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Electronic Supplementary Information

Mono- and Diiodo-1,2,3-Triazoles and Their Mono Nitro Derivatives

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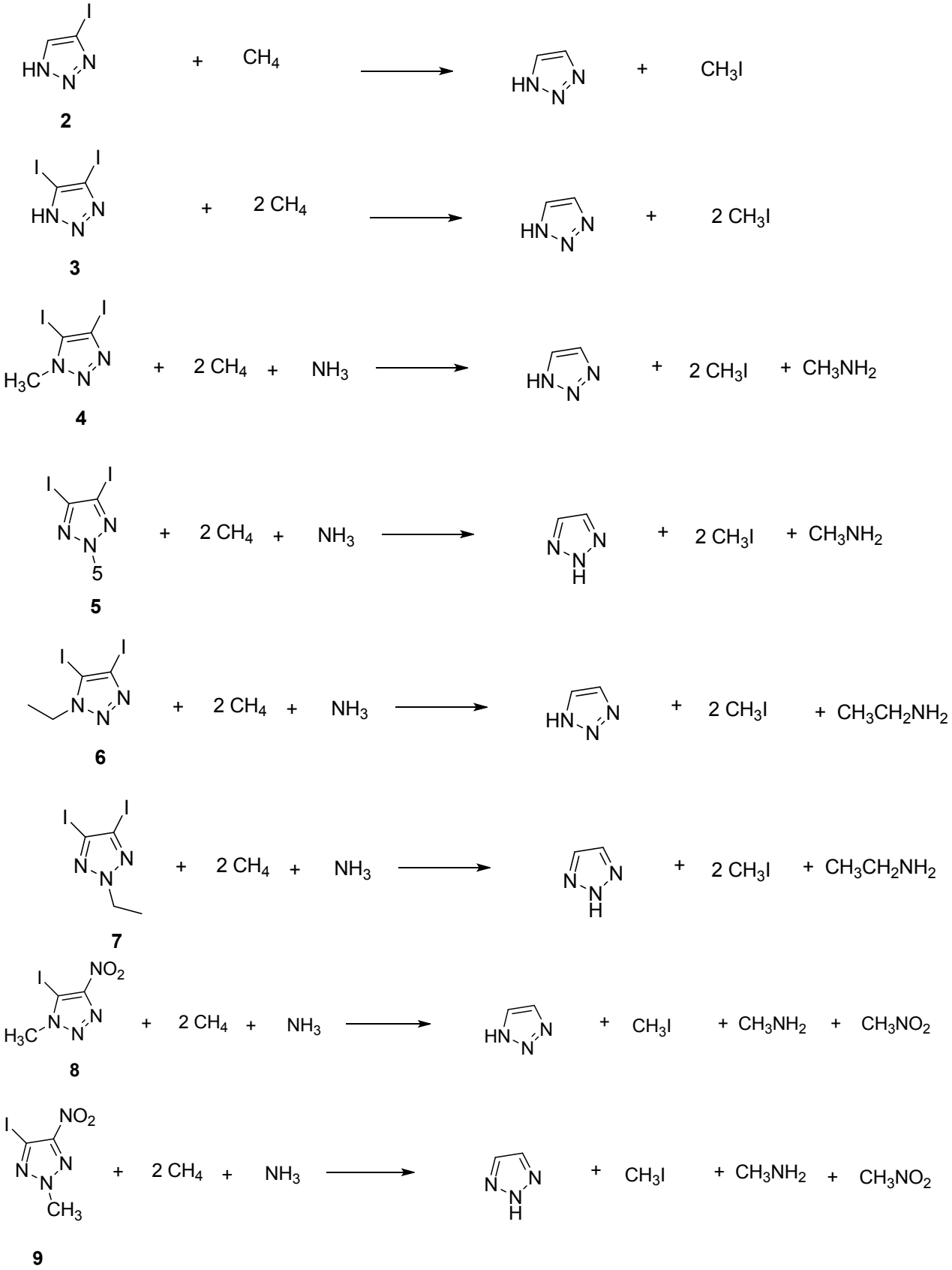
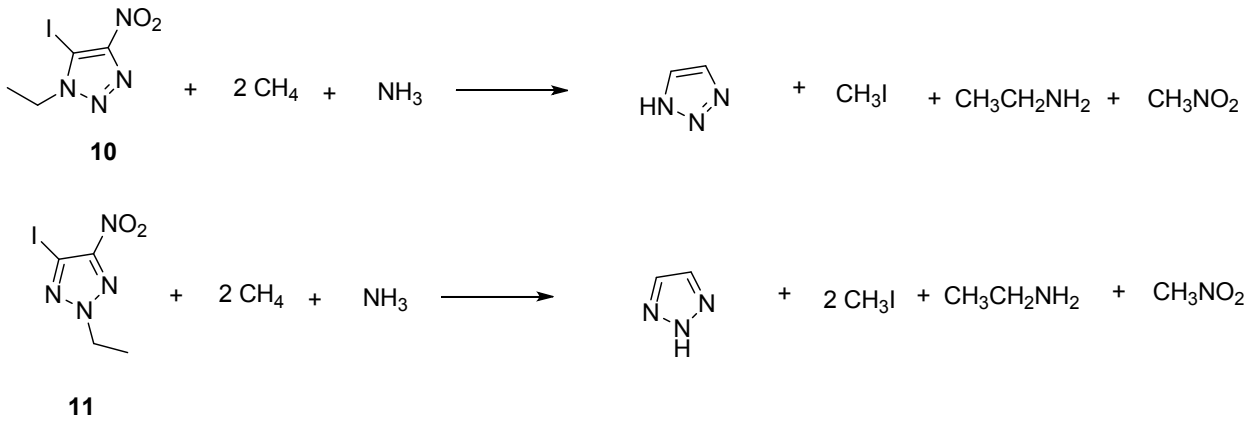

2
+ CH4
+ CH3I
3
+ 2 CH4
+ 2 CH3I
4
+ 2 CH4 + NH3
+ 2 CH3I + CH3NH2
5
+ 2 CH4 + NH3
+ 2 CH3I + CH3NH2
6
+ 2 CH4 + NH3
+ 2 CH3I + CH3CH2NH2
7
+ 2 CH4 + NH3
+ 2 CH3I + CH3CH2NH2
8
+ 2 CH4 + NH3
+ CH3I + CH3NH2 + CH3NO2
9
+ 2 CH4 + NH3
+ CH3I + CH3NH2 + CH3NO2



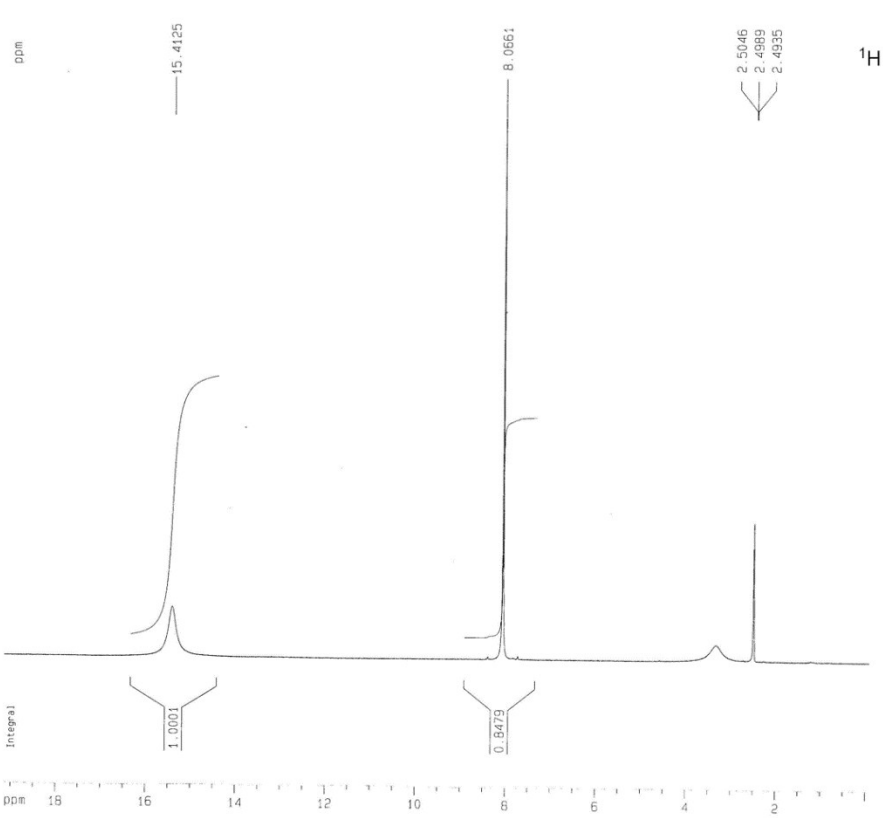
Scheme S1: Isodesmic reactions

Table S1: Crystallographic data for compounds 5, 6, 8 and 10.

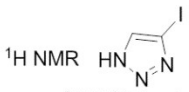
Compound	**5**	**6**	**8**	**10**
Formula	$C_3H_3I_2N_3$	$C_4H_5I_2N_3$	$C_3H_3IN_4O_2$	$C_4H_5IN_4O_2$
CCDC number	1446302	1446304	1446331	1446333
M_w	334.88	348.91	253.99	268.02
Crystal size [mm^3]	0.399 x 0.206 x 0.018	0.316 x 0.115 x 0.104	0.223 x 0.150 x 0.037	0.174 x 0.077 x 0.014
Crystal system	Orthorhombic	Triclinic	Triclinic	Triclinic
Space group	$Pmn2_1$	P-1	P-1	P-1
a [Å]	11.4559(8)	7.274(3)	7.0649(12)	6.9327(11)
b [Å]	4.1982(3)	7.508(3)	7.2001(12)	7.2485(11)
c [Å]	7.7048(5)	7.980(3)	70.362(5)	8.5638(12)
α[°]	90	84.239(4)	64.462(5)	77.511(5)
β [°]	90	83.370(5)	64.462(5)	67.263(4)°
γ [°]	90	68.174(4)	86.027(5)	83.499(5)°
V [Å^3]	370.56(4)	401.1(3)	339.95(10)	387.30(10)
Z	2	2	2	2

T [K]	150(2)	150(2)	150(2)	150(2)
ρ_{calcd} [Mg m^{-3}]	3.001	2.889	2.481	2.298
μ [mm^{-1}]	8.396	7.763	4.654	4.091
F(000)	296	312	236	252
θ[°]	3.186 to 27.485	2.928 to 30.405	3.016 to 25.507	2.626 to 30.413
Index ranges	-14<=h<=14	-9<=h<=10	-8<=h<=8	-9<=h<=9
	-5<=k<=5	-10<=k<=10	-8<=k<=8	-9<=k<=10
	-9<=l<=10	-0<=l<=11	-9<=l<=9	-12<=l<=12
Reflections collected	3581	2117	2656	4209
Independent reflections (R_{int})	838 [R(int) = 0.0397]	2117	1247 [R(int) = 0.0342]	2103 [R(int) = 0.0276]
Data/restraints/parameters	838 / 1 / 41	2117 / 0 / 84	1247 / 0 / 92	2103 / 0 / 101
GOF on F^2	1.088	1.165	1.065	1.049
R_1 ($I > 2\delta(I)$)[a]	0.0186	0.0308	0.0312	0.0283
wR_2 ($I > 2\delta$ (I))[b]	0.0452	0.0808	0.0762	0.0648
R_1 (all data)	0.0187	0.0344	0.0341	0.0351
wR_2 (all data)	0.0453	0.0831	0.0788	0.0675
Largest diff. peak and hole [e. Å-3]	0.816 and -0.716	1.489 and -1.117	1.083 and -1.189	1.243 and -1.382

[a] $R_1 = \sum||F_0| - |F_c|| / \sum|F_0|$ [b] $R_2 = [\sum w(F_0^2 - F_c^2)^2 / \sum w(F_0^2)^2]^{1/2}$



^{1}H NMR



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PROCNO 1

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PULPROG zg
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SOLVENT Acetone
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FIDRES 0.221785 Hz
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RG 512
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TE 300.0 K
D1 1.00000000 sec

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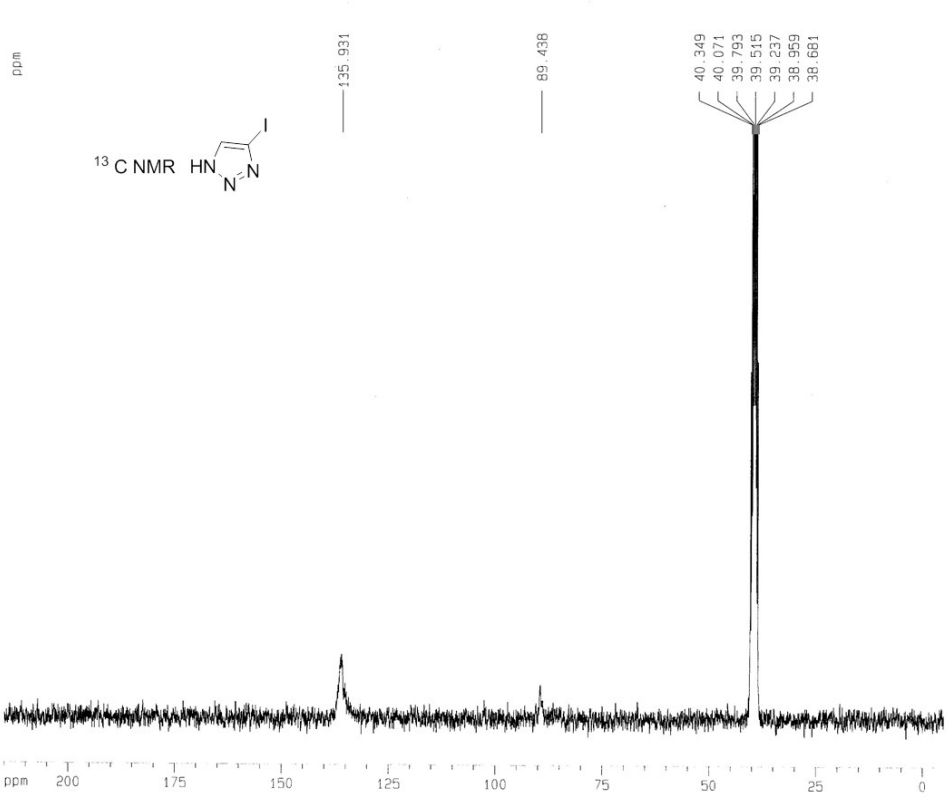

^{13}C NMR

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d11 0.03000000 sec
d12 0.00002000 sec

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PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
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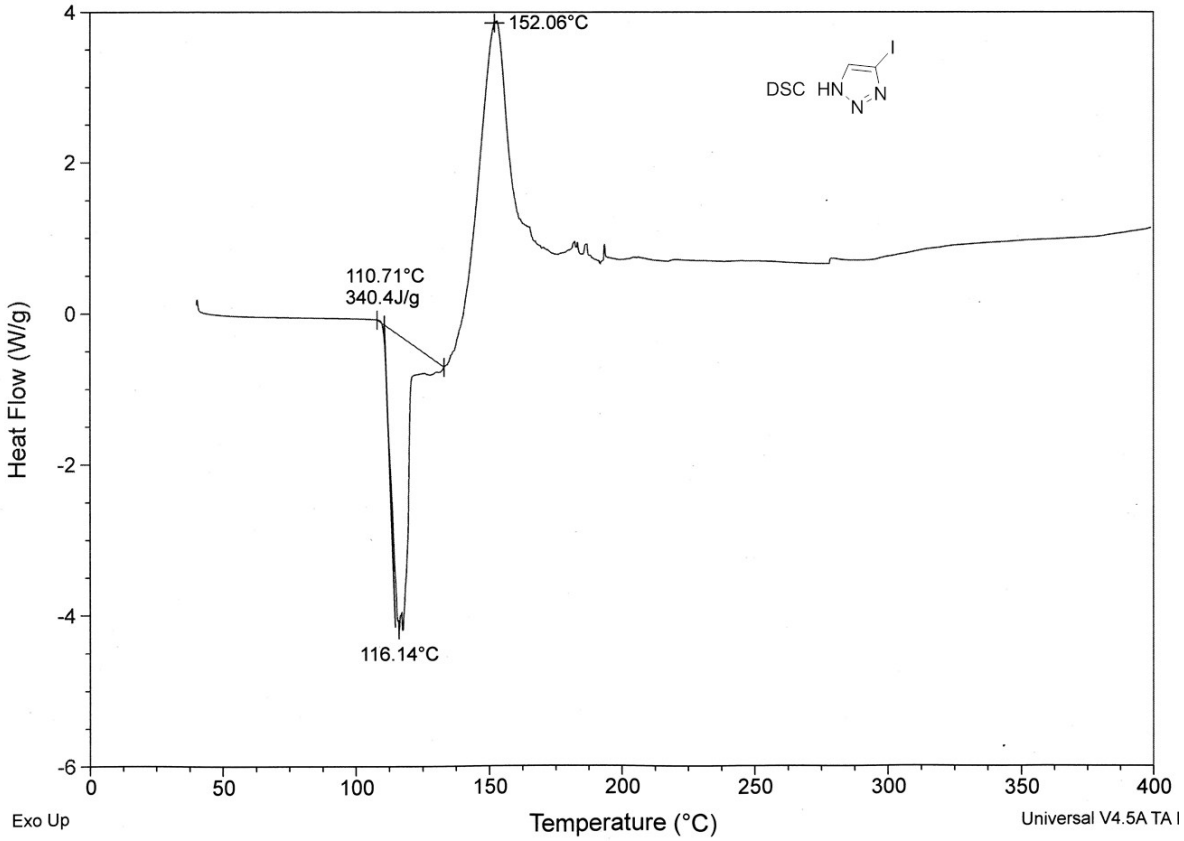
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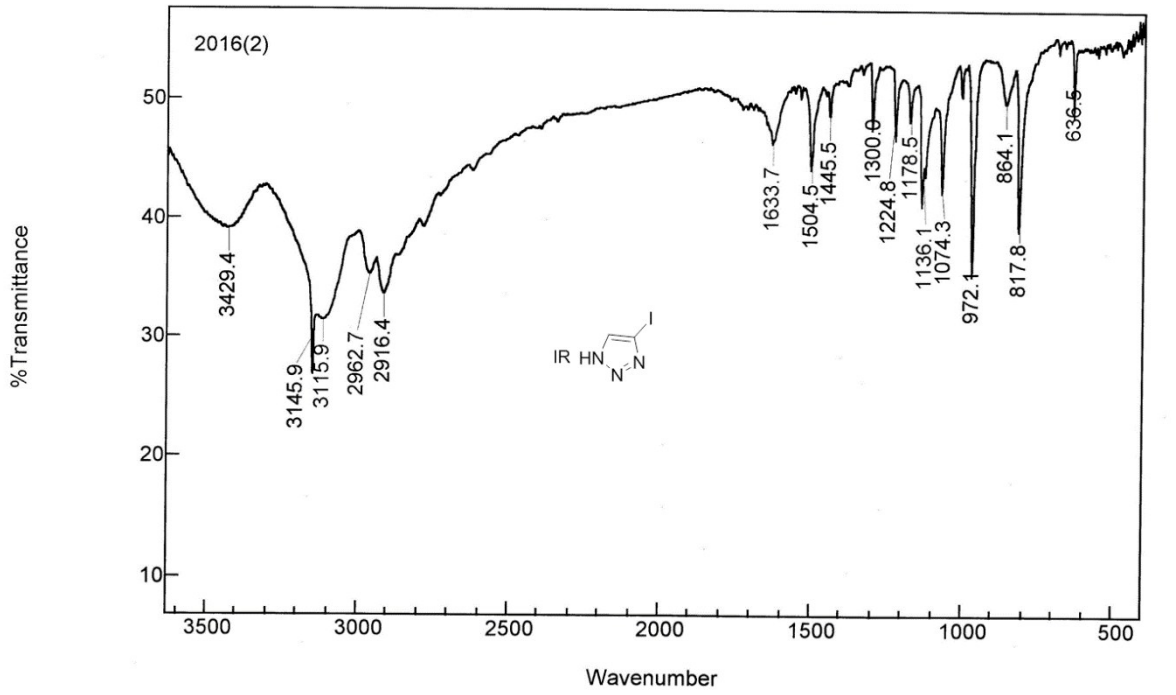
DSC
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA I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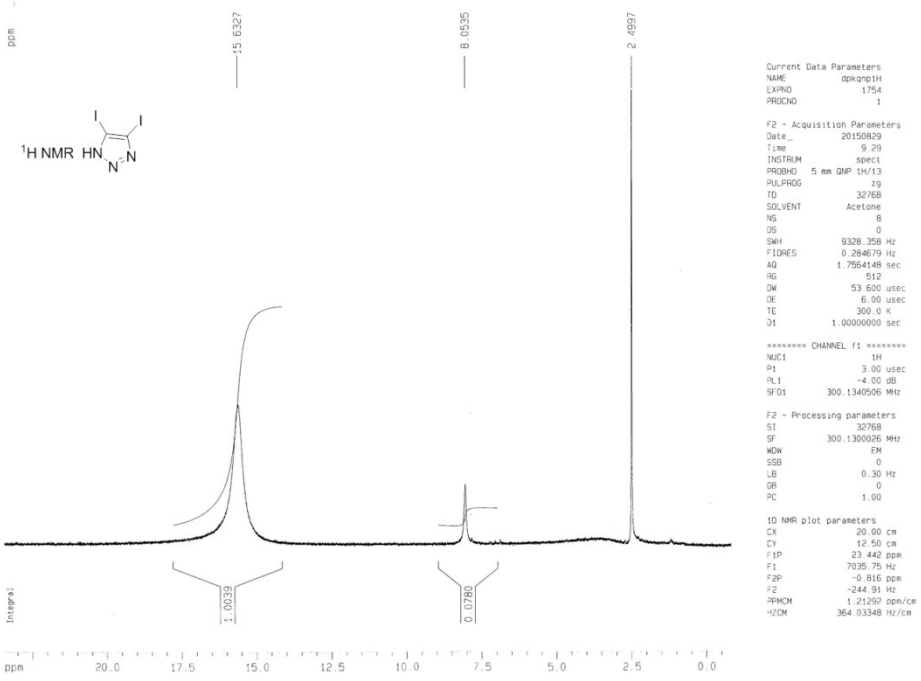
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5.0
2.5
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LB 0.30 Hz
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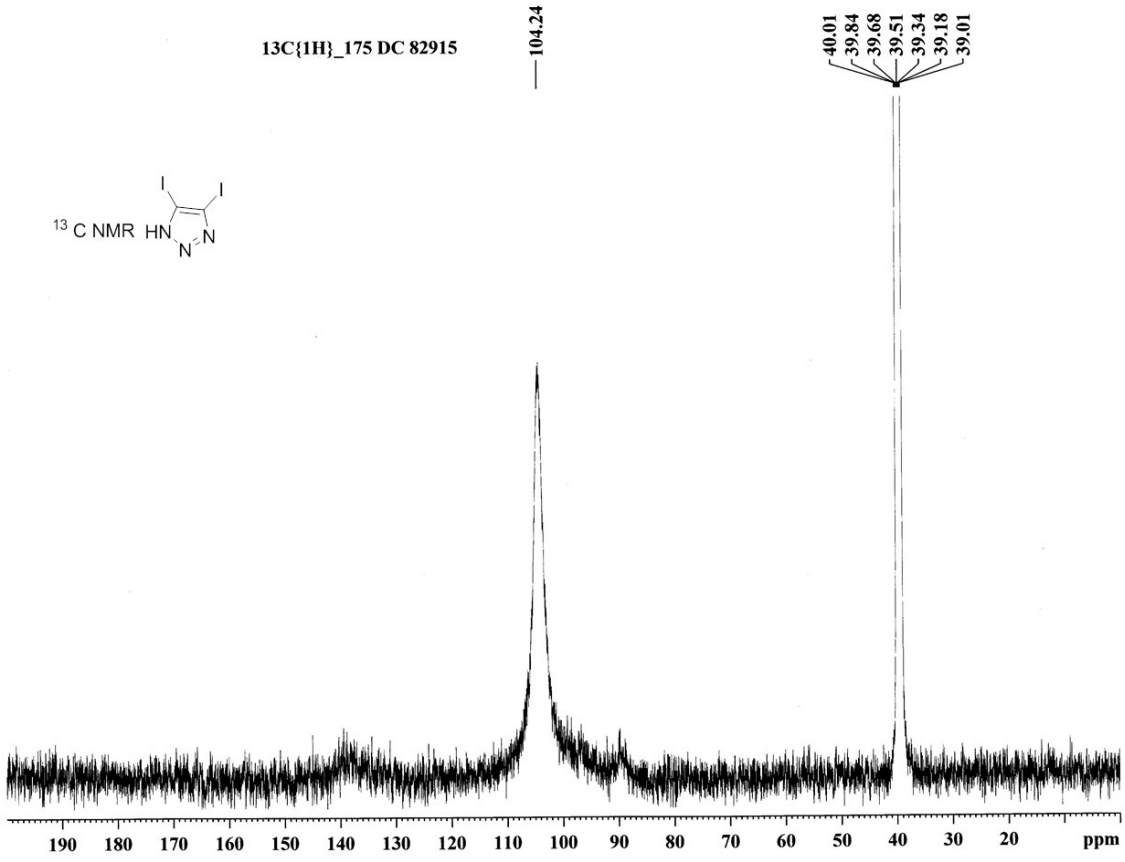
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40.01
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39.68
39.51
39.34
39.18
39.01
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160
150
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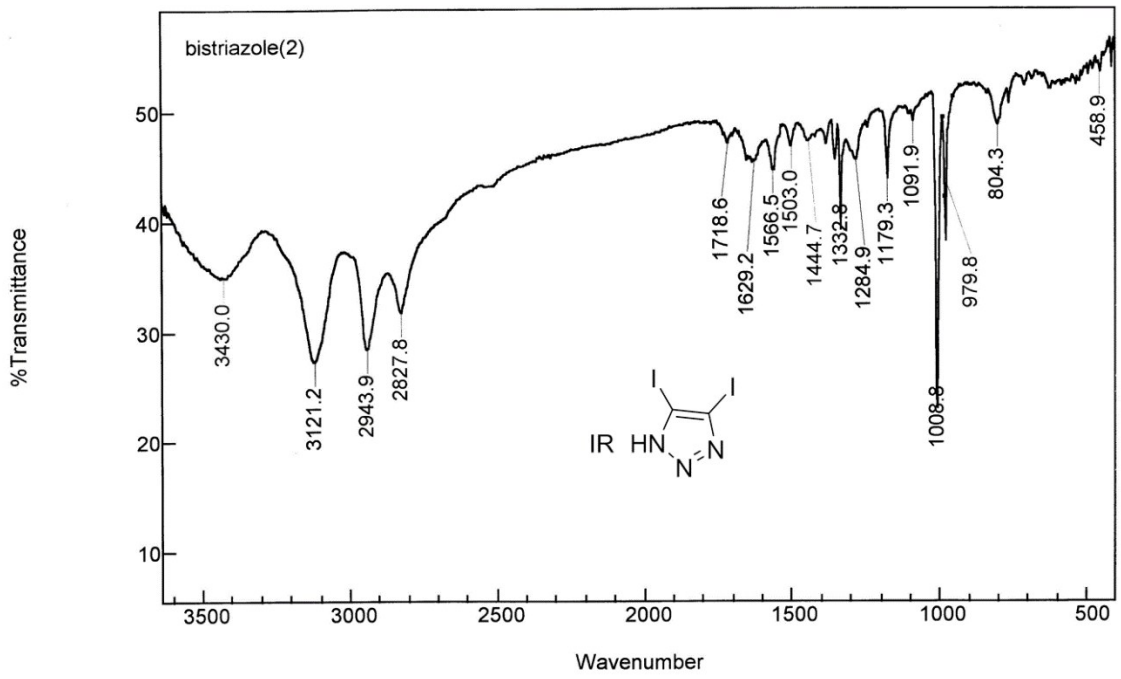
90
80
70
60
50
40
30
20
ppm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1629.2
1566.5
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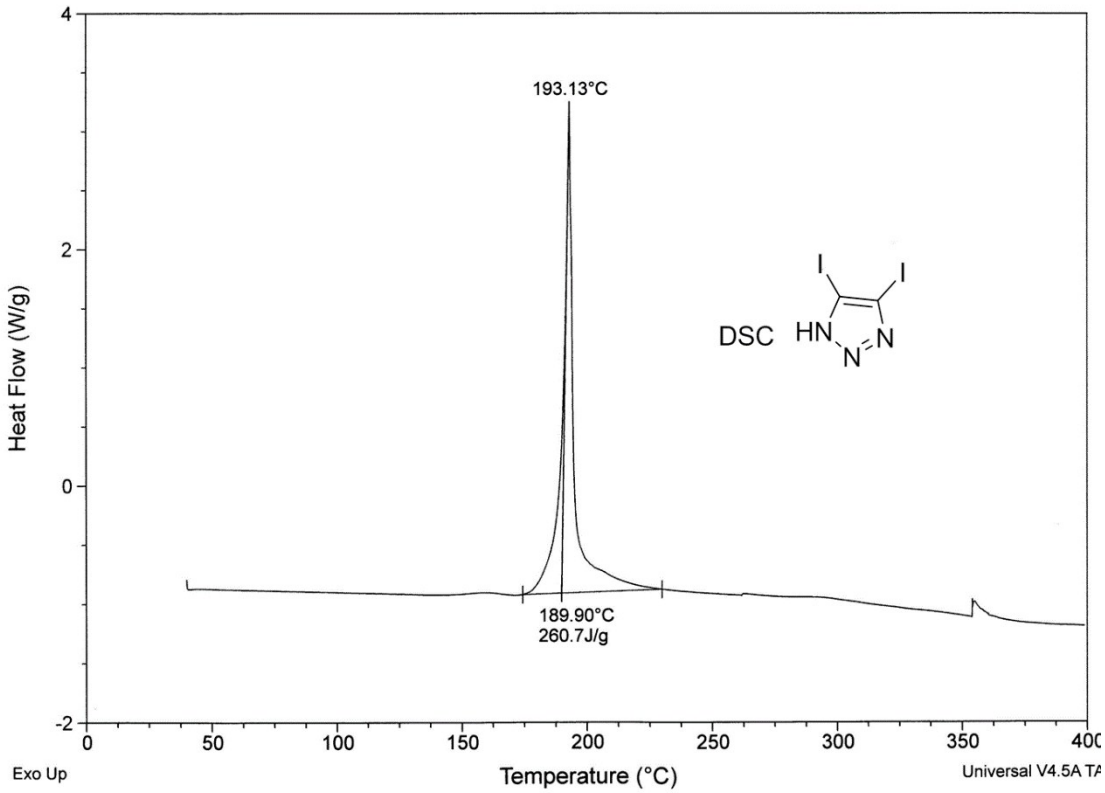
804.3
458.9
IR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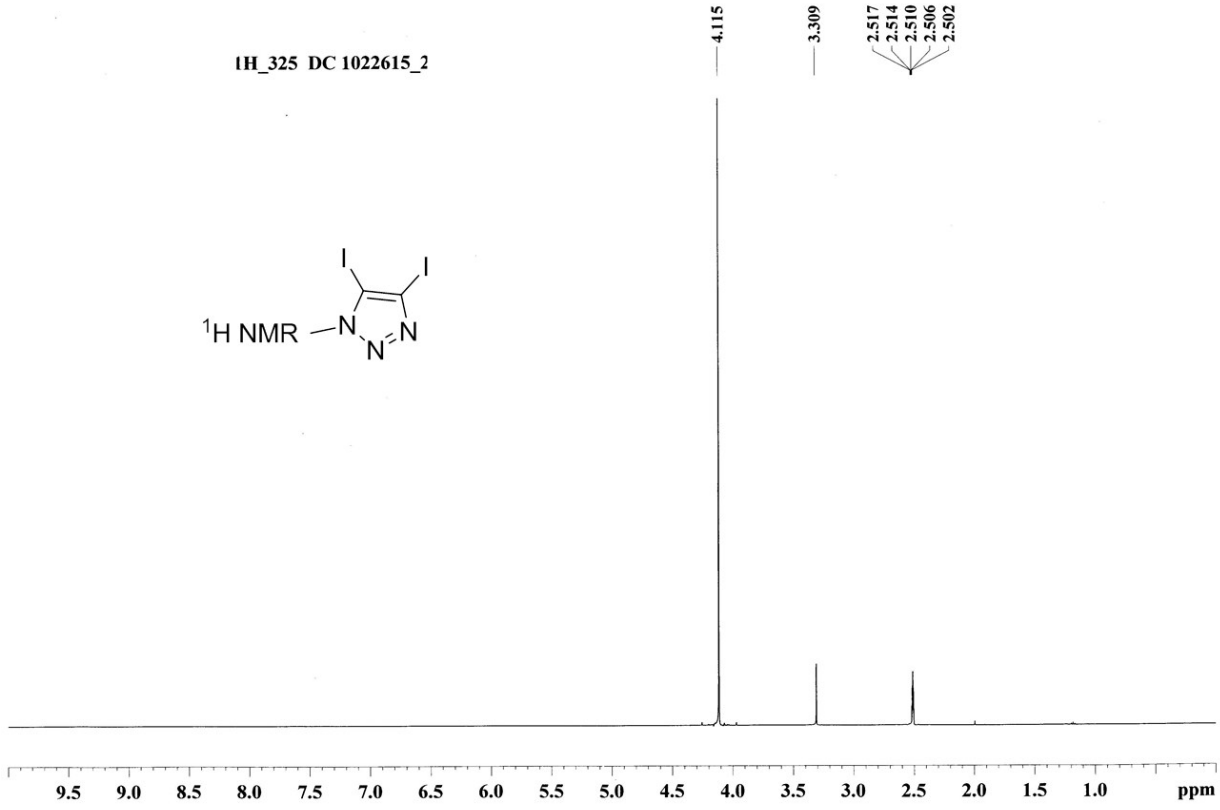
Heat Flow (W/g)
Exo Up
Temperature (°C)
Universal V4.5A TA
DSC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3.309
2.517
2.514
2.510
2.506
2.502
^{1}H NMR
I
I
N
N
N
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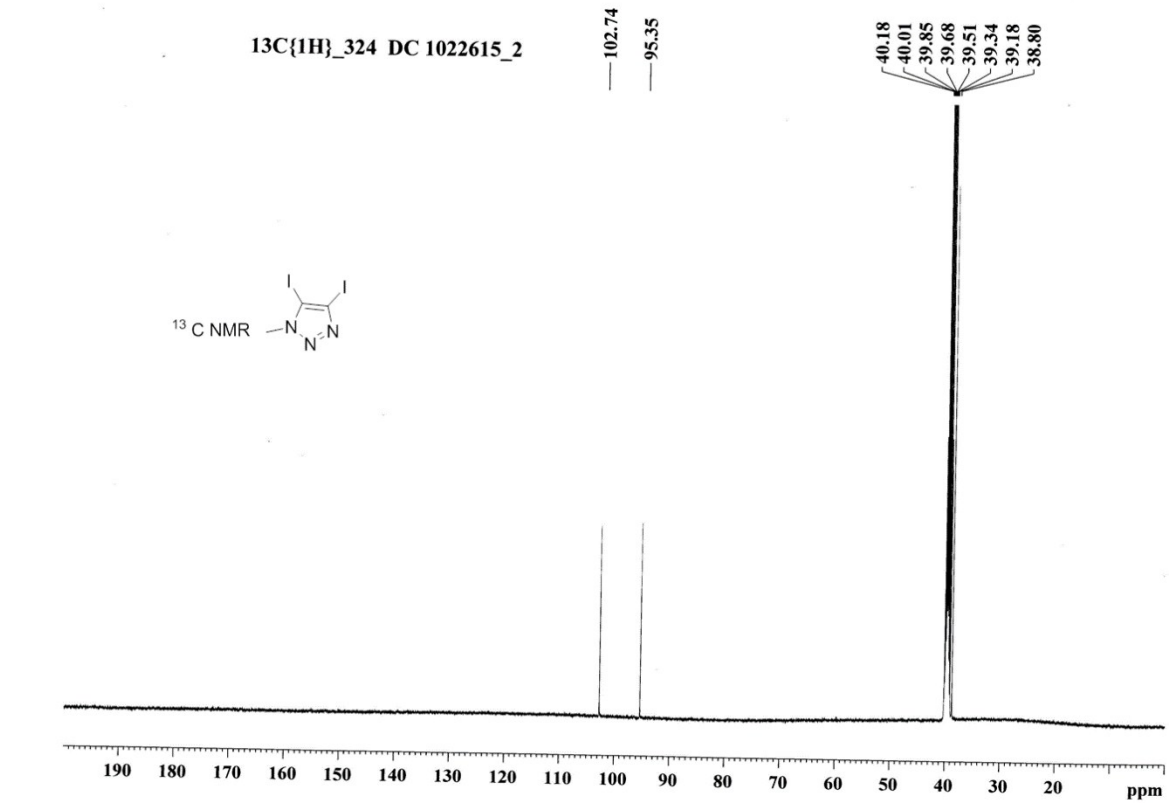
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95.35
40.18
40.01
39.85
39.68
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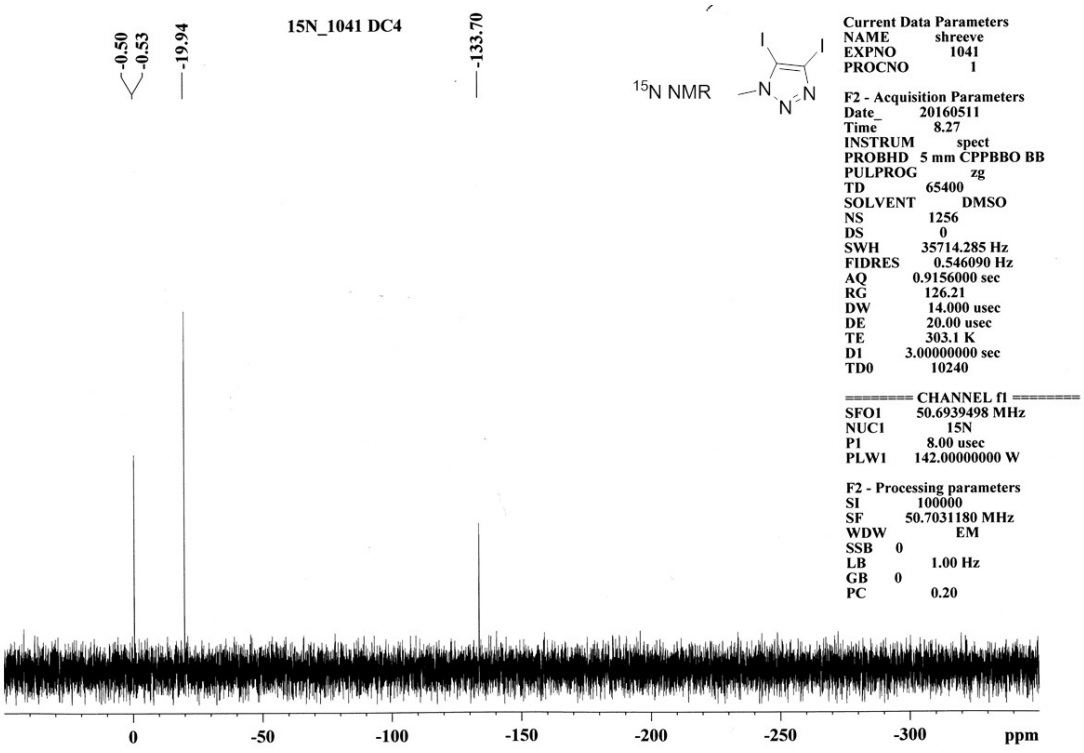
38.80
^{13}C NMR
I
I
N
N
N
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm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PROCNO 1
F2 - Acquisition Parameters
Date_ 20160511
Time 8.27
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg
TD 65400
SOLVENT DMSO
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DS 0
SWH 35714.285 Hz
FIDRES 0.546090 Hz
AQ 0.9156000 sec
RG 126.21
DW 14.000 usec
DE 20.00 usec
TE 303.1 K
D1 3.00000000 sec
TD0 10240
CHANNEL f1
SFO1 50.6939498 MHz
NUC1 15N
P1 8.00 usec
PLW1 142.00000000 W
F2 - Processing parameters
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-150
-200
-250
-300
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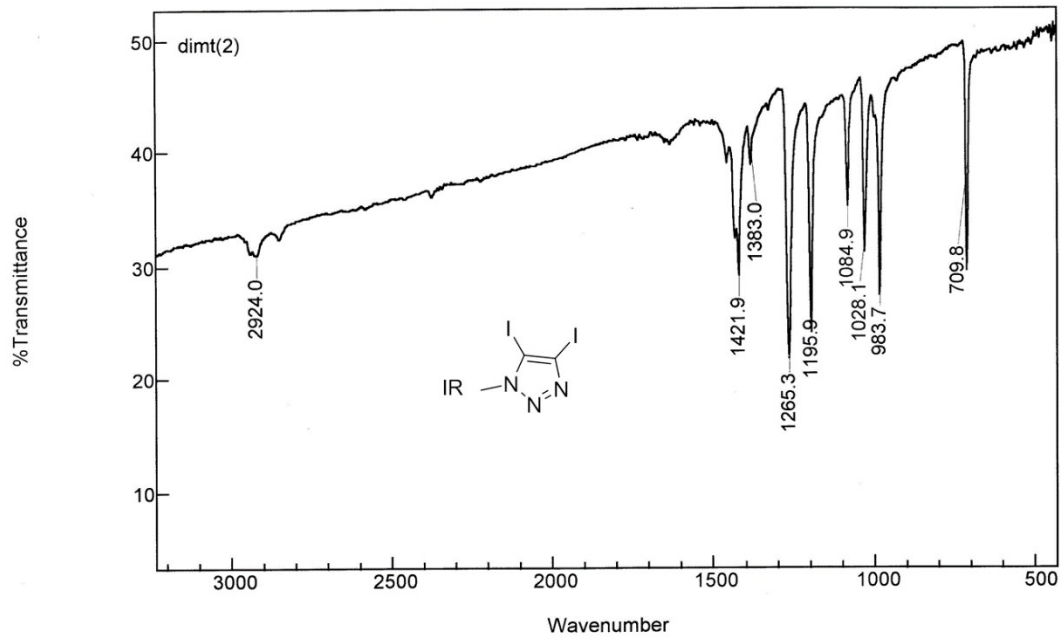
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983.7
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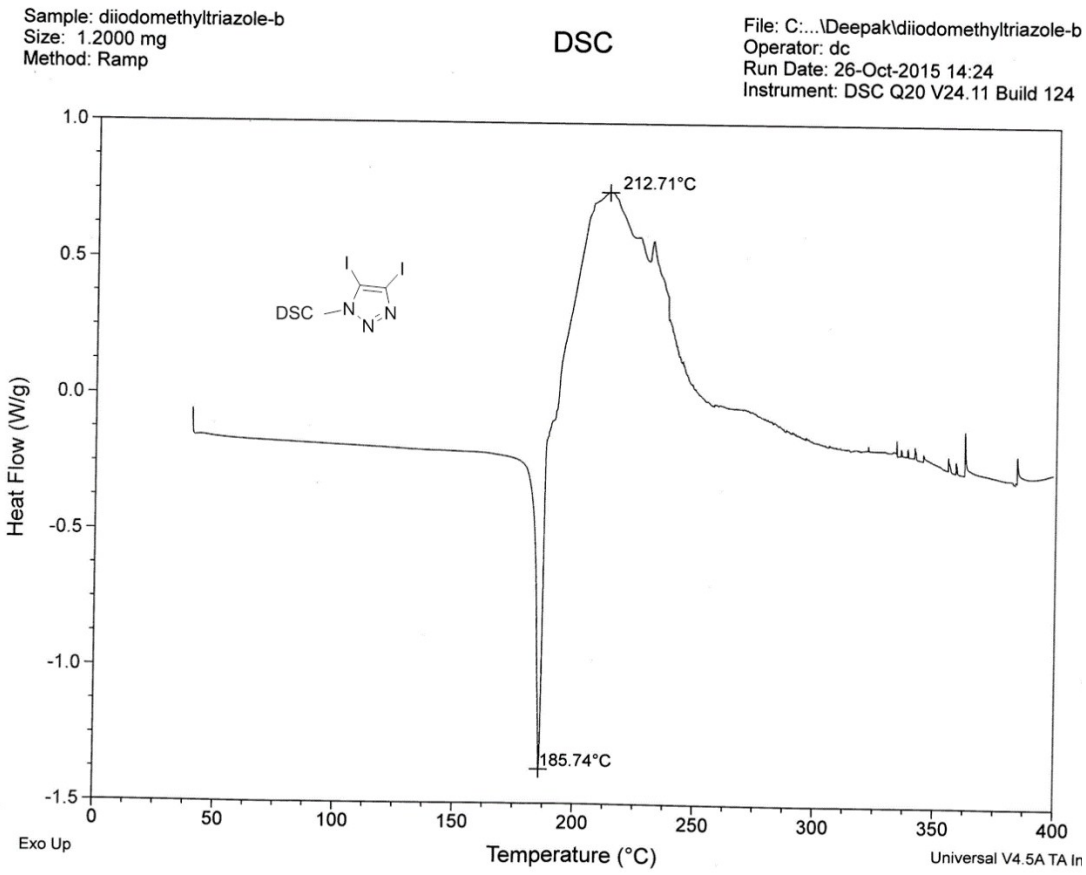
30
20
10
3000
2500
2000
1500
1000
500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Method: Ramp
DSC
File: C:...\Deepak\diiodomethyltriazole-b
Operator: dc
Run Date: 26-Oct-2015 14:24
Instrument: DSC Q20 V24.11 Build 124
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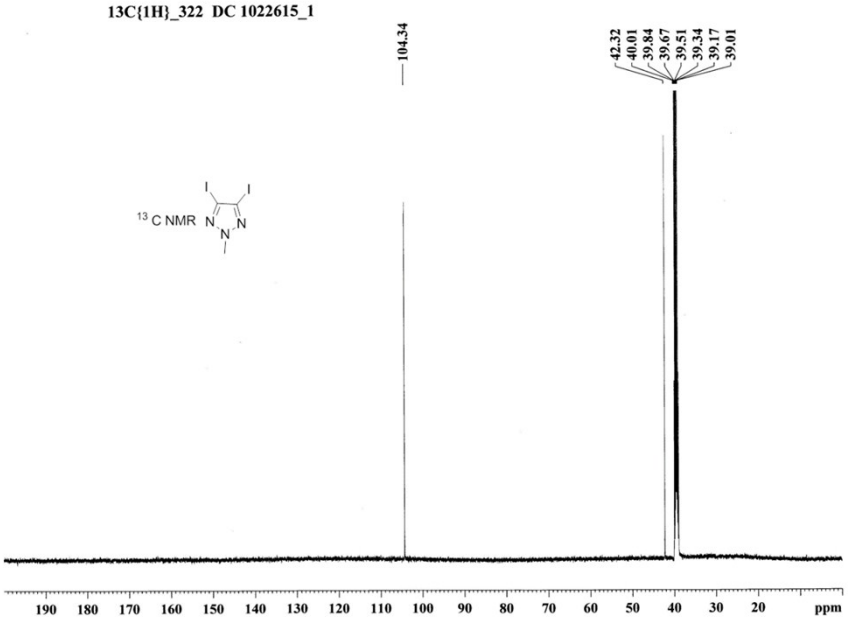
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA In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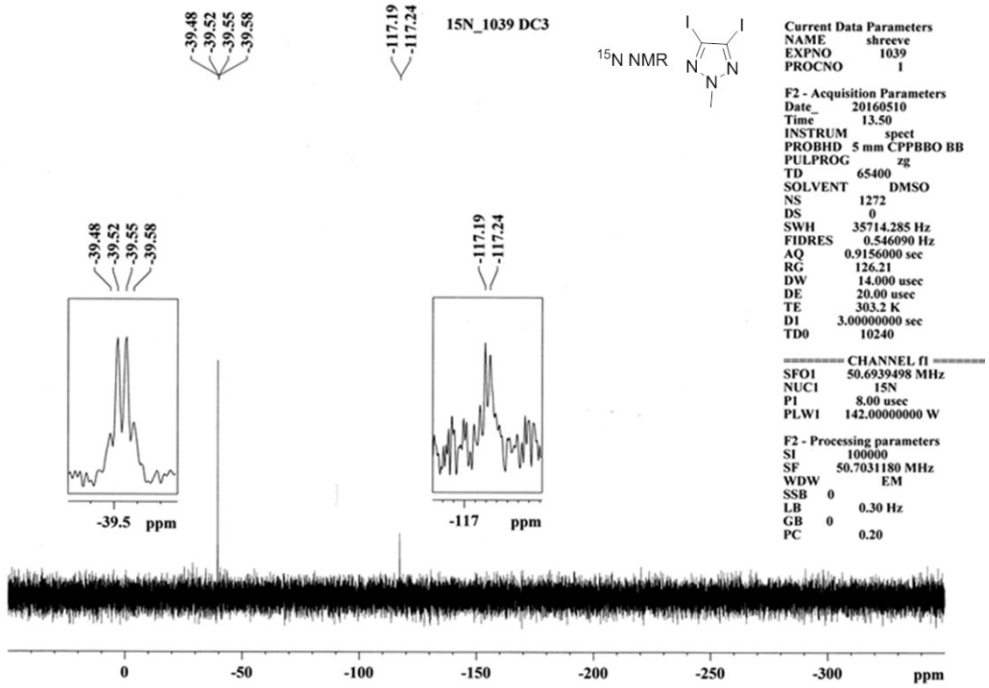
39.17
39.01
ppm


15N_1039 DC3
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15N NMR
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EXPNO 1039
PROCNO 1
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Date_ 20160510
Time 13.50
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PULPROG zg
TD 65400
SOLVENT DMSO
NS 1272
DS 0
SWH 35714.285 Hz
FIDRES 0.546090 Hz
AQ 0.9156000 sec
RG 126.21
DW 14.000 usec
DE 20.00 usec
TE 303.2 K
D1 3.00000000 sec
TD0 10240
CHANNEL f1
SFO1 50.6939498 MHz
NUC1 15N
P1 8.00 usec
PLW1 142.00000000 W
F2 - Processing parameters
SI 100000
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WDW EM
SSB 0
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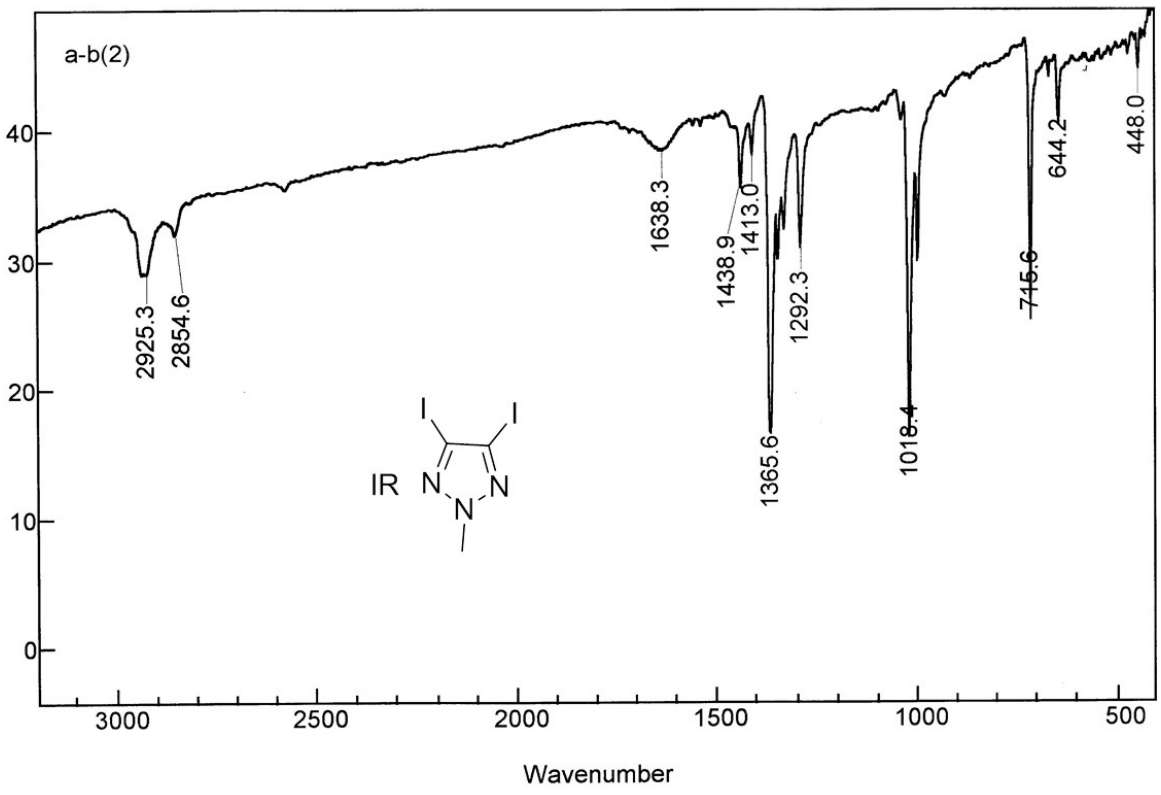
-300
ppm


a-b(2)
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2854.6
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1438.9
1413.0
1365.6
1292.3
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10
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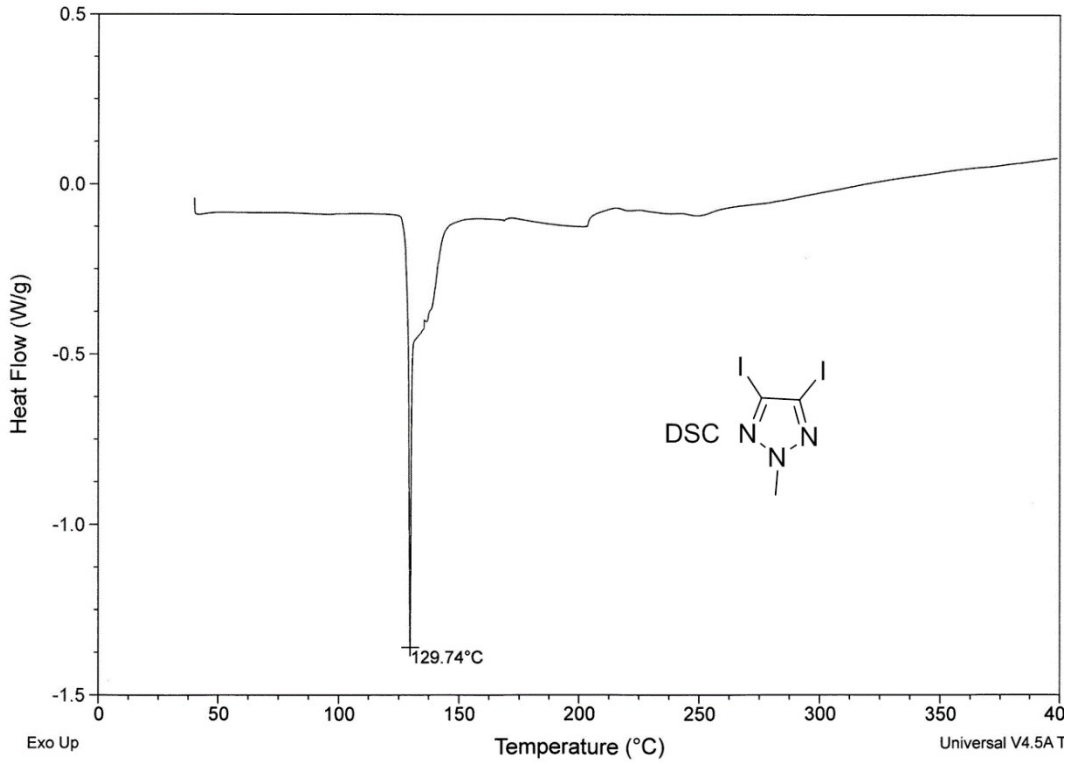
3000
2500
2000
1500
1000
500
Wavenumber


0.5
0.0
-0.5
-1.0
-1.5
Heat Flow (W/g)
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50
100
150
200
250
300
350
40
Exo Up
Temperature (°C)
Universal V4.5A T
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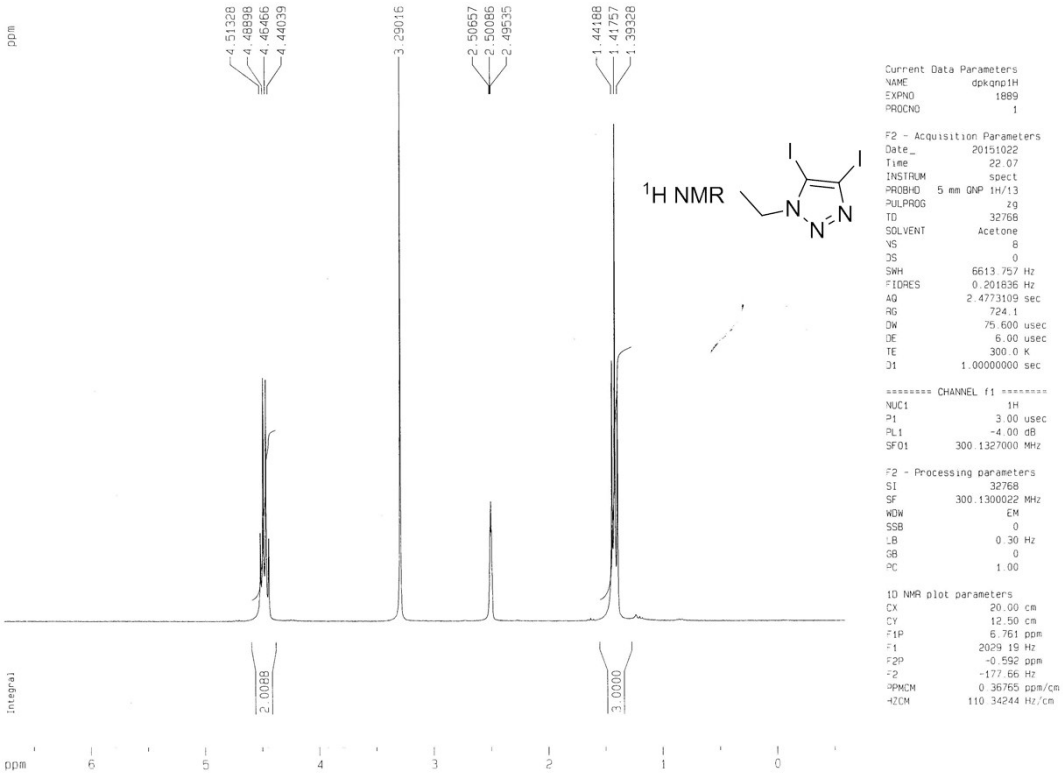
DSC
I
I
N
N
N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1.39328
^{1}H NMR
I
I
N
N
N
integral
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3.0000
ppm
6
5
4
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2
1
0
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NAME dpkqnp1H
EXPNO 1889
PROCNO 1
F2 - Acquisition Parameters
Date_ 20151022
Time 22.07
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PULPROG zg
TD 32768
SOLVENT Acetone
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AQ 2.4773109 sec
RG 724.1
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
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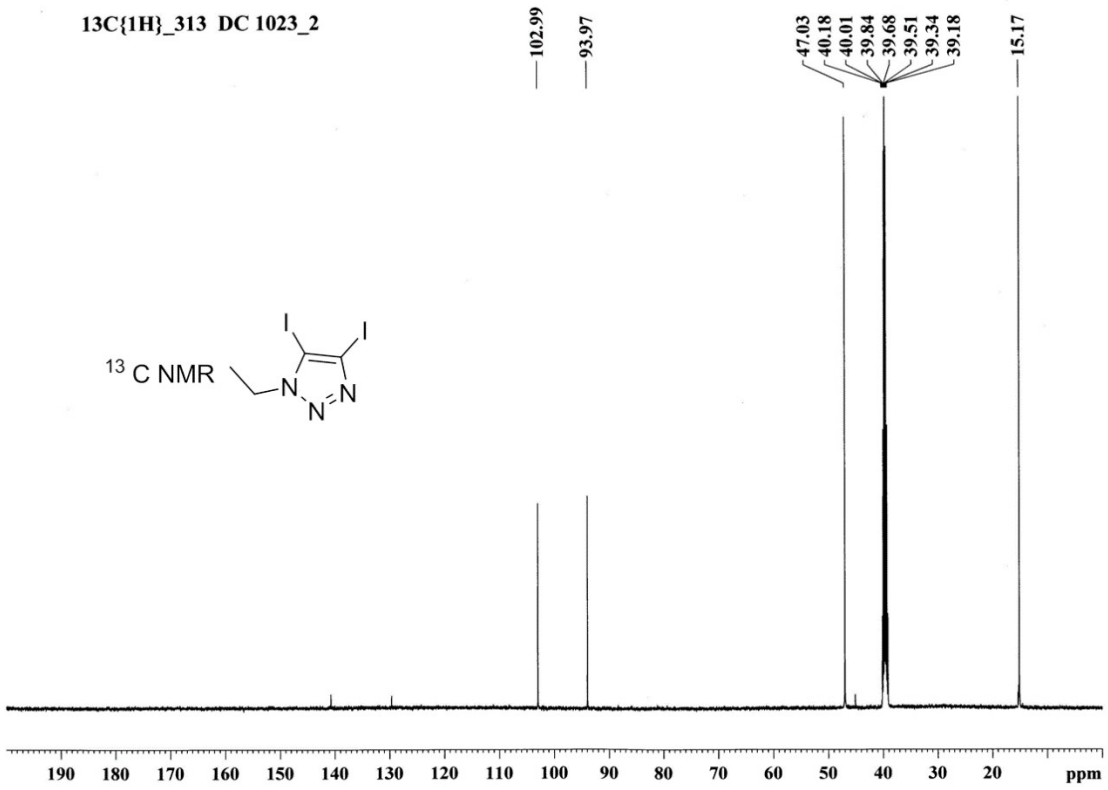
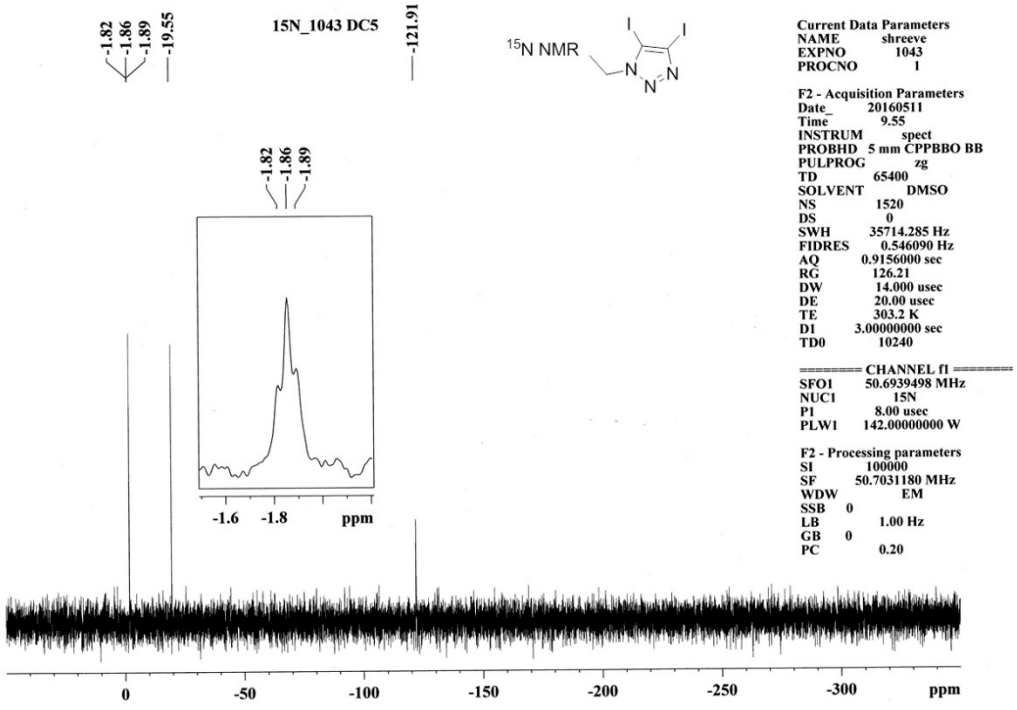
HZCM 110.34244 Hz/cm





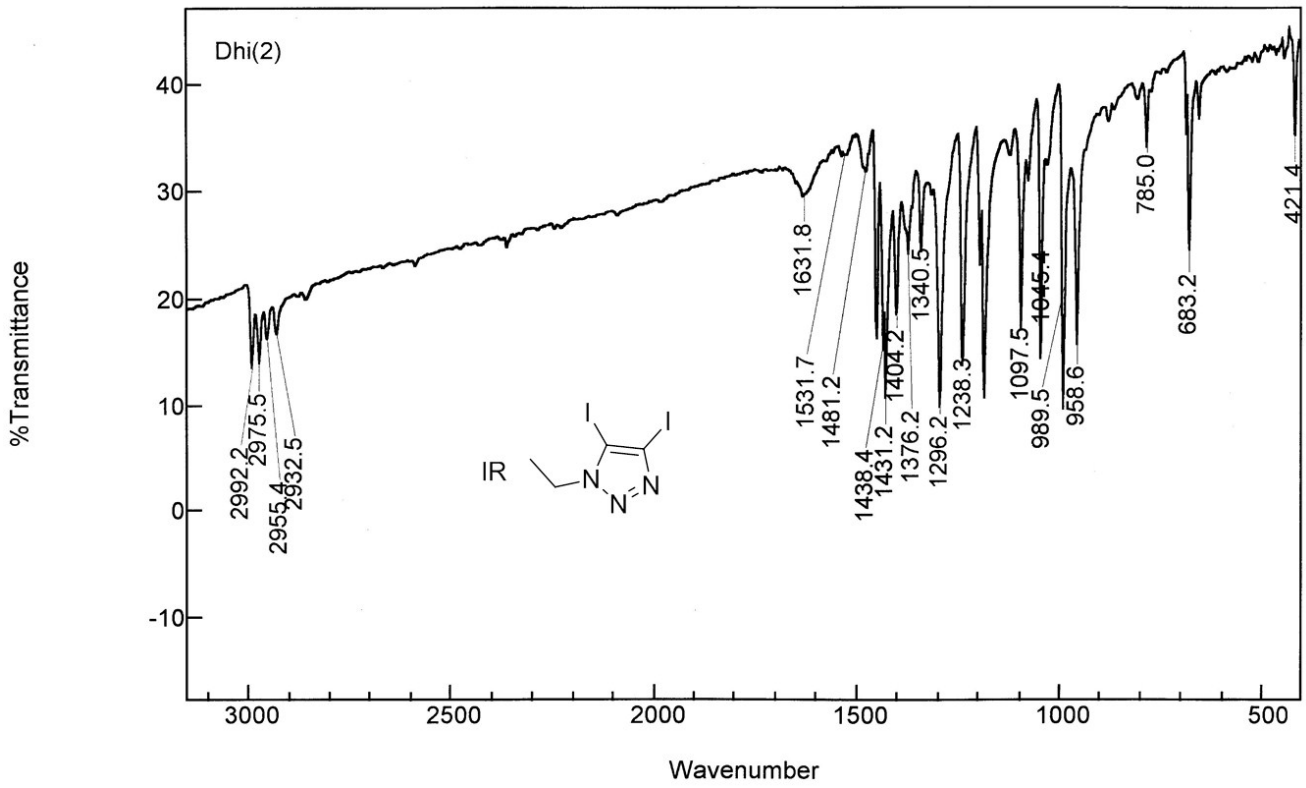
Current Data Parameters
NAME shreeve
EXPNO 1043
PROCNO 1

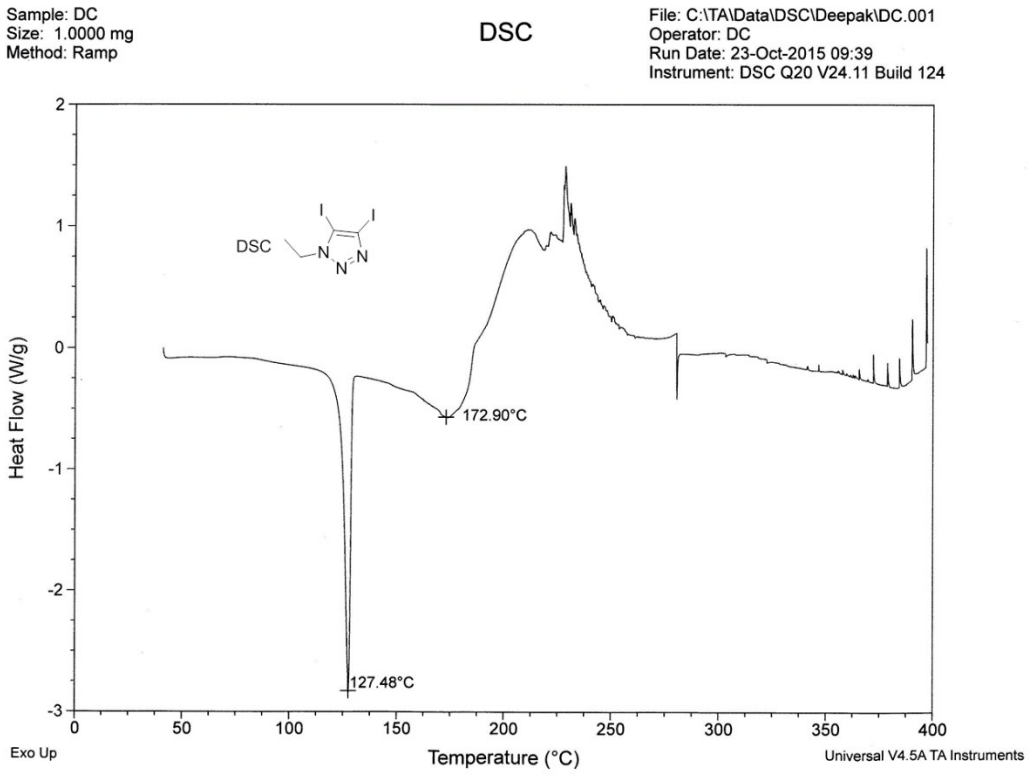
F2 - Acquisition Parameters
Date_ 20160511
Time 9.55
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg
TD 65400
SOLVENT DMSO
NS 1520
DS 0
SWH 35714.285 Hz
FIDRES 0.546090 Hz
AQ 0.9156000 sec
RG 126.21
DW 14.000 usec
DE 20.00 usec
TE 303.2 K
D1 3.00000000 sec
TD0 10240

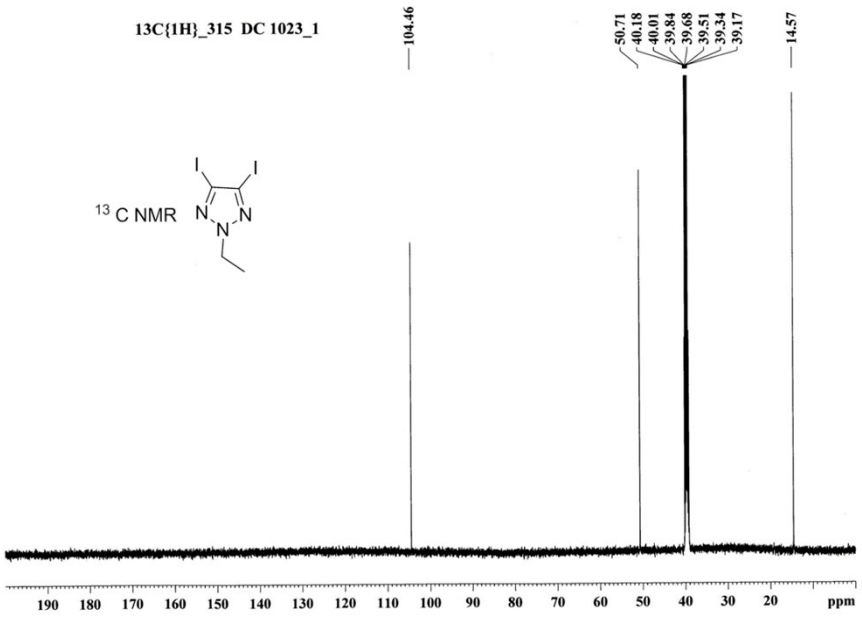
======== CHANNEL f1 ========
SFO1 50.6939498 MHz
NUC1 15N
P1 8.00 usec
PLW1 142.00000000 W

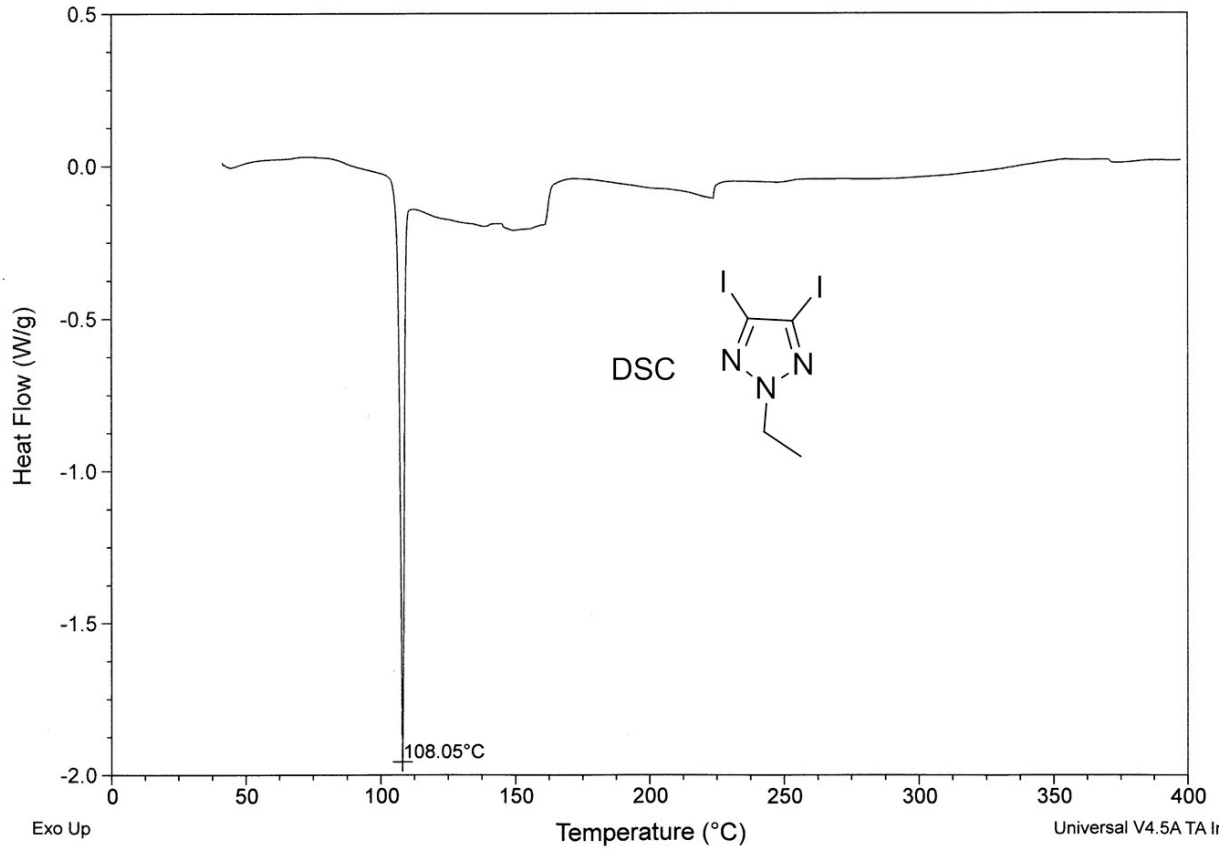
F2 - Processing parameters
SI 100000
SF 50.7031180 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20

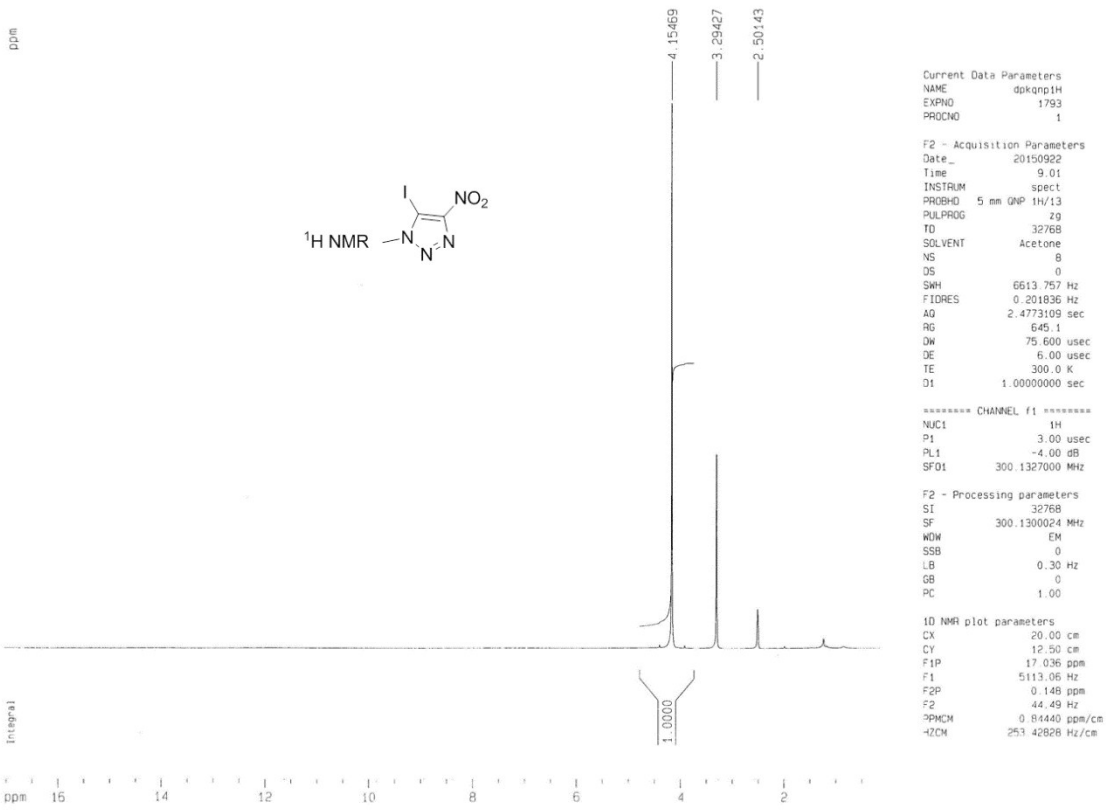
Bio-Rad Merlin

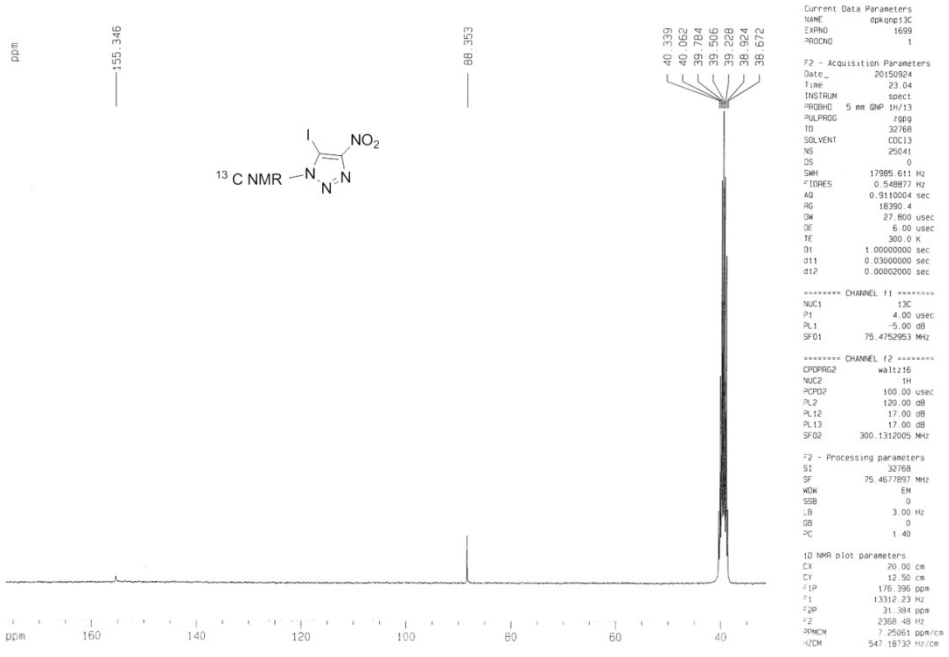


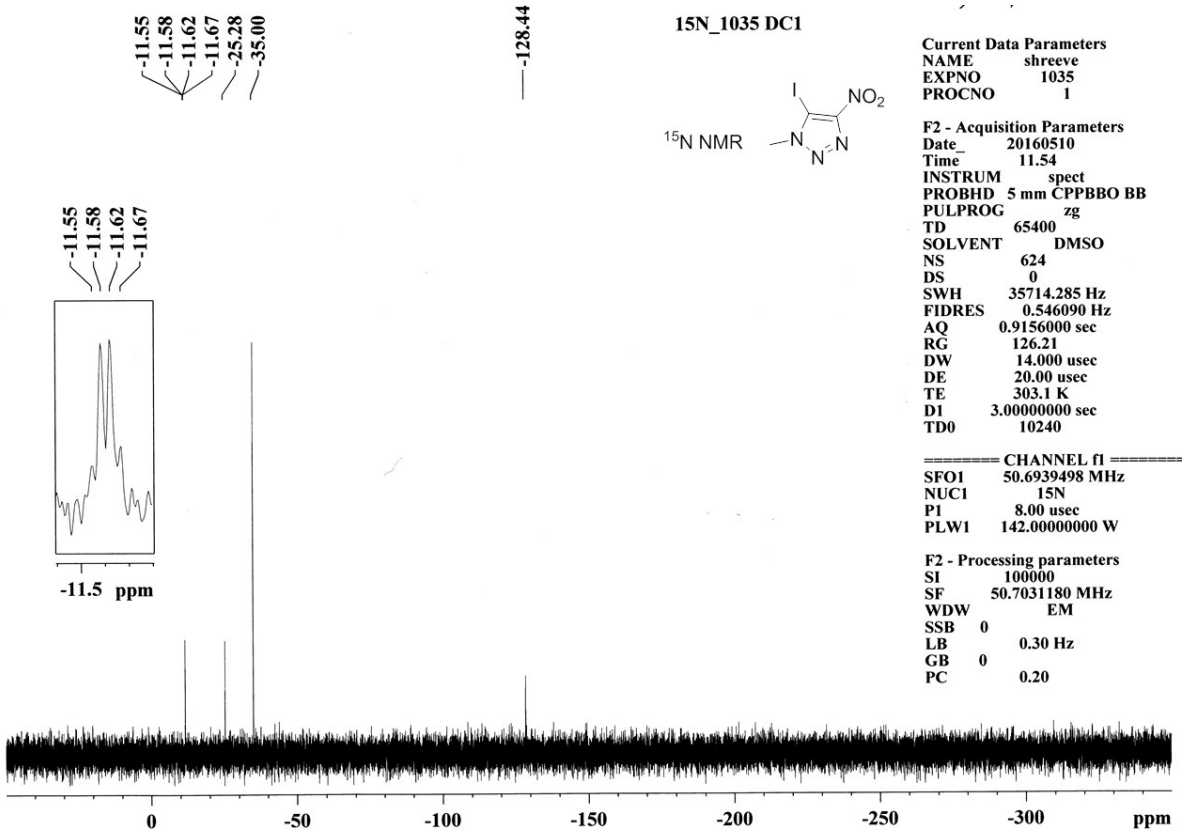


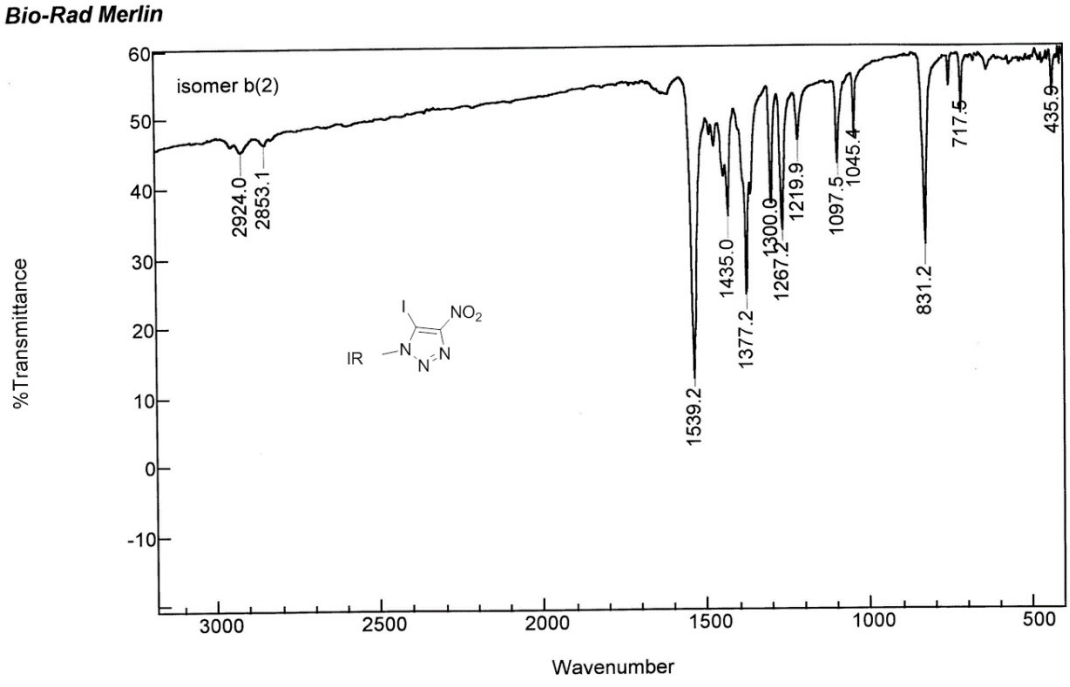

13C{1H}_315 DC 1023_1
104.46
50.71
40.18
40.01
39.84
39.68
39.51
39.34
39.17
14.57
13 C NMR
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm

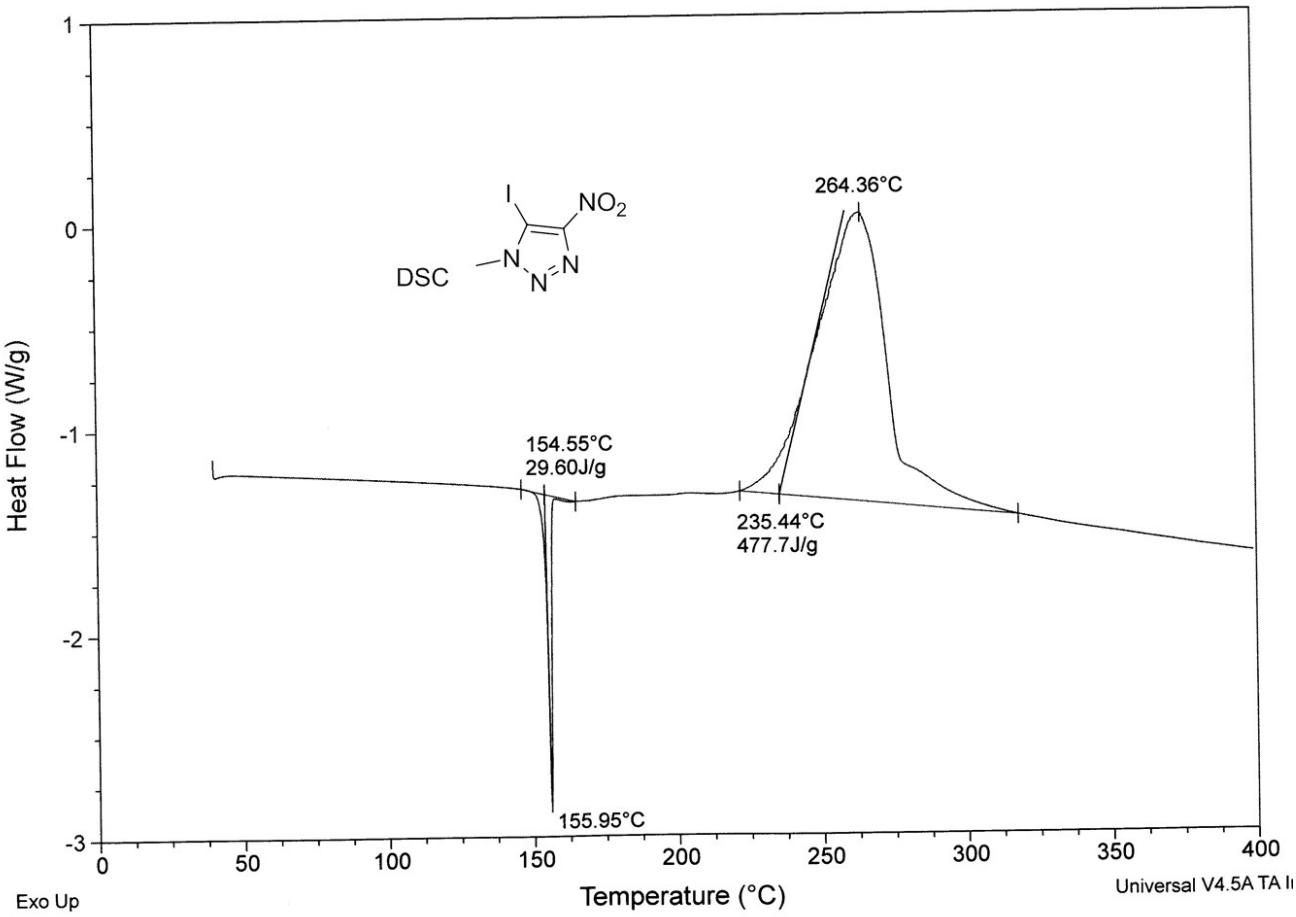

0.5
0.0
-0.5
-1.0
-1.5
-2.0
Heat Flow (W/g)
DSC
108.05°C
0 50 100 150 200 250 300 350 400
Temperature (°C)
Exo Up
Universal V4.5A TA I

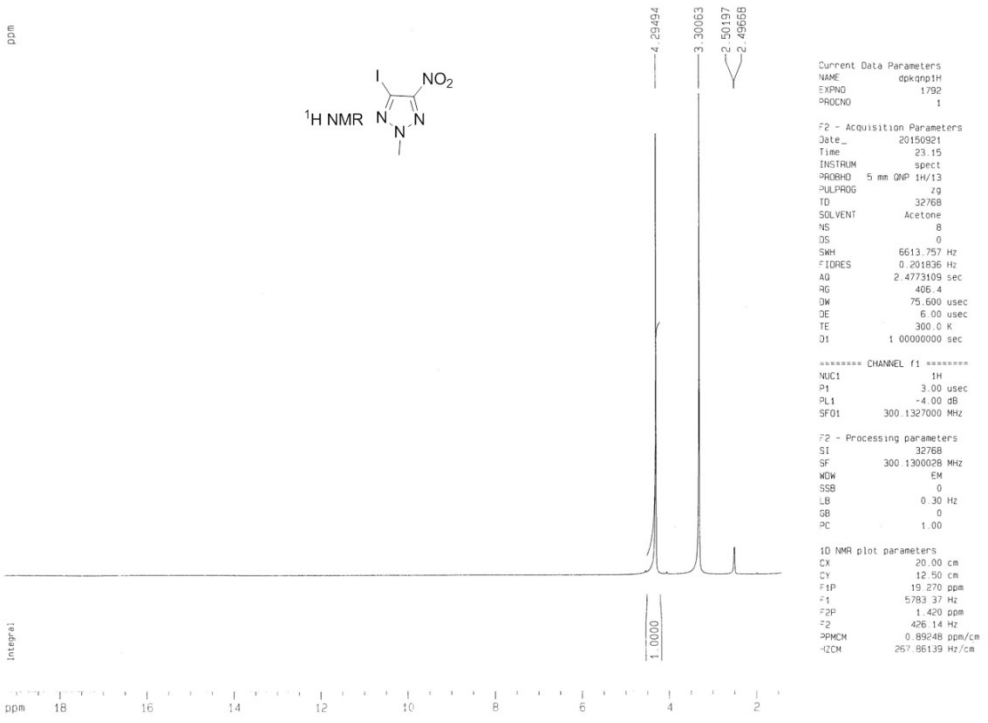

ppm
4.15469
3.29427
2.50143
^{1}H NMR
I
NO$_2$
N
N
N
Integral
1.0000
ppm 16 14 12 10 8 6 4 2
Current Data Parameters
NAME dpkqnp1H
EXPNO 1793
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150922
Time 9.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4773109 sec
RG 645.1
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 17.036 ppm
F1 5113.06 Hz
F2P 0.148 ppm
F2 44.49 Hz
PPMCM 0.84440 ppm/cm
HZCM 253.42828 Hz/cm

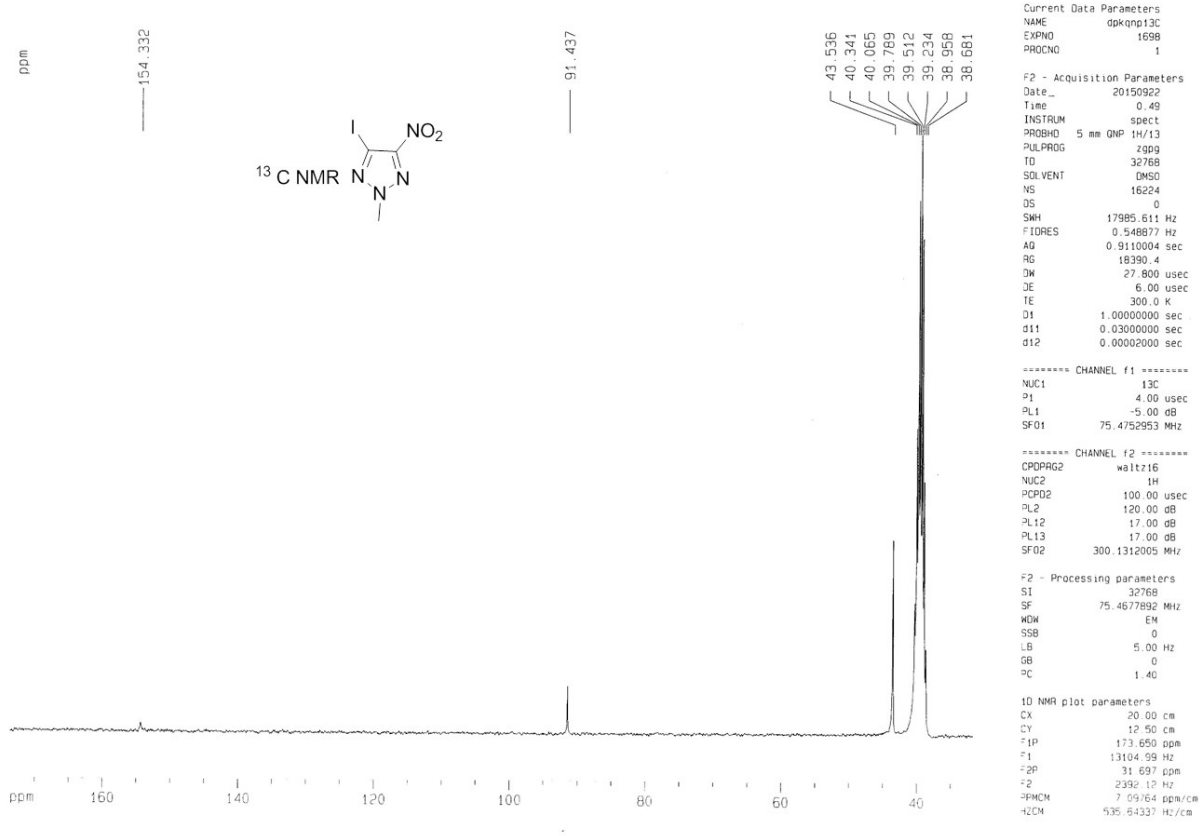

ppm
155.346
88.353
40.339
40.062
39.784
39.506
39.228
38.924
38.672
^{13}C NMR
I
NO$_2$
N
N
N
ppm 160 140 120 100 80 60 40
Current Data Parameters
NAME dpkqnp13C
EXPNO 1699
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150924
Time 23.04
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CDCl3
NS 25041
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677897 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 176.396 ppm
F1 13312.23 Hz
F2P 31.384 ppm
F2 2368.48 Hz
PPMCM 7.25061 ppm/cm
HZCM 547.18732 Hz/cm

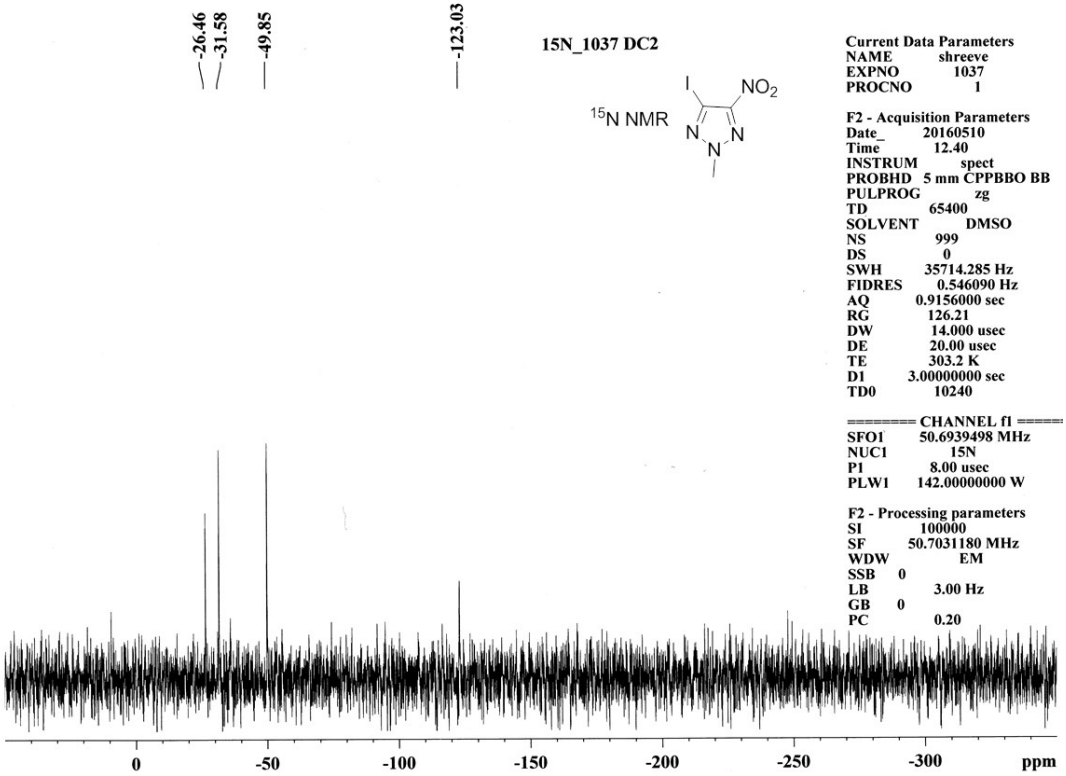

-11.55
-11.58
-11.62
-11.67
-25.28
-35.00
-128.44
15N_1035 DC1
^{15}N NMR
I
NO$_2$
N
N
Current Data Parameters
NAME shreeve
EXPNO 1035
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160510
Time 11.54
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg
TD 65400
SOLVENT DMSO
NS 624
DS 0
SWH 35714.285 Hz
FIDRES 0.546090 Hz
AQ 0.9156000 sec
RG 126.21
DW 14.000 usec
DE 20.00 usec
TE 303.1 K
D1 3.00000000 sec
TD0 10240
CHANNEL f1
SFO1 50.6939498 MHz
NUC1 15N
P1 8.00 usec
PLW1 142.00000000 W
F2 - Processing parameters
SI 100000
SF 50.7031180 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 0.20
-11.5 ppm
0
-50
-100
-150
-200
-250
-300
ppm

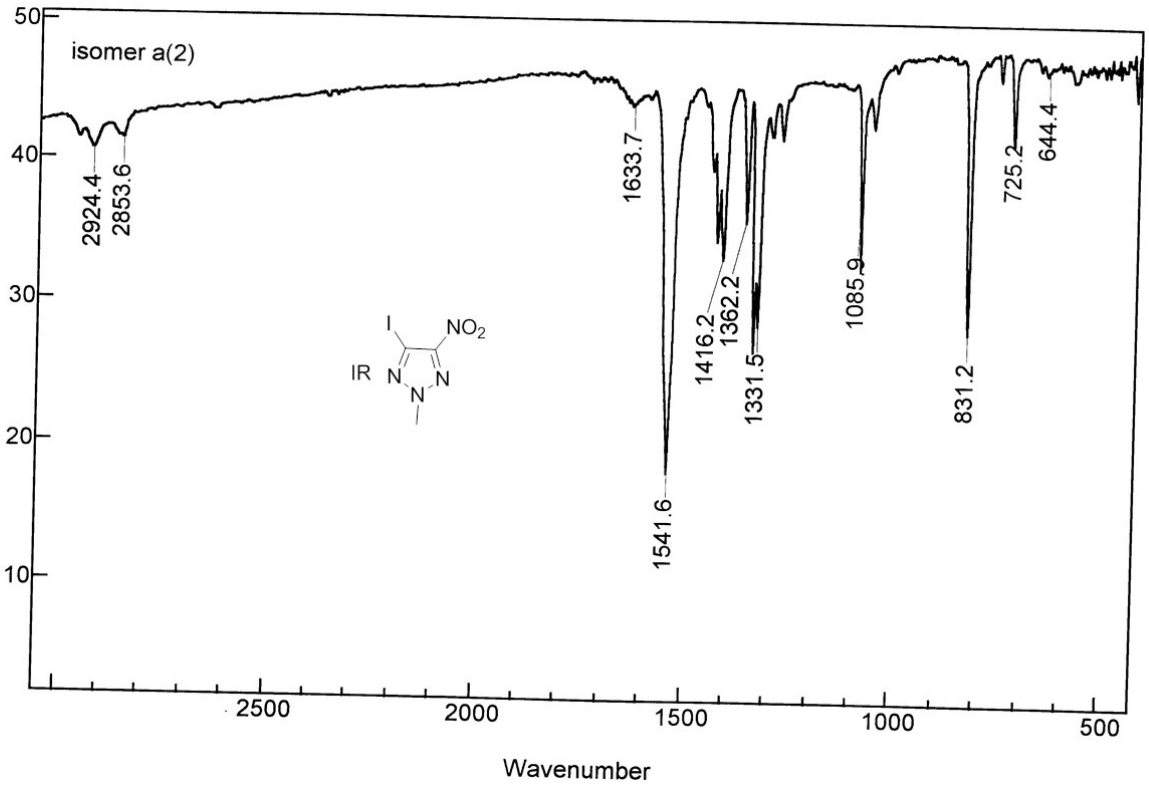

Bio-Rad Merlin
isomer b(2)
IR
%Transmittance
Wavenumber
2924.0
2853.1
1539.2
1435.0
1377.2
1300.0
1267.2
1219.9
1097.5
1045.4
831.2
717.5
435.9
60
50
40
30
20
10
0
-10
3000
2500
2000
1500
1000
500

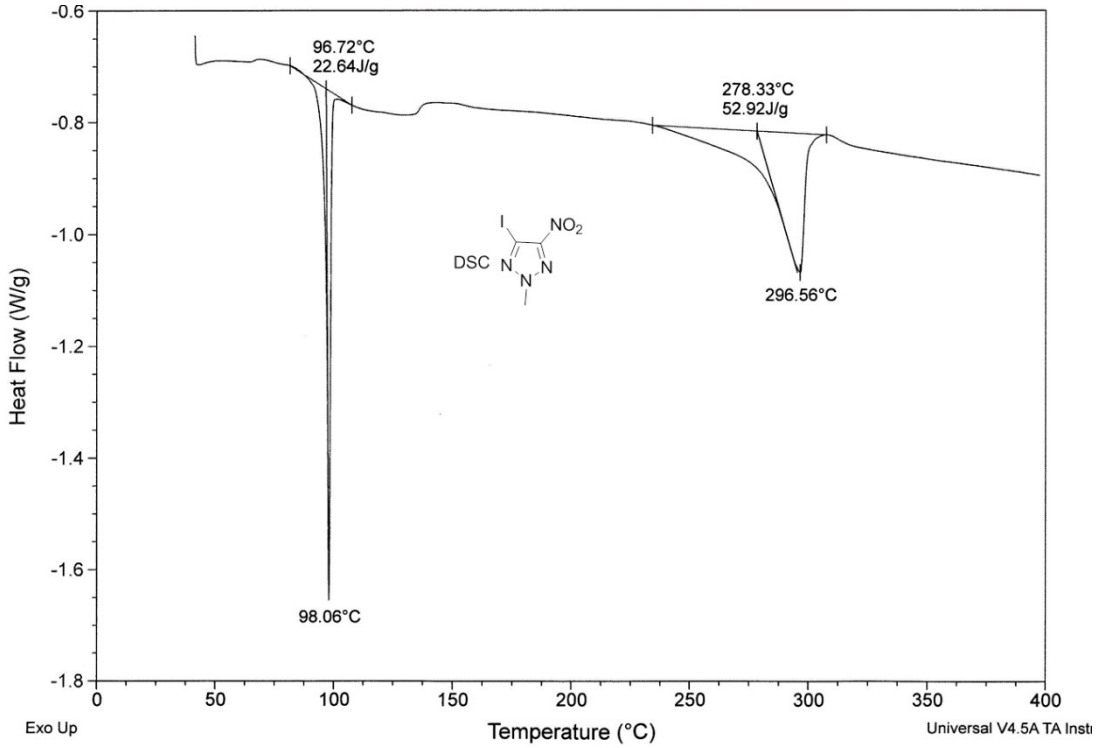

DSC
I
NO2
N
N
N
264.36°C
154.55°C
29.60J/g
235.44°C
477.7J/g
155.95°C
Heat Flow (W/g)
Temperature (°C)
Exo Up
Universal V4.5A TA I
1
0
-1
-2
-3
0
50
100
150
200
250
300
350
400

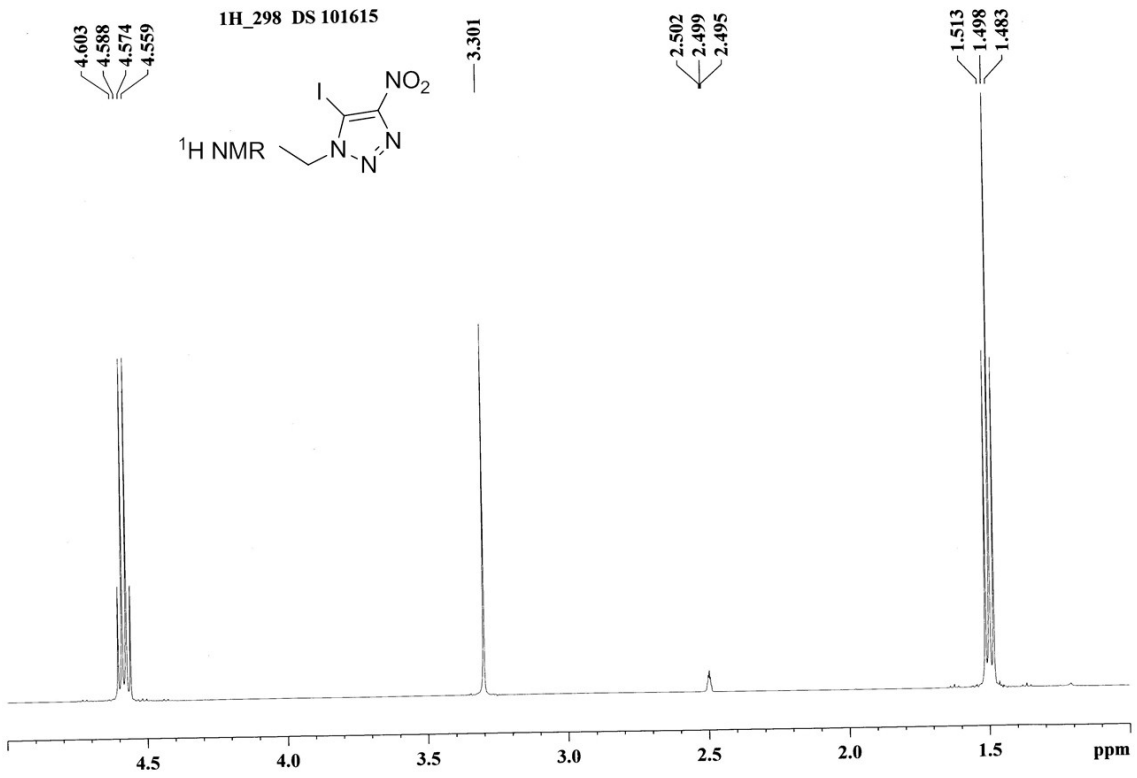

ppm
1H NMR
I
NO2
N
N
N
4.29494
3.30063
2.50197
2.49658
1.0000
Integral
ppm
18
16
14
12
10
8
6
4
2
Current Data Parameters
NAME pkqnp1H
EXPNO 1792
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150921
Time 23.15
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zg
TD 32768
SOLVENT Acetone
NS 8
DS 0
SWH 6613.757 Hz
FIDRES 0.201836 Hz
AQ 2.4773109 sec
RG 406.4
DW 75.600 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1327000 MHz
F2 - Processing parameters
SI 32768
SF 300.1300028 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 19.270 ppm
F1 5783.37 Hz
F2P 1.420 ppm
F2 426.14 Hz
PPMCM 0.89248 ppm/cm
HZCM 267.86139 Hz/cm

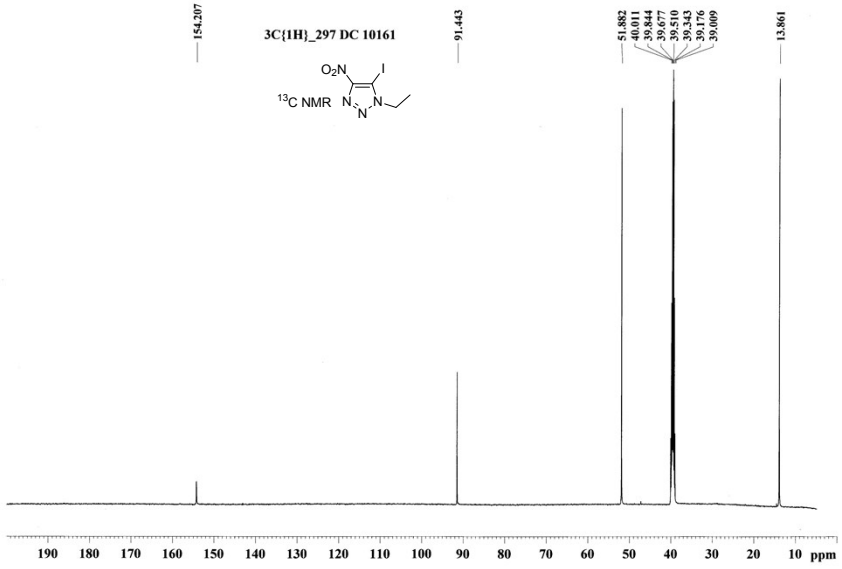

ppm
154.332
91.437
43.536
40.341
40.065
39.789
39.512
39.234
38.958
38.681
^{13}C NMR
I
NO$_2$
N
N
N
ppm
160
140
120
100
80
60
40
Current Data Parameters
NAME dpkqnp13C
EXPNO 1698
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150922
Time 0.49
INSTRUM spect
PROBHD 5 mm GNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 16224
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 18390.4
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677892 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 12.50 cm
F1P 173.650 ppm
F1 13104.99 Hz
F2P 31.697 ppm
F2 2392.12 Hz
PPMCM 7.09764 ppm/cm
HZCM 535.64337 Hz/cm

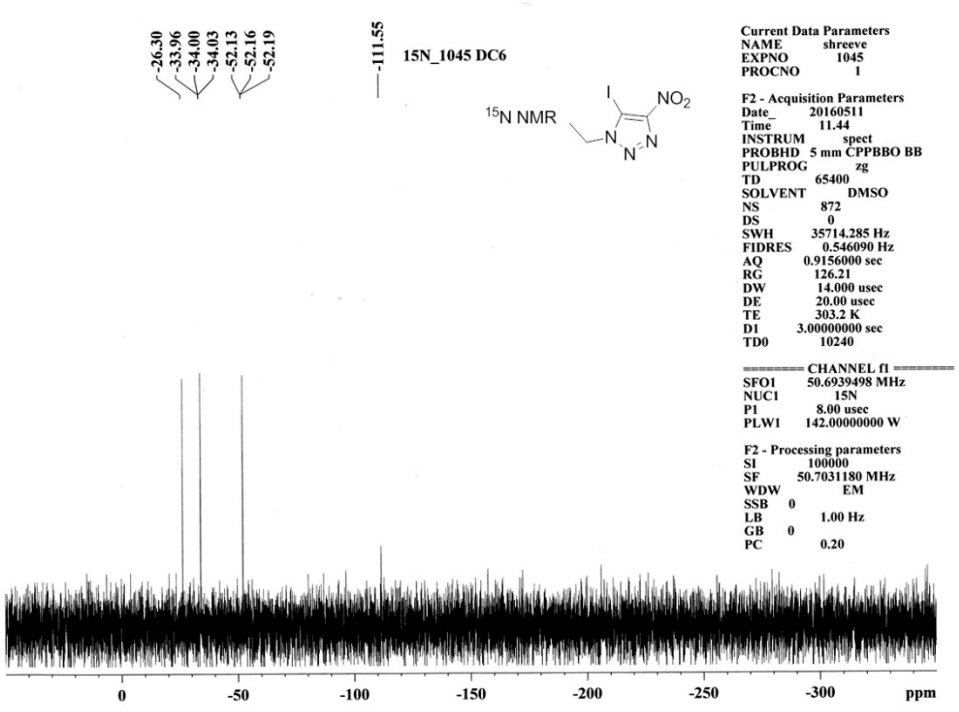

-26.46
-31.58
-49.85
-123.03
15N_1037 DC2
^{15}N NMR
I
NO$_2$
N
N
N
0
-50
-100
-150
-200
-250
-300
ppm
Current Data Parameters
NAME shreeve
EXPNO 1037
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160510
Time 12.40
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg
TD 65400
SOLVENT DMSO
NS 999
DS 0
SWH 35714.285 Hz
FIDRES 0.546090 Hz
AQ 0.9156000 sec
RG 126.21
DW 14.000 usec
DE 20.00 usec
TE 303.2 K
D1 3.00000000 sec
TD0 10240
======== CHANNEL f1 ========
SFO1 50.6939498 MHz
NUC1 15N
P1 8.00 usec
PLW1 142.00000000 W
F2 - Processing parameters
SI 100000
SF 50.7031180 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 0.20

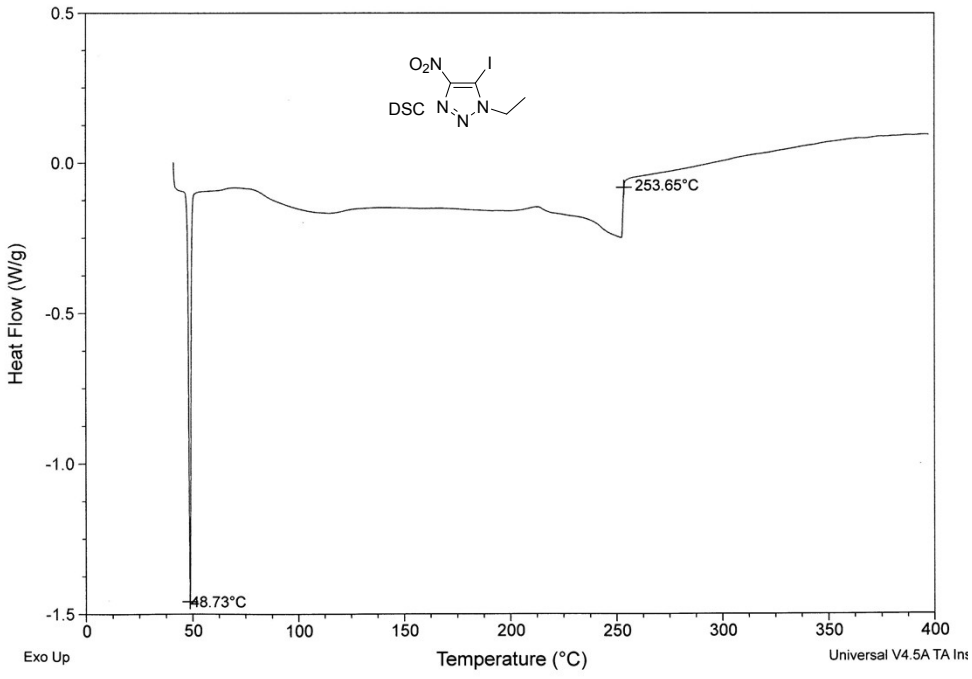

isomer a(2)
IR
2924.4
2853.6
1633.7
1541.6
1416.2
1362.2
1331.5
1085.9
831.2
725.2
644.4
Wavenumber

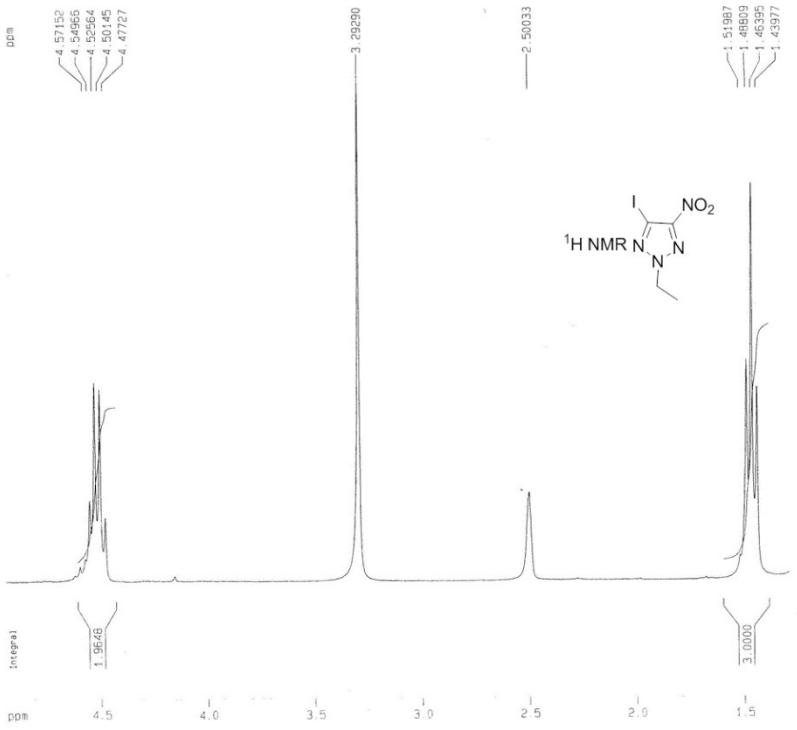

DSC
96.72°C
22.64J/g
278.33°C
52.92J/g
296.56°C
98.06°C
Heat Flow (W/g)
Exo Up
Temperature (°C)
Universal V4.5A TA Instr


1H_298 DS 101615
4.603
4.588
4.574
4.559
3.301
2.502
2.499
2.495
1.513
1.498
1.483
NO2
I
1H NMR
4.5
4.0
3.5
3.0
2.5
2.0
1.5
ppm


154.207
3C{1H}_297 DC 10161
91.443
51.882
40.011
39.844
39.677
39.510
39.343
39.176
39.009
13.861
O2N
I
13C NMR
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm


-26.30
-33.96
-34.00
-34.03
-52.13
-52.16
-52.19
-111.55
15N_1045 DC6
15N NMR
I
NO2
N
N
N
Current Data Parameters
NAME shreeve
EXPNO 1045
PROCNO 1
F2 - Acquisition Parameters
Date_ 20160511
Time 11.44
INSTRUM spect
PROBHD 5 mm CPPBBO BB
PULPROG zg
TD 65400
SOLVENT DMSO
NS 872
DS 0
SWH 35714.285 Hz
FIDRES 0.546090 Hz
AQ 0.9156000 sec
RG 126.21
DW 14.000 usec
DE 20.00 usec
TE 303.2 K
D1 3.00000000 sec
TD0 10240
CHANNEL f1
SFO1 50.6939498 MHz
NUC1 15N
P1 8.00 usec
PLW1 142.00000000 W
F2 - Processing parameters
SI 100000
SF 50.7031180 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 0.20
0
-50
-100
-150
-200
-250
-300
ppm


O2N
I
DSC
N
N
N
253.65°C
48.73°C
Heat Flow (W/g)
0.5
0.0
-0.5
-1.0
-1.5
0
50
100
150
200
250
300
350
400
Exo Up
Temperature (°C)
Universal V4.5A TA Ins



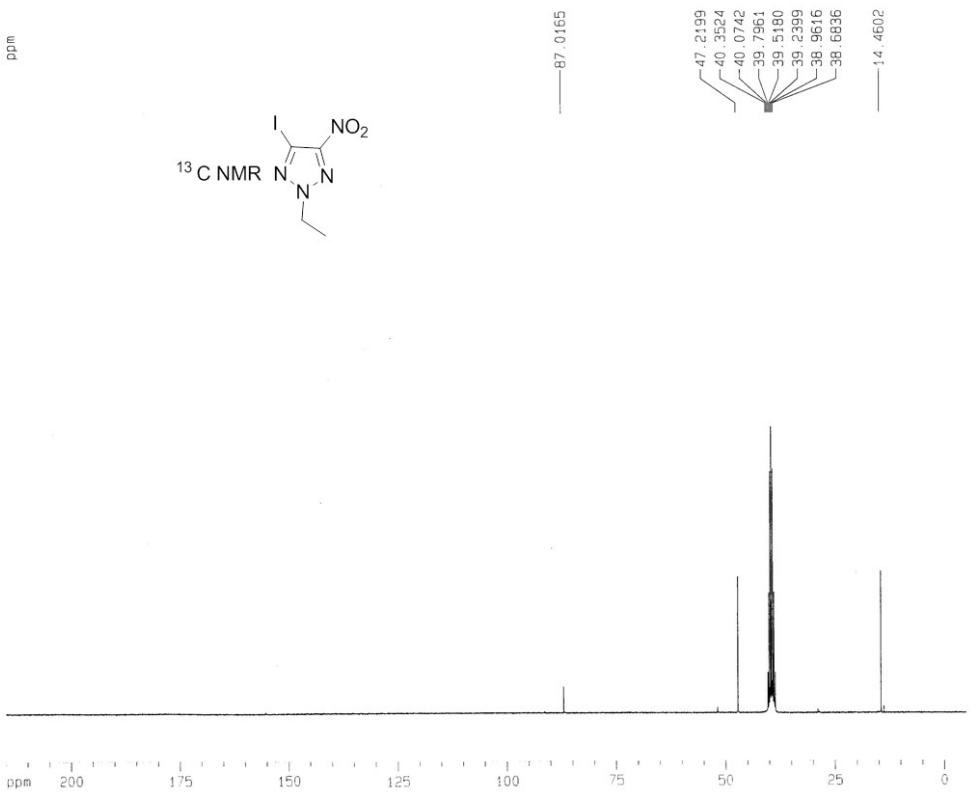

```
Current Data Parameters
NAME                dpkqnp1H
EXPNO                   1806
PROCNO                     1

F2 - Acquisition Parameters
Date_               20151015
Time                   21.51
INSTRUM                spect
PROBHD   5 mm QNP 1H/13
PULPROG                  zg
TD                      32768
SOLVENT              Acetone
NS                         8
DS                         0
SWH                 6613.757 Hz
FIDRES              0.201836 Hz
AQ                  2.4773109 sec
RG                      574.7
DW                     75.600 usec
DE                      6.00 usec
TE                     300.0 K
D1                 1.00000000 sec

======== CHANNEL f1 ========
NUC1                       1H
P1                       3.00 usec
PL1                     -4.00 dB
SFO1               300.1327000 MHz

F2 - Processing parameters
SI                      32768
SF                 300.1300024 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00

1D NMR plot parameters
CX                      20.00 cm
CY                      12.50 cm
F1P                      4.942 ppm
F1                    1483.30 Hz
F2P                      1.291 ppm
F2                     387.46 Hz
PPMCM                 0.18256 ppm/cm
HZCM                 54.79194 Hz/cm
```




```
Current Data Parameters
NAME                dpkqnp13C
EXPNO                   1708
PROCNO                     1

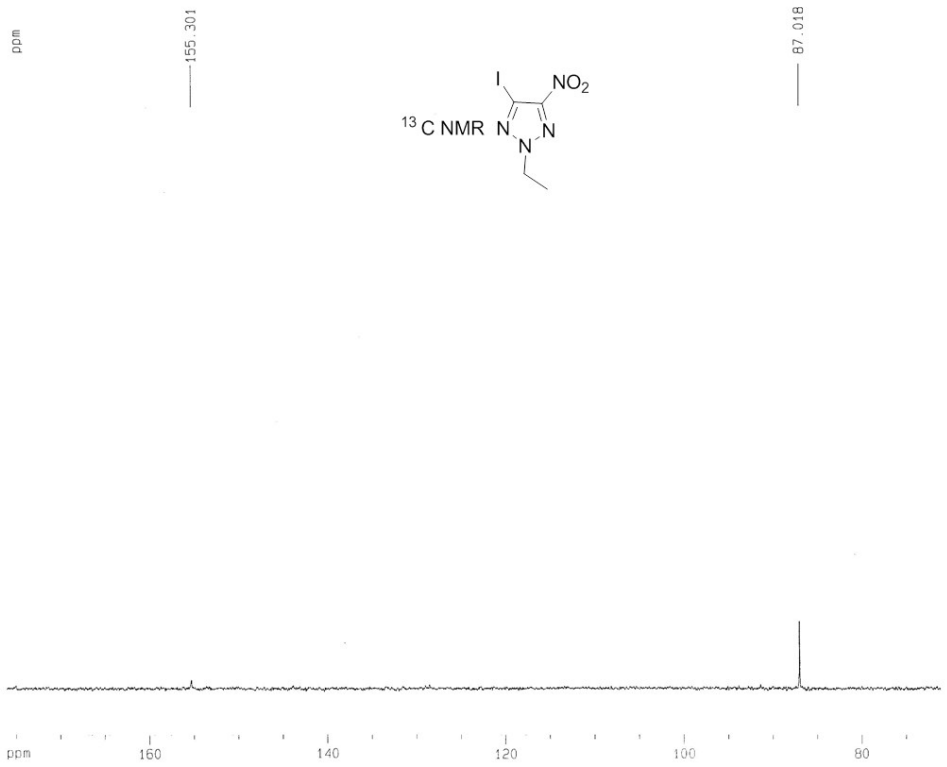
F2 - Acquisition Parameters
Date_               20151019
Time                   22.47
INSTRUM                spect
PROBHD   5 mm QNP 1H/13
PULPROG                zgpg
TD                      32768
SOLVENT              CDCl3
NS                      24253
DS                         0
SWH                17985.611 Hz
FIDRES              0.548877 Hz
AQ                  0.9110004 sec
RG                     18390.4
DW                     27.800 usec
DE                      6.00 usec
TE                     300.0 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec

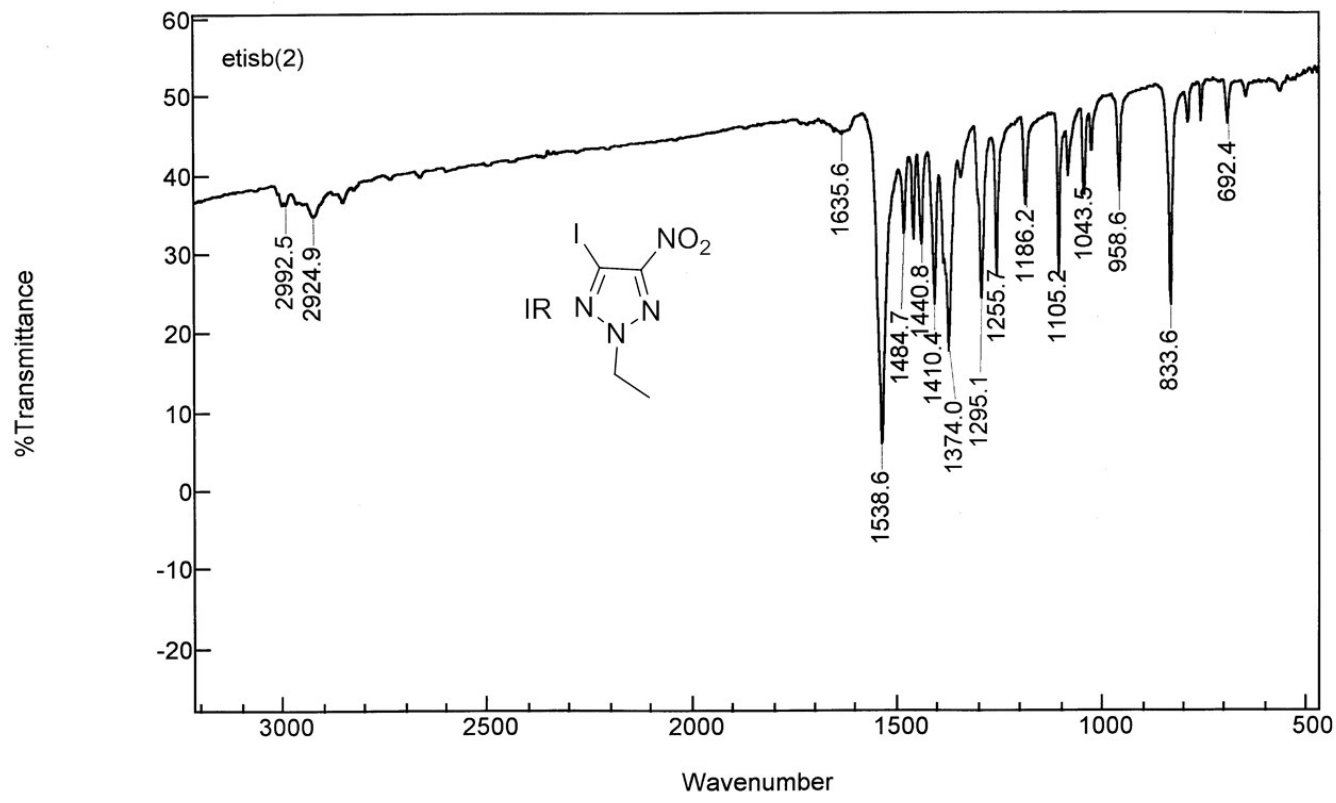
======== CHANNEL f1 ========
NUC1                      13C
P1                       4.00 usec
PL1                     -5.00 dB
SFO1               75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                  100.00 usec
PL2                    120.00 dB
PL12                    17.00 dB
PL13                    17.00 dB
SFO2               300.1312005 MHz

F2 - Processing parameters
SI                      32768
SF                 75.4677892 MHz
WDW                        EM
SSB                         0
LB                       0.50 Hz
GB                          0
PC                       1.40

1D NMR plot parameters
CX                      20.00 cm
CY                       6.00 cm
F1P                   215.000 ppm
F1                  16225.58 Hz
F2P                    -5.000 ppm
F2                     -377.34 Hz
PPMCM                11.00000 ppm/cm
HZCM                830.14563 Hz/cm
```

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Current Data Parameters
NAME            dpkqnp13C
EXPNO                1708
PROCNO                  1

F2 - Acquisition Parameters
Date_           20151019
Time                22.47
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG             zgpg
TD                 32768
SOLVENT             CDCl3
NS                 24253
DS                     0
SWH           17985.611 Hz
FIDRES         0.548877 Hz
AQ             0.9110004 sec
RG                18390.4
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1             1.00000000 sec
d11            0.03000000 sec
d12            0.00002000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 4.00 usec
PL1                -5.00 dB
SFO1          75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2               120.00 dB
PL12               17.00 dB
PL13               17.00 dB
SFO2         300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF            75.4677892 MHz
WDW                   EM
SSB                    0
LB                 3.00 Hz
GB                     0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                25.00 cm
F1P              176.097 ppm
F1             13289.69 Hz
F2P               71.162 ppm
F2              5370.48 Hz
PPMCM           5.24675 ppm/cm
HZCM          395.96051 Hz/cm
```