

Title:

Design, Synthesis, Biological Evaluation and Molecular Modelling Studies of Oxoacetamide warhead containing Indole-Quinazolinone Based Novel Hybrid Analogues as Potential Pancreatic Lipase Inhibitors

Authors and Affiliations:

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[#] Authors with equal contribution

^{*} Corresponding author

Present address of the corresponding author:

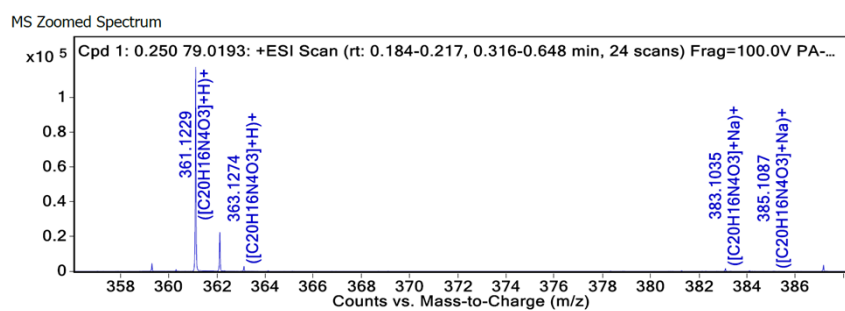
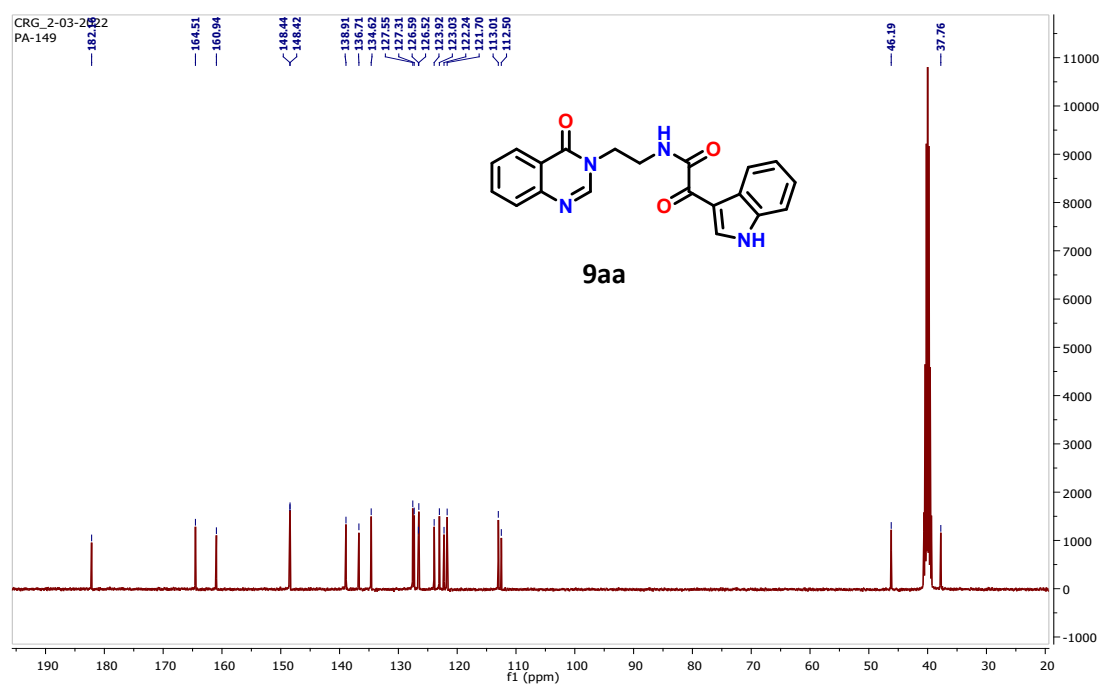
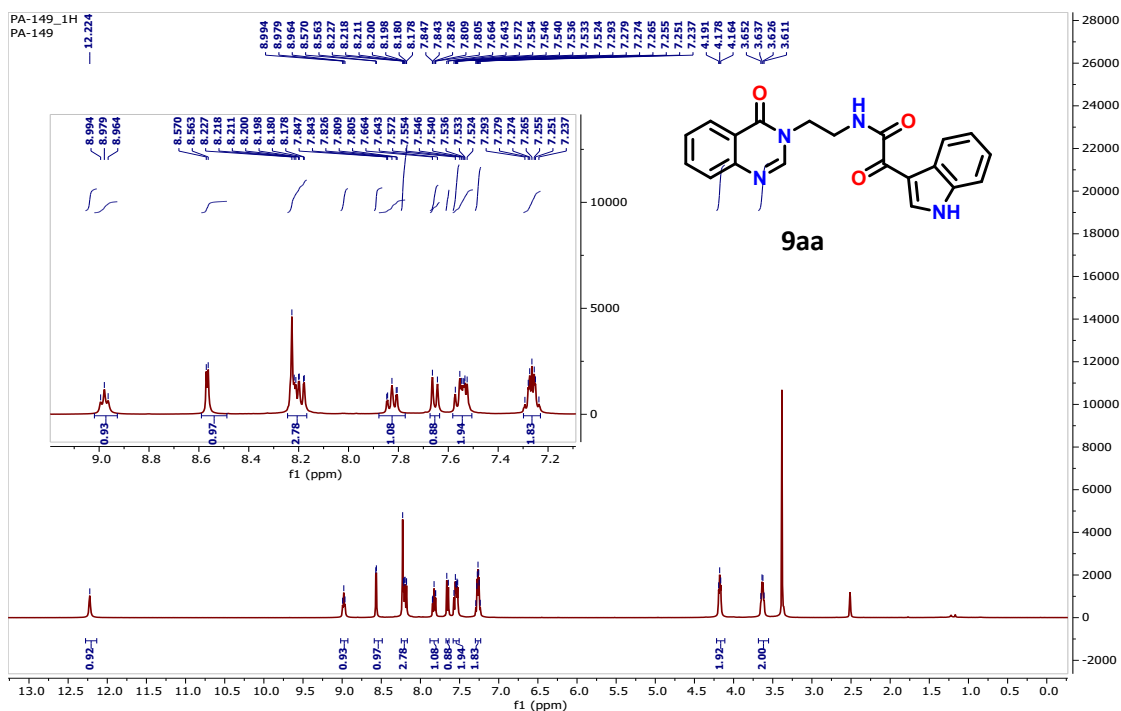
Laboratory of Natural Product Chemistry, Department of Pharmacy, Birla Institute of Technology and Science, Pilani (BITS Pilani), Pilani Campus, Pilani - 333 031, Rajasthan, India

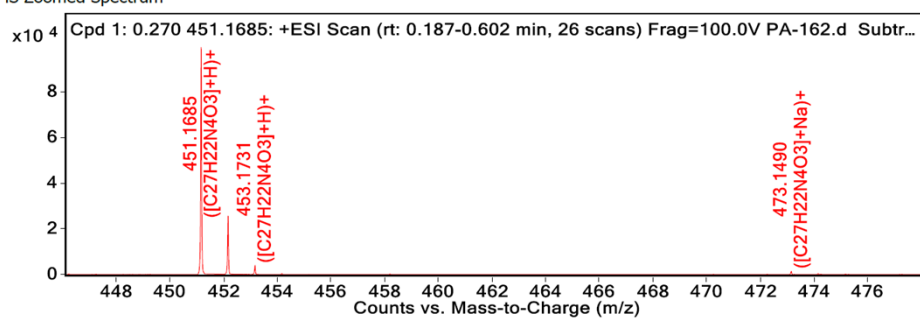
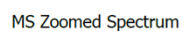
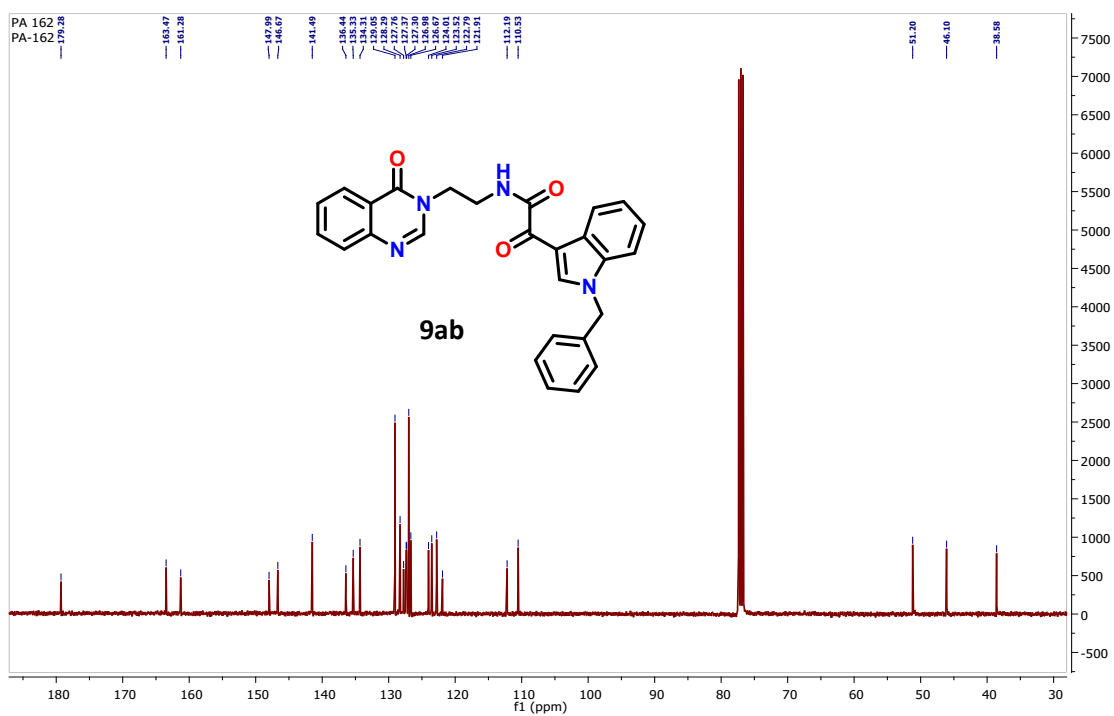
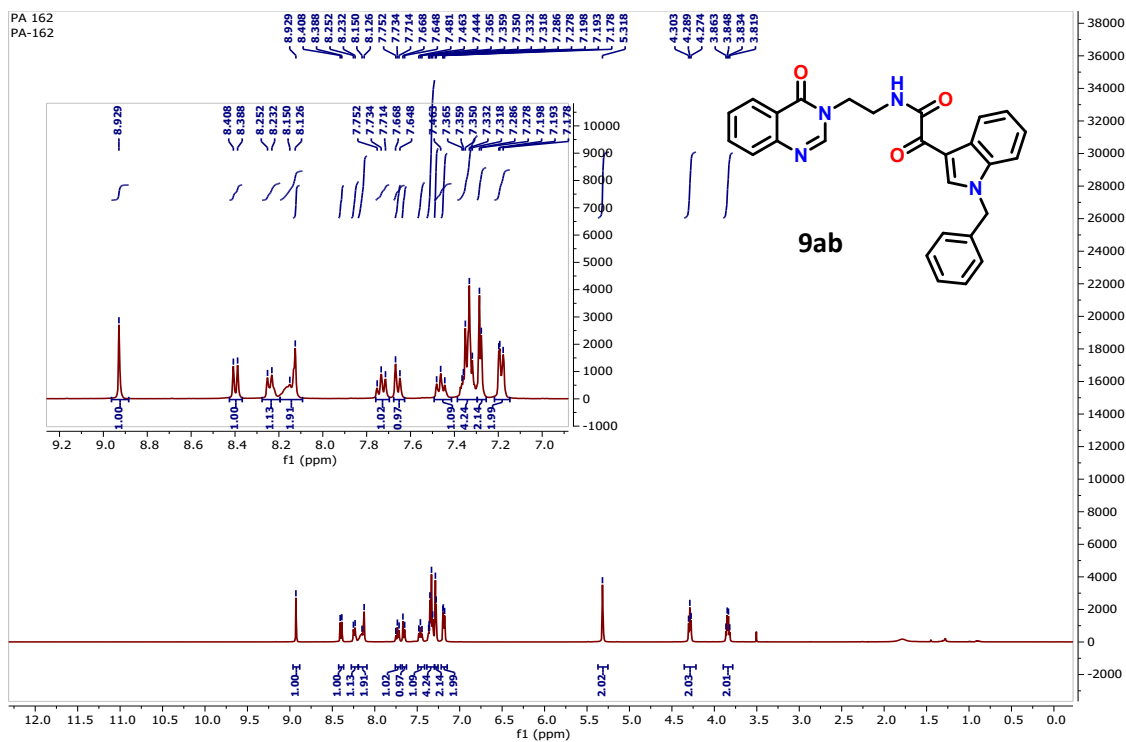
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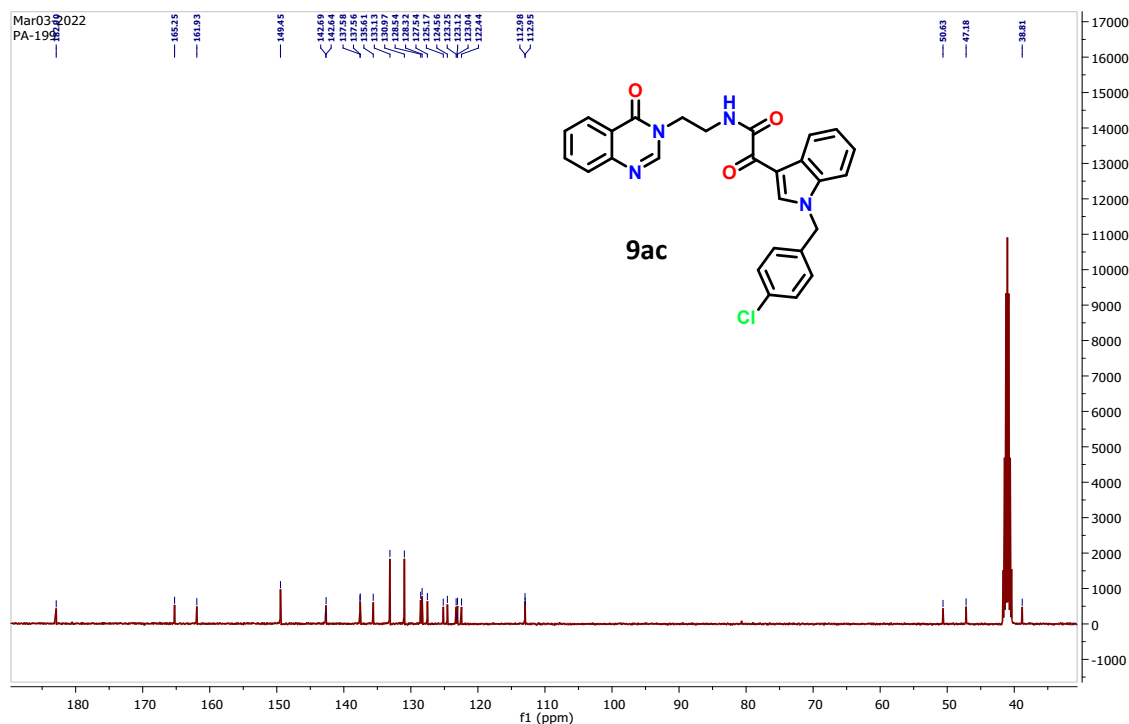
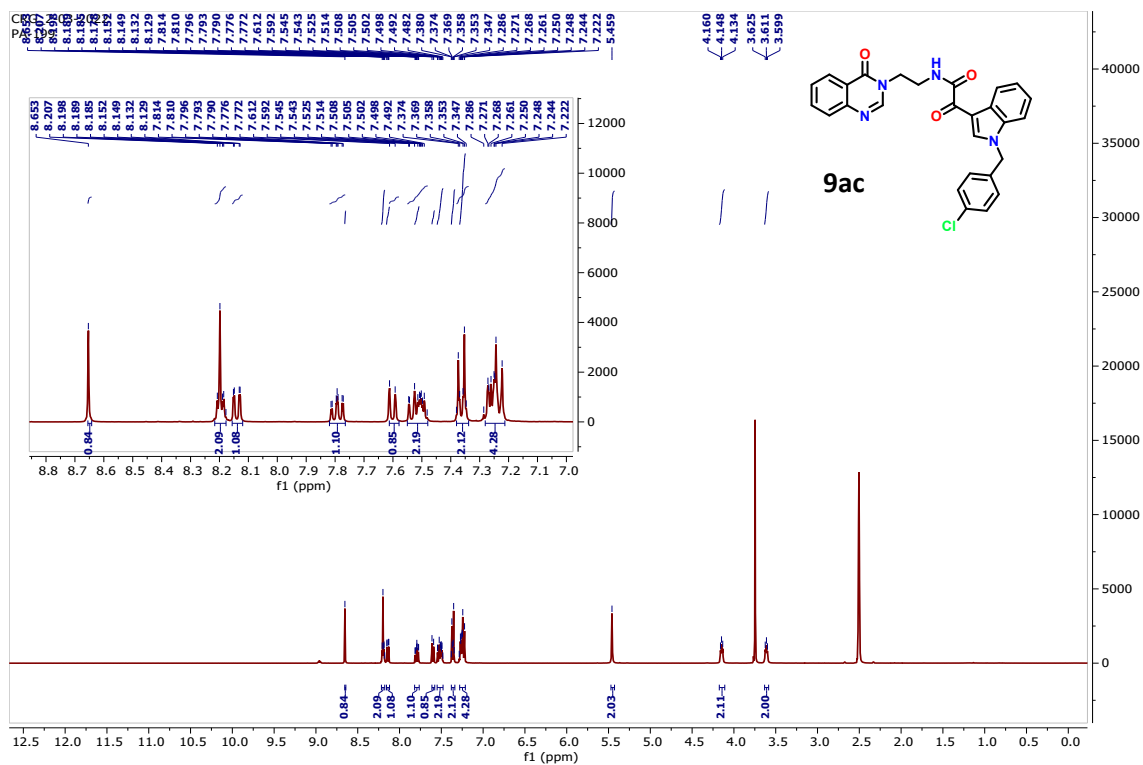
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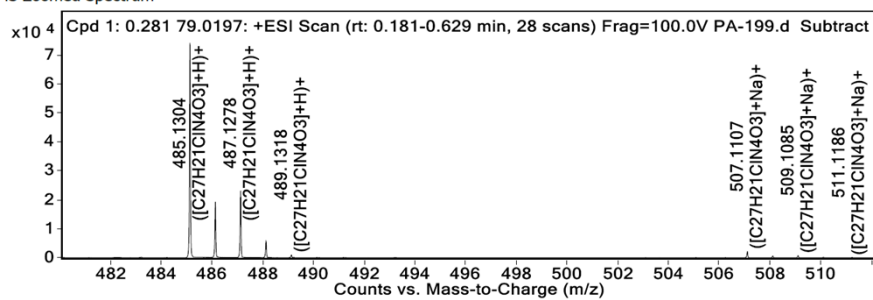
1. ¹H NMR, ¹³C NMR and HRMS Spectra:

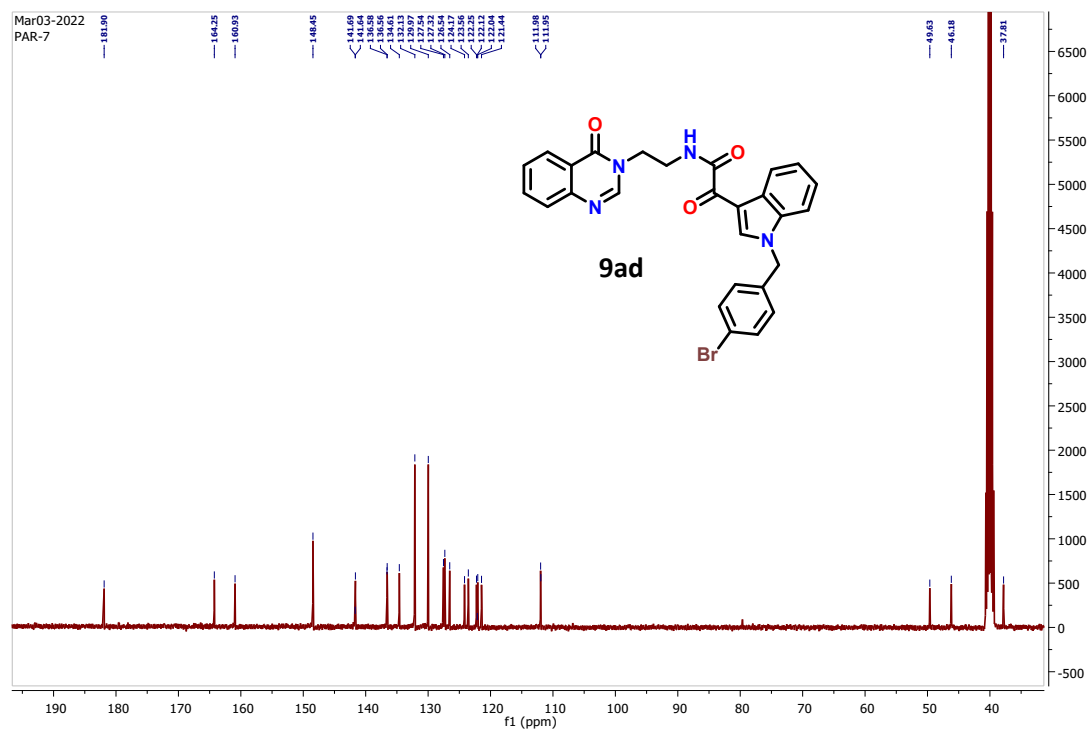
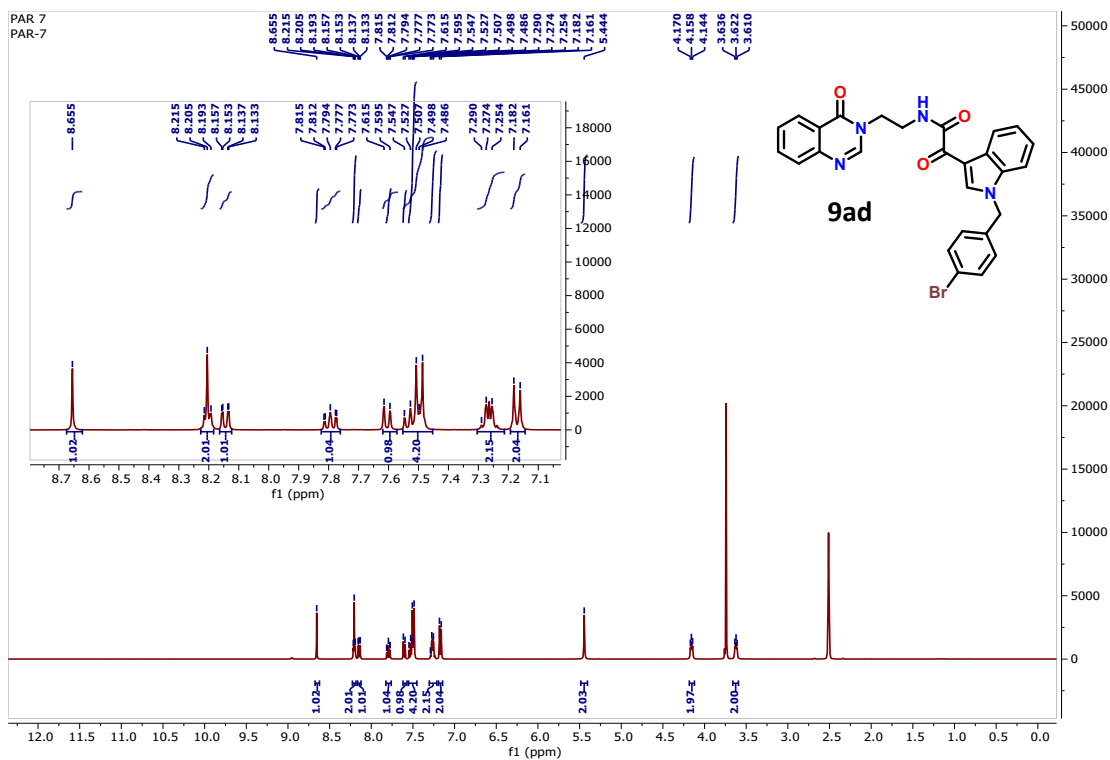




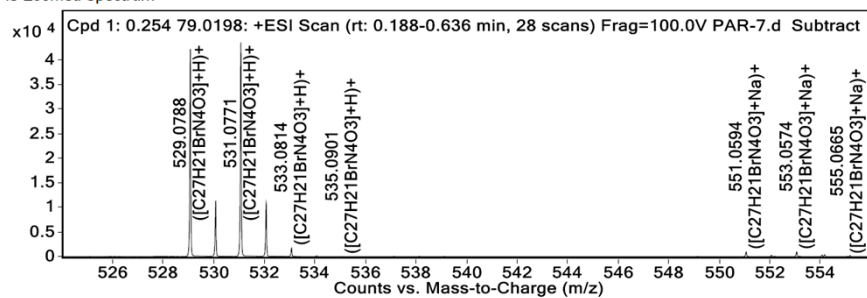


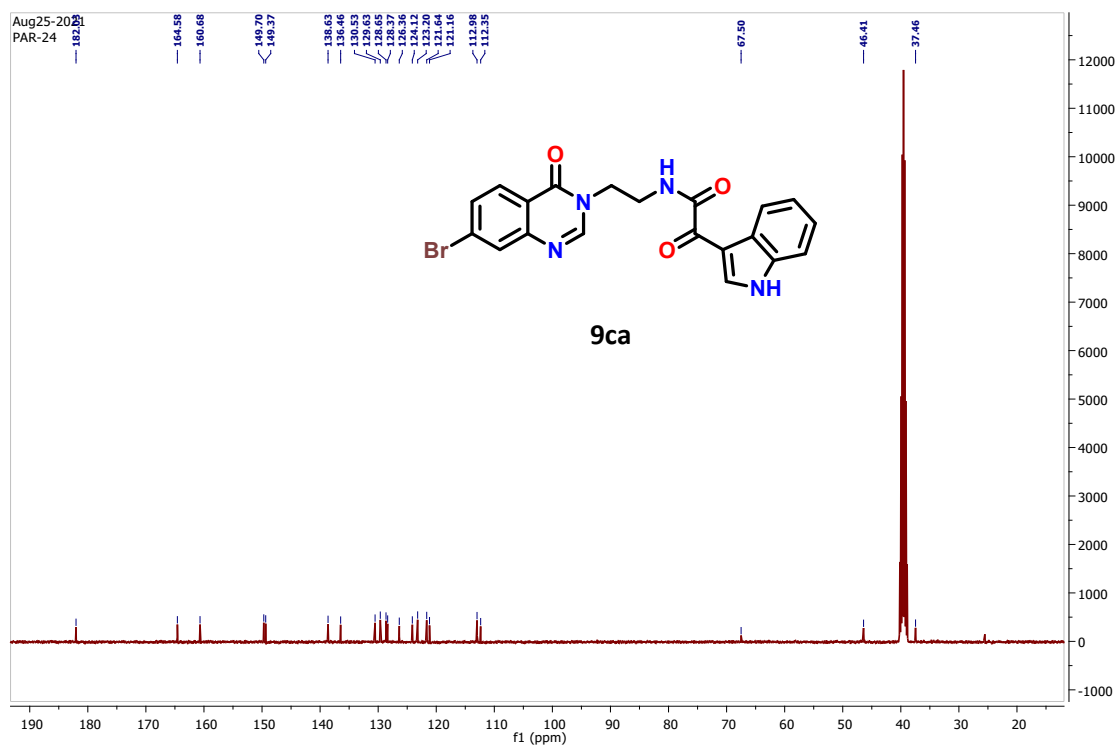
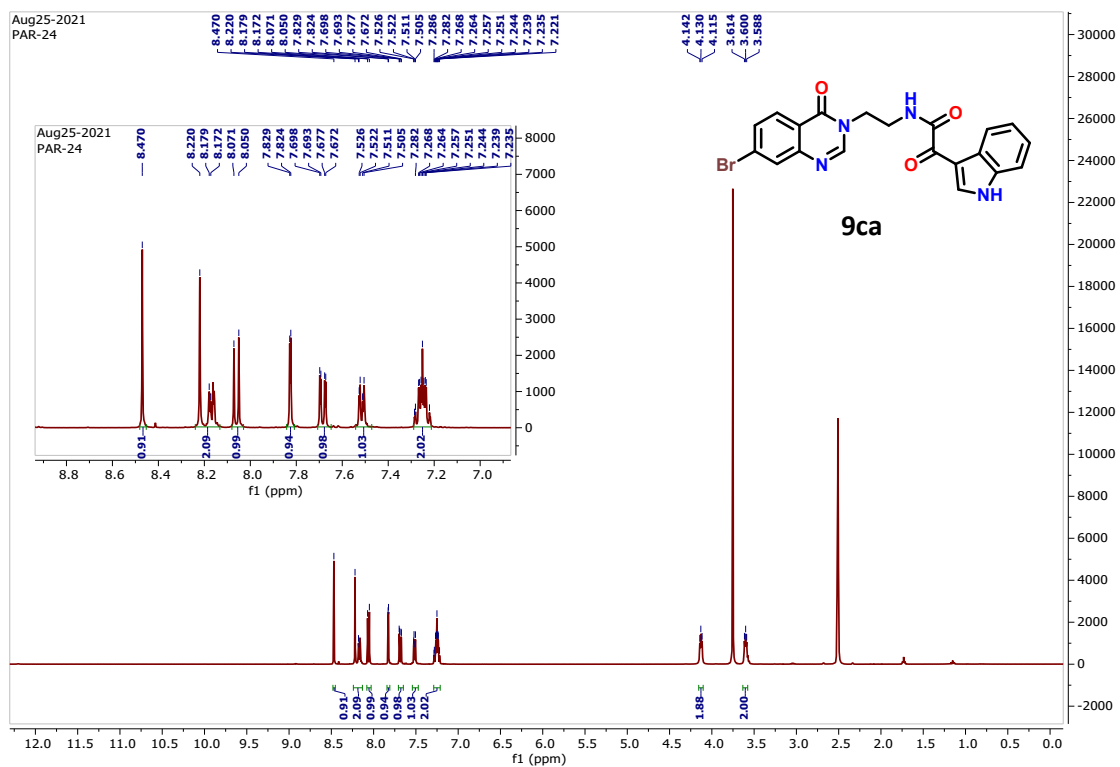
MS Zoomed Spectrum





MS Zoomed Spectrum

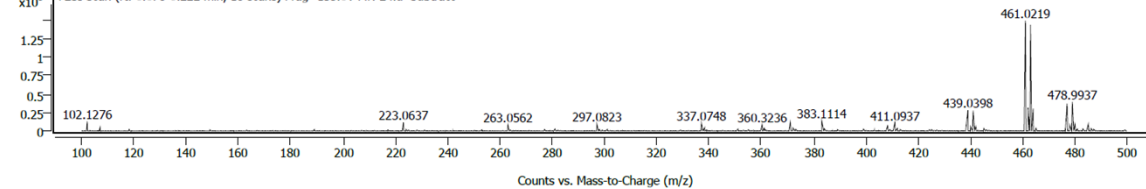


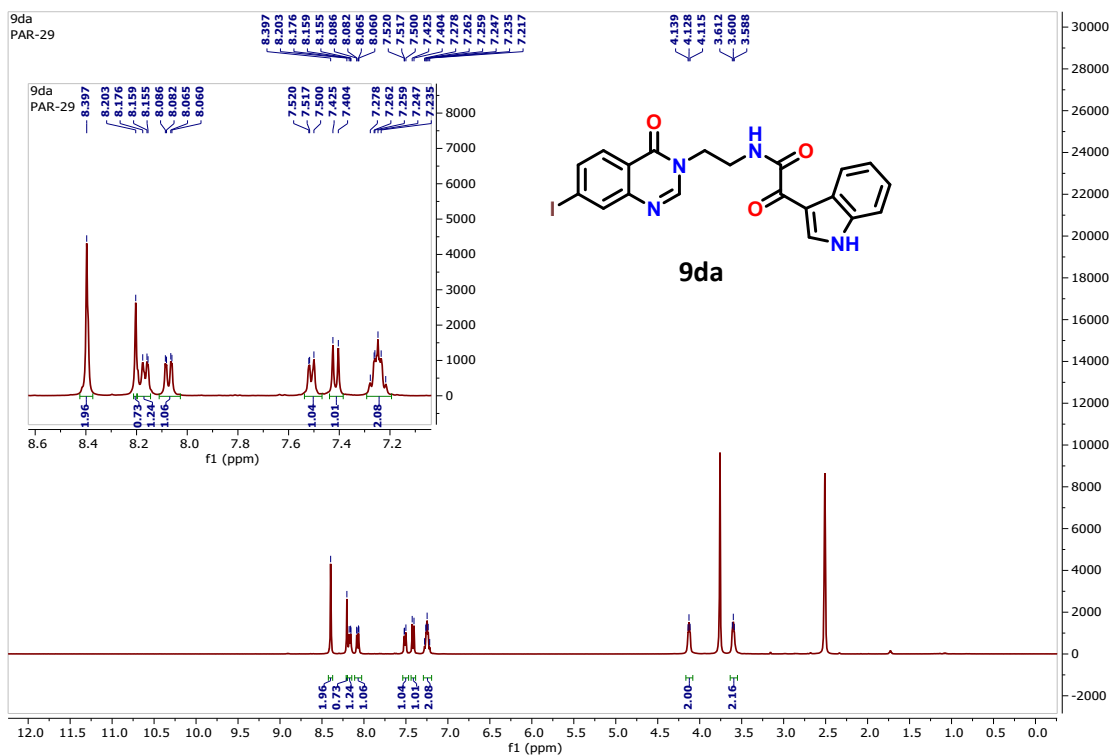


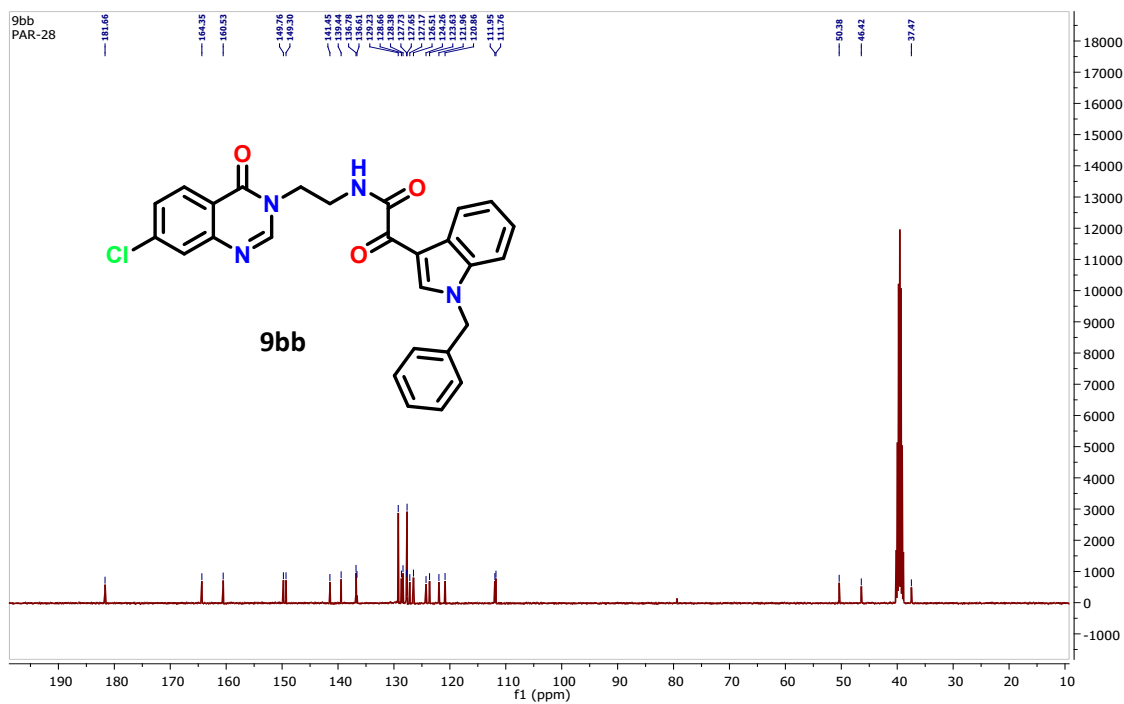
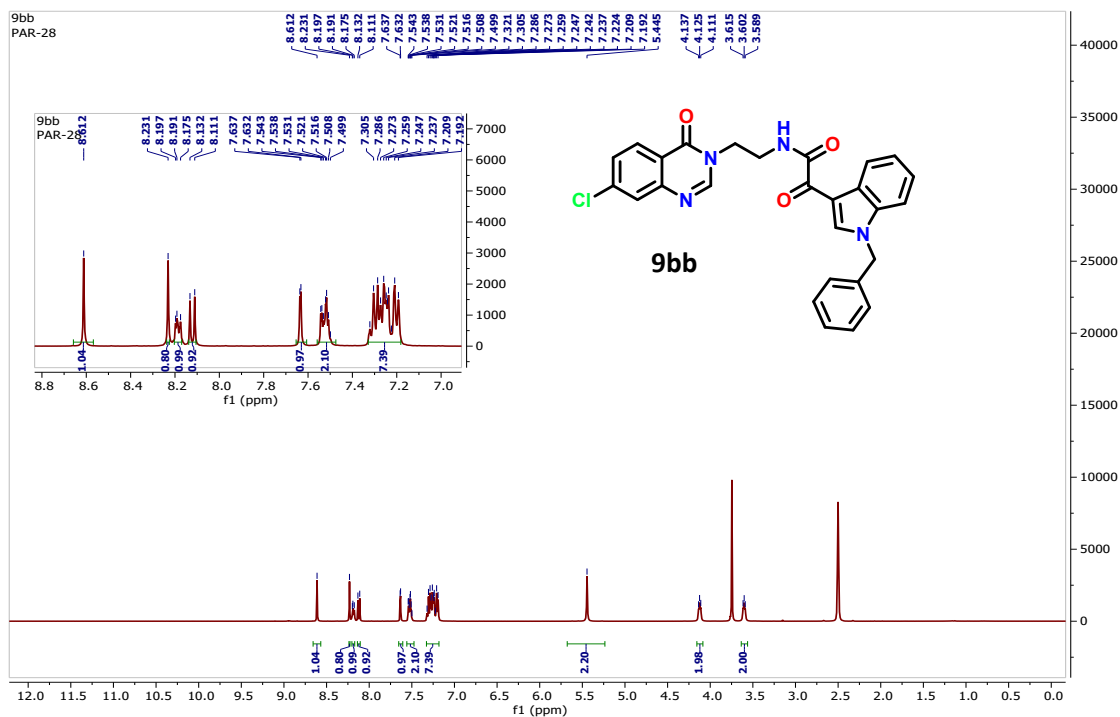
Peak Spec

+ Scan (rt: 0.078-0.222 min) Sub SpectrumIdString

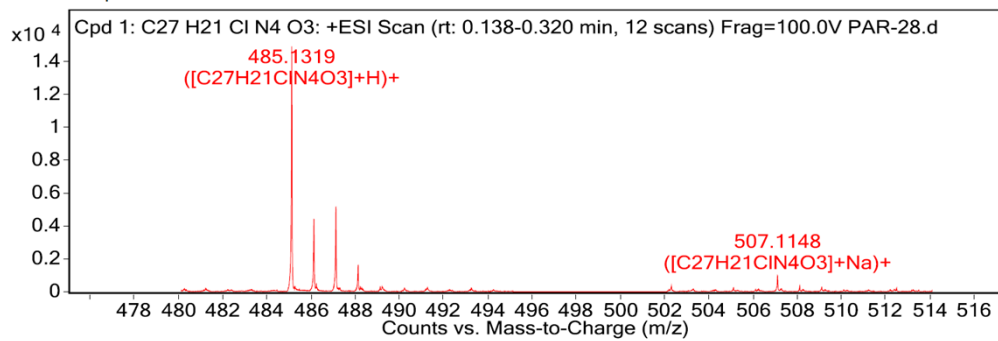
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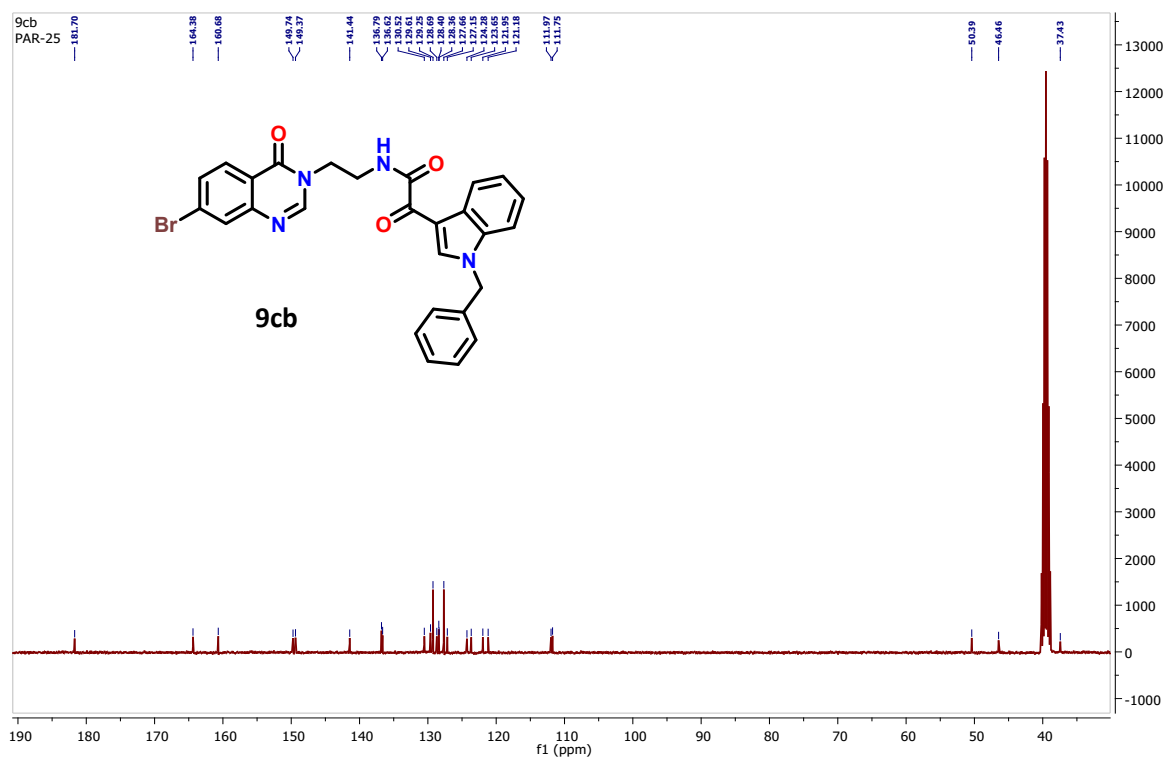
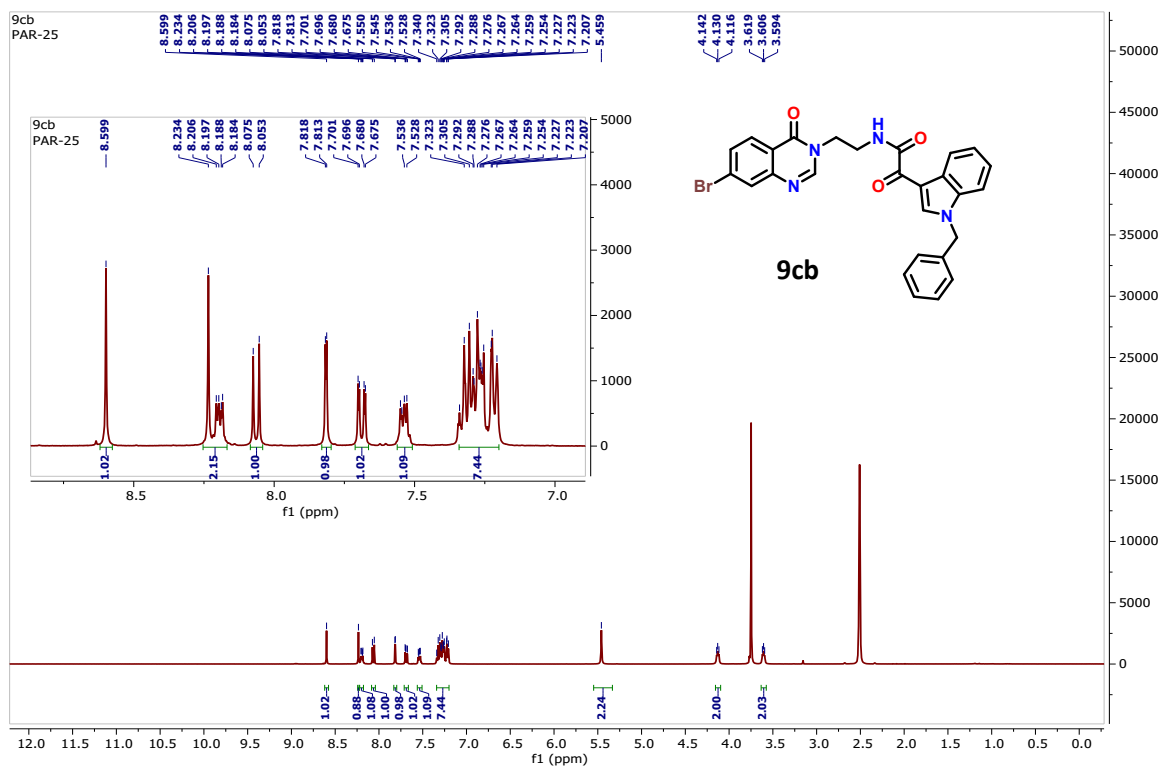






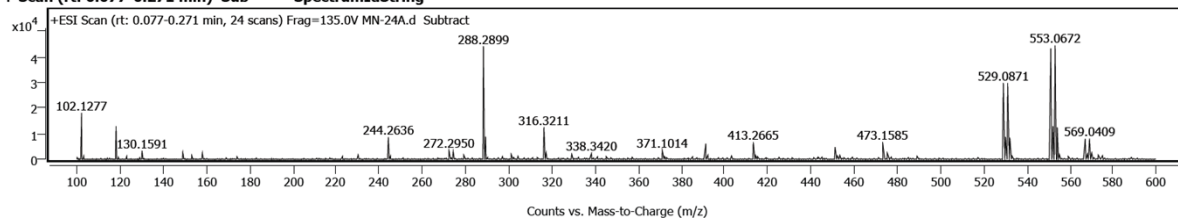
MS Zoomed Spectrum

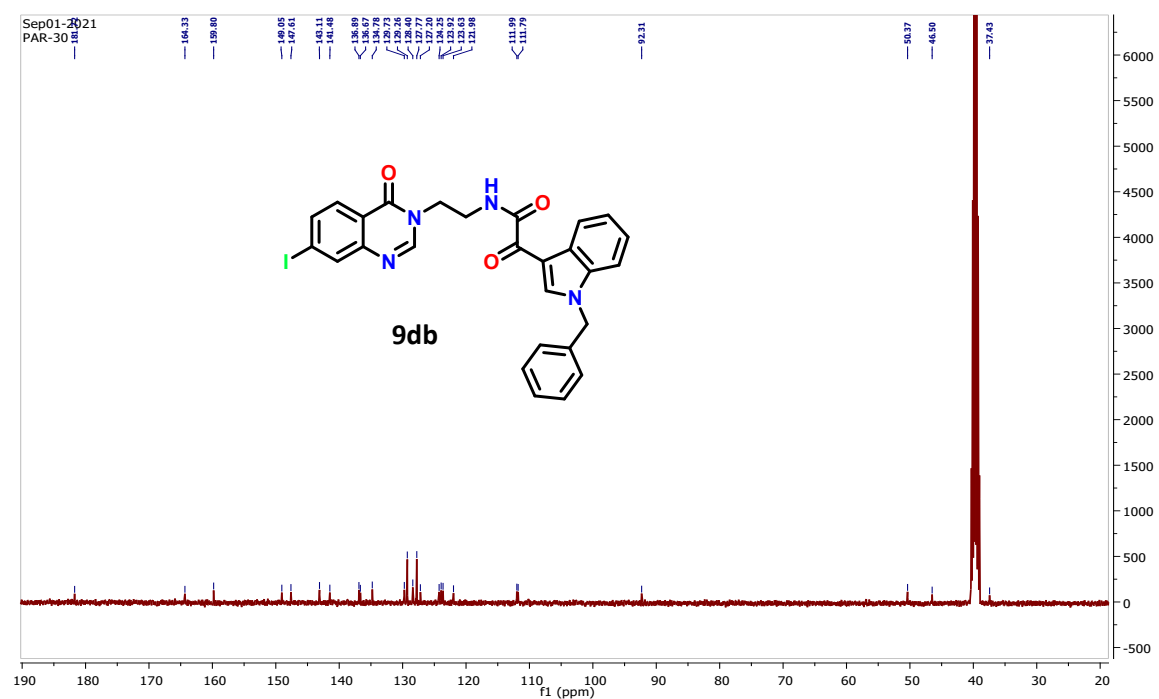
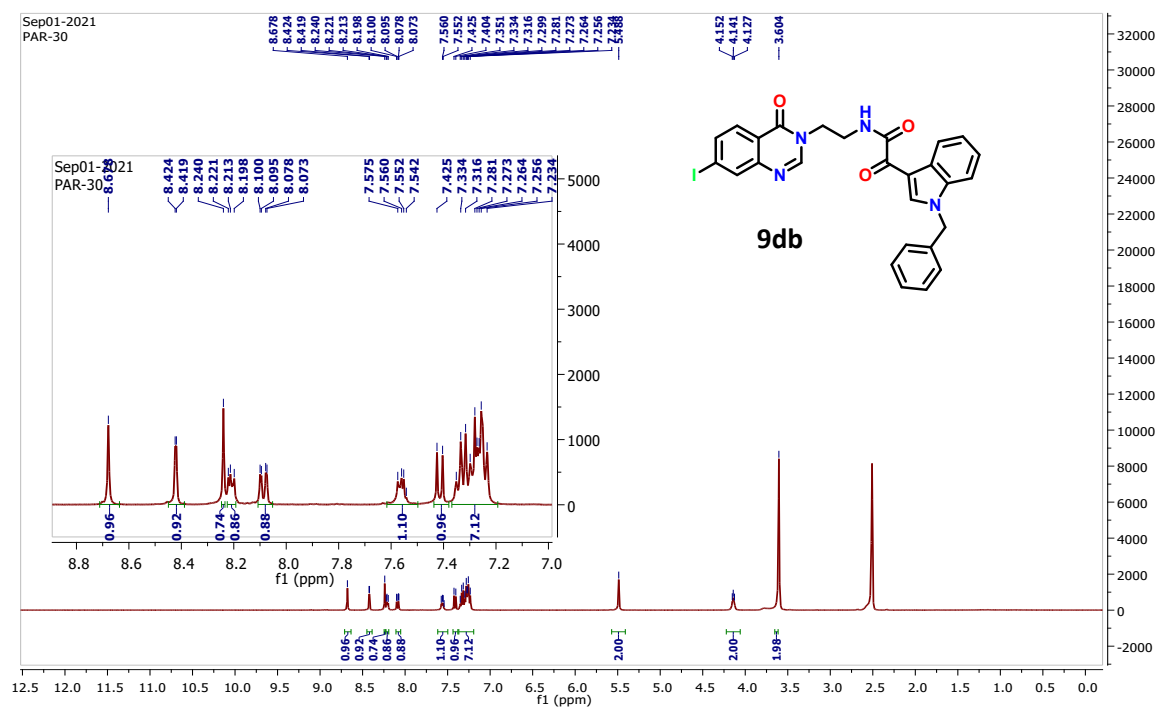




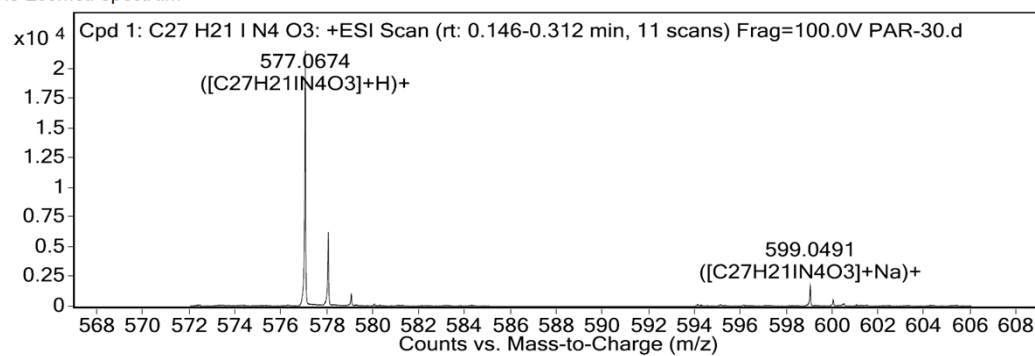
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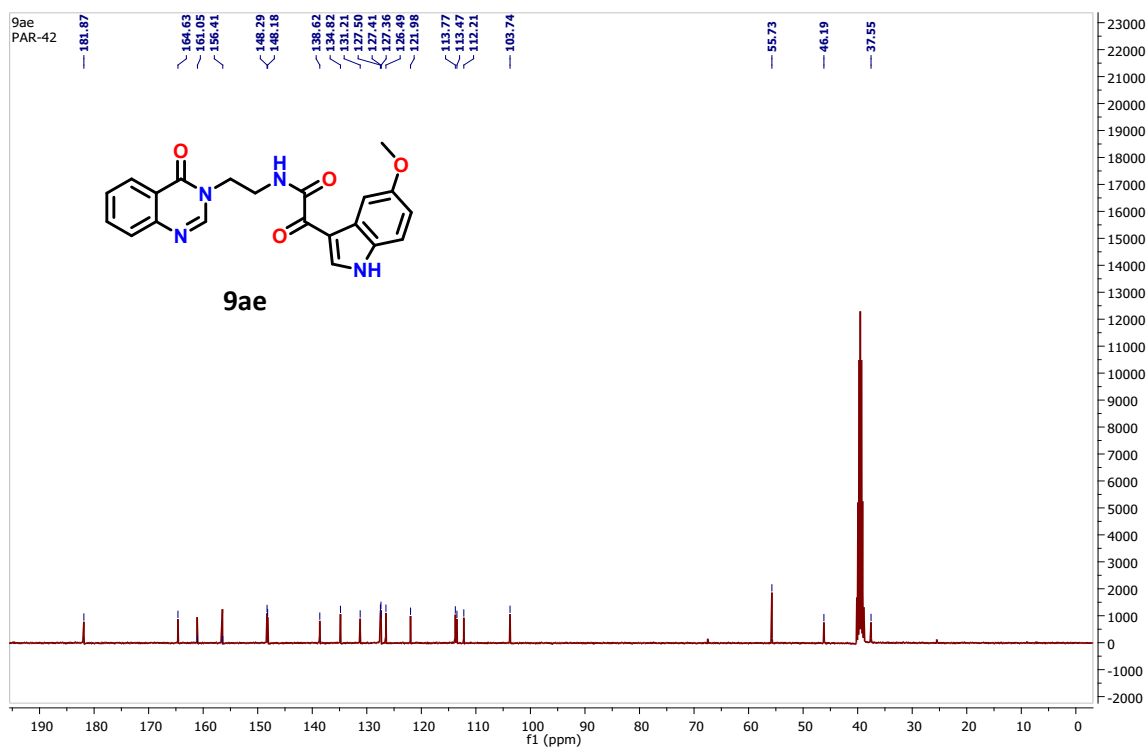
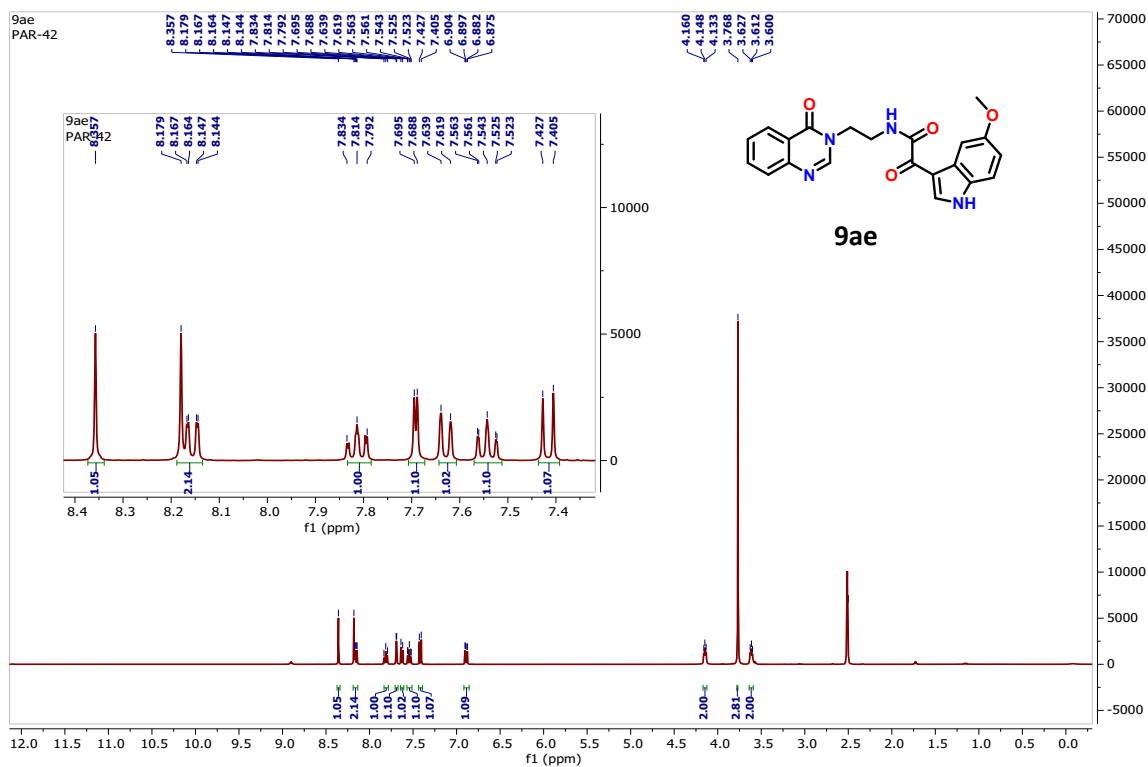
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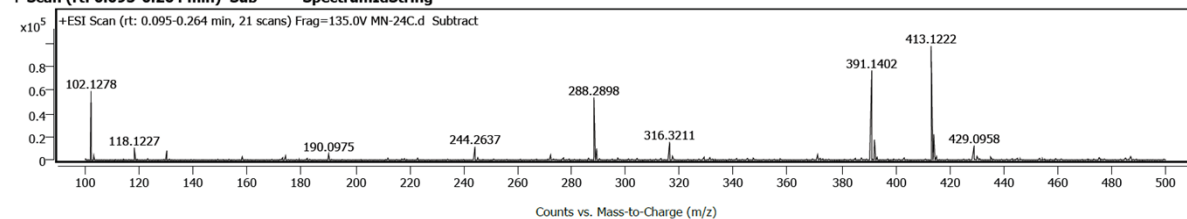
MS Zoomed Spectrum

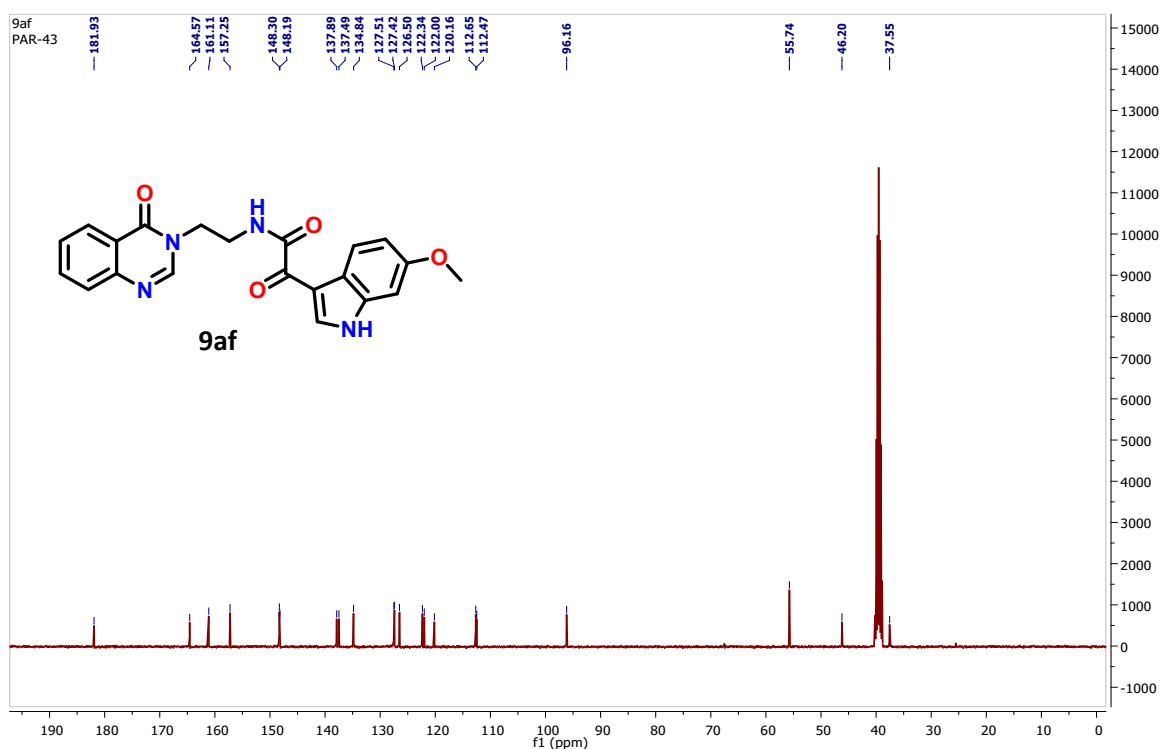
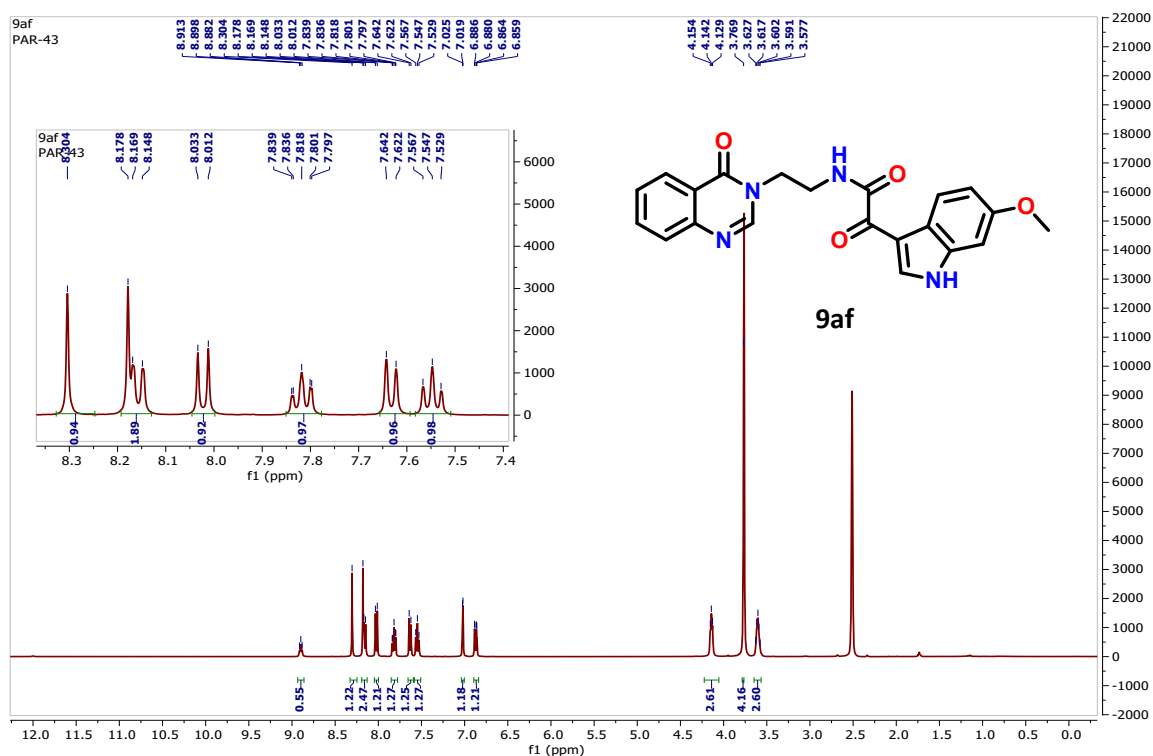




Peak Spec

+ Scan (rt: 0.095-0.264 min) Sub SpectrumIdString

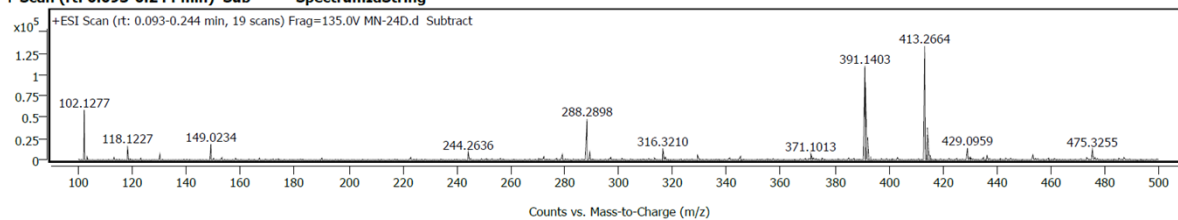


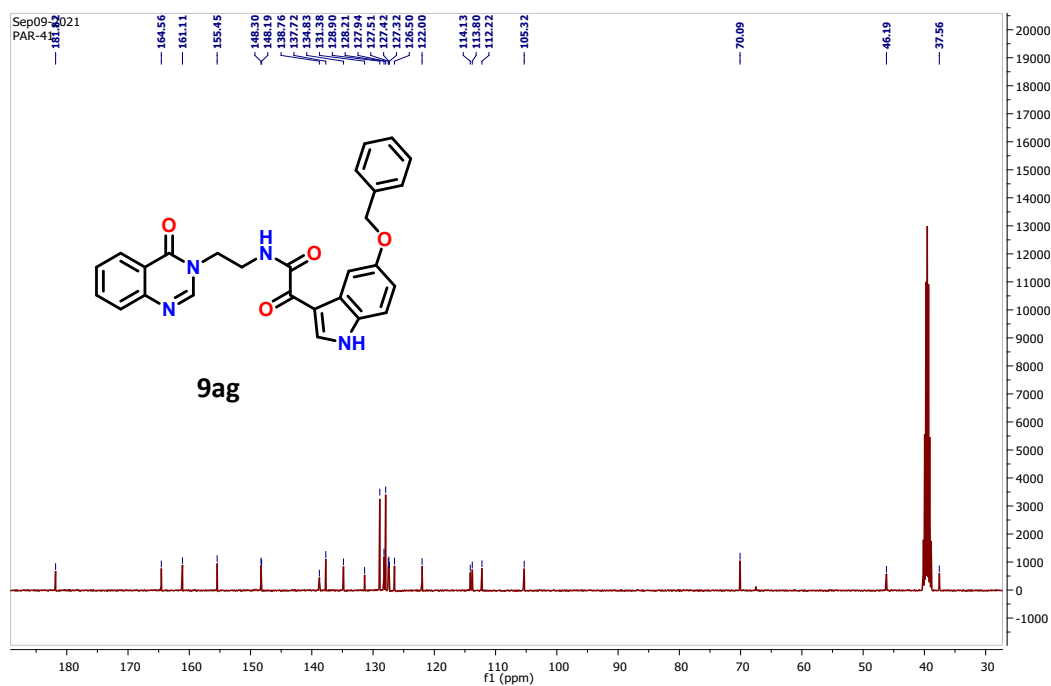
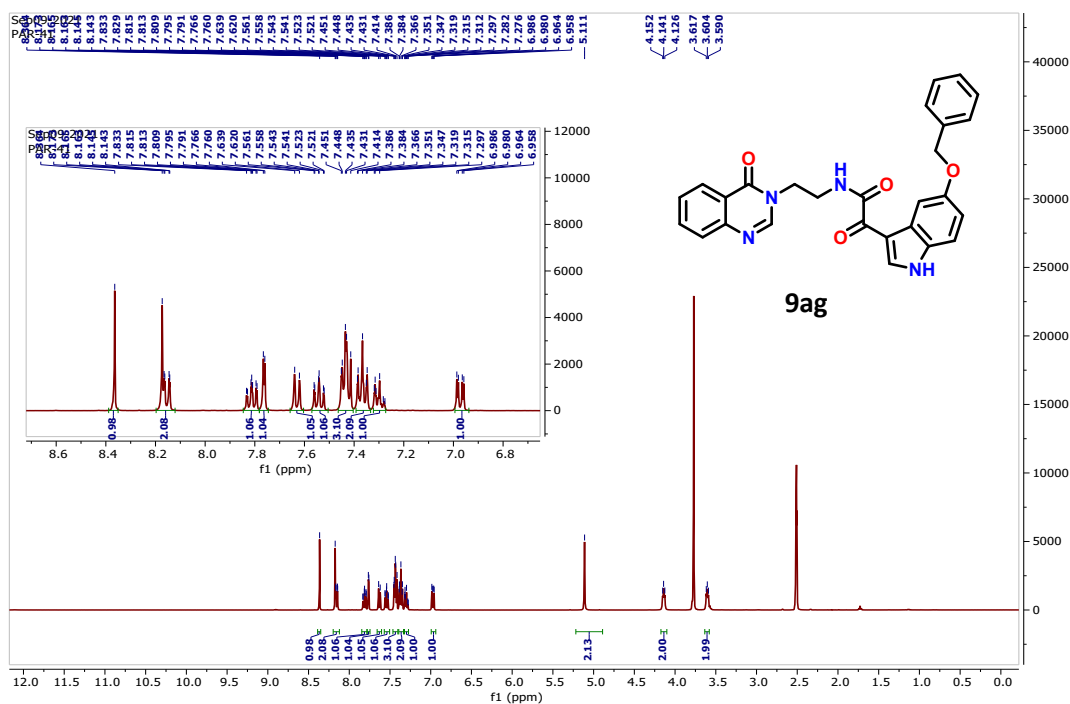


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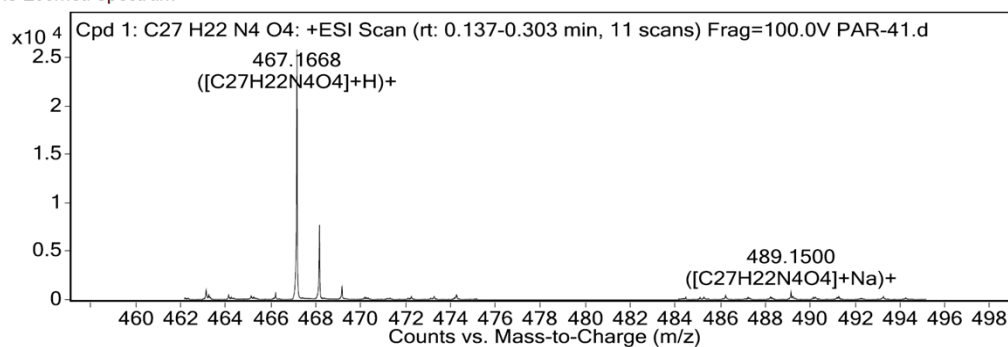
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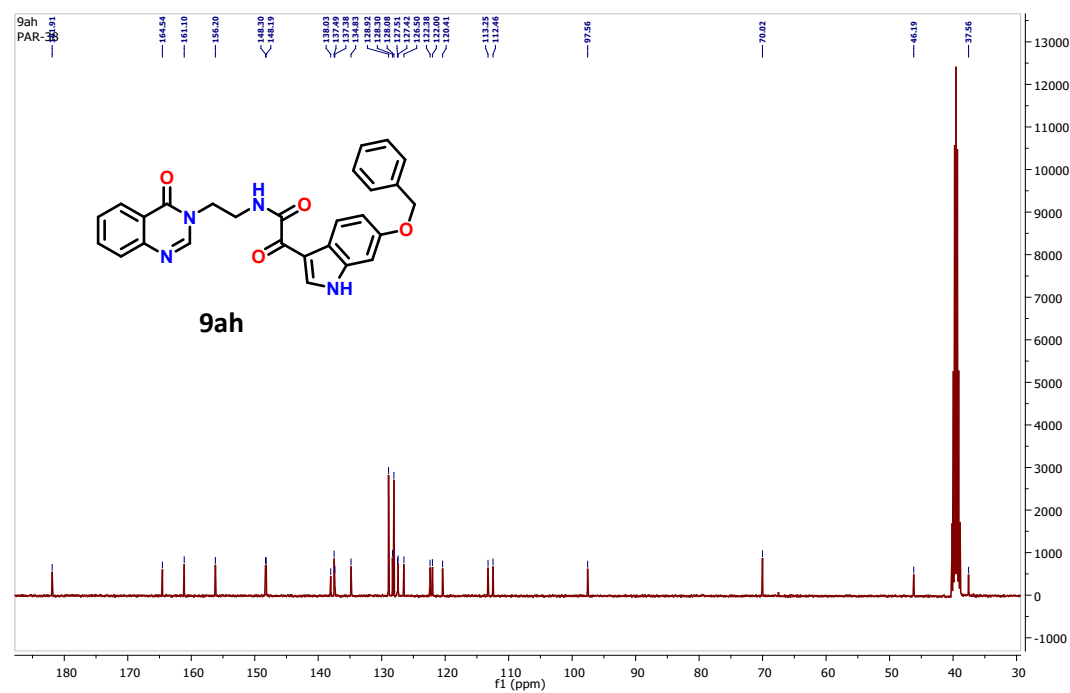
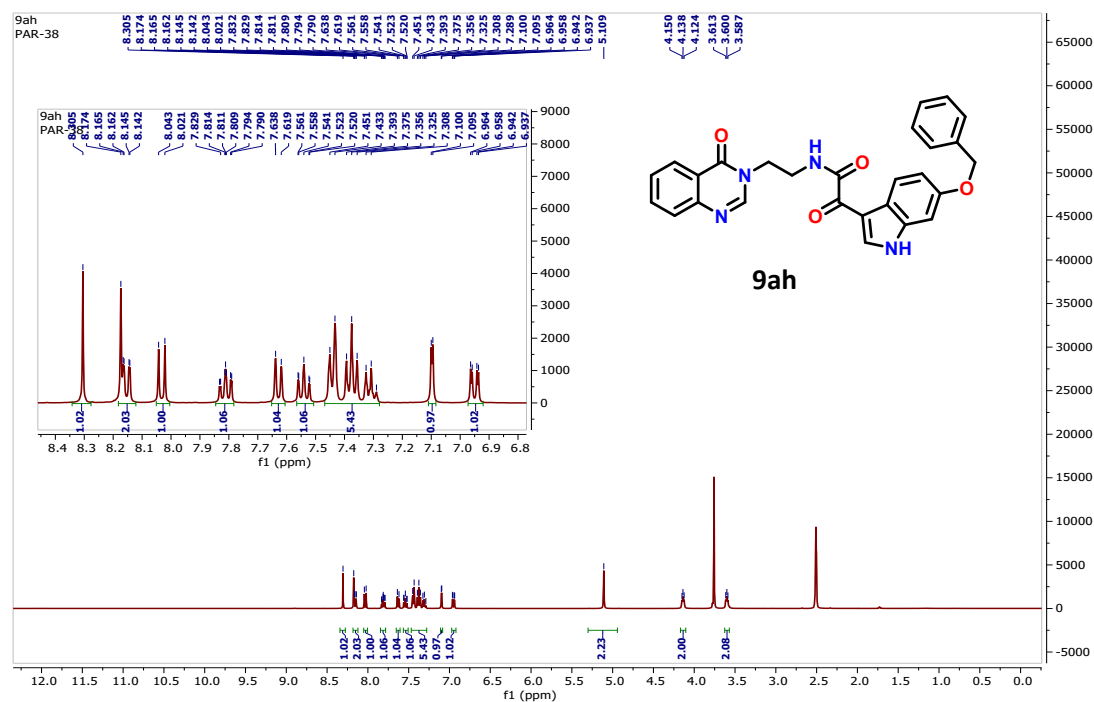
+ESI Scan (rt: 0.093-0.244 min, 19 scans) Frag=135.0V MN-24D.d Subtract



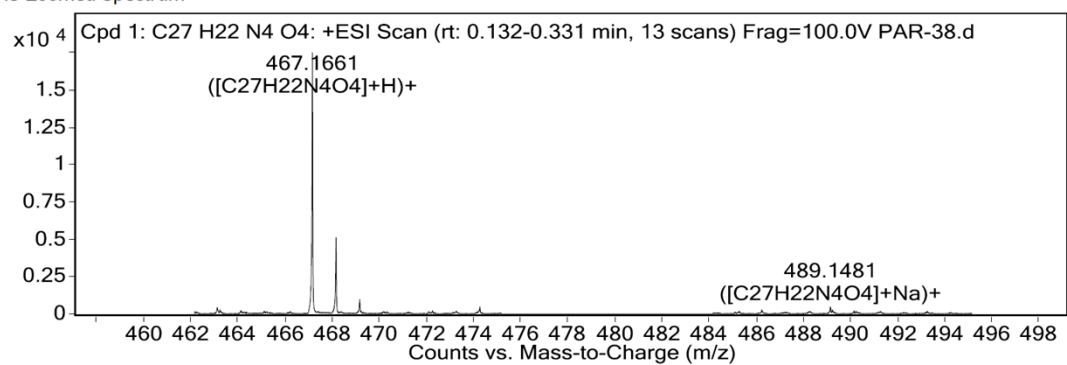


MS Zoomed Spectrum





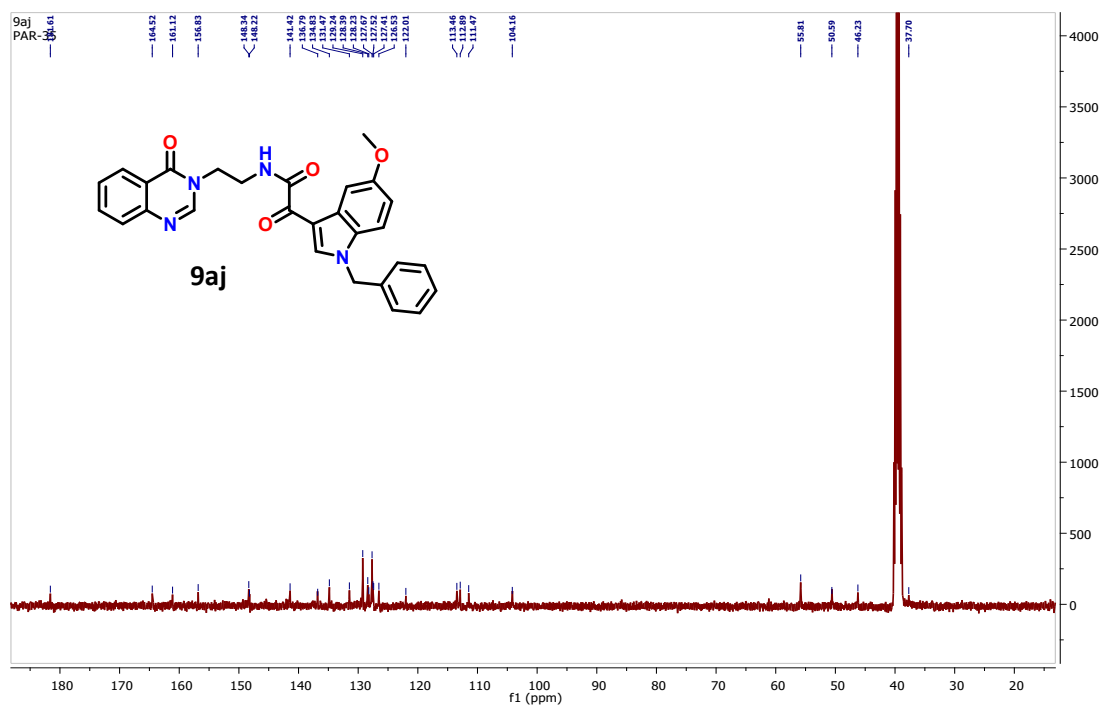
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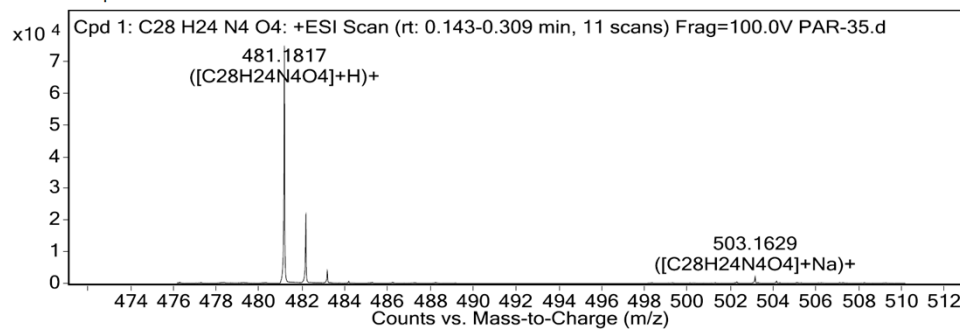
Chemical structure of 9aj: COc1ccc(Cn2cnc3ccccc32)c4c1c(=O)nc4CCn5cnc6ccccc65

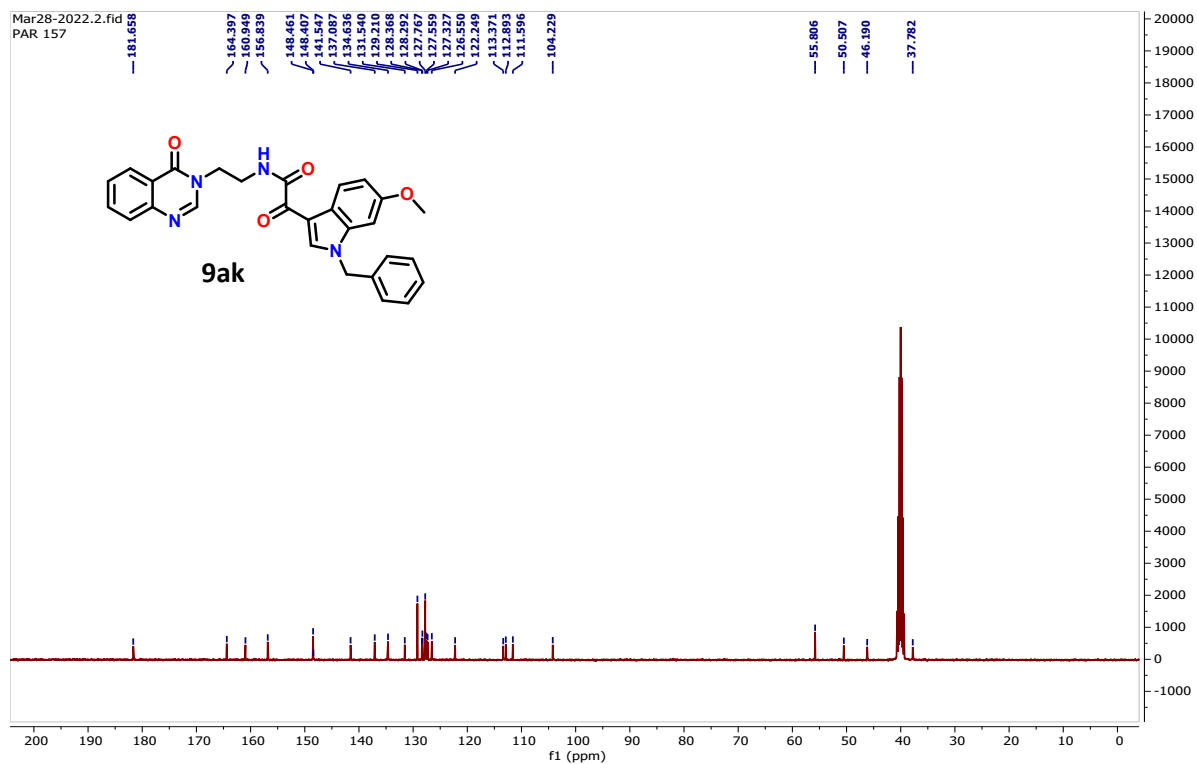
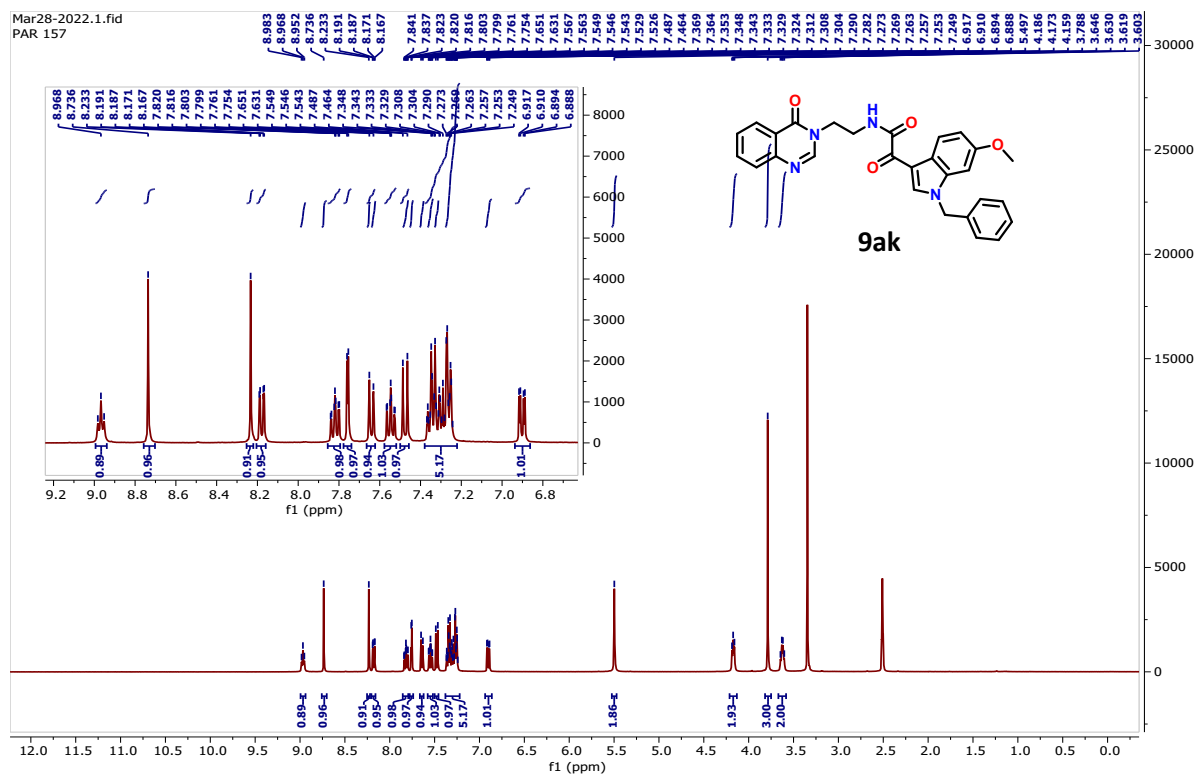
¹H NMR spectrum (CDCl₃):

Chemical Shift (ppm)	Integration
~11.1 (s, 1H)	0.95
~8.2 (d, 2H)	0.96
6.8 - 7.8 (m, 10H)	0.92, 1.00, 0.99, 0.97, 0.98, 5.11, 0.99
~5.5 (s, 2H)	1.92
~4.0 (m, 2H)	1.94
~3.3 (m, 2H)	2.98, 2.00



MS Zoomed Spectrum

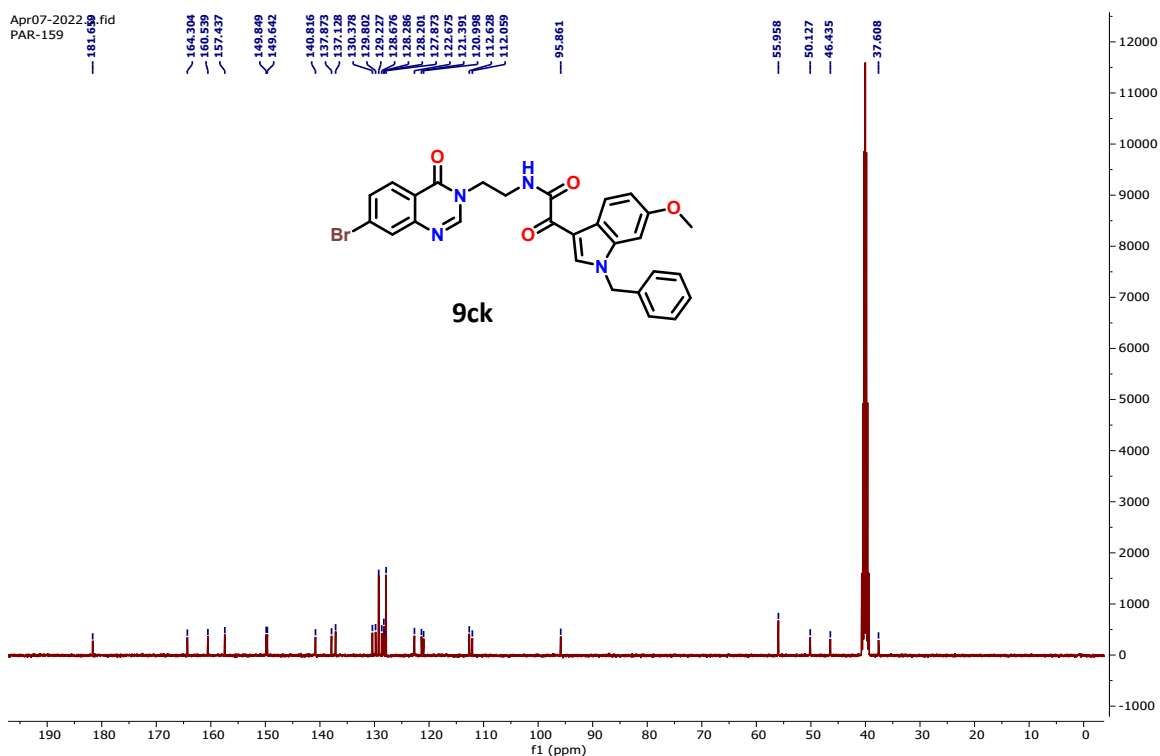
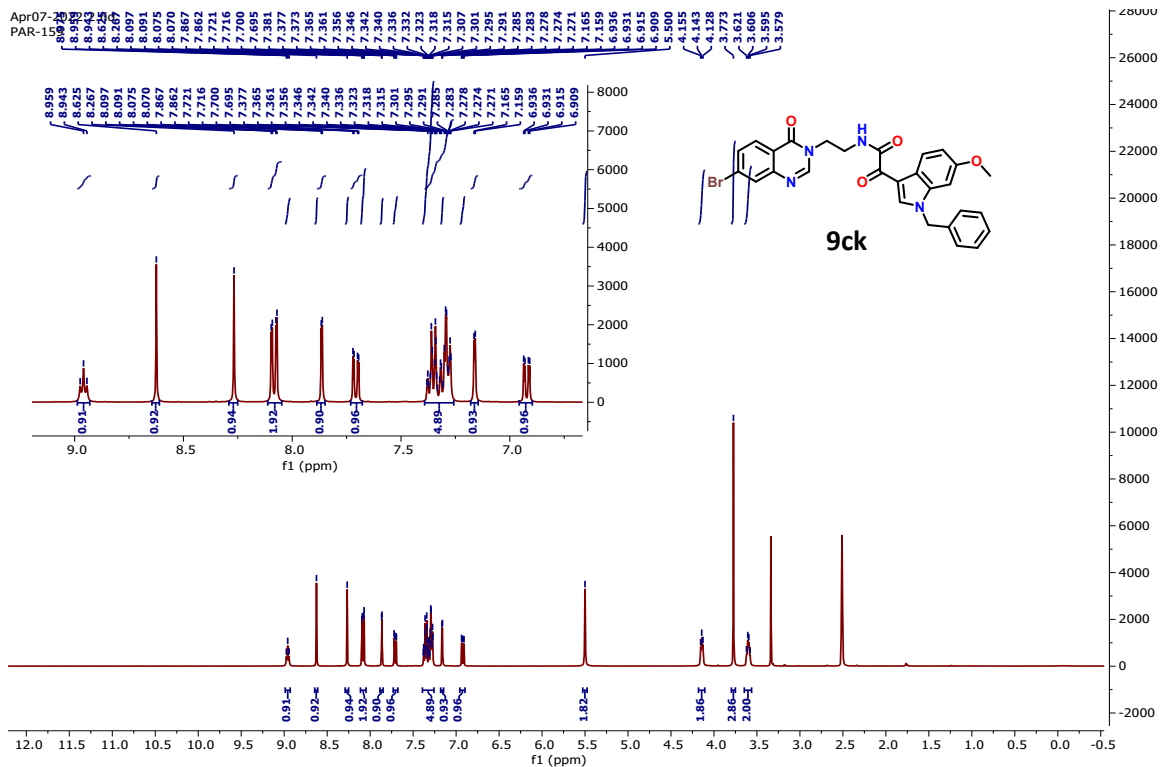
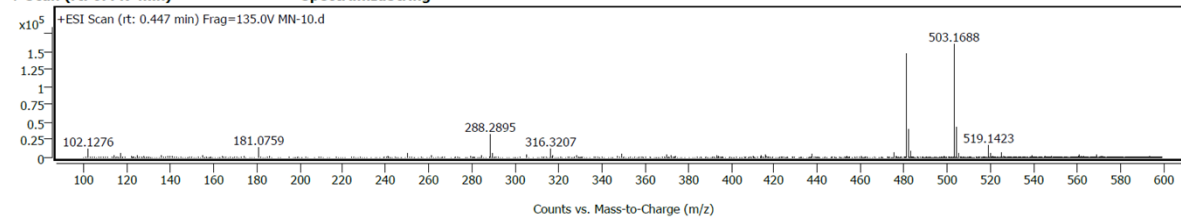




Peak Spec

+ Scan (rt: 0.447 min)

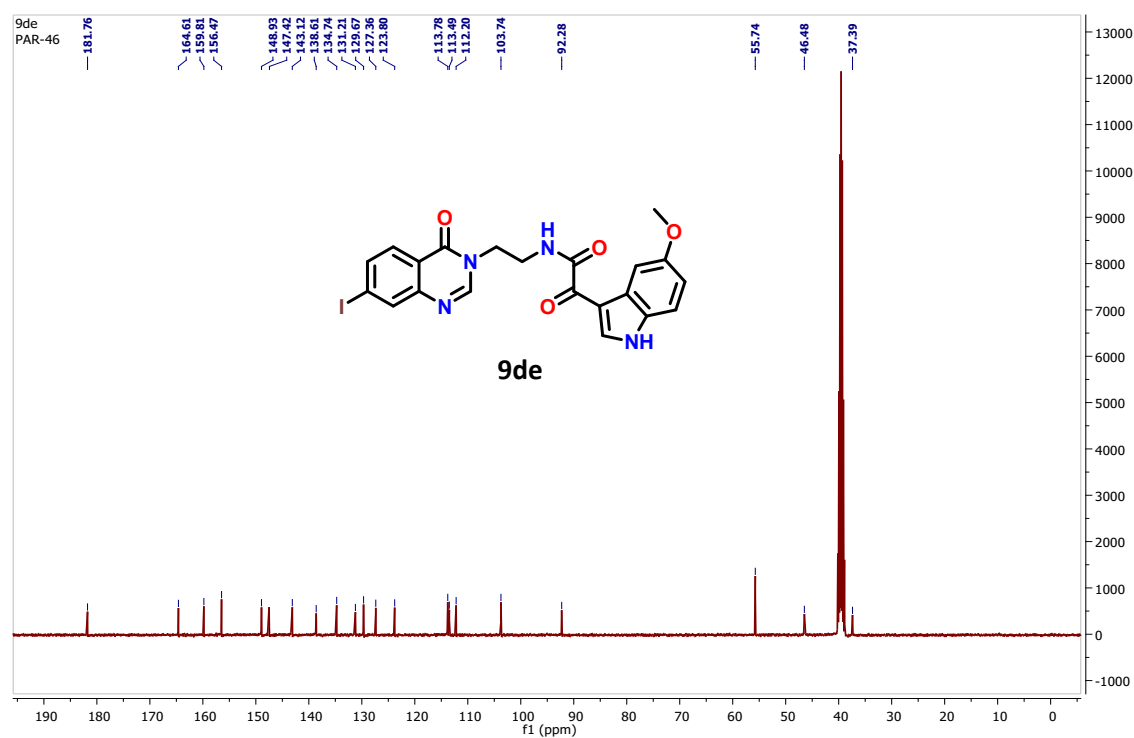
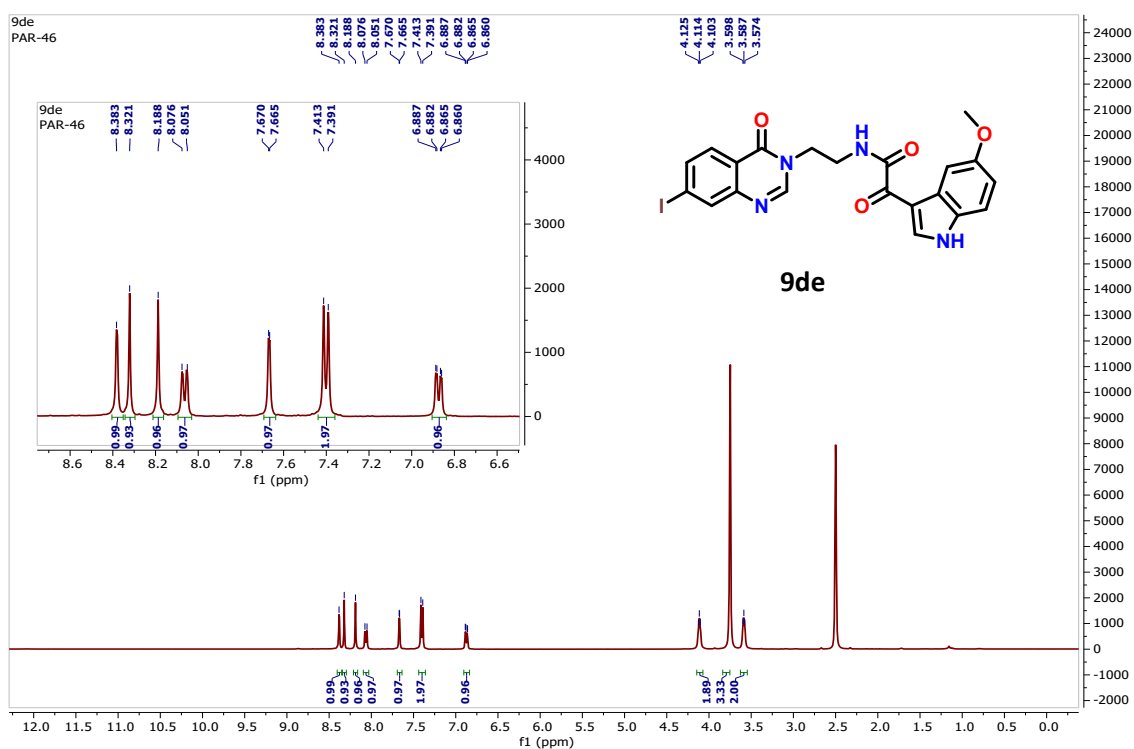
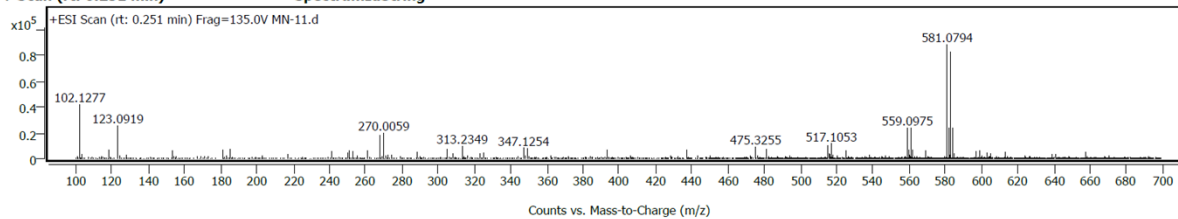
SpectrumIdString



Peak Spec

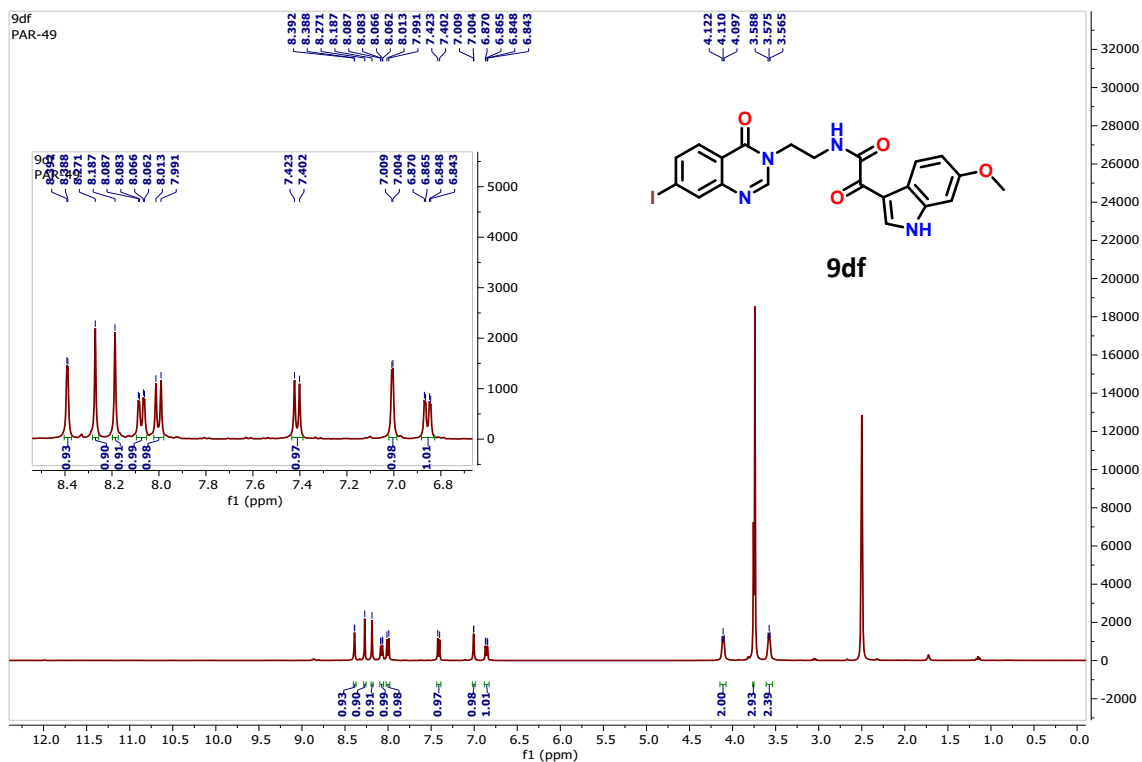
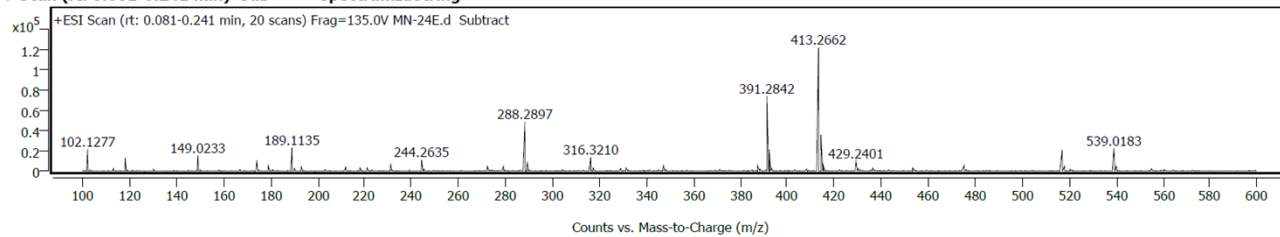
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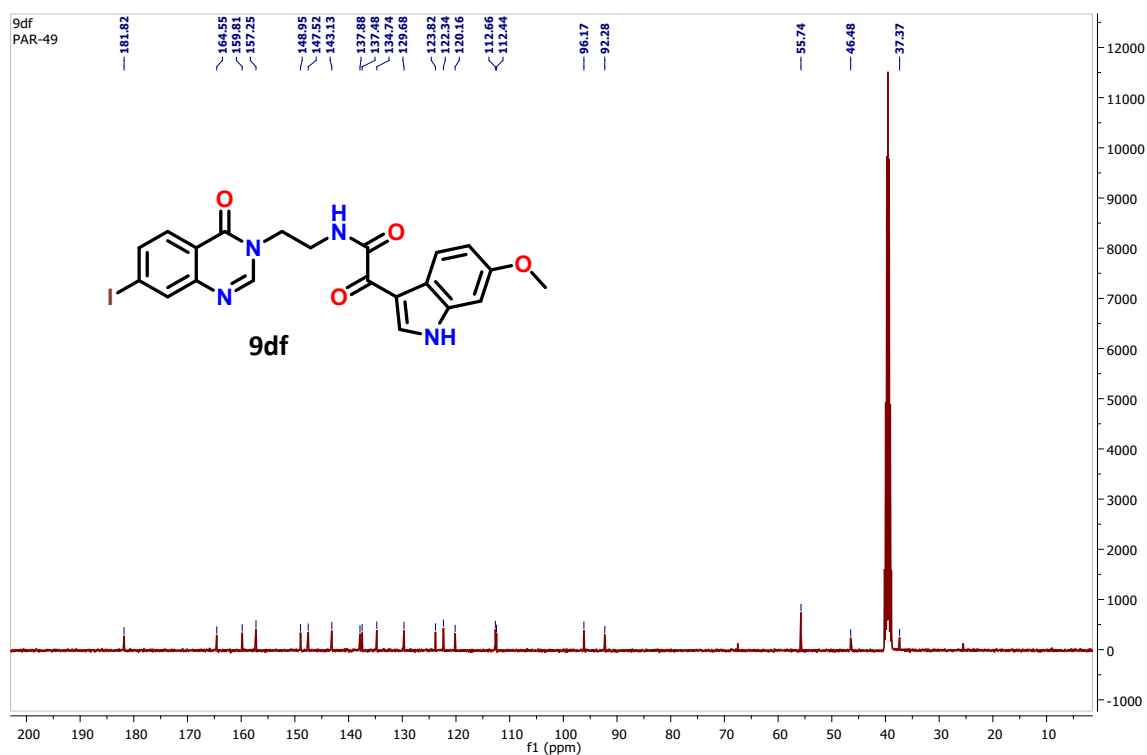
SpectrumIdString



Peak Spec

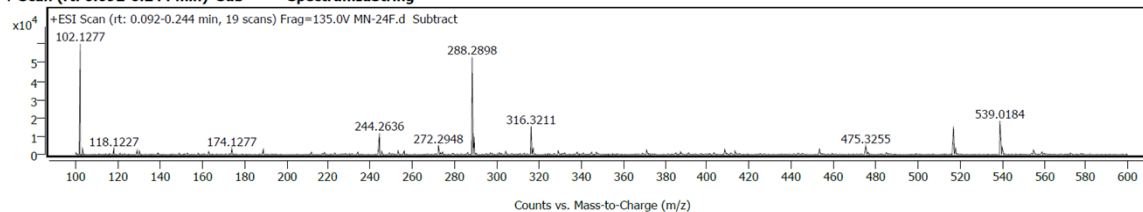
+ Scan (rt: 0.081-0.241 min) Sub SpectrumIdString





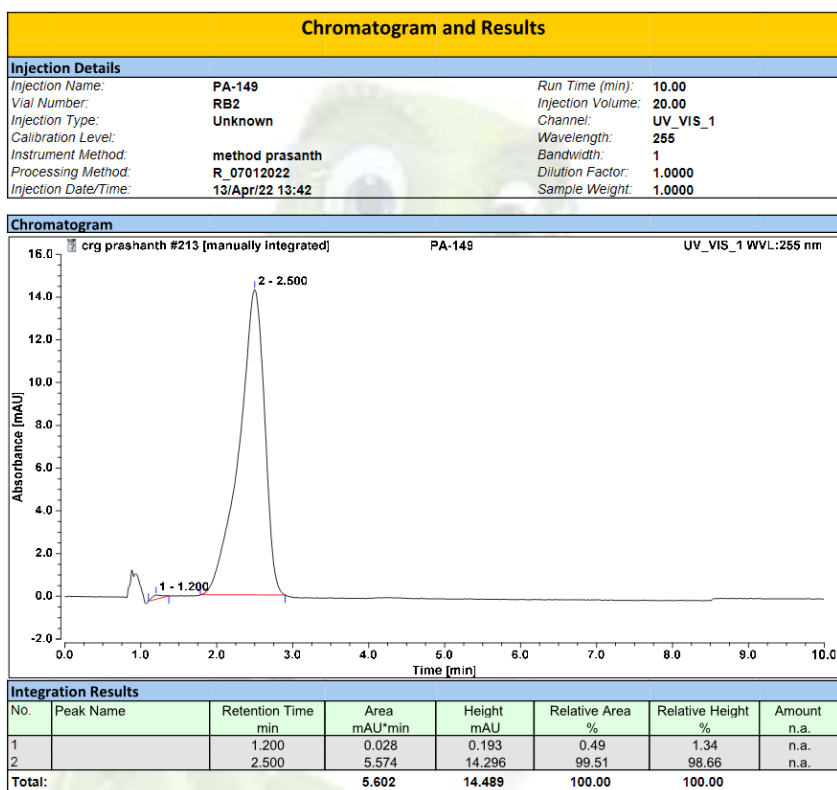
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+ Scan (rt: 0.092-0.244 min) Sub SpectrumIdString

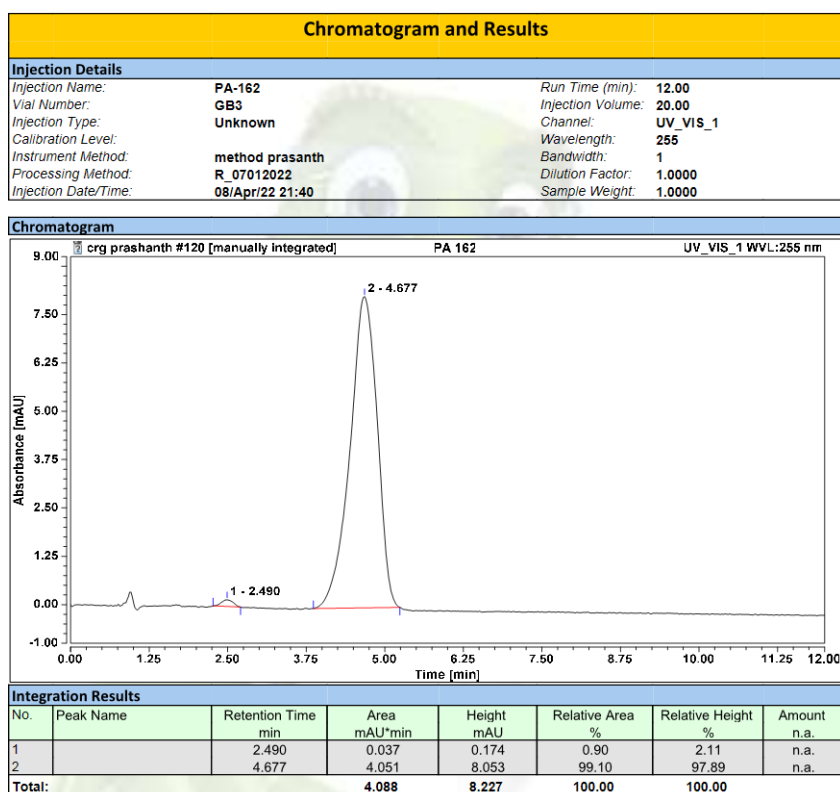


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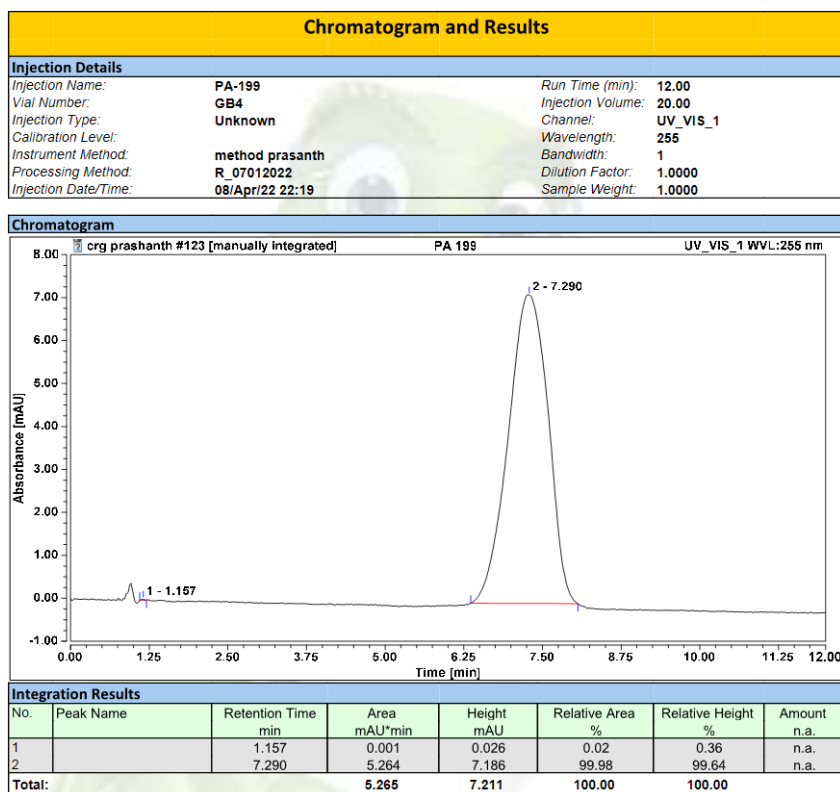
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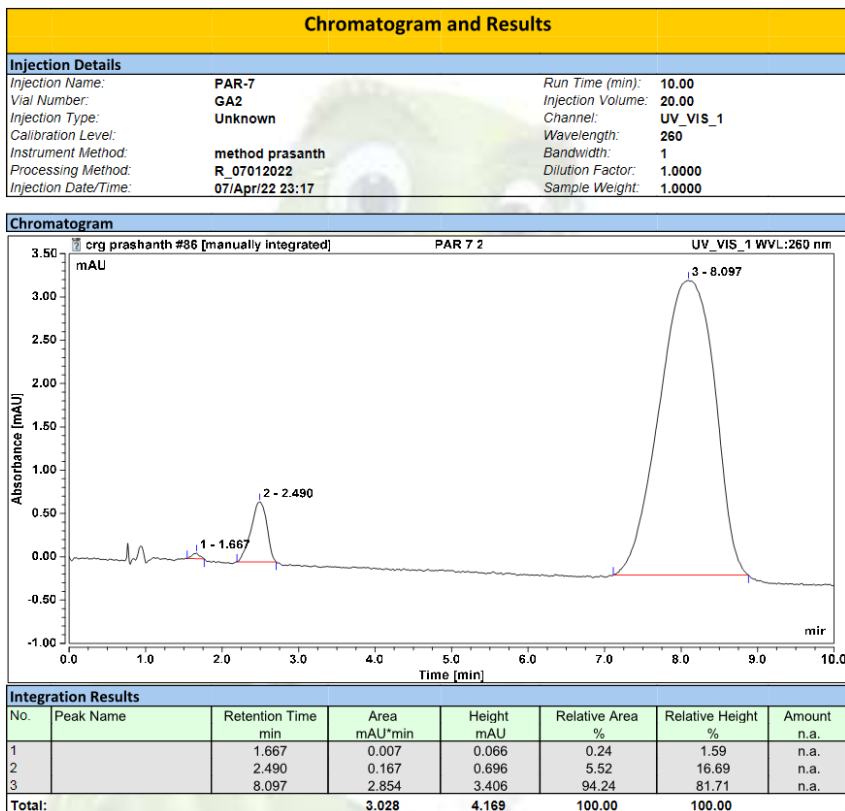
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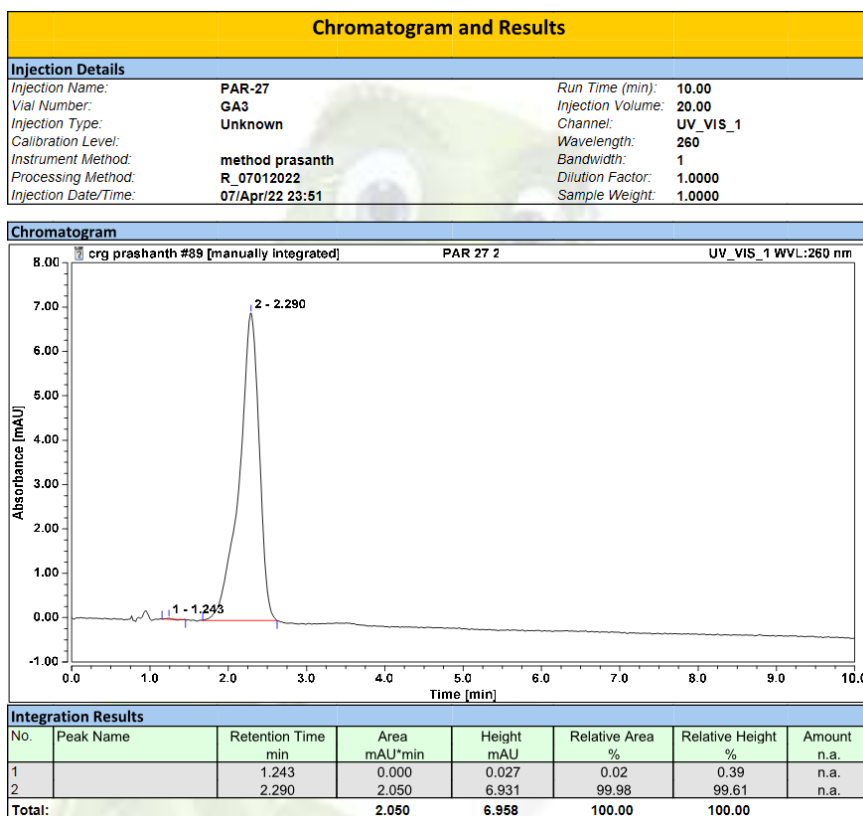
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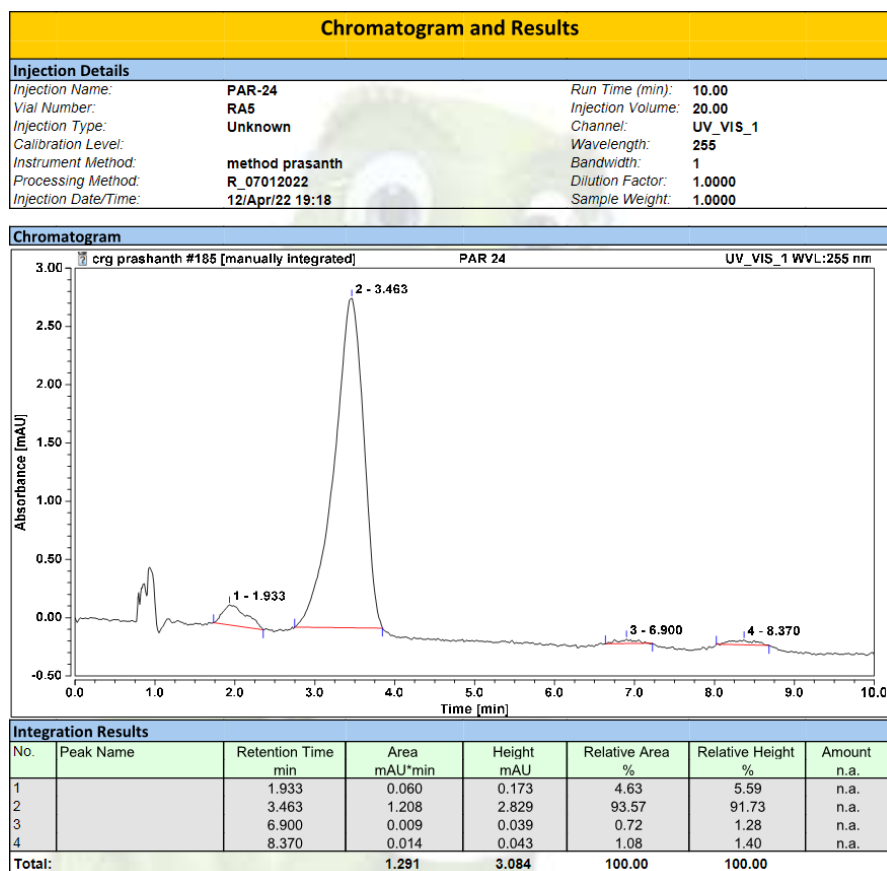
2-(1-(4-bromobenzyl)-1H-indol-3-yl)-2-oxo-N-(2-(4-oxoquinazolin-3(4H)-yl)ethyl)acetamide (9ad)



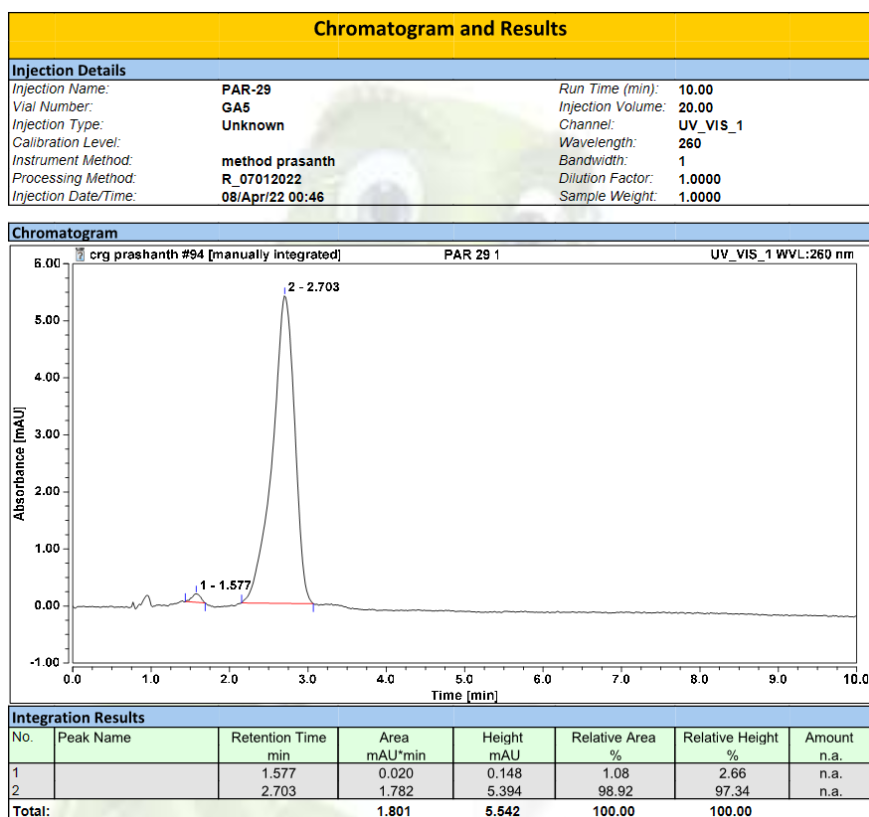
N-(2-(7-chloro-4-oxoquinazolin-3(4H)-yl)ethyl)-2-(1H-indol-3-yl)-2-oxoacetamide(9ba)



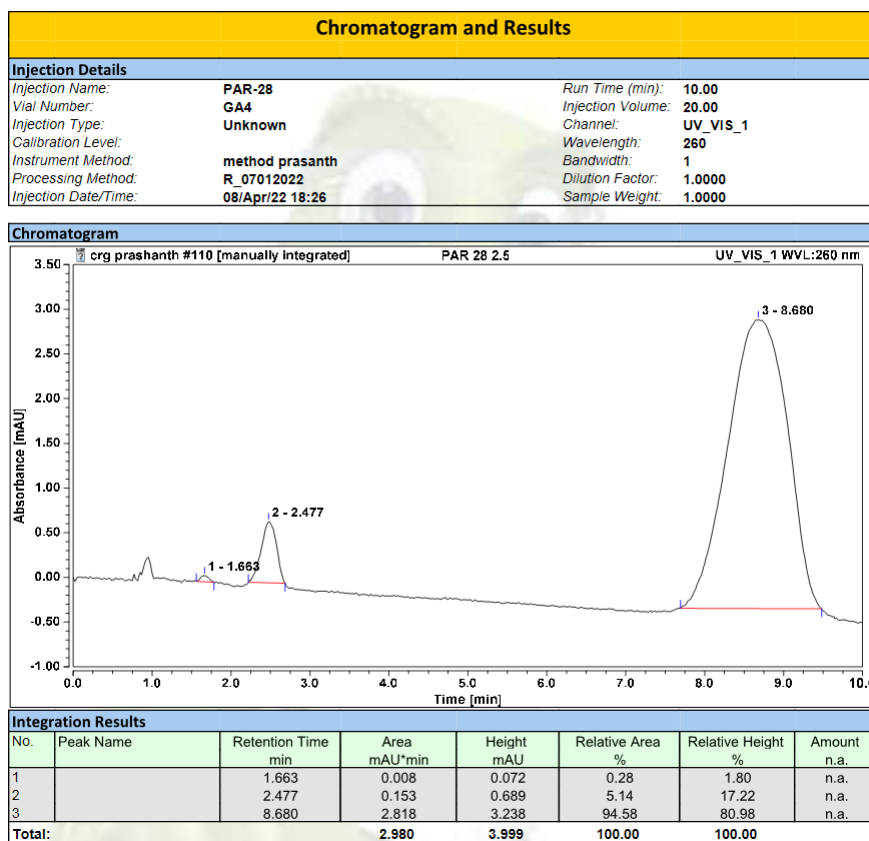
N-(2-(7-bromo-4-oxoquinazolin-3(4H)-yl)ethyl)-2-(1H-indol-3-yl)-2-oxoacetamide(9ca)



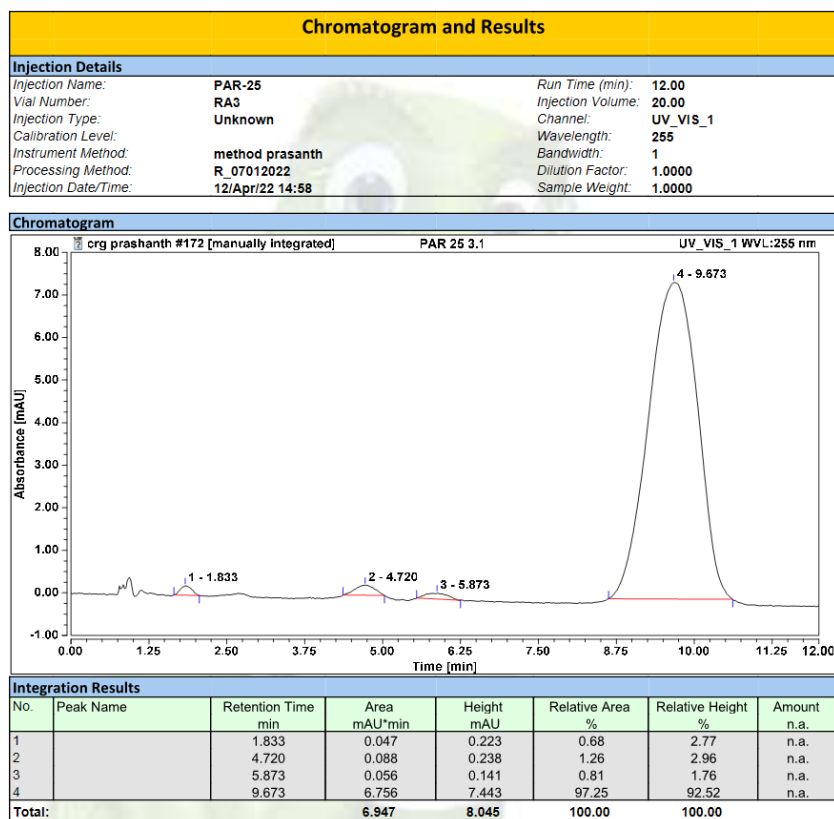
2-(1H-indol-3-yl)-N-(2-(7-iodo-4-oxoquinazolin-3(4H)-yl)ethyl)-2-oxoacetamide(9da)



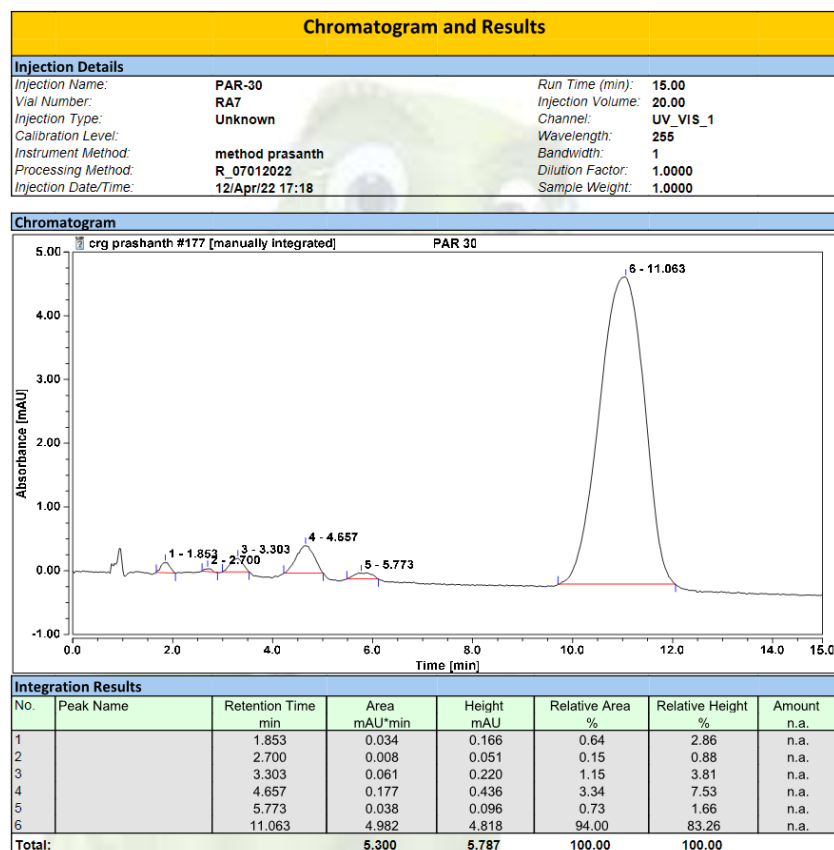
2-(1-benzyl-1H-indol-3-yl)-N-(2-(7-chloro-4-oxoquinazolin-3(4H)-yl)ethyl)-2-oxoacetamide (9bb)



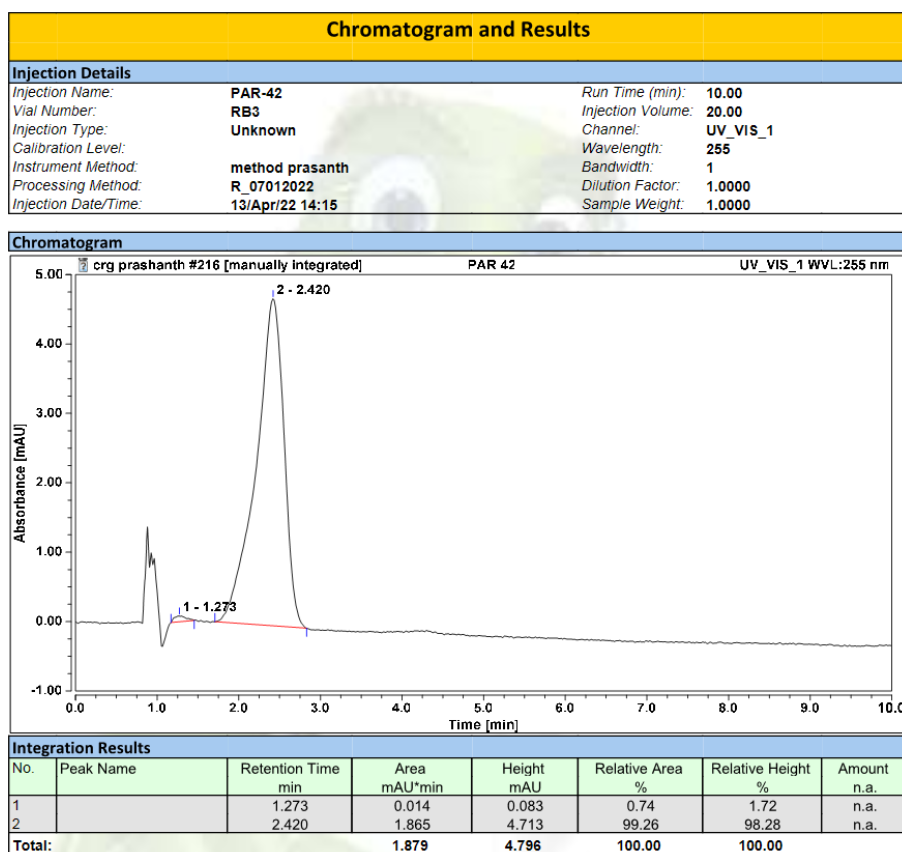
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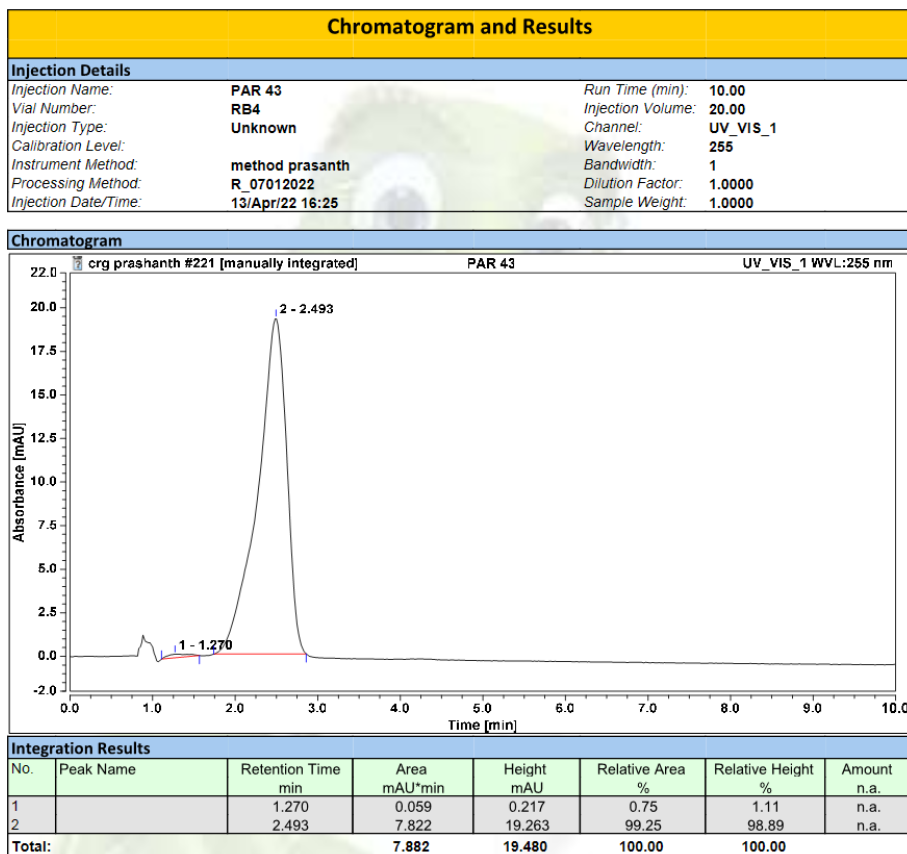
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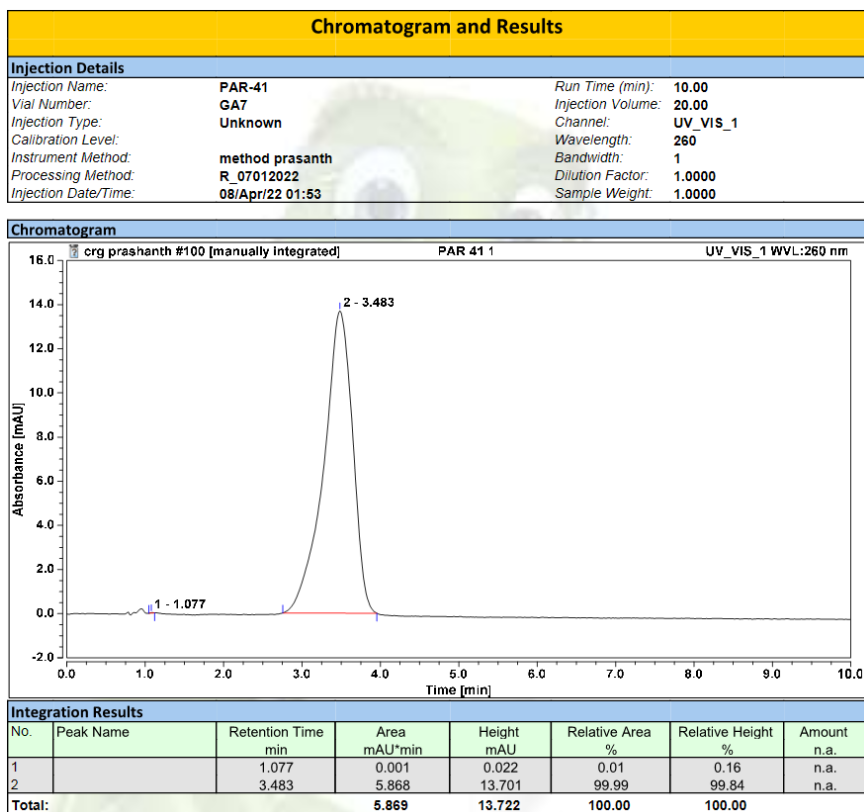
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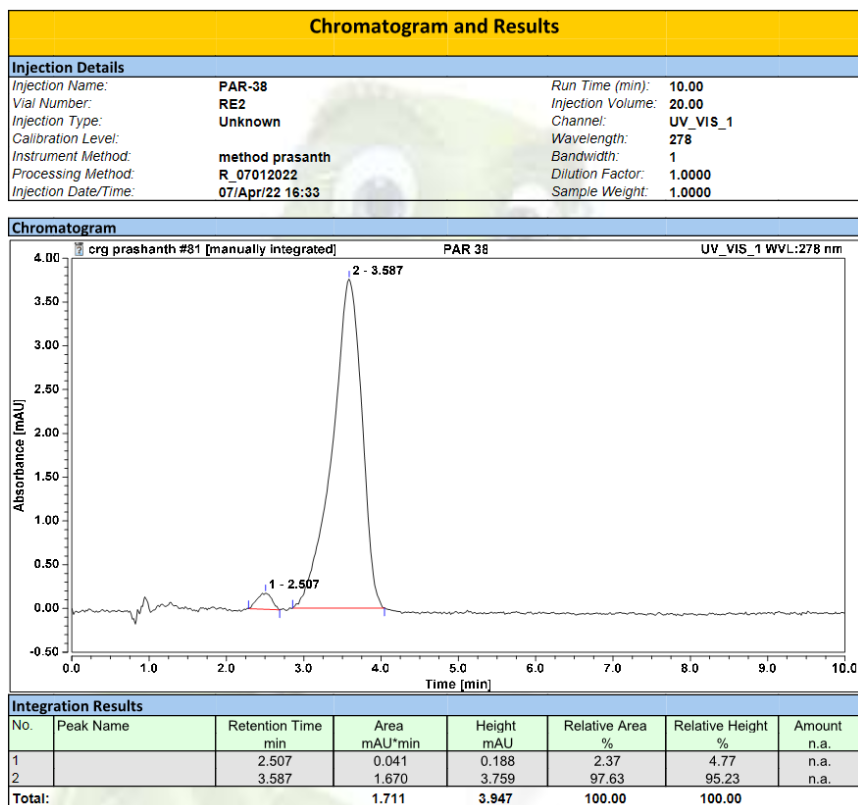
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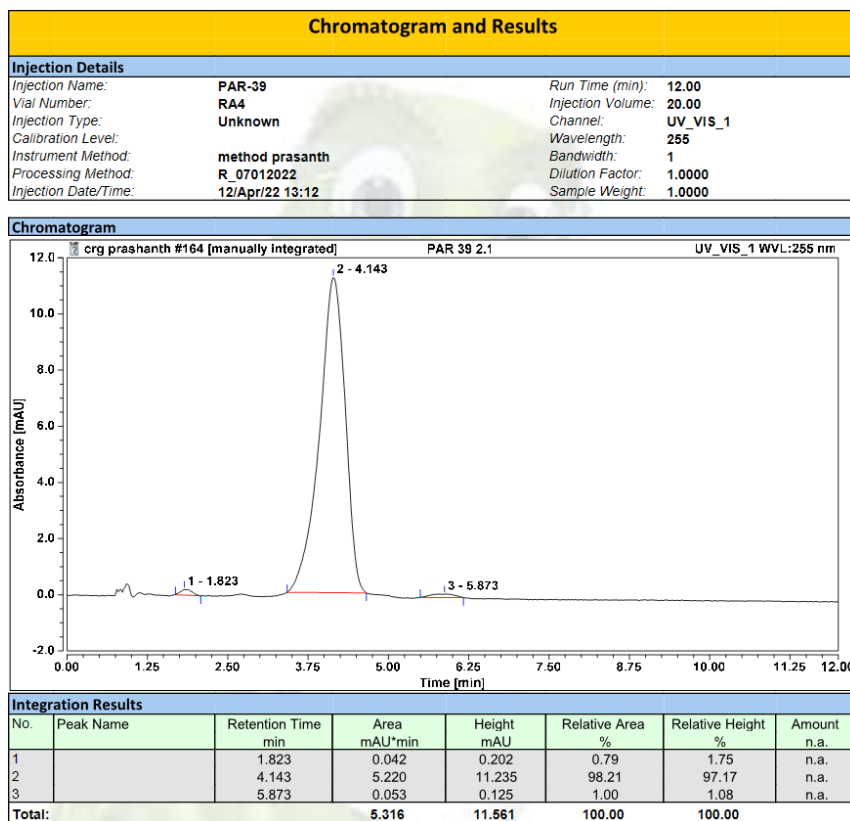
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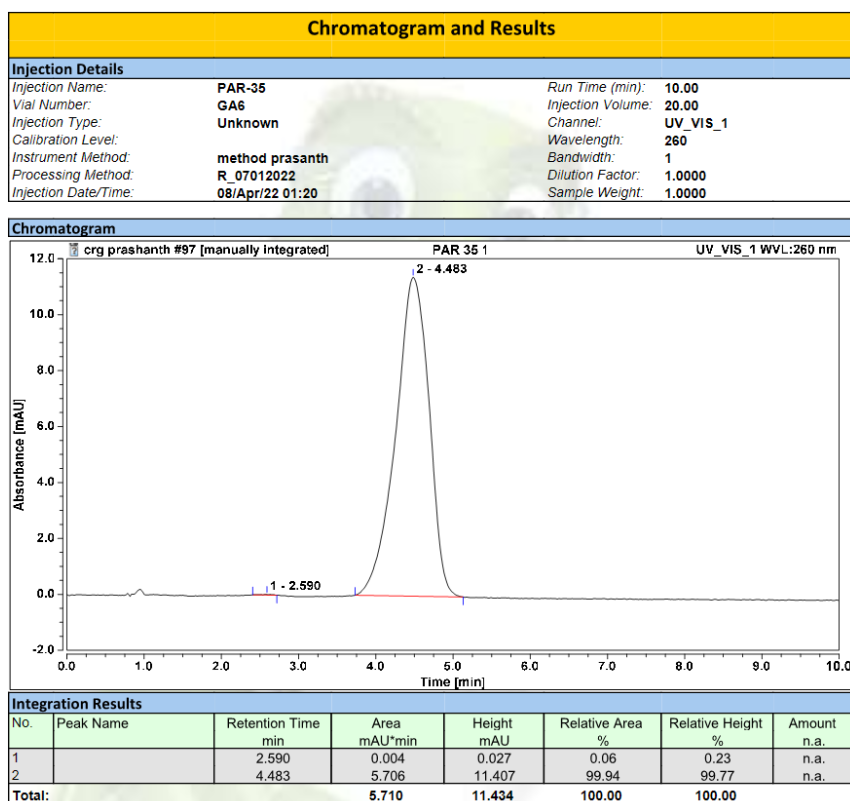
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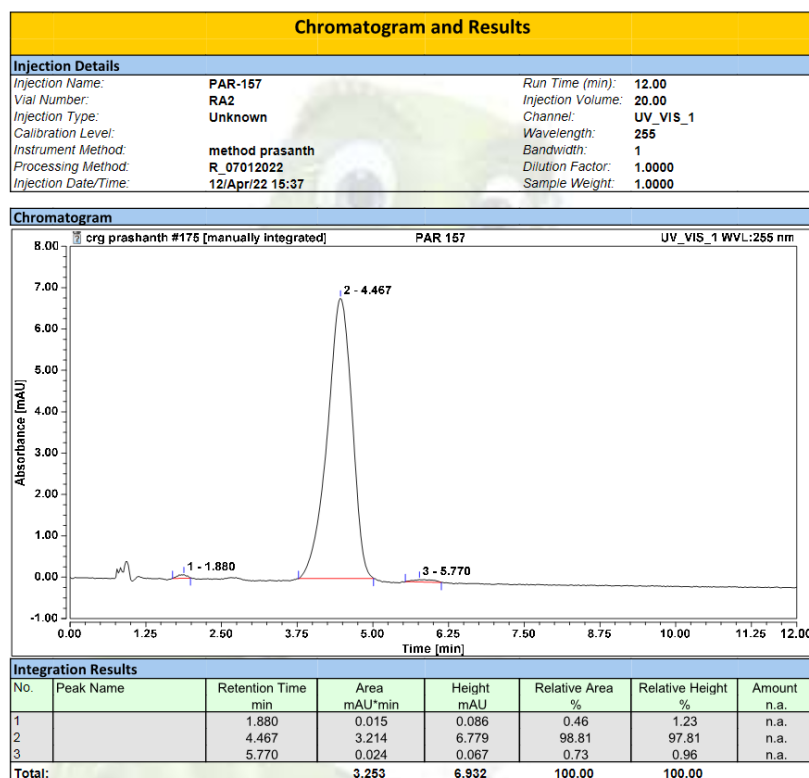
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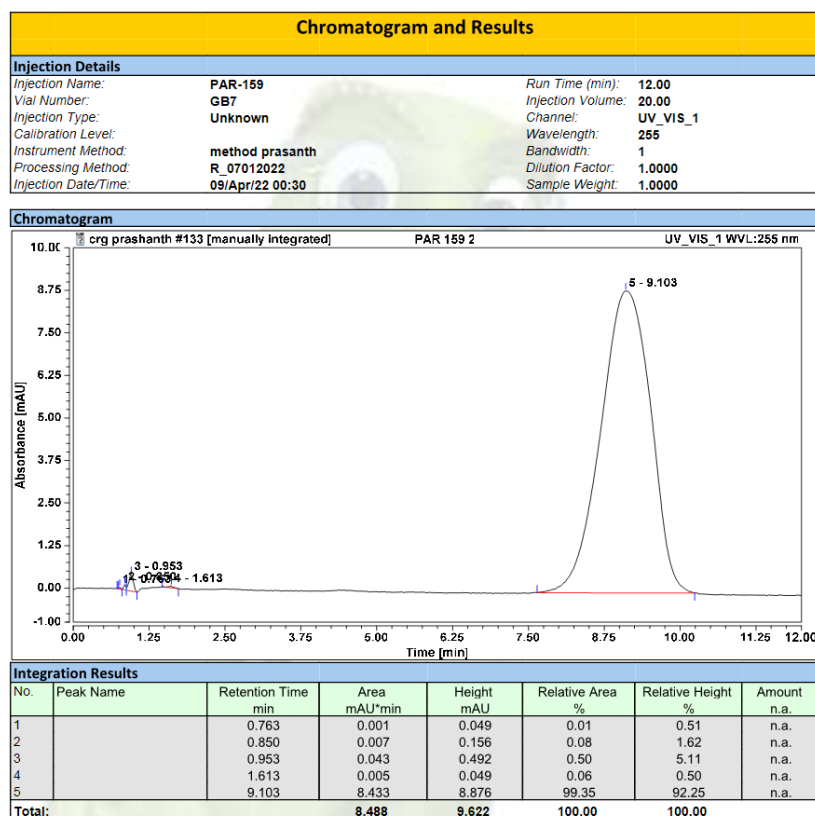
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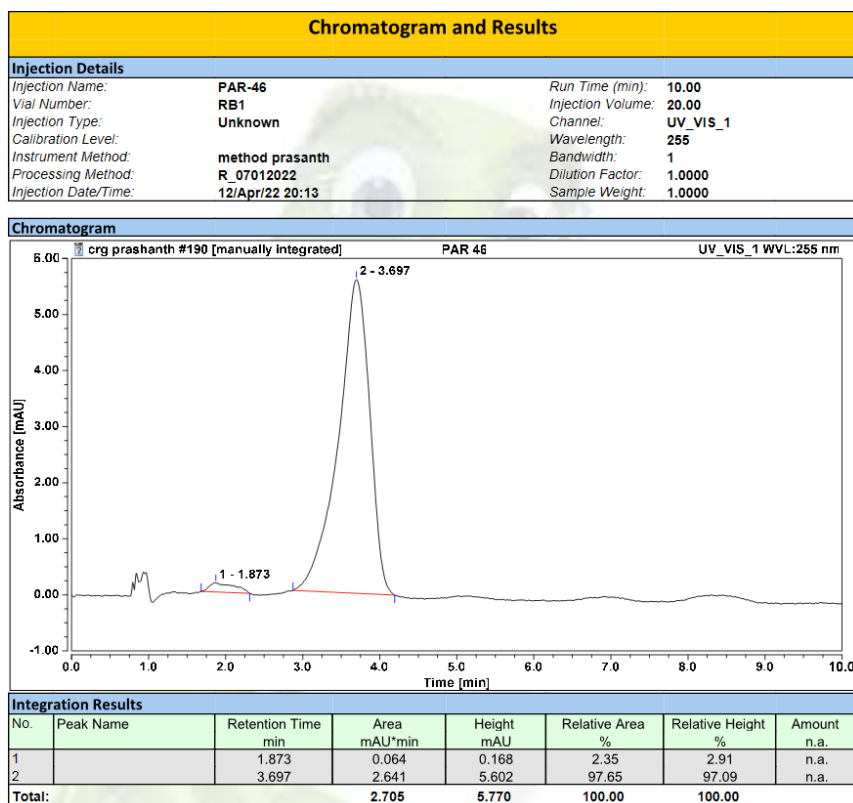
2-(1-benzyl-6-methoxy-1H-indol-3-yl)-2-oxo-N-(2-(4-oxoquinazolin-3(4H)-yl)ethyl)acetamide (9ak)



2-(1-benzyl-6-methoxy-1H-indol-3-yl)-N-(2-(7-bromo-4-oxoquinazolin-3(4H)-yl)ethyl)-2-oxoacetamide (9ck)



N-(2-(7-iodo-4-oxoquinazolin-3(4H)-yl)ethyl)-2-(5-methoxy-1H-indol-3-yl)-2-oxoacetamide(9de)



N-(2-(7-iodo-4-oxoquinazolin-3(4H)-yl)ethyl)-2-(6-methoxy-1H-indol-3-yl)-2-oxoacetamide(9df)

