

## Supplementary materials

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

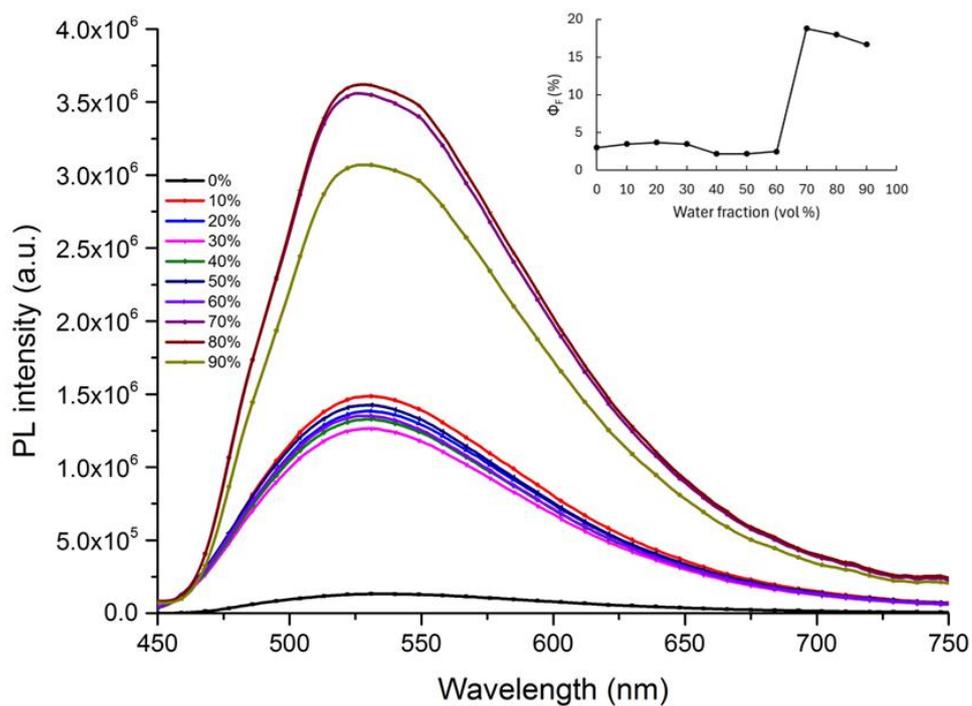
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<sup>1</sup> Department of Organic Chemistry, Kaunas University of Technology, Radvilėnų pl. 19, LT-50254 Kaunas, Lithuania; viktorija.dargyte@ktu.lt

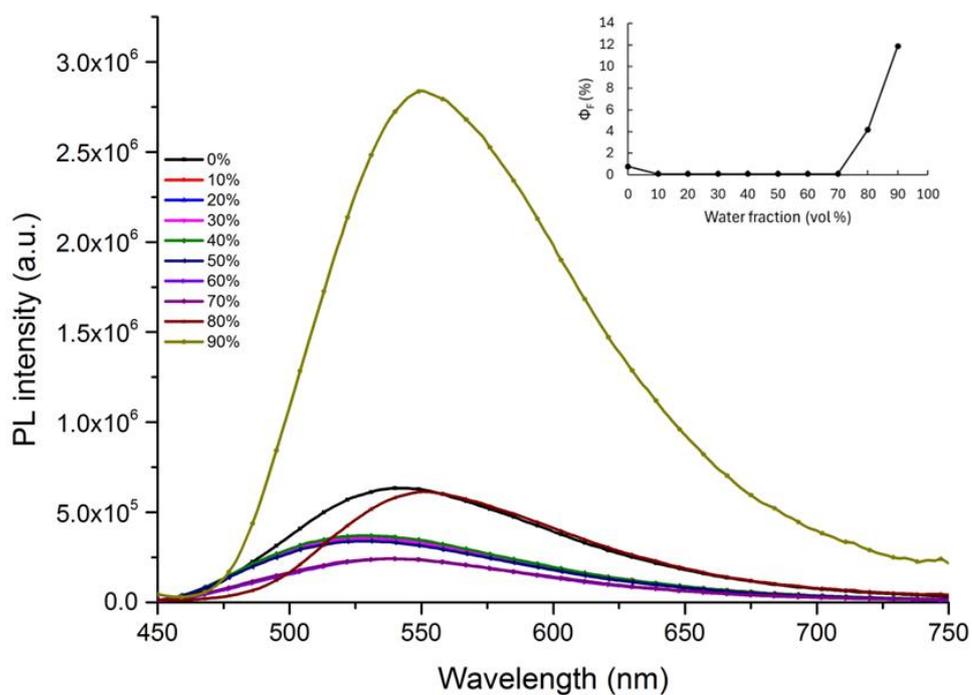
<sup>2</sup> Institute of Synthetic Chemistry, Kaunas University of Technology, K. Baršausko g. 59, LT-51423 Kaunas, Lithuania; aurimas.bieliauskas@ktu.lt

<sup>3</sup> Latvian Institute of Organic Synthesis, Aizkraukles 21, LV-1006 Rīga, Latvia; serg@osi.lv

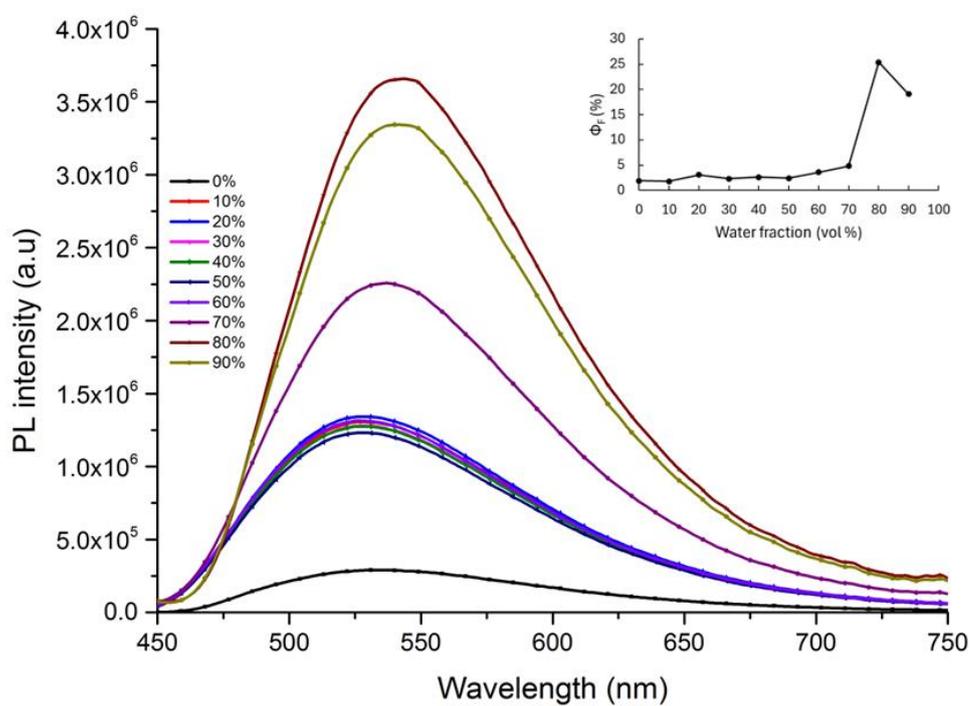
\* Correspondence: egle.arbaciauskiene@ktu.lt (E.A.); algirdas.sackus@ktu.lt (A.Š.)



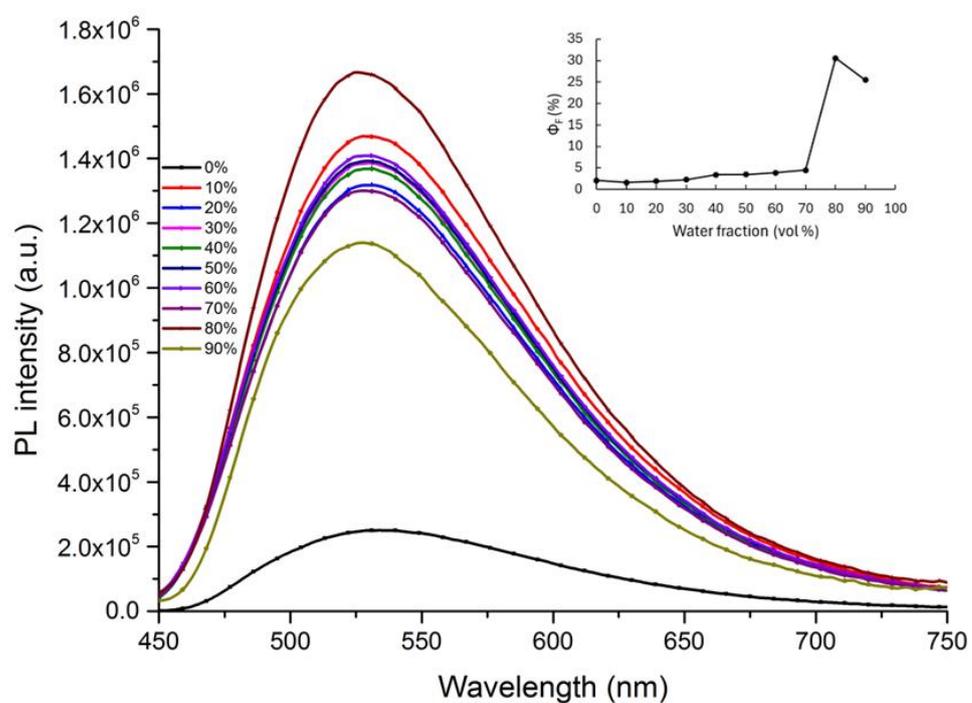
**Figure S1.** Fluorescence emission spectra of compound **4b** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.



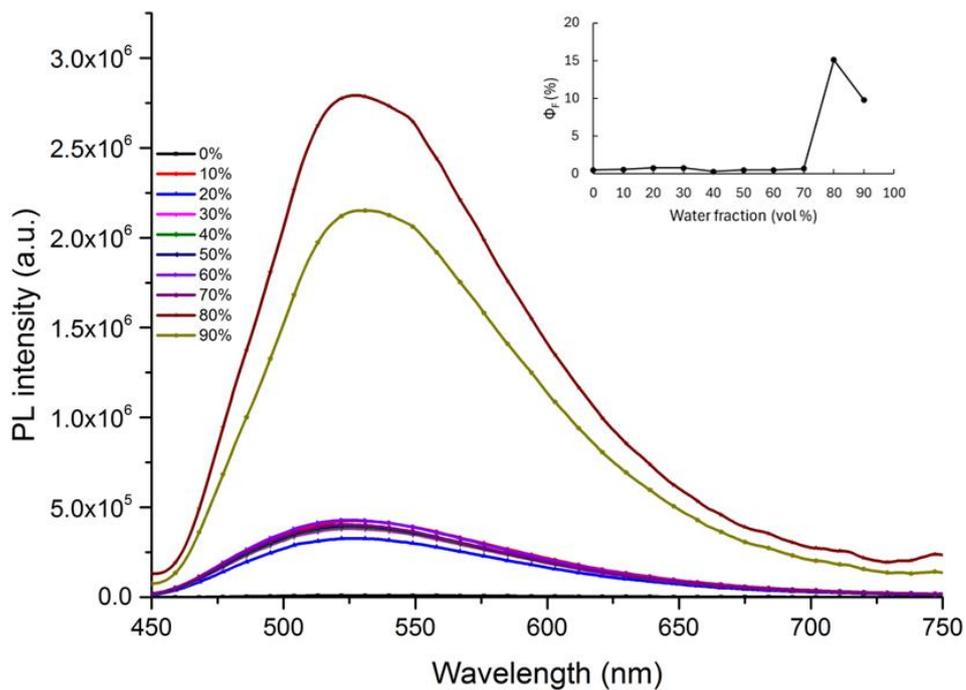
**Figure S2.** Fluorescence emission spectra of compound **4c** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.



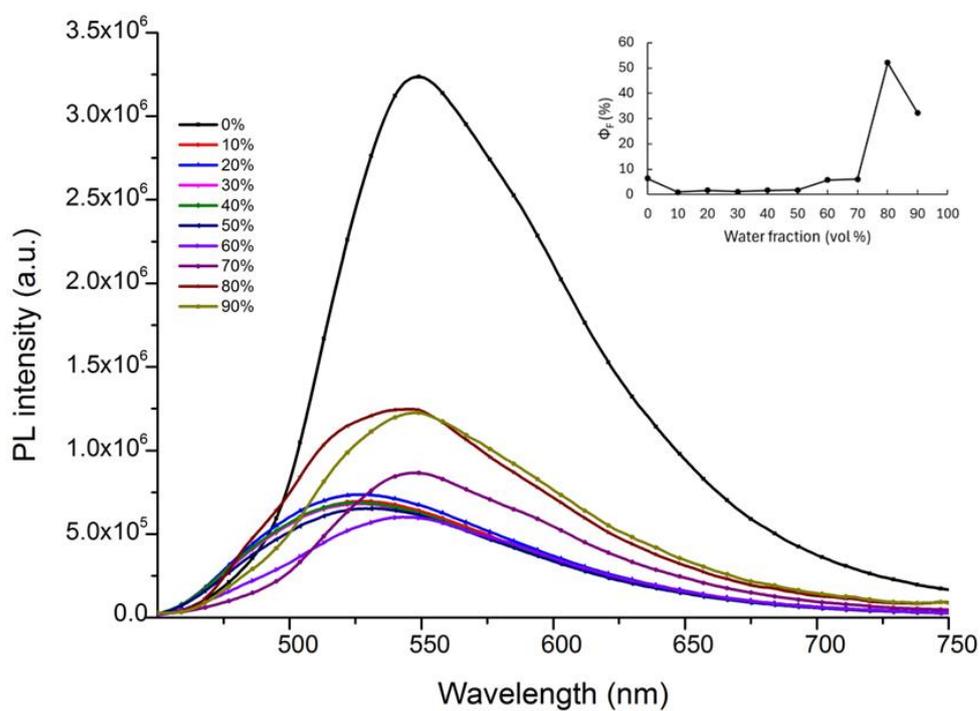
**Figure S3.** Fluorescence emission spectra of compound **4d** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.



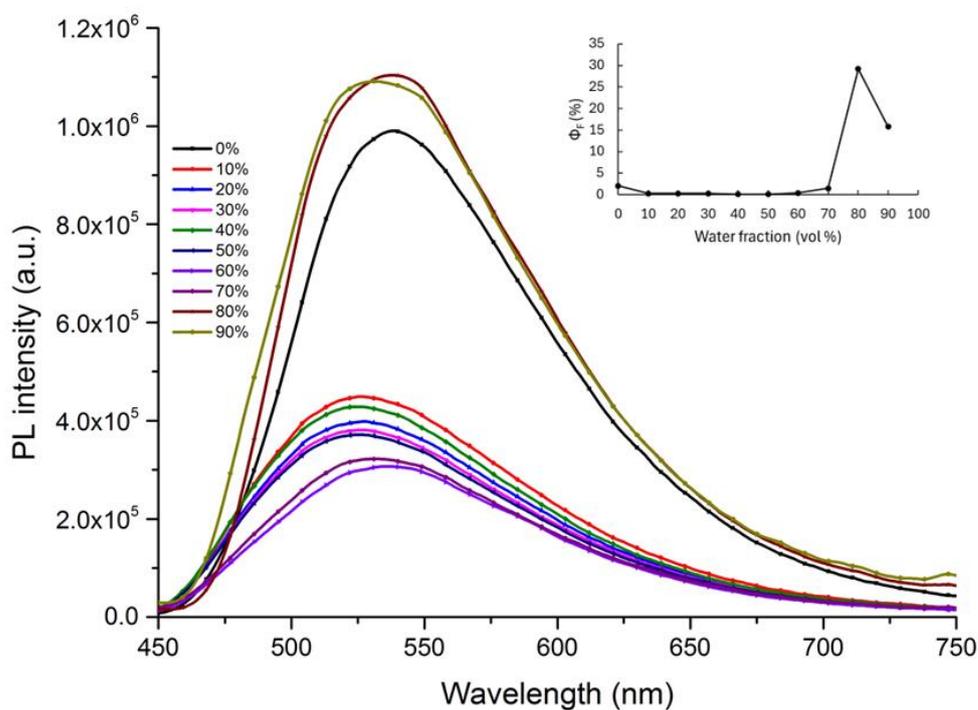
**Figure S4.** Fluorescence emission spectra of compound **4e** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.



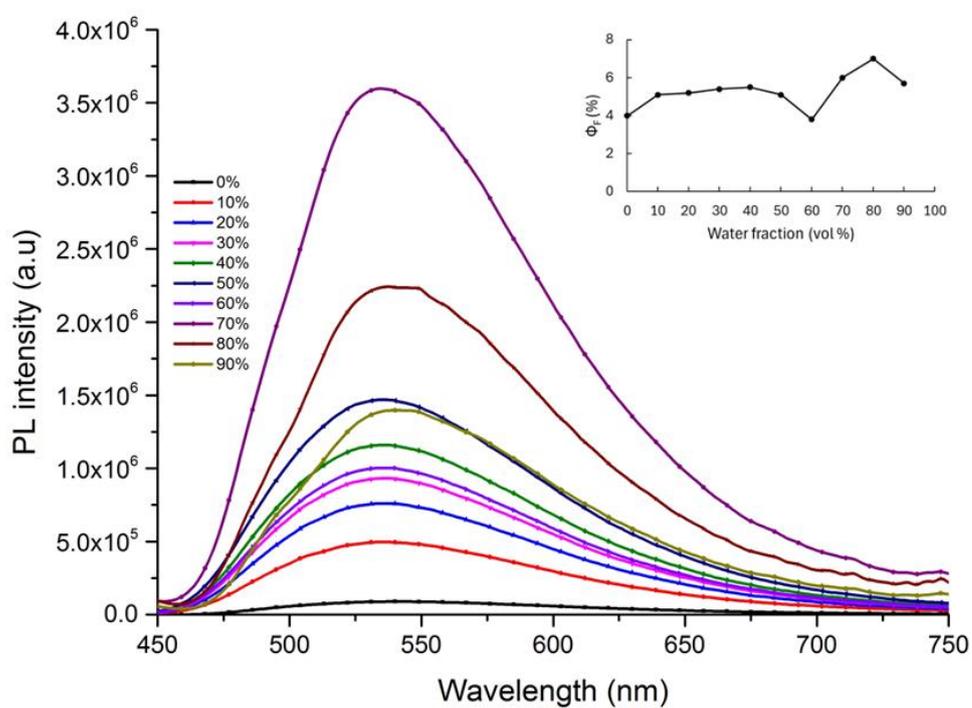
**Figure S5.** Fluorescence emission spectra of compound **4f** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.



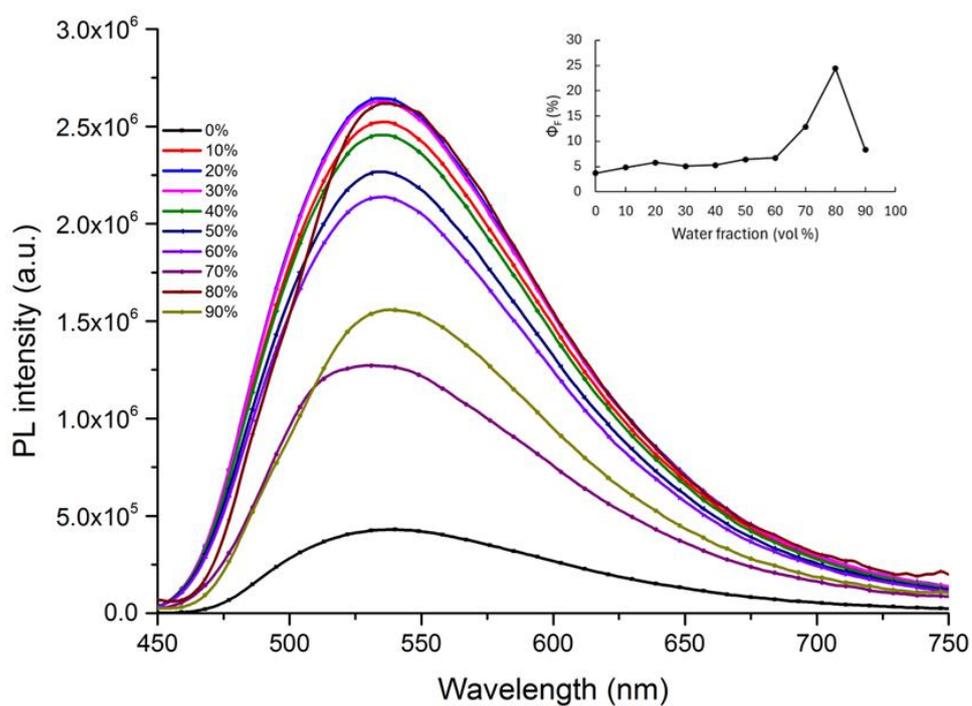
**Figure S6.** Fluorescence emission spectra of compound **4g** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.



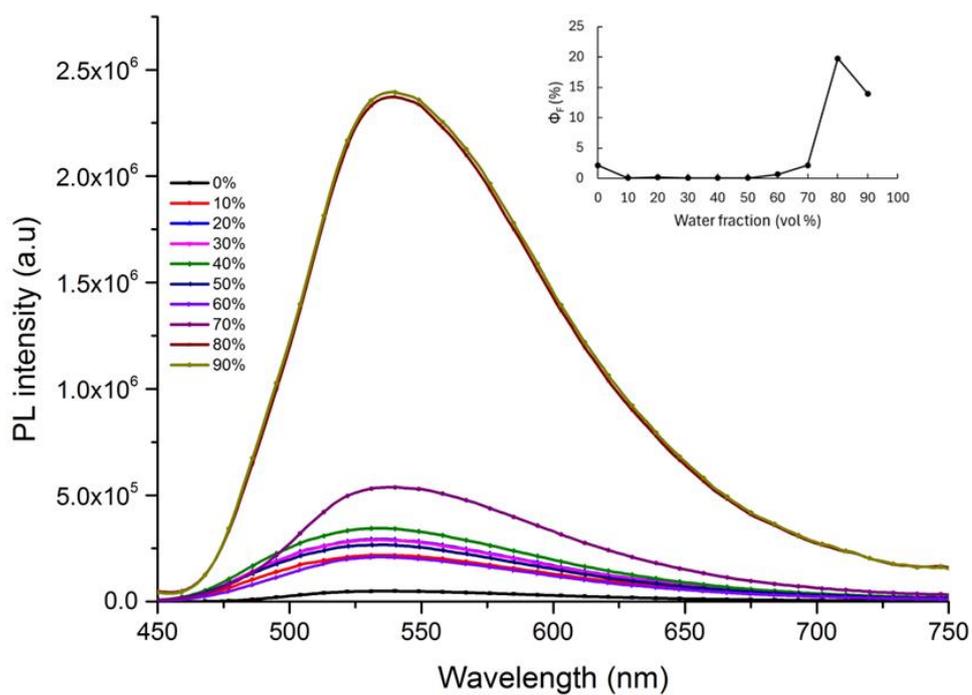
**Figure S7.** Fluorescence emission spectra of compound **4h** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.



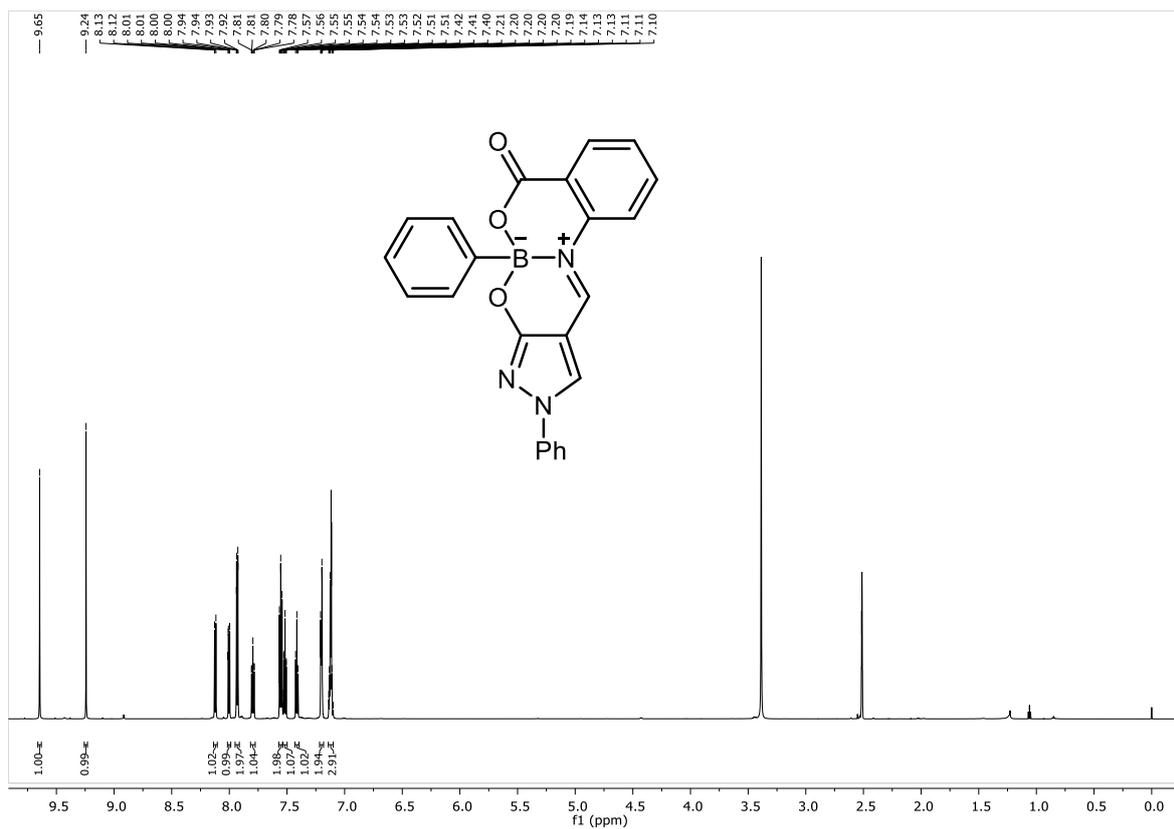
**Figure S8.** Fluorescence emission spectra of compound **4i** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction



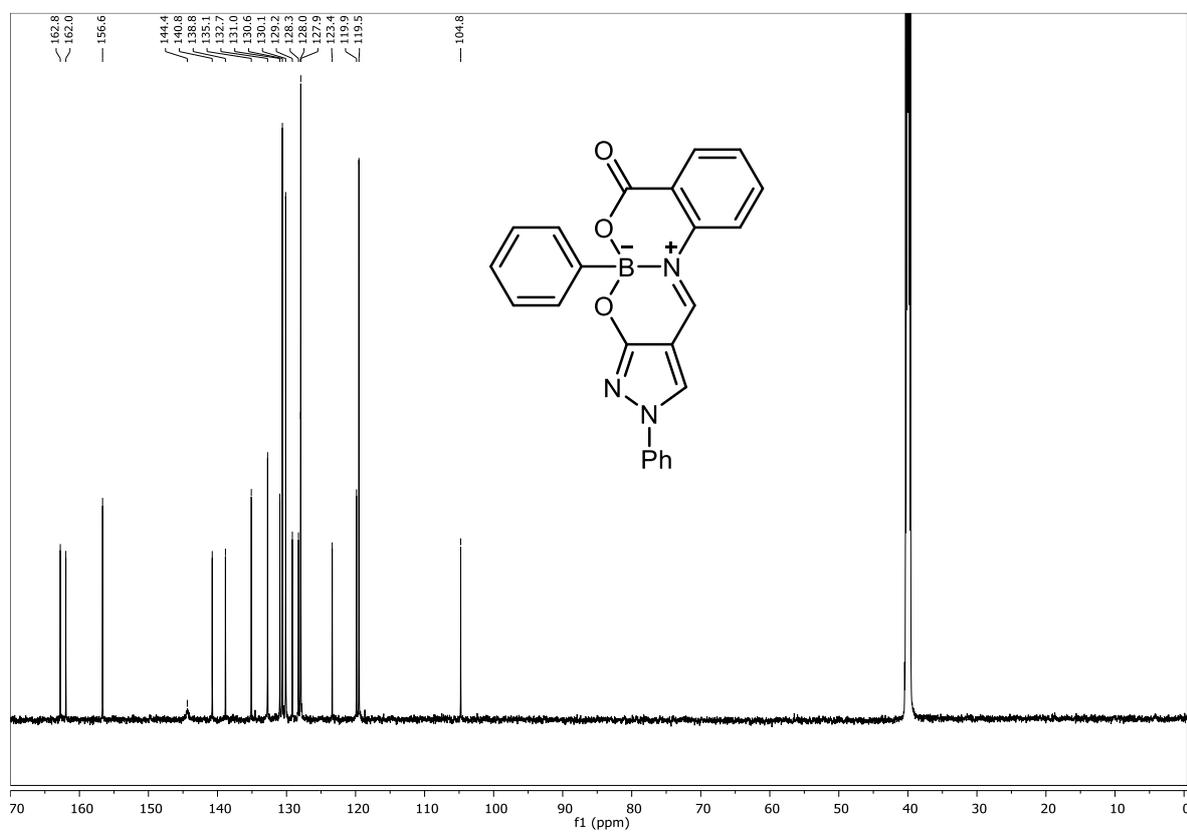
**Figure S9.** Fluorescence emission spectra of compound **4j** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.



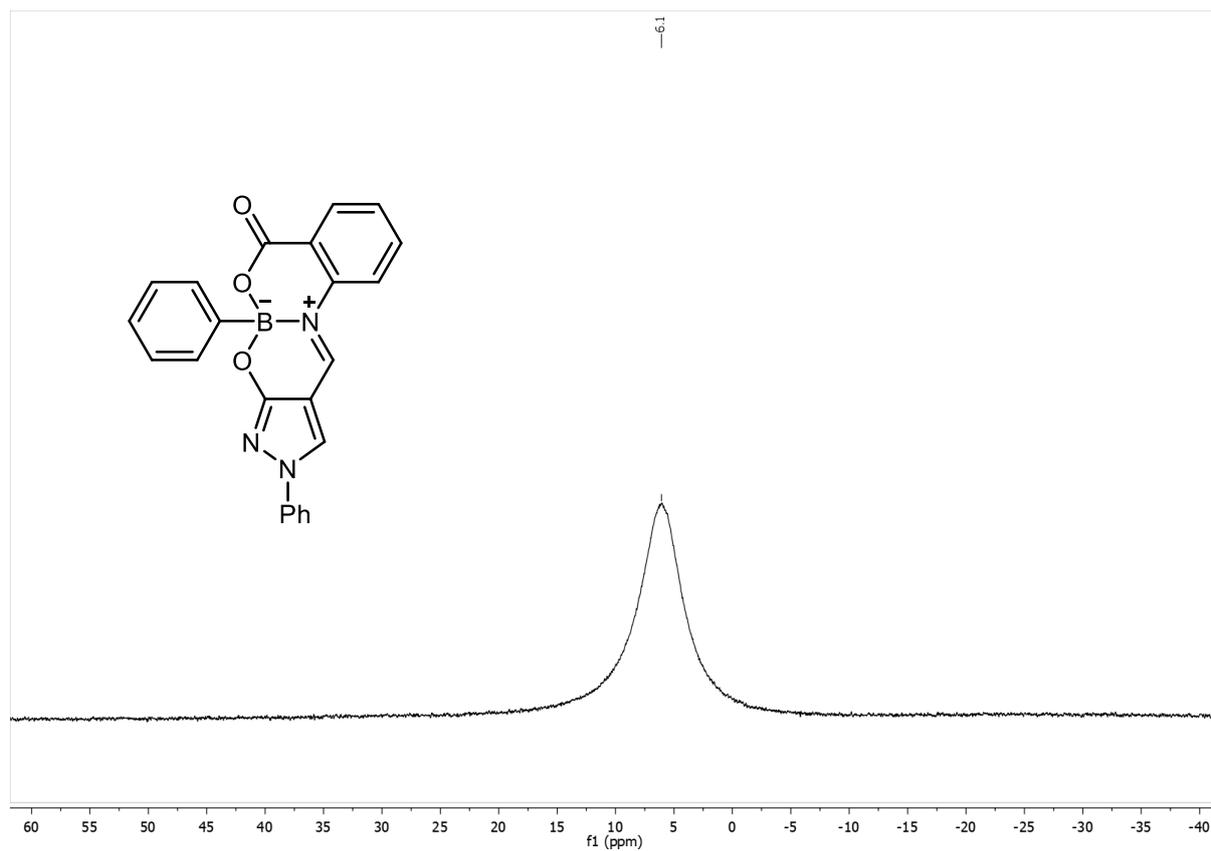
**Figure S10.** Fluorescence emission spectra of compound **4k** in mixed THF–water solutions. The insert shows the relationship between the fluorescence quantum yield and the water fraction.



**Figure S11. <sup>1</sup>H NMR (700 MHz, DMSO-*d*<sub>6</sub>) spectrum of 4a**



**Figure S12. <sup>13</sup>C NMR (176 MHz, DMSO-*d*<sub>6</sub>) spectrum of 4a**



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

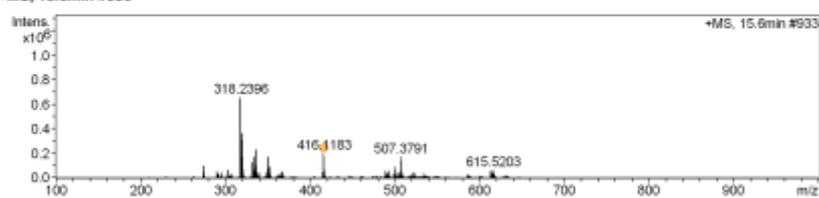
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Sample Name: VDD-224\_Boron  
Comment: AB  
Acquisition Date: 3/28/2023 8:46:51 PM  
Operator: hplc  
Instrument: micrOTOF-Q III 8228888.20448

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

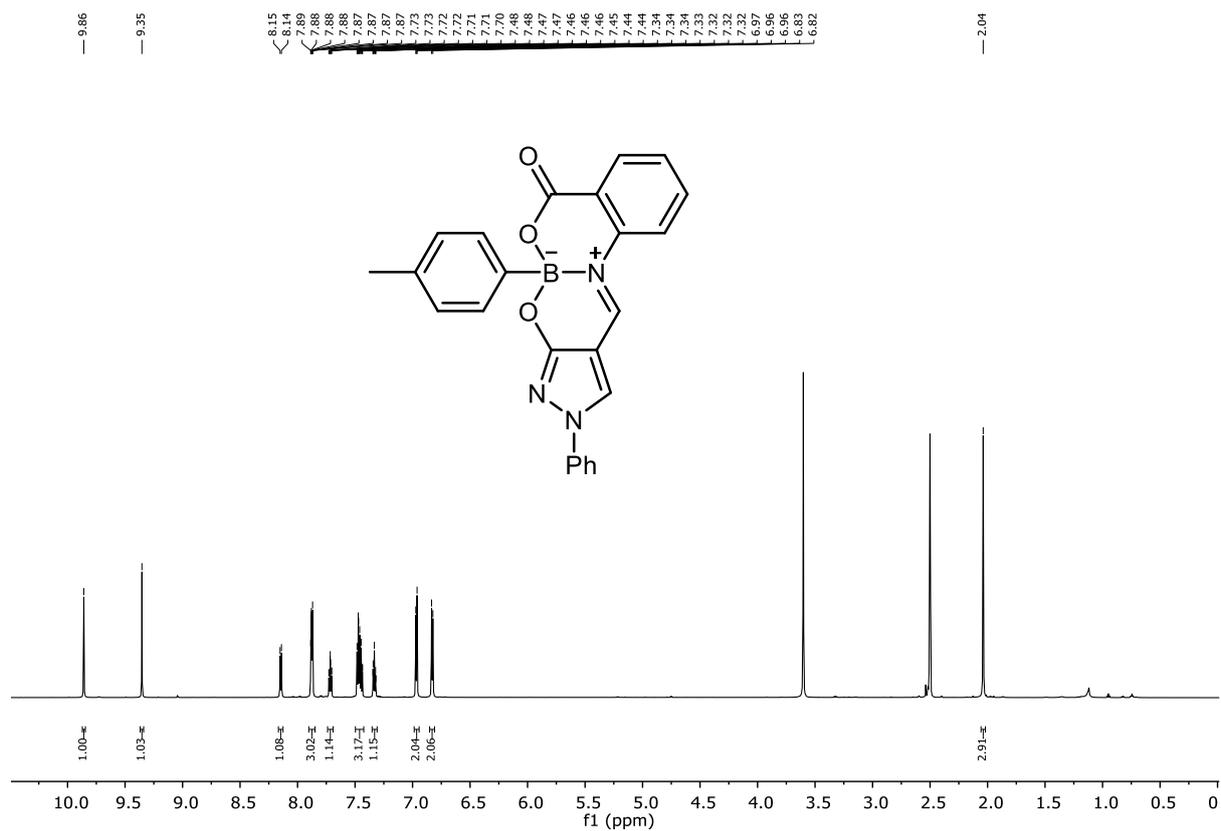
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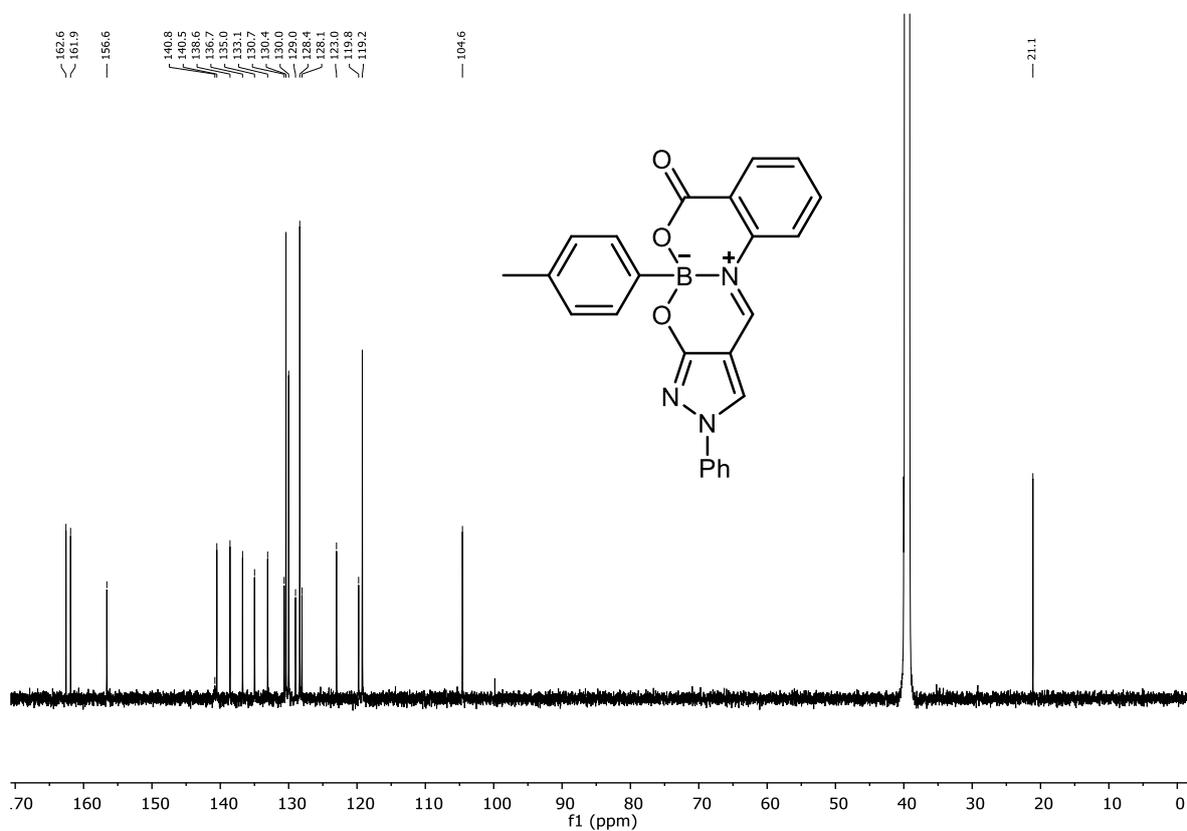


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
416.1183	1	C <sub>23</sub> H <sub>16</sub> BN <sub>3</sub> NaO <sub>3</sub>	416.1181	0.5	4.6	1	100.00	17.5	even	ok

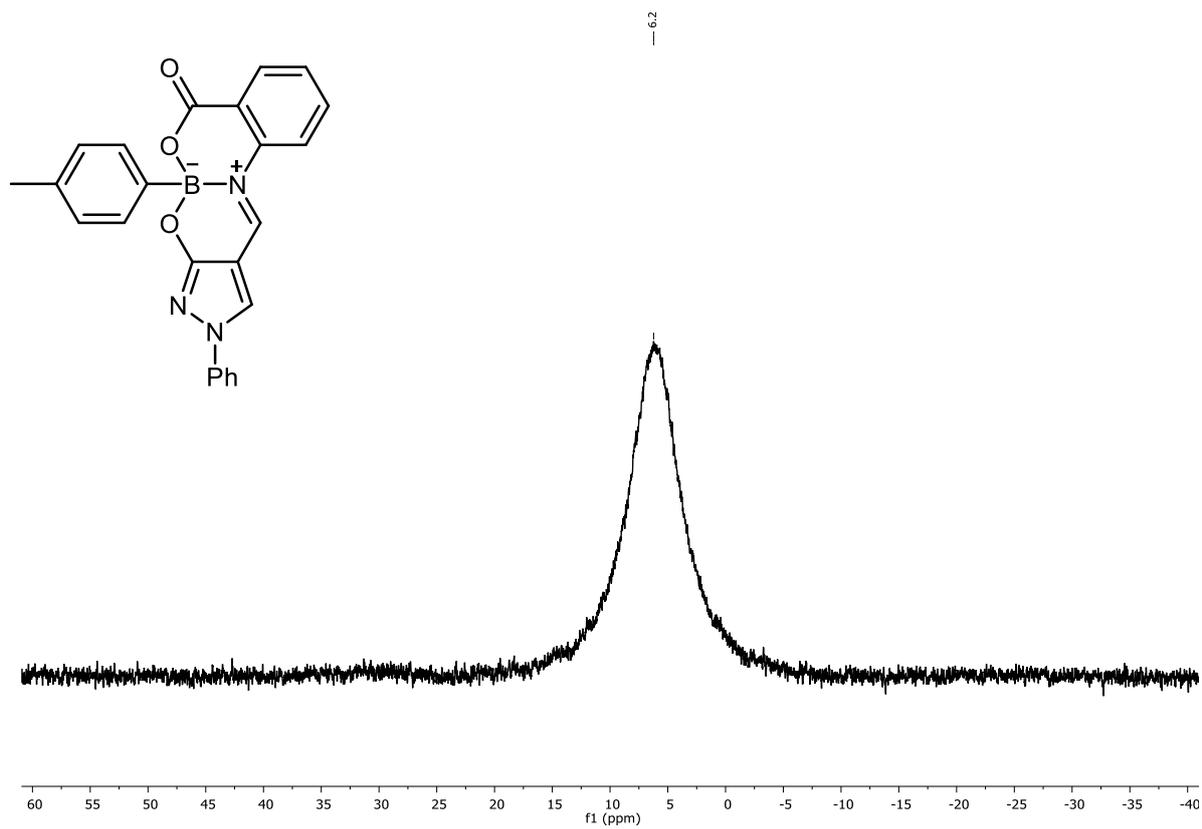
Figure S14. HRMS (ESI<sup>+</sup>) report of **4a**



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



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



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

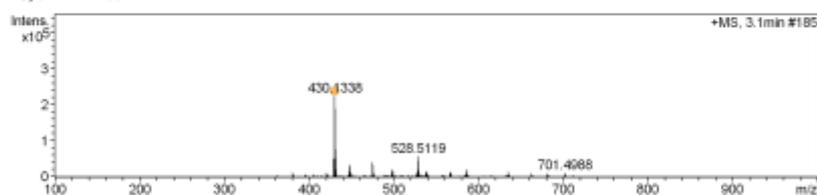
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Sample Name VDD-228  
Comment AB  
Acquisition Date 3/1/2024 7:24:27 PM  
Operator hplc  
Instrument micrOTOF-Q III 8228888.20448

**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

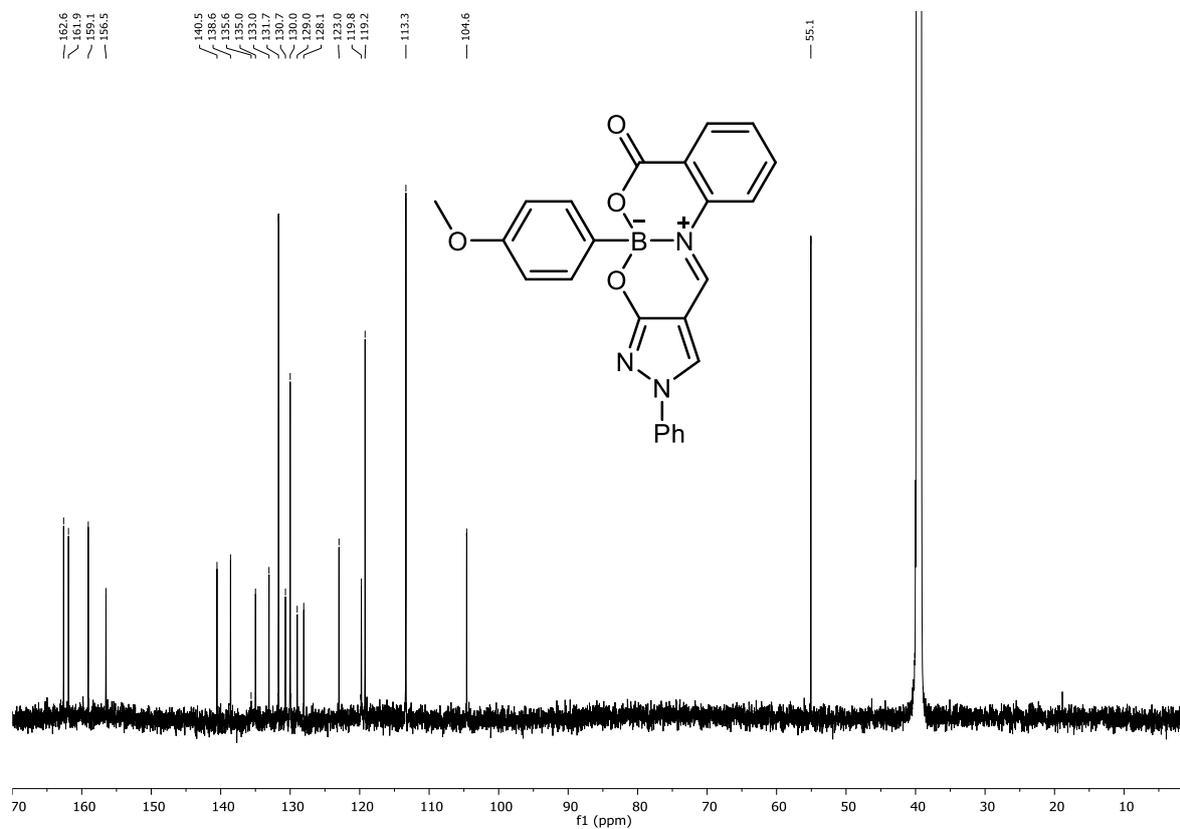
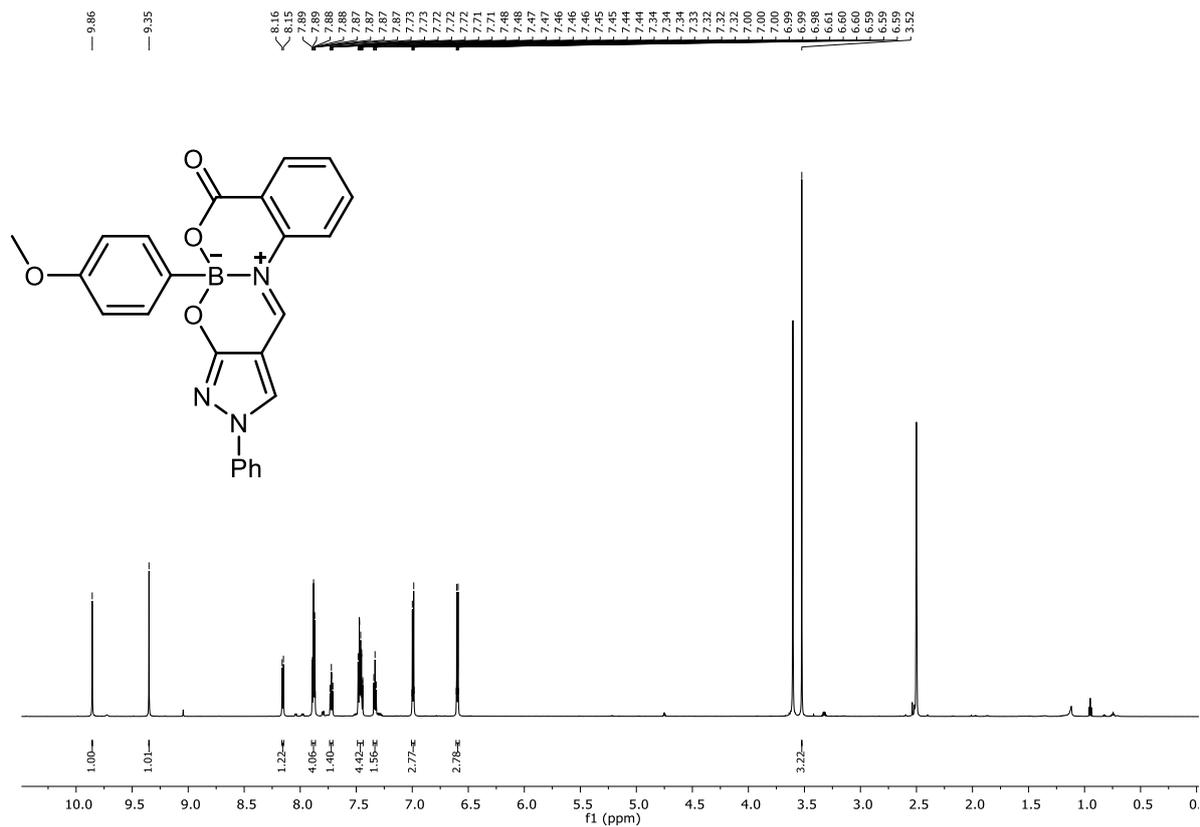
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	3.1	n.a.	Single spectrum	n.a.	n.a.	n.a.	430.1338	n.a.

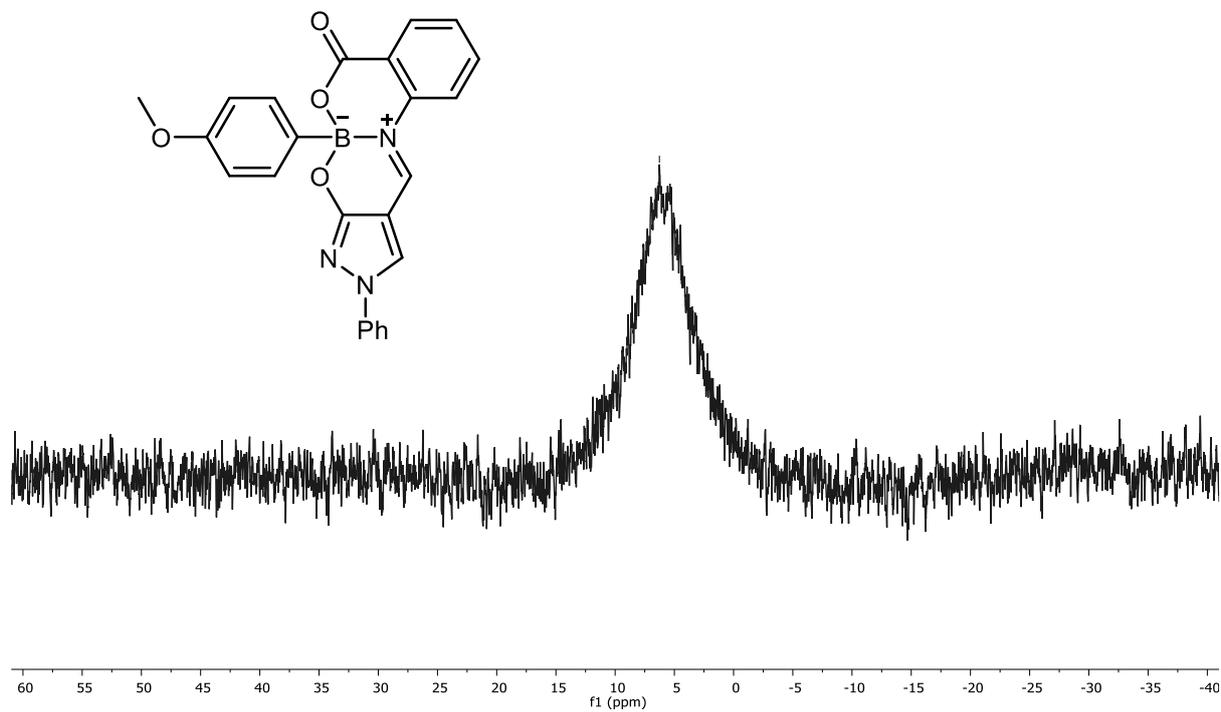
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430.1338	1	C <sub>24</sub> H <sub>18</sub> N <sub>3</sub> NaO <sub>3</sub>	430.1338	-0.1	2.7	1	100.00	17.5	even	ok

**Figure S18.** HRMS (ESI<sup>+</sup>) report of **4b**





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

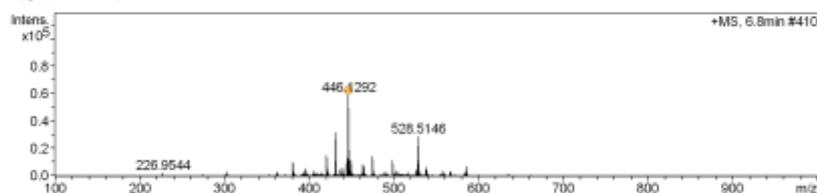
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Sample Name: VDD-227  
Comment: AB  
Acquisition Date: 3/1/2024 6:55:13 PM  
Operator: hplc  
Instrument: micrOTOF-Q III 8228888.20448

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

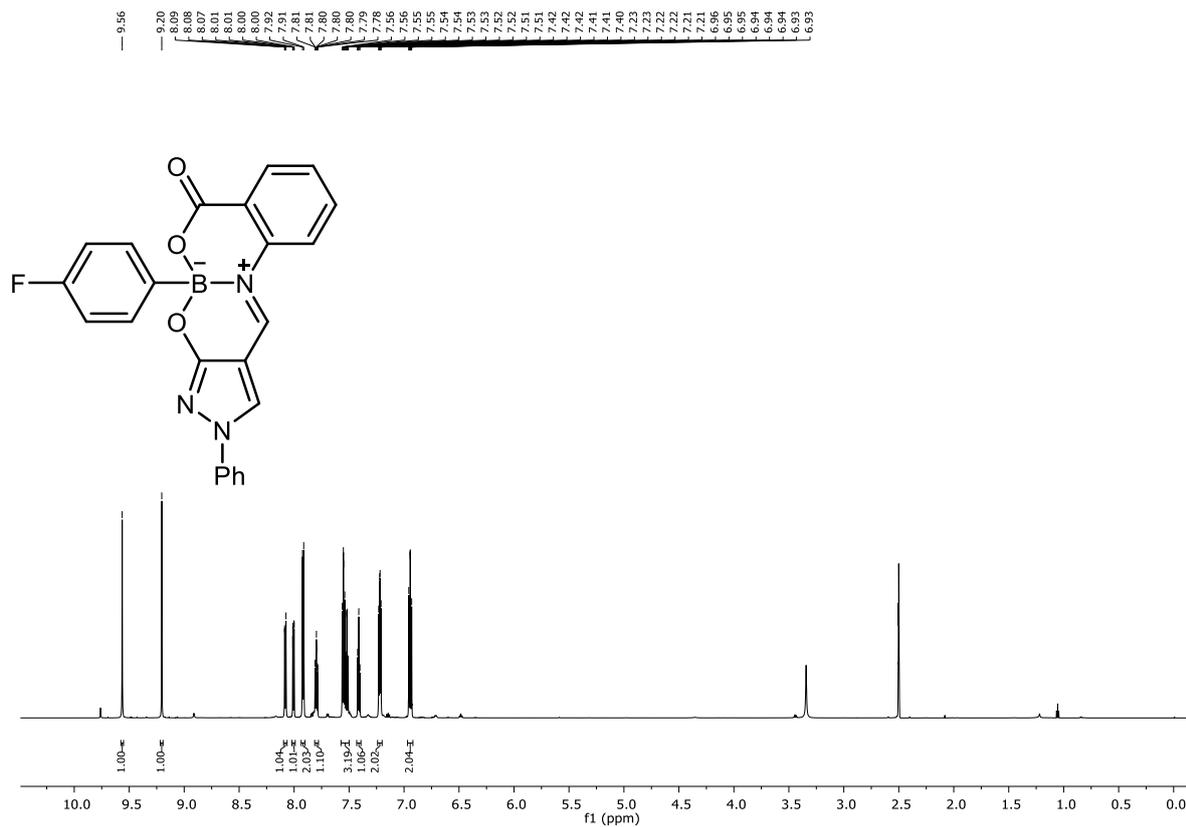
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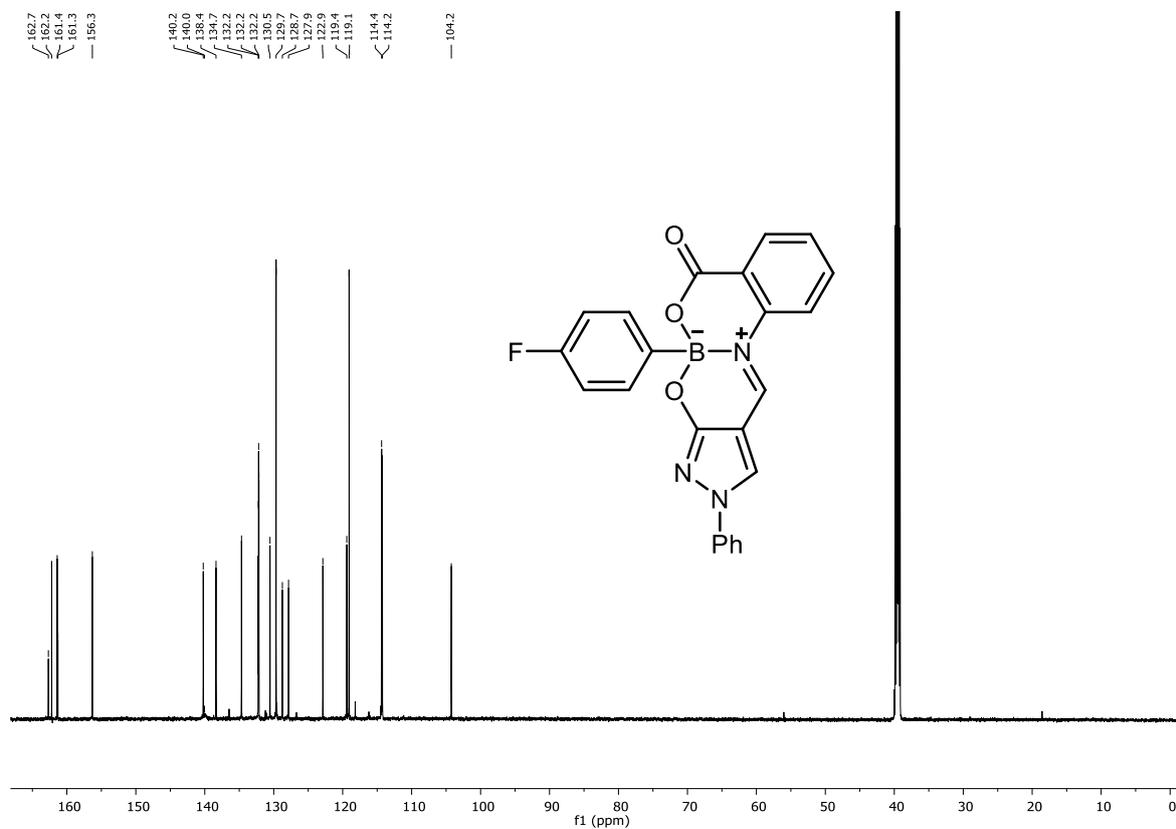


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
446.1292	1	C <sub>24</sub> H <sub>18</sub> N <sub>3</sub> NaO <sub>4</sub>	446.1287	1.3	11.7	4	100.00	17.5	even	ok

Figure S22. HRMS (ESI<sup>+</sup>) report of **4c**



**Figure S23.** <sup>1</sup>H NMR (700 MHz, DMSO-*d*<sub>6</sub>) spectrum of 4d



**Figure S24.** <sup>13</sup>C NMR (176 MHz, DMSO-*d*<sub>6</sub>) spectrum of 4d

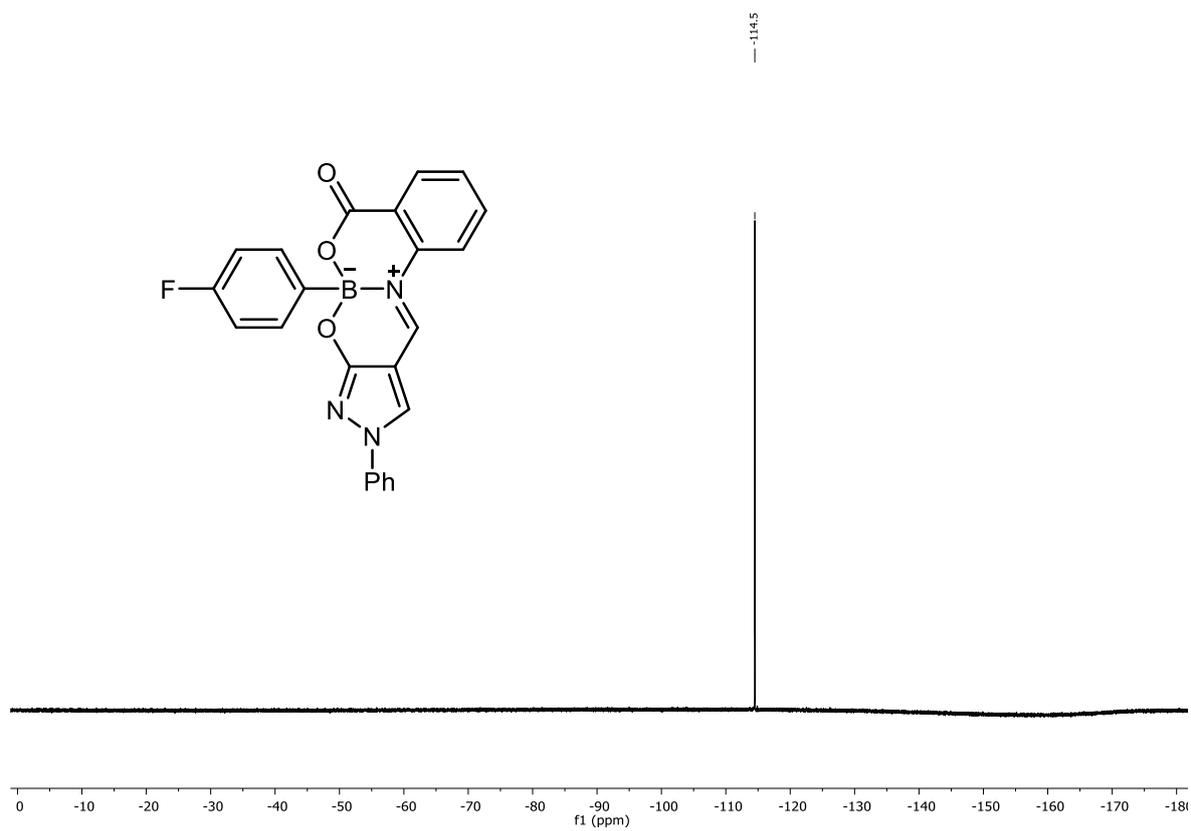


Figure S25.  $^{19}\text{F}$  NMR (376 MHz,  $\text{DMSO-}d_6$ ) spectrum of 4d

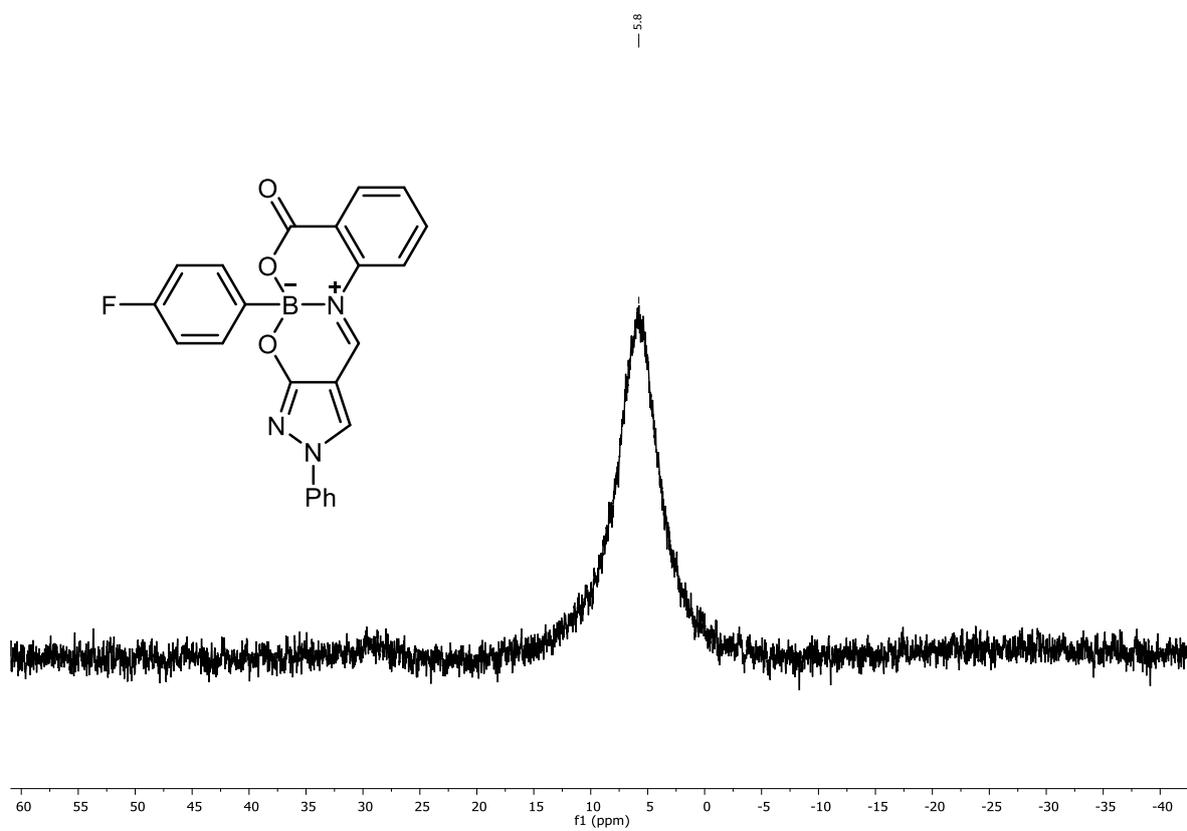


Figure S26.  $^{11}\text{B}$  NMR (128 MHz,  $\text{DMSO-}d_6$ ) spectrum of 4d

## Compound Spectrum SmartFormula Report

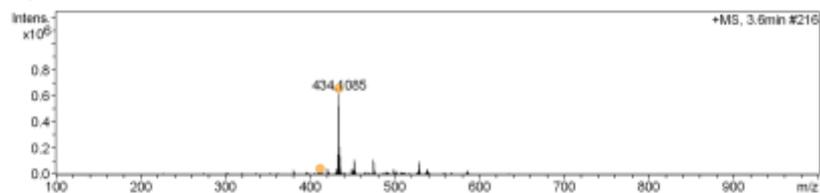
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Method	DirectInfusion_TuneLow_pos.m	Operator hplc
Sample Name	VDD-230	Instrument micrOTOF-Q III 8228888.20448
Comment	AB	

<b>Acquisition Parameter</b>					
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Focus	Not active	Set Capillary	4500 V	Set Dry Heater	180 °C
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Scan End	1000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste



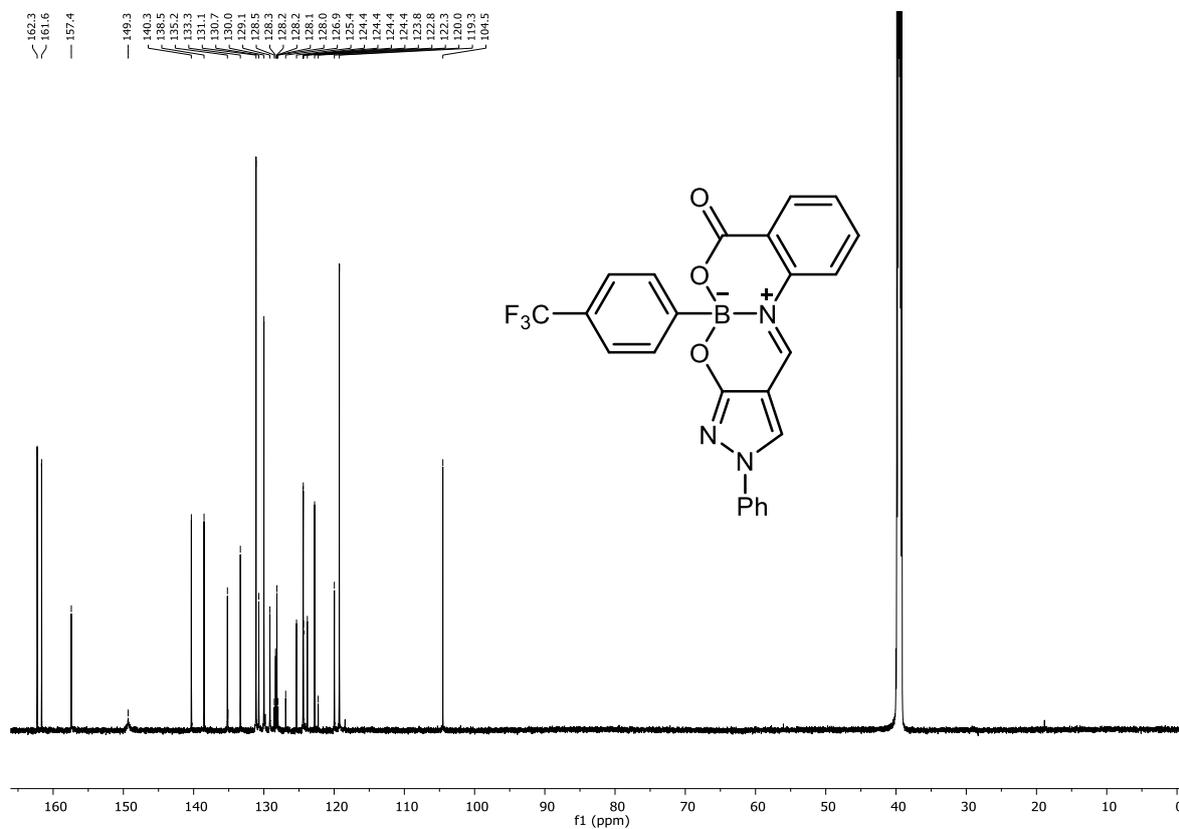
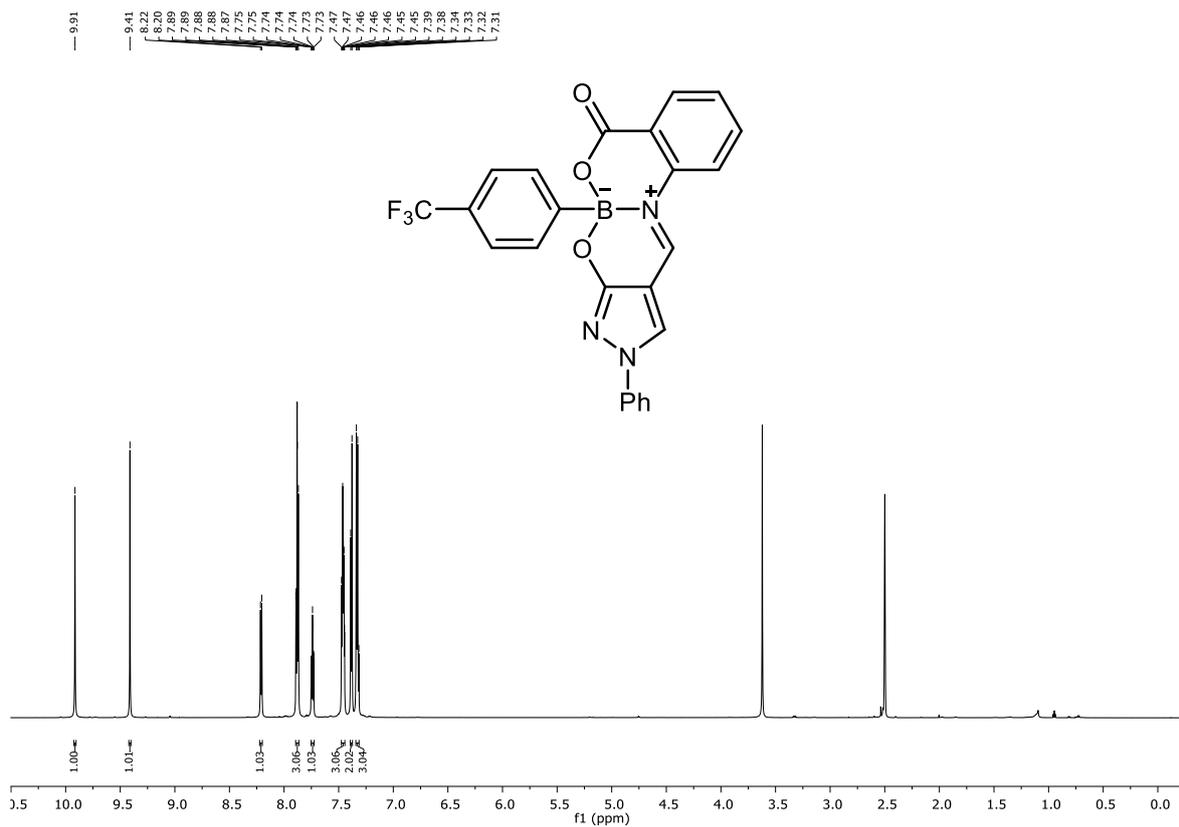
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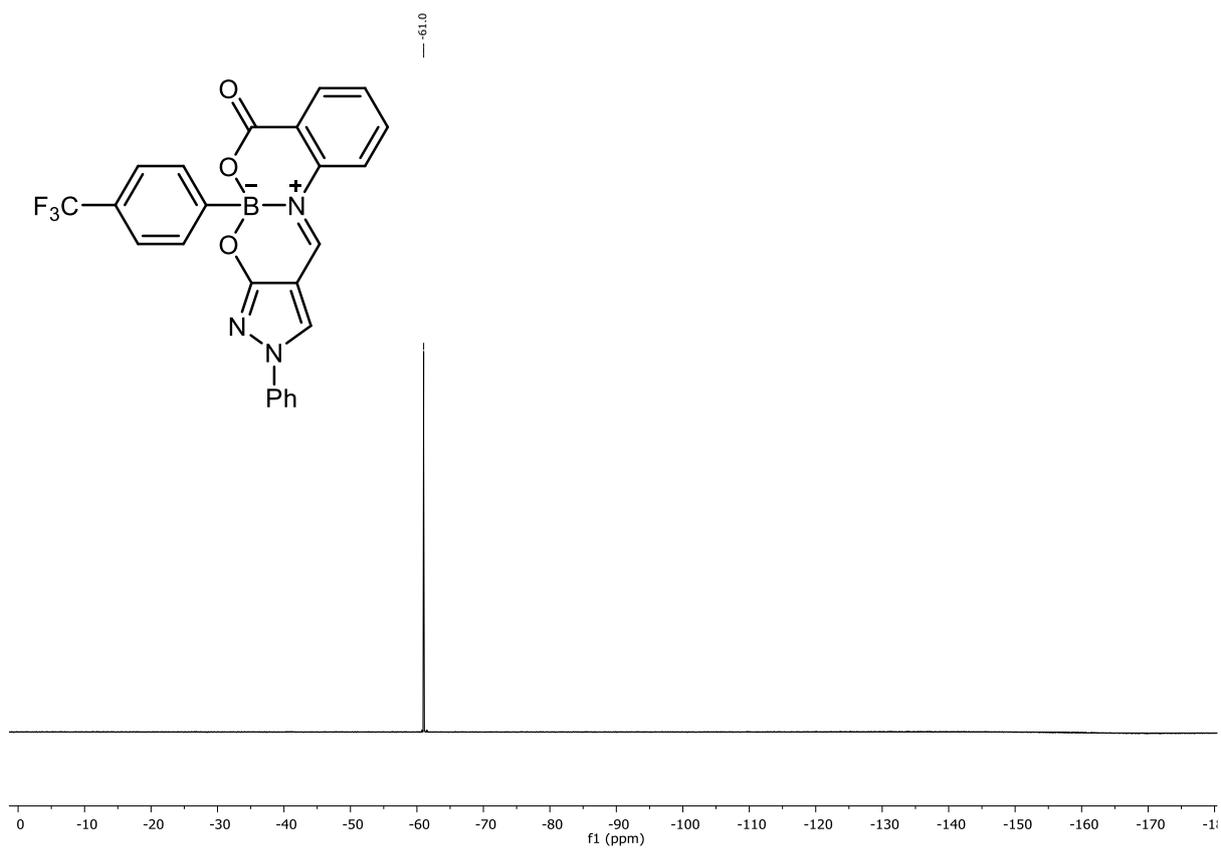
**+MS, 3.6min #216**



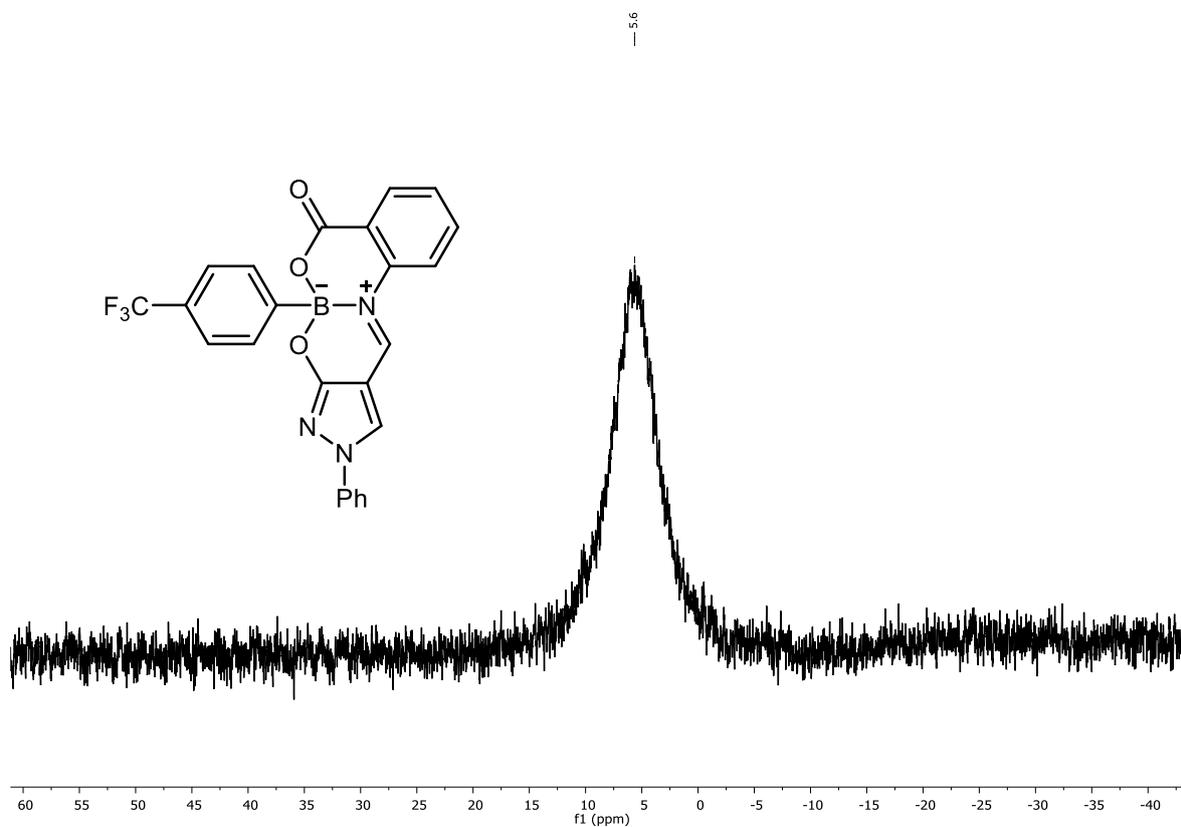
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
412.1257	1	C23H16BFN3O3	412.1257	2.6	84.1	1	100.00	17.5	even	ok
434.1085	1	C23H15BFN3NaO3	434.1087	0.5	8.0	2	100.00	17.5	even	ok

**Figure S27. HRMS (ESI<sup>+</sup>) report of 4d**





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



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

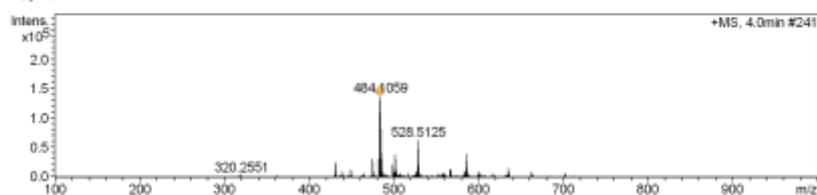
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Sample Name: VDD-231  
Comment: AB  
Acquisition Date: 3/3/2024 6:47:20 PM  
Operator: hplc  
Instrument: micrOTOF-Q III 8228888.20448

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Focus: Not active  
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Scan End: 1000 m/z  
Ion Polarity: Positive  
Set Capillary: 4500 V  
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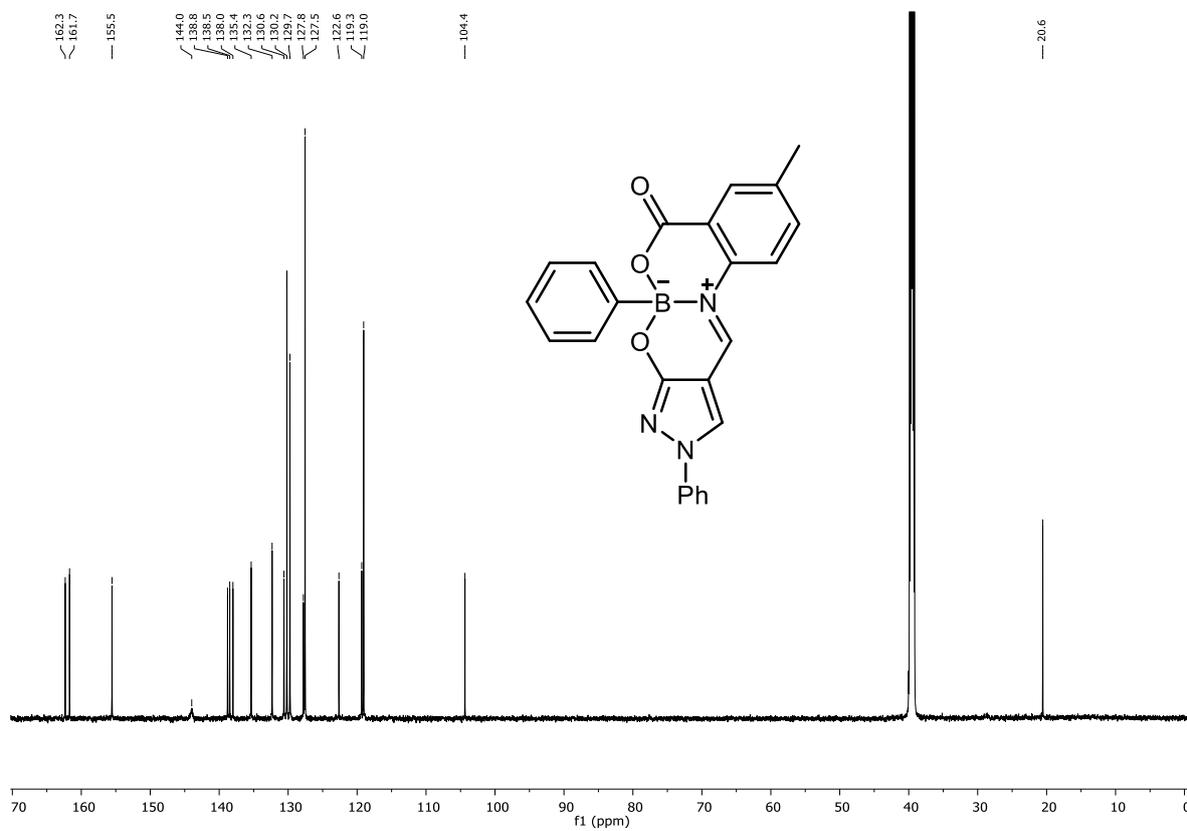
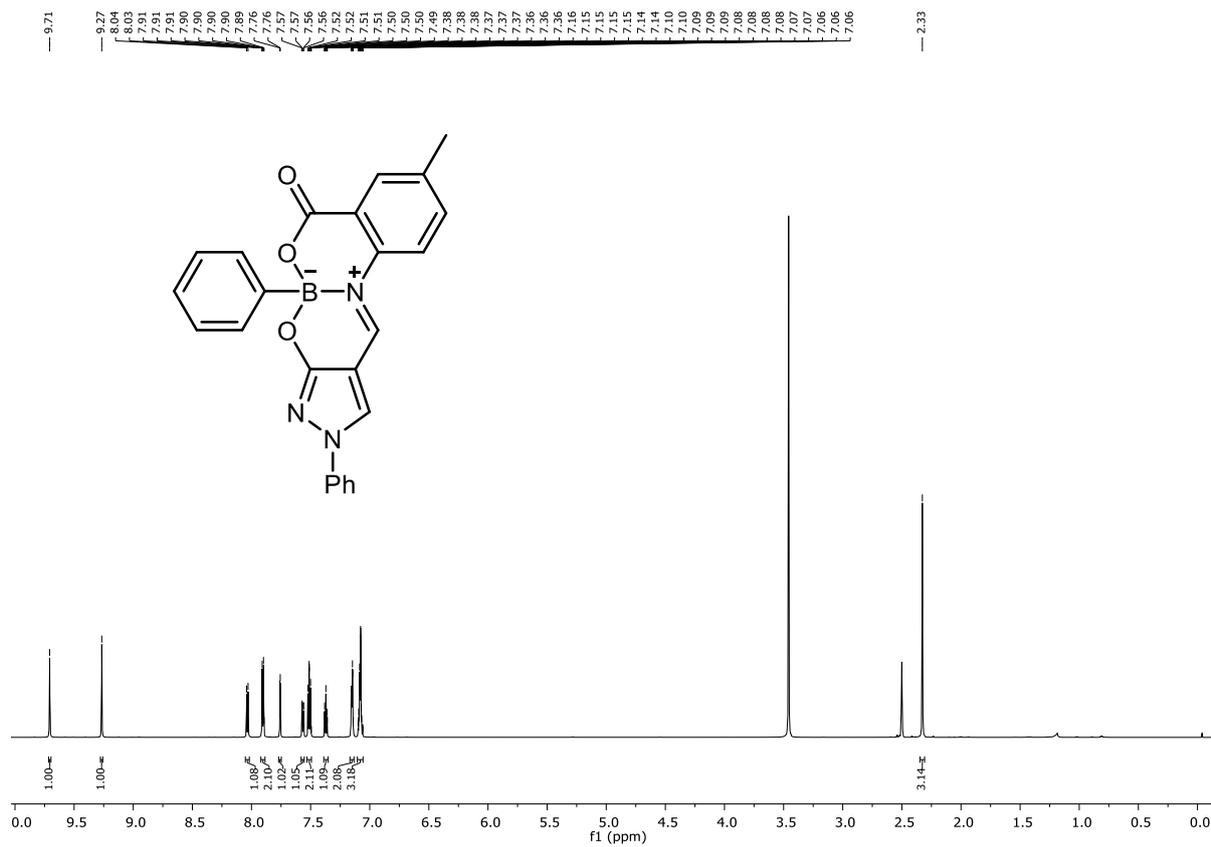
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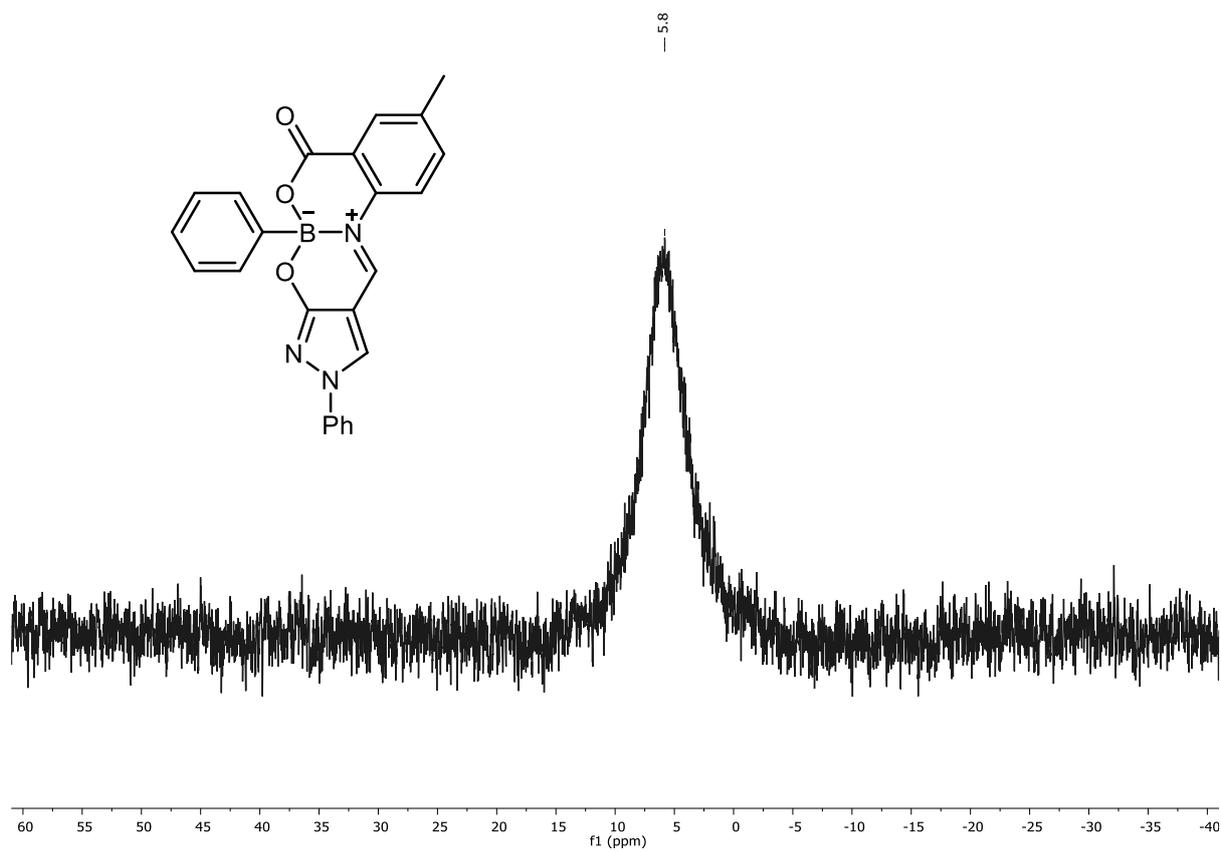
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484.1059	1	C <sub>24</sub> H <sub>15</sub> BF <sub>3</sub> N <sub>3</sub> NaO <sub>3</sub>	484.1055	-0.7	5.7	3	100.00	17.5	even	ck

Figure S32. HRMS (ESI<sup>+</sup>) report of **4e**





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

## Compound Spectrum SmartFormula Report

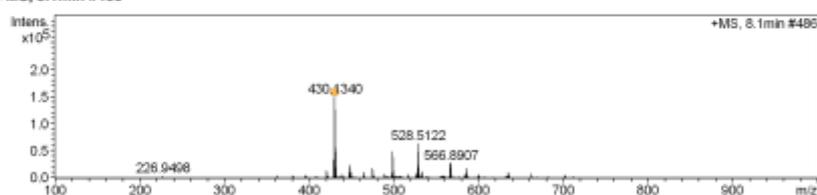
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Method	DirectInfusion_TuneLow_pos.m	Instrument	micrOTOF-Q III 8228888.20448
Sample Name	VDD-242		
Comment	AB		

<b>Acquisition Parameter</b>					
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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



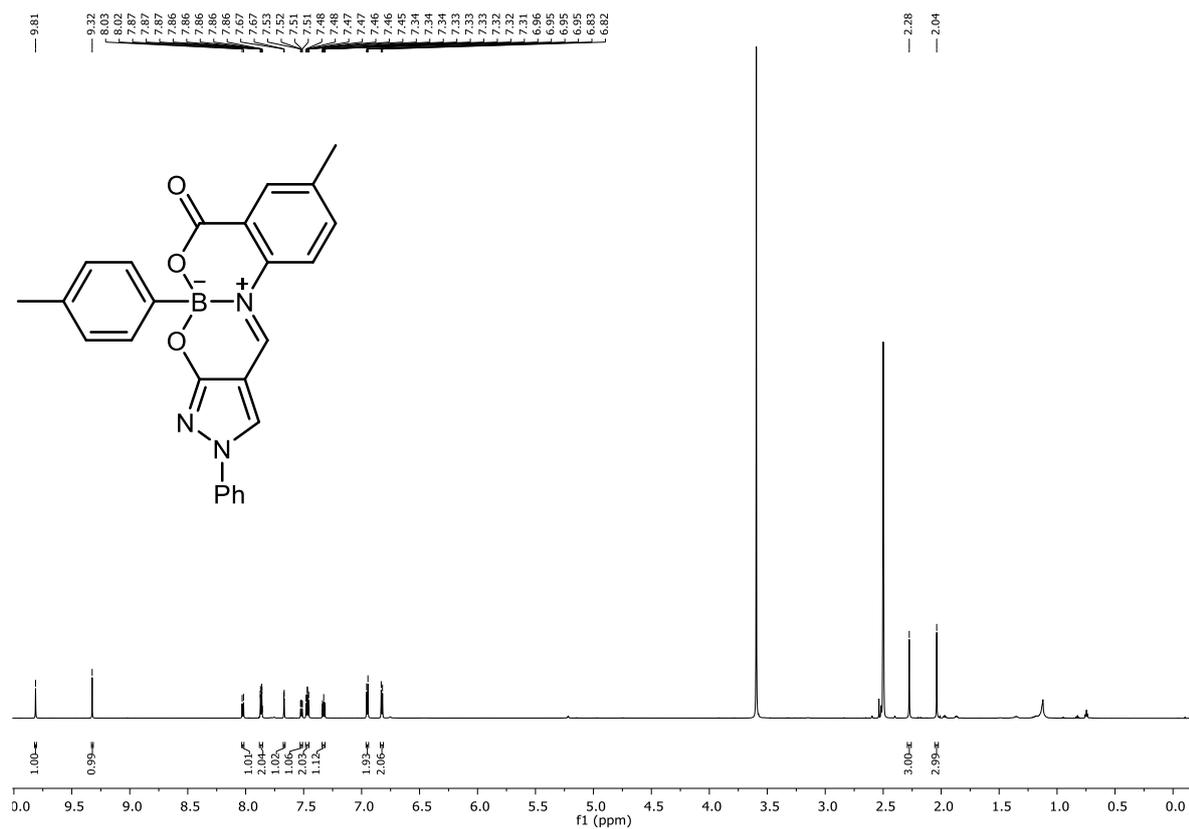
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n.a.	8.1	n.a.	Single spectrum	n.a.	n.a.	n.a.	430.1340	n.a.

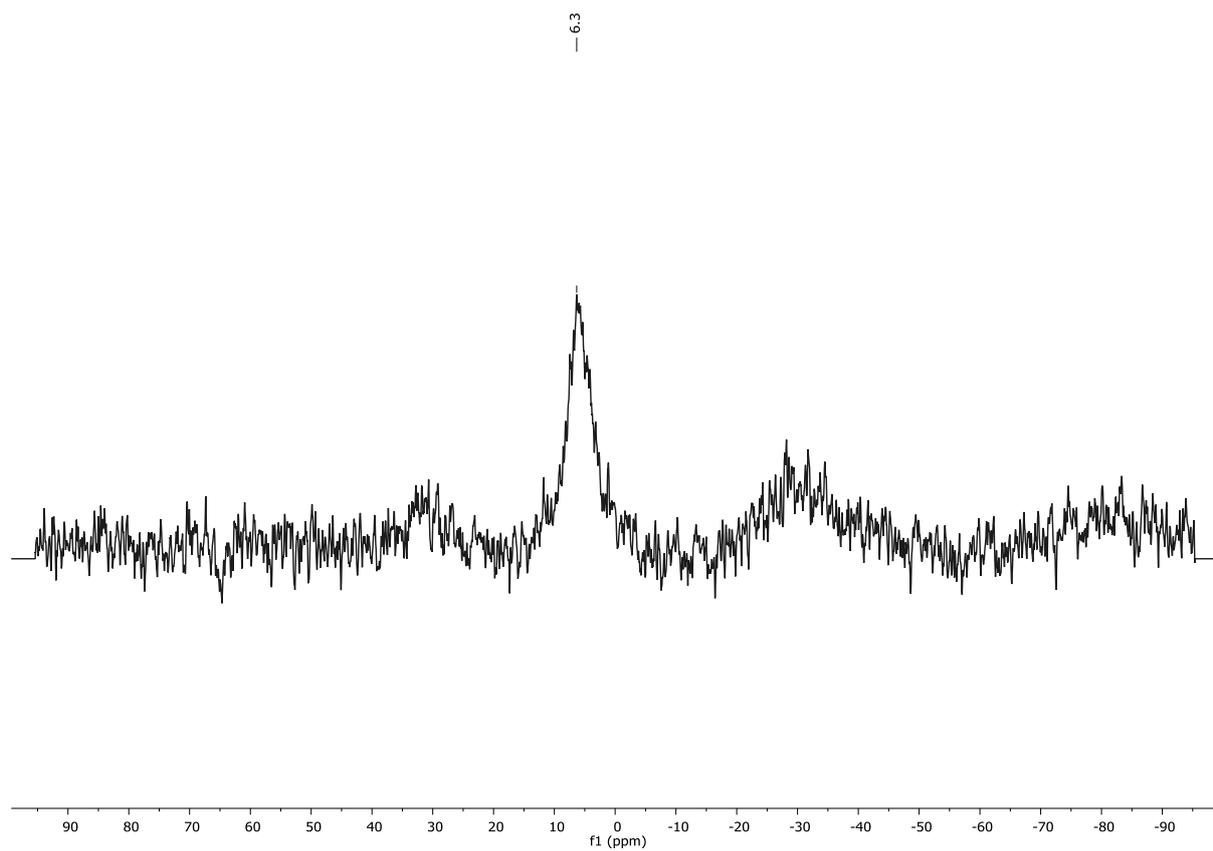
**+MS, 8.1min #486**



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430.1340	1	C <sub>24</sub> H <sub>18</sub> BN <sub>3</sub> NaO <sub>3</sub>	430.1338	0.4	3.6	1	100.00	17.5	even	ok

**Figure S36.** HRMS (ESI<sup>+</sup>) report of **4f**





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

## Compound Spectrum SmartFormula Report

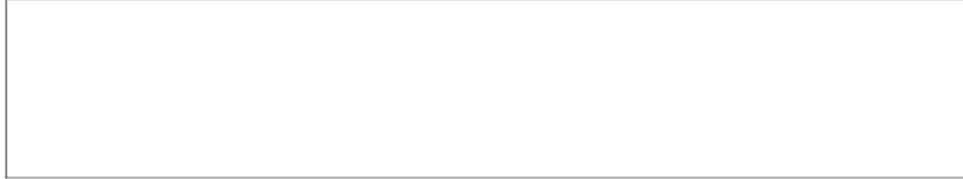
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Method DirectInfusion\_TuneLow\_pos.m  
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Comment AB

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Instrument micrOTOF-Q III 8228888.20448

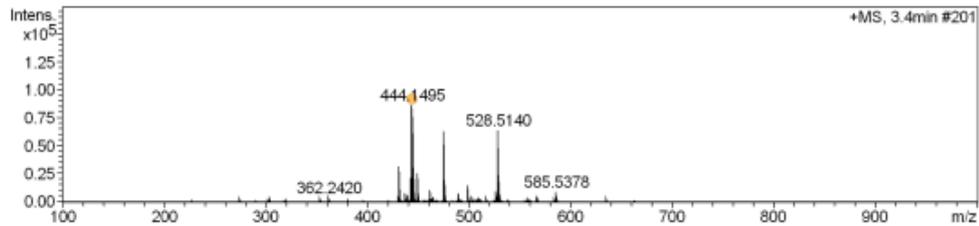
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Scan End	1000 m/z	Set Collision Cell RF	140.0 Vpp	Set Divert Valve	Waste



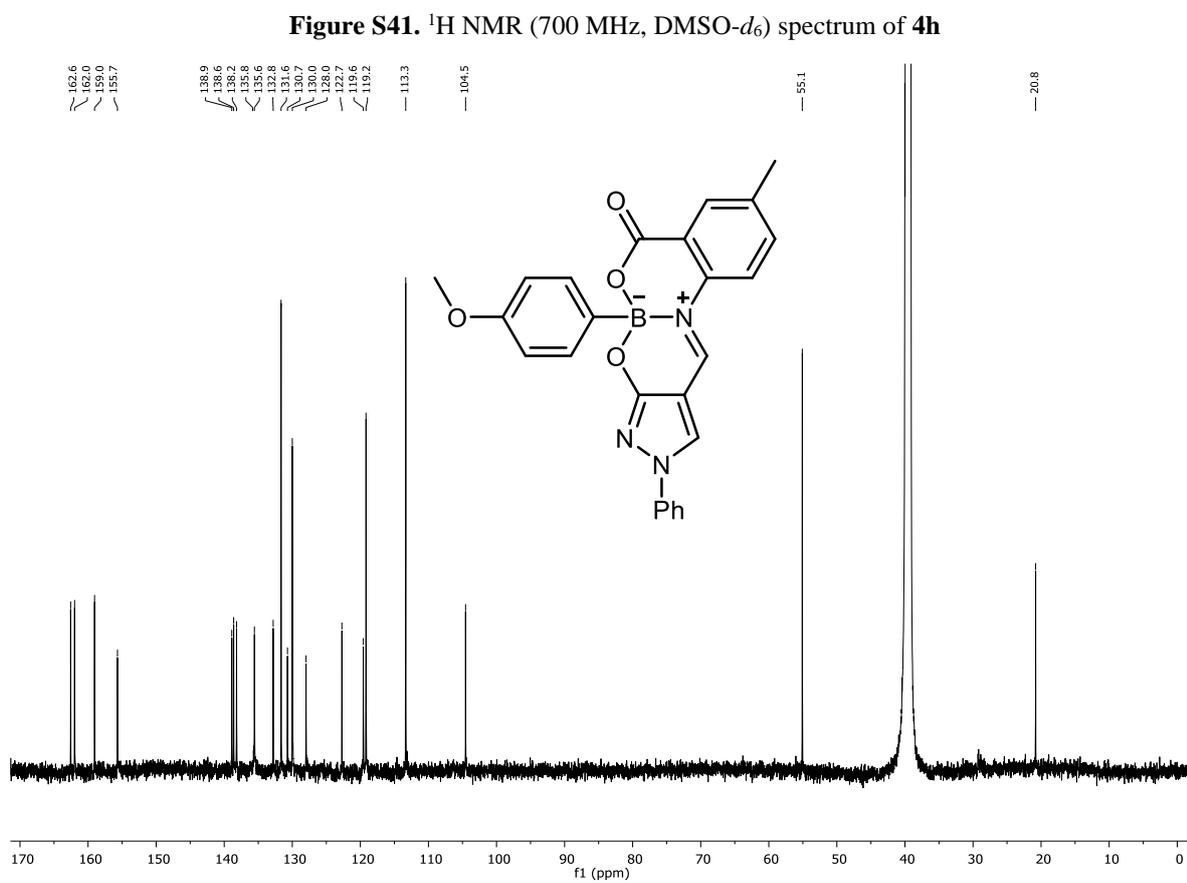
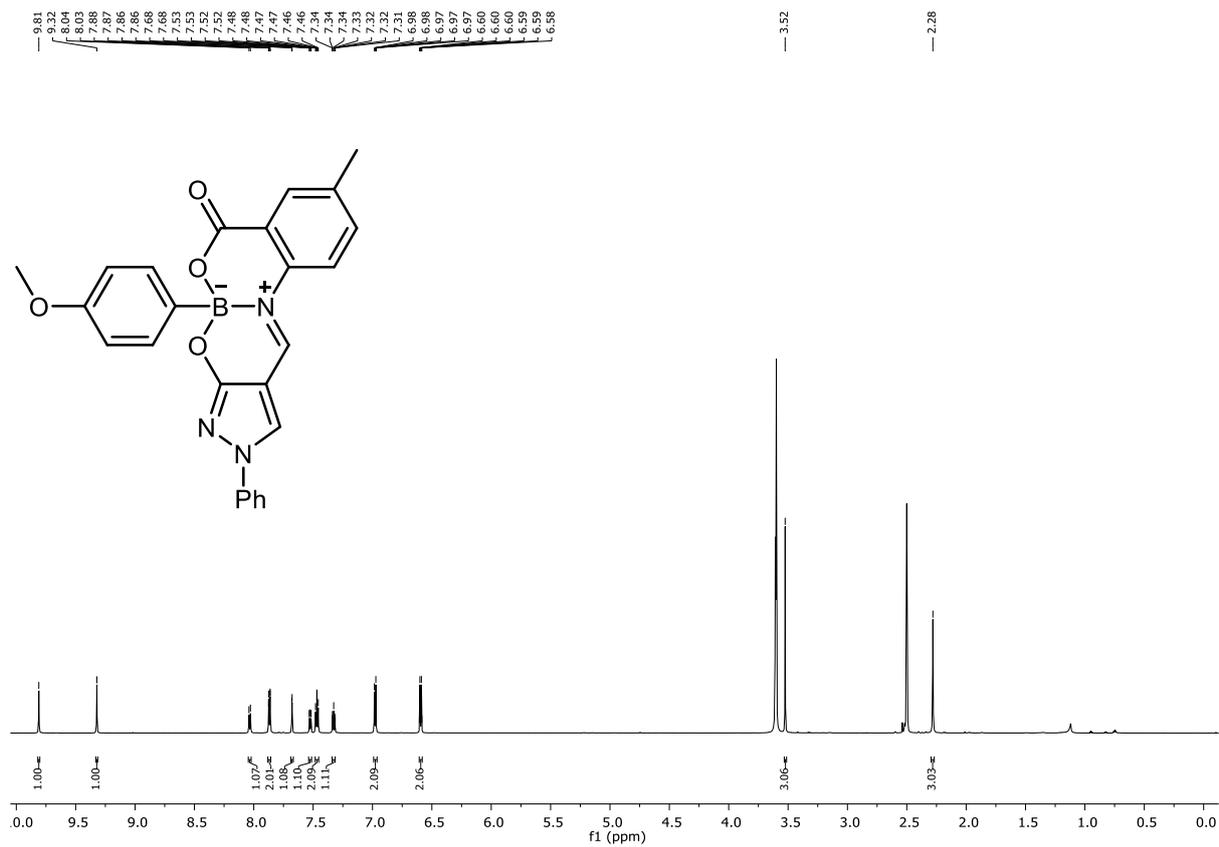
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n.a.	3.4	n.a.	Single spectrum	n.a.	n.a.	n.a.	444.1495	n.a.

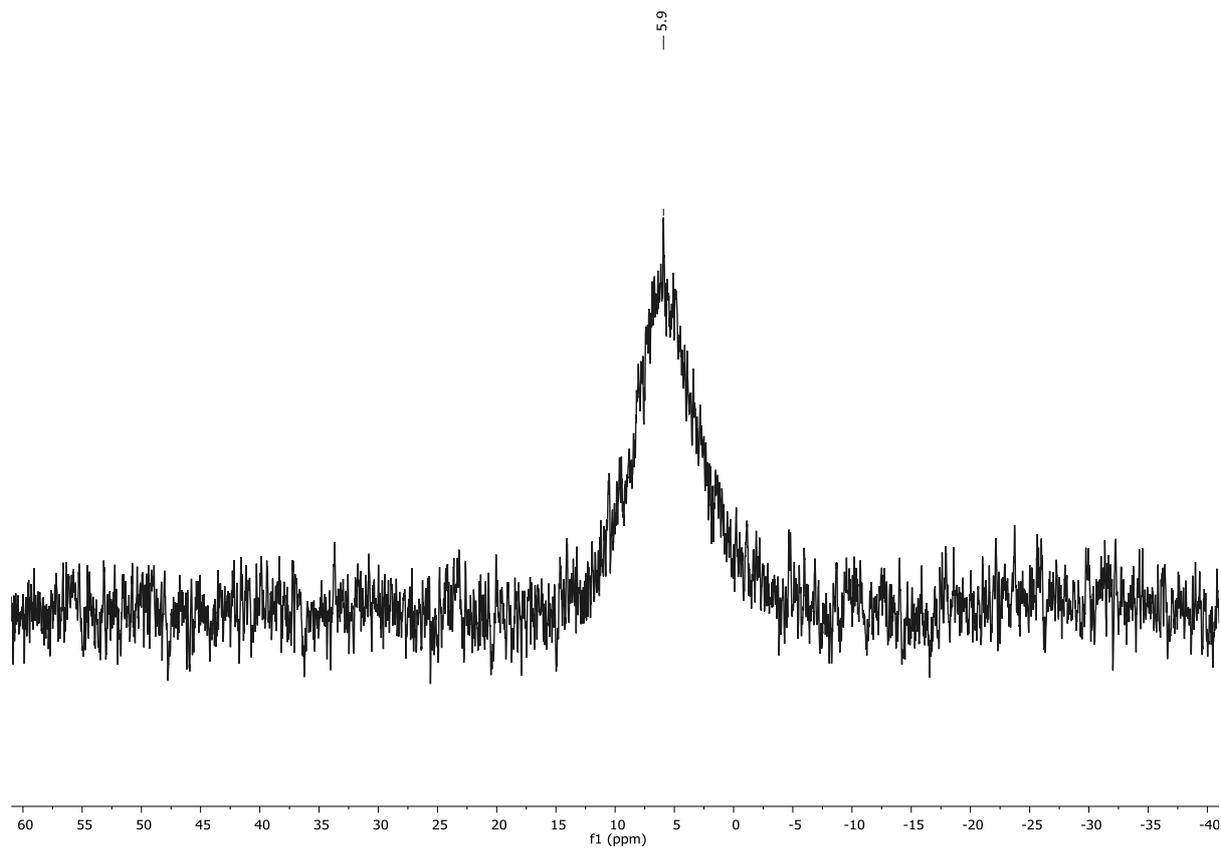
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444.1495	1	C25H20BN3NaO3	444.1494	-0.2	9.6	2	100.00	17.5	even	ok

Figure S40. HRMS (ESI<sup>+</sup>) report of 4g





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

## Compound Spectrum SmartFormula Report

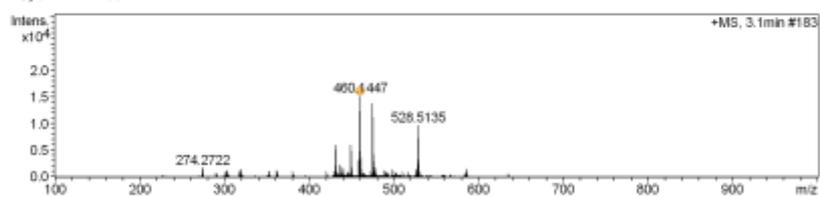
<b>Analysis Info</b>		Acquisition Date	3/3/2024 7:36:01 PM
Analysis Name	D:\Data\VDD-248.d	Operator	hplc
Method	DirectInfusion_TuneLow_pos.m	Instrument	micrOTOF-Q III 822888.20448
Sample Name	VDD-248		
Comment	AB		

<b>Acquisition Parameter</b>					
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.	3.1	n.a.	Single spectrum	n.a.	n.a.	n.a.	460.1447	n.a.

**+MS, 3.1min #183**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdB	e <sup>-</sup> Conf	N-Rule
460.1447	1	C25H20BN3NaO4	460.1444	-0.8	11.5	2	100.00	17.5	even	ok

**Figure S44.** HRMS (ESI<sup>+</sup>) report of **4h**



Figure S45. <sup>1</sup>H NMR (700 MHz, DMSO-*d*<sub>6</sub>) spectrum of **4i**

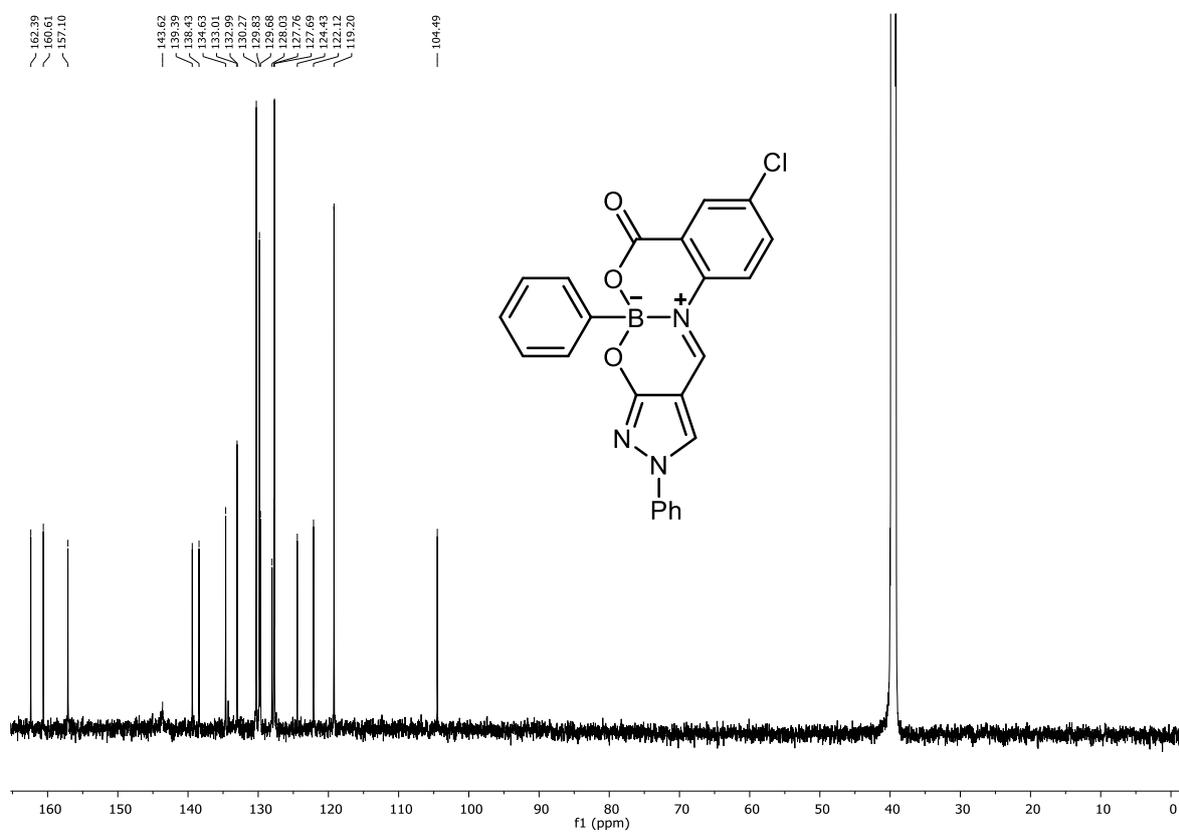
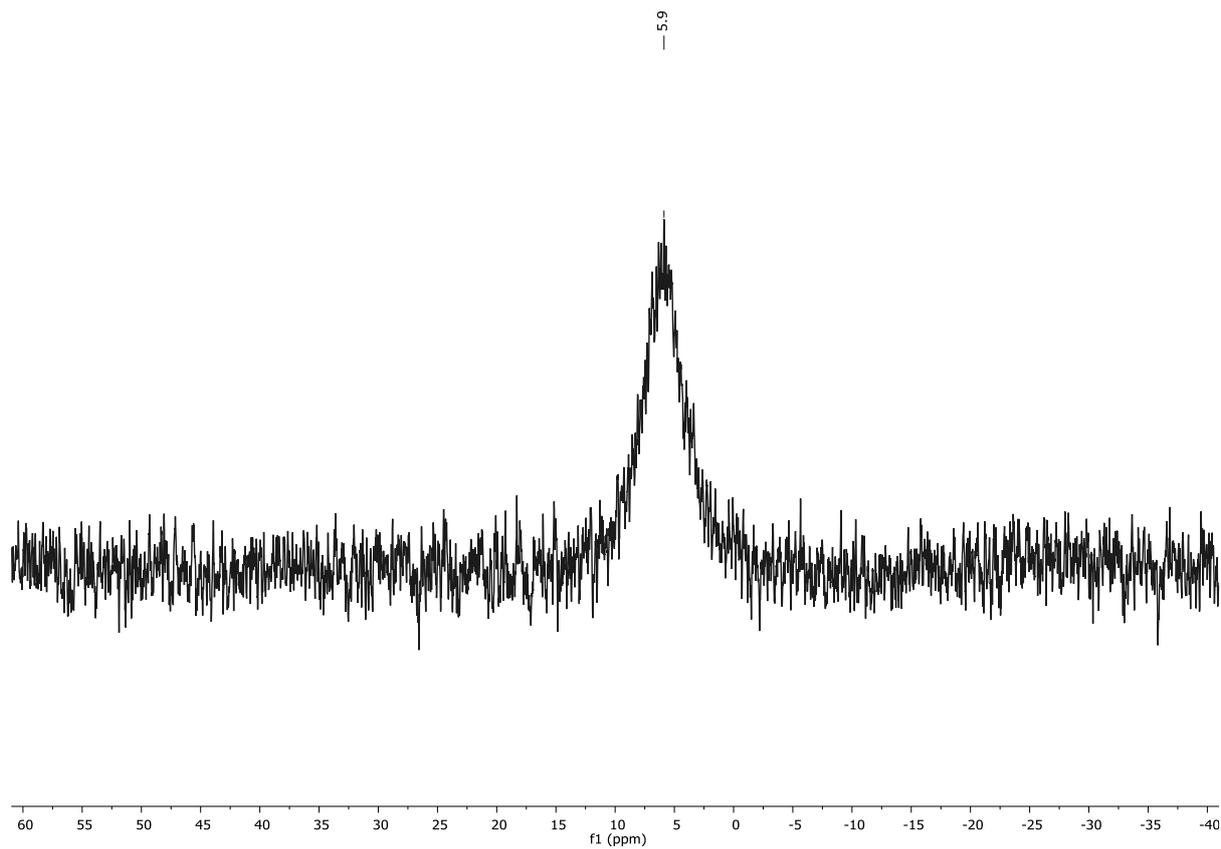


Figure S46. <sup>13</sup>C NMR (176 MHz, DMSO-*d*<sub>6</sub>) spectrum of **4i**



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

## Compound Spectrum SmartFormula Report

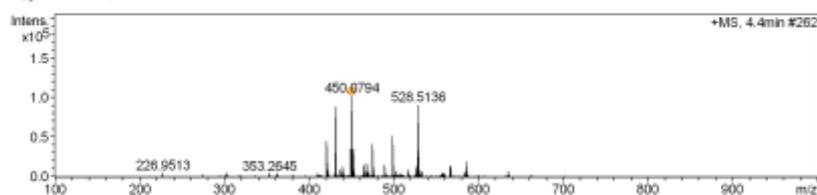
<b>Analysis Info</b>		Acquisition Date	3/1/2024 7:56:46 PM
Analysis Name	D:\Data\VDD-241.d	Operator	hplc
Method	DirectInfusion_TuneLow_pos.m	Instrument	micrOTOF-Q III 8228888.20448
Sample Name	VDD-241		
Comment	AB		

<b>Acquisition Parameter</b>					
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.	4.4	n.a.	Single spectrum	n.a.	n.a.	n.a.	450.0794	n.a.

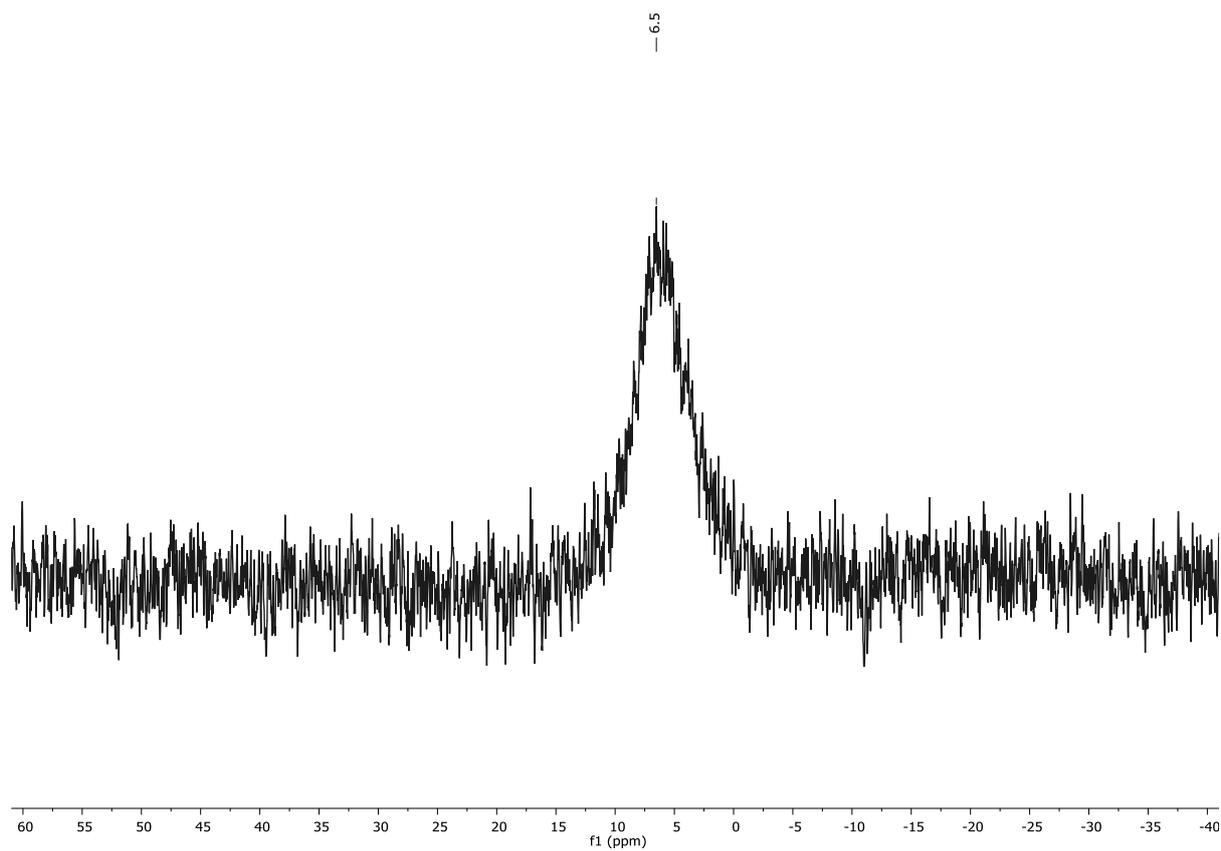
**+MS, 4.4min #262**



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

**Figure S48.** HRMS (ESI<sup>+</sup>) report of **4i**





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

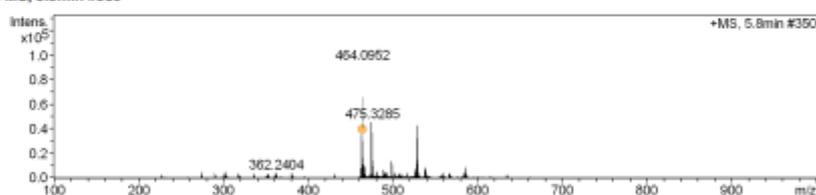
## Compound Spectrum SmartFormula Report

**Analysis Info**  
Analysis Name: D:\Data\VDD-244.d  
Method: DirectInfusion\_TuneLow\_pos.m  
Sample Name: VDD-244  
Comment: AB  
Acquisition Date: 3/3/2024 7:00:35 PM  
Operator: hplc  
Instrument: micrOTOF-Q III 8228888.20448

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

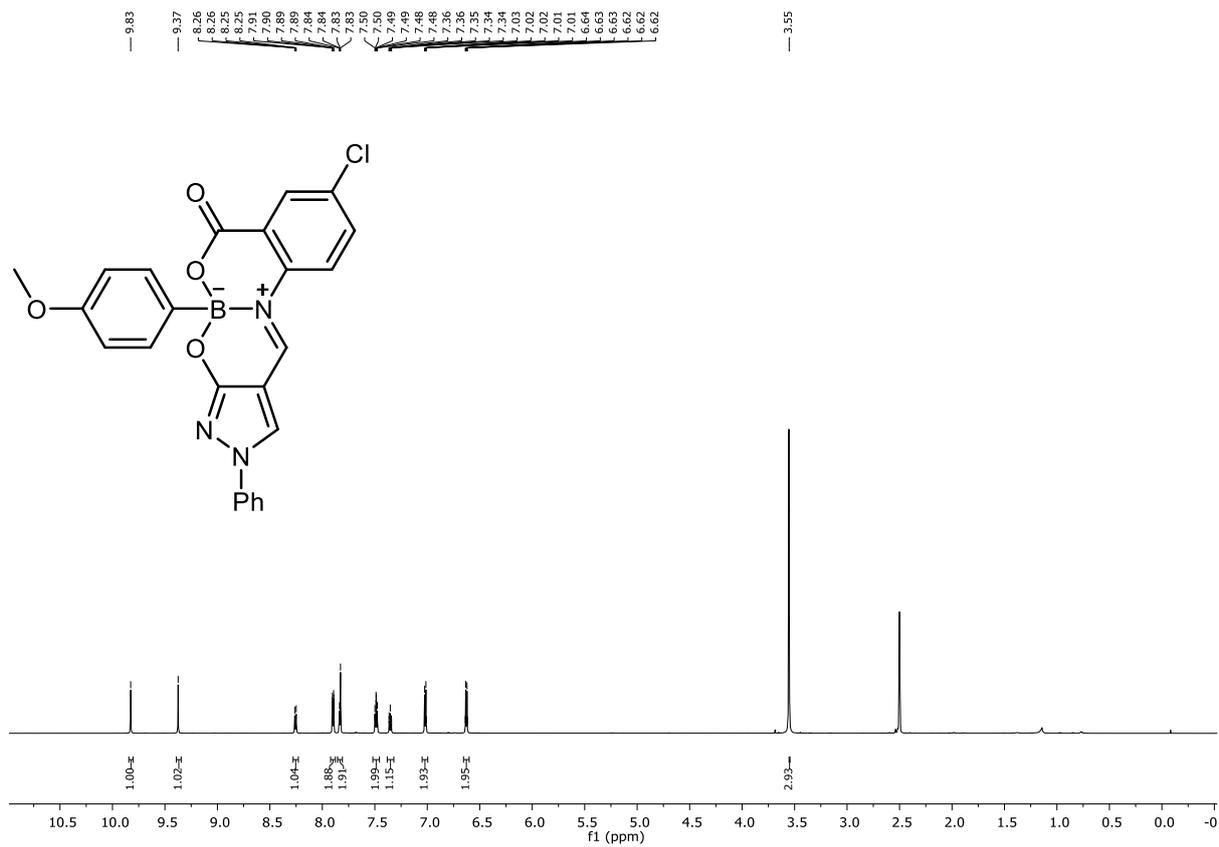
#	RT [min]	Area	Int. Type	I	S/N	Chromatogram	Max. m/z	FWHM [min]
n.a.	5.8	n.a.	Single spectrum	n.a.	n.a.	n.a.	475.3285	n.a.

### +MS, 5.8min #350

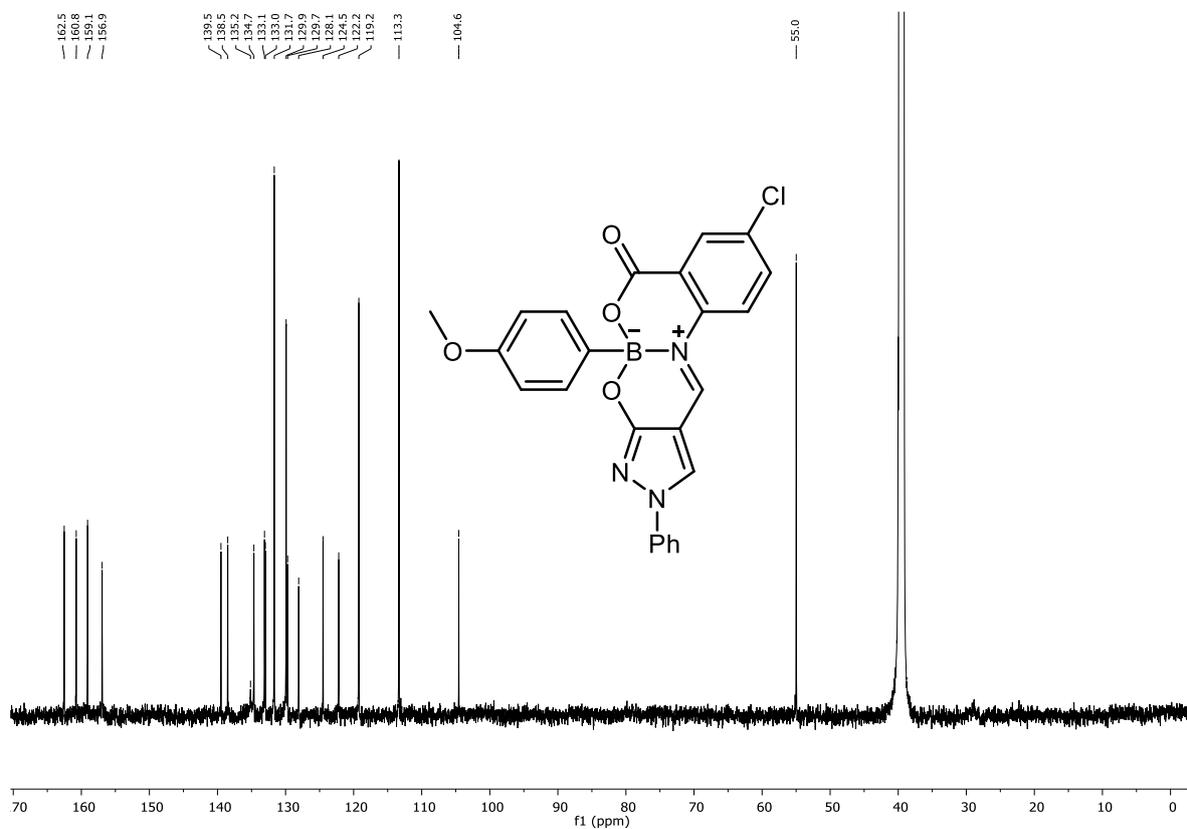


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e <sup>-</sup> Conf	N-Rule
464.0952	1	C <sub>24</sub> H <sub>17</sub> BClN <sub>3</sub> NaO <sub>3</sub>	464.0948	1.0	36.6	1	100.00	17.5	even	ok

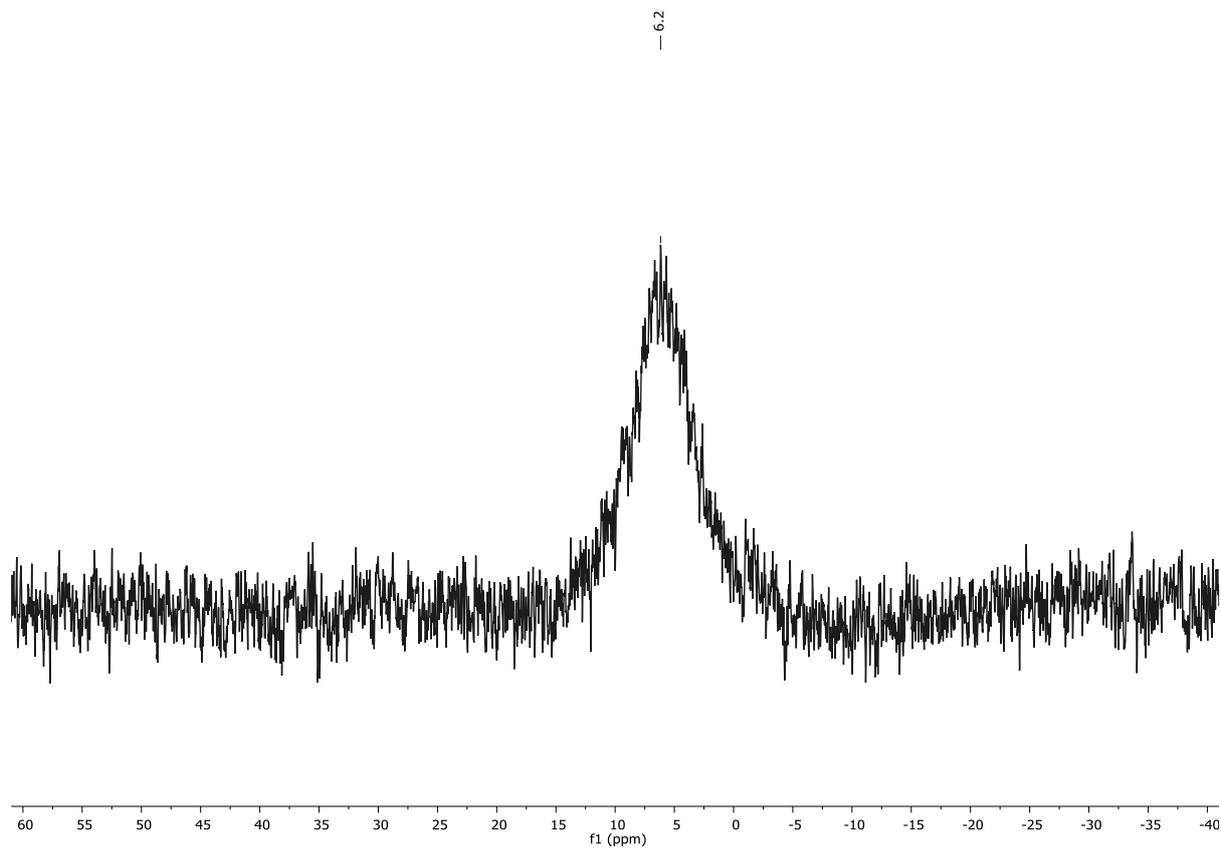
Figure S52. HRMS (ESI<sup>+</sup>) report of 4j



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



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



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

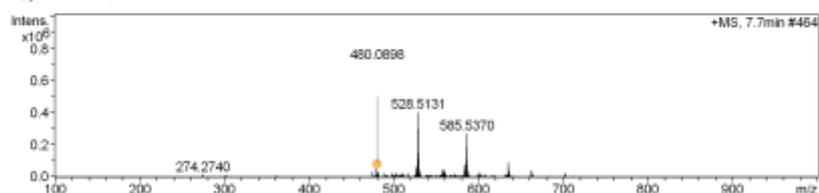
## Compound Spectrum SmartFormula Report

**Analysis Info** Acquisition Date 3/1/2024 8:32:46 PM  
Analysis Name D:\Data\VDD-243.d  
Method DirectInfusion\_TuneLow\_pos.m Operator hplc  
Sample Name VDD-243 Instrument micrOTOF-Q III 8228888.20448  
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 <sup>-</sup> Conf	N-Rule
480.0898	1	C24H17BCIN3NaO4	480.0897	0.1	46.6	4	100.00	17.5	even	ok

Figure S56. HRMS (ESI<sup>+</sup>) report of 4k