Luminescent Properties and Cytotoxic Activity of 2-phenylbenzoxazole Fluorosulfate Derivatives

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Supplementary information



Figure S1. The two-chamber reactor.

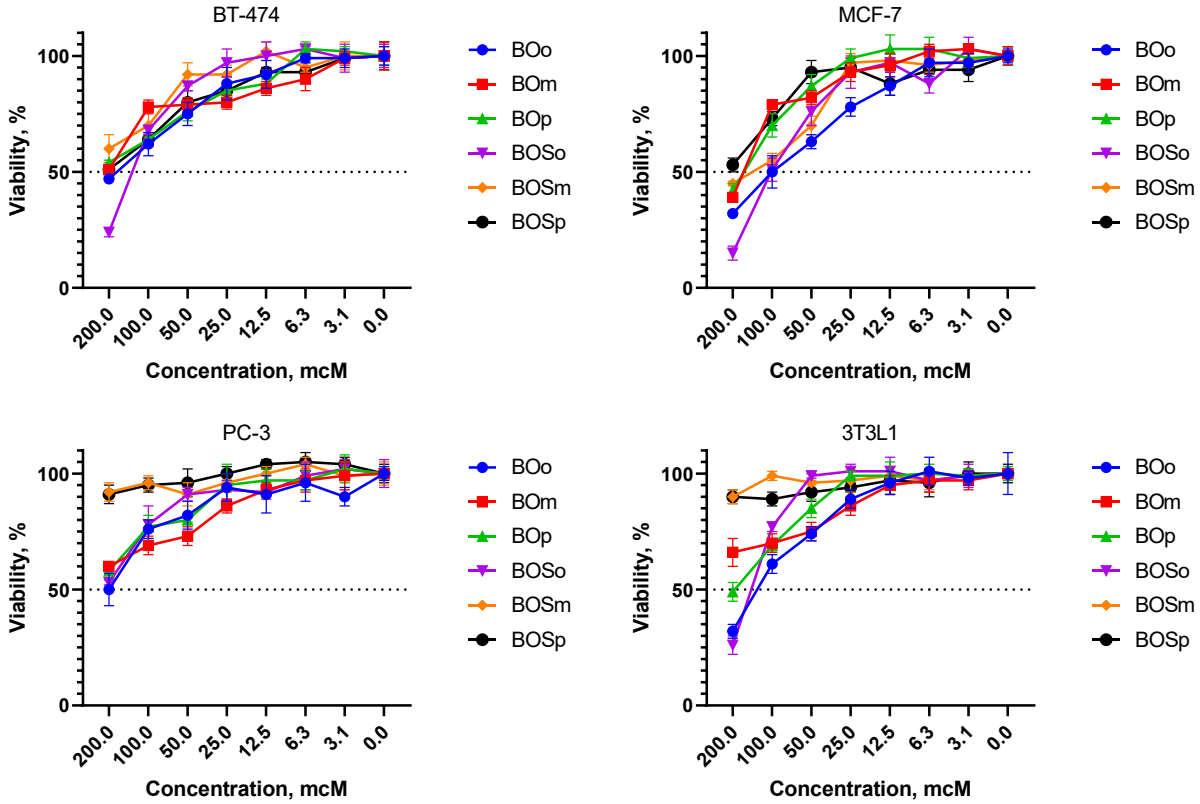


Figure S2. Effect of the tested compounds on the viability of breast cancer, prostate cancer and normal fibroblast cell lines in the concentration range of 0-200 μM.

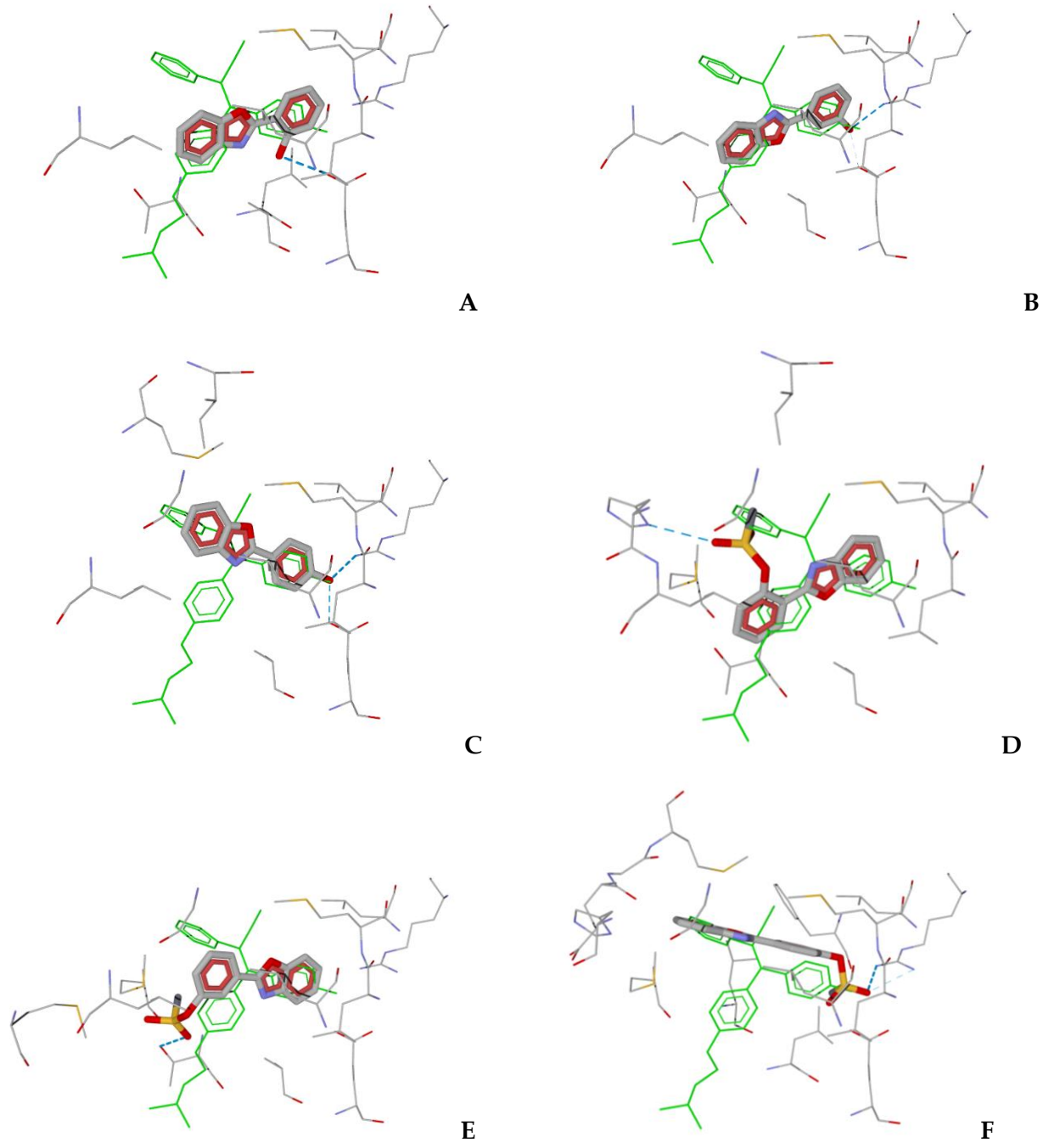


Figure S3. The docking poses (sticks) of compounds **BOo** (Panel A), **BOm** (Panel B), **BOp** (Panel C), **BOSo** (Panel D), **BOSm** (Panel E), and **BOSp** (Panel F) superimposed on the co-crystallized tamoxifen molecule (thin green sticks) in hER protein (PDB: 3ERT). Hydrogen bonds are shown in dashed blue lines. The residues within 3 Å from each pose are visible.

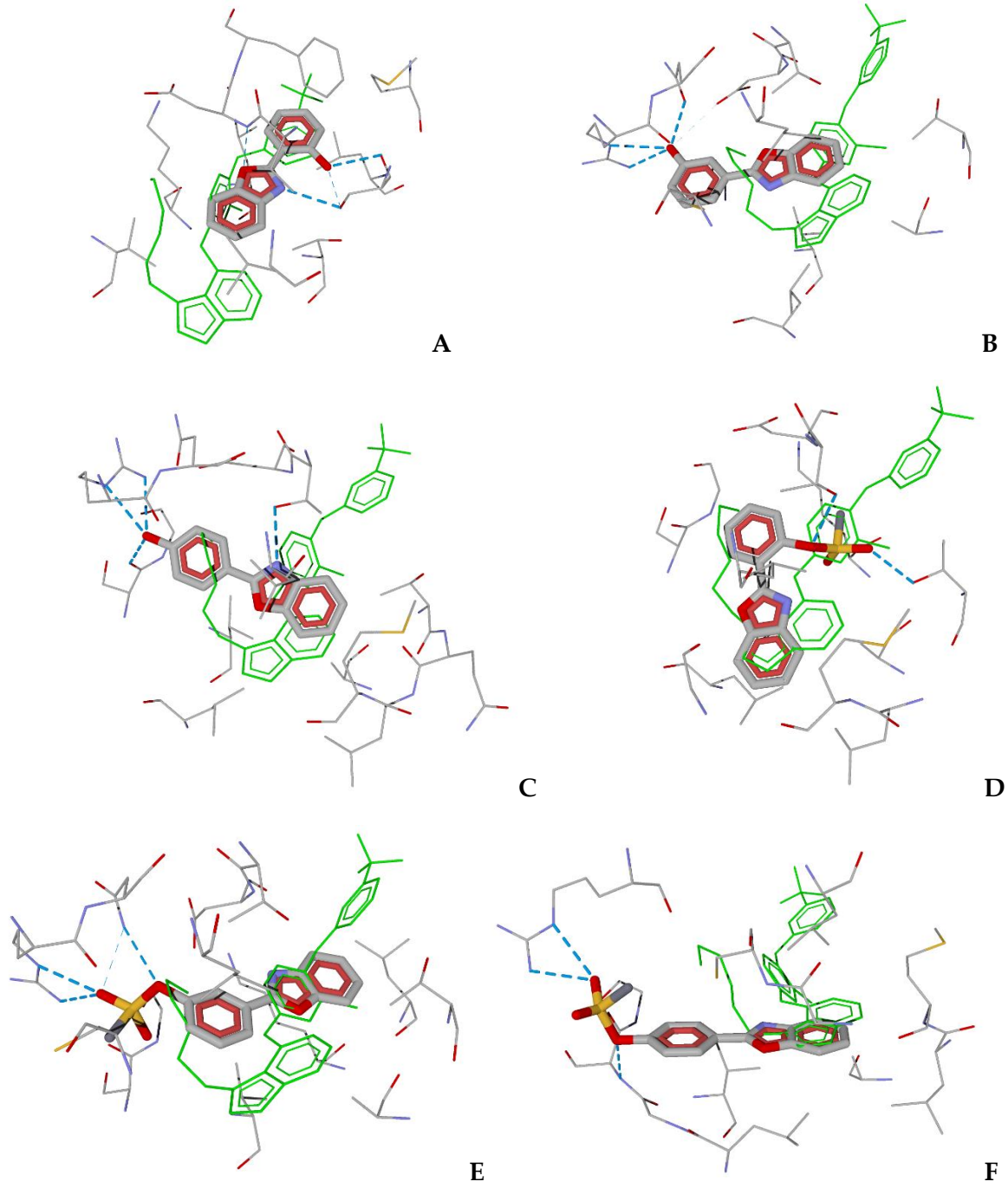


Figure S4. The docking poses (sticks) of compounds **BOo** (Panel A), **BOm** (Panel B), **BOp** (Panel C), **BOSo** (Panel D), **BOSm** (Panel E), and **BOSp** (Panel F) superimposed on the co-crystallized SYR127063 molecule (thin green sticks) in HER2 protein (PDB: 3PP0). Hydrogen bonds are shown in dashed blue lines. The residues within 3 Å from each pose are visible.

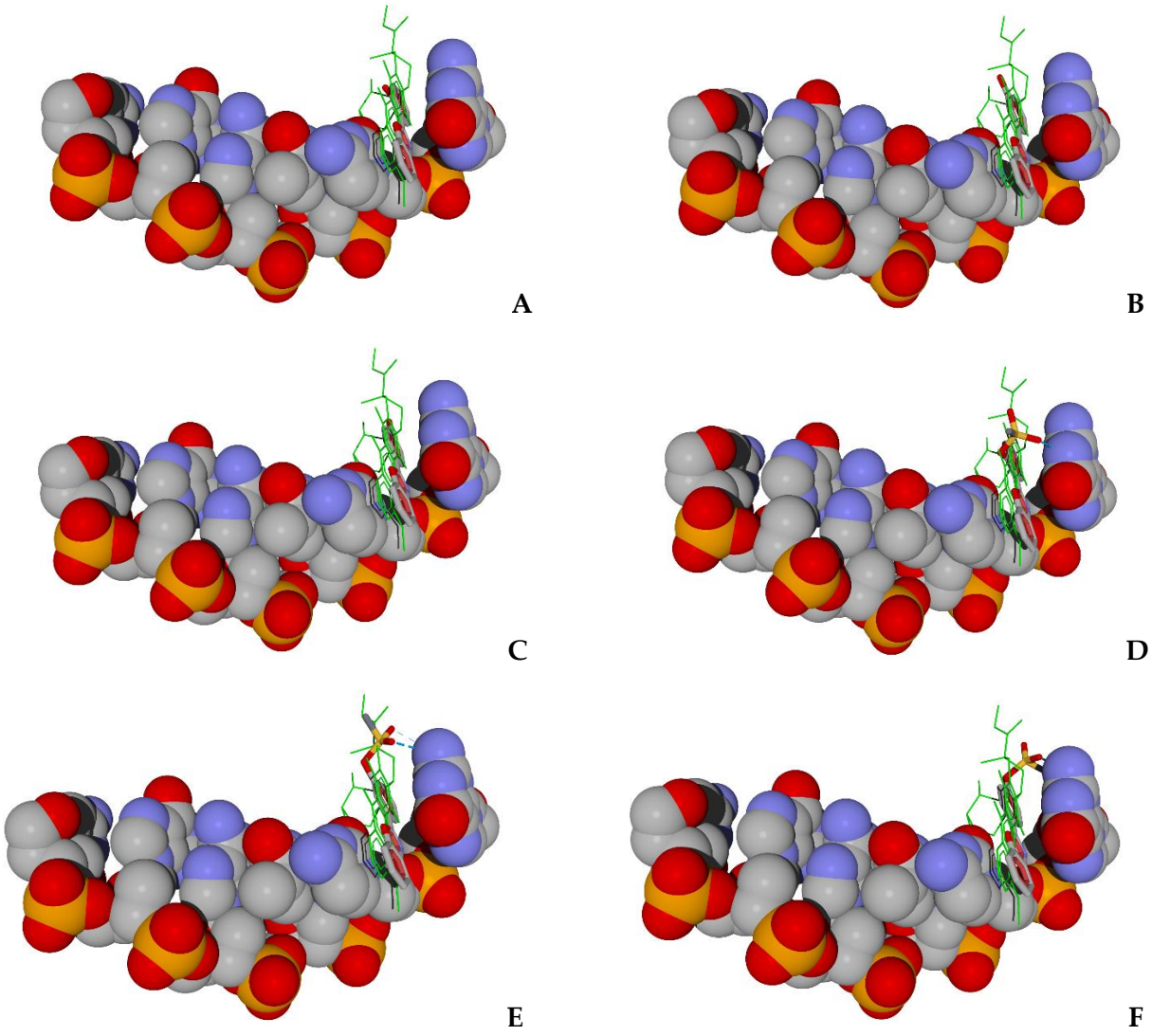


Figure S5. The docking poses (sticks) of compounds **BOo** (Panel A), **BOm** (Panel B), **BOp** (Panel C), **BOSo** (Panel D), **BOSm** (Panel E), and **BOSp** (Panel F) superimposed on the co-crystallized doxorubicin molecule (thin green sticks) in DNA strand (PDB: 151D). Hydrogen bonds are shown in dashed blue lines.

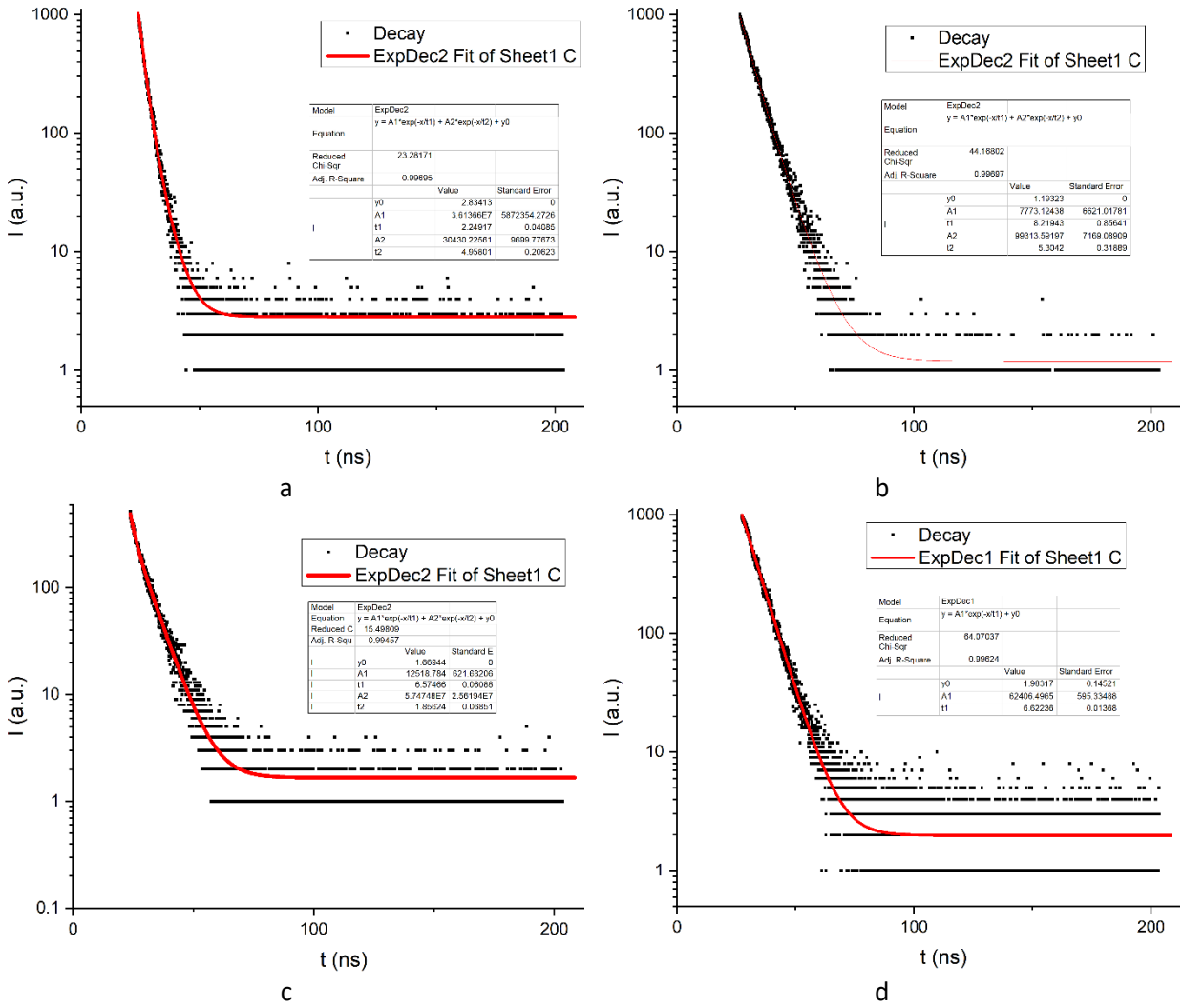


Figure S6. Emission decay plots in the solid state for compounds: (a) **BOo**; (b) **BOSp**; (c) **BOSm**; (d) **BOSo**.

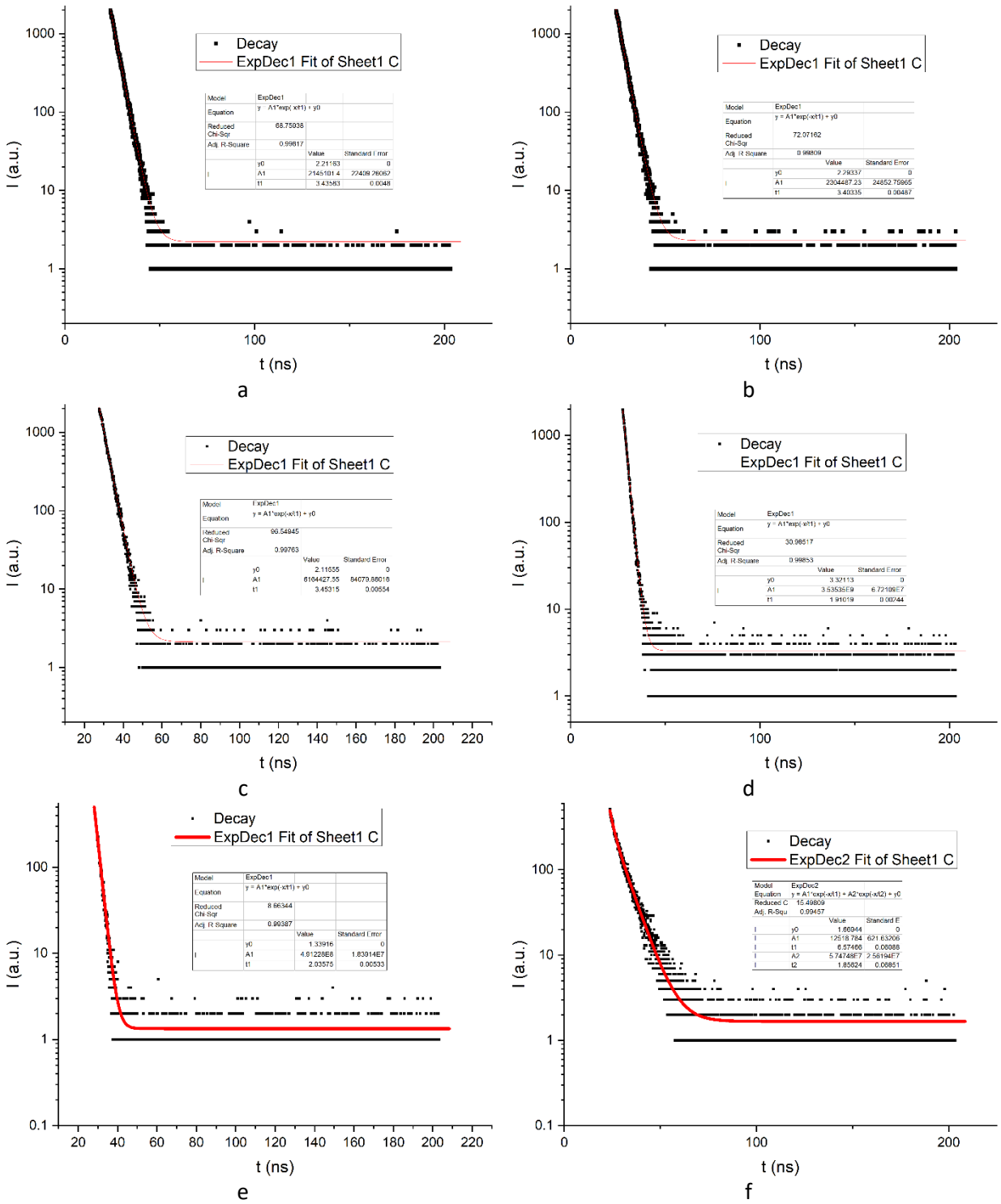


Figure S7. Emission decay plots in acetonitrile solution (C = $1.0 \cdot 10^{-3}$ M) for compounds: (a) **BOo**; (b) **BOp**; (c) **BOm**; (d) **BOSp**; (e) **BOSm**; (f) **BOSo**.

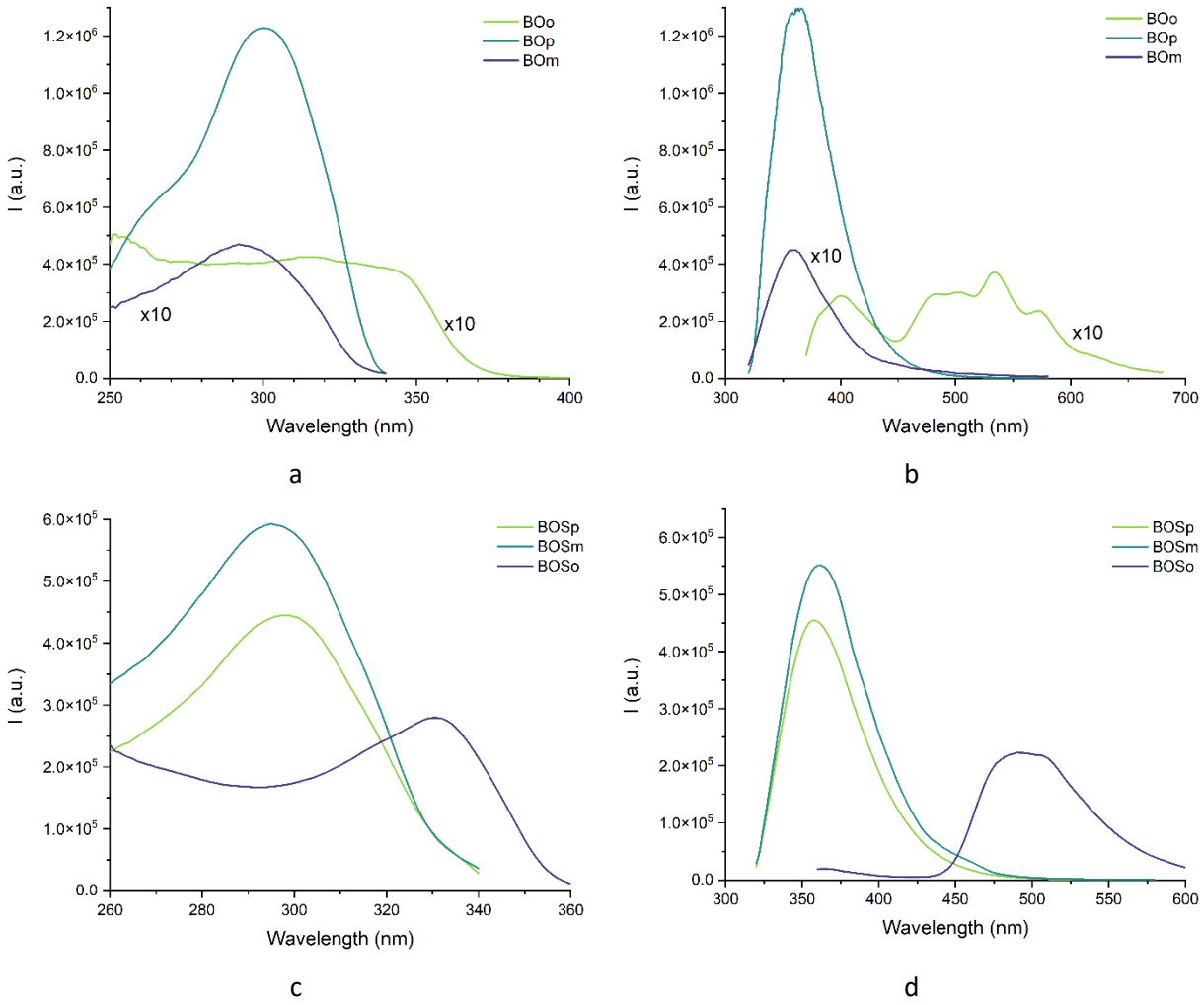


Figure S8. Excitation and emission spectra in phosphate buffer solution ($1.0 \cdot 10^{-3}$ M): (a) normalized excitation spectra of 2-(hydroxyphenyl)benzoxazoles, λ_{em} = 360 nm (**BOp**, **BOm**), 480 nm (**BOo**); (b) normalized emission spectra of 2-(hydroxyphenyl)benzoxazoles, λ_{ex} = 300 nm (**BOp**, **BOm**), 350 nm (**BOo**) (c) excitation spectra of 2-(fluorosulfatophenyl)benzoxazoles, λ_{em} = 360 nm (**BOSp**, **BOSm**), 500 nm (**BOSo**); (d) emission spectra of 2-(fluorosulfatophenyl)benzoxazoles, λ_{ex} = 300 nm (**BOSp**, **BOSm**), 340 nm (**BOSo**).

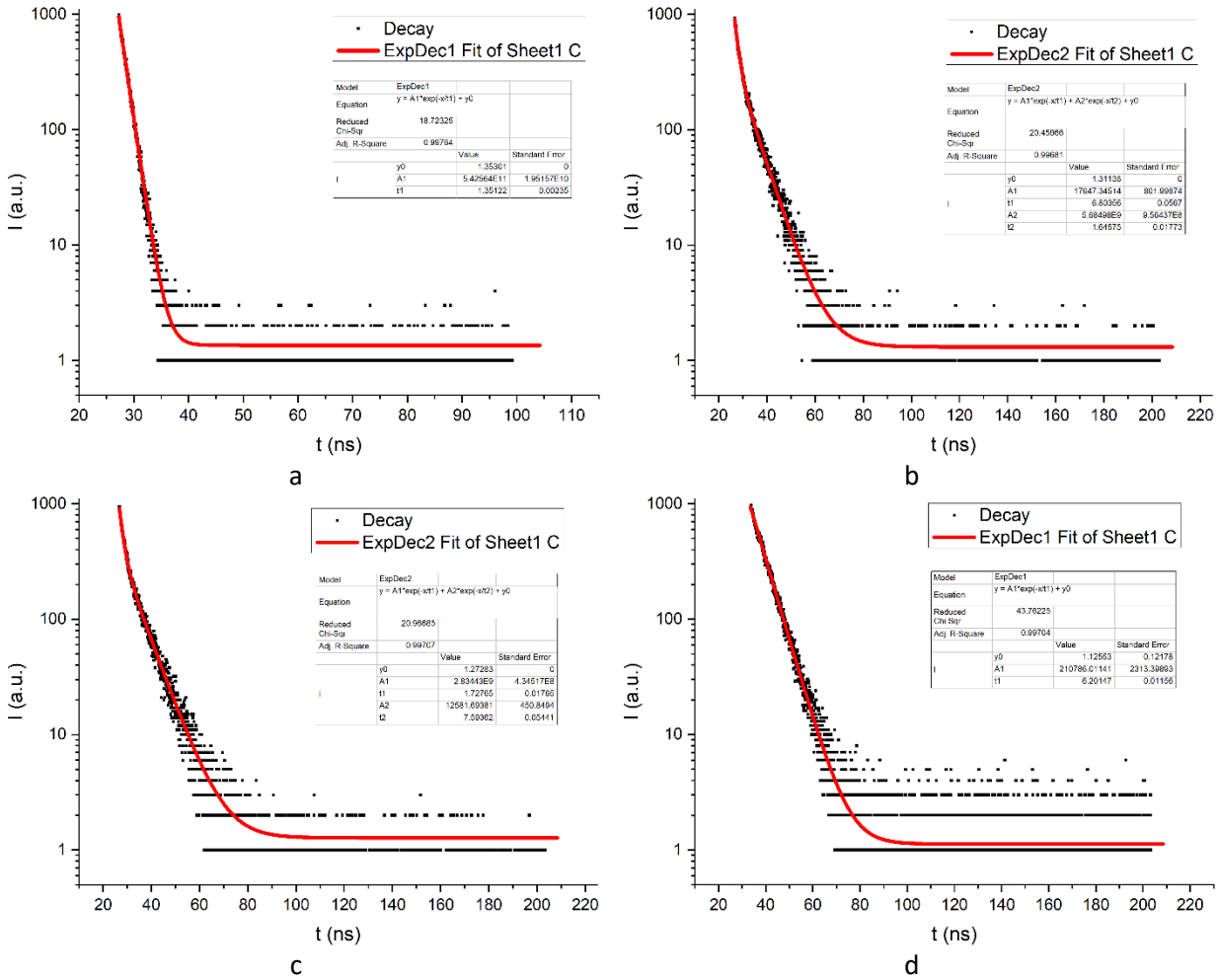


Figure S9. Emission decay plots in phosphate buffer solution (C = $1.0 \cdot 10^{-3}$ M) for compounds: (a) **BOp**; (b) **BOSp**; (c) **BOSm**; (d) **BOSo**.

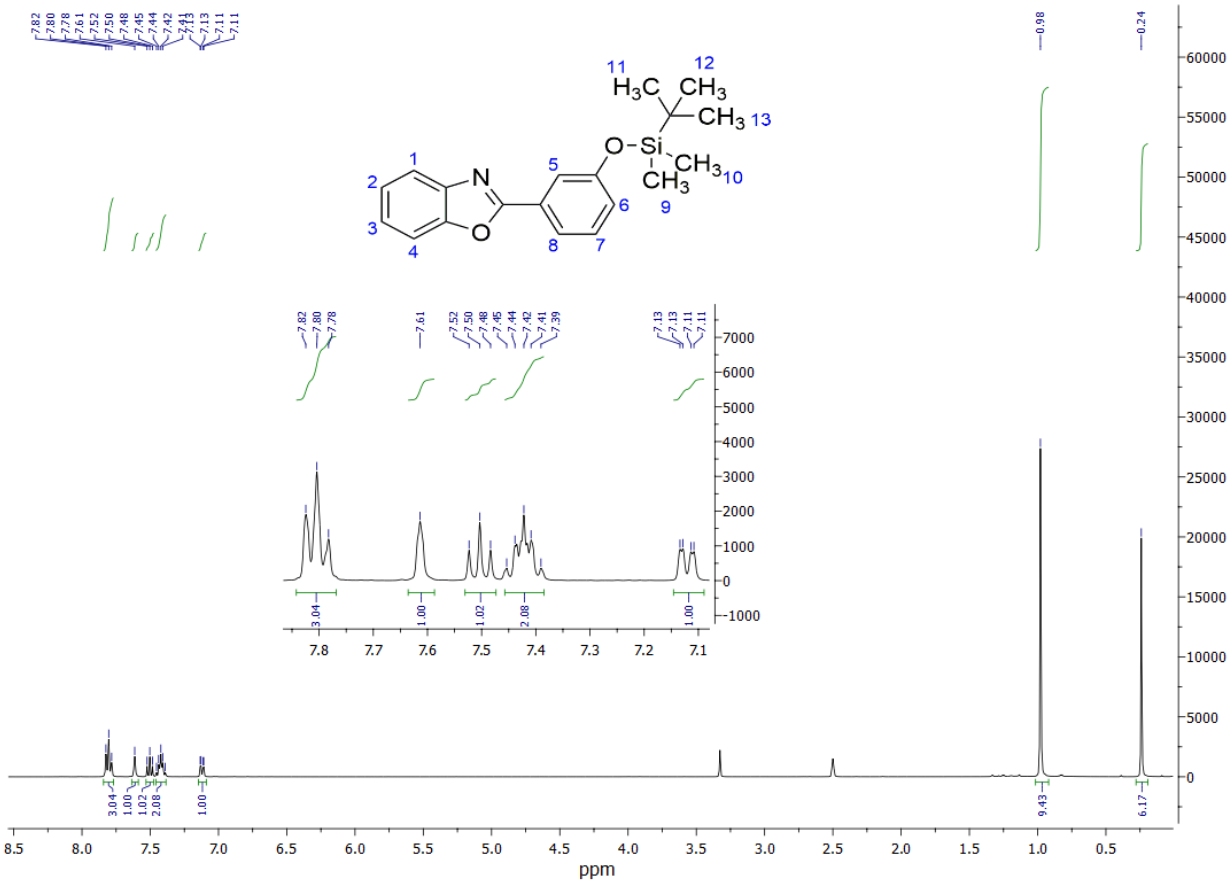


Figure S10. ^{1}H NMR spectrum of compound **BOmTBS** in DMSO-d$_6$ (400 MHz).

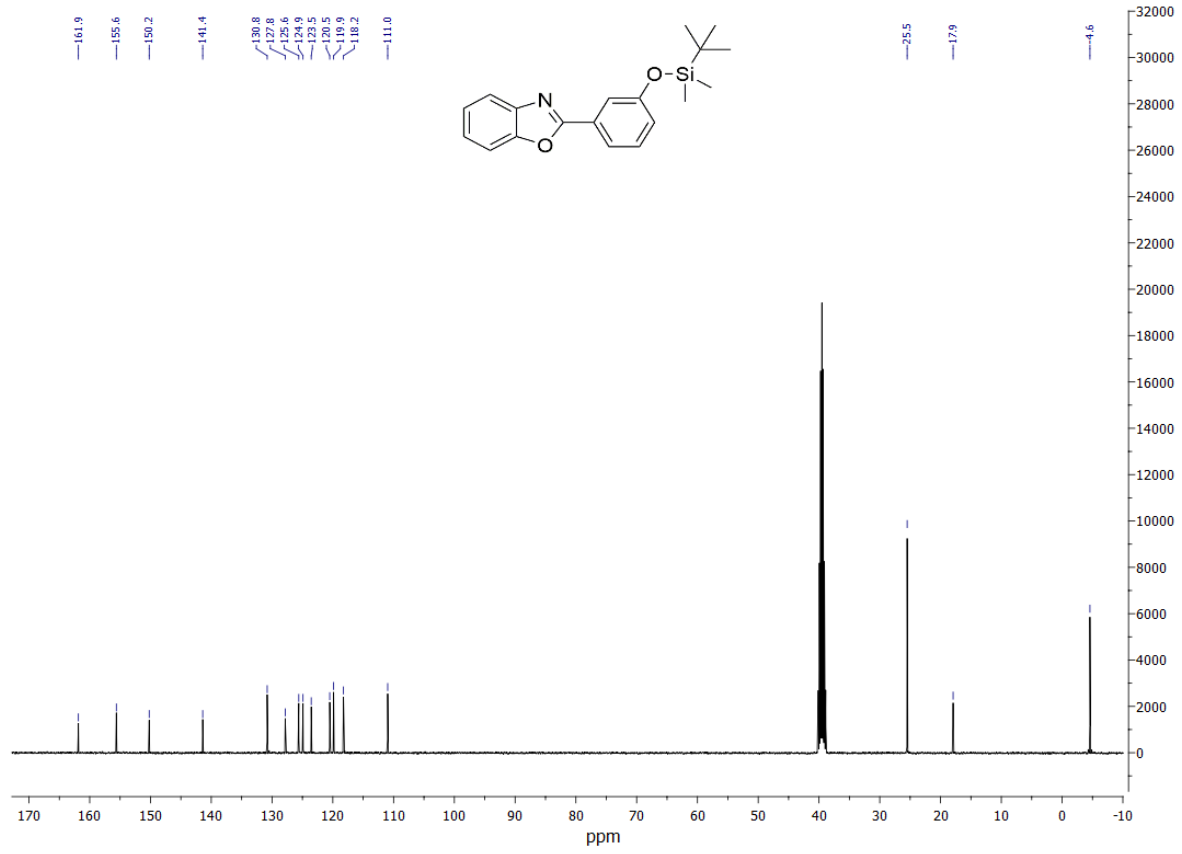


Figure S11. ^{13}C NMR spectrum of compound **BOmTBS** in DMSO-d$_6$ (100 MHz).

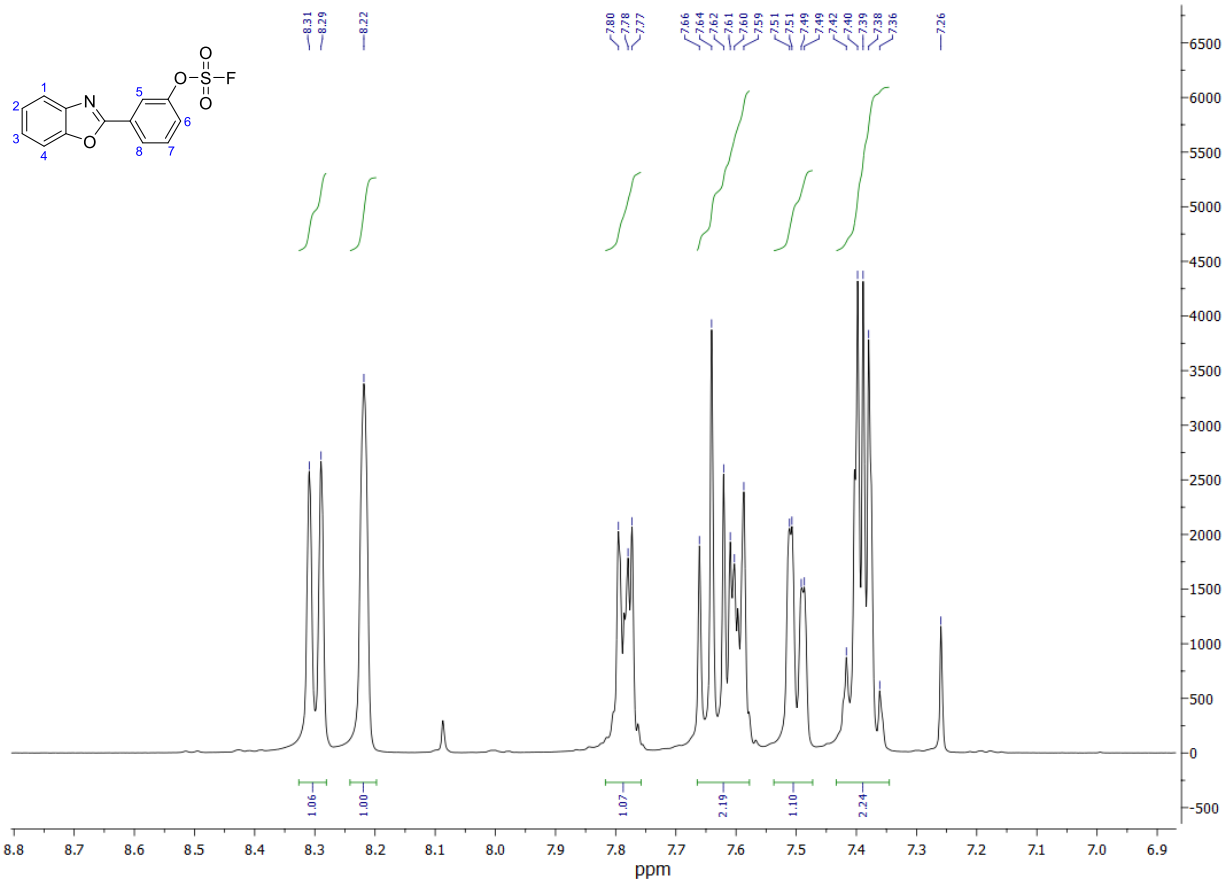


Figure S12. ^{1}H NMR spectrum of compound **BOSm** in $CDCl_3$ (400 MHz).

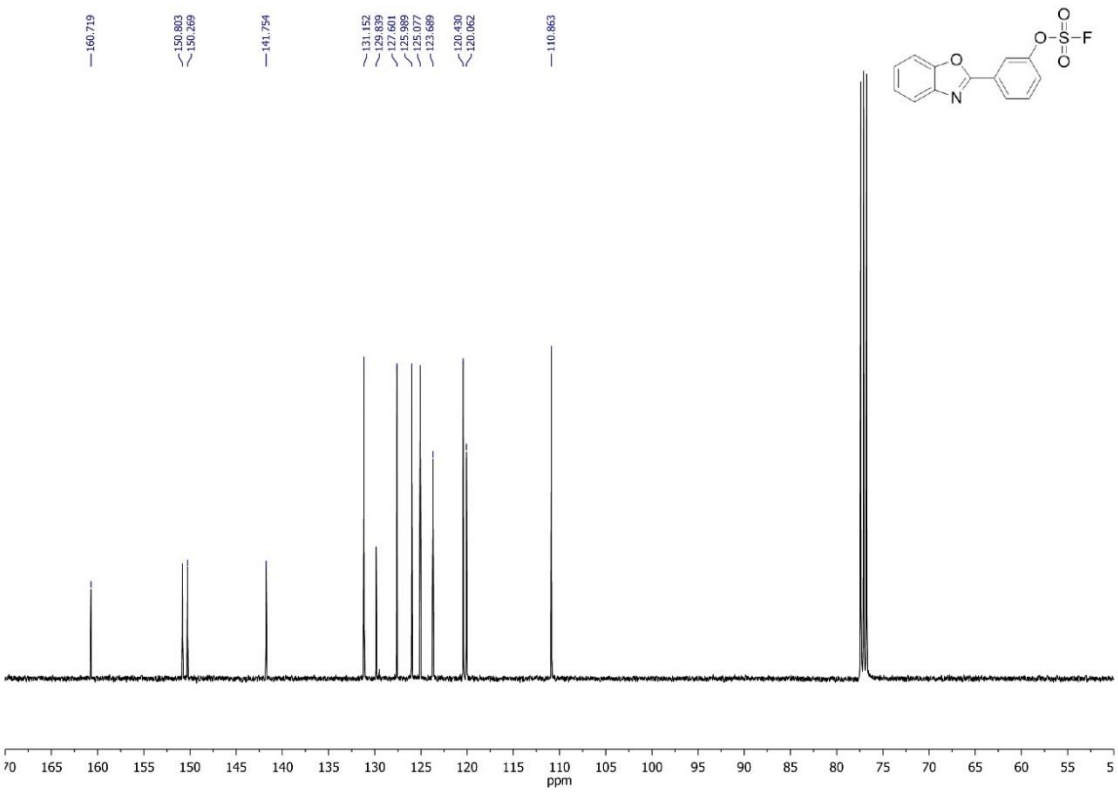


Figure S13. ^{13}C NMR spectrum of compound **BOSm** in $CDCl_3$ (100 MHz).

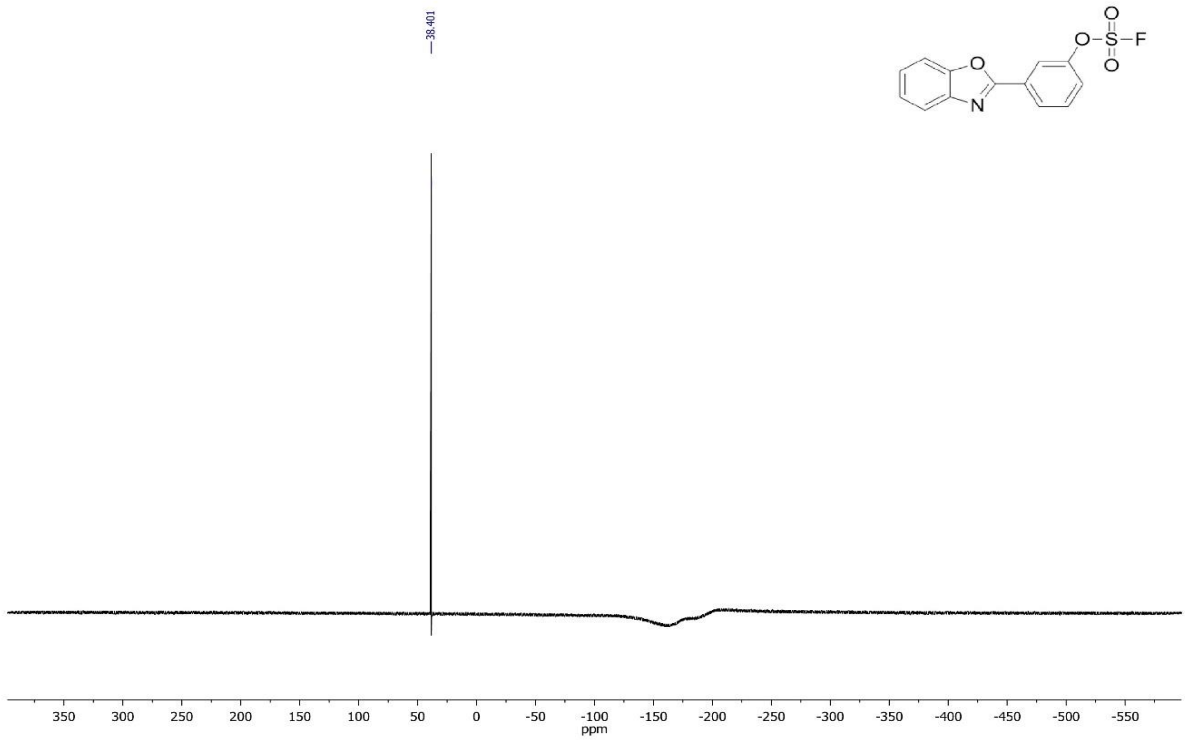


Figure S14. ^{19}F NMR spectrum of compound **BOSm** in $CDCl_3$ (376 MHz).

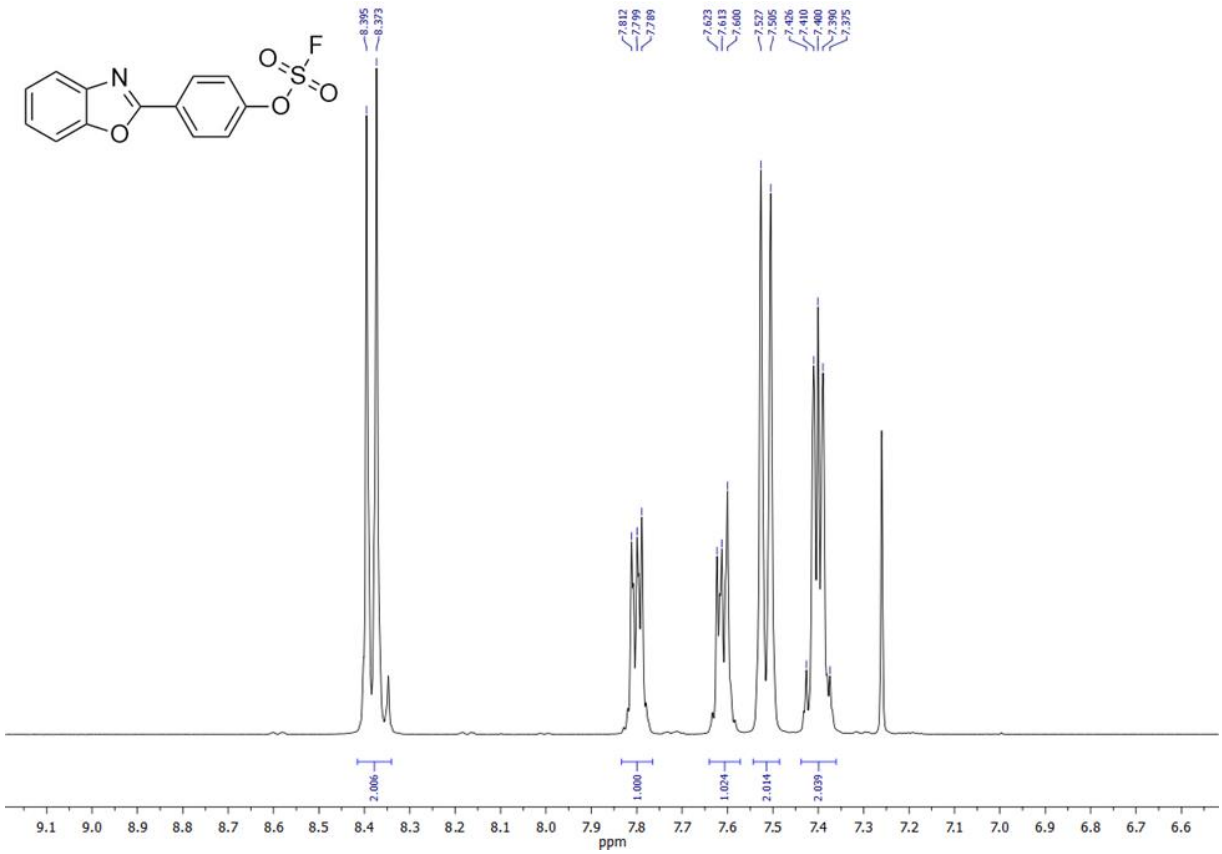


Figure S15. ^{1}H NMR spectrum of compound **BOSp** in $CDCl_3$ (400 MHz).

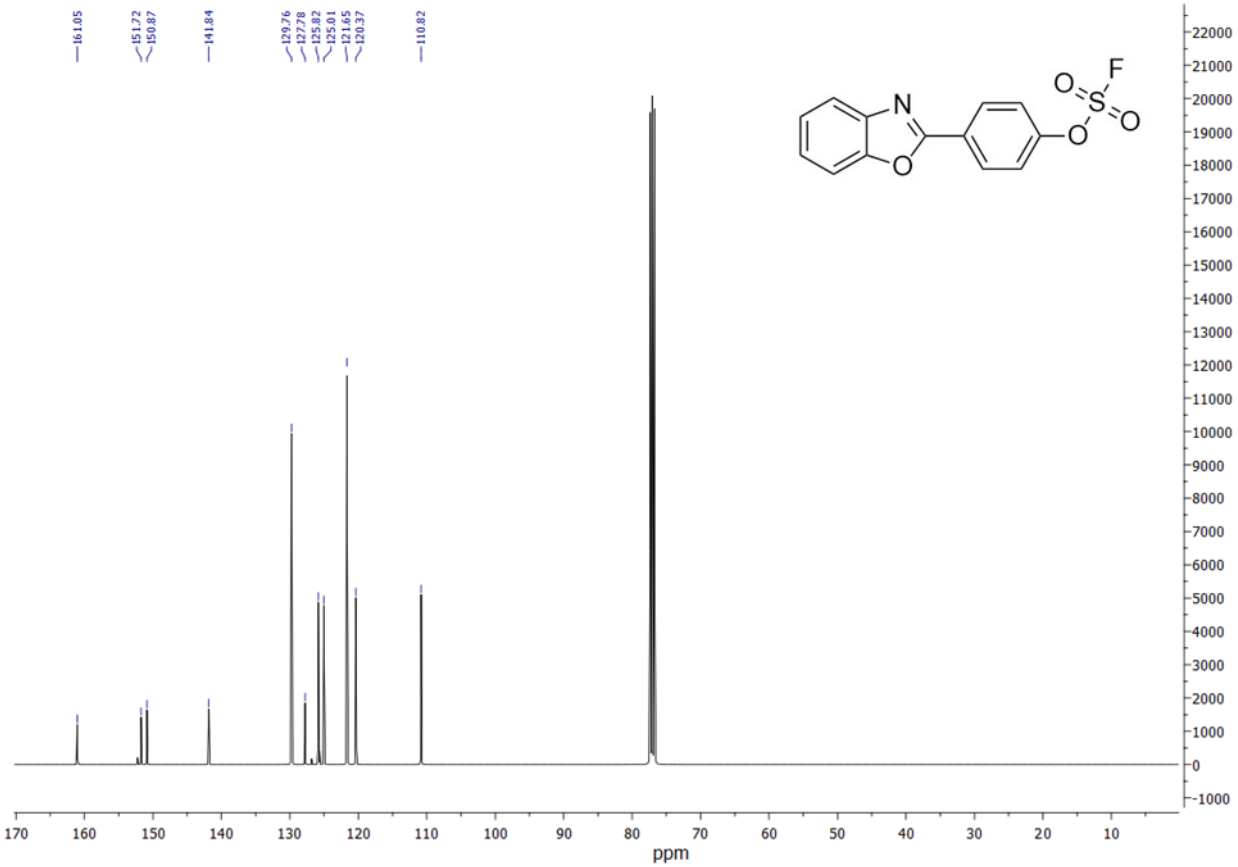


Figure S16. ^{13}C NMR spectrum of compound **BOSp** in $CDCl_3$ (100 MHz).

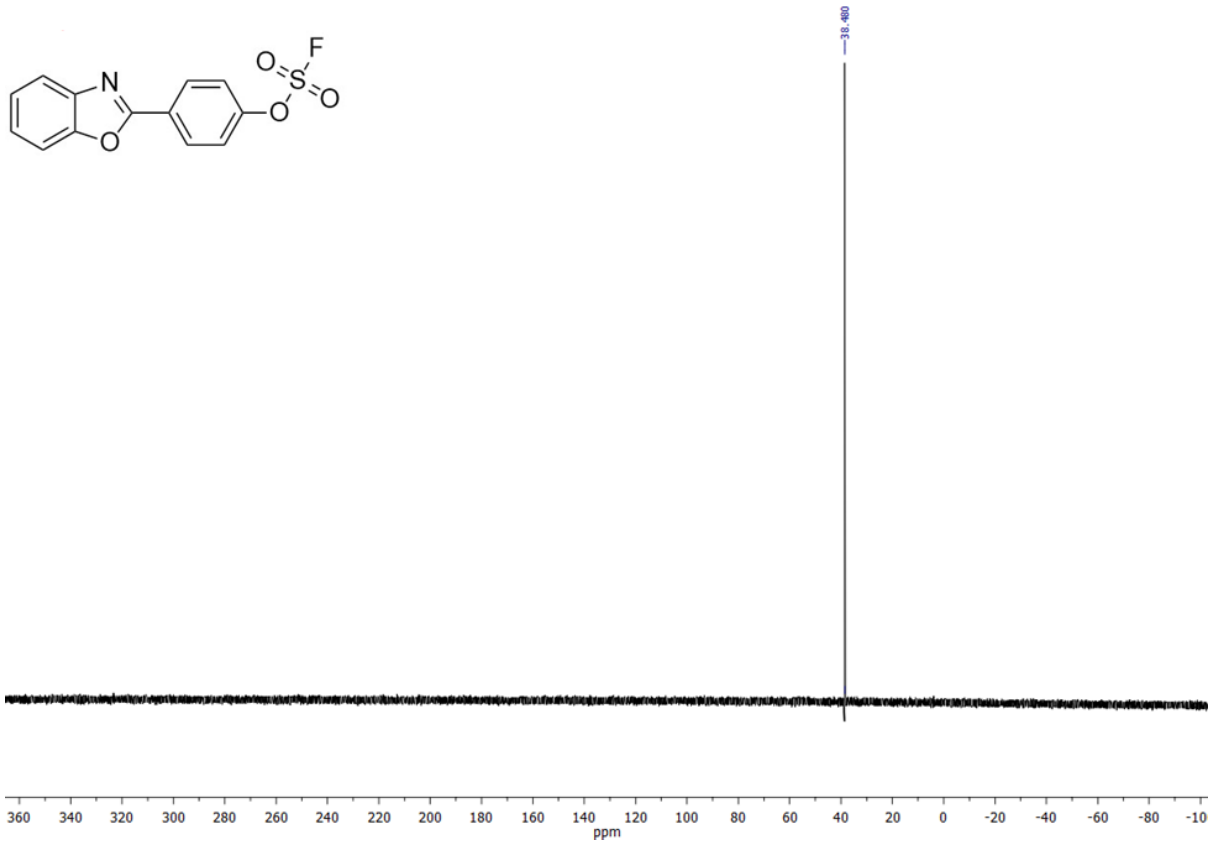


Figure S17. ^{19}F NMR spectrum of compound **BOSp** in $CDCl_3$ (376 MHz).

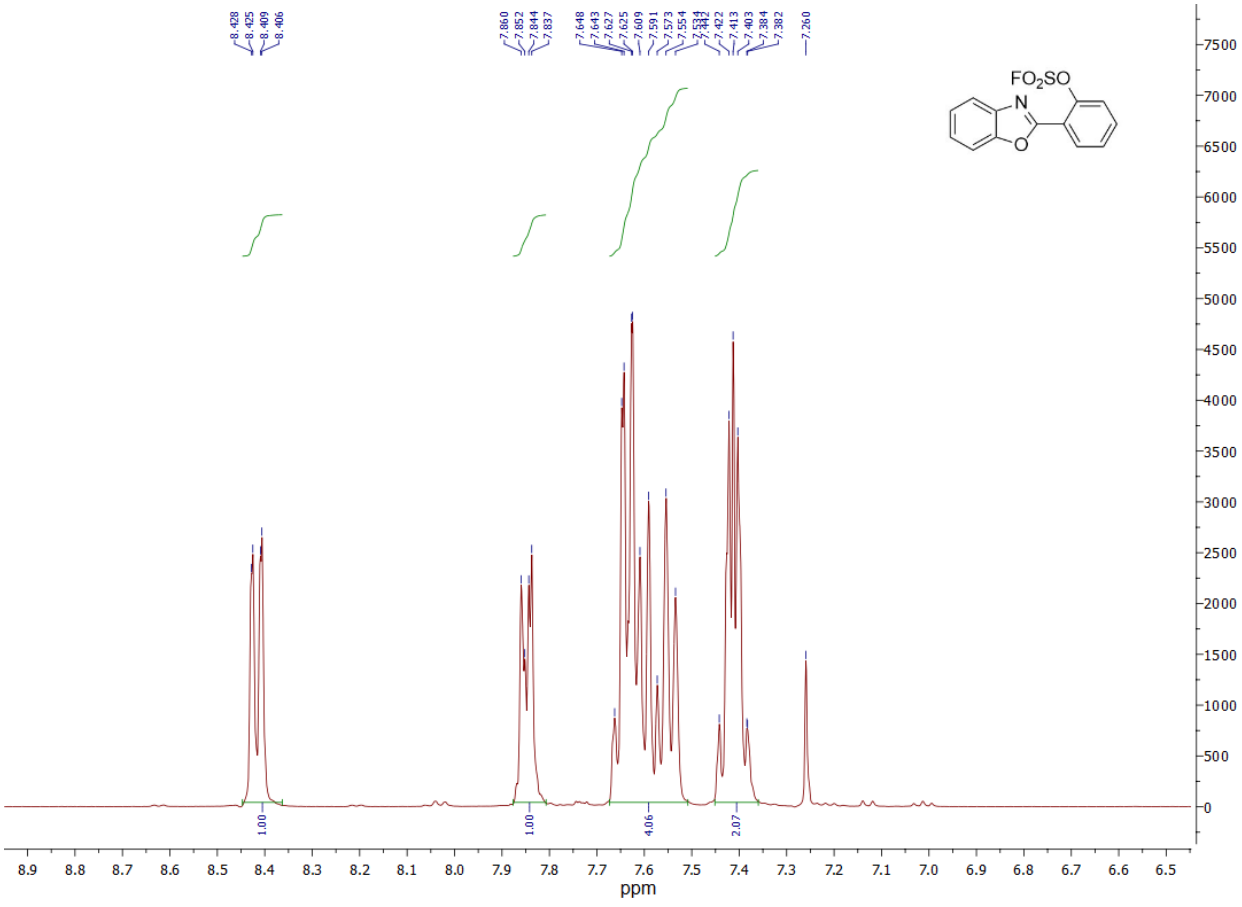


Figure S18. ^{1}H NMR spectrum of compound **BOSo** in $CDCl_3$ (400 MHz).

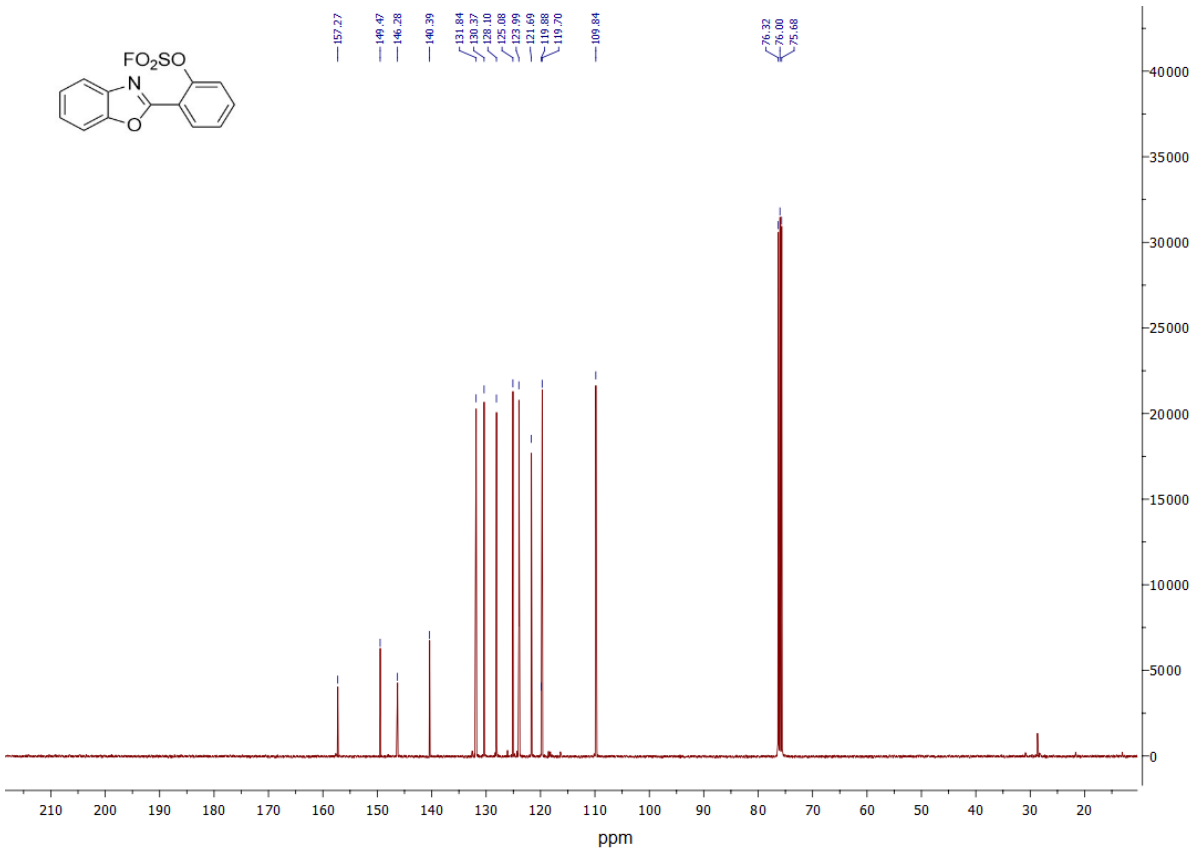


Figure S19. ^{13}C NMR spectrum of compound **BOSo** in $CDCl_3$ (100 MHz)**.**

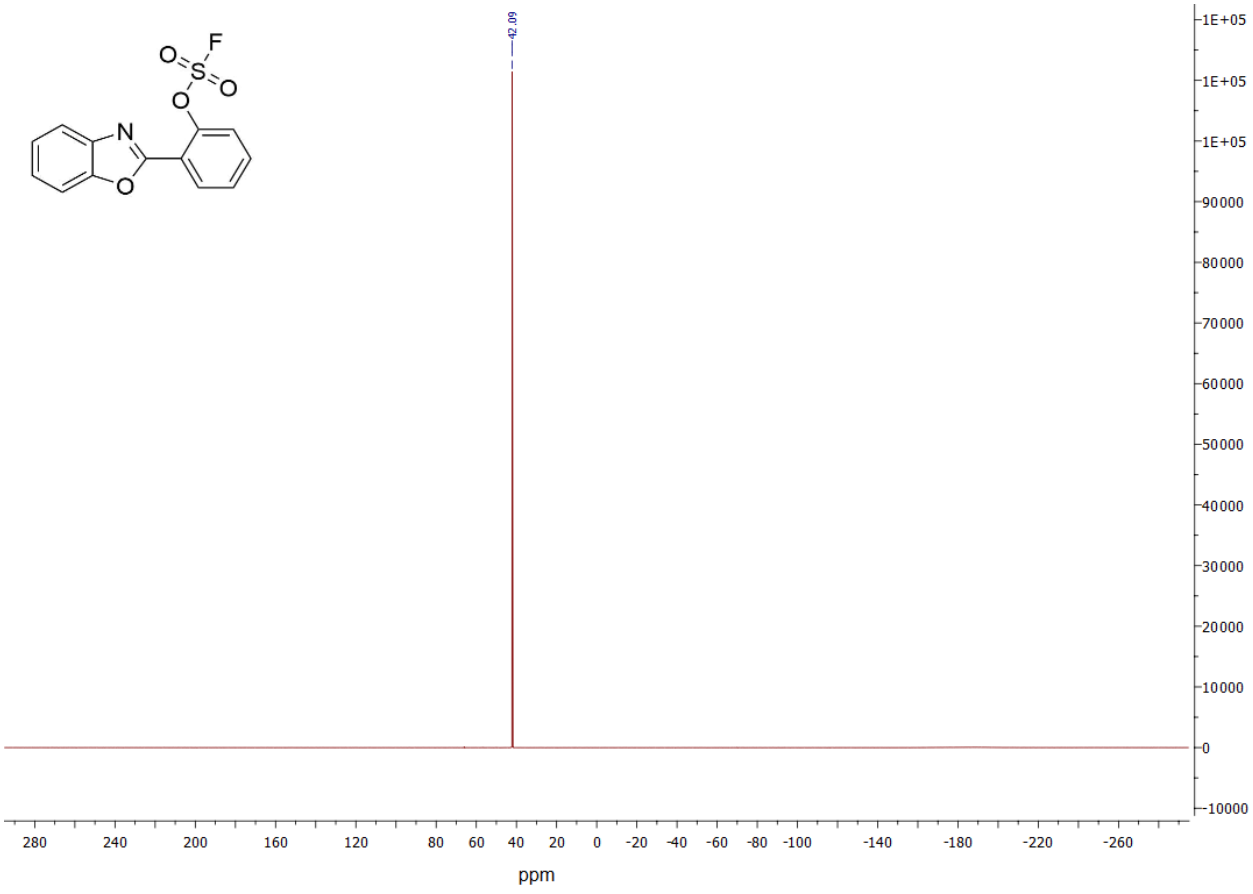


Figure S20. ^{19}F NMR spectrum of compound **BOSo** in $CDCl_3$ (376 MHz).

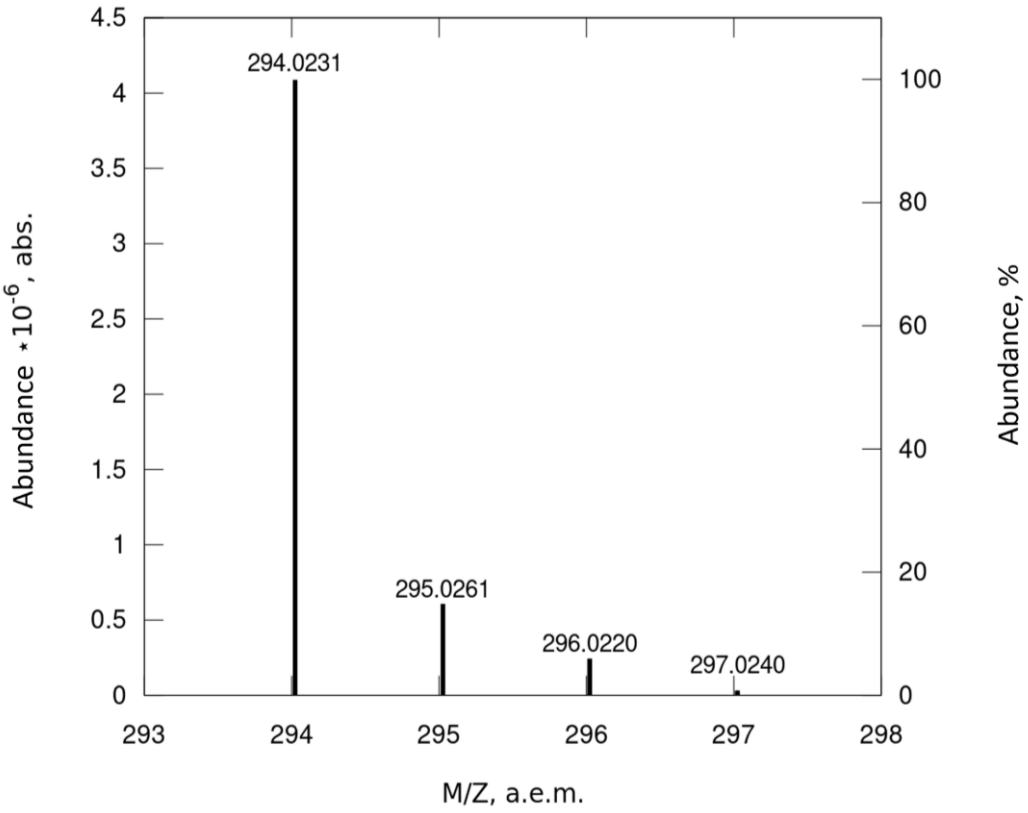


Figure S21. Peaks in the HRMS spectrum of Compound **BOSp**.

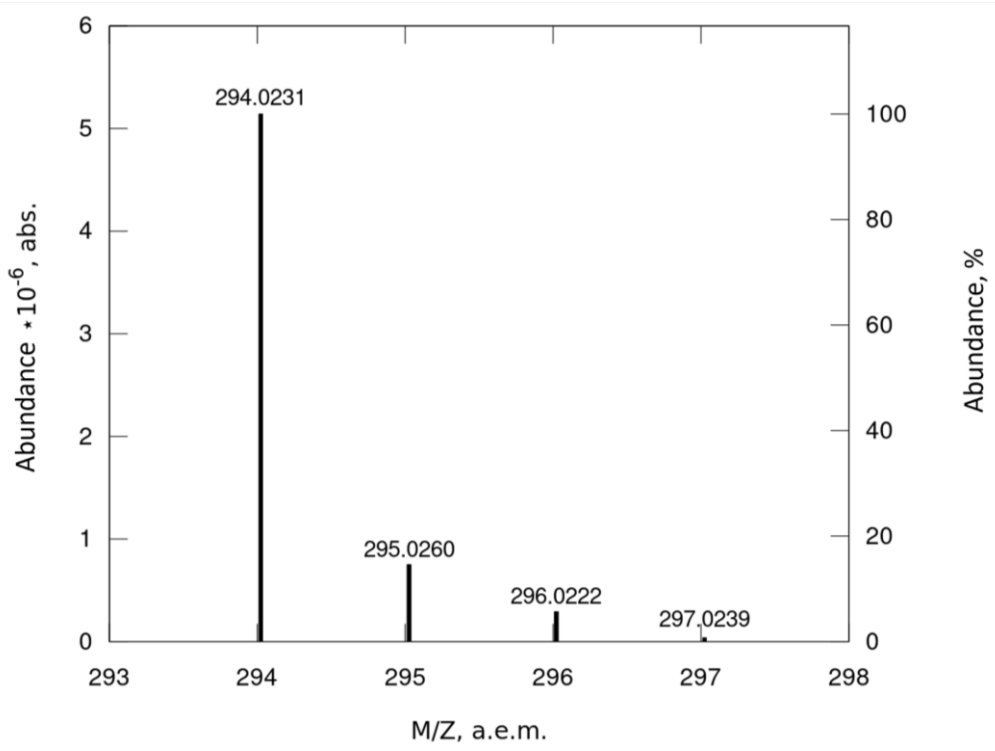


Figure S22. Peaks in the HRMS spectrum of Compound **BOSm**.

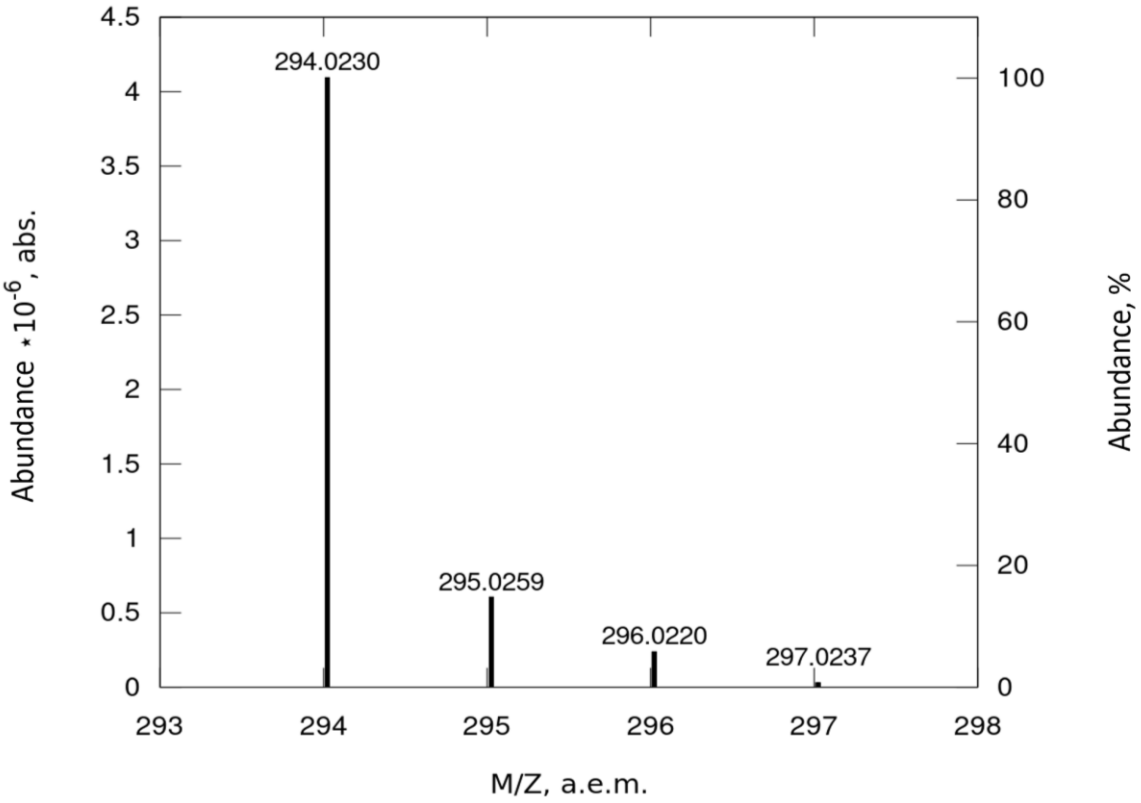


Figure S23. Peaks in the HRMS spectrum of Compound **BOSo**.