688	-1.6484997	-0.4325653
19	B	0.8385972	-1.9906471	-0.0796437
20	F	0.3197058	-2.8109544	-1.0700008
21	F	0.7539192	-2.5712895	1.1833643
22	C	-4.2739711	-0.9831971	0.1428809
23	H	-5.3534523	-1.0884018	0.180874
24	C	-3.4469419	-2.1236945	0.2111409
25	H	-3.8933615	-3.1081909	0.3106399
26	C	-3.7040602	0.2671578	0.0392368
27	H	-4.3236736	1.1548122	-0.0011044
28	C	-2.0717472	-2.0155689	0.1572382
29	H	-1.4596832	-2.902348	0.2136792
30	Cl	-2.566397	3.1517859	-0.1759612

**1d-Q6Cl** ( $S_0$ ):  $E(\text{B3LYP}) = -1391.992891$  Hartree

Row	Symbol	X	Y	Z
1	C	1.1310176	0.1103083	-0.017914
2	C	1.7443851	-1.1723428	-0.1090792
3	C	0.899636	-2.3092536	-0.2037357
4	C	-0.4561378	-2.1602241	-0.1649444
5	C	-1.0463461	-0.8651504	-0.0587075
6	N	-0.2550971	0.229841	-0.0412912
7	H	-1.0972846	-3.0267435	-0.2402545

8	C	-2.4962902	-0.7124863	0.0147436
9	C	-3.0711658	0.5713317	-0.1537525
10	C	-3.3629697	-1.8098319	0.2350761
11	C	-4.4697347	0.7262951	-0.1497647
12	C	-4.7382345	-1.6479582	0.2605506
13	H	-2.9556007	-2.7986118	0.4117132
14	C	-5.291044	-0.370562	0.0559721
15	H	-4.8703605	1.7228961	-0.3000514
16	H	-5.3819541	-2.5021343	0.442314
17	H	-6.3691144	-0.2388031	0.0690079
18	O	-2.3180969	1.6433797	-0.3661694
19	B	-0.91536	1.7280774	-0.0282179
20	F	-0.2736366	2.4910046	-0.9930636
21	F	-0.7102792	2.2262355	1.2562831
22	C	3.933318	-0.1679606	0.0334568
23	C	3.339393	1.1063299	0.1531658
24	H	3.9692326	1.9812423	0.2693863
25	C	3.1548017	-1.295607	-0.0930883
26	H	3.6060257	-2.2788958	-0.17217
27	C	1.966847	1.2468521	0.1269434
28	H	1.5333772	2.230784	0.2216251
29	H	1.3434902	-3.2962922	-0.2995752
30	Cl	5.6799901	-0.3025503	0.0597046

**1d-Q8CI** ( $S_0$ ):  $E(\text{B3LYP}) = -1391.968431$  Hartree

Row	Symbol	X	Y	Z
1	C	-1.5446544	0.4166505	0.0006191
2	C	-1.9006417	1.7905024	-0.2028575
3	C	-0.8728442	2.7669752	-0.1186819
4	C	0.4133213	2.3941116	0.1355393
5	C	0.7538617	1.0115156	0.159357
6	N	-0.1968638	0.0599889	0.0357666
7	H	-1.1329311	3.8141287	-0.2457445
8	H	1.2024899	3.1299518	0.2103583

9	C	2.1650302	0.6303927	0.1908912
10	C	2.5555873	-0.5452797	-0.4888179
11	C	3.1577421	1.4418689	0.7796159
12	C	3.9162734	-0.8619536	-0.6239206
13	C	4.499674	1.1022519	0.6817965
14	H	2.8712868	2.3254364	1.3417319
15	C	4.8751856	-0.046157	-0.037313
16	H	4.1844275	-1.7582653	-1.1726801
17	H	5.2531719	1.720151	1.159046
18	H	5.925906	-0.307138	-0.125505
19	O	1.6250786	-1.3125207	-1.0584586
20	B	0.3573502	-1.4846333	-0.375917
21	F	-0.5515813	-2.0059346	-1.2647914
22	F	0.5179316	-2.1824653	0.8063854
23	C	-4.2485032	1.2427282	-0.3868192
24	H	-5.2813963	1.5228808	-0.5654293
25	C	-3.9364617	-0.0817675	-0.0356531
26	H	-4.7319443	-0.8049134	0.1053498
27	C	-3.2416941	2.1808998	-0.4236714
28	H	-3.4558132	3.2301762	-0.6029153
29	C	-2.63165	-0.4937721	0.1960191
30	Cl	-2.45312	-2.0804236	0.8918652

**1d-P4Cl** ( $S_0$ ):  $E(\text{B3LYP}) = -1391.992768$  Hartree

Row	Symbol	X	Y	Z
1	C	2.3550009	-0.2010497	0.0131541
2	C	2.6277743	-1.5950276	-0.1199387
3	C	1.5297265	-2.4753617	-0.2885393
4	C	0.2521609	-1.9921364	-0.2788705
5	C	0.0062085	-0.5964498	-0.1319344
6	N	1.0431036	0.2642803	-0.0452021
7	H	1.7149257	-3.5384073	-0.4165856
8	H	-0.5823814	-2.6660239	-0.410203
9	C	-1.3626555	-0.0823308	-0.0898347

10	C	-1.5899508	1.3074252	-0.2263184
11	C	-2.4770876	-0.9381533	0.0678088
12	C	-2.9064747	1.8047537	-0.2544848
13	C	-3.7611824	-0.4249616	0.0586857
14	H	-2.3466894	-2.0016622	0.2203028
15	C	-3.9867799	0.9500462	-0.1122702
16	H	-3.0458855	2.8729388	-0.3791887
17	H	-5.0004042	1.3357258	-0.1221248
18	O	-0.5878013	2.1618602	-0.3781194
19	B	0.7797256	1.879515	0.0059059
20	F	1.6252146	2.485737	-0.9102396
21	F	1.047923	2.2735648	1.3139578
22	C	5.0056357	-1.1853411	0.1311572
23	H	6.0288449	-1.5447101	0.174676
24	C	4.7307517	0.1910734	0.2915203
25	H	5.5482872	0.8835182	0.4669735
26	C	3.9641795	-2.0644621	-0.0692621
27	H	4.1455082	-3.1295851	-0.1823517
28	C	3.4411334	0.6829251	0.2339458
29	H	3.2616961	1.7393675	0.3618233
30	Cl	-5.1323958	-1.5066466	0.2715377

**1d-P5F** ( $S_0$ ):  $E(\text{B3LYP}) = -1031.641158$  Hartree

Row	Symbol	X	Y	Z
1	C	-2.1249873	0.0035168	0.0032209
2	C	-2.6798045	1.3143338	-0.0843004
3	C	-1.7854665	2.4101605	-0.1855953
4	C	-0.436357	2.2029218	-0.1570824
5	C	0.0949059	0.8831732	-0.0558413
6	N	-0.7432646	-0.1763661	-0.032695
7	H	-2.1857953	3.4161428	-0.2784375
8	H	0.2412269	3.0407512	-0.2383666
9	C	1.5371652	0.6661304	0.0069288
10	C	2.055043	-0.6434594	-0.1686984

11	C	2.4528744	1.7216127	0.2234215
12	C	3.4433929	-0.8665441	-0.175252
13	C	3.8216829	1.5110919	0.238917
14	H	2.0926999	2.7270725	0.4050403
15	C	4.284038	0.2078662	0.0271167
16	H	3.8274619	-1.8682041	-0.3249229
17	H	4.5245724	2.3165346	0.414829
18	O	1.2563049	-1.6777749	-0.3771864
19	B	-0.1518823	-1.6993245	-0.0294427
20	F	-0.8258953	-2.431312	-0.9944398
21	F	-0.3613843	-2.1964683	1.2537752
22	C	-4.9250849	0.4096116	0.0771741
23	H	-6.0014509	0.5466517	0.1028385
24	C	-4.3725718	-0.8850969	0.1919572
25	H	-5.0310224	-1.7395678	0.3144131
26	C	-4.0851837	1.4936466	-0.0565348
27	H	-4.4819975	2.5020231	-0.1338935
28	C	-3.0073686	-1.0952561	0.155337
29	H	-2.6146189	-2.0962621	0.2470333
30	F	5.6213996	-0.0048877	0.0340452

**1d-P5CI** ( $S_0$ ):  $E(\text{B3LYP}) = -1391.994276$  Hartree

Row	Symbol	X	Y	Z
1	C	-2.4628862	-0.0022196	0.0040891
2	C	-3.0254782	1.3056163	-0.0831083
3	C	-2.1381191	2.4067545	-0.1849274
4	C	-0.7874829	2.2073921	-0.1577479
5	C	-0.2494501	0.8909277	-0.0576621
6	N	-1.0805809	-0.1738687	-0.0334919
7	H	-2.5446368	3.4103177	-0.2768781
8	H	-0.1142896	3.0488116	-0.2386859
9	C	1.1946313	0.6815379	0.0032248
10	C	1.7195241	-0.6226011	-0.1727825
11	C	2.1064467	1.7392303	0.2198618

12	C	3.1099843	-0.8379422	-0.1808599
13	C	3.4757533	1.5338896	0.2346723
14	H	1.7440079	2.7440049	0.4026548
15	C	3.962288	0.2335192	0.0213041
16	H	3.479943	-1.8441694	-0.3350649
17	H	4.1613433	2.3535736	0.411965
18	O	0.927765	-1.6632068	-0.3817727
19	B	-0.4788645	-1.6944567	-0.030866
20	F	-1.1512706	-2.4302323	-0.9938608
21	F	-0.683572	-2.190903	1.2532423
22	C	-5.2650354	0.3873727	0.0810056
23	H	-6.3421725	0.5179597	0.1078385
24	C	-4.704791	-0.9042136	0.1954203
25	H	-5.3582022	-1.7624039	0.3187475
26	C	-4.4320016	1.4764298	-0.053748
27	H	-4.8350323	2.4823525	-0.1306857
28	C	-3.3385566	-1.1063625	0.1572936
29	H	-2.939563	-2.1049348	0.2486639
30	Cl	5.6946761	-0.0350742	0.0261032

**1d-P5Br** ( $S_0$ ):  $E(\text{B3LYP}) = -3503.527529$  Hartree

Row	Symbol	X	Y	Z
1	C	-3.0868605	-0.0042623	0.008624
2	C	-3.6545836	1.3019843	-0.0629579
3	C	-2.7716099	2.4073084	-0.1543558
4	C	-1.4204009	2.2127796	-0.1358852
5	C	-0.8758651	0.8974268	-0.058368
6	N	-1.7034895	-0.1703131	-0.0328064
7	H	-3.1819312	3.4106585	-0.2302707
8	H	-0.7526768	3.059055	-0.2080212
9	C	0.5694426	0.6934638	-0.0121239
10	C	1.0975345	-0.6135857	-0.1521247
11	C	1.4797911	1.7596838	0.1666682
12	C	2.4890568	-0.8253841	-0.1515381

13	C	2.8493463	1.5590199	0.1805905
14	H	1.1173647	2.7697701	0.3155305
15	C	3.337636	0.2533701	0.0141253
16	H	2.8577455	-1.8361927	-0.2747534
17	H	3.5299263	2.3891049	0.3245847
18	O	0.3129391	-1.6635007	-0.3311863
19	B	-1.1059035	-1.6903465	-0.0351259
20	F	-1.7501293	-2.4052754	-1.0336906
21	F	-1.3555771	-2.2115597	1.2312194
22	C	-5.8912196	0.3736772	0.08202
23	H	-6.9689052	0.4998656	0.1072492
24	C	-5.3262251	-0.9172968	0.1776451
25	H	-5.9765952	-1.7800348	0.2841561
26	C	-5.0616	1.4672817	-0.0354203
27	H	-5.4679395	2.4727385	-0.1001512
28	C	-3.9590771	-1.1137613	0.1415398
29	H	-3.5573831	-2.1123935	0.2182544
30	Br	5.2185712	-0.0308389	0.0225655

**1d-P6CI** ( $S_0$ ):  $E(\text{B3LYP}) = -1391.989756$  Hartree

Row	Symbol	X	Y	Z
1	C	-2.2705305	-0.1288161	0.0005537
2	C	-3.035674	1.0646431	-0.157483
3	C	-2.3363732	2.2902597	-0.2920818
4	C	-0.9722926	2.3158549	-0.2247214
5	C	-0.2317775	1.1104161	-0.0516141
6	N	-0.8788267	-0.0730181	-0.0023637
7	H	-2.8972838	3.208977	-0.4410379
8	H	-0.4415802	3.2510289	-0.331261
9	C	1.2279404	1.1472556	0.0569518
10	C	1.9571363	-0.0594559	-0.0821373
11	C	1.9308072	2.3514006	0.2833556
12	C	3.3701776	-0.0134712	-0.0524567
13	C	3.3150527	2.3708386	0.3377389

14	H	1.3910881	3.2770159	0.4433783
15	C	4.03907	1.1829204	0.1569817
16	H	3.84163	3.3006397	0.5241243
17	H	5.123299	1.1850738	0.1897128
18	O	1.3491844	-1.2129515	-0.290584
19	B	-0.0320833	-1.4714585	0.0670874
20	F	-0.5637327	-2.3489989	-0.8626175
21	F	-0.1591519	-1.9356843	1.3719593
22	C	-5.0989214	-0.2005443	0.0072331
23	H	-6.1832774	-0.2473615	0.0078201
24	C	-4.3391316	-1.3769668	0.1933977
25	H	-4.8473249	-2.3241375	0.3457718
26	C	-4.4516891	1.0035641	-0.1630676
27	H	-5.0112871	1.9253945	-0.2944975
28	C	-2.9578808	-1.354182	0.1897035
29	H	-2.4035288	-2.2686403	0.3356448
30	Cl	4.2692632	-1.4938889	-0.2689456

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