

SUPPLEMENTARY DATA

Synthesis and cytotoxicity evaluation of benzimidazole conjugated amino acid derivatives

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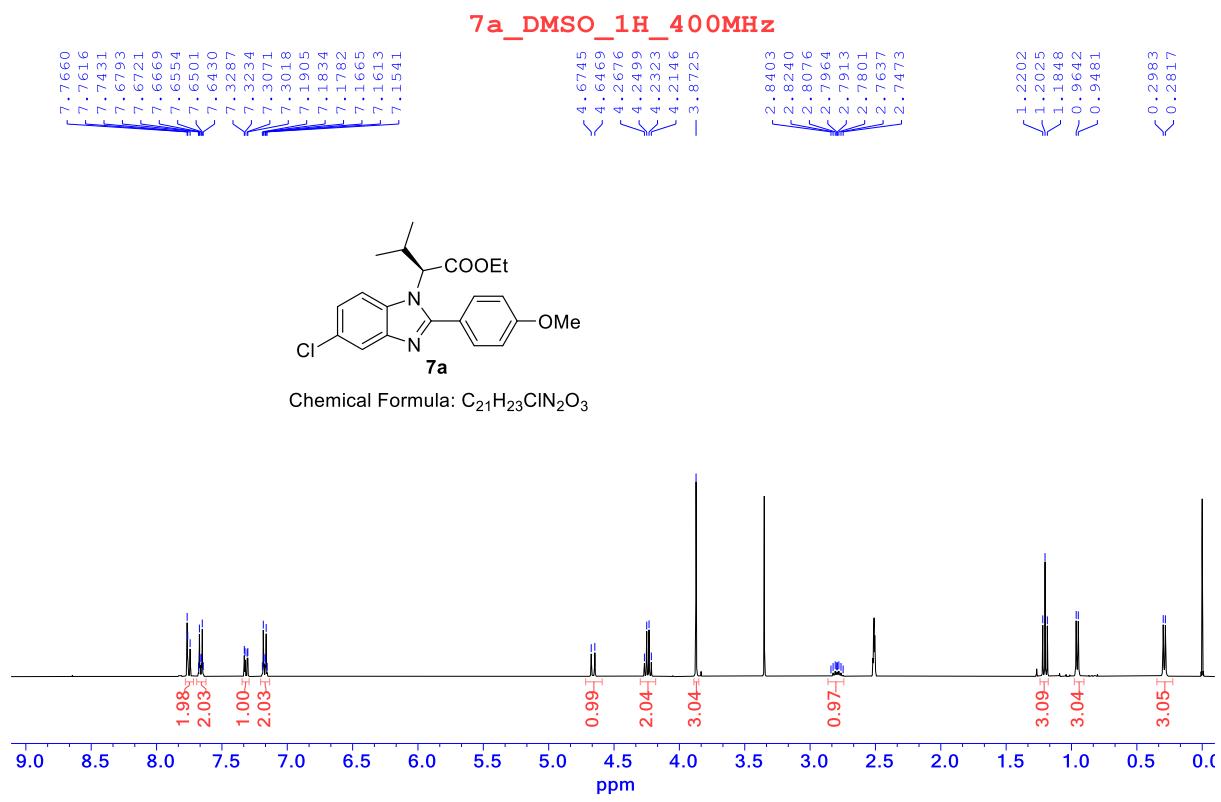


Figure S1. ¹H-NMR spectrum of compound **7a**

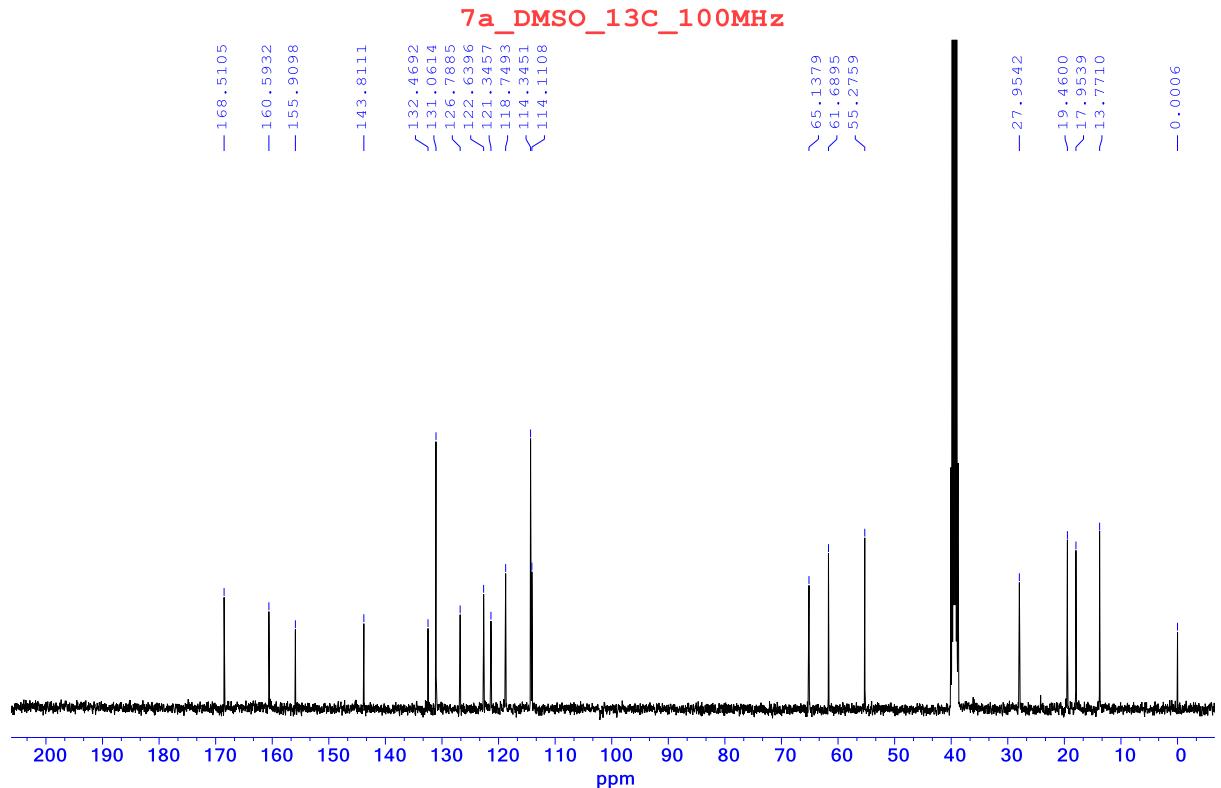


Figure S2. ¹³C-NMR spectrum of compound **7a**

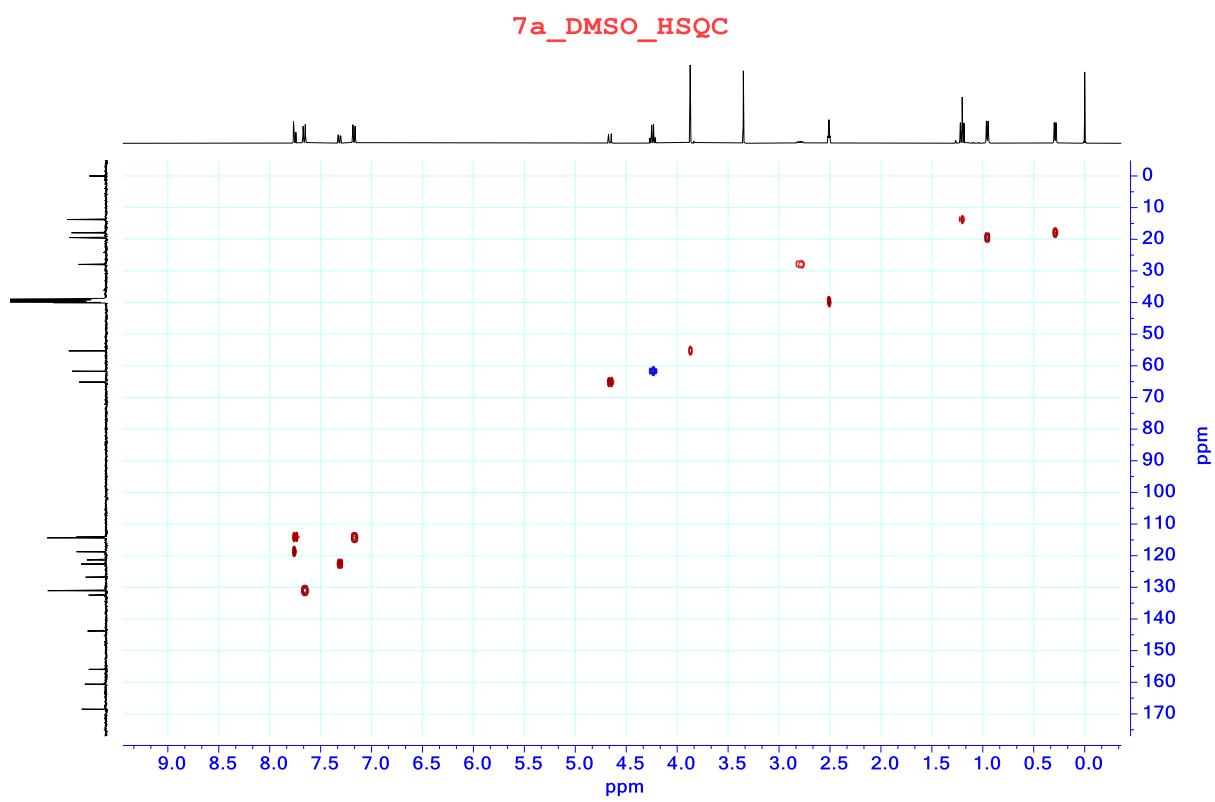


Figure S3. HSQC spectrum of compound **7a**

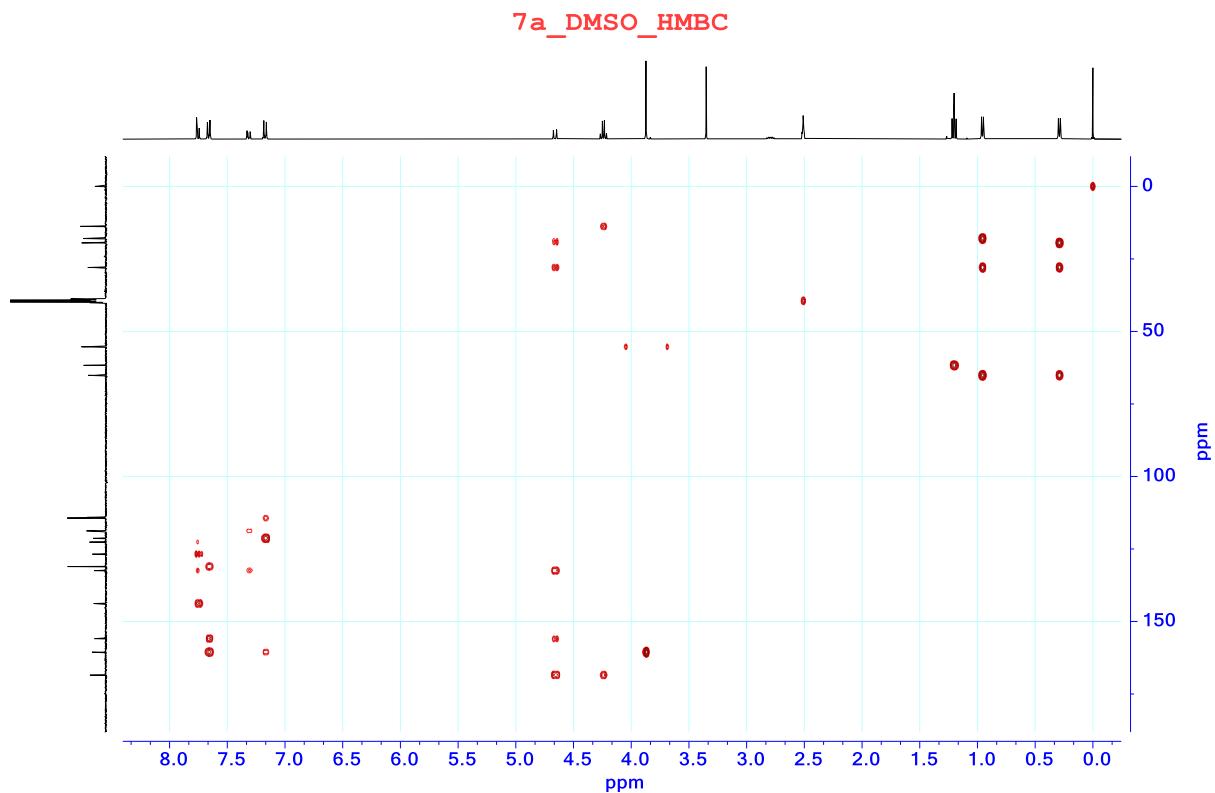


Figure S4. HMBC spectrum of compound **7a**

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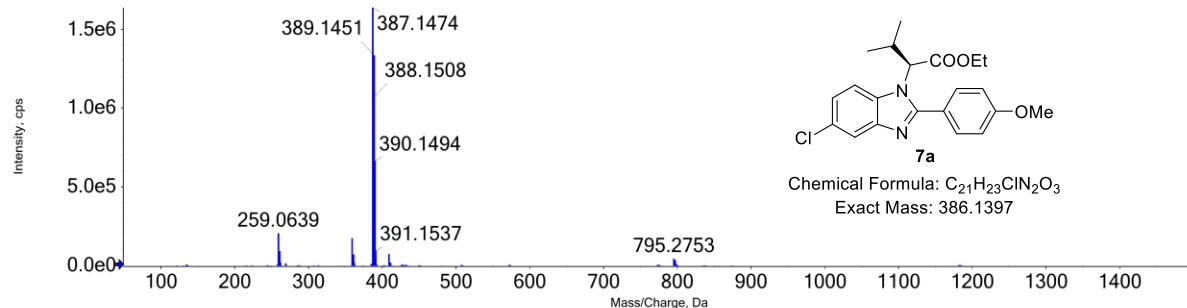
ANALYSIS REPORT

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	X500 _R 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)

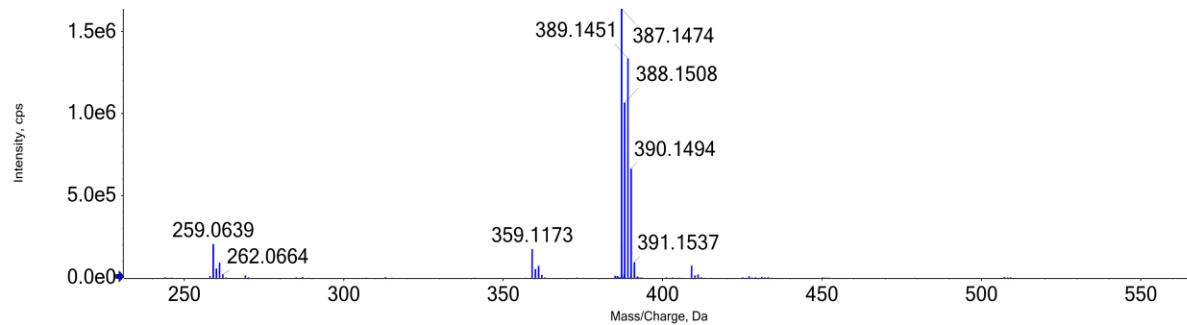


Figure S5. MS spectrum of compound **7a**

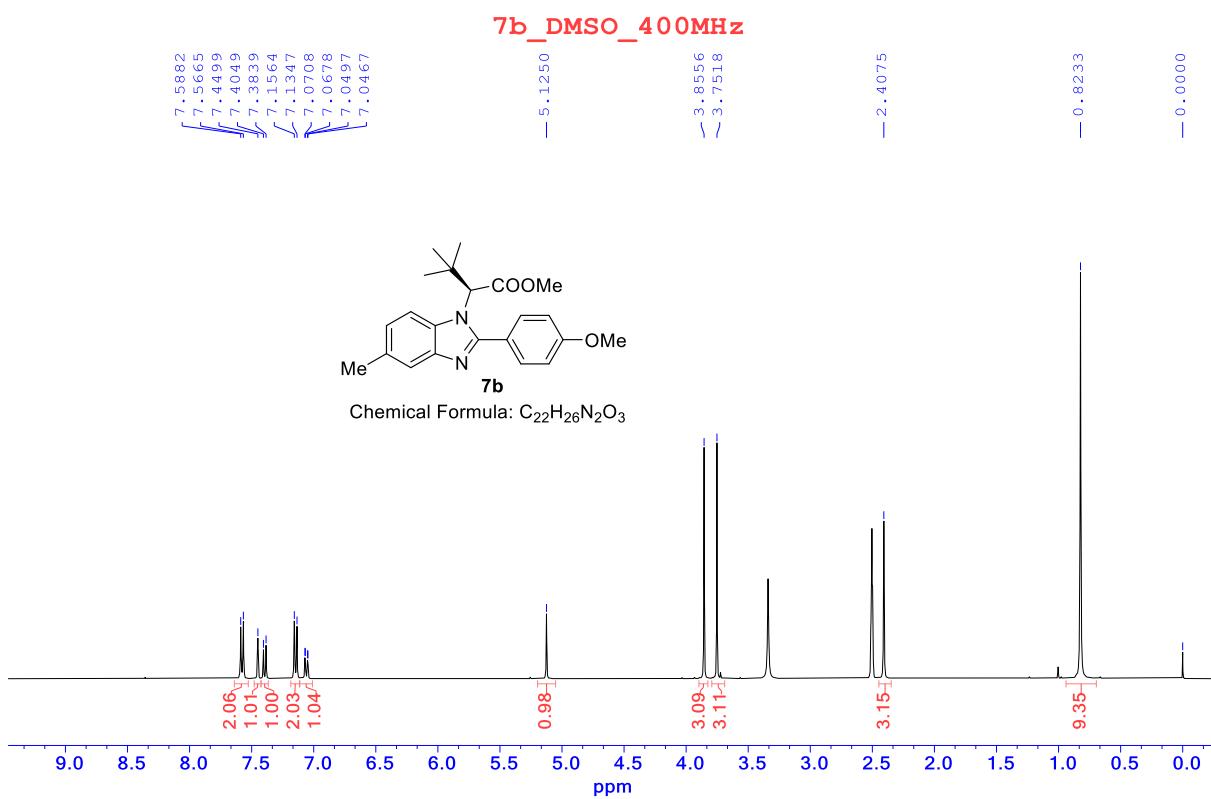


Figure S6. ^1H -NMR spectrum of compound **7b**

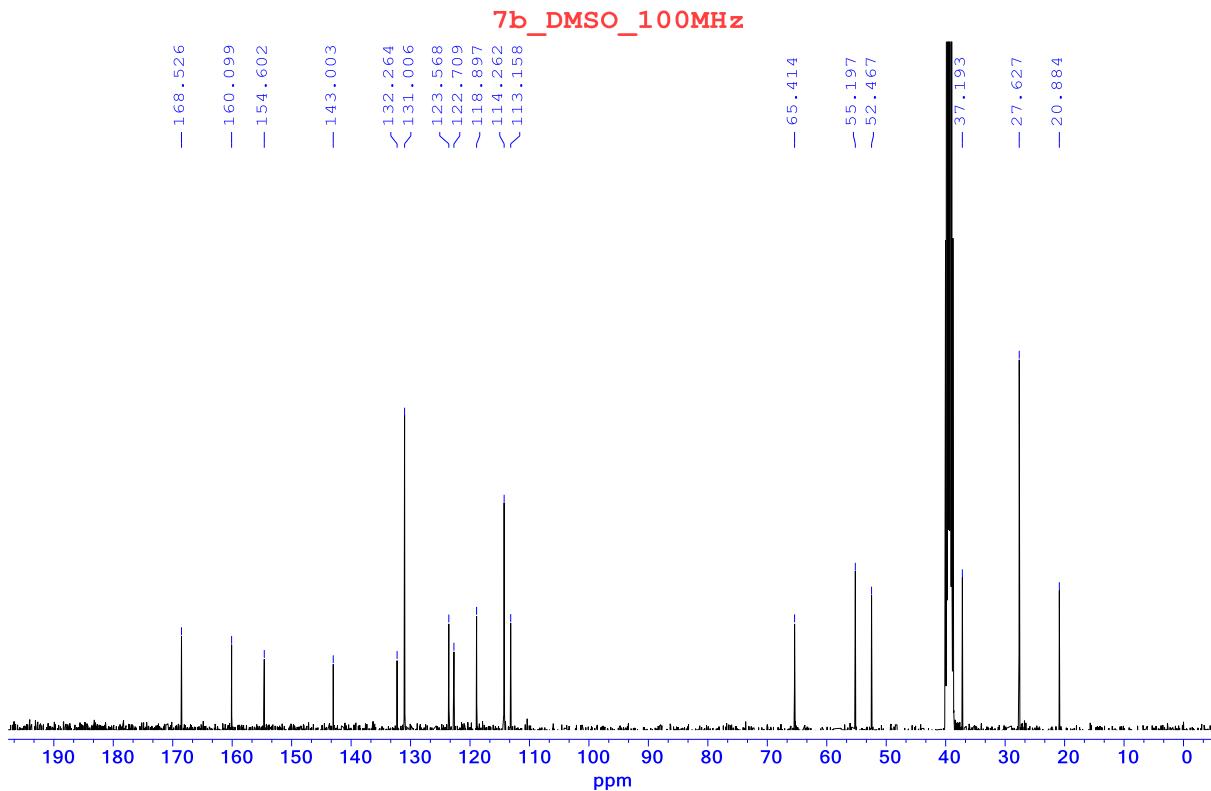


Figure S7. ^{13}C -NMR spectrum of compound **7b**

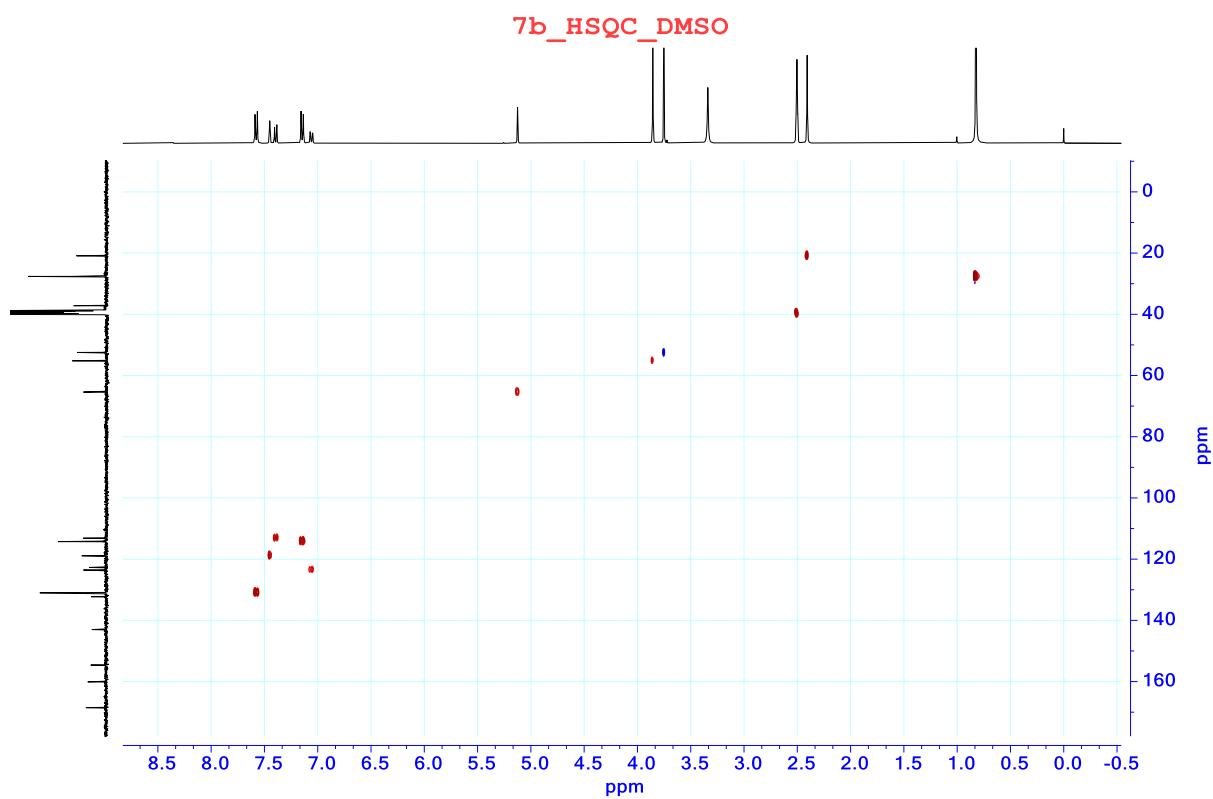


Figure S8. HSQC spectrum of compound 7b

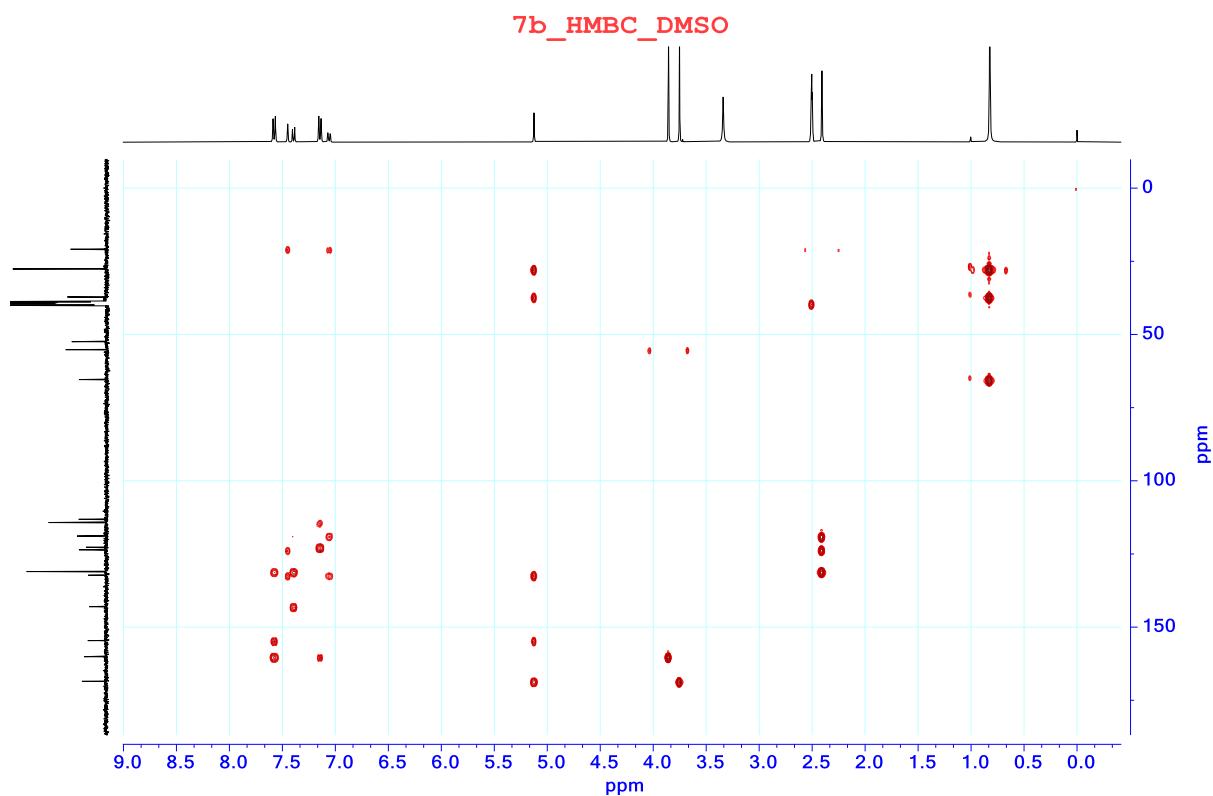


Figure S9. HMBC spectrum of compound 7b

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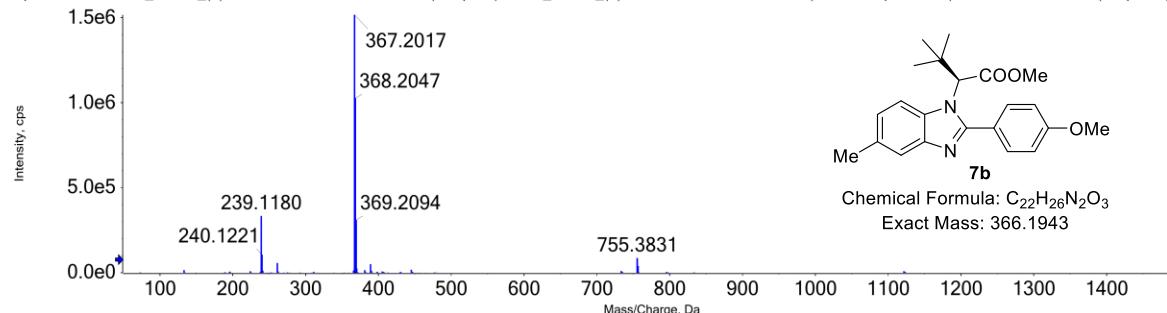
ANALYSIS REPORT

Injection details

<i>Sample name</i>	KA129	<i>Vial position</i>	23
<i>Sample file name</i>	SR. wiff2-HUE	<i>Inject volume</i>	2.00
<i>Acquisition date</i>	08/08/2025 01:18:10 PM	<i>Acquisition method</i>	ESI_POS_SCAN
<i>Operator</i>	CB21261708	<i>Instrument name</i>	X500 _R 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)

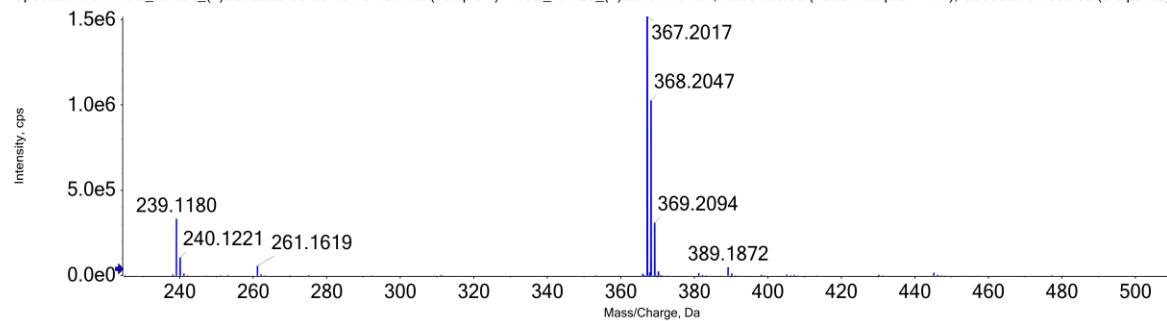


Figure S10. MS spectrum of compound **7b**

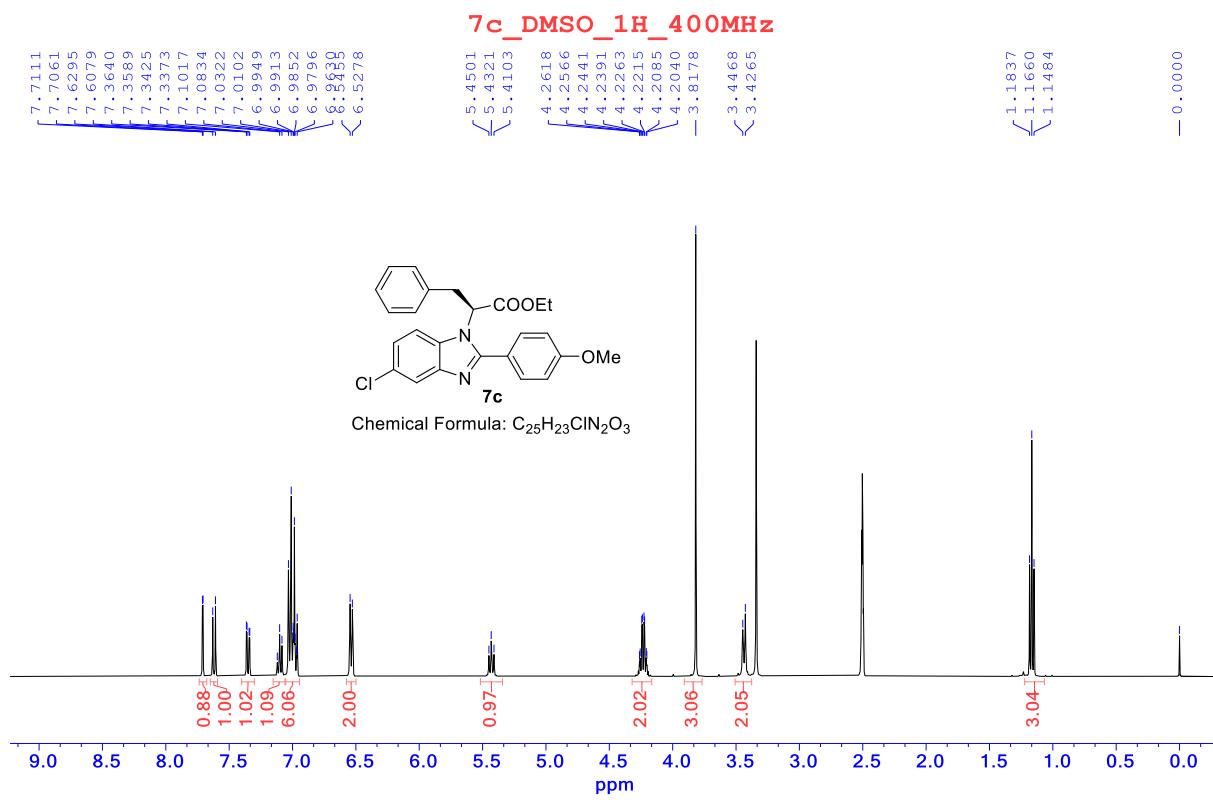


Figure S11. ¹H-NMR spectrum of compound **7c**

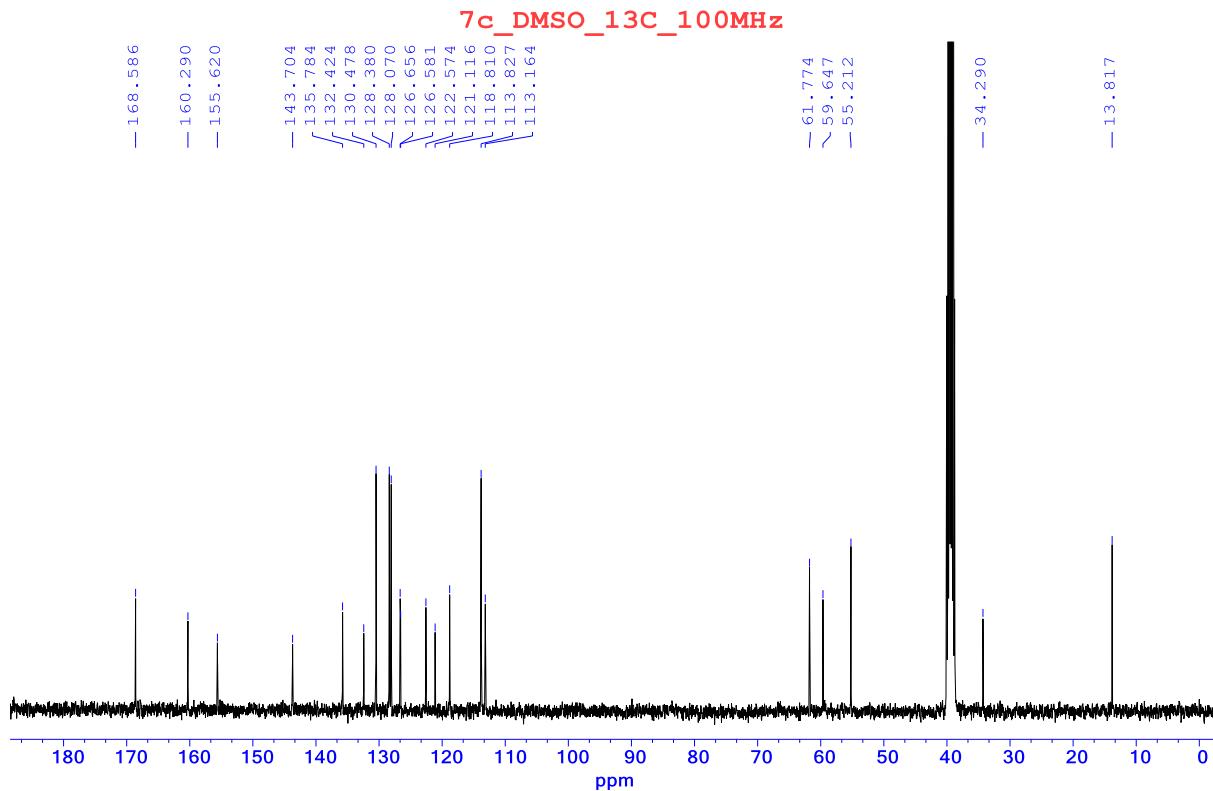


Figure S12. ¹³C-NMR spectrum of compound **7c**

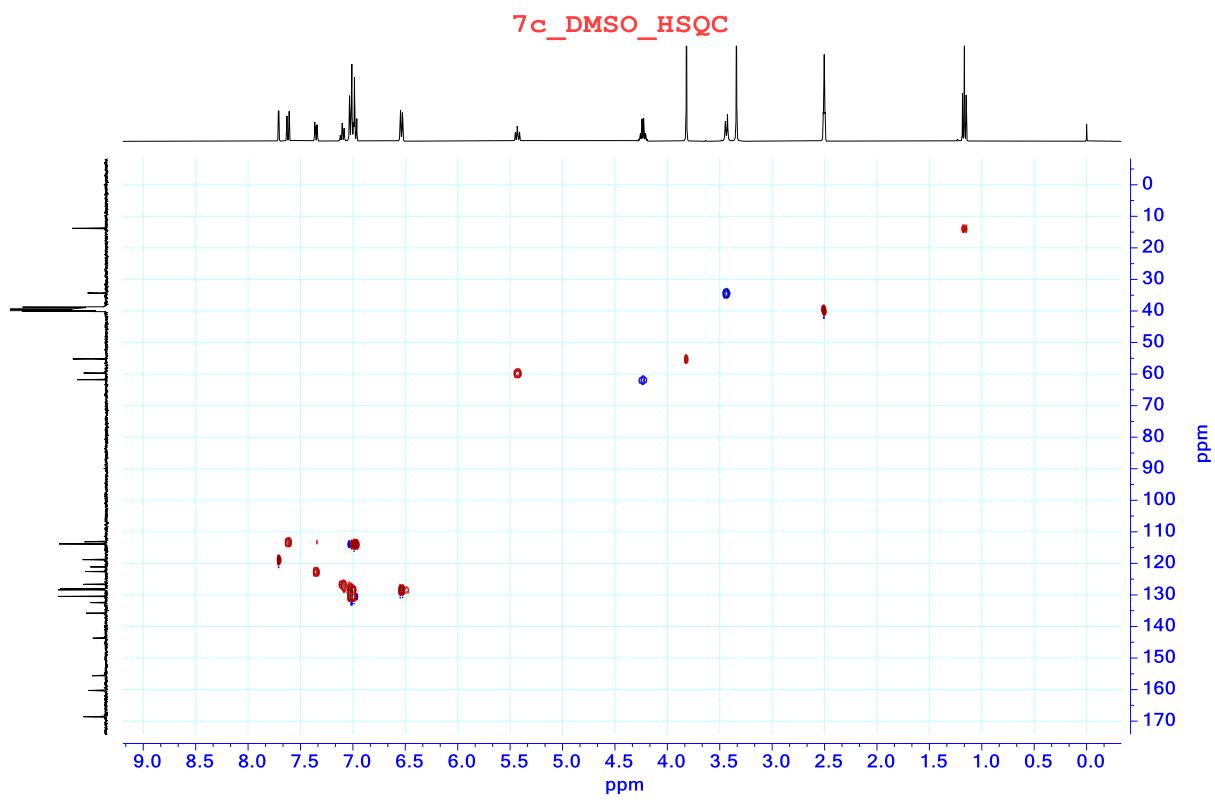


Figure S13. HSQC spectrum of compound **7c**

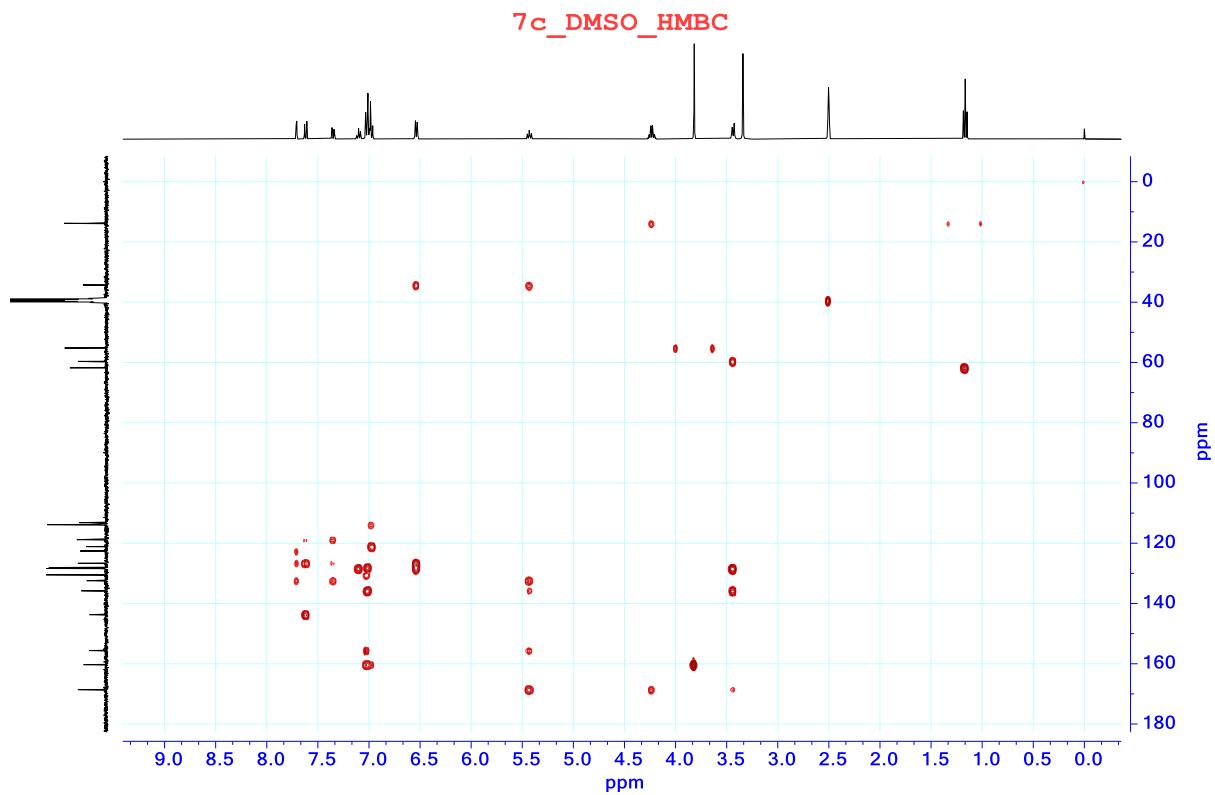


Figure S14. HMBC spectrum of compound **7c**

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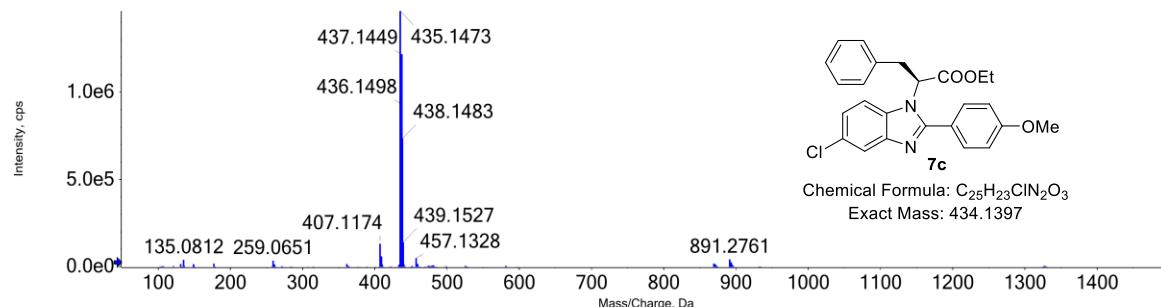
ANALYSIS REPORT

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	X500 _R 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)

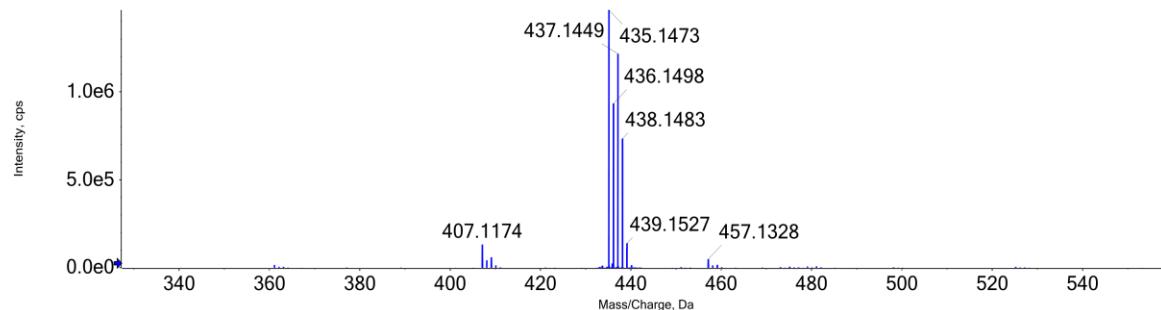


Figure S15. MS spectrum of compound 7c

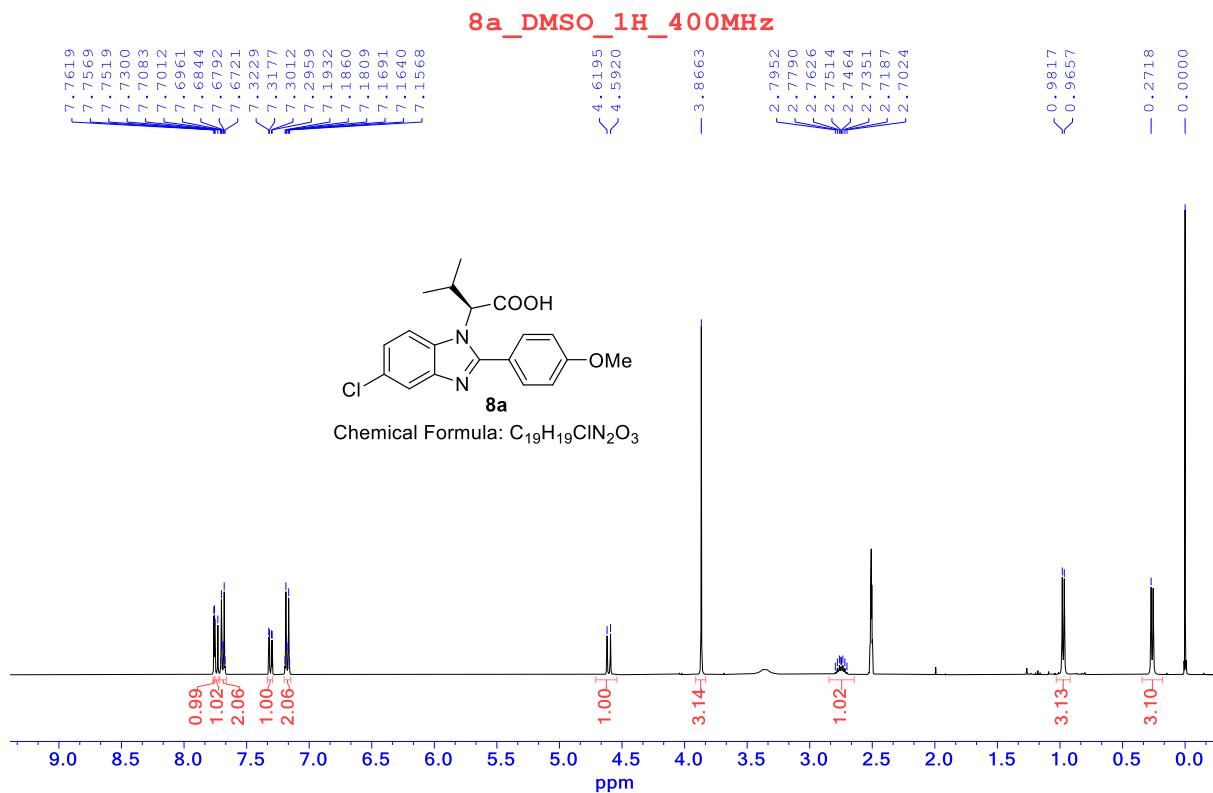


Figure S16. ¹H-NMR spectrum of compound 8a

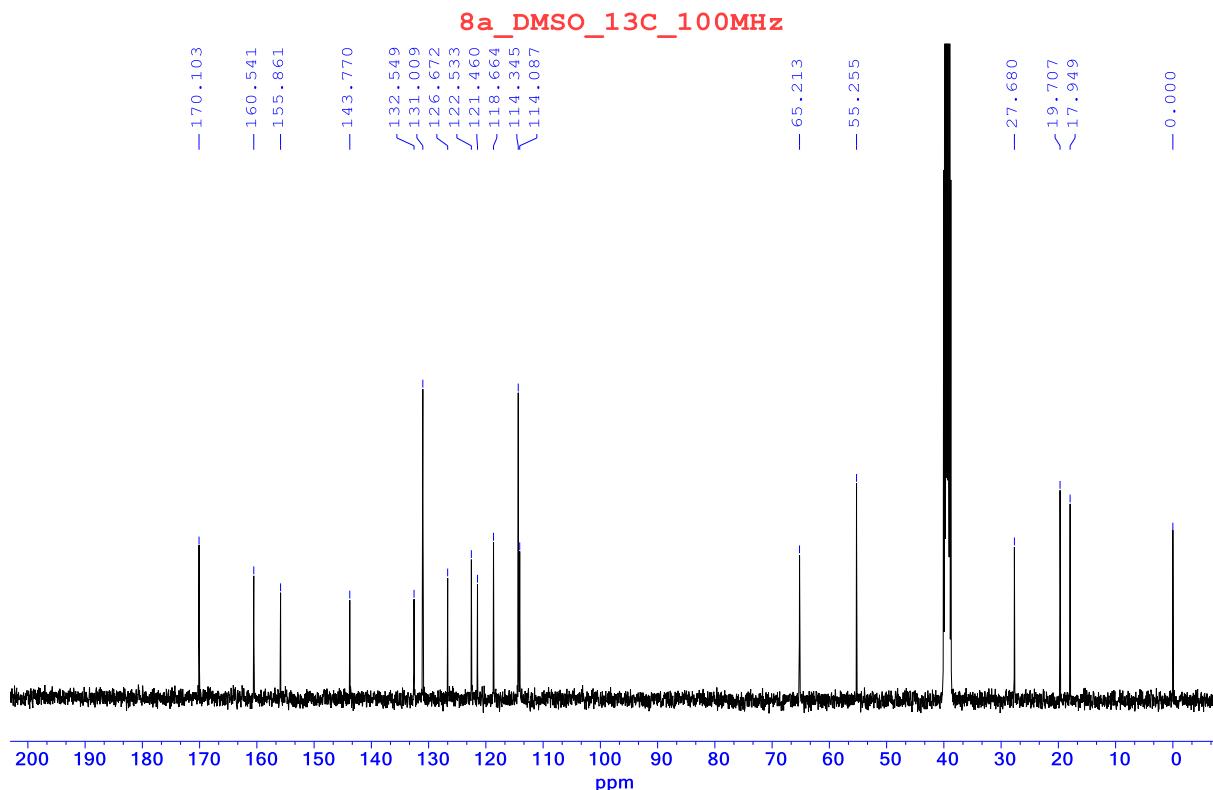


Figure S17. ¹³C-NMR spectrum of compound 8a

8a_DMSO_HSQC

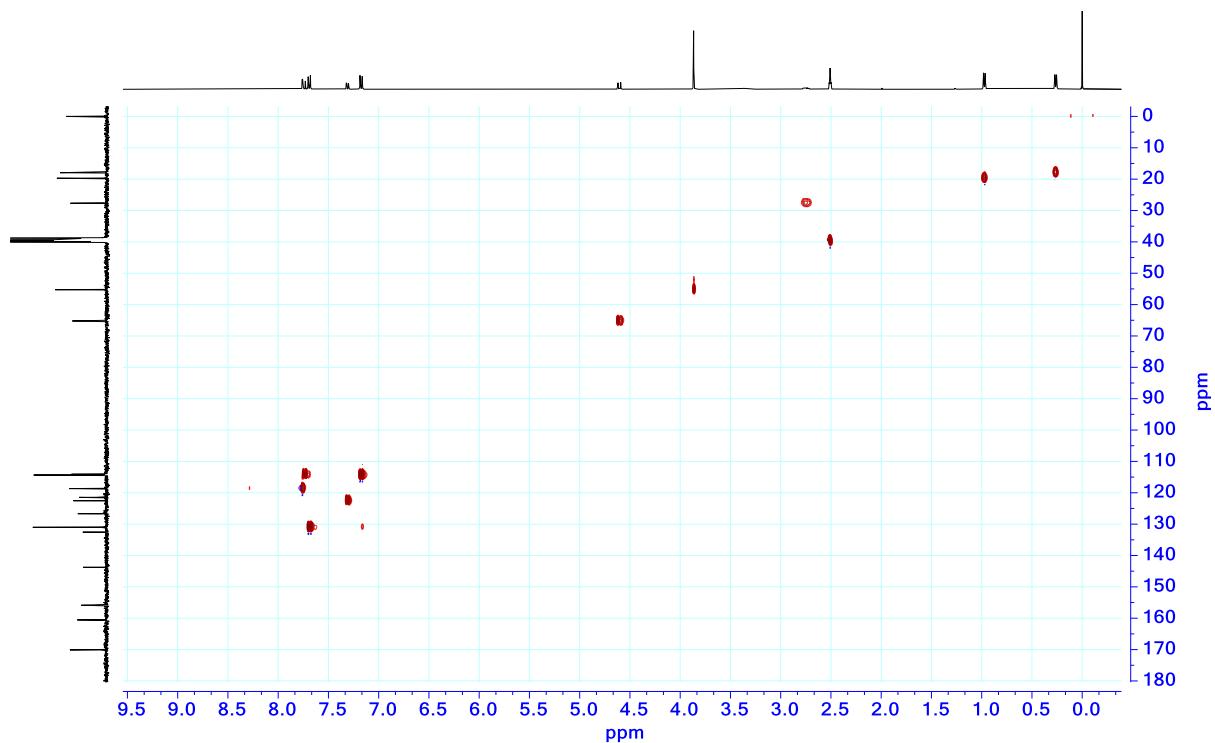


Figure S18. HSQC spectrum of compound 8a

8a_DMSO_HMBC

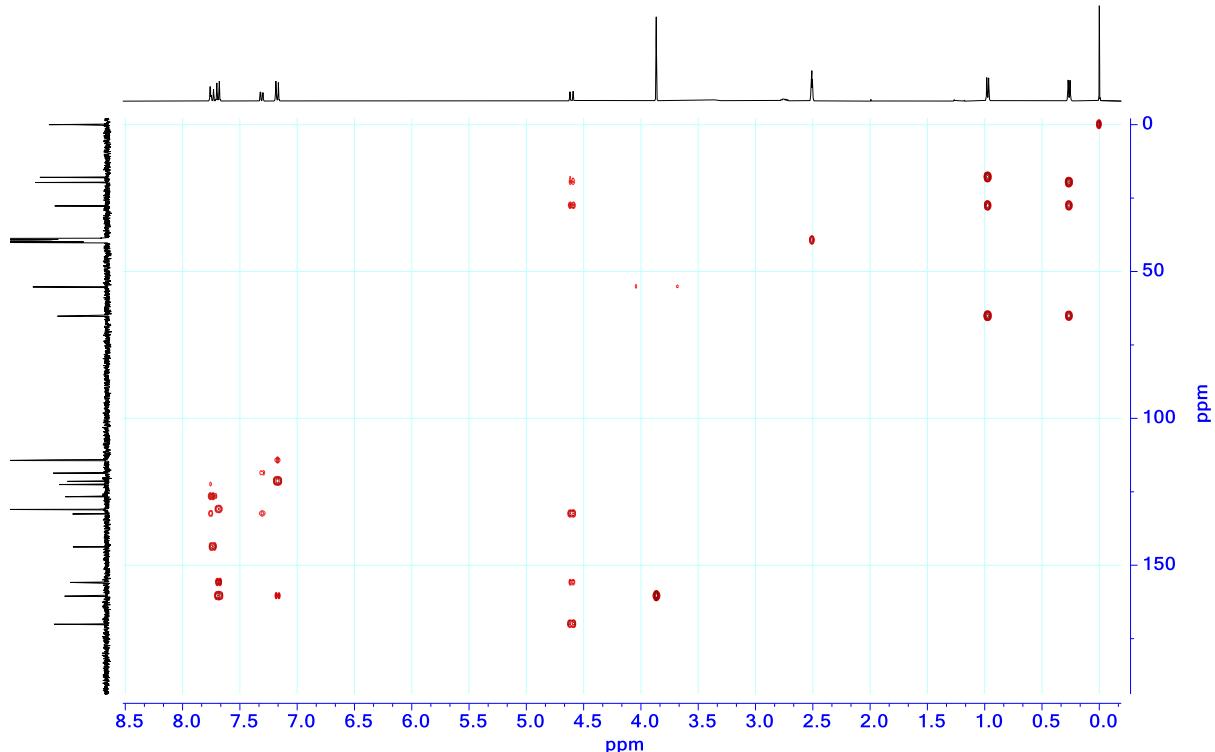


Figure S19. HMBC spectrum of compound 8a

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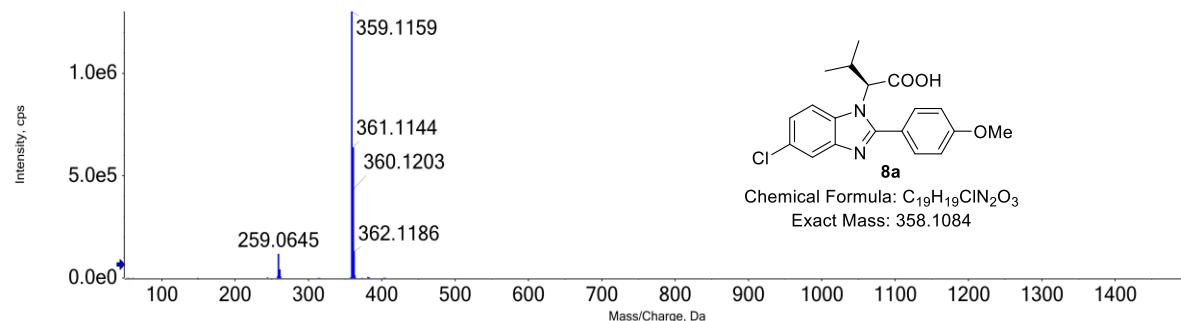
ANALYSIS REPORT

Injection details

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

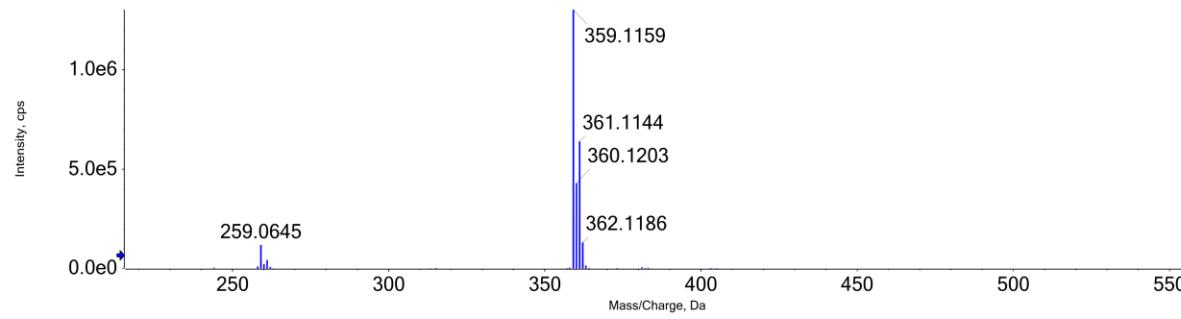


Figure S20. MS spectrum of compound **8a**

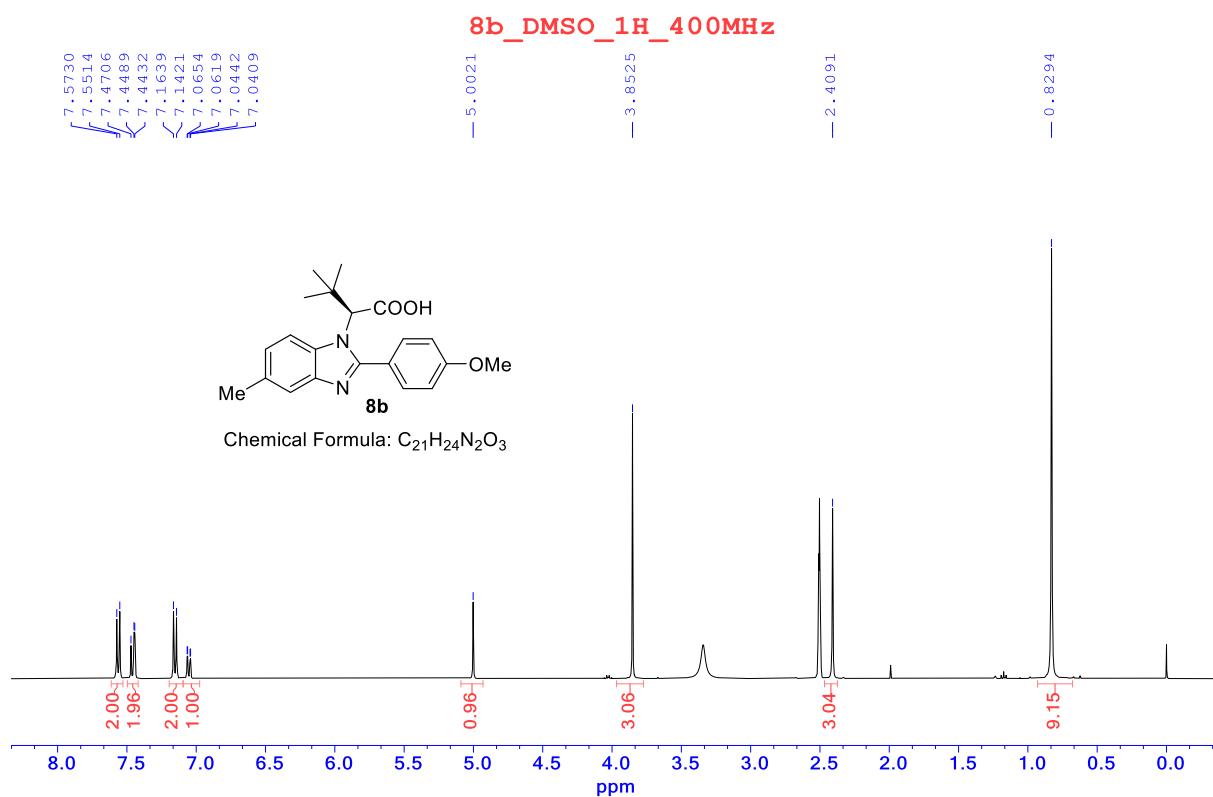


Figure S21. ¹H-NMR spectrum of compound **8b**

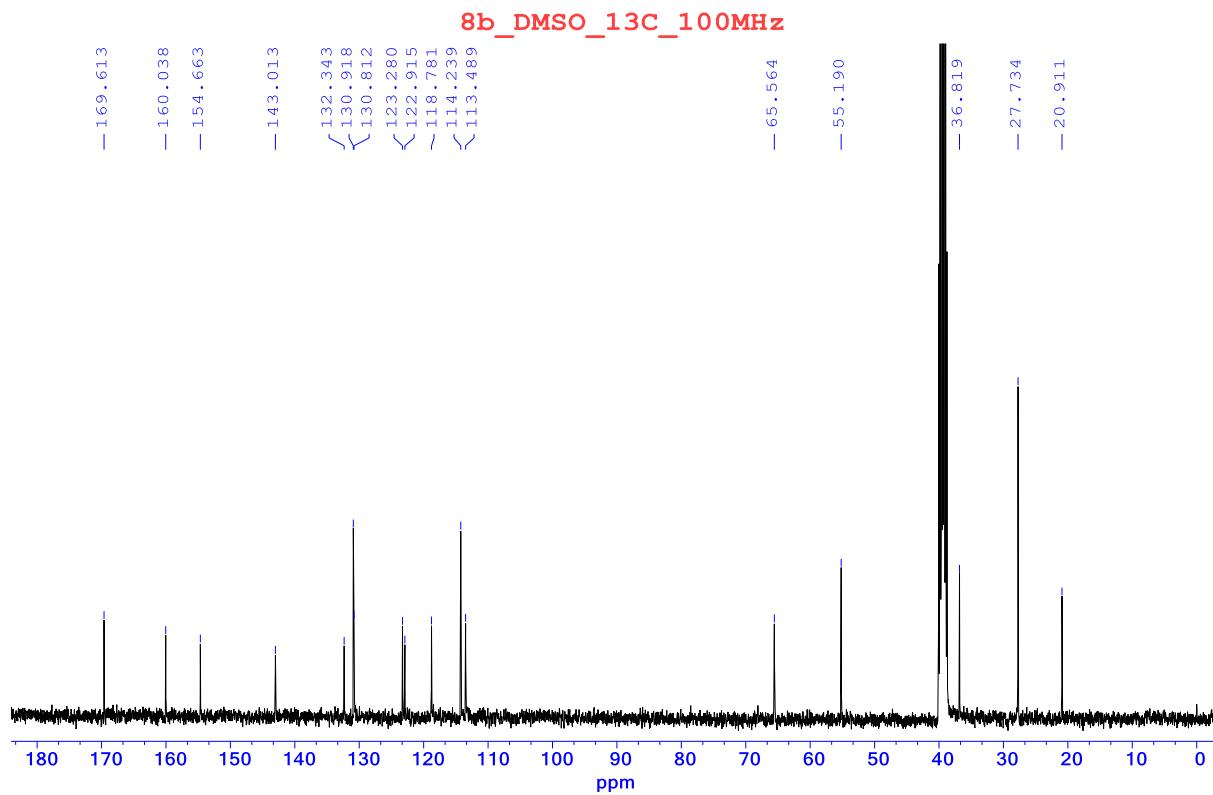


Figure S22. ¹³C-NMR spectrum of compound **8b**

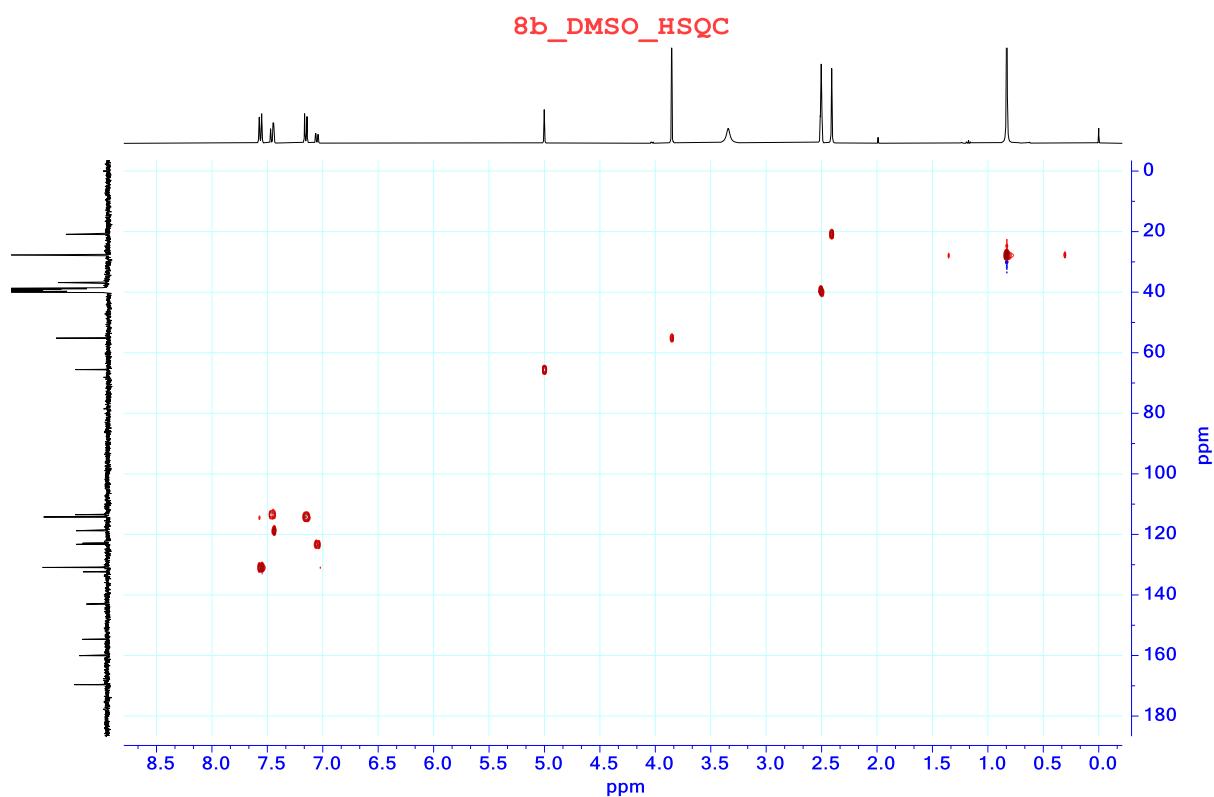


Figure S23. HSQC spectrum of compound **8b**

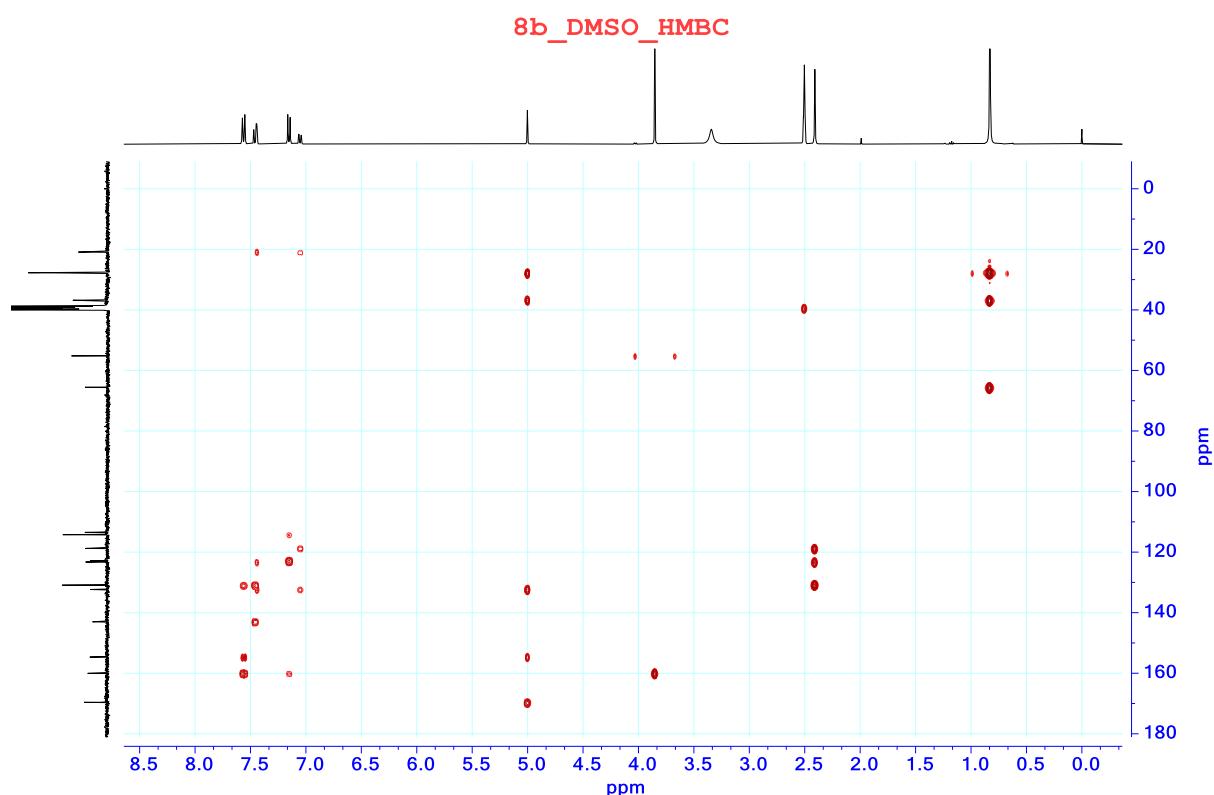


Figure S24. HMBC spectrum of compound **8b**

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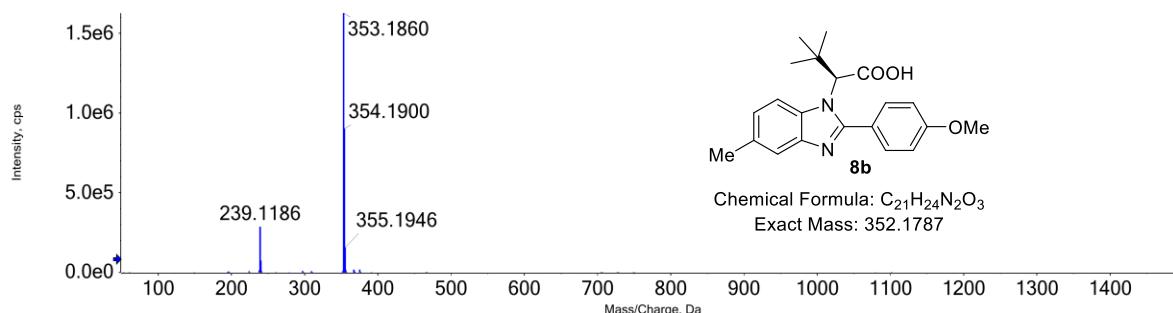
ANALYSIS REPORT

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	ESI_POS_SCAN
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)

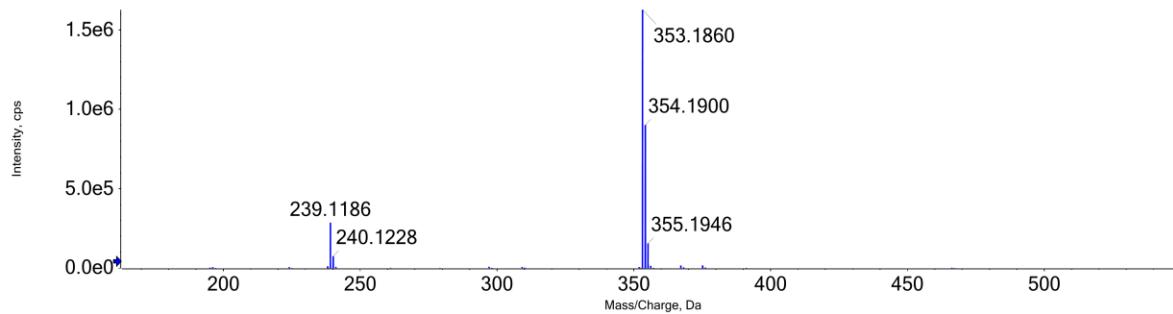


Figure S25. MS spectrum of compound **8b**

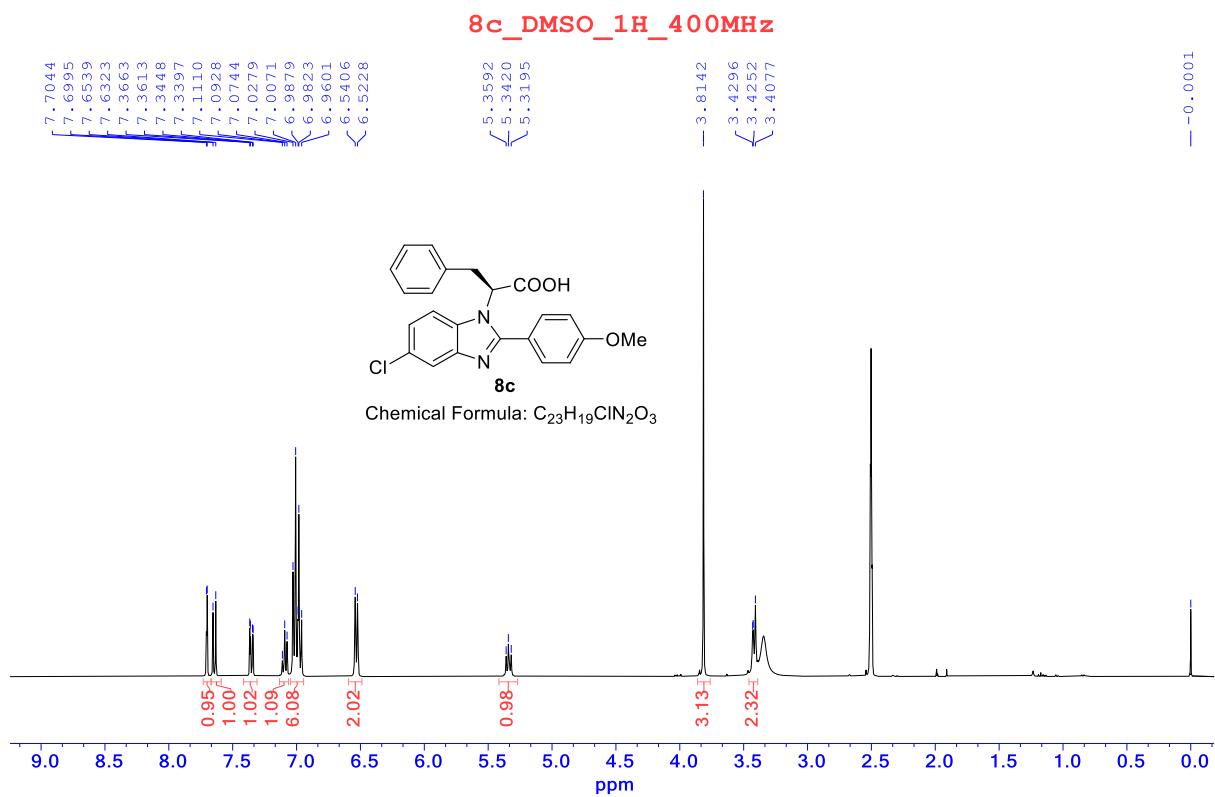


Figure S26. ¹H-NMR spectrum of compound **8c**

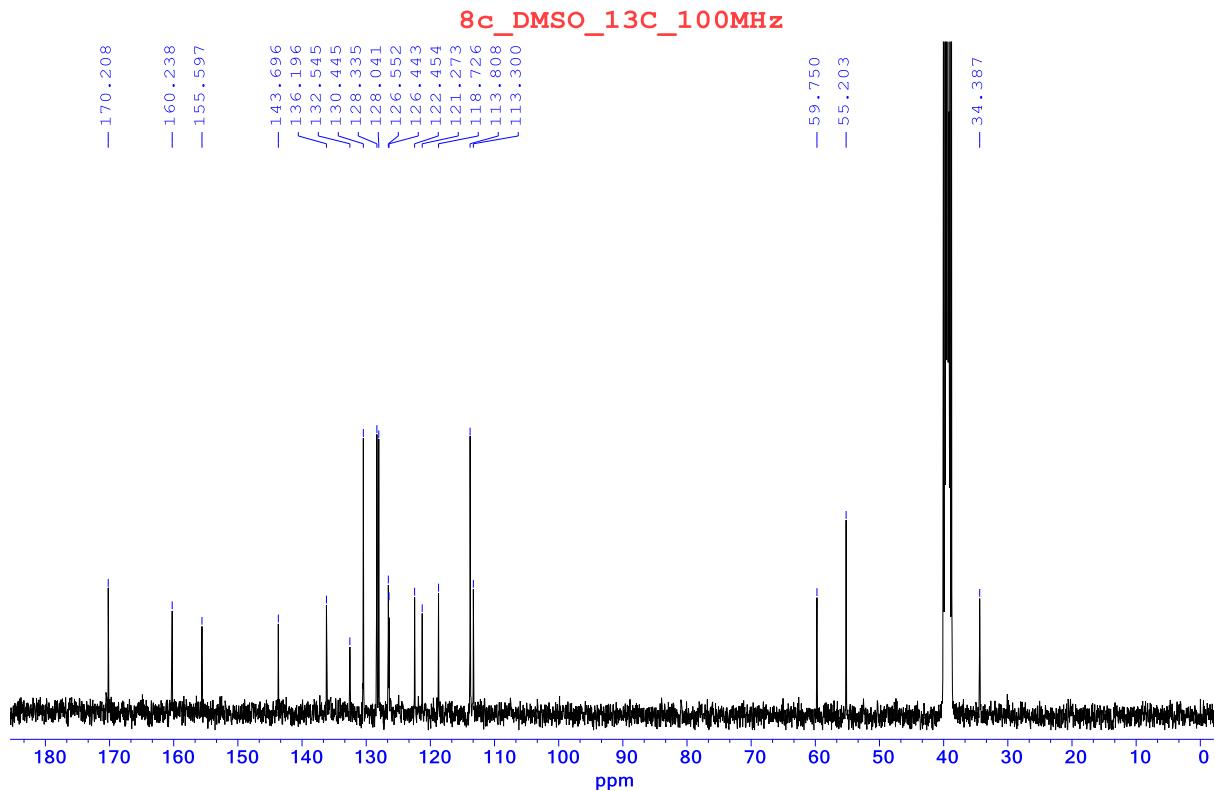


Figure S27. ¹³C-NMR spectrum of compound **8c**

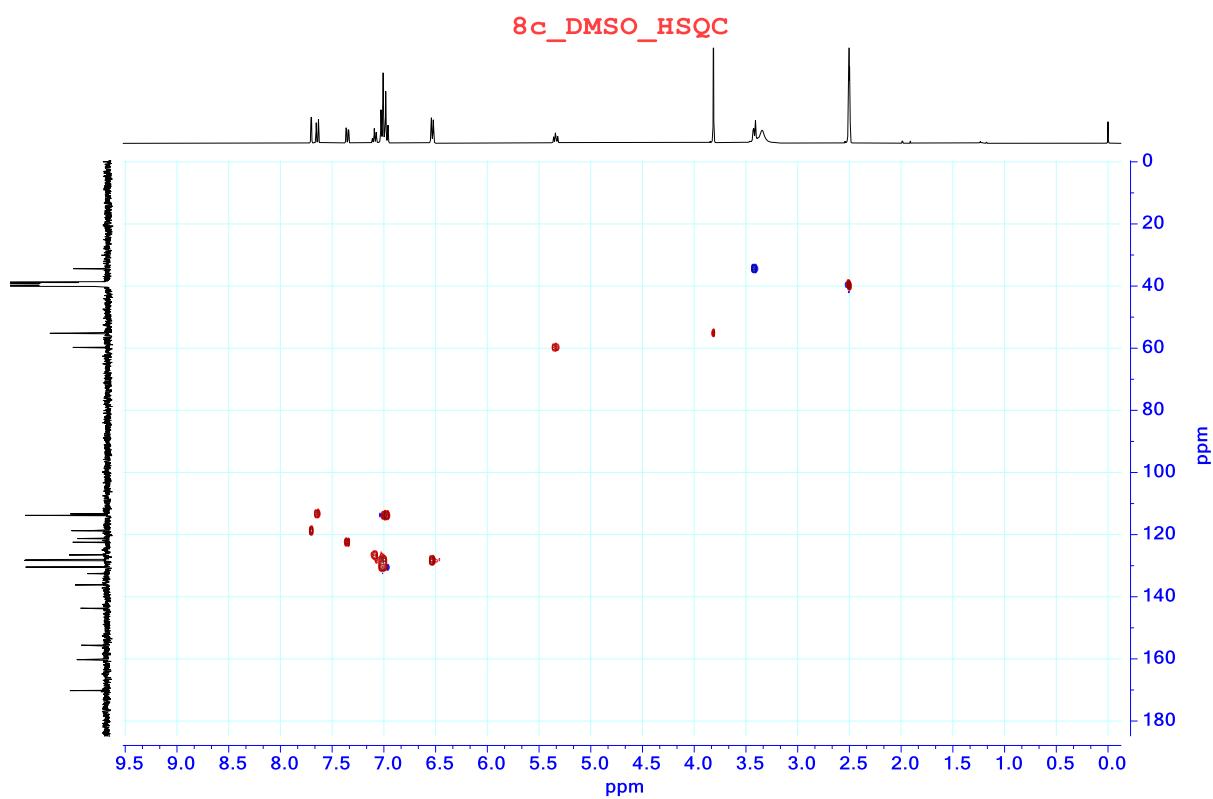


Figure S28. HSQC spectrum of compound **8c**

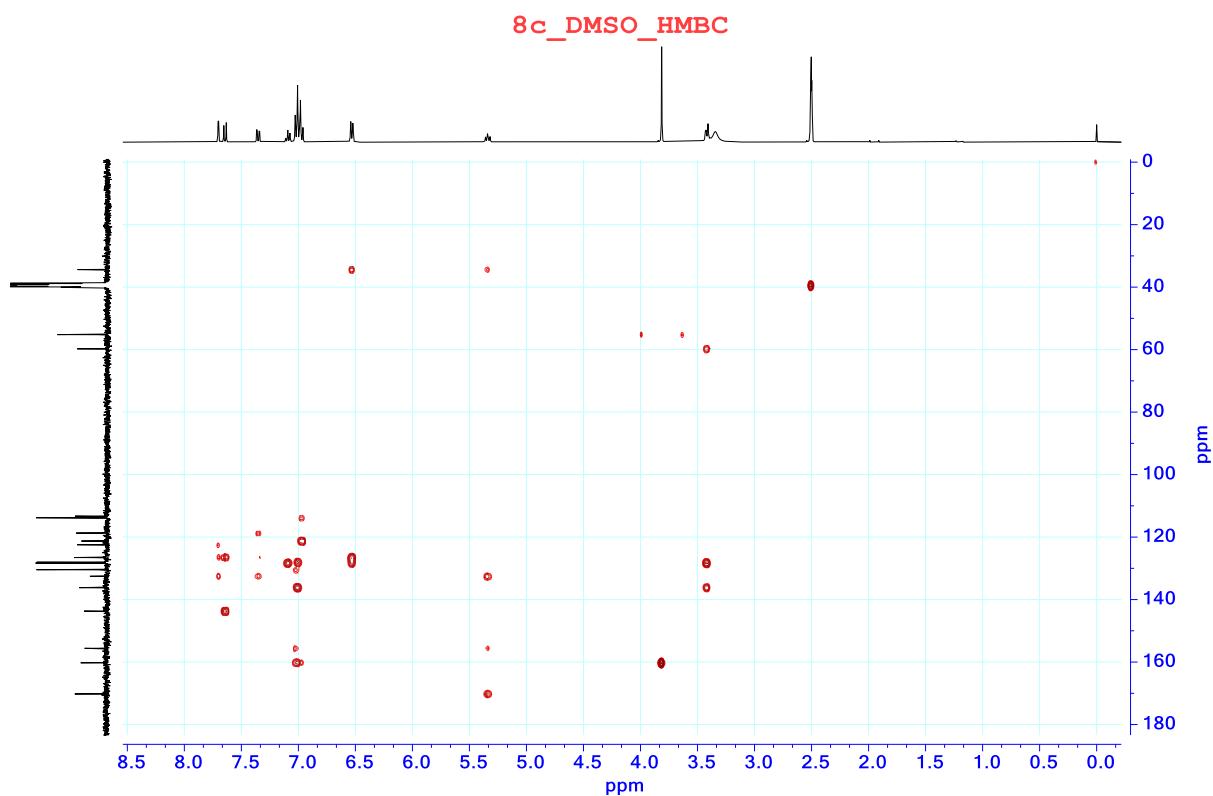


Figure S29. HMBC spectrum of compound **8c**

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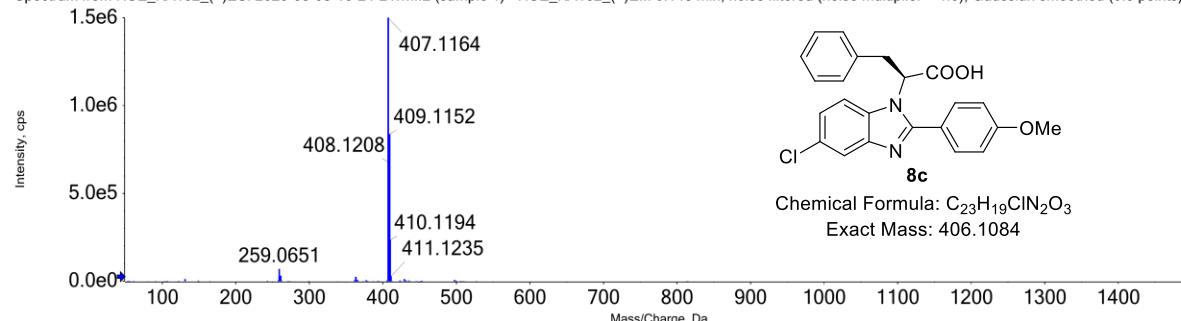
ANALYSIS REPORT

Injection details

<i>Sample name</i>	KA132	<i>Vial position</i>	26
<i>Sample file name</i>	SR. wiff2-HUE	<i>Inject volume</i>	2.00
<i>Acquisition date</i>	08/08/2025 01:24:27 PM	<i>Acquisition method</i>	ESI_POS_SCAN
<i>Operator</i>	CB21261708	<i>Instrument name</i>	X500 _R 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)

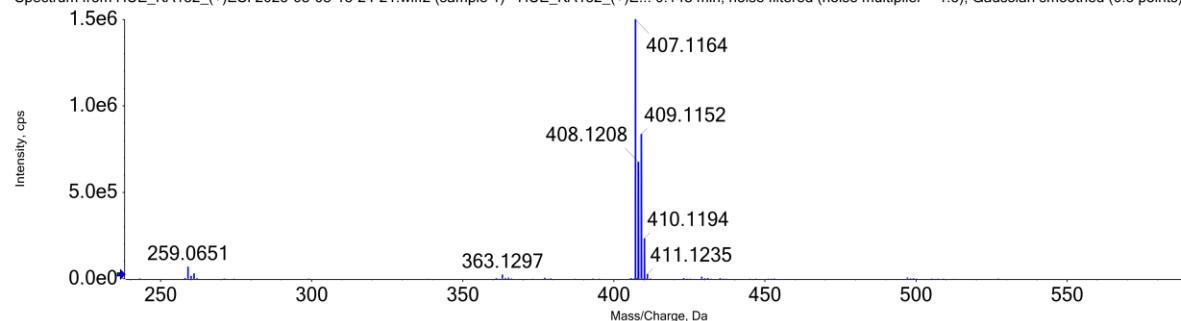


Figure S30. MS spectrum of compound **8c**