

Electronical supporting information for

New luminescent organoboron esters based on damnacanthal: One-Pot multicomponent synthesis, optical behavior, cytotoxicity, and selectivity studies against MDA-MBA-231 breast cancer cells

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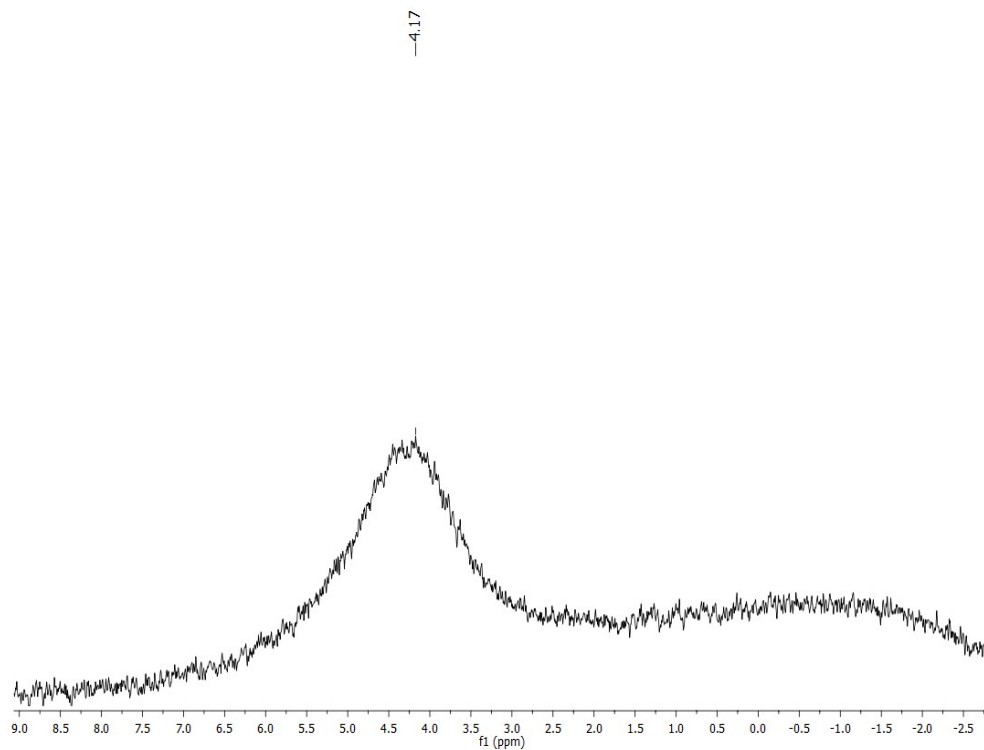


Fig. S1. ^{11}B NMR spectrum of organoboron ester derivative **4a** in $(\text{CD}_3)_2\text{SO}$ at 128 MHz.

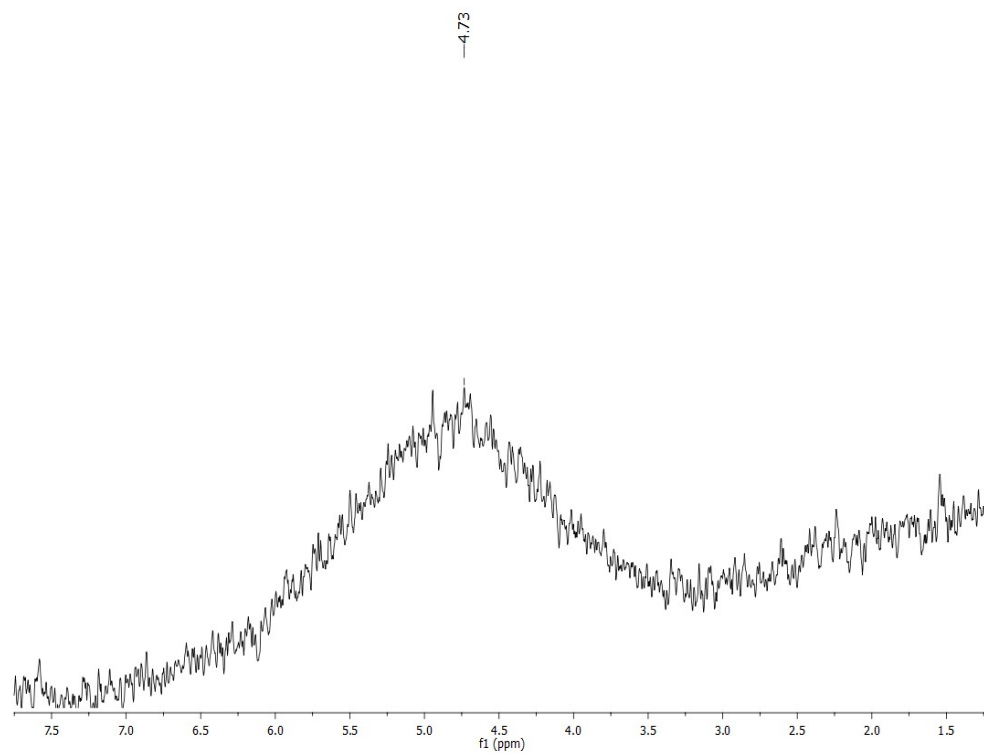


Fig. S2. ^{11}B NMR spectrum of organoboron ester derivative **4b** in CDCl_3 at 128 MHz.

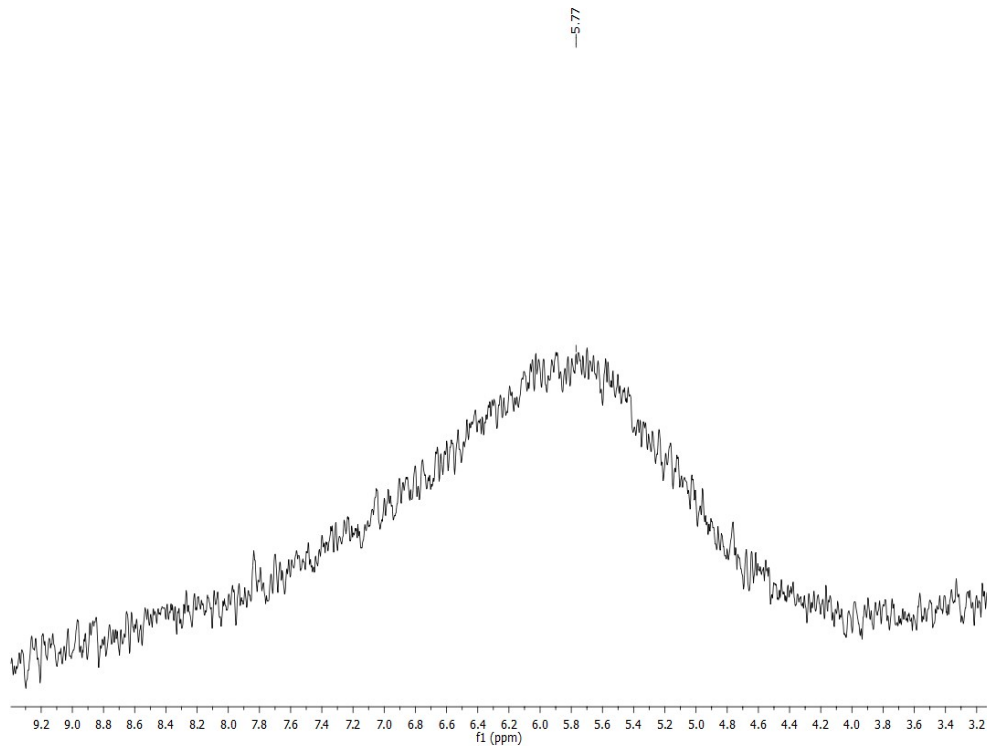


Fig. S3. ^{11}B NMR spectrum of organoboron ester derivative **4c** in CDCl_3 at 128 MHz.

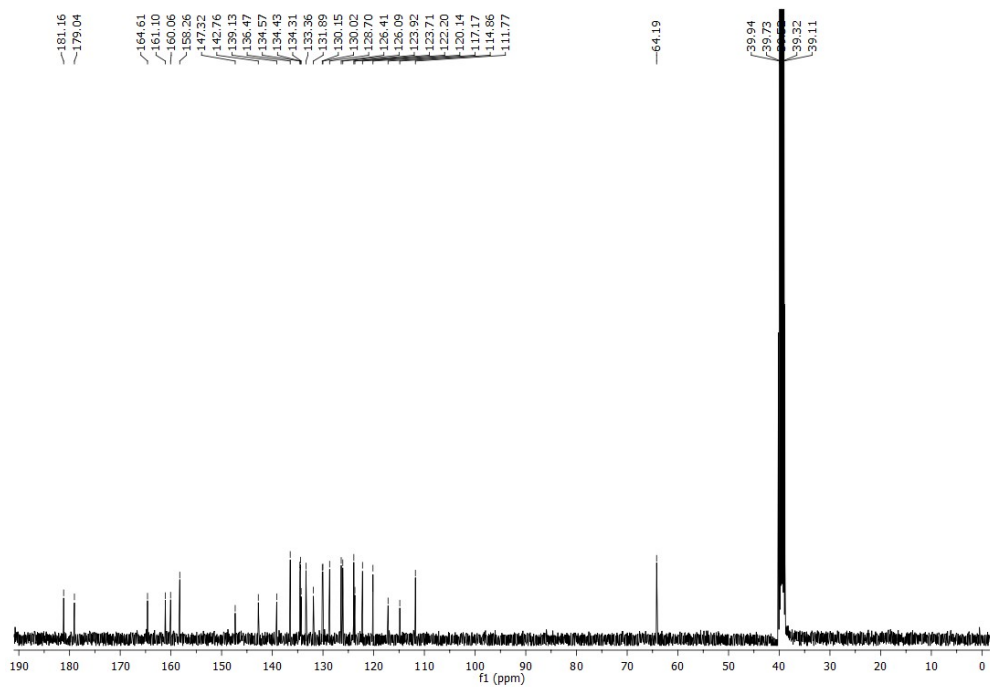


Fig. S4. ^{13}C NMR spectrum of organoboron ester derivative **4a** in $(\text{CD}_3)_2\text{SO}$ at 100.14 MHz.

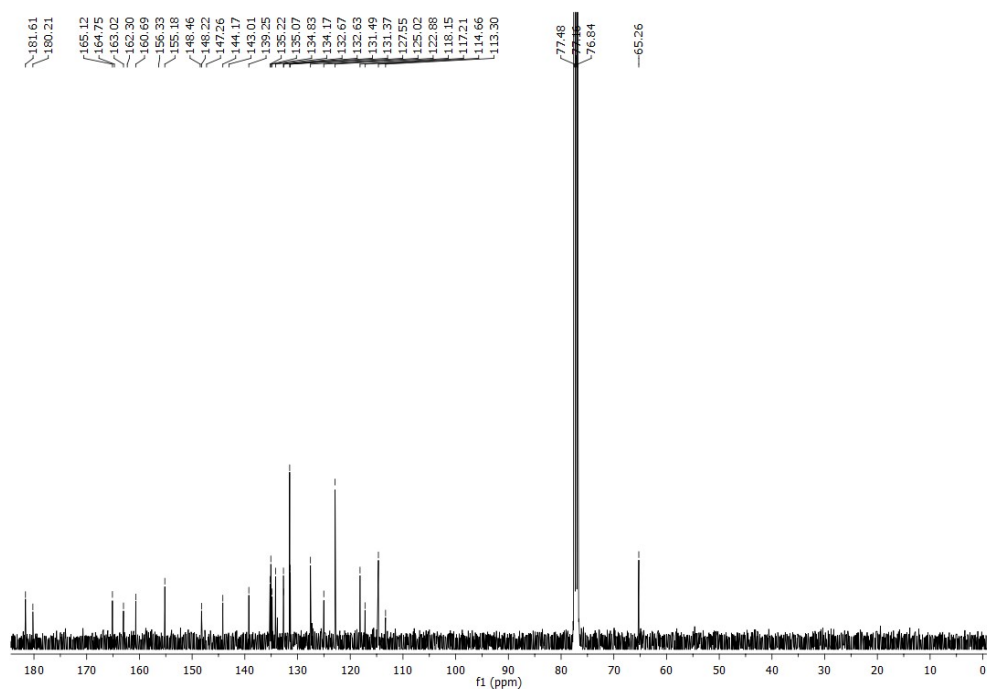


Fig. S5. ^{13}C NMR spectrum of organoboron ester derivative **4b** in CDCl_3 at 100.14 MHz.

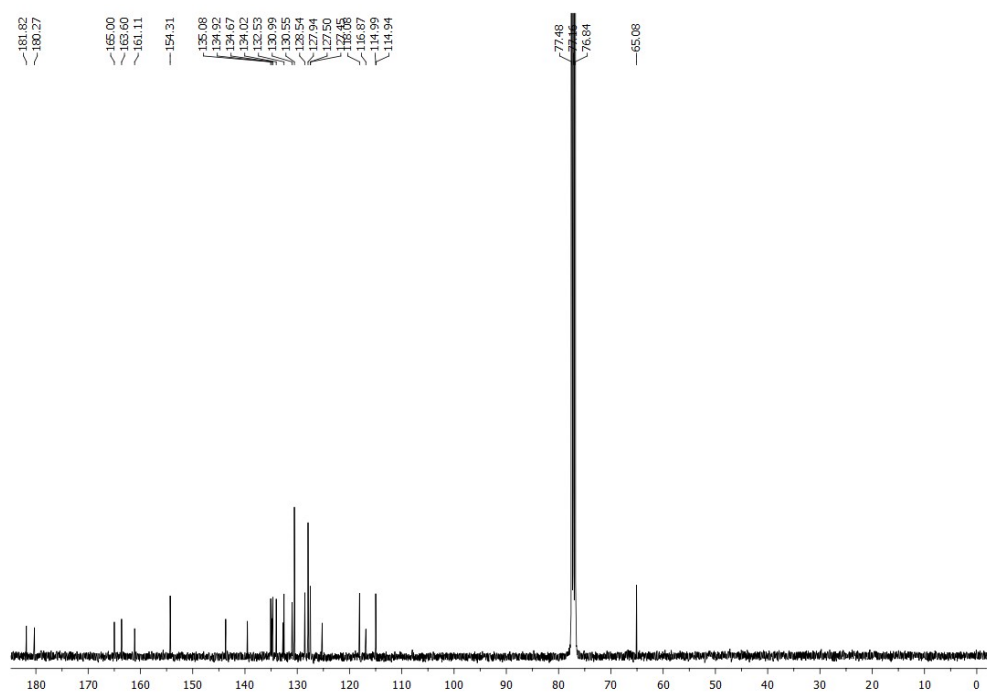


Fig. S6. ^{13}C NMR spectrum of organoboron ester derivative **4c** in CDCl_3 at 100.14 MHz.

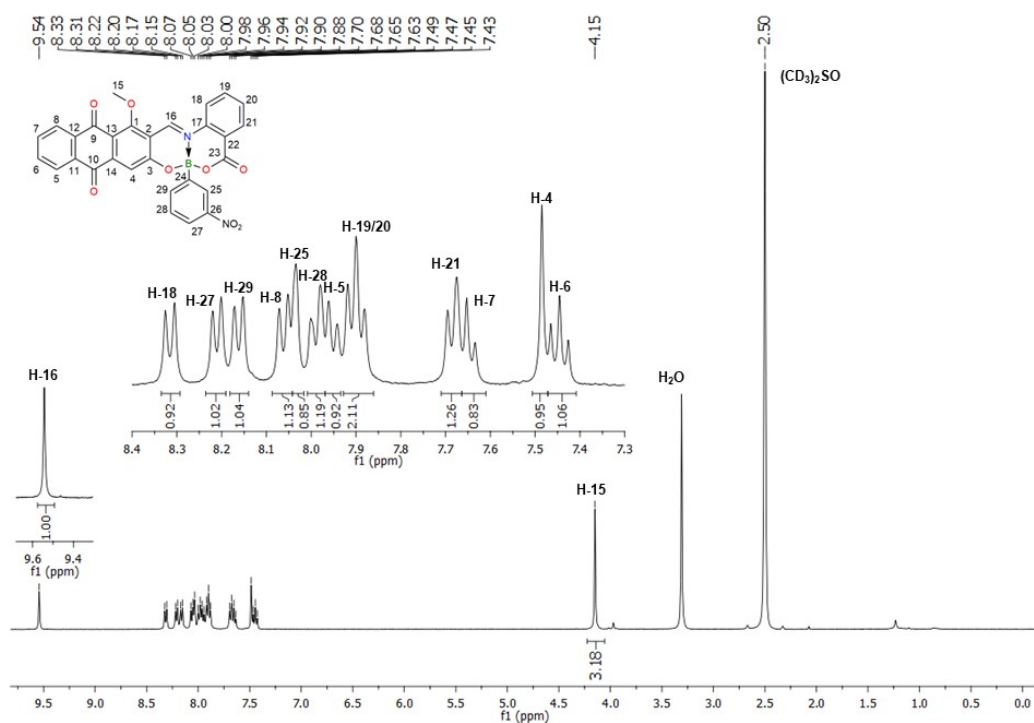


Fig. S7. ^1H NMR $(\text{CD}_3)_2\text{SO}$ spectrum of compound **4a** at 400.14 MHz.

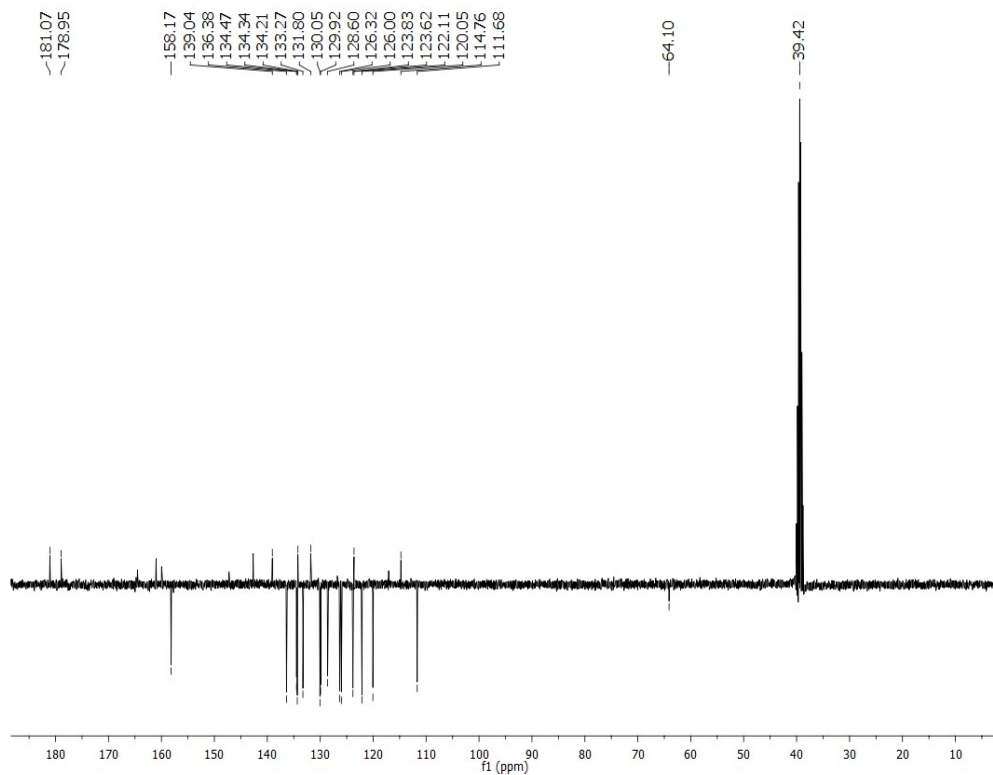


Fig. S8. DEPT 135 spectrum of organoboron ester derivative **4a** in $(\text{CD}_3)_2\text{SO}$ at 100.14 MHz.

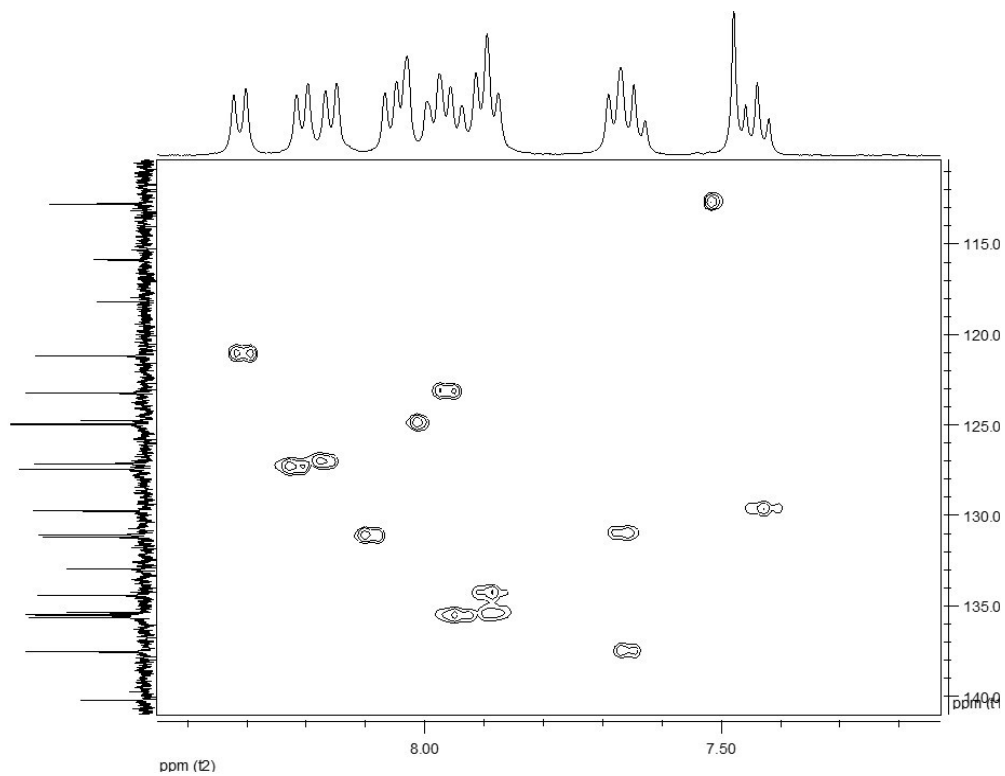


Fig. S9. HETCOR spectrum of organoboron ester derivative **4a** in $(\text{CD}_3)_2\text{SO}$ at 100.14 MHz.

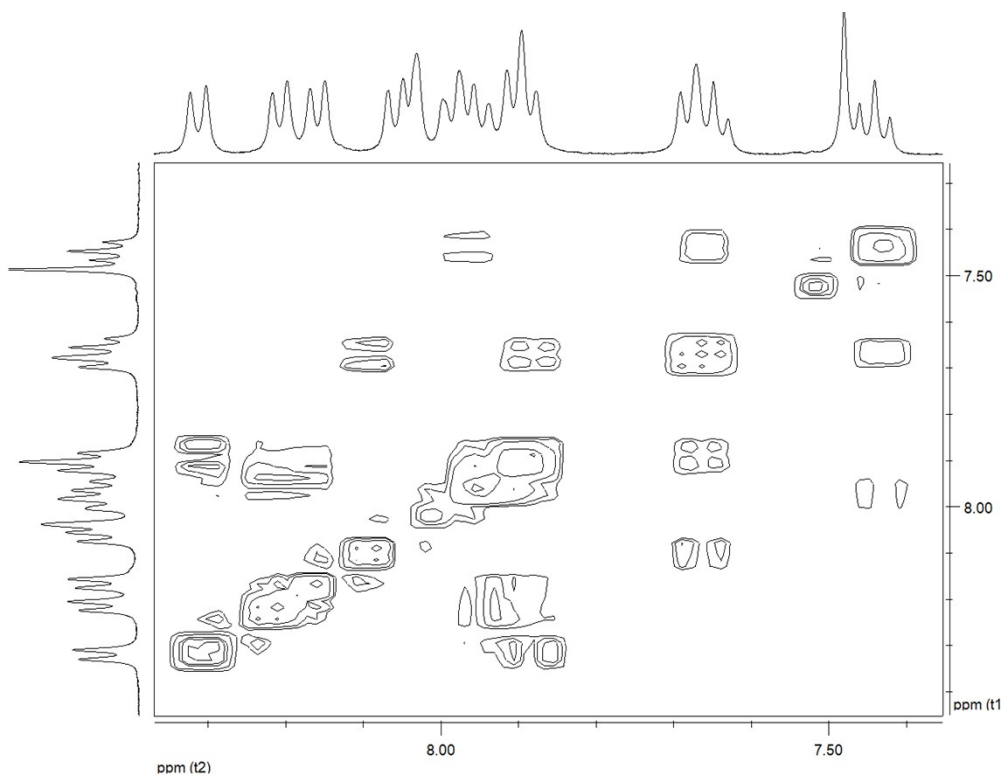


Fig. S10. COSY spectrum of organoboron ester derivative **4a** in $(\text{CD}_3)_2\text{SO}$ at 100.14 MHz.

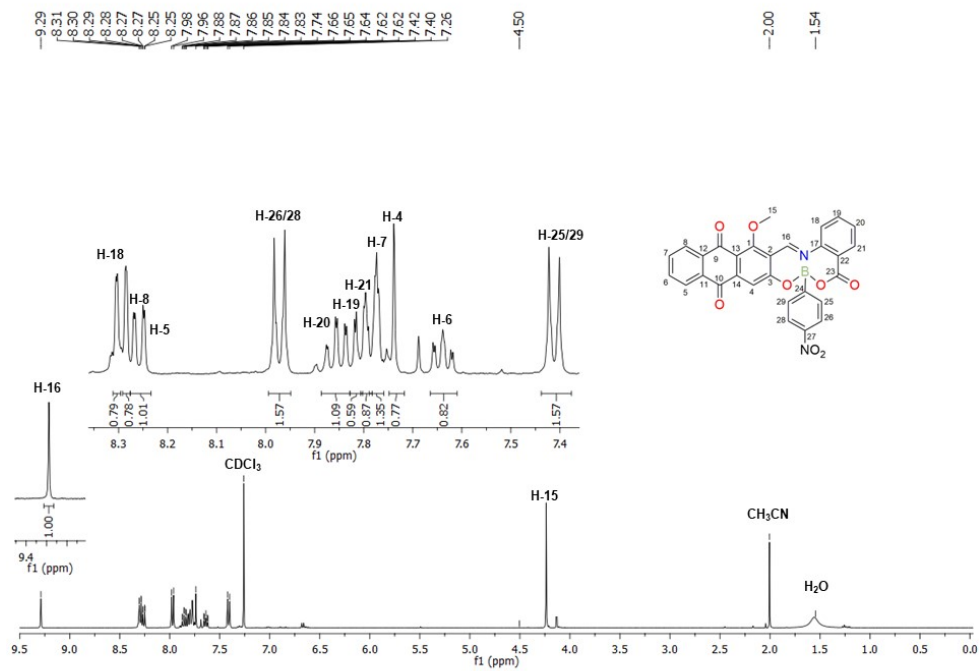


Fig. S11. ¹H NMR spectrum of organoboron ester derivative **4b** in CDCl₃ at 400.16 MHz

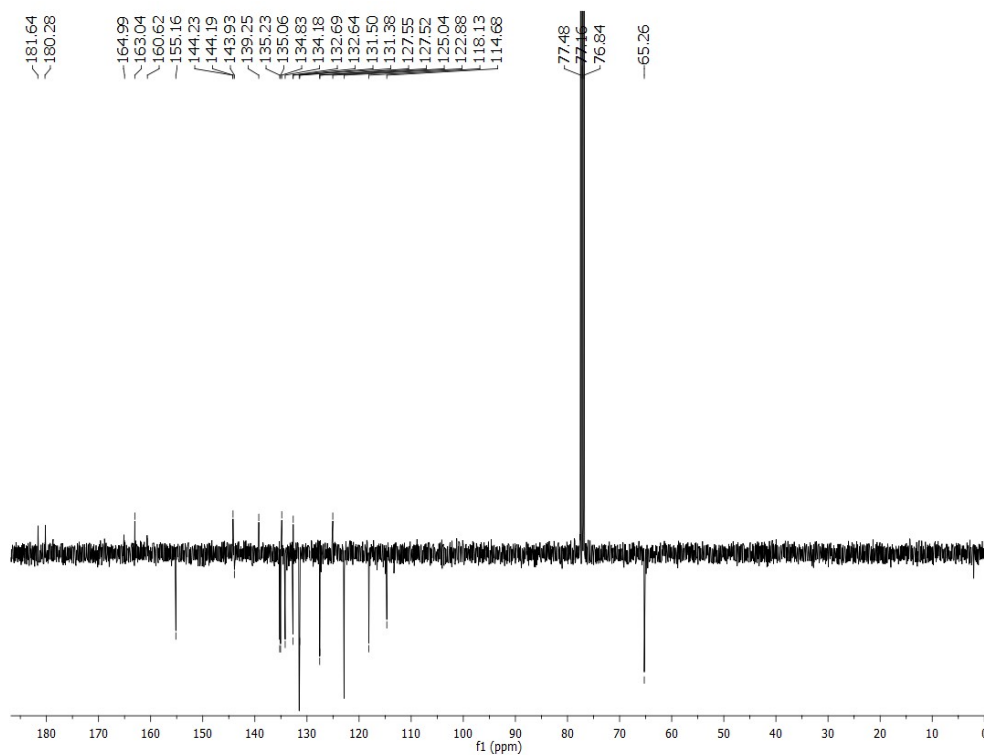


Fig. S12. DEPT 135 spectrum of organoboron ester derivative **4b** in CDCl₃ at 100.14 MHz.

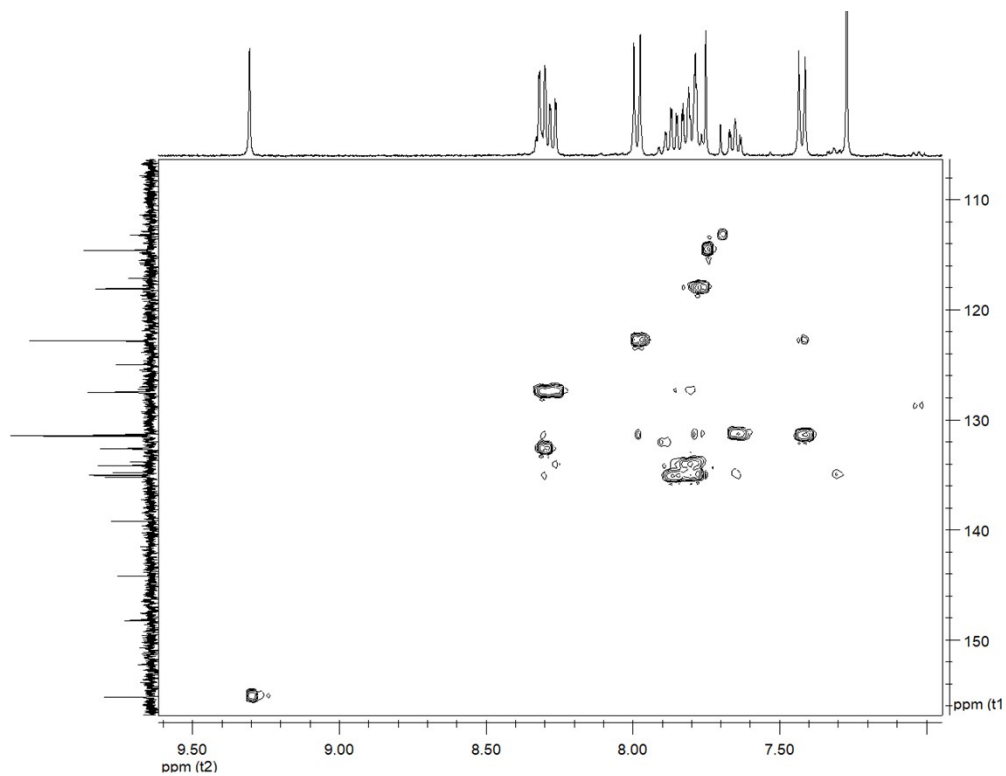


Fig. S13. HETCOR spectrum of organoboron ester derivative **4b** in CDCl_3 at 100.14 MHz.

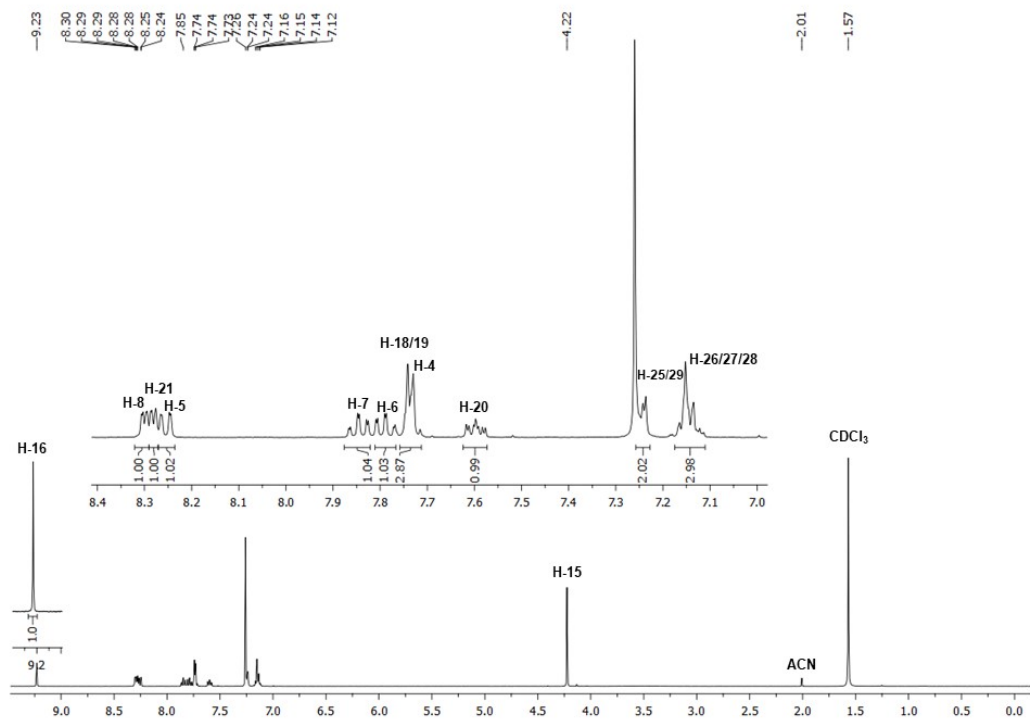


Fig. S14. ^1H NMR ($\text{CD}_3)_2\text{SO}$) spectrum of organoboron ester **4c** at 400.14 MHz.



Fig. S15. ¹³C NMR spectrum of organoboron ester derivative **4c** in (CD₃)₂SO at 100.14 MHz.

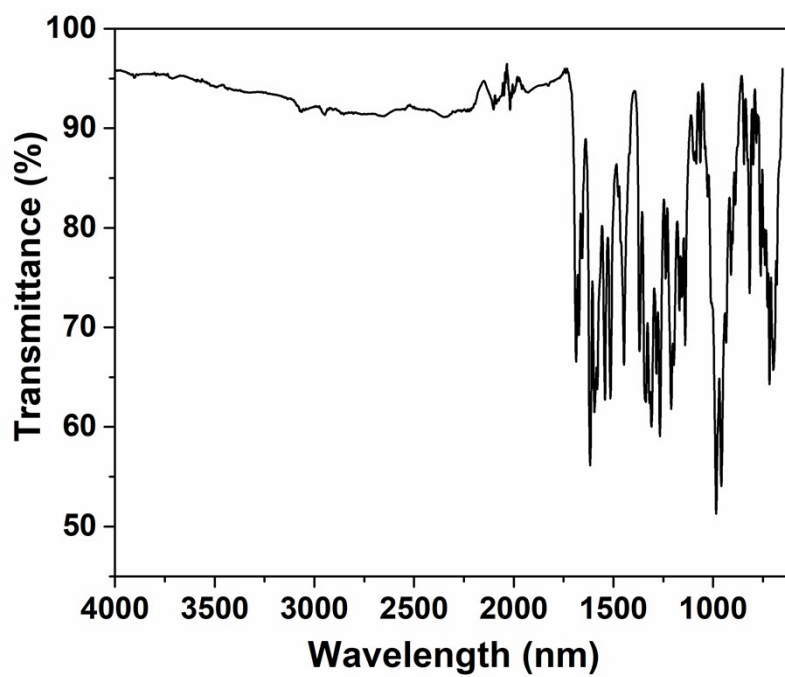


Fig. S16. IR-ATR spectrum of organoboron ester derivative **4a**.

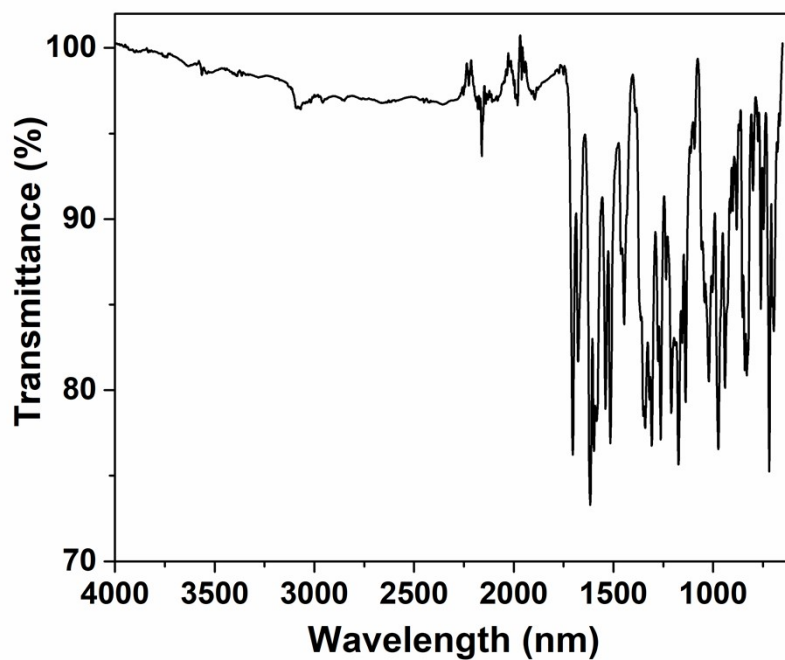


Fig. S17. IR-ATR spectrum of organoboron ester derivative **4b**.

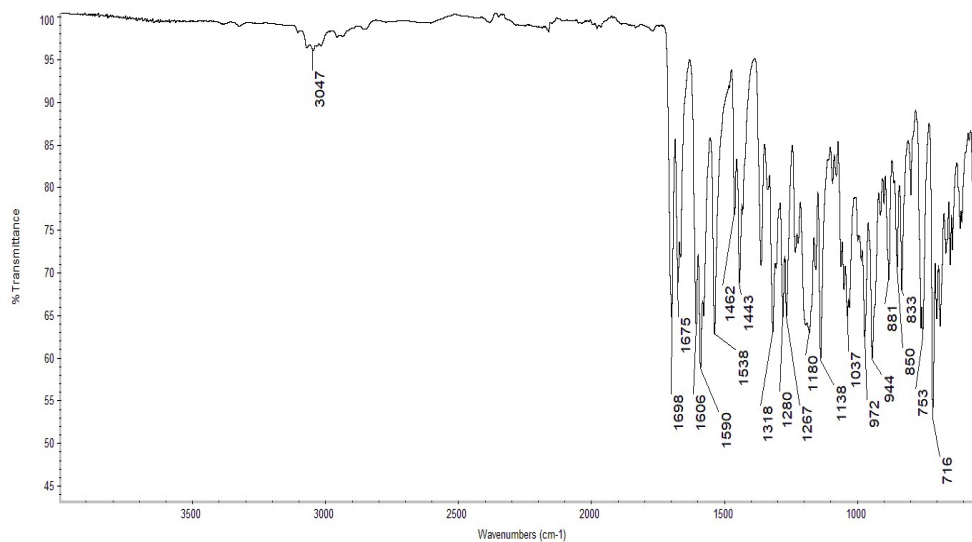


Fig. S18. IR-ATR spectrum of organoboron ester derivative **4c**.

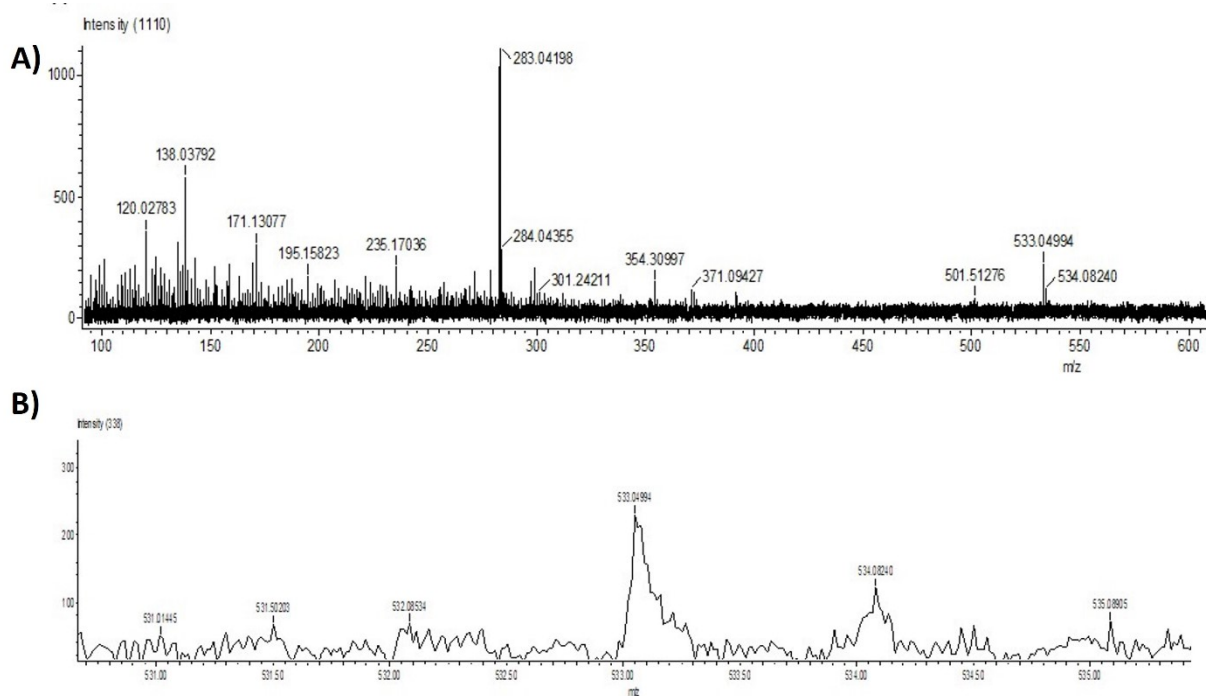


Fig. S.19. DART-HRMS spectrum of organoboron ester **4a** and B) Isotopic pattern of compound **4a**

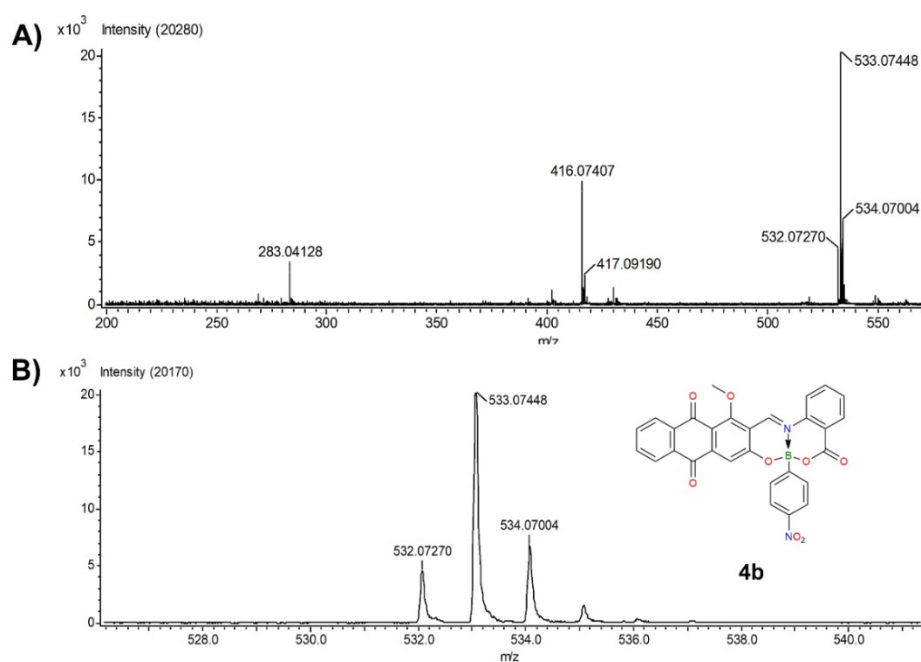


Fig. S.20. DART-HRMS spectrum of organoboron ester **4b** and B) Isotopic pattern of compound **4b**.

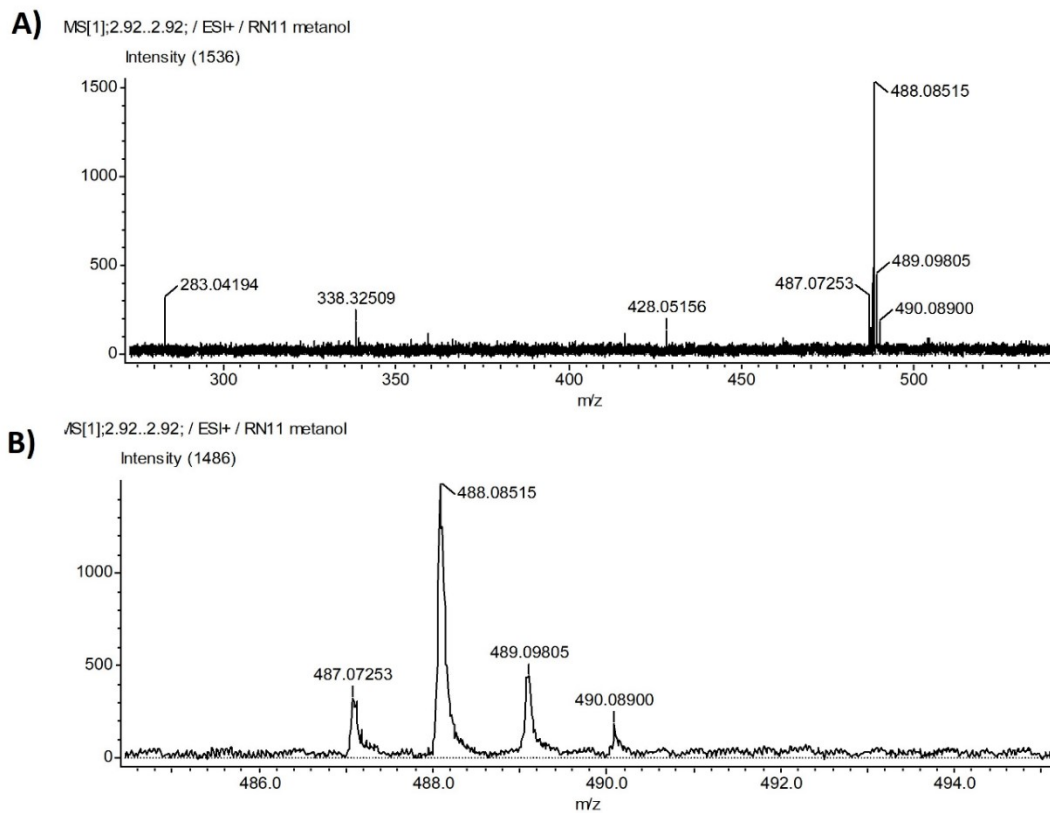


Fig. S.21. DART-HRMS spectrum of organoboron ester **4c** and B) Isotopic pattern of compound **4c**.

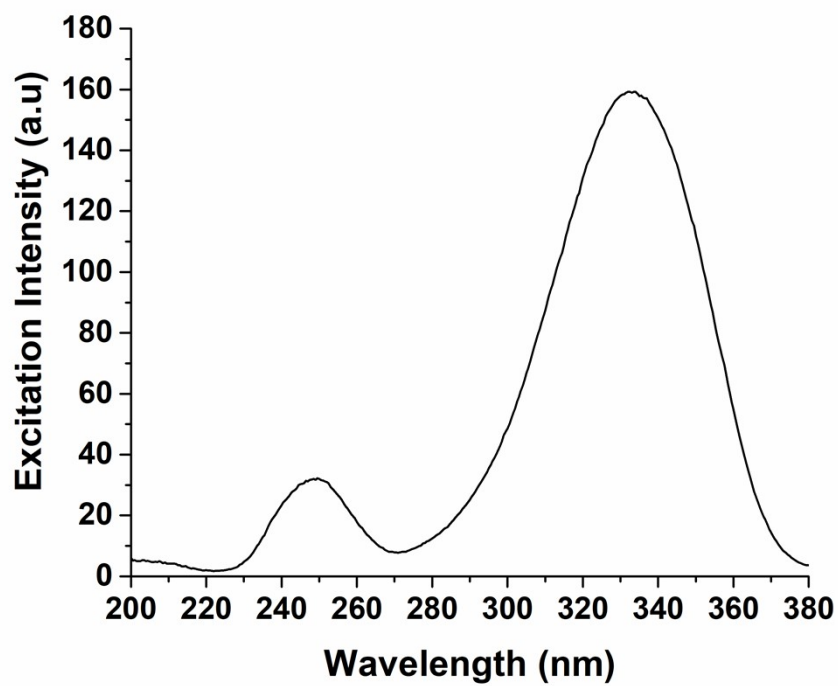


Fig. S22. Excitation spectrum of compound **4a** excited at 256 nm.

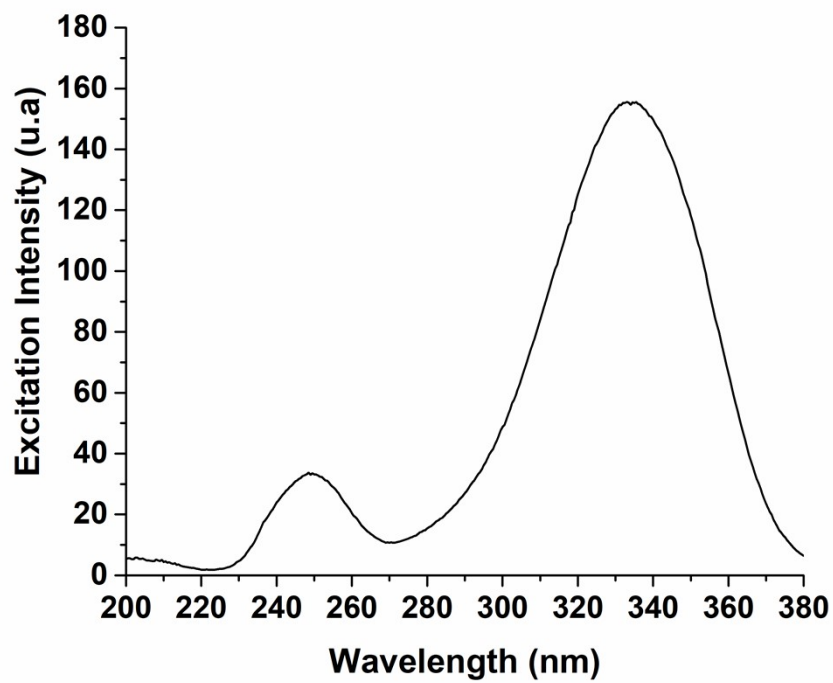


Fig. S23. Excitation spectrum of compound **4b** excited at 257 nm.

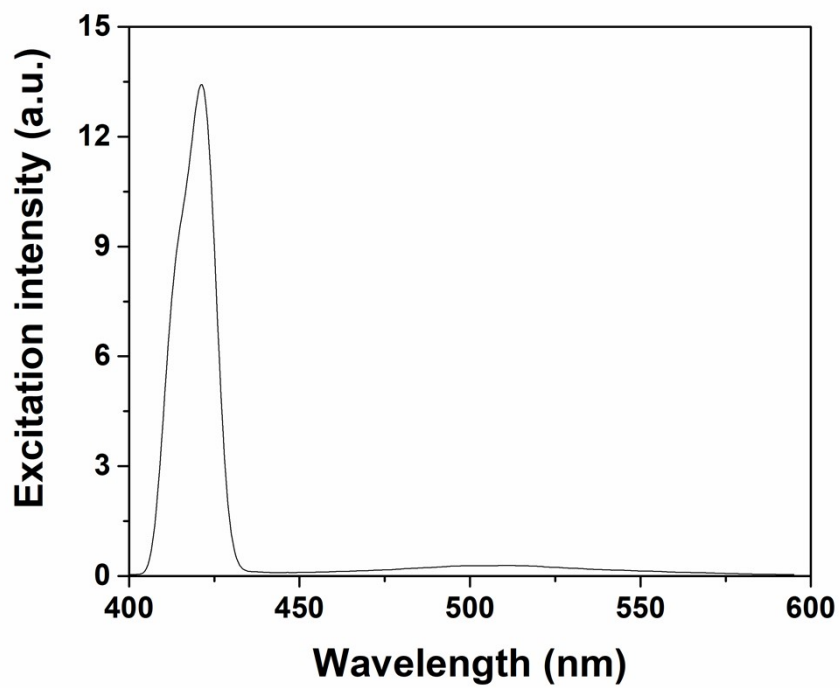


Fig. S24. Excitation spectrum of compound **4a** excited at 415 nm.

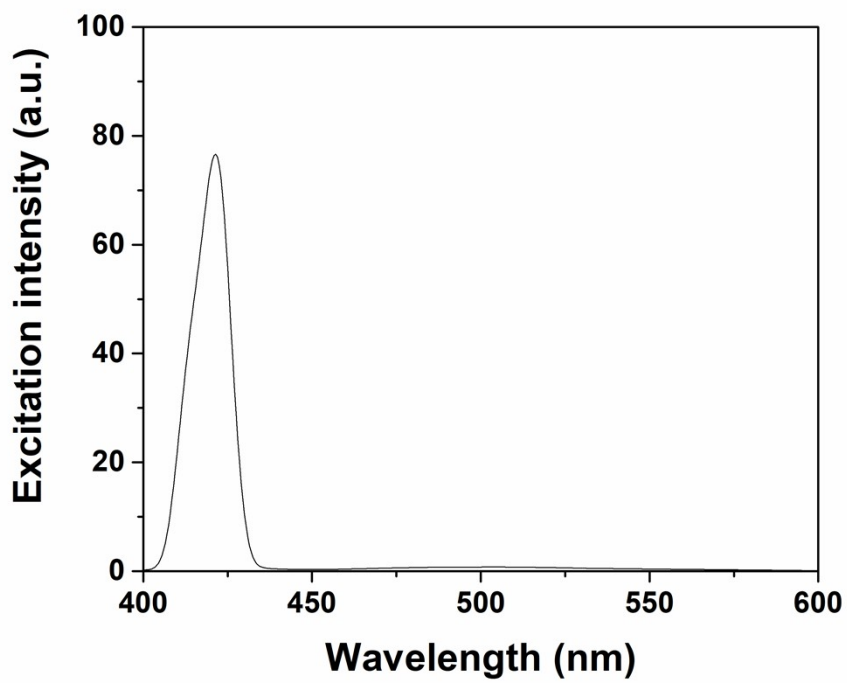


Fig. S25. Excitation spectrum of compound **4b** excited at 416 nm.

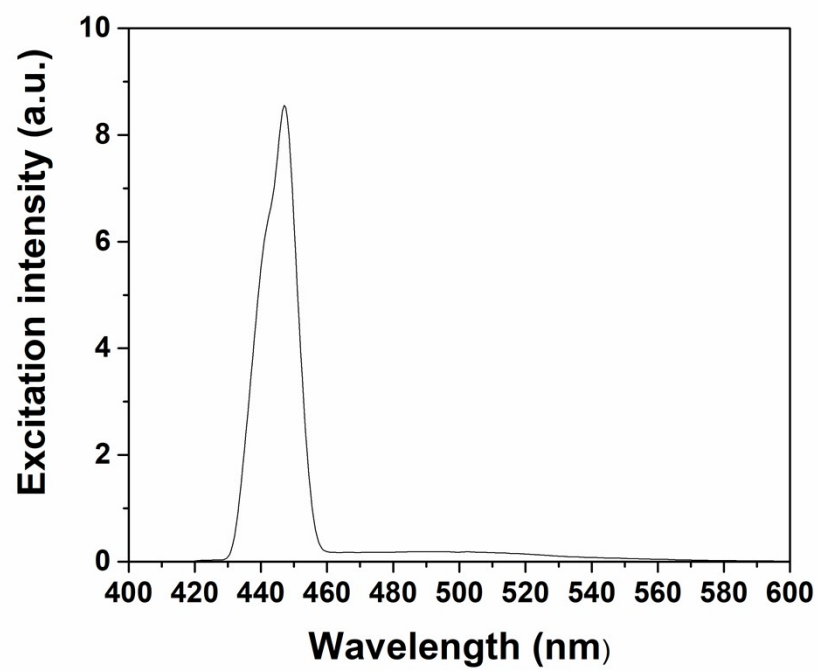


Fig. S26. Excitation spectrum of compound **4c** excited at 440 nm.