

Supplementary materials

Multicomponent Synthesis of New Fluorescent Boron Complexes Derived from 3-Hydroxy-1-phenyl-1H-pyrazole-4-carbaldehyde

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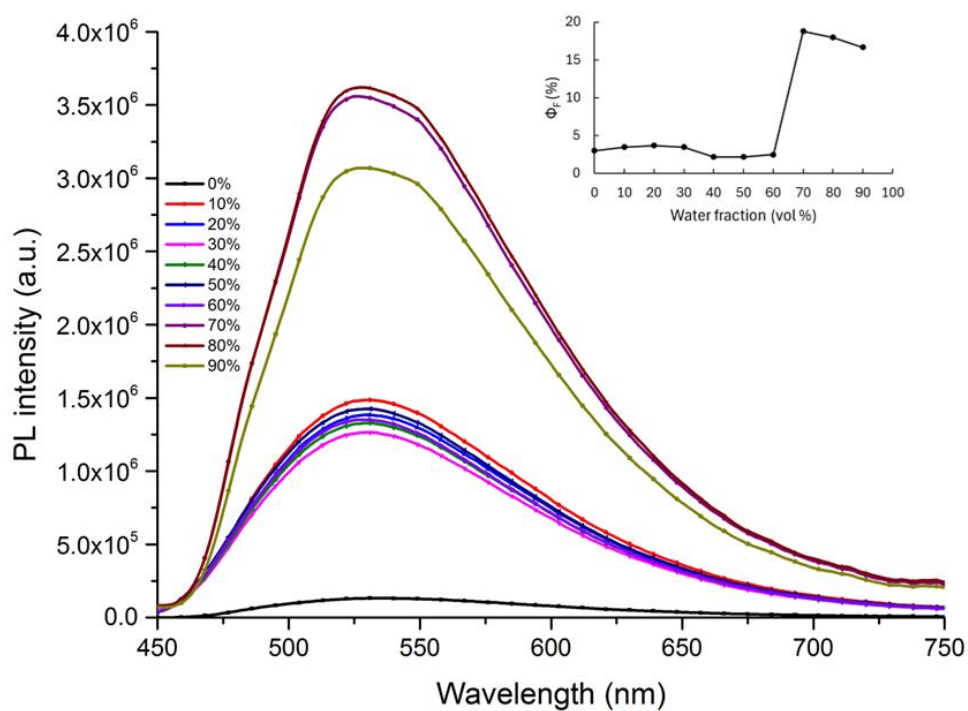


Figure S1. Fluorescence emission spectra of compound **4b** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.

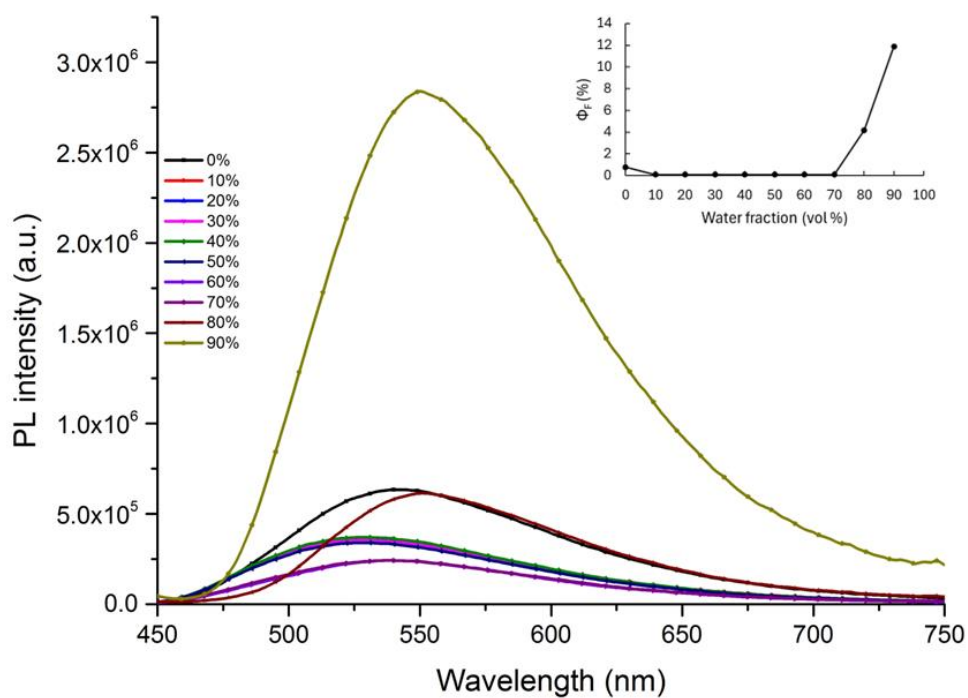


Figure S2. Fluorescence emission spectra of compound **4c** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.

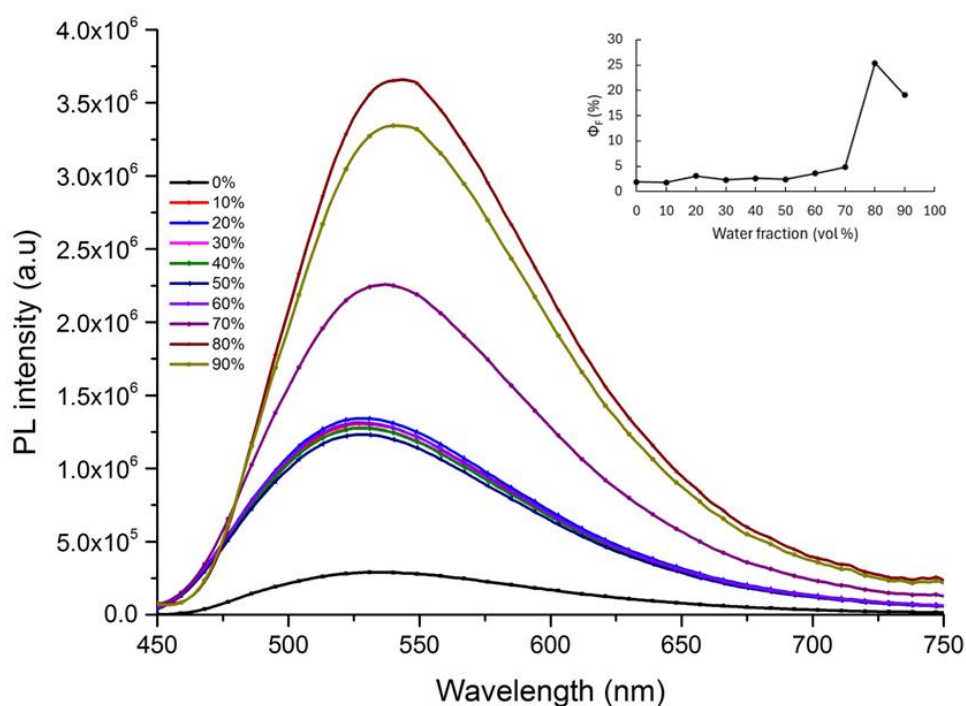


Figure S3. Fluorescence emission spectra of compound **4d** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.

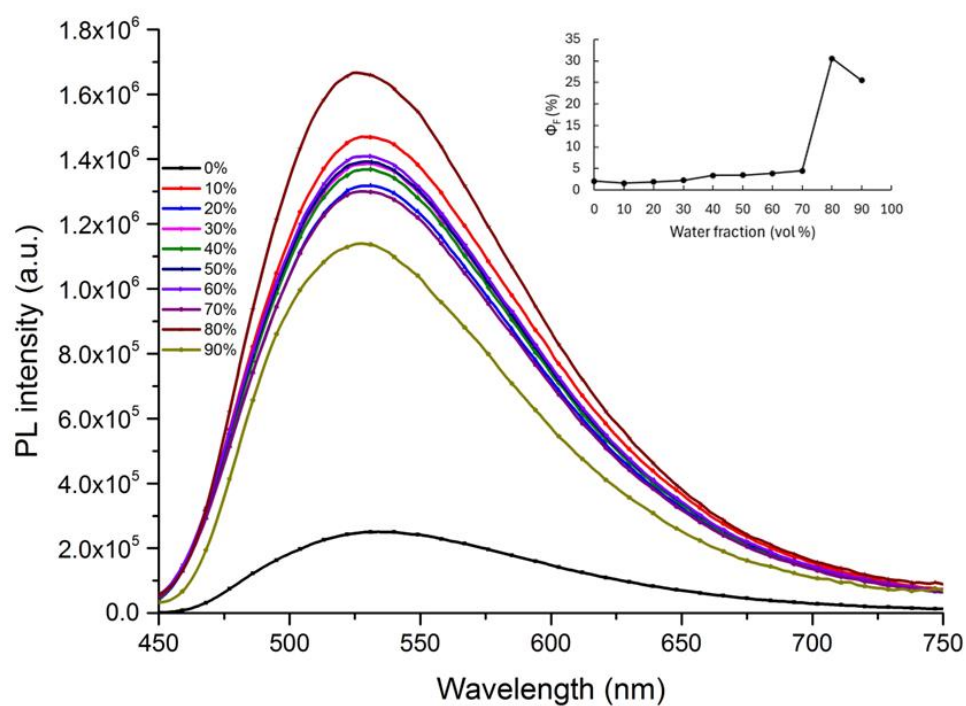


Figure S4. Fluorescence emission spectra of compound **4e** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.

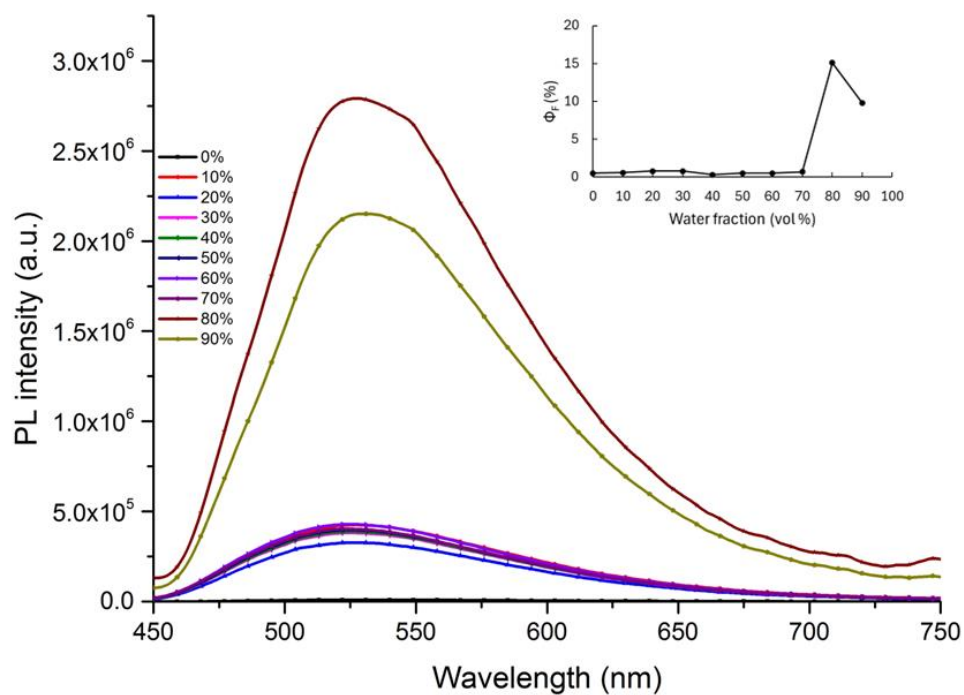


Figure S5. Fluorescence emission spectra of compound **4f** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.

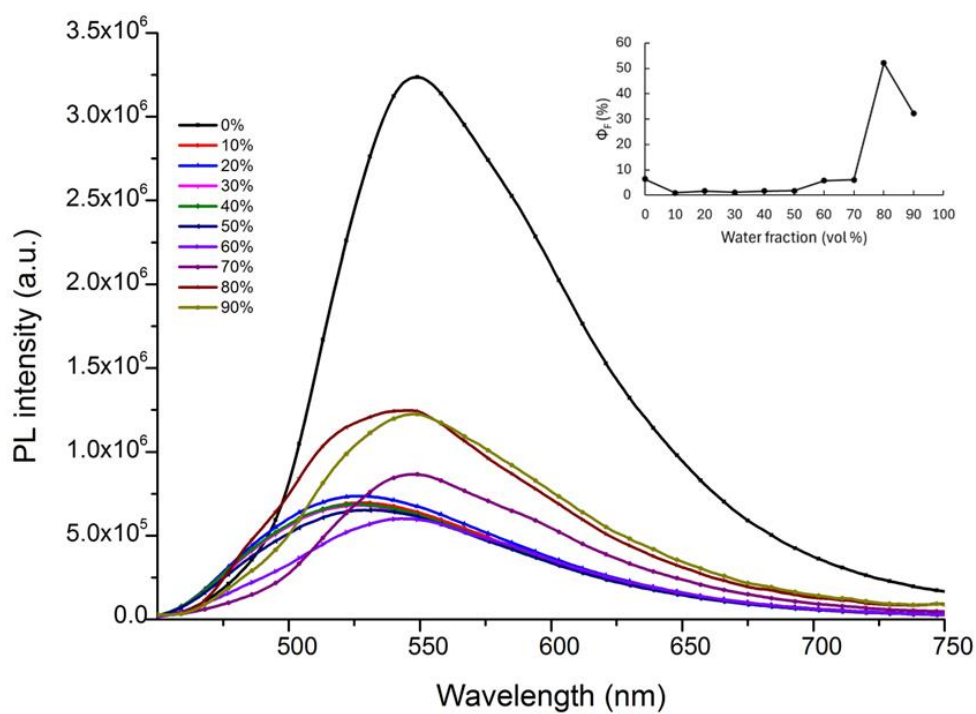


Figure S6. Fluorescence emission spectra of compound **4g** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.

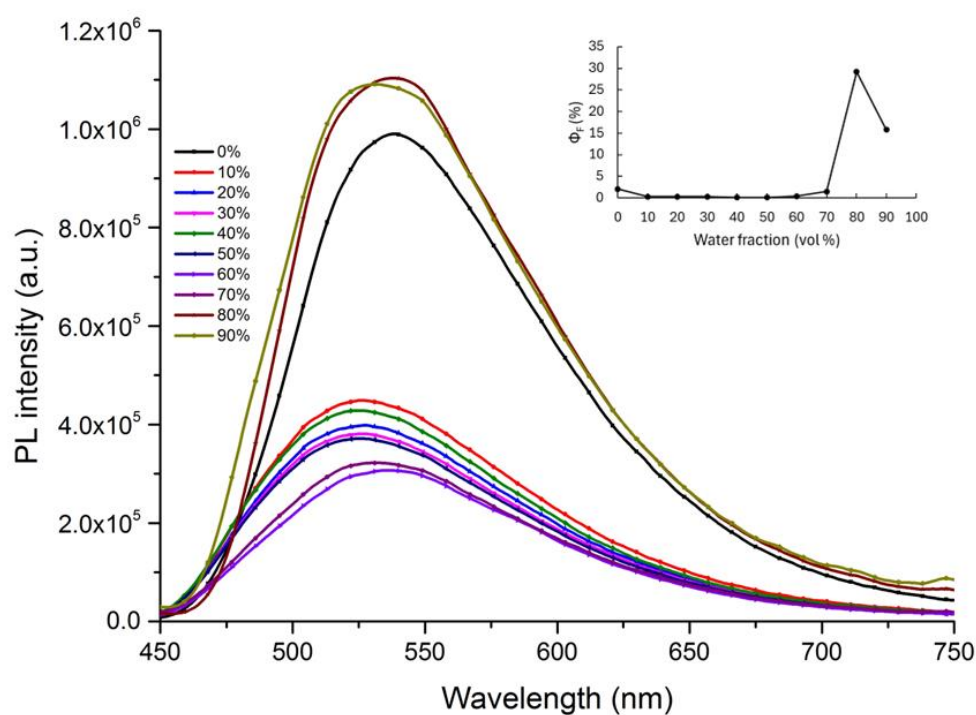


Figure S7. Fluorescence emission spectra of compound **4h** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.

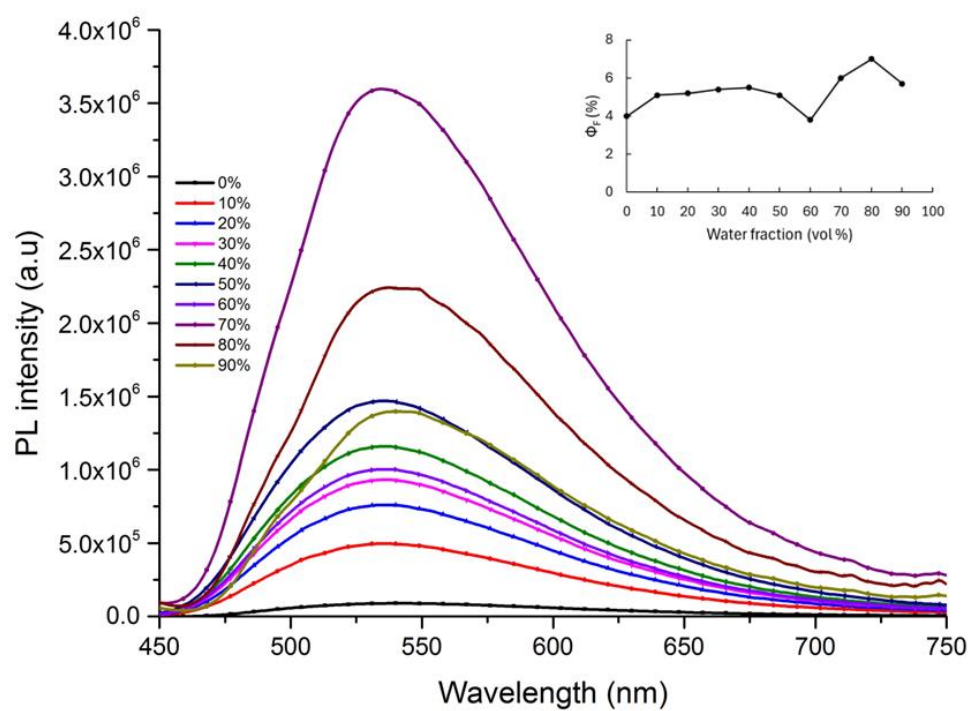


Figure S8. Fluorescence emission spectra of compound **4i** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction

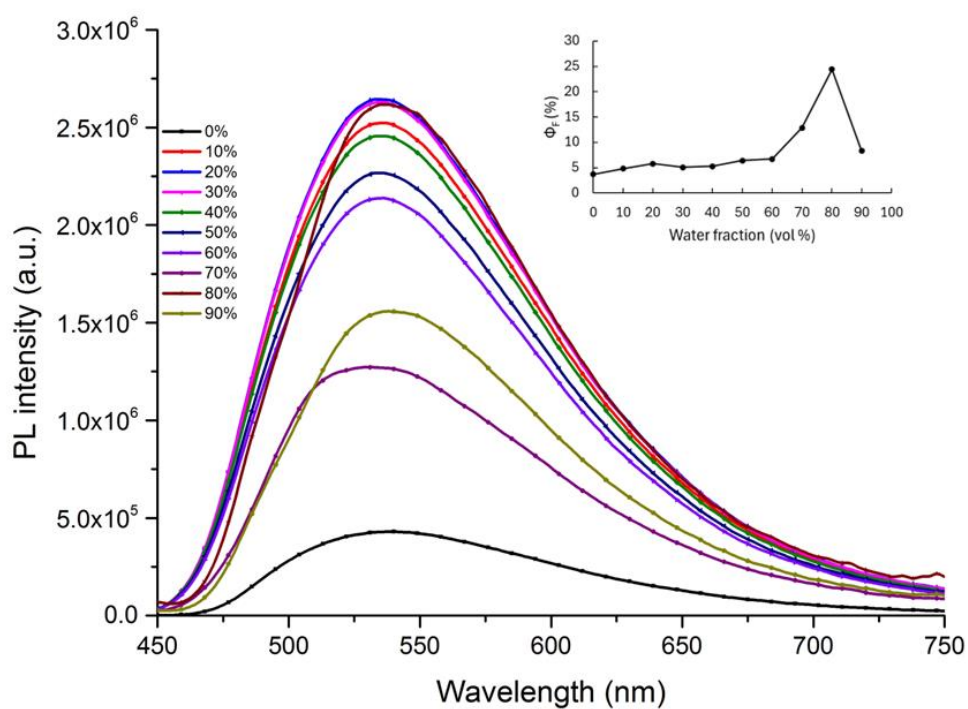


Figure S9. Fluorescence emission spectra of compound **4j** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.

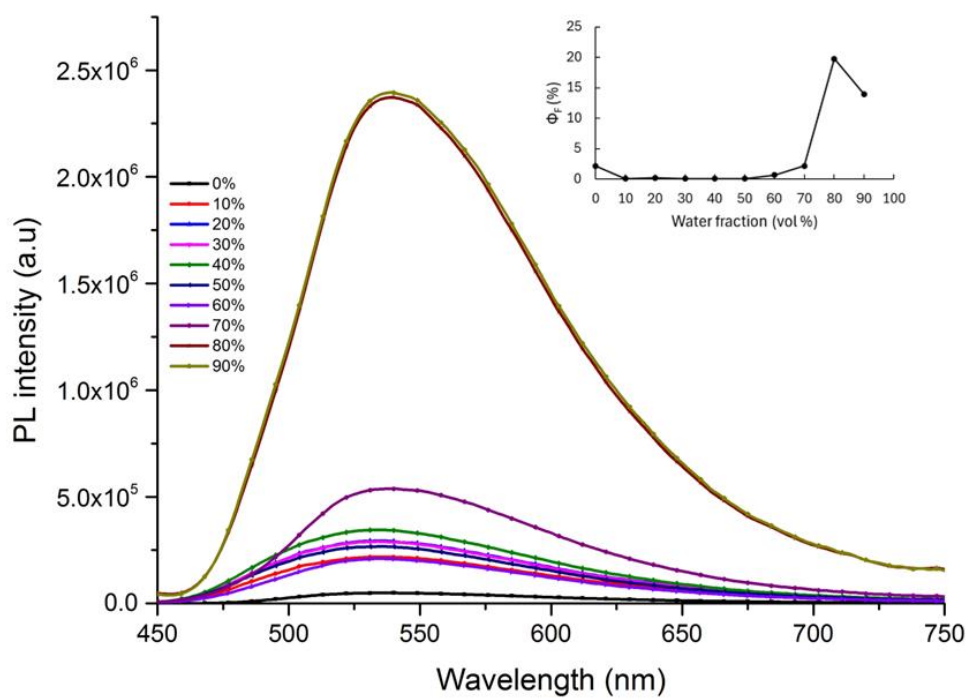


Figure S10. Fluorescence emission spectra of compound **4k** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.

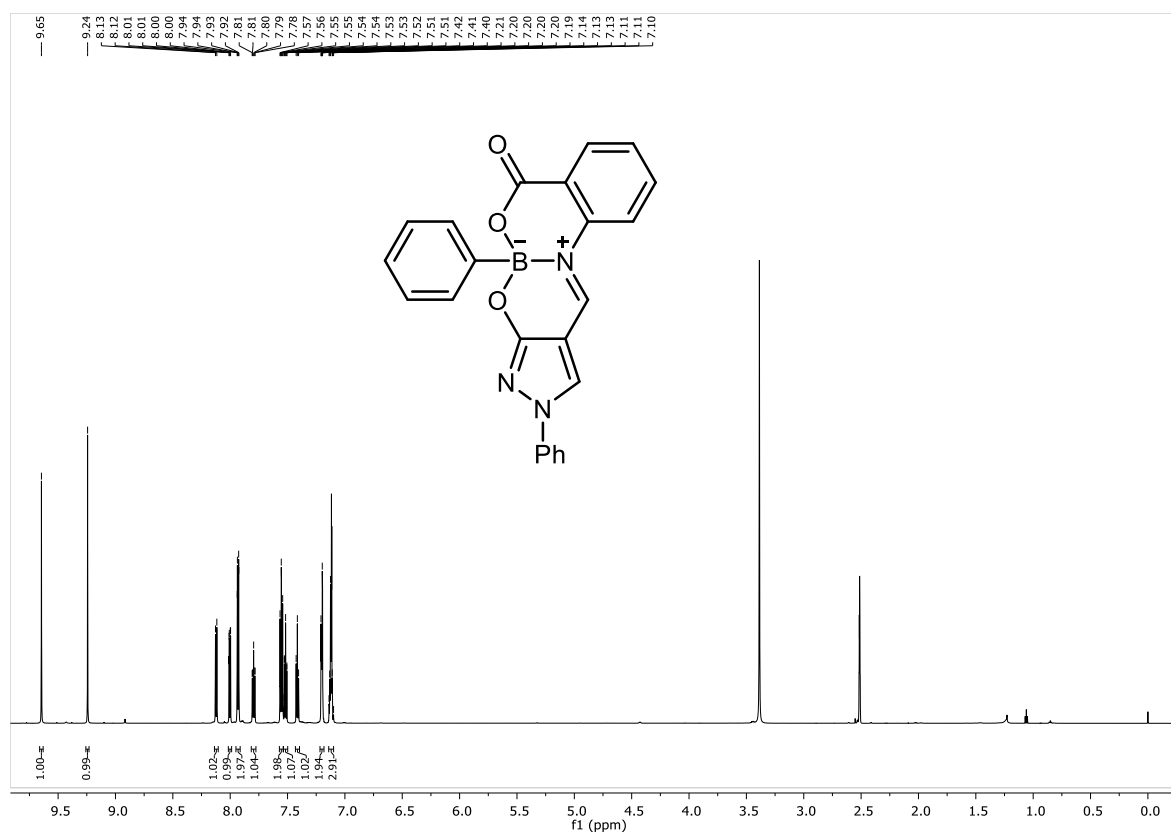


Figure S11. ^1H NMR (700 MHz, $\text{DMSO}-d_6$) spectrum of **4a**

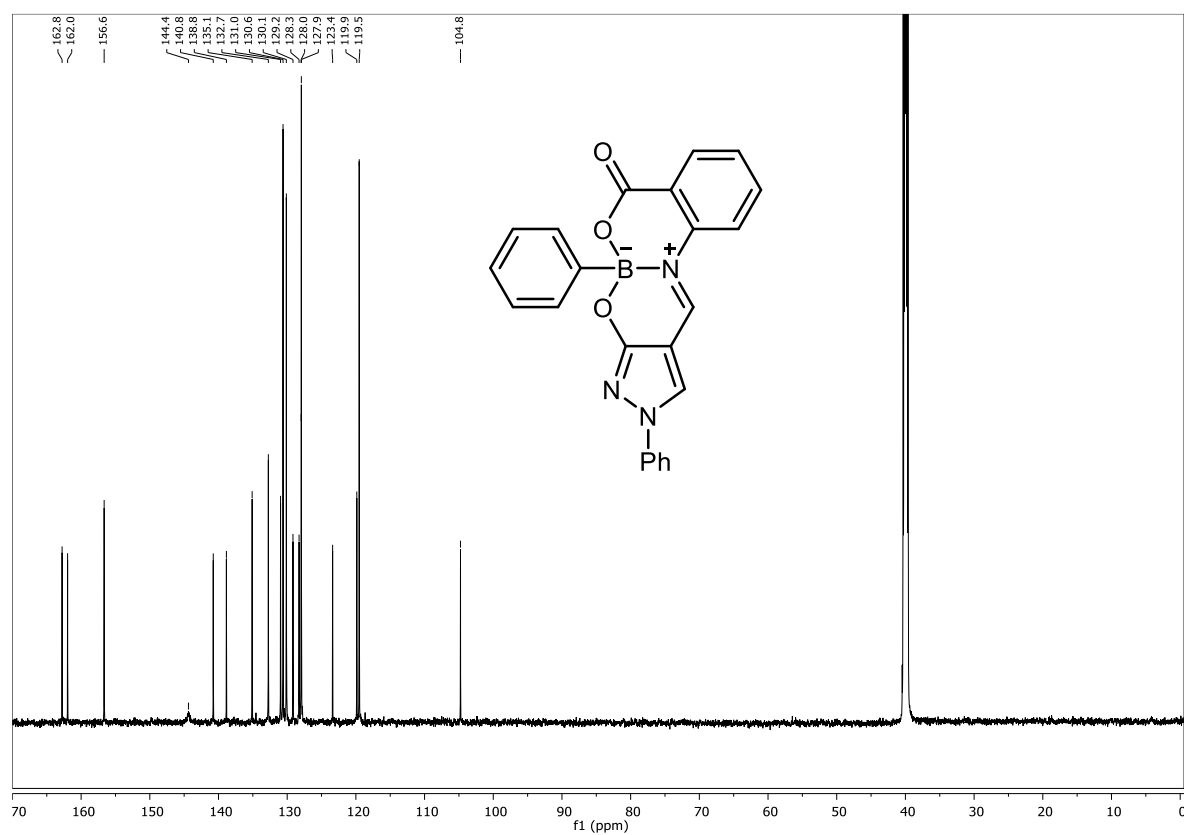


Figure S12. ^{13}C NMR (176 MHz, $\text{DMSO}-d_6$) spectrum of **4a**

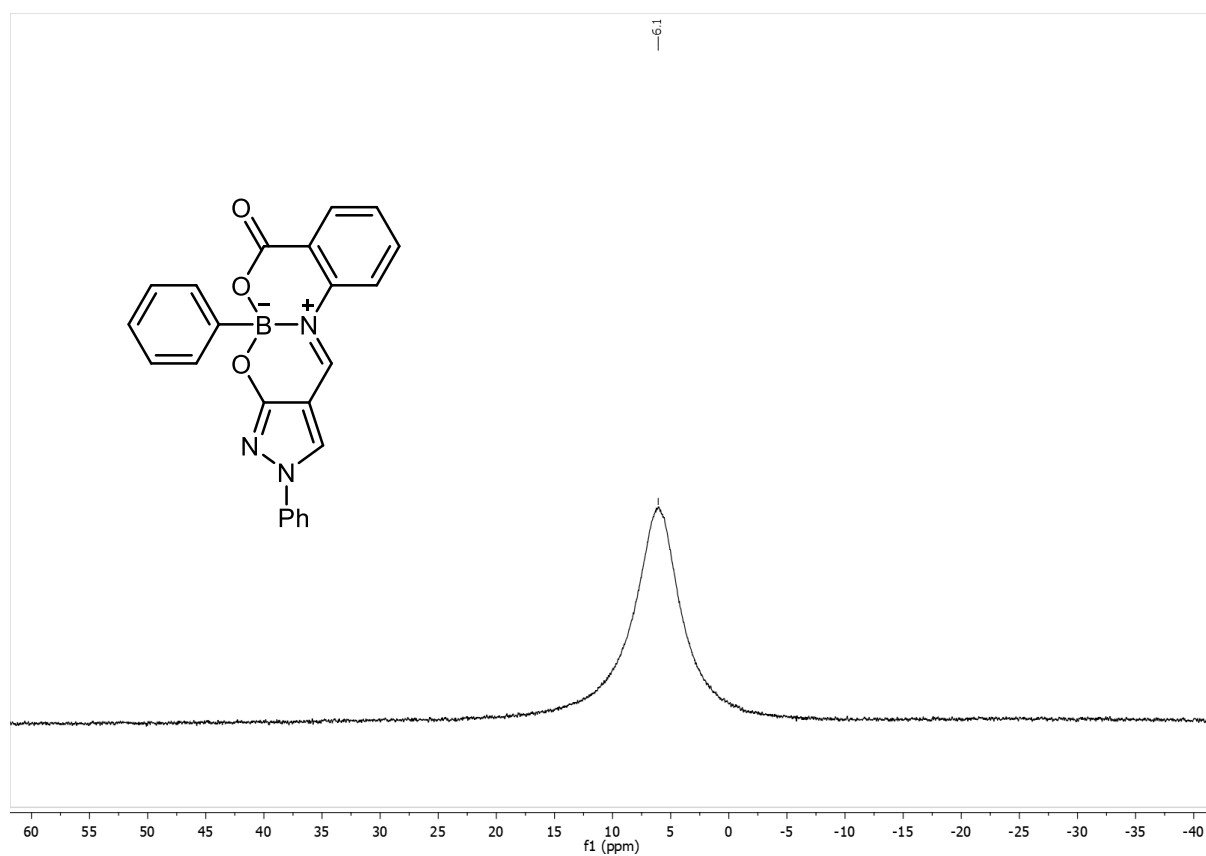


Figure S13. ^{11}B NMR (128 MHz, $\text{DMSO-}d_6$) spectrum of **4a**

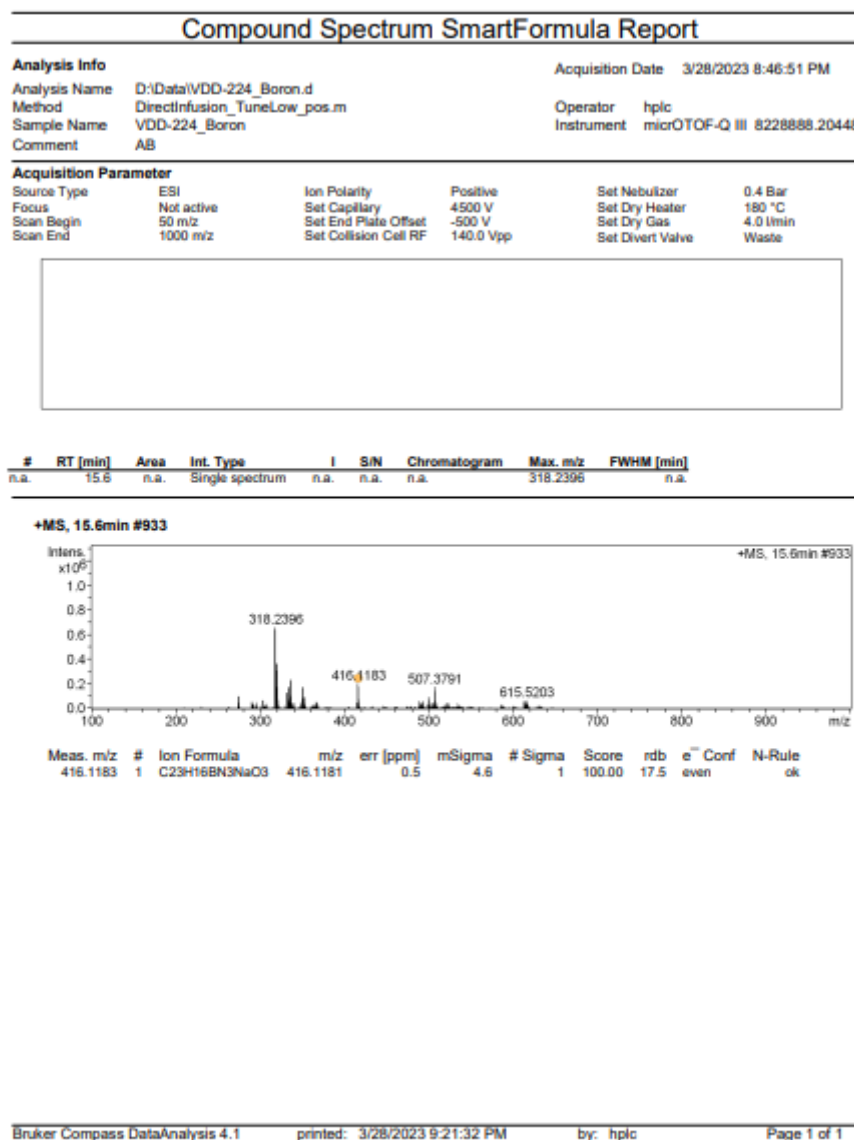


Figure S14. HRMS (ESI⁺) report of **4a**

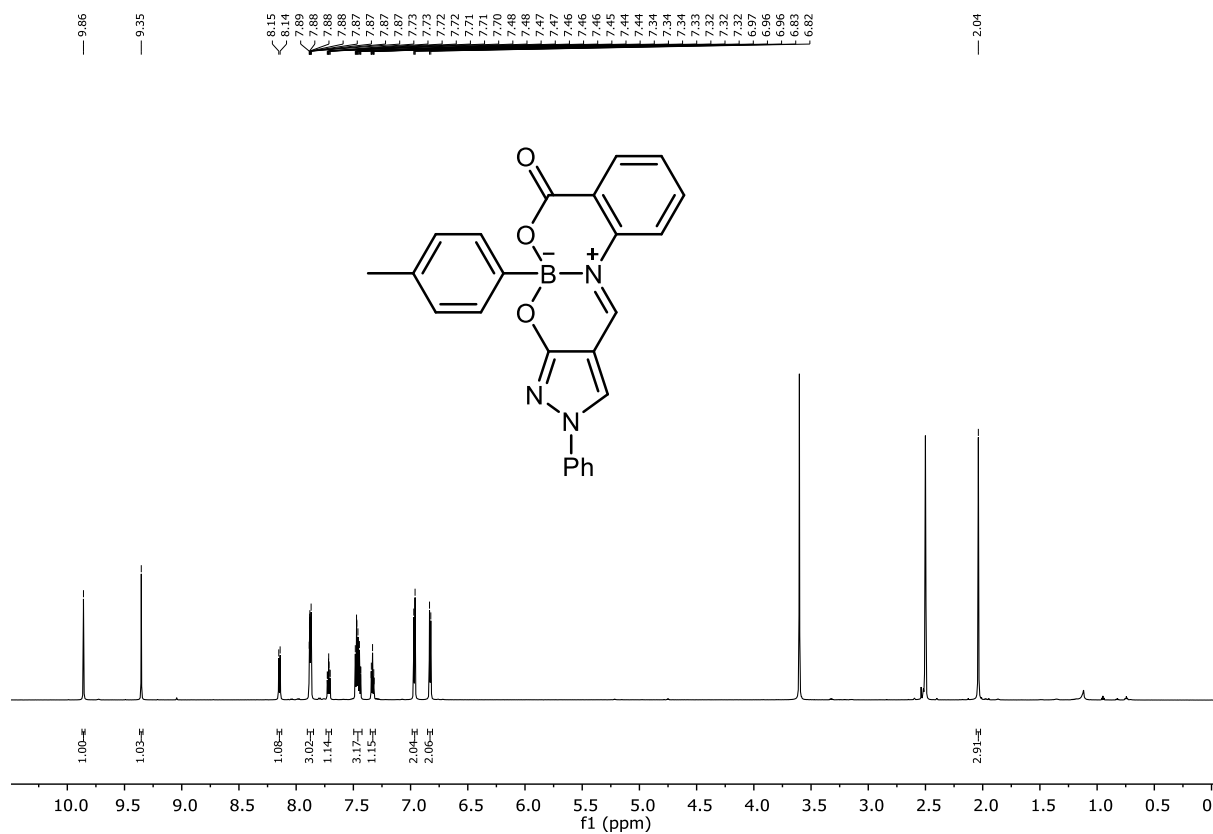


Figure S15. ¹H NMR (700 MHz, DMSO-*d*₆) spectrum of **4b**

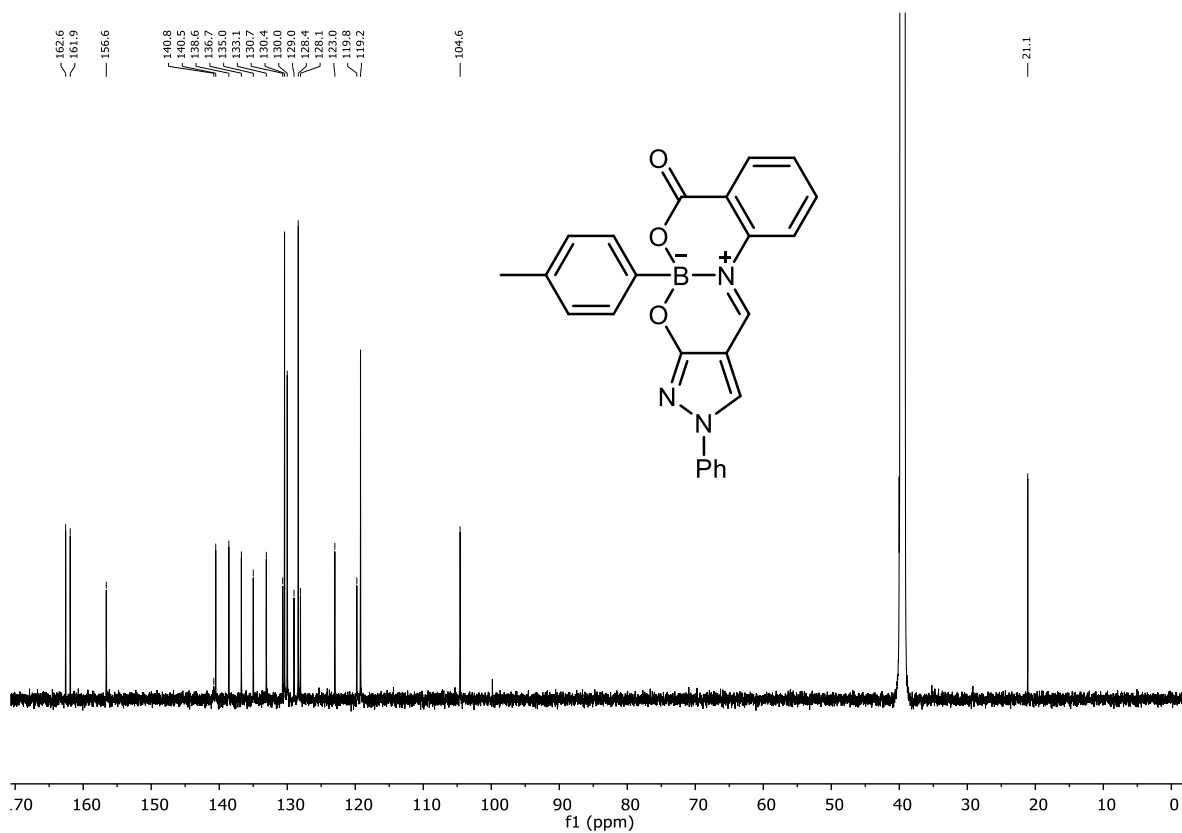


Figure S16. ¹³C NMR (176 MHz, DMSO-*d*₆) spectrum of **4b**

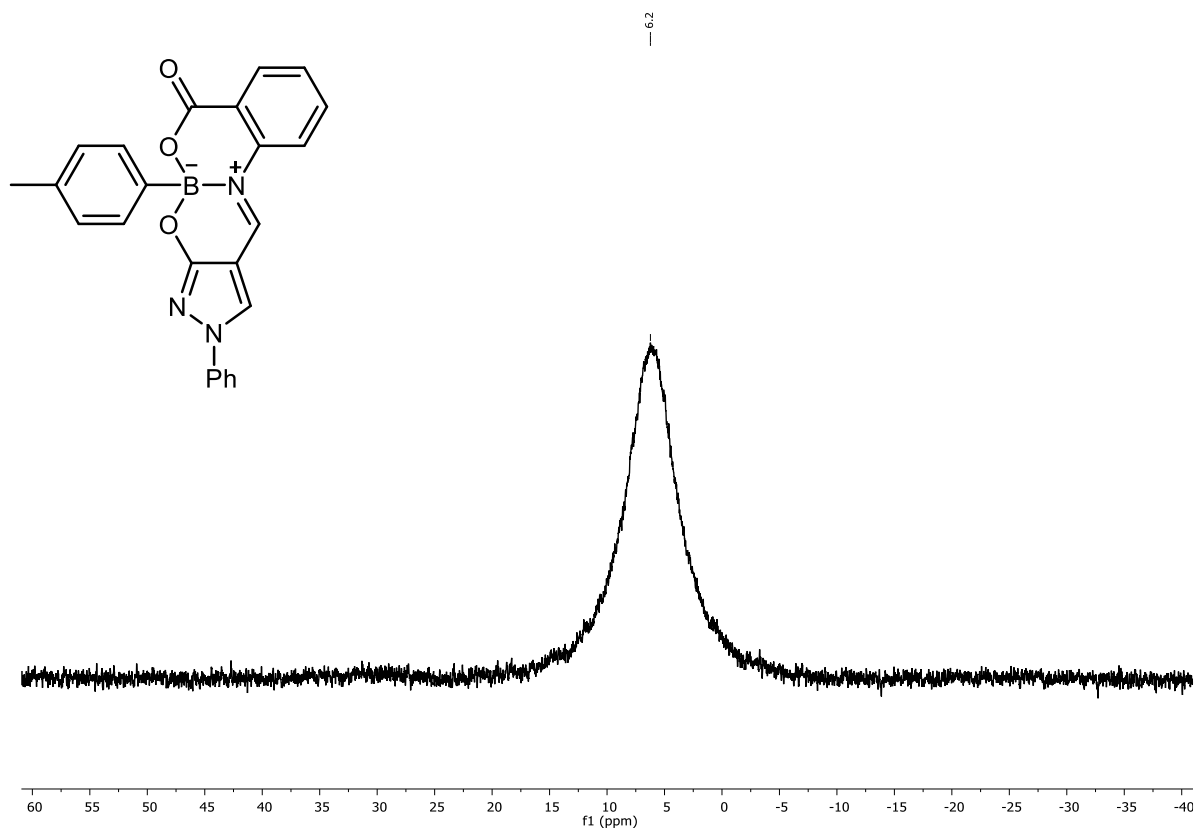


Figure S17. ^{11}B NMR (128 MHz, $\text{DMSO-}d_6$) spectrum of **4b**

Compound Spectrum SmartFormula Report

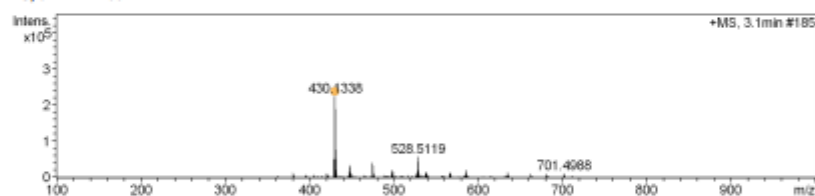
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Comment	AB		

Acquisition Parameter					
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Scan End	1000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste



#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	3.1	n.a.	Single spectrum	n.a.	n.a.	n.a.	430.1338	n.a.

+MS, 3.1min #185



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
430.1338	1	C ₂₄ H ₁₈ BN ₃ NaO ₃	430.1338	-0.1	2.7	1	100.00	17.5	even	ok

Figure S18. HRMS (ESI⁺) report of **4b**

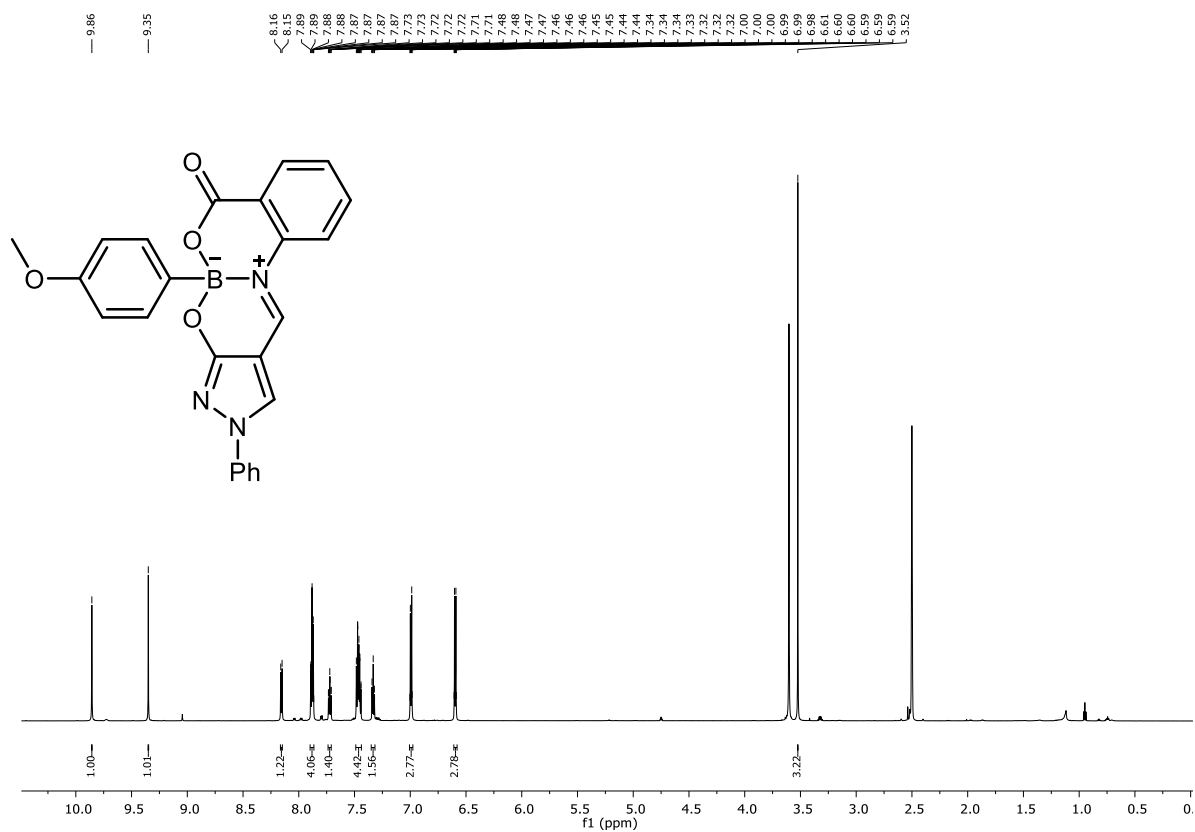


Figure S19. ^1H NMR (700 MHz, $\text{DMSO}-d_6$) spectrum of **4c**

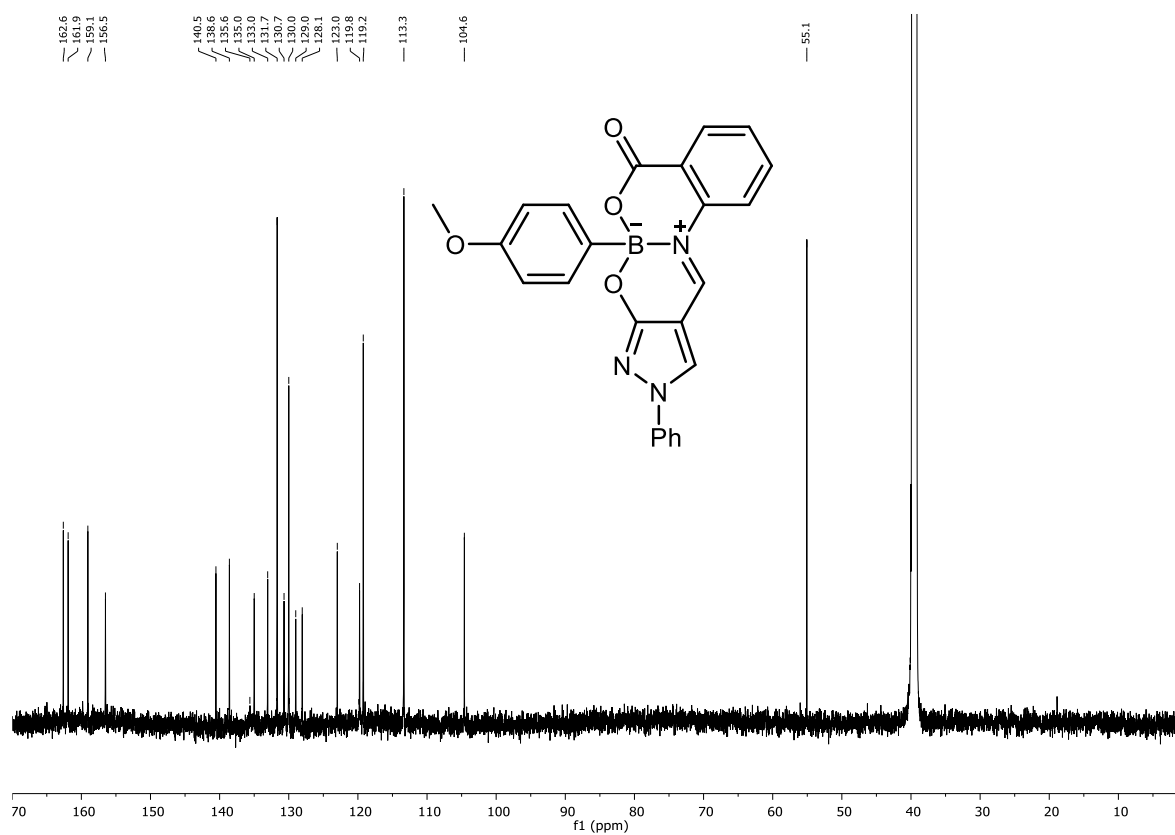


Figure S20. ^{13}C NMR (176 MHz, $\text{DMSO}-d_6$) spectrum of **4c**

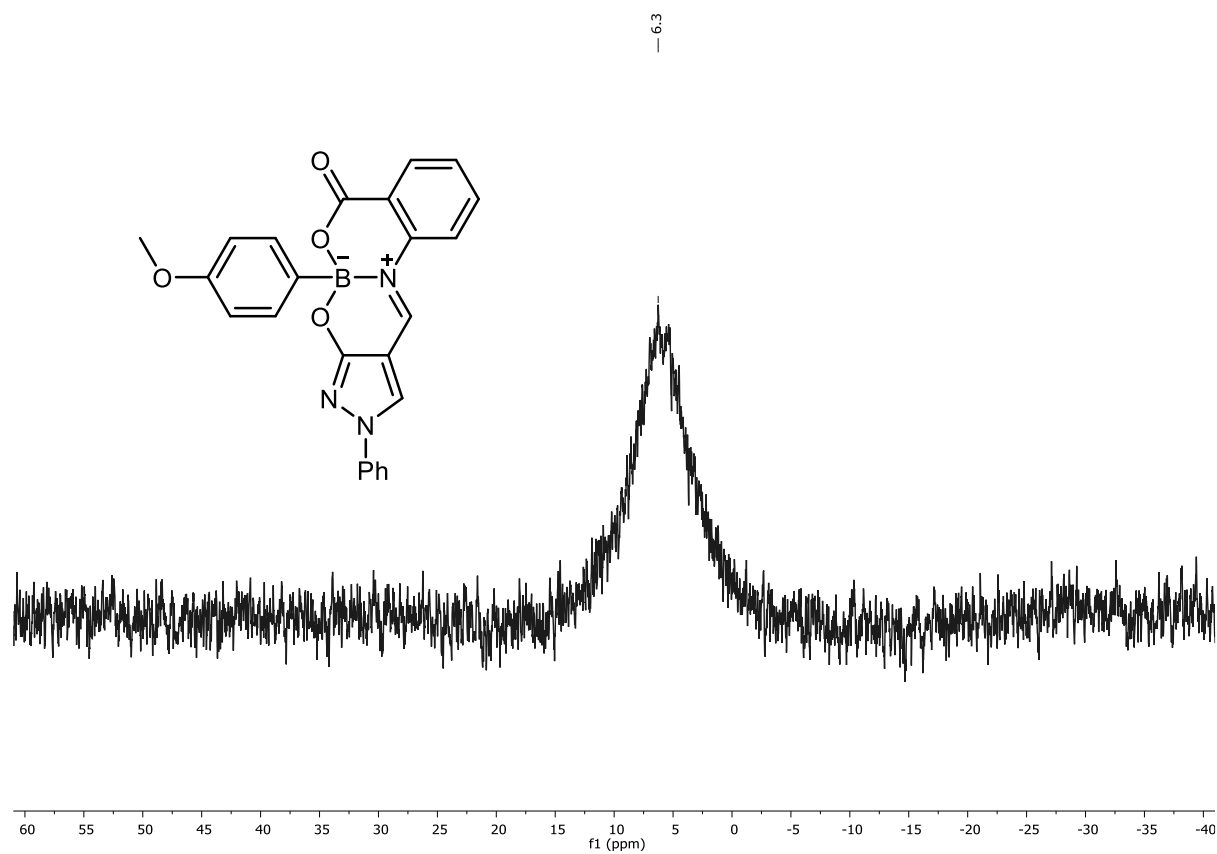


Figure S21. ^{11}B NMR (128 MHz, $\text{DMSO-}d_6$) spectrum of **4c**

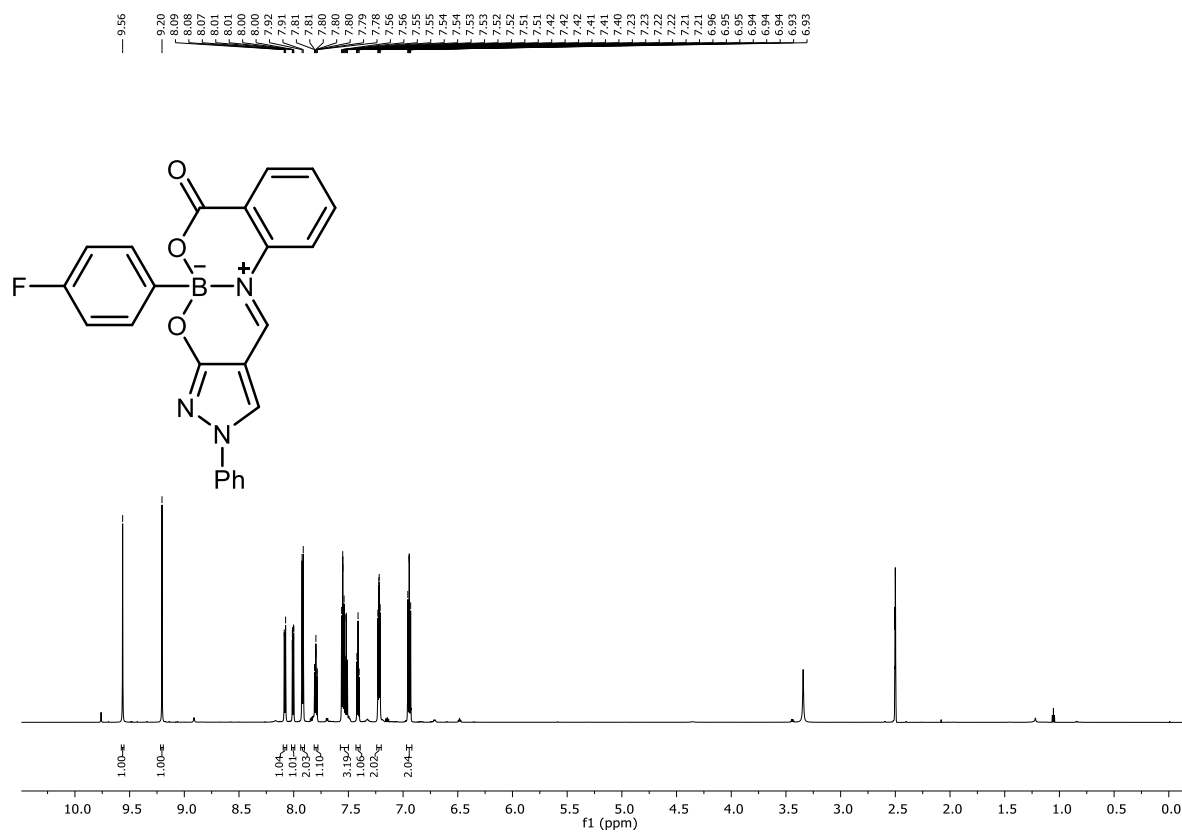


Figure S23. ¹H NMR (700 MHz, DMSO-*d*₆) spectrum of **4d**

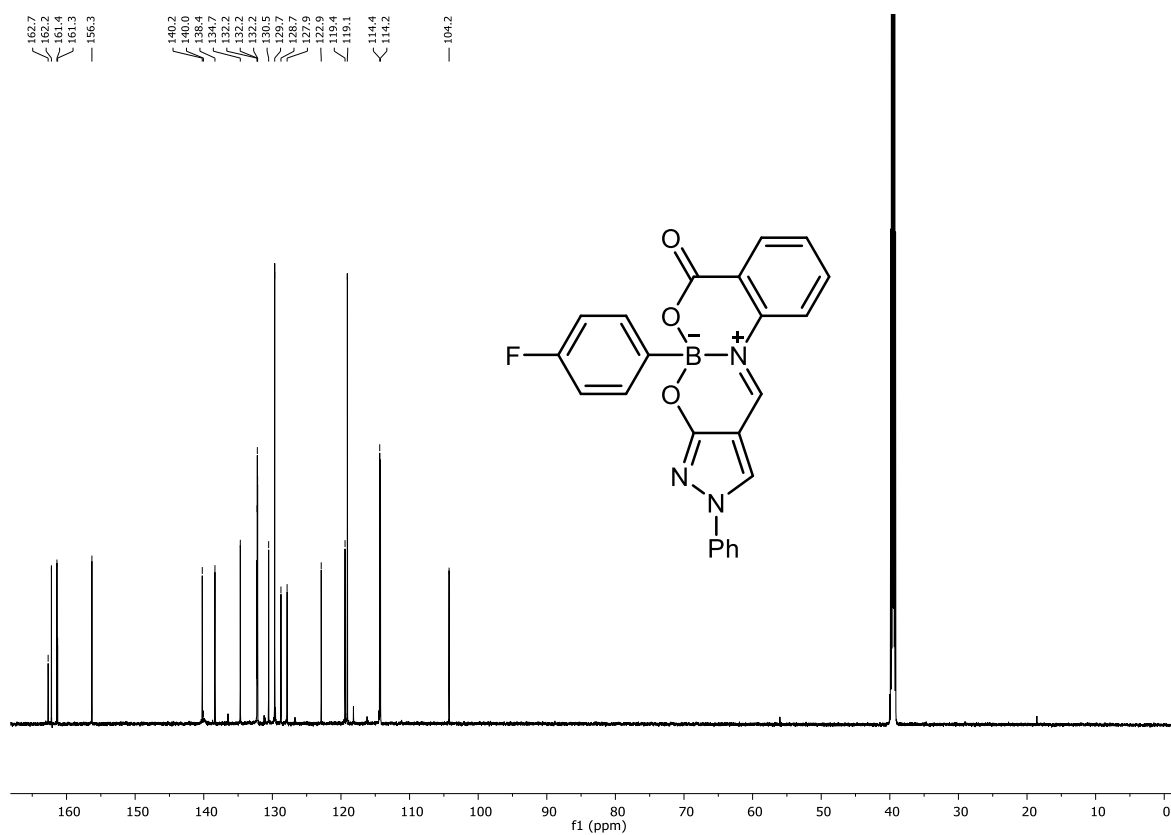


Figure S24. ¹³C NMR (176 MHz, DMSO-*d*₆) spectrum of **4d**

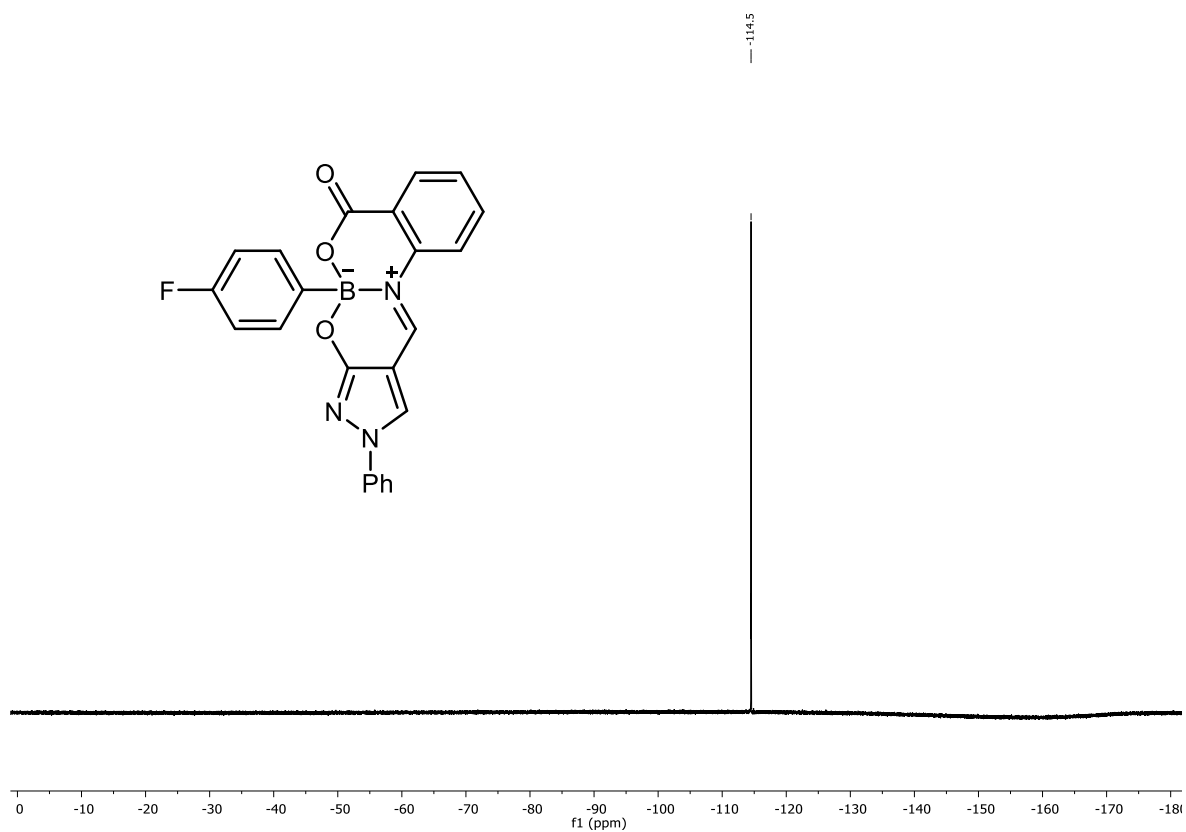


Figure S25. ^{19}F NMR (376 MHz, $\text{DMSO}-d_6$) spectrum of **4d**

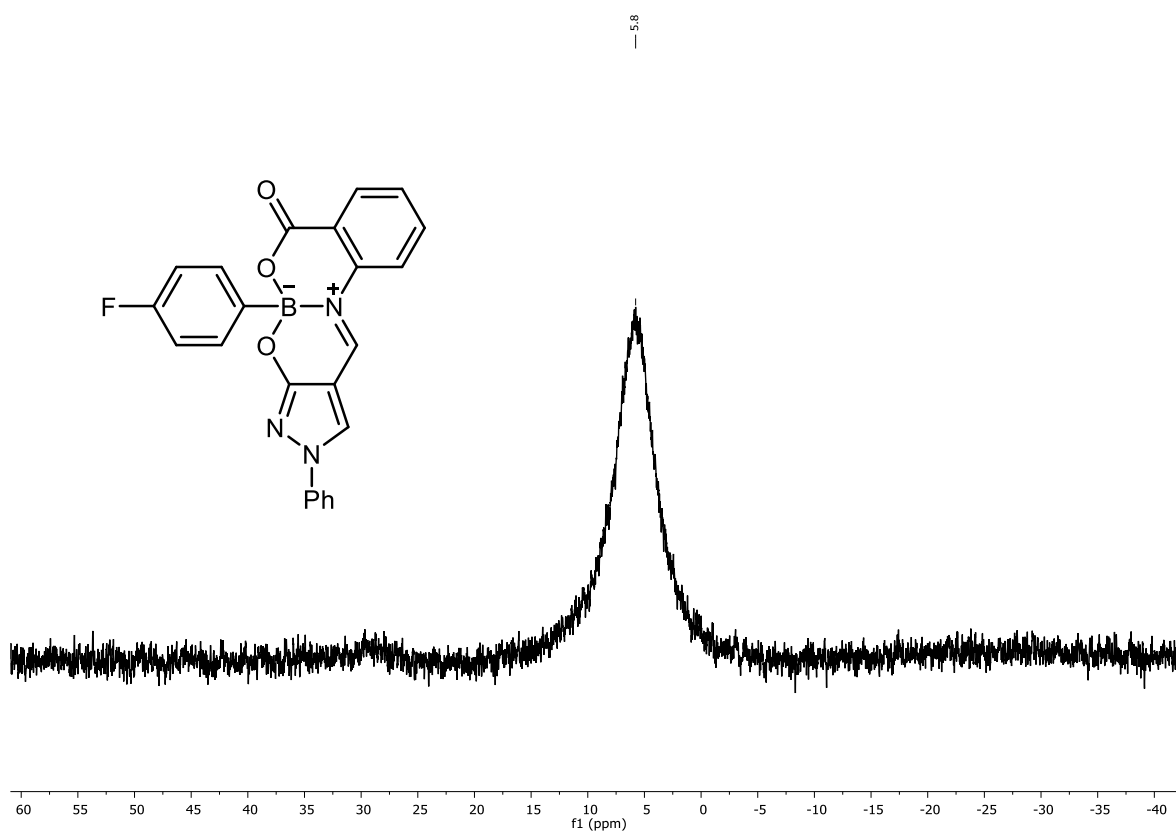


Figure S26. ^{11}B NMR (128 MHz, $\text{DMSO}-d_6$) spectrum of **4d**

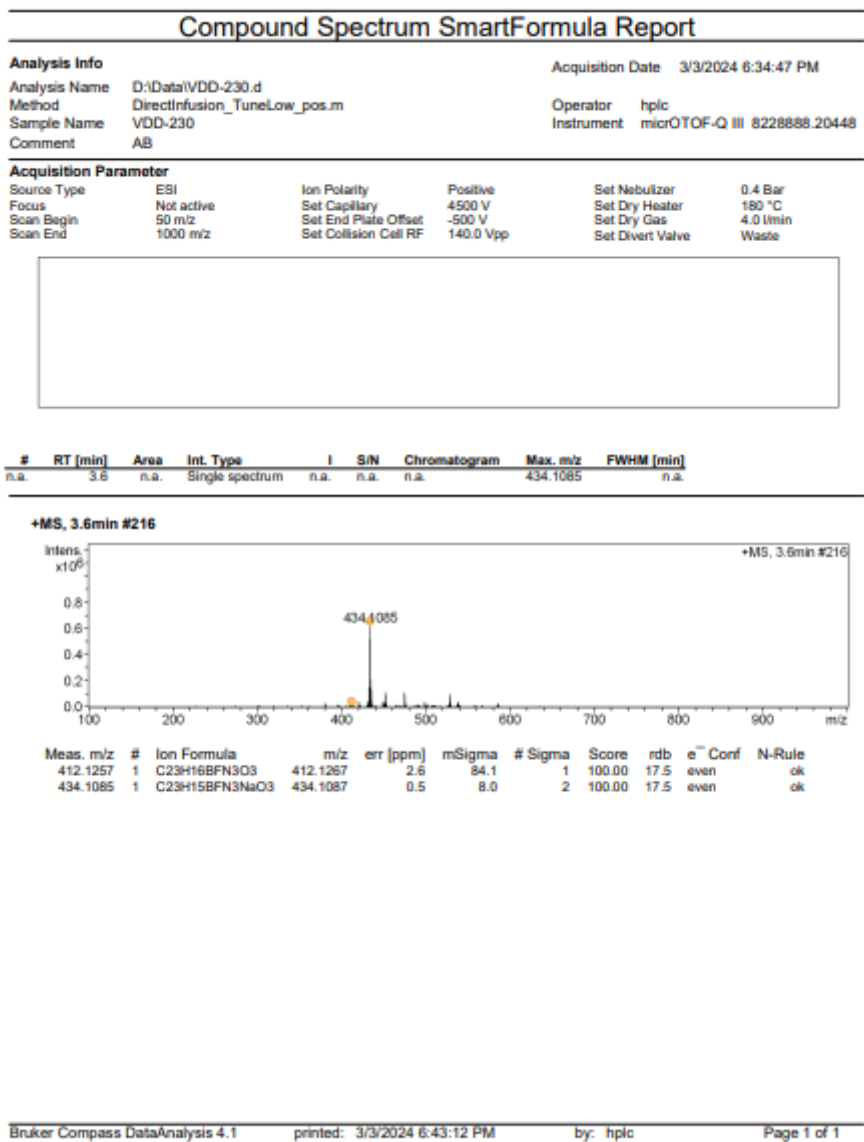


Figure S27. HRMS (ESI⁺) report of **4d**

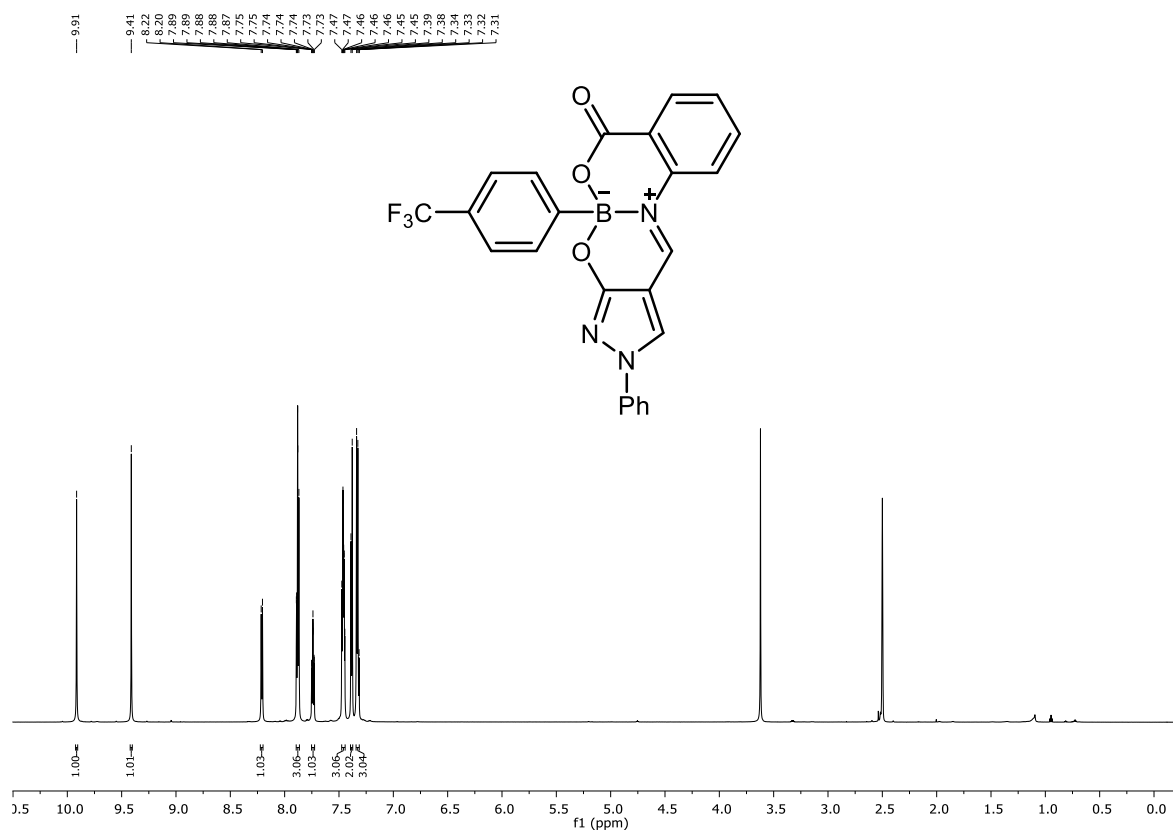


Figure S28. ¹H NMR (700 MHz, DMSO-*d*₆) spectrum of **4e**

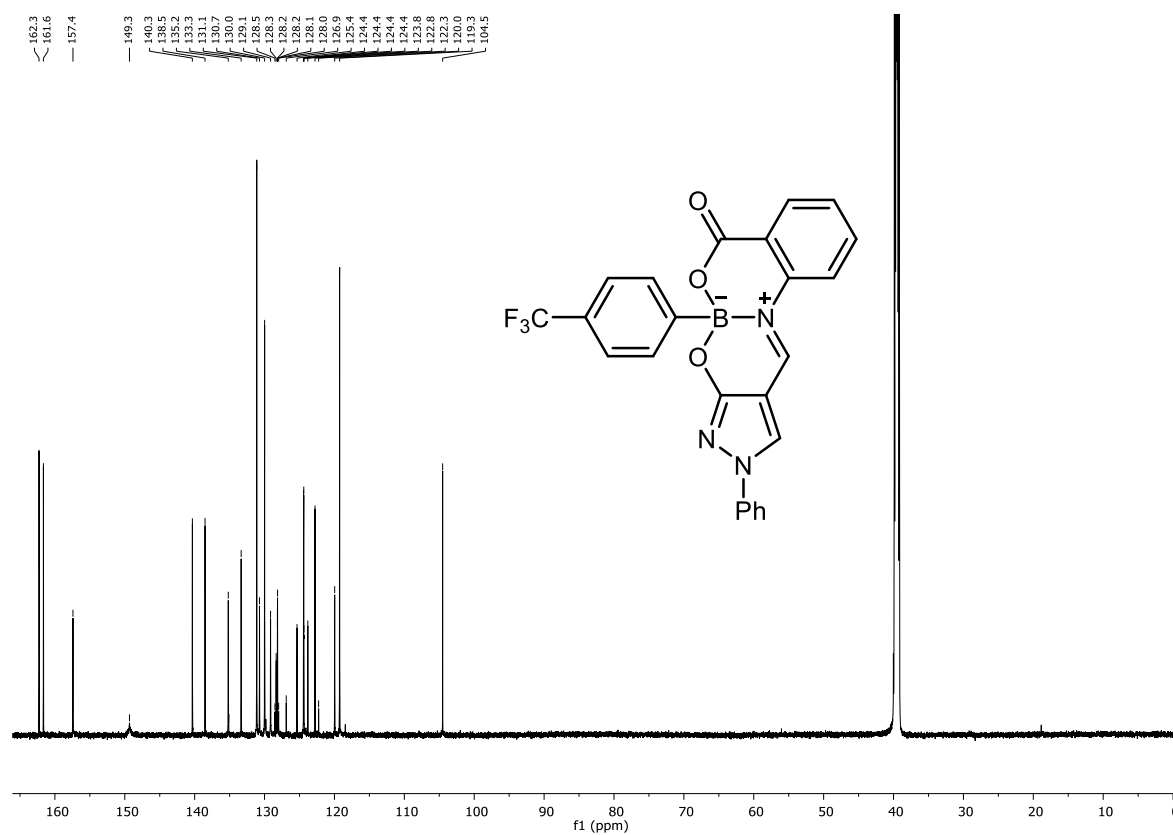


Figure S29. ¹³C NMR (176 MHz, DMSO-*d*₆) spectrum of **4e**

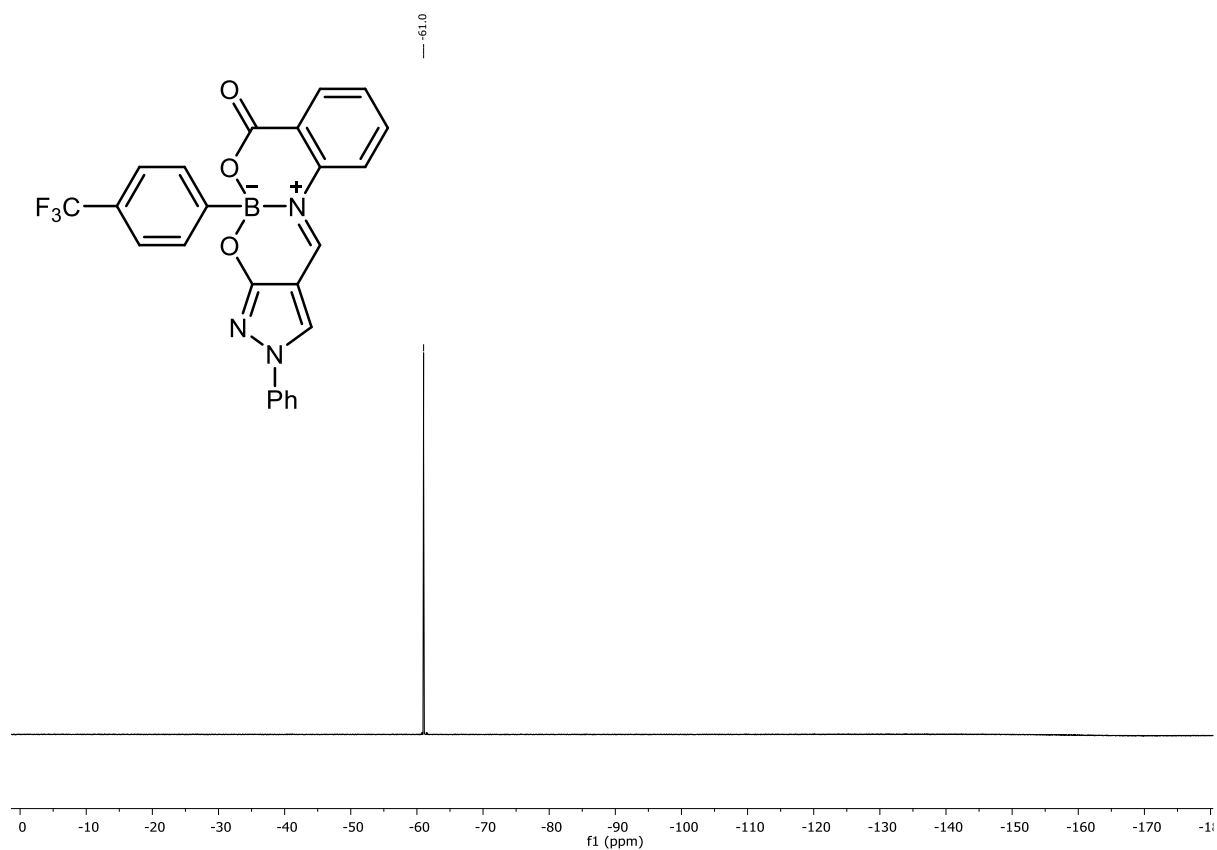


Figure S30. ^{19}F NMR (376 MHz, $\text{DMSO}-d_6$) spectrum of **4e**

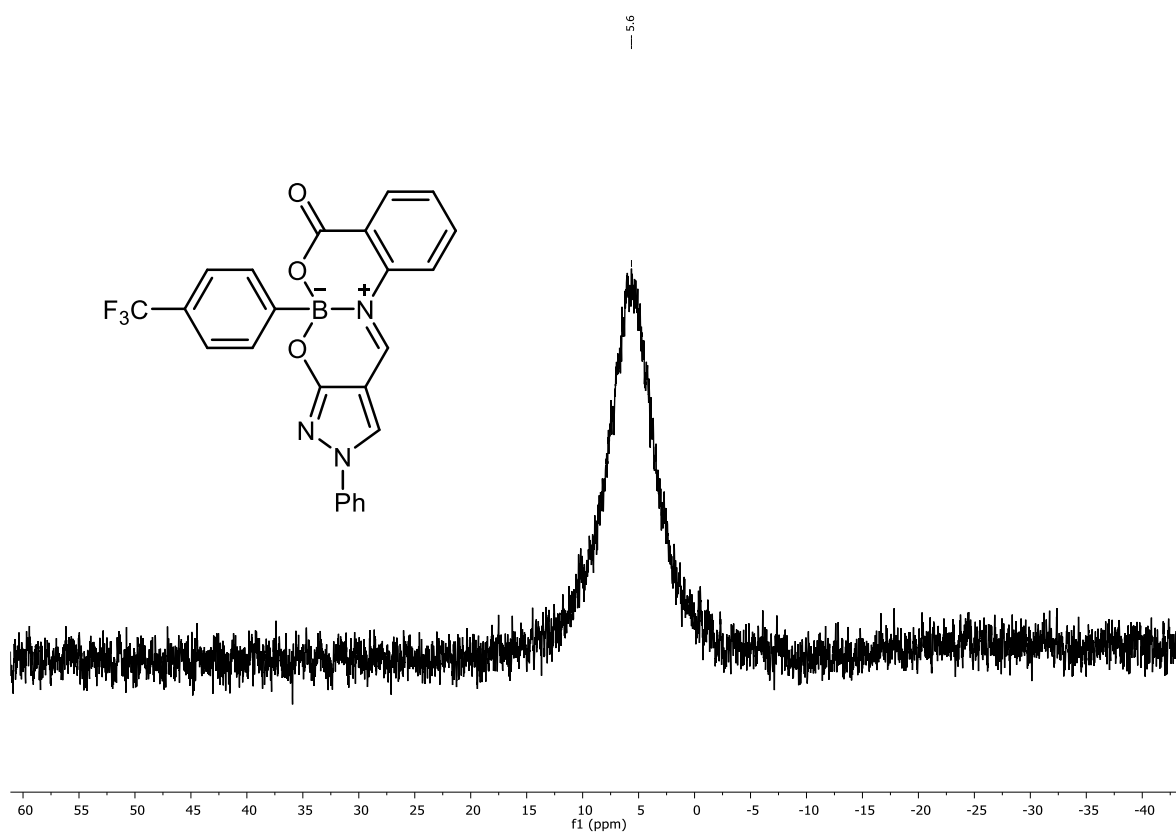


Figure S31. ^{11}B NMR (128 MHz, $\text{DMSO}-d_6$) spectrum of **4e**

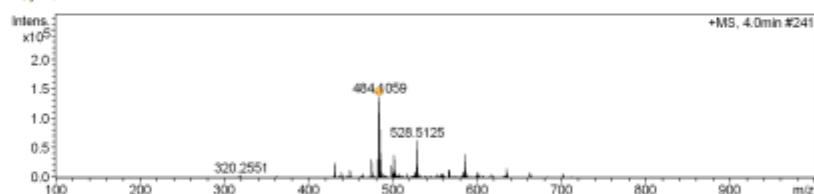
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Comment	AB		

Acquisition Parameter					
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	4.0	n.a.	Single spectrum	n.a.	n.a.	n.a.	484.1059	n.a.

+MS, 4.0min #241



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
484.1059	1	C ₂₄ H ₁₅ BF ₃ N ₃ NaO ₃	484.1055	-0.7	5.7	3	100.00	17.5	even	ok

Figure S32. HRMS (ESI⁺) report of 4e

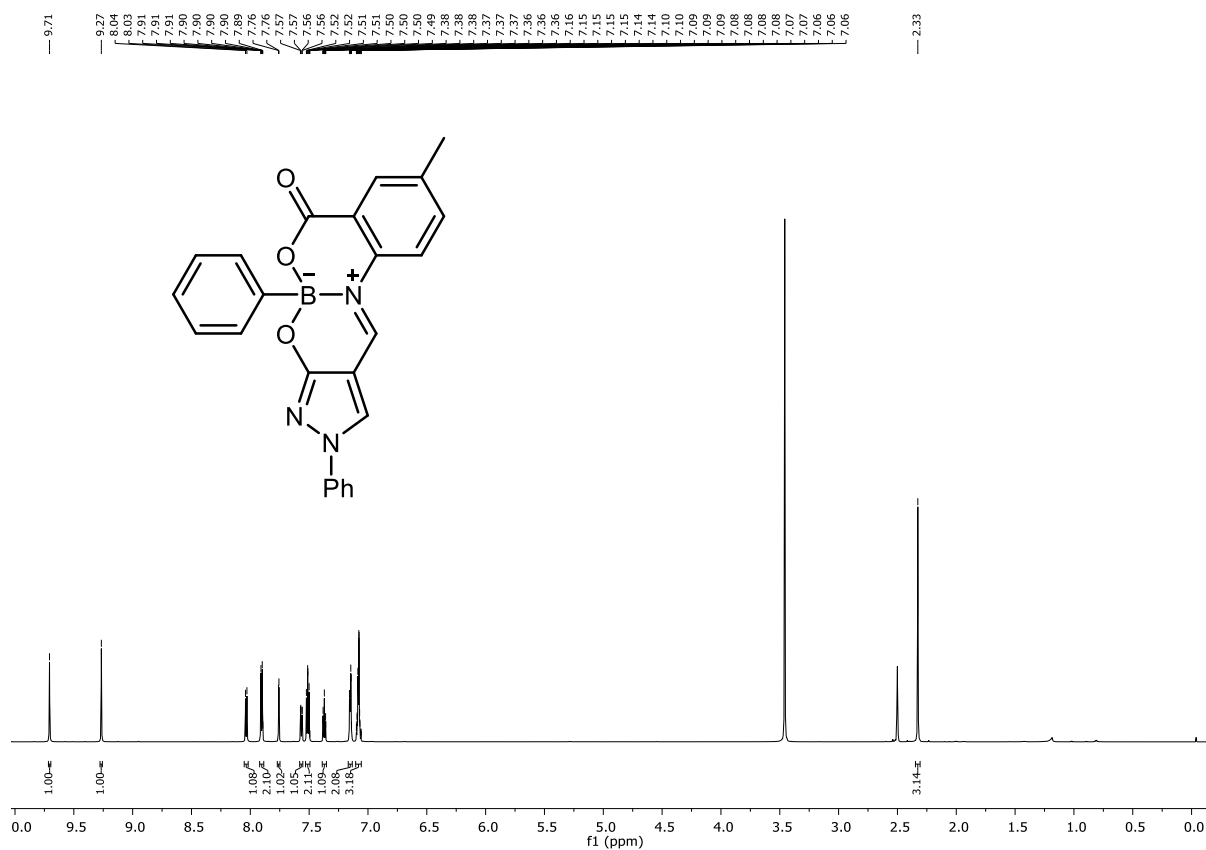


Figure S33. ¹H NMR (700 MHz, DMSO-*d*₆) spectrum of **4f**

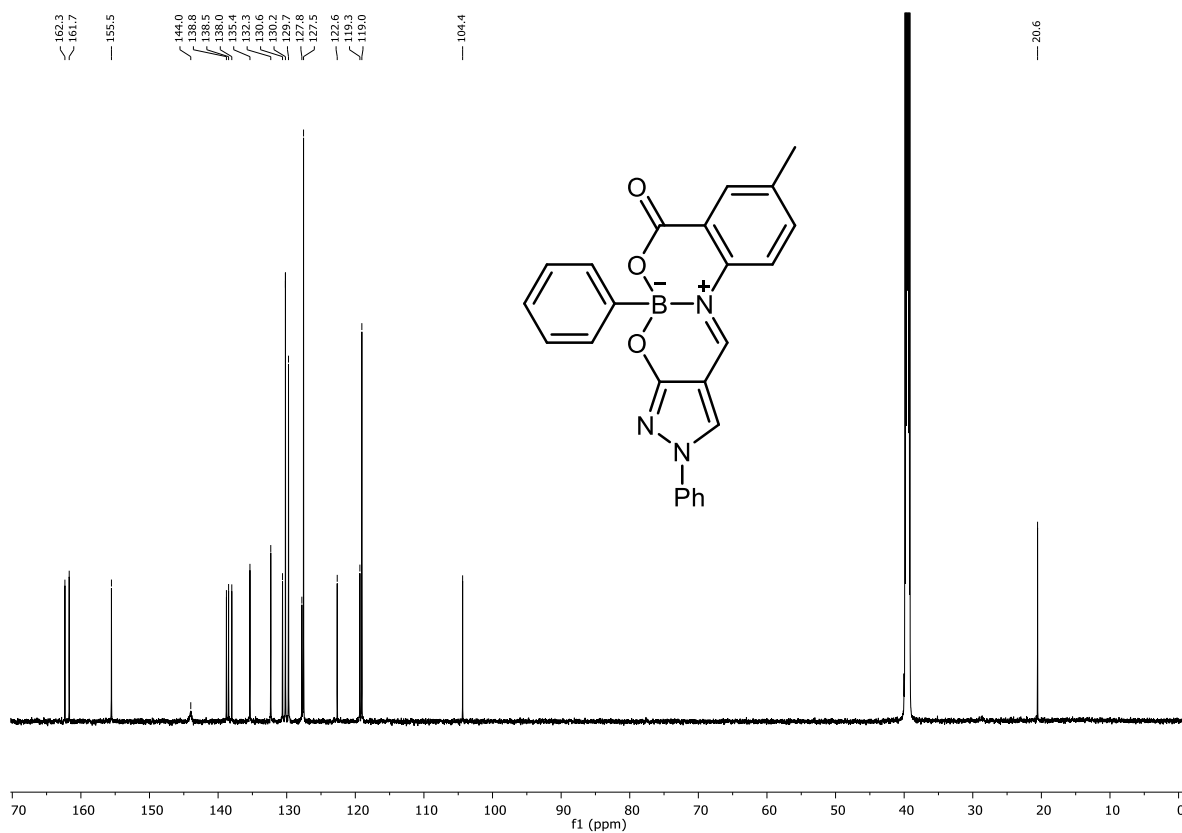


Figure S34. ¹³C NMR (176 MHz, DMSO-*d*₆) spectrum of **4f**

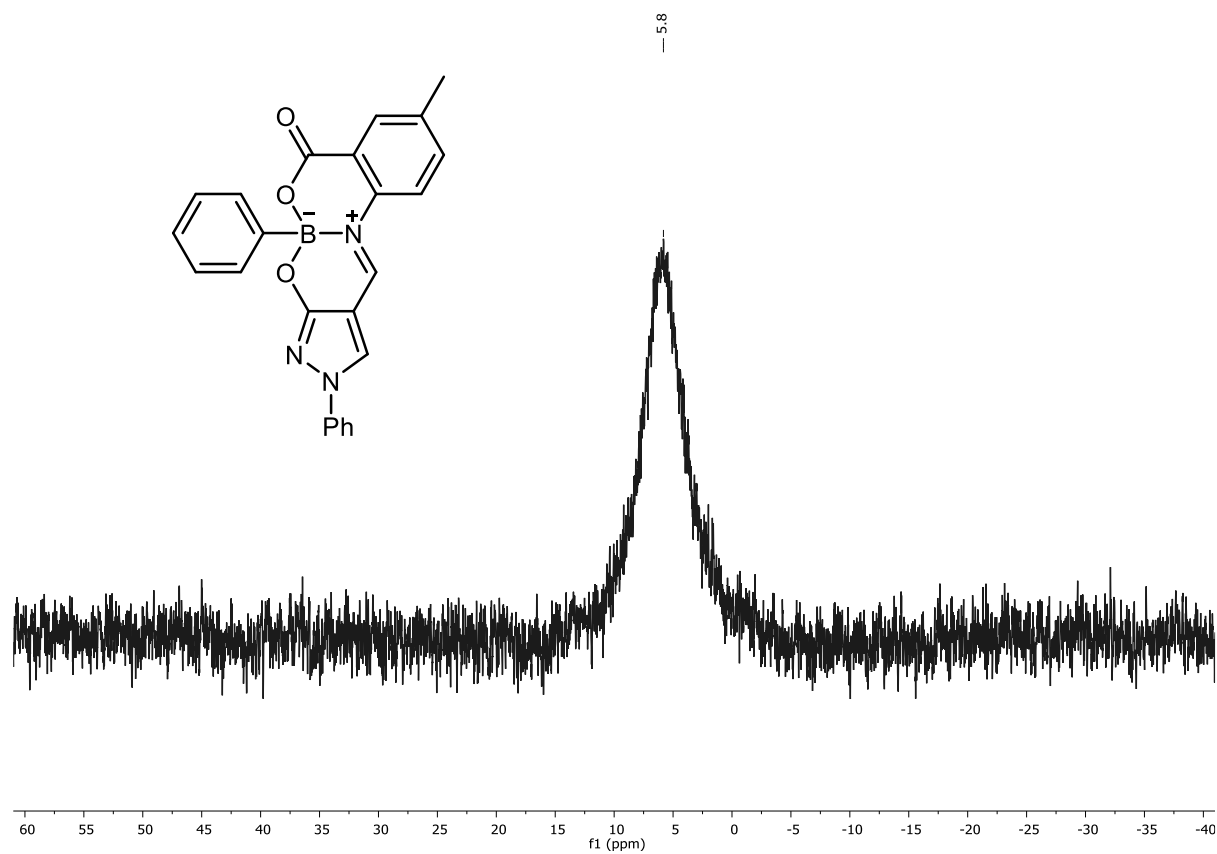


Figure S35. ^{11}B NMR (128 MHz, $\text{DMSO-}d_6$) spectrum of **4f**

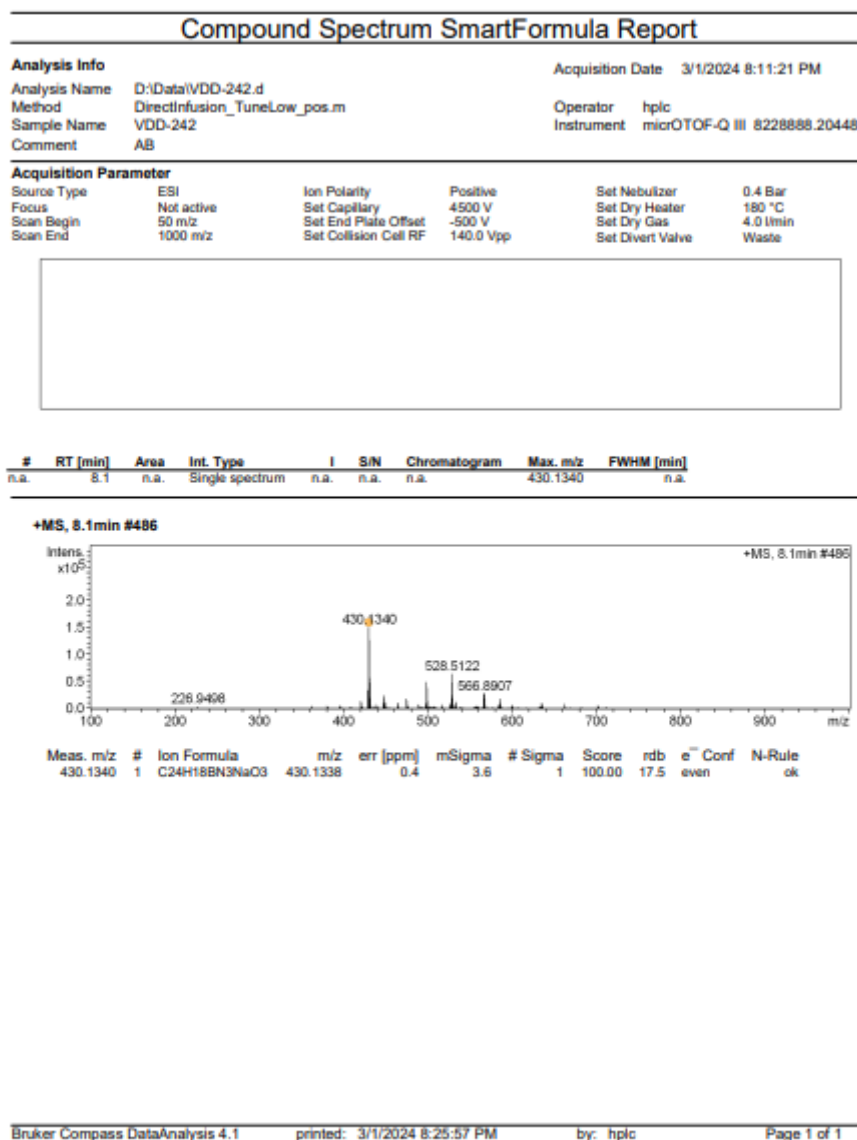


Figure S36. HRMS (ESI⁺) report of **4f**

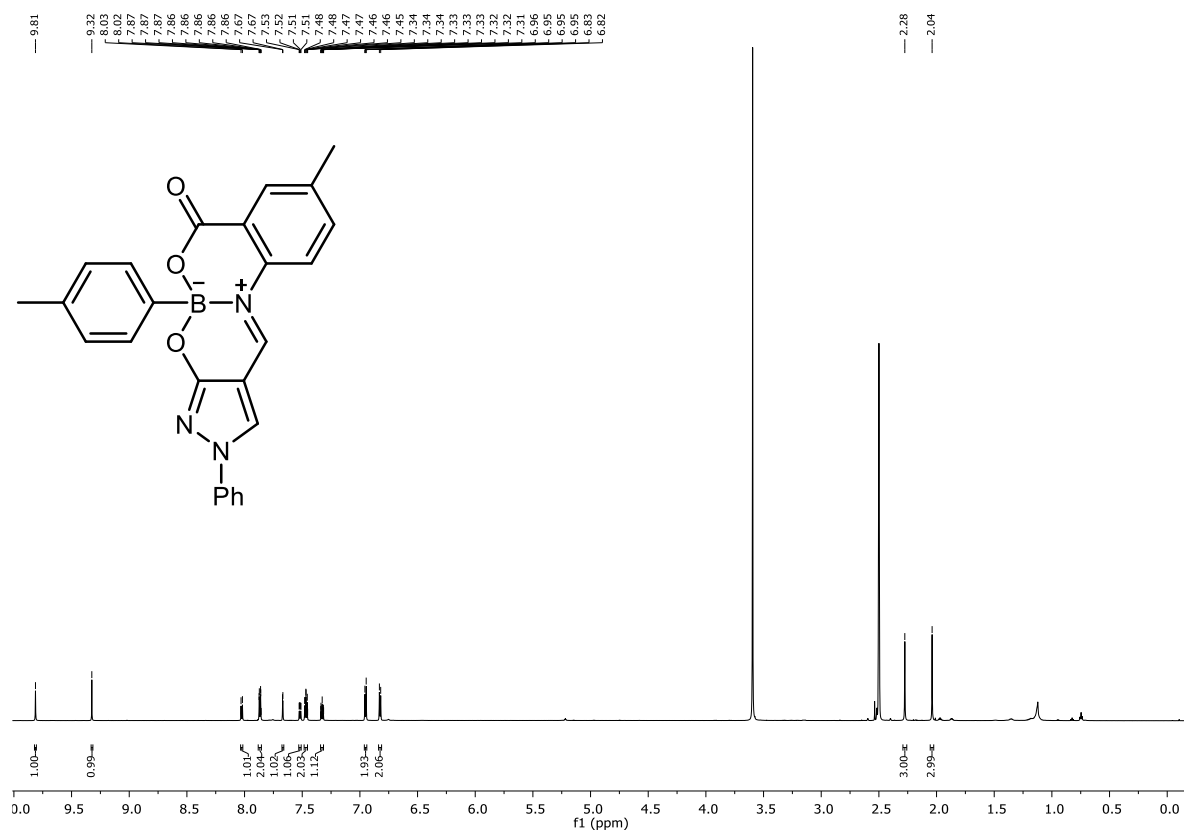


Figure S37. ^1H NMR (700 MHz, $\text{DMSO-}d_6$) spectrum of **4g**

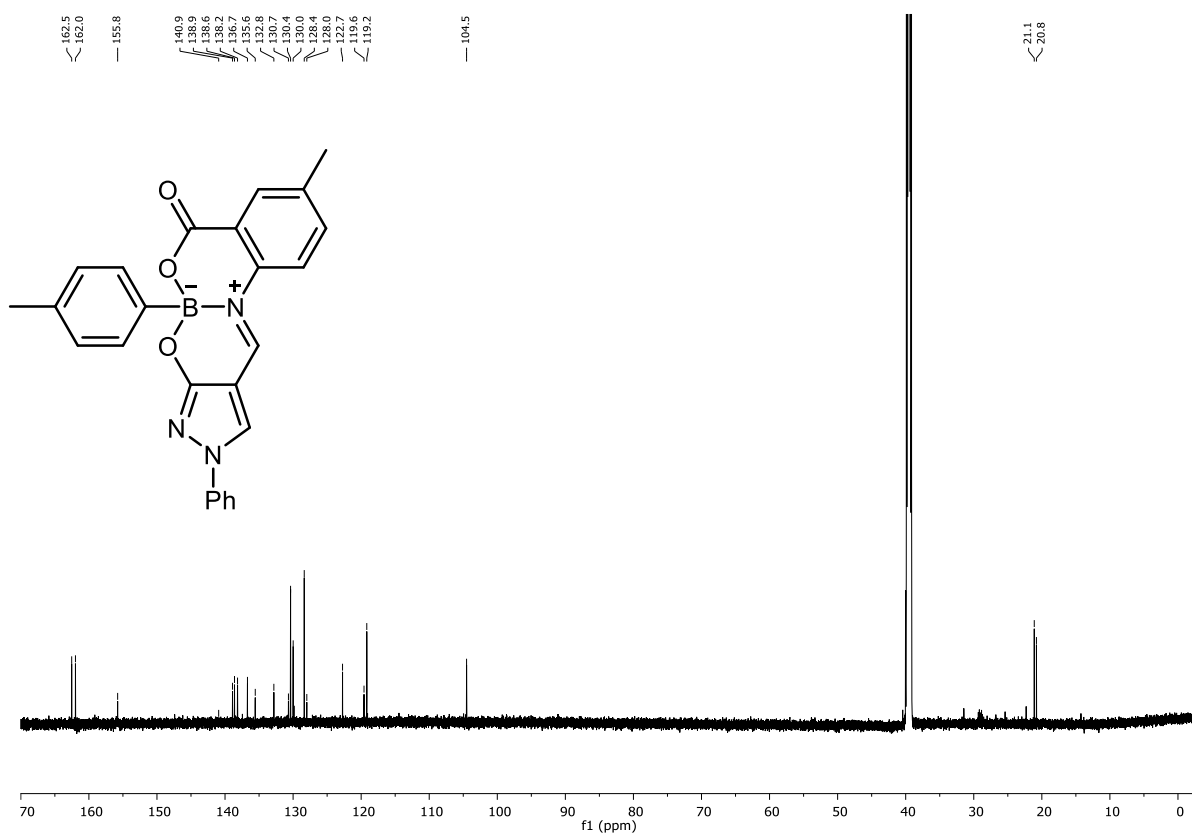


Figure S38. ^{13}C NMR (176 MHz, $\text{DMSO-}d_6$) spectrum of **4g**

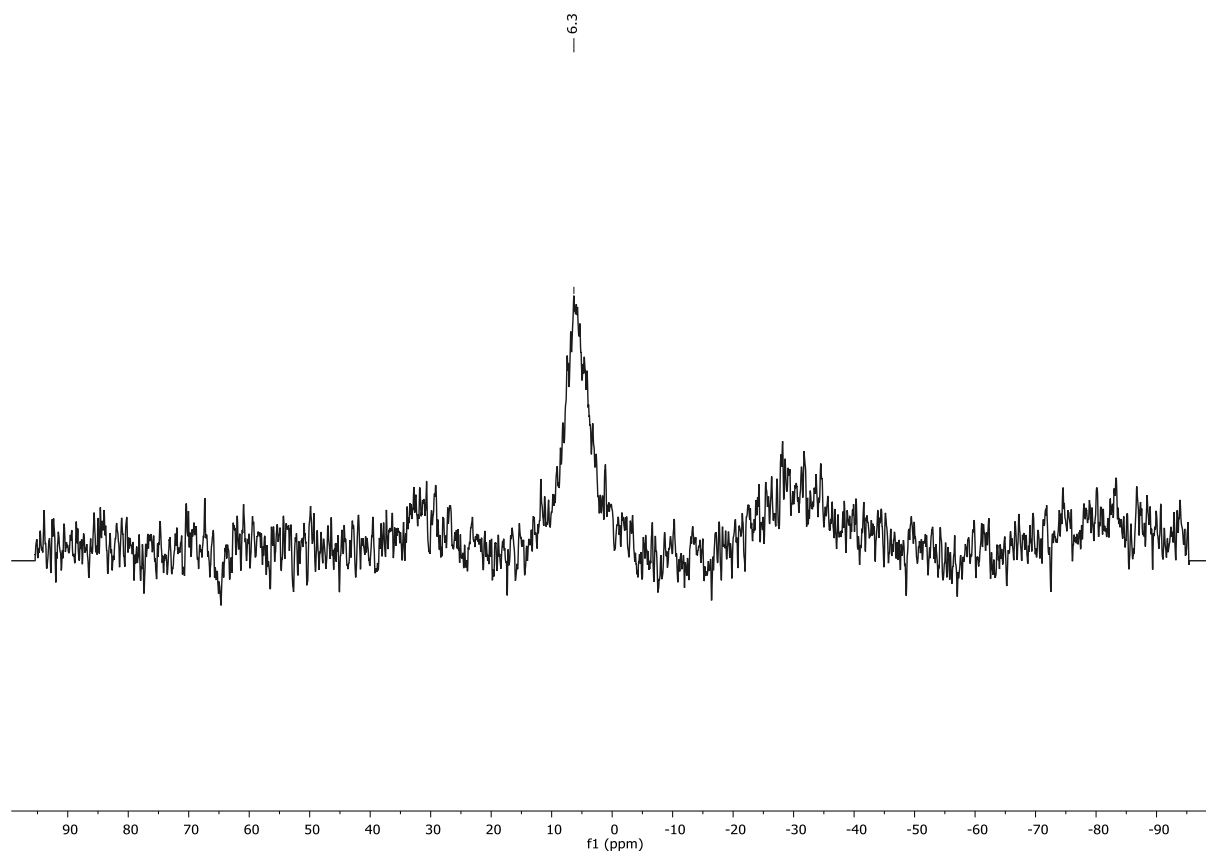


Figure S39. ^{11}B NMR (128 MHz, $\text{DMSO-}d_6$) spectrum of **4g**

Compound Spectrum SmartFormula Report

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Sample Name VDD-249
Comment AB

Acquisition Date 3/3/2024 7:52:58 PM

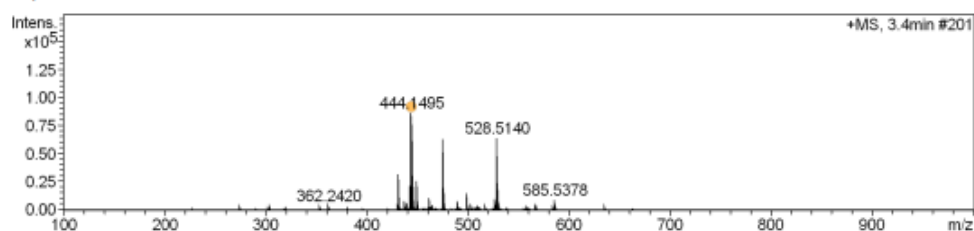
Operator hplc
Instrument microTOF-Q III 8228888.20448

Acquisition Parameter

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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	3.4	n.a.	Single spectrum	n.a.	n.a.	n.a.	444.1495	n.a.

+MS, 3.4min #201



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
444.1495	1	C ₂₅ H ₂₀ BN ₃ NaO ₃	444.1494	-0.2	9.6	2	100.00	17.5	even	ok

Figure S40. HRMS (ESI⁺) report of **4g**

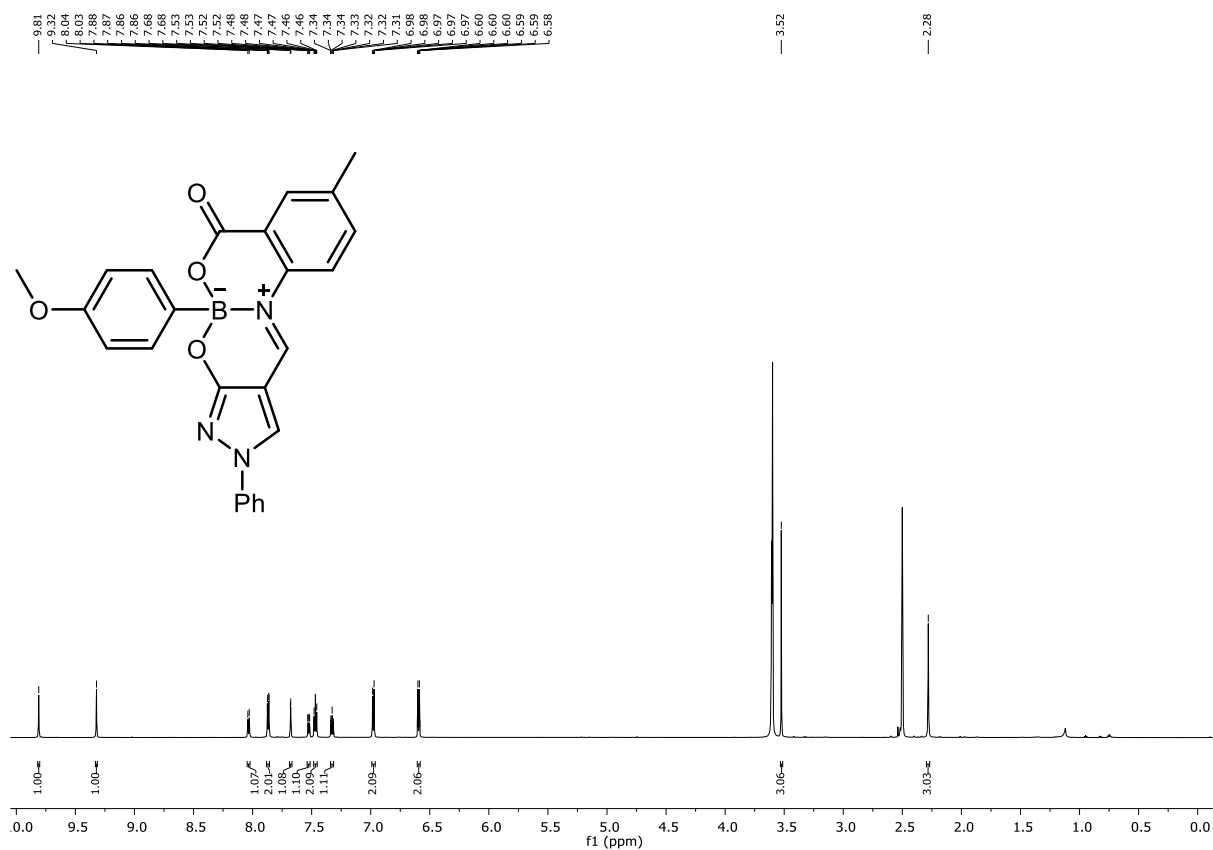


Figure S41. ¹H NMR (700 MHz, DMSO-*d*₆) spectrum of **4h**

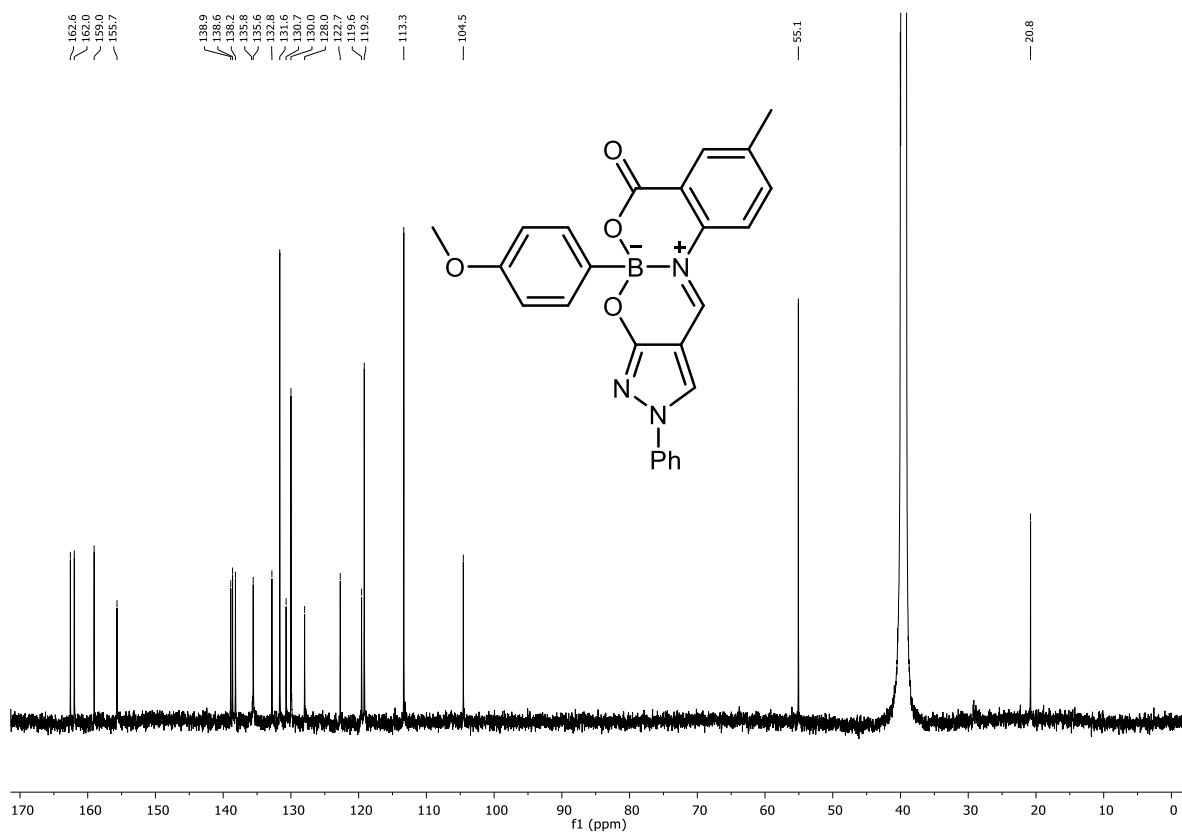


Figure S42. ¹³C NMR (176 MHz, DMSO-*d*₆) spectrum of **4h**

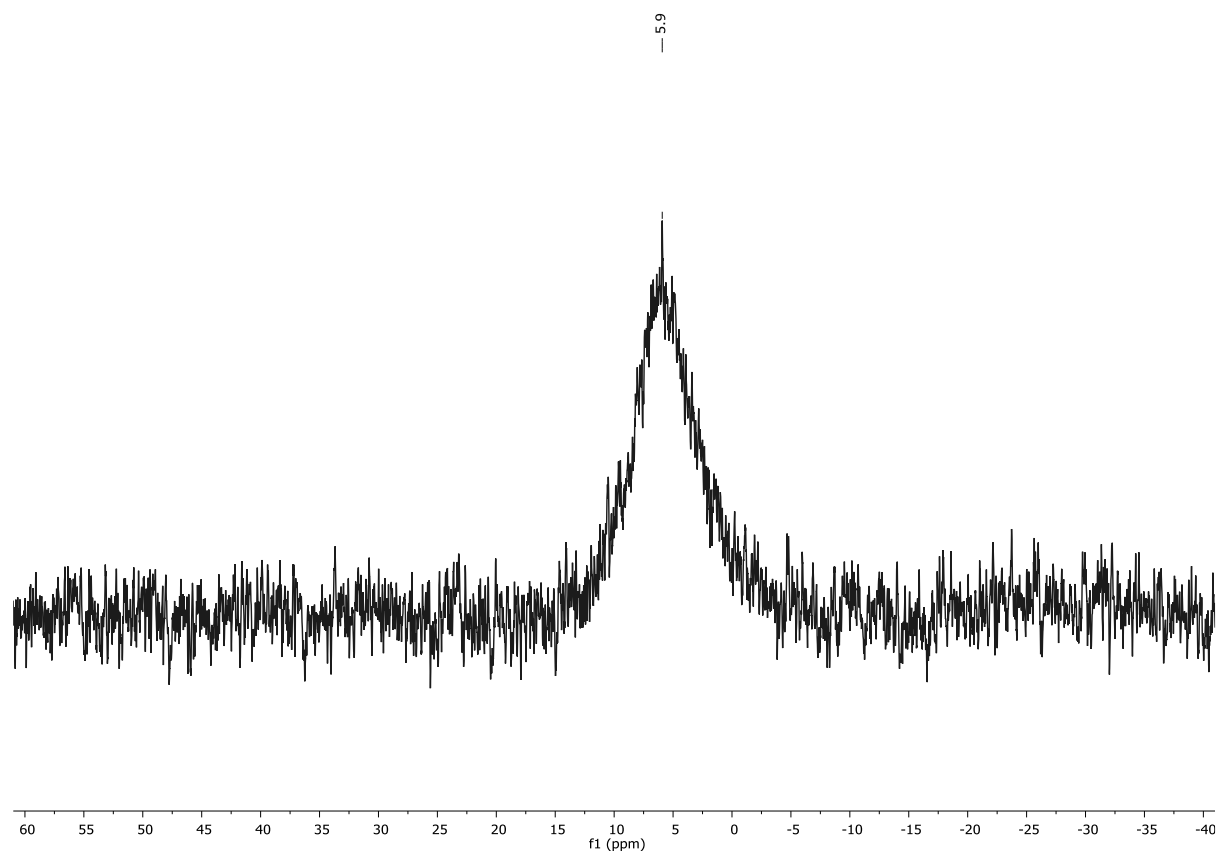


Figure S43. ^{11}B NMR (128 MHz, $\text{DMSO-}d_6$) spectrum of **4h**

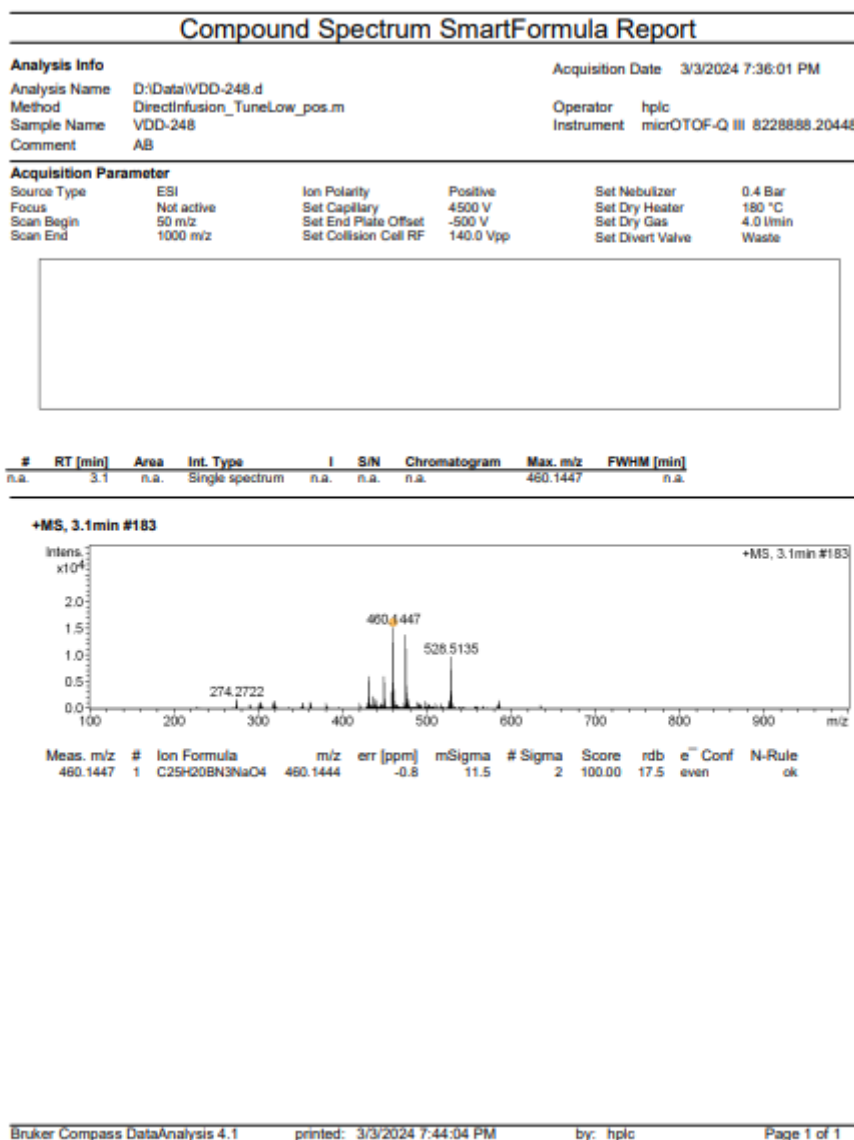
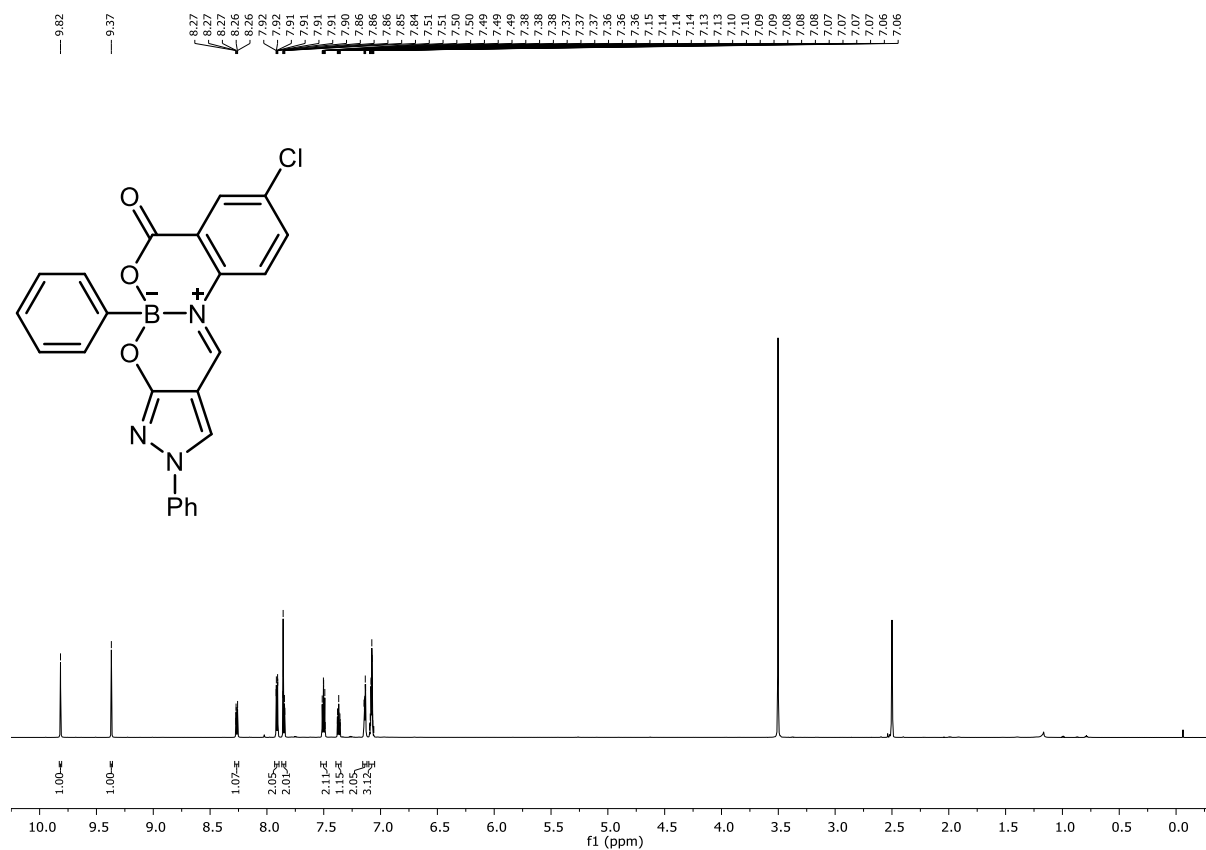


Figure S44. HRMS (ESI⁺) report of **4h**



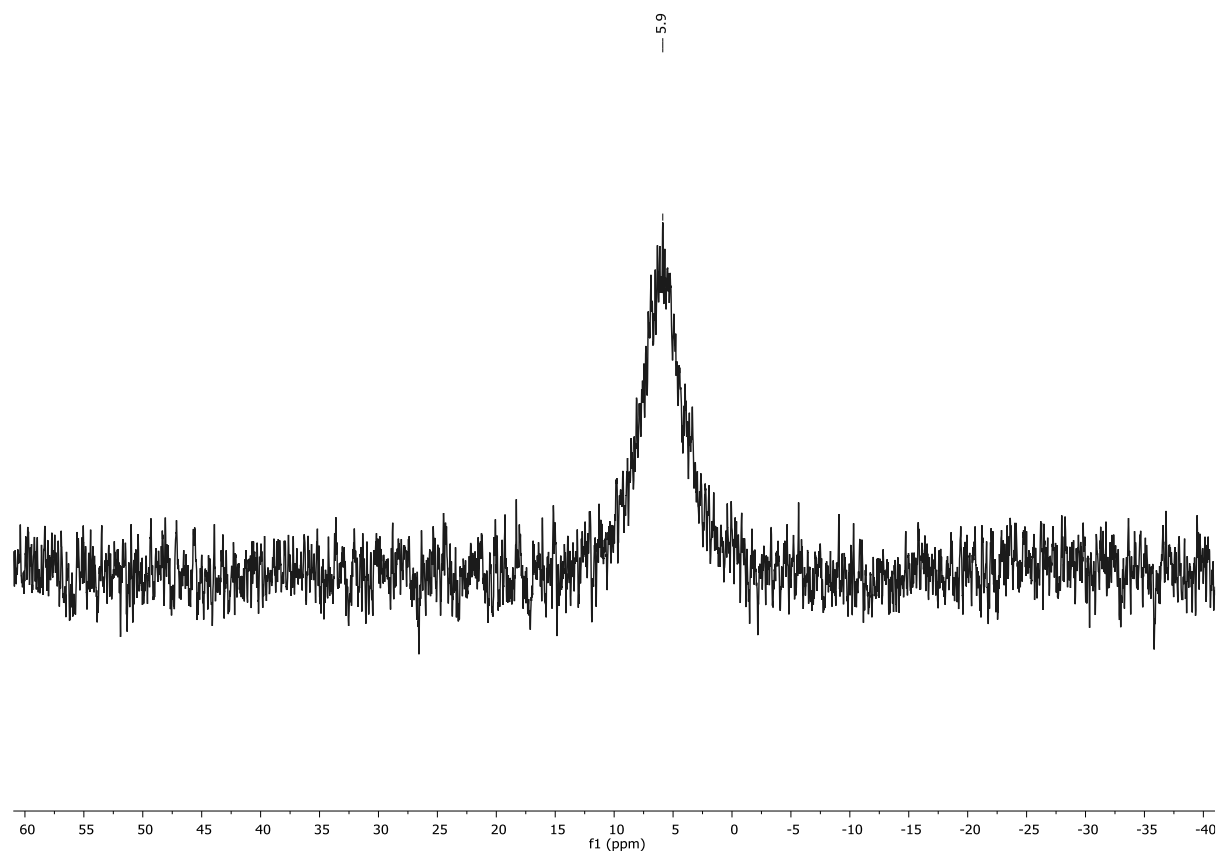


Figure S47. ^{11}B NMR (128 MHz, $\text{DMSO-}d_6$) spectrum of **4i**

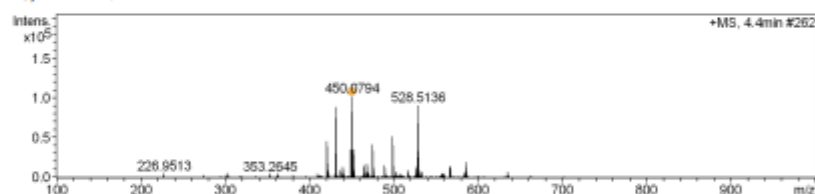
Compound Spectrum SmartFormula Report

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Sample Name	VDD-241		
Comment	AB		

Acquisition Parameter					
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Scan End	1000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	4.4	n.a.	Single spectrum	n.a.	n.a.	n.a.	450.0794	n.a.

+MS, 4.4min #262



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻	Conf	N-Rule
450.0794	1	C23H15BCIN3NaO3	450.0791	-0.6	6.5	1	100.00	17.5	even		ok

Figure S48. HRMS (ESI⁺) report of **4i**

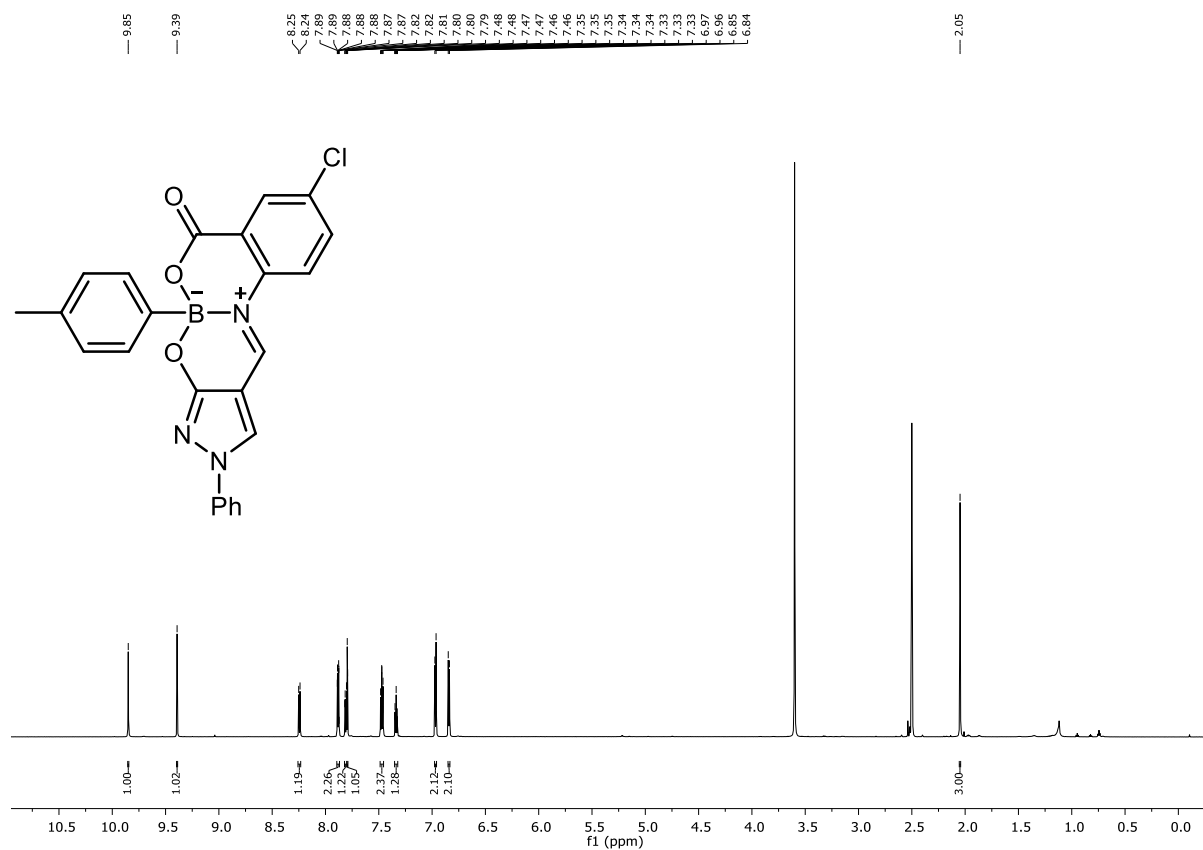


Figure S49. ¹H NMR (700 MHz, DMSO-*d*₆) spectrum of **4j**

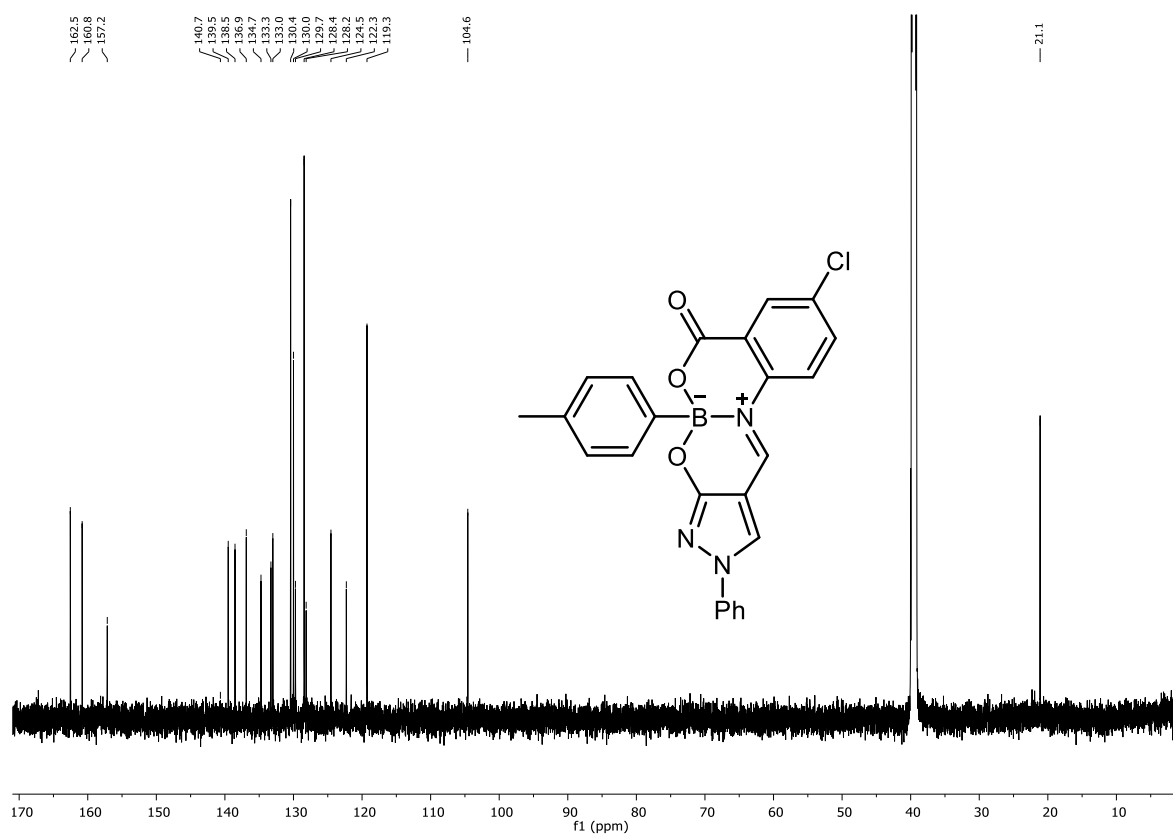


Figure S50. ¹³C NMR (176 MHz, DMSO-*d*₆) spectrum of **4j**

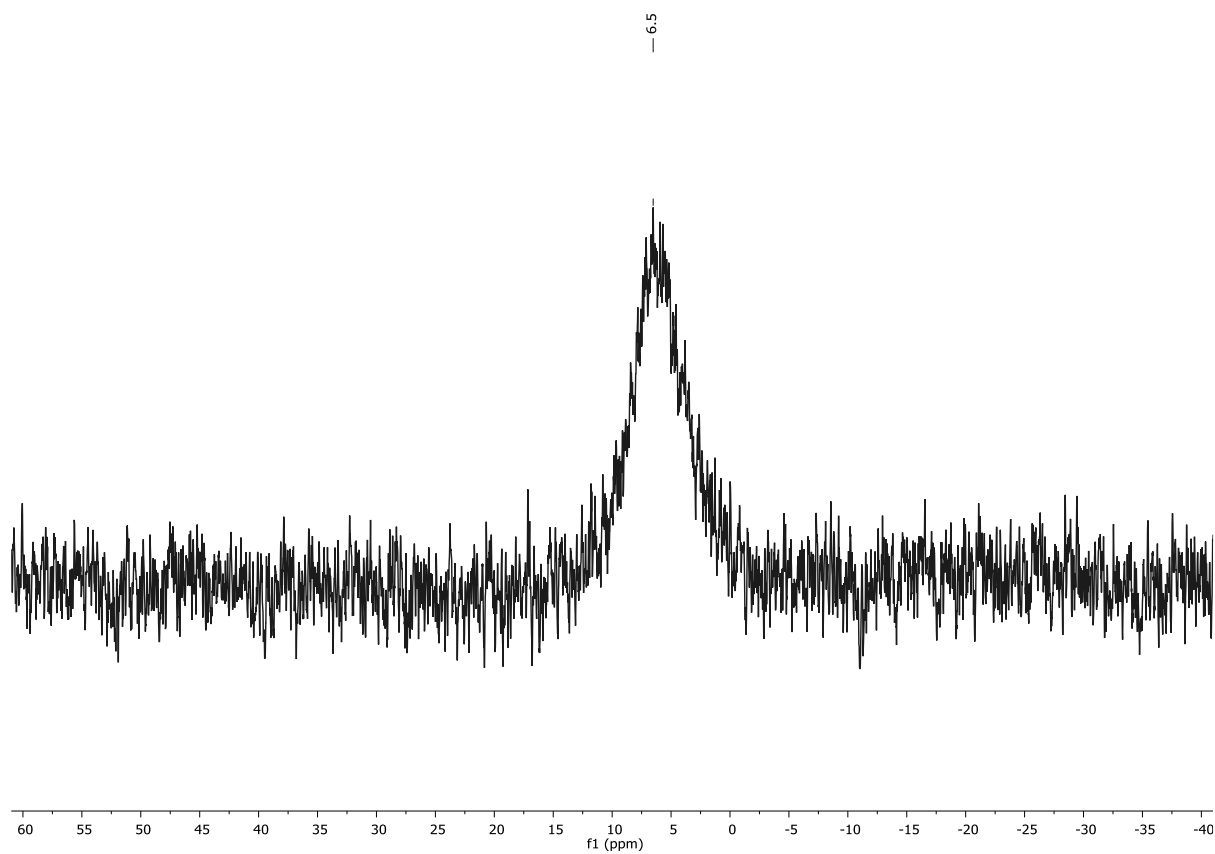


Figure S51. ^{11}B NMR (128 MHz, $\text{DMSO-}d_6$) spectrum of **4j**

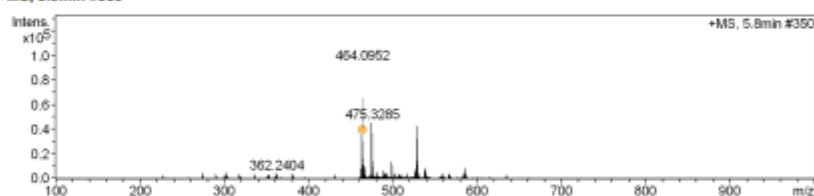
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Sample Name	VDD-244			
Comment	AB			

Acquisition Parameter					
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	5.8	n.a.	Single spectrum	n.a.	n.a.	n.a.	475.3285	n.a.

+MS, 5.8min #350



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdp	e ⁻ Conf	N-Rule
464.0952	1	C ₂₄ H ₁₇ BClN ₃ NaO ₃	464.0948	1.0	36.6	1	100.00	17.5	even	ok

Figure S52. HRMS (ESI⁺) report of **4j**

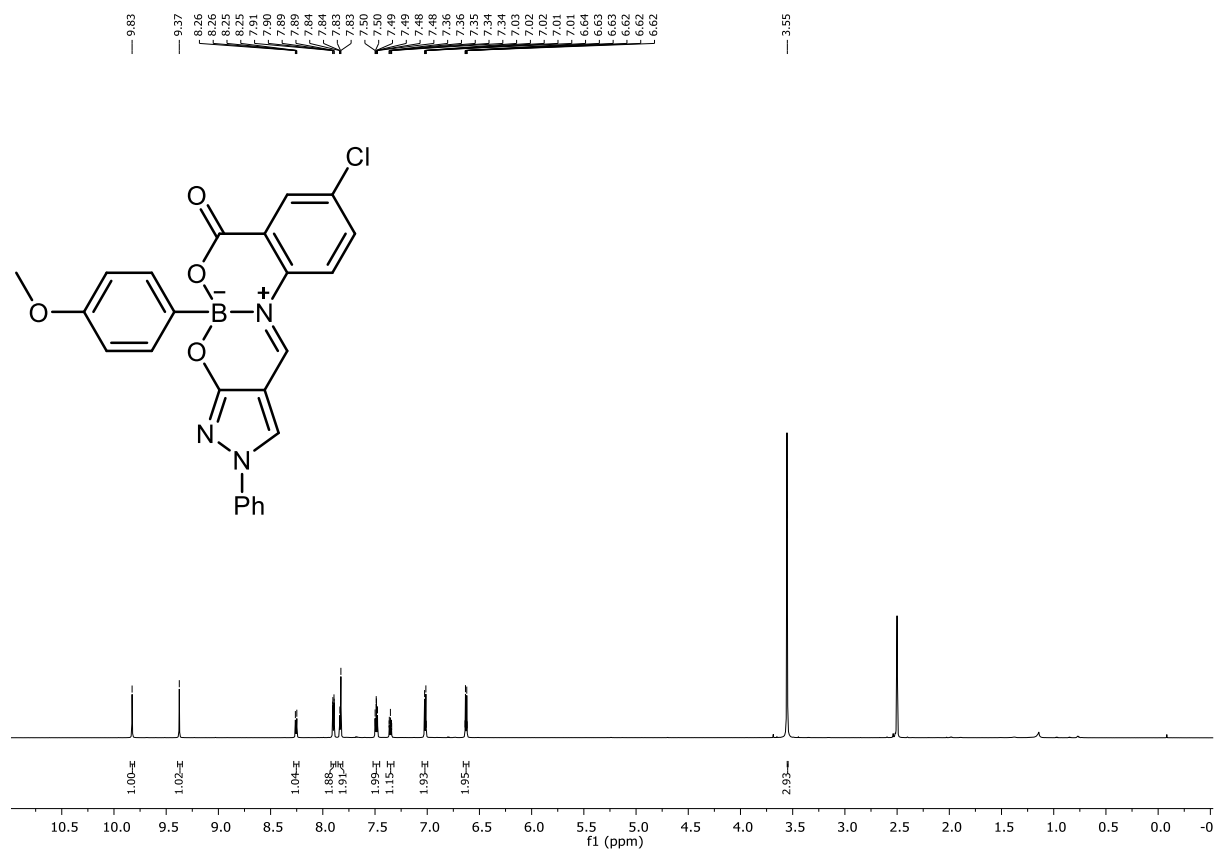


Figure S53. ¹H NMR (700 MHz, DMSO-*d*₆) spectrum of **4k**

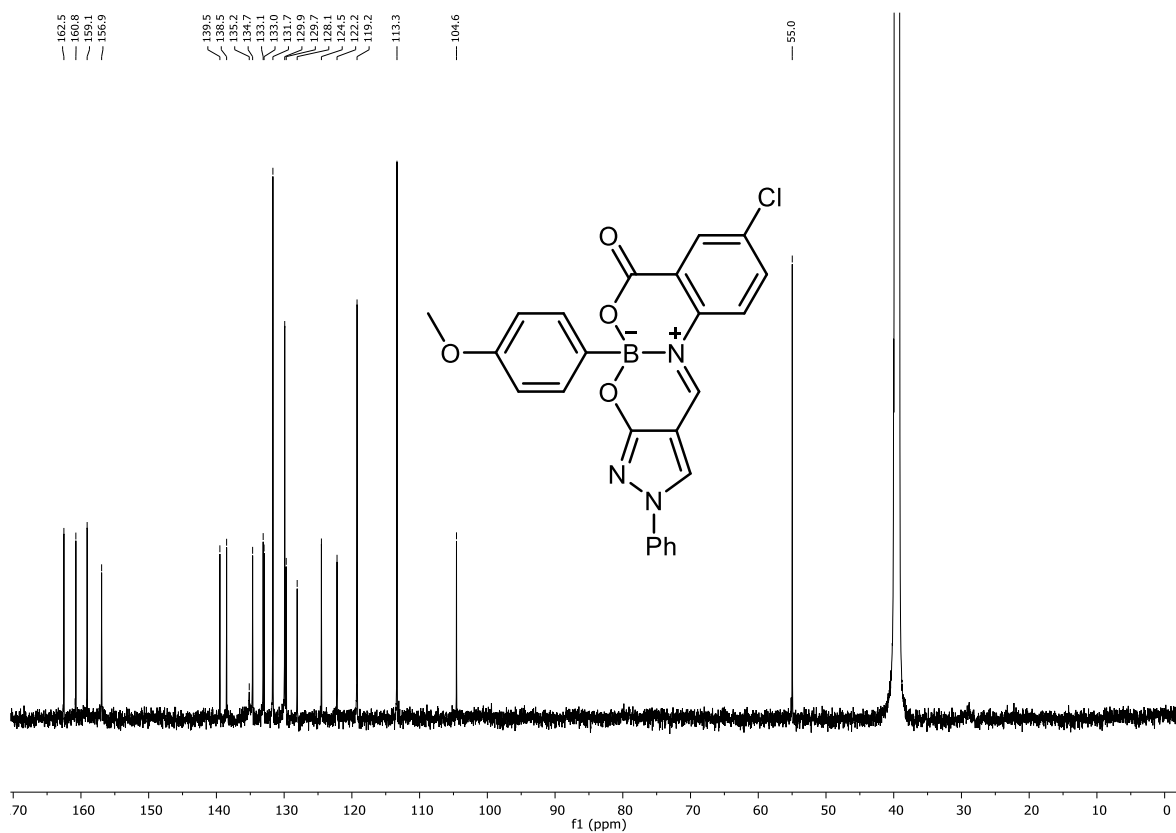


Figure S54. ¹³C NMR (176 MHz, DMSO-*d*₆) spectrum of **4k**

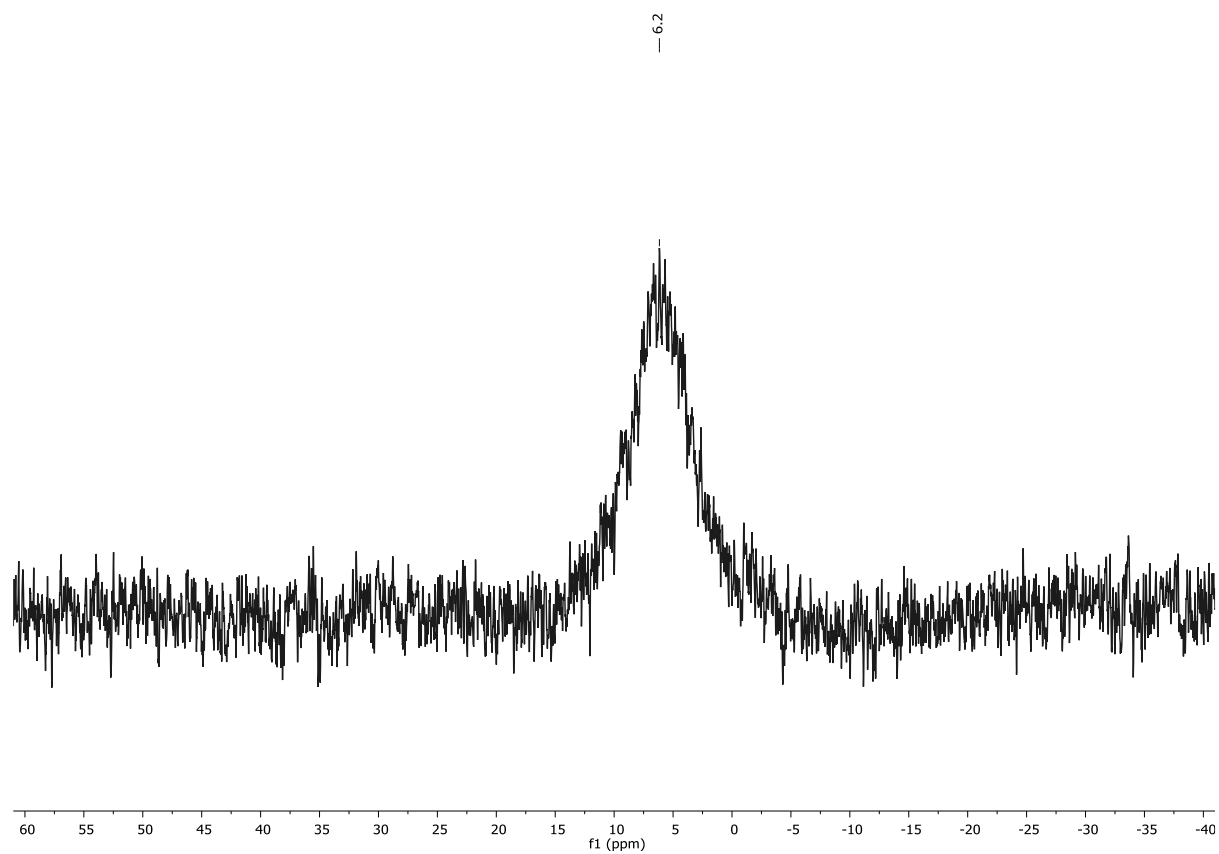


Figure S55. ^{11}B NMR (128 MHz, $\text{DMSO-}d_6$) spectrum of **4k**

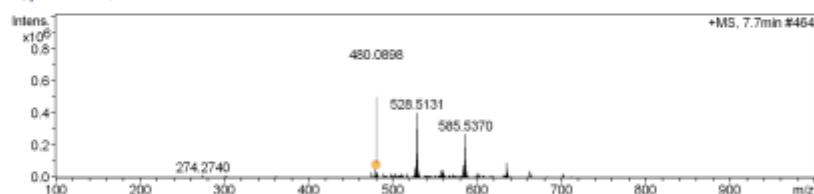
Compound Spectrum SmartFormula Report

Analysis Info		Acquisition Date	3/1/2024 8:32:46 PM
Analysis Name	D:\Data\VDD-243.d	Operator	hplc
Method	DirectInfusion_TuneLow_pos.m	Instrument	micrOTOF-Q III 8228888.20448
Sample Name	VDD-243		
Comment	AB		

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste

#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	7.7	n.a.	Single spectrum	n.a.	n.a.	n.a.	528.5131	n.a.

+MS, 7.7min #464



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e ⁻ Conf	N-Rule
480.0898	1	C ₂₄ H ₁₇ BClN ₃ NaO ₄	480.0897	0.1	46.6	4	100.00	17.5	even	ok

Figure S56. HRMS (ESI⁺) report of **4k**