

## Supplementary Information

### Isatin-Based Benzyloxybenzene Derivatives as Monoamine Oxidase Inhibitors with Neuroprotective Effect Targeting Neurodegenerative Disease Treatment

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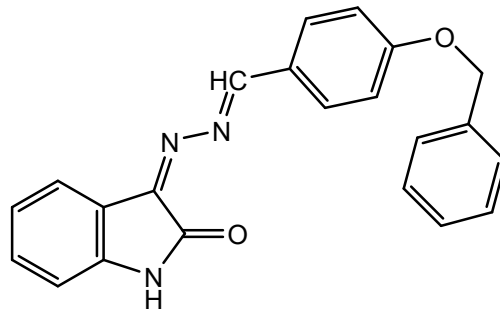
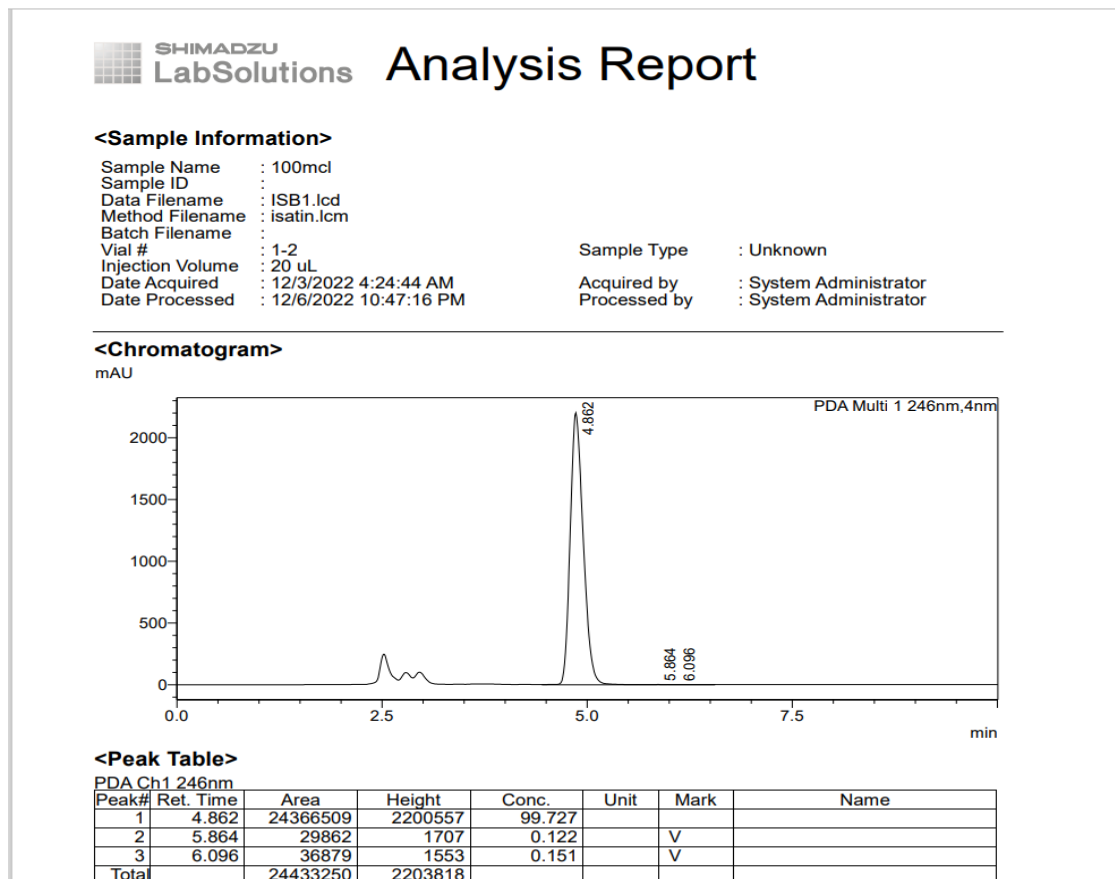


Figure S1. ISB1 structure

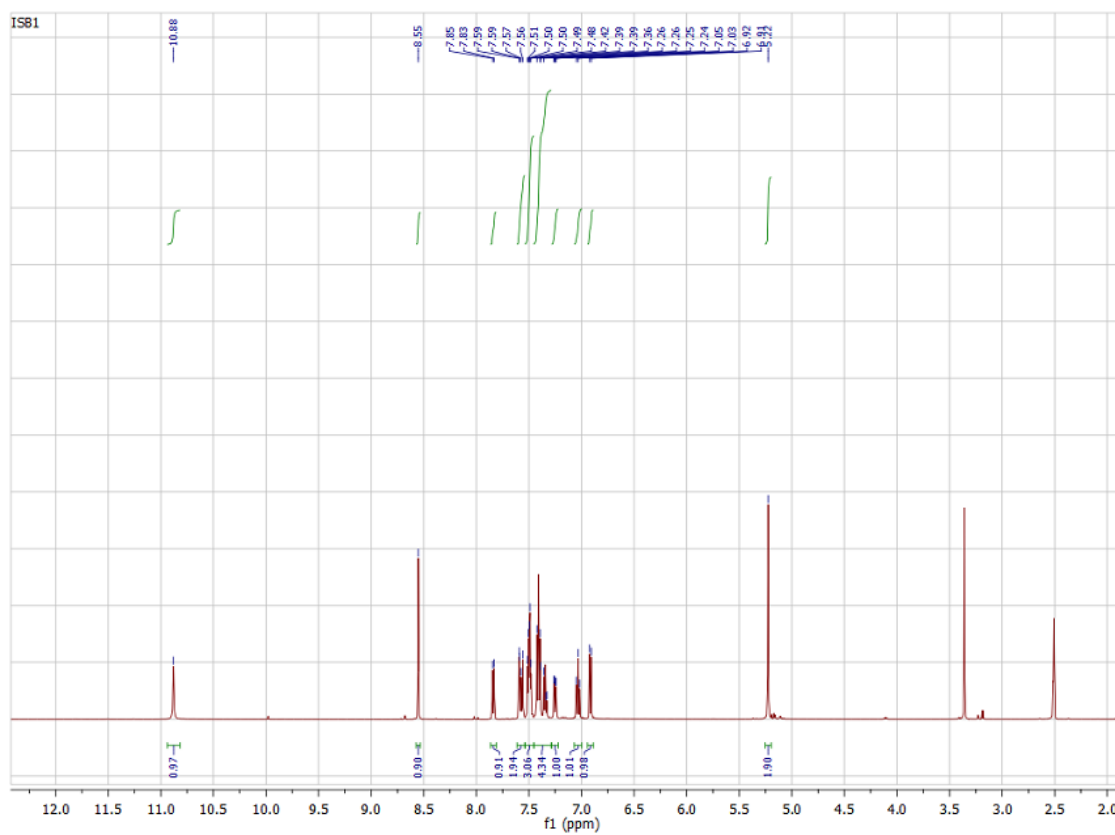
1.1 TLC OF ISB-1. Mobile phase is Hexane: ethyl acetate (70:30)



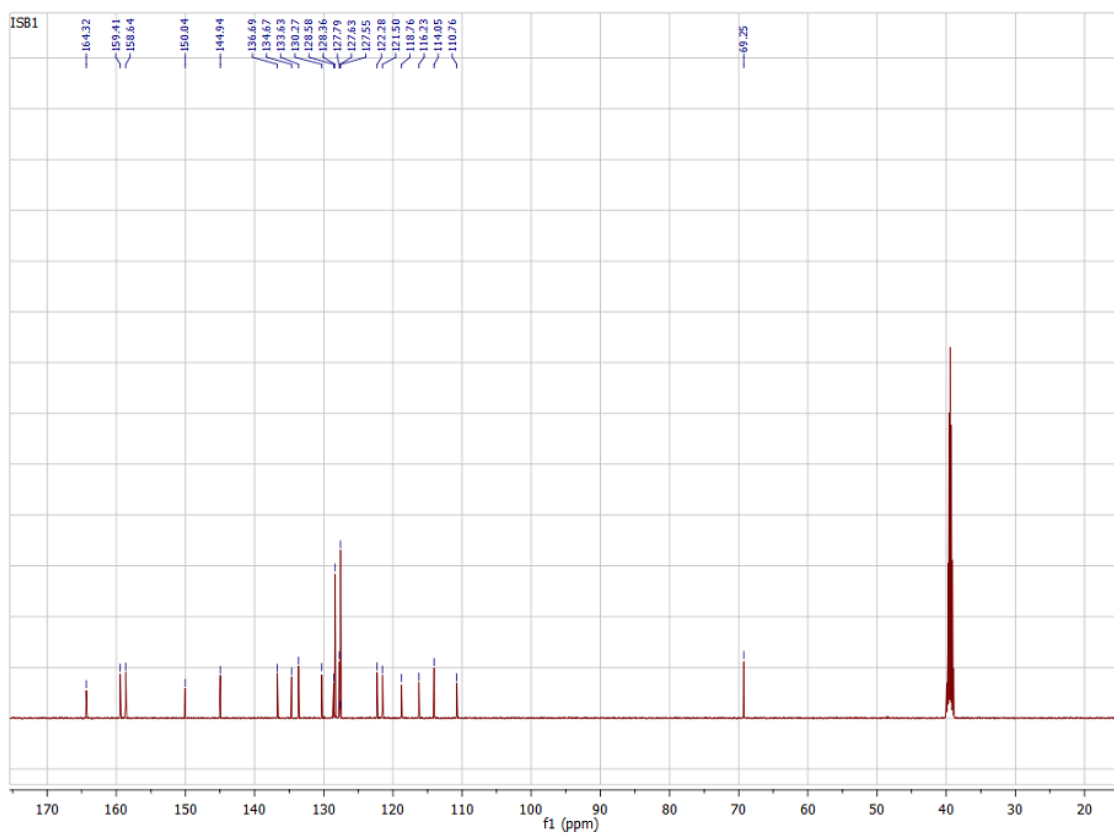
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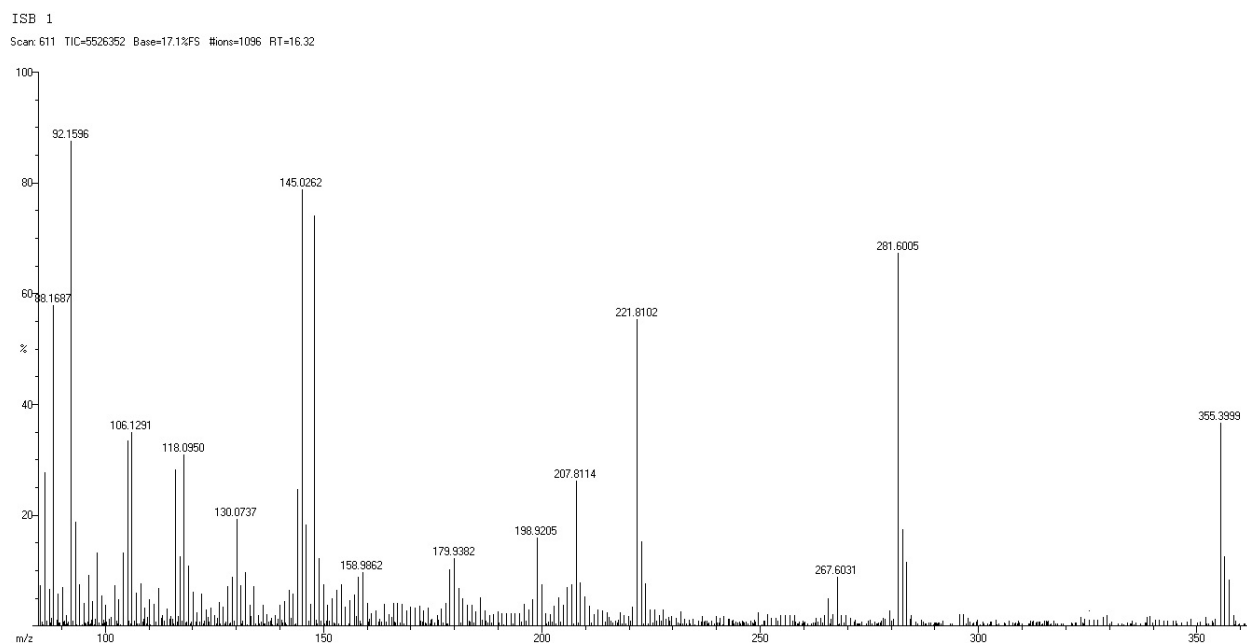
### 1.3 $^1\text{H}$ NMR SPECTRA OF ISB-1



### 1.4 $^{13}\text{C}$ NMR SPECTRA OF ISB-1:



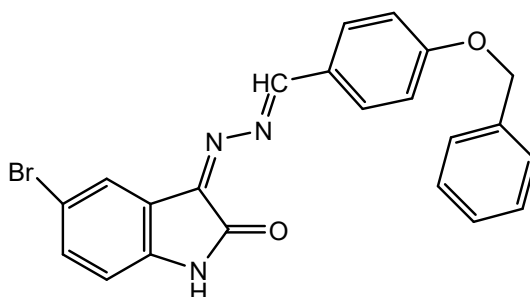
## 1.5 MASS SPECTRA OF ISB-1



## 1.6 SPECTRAL INTERPRETATION:

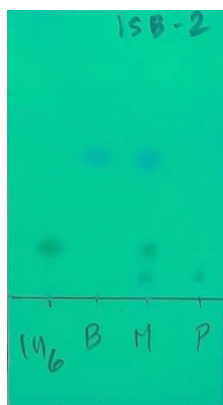
*3-((4-(benzyloxy)benzylidene)hydrazineylidene)indolin-2-one (ISB1)*: Orange, solid, 68%, melting point.  $181 \pm 2^\circ\text{C}$ .  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.85 (s, 1H, NH), 8.55 (s, 1H, =CH-), 7.84-6.92 (m, 13H, ArH), 5.22 (s, 2H, -CH $_2$ -).  $^{13}\text{C NMR}$  (500 MHz, DMSO- $d_6$ ) 164.32,

159.41, 158.64, 150.04, 144.94, 136.69, 134.67, 133.63, 130.27, 128.58, 128.36, 127.67, 122.28, 121.50, 118.76, 116.23, 114.05, 110.76, 69.25. Chemical Formula  $C_{22}H_{16}FN_3O_2$ . EI- HRMS (m/z): Calculated-355.3892, Observed-355.3999.



**Figure S2.** ISB-2 structure

2.1 TLC OF ISB-2: Mobile phase is Hexane: ethyl acetate (70:30)





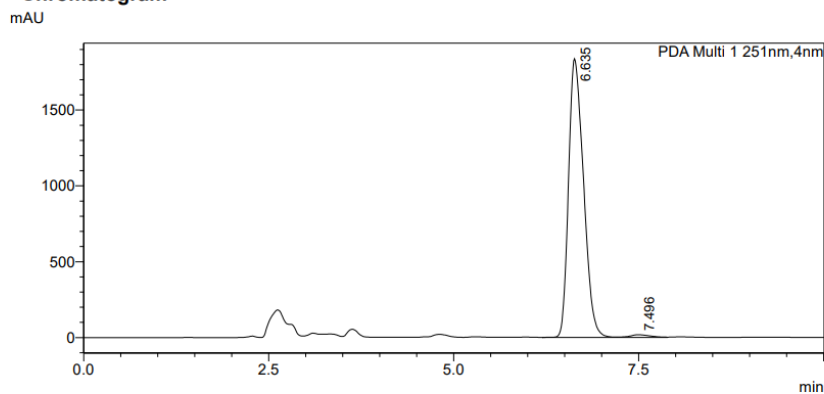
## 2.2 HPLC OF ISB-2

# SHIMADZU LabSolutions Analysis Report

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 Method Filename : isatin.lcm  
 Batch Filename :  
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 Processed by : System Administrator

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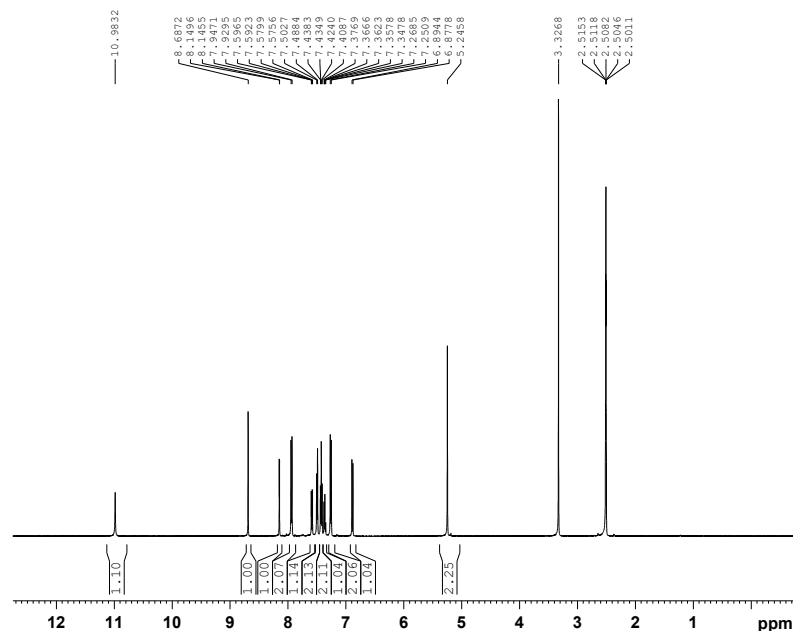
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## 2.3 <sup>1</sup>H NMR OF ISB-2

ISB-2

<sup>1</sup>H\_8scan DMSO {D:\Spectra} nmr 5

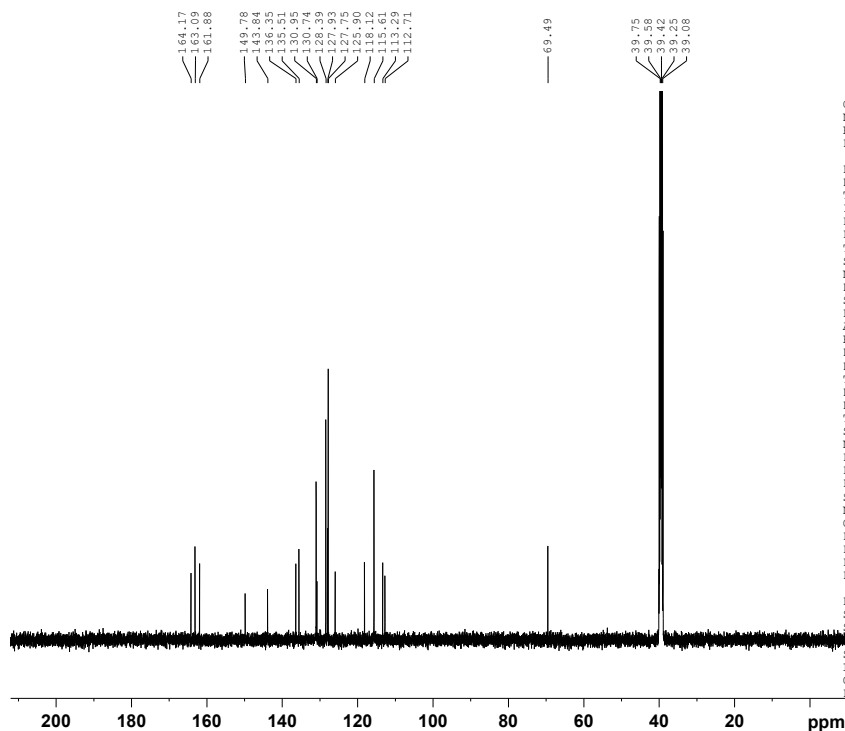


BRUKER  
 AVANCE NEO  
 500 MHz NMR  
 SPECTROMETER  
 SAIF, P.U.

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 PROCNO 1  
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 DE 6.79 usec  
 TE 300.2 K  
 D1 1.00000000 sec  
 TD0 1  
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 FO 3.33 usec  
 P1 10.00 usec  
 PLW1 20.93000031 W  
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 WDW EM  
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## 2.4 <sup>13</sup>C NMR OF ISB-2

ISB-2  
C13CPD DMSO {D:\Spectra} nmr 5



BRUKER  
AVANCE NEO  
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SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

Current Data Parameters  
NAME Nov23-2022  
EXPNO 51  
PROCNO 1

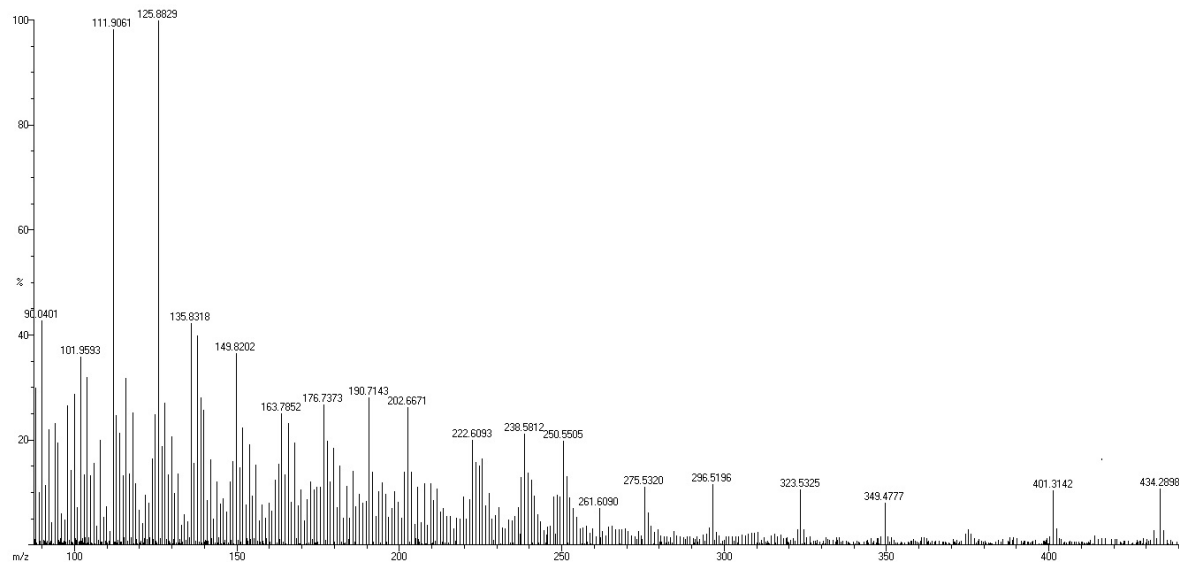
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RG 101  
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DE 6.50 usec  
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D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SFO1 125.7804233 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 83.14099884 W  
SFO2 500.1720007 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 80.00 usec  
PLW2 20.93000031 W  
PLW12 0.32703000 W  
PLW13 0.16449000 W

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## 2.5 MASS SPECTRUM OF ISB-2

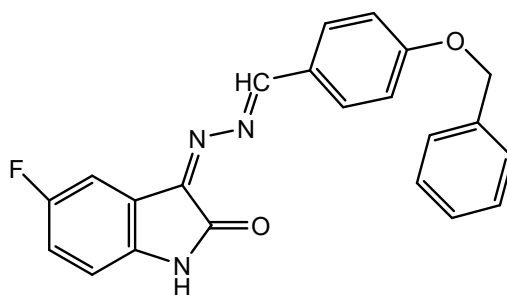
ISB-2

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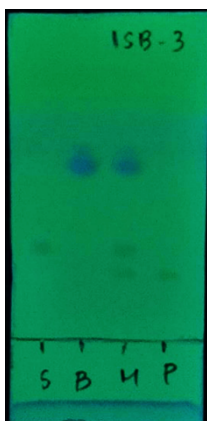
## 2.6 SPECTRAL INTERPRETATION:

3-((4-(benzyloxy)benzylidene)hydrazineylidene)-5-bromoindolin-2-one (**ISB2**): Orange, solid, 81%, melting point.  $244 \pm 2^\circ\text{C}$ .  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.98 (s, 1H, NH), 8.68 (s, 1H, =CH-), 8.14-6.87 (m, 12H, ArH), 5.24 (s, 2H, -CH $_2$ -)  $^{13}\text{C}$  NMR (500 MHz, DMSO- $d_6$ ) 164.17, 163.09, 161.88, 149.78, 143.84, 136.35, 135.51, 130.95, 130.74, 128.39, 127.93, 127.75, 125.90, 118.12, 115.61, 113.29, 112.71, 69.49. Chemical formula  $\text{C}_{22}\text{H}_{15}\text{BrFN}_3\text{O}$  EI-HRMS (m/z): Calculated- 434.2898, Observed-434.2853.



**Figure S3.** ISB3 structure

3.1 TLC OF ISB-3: Mobile phase is Hexane: ethyl acetate (70:30)



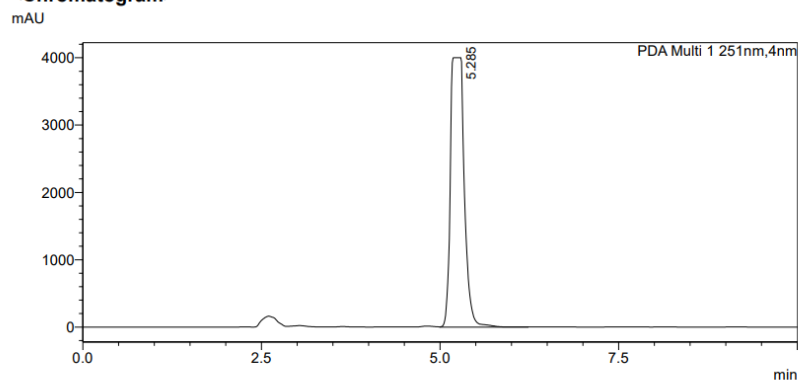
### 3.2 HPLC OF ISB-3

SHIMADZU LabSolutions Analysis Report

<Sample Information>

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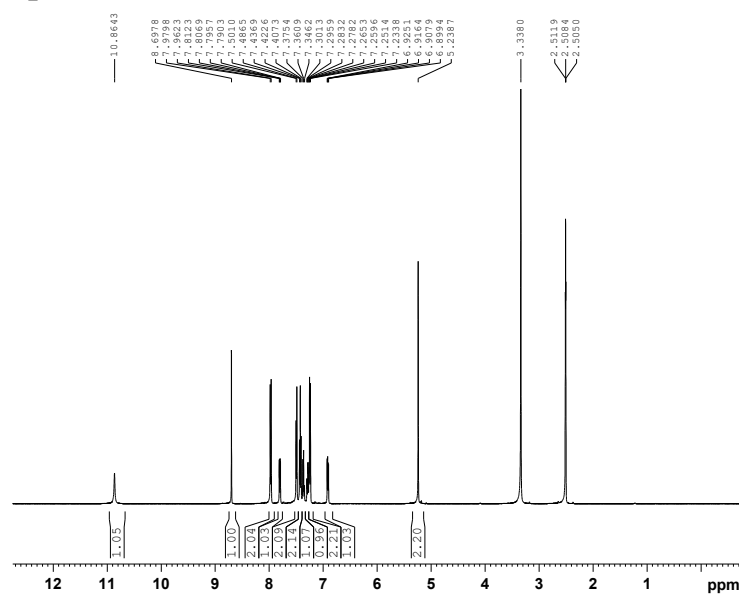


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### 3.3 <sup>1</sup>H NMR OF ISB-3

ISB-3  
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BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P.U.

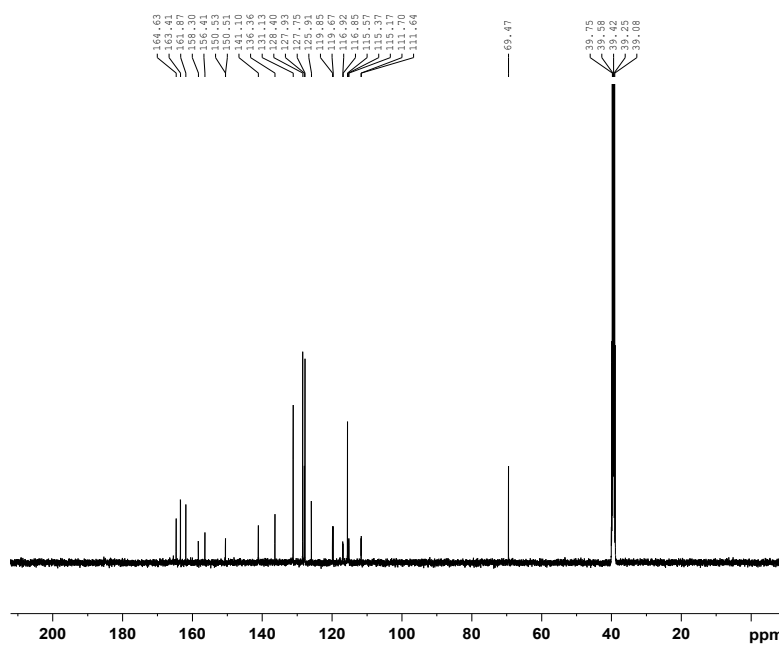
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FIDRES 0.448788 Hz  
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RG 101  
DW 34.000 usec  
DE 6.79 usec  
TE 300.2 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.1730885 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.93000031 W

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PC 1.00

### 3.4 <sup>13</sup>C NMR OF ISB-3

ISB-3  
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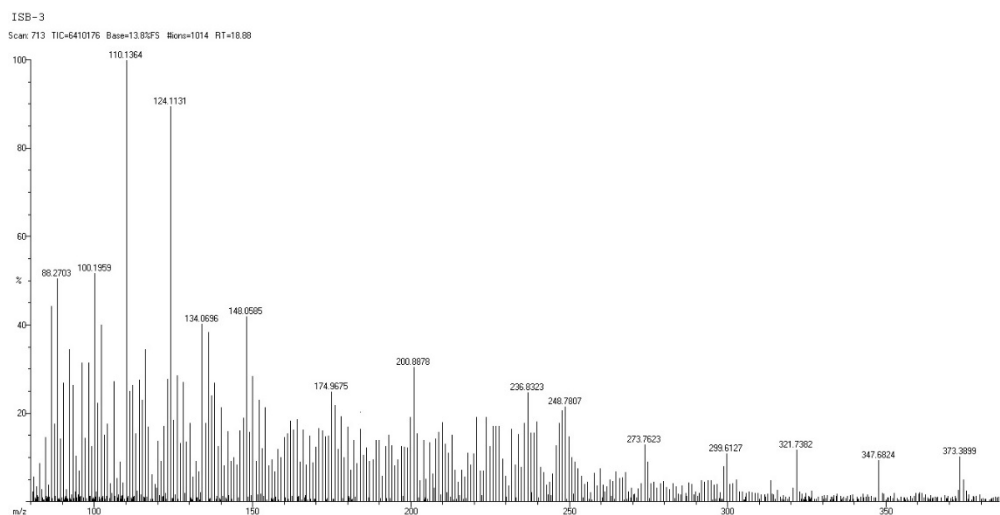
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

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PROCNO 1

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DE 6.50 usec  
TE 300.2 K  
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D11 0.03000000 sec  
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SFO1 125.7804233 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 83.14099884 W  
SFO2 500.1720007 MHz  
NUC2 1H  
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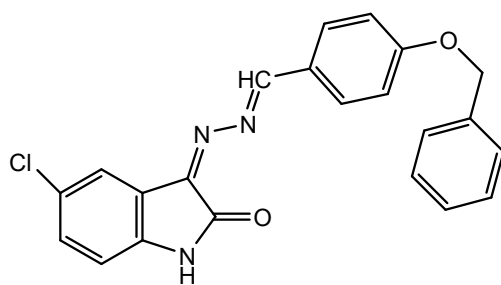
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### 3.5 MASS SPECTRA OF ISB-3



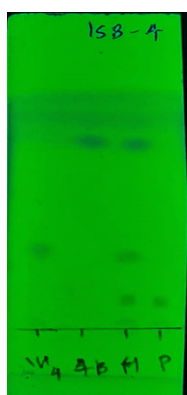
### 3.6 SPECTRAL INTERPRETATION:

*3-((4-(benzyloxy)benzylidene)hydrazineylidene)-5-fluoroindolin-2-one (ISB 3)*: Brick red , solid, 72%, melting point.  $229 \pm 2^\circ\text{C}$ .  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.86 (s, 1H, NH), 8.69 (s, 1H, =CH-), 7.97-6.89 (m, 12H, ArH), 5.23 (s, 2H, -CH<sub>2</sub>-).  $^{13}\text{C}$  NMR (500 MHz, DMSO- $d_6$ ): 164.63, 163.41, 161.87, 158.30, 156.41, 150.53, 141.10, 136.36, 131.13, 128.40, 127.93, 126.91, 119.85, 116.92, 115.87, 111.70, 69.47. Chemical formula C<sub>22</sub>H<sub>15</sub>F<sub>2</sub>N<sub>3</sub>O<sub>2</sub> EI-HRMS (m/z): Calculated- 378.3899, Observed-373.3797.



**Figure S4.** ISB4 structure

4.1 TLC OF ISB-4: Mobile phase is Hexane: ethyl acetate (70:30)



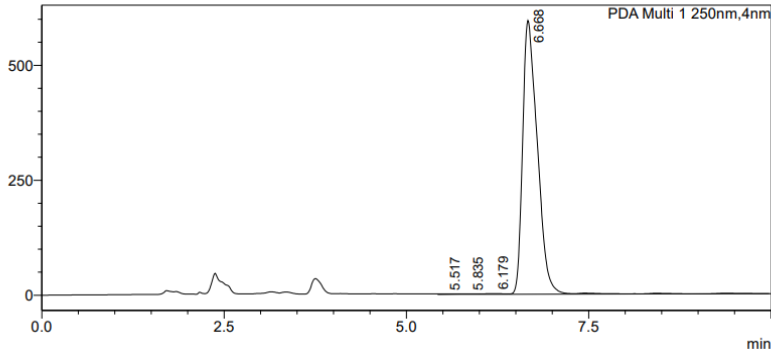
4.2 HPLC OF ISB-4

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 Processed by : System Administrator

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mAU



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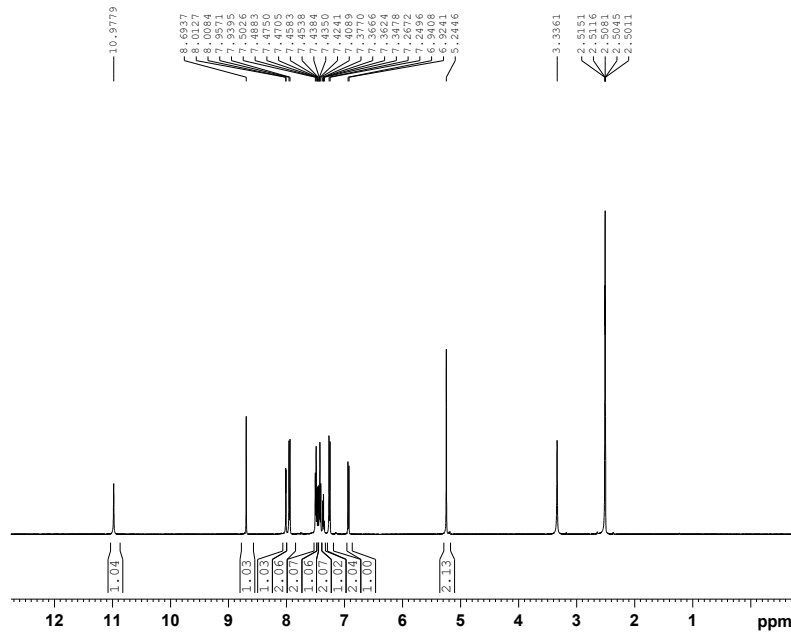
PDA Ch1 250nm

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4	6.668	8435943	595104	99.275		SV	
Total		8497519	598663				

## 4.3 <sup>1</sup>H NMR OF ISB-4

ISB-4

1H\_8scan DMSO {D:\Spectra} nmr 7



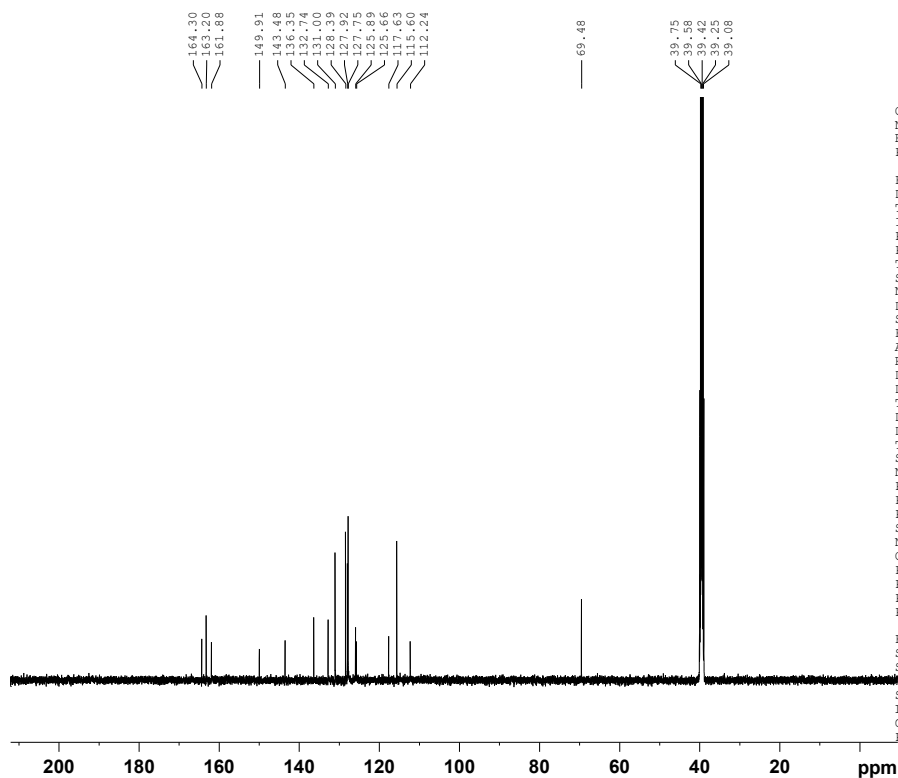
BRUKER  
 AVANCE NEO  
 500 MHz NMR  
 SPECTROMETER  
 SAIF, P.U.

Current Data Parameters  
 NAME Nov23-2022  
 EXPNO 70  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date 20221123  
 Time 10.24 h  
 INSTRUM Avance Neo 500  
 PROBRD z119470\_0333 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 0  
 SWH 14705.883 Hz  
 FIDRES 0.448788 Hz  
 AQ 2.2282240 sec  
 RG 101  
 DW 34.000 usec  
 DE 6.79 usec  
 TE 300.2 K  
 D1 1.0000000 sec  
 TD0 1  
 SFO1 500.1730885 MHz  
 NUC1 1H  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 20.93000031 W  
 F2 - Processing parameters  
 SI 65536  
 SF 500.1700000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

## 4.4 <sup>13</sup>C NMR OF ISB-4



ISB-4  
 C13CPD DMSO {D:\Spectra} nmr 7

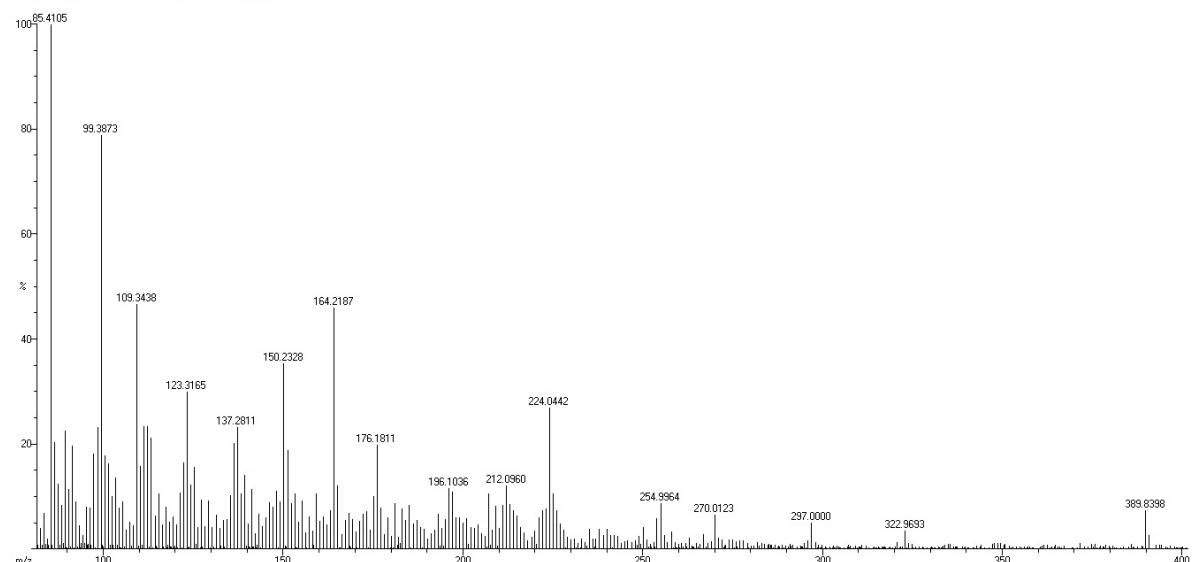


BRUKER  
 AVANCE NEO  
 500 MHz NMR SPECTROMETER  
 SAIF, PANJAB UNIVERSITY,  
 CHANDIGARH

Current Data Parameters  
 NAME Nov23-2022  
 EXPNO 71  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20221123  
 Time\_ 13.00 h  
 INSTRUM Avance Neo 500  
 PROBHD Z119470\_0333 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 512  
 DS 4  
 SWH 37037.035 Hz  
 FIDRES 1.130281 Hz  
 AQ 0.8847360 sec  
 RG 101  
 DW 13.500 usec  
 DE 6.50 usec  
 TE 300.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SFO1 125.7804233 MHz  
 NUC1 13C  
 P0 3.33 usec  
 F1 10.00 usec  
 PLW1 83.14099884 W  
 SFO2 500.1720007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 ECPD2 80.00 usec  
 PLW2 20.93000031 W  
 PLW12 0.32703000 W  
 PLW13 0.16449000 W  
 F2 - Processing parameters  
 SI 32768  
 SF 125.7679215 MHz  
 NDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

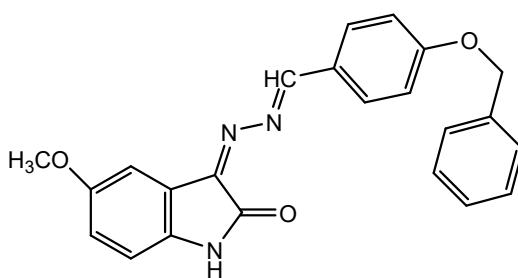
### 4.5 MASS SPECTRA OF ISB-4

ISB 4  
 Scan: 701 TIC=7425776 Base=27.3%FS H ions=1023 RT=18.58



### 4.6 SPECTRAL INTERPRETATION:

3-((4-(benzyloxy)benzylidene)hydrazineylidene)-5-chloroindolin-2-one (**ISB 4**): Orange solid, 78%, melting point.  $240 \pm 2^\circ\text{C}$ .  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.97 (s, 1H, NH), 8.69 (s, 1H, =CH-), 8.01-6.92 (m, 12H, ArH), 5.24 (s, 2H, -CH $_2$ -)  $^{13}\text{C}$  NMR (500 MHz, DMSO- $d_6$ ) 164.30, 163.88, 161.88, 149.91, 143.48, 136.35, 132.74, 131.00, 128.39, 127.92, 126.89, 125.66, 117.63, 116.60, 112.24, 69.48. Chemical Formula  $\text{C}_{22}\text{H}_{15}\text{ClFN}_3\text{O}_2$  EI- HRMS (m/z): Calculated-389.8398, Observed- 389.8343.



**Figure S5.** ISB5 structure

5.1 TLC OF ISB-5: Mobile phase is Hexane: ethyl acetate (70:30)



## 5.2 HPLC OF 15B-5

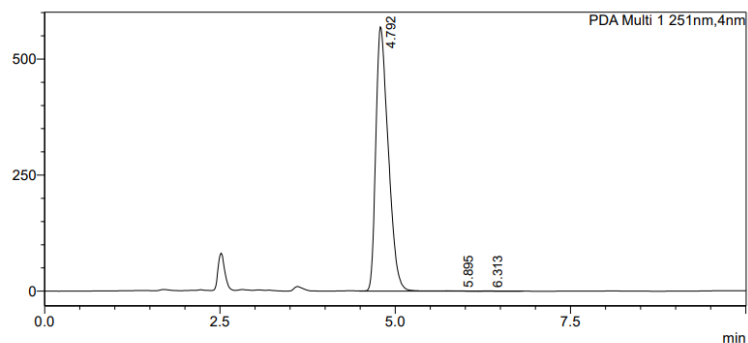
### SHIMADZU LabSolutions Analysis Report

#### <Sample Information>

Sample Name : 100mcl  
 Sample ID :  
 Data Filename : ISB-5 ORG NEW.lcd  
 Method Filename : isatin.lcm  
 Batch Filename :  
 Vial # : 1-2  
 Injection Volume : 20 uL  
 Date Acquired : 12/7/2022 12:46:47 AM  
 Date Processed : 12/7/2022 1:00:09 AM  
 Sample Type : Unknown  
 Acquired by : System Administrator  
 Processed by : System Administrator

#### <Chromatogram>

mAU

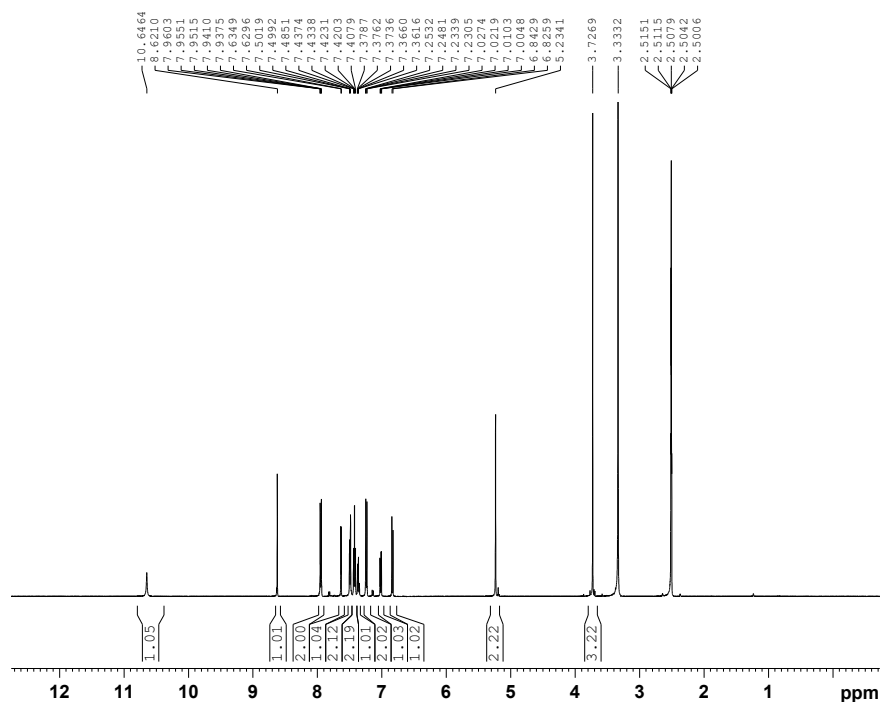


#### <Peak Table>

PDA Ch1 251nm							
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
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2	5.895	1977	181	0.028		T	
3	6.313	5518	338	0.078		T	
Total		7057420	569636				

## 5.3 <sup>1</sup>H NMR OF 15B-5

ISB-5  
1H\_8scan DMSO {D:\Spectra} nmr 8



BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P.U.

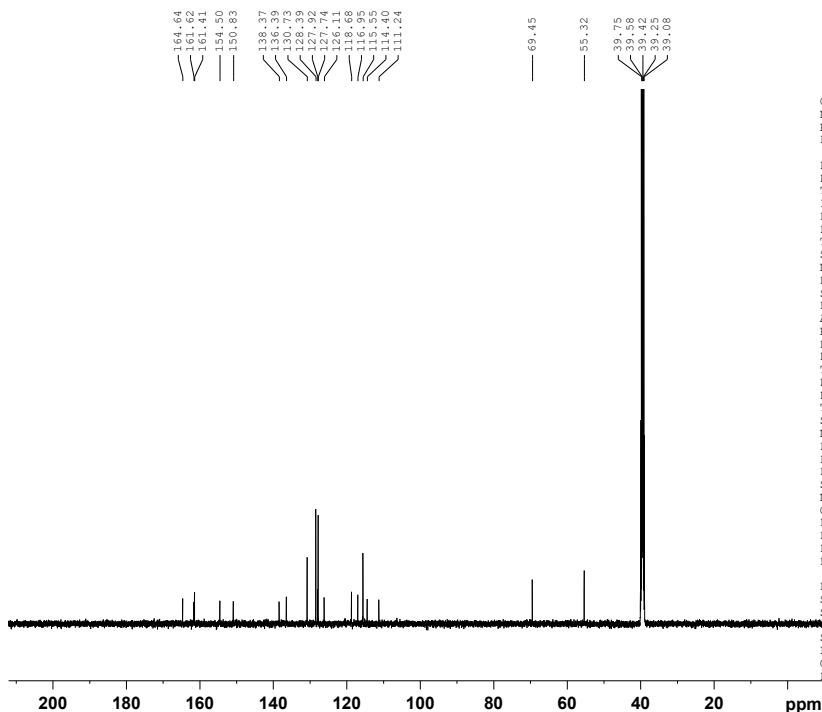
Current Data Parameters  
NAME Nov23-2022  
EXPNO 81  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 11.11 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 ( )  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 0  
SWH 14705.883 Hz  
FIDRES 0.448788 Hz  
AQ 2.2282240 sec  
RG 101  
DW 34.000 usec  
DE 6.79 usec  
TE 300.2 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.1730885 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.93000031 W

F2 - Processing parameters  
SI 65536  
SF 500.1700000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

### 5.4 <sup>13</sup>C NMR OF ISB-5

ISB-5  
C13CPD DMSO {D:\Spectra} nmr 8



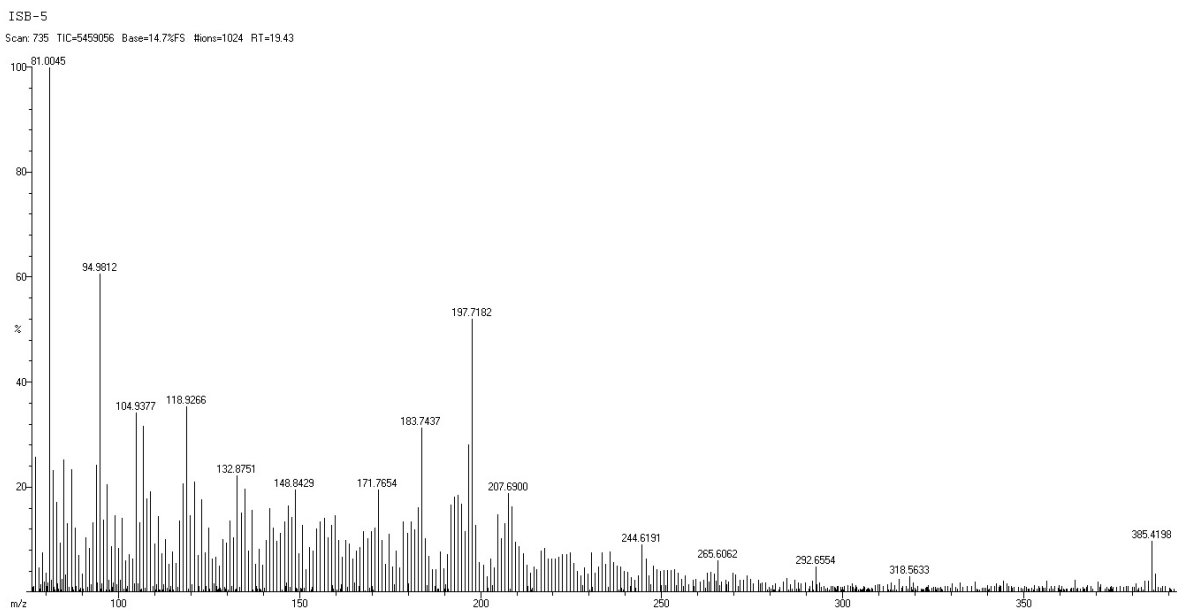
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

Current Data Parameters  
NAME Nov23-2022  
EXPNO 82  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 15.10 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 1024  
DS 4  
SWH 37037.035 Hz  
FIDRES 1.130281 Hz  
AQ 0.8847360 sec  
RG 101  
DW 13.500 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7804233 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 83.14099884 W  
SFO2 500.1720007 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 80.00 usec  
PLW2 20.93000031 W  
PLW12 0.32703000 W  
PLW13 0.16449000 W

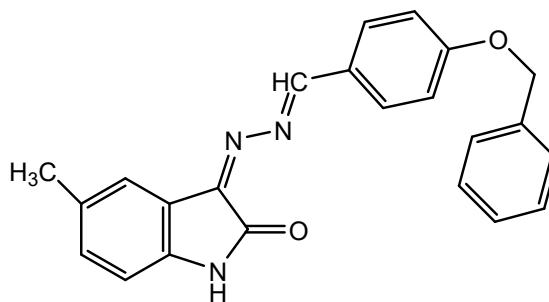
F2 - Processing parameters  
SI 32768  
SF 125.7679202 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

### 5.5 MASS SPECTRA OF ISB-5



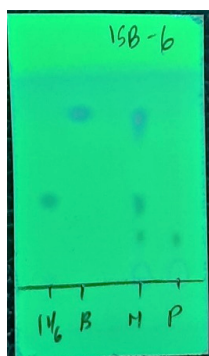
## 5.6 SPECTRAL INTERPRETATION

*3-((4-(benzyloxy)benzylidene)hydrazineylidene)-5-methoxyindolin-2-one (ISB5)*: Reddish brown, solid, 72%, melting point.  $192 \pm 2^\circ\text{C}$ .  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.64 (s, 1H, NH), 8.62 (s, 1H, =CH-), 7.96-6.82(m, 12H, ArH), 5.23 (s, 2H, -CH<sub>2</sub>-), 3.72 (s, 3H, -CH<sub>2</sub>-Ar).  $^{13}\text{C NMR}$  (500 MHz, DMSO- $d_6$ ) 164.64, 161.62, 161.41, 154.50, 150.63, 138.37, 136.39, 130.73, 128.39, 127.92, 126.11, 118.68, 116.98, 115.55, 114.40, 111.28, 69.45, 55.32. Chemical formula C<sub>23</sub>H<sub>18</sub>FN<sub>3</sub>O<sub>3</sub> EI- HRMS (m/z): Calculated-385.4198, Observed- 385.4152.



**Figure S6.** ISB6 structure

6.1 TLC OF ISB-6: Mobile phase is Hexane: ethyl acetate (70:30)



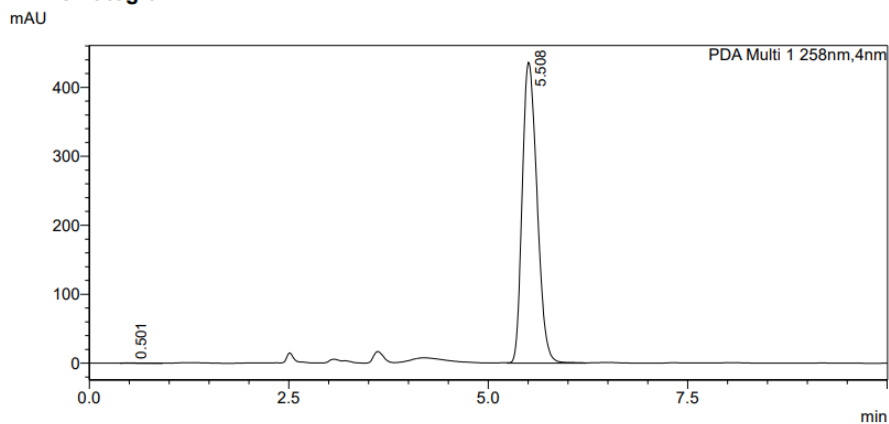
6.2 HPLC OF ISB-6

**SHIMADZU LabSolutions Analysis Report**

**<Sample Information>**

Sample Name	: 100mcl	Sample Type	: Unknown
Sample ID	:	Acquired by	: System Administrator
Data Filename	: ISB6.lcd	Processed by	: System Administrator
Method Filename	: isatin.lcm		
Batch Filename	:		
Vial #	: 1-2		
Injection Volume	: 20 uL		
Date Acquired	: 12/3/2022 4:11:05 AM		
Date Processed	: 12/6/2022 10:55:54 PM		

**<Chromatogram>**

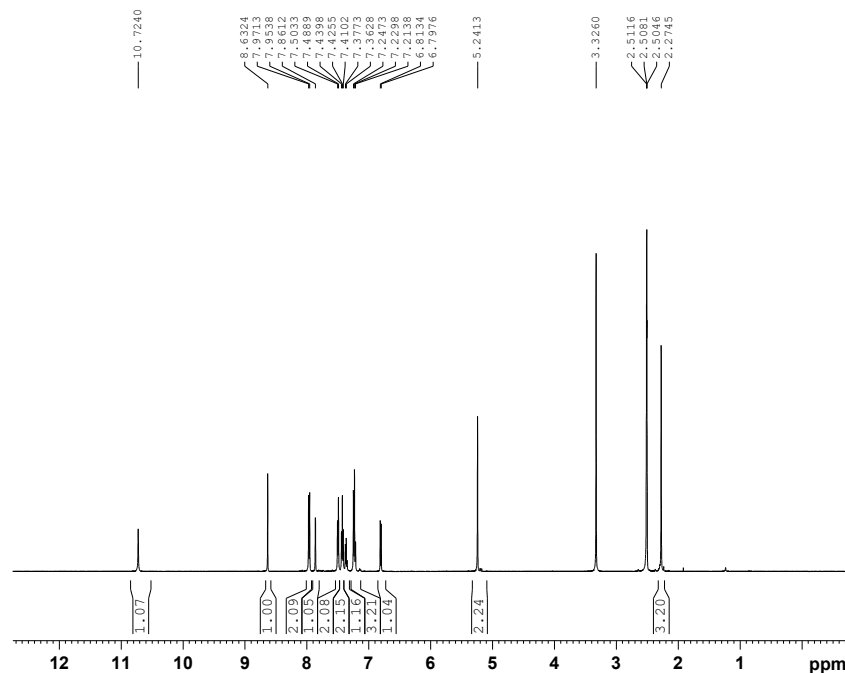


**<Peak Table>**

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	0.501	7008	324	0.124			
2	5.508	5662652	436305	99.876			
Total		5669660	436629				

### 6.3 <sup>1</sup>H NMR OF ISB-6

ISB-6  
1H\_8scan DMSO {D:\Spectra} nmr 9



BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P.U.

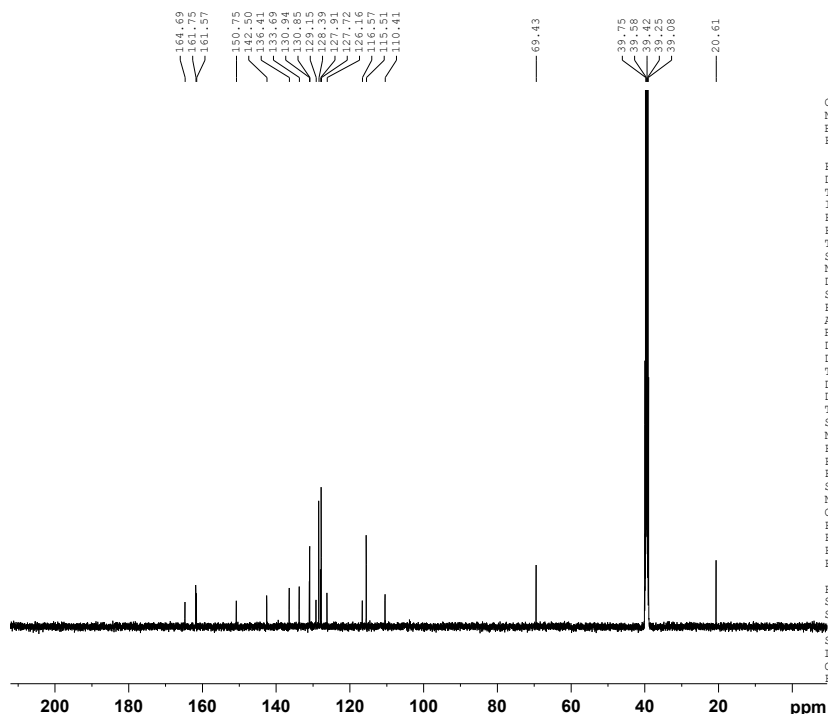
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Current Data Parameters
NAME      Nov23-2022
EXPNO    90
PROCNO   1

F2 - Acquisition Parameters
Date_    20221123
Time     10.29 h
INSTRUM  Avance Neo 500
PROBHD   Z119470_0333 (
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        16
DS        0
SWH       14705.883 Hz
FIDRES    0.448788 Hz
AQ        2.2282240 sec
RG        101
DW        34.000 usec
DE        6.79 usec
TE        300.2 K
D1        1.00000000 sec
TD0       1
SFO1      500.1730885 MHz
NUC1      1H
FO        3.33 usec
P1        10.00 usec
PLW1      20.93000031 W

F2 - Processing parameters
SI        65536
SF        500.1700000 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
```

### 6.4 <sup>13</sup>C NMR OF ISB-6

ISB-6  
C13CPD DMSO {D:\Spectra} nmr 9



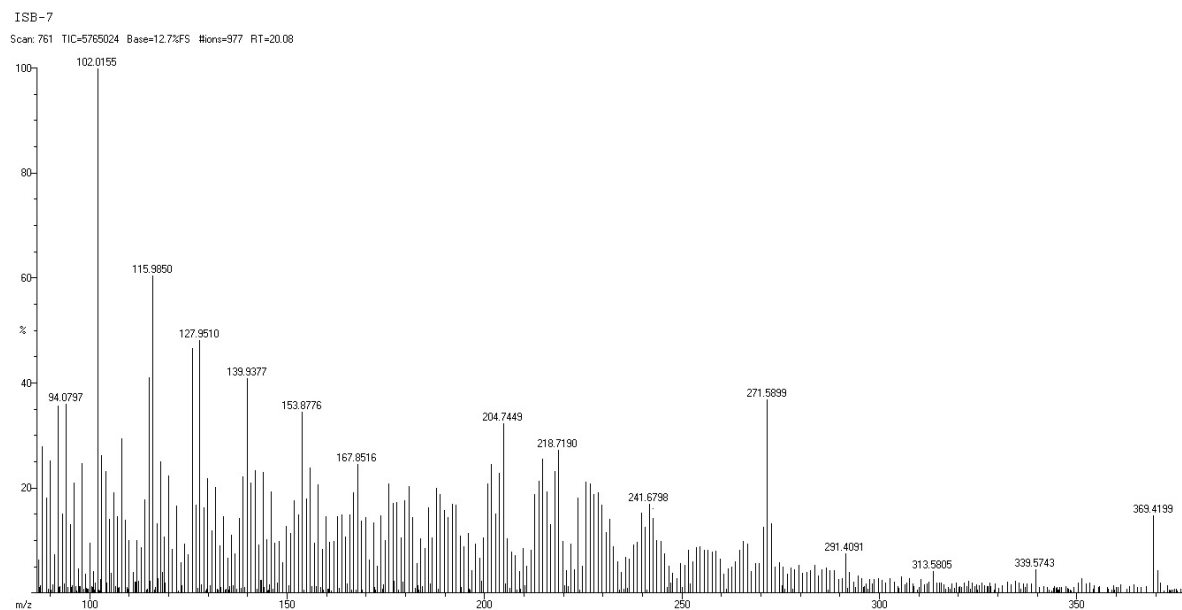
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

```
Current Data Parameters
NAME      Nov23-2022
EXPNO    91
PROCNO   1

F2 - Acquisition Parameters
Date_    20221123
Time     15.39 h
INSTRUM  Avance Neo 500
PROBHD   Z119470_0333 (
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        512
DS        4
SWH       37037.035 Hz
FIDRES    1.130281 Hz
AQ        0.8847360 sec
RG        101
DW        13.500 usec
DE        6.50 usec
TE        300.1 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
SFO1      125.7804233 MHz
NUC1      13C
FO        3.33 usec
P1        10.00 usec
PLW1      83.14099884 W
SFO2      500.1720007 MHz
NUC2      1H
CPDPRG2  waltz65
PCPD2    80.00 usec
PLW2      20.93000031 W
PLW12     0.32703000 W
PLW13     0.16449000 W

F2 - Processing parameters
SI        32768
SF        125.7679212 MHz
WDW       EM
SSB       0
LB        1.00 Hz
GB        0
PC        1.40
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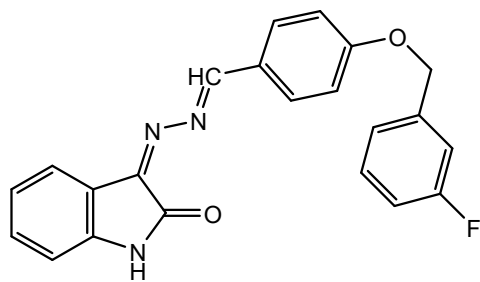
## 6.5 MASS INTERPRETATION OF ISB-6



## 6.6 SPECTRAL INTERPRETATION:

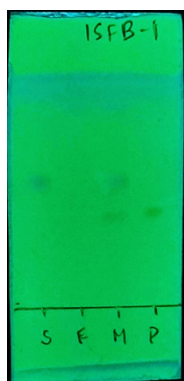
*3-((4-(benzyloxy)benzylidene)hydrazineylidene)-5-methylindolin-2-one (ISB6)*: orange, solid, 68%, melting point.  $210 \pm 2^\circ\text{C}$ .  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.72 (s, 1H, NH), 8.63 (s, 1H, =CH-), 7.97-6.79(m, 12H, ArH), 5.24 (s, 2H, -CH<sub>2</sub>-), 2.27 (s, 3H, -CH<sub>2</sub>-Ar).  $^{13}\text{C}$  NMR (500 MHz, DMSO- $d_6$ ) 164.69, 161.76, 161.87, 160.75, 142.80, 136.41, 133.69, 130.94, 129.18, 128.39, 127.91, 126.16, 116.87, 115.51, 110.41, 69.43, 20.61. Chemical formula  $\text{C}_{23}\text{H}_{19}\text{N}_3\text{O}_2$ . EI- HRMS (m/z): Calculated-369.4199, Observed- 369.4158.





**Figure S7.** ISFB1 structure

7.1 TLC OF ISFB-1: Mobile phase is Hexane: ethyl acetate (70:30)



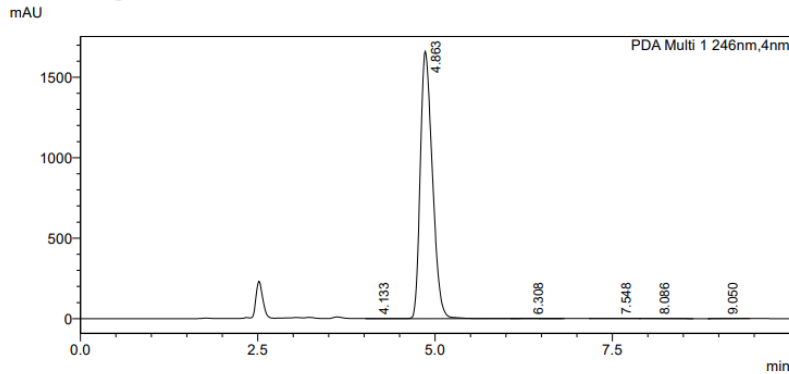
7.2 HPLC OF ISFB-1

## <Sample Information>

Sample Name : isatin001  
 Sample ID : isfb1  
 Data Filename : fluoro and bb\_05-12-2022\_003.lcd  
 Method Filename : isatin.lcm  
 Batch Filename : fluoro and bb.lcb  
 Vial # : 1-2  
 Injection Volume : 20 uL  
 Date Acquired : 12/5/2022 1:39:04 AM  
 Date Processed : 12/6/2022 4:20:08 AM

Sample Type : Standard  
 Level : 1  
 Acquired by : System Administrator  
 Processed by : System Administrator

## <Chromatogram>

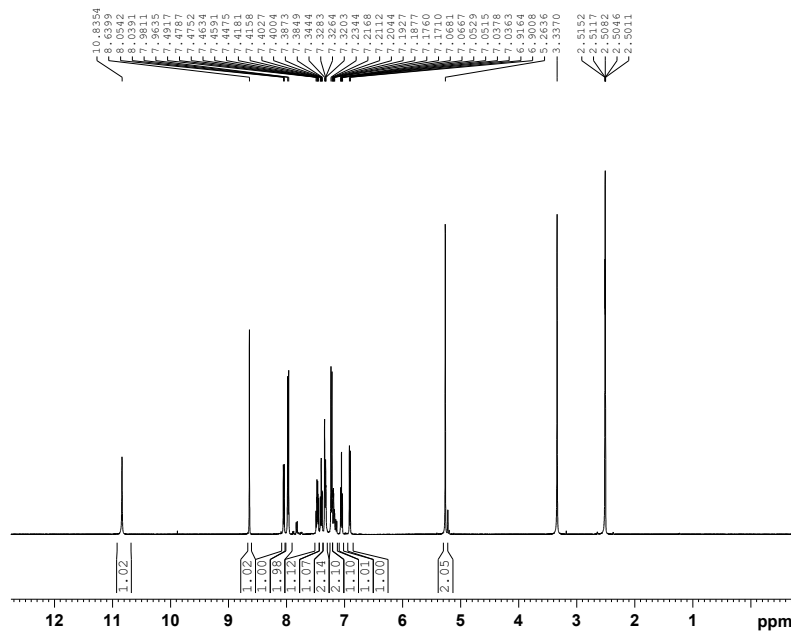


## <Peak Table>

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	4.133	16616	898	0.084			
2	4.863	19734389	1659909	99.606		SV	
3	6.308	34168	1978	0.172		T	
4	7.548	12384	449	0.063			
5	8.086	11333	558	0.057		V	
6	9.050	3584	189	0.018			
Total		19812474	1663981				

## 7.3 <sup>1</sup>H NMR OF ISFB-1

ISFB-1  
 1H\_8scan DMSO {D:\Spectra} nmr 10



BRUKER  
 AVANCE NEO  
 500 MHz NMR  
 SPECTROMETER  
 SAIF, P.U.

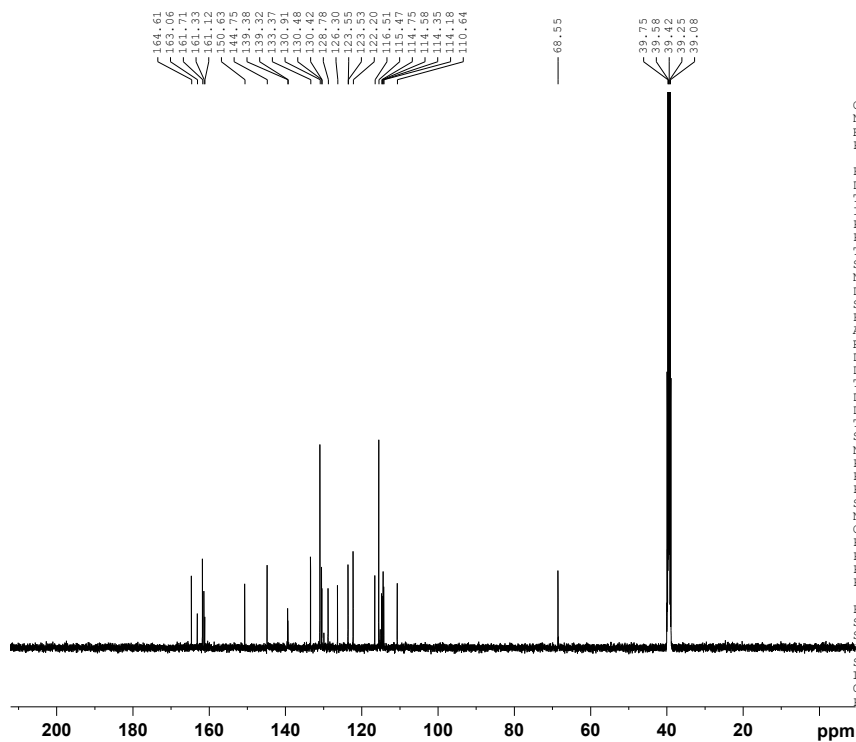
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 NAME Nov23-2022  
 EXPNO 100  
 PROCNO 1

F2 - Acquisition Parameters  
 Date 20221123  
 Time 10.32 h  
 INSTRUM Avance Neo 500  
 PROBHD Z119470\_0333 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 0  
 SWH 14705.883 Hz  
 FIDRES 0.448788 Hz  
 AQ 2.2282240 sec  
 RG 101  
 DW 34.000 usec  
 DE 6.79 usec  
 TE 300.2 K  
 D1 1.00000000 sec  
 TD0 1  
 SFO1 500.1730885 MHz  
 NUC1 1H  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 20.93000031 W

F2 - Processing parameters  
 SI 65536  
 SF 500.1700000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

## 7.4 <sup>13</sup>C NMR OF ISFB-1

ISFB-1  
 C13CPD DMSO {D:\Spectra} nmr 10



BRUKER  
 AVANCE NEO  
 500 MHz NMR SPECTROMETER  
 SAIF, PANJAB UNIVERSITY,  
 CHANDIGARH

Current Data Parameters  
 NAME Nov23-2022  
 EXPNO 101  
 PROCNO 1

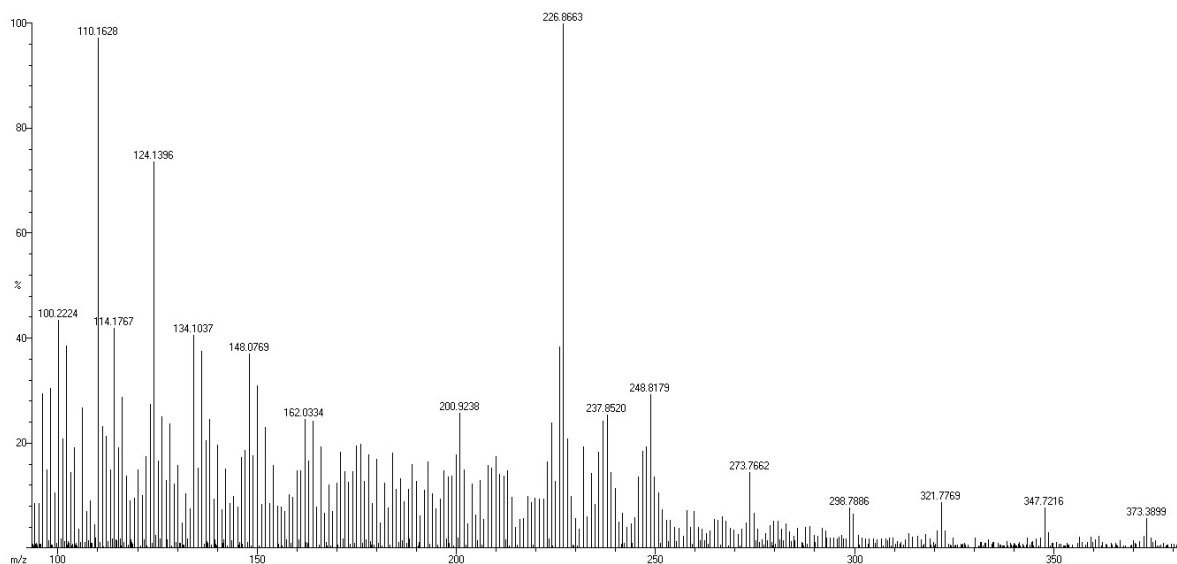
F2 - Acquisition Parameters  
 Date\_ 20221123  
 Time 16.06 h  
 INSTRUM Avance Neo 500  
 PROBHD Z119470\_0333 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 512  
 DS 4  
 SWH 37037.035 Hz  
 FIDRES 1.130281 Hz  
 AQ 0.8847360 sec  
 RG 101  
 DW 13.500 usec  
 DE 6.50 usec  
 TE 300.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDD 1  
 SFO1 125.7804233 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 83.14099884 W  
 SFO2 500.1720007 MHz  
 NUC2 1H  
 CPDPRG[2] waltz65  
 PCPD2 80.00 usec  
 PLW2 20.93000031 W  
 PLW12 0.32703000 W  
 PLW13 0.16449000 W

F2 - Processing parameters  
 SI 32768  
 SF 125.7679210 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

## 7.5 MASS SPECTRA OF ISFB-1

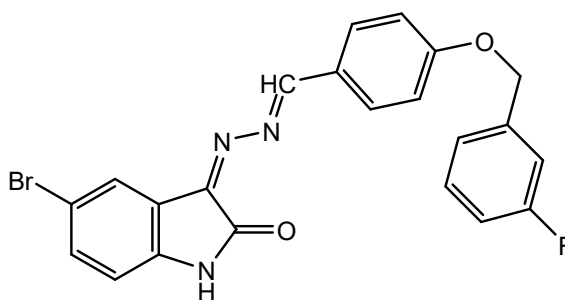
ISFB-1

Scan: 715 TIC=6459648 Base=14.7%FS #Ions=1032 RT=18.93



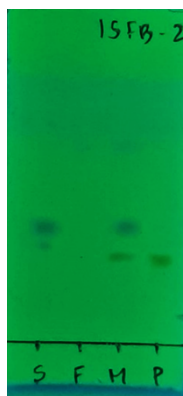
## 7.6 SPECTRAL INTERPRETATION:

3-((4-((3-fluorobenzyl)oxy)benzylidene)hydrazineylidene)indolin-2-one (**ISFB1**): orange, solid, 75%, melting point.  $218 \pm 2^\circ\text{C}$ .  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.83 (s, 1H, NH), 8.63 (s, 1H, =CH-), 8.05-6.90(m, 12H, ArH), 5.26 (s, 2H, -CH $_2$ -).  $^{13}\text{C NMR}$  (500 MHz, DMSO- $d_6$ )  $\delta$ : 164.61, 163.06, 161.71, 150.63, 144.76, 139.38, 133.37, 130.91, 128.78, 126.30, 123.66, 122.20, 116.81, 115.47, 114.75, 110.64, 68.88. Chemical formula  $\text{C}_{22}\text{H}_{16}\text{FN}_3\text{O}_2$ . EI- HRMS (m/z): Calculated-373.3899, Observed- 373.3797.



**Figure S8.** ISFB2 structure

8.1 TLC OF ISFB-2: Mobile phase is Hexane: ethyl acetate (70:30)



## 8.2 HPLC OF ISFB-2

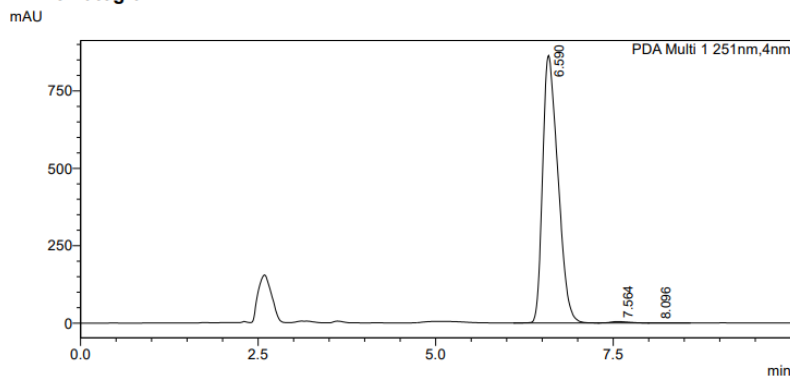
### SHIMADZU LabSolutions Analysis Report

#### <Sample Information>

Sample Name : isatin001  
 Sample ID : isfb2  
 Data Filename : fluoro and bb\_05-12-2022\_004.lcd  
 Method Filename : isatin.lcm  
 Batch Filename : fluoro and bb.lcb  
 Vial # : 1-3  
 Injection Volume : 20 uL  
 Date Acquired : 12/5/2022 1:49:26 AM  
 Date Processed : 12/6/2022 10:37:55 PM

Sample Type : Standard  
 Level : 1  
 Acquired by : System Administrator  
 Processed by : System Administrator

#### <Chromatogram>

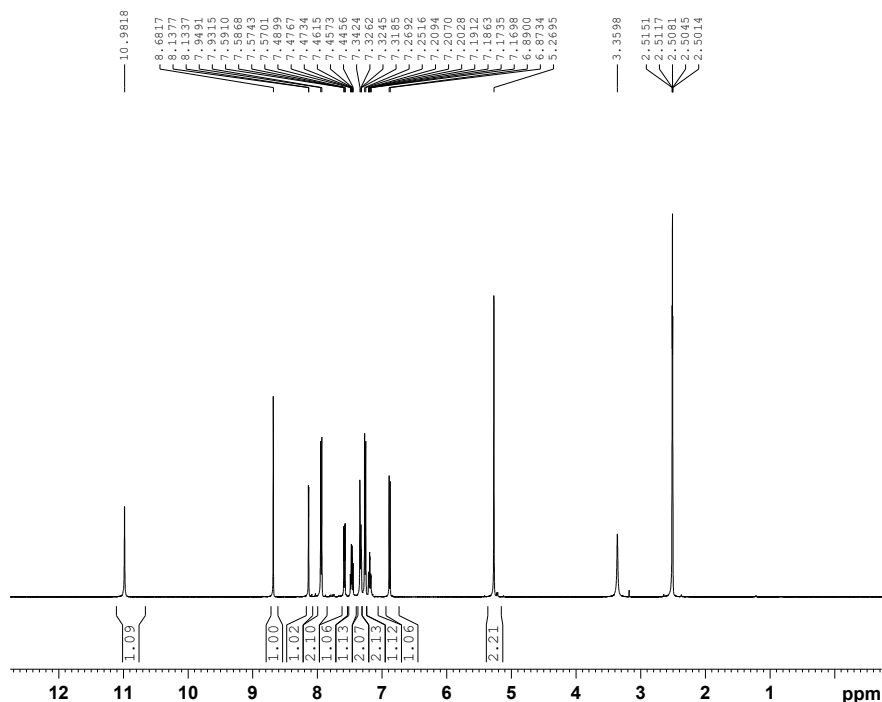


#### <Peak Table>

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.590	12988987	864298	99.271			
2	7.564	89640	4934	0.685		V	
3	8.096	5746	308	0.044		V	
Total		13084373	869540				

## 8.3 <sup>1</sup>H NMR OF ISFB-2

ISFB-2  
 1H\_8scan DMSO {D:\Spectra} nmr 11



BRUKER  
 AVANCE NEO  
 500 MHz NMR  
 SPECTROMETER  
 SAIF, P.U.

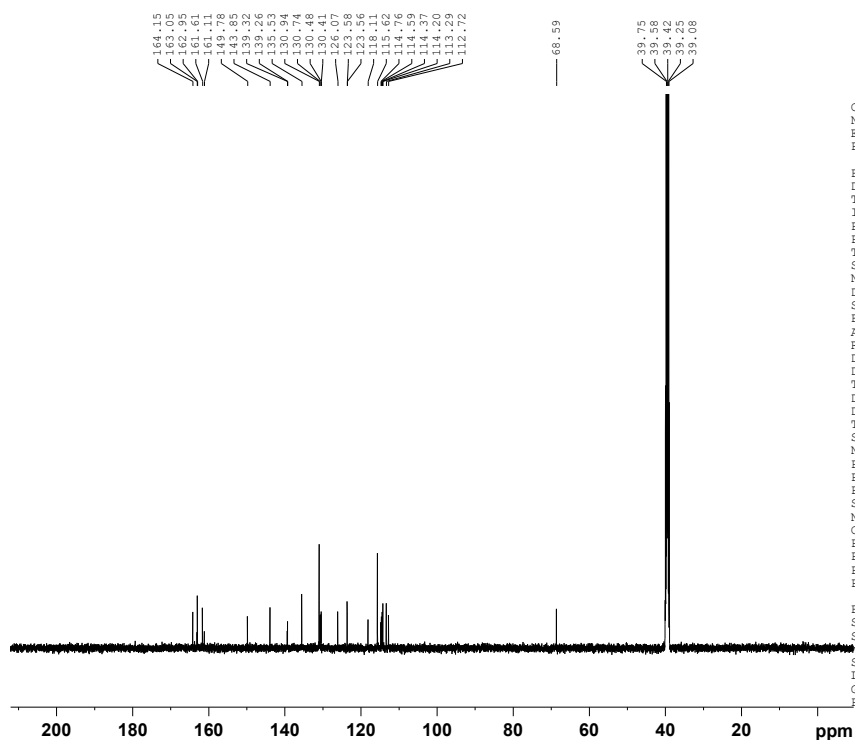
Current Data Parameters  
 NAME Nov23-2022  
 EXPNO 110  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20221123  
 Time\_ 10.34 h  
 INSTRUM Avance Neo 500  
 PROBHD Z119470\_0333 ( )  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 0  
 SWH 14705.883 Hz  
 FIDRES 0.448788 Hz  
 AQ 2.2282240 sec  
 RG 101  
 DW 34.000 usec  
 DE 6.79 usec  
 TE 300.2 K  
 D1 1.0000000 sec  
 TD0 1  
 SFO1 500.1730885 MHz  
 NUC1 1H  
 PU 3.33 usec  
 P1 10.00 usec  
 PLW1 20.93000031 W

F2 - Processing parameters  
 SI 65536  
 SF 500.1700000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

## 8.4 <sup>13</sup>C NMR OF ISFB-2

ISFB-2  
C13CPD DMSO {D:\Spectra} nmr 11



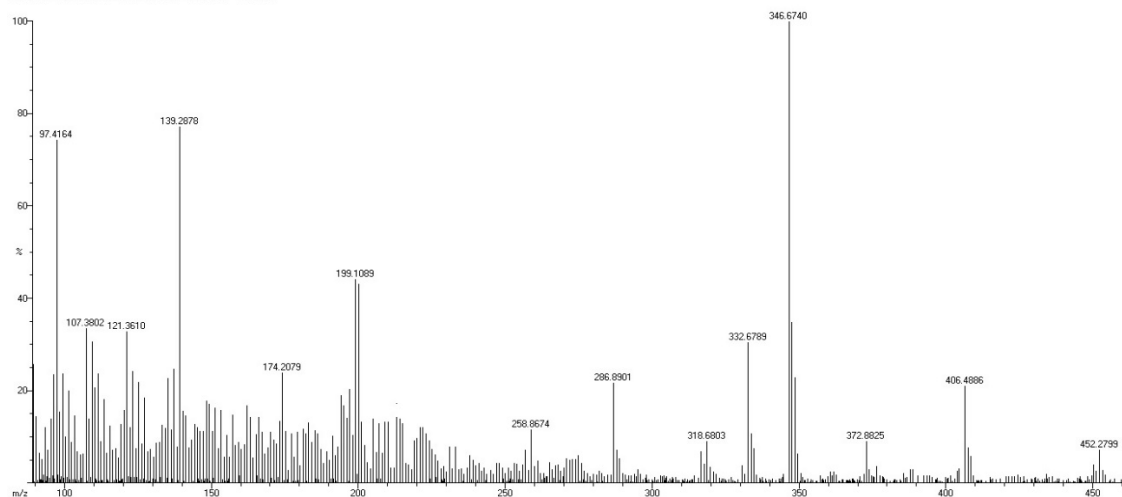
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

Current Data Parameters  
NAME Nov23-2022  
Date 20221123  
Time 19.31 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 37037.035 Hz  
FIDRES 1.130281 Hz  
AQ 0.8847360 sec  
RG 101  
DW 13.500 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1  
SF01 125.7804233 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 83.14099884 W  
SF02 500.1720007 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 80.00 usec  
PLW2 20.9300031 W  
PLW12 0.32703000 W  
PLW13 0.16449000 W

F2 - Processing parameters  
SI 32768  
SF 125.7679213 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## 8.5 MASS SPECTRA OF ISFB-2

ISFB-2  
Scan 712 TIC=7847632 Base=16.94FS # ions=972 RT=18.85

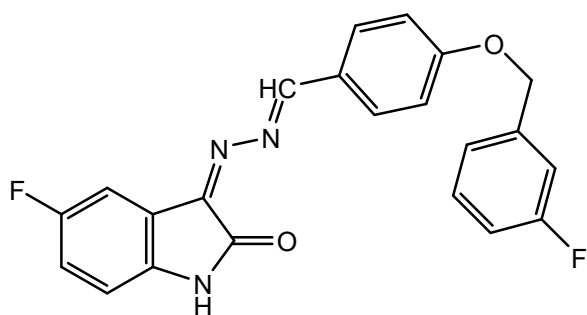


## 8.6 SPECTRAL INTERPRETATION:

*5-bromo-3-((4-((3-fluorobenzyl)oxy)benzylidene)hydrazineylidene)indolin-2-one (ISFB2):*

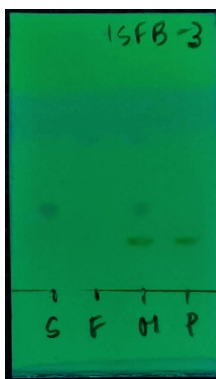
Dark orange, solid, 68%, melting point.  $240 \pm 2^\circ\text{C}$ . <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>)  $\delta$ : 10.98

(s, 1H, NH), 8.68 (s, 1H, =CH-), 8.13-6.87 (m, 11H, ArH), 5.26 (s, 2H, -CH<sub>2</sub>-).<sup>13</sup>C NMR (500 MHz, DMSO-d<sub>6</sub>) 164.18, 163.08, 162.95, 161.61, 149.78, 143.85, 139.32, 136.83, 130.94, 126.07, 123.58, 118.11, 114.76, 113.29, 112.72, 68.69. Chemical formula C<sub>22</sub>H<sub>15</sub>BrFN<sub>3</sub>O<sub>2</sub>. EI-HRMS (m/z): Calculated-452.2799, Observed- 452.2758.



**Figure S9.** ISFB3 structure

9.1 TLC OF ISFB-3: Mobile phase is Hexane: ethyl acetate (70:30)



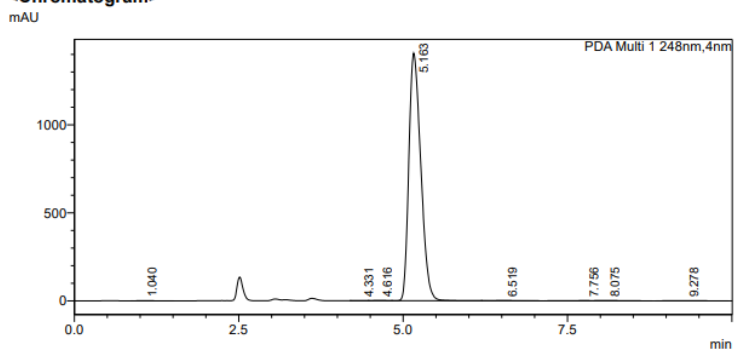
## 9.2 HPLC OF ISFB-3

### SHIMADZU LabSolutions Analysis Report

#### <Sample Information>

Sample Name : isatin001  
 Sample ID : isfb3  
 Data Filename : fluoro and bb\_05-12-2022\_005.lcd  
 Method Filename : isatin.lcm  
 Batch Filename : fluoro and bb.lcb  
 Vial # : 1-4  
 Injection Volume : 20 uL  
 Date Acquired : 12/5/2022 1:59:47 AM  
 Date Processed : 12/6/2022 10:38:58 PM  
 Sample Type : Standard  
 Level : 1  
 Acquired by : System Administrator  
 Processed by : System Administrator

#### <Chromatogram>



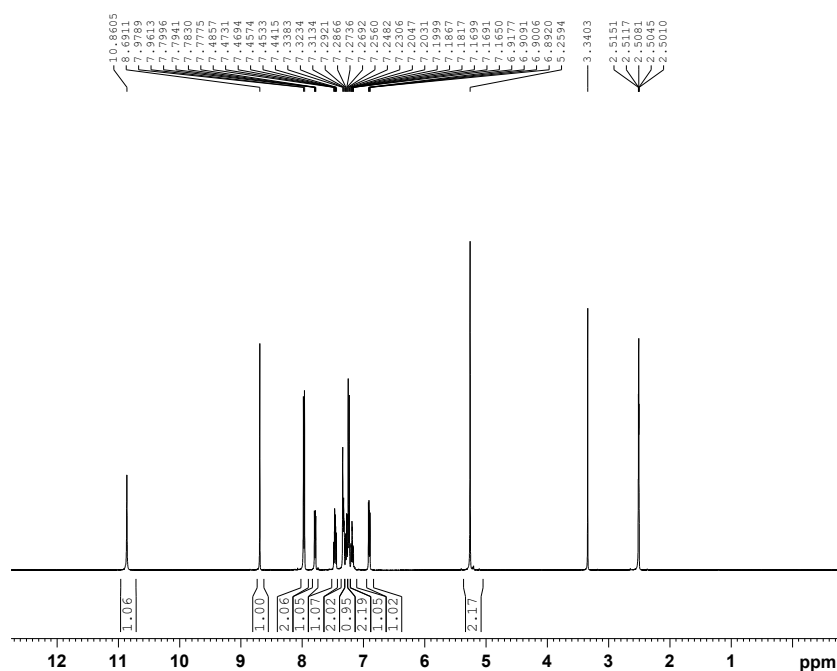
#### <Peak Table>

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	1.040	2803	136	0.016			
2	4.331	1171	138	0.007			
3	4.616	19751	1534	0.110			
4	5.163	17785891	1406472	99.151		V	
5	6.519	35192	1861	0.196		V	
6	7.756	34287	1238	0.191			
7	8.075	44788	2043	0.250		V	
8	9.278	14236	523	0.079			
Total		17938119	1413946				

## 9.3 <sup>1</sup>H NMR OF ISFB-3:



ISFB-3  
1H\_8scan DMSO {D:\Spectra} nmr 12



BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P.U.

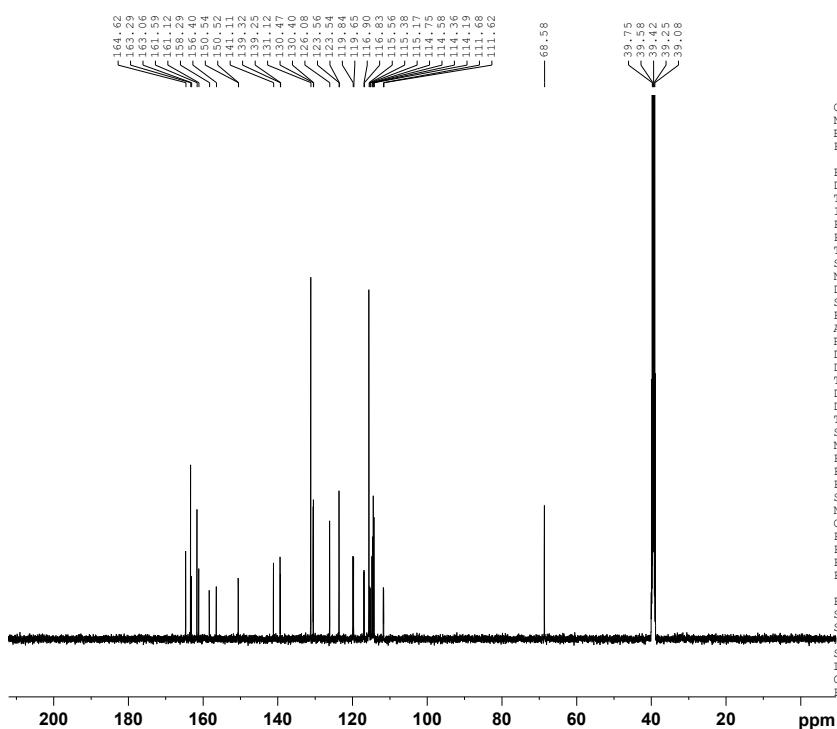
Current Data Parameters  
NAME Nov23-2022  
EXPNO 120  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 10.36 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 0  
SWH 14705.883 Hz  
FIDRES 0.448788 Hz  
AQ 2.2282240 sec  
RG 95.7854  
DW 34.000 usec  
DE 6.79 usec  
TE 300.2 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.1730885 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.93000031 W

F2 - Processing parameters  
SI 65536  
SF 500.1700000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

### 9.4 <sup>13</sup>C NMR OF ISFB-3:

ISFB-3  
C13CPD DMSO {D:\Spectra} nmr 12



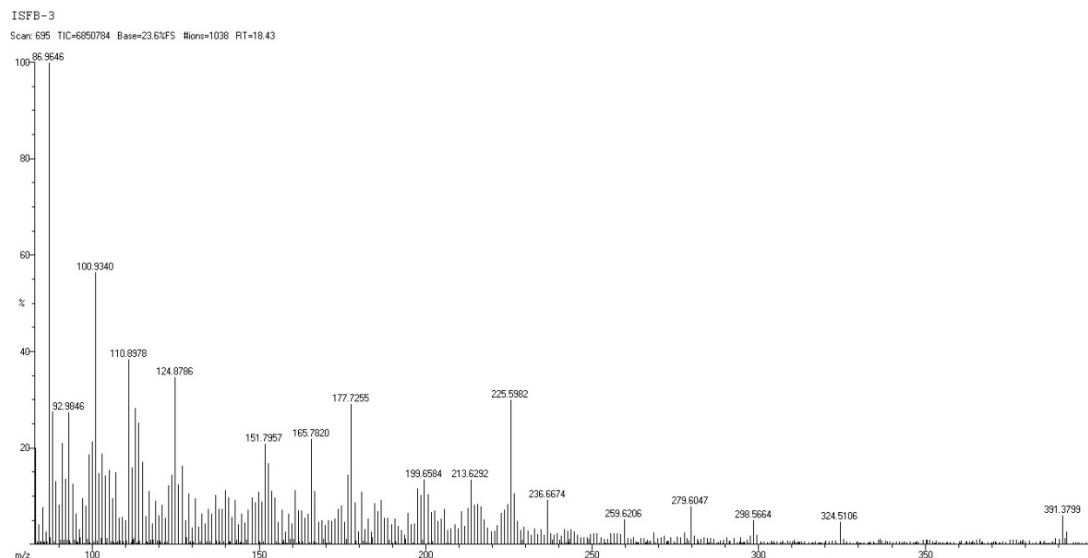
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

Current Data Parameters  
NAME Nov23-2022  
EXPNO 121  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 19.57 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 37037.035 Hz  
FIDRES 1.130281 Hz  
AQ 0.8847360 sec  
RG 101  
DW 13.500 usec  
DE 6.50 usec  
TE 300.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7804233 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 83.14099884 W  
SFO2 500.1720007 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 80.00 usec  
PLW2 20.93000031 W  
PLW12 0.32703000 W  
PLW13 0.16449000 W

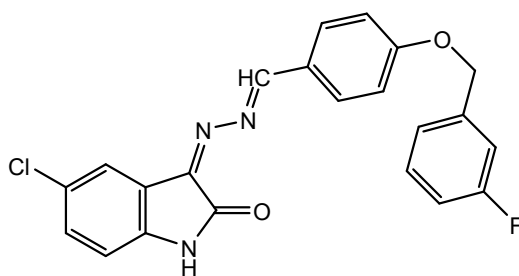
F2 - Processing parameters  
SI 32768  
SF 125.7679208 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

### 9.5 MASS SPECTRUM OF ISFB-3:



## 9.6 SPECTRAL INTERPRETATION:

*5-fluoro-3-((4-((3-fluorobenzyl)oxy)benzylidene)hydrazineylidene)indolin-2-one* (**ISFB3**):  
Brick red, solid, 82%, melting point.  $230 \pm 2^\circ\text{C}$ .  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.86 (s, 1H, NH), 8.69 (s, 1H, =CH-), 7.97-6.89(m, 11H, ArH), 5.25 (s, 2H, -CH<sub>2</sub>-).  $^{13}\text{C NMR}$  (500 MHz, DMSO- $d_6$ ) 164.62, 163.29, 161.89, 158.29, 156.40, 150.54, 141.11, 139.32, 131.12, 130.47, 126.08, 123.86, 119.84, 116.90, 115.66, 114.75, 111.68, 68.58. Chemical formula  $\text{C}_{22}\text{H}_{15}\text{F}_2\text{N}_3\text{O}_2$ . EI- HRMS (m/z): Calculated-391.3799, Observed- 391.3702.



**Figure S10.** ISFB4 structure

10.1 TLC OF ISFB-4: Mobile phase is Hexane: ethyl acetate (70:30)



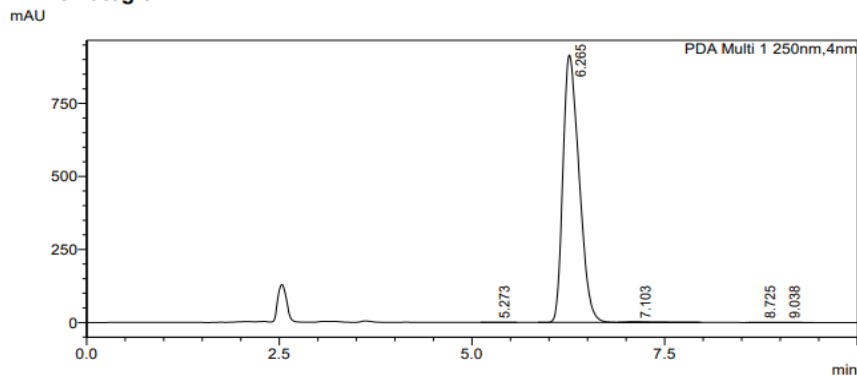
10.2 HPLC OF ISFB-4

SHIMADZU LabSolutions Analysis Report

<Sample Information>

Sample Name : isatin001  
 Sample ID : isfb4  
 Data Filename : fluoro and bb\_05-12-2022\_006.lcd  
 Method Filename : isatin.lcm  
 Batch Filename : fluoro and bb.lcb  
 Vial # : 1-5  
 Injection Volume : 20 uL  
 Date Acquired : 12/5/2022 2:10:10 AM  
 Date Processed : 12/6/2022 4:31:29 AM  
 Sample Type : Standard  
 Level : 1  
 Acquired by : System Administrator  
 Processed by : System Administrator

<Chromatogram>



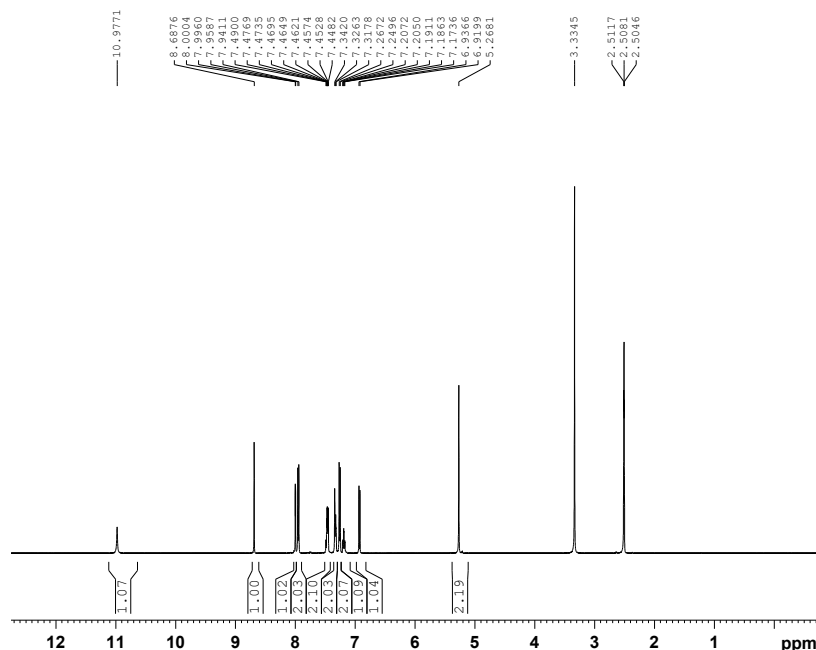
<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	5.273	3583	317	0.027			
2	6.265	13393299	914624	99.620		S	
3	7.103	41061	2069	0.305		T	
4	8.725	2877	172	0.021			
5	9.038	3518	242	0.026		V	
Total		13444337	917424				

### 10.3 <sup>1</sup>H NMR OF ISFB-4

ISFB-4

1H\_8scan DMSO {D:\Spectra} nmr 13



BRUKER  
 AVANCE NEO  
 500 MHz NMR  
 SPECTROMETER  
 SAIF, P.U.

Current Data Parameters  
 NAME Nov23-2022  
 EXPNO 130  
 PROCNO 1

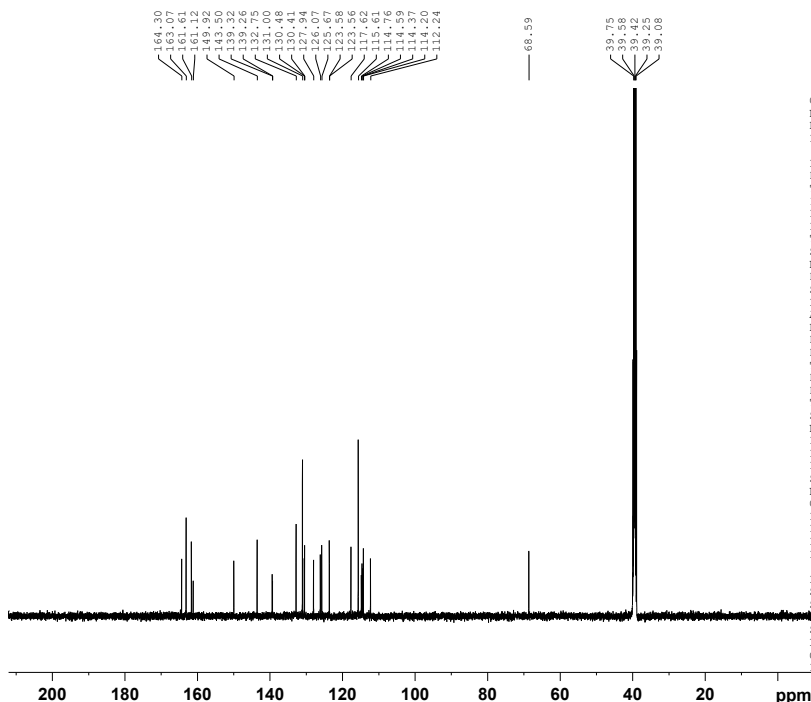
F2 - Acquisition Parameters  
 Date\_ 20221123  
 Time 10.39 h  
 INSTRUM Avance Neo 500  
 PROBHD Z119470\_0333 (  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 0  
 SWH 14705.883 Hz  
 FIDRES 0.448788 Hz  
 AQ 2.2282240 sec  
 RG 101  
 DW 34.000 usec  
 DE 6.79 usec  
 TE 300.2 K  
 D1 1.00000000 sec  
 TDO 1  
 SFO1 500.1730885 MHz  
 NUC1 1H  
 FO 3.33 usec  
 P1 10.00 usec  
 PLW1 20.93000031 W

F2 - Processing parameters  
 SI 65536  
 SF 500.1700000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 FC 1.00

### 10.4 <sup>13</sup>C NMR OF ISFB-4

ISFB-4

C13CPD DMSO {D:\Spectra} nmr 13



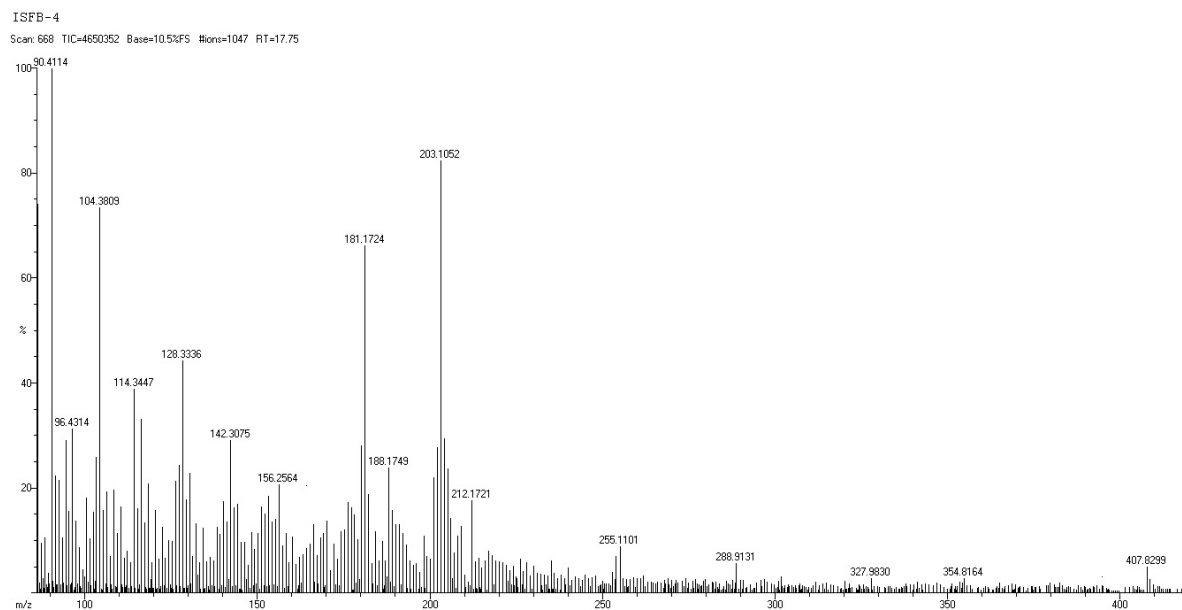
BRUKER  
 AVANCE NEO  
 500 MHz NMR SPECTROMETER  
 SAIF, PANJAB UNIVERSITY,  
 CHANDIGARH

Current Data Parameters  
 NAME Nov23-2022  
 EXPNO 131  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20221123  
 Time 20.24 h  
 INSTRUM Avance Neo 500  
 PROBHD Z119470\_0333 (  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 512  
 DS 4  
 SWH 37037.035 Hz  
 FIDRES 1.130281 Hz  
 AQ 0.8847360 sec  
 RG 101  
 DW 13.500 usec  
 DE 6.50 usec  
 TE 300.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1  
 SFO1 125.7804233 MHz  
 NUC1 13C  
 FO 3.33 usec  
 P1 10.00 usec  
 PLW1 83.14099884 W  
 SFO2 500.1720007 MHz  
 NUC2 1H  
 CPDPRG2 waltz65  
 ECPD2 80.00 usec  
 PLW2 20.93000031 W  
 PLW12 0.32703000 W  
 PLW13 0.16449000 W

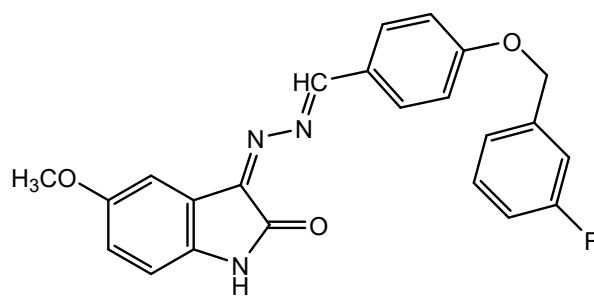
F2 - Processing parameters  
 SI 32768  
 SF 125.7679207 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.40

## 10.5 MASS SPECTRA OF ISFB-4



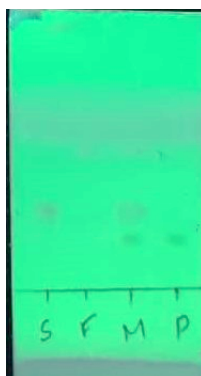
## 10.6 SPECTRAL INTERPRETATION:

*5-chloro-3-((4-((3-fluorobenzyl)oxy)benzylidene)hydrazineylidene)indolin-2-one* (**ISFB4**): Orange, solid, 78%, melting point.  $239 \pm 2^\circ\text{C}$ .  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.97 (s, 1H, NH), 8.68 (s, 1H, =CH-), 8.00-6.91 (m, 11H, ArH), 5.26 (s, 2H, -CH $_2$ -).  $^{13}\text{C}$  NMR (500 MHz, DMSO- $d_6$ ) 164.30, 163.07, 161.61, 149.92, 143.60, 139.32, 132.76, 131.00, 130.46, 127.94, 126.07, 125.67, 123.66, 117.62, 116.61, 114.76, 112.24, 68.69. Chemical formula  $\text{C}_{22}\text{H}_{15}\text{ClFN}_3\text{O}_2$ . EI- HRMS (m/z): Calculated-407.8299, Observed- 407.8248.



**Figure S11.** ISFB5 structure

11.1 TLC OF ISFB-5: Mobile phase is Hexane: ethyl acetate (70:30)



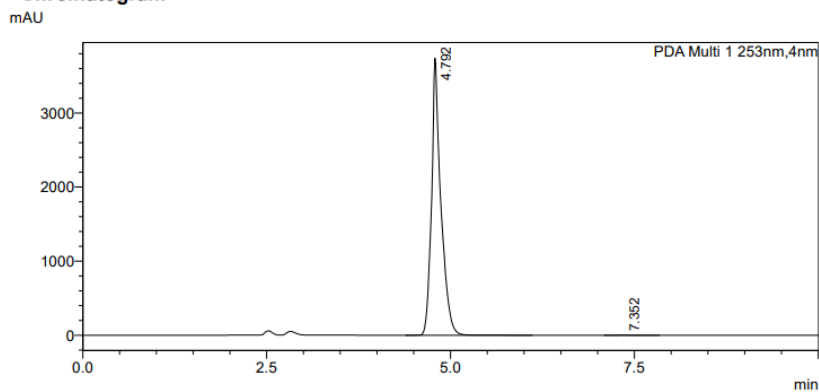
11.2 HPLC OF ISFB-5

**SHIMADZU LabSolutions Analysis Report**

**<Sample Information>**

Sample Name : isatin001  
 Sample ID : isfb5  
 Data Filename : fluoro and bb\_05-12-2022\_007.lcd  
 Method Filename : isatin.lcm  
 Batch Filename : fluoro and bb.lcb  
 Vial # : 1-6  
 Injection Volume : 20 uL  
 Date Acquired : 12/5/2022 2:20:31 AM  
 Date Processed : 12/6/2022 4:33:15 AM  
 Sample Type : Standard  
 Level : 1  
 Acquired by : System Administrator  
 Processed by : System Administrator

**<Chromatogram>**

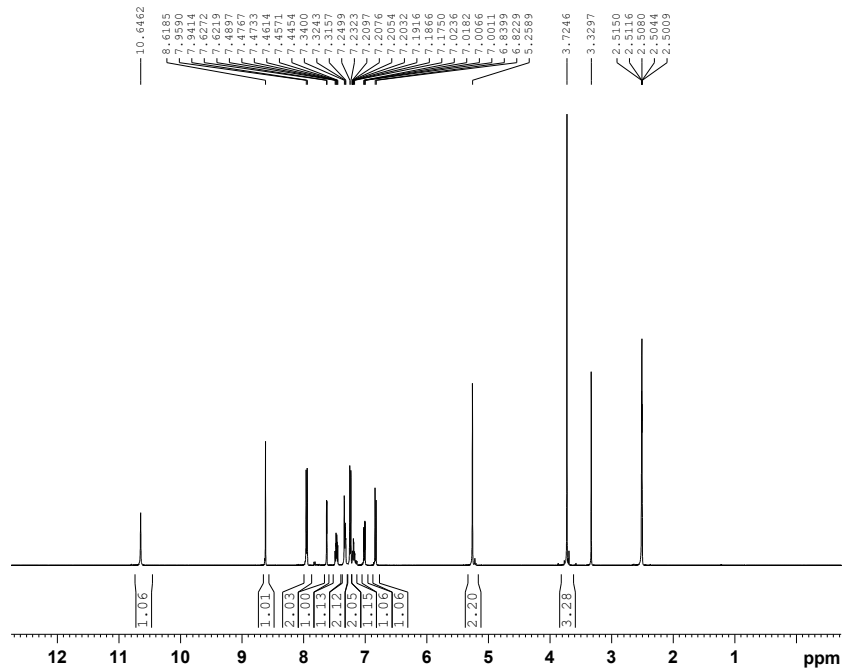


**<Peak Table>**

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1	4.792	33082034	3741328	99.973			
2	7.352	8796	486	0.027			
Total		33090830	3741814				

### 11.3 <sup>1</sup>H NMR OF ISFB-5

ISFB-5  
1H\_8scan DMSO {D:\Spectra} nmr 14



BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P.U.

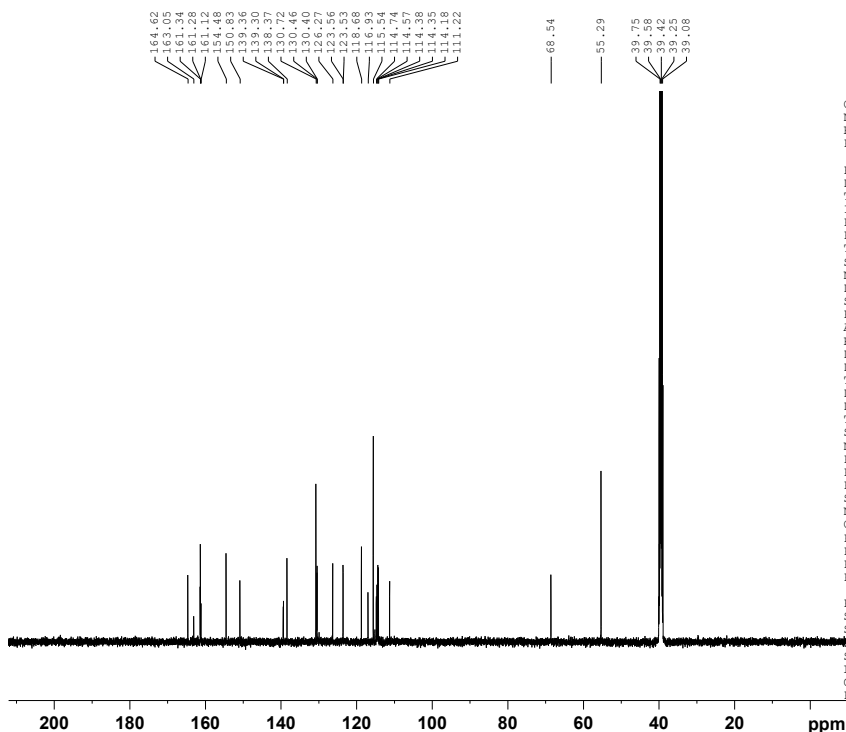
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NAME      Nov23-2022
EXPNO    140
PROCNO   1

F2 - Acquisition Parameters
Date_    20221123
Time     10.41 h
INSTRUM  Avance Neo 500
PROBHD   Z119470_0333 (
PULPROG  zg30
TD        65536
SOLVENT  DMSO
NS        16
DS        0
SWH       14705.883 Hz
FIDRES    0.448788 Hz
AQ         2.2282240 sec
RG         101
DW         34.000 usec
DE         6.79 usec
TE         300.2 K
D1         1.00000000 sec
TD0        1
SF01       500.1730885 MHz
NUC1       1H
P0         3.33 usec
P1         10.00 usec
PLW1       20.93000031 W

F2 - Processing parameters
SI         65536
SF         500.1700000 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

### 11.4 <sup>13</sup>C NMR OF ISFB-5

ISFB-5  
C13CPD DMSO {D:\Spectra} nmr 14



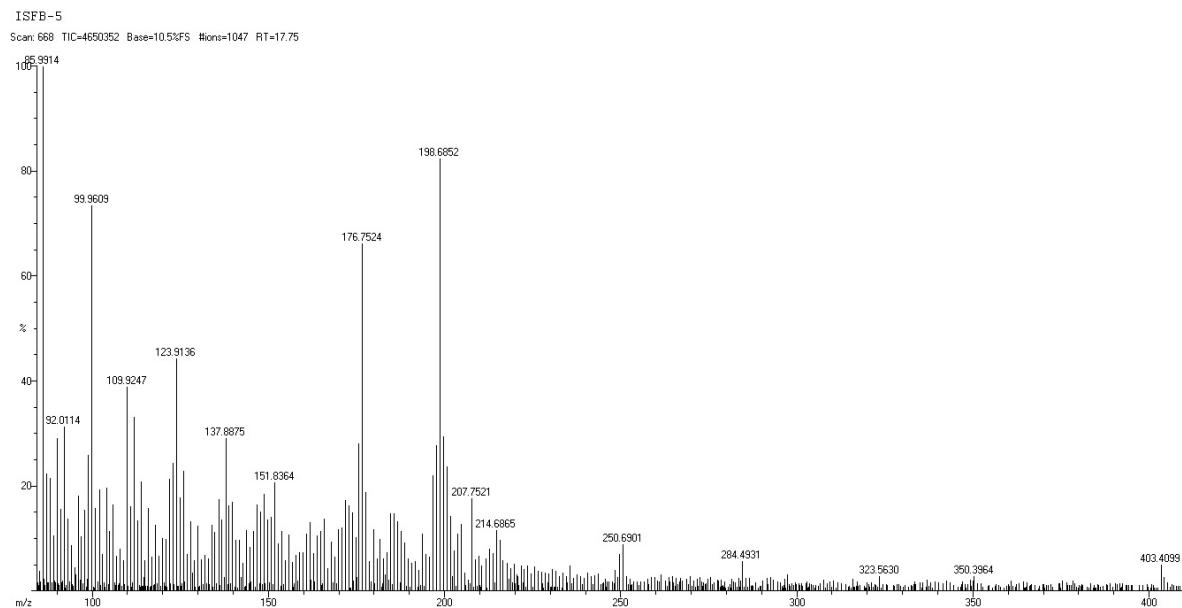
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

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Current Data Parameters
NAME      Nov23-2022
EXPNO    141
PROCNO   1

F2 - Acquisition Parameters
Date_    20221123
Time     20.51 h
INSTRUM  Avance Neo 500
PROBHD   Z119470_0333 (
PULPROG  zgpg30
TD        65536
SOLVENT  DMSO
NS        512
DS        4
SWH       37037.035 Hz
FIDRES    1.130281 Hz
AQ         0.8847360 sec
RG         101
DW         13.500 usec
DE         6.50 usec
TE         300.2 K
D1         2.00000000 sec
D11       0.03000000 sec
TD0        1
SF01       125.7804233 MHz
NUC1       13C
P0         3.33 usec
P1         10.00 usec
PLW1       83.14099884 W
SF02       500.1720007 MHz
NUC2       1H
CPDPRG[2] waltz65
PCPD2     80.00 usec
PLW2       20.93000031 W
PLW12     0.32703000 W
PLW13     0.16449000 W

F2 - Processing parameters
SI         32768
SF         125.7679211 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

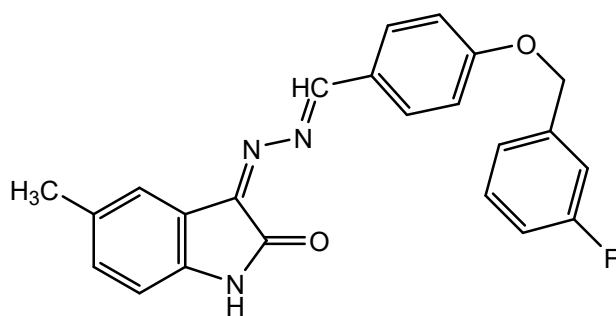
## 11.5 MASS SPECTRA OF ISFB-5



### 11.6 SPECTRAL INTERPRETATION:

*3-((4-((3-fluorobenzyl)oxy)benzylidene)hydrazineylidene)-5-methoxyindolin-2-one (ISFB5):*  
Brown, solid, 76%, melting point.  $195 \pm 2^\circ\text{C}$ .  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.64 (s, 1H, NH), 8.61 (s, 1H, =CH-), 7.95-6.82 (m, 11H, ArH), 5.25 (s, 2H, -CH<sub>2</sub>-), 3.72 (s, 3H, -CH<sub>2</sub>-Ar).  $^{13}\text{C NMR}$  (500 MHz, DMSO- $d_6$ ) 164.62, 163.05, 161.34, 154.48, 150.83, 139.36, 138.37, 130.72, 126.27, 123.56, 118.68, 116.93, 115.54, 114.74, 111.22, 68.54, 55.29. Chemical formula  $\text{C}_{23}\text{H}_{18}\text{FN}_3\text{O}_3$ . EI- HRMS (m/z): Calculated-403.4099, Observed- 403.4057.





**Figure S12.** ISFB6 structure

12.1 TLC OF ISFB-6: Mobile phase is Hexane: ethyl acetate (70:30)



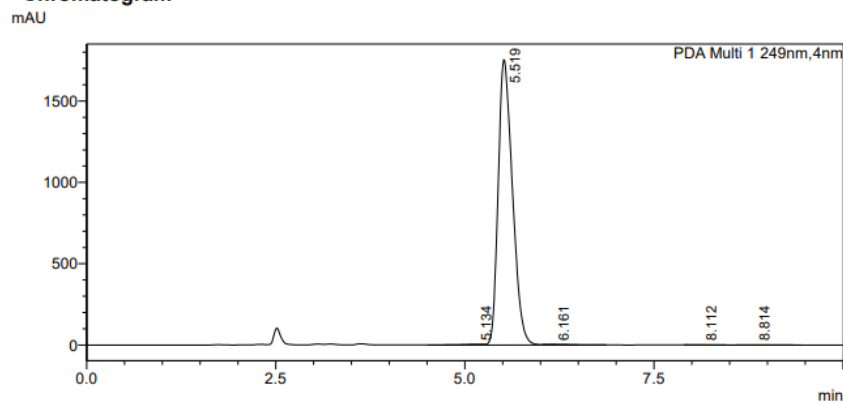
12.2 HPLC OF ISFB-6

**SHIMADZU LabSolutions Analysis Report**

**<Sample Information>**

Sample Name : isatin001  
 Sample ID : isfb6  
 Data Filename : fluoro and bb\_05-12-2022\_008.lcd  
 Method Filename : isatin.lcm  
 Batch Filename : fluoro and bb.lcb  
 Vial # : 1-7  
 Injection Volume : 20 uL  
 Date Acquired : 12/5/2022 2:30:53 AM  
 Date Processed : 12/6/2022 4:38:13 AM  
 Sample Type : Standard  
 Level : 1  
 Acquired by : System Administrator  
 Processed by : System Administrator

**<Chromatogram>**



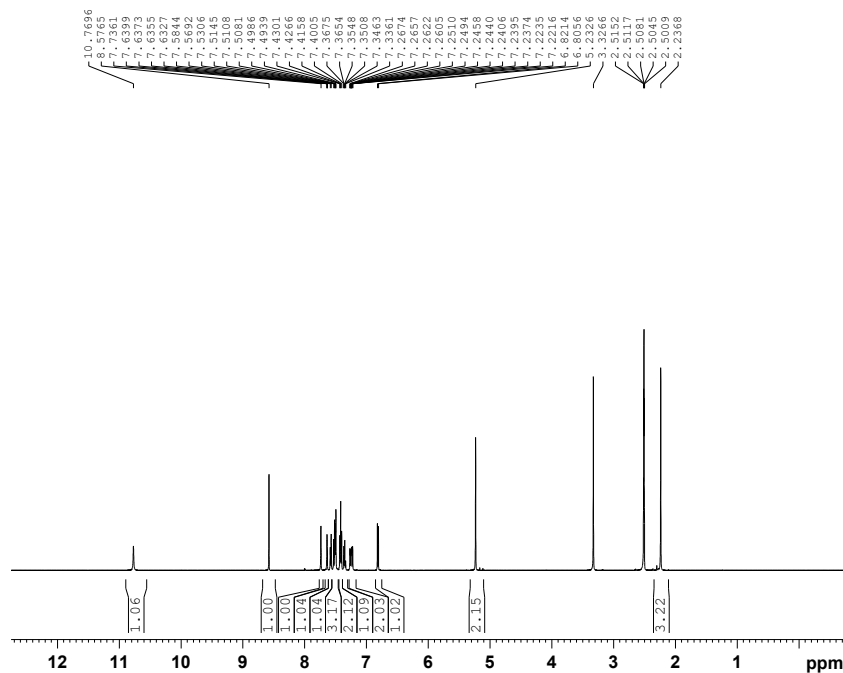
**<Peak Table>**

PDA Ch1 249nm

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	5.134	95496	4313	0.412			
2	5.519	23026214	1752400	99.437		SV	
3	6.161	17833	1371	0.077		T	
4	8.112	4803	293	0.021			
5	8.814	12300	497	0.053			
Total		23156646	1758873				

### 12.3 <sup>1</sup>H NMR OF ISFB-6

ISFB-6  
1H\_8scan DMSO {D:\Spectra} nmr 15



BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P.U.

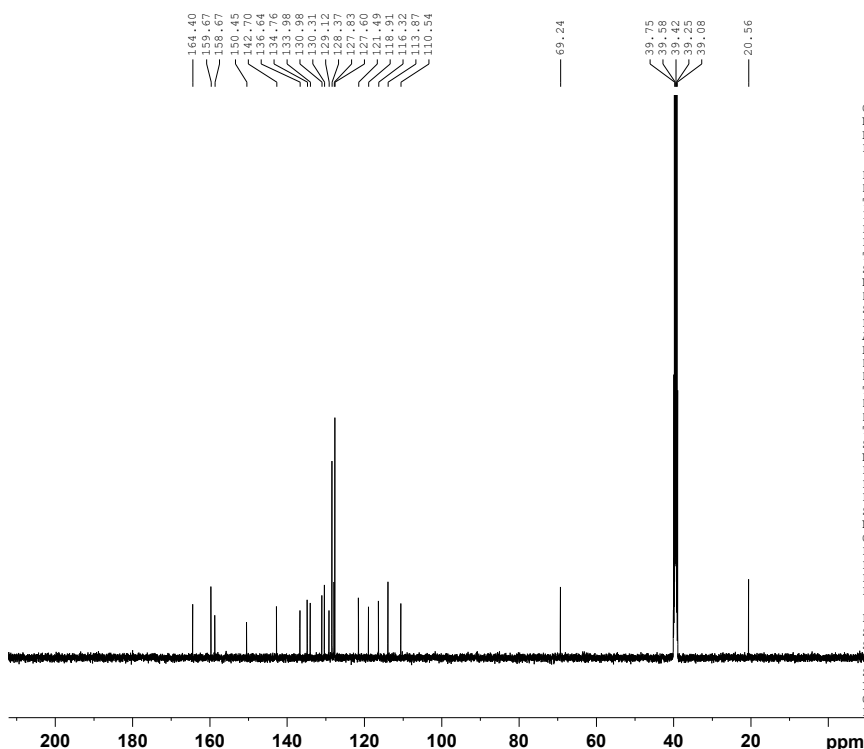
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NAME Nov23-2022  
EXPNO 150  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 10.44 h  
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PROBHD Z119470\_0333 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 0  
SWH 14705.883 Hz  
FIDRES 0.448788 Hz  
AQ 2.2282240 sec  
RG 101  
DW 34.000 usec  
DE 6.79 usec  
TE 300.2 K  
D1 1.00000000 sec  
TD0 1  
SF01 500.1730885 MHz  
NUC1 1H  
PO 3.33 usec  
P1 10.00 usec  
PLW1 20.93000031 W

F2 - Processing parameters  
SI 65536  
SF 500.1700000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

### 12.4 <sup>13</sup>C NMR OF ISFB-6

ISFB-6  
C13CPD DMSO {D:\Spectra} nmr 15



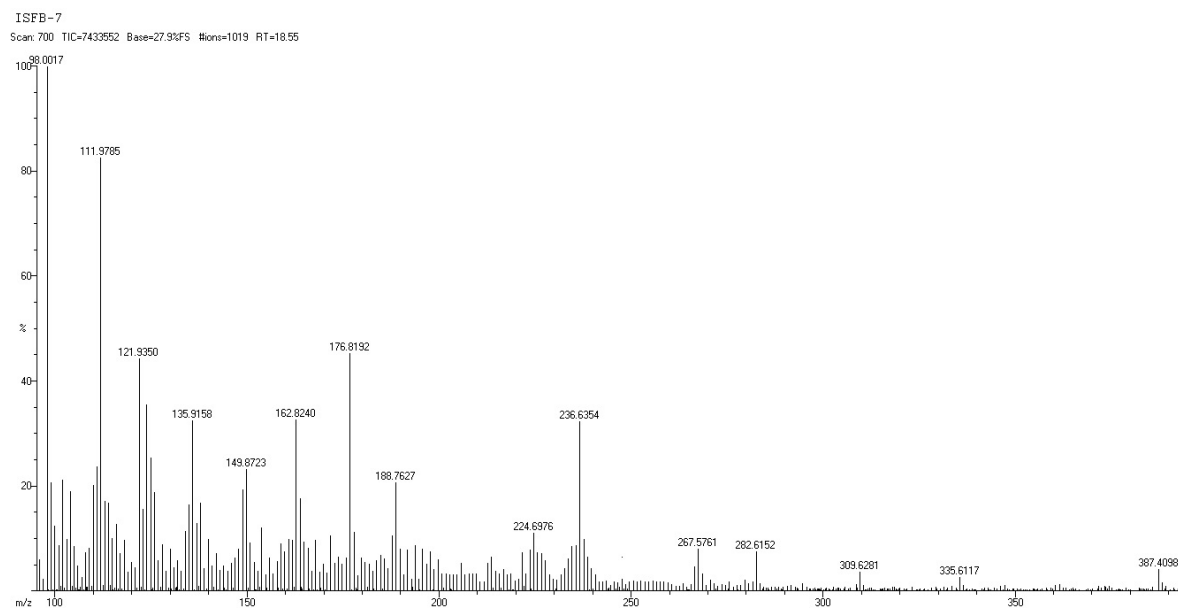
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

Current Data Parameters  
NAME Nov23-2022  
EXPNO 151  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 21.18 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 37037.035 Hz  
FIDRES 1.130281 Hz  
AQ 0.8847360 sec  
RG 101  
DW 13.500 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 125.7804233 MHz  
NUC1 13C  
PO 3.33 usec  
P1 10.00 usec  
PLW1 83.14099884 W  
SF02 500.1720007 MHz  
NUC2 1H  
CPDPRG[2 waltz65  
PCPD2 80.00 usec  
PLW2 20.93000031 W  
PLW12 0.32703000 W  
PLW13 0.16449000 W

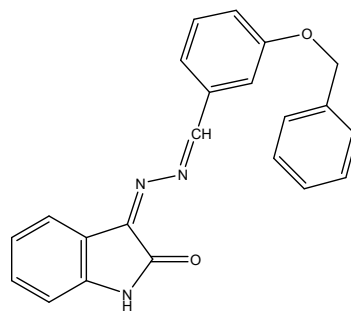
F2 - Processing parameters  
SI 32768  
SF 125.7679213 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## 12.5 MASS SPECTRA OF ISFB-6



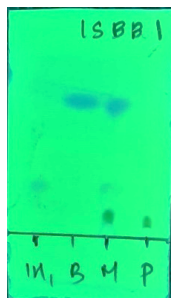
## 12.6 SPECTRAL INTERPRETATION

*3-((4-((3-fluorobenzyl)oxy)benzylidene)hydrazineylidene)-5-methylindolin-2-one* (**ISFB6**): Orange, solid, 88%, melting point.  $212 \pm 2^\circ\text{C}$ .  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.76 (s, 1H, NH), 8.57 (s, 1H, =CH-), 7.73-6.80 (m, 11H, ArH), 5.23 (s, 2H, -CH<sub>2</sub>-), 2.23 (s, 3H, -CH<sub>2</sub>-Ar).  $^{13}\text{C NMR}$  (500 MHz, DMSO- $d_6$ ) 164.40, 169.67, 168.67, 160.48, 142.70, 136.64, 134.76, 133.96, 130.98, 129.12, 128.37, 127.60, 121.49, 118.91, 116.32, 113.87, 110.54, 69.24, 20.56. Chemical formula  $\text{C}_{23}\text{H}_{18}\text{FN}_3\text{O}_2$ . EI- HRMS (m/z): Calculated-387.4098, Observed- 387.4063.



**Figure S13.** ISBB1 structure

13.1 TLC OF ISBB-1: Mobile phase is Hexane: ethyl acetate (70:30)



13.2 HPLC OF ISBB-1

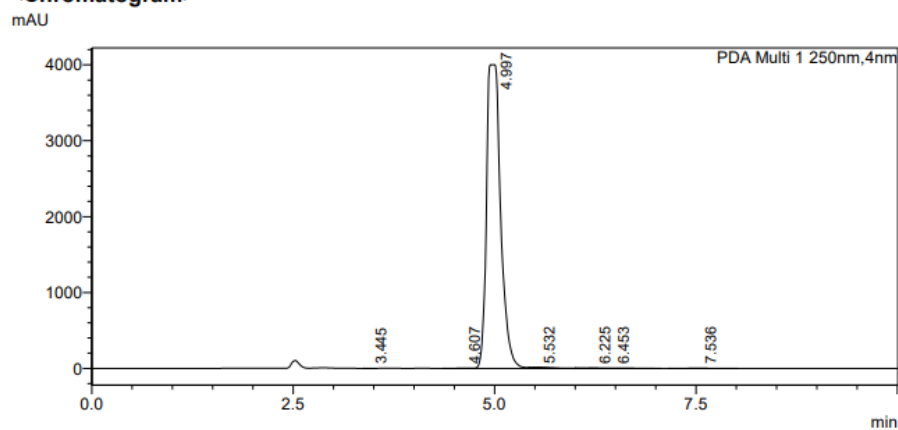


## Analysis Report

### <Sample Information>

Sample Name	: isatin001	Sample Type	: Standard
Sample ID	: isbb1	Level	: 1
Data Filename	: fluoro and bb_05-12-2022_009.lcd	Acquired by	: System Administrator
Method Filename	: isatin.lcm	Processed by	: System Administrator
Batch Filename	: fluoro and bb.lcb		
Vial #	: 1-8		
Injection Volume	: 20 uL		
Date Acquired	: 12/5/2022 2:41:16 AM		
Date Processed	: 12/6/2022 4:41:09 AM		

### <Chromatogram>

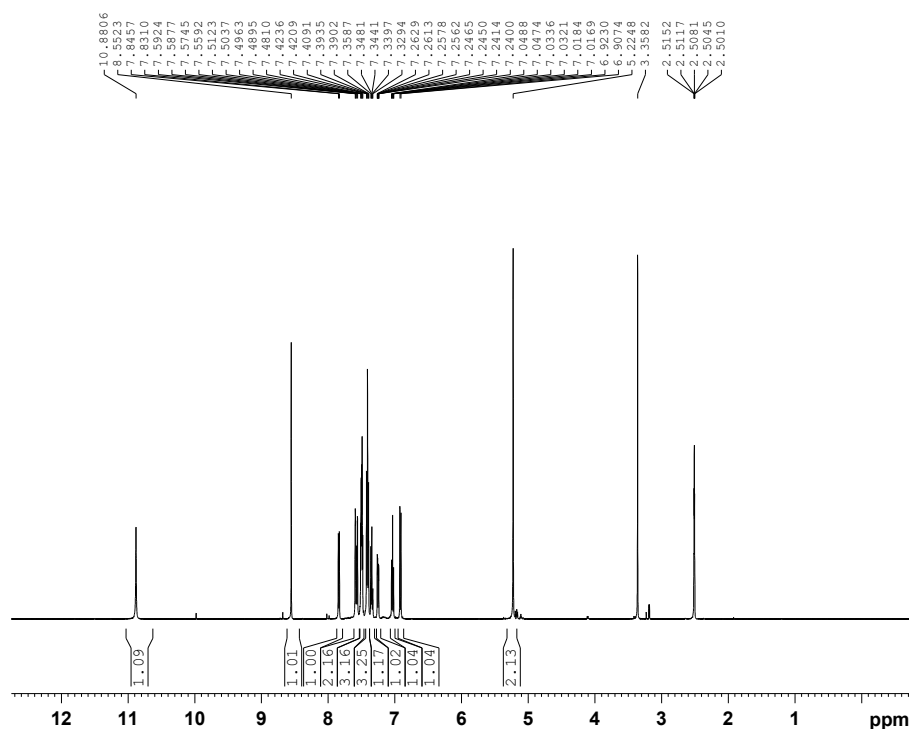


### <Peak Table>

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	3.445	1931	228	0.004			
2	4.607	6937	500	0.014			
3	4.997	48906742	3999836	99.630		SV	
4	5.532	79091	7379	0.161		T	
5	6.225	51237	3427	0.104		T	
6	6.453	29557	2266	0.060		TV	
7	7.536	12683	558	0.026			
Total		49088178	4014195				

### 13.3 <sup>1</sup>H NMR OF ISBB-1

ISBB-1  
1H\_8scan DMSO {D:\Spectra} nmr 16



BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P.U.

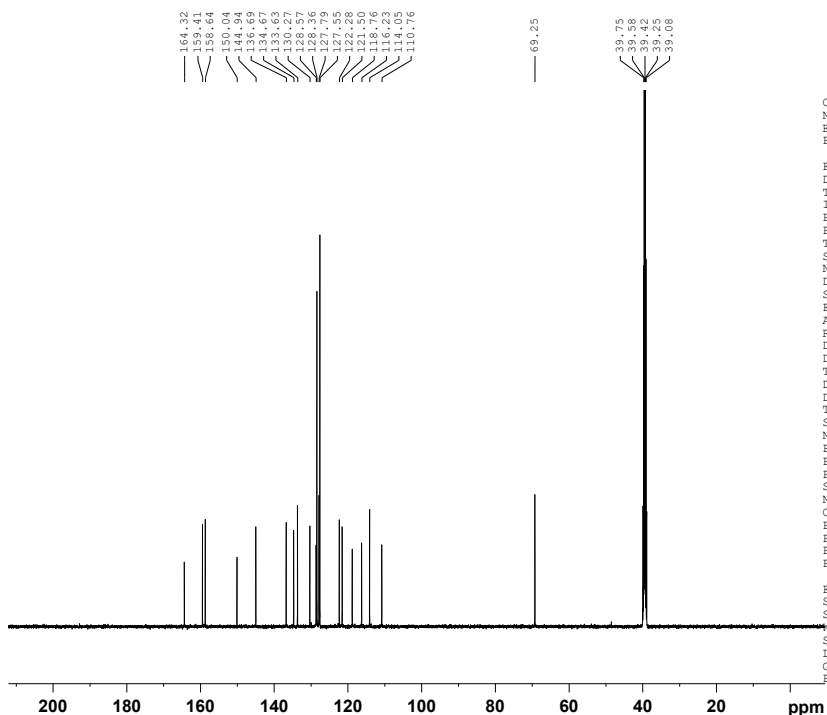
Current Data Parameters  
NAME Nov23-2022  
EXPNO 160  
PROCNO 1

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Date\_ 20221123  
Time\_ 10.46 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 0  
SWH 14705.883 Hz  
FIDRES 0.448788 Hz  
AQ 2.2282240 sec  
RG 95.7854  
DW 34.000 usec  
DE 6.79 usec  
TE 300.2 K  
D1 1.00000000 sec  
TDO 1  
SFO1 500.1730885 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.93000031 W

F2 - Processing parameters  
SI 65536  
SF 500.1700000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
FC 1.00

### 13.4 <sup>13</sup>C NMR OF ISBB-1

ISBB-1  
C13CPD DMSO {D:\Spectra} nmr 16



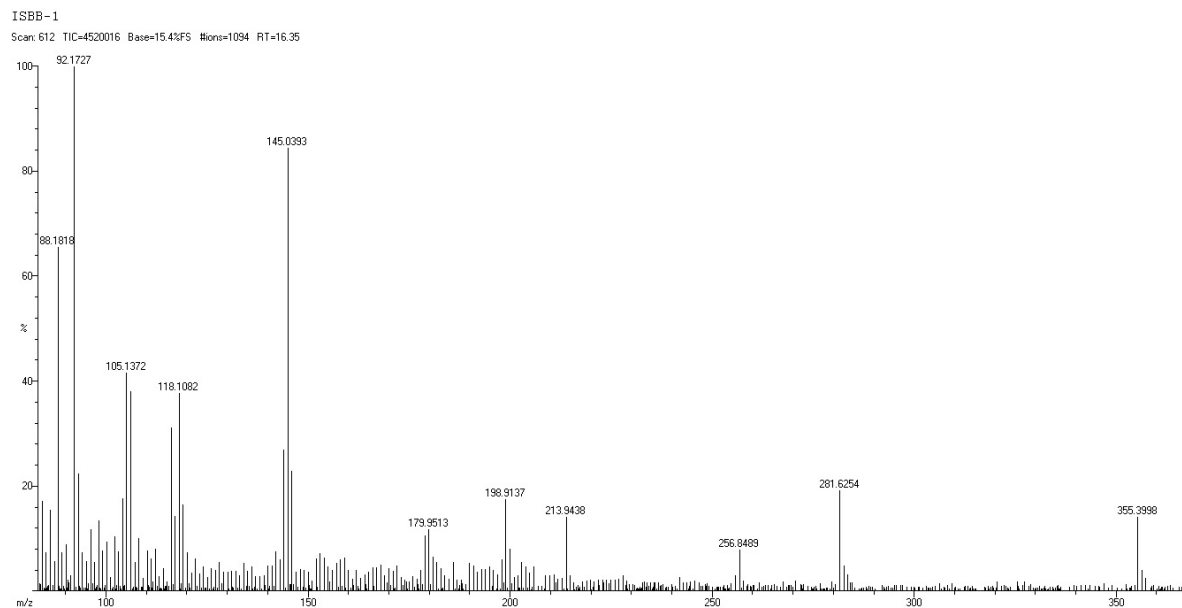
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

Current Data Parameters  
NAME Nov23-2022  
EXPNO 161  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 21.44 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 37037.035 Hz  
FIDRES 1.130281 Hz  
AQ 0.8847360 sec  
RG 101  
DW 13.500 usec  
DE 6.50 usec  
TE 300.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1  
SFO1 125.7804233 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 83.14099884 W  
SFO2 500.1720007 MHz  
NUC2 1H  
CPDPRG2 waltz65  
PCPD2 80.00 usec  
PLW2 20.93000031 W  
PLW12 0.32703000 W  
PLW13 0.16449000 W

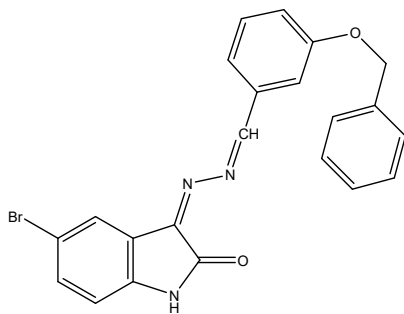
F2 - Processing parameters  
SI 32768  
SF 125.7679210 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
FC 1.40

### 13.5 MASS SPECTRA OF ISBB-1



### 13.6 SPECTRAL INTERPRETATION:

*3-((3-(benzyloxy)benzylidene)hydrazineylidene)indolin-2-one (ISBB1):* Dark red, solid, 78%, melting point.  $228 \pm 2^\circ\text{C}$ .  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.88 (s, 1H, NH), 8.55 (s, 1H, =CH-), 7.84-6.90 (m, 13H, ArH), 5.22 (s, 2H, -CH $_2$ -).  $^{13}\text{C}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 164.32, 159.41, 158.64, 160.04, 144.94, 136.69, 134.37, 133.63, 130.27, 128.57, 127.79, 122.28, 121.80, 116.76, 114.06, 110.76, 69.28. Chemical formula  $\text{C}_{22}\text{H}_{17}\text{N}_3\text{O}_2$ . EI- HRMS (m/z): Calculated-355.3998, Observed- 355.3998.



**Figure S14.** ISBB2 structure

14.1 TLC OF ISBB-2: Mobile phase is Hexane: ethyl acetate (70:30)



14.2 HPLC OF ISBB-2

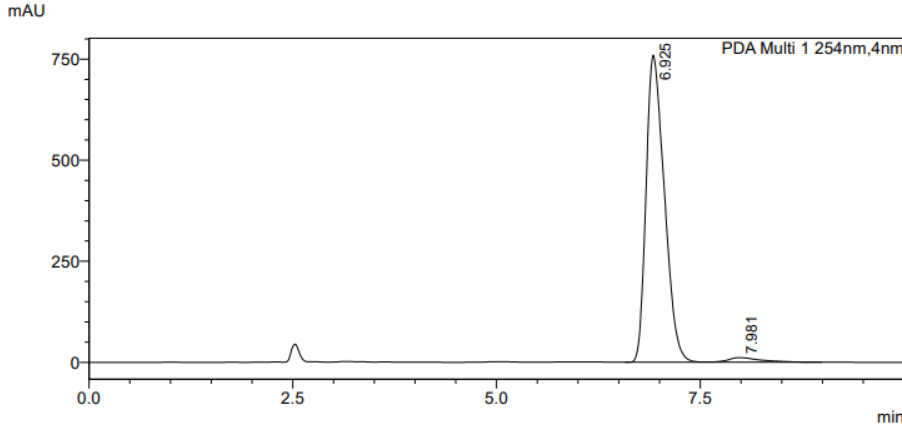
<Sample Information>

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Sample Name       : isatin001
Sample ID        : isbb2
Data Filename    : fluoro and bb_05-12-2022_010.lcd
Method Filename  : isatin.lcm
Batch Filename   : fluoro and bb.lcb
Vial #          : 1-9
Injection Volume : 20 uL
Date Acquired   : 12/5/2022 2:51:39 AM
Date Processed  : 12/6/2022 10:45:14 PM

Sample Type      : Standard
Level           : 1
Acquired by     : System Administrator
Processed by    : System Administrator
    
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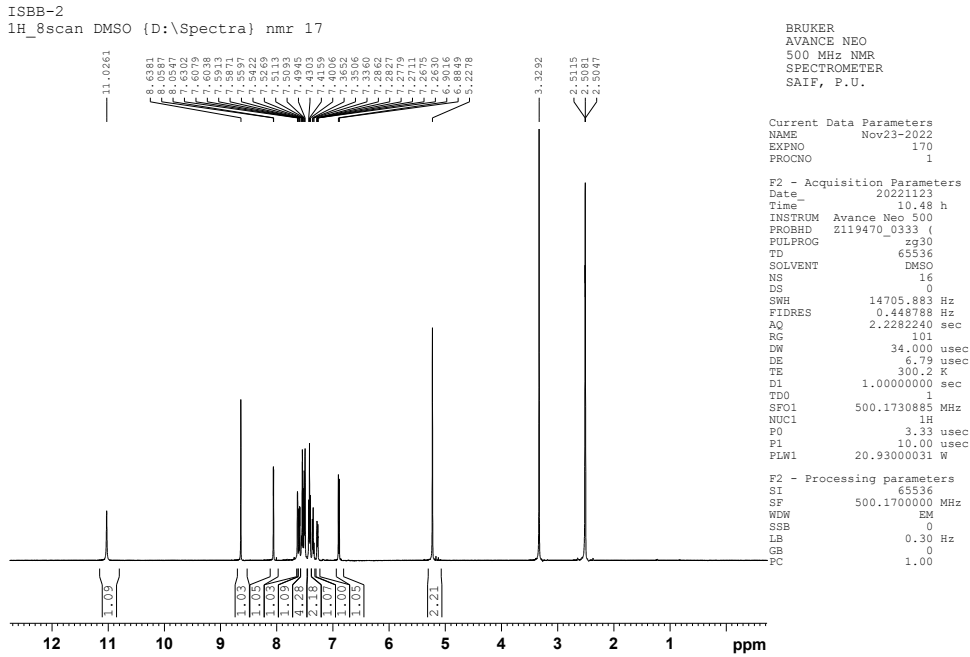
<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	6.925	11885761	759058	97.327			
2	7.981	326456	11494	2.673		V	
Total		12212217	770551				

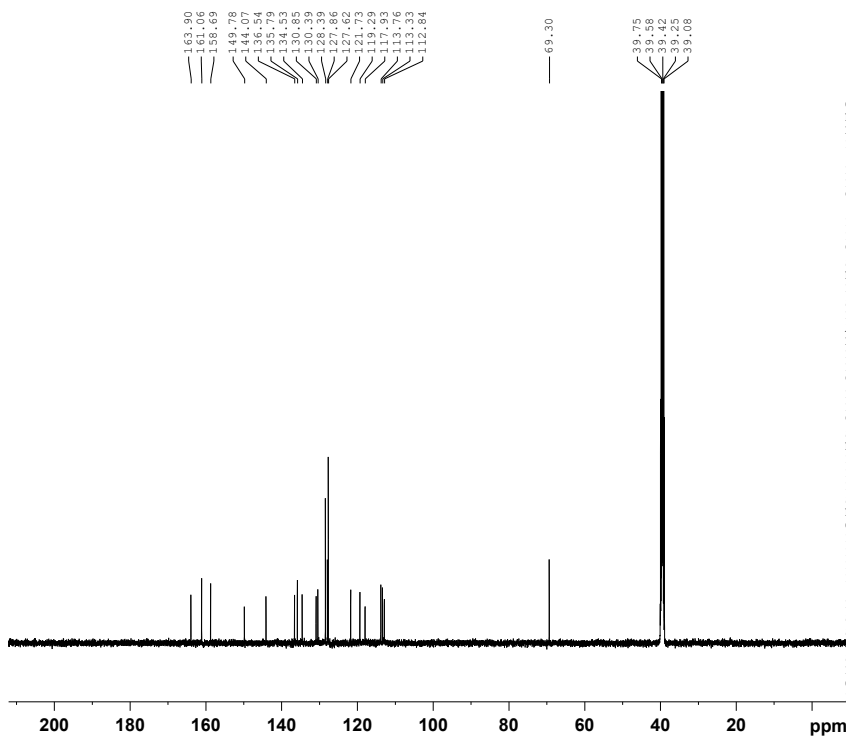
14.3 <sup>1</sup>H NMR OF ISBB-2



14.4 <sup>13</sup>C NMR OF ISBB-2



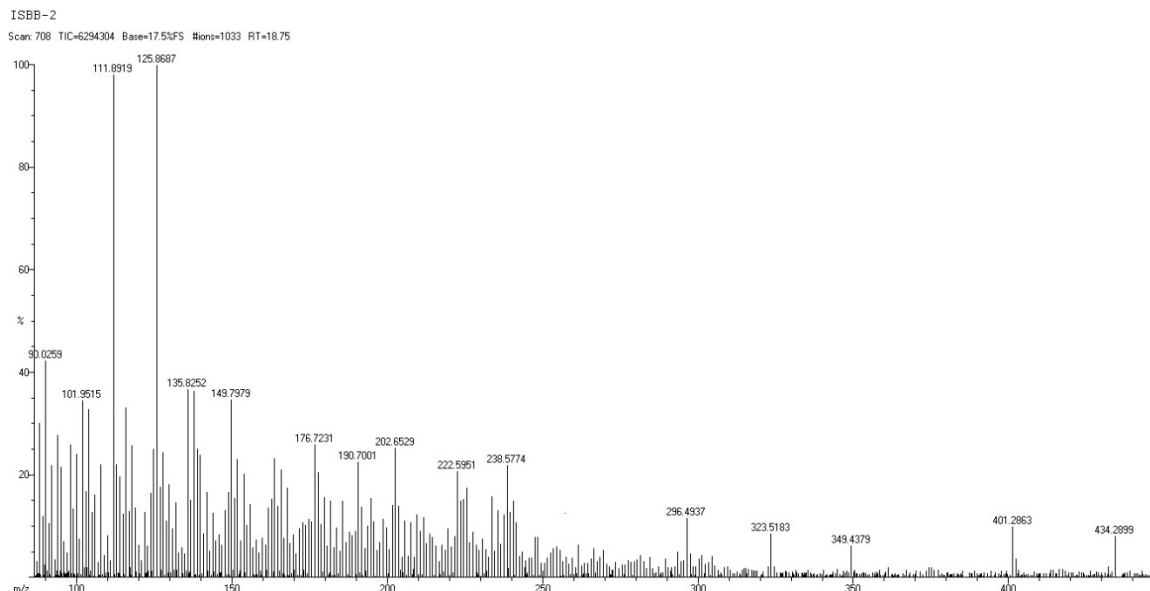
ISBB-2  
 C13CPD DMSO {D:\Spectra} nmr 17



BRUKER  
 AVANCE NEO  
 500 MHz NMR SPECTROMETER  
 SAIF, PANJAB UNIVERSITY,  
 CHANDIGARH

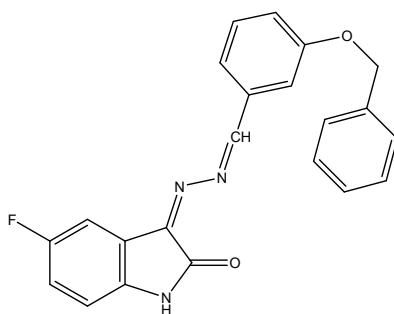
Current Data Parameters  
 NAME Nov23-2022  
 EXPNO 171  
 PROCNO 1  
 F2 - Acquisition Parameters  
 Date\_ 20221123  
 Time 22.11 h  
 INSTRUM Avance Neo 500  
 PROBHD Z119470\_0333 ( )  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 512  
 DS 4  
 SWH 37037.035 Hz  
 FIDRES 1.130281 Hz  
 AQ 0.8847360 sec  
 RG 101  
 DW 13.500 usec  
 DE 6.50 usec  
 TE 300.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1  
 SF01 125.7804233 MHz  
 NUC1 13C  
 P0 3.33 usec  
 P1 10.00 usec  
 PLW1 83.14099984 W  
 SF02 500.1720007 MHz  
 NUC2 1H  
 CPDPRG2 waltz65  
 PCPD2 80.00 usec  
 PLW2 20.93000031 W  
 PLW12 0.32703000 W  
 PLW13 0.16449000 W  
 F2 - Processing parameters  
 SI 32768  
 SF 125.7679213 MHz  
 NDNW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.40

### 14.5 MASS SPECTRA OF ISBB-2



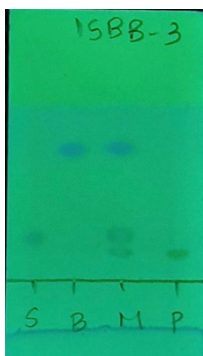
### 14.6 SPECTRAL INTERPRETATION:

*3-((3-(benzyloxy)benzylidene)hydrazineylidene)-5-bromoindolin-2-one (ISBB2)*: Orange, solid, 69%, melting point.  $235 \pm 2^\circ\text{C}$ .  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 11.02 (s, 1H, NH), 8.63 (s, 1H, =CH-), 8.05-6.88 (m, 12H, ArH), 5.22 (s, 2H, -CH $_2$ -)  $^{13}\text{C}$  NMR (500 MHz, DMSO- $d_6$ ) 163.90, 161.06, 158.69, 149.78, 144.07, 136.64, 135.79, 134.53, 130.85, 128.39, 127.62, 121.62, 119.29, 117.93, 113.76, 112.84, 69.30. Chemical formula  $\text{C}_{22}\text{H}_{16}\text{BrN}_3\text{O}_2$ . EI- HRMS (m/z): Calculated-434.2899, Observed- 434.2853.



**Figure S15.** ISBB3 structure

15.1 TLC OF ISBB-3: Mobile phase is Hexane: ethyl acetate (70:30)



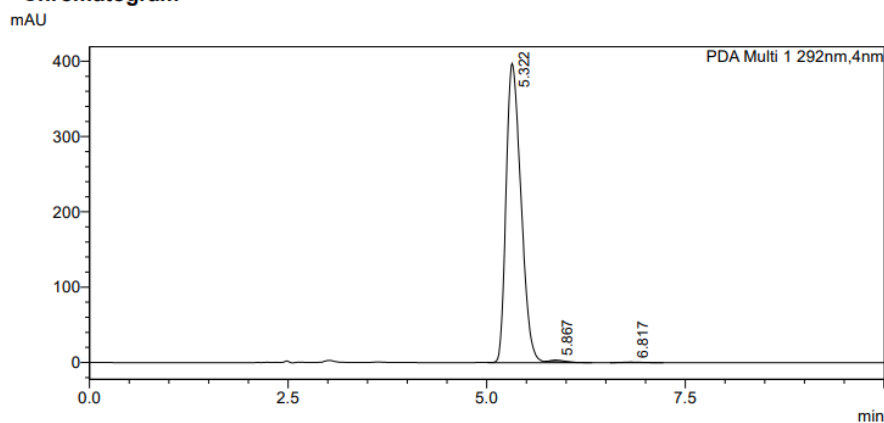
## 15.2 HPLC OF ISBB-3

# SHIMADZU LabSolutions Analysis Report

### <Sample Information>

Sample Name : isatin001  
 Sample ID : isbb3  
 Data Filename : fluoro and bb\_05-12-2022\_011.lcd  
 Method Filename : isatin.lcm  
 Batch Filename : fluoro and bb.lcb  
 Vial # : 1-10  
 Injection Volume : 20 uL  
 Date Acquired : 12/5/2022 3:02:02 AM  
 Date Processed : 12/6/2022 10:25:05 PM  
 Sample Type : Standard  
 Level : 1  
 Acquired by : System Administrator  
 Processed by : System Administrator

### <Chromatogram>



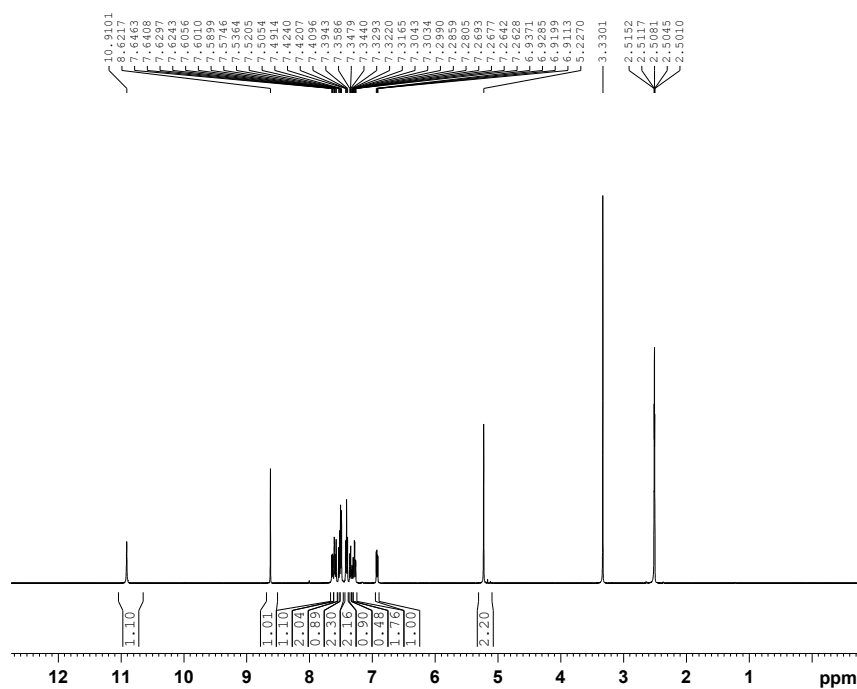
### <Peak Table>

PDA Ch1 292nm

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2	5.867	24549	2149	0.470		T	
3	6.817	10723	673	0.205			
Total		5222621	399970				

## 15.3 <sup>1</sup>H NMR OF ISBB-3

ISBB-3  
1H\_scan DMSO {D:\Spectra} nmr 18



BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P.U.

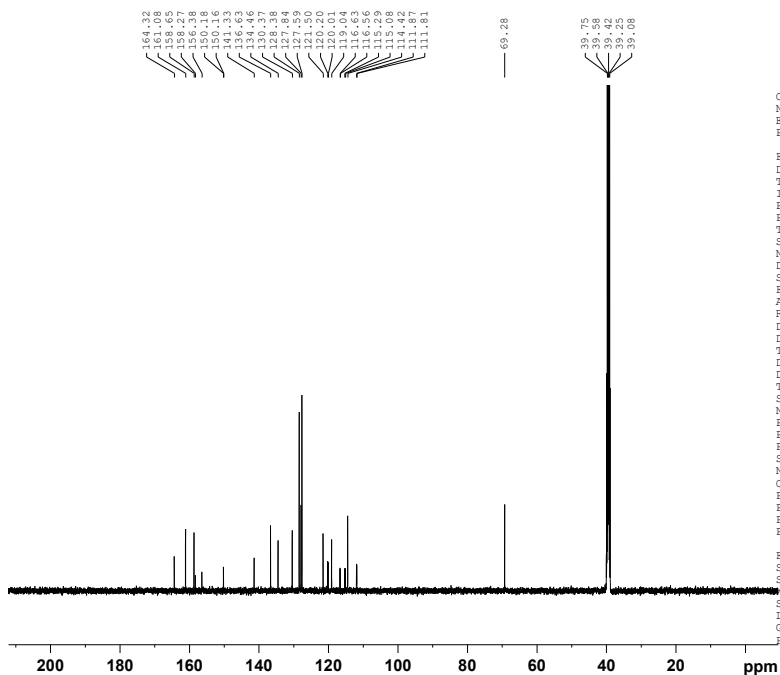
Current Data Parameters  
NAME Nov23-2022  
EXFNO 180  
PROCNO 1

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Date\_ 20221123  
Time\_ 10.51 h  
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PROBHD Z119470\_0333 ( )  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 0  
SWH 14705.883 Hz  
FIDRES 0.448788 Hz  
AQ 2.2282240 sec  
RG 101  
DW 34.000 usec  
DE 6.79 usec  
TE 300.2 K  
D1 1.00000000 sec  
TD0 1  
SF01 500.1730885 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.93000031 W

F2 - Processing parameters  
SI 65536  
SF 500.1700000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

### 15.4 <sup>13</sup>C NMR OF ISBB-3

ISBB-3  
C13CPD DMSO {D:\Spectra} nmr 18



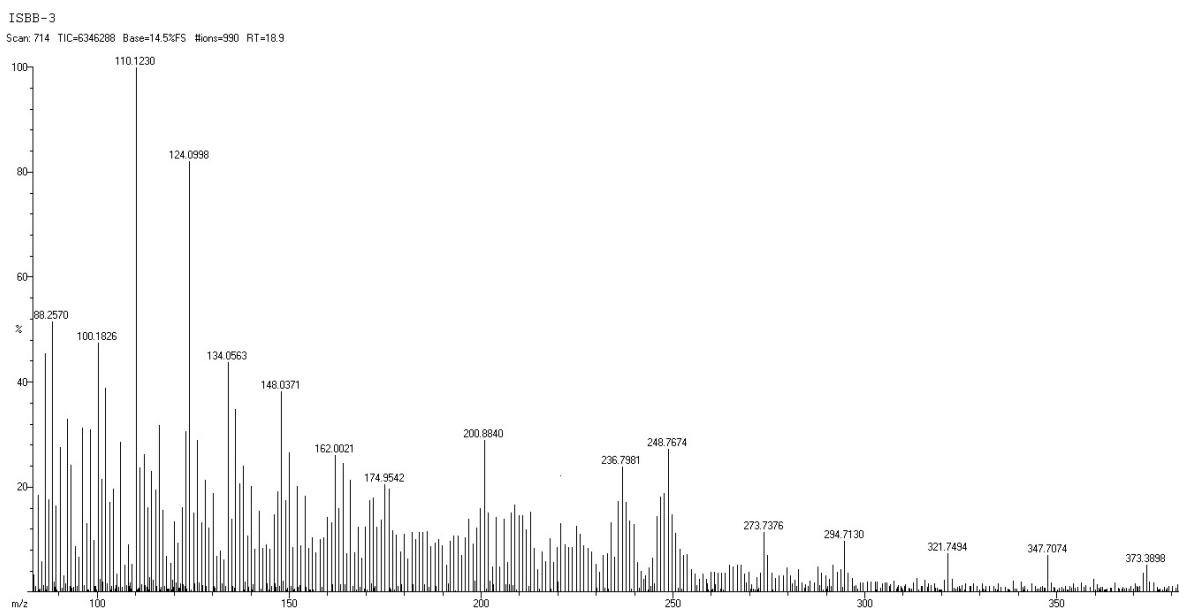
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

Current Data Parameters  
NAME Nov23-2022  
EXFNO 181  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 22.38 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 ( )  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 37037.035 Hz  
FIDRES 1.130281 Hz  
AQ 0.8847360 sec  
RG 101  
DW 13.500 usec  
DE 6.50 usec  
TE 300.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SF01 125.7804233 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 83.14099884 W  
SF02 500.1720007 MHz  
NUC2 1H  
CPDPRG2 waltz65  
PCPD2 80.00 usec  
PLW2 20.93000031 W  
PLW12 0.32703000 W  
PLW13 0.16449000 W

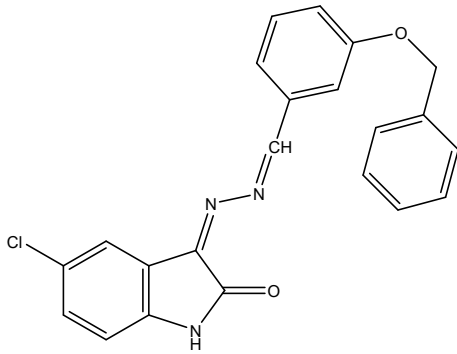
F2 - Processing parameters  
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SF 125.7679210 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

### 15.5 MASS SPECTRUM OF ISBB-3



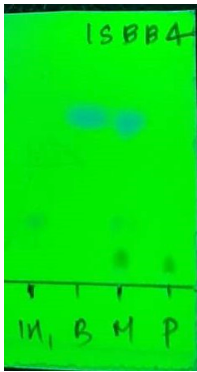
## 15.6 SPECTRAL INTERPRETATION

3-((3-(benzyloxy)benzylidene)hydrazineylidene)-5-fluorindolin-2-one (**ISBB3**): Orange, solid, 86%, melting point.  $210 \pm 2^\circ\text{C}$ .  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 11.02 (s, 1H, NH), 8.63 (s, 1H, =CH-), 8.05-6.88 (m, 12H, ArH), 5.22 (s, 2H, -CH<sub>2</sub>-).  $^{13}\text{C}$  NMR (500 MHz, DMSO- $d_6$ ) 164.32, 161.08, 158.68, 156.38, 150.18, 141.33, 136.63, 134.46, 130.37, 128.38, 127.64, 121.50, 120.20, 119.04, 116.63, 115.29, 114.42, 111.87, 69.28. Chemical formula C<sub>22</sub>H<sub>16</sub>FN<sub>3</sub>O<sub>2</sub>. EI- HRMS (m/z): Calculated-373.3898, Observed- 373.3898.



**Figure S11.** ISBB4 structure

16.1 TLC OF ISBB-4: Mobile phase is Hexane: ethyl acetate (70:30)



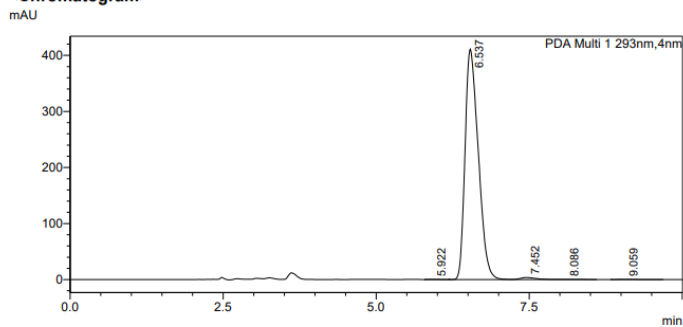
16.2 HPLC OF ISBB-4

SHIMADZU LabSolutions Analysis Report

<Sample Information>

Sample Name : isatin001  
 Sample ID : isbb4  
 Data Filename : fluoro and bb\_05-12-2022\_012.lcd  
 Method Filename : isatin.lcm  
 Batch Filename : fluoro and bb.lcb  
 Vial # : 1-11  
 Injection Volume : 20 uL  
 Date Acquired : 12/5/2022 3:12:23 AM  
 Date Processed : 12/6/2022 10:28:55 PM  
 Sample Type : Standard  
 Level : 1  
 Acquired by : System Administrator  
 Processed by : System Administrator

<Chromatogram>



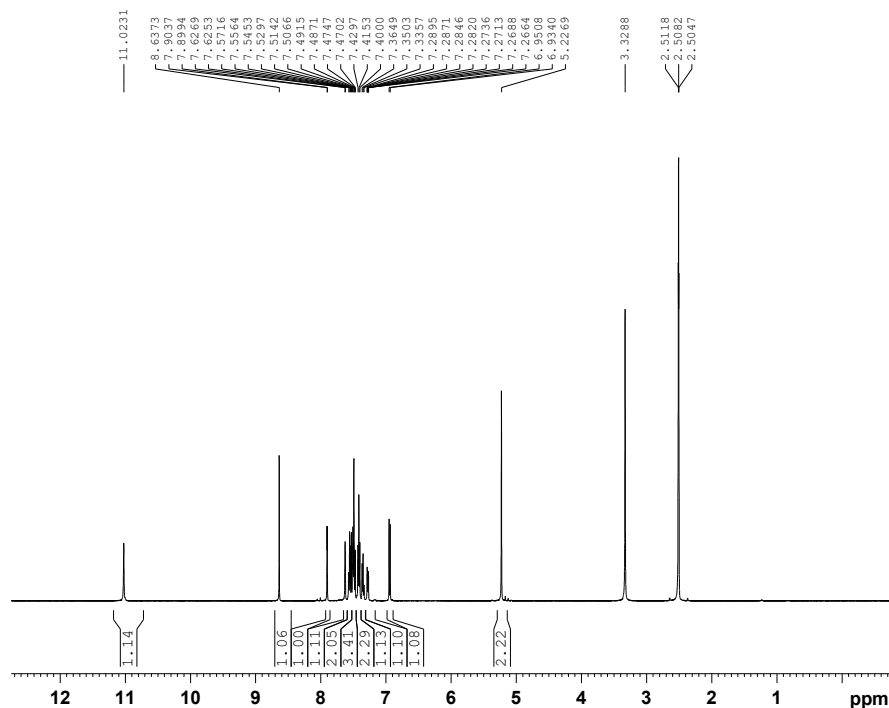
<Peak Table>

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
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2	6.537	6186172	411063	98.701			
3	7.452	66173	3677	1.056		V	
4	8.086	8112	374	0.129		V	
5	9.059	5478	256	0.087			
Total		6267564	415521				

### 16.3 <sup>1</sup>H NMR OF ISBB-4

ISBB-4

<sup>1</sup>H\_8scan DMSO {D:\Spectra} nmr 19



BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P.U.

Current Data Parameters  
NAME Nov23-2022  
EXPNO 190  
PROCNO 1

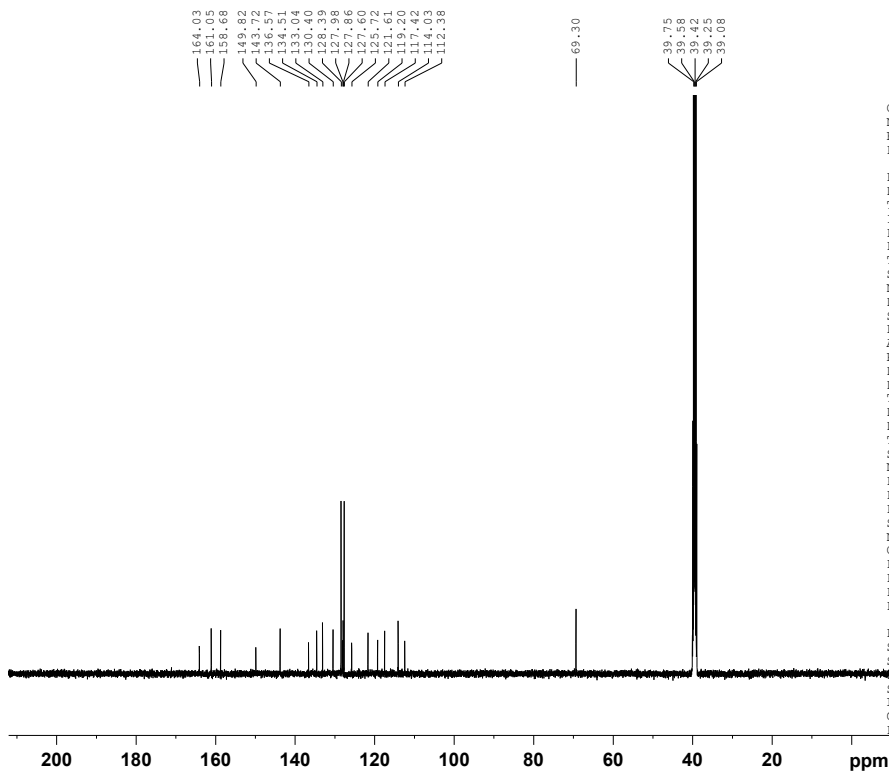
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Time 10.53 h  
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PROBHD z119470\_0333 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 0  
SWH 14705.883 Hz  
FIDRES 0.448788 Hz  
AQ 2.2282240 sec  
RG 101  
DW 34.000 usec  
DE 6.79 usec  
TE 300.2 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.1730885 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.93000031 W

F2 - Processing parameters  
SI 65536  
SF 500.1700000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

### 16.4 <sup>13</sup>C NMR OF ISBB-4

ISBB-4

<sup>13</sup>C13CPD DMSO {D:\Spectra} nmr 19



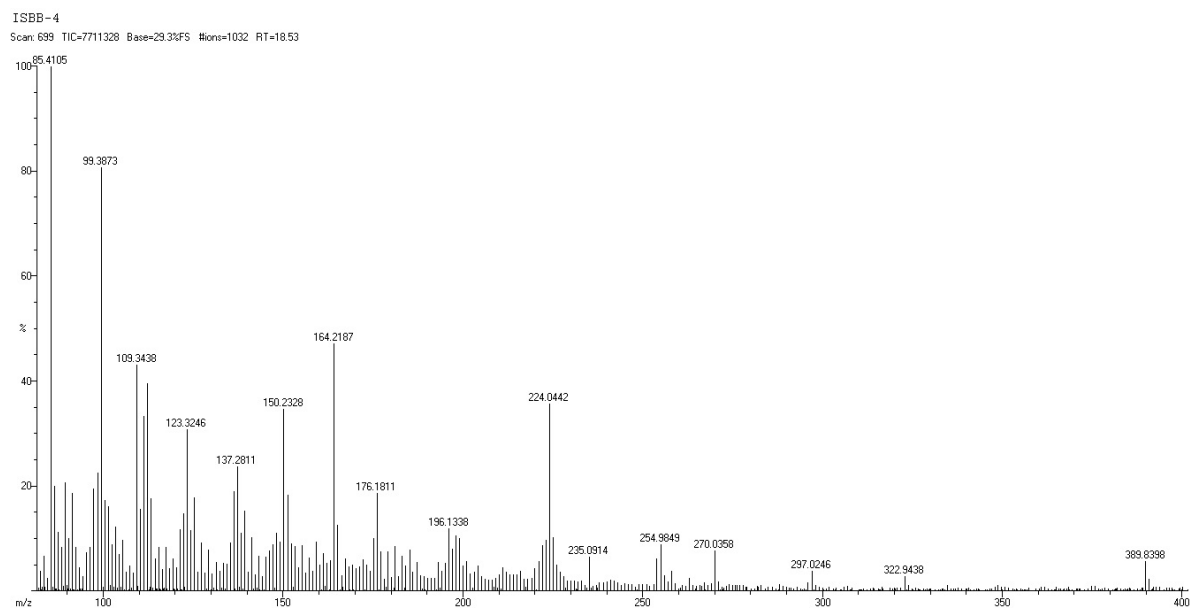
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

Current Data Parameters  
NAME Nov23-2022  
EXPNO 191  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time 23.05 h  
INSTRUM Avance Neo 500  
PROBHD z119470\_0333 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 37037.035 Hz  
FIDRES 1.130281 Hz  
AQ 0.8847360 sec  
RG 101  
DW 13.500 usec  
DE 6.50 usec  
TE 300.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7804233 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 83.14099884 W  
SFO2 500.1720007 MHz  
NUC2 1H  
CPDPRG2 waltz65  
PCPD2 80.00 usec  
PLW2 20.93000031 W  
PLW12 0.32703000 W  
PLW13 0.16449000 W

F2 - Processing parameters  
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SF 125.7679212 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

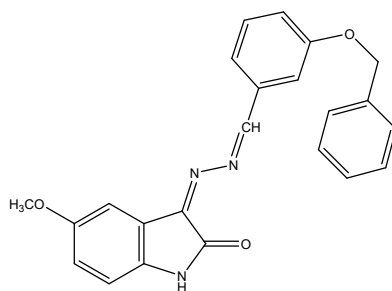
## 16.5 MASS SPECTRA OF ISBB-4



## 16.6 SPECTRAL INTERPRETATION

*3-((3-(benzyloxy)benzylidene)hydrazineylidene)-5-chloroindolin-2-one (ISBB4)*: Orange, solid, 84%, melting point.  $240 \pm 2^\circ\text{C}$ .  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 11.02 (s, 1H, NH), 8.63 (s, 1H, =CH-), 7.90-6.93 (m, 12H, ArH), 5.22 (s, 2H, -CH<sub>2</sub>-)  $^{13}\text{C}$  NMR (500 MHz, DMSO- $d_6$ ) 164.03, 161.05, 158.68, 149.82, 143.72, 136.67, 134.51, 133.04, 130.40, 128.39, 127.98, 126.72, 121.61, 119.20, 117.42, 114.03, 112.36, 69.30. Chemical formula  $\text{C}_{22}\text{H}_{16}\text{ClN}_3\text{O}_2$ . EI- HRMS (m/z): Calculated-389.8398, Observed- 389.8343.





**Figure S17.** ISBB5 structure

17.1 TLC OF ISBB-5: Mobile phase is Hexane: ethyl acetate (70:30)



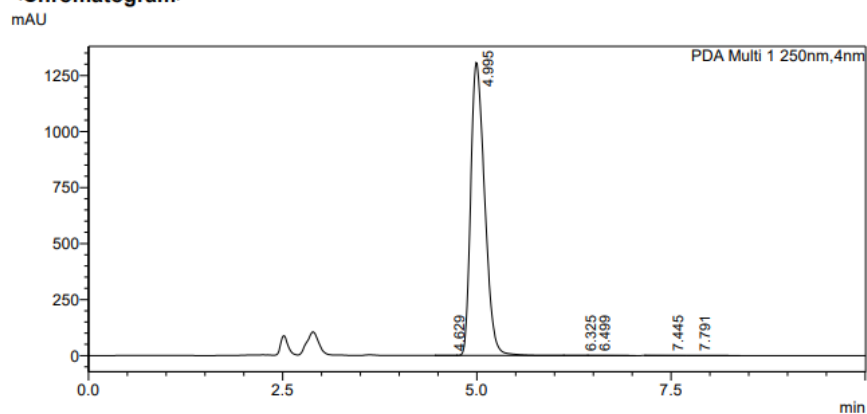
17.2 HPLC OF ISBB-5

**SHIMADZU LabSolutions Analysis Report**

**<Sample Information>**

Sample Name : isatin001  
 Sample ID : isbb5  
 Data Filename : fluoro and bb\_05-12-2022\_013.lcd  
 Method Filename : isatin.lcm  
 Batch Filename : fluoro and bb.lcb  
 Vial # : 1-12  
 Injection Volume : 20 uL  
 Date Acquired : 12/5/2022 3:22:44 AM  
 Date Processed : 12/6/2022 10:32:39 PM  
 Sample Type : Standard  
 Level : 1  
 Acquired by : System Administrator  
 Processed by : System Administrator

**<Chromatogram>**

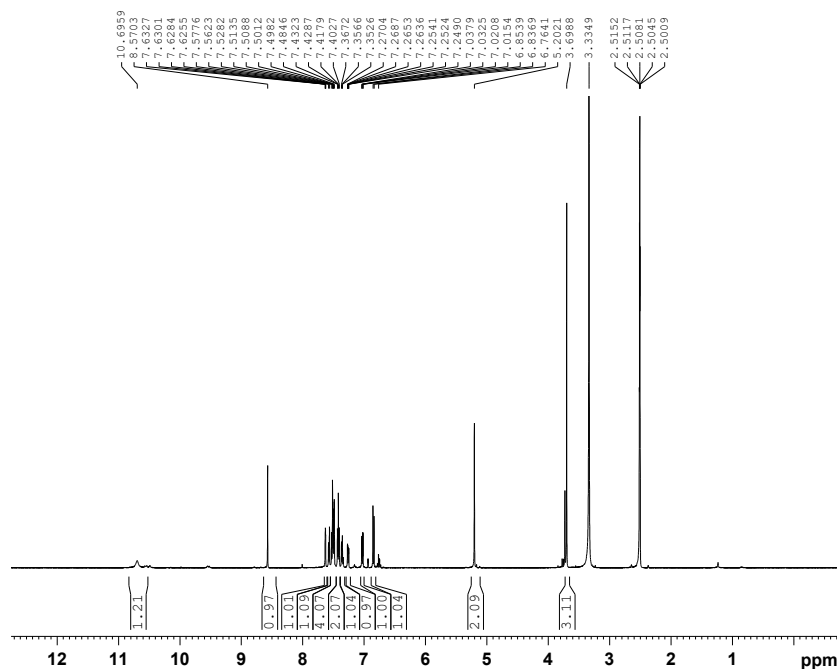


**<Peak Table>**

Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	4.629	1507	161	0.009			
2	4.995	16269042	1306541	99.815		V	
3	6.325	4976	433	0.031			
4	6.499	7545	537	0.046		V	
5	7.445	7884	340	0.048			
6	7.791	8321	429	0.051		V	
Total		16299275	1308441				

### 17.3 <sup>1</sup>H NMR OF 1SBB-5

ISBB-5  
1H\_scan DMSO {D:\Spectra} nmr 20



BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P. U.

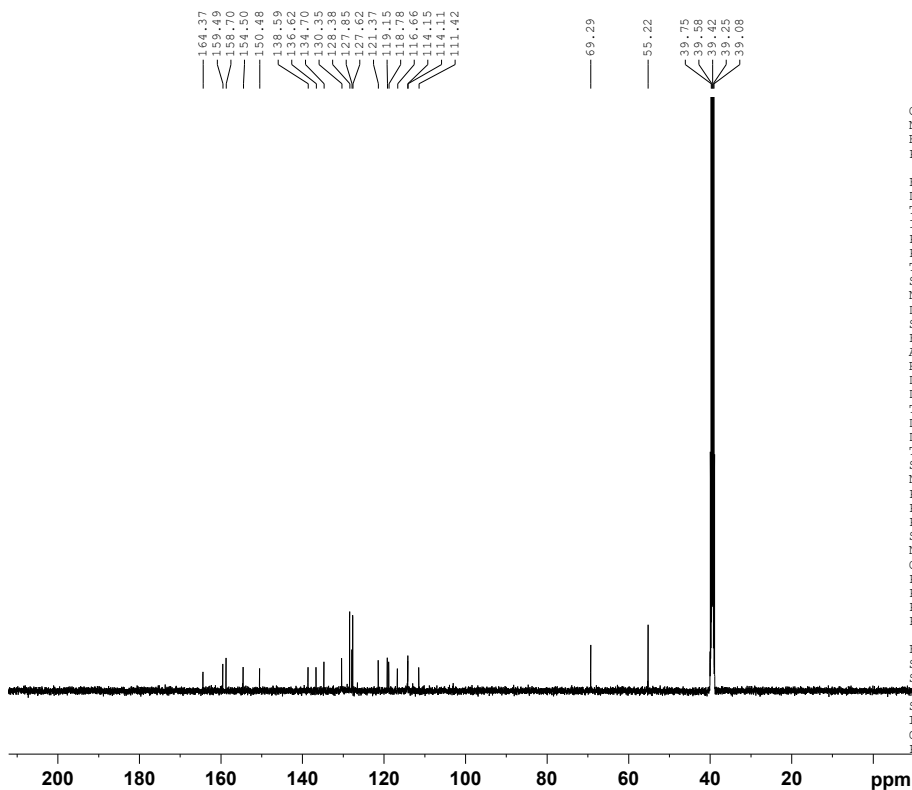
Current Data Parameters  
NAME Nov23-2022  
EXPNO 200  
PROCNO 1

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Time\_ 10.55 h  
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PROBHD Z119470\_0333 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 0  
SWH 14705.883 Hz  
FIDRES 0.448788 Hz  
AQ 2.2282240 sec  
RG 101  
DW 34.000 usec  
DE 6.79 usec  
TE 300.2 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.1730885 MHz  
NUC1 1H  
P0 3.33 usec  
P1 10.00 usec  
PLW1 20.93000031 W

F2 - Processing parameters  
SI 65536  
SF 500.1700000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

### 17.4 <sup>13</sup>C NMR OF ISBB-5

ISBB-5  
C13CPD DMSO {D:\Spectra} nmr 20



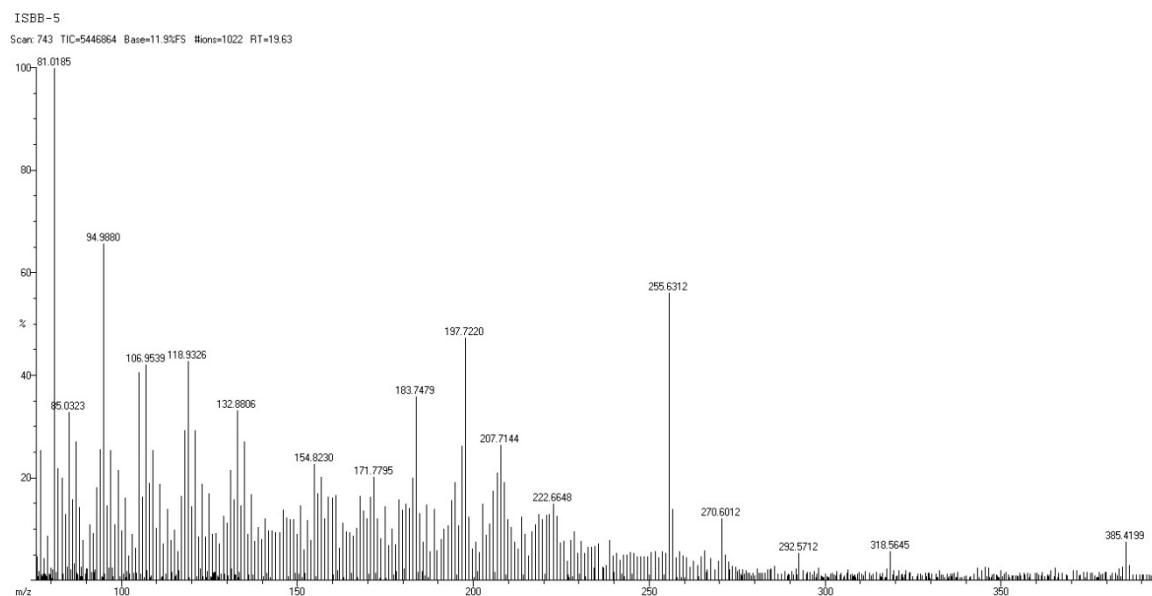
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

Current Data Parameters  
NAME Nov23-2022  
EXPNO 201  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 23.32 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 37037.035 Hz  
FIDRES 1.130281 Hz  
AQ 0.8847360 sec  
RG 101  
DW 13.500 usec  
DE 6.50 usec  
TE 300.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7804233 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 83.14099884 W  
SFO2 500.1720007 MHz  
NUC2 1H  
CPDPRG2 waltz65  
PCPD2 80.00 usec  
PLW2 20.93000031 W  
PLW12 0.32703000 W  
PLW13 0.16449000 W

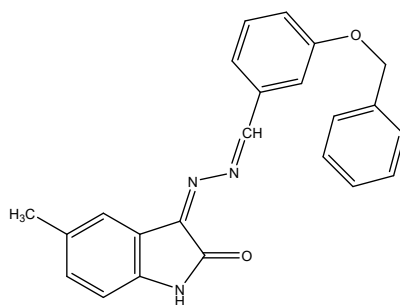
F2 - Processing parameters  
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SF 125.7679198 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## 17.5 MASS SPECTRA OF ISBB-5



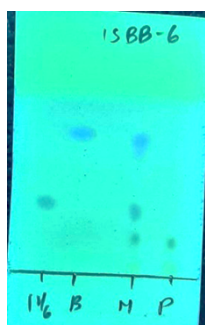
## 17.6 SPECTRAL INTERPRETATION

*3-((3-(benzyloxy)benzylidene)hydrazineylidene)-5-methoxyindolin-2-one (ISBB5)*: Dark brown, solid, 68%, melting point.  $218 \pm 2^\circ\text{C}$ .  $^1\text{H NMR}$  (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.69 (s, 1H, NH), 8.57 (s, 1H, =CH-), 7.63-6.76(m, 12H, Ar-H), 5.20 (s, 2H, -CH<sub>2</sub>-), 3.69 (s, 3H, -CH<sub>2</sub>-Ar).  $^{13}\text{C NMR}$  (500 MHz, DMSO- $d_6$ ) 164.37, 159.49, 158.70, 154.80, 150.48, 138.89, 136.62, 134.70, 130.36, 128.36, 127.85, 121.37, 119.18, 118.78, 116.66, 114.15, 111.42, 69.29, 55.22. Chemical formula C<sub>23</sub>H<sub>19</sub>N<sub>3</sub>O<sub>3</sub>. EI- HRMS (m/z): Calculated-385.4199, Observed- 385.4152.



**Figure S18.** ISBB6 structure

18.1 TLC OF ISBB-6: Mobile phase is Hexane: ethyl acetate (70:30)



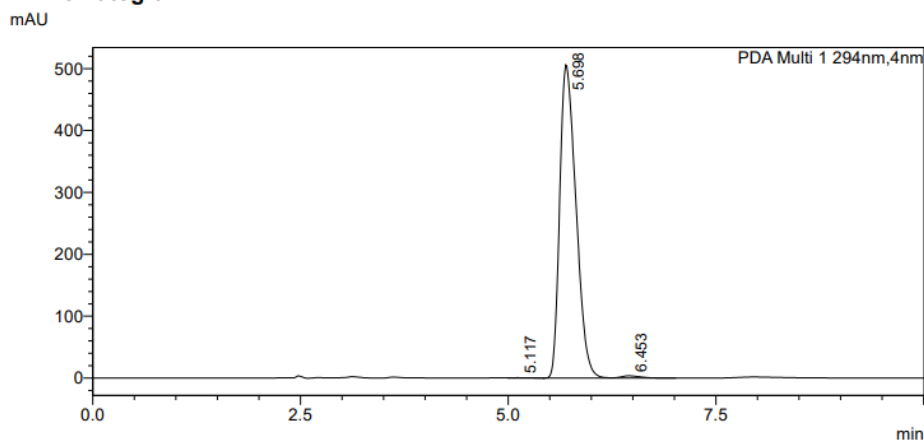
18.2 HPLC OF ISBB-6

**SHIMADZU LabSolutions Analysis Report**

**<Sample Information>**

Sample Name	: isatin001	Sample Type	: Standard
Sample ID	: isbb6	Level	: 1
Data Filename	: fluoro and bb_05-12-2022_014.lcd	Acquired by	: System Administrator
Method Filename	: isatin.lcm	Processed by	: System Administrator
Batch Filename	: fluoro and bb.lcb		
Vial #	: 1-13		
Injection Volume	: 20 uL		
Date Acquired	: 12/5/2022 3:33:06 AM		
Date Processed	: 12/6/2022 10:35:15 PM		

**<Chromatogram>**

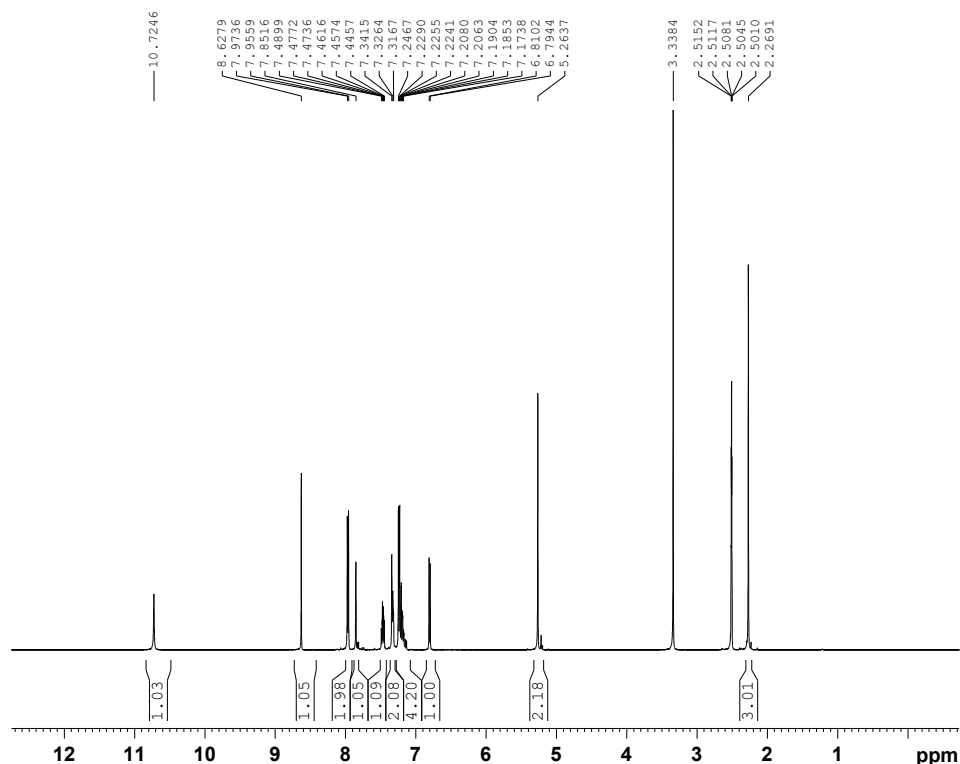


**<Peak Table>**

PDA Ch1 294nm							
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	5.117	7527	509	0.108			
2	5.698	6879649	505641	99.070		V	
3	6.453	57057	3639	0.822		V	
Total		6944233	509789				

### 18.3 <sup>1</sup>H NMR OF ISBB-6

ISBB-6  
1H\_8scan DMSO {D:\Spectra} nmr 21



BRUKER  
AVANCE NEO  
500 MHz NMR  
SPECTROMETER  
SAIF, P.U.

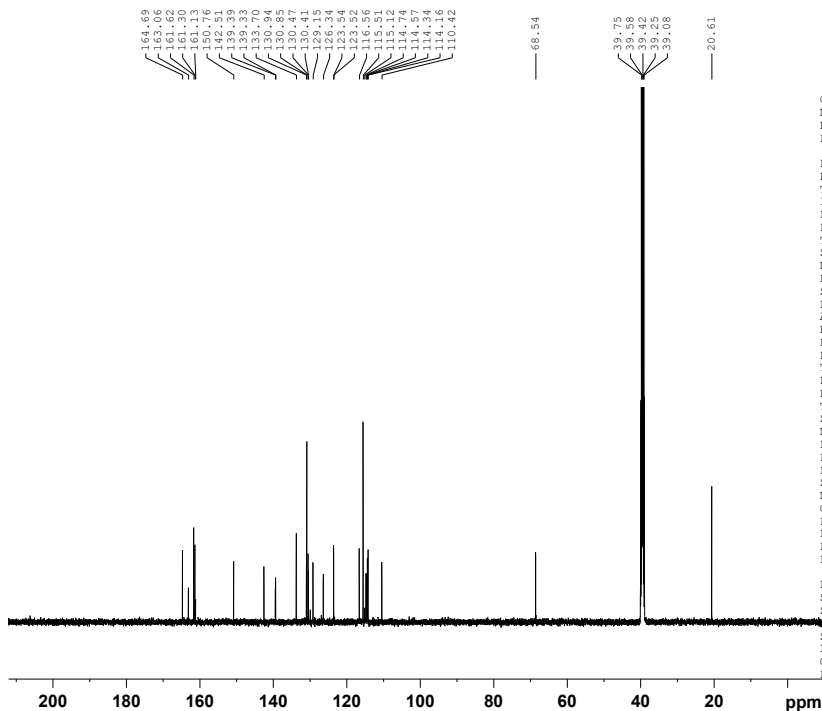
Current Data Parameters  
NAME Nov23-2022  
EXPNO 210  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 10.58 h  
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PROBHD Z119470\_0333 (  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 0  
SWH 14705.883 Hz  
FIDRES 0.448788 Hz  
AQ 2.2282240 sec  
RG 95.7854  
DW 34.000 usec  
DE 6.79 usec  
TE 300.2 K  
D1 1.00000000 sec  
TD0 1  
SFO1 500.1730885 MHz  
NUC1 1H  
P0 3.33  
P1 10.00 usec  
PLW1 20.93000031 W

F2 - Processing parameters  
SI 65536  
SF 500.1700000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

### 18.4 <sup>13</sup>C NMR OF ISBB-6

ISBB-6  
C13CPD DMSO {D:\Spectra} nmr 21



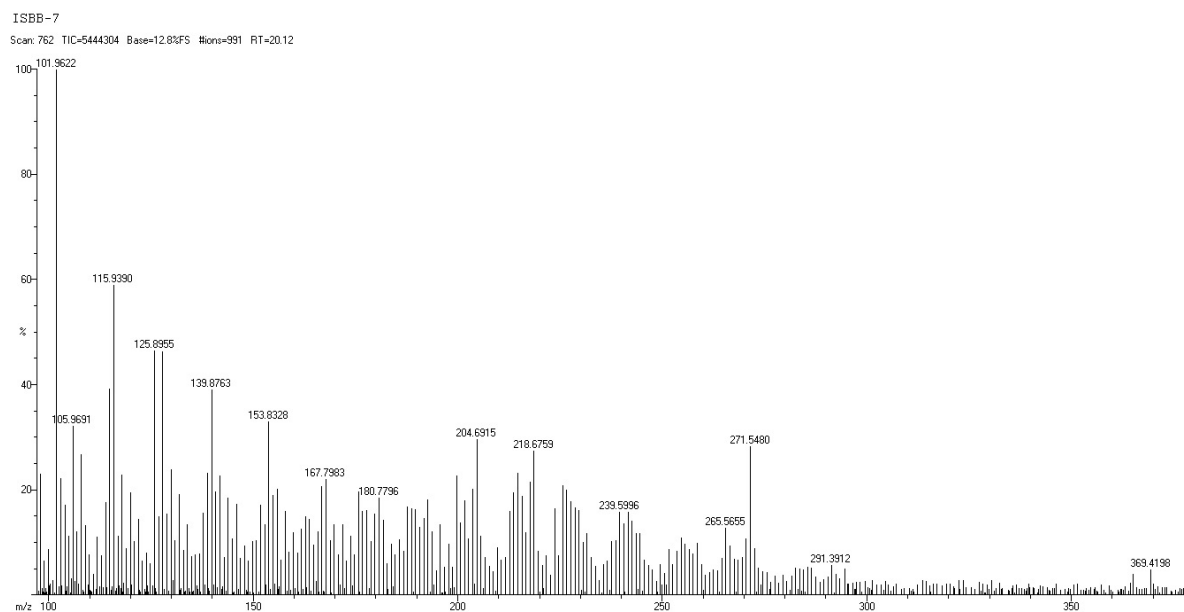
BRUKER  
AVANCE NEO  
500 MHz NMR SPECTROMETER  
SAIF, PANJAB UNIVERSITY,  
CHANDIGARH

Current Data Parameters  
NAME Nov23-2022  
EXPNO 211  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20221123  
Time\_ 23.58 h  
INSTRUM Avance Neo 500  
PROBHD Z119470\_0333 (  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 512  
DS 4  
SWH 37037.035 Hz  
FIDRES 1.130281 Hz  
AQ 0.8847360 sec  
RG 101  
DW 13.500 usec  
DE 6.50 usec  
TE 300.2 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TD0 1  
SFO1 125.7804233 MHz  
NUC1 13C  
P0 3.33 usec  
P1 10.00 usec  
PLW1 83.14009884 W  
SFO2 500.1720007 MHz  
NUC2 1H  
CPDPRG[2] waltz65  
PCPD2 80.00 usec  
PLW2 20.93000031 W  
PLW12 0.32703000 W  
PLW13 0.16449000 W

F2 - Processing parameters  
SI 32768  
SF 125.7679206 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

## 18.5 MASS SPECTRUM OF ISBB-6



## 18.6 SPECTRAL INTERPRETATION:

*3-((3-(benzyloxy)benzylidene)hydrazineylidene)-5-methylindolin-2-one (ISBB6)*: orange solid, 81%, melting point.  $238 \pm 2^\circ\text{C}$ .  $^1\text{H}$  NMR (500 MHz, DMSO- $d_6$ )  $\delta$ : 10.72 (s, 1H, NH), 8.62 (s, 1H, =CH-), 7.97-6.79(m, 12H, ArH), 5.26 (s, 2H, -CH<sub>2</sub>-), 2.26 (s, 3H, -CH<sub>2</sub>-Ar).  $^{13}\text{C}$  NMR (500 MHz, DMSO- $d_6$ ) 164.69, 163.06, 161.62, 150.76, 142.61, 139.39, 133.70, 130.70, 129.15, 126.34, 123.54, 116.86, 115.12, 114.57, 110.42, 68.54, 20.61. Chemical formula C<sub>23</sub>H<sub>19</sub>N<sub>3</sub>O<sub>2</sub> EI- HRMS (m/z): Calculated-369.4198, Observed- 369.4158.