Supporting Information

Tuning of colour and chemical stability of model boranils: a strong effect of structural modifications

Grzegorz Wesela-Bauman,[a,b] * Mateusz Urban,[a] Sergiusz Luliński,[a] * Janusz Serwatowski,[a] Krzysztof Woźniak [b]

[a] Physical Chemistry Department, Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland
[b] Laboratory of Crystallochemistry, Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland.

*Corresponding authors: grzegorz.wesela@chem.uw.edu.pl, serek@ch.pw.edu.pl

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Synthetic procedures and compound characterization

General comments. All used reagents were provided by Aldrich Chemical Company. *n*-BuLi was used as a concentrated solution (10 M) in hexane. Solvents (THF and Et_2O) used for reactions were dried by heating to reflux with sodium/benzophenone and distilled under argon. Ethanol (96%) denatured with Et_2O was used. Reactions and manipulations involving air and moisture-sensitive reagents were carried out under argon atmosphere.

NMR characterization. The ^{1}H, ^{19}F and ^{13}C NMR spectra were recorded on Varian Mercury 400 MHz spectrometer (*VnmrJ*, ver. 3.2 A). The ^{11}B NMR spectra were recorded on Bruker Avance III NMR 300 MHz spectrometer (*TOPSPIN*, ver. 3.2-pl5). Chemical shifts of the ^{1}H and ^{13}C NMR spectra were referenced to TMS by using known chemical shifts of residual solvent peaks. In the ^{13}C NMR spectra of diarylborinic complexes, the resonances of boron-bound carbon atoms were not observed in most cases as a result of their broadening by a quadrupolar boron nucleus. ^{11}B and ^{19}F NMR spectra were referenced to $BF_3 \cdot Et_2O$ in C_6D_6. ^{1}H and ^{13}C NMR resonances for **1-7**, **9-10,** and **8** were assigned according to **Figures S1a** and **S1b**, respectively.

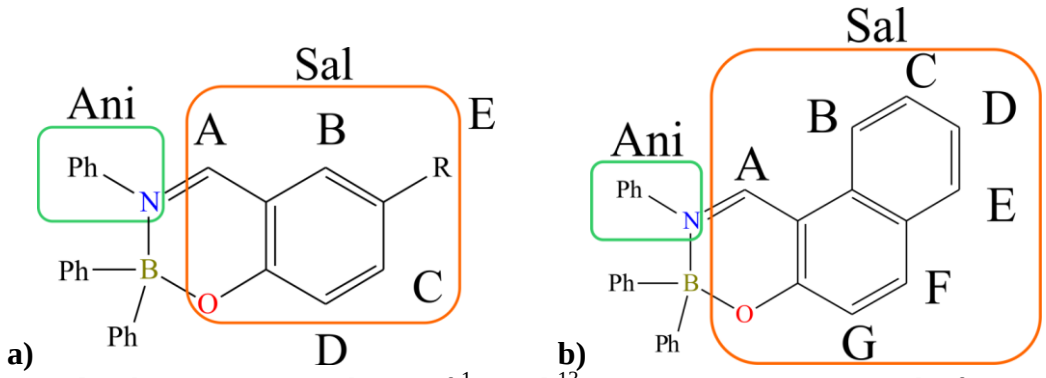


Figure S1a-b. The assignment scheme of ^{1}H and ^{13}C NMR resonances (R is the functional group) for **1-7**, **9-10**, and **8.**

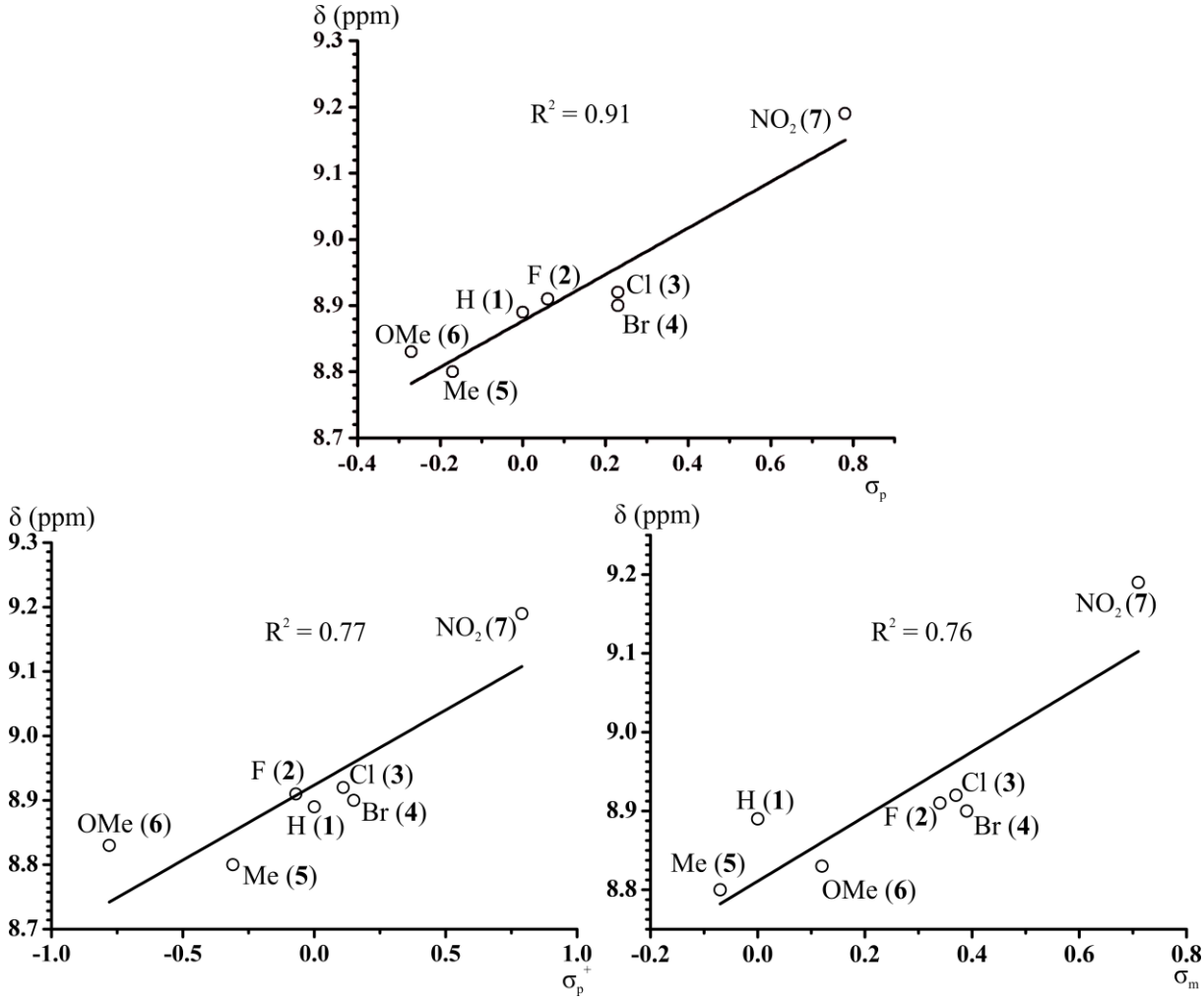
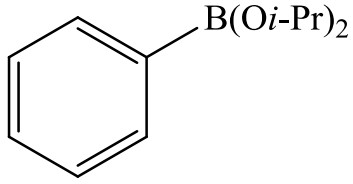
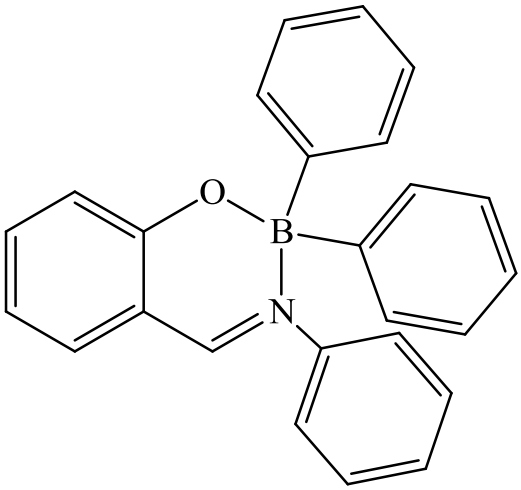


Figure S2. Chemical shifts of the C**H**=N protons for compounds **1**-**7** (ca. 0.1 M solutions in acetone-d_6) *versus* Hammett constants σ_p, σ_p^+ and σ_m.

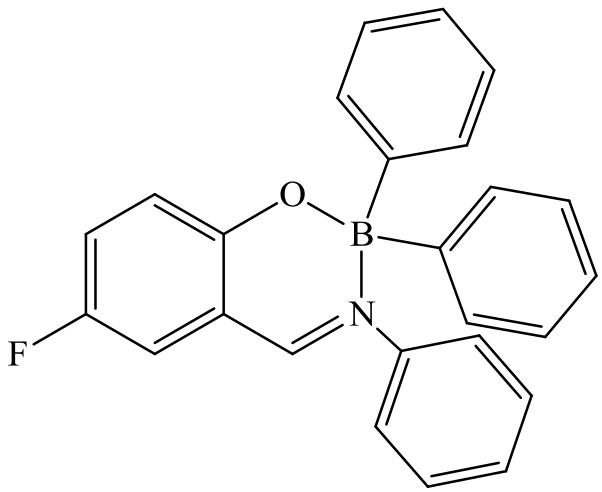


Synthesis of diisopropyl phenylboronate. Bromobenzene (31.4 g, 0.20 mol) was added dropwise to a stirred solution of *n*-BuLi (21.0 mL, 0.21 mol) in THF (100 mL) at −78 °C. After *ca.* 30 min, triisopropyl borate (49.0 mL, 0.21 mol) was added dropwise. The mixture was stirred at −78 °C for 30 min. Then it was warmed to 30 °C and quenched with a solution of 2 M HCl in Et_2O (125 mL, 0.25 mol). Solvents were removed and the residue was subjected to fractional vacuum distillation to give the product as a colourless liquid, b.p. 70-79 °C (2 Tr). Yield 38.62 g (94 %). **^{1}H NMR (400 MHz, acetone-d_6):** δ = 7.41-7.29 (m, 3H, **Ph**), 7.59-7.52 (m, 2H, **Ph**), 4.62 (sept., J_{HH} = 6.1 Hz, 2H, C**H**), 1.21 (d, J_{HH} = 6.1 Hz, 12H, C**H$_3$**) ppm. **^{11}B NMR (64 MHz, Acetone-d_6):** δ = 28 ($w_{1/2}$ = 130 Hz) ppm.



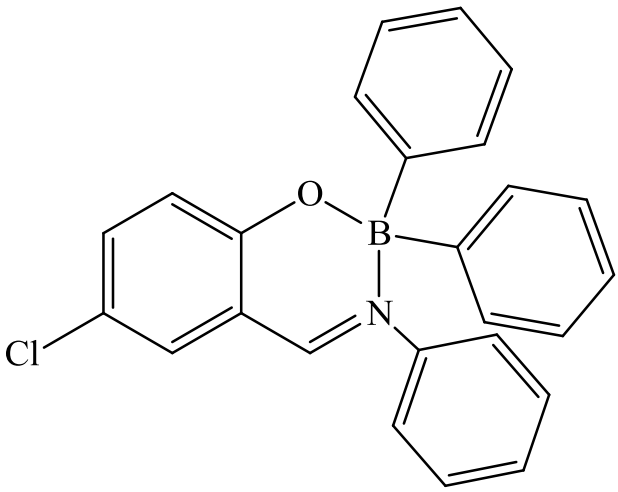
Synthesis of [Ph]$_2$B[6-H-Sal][Ani] (1). Bromobenzene (1.57 g, 10.0 mmol) was added dropwise to a stirred solution of *n*-BuLi (1.02 mL, 10.0 mmol) in THF (30 mL) at −78 °C. After 30 min diisopropyl phenylboronate (2.06 g, 10.0 mmol) was added dropwise. Subsequently the mixture was stirred for *ca.* 30 min and then allowed to reach the room temperature. The solvent was removed under vacuum and the residue was dissolved in EtOH (25 mL). The solution was treated with 2 M HCl in Et_2O (5.0 mL, 10.0 mmol) at 40 °C. After 20 min the mixture was warmed to 50 °C and then aniline (1.21 g, 13.0 mmol) and salicylaldehyde (1.10 g, 9.0 mmol) were simultaneously added resulting in a yellow coloration of the mixture. It was concentrated under vacuum and cooled to 0 °C. The crude product was filtered. The solid was washed with cold ethanol and hexane, and dried under vacuum to give a yellow crystalline material. Yield 3.19 g (8.8 mmol, 98 %). M.p. 151-153 °C, from DSC: 156.8 °C. **^{1}H NMR (400 MHz, CDCl$_3$):** δ = 8.35 (s, 1H, **A**), 7.57-7.39 (m, 5H, **Ar, Ani**), 7.32 (dd, J_{HH} = 7.8, J_{HH} = 1.6 Hz, 1H, **B**), 7.27-7.13 (m, 9H, **Ar**), 7.03 (dd, J_{HH} = 8.2, J_{HH} = 1.6 Hz, 3H, **Ar**), 6.82 (dt, J_{HH} = 7.5, J_{HH} = 0.8 Hz, 1H, **E**) ppm. **^{1}H NMR (400 MHz, acetone-d$_6$):** δ = 8.89 (s, 1H, **A**), 7.60 (dd, J_{HH} = 7.8, J_{HH} = 1.7 Hz, 1H), 7.50 (ddd, J = 8.5, J_{HH} = 7.2, J_{HH} = 1.8 Hz, 1H), 7.40 (dd, J_{HH} = 7.9, 1.6 Hz, 4H), 7.27-7.16 (m, 5H), 7.14-7.03 (m, 6H), 6.91-6.81 (m, 2H). **^{13}C{^{1}H} NMR (100.6 MHz, CDCl$_3$):** δ = 162.8 (N=**C**H), 162.3 (**Sal**, O-**C**), 145.4 (**Ani**, N-**C**), 138.7, 133.6, 132.1, 128.6, 128.2, 126.9, 126.3, 124.4, 120.1, 118.8, 118.1 ppm. **^{11}B NMR (64 MHz, acetone-d$_6$):** δ = 6 ($w_{1/2}$ = 192 Hz) ppm. **Anal. Calcd for C$_{25}$H$_{20}$BNO** (361.24): C 83.21, H 5.58, N 3.88%, found C 83.12, H 5.57, N 3.97%. **UV-Vis**: λ_{max} = 400 nm, ε = 4600 $M^{-1}cm^{-1}$. Fluorescence: λ_{exc} = 400 nm, λ_{em} = 534 nm, Φ = 7 %.

All other compounds were prepared as described for **1**.

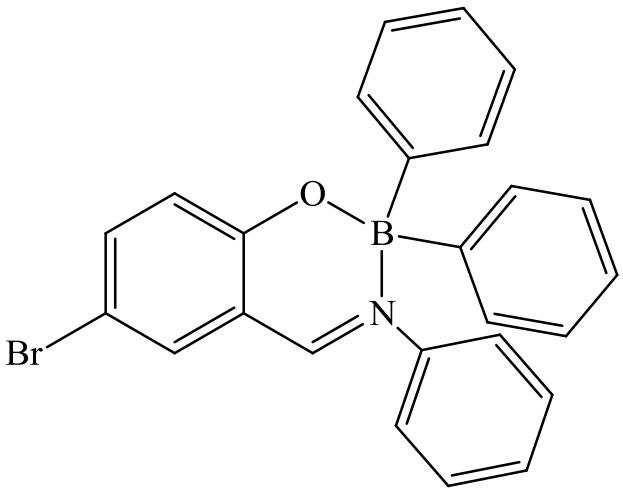


Synthesis of [Ph]$_2$B[6-F-Sal][Ani] (2). Starting materials: THF (20 mL), bromobenzene (0.93 g, 6.0 mmol), *n*-BuLi (0.65 mL, 6.5 mmol), diisopropyl phenylboronate (1.23 g, 6.0 mmol), EtOH

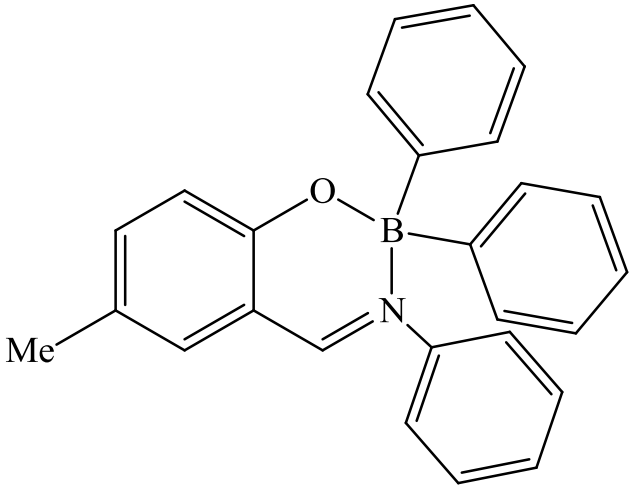
(10 mL), 2 M HCl in Et_2O (3.25 mL, 6.5 mmol), aniline (0.57 g, 6.0 mmol), 5-fluoro-2-hydroxybenzaldehyde (0.77 g, 5.5 mmol). 1.81 g (4.7 mmol, 88%). M.p. 136-138 °C. **^{1}H NMR (400 MHz, acetone-d_6):** δ = 8.91 (s, 1H, **A**), 7.43-7.36 (m, 5H), 7.31 (ddd, J_{HH} = 9.1, 3.2 Hz, J_{HF} = 8.3 Hz, 1H, **C**), 7.27-7.18 (m, 5H), 7.15-7.04 (m, 6H), 6.91 (dd, J_{HH} = 9.1 Hz, J_{HF} = 4.3 Hz, 1H, **D**) ppm. **^{11}B NMR (96 MHz, acetone-d_6):** δ = 6 ($w_{1/2}$ = 170 Hz) ppm. **^{13}C{^{1}H} NMR (100.6 MHz, acetone-d_6):** δ = 164.8 (s, N=CH), 159.5 (d, J_{CF} = 269 Hz, **Sal**, C-F), 154.5 (**Sal**, O-**C**), 146.3 (**Ani**, N-**C**), 134.4, 129.3, 129.0, 127.4, 126.5 (d, J_{CF} = 24 Hz, **Sal**), 126.4, 125.3, 121.7 (d, J_{CF} = 8 Hz, **Sal**), 119.3 (d, J_{CF} = 9 Hz, **Sal**), 117.6 (d, J_{CF} = 24 Hz, **Sal**) ppm. **^{19}F NMR** (376 MHz, acetone-d_6): δ = −125.5 (td, J_{HF} = 8.3 Hz, 4.3 Hz) ppm. **Anal. Calcd for $C_{25}H_{19}BFNO$** (379.23): C 79.18%; H 5.05%; N 3.69%, found C 79.07%, H 5.24%, N 3.86%. **UV-Vis**: λ_{max} = 413 nm, ε = 4900 $M^{-1}cm^{-1}$. Fluorescence: λ_{exc} = 413 nm, λ_{em} = 555 nm, Φ = 2%.



Synthesis of [Ph]$_2$B[6-Cl-Sal][Ani] (3). Starting materials: THF (30 mL), bromobenzene (1.57 g, 10.0 mmol), *n*-BuLi (1.02 mL, 10.0 mmol), diisopropyl phenylboronate (2.06 g, 10.0 mmol), EtOH (25 mL), 2 M HCl in Et_2O (5.0 mL, 10.0 mmol), aniline (1.21 g, 13.0 mmol), 5-chloro-2-hydroxybenzaldehyde (1.41 g, 9.0 mmol). Yield: 3.14 g (7.9 mmol, 88%). M.p. 127-128 °C, from DSC 129.2 °C. **^{1}H NMR (400 MHz, acetone-d_6):** δ = 8.92 (s, 1H, **A**), 7.65 (d, J_{HH} = 2.7 Hz, 1H, **B**), 7.48 (dd, J_{HH} = 8.9, J_{HH} = 2.7 Hz, 1H, **C**), 7.39 (dd, J_{HH} = 7.8, J_{HH} = 1.6 Hz, 4H, **Ar**), 7.29-7.17 (m, 5H, **Ar**), 7.16-7.04 (m, 6H, **Ar**), 6.91 (d, J_{HH} = 8.9 Hz, 1H, **D**) ppm. **^{13}C{^{1}H} NMR (100.6 MHz, acetone-d_6):** δ = 164.9 (N=**C**H), 161.7 (**Sal**, O-**C**), 146.3 (**Ani**, N-**C**), 138.6, 134.5, 132.4, 129.4, 129.1, 127.5, 127.0, 125.4, 123.4, 122.1, 120.5 ppm. **^{11}B NMR (64 MHz, acetone-d_6):** δ = 6 ($w_{1/2}$ = 256 Hz) ppm. **Anal. Calcd for $C_{25}H_{19}BClNO$** (395.69): C 75.88, H 4.84, N 3.54, Cl 8.96%, found C 75.70, H 4.87, N 3.66, Cl 9.08%. **UV-Vis**: λ_{max} = 412 nm, ε = 5300 $M^{-1}cm^{-1}$. Fluorescence: λ_{exc} = 412 nm, λ_{em} = 545 nm, Φ = 7 %.

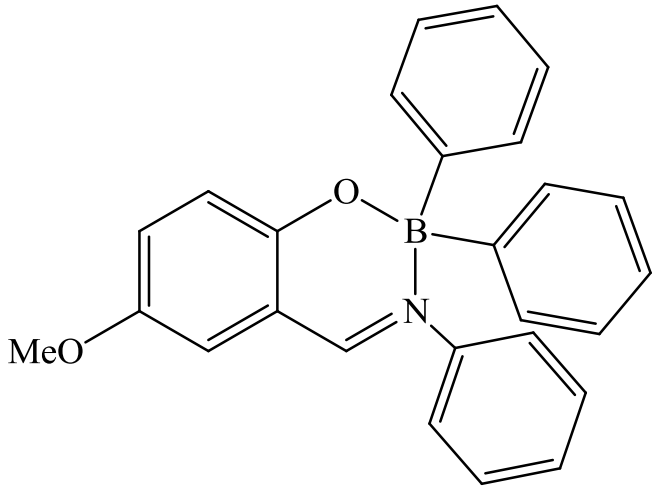


Synthesis of [Ph]$_2$B[6-Br-Sal][Ani] (4). Starting materials: THF (30 mL), bromobenzene (1.57 g, 10.0 mmol), *n*-BuLi (1.02 mL, 10.0 mmol), diisopropyl phenylboronate (2.06 g, 10.0 mmol), EtOH (25 mL), 2 M HCl in Et_2O (5.0 mL, 10.0 mmol), aniline (1.21 g, 13.0 mmol), 5-bromo-2-hydroxybenzaldehyde (1.81 g, 9.0 mmol). Yield 3.55 g (8.1 mmol, 90%). M.p. 137-138 °C, from DSC 142.0 °C. **^{1}H NMR (400 MHz, CDCl$_3$):** δ = 8.30 (s, 1H, **A**), 7.51 (d, J_{HH} = 8.8 Hz, 1H, **C**), 7.45-7.38 (m, 5H, **Ani**), 7.26-7.15 (m, 9H, **Ar**), 7.03 (s, 1H, **Ar**), 7.01 (s, 1H, **Ar**), 6.92 (d, J_{HH} = 8.8 Hz, 1H, **D**) ppm**. ^{1}H NMR (400 MHz, acetone-d$_6$):** δ = 8.90 (s, 1H, **A**), 7.77 (d, *J* = 2.6 Hz, 1H, **B**), 7.58 (dd, *J* = 8.9, 2.6 Hz, 1H, **D**), 7.42 – 7.36 (m, 4H, **Ar**), 7.28 – 7.17 (m, 5H, **Ar**), 7.16 – 7.03 (m, 6H, **Ar**), 6.86 (d, *J* = 8.9 Hz, 1H, **C**). **^{13}C{^{1}H} NMR (100.6 MHz, acetone-d$_6$):** δ = 164.6 (N=**C**H), 161.9 (**Sal**, O-**C**), 146.2 (**Ani**, N-**C**), 141.3, 135.4, 134.4, 129.3, 129.0, 127.4, 126.9, 125.3, 122.4, 121.2, 120.1, 110.1 (**C**-Br) ppm. **^{11}B NMR (64 MHz, DMSO-d$_6$):** δ = 6 ($w_{1/2}$ = 1280 Hz) ppm. **Anal. Calcd for C$_{25}$H$_{19}$BBrNO** (440.14): C 68.22, H 4.35, N 6.91. Br 18.15%, found C 68.01, H 4.50, N 3.31, Br 18.18%. **UV-Vis**: λ_{max} = 415 nm, ε = 5400 $M^{-1}cm^{-1}$. Fluorescence: λ_{exc} = 415 nm, λ_{em} = 536 nm, Φ = 4 %.

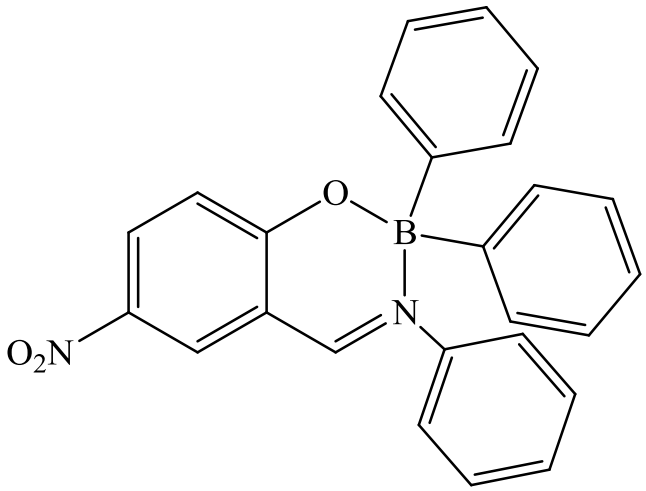


Synthesis of [Ph]$_2$B[6-Me-Sal][Ani] (5). Starting materials: THF (30 mL), bromobenzene (1.57 g, 10.0 mmol), *n*-BuLi (1.02 mL, 10.0 mmol), diisopropyl phenylboronate (2.06 g, 10.0 mmol), EtOH (25 mL), 2 M HCl in Et_2O (5.0 mL, 10.0 mmol), aniline (1.21 g, 13.0 mmol), 5-methyl-2-hydroxybenzaldehyde (1.23 g, 9.0 mmol). Yield 2.91 g (7.8 mmol, 86%). M.p. 143-146 °C, from DSC 145.3 °C. **^{1}H NMR (400 MHz, acetone-d$_6$):** δ = 8.80 (d, J_{HH} = 0.6 Hz, 1H, **A**), 7.40-7.37 (m, 5H, **Ani**), 7.33 (ddd, J_{HH} = 8.4 Hz, J_{HH} = 2.3 Hz, J_{HH} = 0.6 Hz, 1H, **C**), 7.26-7.15 (m, 5H, **Ar**), 7.14-7.02 (m, 6H, **Ar**), 6.79 (d, J_{HH} = 8.4 Hz, 1H, **D**), 2.21 (s, 3H, C**H$_3$**) ppm. **^{13}C{^{1}H} NMR**

(100.6 MHz, acetone-d_6): δ = 165.2 (N=**C**H), 161.1 (**Sal**, O-**C**), 146.5 (**Ani**, N-**C**), 140.4, 135.5, 134.4, 133.0, 129.2, 128.7, 128.5, 127.3, 126.7, 125.3, 119.9, 119.5, 20.1 (**C**H_3) ppm. **^{11}B NMR (64 MHz, acetone-d_6):** δ = 6 ($w_{1/2}$ = 256 Hz) ppm. **Anal. Calcd for $C_{26}H_{22}BNO$** (375.27): C 83.21, H 5.91, N 3.73%, found C 83.14, H 5.90, N 3.84%. **UV-Vis**: λ_{max} = 413 nm, ε = 5100 $M^{-1}cm^{-1}$. Fluorescence: λ_{exc} = 413 nm, λ_{em} = 552 nm, Φ = 17 %.



Synthesis of [Ph]$_2$B[6-OMe-Sal][Ani] (6). Starting materials: THF (30 mL), bromobenzene (1.57 g, 10.0 mmol), *n*-BuLi (1.02 mL, 10.0 mmol), diisopropyl phenylboronate (2.06 g, 10.0 mmol), EtOH (40 mL), 2 M HCl in Et_2O (5.0 mL, 10.0 mmol), aniline (1.21 g, 13.0 mmol), 5-methoxy-2-hydroxybenzaldehyde (1.12 mL, 9.0 mmol). Yield 3.23 g (8.3 mmol, 92%). M.p. 168-169 °C, from DSC 173.9 °C (first cycle) and 173.6 °C (second cycle). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 8.32 (s, 1H, **A**), 7.45-7.43 (m, 4H, **Ar**), 7.25-7.14 (m, 9H, **Ar**), 7.12 (dd, J_{HH} = 9.1, J_{HH} = 3.1 Hz, 1H, **C**), 7.05 (dd, J_{HH} = 8.0, J_{HH} = 1.5 Hz, 2H, **Ar**), 6.98 (d, J_{HH} = 9.1 Hz, 1H, **D**), 6.74 (d, J_{HH} = 3.1 Hz, 1H, **B**), 3.75 (s, 3H, -OC**H**$_3$) ppm. **^{1}H NMR (400 MHz, acetone-d_6):** δ = 8.83 (s, 1H, **A**), 7.42-7.37 (m, 4H, **Ar**), 7.25-7.17 (m, 5H, **Ar**), 7.14-7.02 (m, 8H, **Ar**), 6.84 (d, J_{HH} = 8.8 Hz, 1H, **Ar**), 3.73 (s, 3H, **-OC**H_3). **^{13}C{^{1}H} NMR (100.6 MHz, acetone-d_6):** δ = 164.9 (N=**C**H), 157.8 (**Sal**, O-**C**), 152.8 (**Sal**, MeO-**C**), 146.5 (**Ani**, N-**C**), 134.4, 129.2, 128.7, 128.1, 127.3, 126.7, 125.3, 121.1, 119.2, 114.2, 56.0 (O-**C**H_3) ppm. **^{11}B NMR (64 MHz, acetone-d_6):** δ = 6 ($w_{1/2}$ = 190 Hz) ppm. **Anal. Calcd for $C_{26}H_{22}BNO_2$** (391.27): C 79.81, H 5.67, N 3.58%, found C 79.73, H 5.68, N 3.68%. **UV-Vis**: λ_{max} = 437 nm, ε = 5100 $M^{-1}cm^{-1}$. Fluorescence: λ_{exc} = 437 nm, λ_{em} = 590 nm, Φ = 5 %.

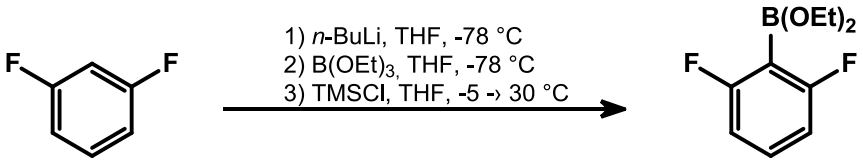


Synthesis of [Ph]$_2$B[6-NO_2-Sal][Ani] (7). Starting materials: THF (30 mL), bromobenzene (1.57 g, 10.0 mmol), *n*-BuLi (1.02 mL, 10.0 mmol), diisopropyl phenylboronate (2.06 g, 10.0 mmol), EtOH

(40 mL), 2 M HCl in Et_2O (5.0 mL, 10.0 mmol), aniline (1.21 g, 13.0 mmol), 5-nitro-2-hydroxybenzaldehyde (1.50 g, 9.0 mmol). A crude product was recrystallized from Et_2O. Yield 3.43 g (8.4 mmol, 89%). M.p. from DSC 167.8 °C. **^{1}H NMR (400 MHz, acetone-d_6):** δ = 9.19 (s, 1H, **A**), 8.65 (d, J_{HH} = 2.8 Hz, 1H, **B**), 8.33 (dd, J_{HH} = 9.0, J_{HH} = 2.8 Hz, 1H, **C**), 7.42-7.40 (m, 4H, **Ar**), 7.30-7.22 (m, 5H, **Ar**), 7.18-7.10 (m, 6H, **Ar**), 8.65 (d, J_{HH} = 9.0 Hz, 1H, **D**) ppm. **^{13}C{^{1}H} NMR (100.6 MHz, acetone-d_6):** δ = 167.5 (N=**C**H), 165.7 (**Sal**, O-**C**), 146.2 (**Ani**, N-**C**), 140.5, 134.5, 133.4, 129.7, 127.8, 127.5, 125.6, 122.5, 121.2, 118.5. **^{11}B NMR (64 MHz, acetone-d_6):** δ = 7 ($w_{1/2}$ = 256 Hz) ppm. **Anal. Calcd for $C_{25}H_{19}BN_2O_3$** (406.24): C 73.91, H 4.71, N 6.90%, found C 73.57, H 4.82, N 6.89 %. **UV-Vis**: λ_{max} = 390 nm, ε = 6400 $M^{-1}cm^{-1}$. Fluorescence: λ_{exc} = 390 nm, λ_{em} = 506 nm, Φ = 1 %.

Synthesis of [Ph]$_2$B[Naft-Sal][Ani] (8). Starting materials: THF (30 mL), bromobenzene (1.57 g, 10.0 mmol), *n*-BuLi (1.02 mL, 10.0 mmol), diisopropyl phenylboronate (2.06 g, 10.0 mmol), EtOH (40 mL), 2 M HCl in Et_2O (5.0 mL, 10.0 mmol), aniline (1.21 g, 13.0 mmol), 2-hydroxynaphthalene-1-aldehyde (1.72 g). Yield 3.78 g (92%). M.p. 210-211 °C, from DSC 217.4 °C. **^{1}H NMR (400 MHz, acetone-d_6):** δ = 9.43 (s, 1H, **A**), 8.34 (dd, J_{HH} = 8.4, J_{HH} = 1.1 Hz, J_{HH} = 0.6 Hz, 1H, **E**), 8.06 (d, J_{HH} = 9.0 Hz, 1H, **G**), 7.81 (ddd, J_{HH} = 8.0, J_{HH} = 1.4 Hz, J_{HH} = 0.6 Hz, 1H, **B**), 7.56 (ddd, J_{HH} = 8.4, J_{HH} = 7.0, J_{HH} = 1.4 Hz, 1H, **D**), 7.46-7.42 (m, 4H, **Ar**), 7.38 (ddd, J_{HH} = 8.0, J_{HH} = 7.0, J_{HH} = 1.1 Hz, 1H, **C**), 7.35-7.31 (m, 2H, **Ar**), 7.28-7.20 (m, 3H, **Ar**), 7.12 (d, J_{HH} = 9.0 Hz, 1H, **F**), 7.12-7.00 (m, 6H, **Ar**) ppm. **^{13}C{^{1}H} NMR (100.6 MHz, acetone-d_6):** δ = 165.1 (N=**C**H), 160.0 (**sal**, O-**C**),146.9 (**Ani**, N-**C**), 140.6, 134.5, 133.4, 129.9, 129.6, 129.2, 128.4, 128.3, 127.3, 126.7, 125.6, 124.9, 121.7, 121.2, 112.7 ppm. **^{11}B NMR (64 MHz, acetone-d_6):** δ = 6 ($w_{1/2}$ = 256 Hz) ppm. **Anal. Calcd for $C_{29}H_{22}BNO$** (411.30): C 84.86, H 5.39, N 3.41%, found C 84.88, H 5.35, N 3.49%. **UV-Vis**: λ_{max} = 424 nm, ε = 7600 $M^{-1}cm^{-1}$. Fluorescence: λ_{exc} = 424 nm, λ_{em} = 534 nm, Φ = 4 %.

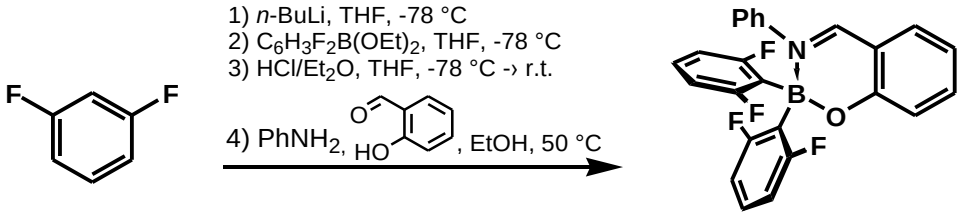
Synthesis of diethyl (2,6-difluorophenyl)boronate



1,3-Difluorobenzene (11.4 g, 0.10 mol) was added dropwise to a stirred solution of *n*-BuLi (10.2 mL, 0.102 mol) in THF (100 mL) at −78 °C. After *ca.* 20 min, triethyl borate (17.0 mL, 0.10 mol) was added dropwise. The mixture was stirred at −78 °C for 30 min, and afterwards warmed to -5 °C. Trimethylsilyl chloride (13.0 mL, 0.102 mol) was added, and the mixture was warmed to 30 °C. Solvents were removed and the residue was subjected to fractional

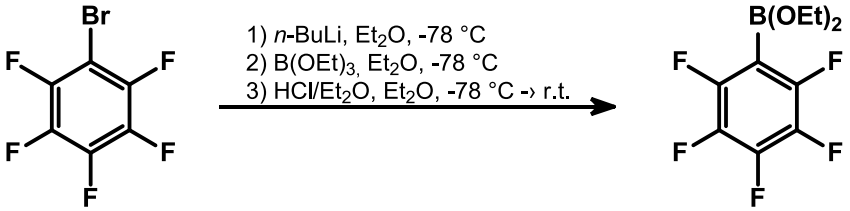
vacuum distillation to give the product as a colourless liquid, b.p. 47-50 °C (2 Tr). Yield 18.4 g (86%). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 7.35-7.24 (m, 1H), 6.88-6.81 (m, 2H), 3.97 (q, *J* = 7.1 Hz, 4H. -OC**H**$_2$-), 1.24 (t, *J* = 7.1 Hz, 6H, -C**H**$_3$) ppm. **^{11}B NMR (64 MHz, $CDCl_3$):** δ = 29 ($w_{1/2}$ = 120 Hz) ppm. **^{19}F NMR (376 MHz, $CDCl_3$):** δ = −103.22 (t, J_{HF} = 6.5 Hz) ppm.

Synthesis of complex [2,6-diFPh]$_2$B[6-H-Sal][Ani] (9).



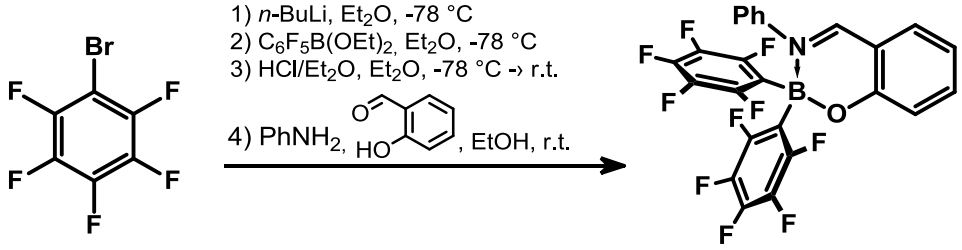
1,3-Difluorobenzene (0.23 g, 2.0 mmol) was added dropwise to a stirred solution of 10 M *n*-BuLi (0.2 mL, 2.0 mmol) in THF (5 mL) at −78 °C. After *ca.* 15 min, diethyl (2,6-difluorophenyl)boronate (0.43 g, 2.0 mmol) in THF (5 mL) was added dropwise. The mixture was stirred at −78 °C for 20 min. Then it was treated with a solution of 2 M HCl in Et_2O (1.1 mL, 2.2 mmol), and slowly warmed up to the room temperature. Aniline (0.20 g, 2.1 mmol) and salicylaldehyde (0.26 g, 2.1 mmol) in ethanol (5 mL) were added to a stirred solution at rt. The mixture was warmed to 50 °C. After *ca.* 1 hr the mixture was cooled to rt and concentrated in vacuo to give a yellow solid. A crude product was obtained by filtration of a cooled solution (*ca.* −30 °C) and washed with a cooled mixture of Et_2O and hexane. Then it was recrystallized from ethanol and dried under vacuum. Yield 0.76 g (1.8 mmol, *ca.* 90%). M.p. 210-212 °C. **^{1}H NMR (300 MHz, acetone-d_6):** δ = 9.00 (s, 1H, N=C**H**), 7.71 (dd, J_{HF} = 7.7, 1.7 Hz, 1H, **Ani**), 7.59-7.44 (m, 3H, Ar), 7.38-7.21 (m, 3H, Ar), 7.13 (tt, *J* = 8.4, 6.5 Hz, 2H, Ph), 6.92 (ddd, *J* = 7.8, 7.2, 1.0 Hz, 1H, **Ph**), 6.84 (ddt, *J* = 8.4, 1.0, 0.6 Hz, **Ph**), 6.71-6.58 (m, 4H, Ar) ppm. **^{11}B NMR (96 MHz, acetone-d_6):** δ = 2 ($w_{1/2}$ = 120 Hz) ppm. **^{13}C NMR (100.6 MHz, acetone-d_6):** δ = 166.2 (dd, J_{CF} = 243, 15 Hz, **C**-F), 164.3 (s, 1H, N=CH), 161.1 (**Sal**, O-**C**), 144.8 (**Ani**, N-**C**), 138.8, 133.3, 129.2 (t, J_{CF} = 12 Hz, **Ph**), 128.6, 128.4, 123.4, 119.2, 119.1, 118.4, 110.6, 110.5, 110.3 ppm. **^{19}F NMR (376 MHz, acetone-d_6):** δ = −103.78 (t, *J* = 6.8 Hz) ppm. **Anal. Calcd for $C_{25}H_{16}BF_4NO$** (433.21): C 69.31, H 3.72, N 3.23, F 17.54, found C 69.30, H 3.84, N 3.40%. **UV-Vis**: λ_{max} = 424 nm, ε = 7600 $M^{-1}cm^{-1}$. Fluorescence: λ_{exc} = 424 nm, λ_{em} = 534 nm, Φ = 4%.

Synthesis of Diethyl pentafluorophenylboronate.



Pentafluorobromobenzene (12.4 g, 50 mmol) was added dropwise to a stirred solution of *n*-BuLi (5.6 mL, 56 mmol) in Et_2O (50 mL) at −78 °C. After *ca.* 15 min, triethyl borate (8.6 g, 50 mmol) was added dropwise. The mixture was stirred in −78 °C for 30 min, and then treated with solution of 2 M HCl in Et_2O (26 mL, 53 mmol). Then it was slowly warmed up to rt and pH was adjusted to *ca.* 2 by addition of *ca.* 1 mL of 2 M HCl in Et_2O and stirred overnight. After filtration, solvents were removed under reduced pressure and the residue was subjected to fractional vacuum distillation to give the product as a colourless liquid, b.p. 65-80 °C (2 Tr).Yield 11.4 g (86 %). **^{1}H NMR (400 MHz, $CDCl_3$):** δ = 3.98 (q, J_{HH} = 7.1 Hz, 4H, -CH_2-), 1.24 (t, J_{HH} = 7.1 Hz, 6H, CH_3) ppm. **^{11}B NMR (128 MHz, $CDCl_3$):** δ = 26 ($w_{1/2}$ = 128 Hz) ppm. **^{19}F NMR (376 MHz, $CDCl_3$):** δ = −132.28 ÷ −132.63 (m, 2F), −153.45 (tt, J_{FF} = 19.8, 2.1 Hz, 1F), −161.82 ÷ −162.15 (m, 2F) ppm.

Synthesis of complex [pentaFPh]$_2$B[6-H-Sal][Ani] (10)



Pentafluorobromobenzene (1.24 g, 5.0 mmol) was added dropwise to a stirred solution of *n*-BuLi (0.53 mL, 5.3 mmol) in Et_2O (20 mL) at −78 °C. After *ca.* 15 min, diethyl pentafluorophenylboronate (1.34 g, 5.0 mmol) was added dropwise. The mixture was stirred at −78 °C for 20 min, treated with solution of 2 M HCl in Et_2O (2.7 mL, 5.4 mmol), and slowly warmed up to room temperature. After 3 hrs aniline (0.60 g, 6.5 mmol) and salicylaldehyde (0.59 g, 4.8 mmol) were added, and the reaction was stirred for 2 hrs at rt. Then volatiles were removed in vacuo. The resulting yellow oil was dissolved in 5 mL of ethanol and a solid precipitated. It was obtained by filtration of a cooled solution. The bright yellow crystalline solid was washed with cold mixture of Et_2O and hexane, and dried under vacuum. Yield 0.84 g (1.6 mmol, 31%). M.p. 152-154°C. **^{1}H NMR (300 MHz, acetone-d_6):** δ = 9.23 (s, 1H, N=C**H**), 7.85 (ddd, J_{HH} = 7.8, 1.8, 0.6 Hz, 1H), 7.68 (ddd, *J* = 8.4, 7.3, 1.8

Hz, 1H), 7.55-7.34 (m, 5H), 7.07 (ddd, *J* = 7.8, 7.3, 1.0 Hz, 1H), 6.98 (ddt, *J* = 8.4, 1.0, 0.6 Hz, 1H) ppm. **^{11}B NMR (96 MHz, acetone-d_6):** δ = 1 ($w_{1/2}$ = 130 Hz) ppm. **^{13}C NMR (75 MHz, acetone-d_6):** δ = 166.0 (N=**C**H), 159.8 (**Sal**, O-**C**), 144.0 (**Ani**, N-**C**), 139.9, 133.9, 129.3, 129.2, 123.2, 120.5, 119.1, 118.2 ppm. **^{19}F NMR (282 MHz, acetone-d_6):** δ = −135.02 (dd, J_{FF} = 23.5, 9.2 Hz, 2F), −158.48 (tt, J_{FF} = 20.0, 2.1 Hz, 1F), −165.68 (ddd, J_{FF} = 23.5, 20.0, 9.2 Hz, 2F) ppm. **Anal. Calcd for $C_{25}H_{10}BF_{10}NO$** (541.15): C 55.49; H 1.86; N 2.59; F 35.11, found C 54.26; H 2.40; N 2.72%. **UV-Vis**: λ_{max} = 396 nm, ε = 4800 $M^{-1}cm^{-1}$. Fluorescence: λ_{exc} = 396 nm, λ_{em} = 509 nm, Φ = 12%.

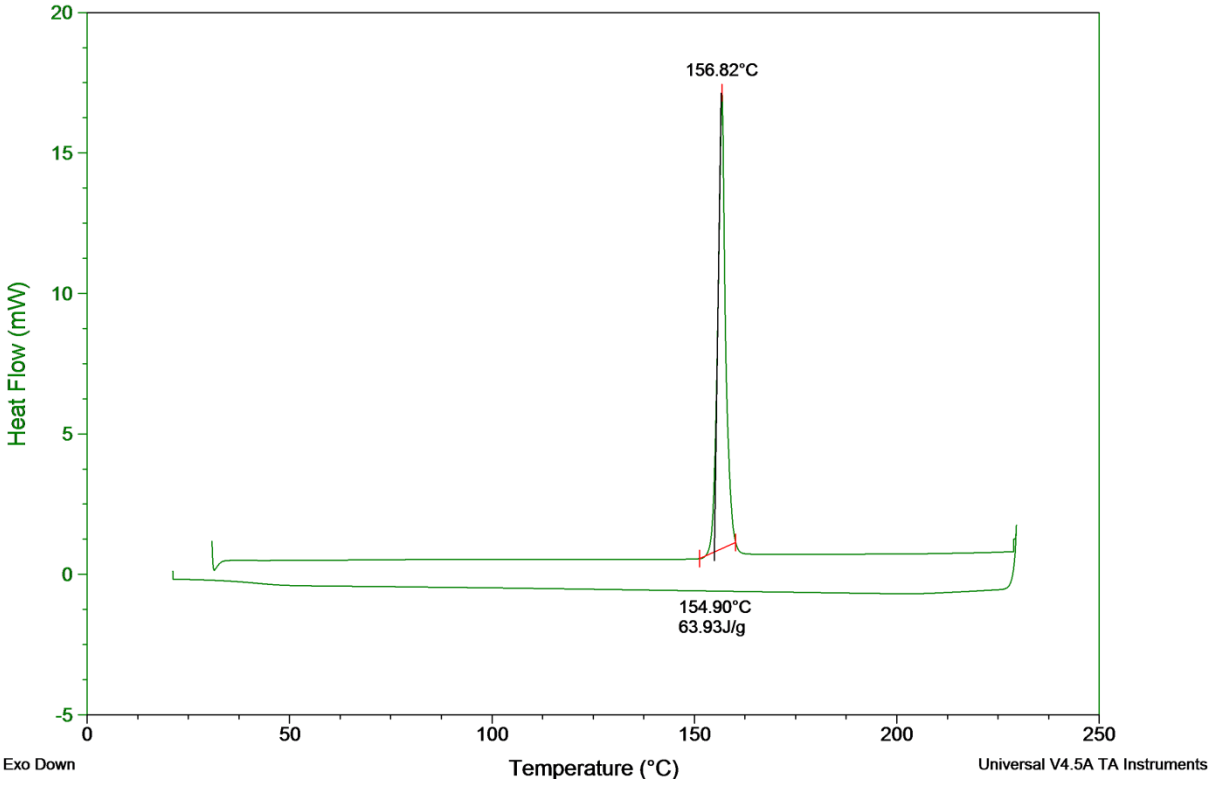
DSC measurements

Differential scanning calorimetric (DSC) measurements were performed on a DSC Q200 from TA Instruments.

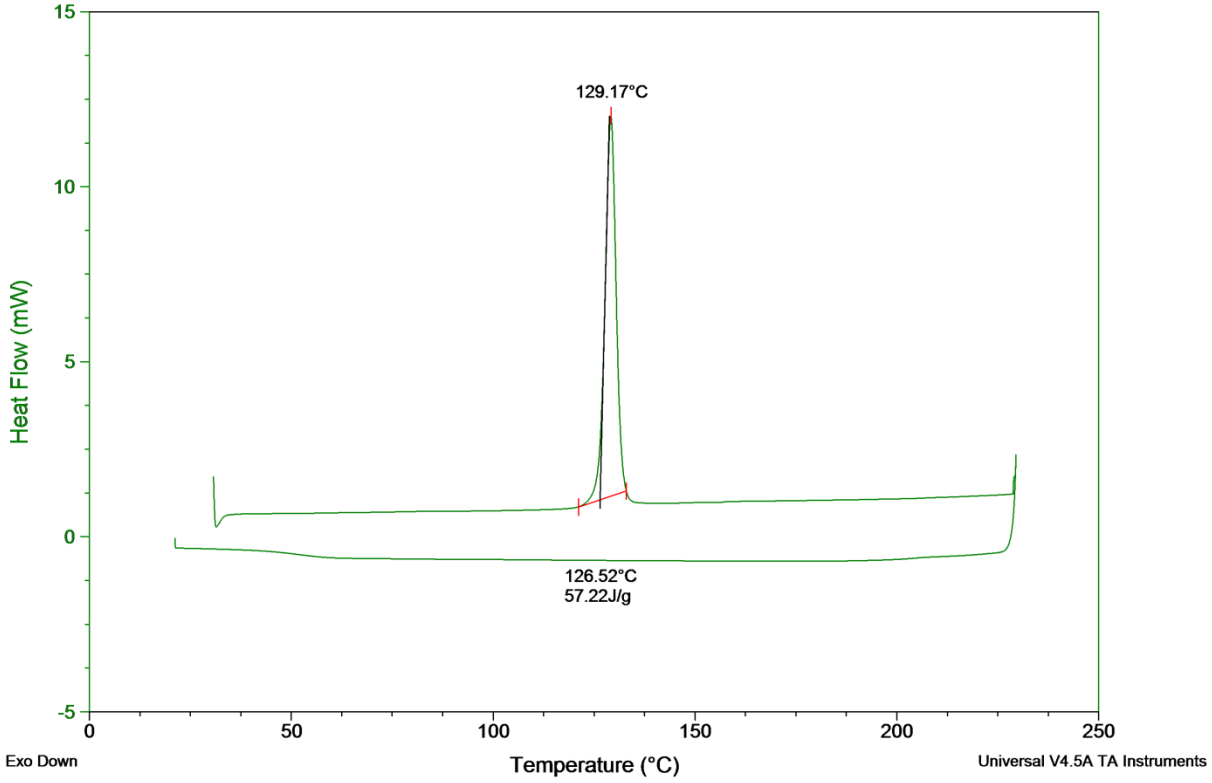
Table S1. The summary of DSC measurements for selected compounds. Melting points (T_m) and crystallization temperatures (T_c)..

		m / mg	T_c / °C	T_m / °C	heating cycle
1	**$[Ph]_2B$[6-H-Sal][an]**	3.5900	--	156.8	first
3	**$[Ph]_2B$[6-Cl-Sal][an]**	3.7480	--	129.2	first
4	**$[Ph]_2B$[6-Br-Sal][an]**	2.1820	--	142.0	first
5	**$[Ph]_2B$[6-Me-Sal][an]**	2.9760	--	145.3	first
6	**$[Ph]_2B$[6-OMe-Sal][an]**	2.1100	--	173.9	first
			111.9	173.6	second
7	**$[Ph]_2B$[6-NO_2-Sal][an]**	3.8560	--	167.8	first
8	**$[Ph]_2B$[Naft-Sal][an]**	2.7780	--	217.4	first

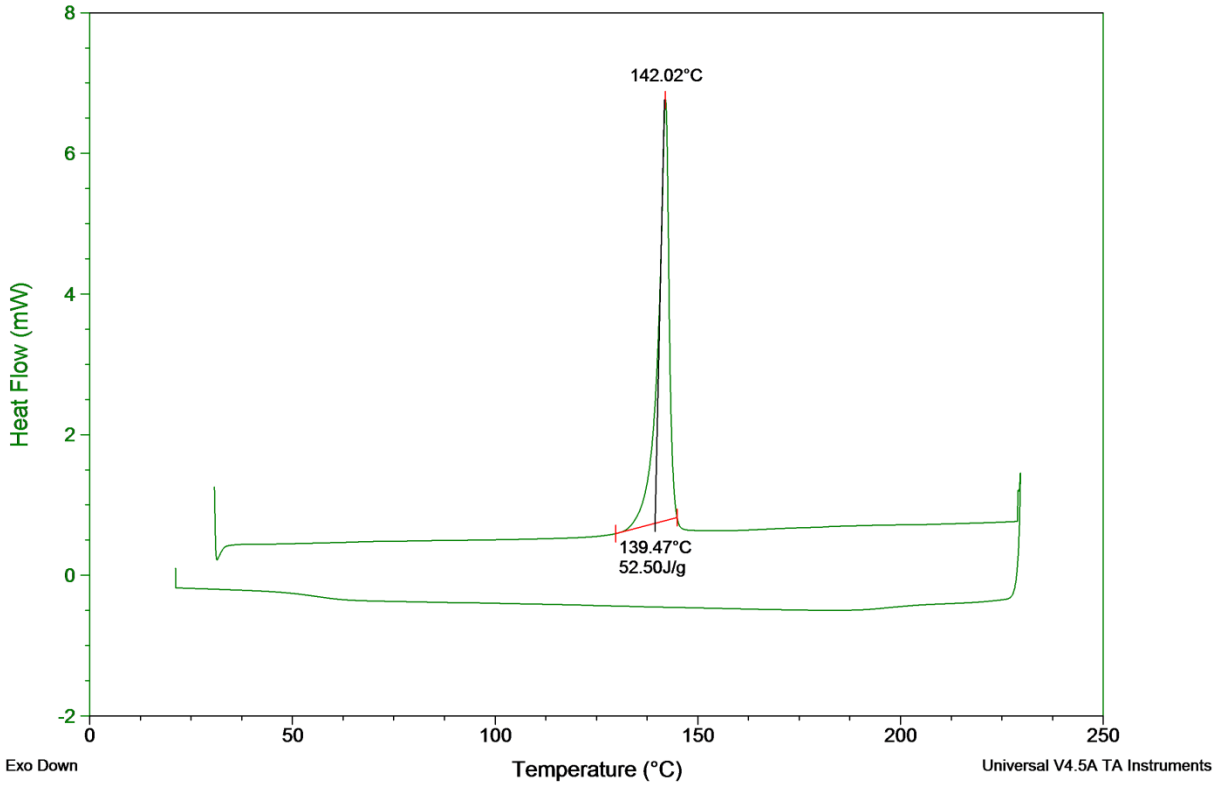
[Ph]$_2$B[6-H-Sal][an] (1)
Cycle 1



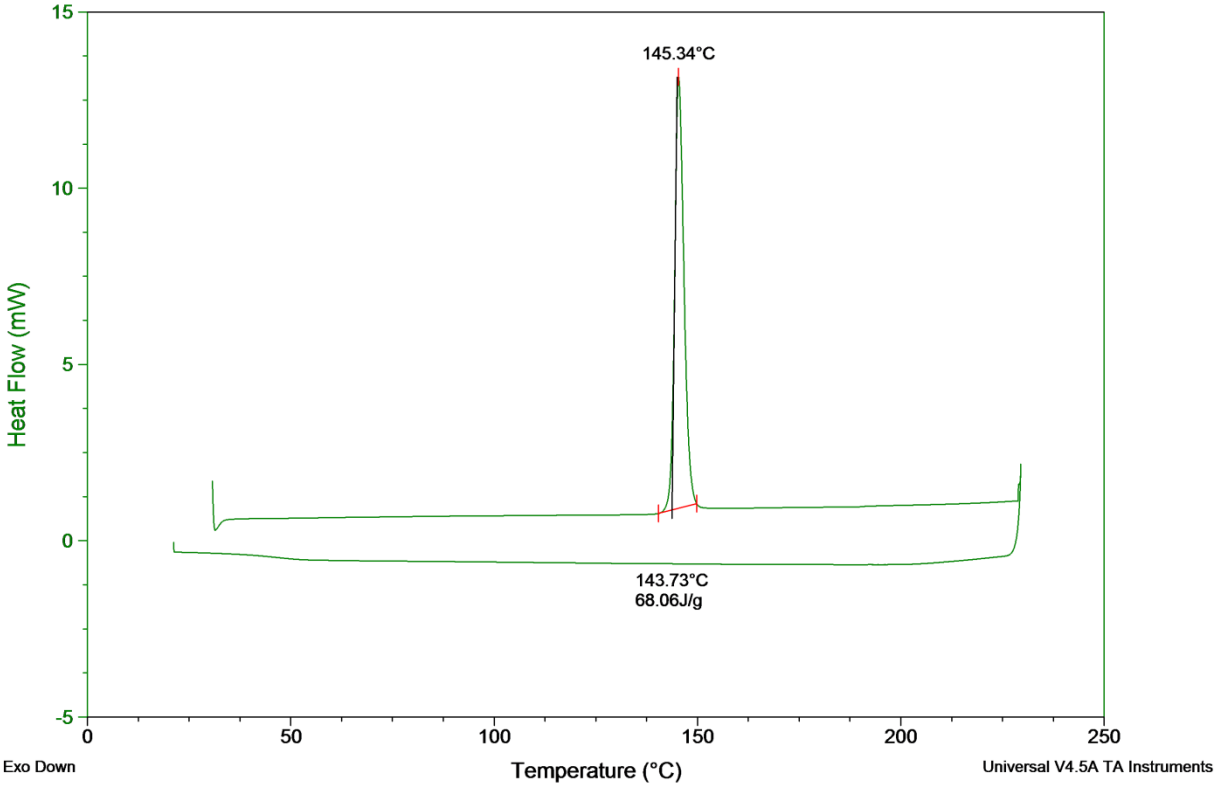
[Ph]$_2$B[6-Cl-Sal][an] (3)
Cycle 1



[Ph]$_2$B[6-Br-Sal][an] (4)
Cycle 1

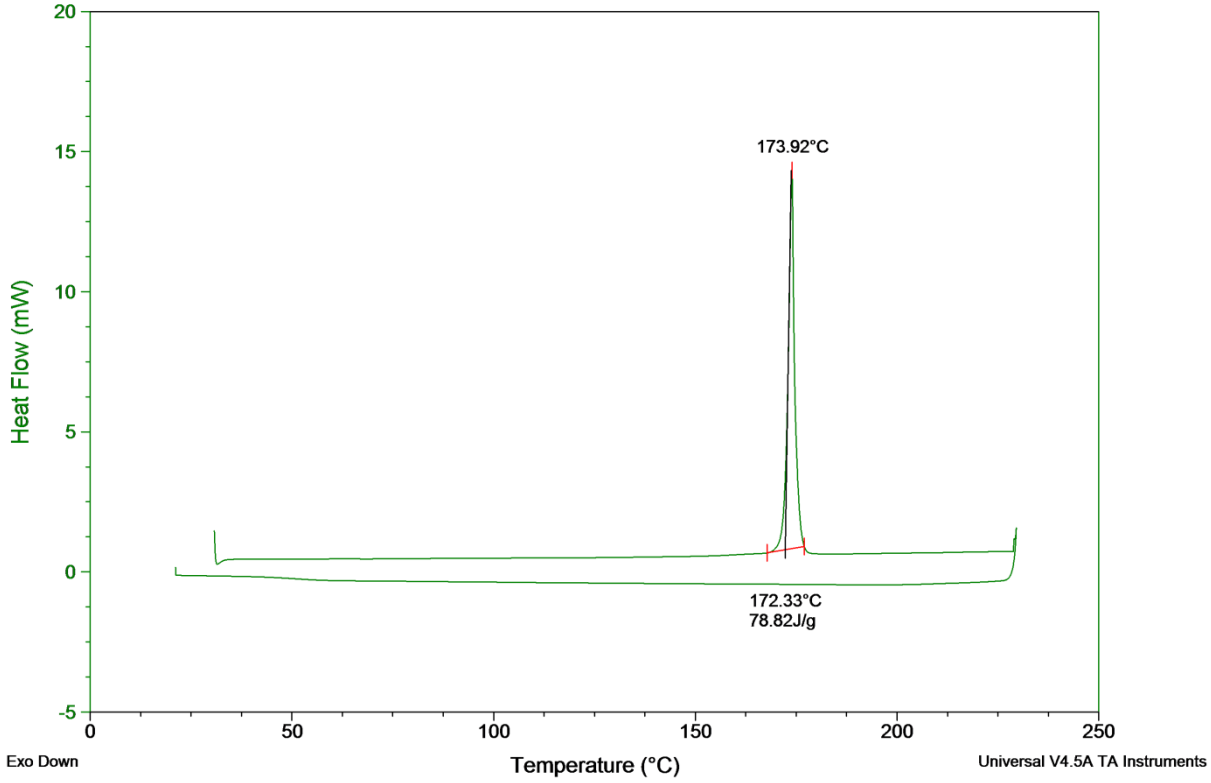


[Ph]$_2$B[6-Me-Sal][an] (5)
Cycle 1

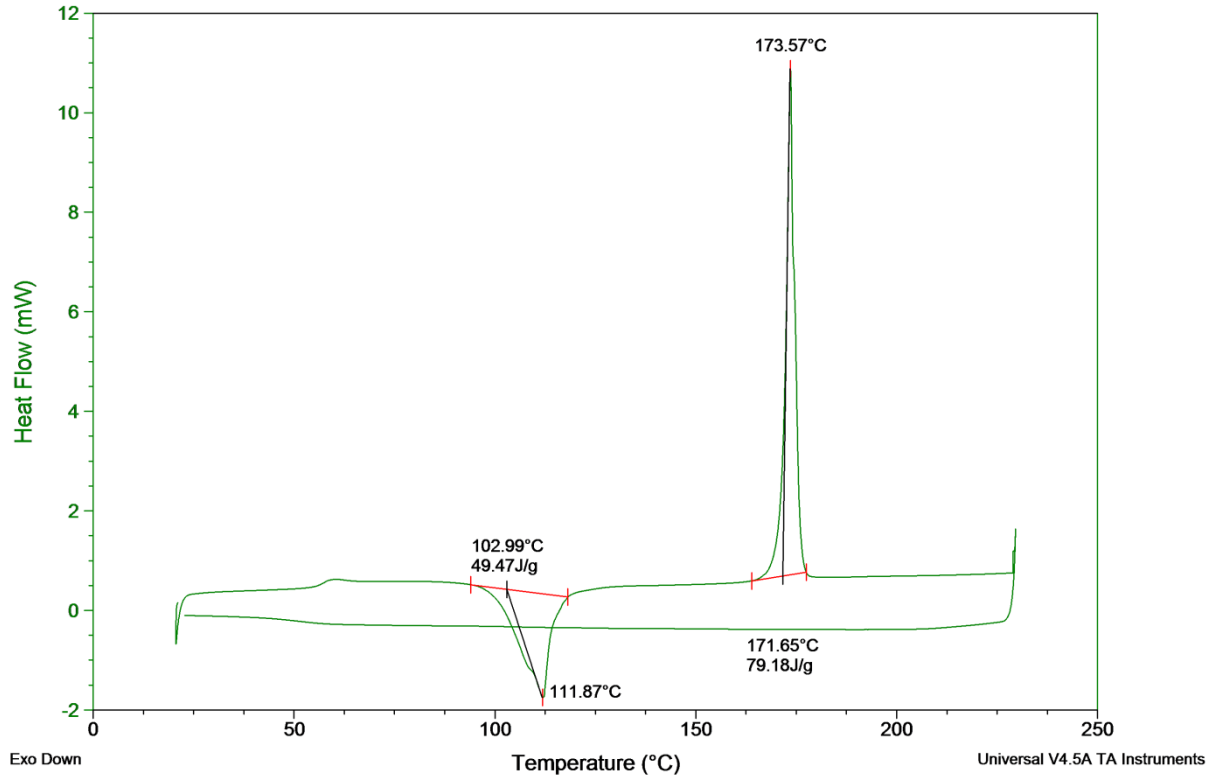


[Ph]$_2$B[6-OMe-Sal][an] (6)

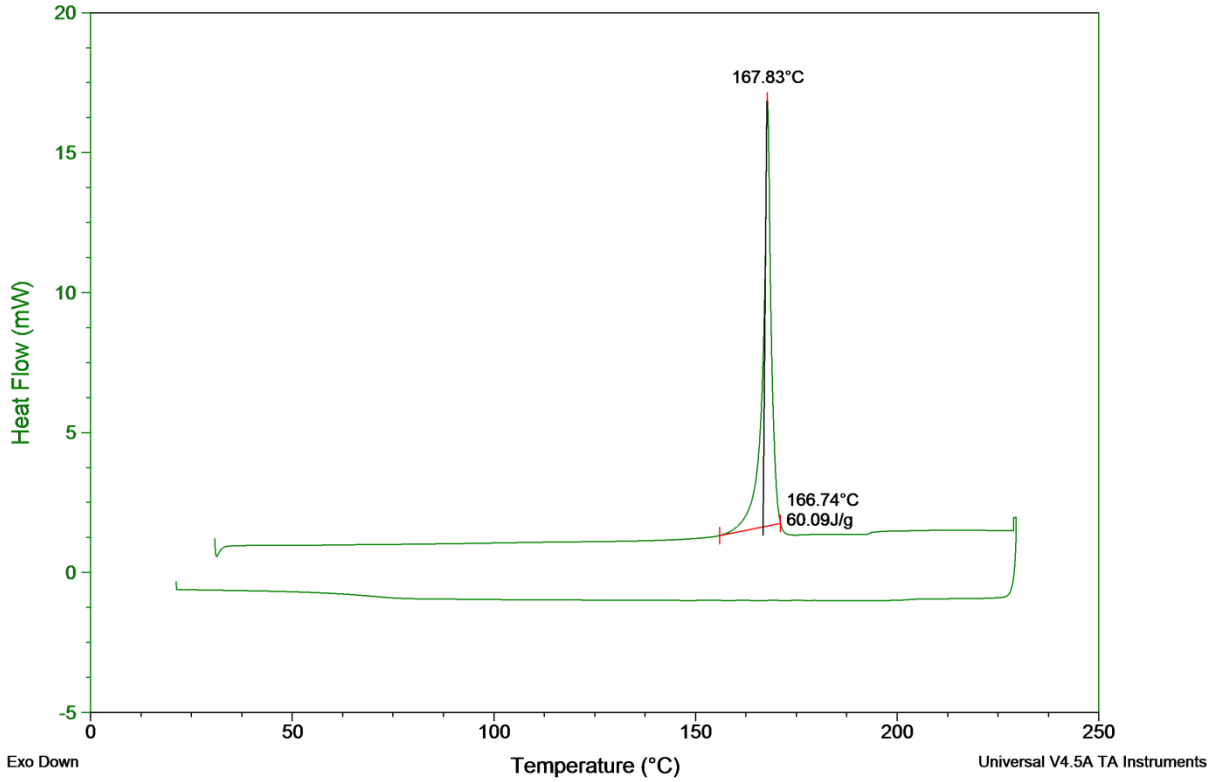
Cycle 1



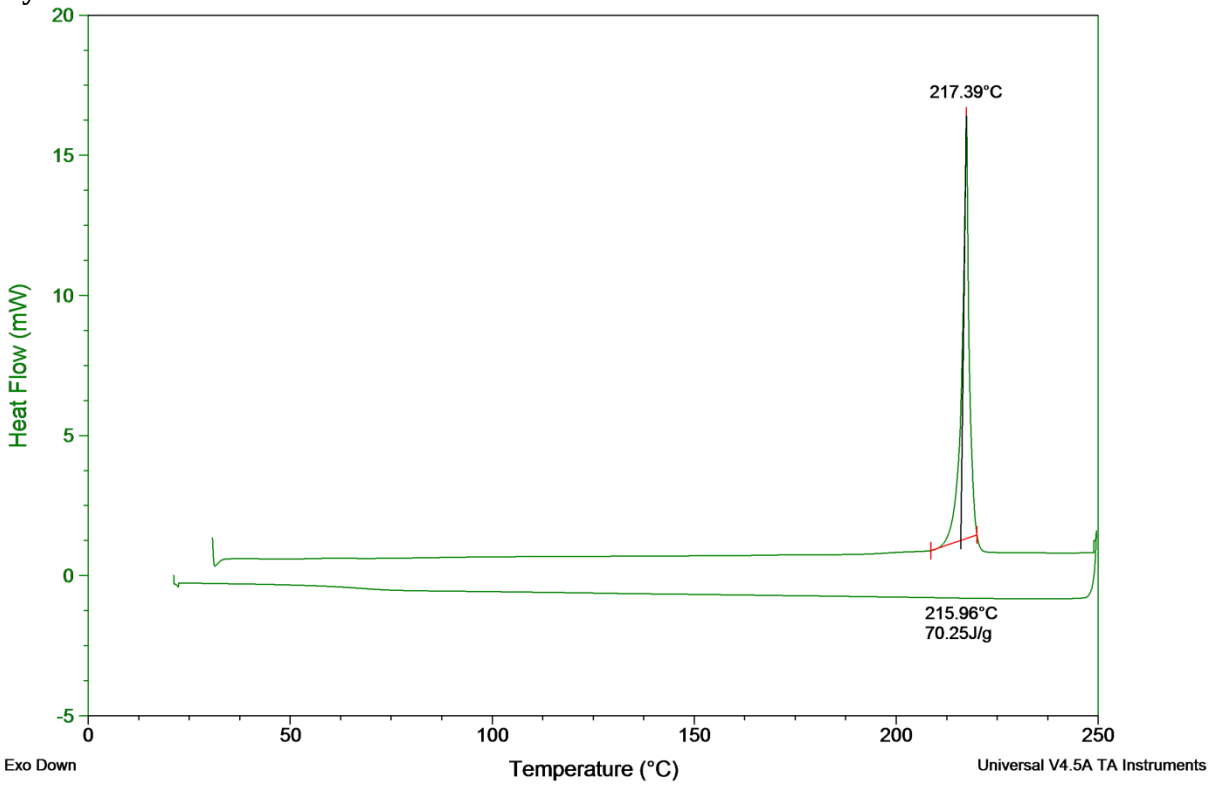
Cycle 2



[Ph]$_2$B[6-NO$_2$-Sal][an] (7)
Cycle 1



[Ph]$_2$B[naft][an] (8)
Cycle 1



X-Ray data

X-ray single crystal data collection, reduction and refinement. Single crystals of **1** were obtained through solvent evaporation from para-filmed vials. Single crystal X-ray measurement were performed on a Kuma KM4CCD κ–axis diffractometer with graphite-monochromated Mo K_α radiation (λ = 0.71073 Å) and an Oxford Cryostream cooling device. Data reduction and analysis were carried out with the *CRYSALISPRO* program.[1] Data set was restricted to 0.7 $Å^{-1}$ resolution. The crystal structure was solved using the *SUPERFLIP* program implemented in *CRYSTALS*.[2] The independent atom model (IAM) refinement based on F^2 was performed with the *CRYSTALS* package with $I > -3.0\sigma(I)$ cut-off. Reflections affected by the beam-stop were carefully removed from the refinement. The *Chebychev* (F^2) weights were applied. Atomic scattering factors in their analytical form were taken from the *International Tables for Crystallography*.[3] All non-hydrogen atoms were refined anisotropically and all of the hydrogen atoms were placed in idealized positions within the riding model for atomic displacement parameters (ADPs) (with $U_{iso}^{H} = 1.2 \cdot U_{eq}^{C}$). All hydrogen atoms (with except to the solvent molecules) were clearly visible on the difference density maps. Weighted *R* factors (*wR2*) and all goodness-of-fit (GooF) values are based on F^2. Conventional *R* factors are based on *F* with *F* set to zero for negative F^2. The $F_o^2 > 2\sigma(F_o^2)$ criterion, adopted form *SHELX*, was used only for calculating *R* factors and is not relevant to the choice of reflections for the refinement. The *R* factors based on F^2 are about twice as large as those based on *F*. *DIAMOND*[4] program has been used for visualization. *CHECKCIFs* alert "B" (and "C" alerts) are a consequence of a disordered position of solvent molecules and ambiguity of finding the positions for H-atoms attached to methyl carbon atoms. Solvent molecules are located on symmetry equivalent positions (transformation though 2-fold axis).

CCDC 1035702 contains the supplementary crystallographic data (CIF file) for a crystal studied in this work. It can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif or from the authors.

Crystal structure analysis. Crystals obtained from a concentrated acetone solution of **1** incorporated solvent molecules trapped inside the crystal lattice. The molecular structure of **1** was depicted in **Figure S3**. The chosen crystallographic parameters were put in **Table S2**. The boron atom possesses a typical tetrahedral geometry. The B-N bond length is in the range typical of single B-N bonds ($d_{B(1)-N(1)}$ = 1.634(3) Å), *i.e.*, it is slightly longer than the ones in 8-oxyquinolinato borinic complexes.[5] Chosen motifs of supramolecular assembly based on weak CH…O and CH…π interactions are depicted in **Figure S4**.

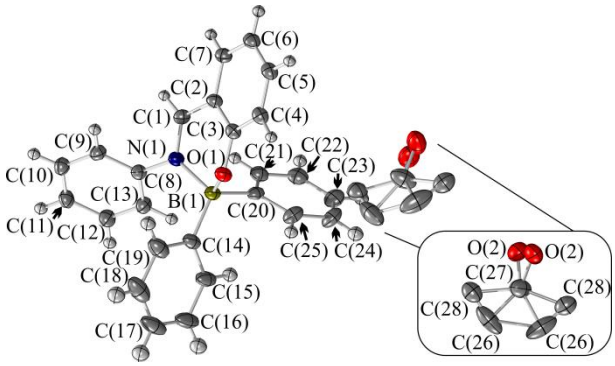


Figure S3. The molecular structure of **1** with atom labelling scheme. Thermal ellipsoids were generated at the 50% level of probability. Occupancies of disordered solvent molecules are *ca.* 0.5:0.5. The most important bond lengths are: $d_{B(1)-N(1)}$ = 1.634(3) Å; $d_{B(1)-O(1)}$ = 1.509(2) Å; $d_{B(1)-C(14)}$ = 1.613(3) Å; $d_{B(1)-C(20)}$ = 1.614(3) Å.

Table S2. Selected crystal data, data collection and refinement parameters for **1**.

	1
Chemical formula	$C_{28}H_{26}BNO_2$
Temperature (K)	100(1)
M_r	419.32
Crystal system, space group	Orthorhombic, *Pcca*
a,	26.7092(14),
b,	9.0357(4),
c (Å)	17.2708(9)
α, β, γ (°)	90, 90, 90
V (Å^3)	4168.1(4)
Z/Z’	4/2
R_{int} (%)	10.0
R[F^2>2σ(F^2)], wR(F^2), GooF	0.0685, 0.1490, 1.000
$\Delta\rho_{max}$, $\Delta\rho_{min}$(e·Å^{-3})	0.85, −0.55

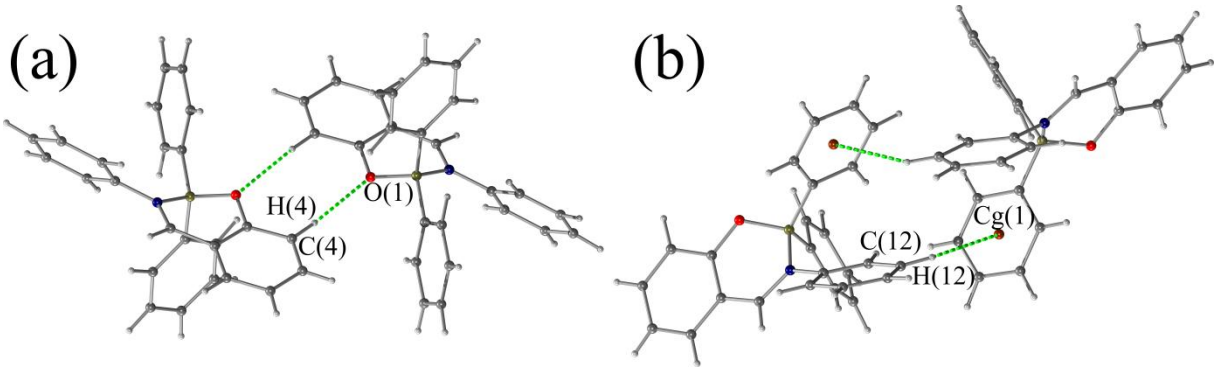


Figure S4. Intermolecular interactions present in the crystal structure of **1**. (a) Symmetry operator: 1−x,1−y,1−z; $d_{C(4)\ldots O(1)}$ = 3.361(2) Å, (b) Symmetry operator: 1.5−x,1−y,z; $d_{C(12)H(12)\ldots Cg(1)}$ = 3.275 Å; Cg(1) is a centroid calculated for C(14), C(15), C(16), C(17), C(18) and C(19) ring. Solvent molecules were omitted for clarity.

Cartesian Coordinates for compound 1

Number	Label	X	Y	Z	Symm. op.
1	H291	0.5576	1.1754	0.1700	x,y,z
2	H292	0.5073	1.1326	0.1312	x,y,z
3	H293	0.5385	1.0135	0.1743	x,y,z
4	H261	0.4957	0.9376	0.2748	x,y,z
5	H262	0.4804	1.0410	0.3425	x,y,z
6	H263	0.4441	1.0166	0.2735	x,y,z
7	O2	0.48500(15)	1.2792(4)	0.2552(3)	x,y,z
8	C26	0.4782(2)	1.0256(8)	0.2881(4)	x,y,z
9	C28	0.5000	1.1518(4)	0.2500	x,y,z
10	C29	0.52874(19)	1.1146(6)	0.1741(3)	x,y,z
11	H291	0.4424	1.1754	0.3300	1−x,y,1/2−z
12	H292	0.4927	1.1326	0.3688	1−x,y,1/2−z
13	H293	0.4615	1.0135	0.3257	1−x,y,1/2−z
14	H261	0.5043	0.9376	0.2252	1−x,y,1/2−z
15	H262	0.5196	1.0410	0.1575	1−x,y,1/2−z
16	H263	0.5559	1.0166	0.2265	1−x,y,1/2−z
17	O2	0.51500(15)	1.2792(4)	0.2448(3)	1−x,y,1/2−z
18	C26	0.5218(2)	1.0256(8)	0.2119(4)	1−x,y,1/2−z
19	C29	0.47126(19)	1.1146(6)	0.3259(3)	1−x,y,1/2−z
20	H1	0.5723	0.5977	0.2885	x,y,z
21	H4	0.4714	0.8747	0.5096	x,y,z
22	H5	0.4174	0.6661	0.5089	x,y,z
23	H6	0.4334	0.4614	0.4268	x,y,z
24	H7	0.5005	0.4587	0.3470	x,y,z
25	H9	0.5909	0.7652	0.1866	x,y,z
26	H10	0.6501	0.7980	0.0867	x,y,z
27	H11	0.7331	0.8319	0.1132	x,y,z
28	H12	0.7623	0.8380	0.2430	x,y,z

29	H13	0.7025	0.8084	0.3449	x,y,z
30	H15	0.6958	0.9892	0.4748	x,y,z
31	H16	0.7344	1.2262	0.4534	x,y,z
32	H17	0.6976	1.3920	0.3663	x,y,z
33	H18	0.6246	1.3388	0.3067	x,y,z
34	H19	0.5858	1.1020	0.3284	x,y,z
35	H21	0.6605	0.5897	0.4260	x,y,z
36	H22	0.6941	0.4627	0.5316	x,y,z
37	H23	0.6889	0.5632	0.6564	x,y,z
38	H24	0.6499	0.7965	0.6727	x,y,z
39	H25	0.6173	0.9242	0.5691	x,y,z
40	N1	0.60666(5)	0.76735(17)	0.33716(9)	x,y,z
41	B1	0.60830(7)	0.8656(2)	0.41658(12)	x,y,z
42	C20	0.63307(6)	0.7688(2)	0.48503(11)	x,y,z
43	C21	0.65808(7)	0.6341(2)	0.47630(12)	x,y,z
44	C22	0.67935(7)	0.5586(2)	0.53881(13)	x,y,z
45	C23	0.67608(8)	0.6178(3)	0.61263(14)	x,y,z
46	C24	0.65152(9)	0.7510(3)	0.62348(14)	x,y,z
47	C25	0.63034(8)	0.8250(3)	0.56064(12)	x,y,z
48	C1	0.57115(6)	0.6685(2)	0.33020(11)	x,y,z
49	C2	0.53011(6)	0.6596(2)	0.38376(10)	x,y,z
50	C3	0.52189(6)	0.78097(19)	0.43336(10)	x,y,z
51	C4	0.47793(7)	0.7853(2)	0.47837(11)	x,y,z
52	C5	0.44526(6)	0.6663(2)	0.47556(11)	x,y,z
53	C6	0.45364(7)	0.5441(2)	0.42753(11)	x,y,z
54	C7	0.49555(7)	0.5417(2)	0.38058(11)	x,y,z
55	C8	0.64199(6)	0.7828(2)	0.27494(10)	x,y,z
56	C9	0.62556(7)	0.7805(2)	0.19830(11)	x,y,z
57	C10	0.66012(7)	0.7975(2)	0.13847(11)	x,y,z
58	C11	0.71066(7)	0.8156(2)	0.15524(11)	x,y,z
59	C12	0.72698(7)	0.8178(2)	0.23155(11)	x,y,z
60	C13	0.69273(7)	0.8015(2)	0.29205(11)	x,y,z
61	C14	0.63550(7)	1.0229(2)	0.40277(12)	x,y,z
62	C15	0.68122(8)	1.0614(3)	0.43895(14)	x,y,z
63	C16	0.70458(11)	1.1977(3)	0.42521(16)	x,y,z
64	C17	0.68350(12)	1.2970(3)	0.37528(18)	x,y,z
65	C18	0.63834(13)	1.2648(3)	0.33926(18)	x,y,z
66	C19	0.61487(10)	1.1276(2)	0.35407(15)	x,y,z
67	O1	0.55392(5)	0.89590(14)	0.43424(8)	x,y,z

Bond lengths for compound 1

Number	Atom(1)	Atom(2)	Length
1	H291	C29	0.949(5)
2	H292	C29	0.950(5)

3	H293	C29	0.950(5)
4	H293	C26	0.795(6)
5	H261	C26	0.951(7)
6	H262	C26	0.952(7)
7	H262	C29	0.764(5)
8	H263	C26	0.949(5)
9	O2	C28	1.222(5)
10	O2	O2	0.821(6)
11	C26	C28	1.440(7)
12	C26	H293	0.795(6)
13	C26	C26	1.757(9)
14	C26	C29	1.052(9)
15	C28	C29	1.556(5)
16	C28	O2	1.222(5)
17	C28	C26	1.440(7)
18	C28	C29	1.556(5)
19	C29	H262	0.764(5)
20	C29	C26	1.052(9)
21	H291	C29	0.949(5)
22	H292	C29	0.950(5)
23	H293	C29	0.950(5)
24	H261	C26	0.951(7)
25	H262	C26	0.952(7)
26	H263	C26	0.949(5)
27	H1	C1	0.964(2)
28	H4	C4	0.987(2)
29	H5	C5	0.941(2)
30	H6	C6	0.922(2)
31	H7	C7	0.957(2)
32	H9	C9	0.958(2)
33	H10	C10	0.933(2)
34	H11	C11	0.953(2)
35	H12	C12	0.981(2)
36	H13	C13	0.951(2)
37	H15	C15	0.980(3)
38	H16	C16	0.968(3)
39	H17	C17	0.950(3)
40	H18	C18	0.948(3)
41	H19	C19	0.924(3)
42	H21	C21	0.959(2)
43	H22	C22	0.960(2)
44	H23	C23	0.965(2)
45	H24	C24	0.945(2)
46	H25	C25	0.973(3)

47	N1	B1	1.634(3)
48	N1	C1	1.308(2)
49	N1	C8	1.437(2)
50	B1	C20	1.613(3)
51	B1	C14	1.614(3)
52	B1	O1	1.509(2)
53	C20	C21	1.397(3)
54	C20	C25	1.403(3)
55	C21	C22	1.398(3)
56	C22	C23	1.385(3)
57	C23	C24	1.383(4)
58	C24	C25	1.395(3)
59	C1	C2	1.437(2)
60	C2	C3	1.409(2)
61	C2	C7	1.411(3)
62	C3	C4	1.409(2)
63	C3	O1	1.346(2)
64	C4	C5	1.386(3)
65	C5	C6	1.399(3)
66	C6	C7	1.382(3)
67	C8	C9	1.395(3)
68	C8	C13	1.397(2)
69	C9	C10	1.394(3)
70	C10	C11	1.390(3)
71	C11	C12	1.388(3)
72	C12	C13	1.397(3)
73	C14	C15	1.415(3)
74	C14	C19	1.381(3)
75	C15	C16	1.401(4)
76	C16	C17	1.366(4)
77	C17	C18	1.388(5)
78	C18	C19	1.413(4)

Angles for compound 1

Number	Atom(1)	Atom(2)	Atom(3)	Angle
1	C29	H293	C26	73.6(6)
2	C26	H262	C29	74.8(6)
3	C28	O2	O2	70.4(5)
4	H261	C26	H262	109.3(6)
5	H261	C26	H263	109.6(6)
6	H261	C26	C28	110.7(6)
7	H261	C26	H293	111.0(7)
8	H261	C26	C26	59.5(4)

9	H261	C26	C29	151.1(8)
10	H262	C26	H263	109.5(6)
11	H262	C26	C28	108.1(6)
12	H262	C26	H293	41.3(3)
13	H262	C26	C26	134.3(6)
14	H262	C26	C29	44.5(4)
15	H263	C26	C28	109.6(6)
16	H263	C26	H293	70.5(5)
17	H263	C26	C26	115.9(6)
18	H263	C26	C29	93.5(6)
19	C28	C26	H293	135.1(7)
20	C28	C26	C26	52.4(3)
21	C28	C26	C29	75.5(5)
22	H293	C26	C26	169.4(7)
23	H293	C26	C29	60.0(5)
24	C26	C26	C29	125.5(6)
25	O2	C28	C26	125.4(4)
26	O2	C28	C29	115.3(4)
27	O2	C28	O2	39.3(3)
28	O2	C28	C26	155.8(4)
29	O2	C28	C29	88.8(4)
30	C26	C28	C29	114.4(4)
31	C26	C28	O2	155.8(4)
32	C26	C28	C26	75.2(4)
33	C26	C28	C29	40.9(3)
34	C29	C28	O2	88.8(4)
35	C29	C28	C26	40.9(3)
36	C29	C28	C29	155.0(4)
37	O2	C28	C26	125.4(4)
38	O2	C28	C29	115.3(4)
39	C26	C28	C29	114.4(4)
40	H291	C29	H292	109.4(5)
41	H291	C29	H293	109.5(5)
42	H291	C29	C28	109.8(4)
43	H291	C29	H262	137.3(7)
44	H291	C29	C26	129.2(6)
45	H292	C29	H293	109.4(5)
46	H292	C29	C28	108.8(4)
47	H292	C29	H262	70.4(4)
48	H292	C29	C26	120.5(6)
49	H293	C29	C28	109.9(4)
50	H293	C29	H262	41.6(3)
51	H293	C29	C26	46.5(4)
52	C28	C29	H262	110.3(5)

53	C28	C29	C26	63.6(5)
54	H262	C29	C26	60.8(5)
55	C26	H293	C29	73.6(6)
56	C29	H262	C26	74.8(6)
57	O2	O2	C28	70.4(5)
58	H293	C26	C26	169.4(7)
59	H293	C26	C28	135.1(7)
60	H293	C26	C29	60.0(5)
61	H293	C26	H261	111.0(7)
62	H293	C26	H262	41.3(3)
63	H293	C26	H263	70.5(5)
64	C26	C26	C28	52.4(3)
65	C26	C26	C29	125.5(6)
66	C26	C26	H261	59.5(4)
67	C26	C26	H262	134.3(6)
68	C26	C26	H263	115.9(6)
69	C28	C26	C29	75.5(5)
70	C28	C26	H261	110.7(6)
71	C28	C26	H262	108.1(6)
72	C28	C26	H263	109.6(6)
73	C29	C26	H261	151.1(8)
74	C29	C26	H262	44.5(4)
75	C29	C26	H263	93.5(6)
76	H261	C26	H262	109.3(6)
77	H261	C26	H263	109.6(6)
78	H262	C26	H263	109.5(6)
79	H262	C29	C26	60.8(5)
80	H262	C29	C28	110.3(5)
81	H262	C29	H291	137.3(7)
82	H262	C29	H292	70.4(4)
83	H262	C29	H293	41.6(3)
84	C26	C29	C28	63.6(5)
85	C26	C29	H291	129.2(6)
86	C26	C29	H292	120.5(6)
87	C26	C29	H293	46.5(4)
88	C28	C29	H291	109.8(4)
89	C28	C29	H292	108.8(4)
90	C28	C29	H293	109.9(4)
91	H291	C29	H292	109.4(5)
92	H291	C29	H293	109.5(5)
93	H292	C29	H293	109.4(5)
94	B1	N1	C1	117.9(1)
95	B1	N1	C8	123.9(1)
96	C1	N1	C8	118.3(1)

97	N1	B1	C20	109.4(1)
98	N1	B1	C14	111.5(1)
99	N1	B1	O1	104.0(1)
100	C20	B1	C14	113.7(1)
101	C20	B1	O1	110.2(1)
102	C14	B1	O1	107.7(1)
103	B1	C20	C21	126.1(2)
104	B1	C20	C25	117.7(2)
105	C21	C20	C25	116.2(2)
106	H21	C21	C20	119.6(2)
107	H21	C21	C22	117.9(2)
108	C20	C21	C22	122.4(2)
109	H22	C22	C21	120.5(2)
110	H22	C22	C23	119.6(2)
111	C21	C22	C23	119.8(2)
112	H23	C23	C22	120.1(2)
113	H23	C23	C24	120.4(2)
114	C22	C23	C24	119.4(2)
115	H24	C24	C23	121.5(2)
116	H24	C24	C25	118.2(2)
117	C23	C24	C25	120.3(2)
118	H25	C25	C20	119.5(2)
119	H25	C25	C24	118.0(2)
120	C20	C25	C24	122.0(2)
121	H1	C1	N1	119.9(2)
122	H1	C1	C2	117.9(2)
123	N1	C1	C2	122.2(2)
124	C1	C2	C3	117.8(2)
125	C1	C2	C7	121.1(2)
126	C3	C2	C7	120.6(2)
127	C2	C3	C4	119.1(2)
128	C2	C3	O1	120.6(2)
129	C4	C3	O1	120.1(2)
130	H4	C4	C3	118.1(2)
131	H4	C4	C5	122.9(2)
132	C3	C4	C5	118.9(2)
133	H5	C5	C4	118.6(2)
134	H5	C5	C6	119.2(2)
135	C4	C5	C6	122.2(2)
136	H6	C6	C5	123.6(2)
137	H6	C6	C7	117.0(2)
138	C5	C6	C7	119.3(2)
139	H7	C7	C2	121.7(2)
140	H7	C7	C6	118.7(2)

141	C2	C7	C6	119.7(2)
142	N1	C8	C9	120.1(2)
143	N1	C8	C13	119.4(2)
144	C9	C8	C13	120.5(2)
145	H9	C9	C8	120.4(2)
146	H9	C9	C10	120.0(2)
147	C8	C9	C10	119.6(2)
148	H10	C10	C9	121.4(2)
149	H10	C10	C11	118.5(2)
150	C9	C10	C11	120.1(2)
151	H11	C11	C10	118.0(2)
152	H11	C11	C12	121.6(2)
153	C10	C11	C12	120.3(2)
154	H12	C12	C11	119.7(2)
155	H12	C12	C13	119.9(2)
156	C11	C12	C13	120.2(2)
157	H13	C13	C8	118.5(2)
158	H13	C13	C12	122.1(2)
159	C8	C13	C12	119.3(2)
160	B1	C14	C15	122.7(2)
161	B1	C14	C19	120.9(2)
162	C15	C14	C19	116.4(2)
163	H15	C15	C14	117.3(2)
164	H15	C15	C16	121.0(2)
165	C14	C15	C16	121.7(2)
166	H16	C16	C15	121.0(3)
167	H16	C16	C17	118.8(3)
168	C15	C16	C17	120.1(3)
169	H17	C17	C16	122.2(3)
170	H17	C17	C18	117.4(3)
171	C16	C17	C18	120.2(3)
172	H18	C18	C17	117.0(3)
173	H18	C18	C19	123.7(3)
174	C17	C18	C19	119.2(3)
175	H19	C19	C14	117.2(2)
176	H19	C19	C18	120.4(2)
177	C14	C19	C18	122.3(2)
178	B1	O1	C3	118.0(1)

Optical properties and theoretical calculations

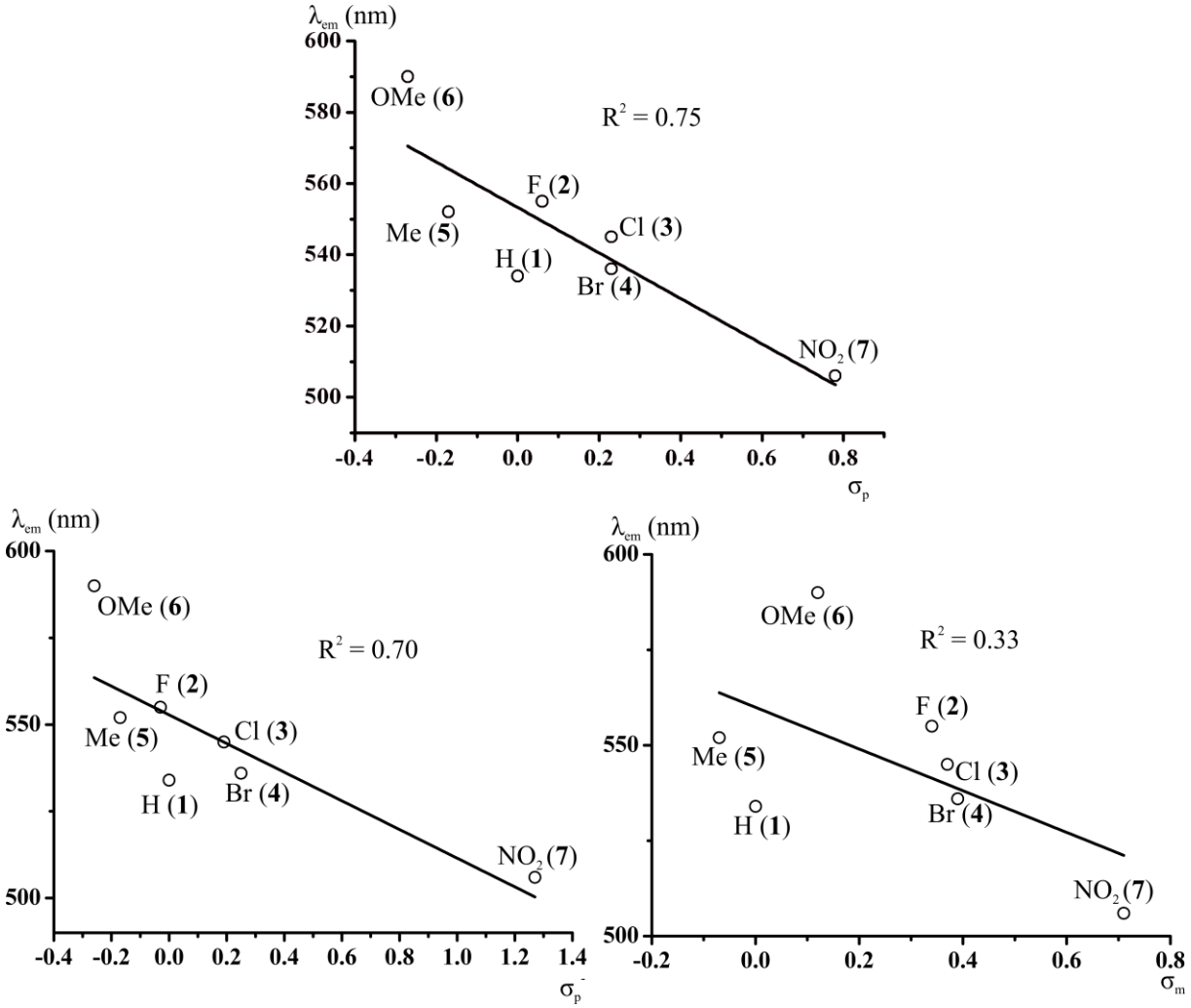


Figure S5. Plots of maxima of emission for compounds **1-7** *versus* Hammett (σ_p, σ_p^- and σ_m) constants. Correlations established for σ_p and σ_p^- are statistically meaningful according to F-test.

Comments on quantum yield quenching: Generally, there is a variety of processes that can be responsible for emission quenching. Quenching can be achieved either by collisions (*collisional* quenching) with small molecules (*e.g.* oxygen, water molecules) or by static (*static* quenching) formation of complexes between molecules in excited state and other species present in the solution. The former process can be distinguished in a series of experiments with varying concentration of a quencher whereas the latter can be observed by the analysis of band shifts in UV-Vis fluorescence spectra.

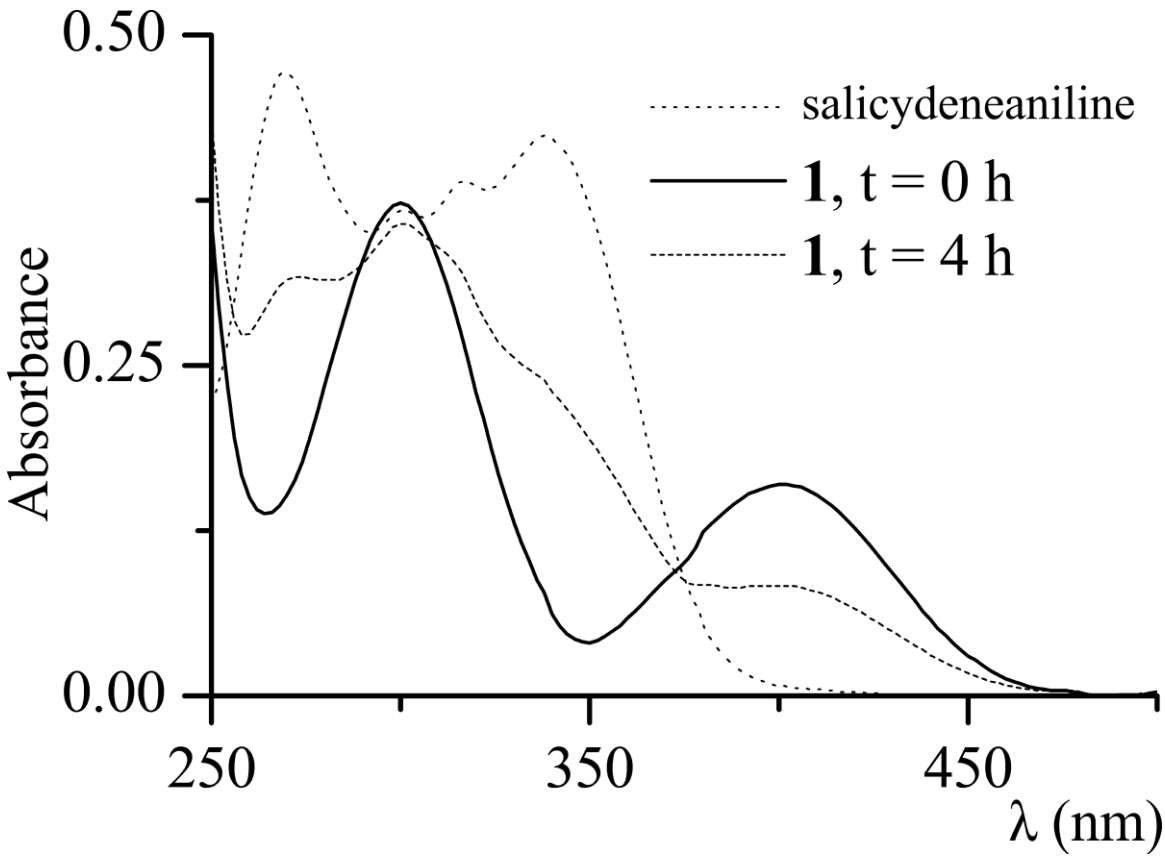


Figure S6. Overlay of the UV-Vis spectra of **1** (directly after preparation and after 4 hrs from preparation) and salicydeneaniline (solutions in CH_2Cl_2).

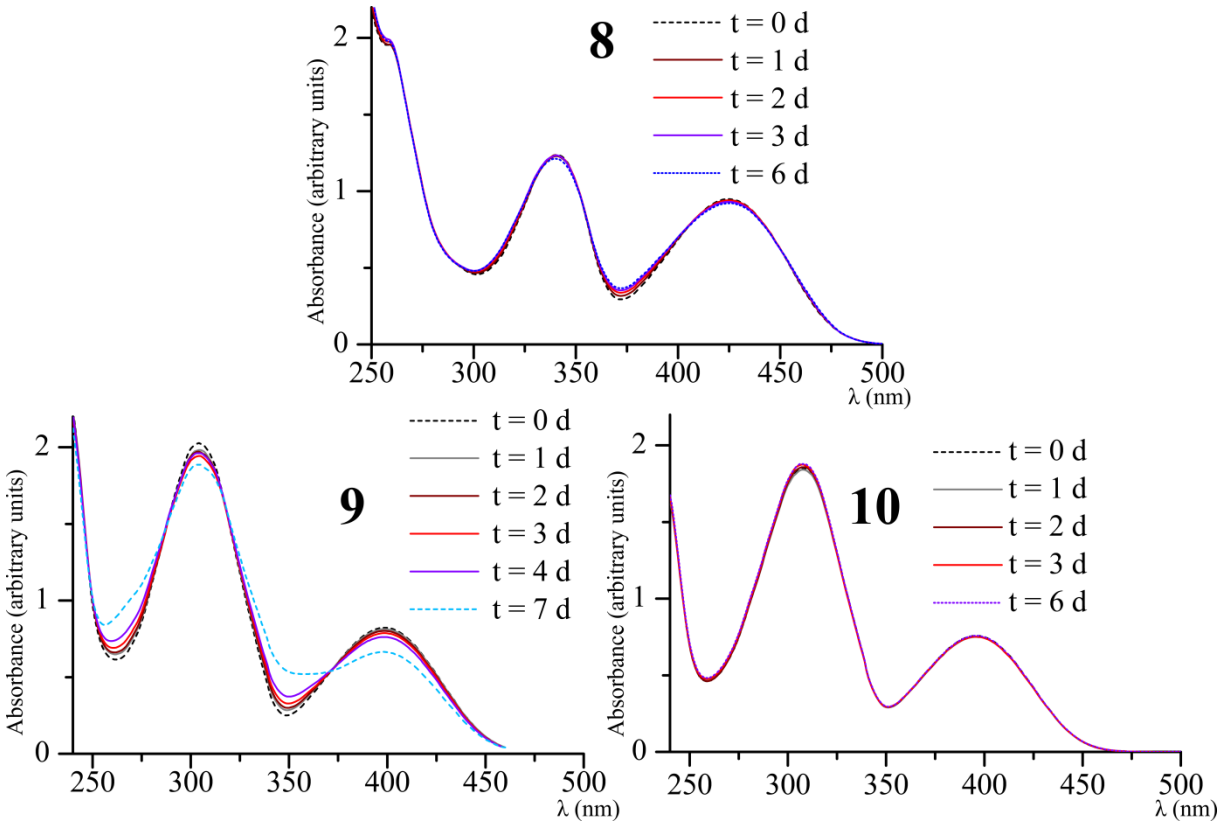


Figure S7. Time-dependent UV-Vis absorption spectra showing the stable nature of complexes **8-10**. Slight changes may be due to the solvent evaporation.

Full geometry optimizations for all compounds were at the RB3LYP/6-31+g(d,p) level of theory. In all cases C-H bond lengths were adjusted to standard neutron distances[6] prior to optimization. Geometries of the excited states along with absorption and emission spectra were obtained using TD-DFT method with the same basis set on the basis of the geometries obtained from ground state optimizations. Subsequently, the vibrational frequencies were calculated (for the ground state and for the first excited singlet state) and the results showed that optimized geometries are stable structures. Tight convergence criteria (*opt=tight*) were used along with high precision integrals (*int=UltraFine*) to obtain good quality wave functions. Wave functions were calculated without the use of symmetry constraints (*nosymm*). All calculations were performed using *Gaussian09*[7] suits of programs. *VMD*[8] and *POV-Ray*[9] programs were used for the visualization of molecular orbitals. AIM analyses[10] were done using *AIMall*[11] suits of programs.

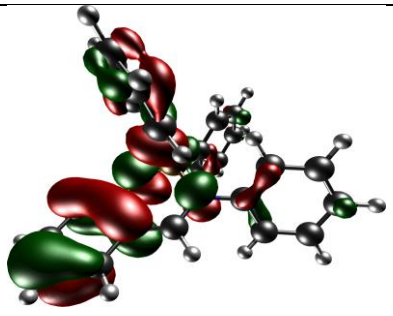
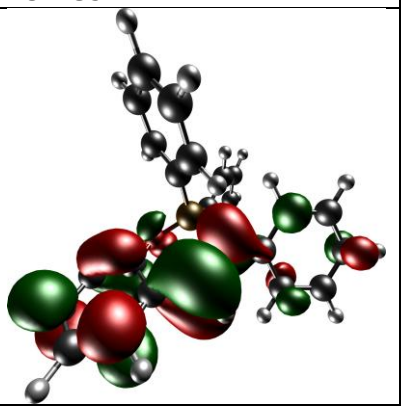
For the evaluation of the charge density distribution (CDD) we have implemented the 6-31+g(d,p) basis set instead of, for instance, the cc-pVDZ one. This is because such a level of theory predicted theoretical UV-Vis spectra correlating with experimental results. Hence, it should give a better description of CDD.

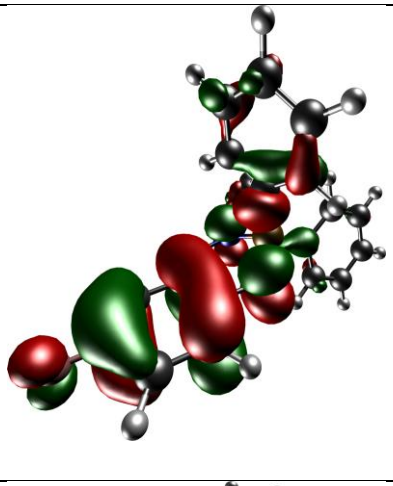
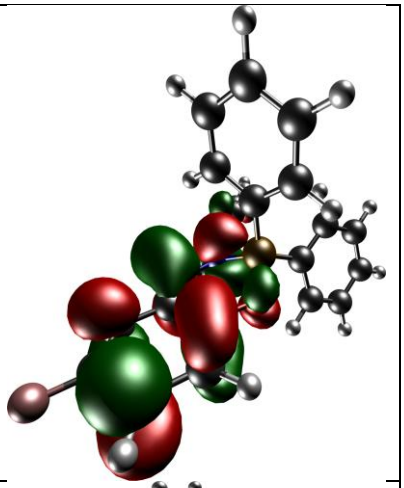
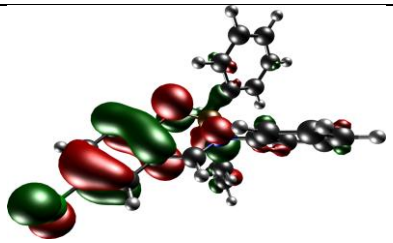
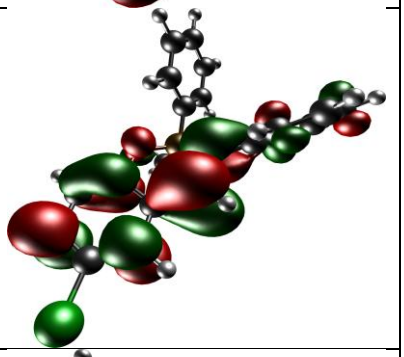
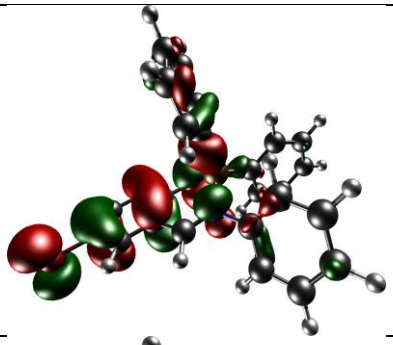
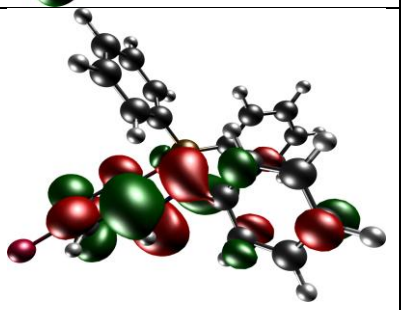
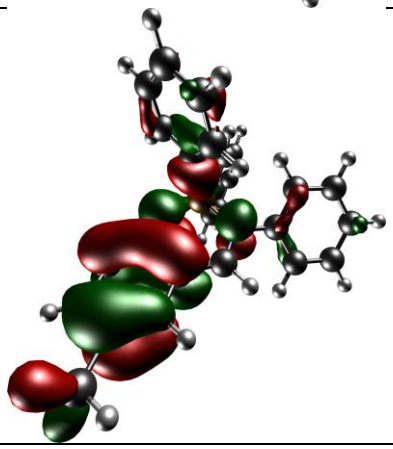
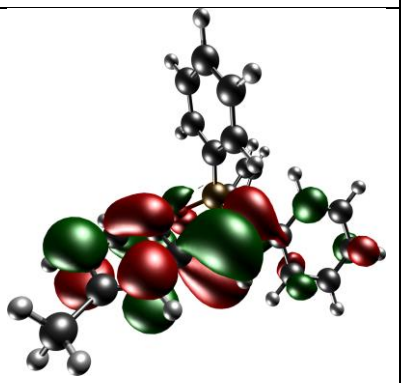
Table S3. Transitions during light excitation and emission calculated at the TD-RB3LYP/6-31+g(d,p) level of theory. Ani – aniline moiety, Sal – salicylaldehyde moiety, IL –intraligand charge transfer, LLCT- ligand to ligand charge transfer.

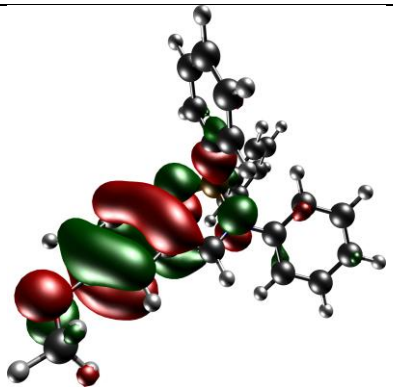
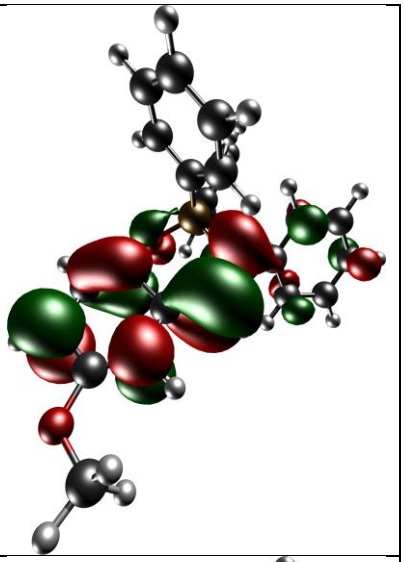
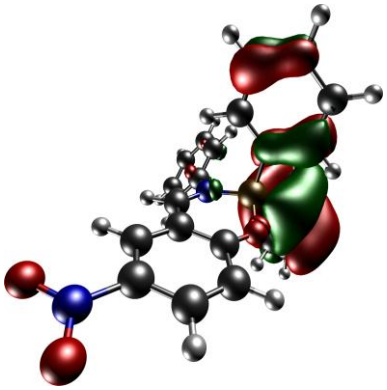
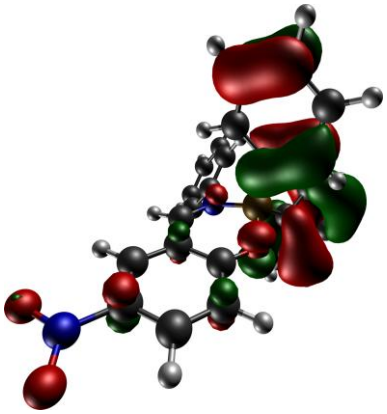
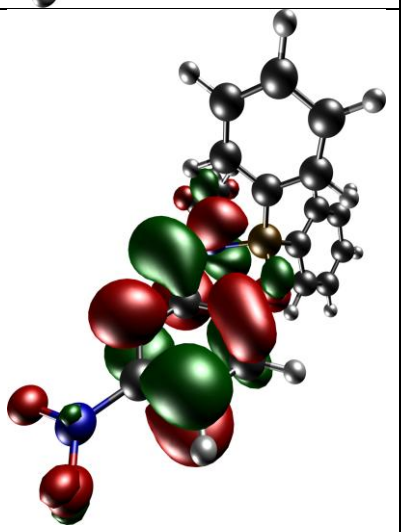
	Compound	transition character	
		Absorption	Emission
1	**$[Ph]_2$B[6-H-Sal][Ani]**	HOMO -> LUMO | π (Sal, Ph); *n* (N, O); *σ* (B-C) -> *π**(Sal, Ani,C-N, Ar-C=N); *n**(O-B) | IL/LLCT	HOMO–3 -> LUMO | *π* (Ph) -> *π**(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | LLCT
			HOMO–4 -> LUMO | *π* (Ph); *n* (O) -> *π**(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | LLCT
2	**$[Ph]_2$B[6-F-Sal][Ani]**	HOMO -> LUMO | *π* (Sal, Ph, Ani); *n* (O, N, F); σ (B-C) -> π*(Sal, Ani, C-N, Ar-C=N); *n**(O, N) | IL/LLCT	HOMO−3 -> LUMO | *π* (Sal, Ph); *n* (O, N) -> π*(Sal, Ani, C-N, Ar-C=N); *n**(O, N) | IL/LLCT
			HOMO−4 -> LUMO | *π* (Ph); *n* (O) -> π*(Sal, Ani, C-N, Ar-C=N); *n**(O, N) | LLCT
3	**$[Ph]_2$B[6-Cl-Sal][Ani]**	HOMO -> LUMO | *π* (Sal, Ph); *n* (Cl, O, N); *σ* (B-C) -> *π**(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT	HOMO–3 -> LUMO | *π* (Ph) -> *π**(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | LLCT
			HOMO–4 -> LUMO | *π* (Ph); *n* (O) -> *π**(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT

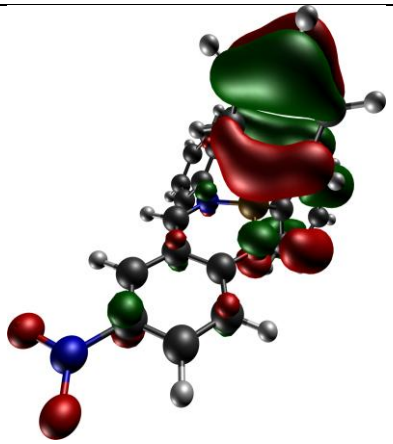
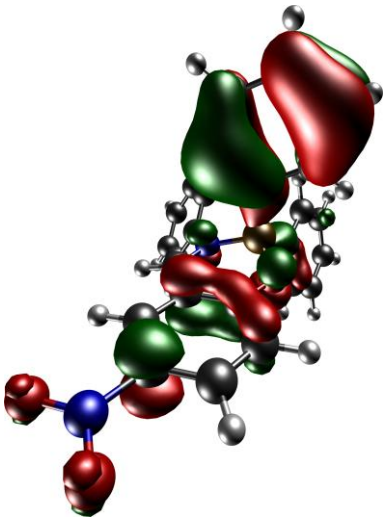
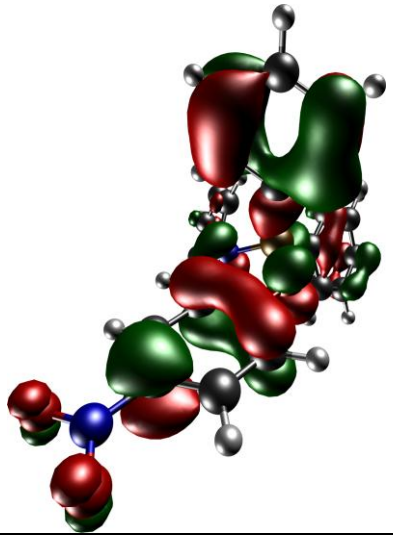
4	**$[Ph]_2B[6\text{-}Br\text{-}Sal][Ani]$**	HOMO -> LUMO | π (Sal, Ph); *n* (Br, O, N); σ (B-C) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT	HOMO–3 -> LUMO | π (Ph) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | LLCT
			HOMO–4 -> LUMO | π (Ph); *n* (O, N) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT
5	**$[Ph]_2B[6\text{-}Me\text{-}Sal][Ani]$**	HOMO -> LUMO | π (Sal, Ph); *n* (O, N); σ (B-C, Me) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT	HOMO -> LUMO | π (Ph, Sal, Ani, C-N); *n* (O-B) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT
6	**$[Ph]_2B[6\text{-}OMe\text{-}Sal][Ani]$**	HOMO -> LUMO | π (Sal, Ph); *n* (O, N, OMe); σ (B-C, Me) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT	HOMO -> LUMO | π (Ph, Sal, Ani, C-N); *n* (O-B) -> π^*(Ph, Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT
7	**$[Ph]_2B[6\text{-}NO_2\text{-}Sal][Ani]$**	HOMO–4-> LUMO | π (Sal, Ph); *n* (O-B, N-B, NO2); σ (B-C) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT	HOMO–3 -> LUMO | π (Ph); *n* (O, N) -> π^*(Sal, Ani, C-N, Ar-C=N); *n* (O-B, N-B, NO_2) | IL/LLCT
		HOMO–3 -> LUMO | π (Sal, Ph); *n* (O-B, N-B, NO2); σ (B-C) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT	HOMO–2 -> LUMO | π (Ph) -> π^*(Sal, Ani, C-N, Ar-C=N); *n* (O-B, N-B, NO_2) | LLCT
			HOMO–4 -> LUMO | π (Sal, Ph, Ani); *n* (O, N,NO_2,NO_2); σ (B-C) -> π^*(Sal, Ani, C-N, Ar-C=N); *n* (O-B, N-B, NO_2) | IL/LLCT
8	**$[Ph]_2B[Naft\text{-}Sal][Ani]$**	HOMO -> LUMO | π (Sal, Ph); *n* (O, N); σ (B-C) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O-B) | IL/LLCT	HOMO -> LUMO | π (Ph); *n* (N) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O,N) | IL/LLCT
9	**$[2,6\text{-}diFPh]_2B[6\text{-}H\text{-}Sal][Ani]$**	HOMO -> LUMO | π (Sal, Ph, Ani); *n* (O, N); σ (B-C) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O, N) | IL/LLCT	HOMO-3 -> LUMO | π (Sal, Ph, Ani); *n* (O, N); σ (B-C) -> π^*(Sal, Ani, , Ph, C-N, Ar-C=N); *n**(O, N) | IL/LLCT
10	**$[pentaFPh]_2B[6\text{-}H\text{-}Sal][Ani]$**	HOMO -> LUMO | π (Sal, Ph, Ani); *n* (O, N); σ (B-C) -> π^*(Sal, Ani, C-N, Ar-C=N); *n**(O, N) | IL/LLCT	--

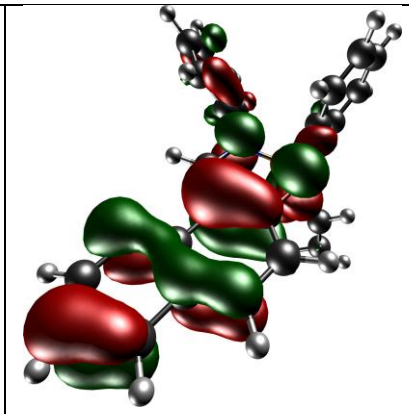
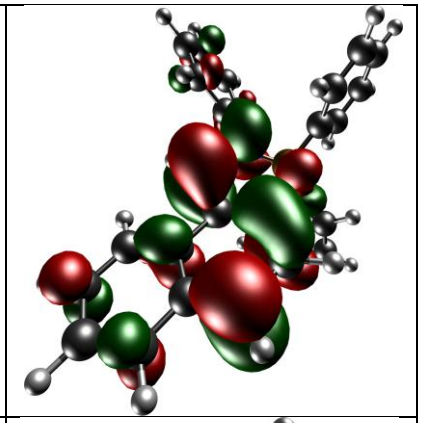
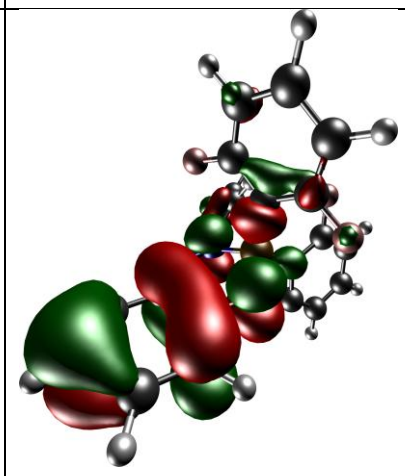
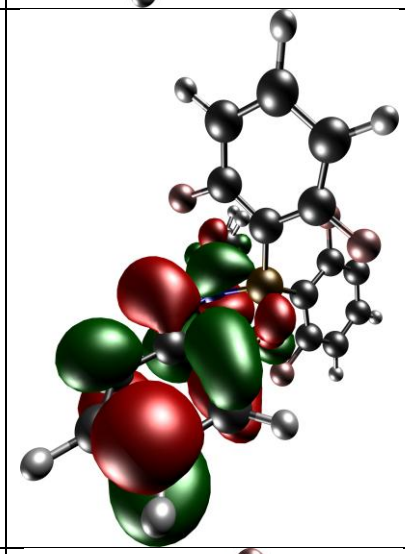
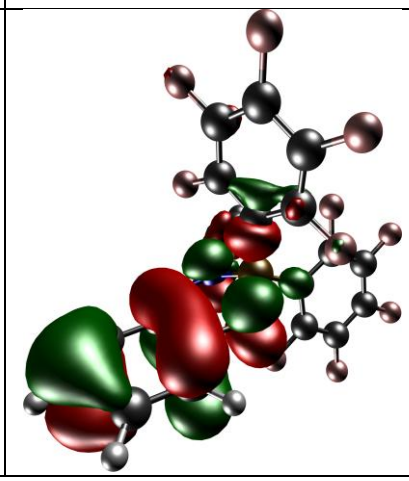
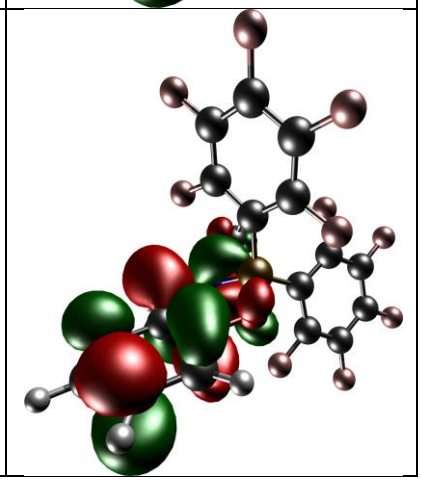
Orbitals generated for ground state geometries (TD-RB3LYP/6-31+g(d,p)).

	HOMOs	LUMOs
$[Ph]_2B[6\text{-}H\text{-}Sal][Ani]$		

$[Ph]_2B[6\text{-}F\text{-}Sal][Ani]$		
$[Ph]_2B[6\text{-}Cl\text{-}Sal][Ani]$		
$[Ph]_2B[6\text{-}Br\text{-}Sal][Ani]$		
$[Ph]_2B[6\text{-}Me\text{-}Sal][Ani]$		

[Ph]$_2$B[6-OMe-Sal][Ani]		
[Ph]$_2$B[6-NO$_2$-Sal][Ani]	HOMO  HOMO−1  HOMO−2	

	 HOMO−3  HOMO−4 	

[Ph]$_2$B[Naft-Sal][Ani]		
[2,6-diFPh]$_2$B[6-H-Sal][Ani]		
[pentaFPh]$_2$B[6-H-Sal][Ani]		

Cartesian coordinates for ground state **[Ph]$_2$B[6-H-Sal][Ani] (1)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	15.29319500	5.43055900	4.82735900
H	12.61890200	7.90284200	8.97499200
H	10.91776300	6.10755900	8.72320100
H	11.25703600	4.25000100	7.10117100
H	13.31006700	4.21255900	5.69536400
H	15.77070300	7.22232700	3.25358700
H	17.46183300	7.33723200	1.44777200
H	19.88771300	7.28184800	2.00713600

H	20.59818400	7.10128700	4.38526200
H	18.90573000	6.95240800	6.18500100
H	18.82702300	8.97027100	7.92358200
H	19.71553000	11.21118300	7.41978700
H	18.32723900	12.85980400	6.17161500
H	16.03103300	12.22449300	5.44277600
H	15.14491100	9.98134800	5.95539800
H	17.48648400	5.15143000	7.28950000
H	18.48643500	3.91989200	9.15965000
H	18.62066900	4.95517900	11.42099800
H	17.72582800	7.25571400	11.76766400
H	16.73015900	8.49586000	9.88648900
N	16.24650300	6.93114700	5.86822300
B	16.30097800	7.81489300	7.26196500
C	17.02617000	6.93803000	8.42093900
C	17.53343100	5.63632700	8.26207400
C	18.10457800	4.92440900	9.32449000
C	18.17897900	5.50215000	10.59240500
C	17.67651800	6.79386600	10.78472100
C	17.11386200	7.49288100	9.71542500
C	15.26221700	6.08594300	5.69795600
C	14.13660400	6.00850700	6.57173700
C	13.95152900	7.05828000	7.51519600
C	12.76263300	7.08992900	8.27132700
C	11.82082400	6.08218000	8.11939200
C	12.00805000	5.02625400	7.20150800
C	13.15297500	5.00287600	6.42562600
C	17.23132200	7.03978200	4.83138900
C	16.82754700	7.15694000	3.49426600
C	17.78348000	7.23748800	2.48011500
C	19.14386300	7.21255000	2.79499700
C	19.54261900	7.11381000	4.13125300
C	18.59455600	7.03307800	5.15100300
C	16.91924600	9.27838900	6.96311200
C	18.20740800	9.66934500	7.36762500
C	18.71568500	10.94250700	7.08788900
C	17.93798400	11.86872900	6.38944900
C	16.64995700	11.50999200	5.98000000
C	16.15548900	10.23521700	6.26702500
O	14.84565800	8.02170600	7.63229000

Cartesian coordinates for ground state **[Ph]$_2$B[6-F-Sal][Ani] (2)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	7.60529600	-0.43683000	9.37601700
H	4.73321500	-1.43674900	4.76902700
H	6.86460000	-0.93798900	3.54176300
H	8.81233200	0.06416200	7.22353100
H	4.13388100	0.67661100	11.35596500
H	4.32740700	0.41658300	13.81003600
H	5.94581200	-1.20862000	14.77504900

H	7.35576400	-2.59123100	13.25836000
H	7.13752800	-2.35190000	10.80293000
H	1.79772300	0.02053200	10.23434100
H	0.19724700	-1.49721900	11.33001600
H	0.48104800	-3.96470200	11.14634000
H	2.39311100	-4.88389500	9.84026500
H	3.98866100	-3.35951900	8.74047900
H	5.31733800	1.95396300	9.49643700
H	4.57181000	4.24006700	9.01769900
H	2.50119300	4.63809300	7.69220900
H	1.19267100	2.68948500	6.85332500
H	1.93631300	0.39275100	7.34286200
N	5.55798900	-0.62946300	9.50318800
O	4.43464000	-1.21066300	7.34647900
B	4.11920100	-0.58062700	8.68820600
C	6.66857900	-0.51033800	8.82370700
C	6.71335900	-0.51282700	7.39522700
C	5.54755100	-0.92733800	6.69445600
C	5.61962700	-1.10209400	5.29639600
C	6.79875900	-0.82773700	4.61936700
C	7.92855000	-0.39773100	5.33049300
C	7.91606200	-0.24895800	6.69712700
C	5.64984000	-0.79321100	10.92510000
C	4.83769600	-0.03193800	11.77440300
C	4.95461700	-0.18151400	13.15607100
C	5.86577200	-1.09254000	13.69853100
C	6.66130700	-1.86401600	12.84860100
C	6.55222600	-1.72021500	11.46439700
C	3.04092100	-1.54073900	9.41333800
C	1.94791500	-1.05281000	10.15026600
C	1.03330100	-1.91035400	10.77120000
C	1.19002400	-3.29427100	10.66780400
C	2.26451800	-3.80848600	9.93540700
C	3.16953600	-2.94007100	9.32008700
C	3.68778400	0.96872800	8.46701900
C	4.40564900	2.09008900	8.91889400
C	3.98872000	3.39975800	8.64919000
C	2.82987600	3.62454700	7.90531000
C	2.09657400	2.52925200	7.43565100
C	2.52189600	1.22964600	7.71597100
F	9.07040900	-0.13574400	4.63644400

Cartesian coordinates for ground state **$[Ph]_2$B[6-Cl-Sal][Ani] (3)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	7.60429800	-0.44284600	9.37503800
H	4.73859700	-1.42787100	4.76054600
H	6.85981100	-0.95421700	3.54469400
H	8.80787800	0.03305500	7.24401700
H	4.14226500	0.69887400	11.34786100
H	4.33321900	0.44594900	13.80303200

H	5.93780700	-1.18919200	14.77409900
H	7.33664800	-2.58879900	13.26269800
H	7.12098100	-2.35622700	10.80628900
H	1.80475800	0.01022300	10.25286700
H	0.21185900	-1.51885000	11.34348500
H	0.49492600	-3.98426700	11.13319300
H	2.39883600	-4.88982800	9.80587700
H	3.98694600	-3.35432000	8.71136900
H	5.33086800	1.95771100	9.47434400
H	4.58366400	4.24436200	9.00185800
H	2.49332700	4.64447300	7.70833700
H	1.16701900	2.69727000	6.89463000
H	1.91244600	0.39993400	7.37762200
N	5.55625300	-0.62624500	9.49987400
O	4.43025700	-1.19542300	7.33813400
B	4.11735000	-0.57493000	8.68747300
C	6.66794500	-0.51377600	8.82170600
C	6.71431600	-0.52026600	7.39302400
C	5.54616400	-0.92499300	6.69065400
C	5.62460800	-1.10094000	5.29373800
C	6.80836600	-0.83748300	4.62221400
C	7.95381500	-0.41485300	5.32573500
C	7.91949500	-0.26964900	6.69825000
C	5.64601500	-0.78514900	10.92294900
C	4.83989300	-0.01416000	11.76906400
C	4.95541200	-0.15976800	13.15129900
C	5.85886100	-1.07640100	13.69715700
C	6.64821600	-1.85742700	12.85021600
C	6.54062600	-1.71763600	11.46547600
C	3.04303500	-1.54239600	9.40819500
C	1.95468700	-1.06213500	10.15699000
C	1.04434300	-1.92612400	10.77514800
C	1.20070000	-3.30890400	10.65689200
C	2.27059200	-3.81548300	9.91261200
C	3.17146500	-2.94067700	9.30023600
C	3.68273700	0.97407900	8.47308800
C	4.41060600	2.09467600	8.91080200
C	3.99271100	3.40470200	8.64464100
C	2.82280600	3.63061300	7.91863800
C	2.07948600	2.53612700	7.46314800
C	2.50583200	1.23608300	7.73980700
Cl	9.43765500	-0.08939900	4.44038500

Cartesian coordinates for ground state **[Ph]$_2$B[6-Br-Sal][Ani] (4)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	0.96984400	14.78450800	7.14329300
H	-1.86315200	13.77633700	11.77387700
H	-3.68502400	12.97295900	10.28250000
H	-1.19100300	13.58632600	6.83588900
H	1.76846700	17.06186900	7.39410400

H	3.63632700	18.22639500	6.25943700
H	5.97840900	17.45400200	6.60303400
H	6.42712200	15.50410400	8.08229300
H	4.55587900	14.32126000	9.18918400
H	2.11320600	12.91057100	12.80406600
H	2.76612600	10.56037800	13.14716000
H	3.49499300	9.16530600	11.21443600
H	3.54551100	10.16663900	8.93469500
H	2.88720400	12.50325100	8.59178100
H	1.18319500	17.04056000	11.23644600
H	2.34476900	18.77442100	12.54839000
H	4.58367200	18.30719600	13.53588500
H	5.63465400	16.07646000	13.18699800
H	4.47206700	14.34962600	11.87025400
B	1.94844800	14.45658300	10.54478200
N	1.95118600	14.89606000	8.95147600
O	0.48870000	14.54092800	10.95021000
C	0.91582700	14.59091400	8.21450600
C	-0.29427300	14.05423500	8.75410400
C	-0.47221800	14.09793400	10.16403600
C	-1.72127600	13.72440100	10.69990200
C	-2.73199500	13.27768800	9.86317400
C	-2.53563200	13.21431700	8.46993900
C	-1.33707300	13.60926000	7.91122900
C	3.04125800	15.59222300	8.33142000
C	2.78540000	16.69961300	7.51127500
C	3.84194500	17.36367700	6.88587600
C	5.15582900	16.93367900	7.08405000
C	5.40789800	15.83984600	7.91733500
C	4.35883600	15.17050400	8.54702200
C	2.44775100	12.91732500	10.67068700
C	2.42701700	12.31793800	11.94803100
C	2.79570400	10.98651800	12.14750700
C	3.20483400	10.20155600	11.06383000
C	3.23416200	10.76459200	9.78755400
C	2.85794900	12.10090800	9.60197900
C	2.73993400	15.55644600	11.42341700
C	2.16720400	16.82365900	11.64593500
C	2.81762600	17.80759000	12.39443100
C	4.07383400	17.54656500	12.95057400
C	4.66253800	16.29574300	12.75246900
C	3.99946900	15.31984900	12.00045500
Br	-3.95704900	12.60908200	7.35237600

Cartesian coordinates for ground state **[Ph]$_2$B[6-Me-Sal][Ani] (5)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	-0.81635500	7.53796600	6.09577000
H	-2.64587900	8.73733100	7.25713100
H	-5.00715500	8.01039700	6.94541300
H	-5.51262000	6.07070700	5.47067300

H	-3.67933900	4.85362800	4.33785200
H	-2.03162500	2.99794200	4.88663600
H	-2.76267400	0.68449900	4.52735900
H	-2.78859600	-0.28610500	2.23361400
H	-2.06165200	1.11549600	0.30465200
H	-1.33689400	3.44206200	0.66541900
H	-0.24043400	7.50488200	2.22122100
H	-1.37075400	9.27905600	0.93441800
H	-3.65030700	8.89307800	0.00602800
H	-4.77327600	6.70304300	0.38854300
H	-3.64132700	4.93737100	1.67951700
C	-0.02233900	5.04749600	5.26324000
C	1.16990600	4.49123900	4.71311700
C	1.33514100	4.54021600	3.30314100
C	2.57724000	4.15417100	2.76072600
C	3.58328700	3.69559700	3.59634300
C	3.43177000	3.61554700	5.00411500
C	2.22427000	4.03230500	5.53986300
C	4.55786500	3.09846700	5.86854900
C	-2.12853600	6.09430100	5.17404400
C	-1.84171000	7.19588500	5.99202200
C	-2.87668500	7.87939300	6.63273800
C	-4.20124400	7.47503700	6.45270300
C	-4.48500900	6.38702800	5.62199100
C	-3.45734600	5.69847100	4.97774700
C	-1.62634700	3.42861000	2.80501500
C	-2.03559100	2.60830400	3.87105700
C	-2.45271500	1.28546900	3.67596300
C	-2.46615600	0.73949400	2.39193100
C	-2.05816800	1.52818700	1.31045800
C	-1.64894100	2.84625000	1.51990500
C	-1.85472300	6.07968900	2.07901800
C	-1.24200500	7.32458000	1.83763100
C	-1.87497400	8.33065100	1.10332500
C	-3.15383900	8.11529500	0.58032000
C	-3.78274600	6.88729600	0.79716700
C	-3.13685500	5.88943000	1.53515300
H	-0.06491500	5.23569200	6.33618200
H	2.71387900	4.20986700	1.68596400
H	4.52745500	3.38407000	3.15461600
H	2.07068000	4.01066200	6.61708000
H	4.30414600	3.16209100	6.93064200
H	5.47978900	3.67011300	5.71025500
H	4.78461600	2.04931600	5.64380600
N	-1.06107900	5.37908700	4.53803500
B	-1.08129000	4.95292500	2.94314400
O	0.37385500	5.00181600	2.52405100

Cartesian coordinates for ground state **$[Ph]_2$B[6-OMe-Sal][Ani] (6)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	1.13855900	3.76890600	5.50383900
H	2.24354200	1.83341900	4.45529100
H	1.19725200	-0.42379300	4.57258800
H	-0.97866500	-0.70517100	5.75306900
H	-2.08273600	1.23786400	6.79572500
H	-1.32501200	5.00777300	4.45470500
H	-0.70822700	7.24717500	3.63354900
H	0.15826700	8.96879900	5.21436200
H	0.38178700	8.40672800	7.63047400
H	-0.24276800	6.18005800	8.44862200
H	1.38360200	4.26308100	8.11645500
H	3.31839700	3.28658200	9.31106300
H	2.96068800	1.65183200	11.15303300
H	0.64328800	0.98358800	11.77286000
H	-1.28971700	1.93720600	10.55305500
H	-2.06999600	4.23246900	10.42090100
H	-5.20293300	4.32098800	5.88988400
H	-6.93674400	5.40193000	7.32588200
H	-4.19388000	5.48686000	10.63298800
H	-5.69952700	7.23368100	11.17627400
H	-6.29298200	5.63036000	11.71510700
H	-7.44801000	6.95785600	11.41347300
O	-6.71756400	6.12387600	9.73116800
N	-1.20126000	3.77253900	8.60973600
B	-1.30808400	3.90483800	6.96758000
C	-2.19399100	4.22150300	9.33791900
C	-3.43513600	4.65450700	8.78635400
C	-3.69956200	4.33212200	7.43147100
C	-4.99078300	4.58663700	6.91986100
C	-5.94800800	5.18340300	7.71761000
C	-5.67786200	5.53238700	9.06394200
C	-4.43301500	5.25568200	9.60079700
C	-6.51319300	6.50232300	11.08513900
C	-0.07757700	3.19233700	9.28362100
C	1.22556000	3.55105500	8.91679200
C	2.31104700	2.99905000	9.59655100
C	2.11042800	2.08274000	10.63318500
C	0.81074900	1.71232400	10.98537400
C	-0.28169100	2.26002400	10.31049600
C	-0.83276600	5.39303100	6.52123600
C	-0.95067400	5.74591600	5.16013500
C	-0.60289500	7.01350100	4.69008300
C	-0.11670600	7.98157800	5.57584100
C	0.00945000	7.66431400	6.92878900
C	-0.34766000	6.38950100	7.38632300
C	-0.55395300	2.66302800	6.25806500
C	0.66932200	2.79105400	5.57763000
C	1.29928800	1.69588800	4.97640500
C	0.71314500	0.42982300	5.03973300
C	-0.50750400	0.27351900	5.70391400

C	-1.12525700	1.37639600	6.29888500
O	-2.78563700	3.74141400	6.68046600

Cartesian coordinates for ground state **$[Ph]_2B[6\text{-}NO_2\text{-}Sal][Ani]$ (7)** calculated at the RB3LYP/6-31+g(d,p) level of theory

N	6.78146300	2.09613100	13.17502400
N	1.93529900	5.42137800	11.50905700
H	6.44967900	4.12338100	13.31705100
H	2.89875400	1.02609900	10.41204500
H	1.46042400	3.07515800	10.32527100
H	4.24944800	5.19734000	12.79509200
H	7.93938100	0.74858100	15.18148500
H	10.23426400	1.08988700	16.04620200
H	11.72066300	2.79862400	15.01642300
H	10.89767500	4.15190300	13.09544200
H	8.61198900	3.78877400	12.21293300
H	7.60347900	-1.58709700	13.93465100
H	9.36890200	-2.97168700	12.92137800
H	10.10304100	-2.55261400	10.57901100
H	9.03324100	-0.72424100	9.26820800
H	7.26376000	0.65633900	10.28454800
H	5.58811600	1.75743600	15.45151400
H	4.26181700	0.83298600	17.29325900
H	3.22542500	-1.42238000	17.09102500
H	3.54509900	-2.73250800	14.99536200
H	4.88416200	-1.80853000	13.14674200
O	5.13359800	0.86935200	11.72931300
O	0.89613300	5.35457700	10.84652600
O	2.30784200	6.42914800	12.11889300
C	6.05009300	3.16146300	12.99681100
C	4.76394300	3.13031900	12.36626200
C	4.37318600	1.93339100	11.69290200
C	3.17954600	1.93418900	10.93355800
C	2.38774000	3.06509900	10.88556600
C	2.77921800	4.23199800	11.57382200
C	3.95993000	4.27857300	12.29689300
C	8.12016900	2.27182800	13.66743600
C	8.58658000	1.49075400	14.73102600
C	9.87912400	1.69129700	15.21504800
C	10.71332900	2.65351500	14.63849200
C	10.25048400	3.41743900	13.56493100
C	8.95741100	3.22638100	13.07520300
C	7.29774500	-0.33499800	12.20301100
C	7.91516300	-1.37841000	12.91456500
C	8.91591600	-2.17080000	12.34257700
C	9.32784200	-1.93792000	11.02853800
C	8.72739000	-0.91061700	10.29459900
C	7.72901200	-0.12698900	10.87861700
C	5.35910200	0.05215500	14.13586100
C	5.15298500	0.76810200	15.32879400

C	4.39640900	0.24884600	16.38652400
C	3.81393700	-1.01408200	16.27408500
C	3.99510400	-1.74831600	15.09703900
C	4.75557100	-1.22065800	14.05219500
B	6.15299400	0.60849500	12.83724500

Cartesian coordinates for ground state **$[Ph]_2$B[Naft-Sal][Ani] (8)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	4.29011700	13.49421400	5.12728300
H	6.70958700	18.20621800	6.56075200
H	4.92804000	19.37262000	5.28466800
H	2.81561000	19.34557500	4.06212600
H	0.87323000	18.11278000	3.13153500
H	0.70637800	15.64692500	3.46614000
H	2.42774000	14.43378100	4.70219600
H	7.07897500	15.82623700	9.92443900
H	5.77005400	16.19491700	11.97916200
H	3.57683500	15.05254800	12.29155200
H	2.71673900	13.54779500	10.50300900
H	4.01502000	13.19263000	8.45062600
H	8.78735400	14.37214200	5.97707200
H	11.06299600	13.46425100	6.24496200
H	11.69941800	12.27883400	8.34182700
H	10.01821200	12.02145400	10.16138300
H	7.74372600	12.92728700	9.88610300
N	5.77183300	13.46169300	6.54766800
B	6.58297900	14.31116700	7.68057500
C	4.89116300	14.09634500	5.80487100
C	4.74038500	15.50871900	5.79519600
C	5.79713600	16.26007700	6.36283400
C	5.86732600	17.66674100	6.14135900
C	4.87855500	18.29705000	5.43601900
C	3.75824200	17.58978100	4.89332200
C	2.73561000	18.26882400	4.18791600
C	1.65306900	17.58338500	3.66998200
C	1.56271000	16.18882900	3.85706100
C	2.54674100	15.50141000	4.54792400
C	3.67668300	16.17430000	5.07354300
C	5.97562300	12.06453000	6.30708300
C	6.03736800	11.16912300	7.38256400
C	6.20862500	9.80661300	7.13943600
C	6.32769200	9.32668000	5.83168800
C	6.28235300	10.22233700	4.76112800
C	6.11307400	11.58819100	4.99559300
C	5.66542500	14.47442600	9.00963100
C	6.12233400	15.32208600	10.04061900
C	5.38479200	15.53373800	11.20691200
C	4.15326800	14.89350900	11.38419900
C	3.67376900	14.04924500	10.38186000
C	4.42237300	13.85071700	9.21496700

C	8.06677300	13.70834600	7.90109100
C	9.04186600	13.84557100	6.89419800
C	10.33500900	13.33833600	7.04267900
C	10.69424000	12.67359800	8.21942300
C	9.74984100	12.52875400	9.23798900
C	8.45831300	13.04179700	9.07493500
O	6.76504500	15.68141700	7.03347400
H	5.94192800	11.53738000	8.39652200
H	6.25021800	9.11838200	7.97822900
H	6.46698800	8.26531400	5.65011900
H	6.39666700	9.86423100	3.74231200
H	6.12448300	12.28839200	4.16565900

Cartesian coordinates for ground state **[2,6-diFPh]$_2$B[6-H-Sal][Ani] (9)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	7.60974700	-0.52934800	9.36943800
H	4.65119500	-1.31649500	4.77577900
H	6.78913500	-0.99361200	3.54675800
H	8.82938000	-0.15868600	7.23808300
H	4.28938800	0.38815800	13.81177000
H	5.89370800	-1.25360100	14.77466100
H	7.31076900	-2.62604400	13.25434900
H	0.14665400	-1.62468300	11.24629800
H	0.55252400	-4.09719400	11.03230300
H	2.62396000	-4.88970500	9.84201400
H	4.56891200	4.36122600	8.96237100
H	2.48158800	4.72163600	7.60557500
H	1.17987800	2.71064000	6.82735400
N	5.55922400	-0.61508600	9.50540900
O	4.37863700	-1.05602500	7.34428400
B	4.14024100	-0.50331300	8.71918900
C	6.67055300	-0.55685300	8.81912800
C	6.71070100	-0.56165100	7.39427900
C	5.51259600	-0.87779800	6.69520000
C	5.56484900	-1.05459500	5.29833500
C	6.76512500	-0.87300800	4.62636900
C	7.95350600	-0.53550200	5.30987900
C	7.92351900	-0.39579600	6.68545000
C	5.63922100	-0.78921200	10.92657500
C	4.82072700	-0.03586300	11.77723700
C	4.92114100	-0.20497300	13.15765200
C	5.82442000	-1.12489800	13.69878600
C	6.62470800	-1.88935800	12.84728100
C	6.52895800	-1.72944100	11.46374100
C	3.07731300	-1.49905900	9.45439600
C	1.92788800	-1.13166100	10.16110000
C	1.01368000	-2.01560700	10.72575100
C	1.25028500	-3.38431600	10.60428500
C	2.39310600	-3.83504900	9.94232200
C	3.25826700	-2.88868200	9.40648700

C	3.69329500	1.06563600	8.51153900
C	4.36549000	2.22745900	8.90103600
C	3.97087200	3.53011800	8.60555300
C	2.81433200	3.71828100	7.85196900
C	2.08609500	2.61027200	7.41414100
C	2.54595500	1.34455500	7.75154200
H	8.87912400	-0.39889400	4.76109400
F	1.80523000	0.29201700	7.30550900
F	5.51712800	2.11918300	9.64249900
F	1.66513400	0.19580300	10.34906000
F	4.38780200	-3.37509400	8.80939400
H	7.11138600	-2.36207800	10.80101700
H	4.12269400	0.68286500	11.36692000

Cartesian coordinates for ground state **[pentaFPh]$_2$B[6-H-Sal][Ani] (10)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	7.61225000	-0.51306300	9.37286200
H	4.65837800	-1.31949600	4.78023100
H	6.79097500	-0.97108400	3.54864800
H	8.82947600	-0.11683800	7.23622100
H	4.16245000	0.70938700	11.39085100
H	4.32409600	0.37689000	13.82997700
H	5.88871900	-1.31628600	14.76740100
H	7.27366100	-2.69938400	13.22810300
H	7.07979600	-2.39804000	10.77817700
N	5.56163500	-0.60723000	9.50631700
O	4.38677300	-1.06372100	7.35191600
B	4.15478400	-0.50697200	8.71561100
C	6.67476100	-0.54159300	8.82006100
C	6.71436500	-0.54226700	7.39585900
C	5.52050200	-0.87087900	6.69659900
C	5.56929000	-1.04672600	5.30190100
C	6.76736900	-0.85145000	4.62815100
C	7.95273200	-0.50186400	5.31009600
C	7.92524500	-0.36334800	6.68551700
C	5.64064600	-0.79644800	10.92773100
C	4.84179000	-0.03407000	11.78868400
C	4.93941600	-0.22329500	13.16692300
C	5.82135300	-1.17178300	13.69361500
C	6.60371500	-1.94278600	12.83137100
C	6.51076500	-1.76275900	11.45007300
C	3.08000500	-1.49189000	9.45910300
C	1.94819400	-1.08941700	10.17119700
C	1.04392500	-1.97645700	10.75285000
C	1.26170200	-3.34546500	10.64374700
C	2.38778400	-3.80171000	9.96512600
C	3.26457700	-2.87889700	9.40137100
C	3.69067600	1.06322500	8.49994400
C	4.36654000	2.21713500	8.89973400
C	3.94852000	3.51145600	8.58672100

C	2.80008600	3.69463000	7.82718100
C	2.08913700	2.57775500	7.39419400
C	2.54412700	1.30774700	7.73147200
F	4.36204000	-3.39428700	8.79902100
F	2.62358100	-5.12183100	9.87295100
F	0.40562500	-4.21519500	11.19804000
F	-0.02756200	-1.52158400	11.42431100
F	1.68012000	0.22546200	10.35731200
F	1.80363100	0.26923900	7.28568400
F	0.97612500	2.73974800	6.65992100
F	2.38323500	4.92883100	7.51153600
F	4.65255600	4.57775200	9.00601200
F	5.50463700	2.14174900	9.64058500
H	8.87551700	-0.35511300	4.75945400

Cartesian coordinates for the first singlet excited state **[Ph]$_2$B[6-H-Sal][Ani] (1)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	15.19634001	5.48064140	4.71782165
H	12.84954347	7.65650259	9.24524749
H	10.87201761	6.17284688	8.77776717
H	10.92564126	4.65424542	6.80183984
H	12.89913084	4.61756519	5.30756234
H	15.91533546	6.87857683	3.17813346
H	17.69492691	6.90685630	1.47772557
H	20.08881464	7.06792330	2.15841869
H	20.65829975	7.18859451	4.58274709
H	18.88841881	7.11438324	6.28430780
H	18.80873579	9.01034646	7.86981958
H	19.54282471	11.32345577	7.48314768
H	18.02886157	12.95182859	6.36143516
H	15.76317073	12.21548266	5.62988466
H	15.02978712	9.89486309	6.01612603
H	17.19950337	5.00555213	7.36975696
H	18.55208090	3.90187868	9.12175565
H	19.06335563	5.09433509	11.24660090
H	18.25759823	7.42772022	11.58782979
H	16.88667236	8.52510652	9.83327949
N	16.24608574	6.91746557	5.84459118
B	16.28505385	7.75190701	7.14203385
C	17.07674906	6.88332642	8.44060363
C	17.43906550	5.53852157	8.28225554
C	18.19772647	4.91711252	9.27608909
C	18.50205353	5.59688989	10.46443045
C	18.04767233	6.90586724	10.65879132
C	17.28588551	7.53028809	9.66956046
C	15.14557353	6.13822971	5.57682645
C	13.99916517	6.11309537	6.41112289
C	13.94120050	6.96314635	7.55147411
C	12.84021692	6.98777180	8.39053247
C	11.73630137	6.15404015	8.12230201

C	11.76980513	5.30388448	7.01388122
C	12.88399429	5.27975550	6.16929795
C	17.26647011	6.97375849	4.86390940
C	16.95347072	6.91139103	3.49127692
C	17.96309497	6.94298833	2.53000203
C	19.30478451	7.04108249	2.90886042
C	19.62119063	7.11181373	4.26854571
C	18.61922725	7.07636698	5.23718147
C	16.86391700	9.25528041	6.96261808
C	18.12946892	9.69829110	7.37231610
C	18.55281042	11.01435268	7.15798592
C	17.70541105	11.92785565	6.52723936
C	16.43538881	11.51325513	6.11616647
C	16.02378500	10.19681025	6.33643495
O	14.99047454	7.79774819	7.80416454

Cartesian coordinates for the first singlet excited state **$[Ph]_2$B[6-F-Sal][Ani] (2)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	7.67742780	-0.57348699	9.37568245
H	4.64289446	-1.00883805	4.75582927
H	6.83410210	-0.98894838	3.47554037
H	8.97585333	-0.63651891	7.17957668
H	3.99919937	0.64269985	11.27438134
H	4.14724463	0.52991529	13.72514626
H	5.90047074	-0.86069396	14.82307933
H	7.48356638	-2.16641271	13.40636642
H	7.30962829	-2.09151528	10.95106656
H	1.83796820	-0.05738990	10.29989978
H	0.19853038	-1.64953624	11.20336053
H	0.45789346	-4.09143698	10.78959204
H	2.39661944	-4.90920615	9.45441877
H	4.04093878	-3.31144987	8.55100850
H	5.50518281	1.98161835	9.18957468
H	4.57457755	4.26923933	9.07199092
H	2.28580174	4.64609014	8.16751013
H	0.90486778	2.70649544	7.43146158
H	1.84933255	0.41346325	7.53575200
N	5.57838942	-0.62720261	9.51161642
O	4.41277410	-0.88386447	7.33022655
B	4.23797269	-0.59750139	8.74485098
C	6.75743513	-0.66054868	8.81082349
C	6.80849364	-0.73518033	7.39673692
C	5.59692121	-0.83942436	6.65391107
C	5.59308794	-0.92910696	5.27312212
C	6.80716566	-0.91927289	4.55610882
C	7.98479685	-0.80989077	5.28436767
C	8.02089697	-0.71609626	6.67069307
C	5.65368059	-0.70154781	10.92583167
C	4.75734800	0.02169351	11.73270113
C	4.84877356	-0.04006479	13.12262244

C	5.83306177	-0.81647822	13.74047071
C	6.72420721	-1.54153361	12.94465479
C	6.63787534	-1.48946974	11.55385483
C	3.08454316	-1.55235756	9.36342295
C	1.97965190	-1.11845743	10.10969957
C	1.04089301	-2.01890659	10.62429950
C	1.18642655	-3.38879013	10.39451348
C	2.27500840	-3.84635987	9.64666803
C	3.20532135	-2.93750352	9.13721571
C	3.67969741	1.04531767	8.49621356
C	4.49920719	2.13574554	8.81741881
C	3.97216835	3.42673753	8.74437508
C	2.67503525	3.63594095	8.25377709
C	1.89986613	2.54844149	7.83697637
C	2.42372556	1.25606321	7.90443134
F	9.16932248	-0.79254486	4.61214093

Cartesian coordinates for the first singlet excited state **[Ph]$_2$B[6-Cl-Sal][Ani] (3)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	7.67689099	-0.56882323	9.36988004
H	4.63938009	-1.00712589	4.75248490
H	6.81143536	-0.99240839	3.47625185
H	8.95959611	-0.63513859	7.19120940
H	3.98539740	0.62538659	11.27628307
H	4.13695910	0.51233211	13.72607604
H	5.90579943	-0.86047119	14.82167599
H	7.50125374	-2.14839235	13.40237690
H	7.32497116	-2.07343942	10.94801097
H	1.81894499	-0.05841695	10.27792311
H	0.18172989	-1.65647245	11.17497278
H	0.46268585	-4.09903657	10.77962925
H	2.42065580	-4.91135900	9.46947933
H	4.06259942	-3.30788832	8.57253139
H	5.50058104	1.98604757	9.21104053
H	4.56739333	4.27256588	9.09838785
H	2.28485079	4.65059112	8.17889570
H	0.91092317	2.71285213	7.42492453
H	1.85873891	0.42109785	7.52378263
N	5.57781610	-0.62421648	9.51060705
O	4.40890133	-0.87622732	7.32785380
B	4.23435911	-0.58871523	8.74700173
C	6.75546391	-0.65688524	8.80761379
C	6.80299368	-0.73237224	7.39266265
C	5.59030848	-0.83605342	6.65292141
C	5.58851825	-0.92779654	5.27213295
C	6.80223695	-0.92013216	4.55686615
C	7.99325417	-0.81049092	5.27337647
C	8.01371016	-0.71528801	6.66596597
C	5.65489332	-0.69986896	10.92426057
C	4.75125230	0.01272548	11.73289518

C	4.84434467	-0.04934229	13.12260873
C	5.83719837	-0.81587794	13.73916752
C	6.73519553	-1.53081382	12.94190680
C	6.64752925	-1.47835619	11.55125603
C	3.08506103	-1.55012135	9.36254607
C	1.96973055	-1.11964969	10.09511961
C	1.03230985	-2.02344914	10.60648747
C	1.18998761	-3.39366857	10.38714419
C	2.28940193	-3.84817425	9.65330783
C	3.21812105	-2.93585429	9.14727648
C	3.68157198	1.04827366	8.50245782
C	4.49702486	2.14048739	8.83246935
C	3.96907119	3.43053337	8.76228382
C	2.67433287	3.64042813	8.26377714
C	1.90313061	2.55387611	7.83675404
C	2.42885353	1.26264758	7.90150706
Cl	9.52304079	-0.79002156	4.40335705

Cartesian coordinates for the first singlet excited state **[Ph]$_2$B[6-Br-Sal][Ani] (4)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	0.89085325	14.91134206	7.11113575
H	-1.69474284	13.36883560	11.76692655
H	-3.74259280	12.99724375	10.35231829
H	-1.52354278	14.21966079	6.86697813
H	1.89517404	16.87108797	7.11115793
H	3.83476161	17.88229559	5.98232570
H	6.14926068	17.14781750	6.54967345
H	6.47550527	15.36930799	8.26575145
H	4.54068814	14.32495384	9.36176531
H	2.33186196	12.95354734	12.79600584
H	3.40405110	10.74598506	13.16523090
H	4.01001327	9.32534696	11.20934512
H	3.61096551	10.15846756	8.89734478
H	2.56011773	12.36613691	8.53434662
H	1.01361278	16.92160007	11.23700235
H	1.99758901	18.65365276	12.68746253
H	4.23380406	18.29556287	13.72692981
H	5.46423231	16.17588697	13.28601170
H	4.48127614	14.44893591	11.83990004
B	1.94273800	14.48813614	10.42077369
N	1.95156761	14.89205558	8.92856928
O	0.59130598	14.22159233	10.90277849
C	0.81803623	14.72392594	8.17528526
C	-0.40395979	14.25523141	8.72101520
C	-0.49667124	13.99567740	10.11832444
C	-1.67214569	13.55150009	10.69764632
C	-2.81857738	13.34340612	9.90613757
C	-2.73274966	13.58874538	8.53721420
C	-1.55543574	14.03448519	7.93518248
C	3.06902554	15.50388623	8.30714999

C	2.89348775	16.51429652	7.34124316
C	3.99497916	17.09600949	6.71469708
C	5.29327669	16.69126257	7.03686939
C	5.47379233	15.69609981	8.00152569
C	4.37868688	15.10537126	8.63034375
C	2.50824093	12.85578160	10.64343726
C	2.64948618	12.35452677	11.94969319
C	3.24225220	11.10778501	12.15415486
C	3.58503917	10.31272513	11.05502303
C	3.34106896	10.77249154	9.75180149
C	2.75270971	12.02058491	9.54325547
C	2.67219617	15.54666130	11.40615734
C	1.99334793	16.75102226	11.67635890
C	2.54692848	17.73498219	12.49859328
C	3.80062034	17.53471518	13.08348842
C	4.48889909	16.34476783	12.83707629
C	3.92424343	15.36702981	12.01098991
Br	-4.26917869	13.30937854	7.44090534

Cartesian coordinates for the first singlet excited state **[Ph]$_2$B[6-Me-Sal][Ani] (5)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	-0.96109940	7.24955110	6.44477700
H	-2.86576015	8.30234367	7.59350397
H	-5.20439474	7.67156971	6.99892203
H	-5.58894949	5.95331694	5.23345646
H	-3.69062161	4.86622613	4.11704136
H	-1.79965714	2.83000853	4.91358411
H	-2.90322858	0.65514505	4.51640973
H	-3.35142456	-0.11750860	2.19209328
H	-2.72473828	1.32894515	0.26192932
H	-1.60435715	3.50363059	0.66382446
H	-0.03398554	7.34470990	2.29551913
H	-0.92895986	9.15950798	0.88905494
H	-3.18810611	8.94770940	-0.14176155
H	-4.53092670	6.88990797	0.26322746
H	-3.63508211	5.07939275	1.66315147
C	0.04723447	5.10893416	5.31803793
C	1.25470186	4.60754563	4.75777198
C	1.32906470	4.36292955	3.35730990
C	2.48667426	3.88517231	2.76935282
C	3.62612015	3.63472406	3.56109783
C	3.59334465	3.85577041	4.94169651
C	2.40433542	4.33845281	5.52277316
C	4.80084937	3.58550785	5.80741473
C	-2.17888499	5.96076127	5.20580020
C	-1.97090775	6.93675096	6.20154131
C	-3.05245673	7.54278542	6.83935280
C	-4.36398709	7.19679177	6.50203631
C	-4.57690056	6.23561164	5.50961657
C	-3.50244406	5.62135640	4.86833064

C	-1.73958518	3.35974870	2.81582223
C	-2.00937003	2.51122932	3.89895969
C	-2.62845122	1.28011879	3.67126267
C	-2.89588841	0.85345309	2.36334493
C	-2.54262348	1.66372979	1.27909622
C	-1.92083208	2.89366908	1.50292187
C	-1.76694720	6.06749290	2.10907184
C	-1.02384052	7.23775147	1.85891213
C	-1.52711261	8.26851439	1.06192135
C	-2.79358141	8.15041016	0.48220812
C	-3.54491107	6.99505907	0.70837552
C	-3.03041072	5.96965832	1.50911846
H	-0.01698556	5.27505474	6.38622750
H	2.49706797	3.71163924	1.69805192
H	4.53197532	3.26232789	3.09249729
H	2.37001516	4.51648118	6.59574969
H	5.12125113	4.49057146	6.33759360
H	5.64580795	3.22908349	5.21182685
H	4.58299215	2.82693806	6.56912798
N	-1.08379343	5.32554146	4.57199924
B	-1.09232797	4.94809043	3.07239700
O	0.24389795	4.63128648	2.58195107

Cartesian coordinates for the first singlet excited state **$[Ph]_2$B[6-OMe-Sal][Ani] (6)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	1.13592858	3.54975191	5.50264148
H	1.92333470	1.48289401	4.42922634
H	0.56402709	-0.59947503	4.56194714
H	-1.59935249	-0.57432995	5.79953955
H	-2.38544696	1.49742719	6.87728053
H	-0.91481182	4.95579657	4.42447902
H	0.07496490	7.04929950	3.55636571
H	0.83209035	8.82000661	5.13857572
H	0.62044769	8.45194212	7.59303993
H	-0.35518826	6.35823987	8.45745793
H	1.38672197	4.24132004	7.85892850
H	3.38418577	3.38162228	9.00004744
H	3.16956332	2.04224457	11.09216280
H	0.89689310	1.54915278	11.99369581
H	-1.10913197	2.36749605	10.82889837
H	-2.09110137	4.27345356	10.46462716
H	-4.99946271	4.88940244	5.77731770
H	-6.94335333	5.57258391	7.23530817
H	-4.45319232	5.03041792	10.71701585
H	-6.07254550	6.53320869	11.50869004
H	-6.60377577	4.82487628	11.62746774
H	-7.81246412	6.13457596	11.52736412
O	-6.91250414	5.73271824	9.77133031
N	-1.16808901	3.88953299	8.61496900
B	-1.27259362	3.99748985	7.06889174

C	-2.23807642	4.23015415	9.39241738
C	-3.50018639	4.60434146	8.83987269
C	-3.68365317	4.57591115	7.43016072
C	-4.90483907	4.92143033	6.85785130
C	-5.98499055	5.30211516	7.66275724
C	-5.81926437	5.34440808	9.05629176
C	-4.58500077	5.00069772	9.64137232
C	-6.82895124	5.80543237	11.19079354
C	-0.01514083	3.38796611	9.26494643
C	1.27155069	3.64679876	8.75485861
C	2.40237163	3.16380871	9.41070394
C	2.28483461	2.41572427	10.58581805
C	1.01047146	2.14820133	11.09440869
C	-0.12741448	2.62543296	10.44636128
C	-0.62735881	5.47478007	6.50177719
C	-0.55501743	5.70822336	5.11857304
C	-0.00340901	6.89490968	4.62907334
C	0.42110517	7.88834018	5.51685190
C	0.29143564	7.68652429	6.89521305
C	-0.25791723	6.49765662	7.38594130
C	-0.67995958	2.69044826	6.29558742
C	0.52774232	2.65271438	5.58414472
C	0.97899623	1.48052854	4.96746850
C	0.21855740	0.31155656	5.04300113
C	-0.99443527	0.32674516	5.73785834
C	-1.43569604	1.50292059	6.34827796
O	-2.65850256	4.19508236	6.63865003

Cartesian coordinates for the first singlet excited state **[Ph]$_2$B[6- NO$_2$-Sal][Ani] (7)** calculated at the RB3LYP/6-31+g(d,p) level of theory

N	6.84622437	2.22650993	13.33063341
N	1.77539475	5.46822188	11.96990677
H	6.21060531	4.11702857	14.03459721
H	3.38167591	1.60550217	9.99069459
H	1.71606617	3.48517473	10.17761523
H	3.92434112	5.11881083	13.47781252
H	7.66729488	2.86383110	15.79128293
H	9.99133251	3.36845639	16.49503175
H	11.84847105	3.26563238	14.83847315
H	11.34901542	2.68046364	12.47063955
H	9.01450414	2.21877612	11.76717090
H	8.58751375	-0.19226255	14.05382824
H	10.06509224	-2.01910750	13.35067810
H	9.62008386	-3.24371558	11.22944327
H	7.68407059	-2.59762103	9.80307401
H	6.18620013	-0.76062822	10.51095371
H	6.70543201	0.31867024	15.42279932
H	5.31408029	-0.95142872	17.01550303
H	3.27531021	-2.13438923	16.21883670
H	2.60926302	-1.99919110	13.82531000

H	3.99184100	-0.70445318	12.23044895
O	5.44345434	1.27254201	11.52095514
O	0.83264633	5.49628389	11.17215089
O	1.94359933	6.30720782	12.86118169
C	5.95003932	3.27031311	13.40829417
C	4.77564334	3.29664772	12.63735085
C	4.56554751	2.28970189	11.63129553
C	3.48847909	2.37075899	10.75237204
C	2.56236959	3.41402211	10.84675437
C	2.74676832	4.37686726	11.85081075
C	3.81639161	4.33992262	12.73298571
C	8.18819302	2.48772235	13.73484439
C	8.47630641	2.82366627	15.06716658
C	9.78659736	3.10746413	15.46052863
C	10.82963957	3.04860656	14.53199610
C	10.54820457	2.71637576	13.20384357
C	9.23665882	2.44972590	12.80391696
C	7.29411569	-0.28051006	12.30605003
C	8.38183873	-0.70534524	13.12235738
C	9.22050535	-1.73925739	12.72858653
C	8.97234587	-2.42612931	11.53152129
C	7.87380698	-2.06704340	10.73142124
C	7.03157722	-1.03983380	11.12890211
C	5.42057404	-0.03909554	13.71146883
C	5.81305007	-0.18659115	15.06876715
C	5.03059200	-0.89800471	15.96847723
C	3.87538694	-1.55864533	15.52047903
C	3.50470282	-1.48928269	14.16801867
C	4.28147676	-0.76481556	13.27373204
B	6.27925327	0.93153593	12.67709275

Cartesian coordinates for the first singlet excited state **[Ph]$_2$B[Naft-Sal][Ani] (8)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	4.13966601	13.45654533	5.18390768
H	6.30661380	18.22630799	6.96676595
H	4.69507766	19.42798479	5.47583374
H	2.84584940	19.36738595	3.87393209
H	1.19208598	18.11282706	2.52682626
H	1.13293061	15.61777890	2.64571705
H	2.70233202	14.41131481	4.07750121
H	7.36844369	15.53265147	10.09007308
H	6.32450482	15.61833081	12.34244141
H	4.05463970	14.65476425	12.70057787
H	2.85148653	13.58028371	10.80336600
H	3.89399960	13.48914325	8.55687520
H	8.76368494	15.01550205	6.19948789
H	11.11016401	14.27855618	6.38166546
H	11.77539781	12.64263468	8.13968523
H	10.05316455	11.75790131	9.70571863
H	7.71766014	12.49662001	9.52589884

N	5.66547290	13.45489627	6.61455178
B	6.53108366	14.29212365	7.54170797
C	4.78150906	14.10252734	5.76733198
C	4.68265266	15.49046609	5.66943816
C	5.58178128	16.29138154	6.42776016
C	5.58761208	17.68361322	6.36193737
C	4.69050642	18.34420734	5.53375147
C	3.74622970	17.61348988	4.75571652
C	2.81735669	18.28146856	3.91494113
C	1.89372663	17.58151451	3.16333758
C	1.86142664	16.17314985	3.22882678
C	2.75616538	15.49436133	4.04061873
C	3.71943576	16.17970328	4.81588092
C	5.81141661	12.05098407	6.43582412
C	5.86649371	11.18307181	7.53809520
C	5.99364731	9.80650188	7.34833118
C	6.05608446	9.26732613	6.06086184
C	5.99706610	10.12579049	4.95940568
C	5.87917243	11.50377686	5.14164397
C	5.71505371	14.44031350	9.23418395
C	6.39227814	15.09159528	10.25625749
C	5.79470647	15.14102101	11.52273072
C	4.52225033	14.59762315	11.72207655
C	3.84251445	14.00169780	10.65844908
C	4.42791947	13.94209488	9.38296501
C	8.04112719	13.78783536	7.82428348
C	9.03659895	14.29334697	6.96317893
C	10.36692496	13.87933402	7.06675740
C	10.74057174	12.96174712	8.05173713
C	9.77327967	12.46519166	8.92968300
C	8.44421515	12.88028876	8.81648217
O	6.49250449	15.68087165	7.23406112
H	5.79077677	11.58307767	8.54123077
H	6.03244479	9.15242171	8.21485948
H	6.15124436	8.19530837	5.91782345
H	6.05870995	9.72522653	3.95142133
H	5.87086864	12.16535993	4.28099782

Cartesian coordinates for the first singlet excited state **[2,6-diFPh]$_2$B[6-H-Sal][Ani] (9)** calculated at the RB3LYP/6-31+g(d,p) level of theory

H	7.63679600	-0.20188600	9.53348400
H	4.91373200	-1.37135600	4.85702500
H	7.07727300	-0.98440500	3.65441700
H	8.96304700	0.02314100	7.39282600
H	4.68750200	0.48801600	14.01652400
H	6.04834600	-1.45701300	14.84657000
H	7.14001000	-2.98215500	13.16935900
H	2.37298900	0.00467500	10.86592400
H	0.83316100	-1.56448100	12.00758800
H	0.50897400	-3.85687900	11.09212200

H	1.75577600	-4.60514900	9.07034900
H	3.30272800	-3.01399300	7.92837000
H	4.26700900	4.37113600	8.44666200
H	2.03334000	4.43463300	7.29868200
H	0.82242800	2.26552200	6.87287900
N	5.55473800	-0.55064700	9.60016300
O	4.55025000	-1.13532500	7.41861000
B	4.26583700	-0.51673000	8.72018400
C	6.76132300	-0.41405500	8.93002600
C	6.86650900	-0.50766700	7.53569000
C	5.72103700	-0.89546600	6.77229700
C	5.80510200	-1.07045700	5.39865500
C	7.02197400	-0.85199800	4.73020300
C	8.15646500	-0.45273500	5.45501600
C	8.08393300	-0.28016300	6.83005100
C	5.64184500	-0.79806600	10.98129800
C	5.05297400	0.01706900	11.96500500
C	5.17064200	-0.20024900	13.33169000
C	5.93295700	-1.27928800	13.78263300
C	6.54786500	-2.12806800	12.85968800
C	6.38301900	-1.87921400	11.50359300
C	3.04810900	-1.43164200	9.38054900
C	2.25428200	-1.00789900	10.50180500
C	1.39006100	-1.87461200	11.12999900
C	1.21156600	-3.18227500	10.61321400
C	1.91148500	-3.60330400	9.45624400
C	2.76970800	-2.73184500	8.82650900
C	3.62364800	0.99699000	8.42893000
C	4.23927400	2.23807200	8.63996200
C	3.70506000	3.46495000	8.24923900
C	2.46717600	3.48946300	7.60951900
C	1.78609400	2.29375300	7.36895200
C	2.38750100	1.11481500	7.78617900
H	9.09629000	-0.27791900	4.93917500
F	6.96070300	-2.73868300	10.62885300
F	4.31043800	1.08284700	11.56051600
F	1.68360300	-0.04462700	7.54504700
F	5.45255700	2.29092700	9.24783100

Structure-properties correlation analysis

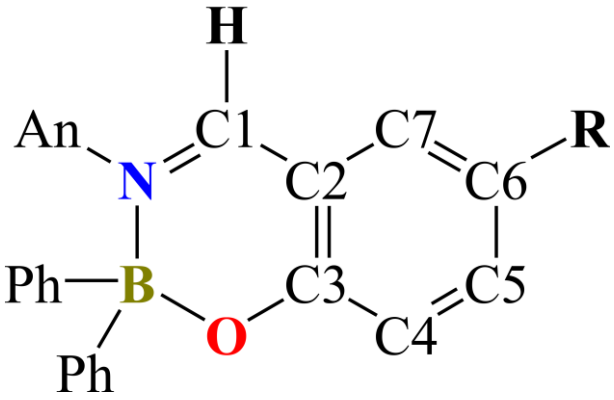


Figure S8. Numbering scheme used for QTAIM analysis of **1-7**.

Table S4. QTAIM analysis of **1**.

					q(atom)	
	$d_{X\cdots A}$ (Å)	$\rho(\mathbf{r}_{BCP})$ (e·Å^{-3})	$\nabla^2\rho$ ($\mathbf{r}_{BCP}$) (e·Å^{-5})	Ellipticity	A	B
B-N	1.6512	0.776	6.628	0.259	2.091	−1.384
B-O	1.5159	0.907	13.376	0.187	2.091	−1.300
B-C(Ph1)	1.6166	1.143	−4.171	0.120	2.091	−0.558
B-C(Ph2)	1.6242	1.169	−4.799	0.066	2.091	−0.015
O-C(3)	1.3196	2.162	−8.256	0.025	−1.300	0.682
C(1)-C(2)	1.4271	2.006	−19.297	0.154	0.667	0.000
C(6)-R	1.0847	1.957	−24.581	0.030	0.004	0.011
C(1)-H	1.0902	1.950	−26.075	0.014	0.670	0.040
N-C(An)	1.4341	1.883	−20.363	0.051	−1.384	0.667
N-C(1)	1.3085	2.411	−19.499	0.152	−1.384	0.667

Table S5. QTAIM analysis of **2**.

					q(atom)	
	$d_{X\cdots A}$ (Å)	$\rho(\mathbf{r}_{BCP})$ (e·Å^{-3})	$\nabla^2\rho$ ($\mathbf{r}_{BCP}$) (e·Å^{-5})	Ellipticity	A	B
B-N	1.6543	0.769	6.603	0.263	2.09	−1.381
B-O	1.5155	0.904	13.423	0.188	2.09	−1.298
B-C(Ph1)	1.6157	1.147	−4.217	0.121	2.09	−0.562
B-C(Ph2)	1.6234	1.174	−4.868	0.065	2.09	−0.562
O-C(3)	1.3206	2.160	−8.724	0.025	−1.298	0.687
C(1)-C(2)	1.4292	1.998	−19.159	0.153	0.674	0.009
C(6)-R	1.3617	1.667	2.169	0.016	0.489	−0.647
C(1)-H	1.0899	1.957	−26.147	0.015	0.674	0.046
N-C(An)	1.4343	1.883	−20.291	0.051	−1.381	0.335
N-C(1)	1.3074	2.416	−19.388	0.158	−1.381	0.674

Table S6. QTAIM analysis of **3**.

					q(atom)	
	$d_{X\cdots A}$ (Å)	$\rho(\mathbf{r}_{BCP})$ (e·Å^{-3})	$\nabla^2\rho(\mathbf{r}_{BCP})$ (e·Å^{-5})	Ellipticity	A	B
B-N	1.6532	0.769	6.603	0.267	2.090	−1.382
B-O	1.5178	0.904	13.327	0.193	2.090	−1.297
B-C(Ph1)	1.6154	1.147	−4.241	0.120	2.090	−0.562
B-C(Ph2)	1.6231	1.168	−4.892	0.066	2.090	−0.563
O-C(3)	1.3182	2.173	−8.386	0.024	−1.297	0.692
C(1)-C(2)	1.4295	1.998	−19.159	0.151	0.675	0.006
C(6)-R	1.7583	1.302	−6.507	0.055	0.055	−0.219
C(1)-H	1.0899	1.957	−26.171	0.015	0.675	0.047
N-C(An)	1.4347	1.876	−20.243	0.051	−1.382	0.333
N-C(1)	1.3071	2.418	−19.347	0.158	−1.382	0.675

Table S7. QTAIM analysis of **4**.

					q(atom)	
	$d_{X\cdots A}$ (Å)	$\rho(\mathbf{r}_{BCP})$ (e·Å^{-3})	$\nabla^2\rho(\mathbf{r}_{BCP})$ (e·Å^{-5})	Ellipticity	A	B
B-N	1.6528	0.776	6.627	0.267	2.091	−1.383
B-O	1.5174	0.904	13.351	0.192	2.091	−1.297
B-C(Ph1)	1.6231	1.147	−4.241	0.121	2.091	−0.562
B-C(Ph2)	1.615	1.174	−4.892	0.065	2.091	−0.562
O-C(3)	1.3182	2.173	−8.459	0.025	−1.297	0.692
C(1)-C(2)	1.4295	1.998	−19.159	0.151	0.675	0.005
C(6)-R	1.9068	1.080	−4.410	0.061	−0.075	−0.088
C(1)-H	1.0899	1.957	−26.171	0.015	0.675	0.047
N-C(An)	1.4344	1.883	−20.243	0.052	−1.383	0.334
N-C(1)	1.3070	2.418	−19.334	0.157	−1.383	0.675

Table S8. QTAIM analysis of **5**.

					q(atom)	
	$d_{X\cdots A}$ (Å)	$\rho(\mathbf{r}_{BCP})$ (e·Å^{-3})	$\nabla^2\rho(\mathbf{r}_{BCP})$ (e·Å^{-5})	Ellipticity	A	B
B-N	1.6510	0.776	6.603	0.254	2.091	−1.384
B-O	1.5151	0.911	13.399	0.184	2.091	−1.300
B-C(Ph1)	1.6247	1.141	−4.145	0.120	2.091	−0.556
B-C(Ph2)	1.6169	1.168	−4.772	0.066	2.091	−0.557
O-C(3)	1.3207	2.160	−8.314	0.024	−1.300	0.679
C(1)-C(2)	1.4260	2.011	−19.327	0.156	0.663	0.000
C(6)-R	1.5109	1.707	−14.339	0.036	0.013	0.075
C(1)-H	1.0902	1.923	−24.581	0.016	0.663	0.042
N-C(An)	1.4337	1.890	−20.436	0.052	−1.384	0.337
N-C(1)	1.3095	2.406	−19.618	0.151	−1.384	0.663

Table S9. QTAIM analysis of **6**.

	$d_{X...A}$ (Å)	$\rho(\mathbf{r}_{BCP})$ (e·Å^{-3})	$\nabla^2\rho(\mathbf{r}_{BCP})$ (e·Å^{-5})	Ellipticity	q(atom) A	q(atom) B
B-N	1.6509	0.776	6.627	0.250	2.092	−1.382
B-O	1.5140	0.911	13.495	0.180	2.092	−1.300
B-C(Ph1)	1.6169	1.168	−4.748	0.065	2.092	−0.556
B-C(Ph2)	1.6248	1.141	−4.121	0.122	2.092	−0.557
O-C(3)	1.3222	2.153	−8.579	0.025	−1.300	0.678
C(1)-C(2)	1.4255	2.011	−19.327	0.161	0.661	0.010
C(6)-R	1.3697	1.917	−9.109	0.037	0.523	−1.103
C(1)-H	1.0901	1.950	−26.003	0.015	0.661	0.039
N-C(An)	1.4330	1.890	−20.484	0.052	−1.382	0.339
N-C(1)	1.3105	2.402	−19.769	0.155	−1.382	0.661

Table S10. QTAIM analysis of **7**.

	$d_{X...A}$ (Å)	$\rho(\mathbf{r}_{BCP})$ (e·Å^{-3})	$\nabla^2\rho(\mathbf{r}_{BCP})$ (e·Å^{-5})	Ellipticity	q(atom) A	q(atom) B
B-N	1.6499	0.776	6.724	0.294	2.085	−1.385
B-O	1.5280	0.871	12.917	0.217	2.085	−1.288
B-C(Ph1)	1.6134	1.181	−5.109	0.070	2.085	−0.570
B-C(Ph2)	1.6206	1.154	−4.458	0.114	2.085	−0.570
O-C(3)	1.3083	2.214	−7.133	0.023	−1.288	0.716
C(1)-C(2)	1.4327	1.991	−19.014	0.145	0.685	0.007
C(6)-R	1.4598	1.809	−18.195	0.166	0.269	0.358
C(1)-H	1.0897	1.957	−26.340	0.014	0.684	0.055
N-C(An)	1.4372	1.863	−19.906	0.050	−1.385	0.328
N-C(1)	1.3045	2.429	−18.975	0.161	−1.385	0.684

Table S11. R^2 factors obtained for correlation between QTAIM topological parameters and $\delta_{C\mathbf{H}=N}$ of **1-7**. For clarity of presentation, R^2 with values 0.9, 0.8 and 0.7 were coloured in red, orange and blue, respectively. Crossed values represent correlations which are not statistically meaningful according to Snedecor's F-test. The reciprocal of the relative standard deviation (Δ_{rel}^{-1}, %) is given in parentheses. The higher value of Δ_{rel}^{-1}, the more meaningful the correlation.

	$d_{X...A}$ (Å)	$\rho(\mathbf{r}_{BCP})$ (e·Å^{-3})	$\nabla^2\rho(\mathbf{r}_{BCP})$ (e·Å^{-5})	Ellipticity	q(atom) A	q(atom) B
B-N	~~0.09 (72)~~	~~0.00 (6)~~	0.80 (450)	0.95 (956)	0.93 (830)	~~0.22 (117)~~
B-O	0.94 (897)	0.91 (1517)	0.90 (722)	0.95 (1030)	0.93 (830)	0.95 (952)
O-C(3)	0.93 (831)	0.93 (787)	0.76 (398)	~~0.49 (220)~~	0.94 (952)	0.94 (950)
C(1)-C(2)	0.82 (474)	0.64 (341)	0.78 (425)	0.61 (279)	0.79 (418)	~~0.12 (61)~~
C(6)-R	~~0.00 (5)~~	~~0.00 (13)~~	~~0.05 (52)~~	0.83	~~0.01 (26)~~	~~0.12~~

				(460)		~~(135)~~
C(1)-H	0.68 (324)	~~0.27 (136)~~	~~0.31 (149)~~	~~0.47 (210)~~	0.79 (438)	0.79 (431)
N-C(An)	0.94 (918)	0.93 (819)	0.94 (871)	0.75 (391)	~~0.22 (117)~~	~~0.02 (29)~~
N-C(1)	0.81 (461)	0.80 (438)	0.83 (489)	0.61 (279)	~~0.22 (117)~~	0.79 (438)

Table S12. R^2 factors obtained for correlation between QTAIM topological parameters and λ_{em} of **1-7**. For clarity of presentation R^2 with values 0.9, 0.8 and 0.7 are coloured in red, orange and blue, respectively. Crossed values represent correlations which are not statistically meaningful according to Snedecor's F-test. The reciprocal of the relative standard deviation (Δ_{rel}^{-1}, %) is given in parentheses. The higher value of Δ_{rel}^{-1}, the more meaningful the correlation.

					q(atom)	
	$d_{X\cdots A}$ (Å)	$\rho(\mathbf{r}_{BCP})$ ($e\cdot Å^{-3}$)	$\nabla^2\rho(\mathbf{r}_{BCP})$ ($e\cdot Å^{-5}$)	Ellipticity	A	B
B-N	~~0.05 (48)~~	~~0.02 (28)~~	~~0.41 (187)~~	0.72 (118)	0.59 (270)	~~0.46 (207)~~
B-O	0.65 (307)	0.71 (244)	0.65 (347)	0.71 (350)	0.59 (270)	0.55 (248)
O-C(3)	0.70 (344)	0.79 (432)	0.59 (269)	~~0.37 (170)~~	0.55 (248)	0.64 (295)
C(1)-C(2)	0.63 (292)	0.44 (239)	0.51 (229)	~~0.16 (99)~~	0.64 (296)	~~0.06 (80)~~
C(6)-R	~~0.01 (25)~~	~~0.03 (37)~~	~~0.17 (100)~~	0.50 (225)	~~0.23 (123)~~	0.79 (479)
C(1)-H	~~0.29 (143)~~	~~0.06 (55)~~	~~0.07 (60)~~	~~0.30 (145)~~	0.64 (296)	0.58 (262)
N-C(An)	0.75 (392)	0.65 (304)	0.71 (410)	~~0.49 (220)~~	~~0.46 (207)~~	~~0.03 (39)~~
N-C(1)	0.75 (383)	0.73 (367)	0.80 (442)	~~0.16 (99)~~	~~0.46 (207)~~	0.64 (296)

NMR spectra

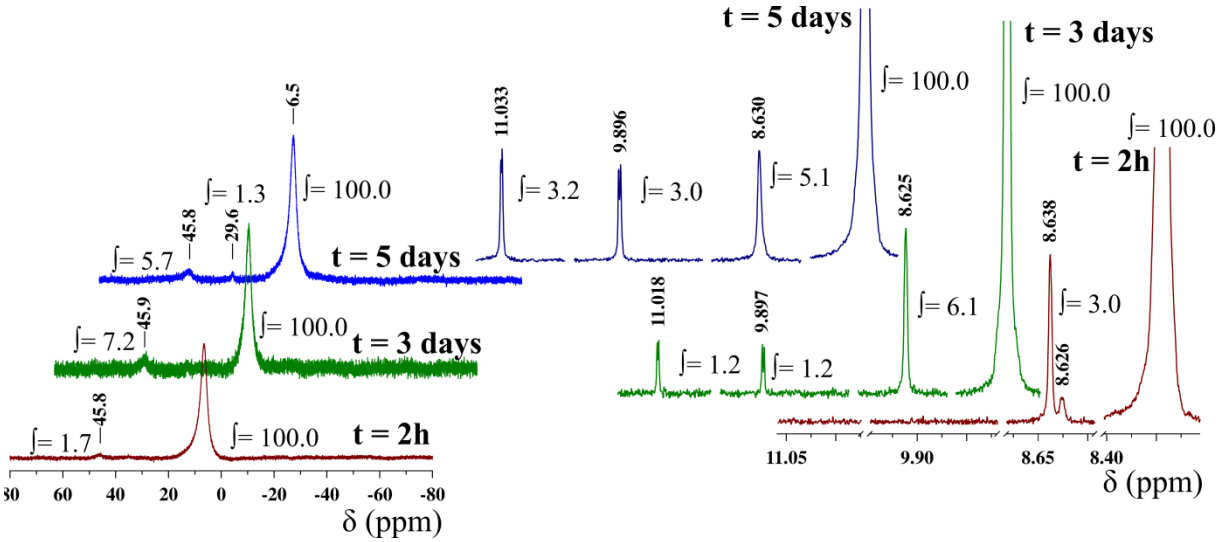
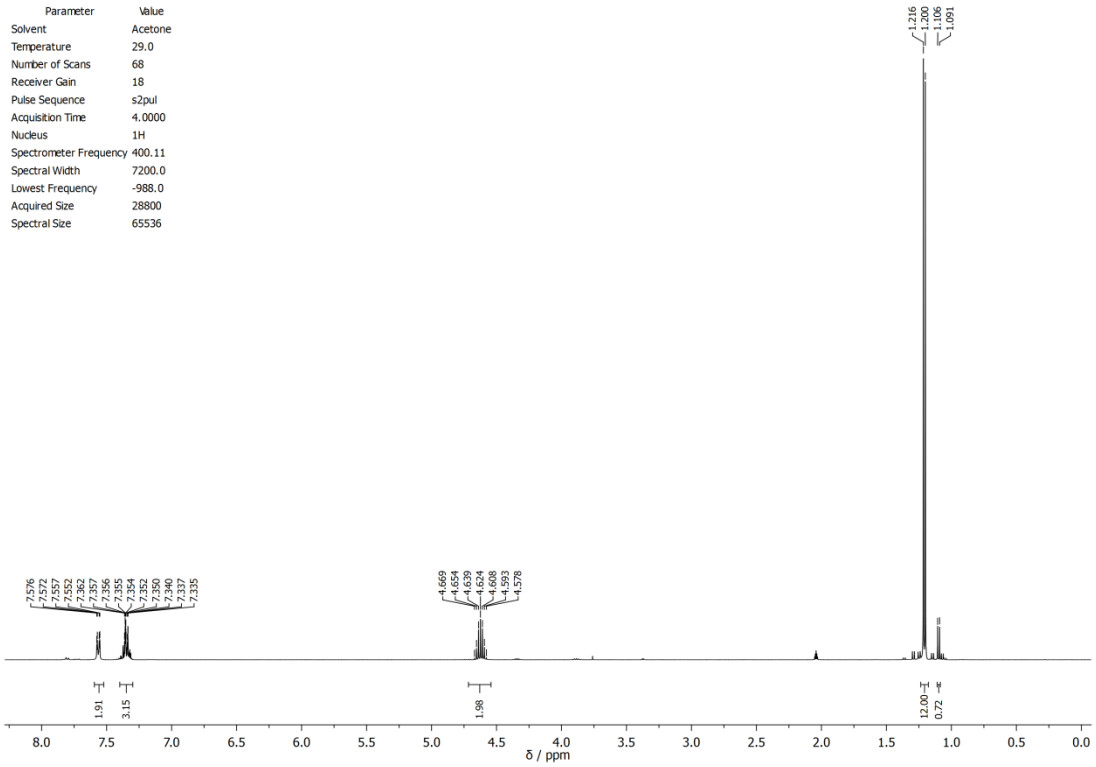


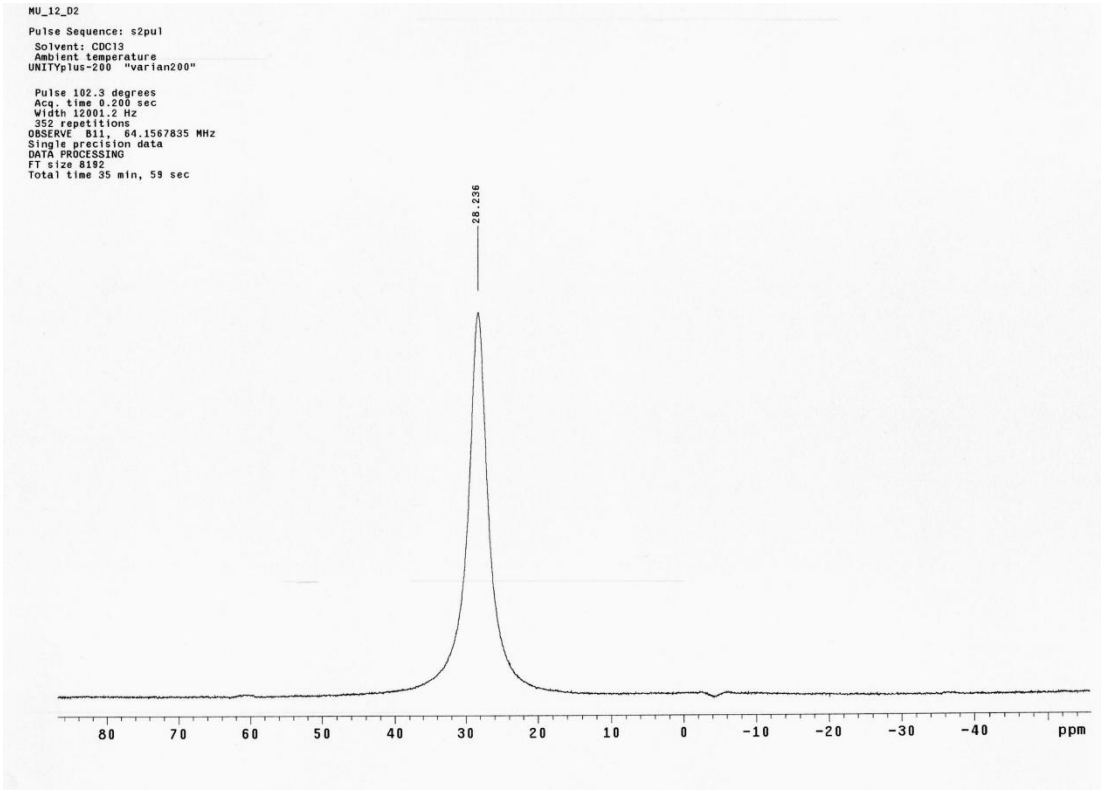
Figure S9. Time-dependent ^{11}B (left) and ^{1}H (right) NMR spectra ($CDCl_3$, rt) of compound **1** showing its gradual decomposition.

Diisopropyl phenylboronate

^{1}H NMR (400 MHz, acetone-d_6)

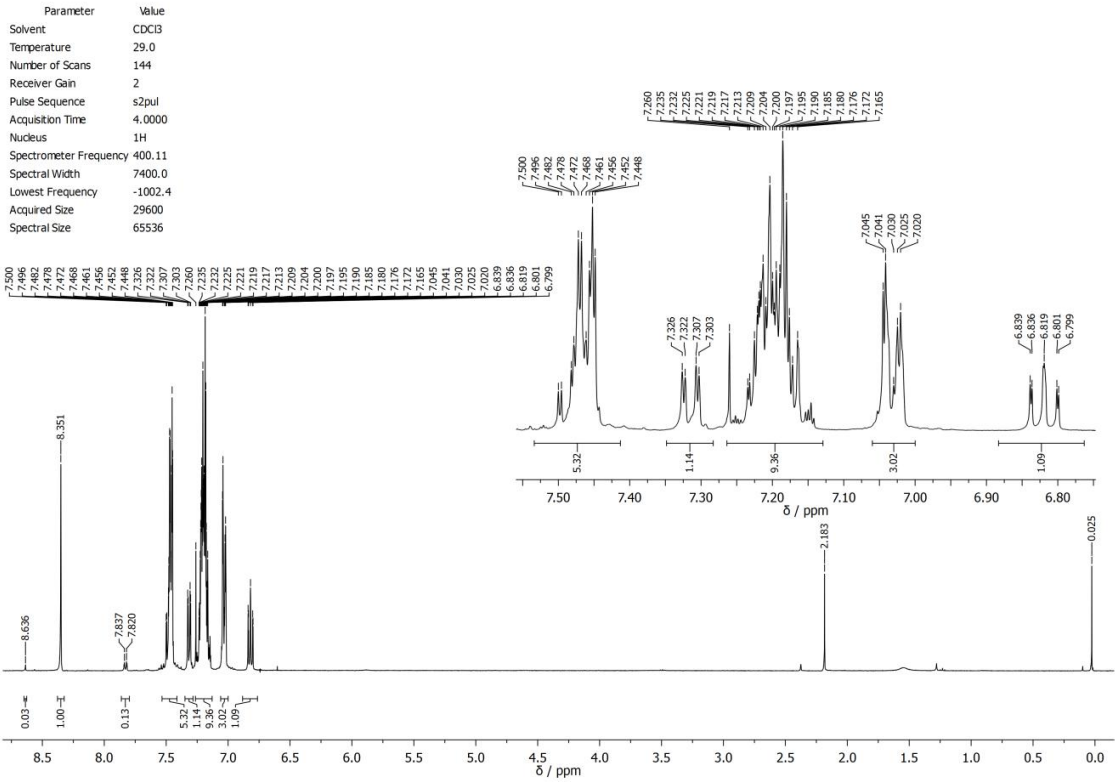


^{11}B NMR (64 MHz, acetone-d_6)

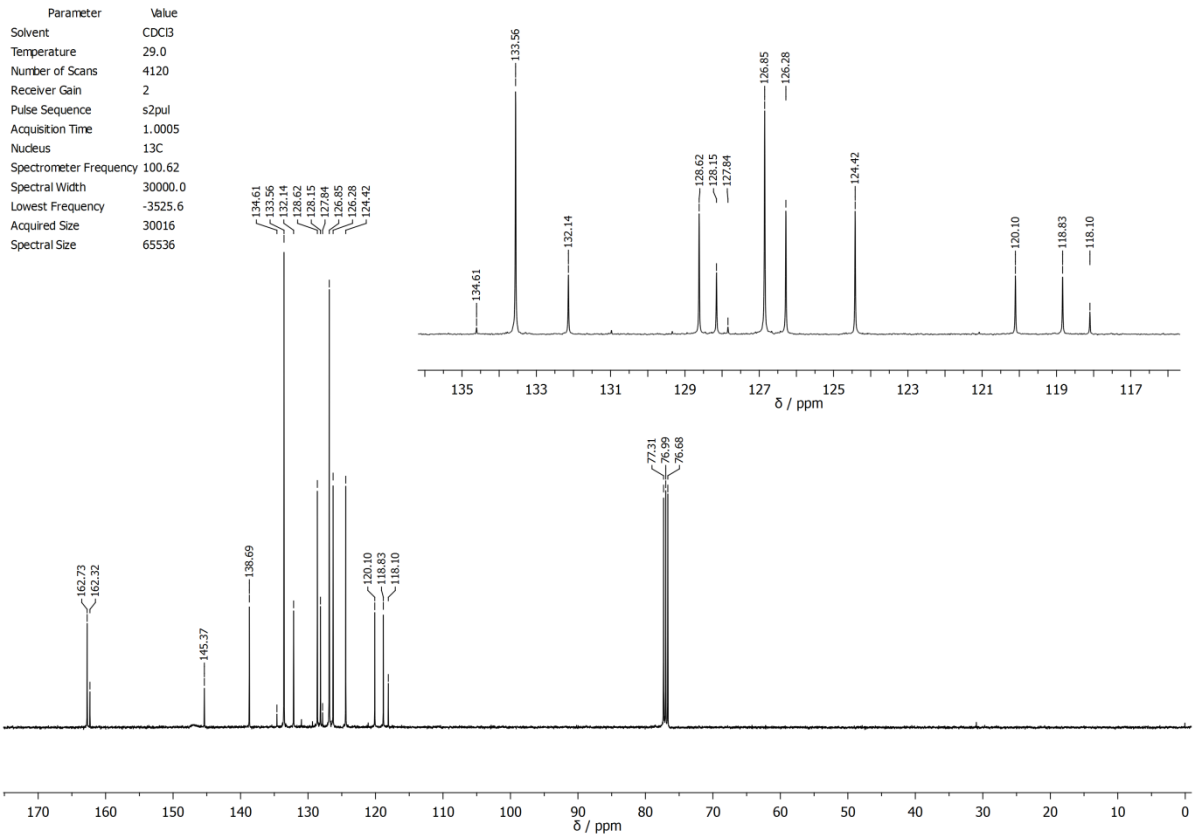


$[Ph]_2B[6\text{-}H\text{-}Sal][Ani]$ (1)

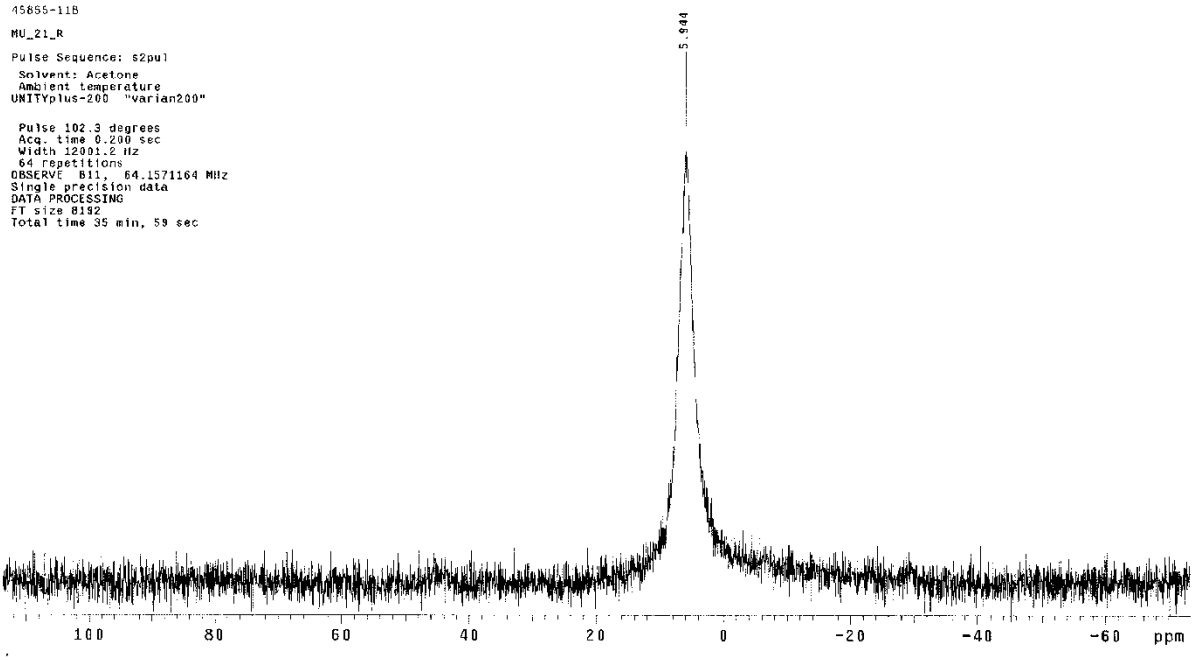
^1H NMR (400 MHz, $CDCl_3$)



$^{3}C\{^{1}H\}$ NMR (100.6 MHz, $CDCl_3$)



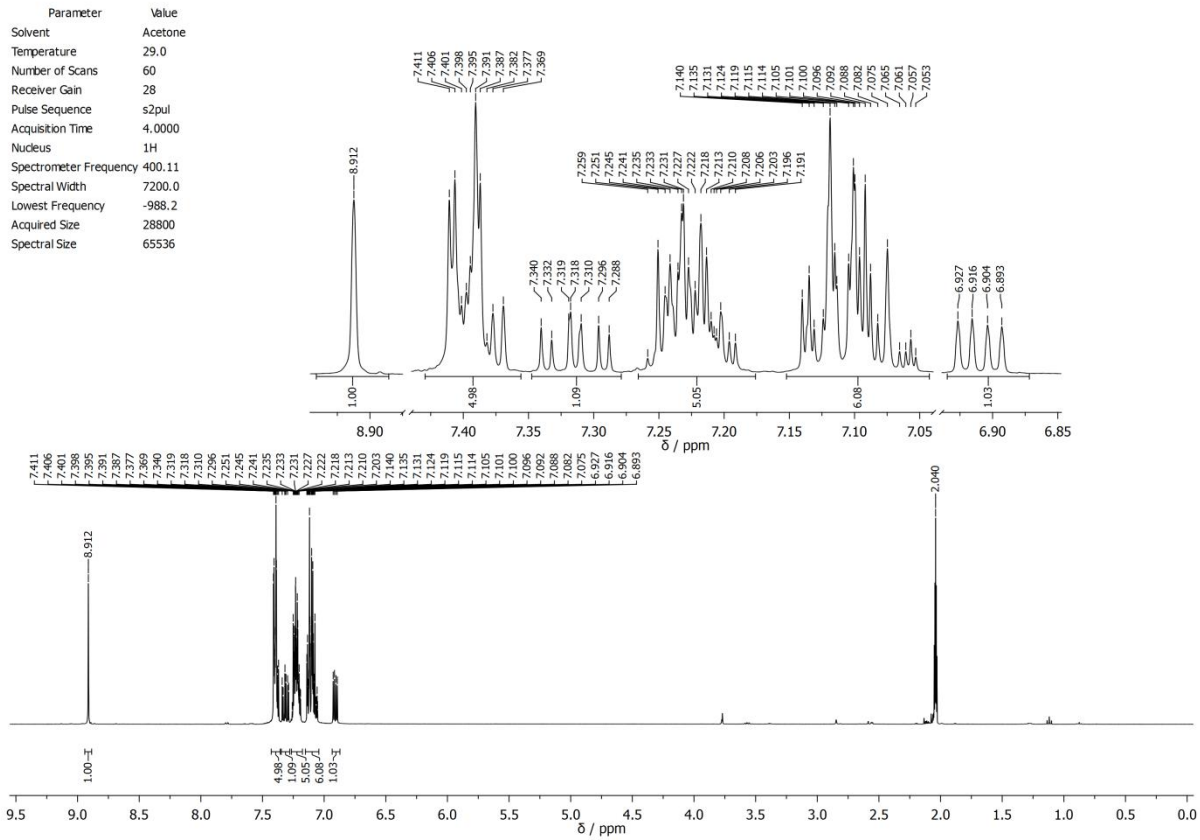
^{11}B NMR (64 MHz, acetone-d_6)



$[Ph]_2B[6\text{-F-Sal}][Ani]$ (2)

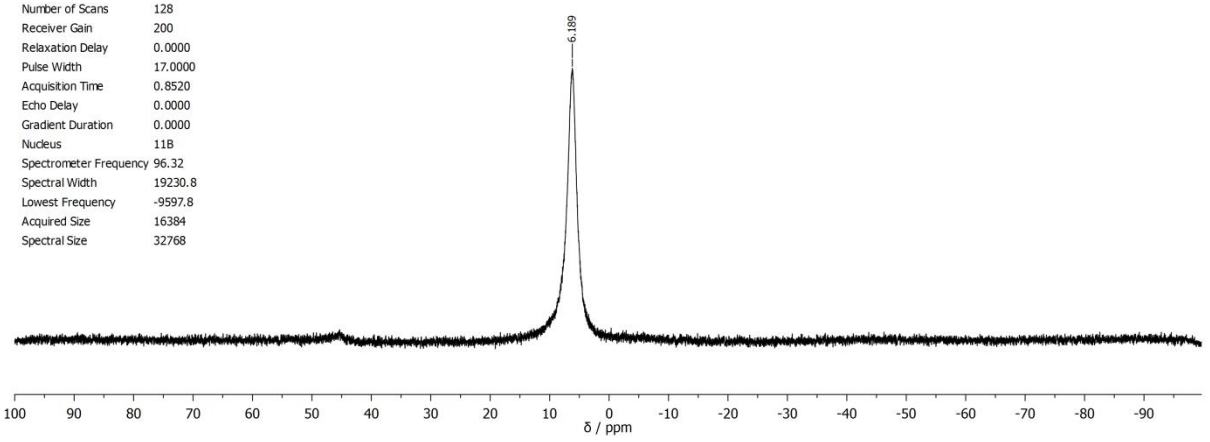
^{1}H NMR (400 MHz, acetone-d_6)

Parameter	Value
Solvent	Acetone
Temperature	29.0
Number of Scans	60
Receiver Gain	28
Pulse Sequence	s2pul
Acquisition Time	4.0000
Nucleus	1H
Spectrometer Frequency	400.11
Spectral Width	7200.0
Lowest Frequency	-988.2
Acquired Size	28800
Spectral Size	65536

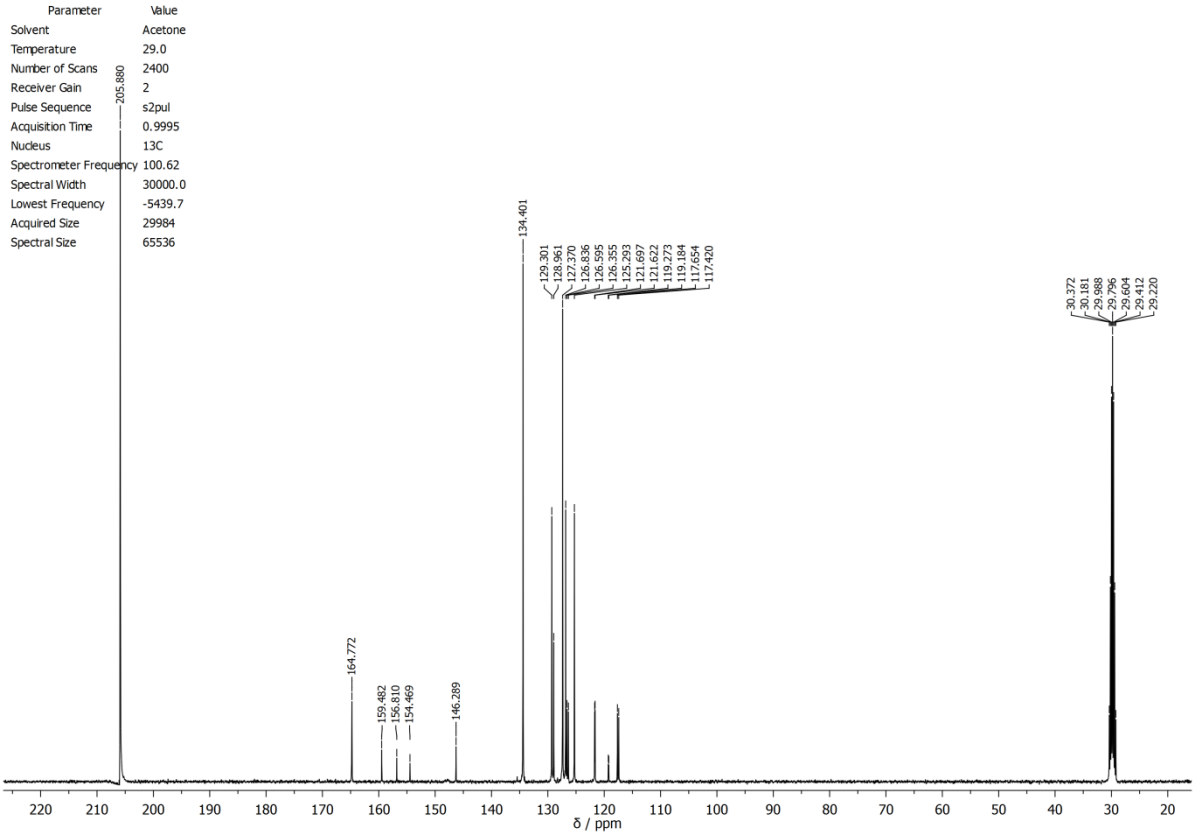


^{11}B NMR (96 MHz, acetone-d_6)

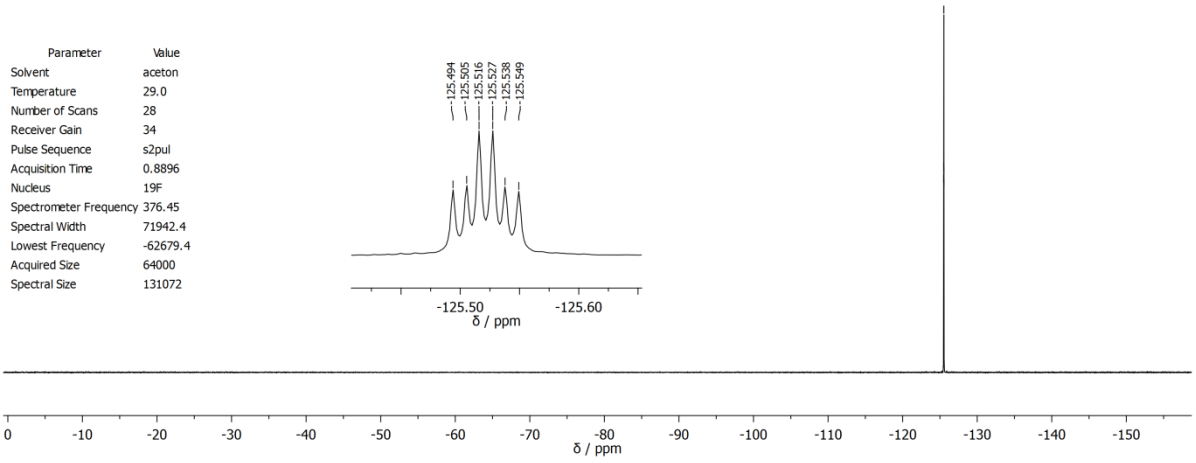
Parameter	Value
Solvent	Acetone
Temperature	298.2
Pulse Sequence	zg_pi
Number of Scans	128
Receiver Gain	200
Relaxation Delay	0.0000
Pulse Width	17.0000
Acquisition Time	0.8520
Echo Delay	0.0000
Gradient Duration	0.0000
Nucleus	11B
Spectrometer Frequency	96.32
Spectral Width	19230.8
Lowest Frequency	-9597.8
Acquired Size	16384
Spectral Size	32768



$^{13}C\{^{1}H\}$ NMR (100.6 MHz, acetone-d_6)

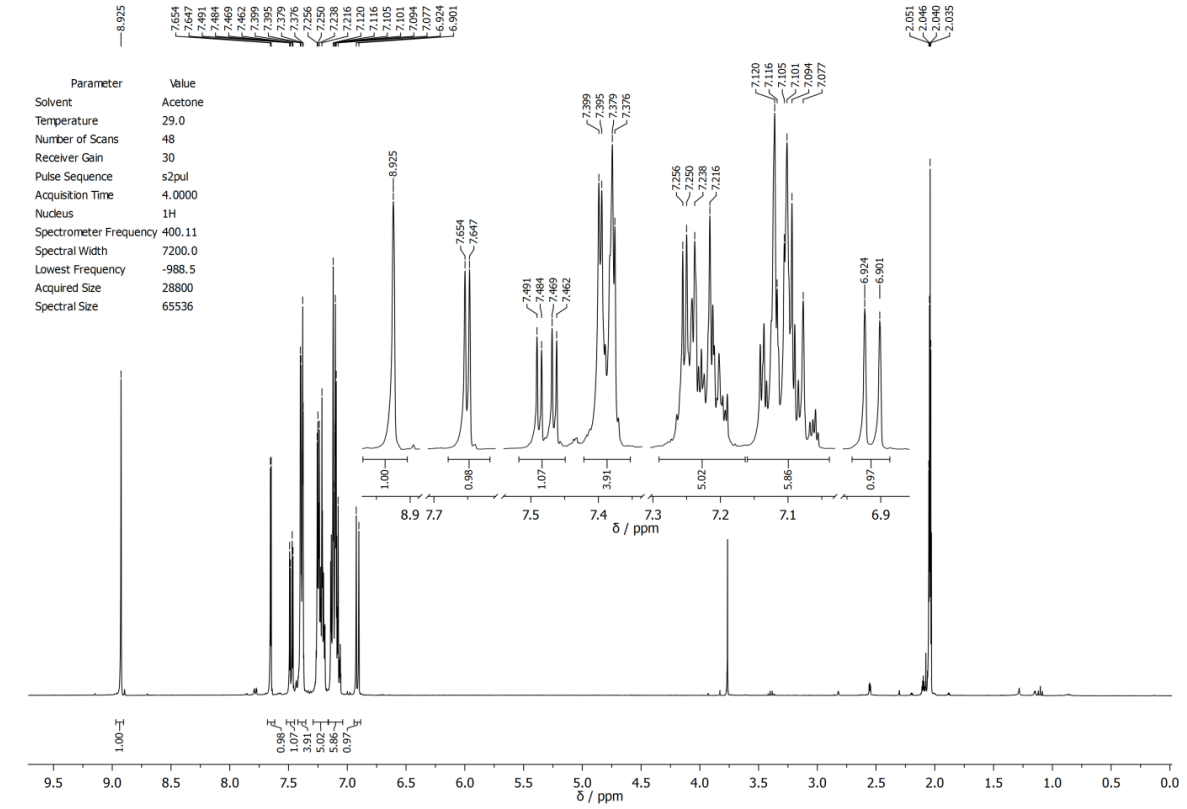


^{19}F NMR (376 MHz, acetone-d_6)

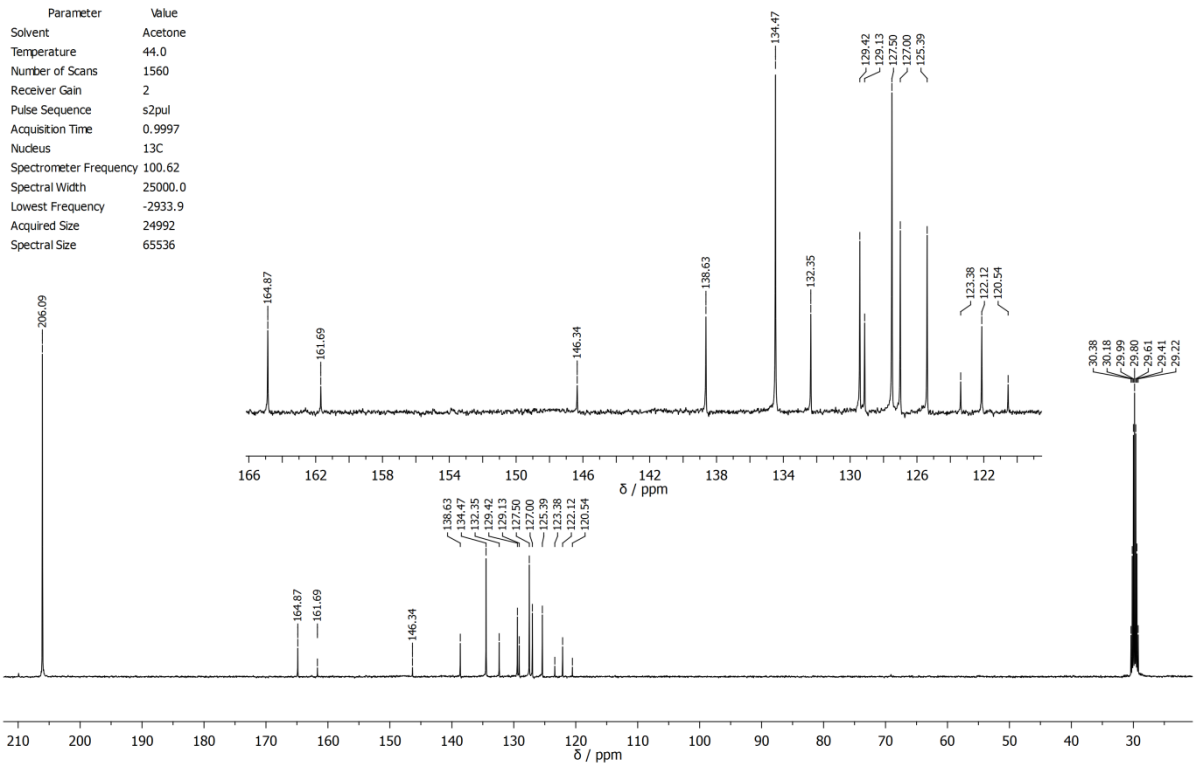


$[Ph]_2B[6\text{-}Cl\text{-}Sal][Ani]$ (3)

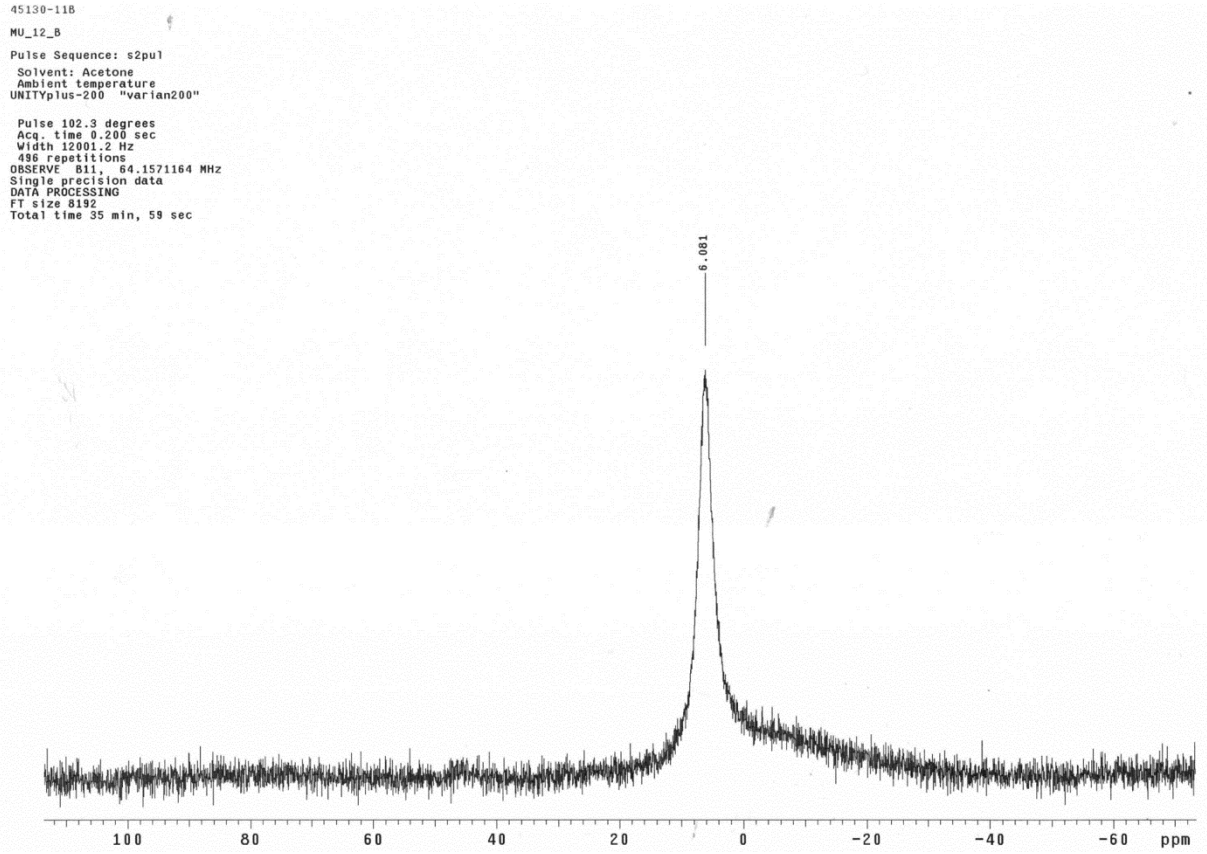
^1H NMR (400 MHz, acetone-d_6)



$^{13}C\{^1H\}$ NMR (100.6 MHz, acetone-d_6)

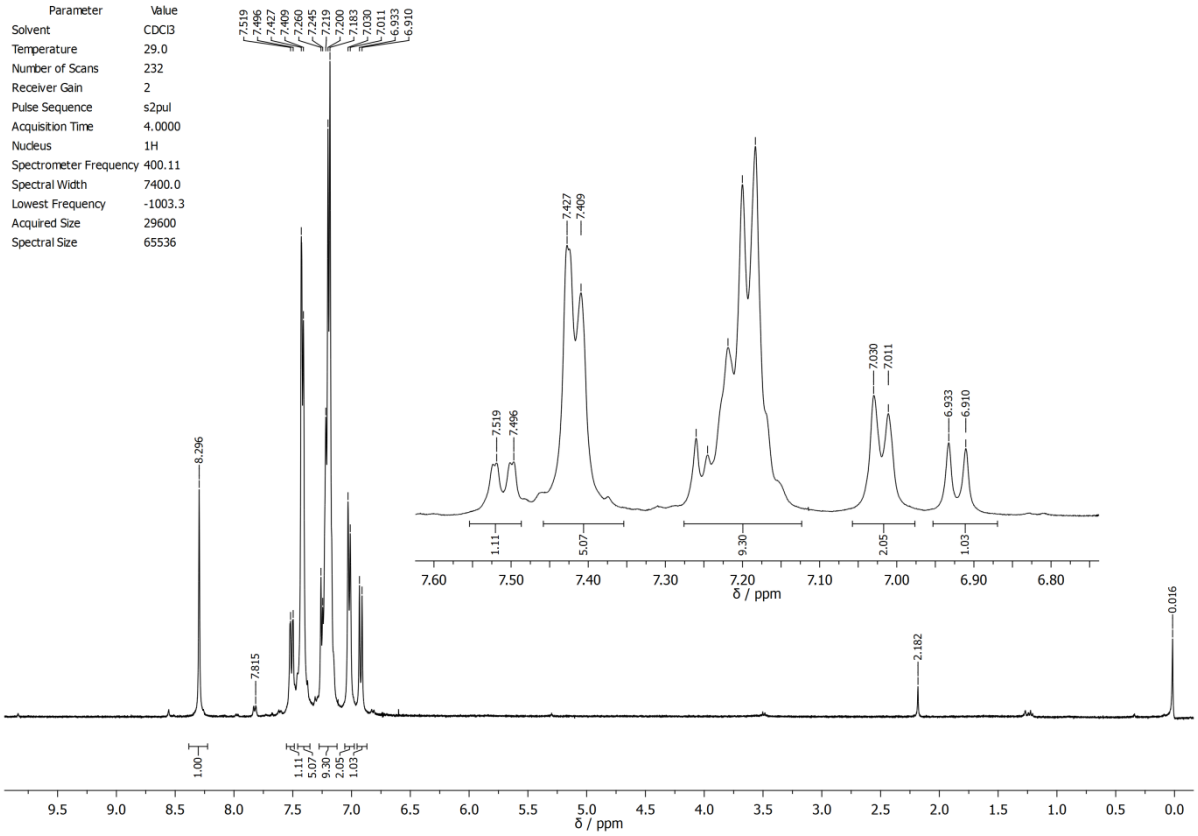


^{11}B NMR (64 MHz, acetone-d_6)

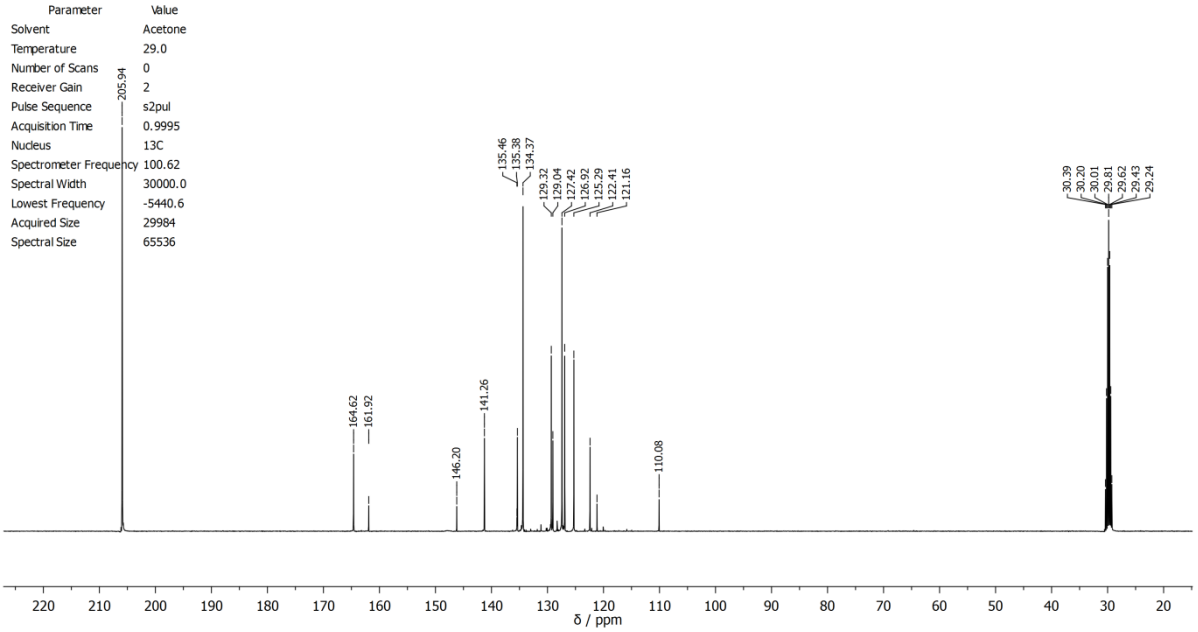


$[Ph]_2B[6\text{-}Br\text{-}Sal][Ani]$ (4)

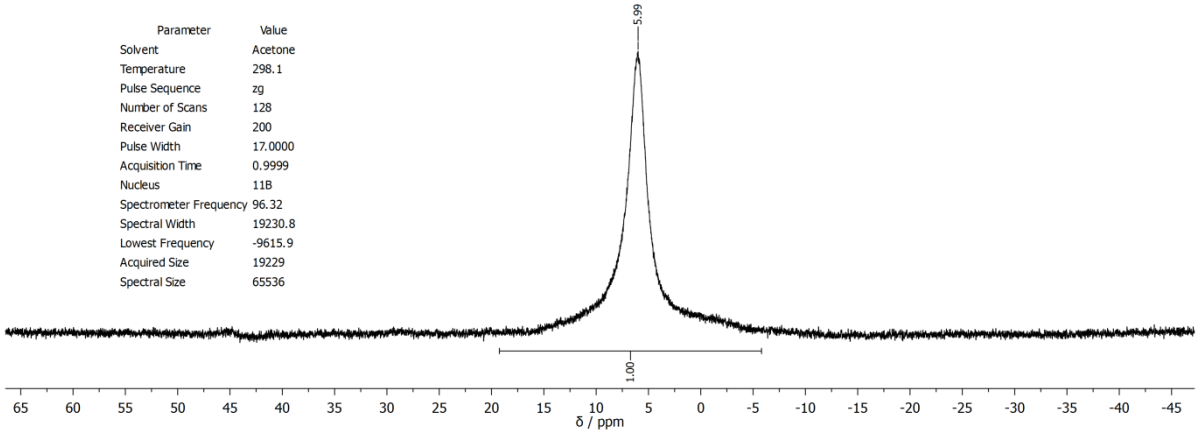
^1H NMR (400 MHz, $CDCl_3$)



$^{13}C\{^1H\}$ NMR (100.6 MHz, acetone-d_6)

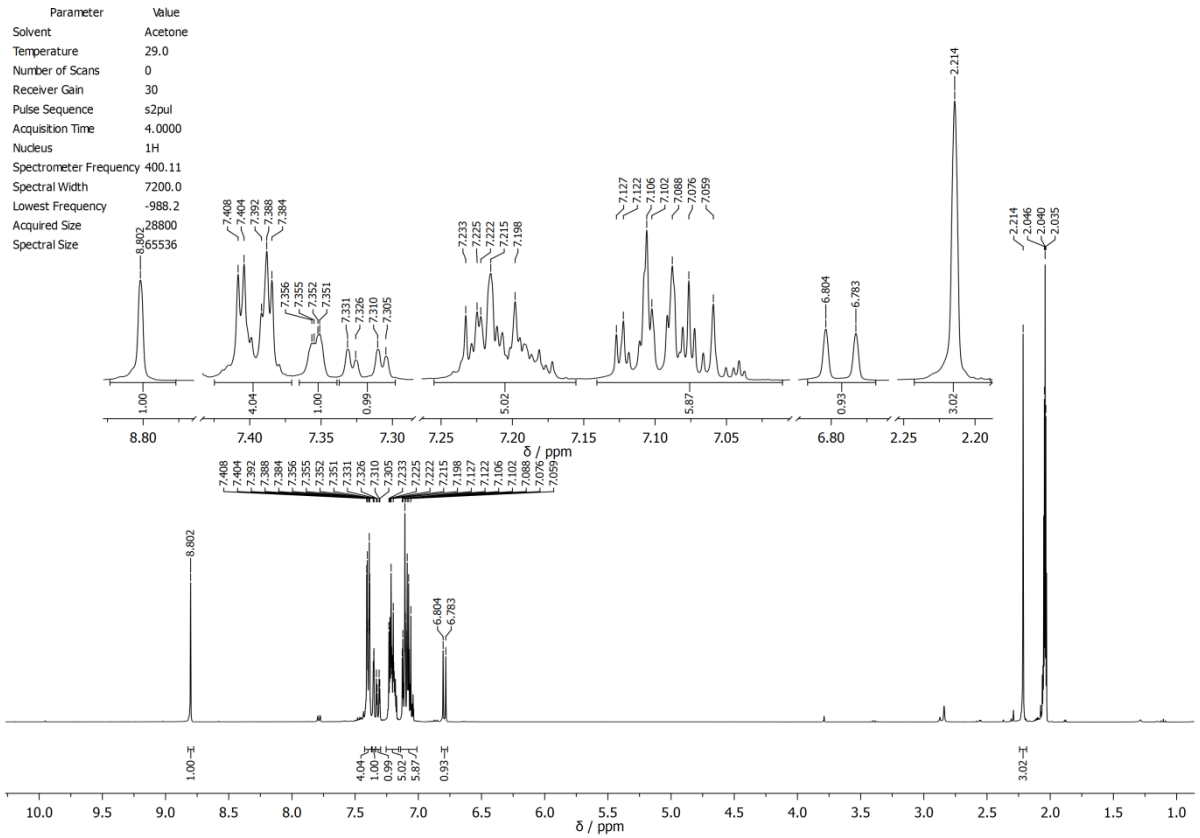


^{11}B NMR (96 MHz, acetone-d_6)

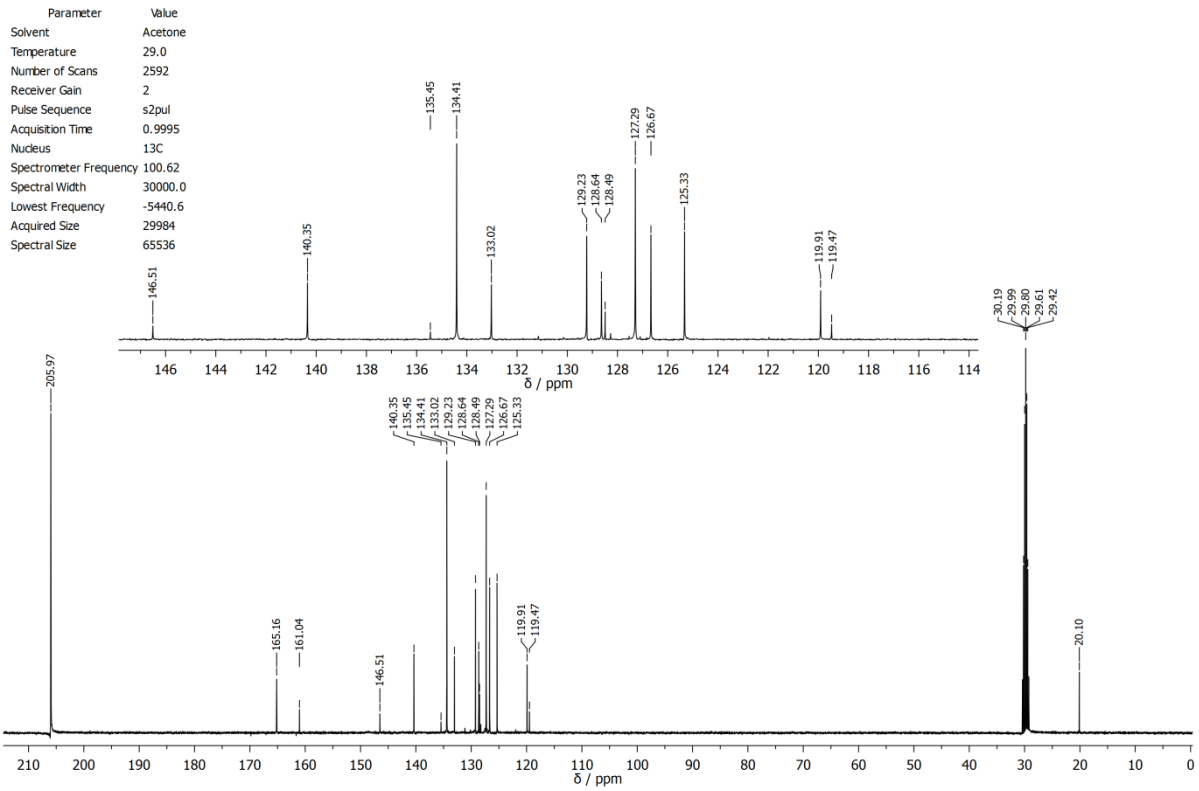


[Ph]$_2$B[6-Me-Sal][Ani] (5)

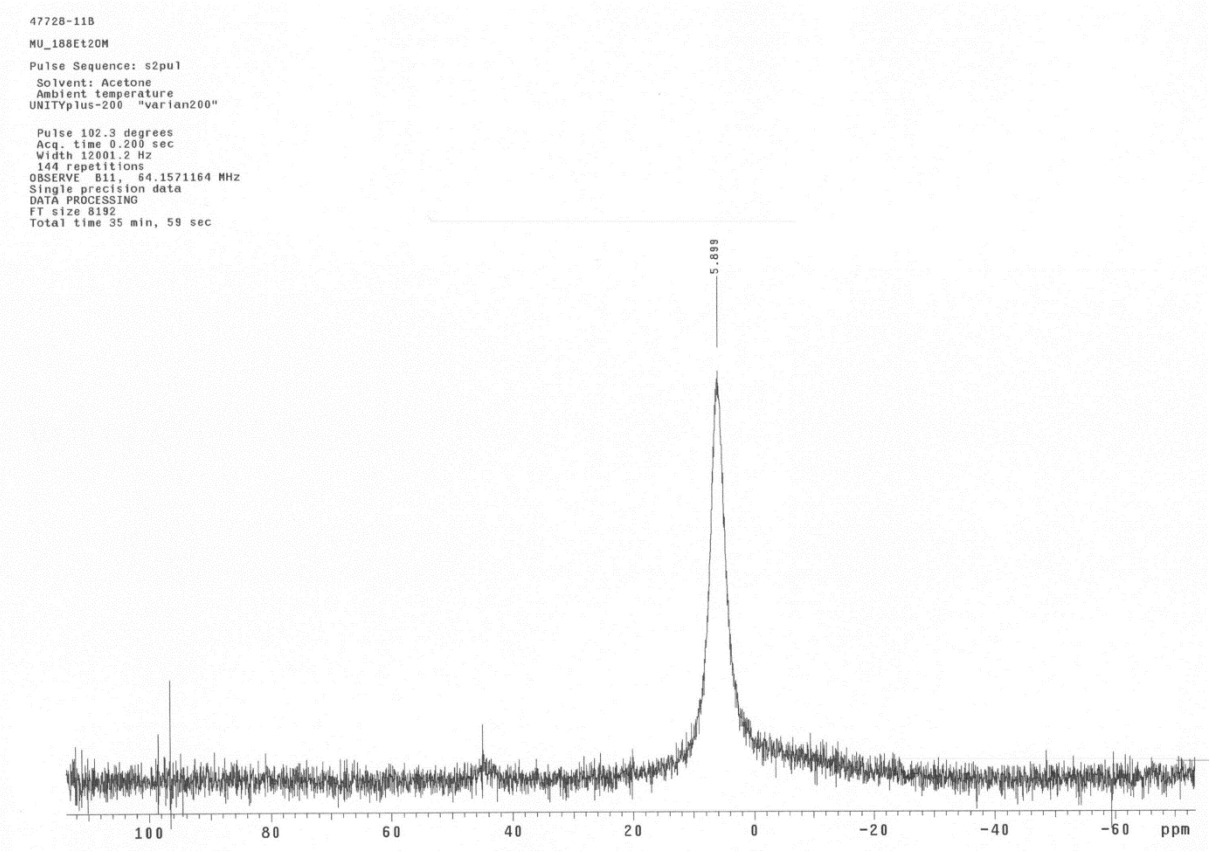
^{1}H NMR (400 MHz, acetone-d_6)



$^{13}C\{^{1}H\}$ NMR (100.6 MHz, acetone-d_6)

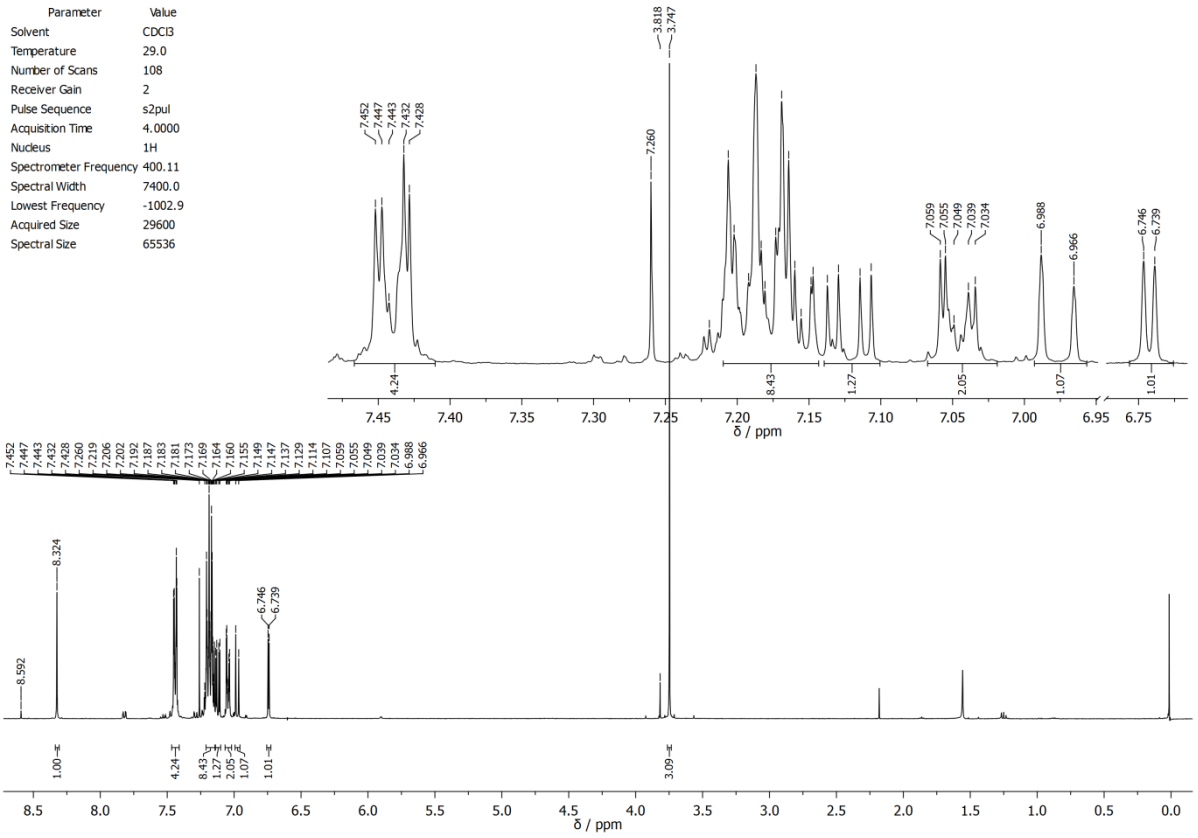


^{11}B NMR (64 MHz, acetone-d_6)

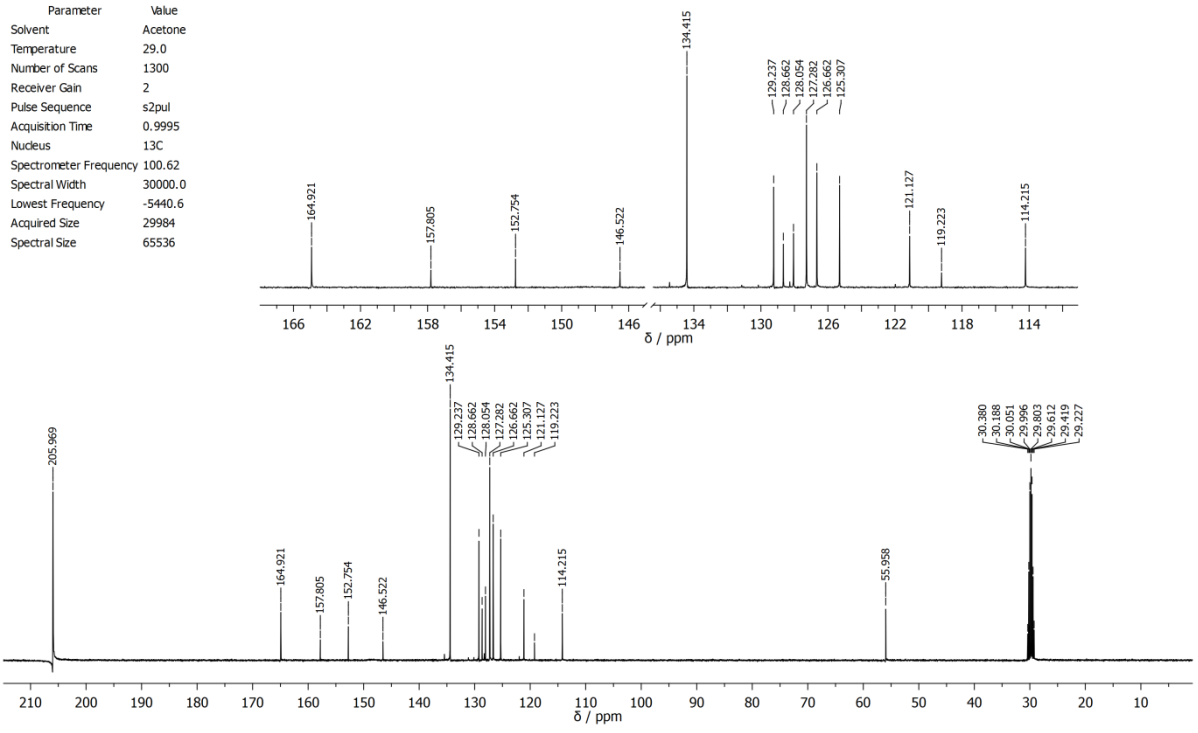


$[Ph]_2B[6\text{-}OMe\text{-}Sal][Ani]$ (6)

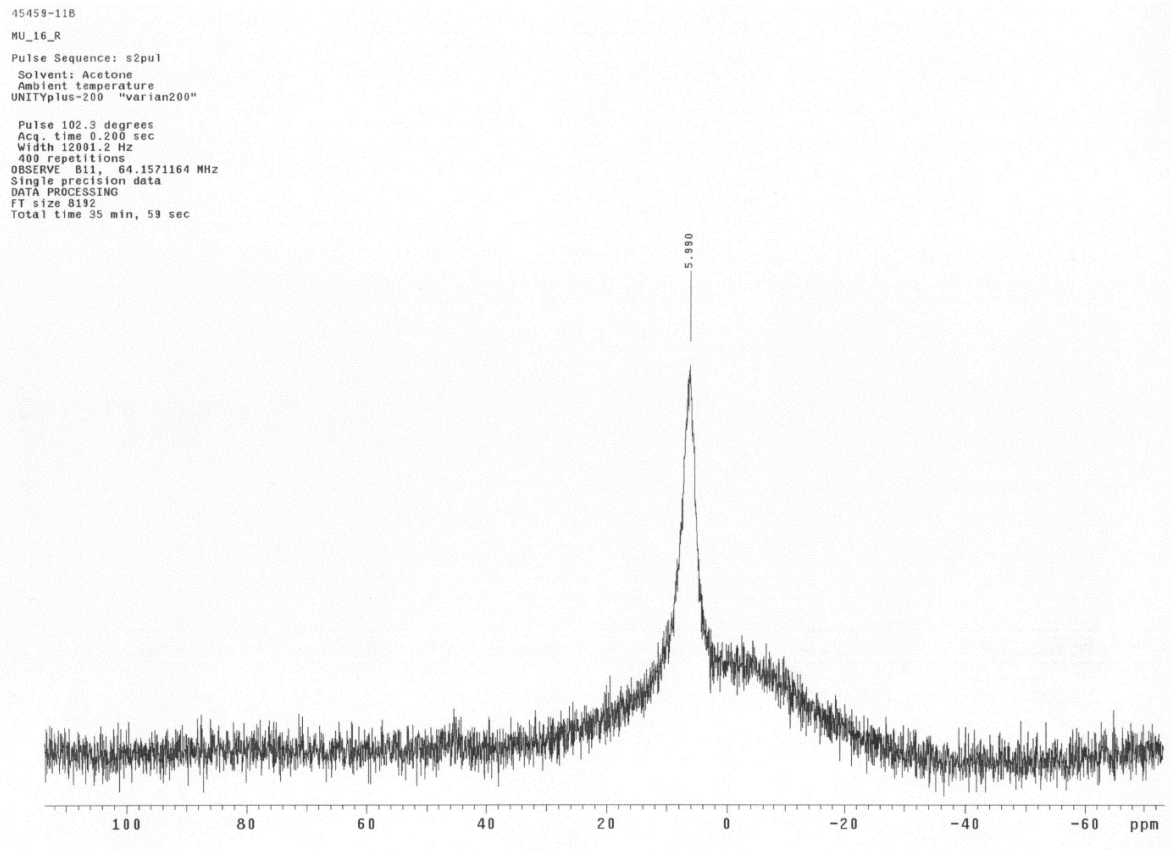
^1H NMR (400 MHz, $CDCl_3$)



$^{13}C\{^1H\}$ NMR (100.6 MHz, acetone-d_6)

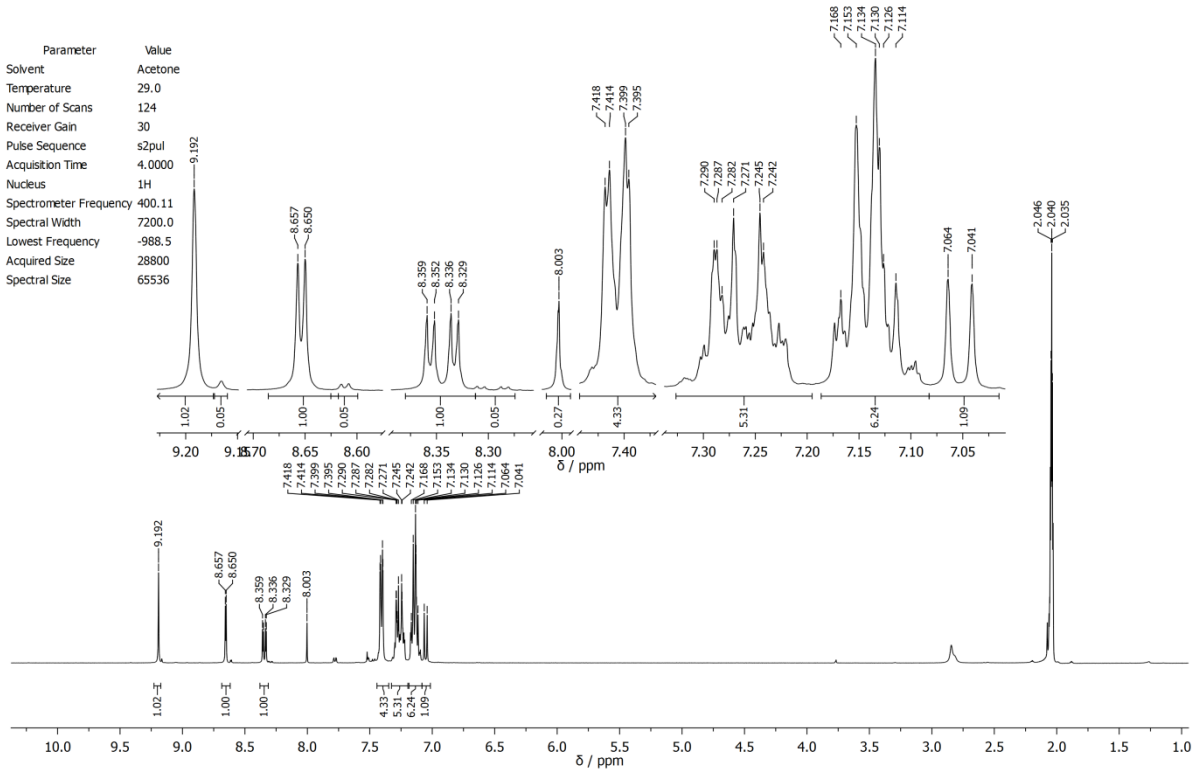


^{11}B NMR (64 MHz, acetone-d_6)

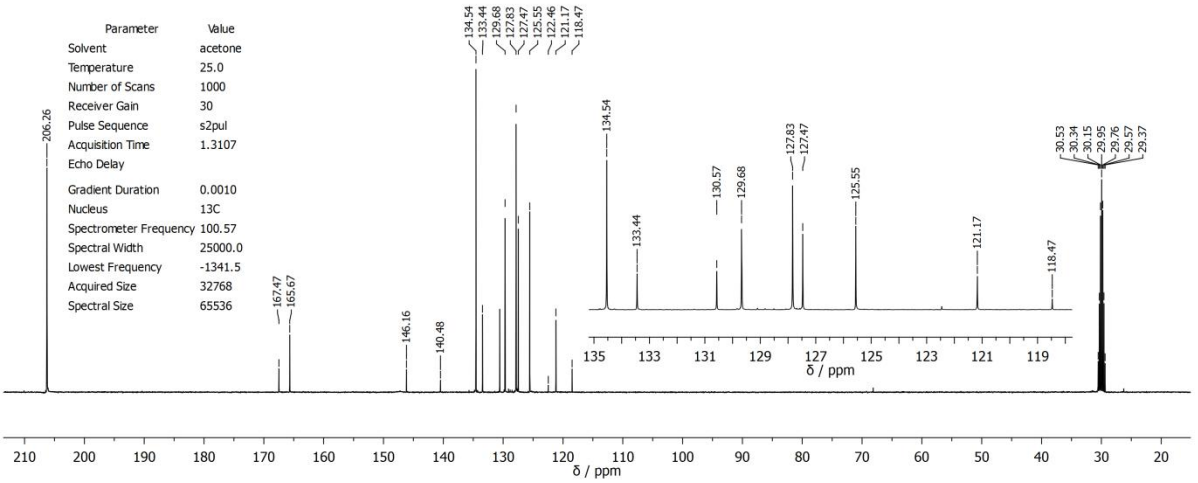


$[Ph]_2B[6\text{-}NO_2\text{-}Sal][Ani]$ (7)

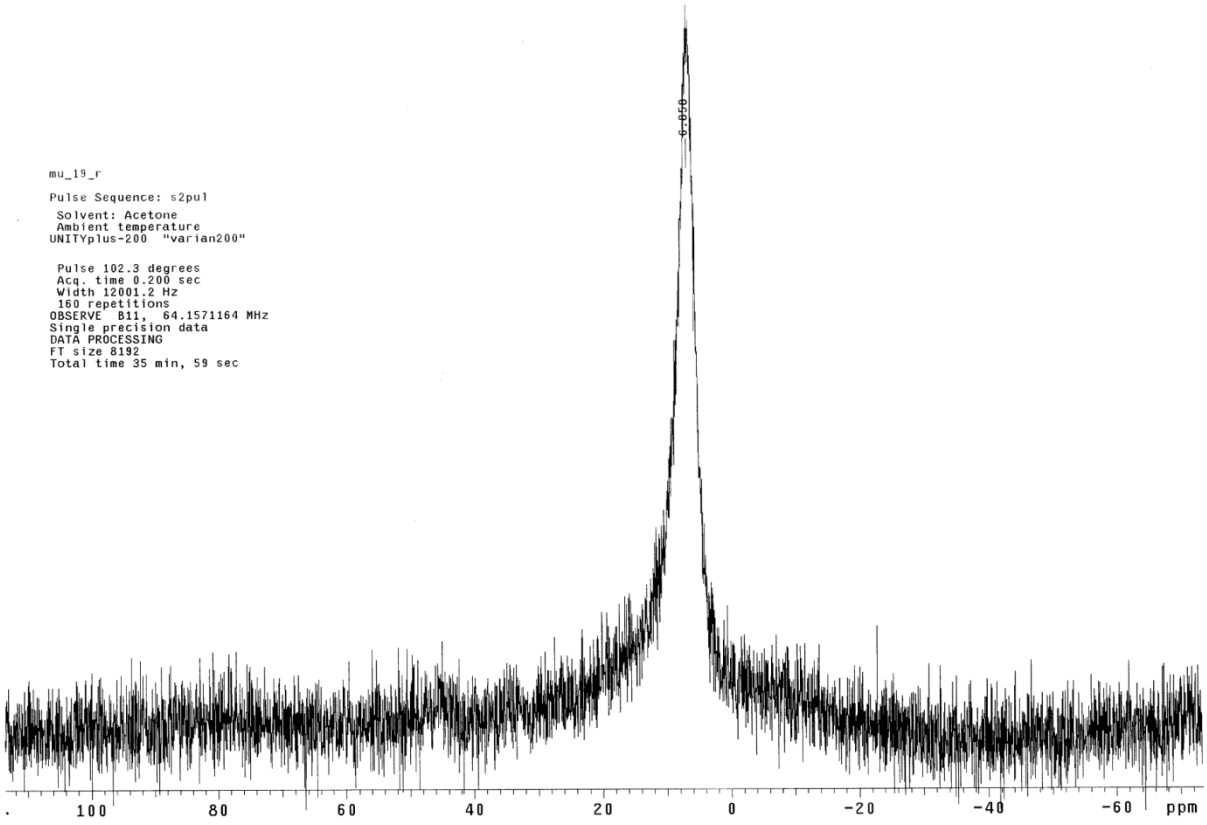
^{1}H NMR (400 MHz, acetone-d_6)



^{13}C NMR (100.6 MHz, acetone-d_6)

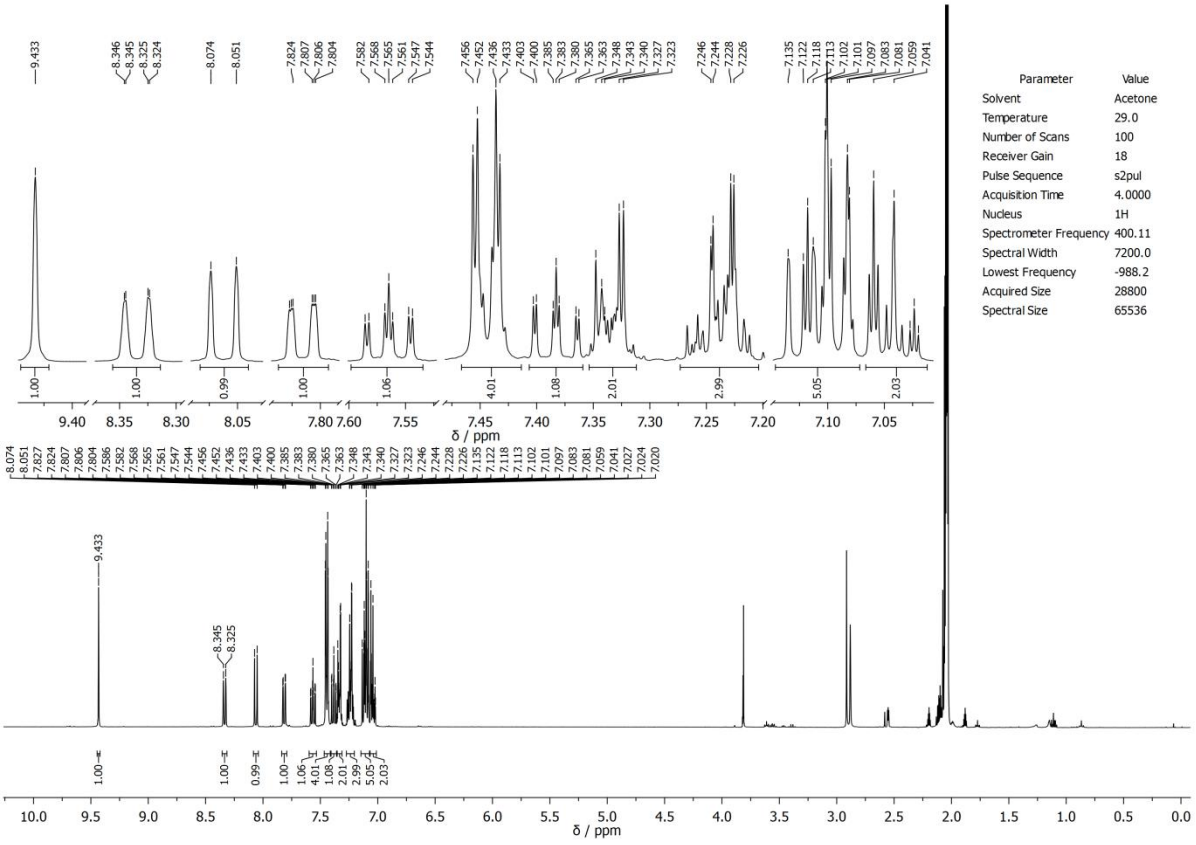


^{11}B NMR (64 MHz, acetone-d_6)

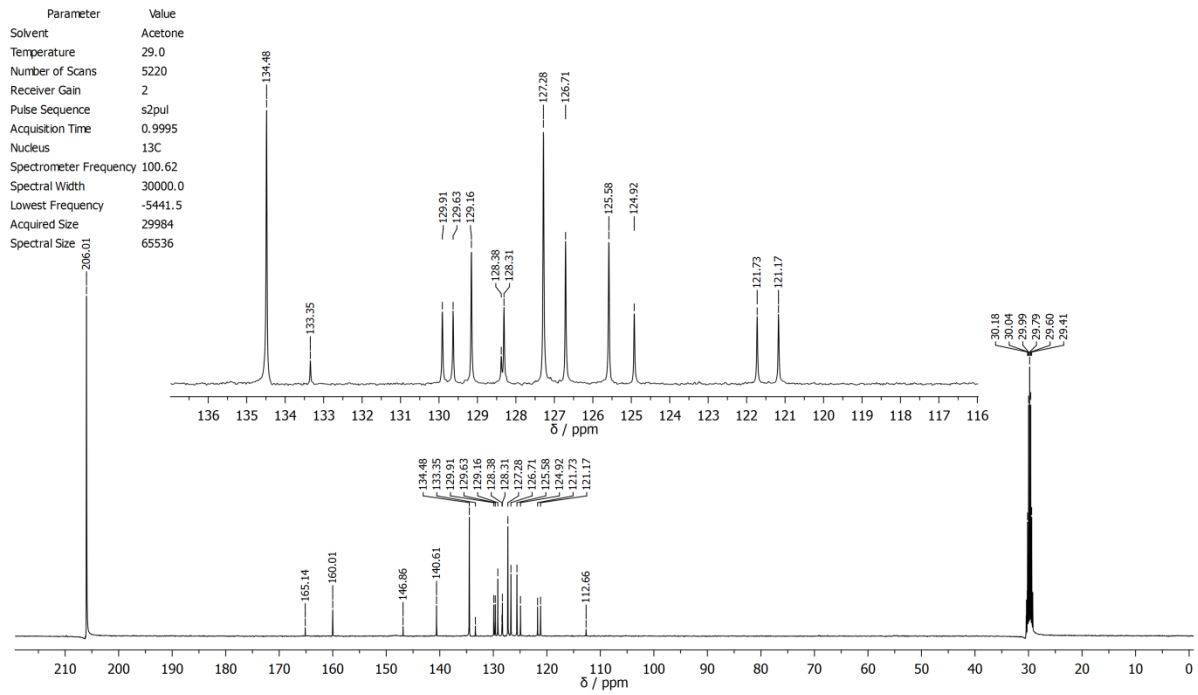


$[Ph]_2B[Naft\text{-}Sal][Ani]$ (8).

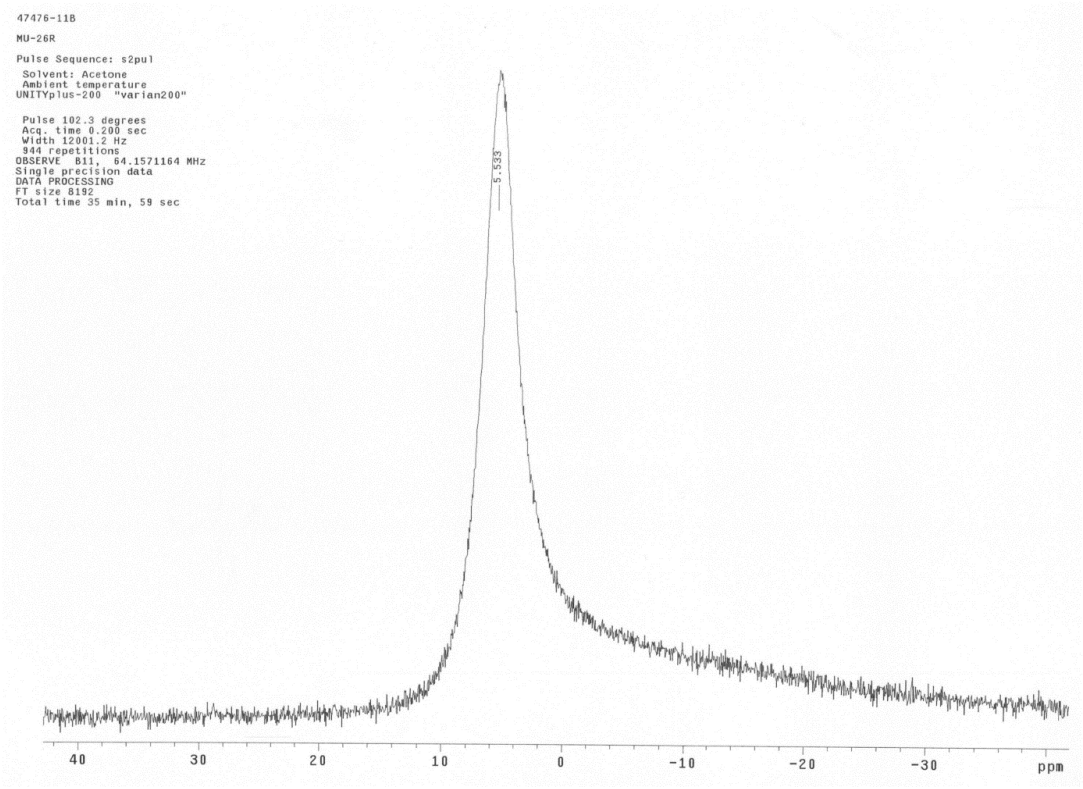
^1H NMR (400 MHz, $CDCl_3$)



$^{13}C\{^1H\}$ NMR (100.6 MHz, $CDCl_3$)

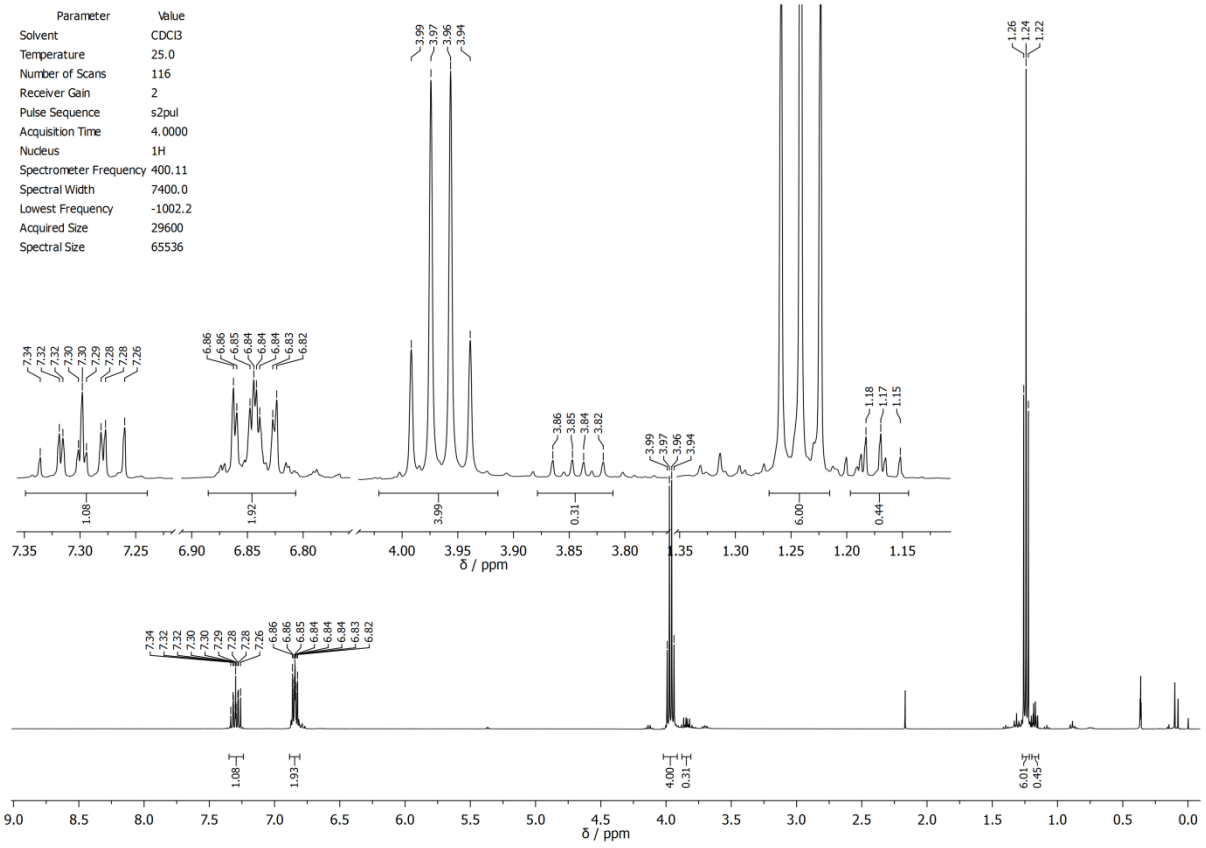


^{11}B NMR (64 MHz, acetone-d_6)

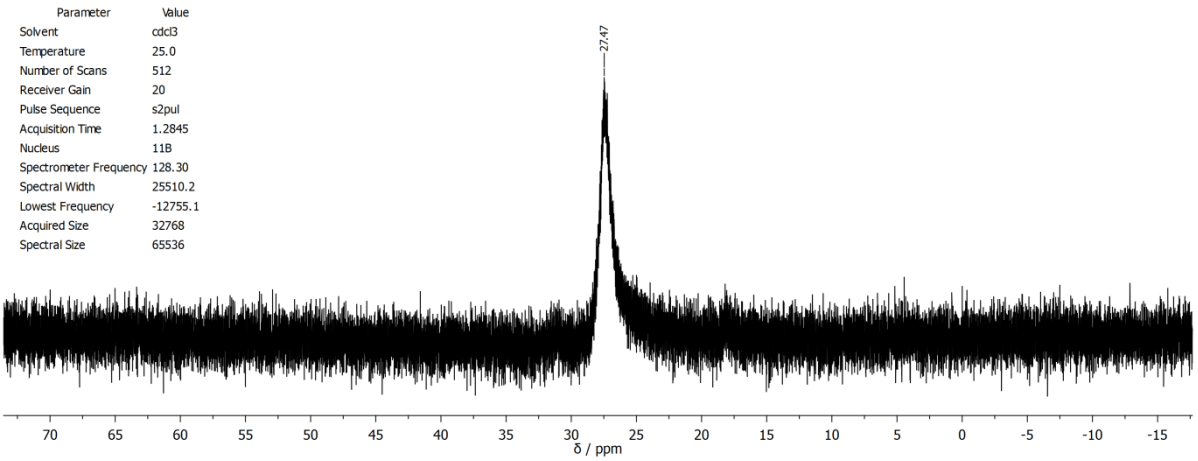


Diethyl 2,6-difluorophenylboronate

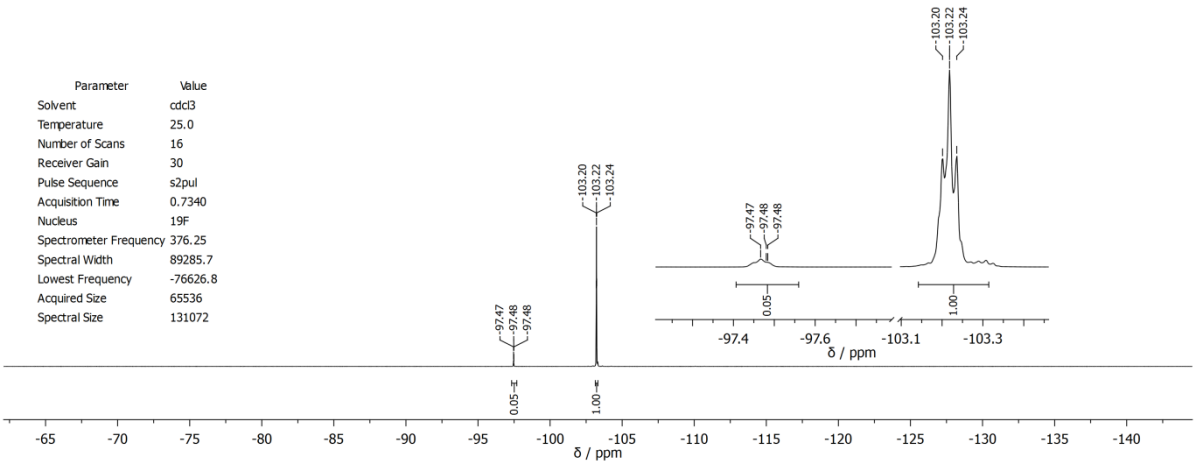
^{1}H NMR (400 MHz, $CDCl_3$)



^{11}B NMR (64 MHz, $CDCl_3$)

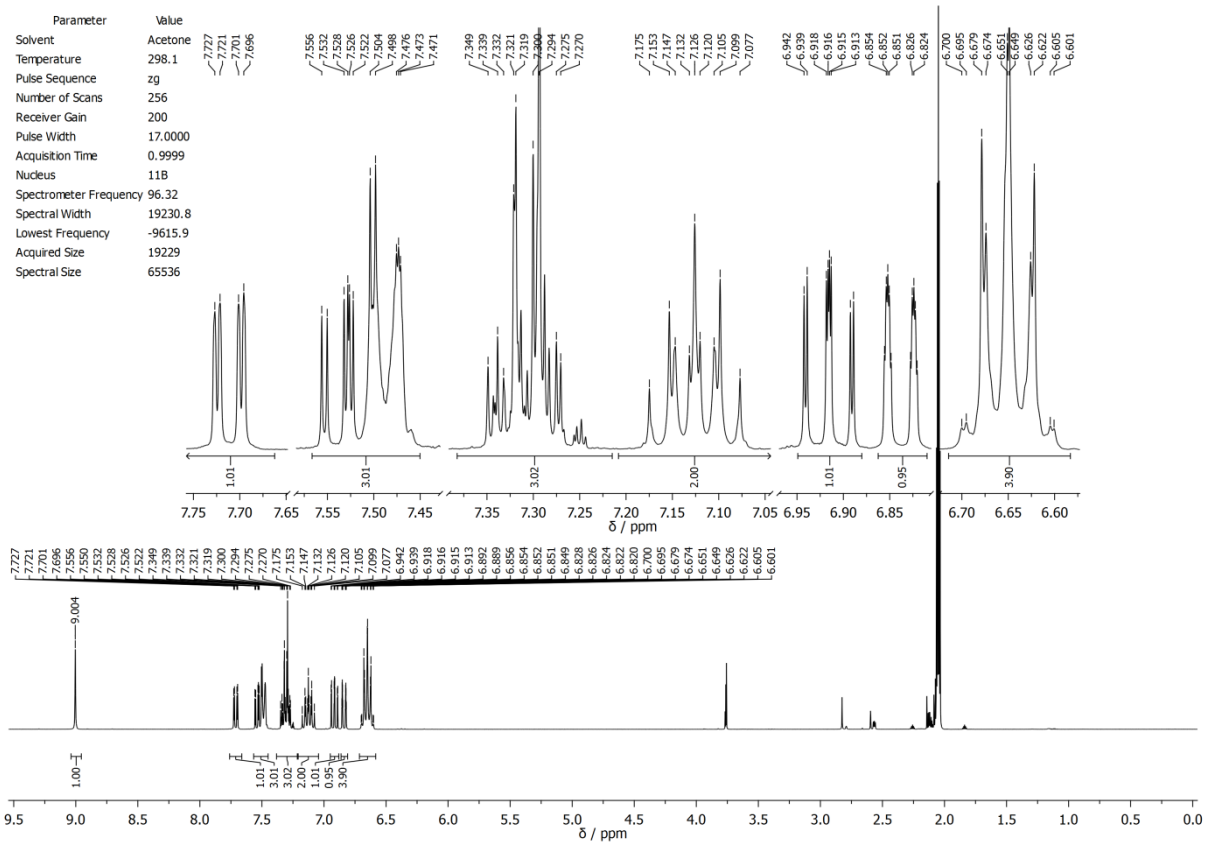


^{19}F NMR (376 MHz, $CDCl_3$)

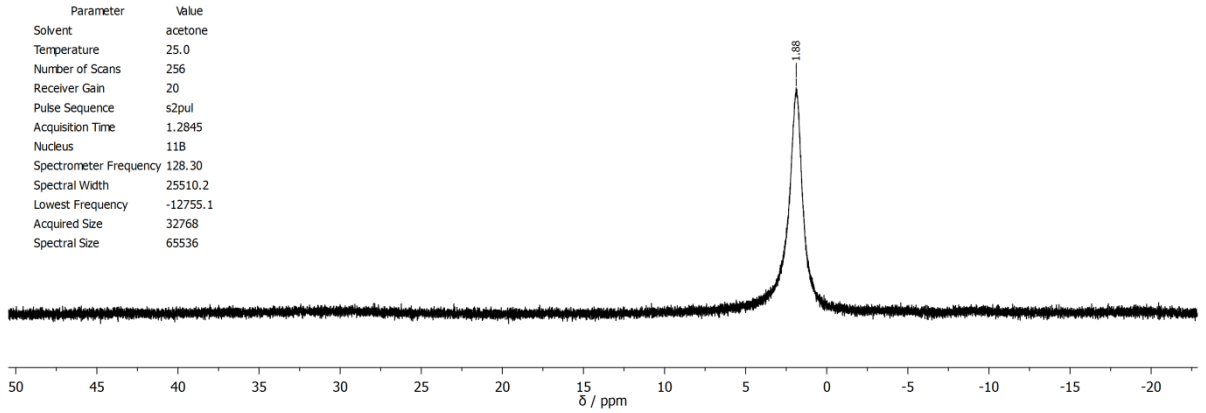


[2,6-diFPh]$_2$B[6-H-Sal][Ani] (9)

^{1}H NMR (300 MHz, acetone-d$_6$)

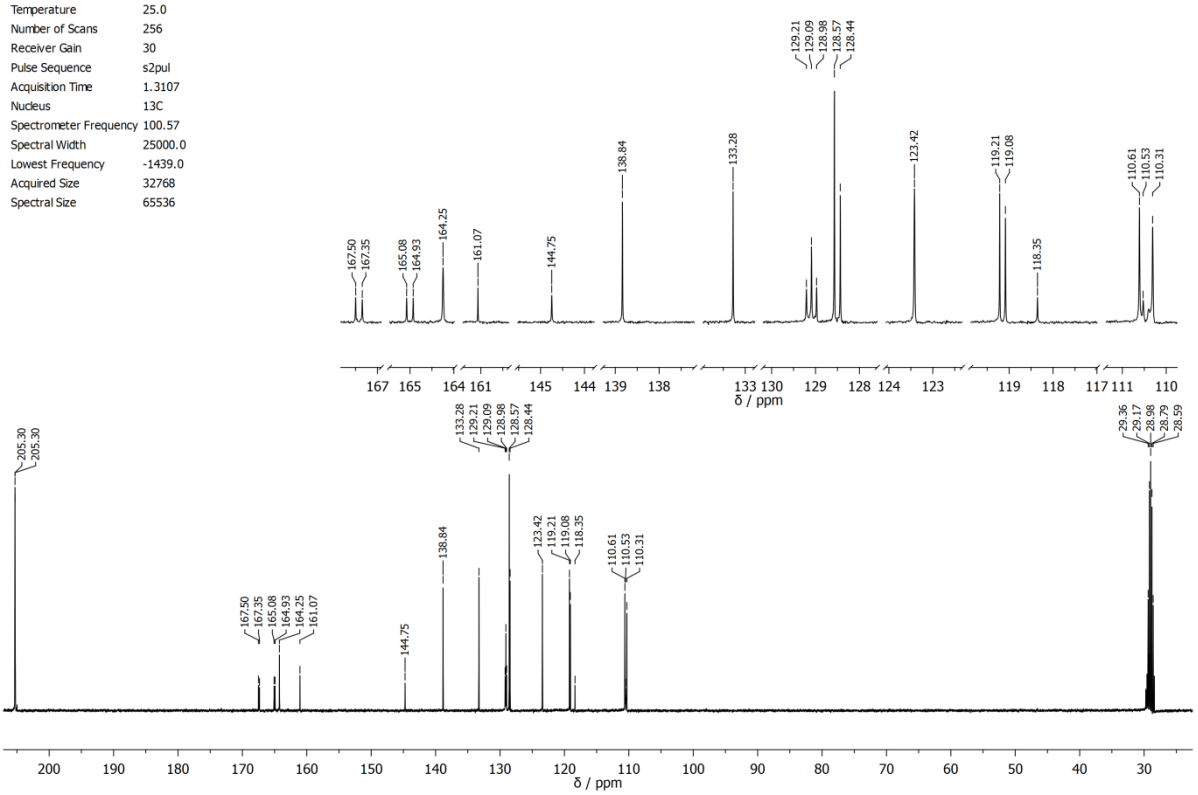


^{11}B NMR (96 MHz, acetone-d$_6$)



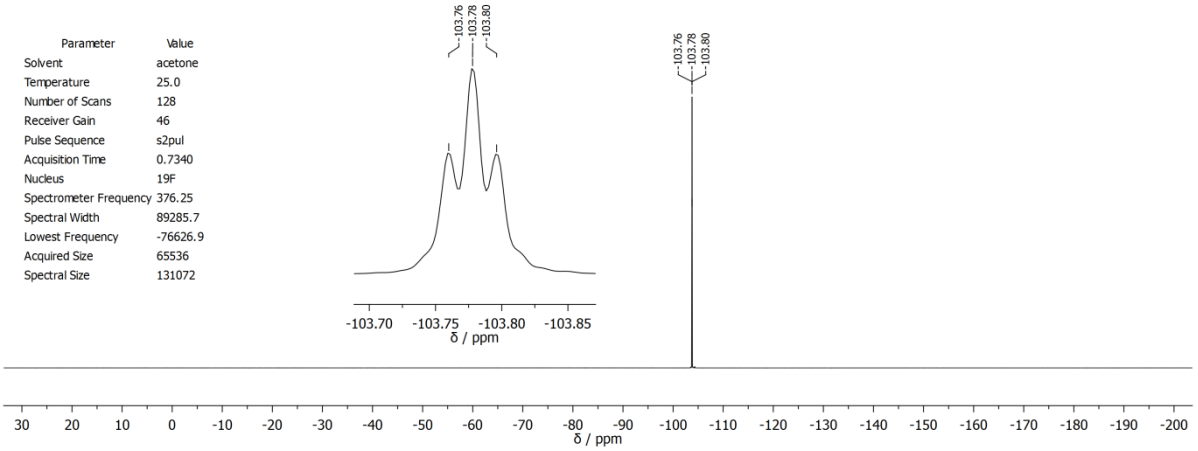
^{13}C NMR (100.6 MHz, acetone-d_6)

Parameter	Value
Solvent	acetone
Temperature	25.0
Number of Scans	256
Receiver Gain	30
Pulse Sequence	s2pul
Acquisition Time	1.3107
Nucleus	13C
Spectrometer Frequency	100.57
Spectral Width	25000.0
Lowest Frequency	-1439.0
Acquired Size	32768
Spectral Size	65536

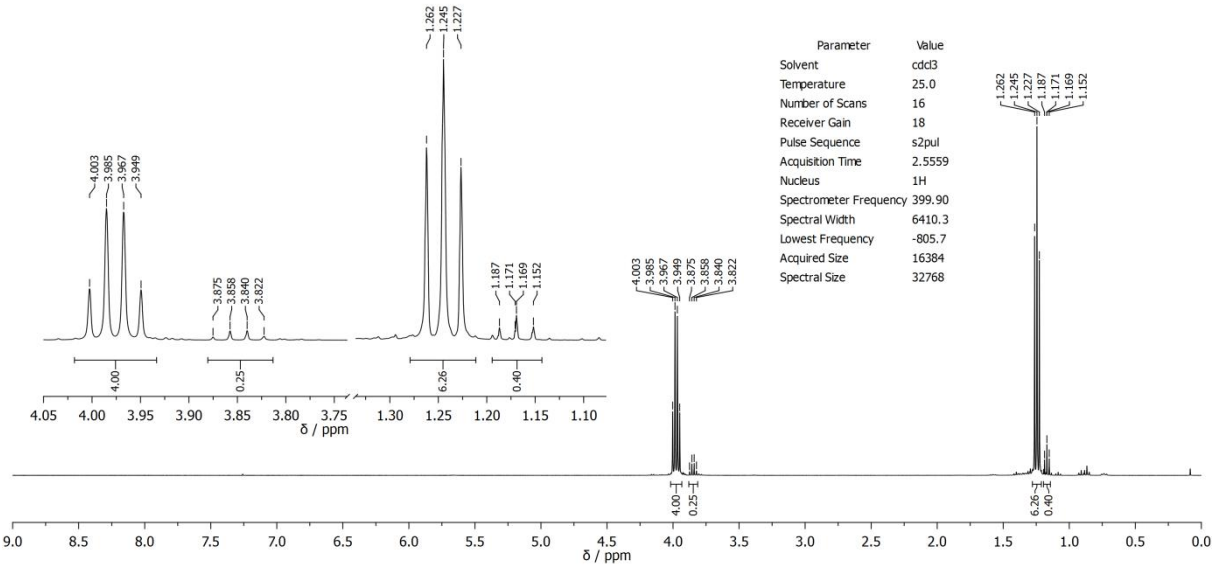


^{19}F NMR (376 MHz, acetone-d_6)

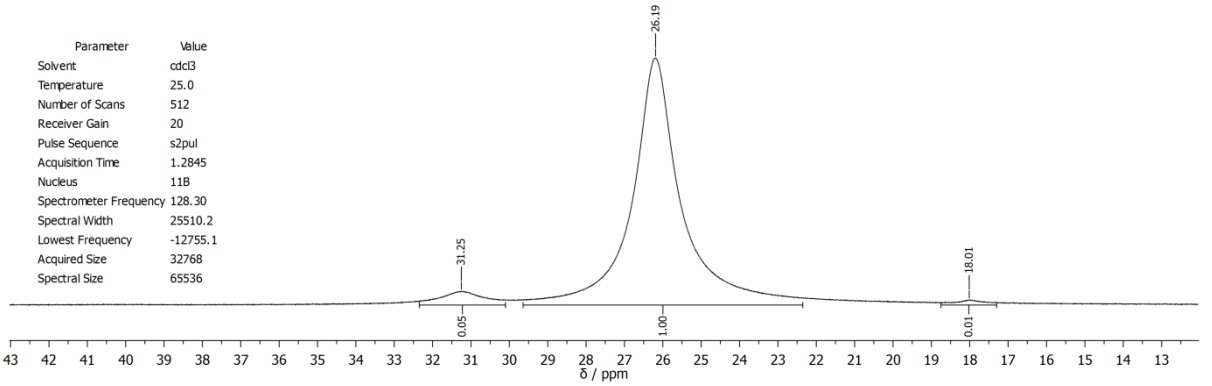
Parameter	Value
Solvent	acetone
Temperature	25.0
Number of Scans	128
Receiver Gain	46
Pulse Sequence	s2pul
Acquisition Time	0.7340
Nucleus	19F
Spectrometer Frequency	376.25
Spectral Width	89285.7
Lowest Frequency	-76626.9
Acquired Size	65536
Spectral Size	131072



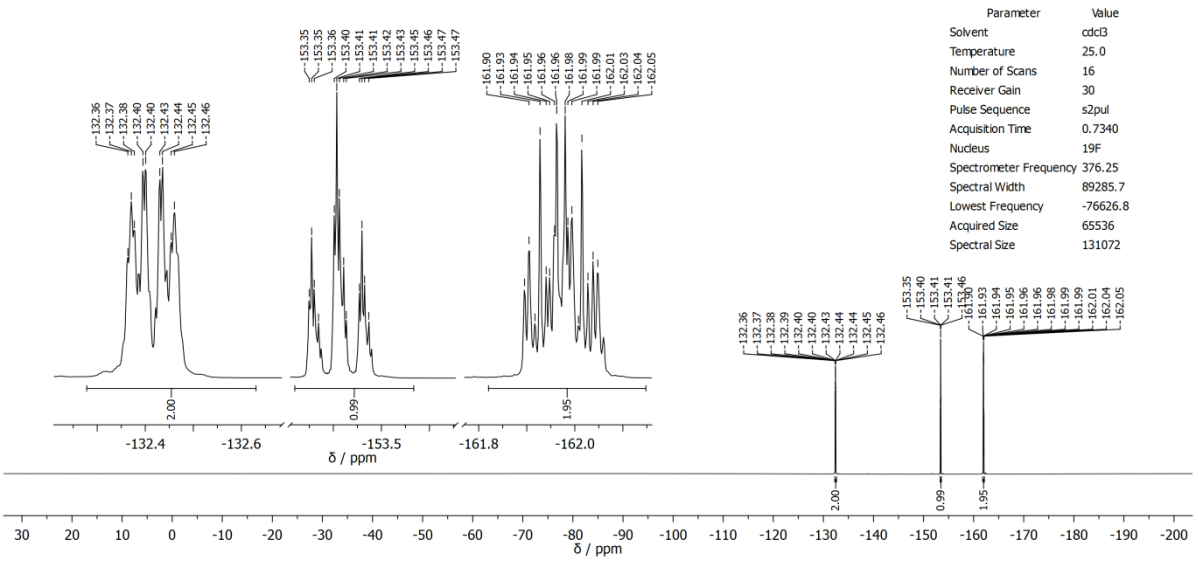
Diethyl pentafluorophenylboronate
^{1}H NMR (400 MHz, $CDCl_3$)



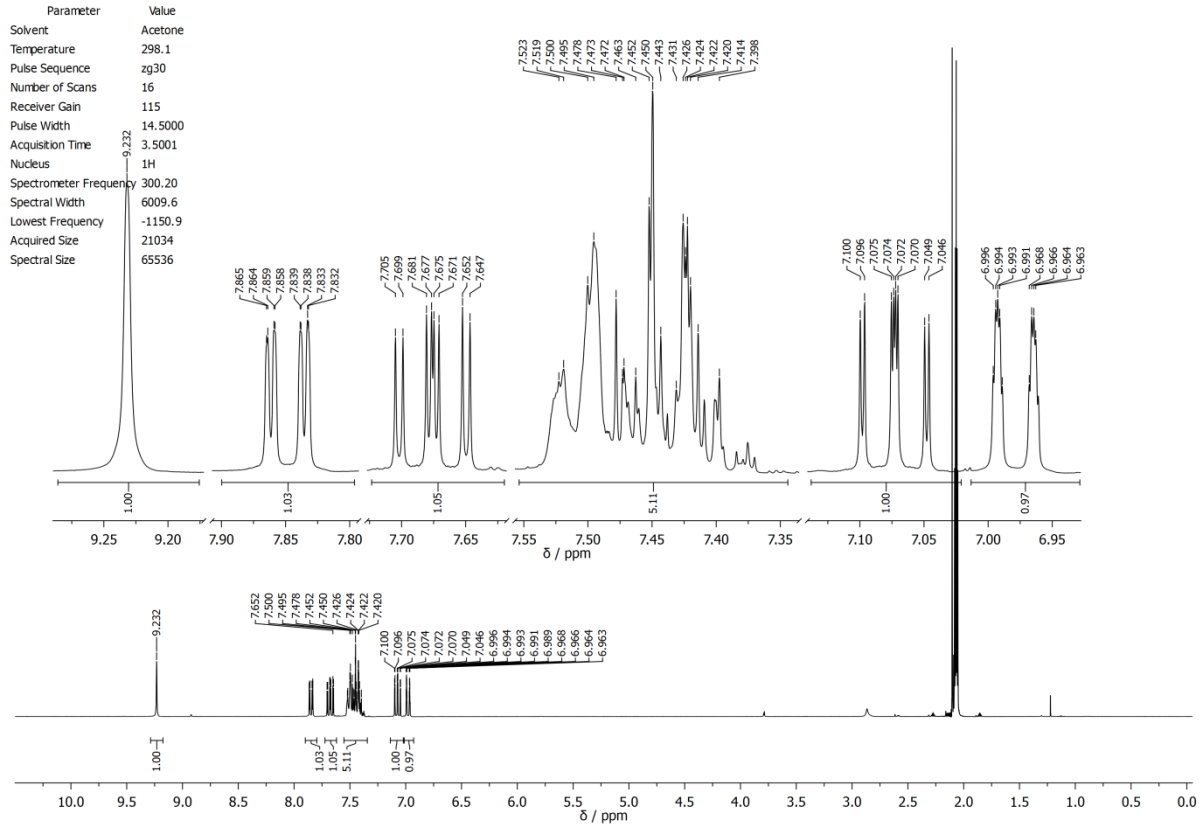
^{11}B NMR (128 MHz, $CDCl_3$)



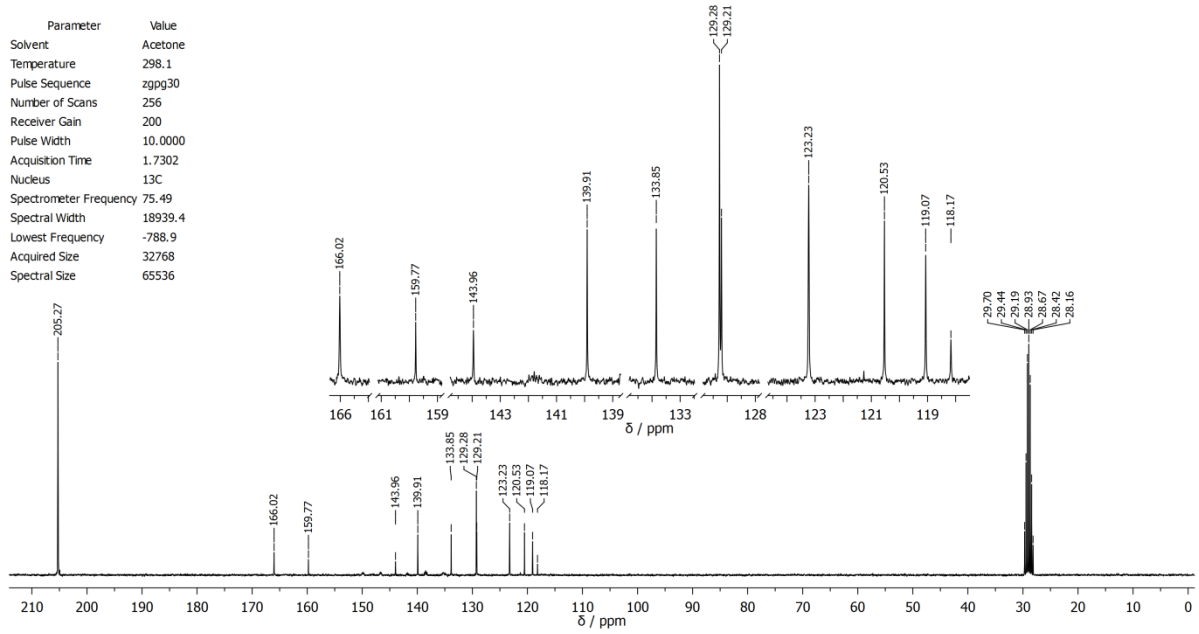
^{19}F NMR (376 MHz, $CDCl_3$)



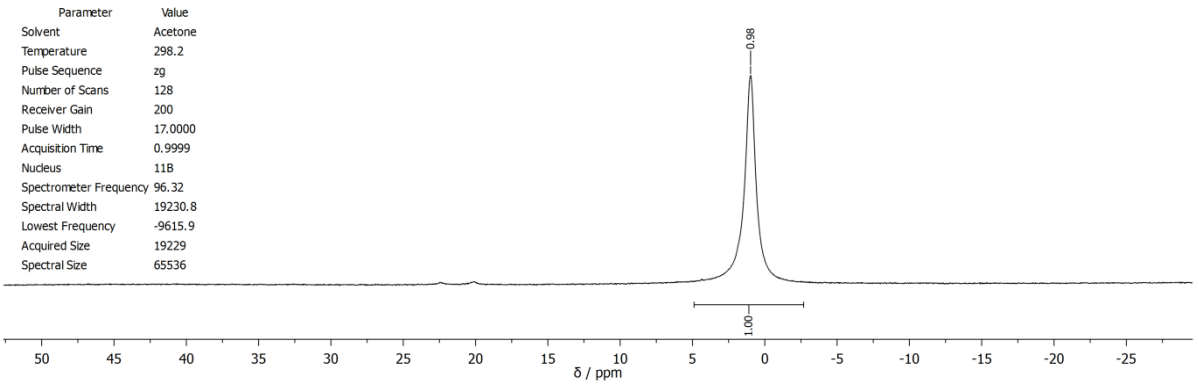
[pentaFPh]$_2$B[6-H-Sal][Ani] (10)
^{1}H NMR (300 MHz, acetone-d_6)



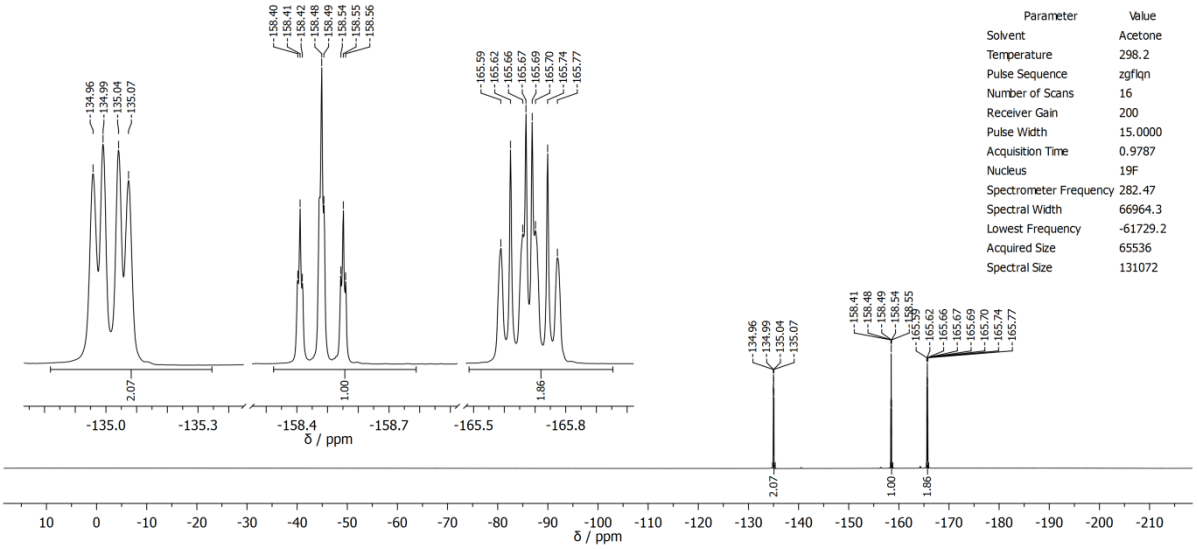
^{13}C NMR (75 MHz, acetone-d_6)



^{11}B NMR (96 MHz, acetone-d_6)



^{19}F NMR (282 MHz, acetone-d_6)



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