

## Supplementary Material

### **Facile Synthesis Of Novel Coumarin Derivatives, Antimicrobial analysis, Enzyme Assay, Docking Study, ADMET Prediction And Toxicity Study.**

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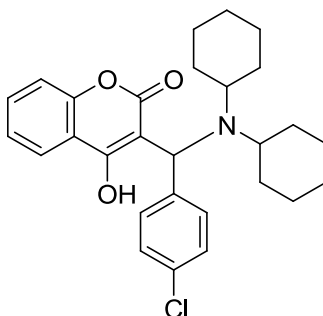
**Table S1** Effect of [Et<sub>3</sub>NH][HSO<sub>4</sub>] catalyst concentration on model reaction **4a**

<b>Entry</b>	<b>[Et<sub>3</sub>NH][HSO<sub>4</sub>] mol%</b>	<b>Time (min)</b>	<b>Yield (%)</b>
1.	No catalyst	90	Trace
2.	5	85	72
3.	10	60	85
4.	15	50	90
5.	20	30	92
6.	25	30	92

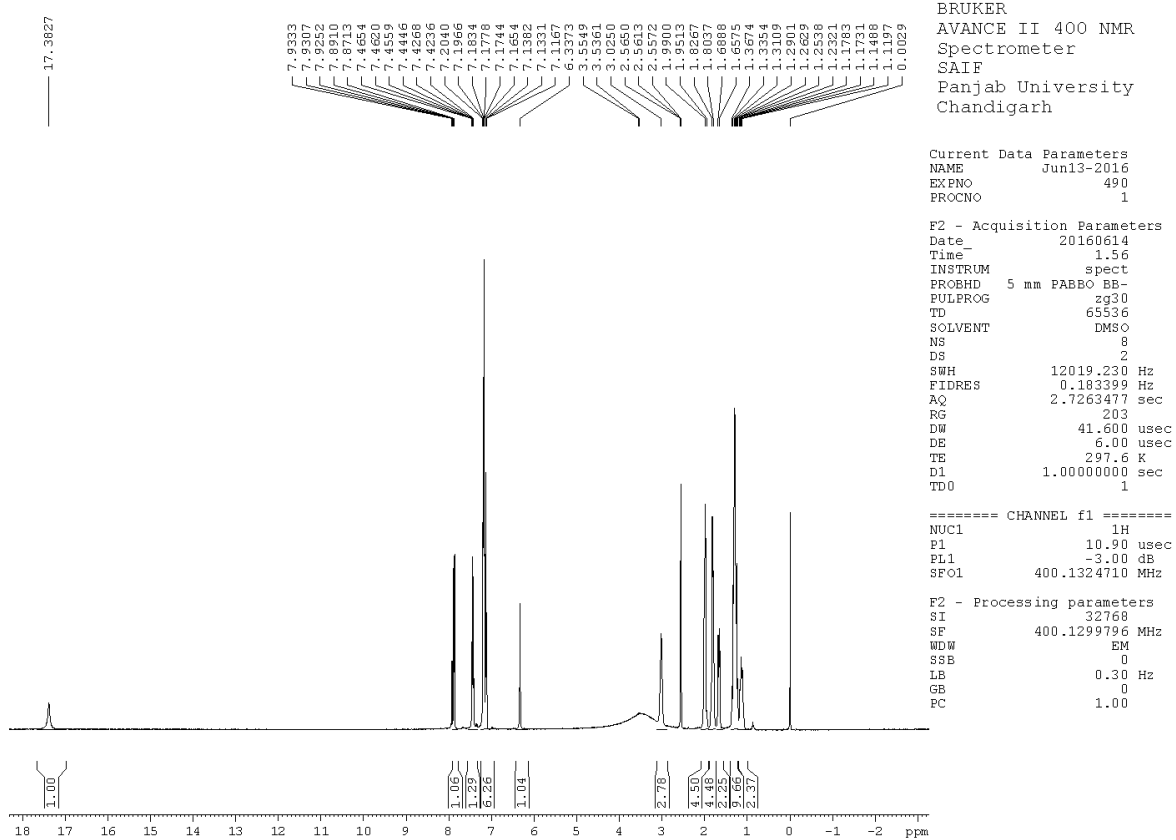
**Table S2** Reusability of [Et<sub>3</sub>NH][HSO<sub>4</sub>] catalyst for model reaction **4a**

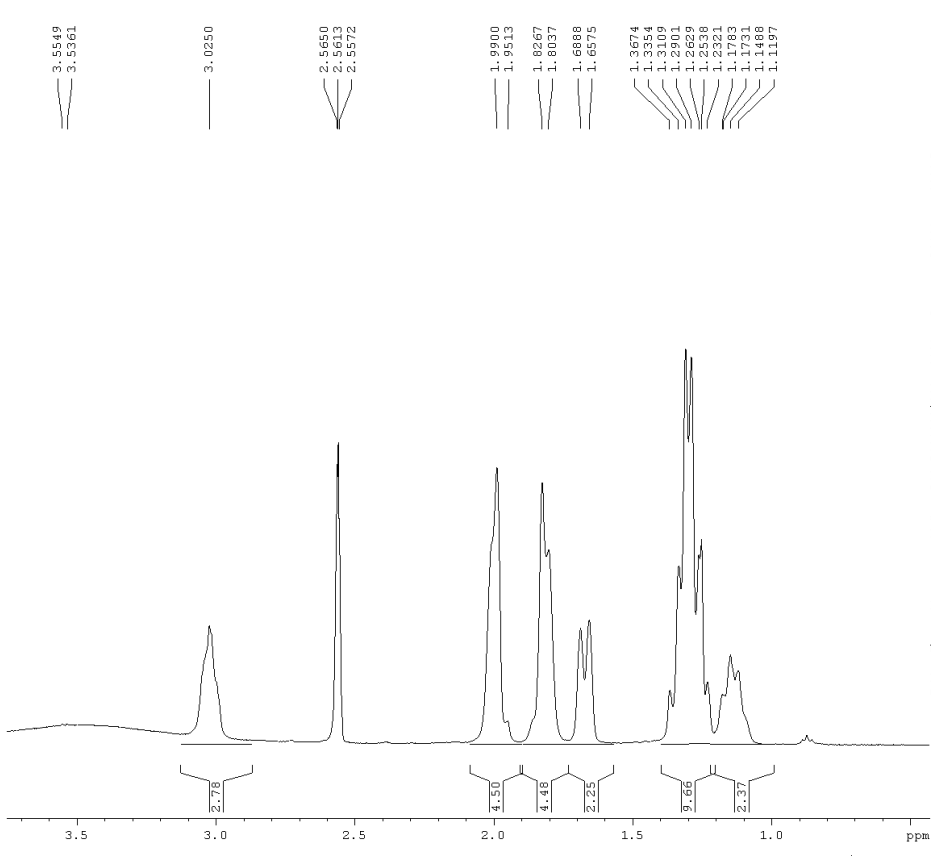
<b>Entry</b>	<b>Run</b>	<b>Time</b>	<b>Yield</b>
1.	1	30	92
2.	2	30	92
3.	3	30	90
4.	4	30	88
5.	5	30	88

<sup>1</sup>H NMR 4b



3-((4-chlorophenyl)(dicyclohexylamino)methyl)-4-hydroxy-2H-chromen-2-one





BRUKER  
 AVANCE II 400 NMR  
 Spectrometer  
 SAIF  
 Panjab University  
 Chandigarh

Current Data Parameters  
 NAME Jun13-2016  
 EXPNO 490  
 PROCNO 1

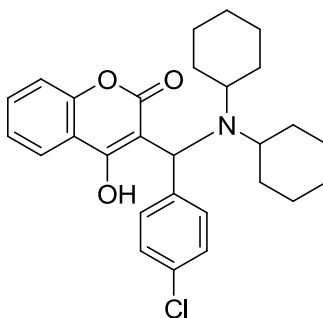
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 SOLVENT DMSO  
 NS 8  
 DS 2  
 SMH 12019.230 Hz  
 FIDRES 0.183399 Hz  
 AQ 2.7263477 sec  
 RG 203  
 DW 41.600 usec  
 DE 6.00 usec  
 TE 297.6 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
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 P1 10.90 usec  
 PL1 -3.00 dB  
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F2 - Processing parameters  
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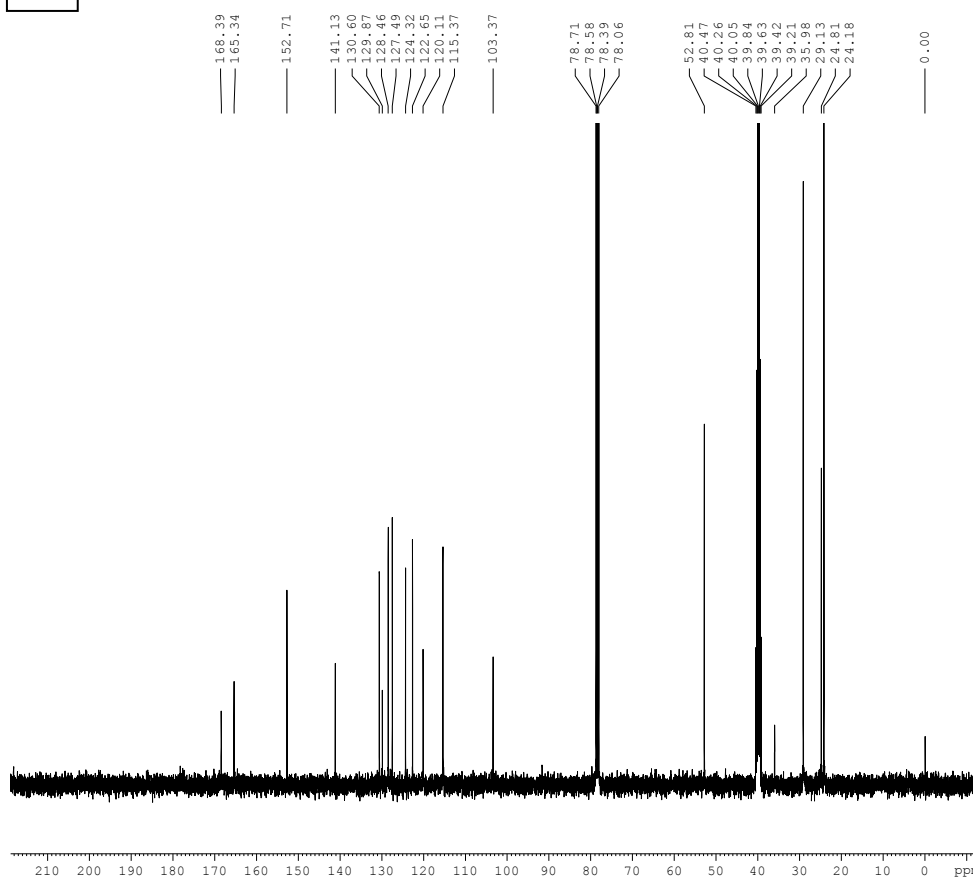
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<sup>13</sup>CNMR 4b



3-((4-chlorophenyl)(dicyclohexylamino)methyl)-4-hydroxy-2H-chromen-2-one

4b



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AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

Current Data Parameters  
NAME Jun13-2016  
EXPNO 491  
PROCNO 1  
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FIDRES 0.454131 Hz  
AQ 1.1010548 sec  
RG 2050  
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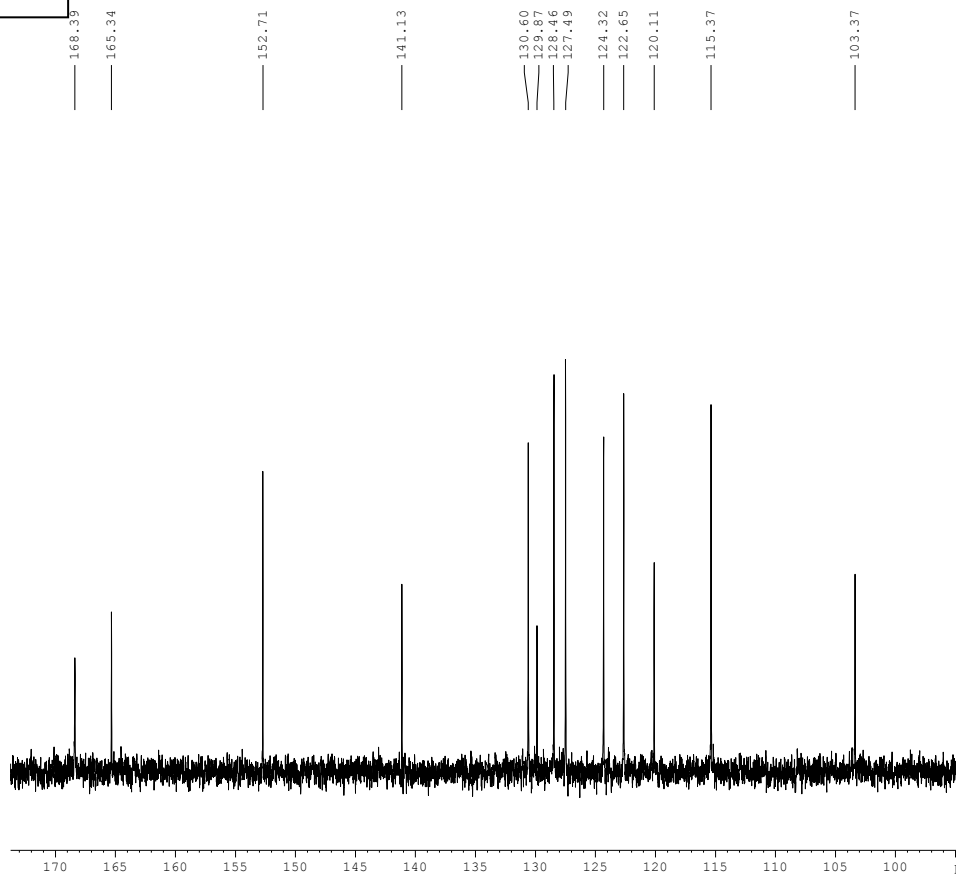
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NUC2 1H  
PCPD2 80.00 usec  
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PL12 14.31 dB  
PL13 18.00 dB  
SFO2 400.1316005 MHz

F2 - Processing parameters  
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SF 100.6127961 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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4b



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Spectrometer  
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Chandigarh

```
Current Data Parameters
NAME      Jun13-2016
EXPNO     491
PROCNO    1

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NS        512
DS        4
SWH       29761.904 Hz
FIDRES    0.454131 Hz
AQ        1.1010548 sec
RG        2050
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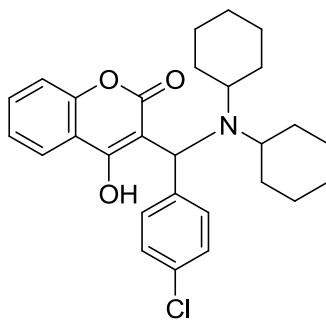
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SFO1     100.6228298 MHz

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NUC2      1H
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PL13      18.00 dB
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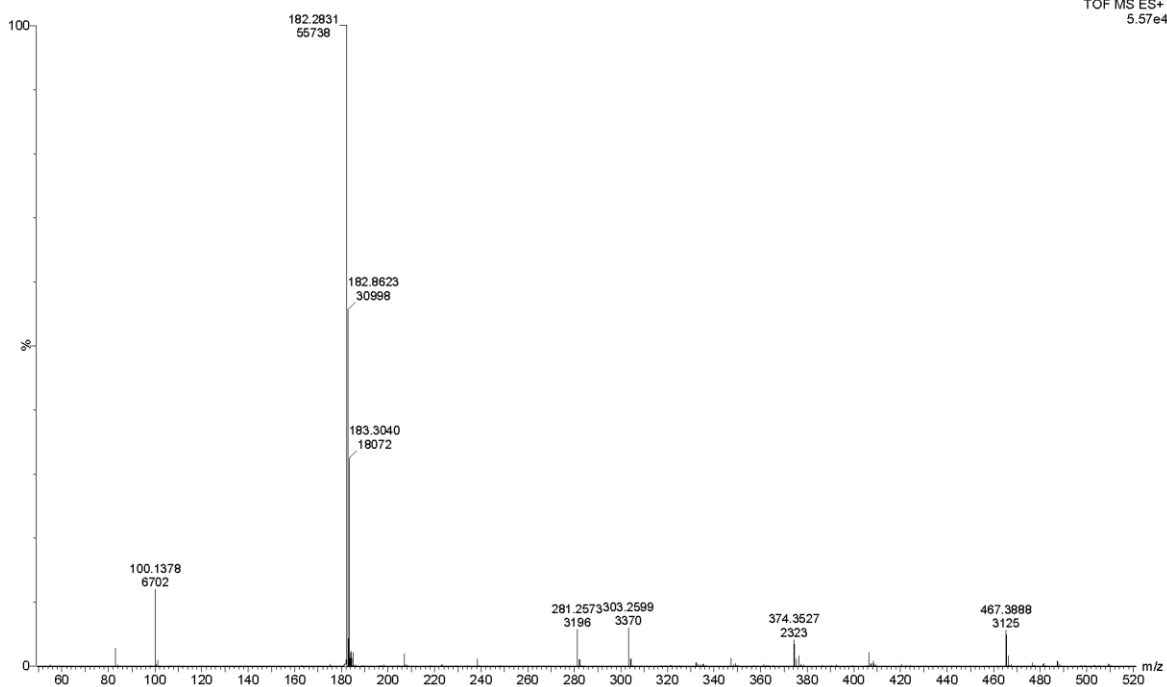
# Mass spectra of **4b**



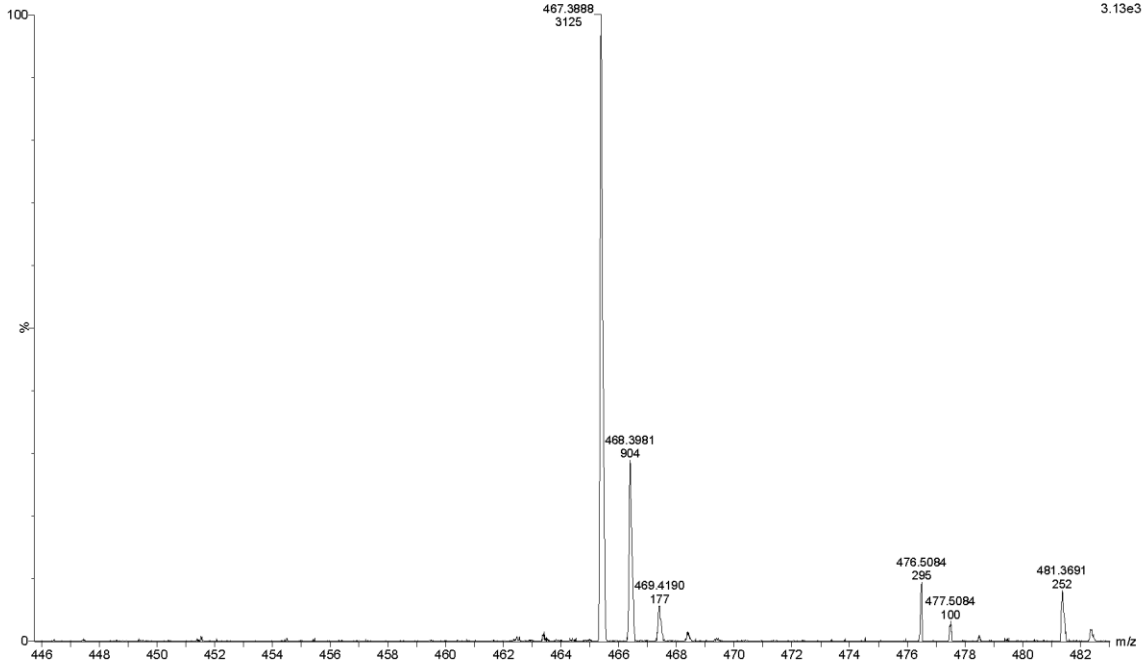
3-((4-chlorophenyl)(dicyclohexylamino)methyl)-4-hydroxy-2*H*-chromen-2-one

WATERS, Q-TOF MICROMASS (ESI-MS)

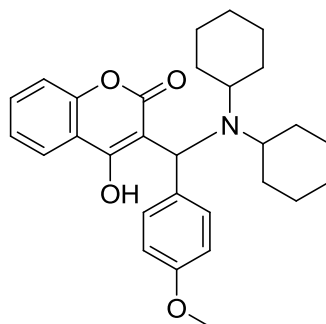
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TOF MS ES+  
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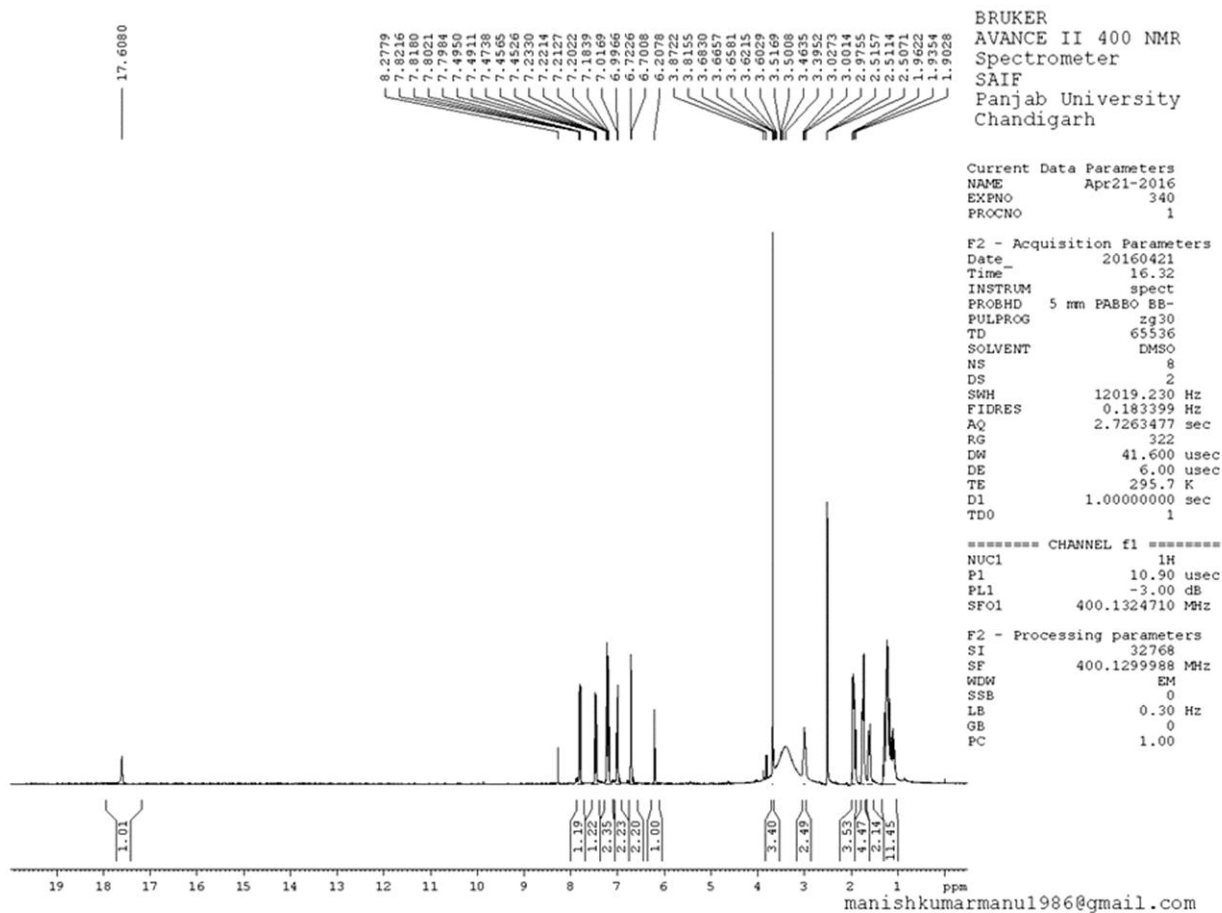


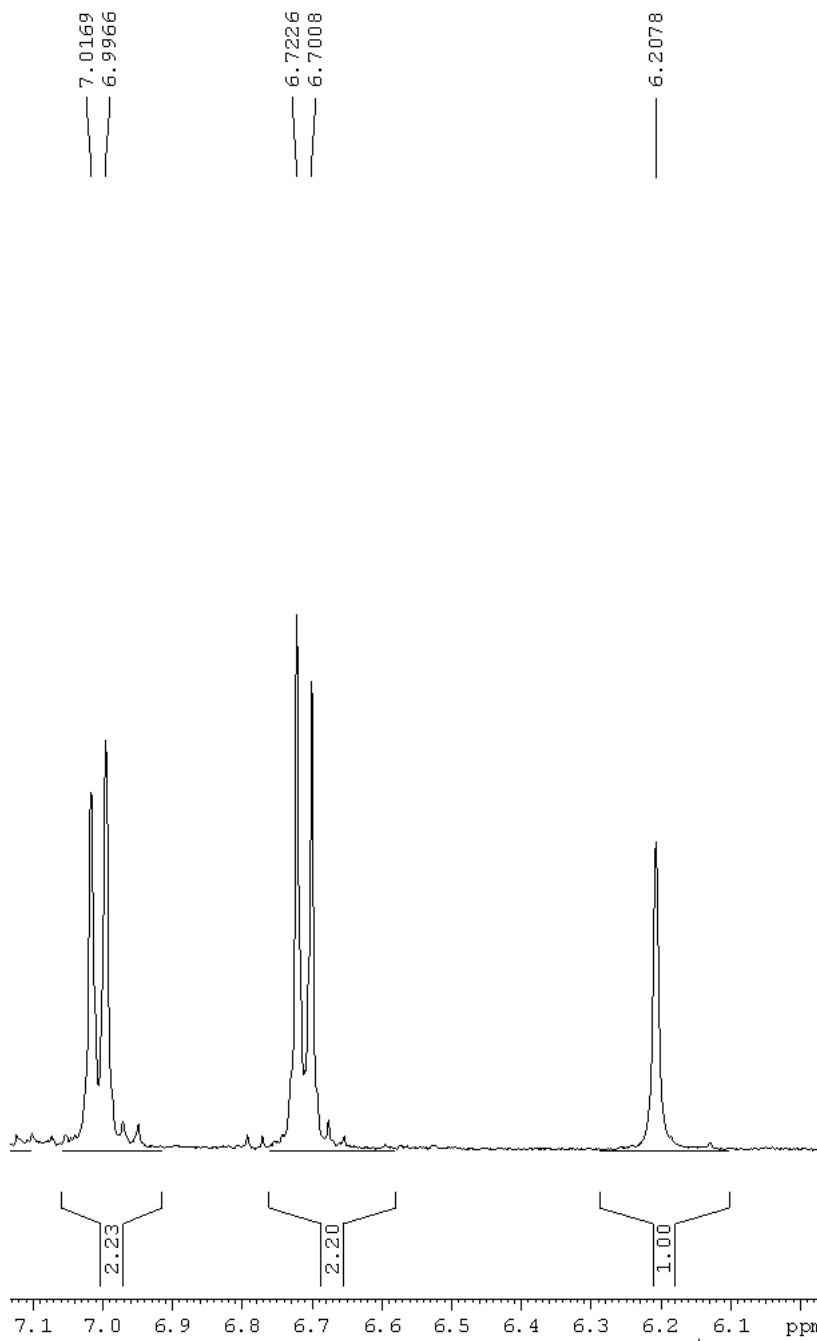


<sup>1</sup>H NMR of 4f



3-((Dicyclohexylamino)(4-methoxyphenyl)methyl)-4-hydroxy-2H-chromen-2-one





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 Spectrometer  
 SAIF  
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 Chandigarh

Current Data Parameters  
 NAME Apr21-2016  
 EXPNO 340  
 PROCNO 1

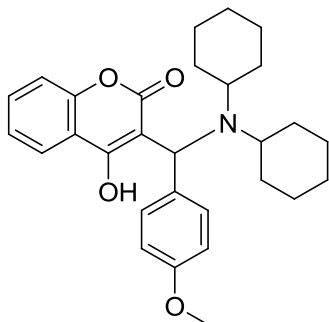
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 FIDRES 0.183399 Hz  
 AQ 2.7263477 sec  
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 TE 295.7 K  
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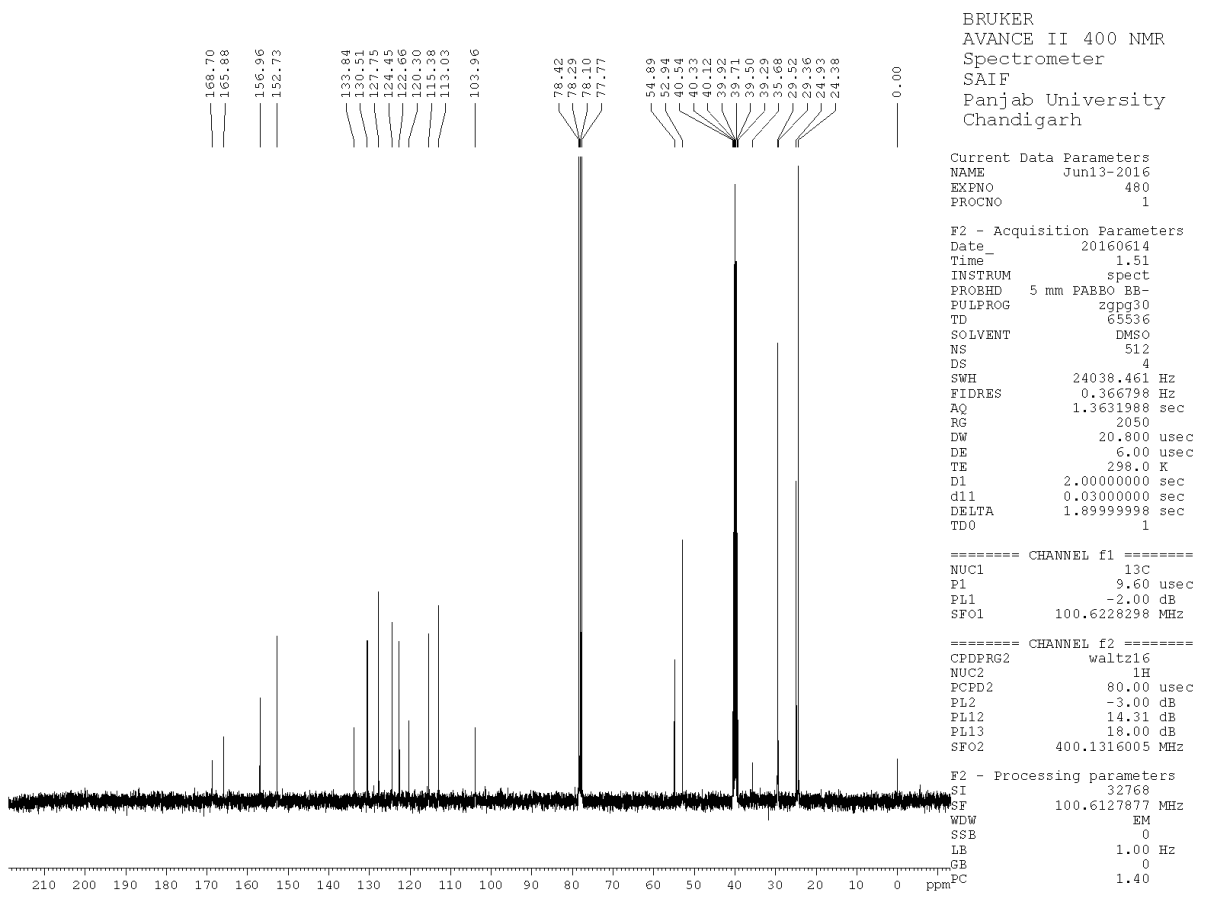
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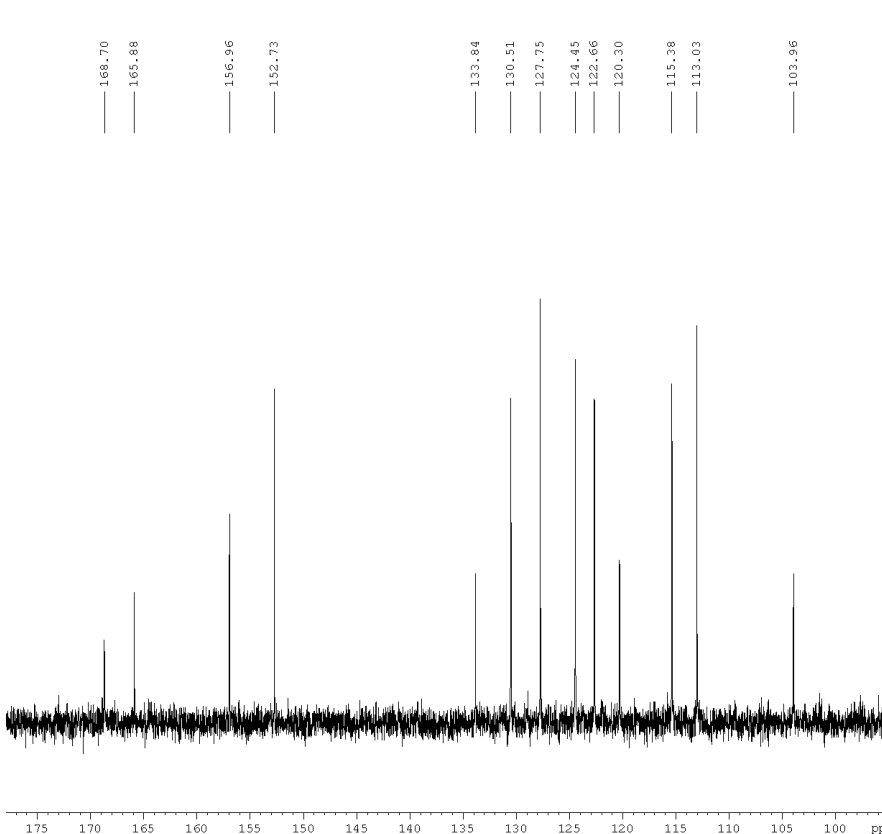
<sup>13</sup>CNMR of 4f



3-((Dicyclohexylamino)(4-methoxyphenyl)methyl)-4-hydroxy-2H-chromen-2-one



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Current Data Parameters  
 NAME Jun13-2016  
 EXPNO 480  
 PROCNO 1

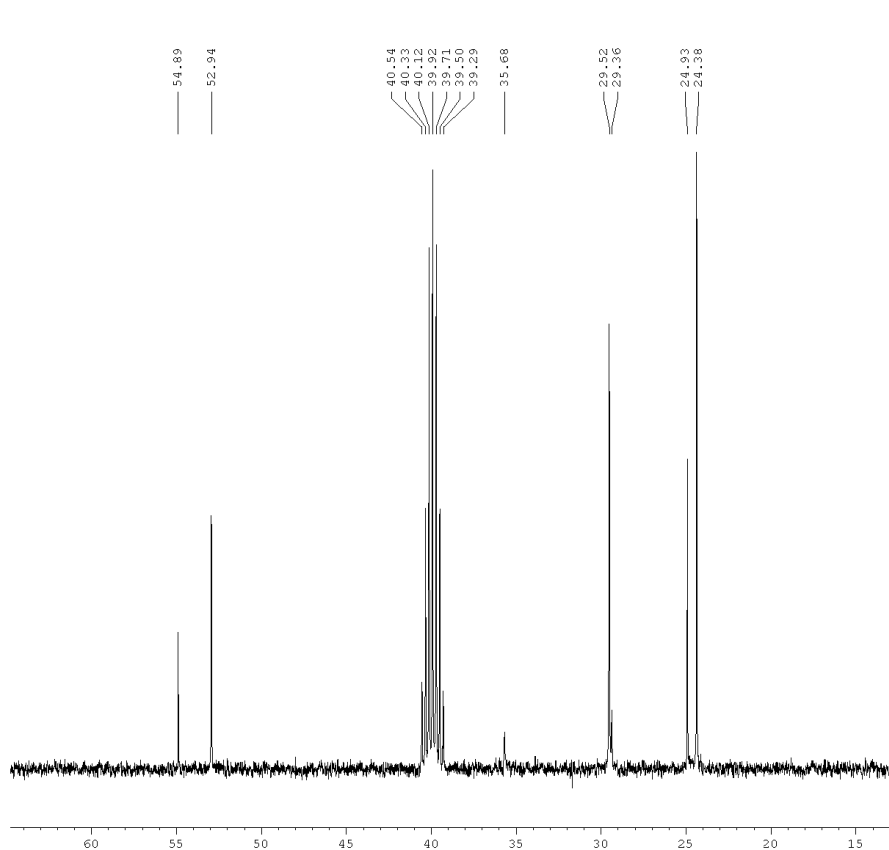
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 PL1 -2.00 dB  
 SFO1 100.6228298 MHz

==== CHANNEL f2 =====  
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 NUC2 1H  
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 PL2 -3.00 dB  
 PL12 14.31 dB  
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 AVANCE II 400 NMR  
 Spectrometer  
 SAIF  
 Panjab University  
 Chandigarh

Current Data Parameters  
 NAME Jun13-2016  
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 FIDRES 0.366798 Hz  
 AQ 1.3631988 sec  
 RG 2050  
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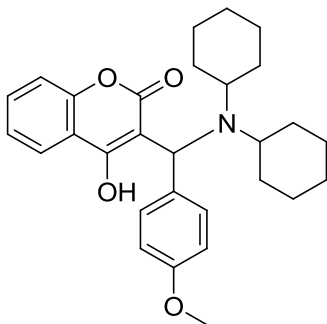
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===== CHANNEL f2 =====  
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 NUC2 1H  
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 PL13 18.00 dB  
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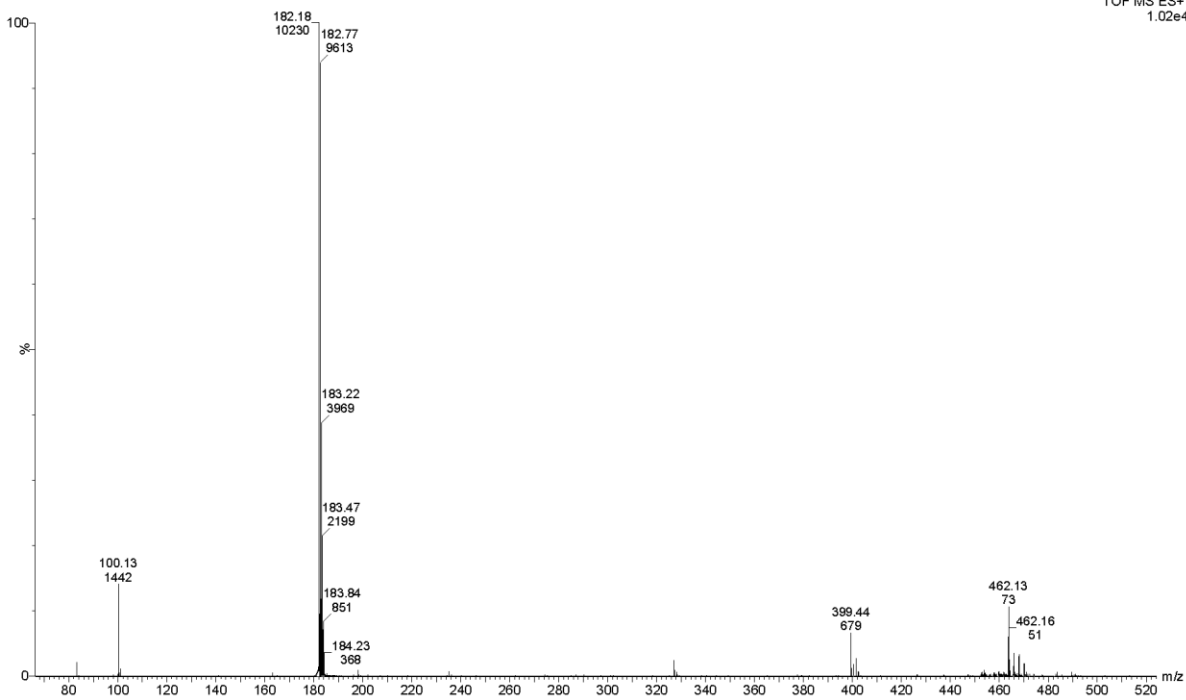
# Mass spectra of **4f**

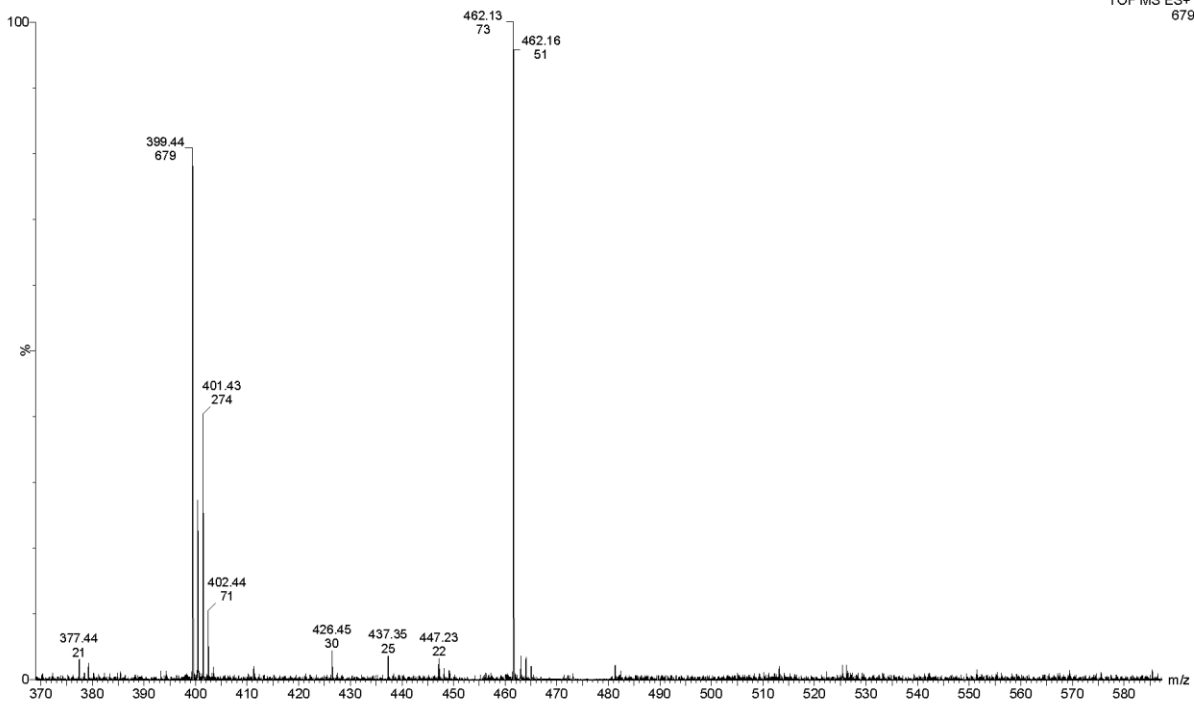


3-((Dicyclohexylamino)(4-methoxyphenyl)methyl)-4-hydroxy-2H-chromen-2-one

WATERS, Q-TOF MICROMASS (ESI-MS)

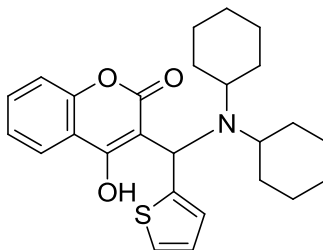
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TOF MS ES+  
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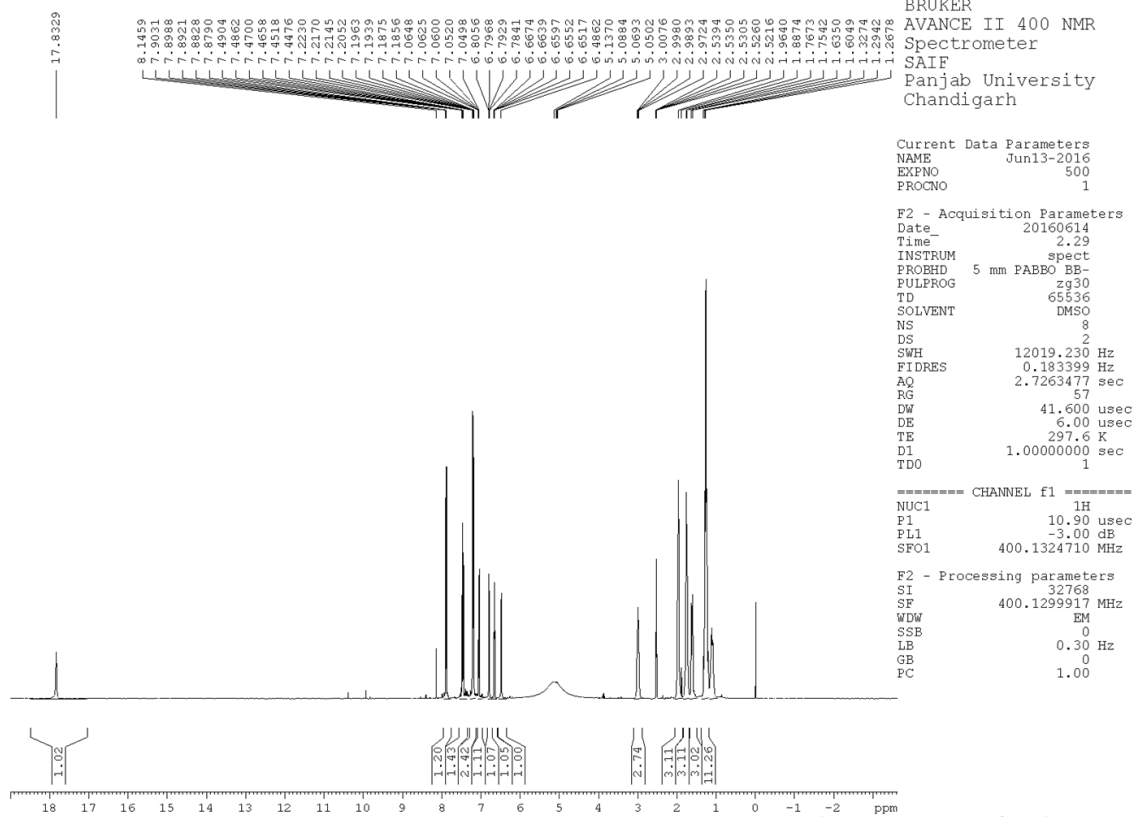


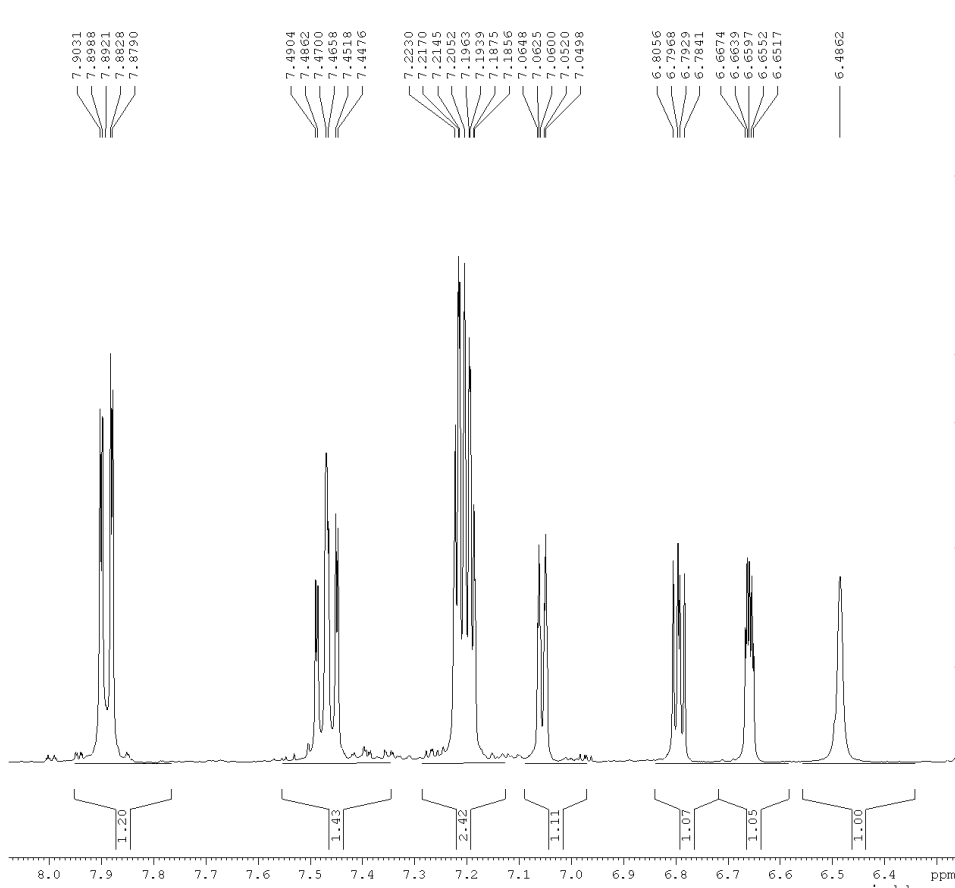


<sup>1</sup>H NMR 4n



3-((Dicyclohexylamino)(thiophen-2-yl)methyl)-4-hydroxy-2H-chromen-2-one





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 AVANCE II 400 NMR  
 Spectrometer  
 SAIF  
 Panjab University  
 Chandigarh

Current Data Parameters  
 NAME Jun13-2016  
 EXPNO 500  
 PROCNO 1

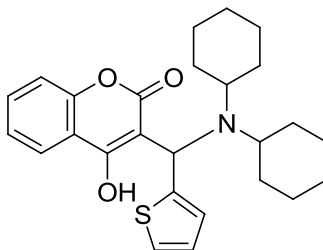
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 FIDRES 0.183399 Hz  
 AQ 2.7263477 sec  
 RG 57  
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 DE 6.00 usec  
 TE 297.6 K  
 D1 1.00000000 sec  
 TDO 1

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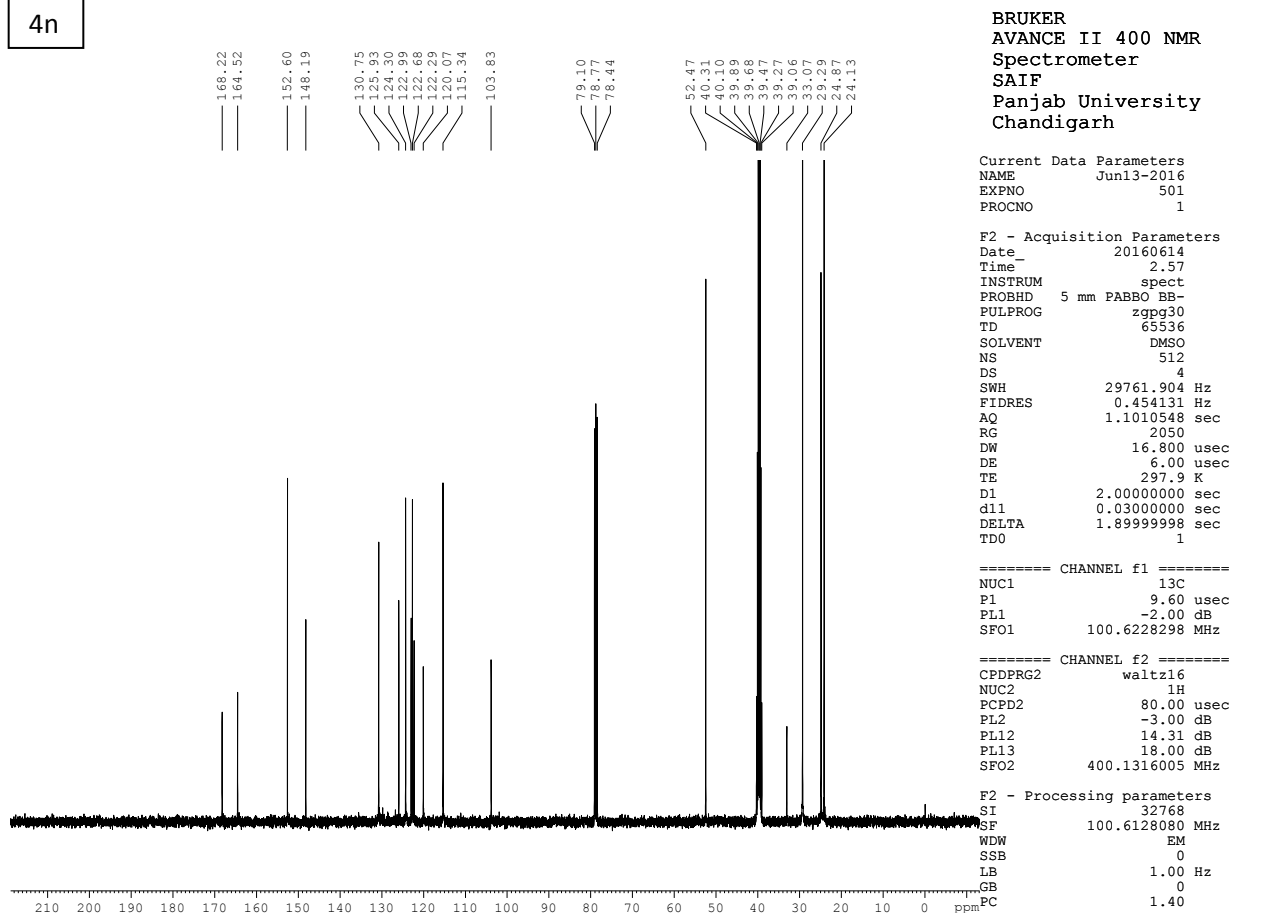
manishkumarmanu1986@gmail.com

<sup>13</sup>CNMR 4n



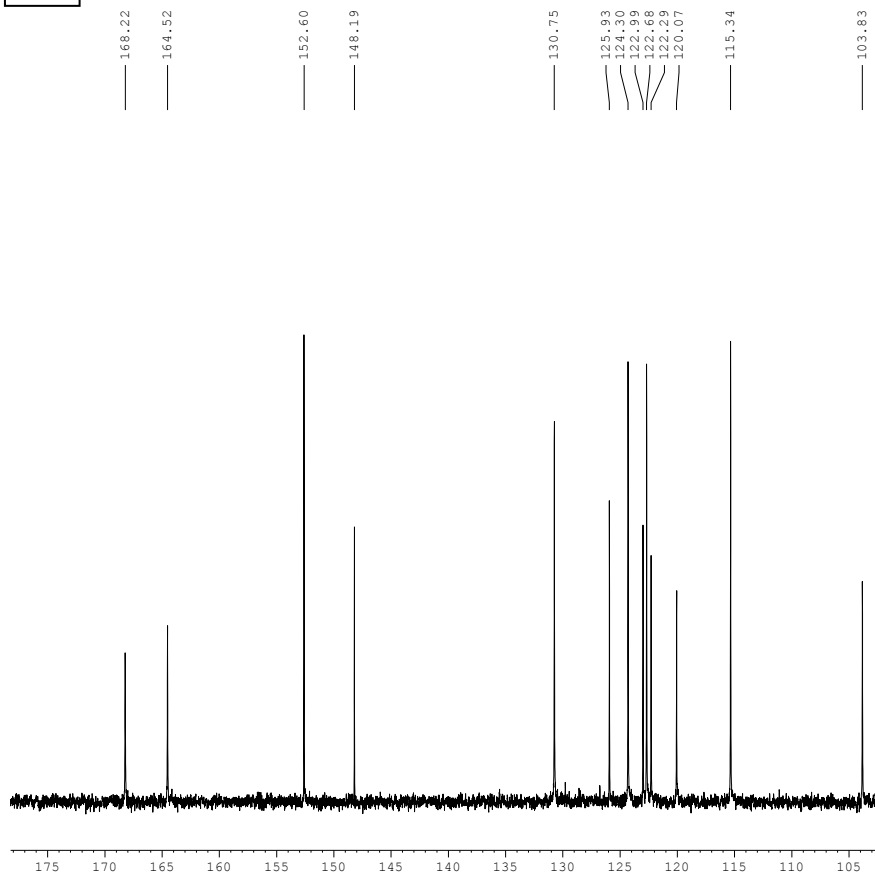
3-((Dicyclohexylamino)(thiophen-2-yl)methyl)-4-hydroxy-2H-chromen-2-one

4n



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4n



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AVANCE II 400 NMR  
Spectrometer  
SAIF  
Panjab University  
Chandigarh

Current Data Parameters  
NAME Jun13-2016  
EXPNO 501  
PROCNO 1

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SWH 29761.904 Hz  
FIDRES 0.454131 Hz  
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RG 2050  
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TE 297.9 K  
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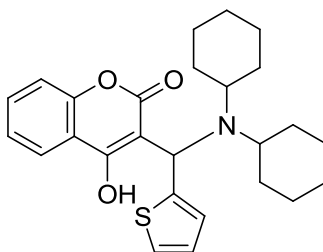
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NUC1 13C  
P1 9.60 usec  
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SFO1 100.6228298 MHz

===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -3.00 dB  
PL12 14.31 dB  
PL13 18.00 dB  
SFO2 400.1316005 MHz

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SI 32768  
SF 100.6128080 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

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# Mass spectra of **4n**



3-((Dicyclohexylamino)(thiophen-2-yl)methyl)-4-hydroxy-2H-chromen-2-one

WATERS, Q-TOF MICROMASS (ESI-MS)

SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH  
TOF MS ES+  
1.85e4

