Design and Synthesis of Carbothioamide/Carboxamide-Based Pyrazoline Analogs as Potential Anticancer Agents: Apoptosis, Molecular Docking, ADME Assay, and DNA Binding Studies

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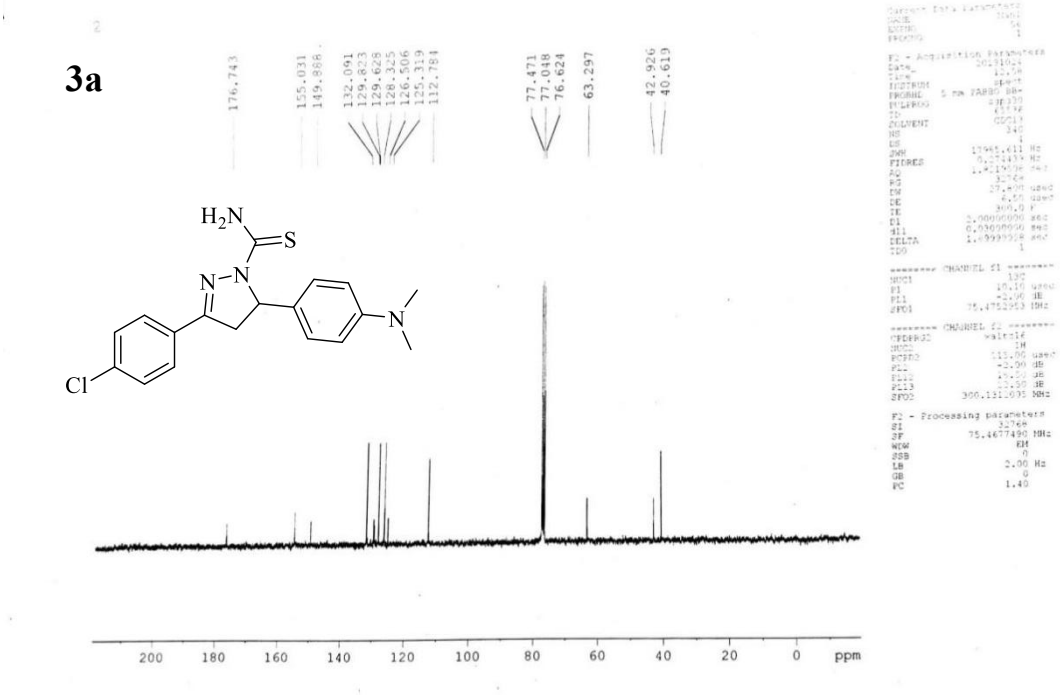
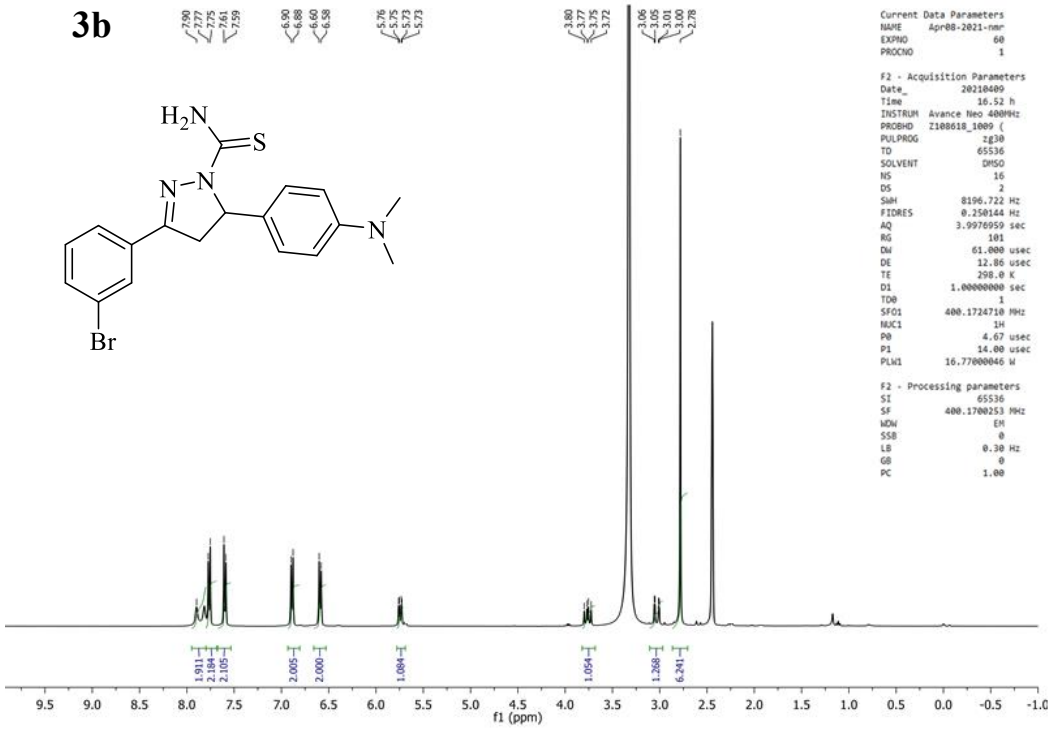


3b

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NAME      Apr08-2021-nmr
EXPNO                 60
PROCNO                 1

F2 - Acquisition Parameters
Date_           20210409
Time              16.52 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH            8196.722 Hz
FIDRES         0.250144 Hz
AQ             3.9976959 sec
RG                   101
DW              61.000 usec
DE              12.86 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         400.1724710 MHz
NUC1                  1H
P0                4.67 usec
P1               14.00 usec
PLW1         16.77000046 W

F2 - Processing parameters
SI                 65536
SF         400.1700253 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                  1.00
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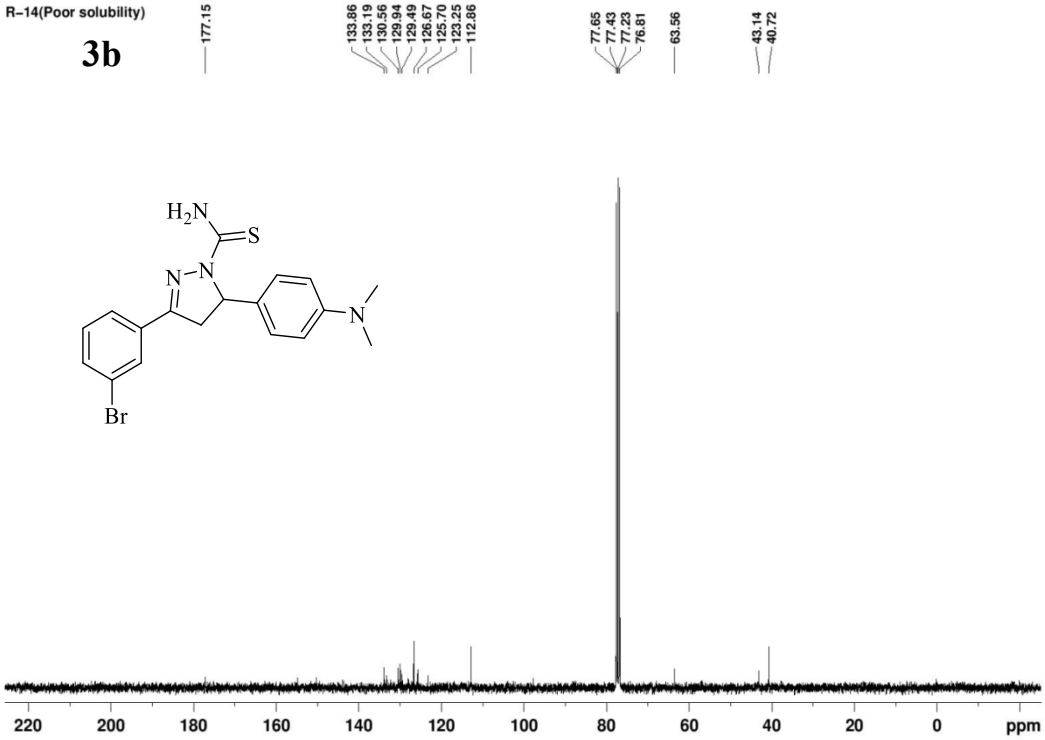
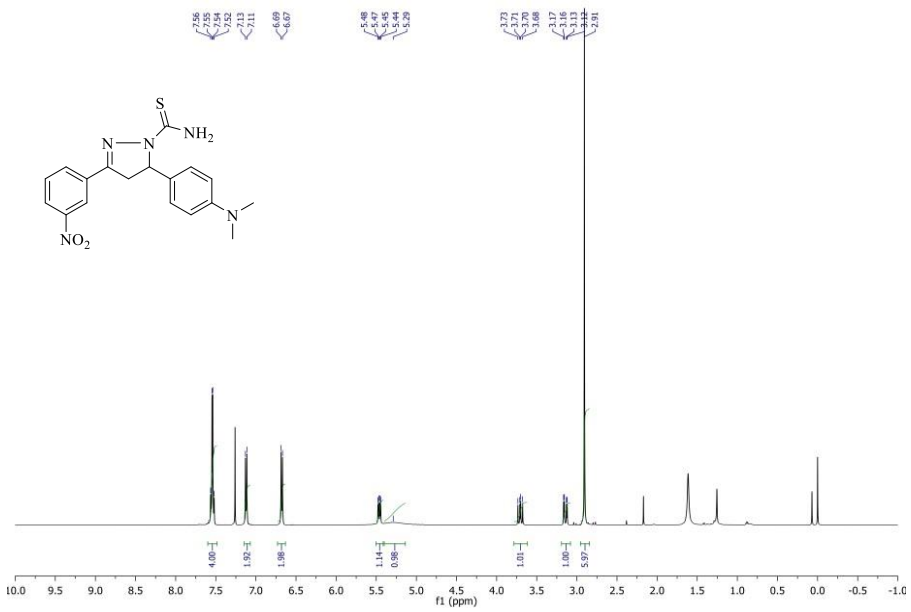
R-14(Poor solubility)

3b



3c



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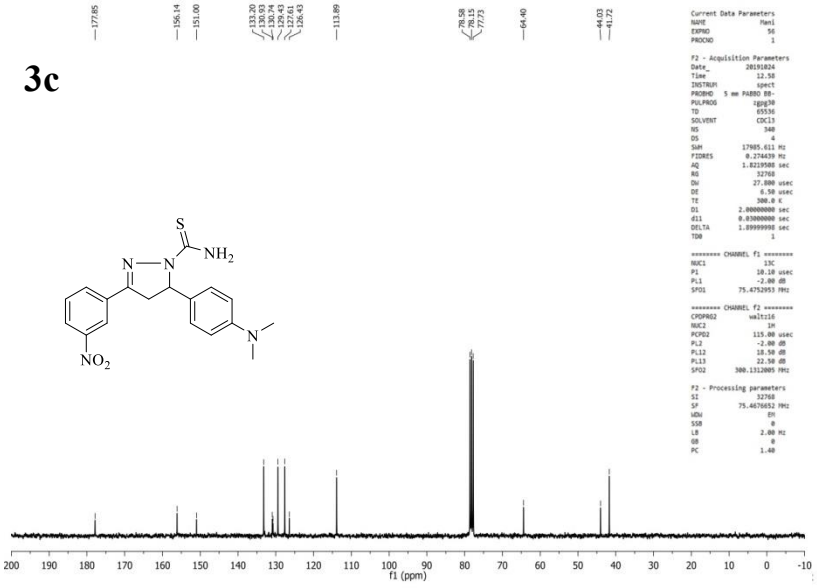


Current Data Parameters
NAME Mani
EXPNO 56
PROCNO 1

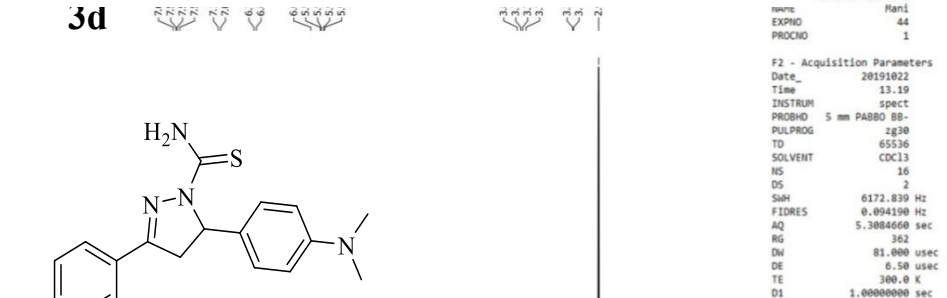
F2 - Acquisition Parameters
Date_ 20191024
Time 12.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 340
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4676652 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

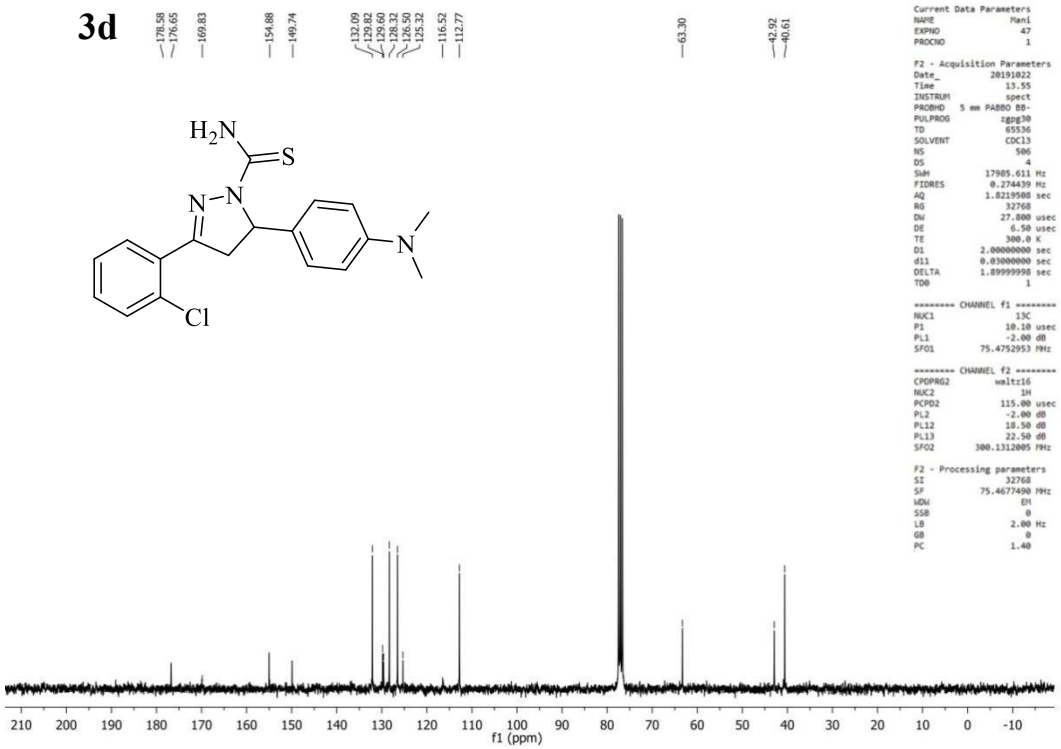
3d



Data Parameters
NAME Mani
EXPNO 44
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191022
Time 13.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 362
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec

3d

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Current Data Parameters
NAME                  Mani
EXPNO                   47
PROCNO                   1

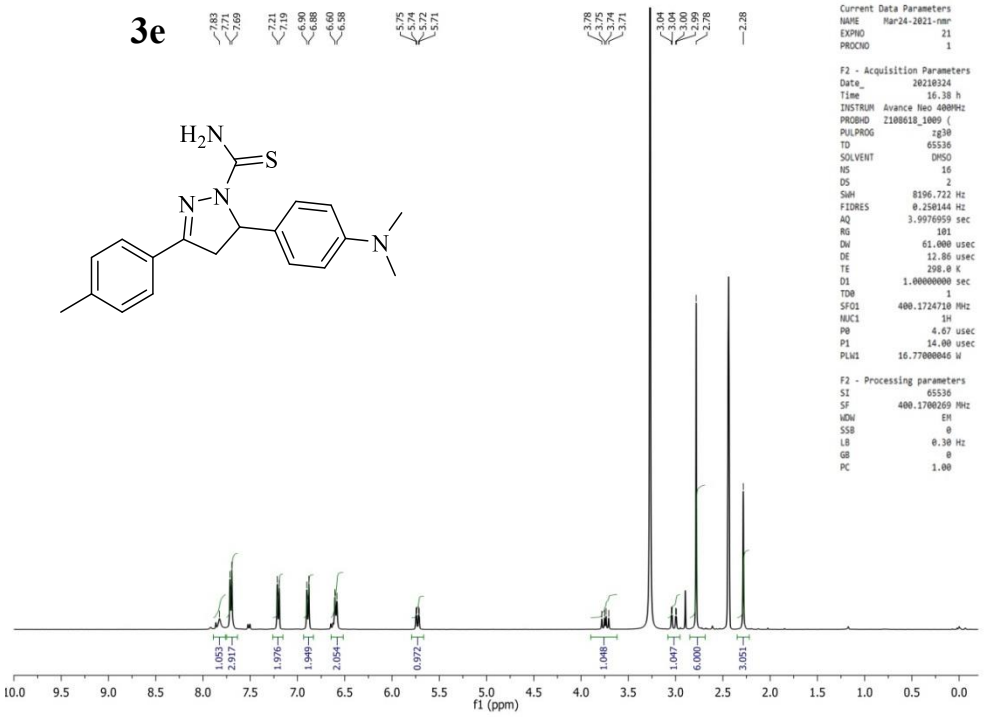
F2 - Acquisition Parameters
Date_               20191022
Time                   13.55
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     506
DS                       4
SWH              17985.611 Hz
FIDRES               0.274439 Hz
AQ                1.8219508 sec
RG                     32768
DW                  27.800 usec
DE                   6.50 usec
TE                   300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                   10.10 usec
PL1                  -2.00 dB
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                    1H
PCPD2               115.00 usec
PL2                  -2.00 dB
PL12                 18.50 dB
PL13                 22.50 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                     32768
SF              75.4677490 MHz
WDW                       EM
SSB                        0
LB                    2.00 Hz
GB                         0
PC                      1.40
```

3e

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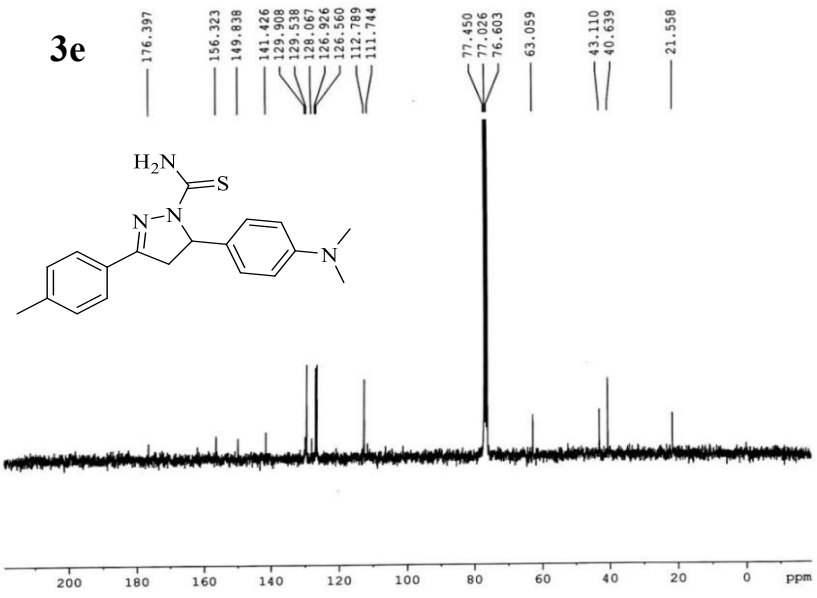
EXPNO               21
PROCNO               1

F2 - Acquisition Parameters
Date_          20210324
Time             16.38 h
INSTRUM  Avance Neo 400MHz
PROBHD   Z108618_1009 (
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH           8196.722 Hz
FIDRES        0.250144 Hz
AQ            3.9976959 sec
RG                   101
DW              61.000 usec
DE              12.86 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1        400.1724710 MHz
NUC1                  1H
P0               4.67 usec
P1              14.00 usec
PLW1        16.77000046 W

F2 - Processing parameters
SI                 65536
SF          400.1700269 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

3e

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Current Data Parameters
NAME                Mani
EXPNO                194
PROCNO                 1

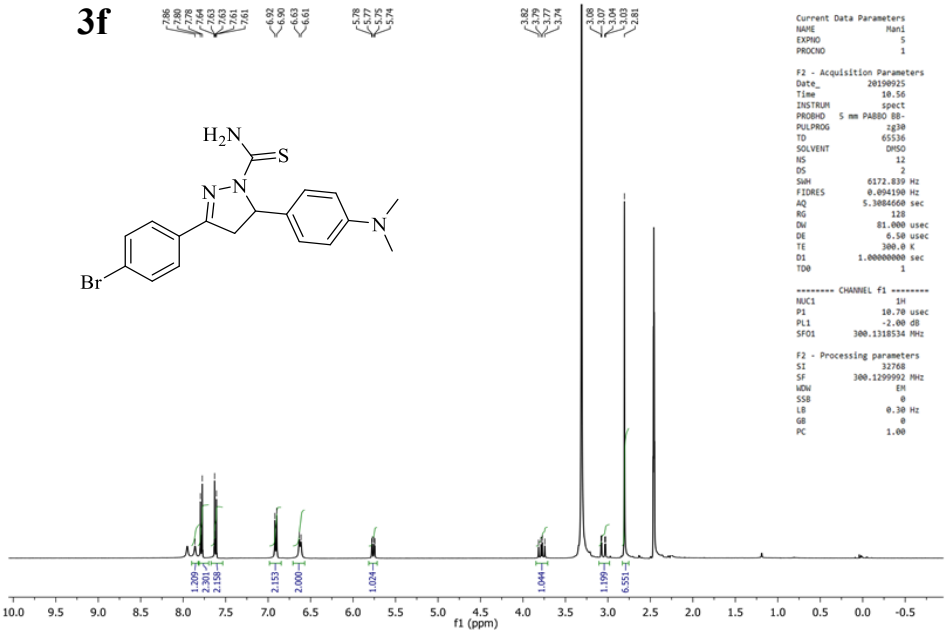
F2 - Acquisition Parameters
Date_           20200226
Time               10.48
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            CDCl3
NS                   711
DS                     4
SWH          17985.611 Hz
FIDRES        0.274439 Hz
AQ            1.8219508 sec
RG                9195.2
DW               27.800 usec
DE                6.50 usec
TE                300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1               10.10 usec
PL1                -2.00 dB
SFO1         75.4752953 MHz

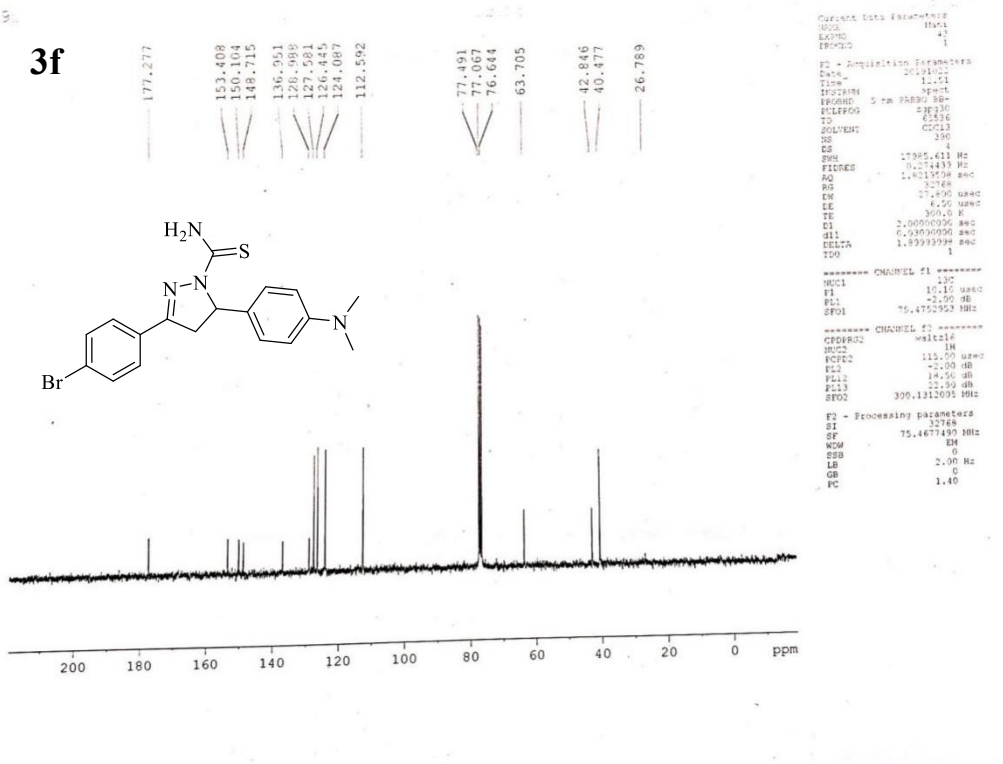
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2           115.00 usec
PL2                -2.00 dB
PL12               18.50 dB
PL13               22.50 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF          75.4677490 MHz
WDW                   EM
SSB                    0
LB                2.00 Hz
GB                     0
PC                1.40
```

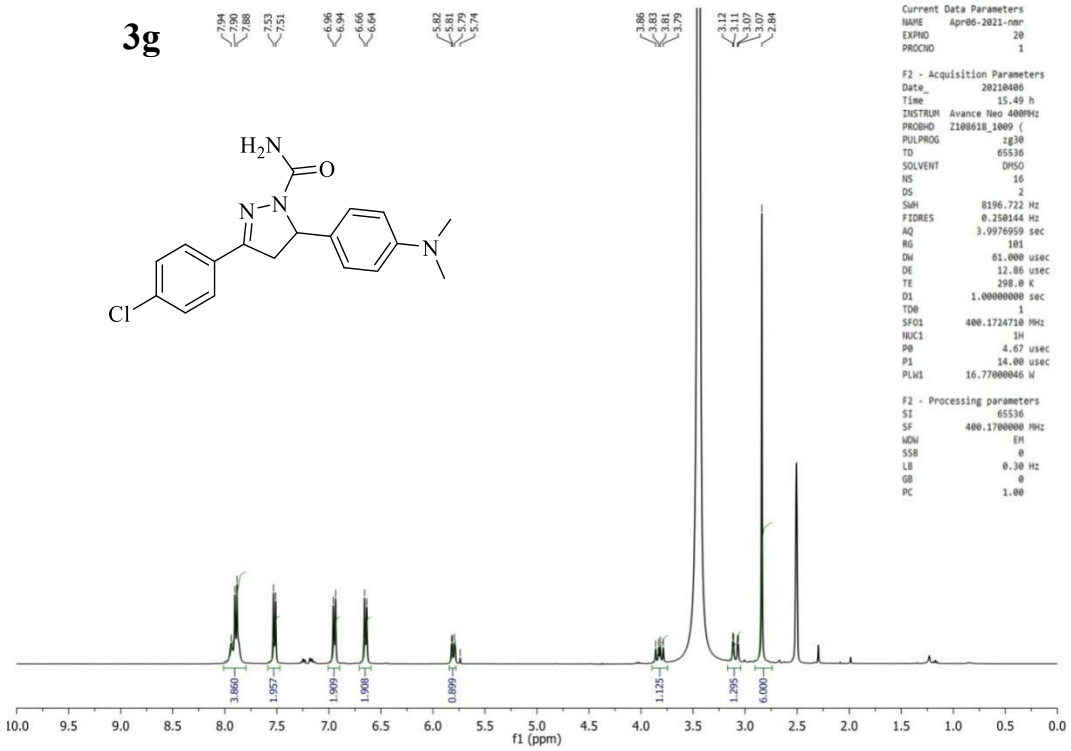
3f


7.86
7.80
7.78
7.64
7.63
7.63
7.61
7.61
6.92
6.90
6.63
6.61
5.78
5.77
5.75
5.74
3.82
3.79
3.77
3.74
3.08
3.07
3.04
3.03
2.81
Current Data Parameters
NAME Man1
EXPNO 5
PROCNO 1
F2 - Acquisition Parameters
Date_ 20190925
Time 10.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 12
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
SFO1 300.1318534 MHz
F2 - Processing parameters
SI 32768
SF 300.1299992 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.209
2.301
2.158
2.153
2.000
1.024
1.044
1.199
6.551
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3f


177.277
153.408
150.104
148.715
136.951
128.998
127.581
126.445
124.087
112.592
77.491
77.067
76.644
63.705
42.846
40.477
26.789
Current Data Parameters
NAME Man1
EXPNO 43
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191002
Time 11.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 390
DS 4
SWH 17985.611 Hz
FIDRES 0.274433 Hz
AQ 1.8219520 sec
RG 32768
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000096 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 14.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677497 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 0 ppm

3g

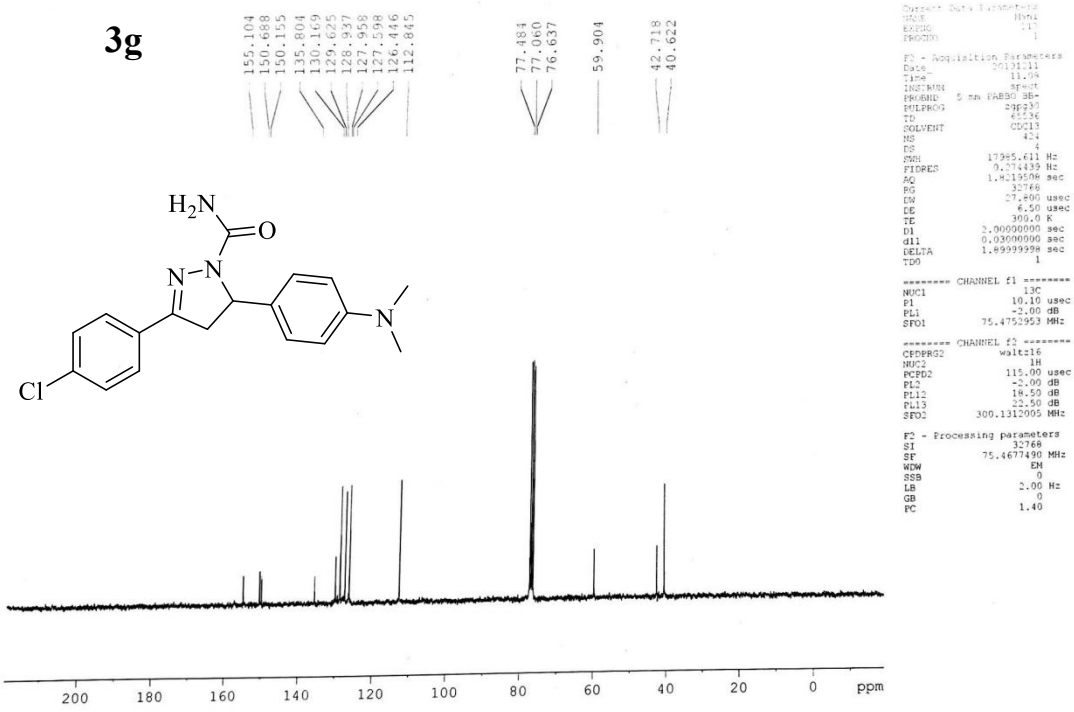


Current Data Parameters
NAME Apr06-2021-nmr
EXPNO 20
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210406
Time 15.49 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 16.77000046 W

F2 - Processing parameters
SI 65536
SF 400.1700000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3g



Current Data Parameters
NAME Hong
EXPNO 11
PROCNO 1

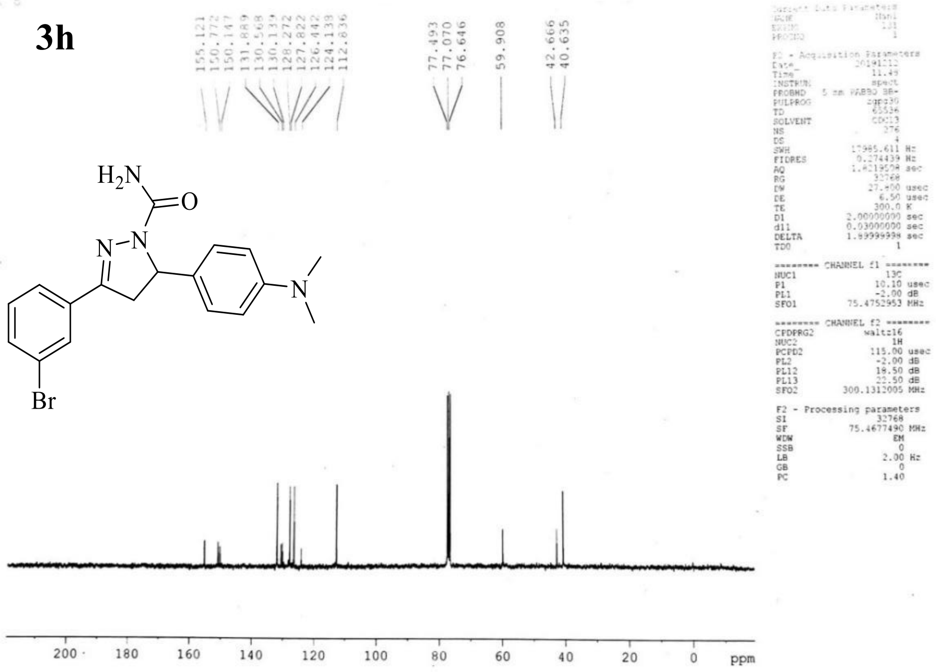
F2 - Acquisition Parameters
Date_ 20191111
Time 11.09
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 424
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32768
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

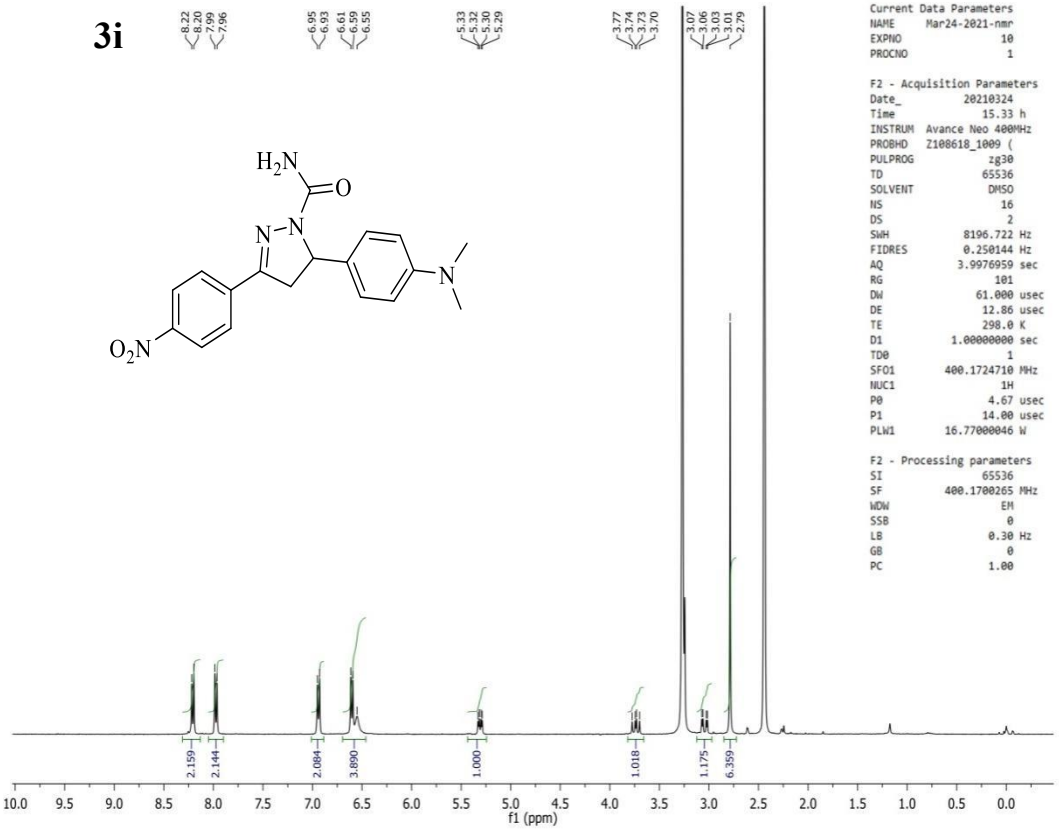
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 19.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

3h


155.121
150.772
150.147
131.889
130.568
130.134
128.272
127.822
126.442
124.133
112.836
77.493
77.070
76.646
59.908
42.666
40.635
H_2N
O
N
N
N
Br
F2 - Acquisition Parameters
Time 11.49
PROBHD 5 mm PABBO BB-
TD 65536
SOLVENT CDCl3
NS 276
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
RG 32768
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

3i

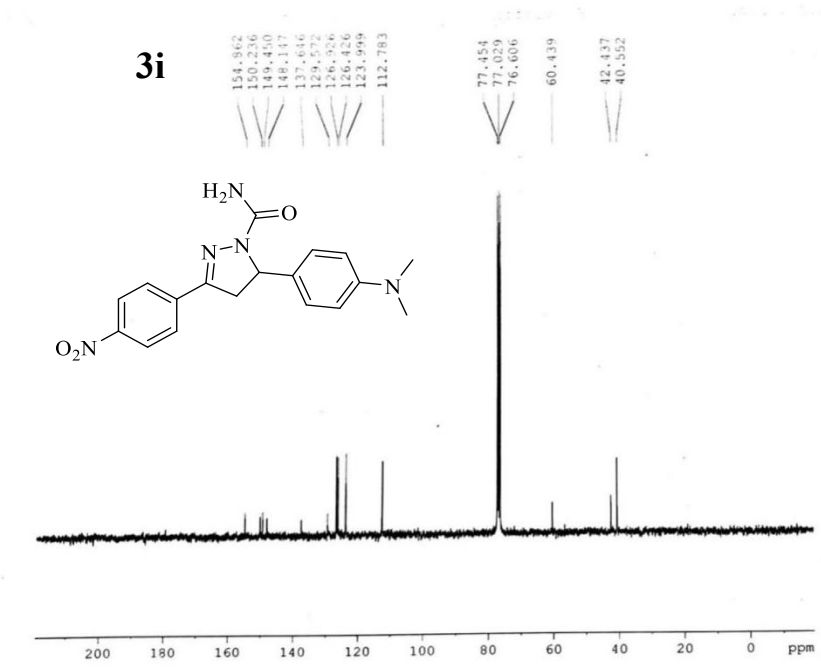


Current Data Parameters
NAME Mar24-2021-nmr
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210324
Time 15.33 h
INSTRUM Avance Neo 400MHz
PROBHD Z108618_1009 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8196.722 Hz
FIDRES 0.250144 Hz
AQ 3.9976959 sec
RG 101
DW 61.000 usec
DE 12.86 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 400.1724710 MHz
NUC1 1H
P0 4.67 usec
P1 14.00 usec
PLW1 16.77000046 W

F2 - Processing parameters
SI 65536
SF 400.1700265 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3i



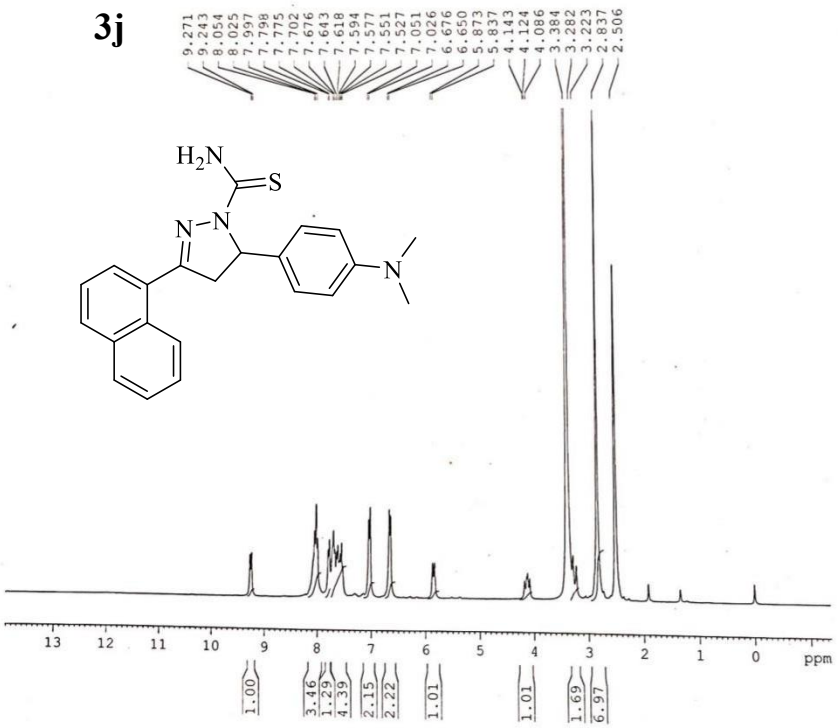
F2 - Acquisition Parameters
Date_ 20210316
Time 13.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 710
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 32749
DW 25.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

3j



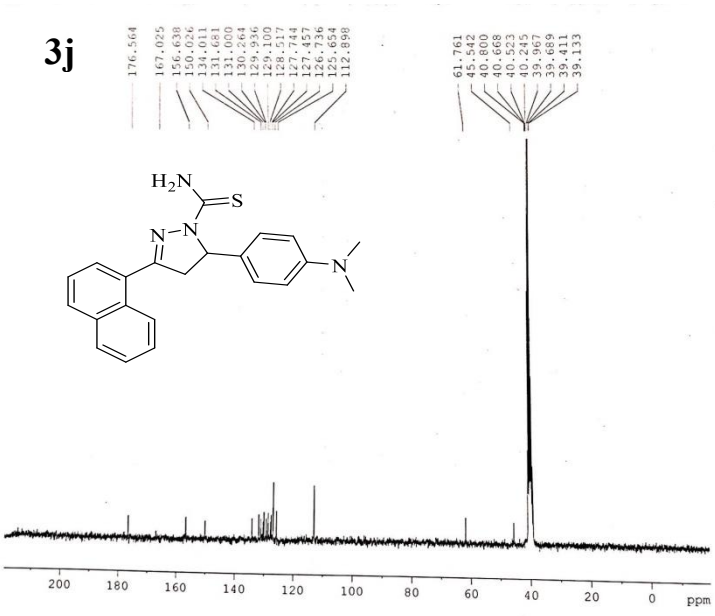
Current Data Parameters
NAME Nani
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190925
Time 10.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 12
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 128
DW 81.000 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 1H
P1 10.70 usec
PL1 -2.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299992 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

3j



Current Data Parameters
NAME 25 sept 2019
EXPNO 1
PROCNO 1

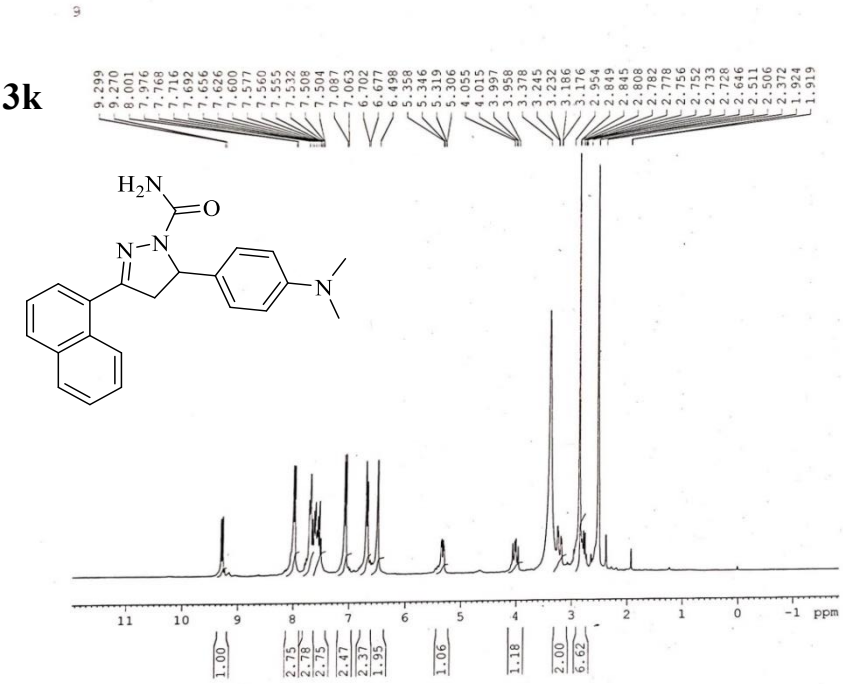
F2 - Acquisition Parameters
Date_ 20190925
Time 13.14
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 419
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219528 sec
RG 32768
DW 27.800 usec
DE 6.50 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 10.10 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 115.00 usec
PL2 -2.00 dB
PL12 18.50 dB
PL13 22.50 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

3k



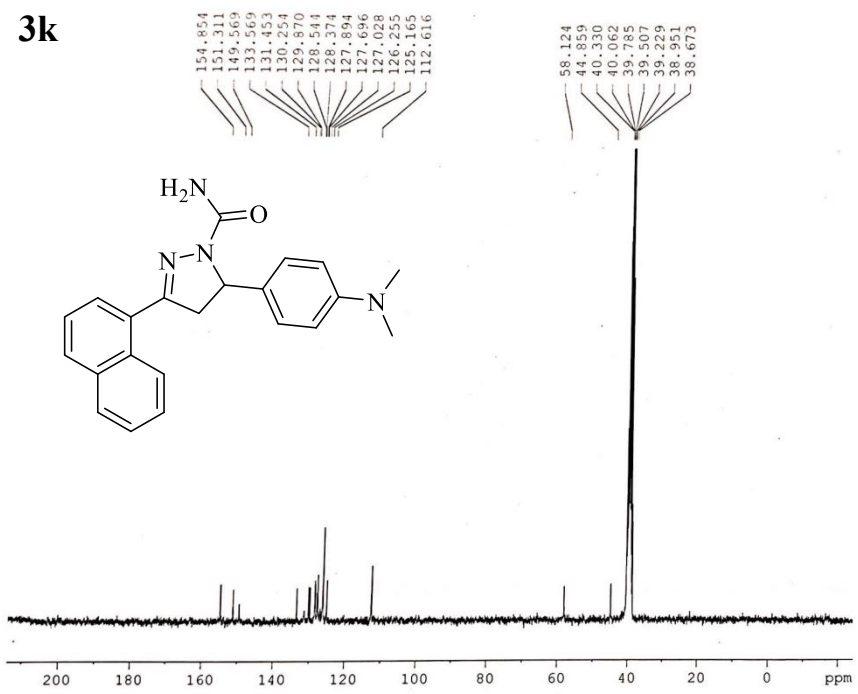

```
Current Data Parameters
NAME                 Nan1
EXPNO                  12
PROCNO                  1

F2 - Acquisition Parameters
Date_               20190926
Time                   10.20
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        12
DS                         2
SWH                6172.839 Hz
FIDRES             0.094190 Hz
AQ                 5.3084660 sec
RG                       128
DW                  81.000 usec
DE                    6.50 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.70 usec
PL1                    -2.00 dB
SFO1             300.1316534 MHz

F2 - Processing parameters
SI                        32768
SF               300.1299980 MHz
WDW                          EM
SSB                           0
LB                         0.30 Hz
GB                            0
PC                         1.00
```

3k



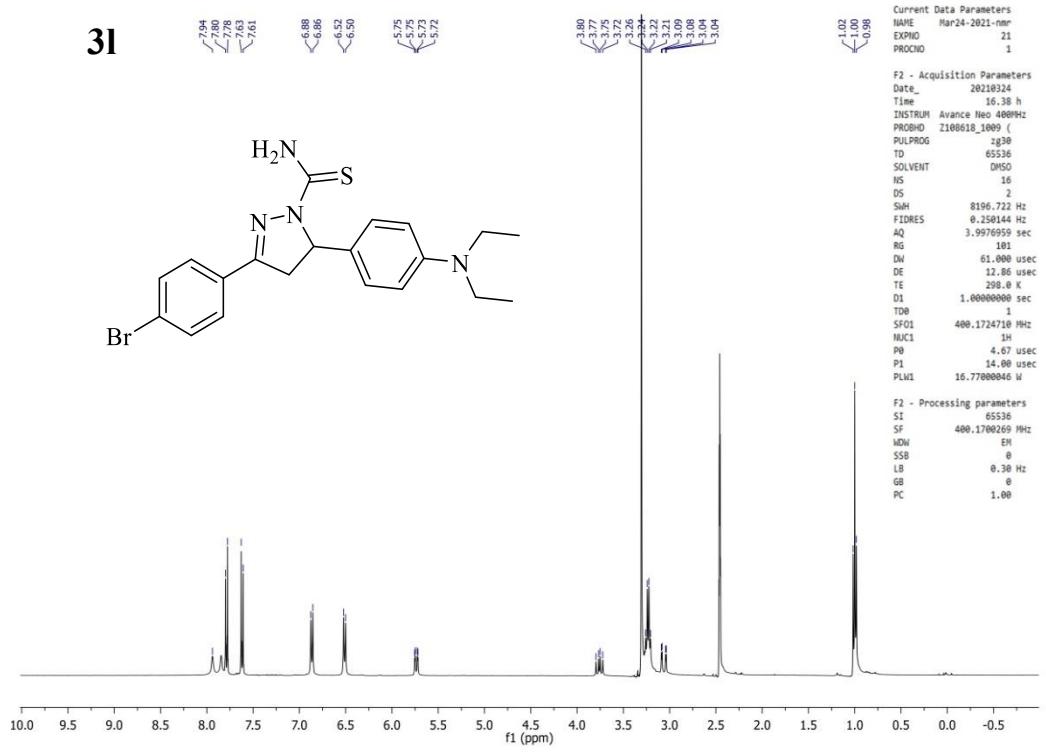

```
Current Data Parameters
NAME                 Nan1
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_               20190926
Time                    9.54
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                       584
DS                         4
SWH               17985.611 Hz
FIDRES             0.274439 Hz
AQ                 1.8219508 sec
RG                     32768
DW                  27.800 usec
DE                    6.50 usec
TE                   300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     13C
P1                     10.10 usec
PL1                    -2.00 dB
SFO1             75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                 115.00 usec
PL2                    -2.00 dB
PL12                   18.50 dB
PL13                   22.50 dB
SFO2             300.1312005 MHz

F2 - Processing parameters
SI                        32768
SF               75.4681433 MHz
WDW                          EM
SSB                           0
LB                         2.00 Hz
GB                            0
PC                         1.40
```



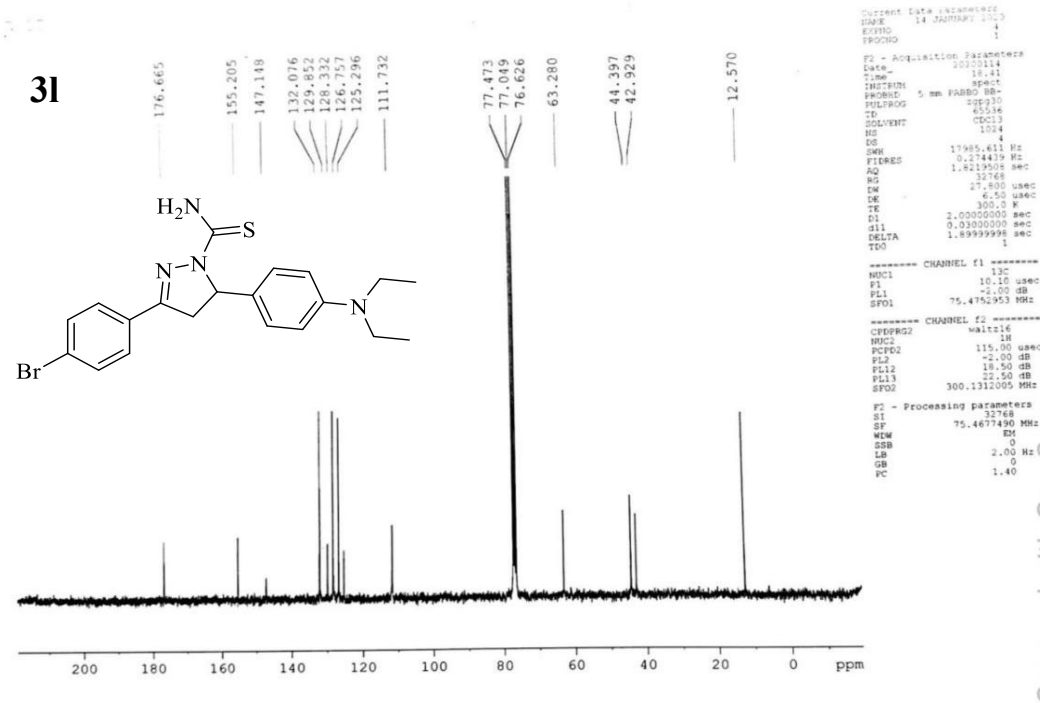
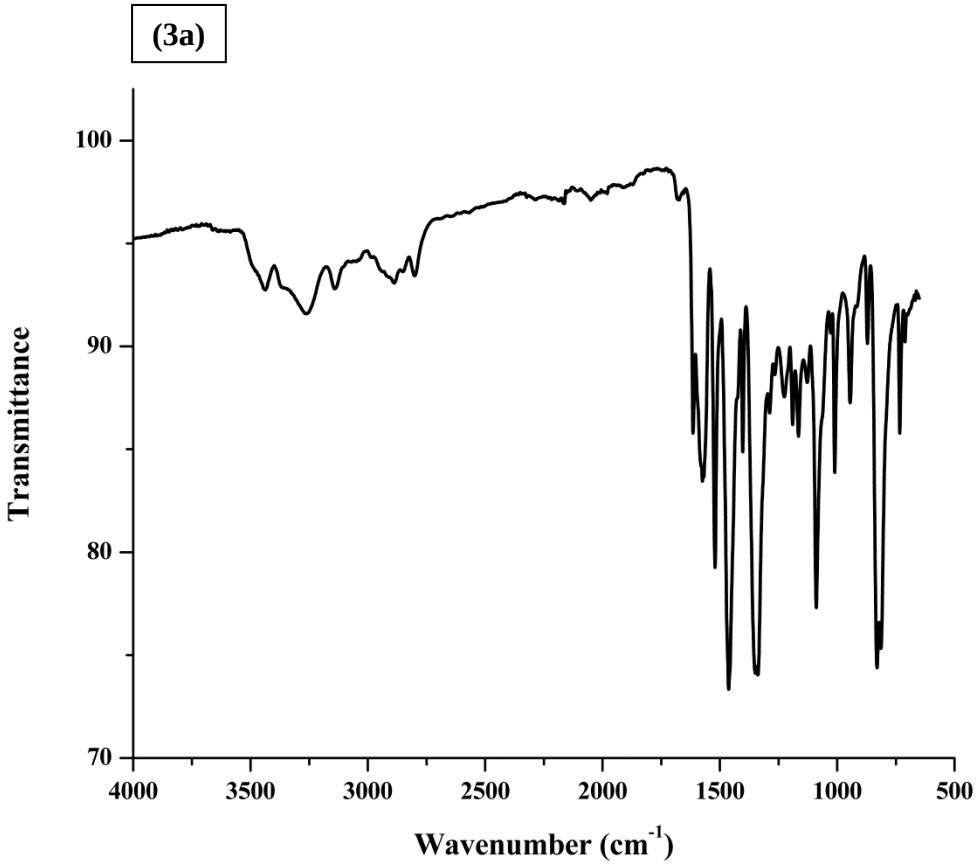
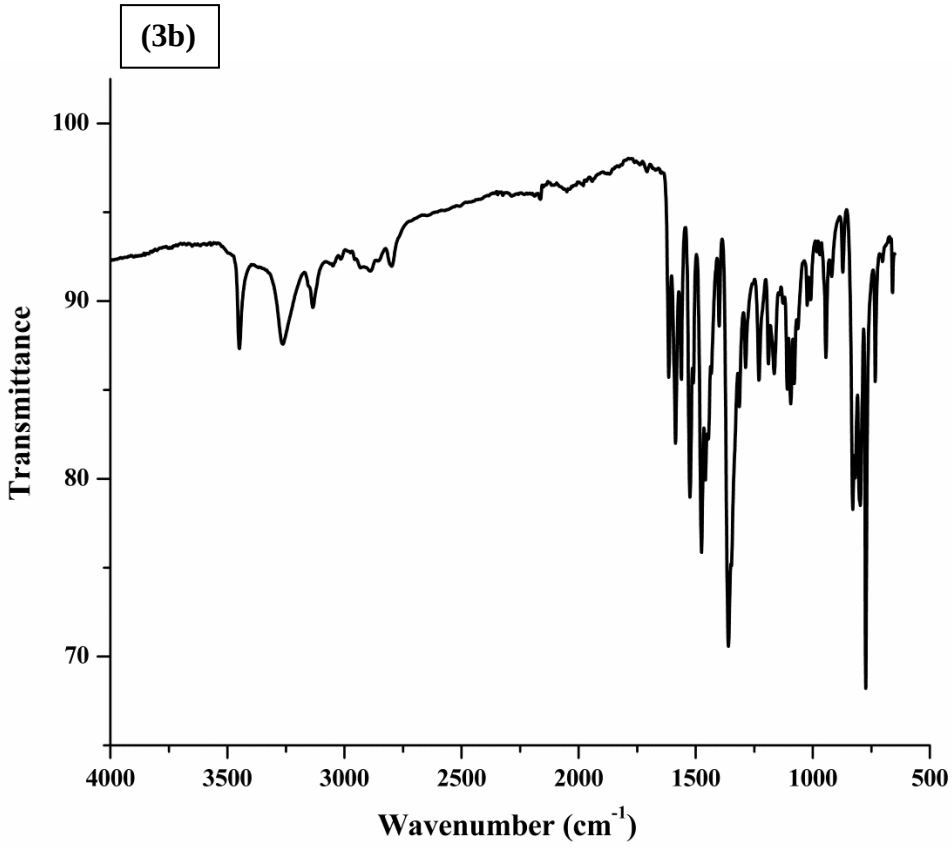
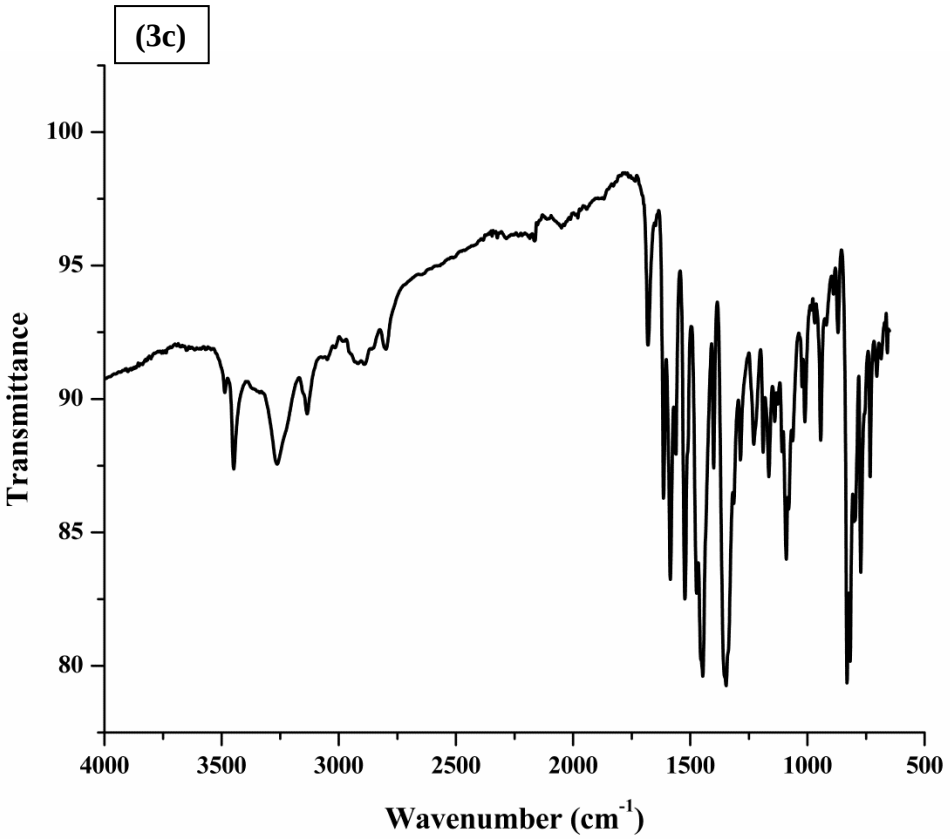
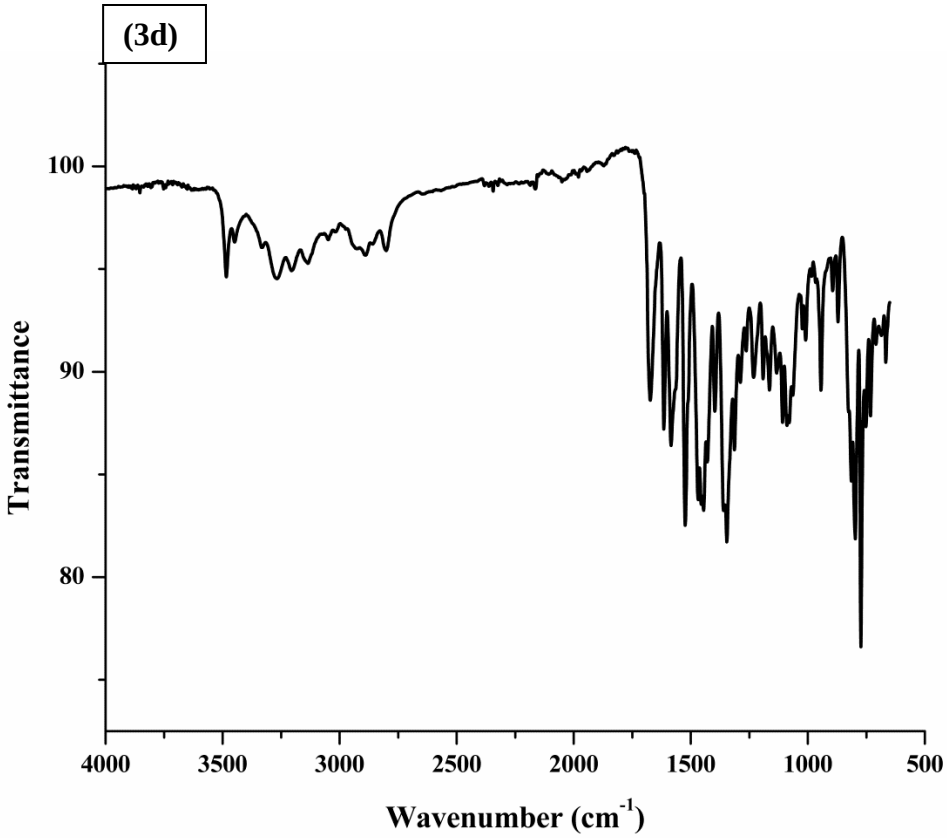


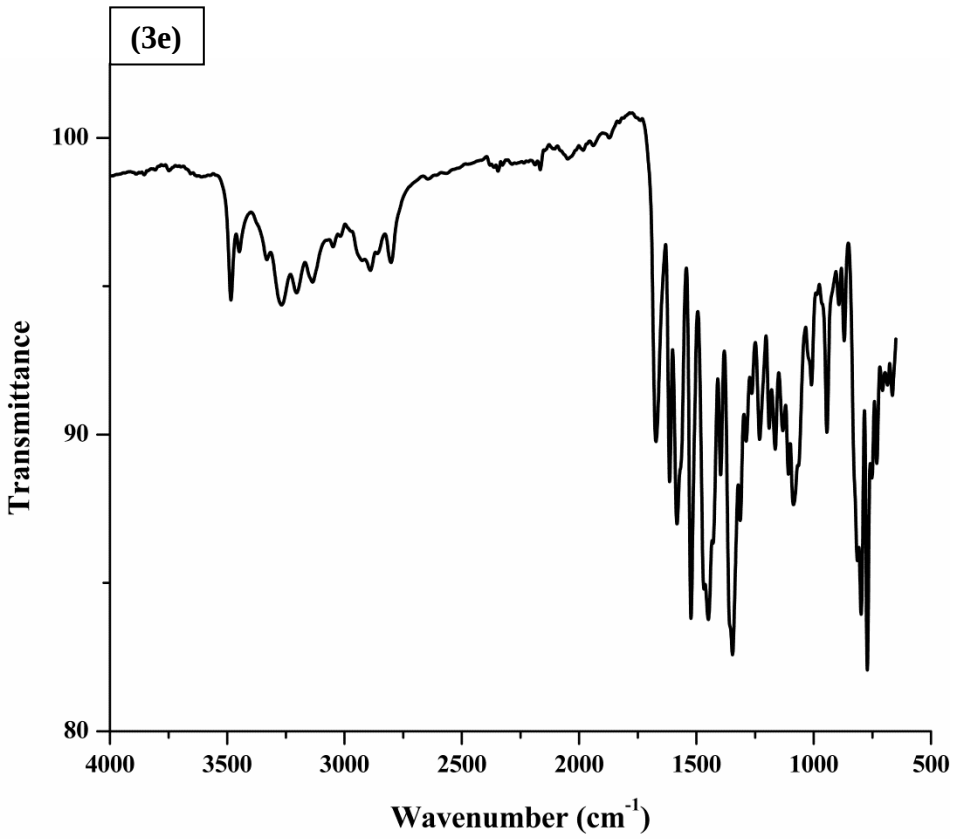
Figure. S1. [1]H NMR spectra of pyrazoline derivatives (3b-3g and 3i-3l) and [13]C-NMR spectra of derivatives 3a-3l.

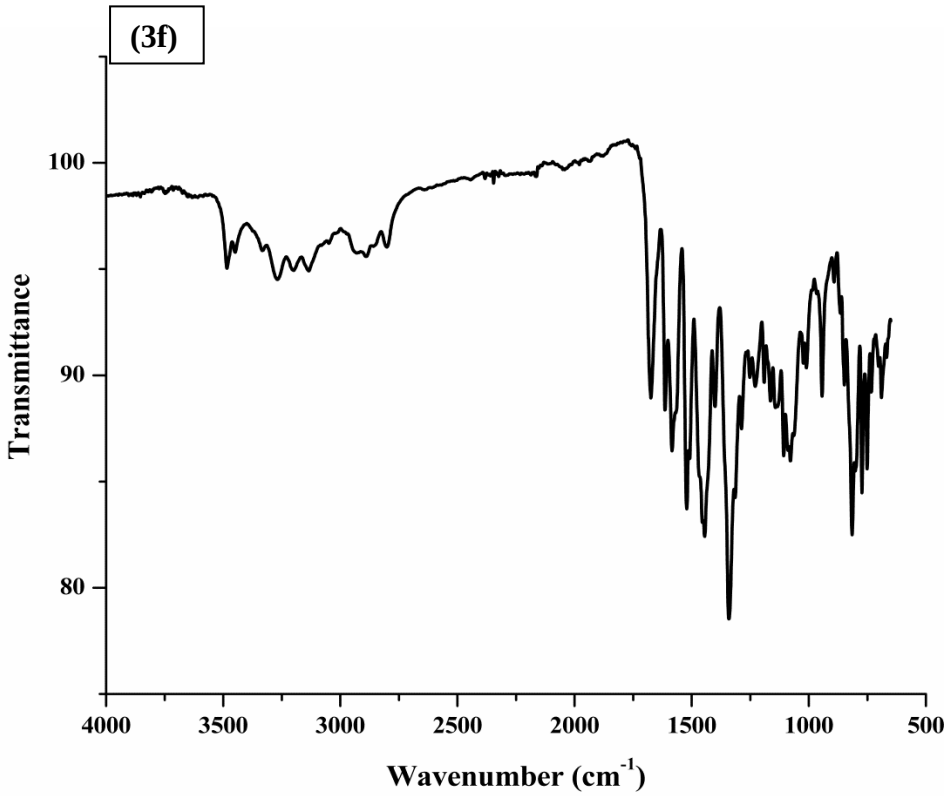

(3a)
Transmittance
100
90
80
70
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

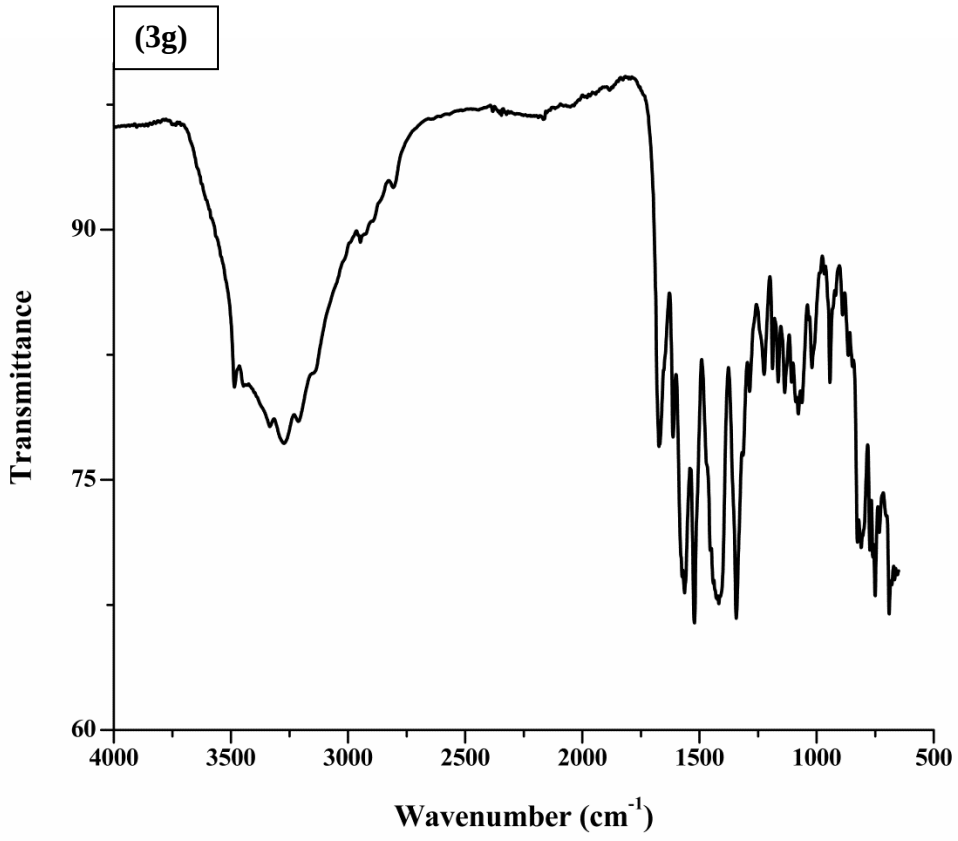

(3b)
Transmittance
100
90
80
70
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

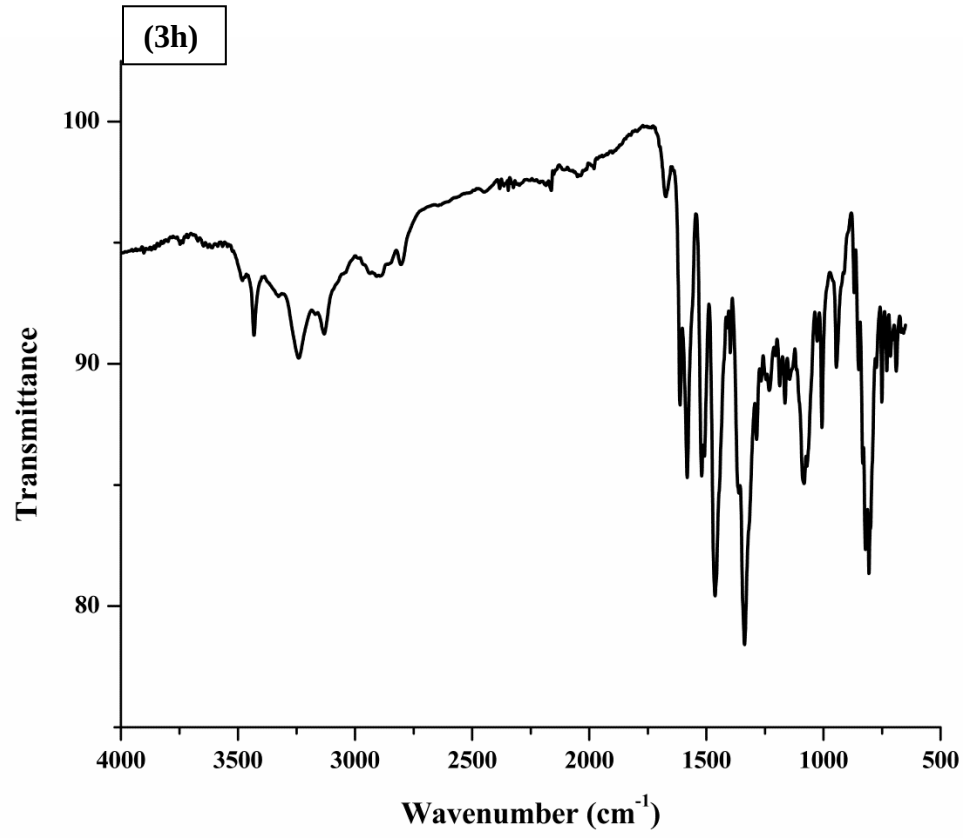

(3c)
Transmittance
100
95
90
85
80
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

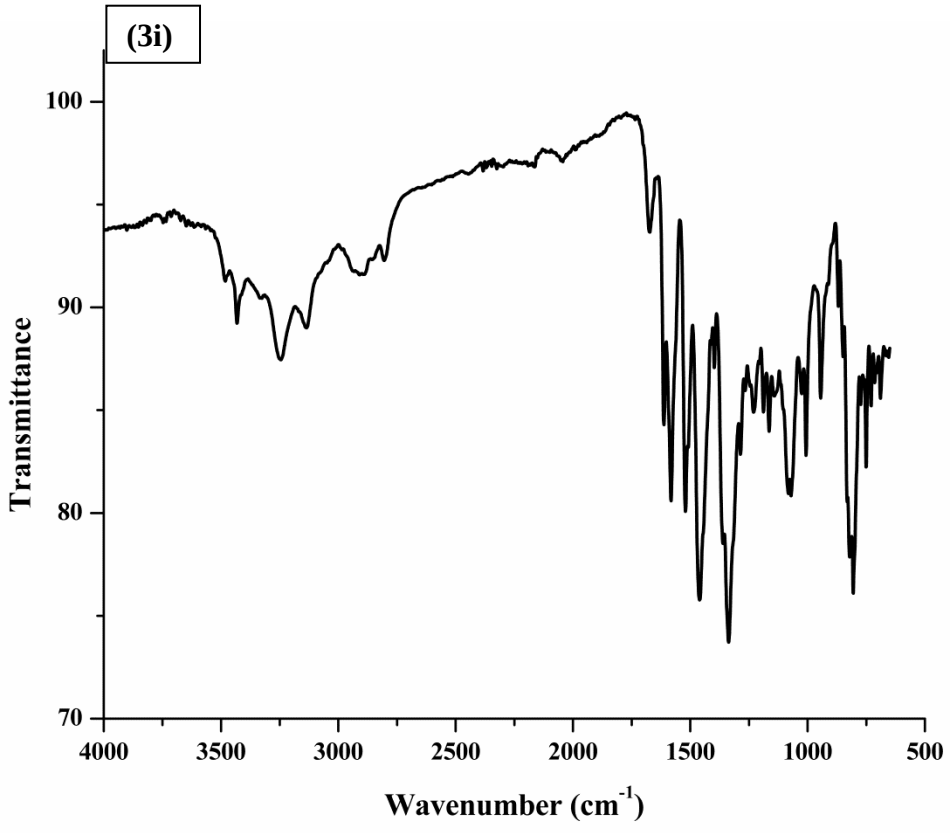

(3d)
Transmittance
100
90
80
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

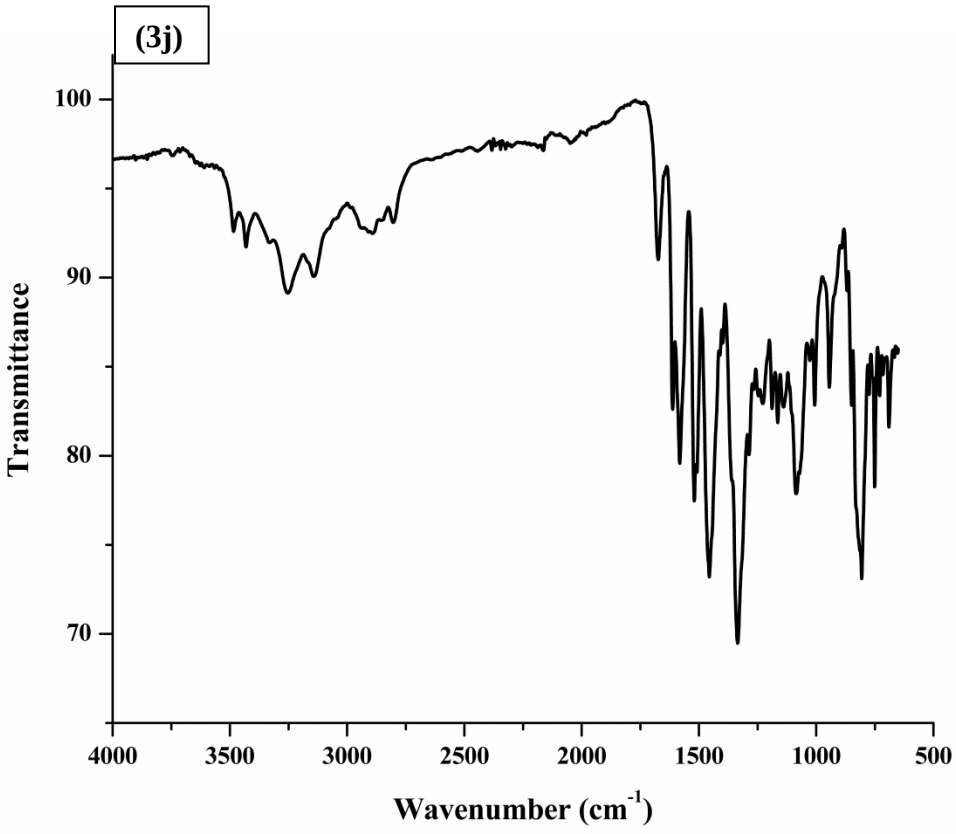

(3e)
100
90
80
Transmittance
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

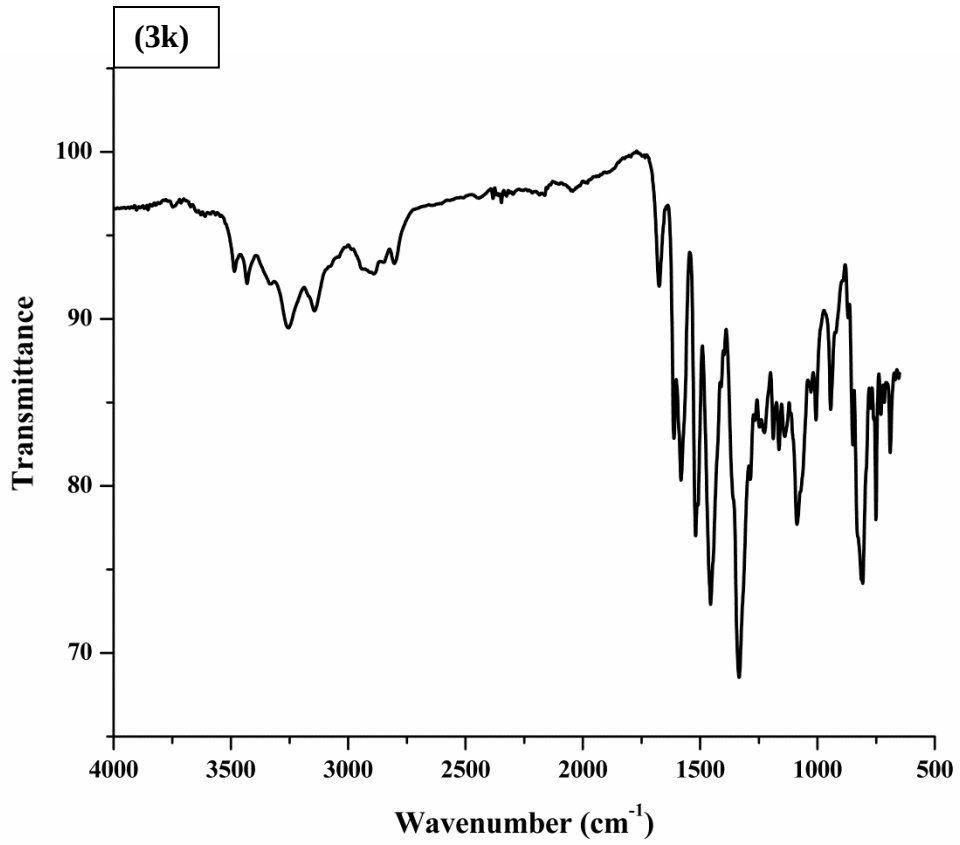

(3f)
100
90
80
Transmittance
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)


(3g)
Transmittance
90
75
60
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)


(3h)
Transmittance
100
90
80
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)


(3i)
Transmittance
100
90
80
70
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)


(3j)
Transmittance
100
90
80
70
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)


(3k)
Transmittance
100
90
80
70
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

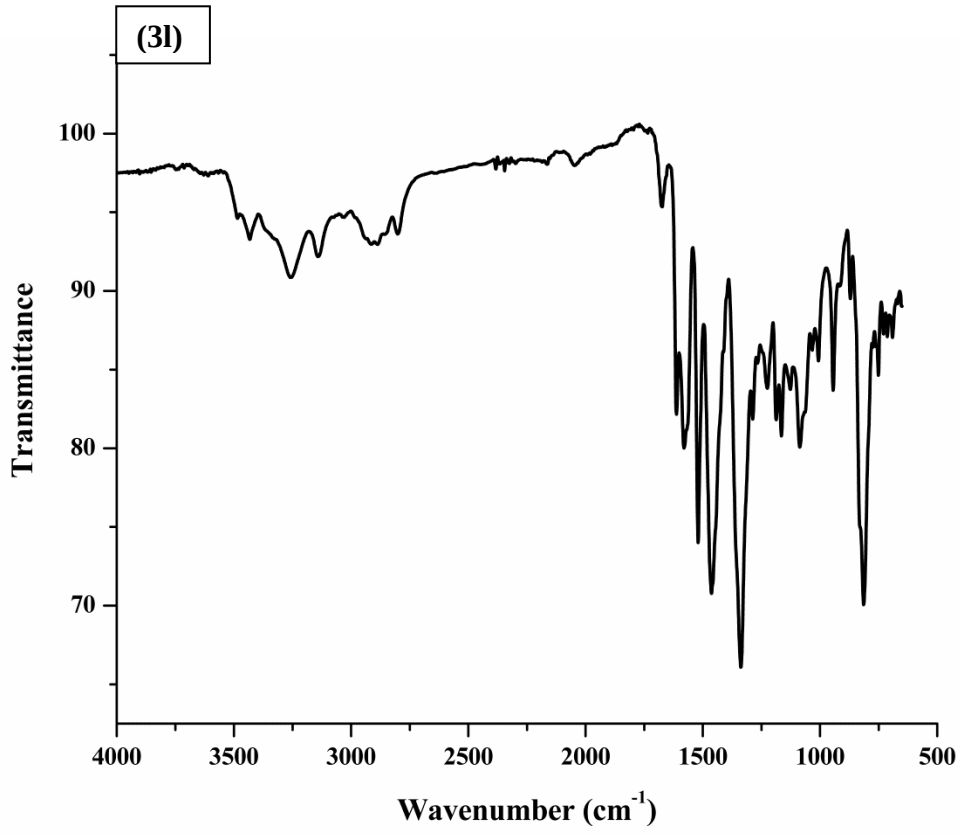
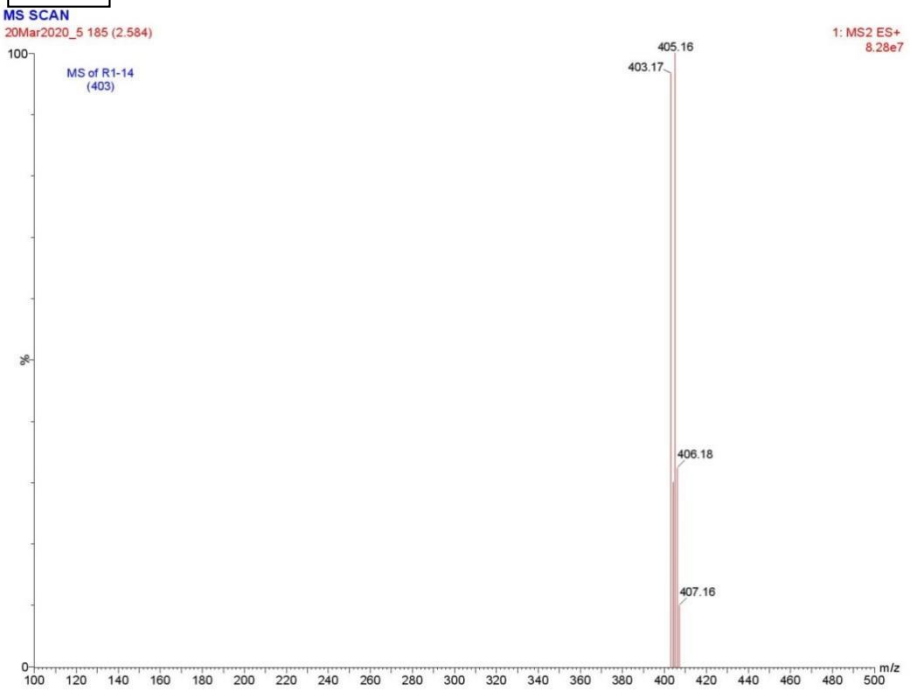
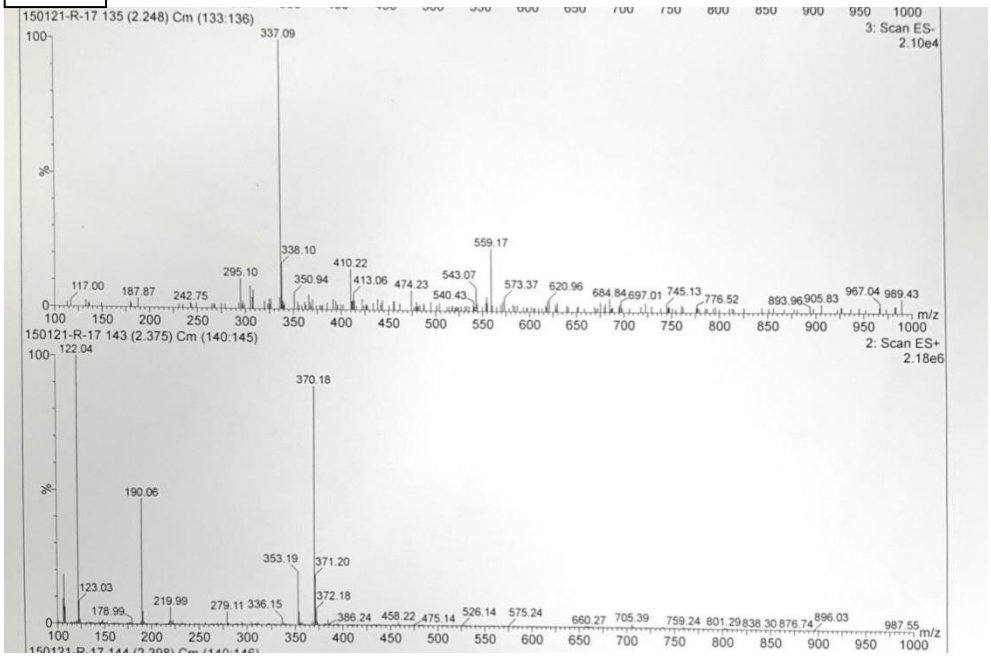

(3l)
Transmittance
100
90
80
70
4000
3500
3000
2500
2000
1500
1000
500
Wavenumber (cm-1)

Figure. S2. FTIR spectra of pyrazoline derivatives (3a-3l).

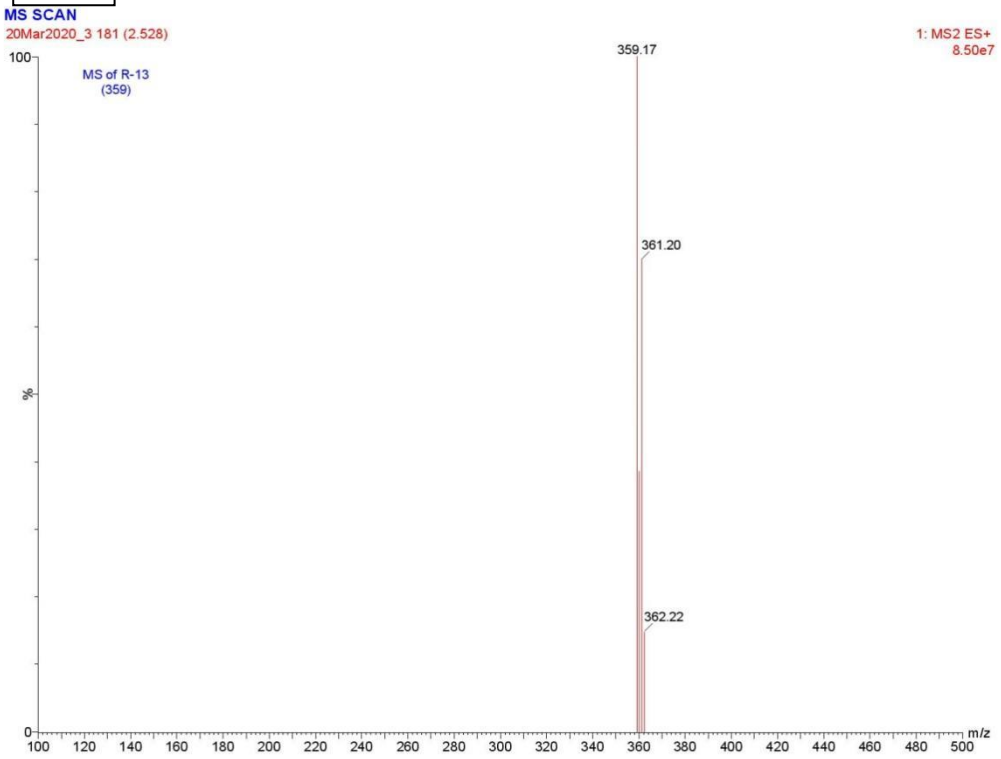
(3b)



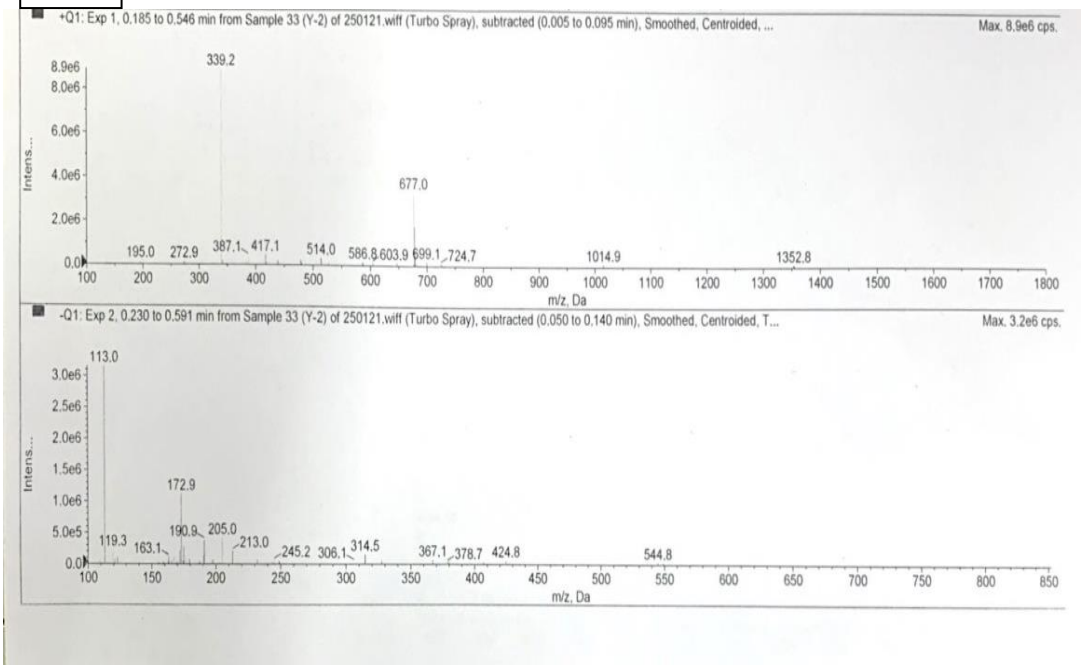
(3c)



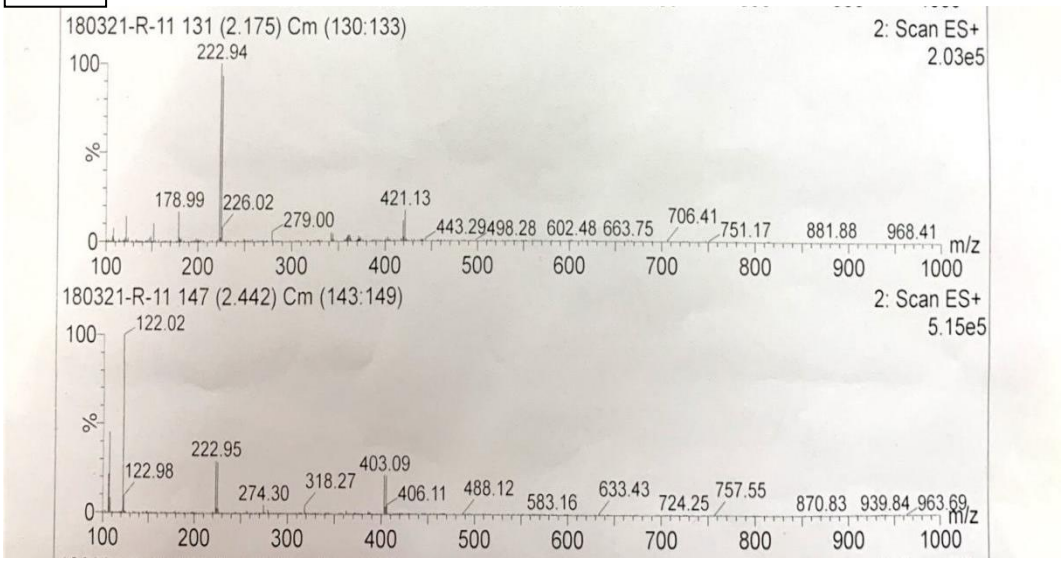
(3d)


MS SCAN
20Mar2020_3 181 (2.528)
1: MS2 ES+
8.50e7
MS of R-13
(359)
359.17
361.20
362.22
%
m/z

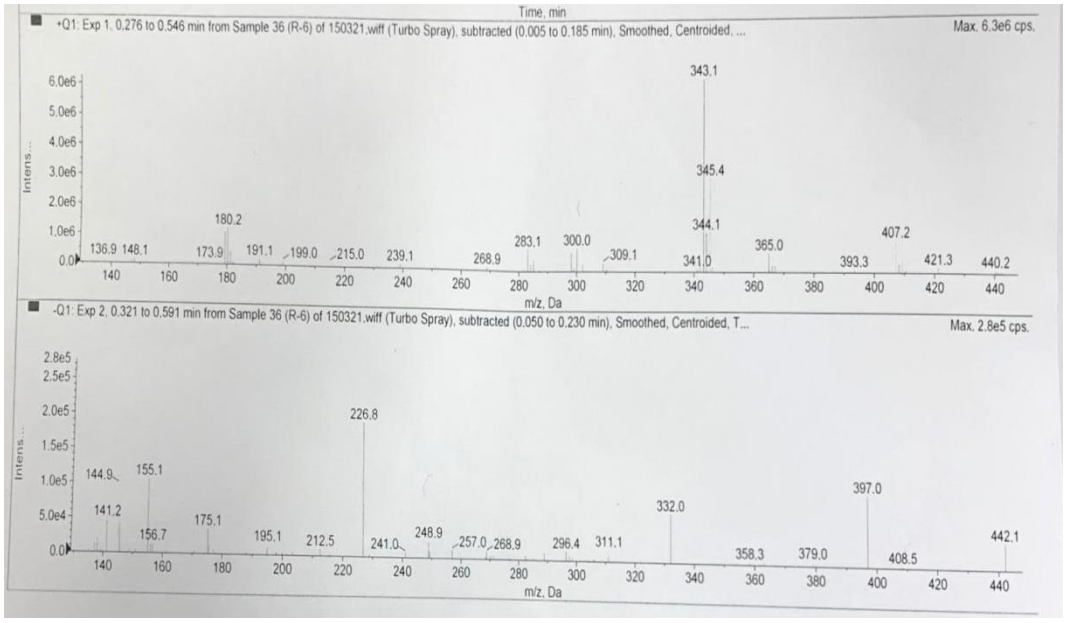
(3e)


+Q1: Exp 1, 0.185 to 0.546 min from Sample 33 (Y-2) of 250121.wiff (Turbo Spray), subtracted (0.005 to 0.095 min), Smoothed, Centroided, ...
Max. 8.9e6 cps.
339.2
677.0
m/z, Da
-Q1: Exp 2, 0.230 to 0.591 min from Sample 33 (Y-2) of 250121.wiff (Turbo Spray), subtracted (0.050 to 0.140 min), Smoothed, Centroided, T...
Max. 3.2e6 cps.
113.0
172.9
m/z, Da

(3f)


180321-R-11 131 (2.175) Cm (130:133)
2: Scan ES+
2.03e5
222.94
178.99
226.02
279.00
421.13
443.29
498.28
602.48
663.75
706.41
751.17
881.88
968.41
m/z
180321-R-11 147 (2.442) Cm (143:149)
2: Scan ES+
5.15e5
122.02
122.98
222.95
274.30
318.27
403.09
406.11
488.12
583.16
633.43
724.25
757.55
870.83
939.84
963.69
m/z

(3g)


Time, min
+Q1: Exp 1, 0.276 to 0.546 min from Sample 36 (R-6) of 150321.wiff (Turbo Spray), subtracted (0.005 to 0.185 min), Smoothed, Centroided, ...
Max. 6.3e6 cps.
343.1
345.4
344.1
180.2
407.2
m/z, Da
-Q1: Exp 2, 0.321 to 0.591 min from Sample 36 (R-6) of 150321.wiff (Turbo Spray), subtracted (0.050 to 0.230 min), Smoothed, Centroided, T...
Max. 2.8e5 cps.
226.8
397.0
332.0
442.1
m/z, Da

(3i)

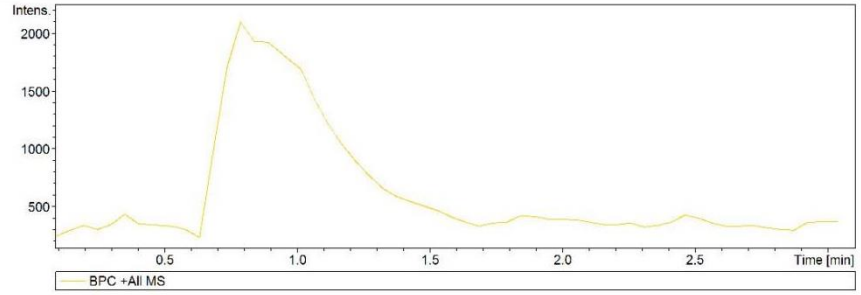
Display Report

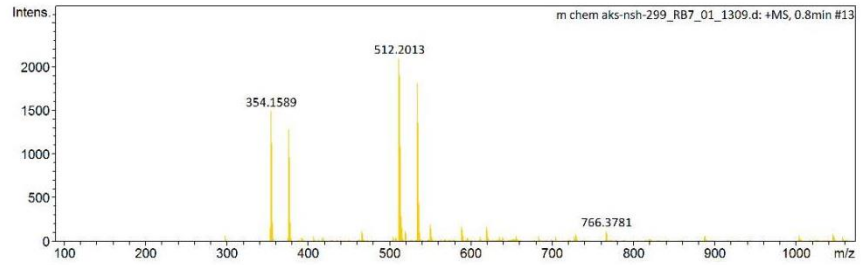
Analysis Info

Analysis Name	D:\Data\March 2020\m chem aks-nsh-299_RB7_01_1309.d	Acquisition Date	3/19/2020 6:04:49 PM
Method	2. LCMS tune wide ACN.m	Operator	IIT Indore
Sample Name	m chem aks-nsh-299	Instrument	micrOTOF-Q 228888.10348
Comment			

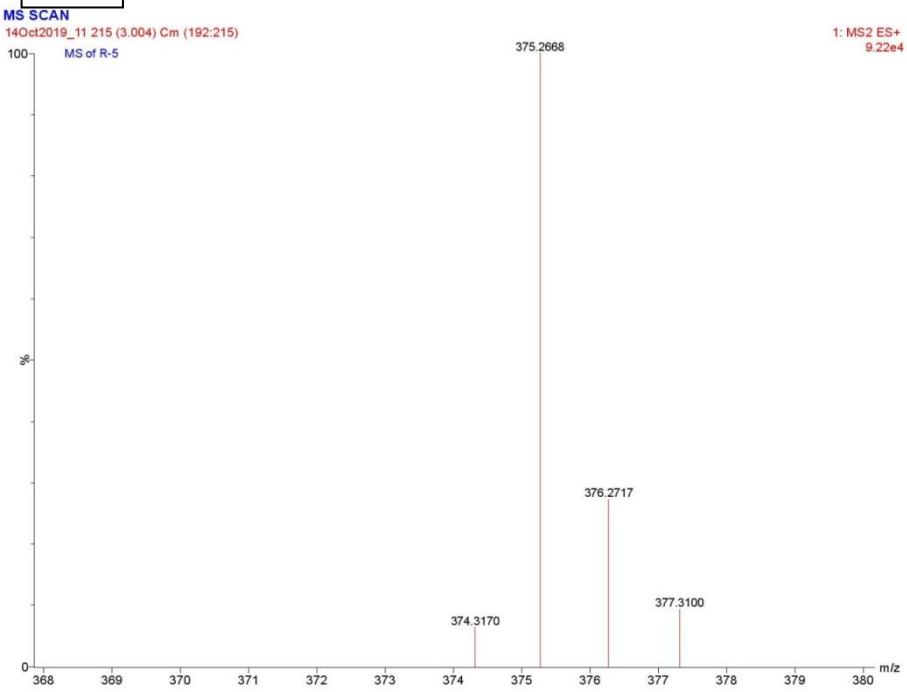
Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	2.0 Bar
Focus	Not active	Set Capillary	4500 V	Set Dry Heater	250 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	7.0 l/min
Scan End	3000 m/z	Set Collision Cell RF	650.0 Vpp	Set Divert Valve	Waste

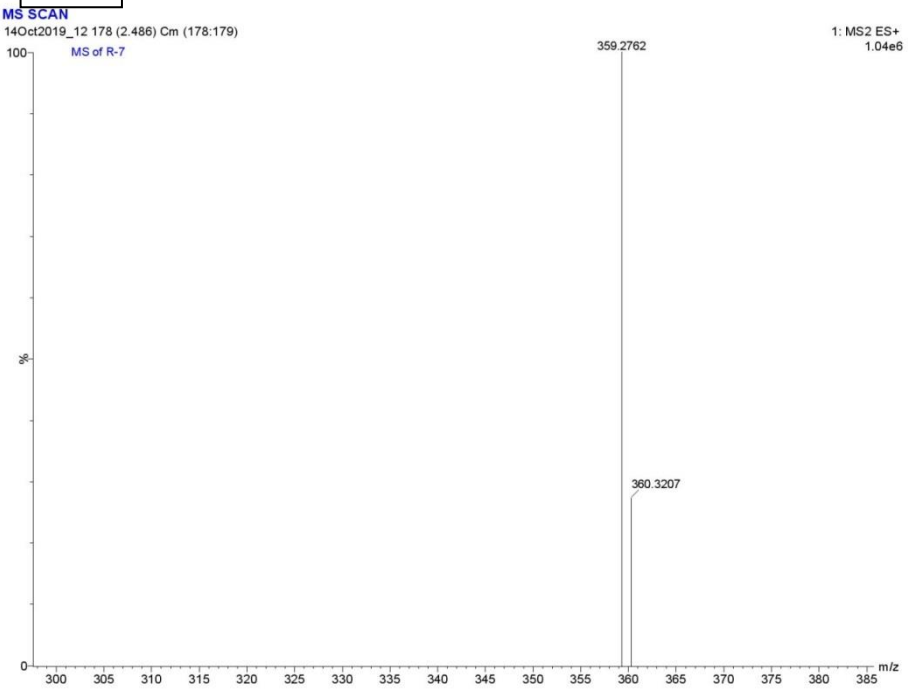




(3j)



(3k)


MS SCAN
14Oct2019_12 178 (2.486) Cm (178:179)
MS of R-7
1: MS2 ES+
1.04e6
359.2762
360.3207
%
m/z

(3l)

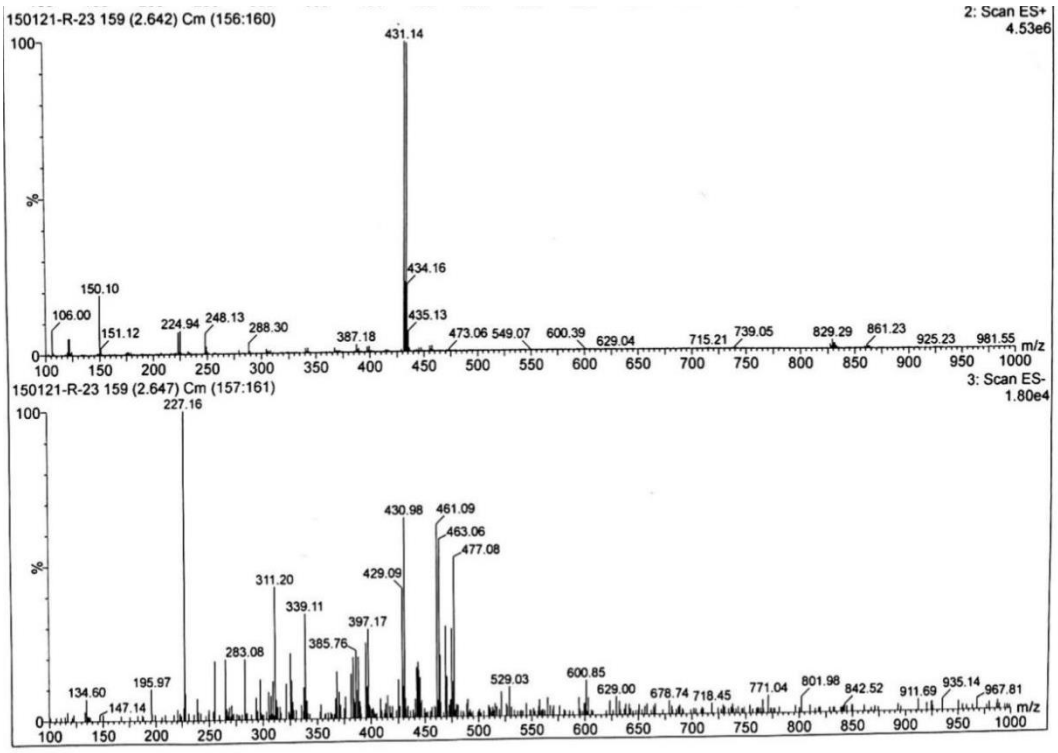

150121-R-23 159 (2.642) Cm (156:160)
2: Scan ES+
4.53e6
431.14
434.16
435.13
150.10
106.00
151.12
224.94
248.13
288.30
387.18
473.06
549.07
600.39
629.04
715.21
739.05
829.29
861.23
925.23
981.55
150121-R-23 159 (2.647) Cm (157:161)
3: Scan ES-
1.80e4
227.16
430.98
461.09
463.06
477.08
429.09
311.20
339.11
397.17
385.76
283.08
134.60
195.97
147.14
529.03
600.85
629.00
678.74
718.45
771.04
801.98
842.52
911.69
935.14
967.81
%
m/z

Figure S3. Mass spectra of pyrazoline derivatives (3a-3l).

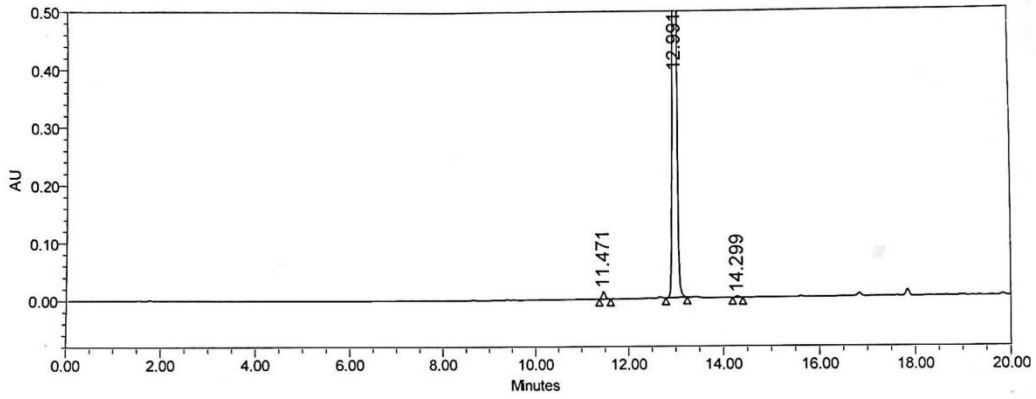
3a

SAMPLE INFORMATION

Sample Name :	A-3-XBS-ABC	Acquired By :	System HPLC_01
Vial :	20	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	3.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 214.0 nm (2998
Date Acquired:	24-02-2022 19:32:26 IST	Date Processed :	24-02-2022 20:01:56 IST

Column Name : XSELECT PHENYL HEXYL (4.6 X 250 mm)5 µ
Mobile phase : C: 5mM ABC in water A : 100% ACN
Flow rate : 1 ml/min, Temperature : Ambient
Flow mode : Gradient , Time/C (%) : 0.0/50.0, 2.0/50.0, 10.0/20.0, 15/05.0, 17.0/05.0, 17.50/50.0. 20.0/50.0

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area
1	11.471	62122	0.91
2	12.991	6780194	98.91
3	14.299	12733	0.19

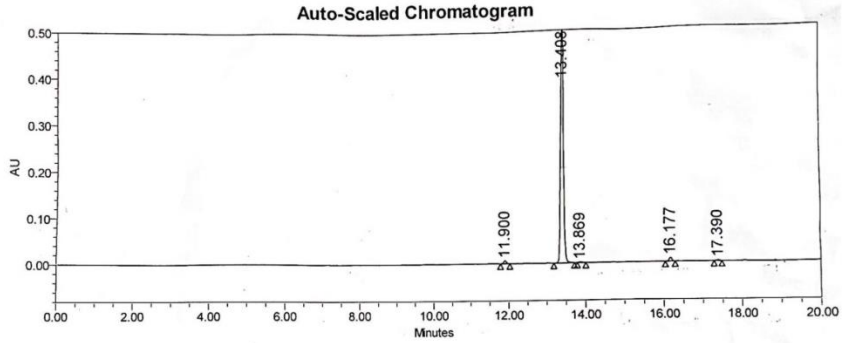
3b

SAMPLE INFORMATION

Sample Name :	B-3-XBS-ABC	Acquired By :	System HPLC_01
Vial :	71	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	3.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 328.0 nm (2998
Date Acquired:	25-02-2022 16:46:00 IST	Date Processed :	25-02-2022 18:23:30 IST

Column Name : XSELECT PHENYL HEXYL (4.6 X 250 mm)5 µ
Mobile phase : C: 5mM ABC in water A : 100% ACN
Flow rate : 1 ml/min, Temperature : Ambient
Flow mode : Gradient , Time/C (%) : 0.0/50.0, 2.0/50.0, 10.0/20.0, 15/05.0, 17.0/05.0, 17.50/50.0. 20.0/50.0

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area
1	11.900	32052	1.20
2	13.408	2589429	96.83
3	13.869	7716	0.29
4	16.177	38247	1.43
5	17.390	6715	0.25

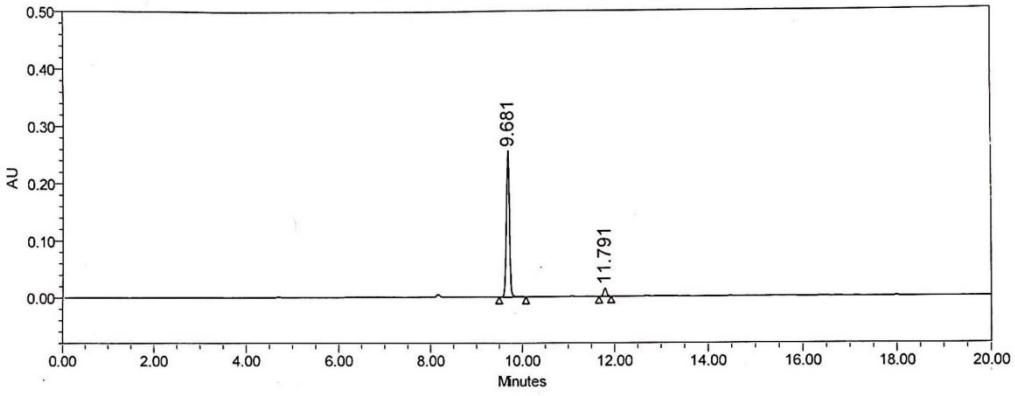
3c

SAMPLE INFORMATION

Sample Name :	C-3-XBS-ABC	Acquired By :	System HPLC_01
Vial :	104	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	3.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 254.0 nm (2998
Date Acquired:	24-02-2022 18:46:40 IST	Date Processed :	24-02-2022 19:16:50 IST

Column Name : XSELECT PHENYL HEXYL (4.6 X 250 mm)5 µ
Mobile phase : C: 5mM ABC in water A : 100% ACN
Flow rate : 1 ml/min, Temperature : Ambient
Flow mode : Gradient , Time/C (%) : 0.0/50.0, 2.0/50.0, 10.0/20.0, 15/05.0, 17.0/05.0, 17.50/50.0. 20.0/50.0

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area
1	9.681	1203403	94.65
2	11.791	68016	5.35

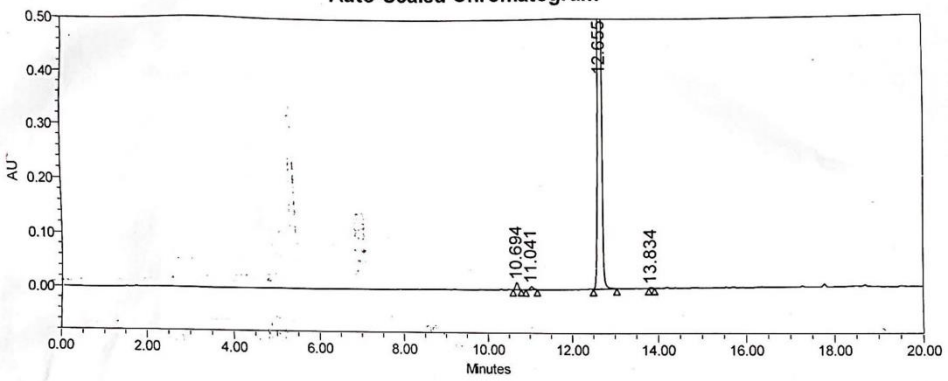
3d

SAMPLE INFORMATION

Sample Name :	D-3-XBS-ABC	Acquired By :	System HPLC_01
Vial :	72	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	3.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 214.0 nm (2998
Date Acquired:	25-02-2022 17:08:46 IST	Date Processed :	25-02-2022 18:21:10 IST

Column Name : XSELECT PHENYL HEXYL (4.6 X 250 mm)5 µ
Mobile phase : C: 5mM ABC in water A : 100% ACN
Flow rate : 1 ml/min, Temperature : Ambient
Flow mode : Gradient , Time/C (%) : 0.0/50.0, 2.0/50.0, 10.0/20.0, 15/05.0, 17.0/05.0, 17.50/50.0. 20.0/50.0

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area
1	10.694	65244	1.11
2	11.041	32983	0.56
3	12.655	5782277	98.21
4	13.834	6952	0.12

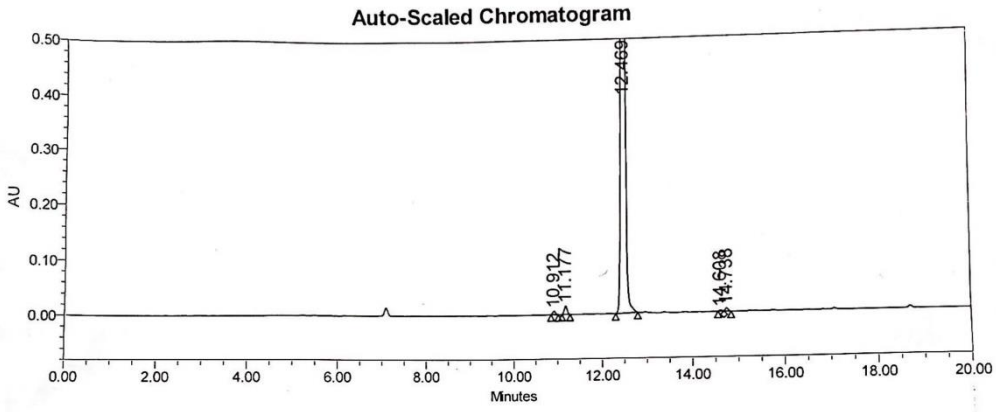
3e

SAMPLE INFORMATION

Name :	E-3-XBS-ABC	Acquired By :	System HPLC_01
Vial :	49	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	3.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 260.0 nm (2998
Date Acquired:	25-02-2022 17:31:29 IST	Date Processed :	25-02-2022 18:19:07 IST

Column Name : XSELECT PHENYL HEXYL (4.6 X 250 mm)5 µ
Mobile phase : C: 5mM ABC in water A : 100% ACN
Flow rate : 1 ml/min, Temperature : Ambient
Flow mode : Gradient , Time/C (%) : 0.0/50.0, 2.0/50.0, 10.0/20.0, 15/05.0, 17.0/05.0, 17.50/50.0. 20.0/50.0

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area
1	10.912	28696	0.29
2	11.177	70449	0.72
3	12.469	9692199	98.61
4	14.608	11032	0.11
5	14.738	26581	0.27

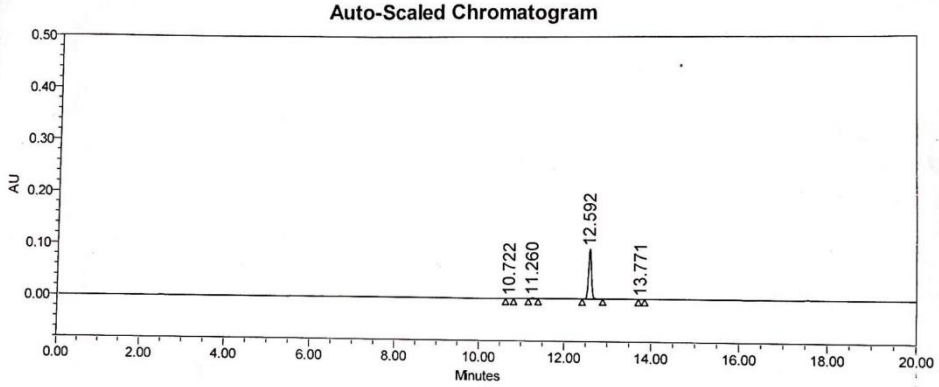
3f

SAMPLE INFORMATION

Sample Name :	S3-XBS-ABC	Acquired By :	System HPLC_01
Vial :	103	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	3.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 258.0 nm (2998
Date Acquired:	23-02-2022 19:17:27 IST	Date Processed :	23-02-2022 19:40:37 IST

Column Name : XSELECT PHENYL HEXYL (4.6 X 250 mm)5 µ
Mobile phase : C: 5mM ABC in water A : 100% ACN
Flow rate : 1 ml/min, Temperature : Ambient
Flow mode : Gradient , Time/C (%) : 0.0/50.0, 2.0/50.0, 10.0/20.0, 15/05.0, 17.0/05.0, 17.50/50.0. 20.0/50.0

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area
1	10.722	2024	0.44
2	11.260	7475	1.63
3	12.592	447879	97.72
4	13.771	930	0.20

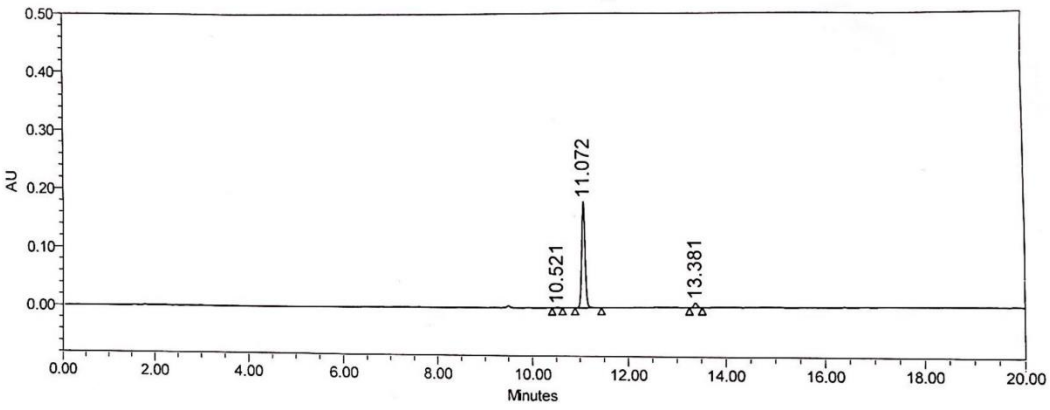
3g

SAMPLE INFORMATION

Sample Name :	G-3-XBS-ABC	Acquired By :	System HPLC_01
Vial :	106	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	3.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 214.0 nm (2998
Date Acquired:	24-02-2022 19:55:28 IST	Date Processed :	24-02-2022 20:17:13 IST

Column Name : XSELECT PHENYL HEXYL (4.6 X 250 mm)5 µ
Mobile phase : C: 5mM ABC in water A : 100% ACN
Flow rate : 1 ml/min, Temperature : Ambient
Flow mode : Gradient , Time/C (%) : 0.0/50.0, 2.0/50.0, 10.0/20.0, 15/05.0, 17.0/05.0, 17.50/50.0. 20.0/50.0

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area
1	10.521	5061	0.55
2	11.072	870230	95.00
3	13.381	40719	4.45

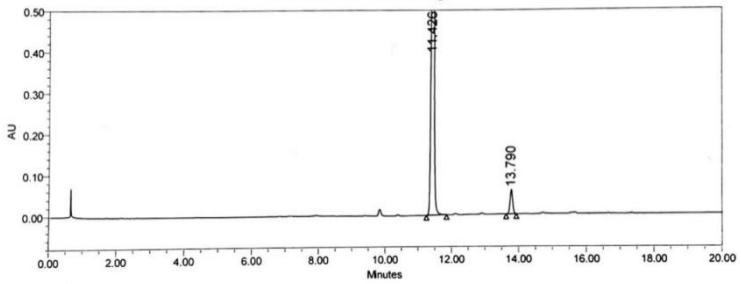
3h

SAMPLE INFORMATION

Sample Name :	H3-XBS-ABC	Acquired By :	System HPLC_01
Vial :	23	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	5.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 214.0 nm (2998
Date Acquired:	02-03-2022 19:01:40 IST	Date Processed :	02-03-2022 19:25:19 IST

Column Name : XSELECT PHENYL HEXYL (4.6 X 250 mm)5 µ
Mobile phase : C: 5mM ABC in water A : 100% ACN
Flow rate : 1 ml/min, Temperature : Ambient
Flow mode : Gradient , Time/C (%) : 0.0/50.0, 2.0/50.0, 10.0/20.0, 15/05.0, 17.0/05.0, 17.50/50.0. 20.0/50.0

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area
1	11.426	7042027	95.57
2	13.790	326588	4.43

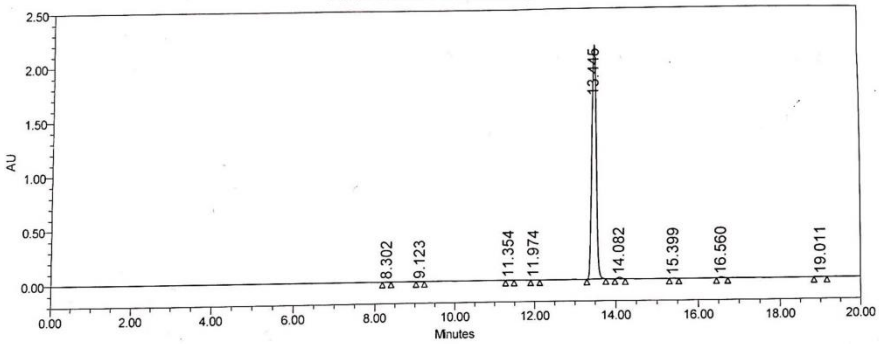
3i

SAMPLE INFORMATION

Sample Name :	I3	Acquired By :	System HPLC_01
Vial :	57	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	3.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 270.0 nm (2998 (190-400)nm)
Date Acquired:	18-02-2022 17:55:39 IST	Date Processed :	18-02-2022 18:31:07 IST

Column Name : XBridgeC8 (4.6 X 250 mm)5 µ
Mobile phase : C : 0.1% AH in Water A : 100% ACN
Flow rate : 1 ml/min, Column Temperature : Ambient.
Flow mode : Gradient , Time/C (%) :: 0.0/60.0, 2.0/60.0, 9.0/25.0, 15.0/5.0, 18.0/5.0, 18.50/60.0, 20.0/60.0

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area
1	8.302	11162	0.07
2	9.123	8228	0.05
3	11.354	7115	0.04
4	11.974	7084	0.04
5	13.445	16191623	98.51
6	14.082	107155	0.65
7	15.399	26533	0.16
8	16.560	66586	0.41

	RT	Area	% Area
9	19.011	11701	0.07

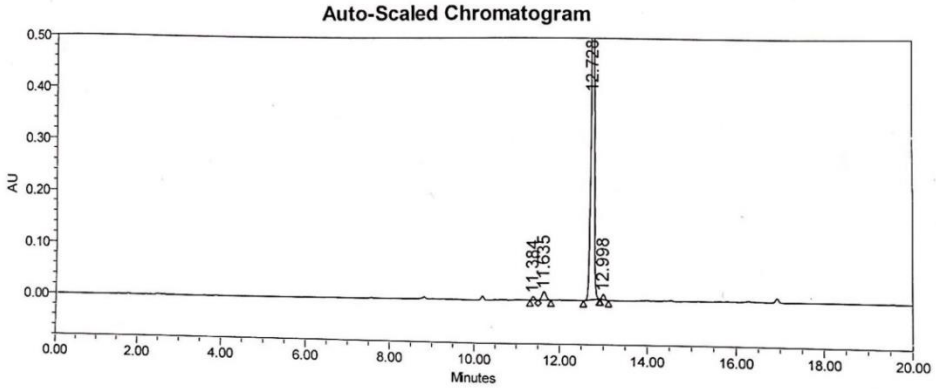
3j

SAMPLE INFORMATION

Sample Name :	J3-XBS-ABC	Acquired By :	System HPLC_01
Vial :	101	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	3.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 214.0 nm (2998
Date Acquired:	23-02-2022 18:32:06 IST	Date Processed :	23-02-2022 18:56:48 IST

Column Name : XSELECT PHENYL HEXYL (4.6 X 250 mm)5 µ
Mobile phase : C: 5mM ABC in water A : 100% ACN
Flow rate : 1 ml/min, Temperature : Ambient
Flow mode : Gradient , Time/C (%) : 0.0/50.0, 2.0/50.0, 10.0/20.0, 15/05.0, 17.0/05.0, 17.50/50.0. 20.0/50.0

Auto-Scaled Chromatogram



Peak Results

	RT	Area	% Area
1	11.384	29812	0.75
2	11.635	101812	2.55
3	12.728	3822752	95.61
4	12.998	43917	1.10

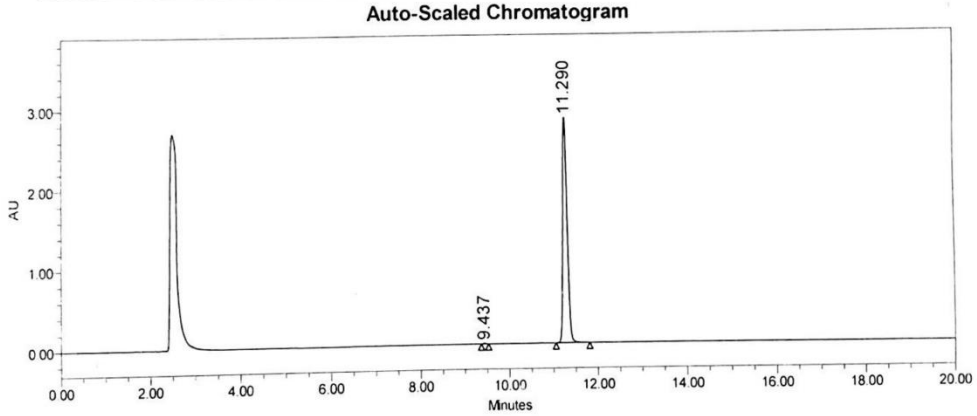
3k

SAMPLE INFORMATION

Sample Name :	K-3-XBS-ABC	Acquired By :	System HPLC_01
Vial :	96	Acq. Method Set :	NON POLAR C@A20MIN 40%
Injection # :	1	Injection Volume :	3.00 ul
Run Time :	20.0 Minutes	Proc. Chnl. Descr.:	2998 PDA 214.0 nm (2998 (190-400)nm)
Date Acquired:	07-03-2022 17:59:11 IST	Date Processed :	07-03-2022 18:49:07 IST

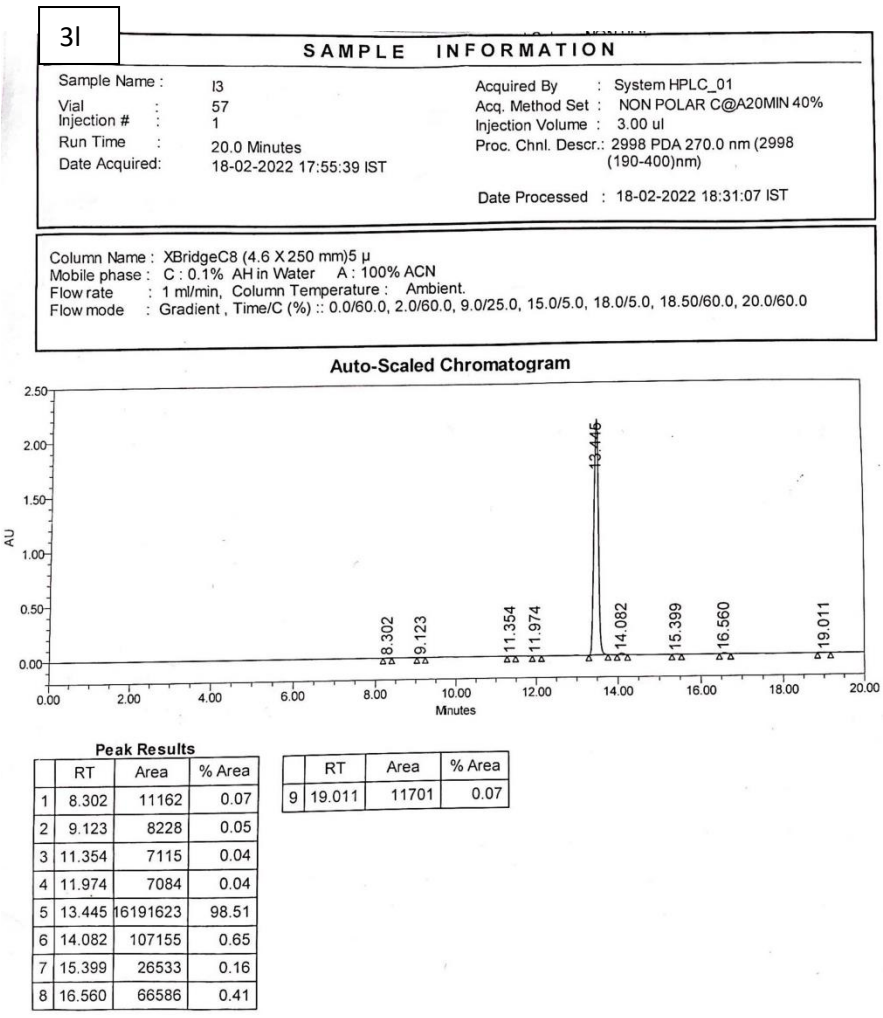
Column Name : XBS(4.6 X 250 mm)5 µ
Mobile phase : C : 5mM ABC in water A : 100% ACN
Flow rate : 1 ml/min, Temperature : Ambient
Flow mode : Gradient , Time/C (%) : 0.0/70.0, 2.0/70.0,6.0/40.0, 12.0/40.0, 15.0/5.0, 18.0/5.0, 18.50/70.0,20.0/70.0

Auto-Scaled Chromatogram



Peak Results

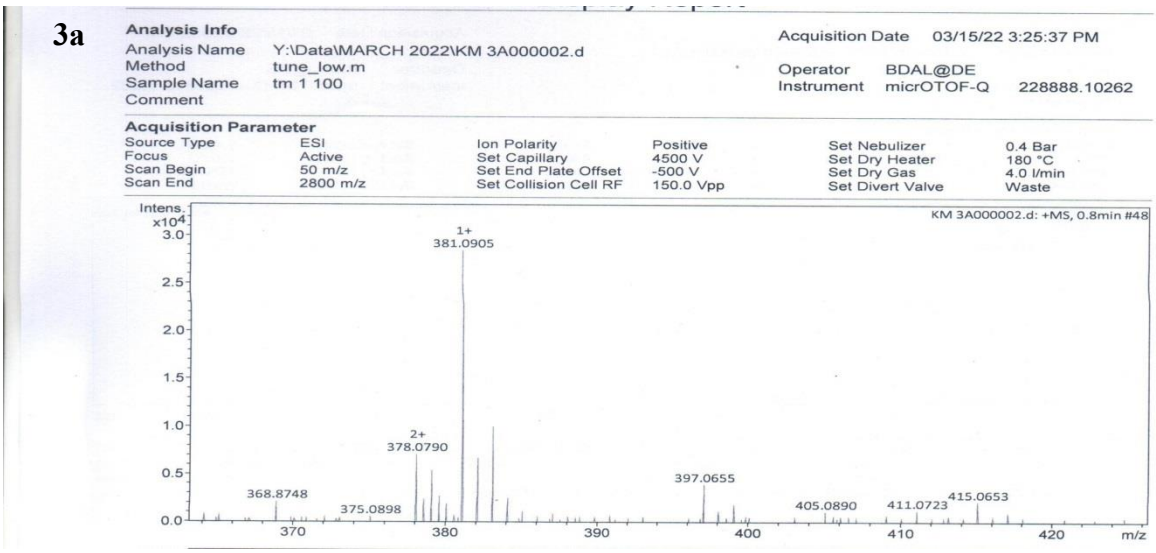
	RT	Area	% Area
1	9.437	42547	0.21
2	11.290	19795397	99.79



	RT	Area	% Area
1	8.302	11162	0.07
2	9.123	8228	0.05
3	11.354	7115	0.04
4	11.974	7084	0.04
5	13.445	16191623	98.51
6	14.082	107155	0.65
7	15.399	26533	0.16
8	16.560	66586	0.41

	RT	Area	% Area
9	19.011	11701	0.07

Figure. S4. HPLC spectra of pyrazoline derivatives (3a-3l).



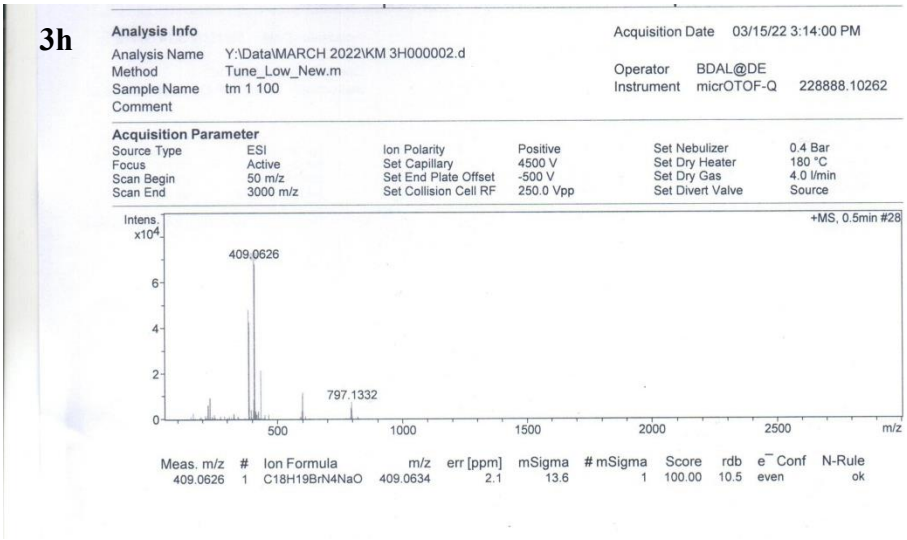


Figure. S5. HRMS spectra of lead compounds (3a and 3h).