

Supporting Information

One-pot Synthesis of 3-Substituted-3-Hydroxyindolin-2-ones: Three Component Coupling of *N*-Protected isatin, Aryne precursor and 1, 3-Cyclodione under Metal-free Conditions

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^a*Applied Organic Chemistry Group, Chemical Science and Technology Division, CSIR-North East Institute of Science and Technology, Jorhat 785006, India*

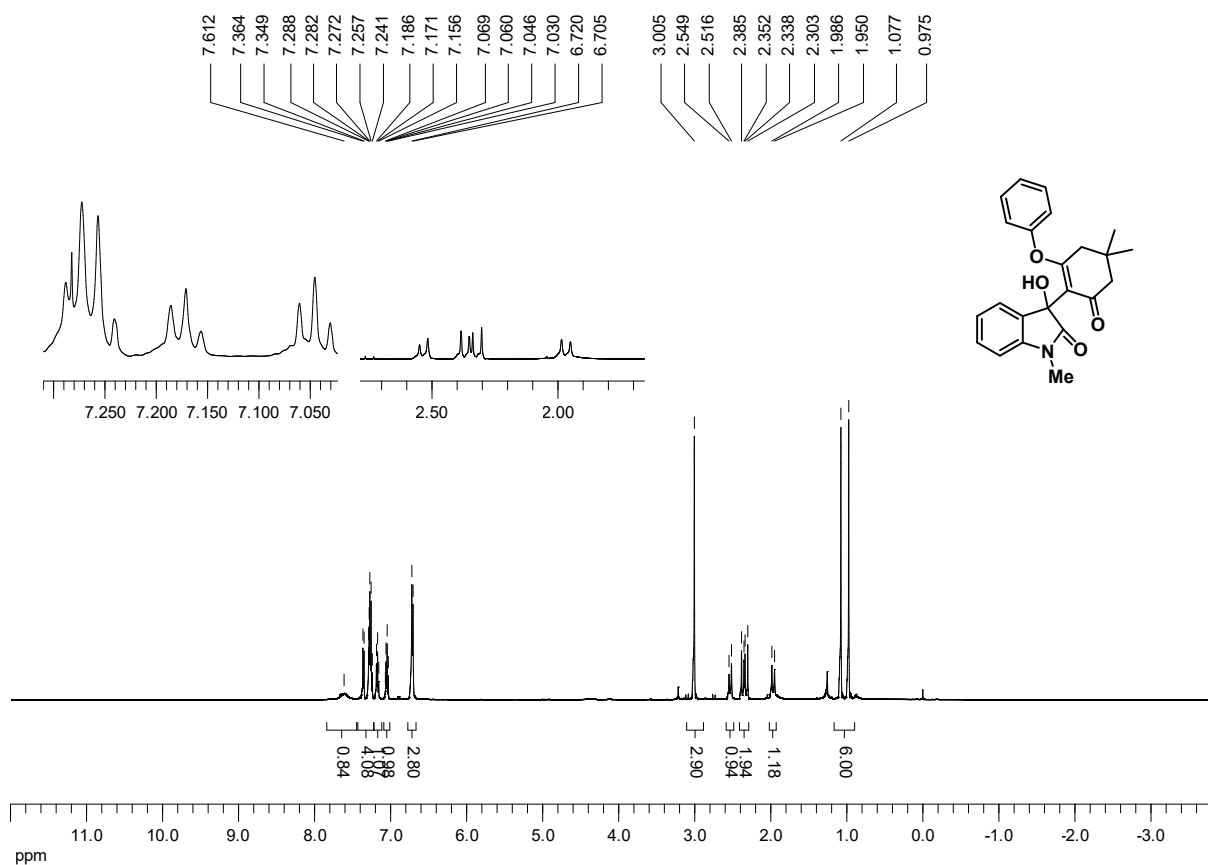
^b*Academy of Scientific and Innovative Research (AcSIR), Ghaziabad, U.P.-201002, India*

^c*Department of Chemistry, Indian Institute of Technology Guwahati, Guwahati-781039, India*

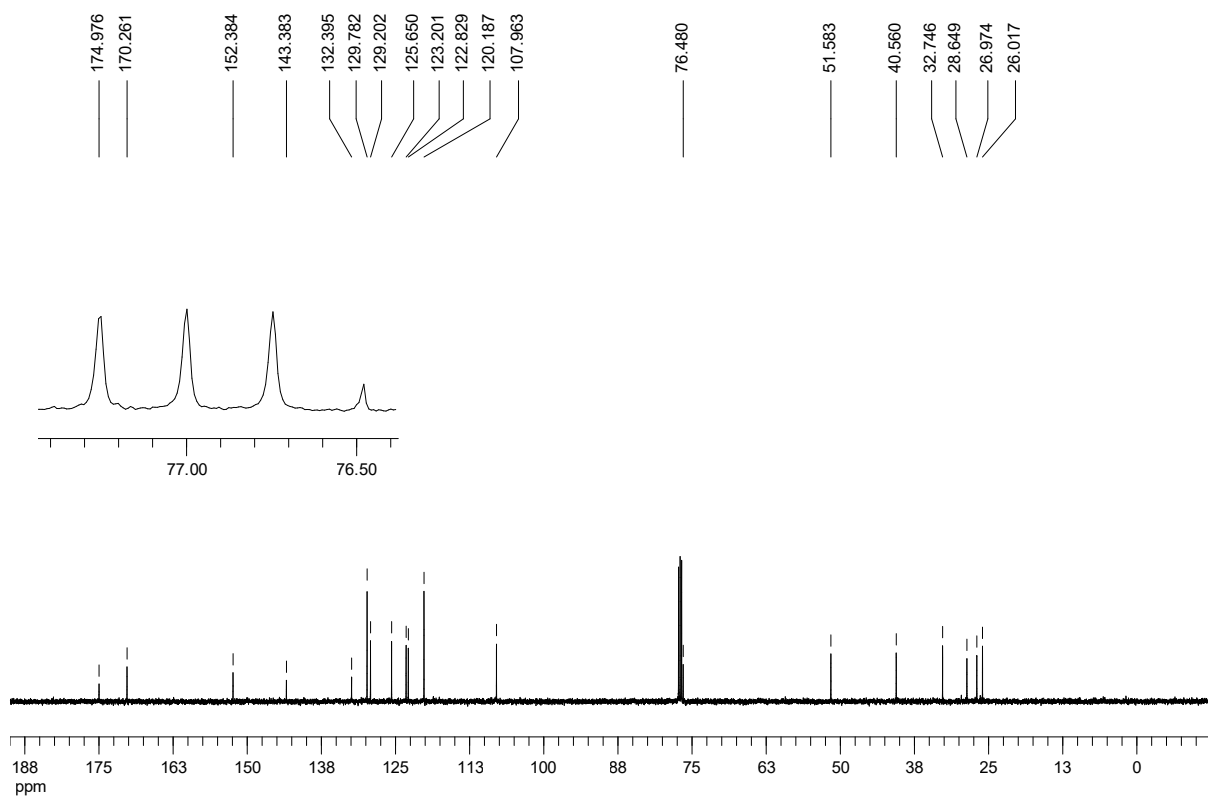
Email: gogoipranj@yahoo.co.uk; gogoipranj@gmail.com

Copies of ¹H, ¹³C, HRMS spectra and Crystallographic data

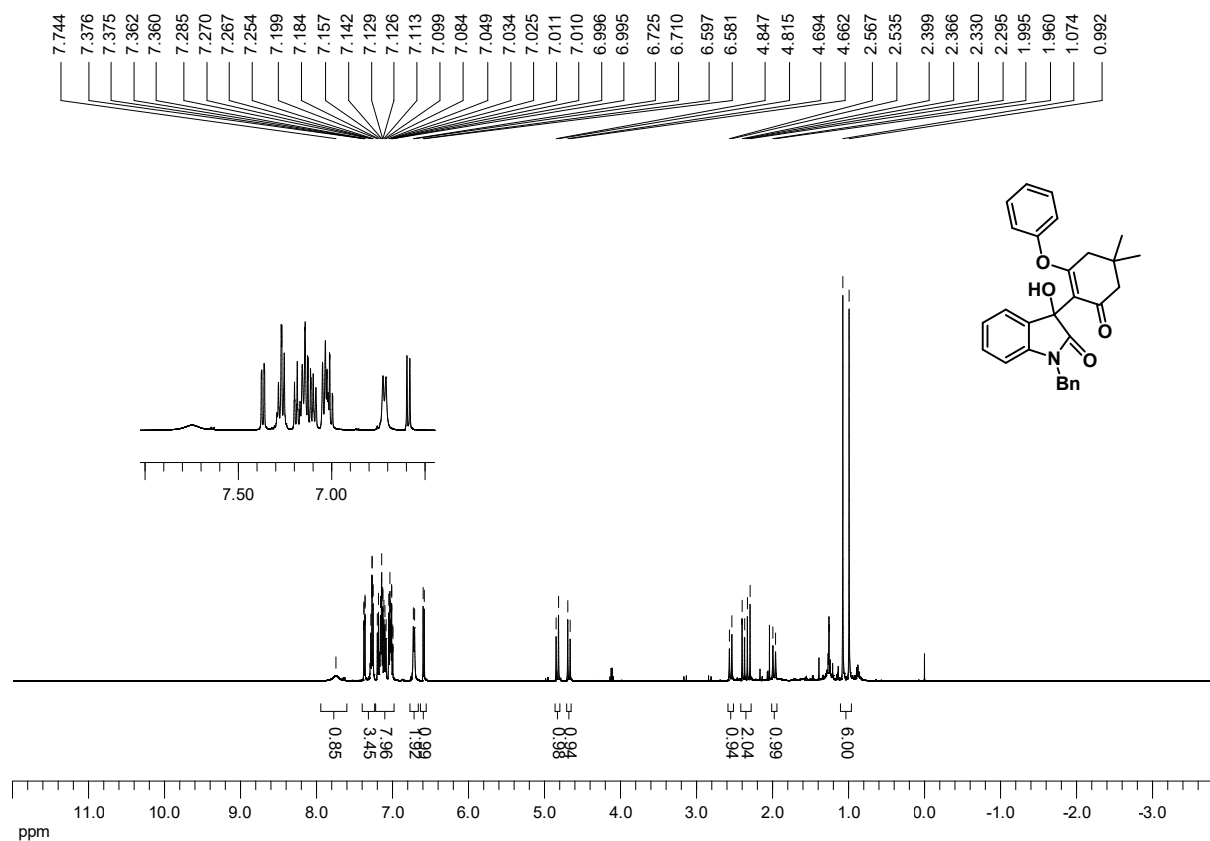
¹H NMR of **4aaa** (CDCl₃, 500 MHz)



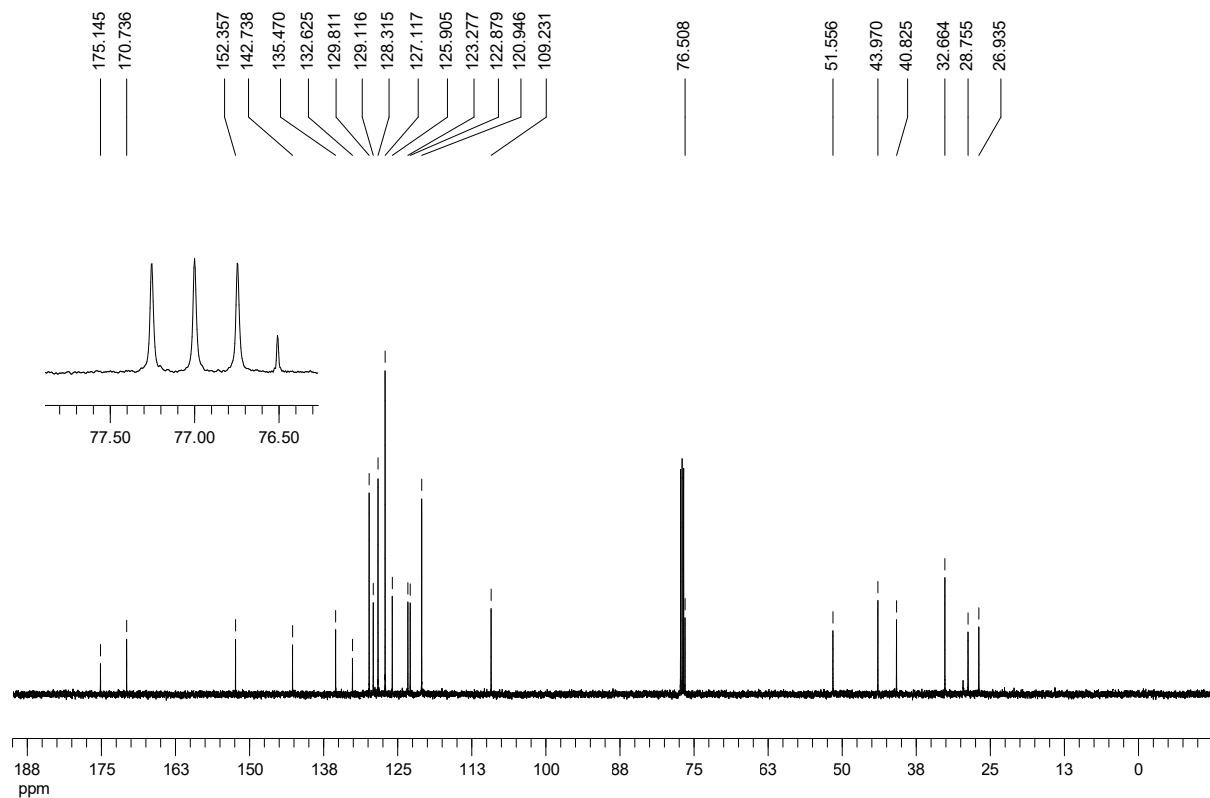
¹³C NMR of **4aaa** (CDCl₃, 126 MHz)



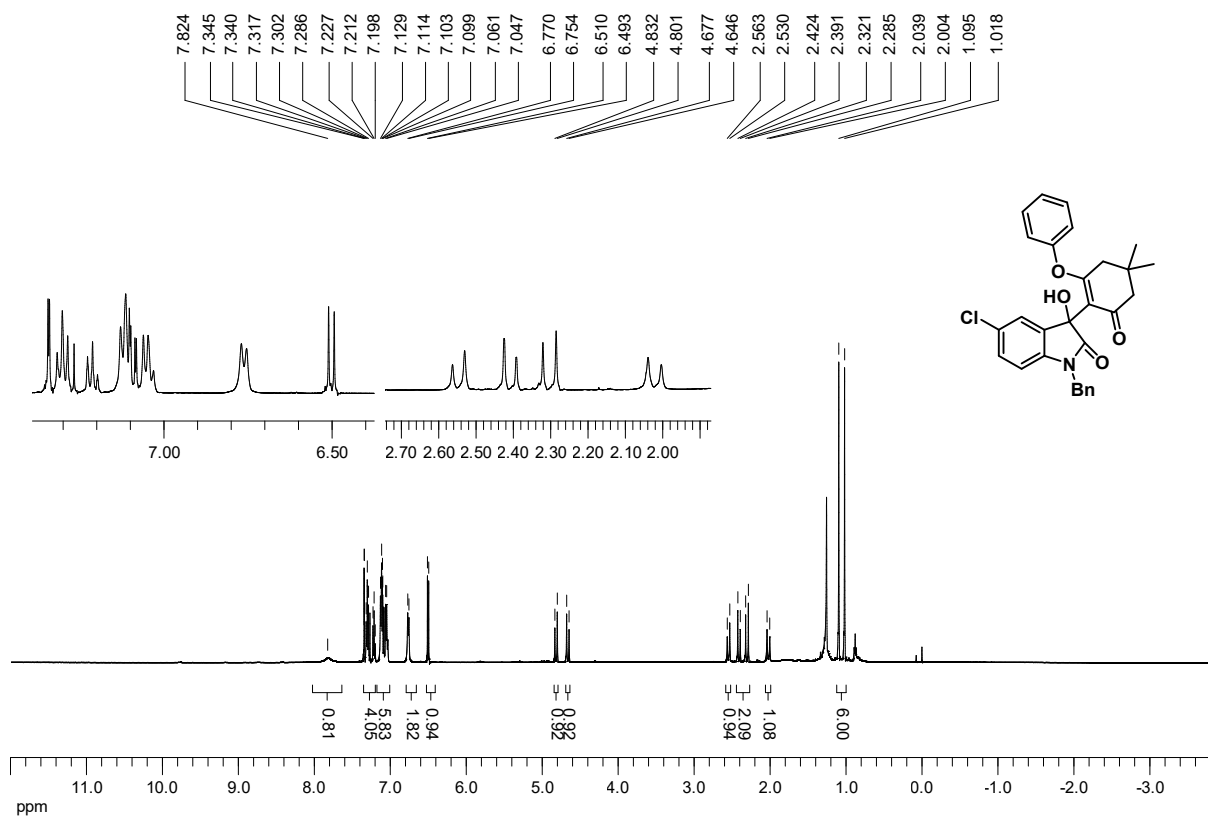
¹H NMR of **4baa** (CDCl₃, 500 MHz)



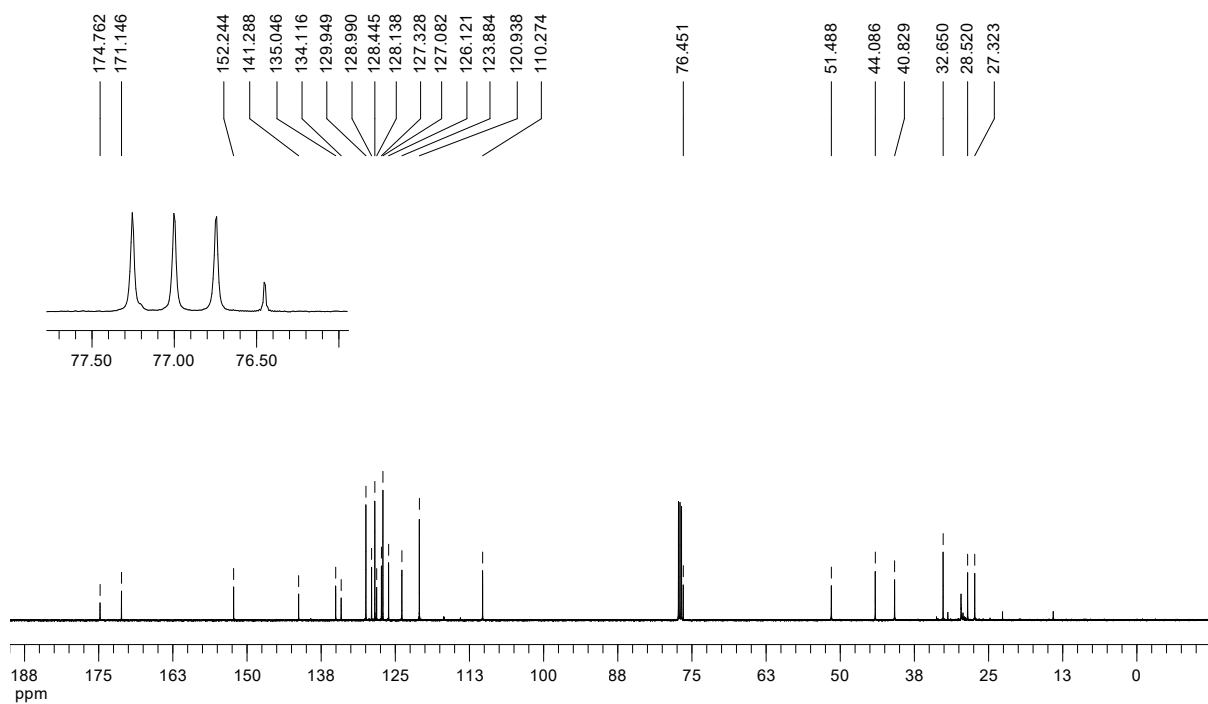
¹³C NMR of **4baa** (CDCl₃, 126 MHz)



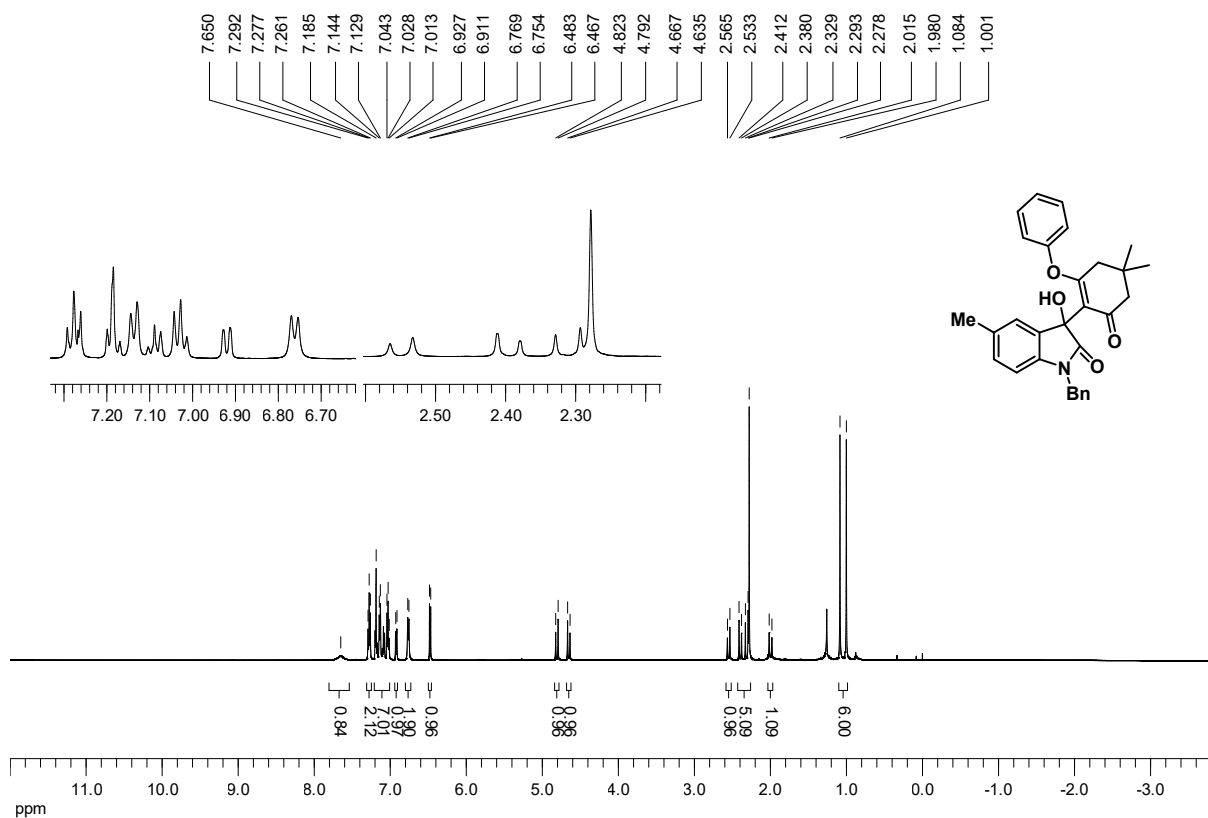
¹H NMR of **4caa** (CDCl₃, 500 MHz)



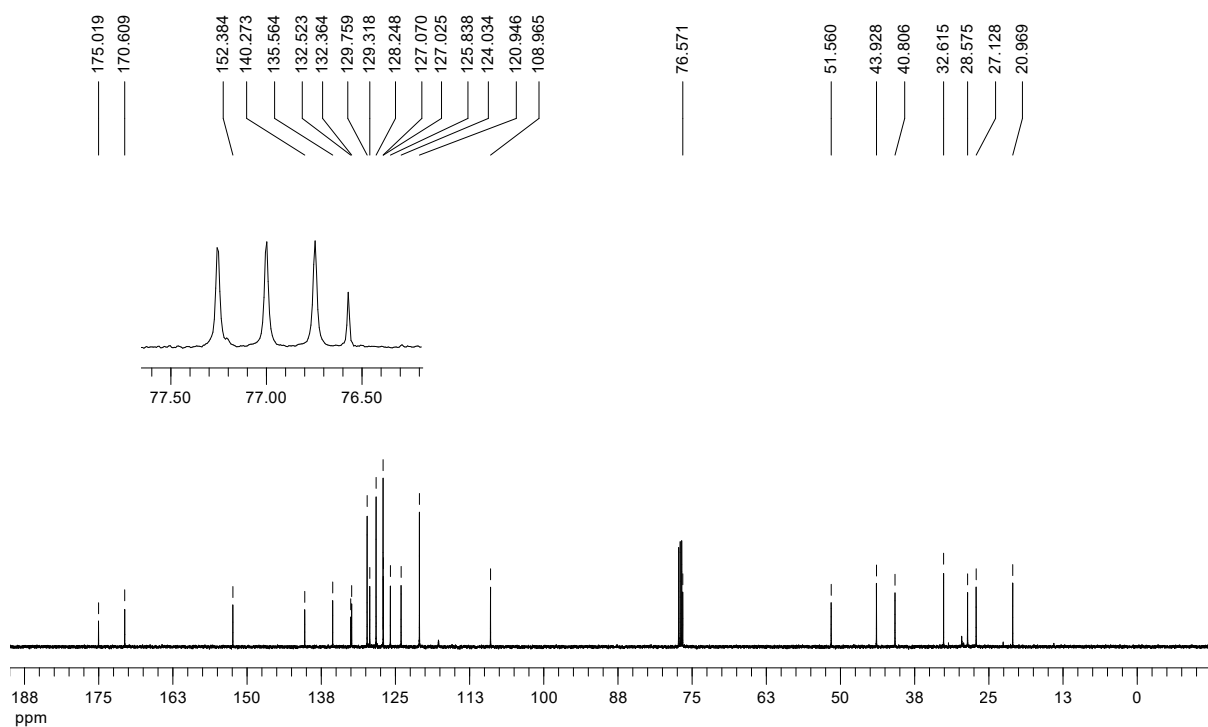
¹³C NMR of **4caa** (CDCl₃, 126 MHz)



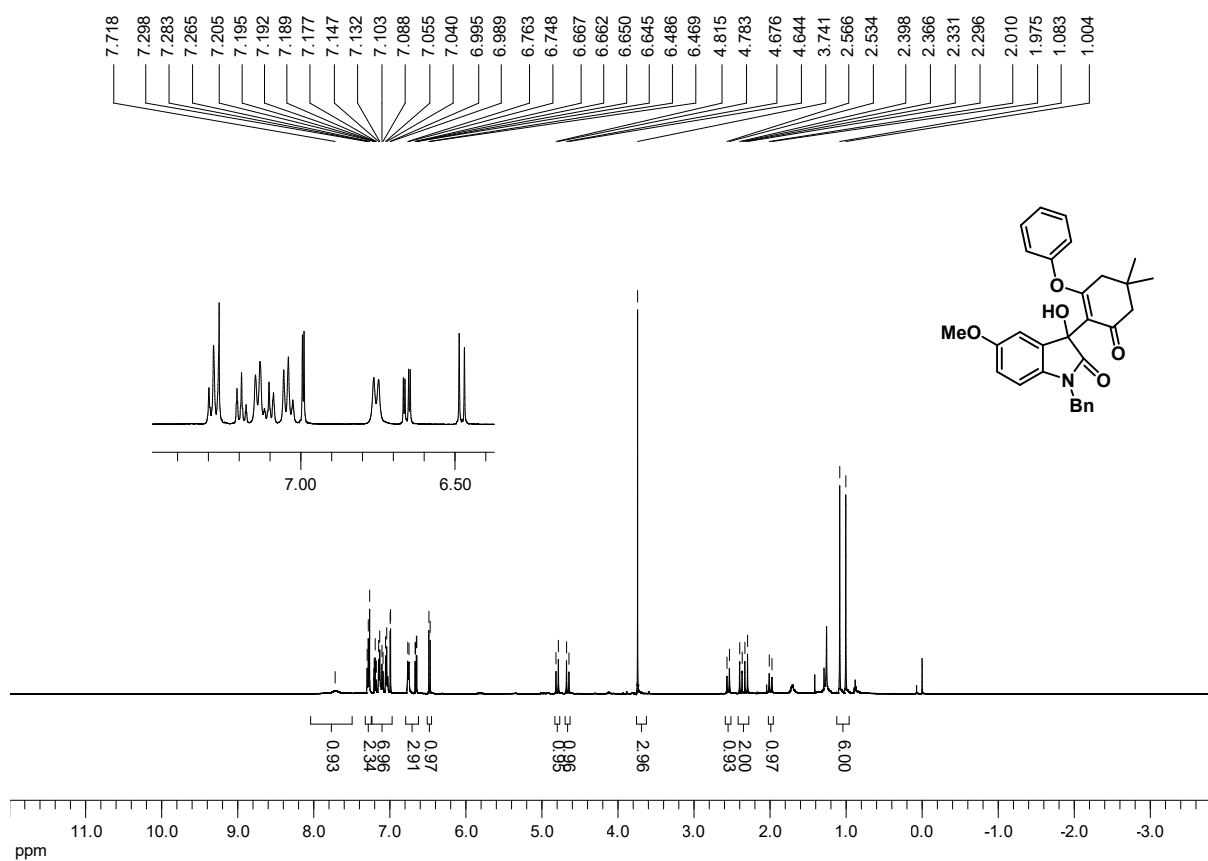
¹H NMR of **4daa** (CDCl₃, 500 MHz)



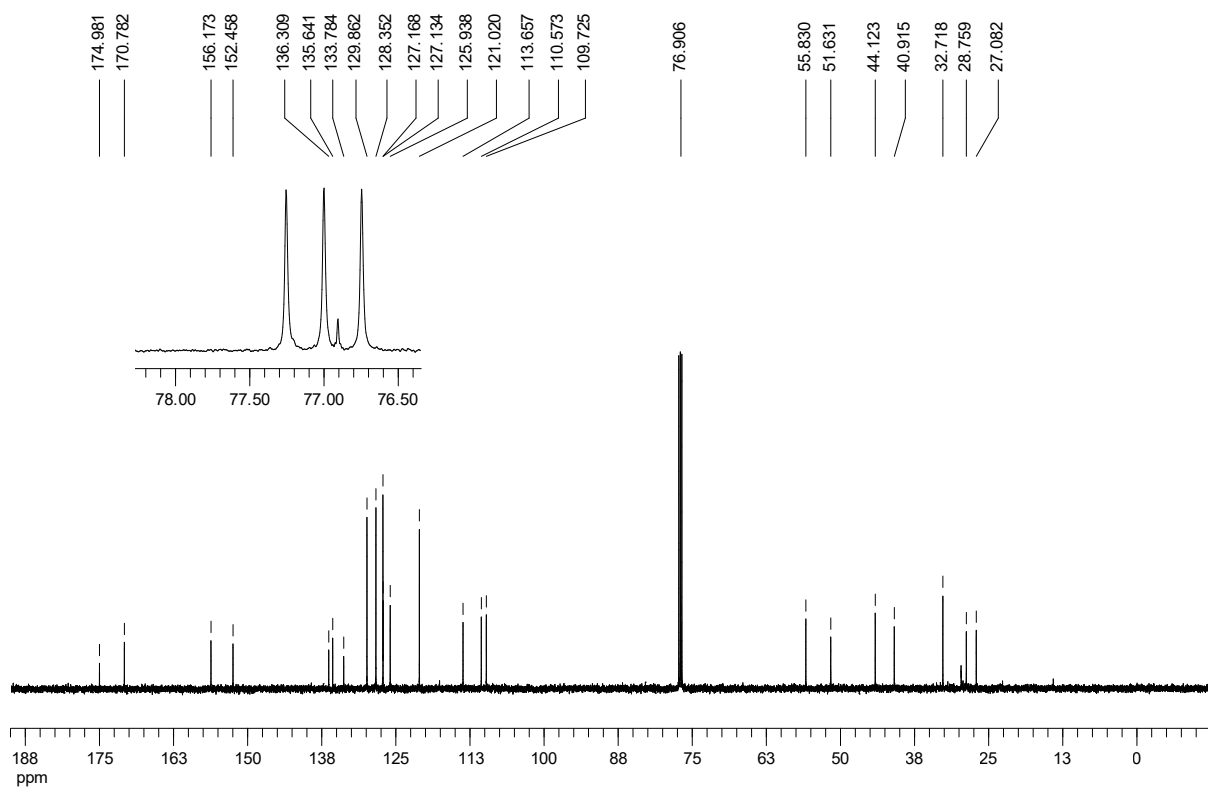
¹³C NMR of **4daa** (CDCl₃, 126 MHz)



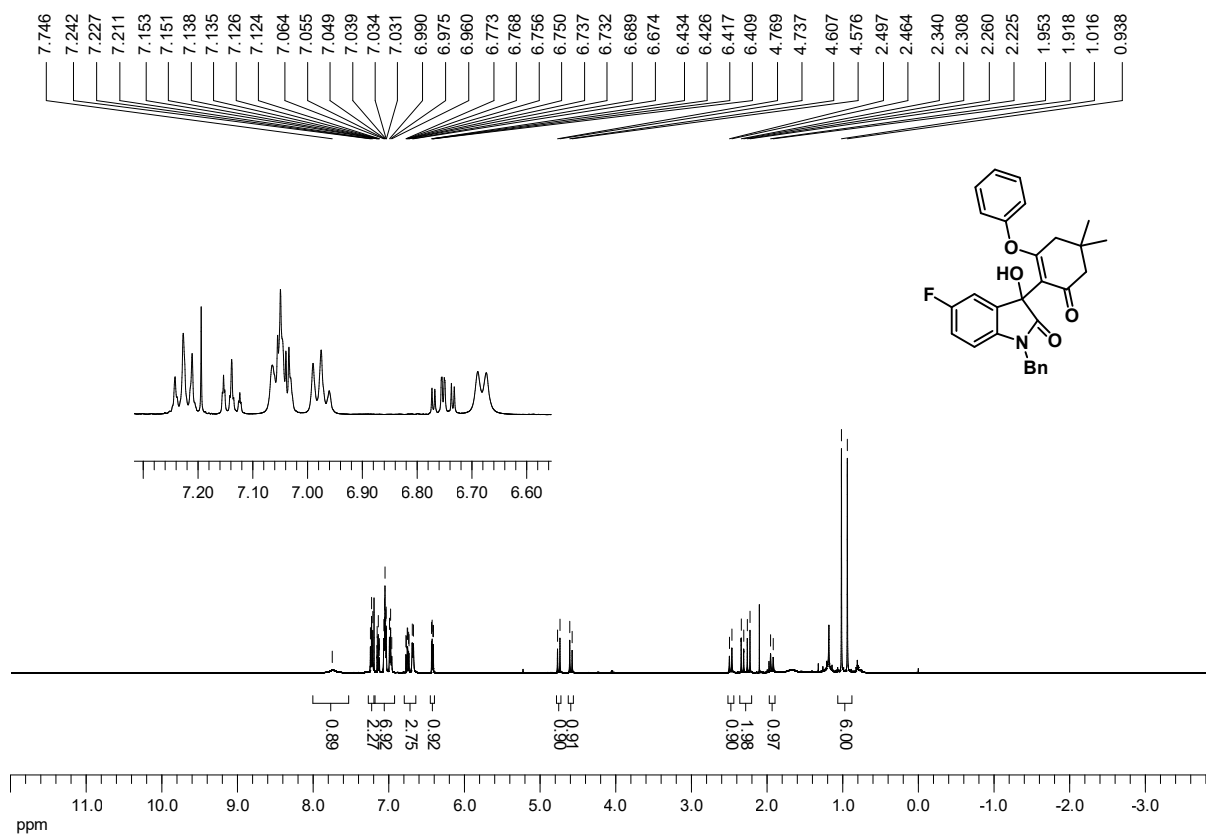
¹H NMR of **4eaa** (CDCl₃, 500 MHz)



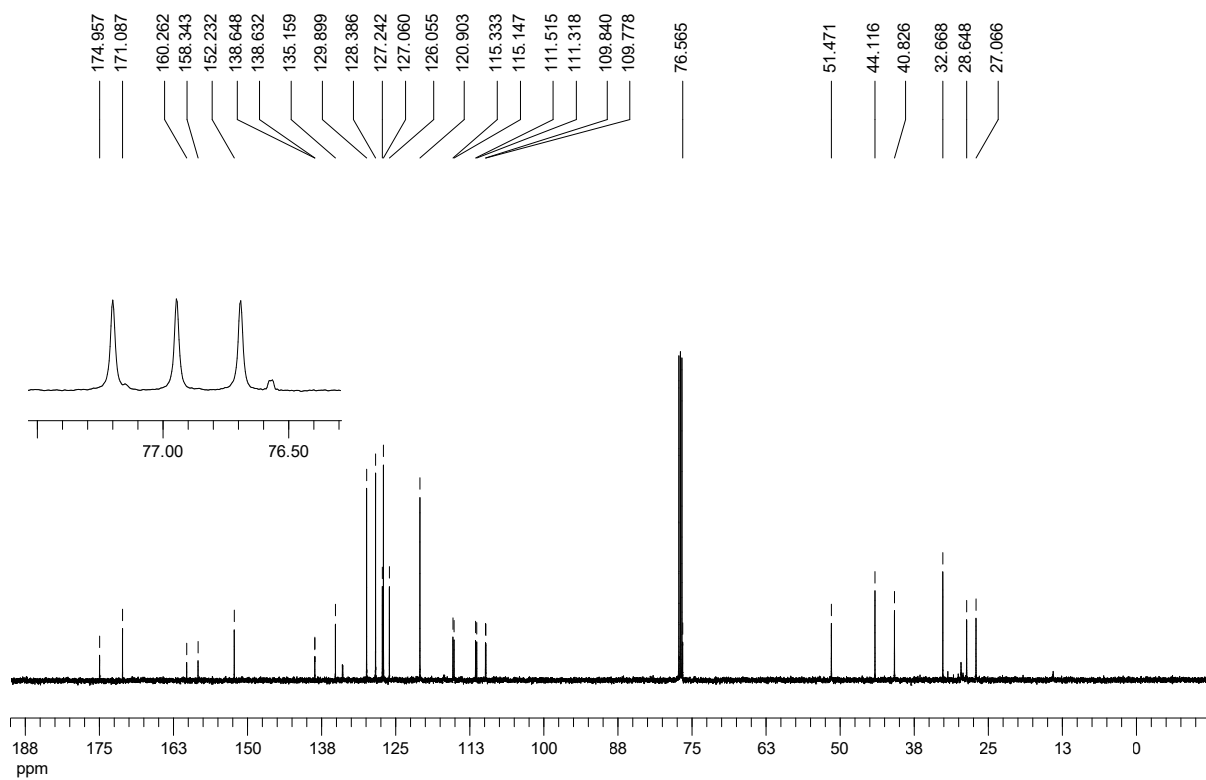
¹³C NMR of **4eaa** (CDCl₃, 126 MHz)



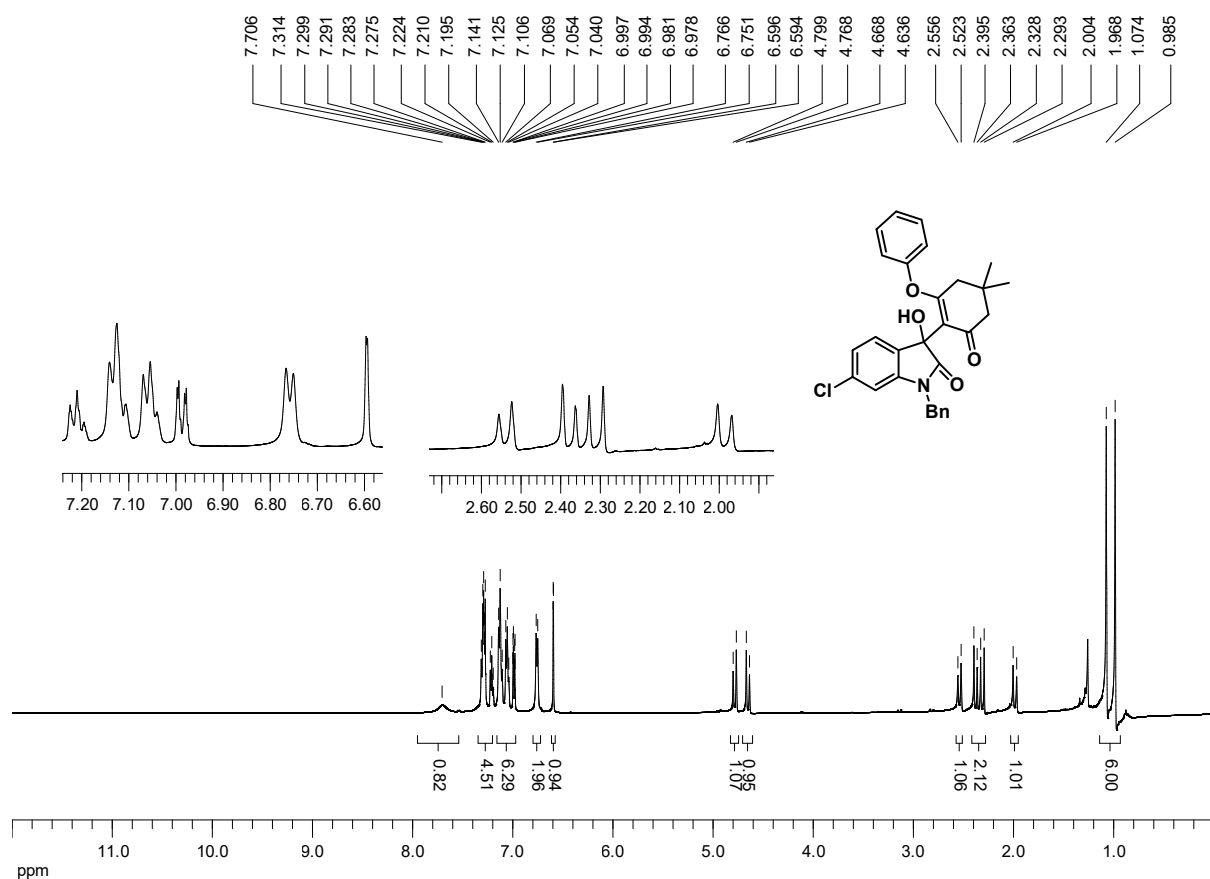
¹H NMR of **4faa** (CDCl₃, 500 MHz)



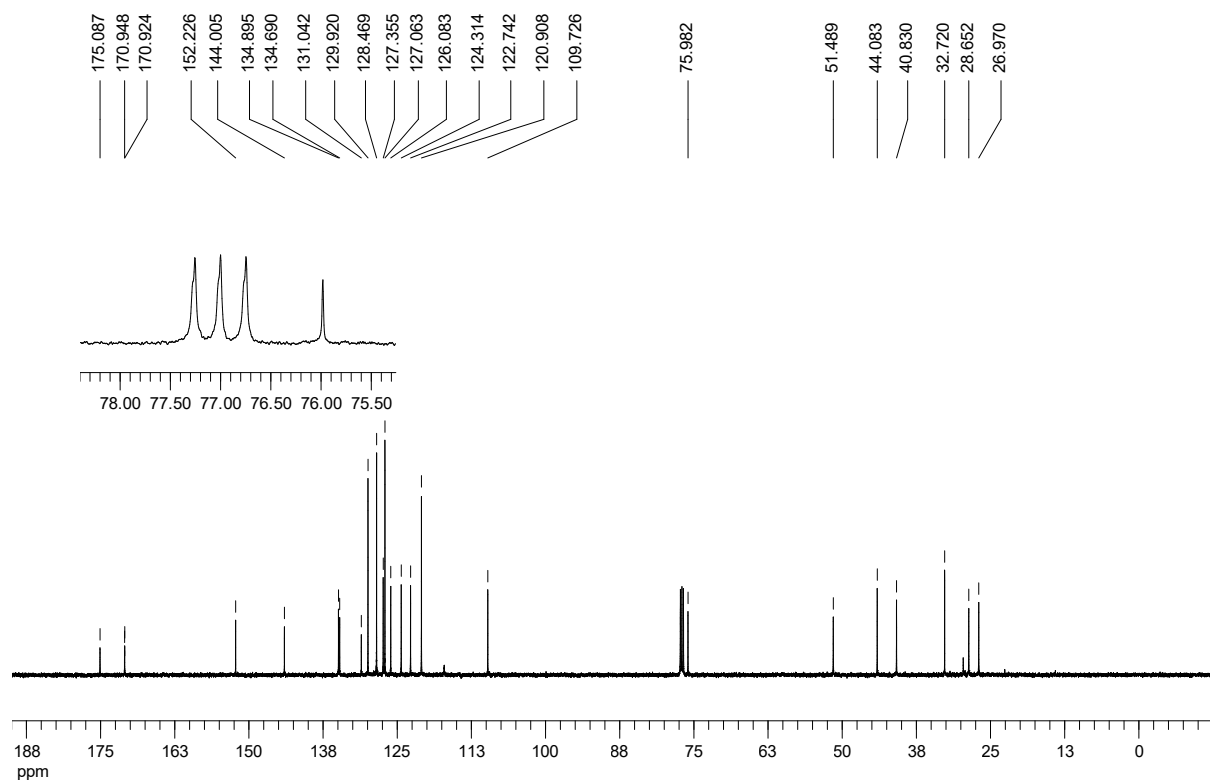
¹³C NMR of **4faa** (CDCl₃, 126 MHz)



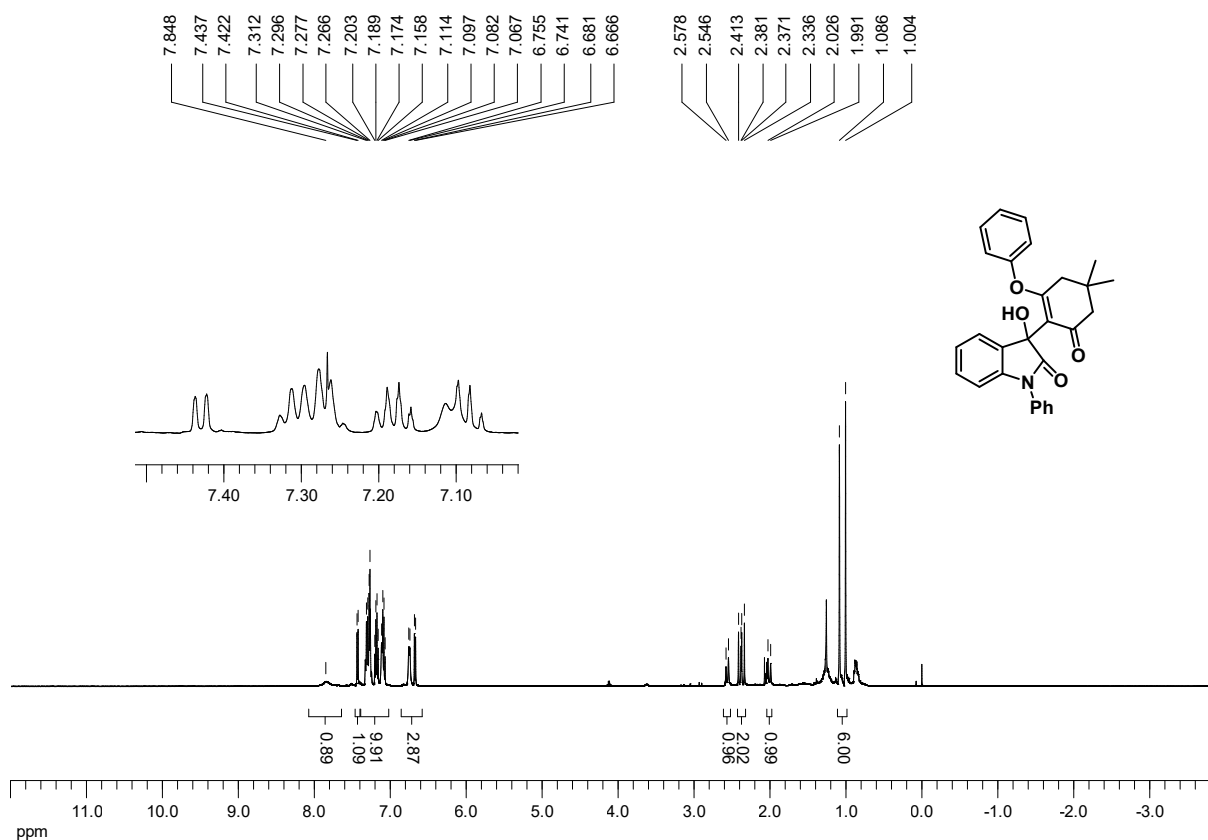
¹H NMR of **4gaa** (CDCl₃, 500 MHz)



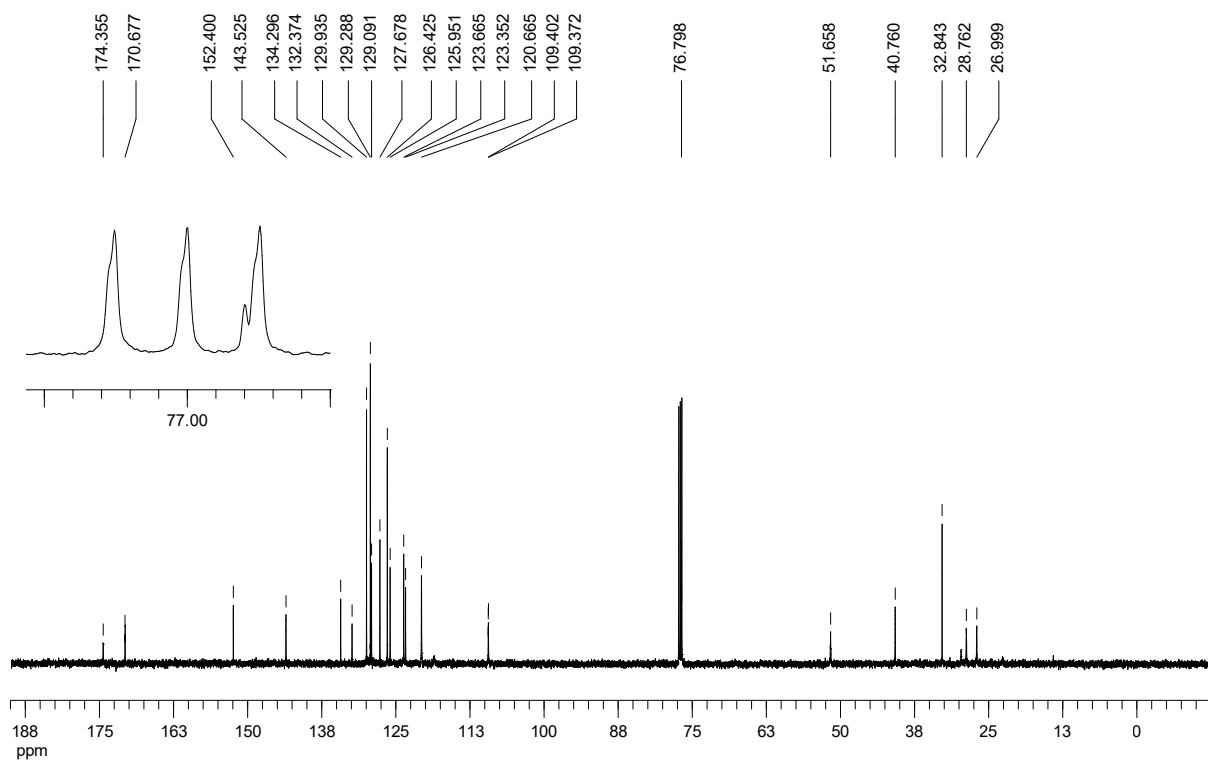
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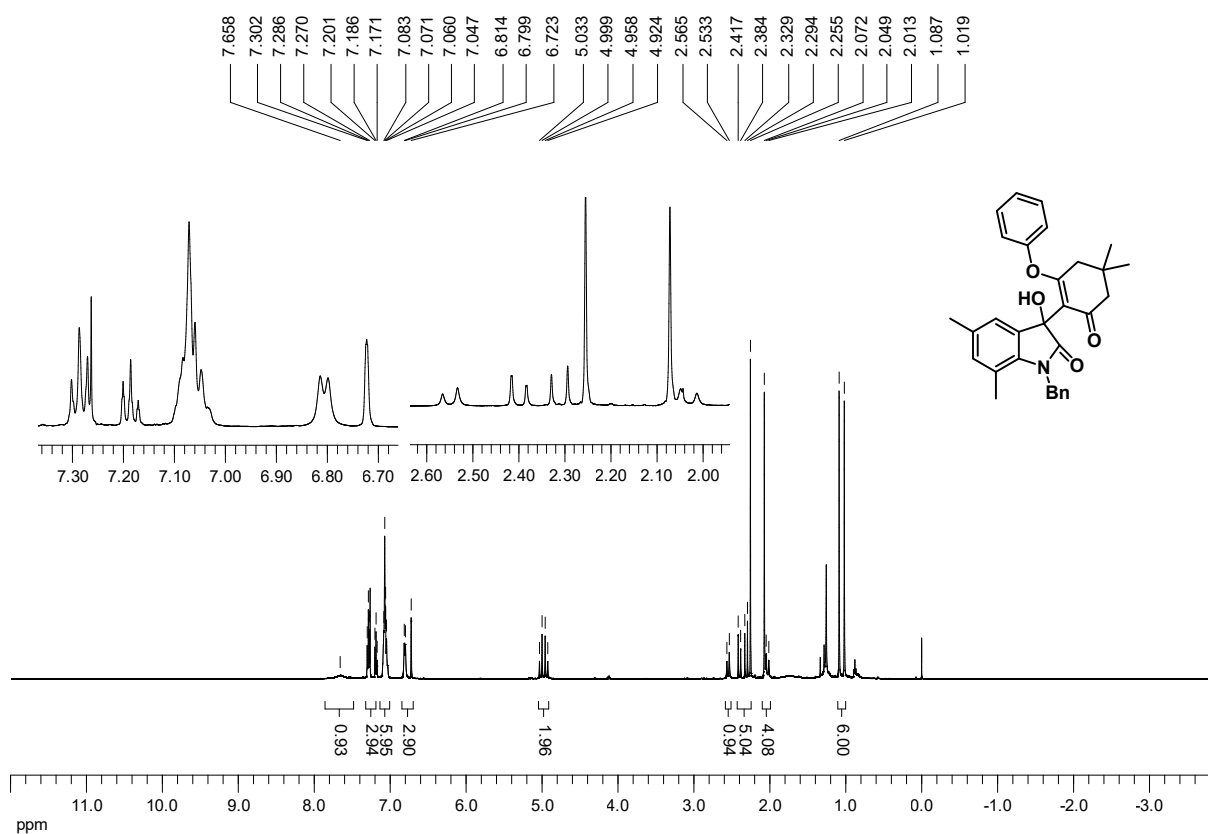
¹H NMR of **4haa** (CDCl₃, 500 MHz)



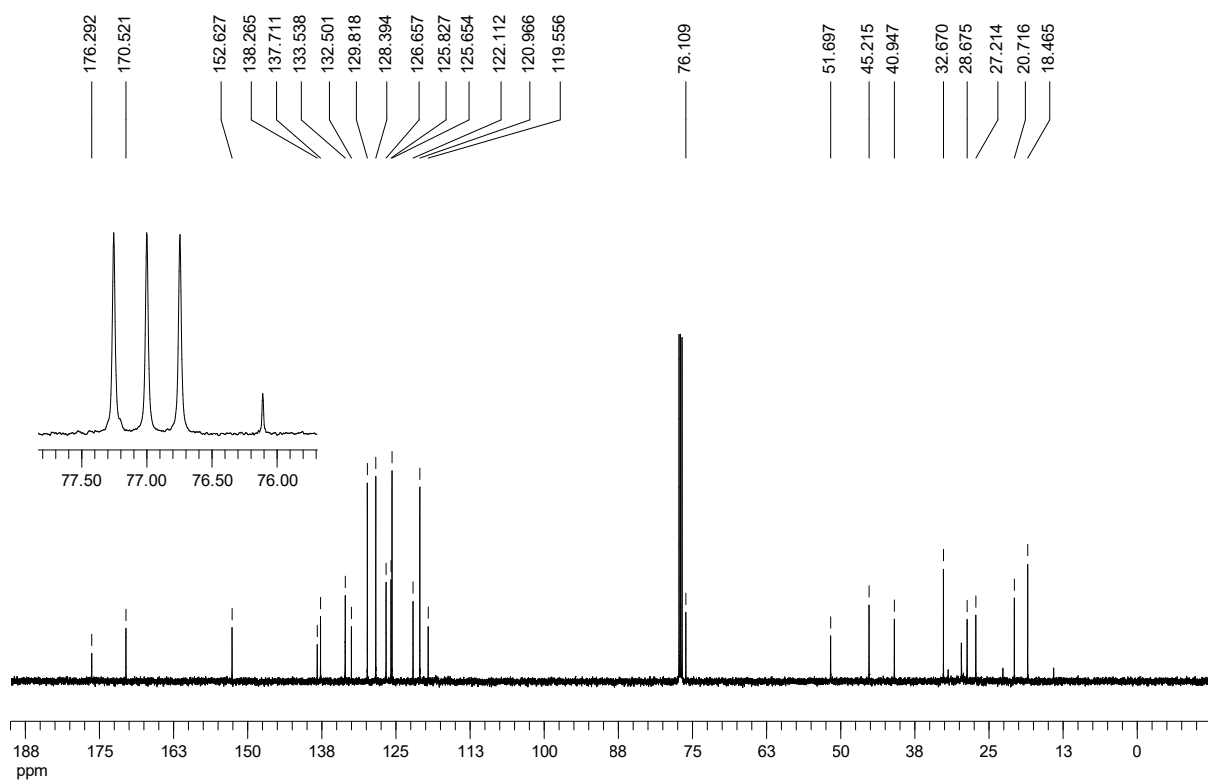
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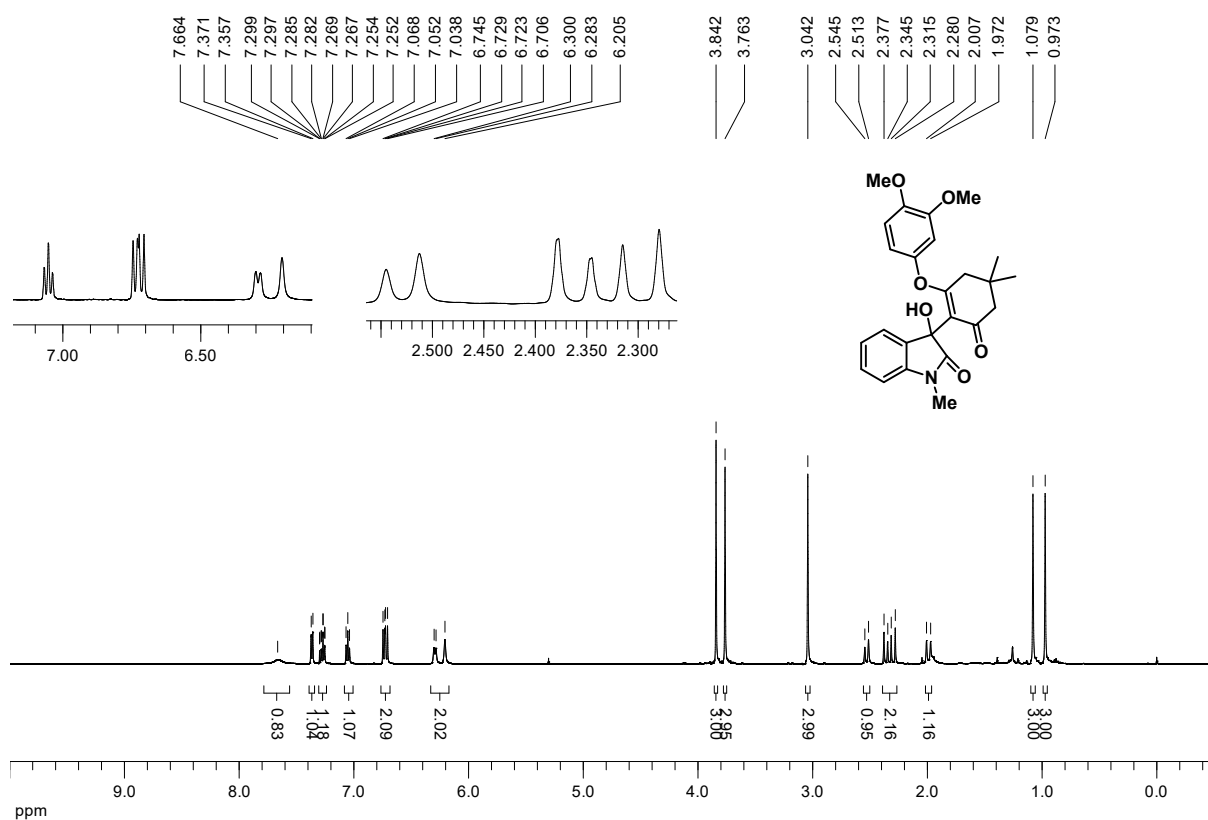
¹H NMR of **4iaa** (CDCl₃, 500 MHz)



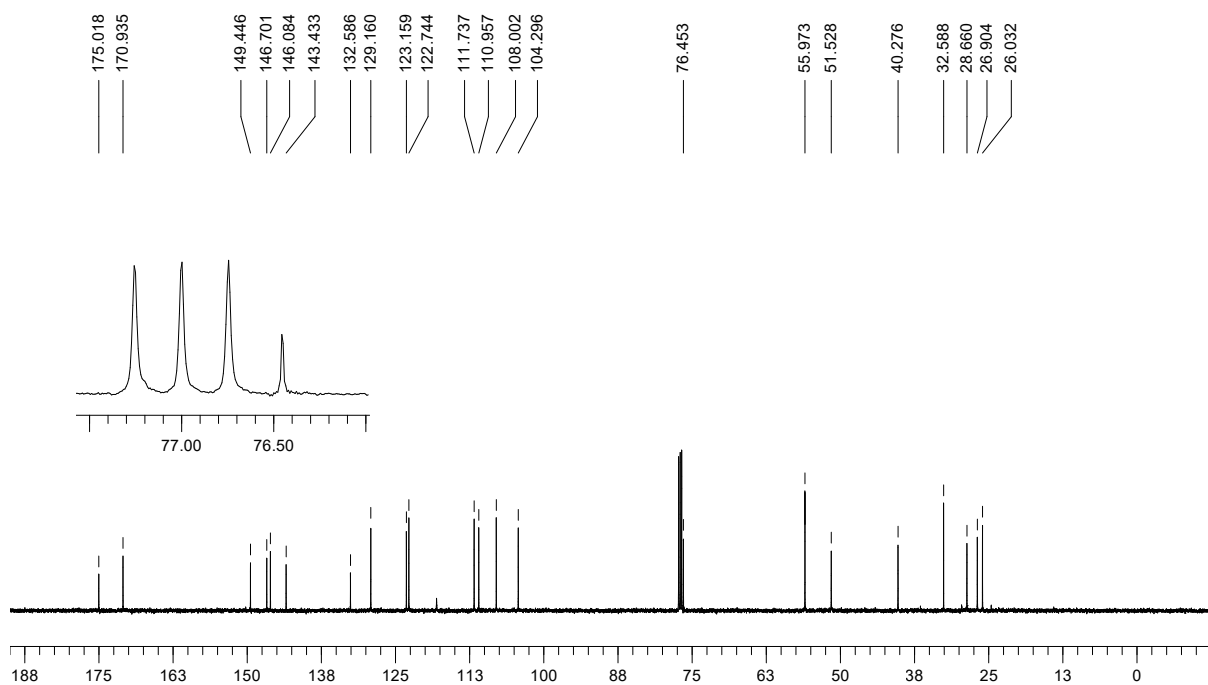
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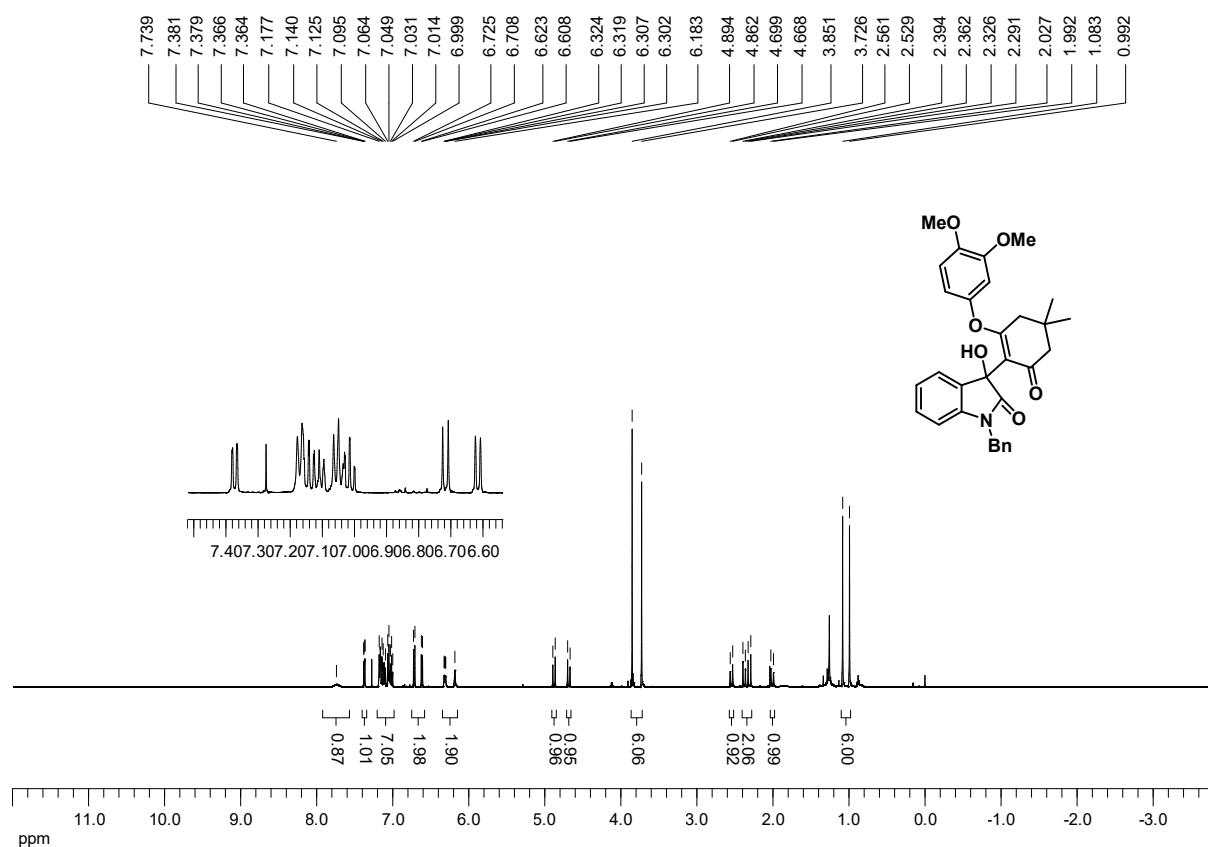
¹H NMR of **4aba** (CDCl₃, 500 MHz)



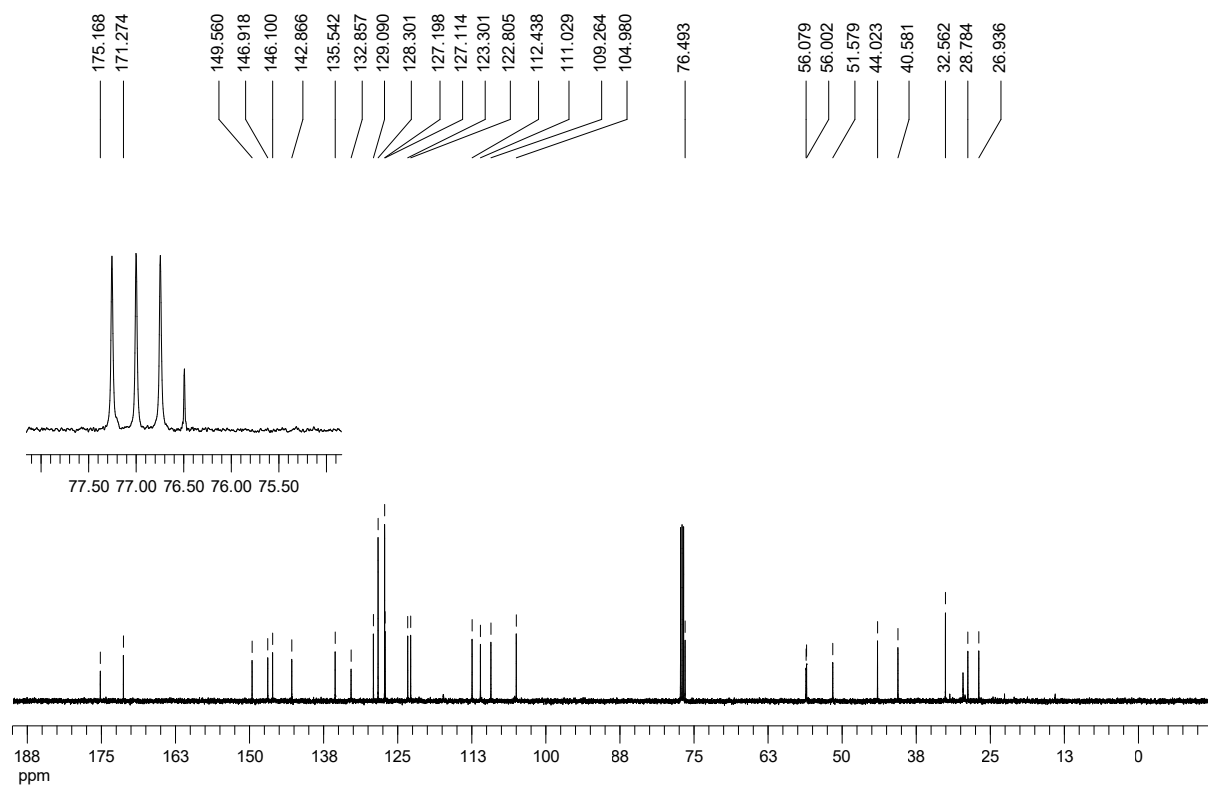
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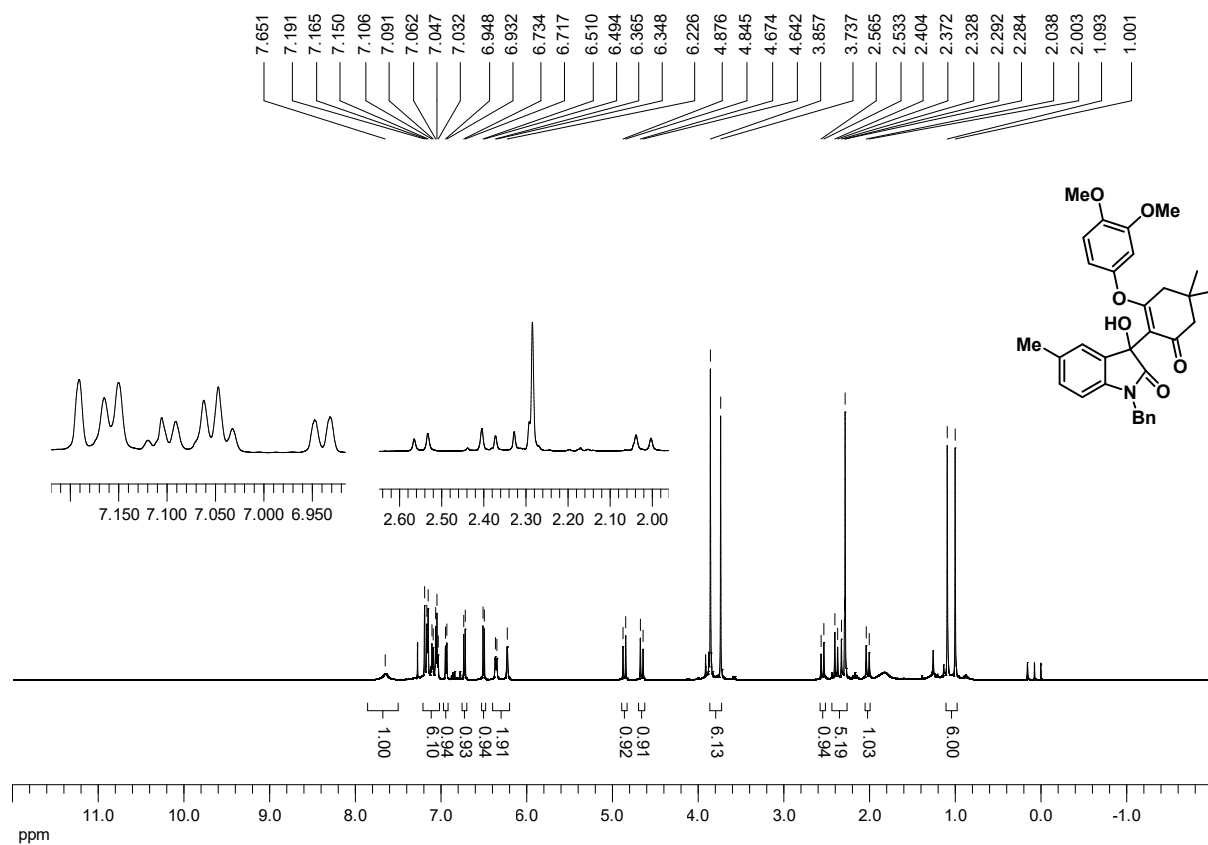
¹H NMR of **4bba** (CDCl₃, 500 MHz)



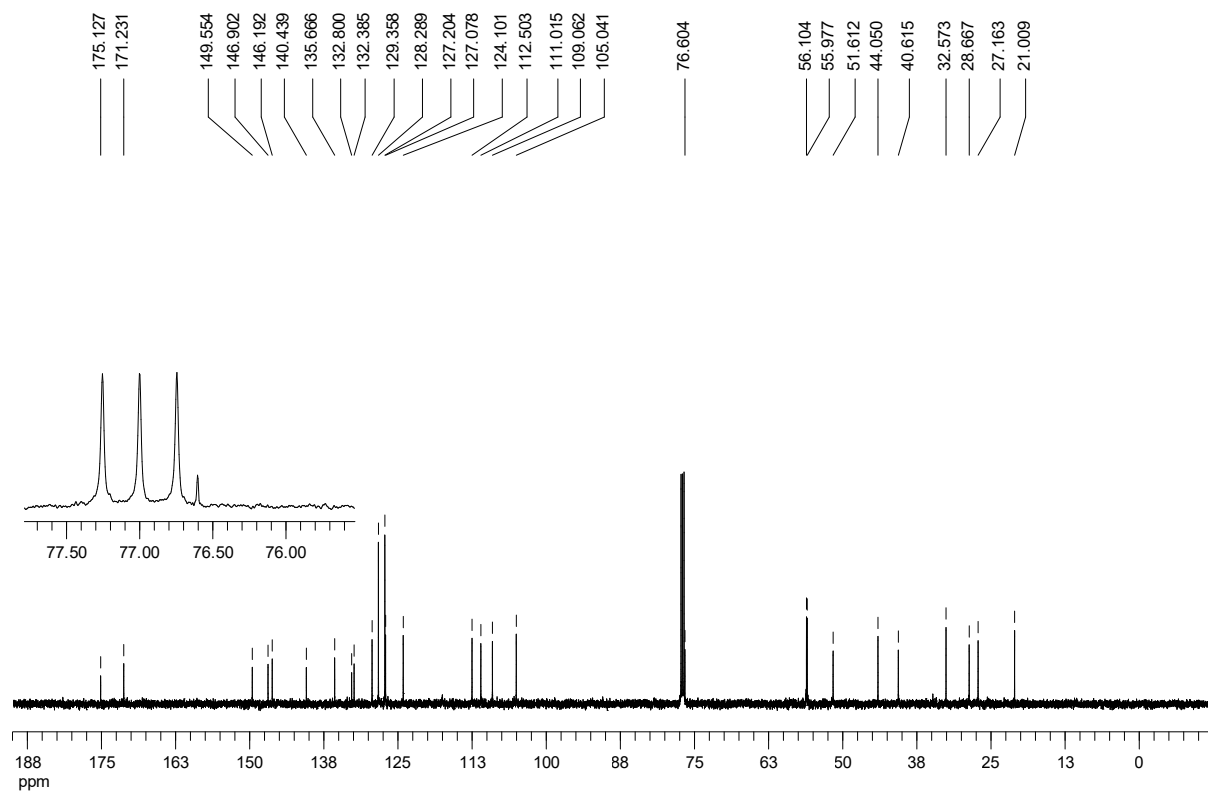
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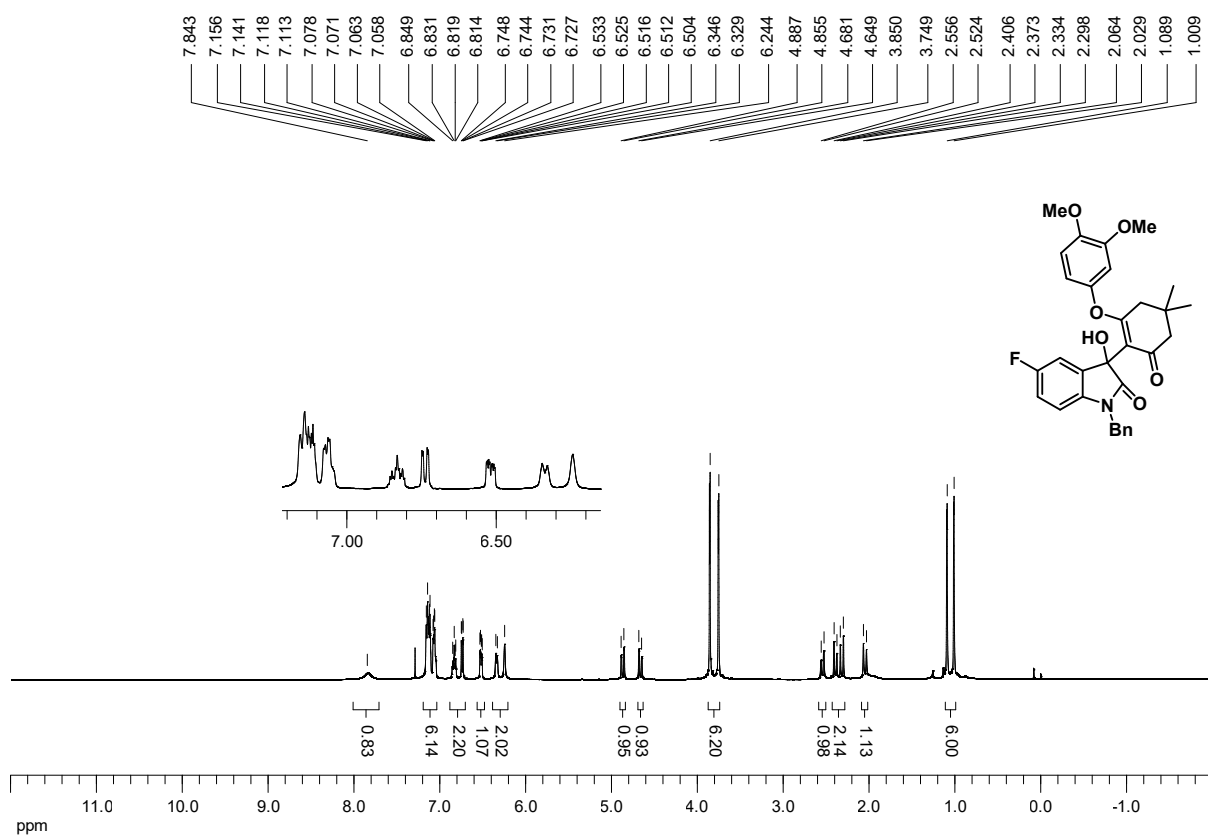
¹H NMR of **4dba** (CDCl₃, 500 MHz)



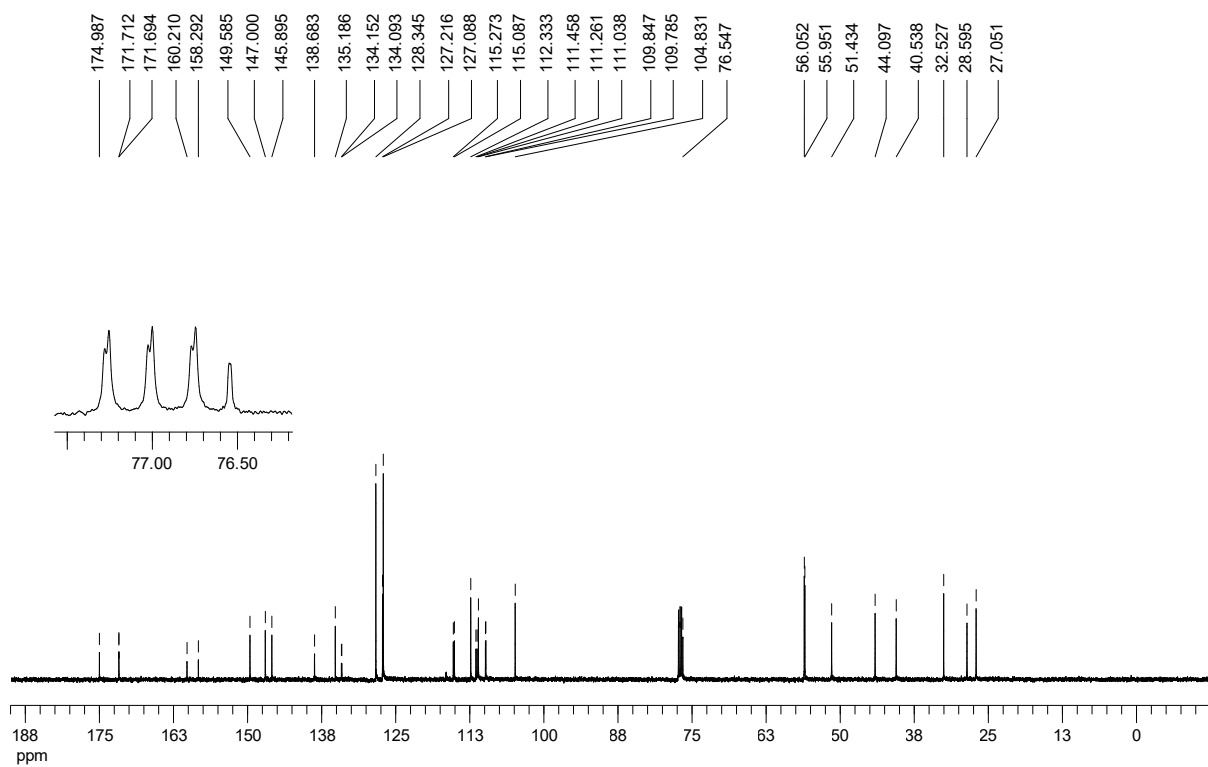
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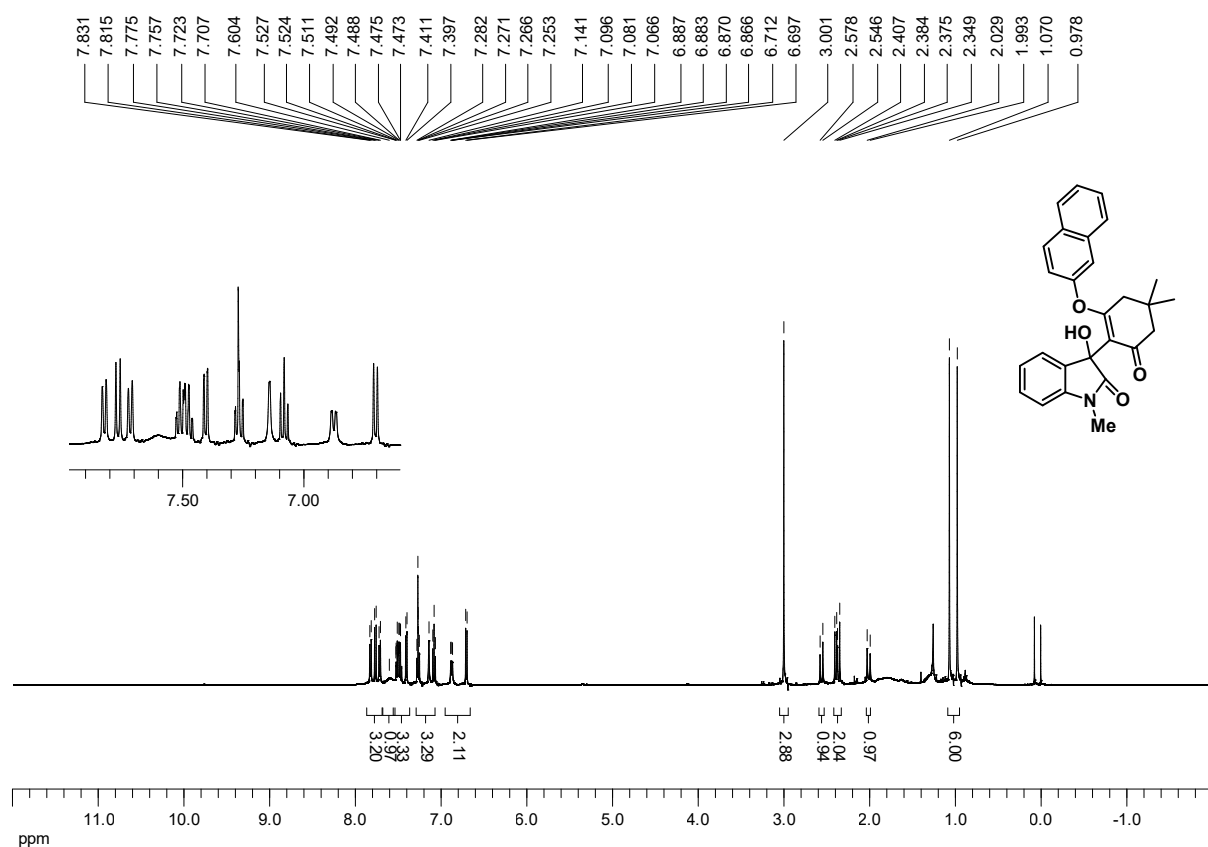
¹H NMR of **4fba** (CDCl₃, 500 MHz)



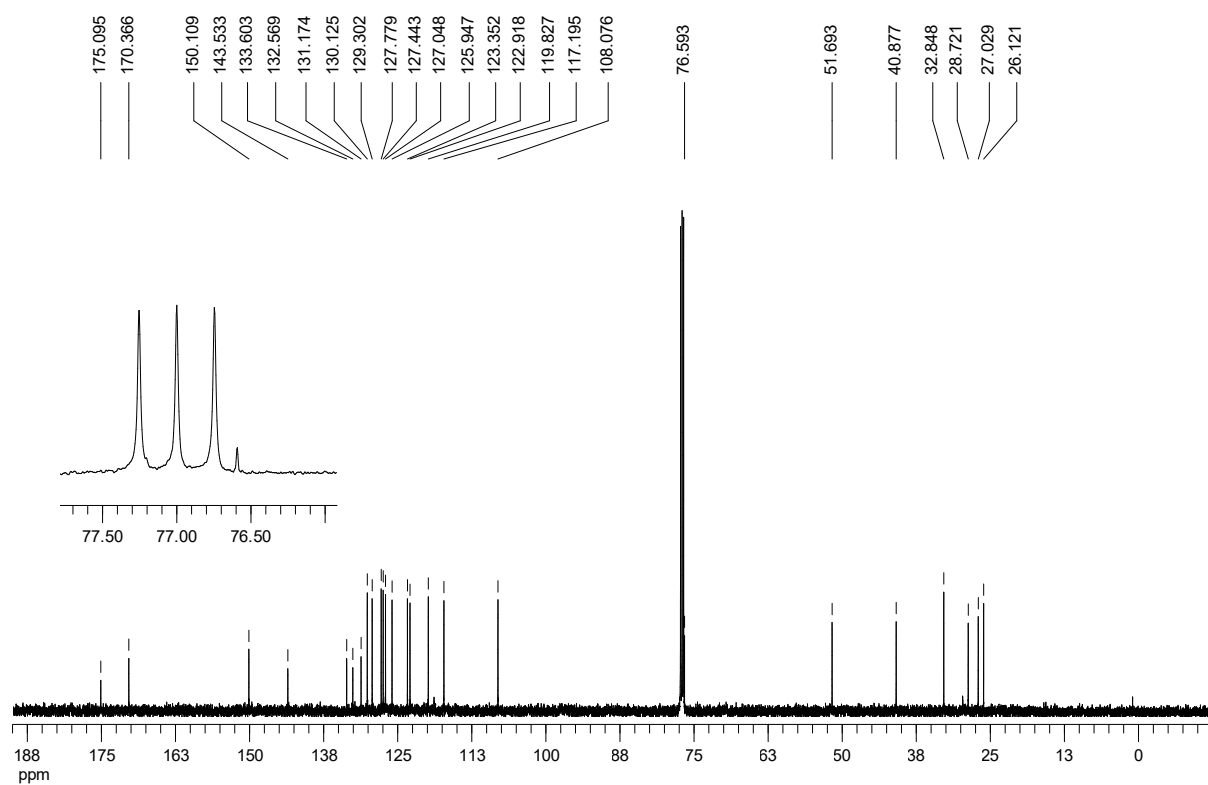
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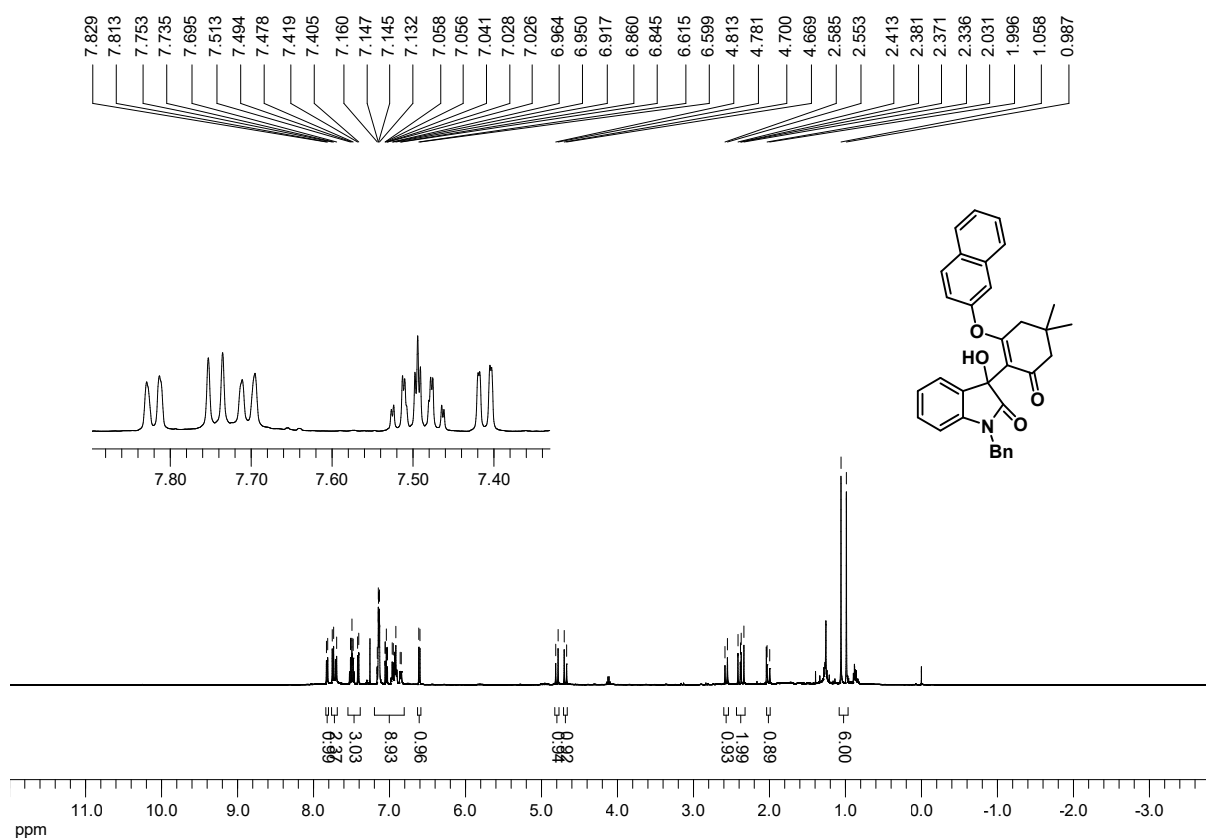
¹H NMR of **4aca** (CDCl₃, 500 MHz)



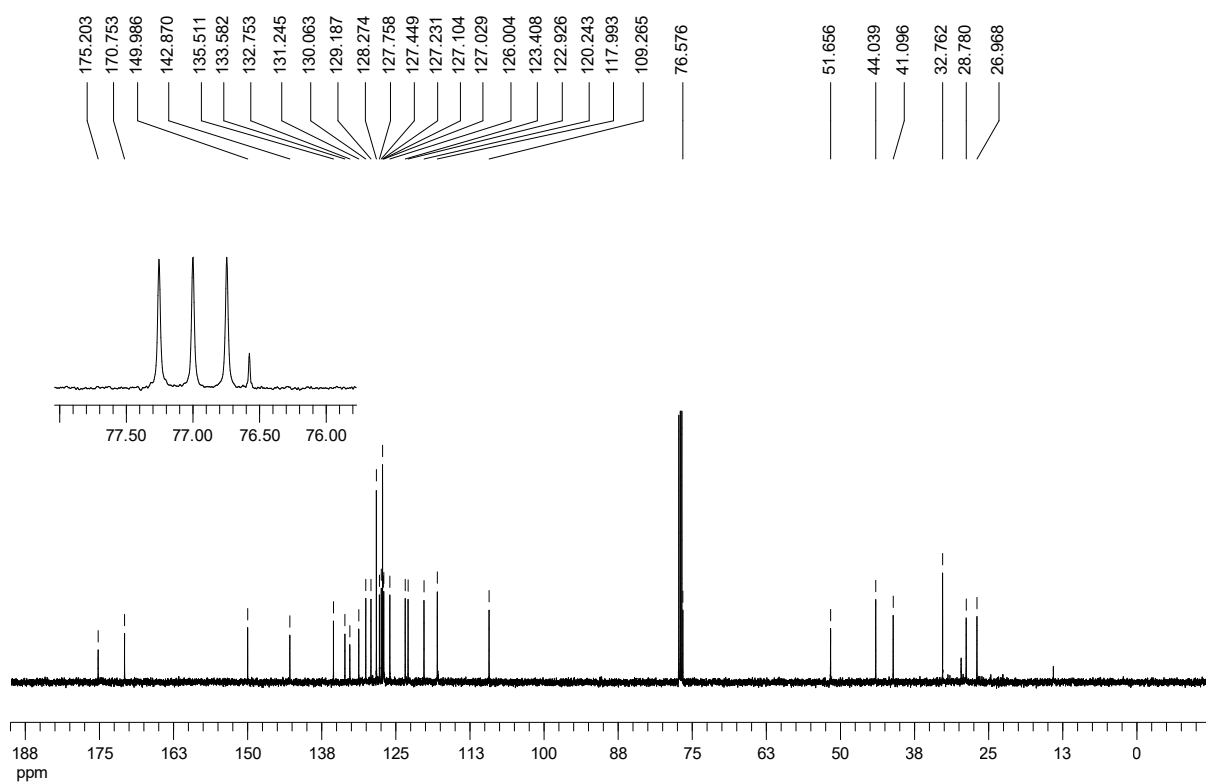
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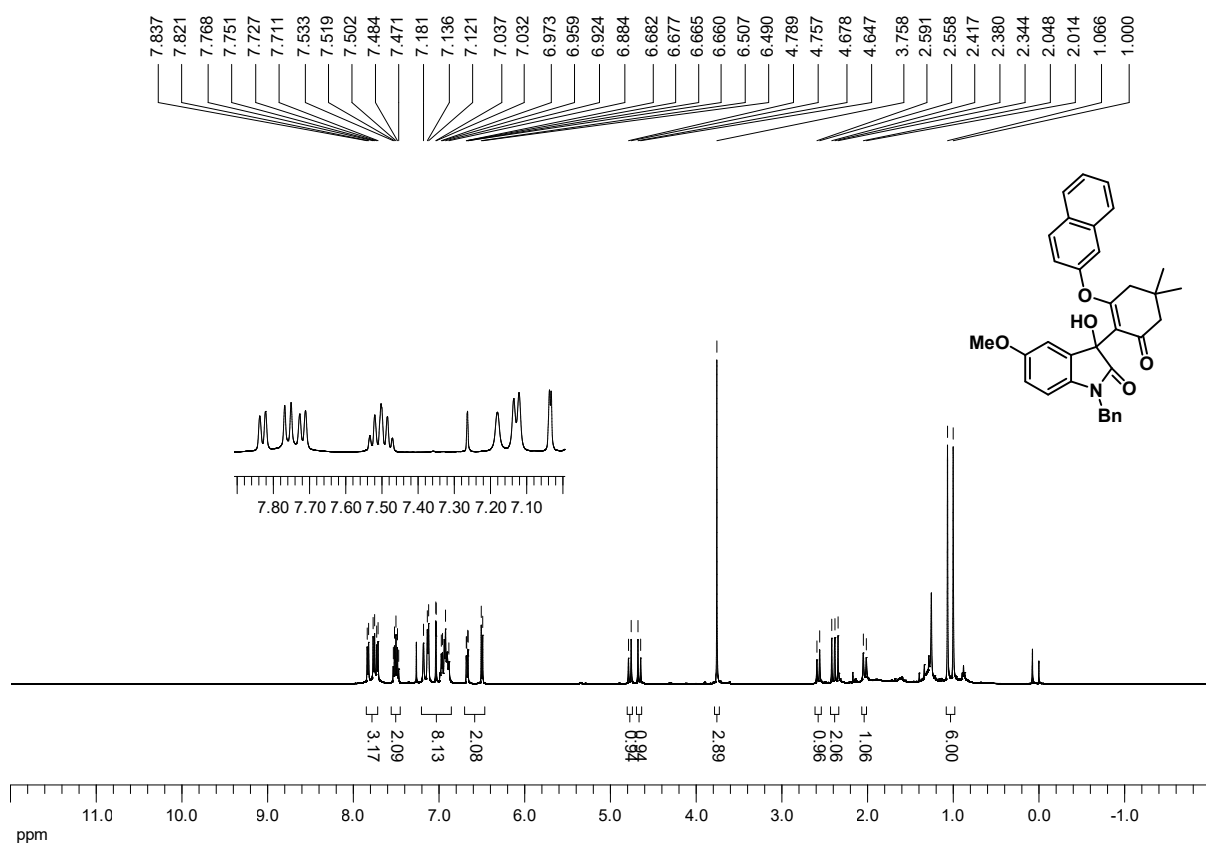
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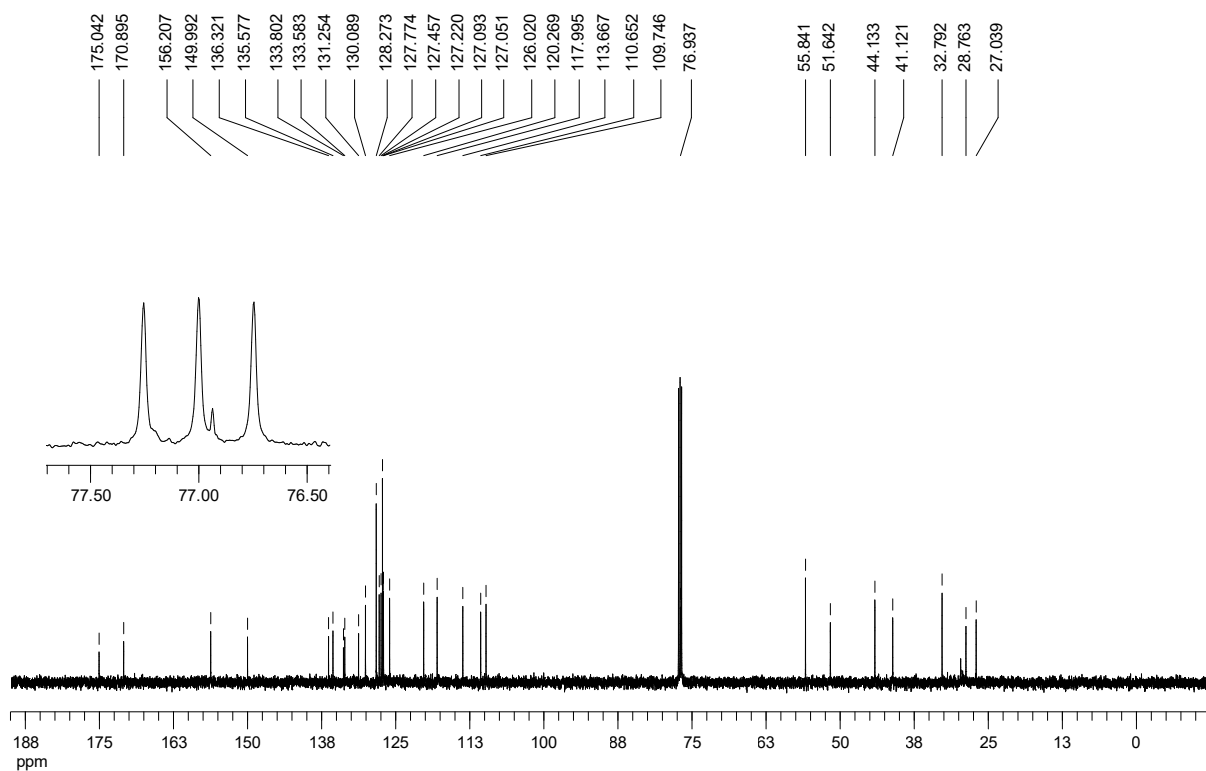
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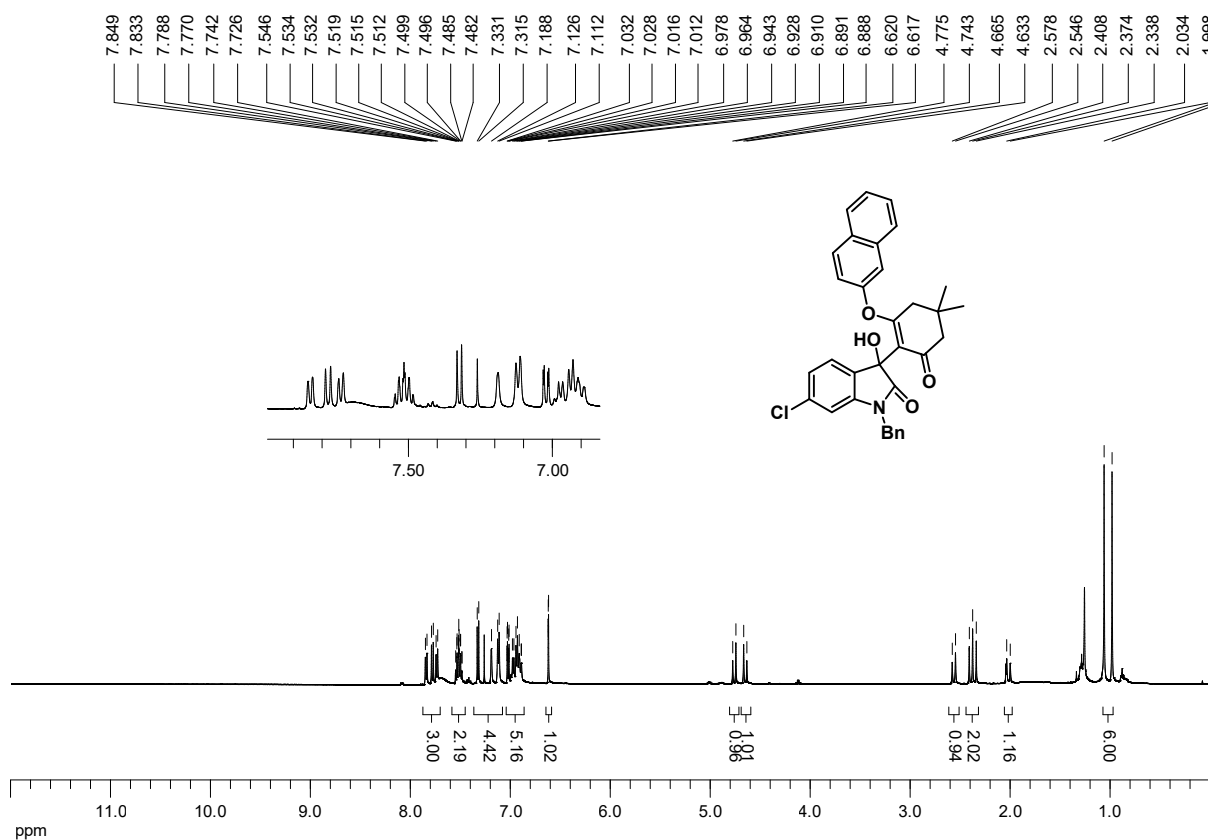
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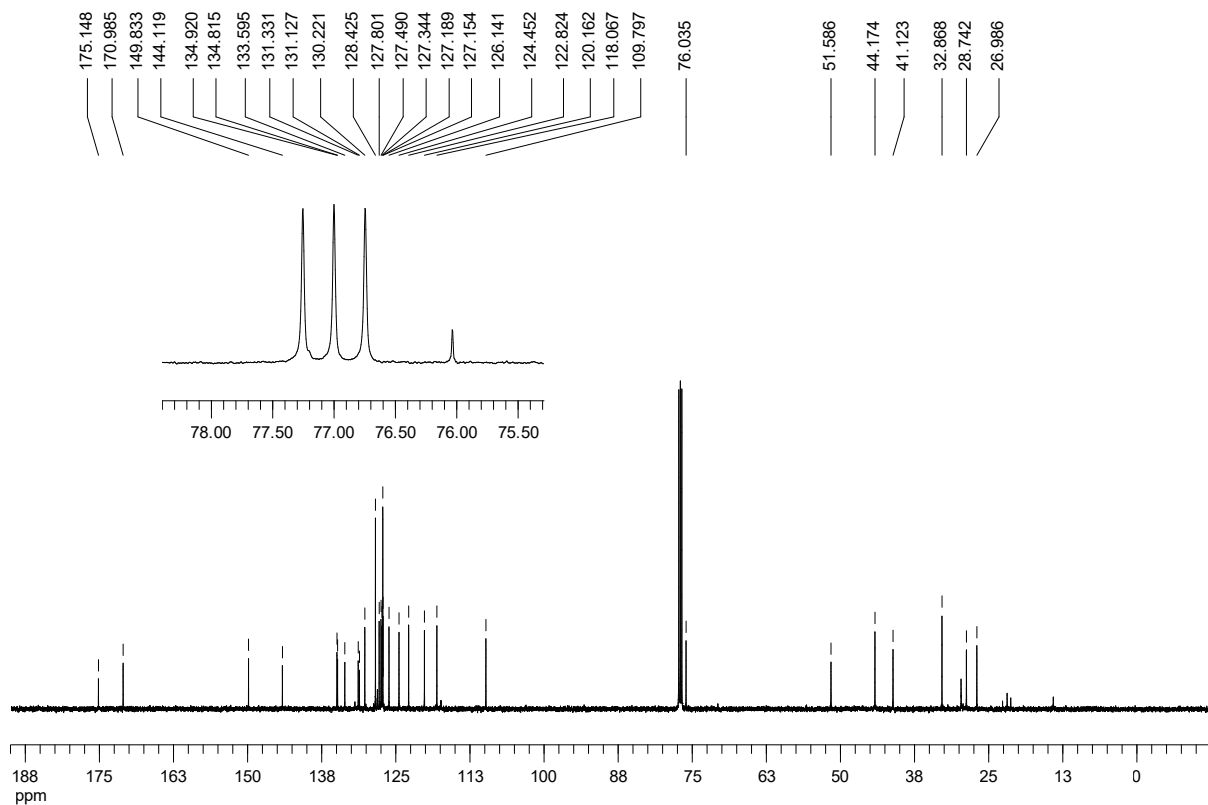
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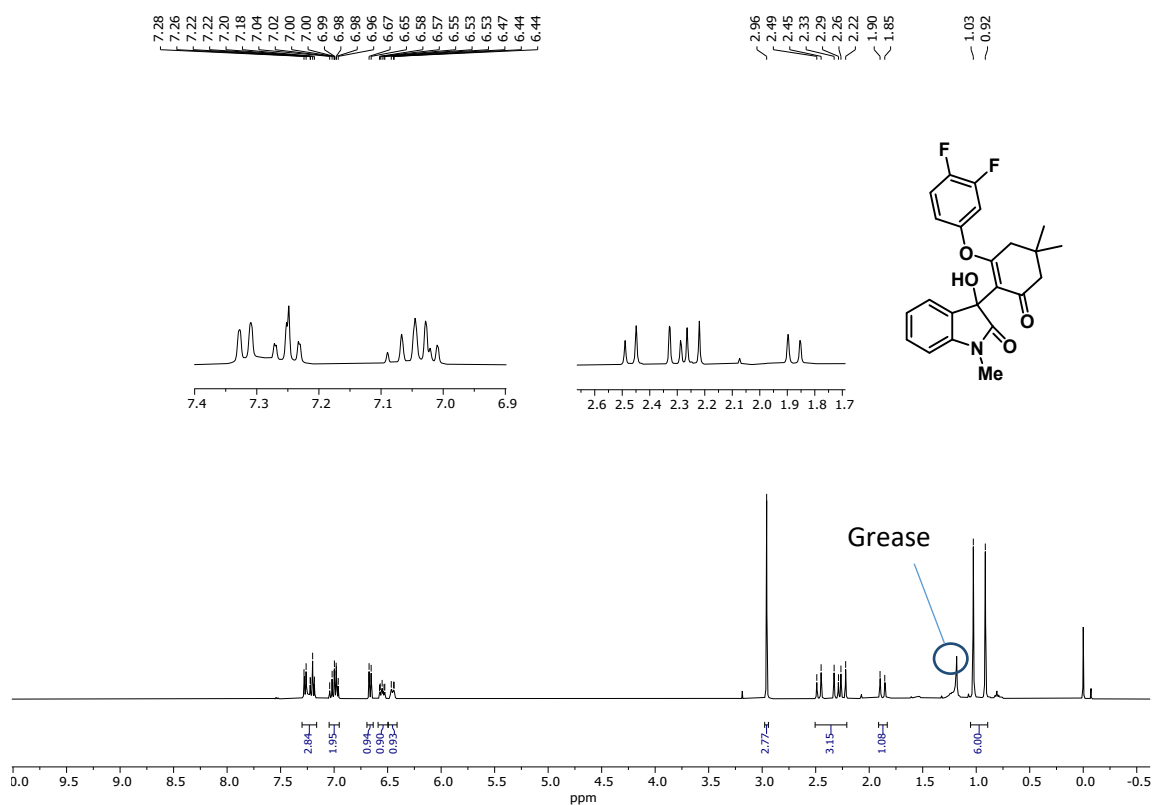
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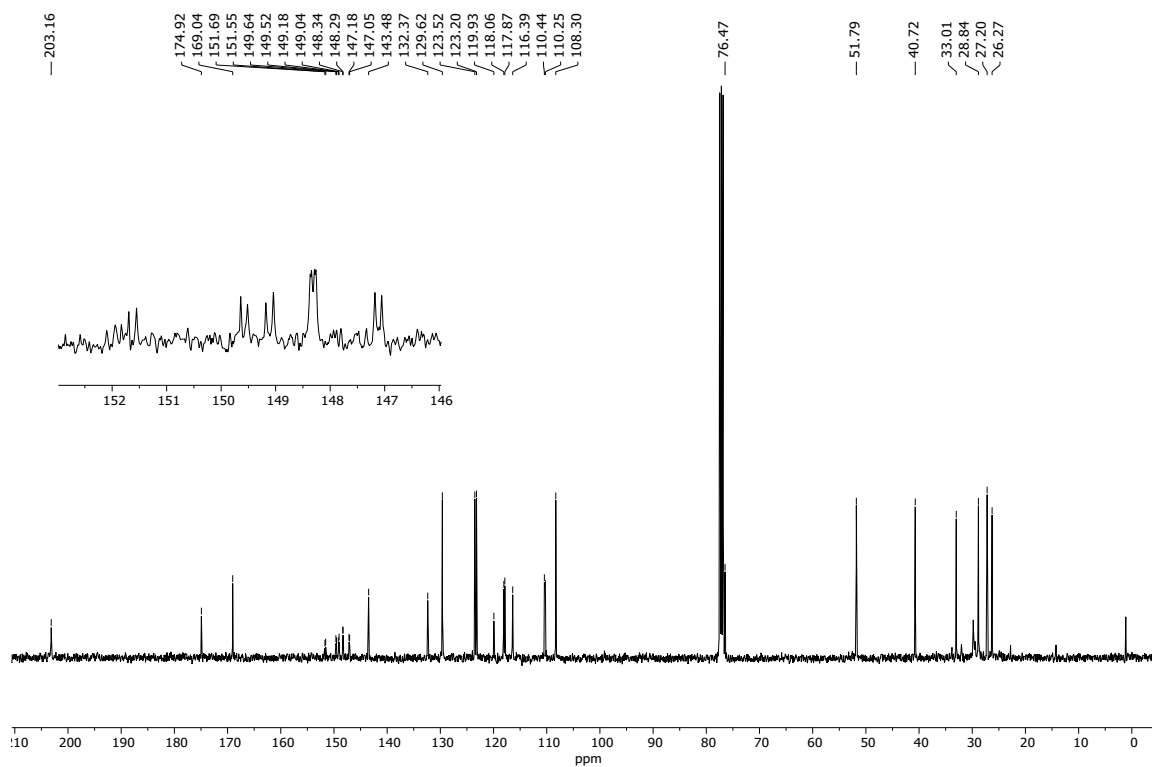
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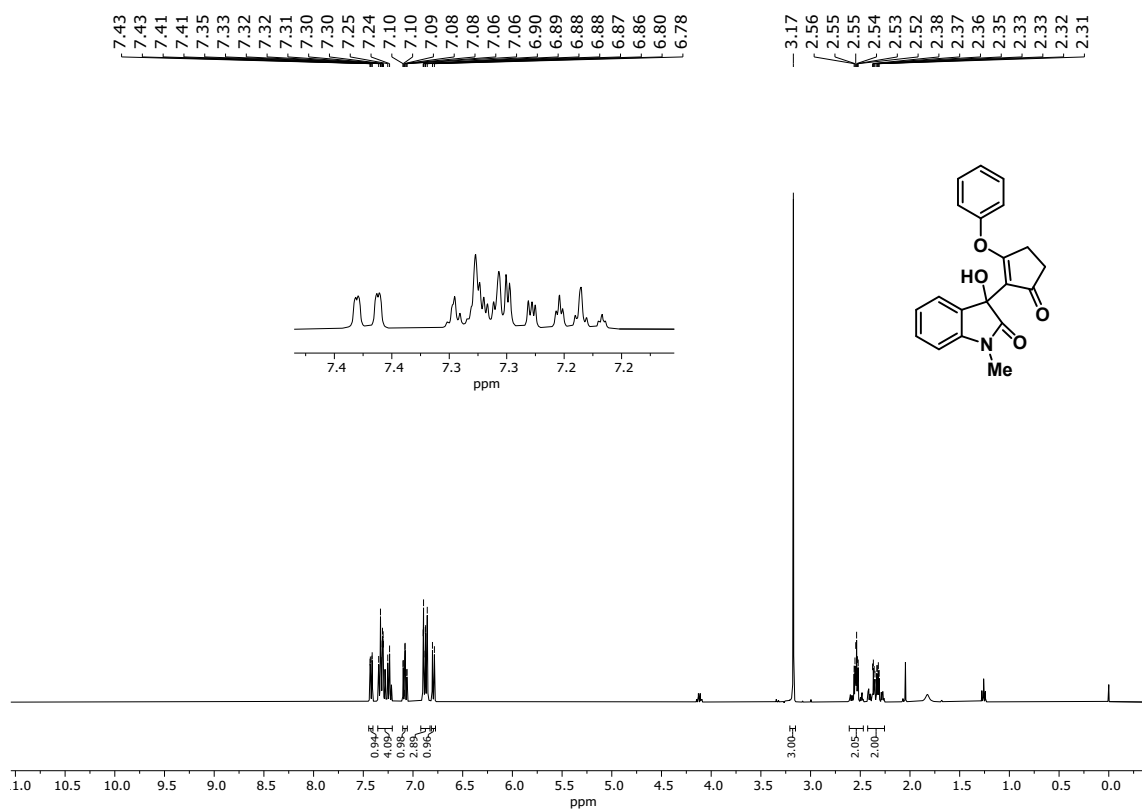
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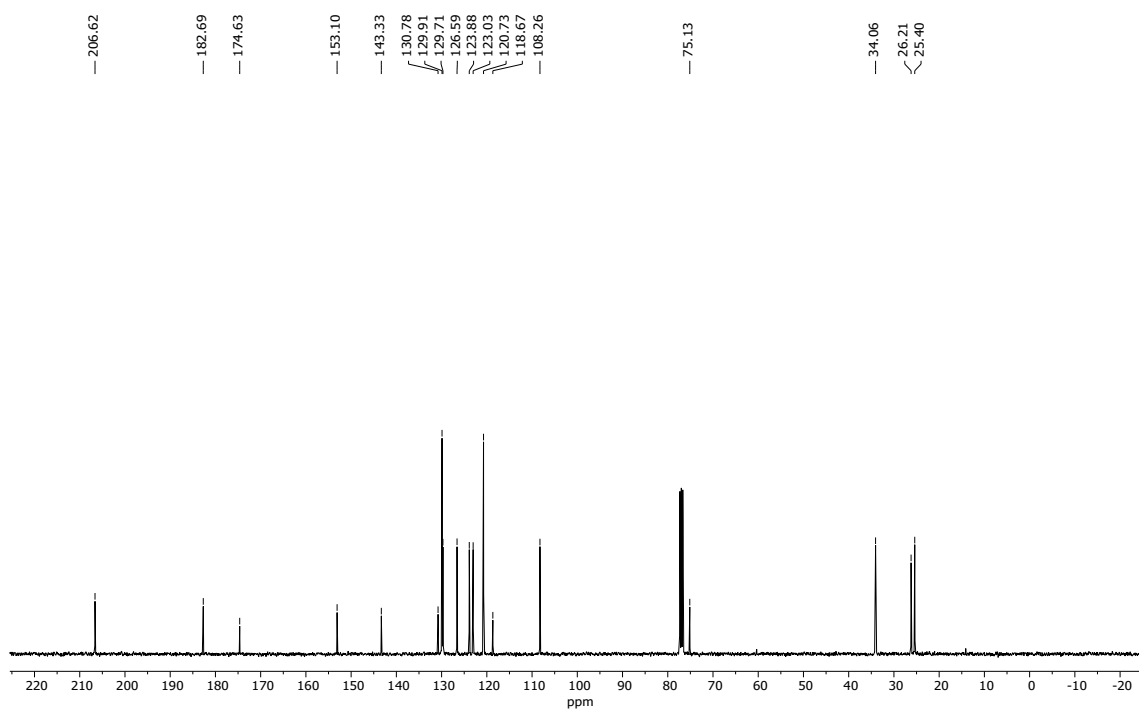
^{13}C NMR of **4ada** (CDCl_3 , 101 MHz)



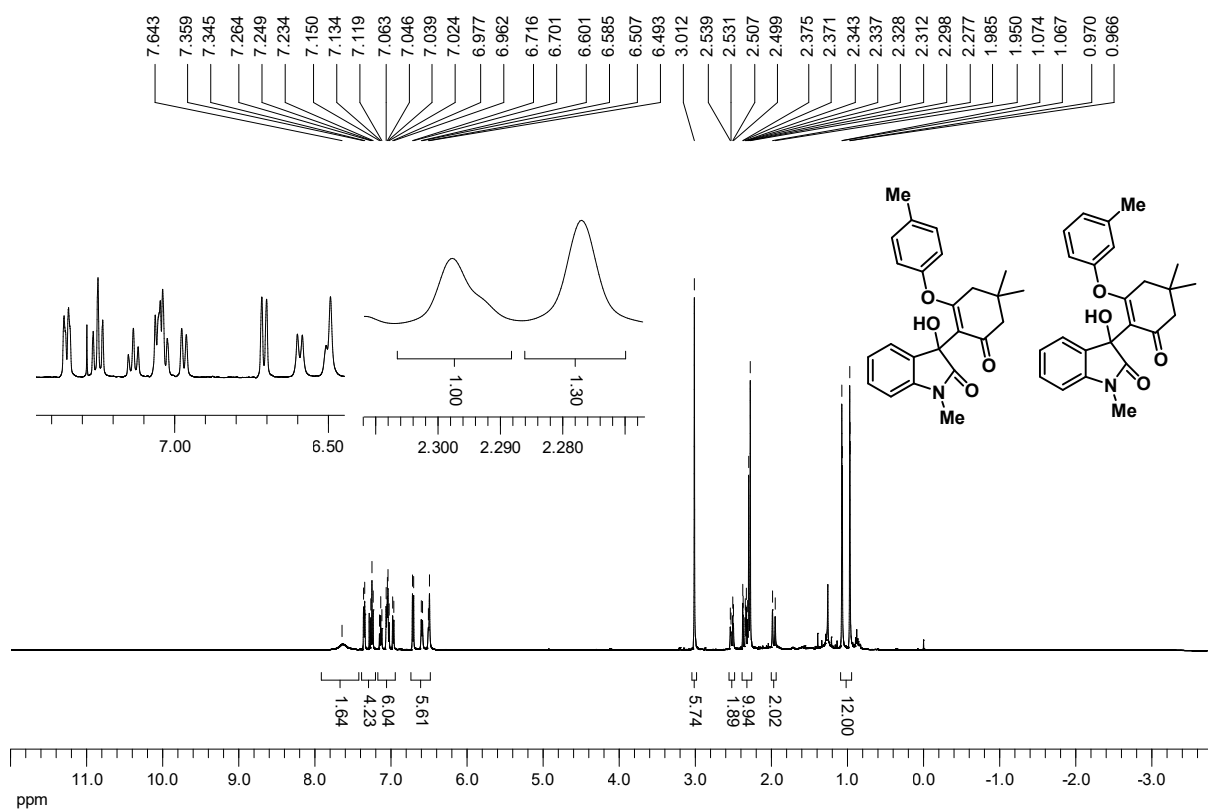
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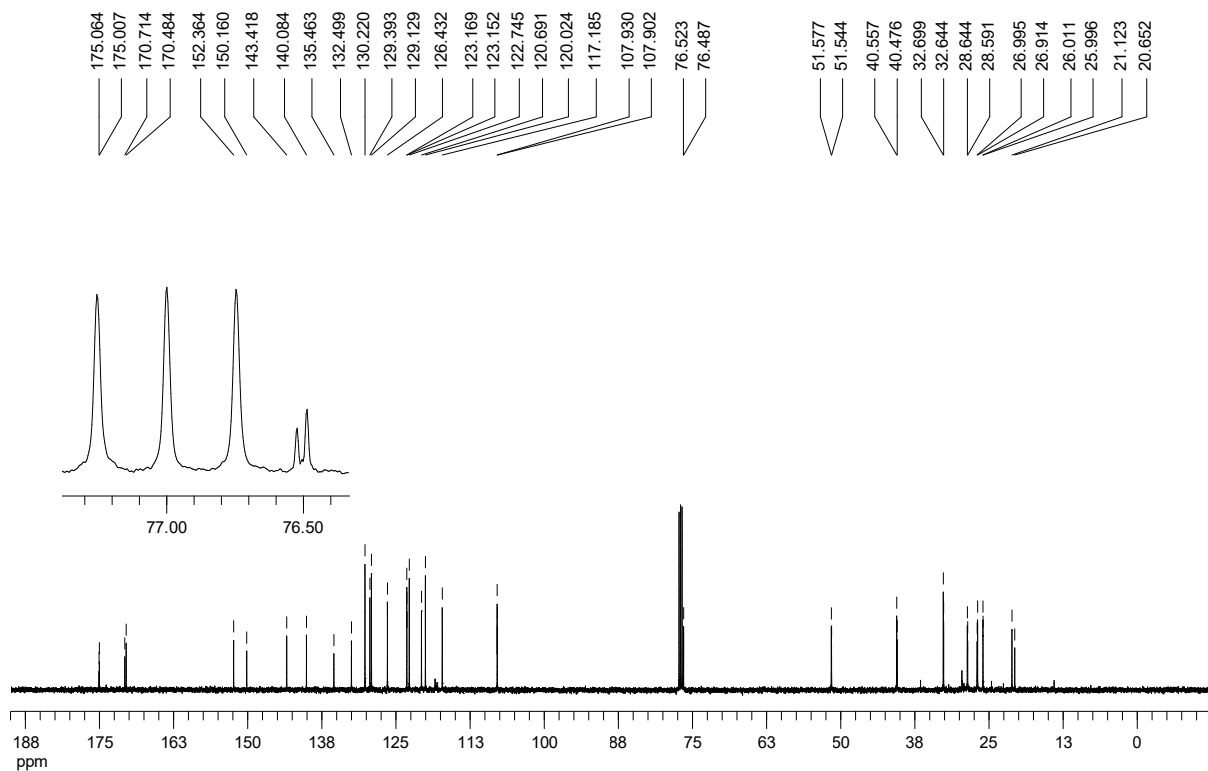
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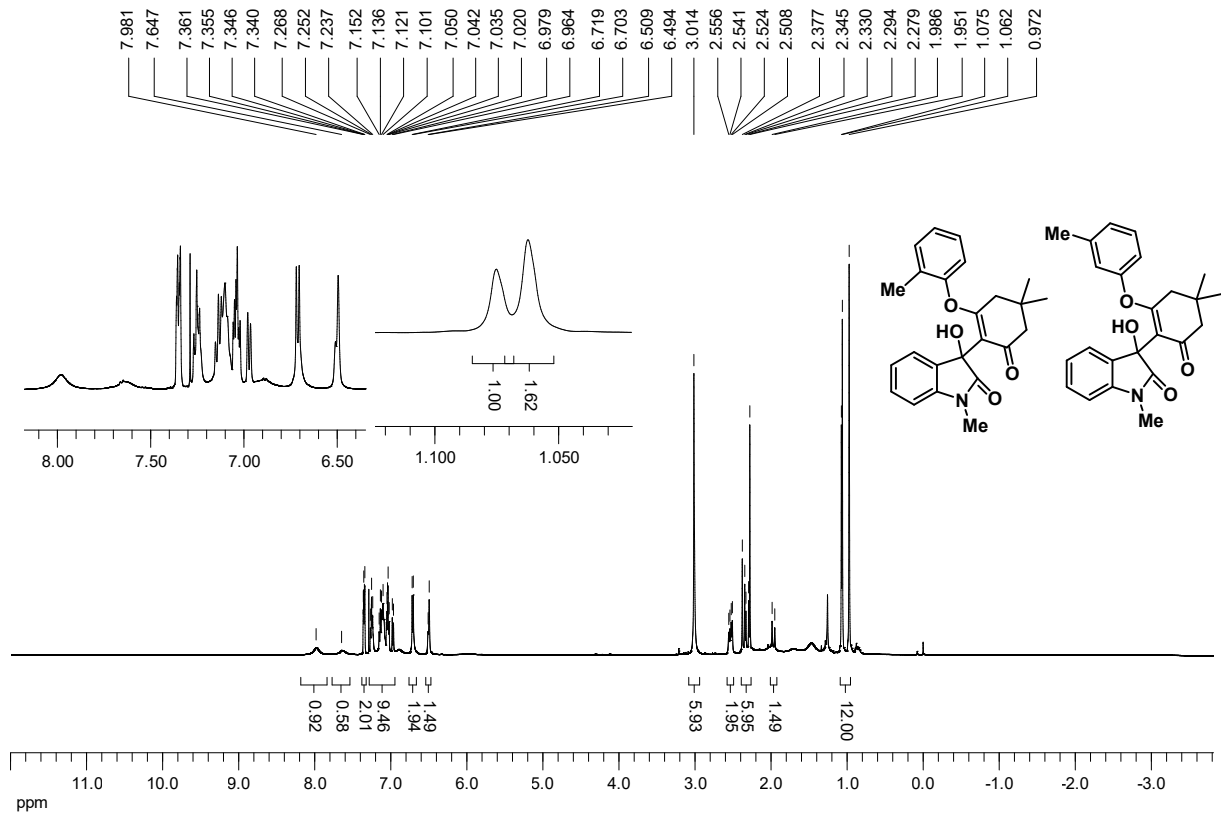
¹H NMR of 4aea & 4ae'a (CDCl₃, 500 MHz)



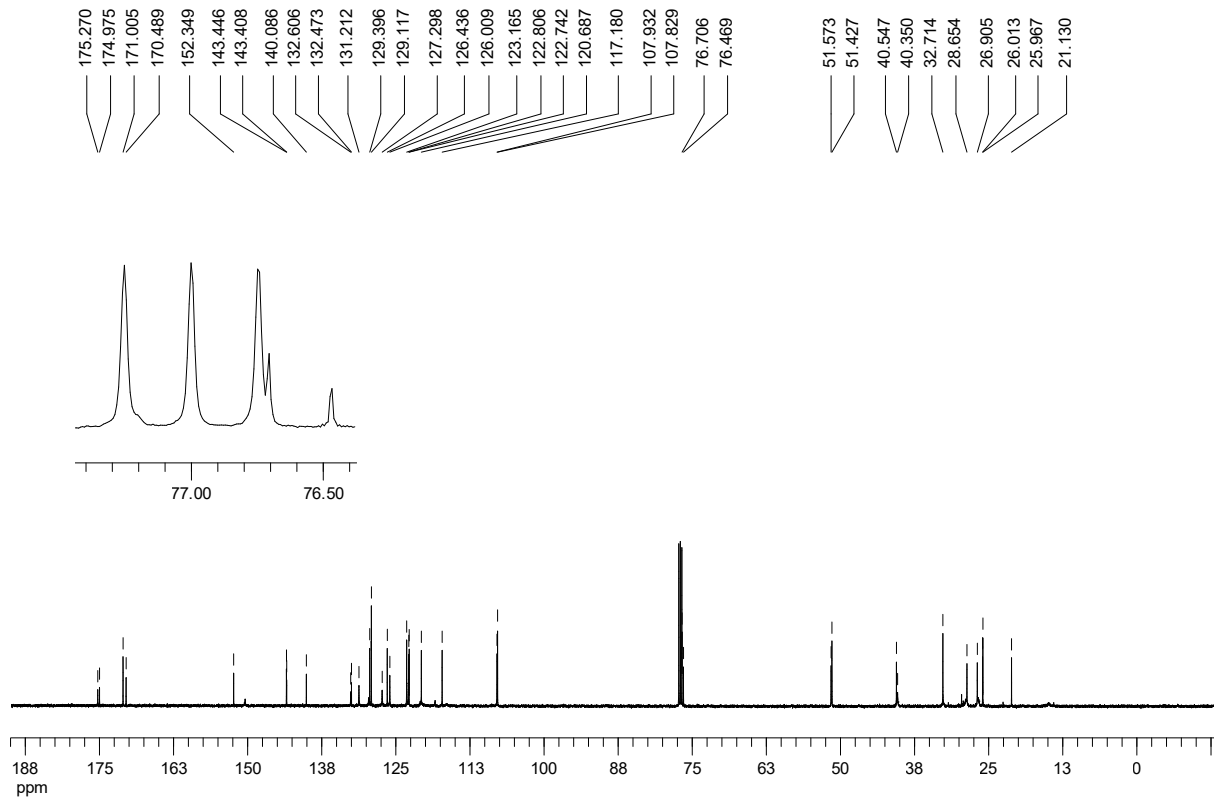
¹³C NMR of 4aea & 4ae'a (CDCl₃, 126 MHz)



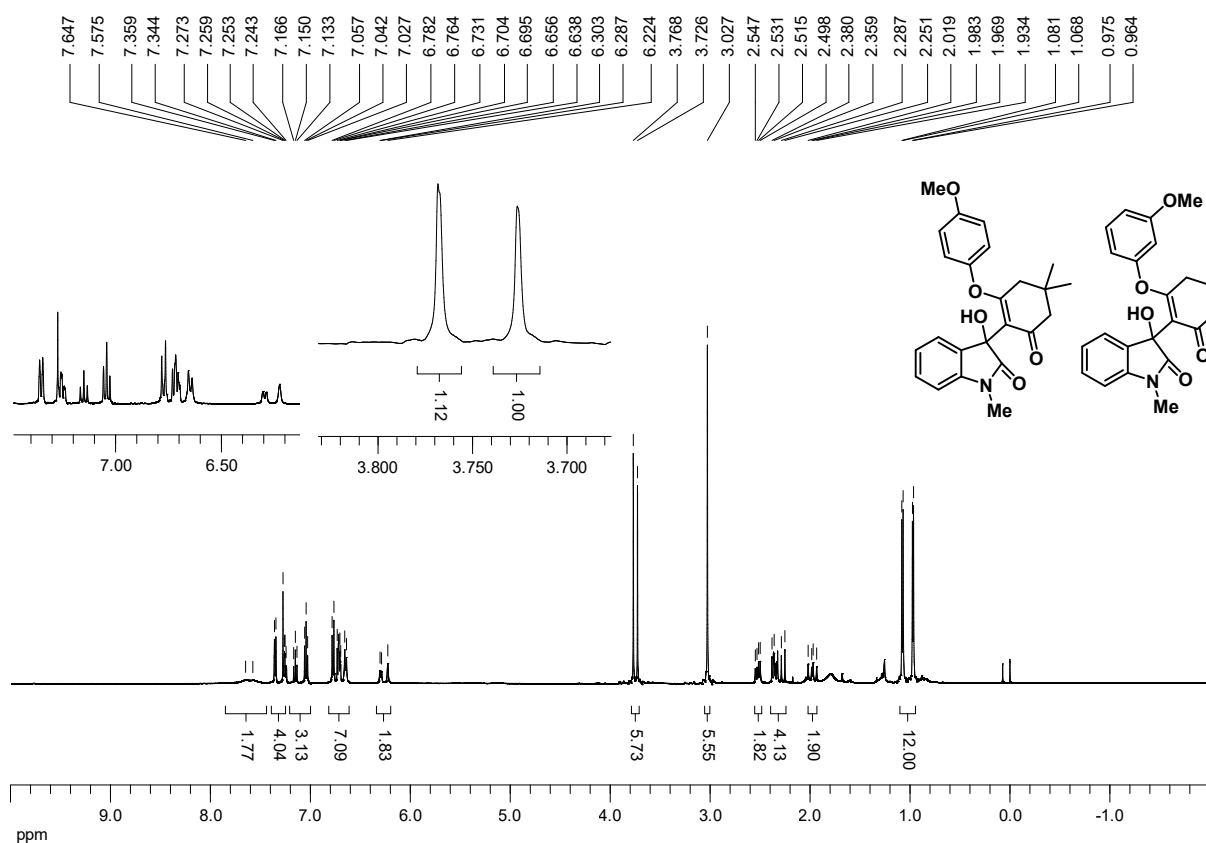
¹H NMR of 4afa & 4af'a (CDCl₃, 500 MHz)



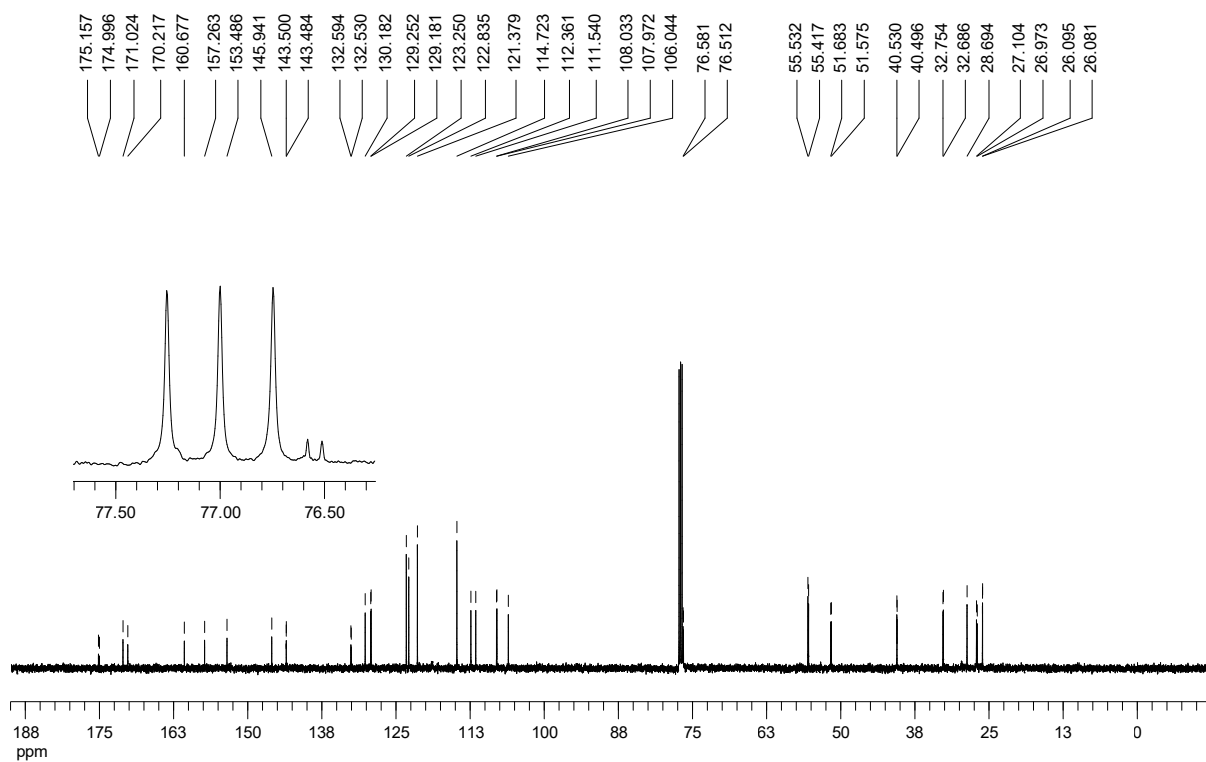
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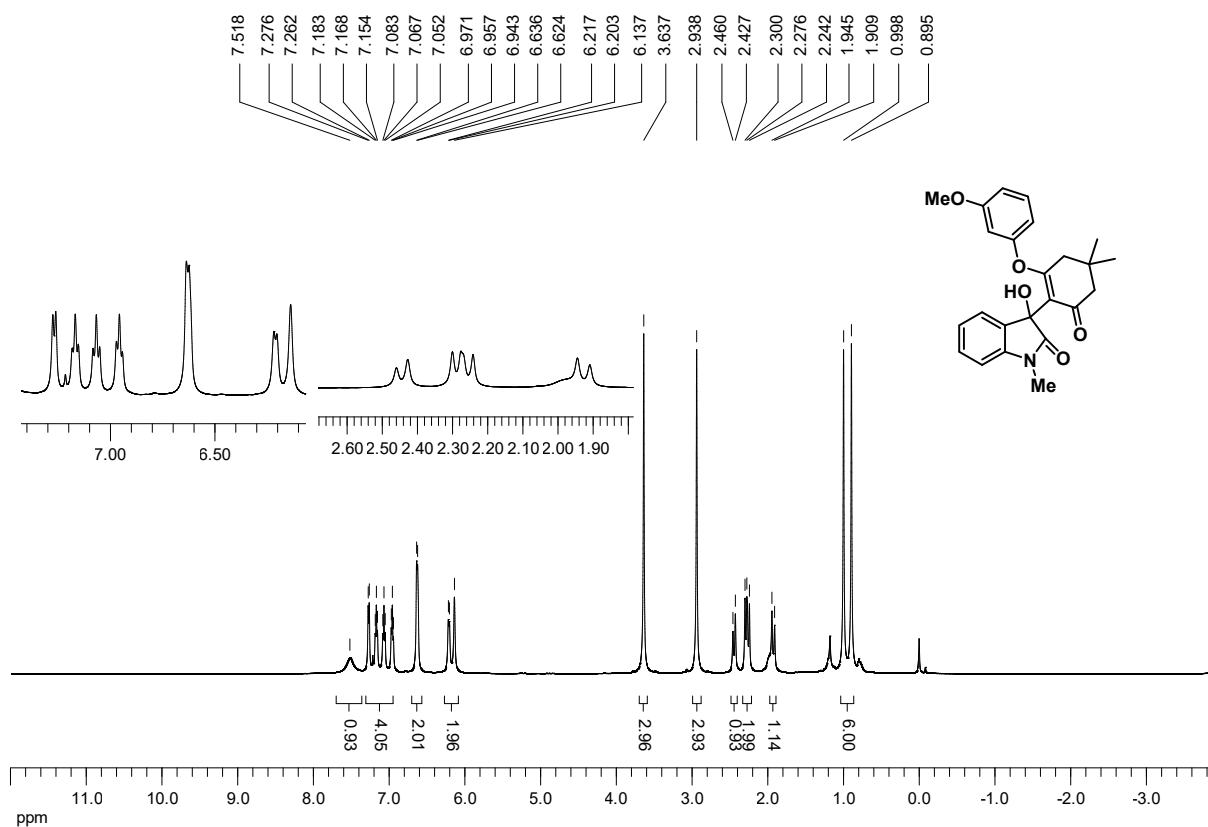
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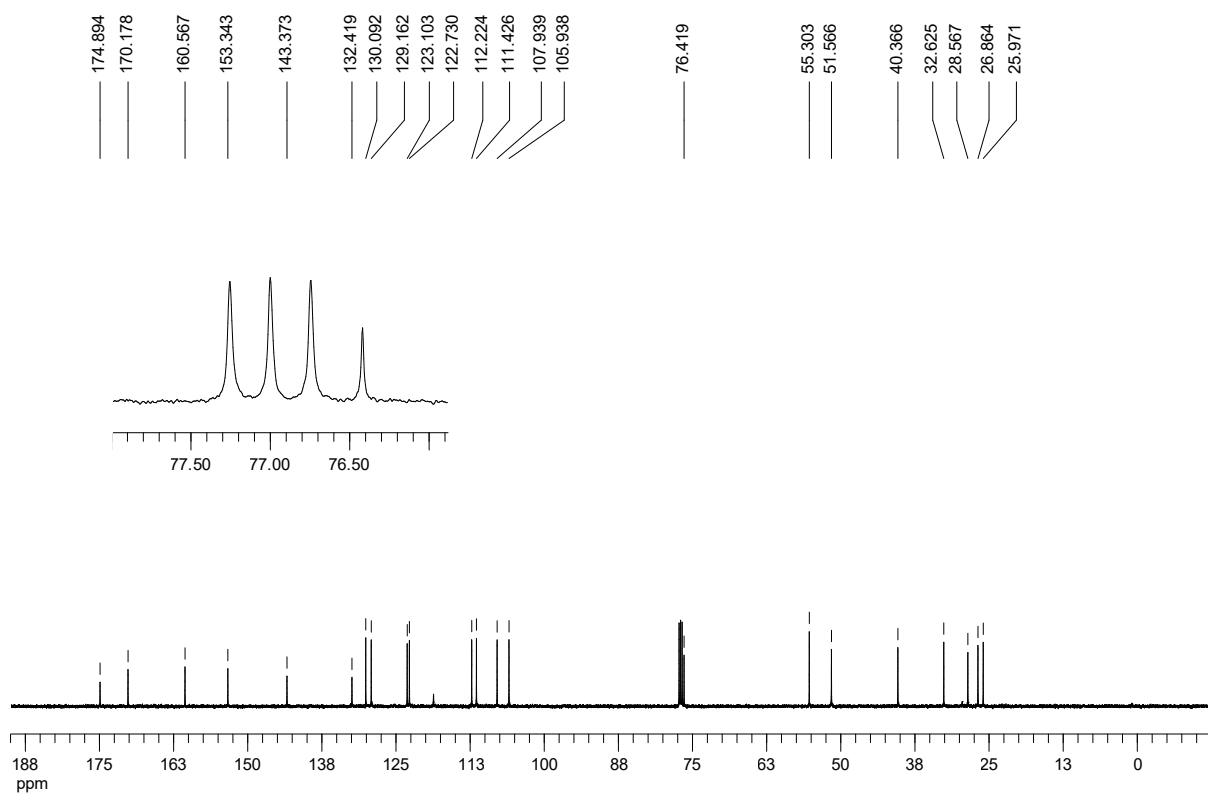
¹³C NMR of 4aga & 4ag'a (CDCl₃, 126 MHz)



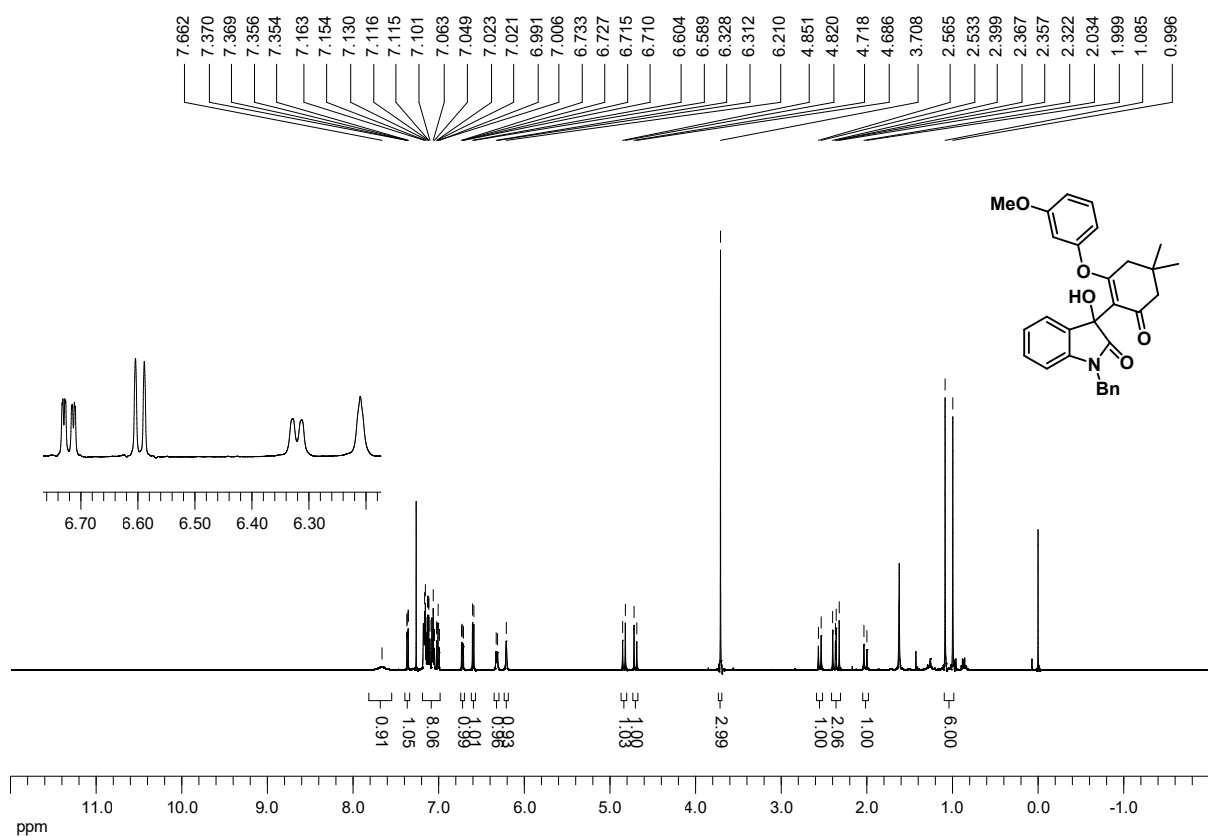
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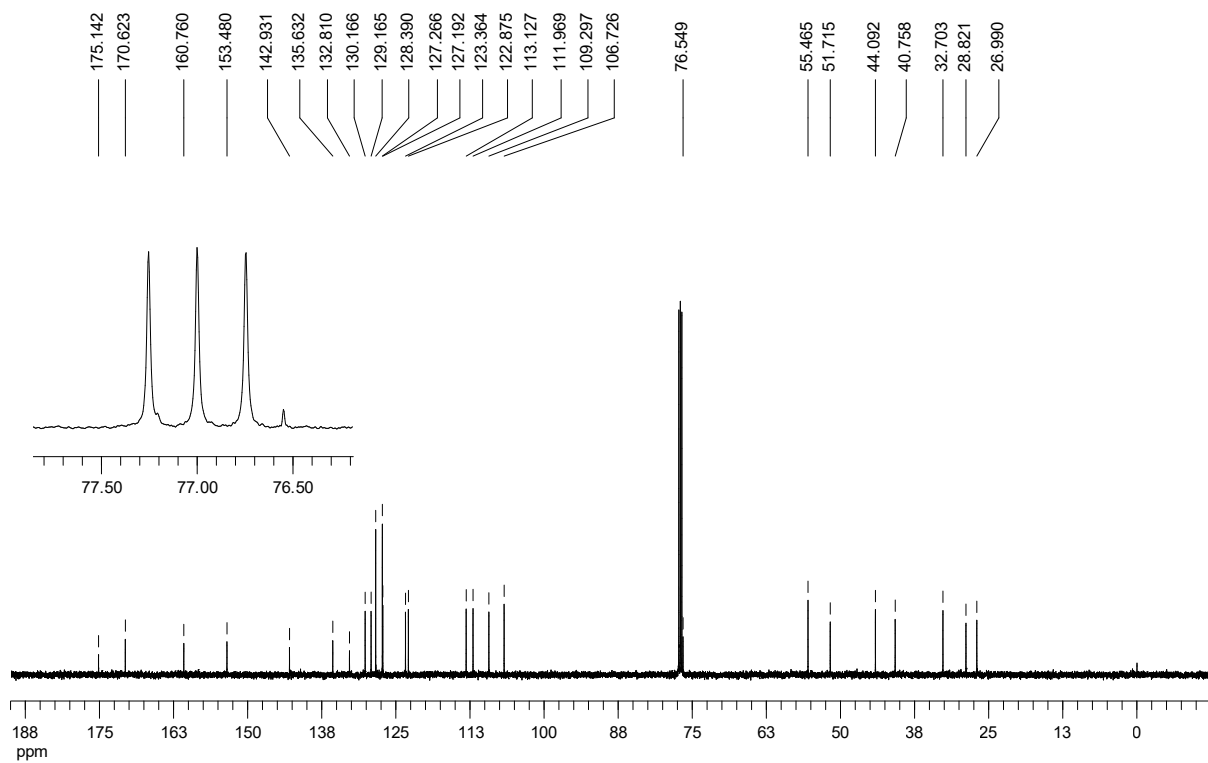
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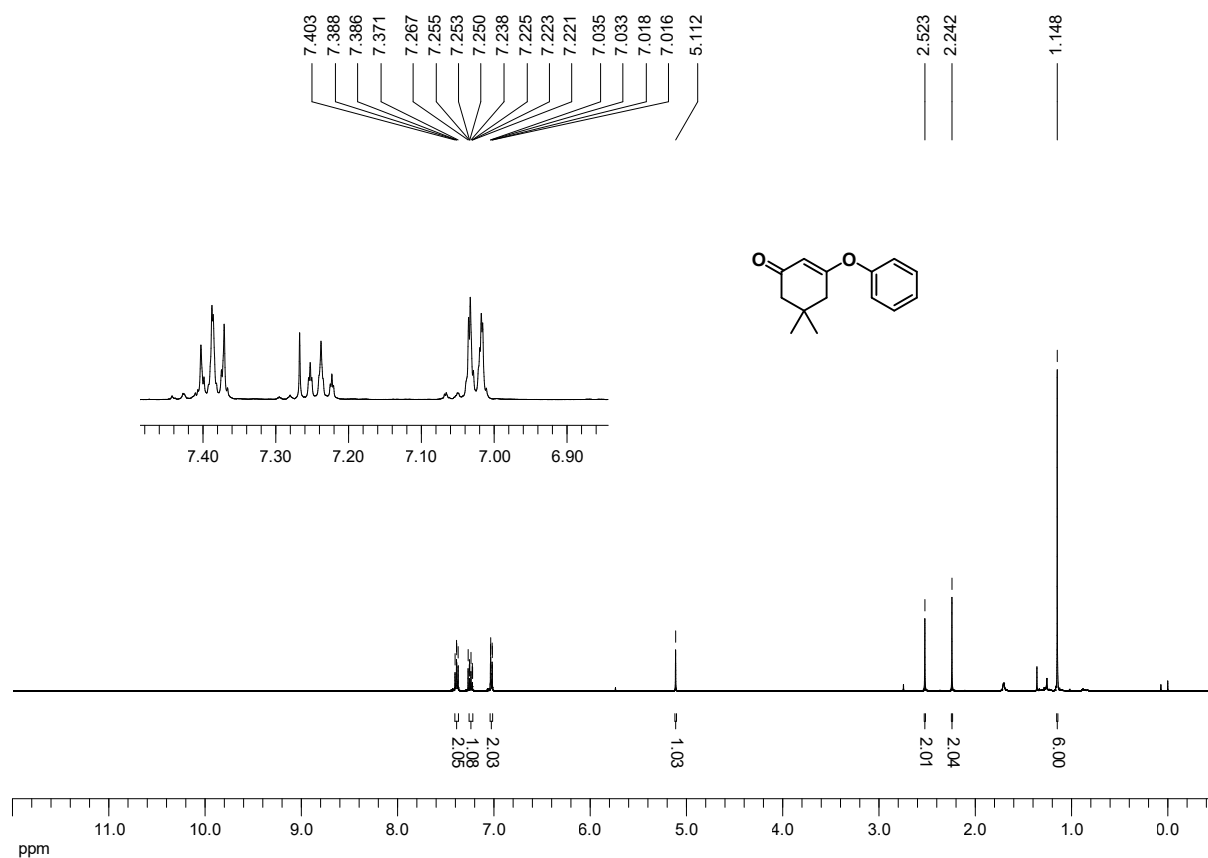
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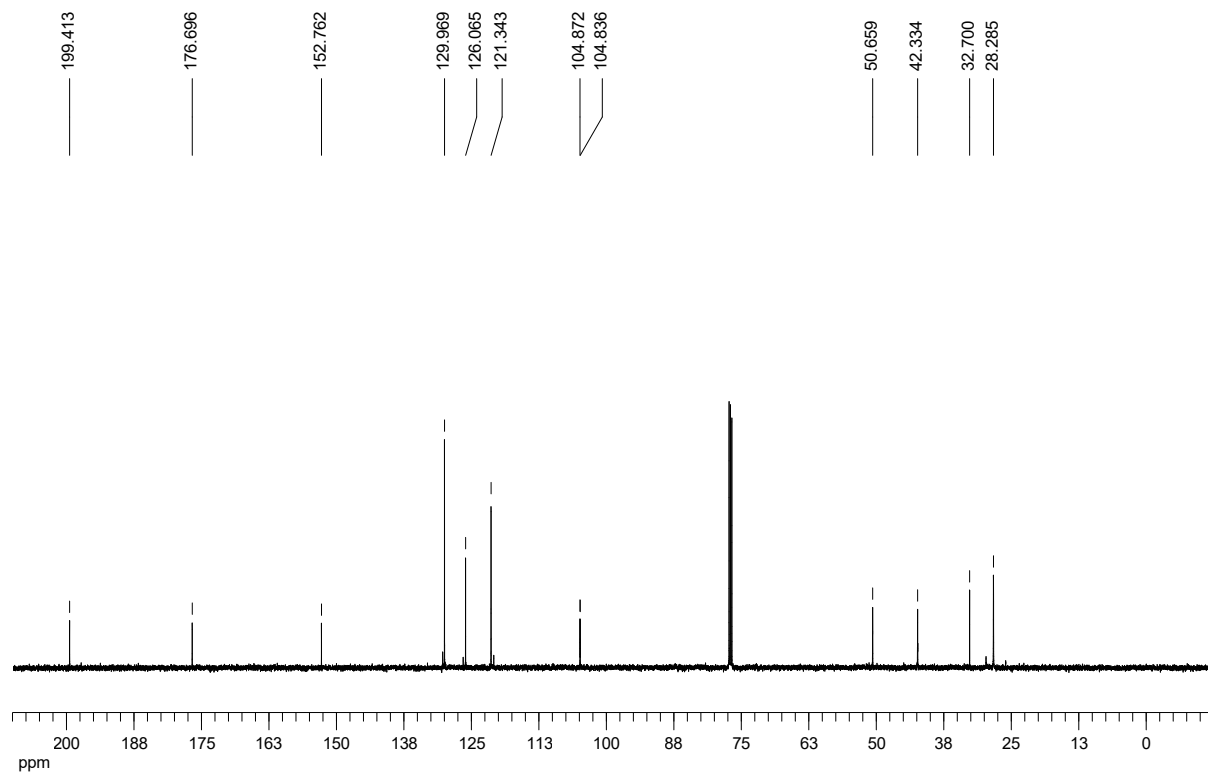
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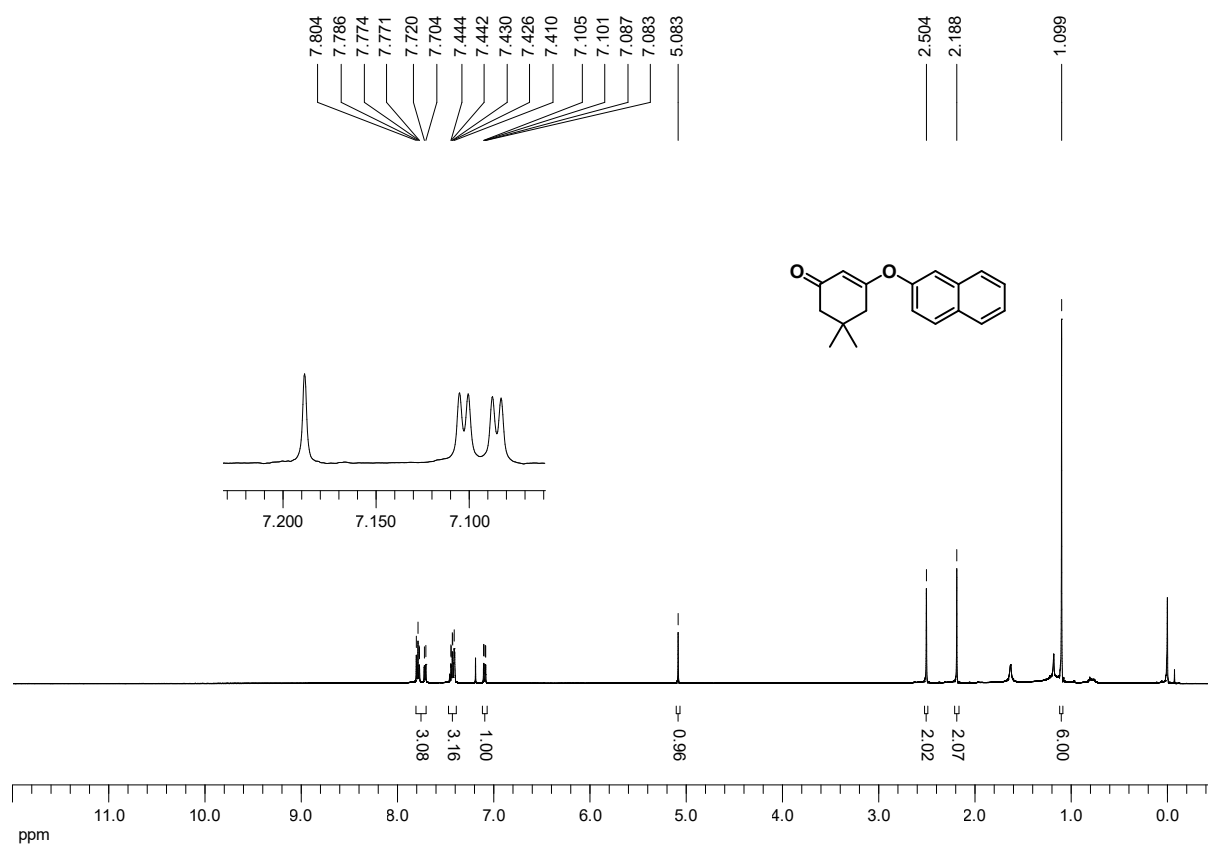
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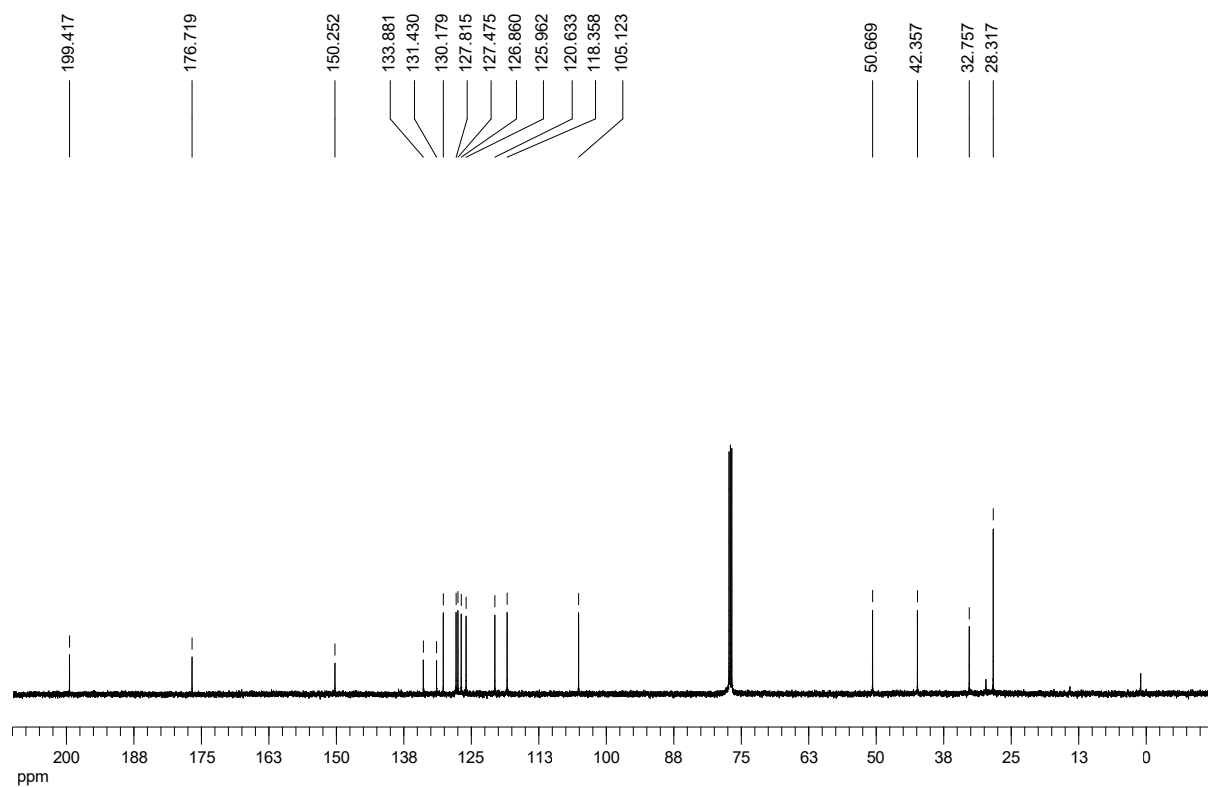
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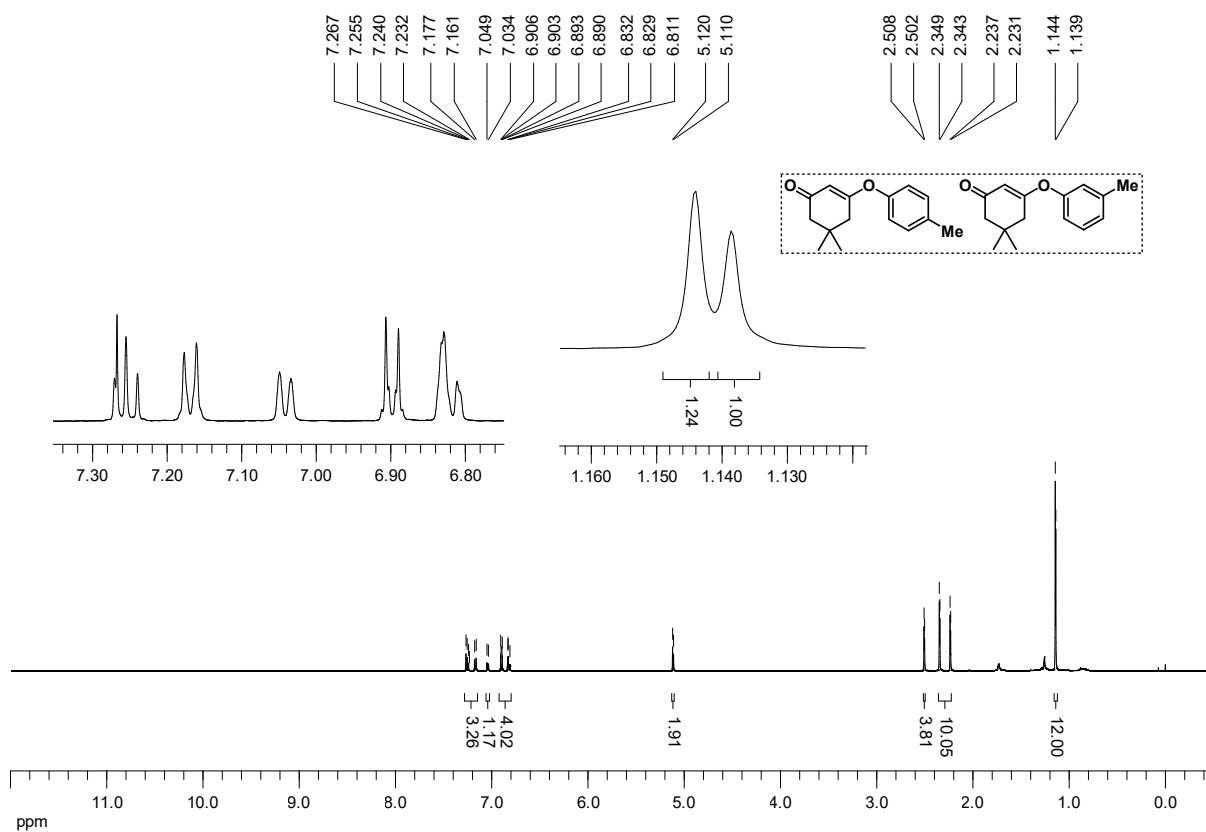
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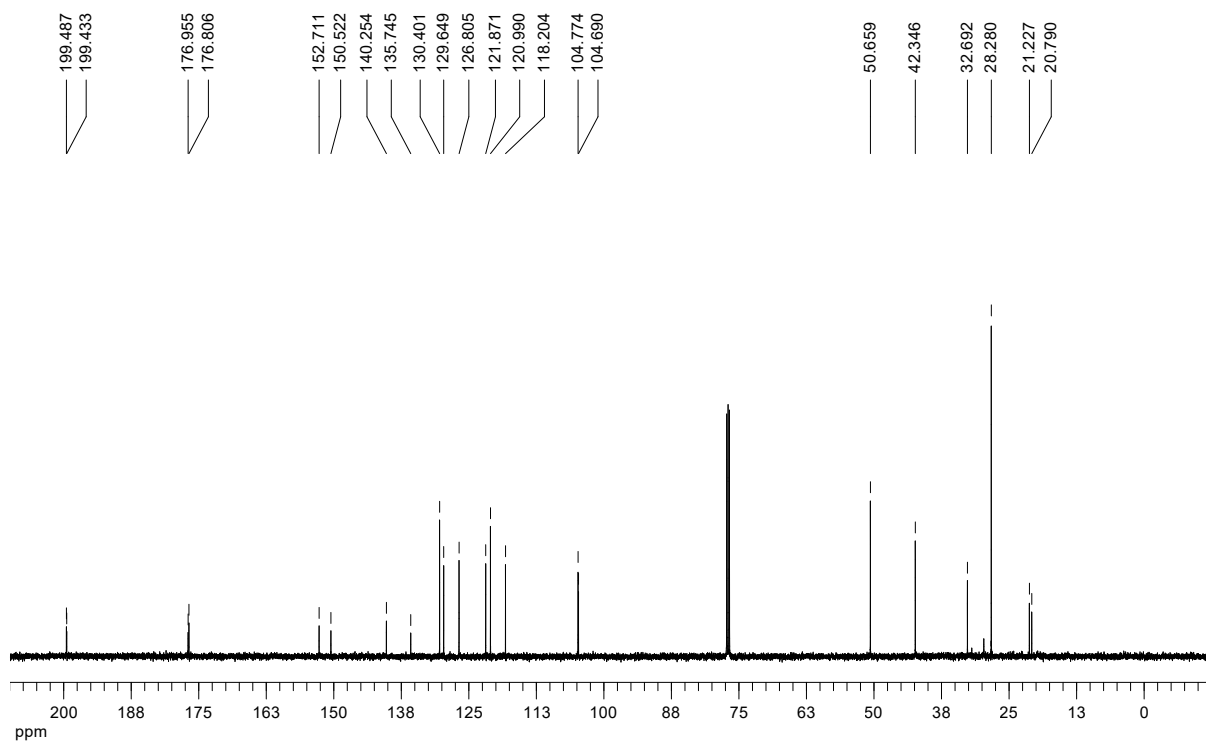
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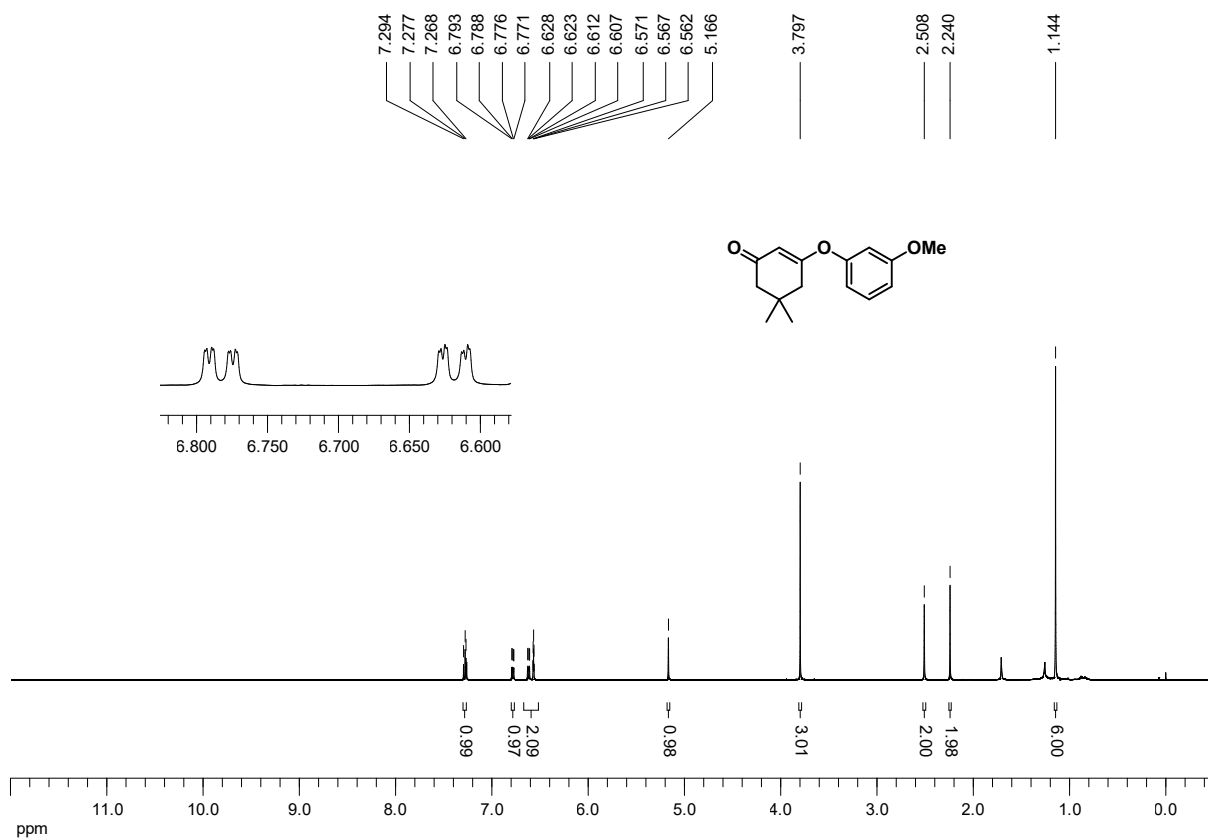
¹H NMR of **5aea** & **5ae'a** (CDCl₃, 500 MHz)



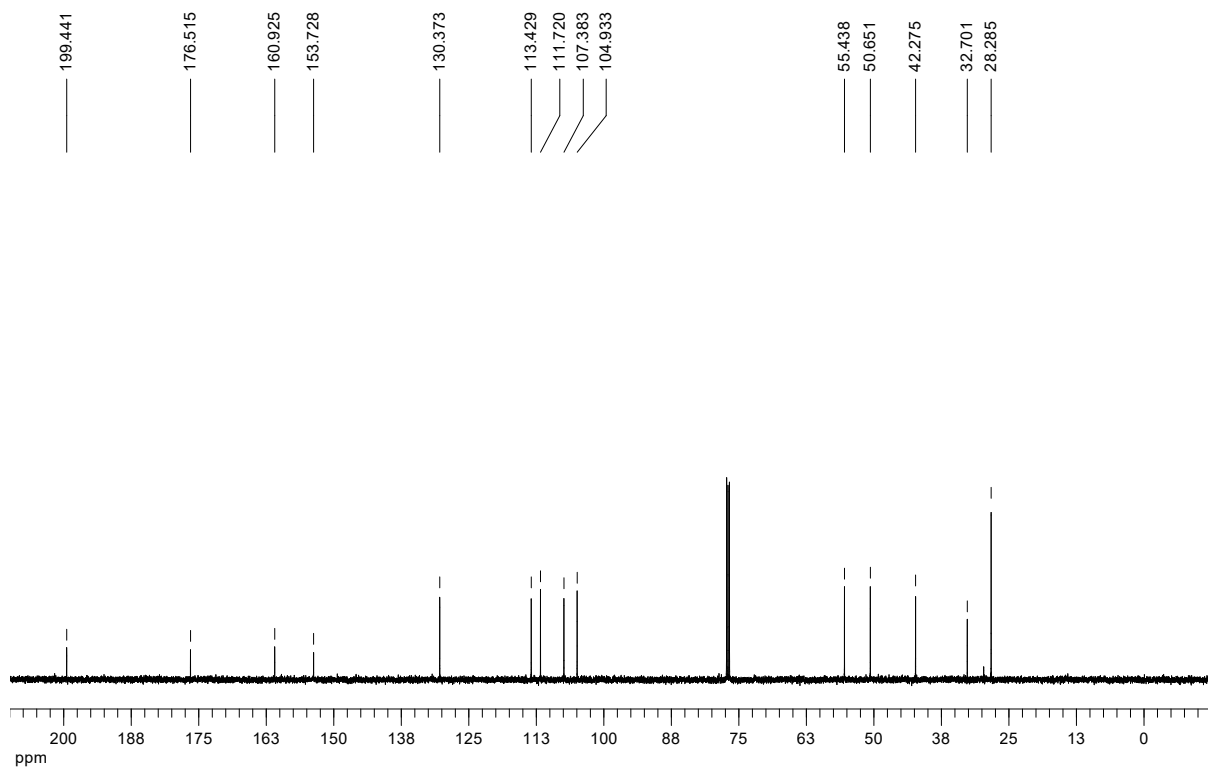
¹³C NMR of **5aea** & **5ae'a** (CDCl₃, 500 MHz)

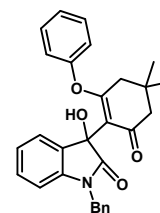
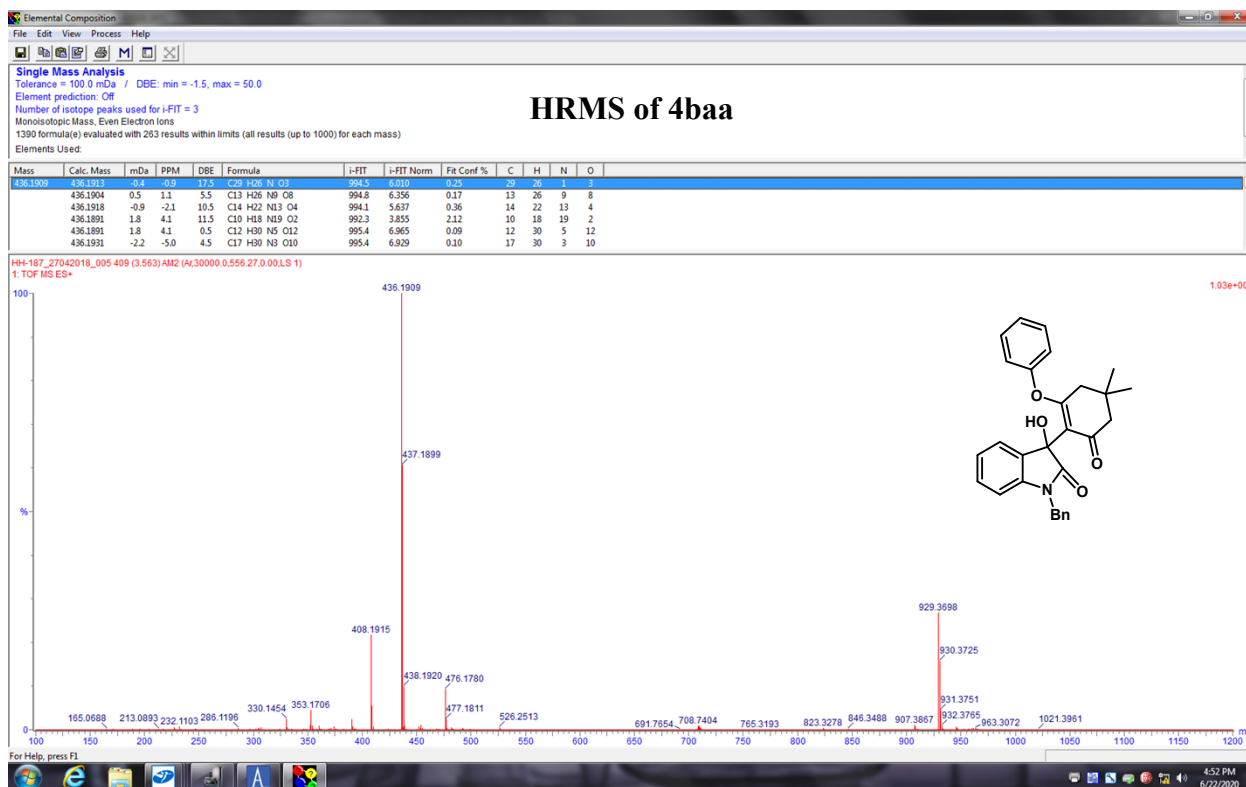
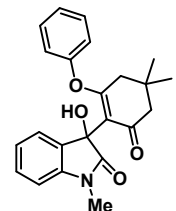
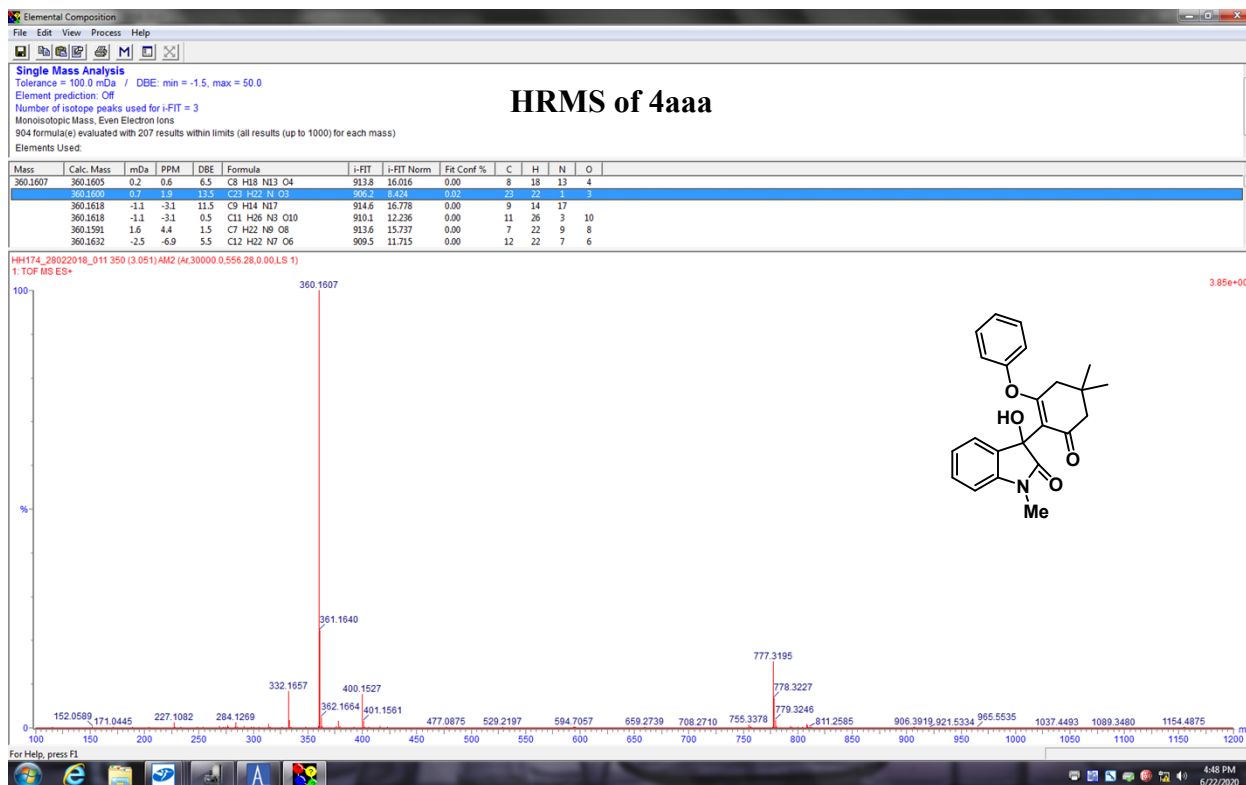


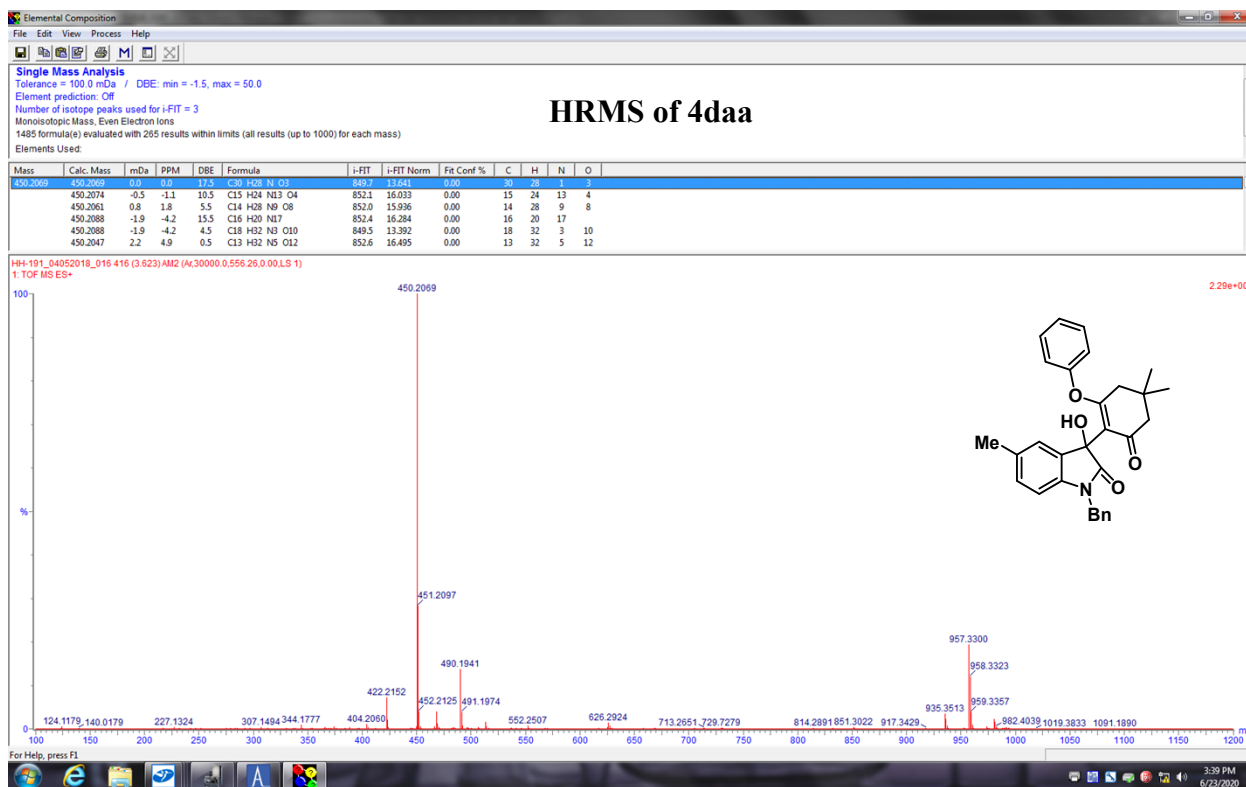
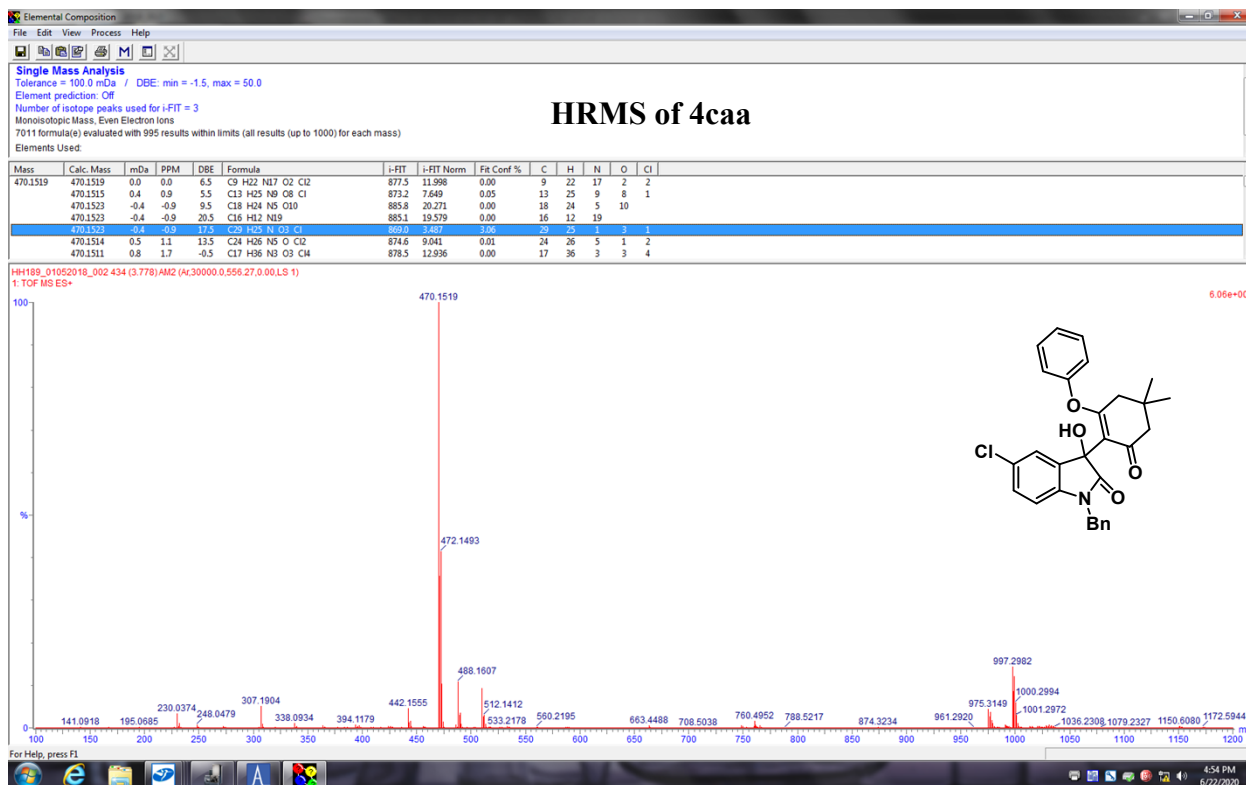
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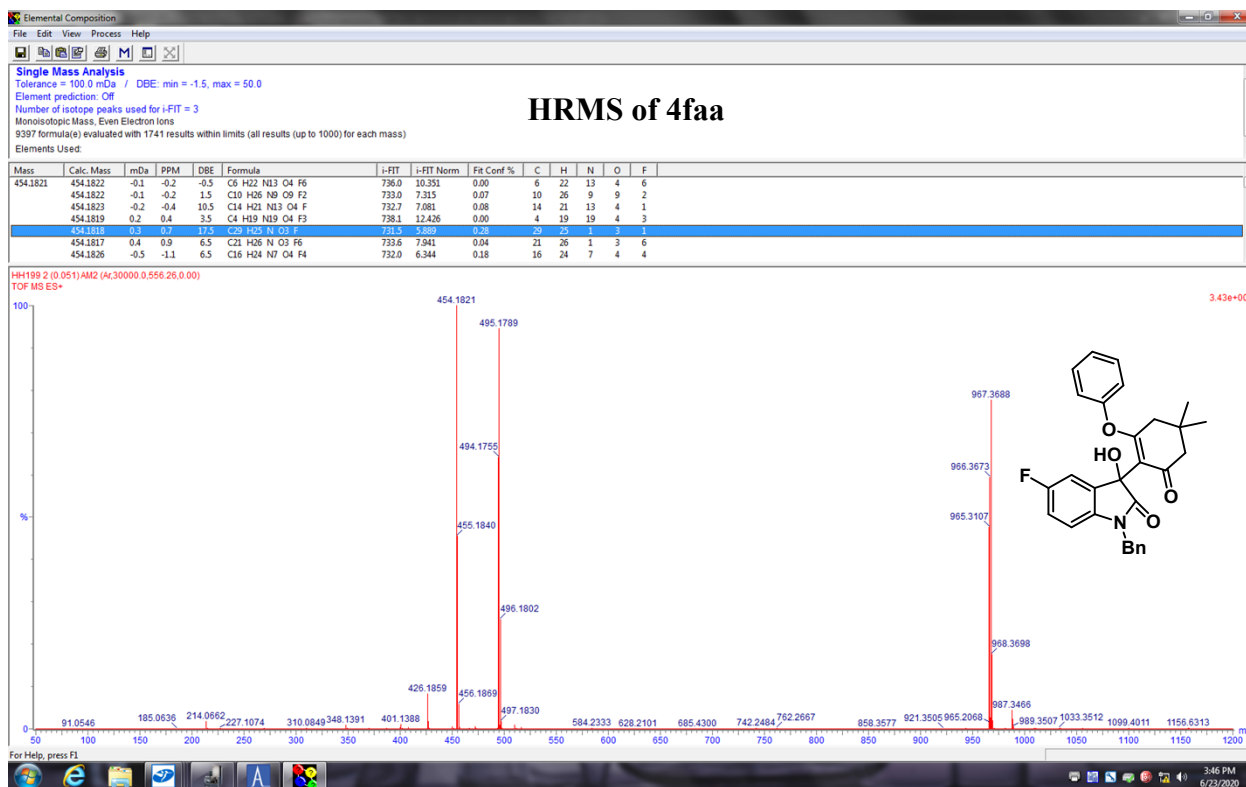
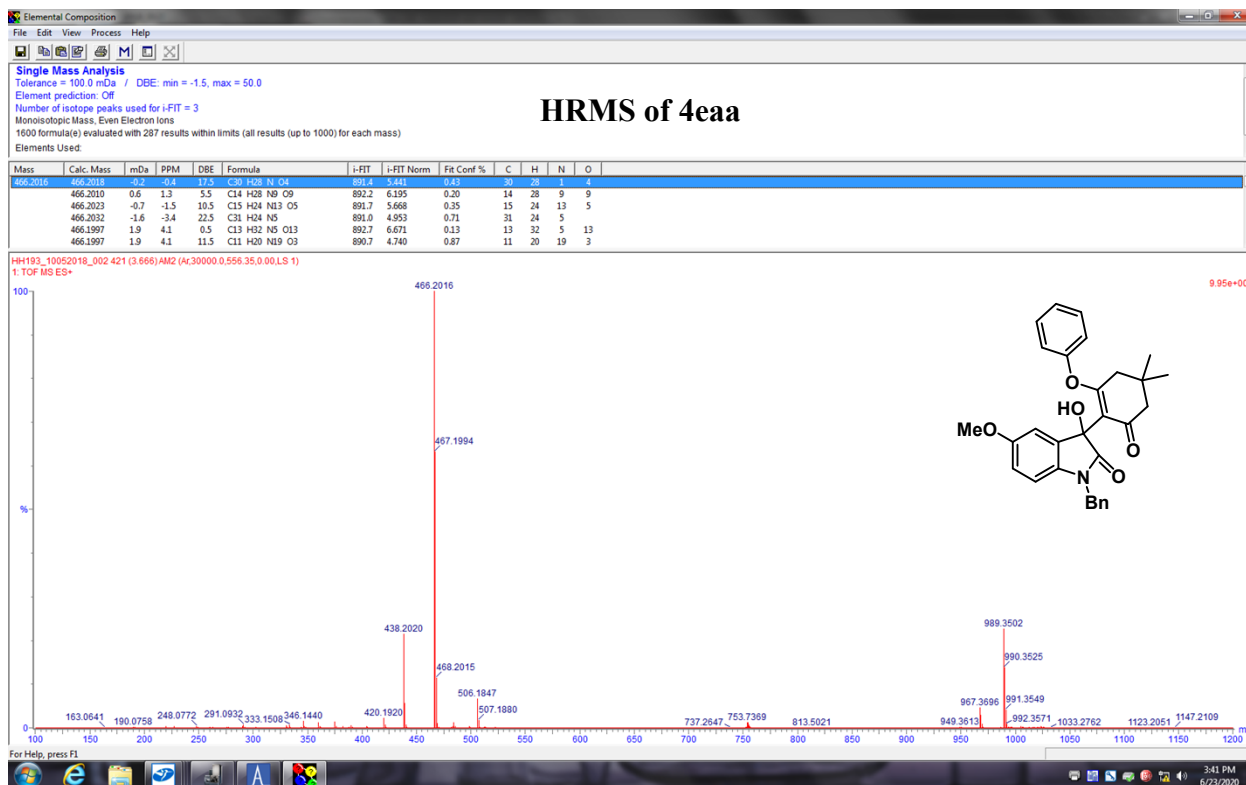


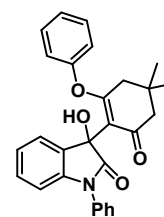
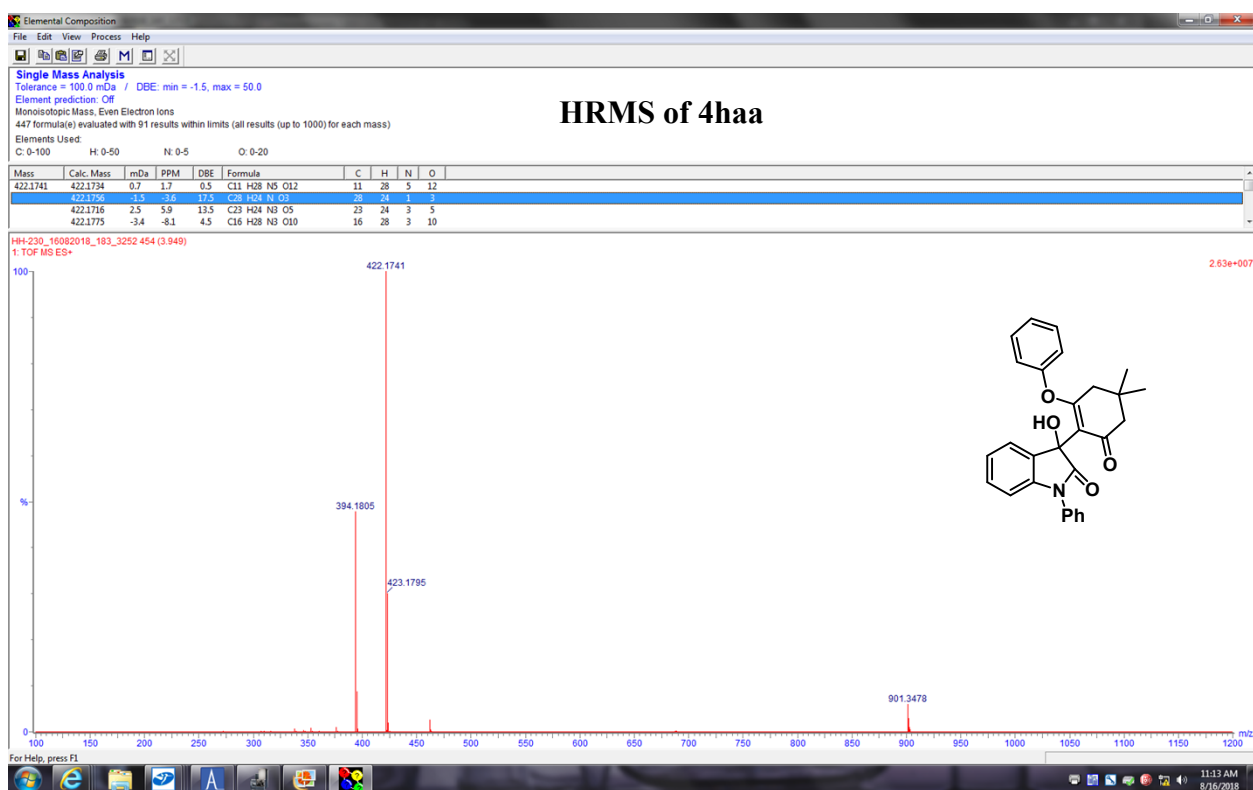
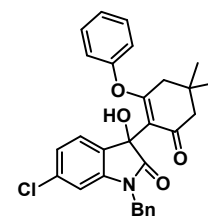
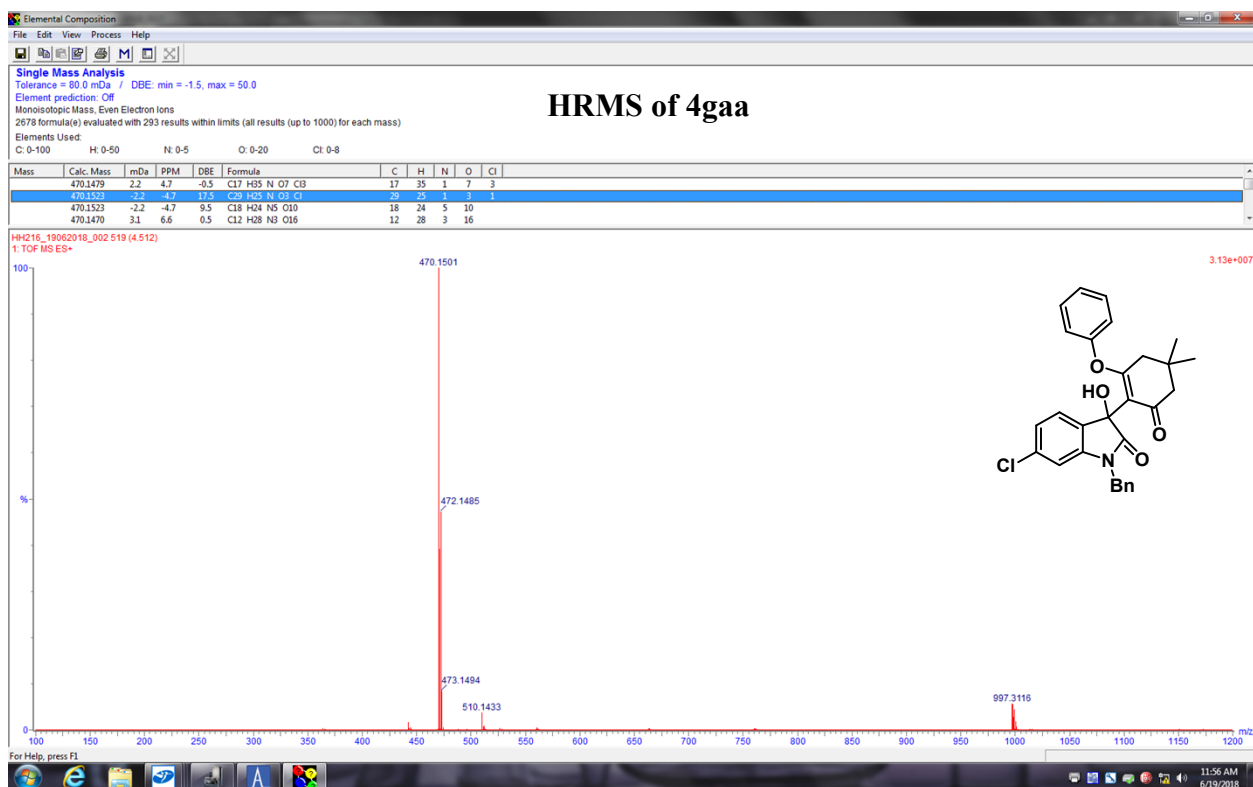
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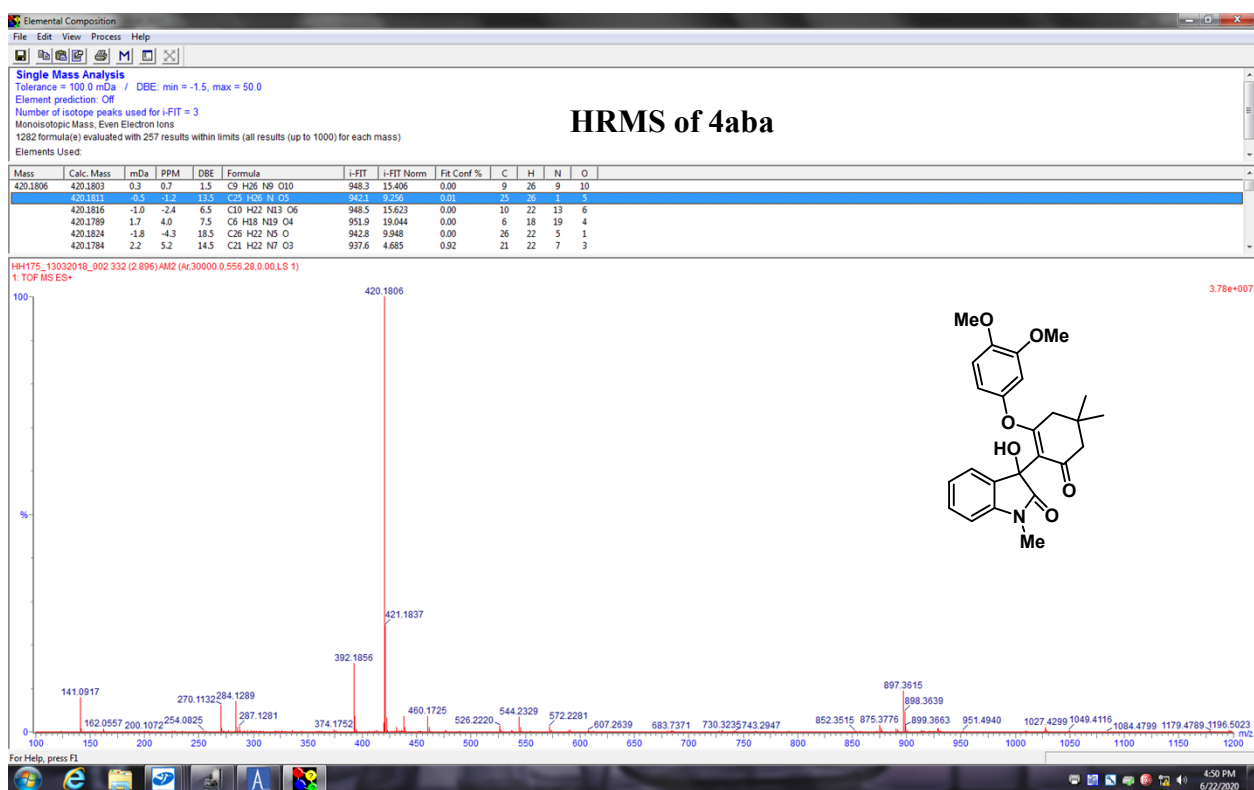
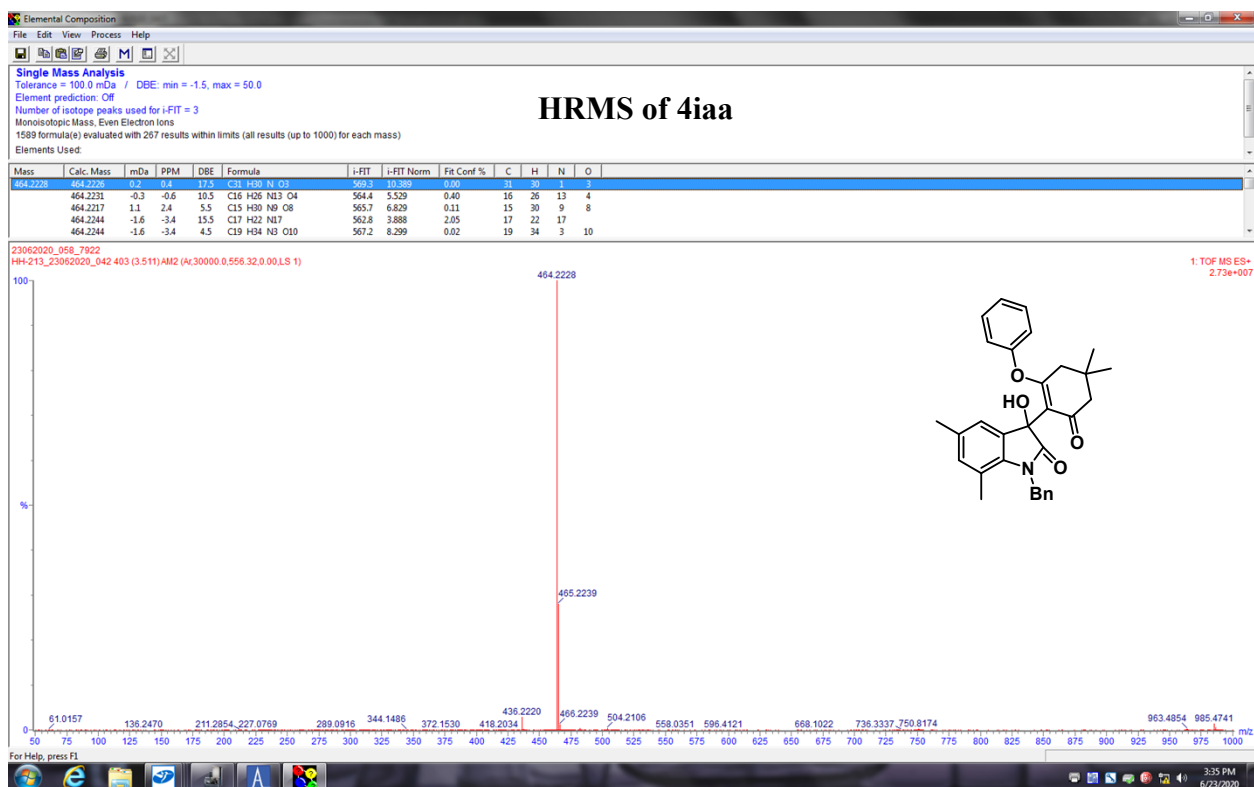


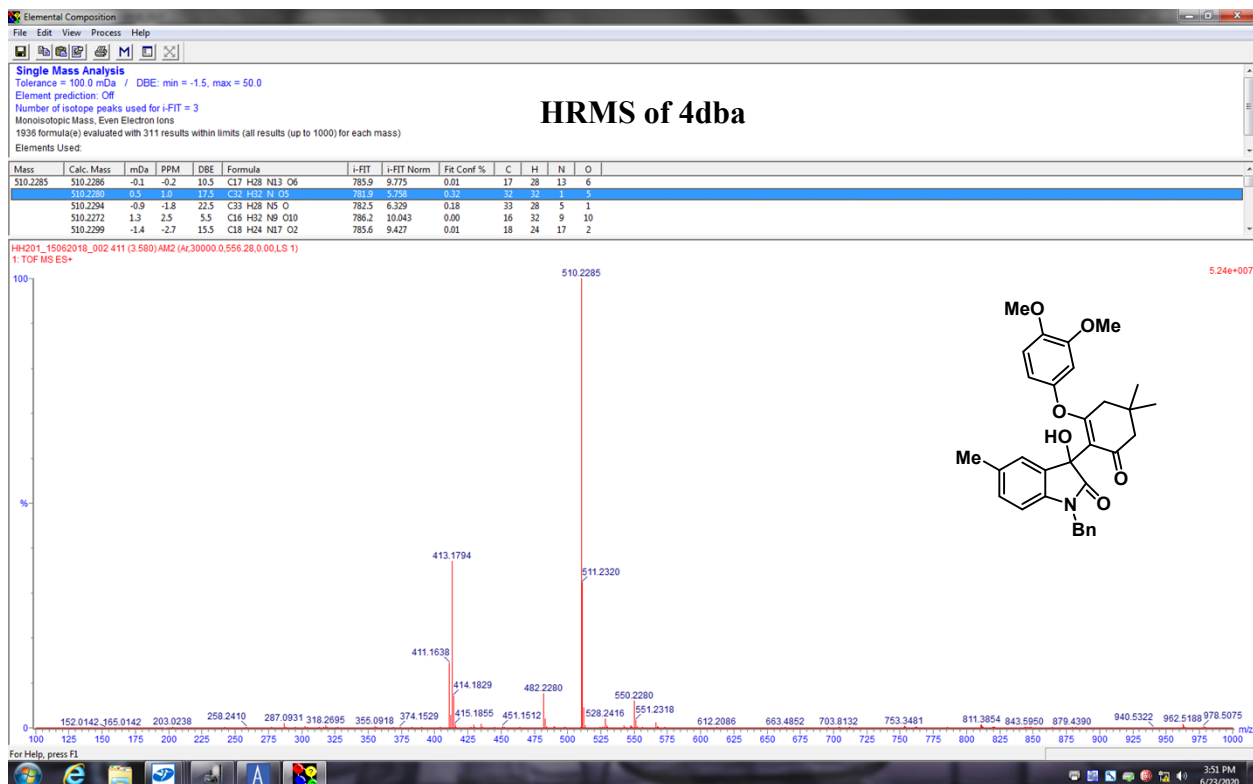
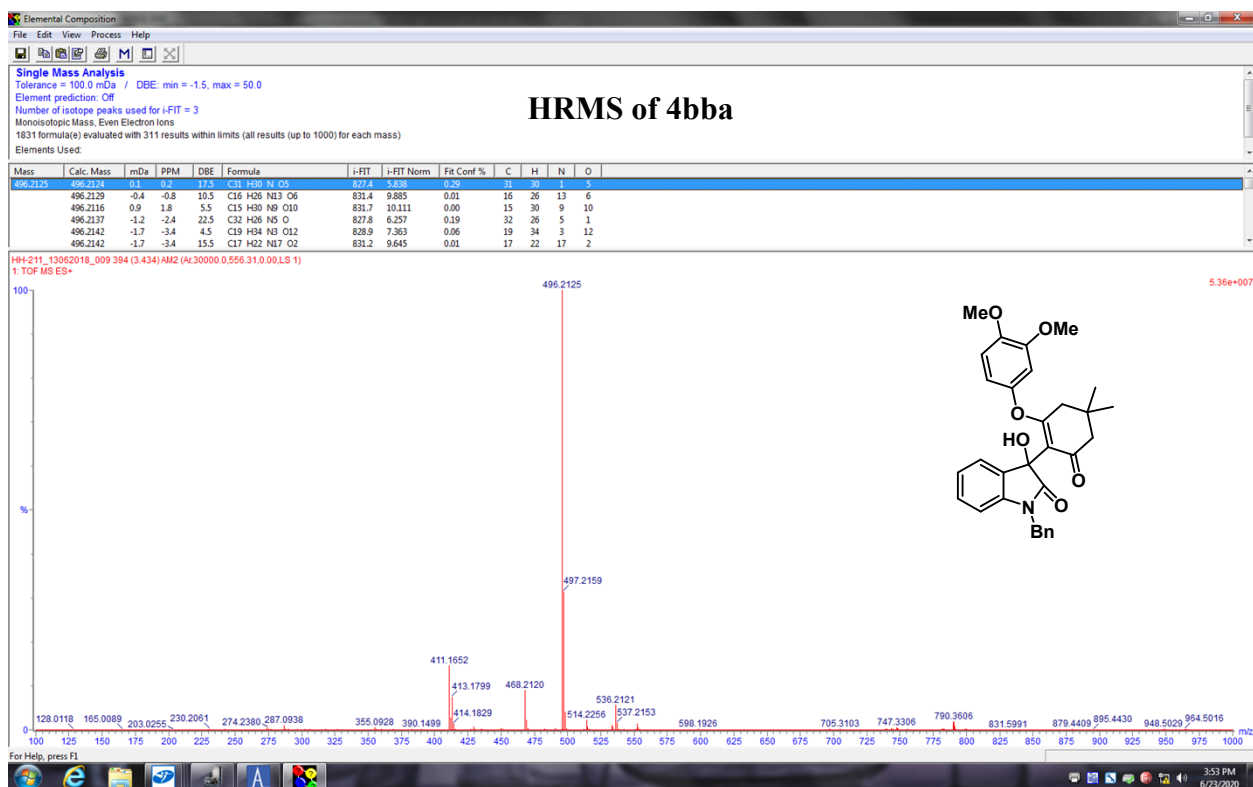


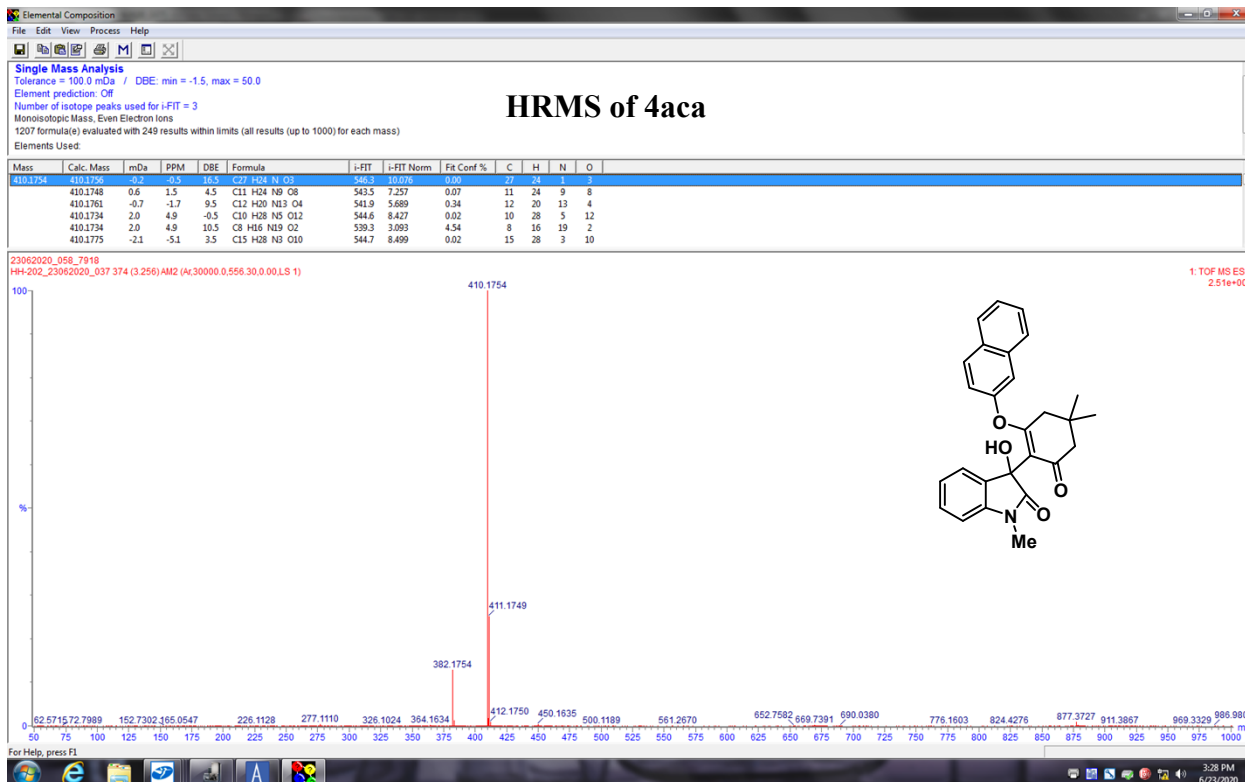
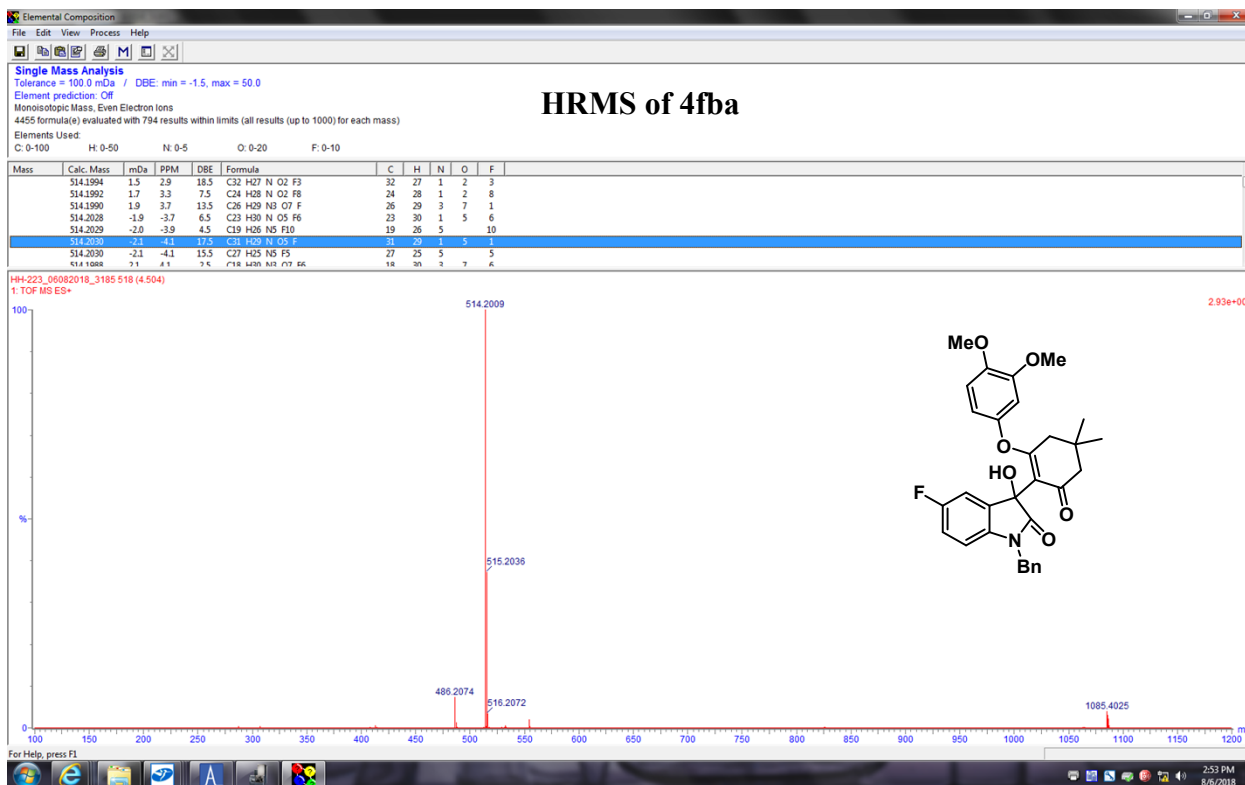


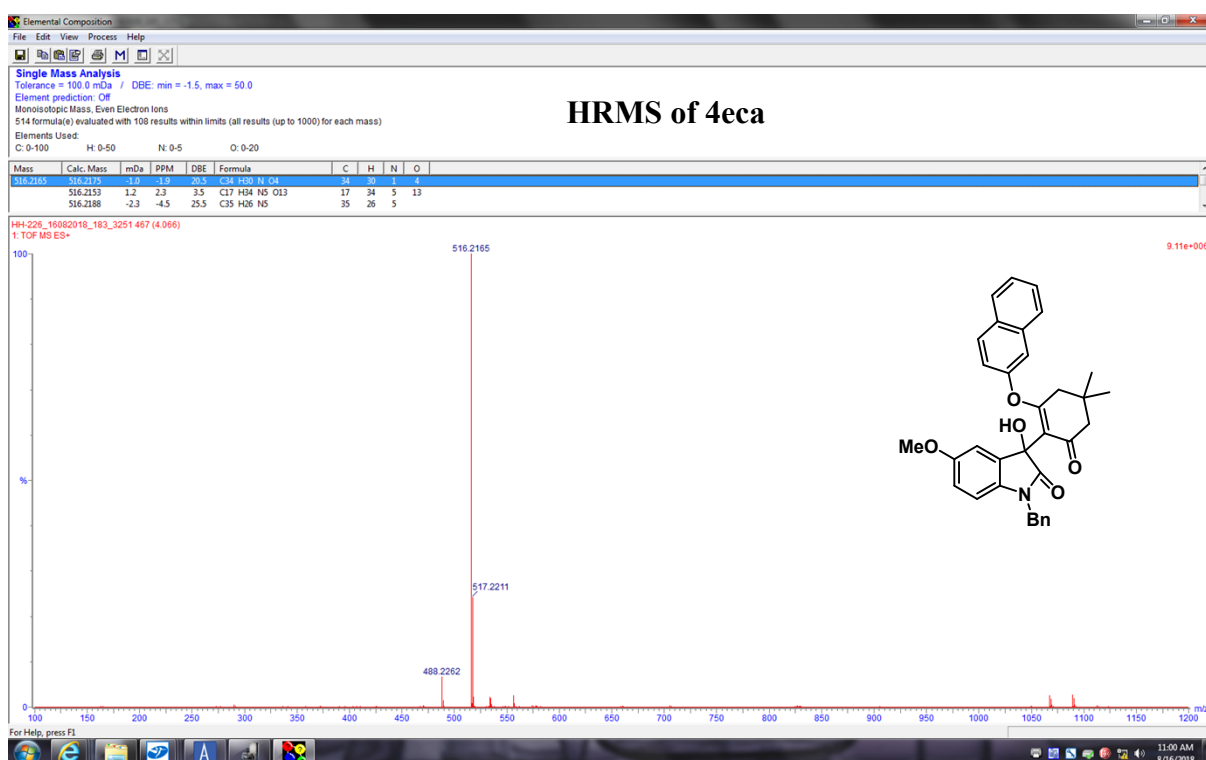
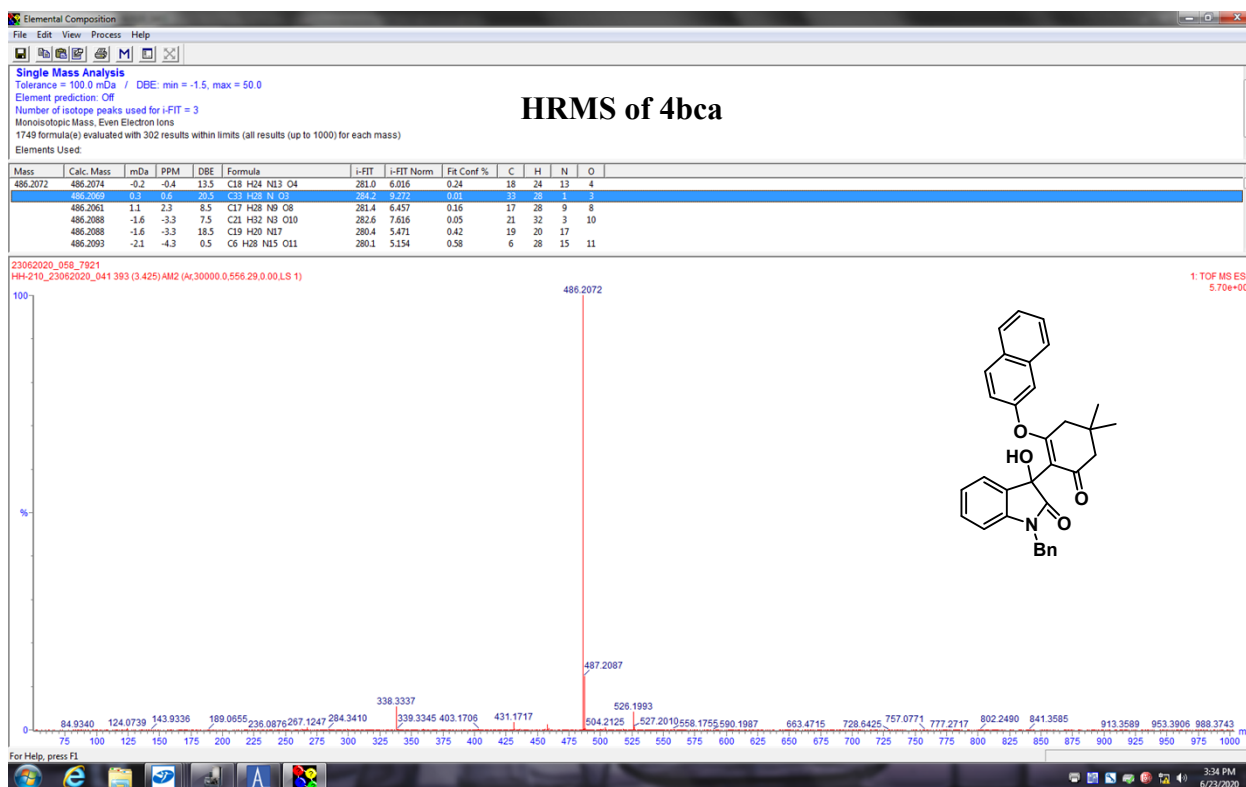


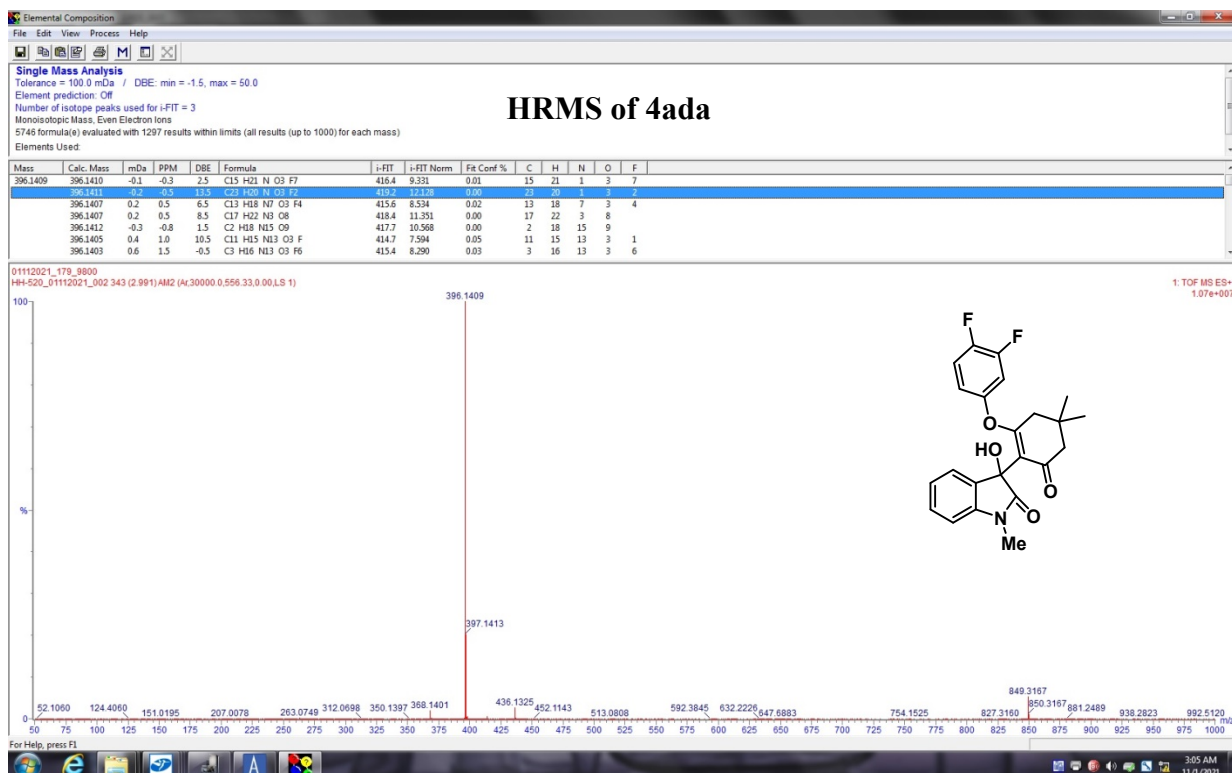
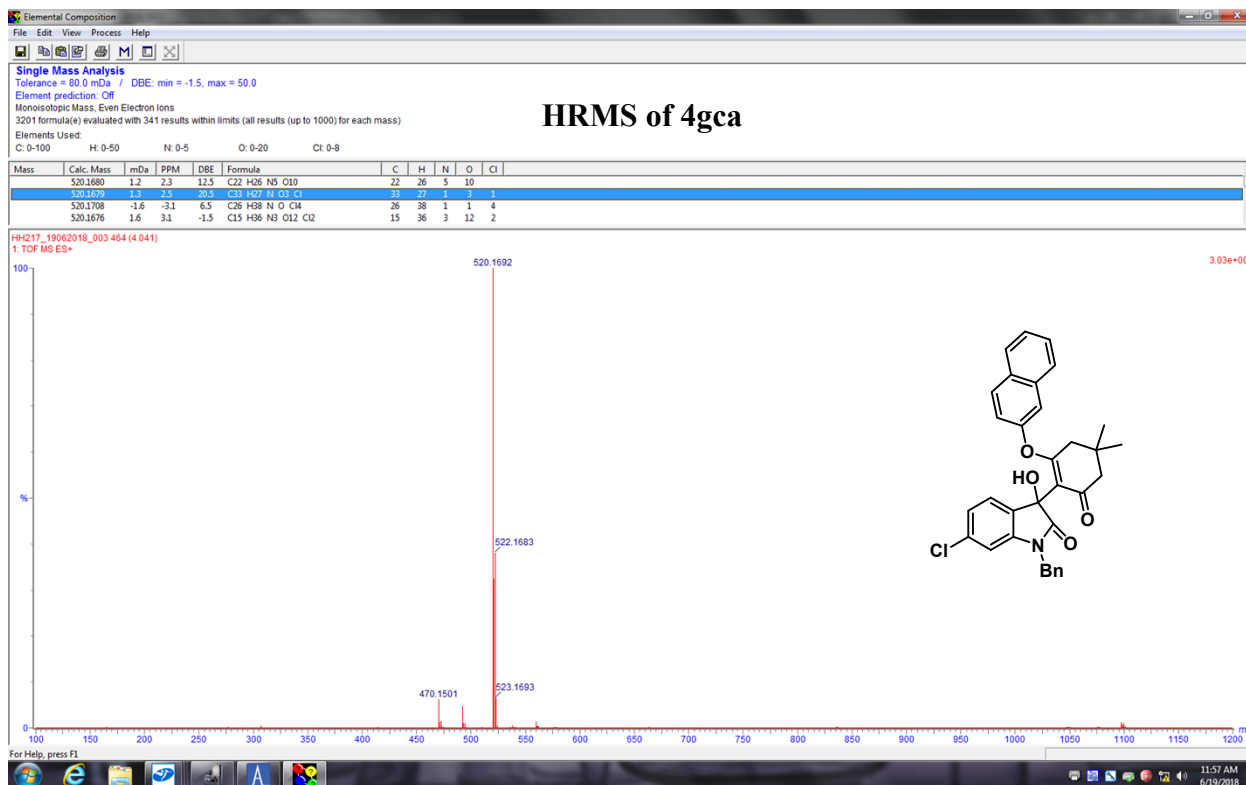


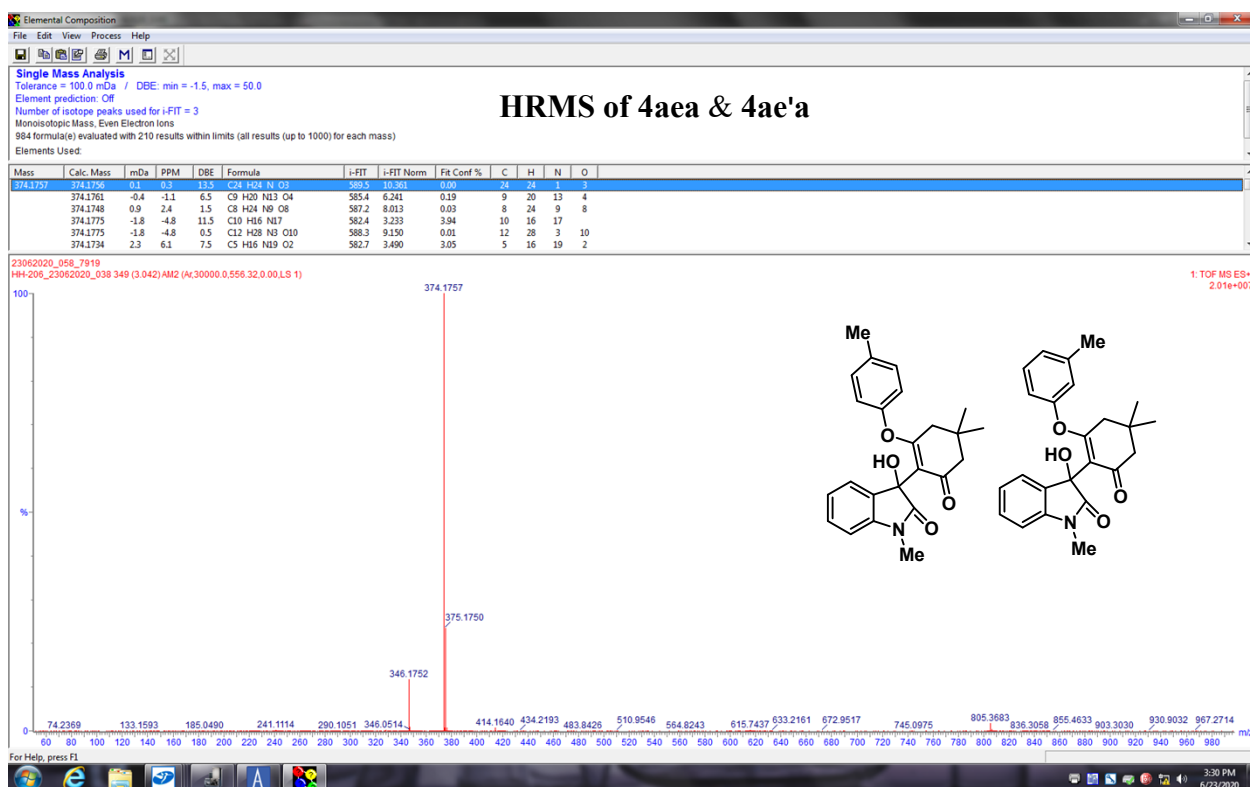
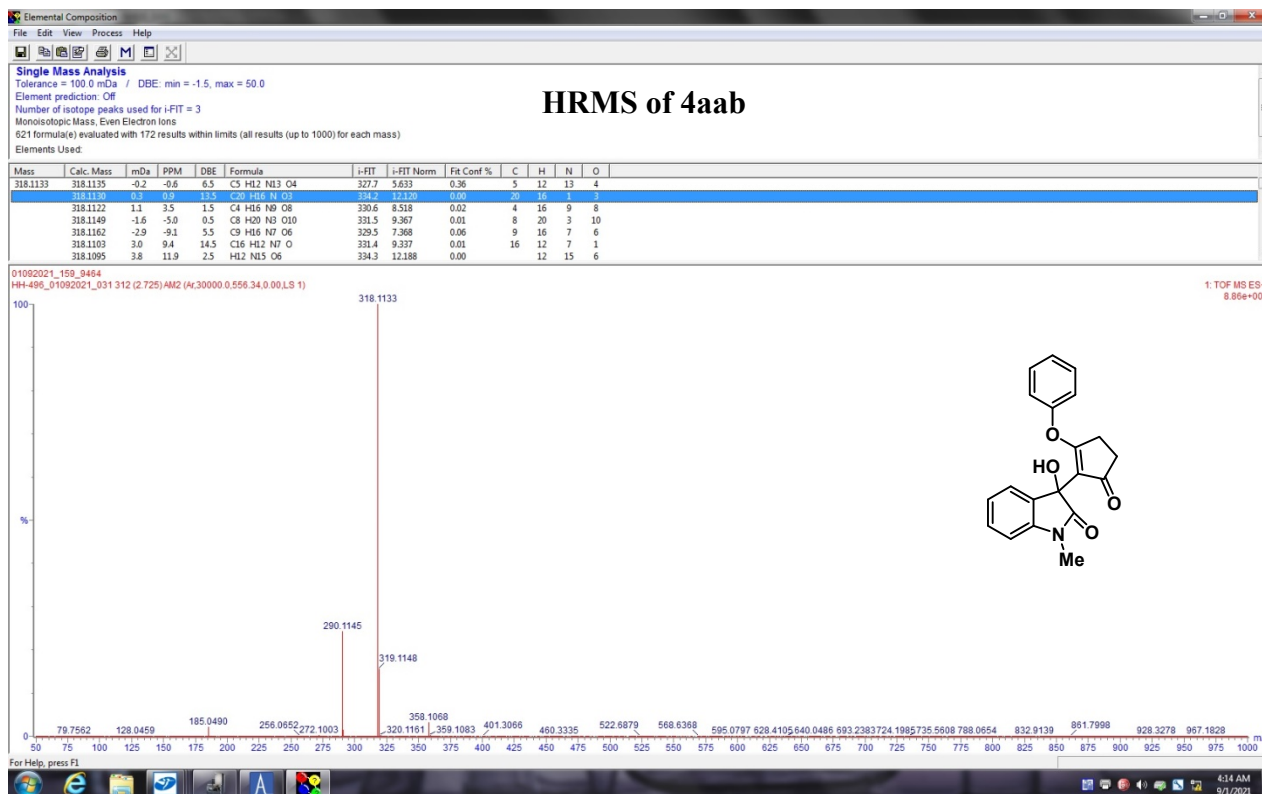


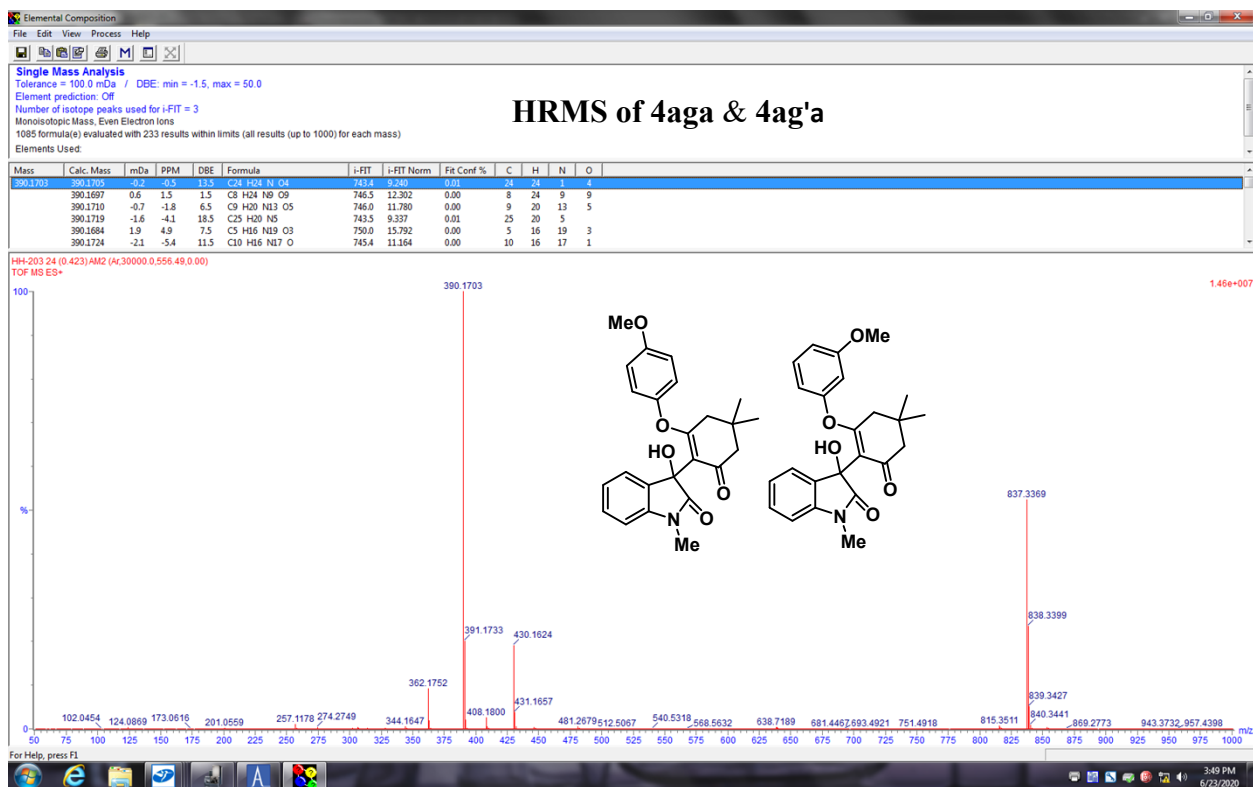
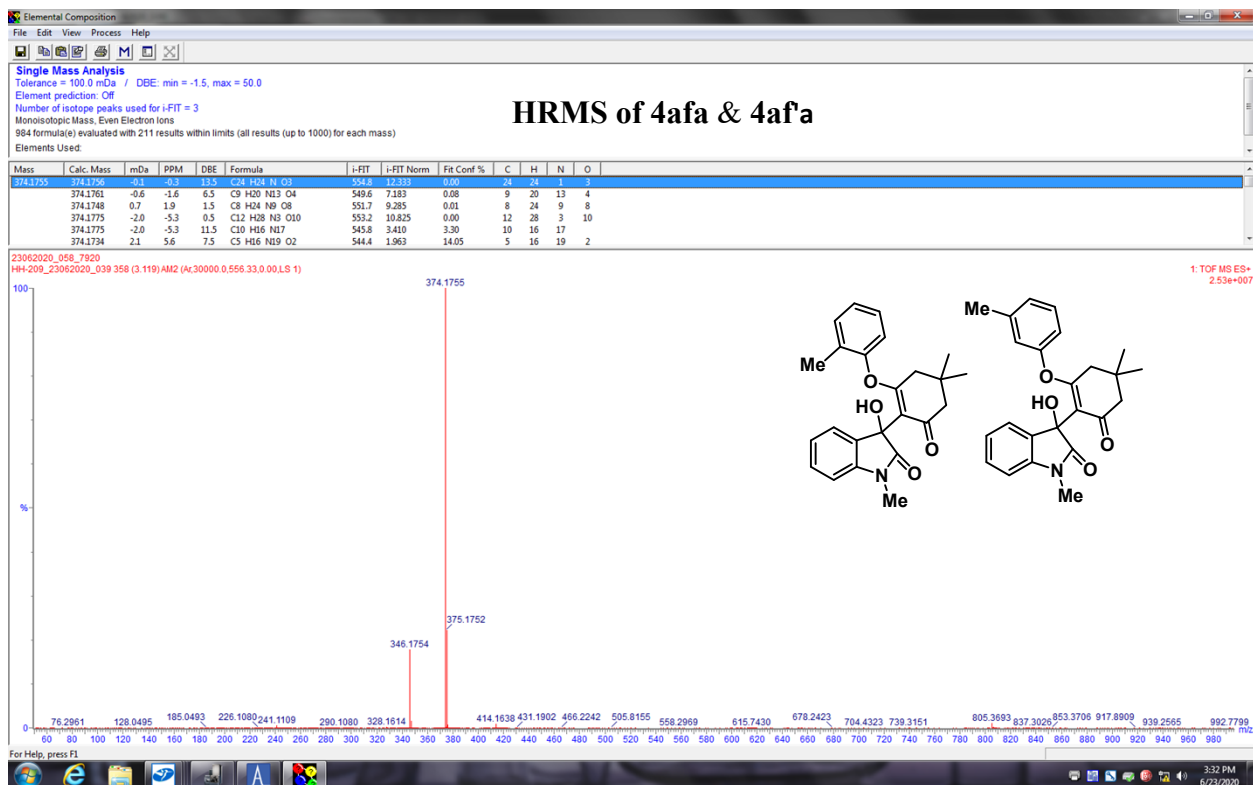


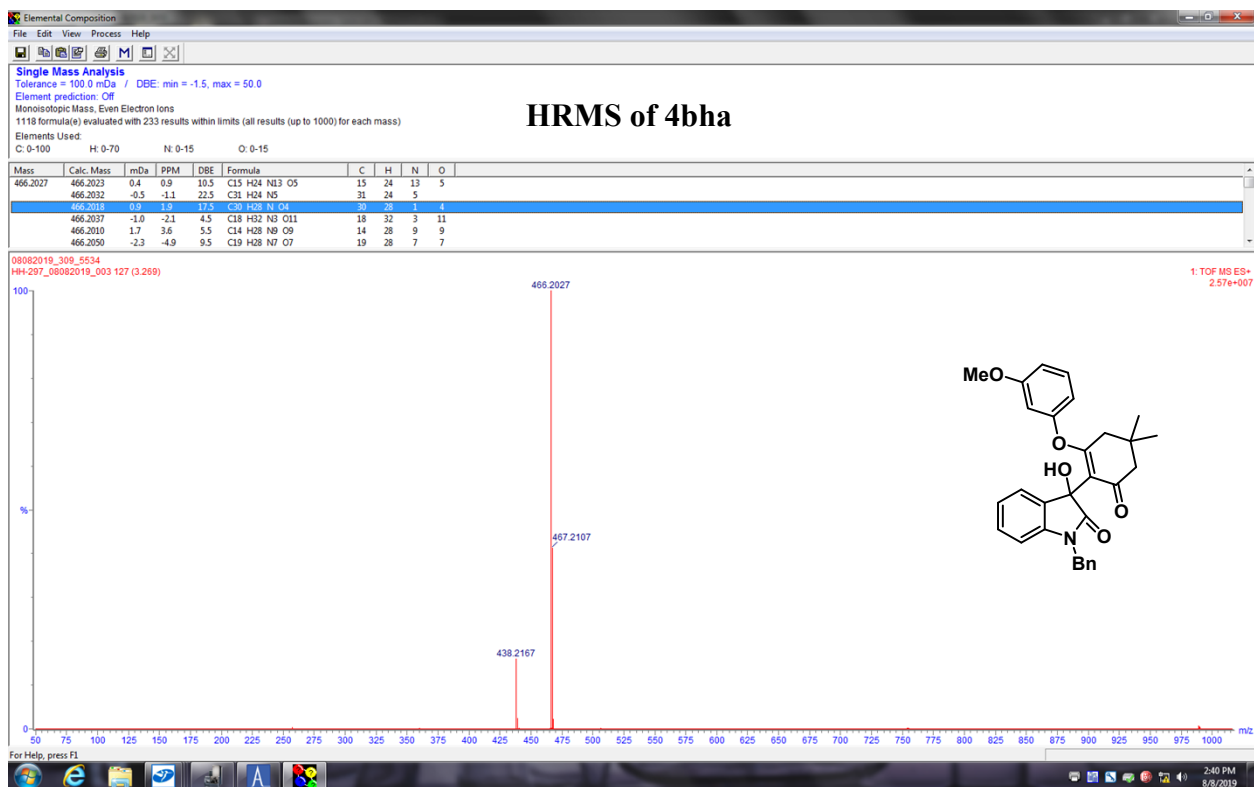
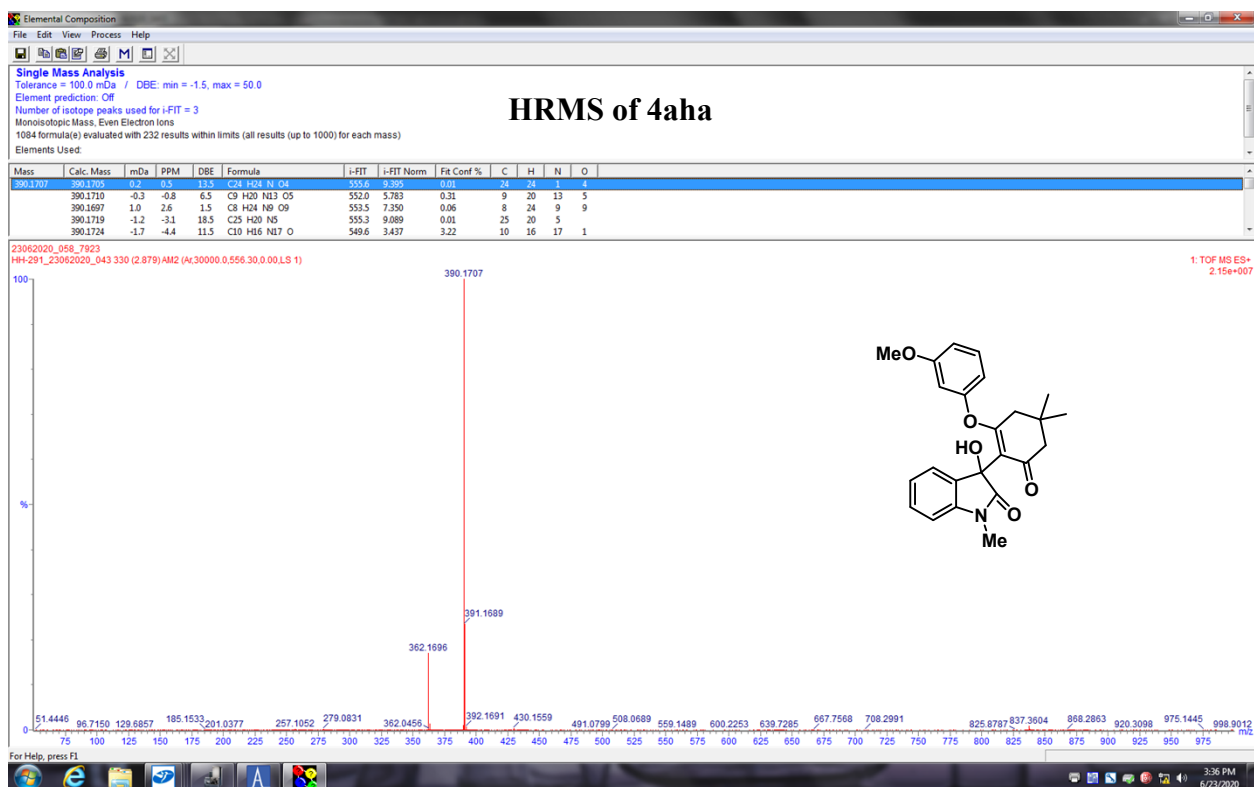


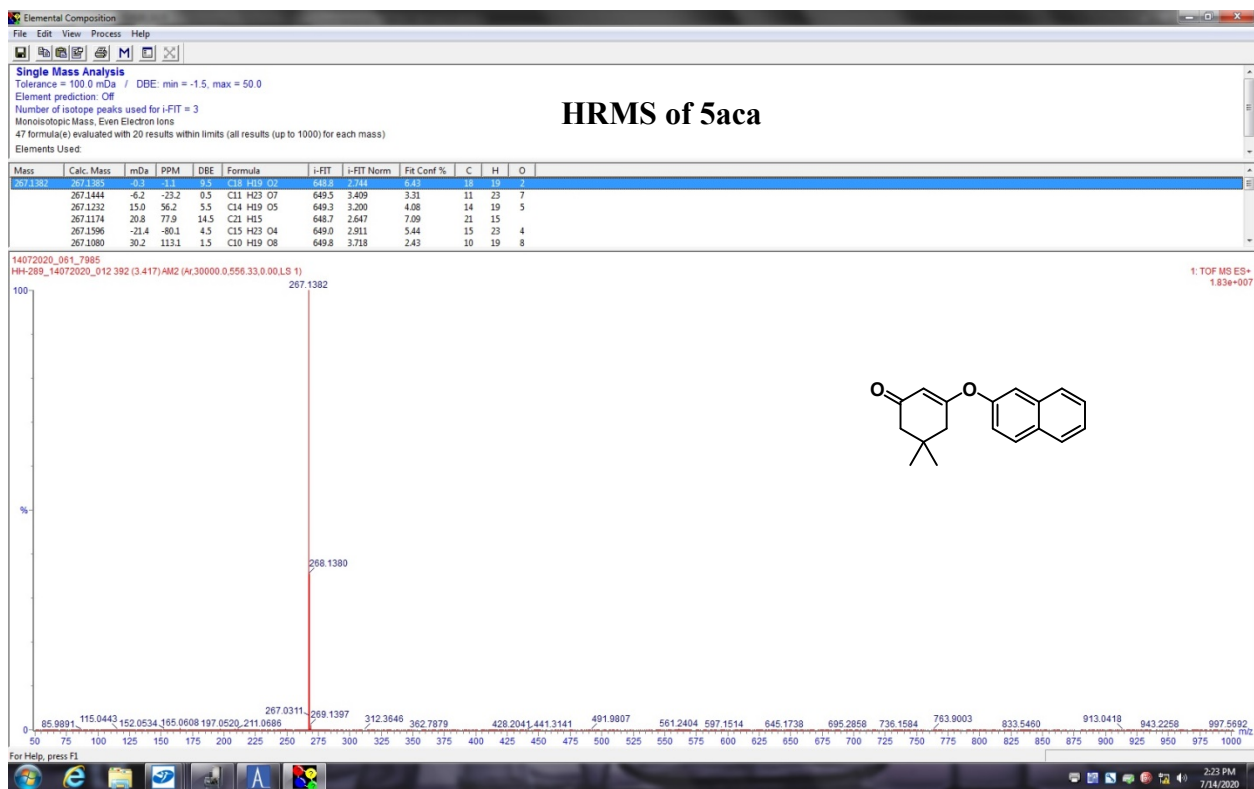
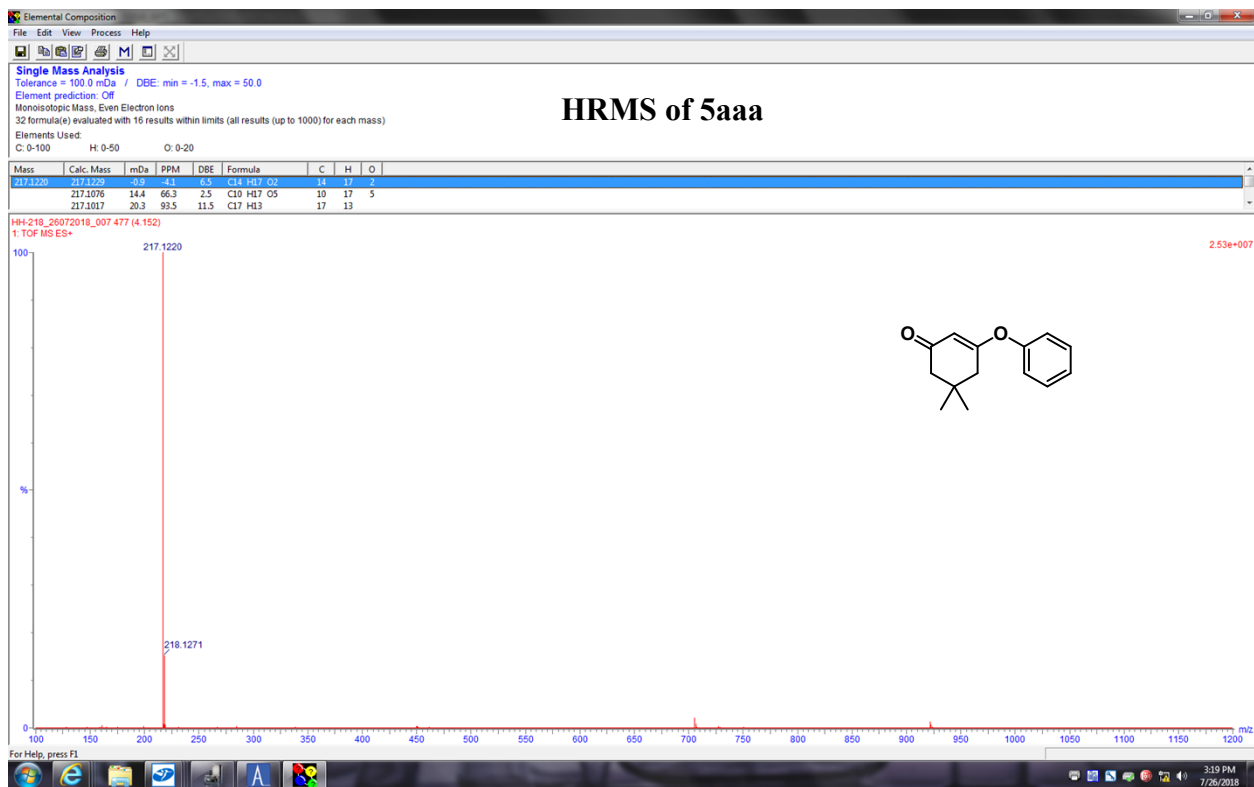


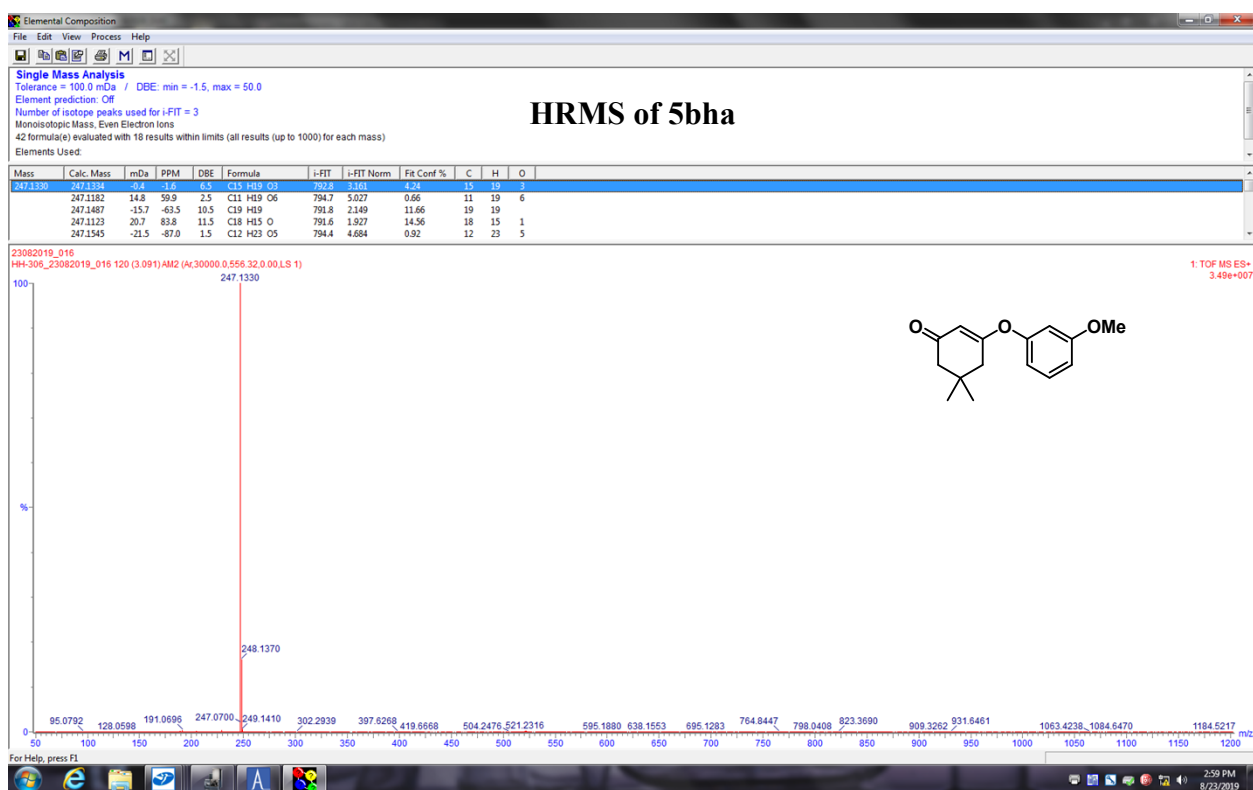
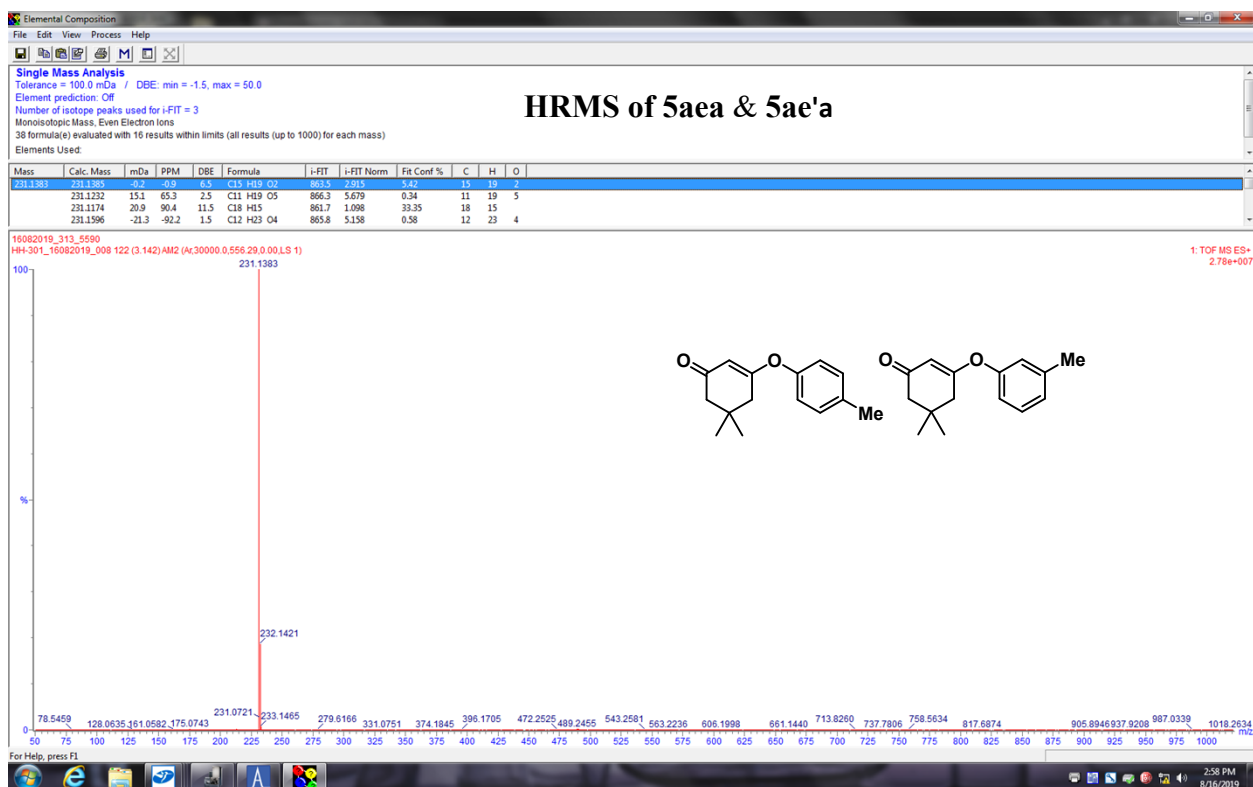












Sample preparation and crystal structure determination of 4baa

The pure compound **4baa** as obtained from column chromatography was crystallized from a mixture solvent of hexanes and EtOH (90:10). [CCDC 2098054 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/conts/retrieving.html]

Check CIF Report of 4baa:

CIF check Report: Datablock: HH-187_0ma_a

Bond precision:	C-C = 0.0033 Å	Wavelength=0.71073
Cell:	a=13.578 (4) b=11.198 (3) c=15.831 (5)	
	alpha=90 beta=94.443 (4) gamma=90	
Temperature:	296 K	
	Calculated	Reported
Volume	2399.8 (12)	2399.8 (13)
Space group	P 21/n	P 21/n
Hall group	-P 2yn	-P 2yn
Moiety formula	C29 H27 N O4	?
Sum formula	C29 H27 N O4	C29 H27 N O4
Mr	453.52	453.51
Dx, g cm ⁻³	1.255	1.255
Z	4	4
Mu (mm ⁻¹)	0.083	0.083
F000	960.0	960.0
F000'	960.45	
h, k, lmax	16, 13, 18	16, 13, 18
Nref	4212	4212
Tmin, Tmax	0.978, 0.989	
Tmin'	0.975	
Correction method=	Not given	
Data completeness=	1.000	Theta (max) = 24.994
R(reflections)=	0.0534 (3013)	wR2(reflections)=
		0.1561 (4212)
S =	1.045	Npar= 311

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

● Alert level C

[RINTA01_ALERT_3_C](#) The value of Rint is greater than 0.12
Rint given 0.130
[PLAT230_ALERT_2_C](#) Hirshfeld Test Diff for C28 --C29 . 5.5
s.u.
[PLAT906_ALERT_3_C](#) Large K Value in the Analysis of Variance 2.034
Check

● Alert level G

[PLAT007_ALERT_5_G](#) Number of Unrefined Donor-H Atoms 1
Report
[PLAT020_ALERT_3_G](#) The Value of Rint is Greater Than 0.12 0.130
Report
[PLAT793_ALERT_4_G](#) Model has Chirality at C15 (Centro SPGR) S
Verify
[PLAT883_ALERT_1_G](#) No Info/Value for _atom_sites_solution_primary . Please
Do !
[PLAT909_ALERT_3_G](#) Percentage of I>2sig(I) Data at Theta(Max) Still 38%
Note
[PLAT978_ALERT_2_G](#) Number C-C Bonds with Positive Residual Density. 3
Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
6 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Datablock HH-187_0ma_a - ellipsoid plot

