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Supplementary Information

"Microwave-Assisted Multi-Component Green Synthesis of Bioactive Pyrazol-5-ol and its Derivatives Using Graphene Oxide as Recyclable Catalyst: A Route to EGFR Inhibitors"

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Supplementary Figures:

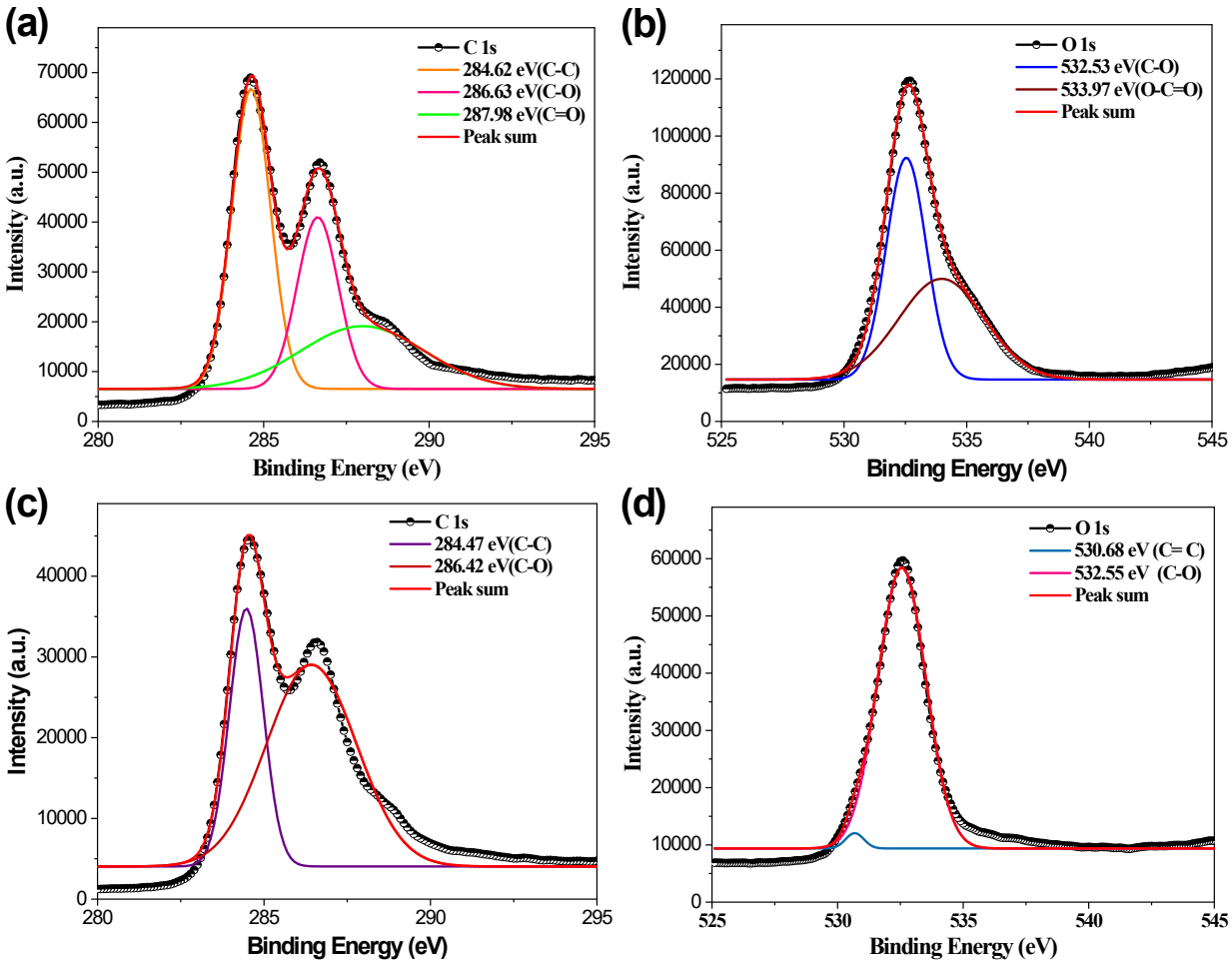
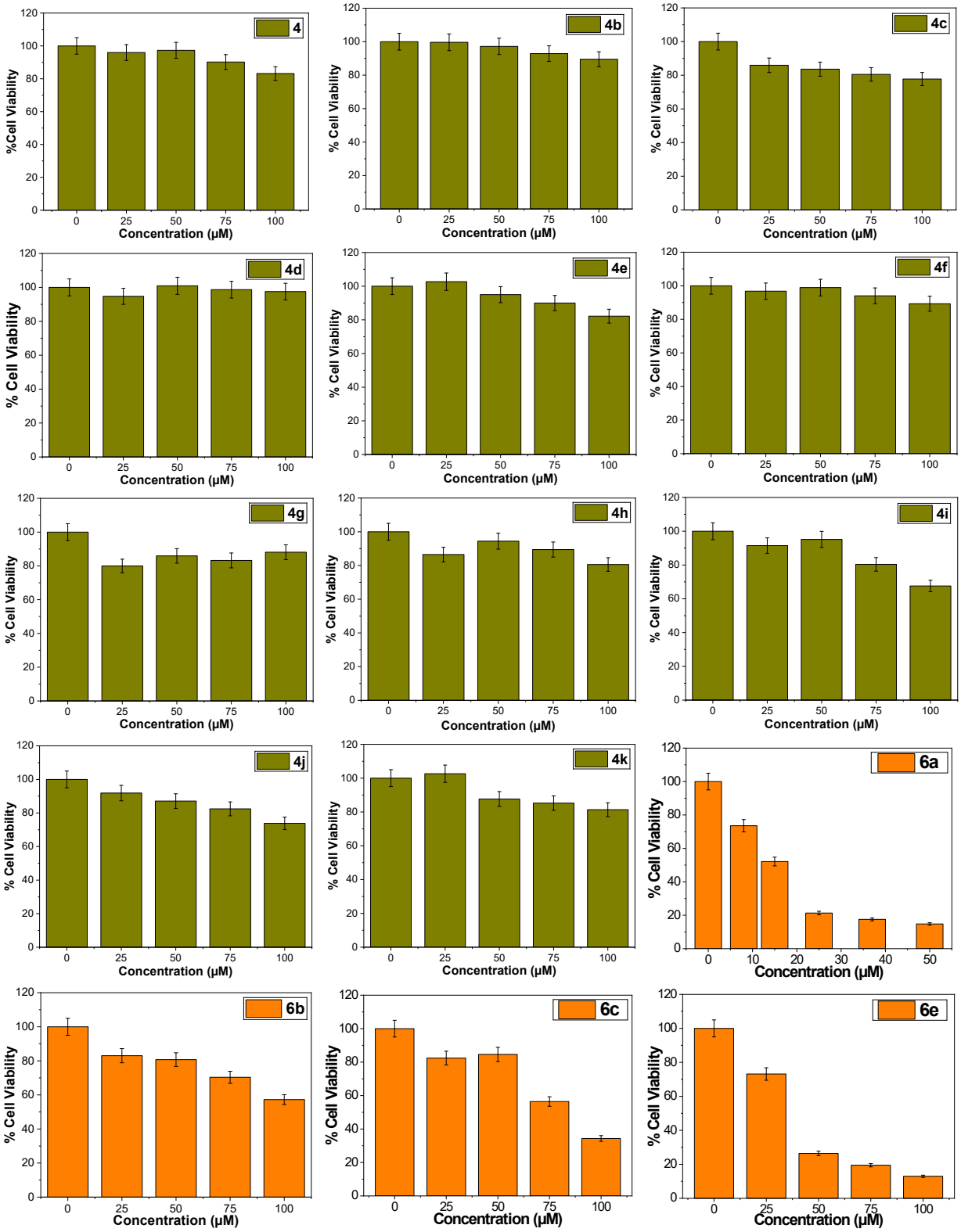


Figure S1. High-resolution C 1s (*a* & *c*) and O 1s (*b* & *d*) XPS spectra of, (*a*, *b*) pure GO (before Cycle I) and (*c*, *d*) GO after Cycle V.


4
4b
4c
4d
4e
4f
4g
4h
4i
4j
4k
6a
6b
6c
6e
%Cell Viability
% Cell Viability
Concentration (μM)

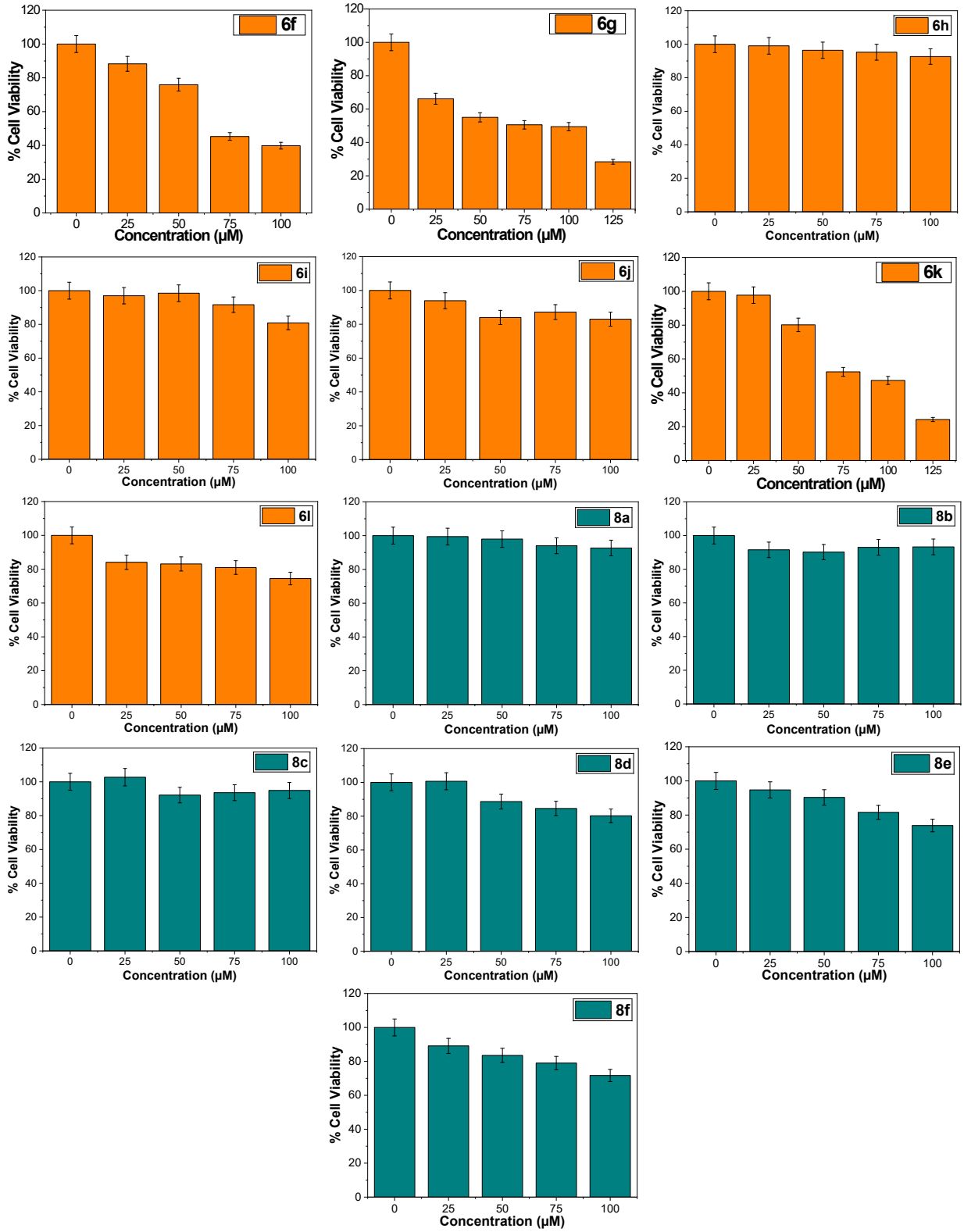
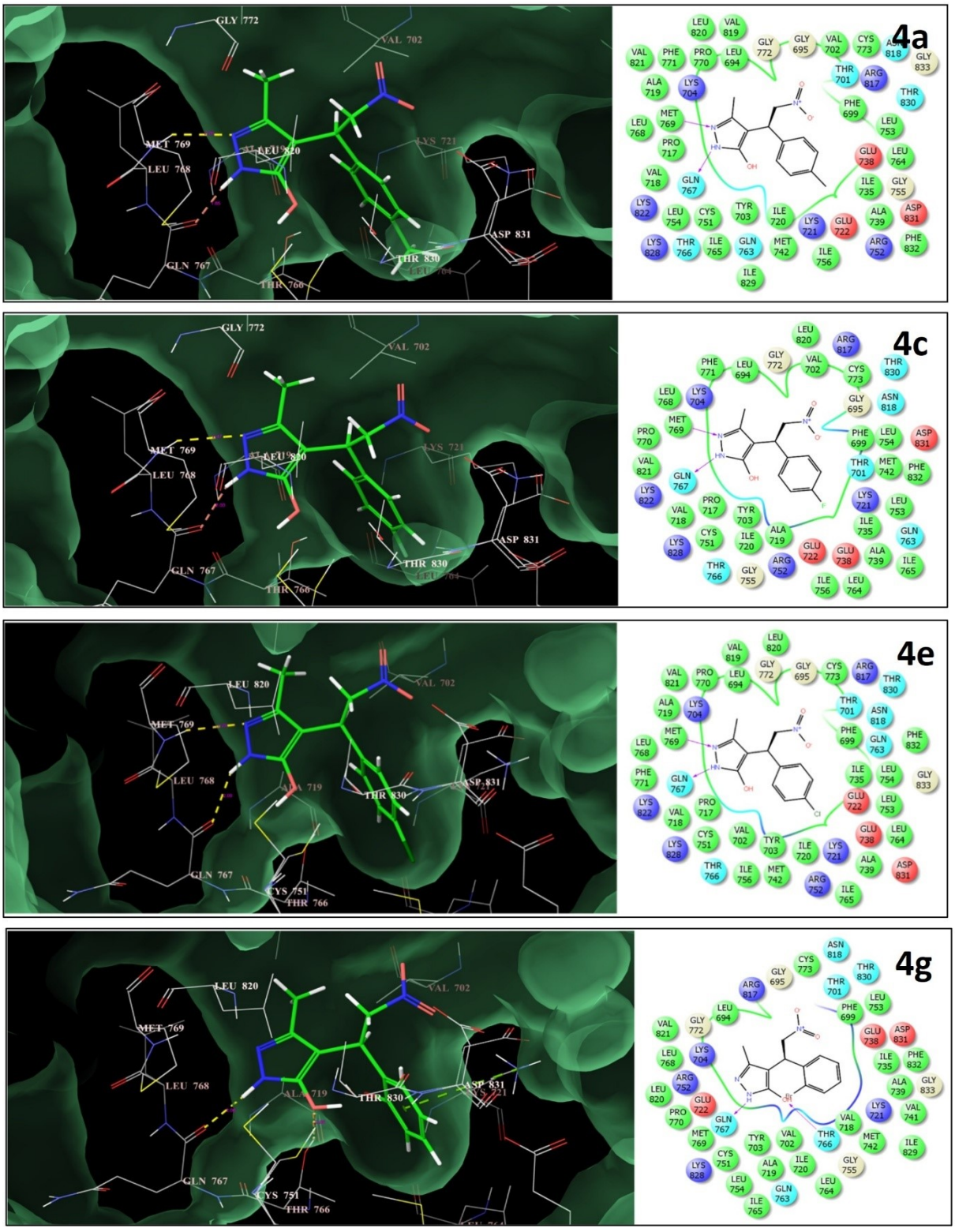


Figure S2. Cell viability (%) *vs* concentration of pyrazol-5-ol derivatives (**4**,**6** & **8** series).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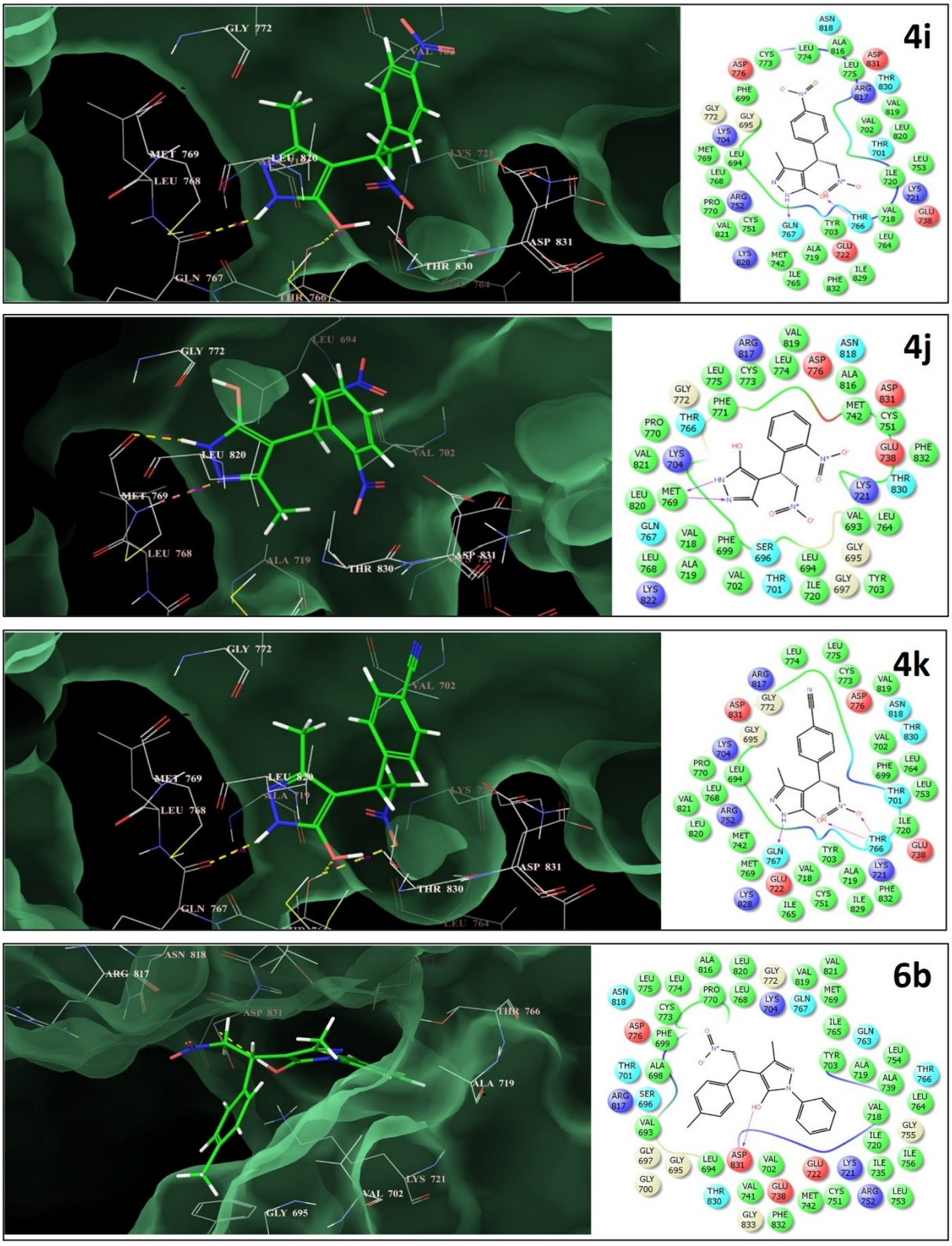
4c
4e
4g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MET 769
LEU 768
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ASP 831
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THR 766
4i
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4j
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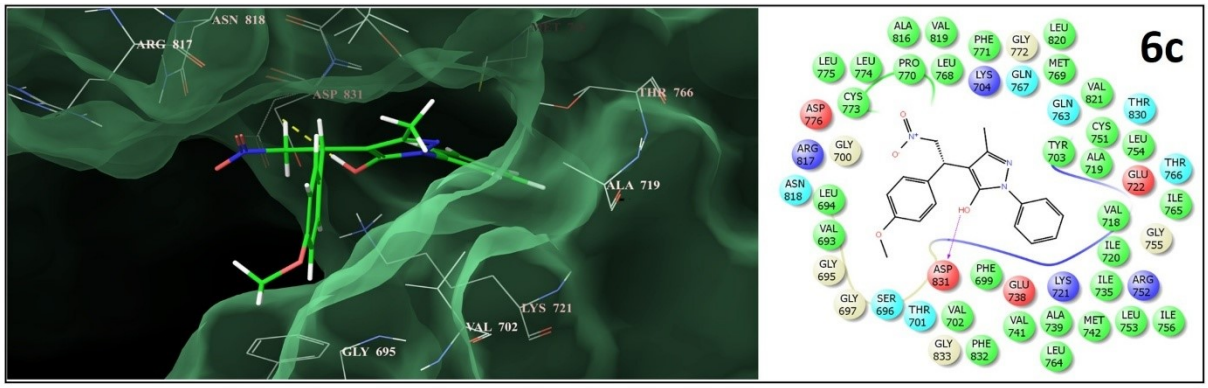
ARG 817
THR 766
ALA 719
VAL 702
GLY 695
6b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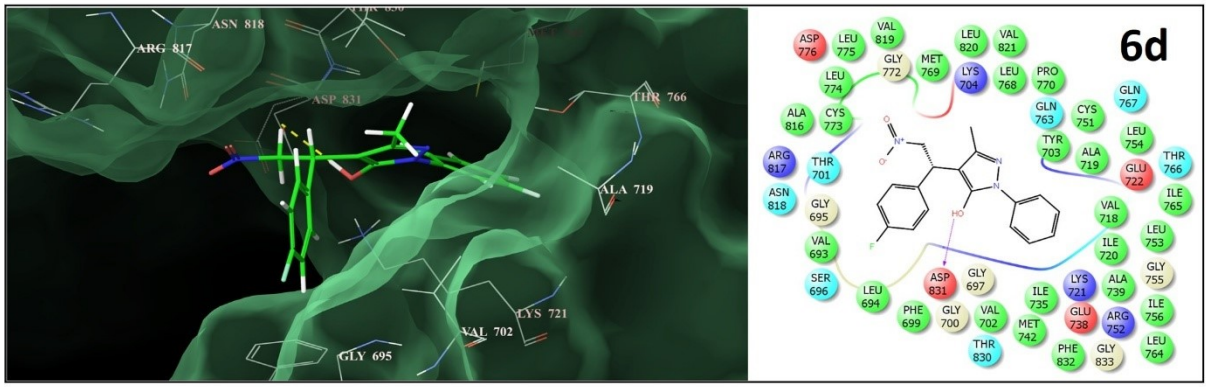
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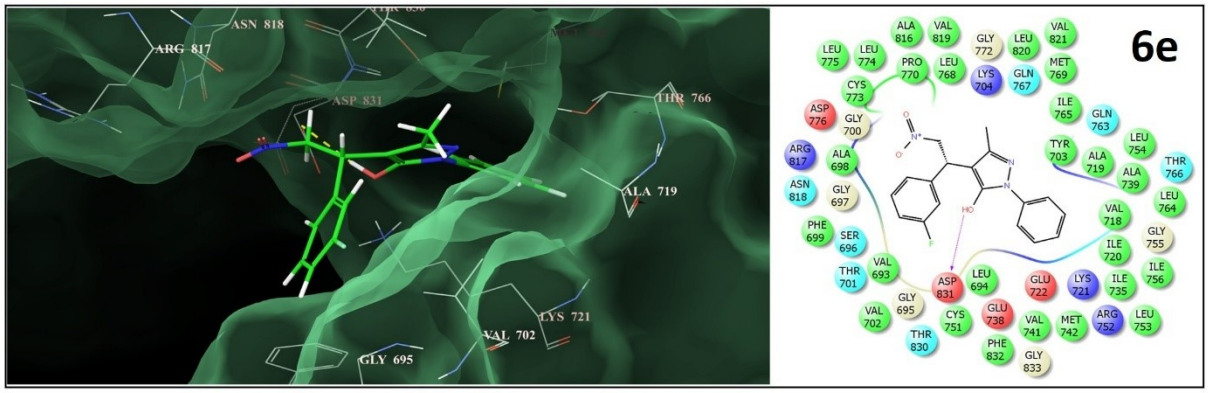
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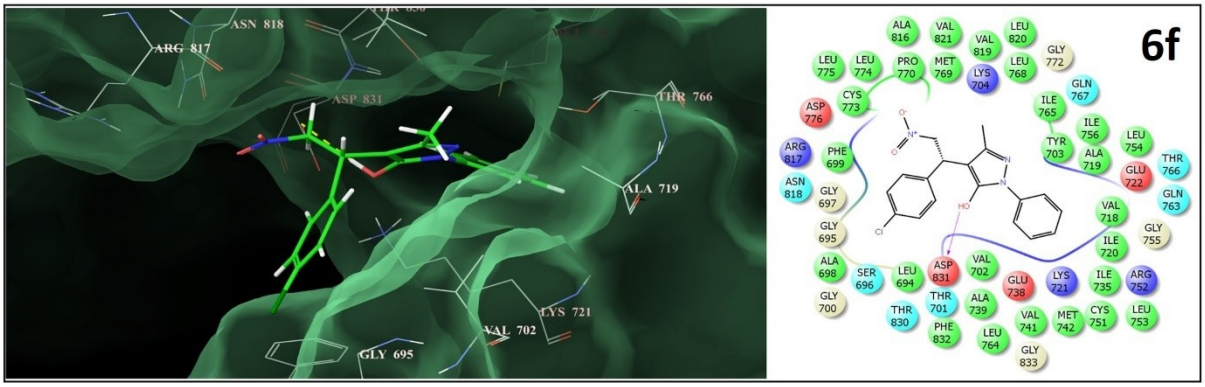
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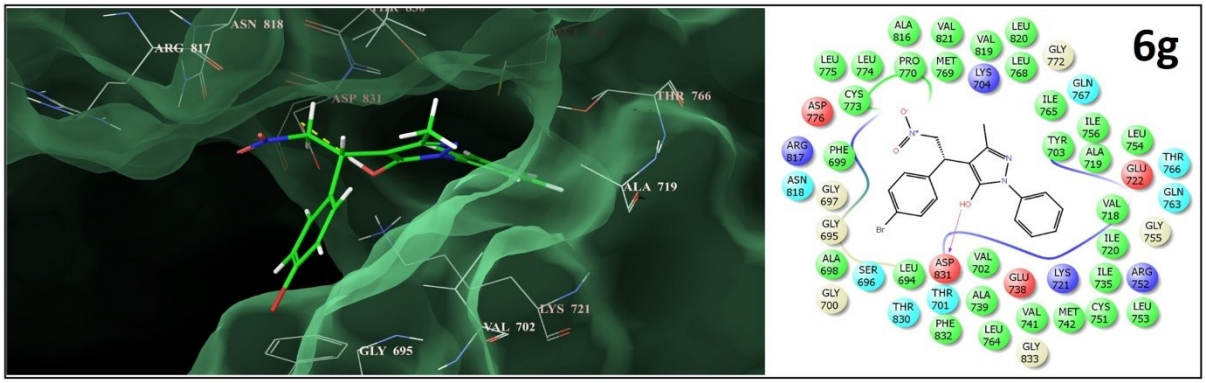
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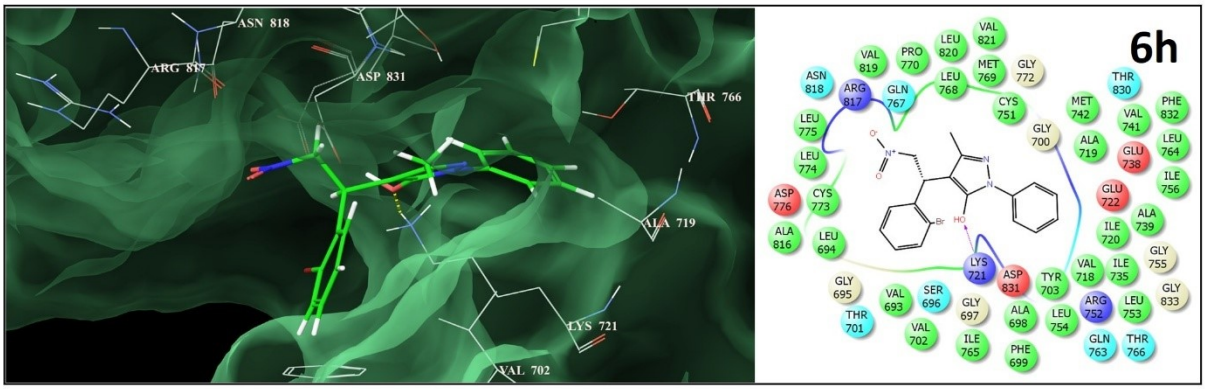
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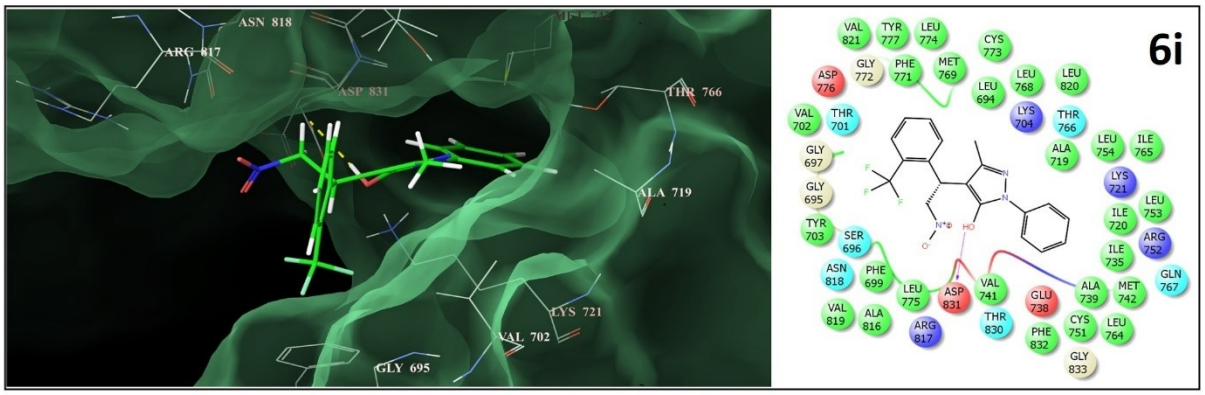
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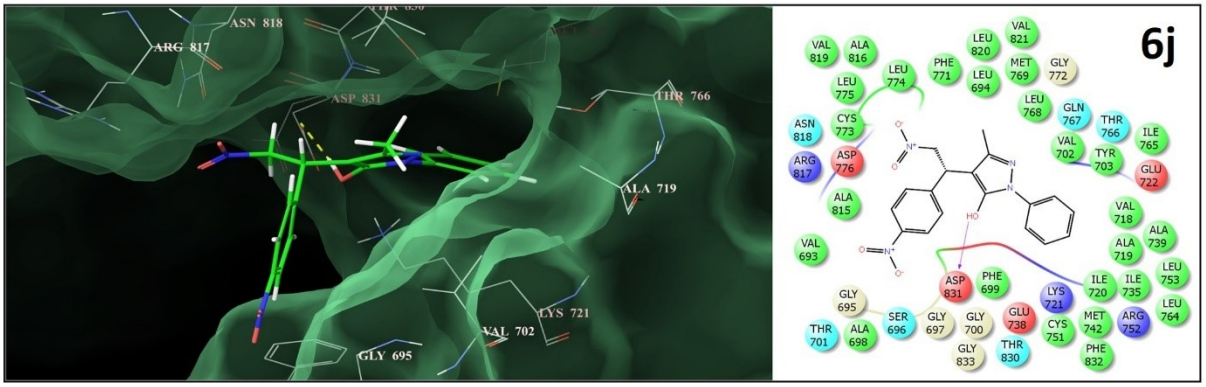
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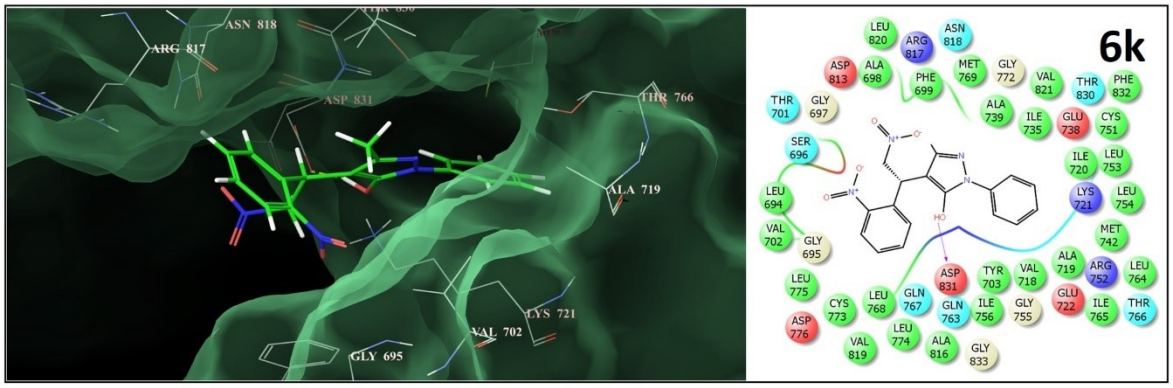
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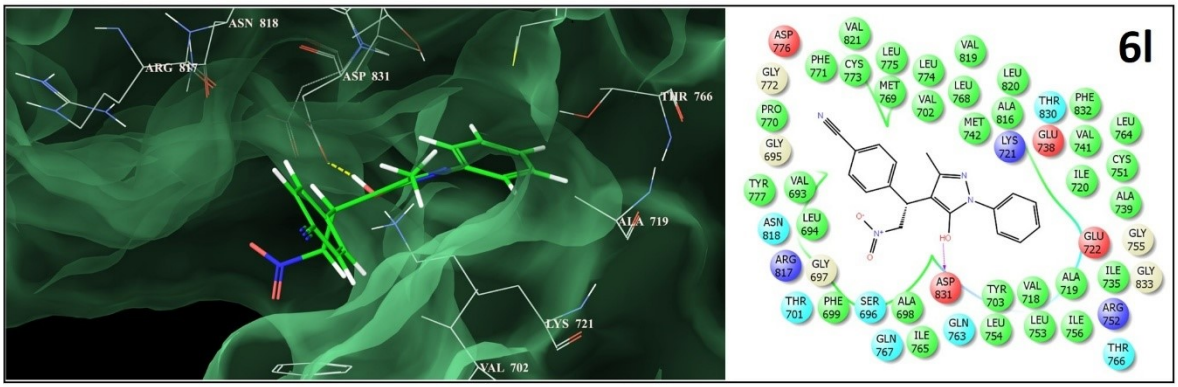
6k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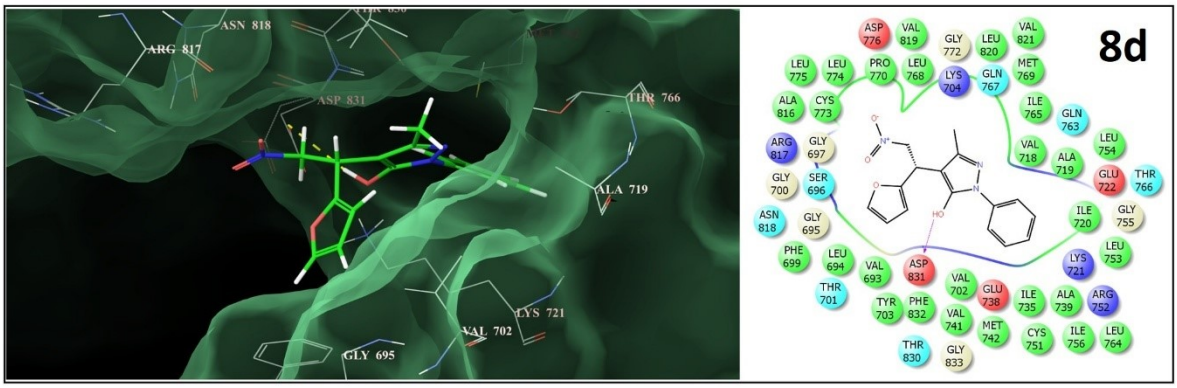
VAL 702
6l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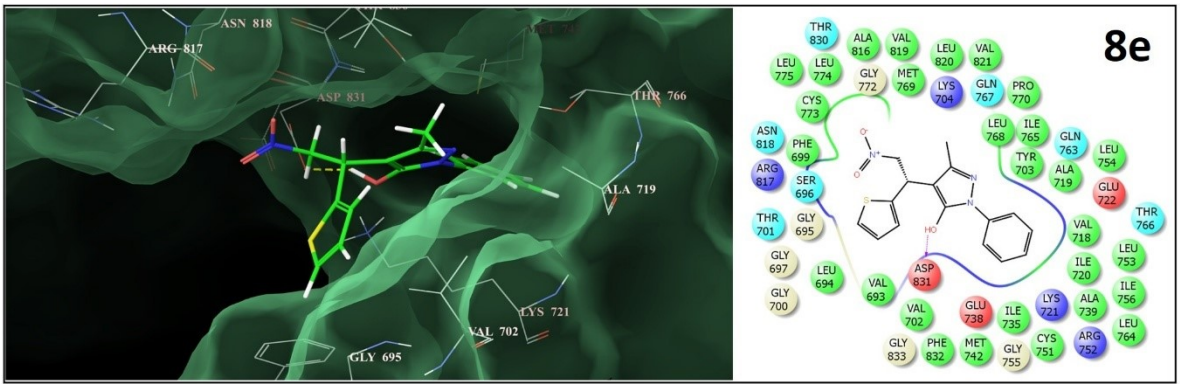
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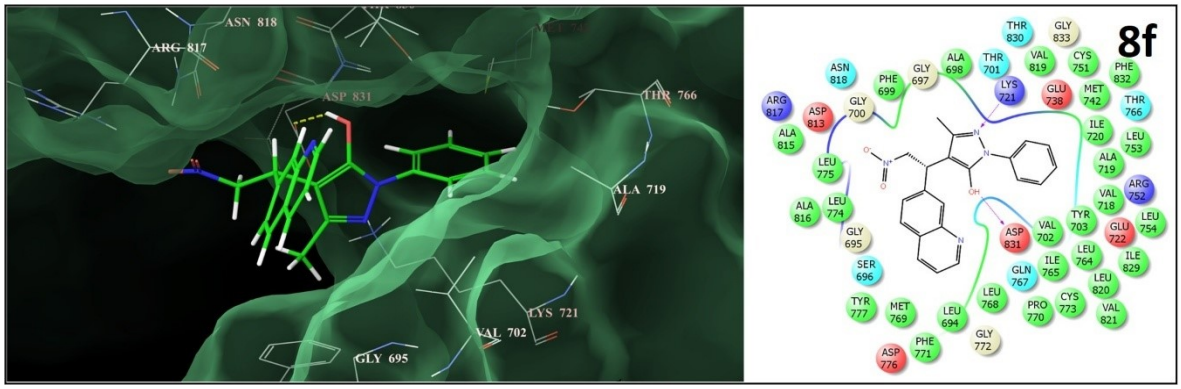


Figure S3. Representative molecular docking of efficient pyrazol-5-ol derivatives (**4**, **6** and **8** series) with their binding mode into the active site of Epidermal Growth Factor Receptor (EPGR) Tyrosine Kinase. (On right side of every docking image binding with pink line of compound with receptor signifies the H-bonding interactions).

Supplementary Tables

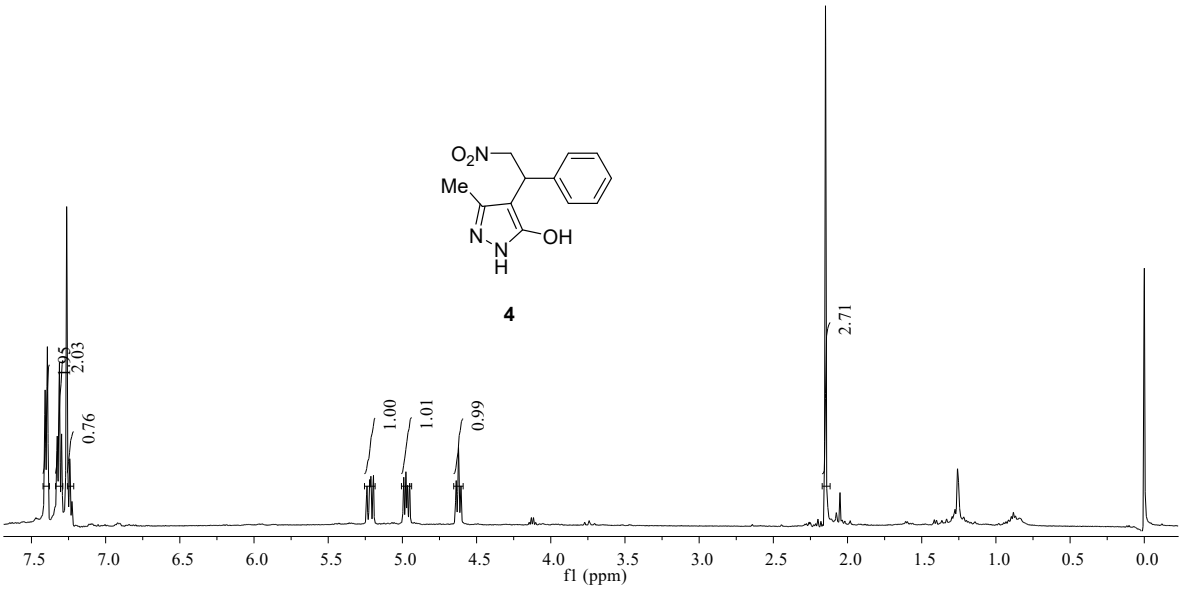
Table S1. X-ray diffraction (XRD) parameters (2θ, full width at half maxim., FWHM, interplanar distance, and crystallite size) of graphene oxide (GO) before Cycle I and after Cycle V.

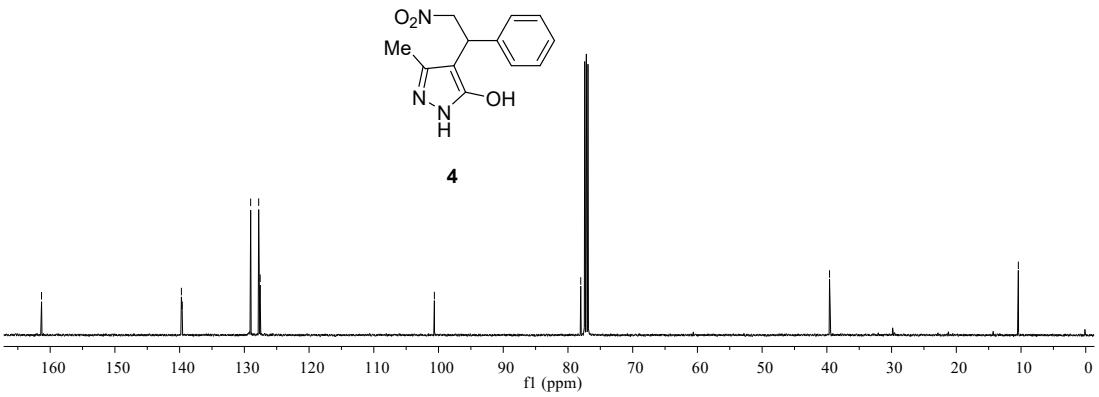
GO	2θ	FWHM	Interplanar distance (nm)	Crystallite Size (nm)
Cycle I	11.47	1.72	0.77	5.16
	42.53	1.45	0.21	4.07
Cycle V	11.01	1.11	0.80	8.66
	42.28	1.02	0.21	6.32

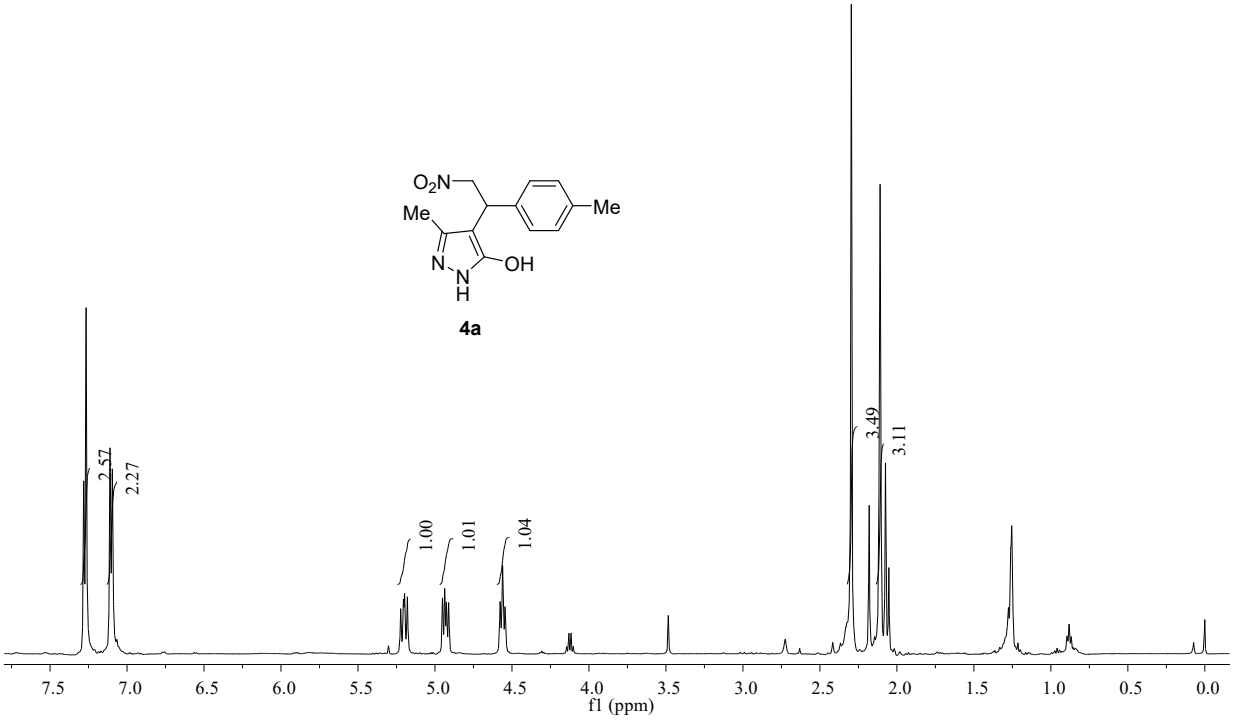
Table S2. X-ray photoelectron spectroscopy (XPS) peak parameters (binding energy, peak area, FWHM, and atomic concentration) and corresponding functional groups of graphene oxide (GO) before Cycle I and after Cycle V.

GO	Peaks	Binding Energy (eV)	Peak Area	FWHW (eV)	At Conc. (%)	(C/O)	Func. Groups
Cycle I	C 1s	284.62	79606.47	1.27	26.64	1.80	C-C
	C 1s	286.63	53759.91	1.47	17.99		C-O
	C 1s	287.98	58730.95	4.39	19.65		C=O
	O 1s	532.53	158792.62	1.92	18.14		O-C=O
	O 1s	533.97	153934.44	4.10	17.58		C=O
Cycle V	C 1s	284.47	40854.58	1.20	24.52	3.06	C-C
	C 1s	286.42	84752.94	3.19	50.86		C-O
	O 1s	530.68	2416.26	0.84	0.49		C=C
	O 1s	532.55	117773.94	2.25	24.12		C-O

Spectral data (^{1}H NMR and ^{13}C NMR) of pyrazol-5-ol derivative (4, 4*a-k*, 6*a-l*, 8*a-d*)



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Me
Me
N
N
H
OH
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2.27
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1.01
1.04
3.49
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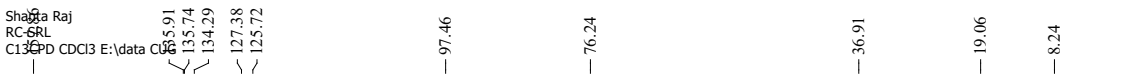
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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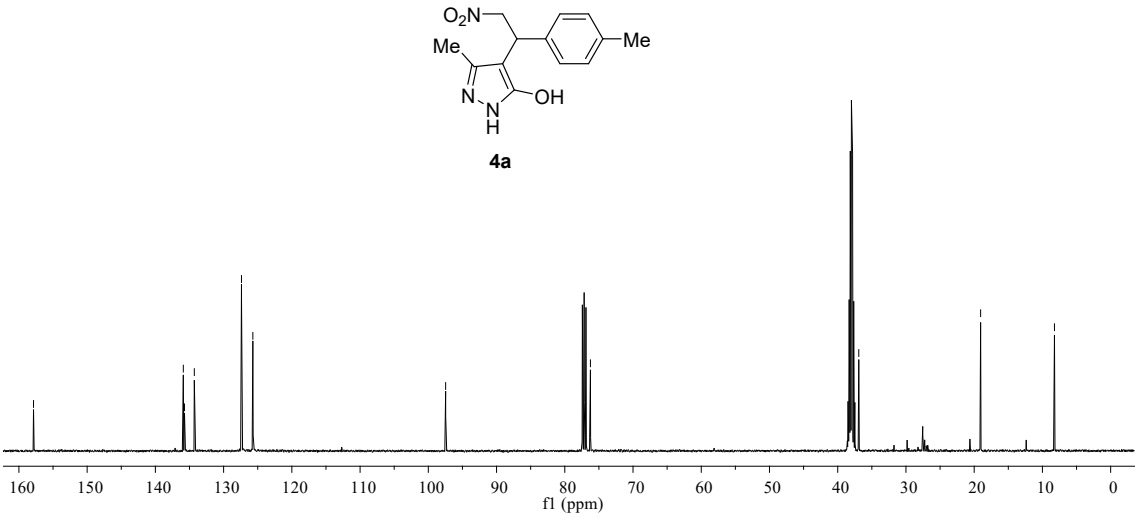
36.91
19.06
8.24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Me
N
N
H
OH
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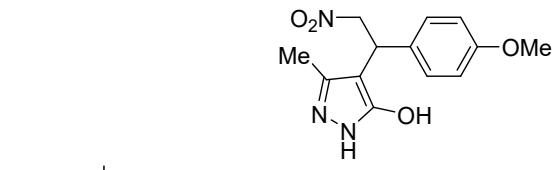
50
40
30
20
10
0
f1 (ppm)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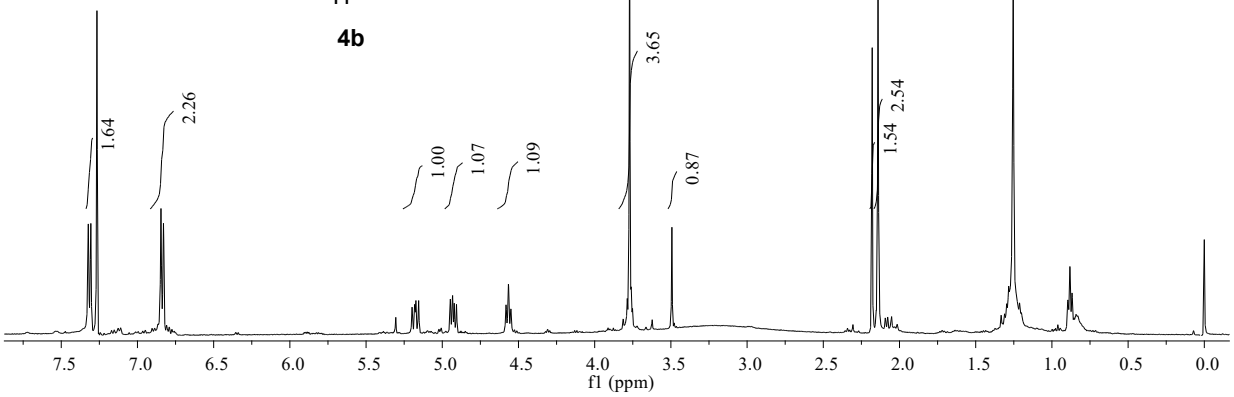
Me
OMe
N
N
H
OH

4b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1.09
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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
f1 (ppm)


Shanta Raj
C13CPD r CDCl3 E:\data CUG
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131.28
127.68
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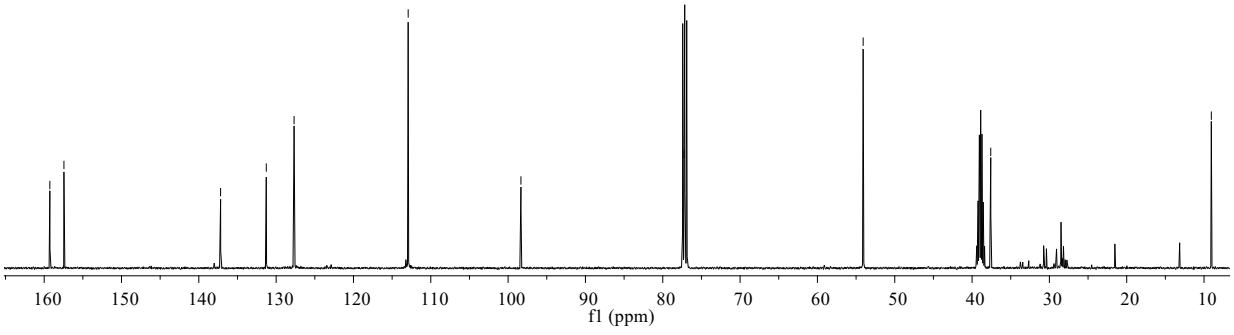
77.24
54.08
37.58
9.06


O2N
Me
OMe
N
N
H
OH

4b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20
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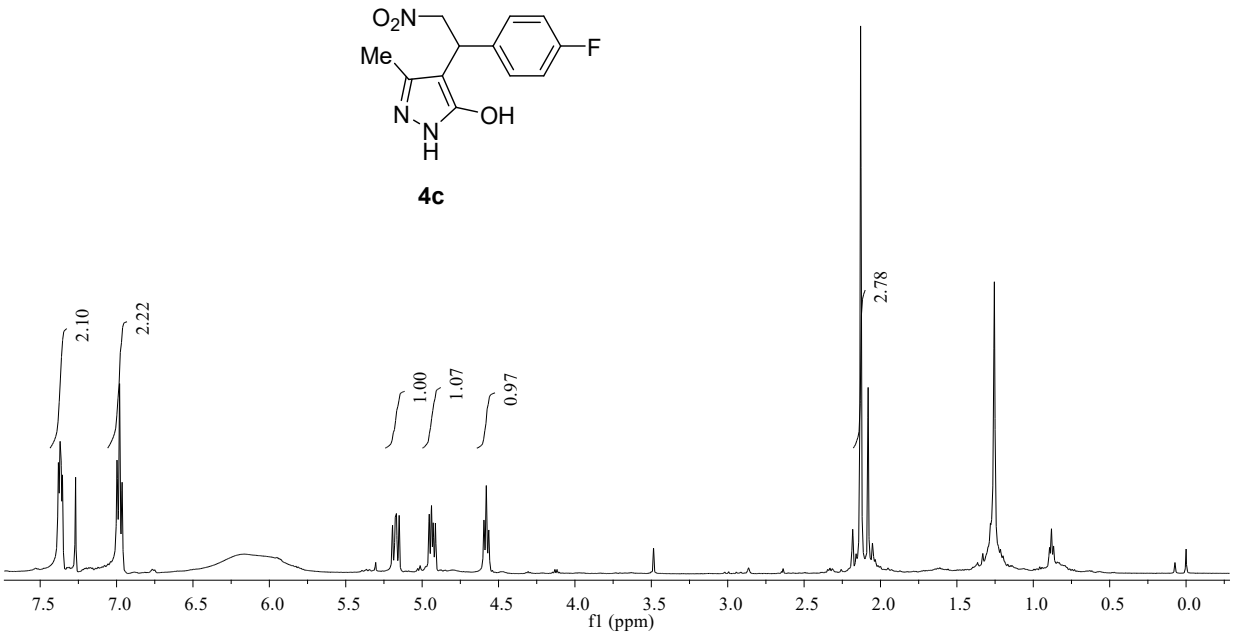
f1 (ppm)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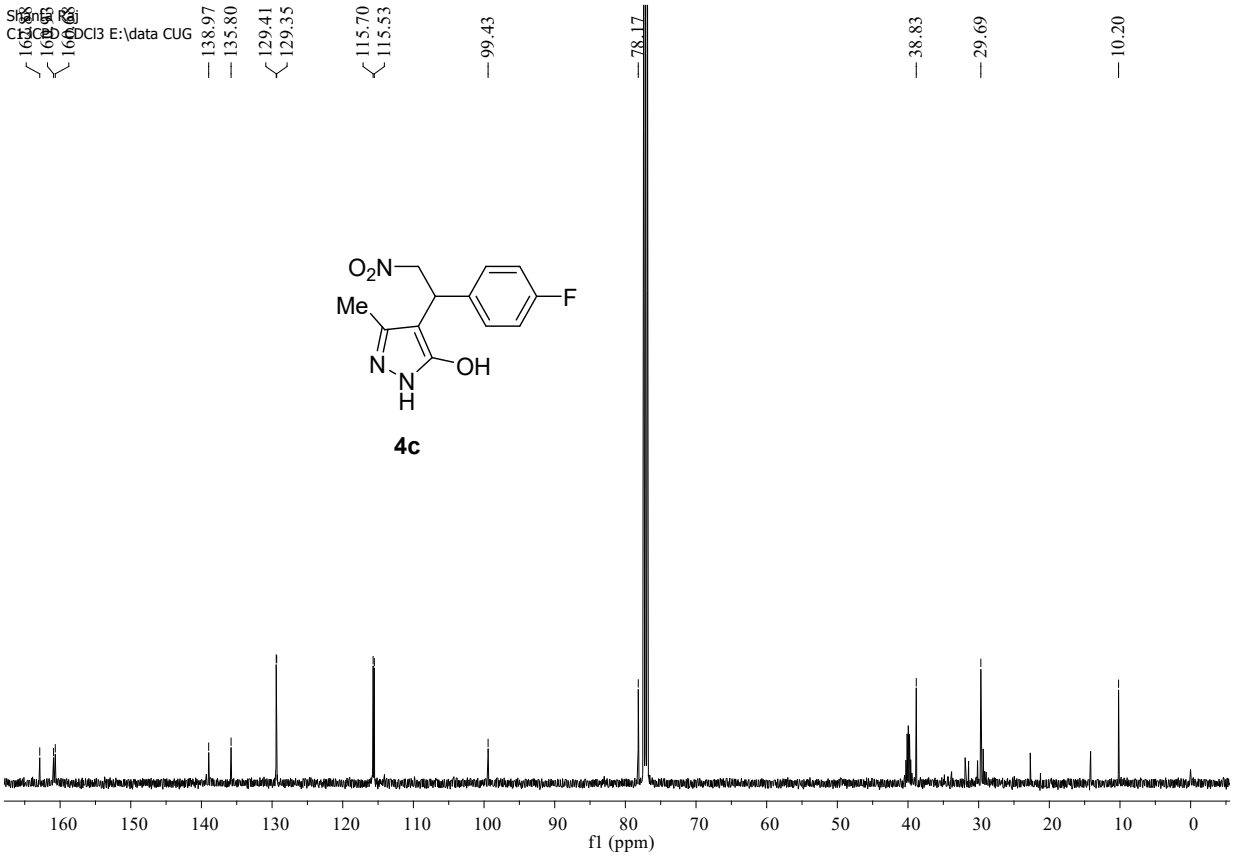
f1 (ppm)

4c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29.69
10.20
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Me
F
N
N
H
OH
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40
30
20
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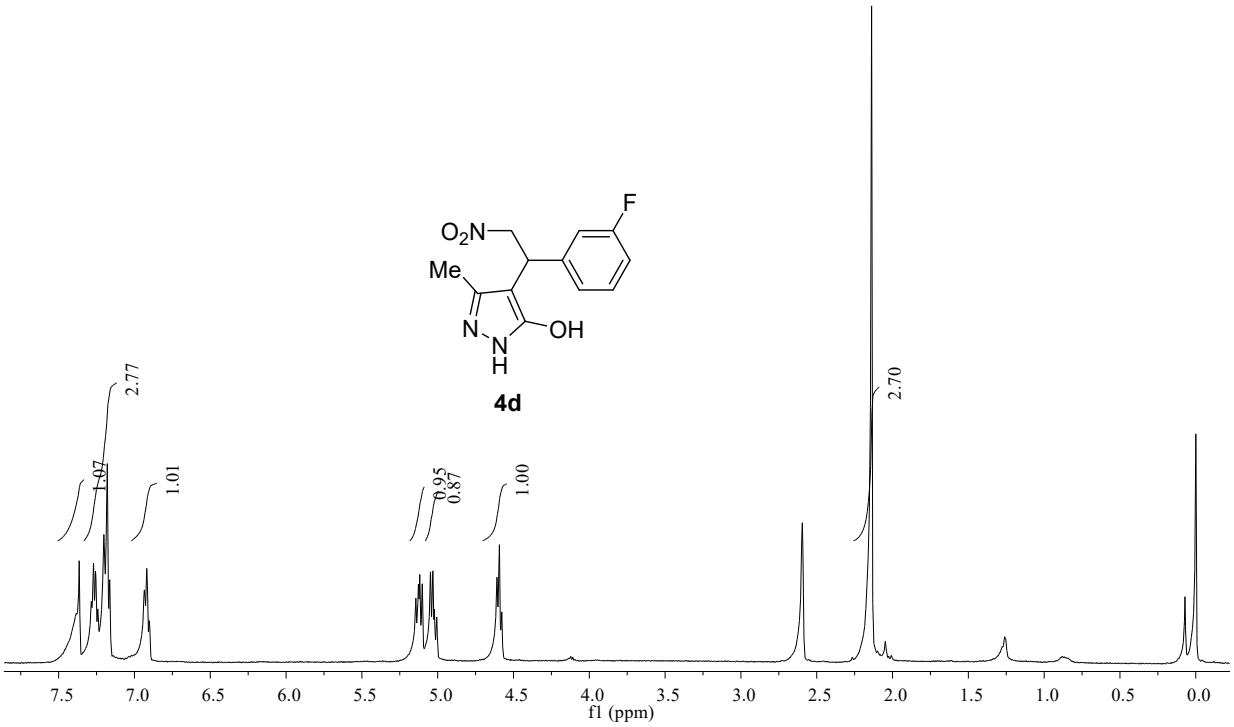
0
f1 (ppm)

4c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6.0
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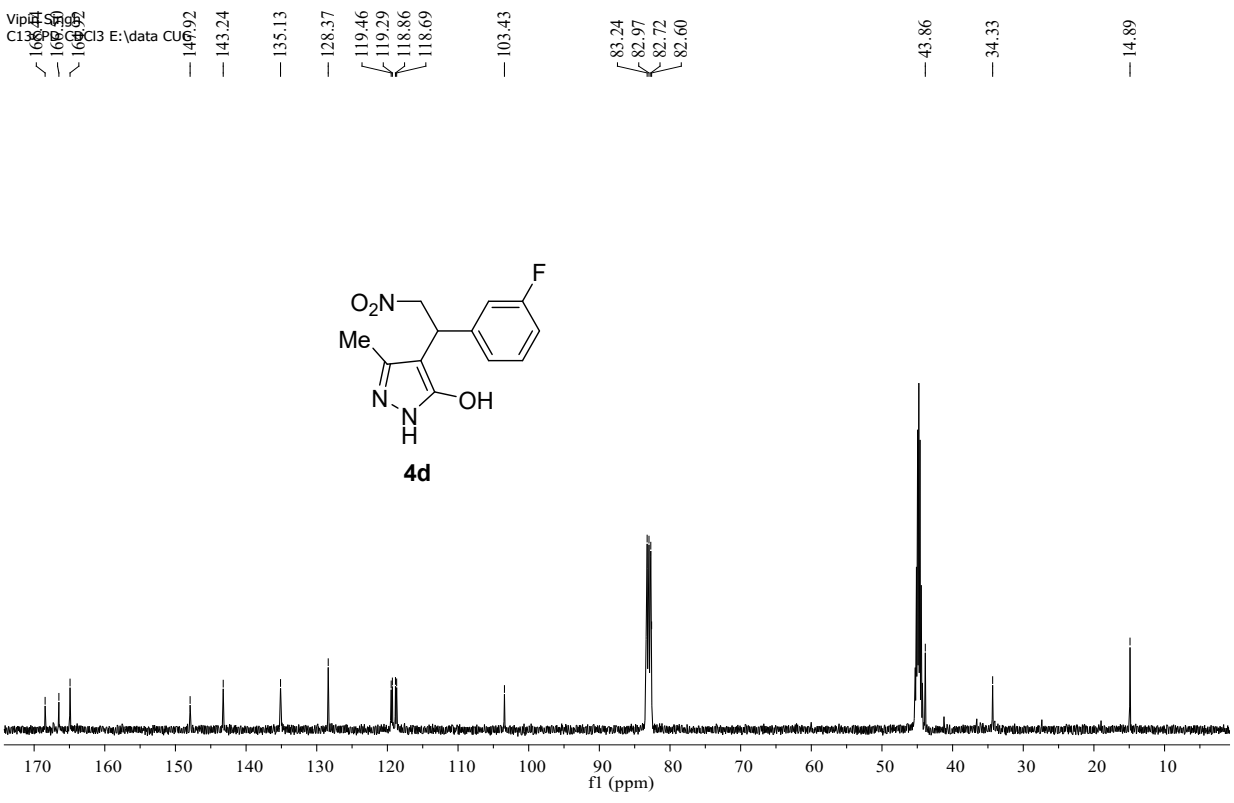
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Me
N
N
H
OH
4d
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120
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100
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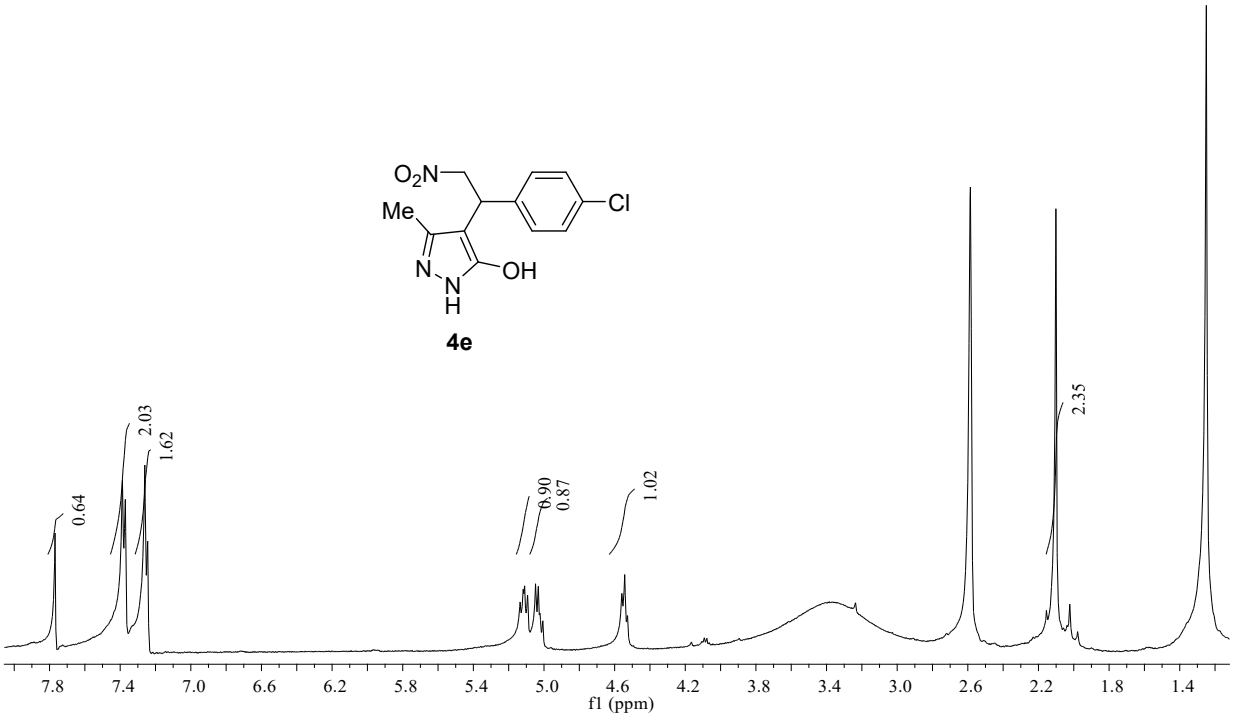
60
50
40
30
20
10
f1 (ppm)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Me
Cl
N
N
H
OH
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7.4
7.0
6.6
6.2
5.8
5.4
5.0
4.6
4.2
3.8
3.4
3.0
2.6
2.2
1.8
1.4
f1 (ppm)


Vipin Singh
RG-VS-105
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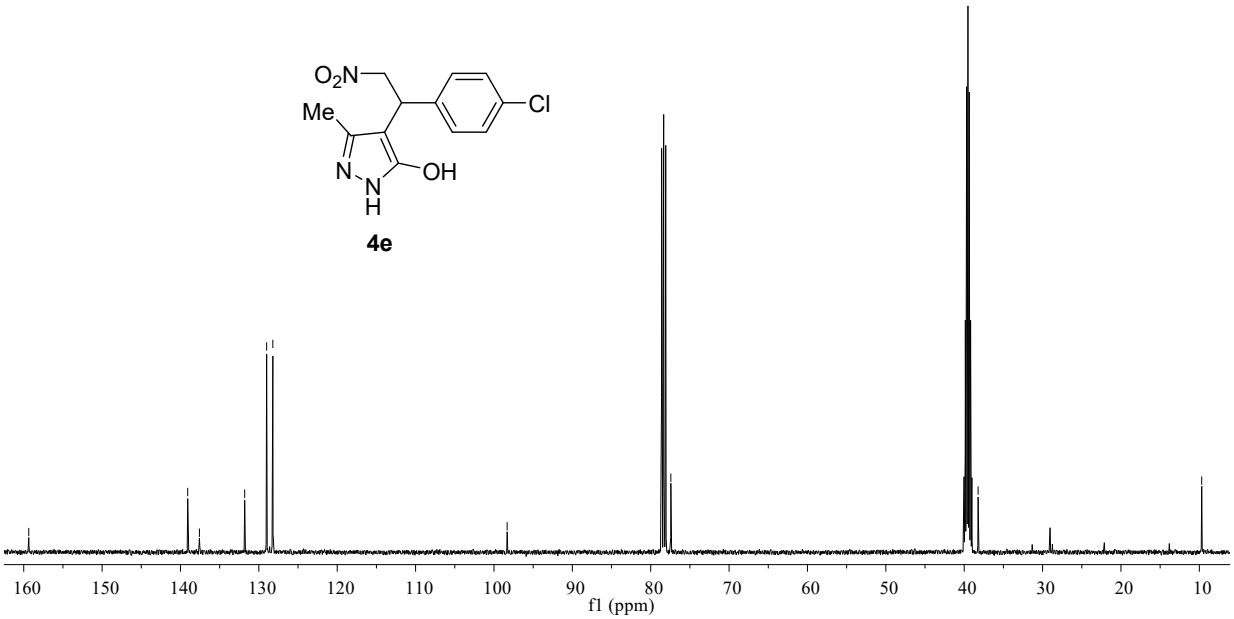
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Cl
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H
OH
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40
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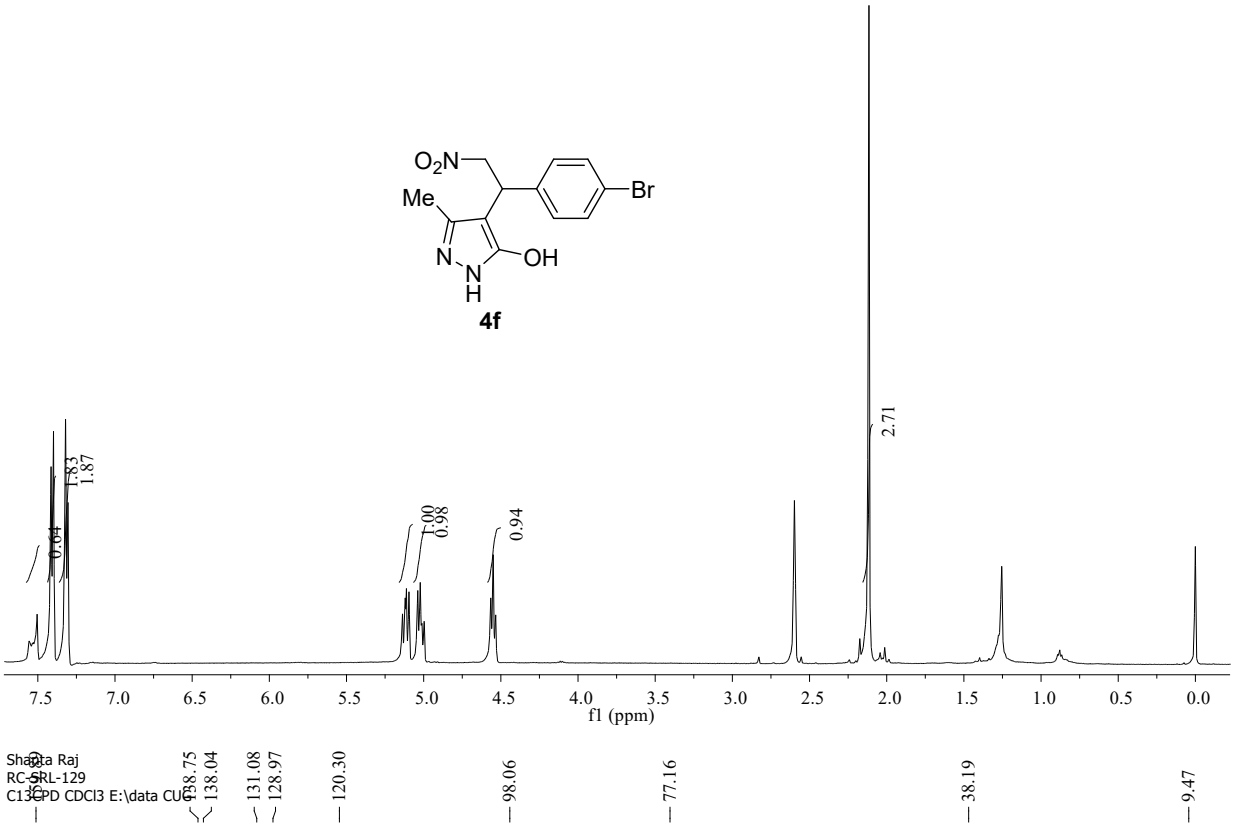
20
10
f1 (ppm)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Br
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N
H
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6.0
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4.0
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3.0
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2.0
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Shagata Raj
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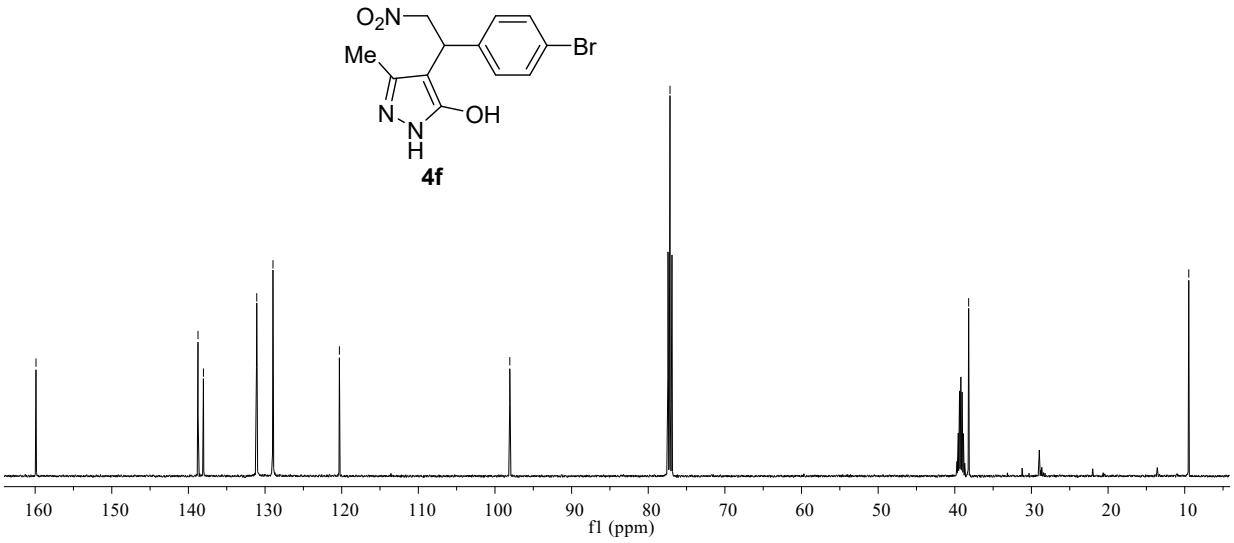
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Me
Br
N
N
H
OH
4f
160
150
140
130
120
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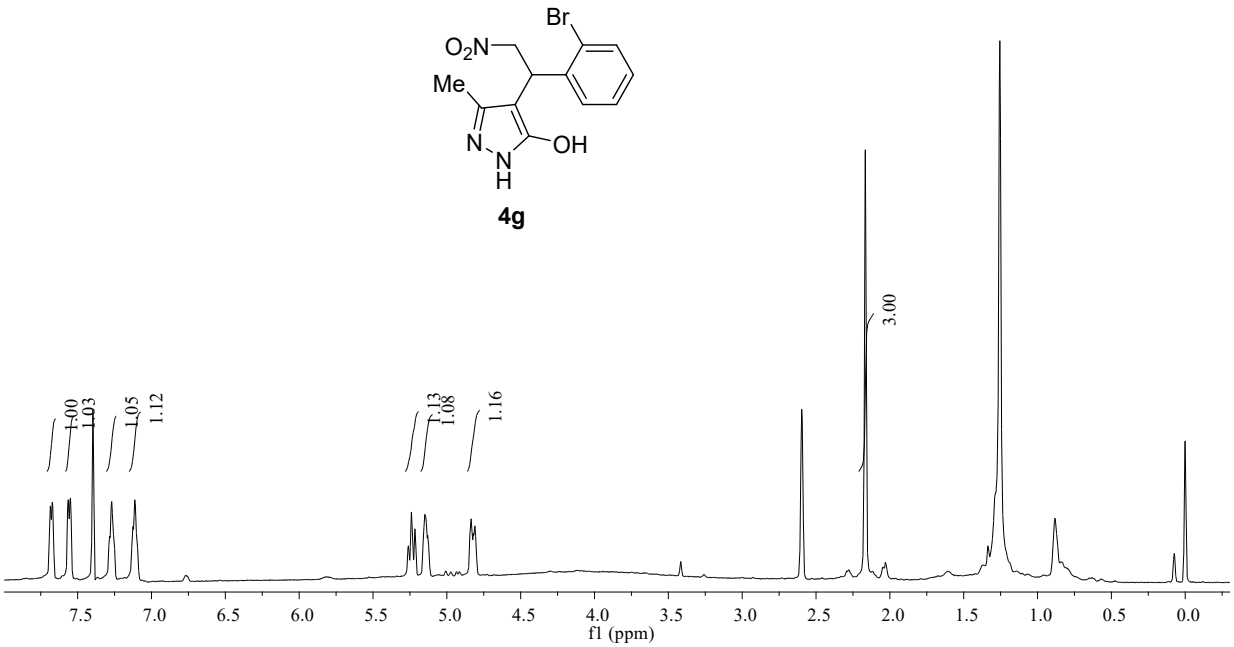
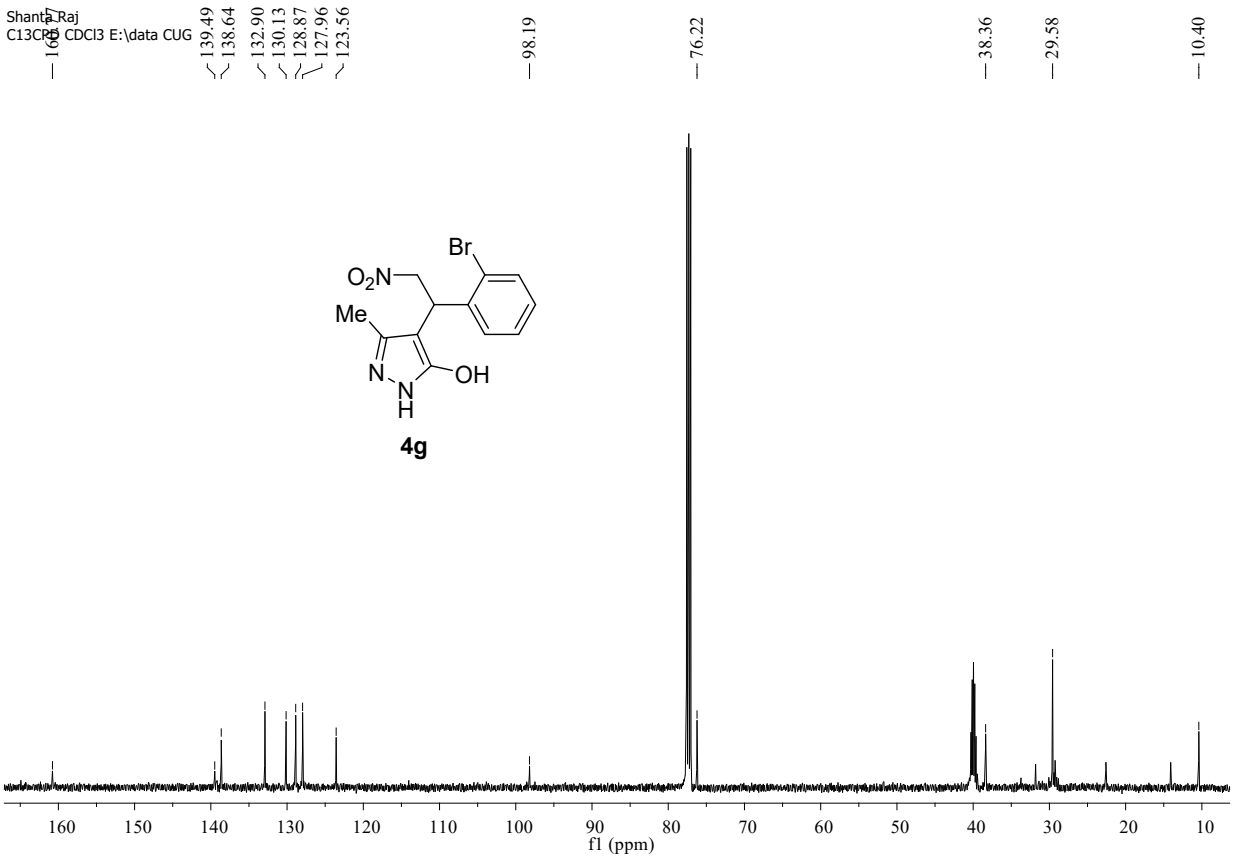
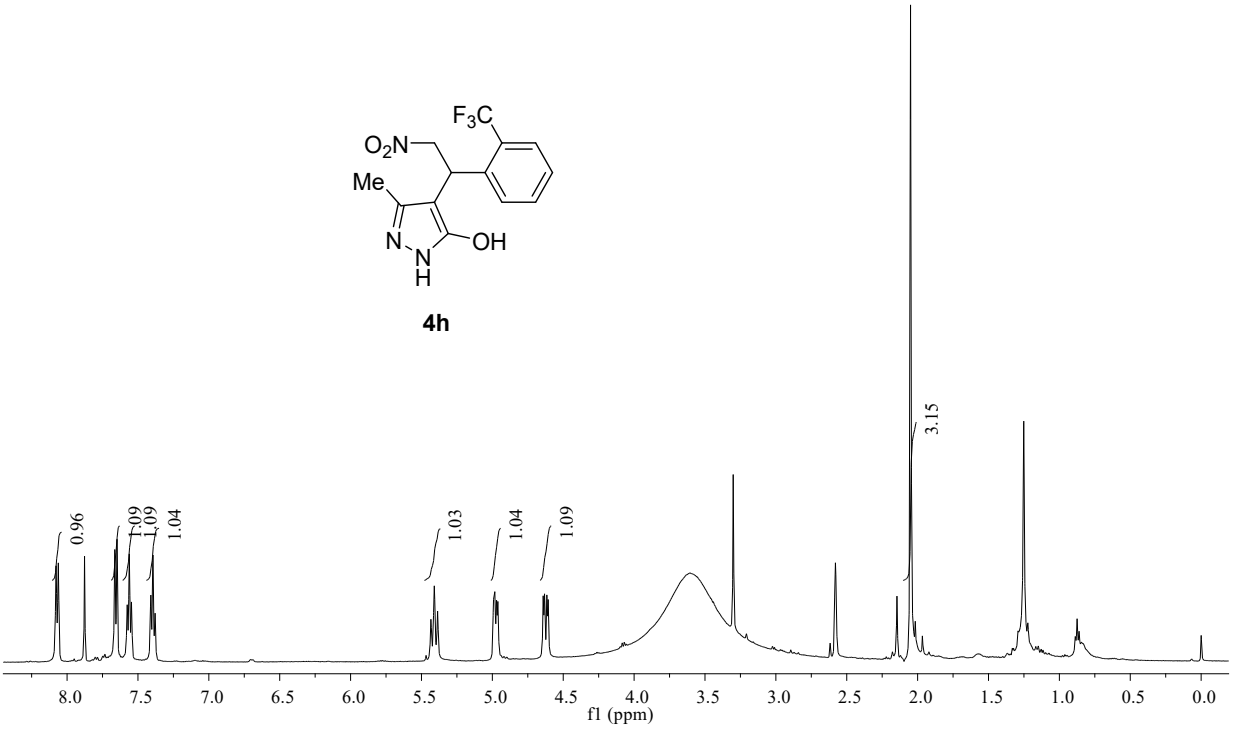
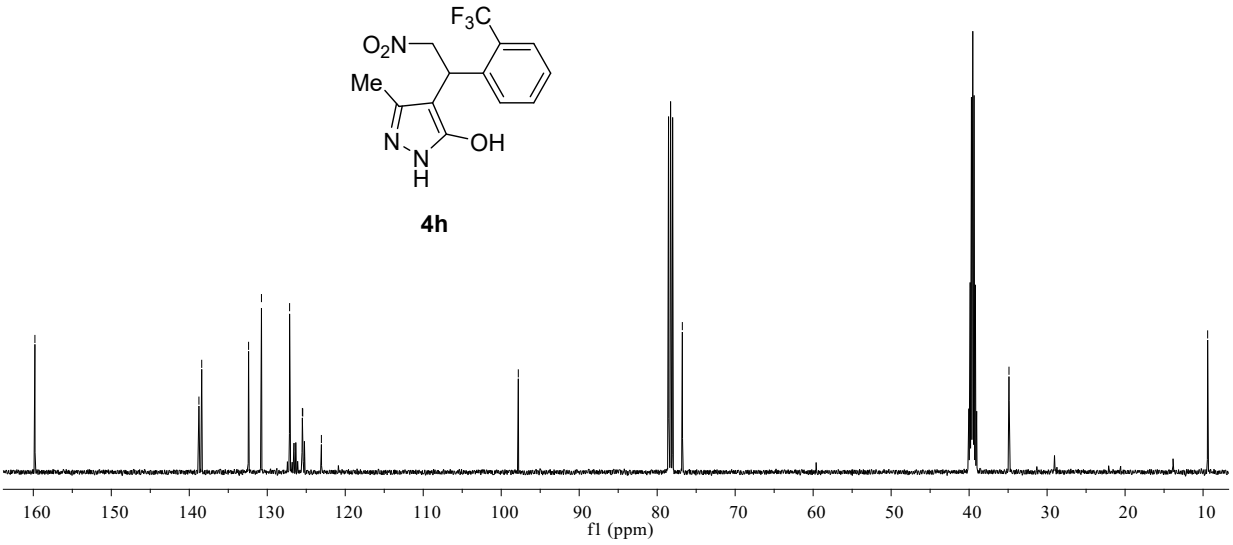
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

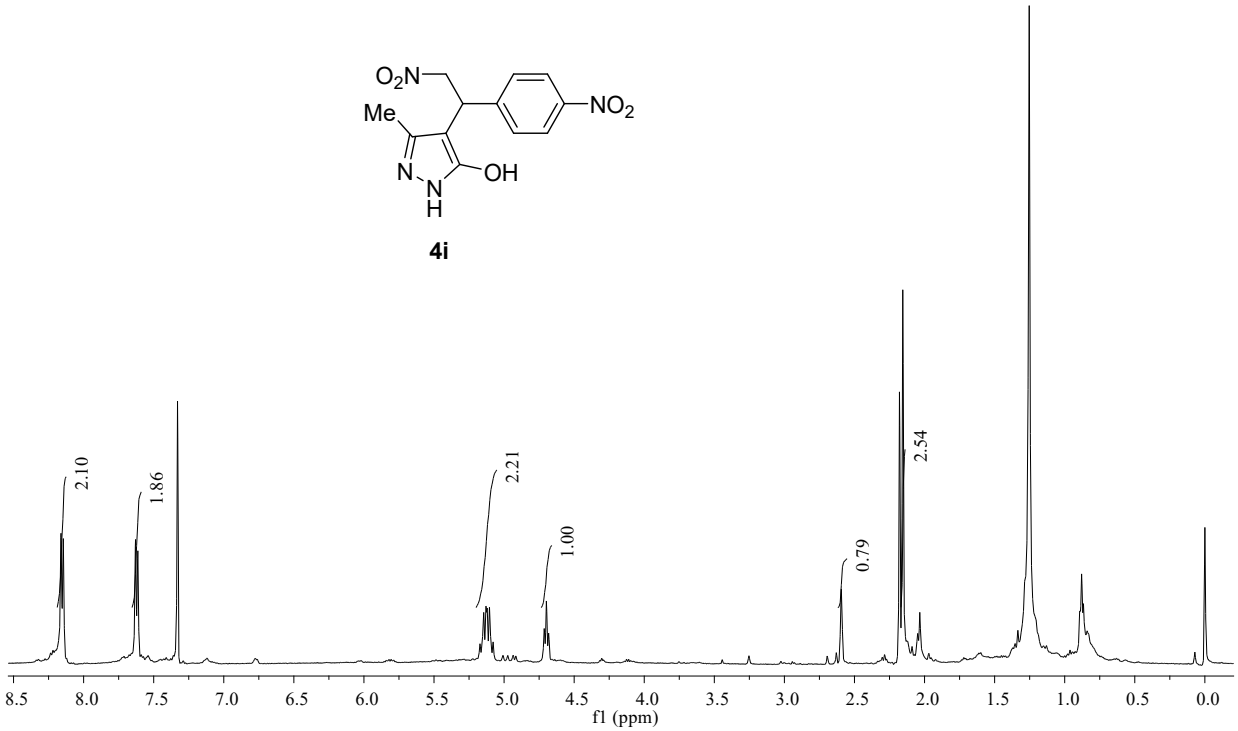

Br
O2N
Me
N
N
H
OH
4g
1.00
1.03
1.05
1.12
1.13
1.08
1.16
3.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

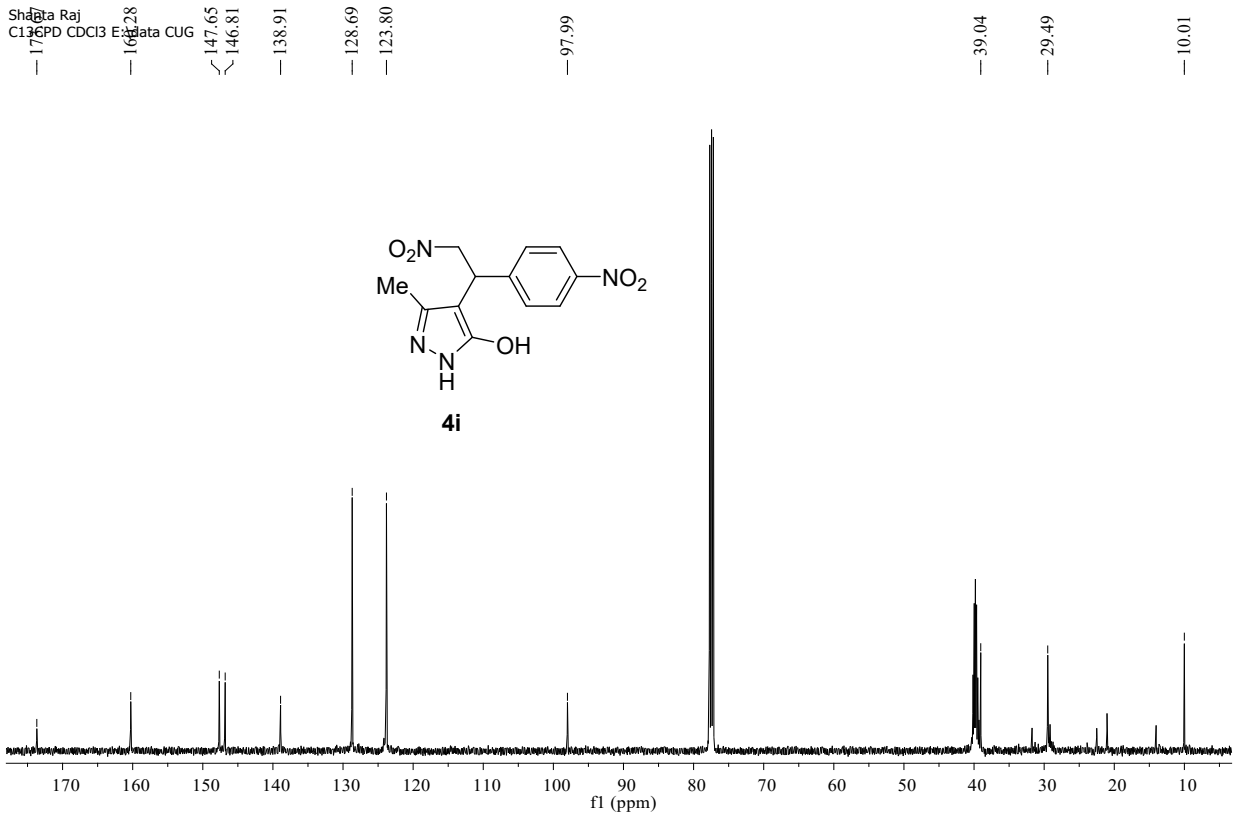

Shanta Raj
C13CPD CDCl3 E:\data CUG
160.57
139.49
138.64
132.90
130.13
128.87
127.96
123.56
98.19
76.22
38.36
29.58
10.40
Br
O2N
Me
N
N
H
OH
4g
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

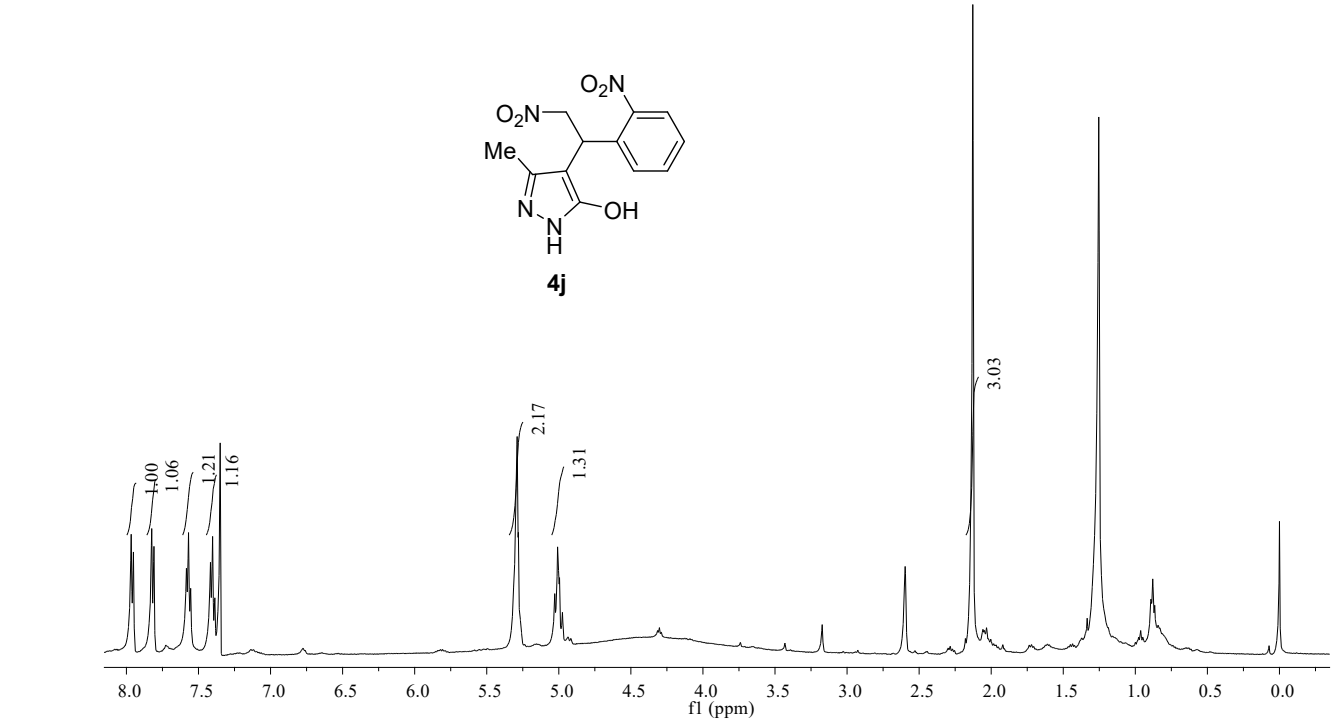

F3C
O2N
Me
N
N
H
OH
4h
0.96
1.09
1.09
1.04
1.03
1.04
1.09
3.15
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

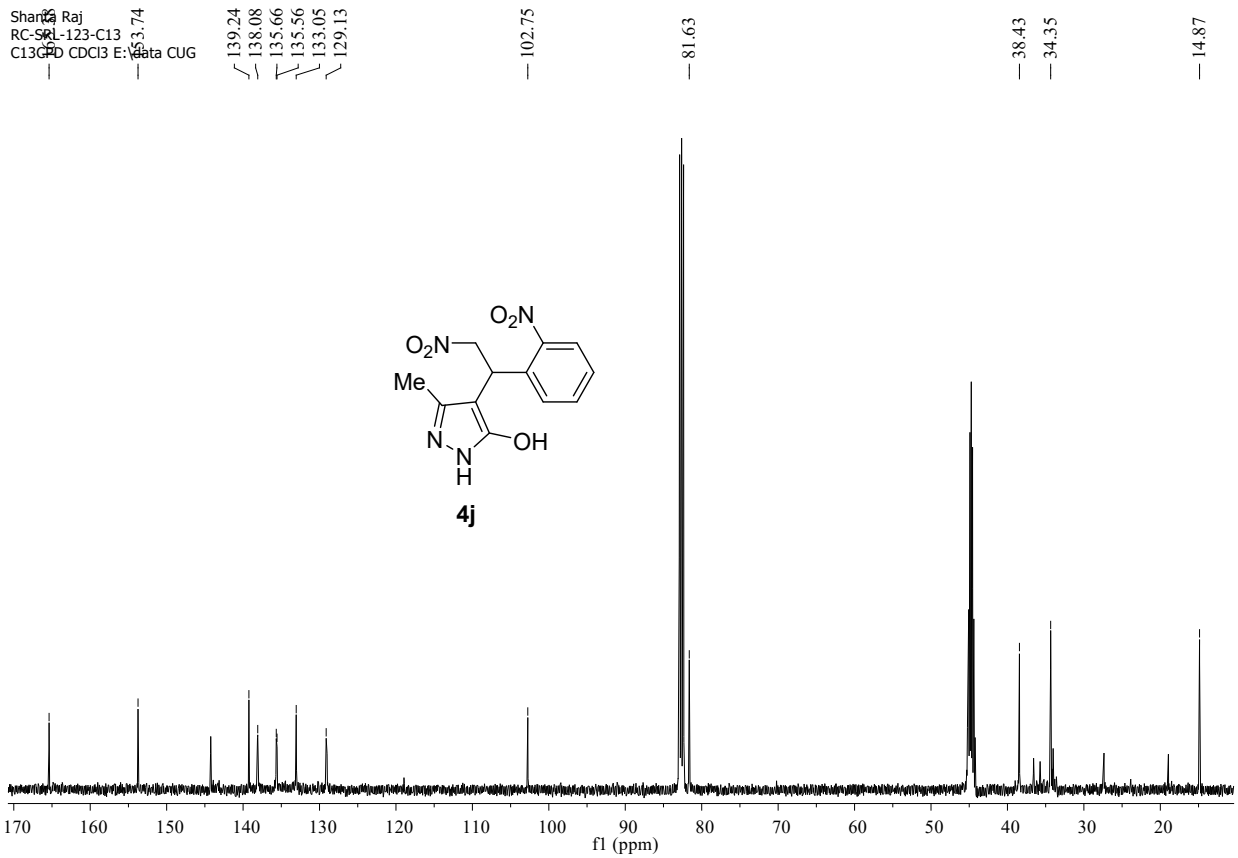

Vipin Singh
RC-VS-108
C13CPD DMSO E:\data CUR
138.76
138.40
132.39
130.74
127.13
125.50
125.45
123.06
97.81
76.77
34.89
9.41

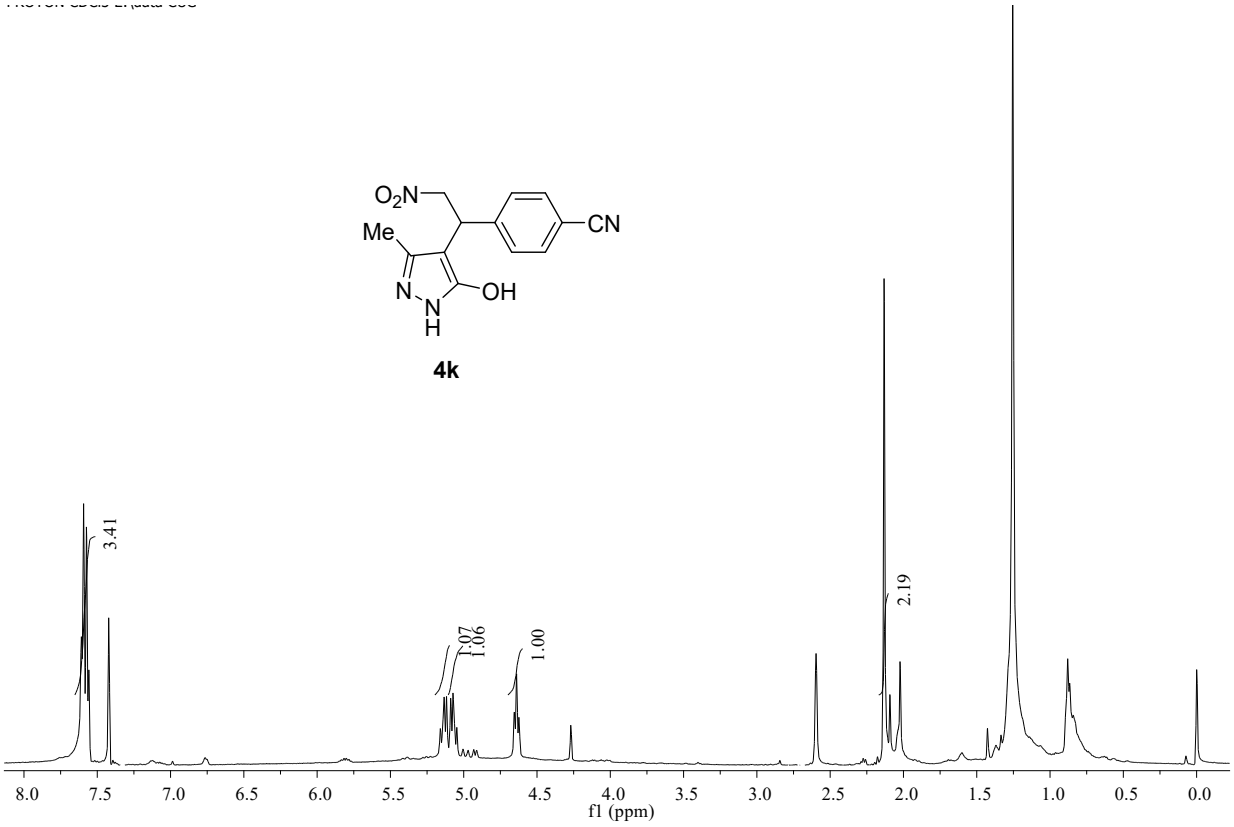

F3C
O2N
Me
N
N
H
OH
4h
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

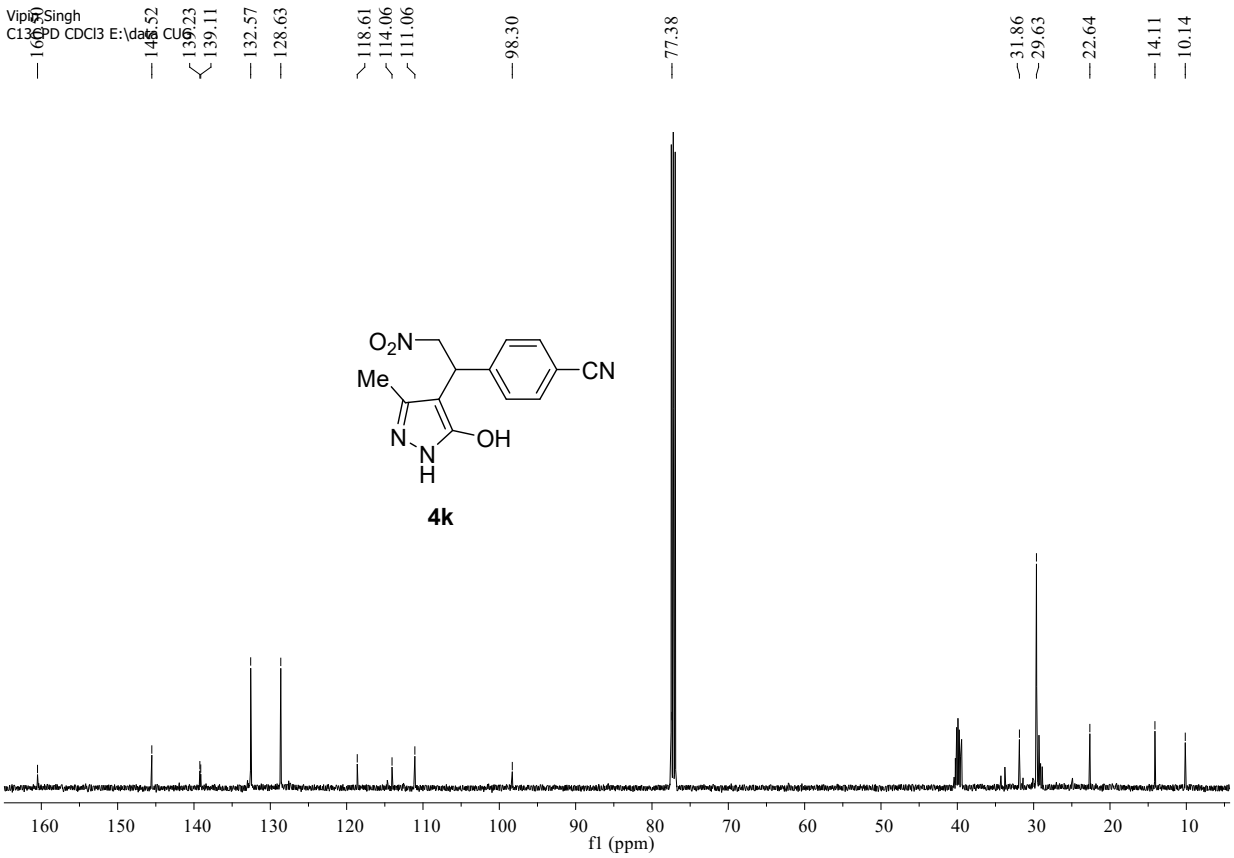

O2N
NO2
Me
N
N
H
OH
4i
2.10
1.86
2.21
1.00
0.79
2.54
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

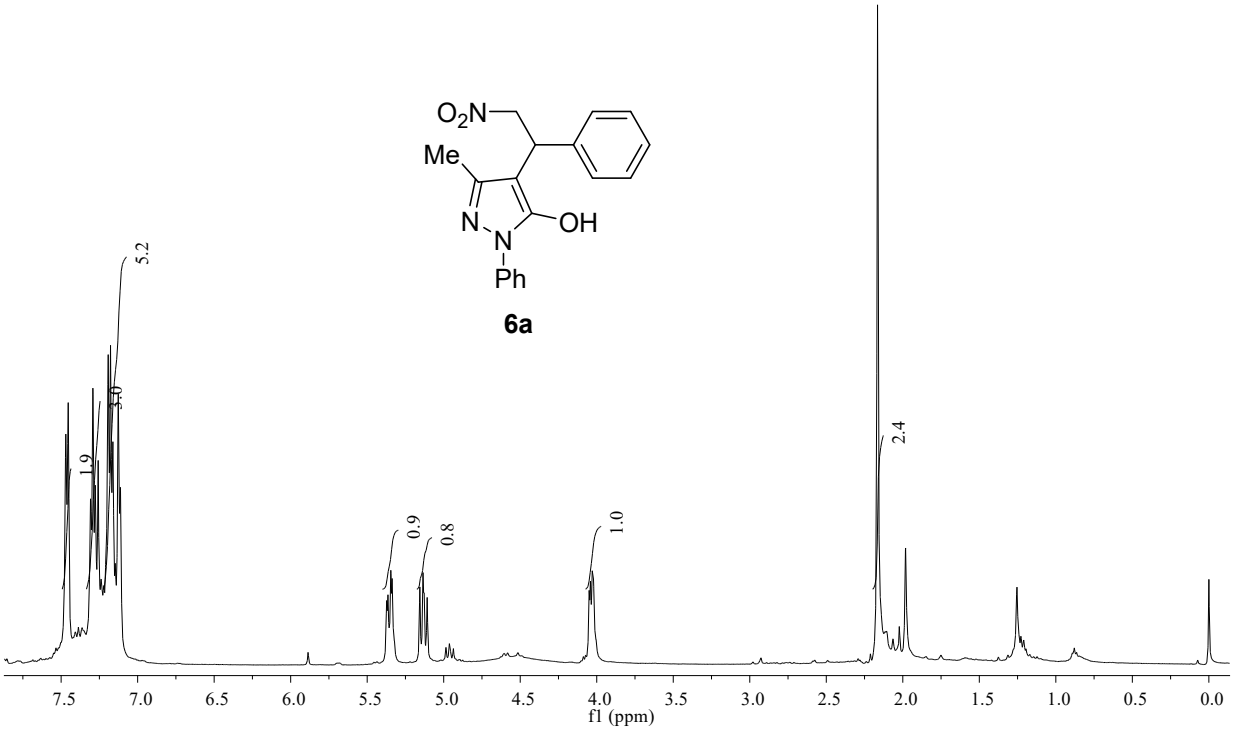

Shaata Raj
C13GPD CDCl3 Exp data CUG
147.65
146.81
138.91
128.69
123.80
97.99
39.04
29.49
10.01
O2N
NO2
Me
N
N
H
OH
4i
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

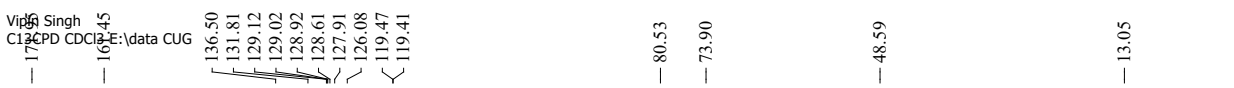

O2N
O2N
Me
N
N
H
OH
4j
1.00
1.06
1.21
1.16
2.17
1.31
3.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

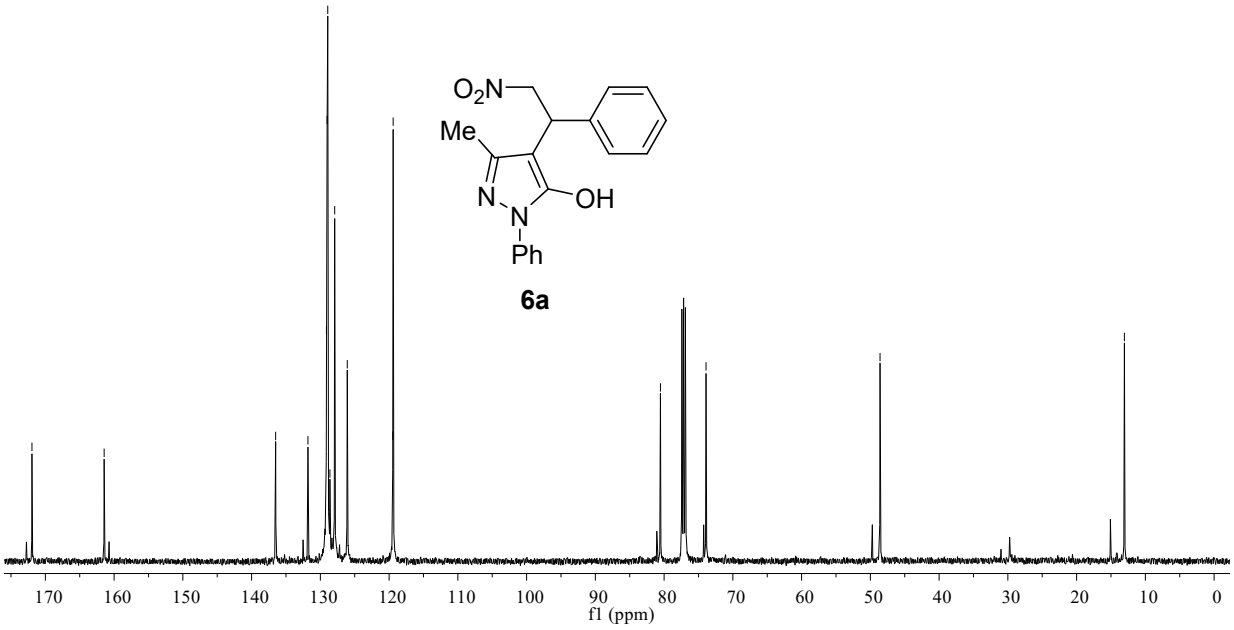

Shanta Raj
RC-SRL-123-C13
C13CPD CDCl3 E:\data CUG
53.74
139.24
138.08
135.66
135.56
133.05
129.13
102.75
81.63
38.43
34.35
14.87
O2N
O2N
Me
N
N
H
OH
4j
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
f1 (ppm)

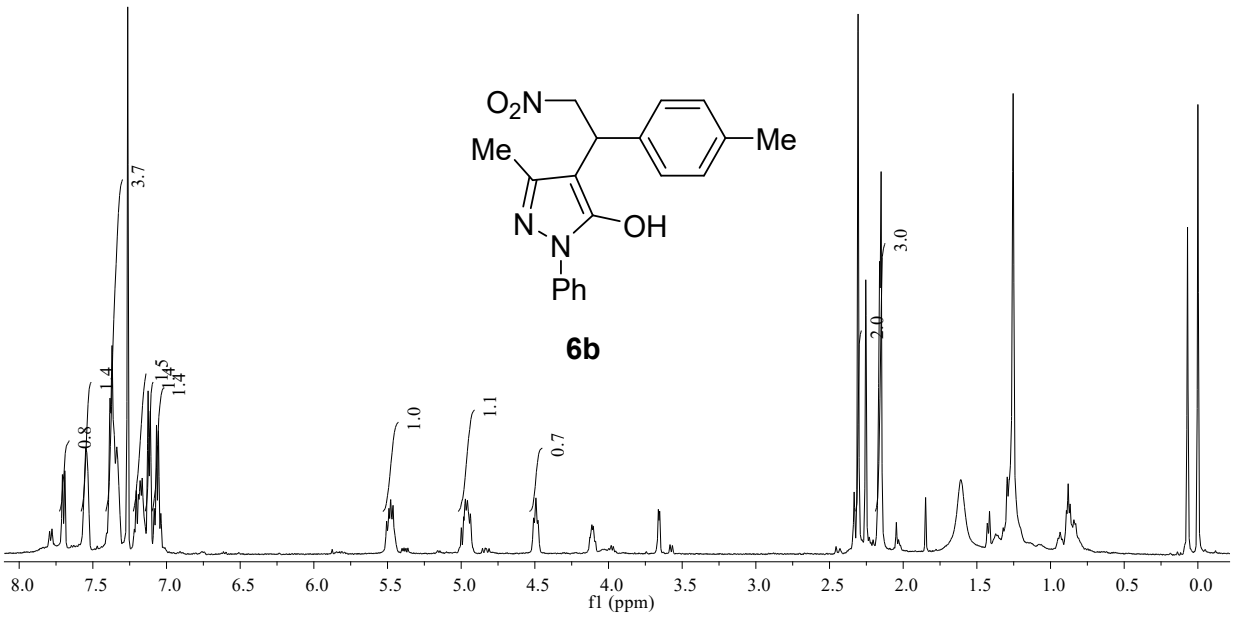

O2N
Me
CN
N
N
H
OH
4k
3.41
1.07
1.06
1.00
2.19
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Vipin Singh
C13CPD CDCl3 E:\data CUG
162.57
144.52
139.23
139.11
132.57
128.63
118.61
114.06
111.06
98.30
77.38
31.86
29.63
22.64
14.11
10.14
O2N
Me
CN
N
N
H
OH
4k
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)


O2N
Me
N
N
OH
Ph
6a
5.2
3.0
1.9
0.9
0.8
1.0
2.4
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
f1 (ppm)

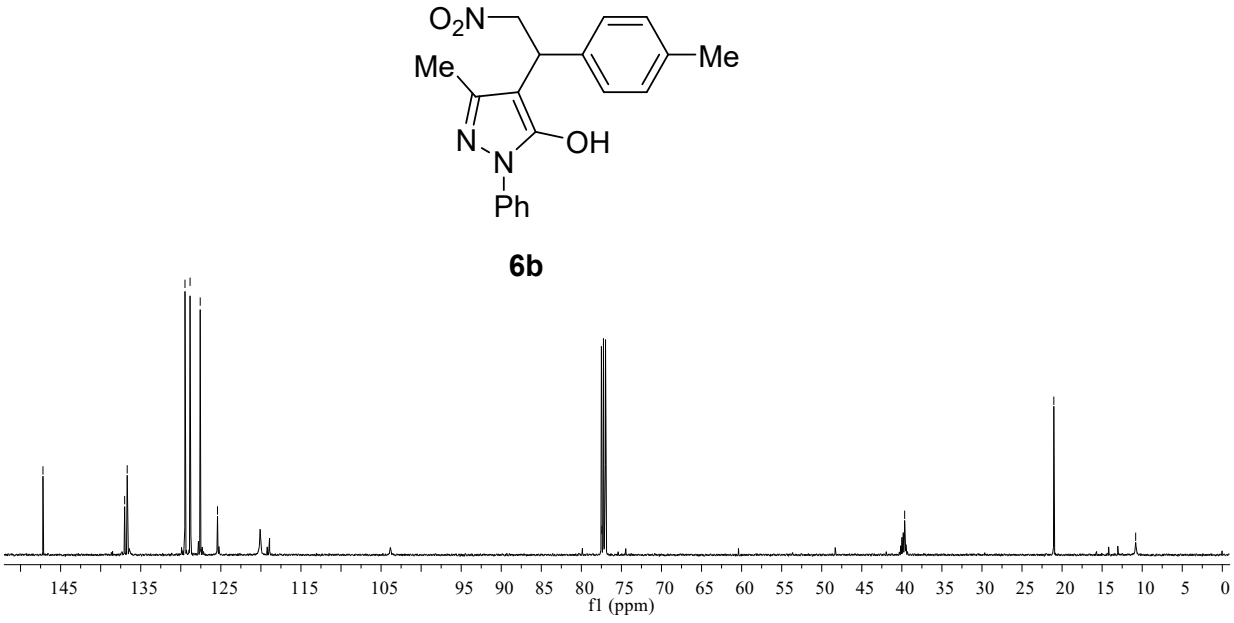

Vipin Singh
C13CPD CDCl3-E:\data CUG
136.50
131.81
129.12
129.02
128.92
128.61
127.91
126.08
119.47
119.41
80.53
73.90
48.59
13.05


O2N
Me
N
N
OH
Ph
6a
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

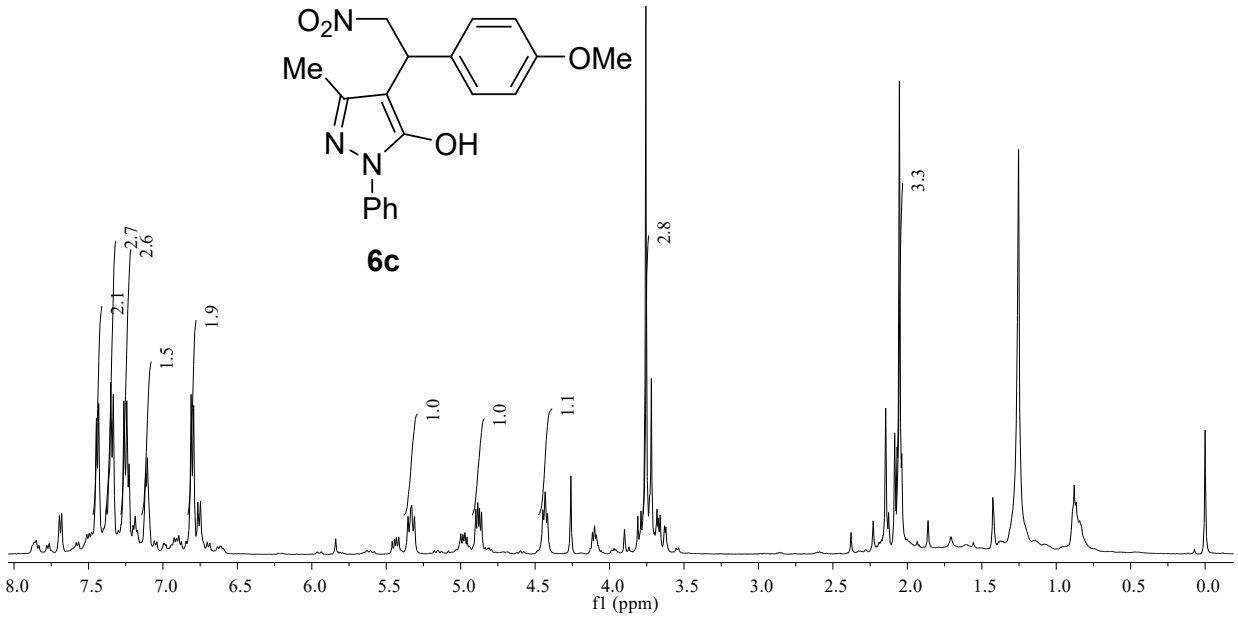

O2N
Me
Me
N
N
OH
Ph
3.7
1.4
0.8
1.4
1.5
1.4
1.0
1.1
0.7
2.0
3.0
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

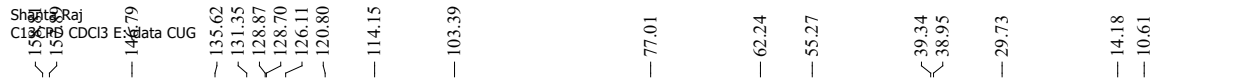
6b

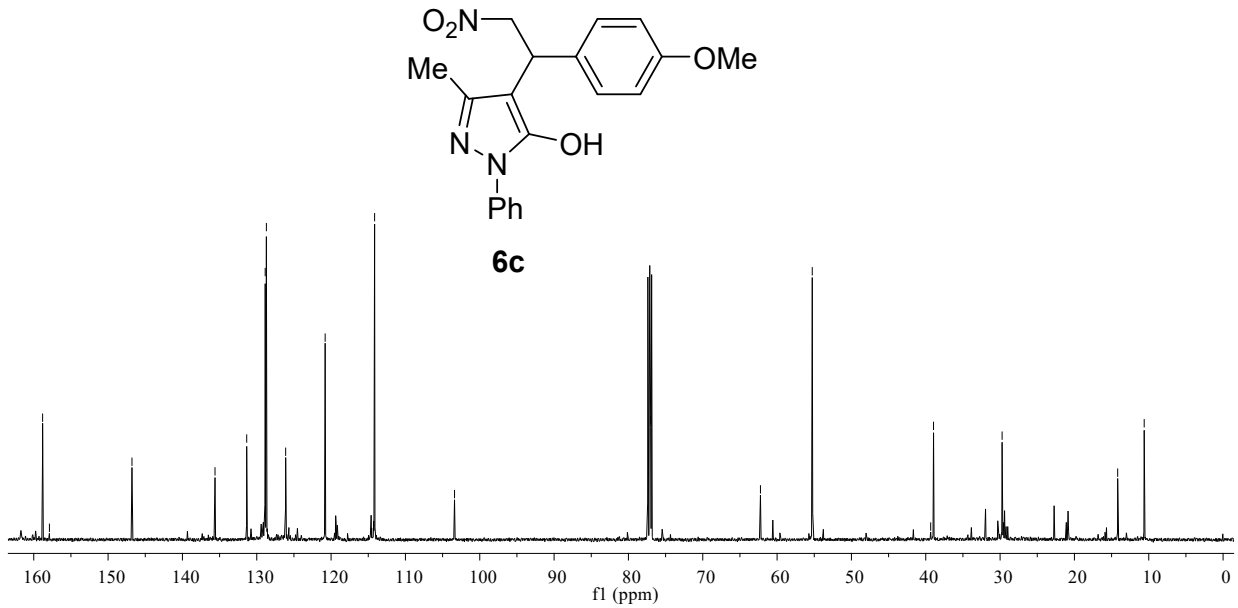

Tapas Sarkar
C13CPD CDCl3 1 1 data 2 26
143.20
137.01
135.69
129.48
128.84
127.57
125.42
77.45
39.65
21.03
10.81

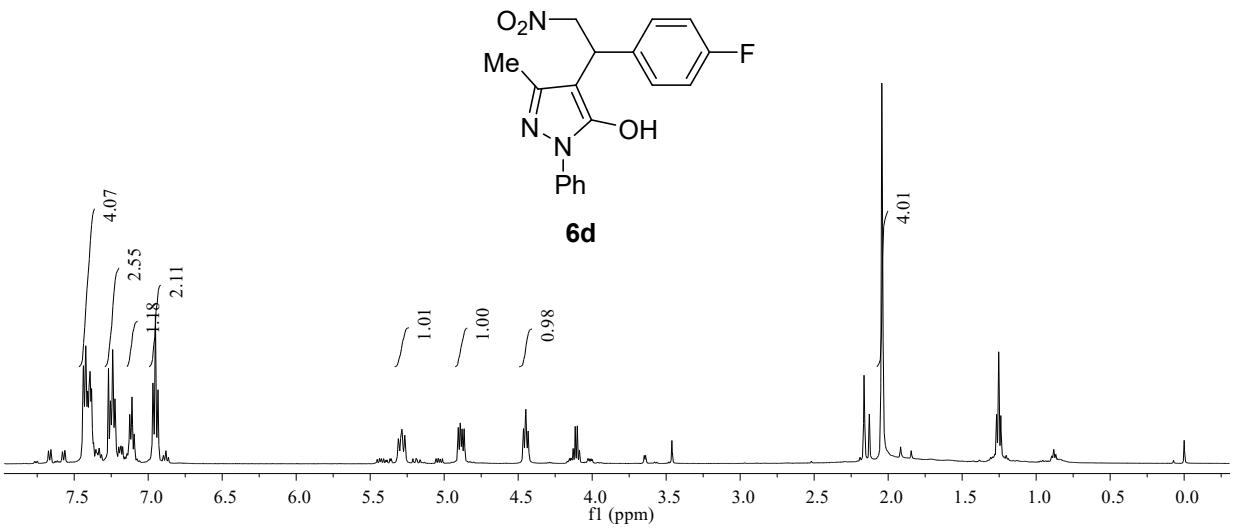

O2N
Me
Me
N
N
OH
Ph
145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0
f1 (ppm)

6b

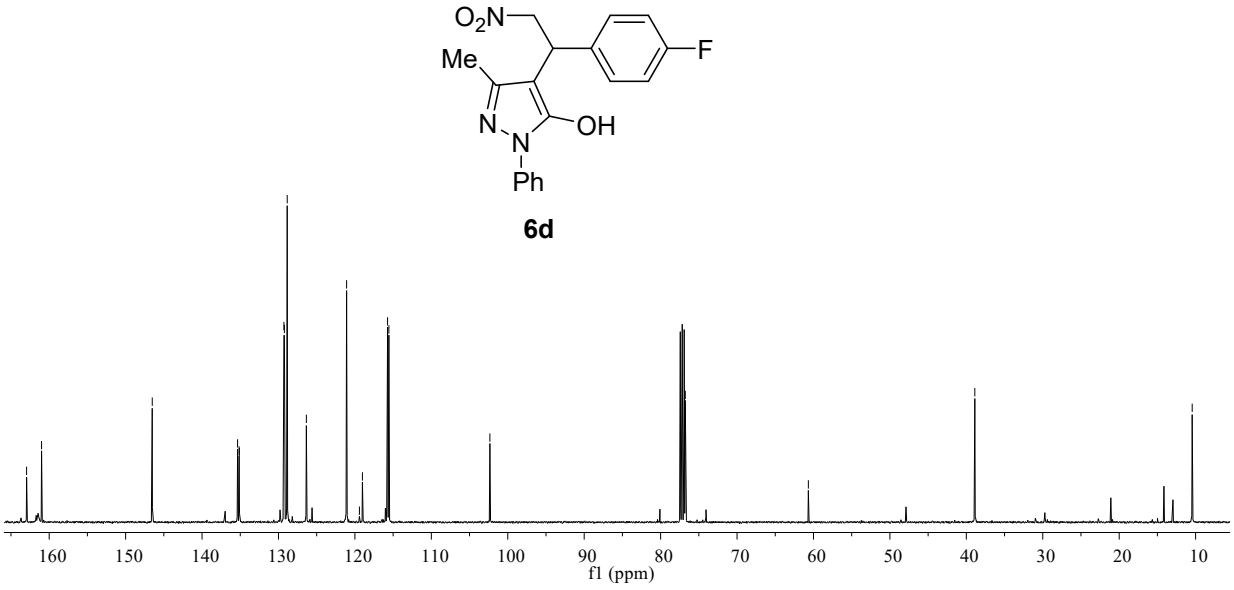

O2N
Me
OMe
N
N
OH
Ph
6c
2.7
2.6
2.1
1.9
1.5
1.0
1.0
1.1
2.8
3.3
8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

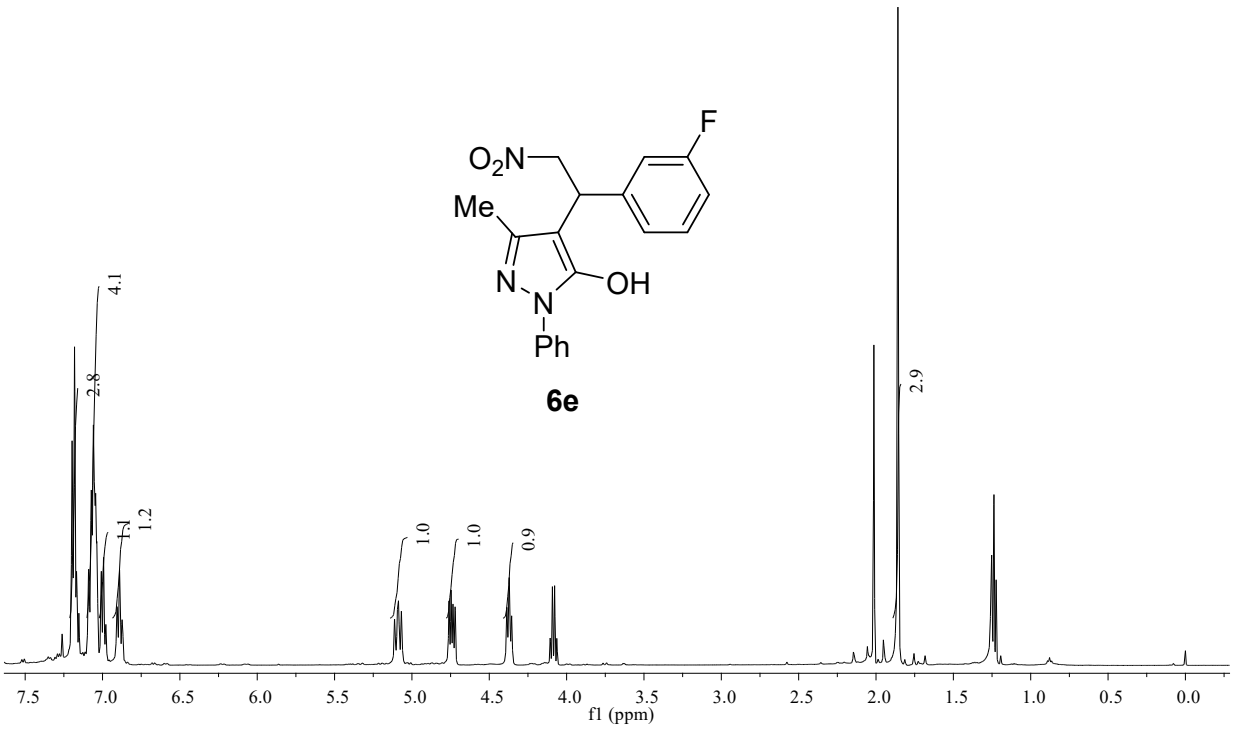

Shanta Raj
C13CPD CDCl3 Exp data CUG
135.62
131.35
128.87
128.70
126.11
120.80
114.15
103.39
77.01
62.24
55.27
39.34
38.95
29.73
14.18
10.61

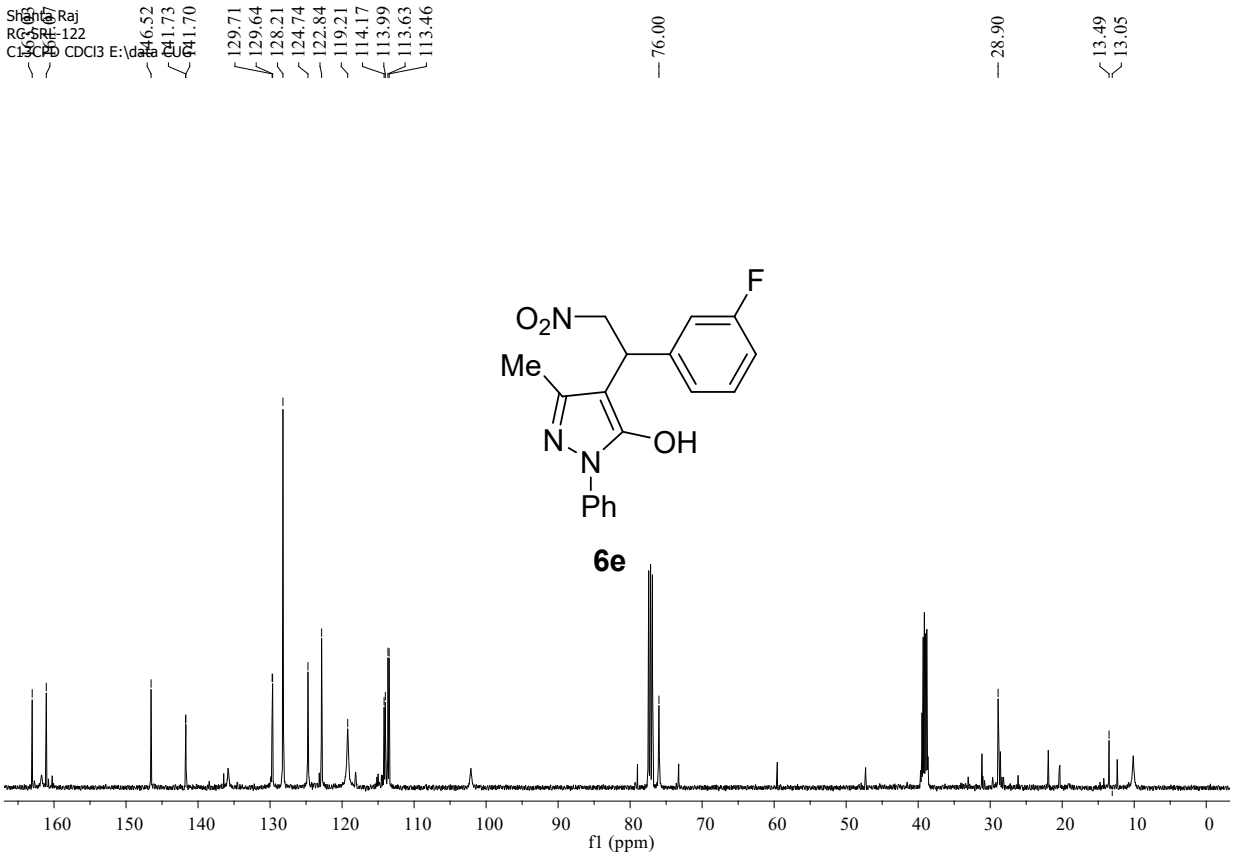

O2N
Me
OMe
N
N
OH
Ph
6c
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

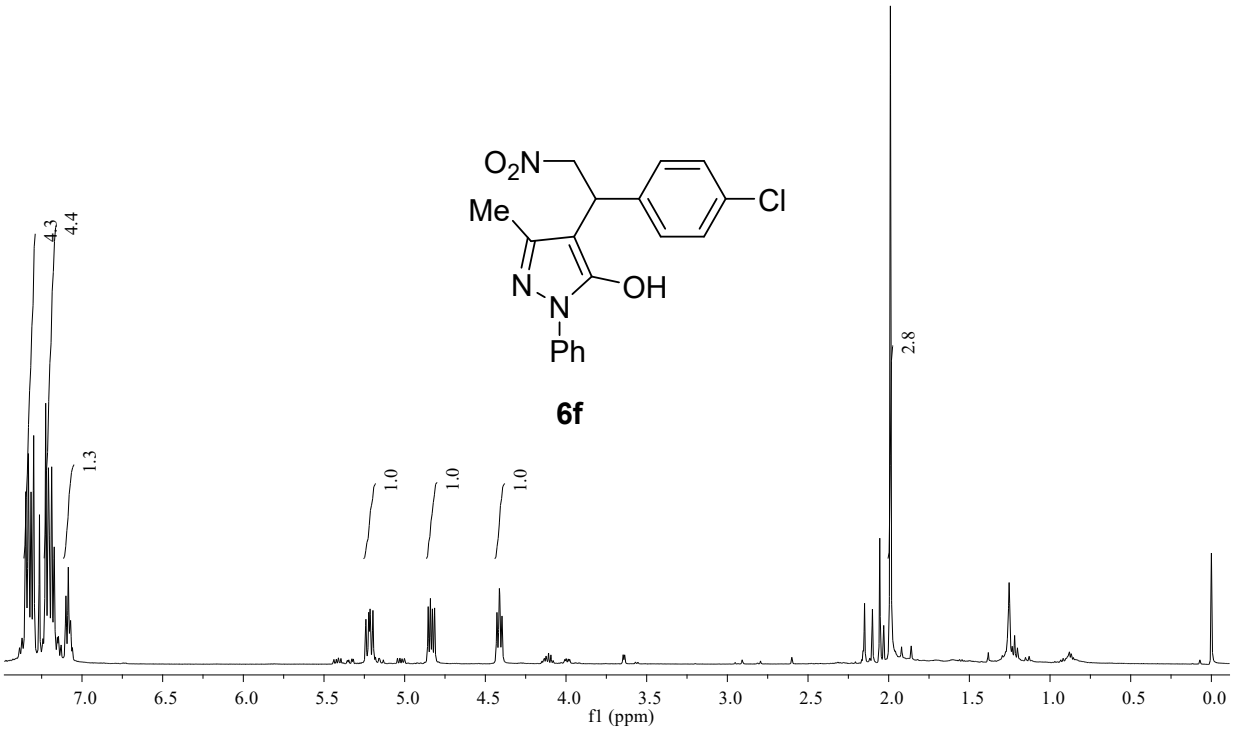

O2N
Me
F
N
OH
N
Ph
6d
4.07
2.55
2.11
1.18
1.01
1.00
0.98
4.01
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Shanta Raj
RC-SRL-114
C13CPD CDCl3 E:\data CUG
146.52
135.35
135.15
135.12
129.29
129.23
128.86
126.35
121.09
119.41
119.02
115.72
115.55
102.34
76.77
60.67
38.89
10.45

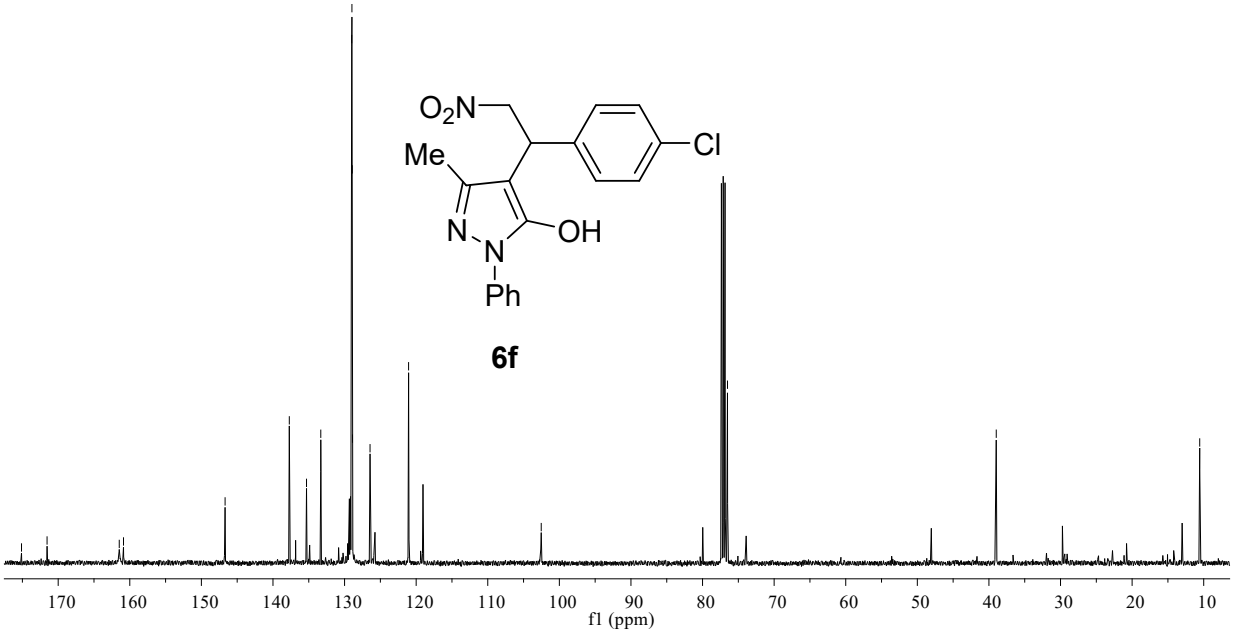

O2N
Me
F
N
OH
N
Ph
6d
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

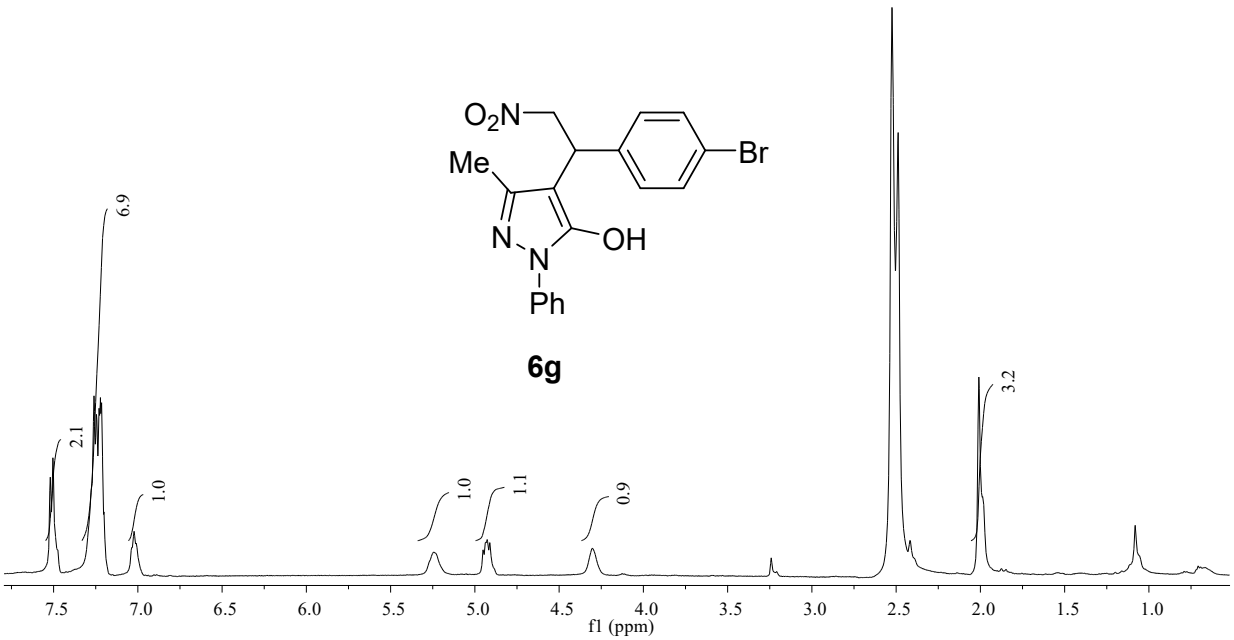

F
O2N
Me
N
N
OH
Ph
6e
4.1
2.8
1.1
1.2
1.0
1.0
0.9
2.9
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

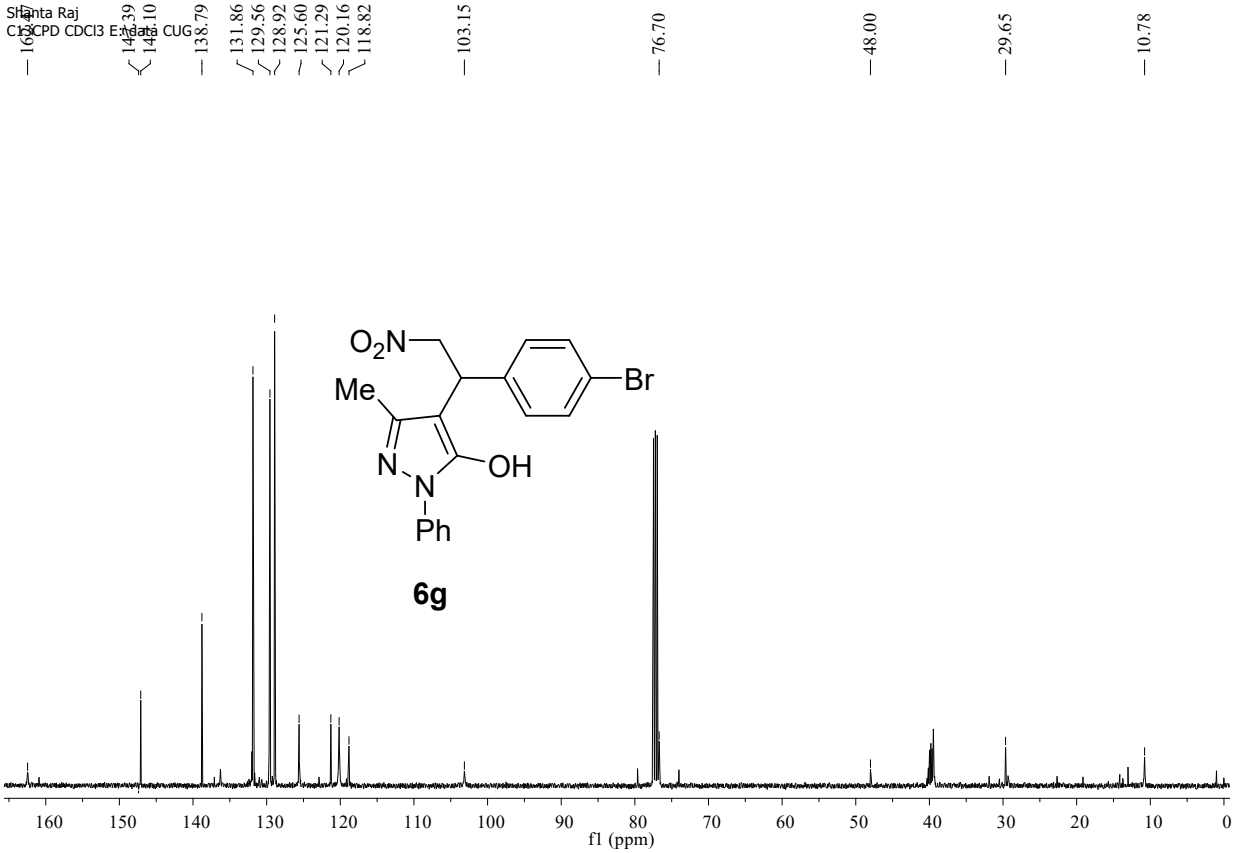

F
O2N
Me
N
N
OH
Ph
6e
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

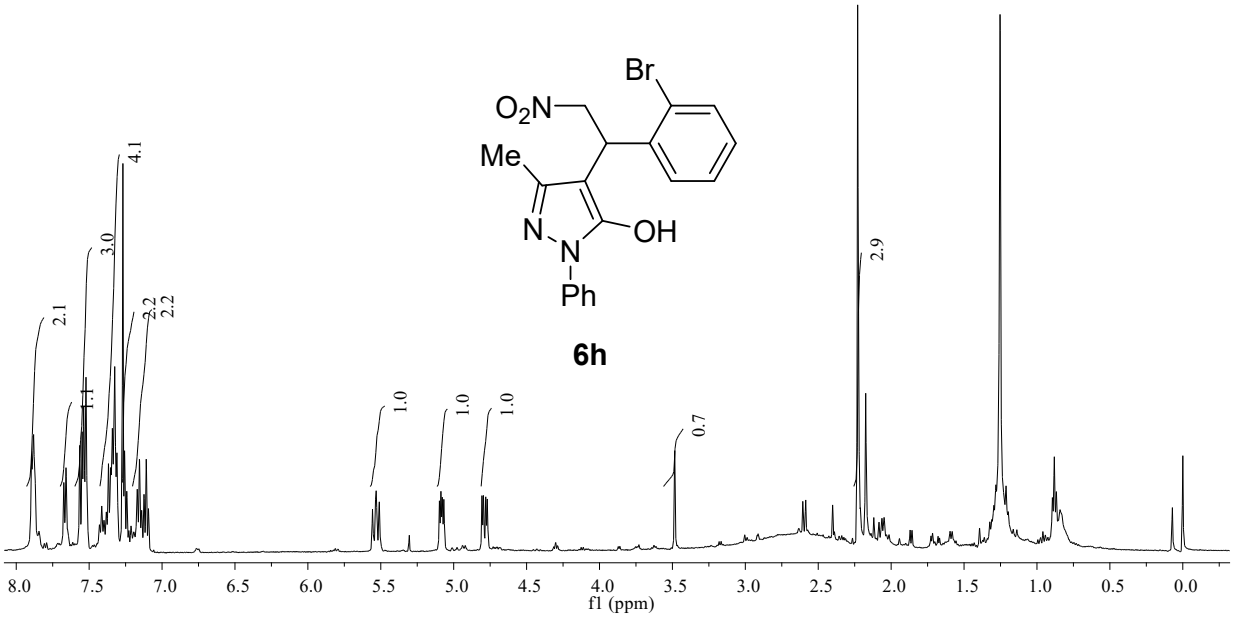

4.3
4.4
1.3
1.0
1.0
1.0
2.8
Me
Cl
OH
Ph
6f
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Shanta Raj
C-13CPD CDCl3 - data CUG
161.47
160.88
146.69
137.72
135.31
133.32
129.01
128.97
128.93
128.89
126.44
121.06
102.53
76.52
38.98
10.56

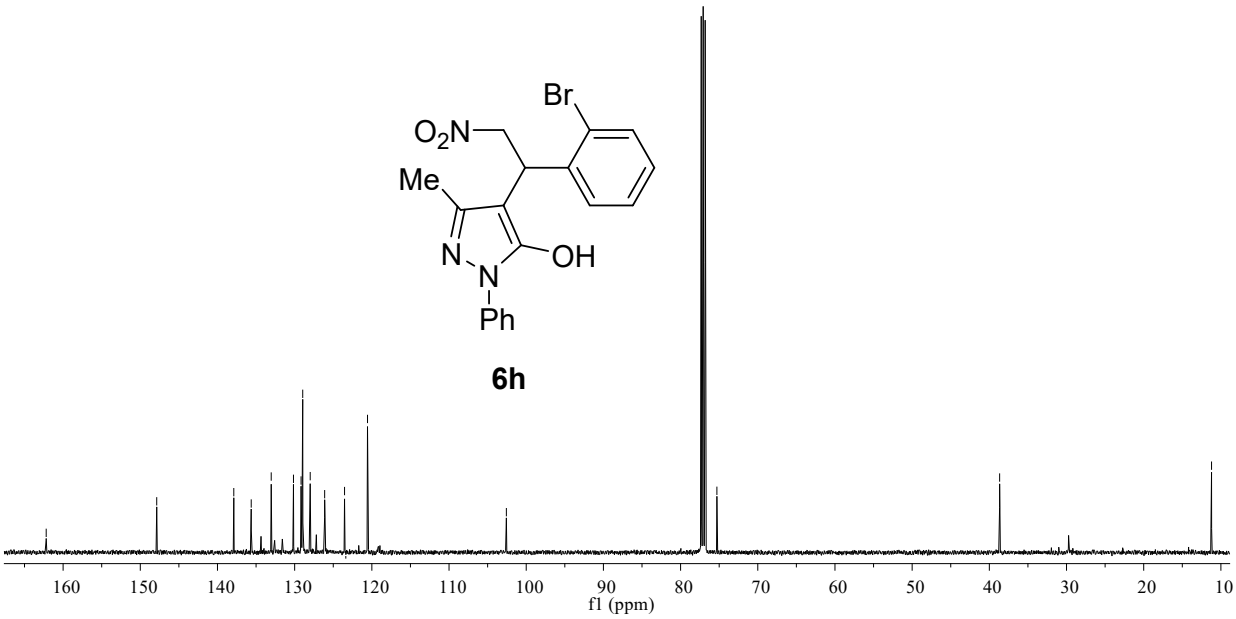

Me
Cl
OH
Ph
6f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

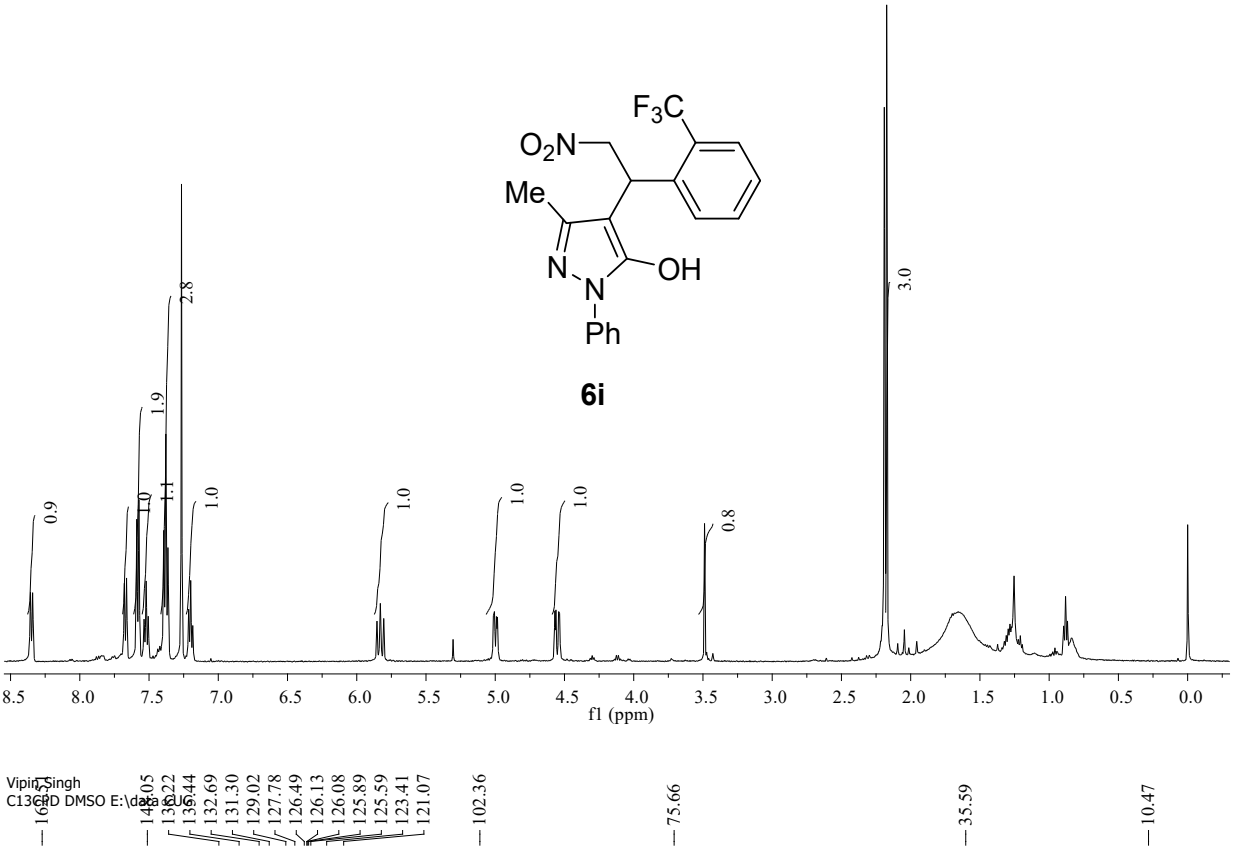

O2N
Me
Br
N
N
OH
Ph
6g
6.9
2.1
1.0
1.0
1.1
0.9
3.2
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)


Shanta Raj
C13CPD CDCl3 Extdata CUG
163.34
144.39
144.10
138.79
131.86
129.56
128.92
125.60
121.29
120.16
118.82
103.15
76.70
48.00
29.65
10.78
O2N
Me
Br
N
N
OH
Ph
6g
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

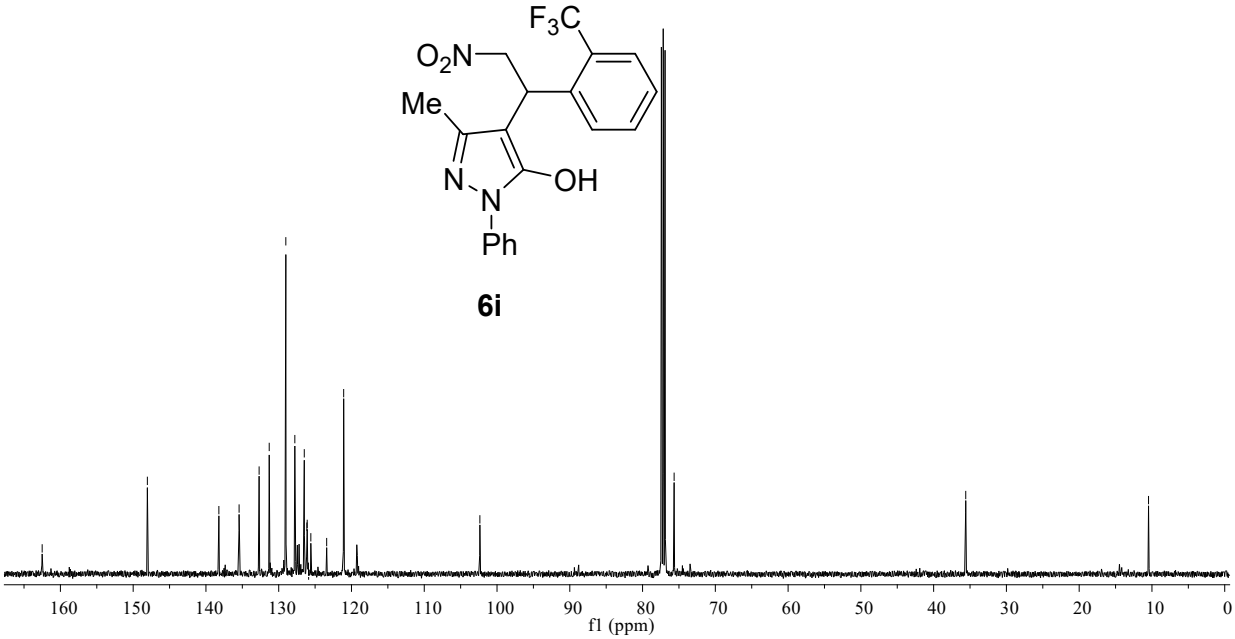

Br
O2N
Me
N
N
OH
Ph
6h
2.1
1.1
3.0
4.1
2.2
2.2
1.0
1.0
1.0
0.7
2.9
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

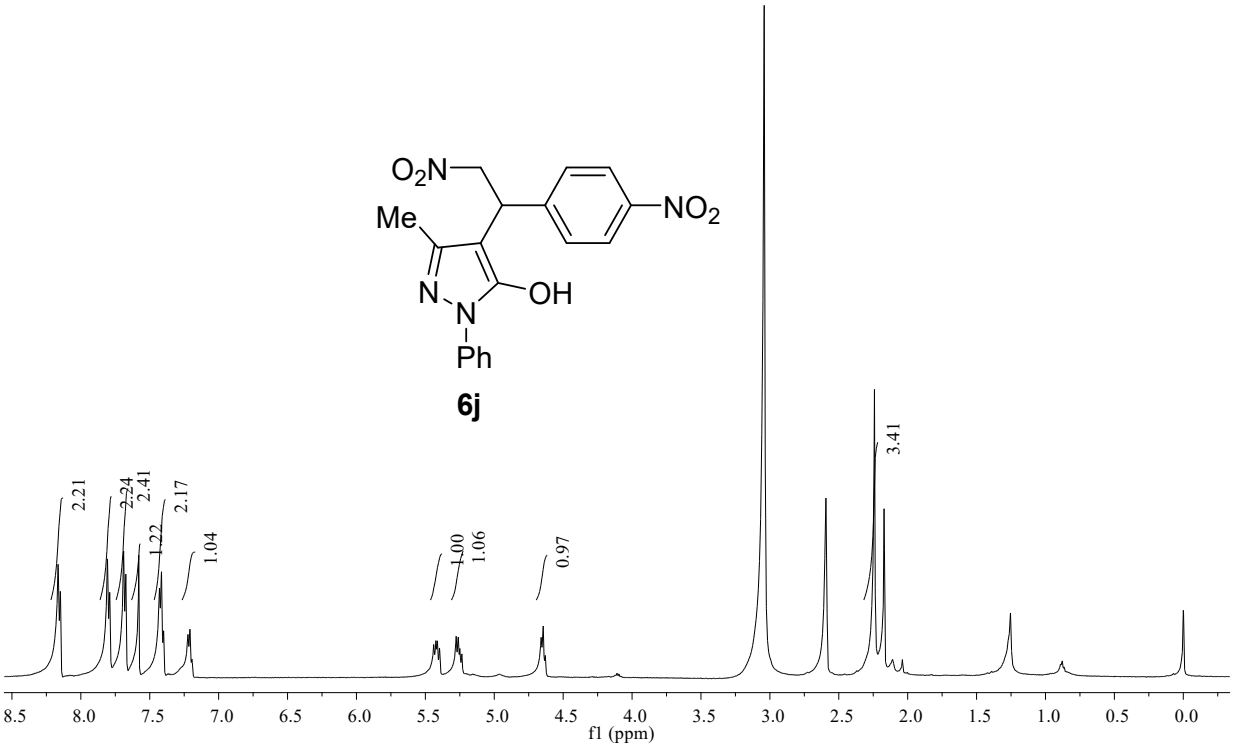

Shanta Raj
C13CPD CDCl3 E:\data-CUG
162.87
147.87
137.89
135.63
133.04
130.15
129.17
128.96
127.99
126.11
123.54
123.37
120.56
102.57
75.30
38.67
11.21

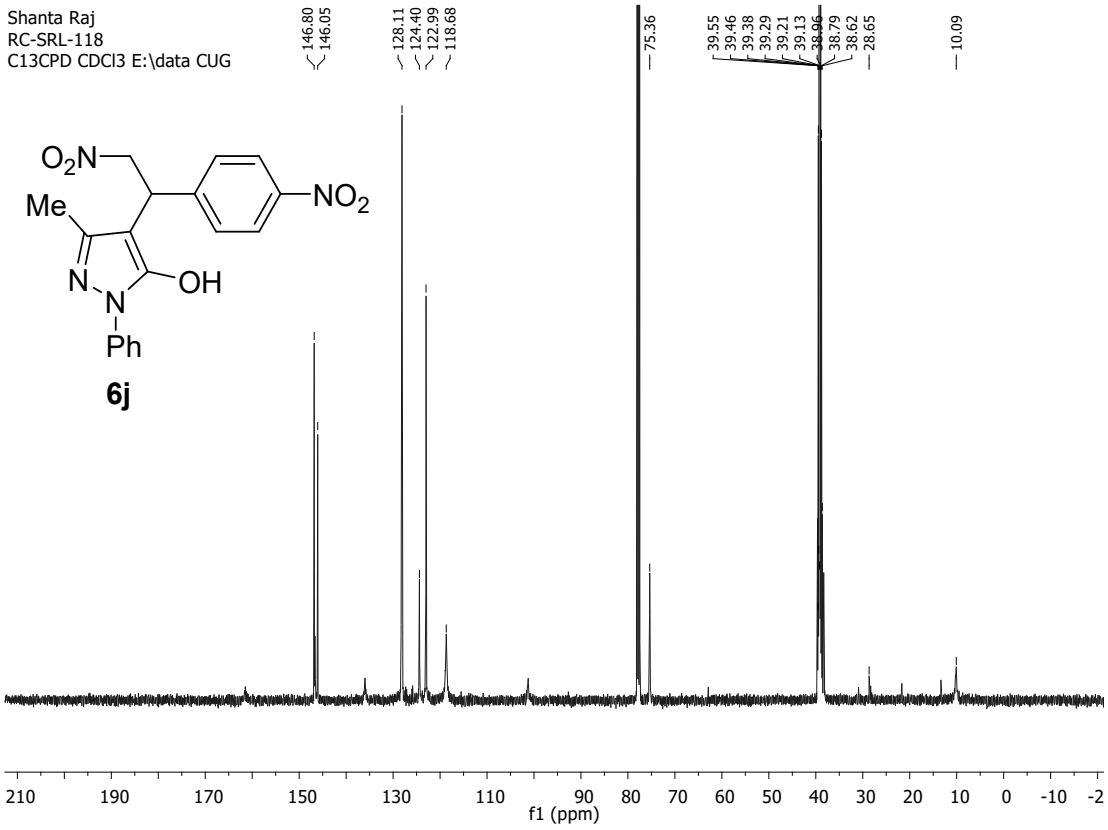

Br
O2N
Me
N
N
OH
Ph
6h
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

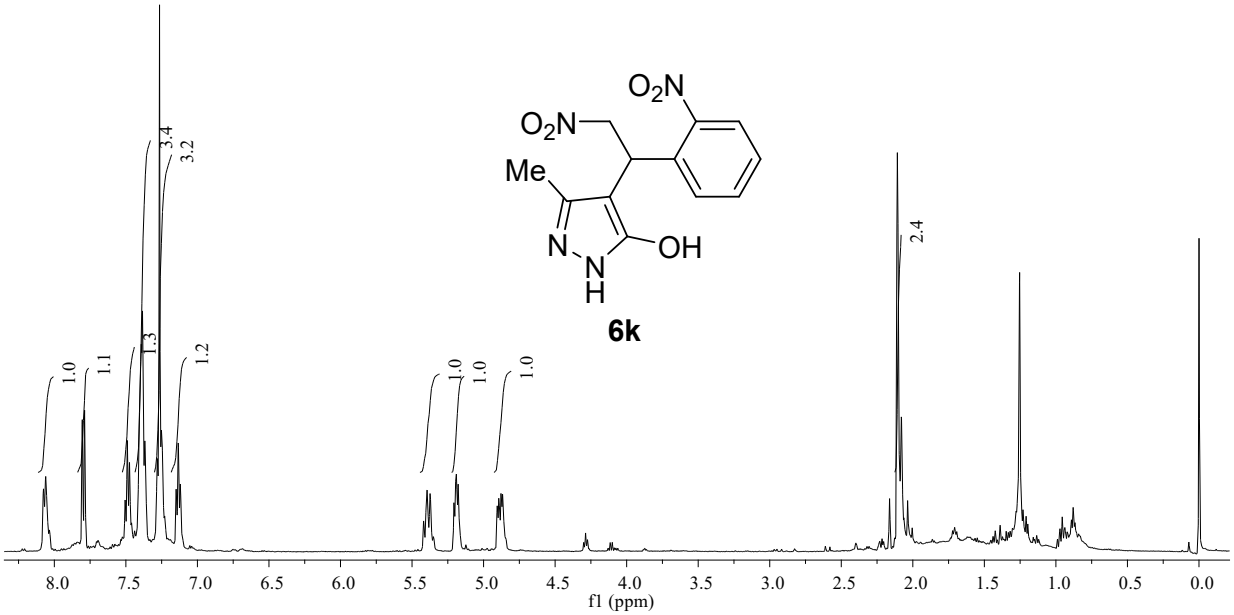

F3C
O2N
Me
N
N
OH
Ph
6i
0.9
1.0
1.9
1.1
2.8
1.0
1.0
1.0
1.0
0.8
3.0
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

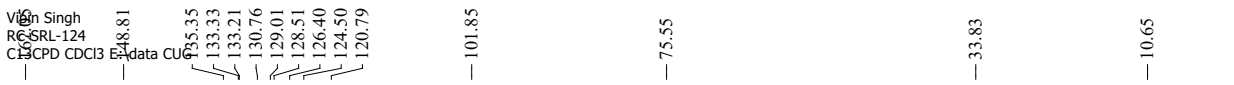
Vipin Singh
C13CPD DMSO E:\data
162.77
144.05
138.22
135.44
132.69
131.30
129.02
127.78
126.49
126.13
126.08
125.89
125.59
123.41
121.07
102.36
75.66
35.59
10.47

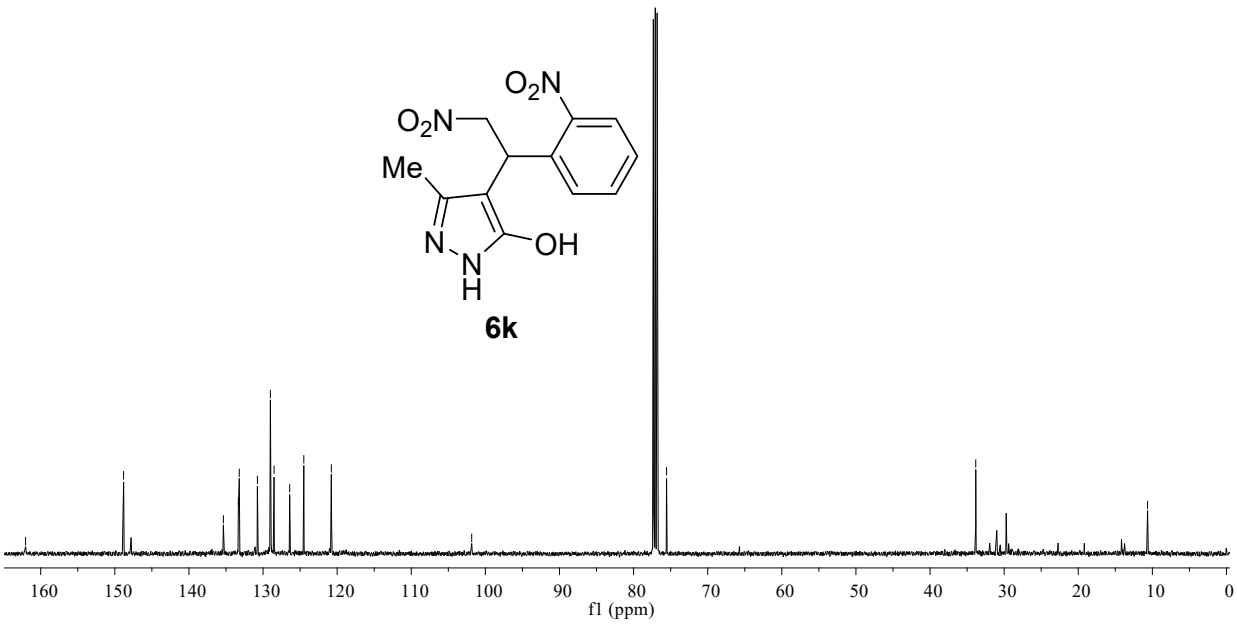

F3C
O2N
Me
N
N
OH
Ph
6i
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

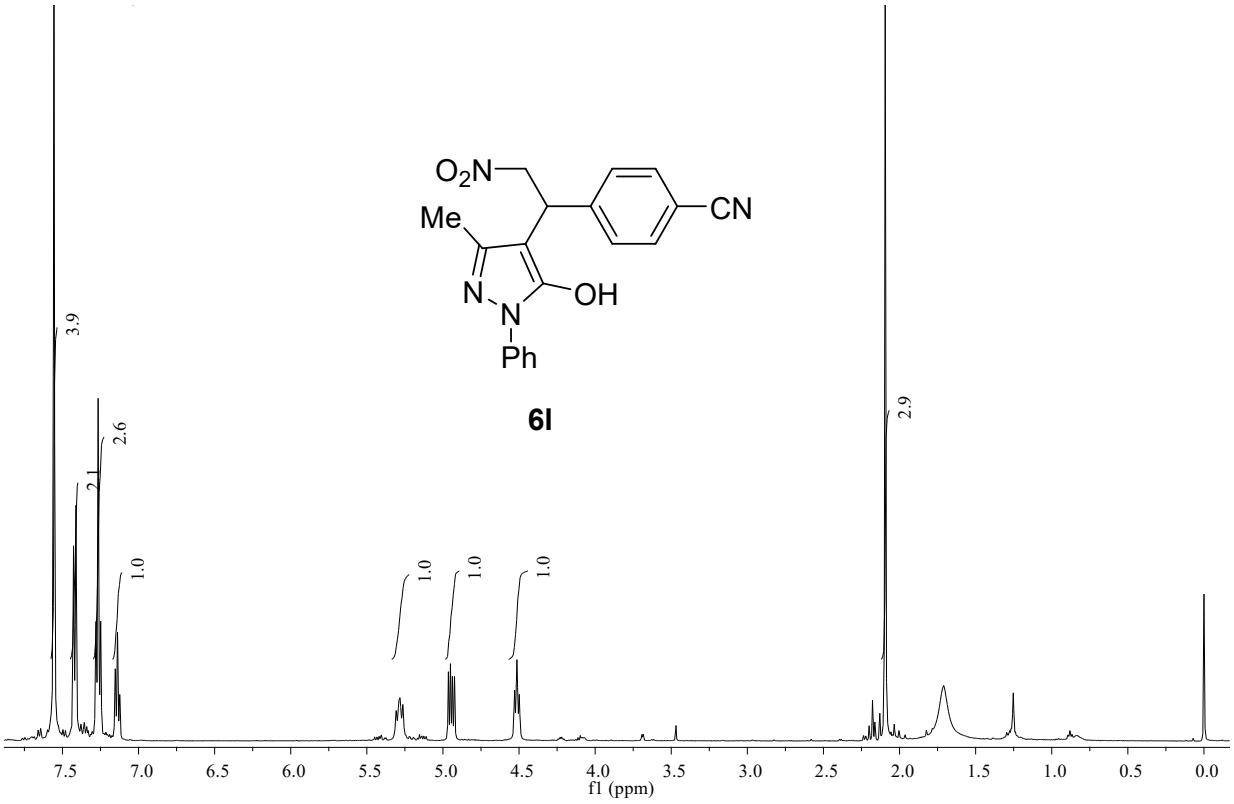

O2N
NO2
Me
OH
N
N
Ph
6j
2.21
2.24
2.41
2.22
2.17
1.04
1.00
1.06
0.97
3.41
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Shanta Raj
RC-SRL-118
C13CPD CDCl3 E:\data CUG
146.80
146.05
128.11
124.40
122.99
118.68
75.36
39.55
39.46
39.38
39.29
39.21
39.13
38.96
38.79
38.62
28.65
10.09
O2N
NO2
Me
OH
N
N
Ph
6j
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-2
f1 (ppm)

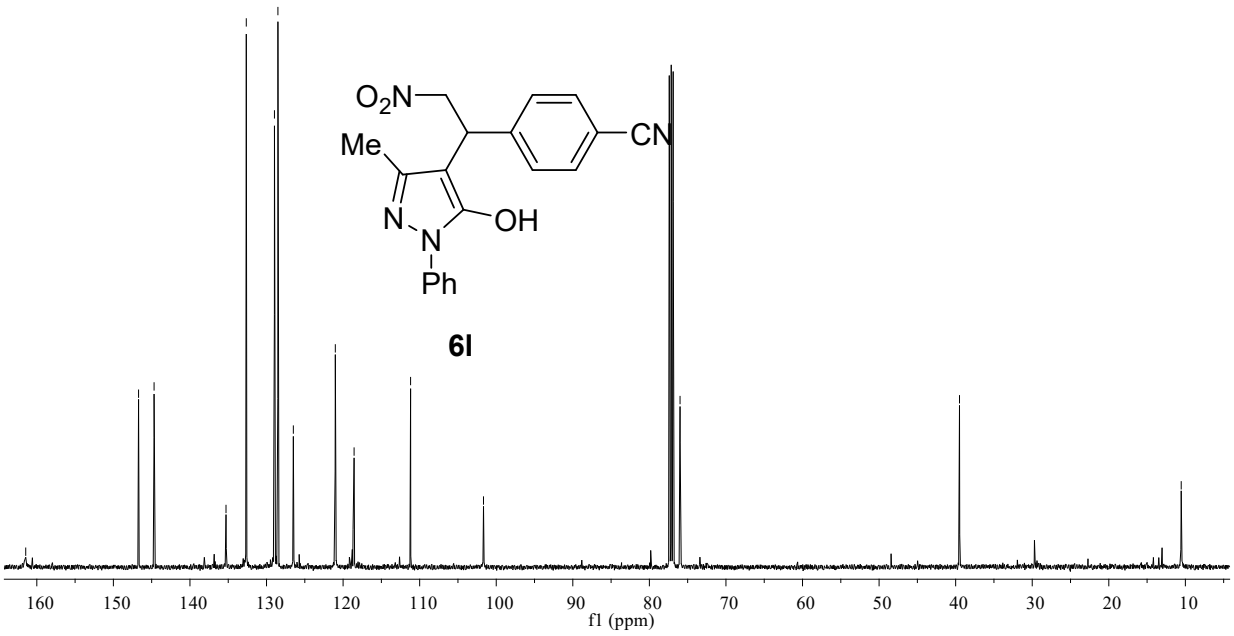

O2N
O2N
Me
N
N
H
OH
6k
1.0
1.1
1.3
3.4
3.2
1.2
1.0
1.0
1.0
2.4
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

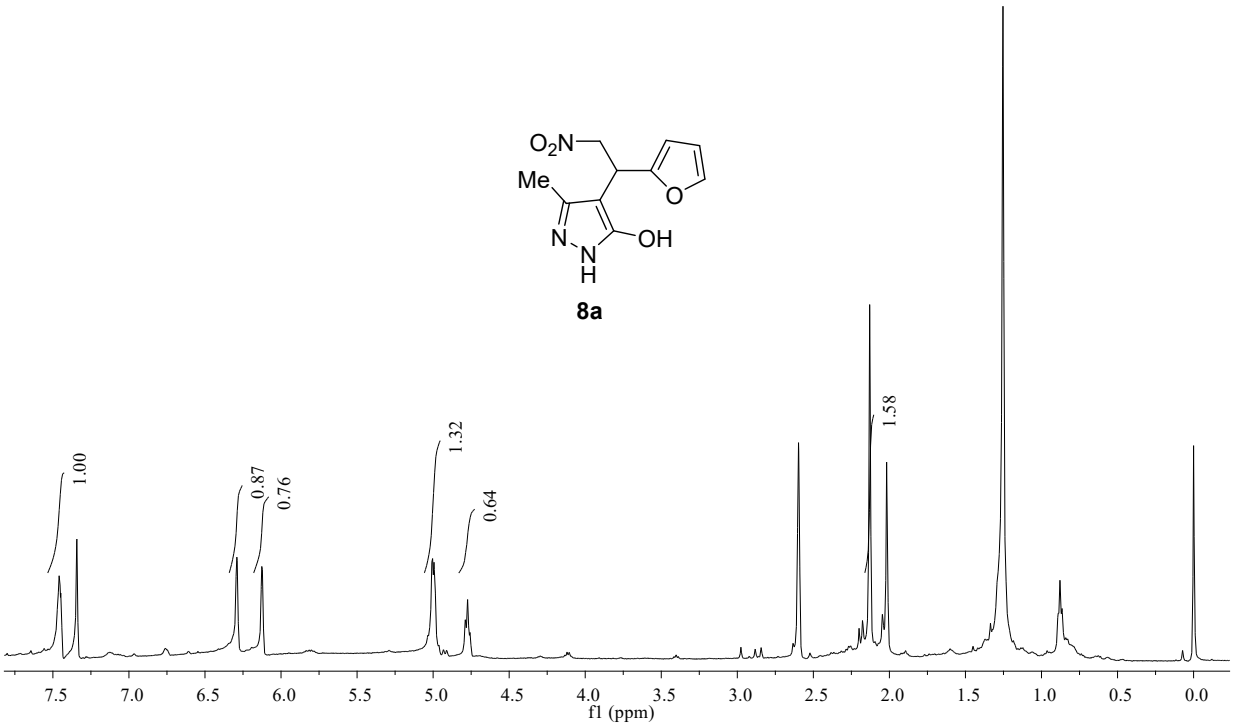

Vipin Singh
RC-SRL-124
C13CPD CDCl3 E:\data CUG
148.81
135.35
133.33
133.21
130.76
129.01
128.51
126.40
124.50
120.79
101.85
75.55
33.83
10.65

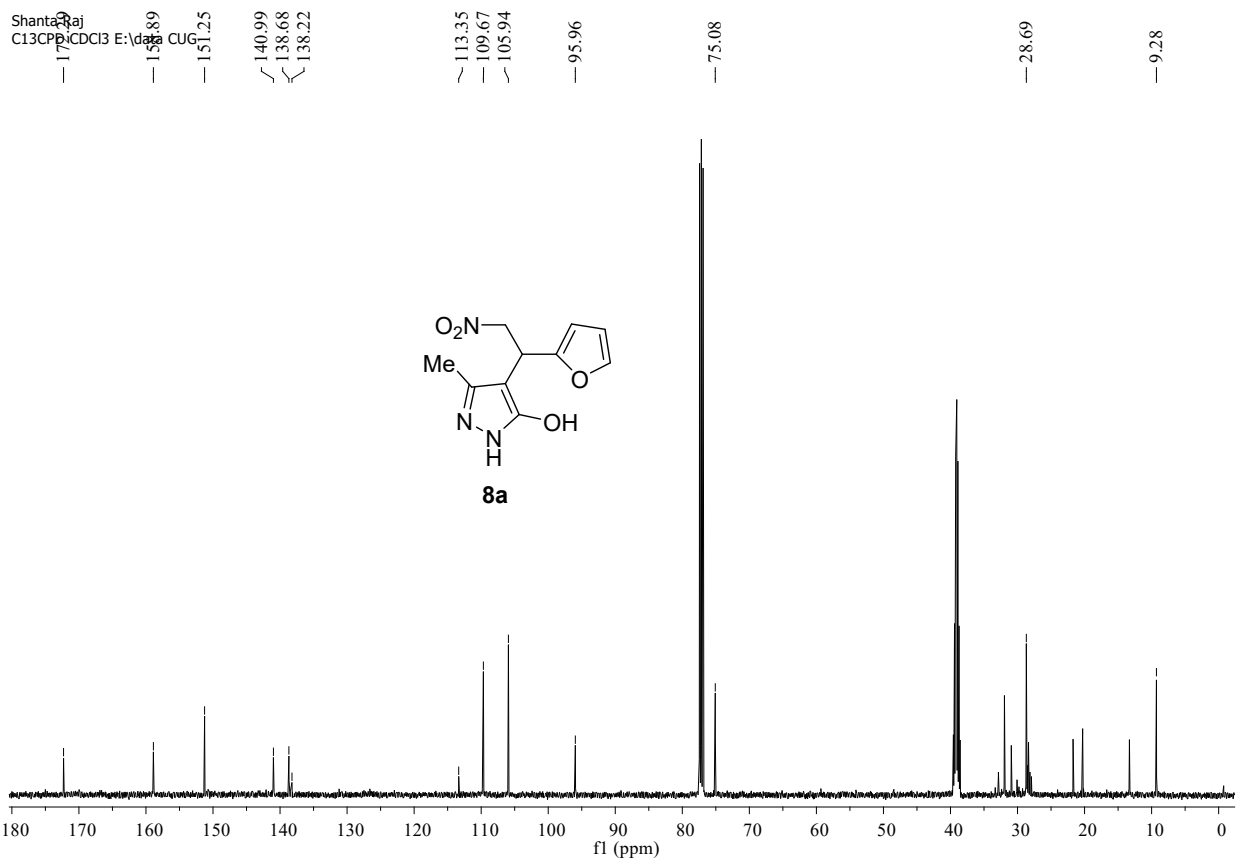

O2N
O2N
Me
N
N
H
OH
6k
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

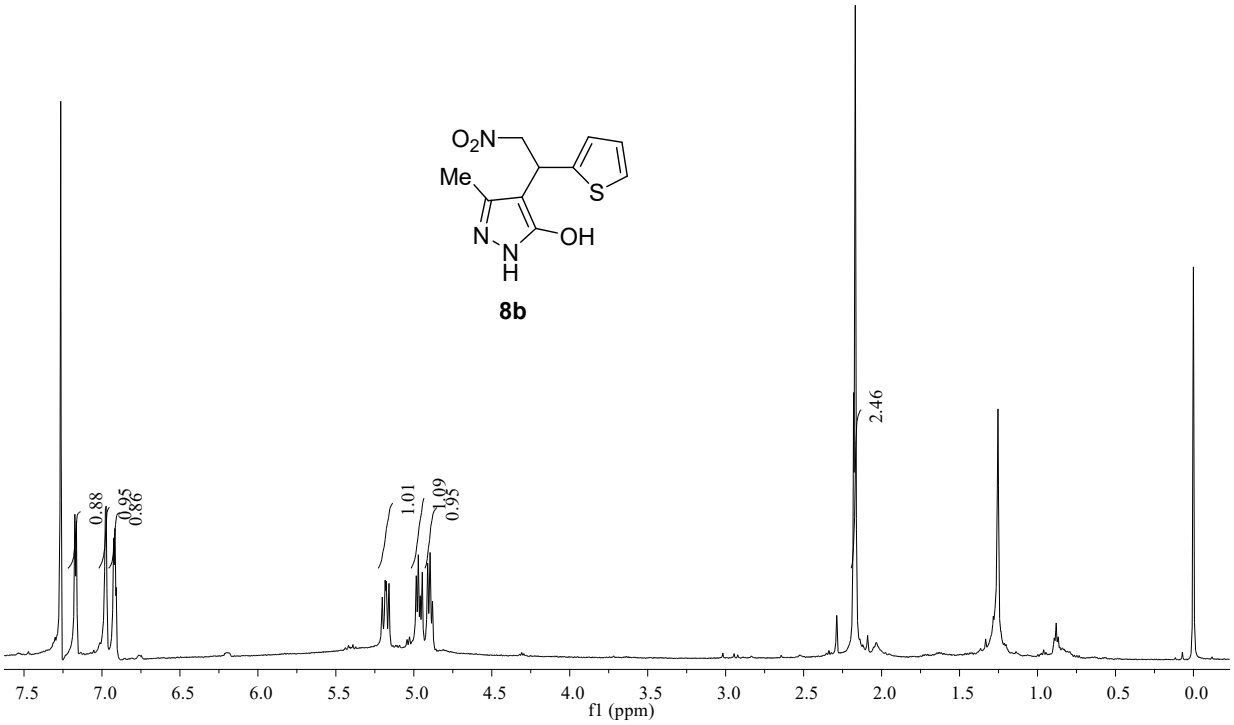

O2N
Me
CN
N
OH
N
Ph
6l
3.9
2.6
2.1
1.0
1.0
1.0
1.0
2.9
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

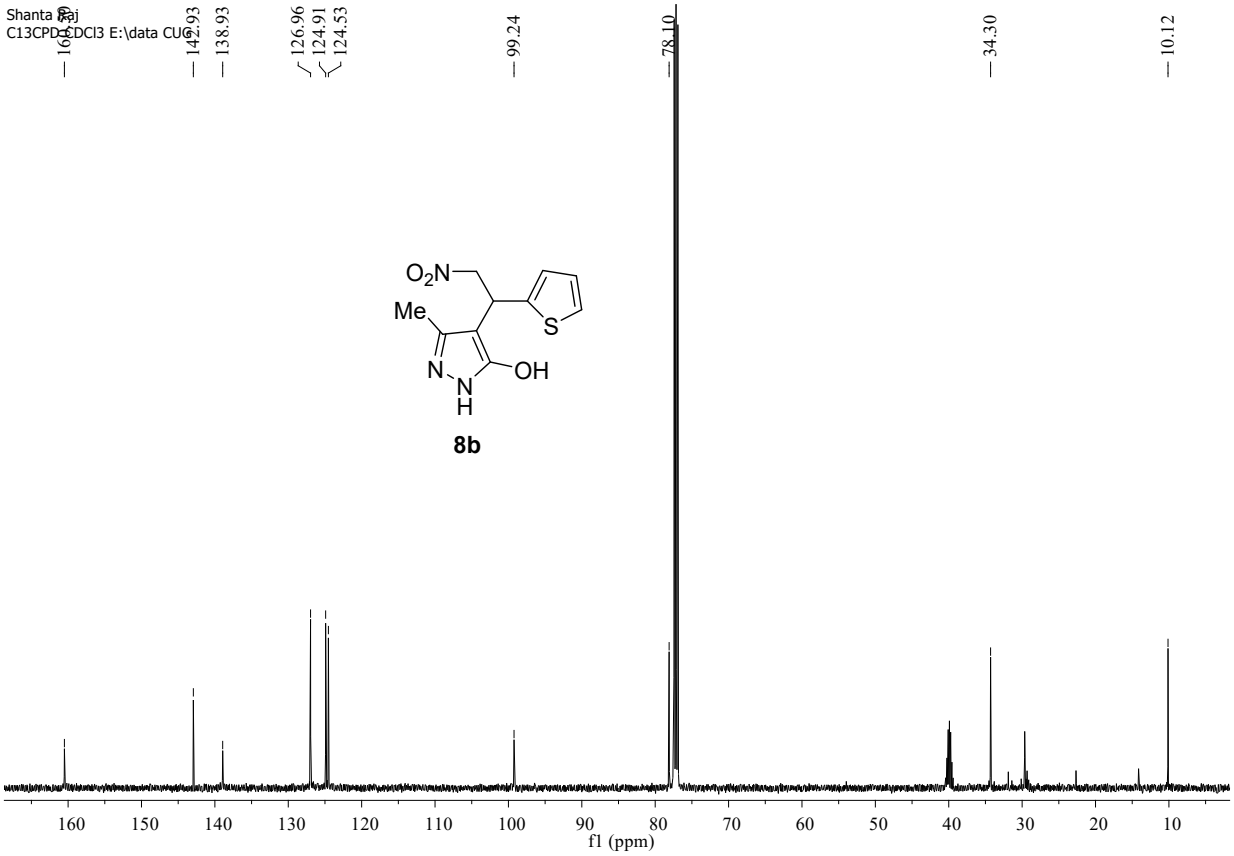

Vikram Singh
C13CPD CDCl3 E:\data\CUG
135.29
132.64
128.96
128.51
126.50
121.02
118.56
111.19
101.66
75.99
39.50
10.54

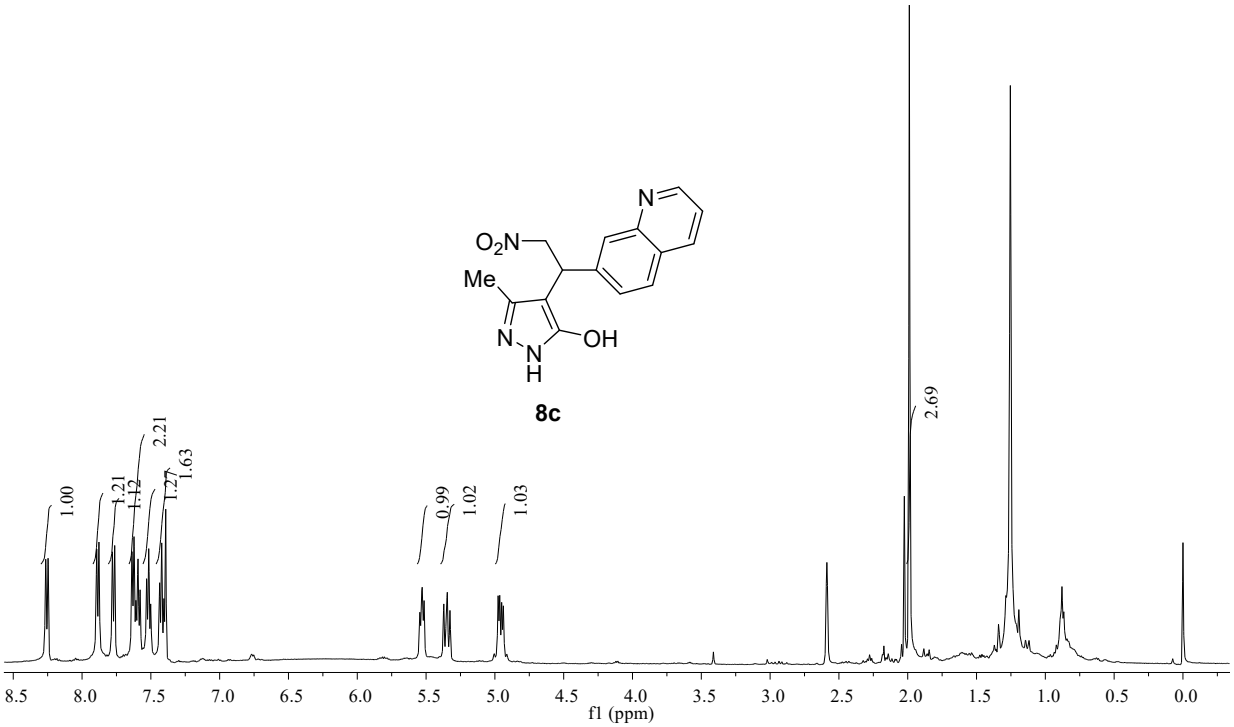

O2N
Me
CN
N
OH
N
Ph
6l
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

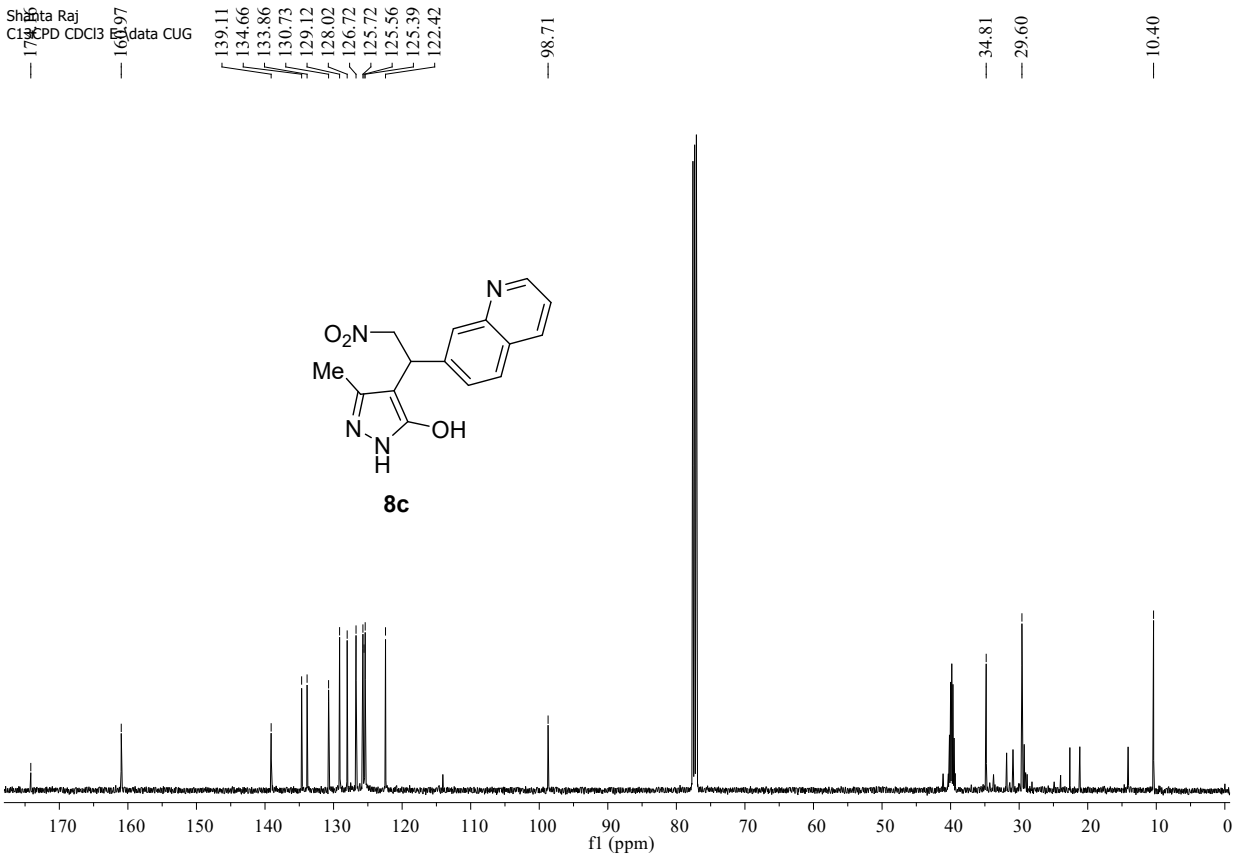

O2N
Me
O
N
N
H
OH
8a
1.00
0.87
0.76
1.32
0.64
1.58
7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

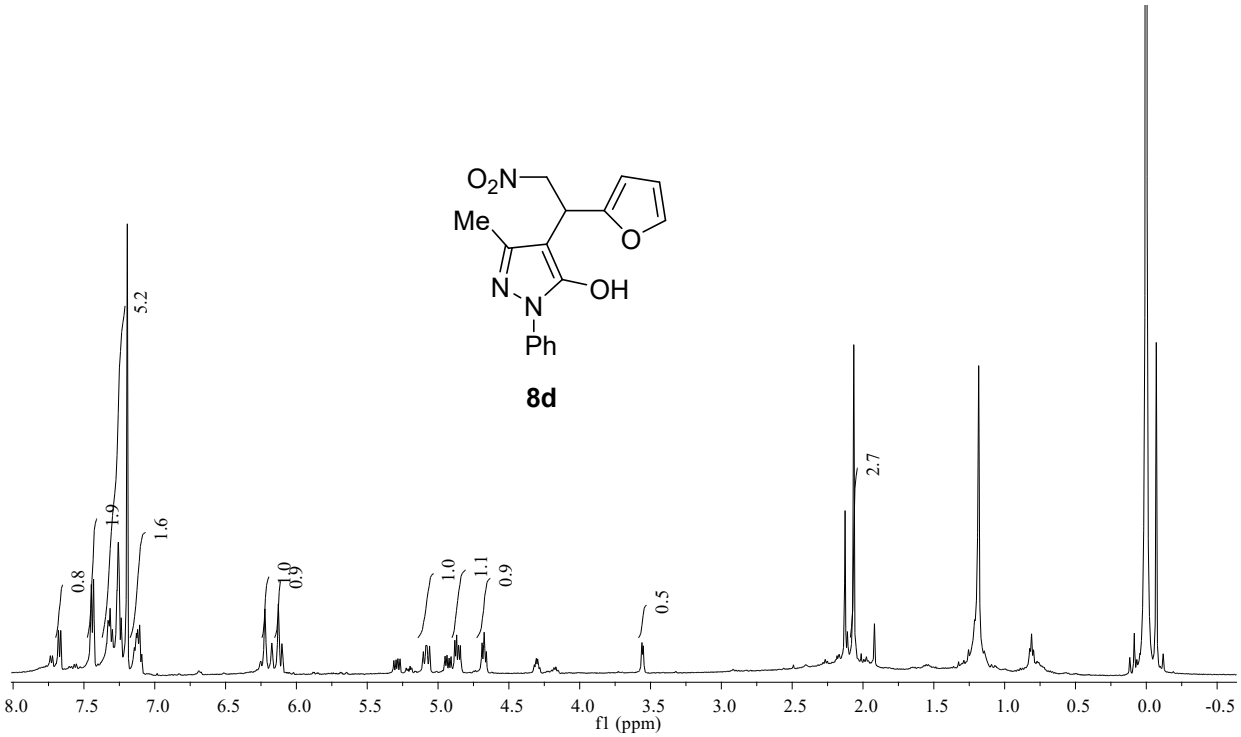

Shanta Raj
C13CPD iCDCl3 E:\data CUG
172.39
158.89
151.25
140.99
138.68
138.22
113.35
109.67
105.94
95.96
75.08
28.69
9.28
O2N
Me
O
N
N
H
OH
8a
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

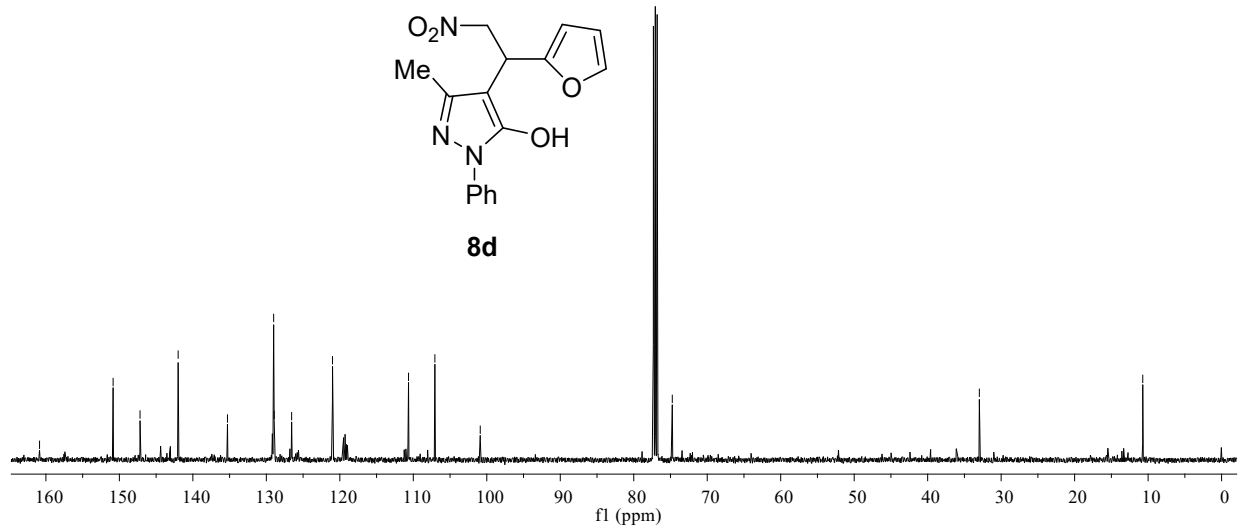

O2N
Me
S
N
N
H
OH
8b
0.88
0.95
0.86
1.01
1.09
0.95
2.46
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

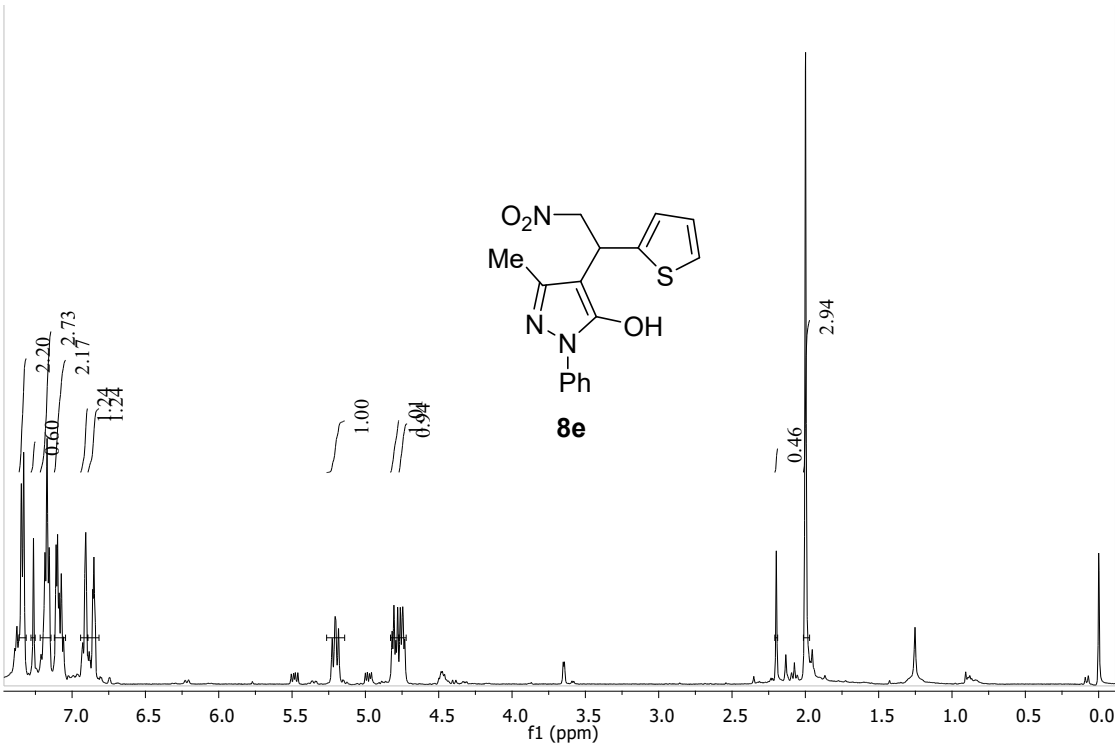

Shanta Raj
C13CPD CDCl3 E:\data CUG
160.46
142.93
138.93
126.96
124.91
124.53
99.24
78.10
34.30
10.12
O2N
Me
S
N
N
H
OH
8b
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

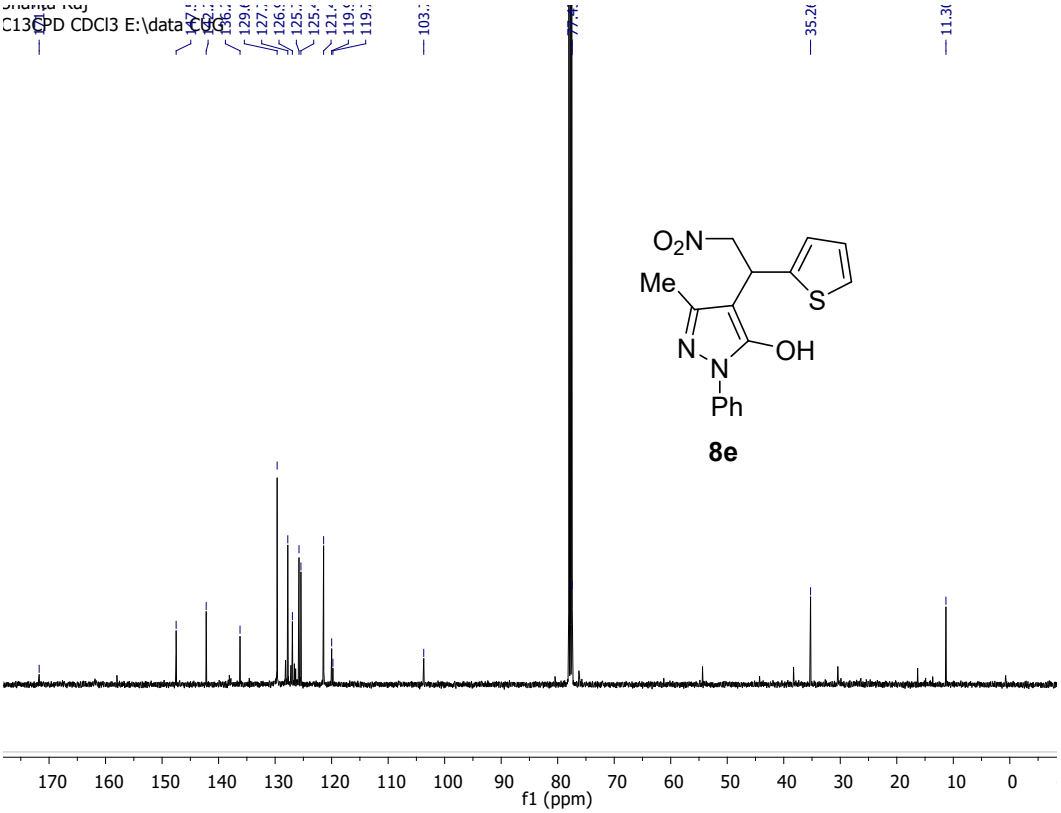

N
O2N
Me
N
N
H
OH
8c
1.00
1.21
1.12
2.21
1.27
1.63
0.99
1.02
1.03
2.69
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

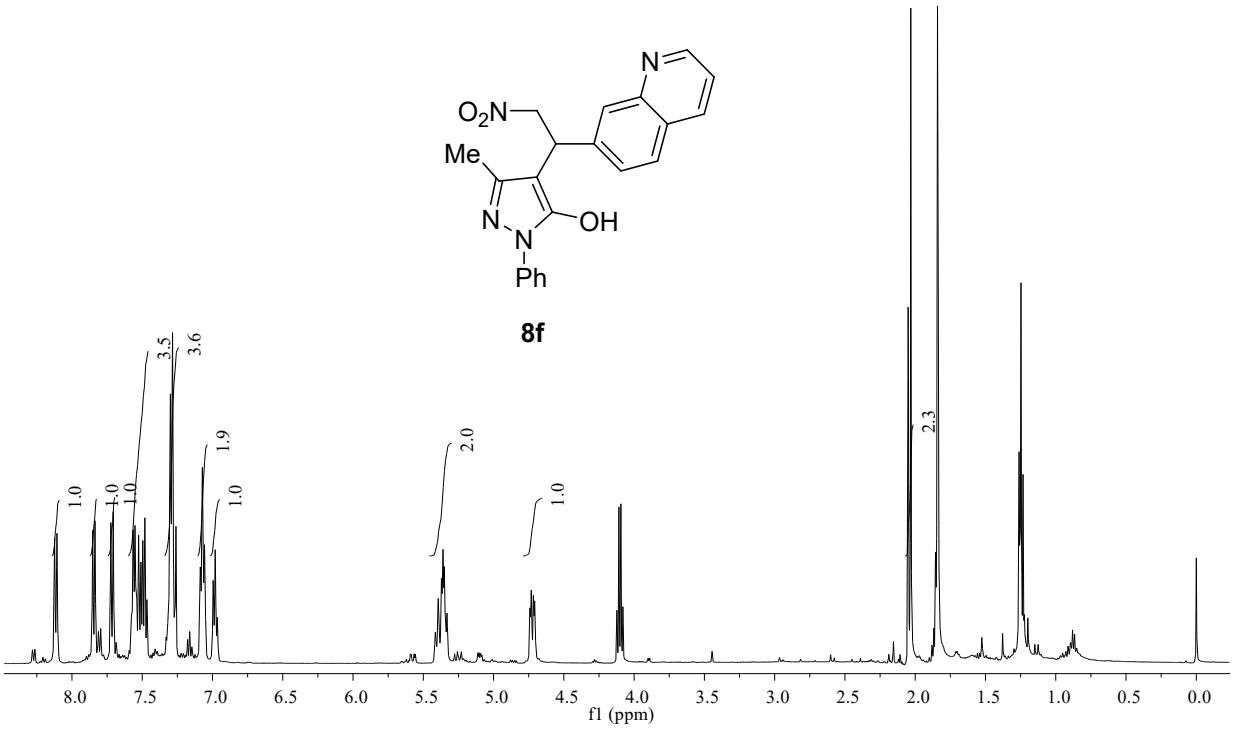

Shazia Raj
C13CPD CDCl3 Tf data CUG
160.97
139.11
134.66
133.86
130.73
129.12
128.02
126.72
125.72
125.56
125.39
122.42
98.71
34.81
29.60
10.40
N
O2N
Me
N
N
H
OH
8c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O2N
Me
O
N
OH
N
Ph
8d
5.2
1.9
1.6
0.8
1.0
0.9
1.0
1.1
0.9
0.5
2.7
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)

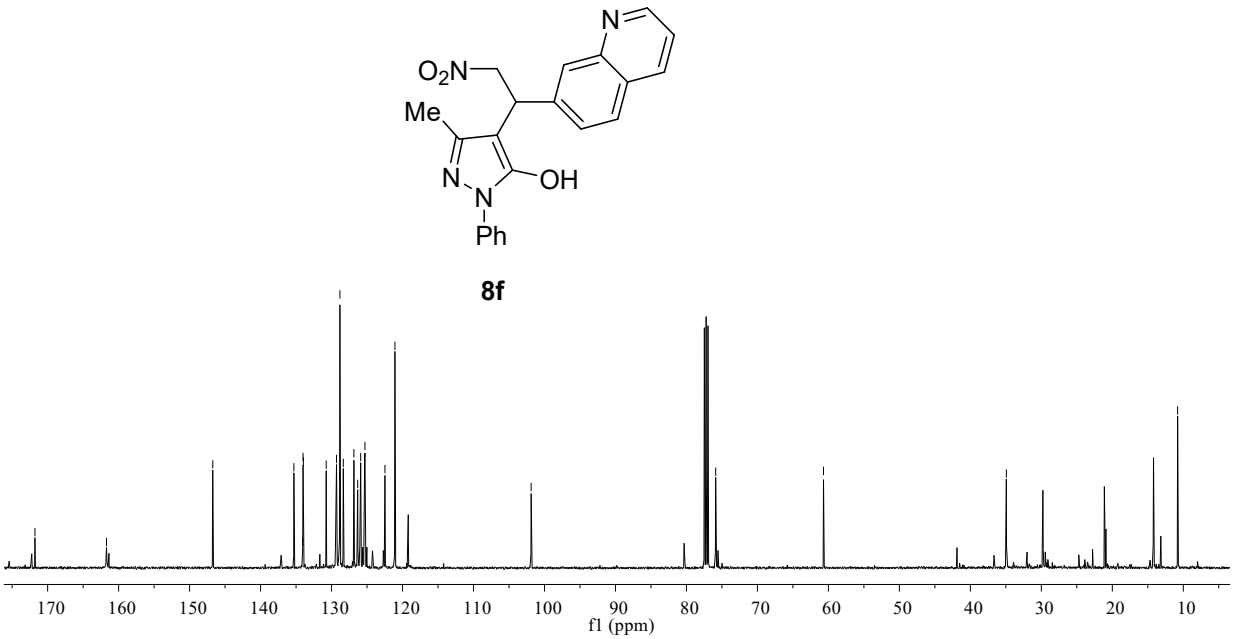

O2N
Me
O
N
OH
N
Ph
8d
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


O2N
Me
S
N
N
OH
Ph
8e
2.20
2.73
2.17
1.24
1.24
0.60
1.00
0.94
0.46
2.94
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
f1 (ppm)

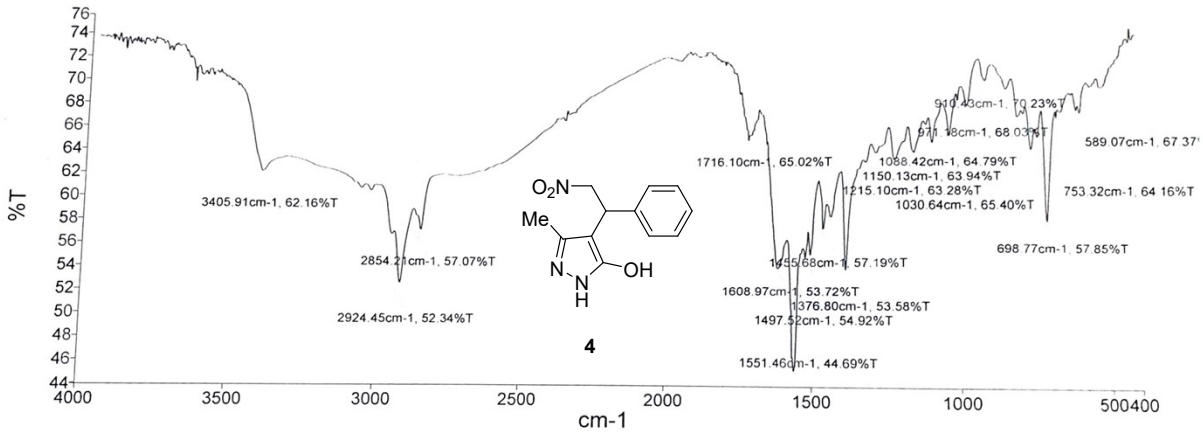

C13CPD CDCl3 E:\data\CDC
O2N
Me
S
N
N
OH
Ph
8e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

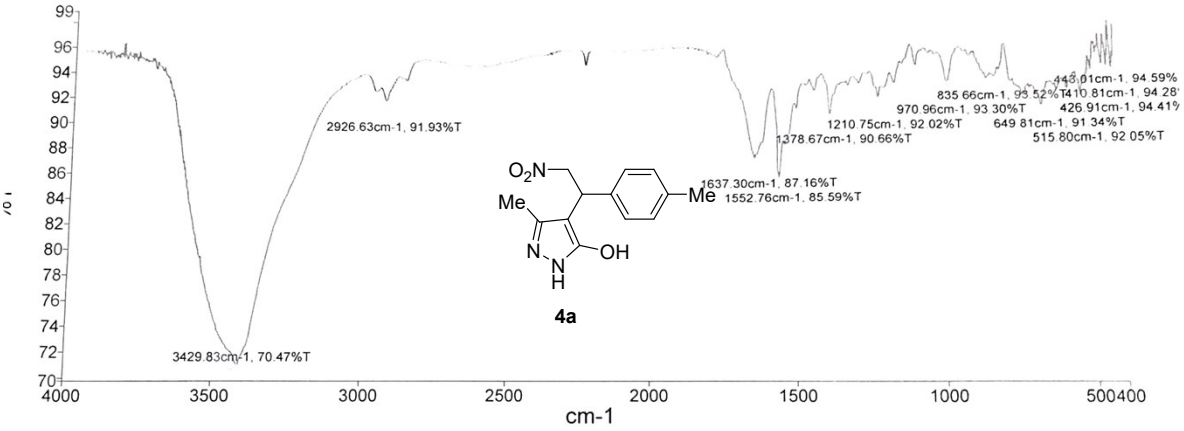

O2N
Me
N
OH
N
Ph
8f
1.0
1.0
1.0
3.5
3.6
1.9
1.0
2.0
1.0
2.3
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

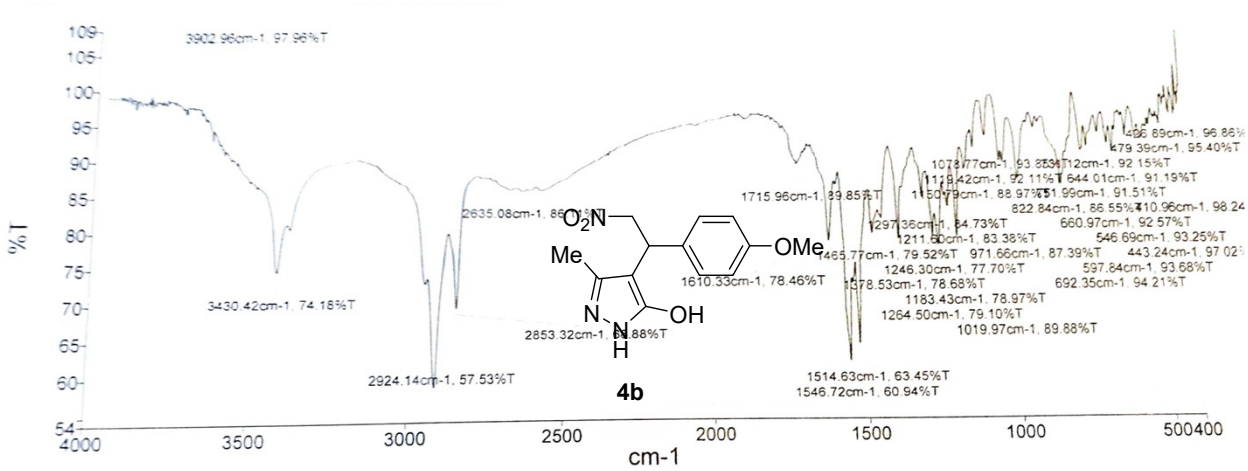

Vipin Singh
RC-SRL-128
C13CPD CDCl3 E:\data CUG
146.74
135.31
134.02
133.97
130.75
129.30
128.82
128.34
126.85
125.90
125.34
125.29
122.48
75.88
60.69
34.93
10.80

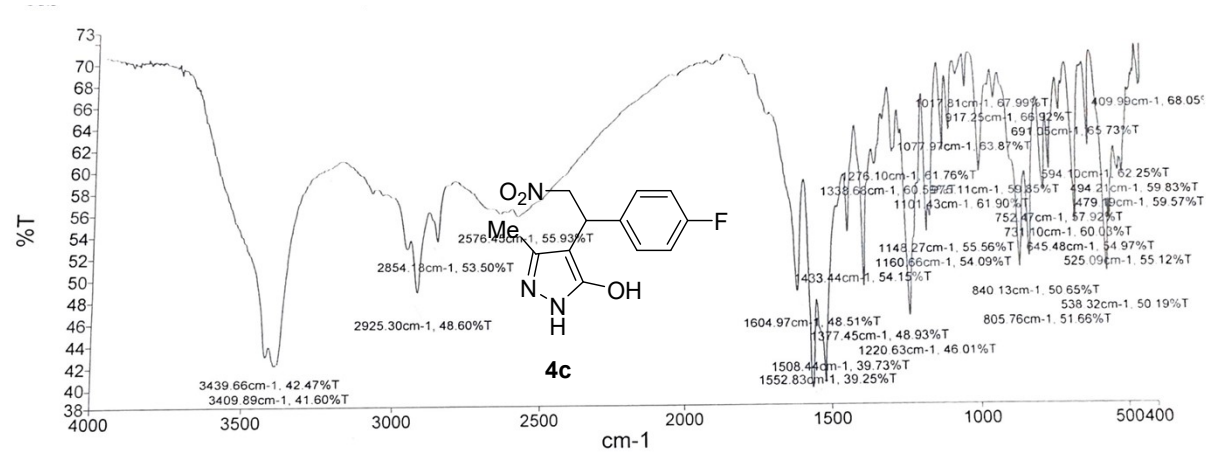

O2N
Me
N
OH
N
Ph
8f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

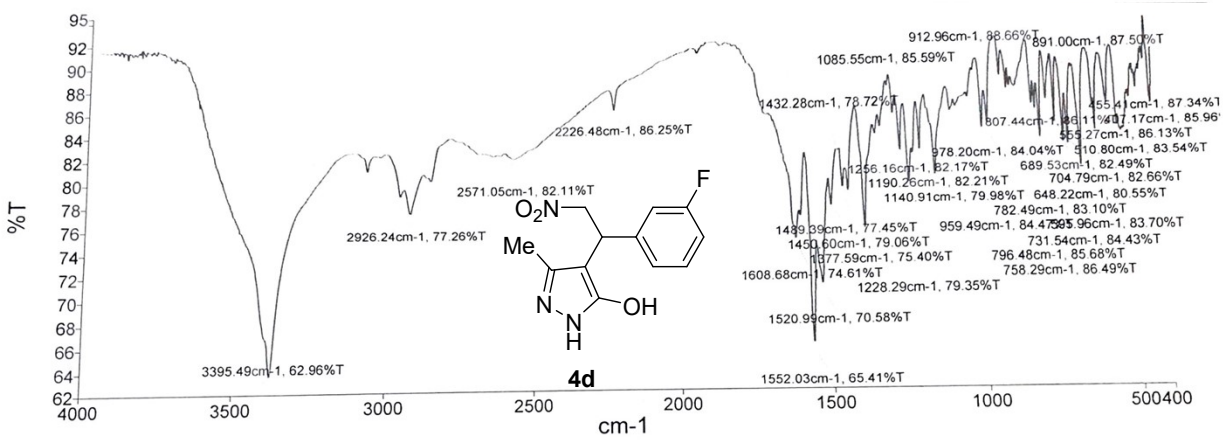
FT-IR Data of pyrazol-5-ol derivative (4, 4*a-k*, 6*a-l*, 8*a-d*)

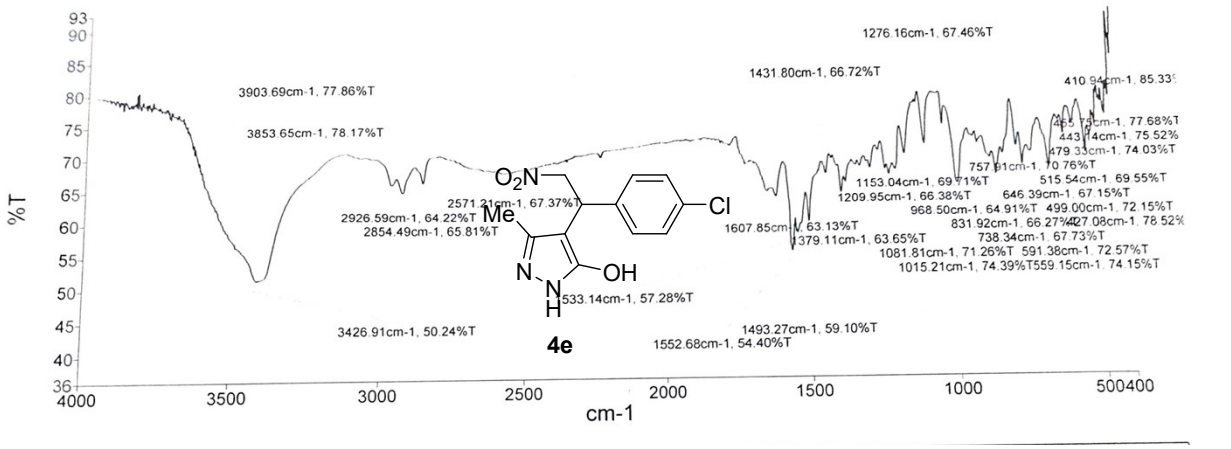


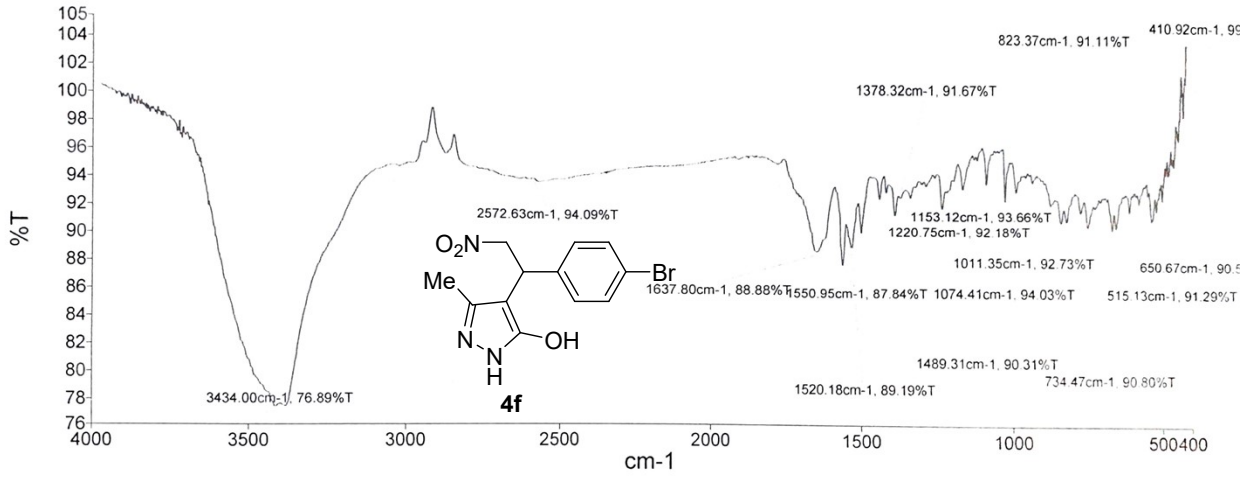


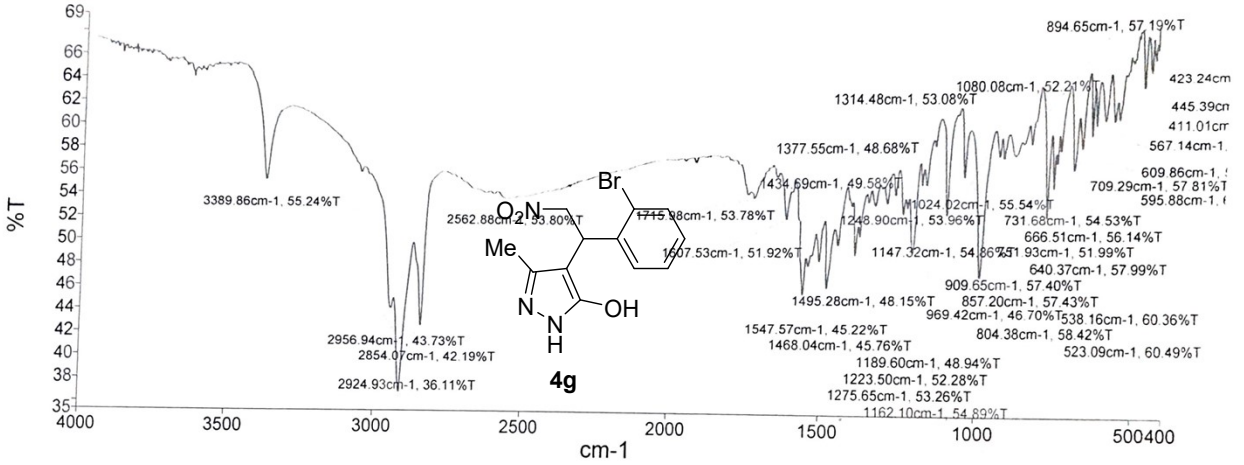


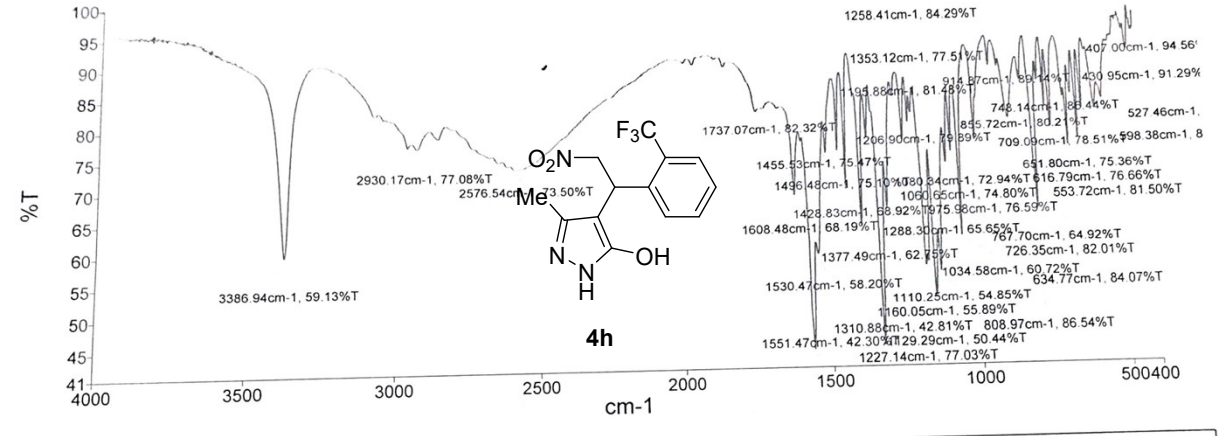

%T
cm-1
4000
3500
3000
2500
2000
1500
1000
500400
O2N
Me
F
OH
N
N
H
4c
3439.66cm-1, 42.47%T
3409.89cm-1, 41.60%T
2925.30cm-1, 48.60%T
2854.18cm-1, 53.50%T
2576.49cm-1, 55.93%T
1604.97cm-1, 48.51%T
1552.83cm-1, 39.25%T
1508.44cm-1, 39.73%T
1377.45cm-1, 48.93%T
1220.63cm-1, 46.01%T
1433.44cm-1, 54.15%T
1017.81cm-1, 67.99%T
917.25cm-1, 66.92%T
691.05cm-1, 65.73%T
1077.97cm-1, 63.87%T
1276.10cm-1, 61.76%T
1338.66cm-1, 60.55%T
1101.43cm-1, 61.90%T
1148.27cm-1, 55.56%T
1160.66cm-1, 54.09%T
840.13cm-1, 50.65%T
805.76cm-1, 51.66%T
752.47cm-1, 57.92%T
731.10cm-1, 60.03%T
645.48cm-1, 54.97%T
525.09cm-1, 55.12%T
538.32cm-1, 50.19%T
594.10cm-1, 62.25%T
494.21cm-1, 59.83%T
479.19cm-1, 59.57%T
409.99cm-1, 68.05%T

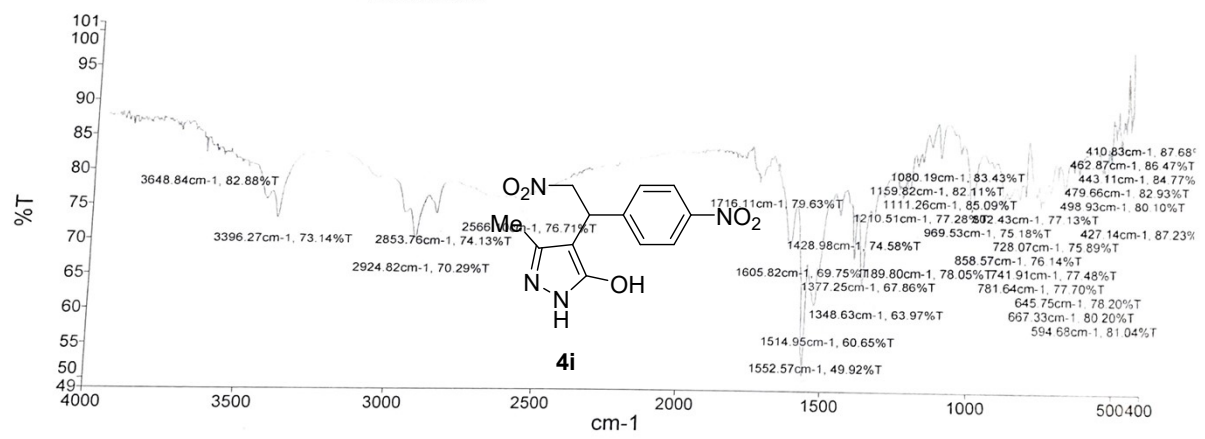

%T
cm-1
4000
3500
3000
2500
2000
1500
1000
500400
O2N
Me
F
OH
N
N
H
4d
3395.49cm-1, 62.96%T
2926.24cm-1, 77.26%T
2571.05cm-1, 82.11%T
2226.48cm-1, 86.25%T
1608.68cm-1, 74.61%T
1552.03cm-1, 65.41%T
1520.99cm-1, 70.58%T
1489.39cm-1, 77.45%T
1450.60cm-1, 79.06%T
1377.59cm-1, 75.40%T
1432.28cm-1, 78.72%T
1228.29cm-1, 79.35%T
1256.16cm-1, 82.17%T
1190.26cm-1, 82.21%T
1140.91cm-1, 79.98%T
1085.55cm-1, 85.59%T
978.20cm-1, 84.04%T
959.49cm-1, 84.47%T
912.96cm-1, 88.66%T
891.00cm-1, 87.50%T
807.44cm-1, 86.11%T
782.49cm-1, 83.10%T
758.29cm-1, 86.49%T
731.54cm-1, 84.43%T
796.48cm-1, 85.68%T
704.79cm-1, 82.66%T
689.53cm-1, 82.49%T
648.22cm-1, 80.55%T
595.96cm-1, 83.70%T
555.27cm-1, 86.13%T
510.80cm-1, 83.54%T
455.41cm-1, 87.34%T
407.17cm-1, 85.96%T

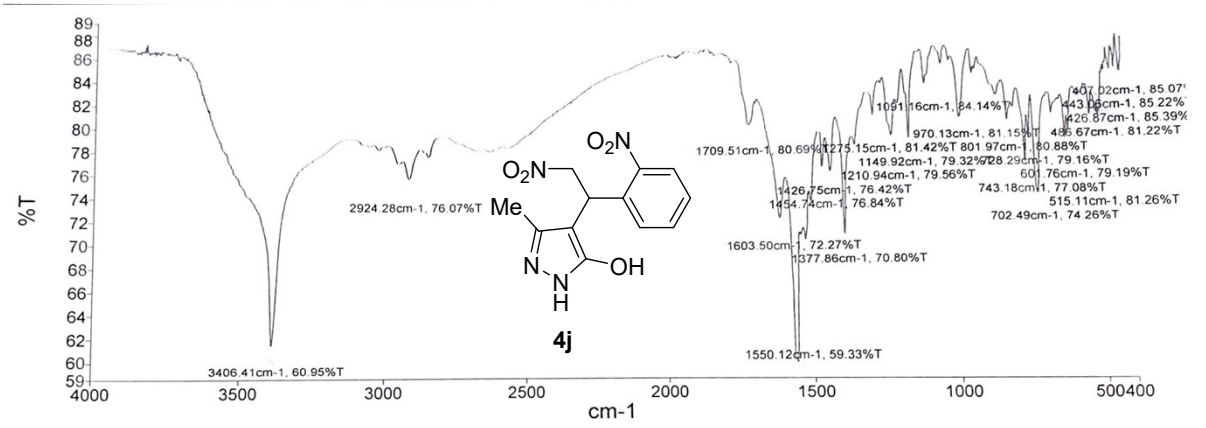

%T
cm-1
4000
3500
3000
2500
2000
1500
1000
500400
O2N
Me
Cl
OH
N
N
H
4e
3903.69cm-1, 77.86%T
3853.65cm-1, 78.17%T
3426.91cm-1, 50.24%T
2926.59cm-1, 64.22%T
2854.49cm-1, 65.81%T
2571.21cm-1, 67.37%T
1607.85cm-1, 63.13%T
1552.68cm-1, 54.40%T
1533.14cm-1, 57.28%T
1493.27cm-1, 59.10%T
1431.80cm-1, 66.72%T
1379.11cm-1, 63.65%T
1276.16cm-1, 67.46%T
1209.95cm-1, 66.38%T
1153.04cm-1, 69.71%T
1081.81cm-1, 71.26%T
1015.21cm-1, 74.39%T
968.50cm-1, 64.91%T
831.92cm-1, 66.27%T
757.91cm-1, 70.76%T
738.34cm-1, 67.73%T
646.39cm-1, 67.15%T
591.38cm-1, 72.57%T
559.15cm-1, 74.15%T
515.54cm-1, 69.55%T
499.00cm-1, 72.15%T
479.33cm-1, 74.03%T
443.14cm-1, 75.52%T
427.08cm-1, 78.52%T
410.94cm-1, 85.33%T

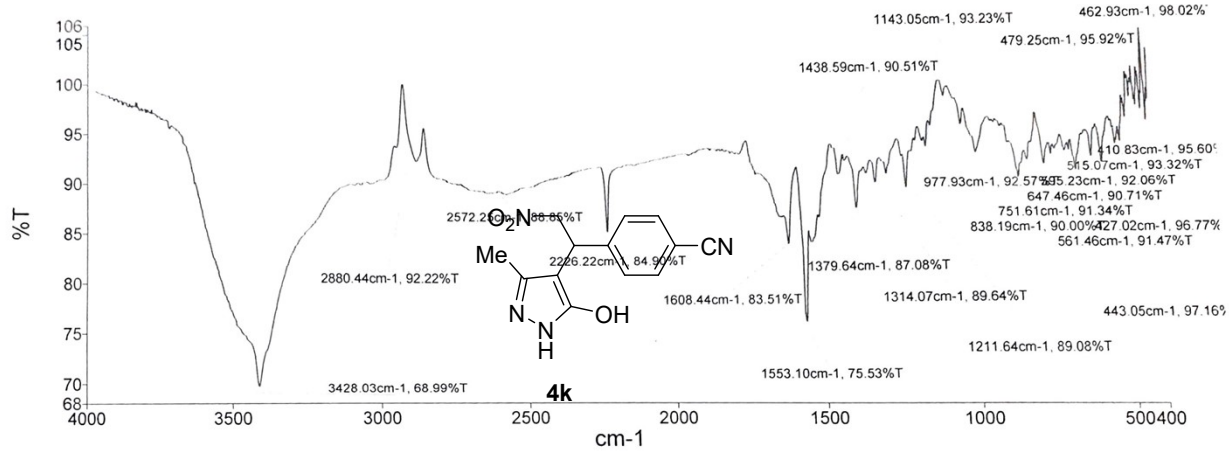

%T
cm-1
823.37cm-1, 91.11%T
410.92cm-1, 99
1378.32cm-1, 91.67%T
2572.63cm-1, 94.09%T
1153.12cm-1, 93.66%T
1220.75cm-1, 92.18%T
1011.35cm-1, 92.73%T
650.67cm-1, 90.5
1637.80cm-1, 88.88%T
1550.95cm-1, 87.84%T
1074.41cm-1, 94.03%T
515.13cm-1, 91.29%T
1489.31cm-1, 90.31%T
734.47cm-1, 90.80%T
1520.18cm-1, 89.19%T
3434.00cm-1, 76.89%T
4f

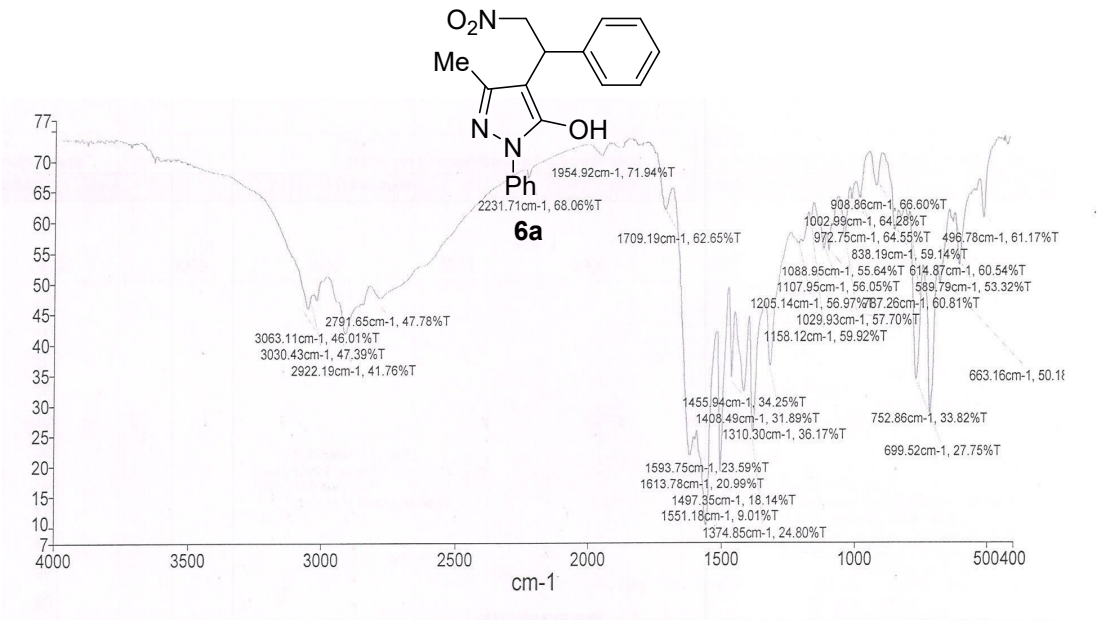

%T
cm-1
894.65cm-1, 57.19%T
423.24cm
445.39cm
411.01cm
567.14cm-1,
1080.08cm-1, 52.21%T
1314.48cm-1, 53.08%T
1377.55cm-1, 48.68%T
609.86cm-1,
709.29cm-1, 57.81%T
595.88cm-1,
1434.69cm-1, 49.58%T
1715.98cm-1, 53.78%T
1248.90cm-1, 53.96%T
731.68cm-1, 54.53%T
666.51cm-1, 56.14%T
1147.32cm-1, 54.86%T
640.37cm-1, 57.99%T
909.65cm-1, 57.40%T
1495.28cm-1, 48.15%T
857.20cm-1, 57.43%T
969.42cm-1, 46.70%T
538.16cm-1, 60.36%T
804.38cm-1, 58.42%T
523.09cm-1, 60.49%T
1547.57cm-1, 45.22%T
1468.04cm-1, 45.76%T
1189.60cm-1, 48.94%T
1223.50cm-1, 52.28%T
1275.65cm-1, 53.26%T
1162.10cm-1, 54.89%T
3389.86cm-1, 55.24%T
2956.94cm-1, 43.73%T
2854.07cm-1, 42.19%T
2924.93cm-1, 36.11%T
4g

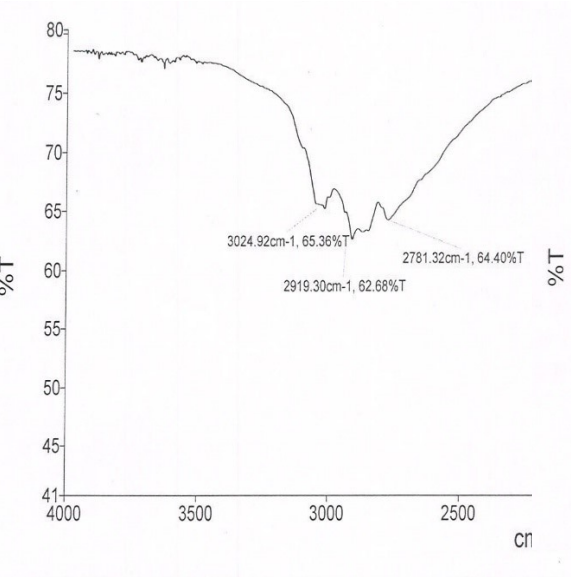

%T
cm-1
1258.41cm-1, 84.29%T
1353.12cm-1, 77.51%T
1737.07cm-1, 82.32%T
1455.53cm-1, 75.47%T
1496.48cm-1, 75.10%T
1428.83cm-1, 68.92%T
1608.48cm-1, 68.19%T
1377.49cm-1, 62.75%T
1530.47cm-1, 58.20%T
1551.47cm-1, 42.30%T
1227.14cm-1, 77.03%T
2930.17cm-1, 77.08%T
2576.54cm-1, 73.50%T
3386.94cm-1, 59.13%T
4h


%T
cm-1
3648.84cm-1, 82.88%T
3396.27cm-1, 73.14%T
2853.76cm-1, 74.13%T
2924.82cm-1, 70.29%T
1716.11cm-1, 79.63%T
1605.82cm-1, 69.75%T
1514.95cm-1, 60.65%T
1552.57cm-1, 49.92%T
1428.98cm-1, 74.58%T
1377.25cm-1, 67.86%T
1348.63cm-1, 63.97%T
1080.19cm-1, 83.43%T
1159.82cm-1, 82.11%T
1111.26cm-1, 85.09%T
1210.51cm-1, 77.28%T
969.53cm-1, 75.18%T
728.07cm-1, 75.89%T
858.57cm-1, 76.14%T
741.91cm-1, 77.48%T
781.64cm-1, 77.70%T
645.75cm-1, 78.20%T
667.33cm-1, 80.20%T
594.68cm-1, 81.04%T
410.83cm-1, 87.68%T
462.87cm-1, 86.47%T
443.11cm-1, 84.77%T
479.66cm-1, 82.93%T
498.93cm-1, 80.10%T
427.14cm-1, 87.23%T
O2N
NO2
Me
OH
N
H
4i


%T
cm-1
3406.41cm-1, 60.95%T
2924.28cm-1, 76.07%T
1709.51cm-1, 80.69%T
1603.50cm-1, 72.27%T
1550.12cm-1, 59.33%T
1377.86cm-1, 70.80%T
1454.74cm-1, 76.84%T
1426.75cm-1, 76.42%T
1275.15cm-1, 81.42%T
1210.94cm-1, 79.56%T
1149.92cm-1, 79.32%T
1091.16cm-1, 84.14%T
970.13cm-1, 81.15%T
801.97cm-1, 80.88%T
728.29cm-1, 79.16%T
601.76cm-1, 79.19%T
743.18cm-1, 77.08%T
515.11cm-1, 81.26%T
702.49cm-1, 74.26%T
O2N
Me
OH
N
H
4j


%T
cm-1
3428.03cm-1, 68.99%T
2880.44cm-1, 92.22%T
2226.22cm-1, 84.90%T
1608.44cm-1, 83.51%T
1553.10cm-1, 75.53%T
1379.64cm-1, 87.08%T
1314.07cm-1, 89.64%T
1211.64cm-1, 89.08%T
1143.05cm-1, 93.23%T
1438.59cm-1, 90.51%T
977.93cm-1, 92.57%T
751.61cm-1, 91.34%T
838.19cm-1, 90.00%T
561.46cm-1, 91.47%T
647.46cm-1, 90.71%T
515.07cm-1, 93.32%T
479.25cm-1, 95.92%T
462.93cm-1, 98.02%T
443.05cm-1, 97.16%T
O2N
Me
CN
OH
N
H
4k


O2N
Me
N
N
Ph
OH
6a
2231.71cm-1, 68.06%T
1954.92cm-1, 71.94%T
1709.19cm-1, 62.65%T
908.86cm-1, 66.60%T
1002.99cm-1, 64.28%T
972.75cm-1, 64.55%T
838.19cm-1, 59.14%T
496.78cm-1, 61.17%T
1088.95cm-1, 55.64%T
614.87cm-1, 60.54%T
1107.95cm-1, 56.05%T
589.79cm-1, 53.32%T
1205.14cm-1, 56.97%T
787.26cm-1, 60.81%T
1029.93cm-1, 57.70%T
1158.12cm-1, 59.92%T
663.16cm-1, 50.18
2791.65cm-1, 47.78%T
3063.11cm-1, 46.01%T
3030.43cm-1, 47.39%T
2922.19cm-1, 41.76%T
1455.94cm-1, 34.25%T
1408.49cm-1, 31.89%T
1310.30cm-1, 36.17%T
752.86cm-1, 33.82%T
699.52cm-1, 27.75%T
1593.75cm-1, 23.59%T
1613.78cm-1, 20.99%T
1497.35cm-1, 18.14%T
1551.18cm-1, 9.01%T
1374.85cm-1, 24.80%T
77
70
65
60
55
50
45
40
35
30
25
20
15
10
7
4000
3500
3000
2500
2000
1500
1000
500400
cm-1


%T
3024.92cm-1, 65.36%T
2919.30cm-1, 62.68%T
2781.32cm-1, 64.40%T
cm

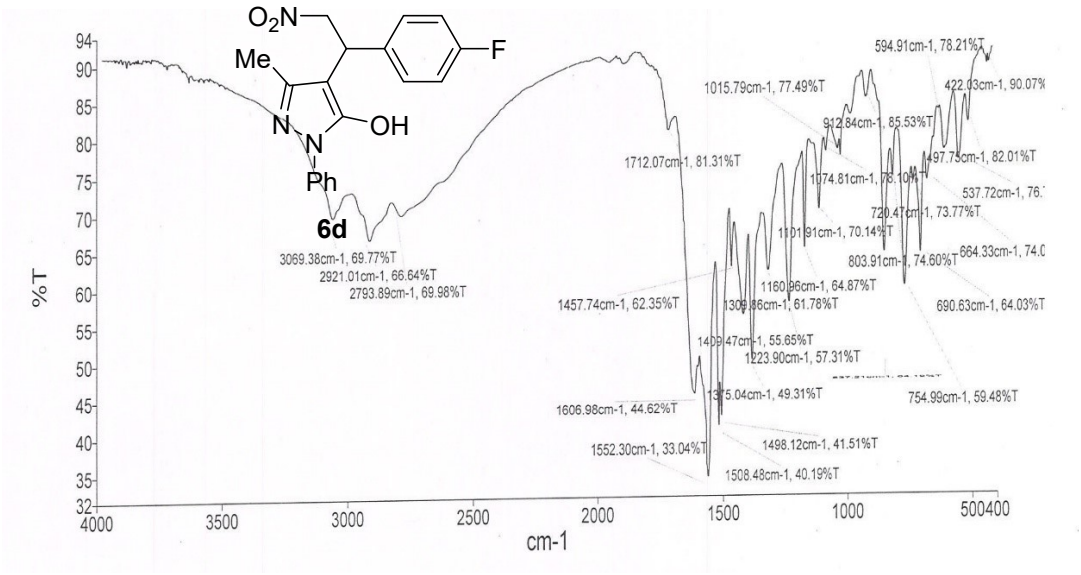
O2N
Me
Me
N
N
OH
Ph

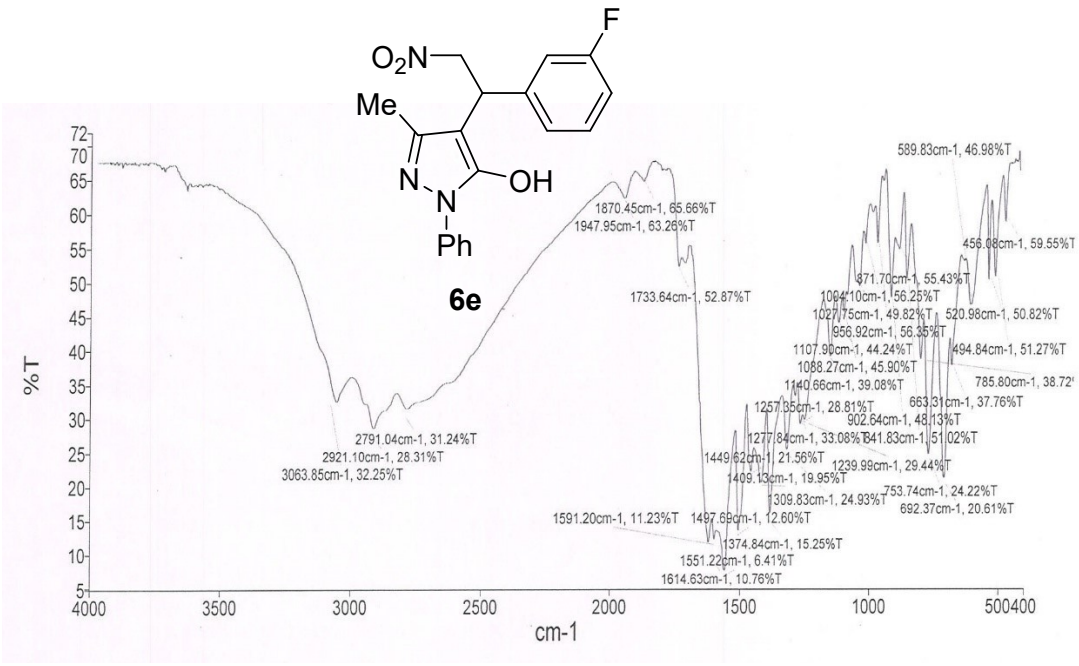
6b

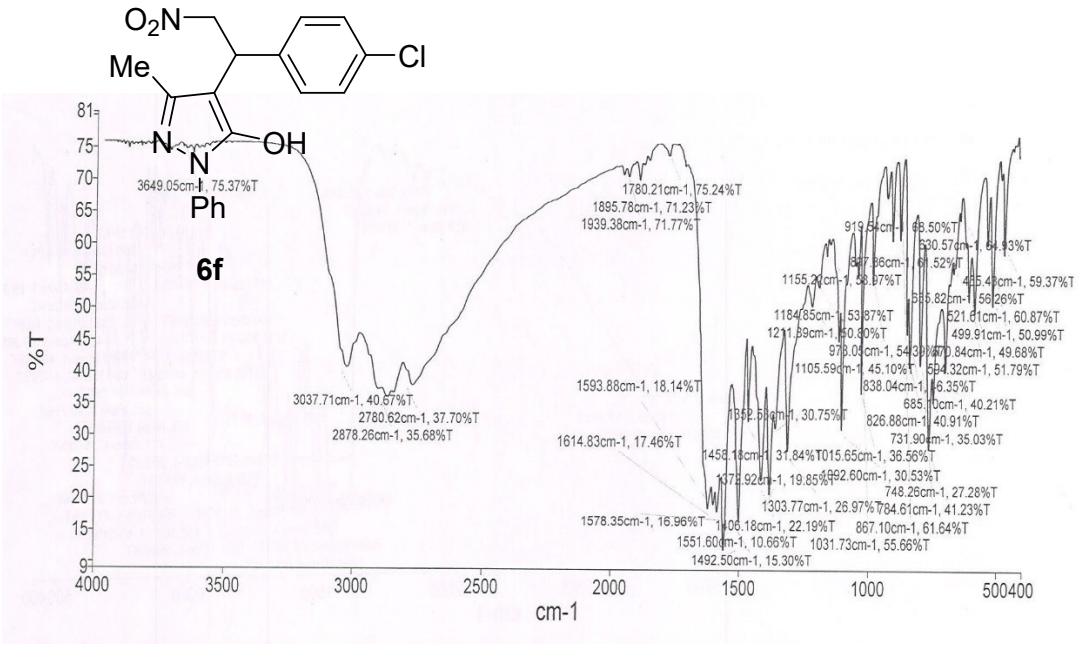
%T
3063.77cm-1, 53.10%T
2924.00cm-1, 44.56%T
1712.83cm-1, 61.62%T
910.20cm-1, 70.31%T
786.09cm-1, 62.87%T
974.20cm-1, 64.44%T
1075.08cm-1, 60.46%T
1112.83cm-1, 52.97%T
832.02cm-1, 51.38%T
690.27cm-1, 48.41%T
1030.63cm-1, 44.52%T
754.26cm-1, 44.55%T
1457.42cm-1, 41.10%T
1178.70cm-1, 41.26%T
1248.49cm-1, 34.36%T
1374.40cm-1, 35.44%T
1550.80cm-1, 21.97%T
1512.40cm-1, 25.72%T
cm-1

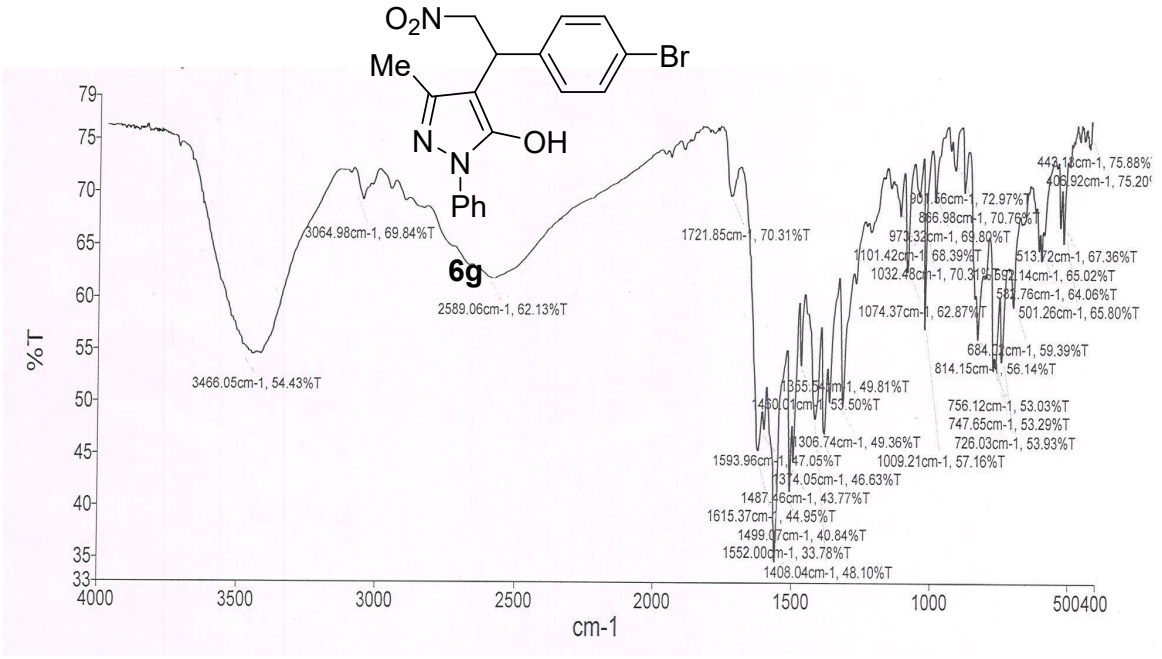
O2N
Me
OMe
N
N
OH
Ph

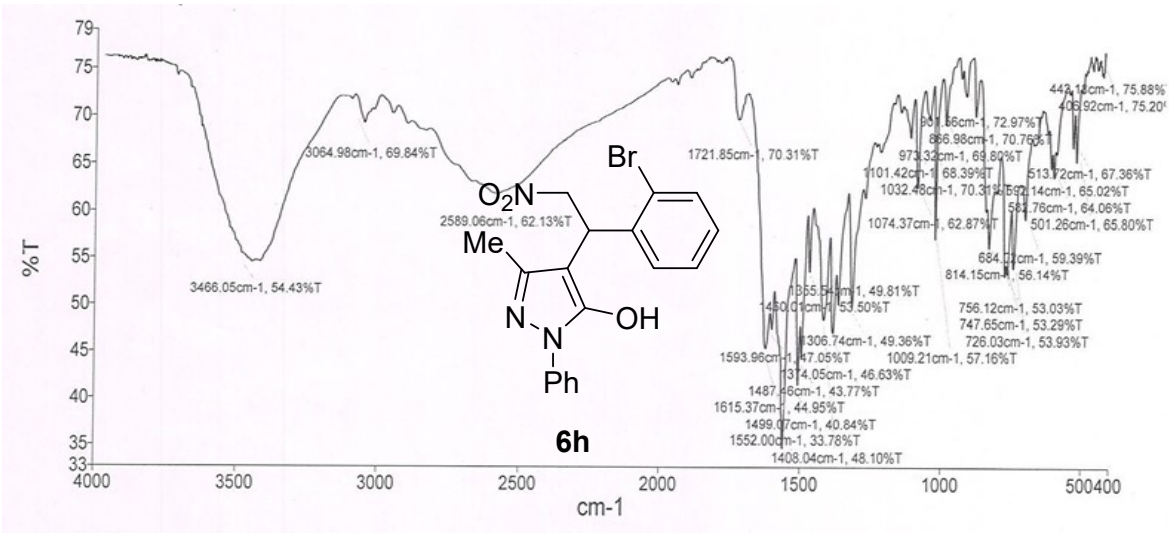
6c

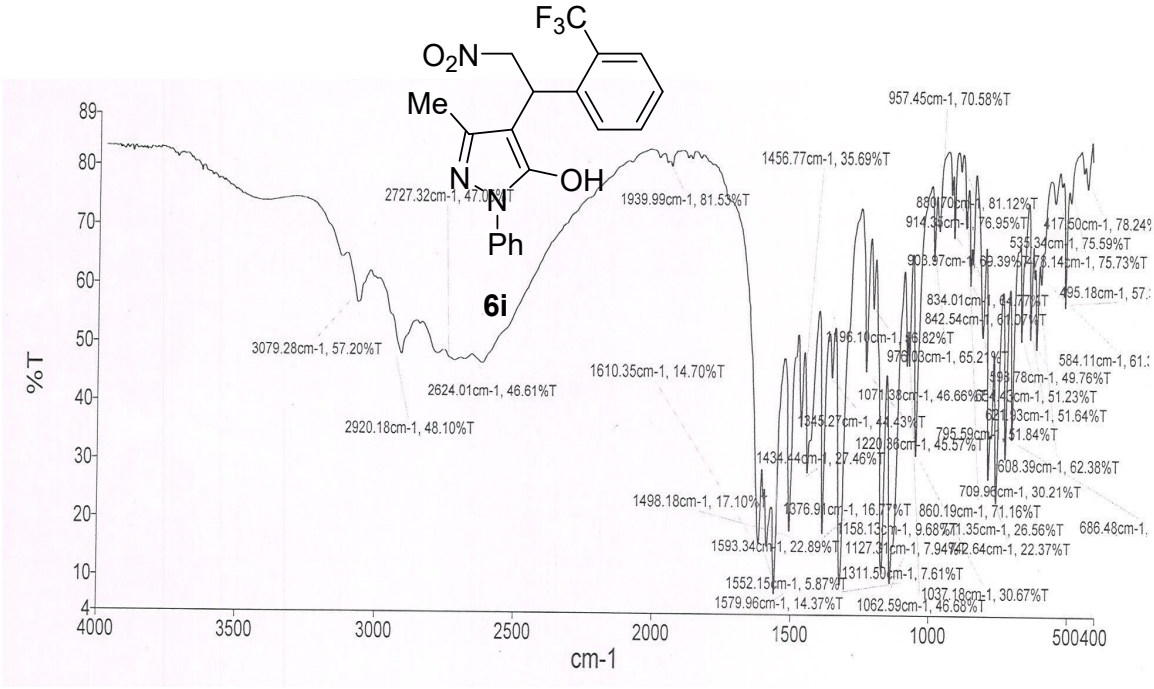

O2N
Me
F
N
N
OH
Ph
6d
%T
cm-1
3069.38cm-1, 69.77%T
2921.01cm-1, 66.64%T
2793.89cm-1, 69.98%T
1712.07cm-1, 81.31%T
1606.98cm-1, 44.62%T
1552.30cm-1, 33.04%T
1508.48cm-1, 40.19%T
1498.12cm-1, 41.51%T
1457.74cm-1, 62.35%T
1375.04cm-1, 49.31%T
1223.90cm-1, 57.31%T
1160.96cm-1, 64.87%T
1101.91cm-1, 70.14%T
1074.81cm-1, 78.10%T
1015.79cm-1, 77.49%T
912.84cm-1, 85.53%T
803.91cm-1, 74.60%T
754.99cm-1, 59.48%T
690.63cm-1, 64.03%T
664.33cm-1, 74.0
594.91cm-1, 78.21%T
422.03cm-1, 90.07%

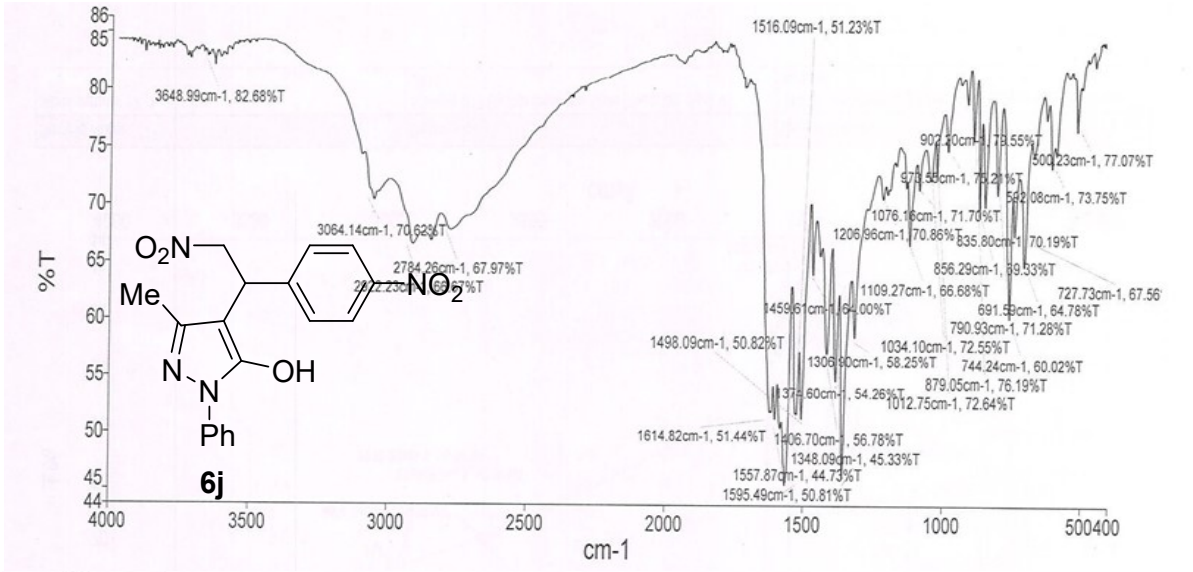

F
O2N
Me
N
N
OH
Ph
6e
%T
cm-1
4000
3500
3000
2500
2000
1500
1000
500400
3063.85cm-1, 32.25%T
2921.10cm-1, 28.31%T
2791.04cm-1, 31.24%T
1870.45cm-1, 65.66%T
1947.95cm-1, 63.26%T
1733.64cm-1, 52.87%T
1591.20cm-1, 11.23%T
1614.63cm-1, 10.76%T
1551.22cm-1, 6.41%T
1497.69cm-1, 12.60%T
1449.62cm-1, 21.56%T
1409.13cm-1, 19.95%T
1374.84cm-1, 15.25%T
1309.83cm-1, 24.93%T
1277.84cm-1, 33.08%T
1257.35cm-1, 28.81%T
1239.99cm-1, 29.44%T
1140.66cm-1, 39.08%T
1088.27cm-1, 45.90%T
1107.90cm-1, 44.24%T
1027.75cm-1, 49.82%T
1004.10cm-1, 56.25%T
956.92cm-1, 56.35%T
902.64cm-1, 48.13%T
871.70cm-1, 55.43%T
841.83cm-1, 51.02%T
753.74cm-1, 24.22%T
692.37cm-1, 20.61%T
663.31cm-1, 37.76%T
589.83cm-1, 46.98%T
520.98cm-1, 50.82%T
494.84cm-1, 51.27%T
456.08cm-1, 59.55%T
785.80cm-1, 38.72%T

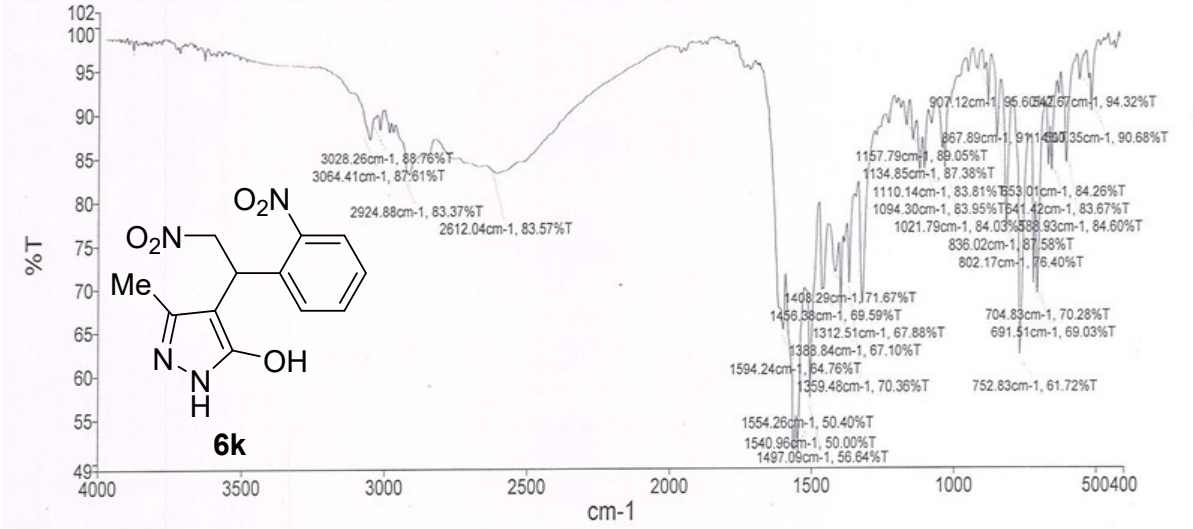

O2N
Me
Cl
N
N
OH
Ph
6f
%T
cm-1
3649.05cm-1, 75.37%T
3037.71cm-1, 40.67%T
2780.62cm-1, 37.70%T
2878.26cm-1, 35.68%T
1780.21cm-1, 75.24%T
1895.78cm-1, 71.23%T
1939.38cm-1, 71.77%T
1593.88cm-1, 18.14%T
1614.83cm-1, 17.46%T
1578.35cm-1, 16.96%T
1551.60cm-1, 10.66%T
1492.50cm-1, 15.30%T
1406.18cm-1, 22.19%T
1303.77cm-1, 26.97%T
1031.73cm-1, 55.66%T
867.10cm-1, 61.64%T
784.61cm-1, 41.23%T
748.26cm-1, 27.28%T
731.90cm-1, 35.03%T
826.88cm-1, 40.91%T
685.10cm-1, 40.21%T
838.04cm-1, 46.35%T
1105.59cm-1, 45.10%T
1211.89cm-1, 50.60%T
1184.85cm-1, 53.87%T
1155.20cm-1, 58.97%T
919.54cm-1, 68.50%T
530.57cm-1, 64.93%T
455.43cm-1, 59.37%T
521.61cm-1, 60.87%T
499.91cm-1, 50.99%T
670.84cm-1, 49.68%T
594.32cm-1, 51.79%T
1458.13cm-1, 31.84%T
1373.92cm-1, 19.85%T
1015.65cm-1, 36.56%T
892.60cm-1, 30.53%T

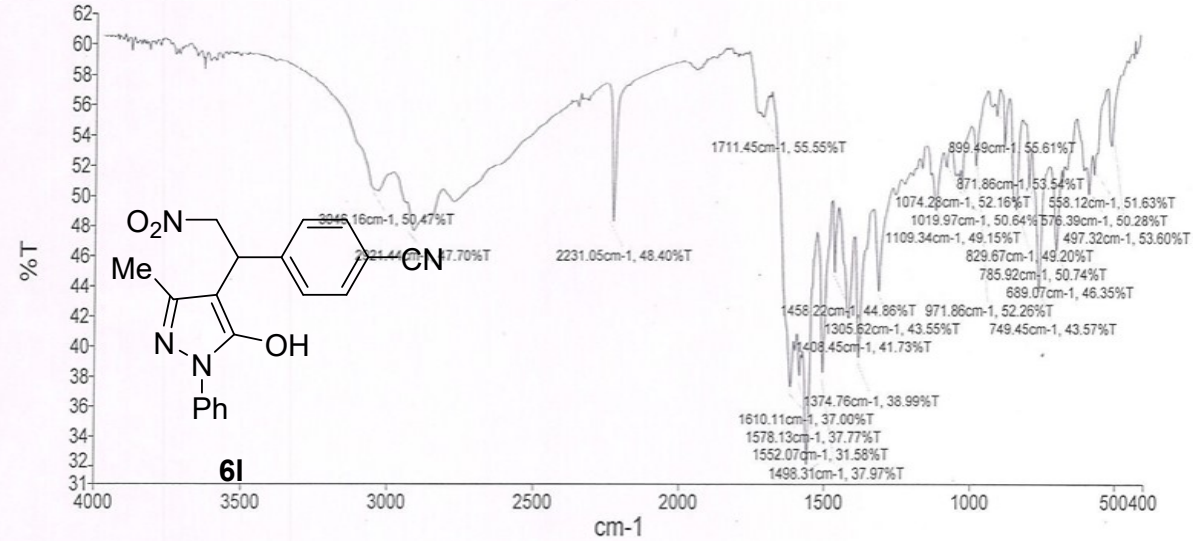

O2N
Me
Br
N
N
OH
Ph
6g
%T
cm-1
3466.05cm-1, 54.43%T
3064.98cm-1, 69.84%T
2589.06cm-1, 62.13%T
1721.85cm-1, 70.31%T
1593.96cm-1, 47.05%T
1615.37cm-1, 44.95%T
1499.07cm-1, 40.84%T
1552.00cm-1, 33.78%T
1408.04cm-1, 48.10%T
1487.46cm-1, 43.77%T
1374.05cm-1, 46.63%T
1306.74cm-1, 49.36%T
1009.21cm-1, 57.16%T
1074.37cm-1, 62.87%T
1032.48cm-1, 70.31%T
1101.42cm-1, 68.39%T
973.32cm-1, 69.80%T
866.98cm-1, 70.76%T
814.15cm-1, 56.14%T
756.12cm-1, 53.03%T
747.65cm-1, 53.29%T
726.03cm-1, 53.93%T
513.72cm-1, 67.36%T
501.26cm-1, 65.80%T

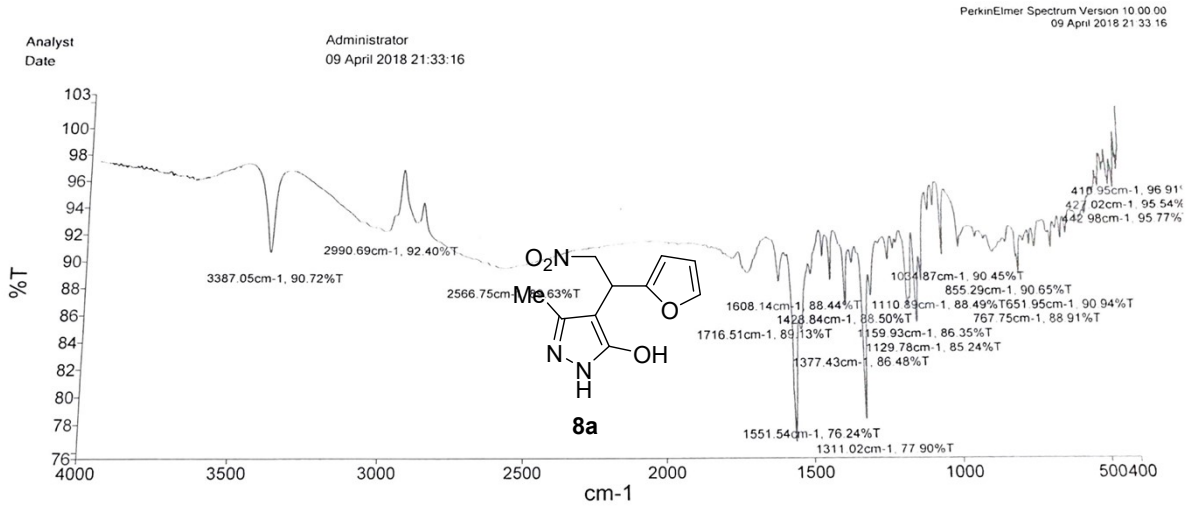

O2N
Me
Br
N
N
OH
Ph
6h
%T
cm-1
3466.05cm-1, 54.43%T
3064.98cm-1, 69.84%T
2589.06cm-1, 62.13%T
1721.85cm-1, 70.31%T
1593.96cm-1, 47.05%T
1615.37cm-1, 44.95%T
1499.07cm-1, 40.84%T
1552.00cm-1, 33.78%T
1408.04cm-1, 48.10%T
1487.46cm-1, 43.77%T
1374.05cm-1, 46.63%T
1306.74cm-1, 49.36%T
1009.21cm-1, 57.16%T
1074.37cm-1, 62.87%T
1032.48cm-1, 70.31%T
1101.42cm-1, 68.39%T
973.32cm-1, 69.80%T
866.98cm-1, 70.76%T
814.15cm-1, 56.14%T
756.12cm-1, 53.03%T
747.65cm-1, 53.29%T
726.03cm-1, 53.93%T
513.72cm-1, 67.36%T
501.26cm-1, 65.80%T


F3C
O2N
Me
N
OH
N
Ph
6i
%T
cm-1
957.45cm-1, 70.58%T
1456.77cm-1, 35.69%T
2727.32cm-1, 47.00%T
1939.99cm-1, 81.53%T
3079.28cm-1, 57.20%T
2624.01cm-1, 46.61%T
2920.18cm-1, 48.10%T
1610.35cm-1, 14.70%T
1498.18cm-1, 17.10%T
1593.34cm-1, 22.89%T
1552.15cm-1, 5.87%T
1579.96cm-1, 14.37%T
1062.59cm-1, 46.68%T
1311.50cm-1, 7.61%T
1127.31cm-1, 7.94%T
1376.91cm-1, 16.77%T
1434.44cm-1, 27.46%T
1345.27cm-1, 44.43%T
1220.86cm-1, 45.57%T
1158.13cm-1, 9.68%T
1071.38cm-1, 46.66%T
976.03cm-1, 65.21%T
842.54cm-1, 61.07%T
834.01cm-1, 64.77%T
709.96cm-1, 30.21%T
608.39cm-1, 62.38%T
584.11cm-1, 61.
535.34cm-1, 75.59%T
495.18cm-1, 57.
417.50cm-1, 78.24%
686.48cm-1,

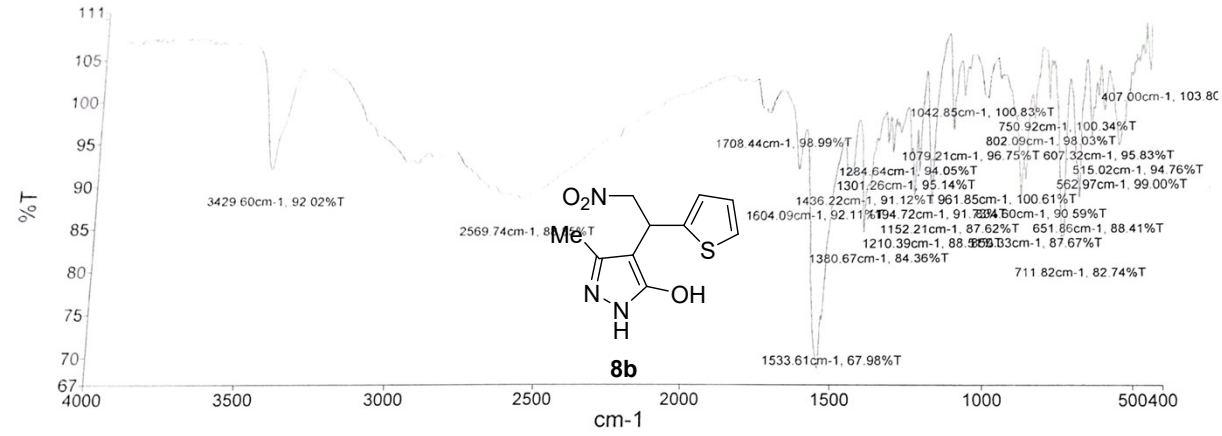

%T
cm-1
3648.99cm-1, 82.68%T
3064.14cm-1, 70.62%T
2784.26cm-1, 67.97%T
1516.09cm-1, 51.23%T
1498.09cm-1, 50.82%T
1614.82cm-1, 51.44%T
1406.70cm-1, 56.78%T
1348.09cm-1, 45.33%T
1557.87cm-1, 44.73%T
1595.49cm-1, 50.81%T
1459.61cm-1, 54.00%T
1306.80cm-1, 58.25%T
1034.10cm-1, 72.55%T
1109.27cm-1, 66.68%T
1206.96cm-1, 70.86%T
1076.16cm-1, 71.70%T
856.29cm-1, 69.33%T
835.80cm-1, 70.19%T
727.73cm-1, 67.56
691.53cm-1, 64.78%T
790.93cm-1, 71.28%T
744.24cm-1, 60.02%T
879.05cm-1, 76.19%T
1012.75cm-1, 72.64%T
Me
OH
Ph
6j

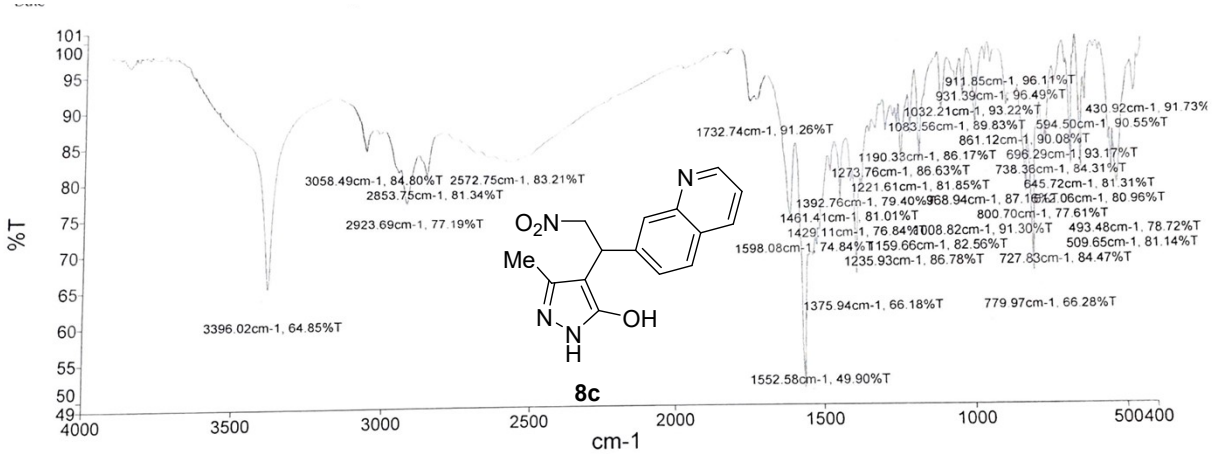

%T
cm-1
3028.26cm-1, 88.76%T
3064.41cm-1, 87.61%T
2924.88cm-1, 83.37%T
2612.04cm-1, 83.57%T
1554.26cm-1, 50.40%T
1540.96cm-1, 50.00%T
1497.09cm-1, 56.64%T
1408.29cm-1, 71.67%T
1456.38cm-1, 69.59%T
1312.51cm-1, 67.88%T
1388.84cm-1, 67.10%T
1594.24cm-1, 64.76%T
1359.48cm-1, 70.36%T
907.12cm-1, 95.60%T
867.89cm-1, 91.14%T
842.67cm-1, 94.32%T
1157.79cm-1, 89.05%T
1134.85cm-1, 87.38%T
1110.14cm-1, 83.81%T
1094.30cm-1, 83.95%T
1021.79cm-1, 84.03%T
836.02cm-1, 87.58%T
802.17cm-1, 76.40%T
753.01cm-1, 84.26%T
741.42cm-1, 83.67%T
588.93cm-1, 84.60%T
704.83cm-1, 70.28%T
691.51cm-1, 69.03%T
752.83cm-1, 61.72%T
Me
OH
6k

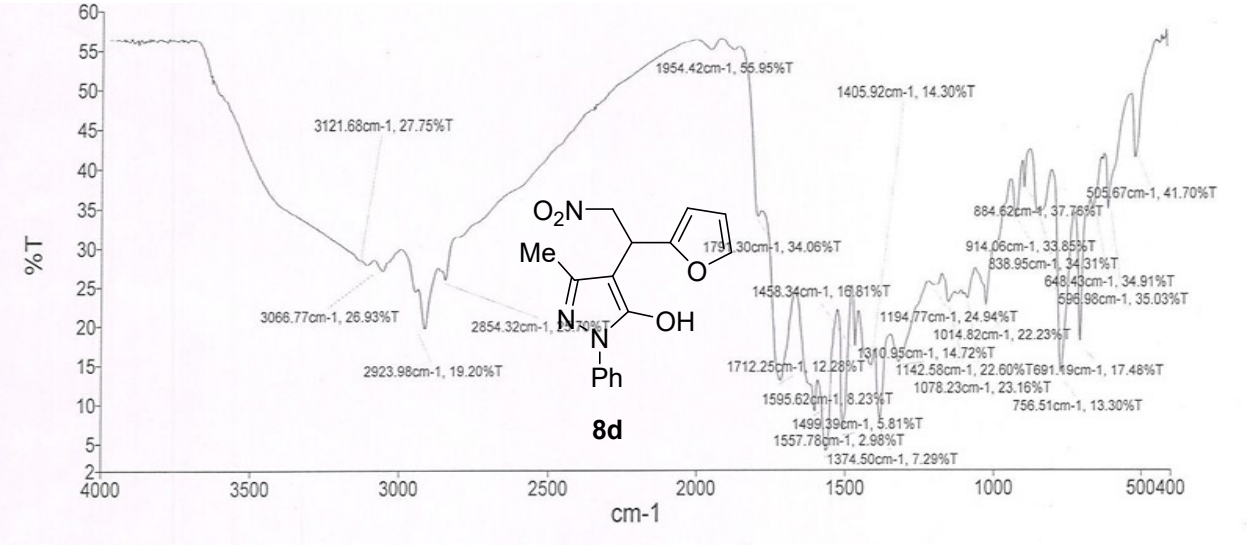

%T
cm-1
3015.16cm-1, 50.47%T
2231.05cm-1, 48.40%T
1711.45cm-1, 55.55%T
1610.11cm-1, 37.00%T
1578.13cm-1, 37.77%T
1552.07cm-1, 31.58%T
1498.31cm-1, 37.97%T
1458.22cm-1, 44.86%T
1408.45cm-1, 41.73%T
1374.76cm-1, 38.99%T
1305.62cm-1, 43.55%T
971.86cm-1, 52.26%T
899.49cm-1, 55.61%T
871.86cm-1, 53.54%T
749.45cm-1, 43.57%T
1074.28cm-1, 52.16%T
1019.97cm-1, 50.64%T
1109.34cm-1, 49.15%T
829.67cm-1, 49.20%T
785.92cm-1, 50.74%T
689.07cm-1, 46.35%T
558.12cm-1, 51.63%T
576.39cm-1, 50.28%T
497.32cm-1, 53.60%T
Me
OH
Ph
6l

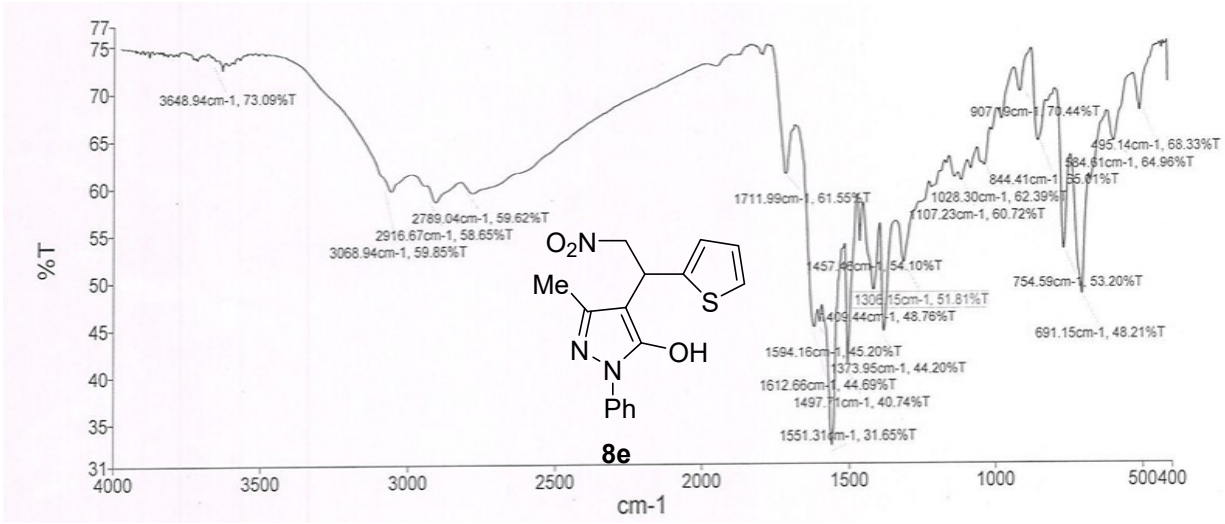


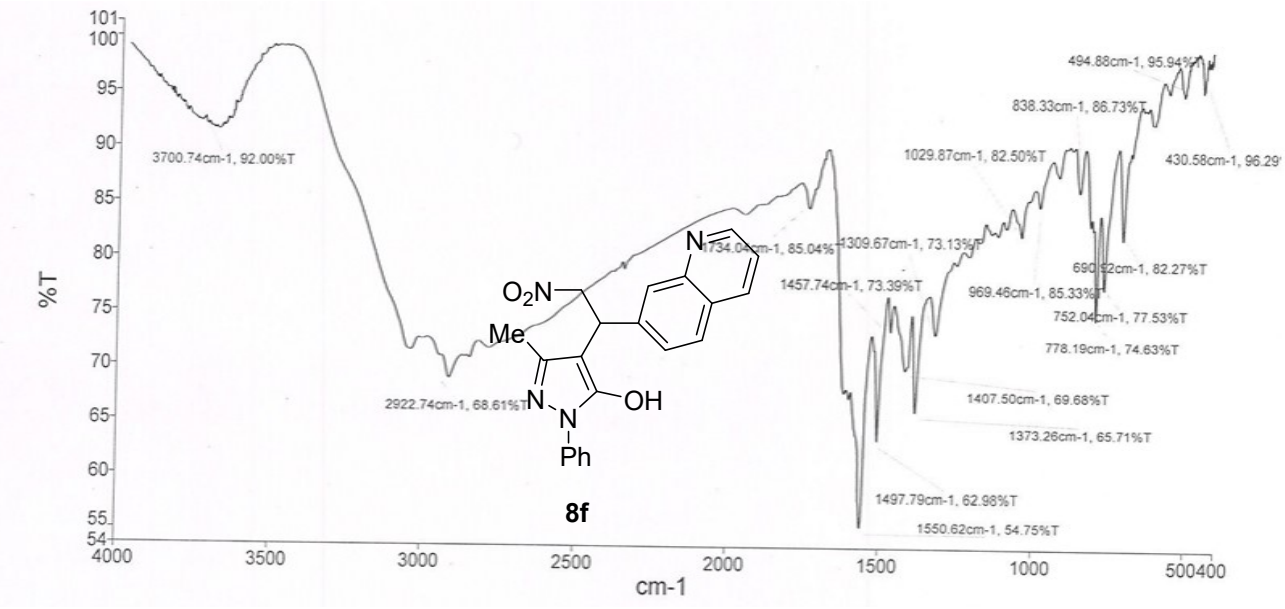
Sample Name	Description	Quality Checks
FURFUIRAL HH_1	Sample 007 By Administrator Date Monday, April 09 2018	The Quality Checks give rise to a Weak Bands warning for the sample.






%T
cm-1
3121.68cm-1, 27.75%T
3066.77cm-1, 26.93%T
2923.98cm-1, 19.20%T
1954.42cm-1, 55.95%T
1405.92cm-1, 14.30%T
1791.30cm-1, 34.06%T
1458.34cm-1, 16.81%T
1712.25cm-1, 12.28%T
1595.62cm-1, 8.23%T
1499.39cm-1, 5.81%T
1557.78cm-1, 2.98%T
1374.50cm-1, 7.29%T
1310.95cm-1, 14.72%T
1194.77cm-1, 24.94%T
1142.58cm-1, 22.60%T
1078.23cm-1, 23.16%T
1014.82cm-1, 22.23%T
914.06cm-1, 33.85%T
884.62cm-1, 37.76%T
838.95cm-1, 34.31%T
756.51cm-1, 13.30%T
691.19cm-1, 17.48%T
648.43cm-1, 34.91%T
596.98cm-1, 35.03%T
505.67cm-1, 41.70%T
O2N
Me
O
N
N
OH
Ph
8d


%T
cm-1
3648.94cm-1, 73.09%T
2789.04cm-1, 59.62%T
2916.67cm-1, 58.65%T
3068.94cm-1, 59.85%T
1711.99cm-1, 61.55%T
1457.96cm-1, 54.10%T
1306.15cm-1, 51.81%T
1409.44cm-1, 48.76%T
1594.16cm-1, 45.20%T
1373.95cm-1, 44.20%T
1612.66cm-1, 44.69%T
1497.71cm-1, 40.74%T
1551.31cm-1, 31.65%T
1107.23cm-1, 60.72%T
1028.30cm-1, 62.39%T
907.19cm-1, 70.44%T
844.41cm-1, 65.01%T
754.59cm-1, 53.20%T
691.15cm-1, 48.21%T
584.61cm-1, 64.96%T
495.14cm-1, 68.33%T
O2N
Me
S
N
N
OH
Ph
8e


%T
cm-1
3700.74cm-1, 92.00%T
2922.74cm-1, 68.61%T
1734.04cm-1, 85.04%T
1457.74cm-1, 73.39%T
1309.67cm-1, 73.13%T
1497.79cm-1, 62.98%T
1550.62cm-1, 54.75%T
1407.50cm-1, 69.68%T
1373.26cm-1, 65.71%T
1029.87cm-1, 82.50%T
969.46cm-1, 85.33%T
838.33cm-1, 86.73%T
778.19cm-1, 74.63%T
752.04cm-1, 77.53%T
690.52cm-1, 82.27%T
494.88cm-1, 95.94%T
430.58cm-1, 96.29
O2N
Me
N
N
OH
Ph
8f