New Journal of Chemistry

Supporting Information for

Aggregation-Induced Emission Enhancement of Chiral Boranils

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Contenu

NMR spectra

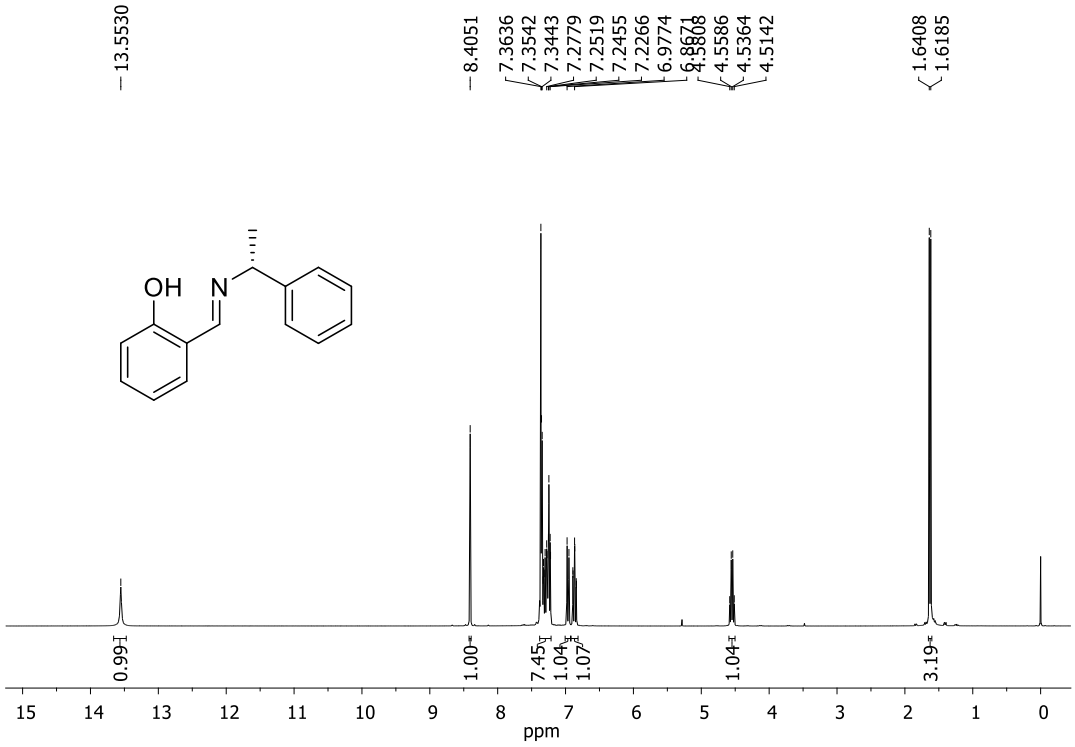

*Figure S 1 - ^{1}H NMR spectrum of (R,E)-2-(((3,3-dimethylbutan-2-yl)imino)methyl)phenol **2a-R** in $CDCl_3$.*

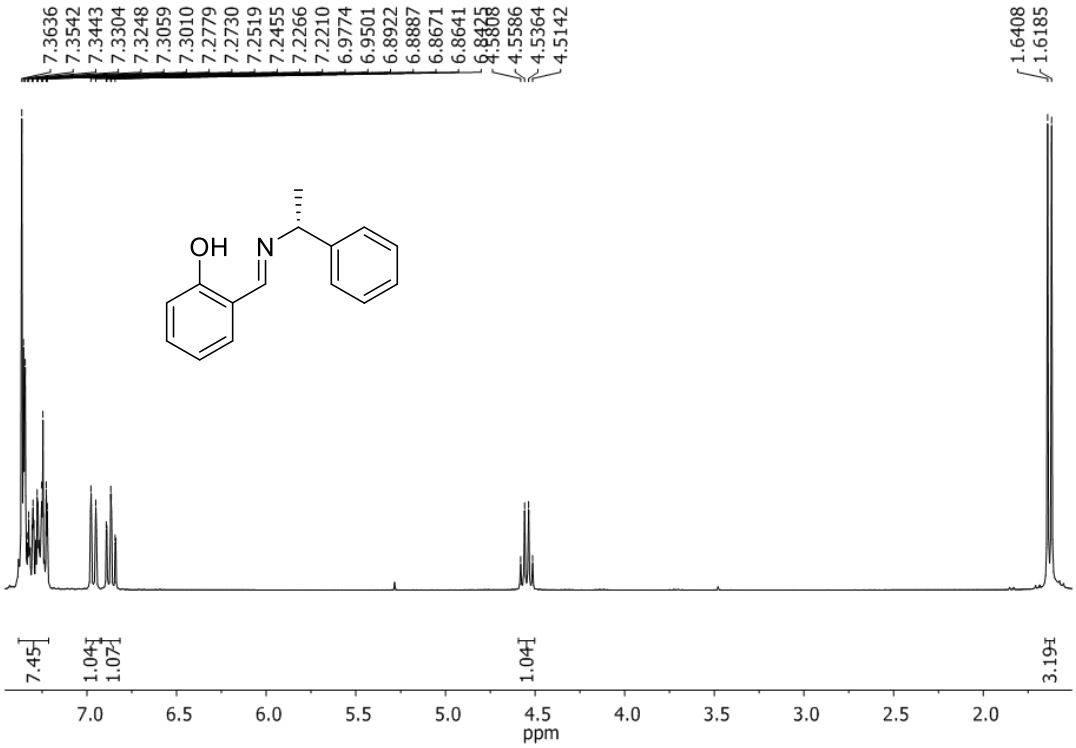

*Figure S 2 - ^{1}H NMR spectrum expansion of (R,E)-2-(((3,3-dimethylbutan-2-yl)imino)methyl)phenol **2a-R** in $CDCl_3$.*

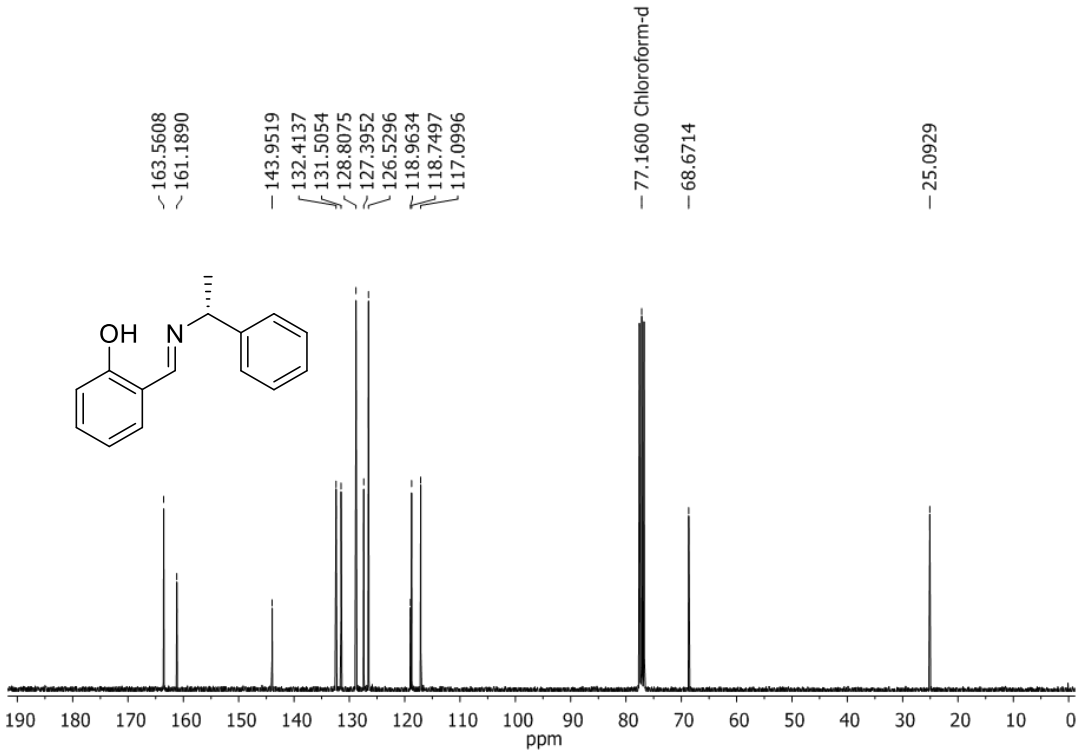

*Figure S 3 – ^{13}C NMR spectrum of (R,E)-2-(((3,3-dimethylbutan-2-yl)imino)methyl)phenol **2a-R** in $CDCl_3$.*

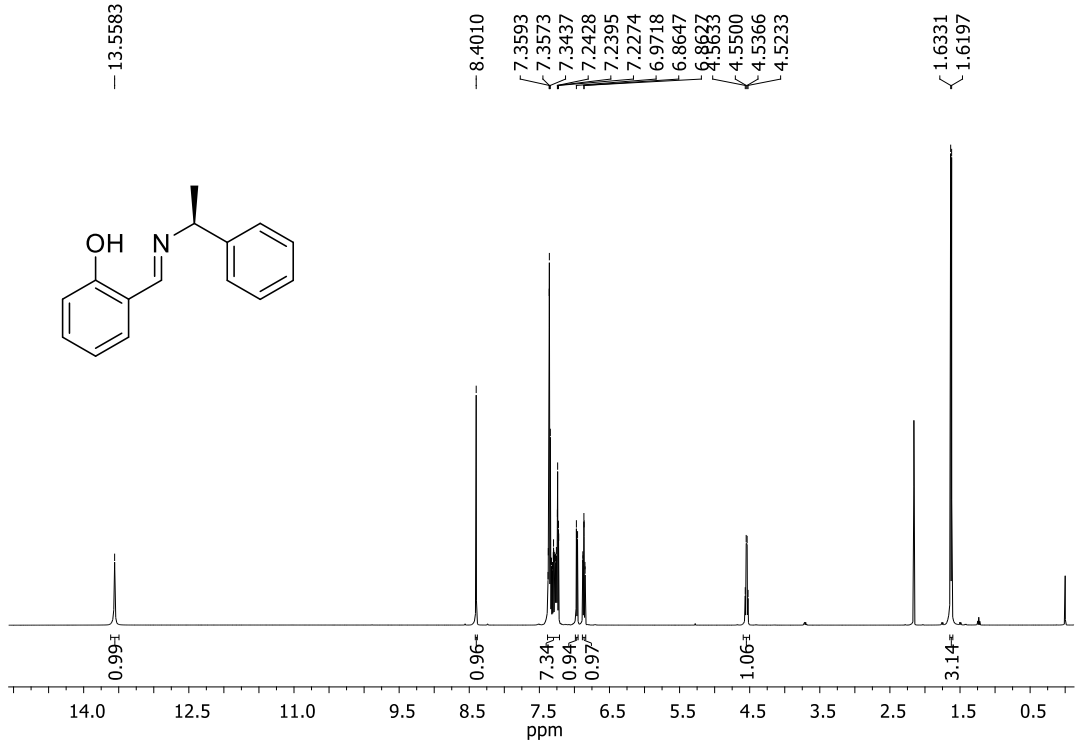

*Figure S 4 - ^{1}H NMR spectrum of (S,E)-2-(((3,3-dimethylbutan-2-yl)imino)methyl)phenol **2a-S** in $CDCl_3$.*

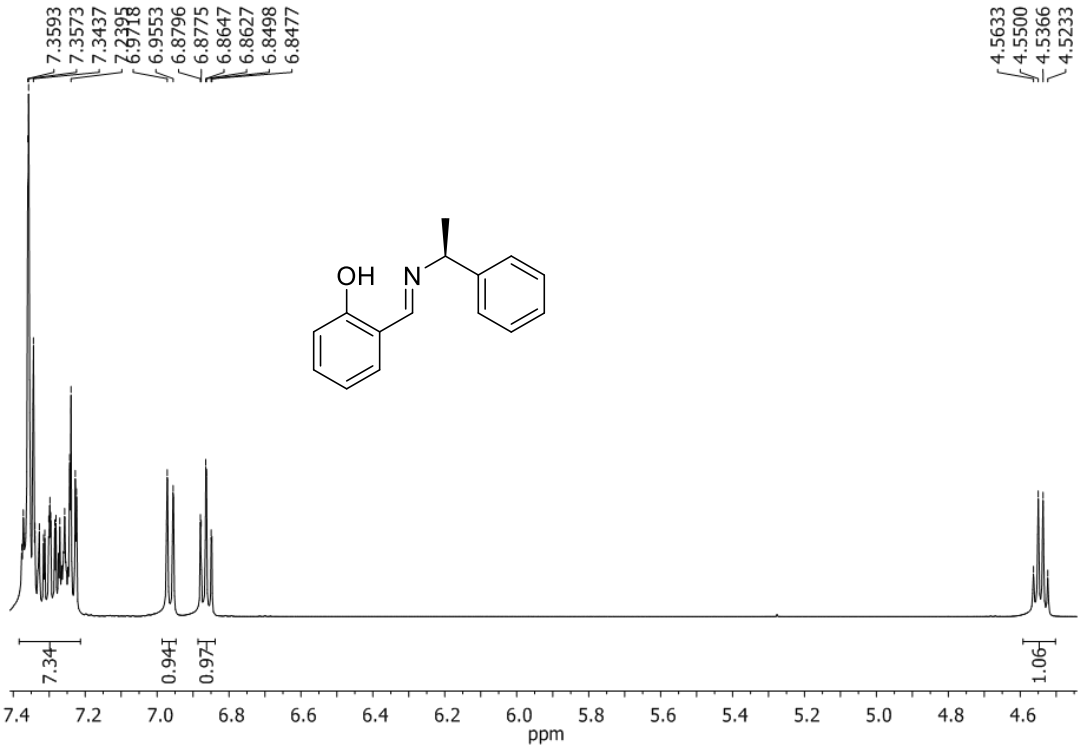

*Figure S 5 - ^{1}H NMR spectrum expansion of (S,E)-2-(((3,3-dimethylbutan-2-yl)imino)methyl)phenol **2a-S** in $CDCl_3$.*

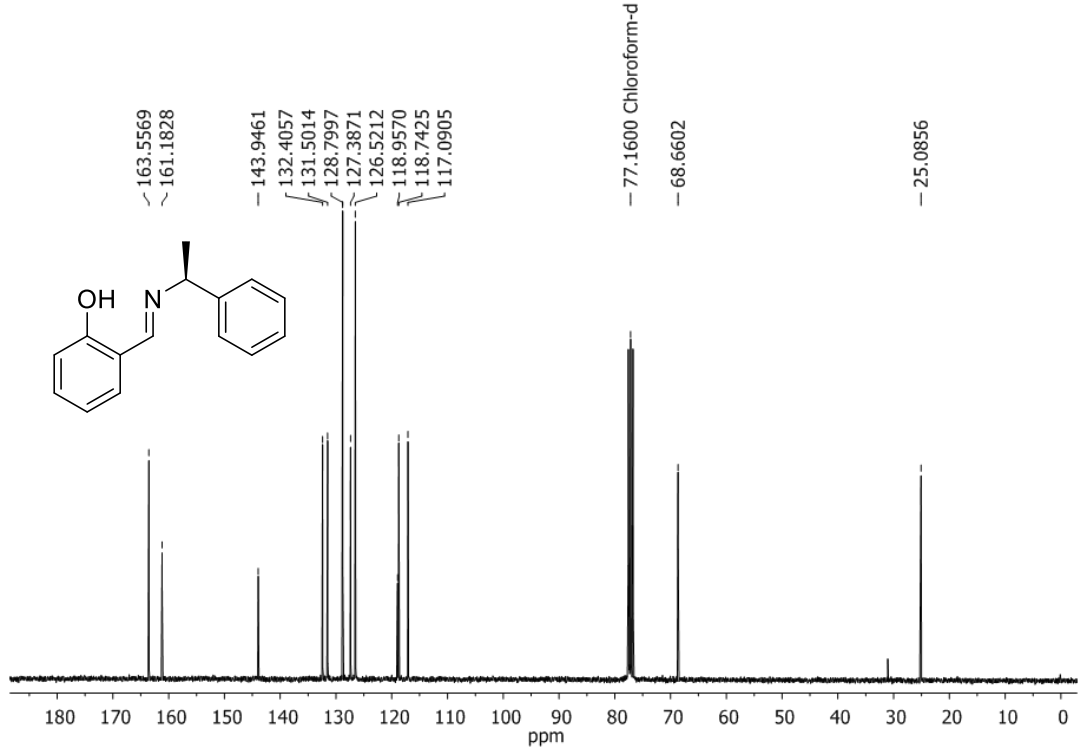

*Figure S 6– ^{13}C NMR spectrum of (S,E)-2-(((3,3-dimethylbutan-2-yl)imino)methyl)phenol **2a-S** in $CDCl_3$.*

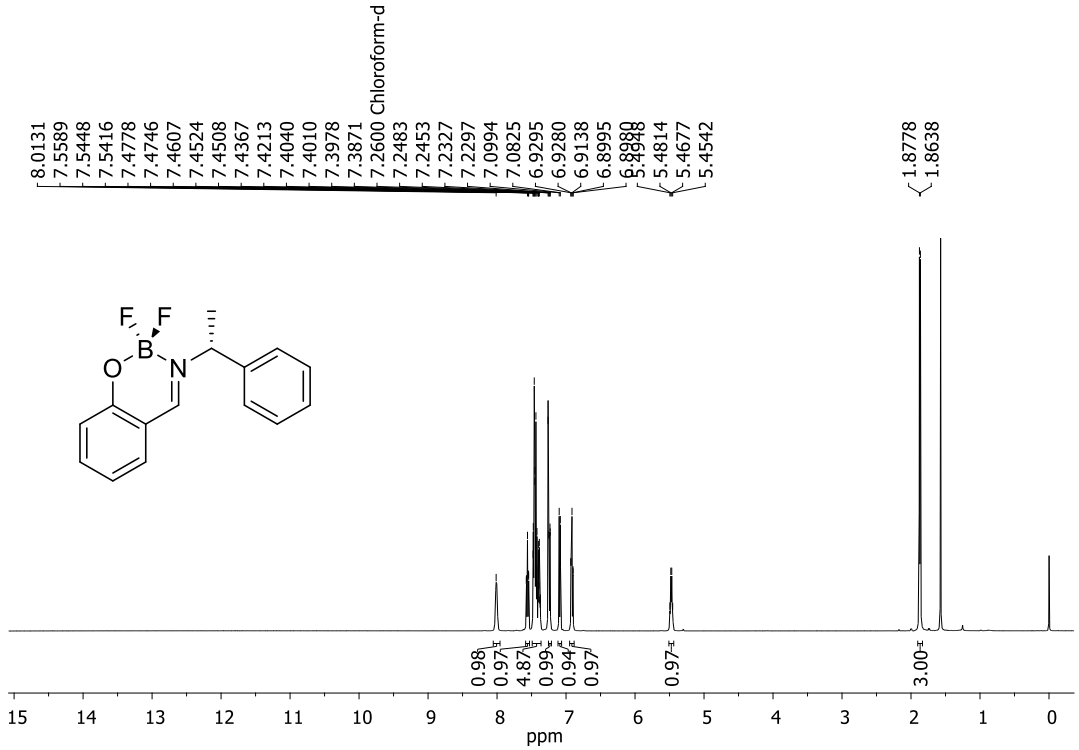

Figure S 7 - ^{1}H NMR spectrum of (R)-2,2-difluoro-3-(1-phenylethyl)-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide 3a-R in CDCl3.

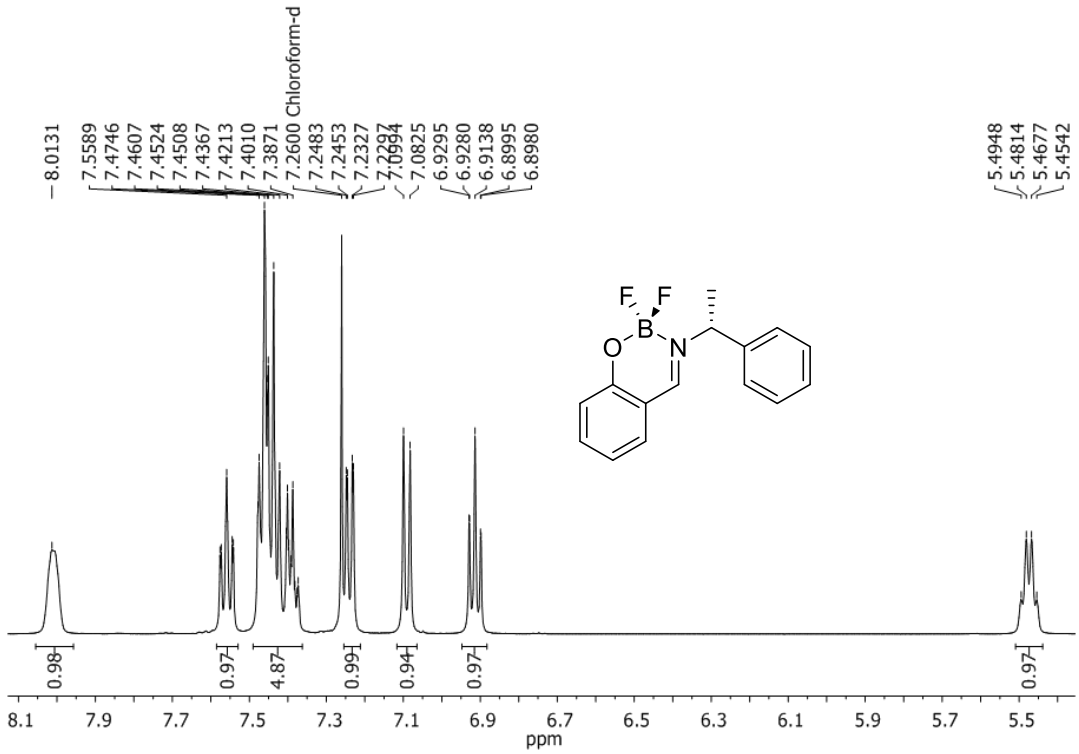

*Figure S 8 - ^{1}H NMR spectrum of (R)-2,2-difluoro-3-(1-phenylethyl)-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3a-R** in $CDCl_3$.*

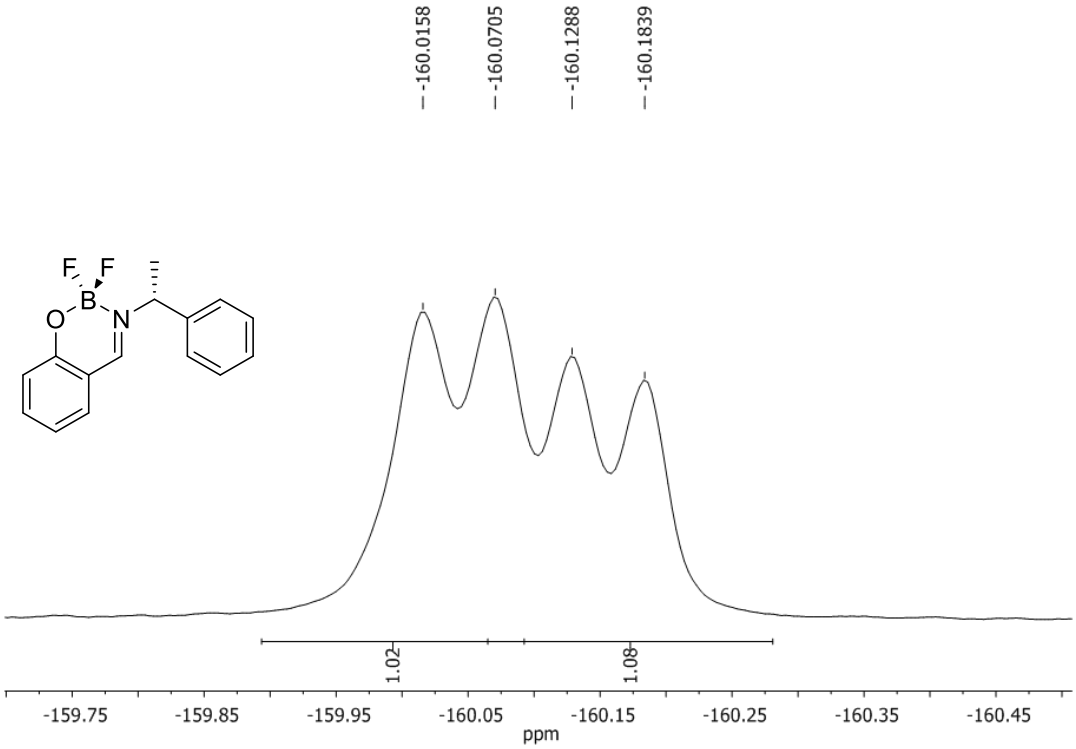

*Figure S 9 -[19]F NMR spectrum of (R)-2,2-difluoro-3-(1-phenylethyl)-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3a-R** in $CDCl_3$.*

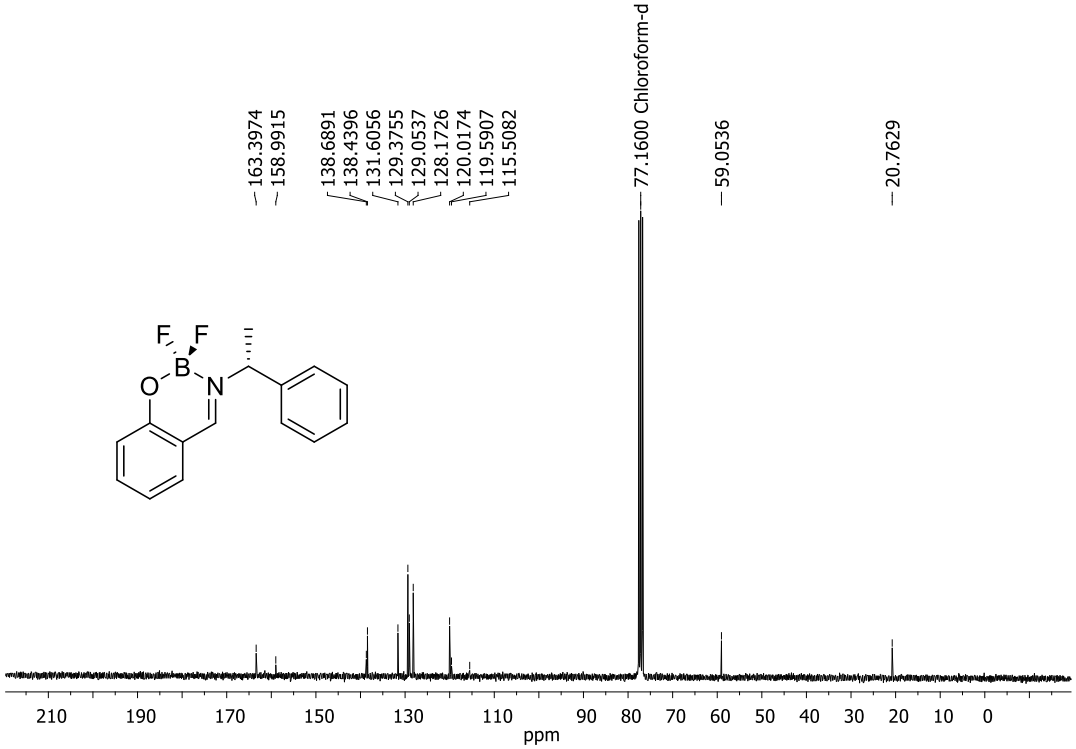

*Figure S 10 - [13]C NMR spectrum of (R)-2,2-difluoro-3-(1-phenylethyl)-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3a-R** in $CDCl_3$.*

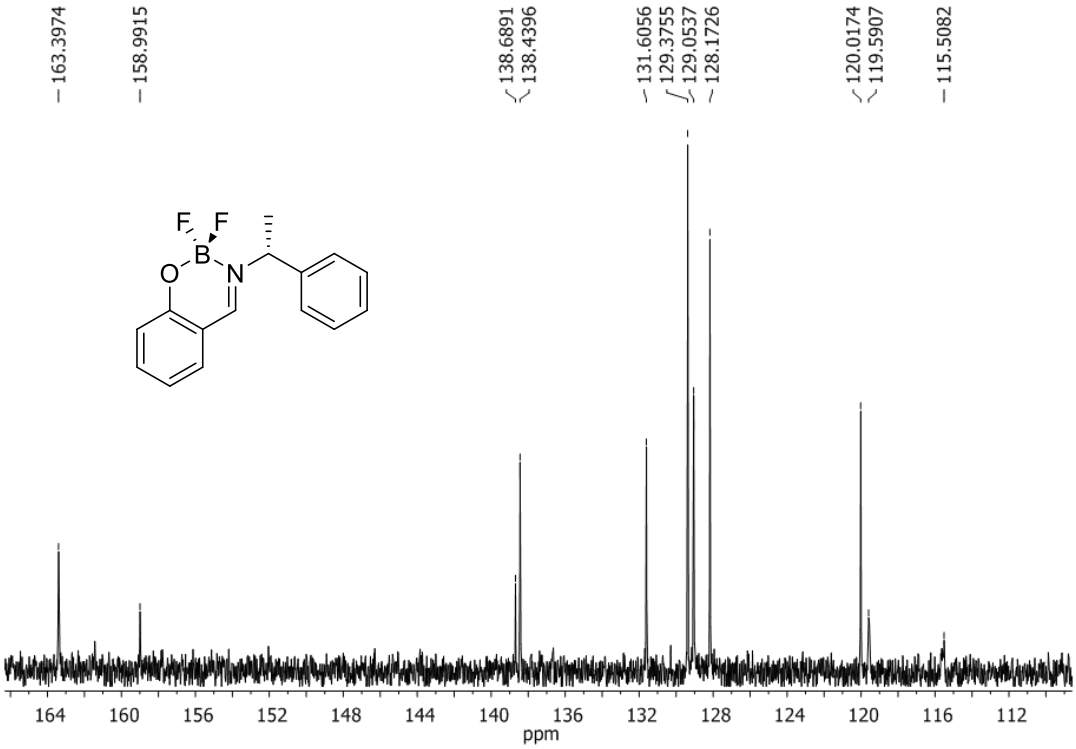

*Figure S 11 - •^{13}C NMR spectrum expansion of (R)-2,2-difluoro-3-(1-phenylethyl)-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3a-R** in $CDCl_3$.*

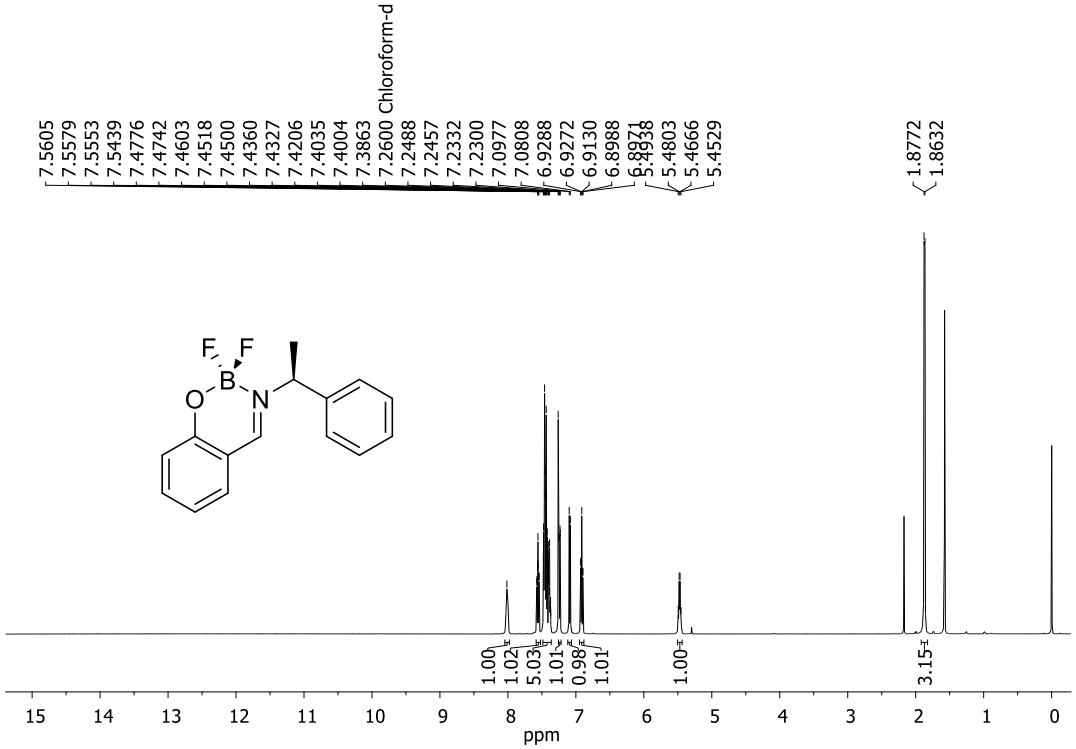

*Figure S 12 - ^{1}H NMR spectrum of (S)-2,2-difluoro-3-(1-phenylethyl)-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3a-S** in $CDCl_3$.*

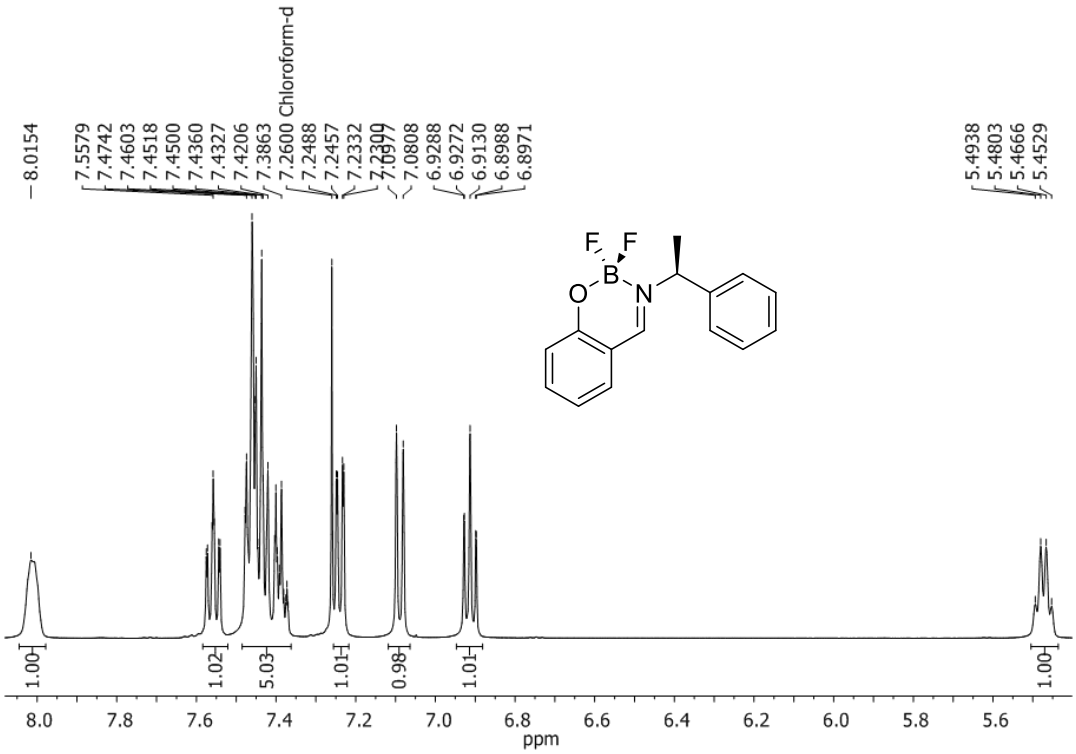

*Figure S 13 - ^{1}H NMR spectrum expansion of (S)-2,2-difluoro-3-(1-phenylethyl)-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3a-S** in $CDCl_3$.*

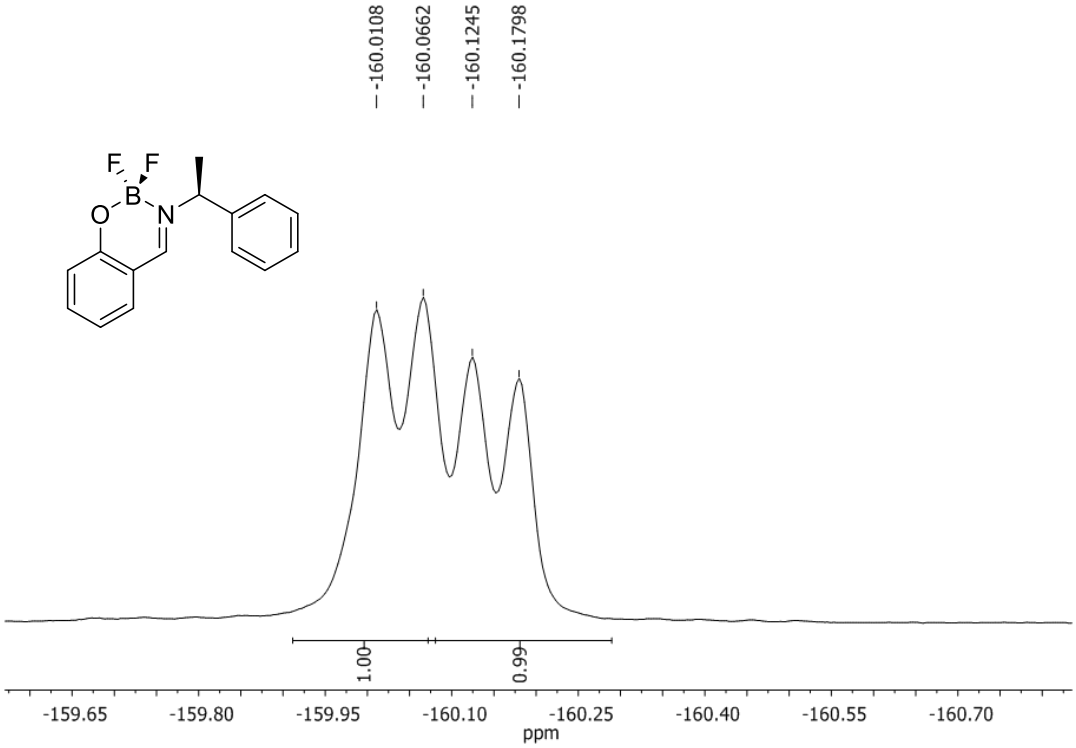

*Figure S 14 - ^{19}F NMR spectrum of (S)-2,2-difluoro-3-(1-phenylethyl)-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3a-S** in $CDCl_3$.*

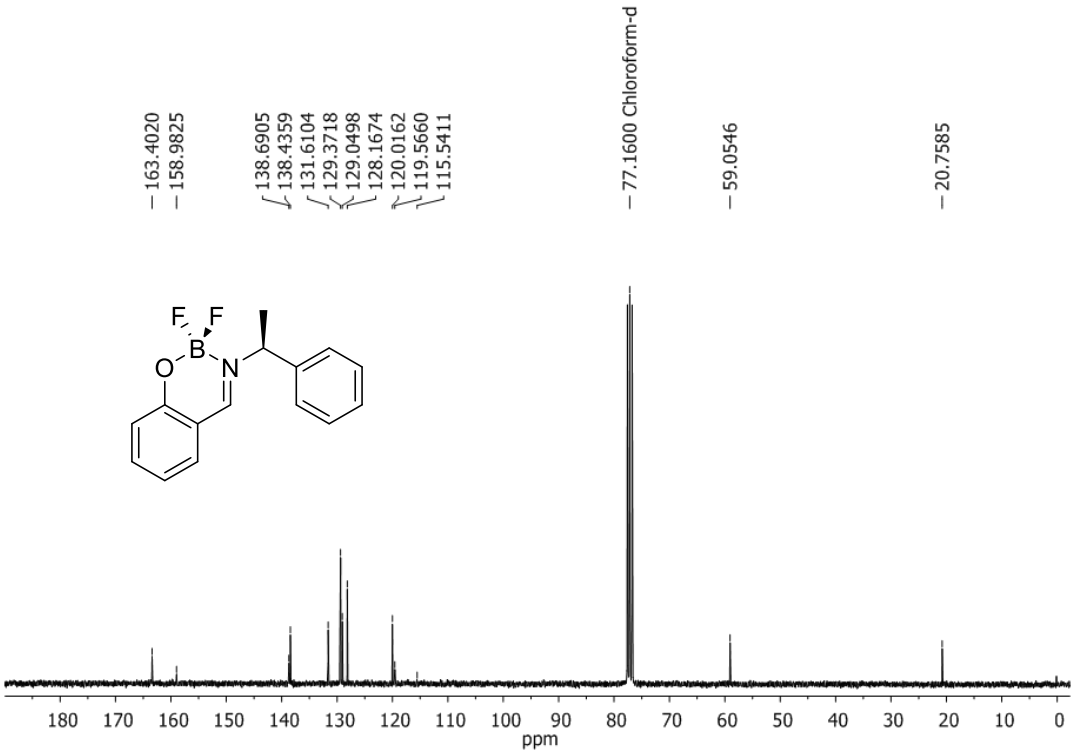

*Figure S 15 – ^{13}C NMR spectrum of (S)-2,2-difluoro-3-(1-phenylethyl)-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3a-S** in $CDCl_3$.*

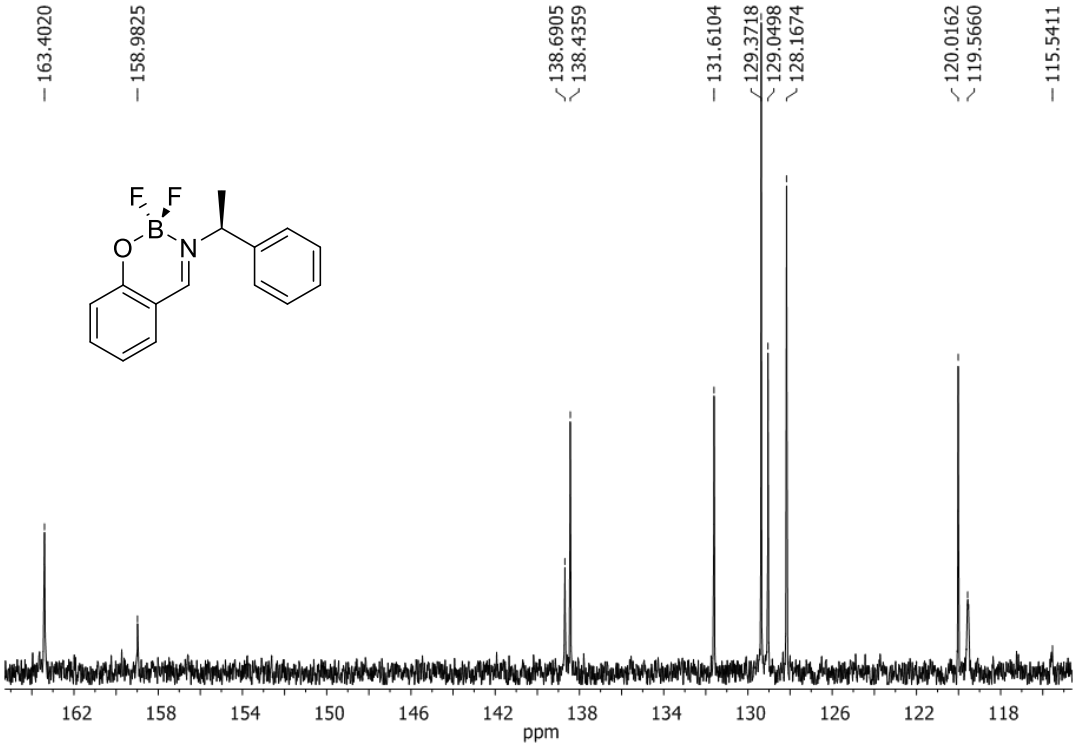

*Figure S 16 – ^{13}C NMR spectrum expansion of (S)-2,2-difluoro-3-(1-phenylethyl)-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3a-S** in $CDCl_3$.*

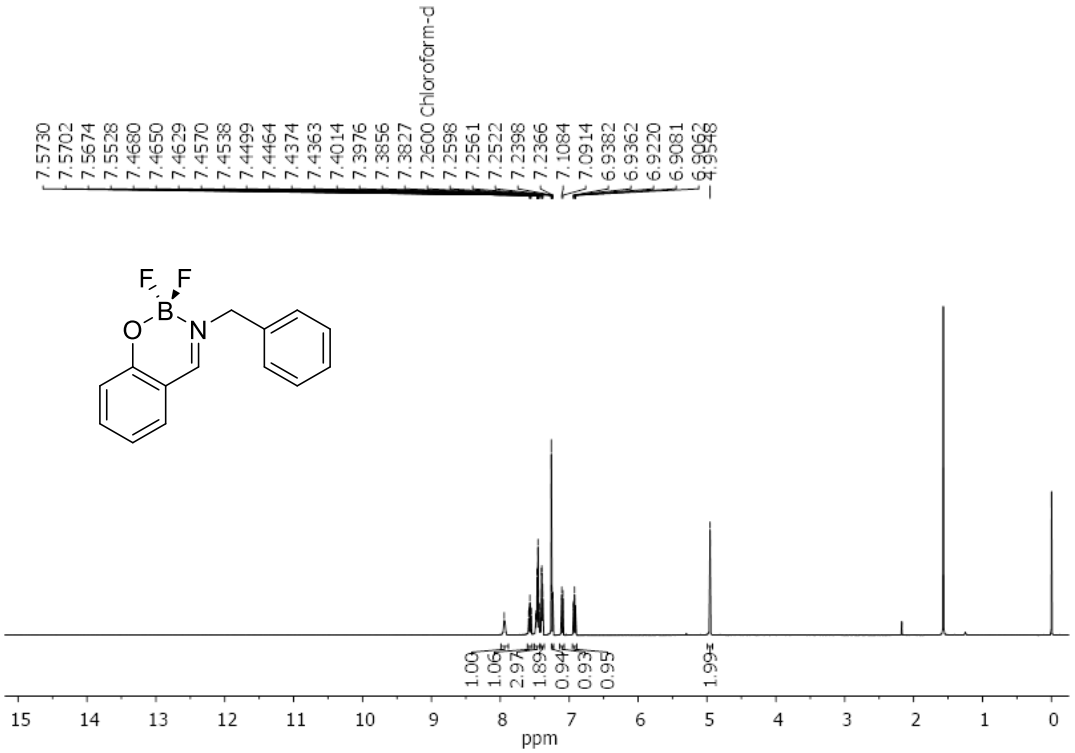

*Figure S 17 – [1]H NMR spectrum of 3-benzyl-2,2-difluoro-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3b** in $CDCl_3$.*

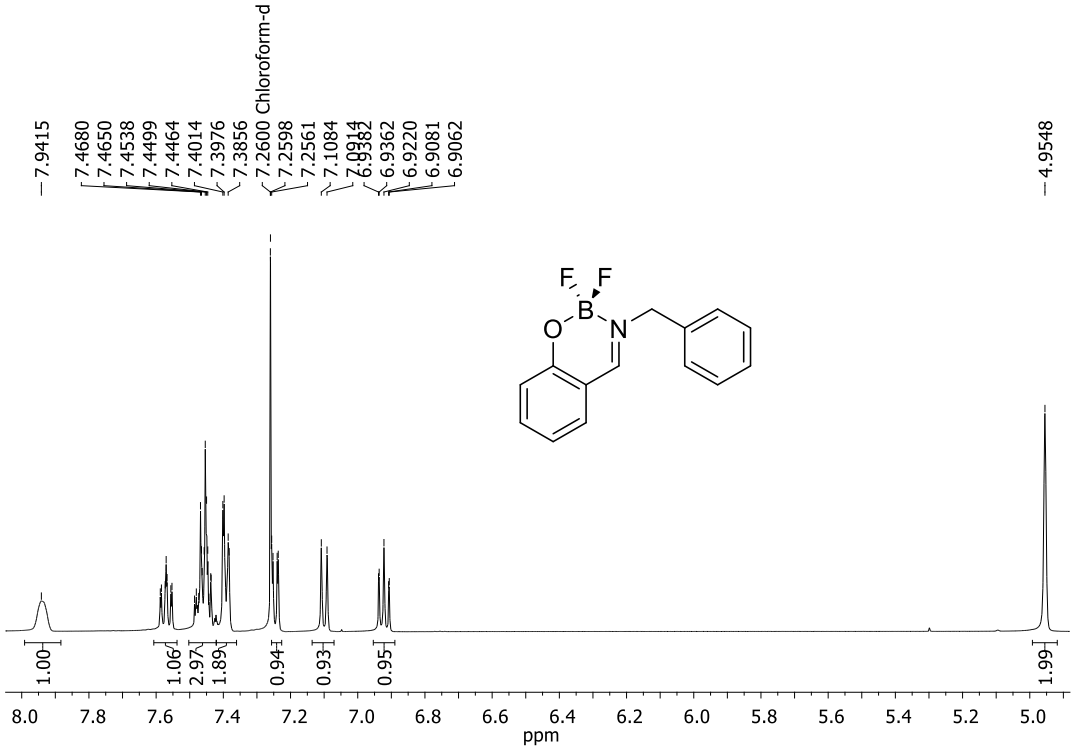

*Figure S 18 - [1]H NMR spectrum expansion of 3-benzyl-2,2-difluoro-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3b** in $CDCl_3$.*

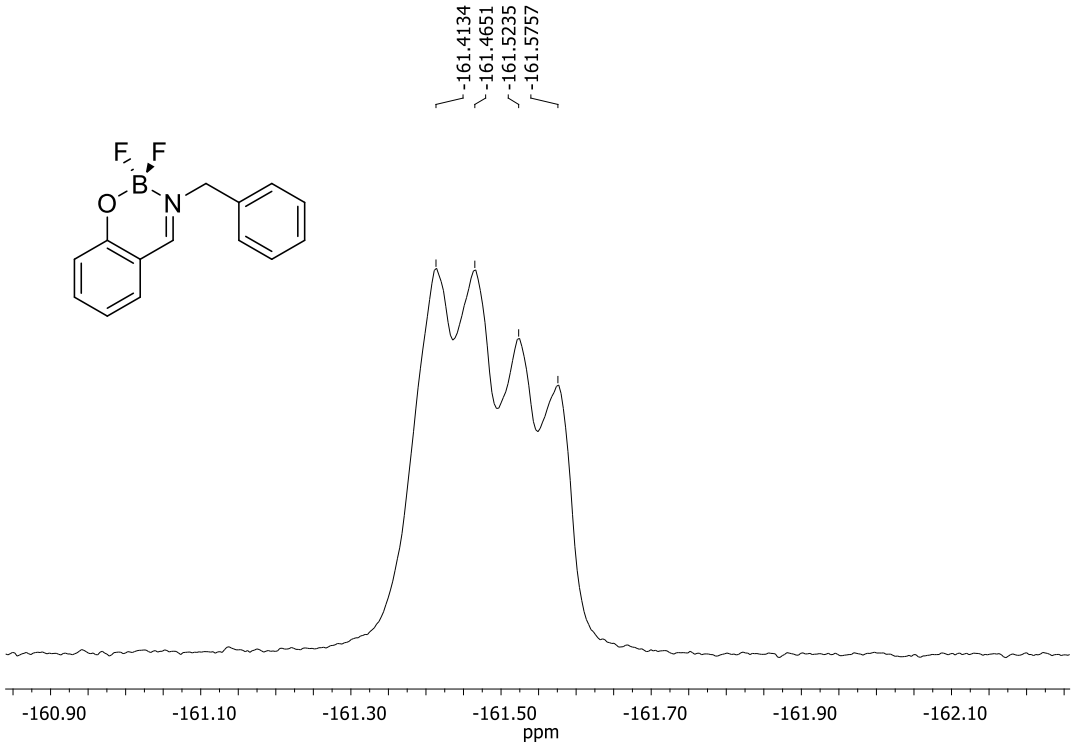

*Figure S 19 – ^{19}F NMR spectrum of 3-benzyl-2,2-difluoro-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3b** in $CDCl_3$.*

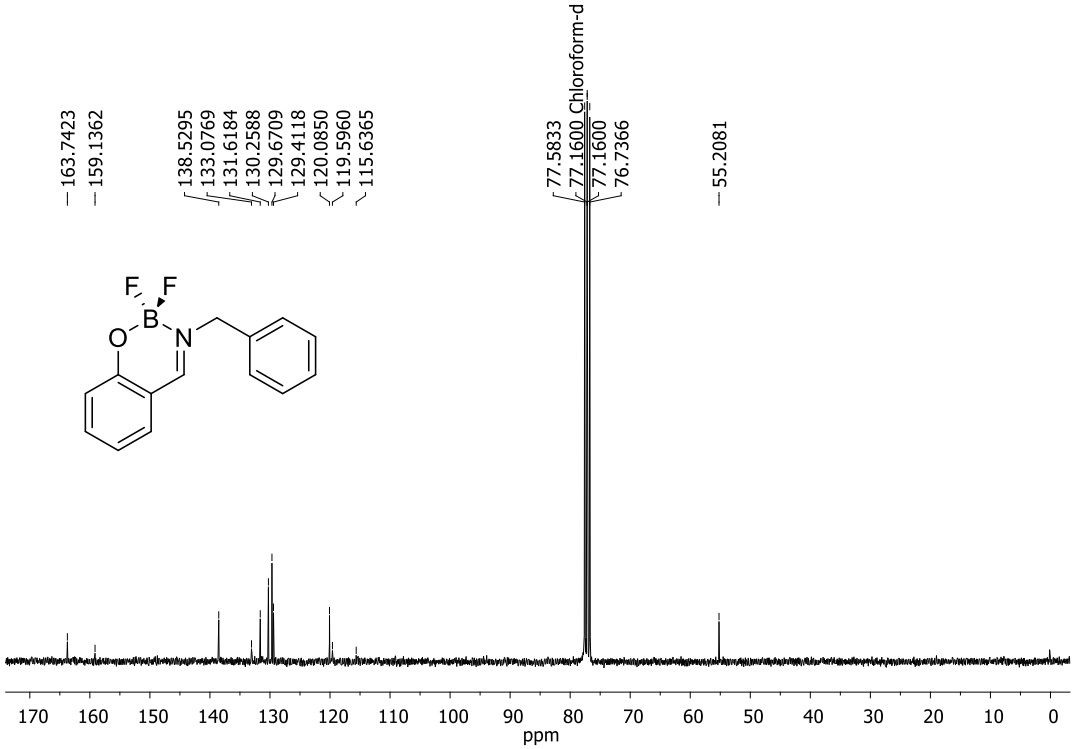

*Figure S 20 – ^{13}C NMR spectrum of 3-benzyl-2,2-difluoro-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3b** in $CDCl_3$.*

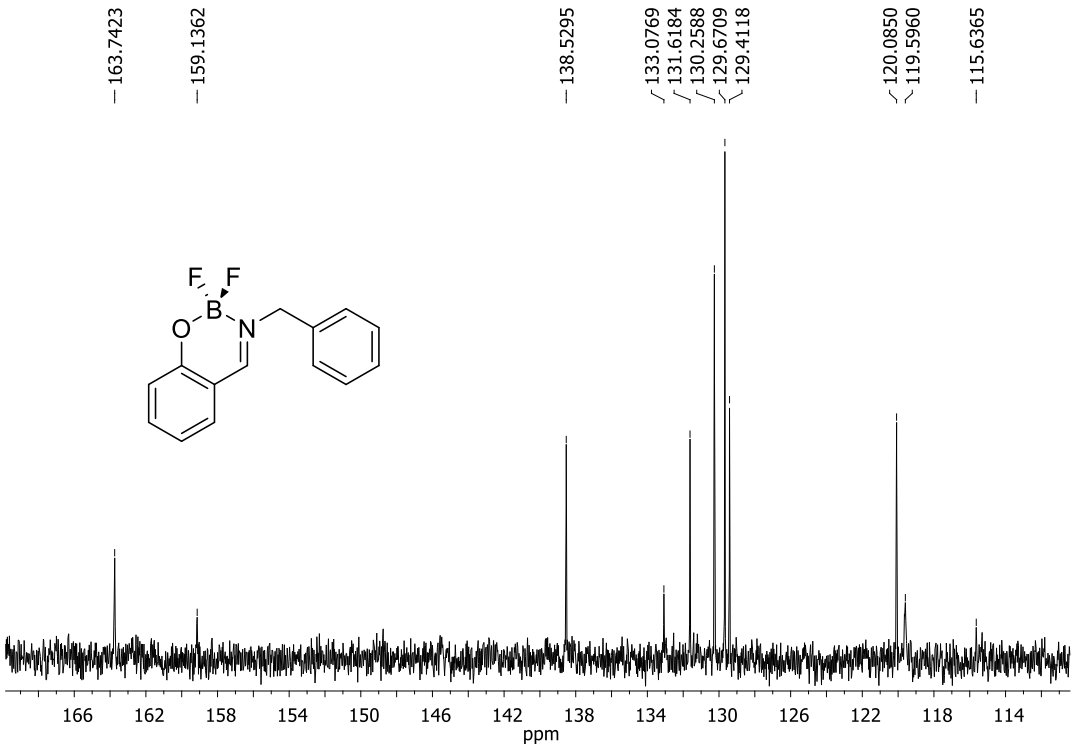

*Figure S 21 – ^{13}C NMR spectrum expansion of 3-benzyl-2,2-difluoro-2H-benzo[e][1,3,2]oxazaborinin-3-ium-2-uide **3b** in $CDCl_3$.*

Absorption, excitation and emission spectra

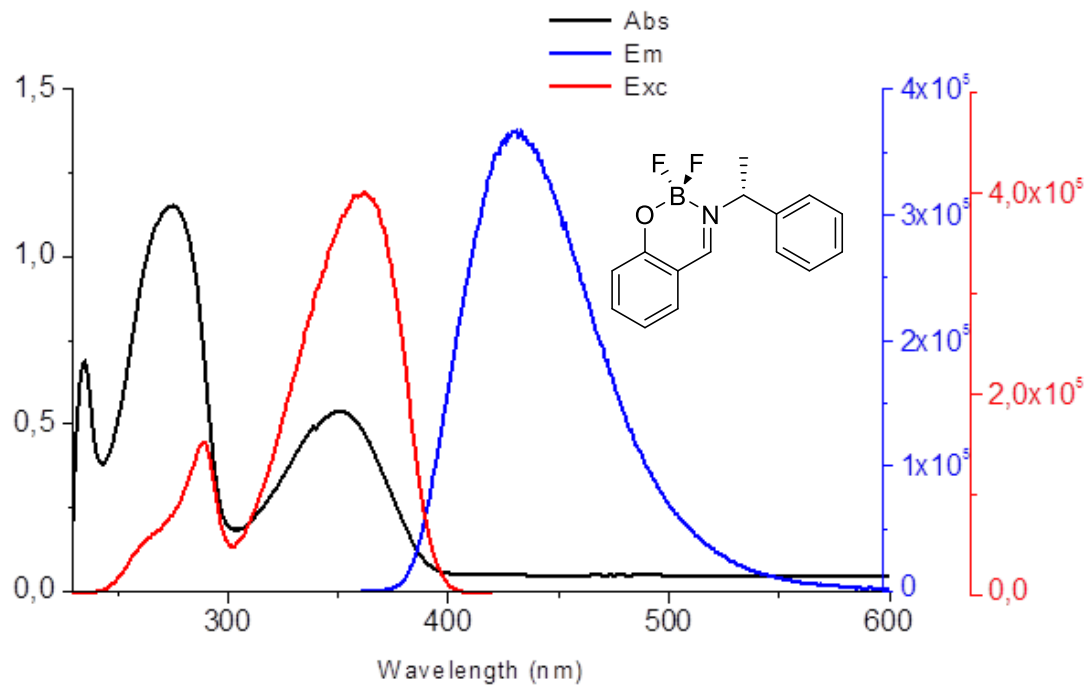

Figure S 22 – Absorption (black line), excitation (red line) and emission (blue line) spectra of ***(+)-3a-R*** *at room temperature (c.a* 10^{-4}*M in dichloromethane).*

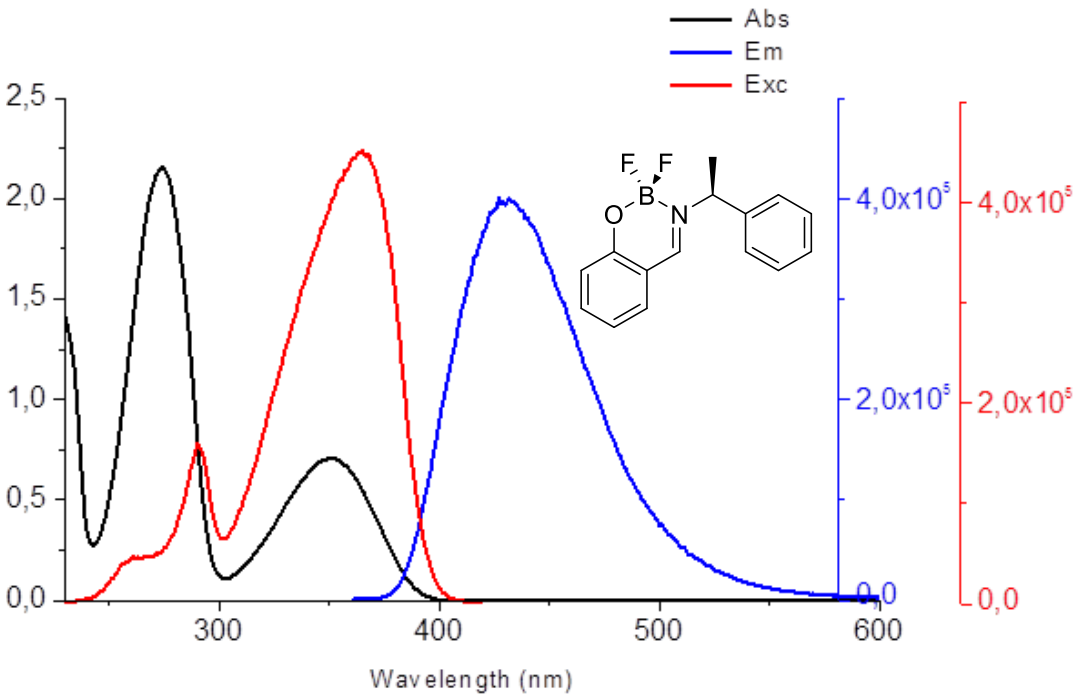

Figure S 23 - Absorption (black line), excitation (red line) and emission (blue line) spectrum of ***(-)-3a-S*** *at room temperature (c.a* 10^{-4}*M in dichloromethane).*

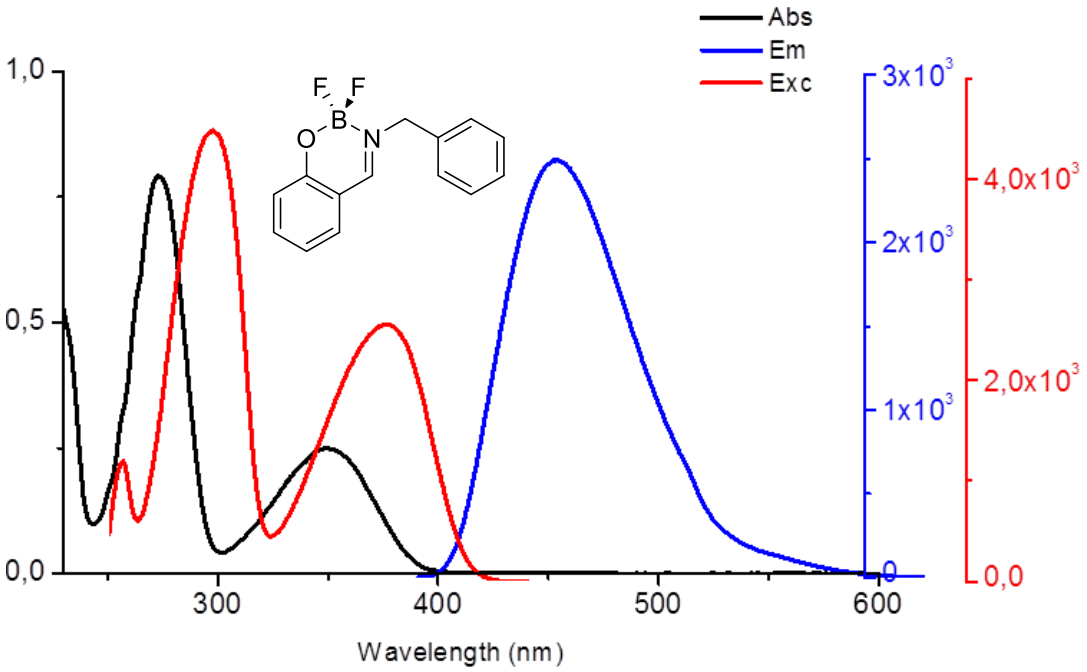

*Figure S 24 – Absorption (black line), excitation (red line) and emission (blue line) spectrum of **3b** at room temperature (c.a 10^{-4}M in dichloromethane)*

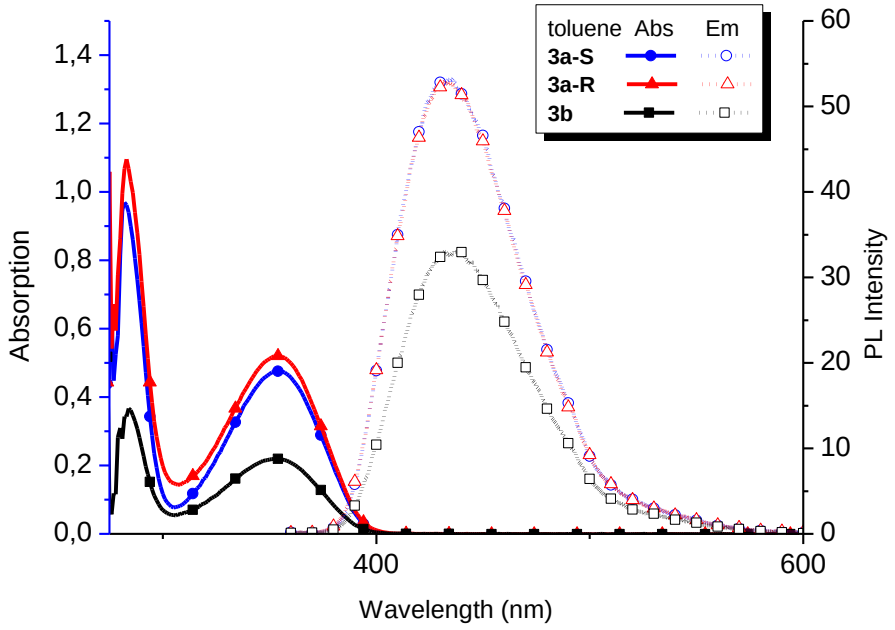

Figure S 25 – Absorption and emission spectra of the dyes at room temperature (10^{-5}M in toluene)

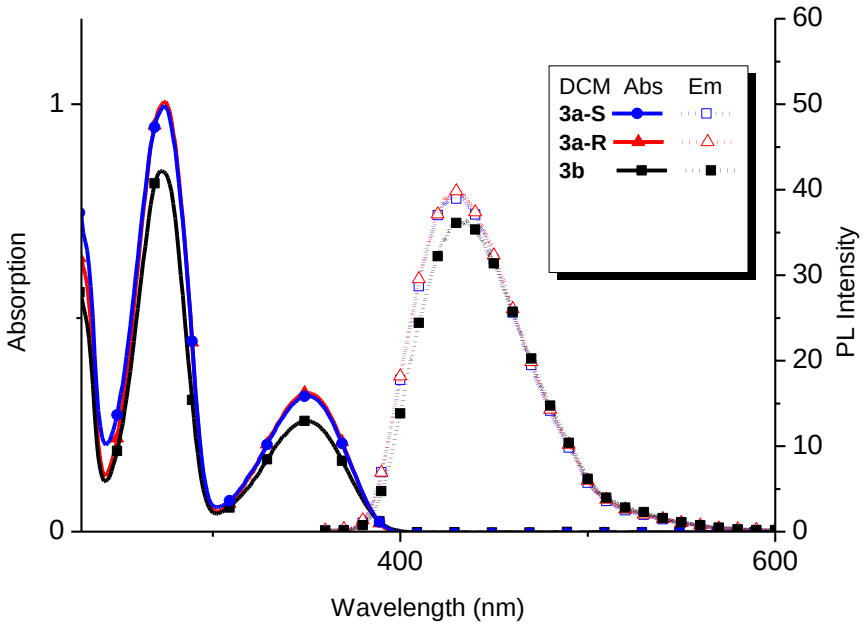

Figure S 26 – Absorption and emission spectra of the dyes at room temperature (10^{-5}M in dichloromethane)

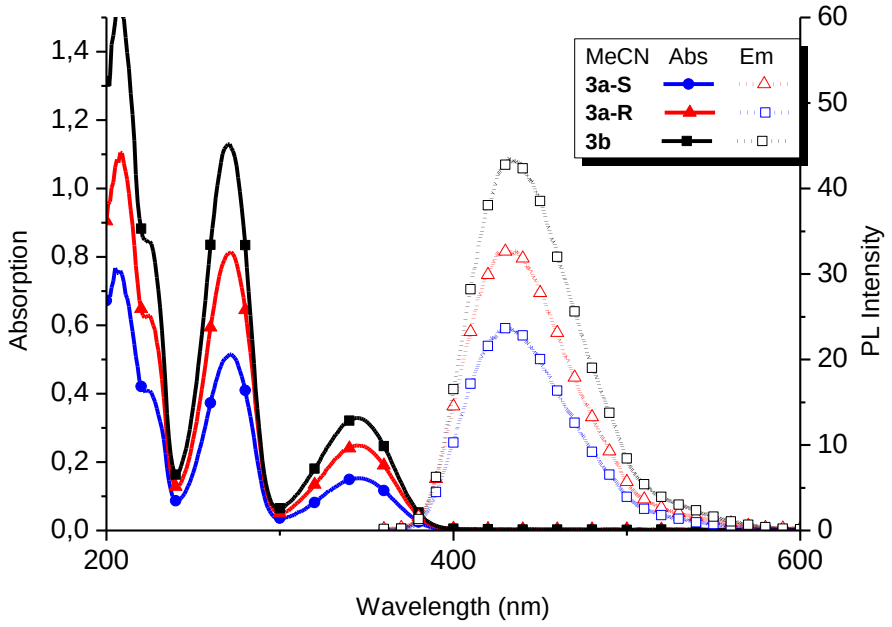

Figure S 27 – Absorption and emission spectra of the dyes at room temperature (10^{-5}M in MeCN)

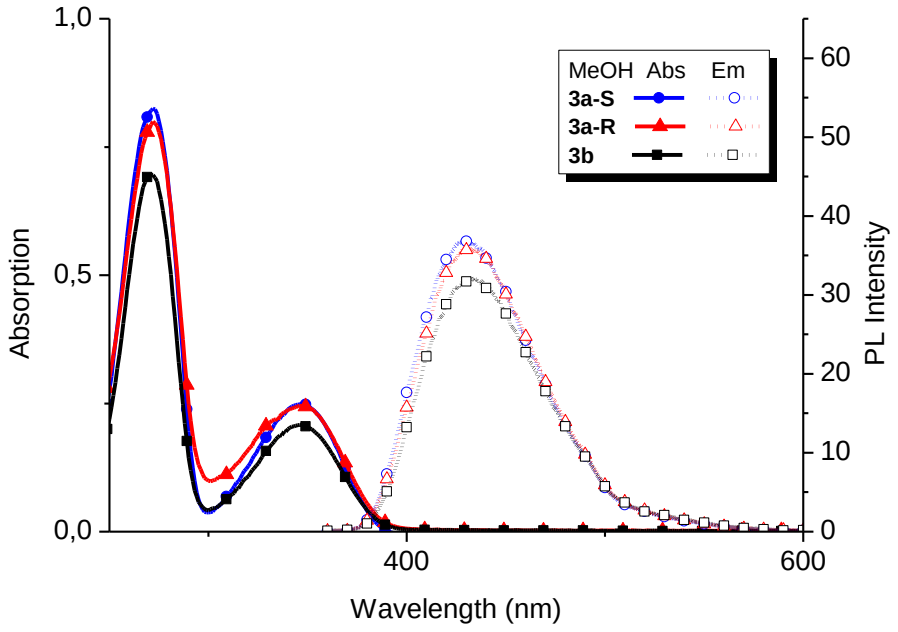

Figure S 28 – Absorption and emission spectra of the dyes at room temperature (10^{-5}M in MeOH)

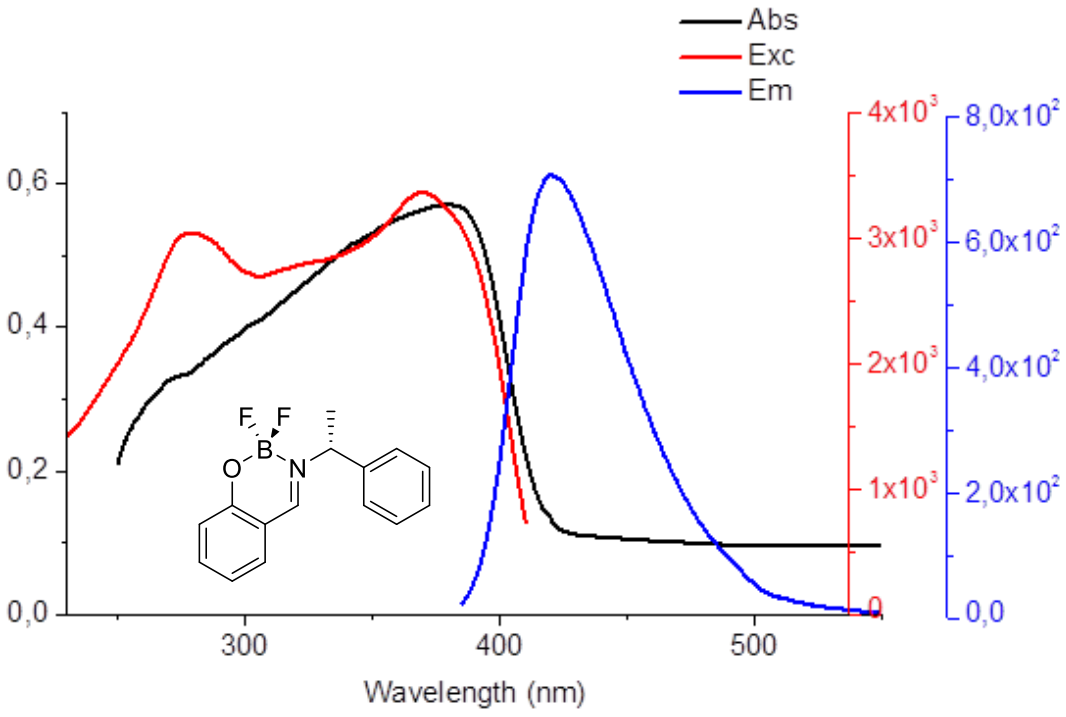

Figure S 29- Absorption (black line), excitation (red line) and emission (blue line) spectrum of **(+)-3a-R** (solid state)

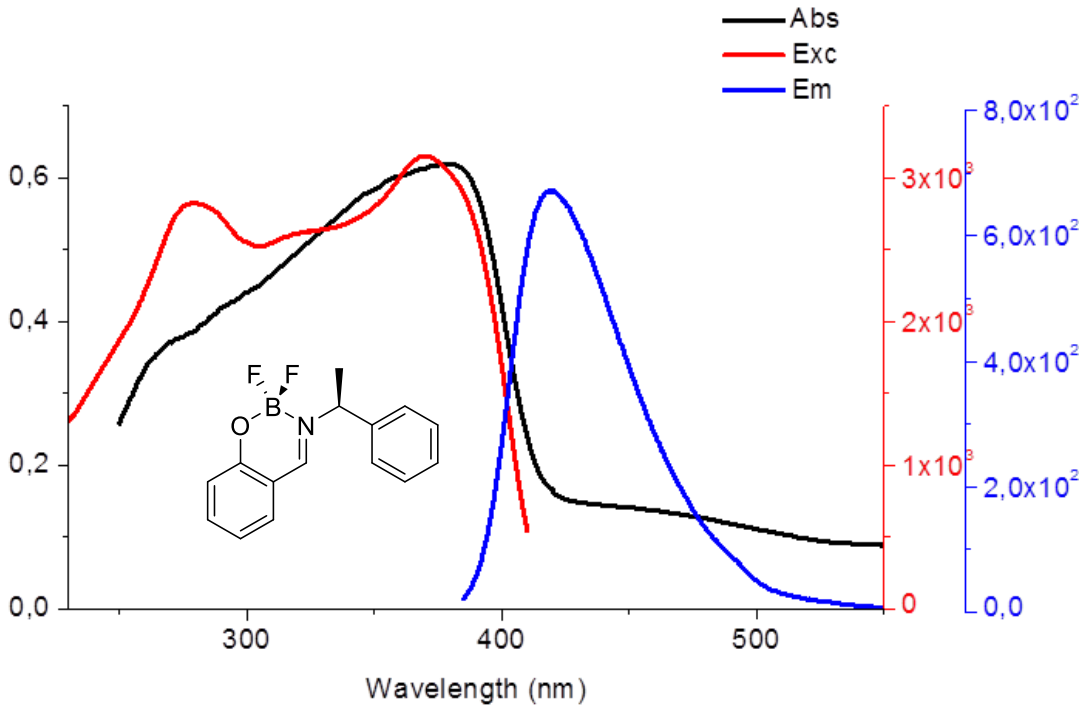

Figure S 30- Absorption (black line), excitation (red line) and emission (blue line) spectrum of **(-)-3a-S** (solid state).

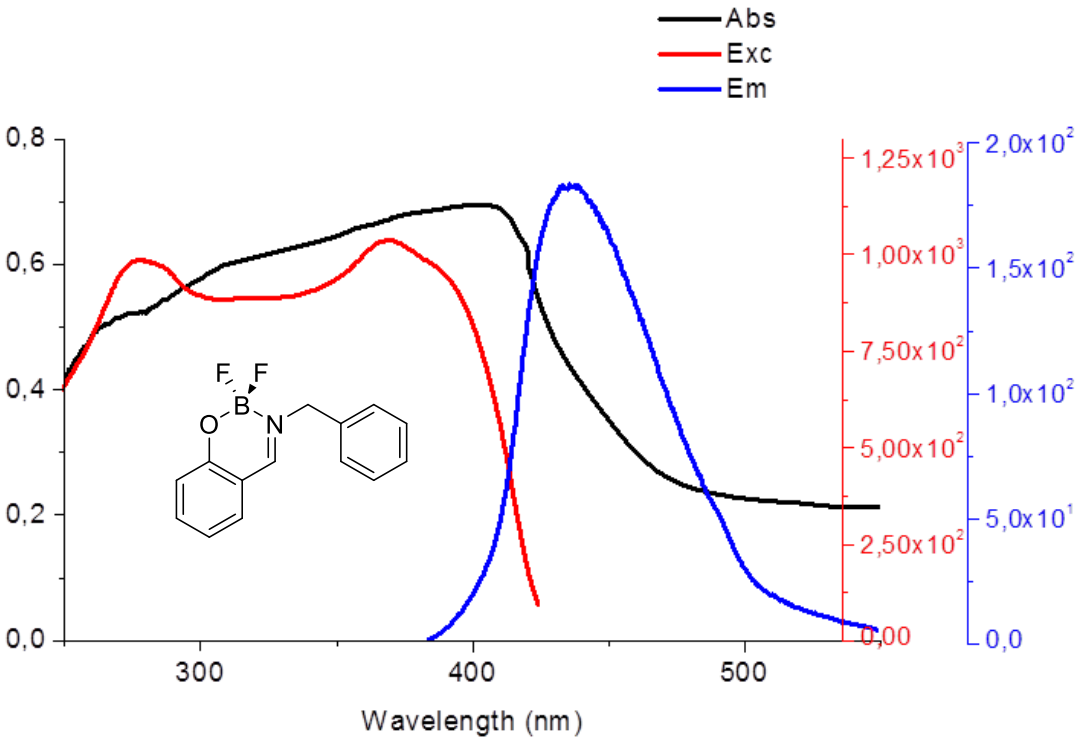

Figure S 31- Absorption (black line), excitation (red line) and emission (blue line) spectrum of **3b** (solid state).

X-ray diffraction

Single-crystals of compound **2a-*R***, **2a-*S***, **3a-*R***, **3a-*S*** and **3b** were manually selected from the crystallization vial. A suitable single-crystal was mounted on a glass fiber with the help of silicon grease. Data were collected at 180(2) K on a Bruker X8 Kappa APEX II charge-coupled device (CCD) area-detector diffractometer (Mo K_a graphite-monochromated radiation, λ = 0.71073 Å) controlled by the APEX2 software package,[1] and equipped with an Oxford Cryosystems Series 700 cryostream monitored remotely using the software interface Cryopad.[2] Images were processed using the software package SAINT+,[3] and data were corrected for absorption by the multi-scan semi-empirical method implemented in SADABS.[4] The structure was solved using the direct methods algorithm implemented in SHELXS-97,[5,6] which allowed the immediate location of the majority of the atoms. All remaining non-hydrogen atoms were located from difference Fourier maps calculated from successive full-matrix least squares refinement cycles on F^2 using SHELXL-97.[5,7] All non-hydrogen atoms were successfully refined using anisotropic displacement parameters.

Hydrogen atoms bound to carbon were located at their idealized positions using appropriate *HFIX* instructions in SHELXL (*43* for the aromatic and vinylic, *23* for the $-CH_2-$ moieties and *13* for the chiral tertiary carbon atoms) and included in subsequent refinement cycles in riding-motion approximation with isotropic thermal displacements parameters (U_{iso}) fixed at 1.2 times U_{eq} of the atom to which they are attached.

Crystallographic data for the structure reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication No. CCDC 1852252-1852256. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB2 2EZ, U.K. FAX: (+44) 1223 336033. E-mail: deposit@ccdc.cam.ac.uk.

(1) APEX2, *Data Collection Software Version 2.1-RC13, Bruker AXS, Delft, The Netherlands* **2006**.

(2) Cryopad, *Remote monitoring and control, Version 1.451, Oxford Cryosystems, Oxford, United Kingdom* **2006**.

(3) SAINT+, *Data Integration Engine v. 7.23a* © 1997-2005, *Bruker AXS, Madison, Wisconsin, USA*.

(4) G. M. Sheldrick, *SADABS v.2.01, Bruker/Siemens Area Detector Absorption Correction Program* **1998**, *Bruker AXS, Madison, Wisconsin, USA*.

(5) G. M. Sheldrick, *Acta Cryst. A* **2008**, *64*, 112-122.

(6) G. M. Sheldrick, *SHELXS-97, Program for Crystal Structure Solution, University of Göttingen* **1997**.

(7) G. M. Sheldrick, *SHELXL-97, Program for Crystal Structure Refinement, University of Göttingen* **1997**.