

Electronic Supplementary (ESI)

Highly Photostable NIR Indicators for Optical Carbon Dioxide Sensors

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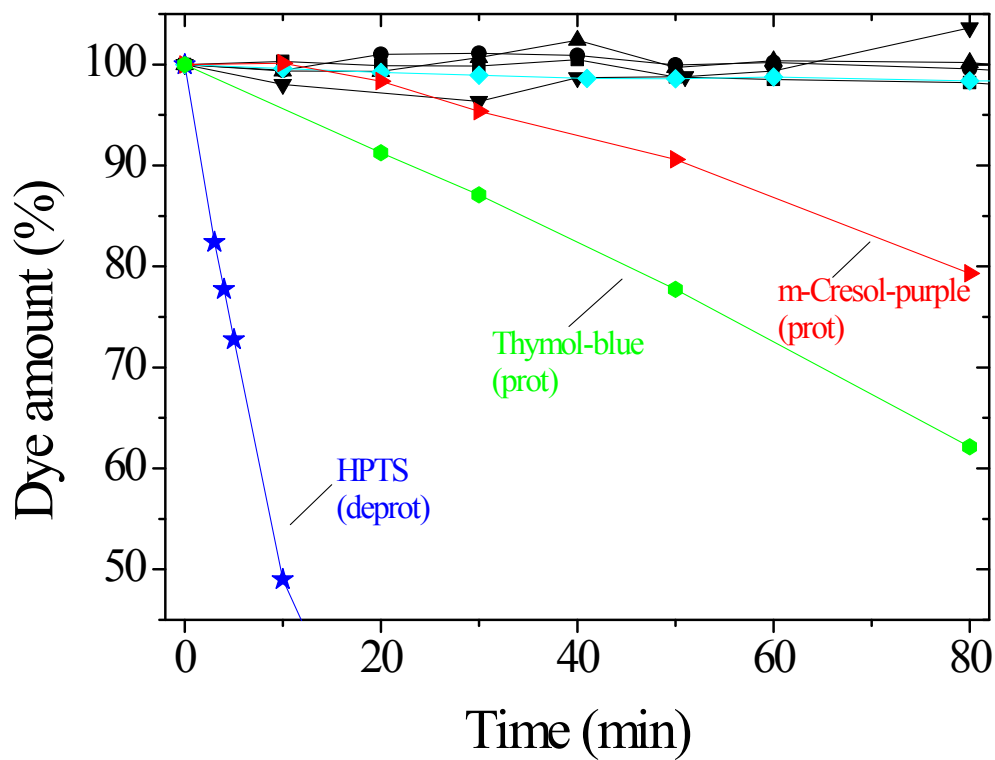


Figure S1. Photodegradation profiles for carbon dioxide sensors (EC49; base: TOAOH; T=25°C) based on the di-OH-aza-BODIPY dyes (black), m-cresol-purple (red triangles), thymol-blue (green dots) obtained from the absorption spectra of the respective neutral form and the absorption spectra of the deprotonated forms of the di-Cl-di-OH-complex (cyan) and HPTS(TOA)₃ (blue stars).

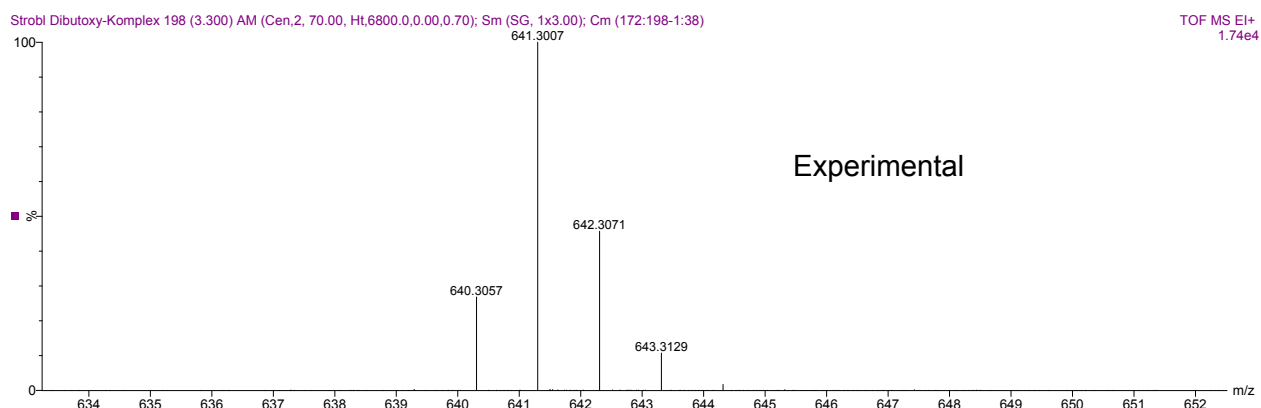
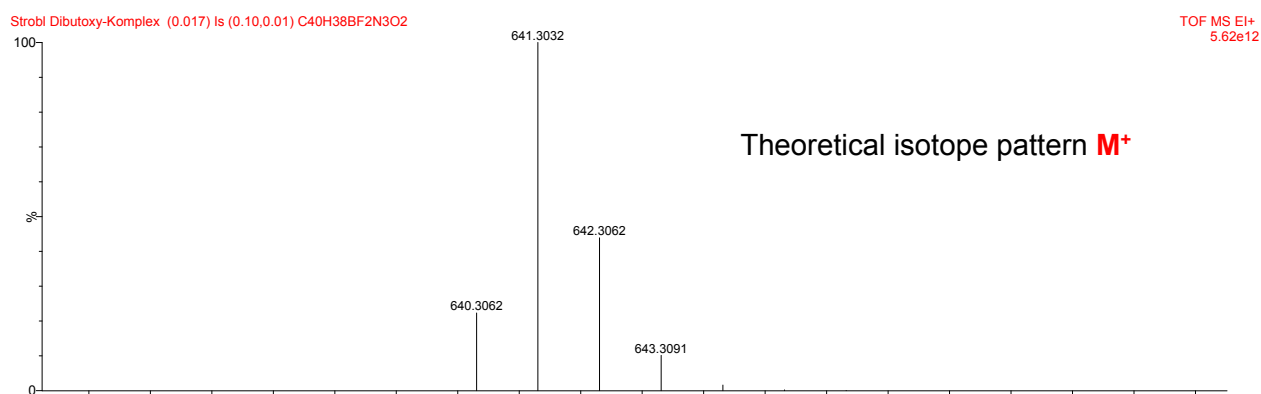
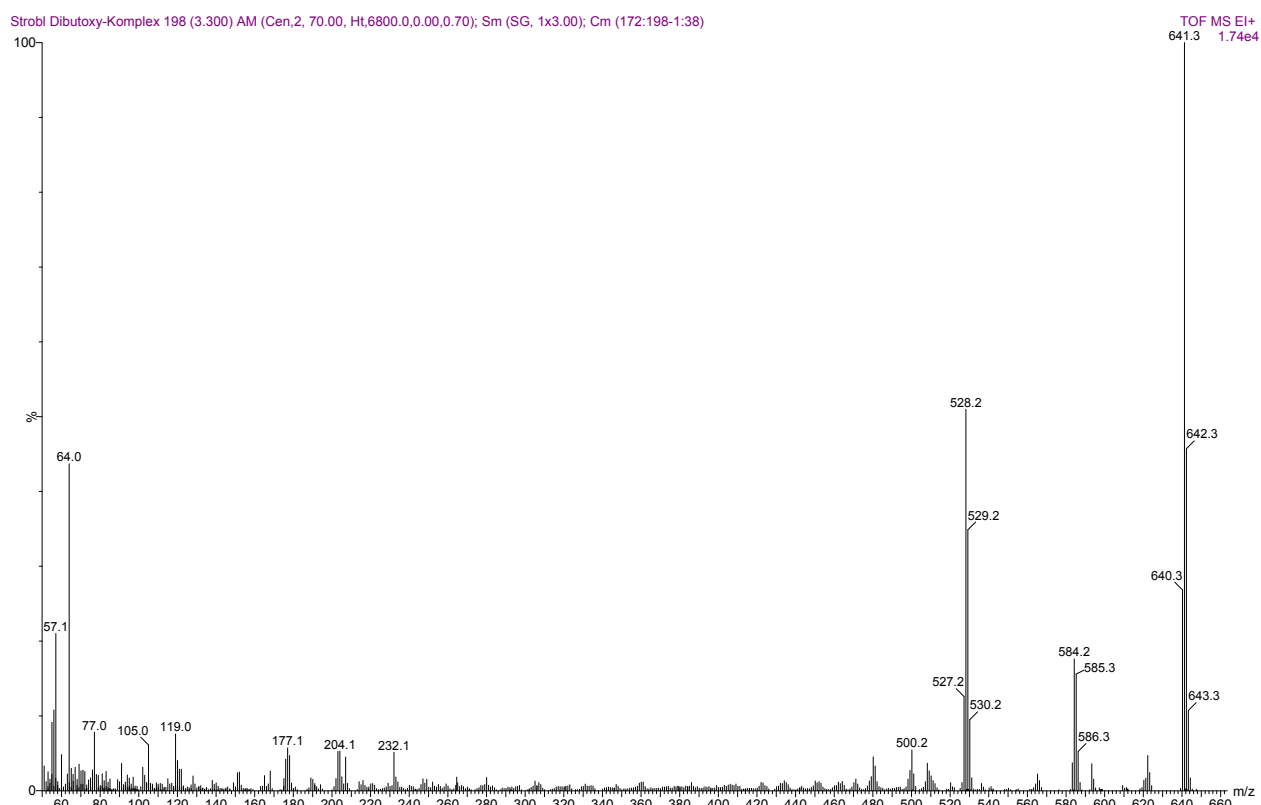


Figure S2. EI-DI Mass spectrum of 3,7-bis(4-butoxyphenyl)-5,5-difluoro-1,9-diphenyl-5*H*-4 λ^4 ,5 λ^4 -dipyrrolo[1,2-*c*:2',1'-*f*][1,3,5,2]triazaborinine (di-butoxy-complex).

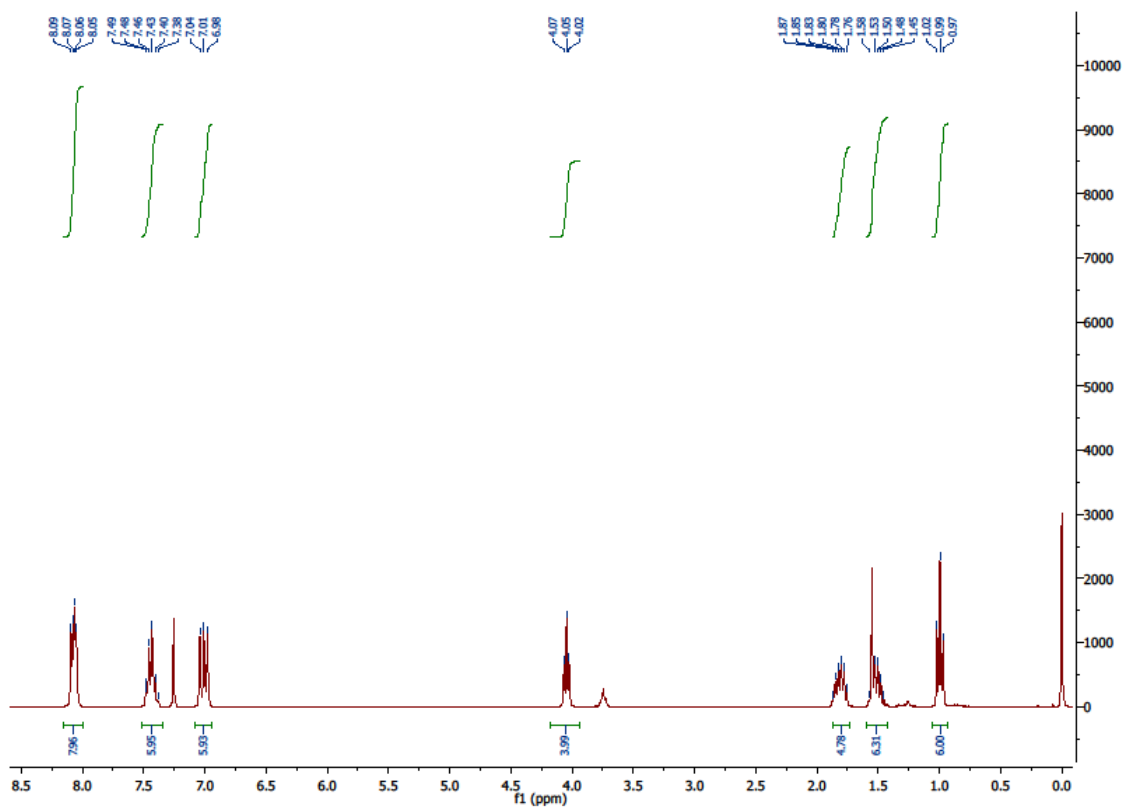


Figure S3. ¹H NMR of 3,7-bis(4-butoxyphenyl)-5,5-difluoro-1,9-diphenyl-5H-4λ⁴,5λ⁴-dipyrrolo[1,2-c:2',1'-f][1,3,5,2]triazaborinine (di-butoxy-complex).

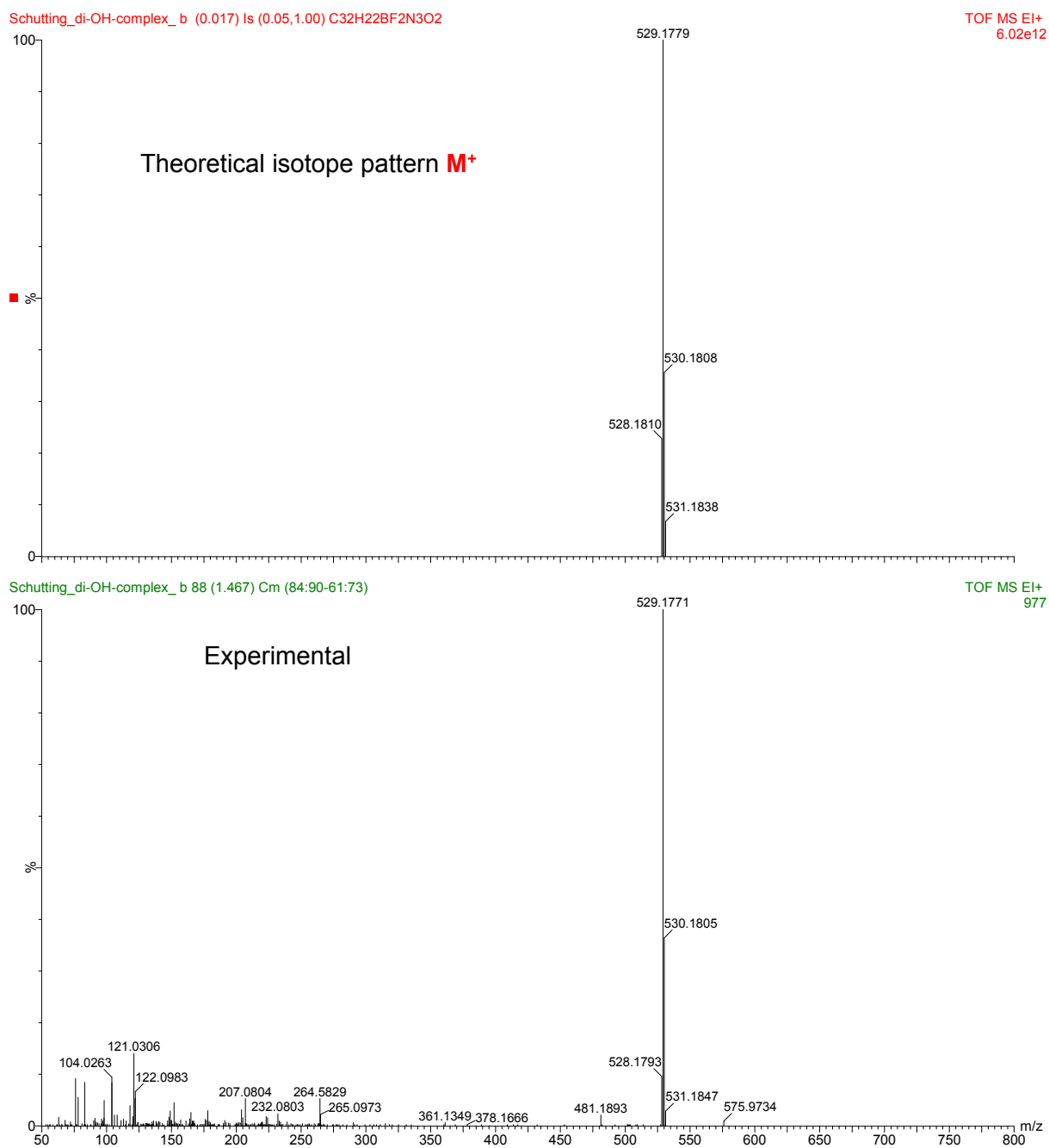


Figure S4. EI-DI Mass spectrum of 4,4'-(5,5-difluoro-1,9-diphenyl-5*H*-4λ⁴,5λ⁴-dipyrrolo[1,2-*c*:2',1'-*f*][1,3,5,2]triazaborinine-3,7-diyl)diphenol (di-OH-complex).

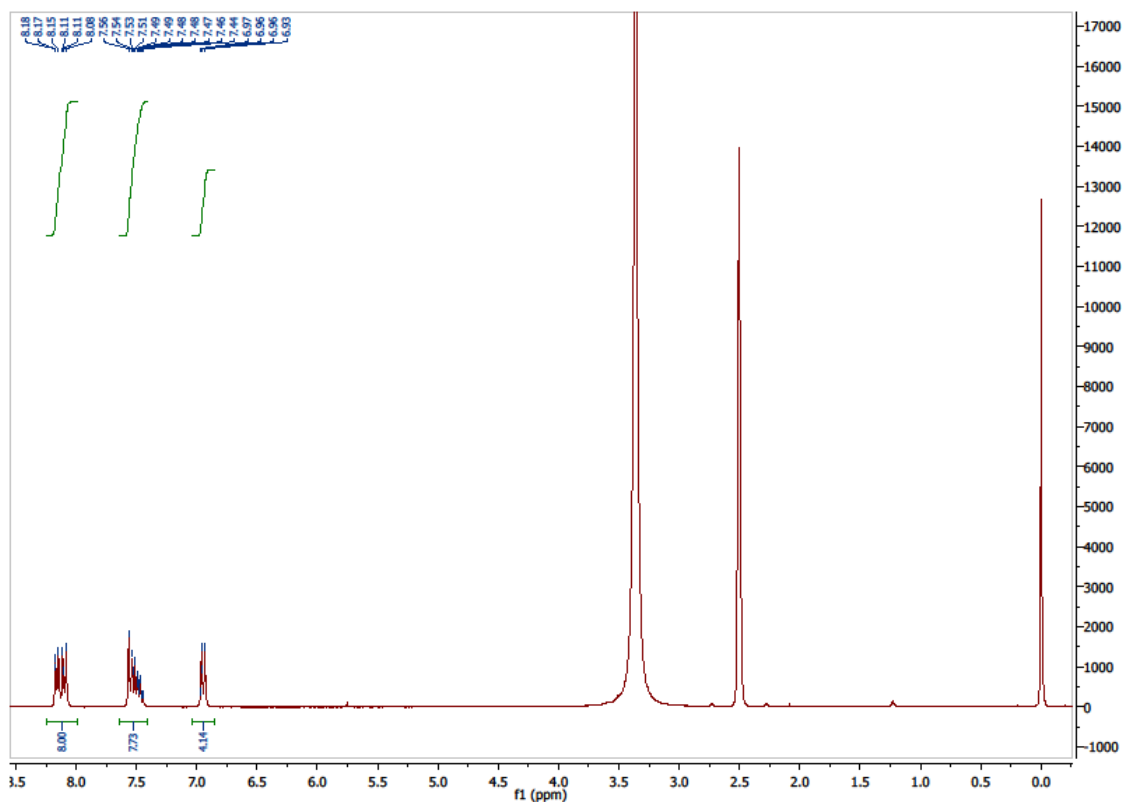


Figure S5. ^1H NMR of 4,4'-(5,5-difluoro-1,9-diphenyl-5H-4 λ^4 ,5 λ^4 -dipyrrolo[1,2-c:2',1'-f][1,3,5,2]triazaborinine-3,7-diyl)diphenol (di-OH-complex).

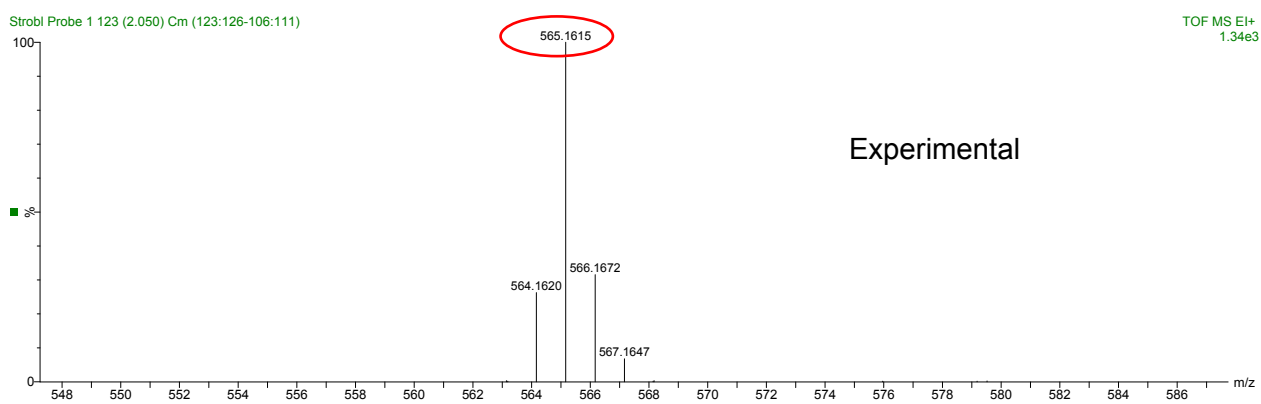
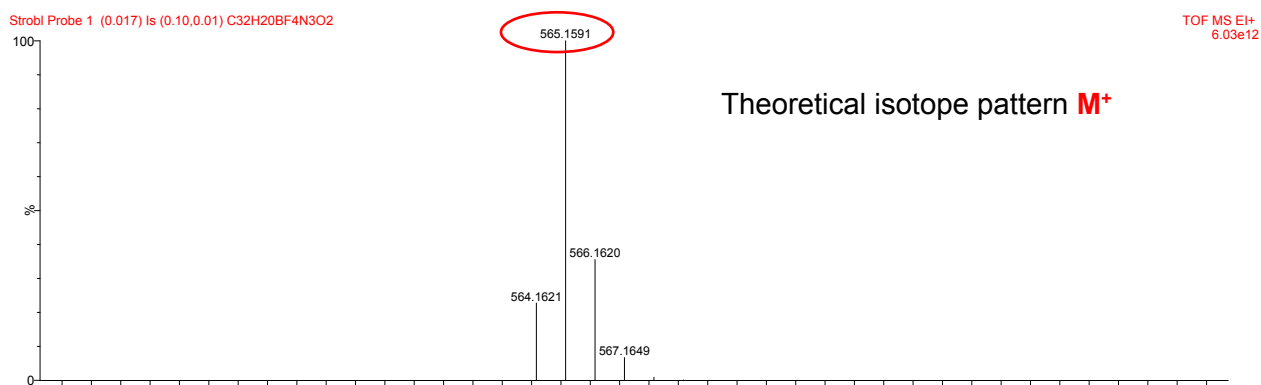
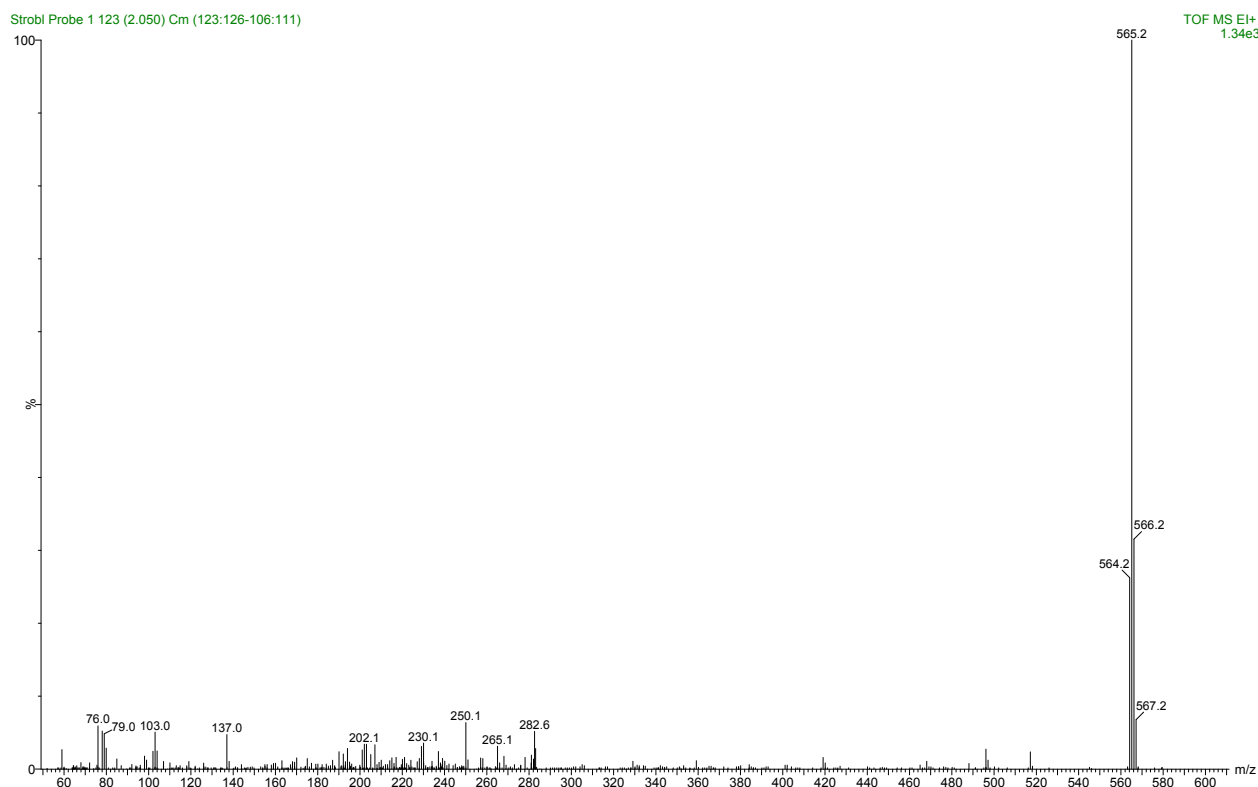


Figure S6. DI-EI Mass spectrum of 4,4'-(5,5-difluoro-1,9-diphenyl-5*H*-4 λ^4 ,5 λ^4 -dipyrrolo[1,2-*c*:2',1'-*f*][1,3,5,2]triazaborinine-3,7-diyl)bis(3-fluorophenol) (di-F-di-OH-complex).

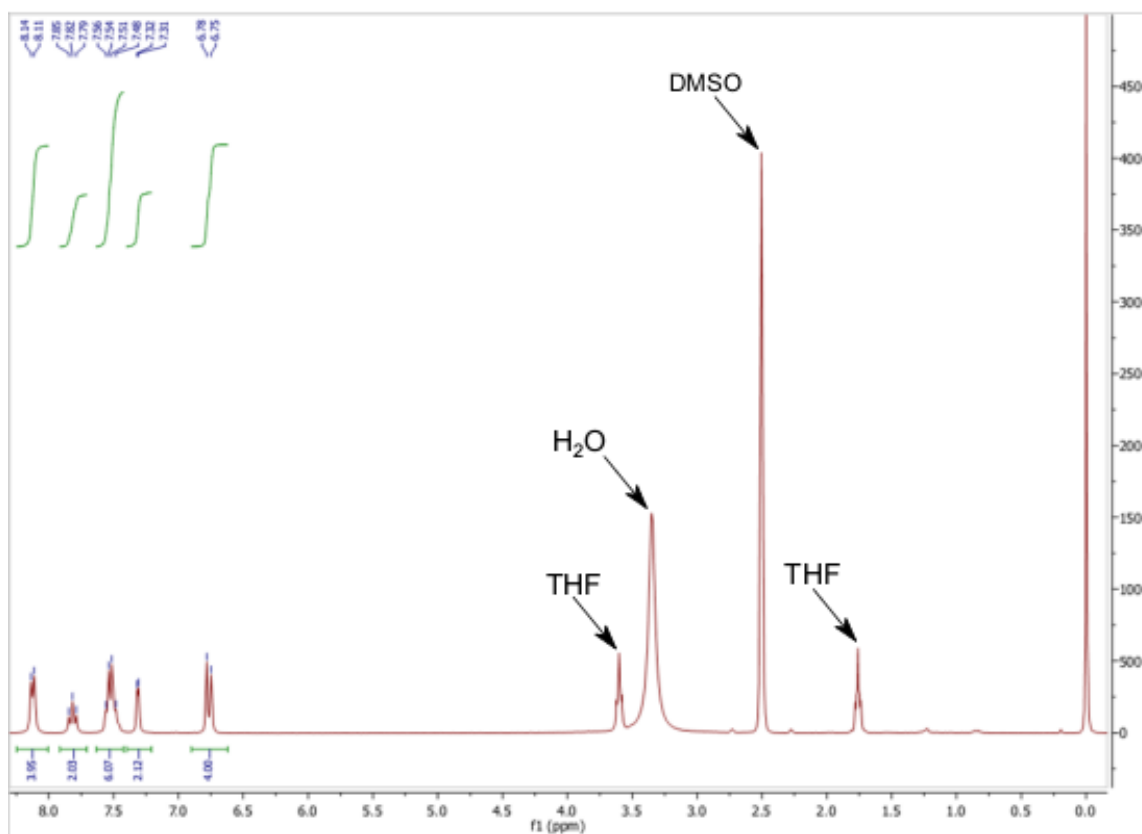


Figure S7. ¹H NMR of 4,4'-(5,5-difluoro-1,9-diphenyl-5H-4λ⁴,5λ⁴-dipyrrolo[1,2-c:2',1'-f][1,3,5,2]triazaborinine-3,7-diyl)bis(3-fluorophenol) (di-F-di-OH-complex).

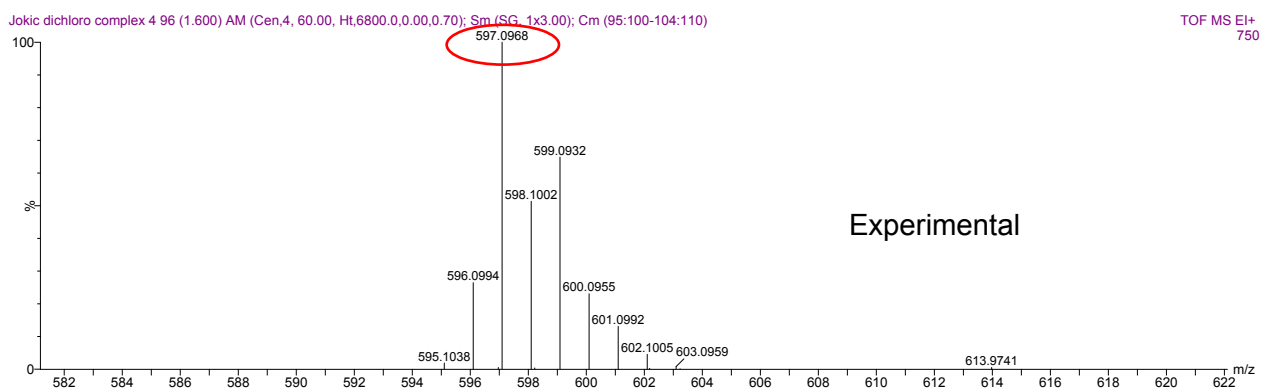
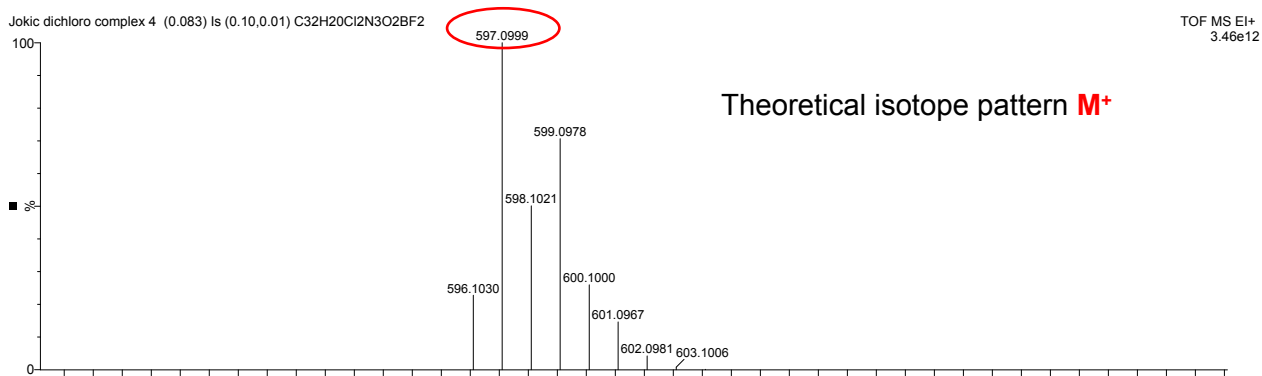
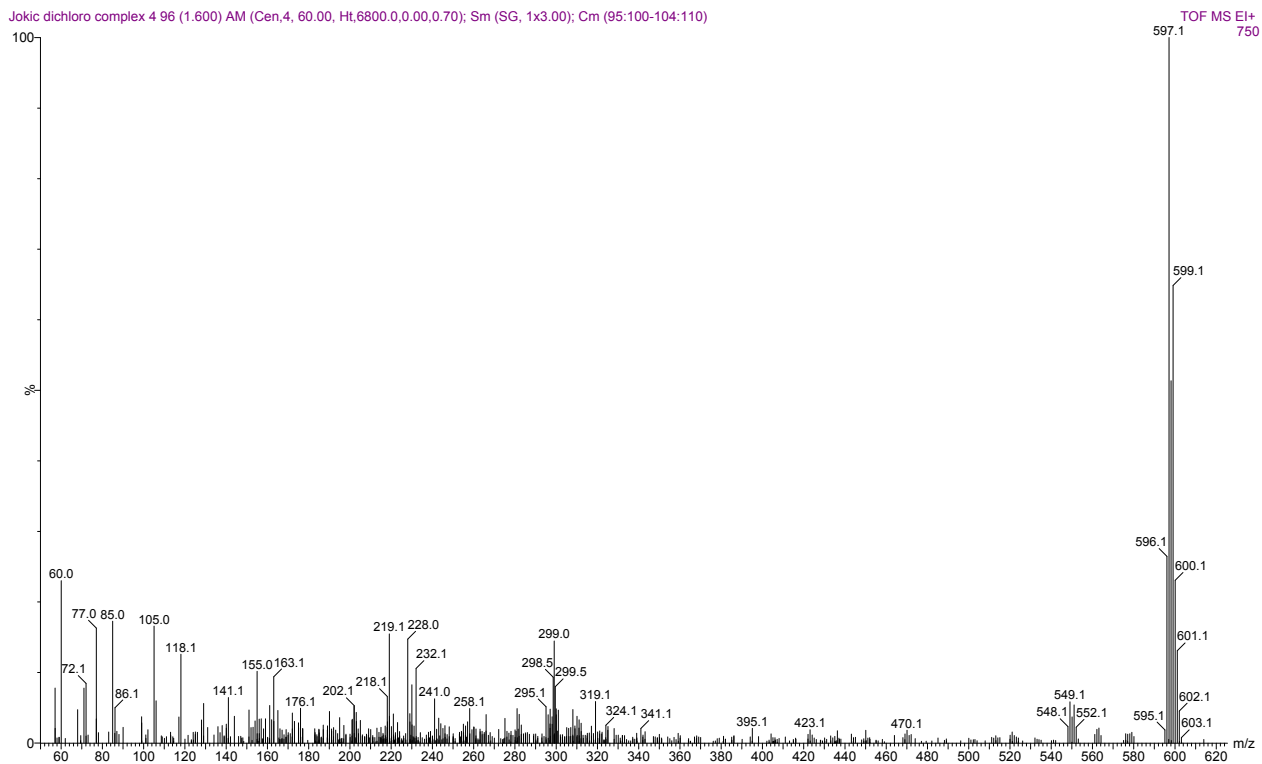


Figure S8. EI-DI Mass spectrum of 4,4'-(5,5-difluoro-1,9-diphenyl-5*H*-4 λ^4 ,5 λ^4 -dipyrrolo[1,2-*c*:2',1'-*f*][1,3,5,2]triazaborinine-3,7-diyl)bis(2-chlorophenol) (di-Cl-di-OH-complex).

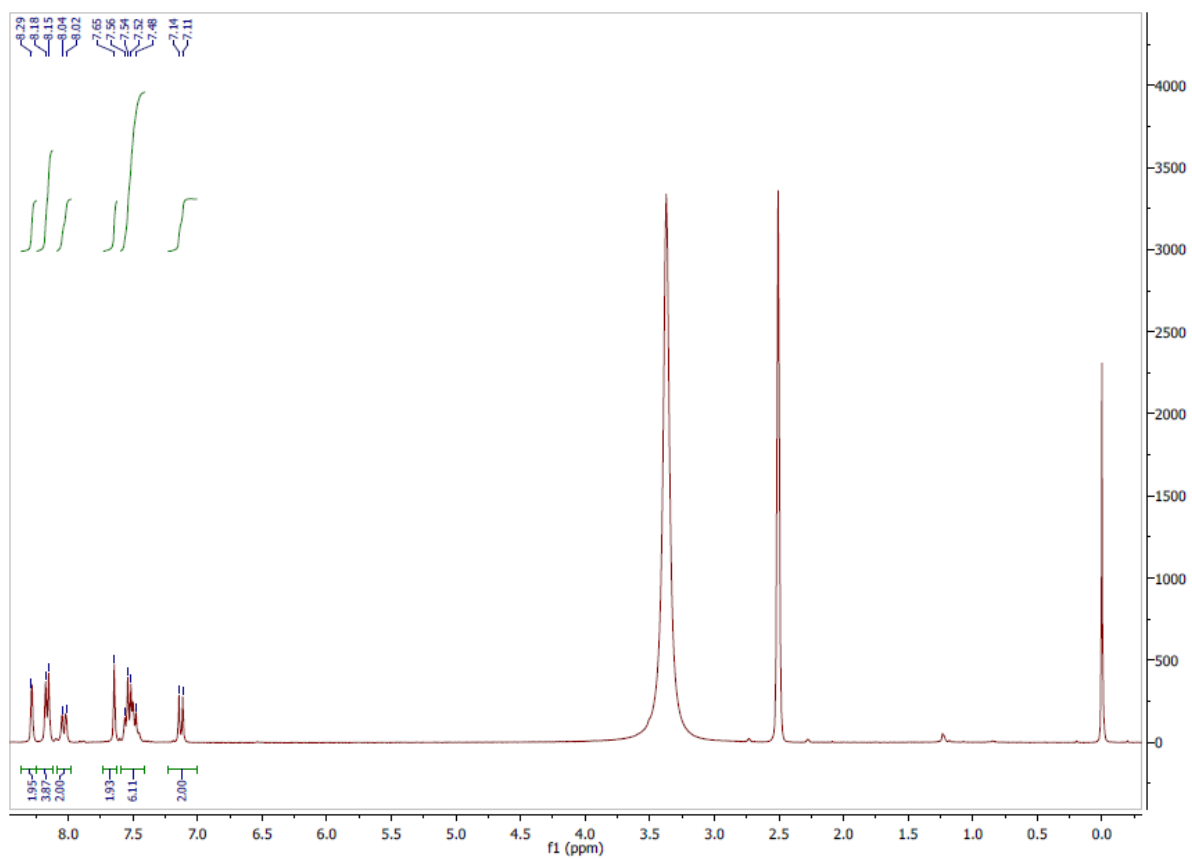


Figure S9. ¹H NMR of 4,4'-(5,5-difluoro-1,9-diphenyl-5H-4λ⁴,5λ⁴-dipyrrolo[1,2-c:2',1'-f][1,3,5,2]triazaborinine-3,7-diyl)bis(2-chlorophenol) (di-Cl-di-OH-complex).

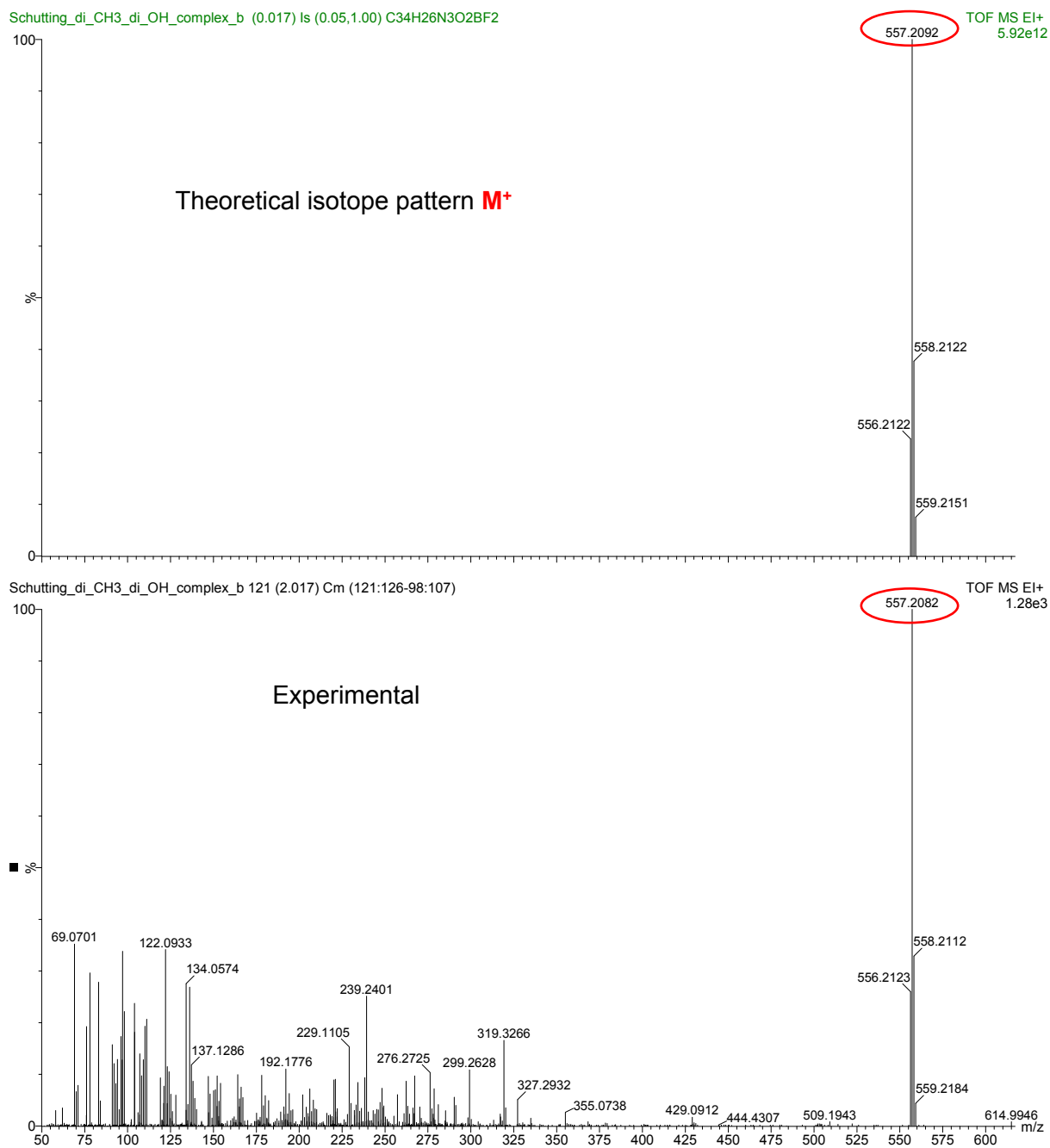


Figure S10. EI-DI Mass spectrum of 4,4'-(5,5-difluoro-1,9-diphenyl-5*H*-4 λ ,5 λ -dipyrrolo[1,2-*c*:2',1'-*f*][1,3,5,2]triazaborinine-3,7-diyl)bis(2-methylphenol) (di-CH₃-di-OH-complex).

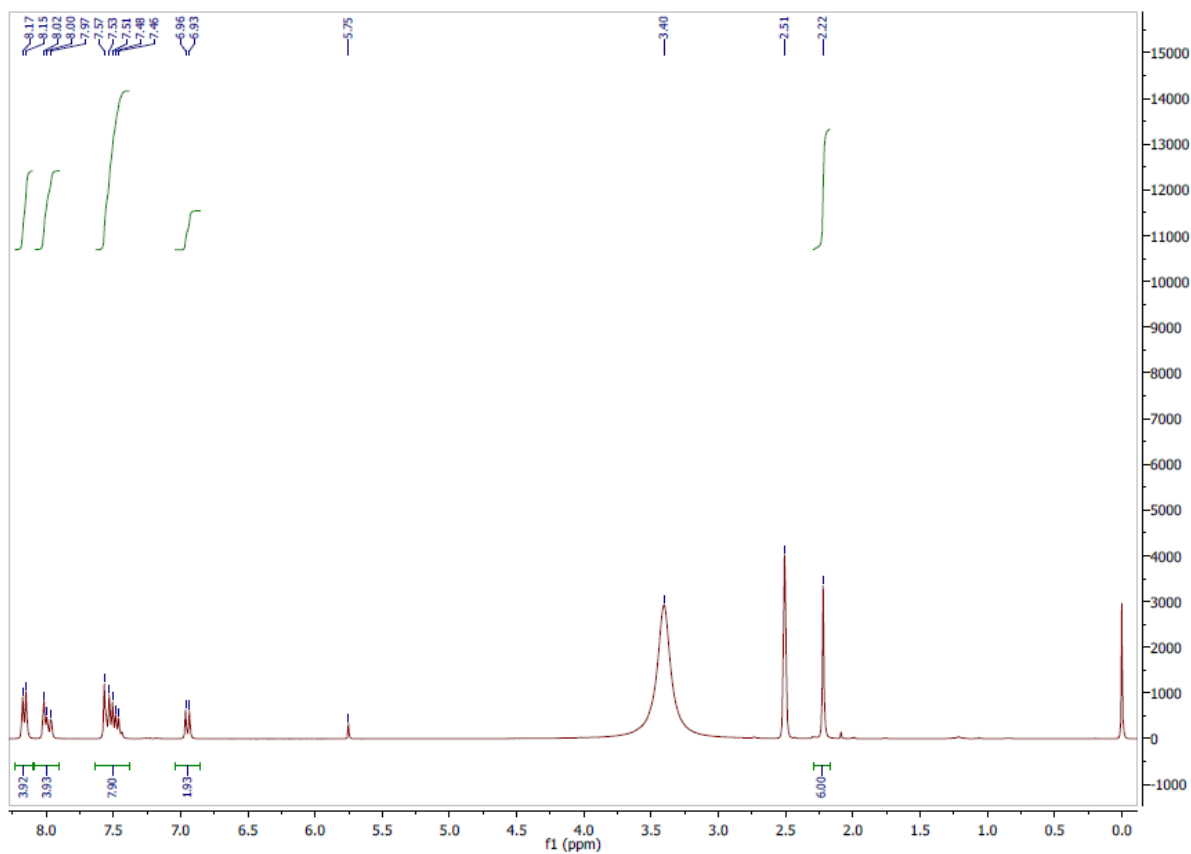


Figure S11. ¹H NMR of 4,4'-(5,5-difluoro-1,9-diphenyl-5H-4λ⁴,5λ⁴-dipyrrolo[1,2-c:2',1'-f][1,3,5,2]triazaborinine-3,7-diyl)bis(2-methylphenol) (di-CH₃-di-OH-complex).