

Identification of pyrazole–rhodanine hybrid scaffolds as potent inhibitors of aldose reductase: design, synthesis, biological evaluation and molecular docking analysis

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Shahid Hameed^{a*}

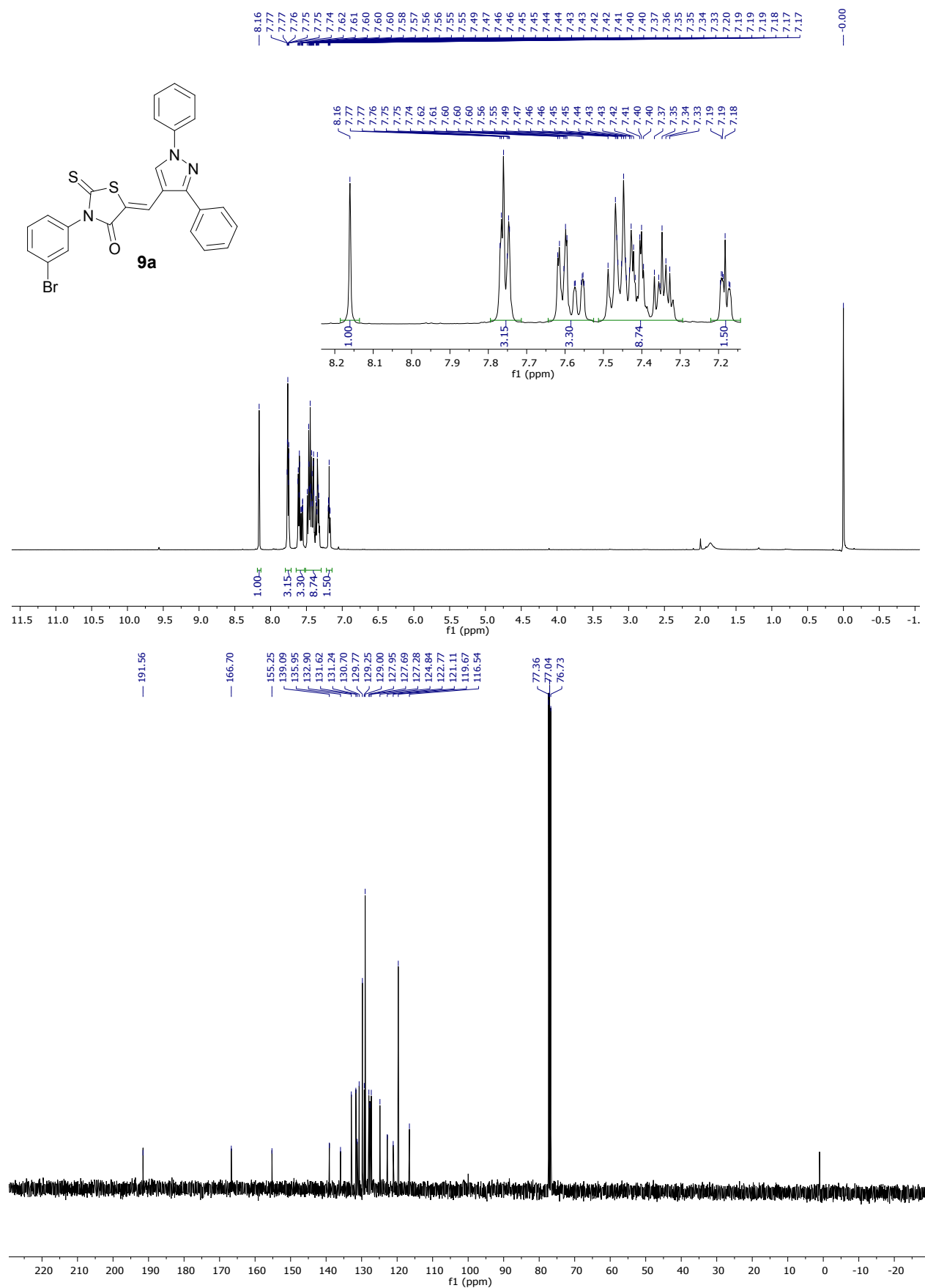
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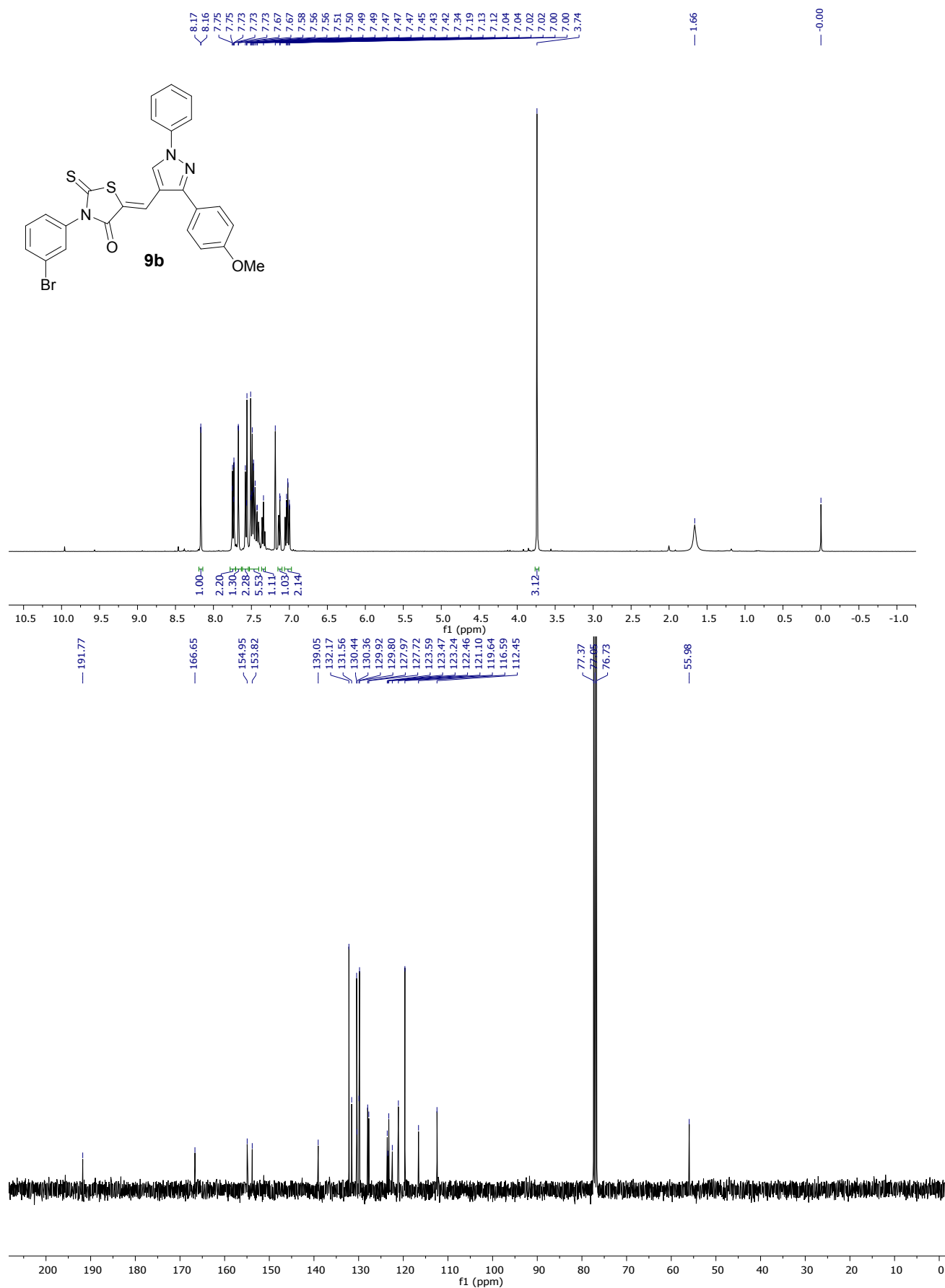
^b*Centre for Advanced Drug Research, COMSATS Institute of Information Technology,
Abbottabad-22060, Pakistan*

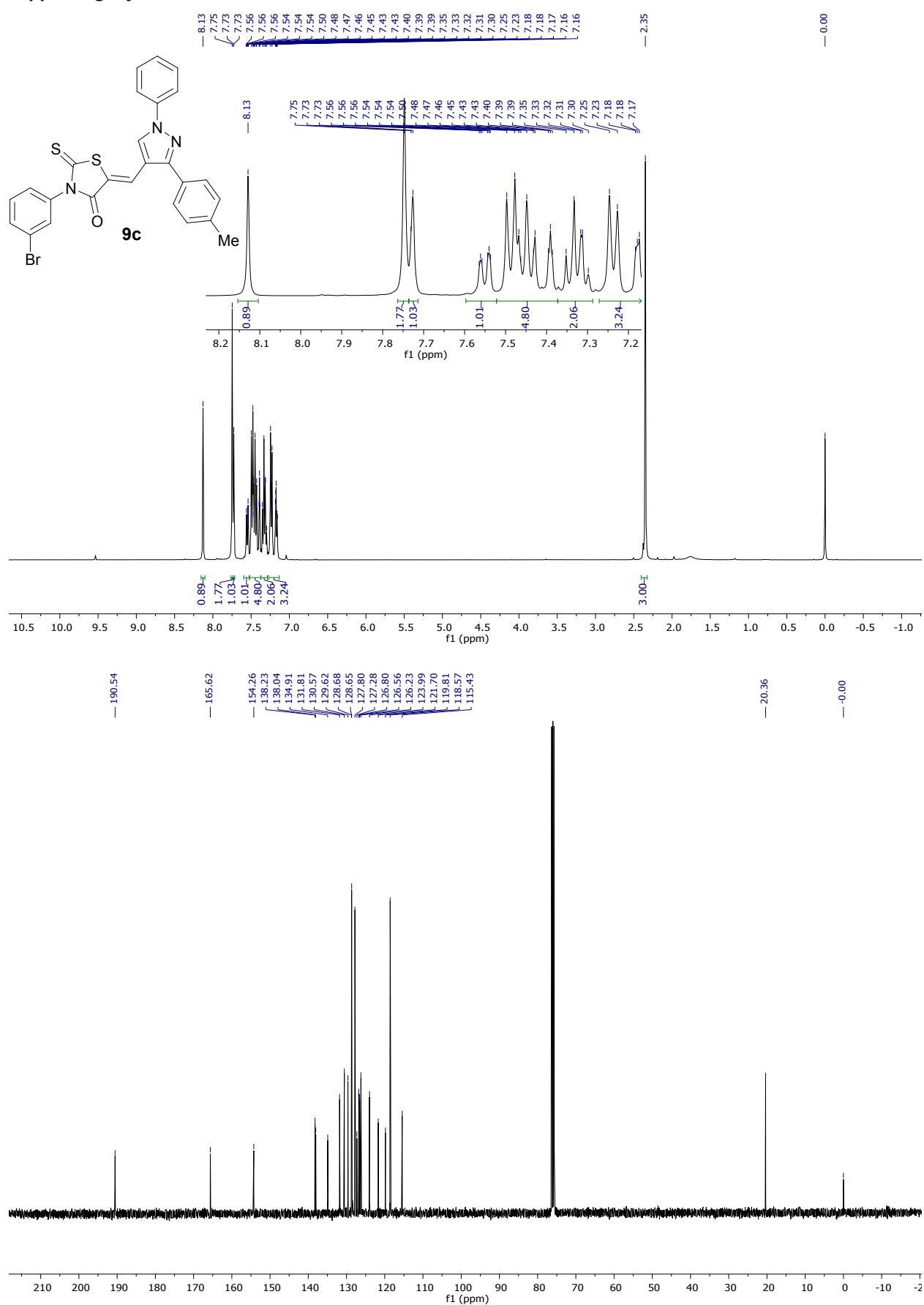
Corresponding authors: E-mail: drjamshed@ciit.net.pk (J. Iqbal); Fax: +92-992-383441; Tel: +92-992-383591, +92-992-383596; Email: shameed@qau.edu.pk (S. Hameed); Fax: +92-51-9064-2241; Tel: +92-51-9064-2133;

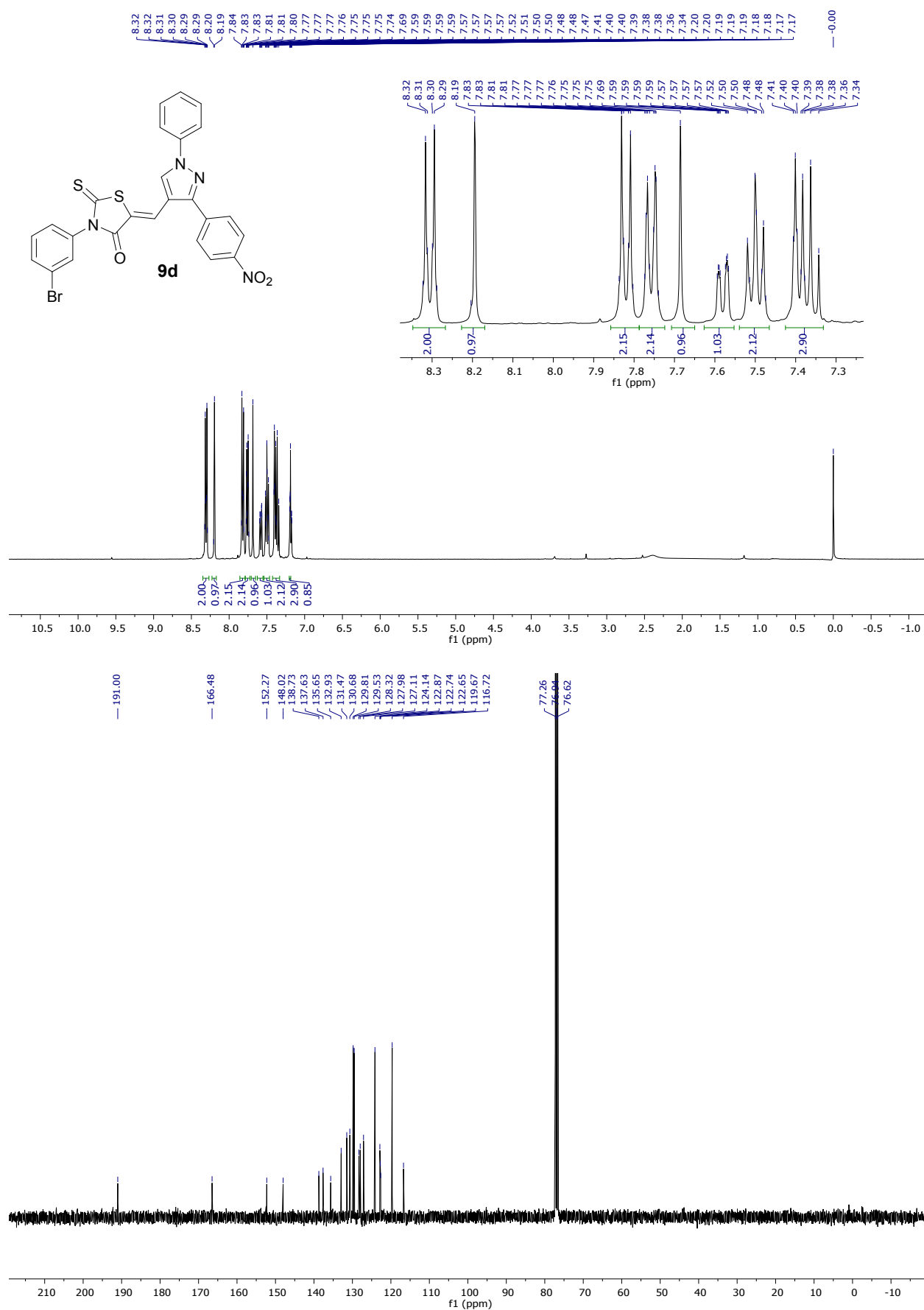
Supporting Information

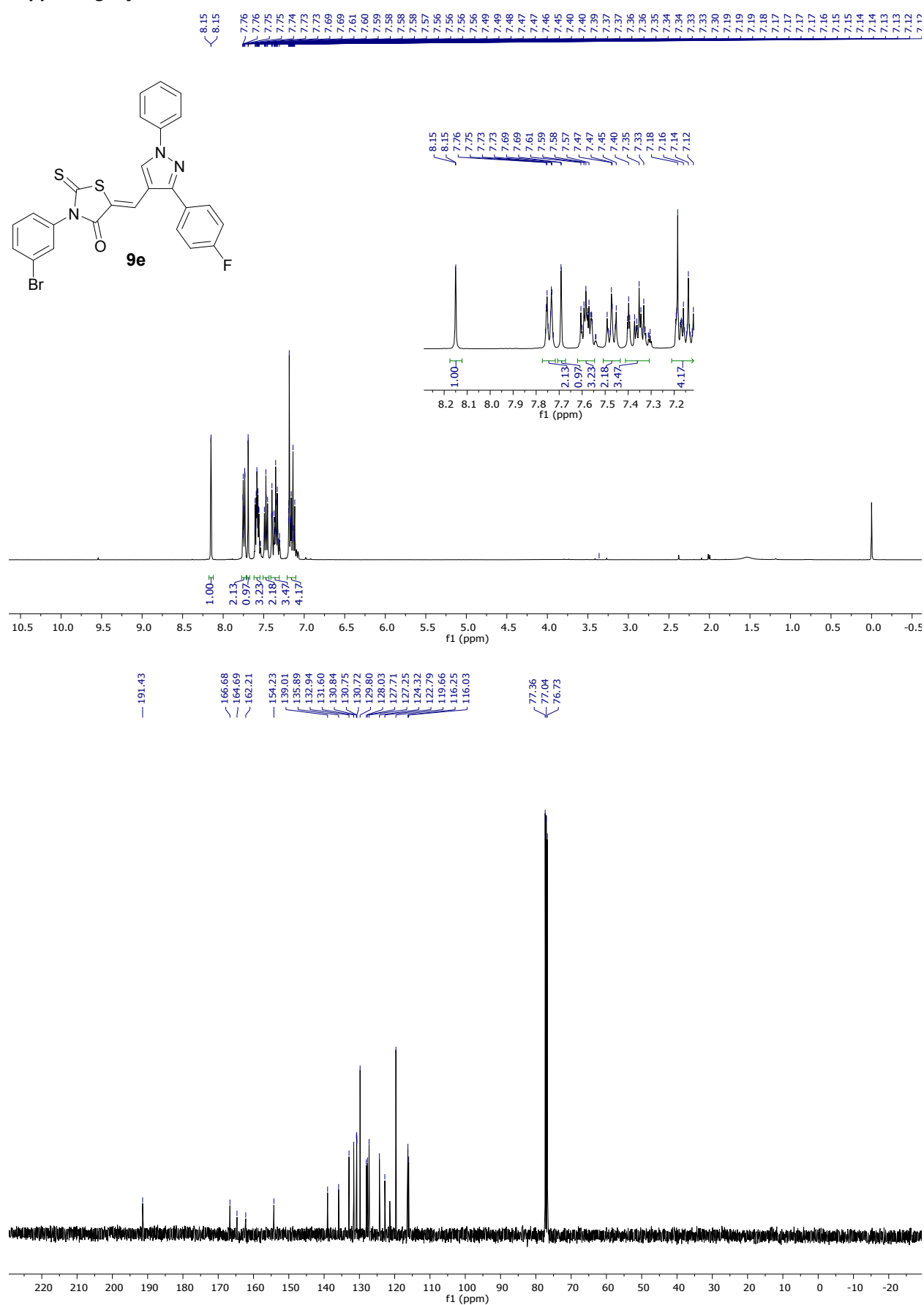
¹H NMR, ¹³C NMR and Mass spectra of synthesized compounds

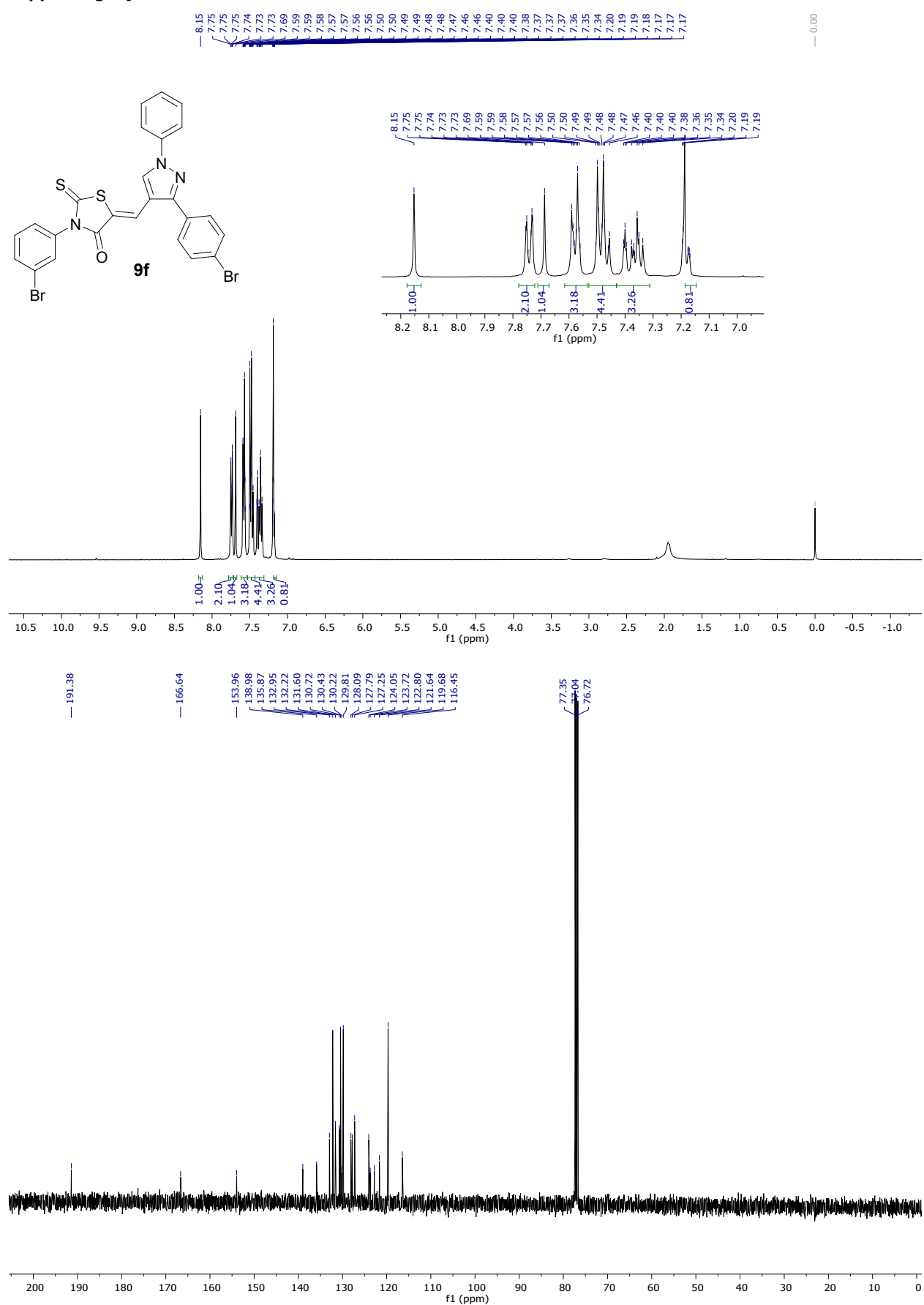


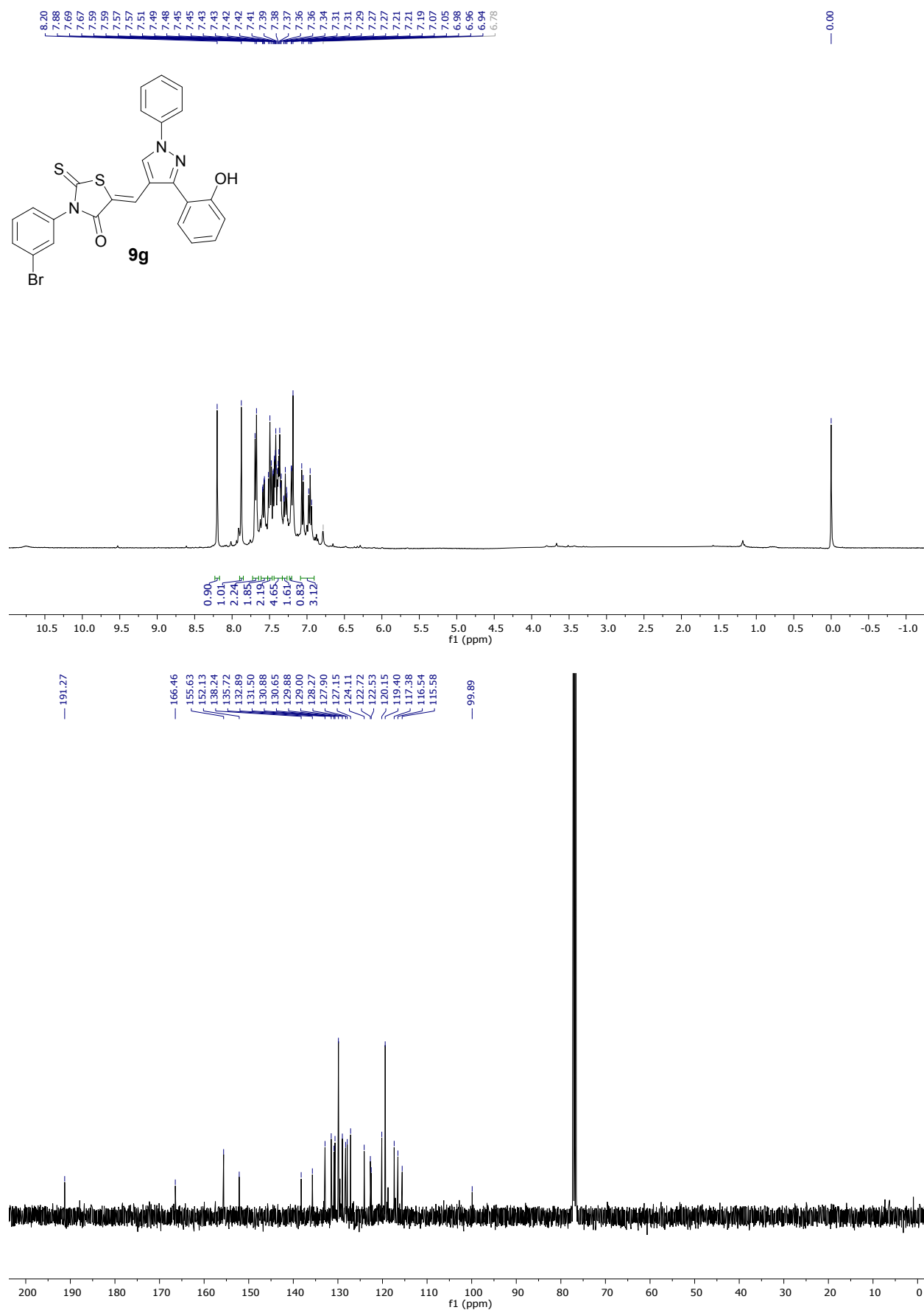


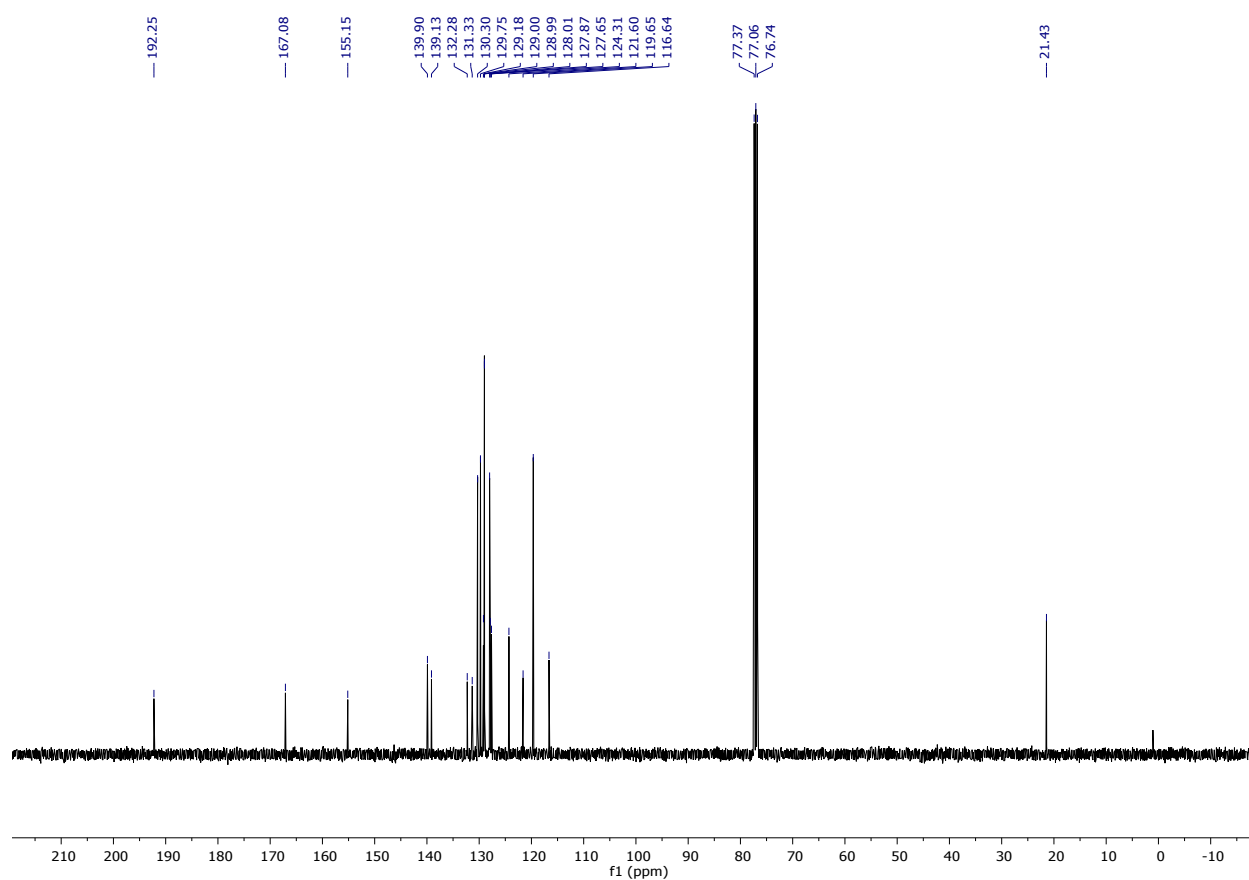
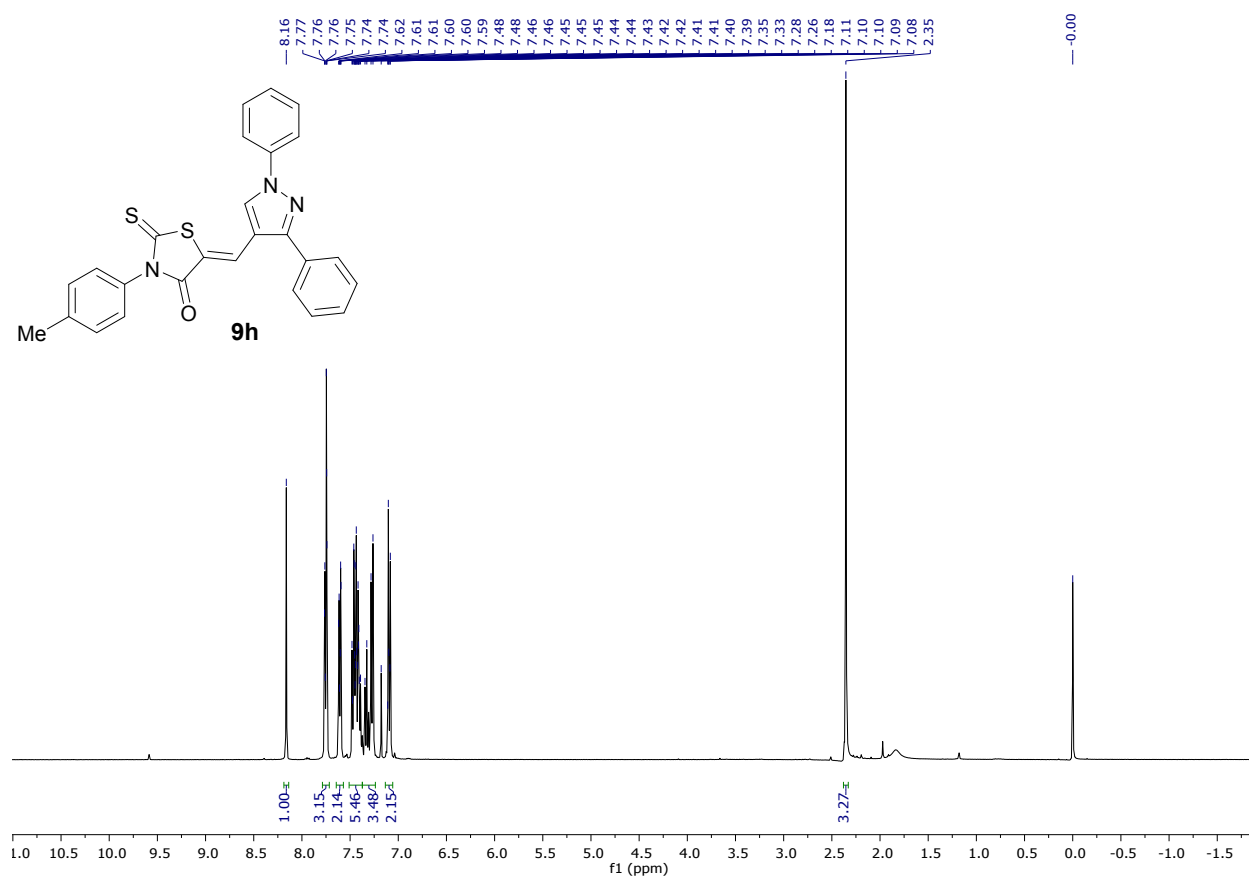


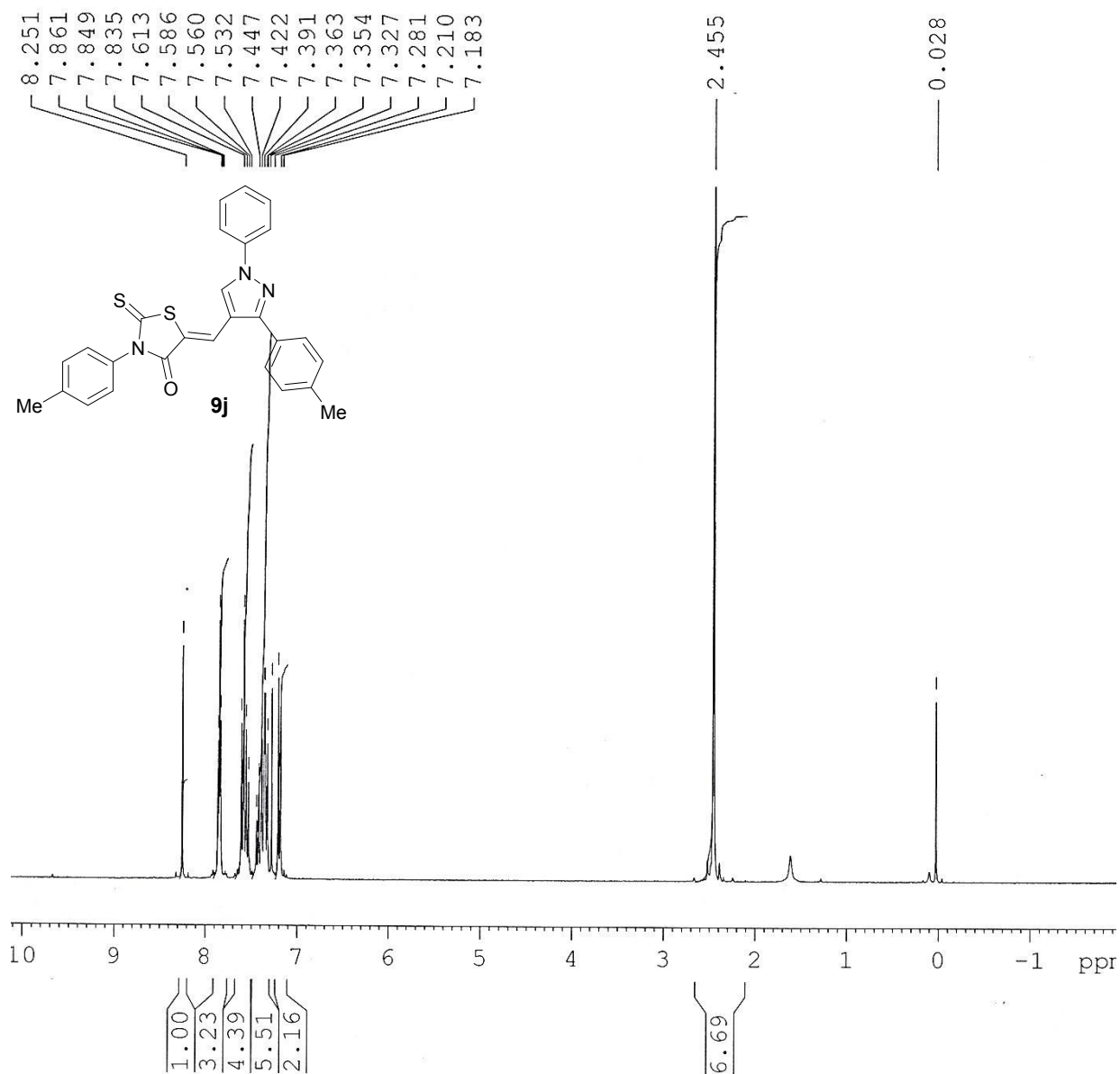


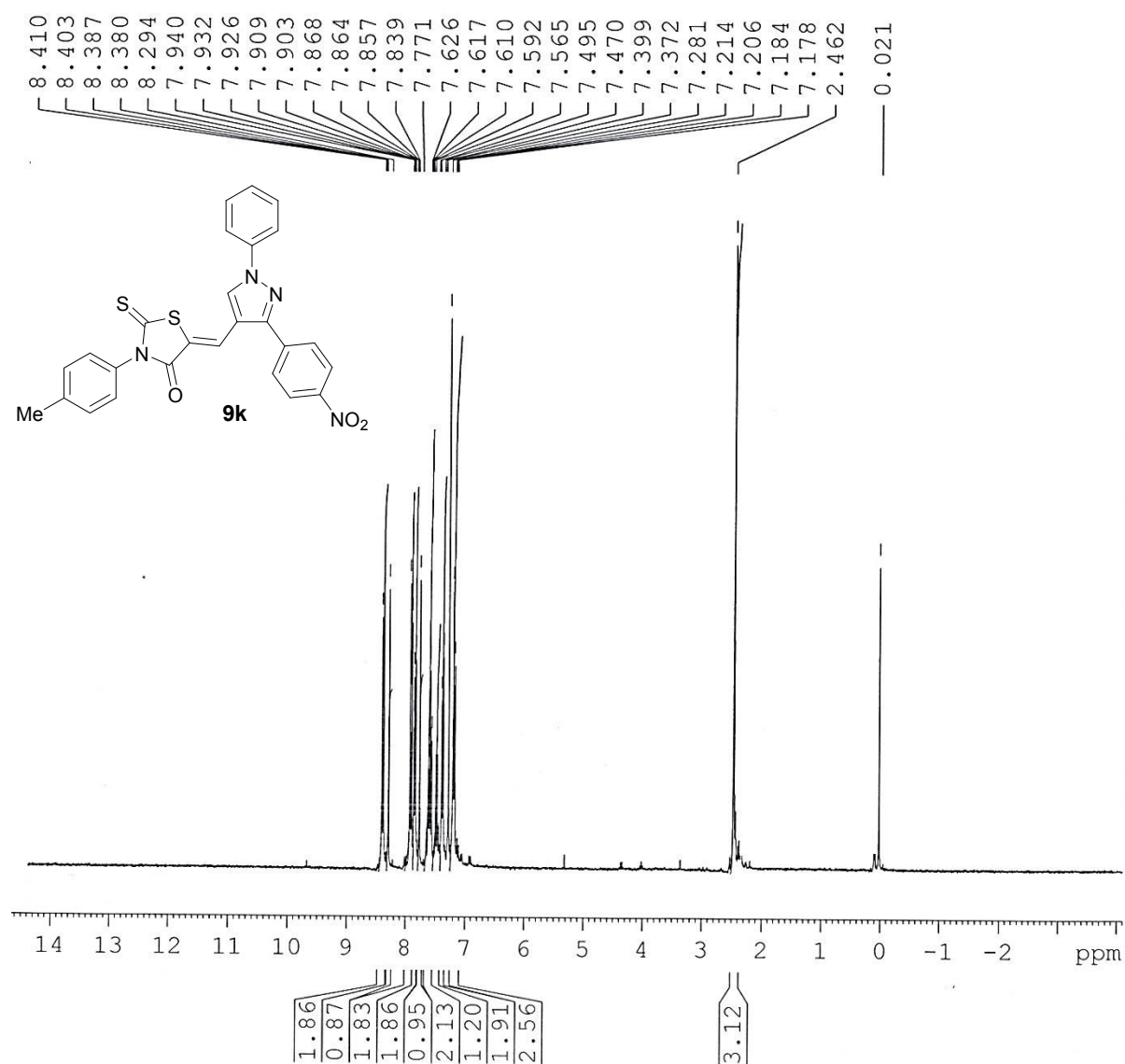


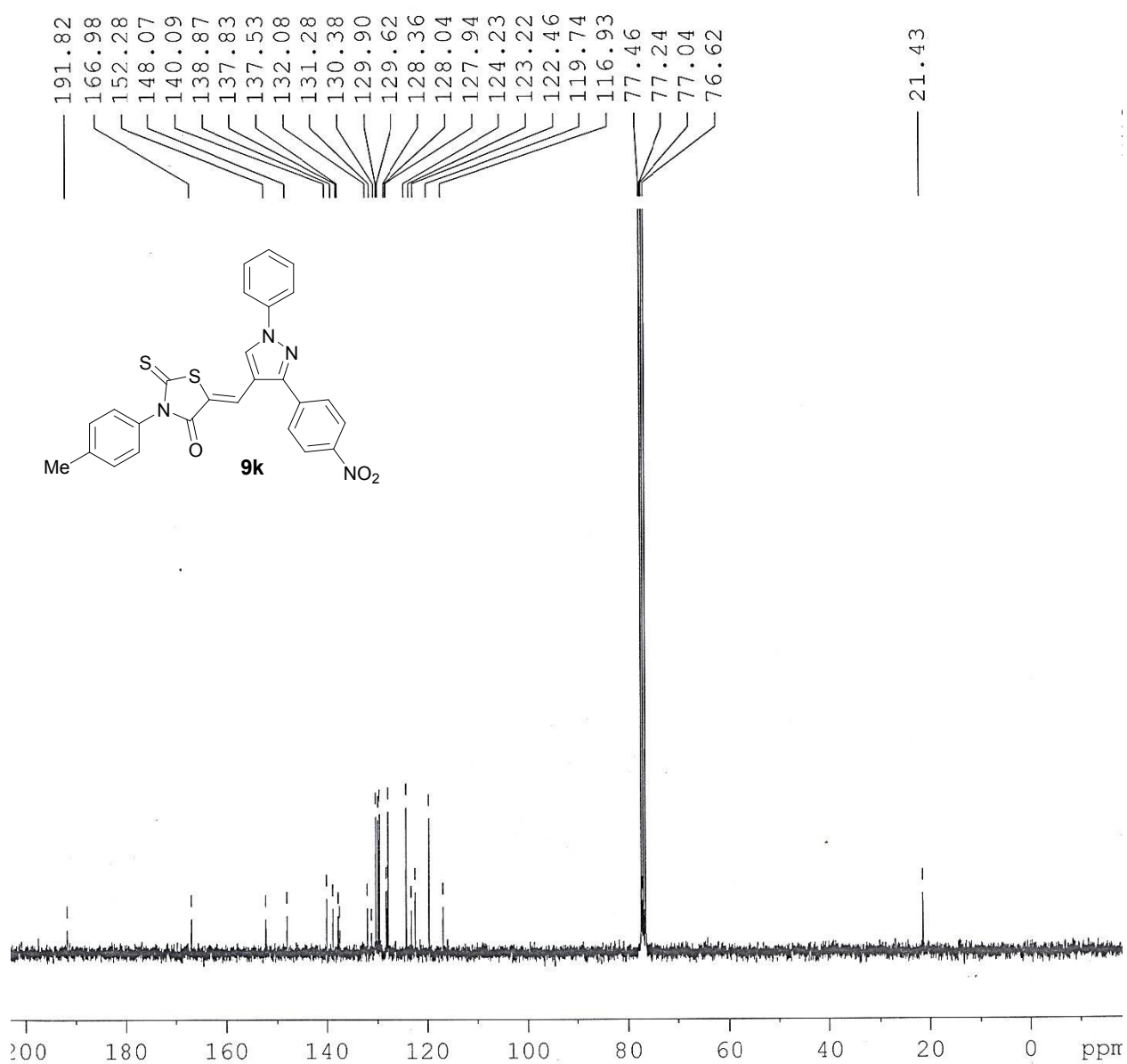


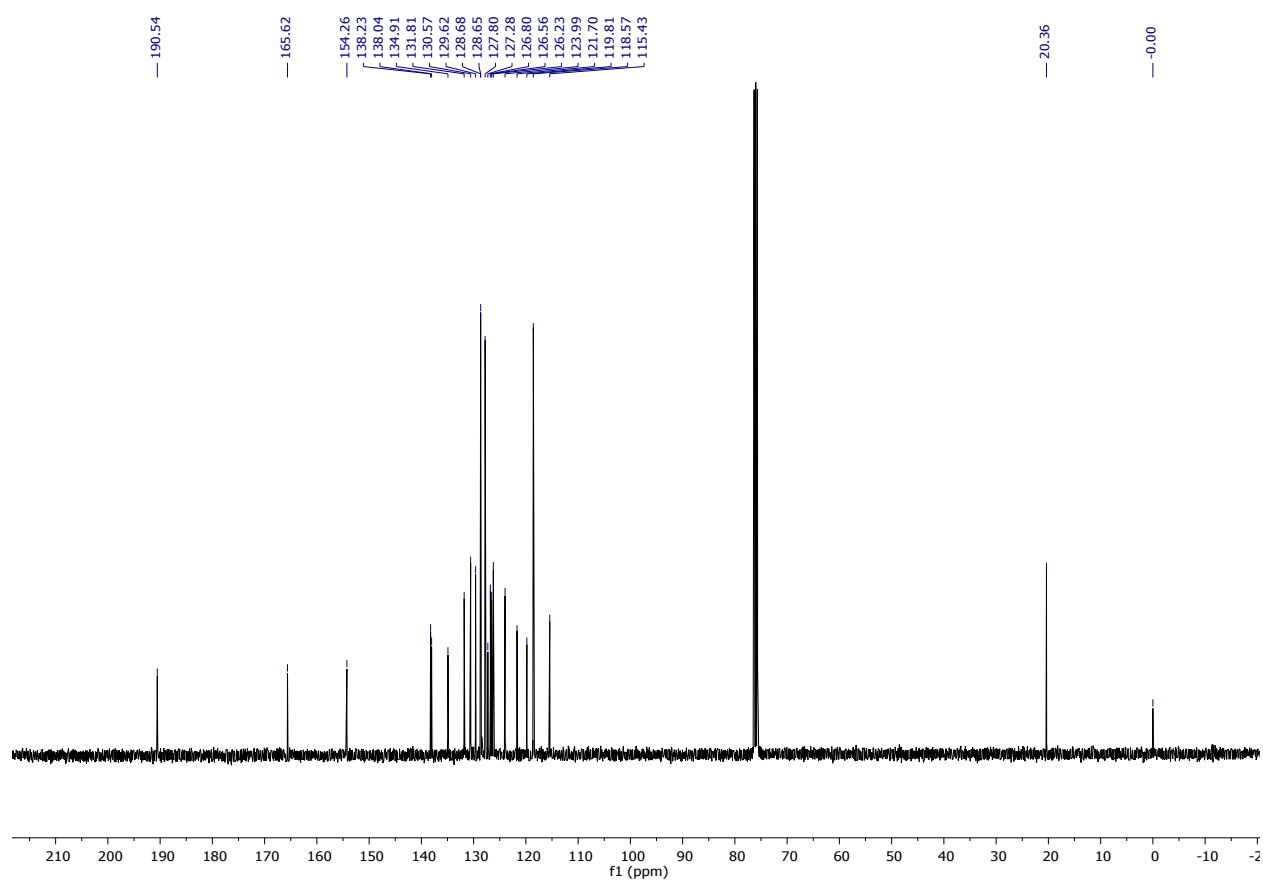
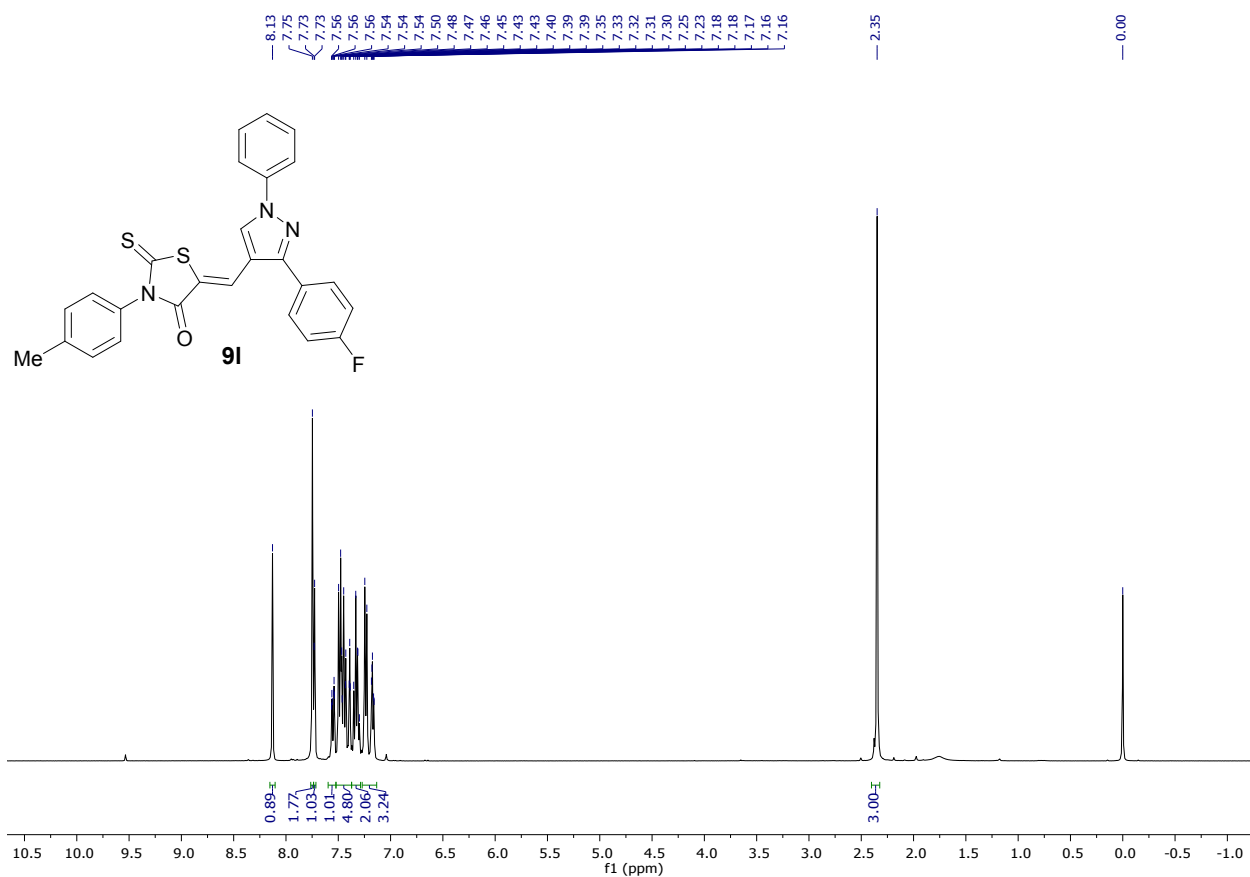


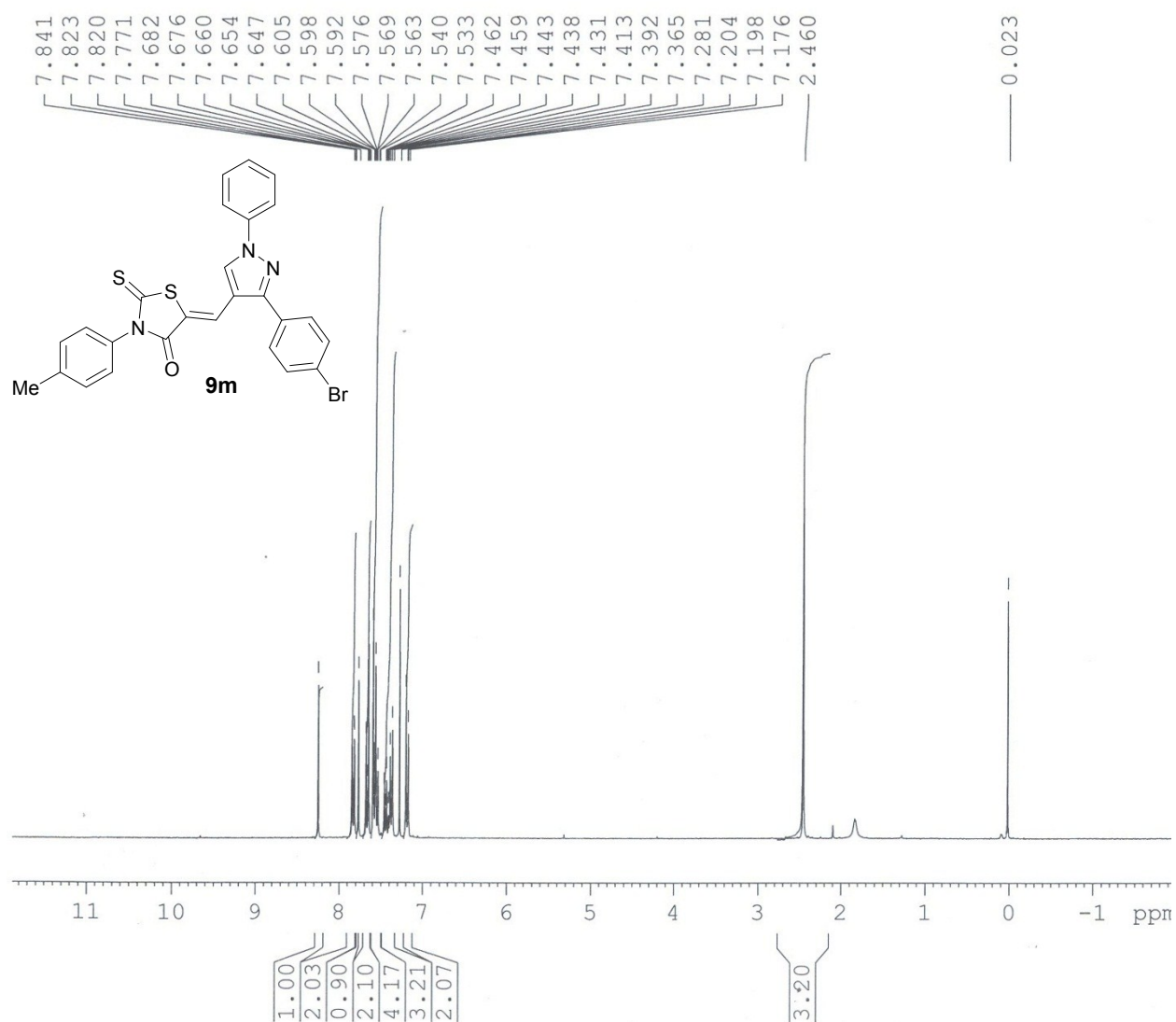


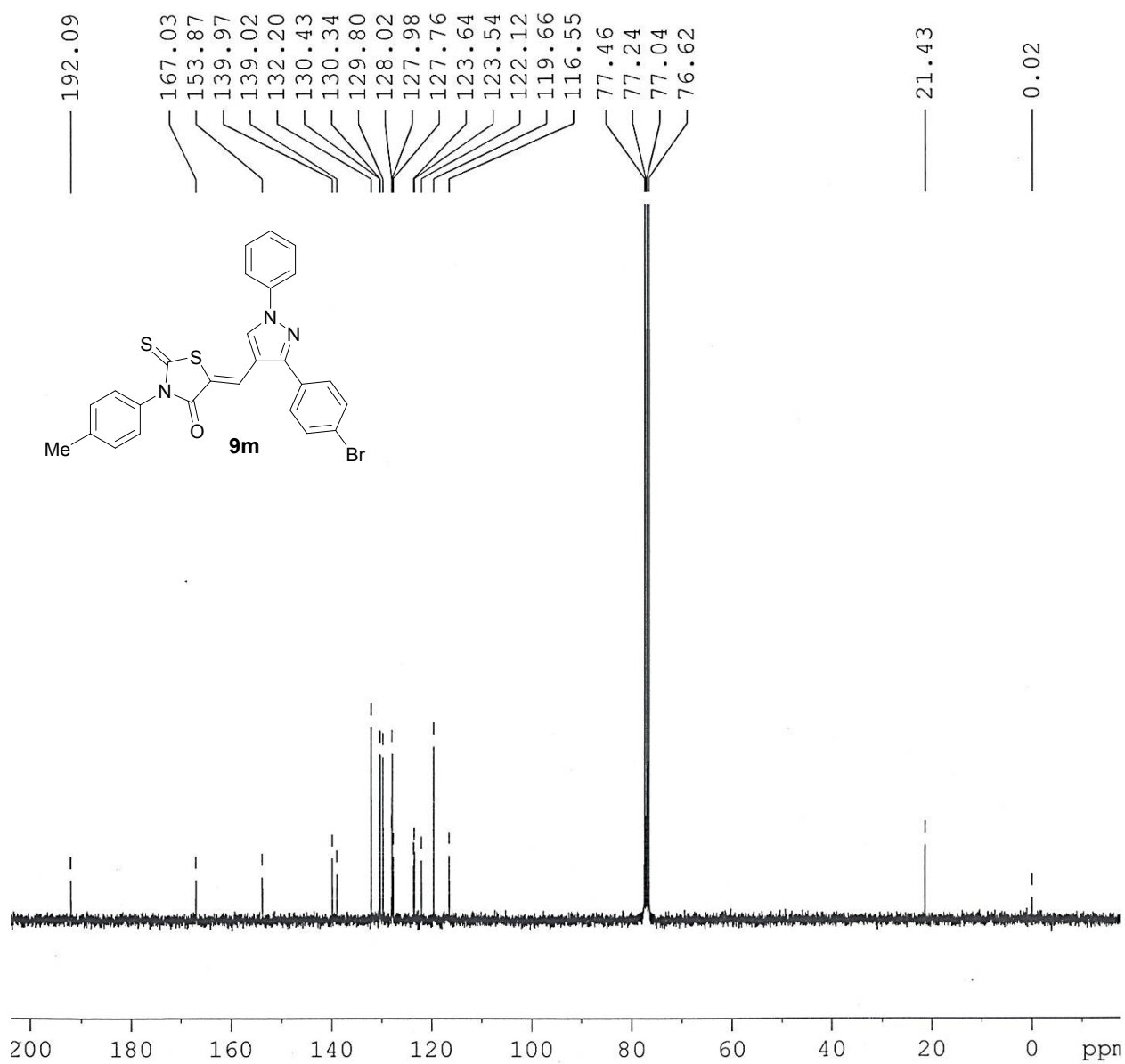


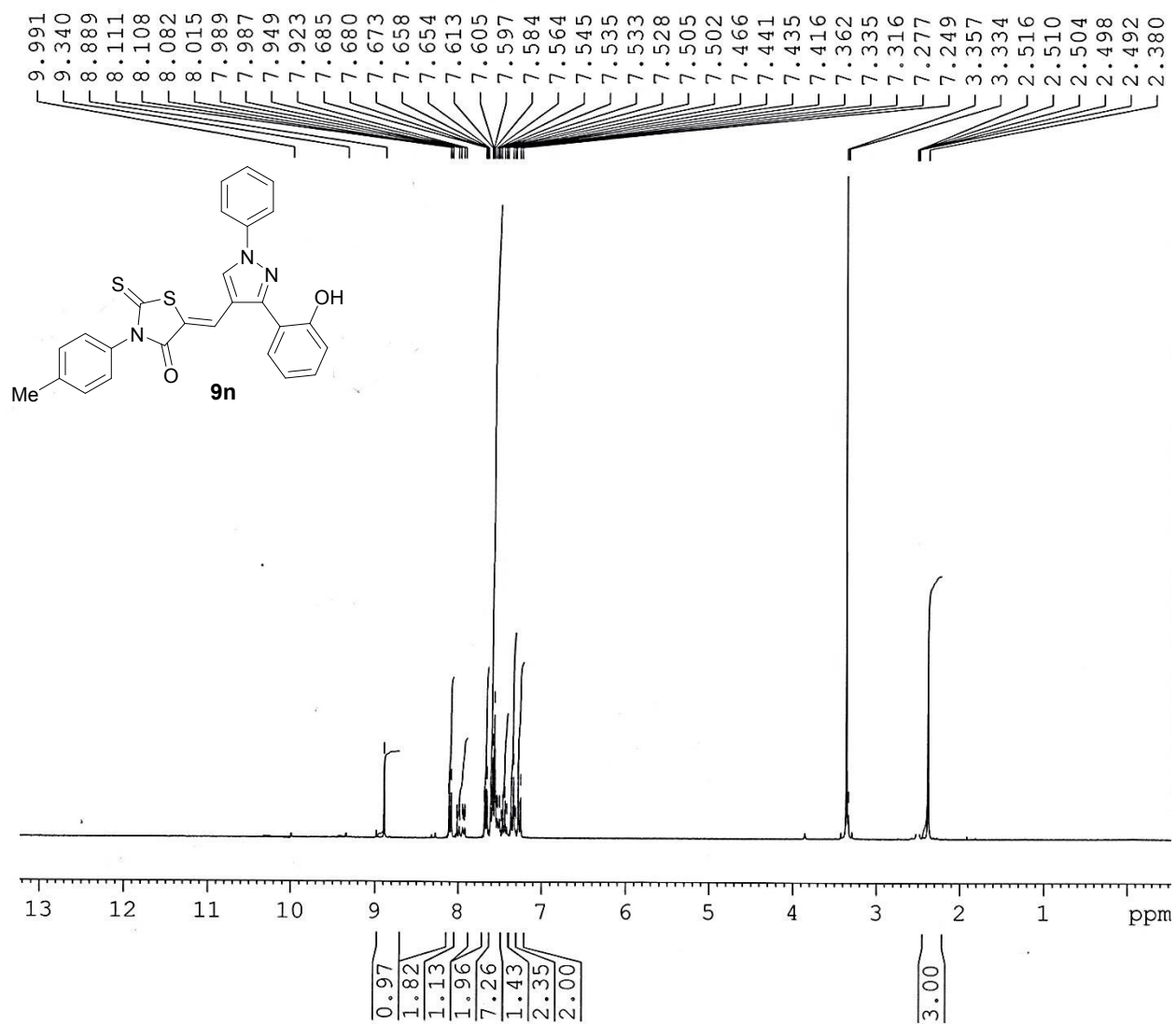


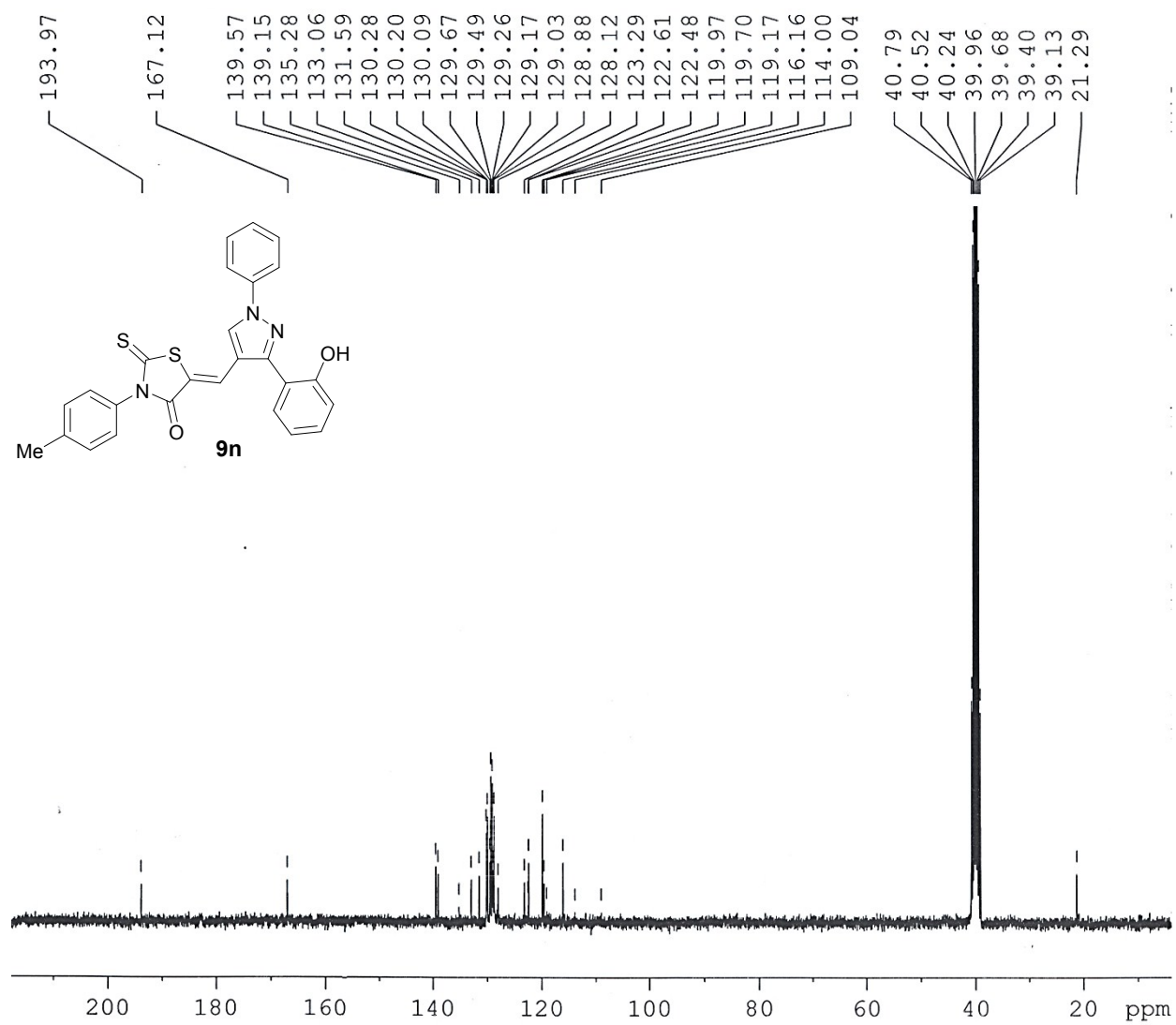


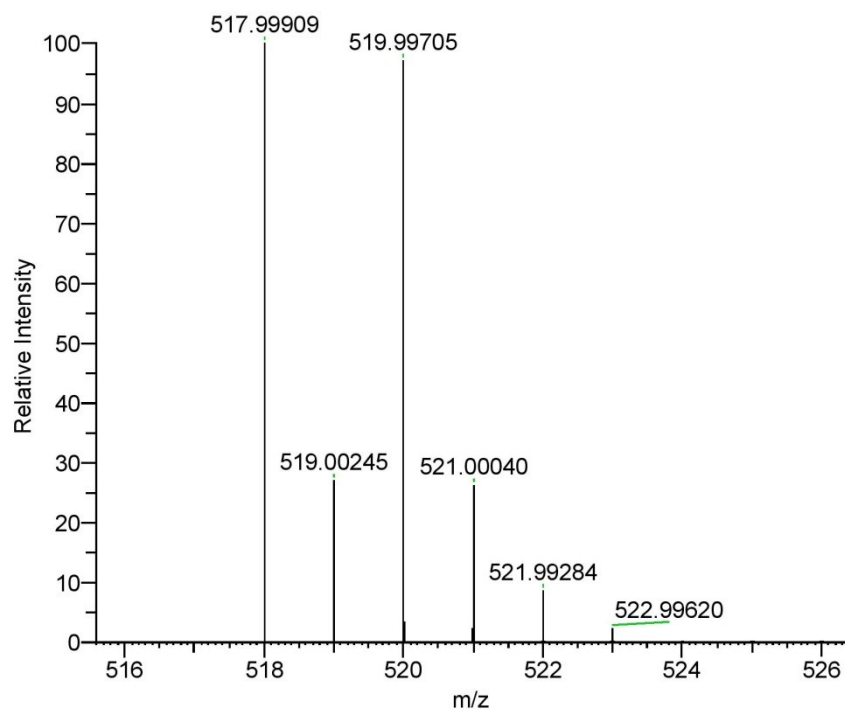
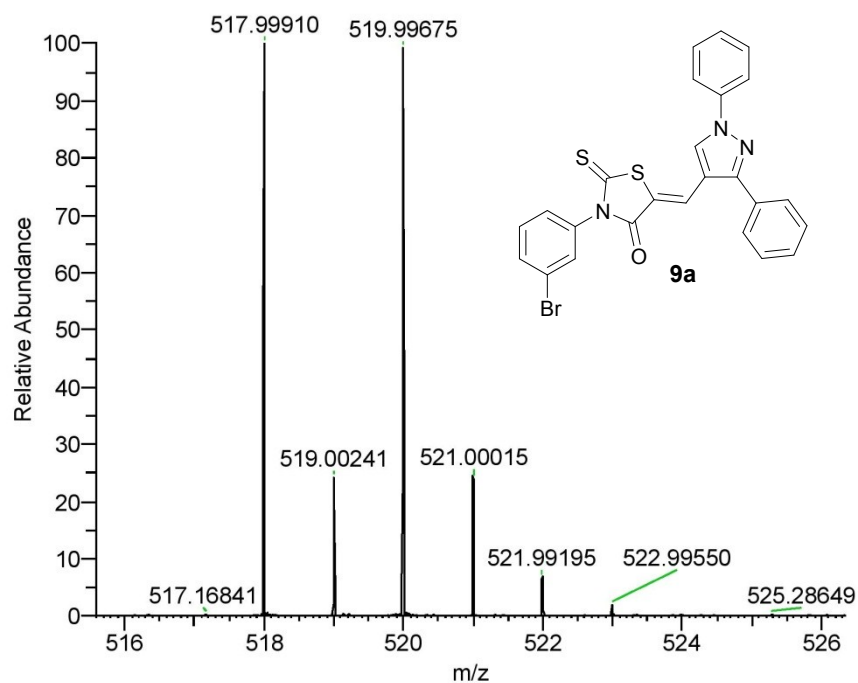




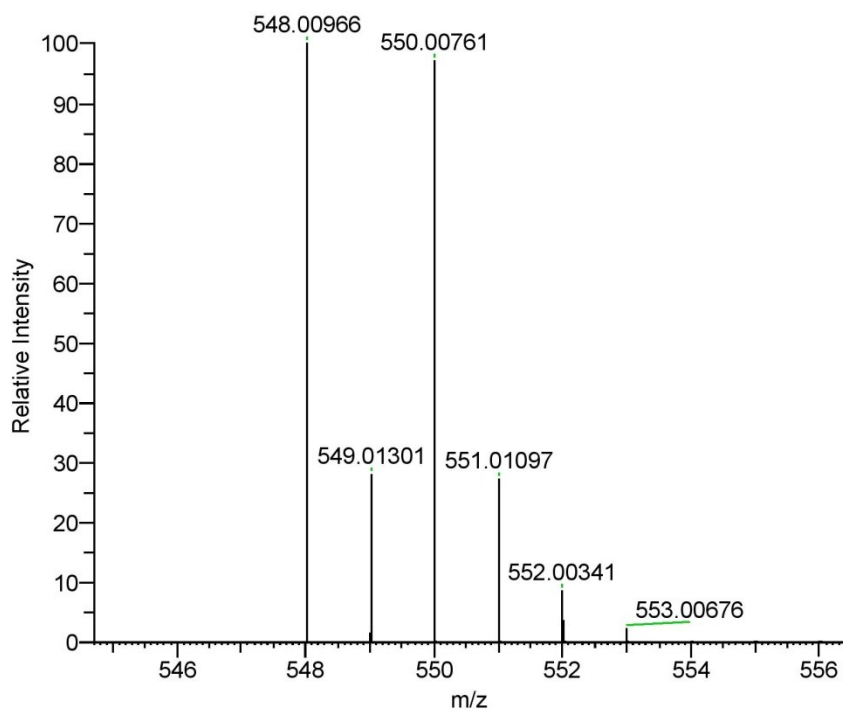
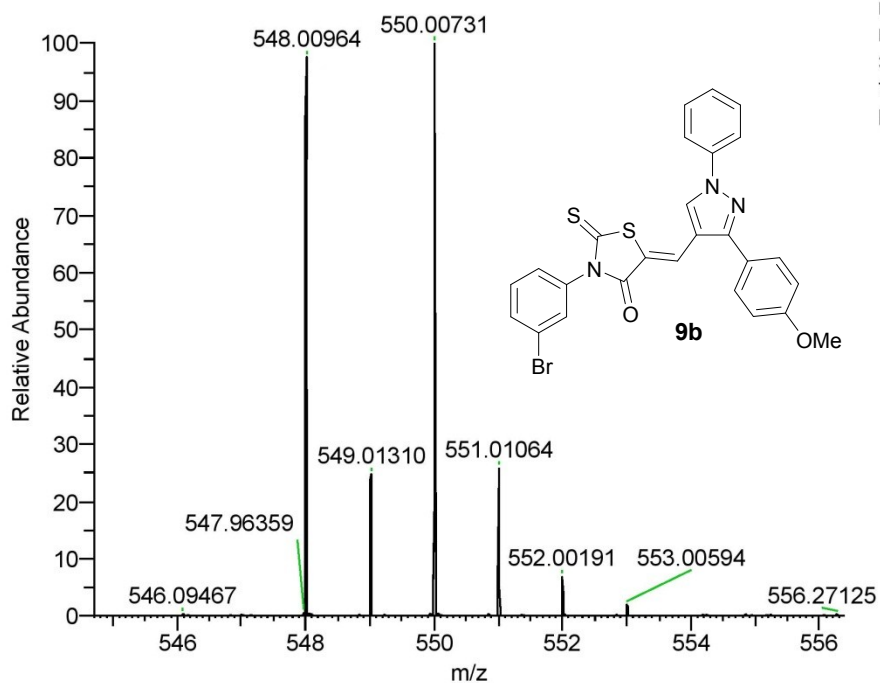




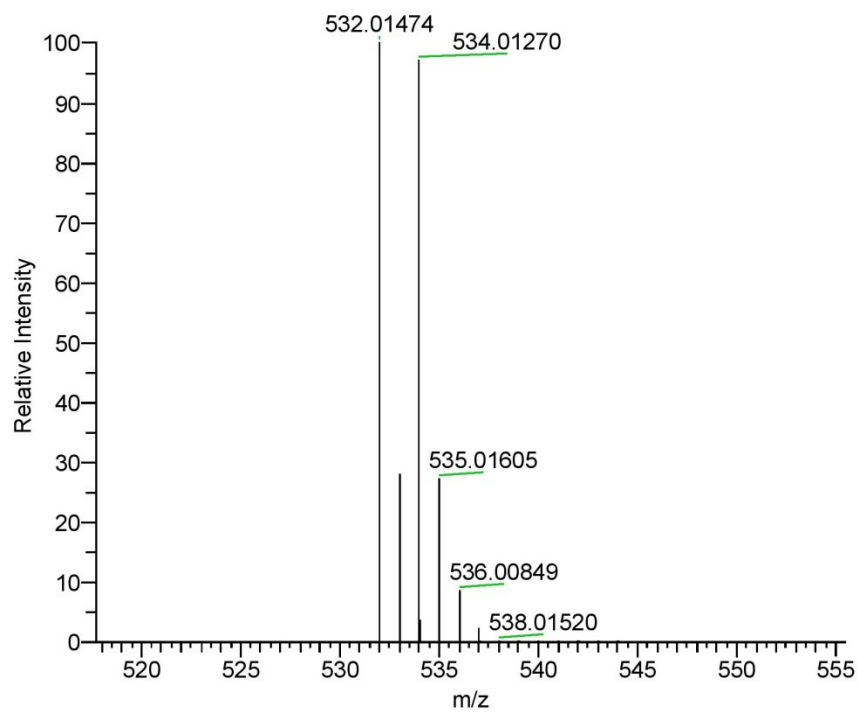
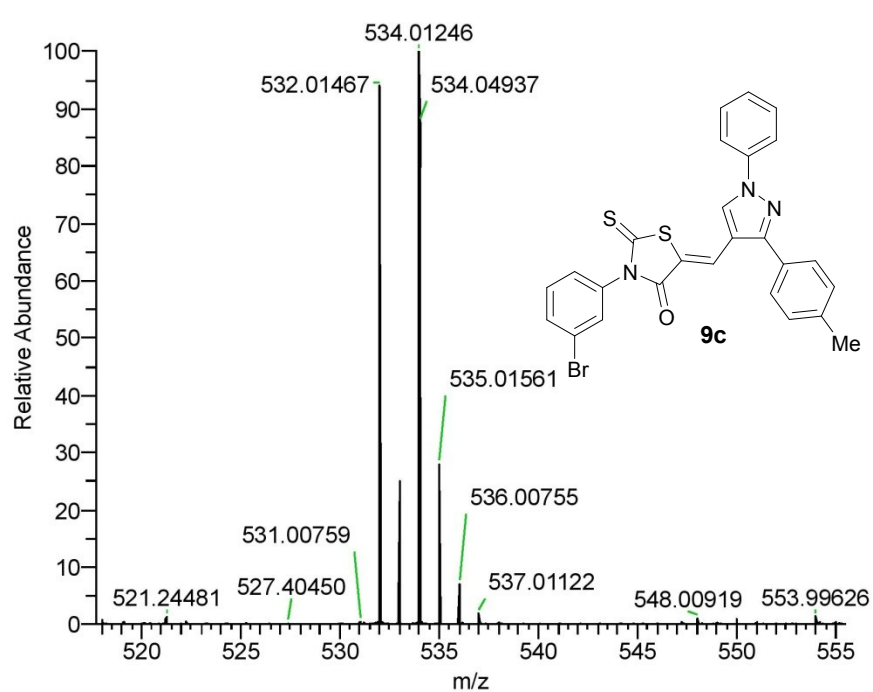




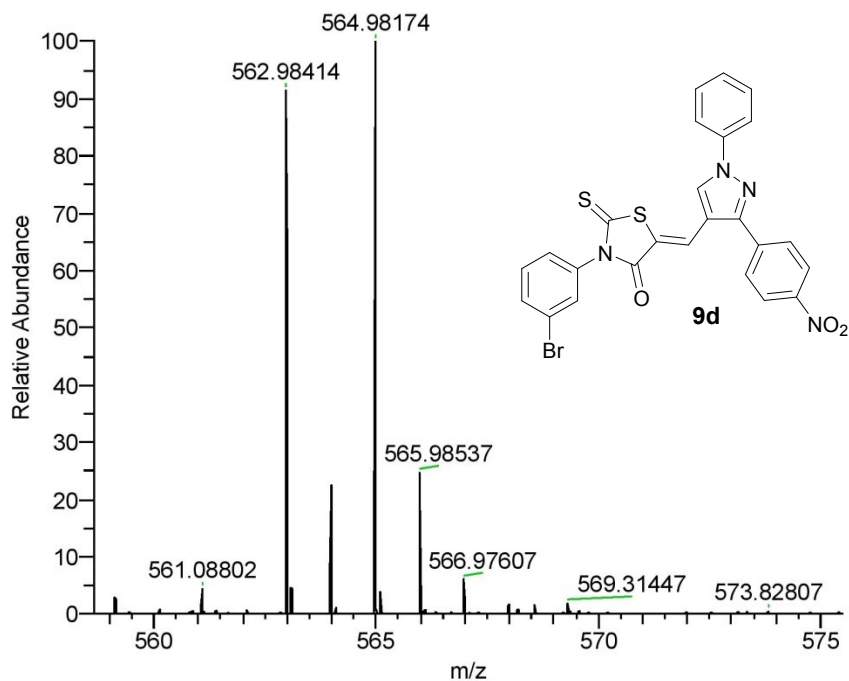
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1	517.99908	C ₂₅ H ₁₇ ON ₃ ⁷⁹ Br...	0	18.5	-0.02	C ₂₅ H ₁₇ O ₁ N ₃ ...	517.99909



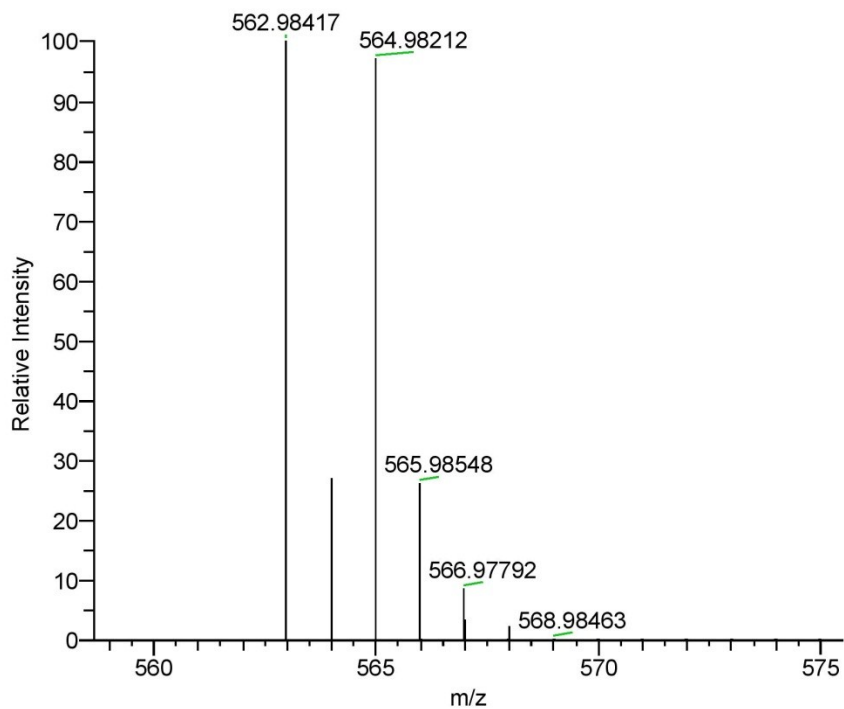
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1	548.00964	C ₂₆ H ₁₉ O ₂ N ₃ ⁷⁹ B...	0	18.5	-0.03	C ₂₆ H ₁₉ O ₂ N ₃ ...	548.00966



Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	532.01465	C ₂₆ H ₁₉ ON ₃ ⁷⁹ Br...	0	18.5	-0.18	C26H19O1N3...	532.01474

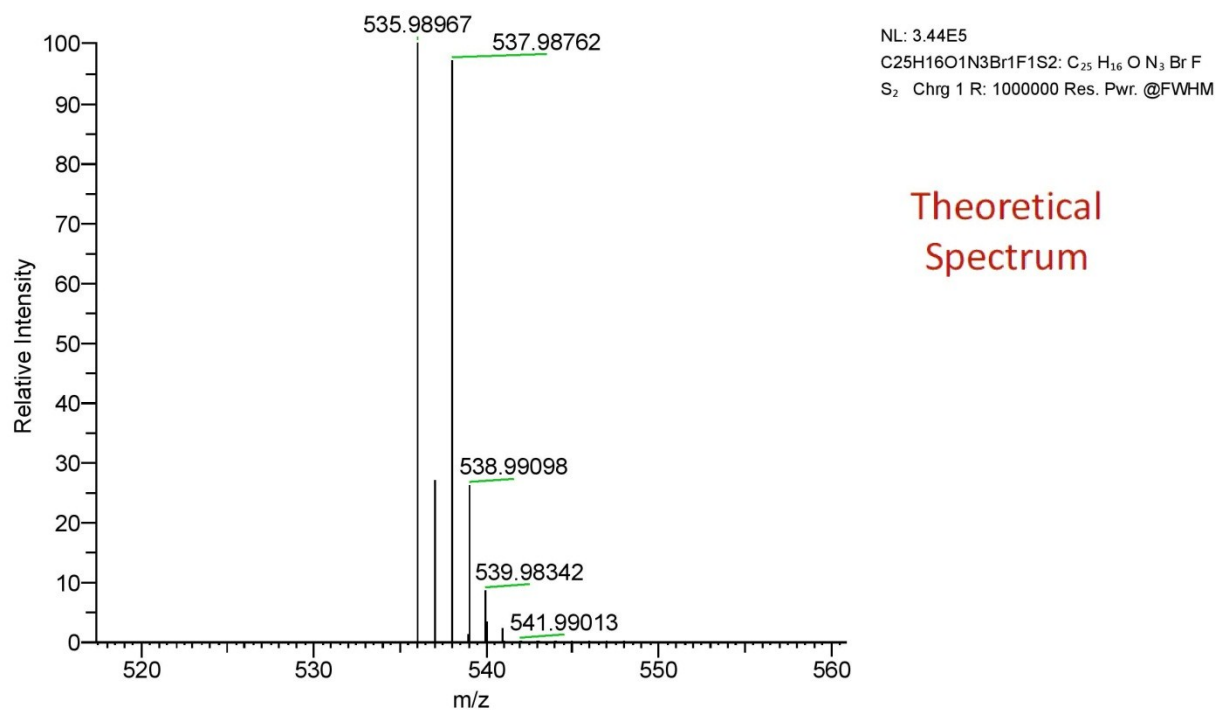
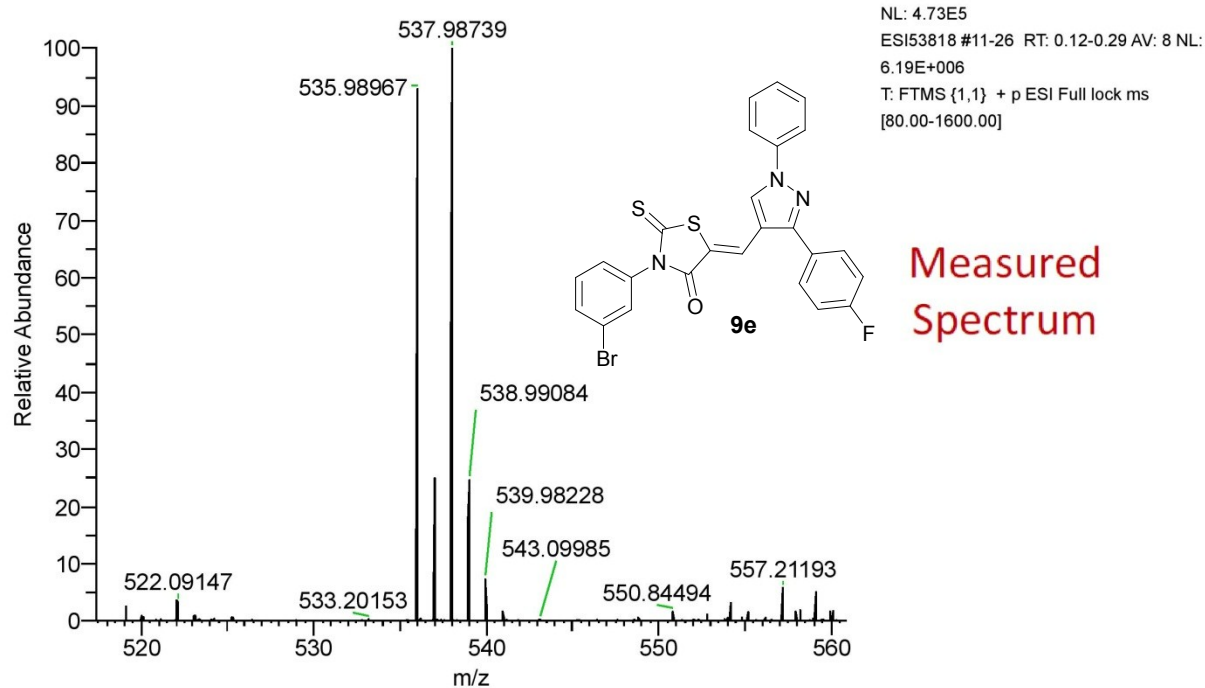


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[80.00-1600.00]

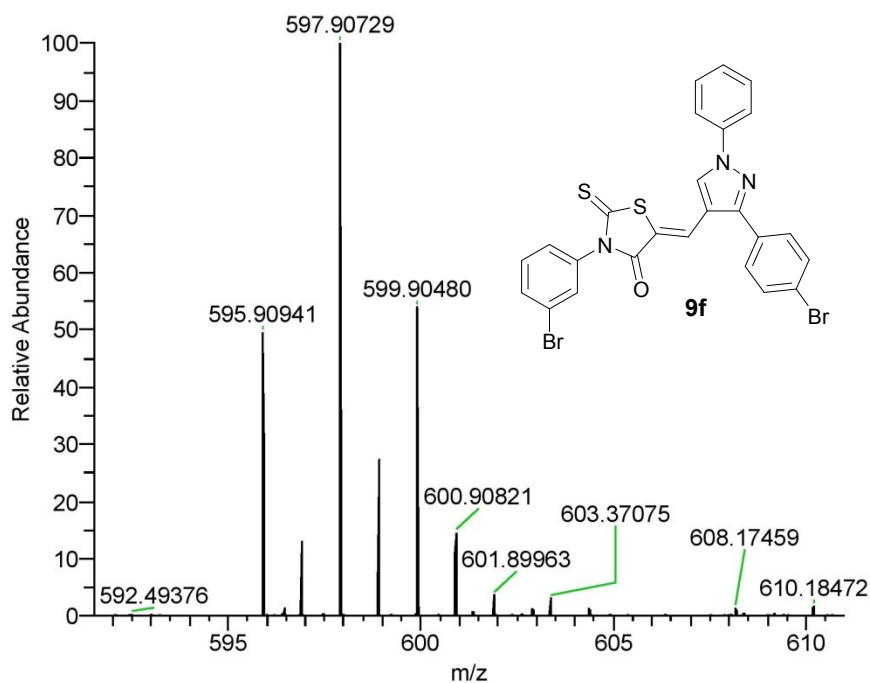


NL: 3.41E5
C25H16O3N4Br1S2: C₂₅ H₁₆ O₃ N₄ Br S₂
Chrg 1 R: 1000000 Res. Pwr. @FWHM

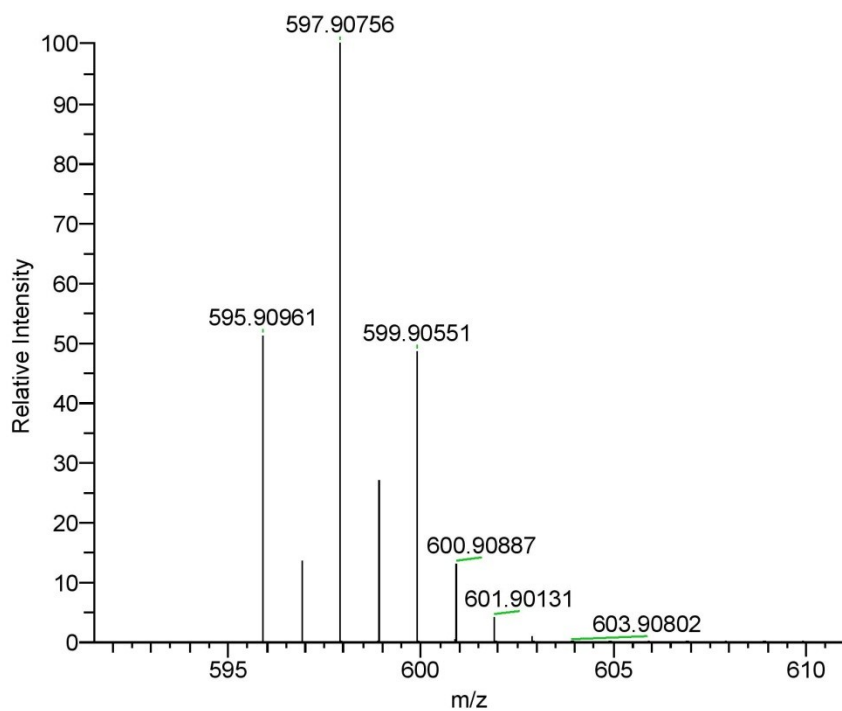
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Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	535.98969	C ₂₅ H ₁₆ ON ₃ ⁷⁹ Br...	0	18.5	0.03	C25H16O1N3...	535.98967

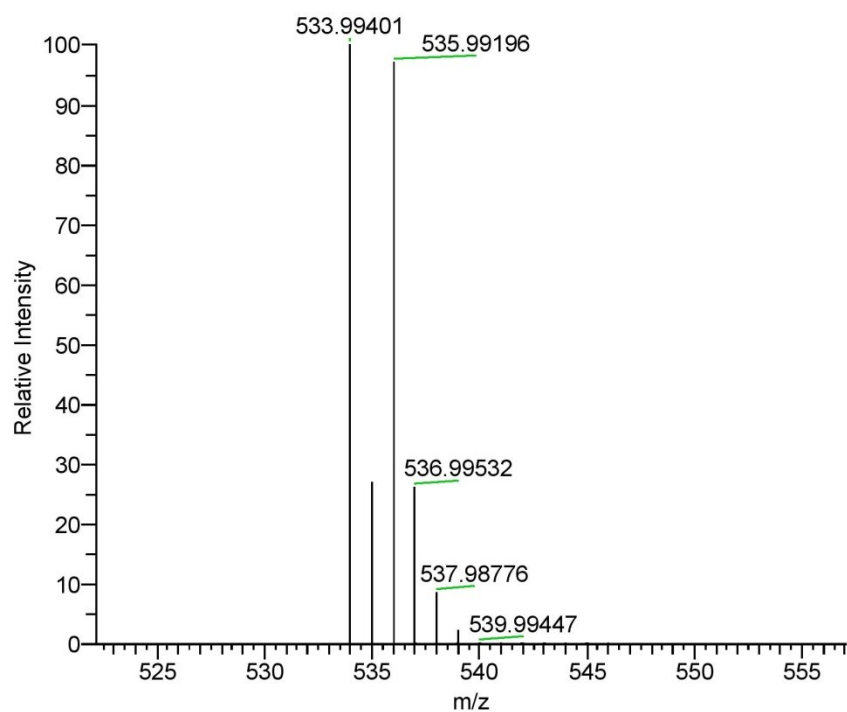
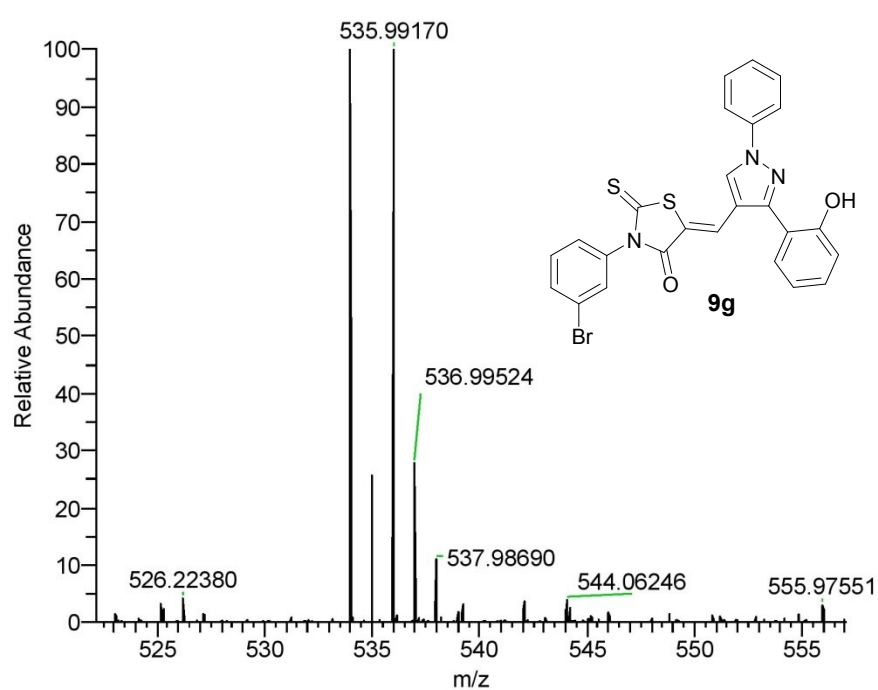


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[80.00-1600.00]

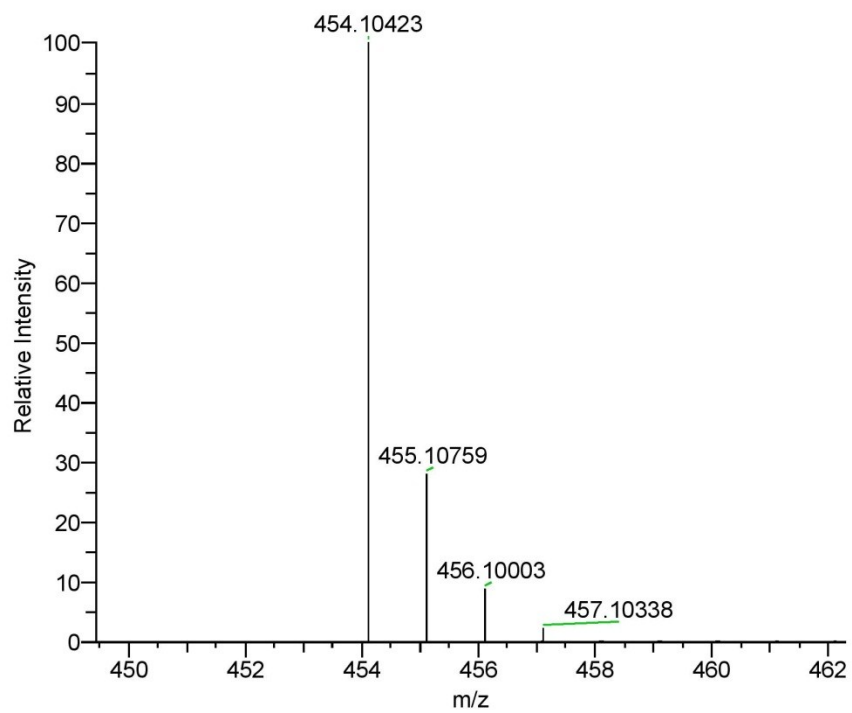
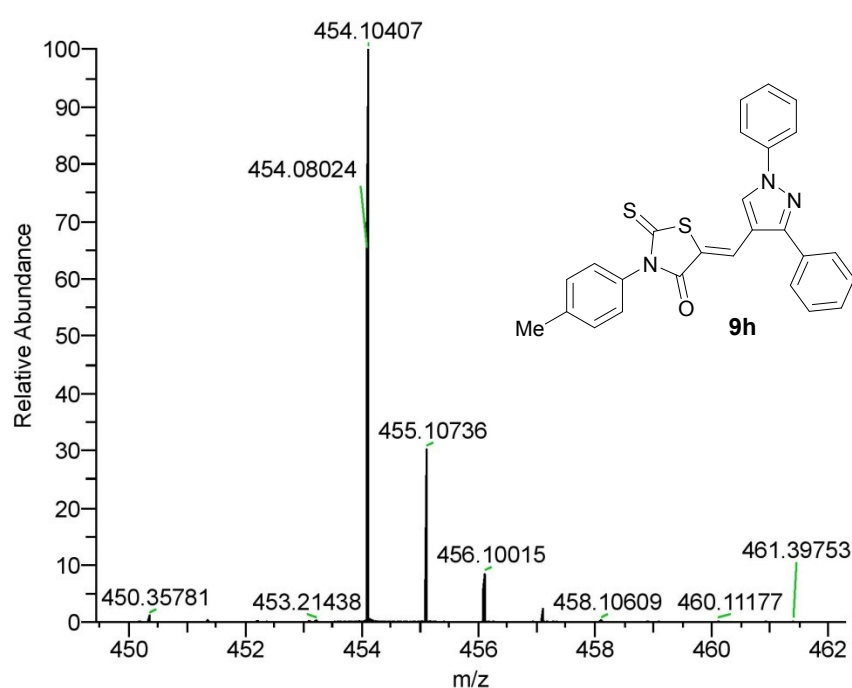


NL: 3.39E5
C₂₅H₁₆O₁N₃Br₂S₂: C₂₅ H₁₆ O N₃ Br₂ S₂
Chrg 1 R: 1000000 Res. Pwr. @FWHM

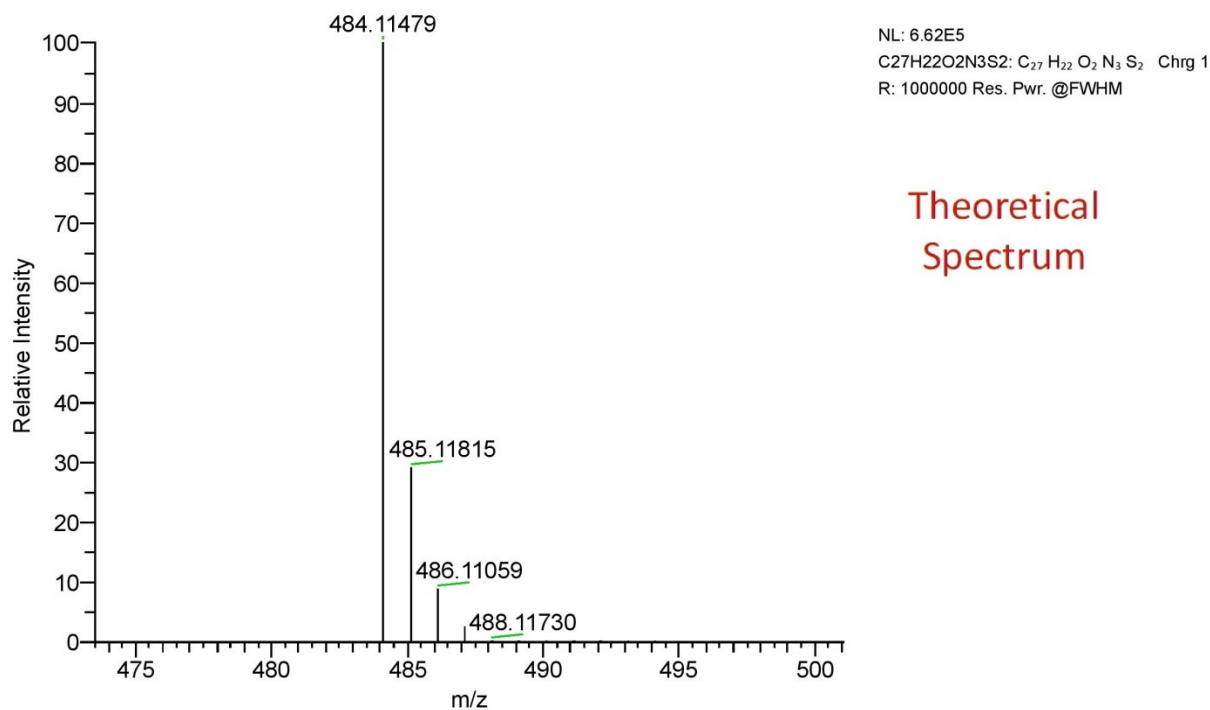
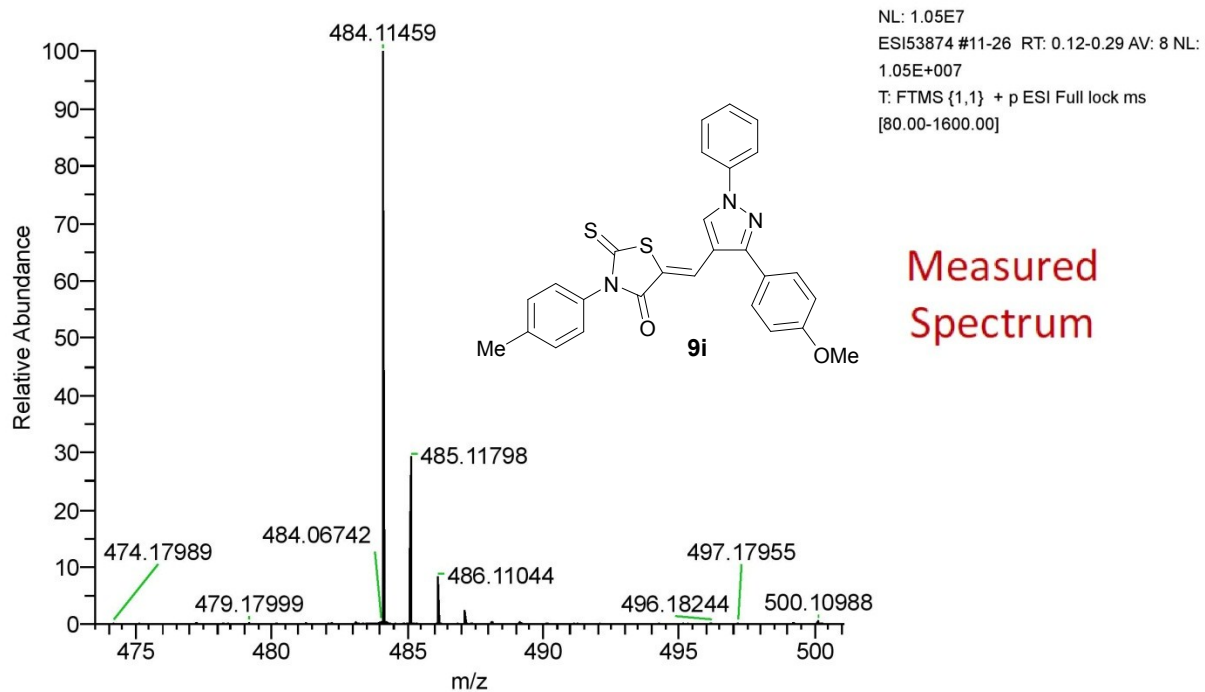
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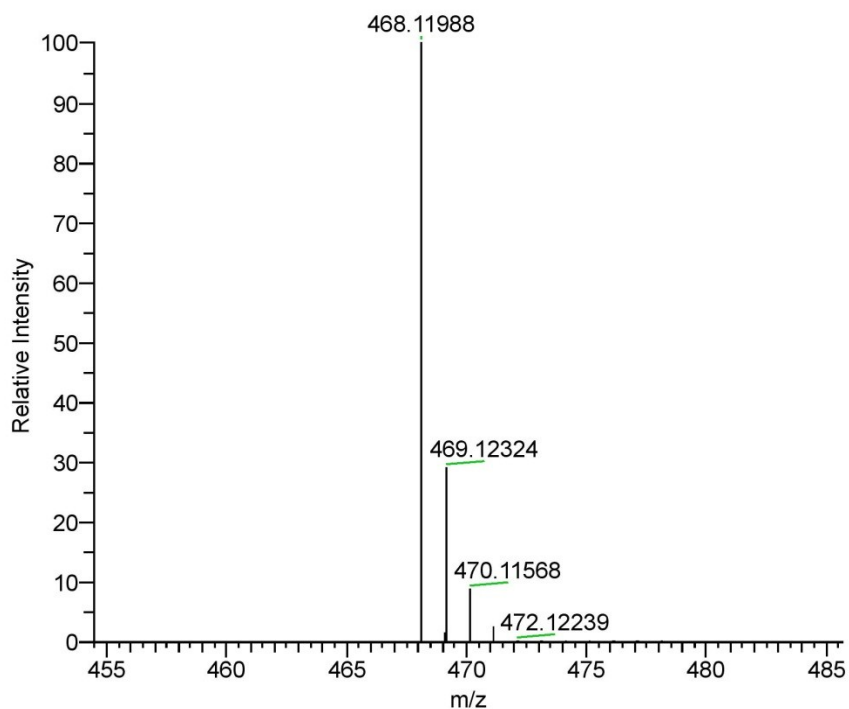
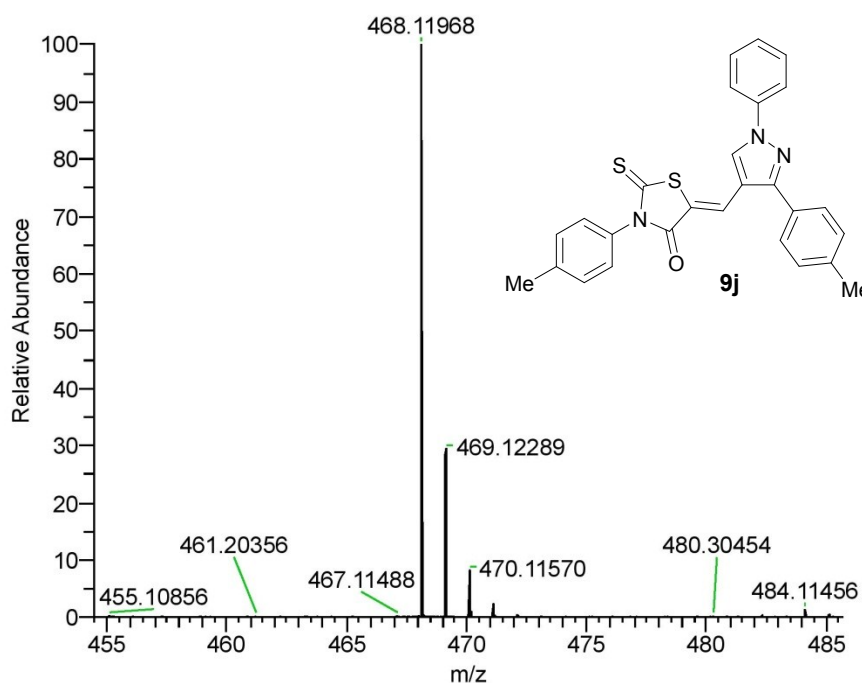
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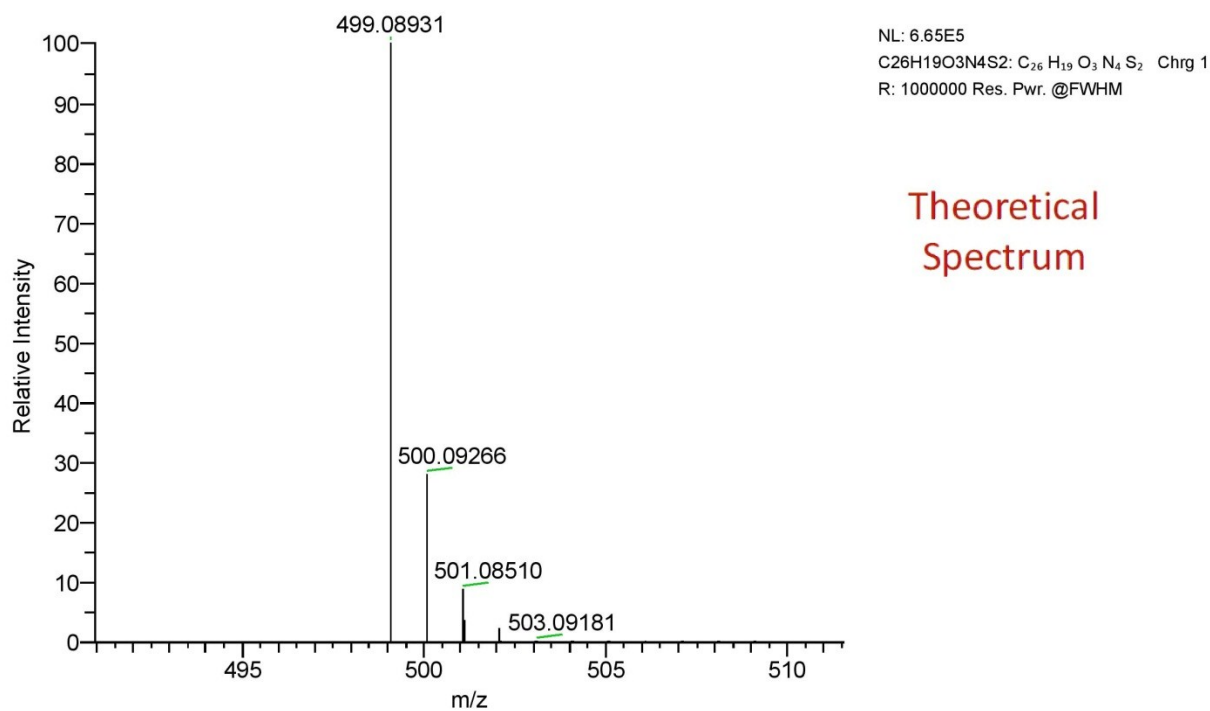
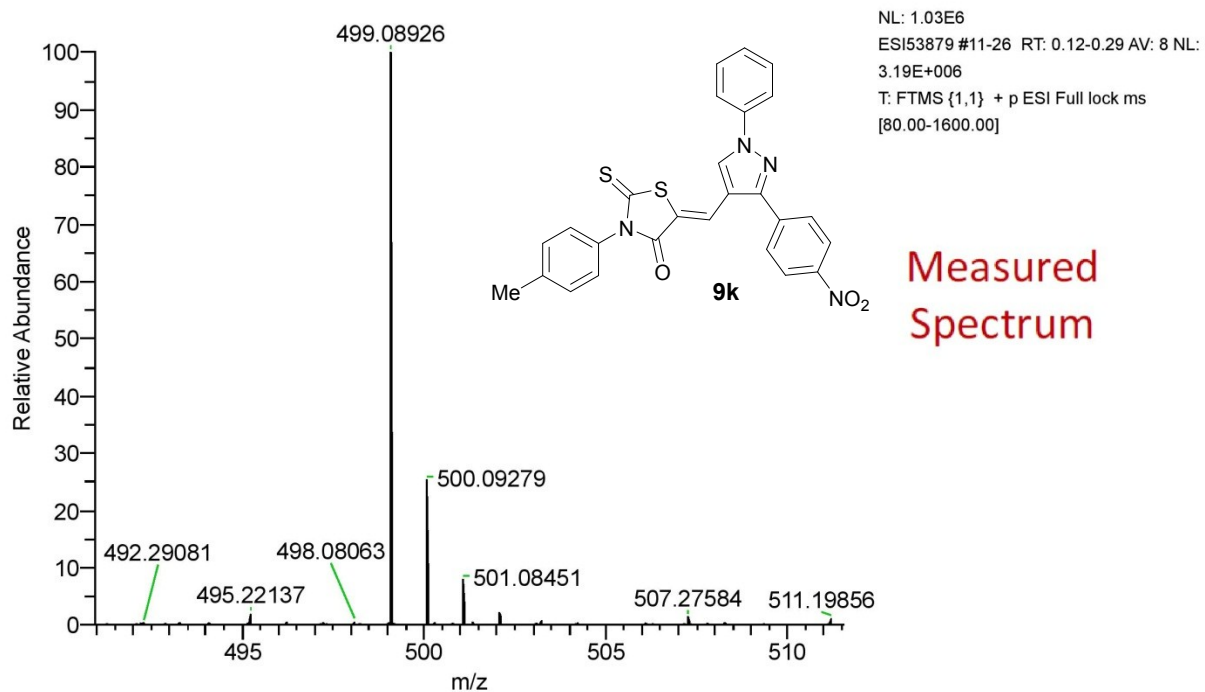
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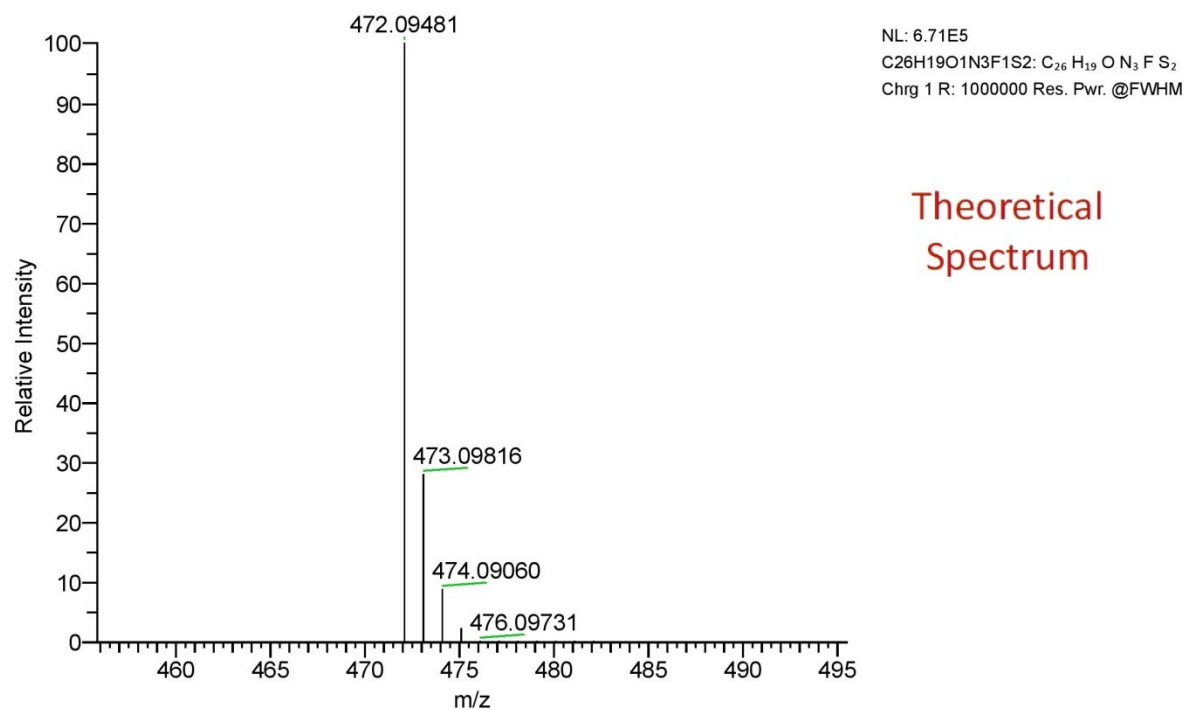
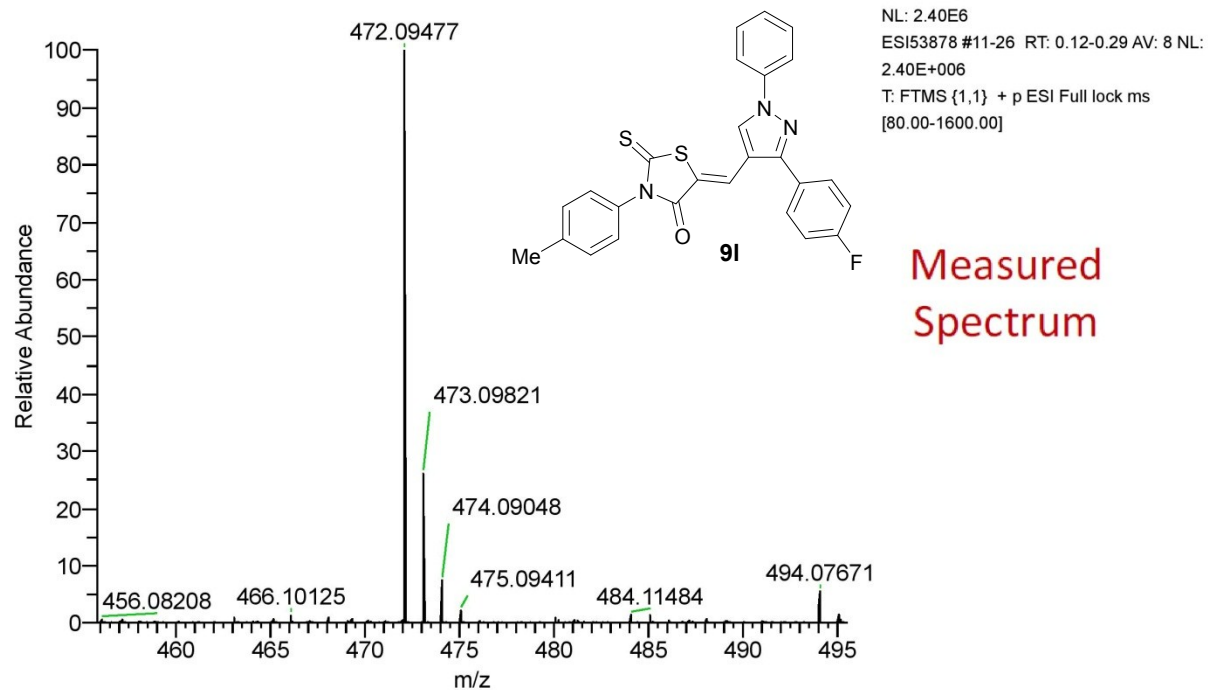
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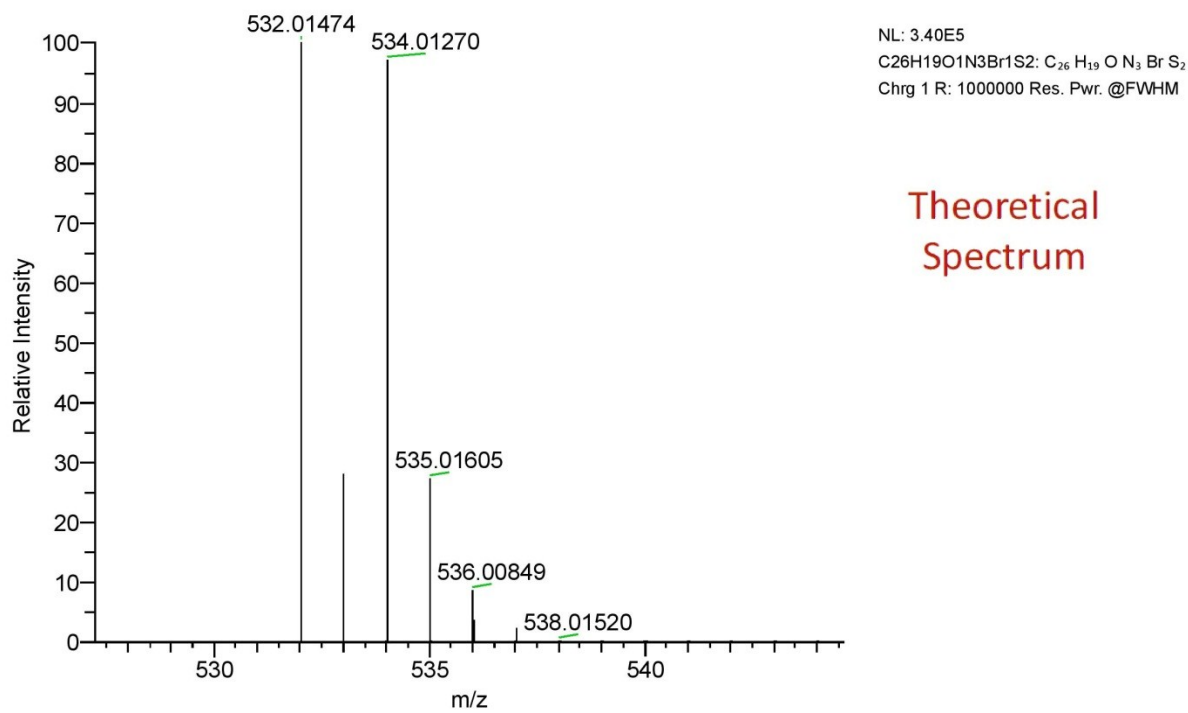
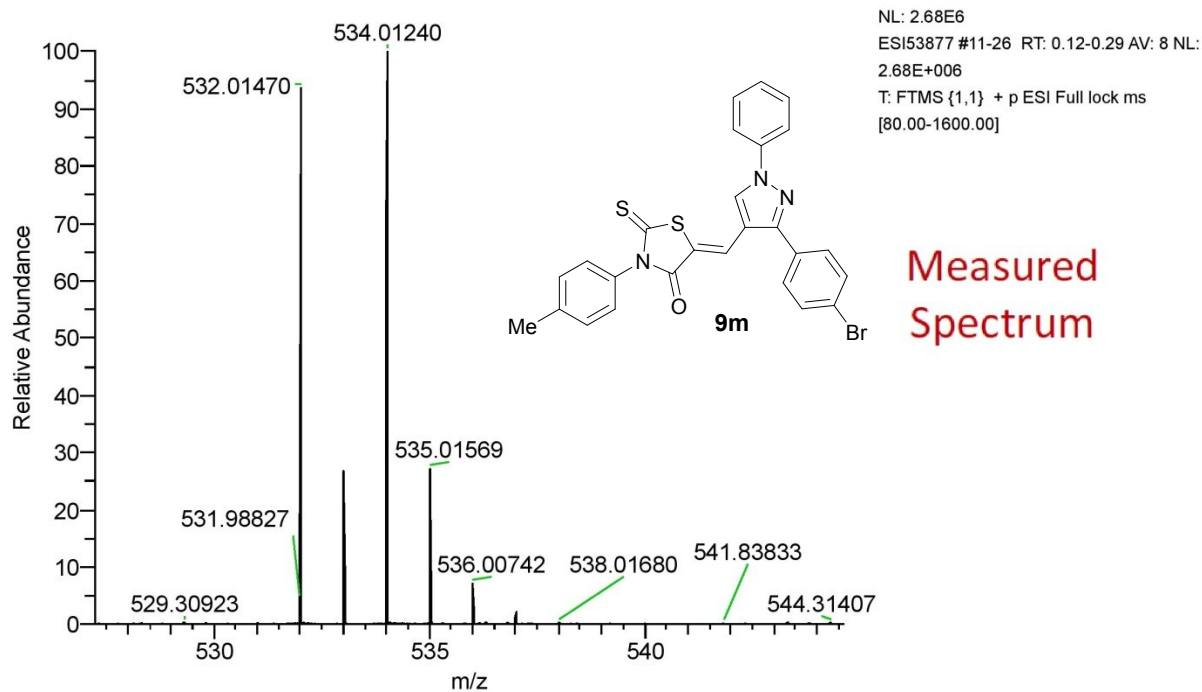
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1	468.11969	C ₂₇ H ₂₂ ON ₃ ³² S ₂	0	18.5	-0.41	C27H22O1N3...	468.11988



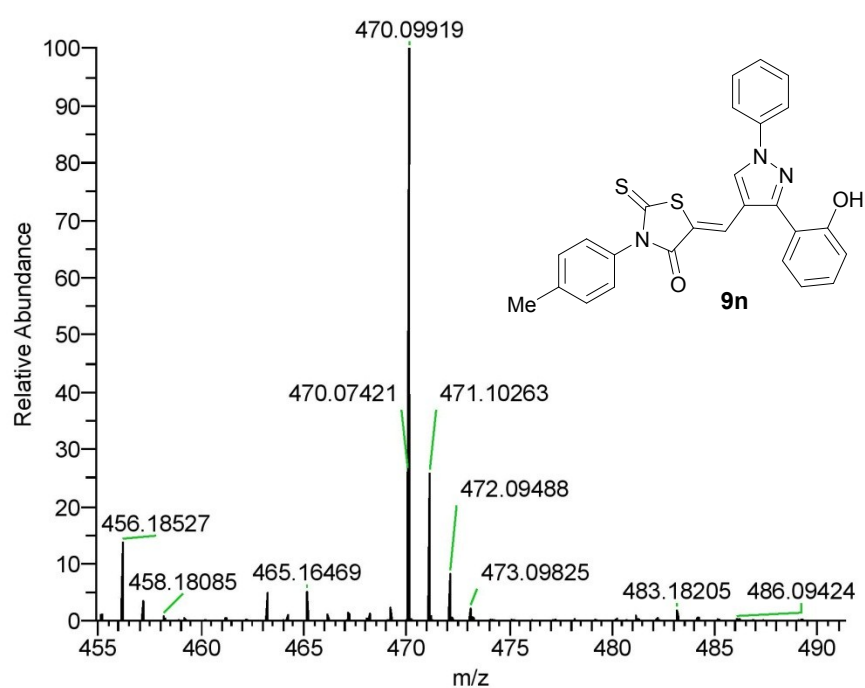
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1	499.08926	C ₂₆ H ₁₉ O ₃ N ₄ ³² S ₂	0	19.5	-0.09	C26H19O3N4...	499.08931



Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
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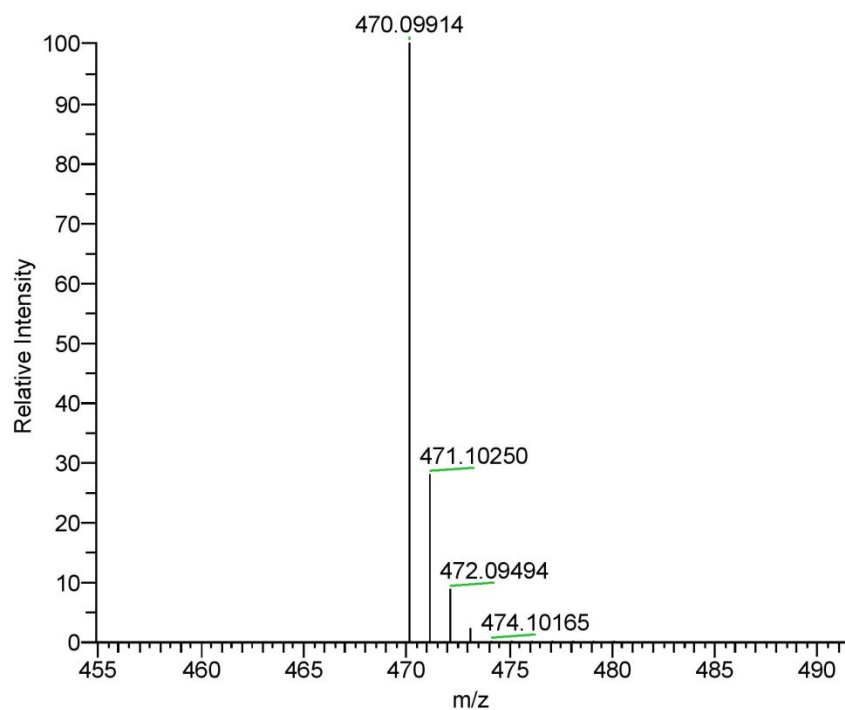


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NL: 2.69E6
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2.40E+007
T: FTMS {1,1} + p ESI Full lock ms
[80.00-1600.00]

Measured
Spectrum



NL: 6.69E5
C26H20O2N3S2: C₂₆ H₂₀ O₂ N₃ S₂ Chrg 1
R: 1000000 Res. Pwr. @FWHM

Theoretical
Spectrum

Index	m/z	Formula	Score	RDB	Delta ppm	OriginalFormula	Theo. Mass
1	470.09918	C ₂₆ H ₂₀ O ₂ N ₃ ³² S ₂	0	18.5	0.08	C26H20O2N3...	470.09914