

## **SUPPLEMENTARY DATA**

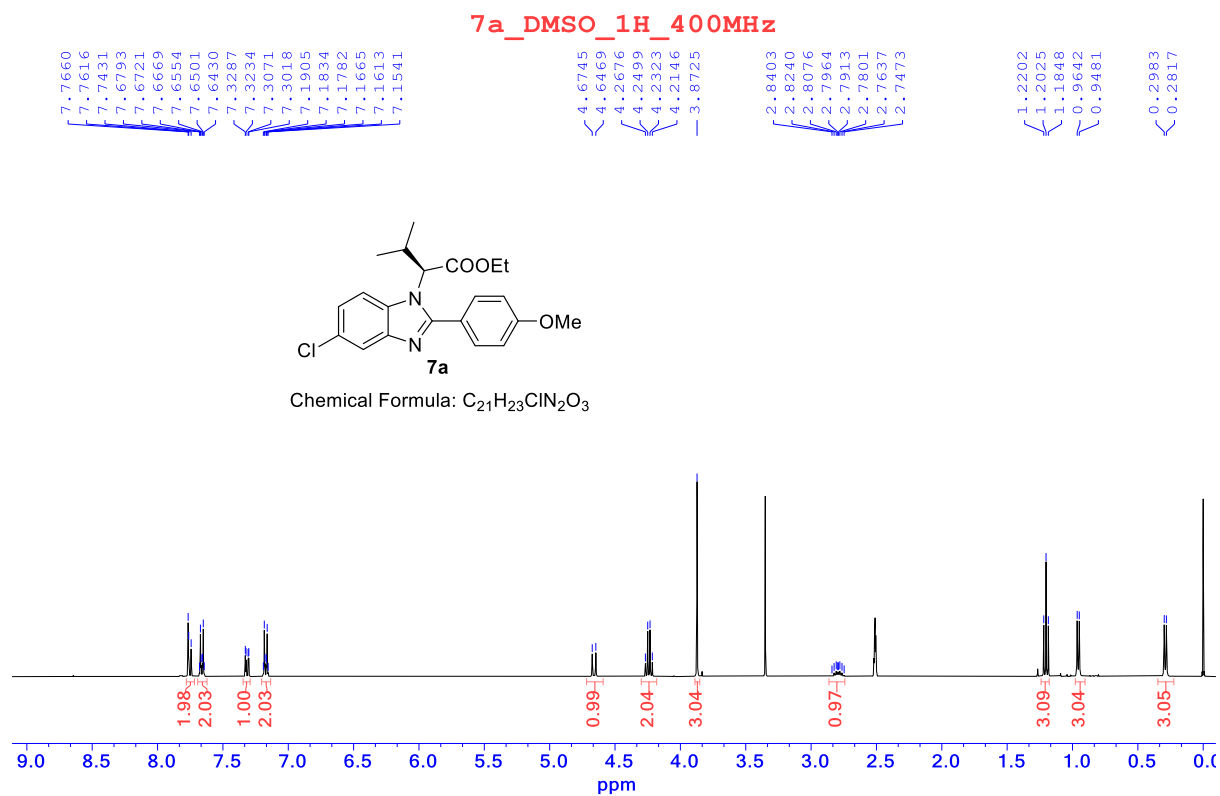
### **Synthesis and cytotoxicity evaluation of benzimidazole conjugated amino acid derivatives**

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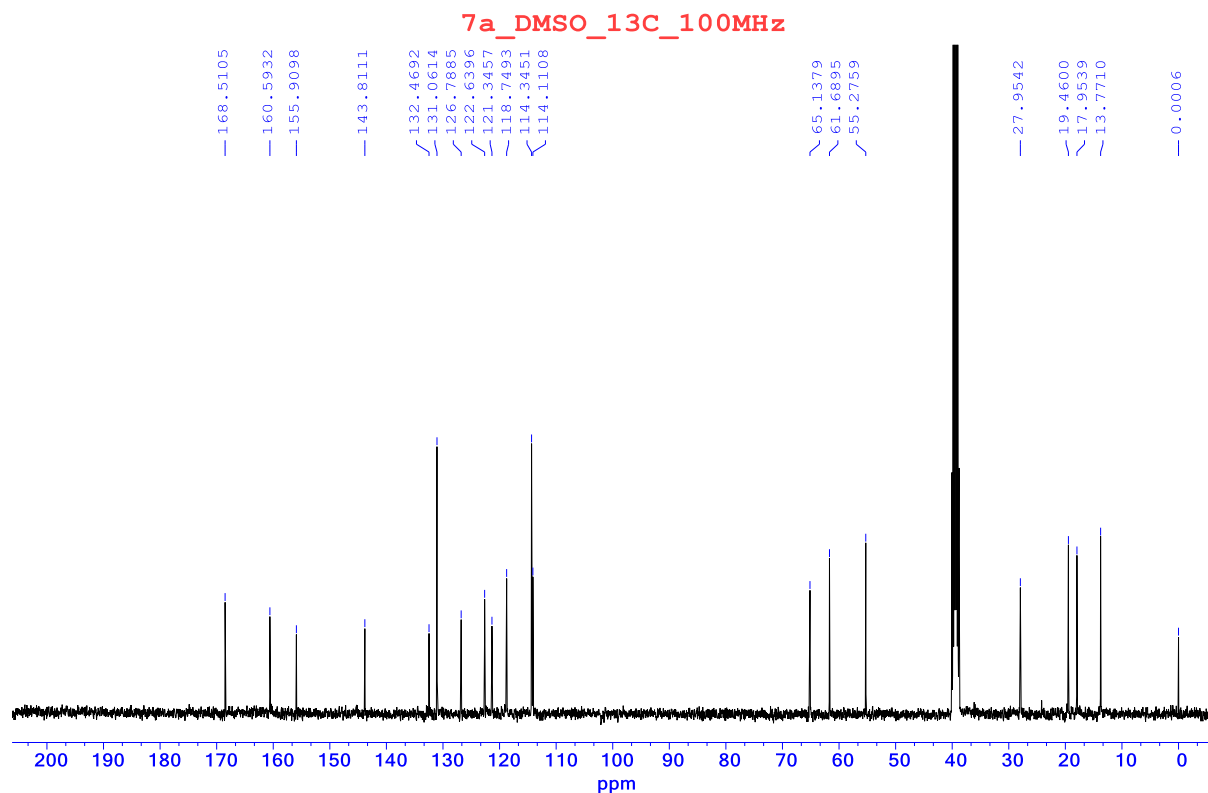
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**Figure S1.** <sup>1</sup>H-NMR spectrum of compound **7a**



**Figure S2.** <sup>13</sup>C-NMR spectrum of compound **7a**

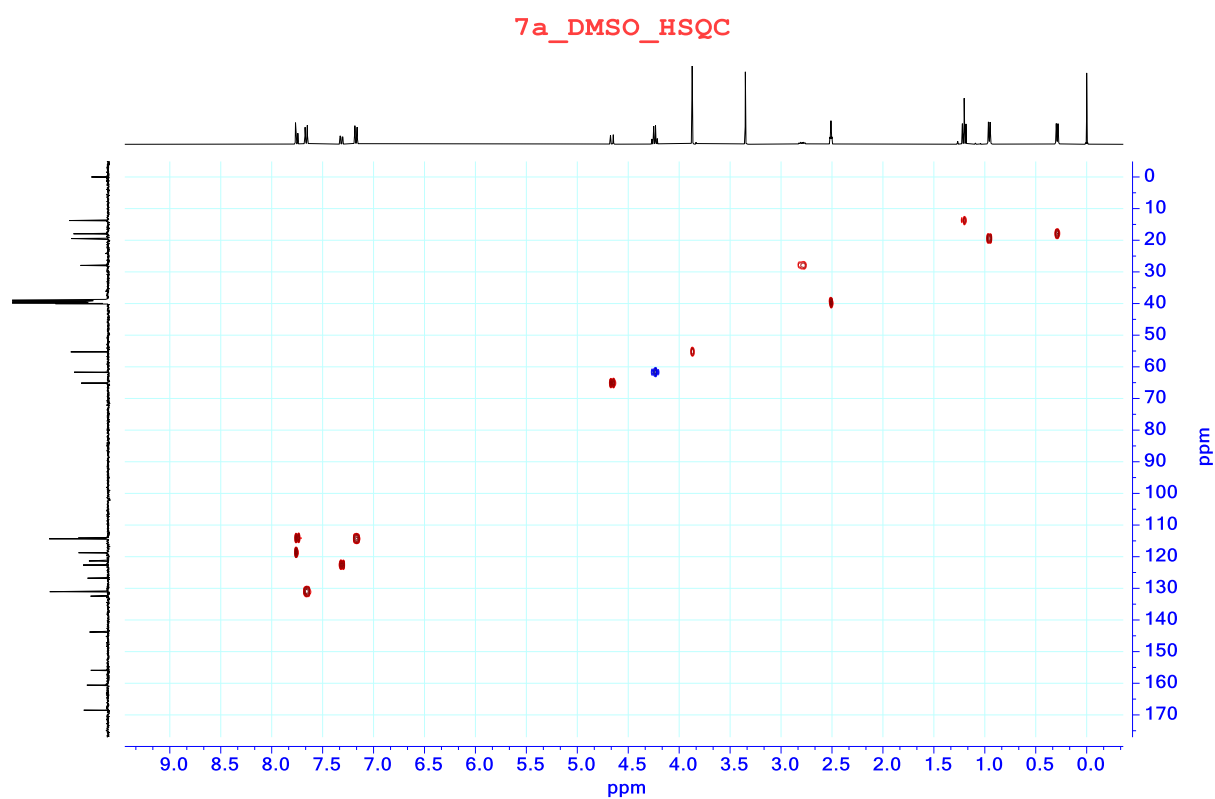


Figure S3. HSQC spectrum of compound **7a**

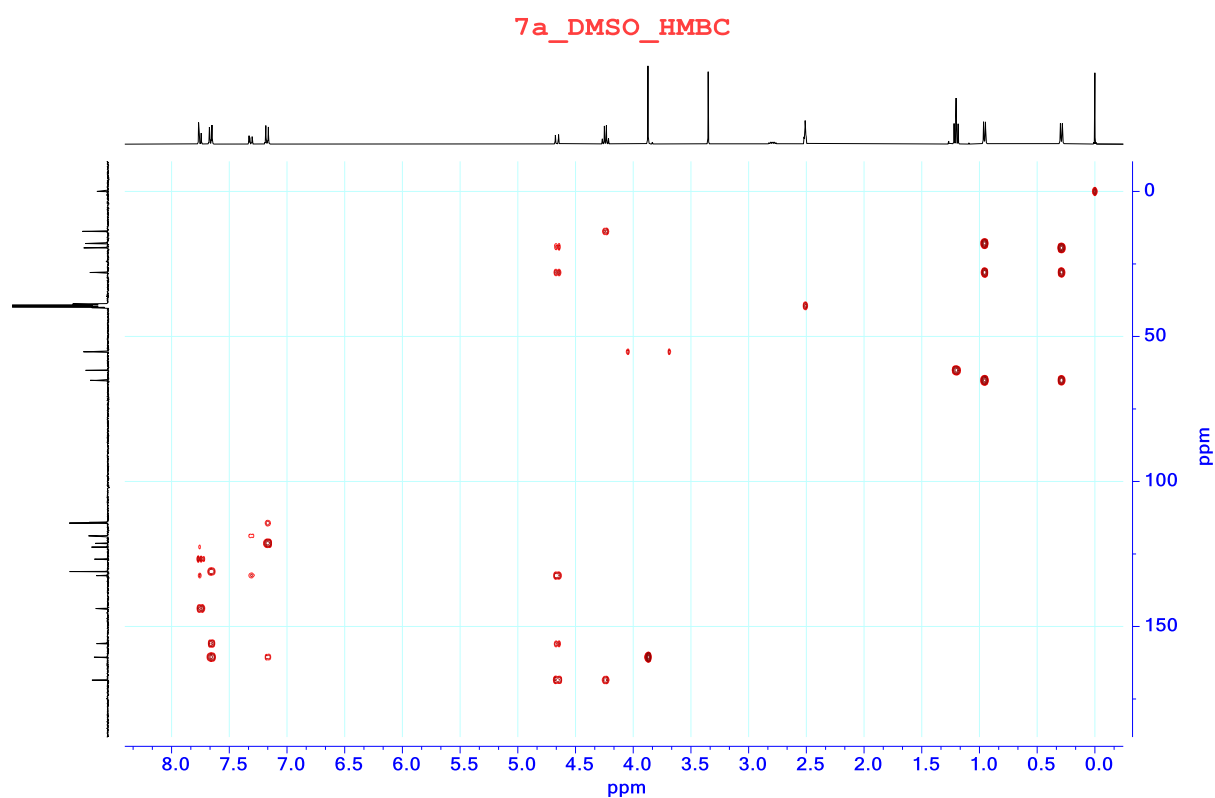


Figure S4. HMBC spectrum of compound **7a**

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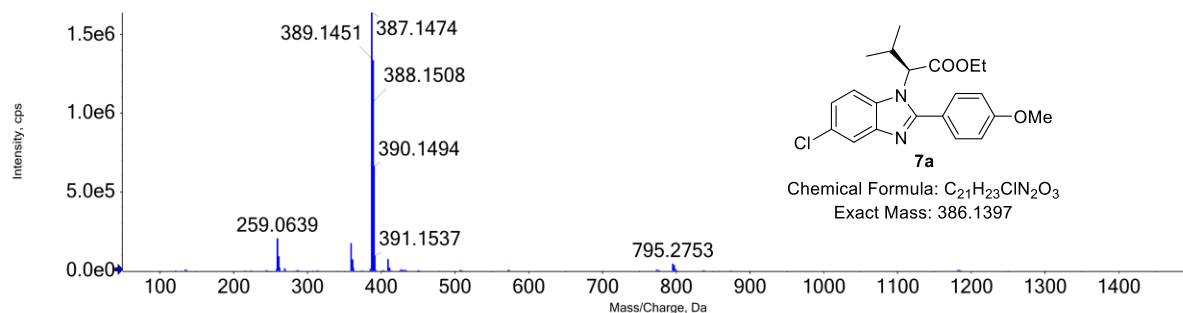
## ANALYSIS REPORT

### Injection details

Sample name	KA96	Vial position	22
Sample file name	SR. wiff2-HUE	Inject volume	2.00
Acquisition date	08/08/2025 01:16:06 PM	Acquisition method	ESI_POS_SCAN
Operator	CB21261708	Instrument name	X500R QTOF

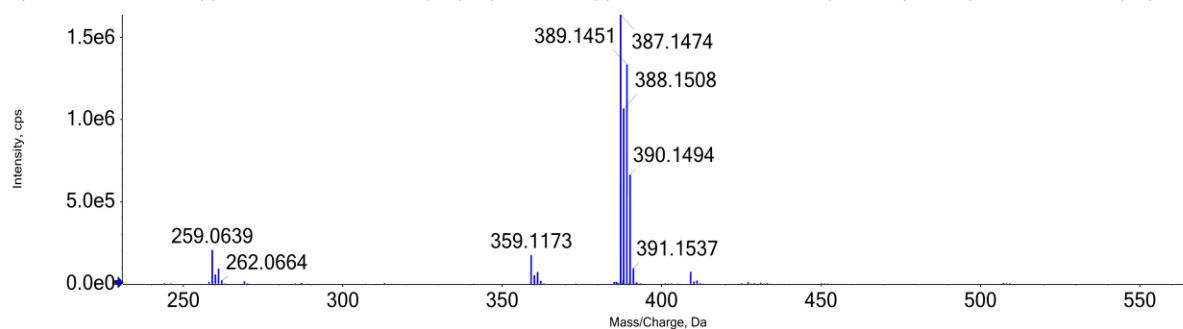
### Full mass spectrum

Spectrum from HUE\_KA96\_(+)ESI 2025-08-08-13-16-06.wiff2 (sample 1) - HUE\_KA96\_(+)ESI...m 0.148 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)

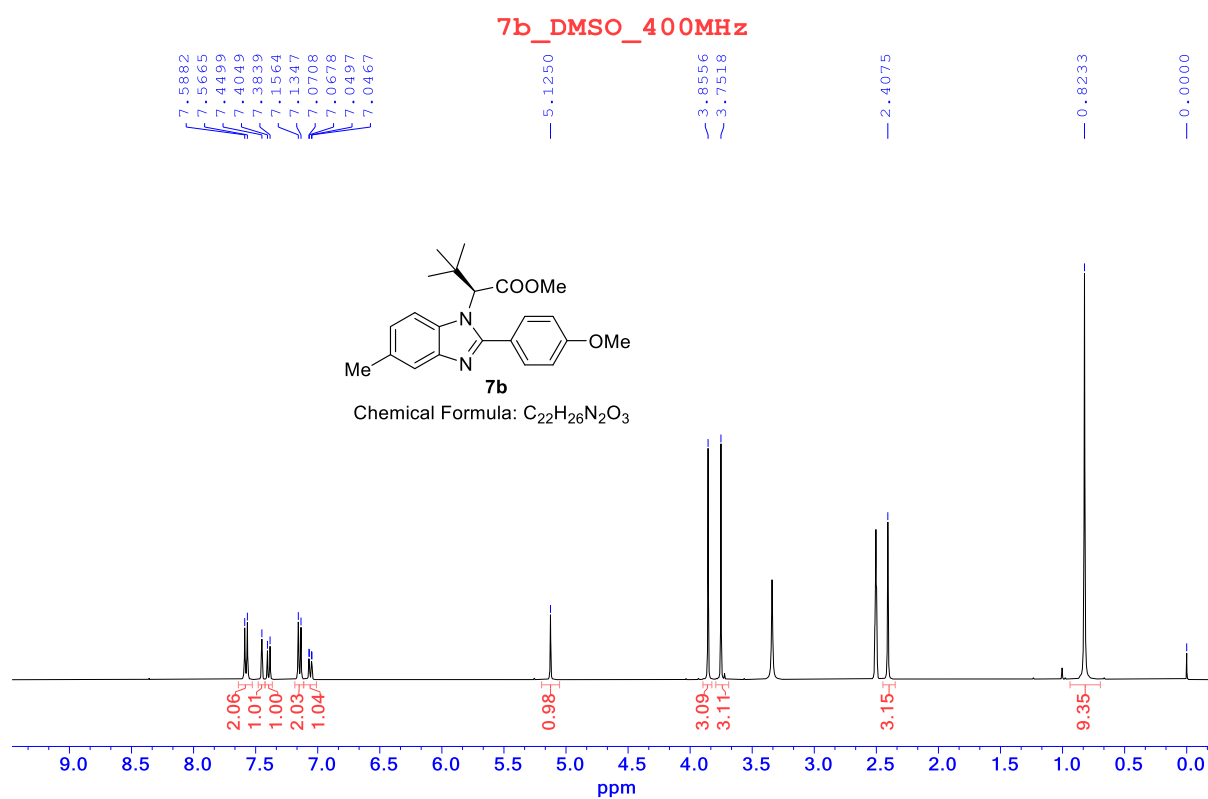


### Expanded spectrum

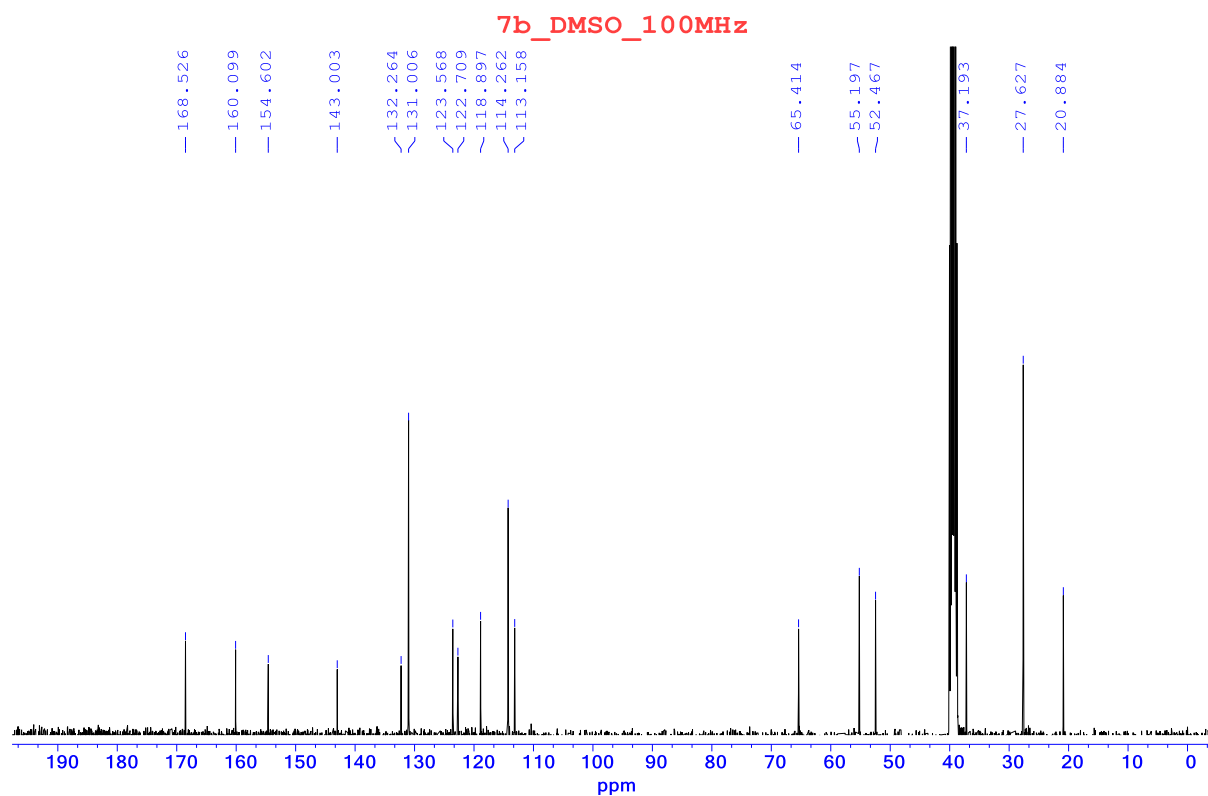
Spectrum from HUE\_KA96\_(+)ESI 2025-08-08-13-16-06.wiff2 (sample 1) - HUE\_KA96\_(+)ESI...m 0.148 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



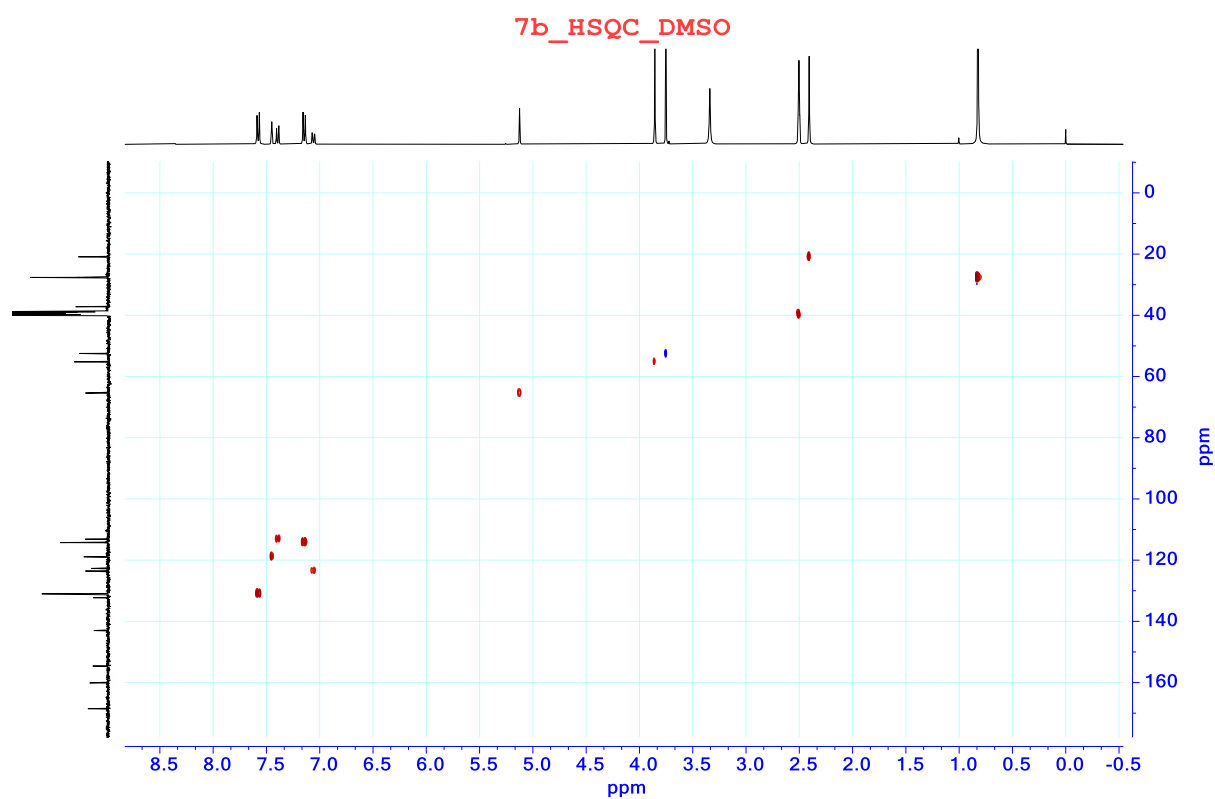
**Figure S5. MS spectrum of compound 7a**



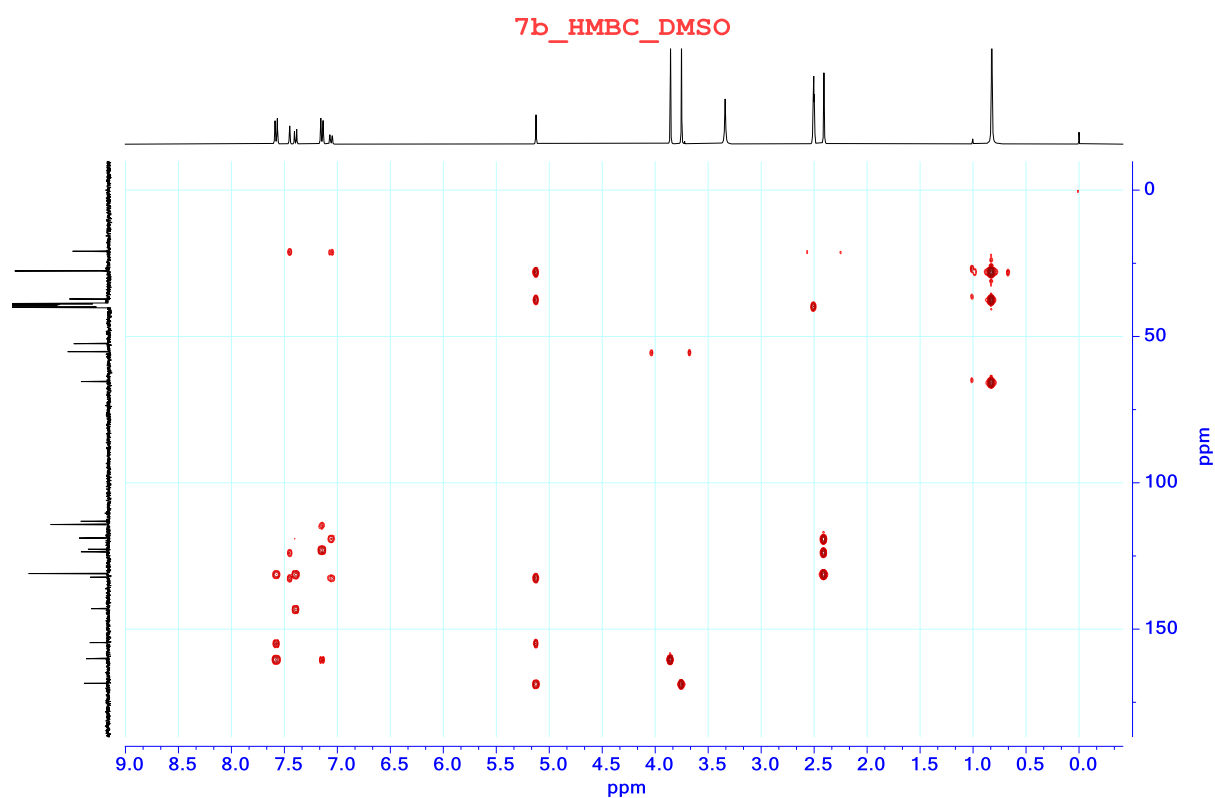
**Figure S6.** <sup>1</sup>H-NMR spectrum of compound **7b**



**Figure S7.** <sup>13</sup>C-NMR spectrum of compound **7b**



**Figure S8.** HSQC spectrum of compound **7b**



**Figure S9.** HMBC spectrum of compound **7b**

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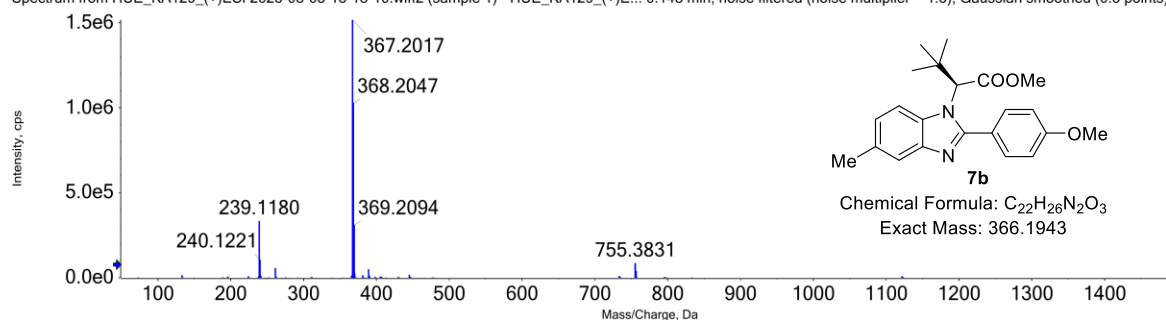
## ANALYSIS REPORT

### Injection details

Sample name	KA129	Vial position	23
Sample file name	SR. wiff2-HUE	Inject volume	2.00
Acquisition date	08/08/2025 01:18:10 PM	Acquisition method	ESI_POS_SCAN
Operator	CB21261708	Instrument name	X500R QTOF

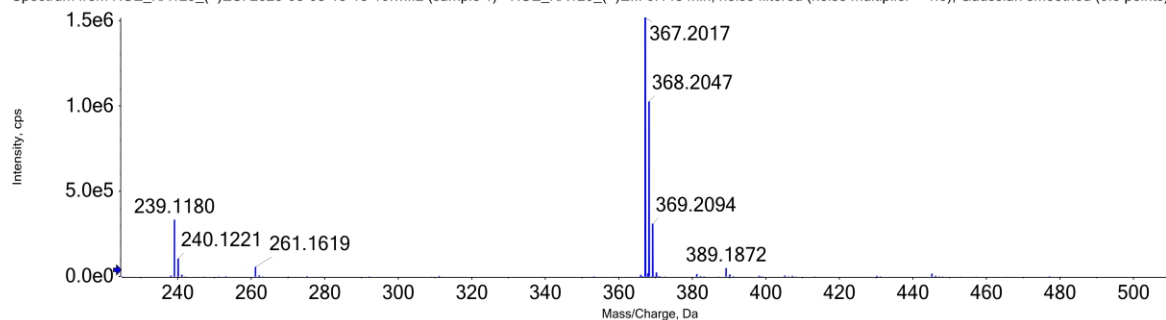
### Full mass spectrum

Spectrum from HUE\_KA129\_(+)ESI 2025-08-08-13-18-10.wiff2 (sample 1) - HUE\_KA129\_(+)E... 0.148 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)

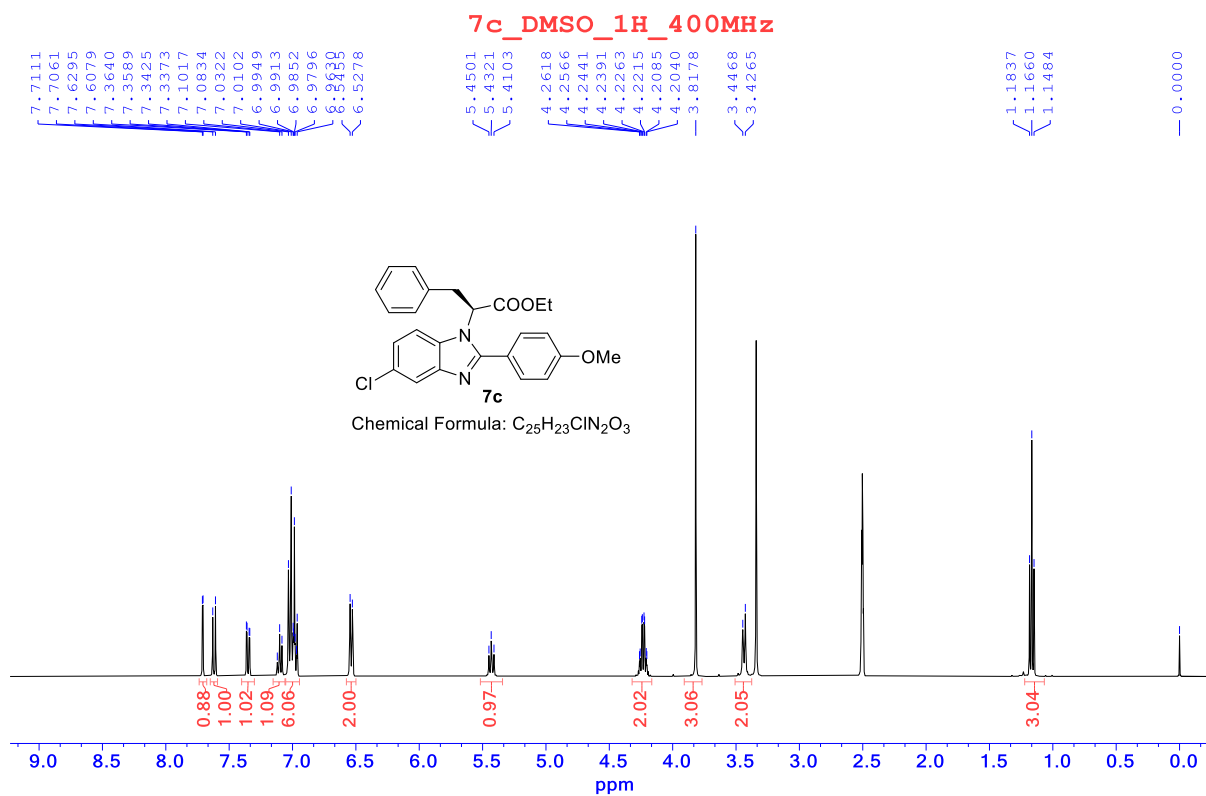


### Expanded spectrum

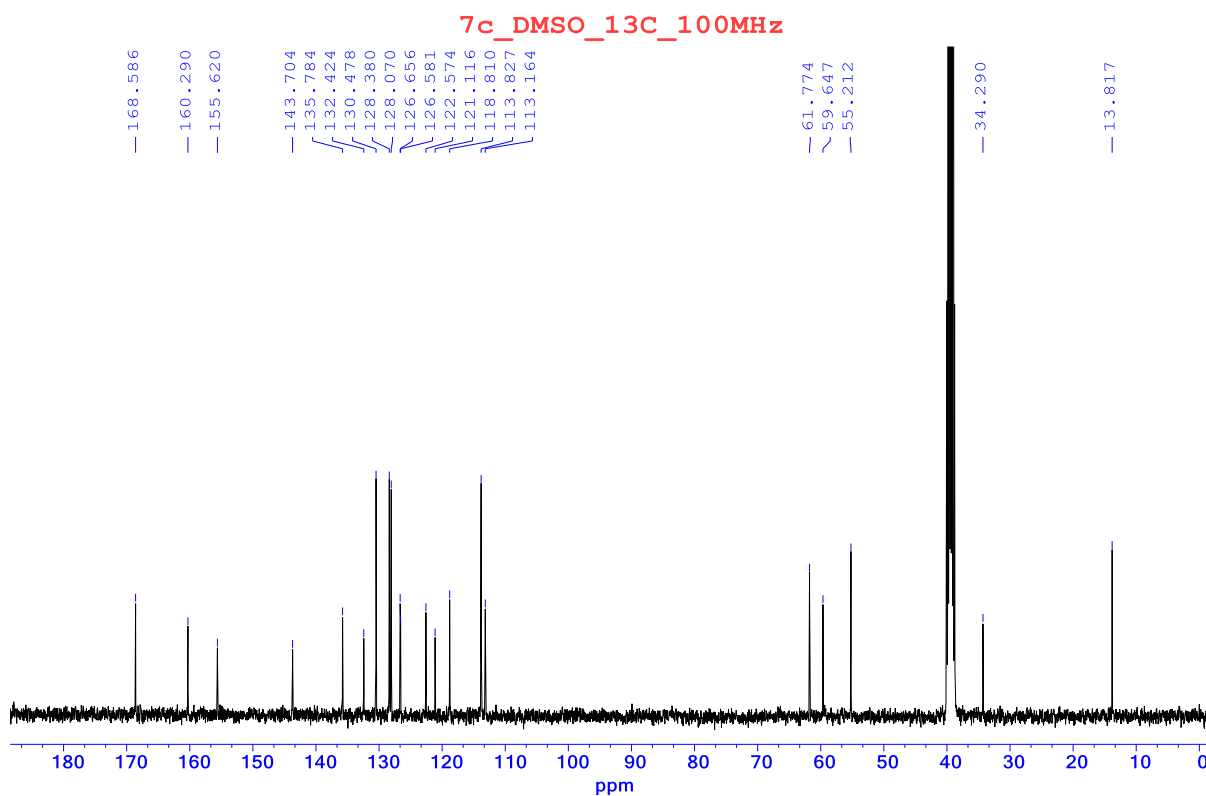
Spectrum from HUE\_KA129\_(+)ESI 2025-08-08-13-18-10.wiff2 (sample 1) - HUE\_KA129\_(+)E... 0.148 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



**Figure S10. MS spectrum of compound 7b**



**Figure S11.** <sup>1</sup>H-NMR spectrum of compound **7c**



**Figure S12.** <sup>13</sup>C-NMR spectrum of compound **7c**



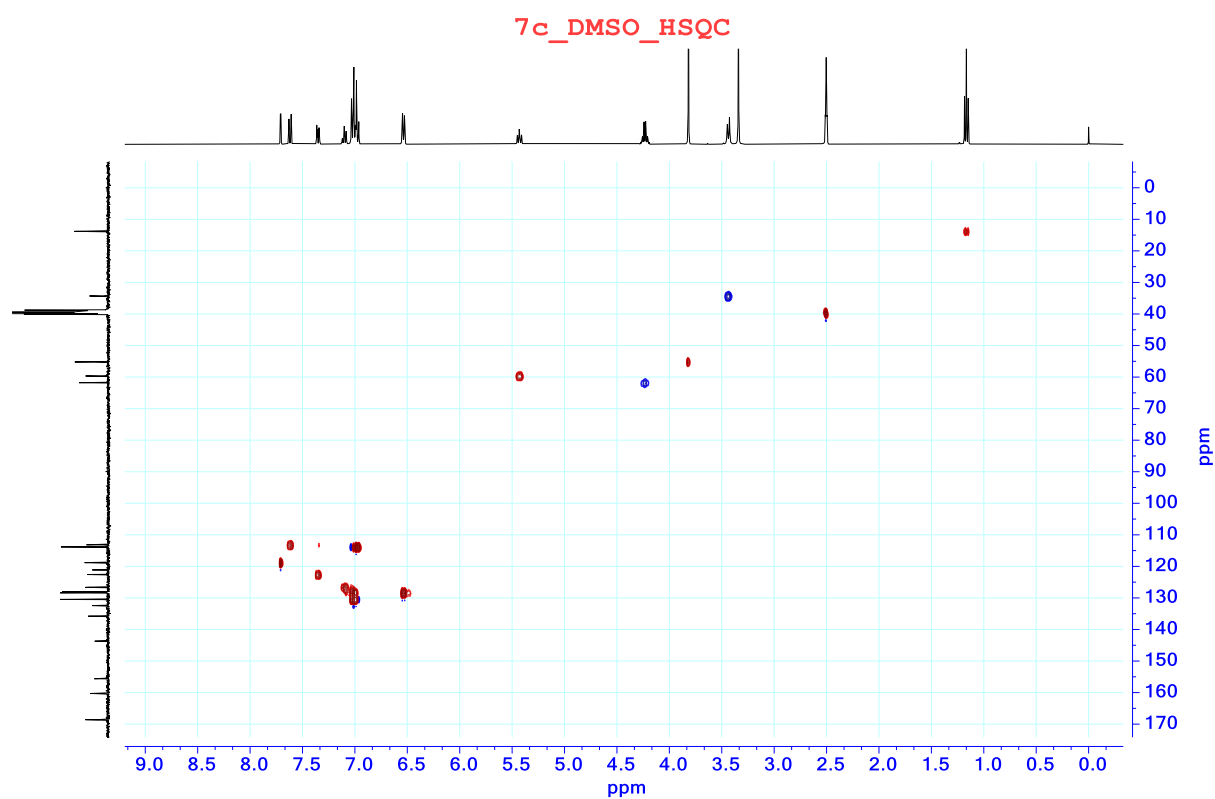


Figure S13. HSQC spectrum of compound **7c**

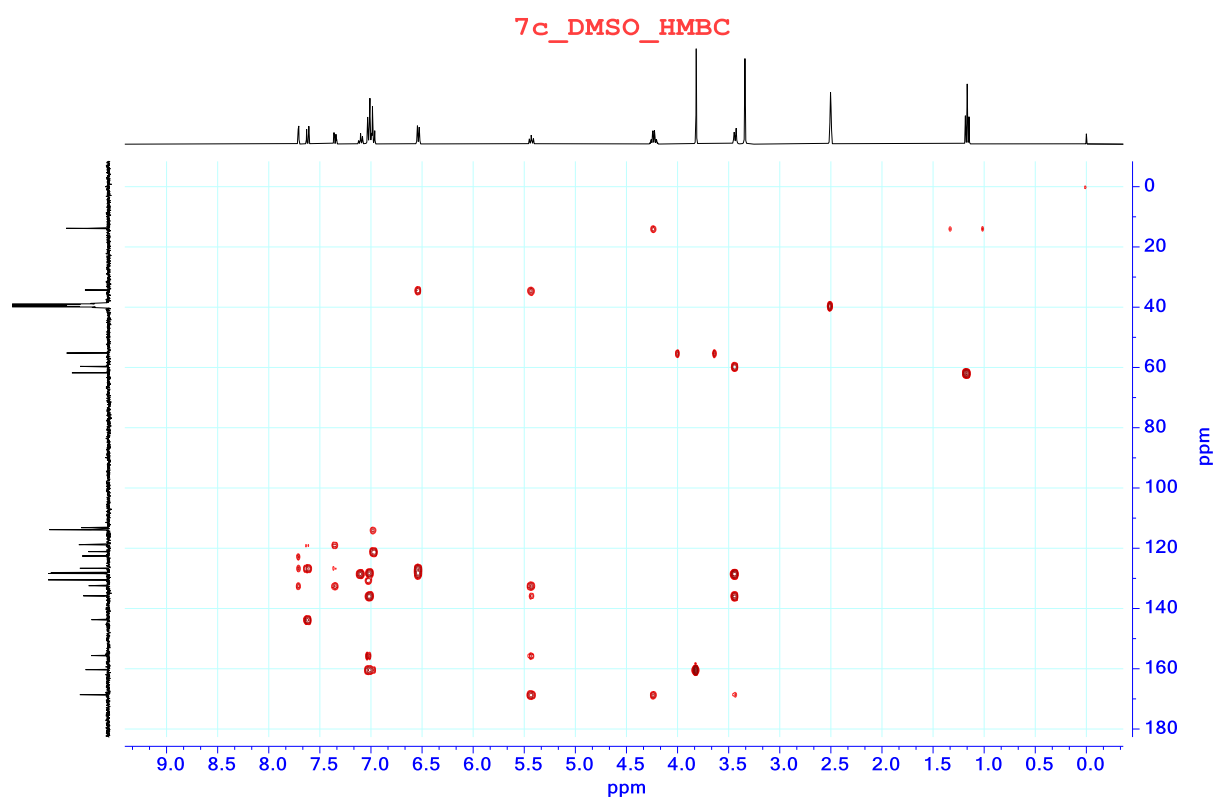


Figure S14. HMBC spectrum of compound **7c**

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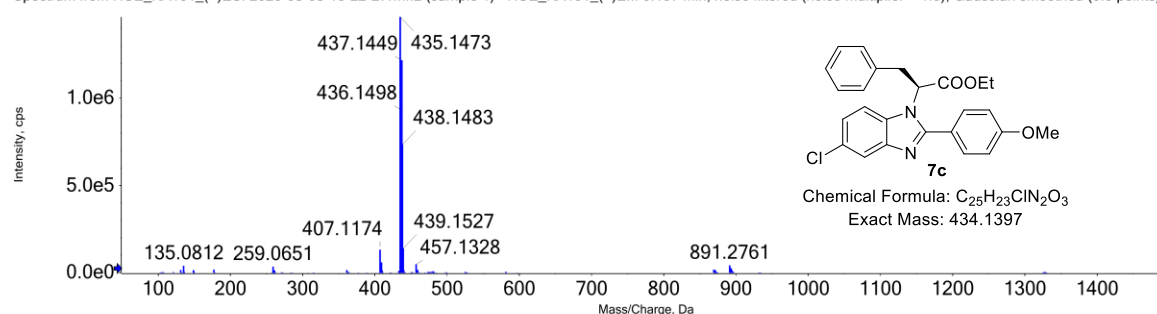
## ANALYSIS REPORT

### Injection details

Sample name	KA131	Vial position	25
Sample file name	SR. wiff2-HUE	Inject volume	2.00
Acquisition date	08/08/2025 01:22:27 PM	Acquisition method	ESI_POS_SCAN
Operator	CB21261708	Instrument name	X500R QTOF

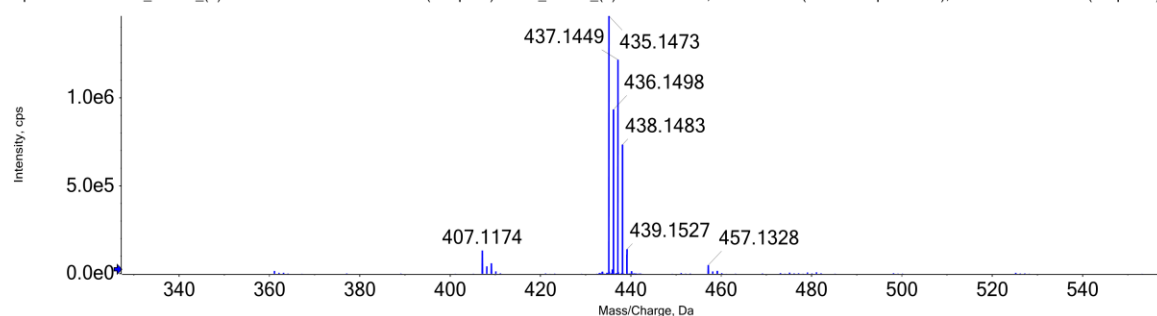
### Full mass spectrum

Spectrum from HUE\_KA131\_(+)ESI 2025-08-08-13-22-27.wiff2 (sample 1) - HUE\_KA131\_(+)E... 0.157 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)

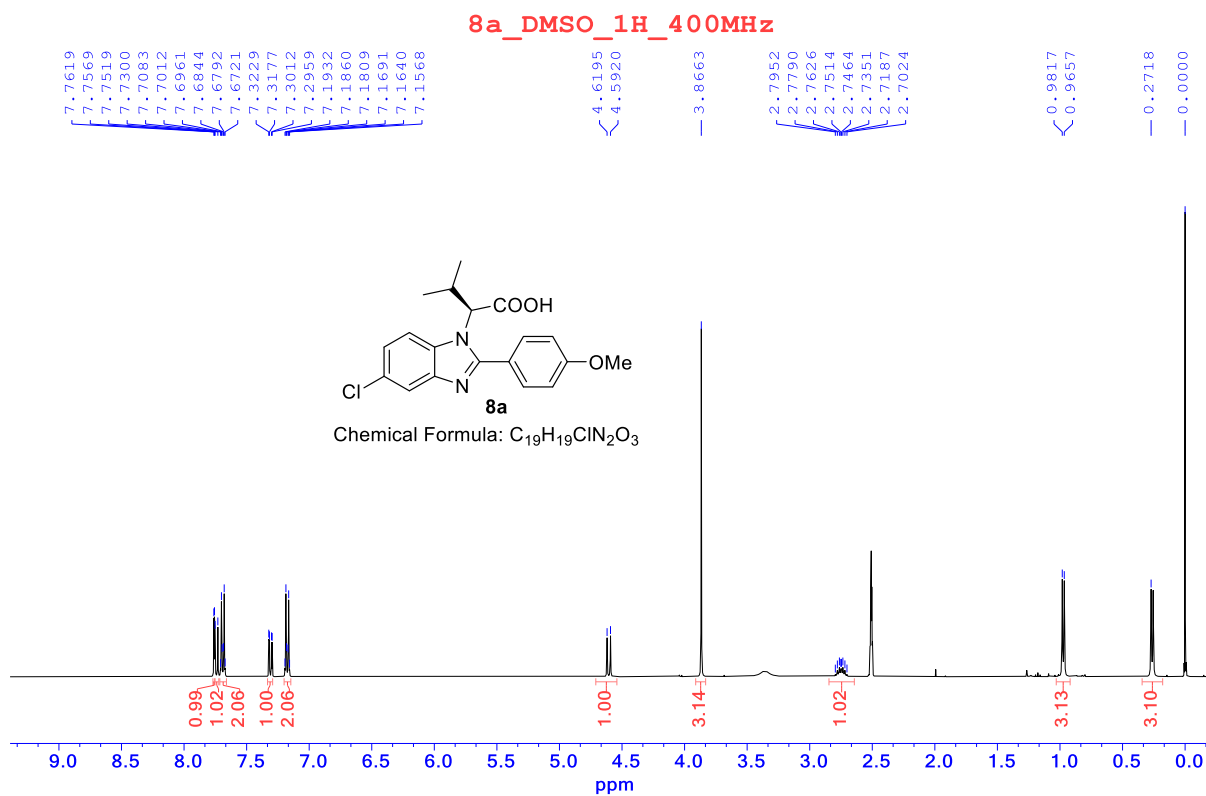


### Expanded spectrum

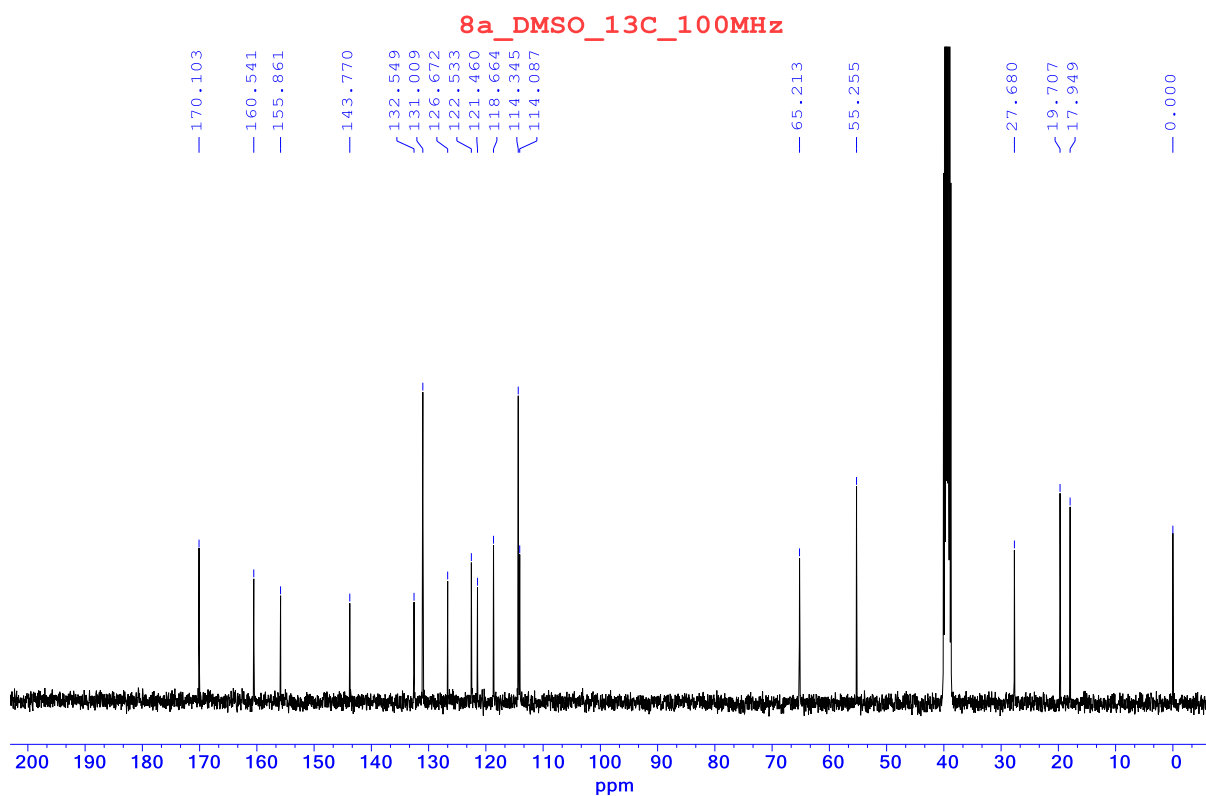
Spectrum from HUE\_KA131\_(+)ESI 2025-08-08-13-22-27.wiff2 (sample 1) - HUE\_KA131\_(+)E... 0.157 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



**Figure S15. MS spectrum of compound 7c**



**Figure S16.** <sup>1</sup>H-NMR spectrum of compound **8a**



**Figure S17.** <sup>13</sup>C-NMR spectrum of compound **8a**

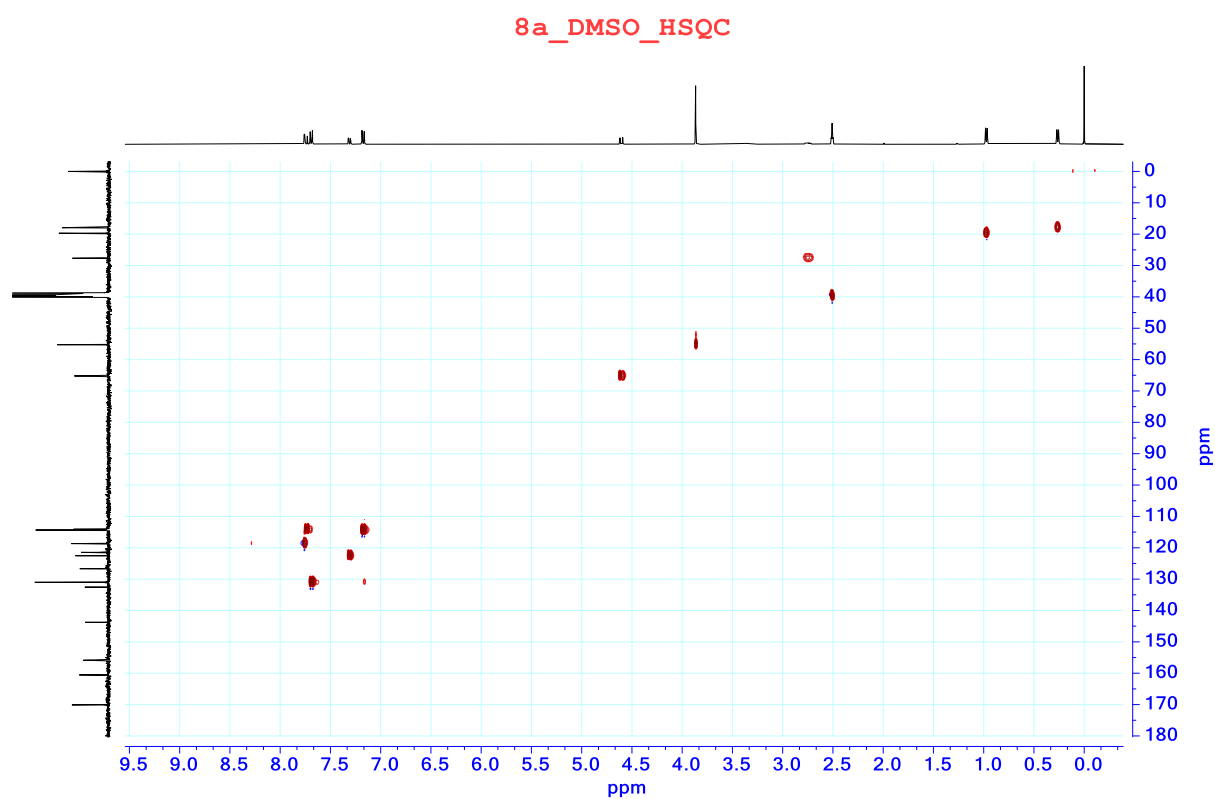


Figure S18. HSQC spectrum of compound **8a**

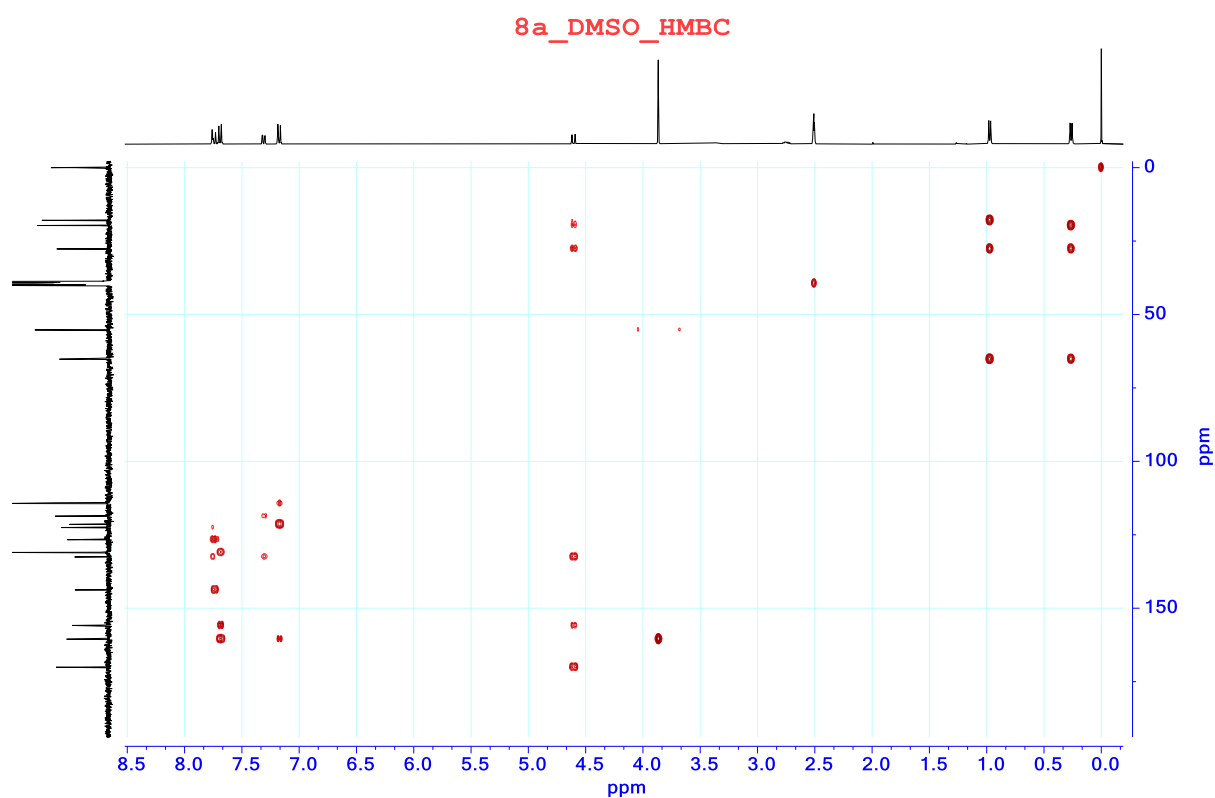


Figure S19. HMBC spectrum of compound **8a**

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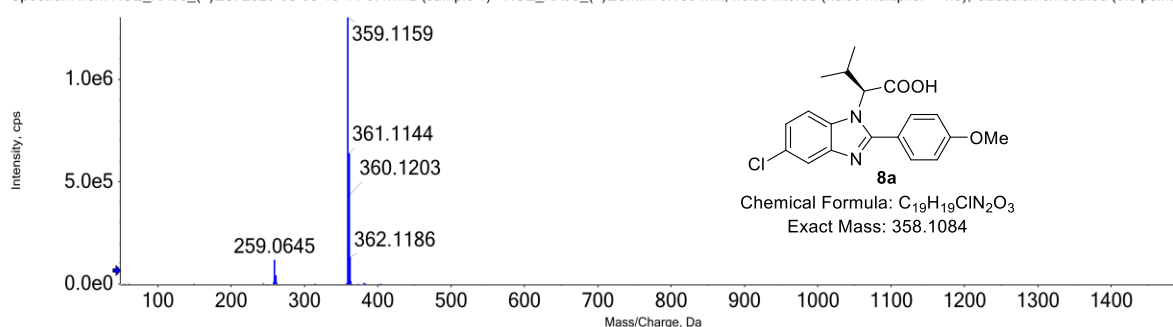
## ANALYSIS REPORT

### Injection details

Sample name	KA95	Vial position	21
Sample file name	SR. wiff2-HUE	Inject volume	2.00
Acquisition date	08/08/2025 01:14:07 PM	Acquisition method	ESI_POS_SCAN
Operator	CB21261708	Instrument name	X500R QTOF

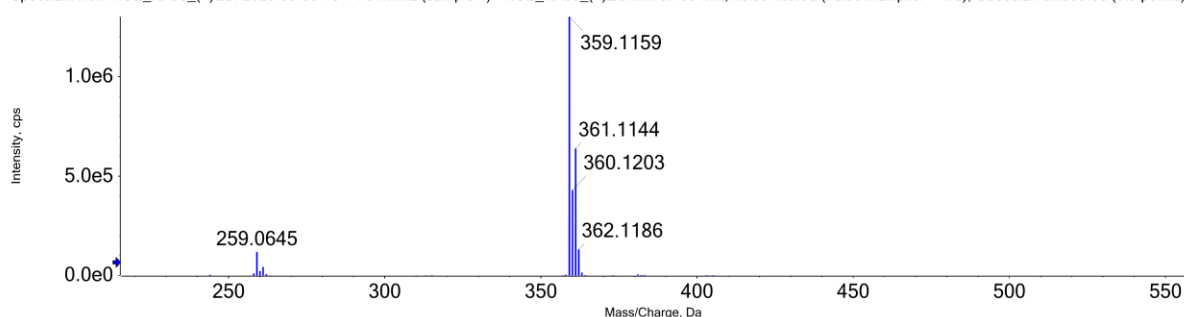
### Full mass spectrum

Spectrum from HUE\_KA95\_(+)ESI 2025-08-08-13-14-07.wiff2 (sample 1) - HUE\_KA95\_(+)ESI...m 0.139 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)

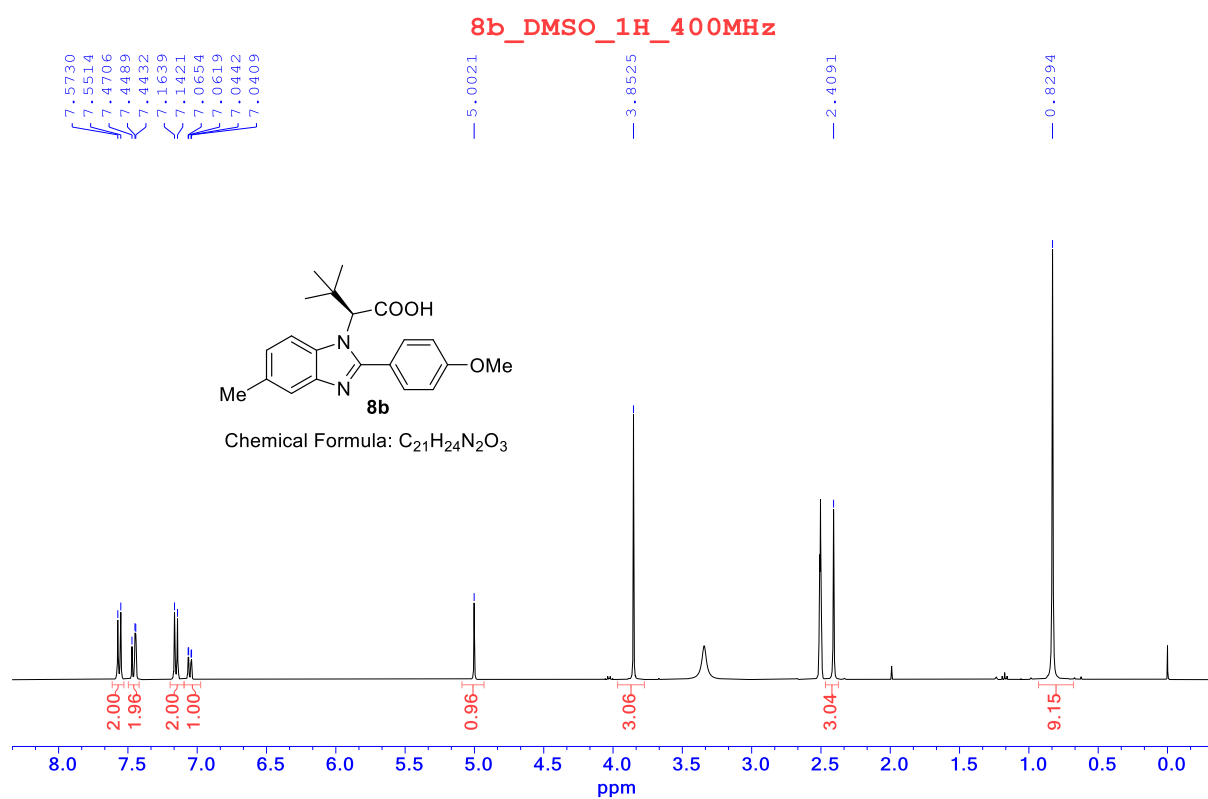


### Expanded spectrum

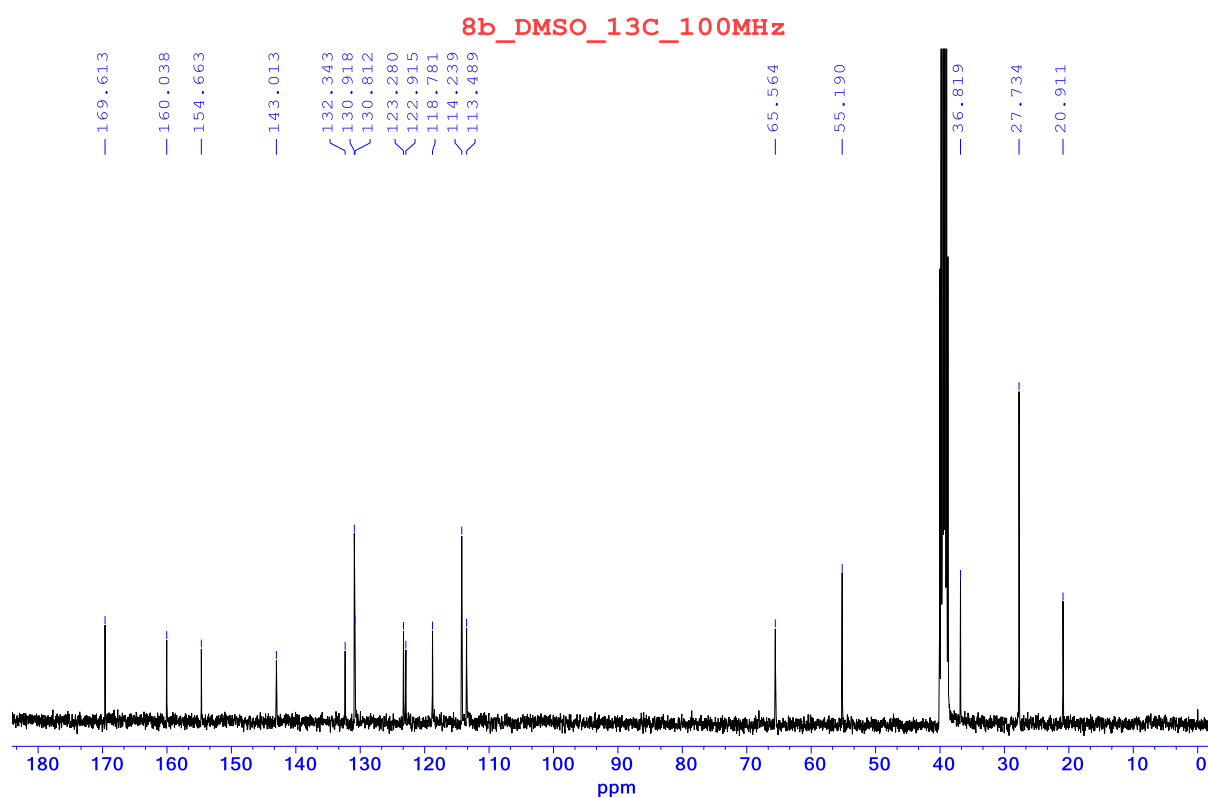
Spectrum from HUE\_KA95\_(+)ESI 2025-08-08-13-14-07.wiff2 (sample 1) - HUE\_KA95\_(+)ESI...m 0.139 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



**Figure S20. MS spectrum of compound 8a**



**Figure S21.** <sup>1</sup>H-NMR spectrum of compound **8b**



**Figure S22.** <sup>13</sup>C-NMR spectrum of compound **8b**

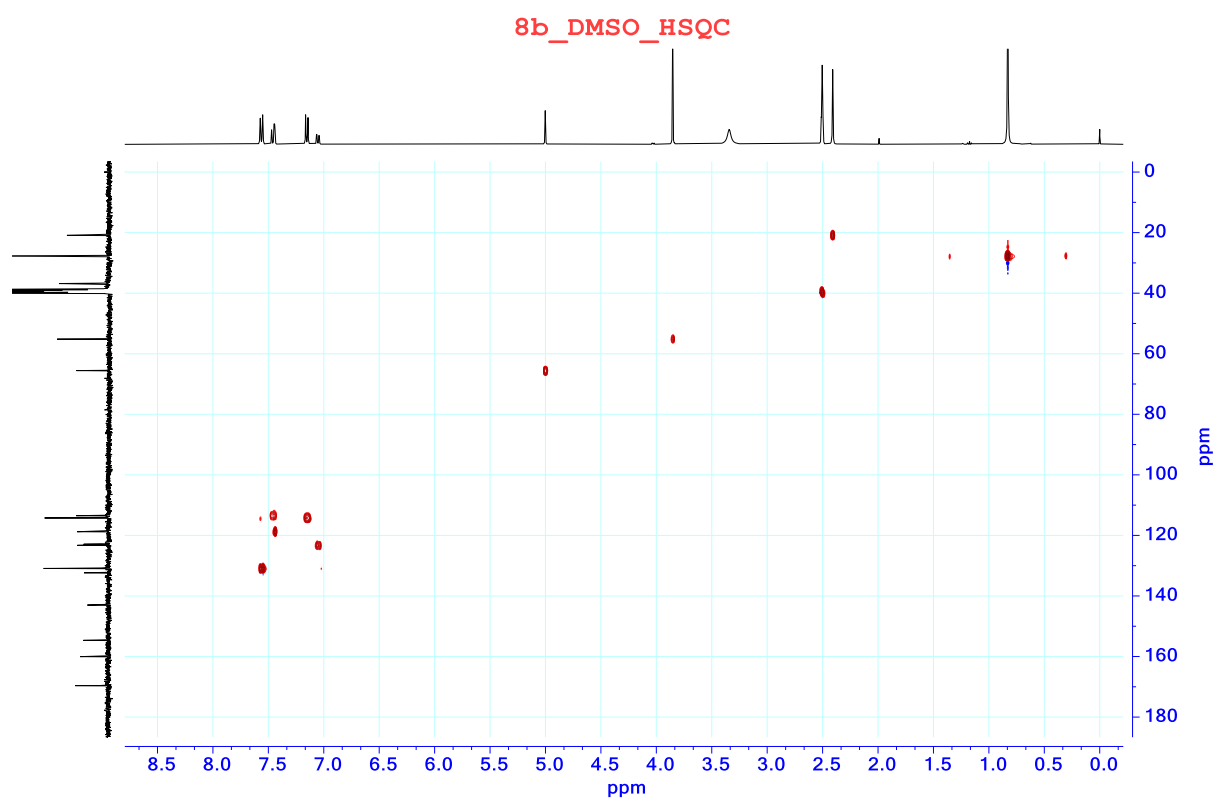


Figure S23. HSQC spectrum of compound **8b**

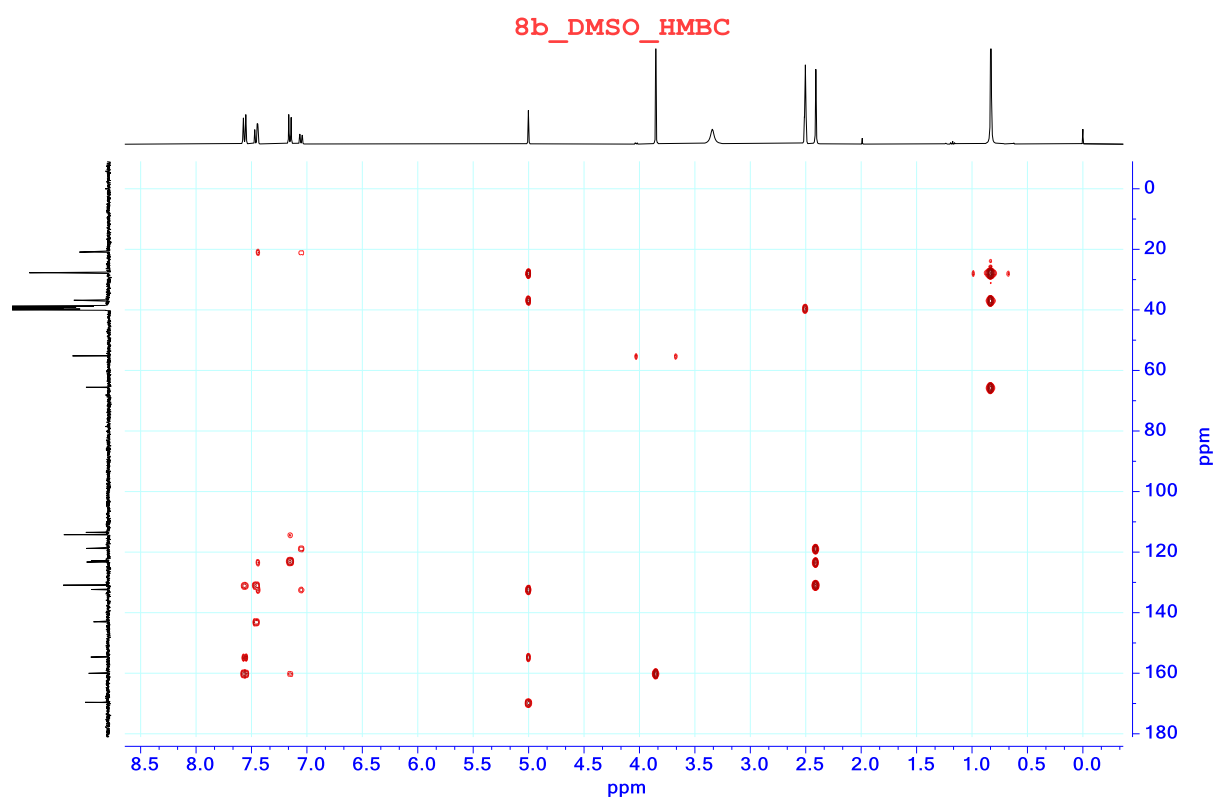


Figure S24. HMBC spectrum of compound **8b**

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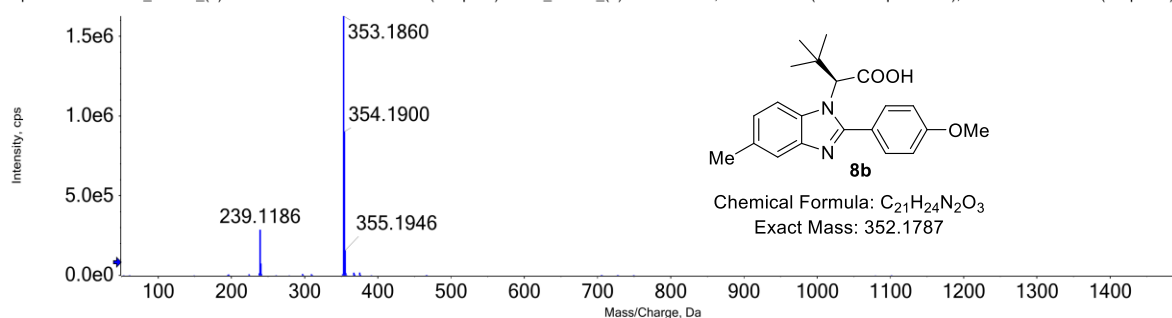
## ANALYSIS REPORT

### Injection details

Sample name	KA130	Vial position	24
Sample file name	SR. wiff2-HUE	Inject volume	2.00
Acquisition date	08/08/2025 01:20:18 PM	Acquisition method	<b>ESI_POS_SCAN</b>
Operator	CB21261708	Instrument name	X500R QTOF

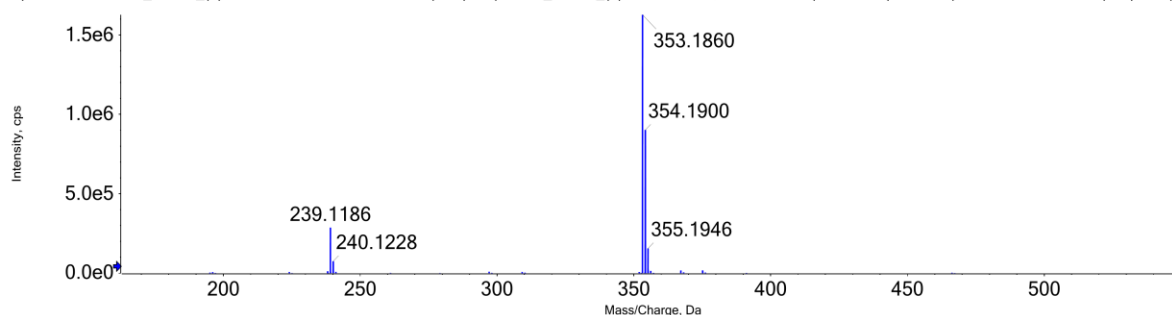
### Full mass spectrum

Spectrum from HUE\_KA130\_(+)ESI 2025-08-08-13-20-18.wiff2 (sample 1) - HUE\_KA130\_(+)E... 0.148 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



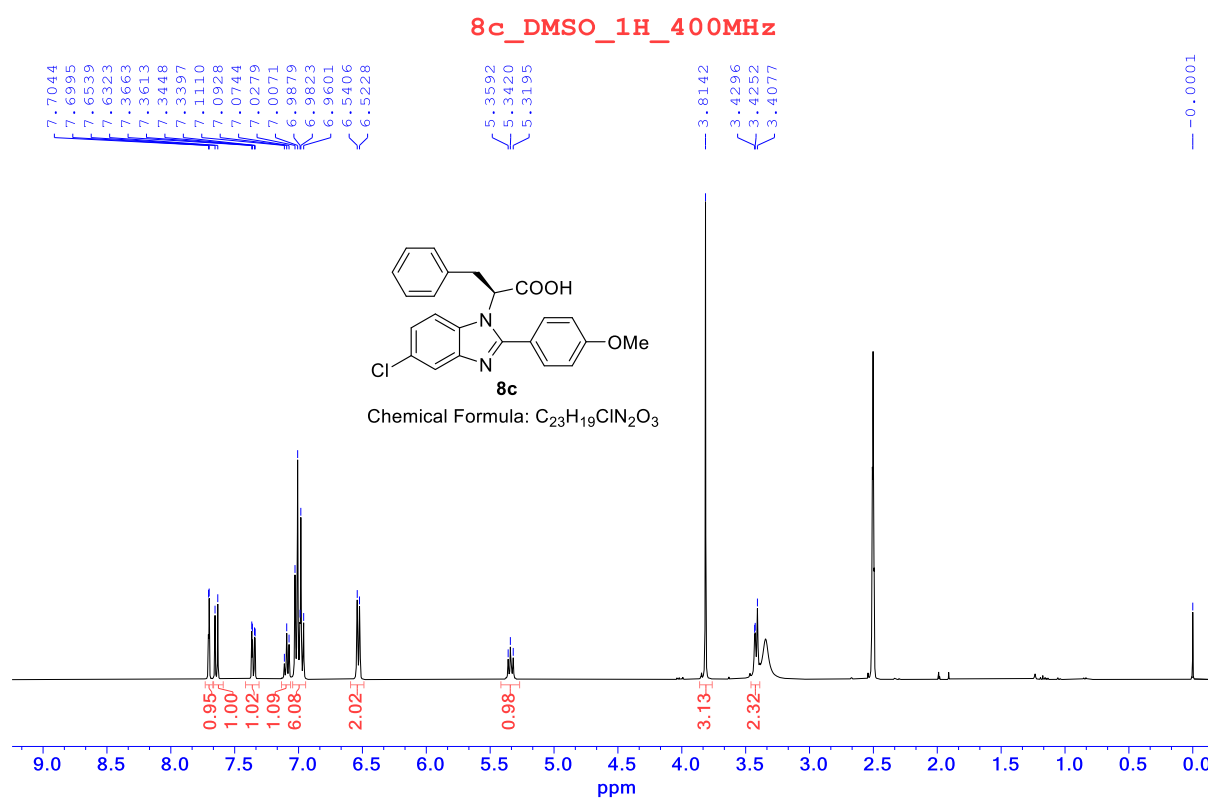
### Expanded spectrum

Spectrum from HUE\_KA130\_(+)ESI 2025-08-08-13-20-18.wiff2 (sample 1) - HUE\_KA130\_(+)E... 0.148 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)

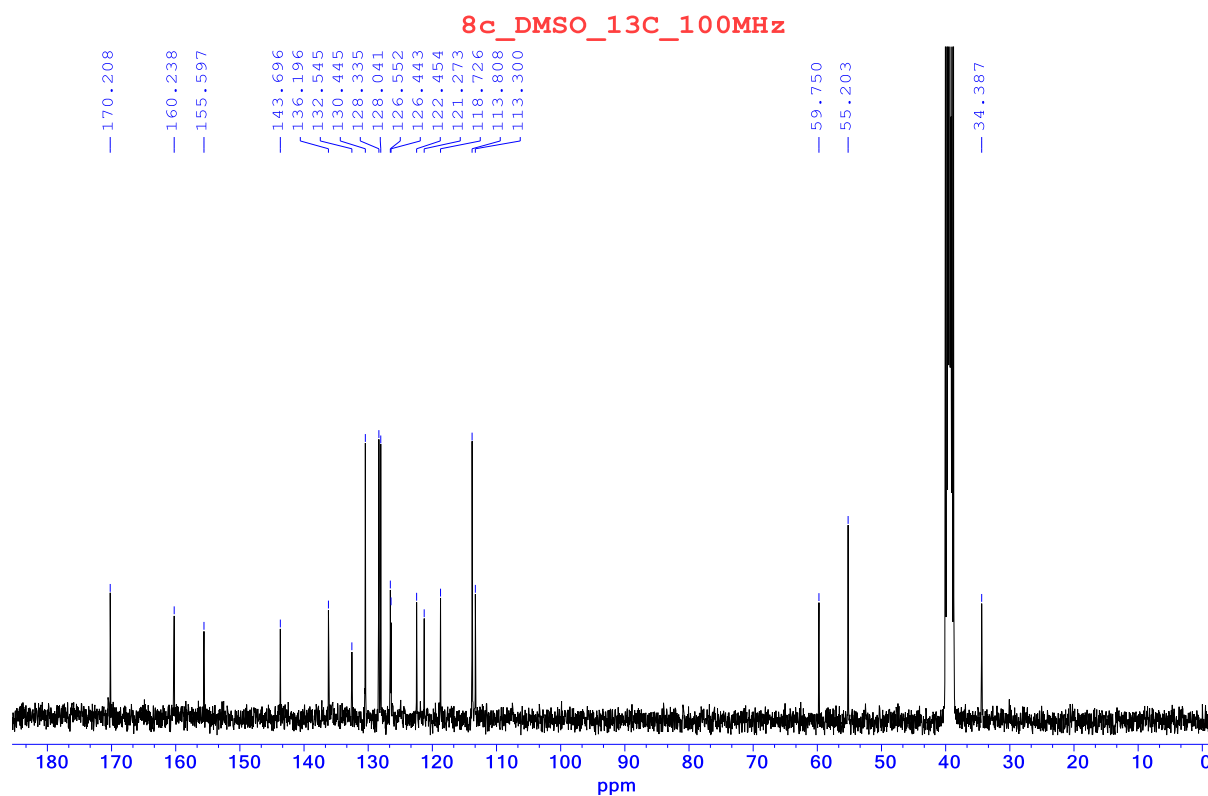


**Figure S25.** MS spectrum of compound **8b**





**Figure S26.** <sup>1</sup>H-NMR spectrum of compound **8c**



**Figure S27.** <sup>13</sup>C-NMR spectrum of compound **8c**

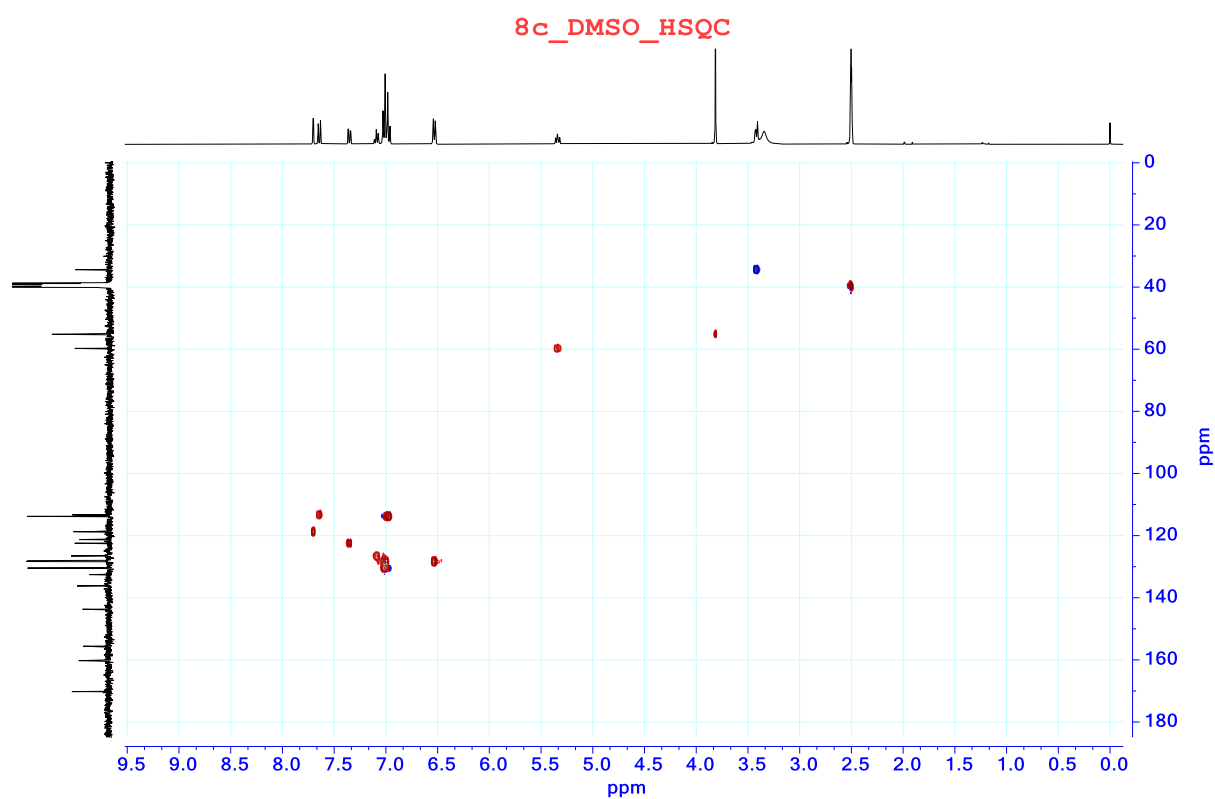


Figure S28. HSQC spectrum of compound **8c**

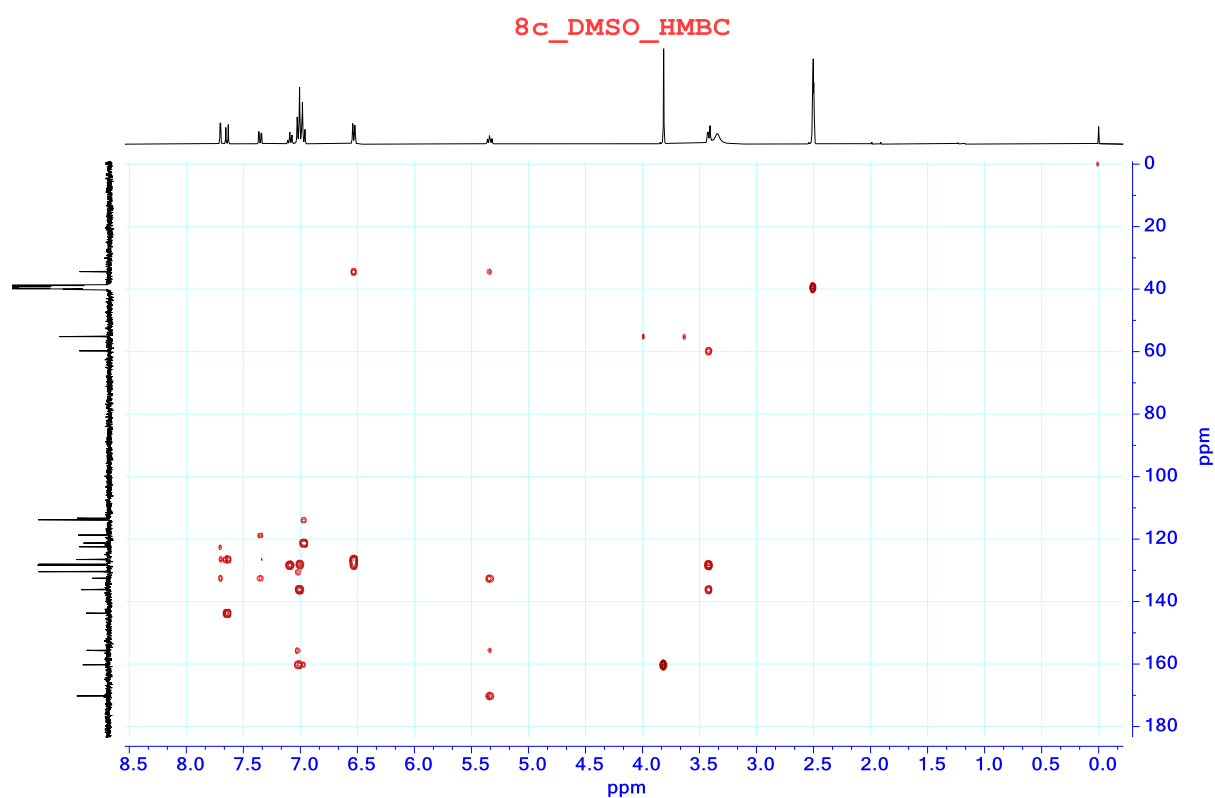


Figure S29. HMBC spectrum of compound **8c**

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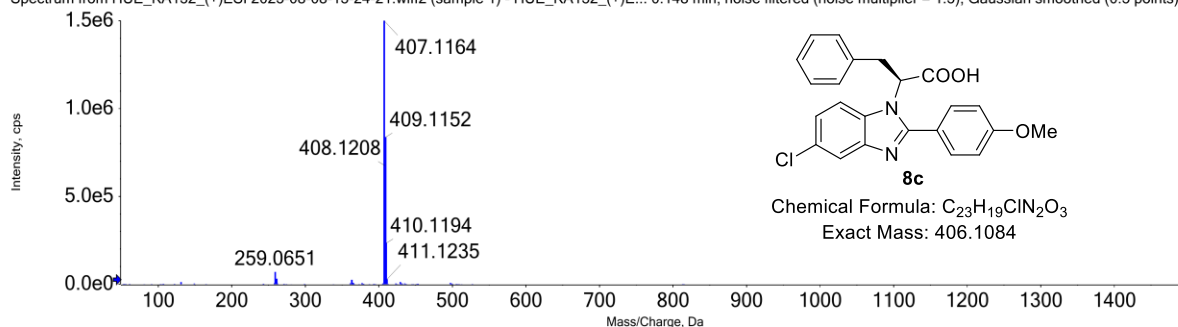
## ANALYSIS REPORT

### Injection details

Sample name	KA132	Vial position	26
Sample file name	SR. wiff2-HUE	Inject volume	2.00
Acquisition date	08/08/2025 01:24:27 PM	Acquisition method	ESI_POS_SCAN
Operator	CB21261708	Instrument name	X500R QTOF

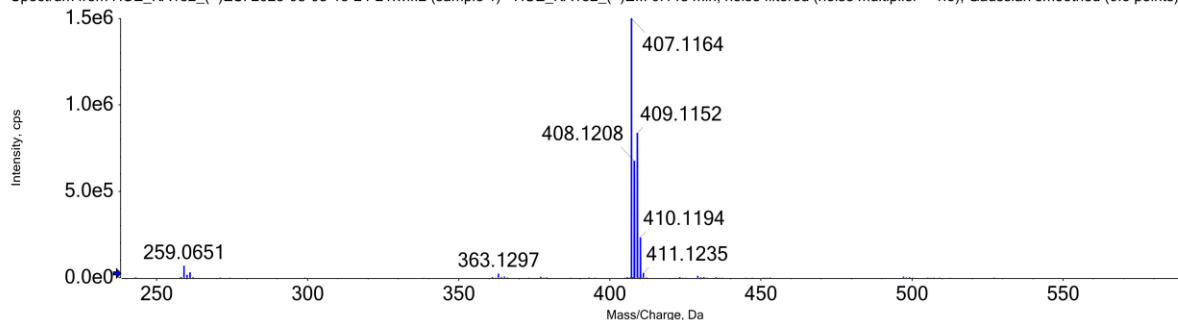
### Full mass spectrum

Spectrum from HUE\_KA132\_(+)ESI 2025-08-08-13-24-21.wiff2 (sample 1) - HUE\_KA132\_(+)E... 0.148 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



### Expanded spectrum

Spectrum from HUE\_KA132\_(+)ESI 2025-08-08-13-24-21.wiff2 (sample 1) - HUE\_KA132\_(+)E... 0.148 min, noise filtered (noise multiplier = 1.5), Gaussian smoothed (0.5 points)



**Figure S30. MS spectrum of compound 8c**