Supporting Information for

Functional Group Transformations in Derivatives of 6-Oxoverdazyl

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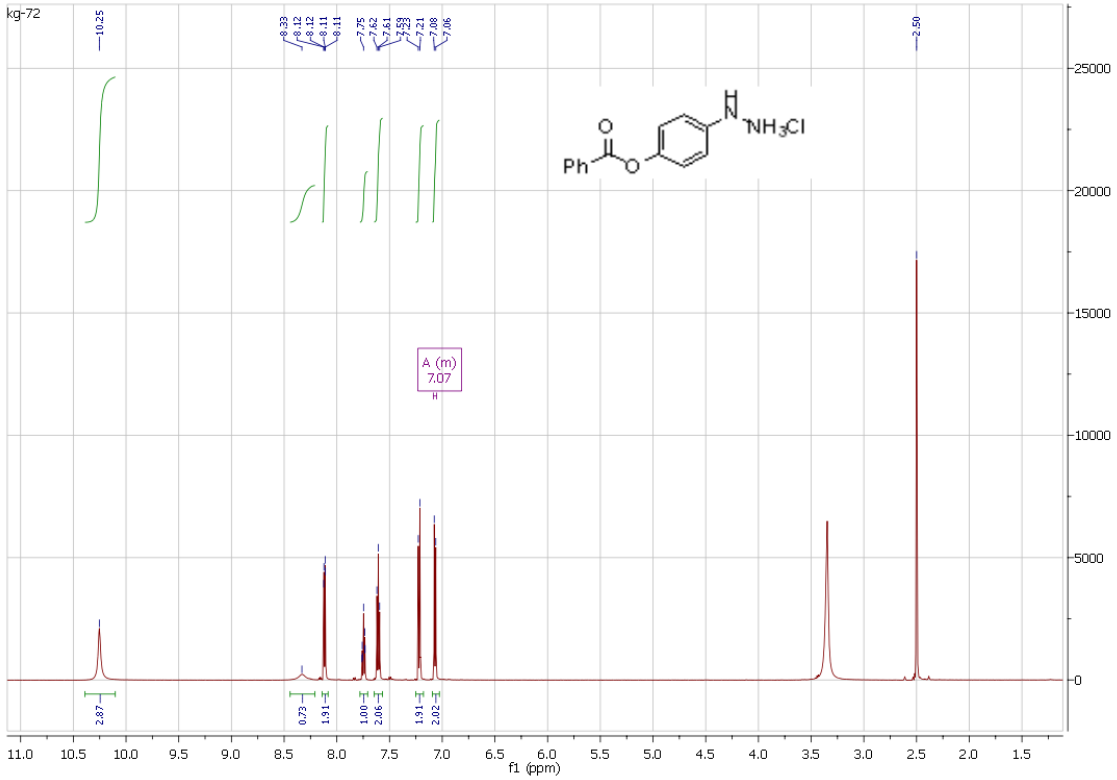
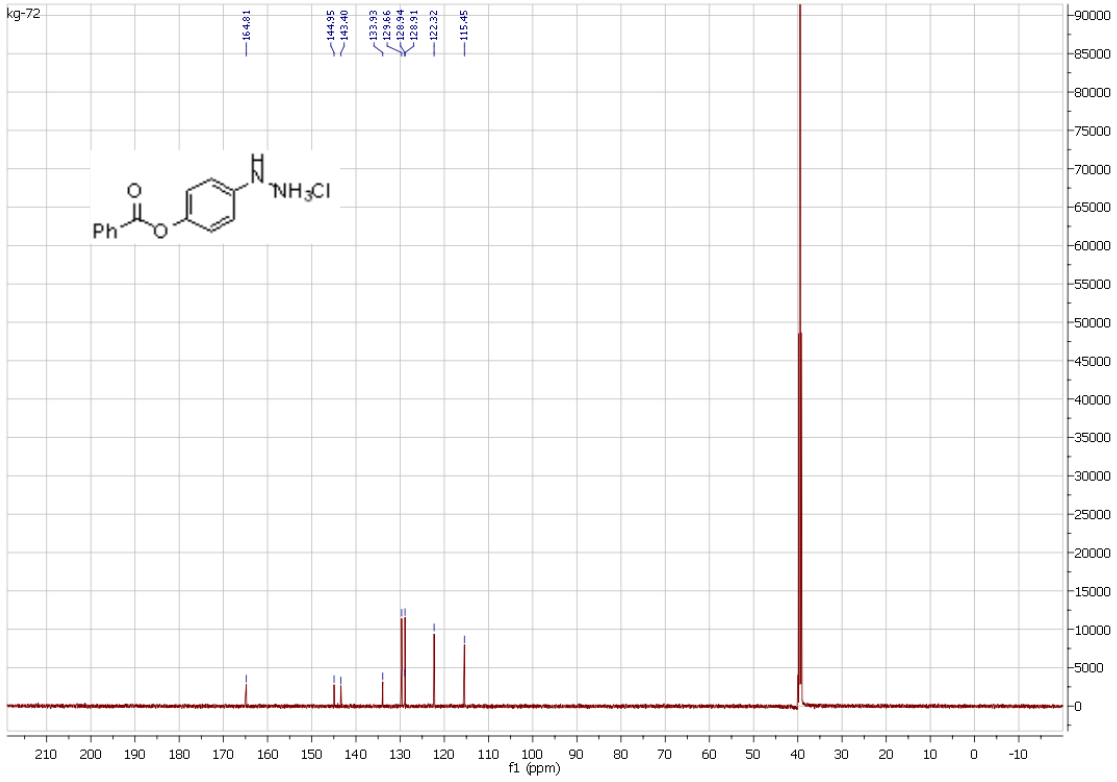
Table of Content:

1. ^{1}H NMR and ^{13}C NMR spectra for selected compounds

2c•HCl





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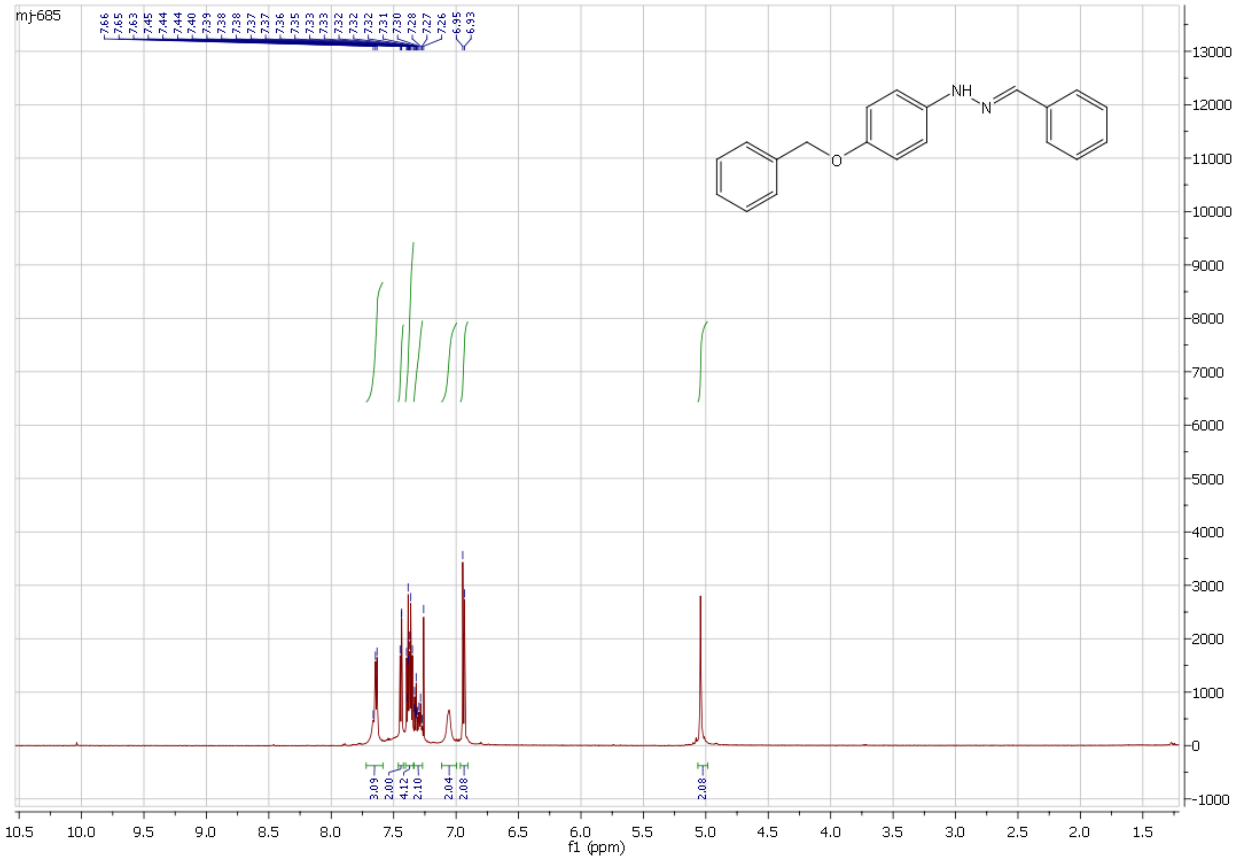
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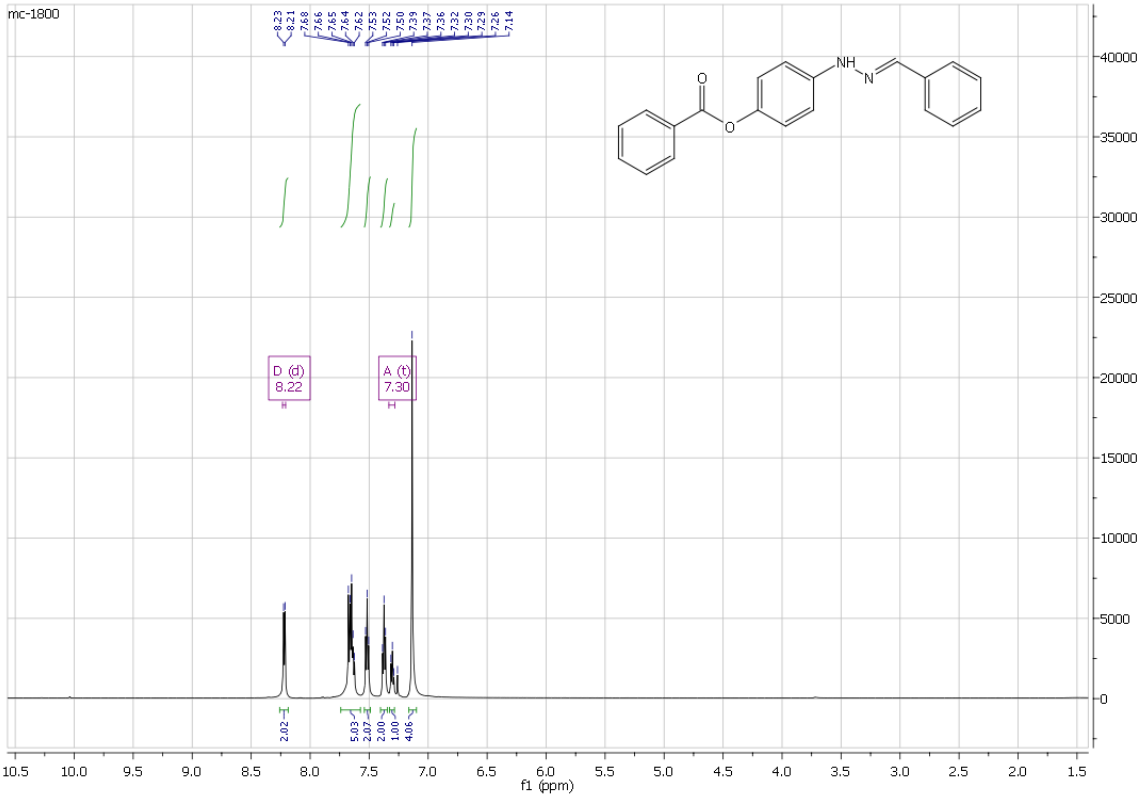
7.37
7.36
7.35
7.33
7.33
7.32
7.32
7.32
7.31
7.30
7.28
7.27
7.26
6.95
6.93
NH
N
O
3.09
2.00
4.12
2.10
2.04
2.08
2.08
f1 (ppm)

3c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7.64
7.62
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7.52
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7.39
7.37
7.36
7.32
7.30
7.29
7.26
7.14
D (d)
8.22
H
A (t)
7.30
H
2.02
5.03
2.07
2.00
1.00
4.06
NH
N
O
O
40000
35000
30000
25000
20000
15000
10000
5000
0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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4.5
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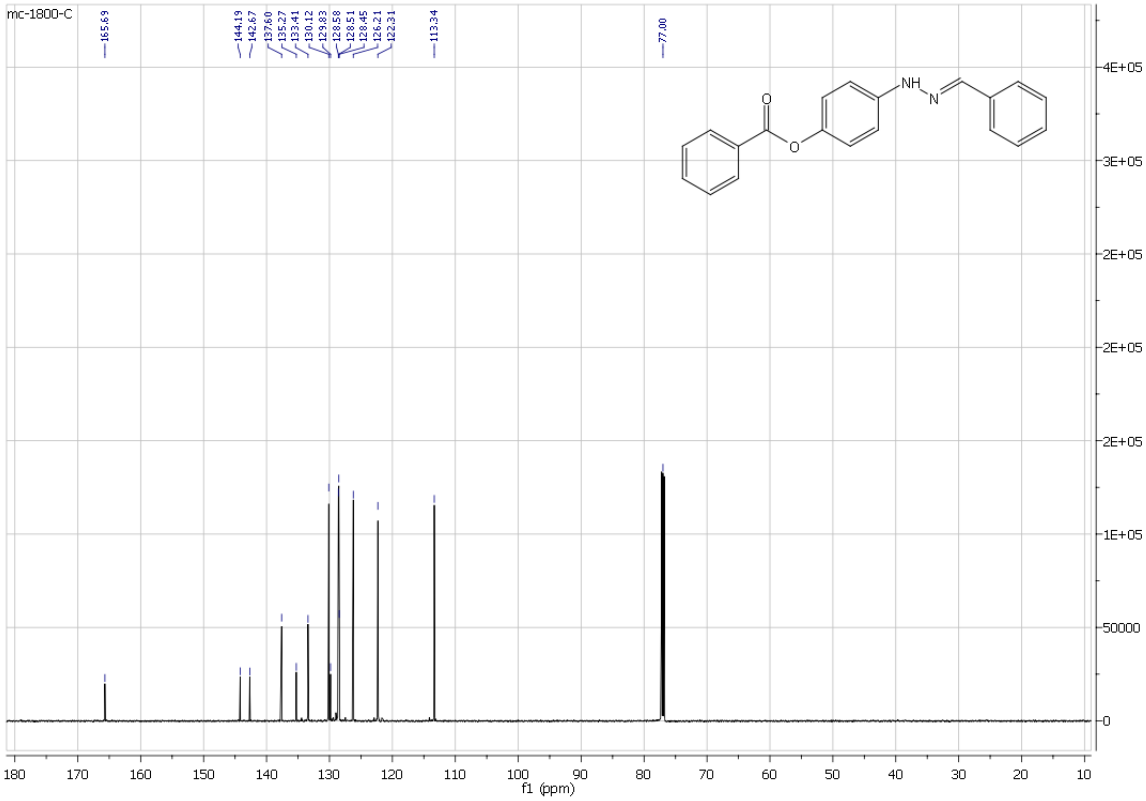
3.0
2.5
2.0
1.5
f1 (ppm)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144.19
142.67
137.60
135.27
133.41
130.12
129.83
128.58
128.51
128.45
126.21
122.31
113.34
77.00
NH
N
O
O
4E+05
3E+05
2E+05
2E+05
2E+05
1E+05
50000
0
180
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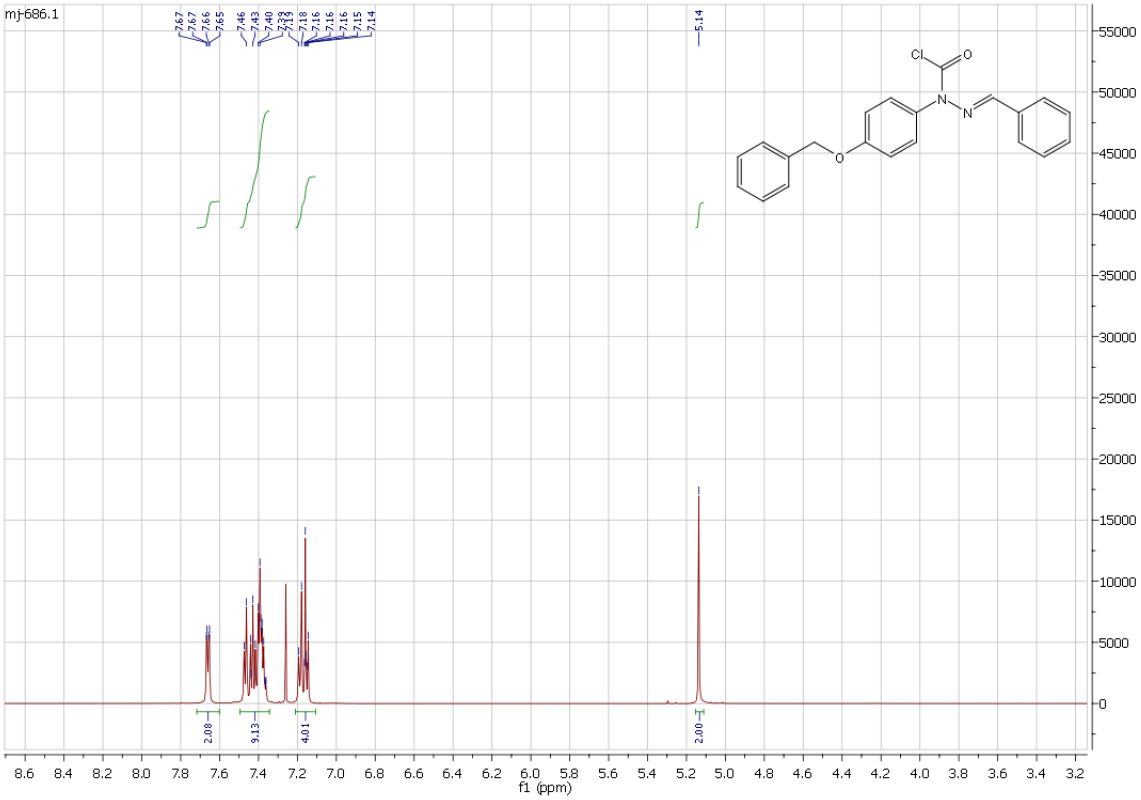
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

4b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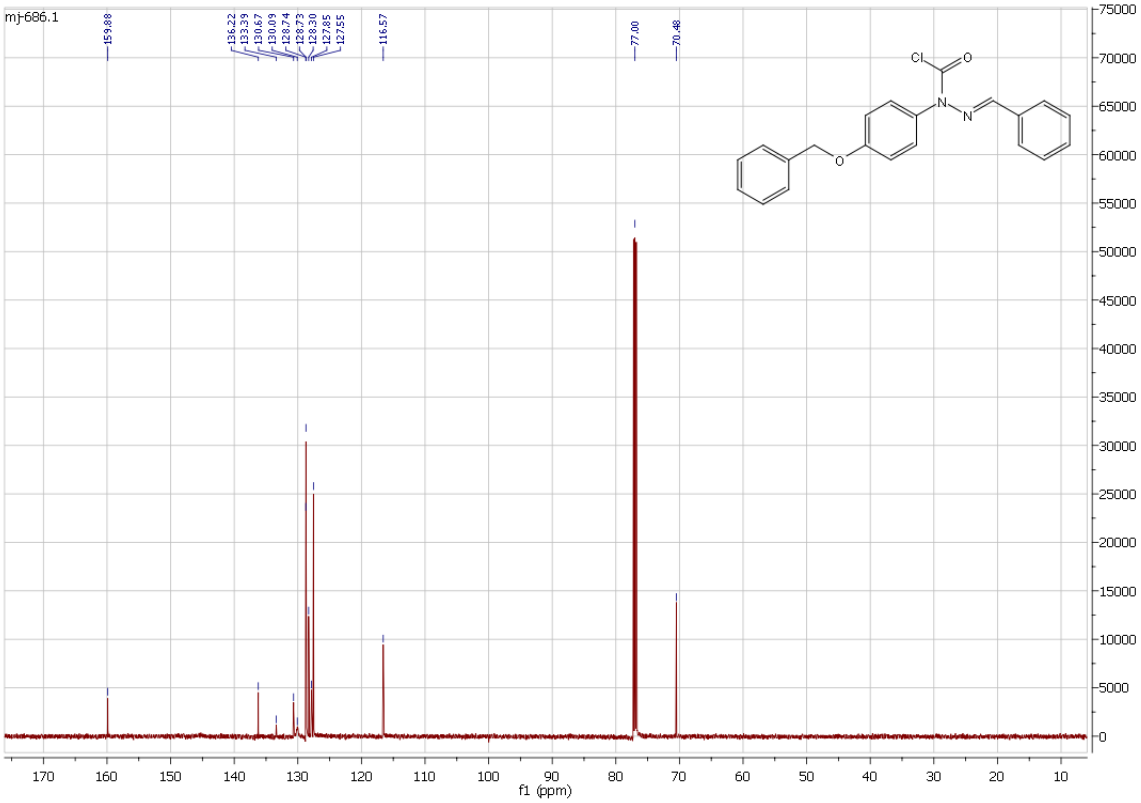
7.16
7.15
7.14
5.14
2.08
9.13
4.01
2.00
f1 (ppm)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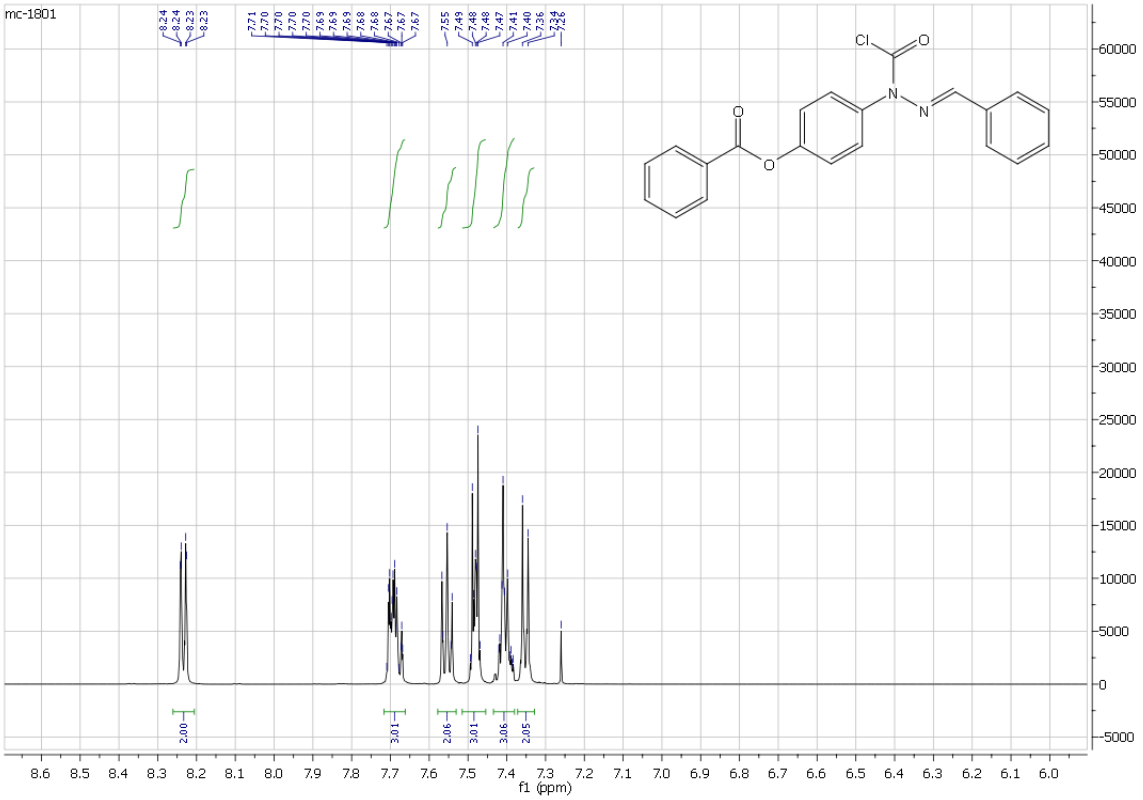
f1 (ppm)

4c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7.70
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7.70
7.69
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7.55
7.49
7.48
7.48
7.47
7.41
7.40
7.36
7.28
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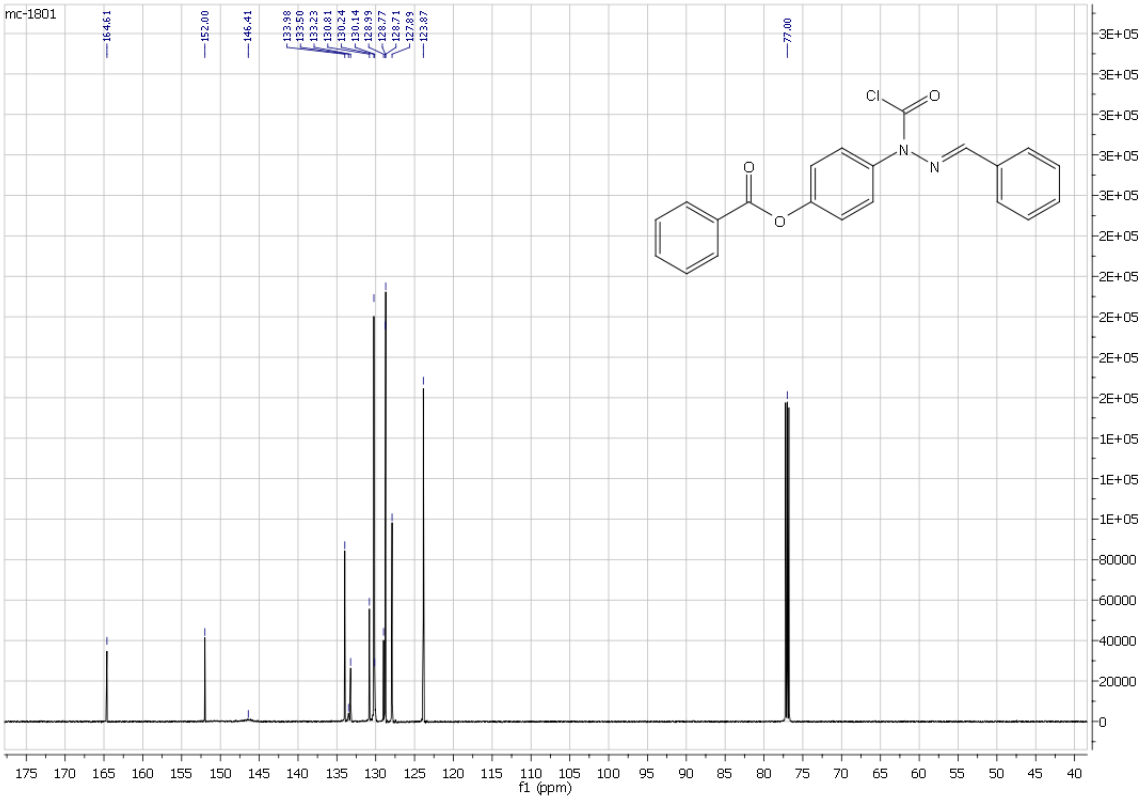
3.01
2.06
3.01
3.06
2.05
Cl
O
N
N
O
O
f1 (ppm)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152.00
146.41
133.98
133.56
133.23
131.61
130.24
130.14
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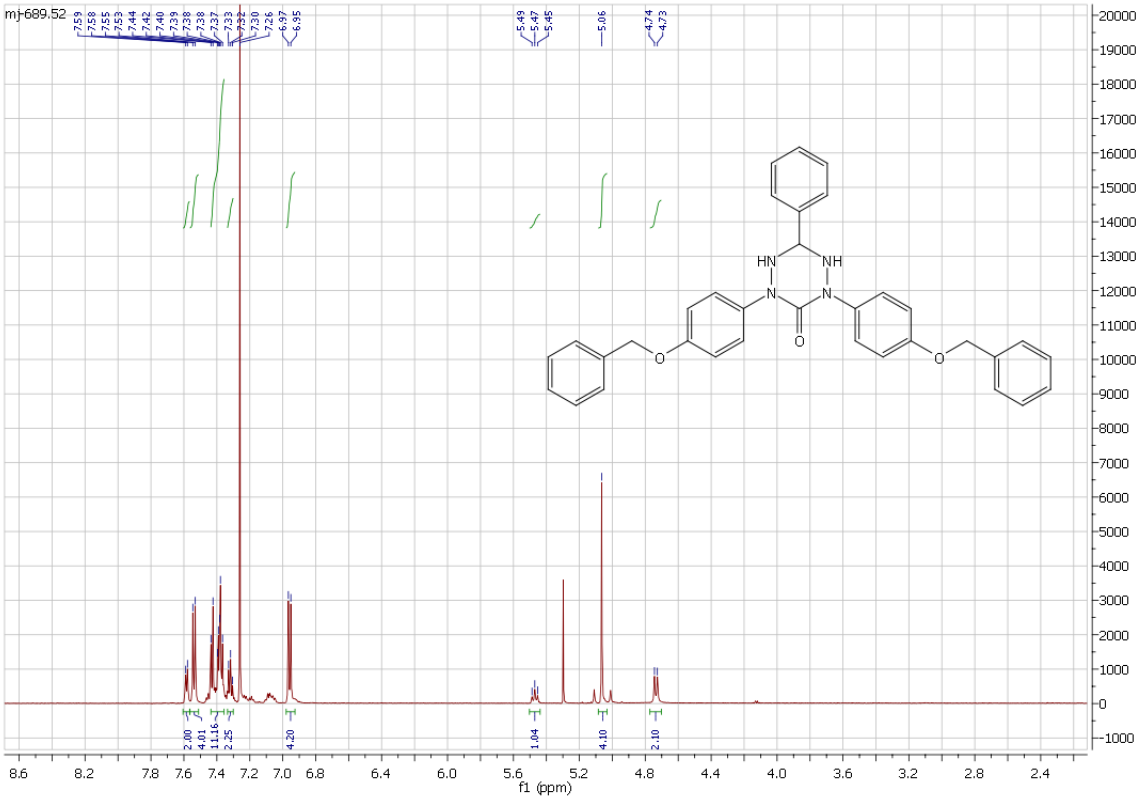
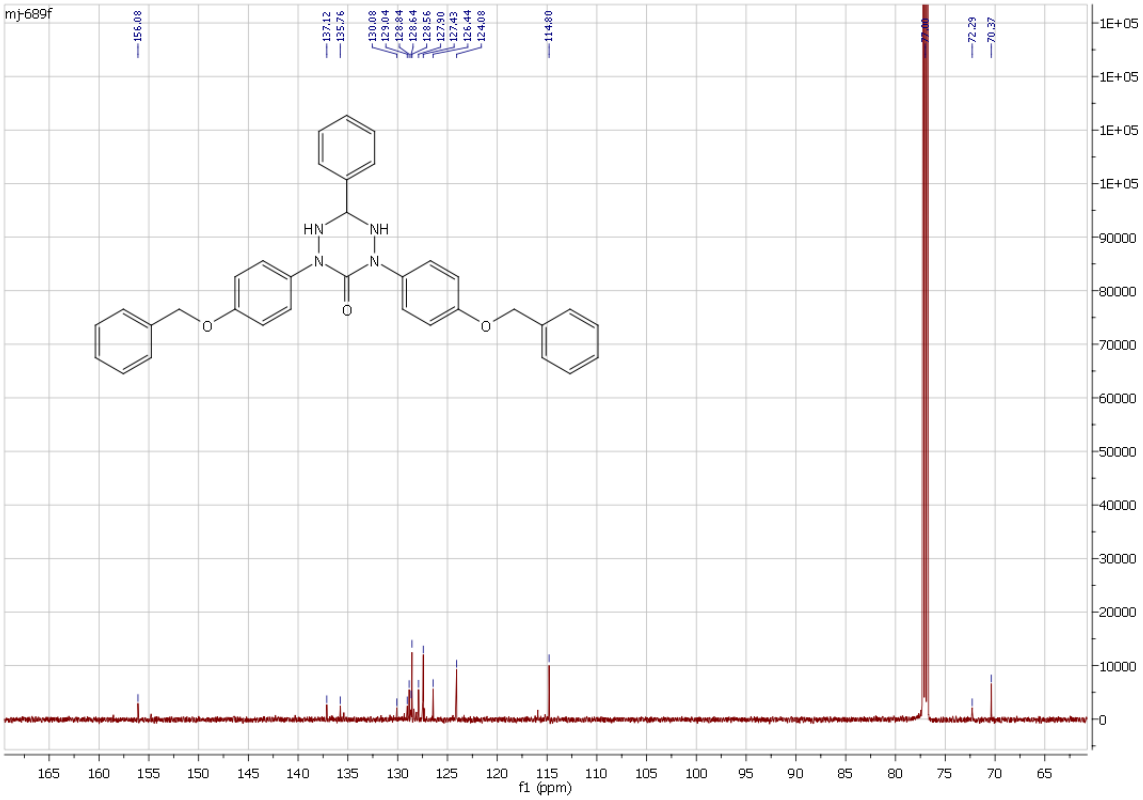
128.71
127.89
123.87
77.00
Cl
O
N
N
O
O
f1 (ppm)

5a





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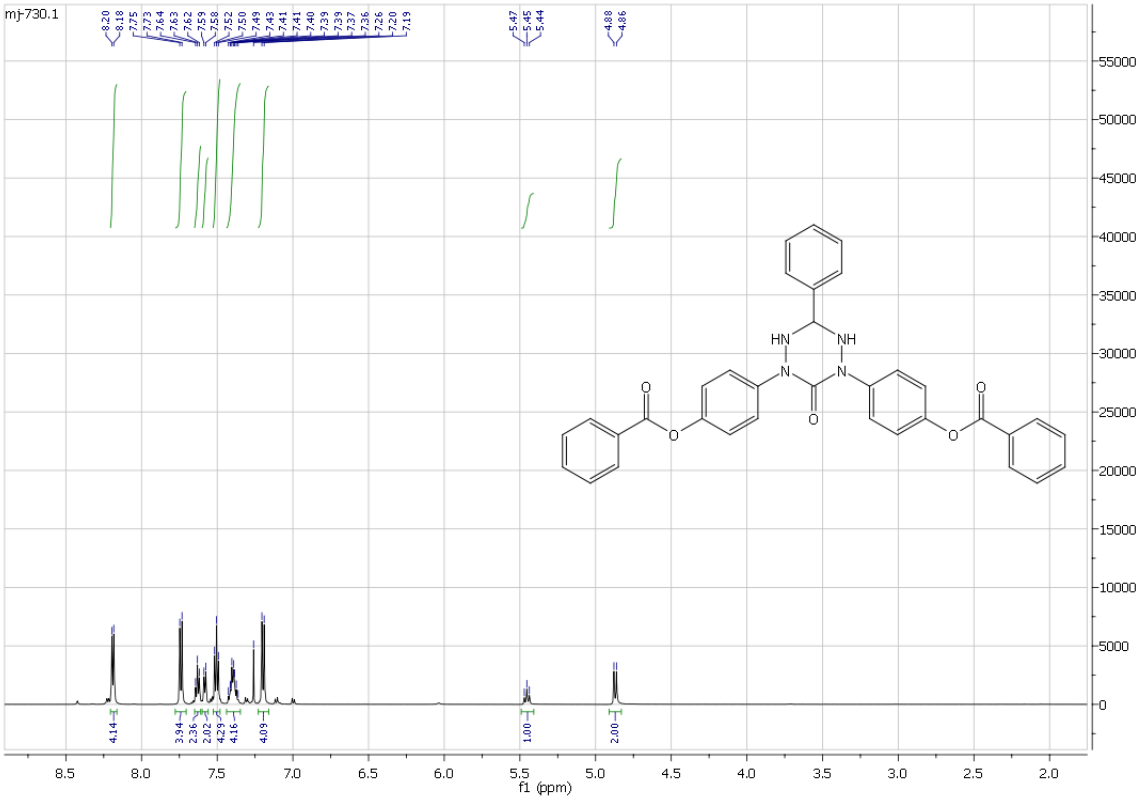

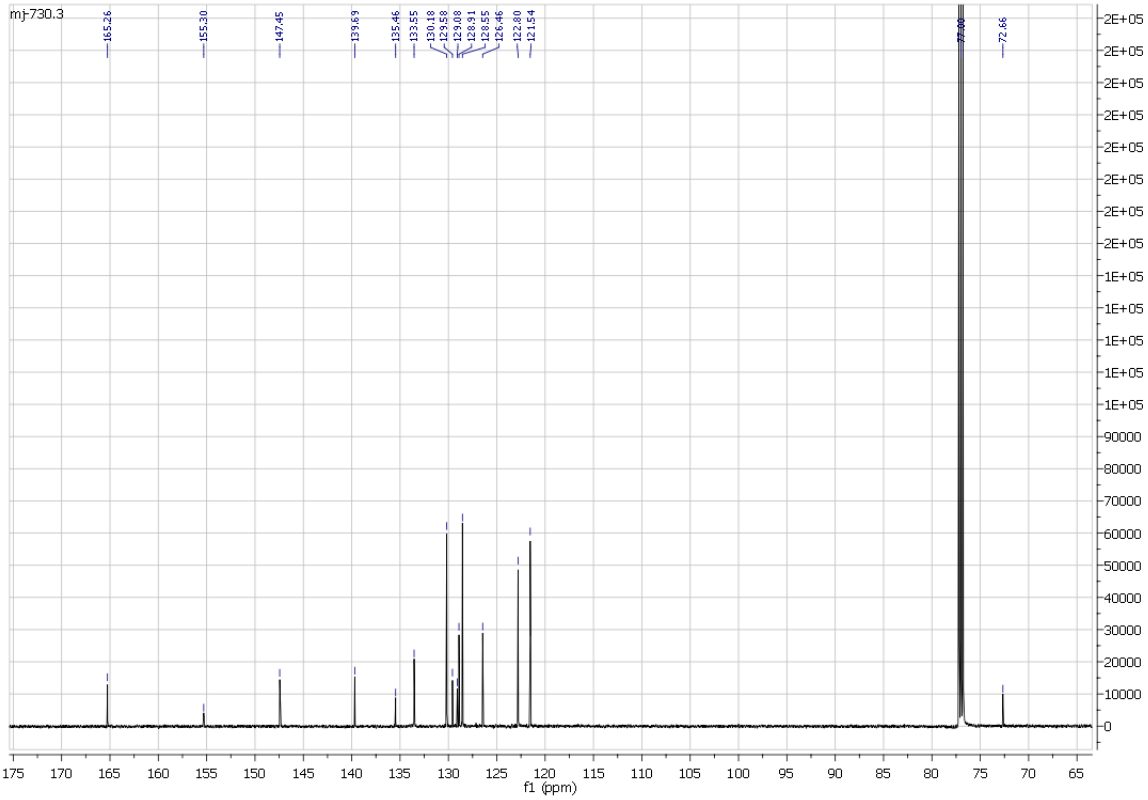

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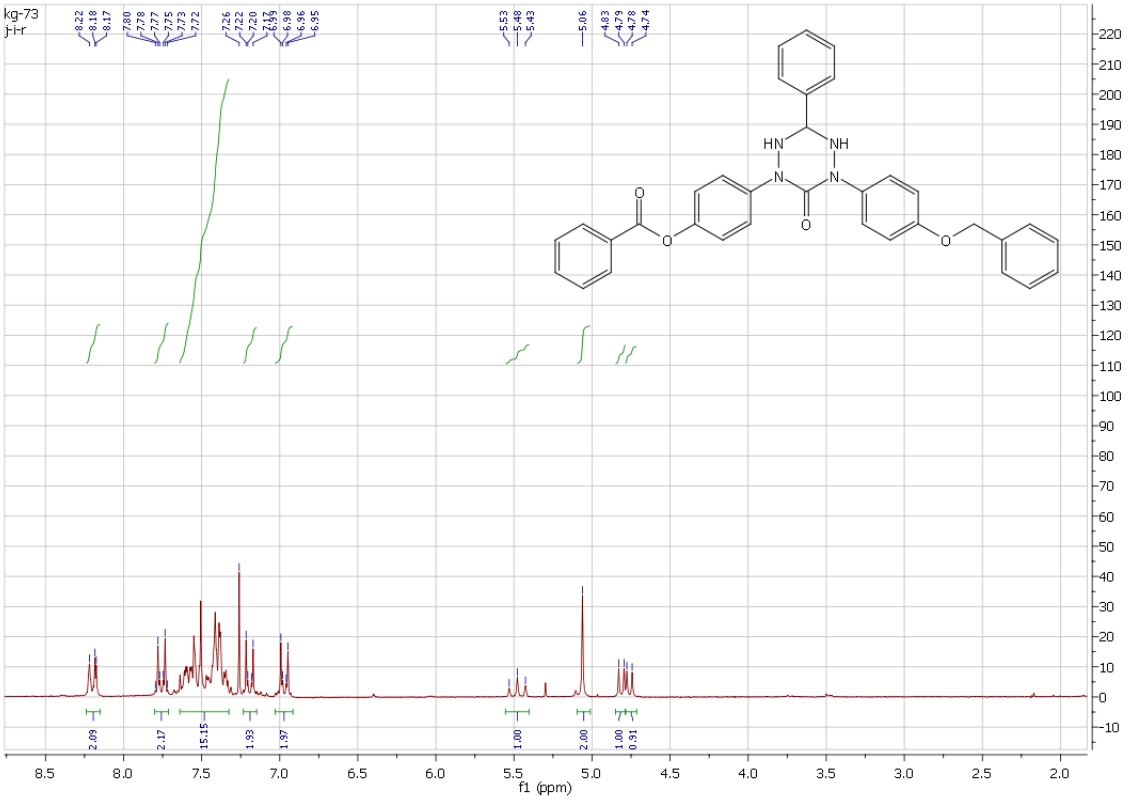
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8.17
7.80
7.78
7.77
7.75
7.73
7.72
7.26
7.22
7.20
7.17
6.99
6.98
6.96
6.95
5.53
5.48
5.43
5.06
4.83
4.79
4.78
4.74
HN
NH
N
N
N
O
O
O
O
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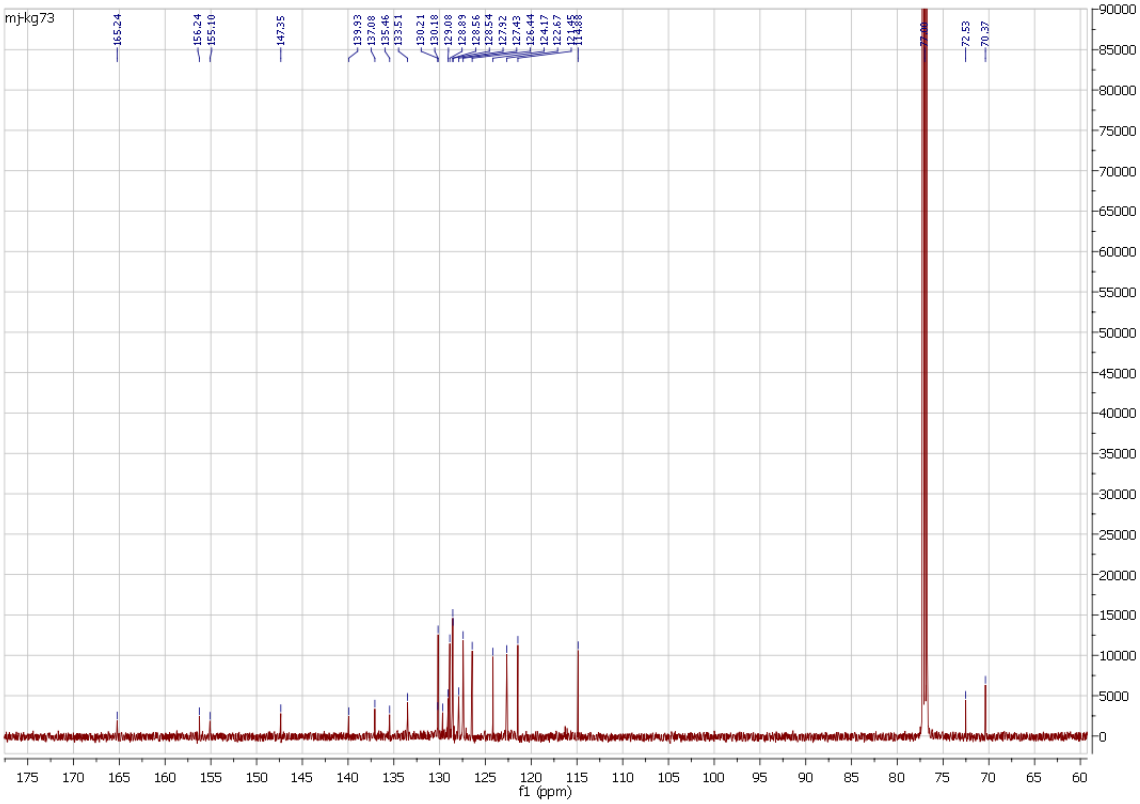
2.17
15.15
1.93
1.97
1.00
2.00
1.00
0.91
f1 (ppm)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130.18
129.08
128.89
128.56
128.54
127.92
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124.17
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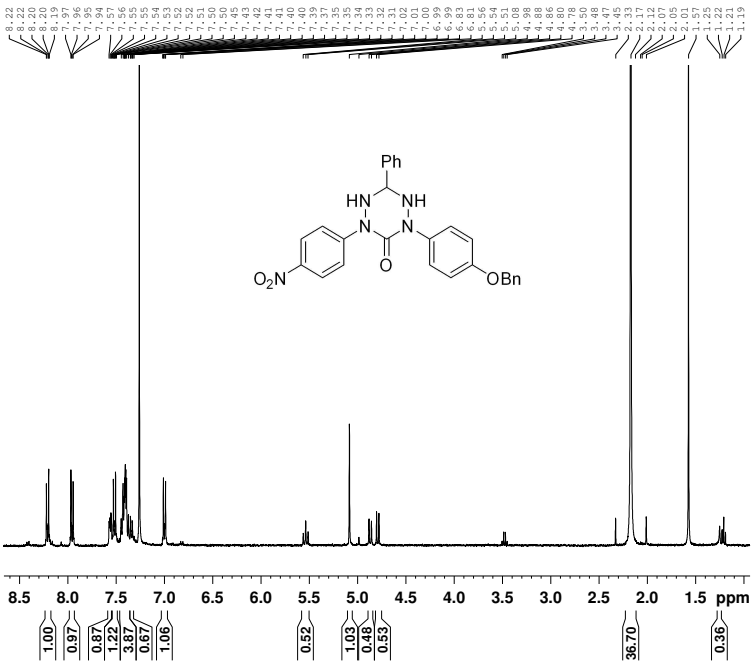
114.68
77.00
72.53
70.37
f1 (ppm)

5d

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PROCNO                1

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TD                 32768
SOLVENT            CDCl3
NS                    16
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SWH             5208.333 Hz
FIDRES          0.158946 Hz
AQ              3.1457779 sec
RG                 456.1
DW                96.000 usec
DE                25.61 usec
TE                295.4 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.38 usec
PL1                -2.50 dB
PL1W         18.35869598 W
SFO1         400.1320007 MHz

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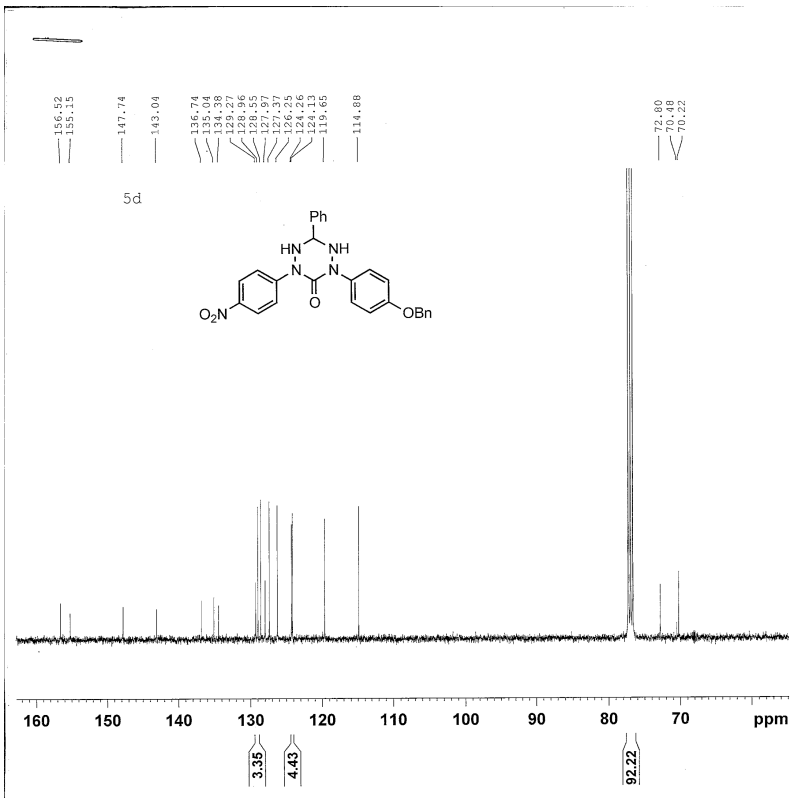


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PROCNO                1

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TD                 32768
SOLVENT            CDCl3
NS                  1280
DS                     8
SWH            26178.010 Hz
FIDRES          0.798889 Hz
AQ              0.6259188 sec
RG                 16384
DW                19.100 usec
DE                 6.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 12.00 usec
PL1                -1.00 dB
PL1W         37.63110352 W
SFO1        100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -2.50 dB
PL12               14.44 dB
PL13               14.44 dB
PL2W         18.35869598 W
PL12W         0.37139997 W
PL13W         0.37139997 W
SFO2        400.1320007 MHz

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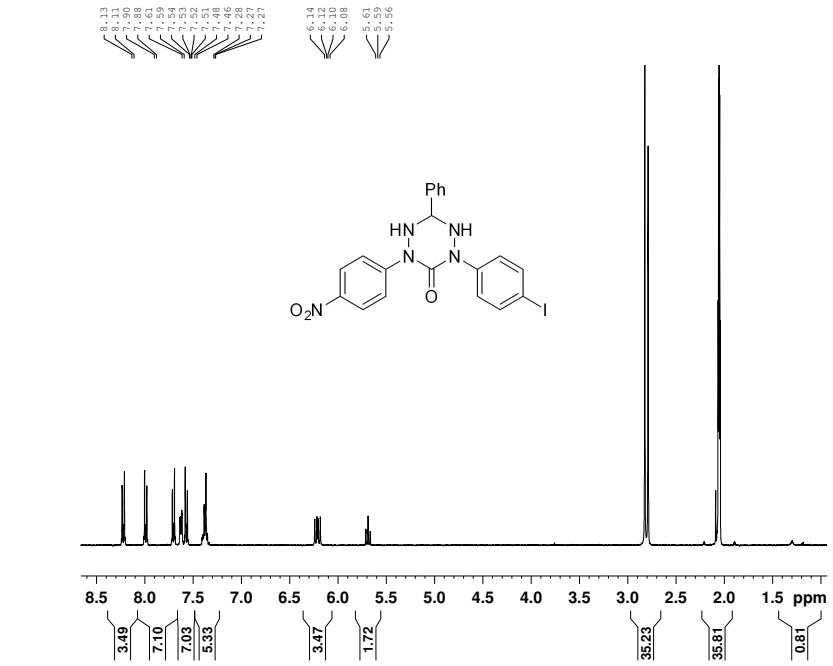
SF          100.6127772 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

5e

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PULPROG               zg30
TD                   32768
SOLVENT           Acetone
NS                       16
DS                        0
SWH                5208.333 Hz
FIDRES            0.158946 Hz
AQ                3.1457779 sec
RG                    574.7
DW                   96.000 usec
DE                   25.61 usec
TE                   298.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    11.38 usec
PL1                   -2.50 dB
PL1W           18.35869598 W
SFO1           400.1320007 MHz

F2 - Processing parameters
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WDW                     EM
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LB                    0.30 Hz
GB        0
PC                    1.00
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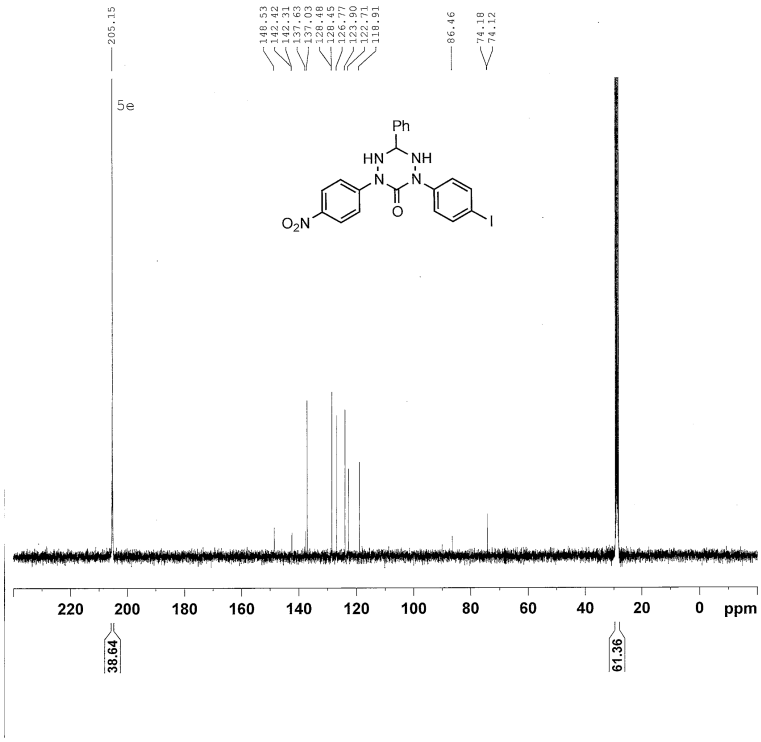


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INSTRUM               spect
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PULPROG             zgpg30
TD                   32768
SOLVENT           Acetone
NS                    1280
DS                       8
SWH               26178.010 Hz
FIDRES            0.798889 Hz
AQ                0.6259188 sec
RG                    16384
DW                   19.100 usec
DE                    6.00 usec
TE                   298.0 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    13C
P1                    12.00 usec
PL1                   -1.00 dB
PL1W           37.63110352 W
SFO1           100.6238364 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                   -2.50 dB
PL12                  14.44 dB
PL13                  14.44 dB
PL2W           18.35869598 W
PL12W           0.37139997 W
PL13W           0.37139997 W
SFO2           400.1320007 MHz

F2 - Processing parameters
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PC                    1.40
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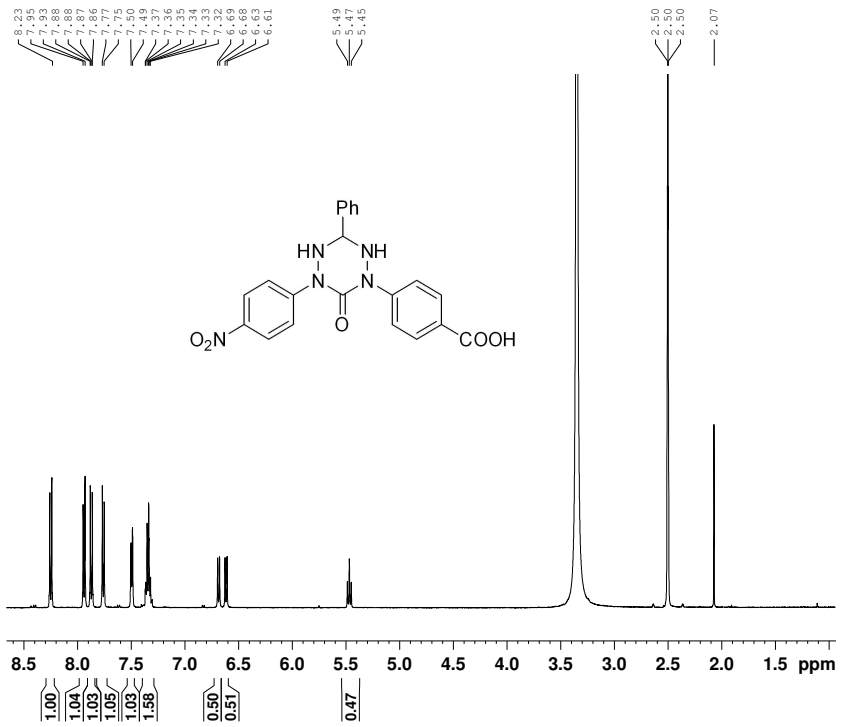
5f

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PULPROG            zg30
TD                32768
SOLVENT            DMSO
NS                    9
DS                    0
SWH            6510.417 Hz
FIDRES         0.198682 Hz
AQ            2.5166323 sec
RG                203.2
DW               76.800 usec
DE                6.00 usec
TE               298.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                11.31 usec
PL1       0 dB
SFO1        500.1325007 MHz

F2 - Processing parameters
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WDW                  EM
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PC                1.00
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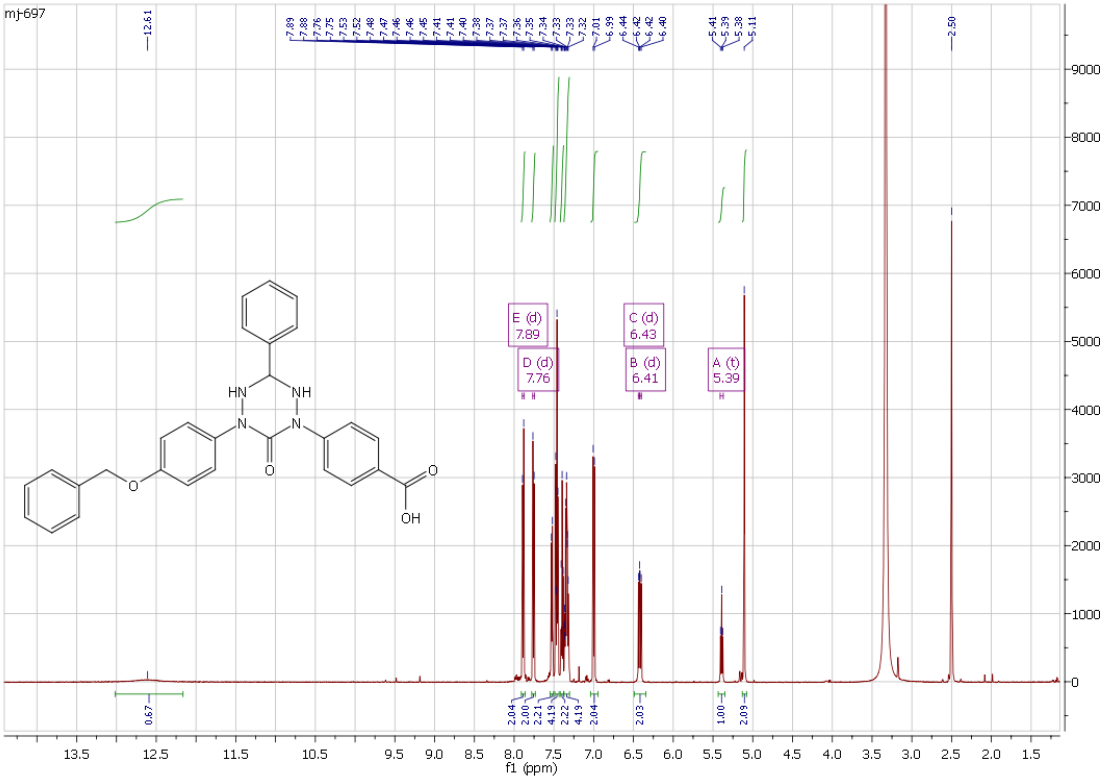
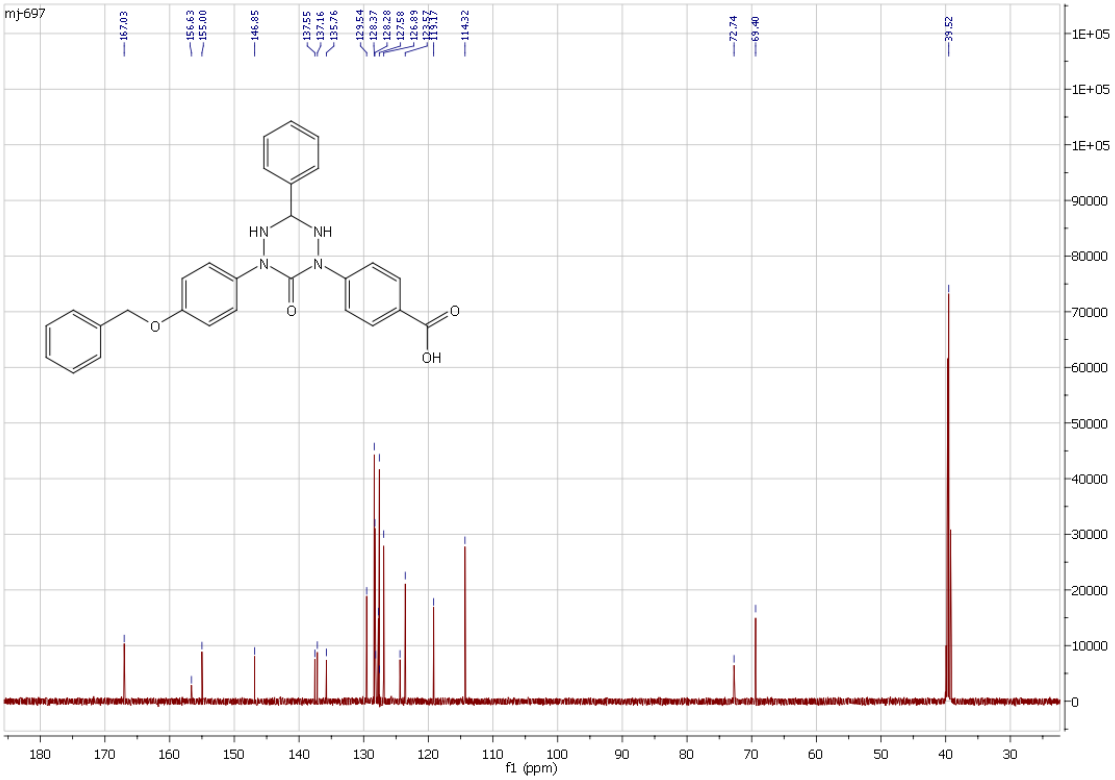
5g


mj-697
E (d) 7.89
D (d) 7.76
C (d) 6.43
B (d) 6.41
A (t) 5.39
HN
NH
N
N
N
O
O
O
OH
f1 (ppm)


mj-697
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N
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N
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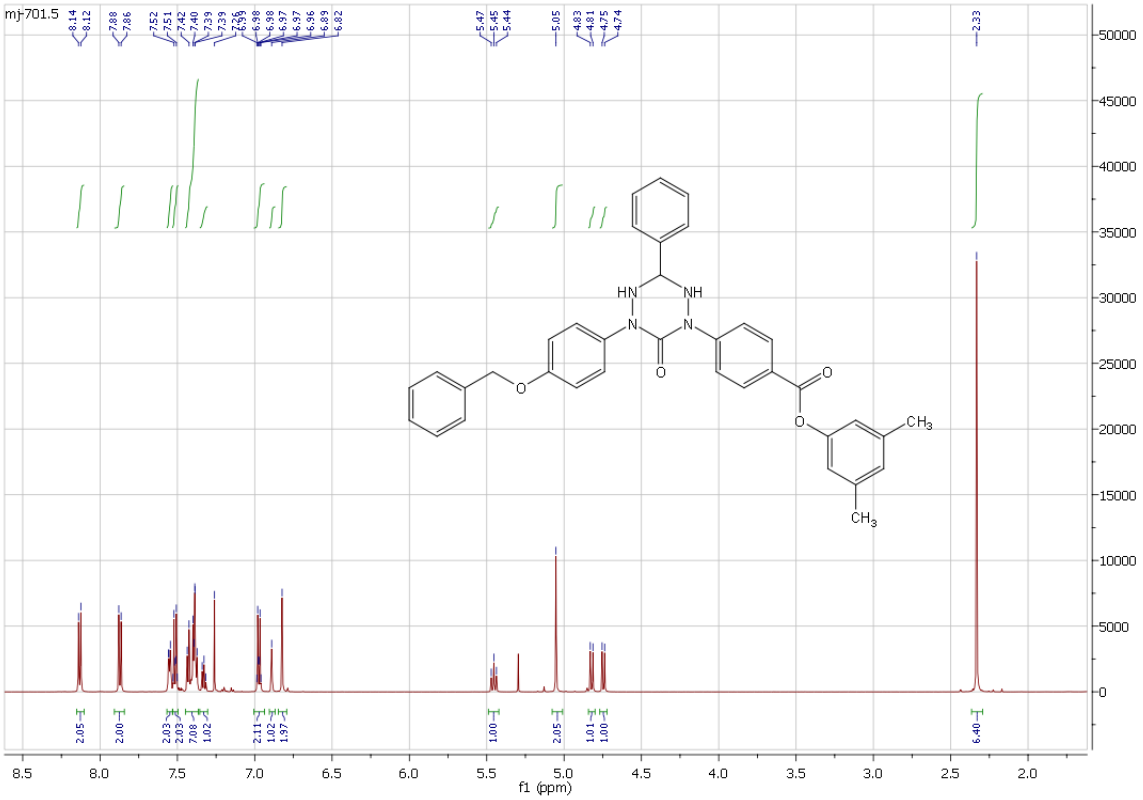
O
O
OH
f1 (ppm)

5t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8.12
7.88
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7.42
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7.36
6.98
6.98
6.97
6.97
6.96
6.89
6.82
5.47
5.45
5.44
5.05
4.83
4.81
4.75
4.74
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CH3
CH3
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2.00
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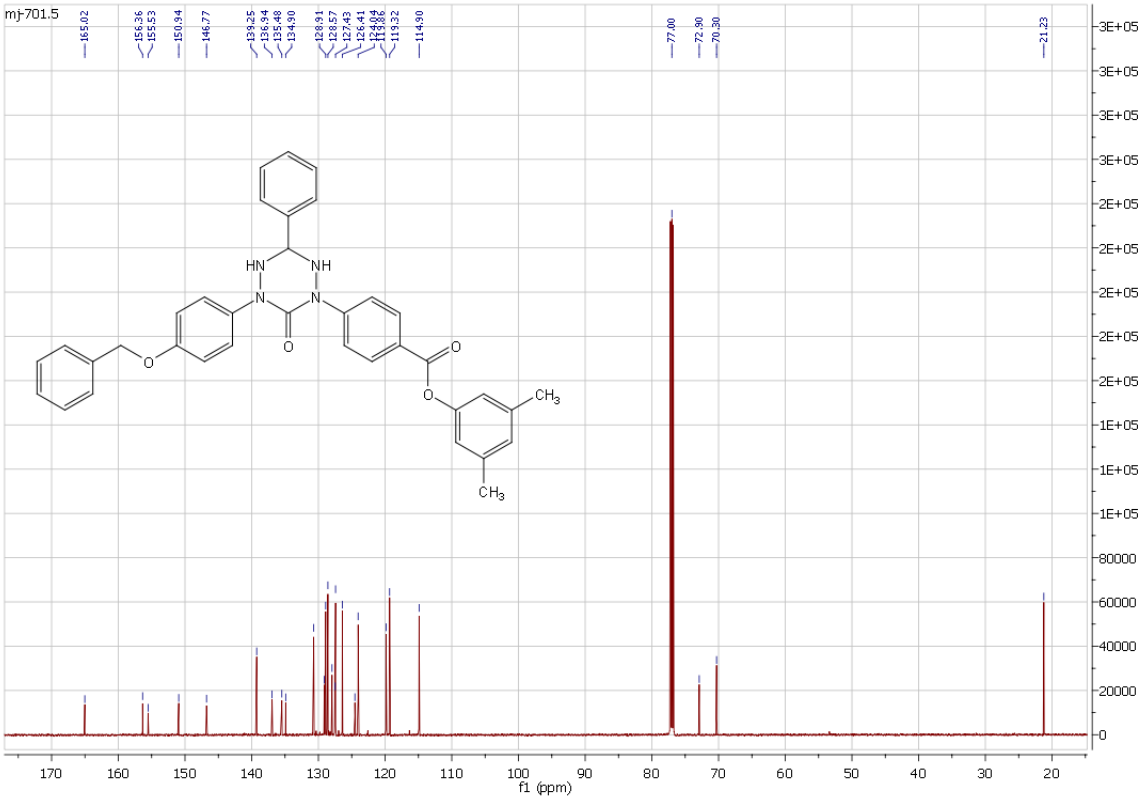
2.05
1.01
1.00
6.40
f1 (ppm)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139.25
136.94
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134.90
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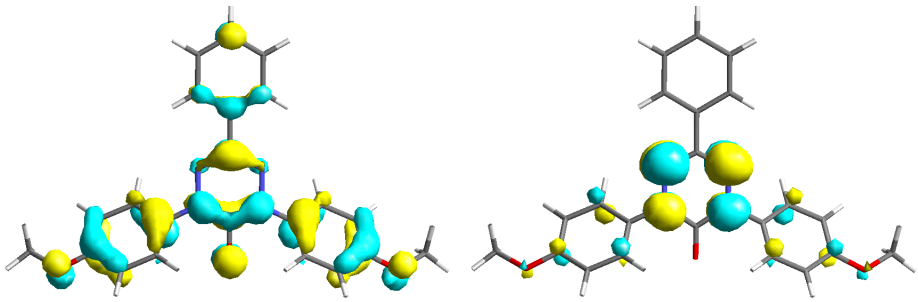
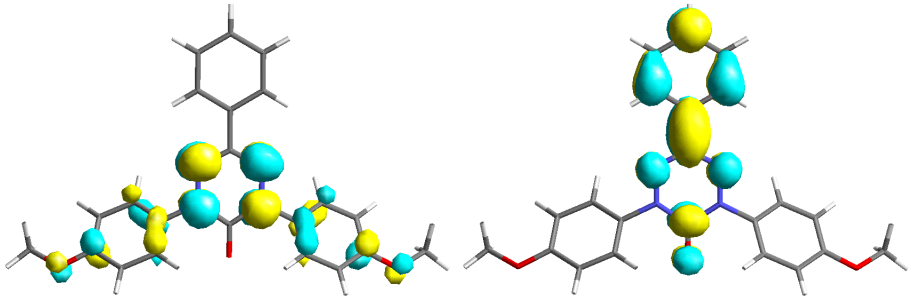
128.57
127.43
126.41
119.32
114.90
77.00
72.90
70.30
21.23
HN
NH
N
N
N
O
O
O
O
CH3
CH3
f1 (ppm)

2. Partial data for TD-DFT calculation (B3LYP/6-31G(2d,p)) for 1v-1z.



β-HOMO β-LUMO



α-HOMO α-LUMO

Figure S1. B3LYP/6-31G(2d,p) derived contours and energies of frontier molecular orbitals for **1v**.

Excitation energies oscillator strength

1v

```
 Excited State   1:  2.025-A      2.2388 eV  553.79 nm  f=0.1056
<S**2>=0.776
    102A ->103A       -0.22192
     99B ->102B       -0.16555
    101B ->102B        0.93865

 Excited State   2:  2.075-A      2.5861 eV  479.42 nm  f=0.0257
<S**2>=0.826
     92B ->102B        0.10398
     96B ->102B        0.37333
     97B ->102B       -0.41023
     98B ->102B       -0.13098
    100B ->102B        0.79416

 Excited State   3:  2.054-A      2.7208 eV  455.69 nm  f=0.0241
<S**2>=0.804
    100A ->103A       -0.13279
```

```
    102A ->103A        0.83756
    102A ->104A        0.12826
     99B ->102B        0.38945
    101B ->102B        0.25977

 Excited State   4:  2.122-A      2.8923 eV  428.67 nm  f=0.0243
<S**2>=0.876
    102A ->108A       -0.10379
     93B ->102B       -0.13662
     96B ->102B       -0.48992
     97B ->102B        0.58649
     98B ->102B        0.19539
    100B ->102B        0.54603
```

1w

```
 Excited State   1:  2.039-A      2.1610 eV  573.73 nm  f=0.0864
<S**2>=0.790
    105A ->107A       -0.15901
    103B ->105B        0.23692
    104B ->105B        0.92828

 Excited State   2:  2.177-A      2.4918 eV  497.56 nm  f=0.0507
<S**2>=0.935
    104A ->106A        0.11874
    105A ->106A        0.61018
    100B ->105B        0.36002
    101B ->105B       -0.26578
    103B ->105B       -0.56261
    104B ->105B        0.18092

 Excited State   3:  2.111-A      2.5584 eV  484.62 nm  f=0.0576
<S**2>=0.864
    105A ->106A        0.68986
    105A ->107A       -0.29205
     98B ->105B        0.11411
     99B ->105B        0.26979
    100B ->105B       -0.18875
    101B ->105B        0.15566
    103B ->105B        0.46674
    103B ->106B       -0.11254

 Excited State   4:  2.060-A      2.7373 eV  452.95 nm  f=0.0325
<S**2>=0.811
    105A ->107A       -0.33310
     93B ->105B        0.11676
     98B ->105B       -0.14759
     99B ->105B       -0.31506
    100B ->105B        0.52505
    101B ->105B       -0.41659
    103B ->105B        0.43597
    104B ->105B       -0.22963
```

1x

```
Excited State   1:  2.029-A      2.2204 eV  558.39 nm  f=0.0940  <S**2>=0.779
    109A ->111A       -0.19997
    107B ->109B        0.22024
    108B ->109B        0.93076

 Excited State   2:  2.063-A      2.5701 eV  482.42 nm  f=0.0160
<S**2>=0.814
    109A ->111A       -0.17360
     98B ->109B       -0.10738
    102B ->109B       -0.47441
    105B ->109B        0.32045
    106B ->109B        0.28761
    107B ->109B        0.68759
    108B ->109B       -0.15880

 Excited State   3:  2.083-A      2.7632 eV  448.69 nm  f=0.0149
<S**2>=0.834
    109A ->110A        0.57643
    109A ->111A        0.35299
    102B ->109B       -0.28487
    105B ->109B        0.33324
    106B ->109B        0.36202
    107B ->109B       -0.30194
    108B ->109B        0.22953

 Excited State   4:  2.245-A      2.8988 eV  427.71 nm  f=0.0249
<S**2>=1.010
    108A ->110A       -0.15718
    109A ->110A        0.59537
    102B ->109B        0.49115
    104B ->109B       -0.16349
    105B ->109B       -0.13888
    107B ->109B        0.47982
```

1y

```
Excited State   1:  2.017-A      1.4245 eV  870.37 nm  f=0.2594  <S**2>=0.767
     97B -> 98B        0.98846
     97B <- 98B       -0.11672

 Excited State   2:  2.054-A      1.6191 eV  765.77 nm  f=0.0020
<S**2>=0.805
     96B -> 98B        0.98091
     96B ->106B        0.11575

 Excited State   3:  2.409-A      1.9545 eV  634.35 nm  f=0.0036
<S**2>=1.201
     97A -> 99A        0.24973
     98A -> 99A        0.86530
     97B -> 99B       -0.37210

 Excited State   4:  2.851-A      2.4342 eV  509.35 nm  f=0.0003
<S**2>=1.782
     97A -> 99A       -0.12295
```

```
     98A -> 99A        0.41390
     97B -> 99B        0.87872
```

1z

```
 Excited State   1:  2.034-A      2.1924 eV  565.51 nm  f=0.1199
<S**2>=0.784
     98A -> 99A       -0.18019
     95B -> 98B        0.15978
     96B -> 98B        0.16831
     97B -> 98B        0.93376

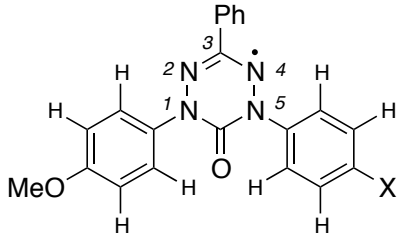
 Excited State   2:  2.074-A      2.5342 eV  489.25 nm  f=0.0324
<S**2>=0.825
     98A -> 99A       -0.25787
     91B -> 98B        0.13765
     92B -> 98B       -0.20486
     93B -> 98B       -0.19757
     94B -> 98B       -0.24472
     96B -> 98B        0.82489
     97B -> 98B       -0.20112

 Excited State   3:  2.051-A      2.6835 eV  462.02 nm  f=0.0192
<S**2>=0.802
     96A -> 99A       -0.12518
     98A -> 99A        0.77905
     98A ->100A       -0.10937
     92B -> 98B       -0.15259
     93B -> 98B       -0.14536
     94B -> 98B       -0.18580
     95B -> 98B       -0.39373
     96B -> 98B        0.19332
     97B -> 98B        0.18740

 Excited State   4:  2.085-A      2.8563 eV  434.07 nm  f=0.0161
<S**2>=0.837
     98A -> 99A        0.23452
     89B -> 98B        0.11778
     91B -> 98B       -0.26363
     92B -> 98B        0.40705
     93B -> 98B        0.40917
     94B -> 98B        0.52369
     96B -> 98B        0.43574
```

3. Theoretical hfcc values for model radicals

Table S1. Calculated hyperfine coupling constants (G) for selected radicals.



compound	$a_{N(1)}$	$a_{N(2)}$	$a_{N(4)}$	$a_{N(5)}$	at N(1)		at C(3)			at N(5)	
					$a_{H(o)}$	$a_{H(m)}$	$a_{H(o)}$	$a_{H(m)}$	$a_{H(p)}$	$a_{H(o)}$	$a_{H(m)}$
1v X = MeO	3.53	5.08	5.08	3.53	-0.93	0.47	0.63	-0.34	0.55	-0.93	0.47
1w X = NO_2	3.54	5.27	5.19	2.77	-0.86	0.46	0.64	-0.34	0.55	-0.94	0.50
1x X= COOMe	3.56	5.23	5.18	3.08	-0.89	0.46	0.64	-0.34	0.56	-0.92	0.53
1y X = O^-	1.74	2.18	2.18	3.38	-0.70	0.29	0.23	-0.14	0.19	0.17	-2.51
1z X = NH_2	3.49	5.03	5.03	3.62	-0.91	0.46	0.62	-0.34	0.54	-0.92	0.45

[a] B3LYP/EPR-II//B3LYP/6-31G(2d,p). The hfcc calculated by averaging values for equivalent nuclei.

4. EPR Spectra Simulation

Simulation of the EPR spectra was done with the PEST program (EPR-WinSim.2002 version 0.98 for Windows; available at: http://www.niehs.nih.gov/research/resources/software/tox-pharm/tools/index.cfm) using results of B3LYP/EPR-II//B3LYP/6-31G(2d,p) for initial input. The resulting *hfcc* values were perturbed until the global minimum for the fit was achieved. Spectra used for simulation were generated by reflection of the left half of each spectrum.

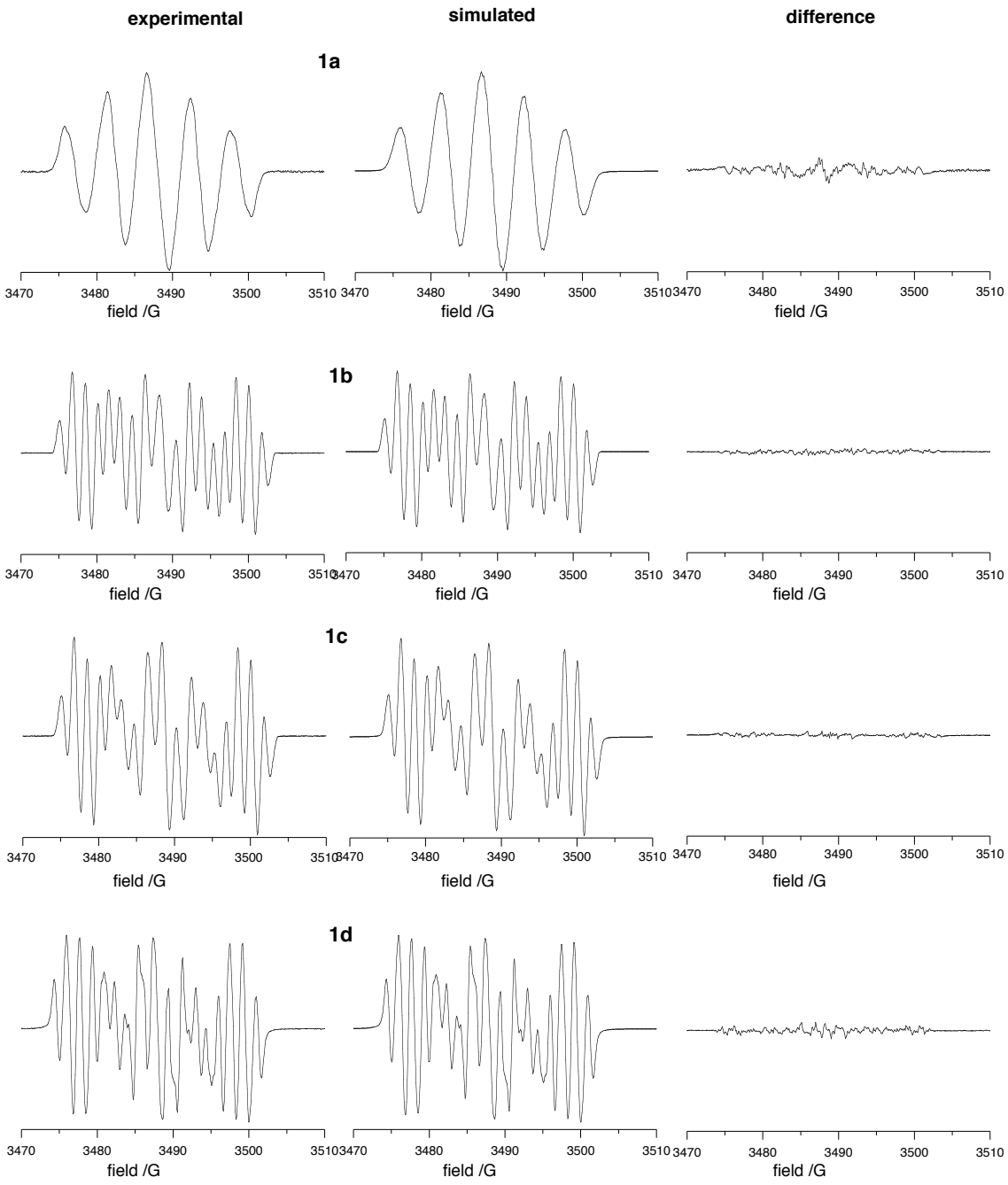


Figure S2. A comparison for experimental, simulate and difference spectra for four radicals.

5. Archive files for DFT calculations

1v


```
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 m=(NoDistance,NoAngle,check) TD(NStates=15)\\Di(4-MeOphenyl)-3-Ph 6-ox
 overdazyl, C1 at the DFT geom\\0,2\O,0,0.0014650954,-0.0024308737,0.00
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```


1w


```
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 m=(NoDistance,NoAngle,check) TD(NStates=15)\\1-(4-MeOphenyl)-5-(4-NO2p
 henyl)-3-Ph 6-oxoverdazyl, C1 at the DFT geom\\0,2\O,0,-0.0203427515,-
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1x

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1y

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1z

1\1\GINC-OCTOPUS\FOpt\UB3LYP\6-31G(2d,p)\C21H18N5O2(2)\PIOTR\01-Apr-20
13\0\\#P UB3LYP/6-31G(2d,p) FOpt=tight freq(noraman) SCF=Direct #P Geo
m=(NoDistance,NoAngle) fcheck\\1-(4-MeOphenyl)-5-(4-NH2phenyl)-3-Ph 6-
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