Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

A Palladium-Catalyzed Cascade Process for Spirooxindole: An Alternative Way for the Synthesis of Spiro(indoline-3,2′-quinazolin)-2-ones

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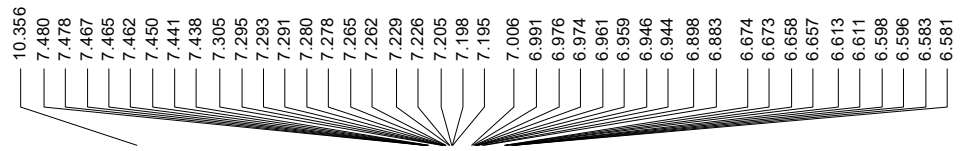
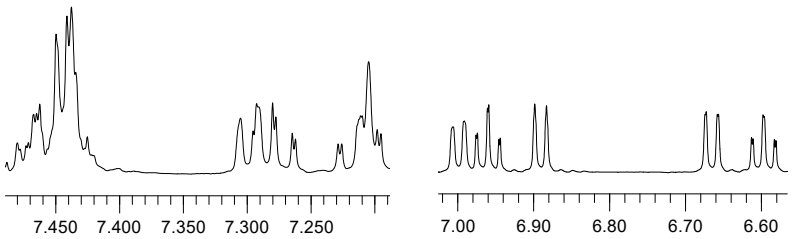
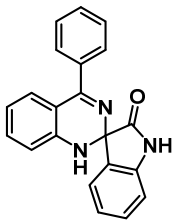
Copies of ^{1}H, ^{13}C NMR and HRMS spectra of all products

^{1}H-NMR (500 MHz, DMSO-d_6)







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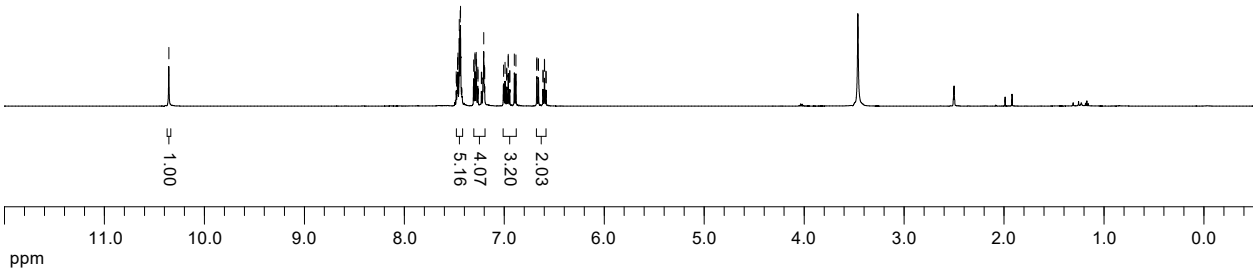
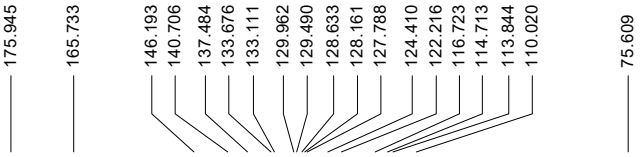
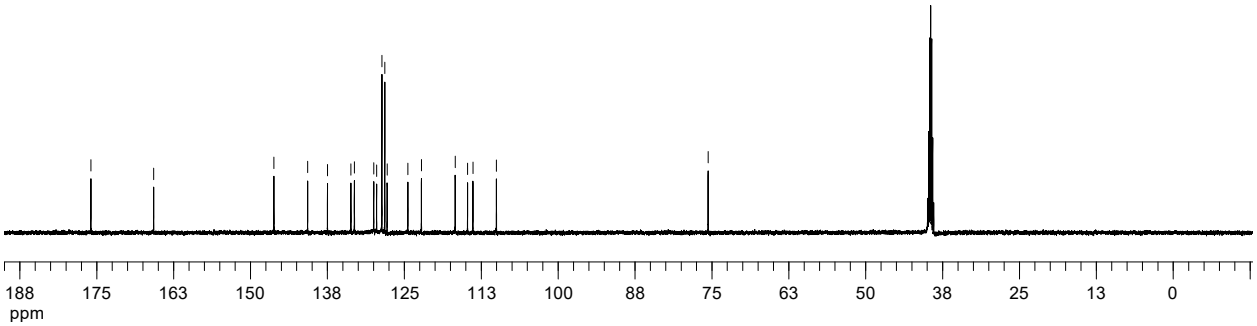


^{13}C-NMR (126 MHz, DMSO-d_6)





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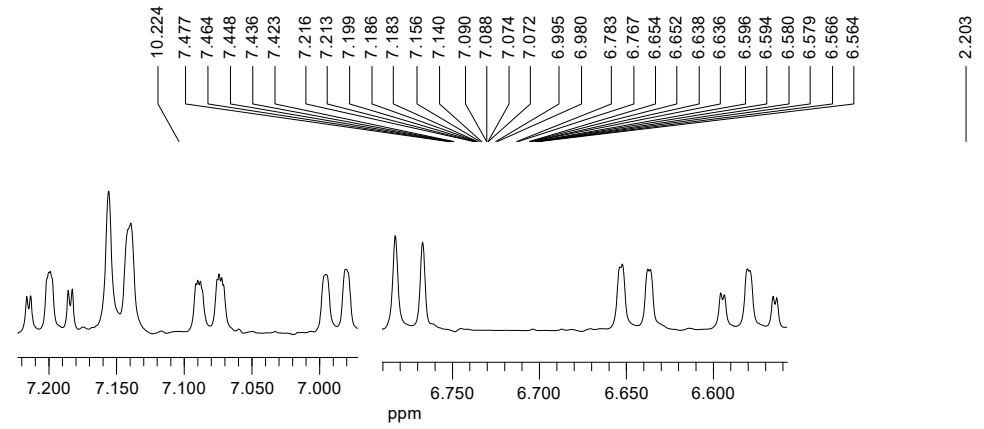

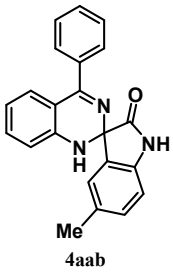

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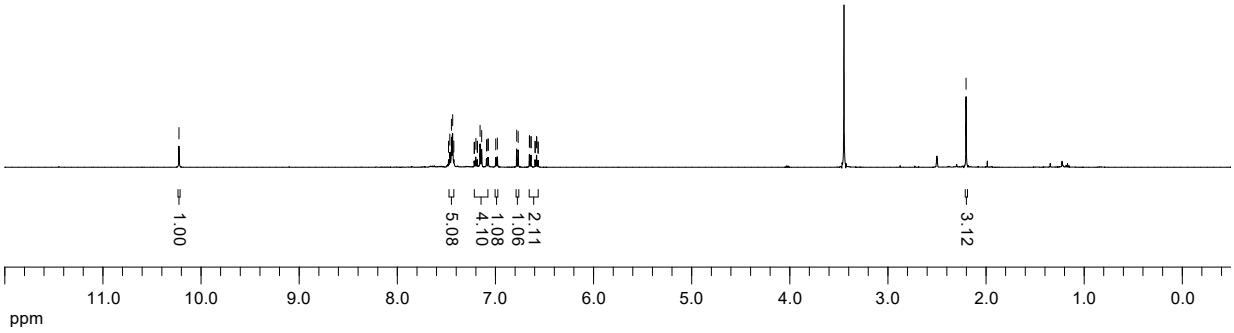

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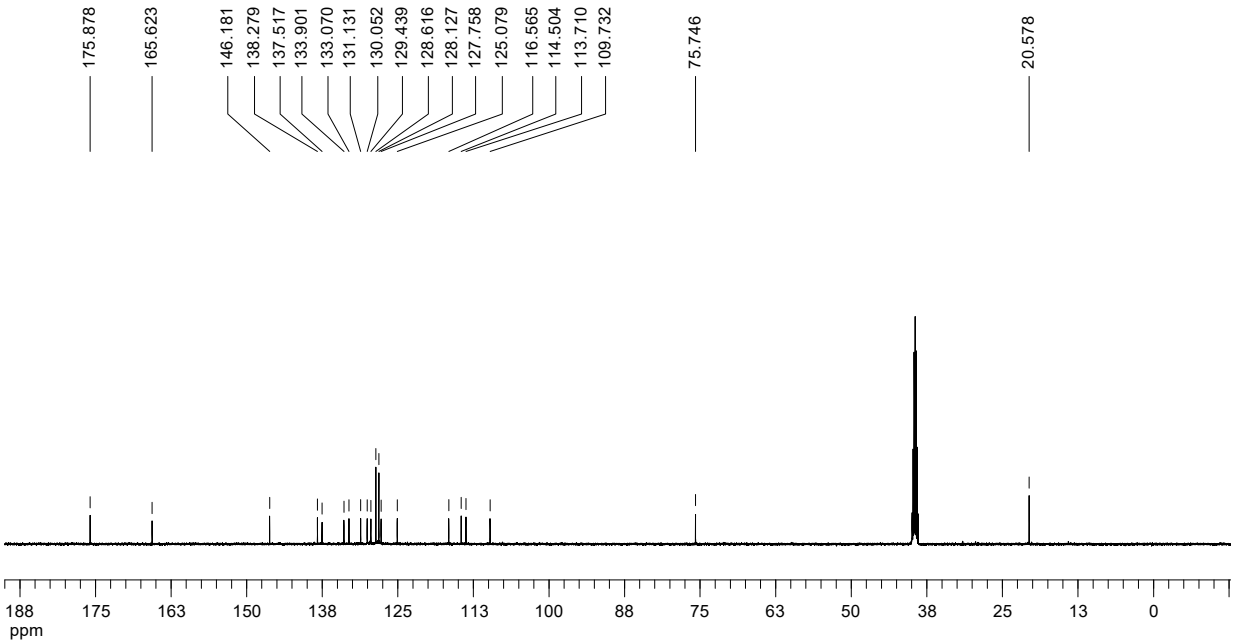

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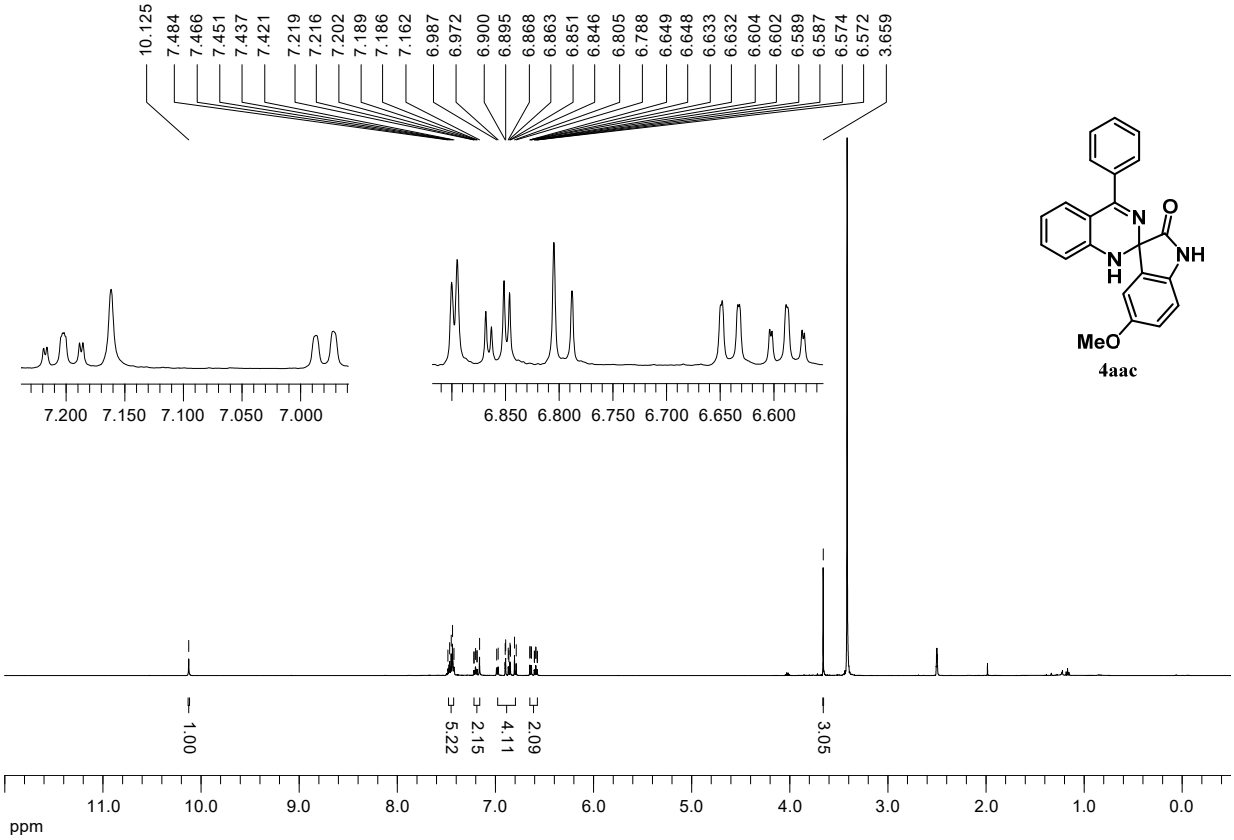

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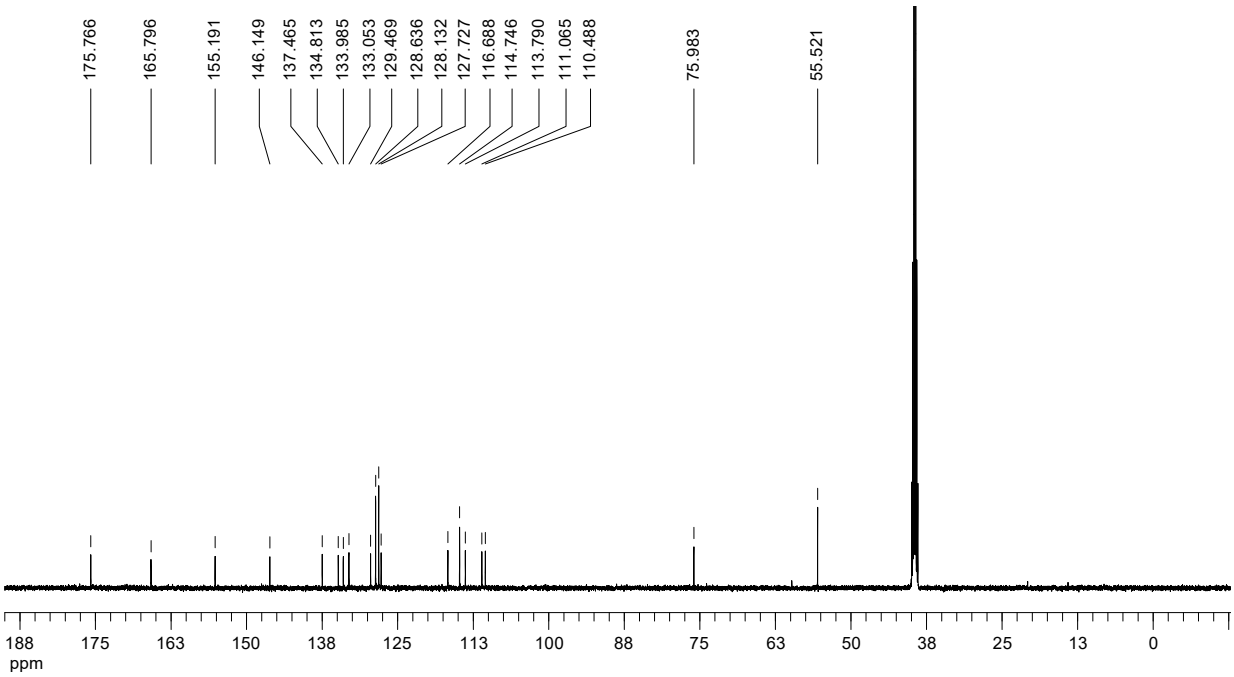

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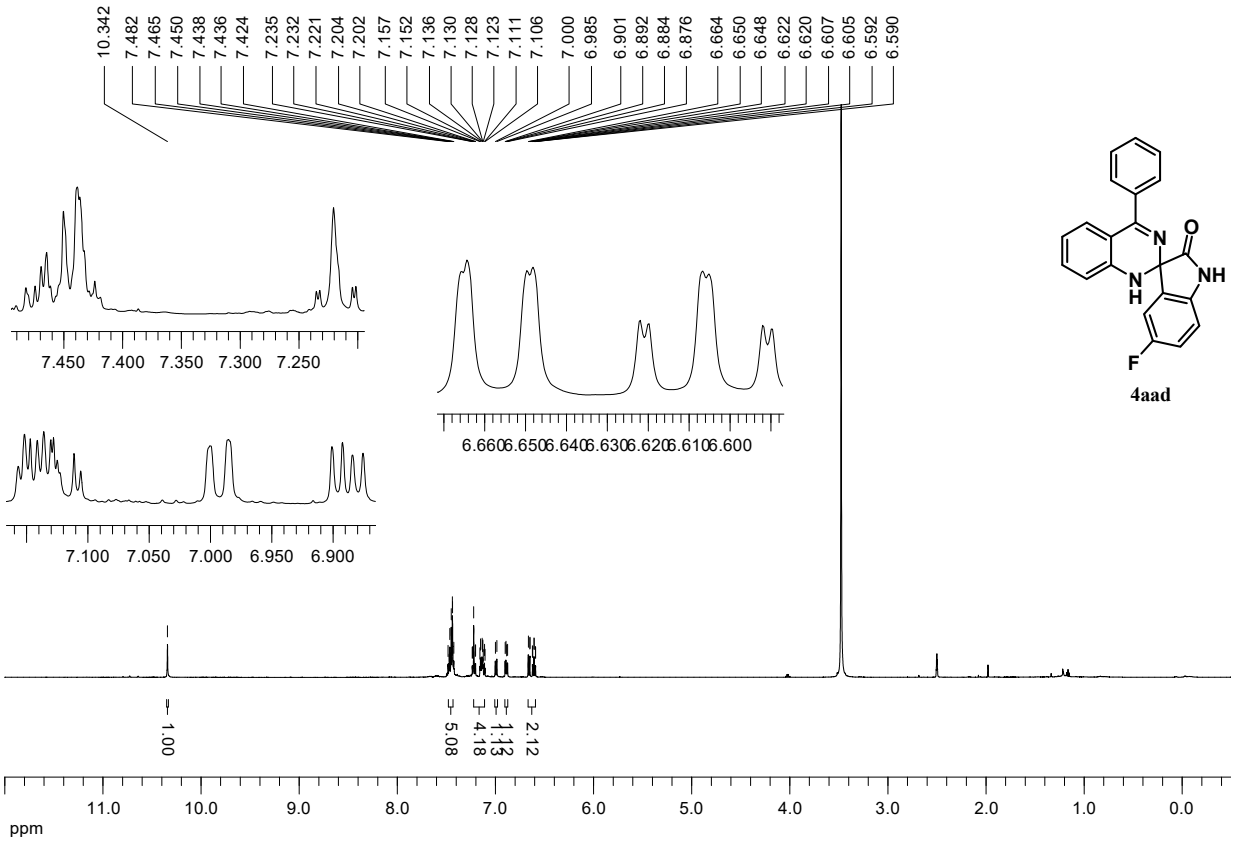

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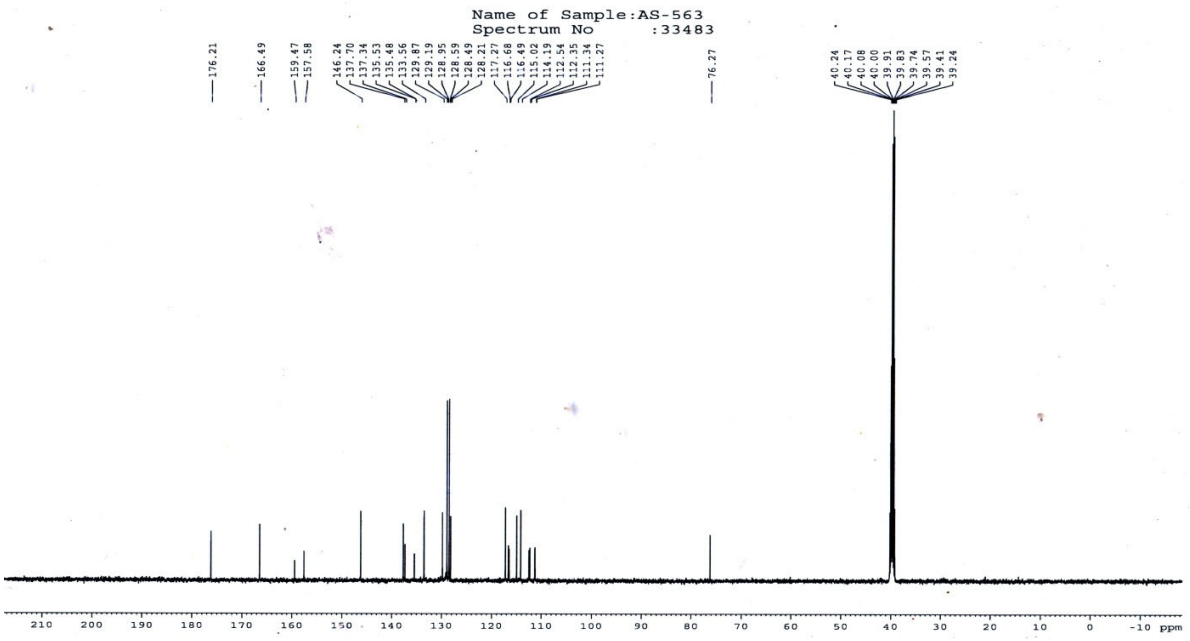

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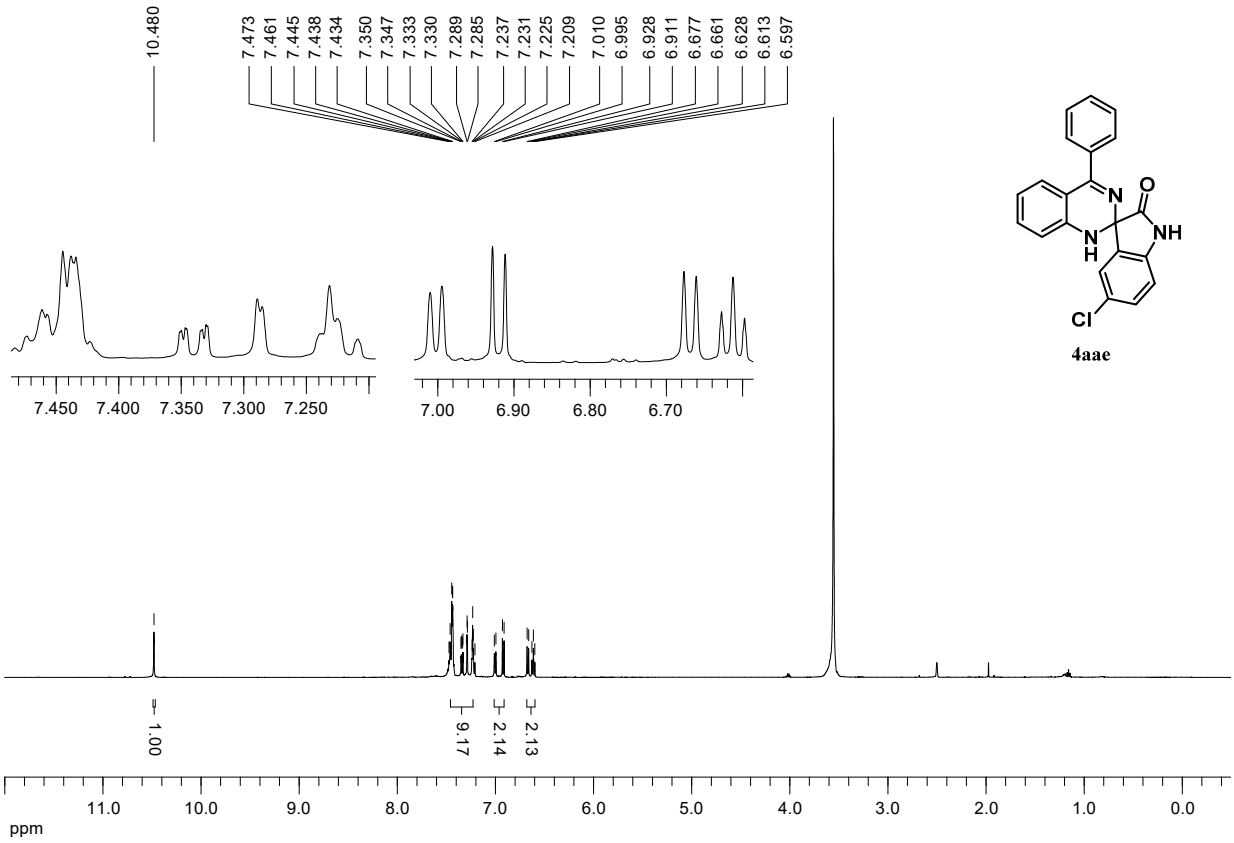

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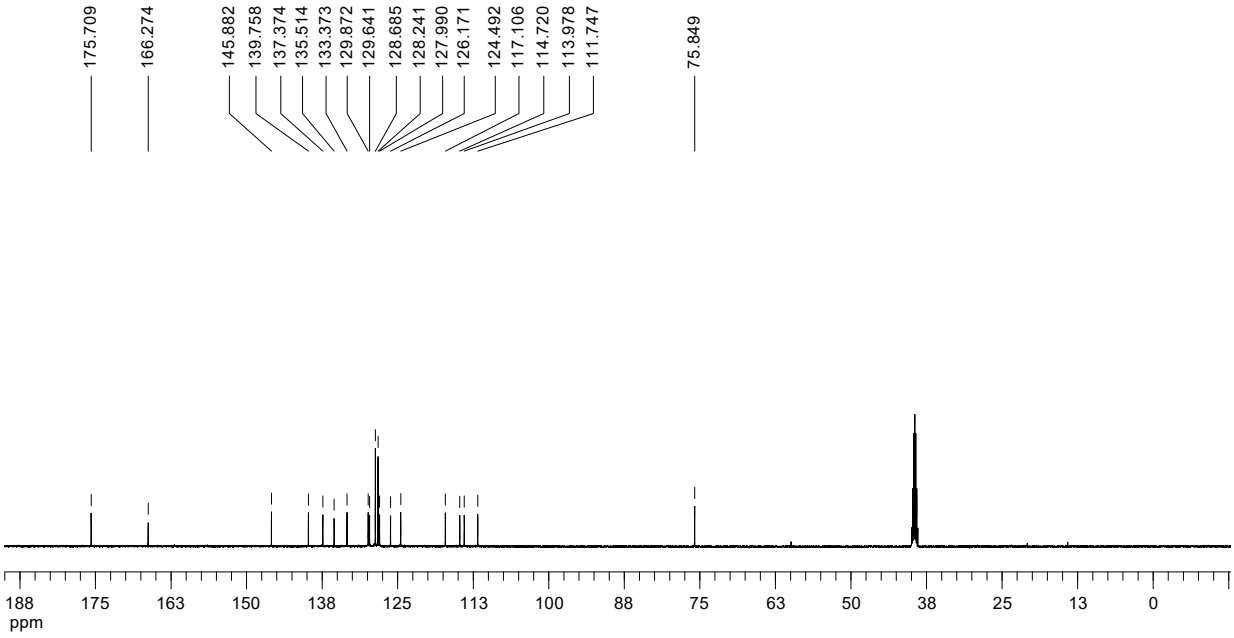

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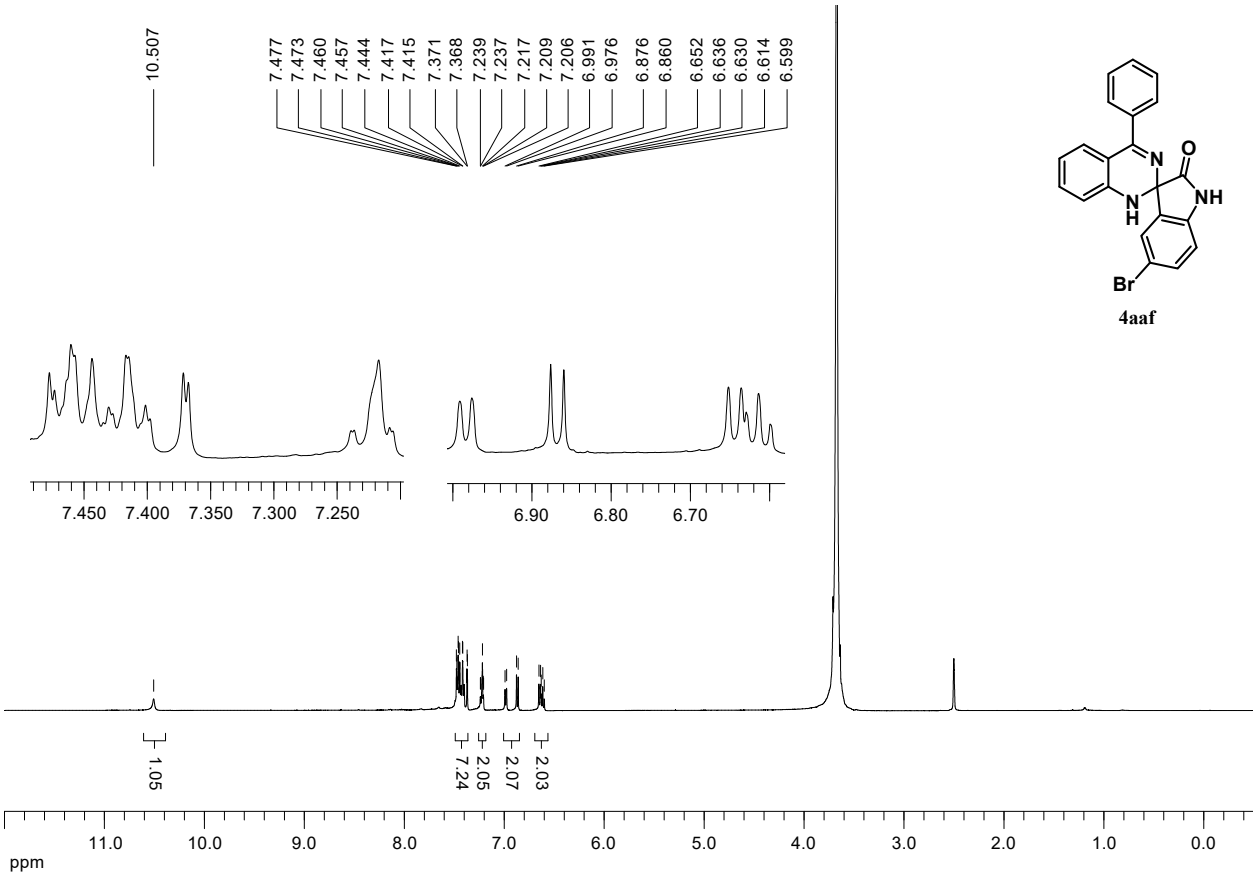

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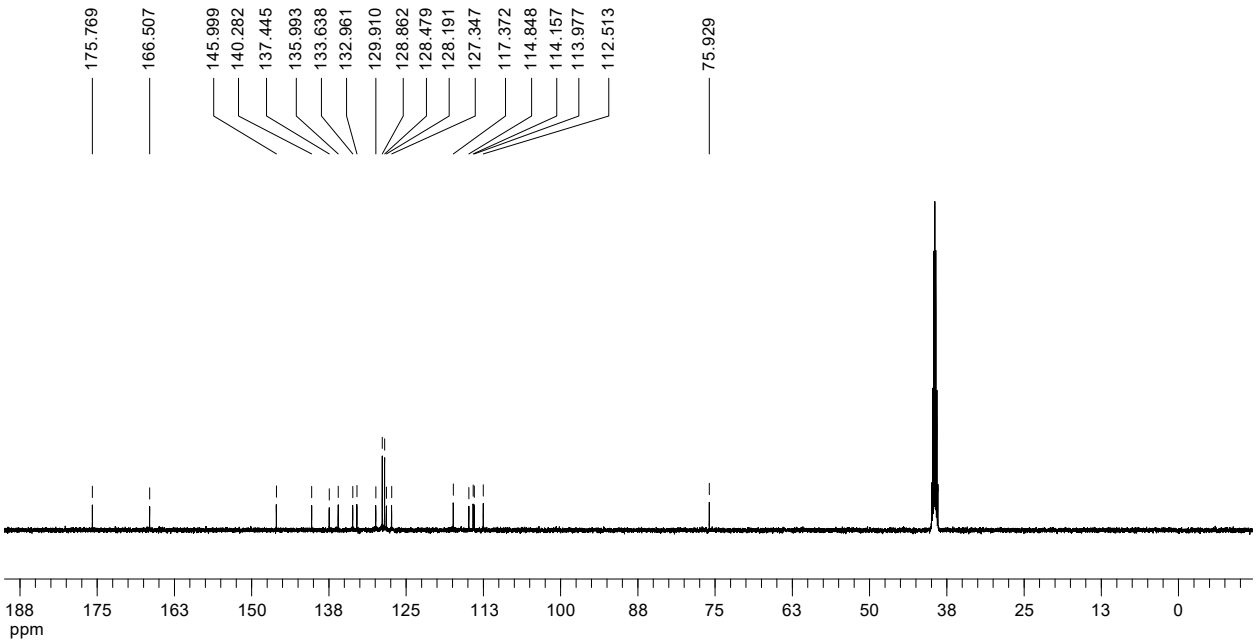

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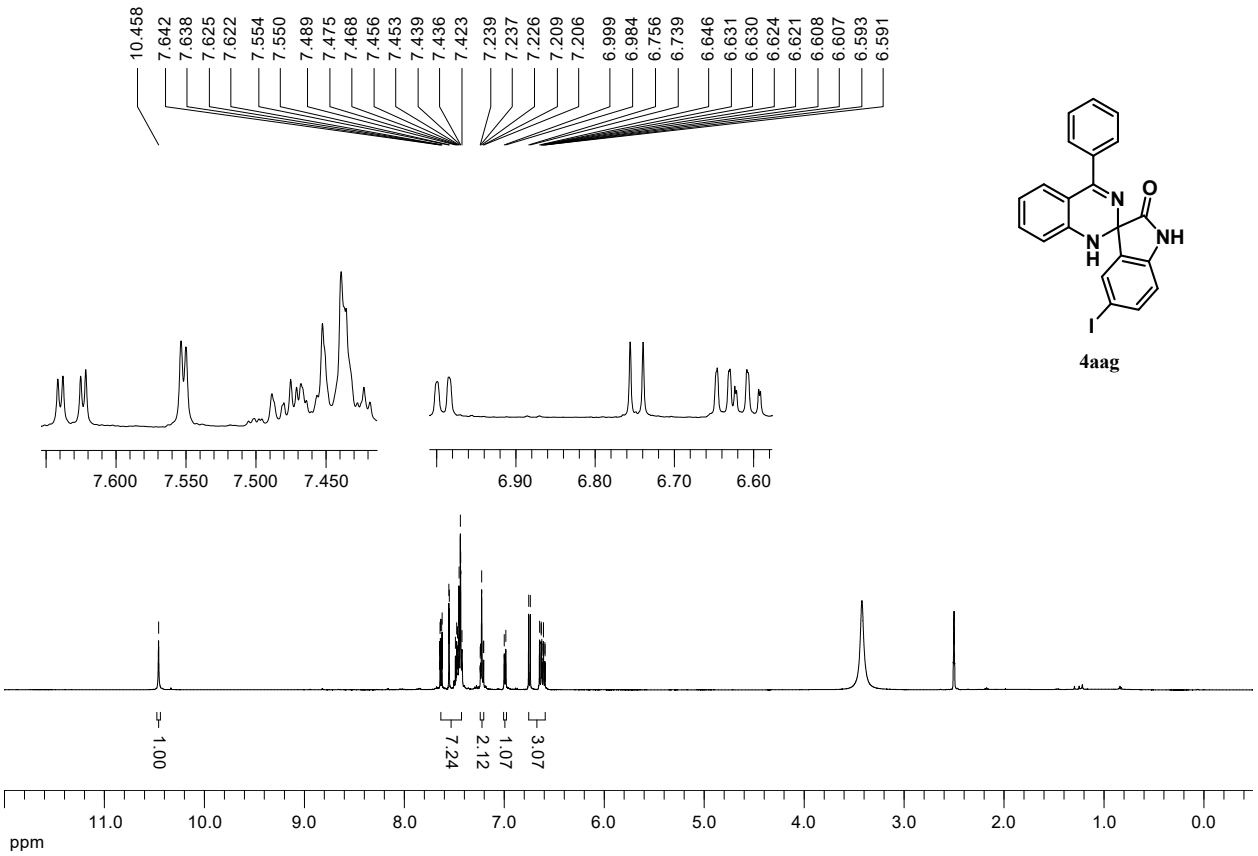

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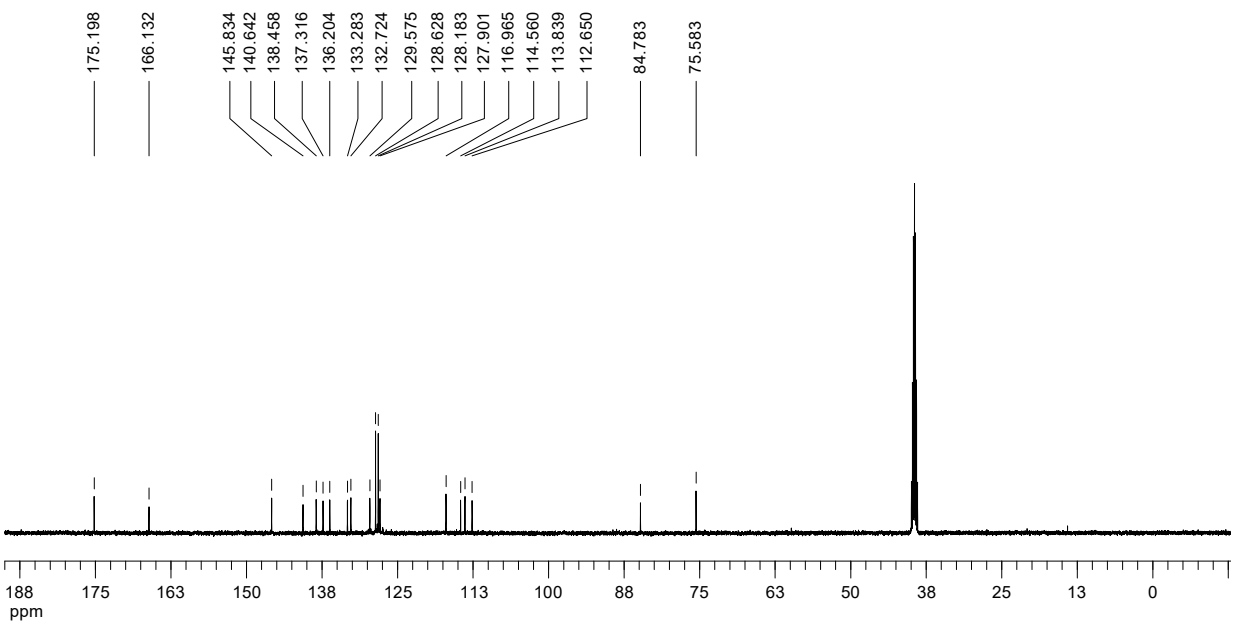

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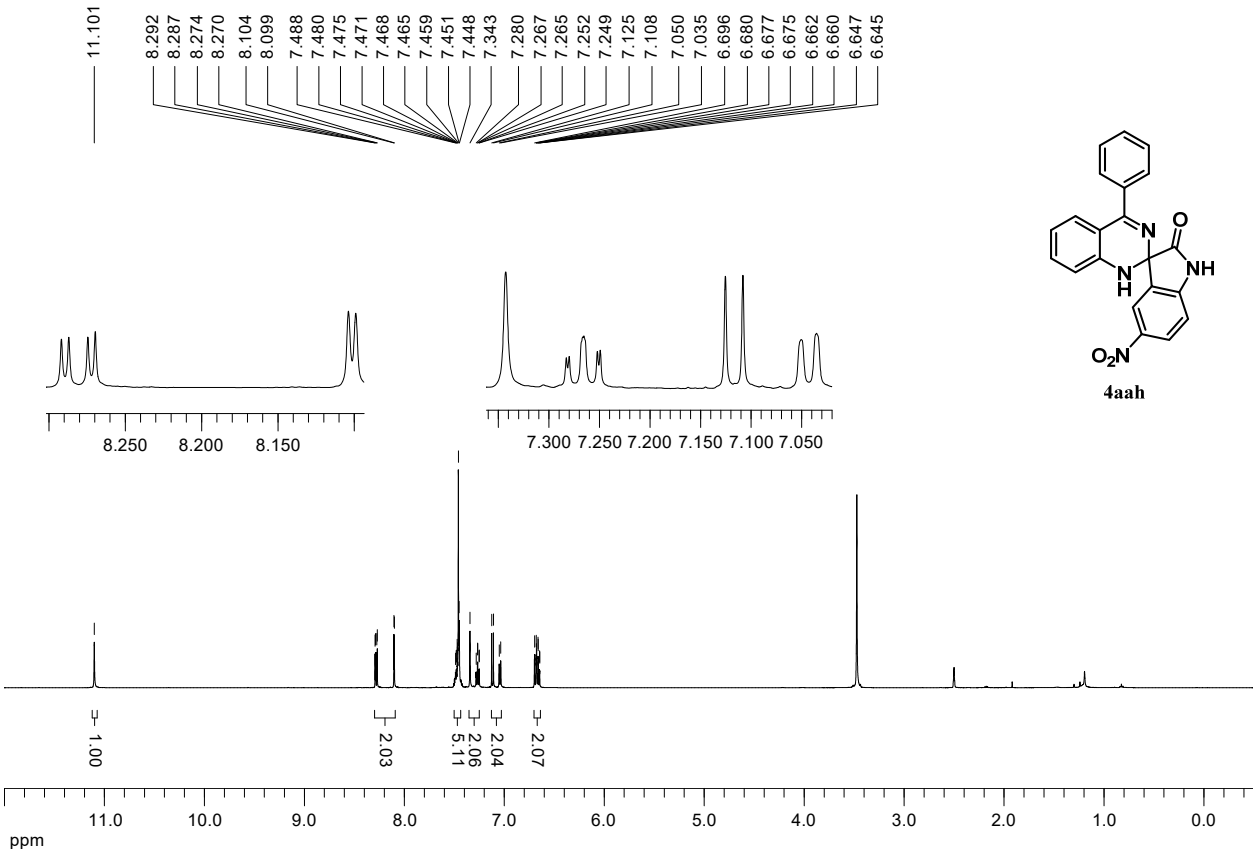

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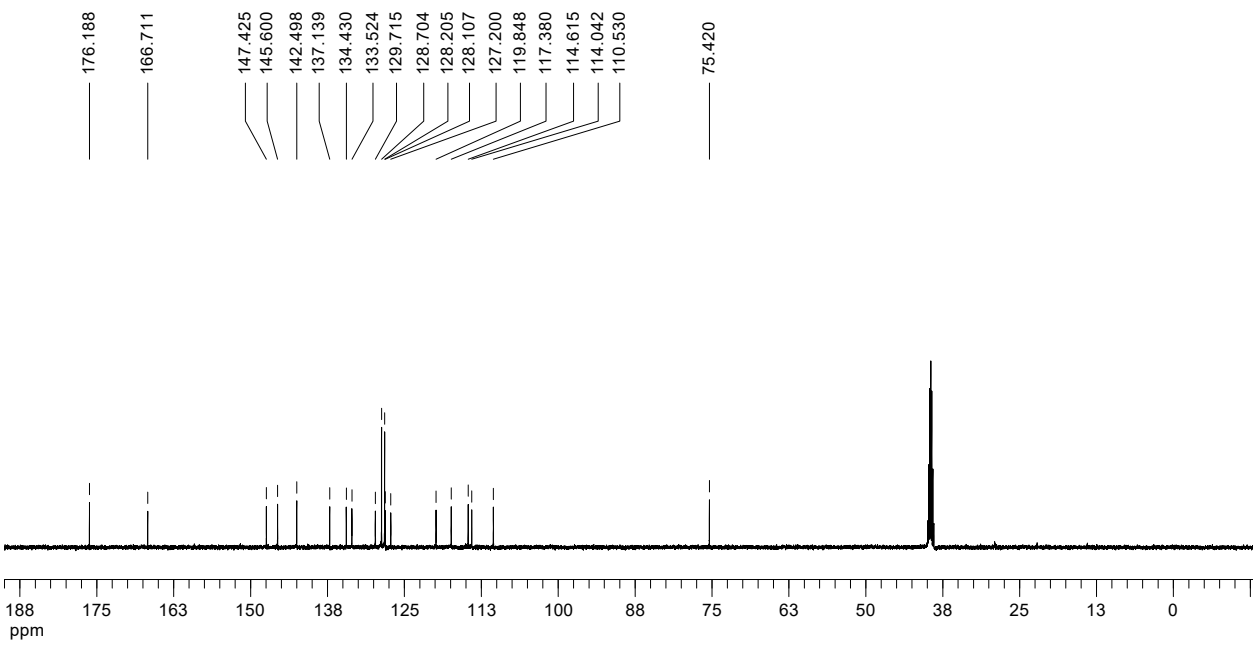

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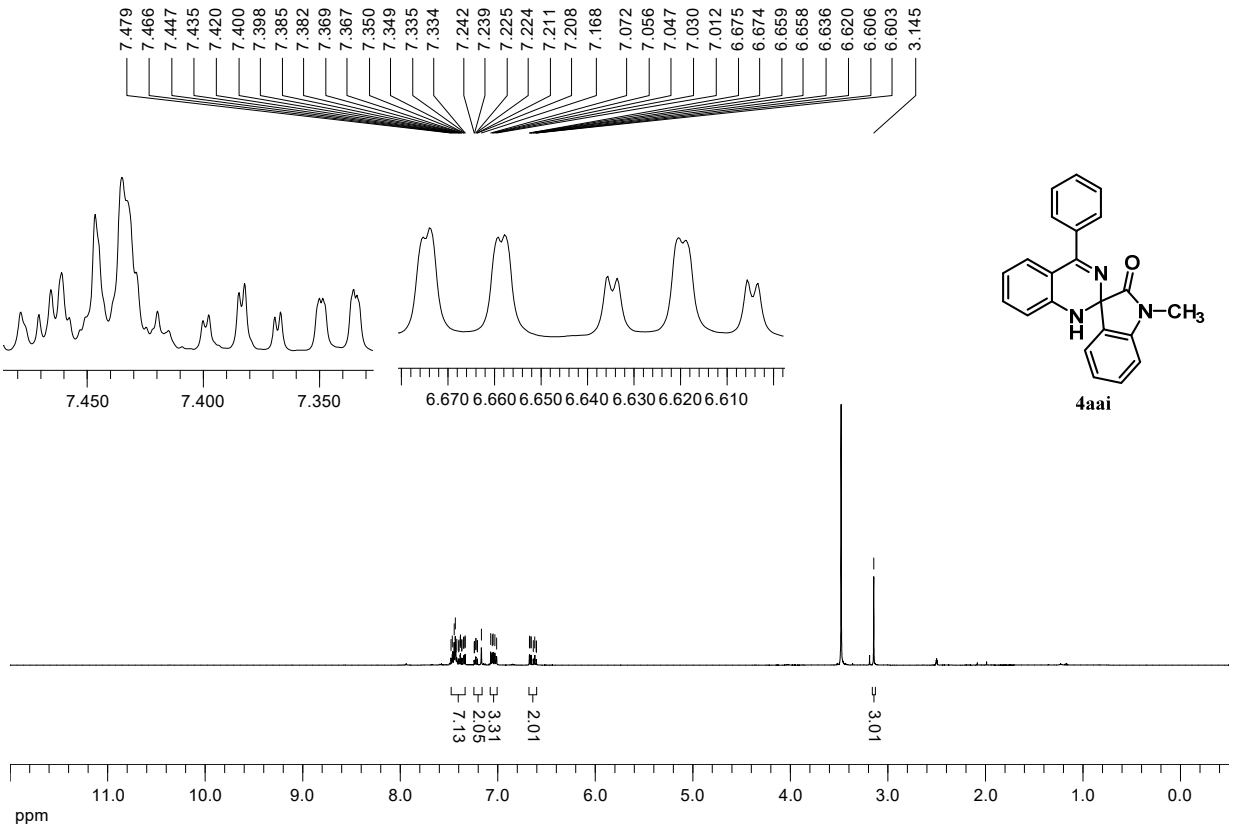

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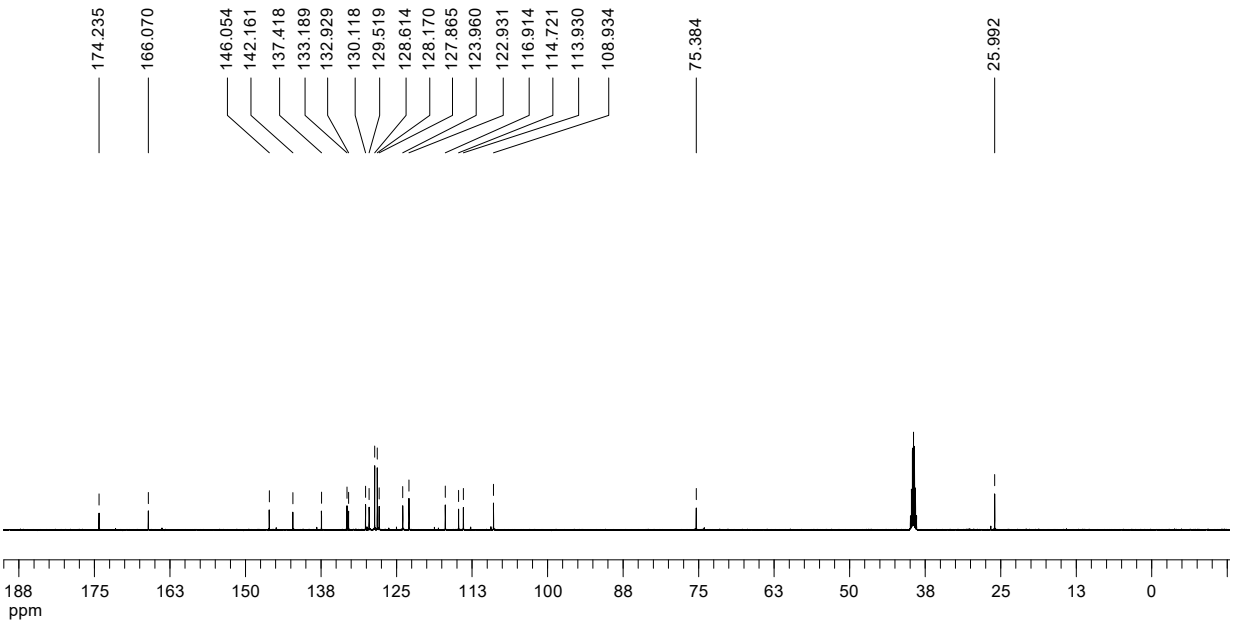

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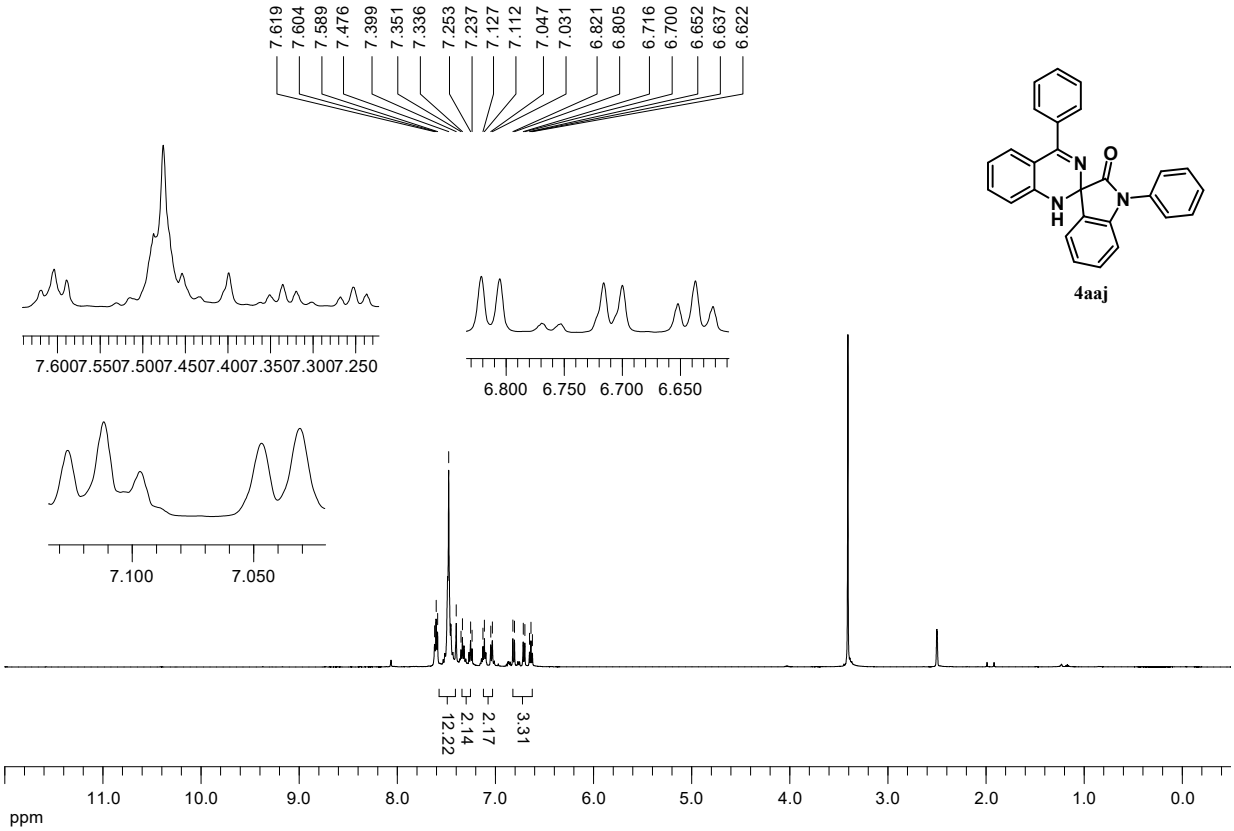

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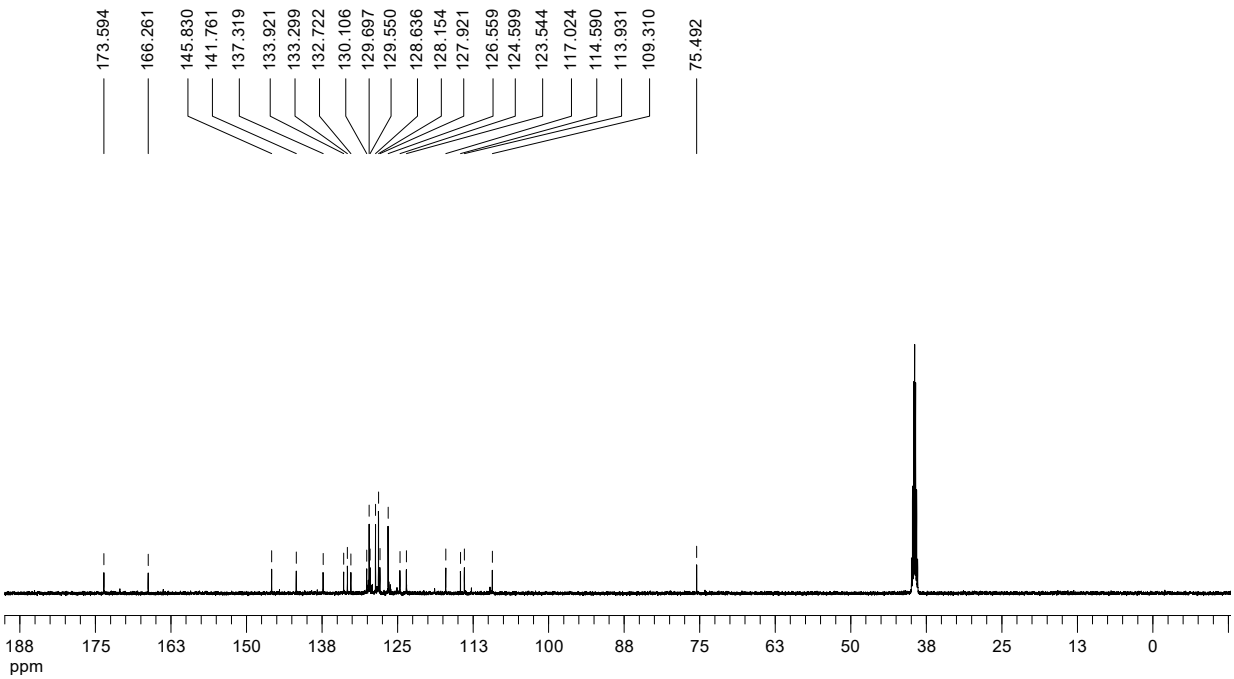

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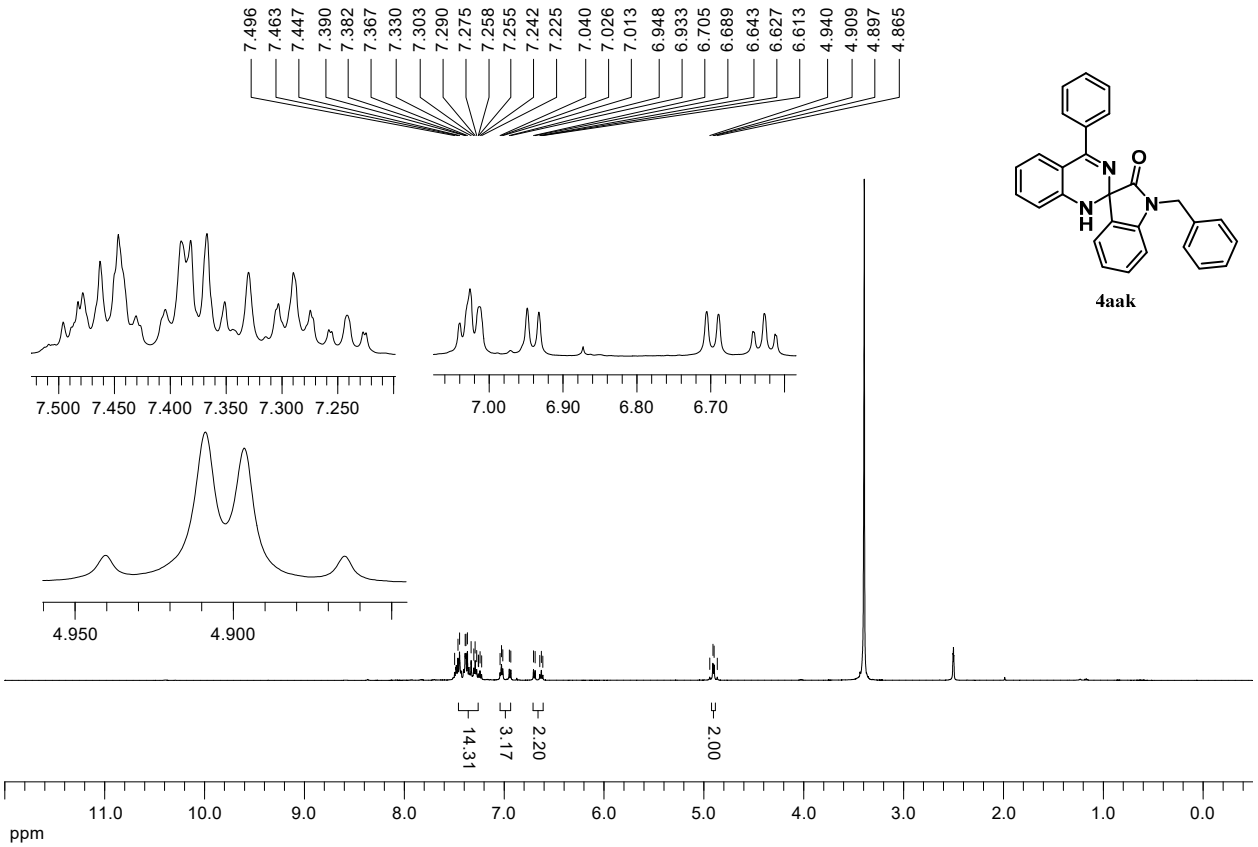

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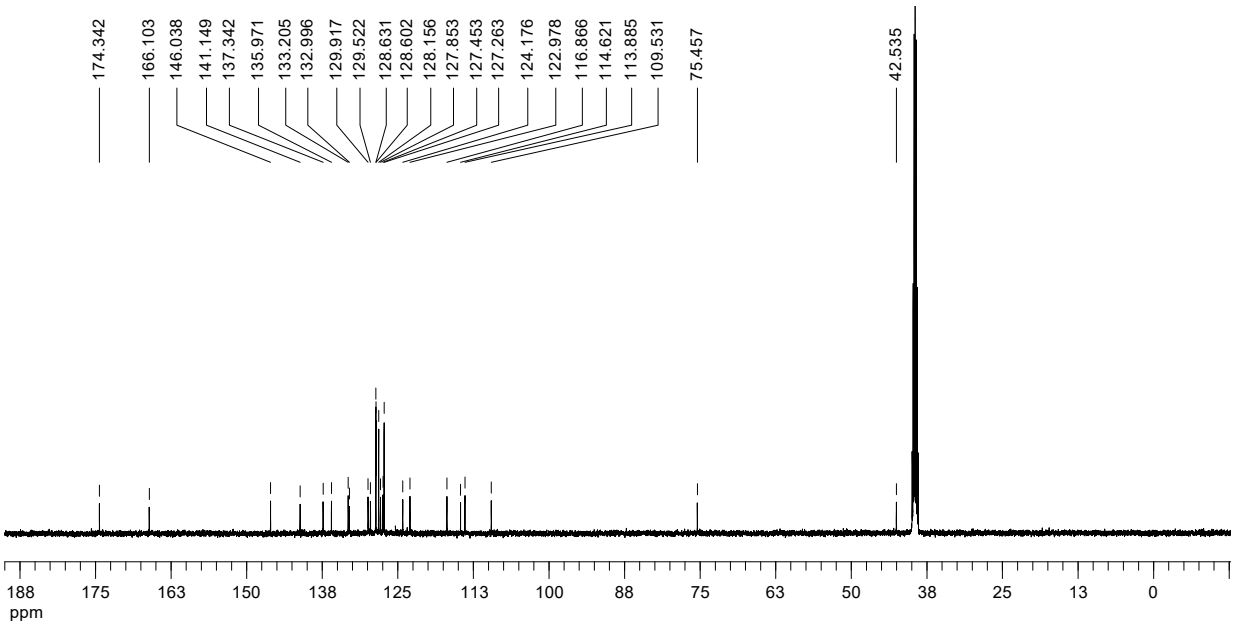

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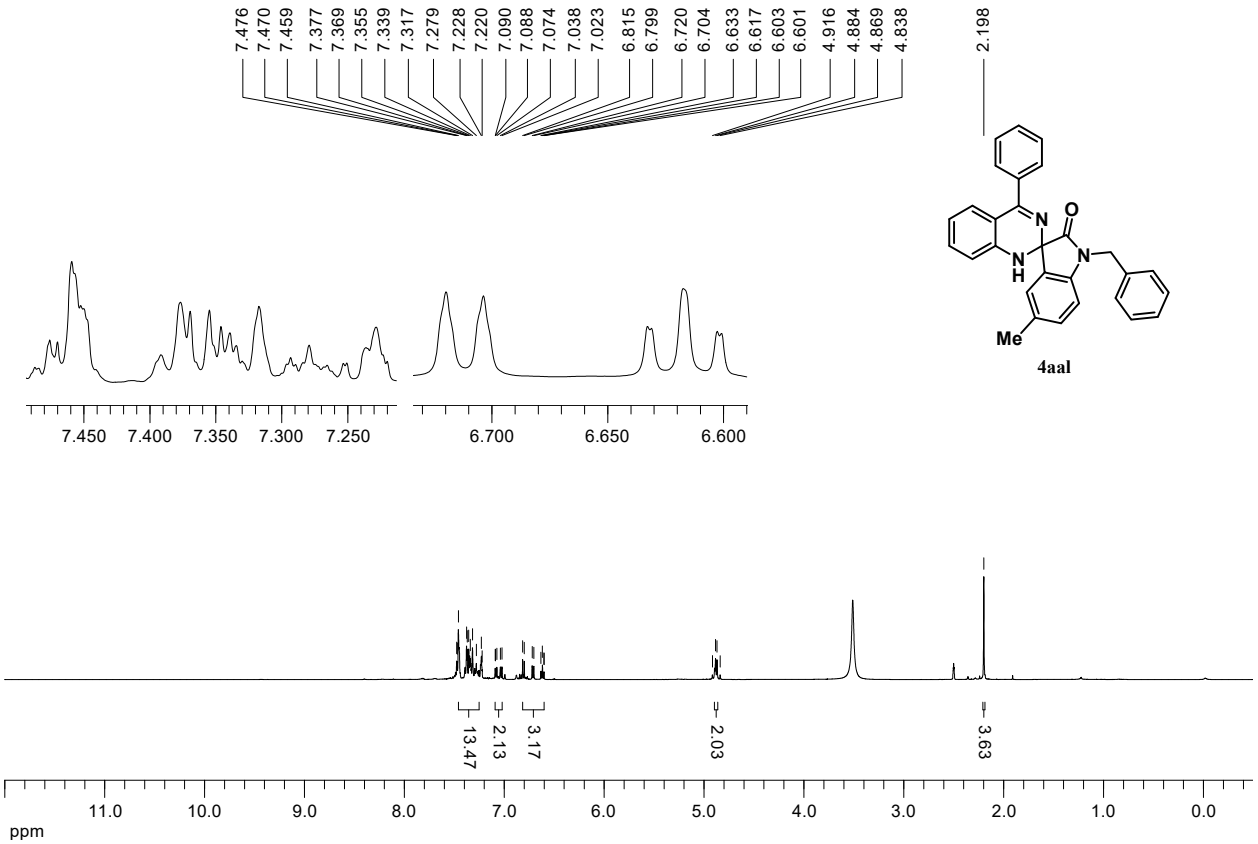

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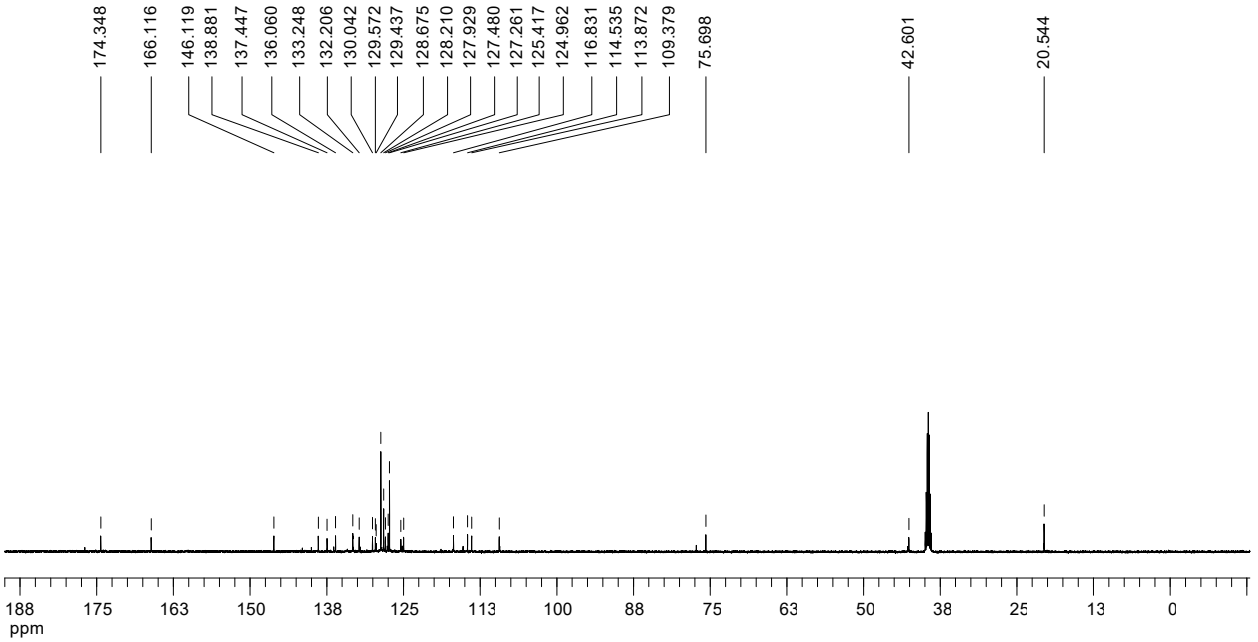

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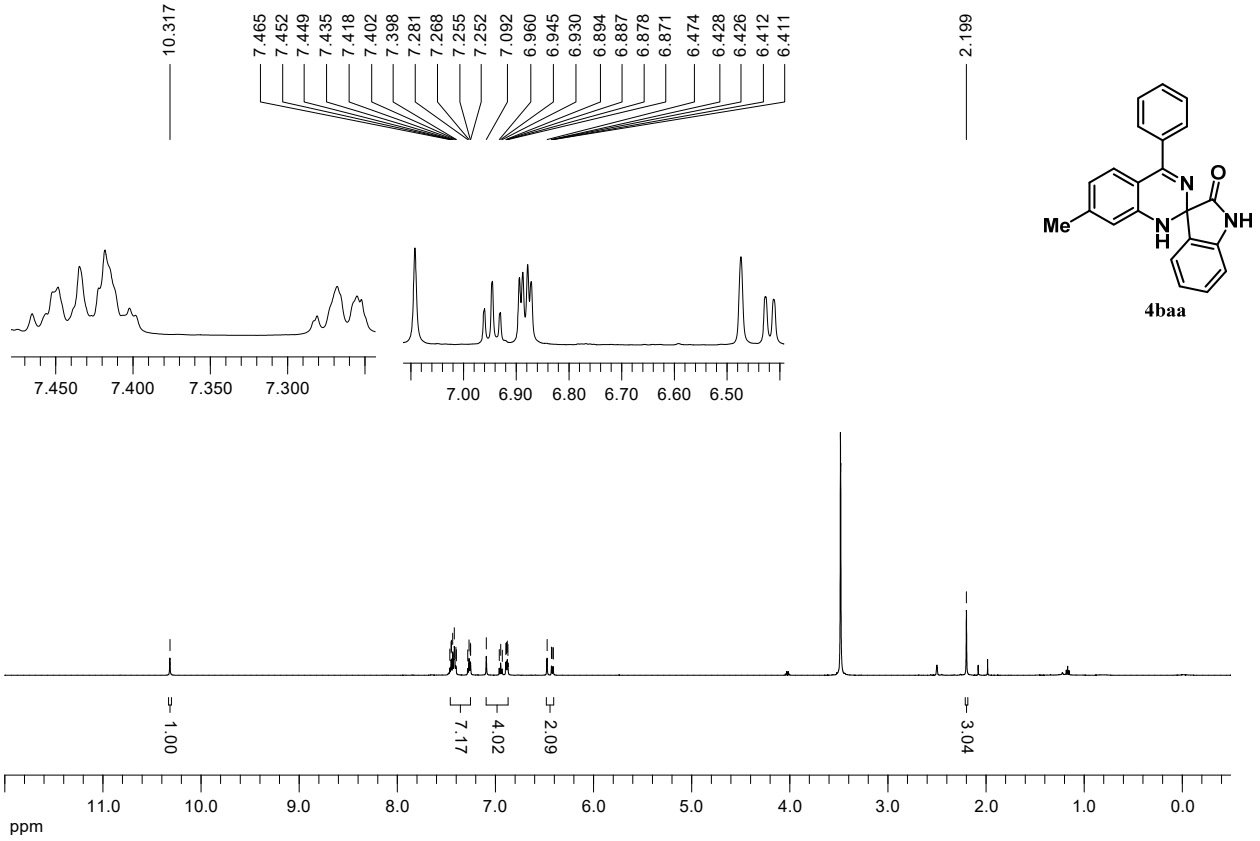

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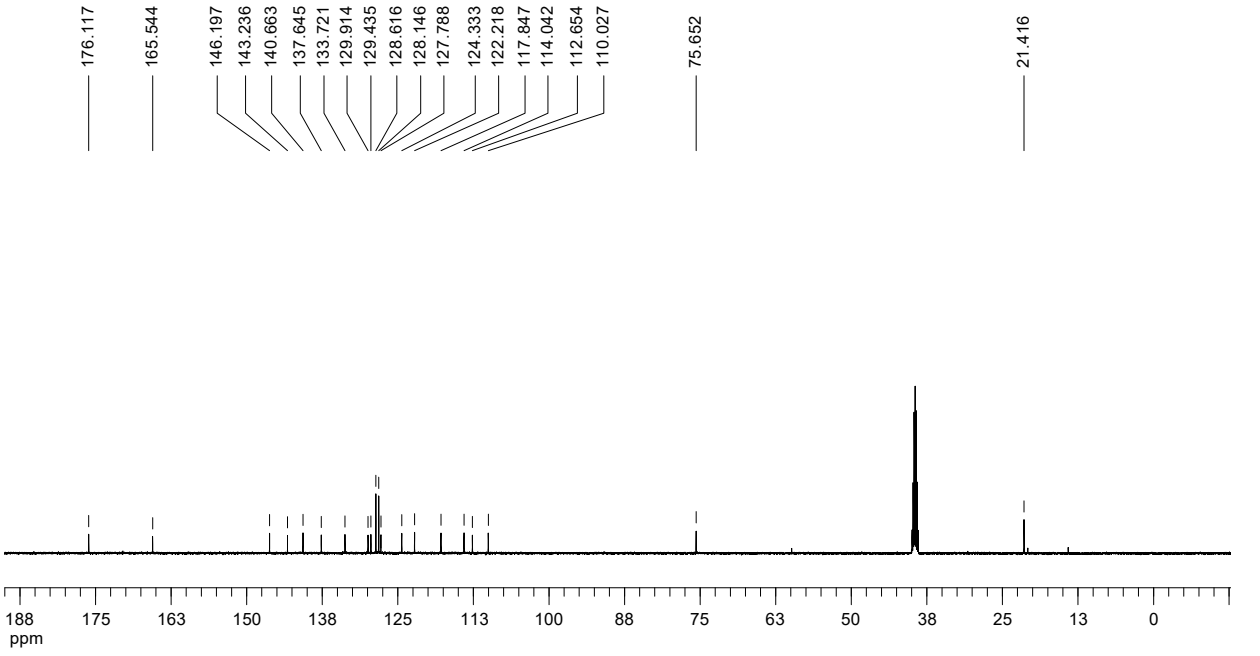

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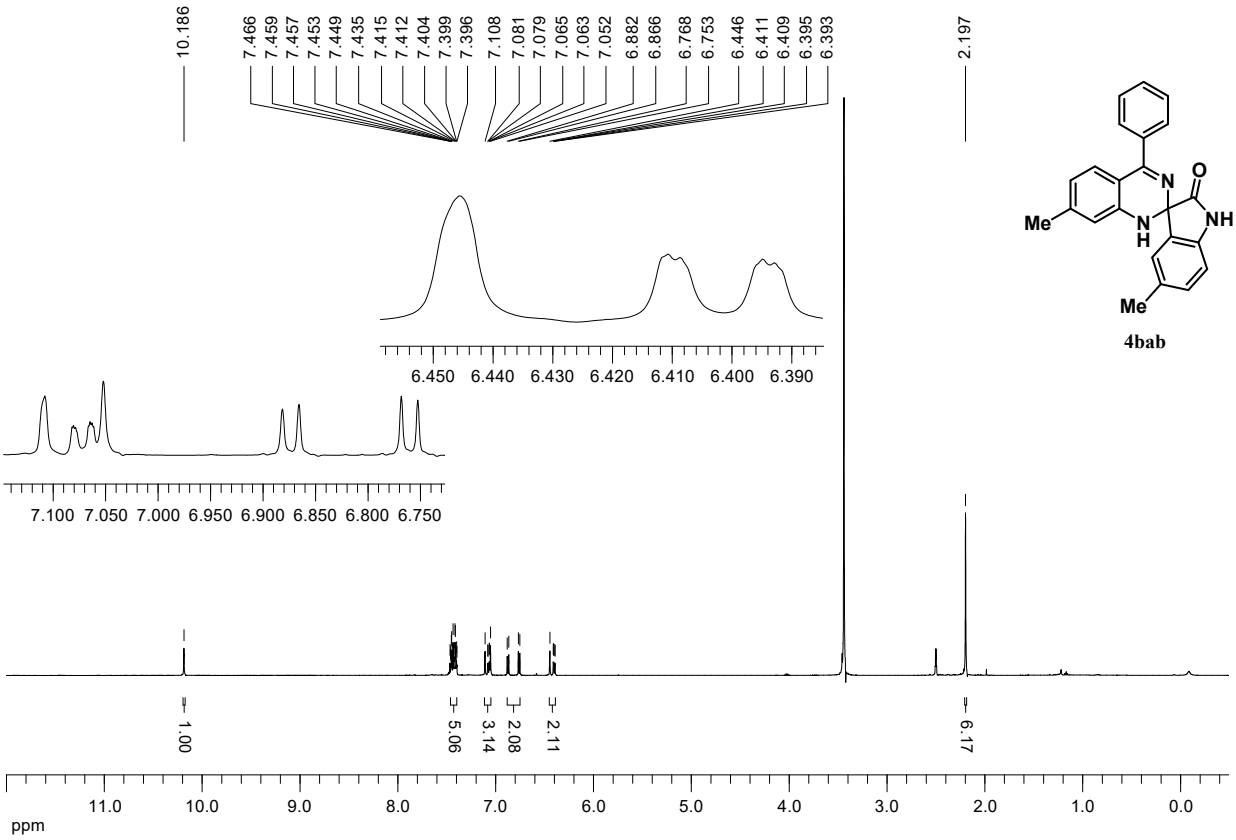

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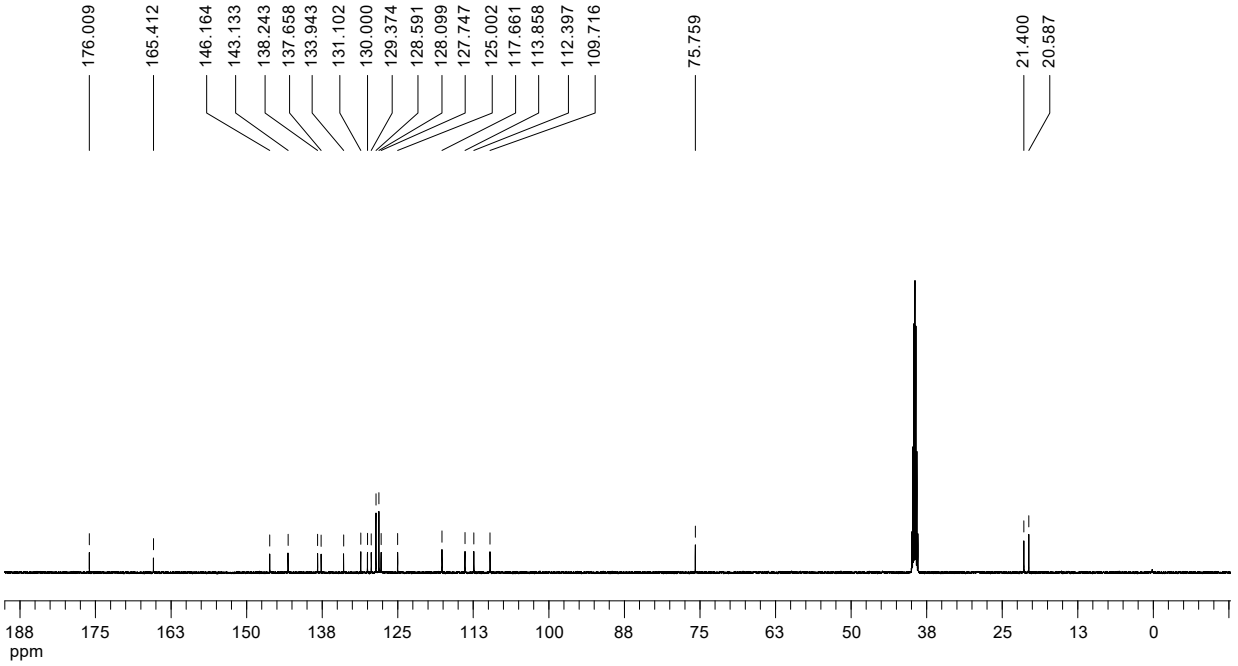

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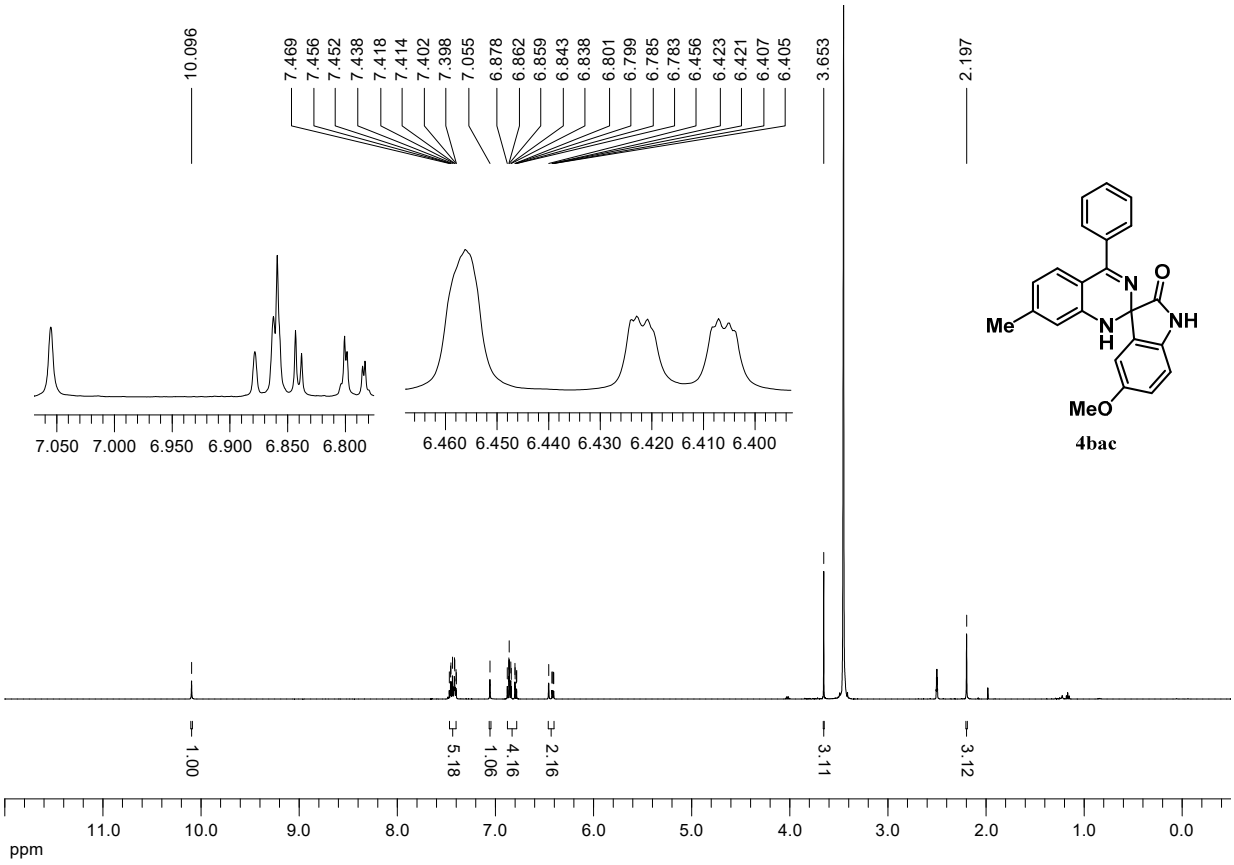

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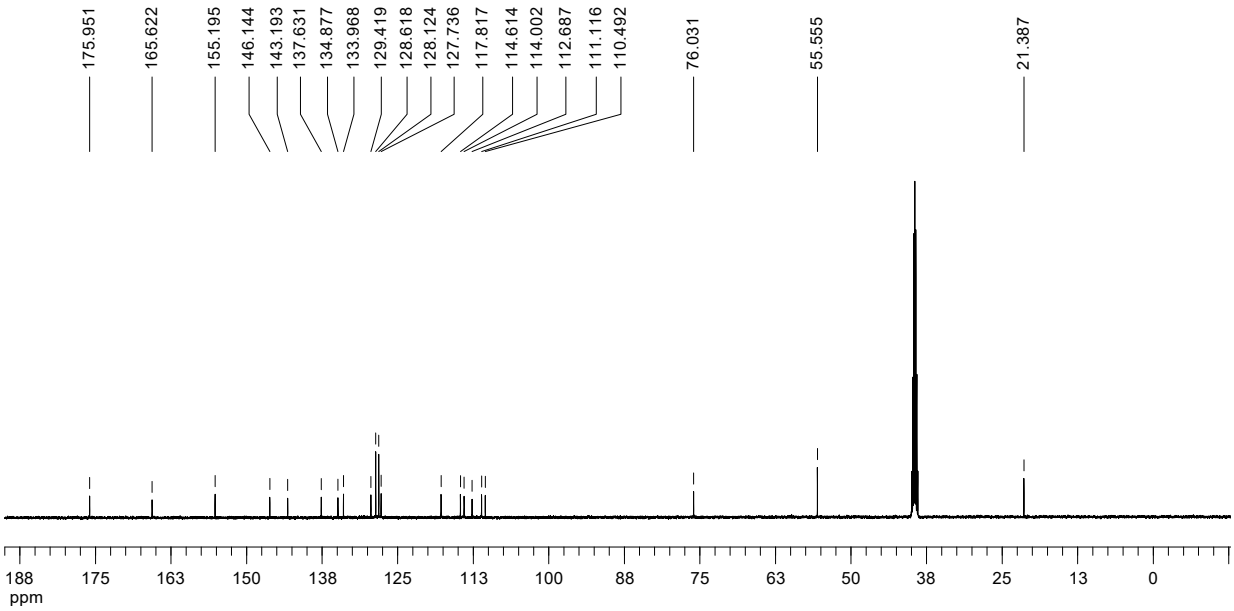

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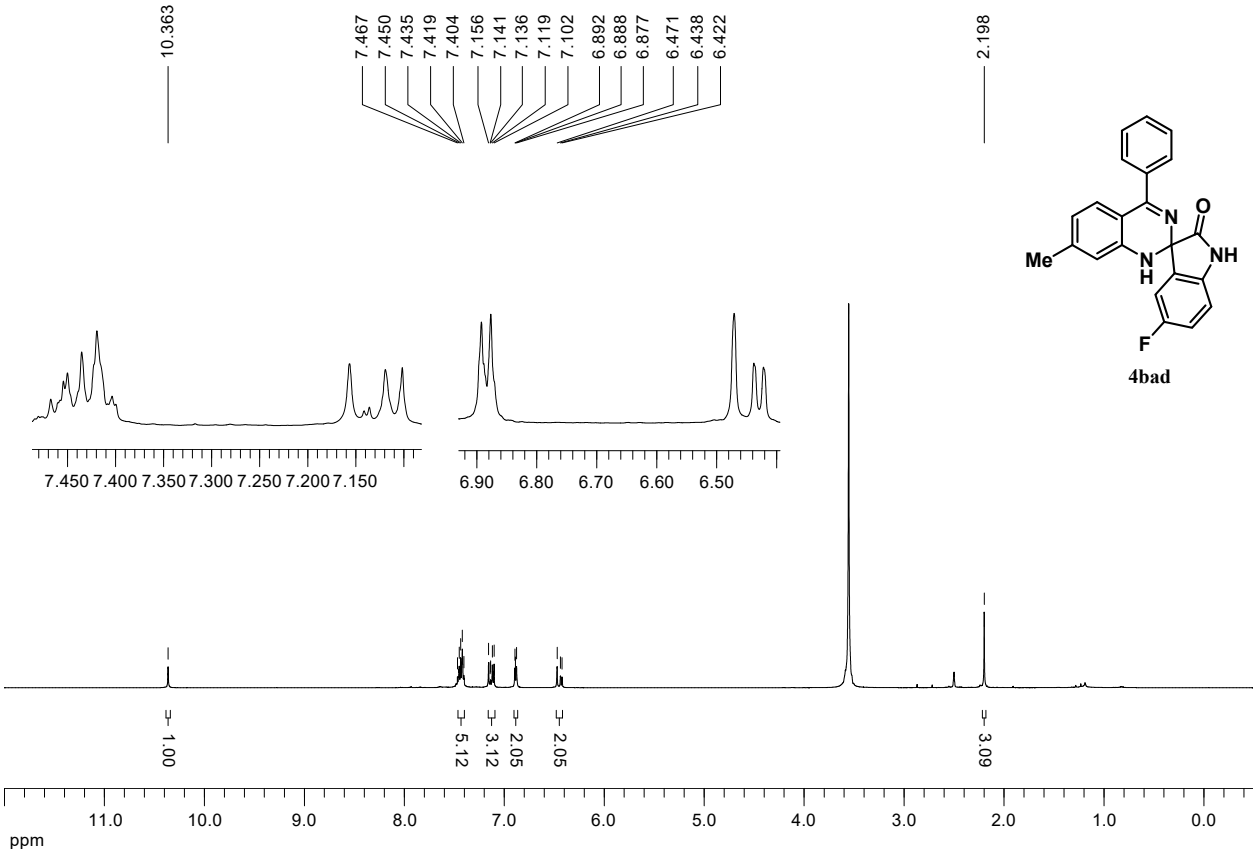

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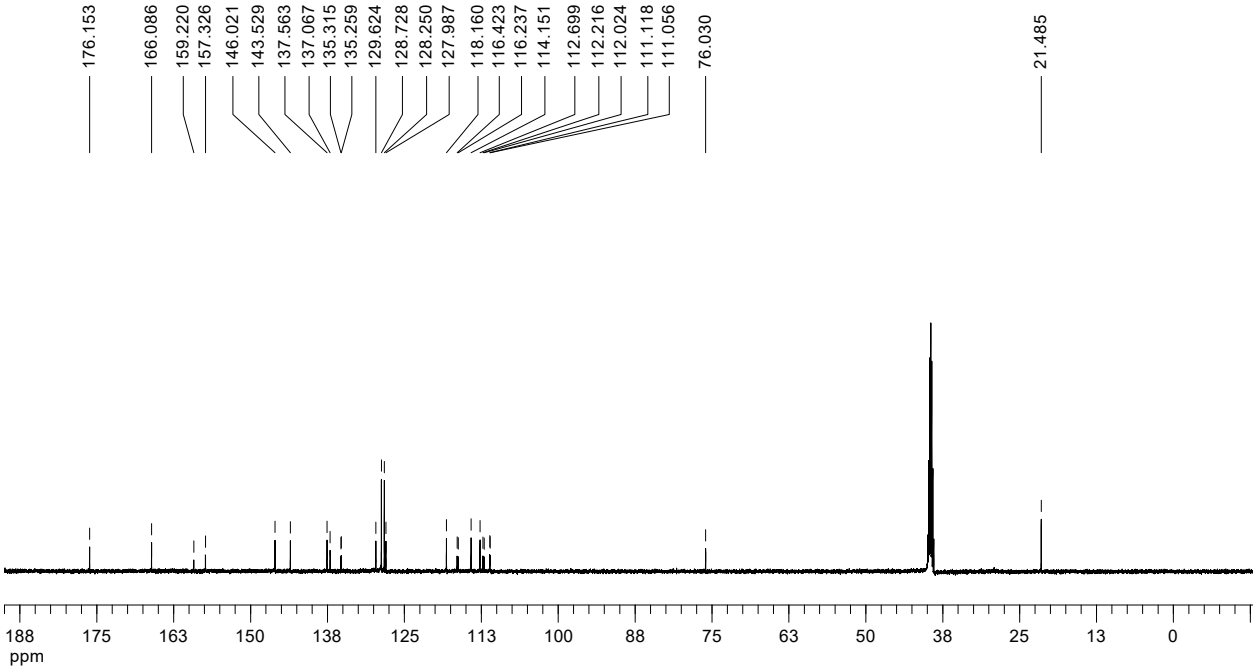

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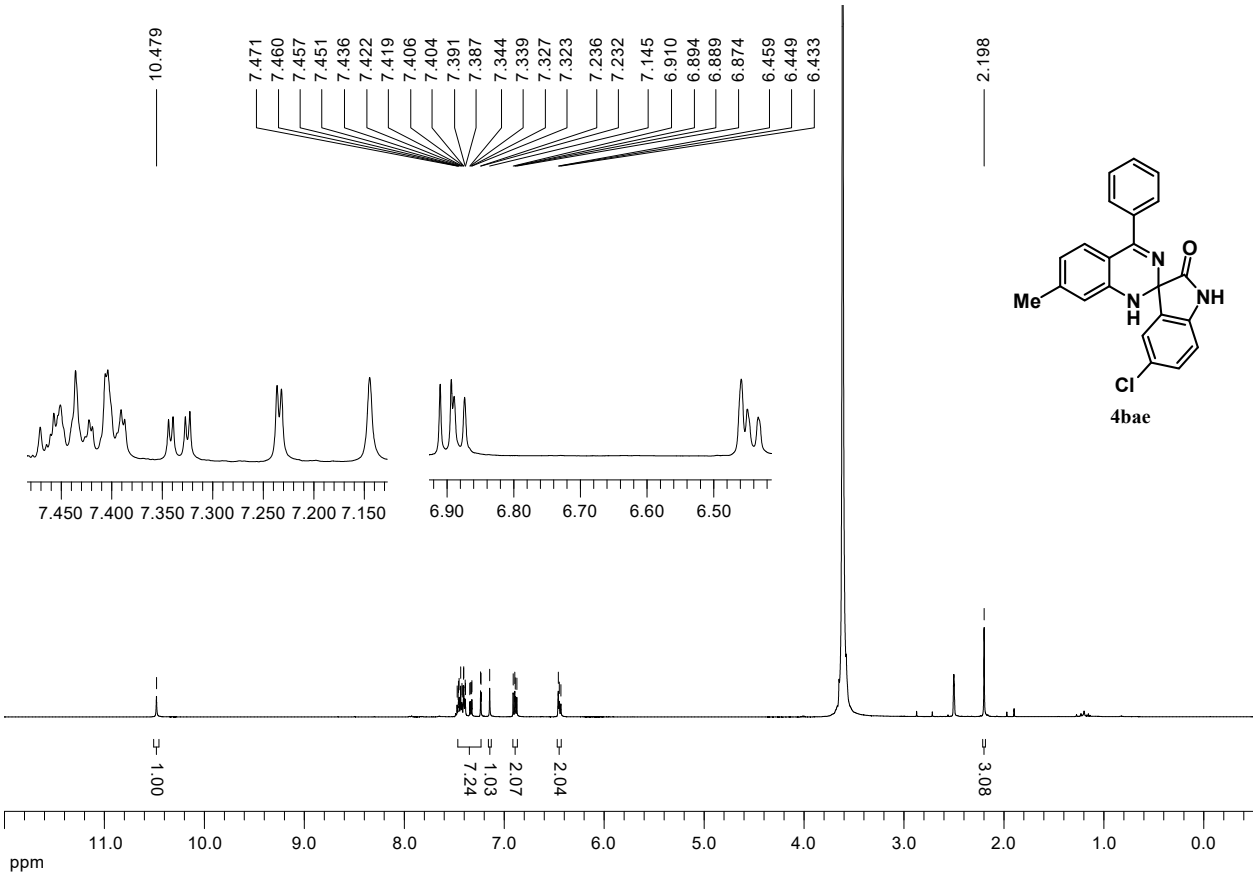

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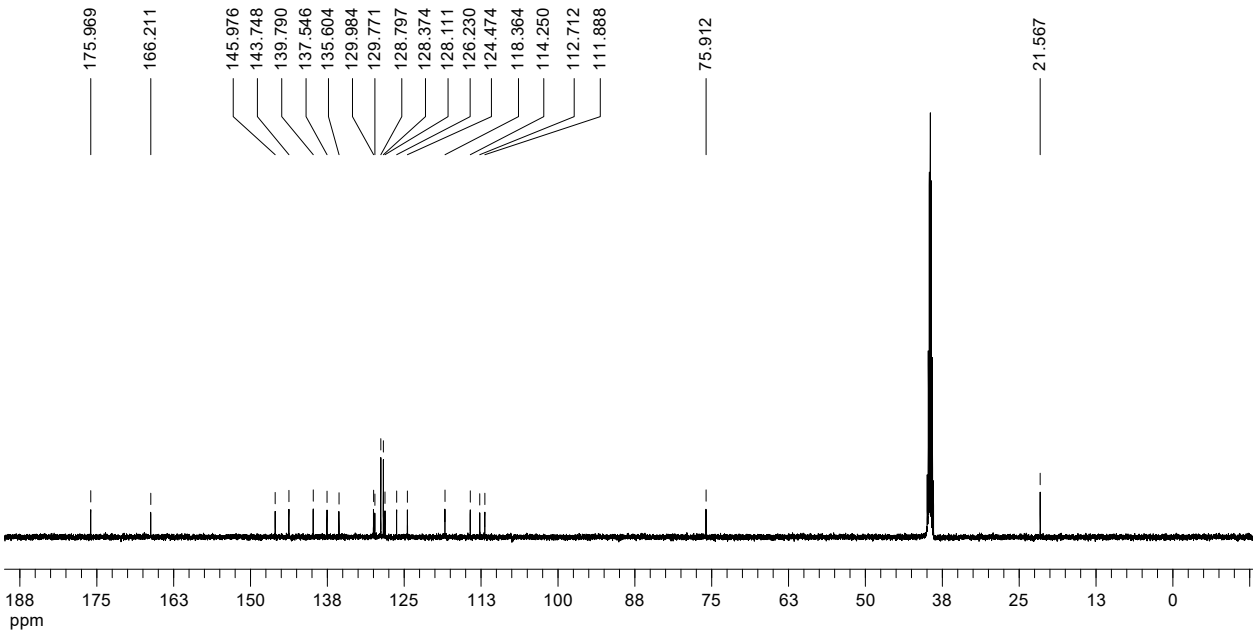

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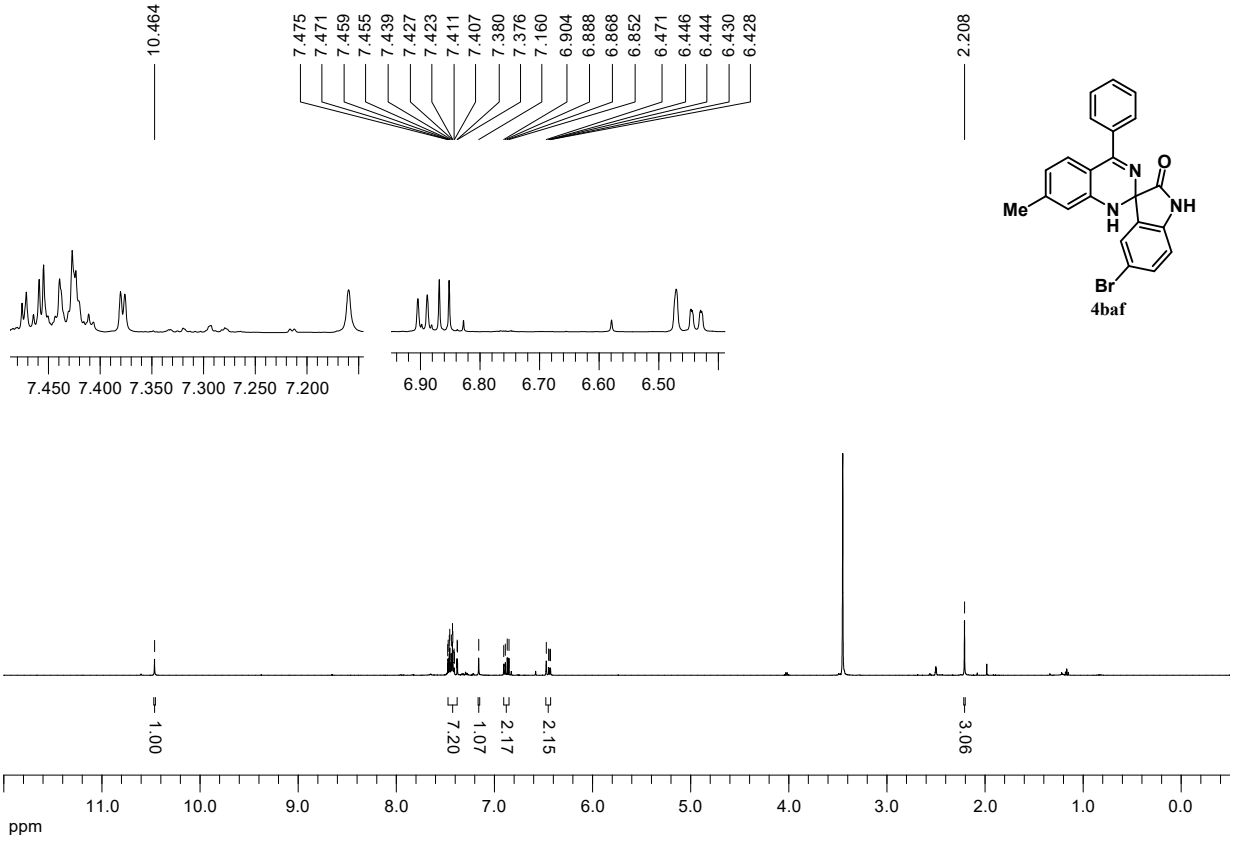

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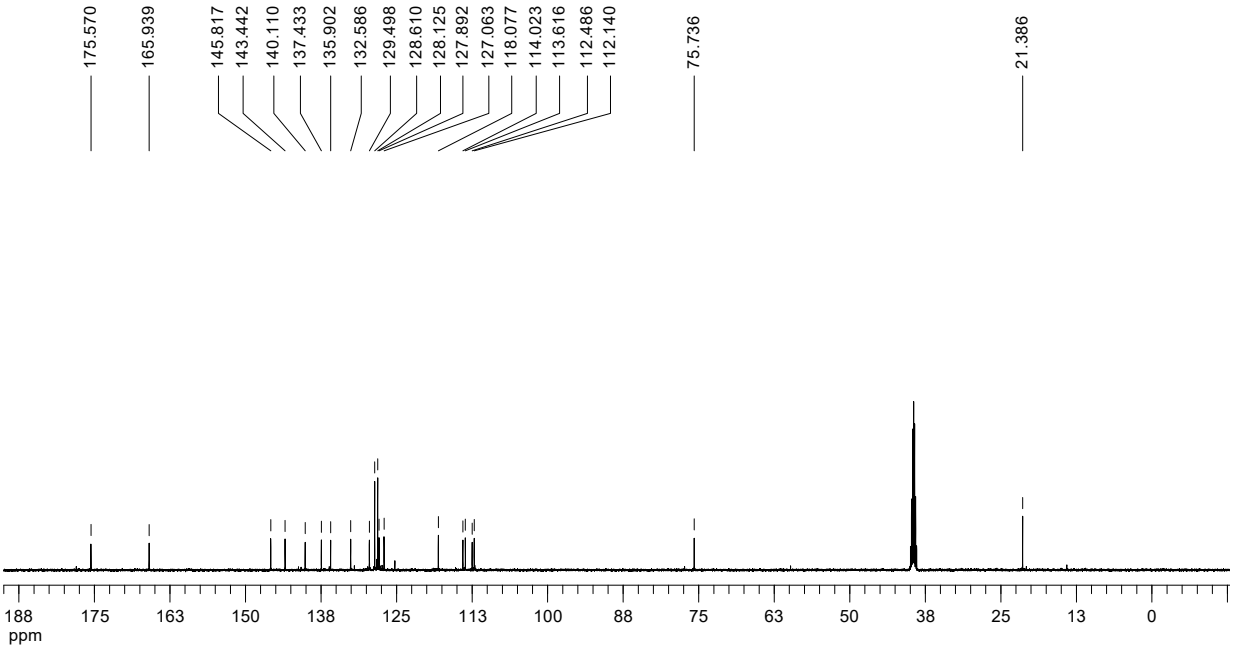

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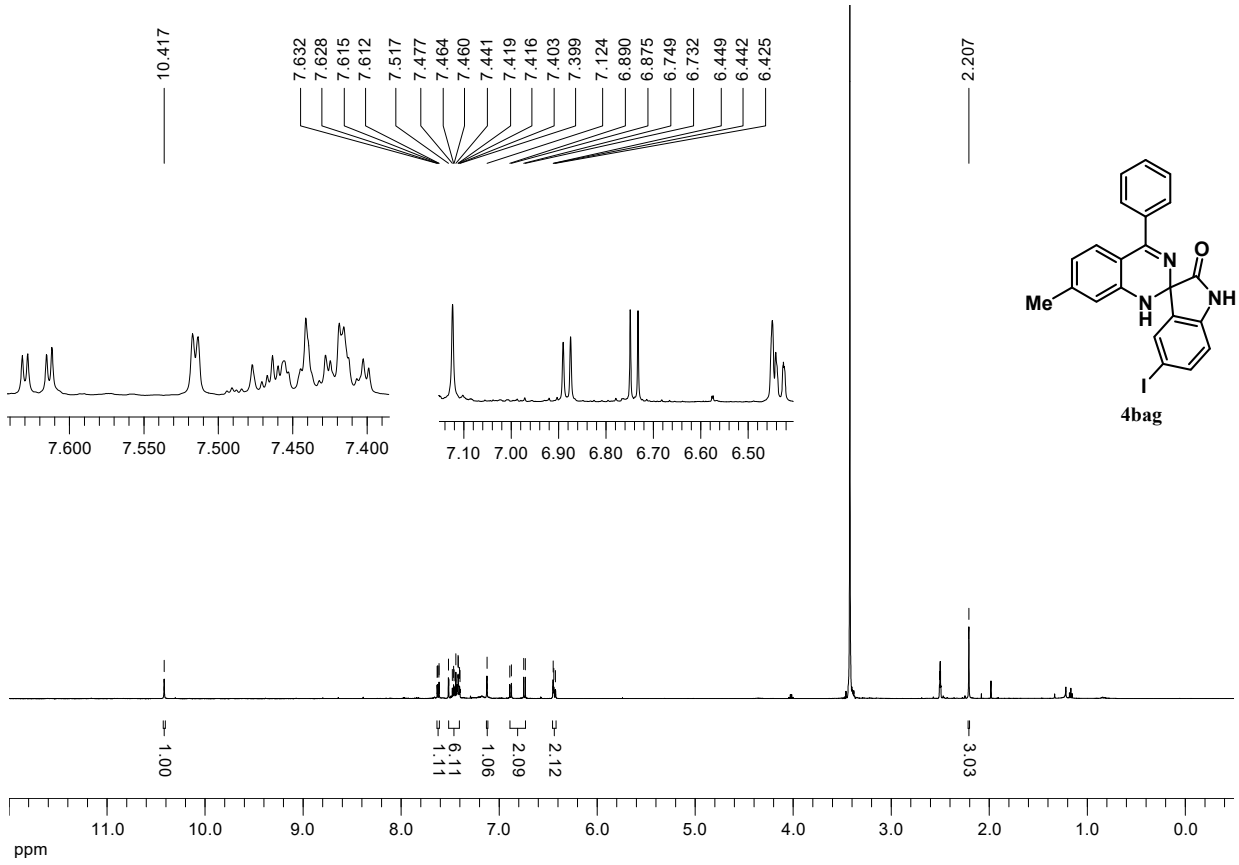

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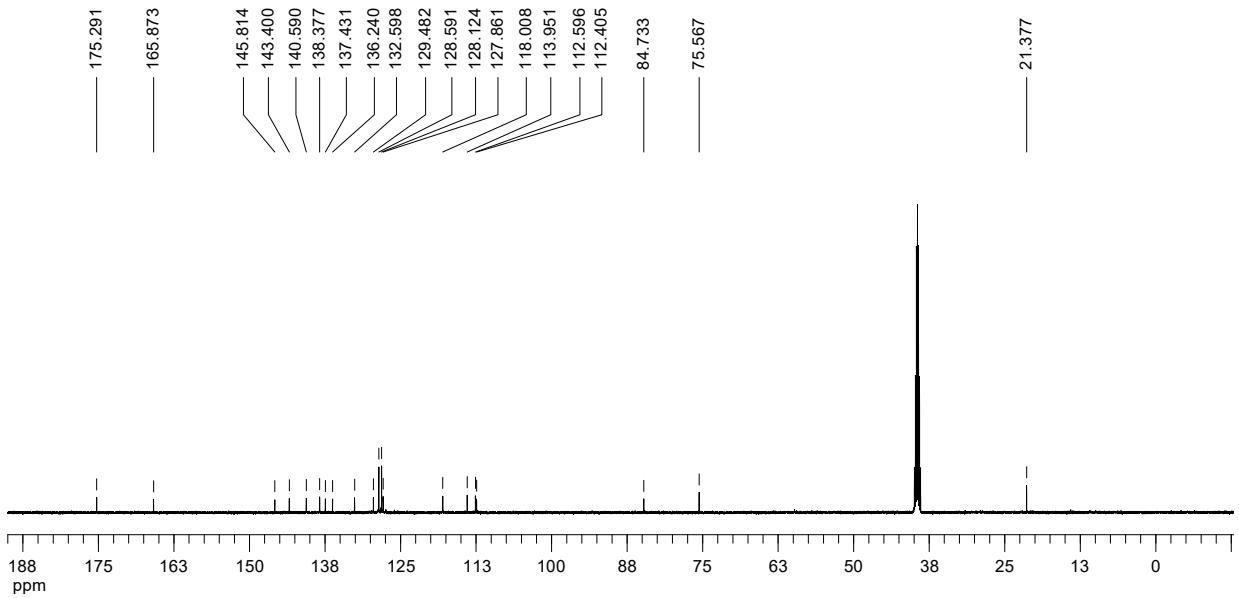

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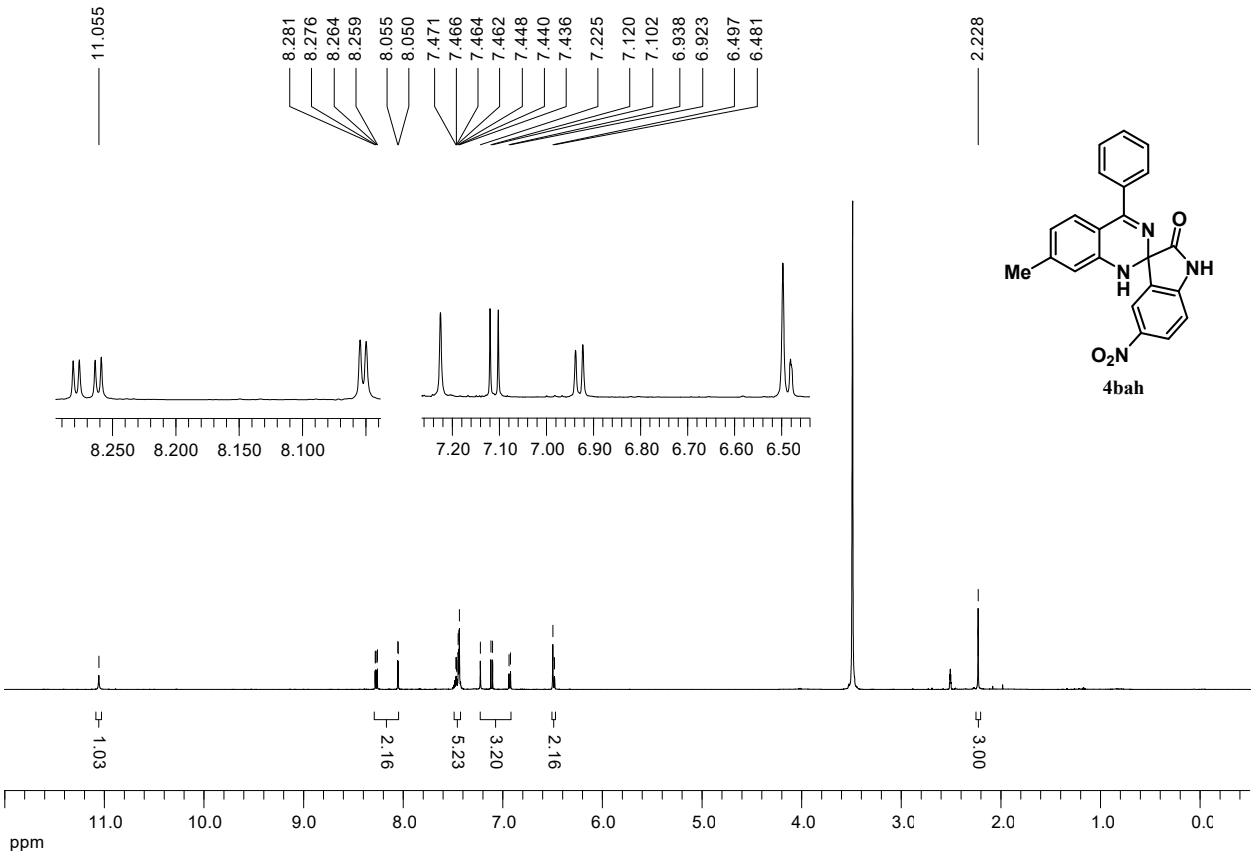

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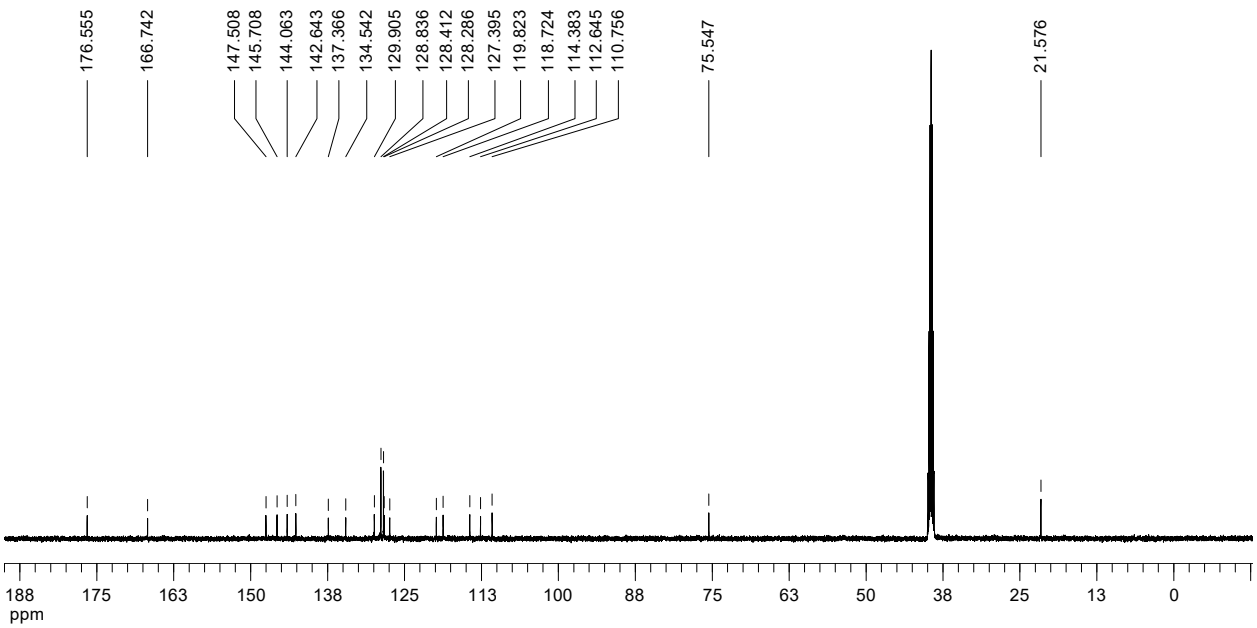

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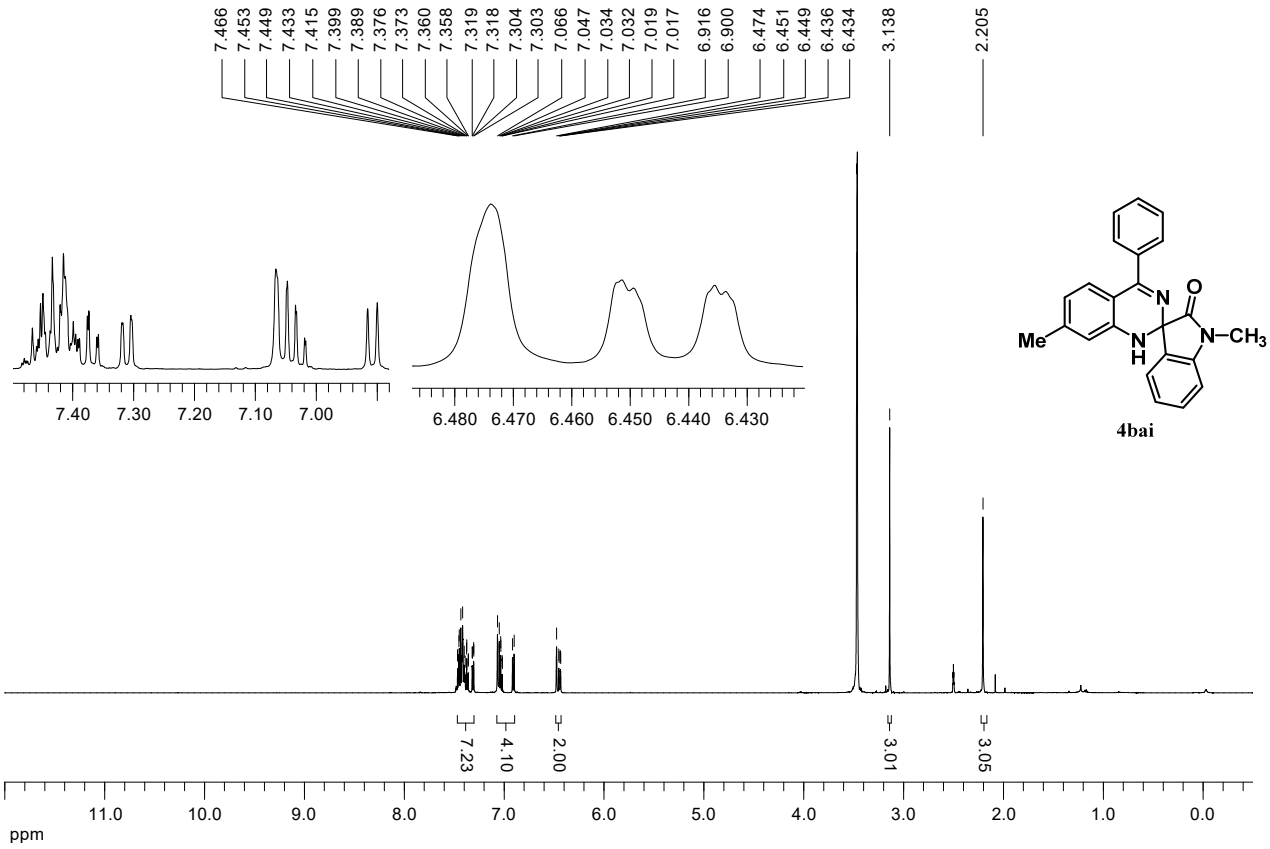

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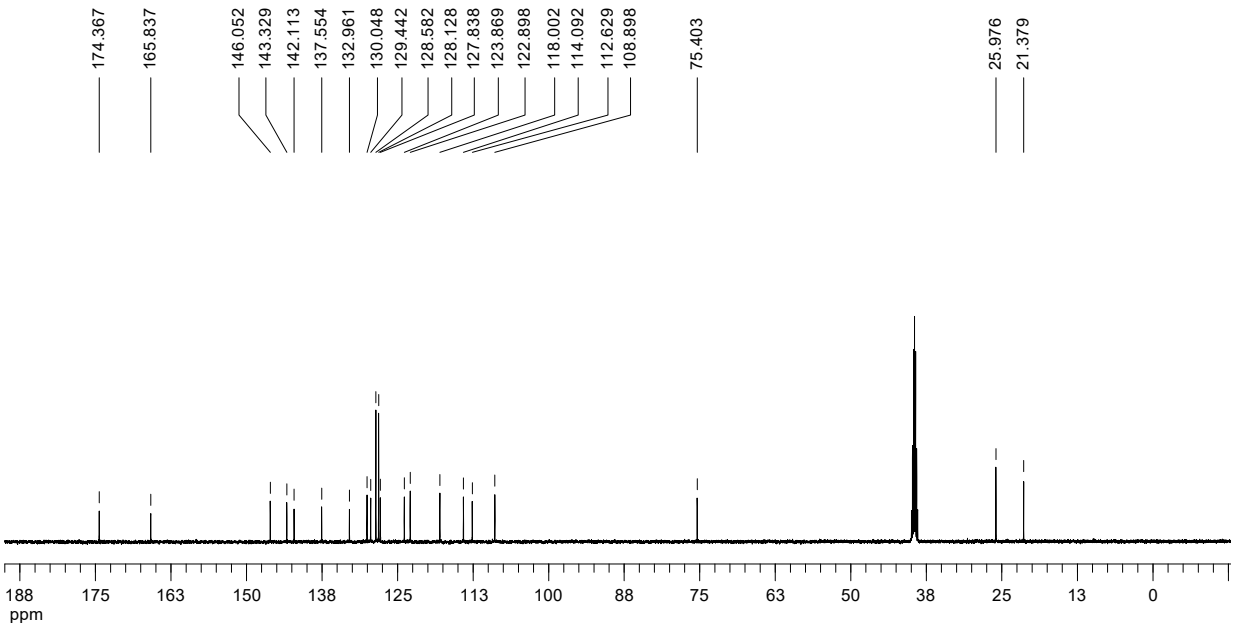

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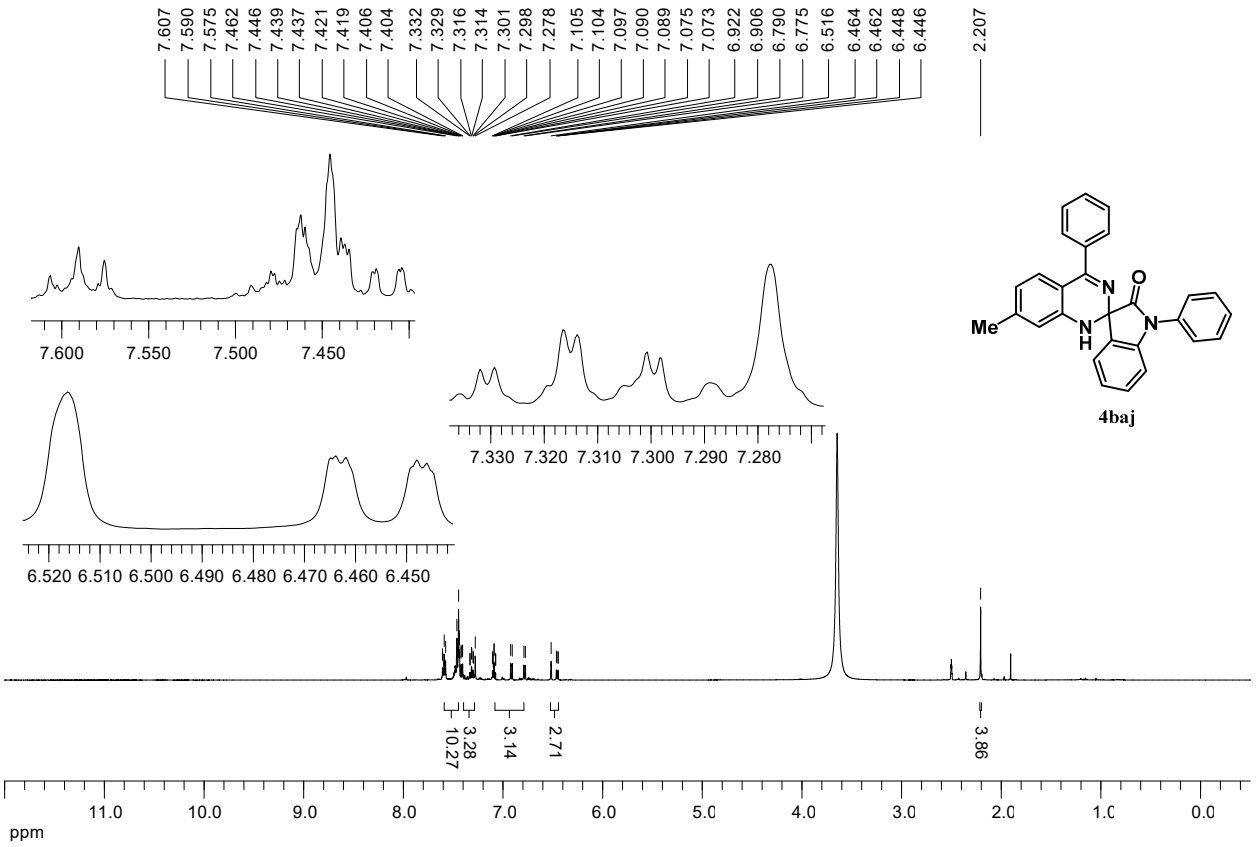

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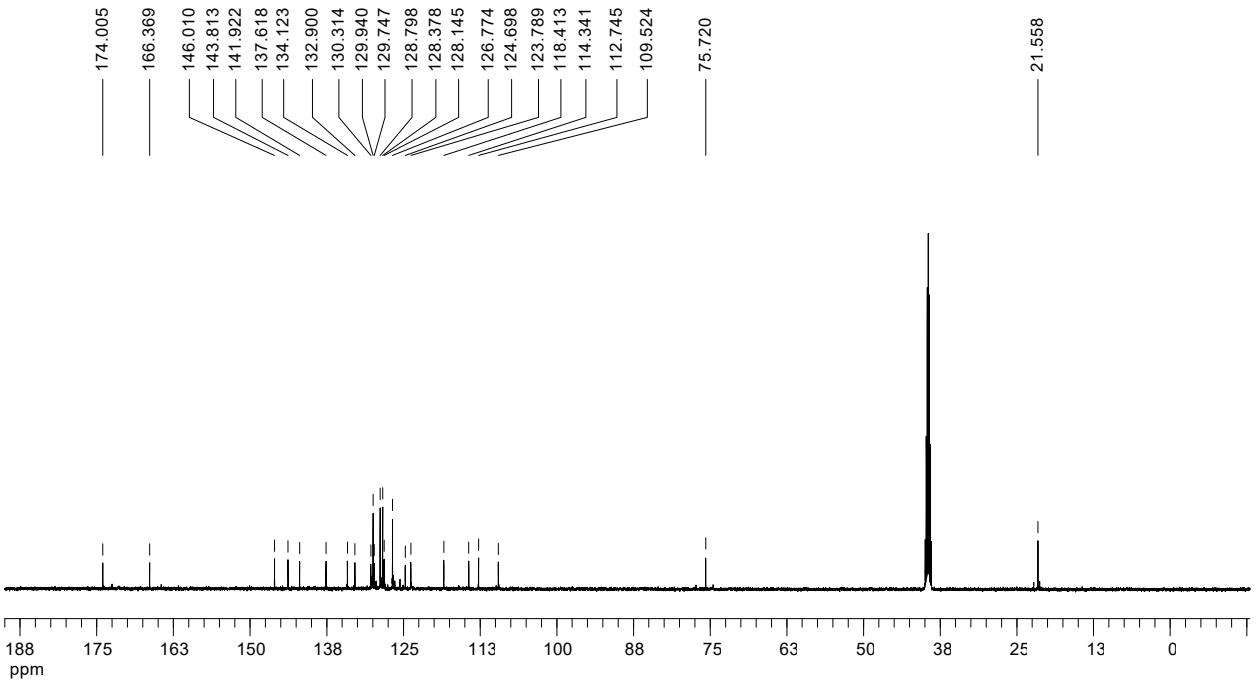

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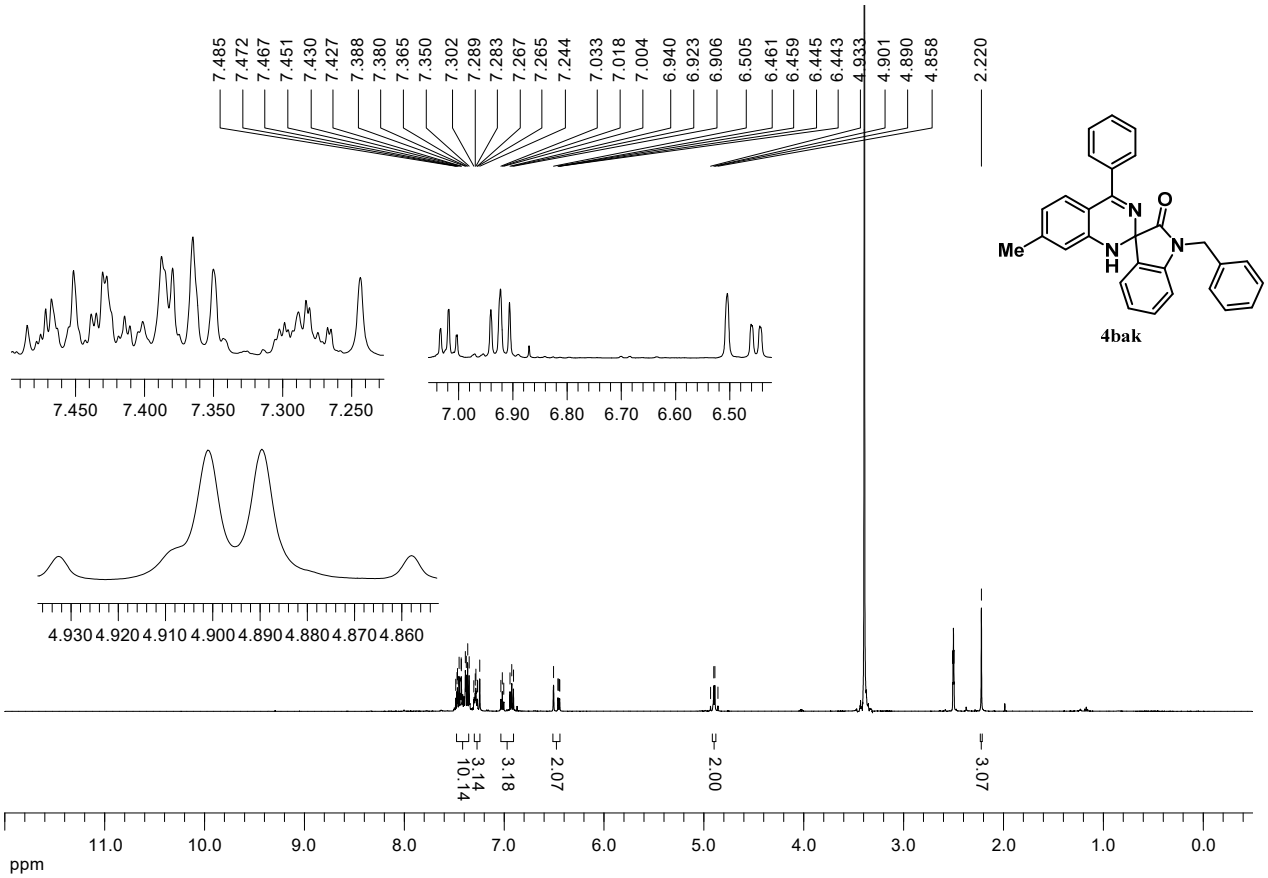

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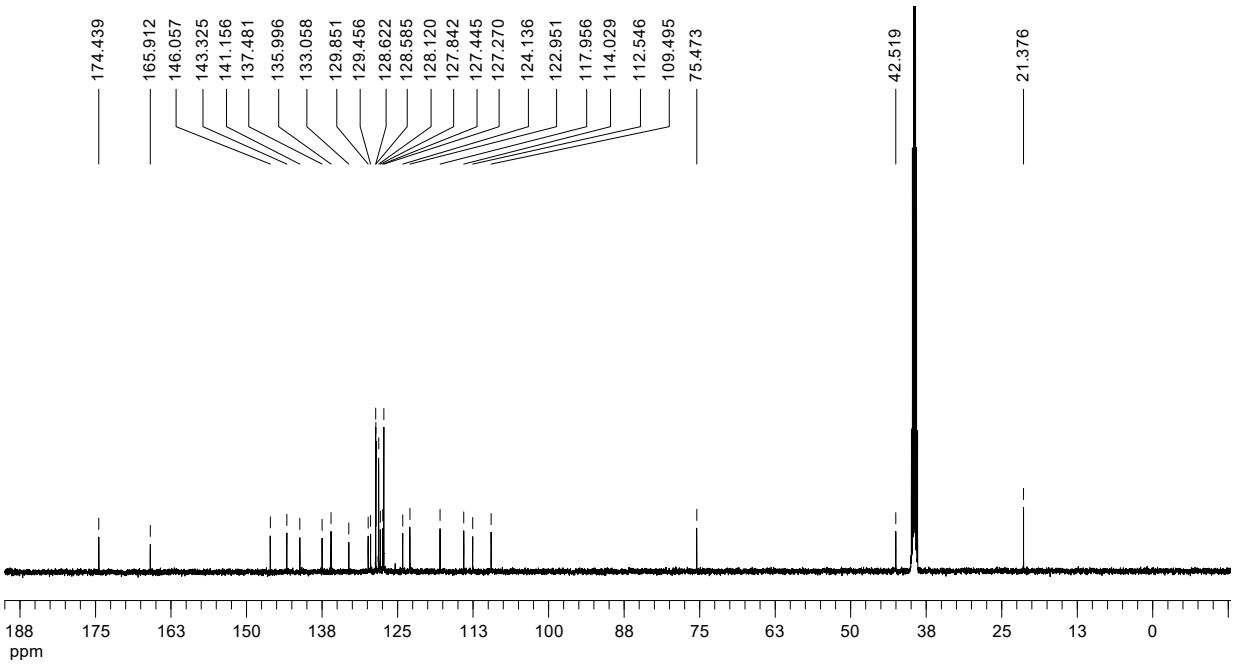

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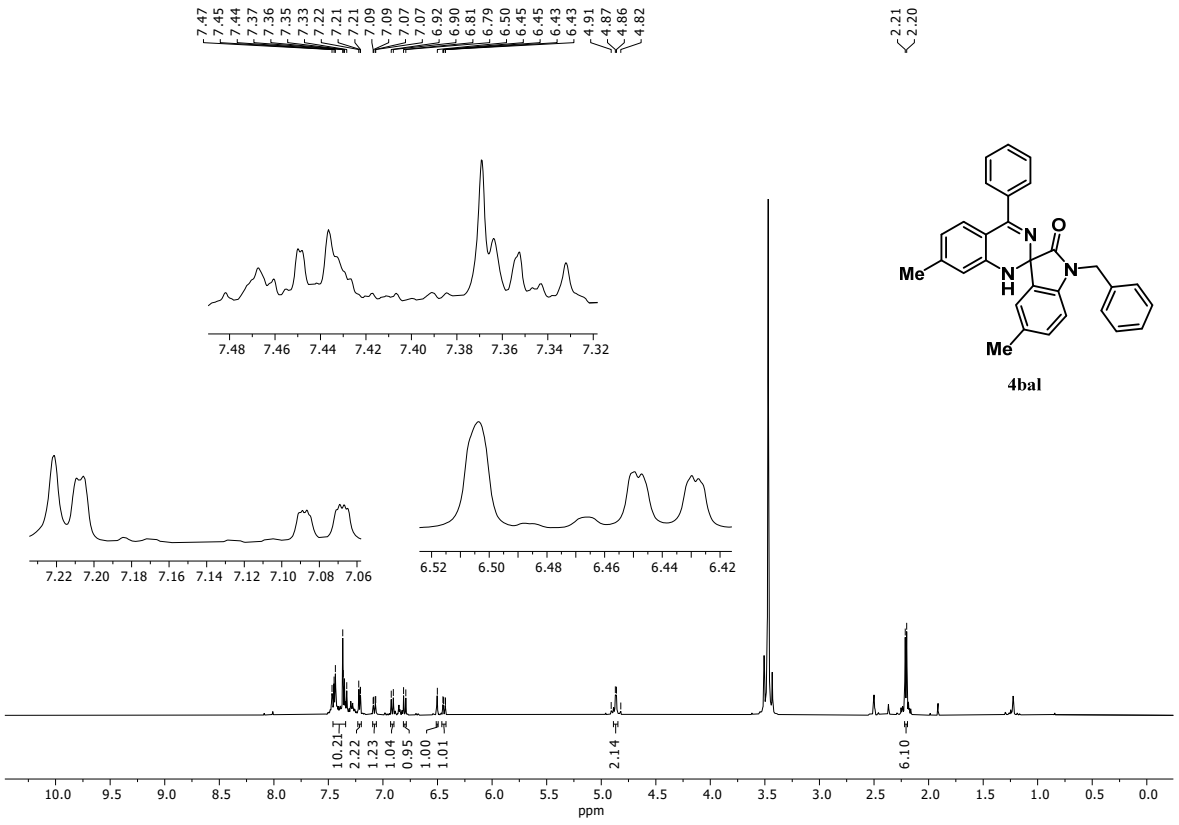

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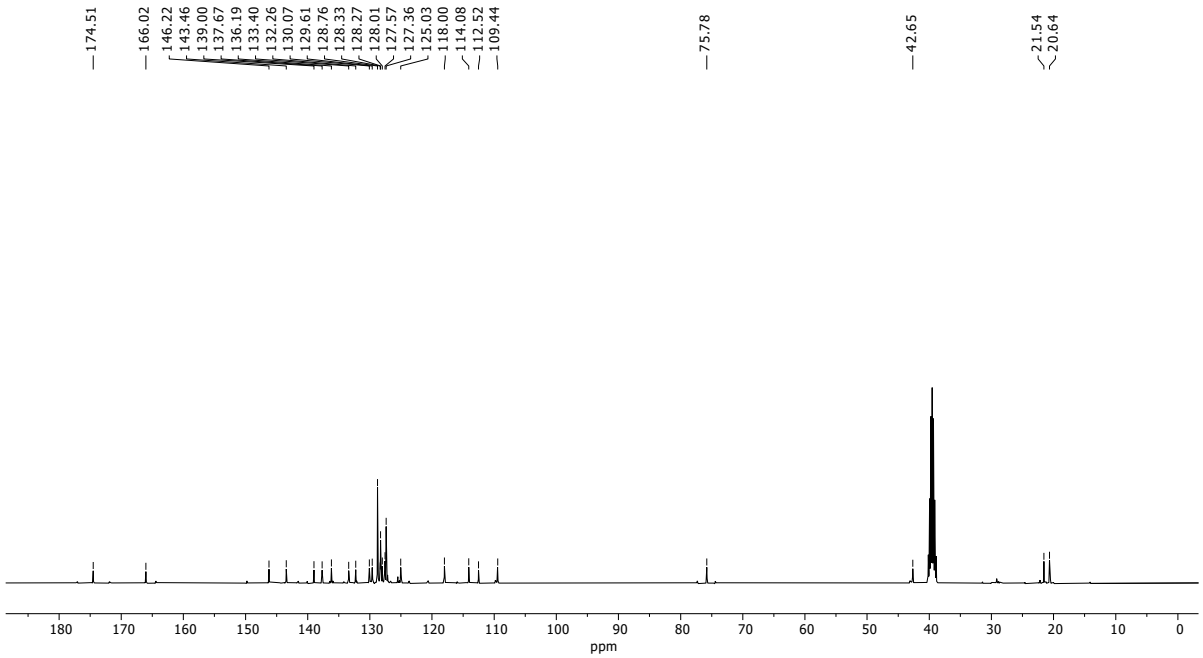
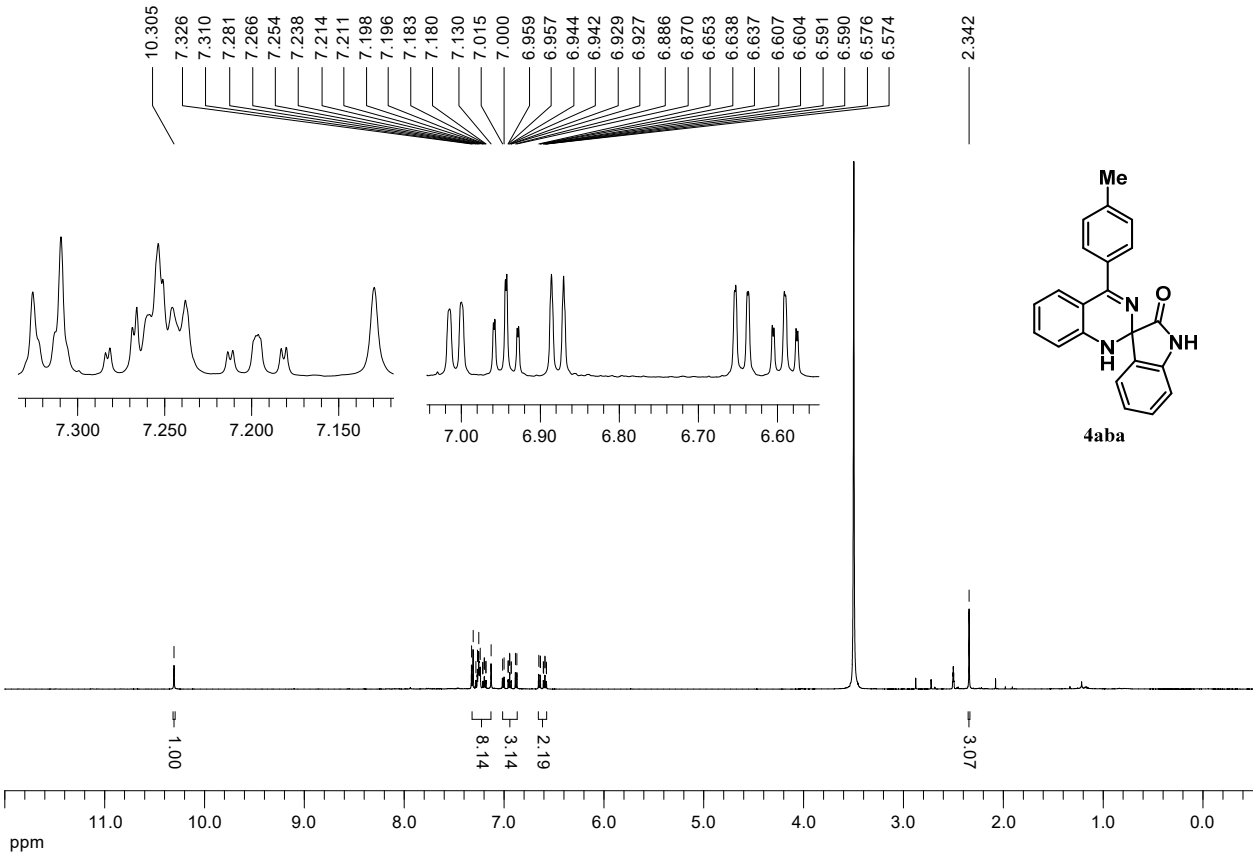
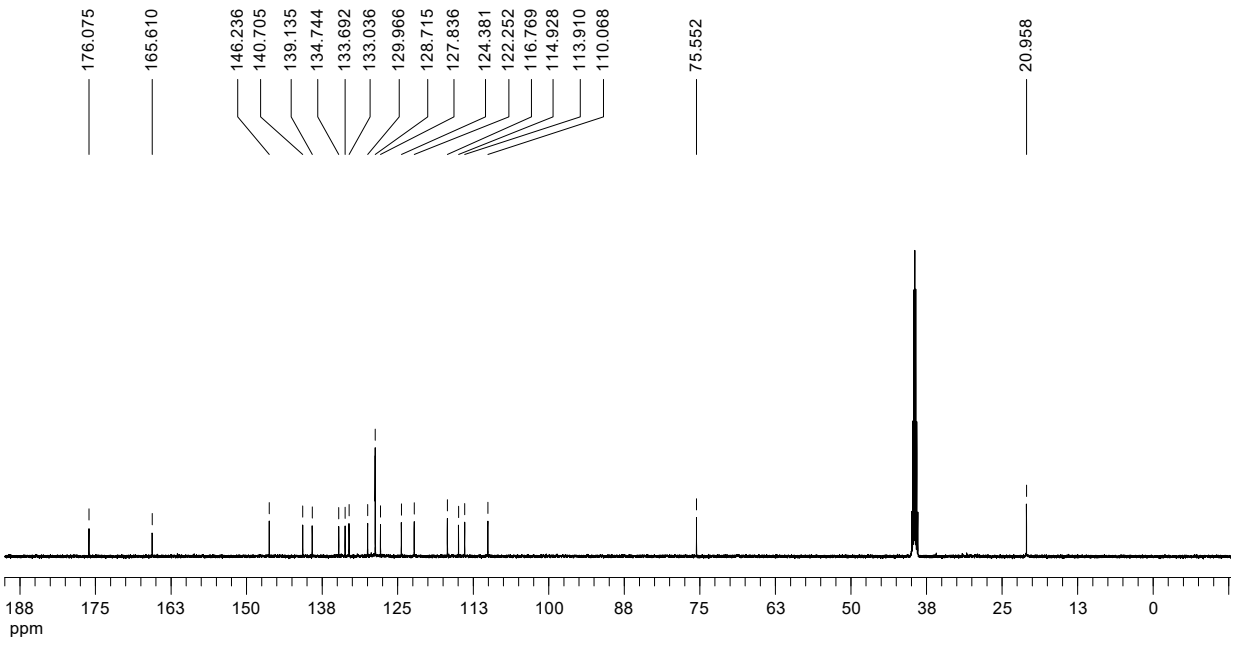


^{1}H-NMR (500 MHz, DMSO-d_6)



^{13}C-NMR (126 MHz, DMSO-d_6)



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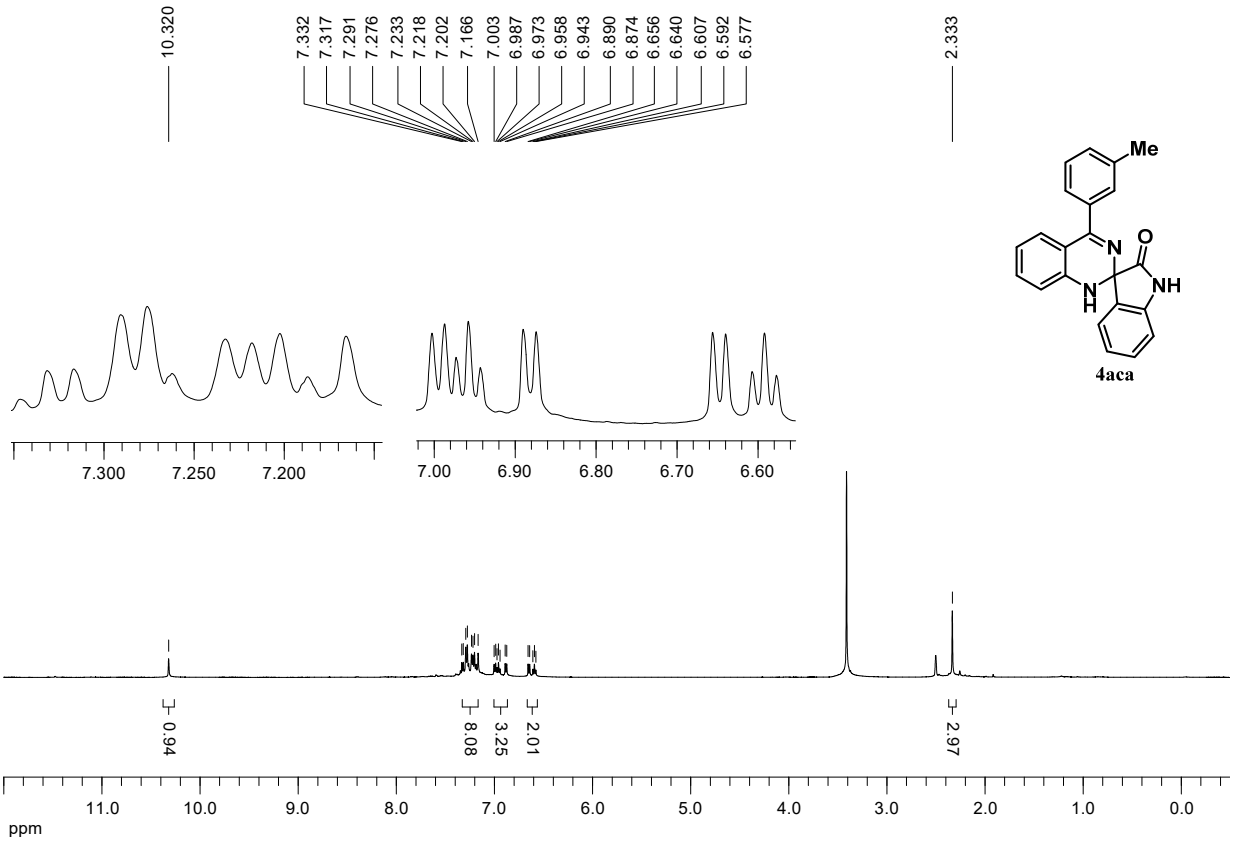
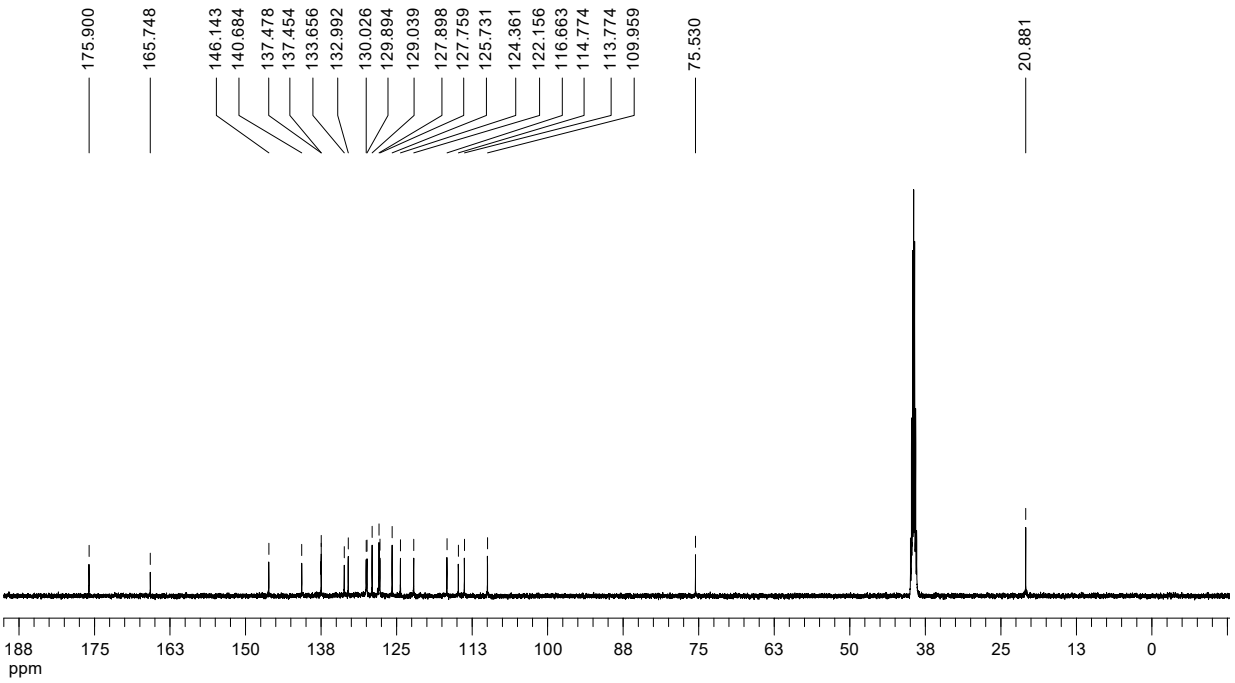


^{13}C-NMR (126 MHz, DMSO-d_6)



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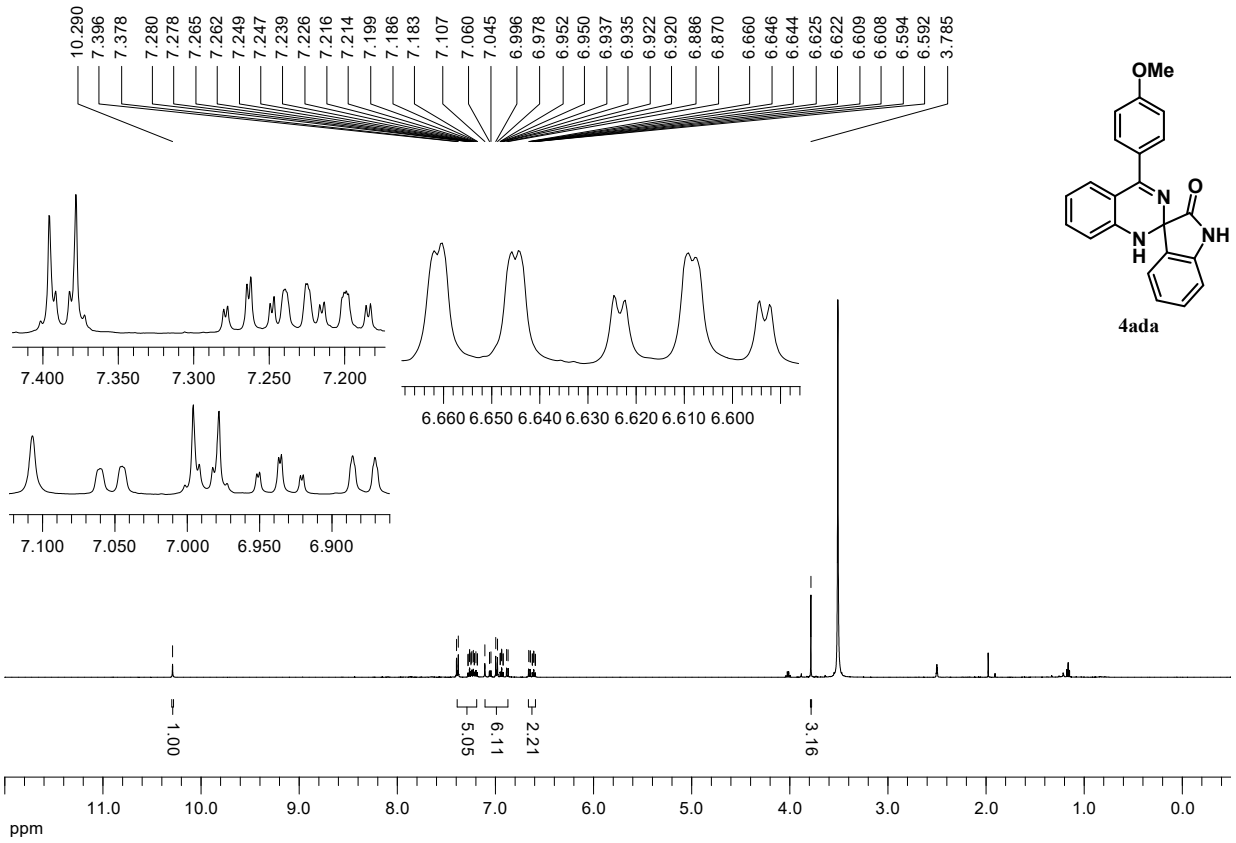
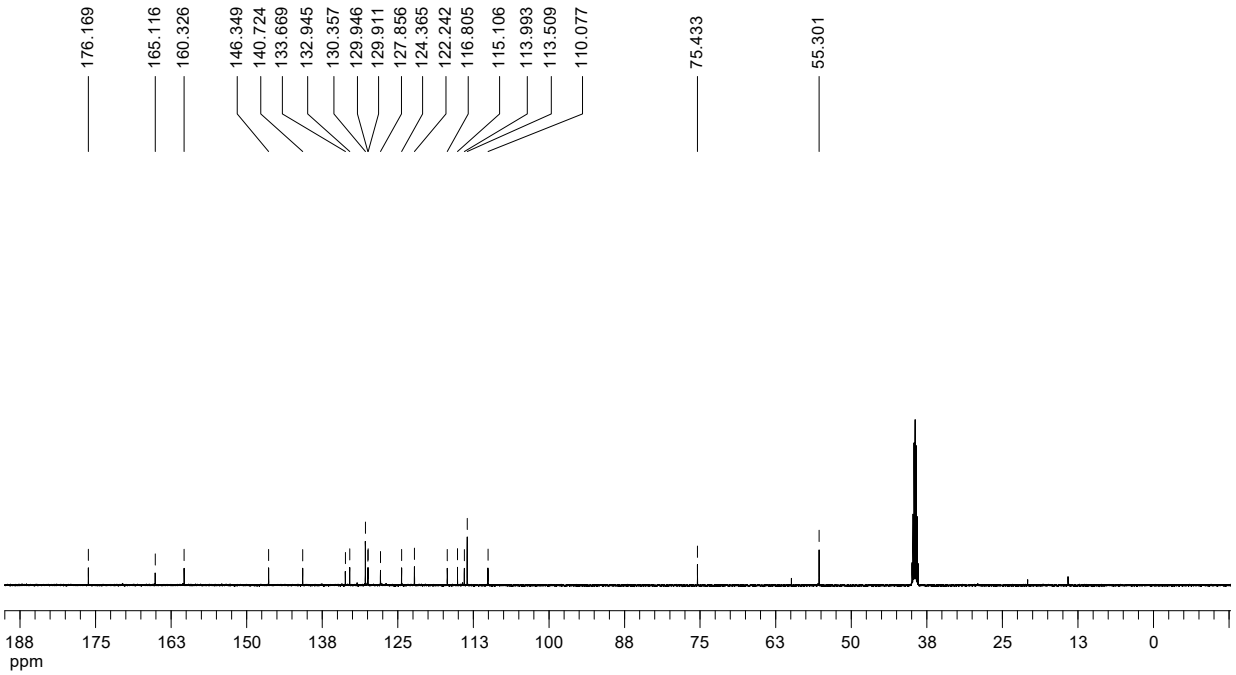


^{13}C-NMR (126 MHz, DMSO-d_6)



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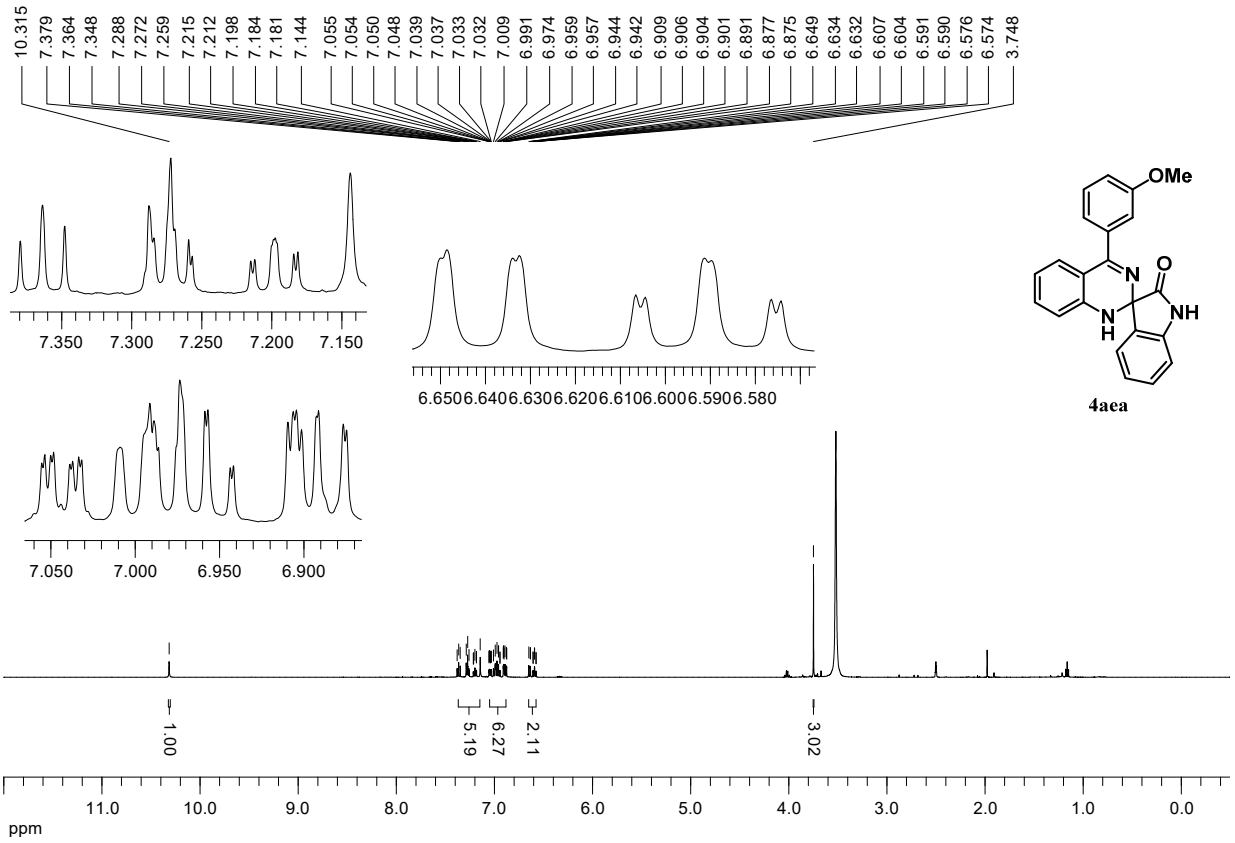
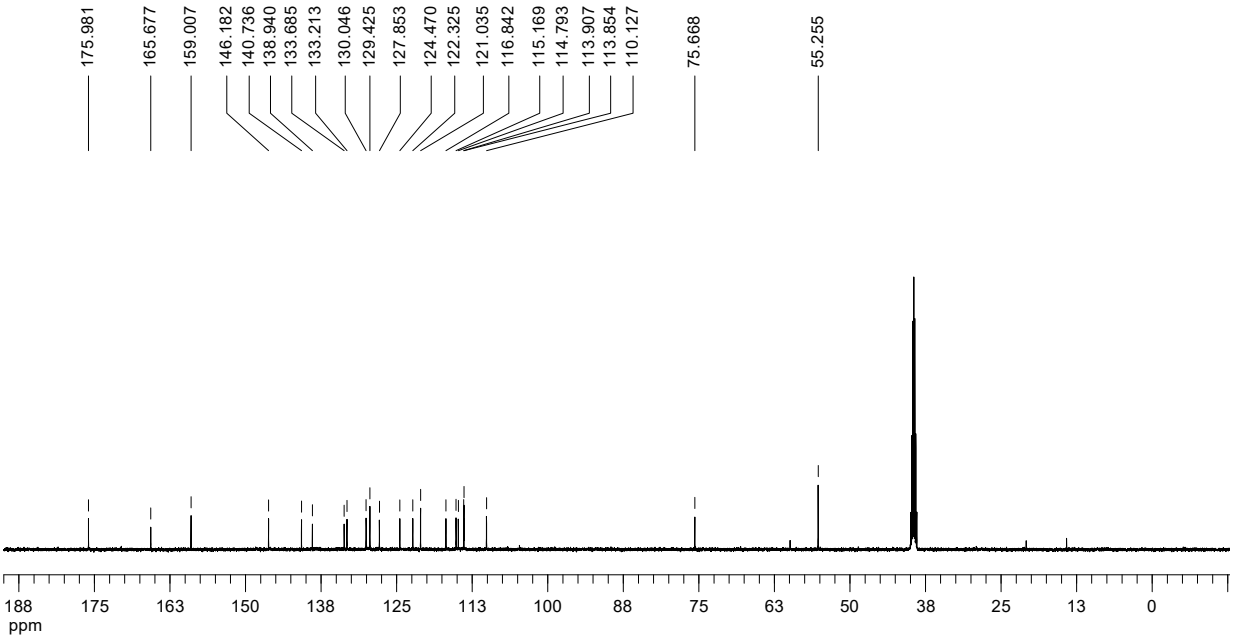
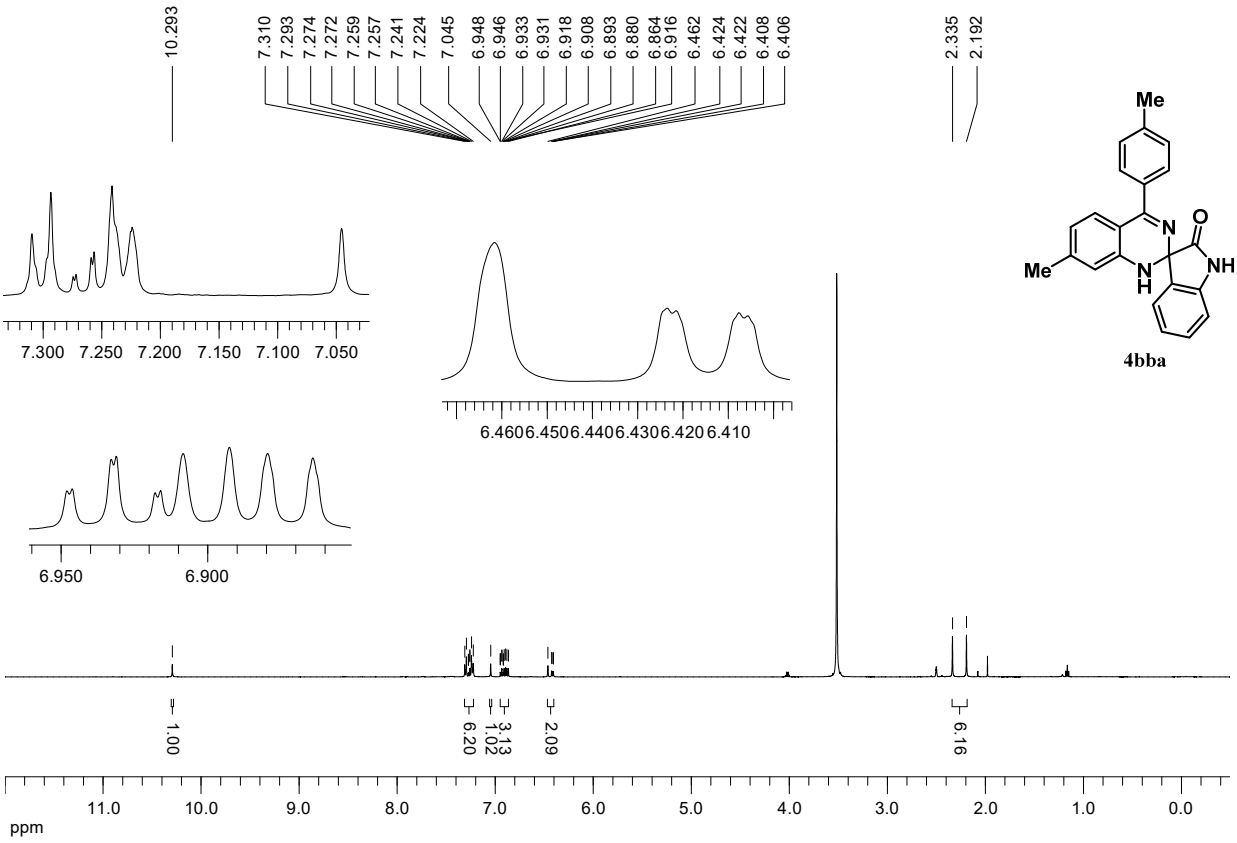


^{13}C-NMR (126 MHz, DMSO-d_6)

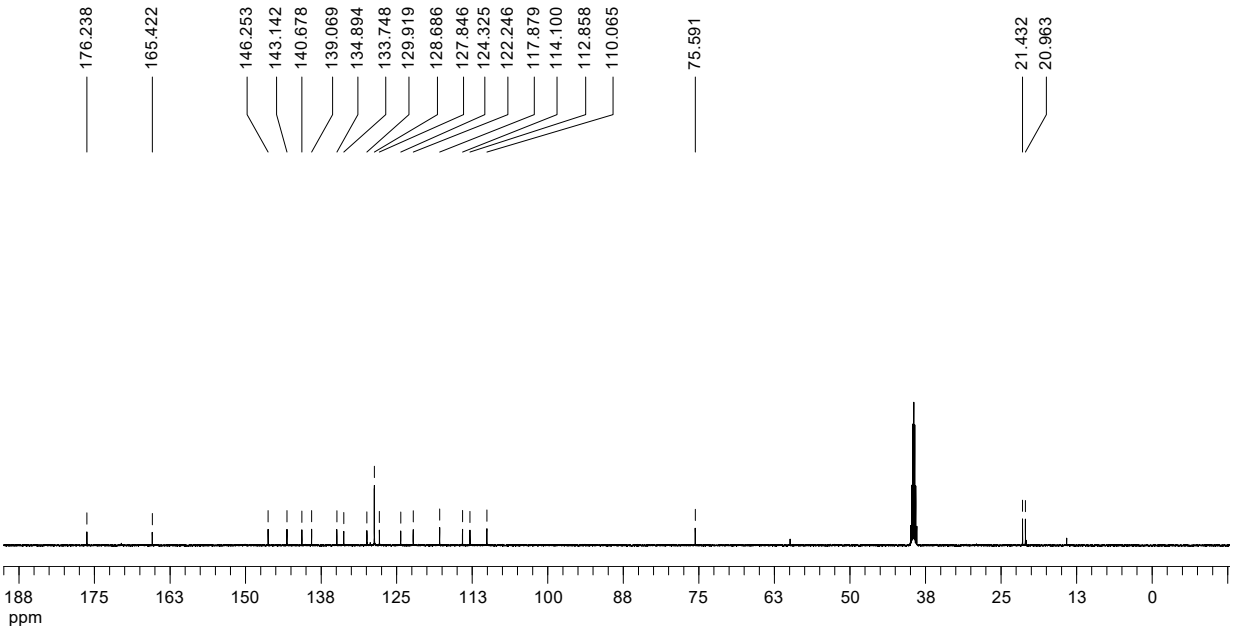


^{1}H-NMR (500 MHz, DMSO-d_6)

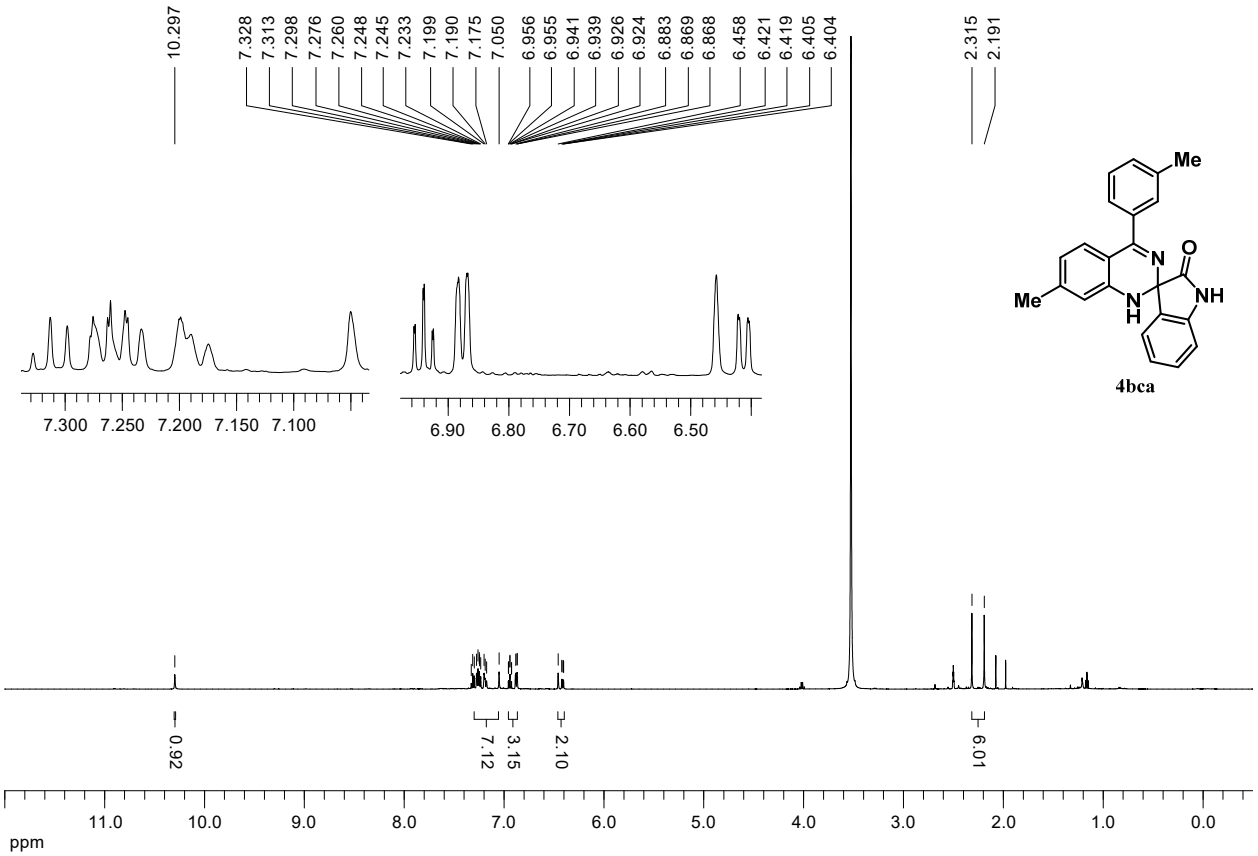


4bba

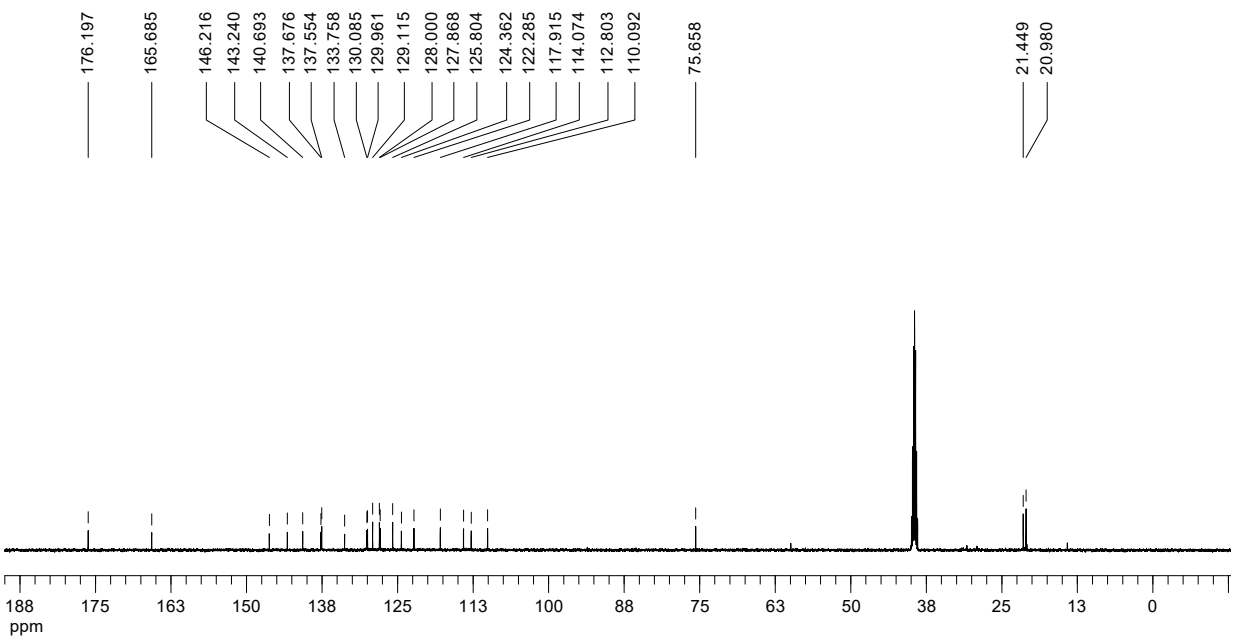
^{13}C-NMR (126 MHz, DMSO-d_6)



^{1}H-NMR (500 MHz, DMSO-d_6)



^{13}C-NMR (126 MHz, DMSO-d_6)



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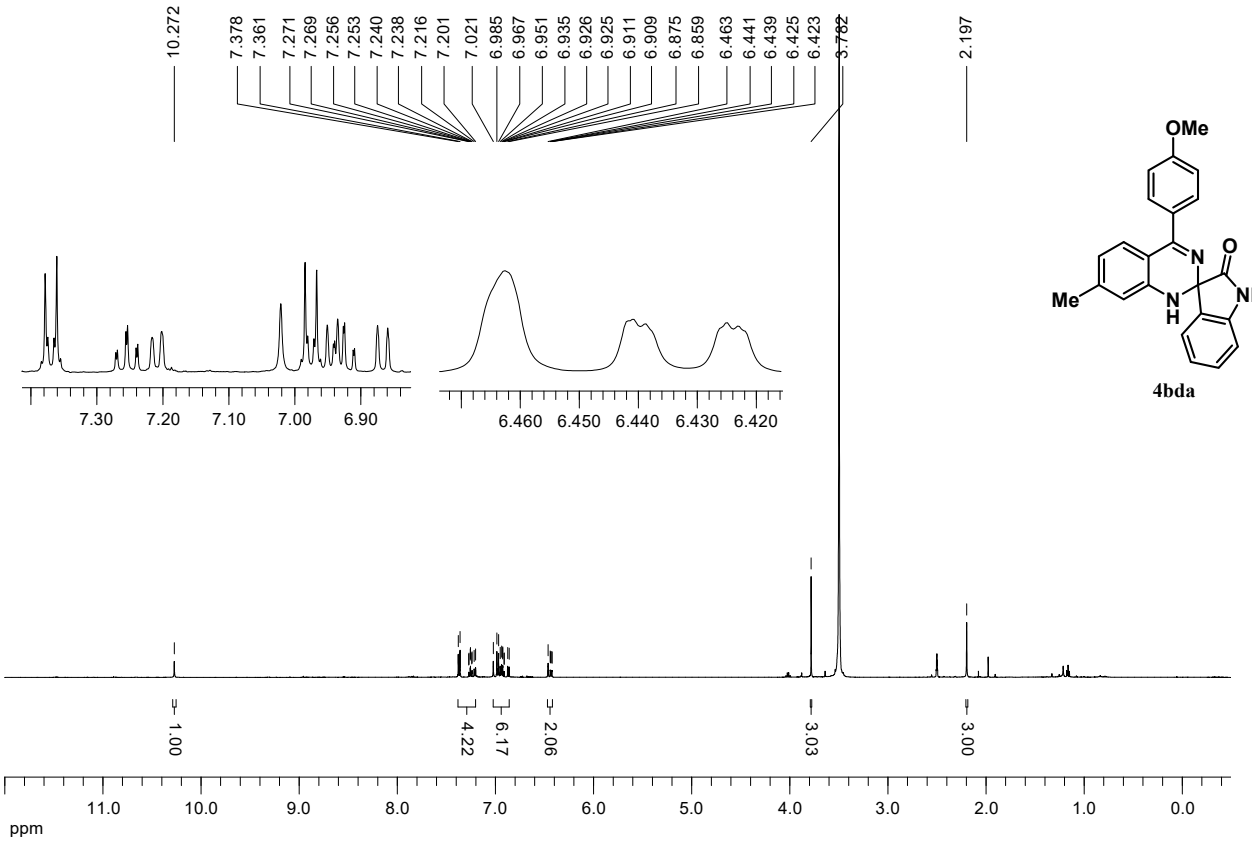

4bda

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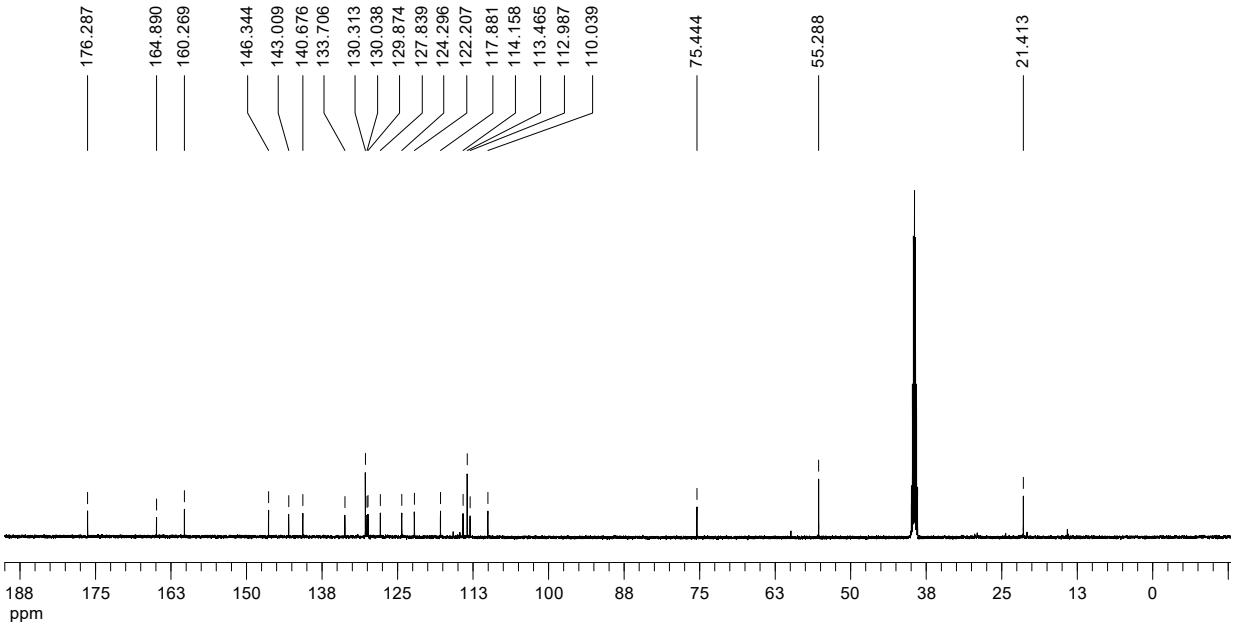

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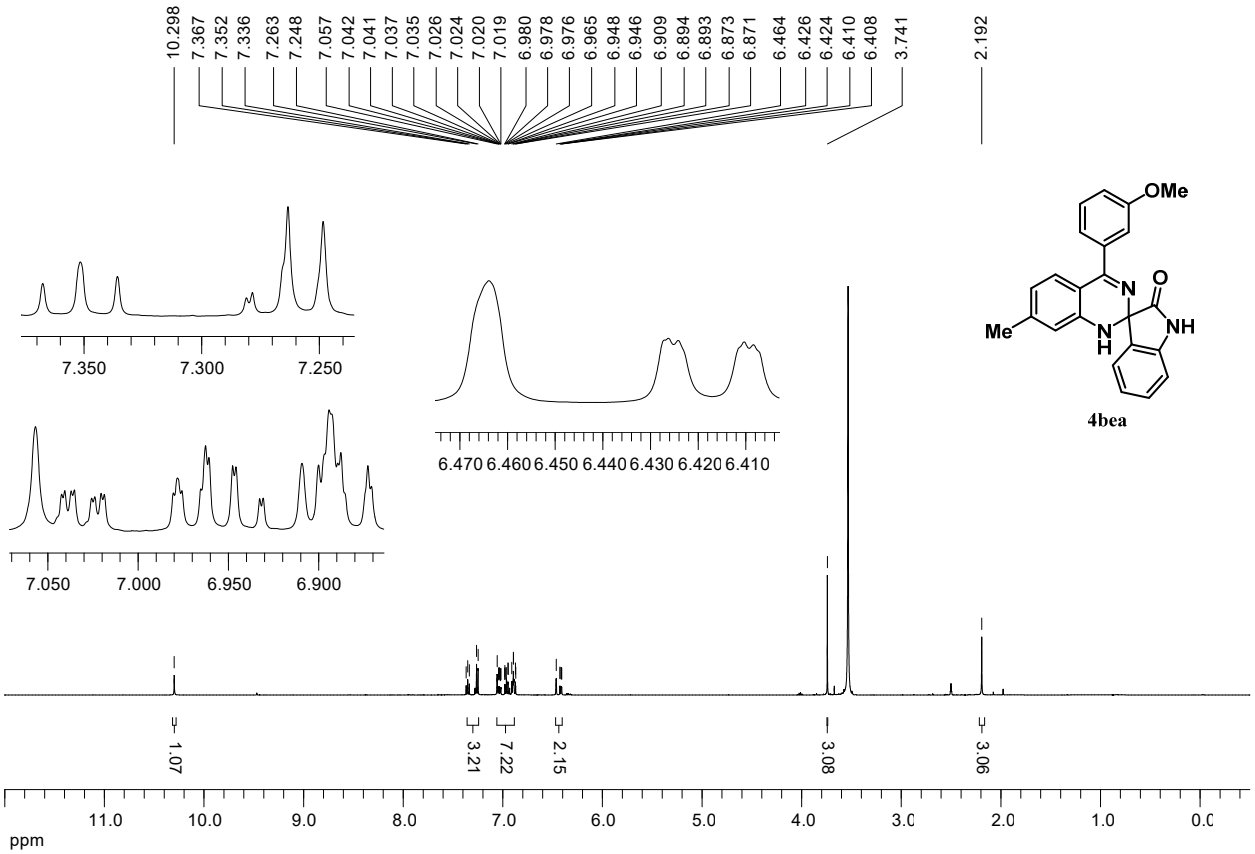

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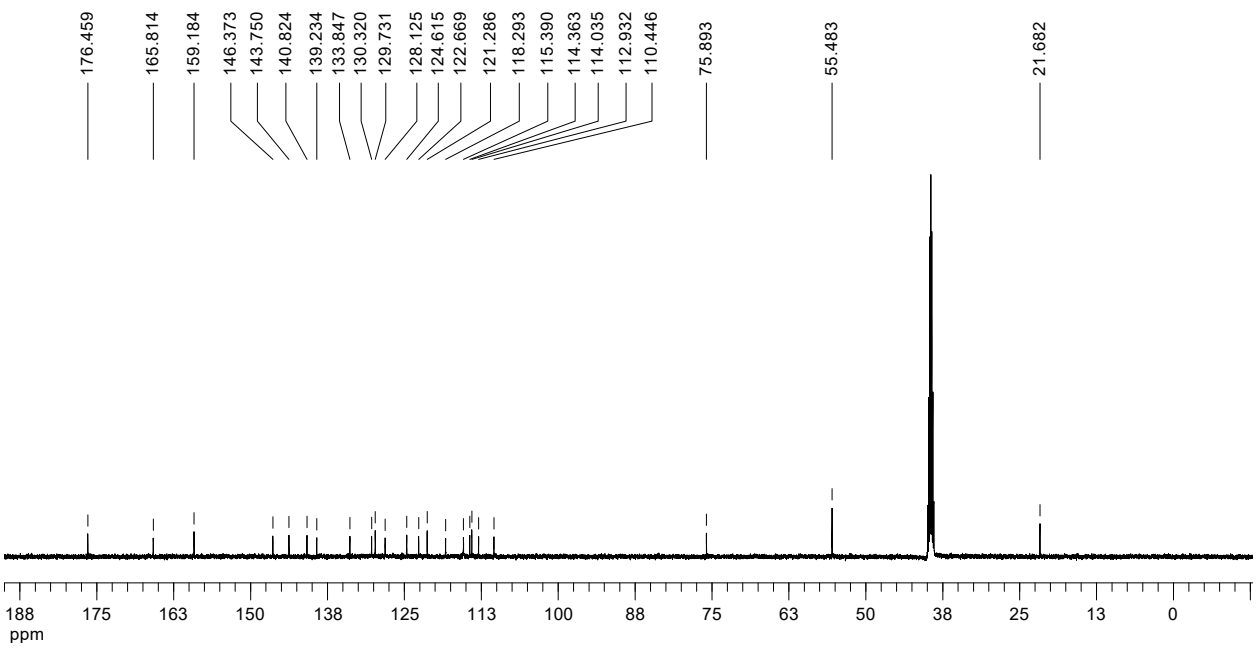

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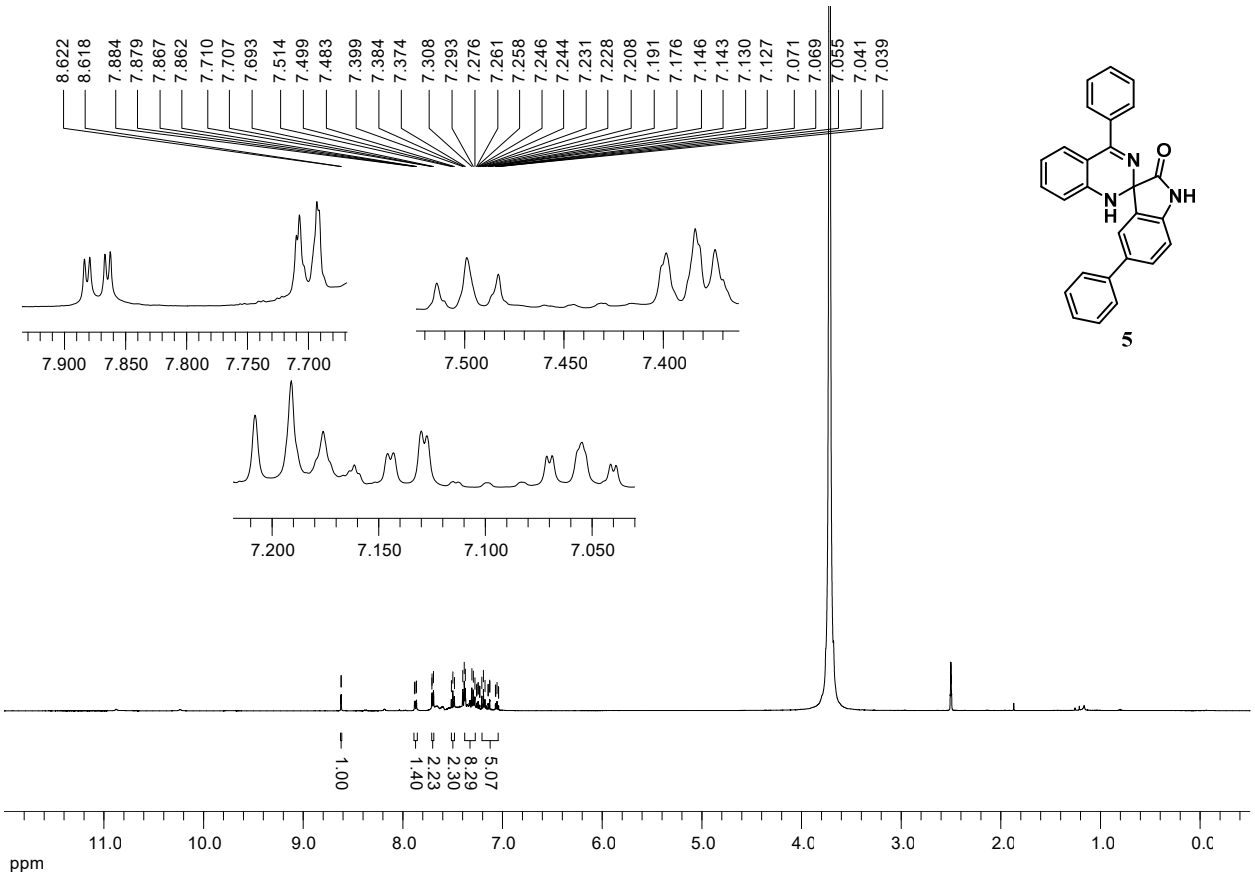

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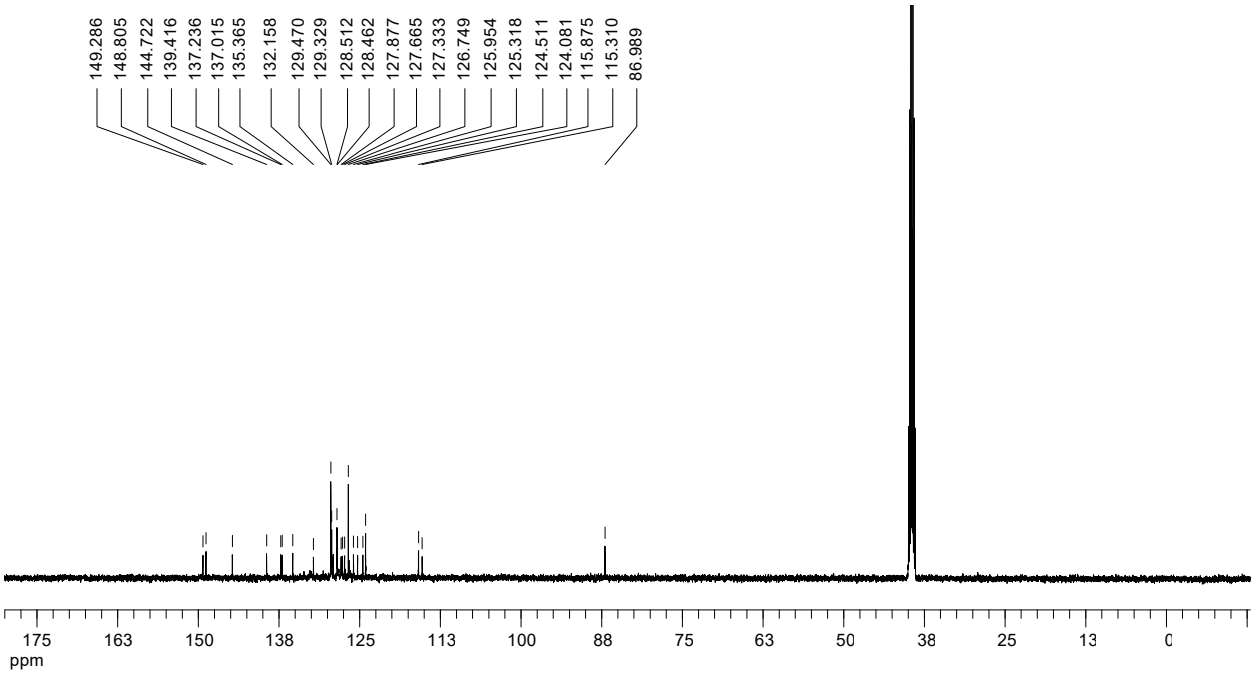

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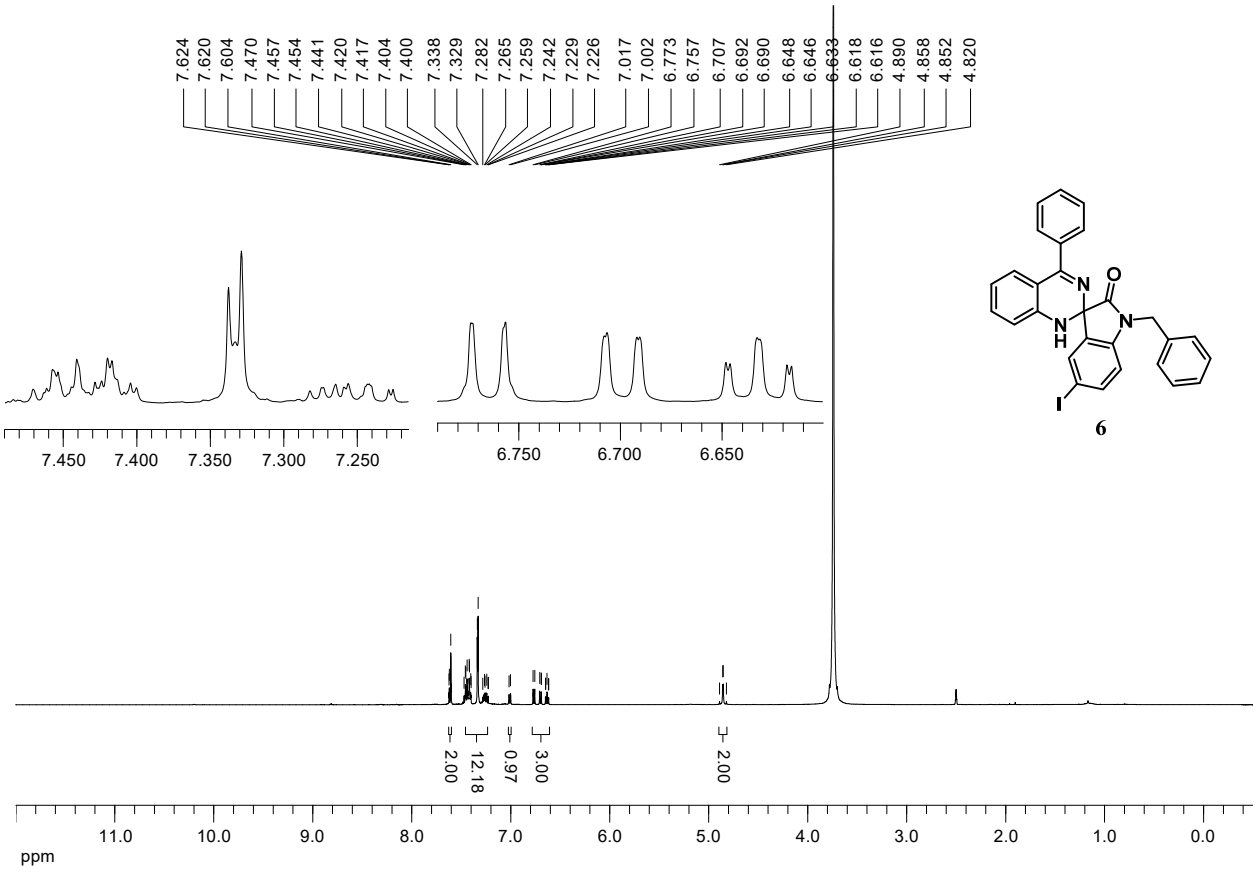
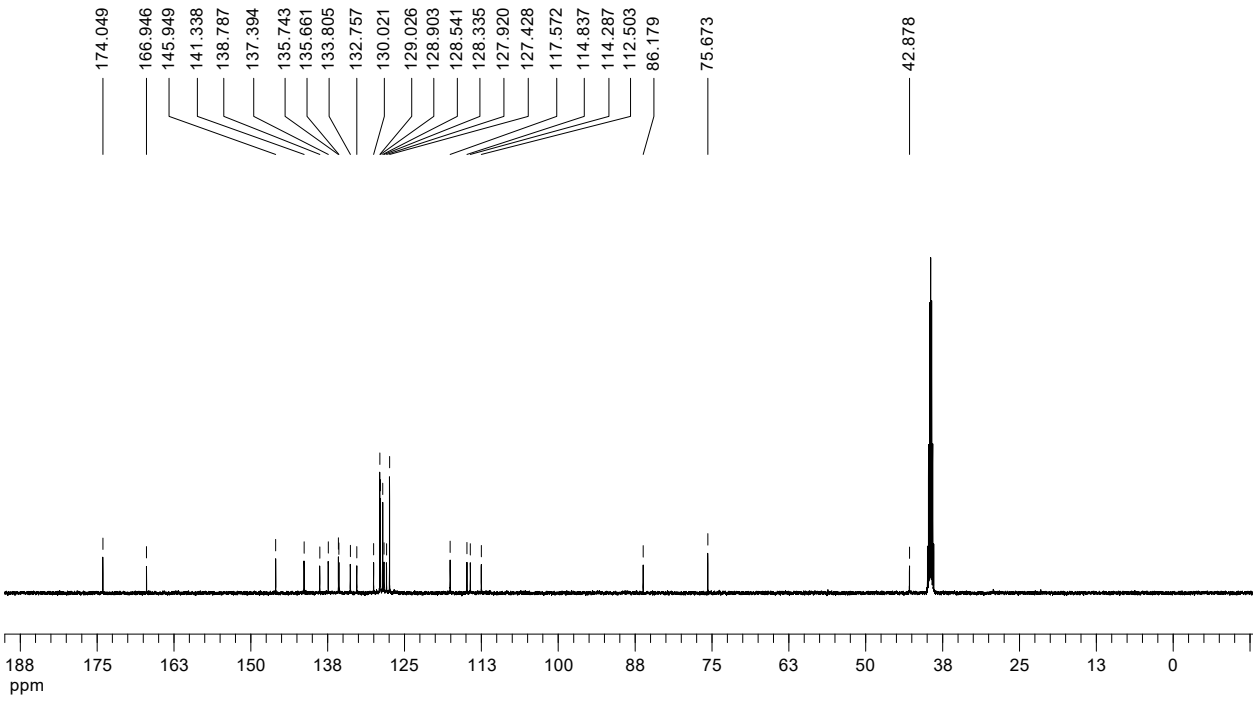
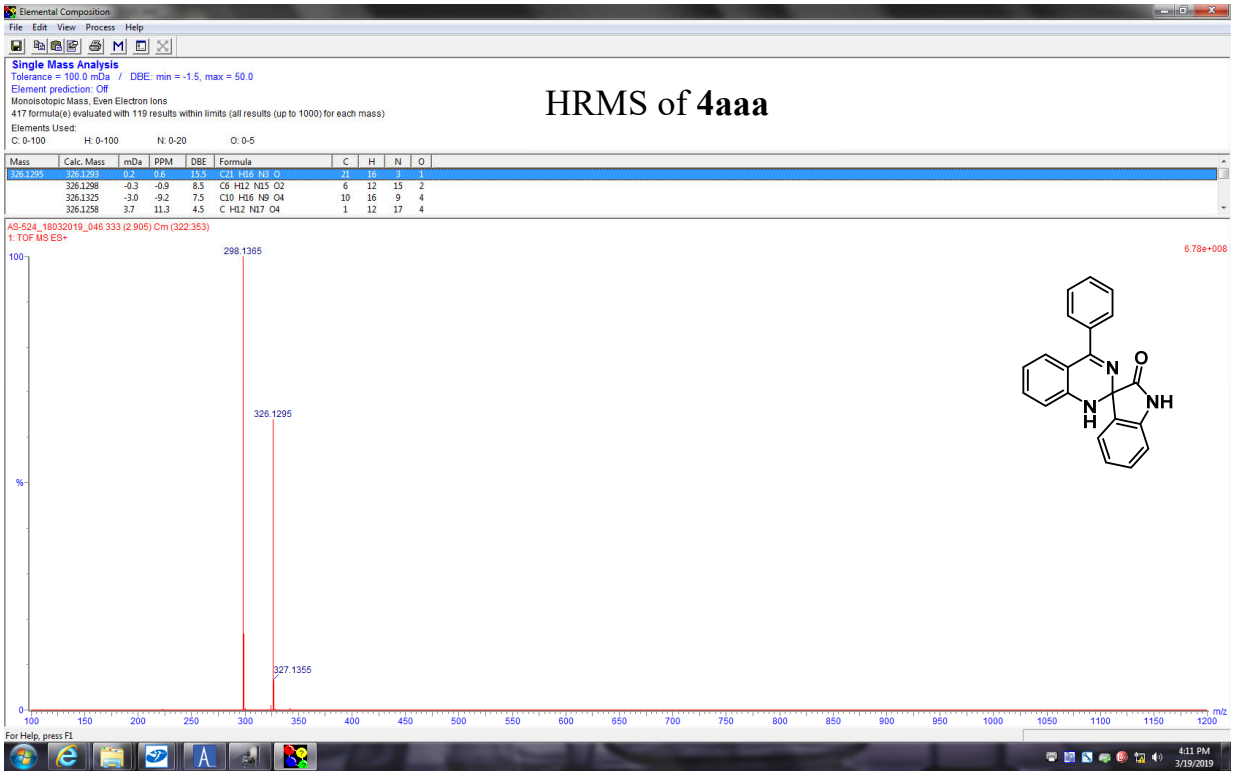


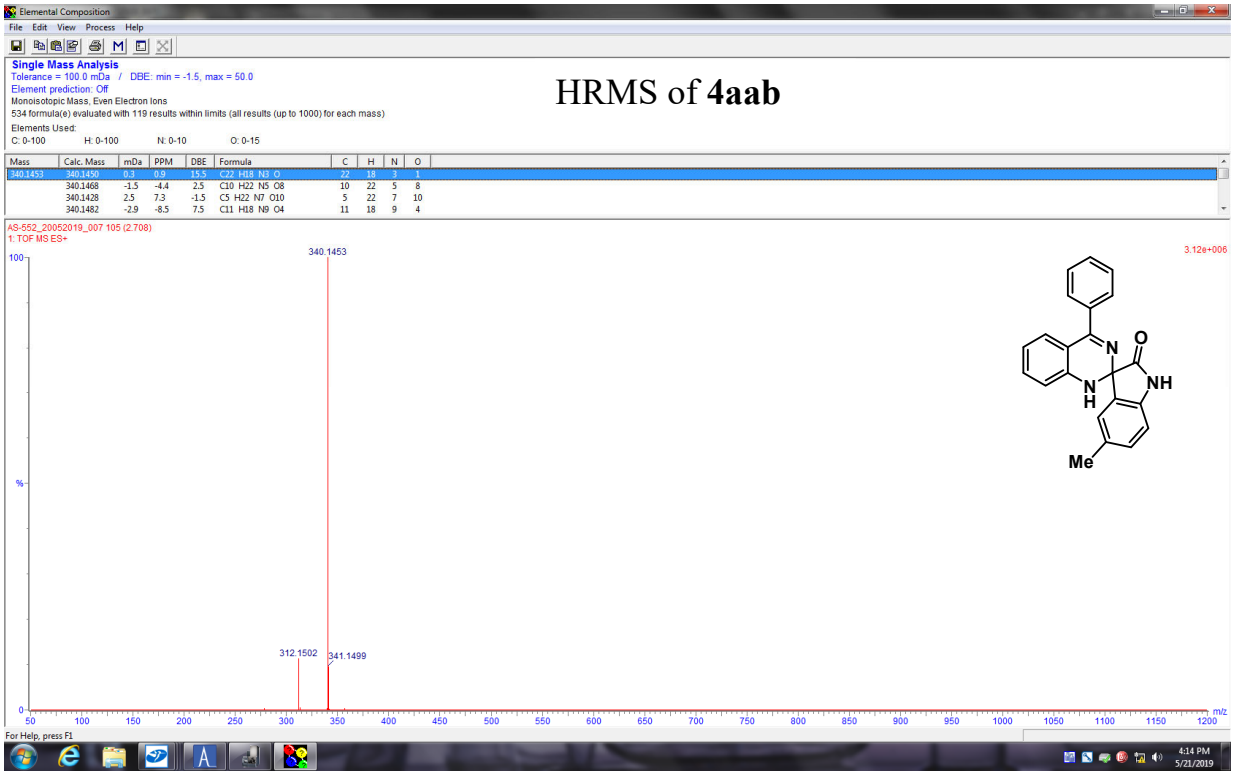
6

^{13}C-NMR (126 MHz, DMSO-d_6)





HRMS of **4aaa**



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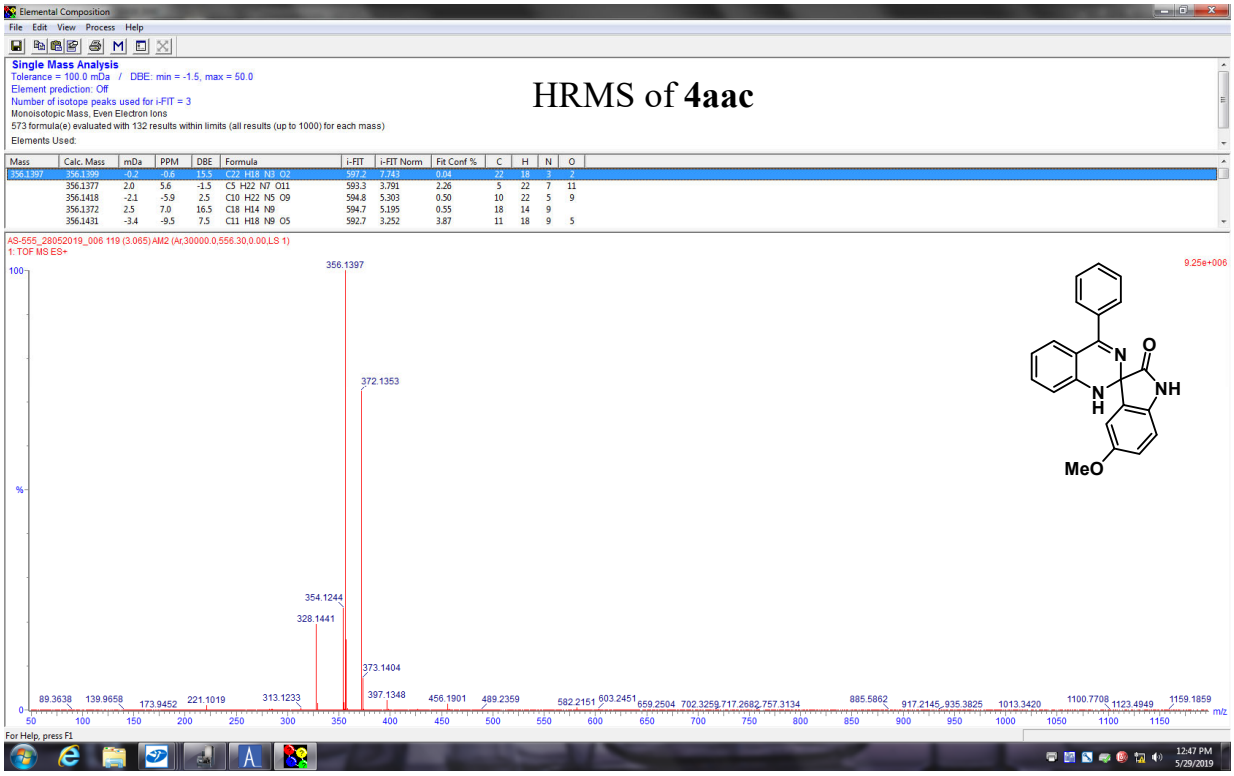
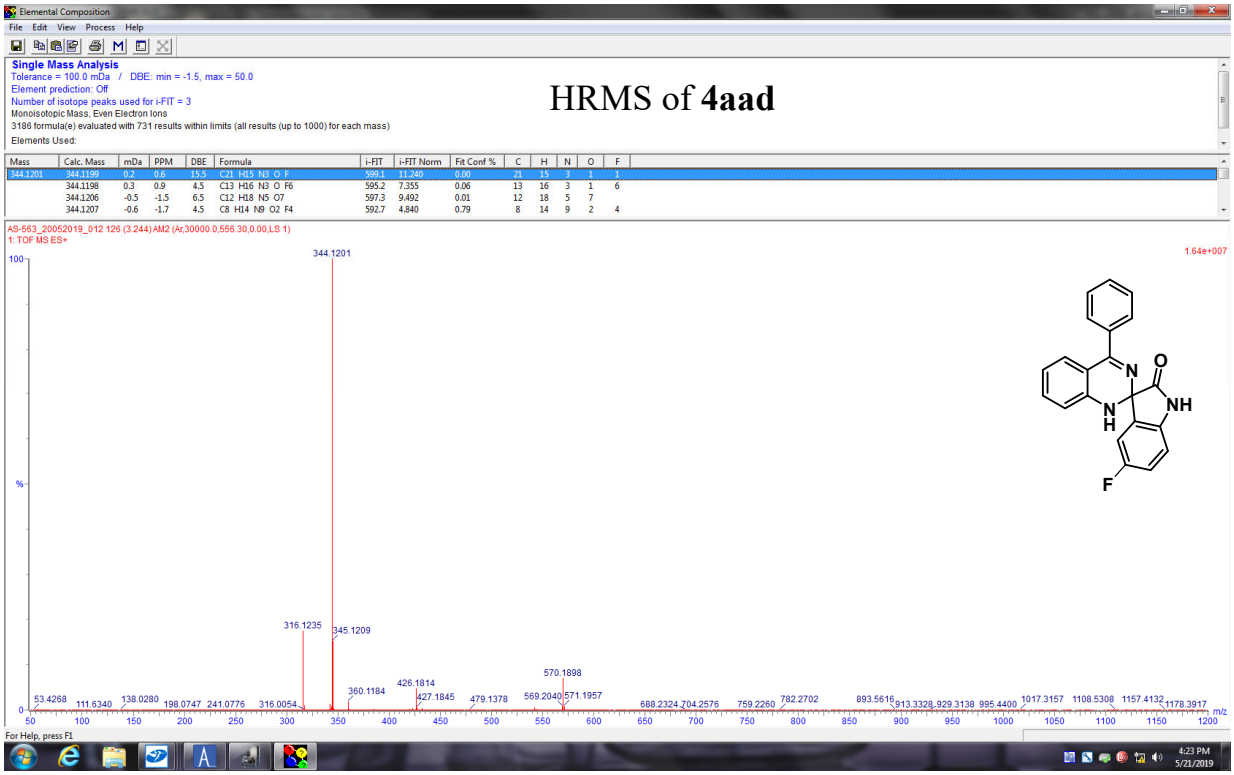
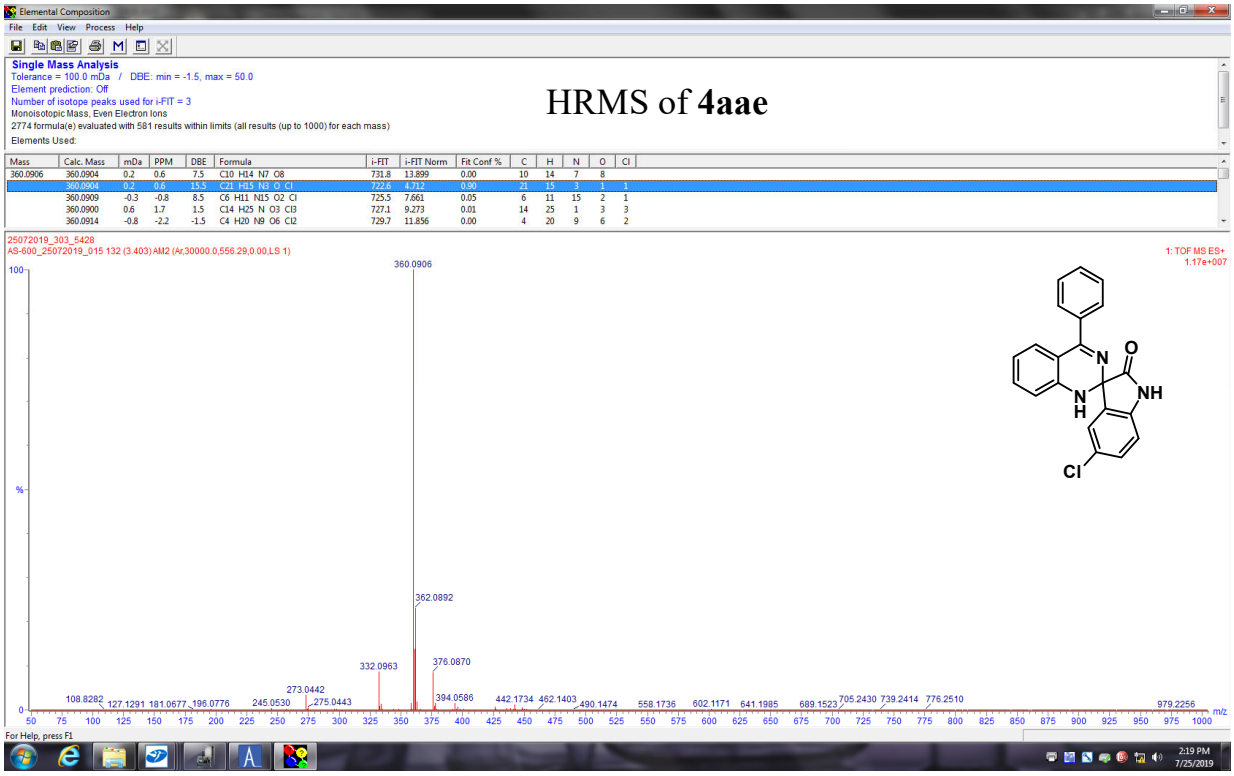


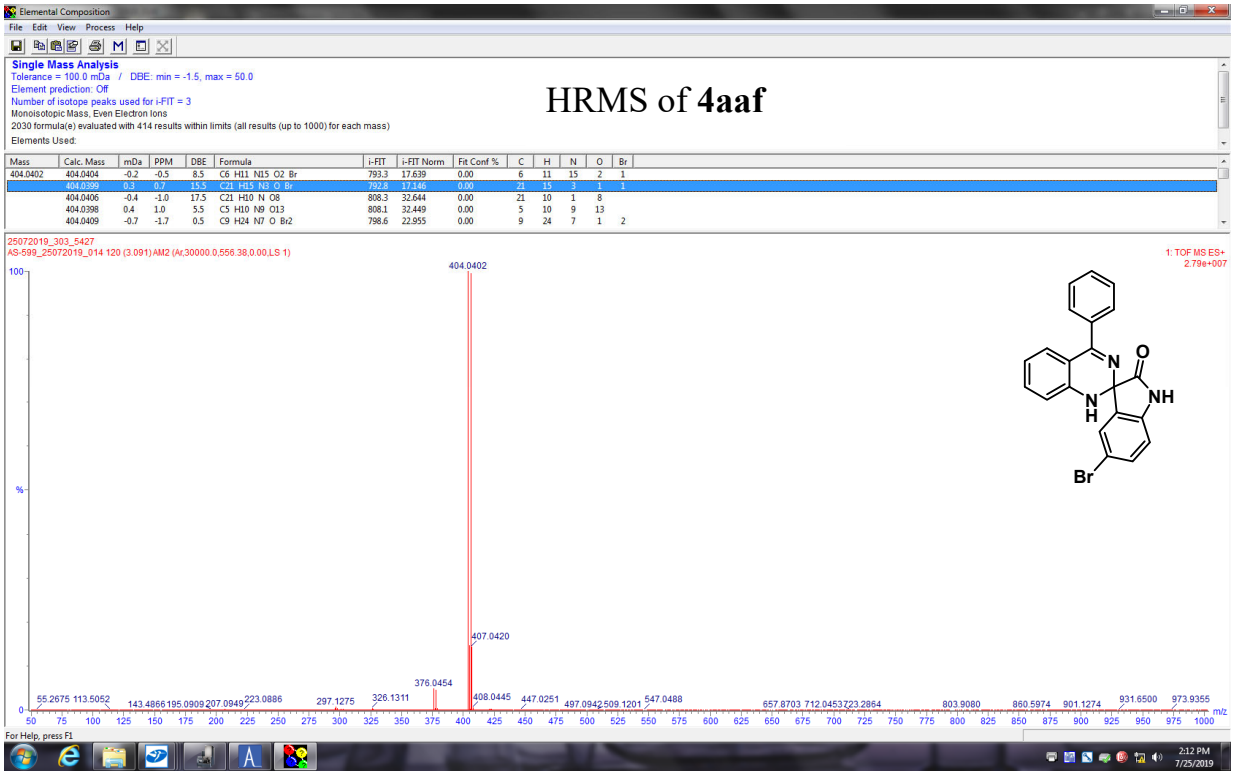
HRMS of **4aac**



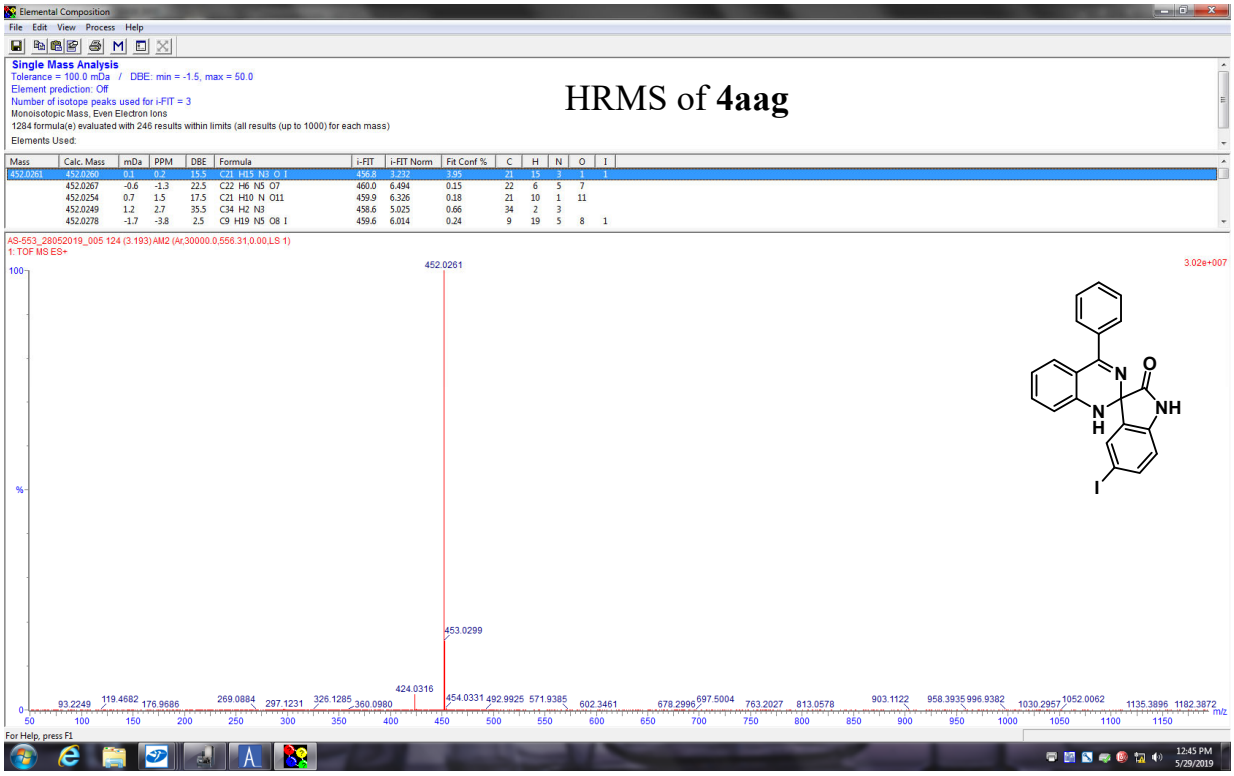
HRMS of **4aad**



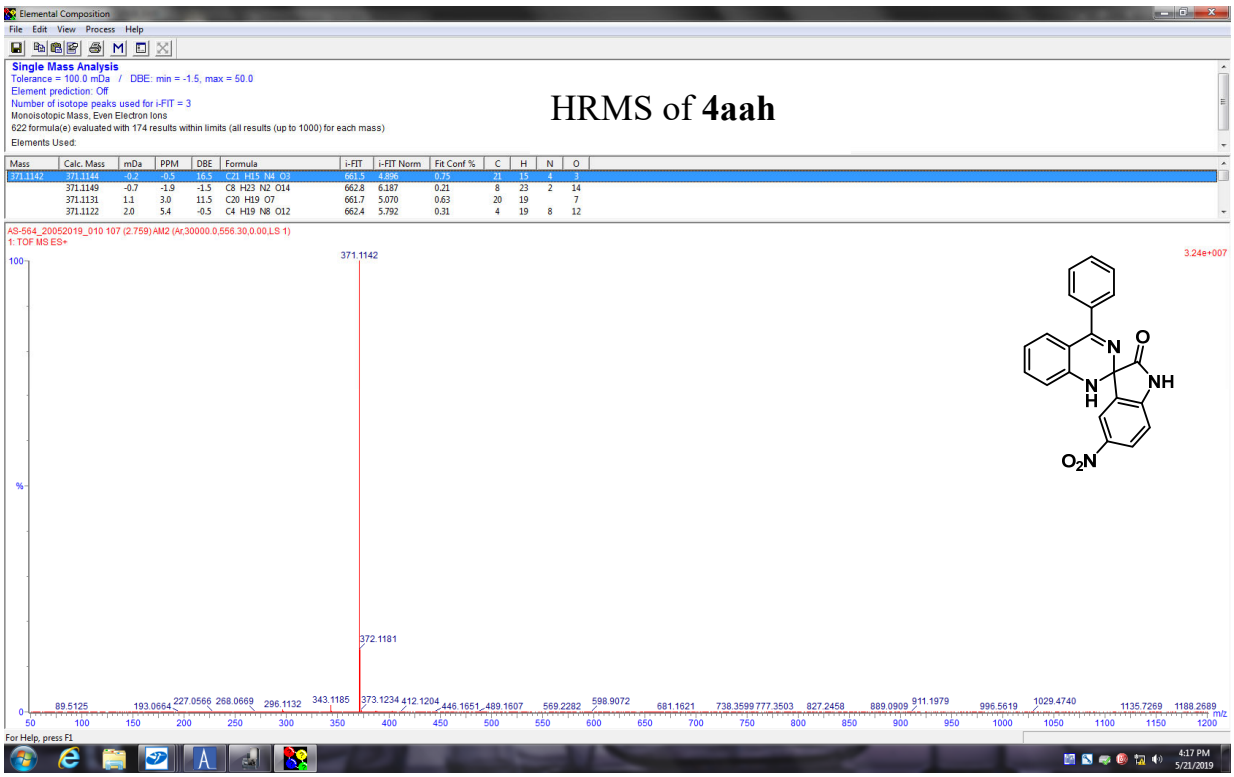
HRMS of **4aae**



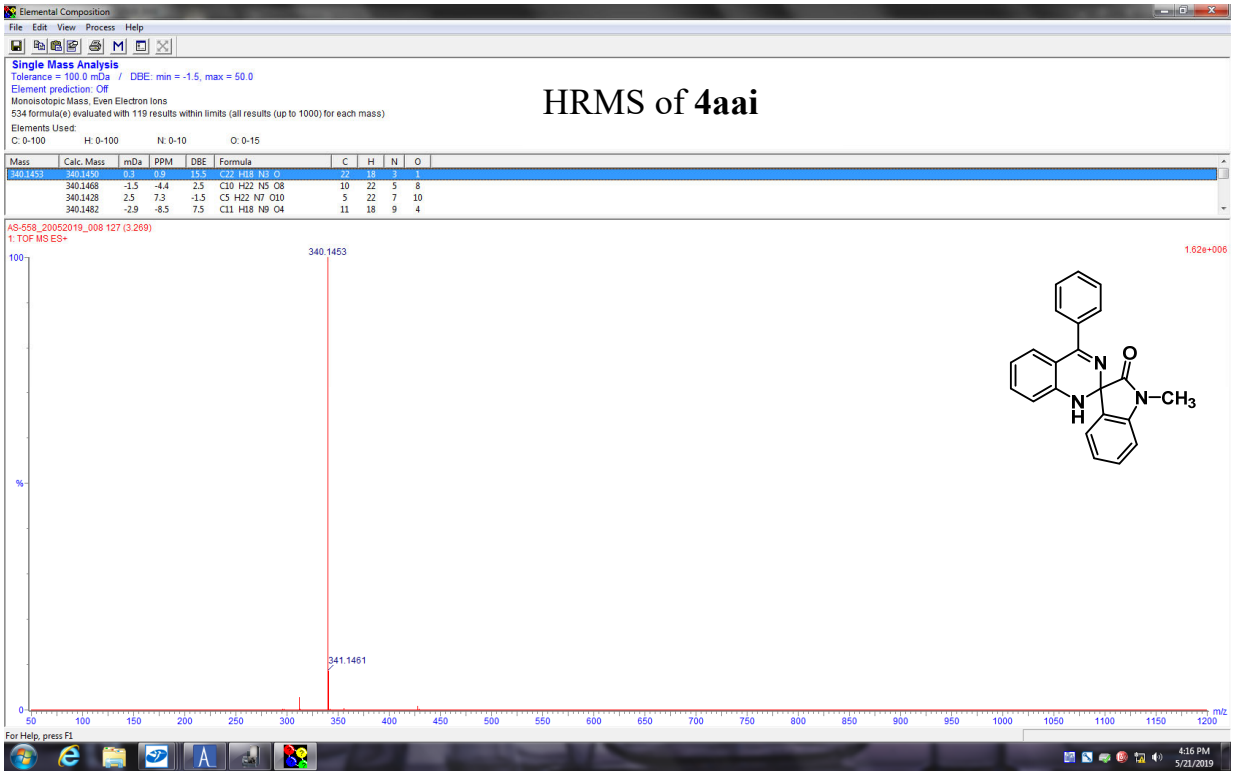
HRMS of **4aaf**



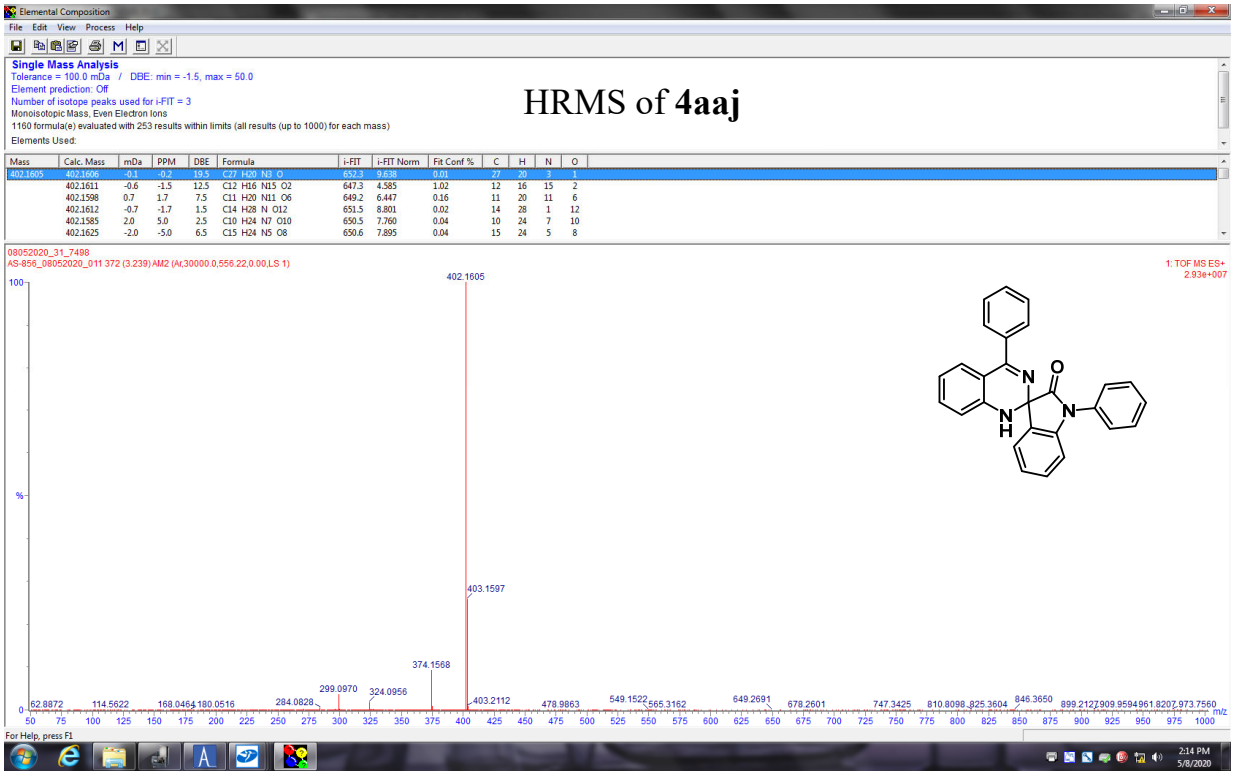
HRMS of **4aag**



HRMS of **4aah**



HRMS of **4aai**



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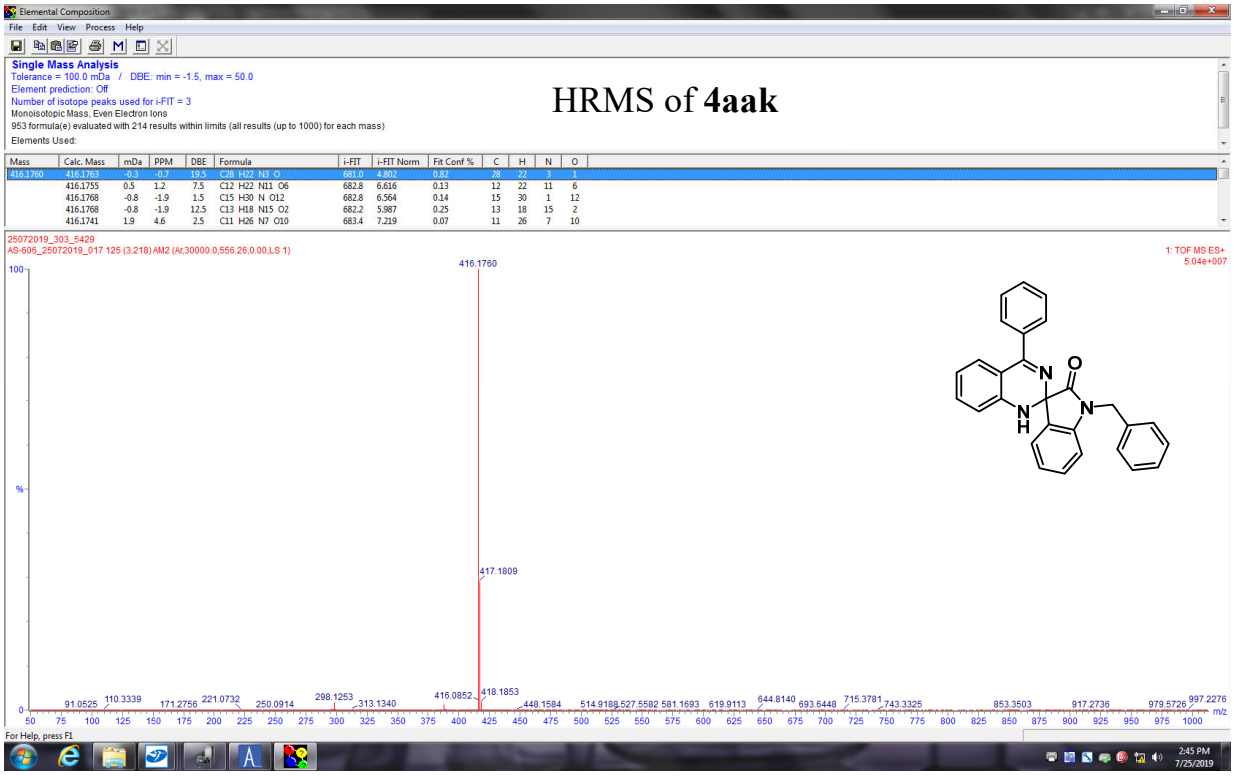
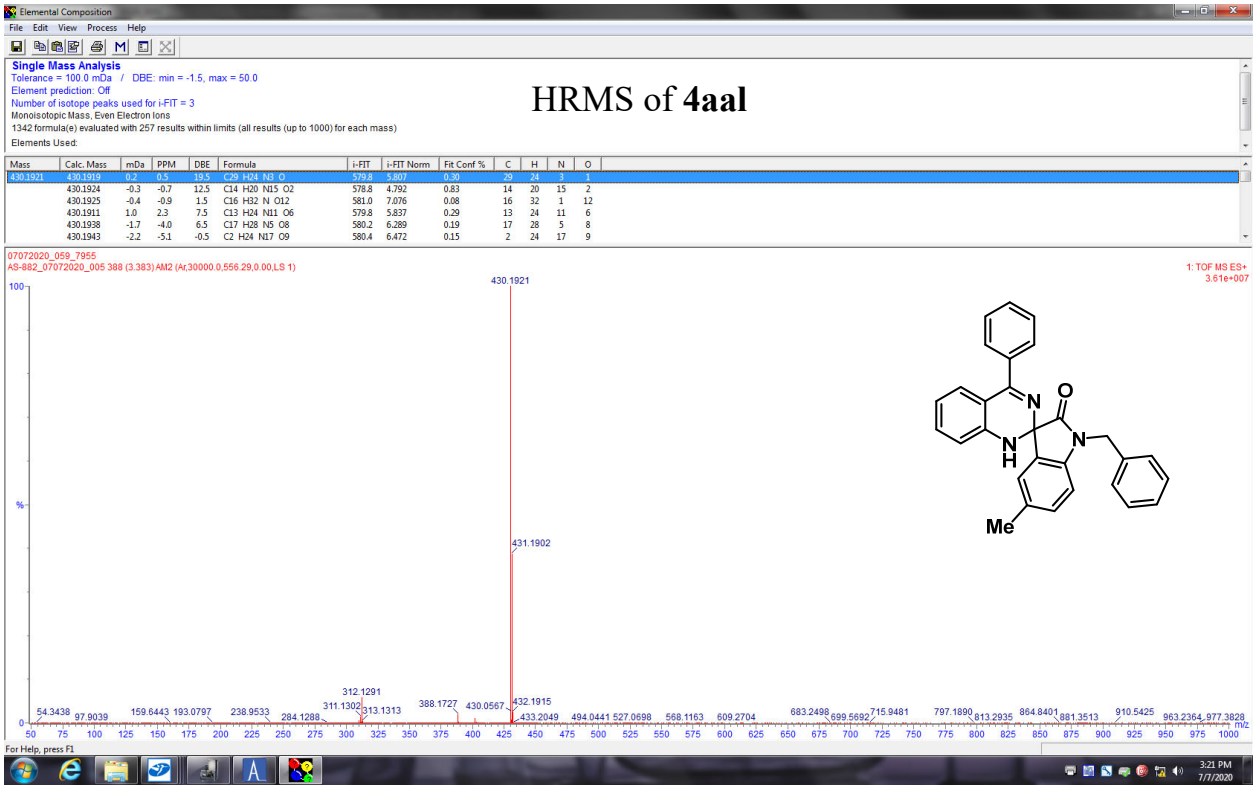


HRMS of **4aak**



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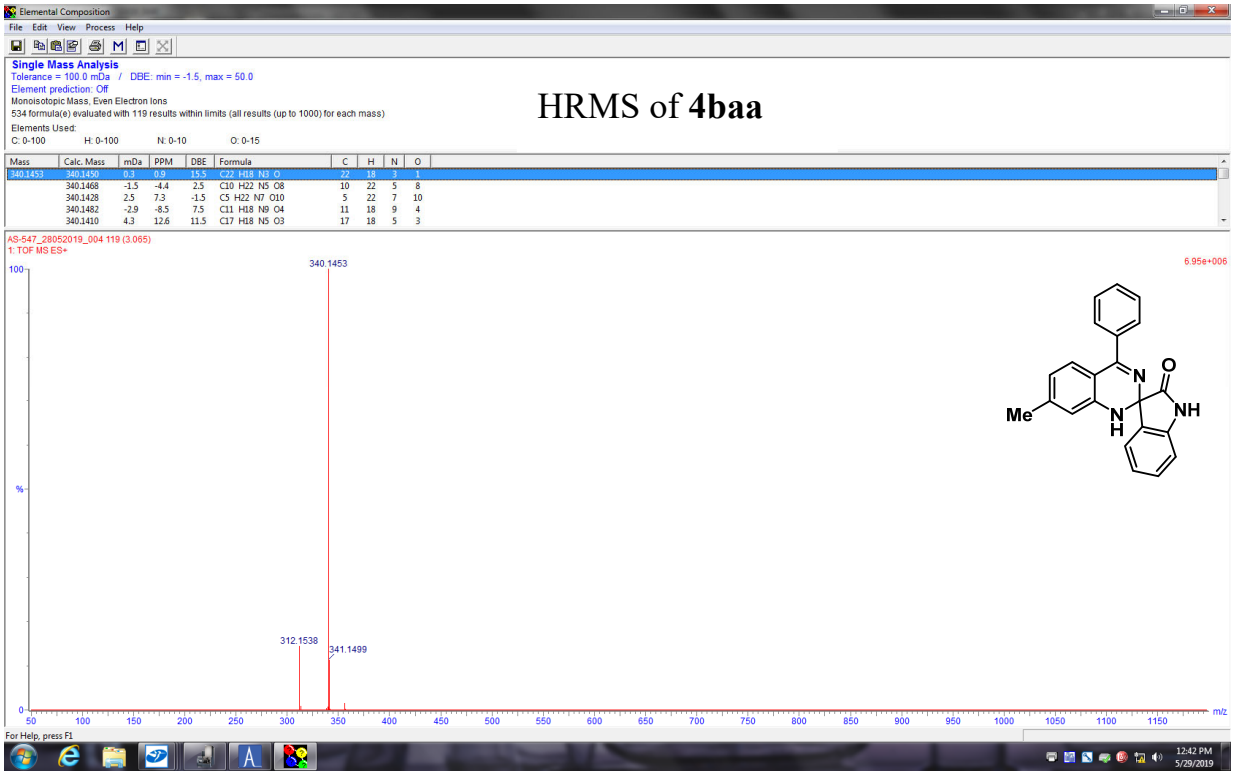
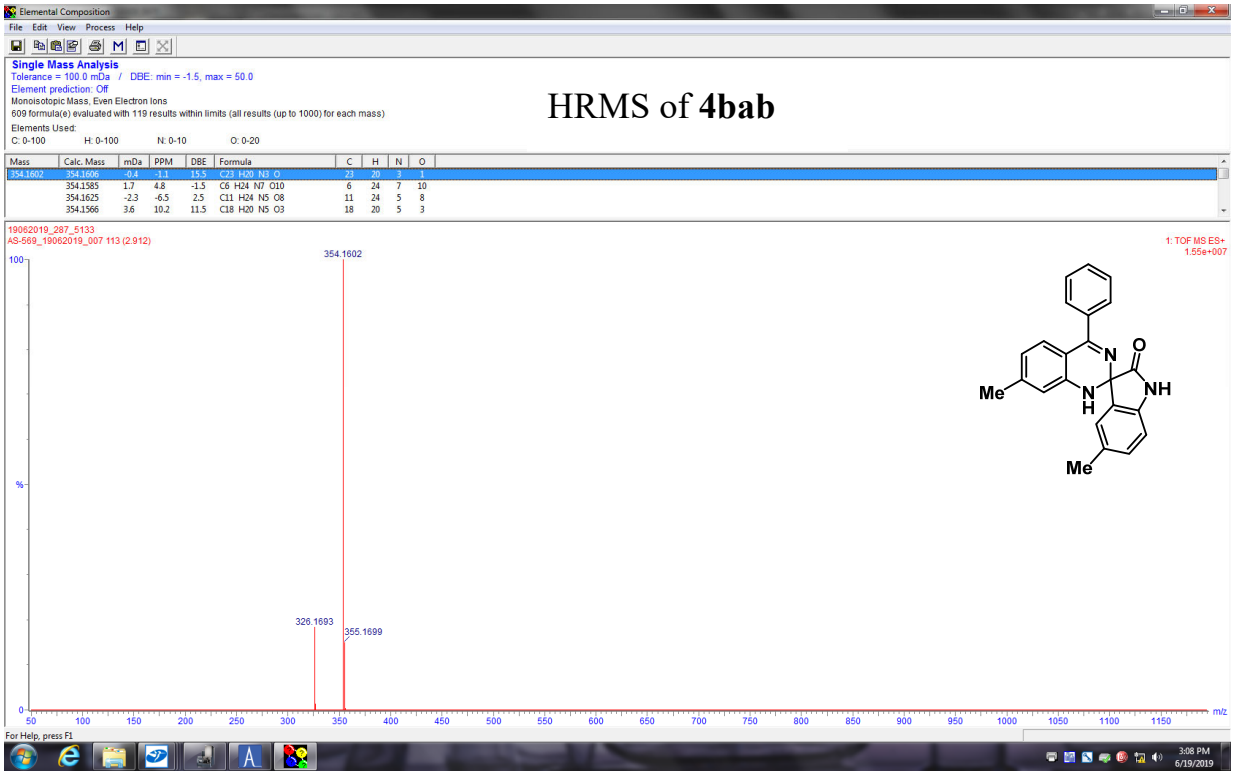
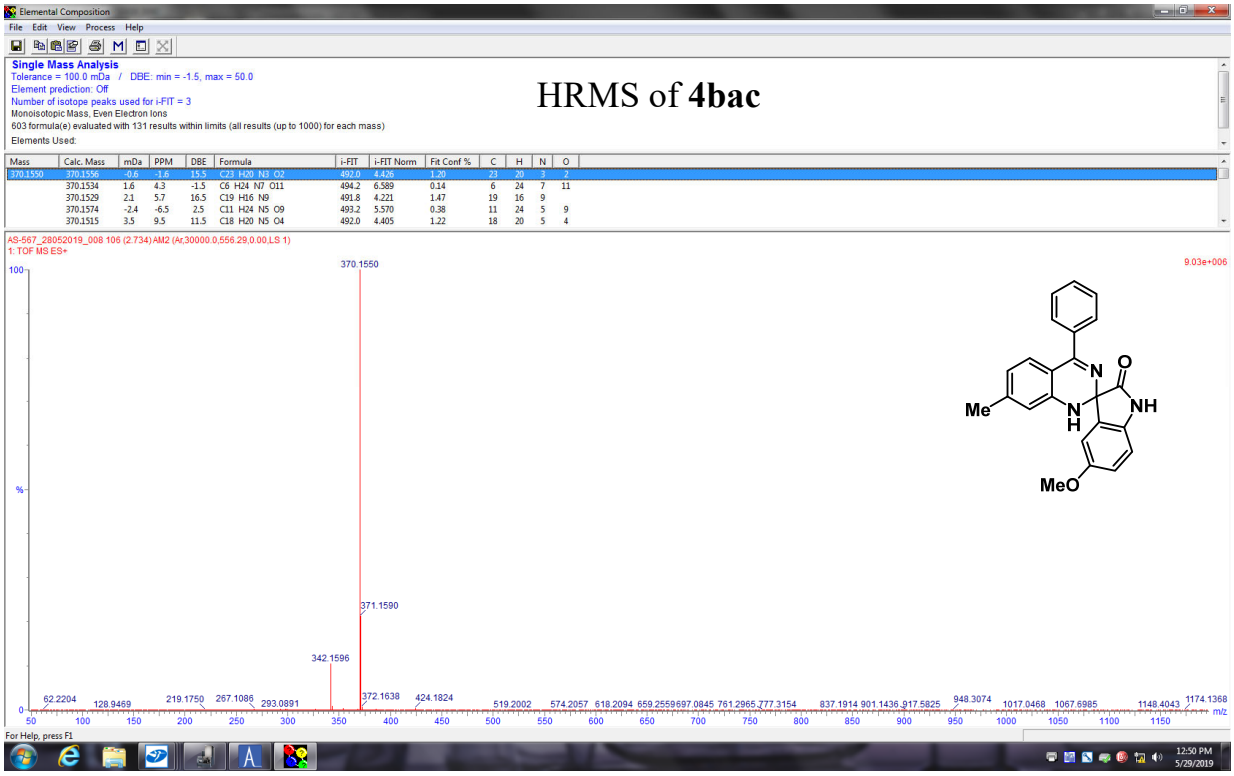


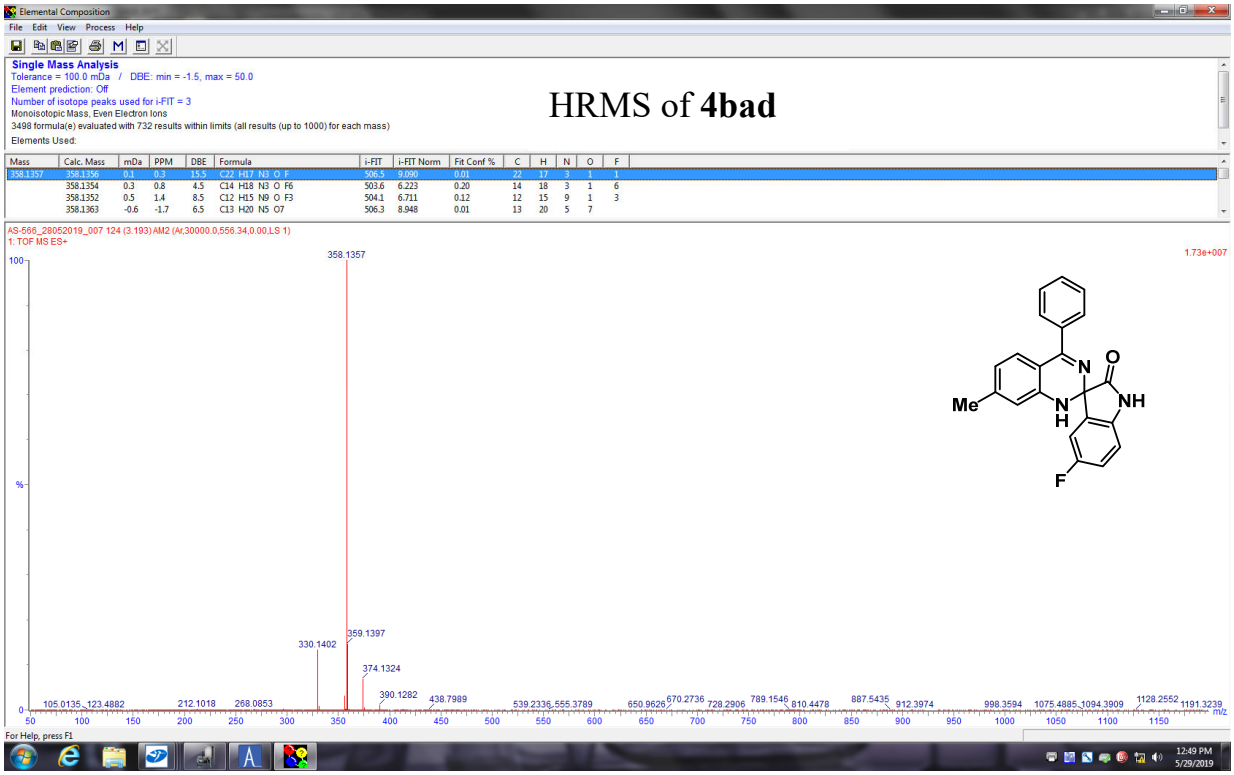
HRMS of **4baa**



HRMS of **4bab**



HRMS of **4bac**



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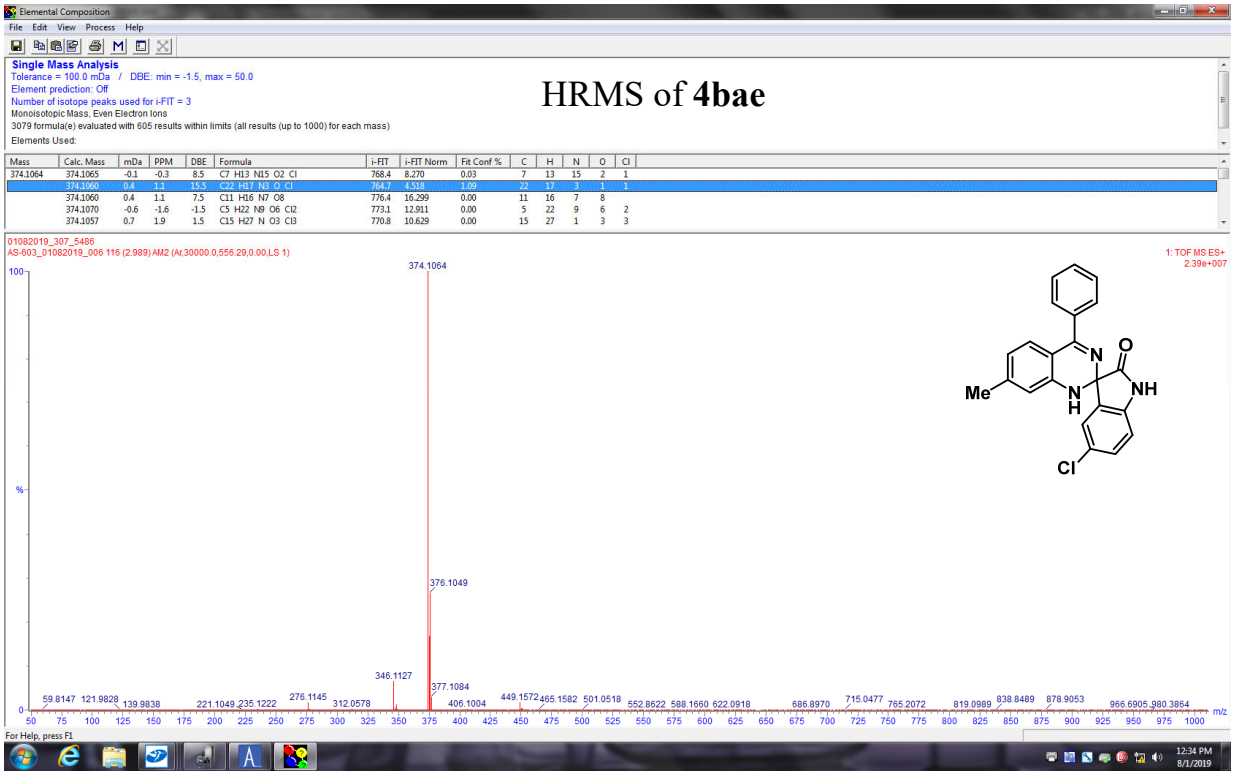
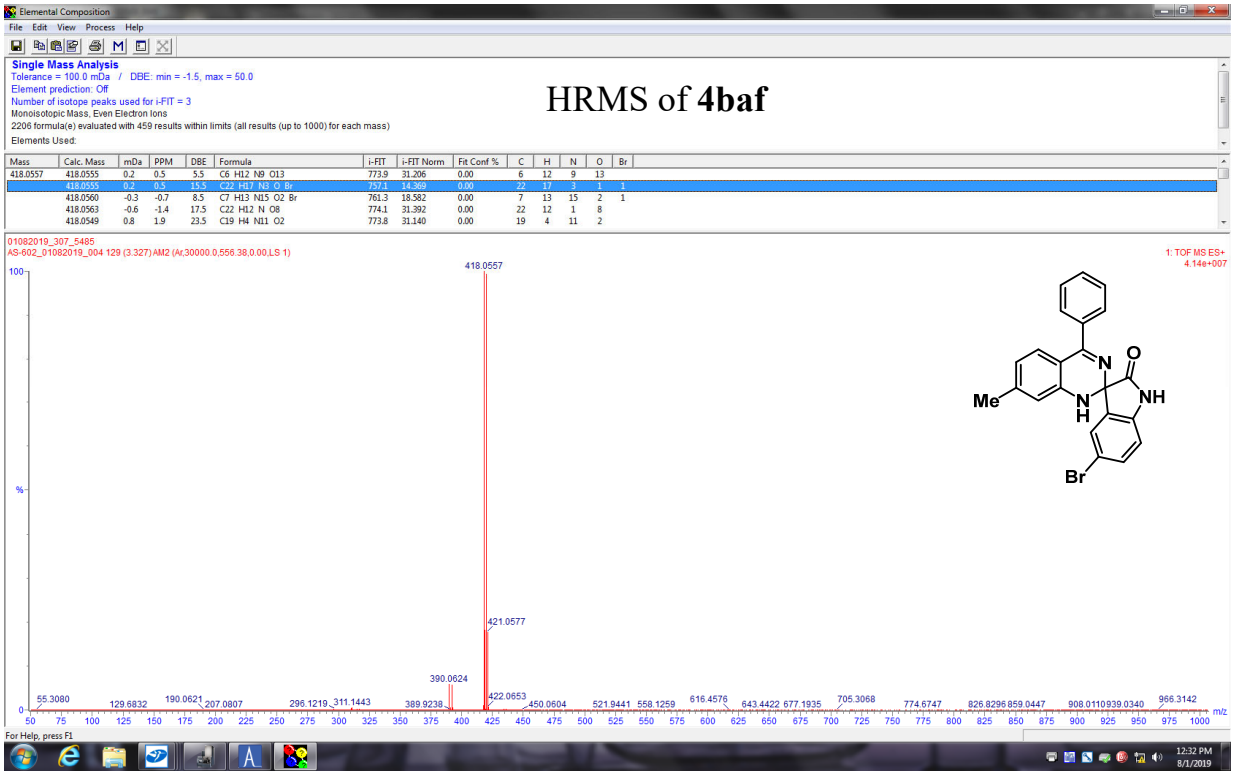


HRMS of **4bae**



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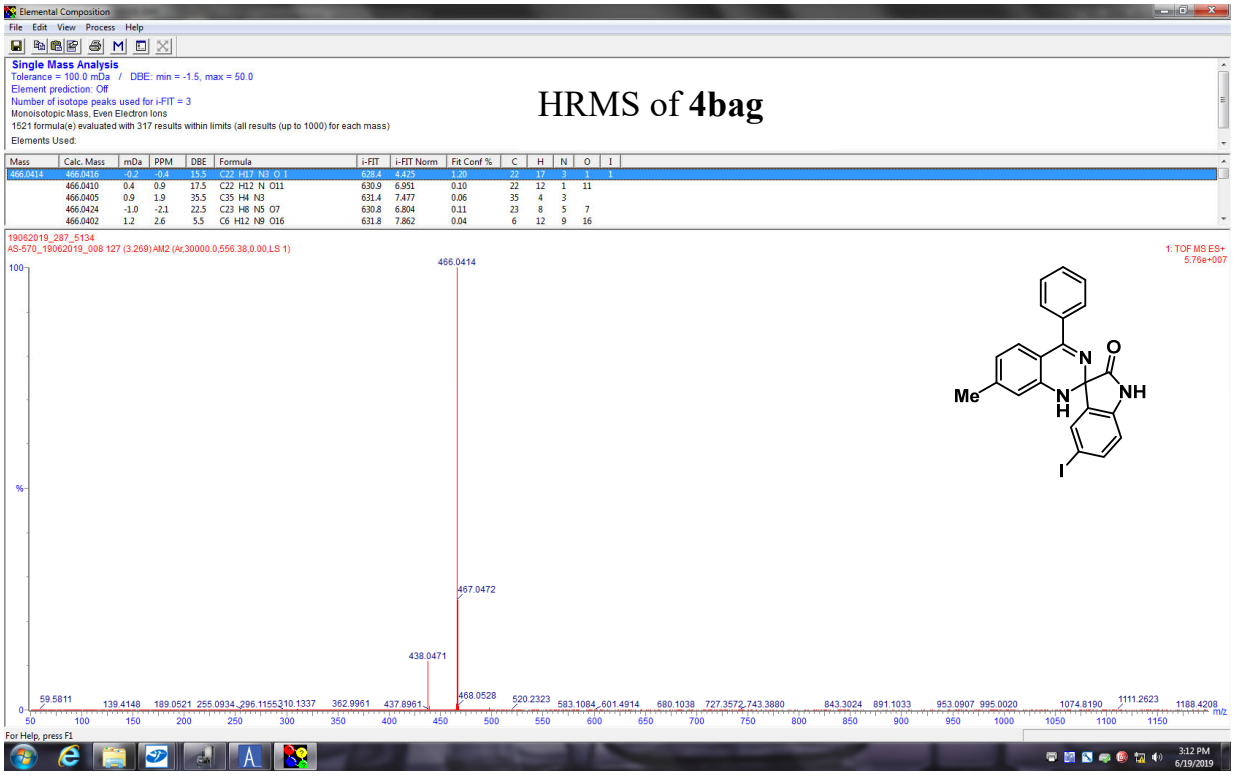

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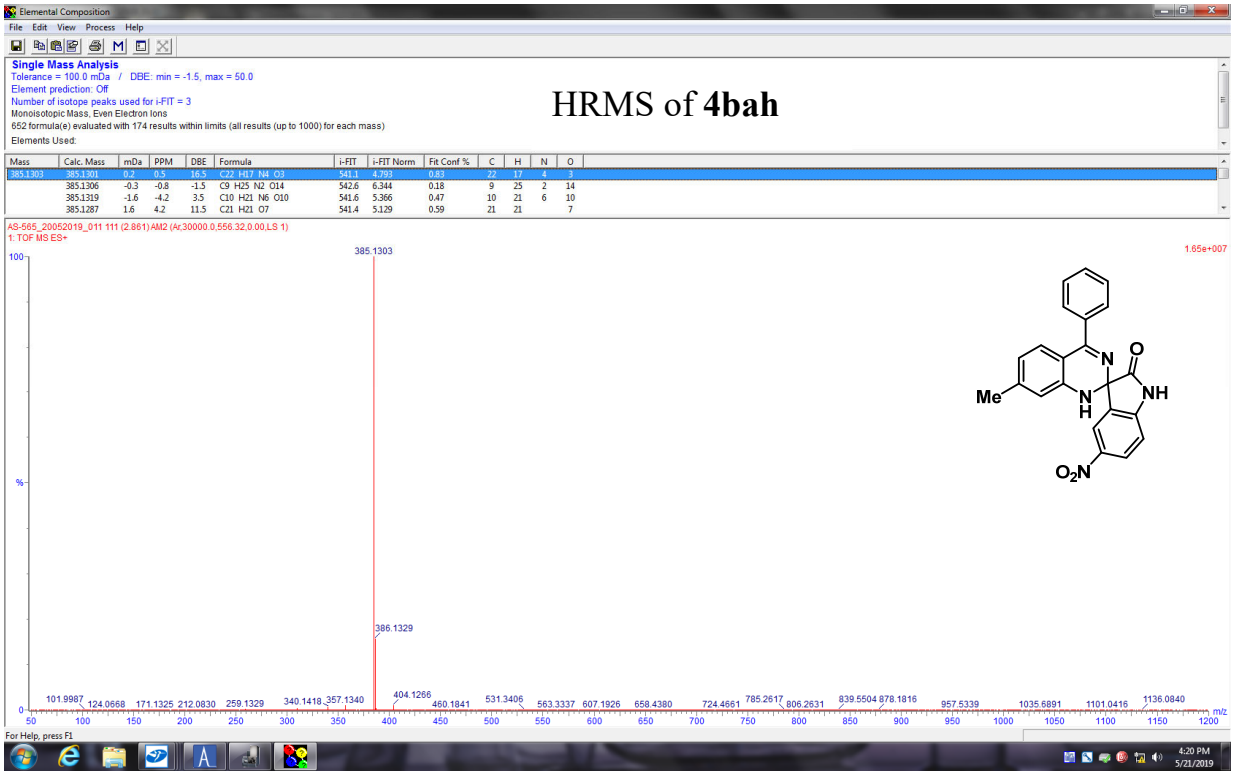

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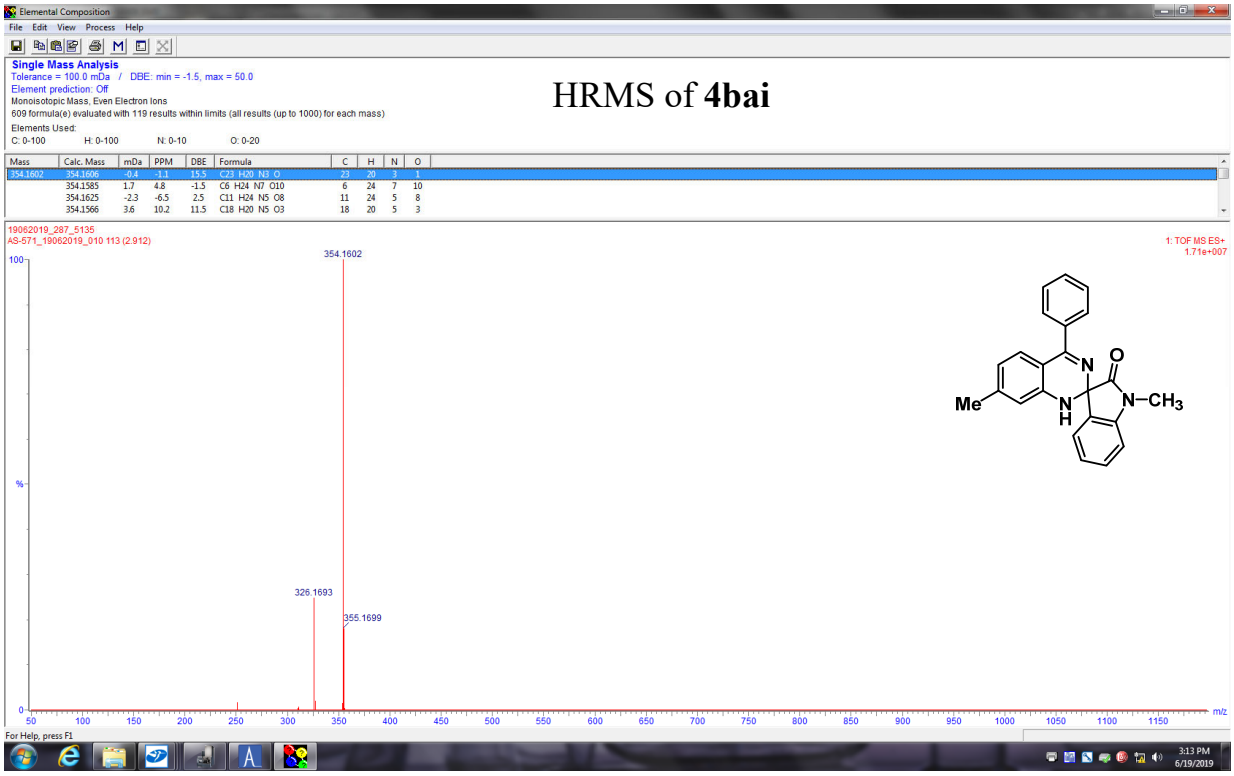

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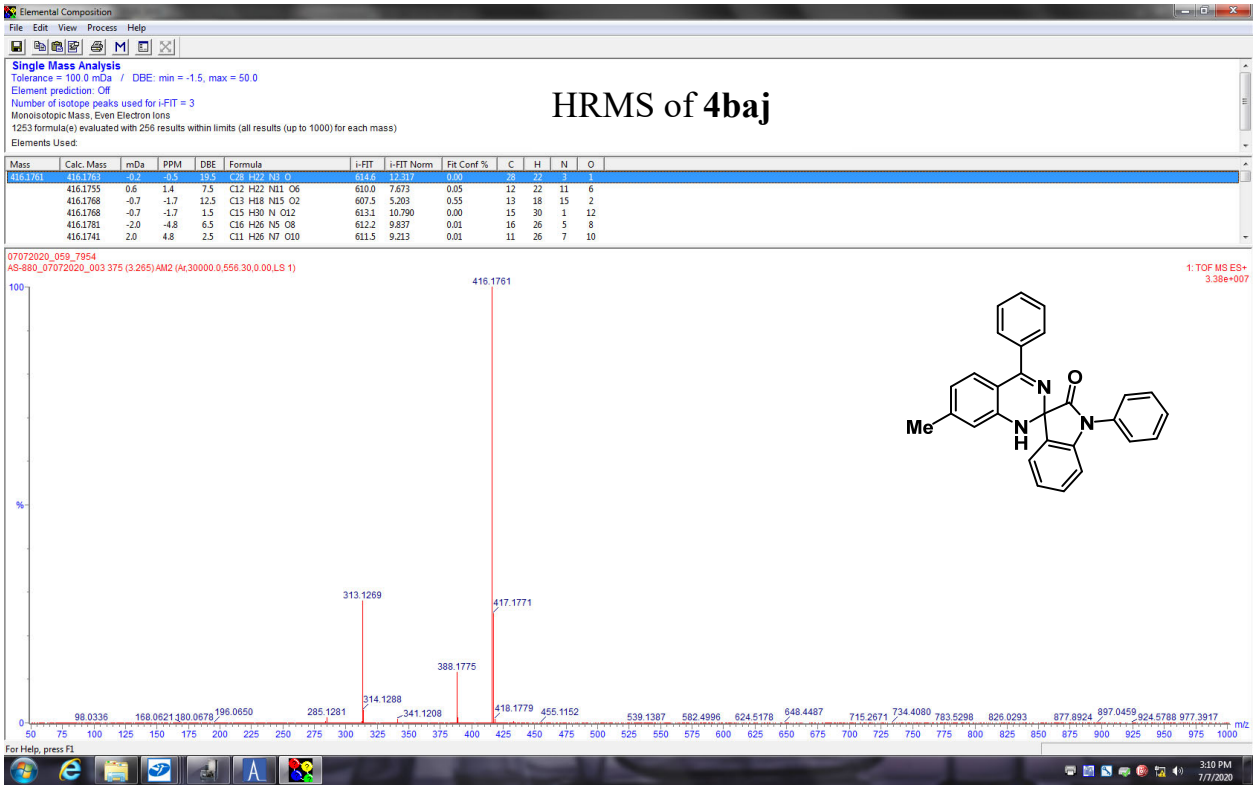
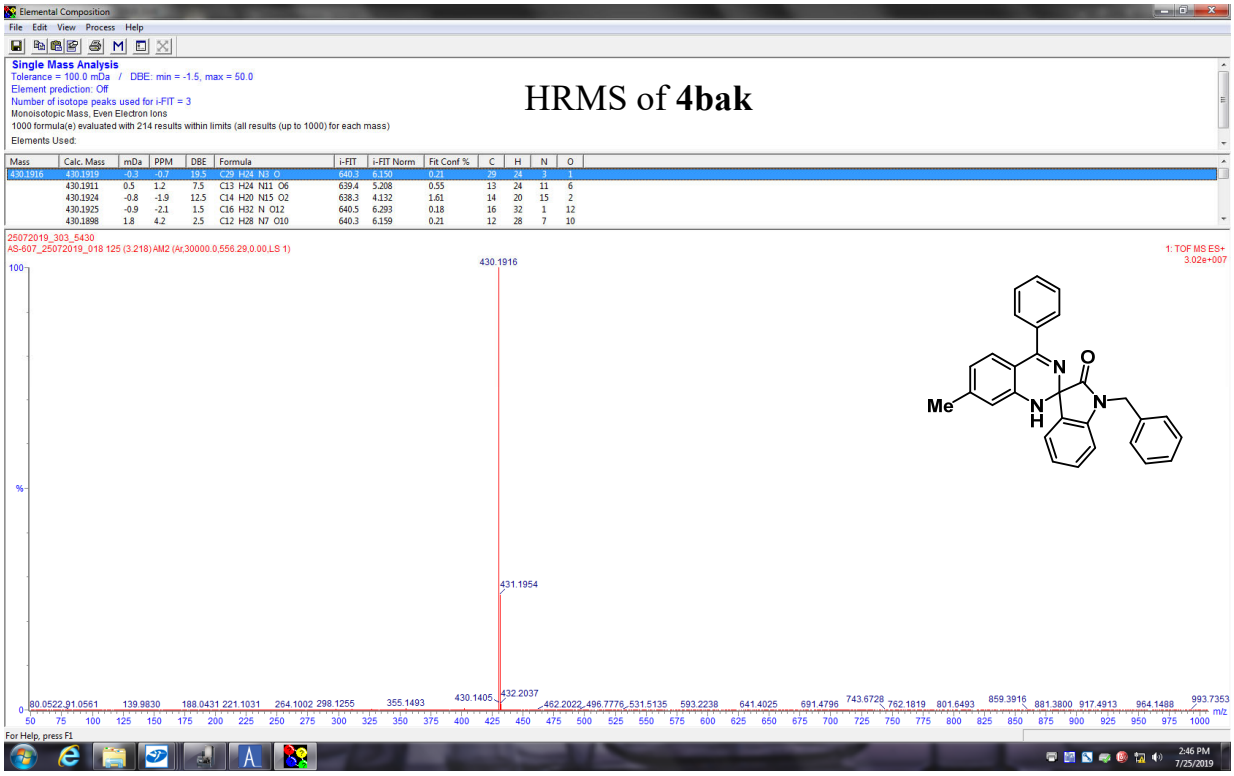


HRMS of **4baj**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Monoisotopic Mass, Even Electron Ions
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HRMS of 4bak
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430.1911 0.5 1.2 7.5 C13 H24 N11 O6 639.4 5.208 0.55 13 24 11 6
430.1924 -0.8 -1.9 12.5 C14 H20 N15 O2 638.3 4.132 1.61 14 20 15 2
430.1925 -0.9 -2.1 1.5 C16 H32 N O12 640.5 6.293 0.18 16 32 1 12
430.1898 1.8 4.2 2.5 C12 H28 N7 O10 640.3 6.159 0.21 12 28 7 10
25072019_303_5430
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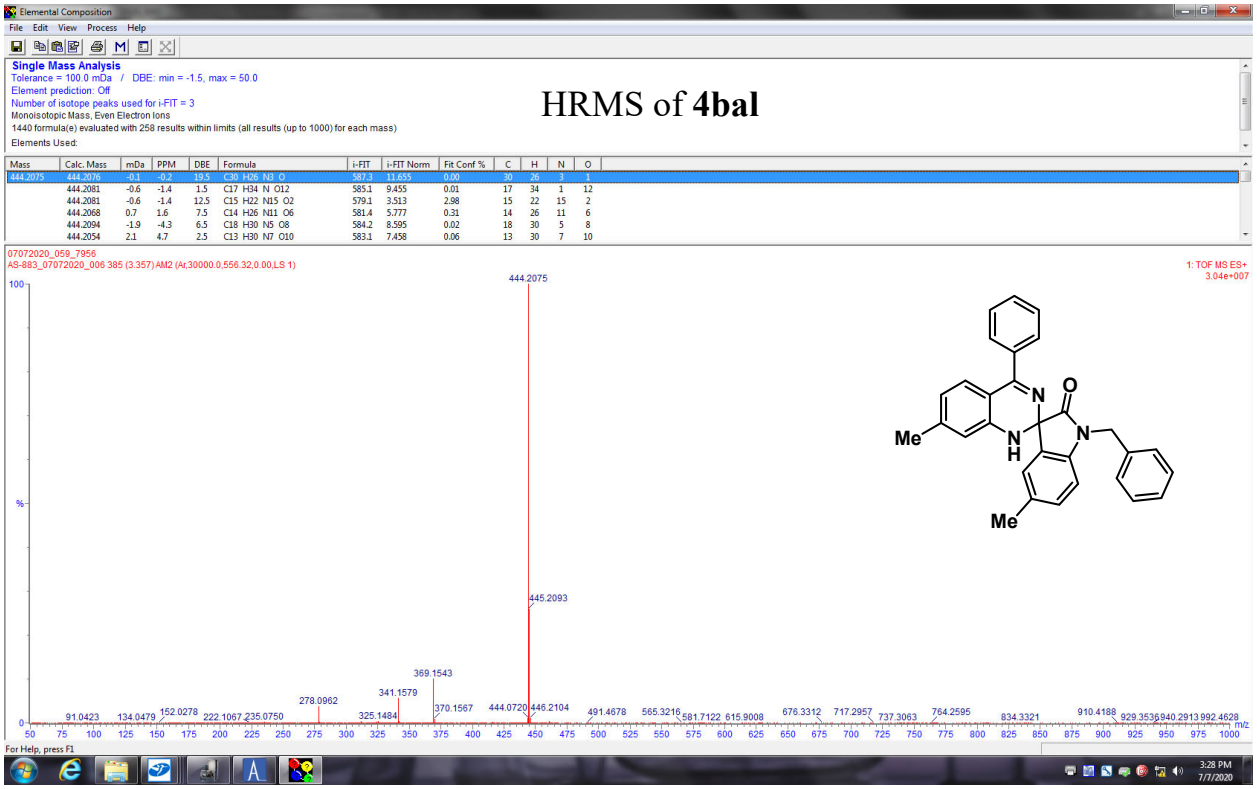
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File Edit View Process Help
Single Mass Analysis
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Element prediction: Off
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Monoisotopic Mass, Even Electron Ions
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07072020_059_7956
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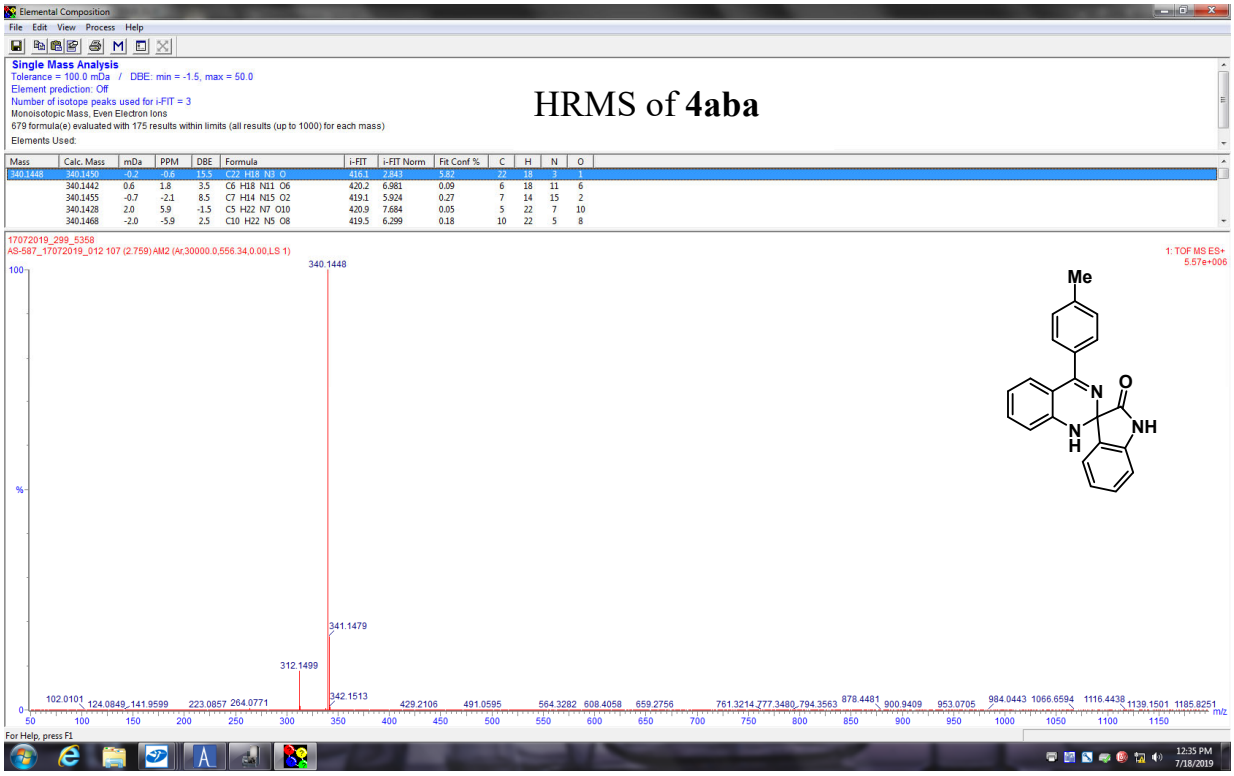
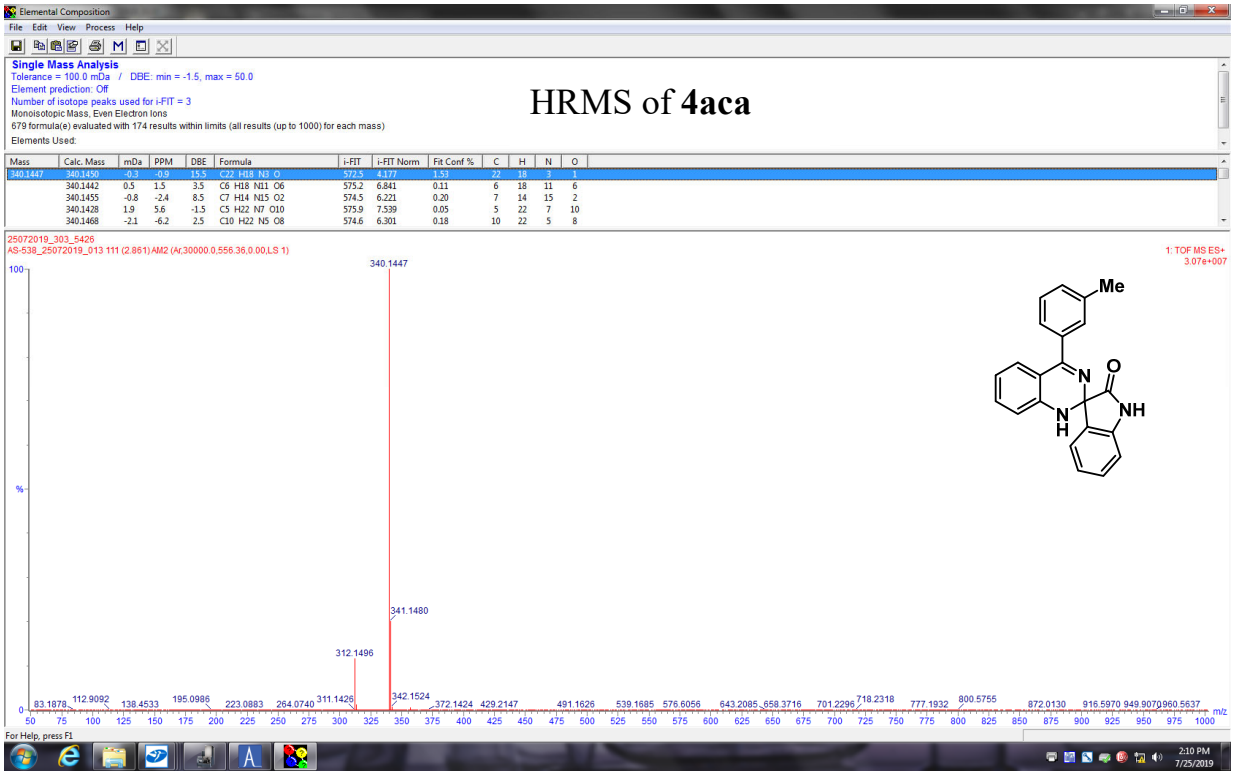


HRMS of **4aba**



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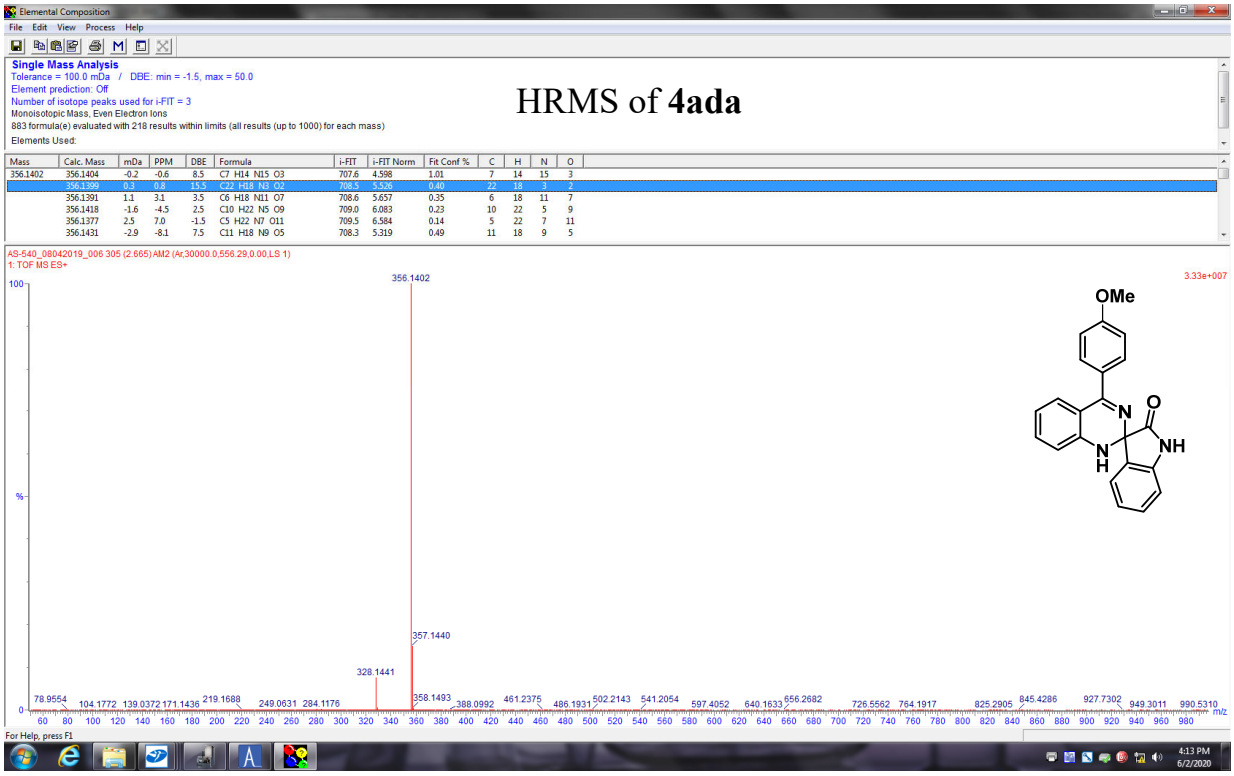

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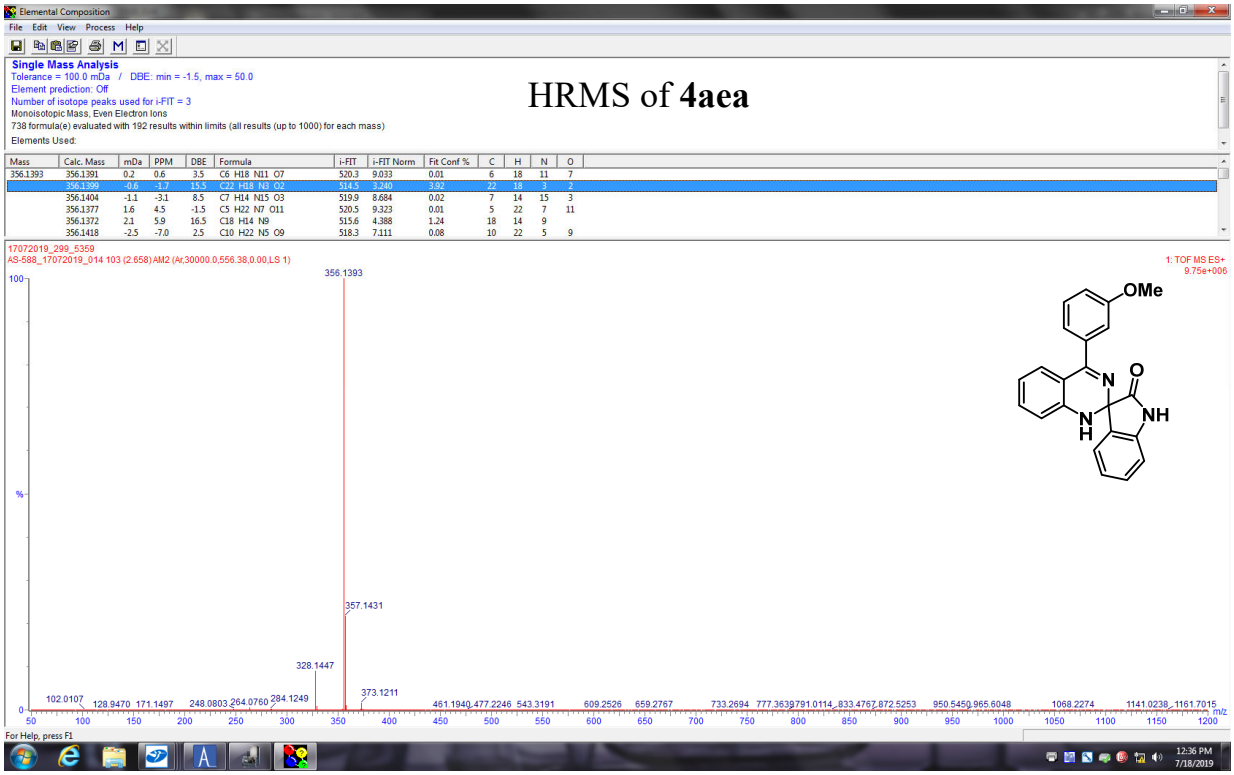

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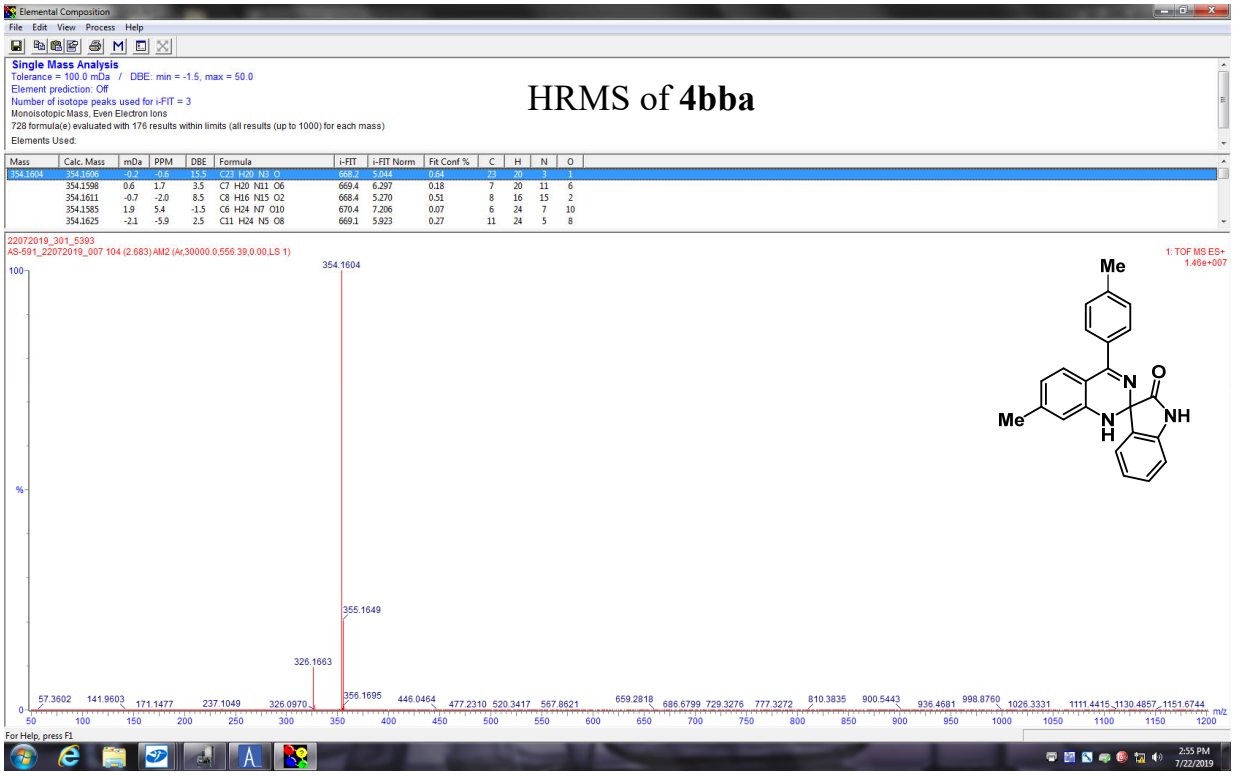
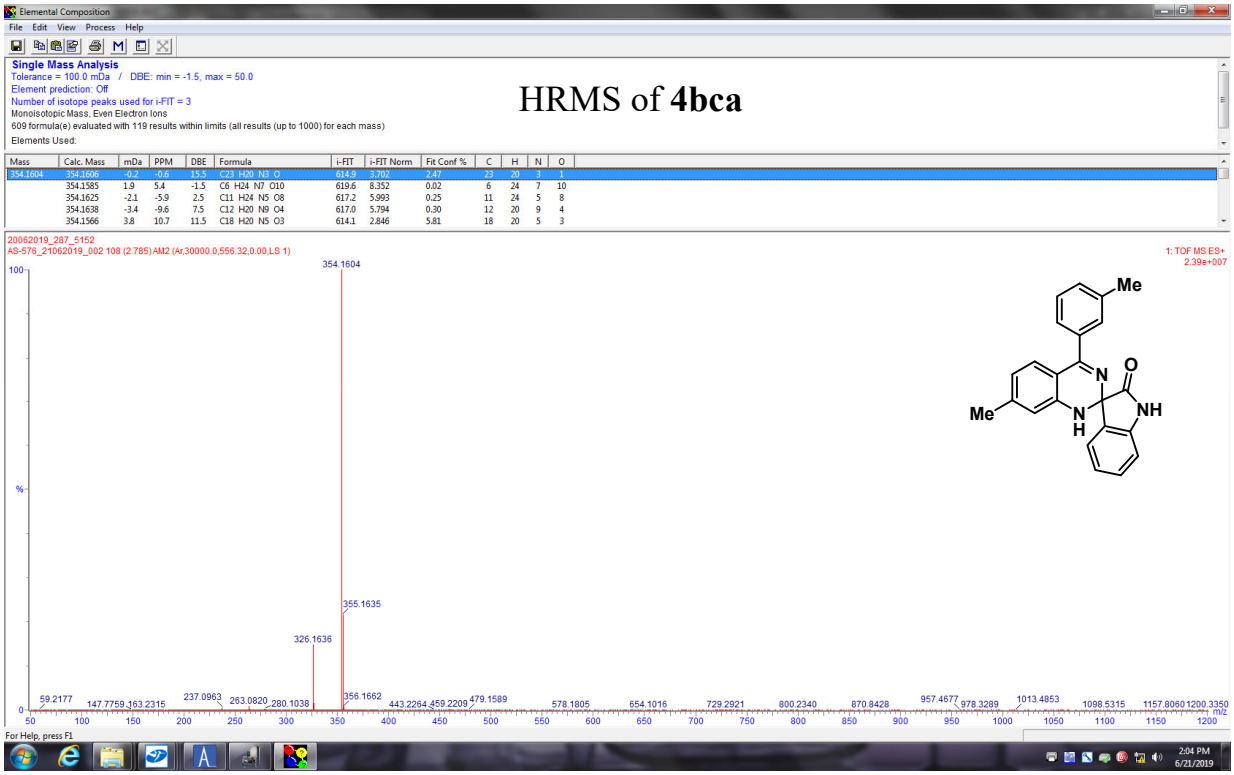
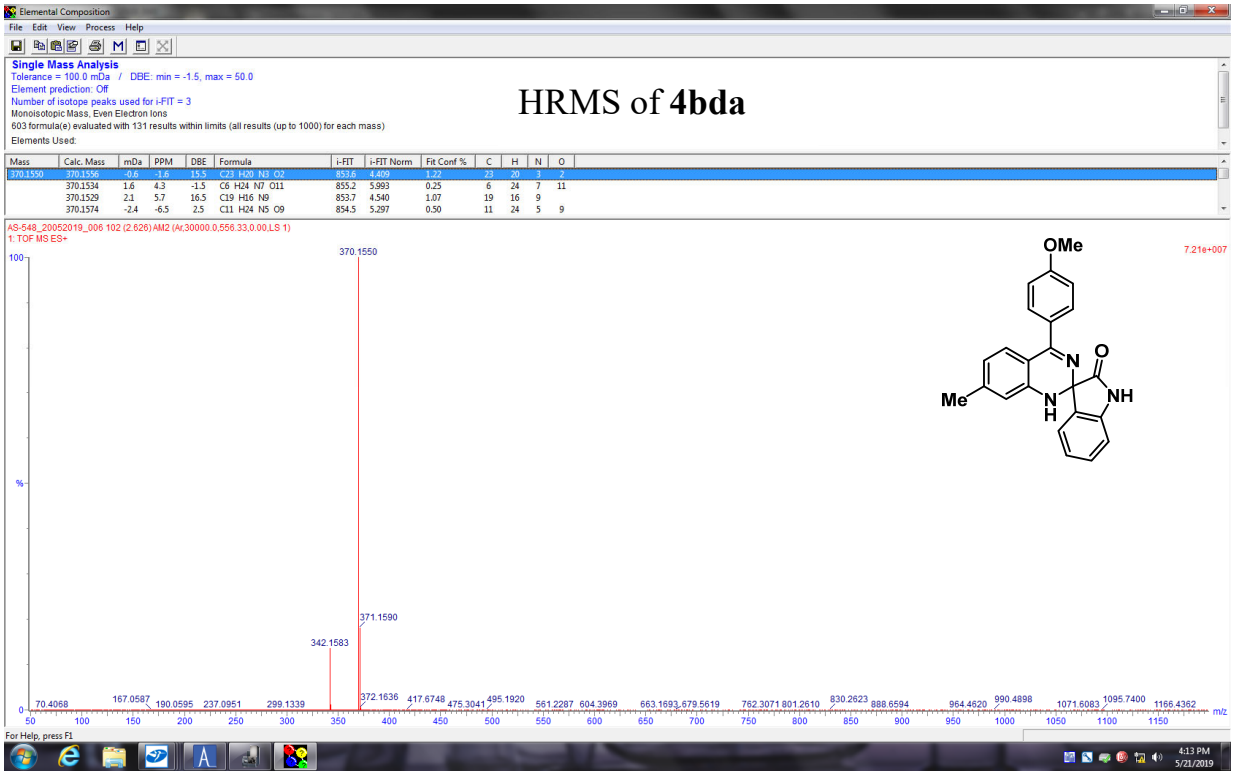
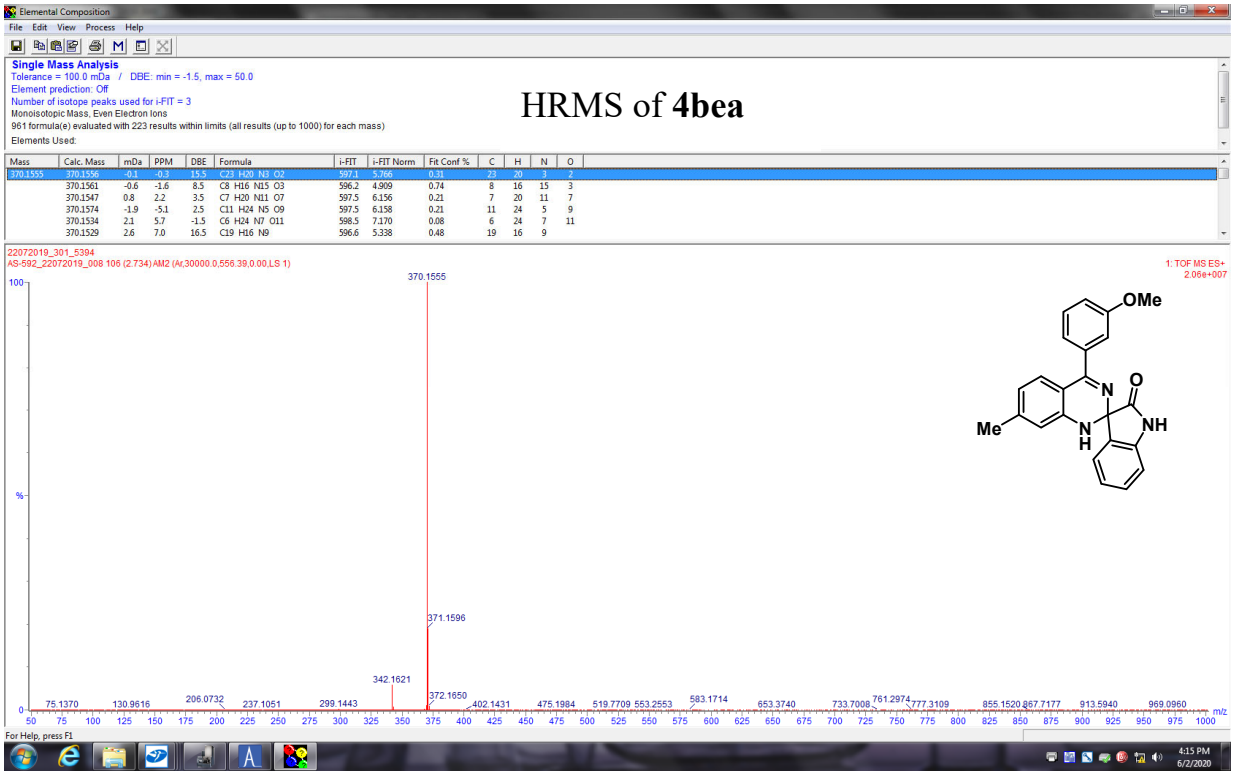


HRMS of **4bba**

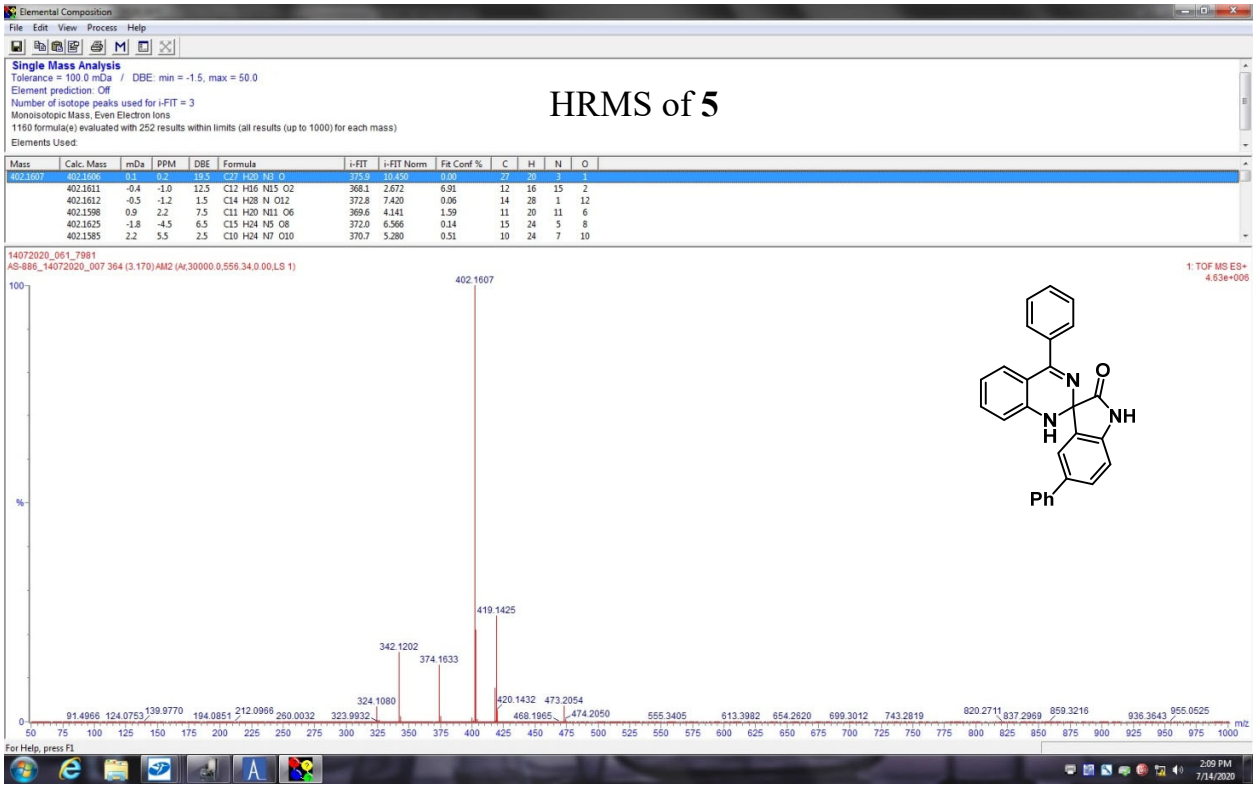


HRMS of **4bca**


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
603 formula(e) evaluated with 131 results within limits (all results (up to 1000) for each mass)
Elements Used:
HRMS of 4bda
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O
370.1550 370.1556 -0.6 -1.6 15.5 C23 H20 N3 O2 853.6 4.409 1.22 23 20 3 2
370.1534 1.6 4.3 -1.5 C6 H24 N7 O11 855.2 5.993 0.25 6 24 7 11
370.1529 2.1 5.7 16.5 C19 H16 N9 853.7 4.540 1.07 19 16 9
370.1574 -2.4 -6.5 2.5 C11 H24 N5 O9 854.5 5.297 0.50 11 24 5 9
AS-548_20052019_006 102 (2.626) AM2 (Ar,30000.0,556.33,0.00,LS 1)
1: TOF MS ES+
7.21e+007
370.1550
371.1590
342.1583
OMe
N
O
Me
N
H
NH
For Help, press F1
4:13 PM
5/21/2019


Elemental Composition
File Edit View Process Help
Single Mass Analysis
Tolerance = 100.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3
Monoisotopic Mass, Even Electron Ions
961 formula(e) evaluated with 223 results within limits (all results (up to 1000) for each mass)
Elements Used:
HRMS of 4bea
Mass Calc. Mass mDa PPM DBE Formula i-FIT i-FIT Norm Fit Conf % C H N O
370.1555 370.1556 -0.1 -0.3 15.5 C23 H20 N3 O2 597.1 5.766 0.31 23 20 3 2
370.1561 -0.6 -1.6 8.5 C8 H16 N15 O3 596.2 4.909 0.74 8 16 15 3
370.1547 0.8 2.2 3.5 C7 H20 N11 O7 597.5 6.156 0.21 7 20 11 7
370.1574 -1.9 -5.1 2.5 C11 H24 N5 O9 597.5 6.158 0.21 11 24 5 9
370.1534 2.1 5.7 -1.5 C6 H24 N7 O11 598.5 7.170 0.08 6 24 7 11
370.1529 2.6 7.0 16.5 C19 H16 N9 596.6 5.338 0.48 19 16 9
22072019_301_5394
AS-592_22072019_008 106 (2.734) AM2 (Ar,30000.0,556.39,0.00,LS 1)
1: TOF MS ES+
2.06e+007
370.1555
371.1596
342.1621
OMe
N
O
Me
N
H
NH
For Help, press F1
4:15 PM
6/2/2020

HRMS of **5**



HRMS of **6**