Supporting information

Synthesis of Indole-Linked β-Cyano-Enones: A Pathway to Indolyl-2-Pyrrolones

Nurabul Mondal, Vidya Kumari, Danish Ali and Lokman H. Choudhury*

Department of Chemistry, Indian Institute of Technology Patna, Patna-801106, India

Email: lokman@iitp.ac.in; lokman.iitp@gmail.com

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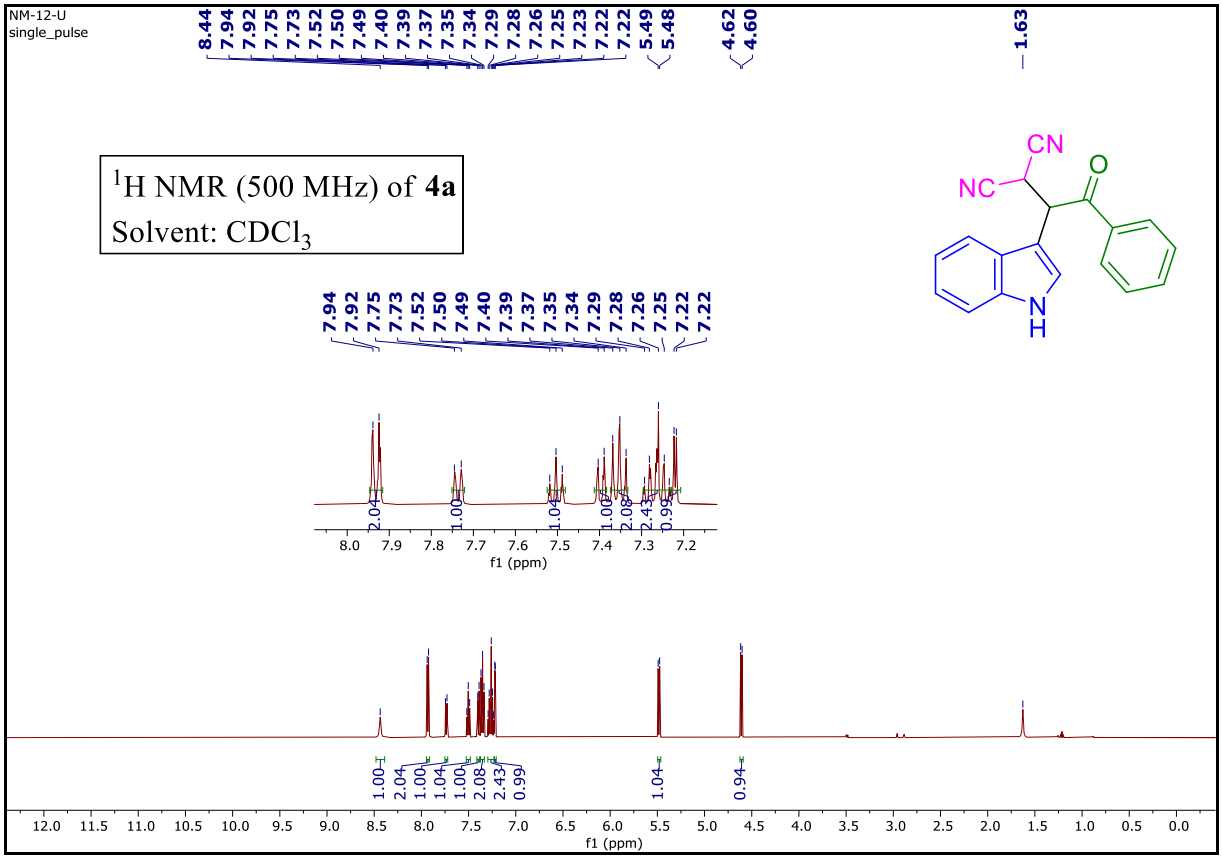
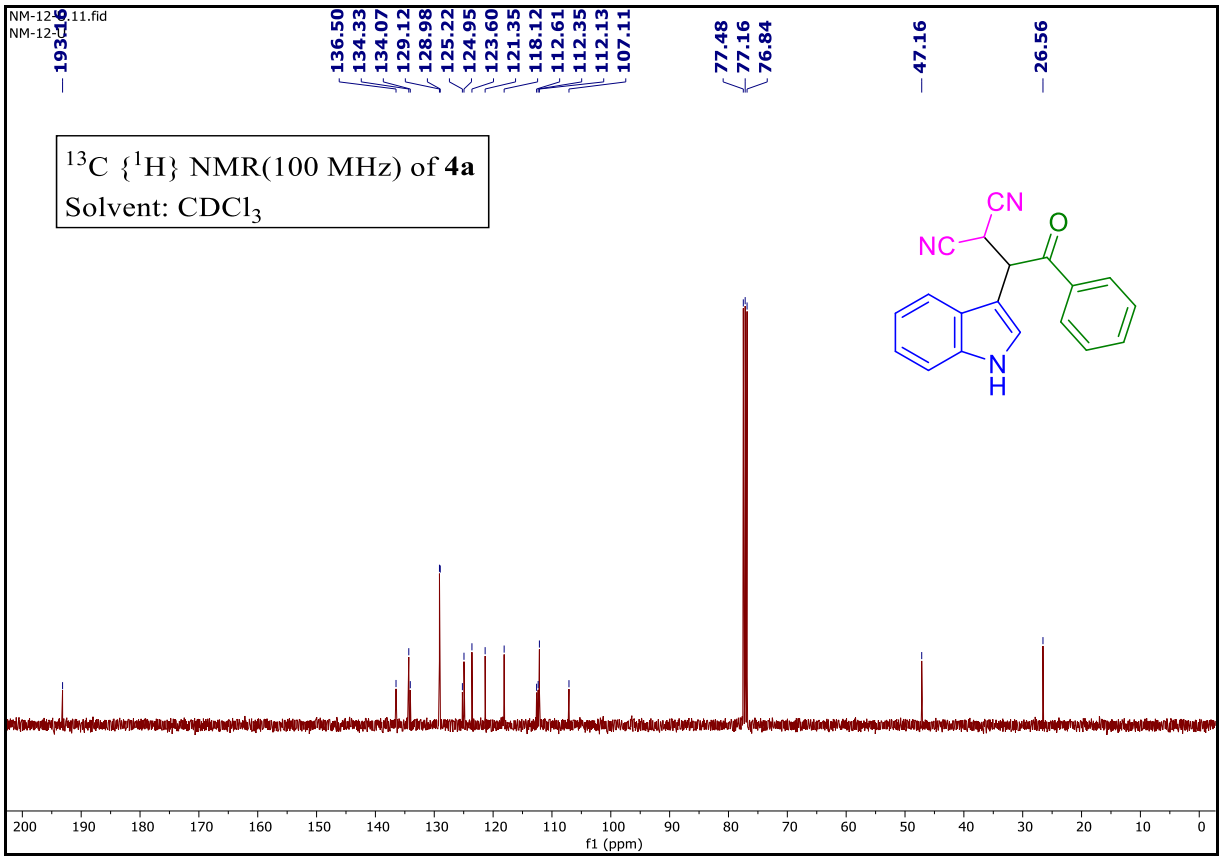
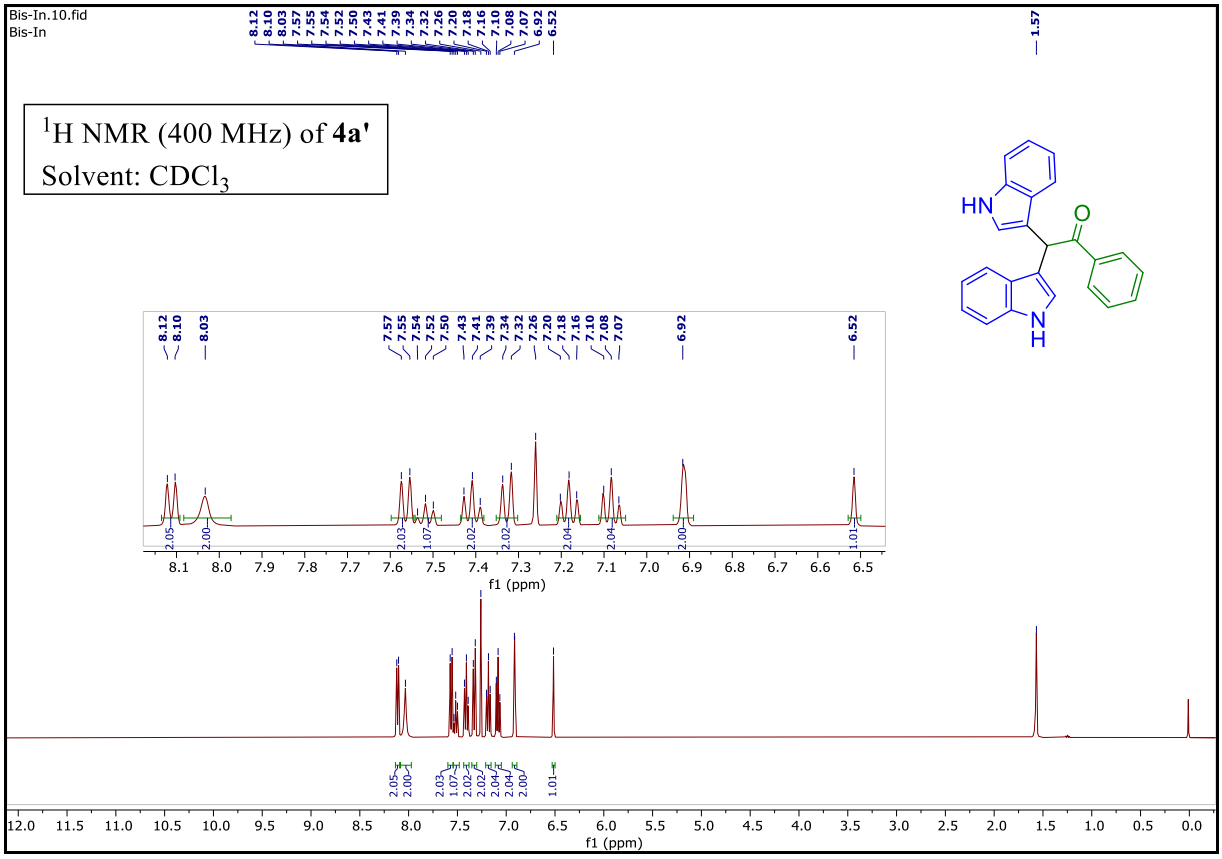
1. ^{1}H and ^{13}C {^{1}H} NMR spectra of all compounds



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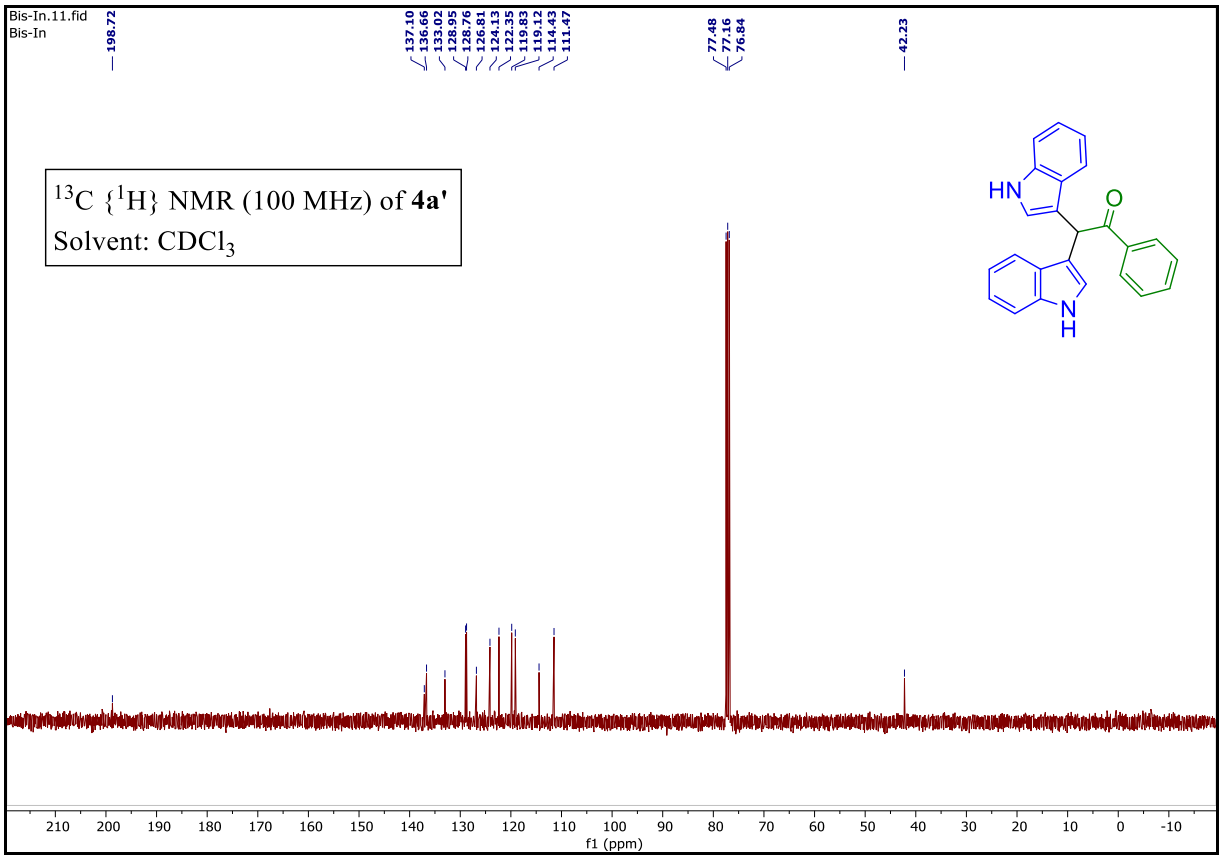
Bis-In
^{1}H NMR (400 MHz) of **4a'**
Solvent: $CDCl_3$
f1 (ppm)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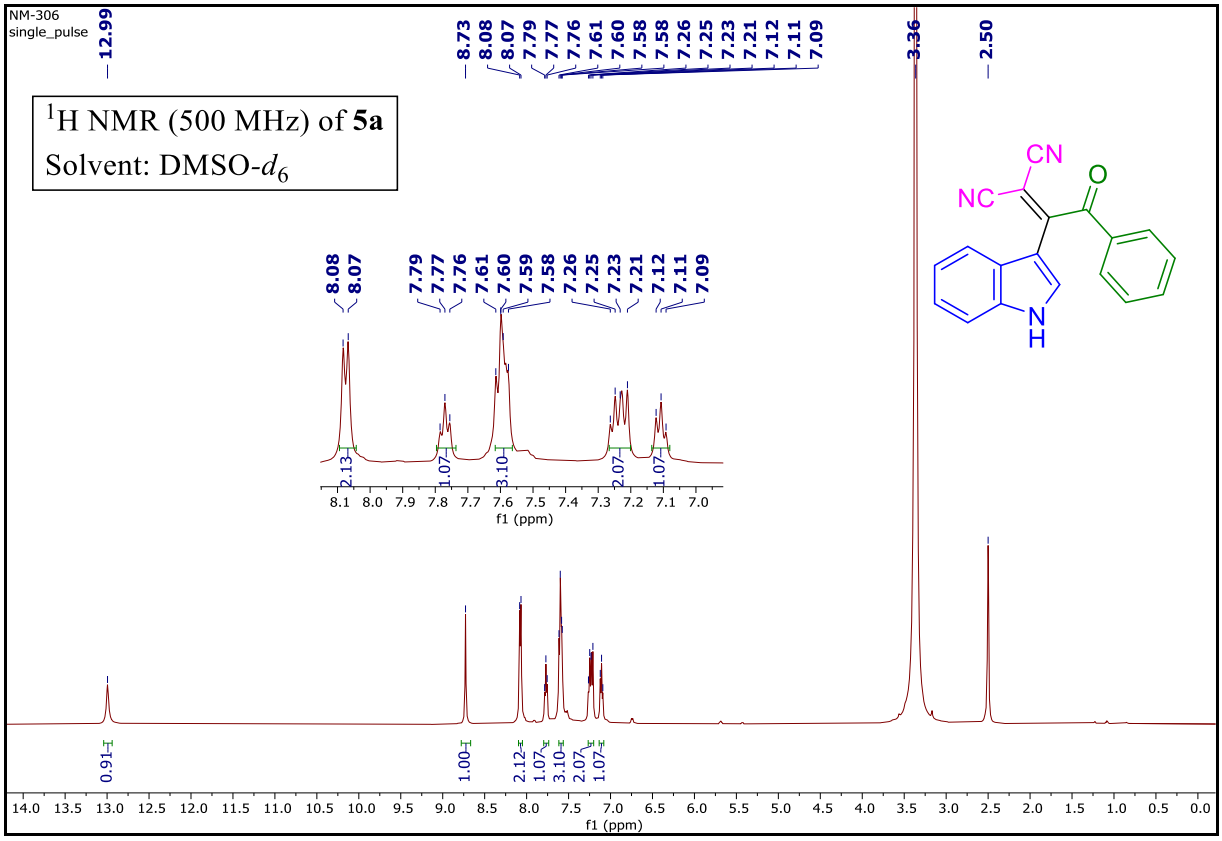
^{13}C {^{1}H} NMR (100 MHz) of **4a'**
Solvent: $CDCl_3$
f1 (ppm)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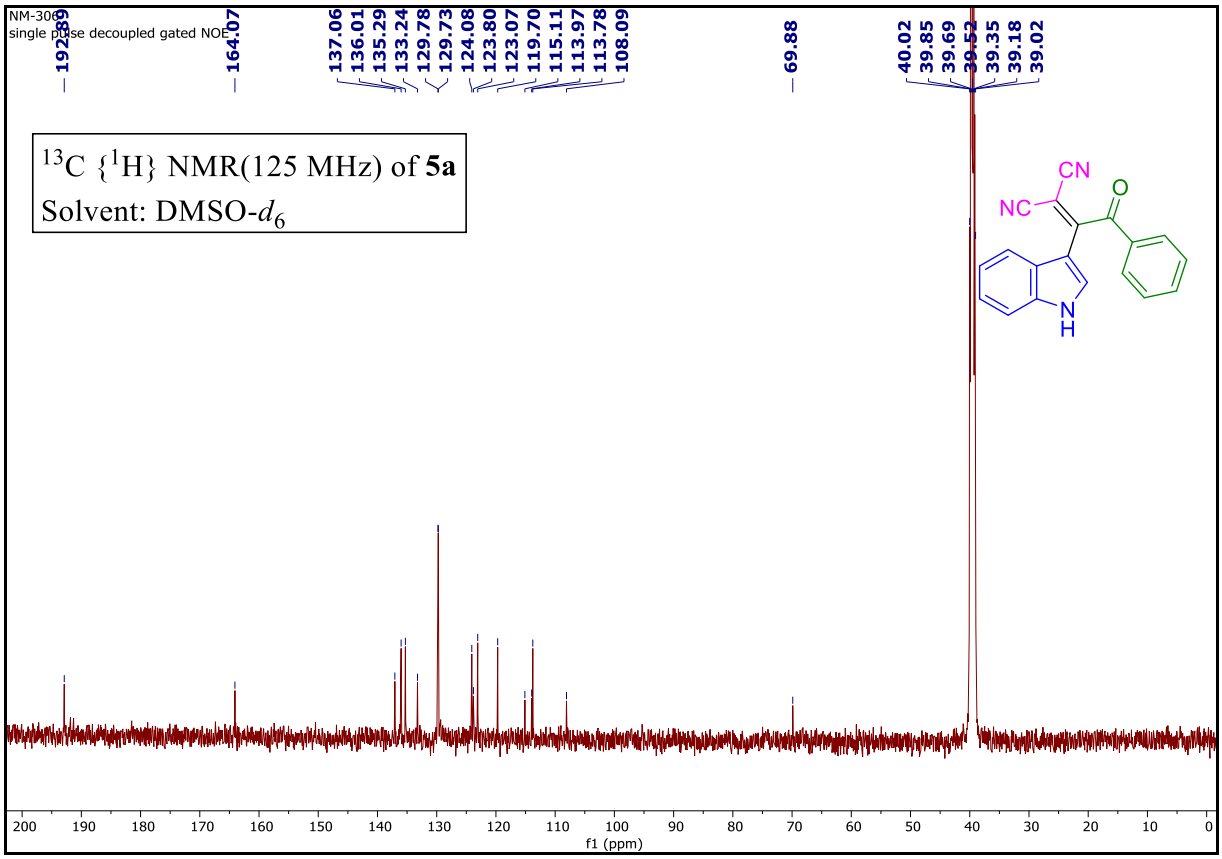
8.08
8.07
7.79
7.77
7.76
7.61
7.60
7.58
7.58
7.26
7.25
7.23
7.21
7.12
7.11
7.09
3.36
2.50
1H NMR (500 MHz) of 5a
Solvent: DMSO-d6
CN
NC
O
N
H
f1 (ppm)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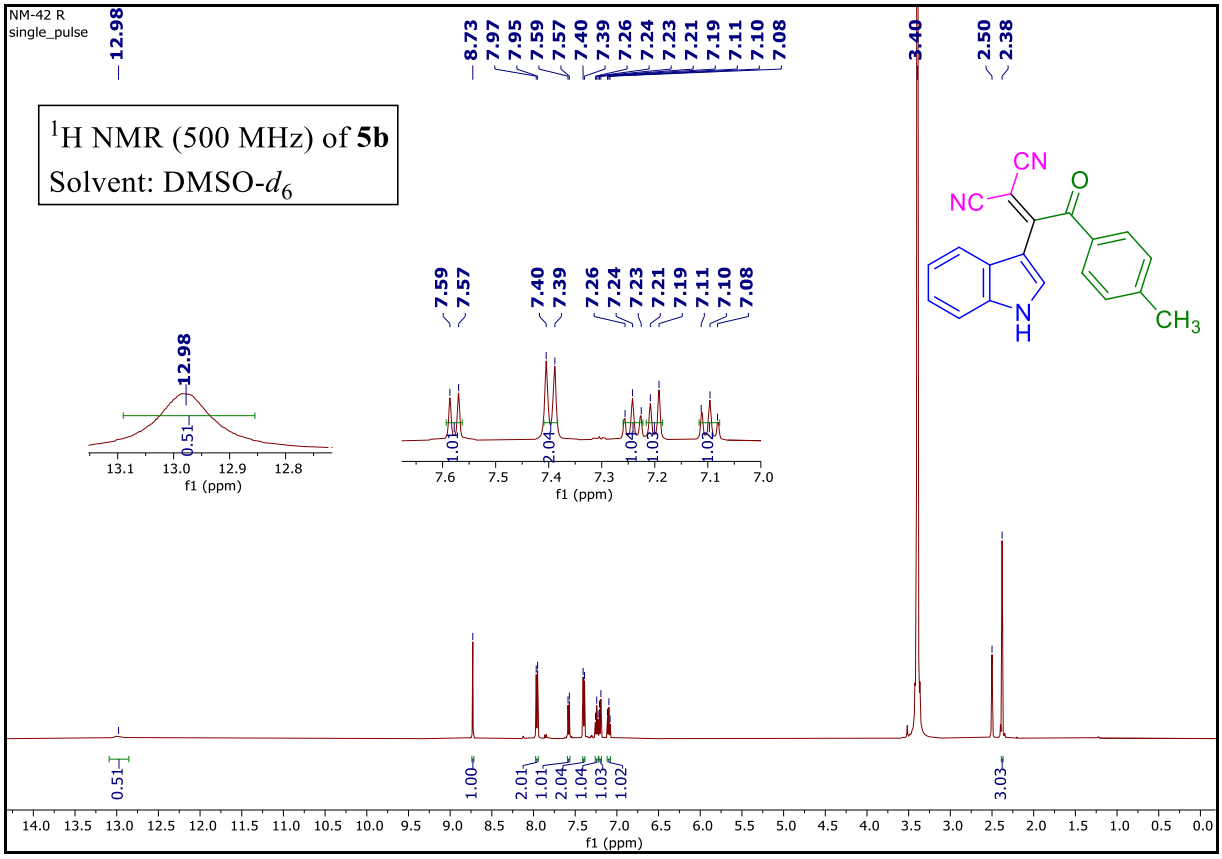
192.89
164.07
137.06
136.01
135.29
133.24
129.78
129.73
124.08
123.80
123.07
119.70
115.11
113.97
113.78
108.09
69.88
40.02
39.85
39.69
39.52
39.35
39.18
39.02
13C {1H} NMR(125 MHz) of 5a
Solvent: DMSO-d6
CN
NC
O
N
H
f1 (ppm)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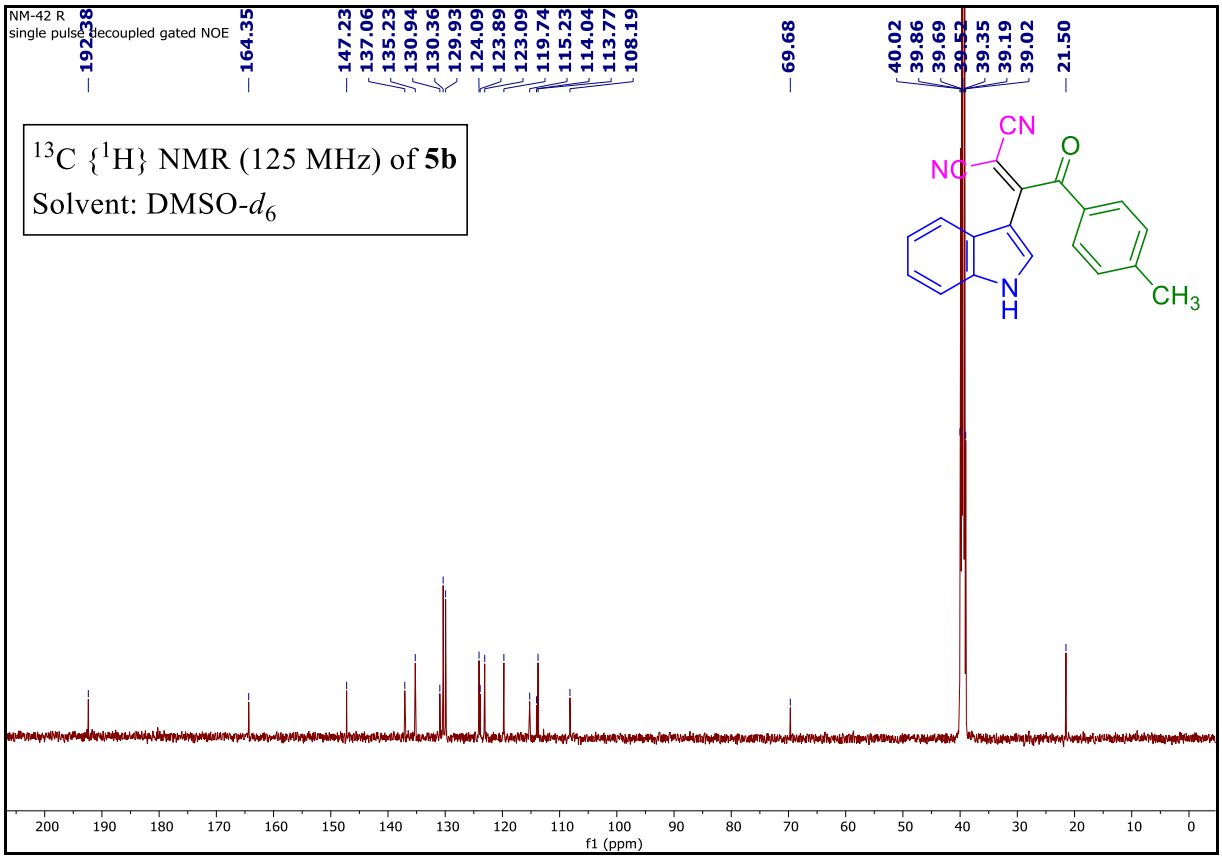
8.73
7.97
7.95
7.59
7.57
7.40
7.39
7.26
7.24
7.23
7.21
7.19
7.11
7.10
7.08
3.40
2.50
2.38
^{1}H NMR (500 MHz) of **5b**
Solvent: DMSO-d_6
CN
NC
O
N
H
CH$_3$
f1 (ppm)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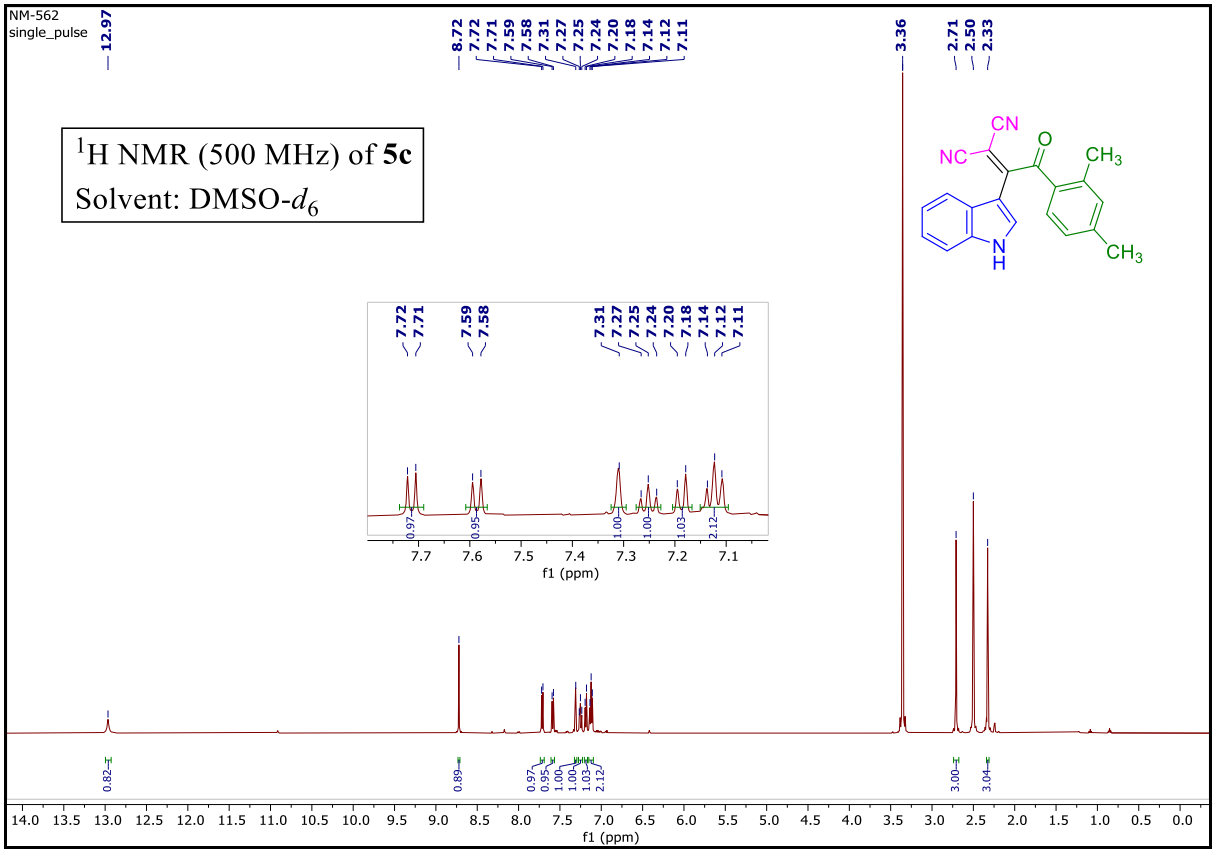
single pulse decoupled gated NOE
192.38
164.35
147.23
137.06
135.23
130.94
130.36
129.93
124.09
123.89
123.09
119.74
115.23
114.04
113.77
108.19
69.68
40.02
39.86
39.69
39.52
39.35
39.19
39.02
21.50
^{13}C {^{1}H} NMR (125 MHz) of **5b**
Solvent: DMSO-d_6
CN
NC
O
N
H
CH$_3$
f1 (ppm)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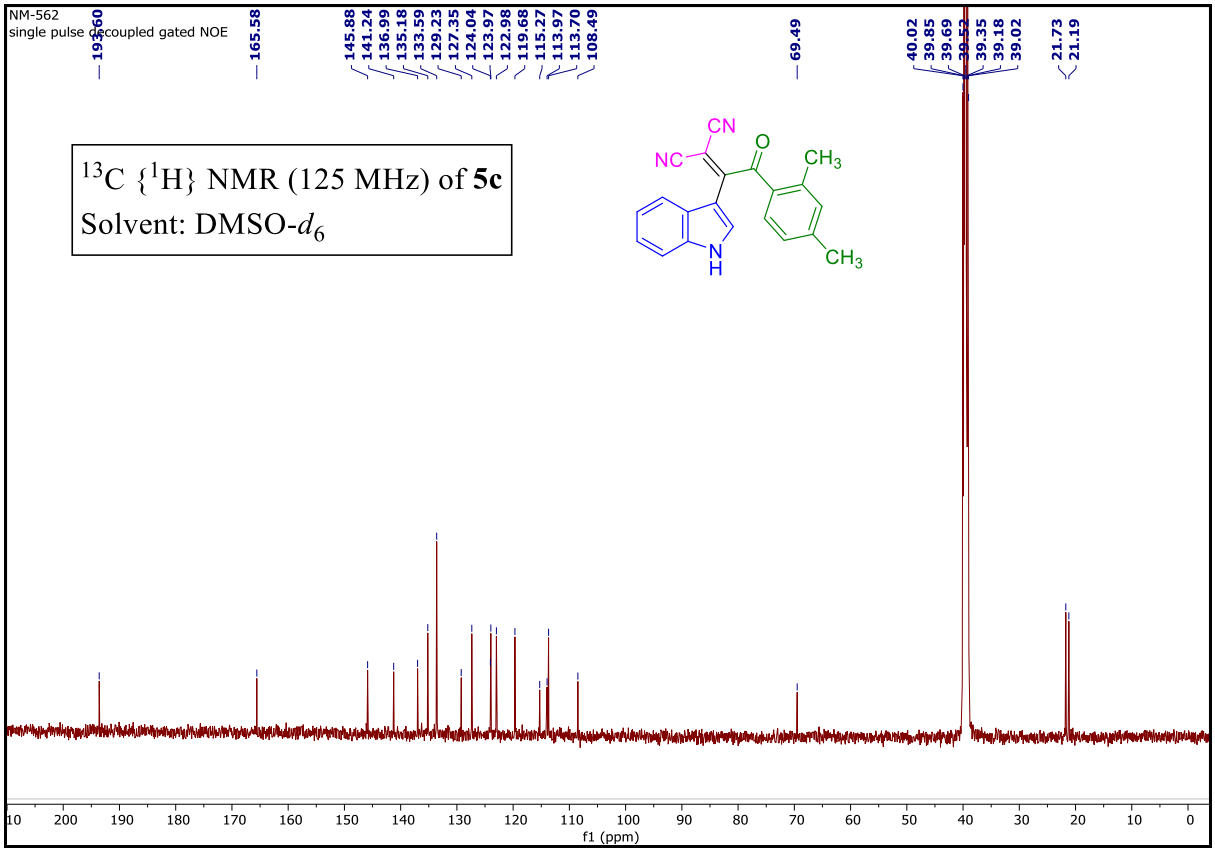
^{1}H NMR (500 MHz) of **5c**
Solvent: DMSO-d_6
f1 (ppm)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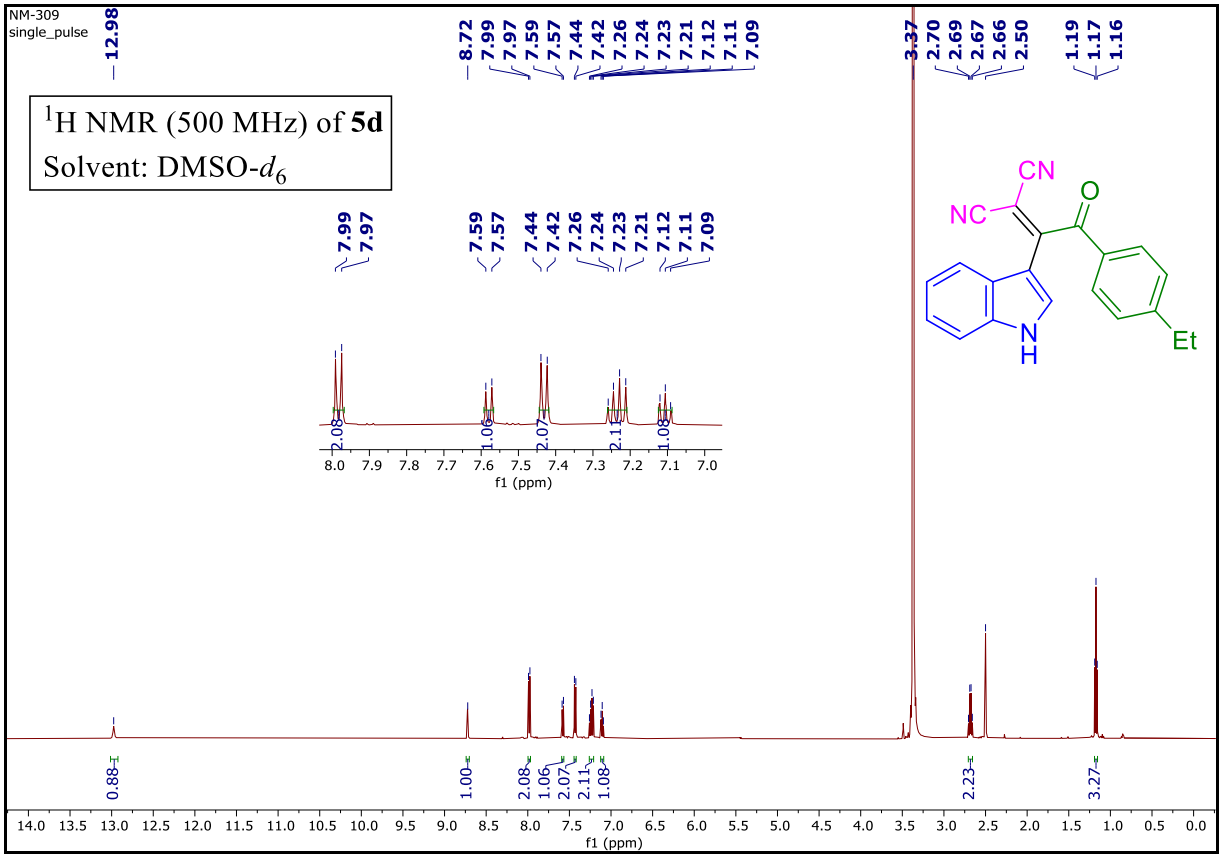
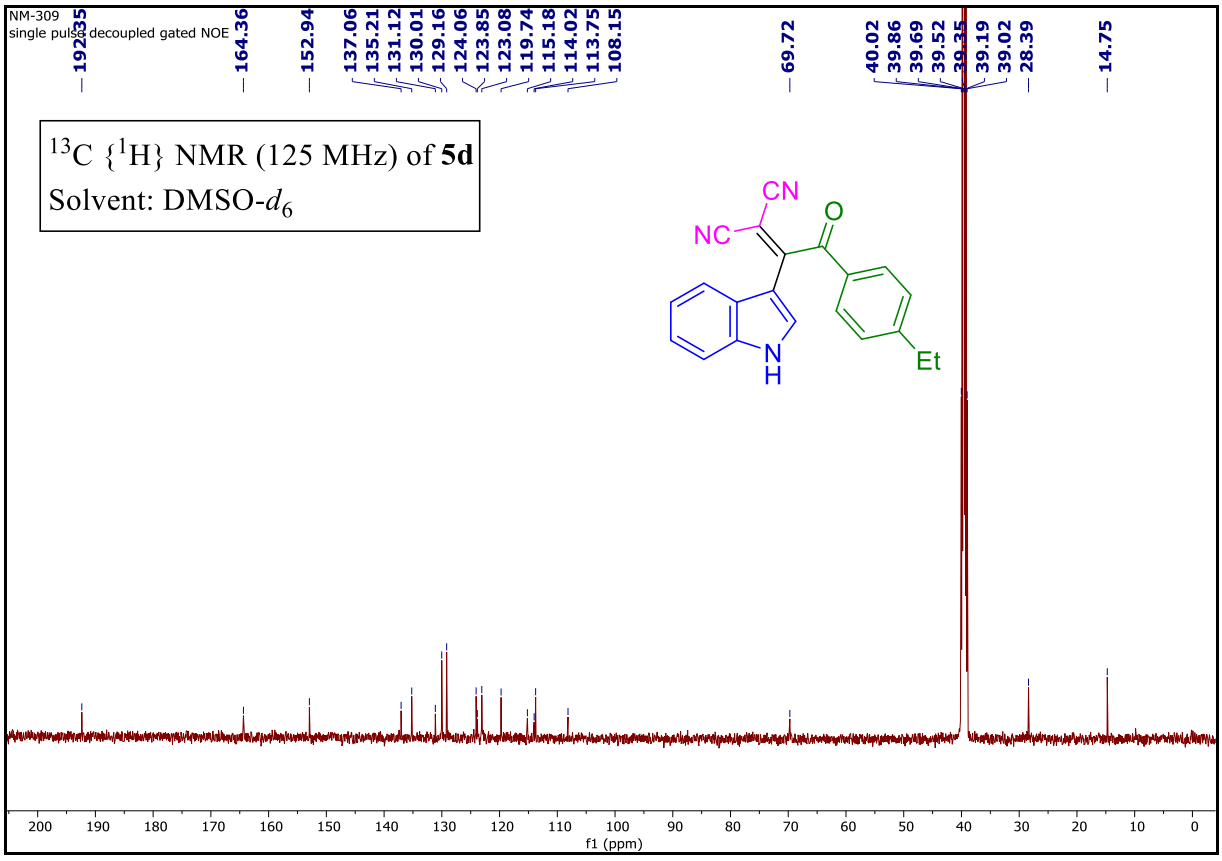
single pulse decoupled gated NOE
^{13}C {^{1}H} NMR (125 MHz) of **5c**
Solvent: DMSO-d_6
f1 (ppm)


NM-309
single_pulse
^{1}H NMR (500 MHz) of **5d**
Solvent: DMSO-d_6
CN
NC
O
N
H
Et
f1 (ppm)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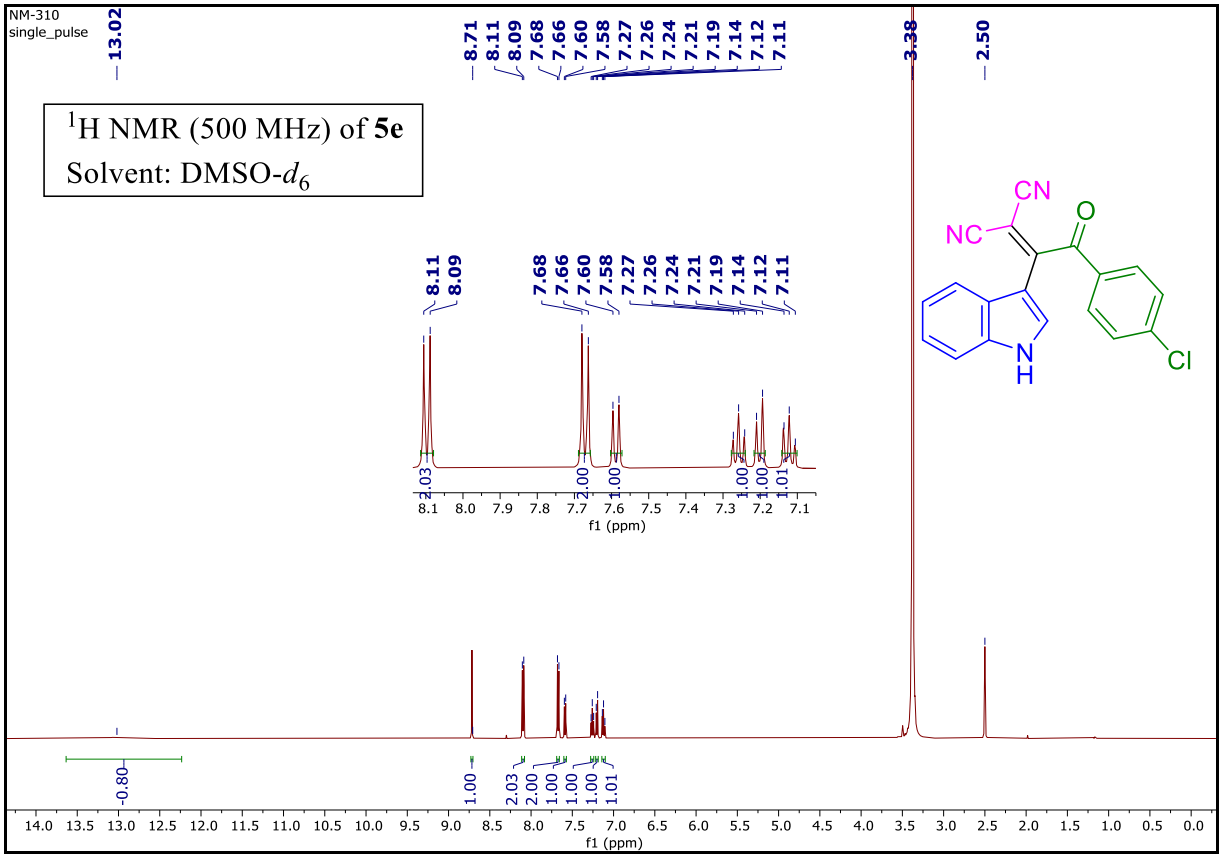
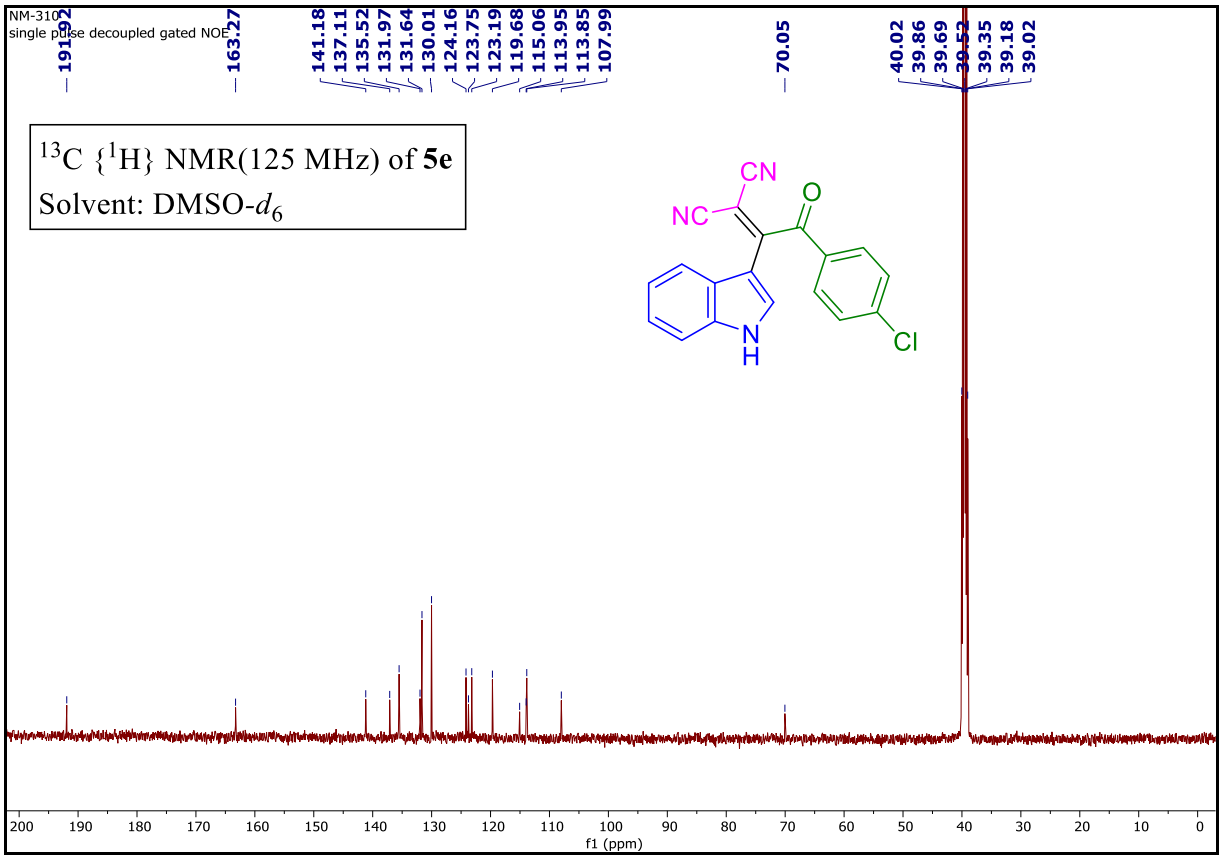
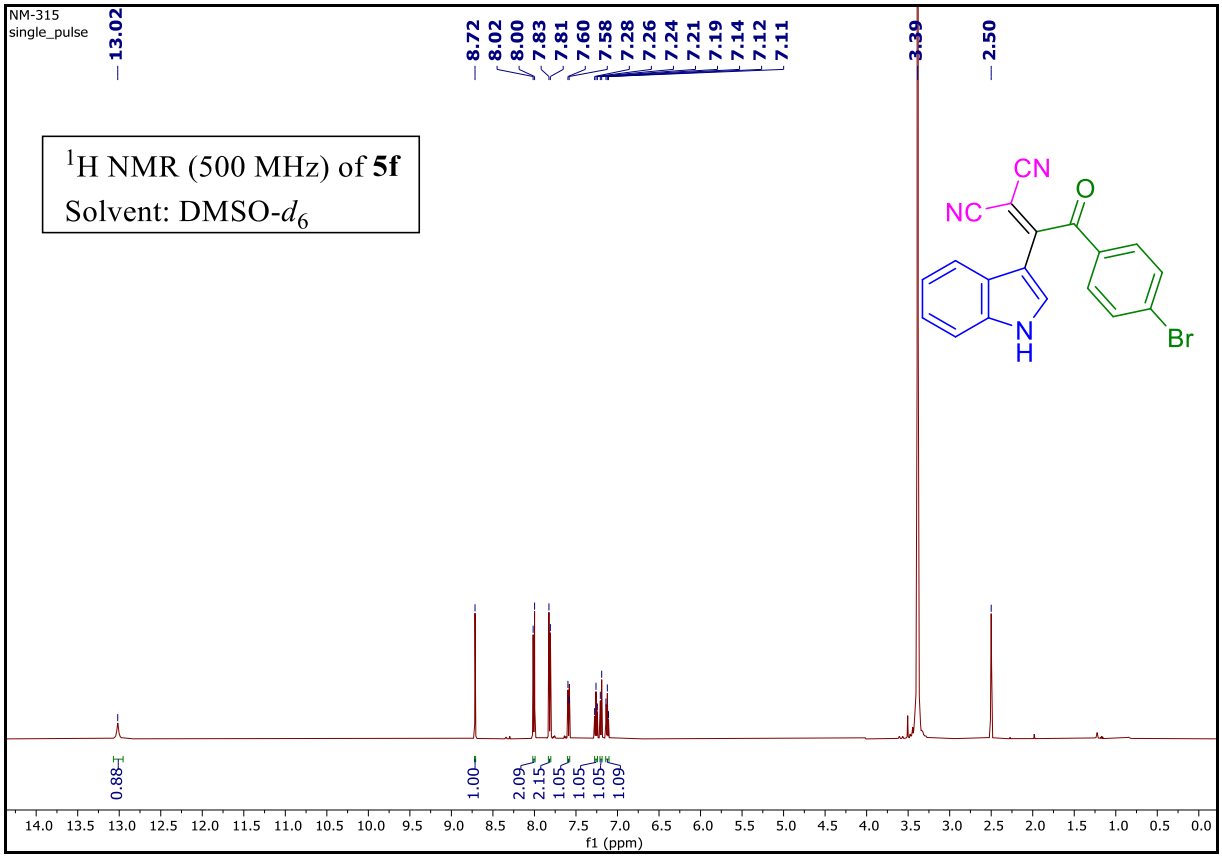
single pulse decoupled gated NOE
^{13}C {^{1}H} NMR (125 MHz) of **5d**
Solvent: DMSO-d_6
CN
NC
O
N
H
Et
f1 (ppm)


NM-310
single_pulse
^{1}H NMR (500 MHz) of **5e**
Solvent: DMSO-d_6
13.02
8.71
8.11
8.09
7.68
7.66
7.60
7.58
7.27
7.26
7.24
7.21
7.19
7.14
7.12
7.11
3.38
2.50
CN
NC
O
Cl
N
H
f1 (ppm)


NM-310
single pulse decoupled gated NOE
^{13}C {^{1}H} NMR(125 MHz) of **5e**
Solvent: DMSO-d_6
191.92
163.27
141.18
137.11
135.52
131.97
131.64
130.01
124.16
123.75
123.19
119.68
115.06
113.95
113.85
107.99
70.05
40.02
39.86
39.69
39.52
39.35
39.18
39.02
CN
NC
O
Cl
N
H
f1 (ppm)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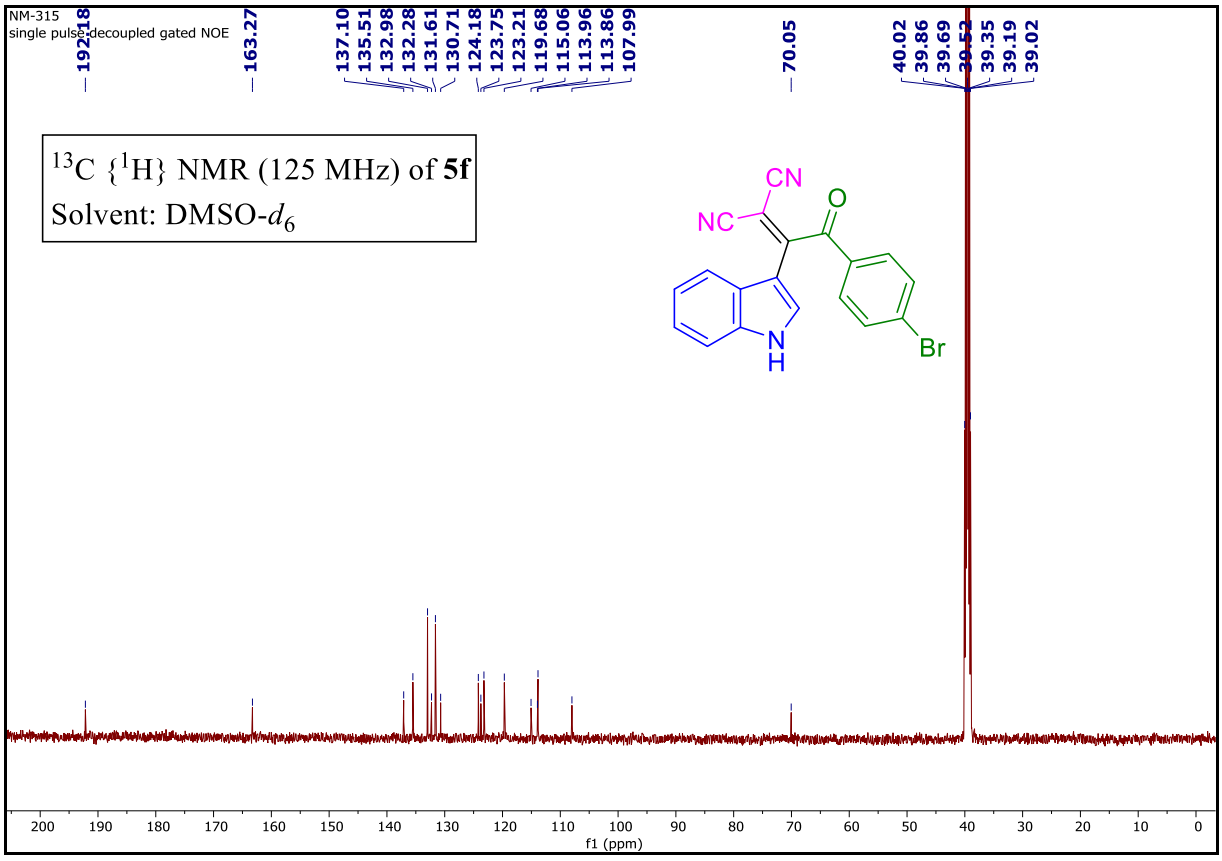
13.02
8.72
8.02
8.00
7.83
7.81
7.60
7.58
7.28
7.26
7.24
7.21
7.19
7.14
7.12
7.11
3.39
2.50
^{1}H NMR (500 MHz) of **5f**
Solvent: DMSO-d_6
CN
NC
O
N
H
Br
0.88
1.00
2.09
2.15
1.05
1.05
1.09
f1 (ppm)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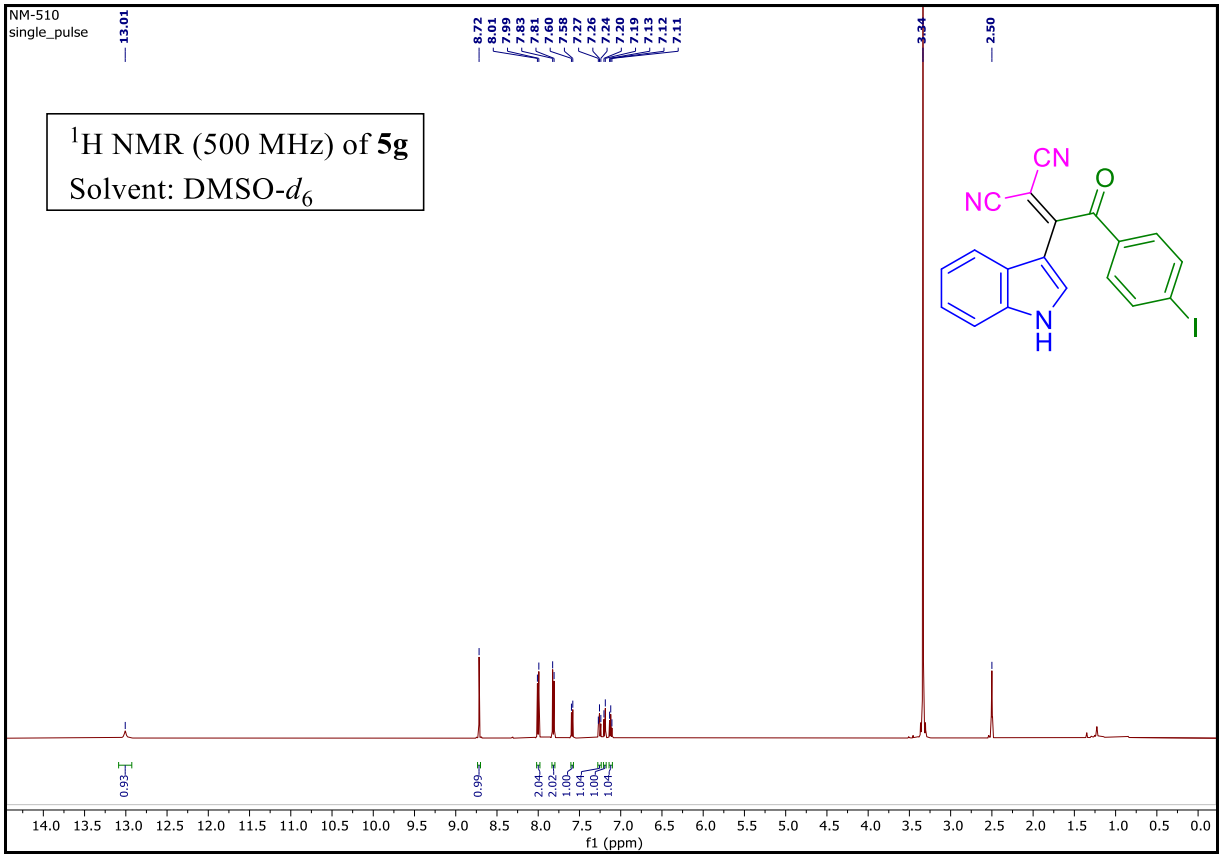
single pulse decoupled gated NOE
192.18
163.27
137.10
135.51
132.98
132.28
131.61
130.71
124.18
123.75
123.21
119.68
115.06
113.96
113.86
107.99
70.05
40.02
39.86
39.69
39.52
39.35
39.19
39.02
^{13}C {^{1}H} NMR (125 MHz) of **5f**
Solvent: DMSO-d_6
CN
NC
O
N
H
Br
f1 (ppm)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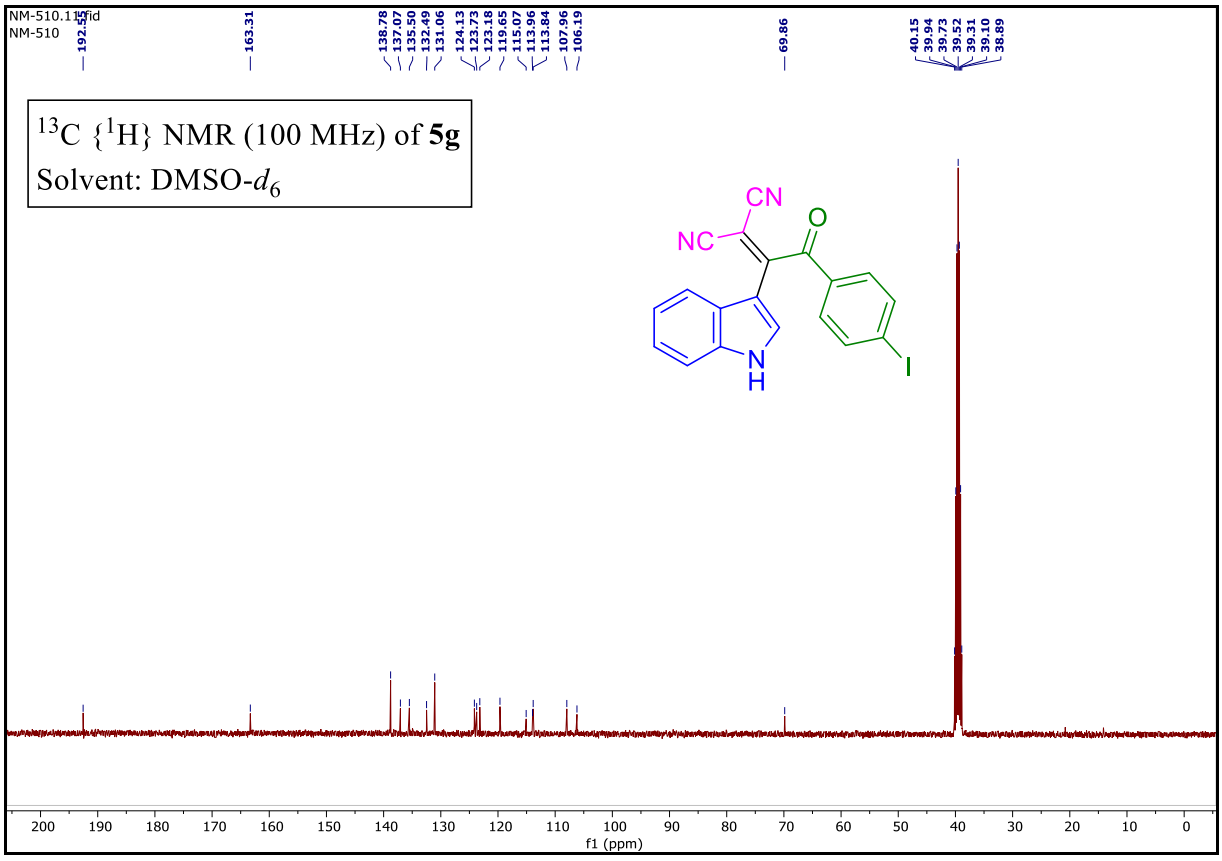
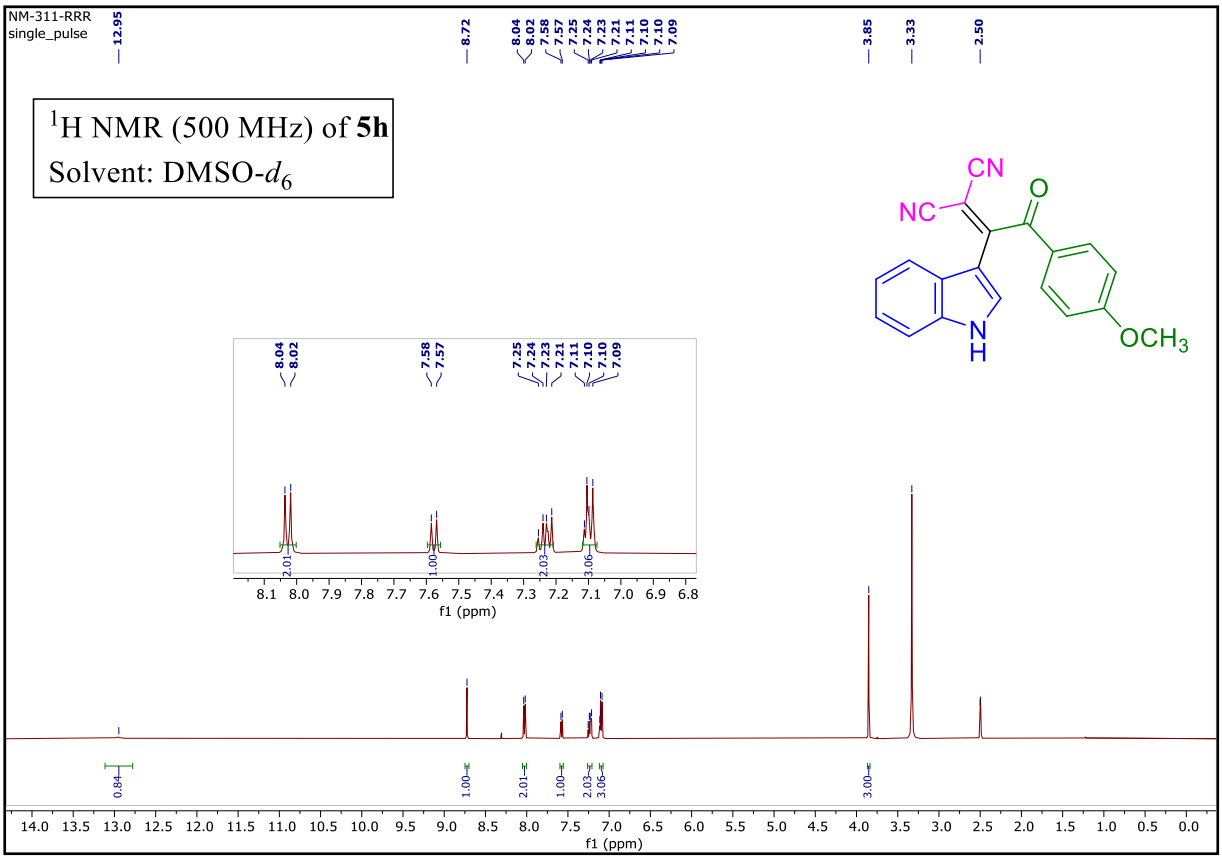
8.72
8.01
7.99
7.83
7.81
7.60
7.58
7.27
7.26
7.24
7.20
7.19
7.13
7.12
7.11
3.34
2.50
0.93
0.99
2.04
2.02
1.00
1.04
1.00
1.04
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
^{1}H NMR (500 MHz) of **5g**
Solvent: DMSO-d_6
CN
NC
O
N
H
I


NM-510.1.fid
NM-510
192.55
163.31
138.78
137.07
135.50
132.49
131.06
124.13
123.73
123.18
119.65
115.07
113.96
113.84
107.96
106.19
69.86
40.15
39.94
39.73
39.52
39.31
39.10
38.89
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
^{13}C {^{1}H} NMR (100 MHz) of **5g**
Solvent: DMSO-d_6
CN
NC
O
N
H
I


NM-311-RRR
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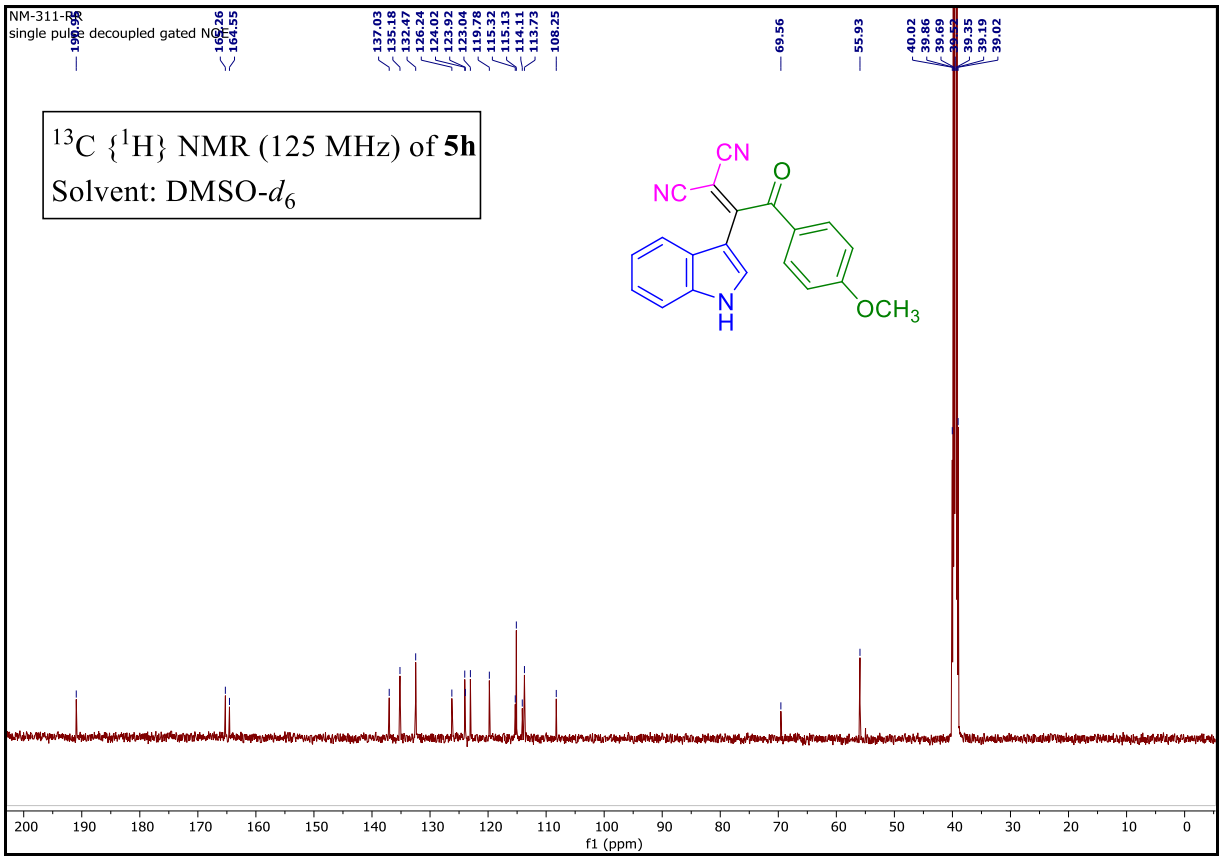
12.95
8.72
8.04
8.02
7.58
7.57
7.25
7.24
7.23
7.21
7.11
7.10
7.09
3.85
3.33
2.50
^{1}H NMR (500 MHz) of **5h**
Solvent: DMSO-d_6
CN
NC
O
N
H
OCH$_3$
f1 (ppm)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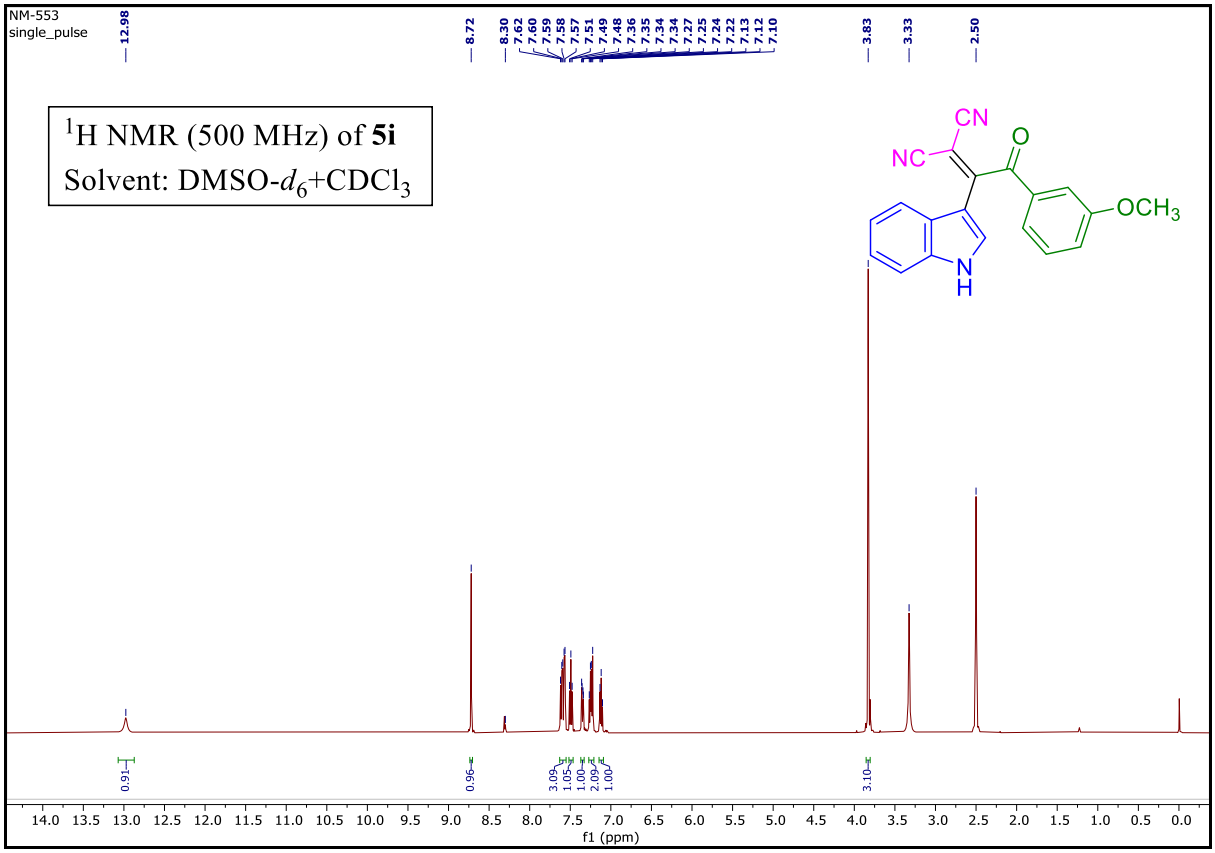
single pulse decoupled gated NOE
164.55
137.03
135.18
132.47
126.24
124.02
123.92
123.04
119.78
115.32
115.13
114.11
113.73
108.25
69.56
55.93
40.02
39.86
39.69
39.52
39.35
39.19
39.02
^{13}C {^{1}H} NMR (125 MHz) of **5h**
Solvent: DMSO-d_6
CN
NC
O
N
H
OCH$_3$
f1 (ppm)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8.30
7.62
7.60
7.59
7.58
7.57
7.51
7.49
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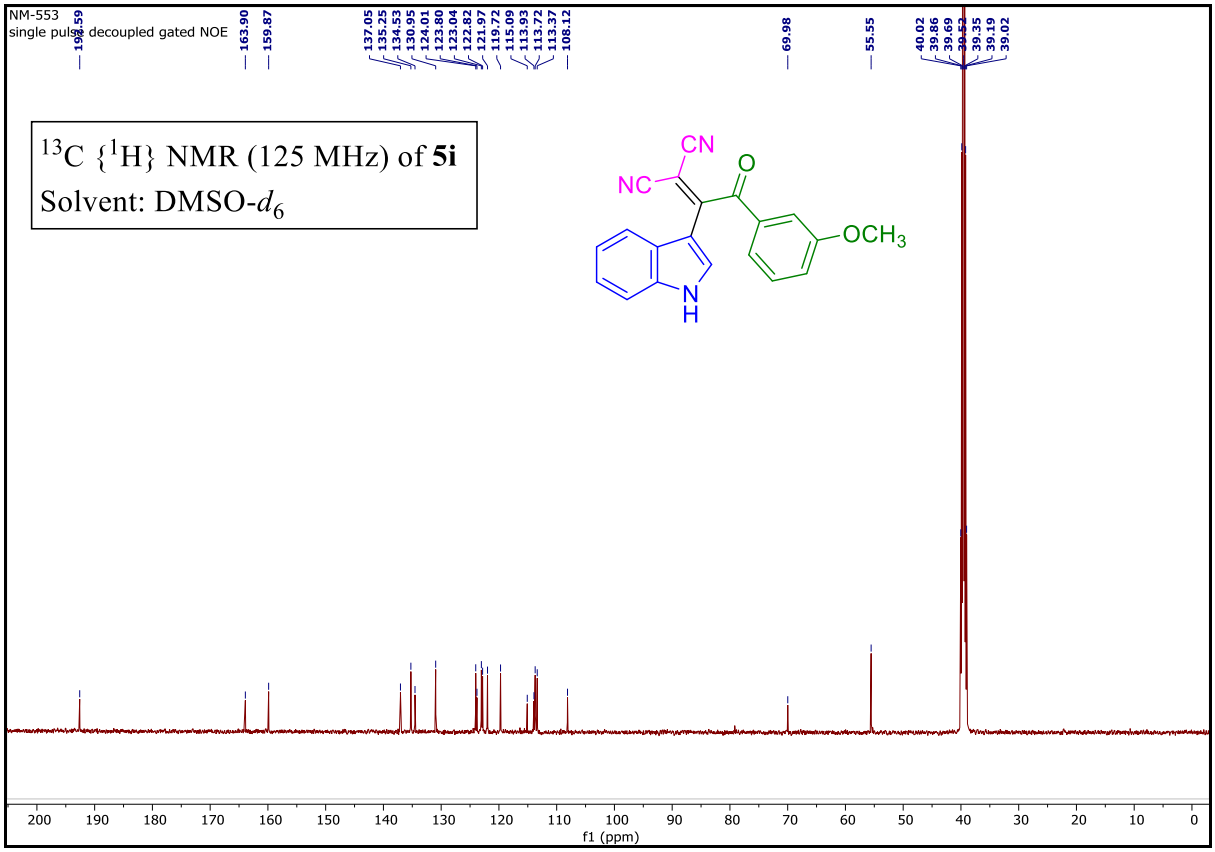
7.36
7.35
7.34
7.34
7.27
7.25
7.24
7.22
7.13
7.12
7.10
3.83
3.33
2.50
^{1}H NMR (500 MHz) of **5i**
Solvent: DMSO-d_6+$CDCl_3$
CN
NC
O
OCH3
N
H
0.91
0.96
3.09
1.05
1.00
2.09
1.00
3.10
f1 (ppm)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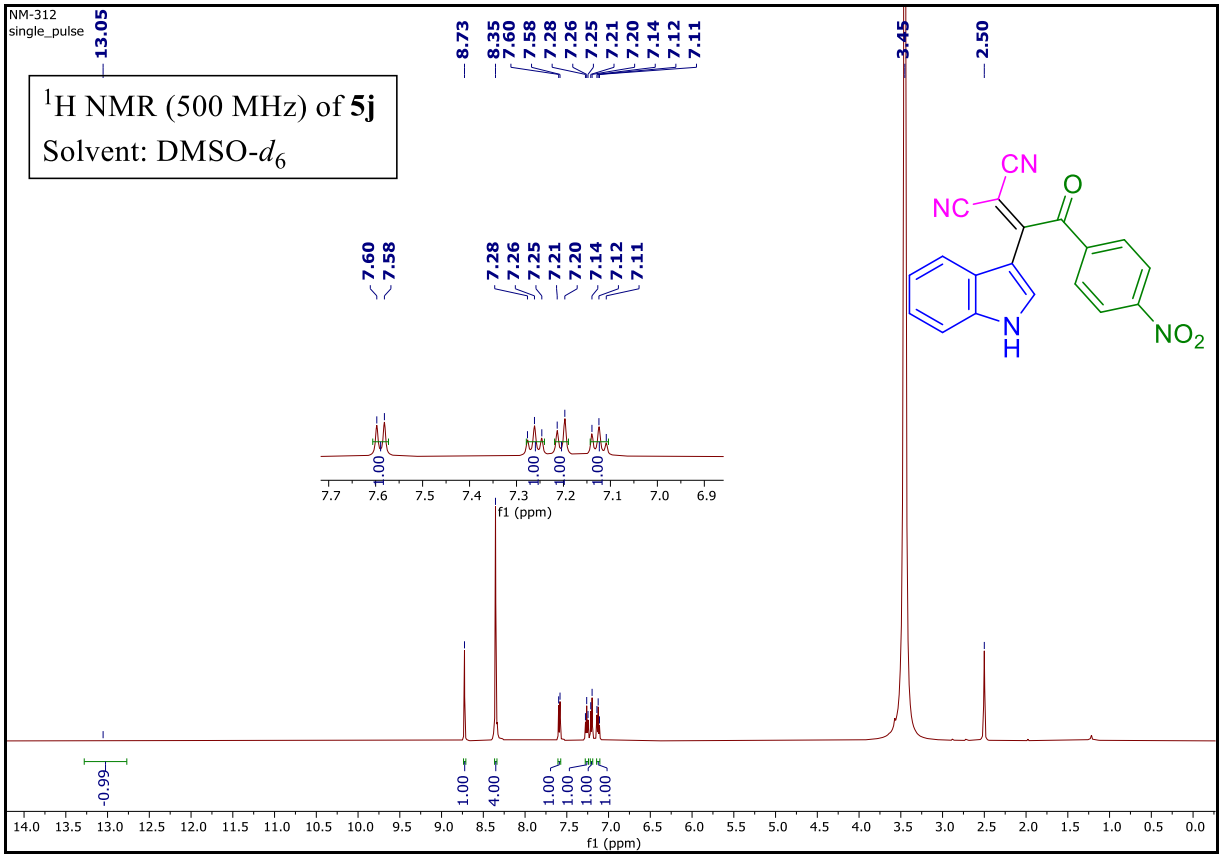
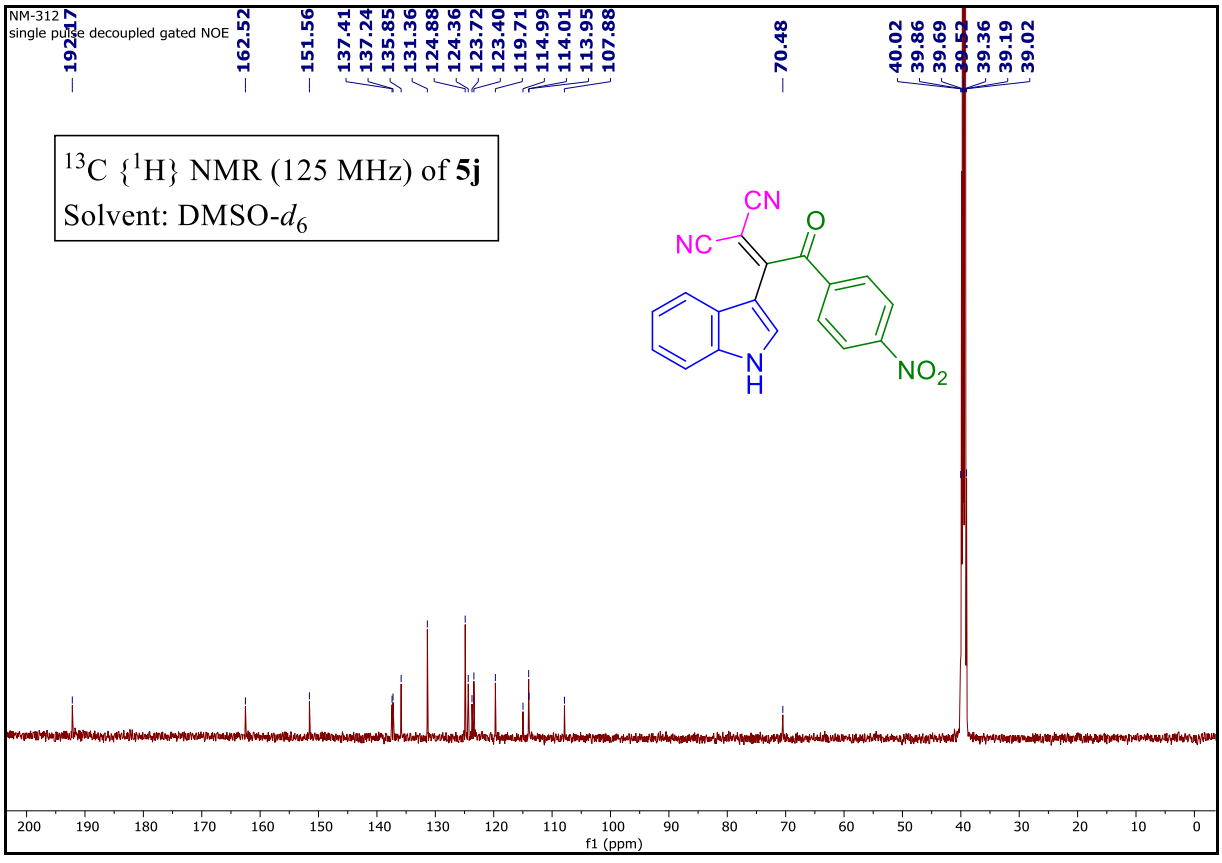
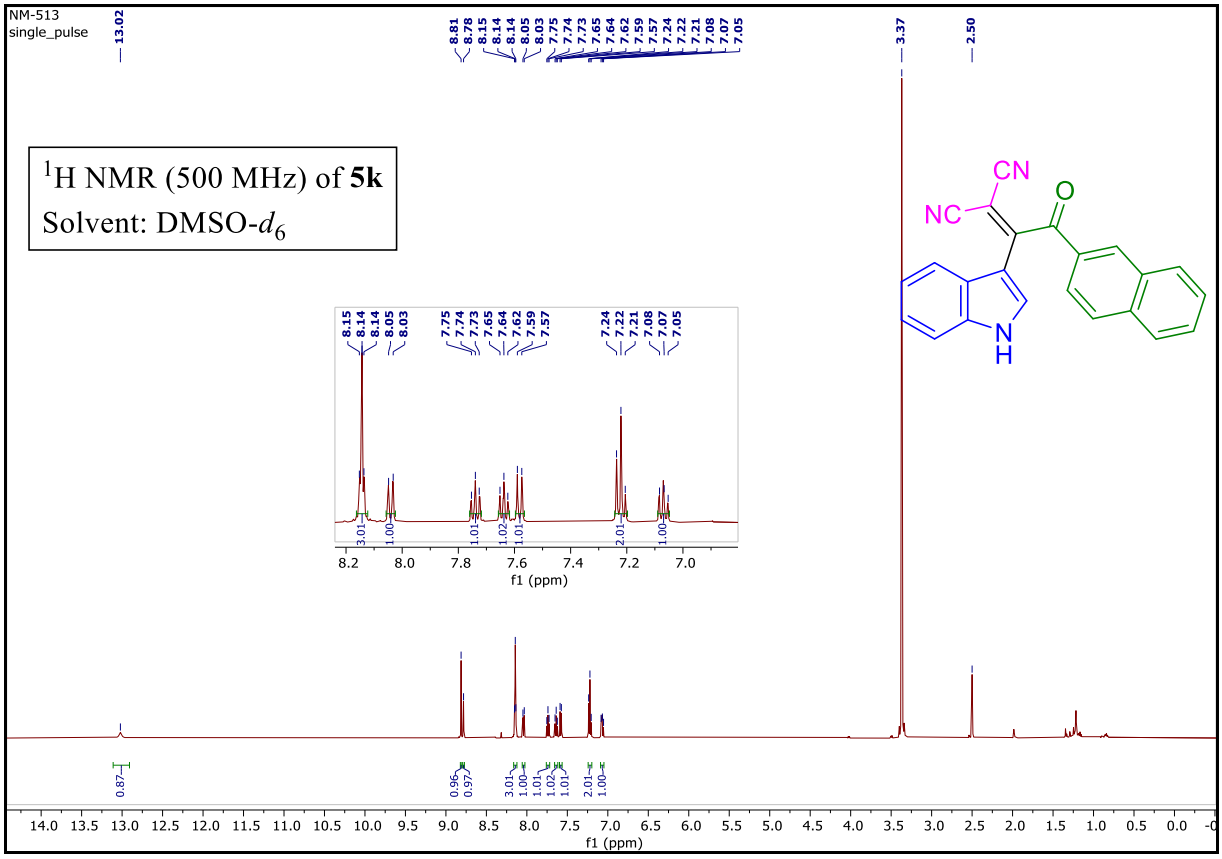
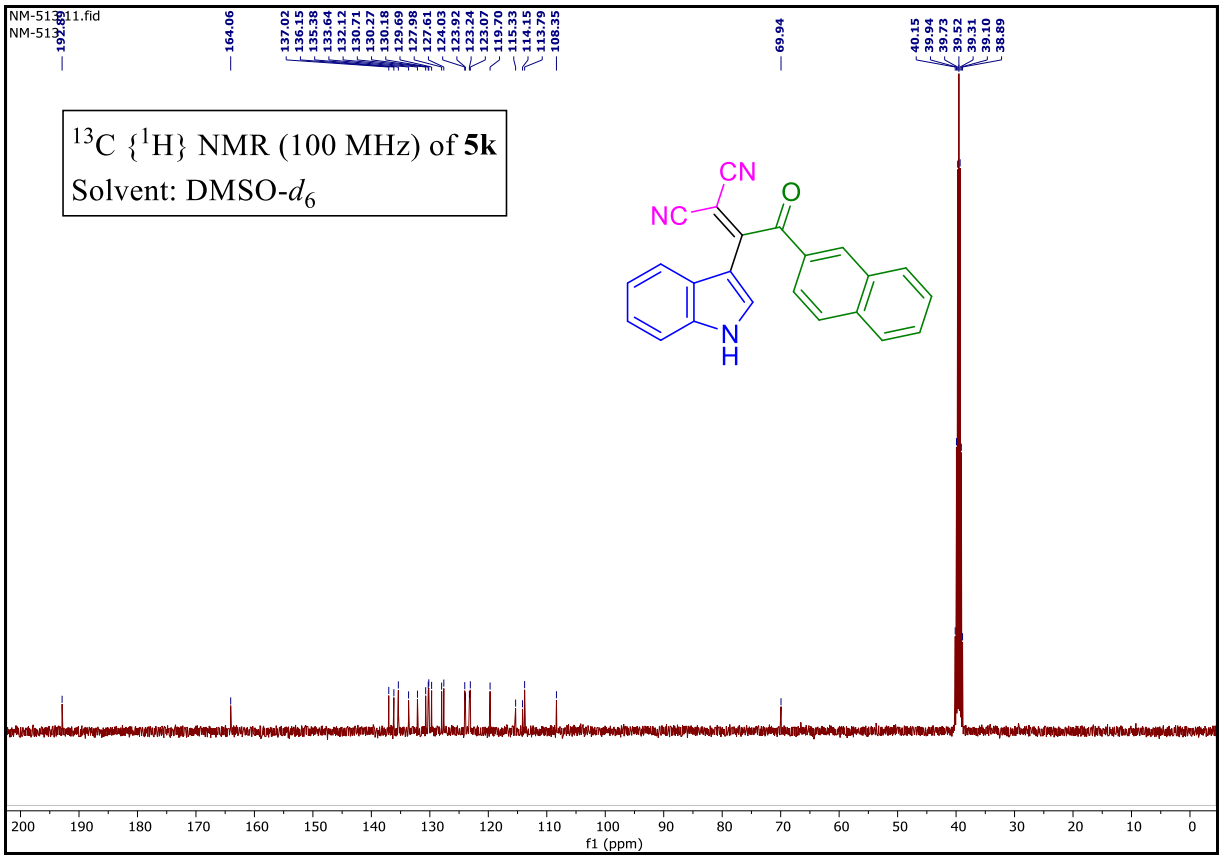
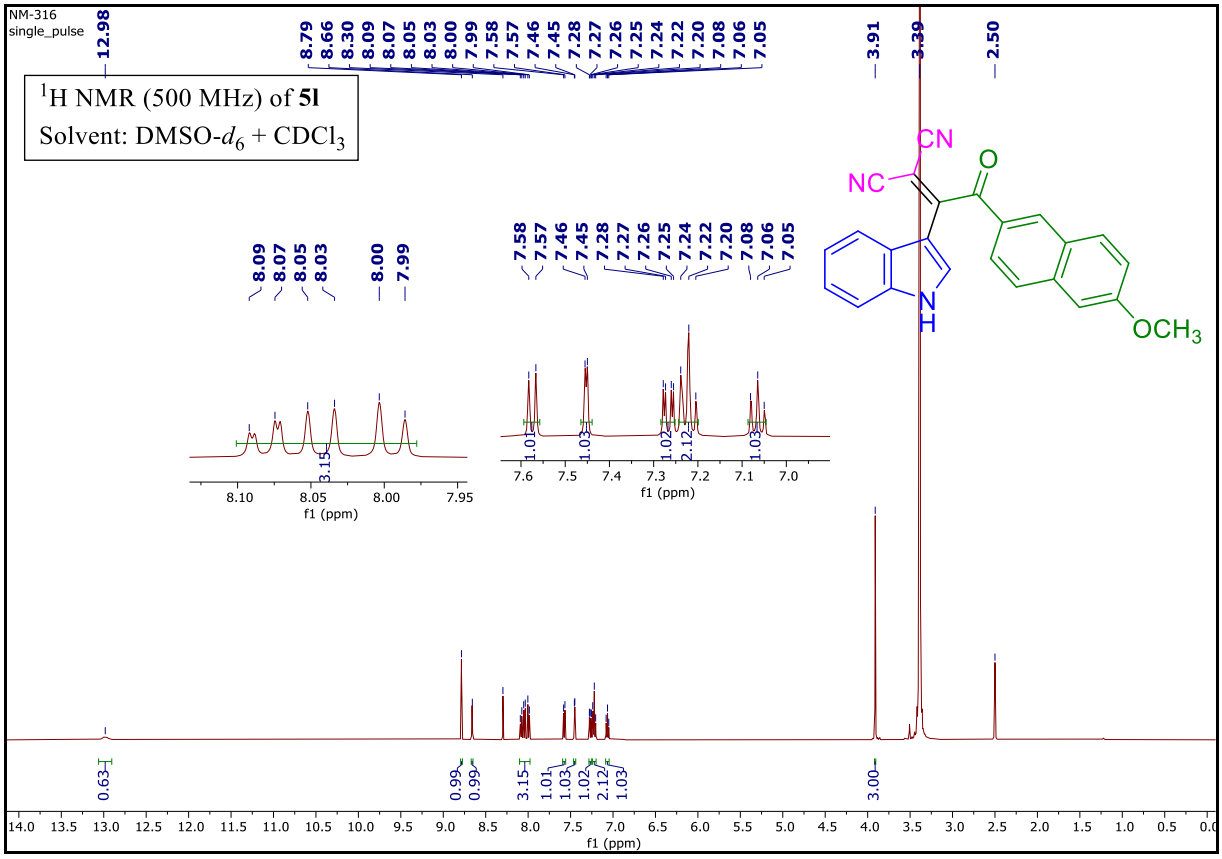
196.59
163.90
159.87
137.05
135.25
134.53
130.95
124.01
123.80
123.04
122.82
121.97
119.72
115.09
113.93
113.72
113.37
108.12
69.98
55.55
40.02
39.86
39.69
39.53
39.35
39.19
39.02
^{13}C {^{1}H} NMR (125 MHz) of **5i**
Solvent: DMSO-d_6
CN
NC
O
OCH3
N
H
f1 (ppm)

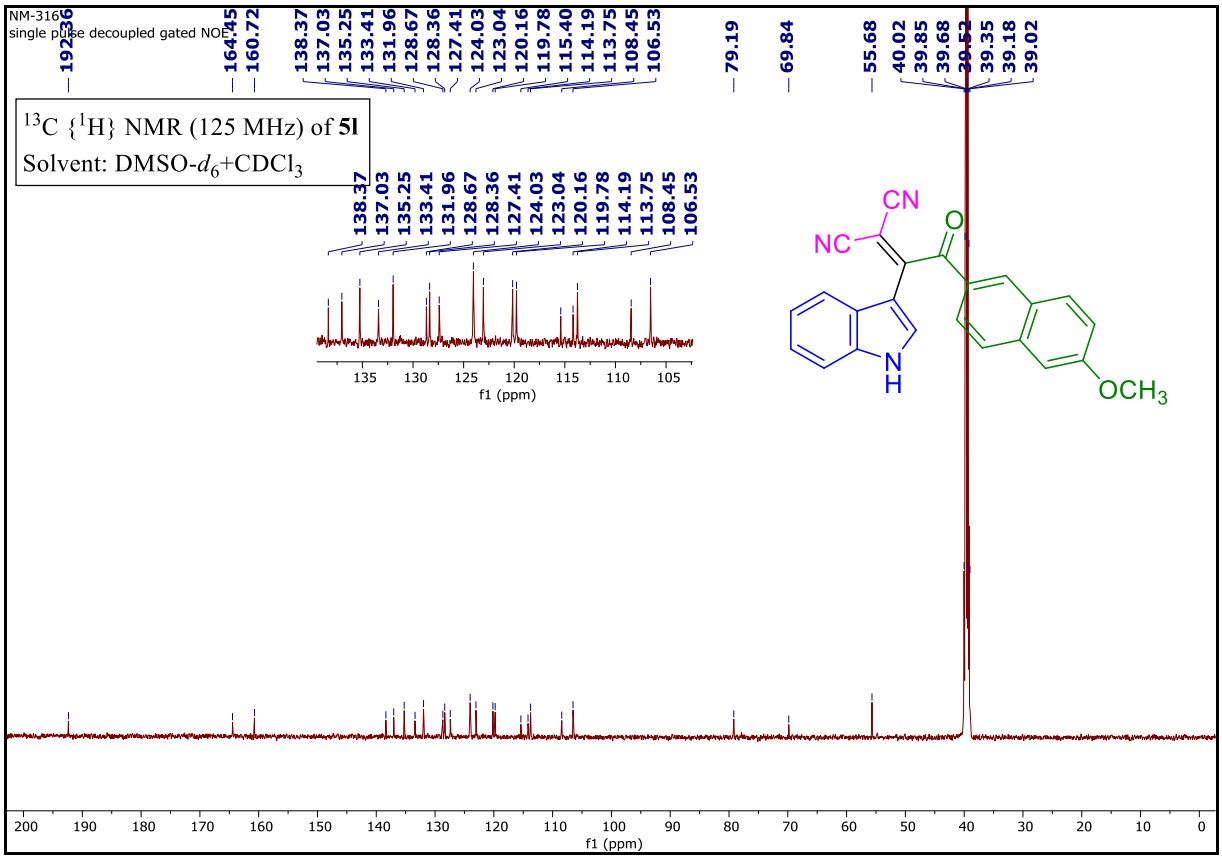

NM-312
single_pulse
^{1}H NMR (500 MHz) of **5j**
Solvent: DMSO-d_6
13.05
8.73
8.35
7.60
7.58
7.28
7.26
7.25
7.21
7.20
7.14
7.12
7.11
3.45
2.50
CN
NC
O
NH
NO2
f1 (ppm)

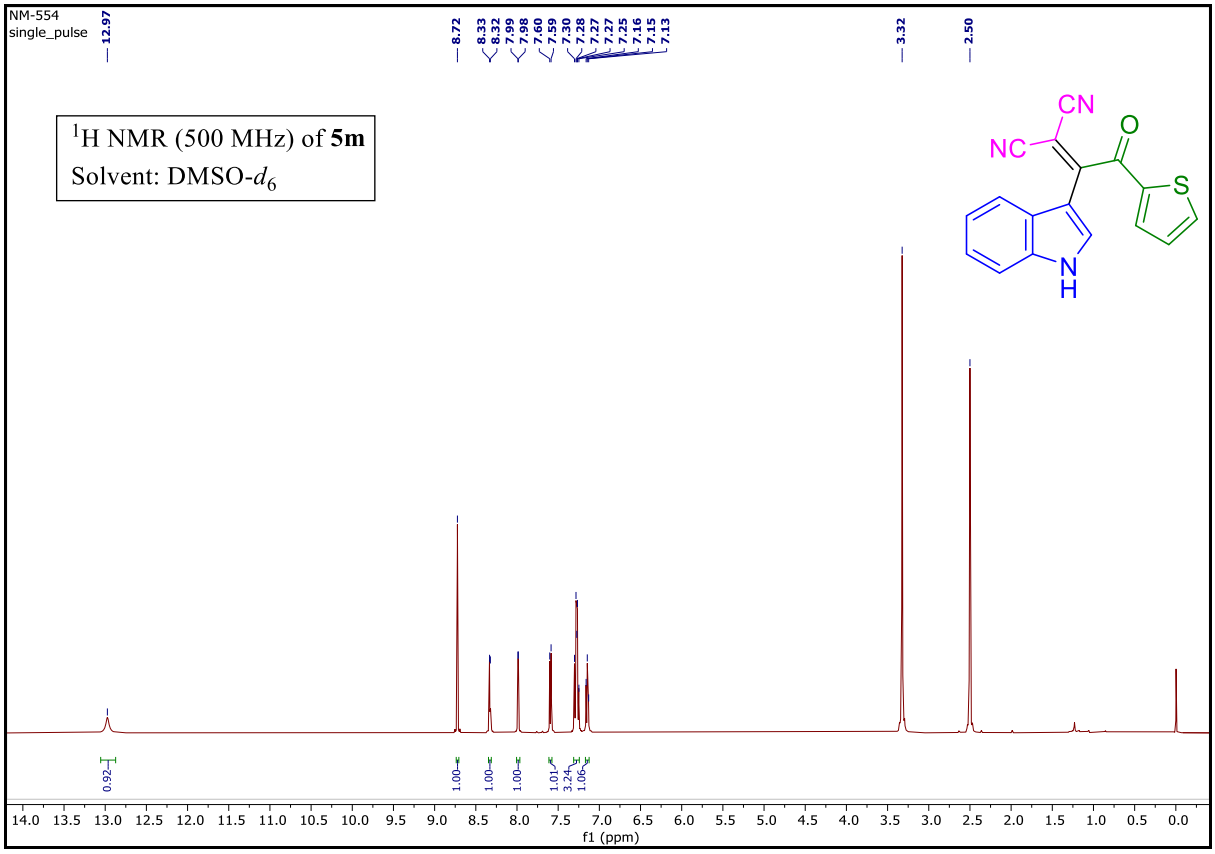

NM-312
single pulse decoupled gated NOE
^{13}C {^{1}H} NMR (125 MHz) of **5j**
Solvent: DMSO-d_6
192.17
162.52
151.56
137.41
137.24
135.85
131.36
124.88
124.36
123.72
123.40
119.71
114.99
114.01
113.95
107.88
70.48
40.02
39.86
39.69
39.52
39.36
39.19
39.02
CN
NC
O
NH
NO2
f1 (ppm)

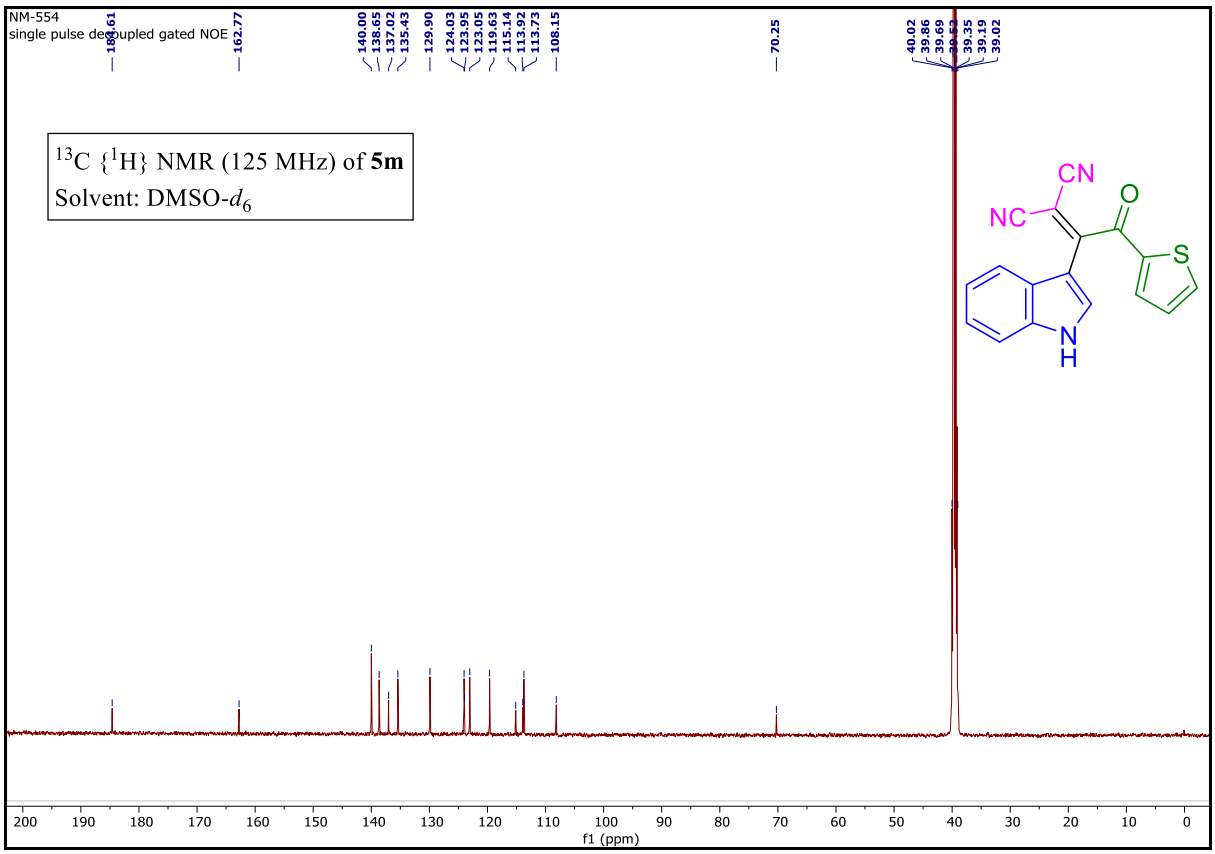

NM-513
single_pulse
^{1}H NMR (500 MHz) of **5k**
Solvent: DMSO-d_6
CN
NC
O
N
H
f1 (ppm)

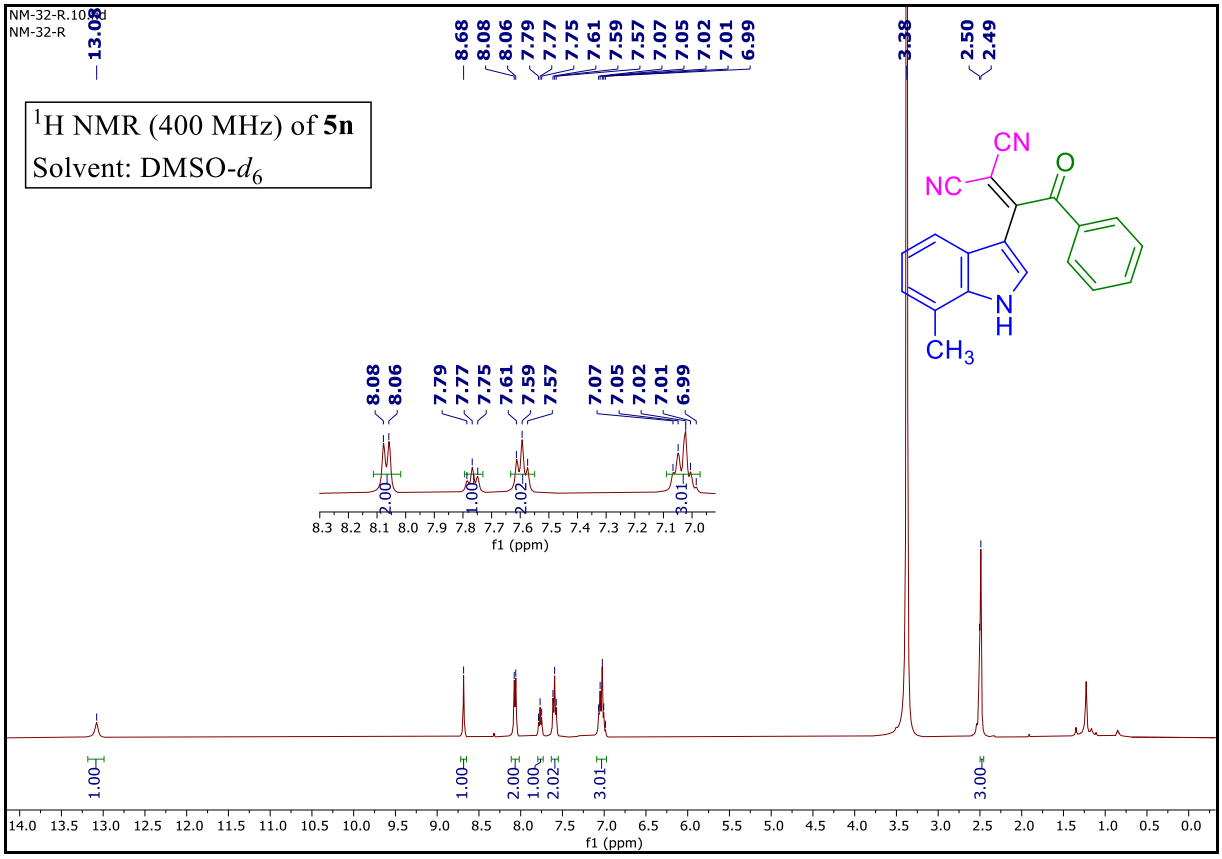

NM-513-11.fid
^{13}C {^{1}H} NMR (100 MHz) of **5k**
Solvent: DMSO-d_6
CN
NC
O
N
H
f1 (ppm)

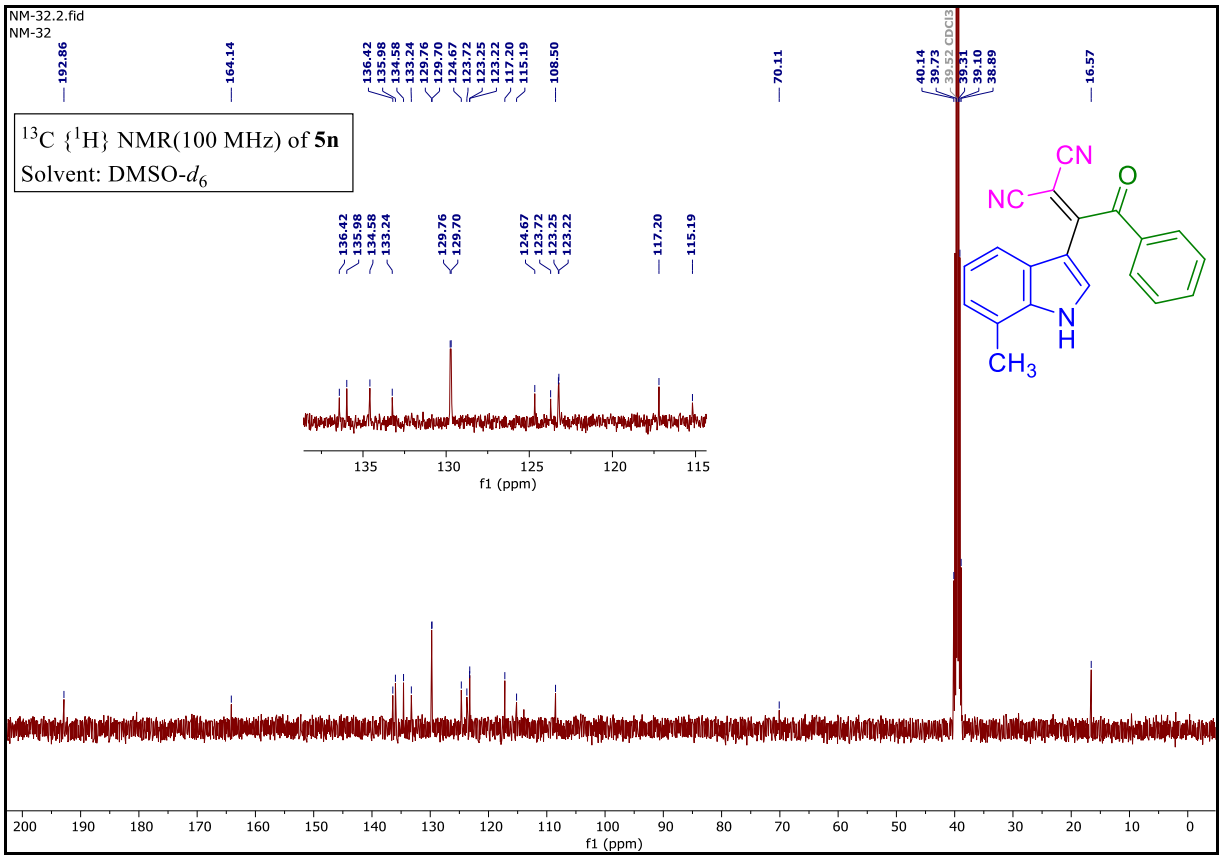

NM-316
single_pulse
^{1}H NMR (500 MHz) of **5l**
Solvent: DMSO-d_6 + $CDCl_3$
CN
NC
O
N
H
OCH_3
f1 (ppm)

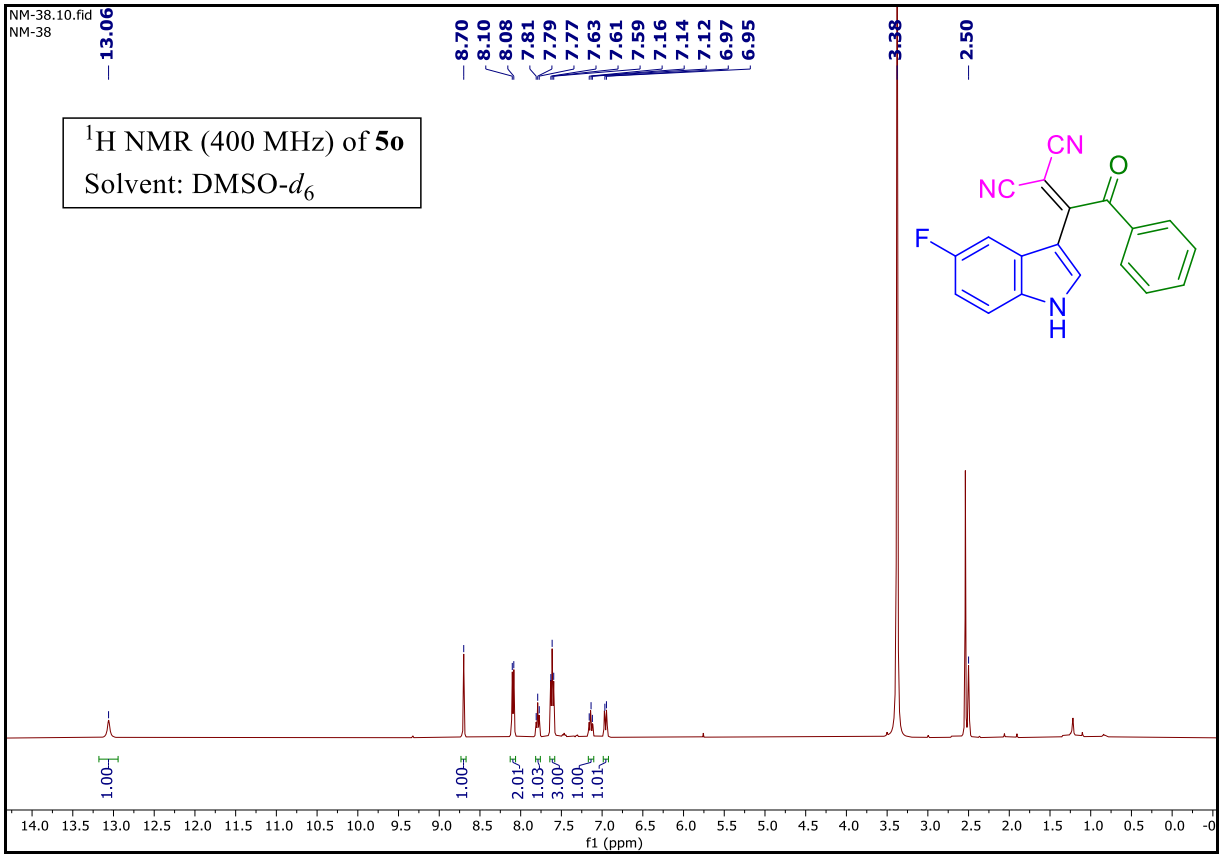

NM-316
single pulse decoupled gated NOE
^{13}C {^{1}H} NMR (125 MHz) of **5l**
Solvent: DMSO-d_6+$CDCl_3$
CN
NC
O
N
H
OCH_3
f1 (ppm)

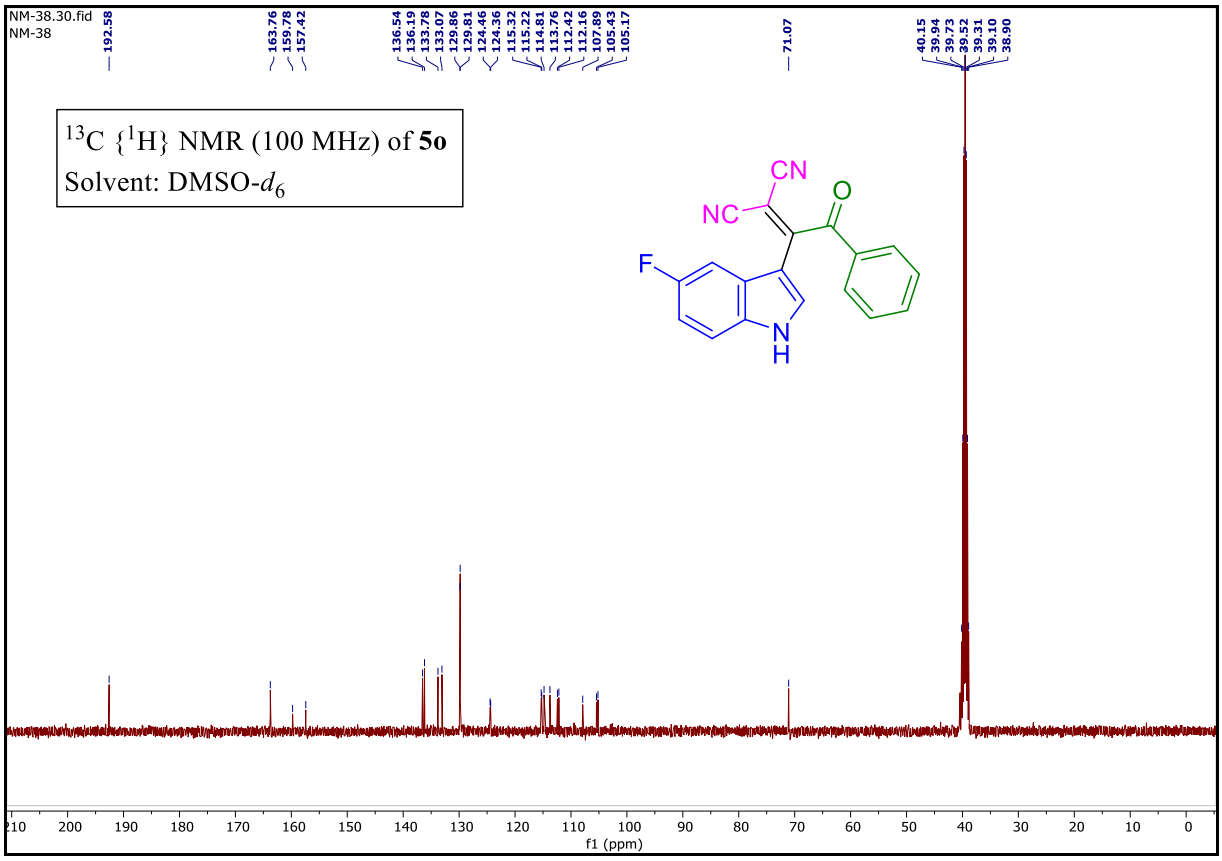

NM-554
single_pulse
12.97
8.72
8.33
8.32
7.99
7.98
7.60
7.59
7.30
7.28
7.27
7.25
7.16
7.15
7.13
3.32
2.50
^{1}H NMR (500 MHz) of **5m**
Solvent: DMSO-d_6
CN
NC
O
S
N
H
0.92
1.00
1.00
1.00
1.01
3.24
1.06
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

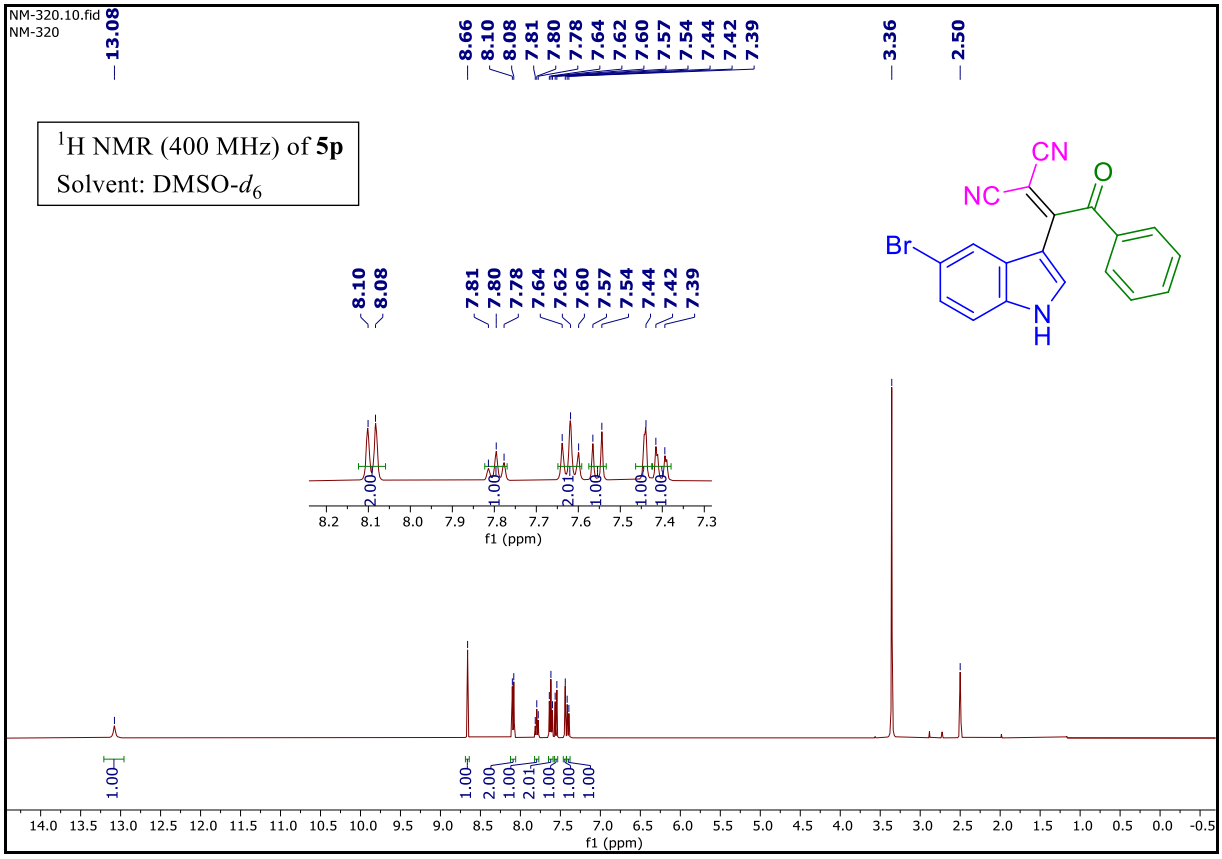

NM-554
single pulse decoupled gated NOE
183.61
162.77
140.00
138.65
137.02
135.43
129.90
124.03
123.95
123.05
119.63
115.14
113.92
113.73
108.15
70.25
40.02
39.86
39.69
39.53
39.35
39.19
39.02
^{13}C {^{1}H} NMR (125 MHz) of **5m**
Solvent: DMSO-d_6
CN
NC
O
S
N
H
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

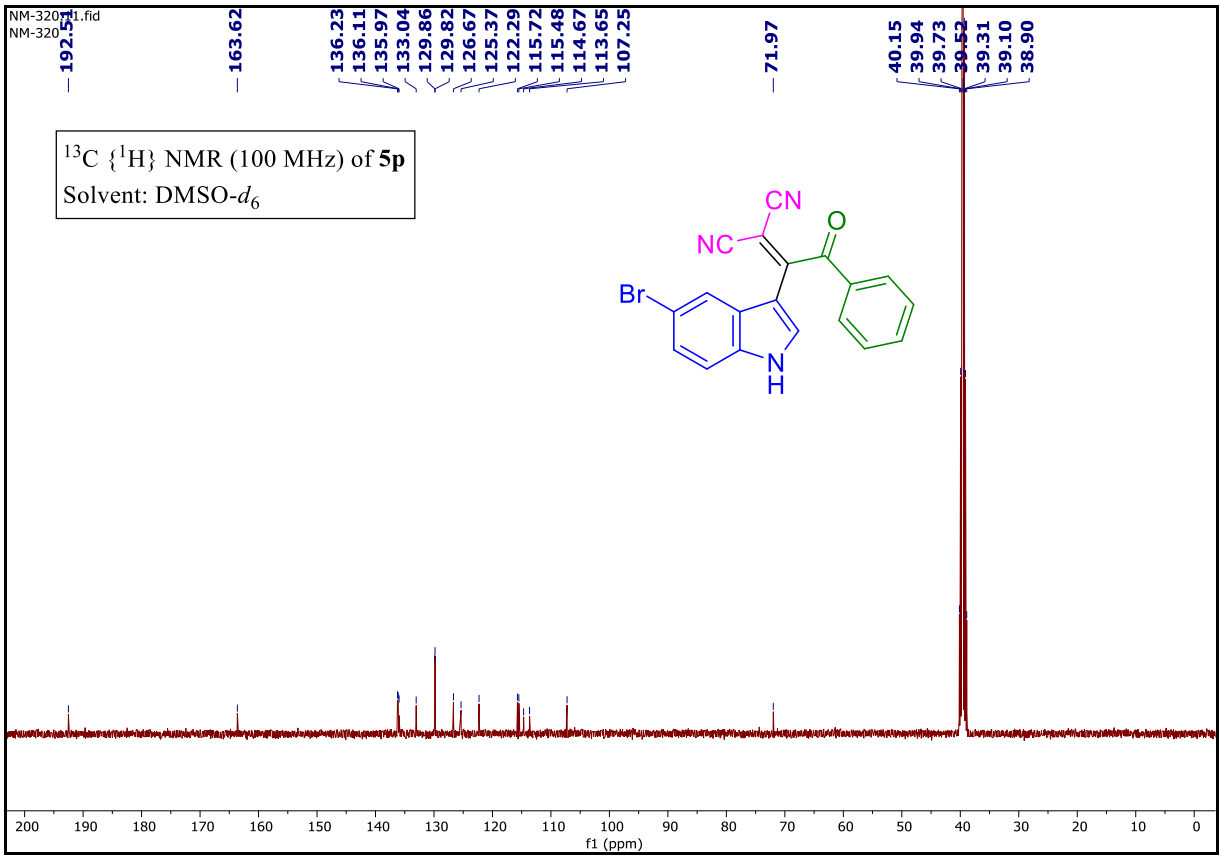

NM-32-R.10.fid
NM-32-R
13.02
8.68
8.08
8.06
7.79
7.77
7.75
7.61
7.59
7.57
7.07
7.05
7.02
7.01
6.99
3.38
2.50
2.49
^{1}H NMR (400 MHz) of **5n**
Solvent: DMSO-d_6
CN
NC
O
N
H
CH$_3$
f1 (ppm)

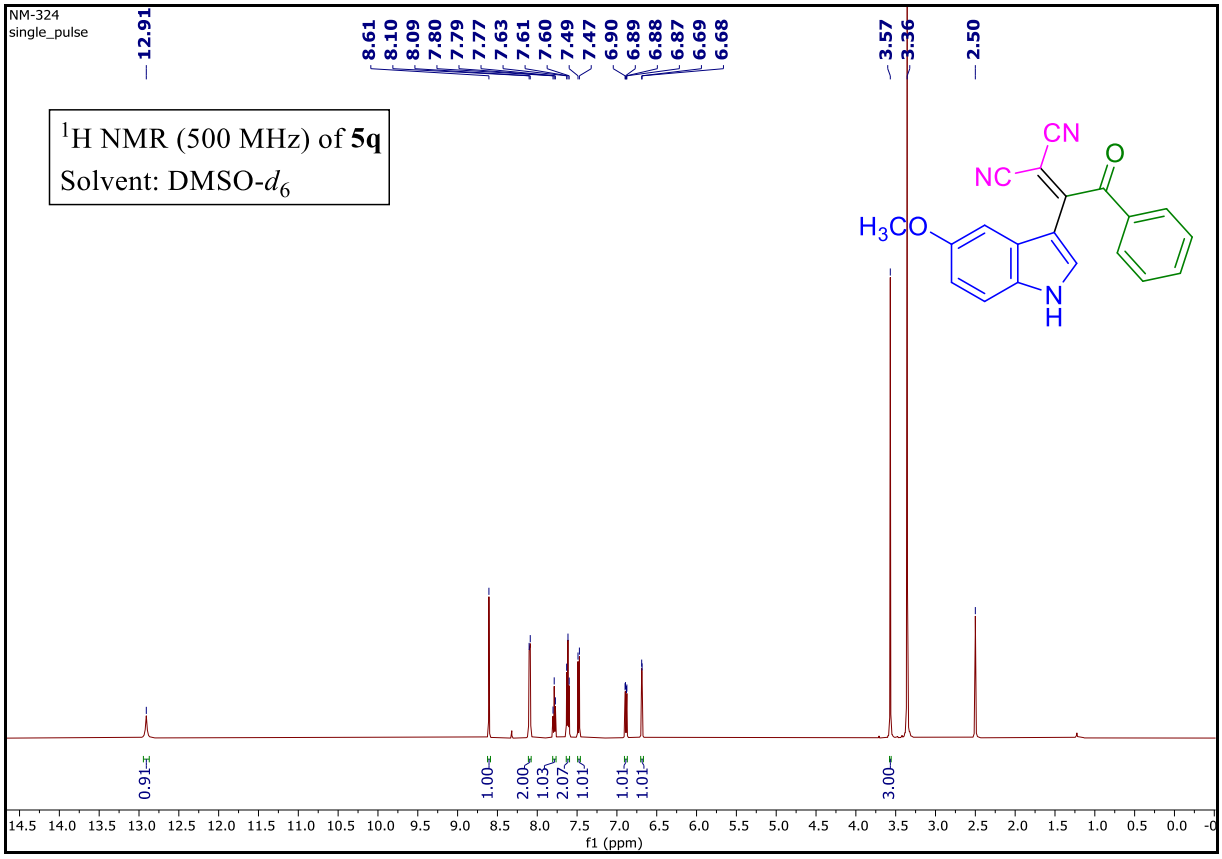

NM-32.2.fid
NM-32
192.86
164.14
136.42
135.98
134.58
133.24
129.76
129.70
124.67
123.72
123.25
123.22
117.20
115.19
108.50
70.11
40.14
39.73
39.52 CDCl3
39.31
39.10
38.89
16.57
^{13}C {^{1}H} NMR(100 MHz) of **5n**
Solvent: DMSO-d_6
CN
NC
O
N
H
CH$_3$
f1 (ppm)

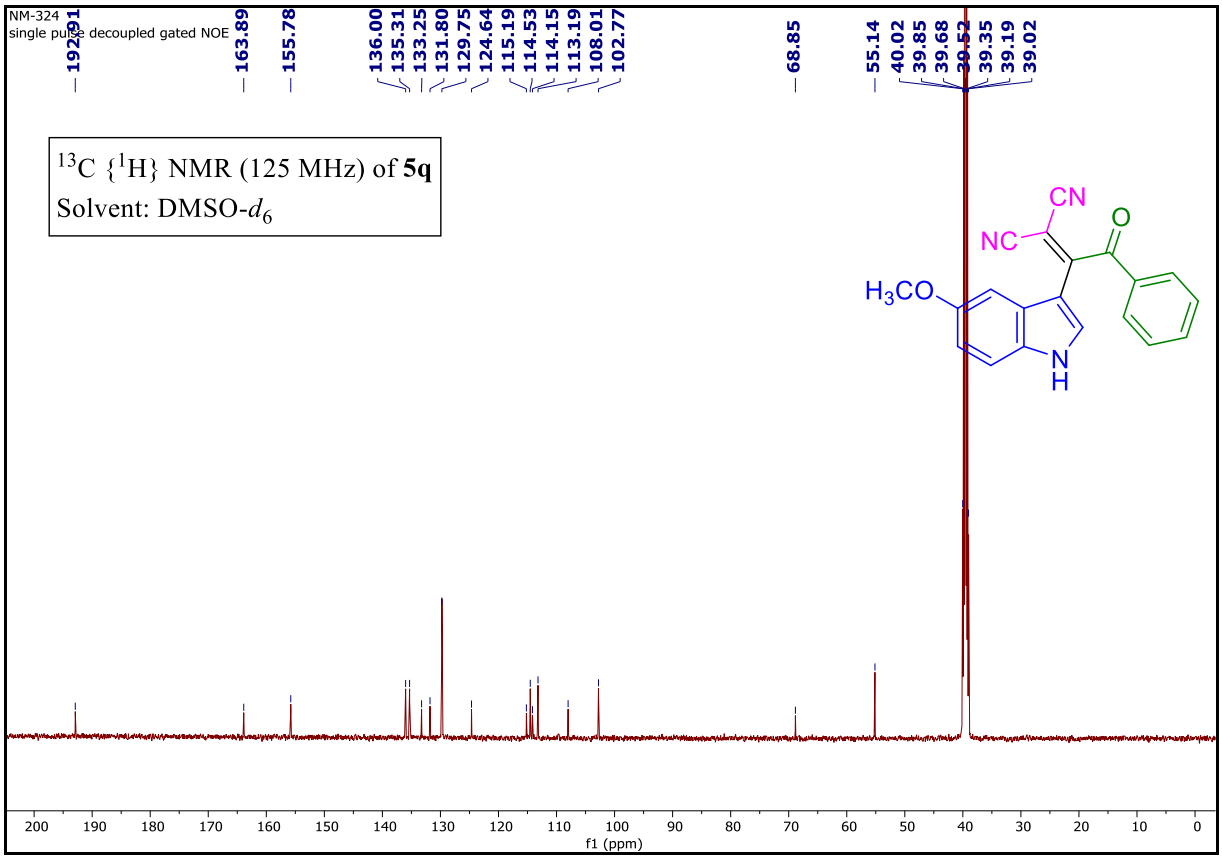

NM-38.10.fid
NM-38
13.06
8.70
8.10
8.08
7.81
7.79
7.77
7.63
7.61
7.59
7.16
7.14
7.12
6.97
6.95
3.38
2.50
1H NMR (400 MHz) of 5o
Solvent: DMSO-d6
CN
NC
O
F
N
H
1.00
1.00
2.01
1.03
3.00
1.00
1.01
f1 (ppm)

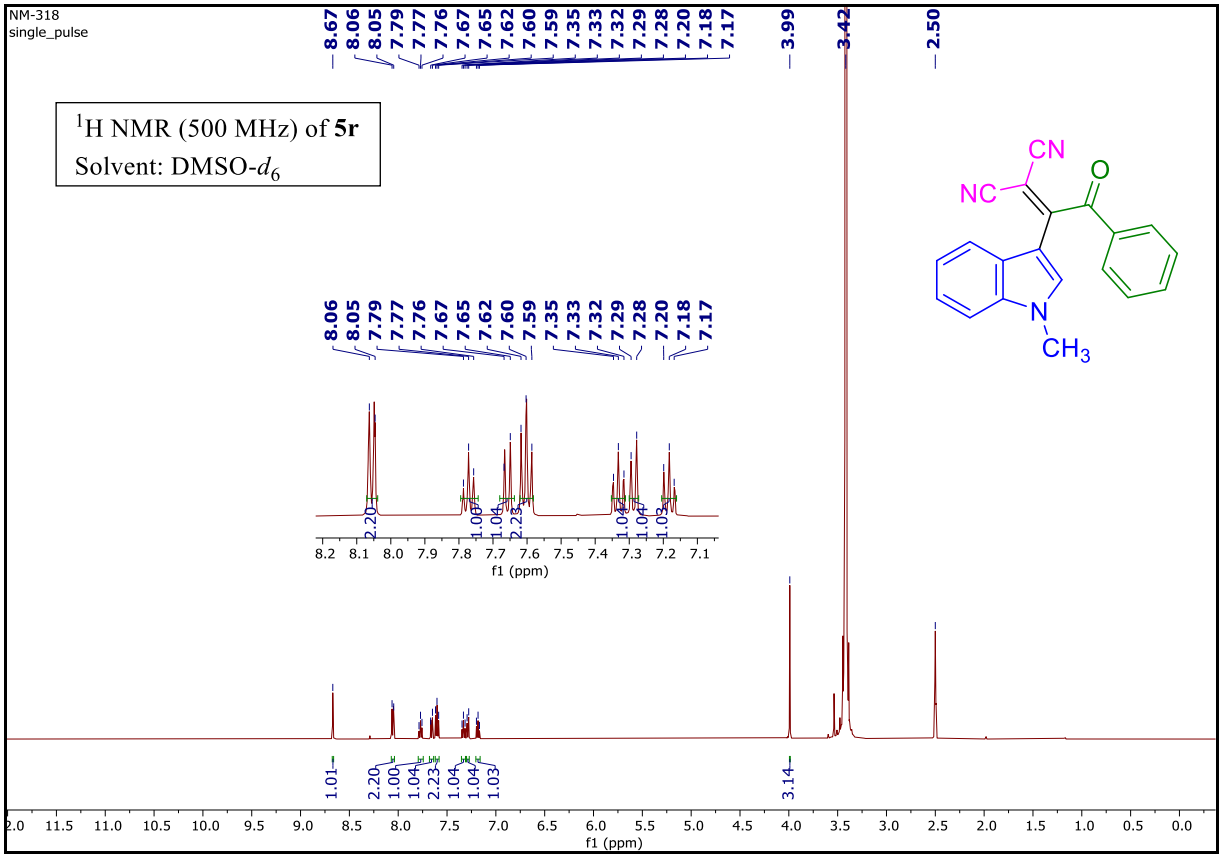

NM-38.30.fid
NM-38
192.58
163.76
159.78
157.42
136.54
136.19
133.78
133.07
129.86
129.81
124.46
124.36
115.32
115.22
114.81
113.76
112.42
112.16
107.89
105.43
105.17
71.07
40.15
39.94
39.73
39.52
39.31
39.10
38.90
13C {1H} NMR (100 MHz) of 5o
Solvent: DMSO-d6
CN
NC
O
F
N
H
f1 (ppm)

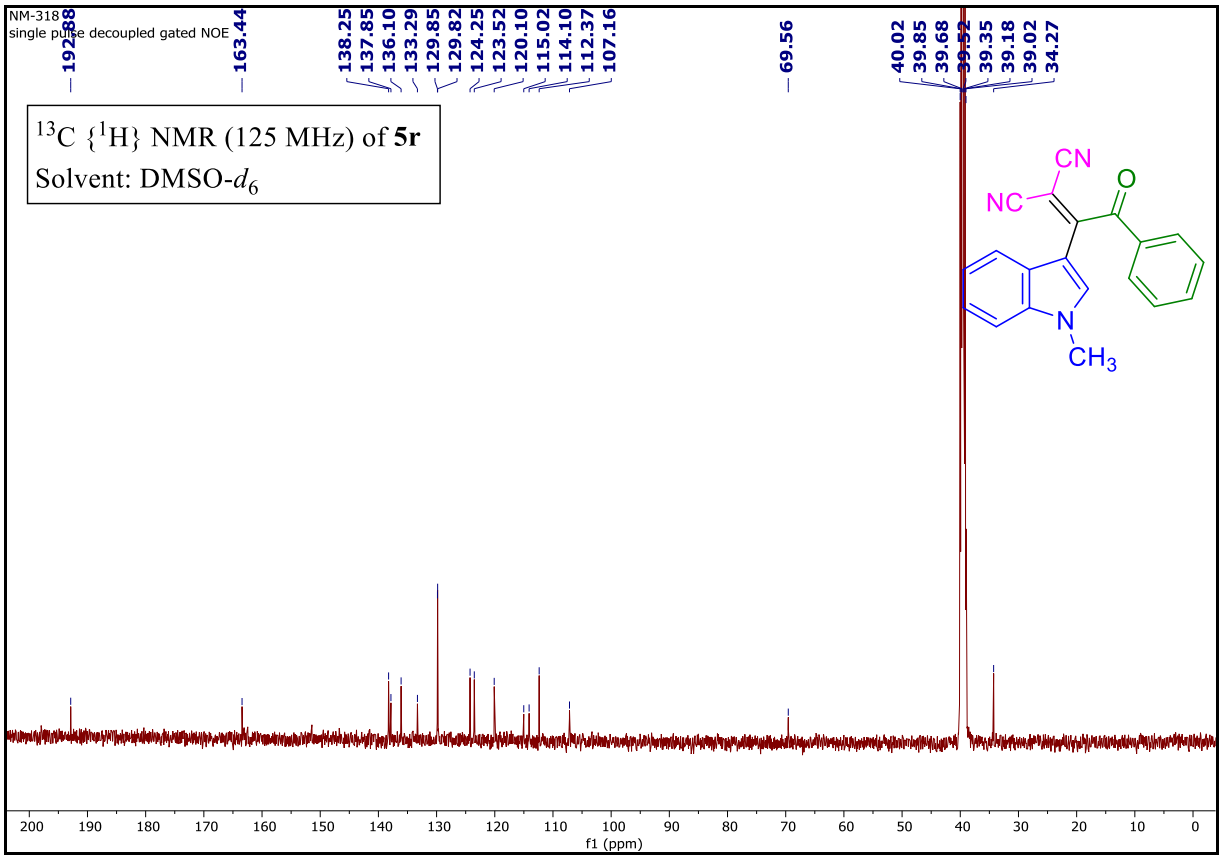

NM-320.10.fid
NM-320
13.08
8.66
8.10
8.08
7.81
7.80
7.78
7.64
7.62
7.60
7.57
7.54
7.44
7.42
7.39
3.36
2.50
^{1}H NMR (400 MHz) of **5p**
Solvent: DMSO-d_6
CN
NC
O
Br
N
H
f1 (ppm)

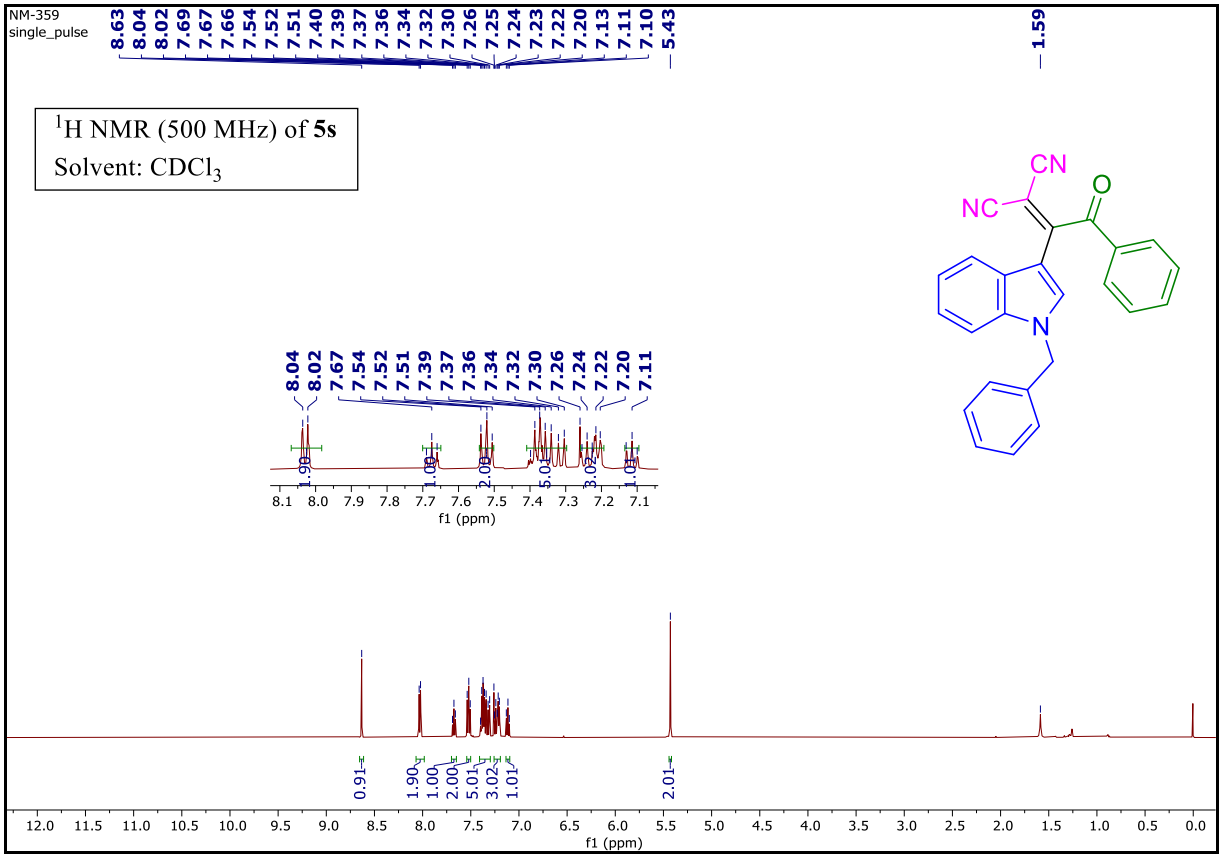

NM-320-C1.fid
NM-320
192.51
163.62
136.23
136.11
135.97
133.04
129.86
129.82
126.67
125.37
122.29
115.72
115.48
114.67
113.65
107.25
71.97
40.15
39.94
39.73
39.52
39.31
39.10
38.90
^{13}C {^{1}H} NMR (100 MHz) of **5p**
Solvent: DMSO-d_6
CN
NC
O
Br
N
H
f1 (ppm)

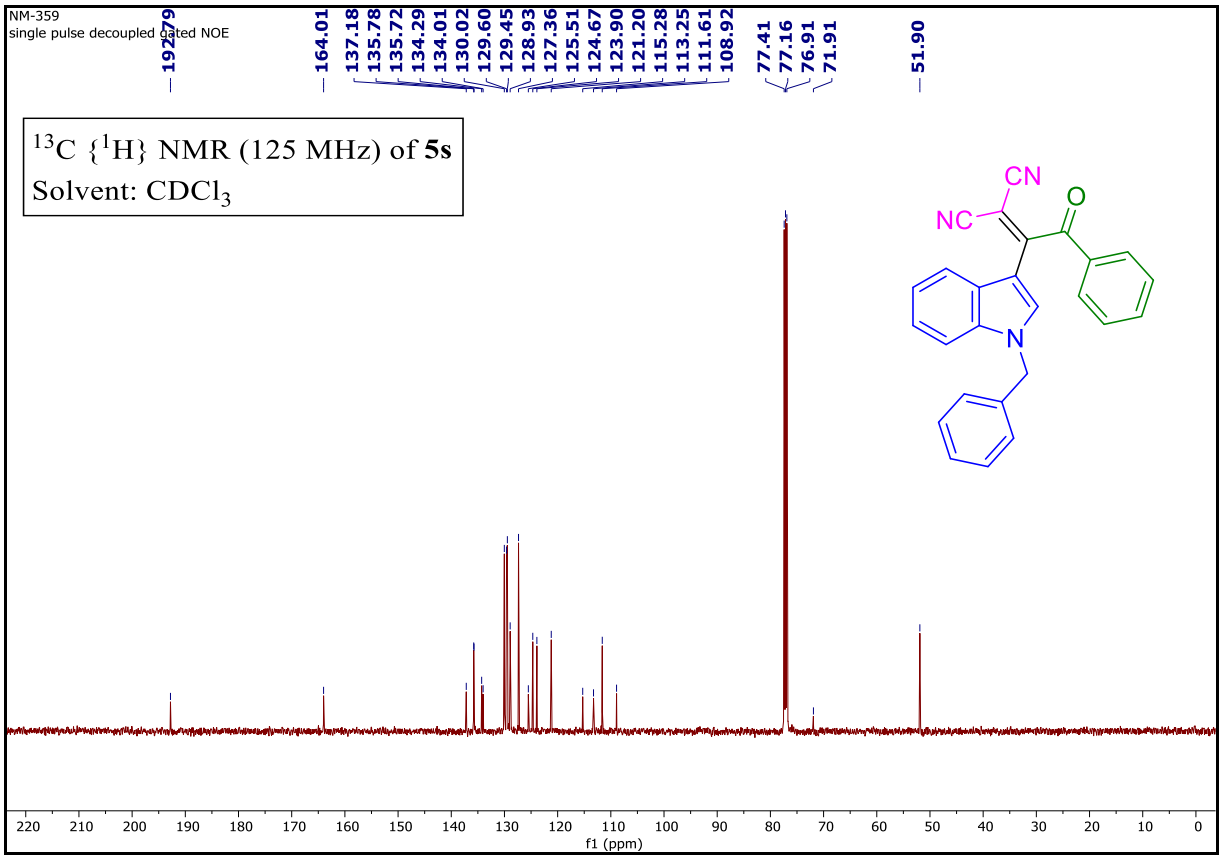

NM-324
single_pulse
12.91
8.61
8.10
8.09
7.80
7.79
7.77
7.63
7.61
7.60
7.49
7.47
6.90
6.89
6.88
6.87
6.69
6.68
3.57
3.36
2.50
^{1}H NMR (500 MHz) of **5q**
Solvent: DMSO-d_6
CN
NC
O
H_3CO
N
H
0.91
1.00
2.00
1.03
2.07
1.01
1.01
1.01
3.00
f1 (ppm)

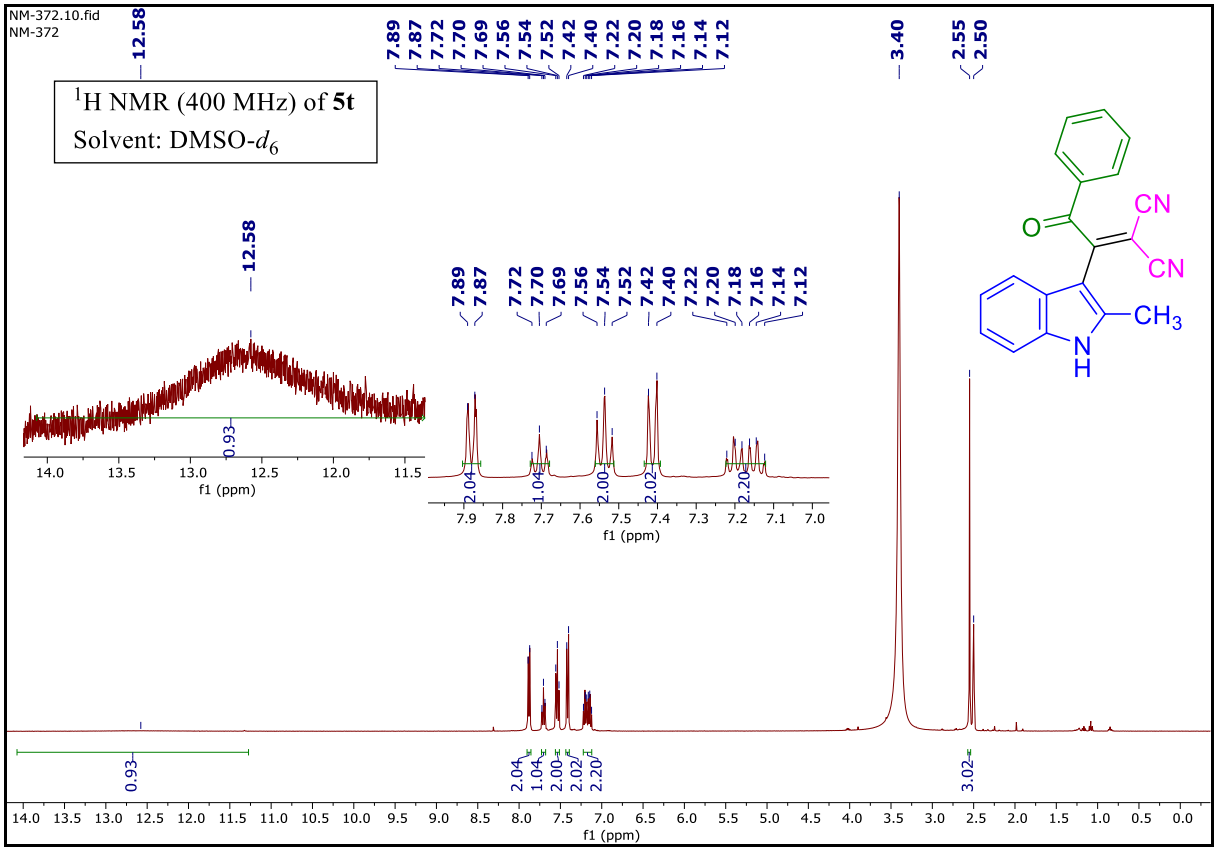

NM-324
single pulse decoupled gated NOE
192.91
163.89
155.78
136.00
135.31
133.25
131.80
129.75
124.64
115.19
114.53
114.15
113.19
108.01
102.77
68.85
55.14
40.02
39.85
39.68
39.52
39.35
39.19
39.02
^{13}C {^{1}H} NMR (125 MHz) of **5q**
Solvent: DMSO-d_6
CN
NC
O
H_3CO
N
H
f1 (ppm)

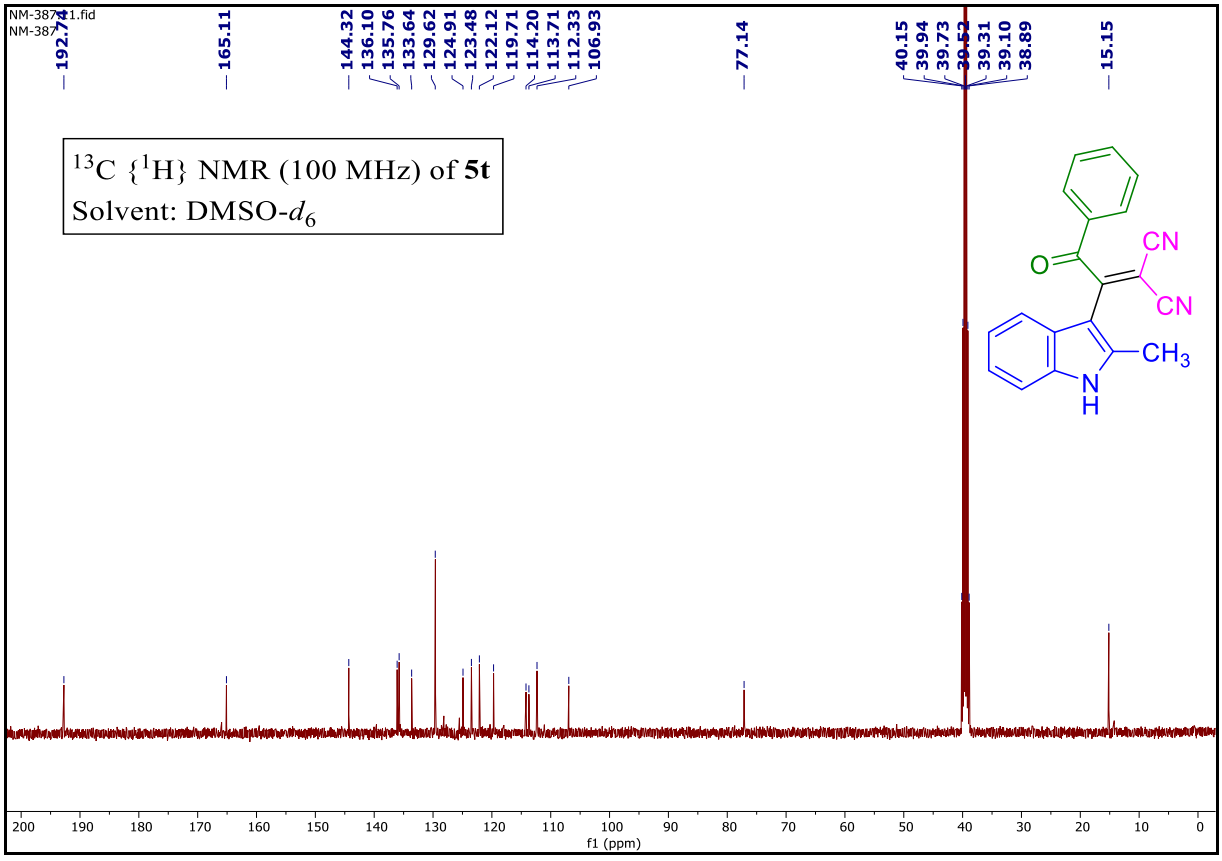

NM-318
single_pulse
^{1}H NMR (500 MHz) of **5r**
Solvent: DMSO-d_6
f1 (ppm)

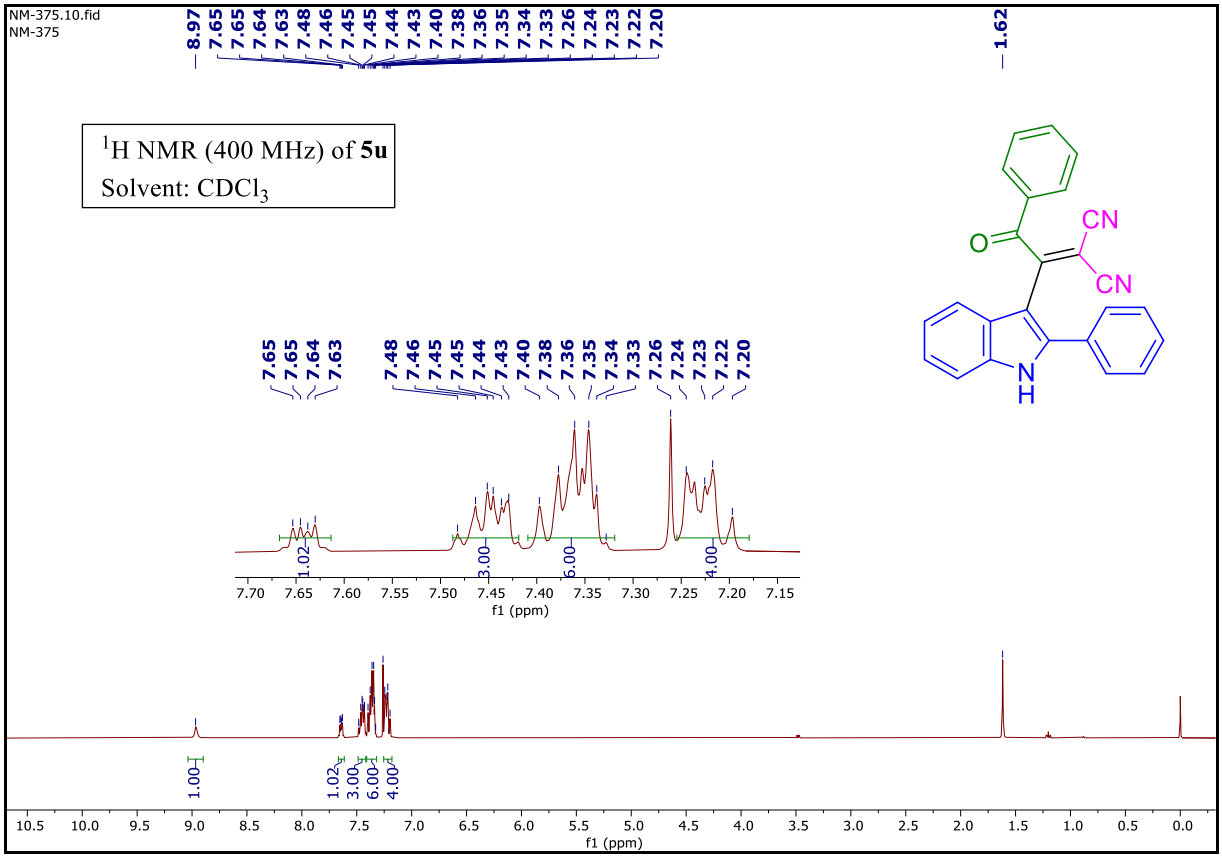

NM-318
single pulse decoupled gated NOE
^{13}C {^{1}H} NMR (125 MHz) of **5r**
Solvent: DMSO-d_6
f1 (ppm)

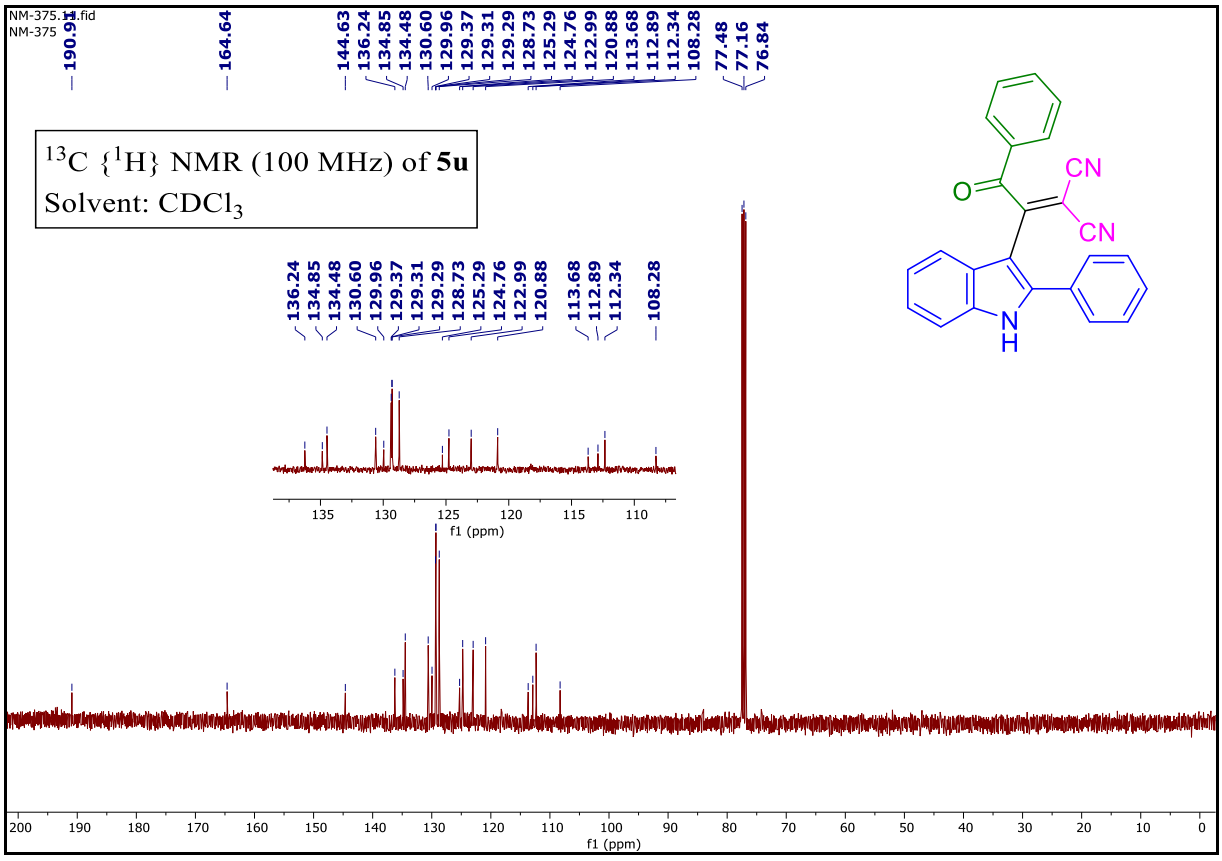

NM-359
single_pulse
8.63 8.04 8.02 7.69 7.67 7.66 7.54 7.52 7.51 7.40 7.39 7.37 7.36 7.34 7.32 7.30 7.26 7.25 7.24 7.23 7.22 7.20 7.13 7.11 7.10 5.43
1.59
^{1}H NMR (500 MHz) of **5s**
Solvent: $CDCl_3$
CN
NC
O
N
8.04 8.02 7.67 7.54 7.52 7.51 7.39 7.37 7.36 7.34 7.32 7.30 7.26 7.24 7.22 7.20 7.11
1.90 1.00 2.00 5.01 3.02 1.01
f1 (ppm)
0.91 1.90 1.00 2.00 5.01 3.02 1.01 2.01
f1 (ppm)

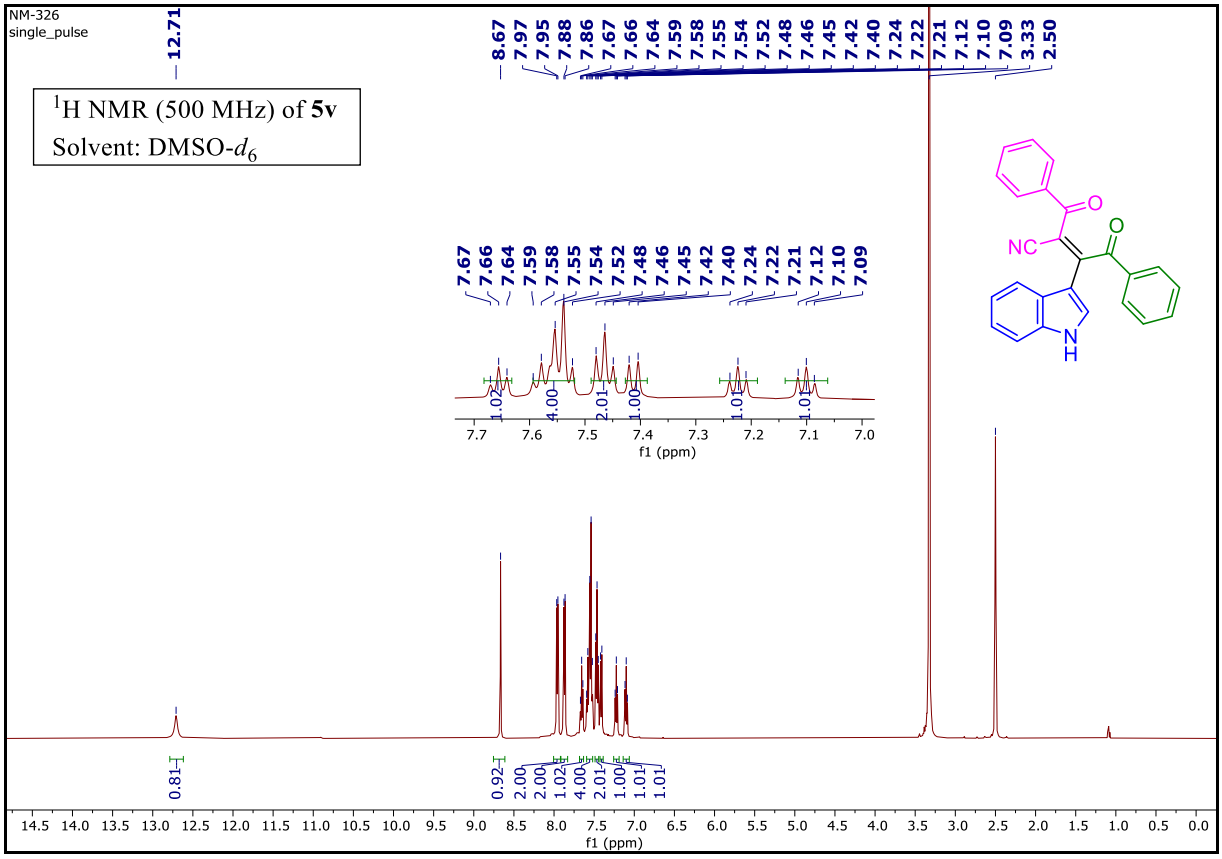

NM-359
single pulse decoupled gated NOE
192.79
164.01 137.18 135.78 135.72 134.29 134.01 130.02 129.60 129.45 128.93 127.36 125.51 124.67 123.90 121.20 115.28 113.25 111.61 108.92
77.41 77.16 76.91 71.91
51.90
^{13}C {^{1}H} NMR (125 MHz) of **5s**
Solvent: $CDCl_3$
CN
NC
O
N
f1 (ppm)

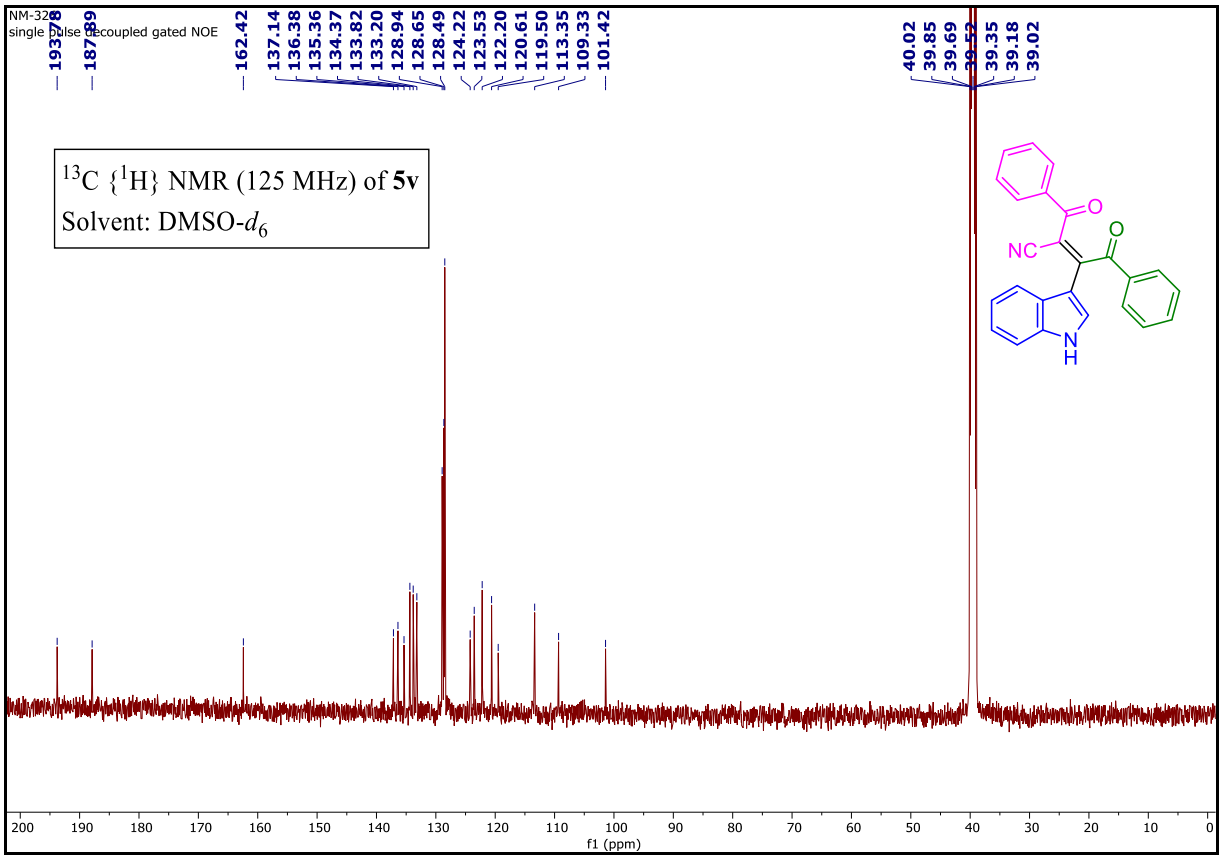

NM-372.10.fid
NM-372
12.58
7.89 7.87 7.72 7.70 7.69 7.56 7.54 7.52 7.42 7.40 7.22 7.20 7.18 7.16 7.14 7.12
3.40
2.55 2.50
^{1}H NMR (400 MHz) of **5t**
Solvent: DMSO-d_6
CN
O
CN
CH3
N
H
f1 (ppm)

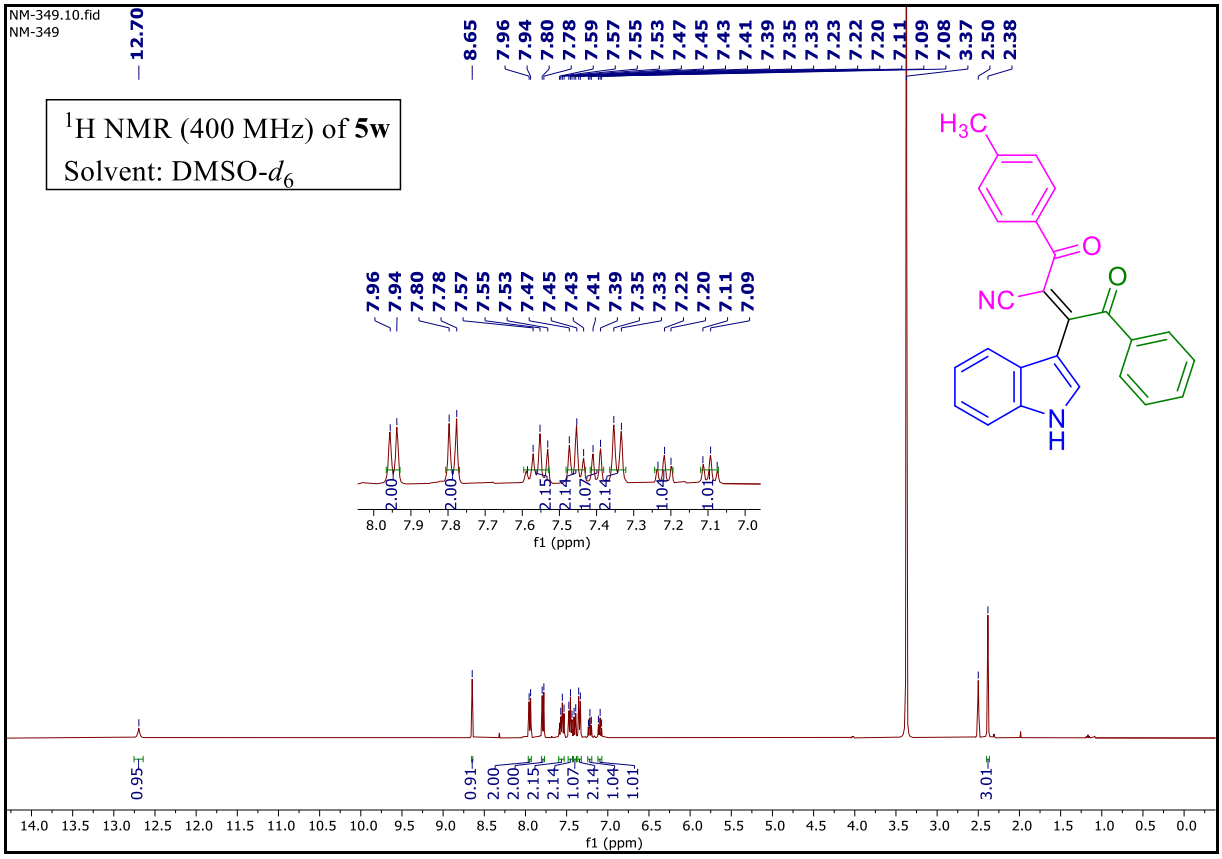

192.74
165.11
144.32 136.10 135.76 133.64 129.62 124.91 123.48 122.12 119.71 114.20 113.71 112.33 106.93
77.14
40.15 39.94 39.73 39.52 39.31 39.10 38.89
15.15
^{13}C {^{1}H} NMR (100 MHz) of **5t**
Solvent: DMSO-d_6
CN
O
CN
CH3
N
H
f1 (ppm)

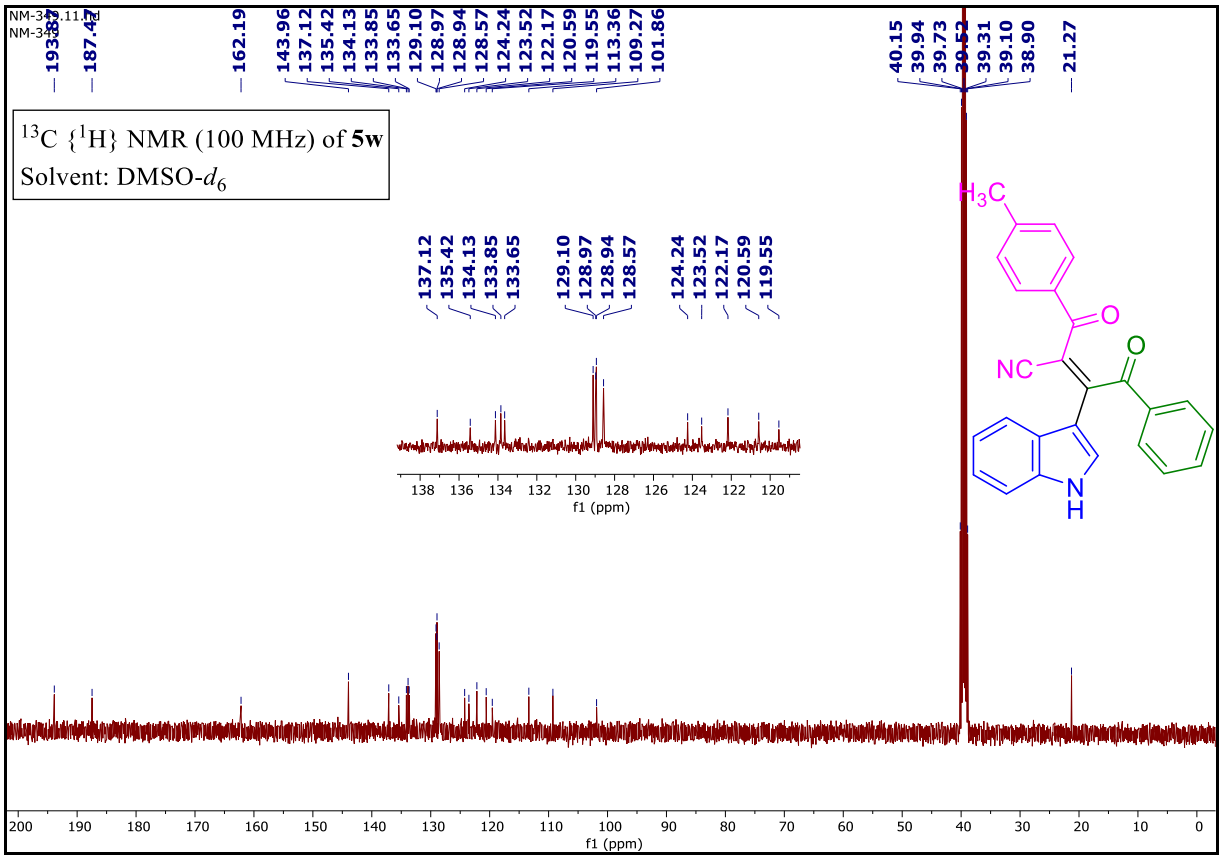

NM-375.10.fid
NM-375
8.97
7.65
7.65
7.64
7.63
7.48
7.46
7.45
7.45
7.44
7.43
7.40
7.38
7.36
7.35
7.34
7.33
7.26
7.24
7.23
7.22
7.20
1.62
^{1}H NMR (400 MHz) of **5u**
Solvent: $CDCl_3$
CN
O
CN
N
H
1.02
3.00
6.00
4.00
f1 (ppm)
1.00
1.02
3.00
6.00
4.00
f1 (ppm)

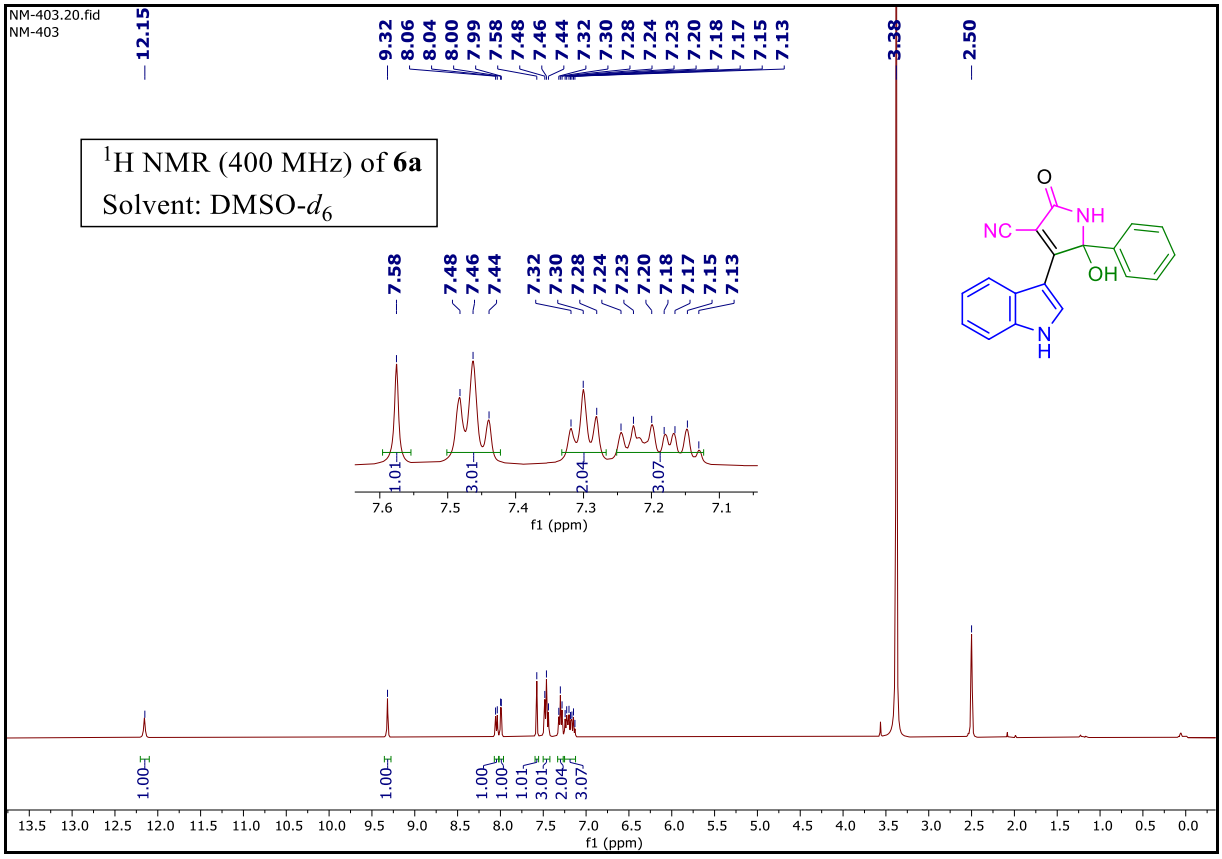

NM-375.11.fid
NM-375
190.91
164.64
144.63
136.24
134.85
134.48
130.60
129.96
129.37
129.31
129.29
128.73
125.29
124.76
122.99
120.88
113.68
112.89
112.34
108.28
77.48
77.16
76.84
^{13}C {^{1}H} NMR (100 MHz) of **5u**
Solvent: $CDCl_3$
CN
O
CN
N
H
f1 (ppm)
f1 (ppm)

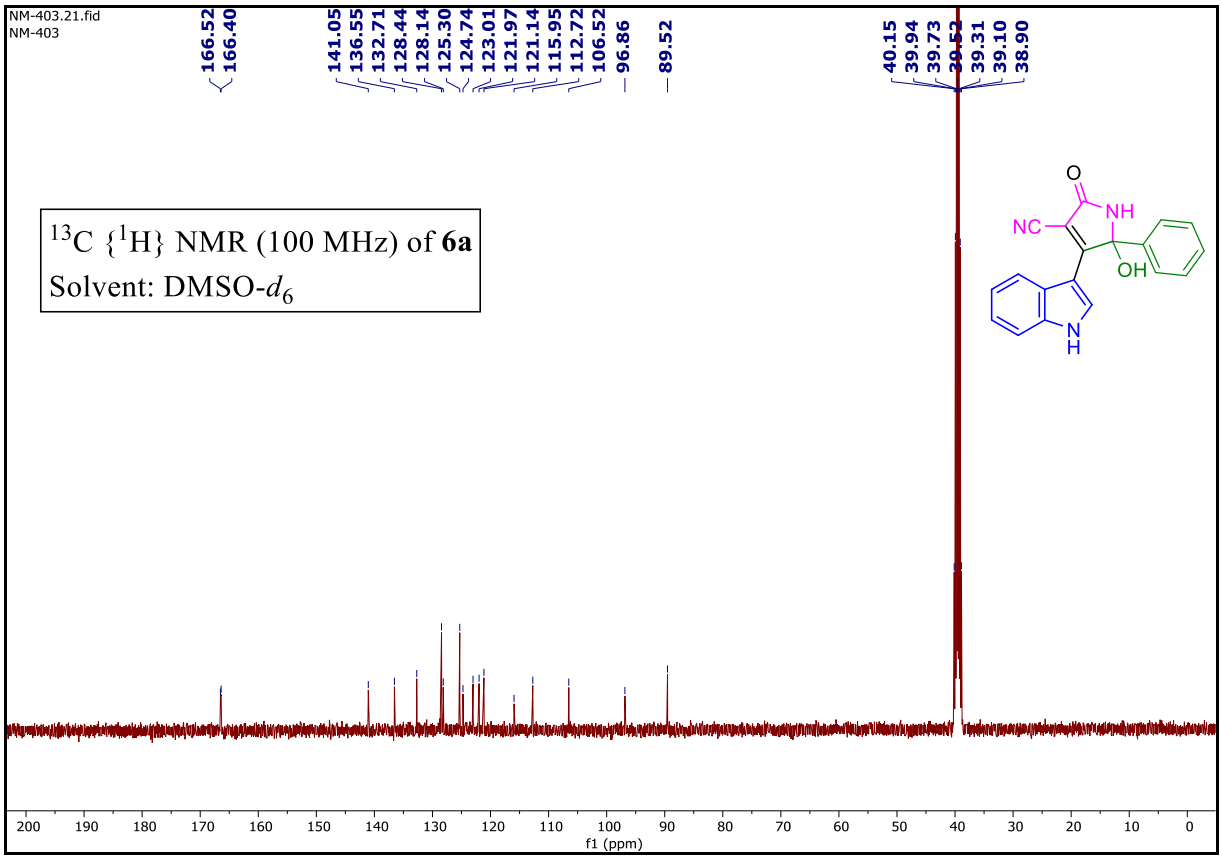

NM-326
single_pulse
^{1}H NMR (500 MHz) of **5v**
Solvent: DMSO-d_6
f1 (ppm)

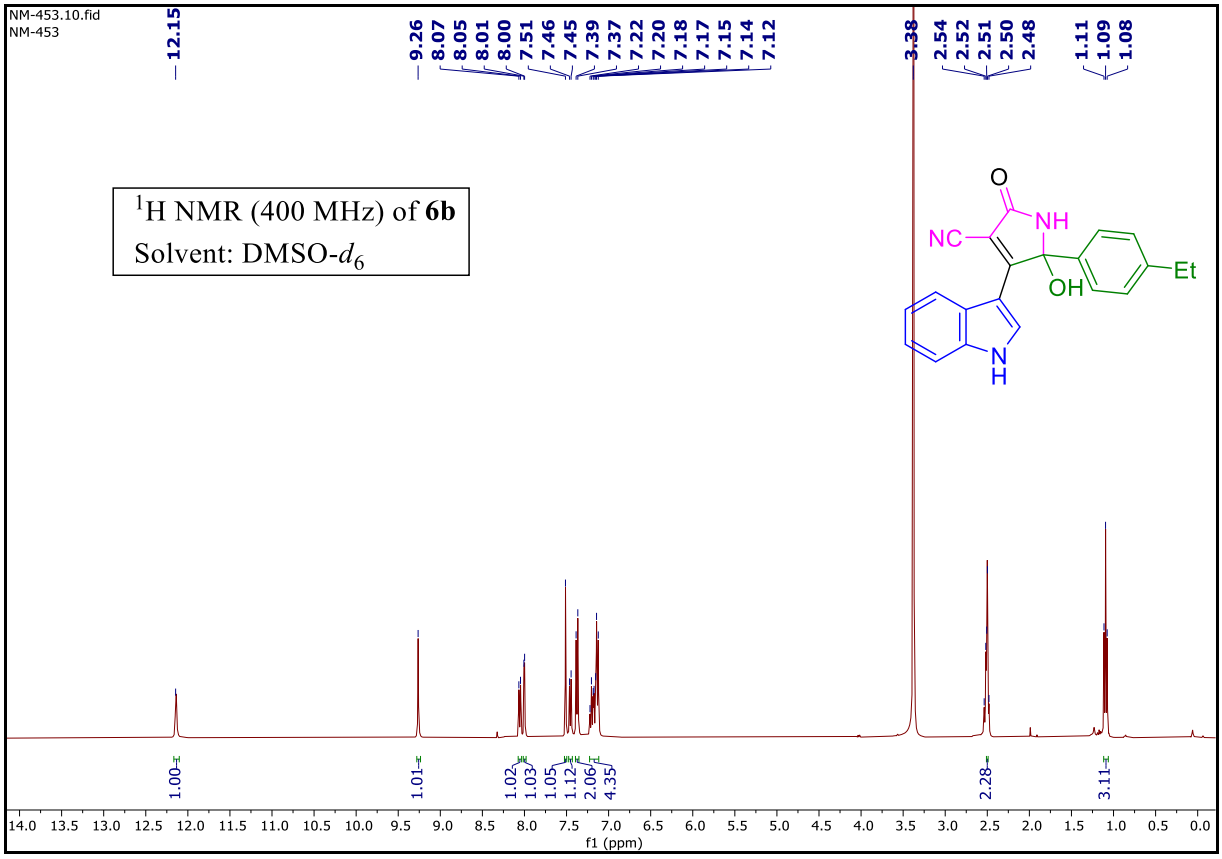

NM-326
single pulse decoupled gated NOE
^{13}C {^{1}H} NMR (125 MHz) of **5v**
Solvent: DMSO-d_6
f1 (ppm)

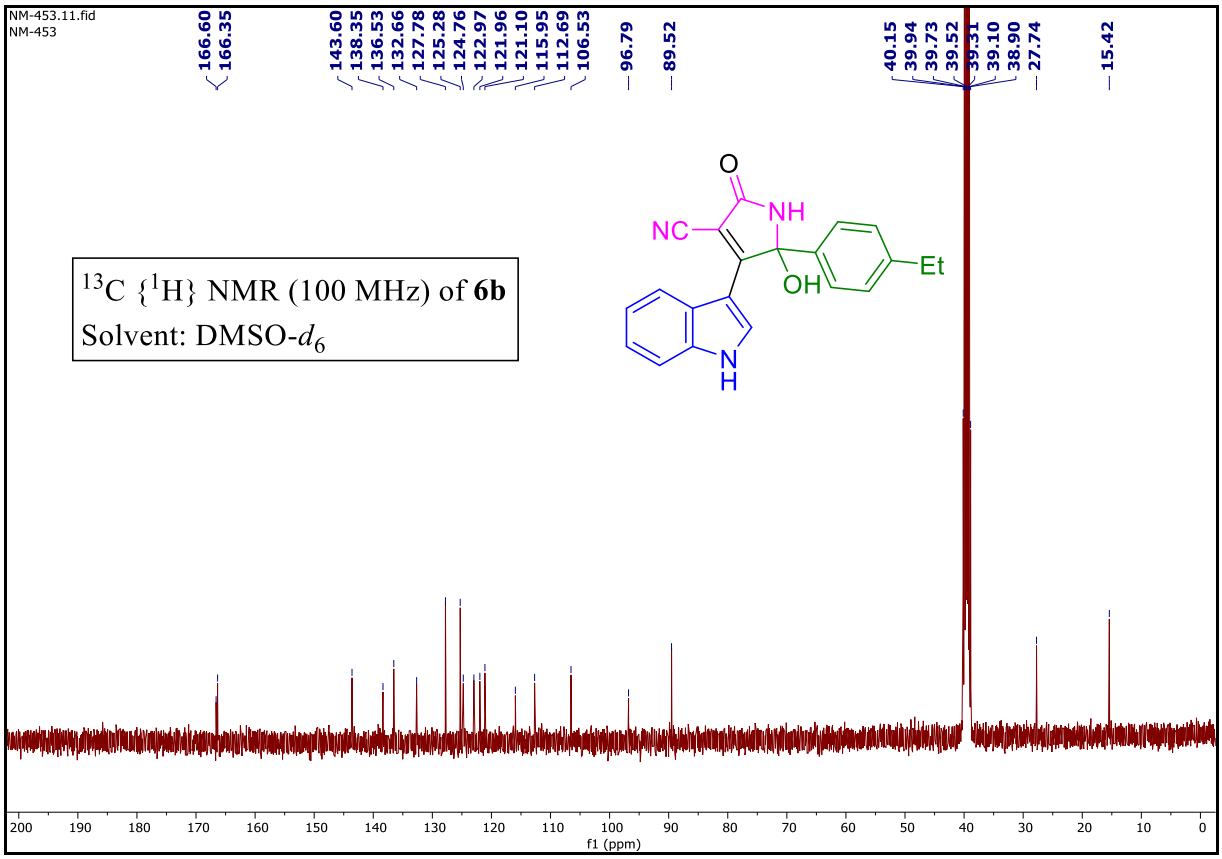

NM-349.10.fid
NM-349
^{1}H NMR (400 MHz) of **5w**
Solvent: DMSO-d_6
f1 (ppm)

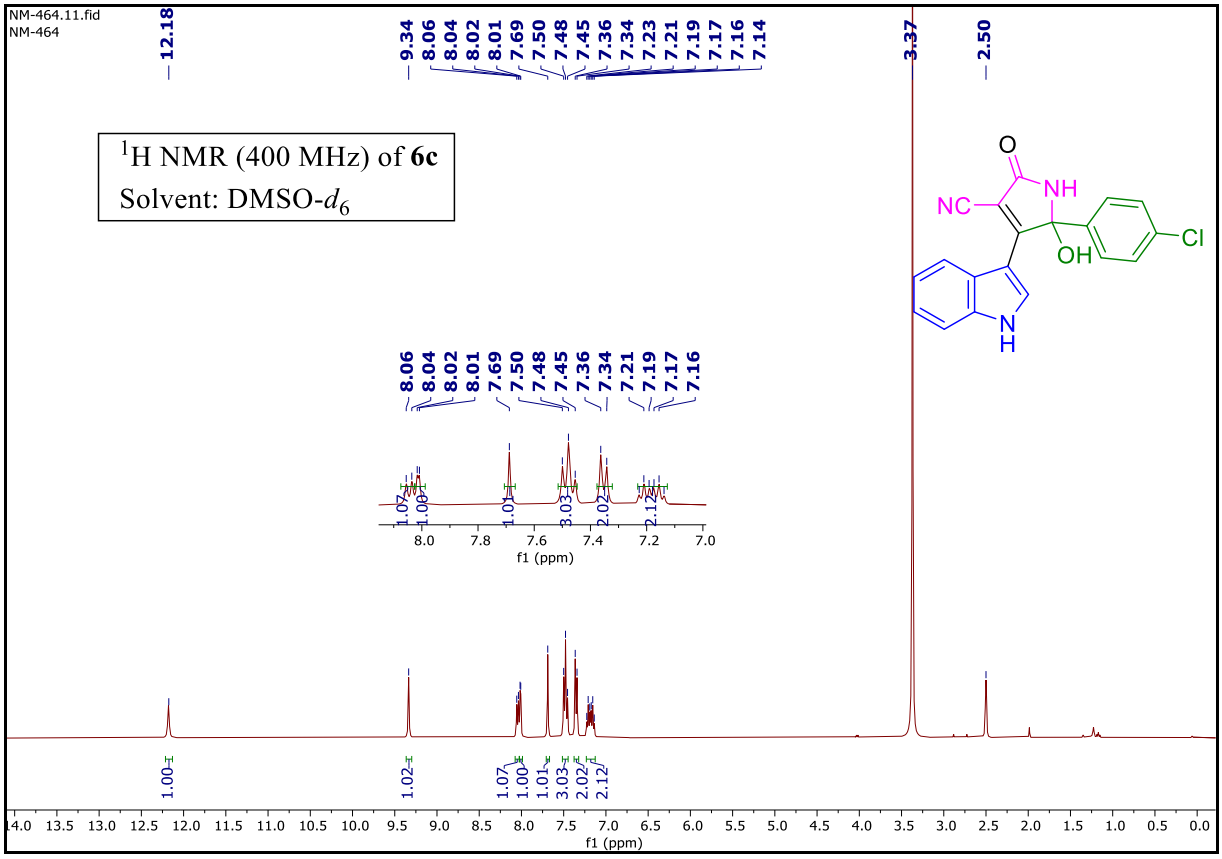

^{13}C {^{1}H} NMR (100 MHz) of **5w**
Solvent: DMSO-d_6
f1 (ppm)

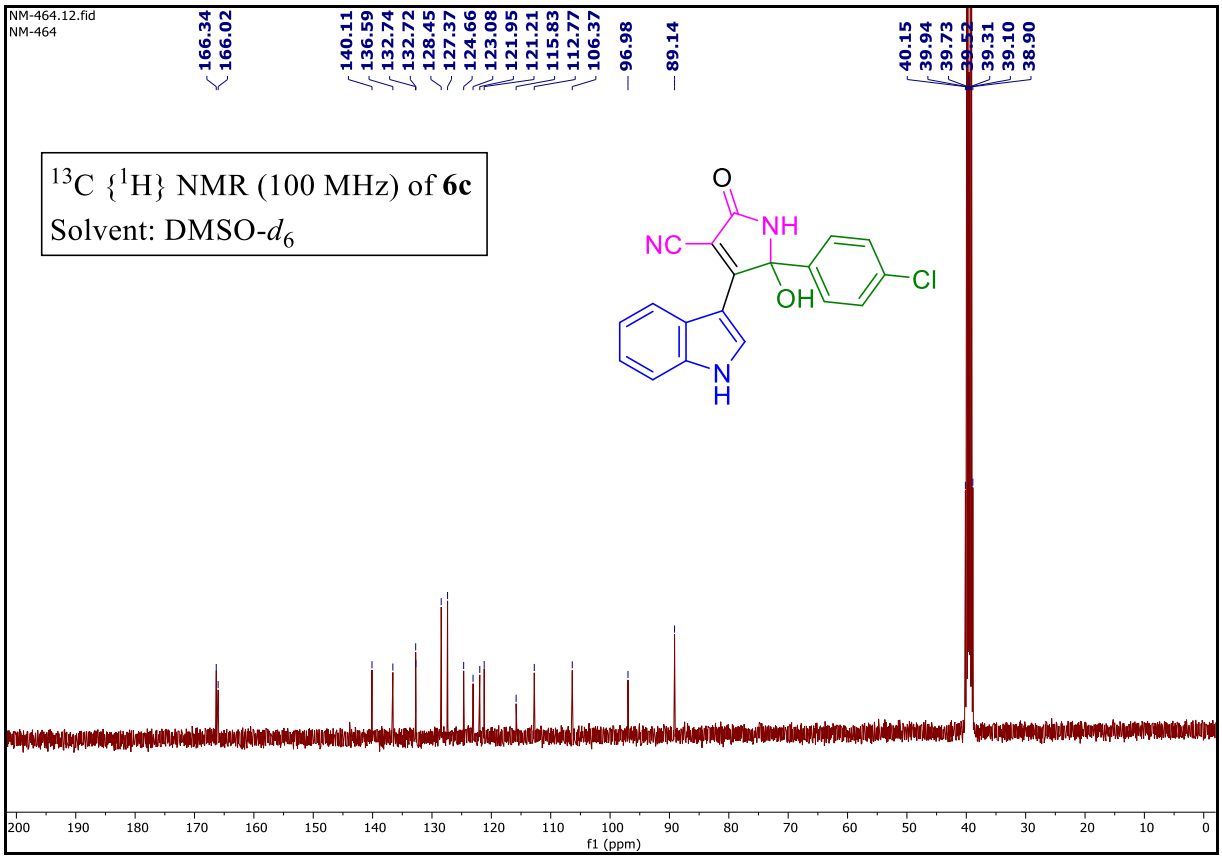

NM-403.20.fid
NM-403
12.15
9.32
8.06
8.04
8.00
7.99
7.58
7.48
7.46
7.44
7.32
7.30
7.28
7.24
7.23
7.20
7.18
7.17
7.15
7.13
3.38
2.50
^{1}H NMR (400 MHz) of **6a**
Solvent: DMSO-d_6
1.01
3.01
2.04
3.07
f1 (ppm)
NC
NH
OH
N
H

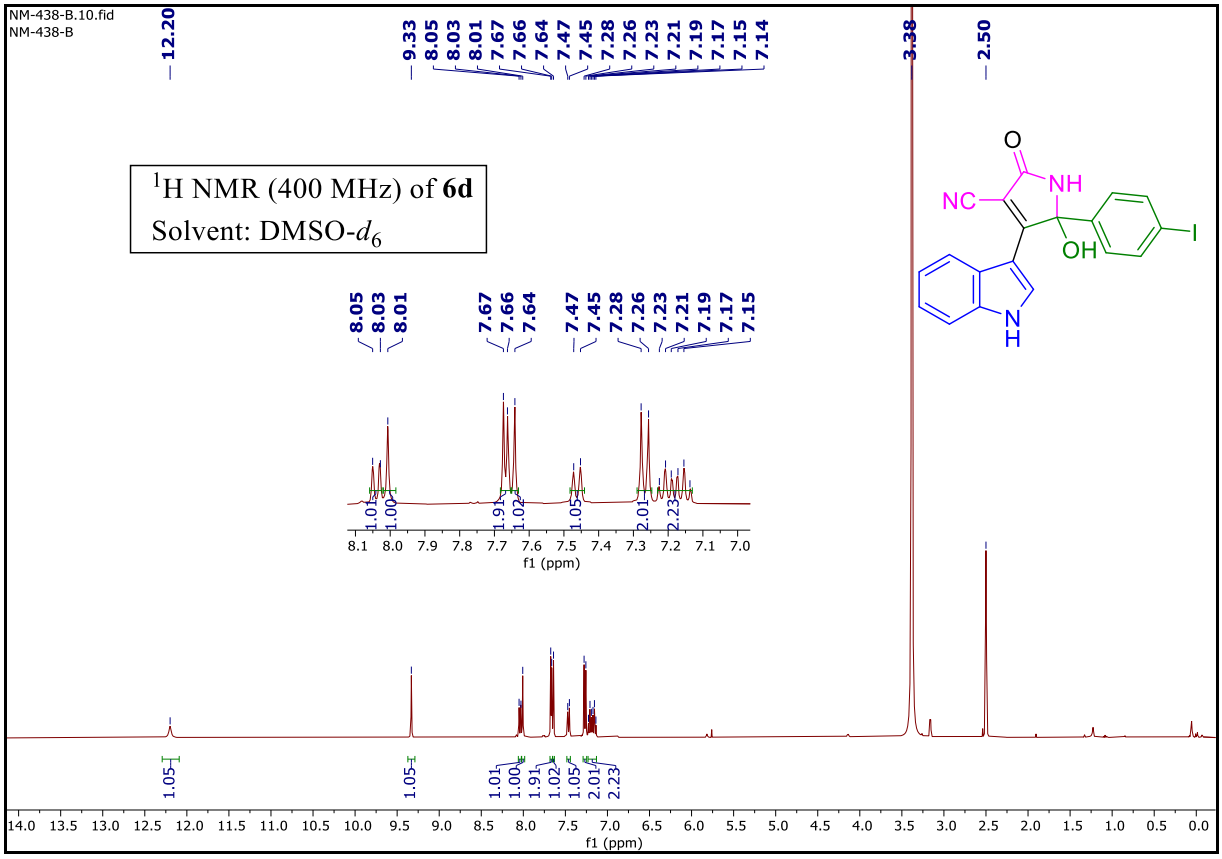

NM-403.21.fid
NM-403
166.52
166.40
141.05
136.55
132.71
128.44
128.14
125.30
124.74
123.01
121.97
121.14
115.95
112.72
106.52
96.86
89.52
40.15
39.94
39.73
39.52
39.31
39.10
38.90
^{13}C {^{1}H} NMR (100 MHz) of **6a**
Solvent: DMSO-d_6
f1 (ppm)
NC
NH
OH
N
H

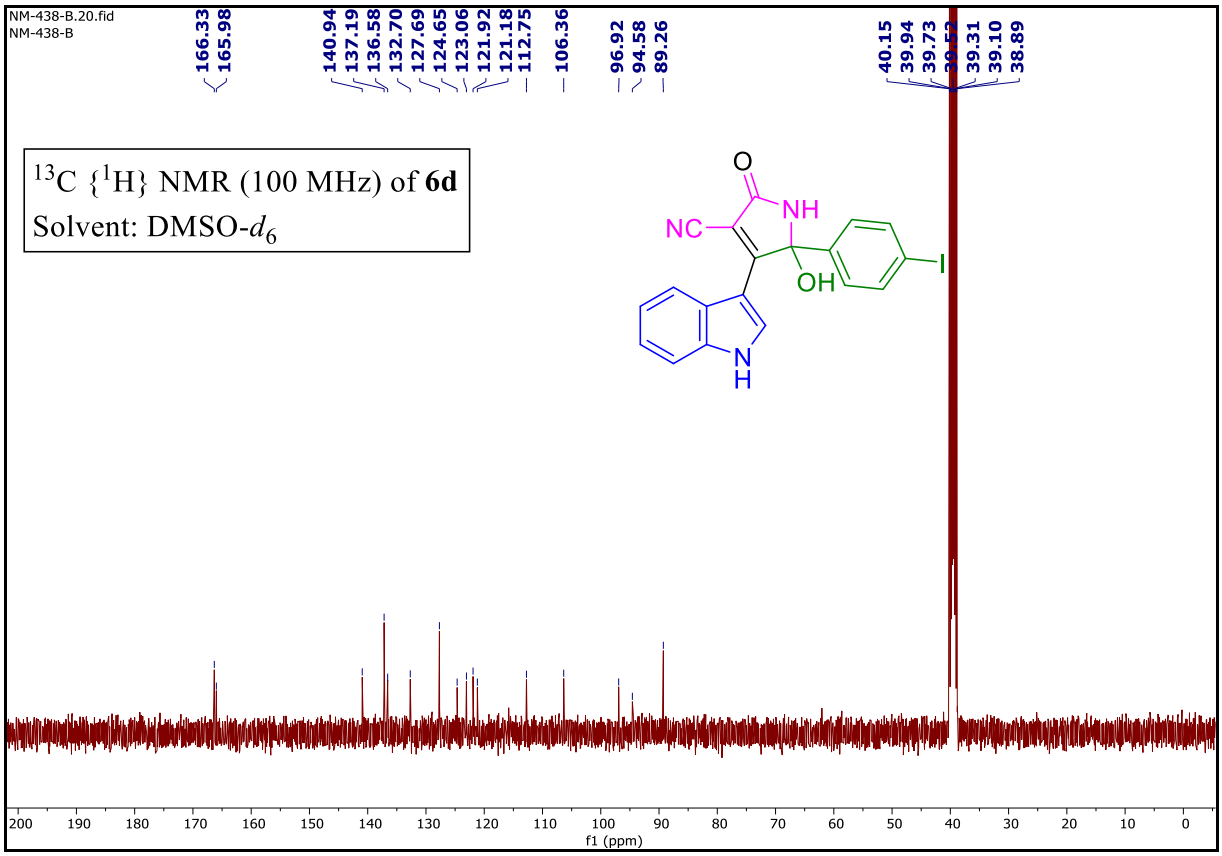

NM-453.10.fid
NM-453
12.15
9.26
8.07
8.05
8.01
8.00
7.51
7.46
7.45
7.39
7.37
7.22
7.20
7.18
7.17
7.15
7.14
7.12
3.38
2.54
2.52
2.51
2.50
2.48
1.11
1.09
1.08
1H NMR (400 MHz) of 6b
Solvent: DMSO-d6
O
NH
NC
OH
Et
N
H
1.00
1.01
1.02
1.03
1.05
1.12
2.06
4.35
2.28
3.11
f1 (ppm)

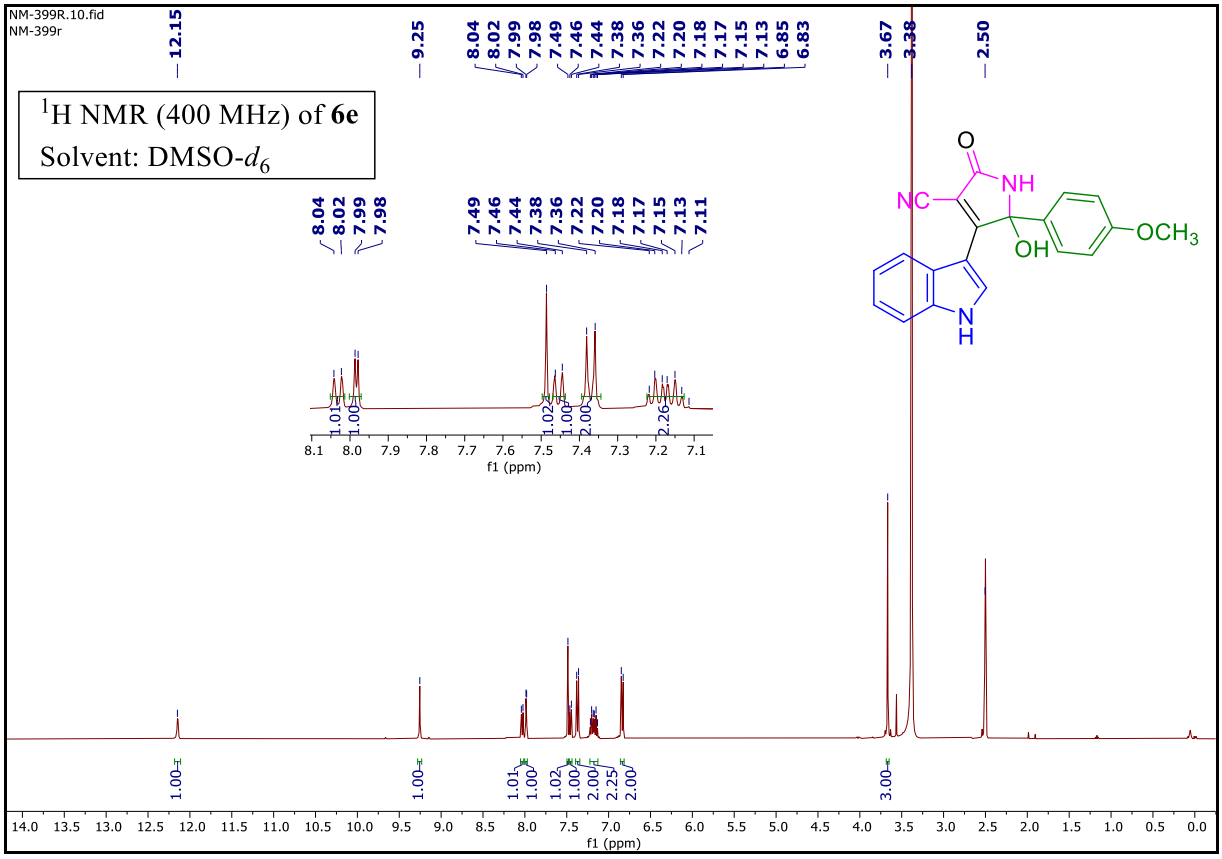

NM-453.11.fid
NM-453
166.60
166.35
143.60
138.35
136.53
132.66
127.78
125.28
124.76
122.97
121.96
121.10
115.95
112.69
106.53
96.79
89.52
40.15
39.94
39.73
39.52
39.31
39.10
38.90
27.74
15.42
13C {1H} NMR (100 MHz) of 6b
Solvent: DMSO-d6
O
NH
NC
OH
Et
N
H
f1 (ppm)

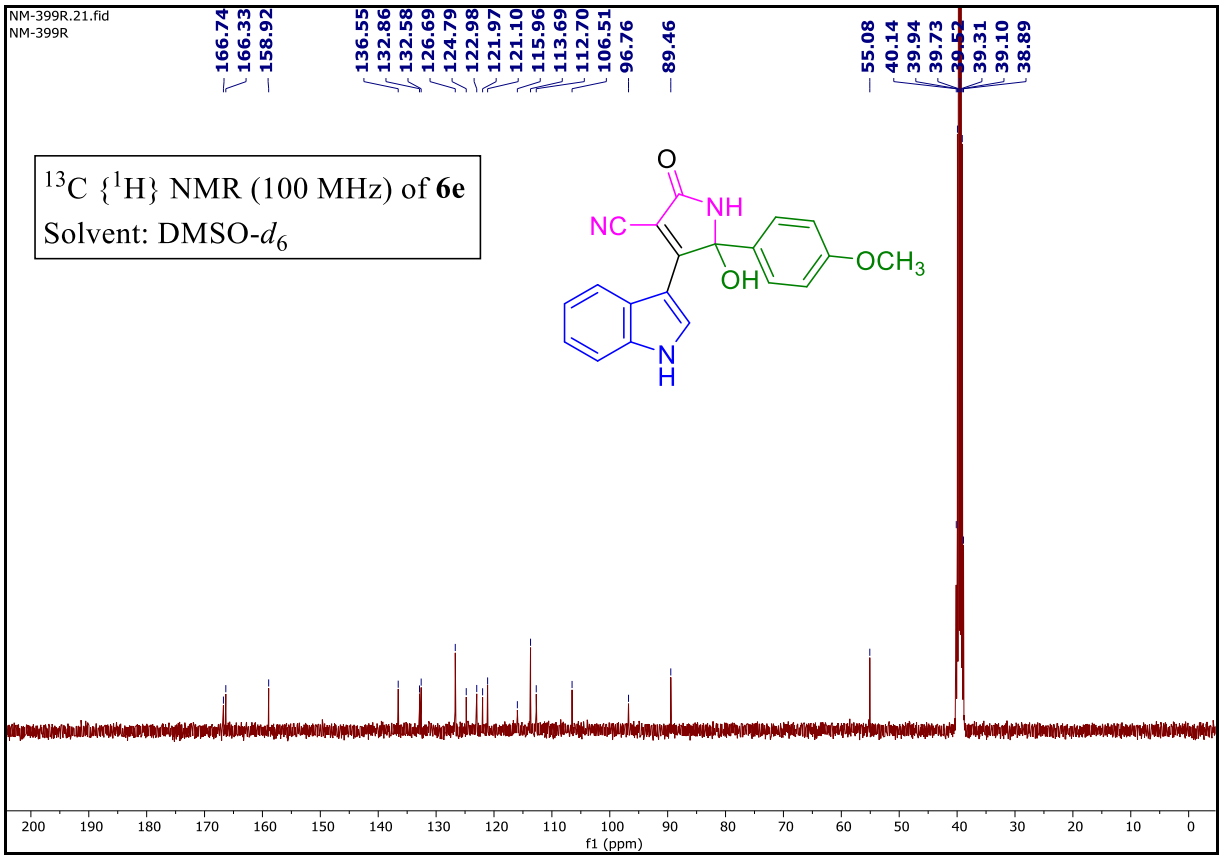

NM-464.11.fid
NM-464
12.18
9.34
8.06
8.04
8.02
8.01
7.69
7.50
7.48
7.45
7.36
7.34
7.23
7.21
7.19
7.17
7.16
7.14
3.37
2.50
^{1}H NMR (400 MHz) of **6c**
Solvent: DMSO-d_6
O
NH
NC
OH
Cl
N
H
f1 (ppm)

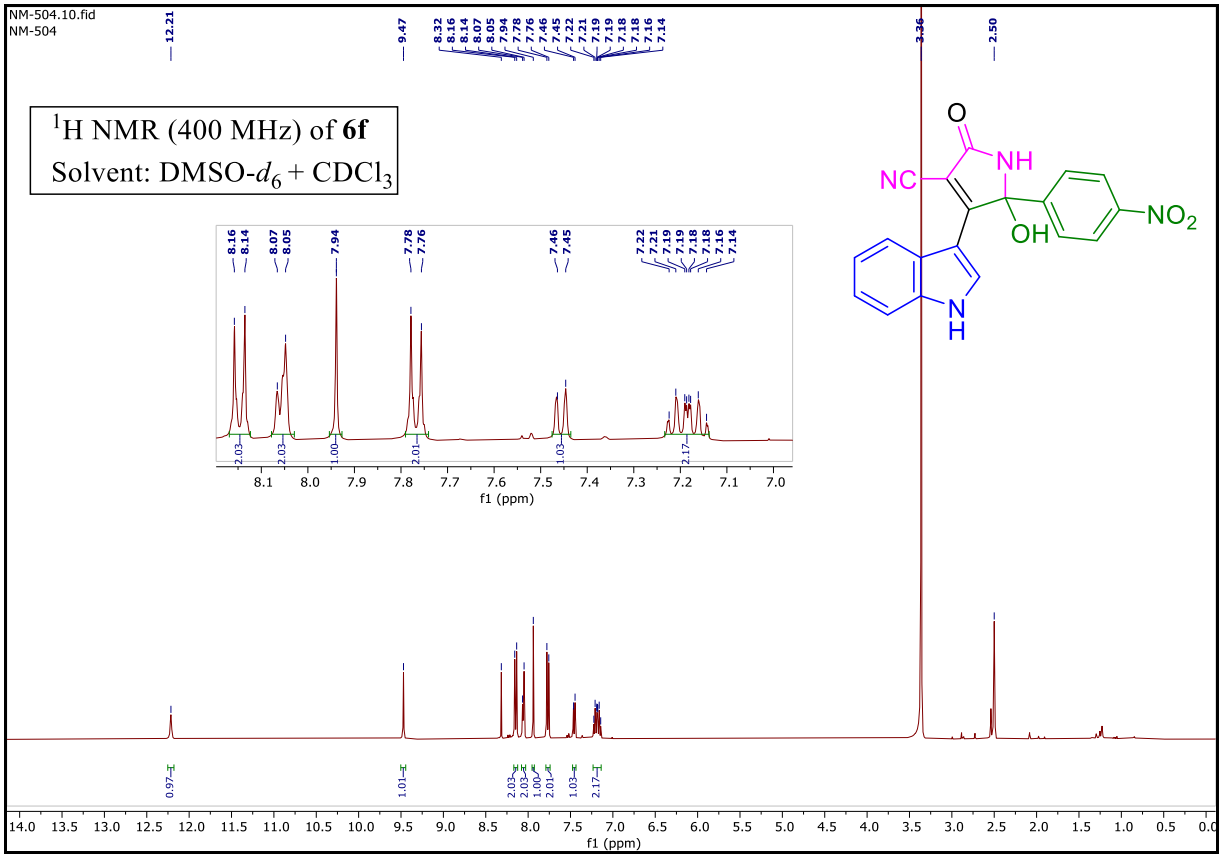

NM-464.12.fid
NM-464
166.34
166.02
140.11
136.59
132.74
132.72
128.45
127.37
124.66
123.08
121.95
121.21
115.83
112.77
106.37
96.98
89.14
40.15
39.94
39.73
39.52
39.31
39.10
38.90
^{13}C {^{1}H} NMR (100 MHz) of **6c**
Solvent: DMSO-d_6
O
NH
NC
OH
Cl
N
H
f1 (ppm)

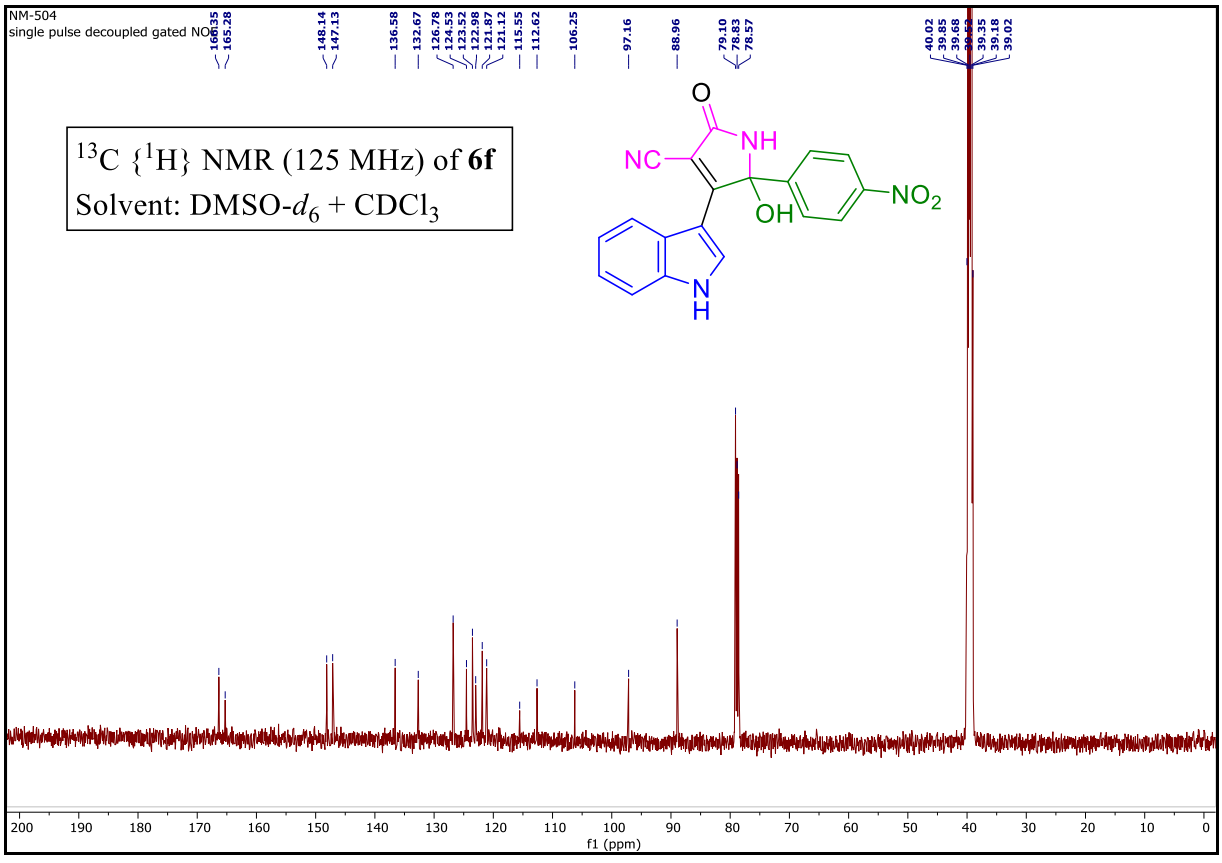

NM-438-B.10.fid
NM-438-B
12.20
9.33
8.05
8.03
8.01
7.67
7.66
7.64
7.47
7.45
7.28
7.26
7.23
7.21
7.19
7.17
7.15
7.14
3.38
2.50
^{1}H NMR (400 MHz) of **6d**
Solvent: DMSO-d_6
O
NH
NC
OH
I
N
H
f1 (ppm)

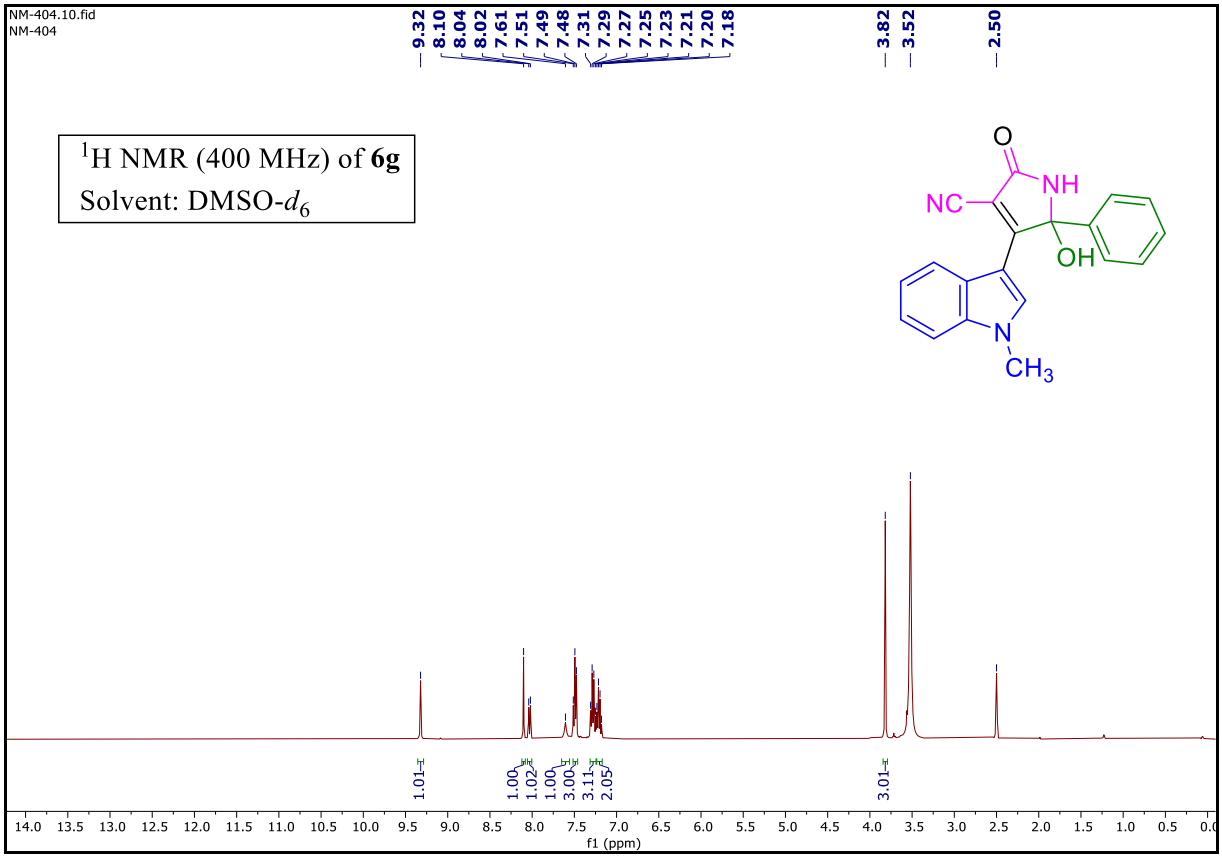

NM-438-B.20.fid
NM-438-B
166.33
165.98
140.94
137.19
136.58
132.70
127.69
124.65
123.06
121.92
121.18
112.75
106.36
96.92
94.58
89.26
40.15
39.94
39.73
39.52
39.31
39.10
38.89
^{13}C {^{1}H} NMR (100 MHz) of **6d**
Solvent: DMSO-d_6
O
NH
NC
OH
I
N
H
f1 (ppm)

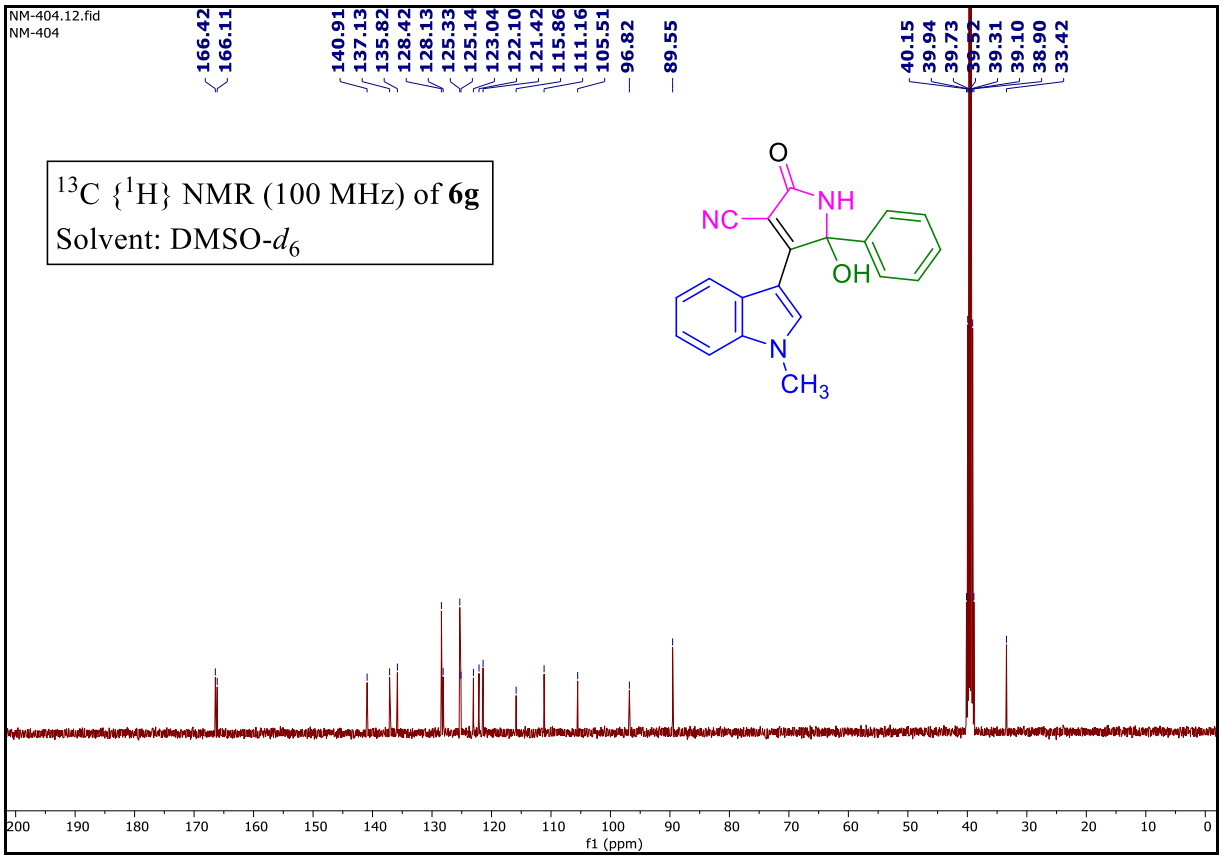

NM-399R.10.fid
NM-399r
^{1}H NMR (400 MHz) of **6e**
Solvent: DMSO-d_6
12.15
9.25
8.04
8.02
7.99
7.98
7.49
7.46
7.44
7.38
7.36
7.22
7.20
7.18
7.17
7.15
7.13
6.85
6.83
3.67
3.38
2.50
NC
O
NH
OH
OCH3
N
H
f1 (ppm)

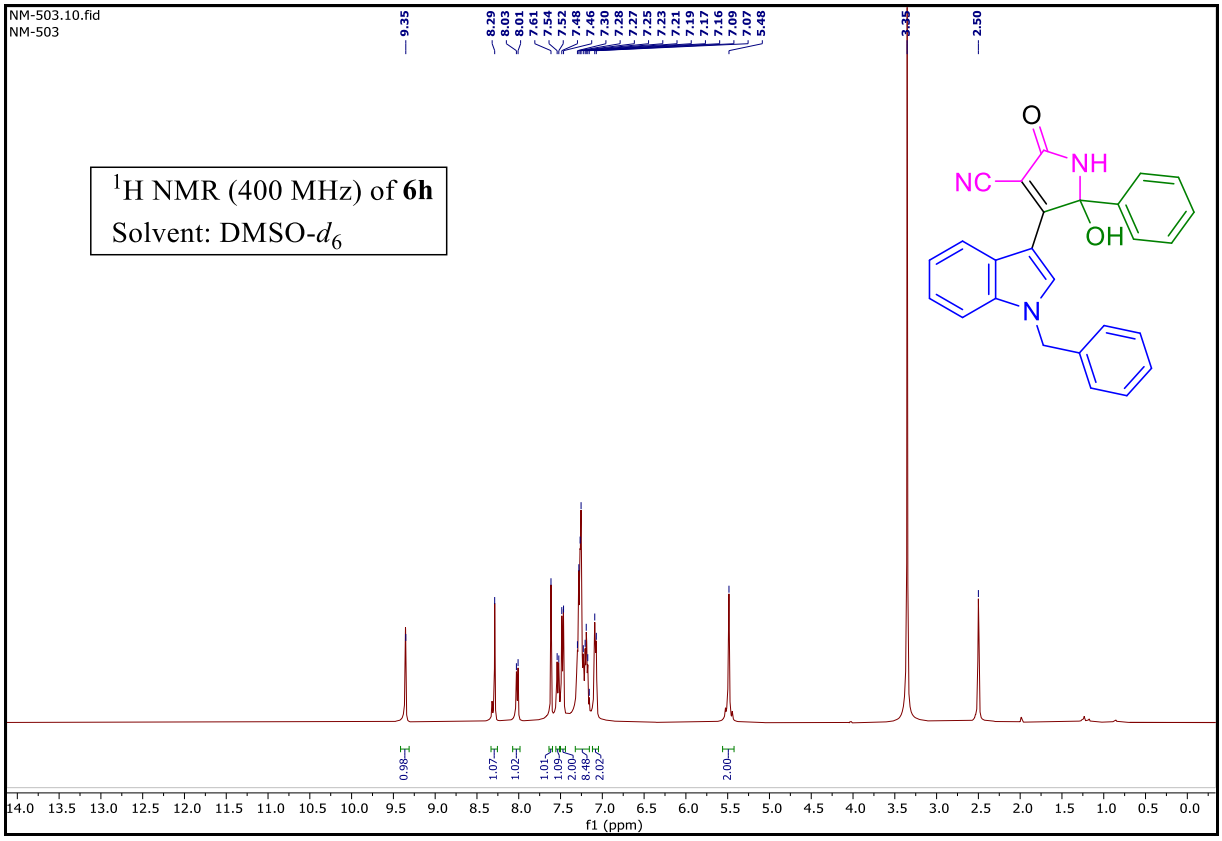

NM-399R.21.fid
NM-399R
^{13}C {^{1}H} NMR (100 MHz) of **6e**
Solvent: DMSO-d_6
166.74
166.33
158.92
136.55
132.86
132.58
126.69
124.79
122.98
121.97
121.10
115.96
113.69
112.70
106.51
96.76
89.46
55.08
40.14
39.94
39.73
39.52
39.31
39.10
38.89
NC
O
NH
OH
OCH3
N
H
f1 (ppm)

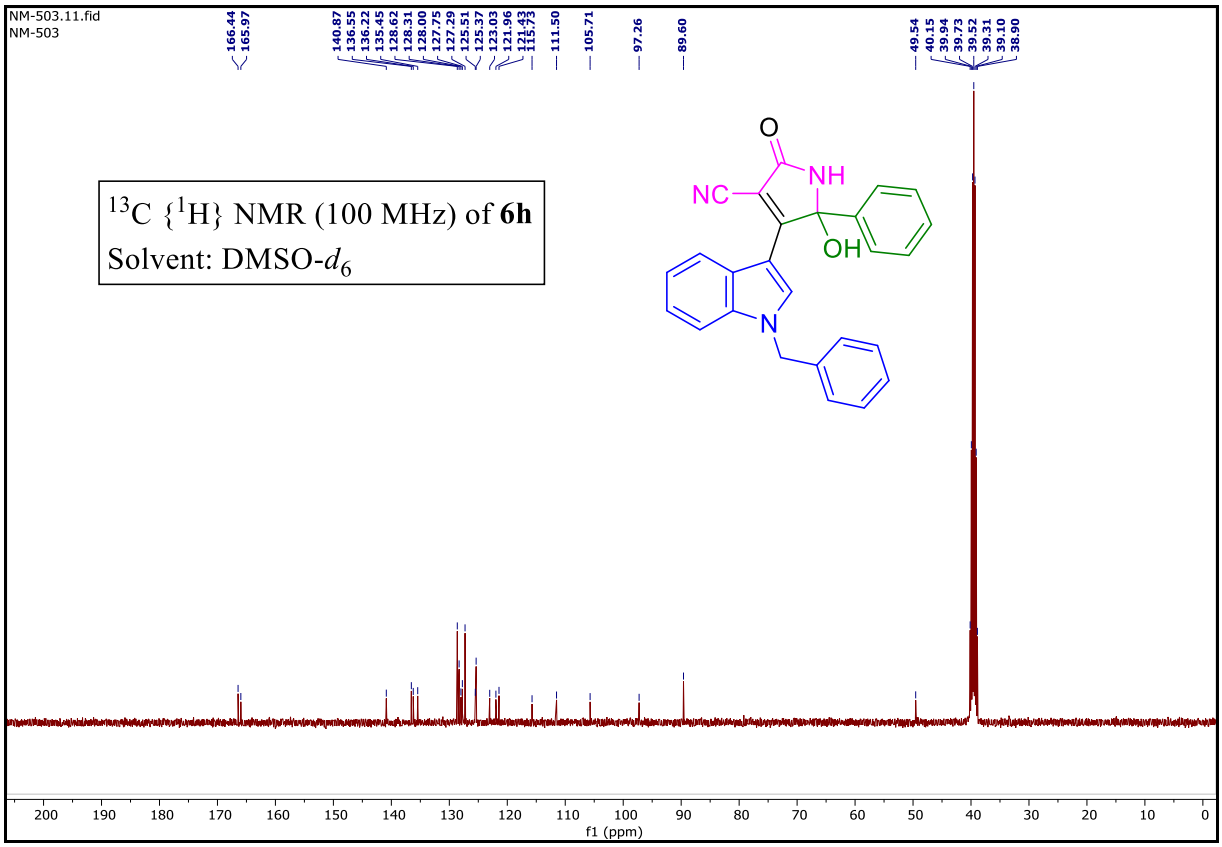

NM-504.10.fid
NM-504
^{1}H NMR (400 MHz) of **6f**
Solvent: DMSO-d_6 + $CDCl_3$
f1 (ppm)

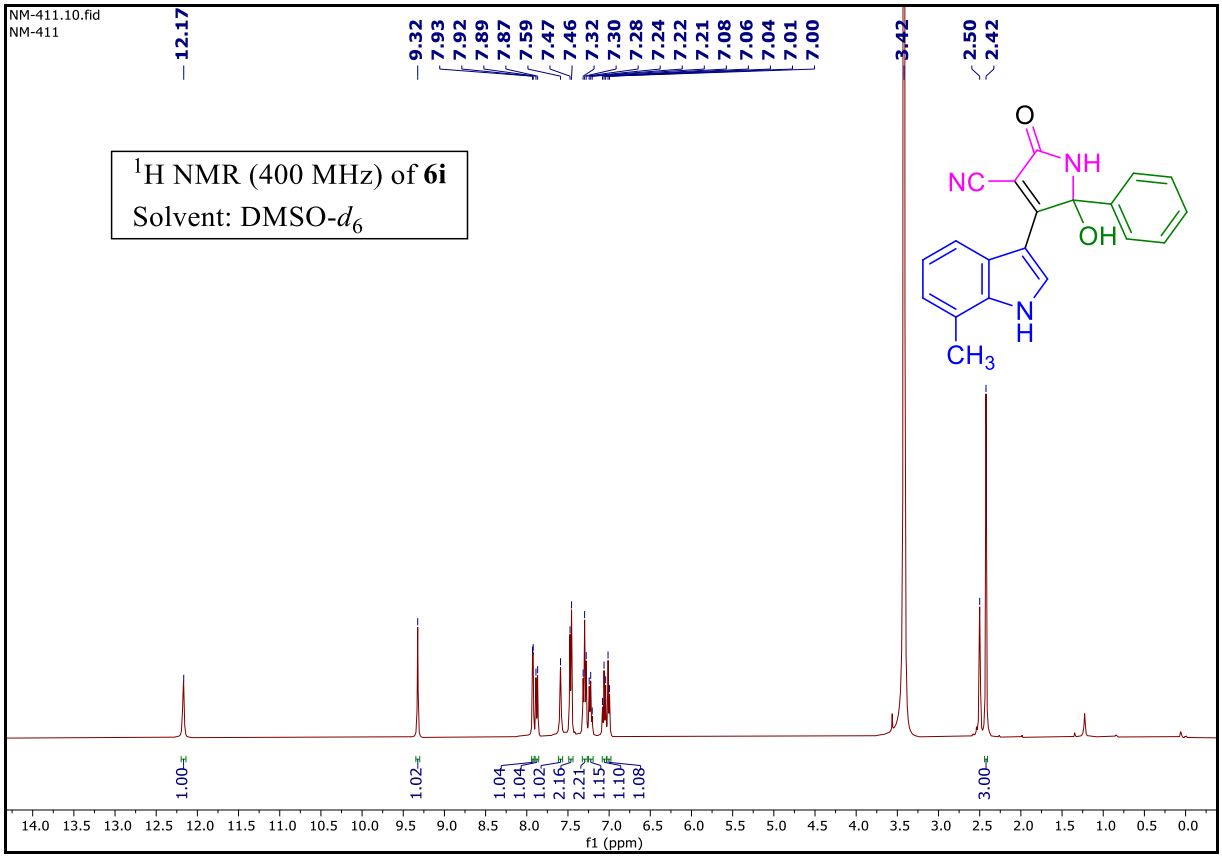

NM-504
single pulse decoupled gated NOE
^{13}C {^{1}H} NMR (125 MHz) of **6f**
Solvent: DMSO-d_6 + $CDCl_3$
f1 (ppm)

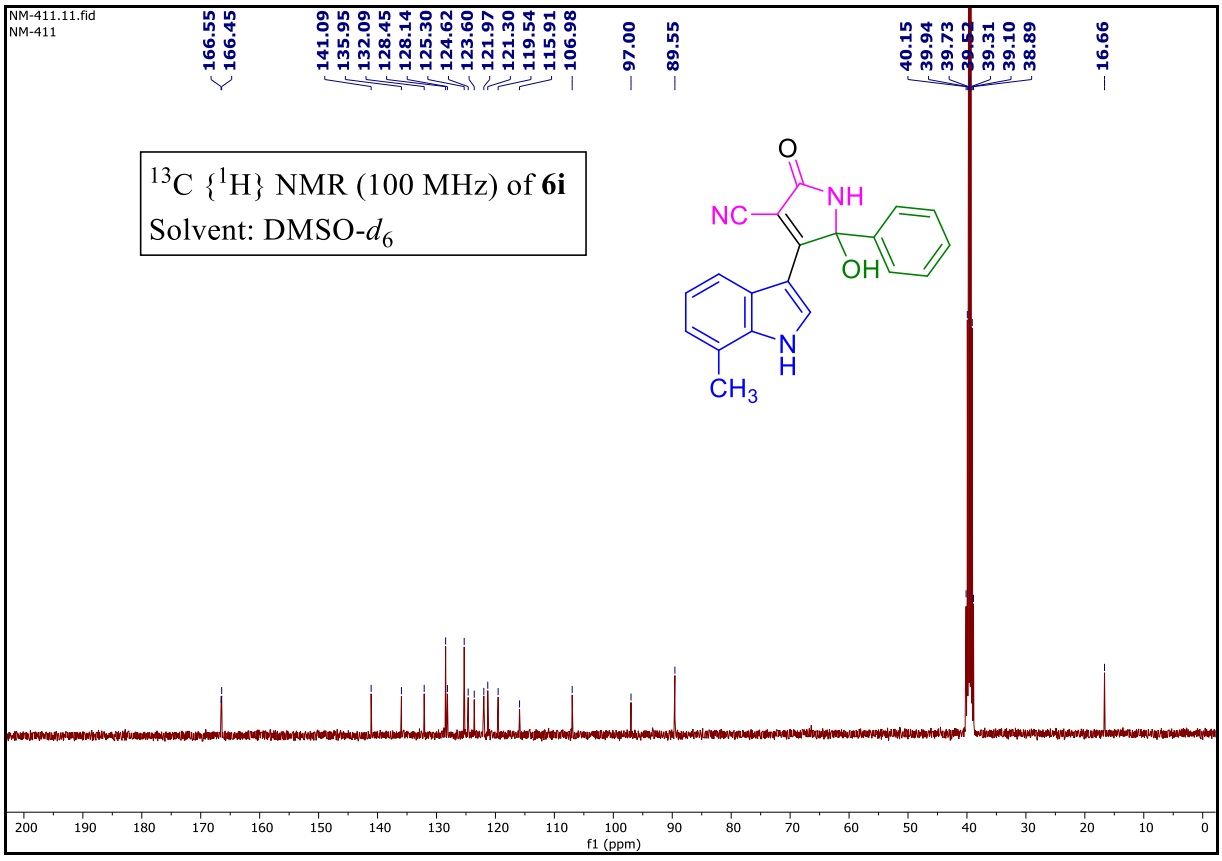

NM-404.10.fid
NM-404
9.32
8.10
8.04
8.02
7.61
7.51
7.49
7.48
7.31
7.29
7.27
7.25
7.23
7.21
7.20
7.18
3.82
3.52
2.50
1H NMR (400 MHz) of 6g
Solvent: DMSO-d6
O
NH
NC
OH
N
CH3
1.01
1.00
1.02
1.00
3.00
3.11
2.05
3.01
f1 (ppm)

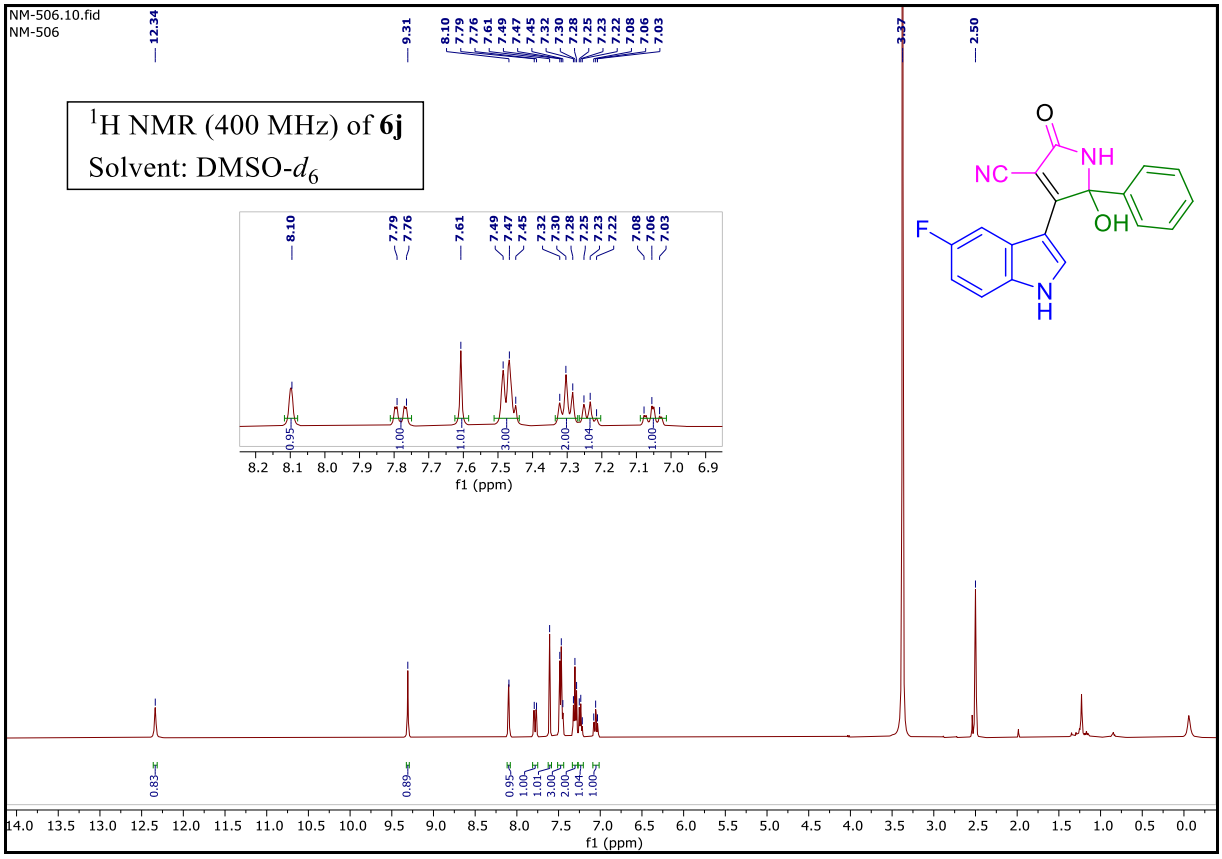

NM-404.12.fid
NM-404
166.42
166.11
140.91
137.13
135.82
128.42
128.13
125.33
125.14
123.04
122.10
121.42
115.86
111.16
105.51
96.82
89.55
40.15
39.94
39.73
39.52
39.31
39.10
38.90
33.42
13C {1H} NMR (100 MHz) of 6g
Solvent: DMSO-d6
O
NH
NC
OH
N
CH3
f1 (ppm)

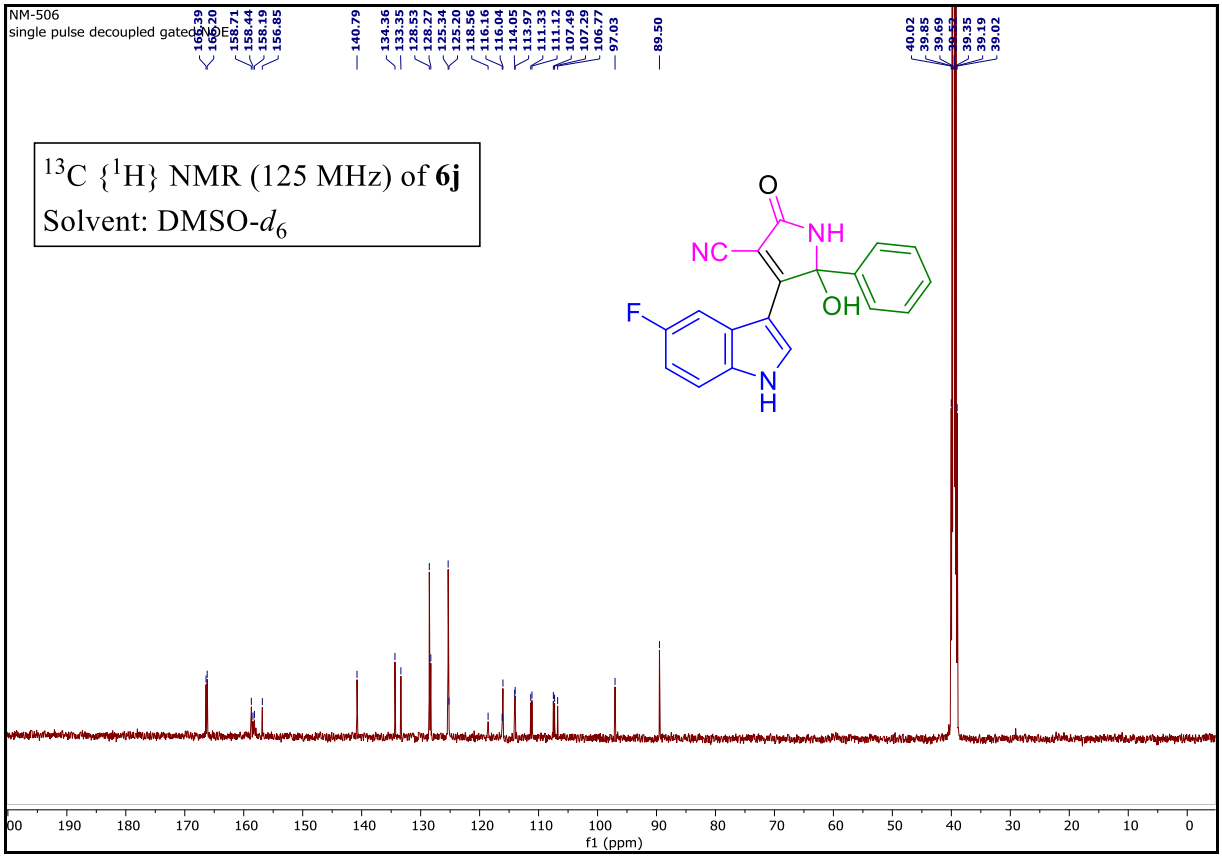

NM-503.10.fid
NM-503
9.35
8.29
8.03
8.01
7.61
7.54
7.52
7.48
7.46
7.30
7.28
7.27
7.25
7.23
7.21
7.19
7.17
7.16
7.09
7.07
5.48
3.35
2.50
0.98
1.07
1.02
1.01
1.09
2.00
8.48
2.02
2.00
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)
^{1}H NMR (400 MHz) of **6h**
Solvent: DMSO-d_6
O
NH
NC
OH
N

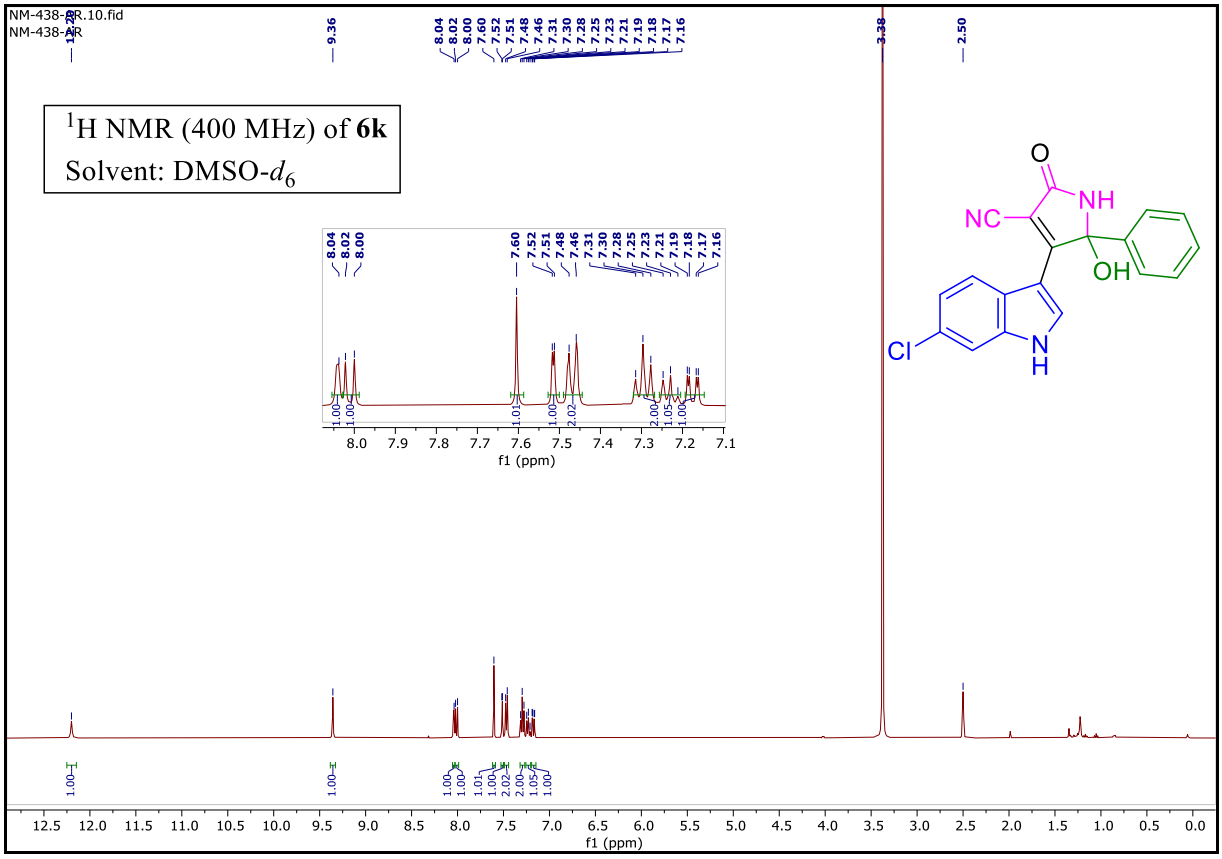

NM-503.11.fid
NM-503
166.44
165.97
140.87
136.55
136.22
135.45
128.62
128.31
128.00
127.75
127.29
125.51
125.37
123.03
121.96
121.43
115.73
111.50
105.71
97.26
89.60
49.54
40.15
39.94
39.73
39.52
39.31
39.10
38.90
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
^{13}C {^{1}H} NMR (100 MHz) of **6h**
Solvent: DMSO-d_6
O
NH
NC
OH
N

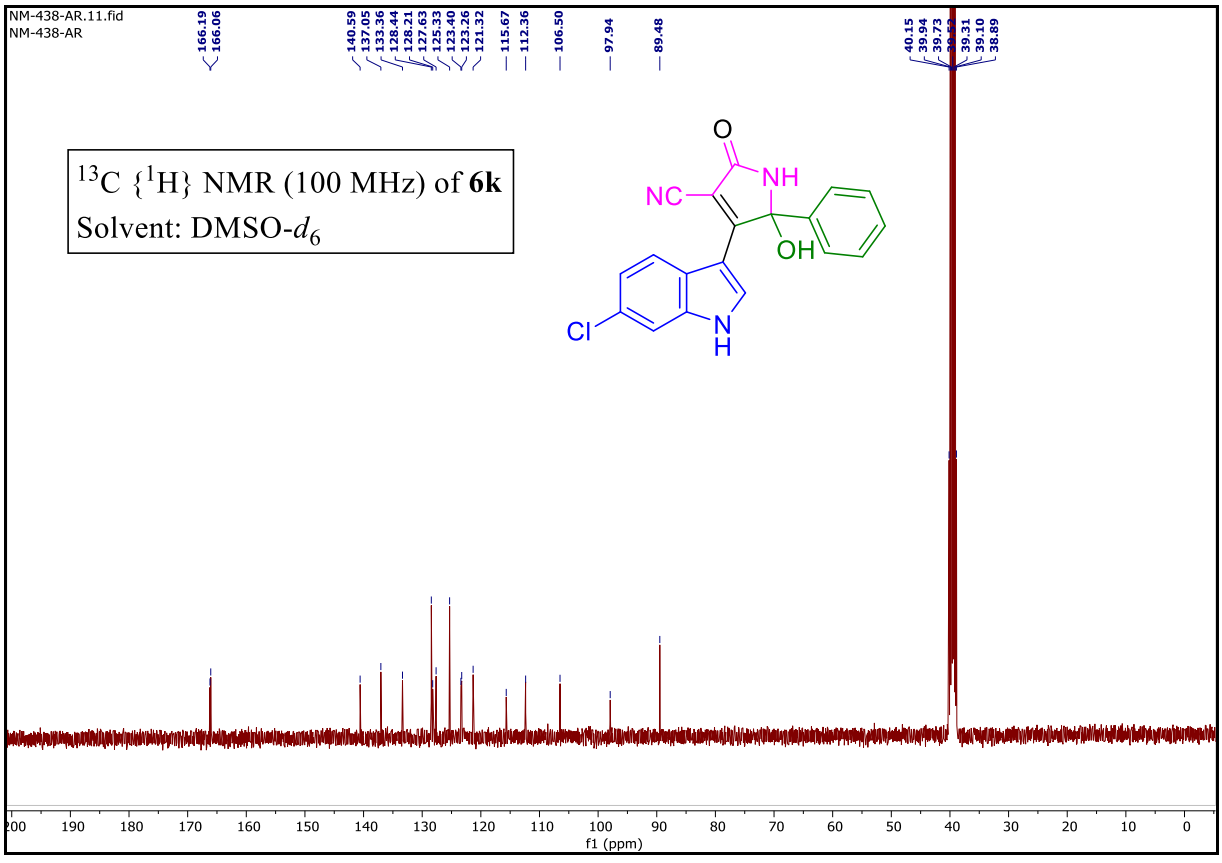

NM-411.10.fid
NM-411
12.17
9.32
7.93
7.92
7.89
7.87
7.59
7.47
7.46
7.32
7.30
7.28
7.24
7.22
7.21
7.08
7.06
7.04
7.01
7.00
3.42
2.50
2.42
^{1}H NMR (400 MHz) of **6i**
Solvent: DMSO-d_6
O
NH
NC
OH
N
H
CH$_3$
1.00
1.02
1.04
1.04
1.02
2.16
2.21
1.15
1.10
1.08
3.00
f1 (ppm)

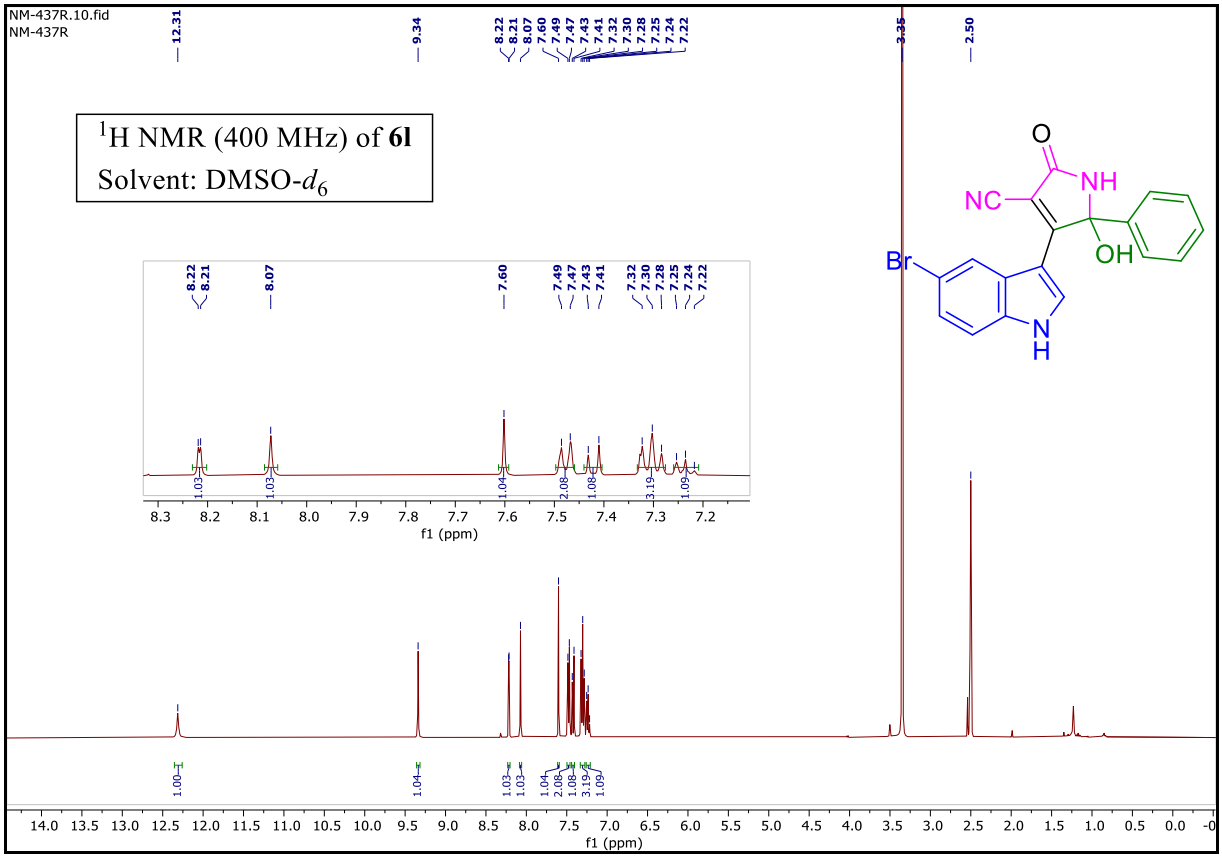

NM-411.11.fid
NM-411
166.55
166.45
141.09
135.95
132.09
128.45
128.14
125.30
124.62
123.60
121.97
121.30
119.54
115.91
106.98
97.00
89.55
40.15
39.94
39.73
39.52
39.31
39.10
38.89
16.66
^{13}C {^{1}H} NMR (100 MHz) of **6i**
Solvent: DMSO-d_6
O
NH
NC
OH
N
H
CH$_3$
f1 (ppm)

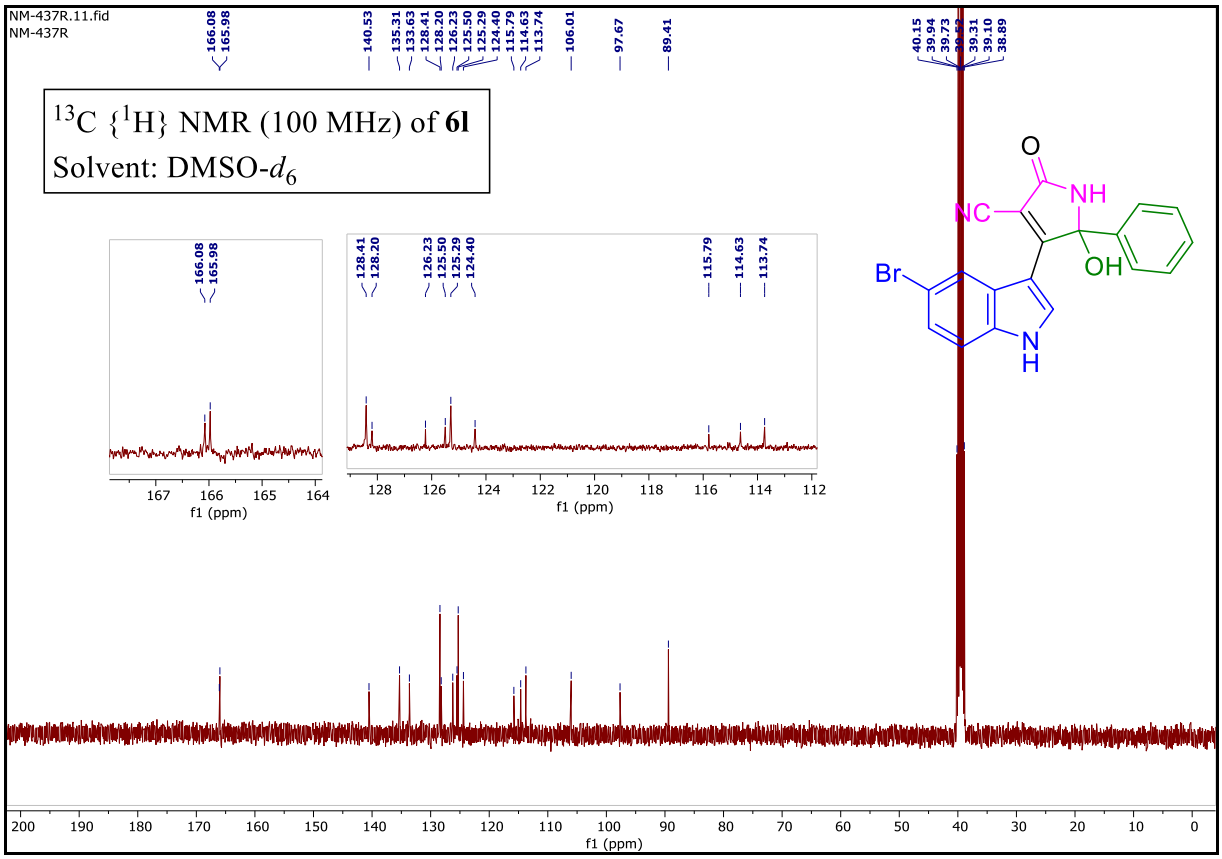

NM-506.10.fid
NM-506
^{1}H NMR (400 MHz) of **6j**
Solvent: DMSO-d_6
f1 (ppm)

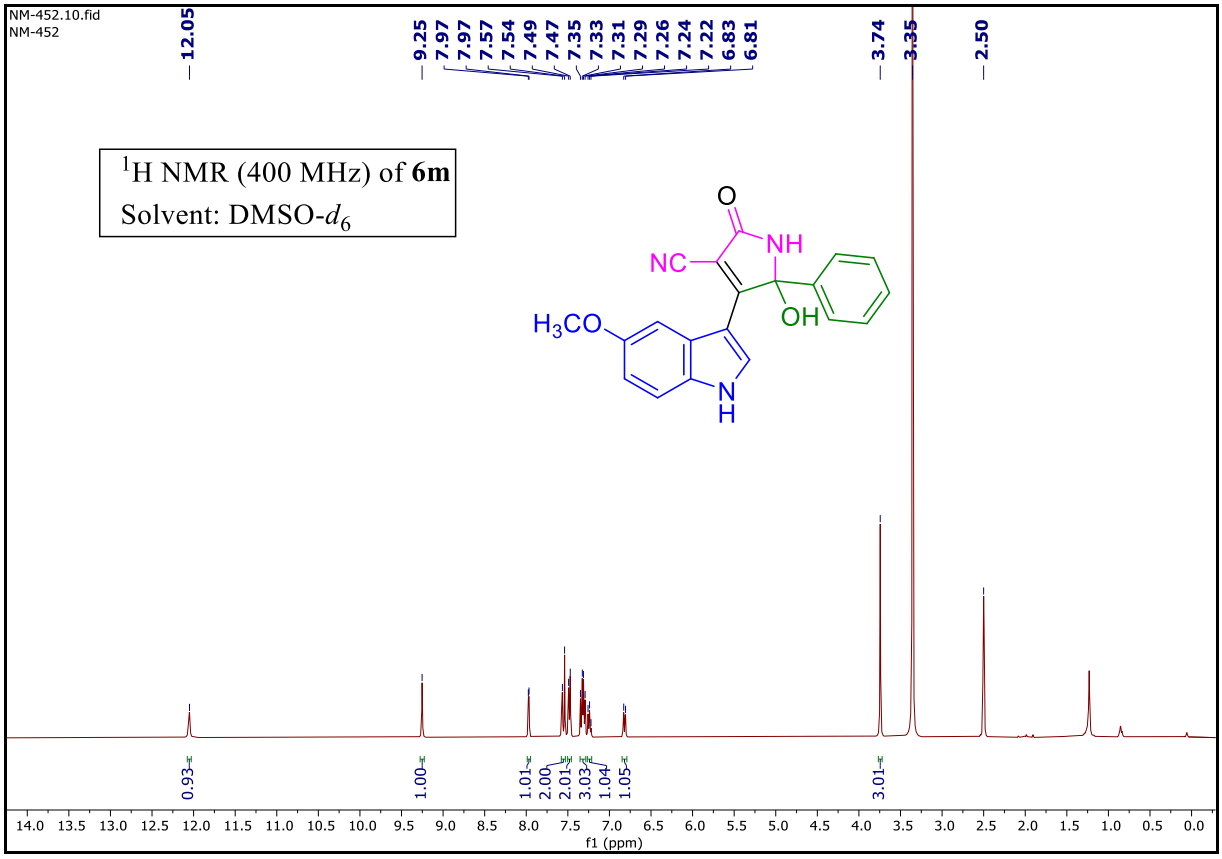

NM-506
single pulse decoupled gated NOE
^{13}C {^{1}H} NMR (125 MHz) of **6j**
Solvent: DMSO-d_6
f1 (ppm)

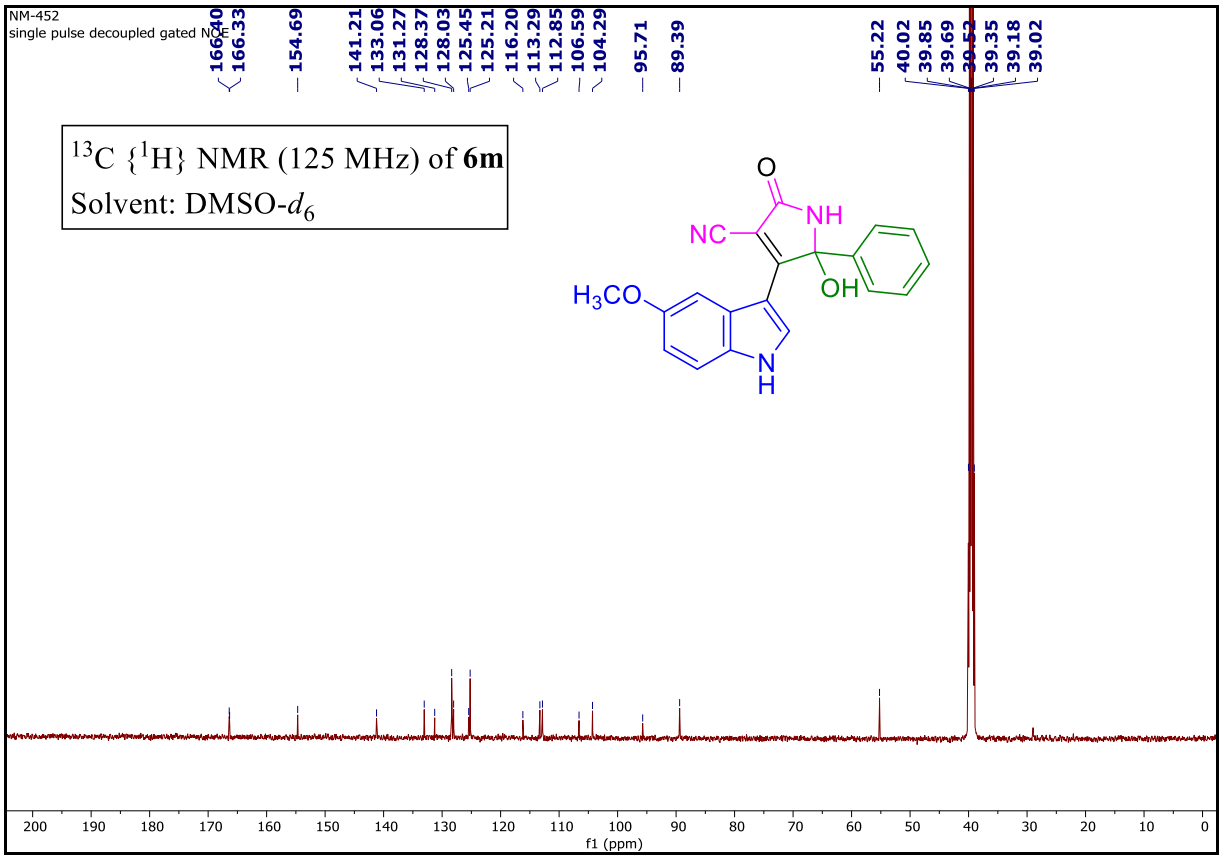

NM-438-AR.10.fid
NM-438-AR
^{1}H NMR (400 MHz) of **6k**
Solvent: DMSO-d_6
f1 (ppm)

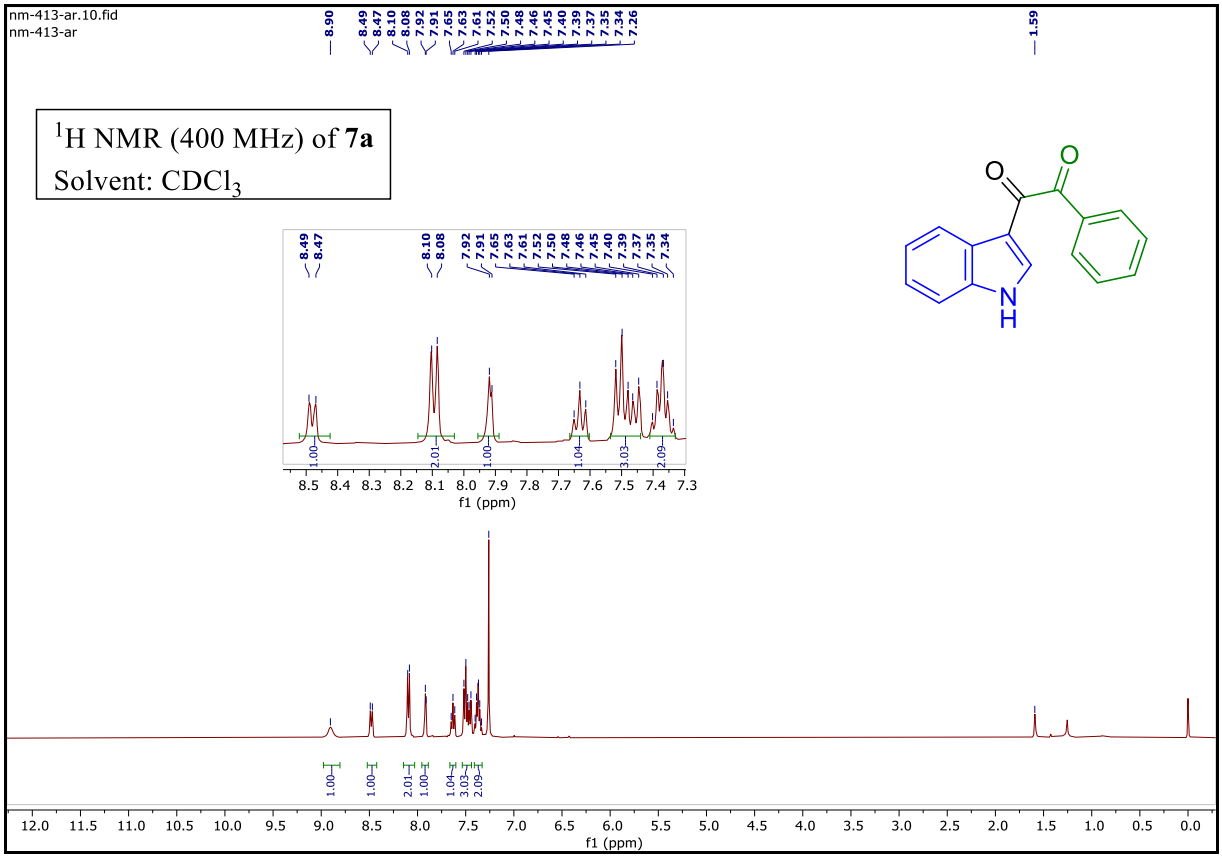

NM-438-AR.11.fid
NM-438-AR
^{13}C {^{1}H} NMR (100 MHz) of **6k**
Solvent: DMSO-d_6
f1 (ppm)

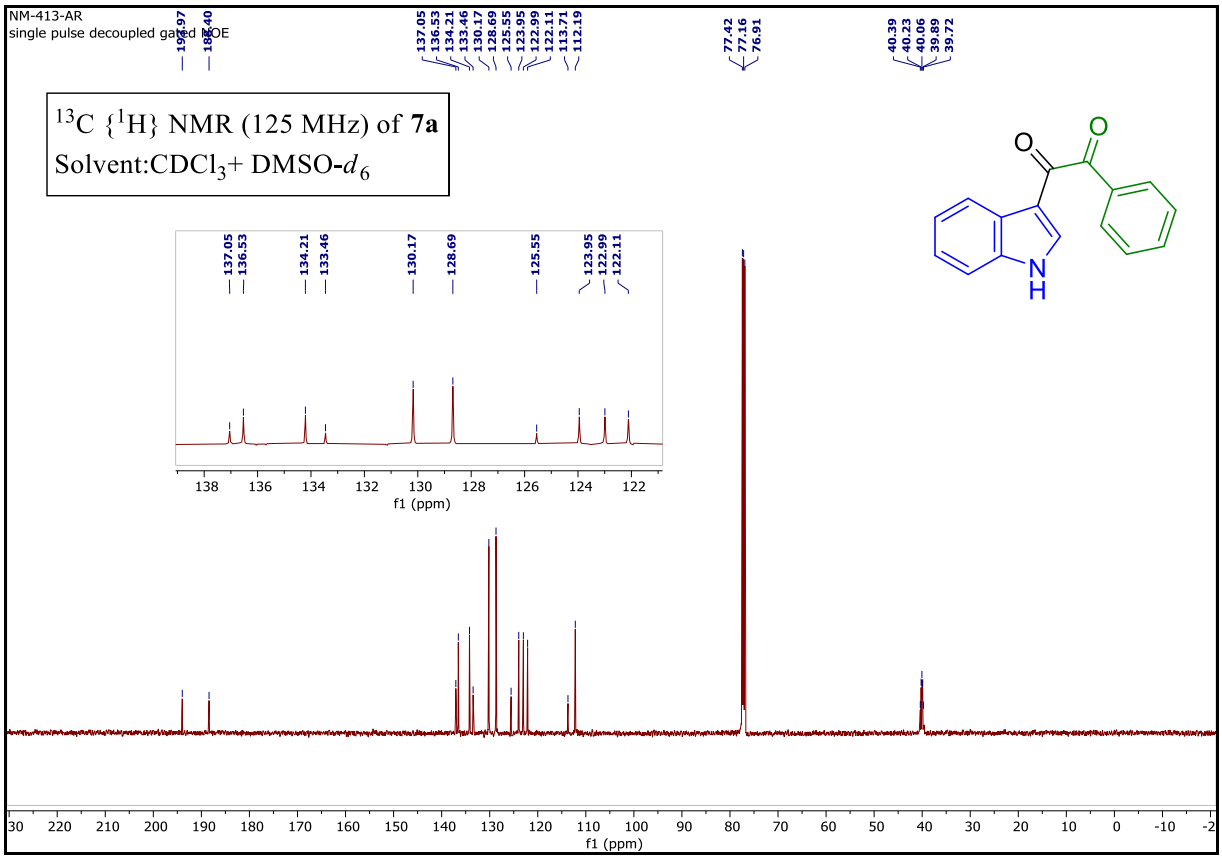

NM-437R.10.fid
NM-437R
^{1}H NMR (400 MHz) of **6l**
Solvent: DMSO-d_6
f1 (ppm)

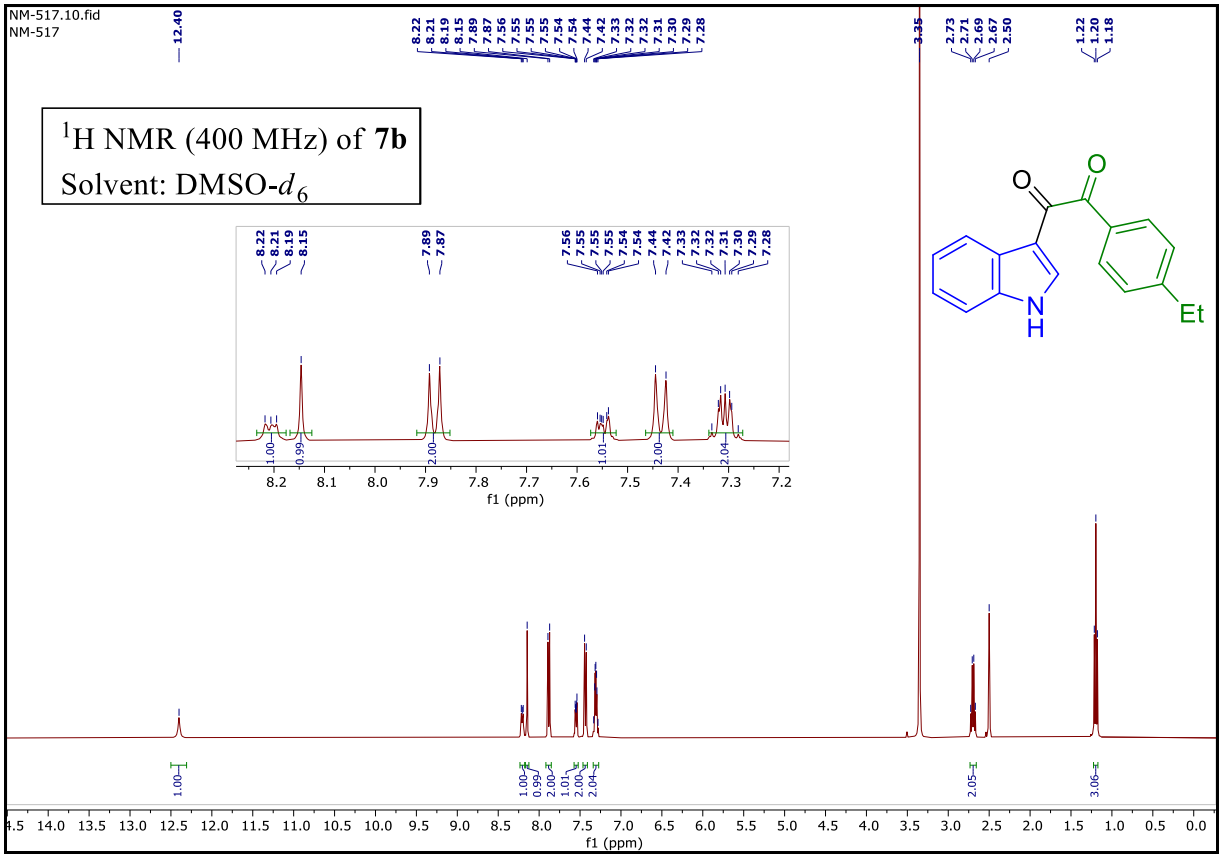

NM-437R.11.fid
NM-437R
^{13}C {^{1}H} NMR (100 MHz) of **6l**
Solvent: DMSO-d_6
f1 (ppm)

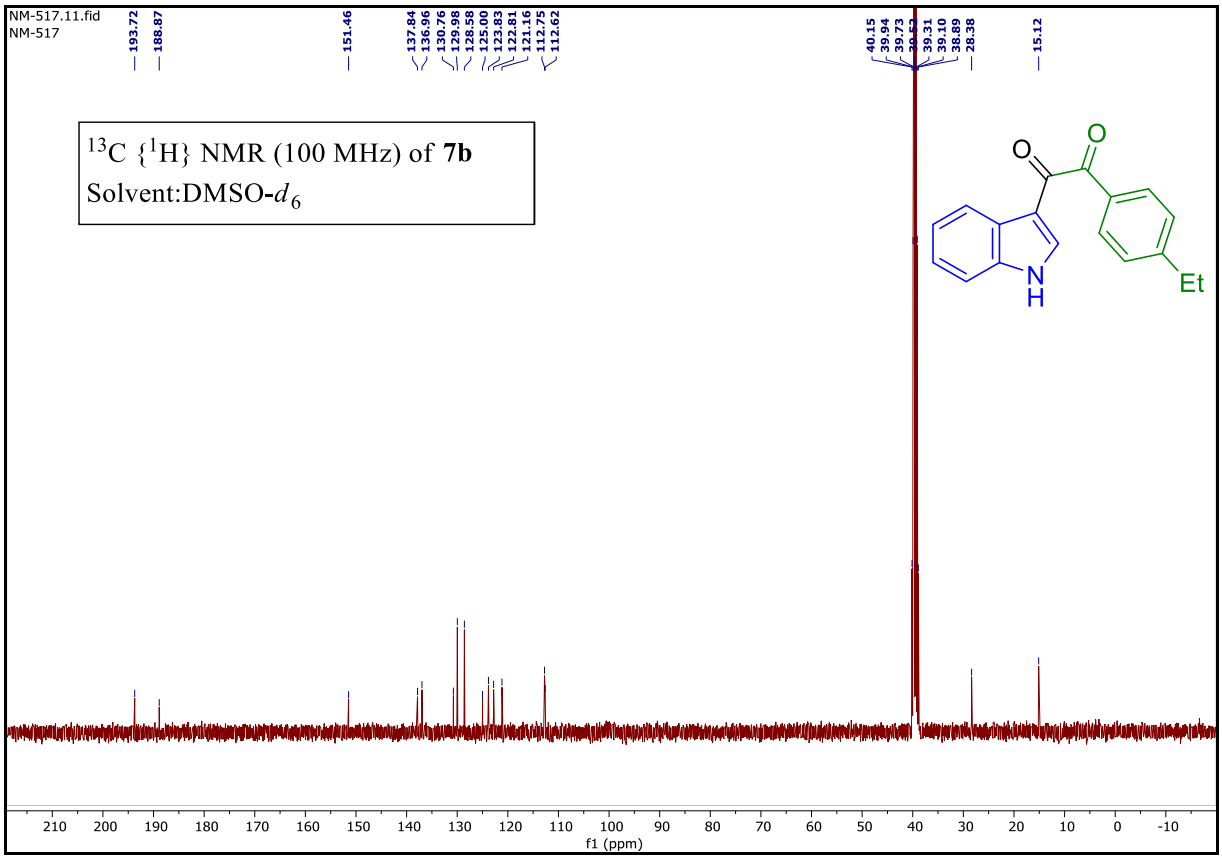

NM-452.10.fid
NM-452
12.05
9.25
7.97
7.97
7.57
7.54
7.49
7.47
7.35
7.33
7.31
7.29
7.26
7.24
7.22
6.83
6.81
3.74
3.35
2.50
^{1}H NMR (400 MHz) of **6m**
Solvent: DMSO-d_6
O
NH
NC
OH
H_3CO
N
H
0.93
1.00
1.01
2.00
2.01
3.03
1.04
1.05
3.01
14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 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
f1 (ppm)

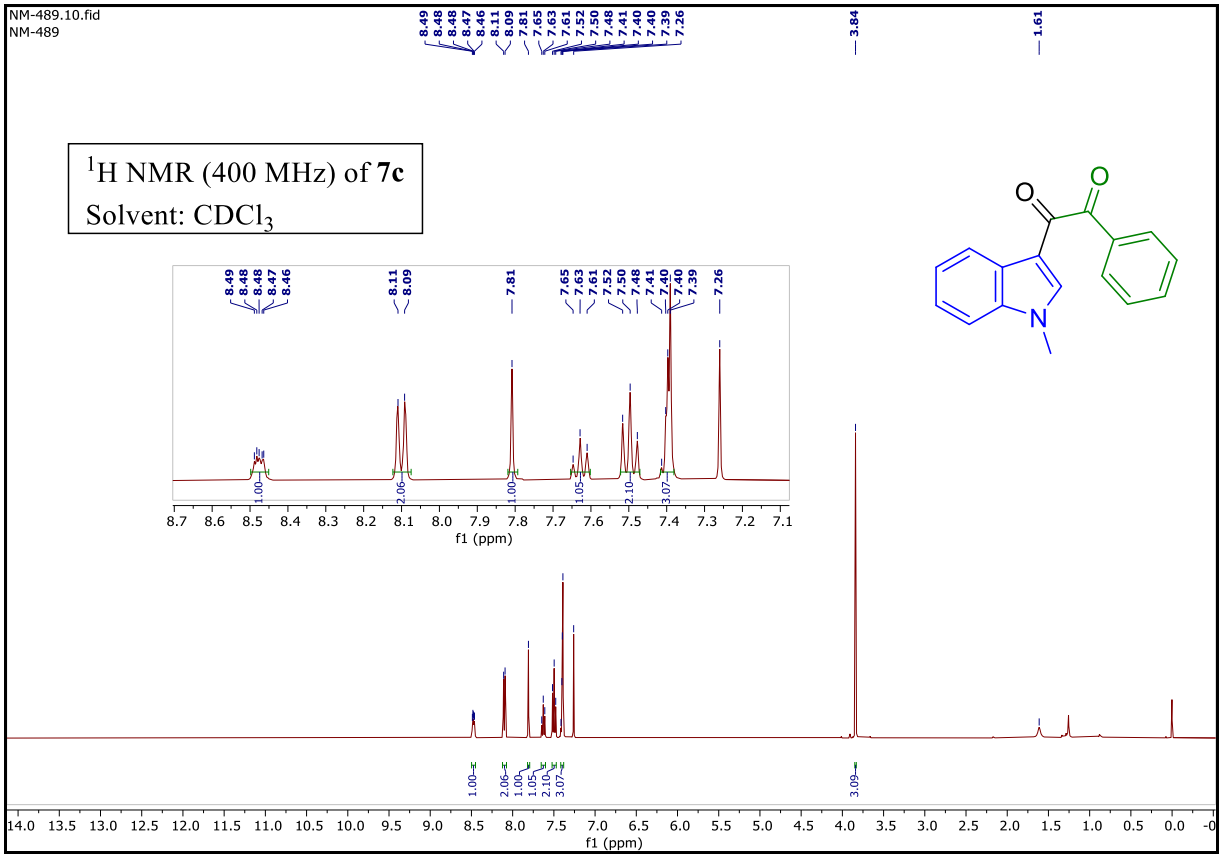

NM-452
single pulse decoupled gated NOE
166.40
166.33
154.69
141.21
133.06
131.27
128.37
128.03
125.45
125.21
116.20
113.29
112.85
106.59
104.29
95.71
89.39
55.22
40.02
39.85
39.69
39.52
39.35
39.18
39.02
^{13}C {^{1}H} NMR (125 MHz) of **6m**
Solvent: DMSO-d_6
O
NH
NC
OH
H_3CO
N
H
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

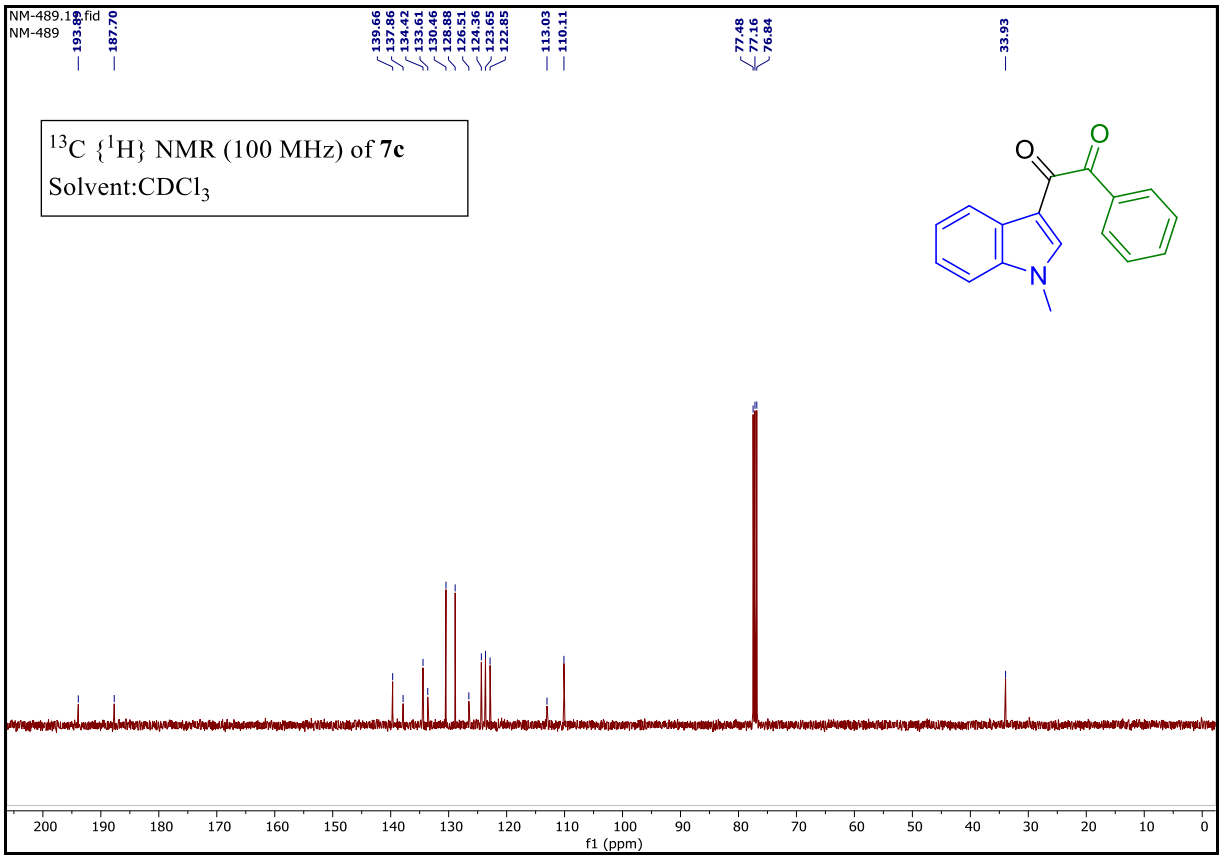

nm-413-ar.10.fid
nm-413-ar
^{1}H NMR (400 MHz) of **7a**
Solvent: $CDCl_3$
f1 (ppm)

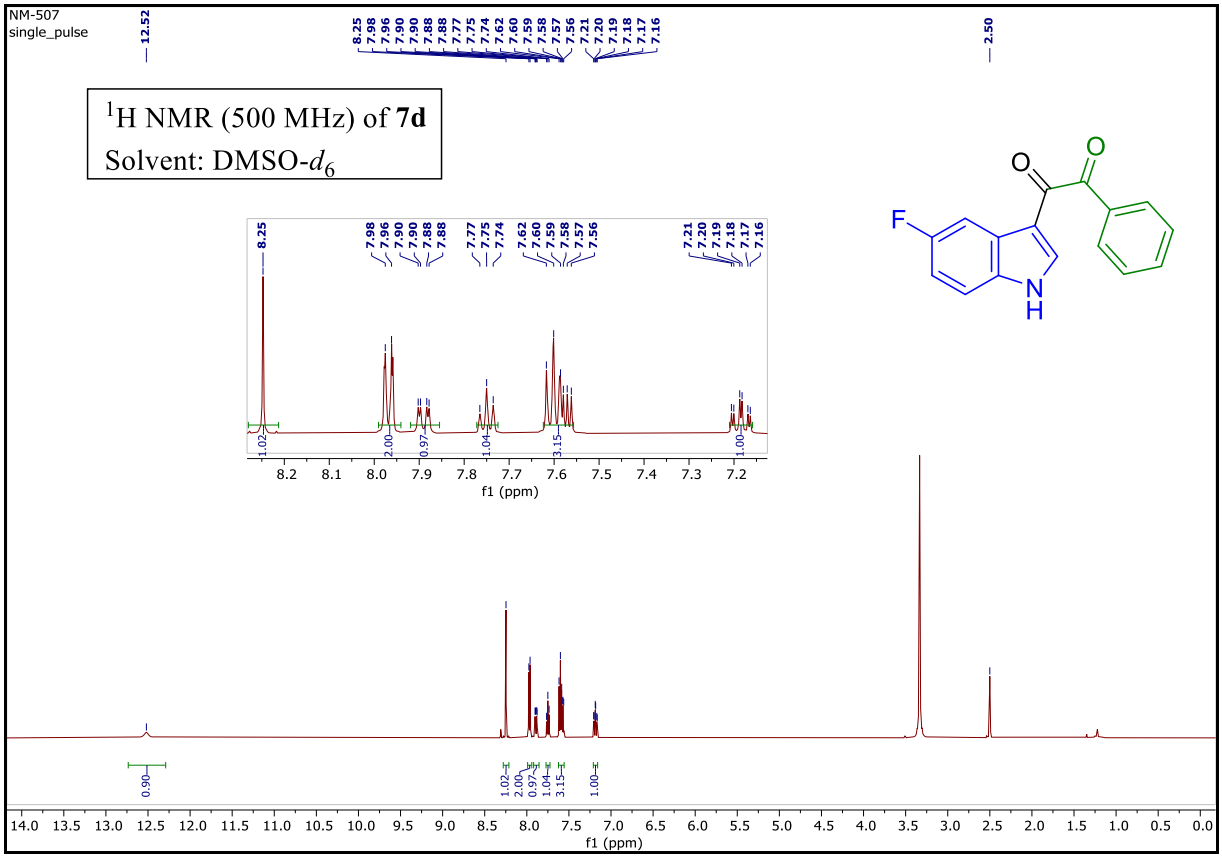

NM-413-AR
single pulse decoupled gated NOE
^{13}C {^{1}H} NMR (125 MHz) of **7a**
Solvent:$CDCl_3$+ DMSO-d_6
f1 (ppm)

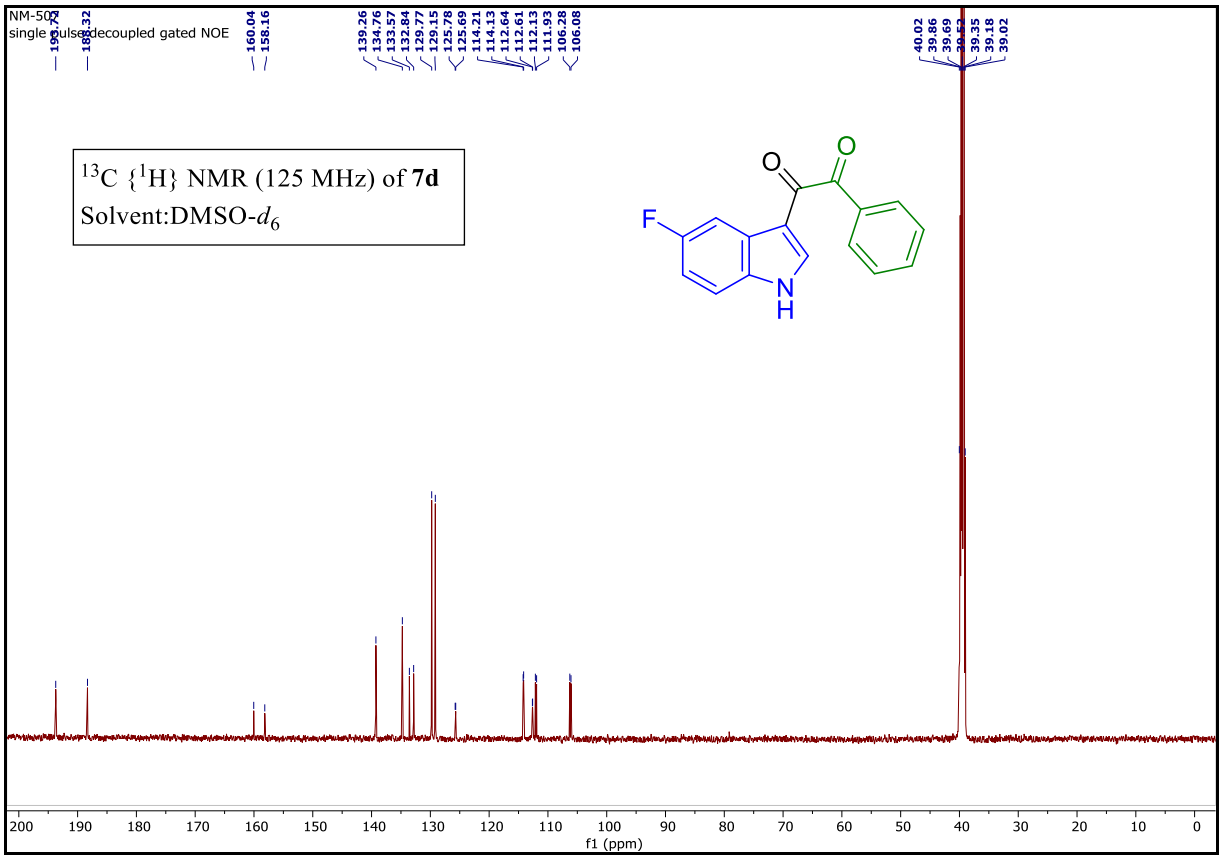

NM-517.10.fid
NM-517
^{1}H NMR (400 MHz) of **7b**
Solvent: DMSO-d_6
f1 (ppm)

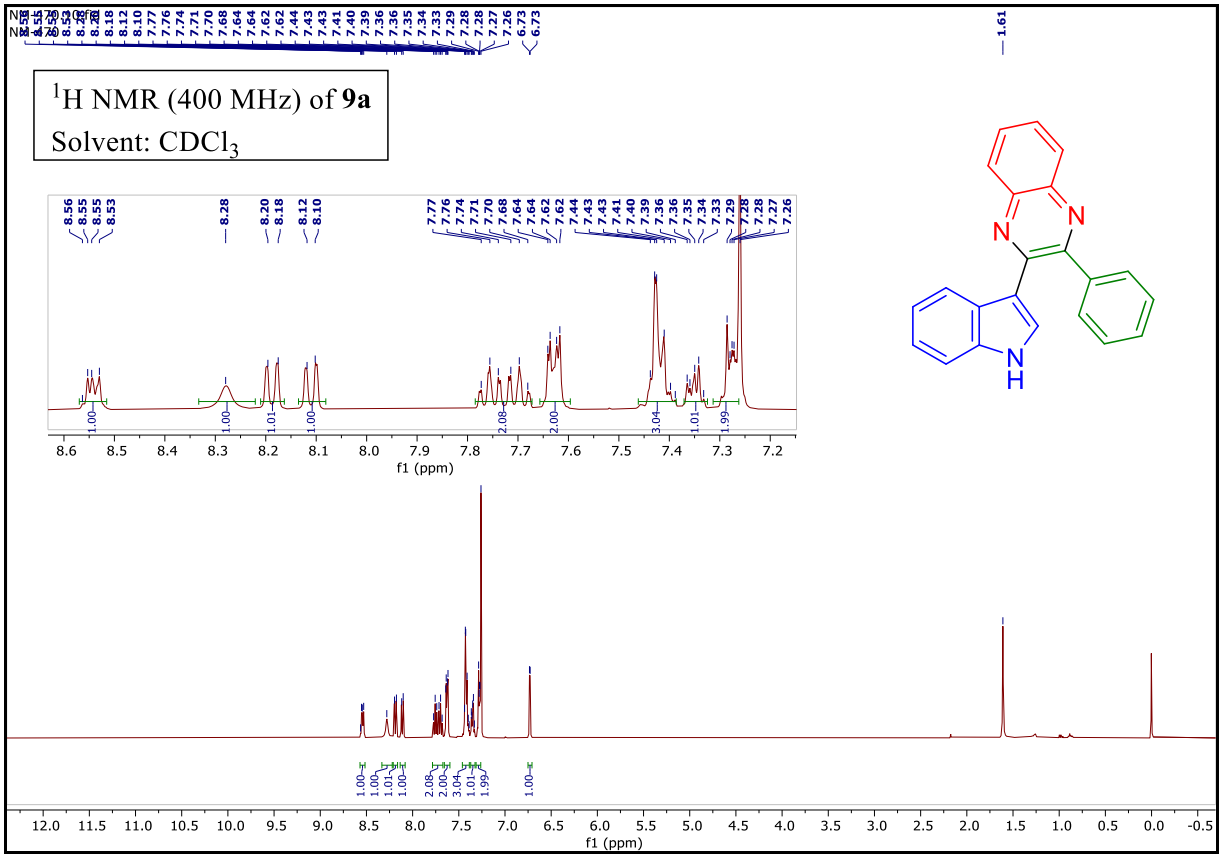

NM-517.11.fid
NM-517
^{13}C {^{1}H} NMR (100 MHz) of **7b**
Solvent:DMSO-d_6
f1 (ppm)

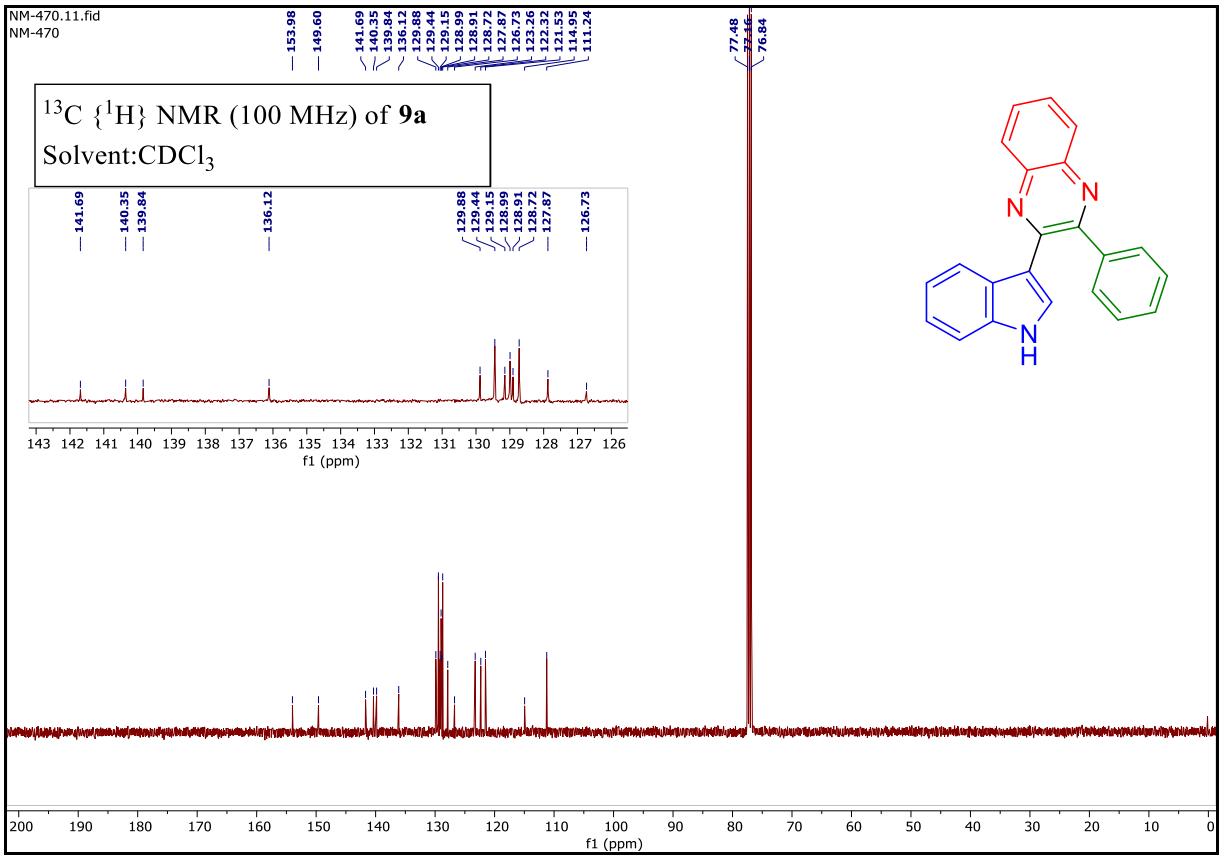

NM-489.10.fid
NM-489
^{1}H NMR (400 MHz) of **7c**
Solvent: $CDCl_3$
f1 (ppm)

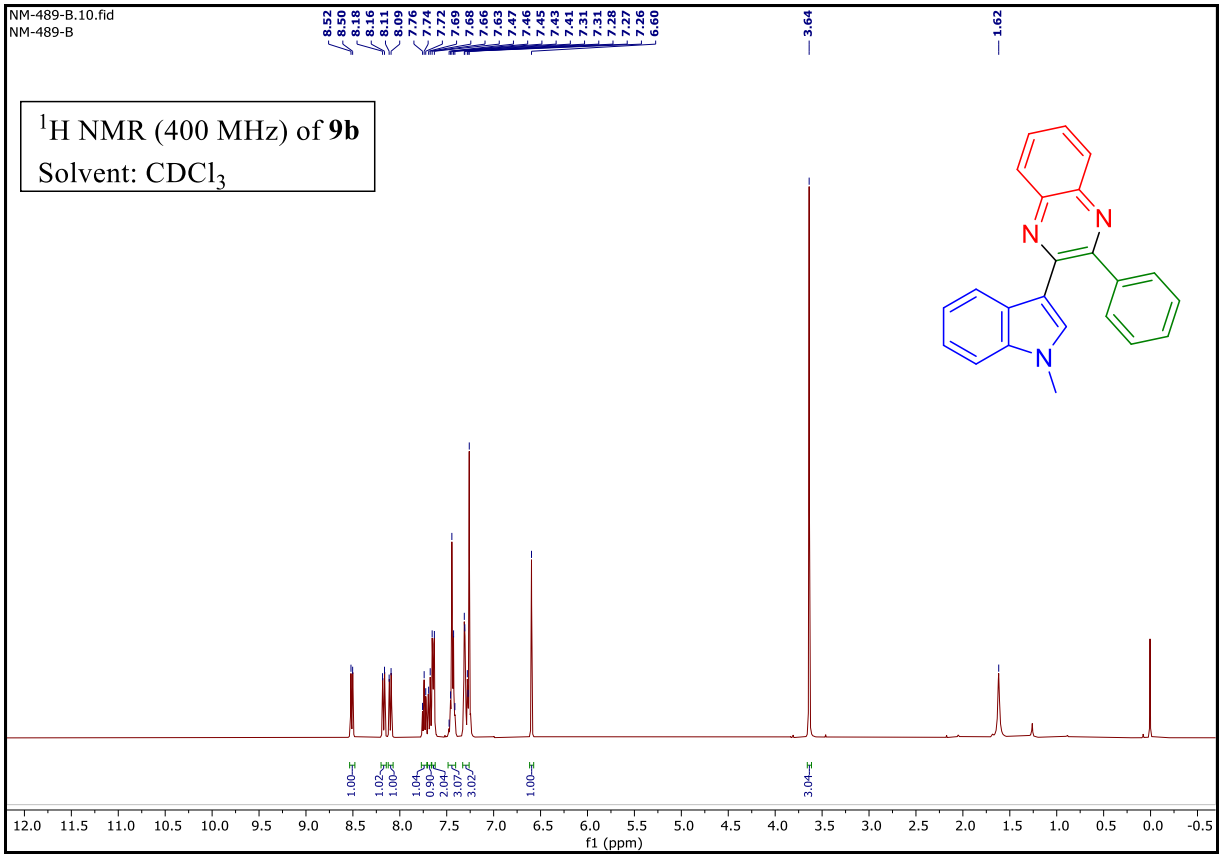

NM-489.11.fid
NM-489
^{13}C {^{1}H} NMR (100 MHz) of **7c**
Solvent:$CDCl_3$
f1 (ppm)

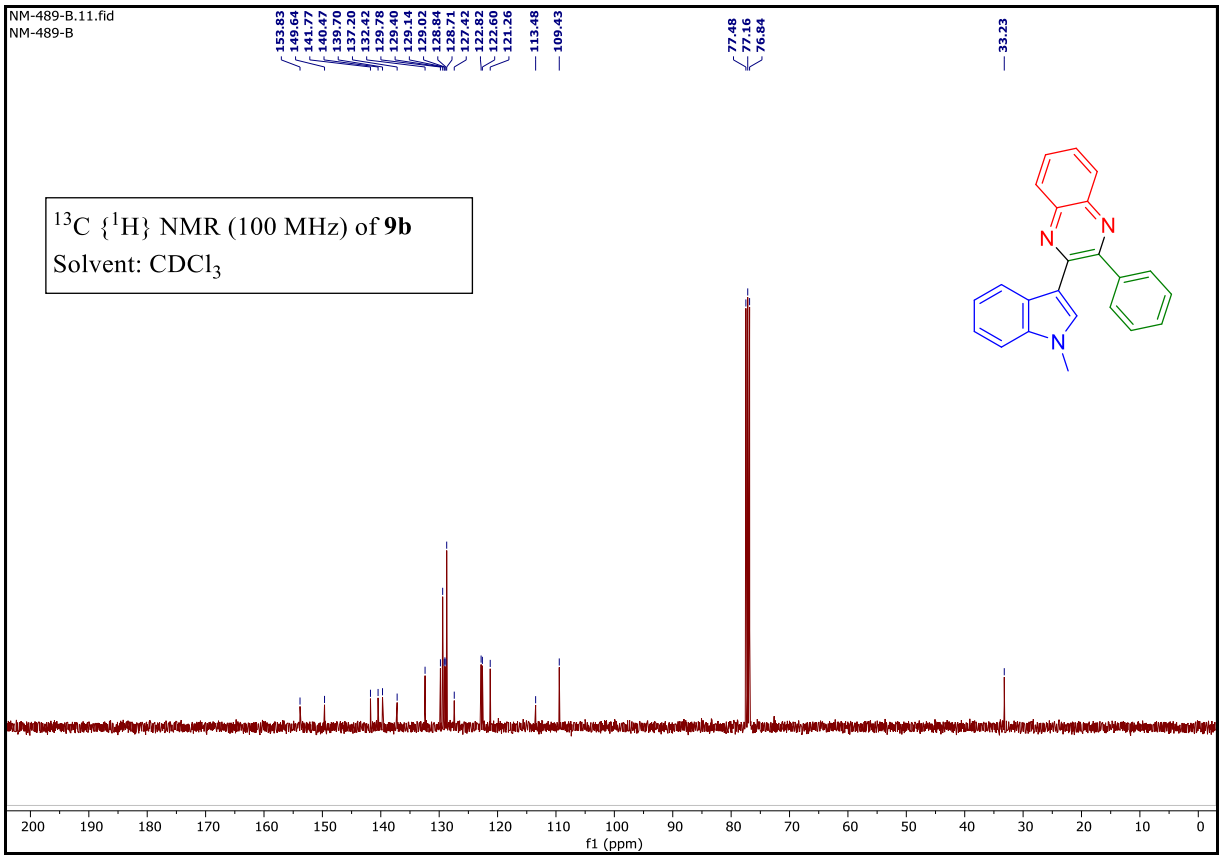

NM-507
single_pulse
^{1}H NMR (500 MHz) of **7d**
Solvent: DMSO-d_6
f1 (ppm)


NM-507
single_pulse_decoupled gated NOE
^{13}C {^{1}H} NMR (125 MHz) of **7d**
Solvent:DMSO-d_6
f1 (ppm)

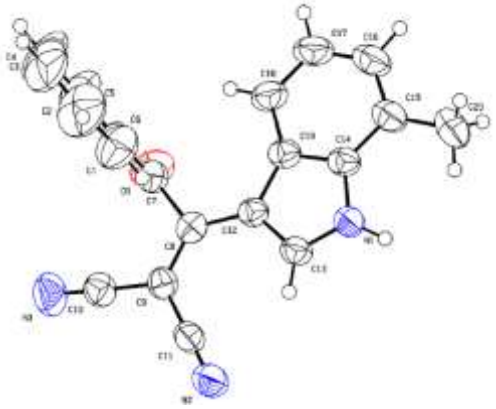

^{1}H NMR (400 MHz) of **9a**
Solvent: $CDCl_3$
f1 (ppm)


NM-470.11.fid
NM-470
^{13}C {^{1}H} NMR (100 MHz) of **9a**
Solvent:$CDCl_3$
f1 (ppm)


NM-489-B.10.fid
NM-489-B
^{1}H NMR (400 MHz) of **9b**
Solvent: $CDCl_3$
f1 (ppm)


NM-489-B.11.fid
NM-489-B
^{13}C {^{1}H} NMR (100 MHz) of **9b**
Solvent: $CDCl_3$
f1 (ppm)

2. Crystallographic description of compound 5n



Ellipsoid plot

Table S1. Crystal data and structure refinement for 5n

CCDC No.	2376014
Empirical formula	$C_{20}H_{13}N_3O$
Formula weight	311.33
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P 21/n
Unit cell dimensions	a = 13.5858(8) Å α = 90°. b = 7.0142(4) Å β = 95.905(2)°. c = 19.7041(11) Å γ = 90°.
Volume	1867.71(19) $Å^3$
Z	4
Density (calculated)	1.107 Mg/m^3
Absorption coefficient	0.071 mm^{-1}
F(000)	648
Crystal size	0.184 x 0.128 x 0.075 mm^3
Theta range for data collection	3.272 to 24.998°.
Index ranges	-16<=h<=16, -8<=k<=8, -23<=l<=23
Reflections collected	49056
Independent reflections	3285 [R(int) = 0.0734]
Completeness to theta = 24.998°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9602 and 0.6988

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3285 / 0 / 221
Goodness-of-fit on F^2	1.054
Final R indices [I>2sigma(I)]	R1 = 0.0614, wR2 = 0.1670
R indices (all data)	R1 = 0.0763, wR2 = 0.1784
Extinction coefficient	n/a
Largest diff. peak and hole	0.235 and -0.221 e.Å^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 5n. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7721(2)	4536(5)	3478(2)	89(1)
C(2)	8550(3)	4495(8)	3112(2)	123(2)
C(3)	8975(3)	2831(10)	2987(2)	136(2)
C(4)	8602(4)	1186(9)	3214(3)	146(2)
C(5)	7779(3)	1180(6)	3576(2)	106(1)
C(6)	7333(2)	2901(4)	3702(1)	62(1)
C(7)	6459(2)	2875(3)	4088(1)	52(1)
C(8)	5972(2)	4769(3)	4220(1)	44(1)
C(9)	5241(2)	5315(3)	3723(1)	46(1)
C(10)	4997(2)	4121(3)	3139(1)	54(1)
C(11)	4693(2)	7038(3)	3727(1)	50(1)
C(12)	6311(2)	5742(3)	4837(1)	43(1)
C(13)	5988(2)	7508(3)	5047(1)	47(1)
C(14)	7127(2)	6554(3)	5869(1)	47(1)
C(15)	7762(2)	6517(4)	6476(1)	58(1)
C(16)	8341(2)	4897(4)	6568(1)	68(1)
C(17)	8283(2)	3429(4)	6096(1)	71(1)
C(18)	7655(2)	3501(4)	5499(1)	60(1)
C(19)	7054(2)	5110(3)	5376(1)	47(1)
C(20)	7803(2)	8130(5)	6977(1)	83(1)
N(1)	6462(1)	7981(3)	5649(1)	52(1)
N(2)	4263(2)	8441(3)	3719(1)	68(1)
N(3)	4810(2)	3173(4)	2672(1)	80(1)
O(1)	6110(1)	1431(2)	4299(1)	76(1)

Table S3. Bond lengths [Å] for 5n

C(1)-C(6)	1.355(4)		C(1)-C(6)	1.355(4)
C(1)-C(2)	1.398(5)		C(1)-C(2)	1.398(5)
C(1)-H(1)	0.9300		C(1)-H(1)	0.9300
C(2)-C(3)	1.336(7)		C(2)-C(3)	1.336(7)
C(2)-H(2)	0.9300		C(2)-H(2)	0.9300
C(3)-C(4)	1.355(7)		C(3)-C(4)	1.355(7)
C(3)-H(3)	0.9300		C(3)-H(3)	0.9300
C(4)-C(5)	1.386(6)		C(4)-C(5)	1.386(6)
C(4)-H(4)	0.9300		C(4)-H(4)	0.9300
C(5)-C(6)	1.385(4)		C(5)-C(6)	1.385(4)
C(5)-H(5)	0.9300		C(5)-H(5)	0.9300
C(6)-C(7)	1.474(3)		C(6)-C(7)	1.474(3)
C(7)-O(1)	1.210(3)		C(7)-O(1)	1.210(3)
C(7)-C(8)	1.519(3)		C(7)-C(8)	1.519(3)
C(8)-C(9)	1.375(3)		C(8)-C(9)	1.375(3)
C(8)-C(12)	1.428(3)		C(8)-C(12)	1.428(3)
C(9)-C(11)	1.421(3)		C(9)-C(11)	1.421(3)
C(9)-C(10)	1.435(3)		C(9)-C(10)	1.435(3)
C(10)-N(3)	1.142(3)		C(10)-N(3)	1.142(3)
C(11)-N(2)	1.143(3)			

Table S4. Bond angles [°] for 5n

C(6)-C(1)-C(2)	120.8(4)		C(9)-C(8)-C(12)	128.2(2)		C(15)-C(16)-C(17)	122.1(2)
C(6)-C(1)-H(1)	119.6		C(9)-C(8)-C(7)	114.64(18)		C(15)-C(16)-H(16)	119.0
C(2)-C(1)-H(1)	119.6		C(12)-C(8)-C(7)	117.12(18)		C(17)-C(16)-H(16)	119.0
C(3)-C(2)-C(1)	119.9(4)		C(8)-C(9)-C(11)	125.01(19)		C(18)-C(17)-C(16)	122.1(2)
C(3)-C(2)-H(2)	120.0		C(8)-C(9)-C(10)	120.0(2)		C(18)-C(17)-H(17)	118.9
C(1)-C(2)-H(2)	120.0		C(11)-C(9)-C(10)	115.00(19)		C(16)-C(17)-H(17)	118.9
C(2)-C(3)-C(4)	120.0(4)		N(3)-C(10)-C(9)	179.4(3)		C(17)-C(18)-C(19)	118.4(2)
C(2)-C(3)-H(3)	120.0		N(2)-C(11)-C(9)	178.5(3)		C(17)-C(18)-H(18)	120.8
C(4)-C(3)-H(3)	120.0		C(13)-C(12)-C(8)	126.51(18)		C(19)-C(18)-H(18)	120.8
C(3)-C(4)-C(5)	121.4(4)		C(13)-C(12)-C(19)	105.65(17)		C(14)-C(19)-C(18)	117.7(2)
C(3)-C(4)-H(4)	119.3		C(8)-C(12)-C(19)	127.85(19)		C(14)-C(19)-C(12)	106.22(18)
C(5)-C(4)-H(4)	119.3		N(1)-C(13)-C(12)	110.42(18)		C(18)-C(19)-C(12)	136.0(2)
C(6)-C(5)-C(4)	118.7(4)		N(1)-C(13)-H(13)	124.8		C(15)-C(20)-H(20A)	109.5
C(6)-C(5)-H(5)	120.6		C(12)-C(13)-H(13)	124.8		C(15)-C(20)-H(20B)	109.5
C(4)-C(5)-H(5)	120.6		N(1)-C(14)-C(19)	108.00(18)		H(20A)-C(20)-H(20B)	109.5
C(1)-C(6)-C(5)	119.1(3)		N(1)-C(14)-C(15)	127.1(2)		C(15)-C(20)-H(20C)	109.5
C(1)-C(6)-C(7)	122.6(2)		C(19)-C(14)-C(15)	124.9(2)		H(20A)-C(20)-H(20C)	109.5
C(5)-C(6)-C(7)	118.2(3)		C(16)-C(15)-C(14)	114.8(2)		H(20B)-C(20)-H(20C)	109.5
O(1)-C(7)-C(6)	123.5(2)		C(16)-C(15)-C(20)	123.4(2)		C(13)-N(1)-C(14)	109.71(19)
O(1)-C(7)-C(8)	118.7(2)		C(14)-C(15)-C(20)	121.8(2)		C(13)-N(1)-H(1A)	126.5(17)
C(6)-C(7)-C(8)	117.8(2)		C(15)-C(16)-C(17)	122.1(2)		C(14)-N(1)-H(1A)	123.7(17)

Table S5. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 5n. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U11	U22	U33	U23	U13	U12
C(1)	76(2)	98(2)	98(2)	-6(2)	34(2)	-3(2)
C(2)	92(3)	163(4)	123(3)	-11(3)	54(2)	-18(3)
C(3)	81(3)	216(6)	119(3)	-51(4)	46(2)	6(3)

C(4)	117(4)	166(5)	163(4)	-60(4)	56(3)	38(3)
C(5)	98(2)	98(3)	125(3)	-35(2)	33(2)	21(2)
C(6)	56(1)	71(2)	59(1)	-15(1)	5(1)	5(1)
C(7)	53(1)	46(1)	55(1)	-4(1)	0(1)	-2(1)
C(8)	44(1)	42(1)	49(1)	1(1)	11(1)	-4(1)
C(9)	49(1)	44(1)	45(1)	-1(1)	4(1)	-3(1)
C(10)	53(1)	54(1)	56(1)	-4(1)	3(1)	-6(1)
C(11)	51(1)	51(1)	45(1)	-2(1)	-5(1)	-1(1)
C(12)	42(1)	43(1)	44(1)	4(1)	6(1)	2(1)
C(13)	47(1)	44(1)	47(1)	4(1)	-3(1)	4(1)
C(14)	45(1)	50(1)	47(1)	8(1)	4(1)	4(1)
C(15)	51(1)	72(2)	50(1)	9(1)	-1(1)	2(1)
C(16)	57(1)	89(2)	54(1)	18(1)	-6(1)	10(1)
C(17)	64(2)	76(2)	70(2)	19(1)	2(1)	26(1)
C(18)	59(1)	58(2)	63(1)	8(1)	7(1)	18(1)
C(19)	44(1)	48(1)	48(1)	9(1)	7(1)	4(1)
C(20)	87(2)	96(2)	60(2)	-12(2)	-20(1)	3(2)
N(1)	57(1)	48(1)	48(1)	-4(1)	-4(1)	7(1)
N(2)	72(1)	61(1)	68(1)	-5(1)	-14(1)	11(1)
N(3)	82(2)	83(2)	71(2)	-26(1)	-2(1)	-13(1)
O(1)	79(1)	46(1)	104(2)	7(1)	16(1)	0(1)

Table S6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for 5n

	x	y	z	U(eq)
H(1)	7433	5699	3568	107
H(2)	8805	5625	2956	148
H(3)	9527	2803	2745	163
H(4)	8905	36	3125	175
H(5)	7532	42	3731	127
H(13)	5509	8253	4802	56
H(16)	8783	4791	6959	81
H(17)	8680	2359	6184	85
H(18)	7633	2505	5186	72
H(20A)	7342	9101	6812	125
H(20B)	7635	7668	7409	125

H(20C)	8460	8653	7032	125
H(1A)	6350(20)	9050(40)	5900(14)	75(8)

Table S7. Torsion angles [°] for 5n

C(6)-C(1)-C(2)-C(3)	-0.8(6)		C(8)-C(12)-C(13)-N(1)	179.8(2)
C(1)-C(2)-C(3)-C(4)	0.1(7)		C(19)-C(12)-C(13)-N(1)	0.1(2)
C(2)-C(3)-C(4)-C(5)	0.1(8)		N(1)-C(14)-C(15)-C(16)	179.3(2)
C(3)-C(4)-C(5)-C(6)	0.4(7)		C(19)-C(14)-C(15)-C(16)	-0.1(3)
C(2)-C(1)-C(6)-C(5)	1.3(5)		N(1)-C(14)-C(15)-C(20)	-1.0(4)
C(2)-C(1)-C(6)-C(7)	-179.9(3)		C(19)-C(14)-C(15)-C(20)	179.5(2)
C(4)-C(5)-C(6)-C(1)	-1.1(5)		C(14)-C(15)-C(16)-C(17)	-0.6(4)
C(4)-C(5)-C(6)-C(7)	-179.9(3)		C(20)-C(15)-C(16)-C(17)	179.8(3)
C(1)-C(6)-C(7)-O(1)	-179.1(3)		C(15)-C(16)-C(17)-C(18)	1.0(4)
C(5)-C(6)-C(7)-O(1)	-0.2(4)		C(16)-C(17)-C(18)-C(19)	-0.7(4)
C(1)-C(6)-C(7)-C(8)	1.4(4)		N(1)-C(14)-C(19)-C(18)	-179.1(2)
C(5)-C(6)-C(7)-C(8)	-179.7(2)		C(15)-C(14)-C(19)-C(18)	0.4(3)
O(1)-C(7)-C(8)-C(9)	-89.8(3)		N(1)-C(14)-C(19)-C(12)	0.5(2)
C(6)-C(7)-C(8)-C(9)	89.7(2)		C(15)-C(14)-C(19)-C(12)	-180.0(2)
O(1)-C(7)-C(8)-C(12)	89.5(3)		C(17)-C(18)-C(19)-C(14)	0.0(3)
C(6)-C(7)-C(8)-C(12)	-91.0(2)		C(17)-C(18)-C(19)-C(12)	-179.5(2)
C(12)-C(8)-C(9)-C(11)	2.0(4)		C(13)-C(12)-C(19)-C(14)	-0.4(2)
C(7)-C(8)-C(9)-C(11)	-178.8(2)		C(8)-C(12)-C(19)-C(14)	179.90(19)
C(12)-C(8)-C(9)-C(10)	-179.3(2)		C(13)-C(12)-C(19)-C(18)	179.1(3)
C(7)-C(8)-C(9)-C(10)	-0.1(3)		C(8)-C(12)-C(19)-C(18)	-0.6(4)
C(9)-C(8)-C(12)-C(13)	-2.8(3)		C(12)-C(13)-N(1)-C(14)	0.2(3)
C(7)-C(8)-C(12)-C(13)	178.0(2)		C(19)-C(14)-N(1)-C(13)	-0.5(2)
C(9)-C(8)-C(12)-	176.8(2)		C(15)-C(14)-N(1)-C(13)	-180.0(2)

C(19)				
C(7)-C(8)-C(12)-C(19)	-2.3(3)			

Symmetry transformations used to generate equivalent atoms:

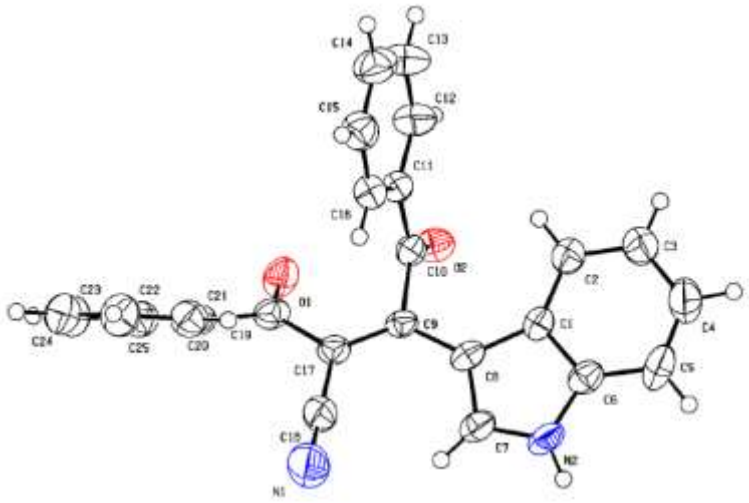
Table S8. Hydrogen bonds for 5n [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(13)-H(13)...N(2)	0.93	2.59	3.392(3)	145.1
C(13)-H(13)...O(1)#1	0.93	2.60	3.134(3)	116.6
N(1)-H(1A)...N(2)#2	0.92(3)	2.12(3)	3.012(3)	164(2)

Symmetry transformations used to generate equivalent atoms:

#1 x,y+1,z #2 -x+1,-y+2,-z+1

3. Crystallographic description of compound 5v



Ellipsoid plot

Table S9. Crystal data and structure refinement for 5v	
CCDC no.	2354497
Empirical formula	$C_{25}H_{16}N_2O_2$
Formula weight	376.40
Temperature/K	298
Crystal system	triclinic
Space group	P-1
a/Å	9.2194(12)
b/Å	10.0506(14)
c/Å	10.4838(14)
α/°	101.017(8)

β/°	101.391(7)
γ/°	93.642(7)
Volume/Å^3	929.6(2)
Z	2
ρ_{calc}g/cm^3	1.345
μ/mm^{-1}	0.086
F(000)	392.0
Crystal size/mm^3	0.089 × 0.056 × 0.045
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.532 to 50.002
Index ranges	-10 ≤ h ≤ 10, -11 ≤ k ≤ 11, -12 ≤ l ≤ 12
Reflections collected	12101
Independent reflections	3197 [R_{int} = 0.0730, R_{sigma} = 0.0826]
Data/restraints/parameters	3197/0/264
Goodness-of-fit on F^2	1.242
Final R indexes [I>=2σ (I)]	R_1 = 0.1078, wR_2 = 0.1599
Final R indexes [all data]	R_1 = 0.1669, wR_2 = 0.1812
Largest diff. peak/hole / e Å^{-3}	0.27/-0.23

Table S10. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5v. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O_2	2656(4)	7362(4)	420(3)	44.7(10)
O_1	969(4)	5335(4)	1399(4)	52.5(11)
N_2	7817(5)	5821(5)	1198(4)	45.5(12)
C_{10}	3147(5)	7205(5)	1531(5)	34.6(12)
C_9	4075(5)	6031(5)	1734(5)	32.8(12)
C_8	5564(5)	6252(5)	1541(5)	35.2(12)
C_1	6307(5)	7484(5)	1325(5)	36.2(12)
C_{11}	3012(5)	8194(5)	2734(5)	38.3(13)
C_{20}	1290(6)	4062(5)	3072(5)	37.3(13)
C_{17}	3444(5)	4952(5)	2122(5)	36.3(13)
C_{19}	1843(5)	4812(5)	2149(5)	41.0(13)
C_7	6569(6)	5288(6)	1442(5)	43.4(14)
C_2	5966(6)	8818(5)	1292(5)	46.6(14)
C_6	7714(6)	7166(6)	1124(5)	41.4(14)
C_{16}	3576(6)	8023(5)	4020(5)	43.9(14)
C_{25}	-115(6)	3361(5)	2688(6)	47.6(15)
C_3	6994(6)	9731(6)	1055(6)	55.1(16)
C_{18}	4293(6)	3897(6)	2491(6)	53.1(16)
C_{21}	2079(6)	4171(6)	4352(5)	49.6(15)
C_{12}	2356(6)	9370(6)	2576(6)	53.2(16)

Table S10. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 5v. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.				
Atom	***x***	***y***	***z***	**U(eq)**
C_4	8384(7)	9376(7)	868(6)	61.6(18)
C_{15}	3441(6)	8994(6)	5101(6)	52.7(16)
N_1	4956(6)	3045(6)	2776(7)	92(2)
C_{22}	1444(7)	3605(6)	5237(6)	58.1(17)
C_{24}	-725(7)	2795(6)	3576(6)	57.9(17)
C_{23}	49(7)	2920(6)	4852(7)	62.4(18)
C_{14}	2753(7)	10120(6)	4917(6)	62.9(18)
C_5	8758(6)	8088(7)	881(6)	58.6(17)
C_{13}	2226(7)	10316(6)	3656(7)	67.5(19)

Table S11. Anisotropic Displacement Parameters (Å^2×10^3) for 5v. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
O_2	44(2)	51(2)	40(2)	11.9(18)	3.3(18)	15.5(18)
O_1	35(2)	69(3)	63(3)	33(2)	12.5(19)	17(2)
N_2	36(3)	58(3)	51(3)	16(2)	19(2)	22(2)
C_{10}	24(3)	36(3)	42(3)	8(3)	5(2)	3(2)
C_9	37(3)	35(3)	30(3)	10(2)	10(2)	14(2)
C_8	29(3)	45(3)	32(3)	5(2)	7(2)	11(2)
C_1	31(3)	44(3)	35(3)	9(3)	8(2)	4(2)
C_{11}	34(3)	37(3)	45(3)	10(3)	11(2)	6(2)
C_{20}	38(3)	38(3)	38(3)	9(3)	9(2)	11(2)
C_{17}	38(3)	37(3)	39(3)	14(2)	11(2)	14(2)
C_{19}	30(3)	41(3)	48(3)	3(3)	4(3)	7(2)
C_7	44(3)	50(4)	41(3)	9(3)	18(3)	15(3)
C_2	40(3)	49(4)	55(4)	14(3)	15(3)	5(3)
C_6	37(3)	53(4)	38(3)	13(3)	9(2)	14(3)
C_{16}	44(3)	40(3)	49(4)	11(3)	13(3)	4(3)
C_{25}	45(3)	49(4)	49(4)	11(3)	11(3)	8(3)
C_3	52(4)	51(4)	69(4)	22(3)	19(3)	8(3)
C_{18}	51(4)	49(4)	70(4)	28(3)	23(3)	14(3)
C_{21}	50(4)	47(4)	50(4)	6(3)	10(3)	3(3)
C_{12}	57(4)	50(4)	53(4)	8(3)	11(3)	20(3)
C_4	51(4)	65(5)	75(5)	28(4)	18(3)	-3(3)
C_{15}	58(4)	52(4)	49(4)	10(3)	13(3)	3(3)
N_1	75(4)	83(4)	154(6)	77(4)	48(4)	41(4)
C_{22}	77(5)	64(4)	36(3)	12(3)	19(3)	6(4)
C_{24}	51(4)	58(4)	68(5)	14(4)	20(3)	0(3)

Table S11. Anisotropic Displacement Parameters ($Å^2×10^3$) for 5v. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C_{23}	70(5)	62(4)	66(5)	19(4)	34(4)	9(4)
C_{14}	66(4)	60(4)	61(4)	-3(3)	22(4)	12(3)
C_5	40(4)	84(5)	61(4)	27(4)	23(3)	5(3)
C_{13}	75(5)	53(4)	70(5)	1(4)	7(4)	32(3)

Table S12. Bond Lengths for 5v.					
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O_2	C_{10}	1.207(5)	C_{20}	C_{21}	1.375(7)
O_1	C_{19}	1.227(6)	C_{17}	C_{19}	1.480(7)
N_2	C_7	1.328(6)	C_{17}	C_{18}	1.424(7)
N_2	C_6	1.377(6)	C_2	C_3	1.368(7)
C_{10}	C_9	1.524(6)	C_6	C_5	1.386(7)
C_{10}	C_{11}	1.481(7)	C_{16}	C_{15}	1.379(7)
C_9	C_8	1.436(6)	C_{25}	C_{24}	1.369(7)
C_9	C_{17}	1.365(7)	C_3	C_4	1.392(8)
C_8	C_1	1.454(7)	C_{18}	N_1	1.135(7)
C_8	C_7	1.387(6)	C_{21}	C_{22}	1.378(7)
C_1	C_2	1.402(7)	C_{12}	C_{13}	1.363(7)
C_1	C_6	1.402(6)	C_4	C_5	1.363(8)
C_{11}	C_{16}	1.393(7)	C_{15}	C_{14}	1.359(8)
C_{11}	C_{12}	1.384(7)	C_{22}	C_{23}	1.366(8)
C_{20}	C_{19}	1.480(7)	C_{24}	C_{23}	1.365(8)
C_{20}	C_{25}	1.381(7)	C_{14}	C_{13}	1.371(8)

Table S13. Bond Angles for 5v.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C_7	N_2	C_6	110.1(4)	O_1	C_{19}	C_{20}	119.8(5)
O_2	C_{10}	C_9	119.9(4)	O_1	C_{19}	C_{17}	119.3(5)
O_2	C_{10}	C_{11}	122.5(5)	C_{20}	C_{19}	C_{17}	120.9(5)
C_{11}	C_{10}	C_9	117.4(4)	N_2	C_7	C_8	110.5(5)
C_8	C_9	C_{10}	113.8(4)	C_3	C_2	C_1	119.4(5)
C_{17}	C_9	C_{10}	118.0(4)	N_2	C_6	C_1	107.6(5)
C_{17}	C_9	C_8	128.2(4)	N_2	C_6	C_5	128.7(5)
C_9	C_8	C_1	128.2(4)	C_5	C_6	C_1	123.7(5)
C_7	C_8	C_9	126.4(5)	C_{15}	C_{16}	C_{11}	120.1(5)
C_7	C_8	C_1	105.3(4)	C_{24}	C_{25}	C_{20}	120.4(6)
C_2	C_1	C_8	136.4(5)	C_2	C_3	C_4	121.6(6)

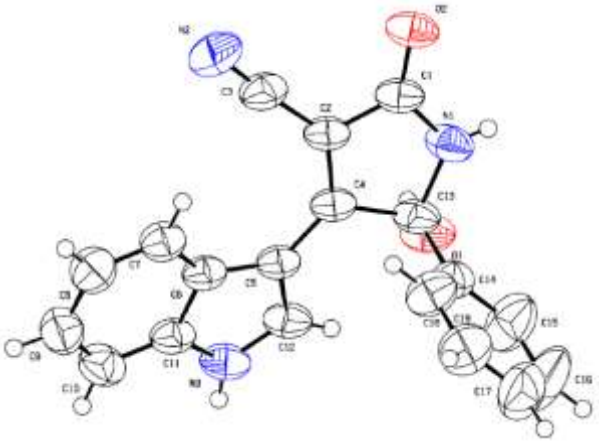
Table S13. Bond Angles for 5v.							
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C_6	C_1	C_8	106.4(4)	N_1	C_{18}	C_{17}	179.2(8)
C_6	C_1	C_2	117.2(5)	C_{20}	C_{21}	C_{22}	119.6(6)
C_{16}	C_{11}	C_{10}	122.9(5)	C_{13}	C_{12}	C_{11}	120.6(6)
C_{12}	C_{11}	C_{10}	118.6(5)	C_5	C_4	C_3	121.0(6)
C_{12}	C_{11}	C_{16}	118.4(5)	C_{14}	C_{15}	C_{16}	120.2(6)
C_{25}	C_{20}	C_{19}	119.2(5)	C_{23}	C_{22}	C_{21}	120.8(6)
C_{21}	C_{20}	C_{19}	121.2(5)	C_{23}	C_{24}	C_{25}	120.3(6)
C_{21}	C_{20}	C_{25}	119.3(5)	C_{24}	C_{23}	C_{22}	119.6(6)
C_9	C_{17}	C_{19}	121.4(4)	C_{15}	C_{14}	C_{13}	120.2(6)
C_9	C_{17}	C_{18}	121.4(5)	C_4	C_5	C_6	117.2(5)
C_{18}	C_{17}	C_{19}	117.2(5)	C_{12}	C_{13}	C_{14}	120.4(6)

Table S14. Torsion Angles for 5v.									
A	B	C	D	Angle/°	A	B	C	D	Angle/°
O_2	C_{10}	C_9	C_8	75.6(6)	C_{20}	C_{25}	C_{24}	C_{23}	0.1(9)
O_2	C_{10}	C_9	C_{17}	-107.2(6)	C_{20}	C_{21}	C_{22}	C_{23}	1.0(9)
O_2	C_{10}	C_{11}	C_{16}	-179.9(5)	C_{17}	C_9	C_8	C_1	-169.8(5)
O_2	C_{10}	C_{11}	C_{12}	-2.9(8)	C_{17}	C_9	C_8	C_7	14.5(8)
N_2	C_6	C_5	C_4	-179.5(6)	C_{19}	C_{20}	C_{25}	C_{24}	-172.2(5)
C_{10}	C_9	C_8	C_1	7.1(7)	C_{19}	C_{20}	C_{21}	C_{22}	171.5(5)
C_{10}	C_9	C_8	C_7	-168.6(5)	C_7	N_2	C_6	C_1	-0.5(6)
C_{10}	C_9	C_{17}	C_{19}	9.2(7)	C_7	N_2	C_6	C_5	-179.6(5)
C_{10}	C_9	C_{17}	C_{18}	-172.1(5)	C_7	C_8	C_1	C_2	-179.7(6)
C_{10}	C_{11}	C_{16}	C_{15}	178.7(5)	C_7	C_8	C_1	C_6	-0.6(5)
C_{10}	C_{11}	C_{12}	C_{13}	-179.1(5)	C_2	C_1	C_6	N_2	179.9(5)
C_9	C_{10}	C_{11}	C_{16}	-5.9(7)	C_2	C_1	C_6	C_5	-0.9(8)
C_9	C_{10}	C_{11}	C_{12}	171.1(5)	C_2	C_3	C_4	C_5	1.7(10)
C_9	C_8	C_1	C_2	3.9(10)	C_6	N_2	C_7	C_8	0.1(6)
C_9	C_8	C_1	C_6	-177.0(5)	C_6	C_1	C_2	C_3	0.7(8)
C_9	C_8	C_7	N_2	176.8(5)	C_{16}	C_{11}	C_{12}	C_{13}	-2.0(9)
C_9	C_{17}	C_{19}	O_1	26.7(8)	C_{16}	C_{15}	C_{14}	C_{13}	-1.8(9)
C_9	C_{17}	C_{19}	C_{20}	-152.8(5)	C_{25}	C_{20}	C_{19}	O_1	32.9(7)
C_8	C_9	C_{17}	C_{19}	-174.0(5)	C_{25}	C_{20}	C_{19}	C_{17}	-147.6(5)
C_8	C_9	C_{17}	C_{18}	4.7(8)	C_{25}	C_{20}	C_{21}	C_{22}	-1.4(8)
C_8	C_1	C_2	C_3	179.7(6)	C_{25}	C_{24}	C_{23}	C_{22}	-0.6(9)
C_8	C_1	C_6	N_2	0.6(6)	C_3	C_4	C_5	C_6	-1.8(9)
C_8	C_1	C_6	C_5	179.8(5)	C_{18}	C_{17}	C_{19}	O_1	-152.0(5)
C_1	C_8	C_7	N_2	0.3(6)	C_{18}	C_{17}	C_{19}	C_{20}	28.5(7)
C_1	C_2	C_3	C_4	-1.1(9)	C_{21}	C_{20}	C_{19}	O_1	-140.1(5)
C_1	C_6	C_5	C_4	1.5(9)	C_{21}	C_{20}	C_{19}	C_{17}	39.5(7)

Table S14. Torsion Angles for 5v.									
A	B	C	D	Angle/°	A	B	C	D	Angle/°
C_{11}	C_{10}	C_9	C_8	-98.6(5)	C_{21}	C_{20}	C_{25}	C_{24}	0.9(8)
C_{11}	C_{10}	C_9	C_{17}	78.7(6)	C_{21}	C_{22}	C_{23}	C_{24}	0.0(9)
C_{11}	C_{16}	C_{15}	C_{14}	0.2(8)	C_{12}	C_{11}	C_{16}	C_{15}	1.7(8)
C_{11}	C_{12}	C_{13}	C_{14}	0.5(10)	C_{15}	C_{14}	C_{13}	C_{12}	1.5(10)

Table S15. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 5v.				
Atom	*x*	*y*	*z*	U(eq)
H_2	8576.79	5389.85	1101.03	55
H_7	6395.02	4392.83	1532.46	52
H_{2A}	5050.03	9079.48	1428.77	56
H_{16}	4045.18	7251.9	4149.85	53
H_{25}	-650.21	3272.01	1820.11	57
H_3	6758.89	10611.17	1018.25	66
H_{21}	3035.01	4622.99	4619.85	59
H_{12}	2001.06	9515.63	1725.56	64
H_4	9067.39	10028.11	732.55	74
H_{15}	3821.54	8878.19	5957.93	63
H_{22}	1971.76	3690.46	6106.3	70
H_{24}	-1671.1	2322.18	3307.65	69
H_{23}	-370.3	2542.22	5456.25	75
H_{14}	2639.85	10760.42	5648.76	75
H_5	9673.61	7836.86	732.02	70
H_{13}	1776.19	11099	3537.05	81

4. Crystallographic description of compound 6a



Ellipsoid plot

Table S16. Crystal data and structure refinement for 6a.	
CCDC No.	2361275
Empirical formula	$C_{19}H_{13}N_3O_2$
Formula weight	315.32
Temperature/K	298
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.4772(6)
b/Å	22.4464(13)
c/Å	9.0718(4)
α/°	90
β/°	96.262(2)
γ/°	90
Volume/Å^3	2120.7(2)
Z	4
ρ_{calc}g/cm^3	0.988
μ/mm^{-1}	0.066
F(000)	656.0
Crystal size/mm^3	0.214 × 0.136 × 0.123
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.868 to 52.84
Index ranges	-13 ≤ h ≤ 13, -28 ≤ k ≤ 28, -11 ≤ l ≤ 11
Reflections collected	20924
Independent reflections	4323 [R_{int} = 0.0503, R_{sigma} = 0.0335]
Data/restraints/parameters	4323/0/222
Goodness-of-fit on F^2	1.034
Final R indexes [I>=2σ (I)]	R_1 = 0.0735, wR_2 = 0.2339
Final R indexes [all data]	R_1 = 0.0826, wR_2 = 0.2429
Largest diff. peak/hole / e Å^{-3}	0.26/-0.27

Table S17. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 6a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
O_2	6337.9(17)	5241.9(9)	6965.8(16)	64.5(5)
O_1	5208.8(15)	5670.7(10)	2215.1(18)	67.1(5)
N_3	7821(2)	4790.9(10)	-375(2)	62.3(6)
N_1	5933(2)	5749.2(12)	4768(2)	63.8(6)
C_6	8780(2)	4568.0(10)	1903(2)	50.6(5)
C_{14}	7007(2)	6290.1(11)	2897(2)	56.1(6)
C_4	7162(2)	5169.4(10)	3324(2)	49.6(5)
C_5	7701(2)	4956.9(10)	2036(2)	49.8(5)
C_2	7254(2)	4959.3(11)	4745(2)	52.1(5)
C_1	6482(2)	5324.4(11)	5638(2)	54.0(5)

Table S17. Fractional Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Parameters (Å^2×10^3) for 6a. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	*x*	*y*	*z*	U(eq)
C_{12}	7179(2)	5086.1(12)	587(2)	59.0(6)
C_7	9782(2)	4324.7(11)	2877(3)	59.5(6)
C_{11}	8817(2)	4472.2(10)	364(2)	54.2(5)
N_2	8334(3)	4050.0(13)	6041(3)	92.5(8)
C_{13}	6295(2)	5722.8(11)	3254(2)	54.5(6)
C_3	7862(3)	4447.7(12)	5413(2)	63.0(6)
C_{19}	8290(3)	6363.7(13)	3368(3)	72.0(7)
C_{10}	9755(3)	4130.0(12)	-196(3)	67.0(7)
C_8	10705(3)	3987.5(13)	2319(3)	70.1(7)
C_9	10691(3)	3882.7(13)	795(3)	72.4(7)
C_{18}	8941(4)	6880.1(15)	3071(4)	88.3(9)
C_{15}	6379(3)	6750.4(16)	2134(5)	96.8(11)
C_{17}	8297(4)	7326.7(15)	2309(5)	102.3(12)
C_{16}	7033(5)	7271.1(17)	1825(6)	125.5(16)

Table S18. Anisotropic Displacement Parameters (Å^2×10^3) for 6a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O_2	66.5(10)	93.7(13)	32.7(8)	6.9(7)	2.8(7)	-9.5(9)
O_1	49.9(9)	101.8(14)	47.4(9)	20.0(8)	-4.6(7)	-4.1(9)
N_3	72.8(13)	82.1(14)	30.9(9)	5.7(8)	0.7(8)	-6.5(11)
N_1	56.6(12)	92.9(16)	42.7(10)	11.4(10)	9.3(9)	11.0(11)
C_6	58.7(12)	54.5(12)	37.6(10)	4.1(8)	1.2(9)	-10.4(10)
C_{14}	60.2(13)	64.8(14)	43.9(11)	5.5(9)	8.4(9)	7.0(10)
C_4	52.0(11)	61.2(12)	34.3(10)	8.0(8)	-1.4(8)	-9.7(9)
C_5	57.6(12)	58.4(12)	32.3(9)	7.0(8)	-0.2(8)	-5.1(10)
C_2	58.7(12)	64.0(13)	32.7(10)	6.4(9)	0.5(8)	-6.8(10)
C_1	51.2(12)	73.6(14)	36.2(10)	7.8(9)	-0.5(8)	-10.6(10)
C_{12}	62.7(14)	78.8(16)	34.6(10)	9.7(10)	0.9(9)	-2.8(11)
C_7	65.5(14)	66.5(14)	45.0(12)	5.4(10)	-1.4(10)	-1.1(11)
C_{11}	66.5(14)	57.3(12)	38.3(10)	2.6(9)	2.9(9)	-10.9(10)
N_2	119(2)	84.2(17)	73.8(16)	30.5(13)	7.9(15)	13.8(16)
C_{13}	49.4(11)	80.2(15)	33.0(10)	11.7(9)	0.6(8)	2.0(10)
C_3	78.1(16)	69.2(15)	40.5(11)	11.5(10)	0.8(11)	-2.3(13)
C_{19}	66.9(16)	74.3(17)	72.1(17)	13.2(13)	-4.8(12)	-5.9(13)
C_{10}	78.8(17)	71.0(15)	52.4(13)	-9.9(11)	12.9(12)	-9.3(13)
C_8	69.2(16)	73.0(16)	66.9(15)	4.3(12)	1.7(12)	4.1(13)
C_9	75.8(17)	66.8(16)	76.5(17)	-7.3(13)	17.1(14)	1.8(13)

Table S18. Anisotropic Displacement Parameters ($Å^2×10^3$) for 6a. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.						
Atom	**U_{11}**	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C_{18}	88(2)	77(2)	100(2)	0.8(17)	9.2(18)	-18.5(17)
C_{15}	71.1(19)	86(2)	130(3)	27(2)	-5.5(19)	14.0(16)
C_{17}	108(3)	59.6(18)	143(3)	2.7(19)	31(2)	-4.2(18)
C_{16}	115(3)	69(2)	191(5)	40(3)	7(3)	20(2)

Table S19. Bond Lengths for 6a.					
Atom	**Atom**	**Length/Å**	**Atom**	**Atom**	**Length/Å**
O_2	C_1	1.244(2)	C_4	C_{13}	1.536(3)
O_1	C_{13}	1.402(3)	C_5	C_{12}	1.398(3)
N_3	C_{12}	1.334(3)	C_2	C_1	1.457(3)
N_3	C_{11}	1.378(3)	C_2	C_3	1.417(3)
N_1	C_1	1.328(3)	C_7	C_8	1.368(4)
N_1	C_{13}	1.465(3)	C_{11}	C_{10}	1.386(4)
C_6	C_5	1.444(3)	N_2	C_3	1.142(3)
C_6	C_7	1.407(3)	C_{19}	C_{18}	1.386(4)
C_6	C_{11}	1.417(3)	C_{10}	C_9	1.373(4)
C_{14}	C_{13}	1.528(3)	C_8	C_9	1.401(4)
C_{14}	C_{19}	1.376(4)	C_{18}	C_{17}	1.355(5)
C_{14}	C_{15}	1.371(4)	C_{15}	C_{16}	1.399(5)
C_4	C_5	1.434(3)	C_{17}	C_{16}	1.355(6)
C_4	C_2	1.366(3)			

Table S20. Bond Angles for 6a.							
Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
C_{12}	N_3	C_{11}	110.40(18)	N_3	C_{12}	C_5	109.8(2)
C_1	N_1	C_{13}	112.9(2)	C_8	C_7	C_6	119.4(2)
C_7	C_6	C_5	136.0(2)	N_3	C_{11}	C_6	107.4(2)
C_7	C_6	C_{11}	117.4(2)	N_3	C_{11}	C_{10}	129.7(2)
C_{11}	C_6	C_5	106.28(19)	C_{10}	C_{11}	C_6	122.8(2)
C_{19}	C_{14}	C_{13}	121.2(2)	O_1	C_{13}	N_1	111.07(18)
C_{15}	C_{14}	C_{13}	121.1(2)	O_1	C_{13}	C_{14}	107.83(18)
C_{15}	C_{14}	C_{19}	117.7(3)	O_1	C_{13}	C_4	113.2(2)
C_5	C_4	C_{13}	121.26(18)	N_1	C_{13}	C_{14}	110.3(2)
C_2	C_4	C_5	131.4(2)	N_1	C_{13}	C_4	101.90(17)
C_2	C_4	C_{13}	107.38(19)	C_{14}	C_{13}	C_4	112.52(18)
C_4	C_5	C_6	130.61(19)	N_2	C_3	C_2	175.4(3)
C_{12}	C_5	C_6	106.0(2)	C_{14}	C_{19}	C_{18}	121.7(3)

Table S20. Bond Angles for 6a.							
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C_{12}	C_5	C_4	123.3(2)	C_9	C_{10}	C_{11}	117.9(2)
C_4	C_2	C_1	110.1(2)	C_7	C_8	C_9	121.8(3)
C_4	C_2	C_3	131.7(2)	C_{10}	C_9	C_8	120.6(3)
C_3	C_2	C_1	117.97(19)	C_{17}	C_{18}	C_{19}	119.3(3)
O_2	C_1	N_1	126.3(2)	C_{14}	C_{15}	C_{16}	120.8(3)
O_2	C_1	C_2	126.0(2)	C_{16}	C_{17}	C_{18}	120.8(3)
N_1	C_1	C_2	107.69(19)	C_{17}	C_{16}	C_{15}	119.7(3)

Table S21. Torsion Angles for 6a.									
A	B	C	D	Angle/°	A	B	C	D	Angle/°
N_3	C_{11}	C_{10}	C_9	176.4(2)	C_7	C_6	C_{11}	N_3	-174.7(2)
C_6	C_5	C_{12}	N_3	2.4(3)	C_7	C_6	C_{11}	C_{10}	3.1(3)
C_6	C_7	C_8	C_9	0.8(4)	C_7	C_8	C_9	C_{10}	1.5(4)
C_6	C_{11}	C_{10}	C_9	-0.9(4)	C_{11}	N_3	C_{12}	C_5	-2.2(3)
C_{14}	C_{19}	C_{18}	C_{17}	0.6(5)	C_{11}	C_6	C_5	C_4	175.6(2)
C_{14}	C_{15}	C_{16}	C_{17}	-1.3(7)	C_{11}	C_6	C_5	C_{12}	-1.7(2)
C_4	C_5	C_{12}	N_3	-175.1(2)	C_{11}	C_6	C_7	C_8	-3.0(3)
C_4	C_2	C_1	O_2	178.2(2)	C_{11}	C_{10}	C_9	C_8	-1.5(4)
C_4	C_2	C_1	N_1	-0.1(3)	C_{13}	N_1	C_1	O_2	-179.6(2)
C_5	C_6	C_7	C_8	-176.3(3)	C_{13}	N_1	C_1	C_2	-1.4(3)
C_5	C_6	C_{11}	N_3	0.5(2)	C_{13}	C_{14}	C_{19}	C_{18}	-179.0(3)
C_5	C_6	C_{11}	C_{10}	178.3(2)	C_{13}	C_{14}	C_{15}	C_{16}	179.3(4)
C_5	C_4	C_2	C_1	-177.9(2)	C_{13}	C_4	C_5	C_6	160.7(2)
C_5	C_4	C_2	C_3	-3.2(4)	C_{13}	C_4	C_5	C_{12}	-22.4(3)
C_5	C_4	C_{13}	O_1	58.0(3)	C_{13}	C_4	C_2	C_1	1.4(2)
C_5	C_4	C_{13}	N_1	177.28(19)	C_{13}	C_4	C_2	C_3	176.0(3)
C_5	C_4	C_{13}	C_{14}	-64.6(3)	C_3	C_2	C_1	O_2	2.7(4)
C_2	C_4	C_5	C_6	-20.1(4)	C_3	C_2	C_1	N_1	-175.5(2)
C_2	C_4	C_5	C_{12}	156.7(2)	C_{19}	C_{14}	C_{13}	O_1	-157.9(2)
C_2	C_4	C_{13}	O_1	-121.38(19)	C_{19}	C_{14}	C_{13}	N_1	80.6(3)
C_2	C_4	C_{13}	N_1	-2.0(2)	C_{19}	C_{14}	C_{13}	C_4	-32.4(3)
C_2	C_4	C_{13}	C_{14}	116.1(2)	C_{19}	C_{14}	C_{15}	C_{16}	1.1(6)
C_1	N_1	C_{13}	O_1	122.9(2)	C_{19}	C_{18}	C_{17}	C_{16}	-0.7(6)

Table S21. Torsion Angles for 6a.									
A	B	C	D	Angle/°	A	B	C	D	Angle/°
C_1	N_1	C_{13}	C_{14}	-117.6(2)	C_{18}	C_{17}	C_{16}	C_{15}	1.0(7)
C_1	N_1	C_{13}	C_4	2.1(3)	C_{15}	C_{14}	C_{13}	O_1	24.0(3)
C_{12}	N_3	C_{11}	C_6	1.0(3)	C_{15}	C_{14}	C_{13}	N_1	-97.5(3)
C_{12}	N_3	C_{11}	C_{10}	-176.6(3)	C_{15}	C_{14}	C_{13}	C_4	149.5(3)
C_7	C_6	C_5	C_4	-10.7(4)	C_{15}	C_{14}	C_{19}	C_{18}	-0.8(5)
C_7	C_6	C_5	C_{12}	172.1(3)					

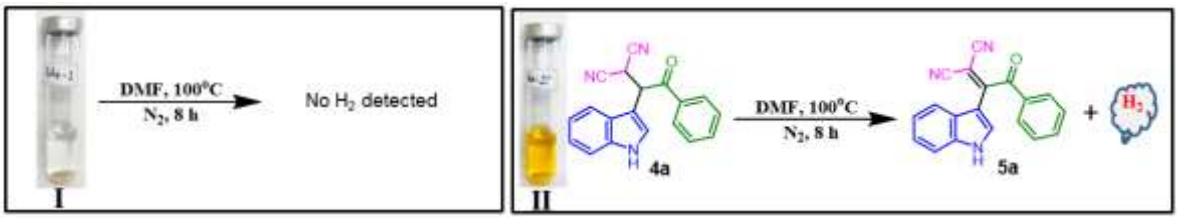
Table S22. Hydrogen Atom Coordinates (Å×10⁴) and Isotropic Displacement Parameters (Å²×10³) for 6a.				
Atom	*x*	*y*	*z*	U(eq)
H_1	4818.34	5365.24	2377.65	101
H_3	7639.26	4798.66	-1322.35	75
H_{12}	6488.59	5339.65	331.35	71
H_7	9817.11	4392.61	3892.24	71
H_{19}	8732.43	6059.18	3898.26	86
H_{10}	9750.64	4069.94	-1210.64	80
H_8	11359.34	3823.4	2968.8	84
H_9	11320.16	3643.64	451.6	87
H_{18}	9811.23	6919.53	3390.64	106
H_{15}	5507.58	6715.97	1817.93	116
H_{17}	8728.15	7675.7	2116.67	123
H_{16}	6602.79	7577.51	1289.03	151
H_{1A}	5480(40)	5947(16)	5100(40)	86(11)

Table S23. Solvent masks information for 6a.						
Number	X	Y	Z	Volume	Electron count	Content
1	-0.340	0.250	-0.157	369.2	90.5	2 C3H6O2,2
2	0.340	0.750	-0.959	369.2	90.5	2 C3H6O2,2

5. Detection of H_2 using gas chromatography (GC)

Gas Chromatography (GC) was performed using a GC-5800 gas chromatograph, Ar was used as carrier gas, thermal conductivity detector (TCD temperature was 50 ^oC) equipped with carbo-sieve column.

Reaction setup for the H_2 evolution of 4a



UV and HPLC spectroscopy-graded DMF was degassed by using a vacuum pump and sonicator for an hour to remove dissolved oxygen. Then, to a 10 mL cleaned and dried glass-sealed tube **II**, 76 mg (0.5 mmol) of **4a** and a magnetic bead were added. Then **4** mL of degassed DMF was injected and purged with N_2 for an hour. In a similar fashion sealed tube **I** was prepared without compound **4a**. Both tube **I** and tube **II** were heated with continuous stirring at 100 ^oC for 8 hours. After 8 hours of reaction, tube **I** and tube **II** were sent to the GC lab for analysis. 1 mL of gas from each of the tubes was injected in GC for the analysis.

The standard H_2 shows a retention time of 0.25 min (Fig. S1). The gas from the tube **I** show only one peak of N_2 gas with the retention time of 0.61 min. (Fig. S2). Tube **II** shows two peaks with a retention time of 0.19 min and 0.61 min for H_2 and N_2 respectively (Fig. S3).

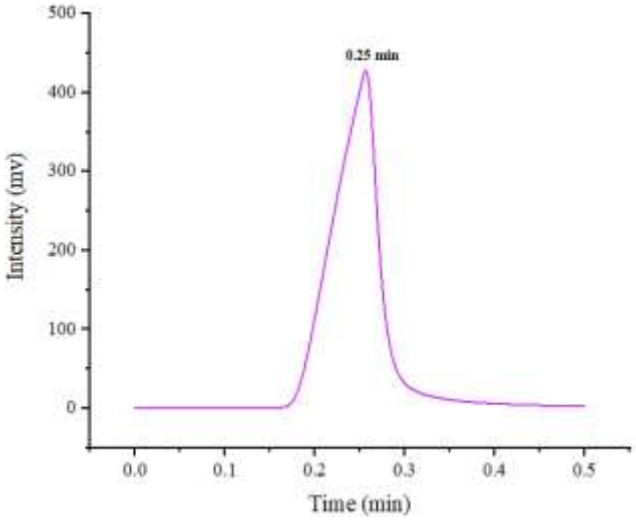


Fig. S1 Chromatogram of reference substance **H_2**

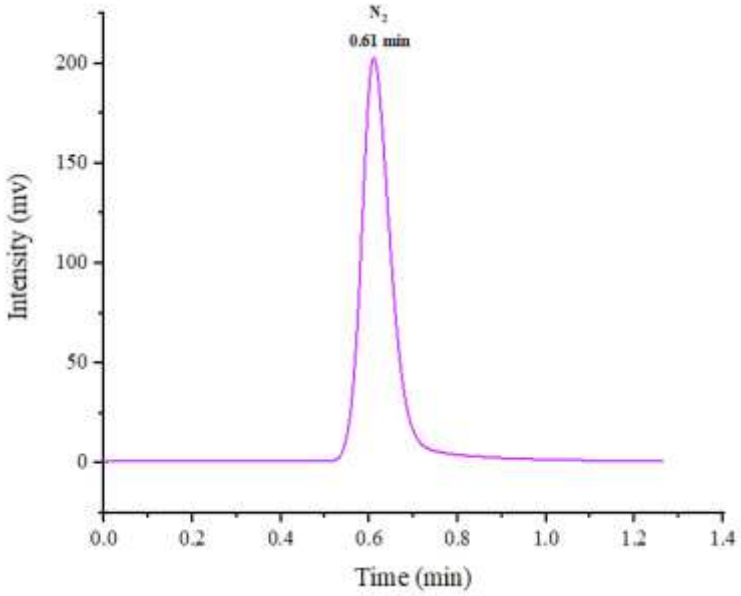


Fig. S2. Chromatogram of gas in the tube **I**

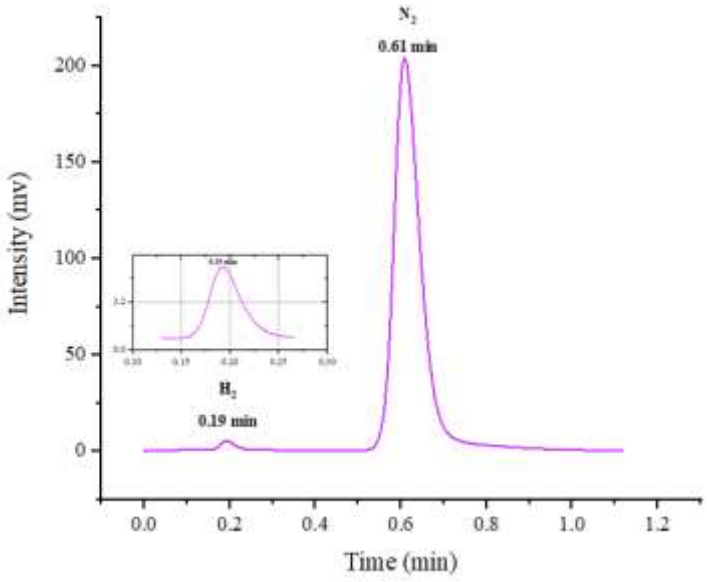
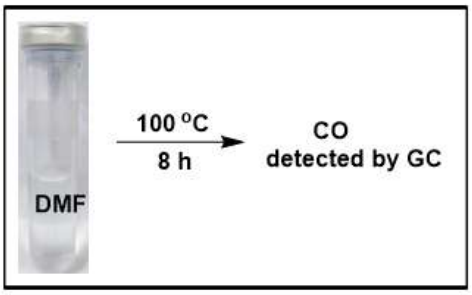


Fig. S3 Chromatogram of gas in the tube **II**

6. Detection of CO using gas chromatography

The presence of CO during the heating of DMF could indeed indicate the formation of dimethylamine. This transformation typically occurs via decarbonylation, where the carbonyl group (-C=O) in DMF is eliminated as carbon monoxide (CO).



A 10 mL cleaned and dried glass-sealed tube was charged with 4 mL of UV and HPLC grade DMF, which was then degassed using a vacuum pump and sonicated for one hour. The sealed tube containing the DMF was subsequently heated at 100°C for 8 hours. Afterward, 1 mL of gas from the tube was collected and injected into a gas chromatograph

(GC) for CO analysis. The output is presented in Fig. S5. A GC analysis of atmospheric air was also conducted to ensure that CO was only detected from the sealed tube.

The standard CO shows the retention time of 0.9 min (Fig. S4). The CO from DMF was shown at 0.87 min (Fig. S5). The Figure S6 is the chromatogram of atmospheric air.

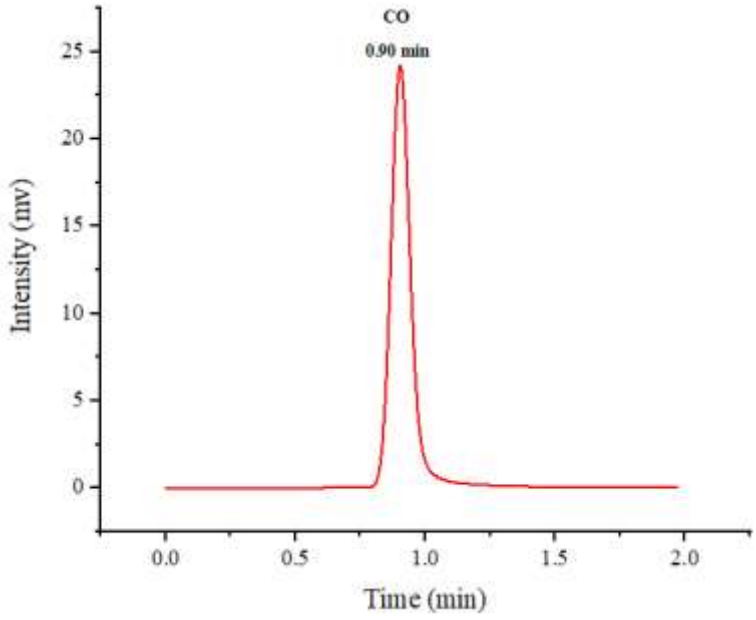


Fig. S4 Chromatogram of reference substance CO

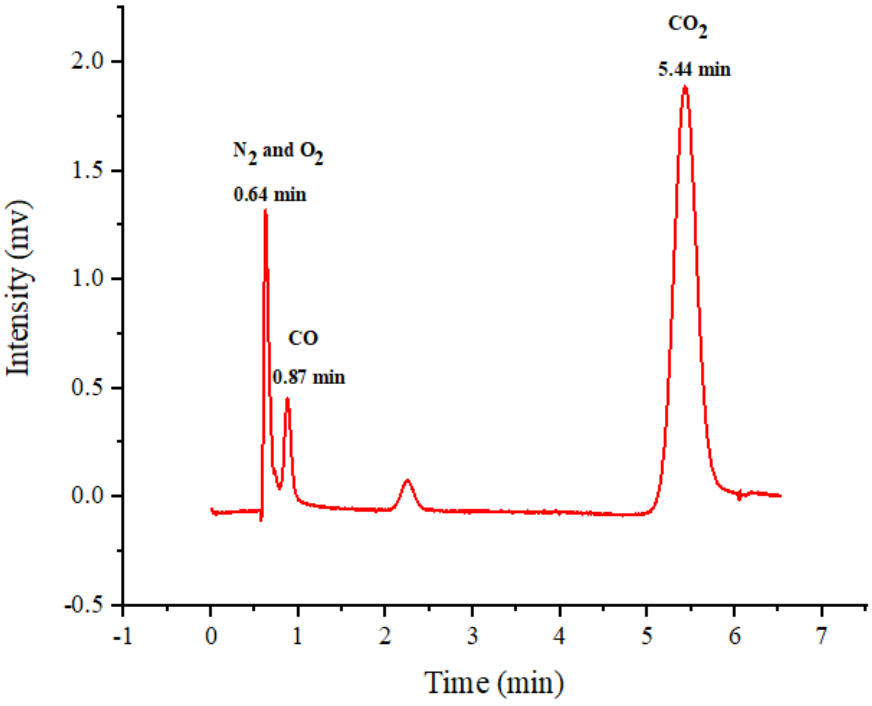


Fig. S5 Chromatogram of gas from heated DMF

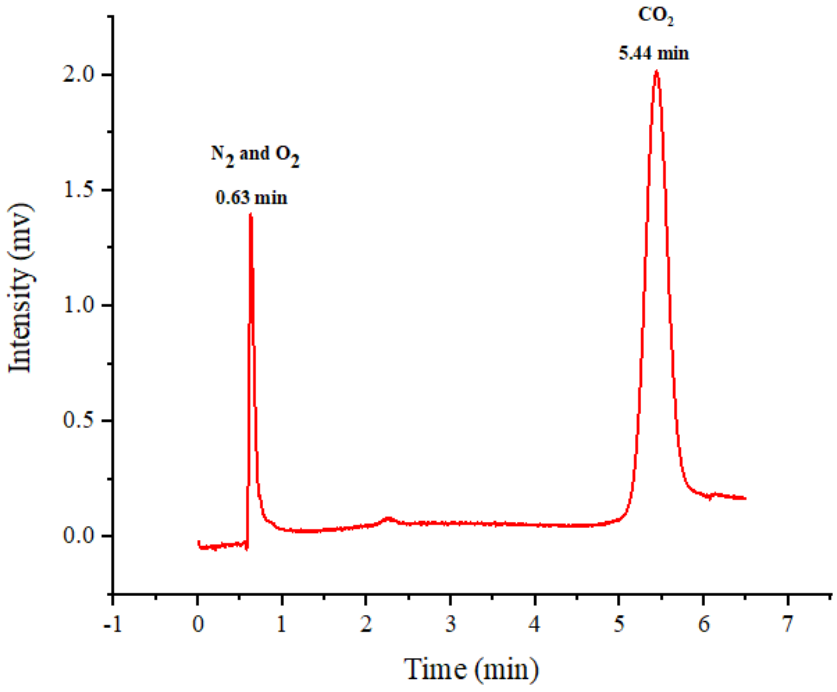


Fig. S6 Chromatogram of atmospheric air