

Electronic Supplementary Material (ESI) for New Journal of Chemistry

Supporting Information

D-A systems based on oxazolone-coumarin triazoles as solid-state emitters and inhibitors of human cervical cancer cells (HeLa)

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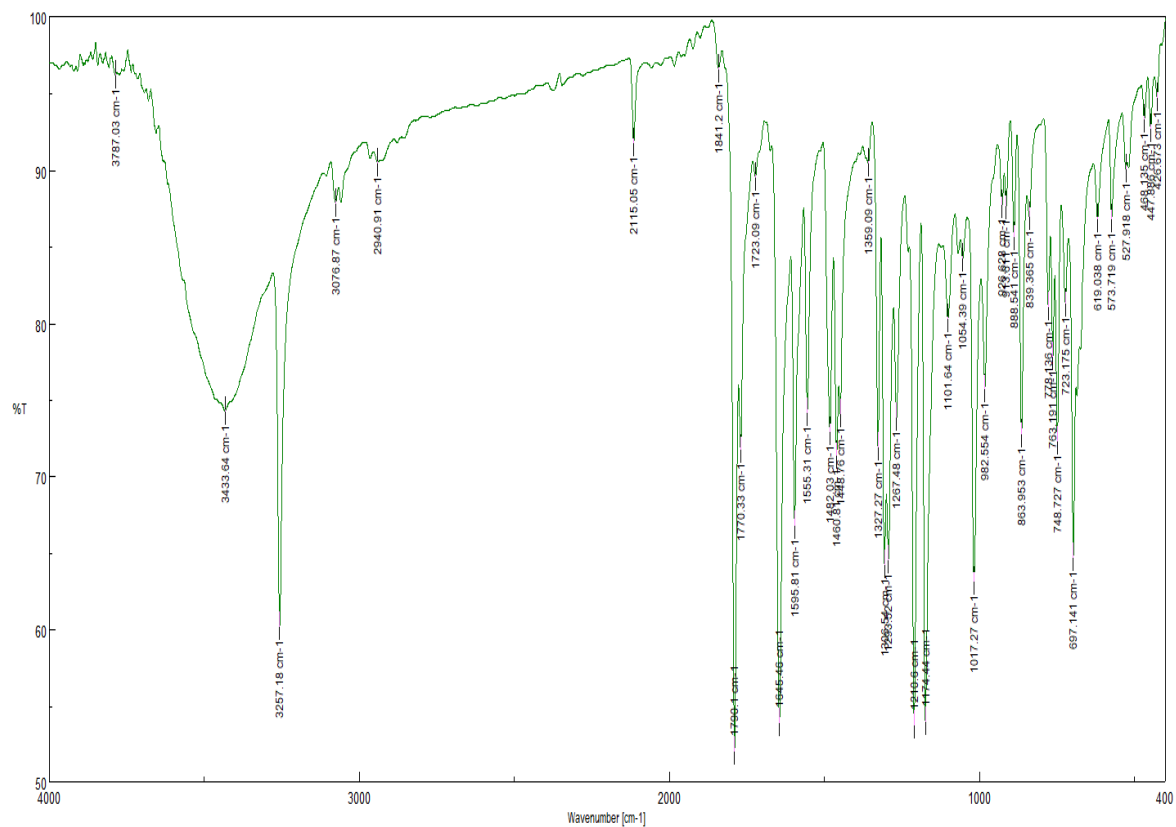
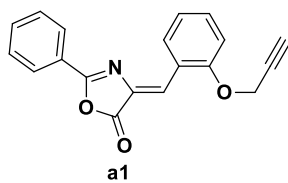
Pages 2-13: FT-IR, ¹H NMR, ¹³C NMR, and mass spectrum of compound **a1-a3**

Pages 14-25: FT-IR, ¹H NMR, ¹³C NMR, and mass spectrum of compound **b1-b3**

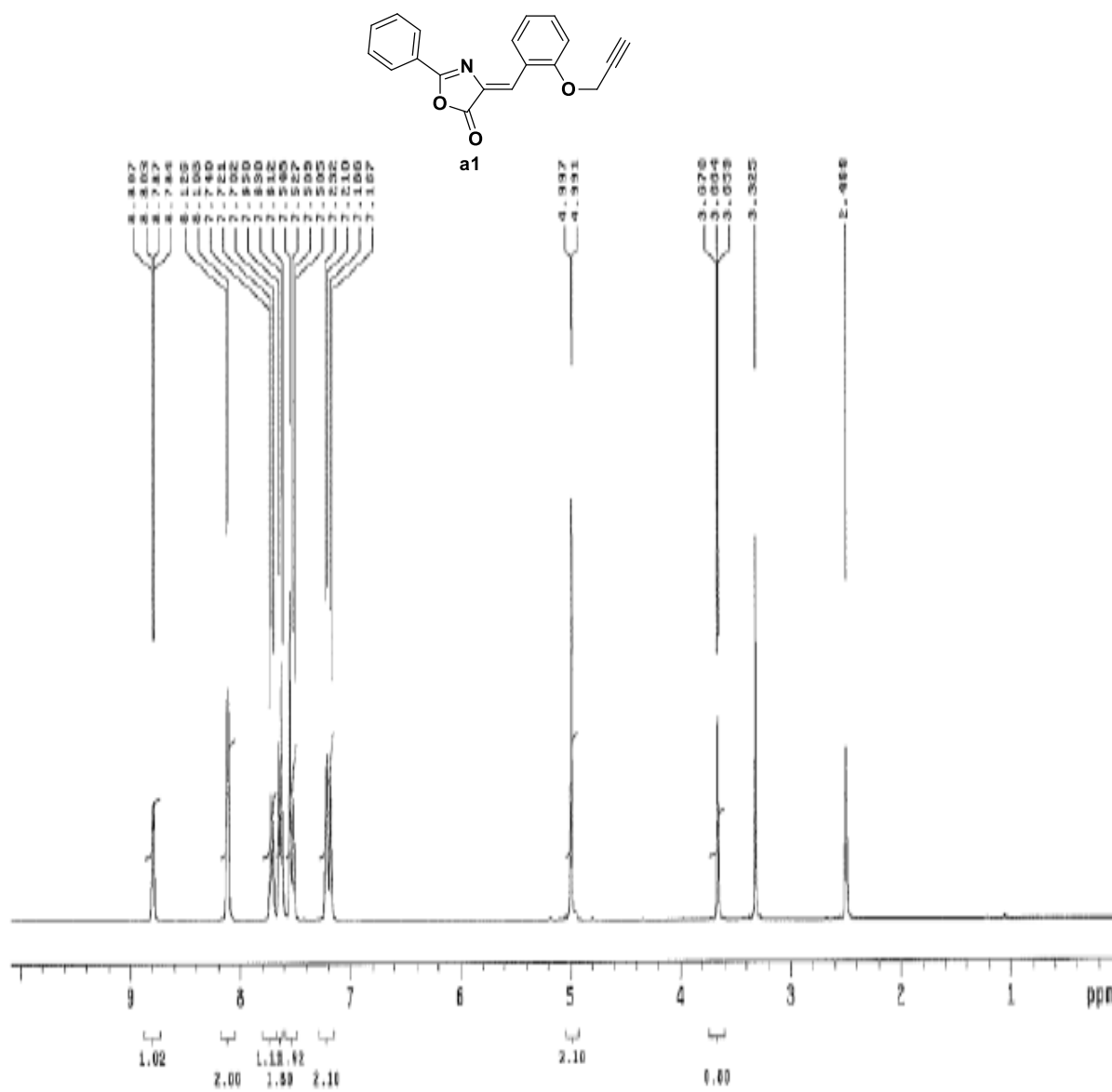
Pages 26-37: FT-IR, ¹H NMR, ¹³C NMR, and mass spectrum of compound **c1-c3**

Pages 38-55: FT-IR, ¹H NMR, and mass spectrum of compound **OC1-OC3**

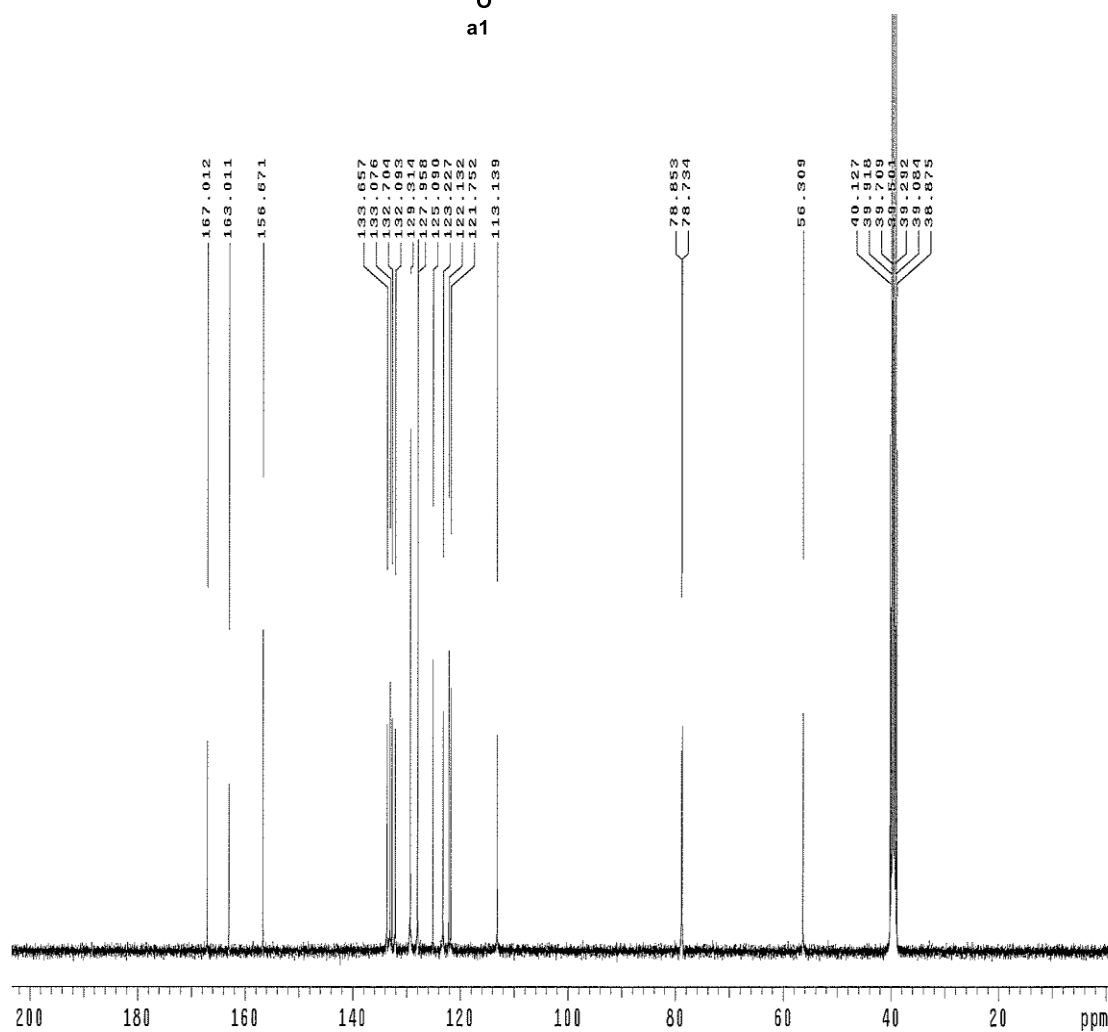
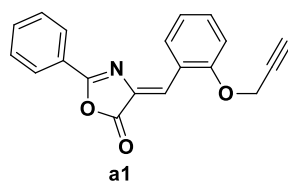
Pages 56: Mechanism of the formation of coumarin bromides (**b1-b3**)



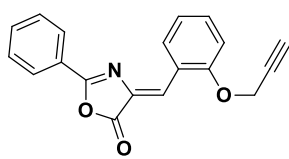
FT-IR Spectrum of **a1**



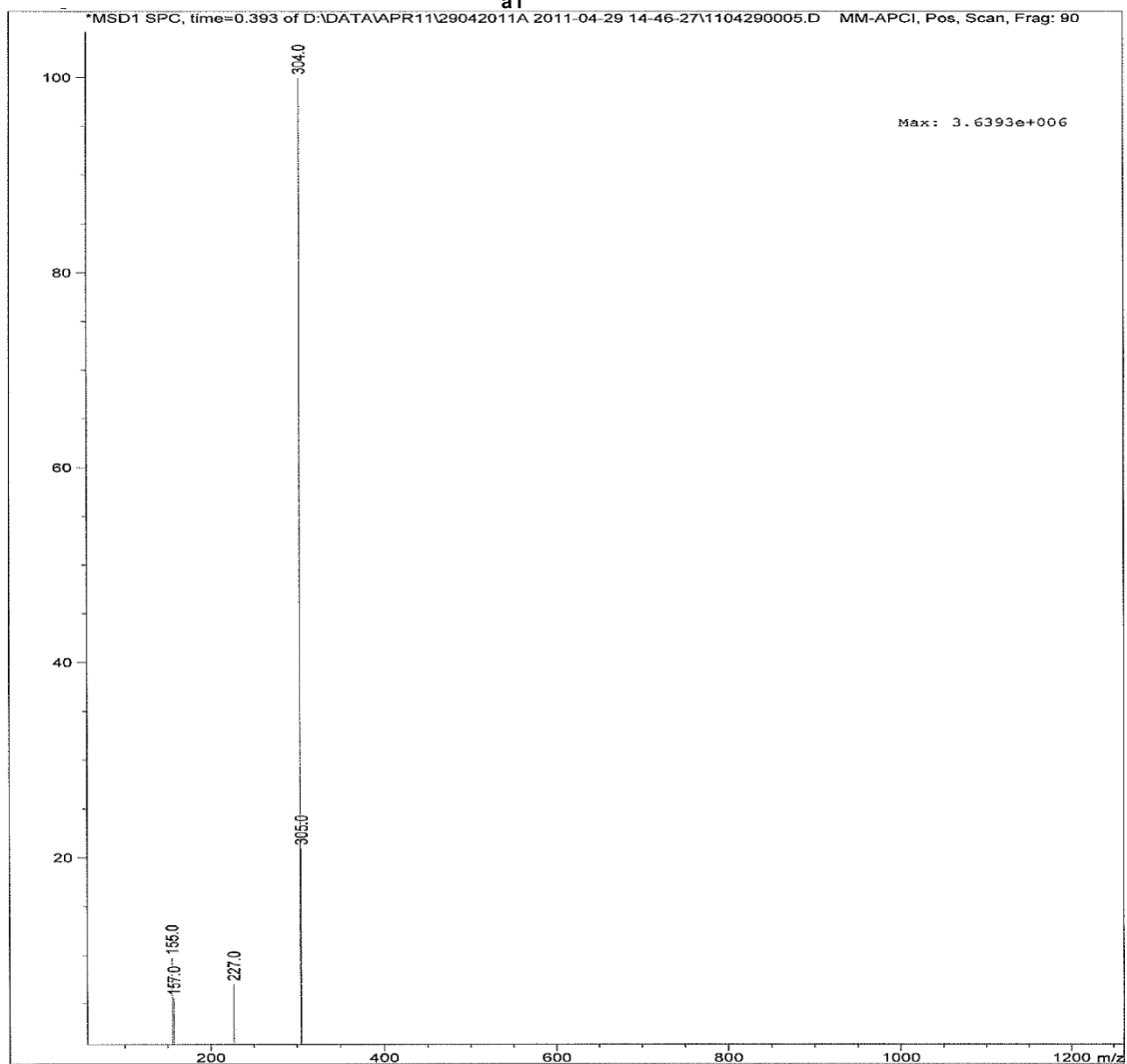
¹H NMR spectrum of **a1** in DMSO



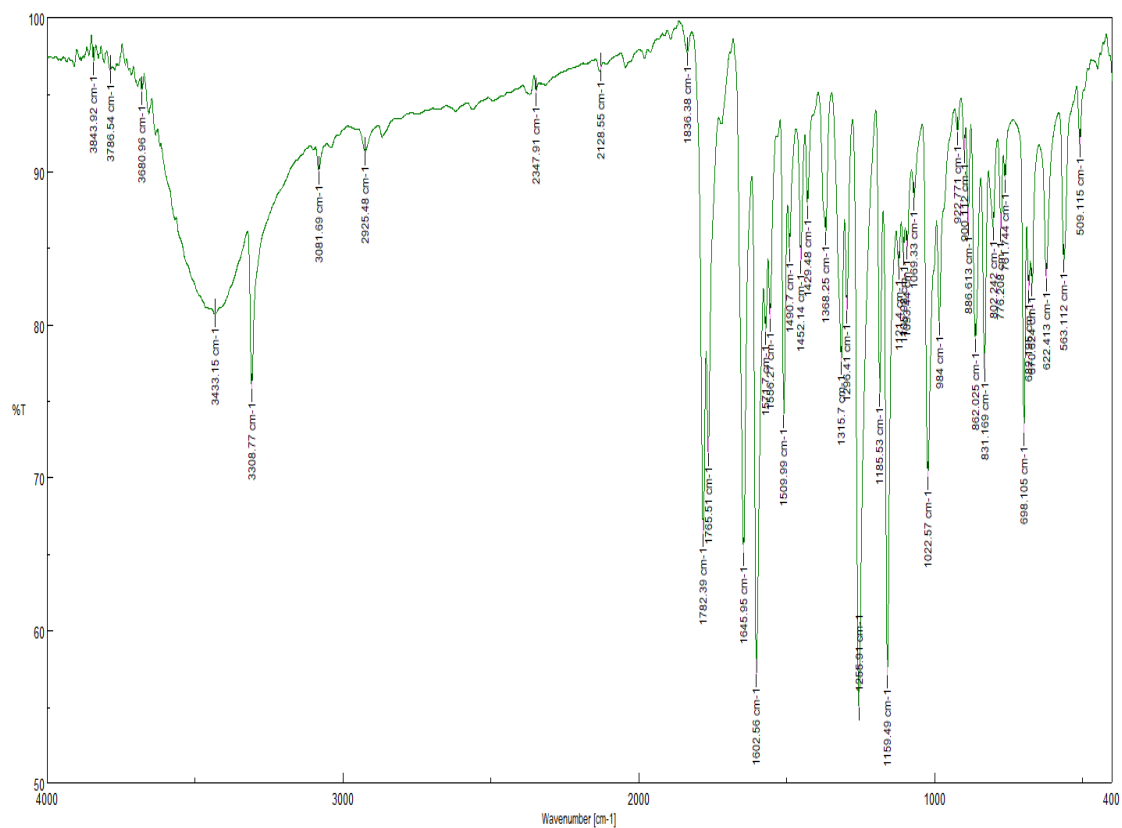
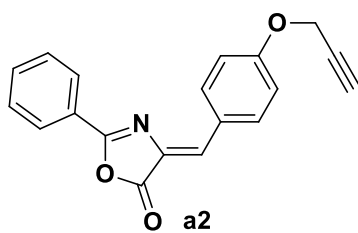
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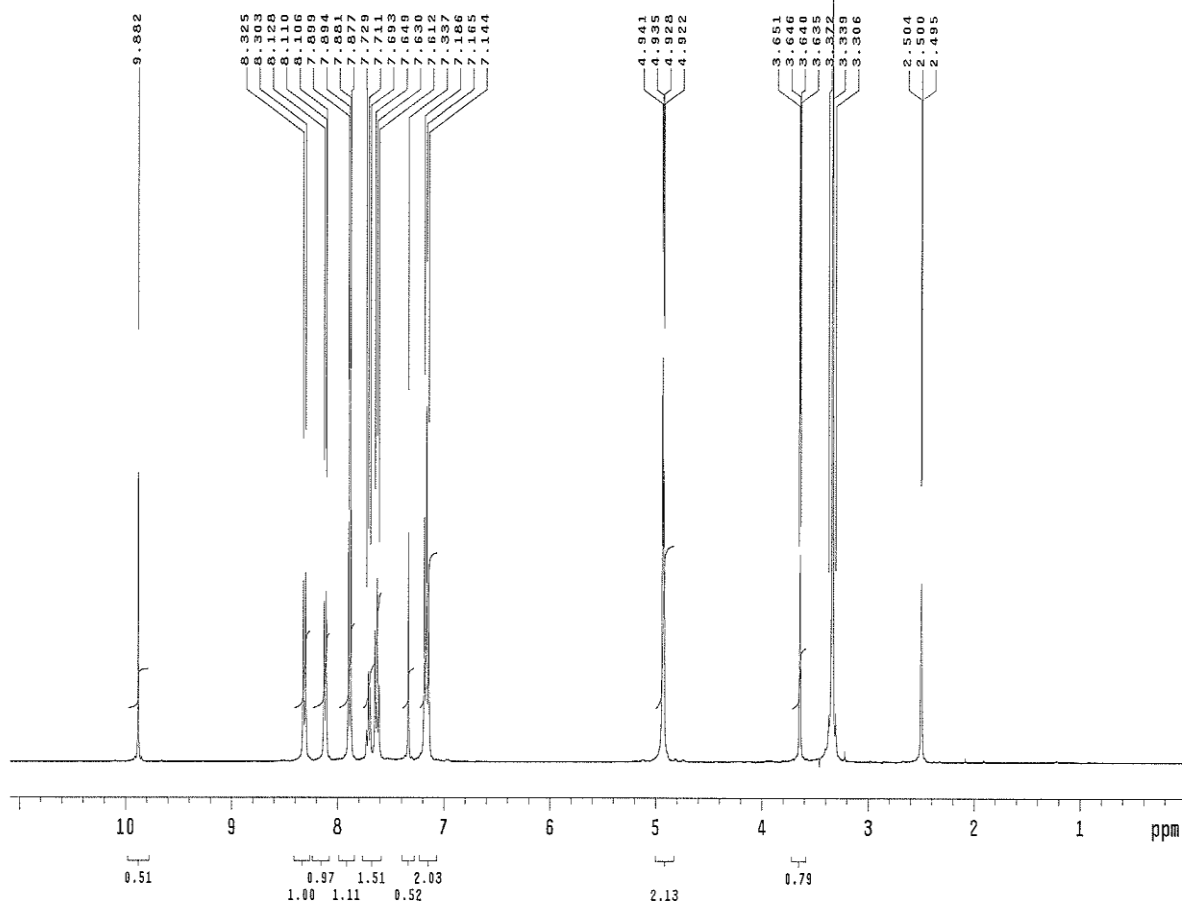
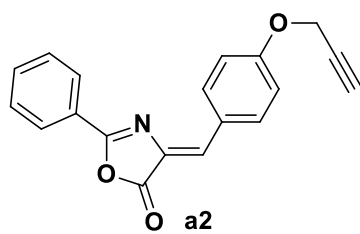
a1



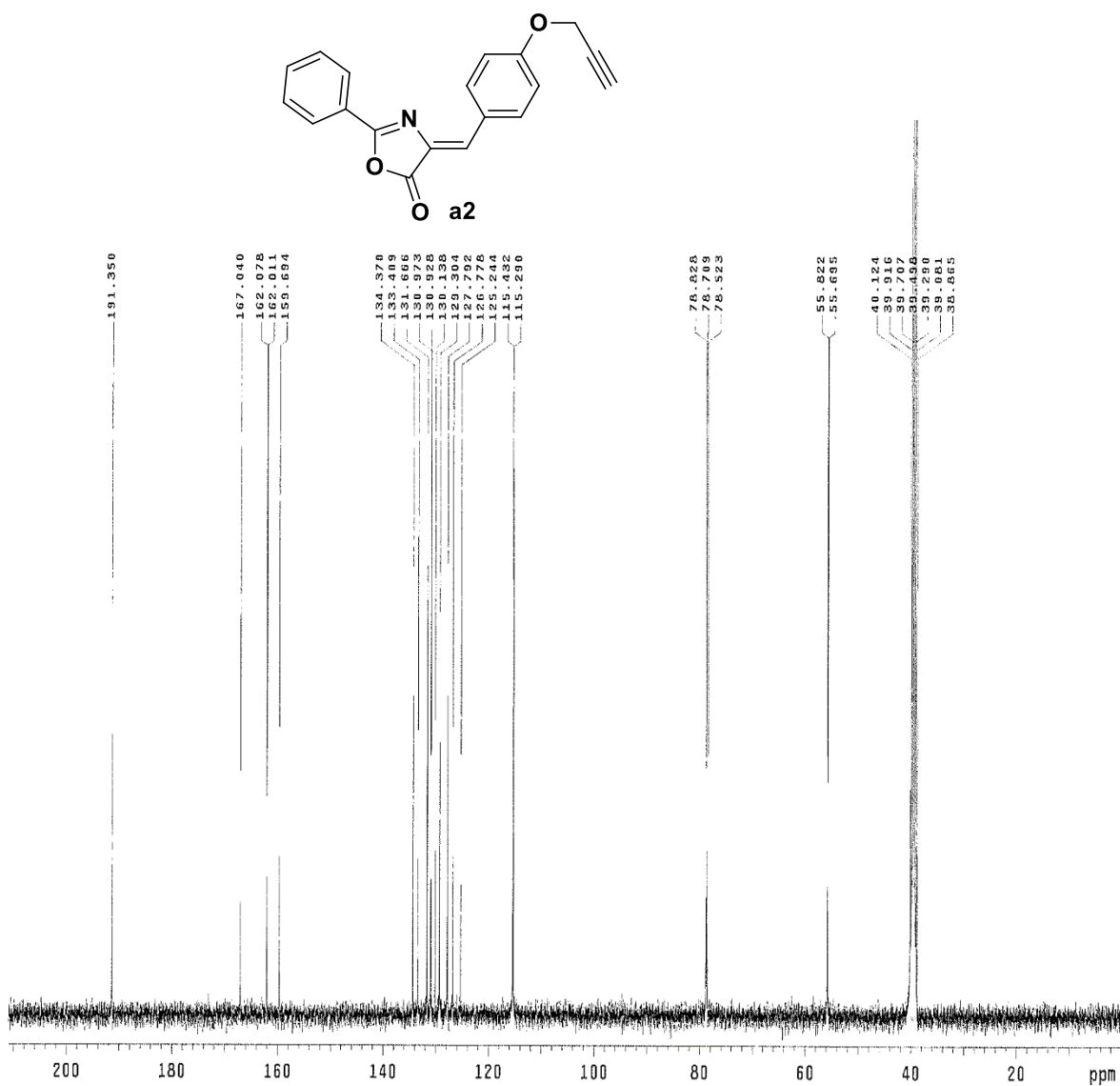
EIMS of **a1**



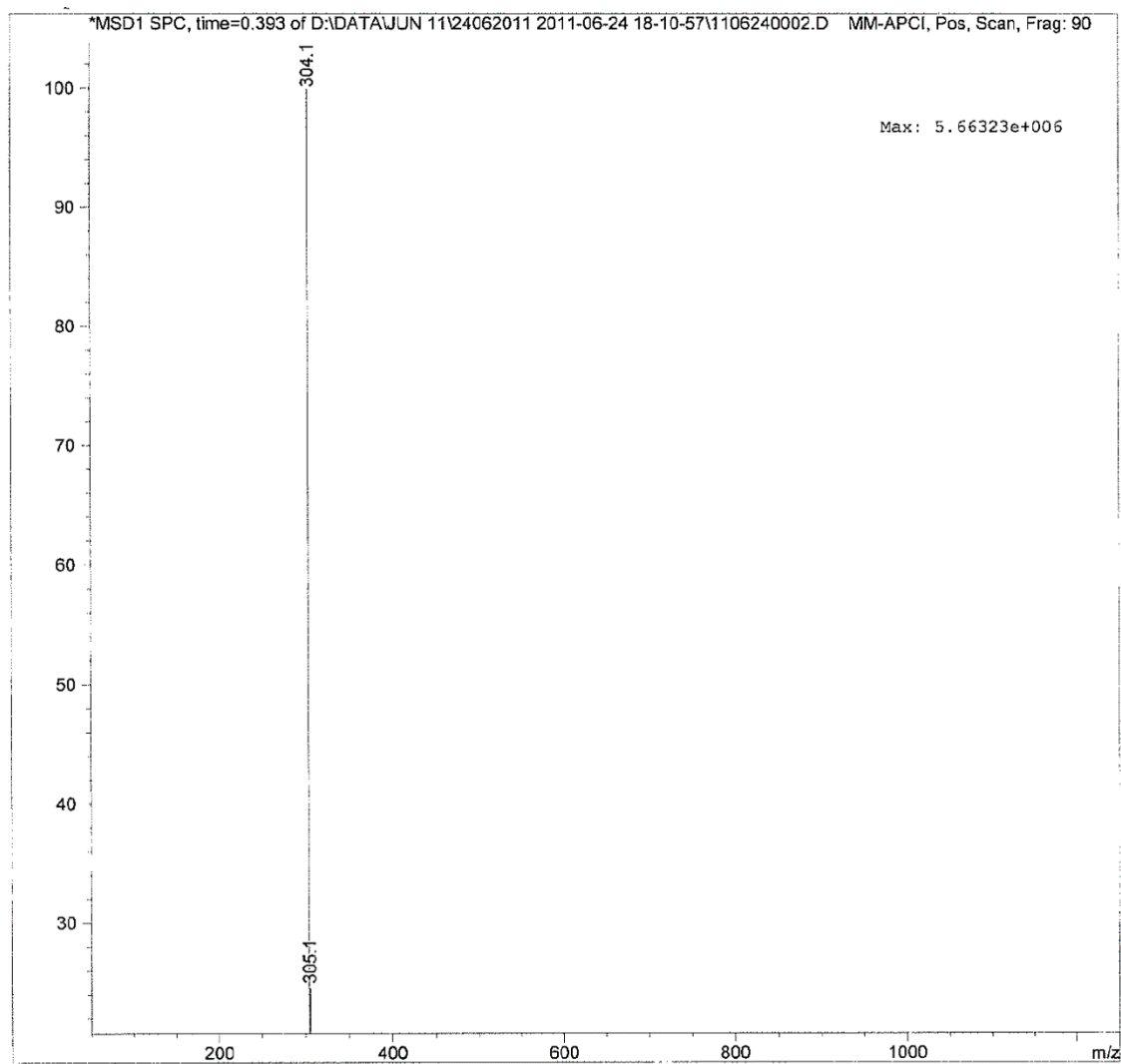
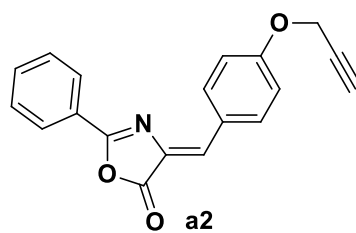
FT-IR Spectrum of **a2**



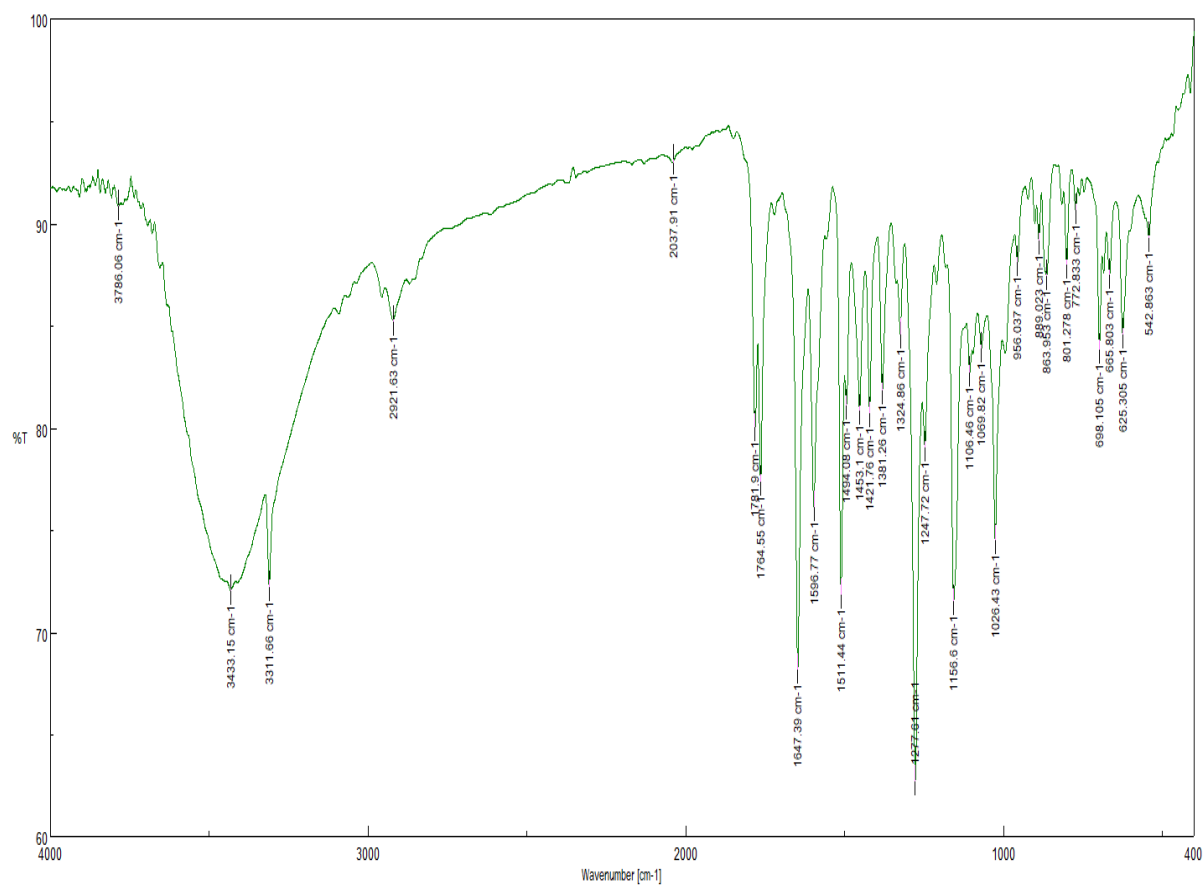
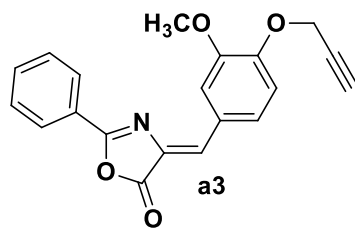
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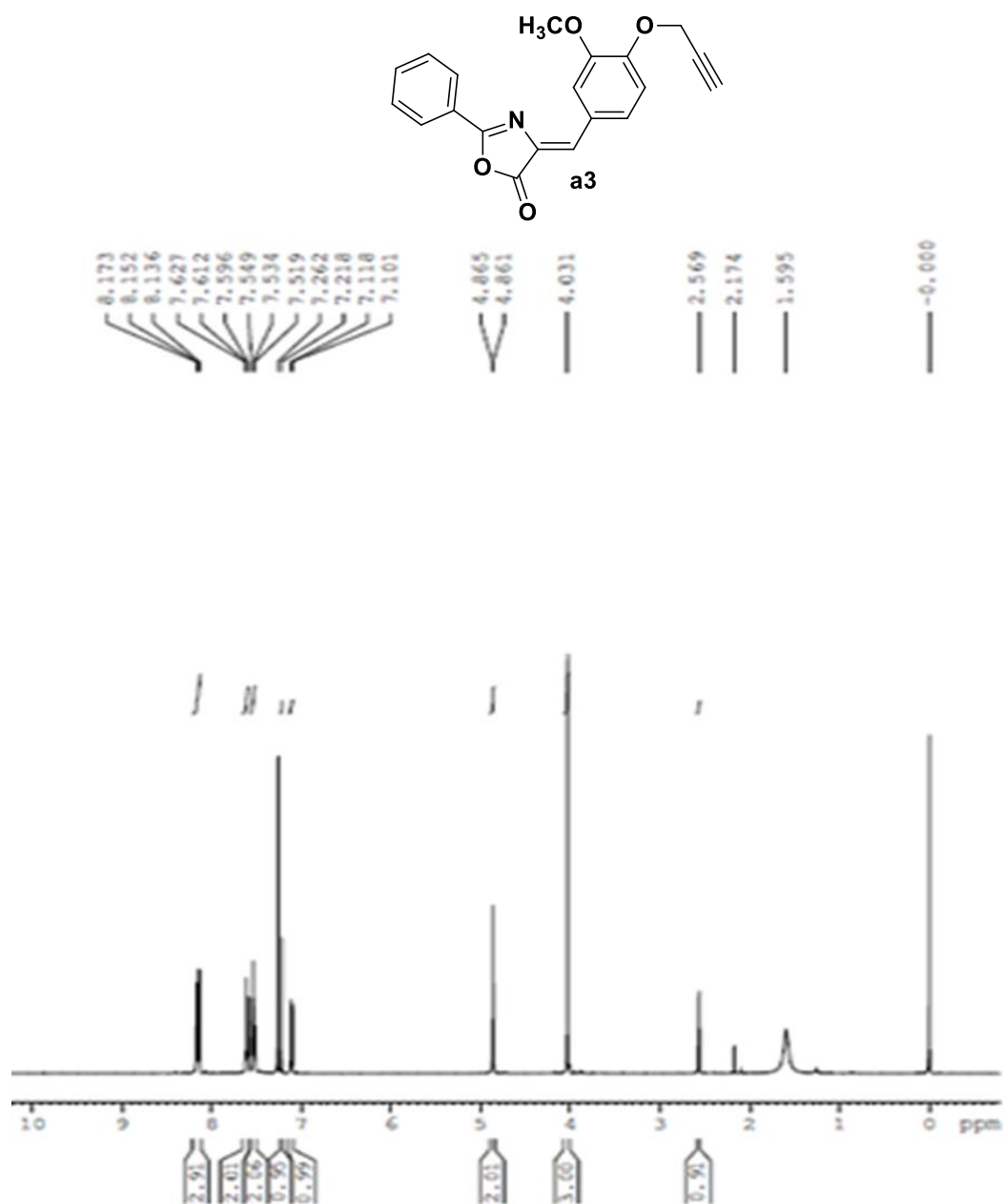
^{13}C NMR spectrum of **a2** in DMSO-d_6



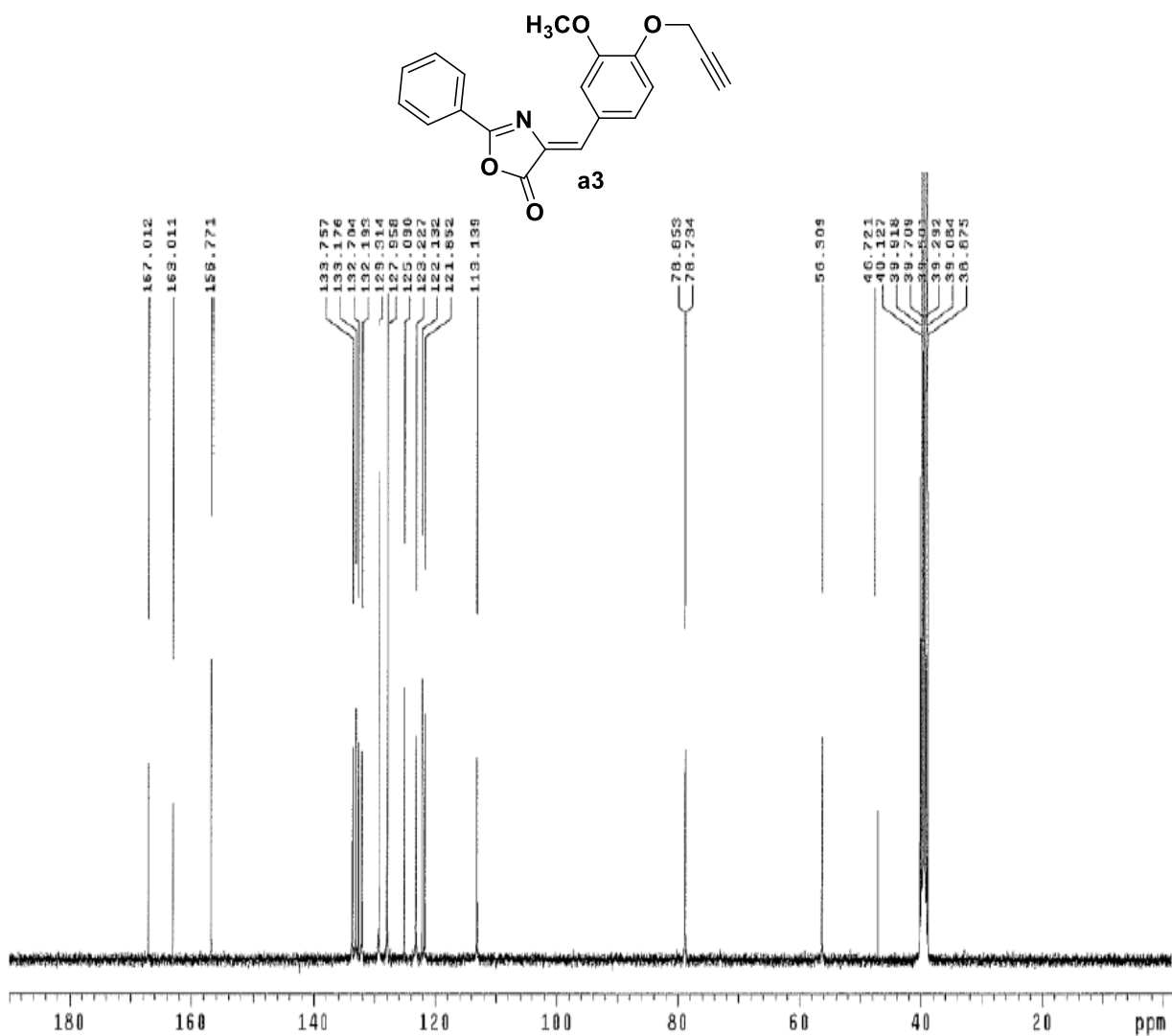
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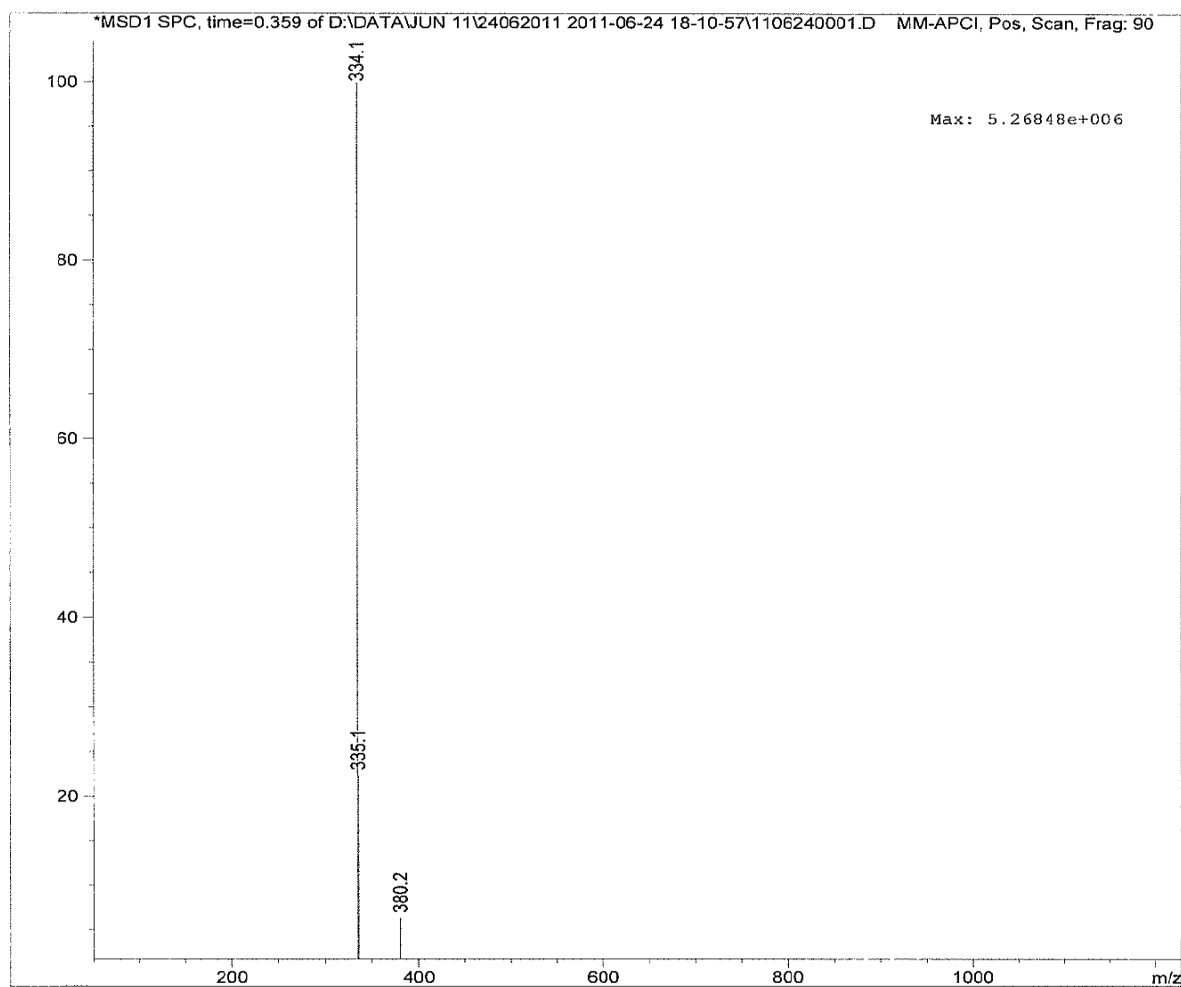
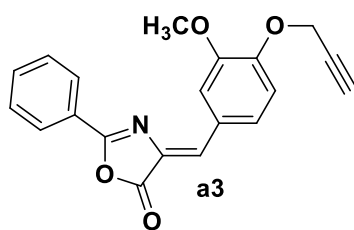
FT-IR Spectrum of **a3**



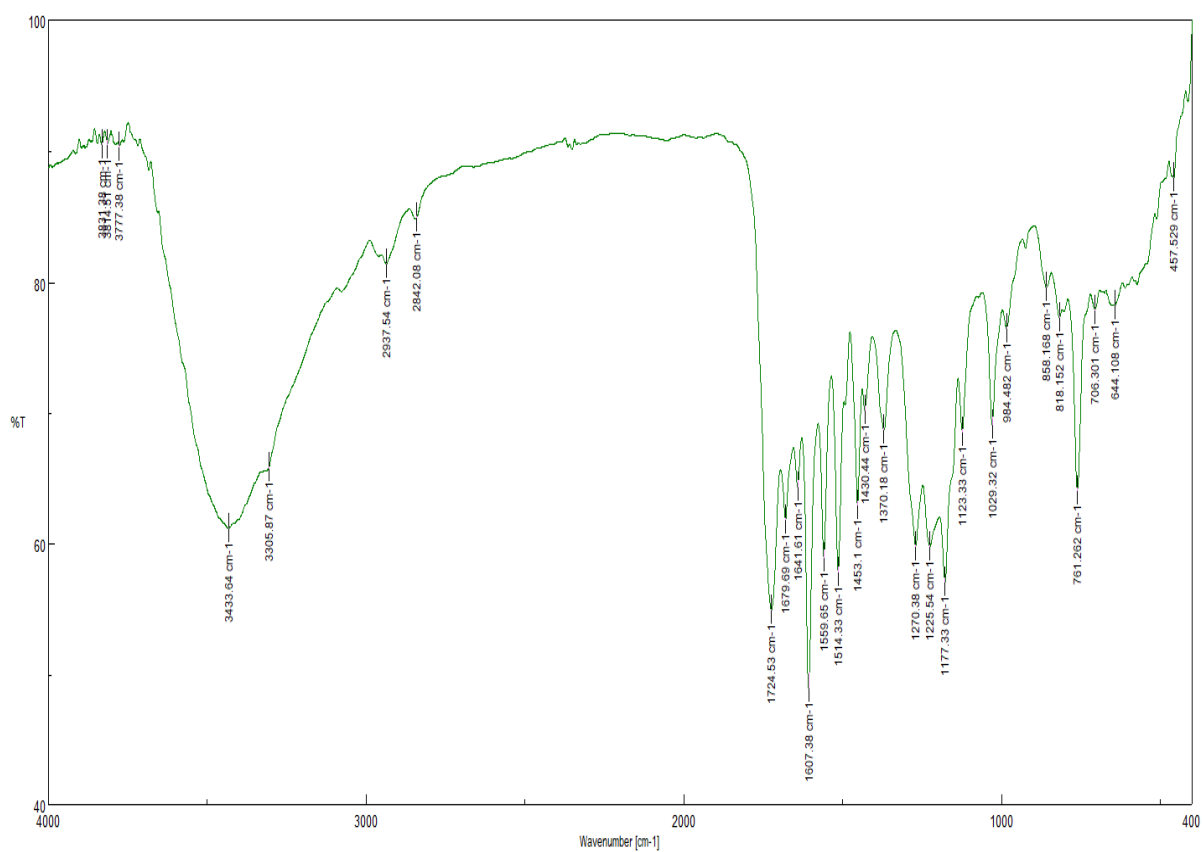
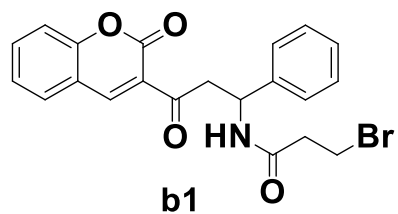
^1H NMR spectrum of **a3** in DMSO d_6



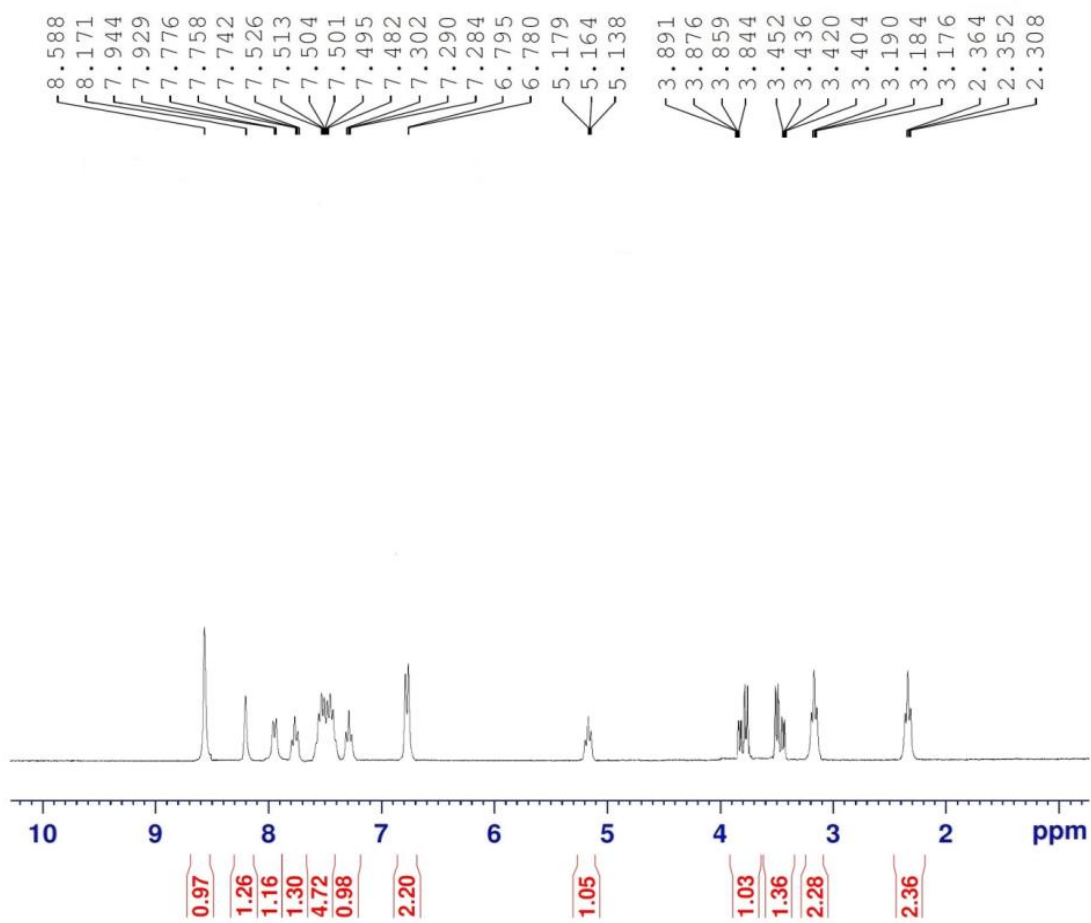
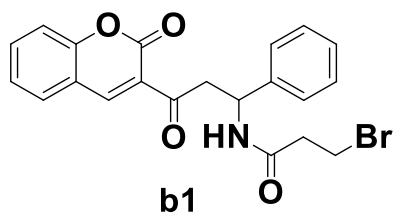
¹³C NMR spectrum of **a3** in DMSO-d₆



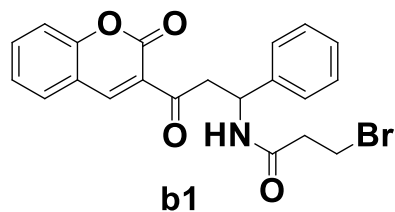
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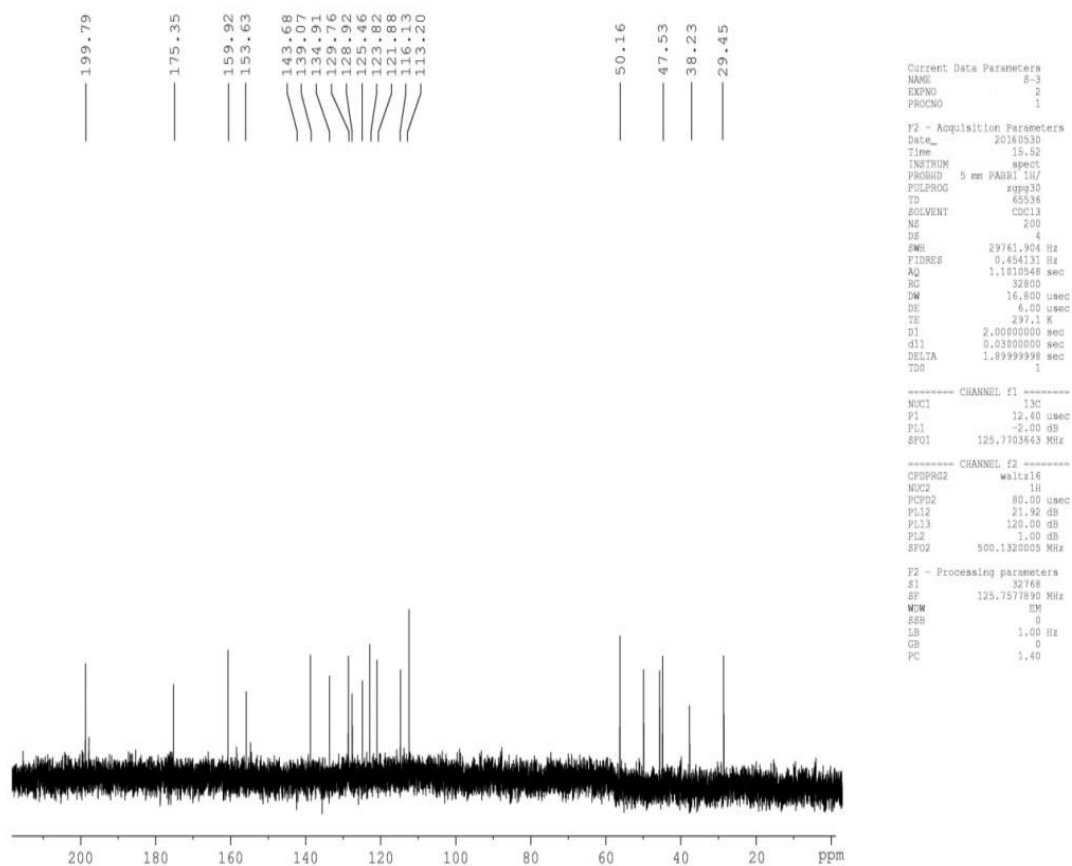
FT-IR Spectrum of **b1**



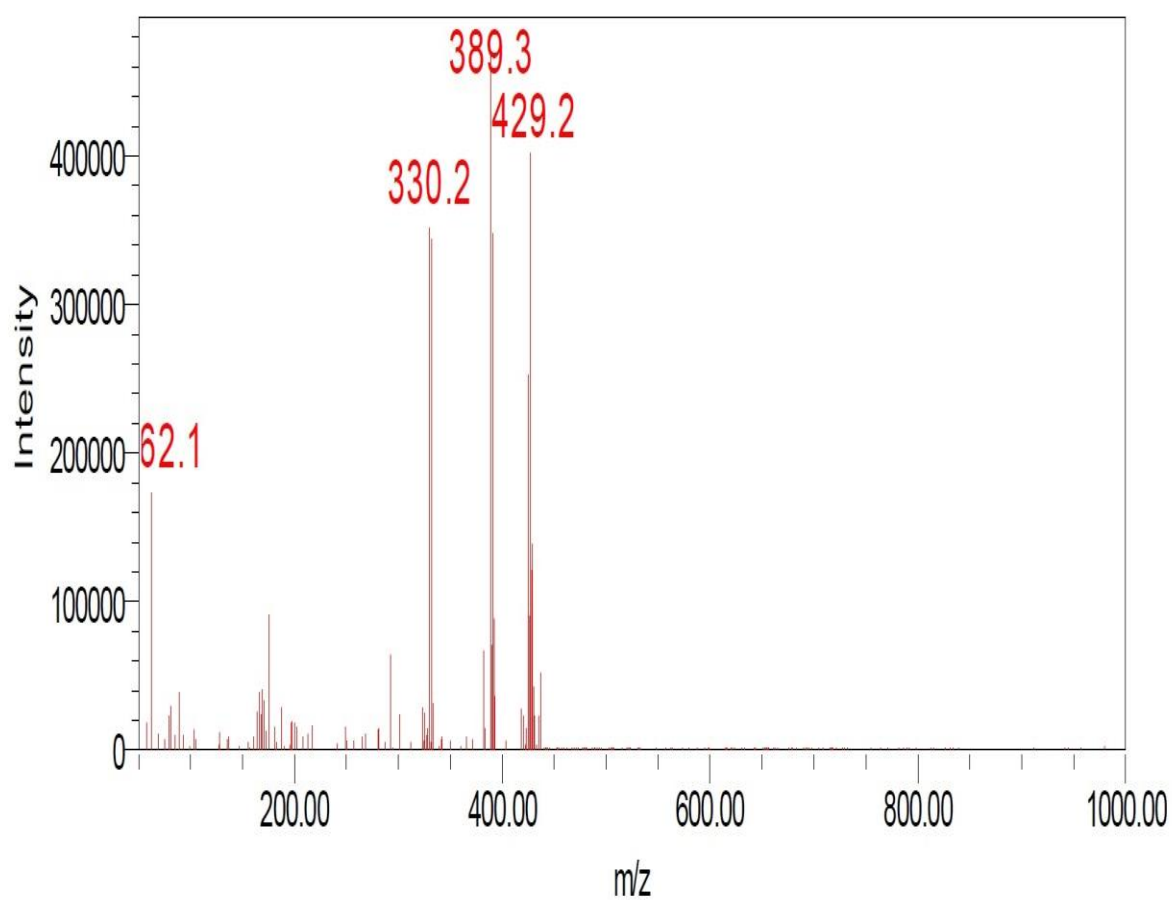
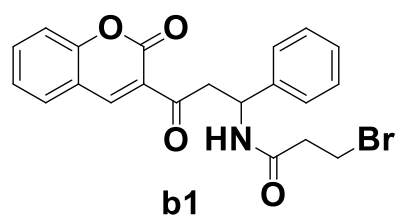
^1H NMR spectrum of **b1** in DMSOd₆



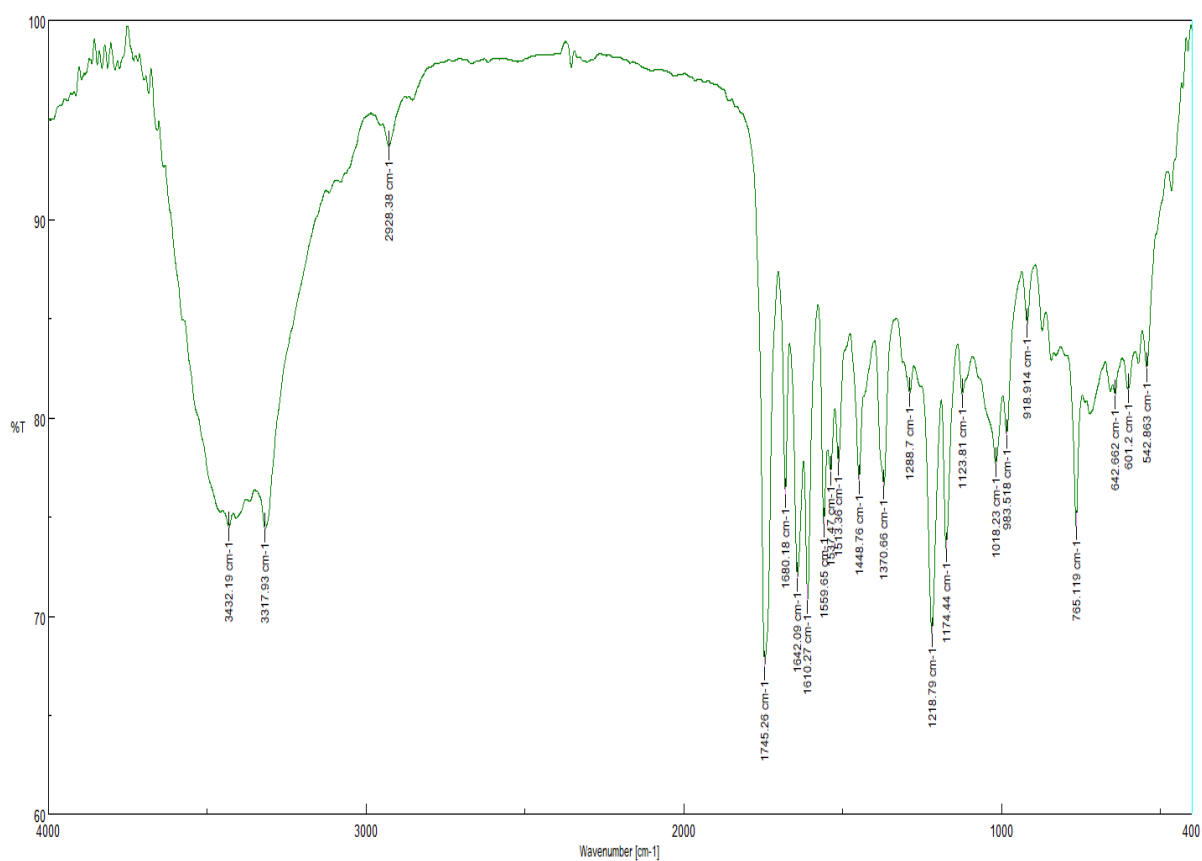
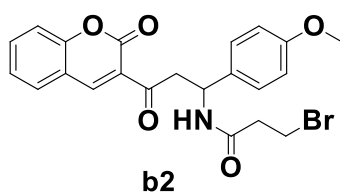
S-3
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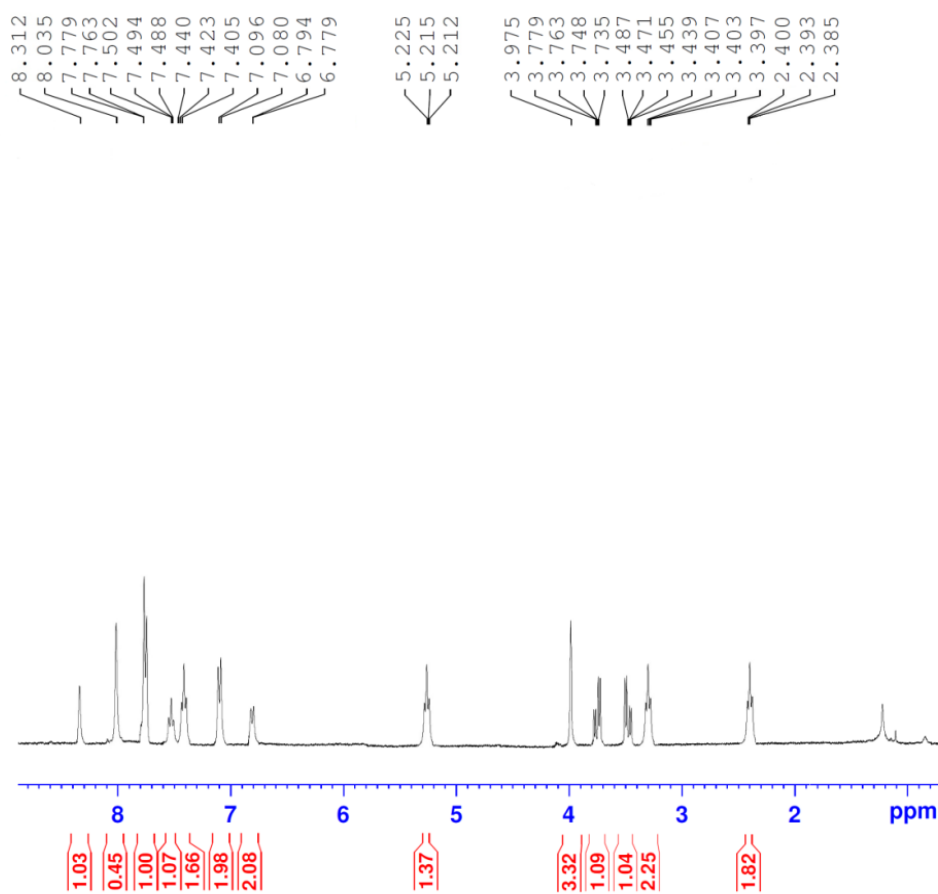
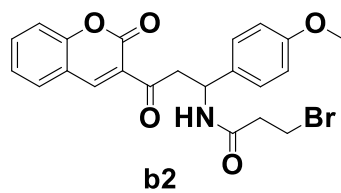
^{13}C NMR spectrum of **b1** in DMSOd6



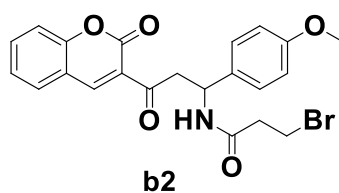
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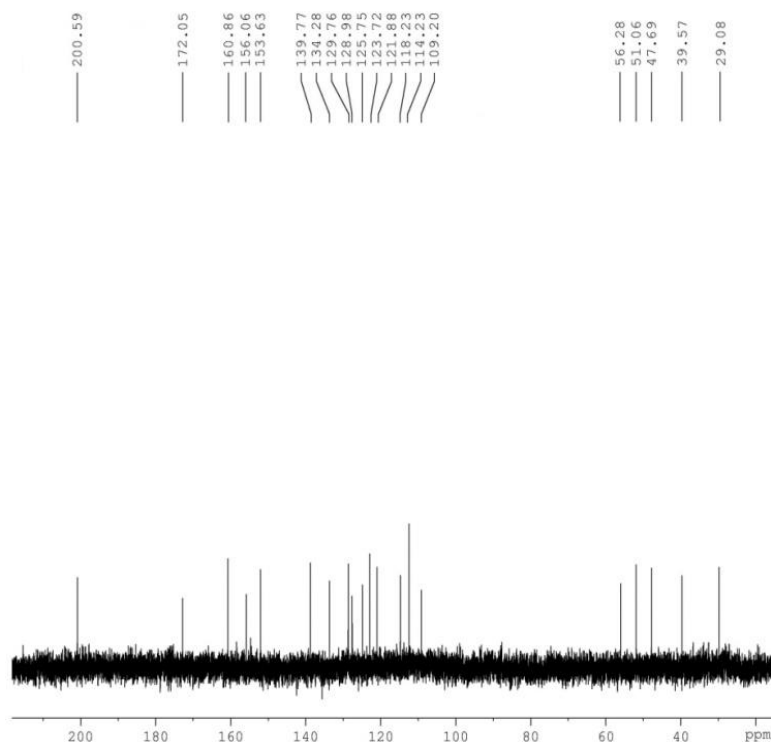
FT-IR Spectrum of **b2**



^1H NMR spectrum of **b2** in DMSOd6



S-1
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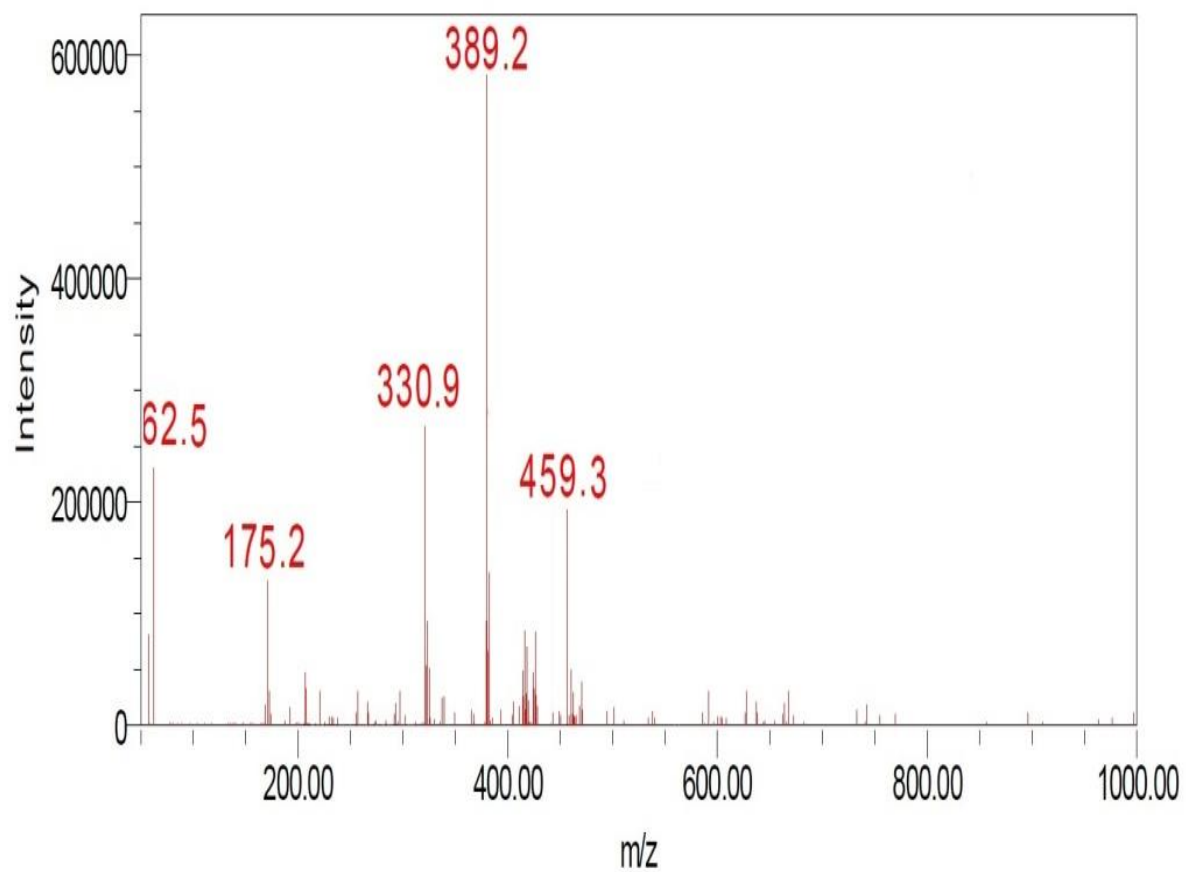
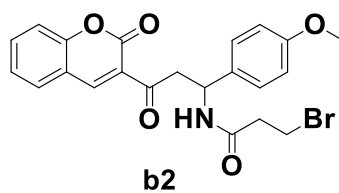
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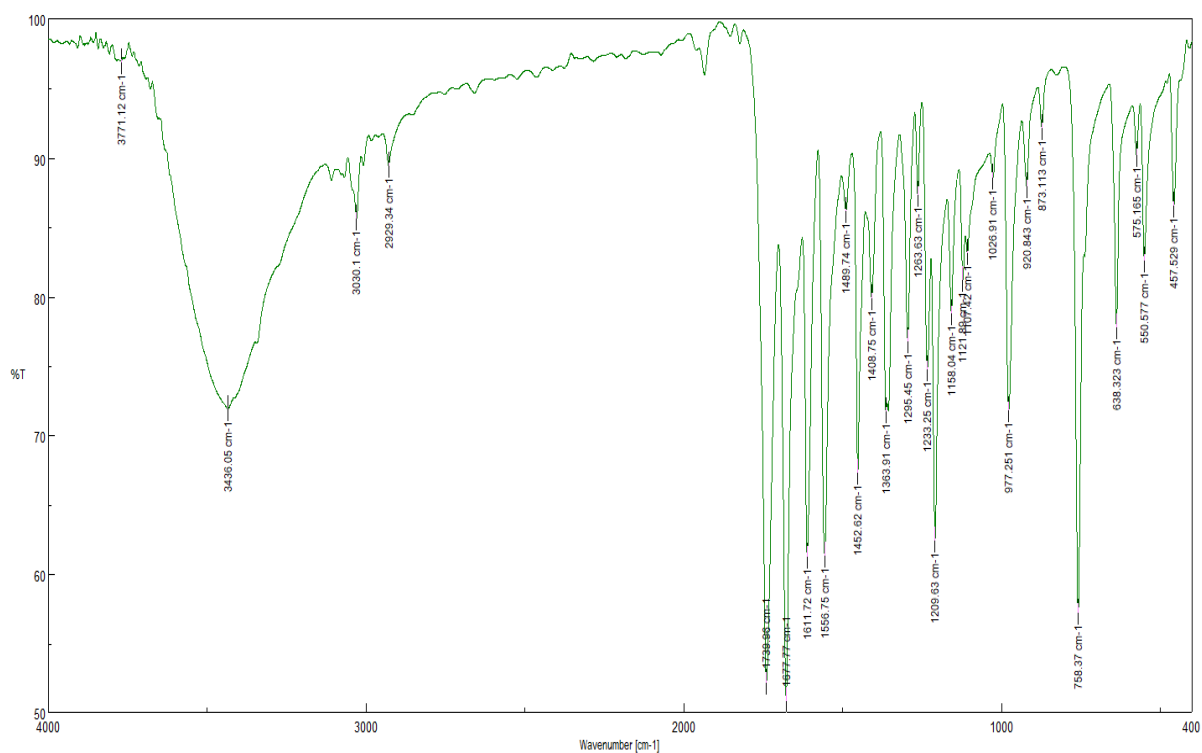
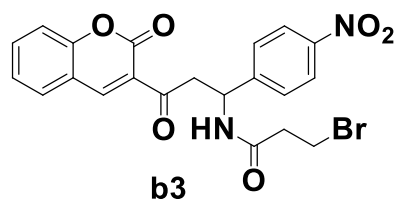
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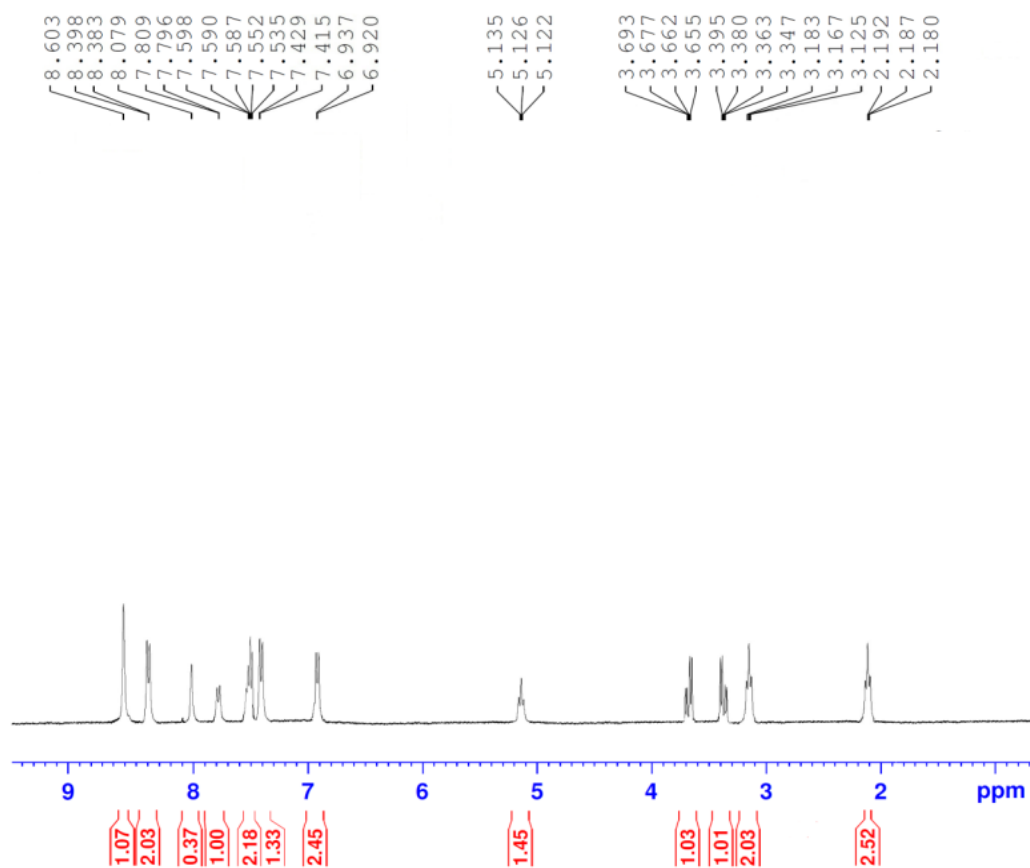
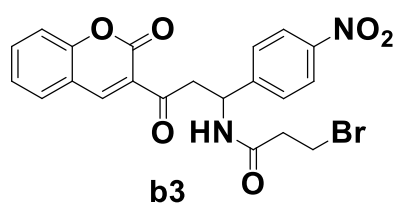
¹³C NMR spectrum of **b2** in DMSOd6



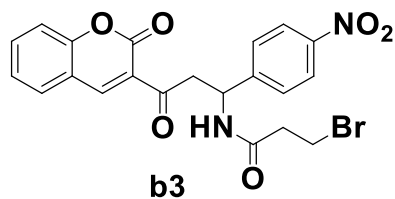
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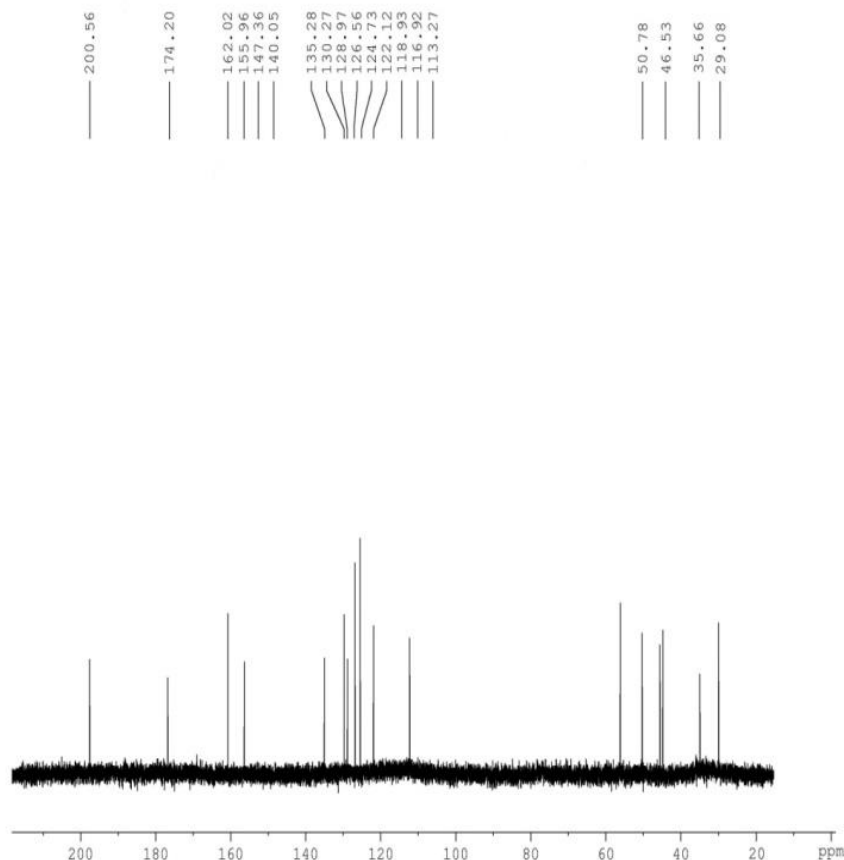
FT-IR Spectrum of **b3**



^1H NMR spectrum of **b3** in DMSO d_6



S-2
C13CPD CDC13 {D:\Yoosuf} NIIST 21



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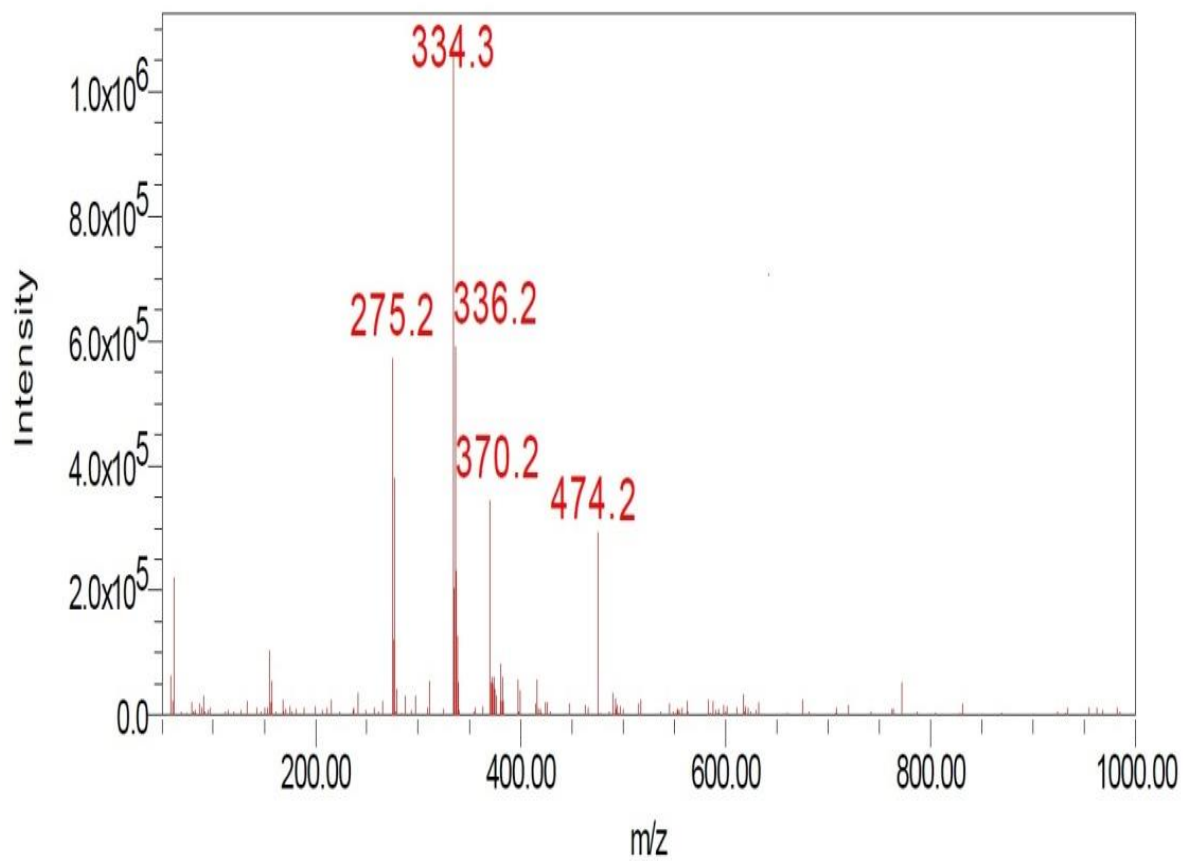
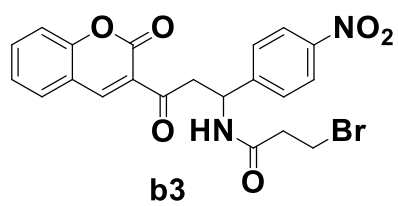
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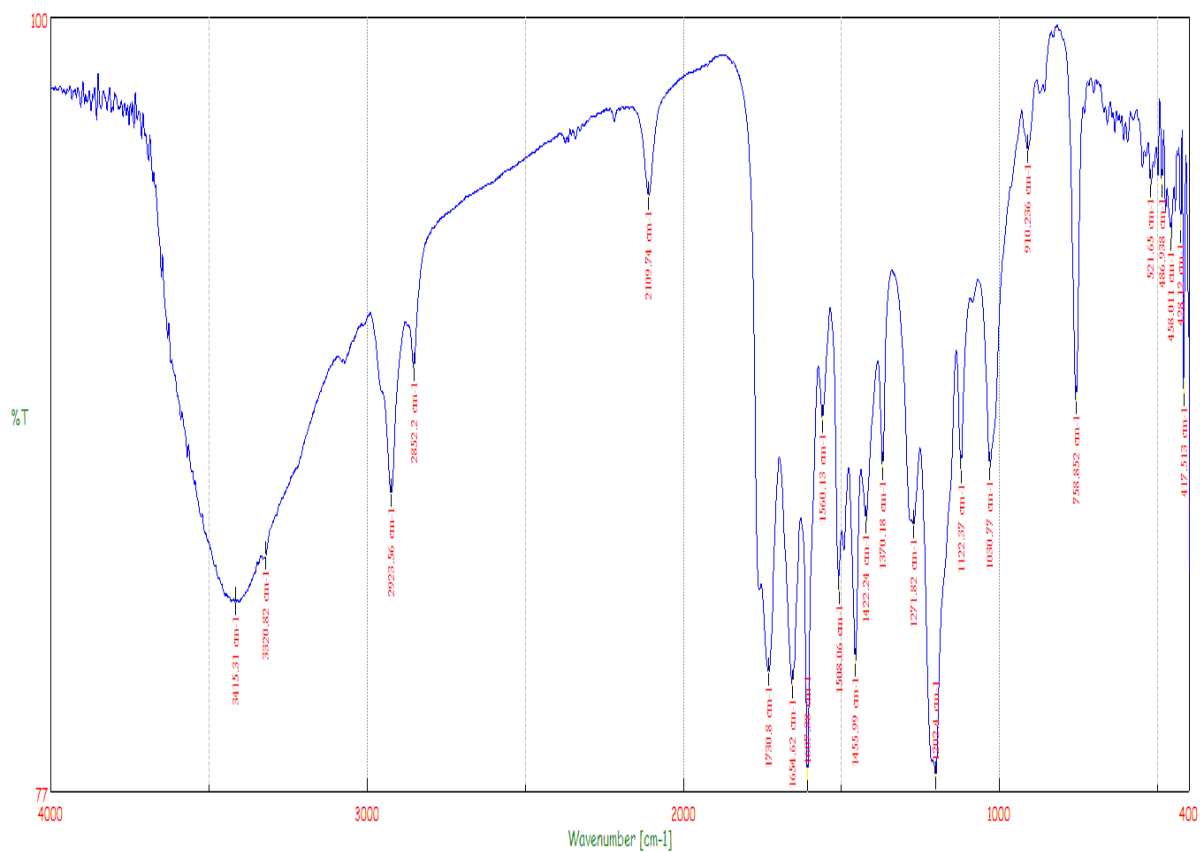
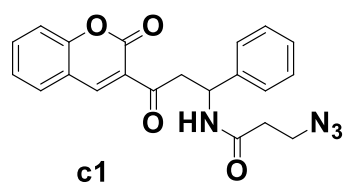
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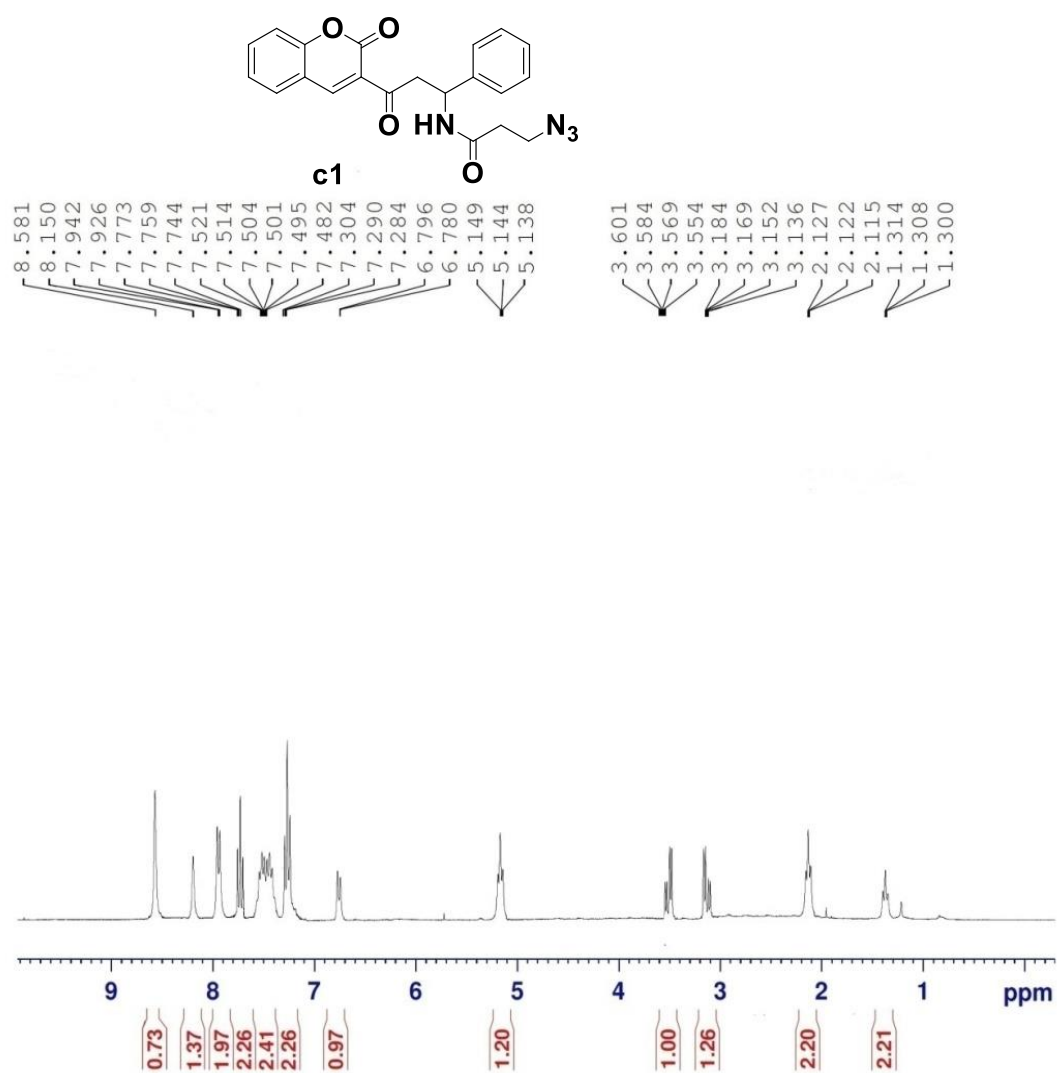
^{13}C NMR spectrum of **b3** in DMSOd6



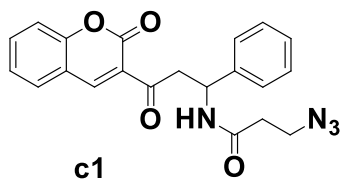
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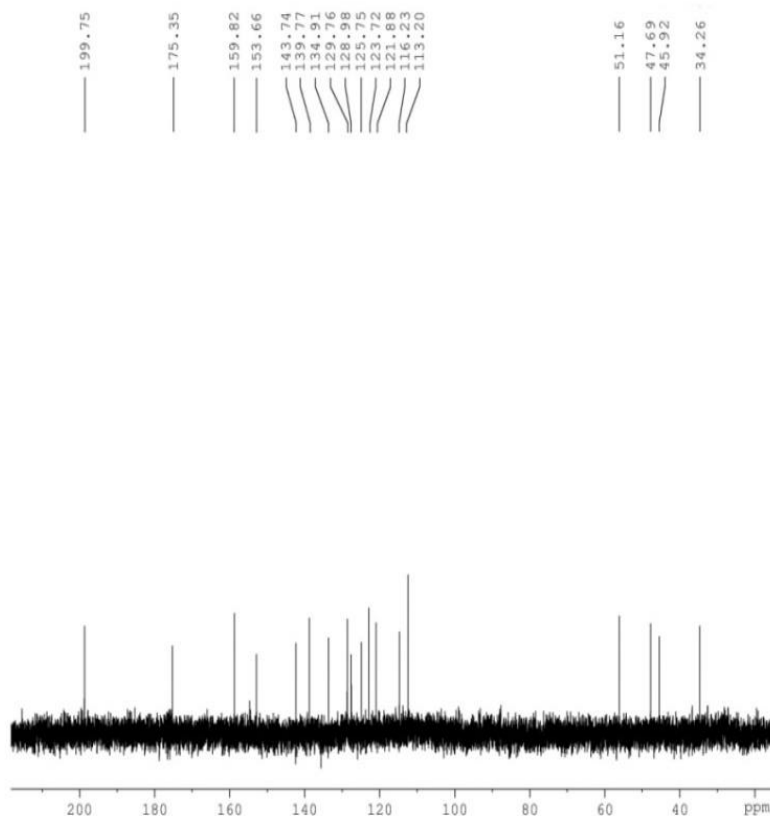
FT-IR Spectrum of **c1**



¹H NMR spectrum of **c1** in DMSOd6



S-73
C13CPD CDCl3 {D:\Yoosuf} NIIST 17



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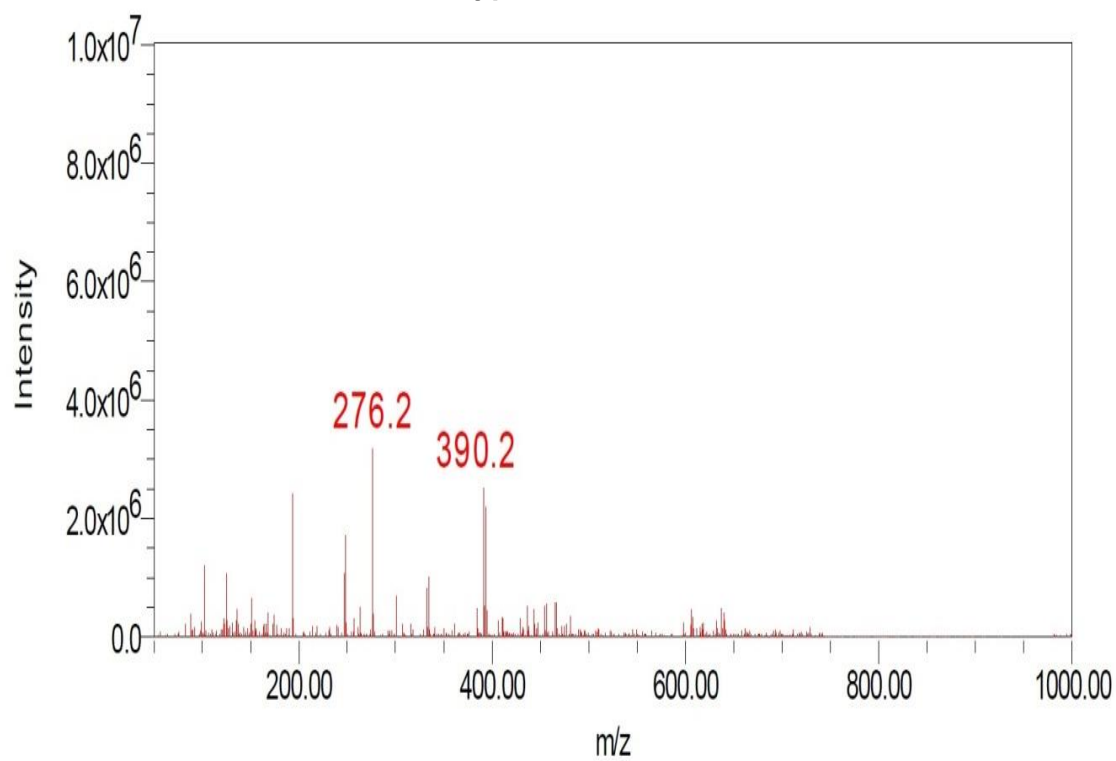
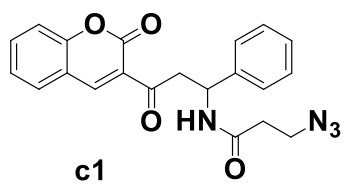
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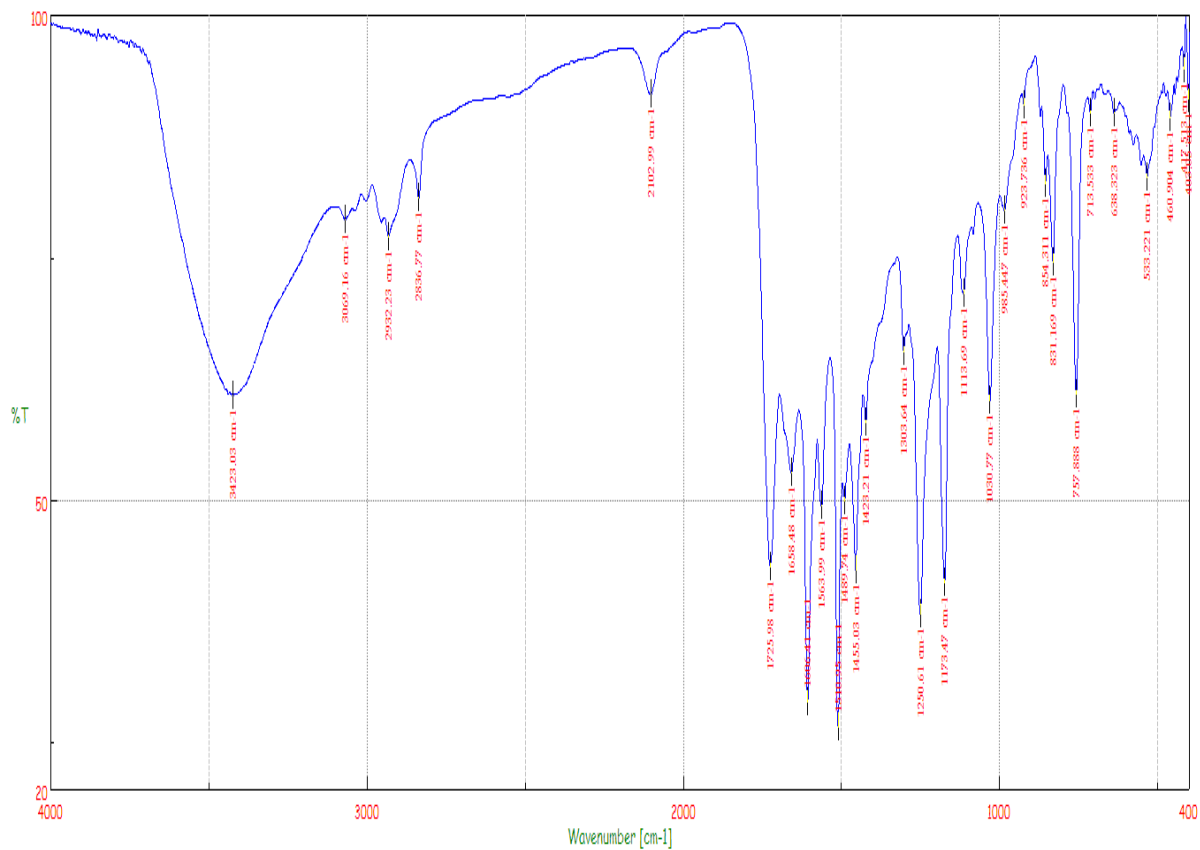
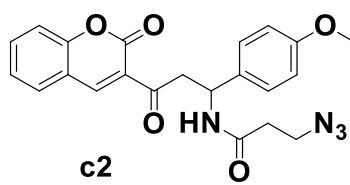
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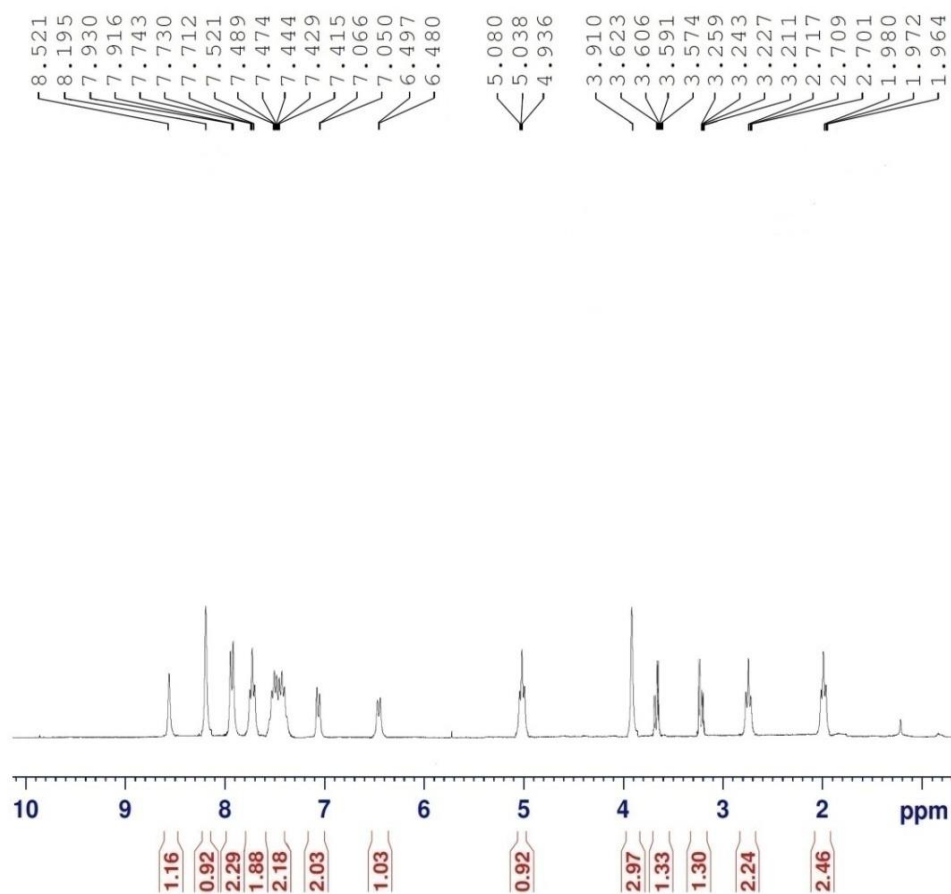
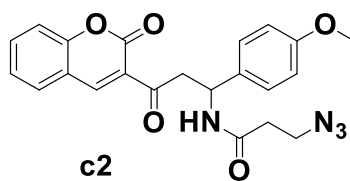
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¹³C NMR spectrum of **c1** in DMSOd6



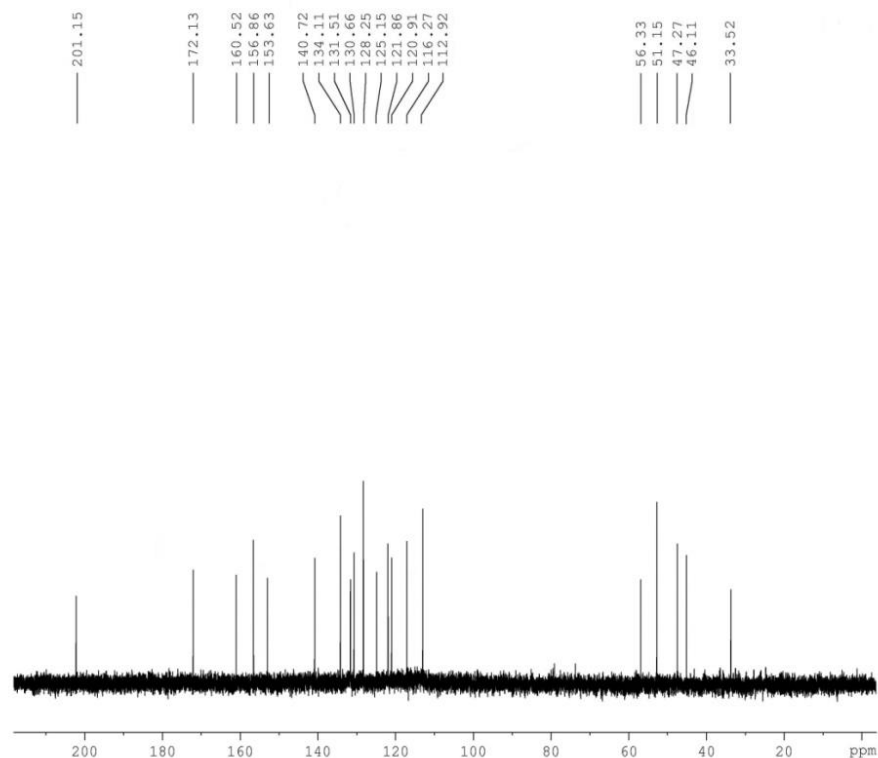
EIMS of **c1**





¹H NMR spectrum of **c2** in DMSO-d₆

S-5
C13CPD CDC13 {D:\Yoosuf} NIIST 16



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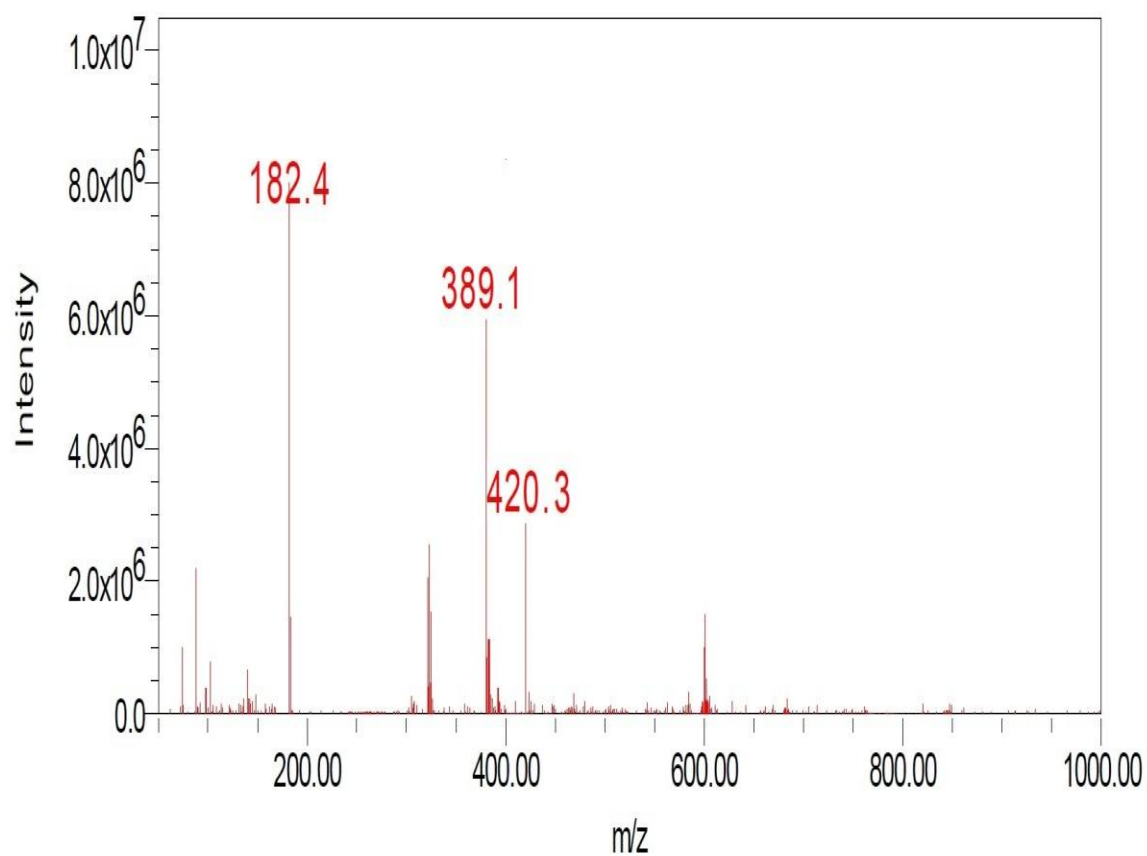
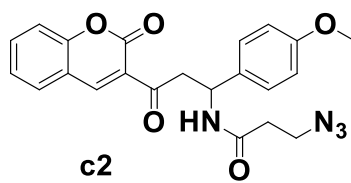
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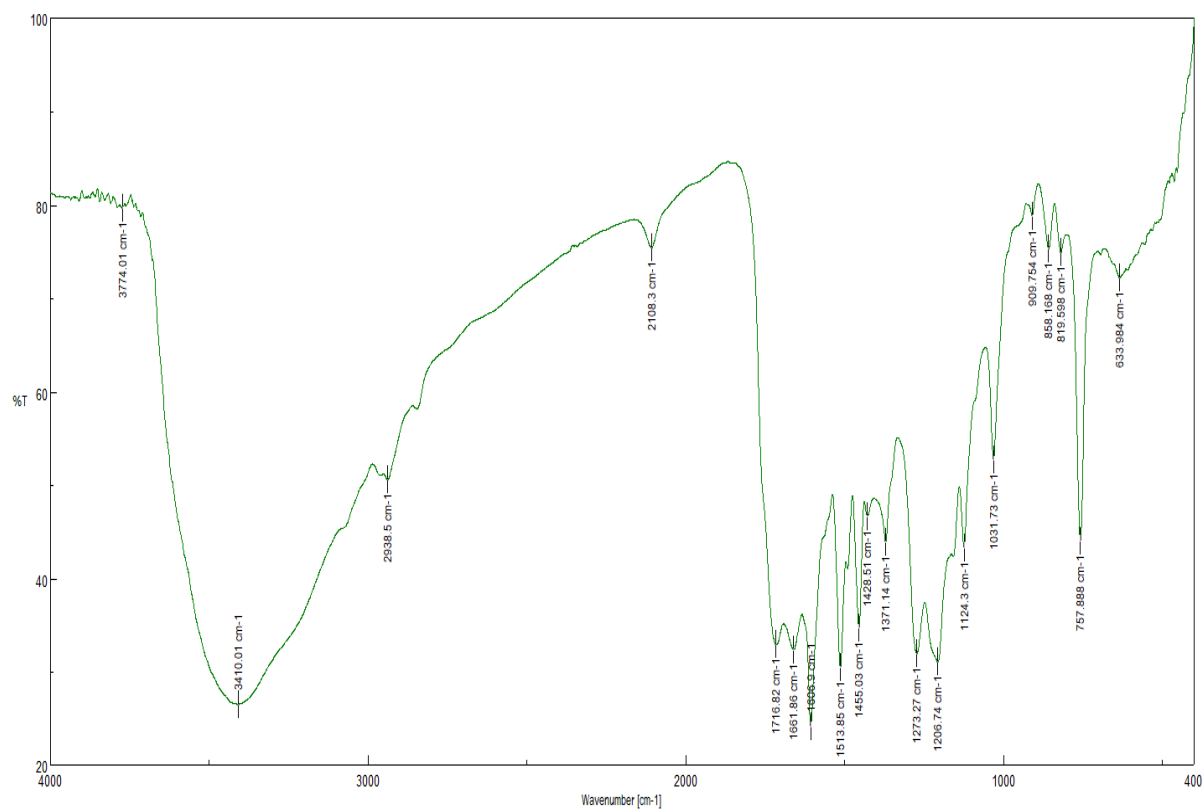
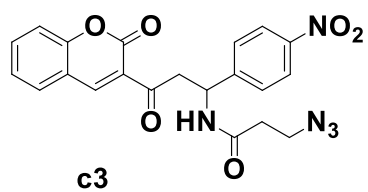
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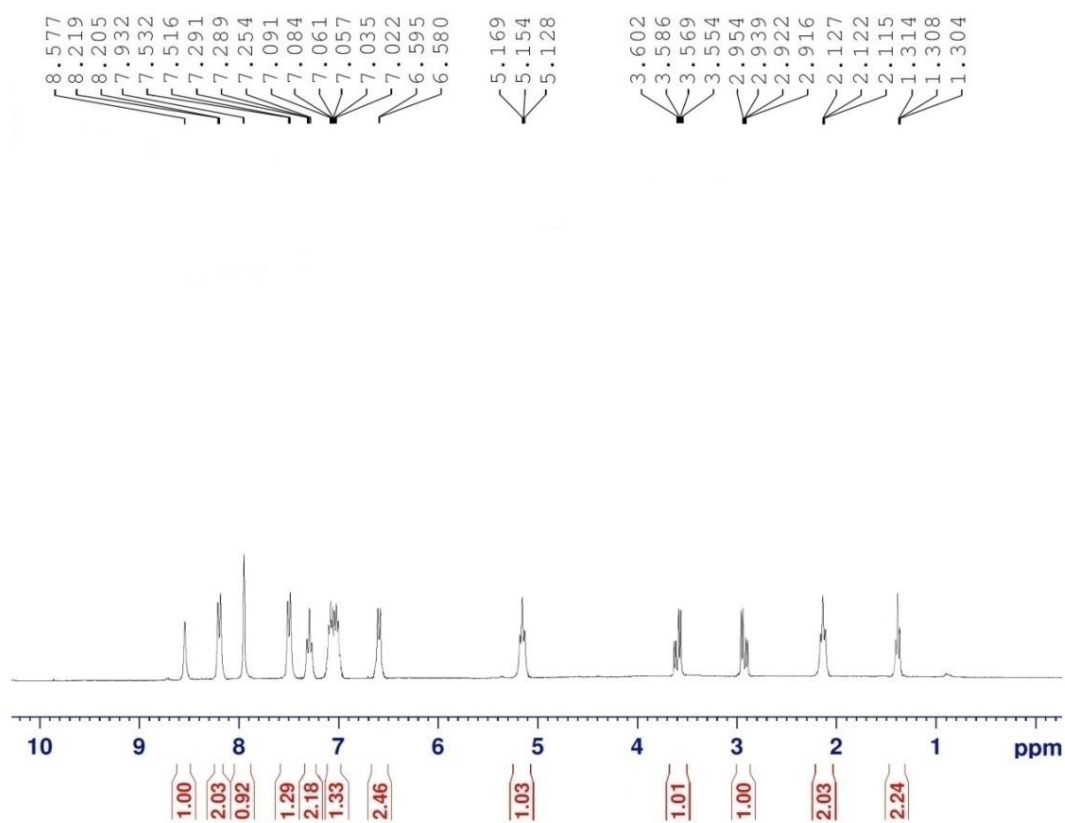
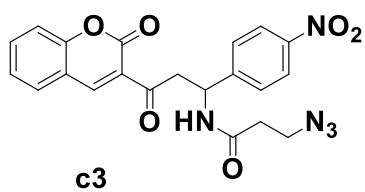
¹³C NMR spectrum of **c2** in DMSOd6



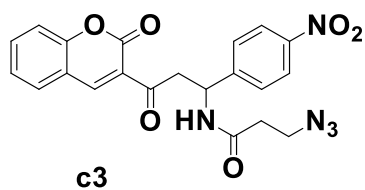
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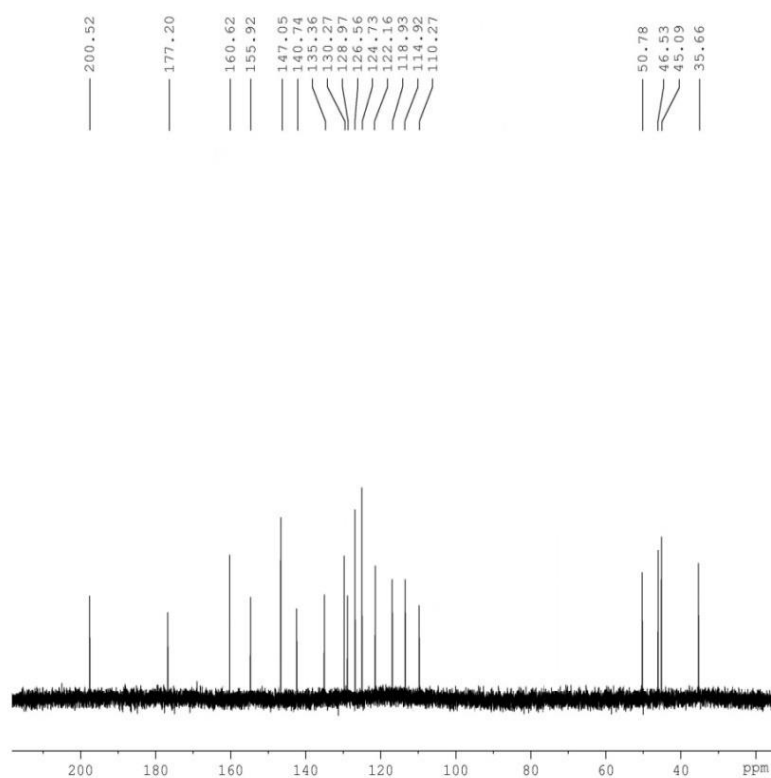
FT-IR Spectrum of **c3**



¹H NMR spectrum of **c3** in DMSO-d₆



S-6
C13CPD CDCl3 {D:\Yoosuf} NIIST 21



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FIDRES     0.454131 Hz
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TD0        1

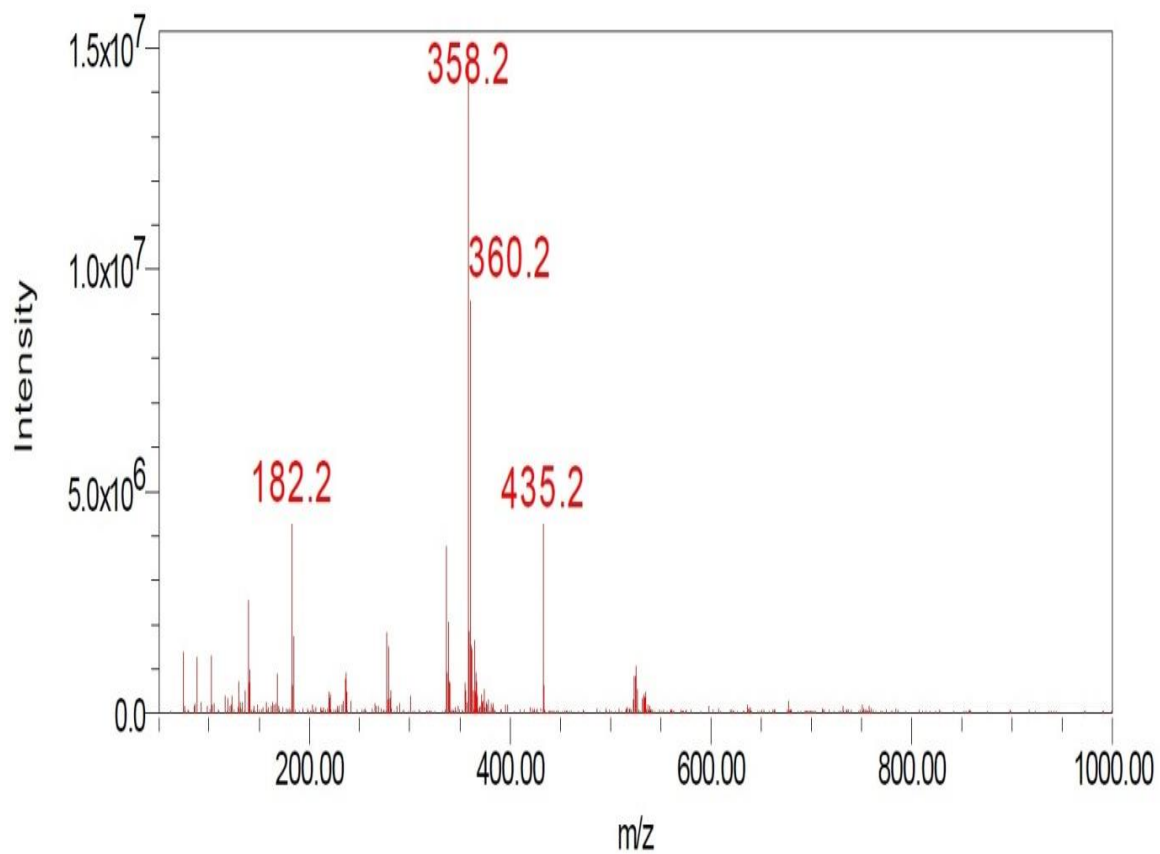
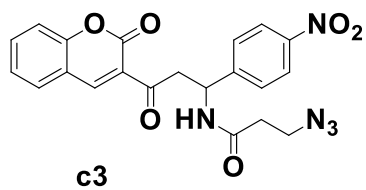
===== CHANNEL f1 =====
NUC1       13C
P1         12.40 usec
PL1        -2.00 dB
SFO1       125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL12       21.92 dB
PL13       120.00 dB
PL2        1.00 dB
SFO2       500.1320005 MHz

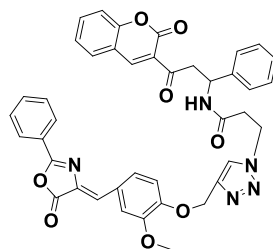
F2 - Processing parameters
S1         32768
SF         125.7577890 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40

```

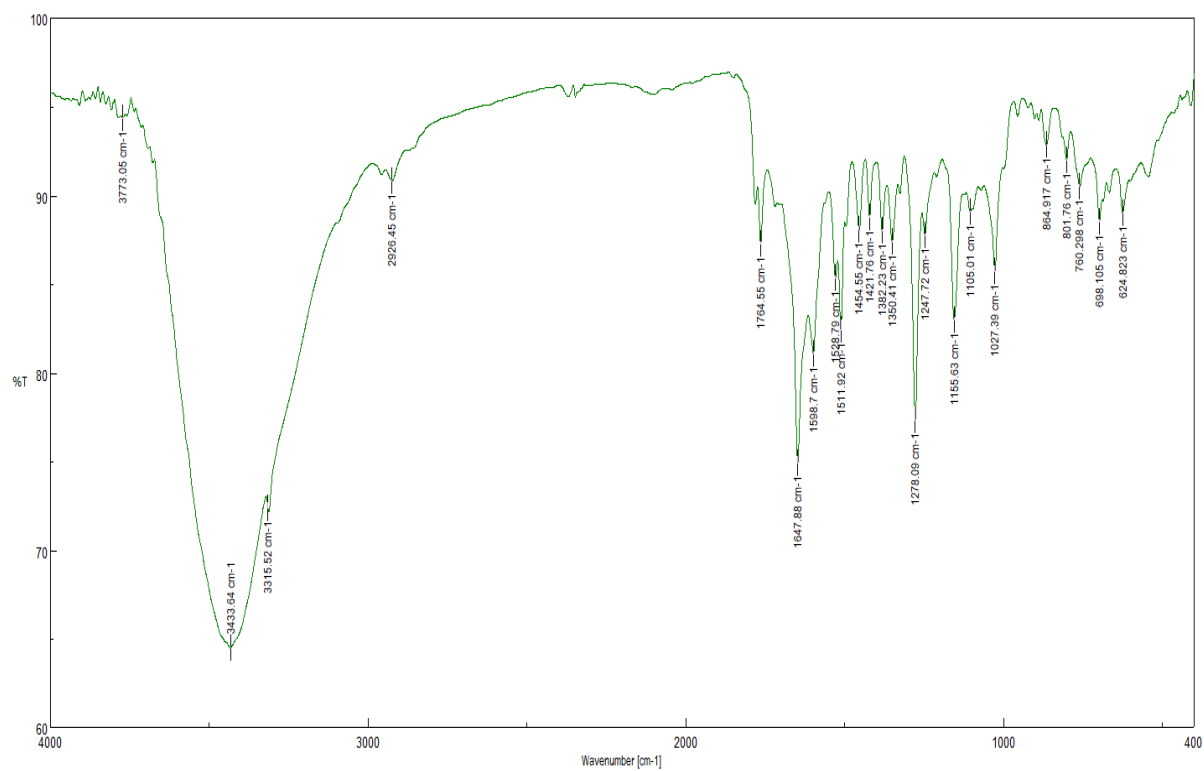
¹³C NMR spectrum of **c3** in DMSOd6



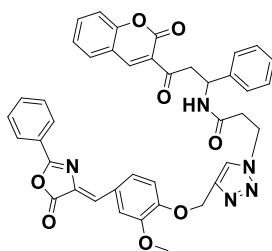
EIMS of **c3**



OC1

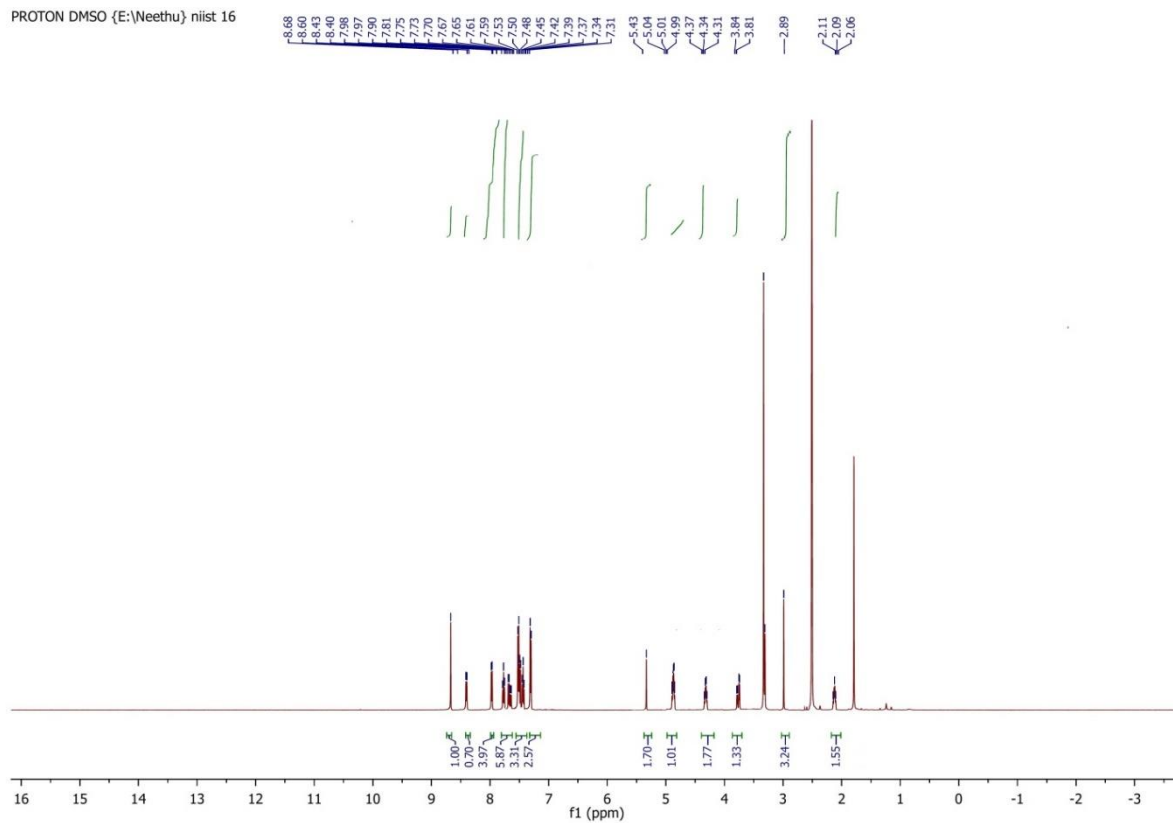


FT-IR Spectrum of OC1

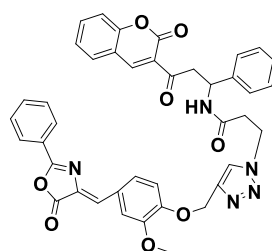


OC1

PROTON DMSO {E:\Neethu} niist 16

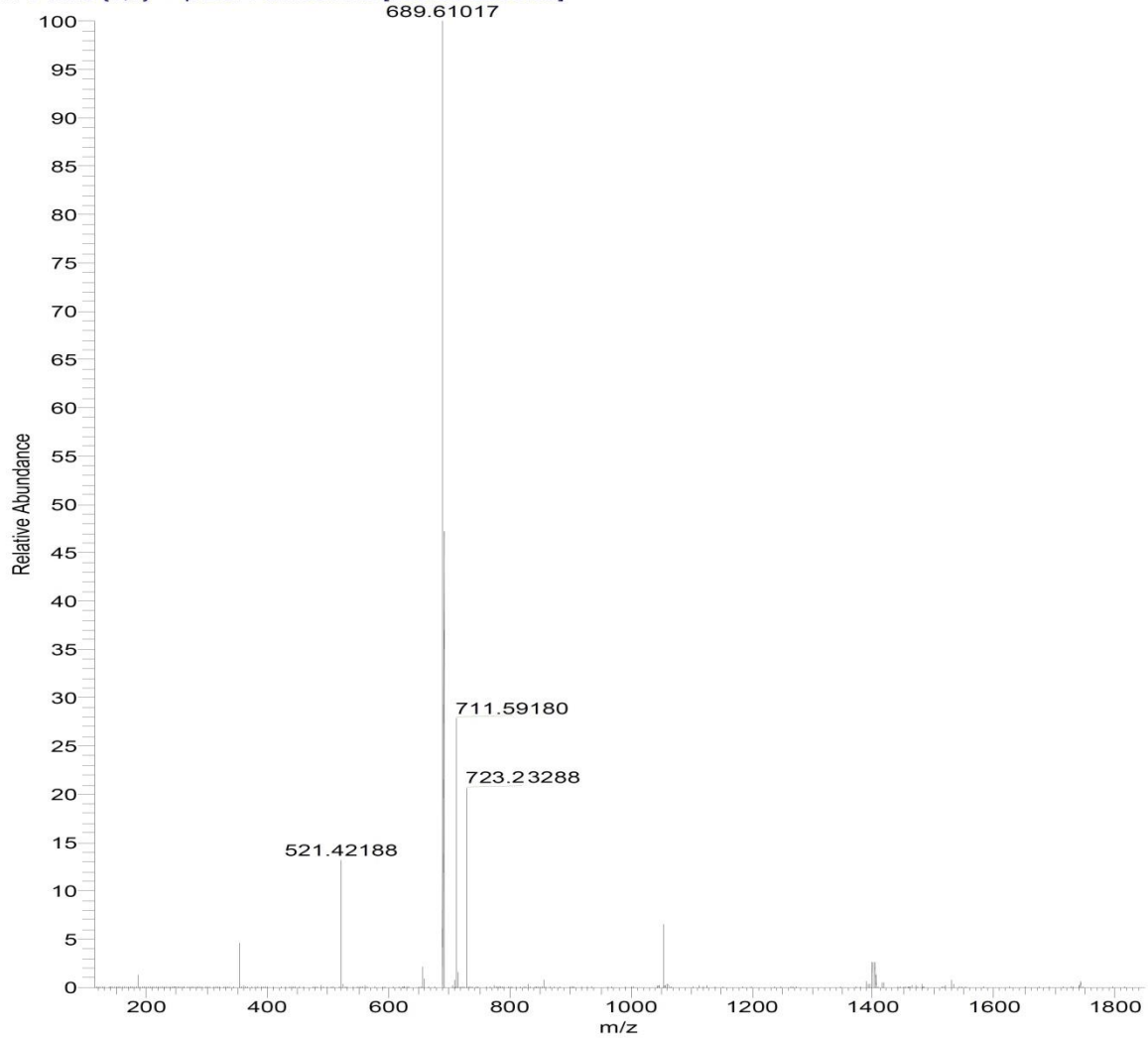


^1H NMR spectrum of **OC1** in DMSOd6



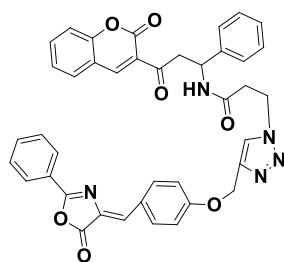
OC1

T: FTMS {1,1} + p ESI Full lock ms [100.00-2000.00]
689.61017

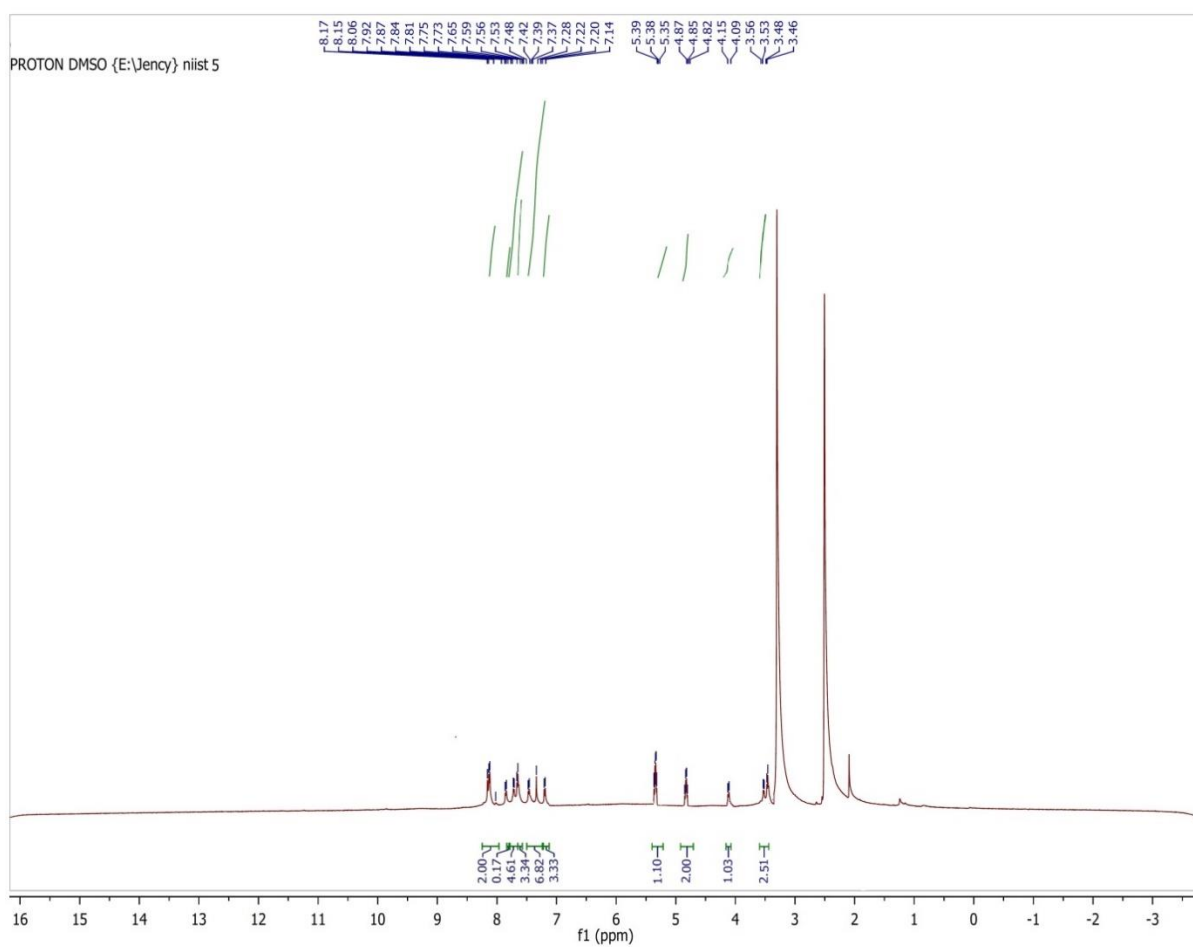


HRMS of OC1

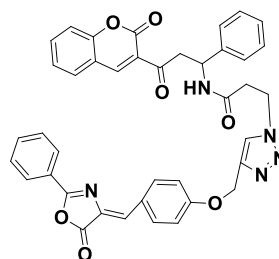




OC2

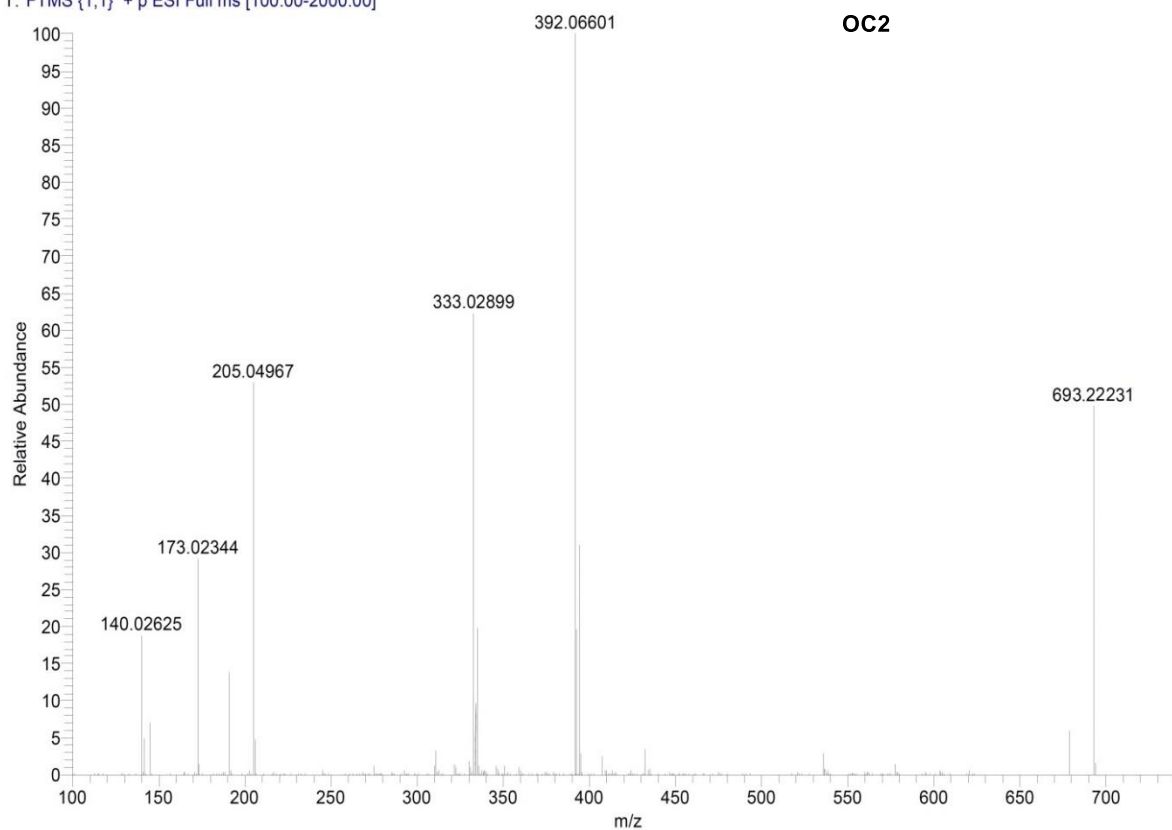


^1H NMR spectrum of **OC2** in DMSO-d₆

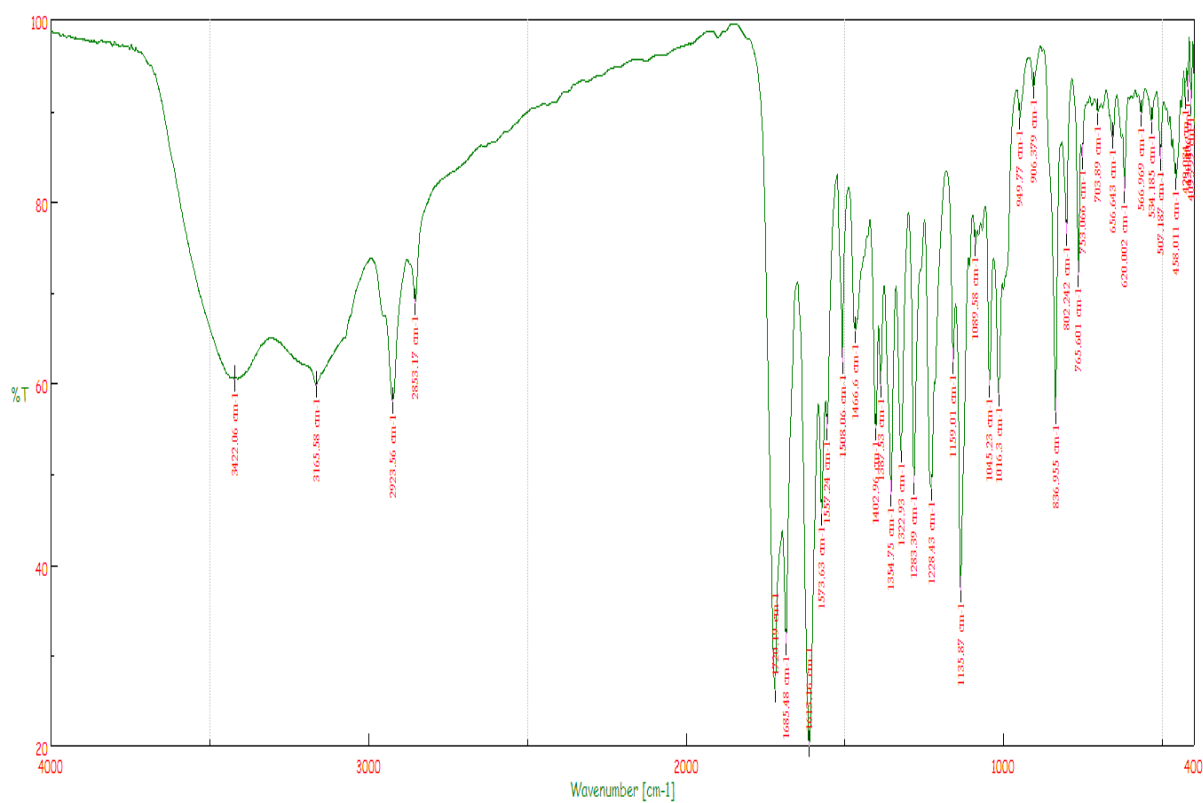
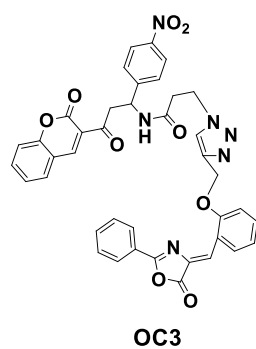


OC2

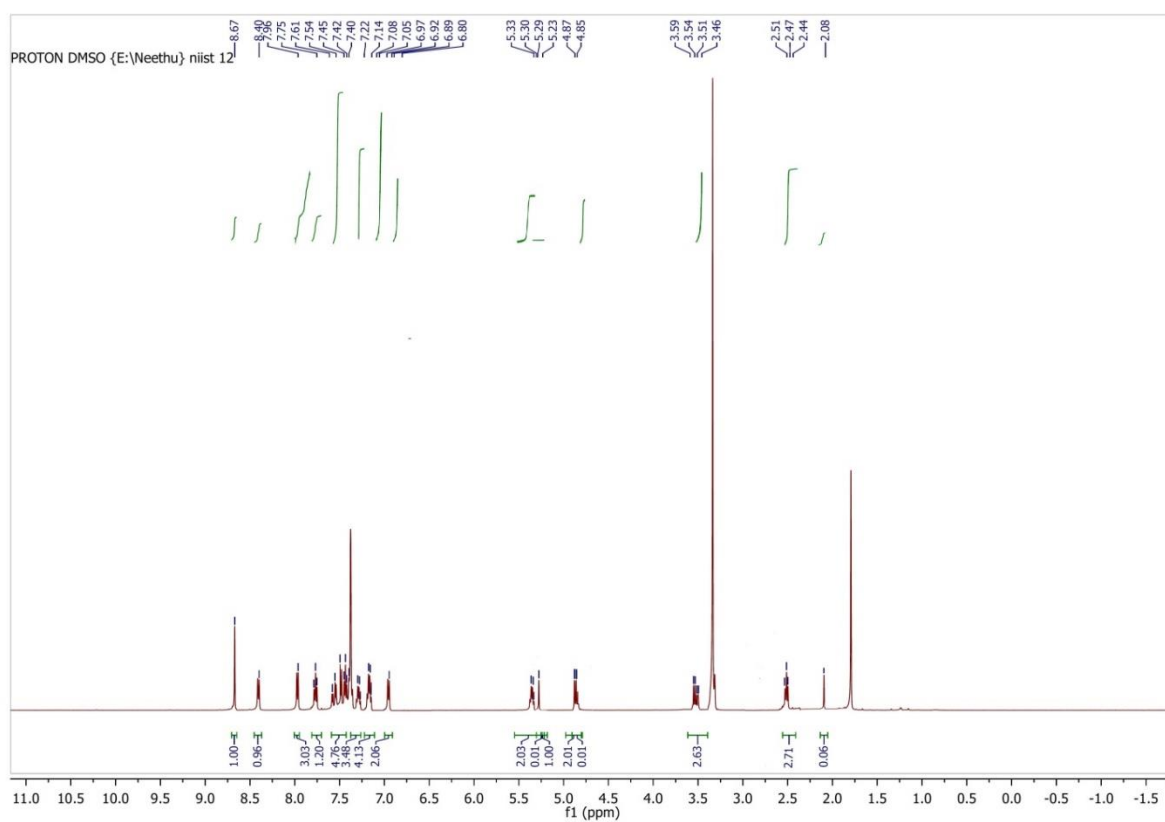
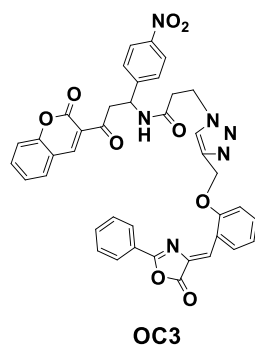
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



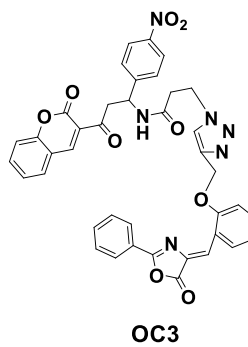
HRMS of **OC2**



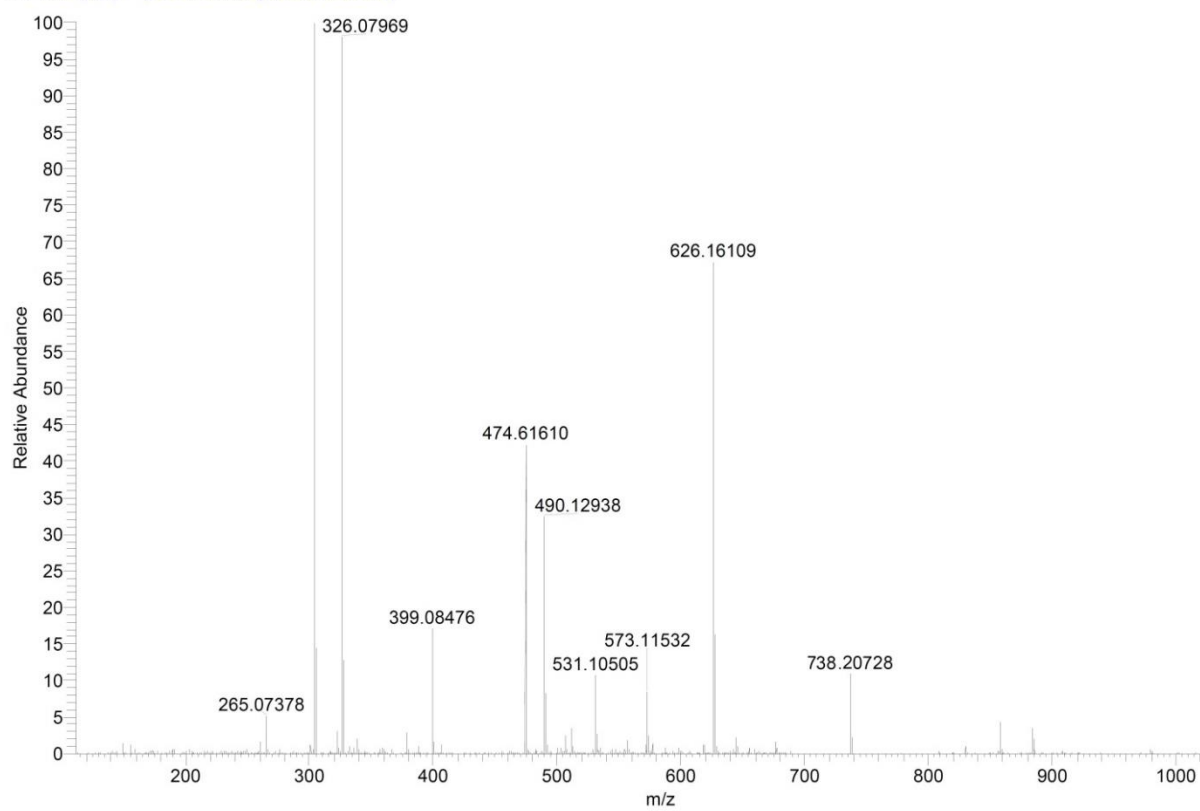
FT-IR Spectrum of OC3



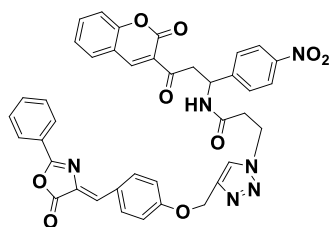
¹H NMR spectrum of **OC3** in DMSOd6



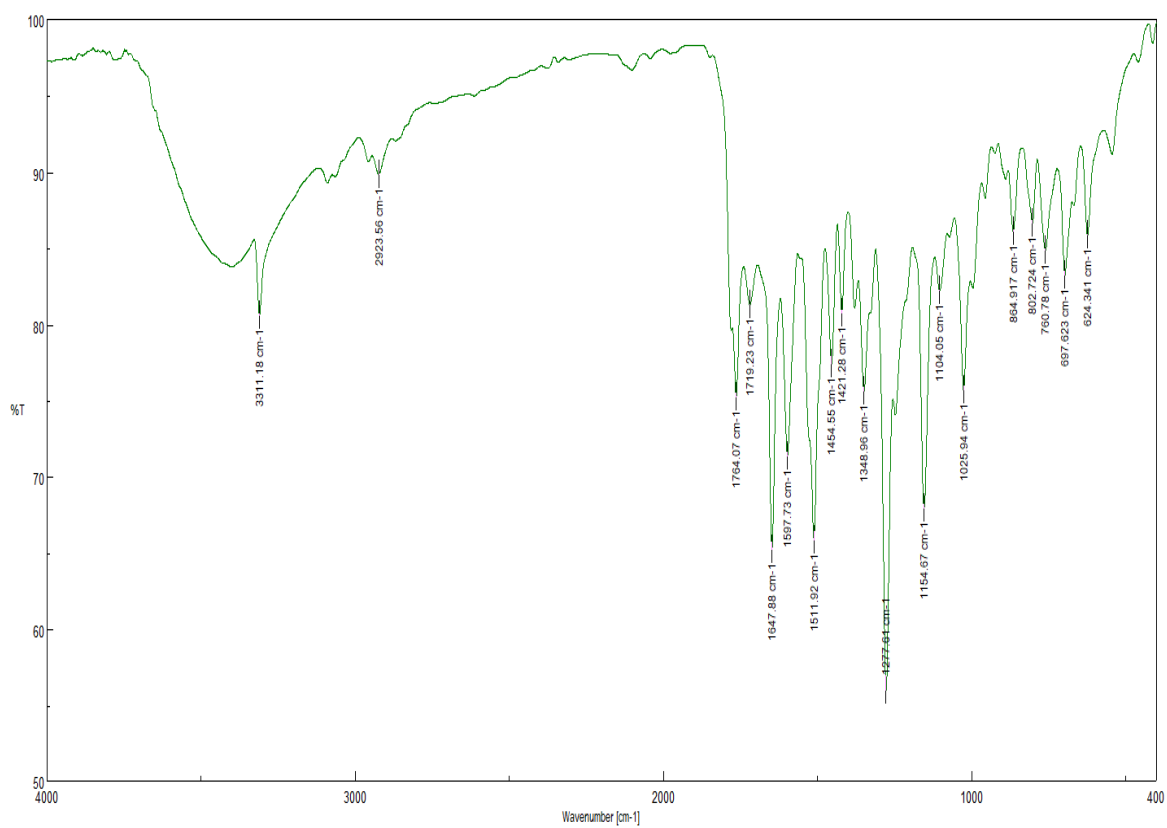
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]



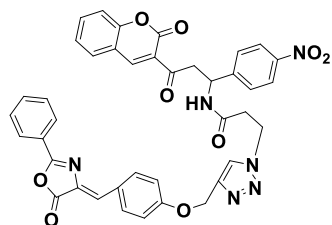
HRMS of **OC3**



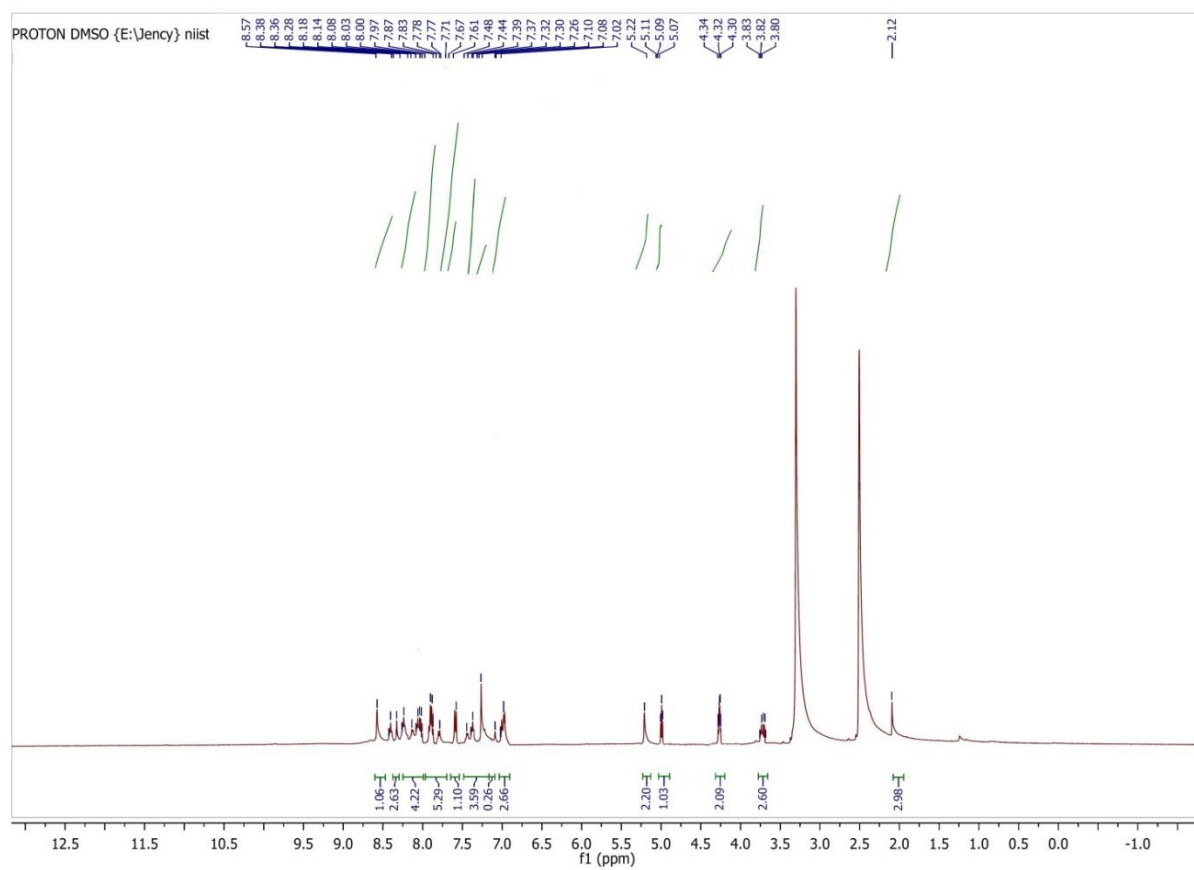
OC4



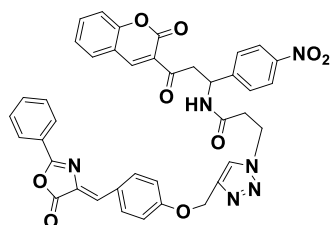
FT-IR Spectrum of OC4



OC4

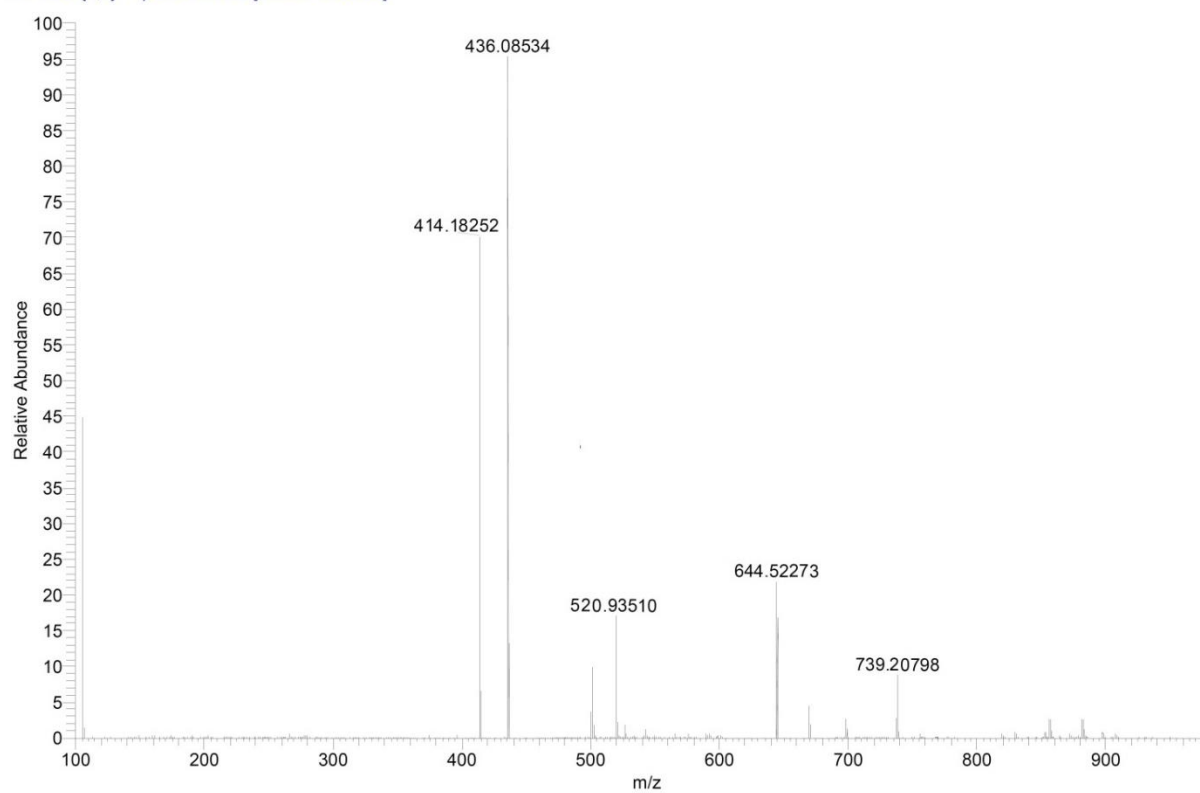


^1H NMR spectrum of **OC4** in DMSO-d₆

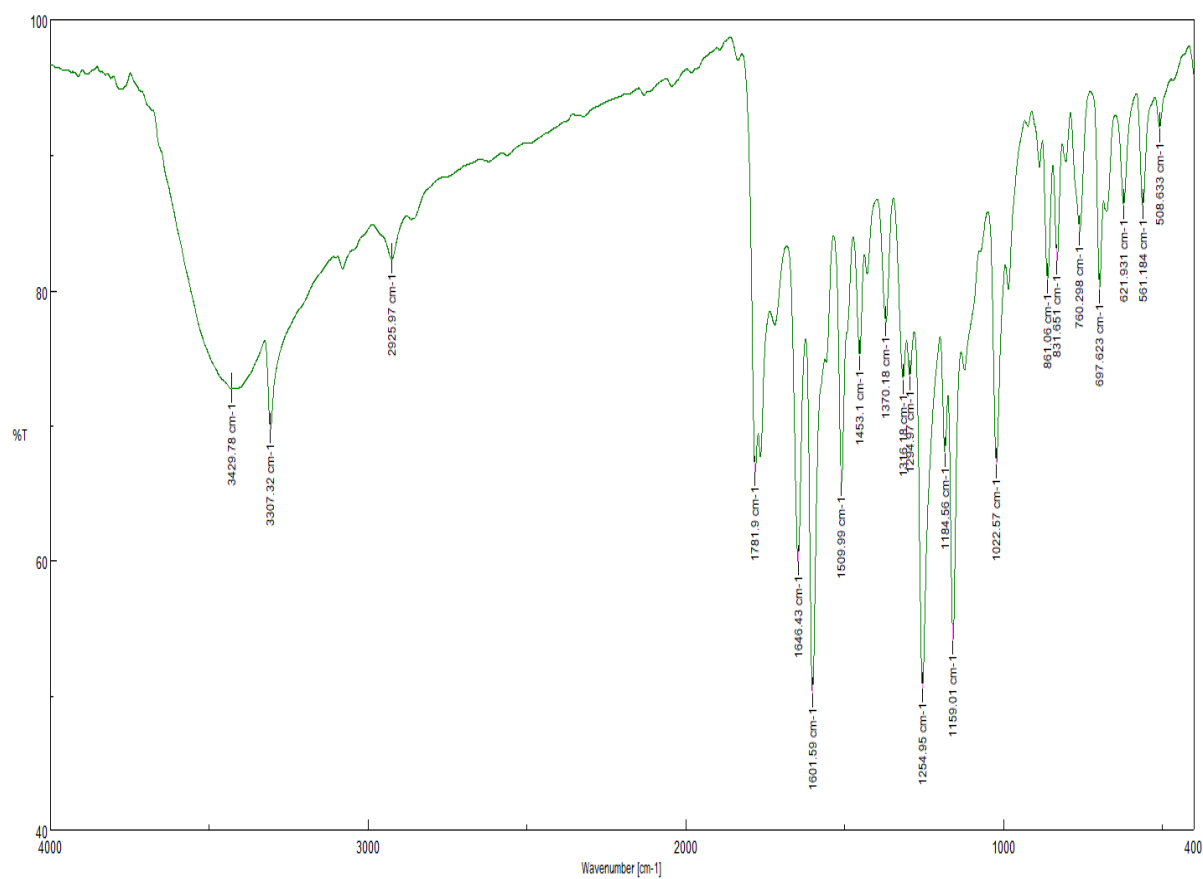
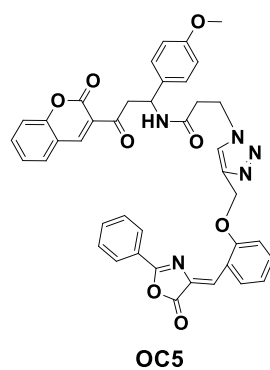


OC4

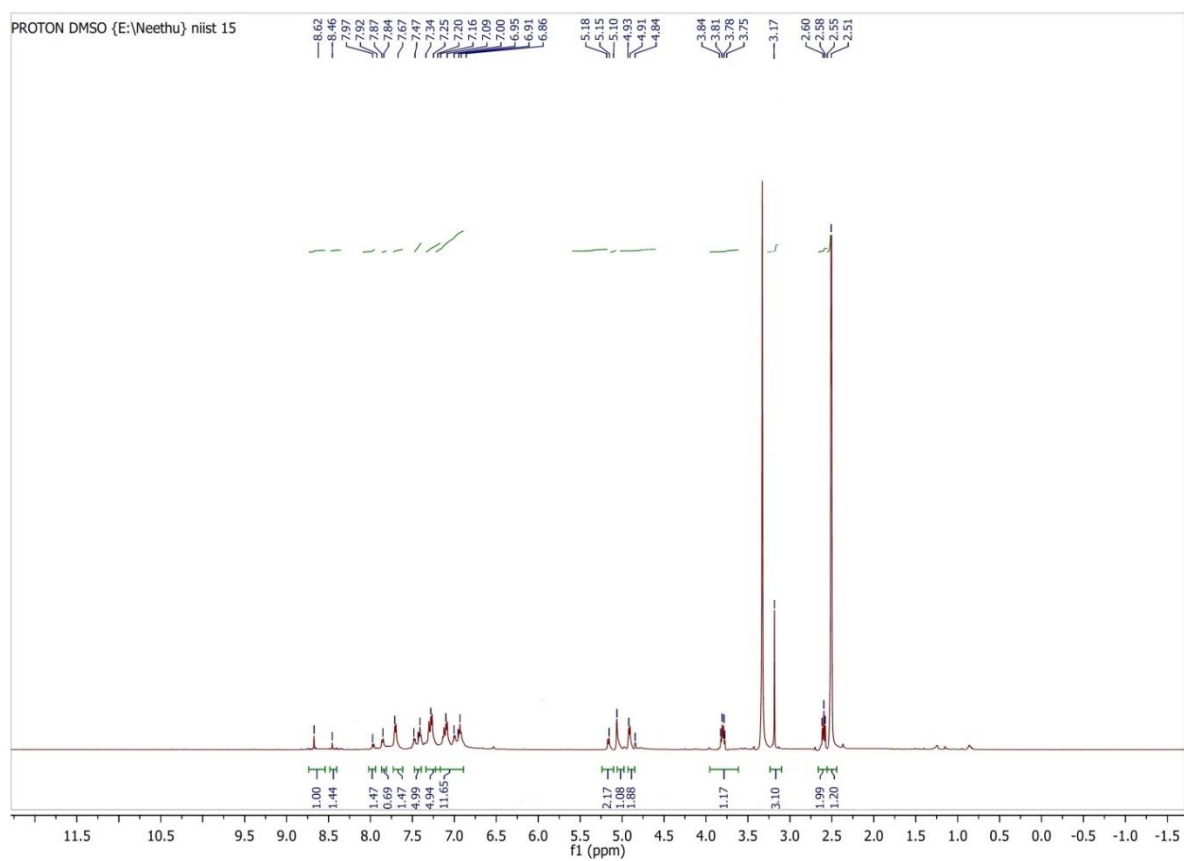
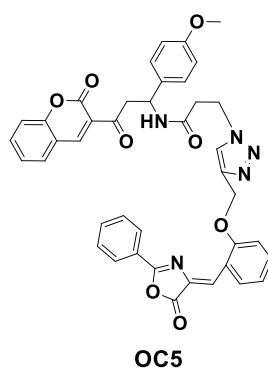
T: FTMS (1,1) + p ESI Full ms [100.00-2000.00]



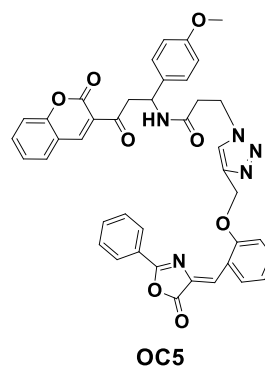
HRMS of OC4



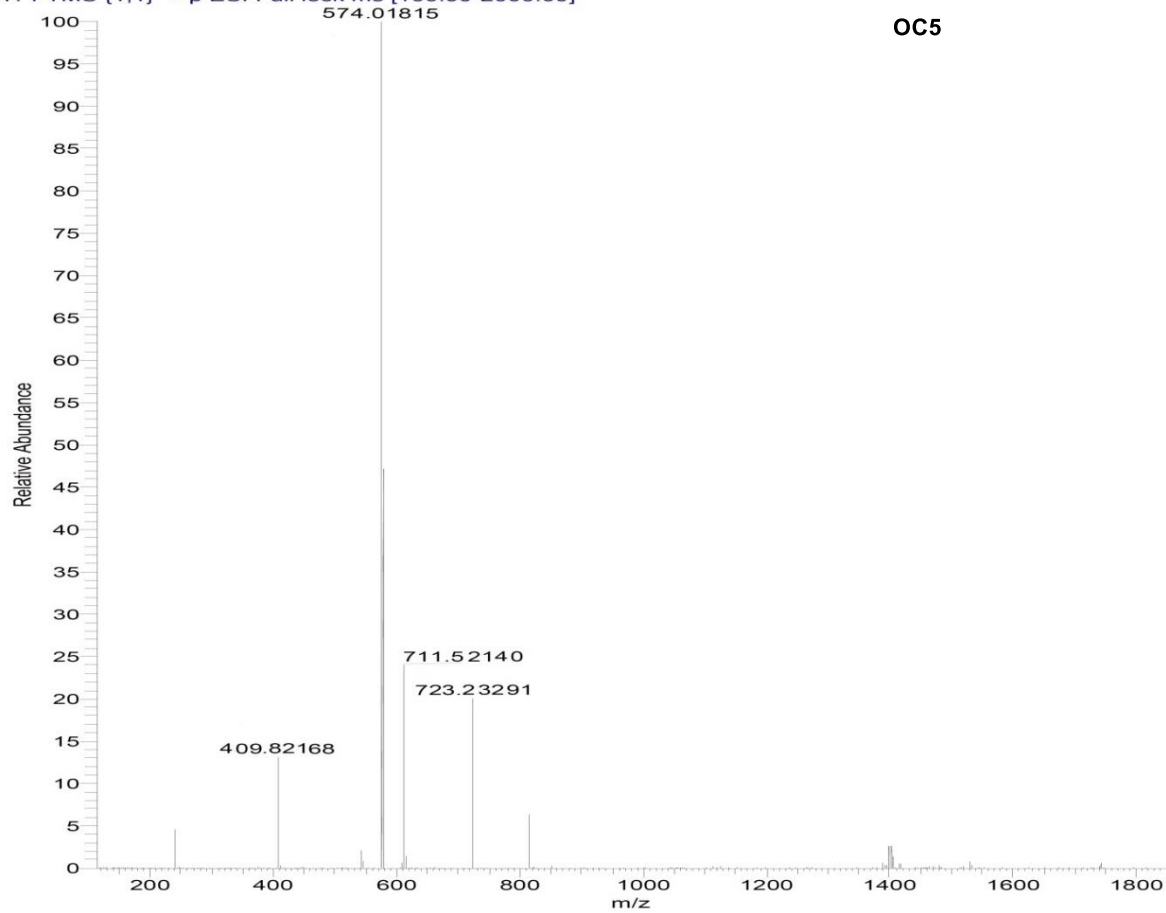
FT-IR Spectrum of OC5



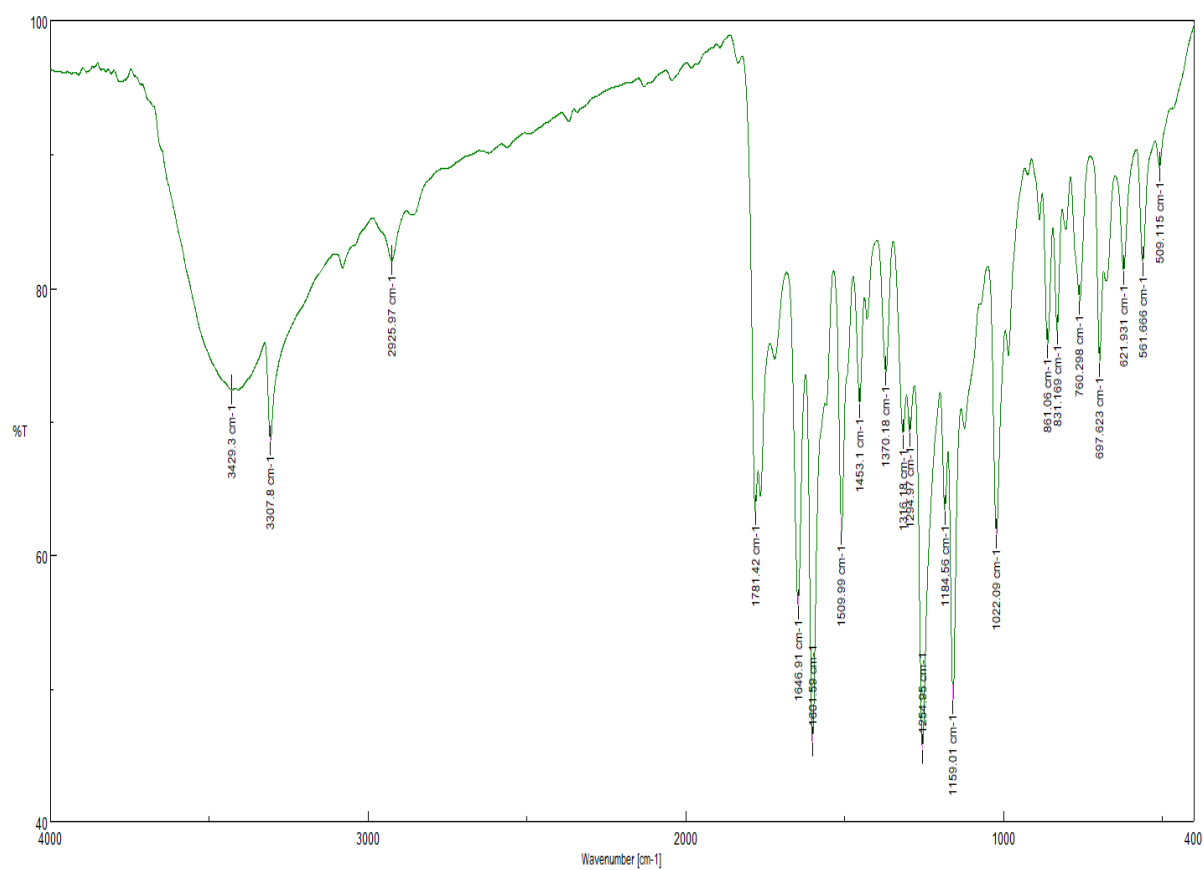
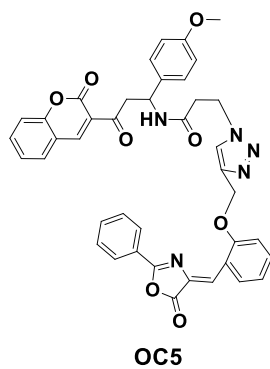
^1H NMR spectrum of **OC5** in DMSOd6



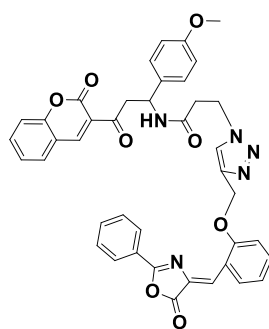
T: FTMS {1,1} + p ESI Full lock ms [100.00-2000.00]
574.01815



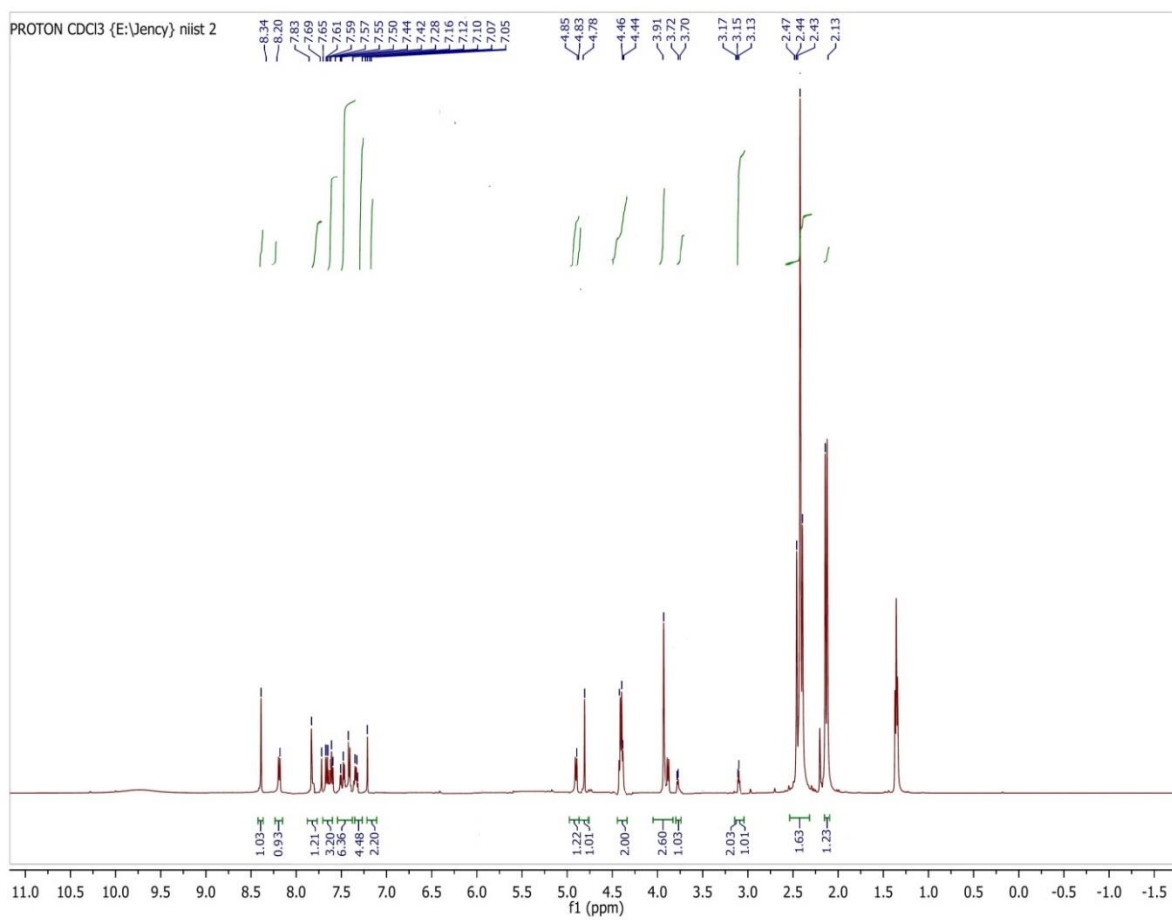
HRMS of **OC5**



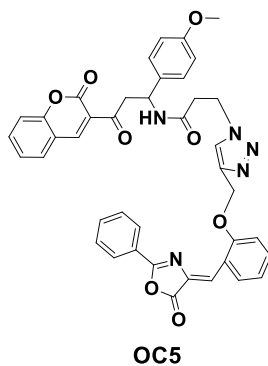
FT-IR Spectrum of OC6



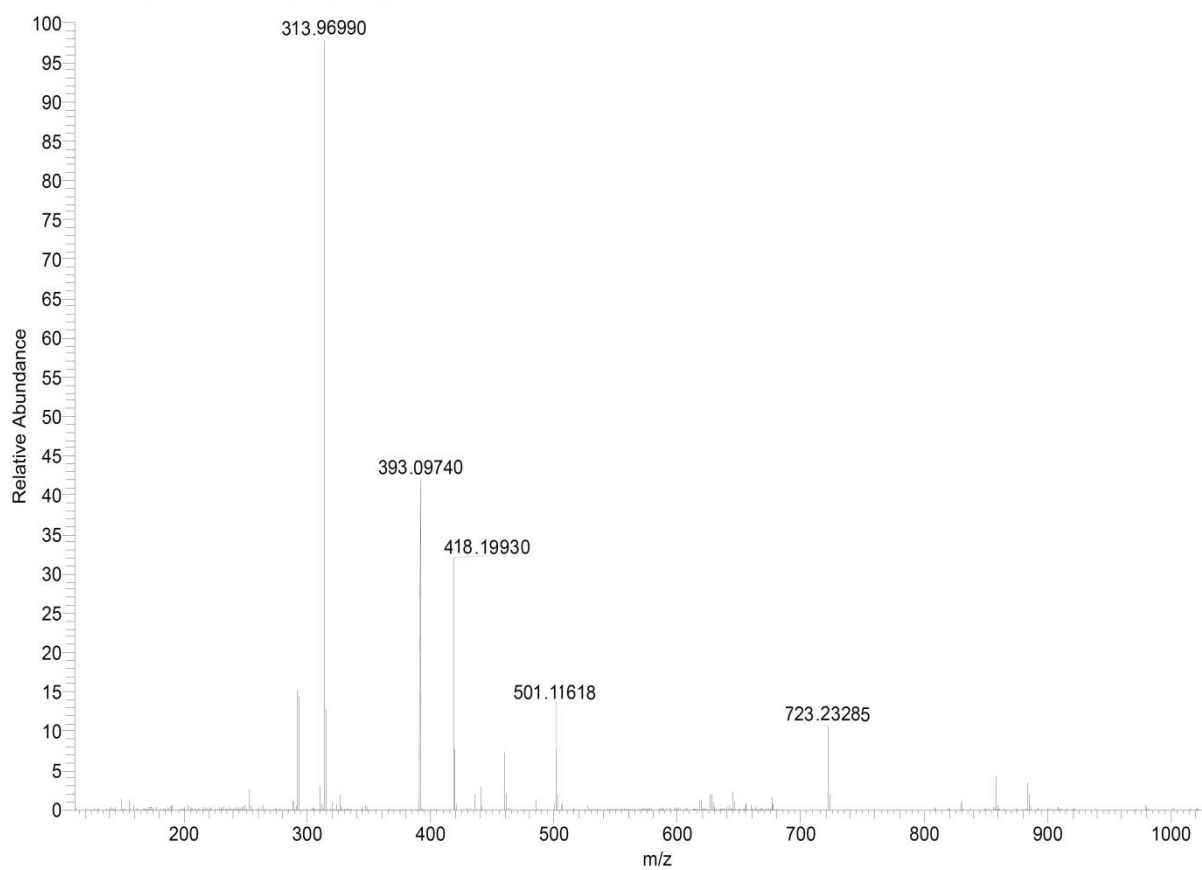
OC5



¹H NMR spectrum of **OC6** in DMSOd₆



T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]



HRMS of OC6

