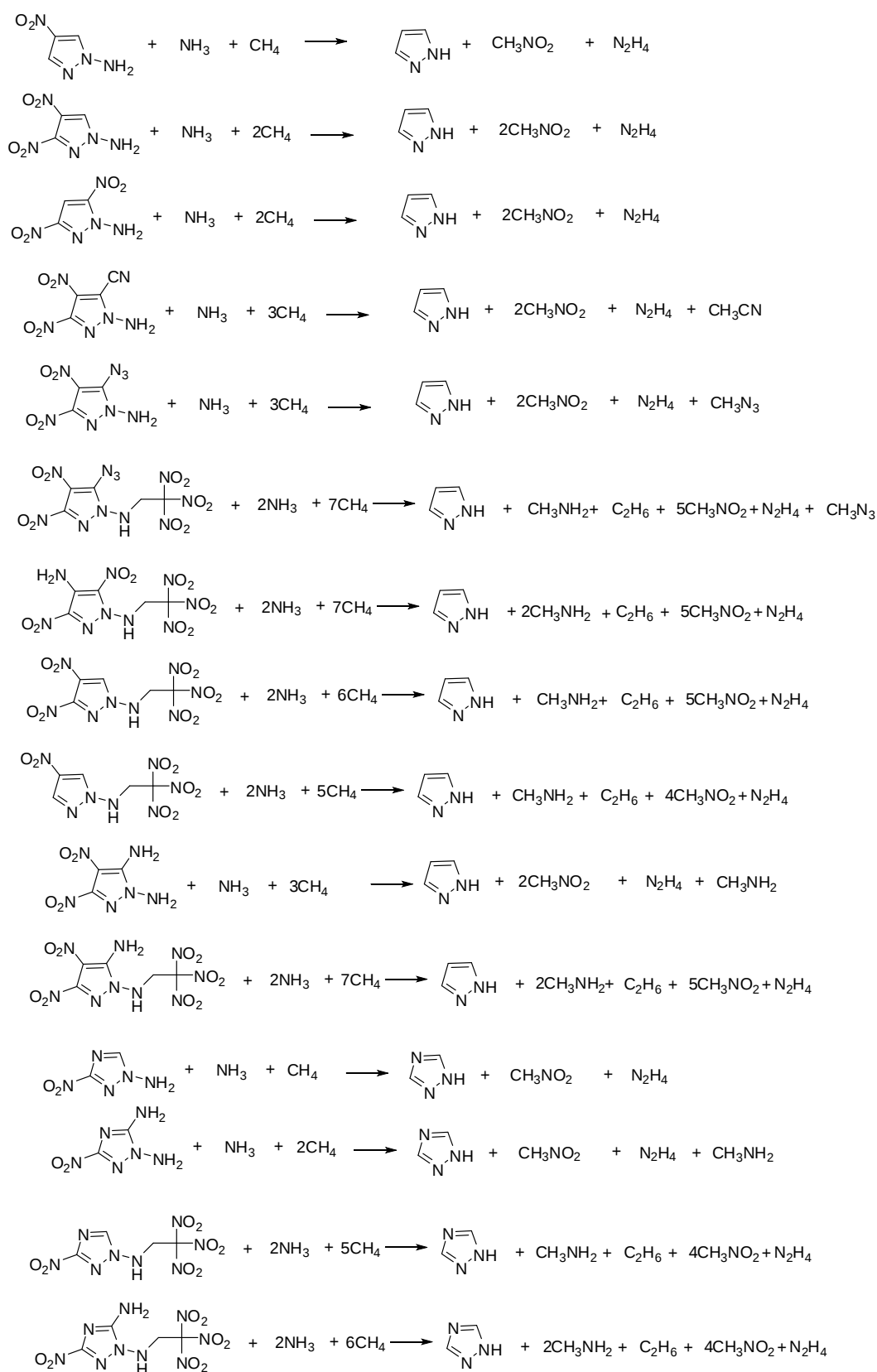


Polynitro-substituted Pyrazoles and Triazoles as Potential Energetic Materials and Oxidizers

Ping Yin, Jiaheng Zhang, Chunlin He, Damon A. Parrish and Jean'ne M. Shreeve*

Table of Contents

	Page
Isodesmic reactions for N-amino and N-trinitroethylamino nitroazoles	S3
The heats of formation (HOF) for <i>N</i> -amino and <i>N</i> -trinitroethylamino nitroazoles	S4
Ball and stick packing diagram of crystals 10 , 11 and 15	S5
¹ H, ¹³ C, ¹⁵ N NMR, ¹⁵ N- ¹ H HMBC, and DSC	S7



Scheme S1. Isodesmic reactions for *N*-amino and *N*-trinitroethylamino nitroazoles

Table S1. The heats of formation (HOF) for *N*-amino and *N*-trinitroethylamino nitroazoles

Compounds	E₀ [Hartree/Particle]	ZPE [Hartree/Particle]	H_T [Hartree/Particle]	HoF(gas) [kJ mol ⁻¹]
4	0.09069	0.099104	0.0870624	231.11472
5	0.092505	0.103419	0.0888048	243.74523
6	0.092159	0.103469	0.08847264	262.59369
7	0.090571	0.103771	0.08694816	404.71982
8	0.094698	0.108776	0.09091008	622.08289
10	0.157737	0.182037	0.15142752	565.58553
12	0.155427	0.176842	0.14920992	209.95117
13	0.153269	0.171875	0.14713824	212.67323
15	0.10892	0.121503	0.1045632	249.36925
16	0.172196	0.195017	0.16530816	184.58040
17	0.078226	0.086692	0.07509696	279.16537
18	0.09562	0.105348	0.0917952	247.56112
19	0.141304	0.159818	0.13565184	240.26836
20	0.158003	0.178156	0.15168288	201.80977

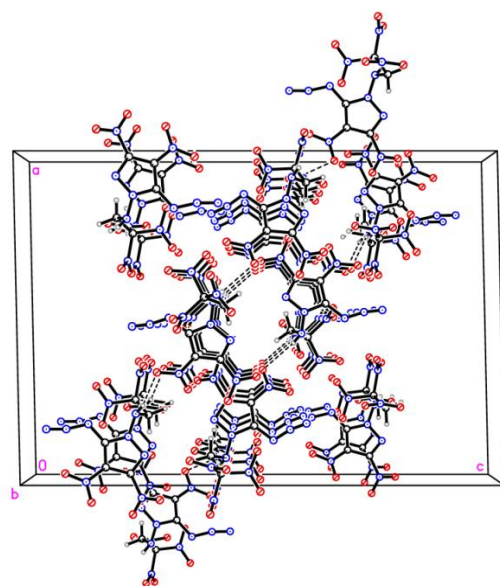


Figure S1. Ball and stick packing diagram of **10** viewed down the b axis. The dashed lines indicate strong hydrogen bonding.

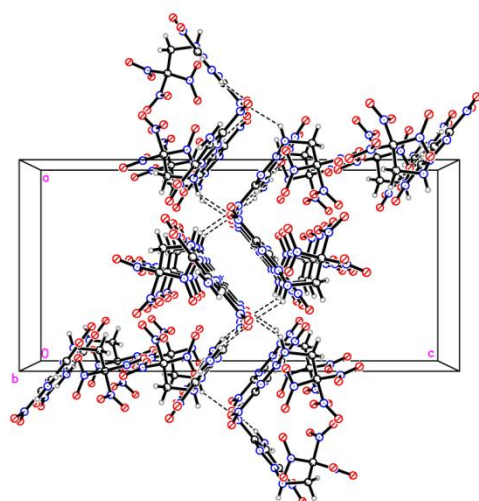


Figure S2. Ball and stick packing diagram of **11** viewed down the b axis. The dashed lines indicate strong hydrogen bonding.

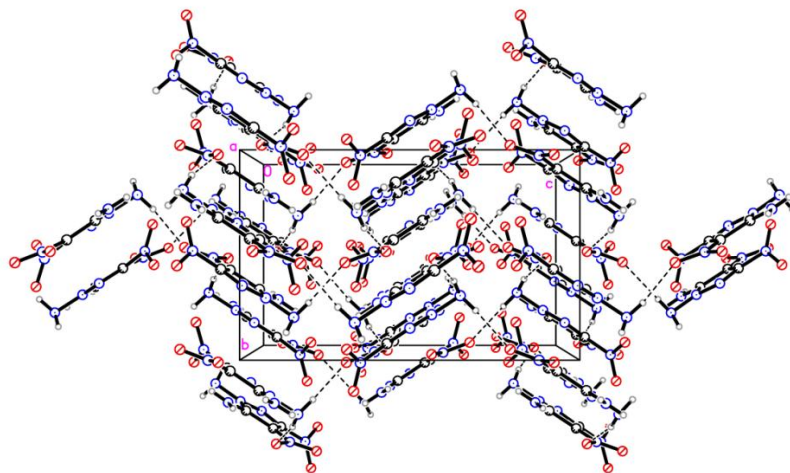
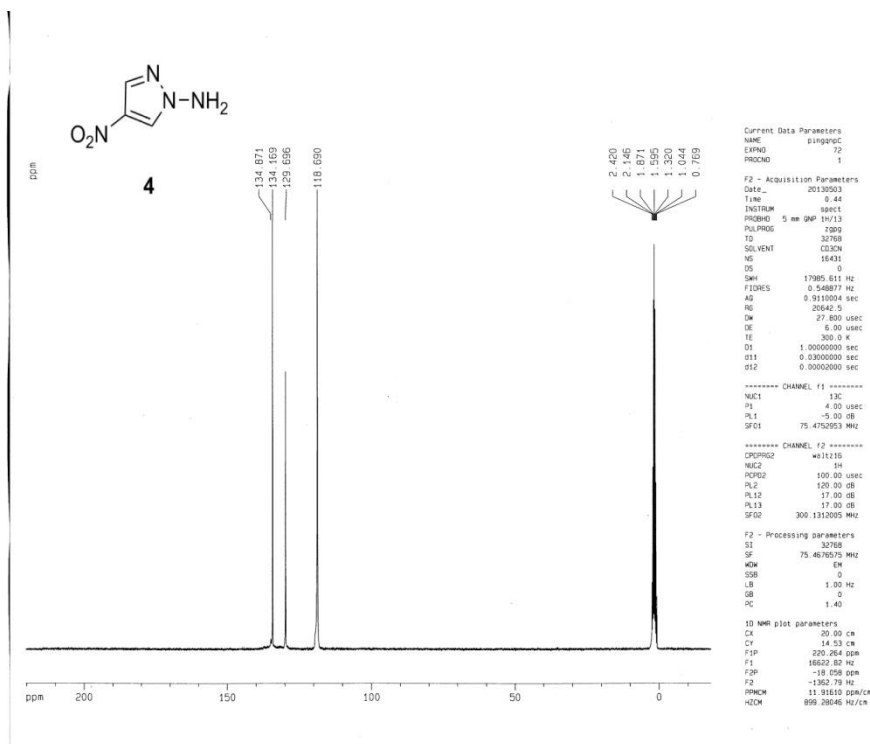
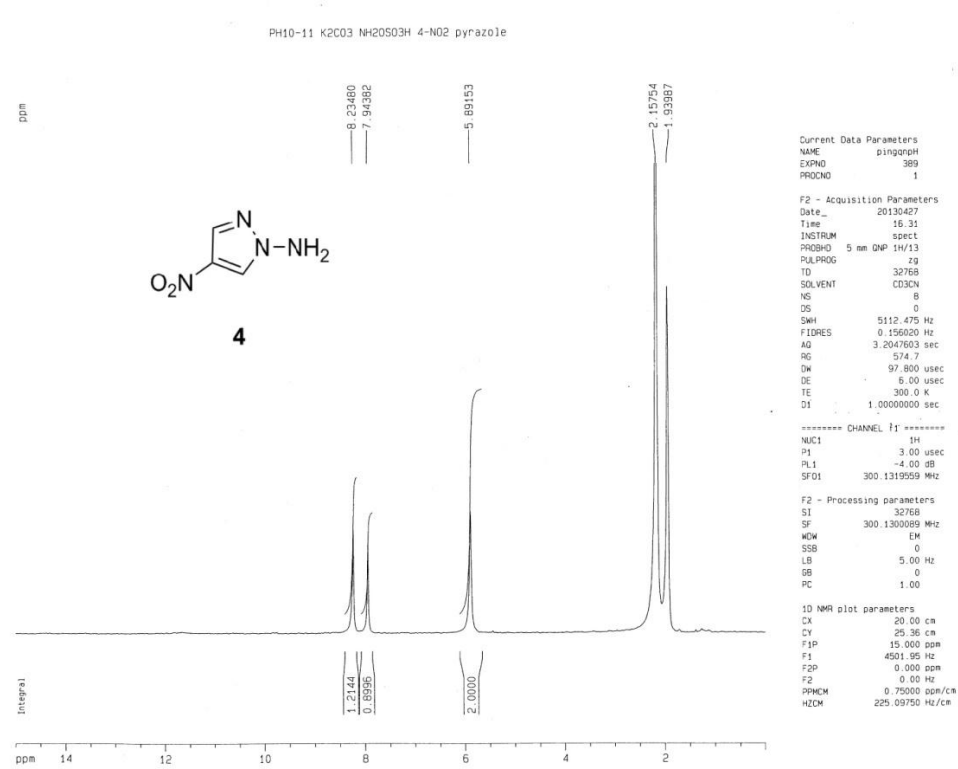
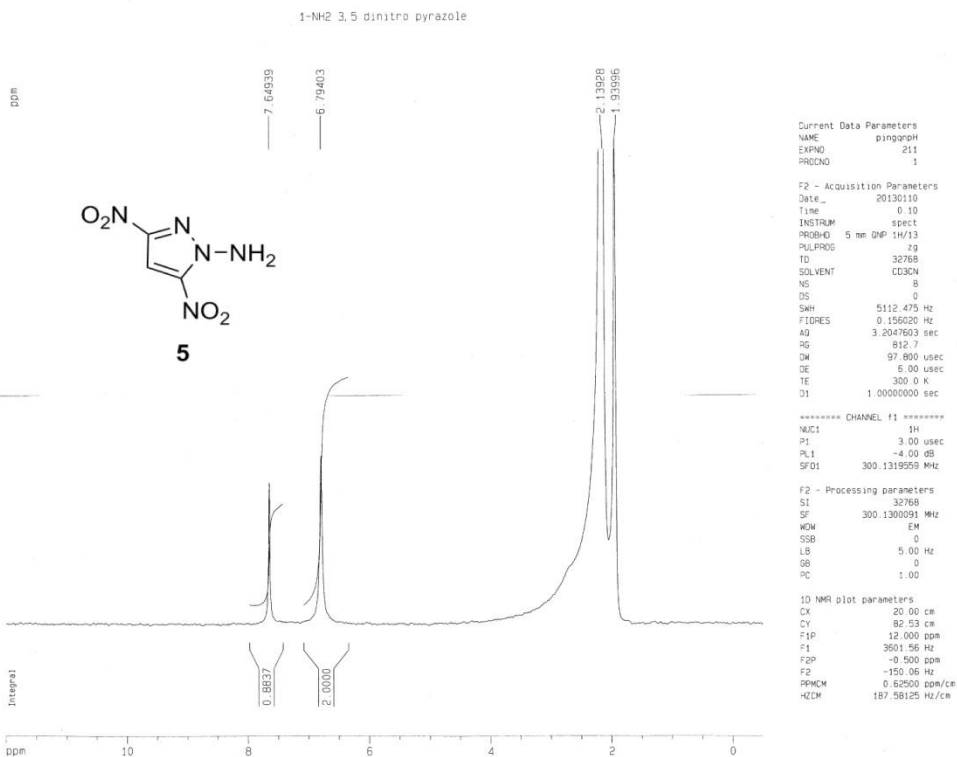
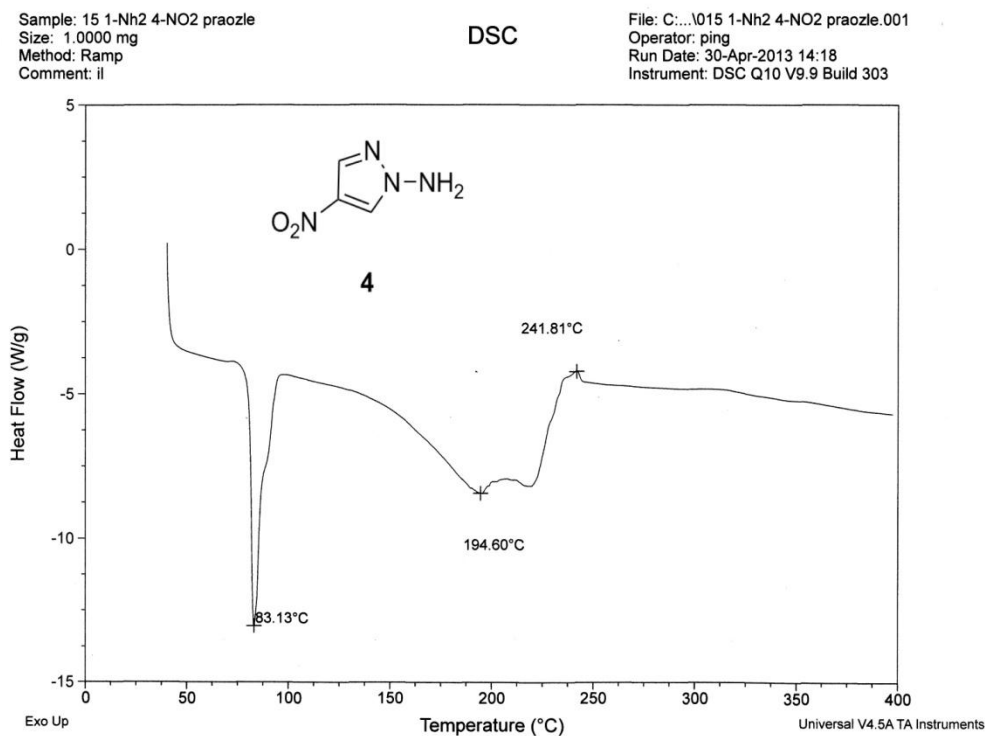
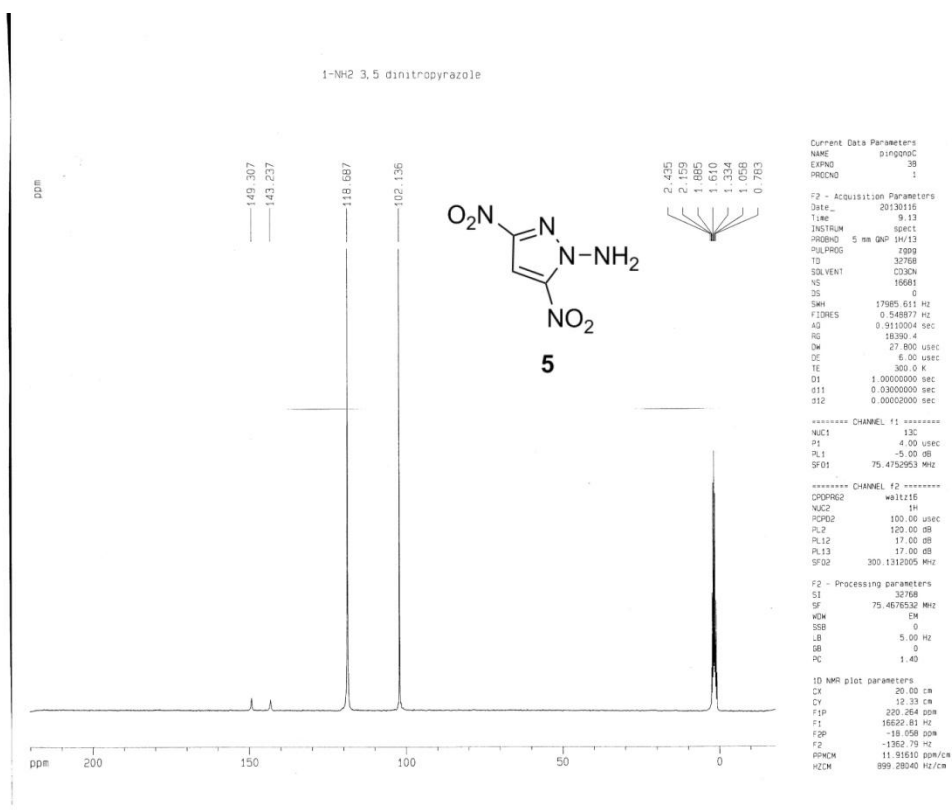


Figure S3. Ball and stick packing diagram of **15** viewed down the a axis. The dashed lines indicate strong hydrogen bonding.

¹H, ¹³C, ¹⁵N NMR, ¹⁵N-¹H HMBC, and DSC for *N*-amino and *N*-trinitroethylamino nitroazoles



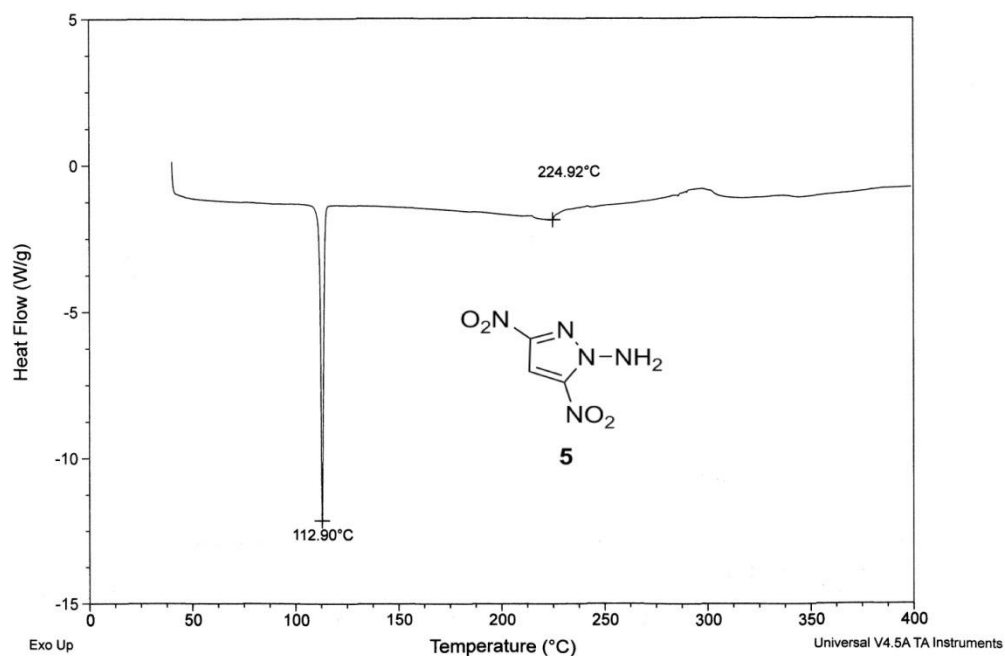


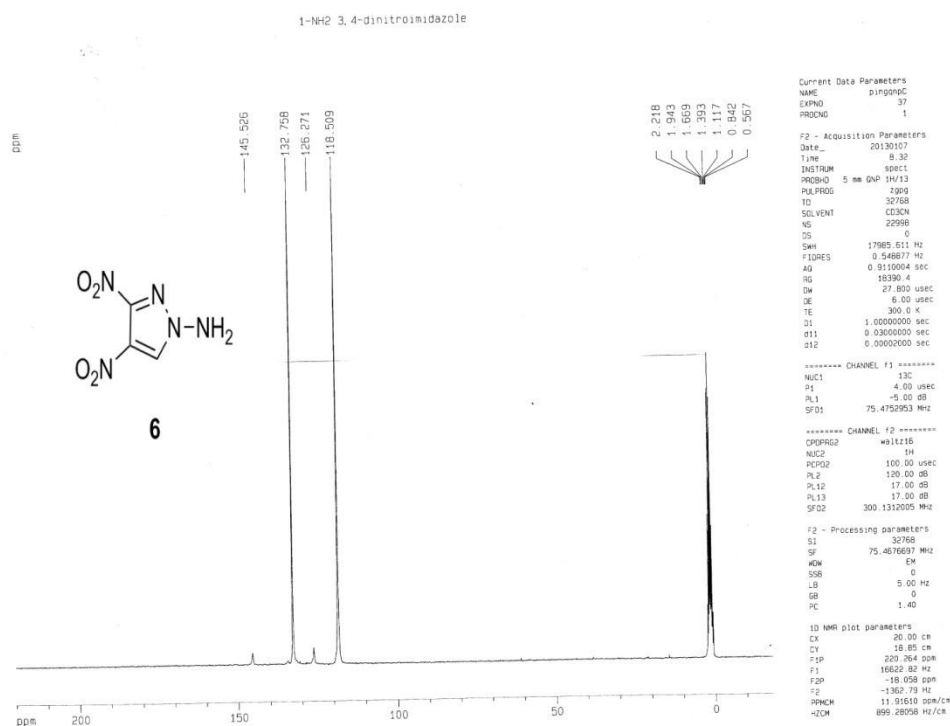
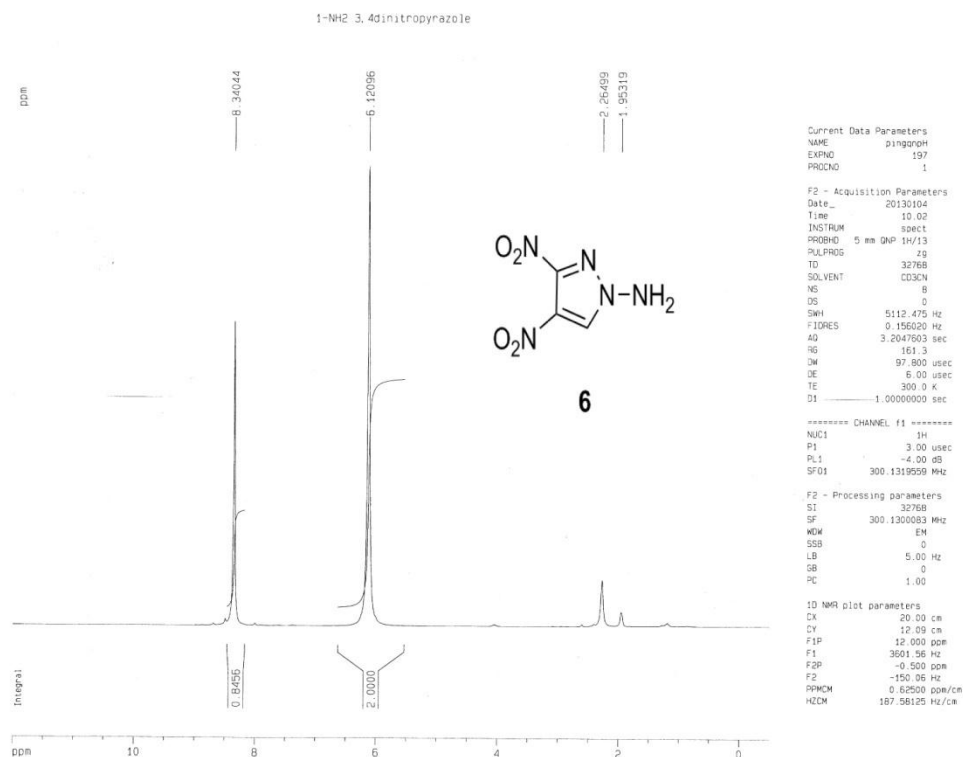


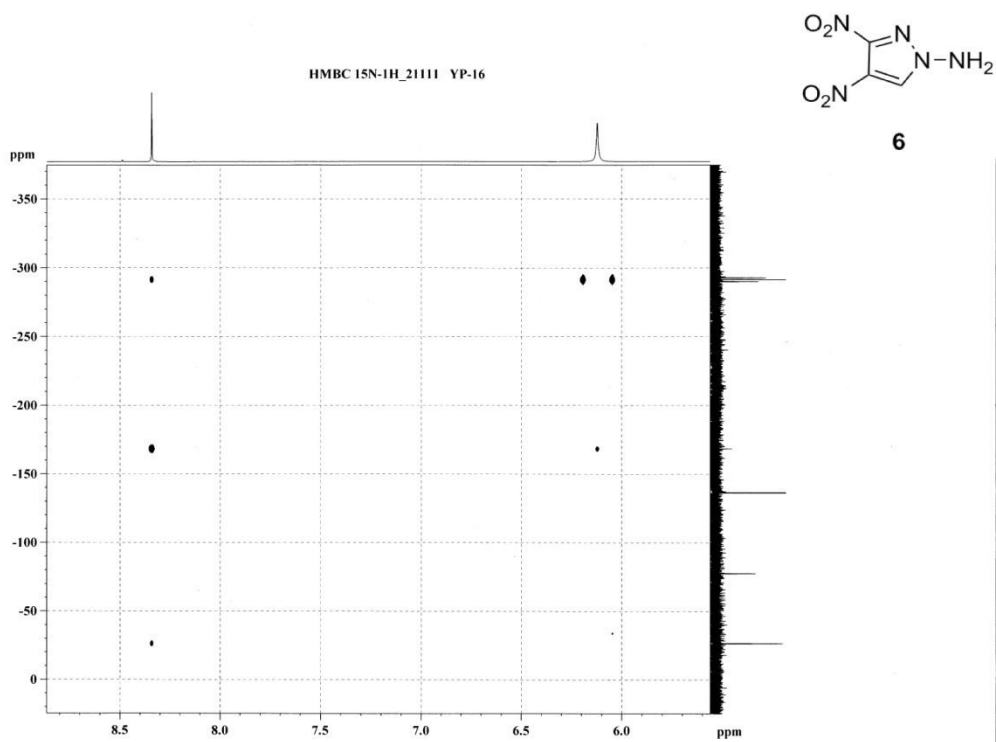
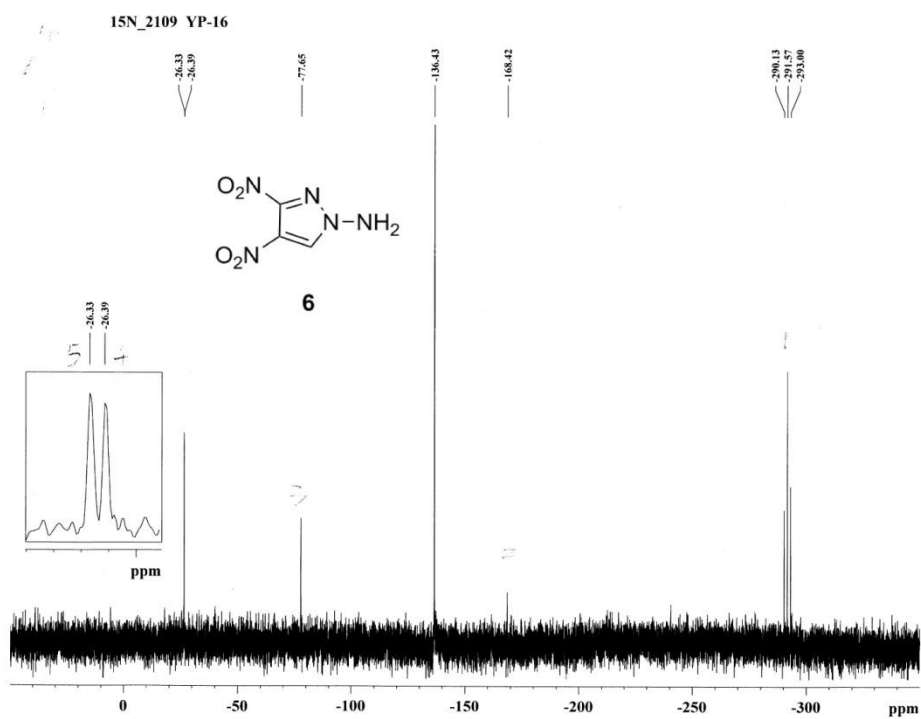
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Method: Ramp

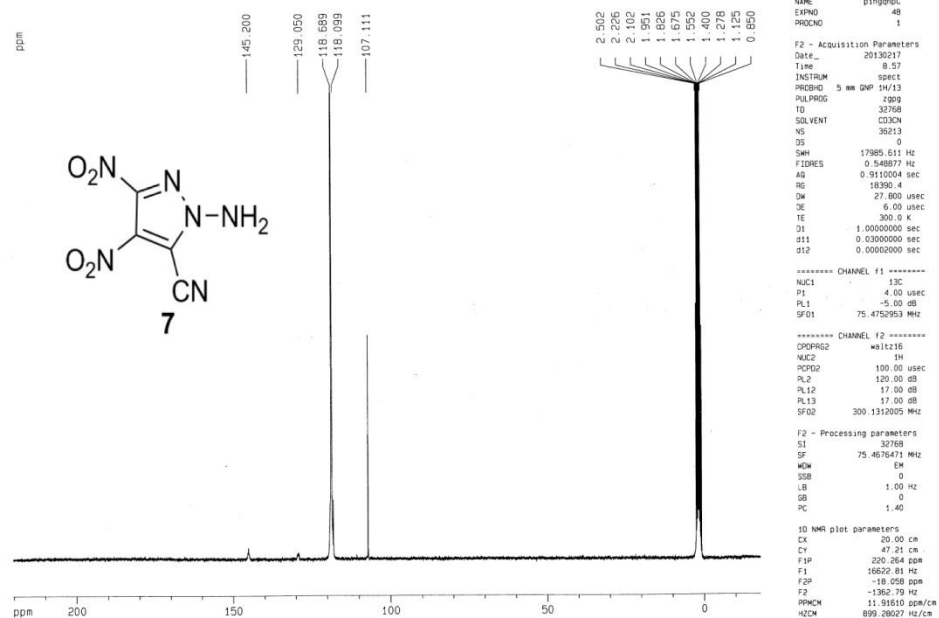
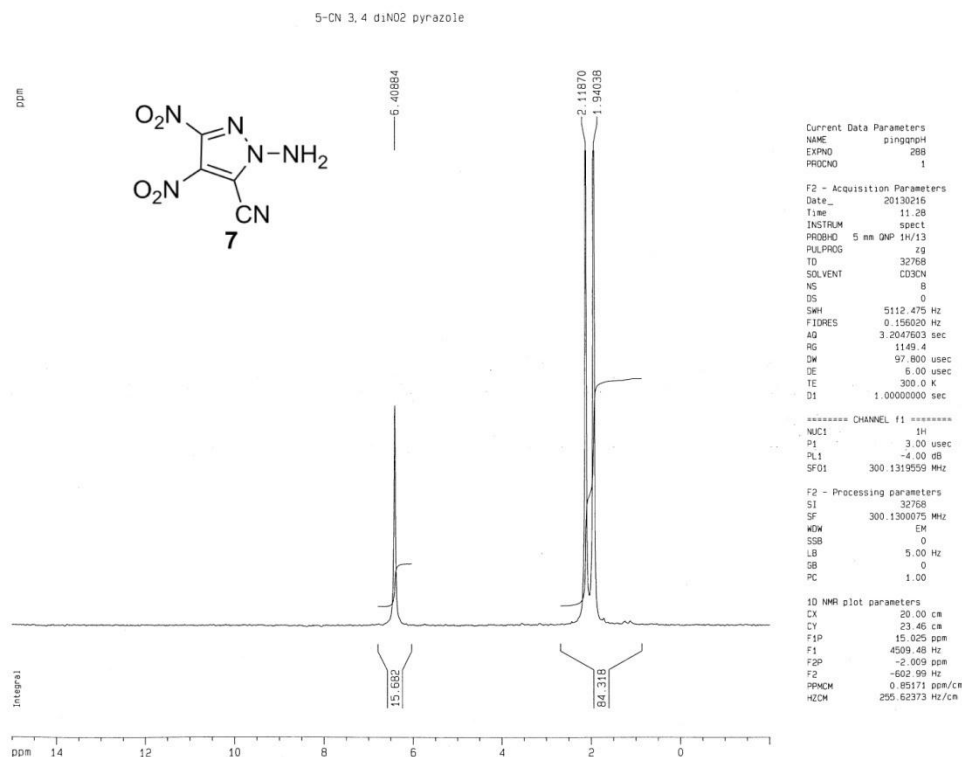
DSC

File: 009 (5oC) 1-NH2 , 3,5-diNO2 pyrazole.001
Operator: ping
Run Date: 19-Feb-2013 21:02
Instrument: DSC Q10 V9.9 Build 303





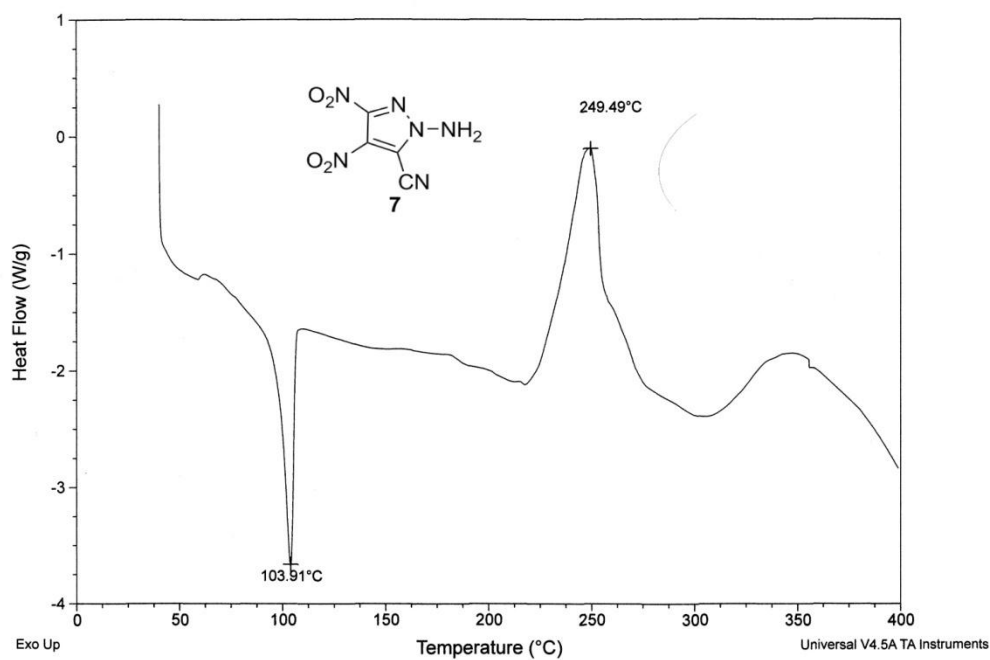




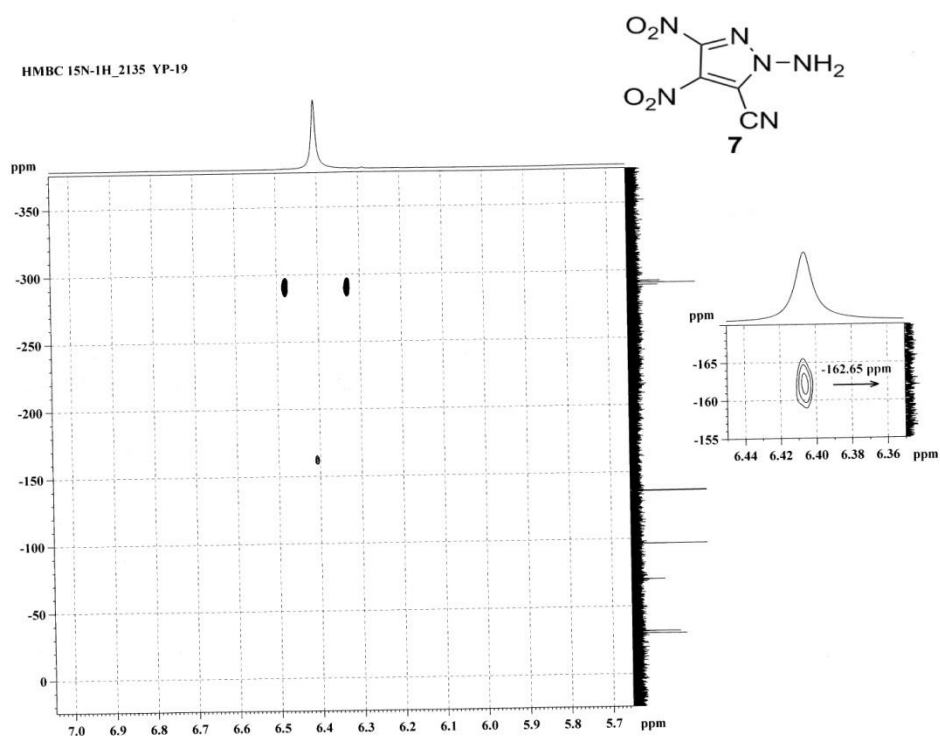
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Size: 1.1000 mg
Method: Ramp

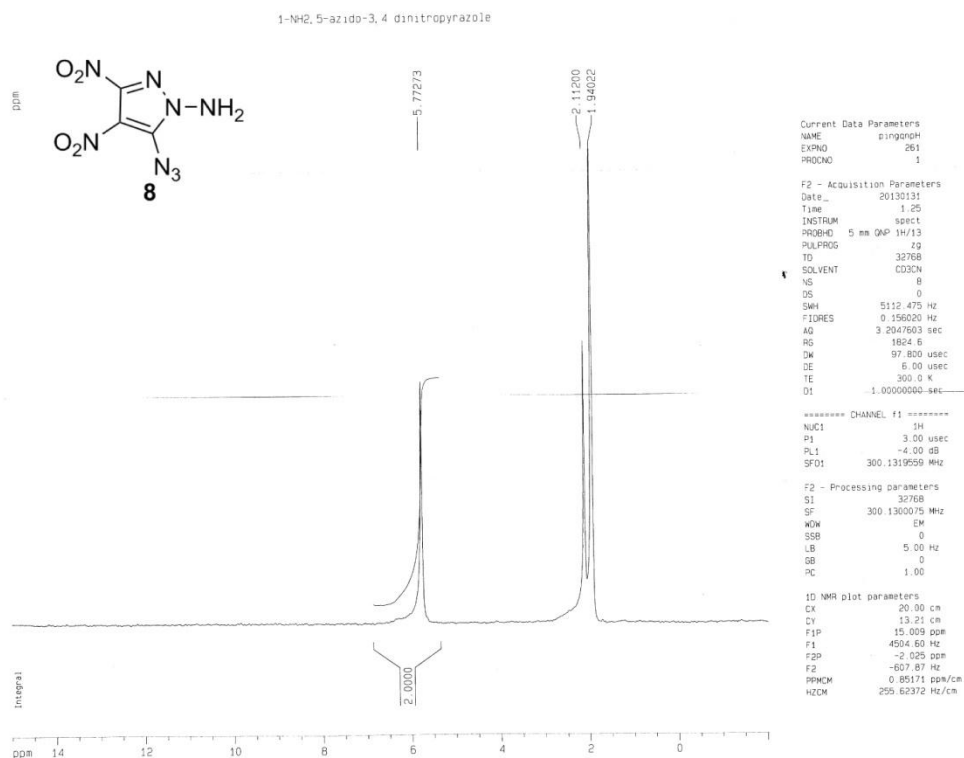
DSC

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Run Date: 05-Feb-2013 21:06
Instrument: DSC Q10 V9.9 Build 303



HMBC 15N-1H_2135 YP-19

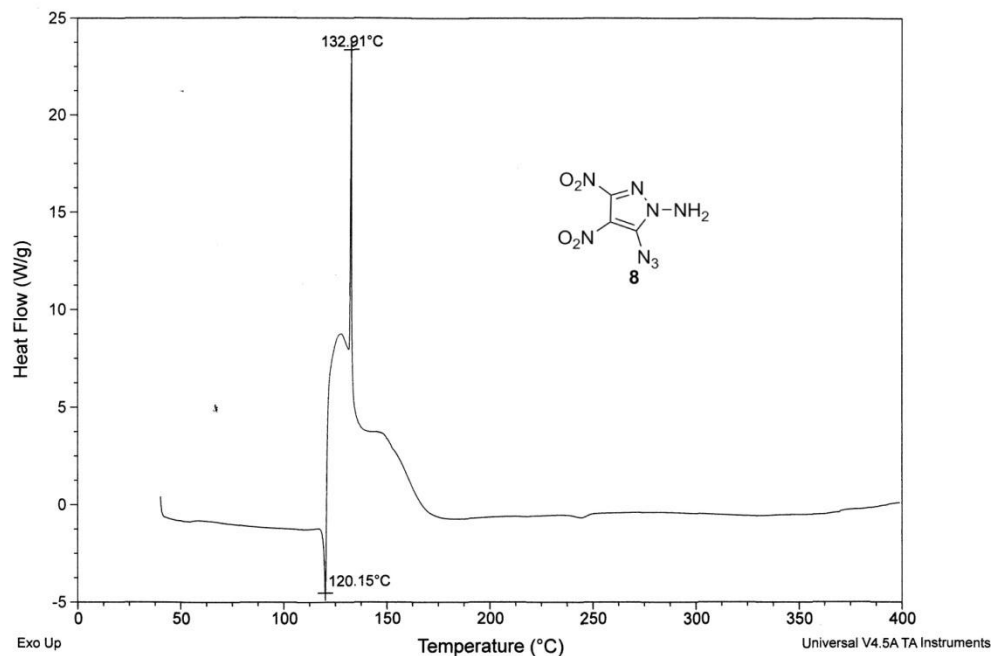


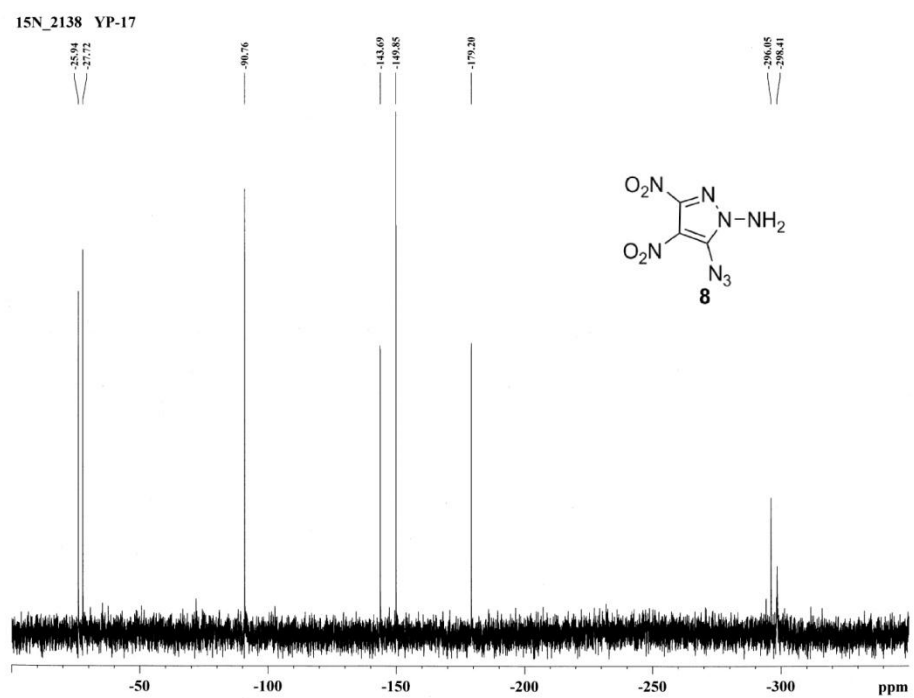
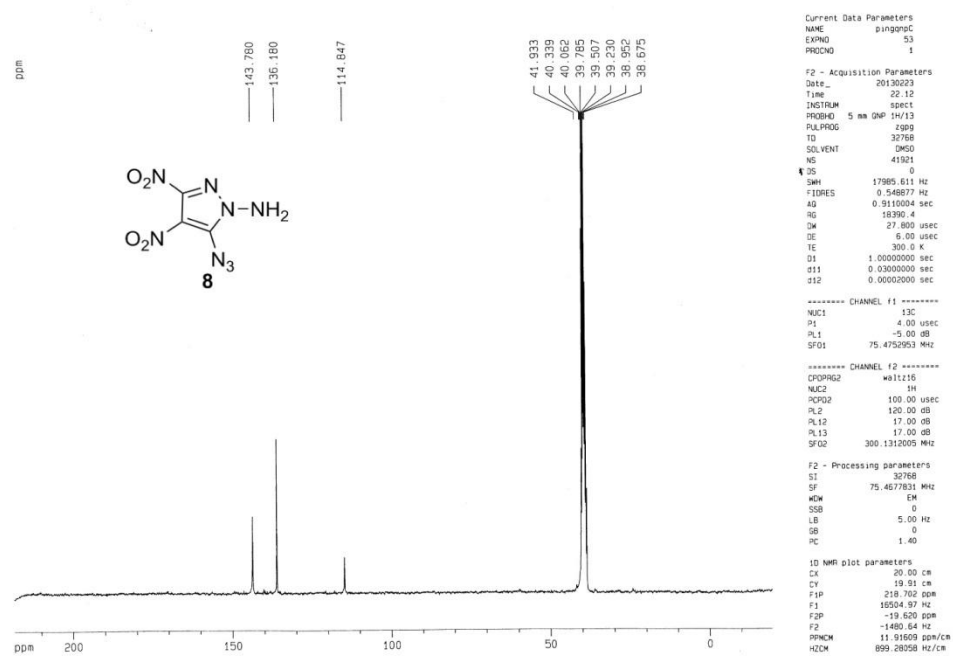


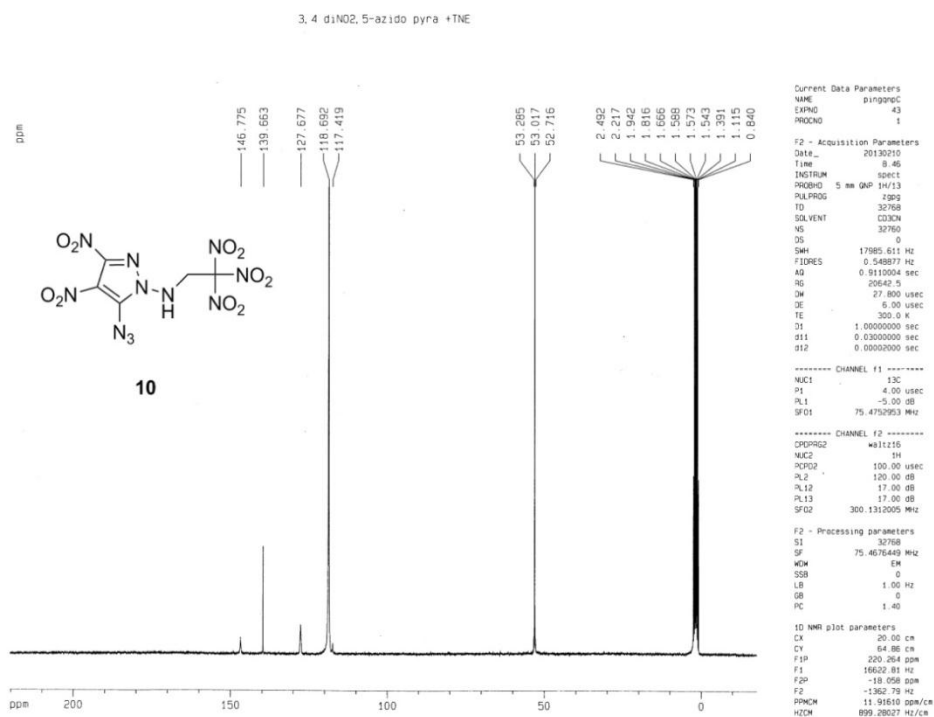
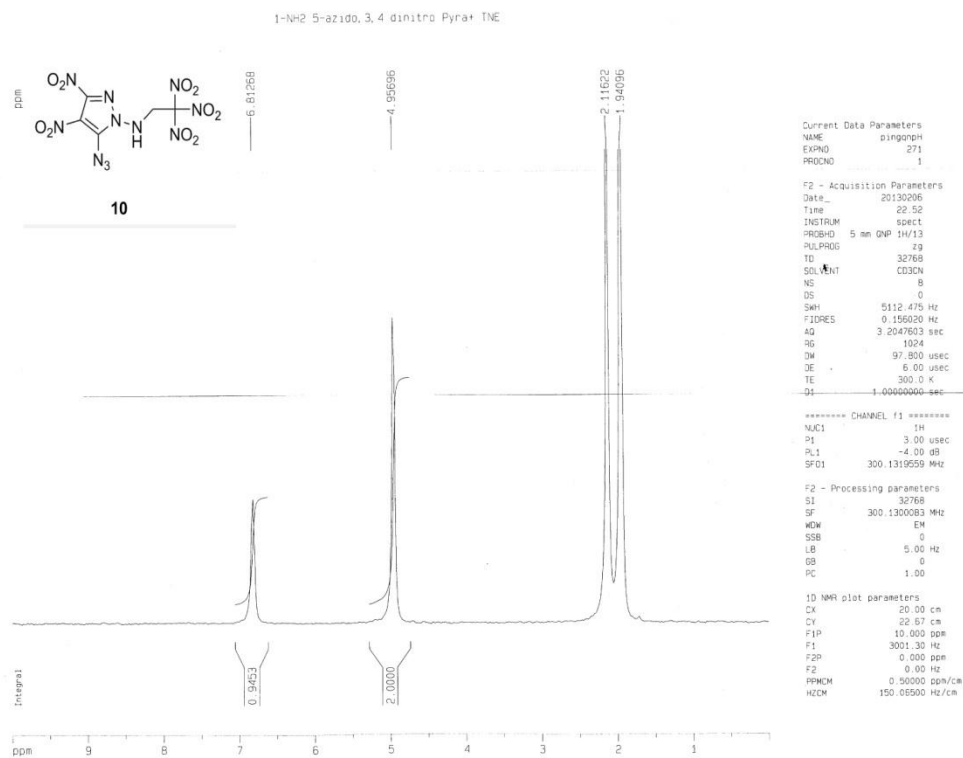
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Size: 0.8000 mg
Method: Ramp
Comment: diaminobistetrazole

DSC

File: 004 crystals 3,4dinitro 5-azido p...
Operator: ping
Run Date: 31-Jan-2013 16:30
Instrument: DSC Q10 V9.9 Build 303



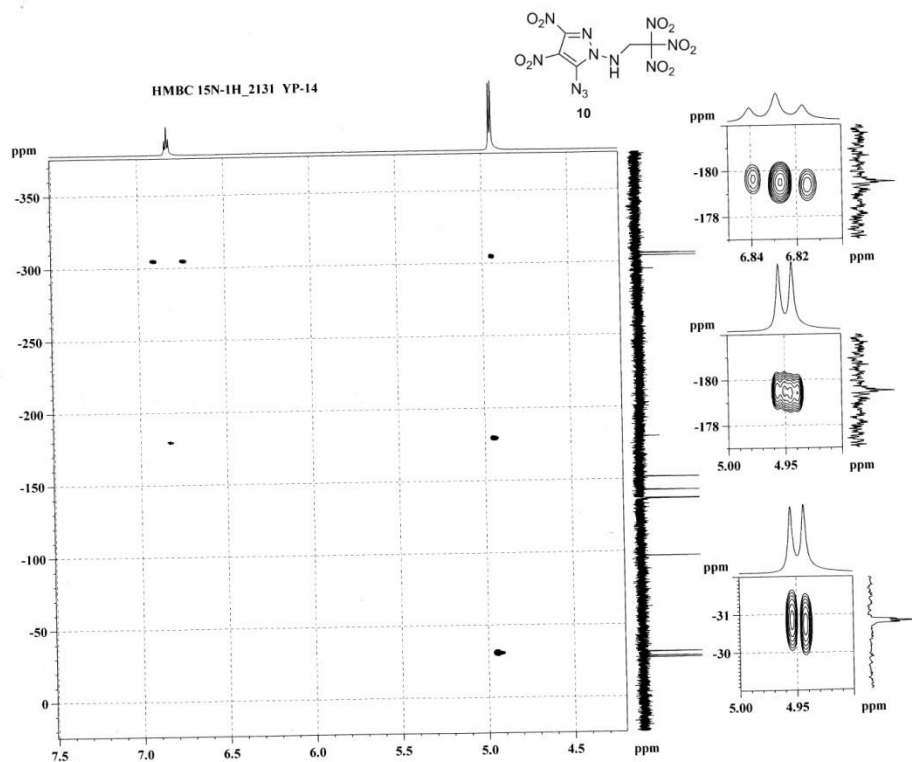
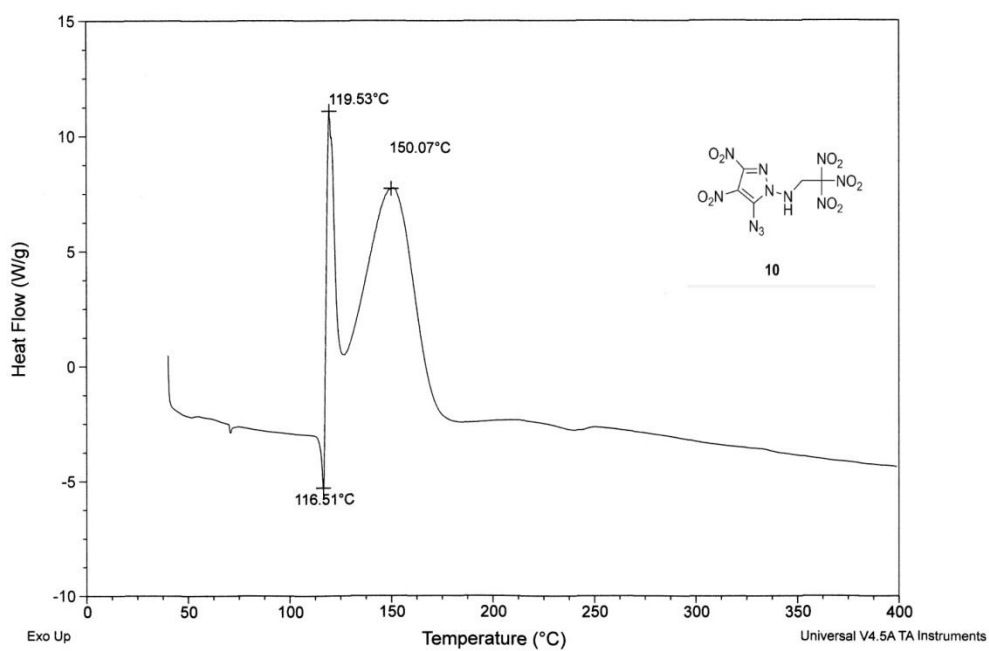


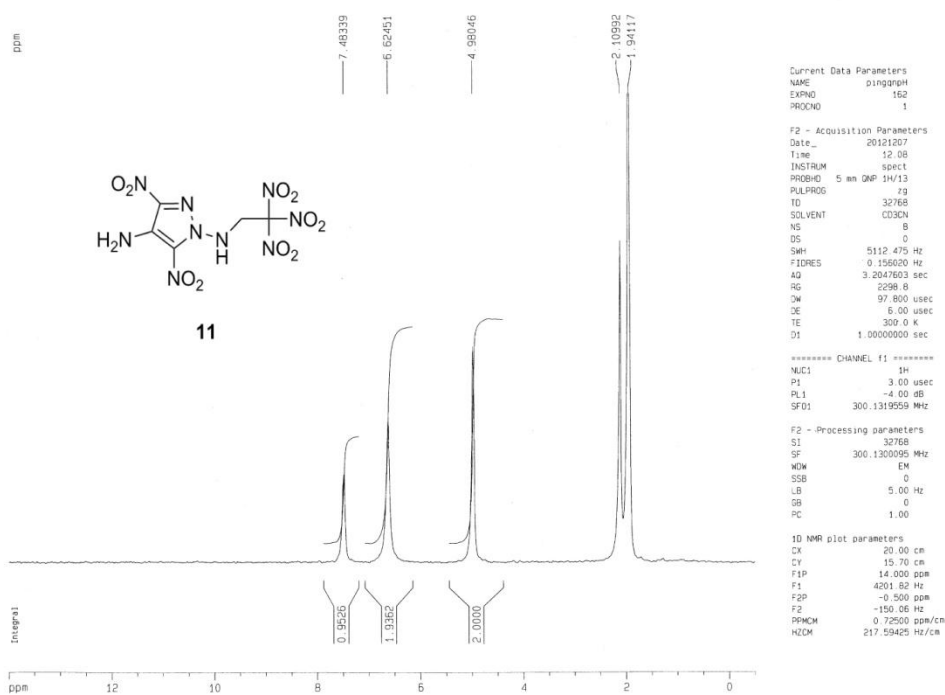
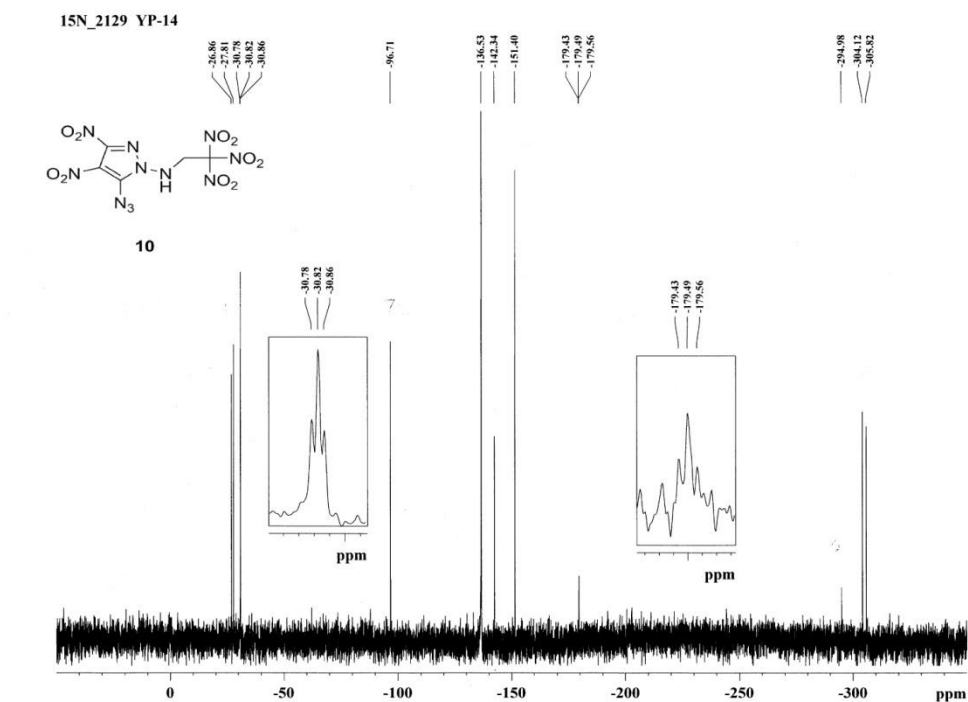


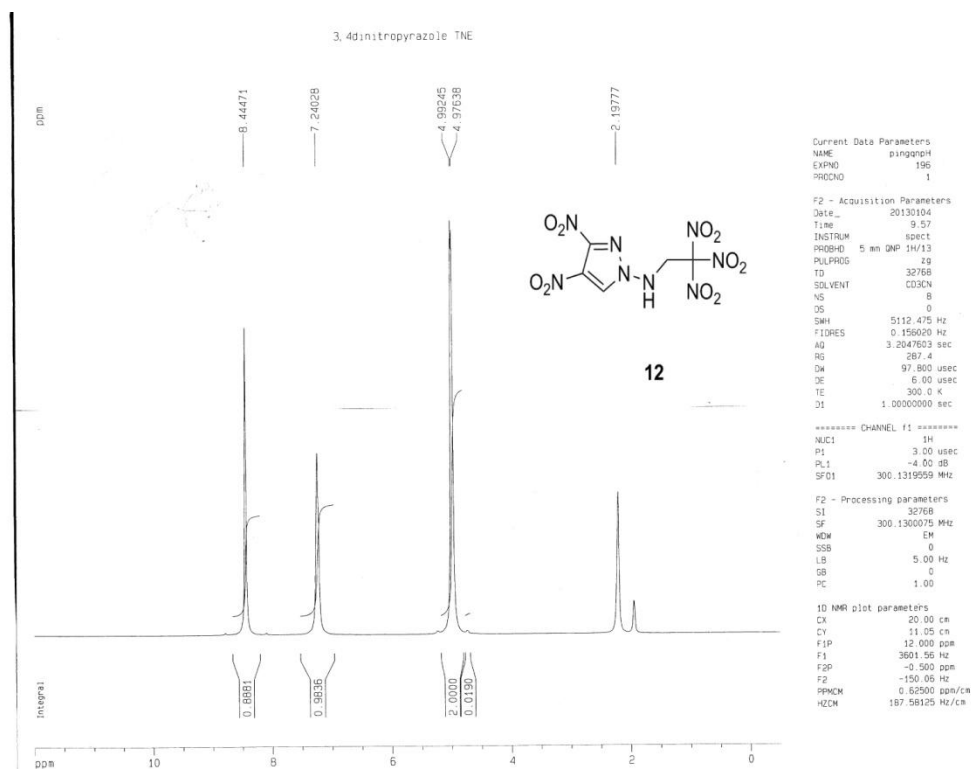
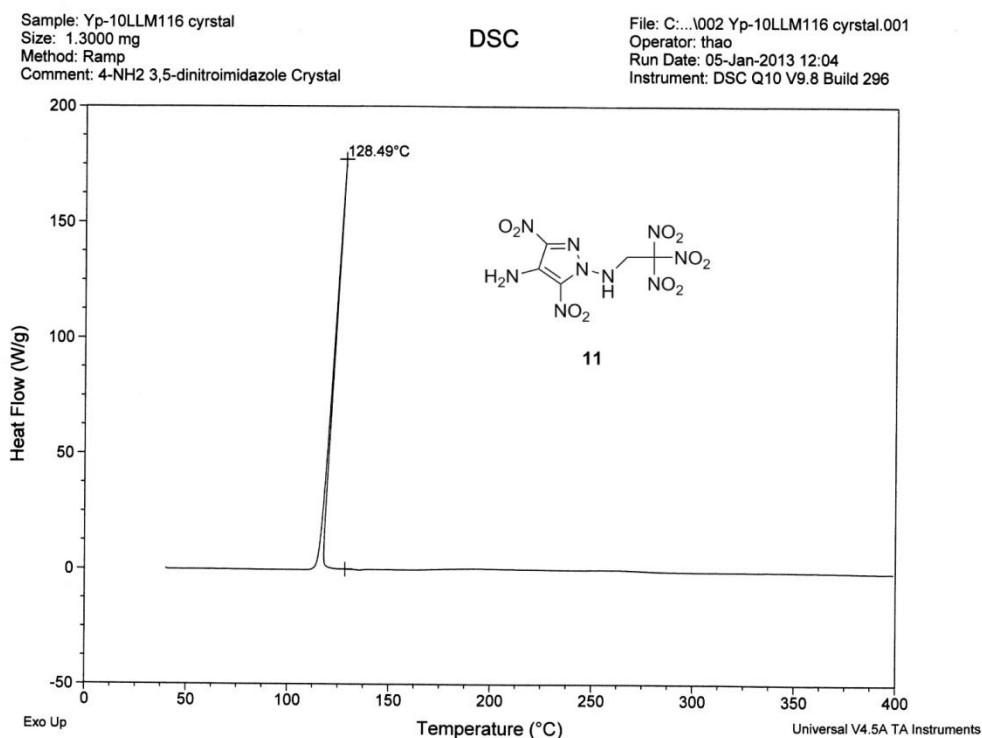
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Size: 0.6000 mg
Method: Ramp
Comment: 06 1-NH2 3,4dinitro 5-azido pyrazoleTNE

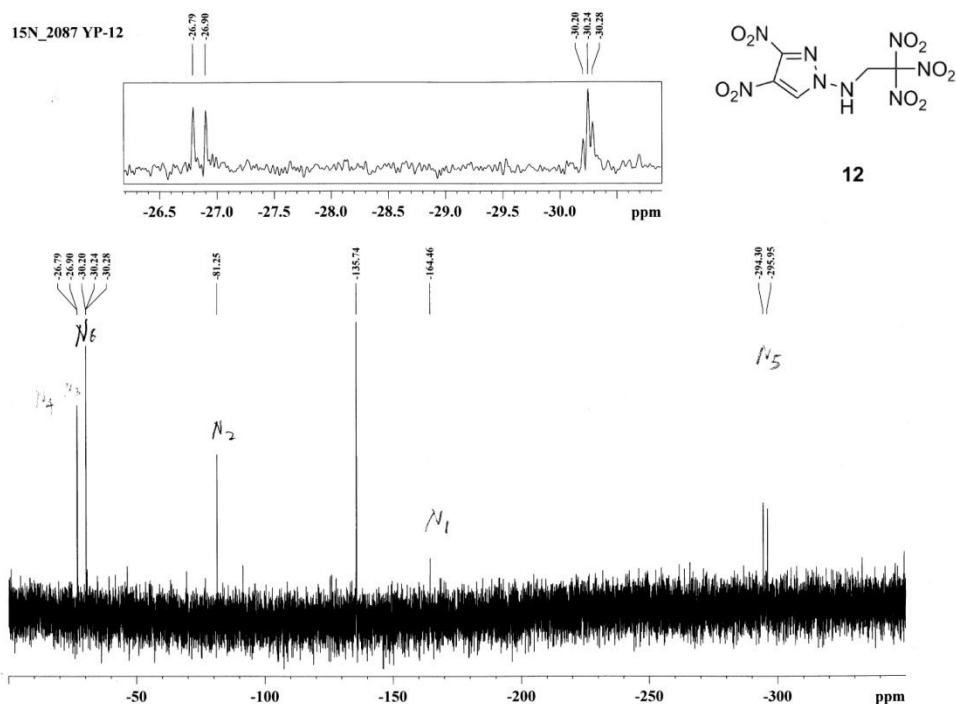
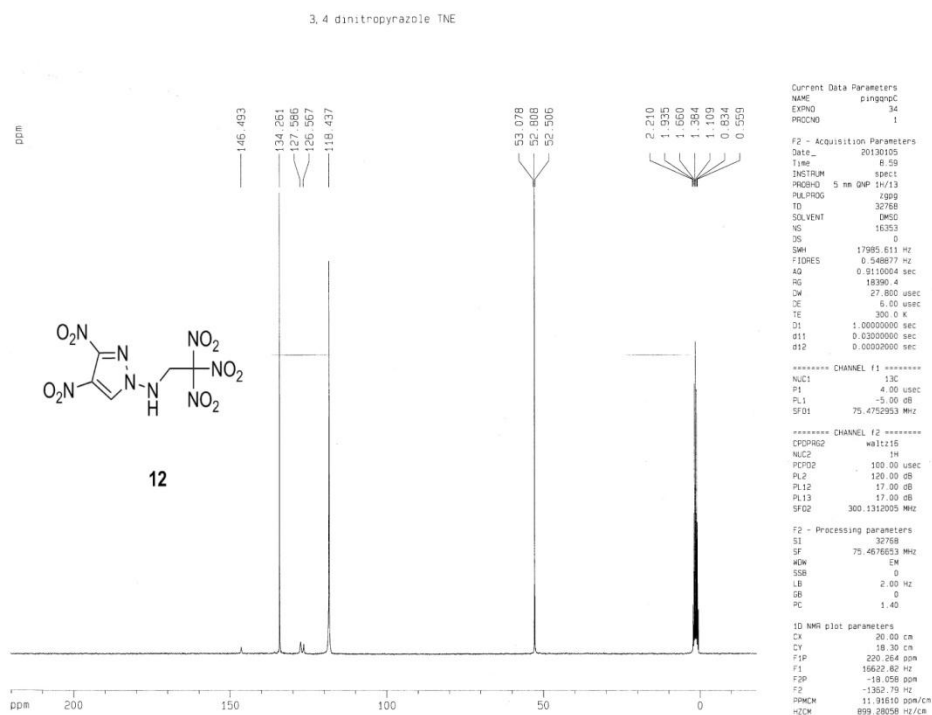
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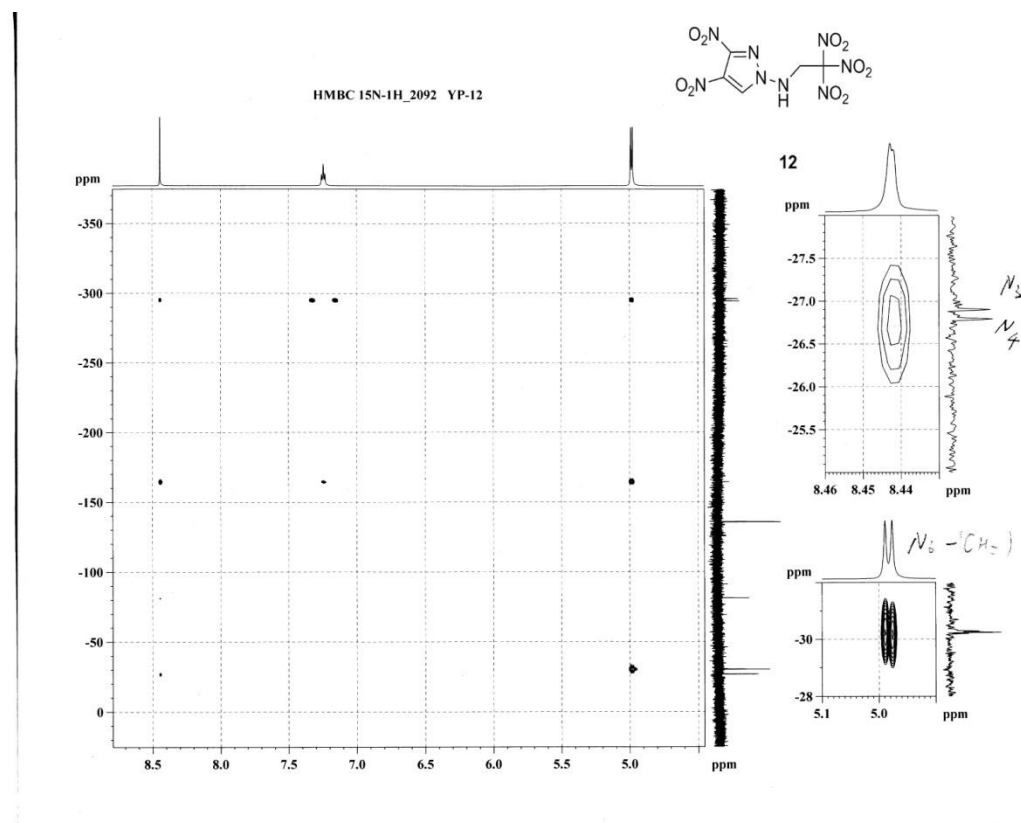
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Operator: ping
Run Date: 07-Feb-2013 15:01
Instrument: DSC Q10 V9.9 Build 303







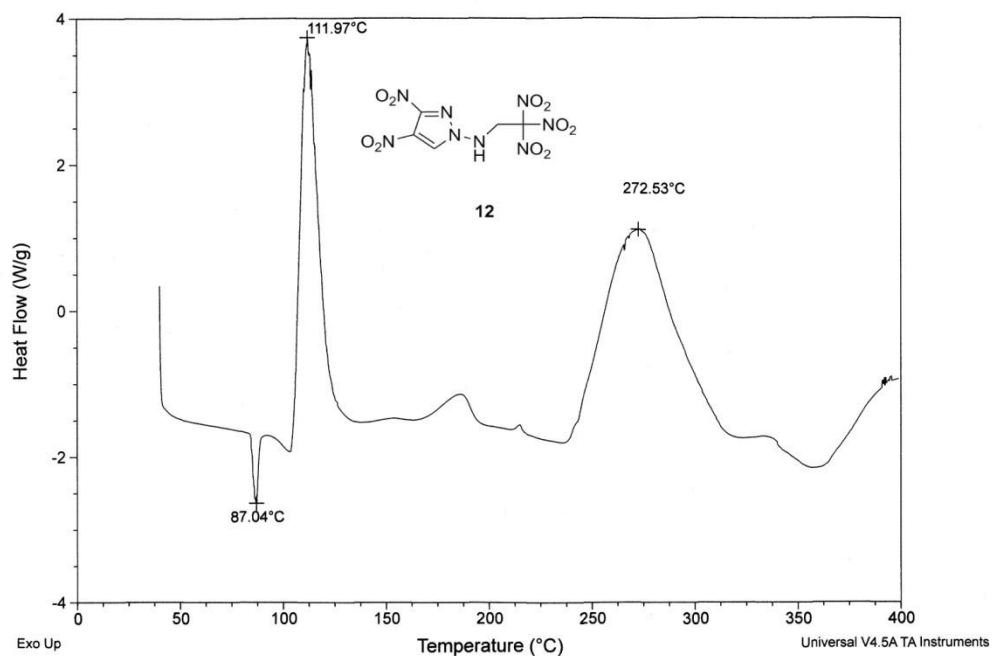


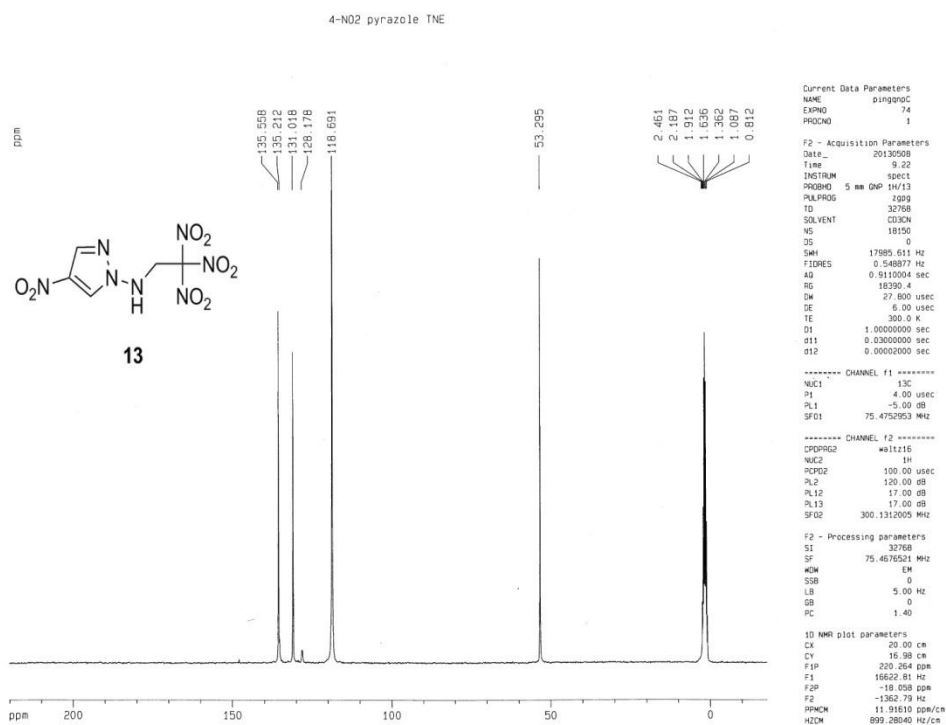
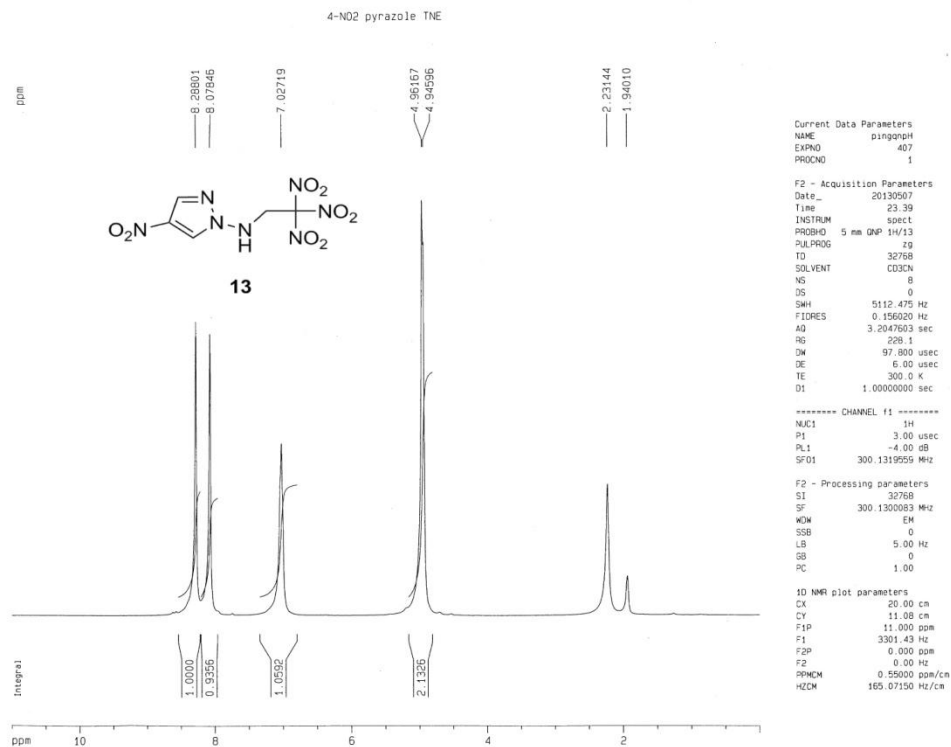


Sample: 1-NH2 , 3,4-diNO2 pyrazole TNE
Size: 0.7000 mg
Method: Ramp

DSC

File: 006 TNE 1-NH2 , 3,4-diNO2 pyrazole TN...
Operator: deep
Run Date: 19-Feb-2013 17:02
Instrument: DSC Q10 V9.9 Build 303

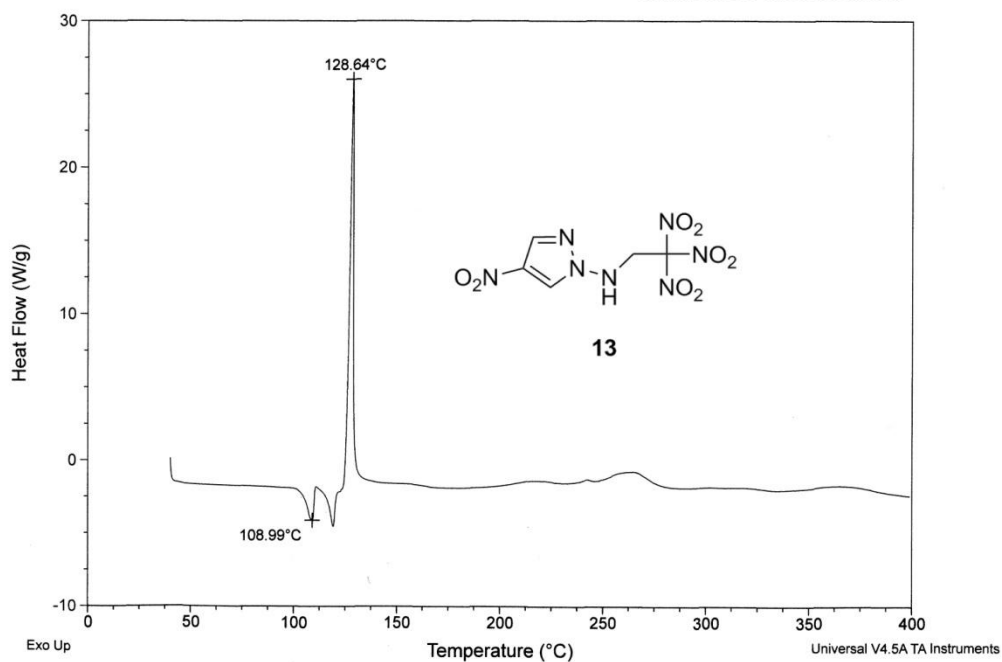




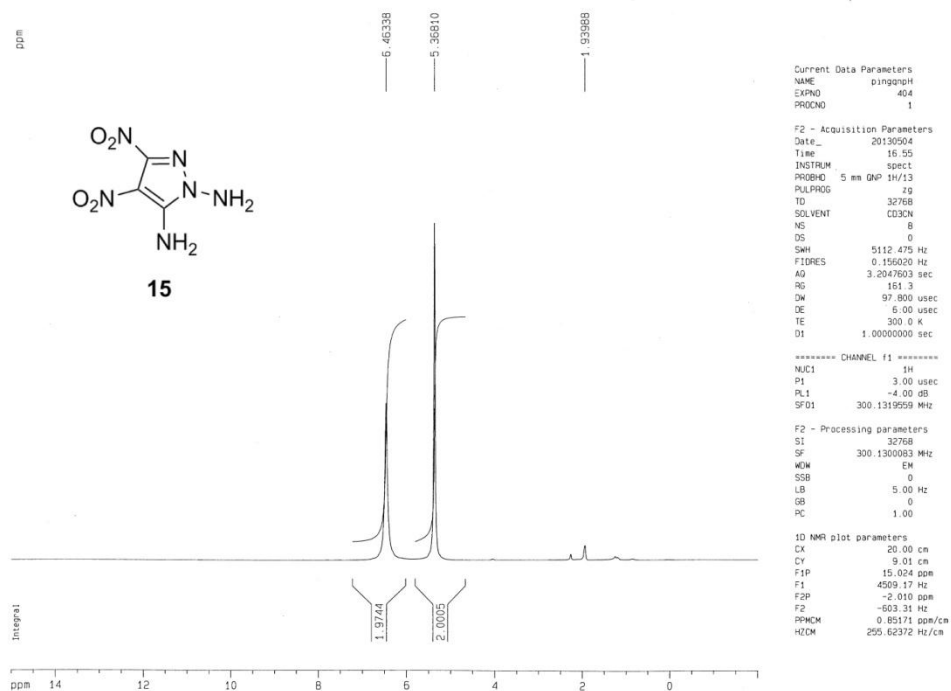
Sample: 015 4 iNO2 pyrazole TNE.001
Size: 1.0000 mg
Method: Ramp

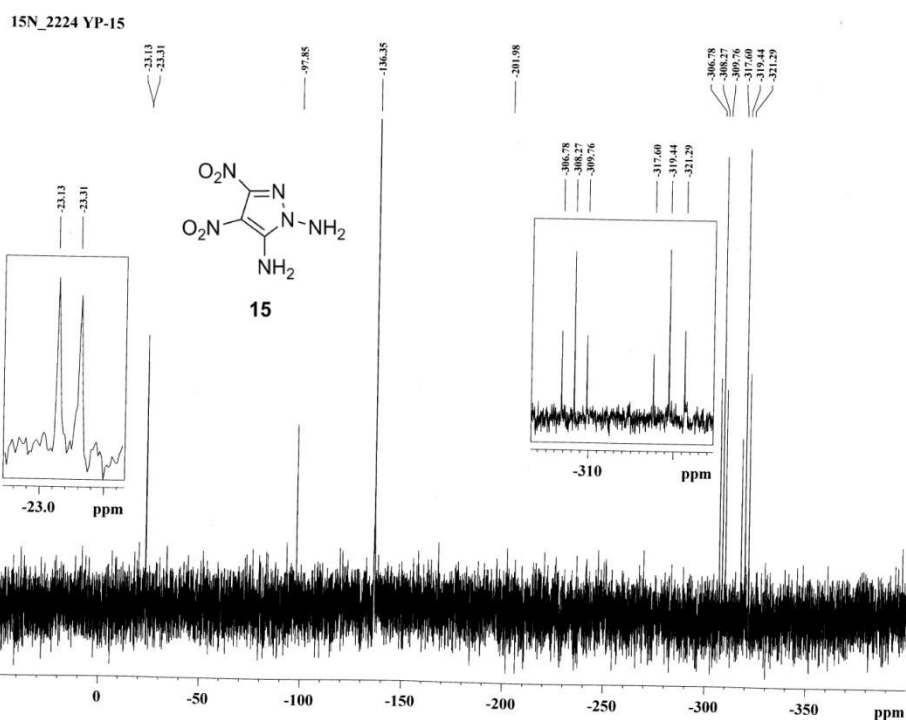
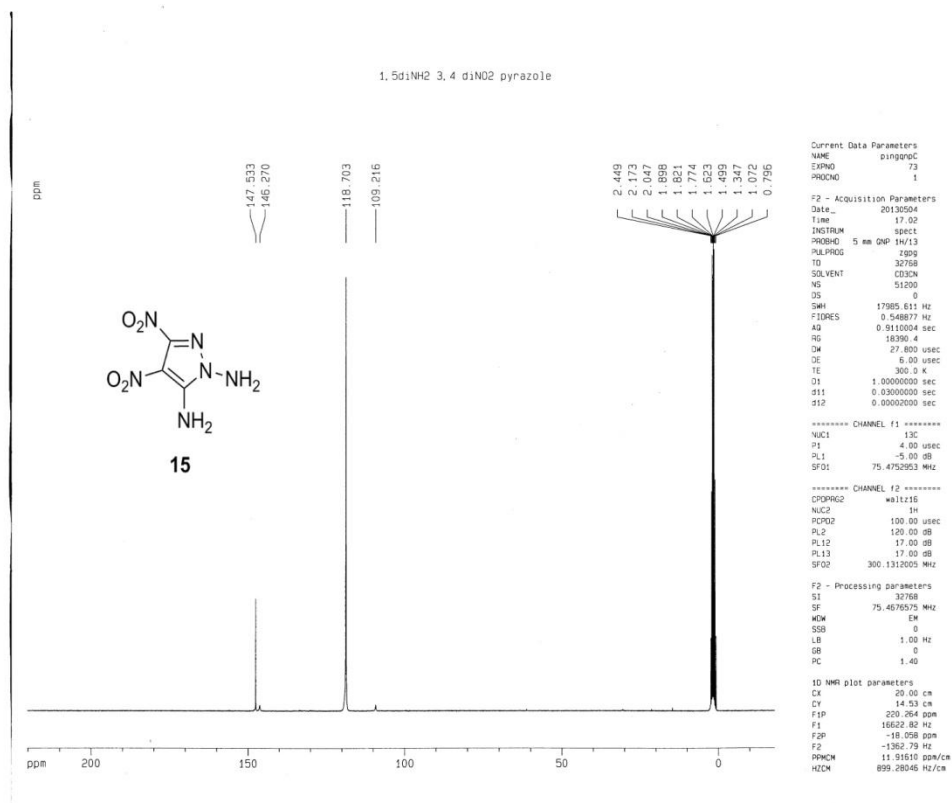
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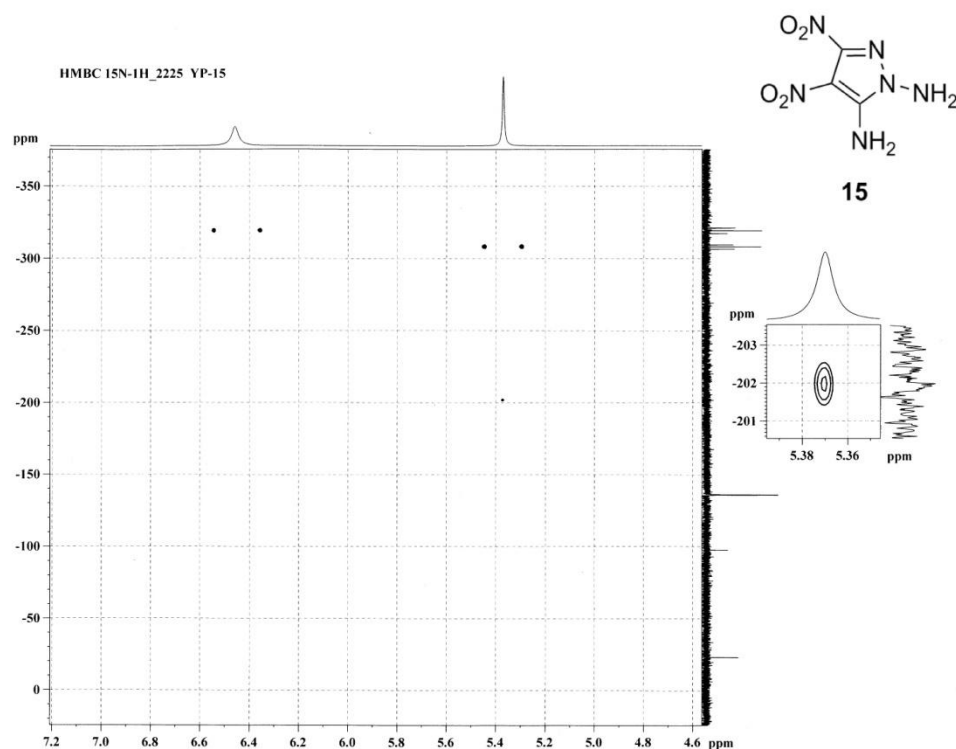
File: C:\015 4 iNO2 pyrazole TNE.001
Operator: ping
Run Date: 30-Apr-2013 15:20
Instrument: DSC Q10 V9.9 Build 303



1,5-d₃NH₂ 3,4-d₂NO₂ pyrazole



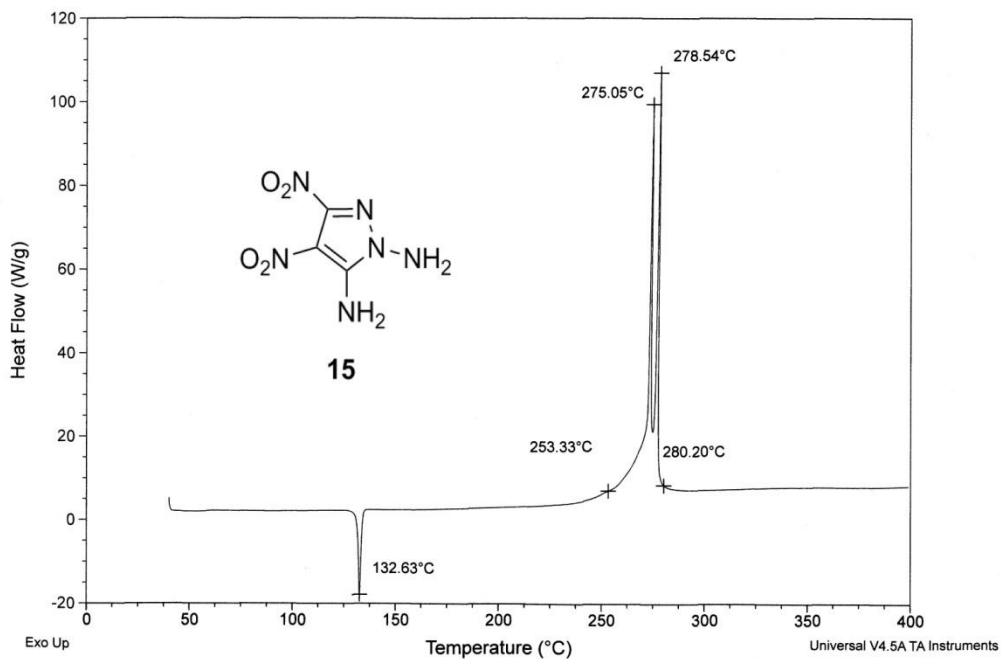


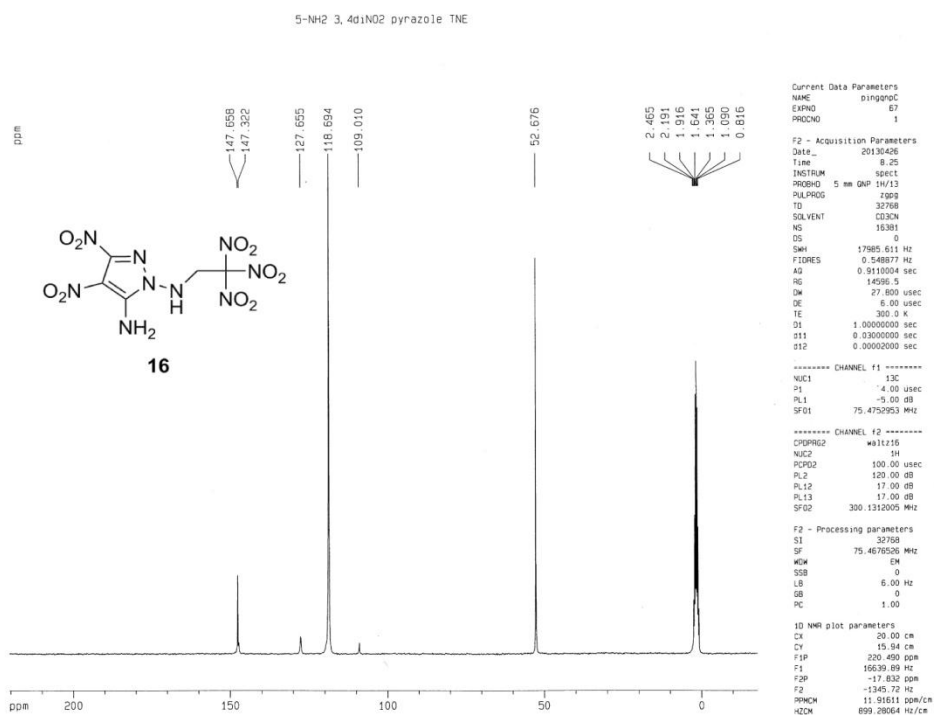
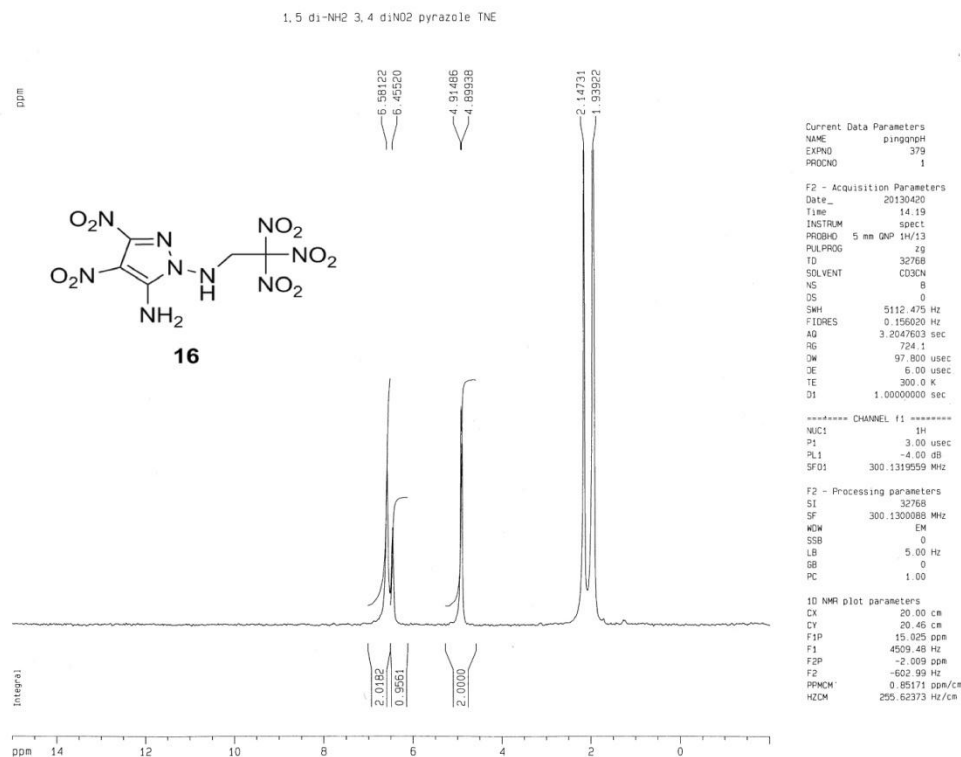


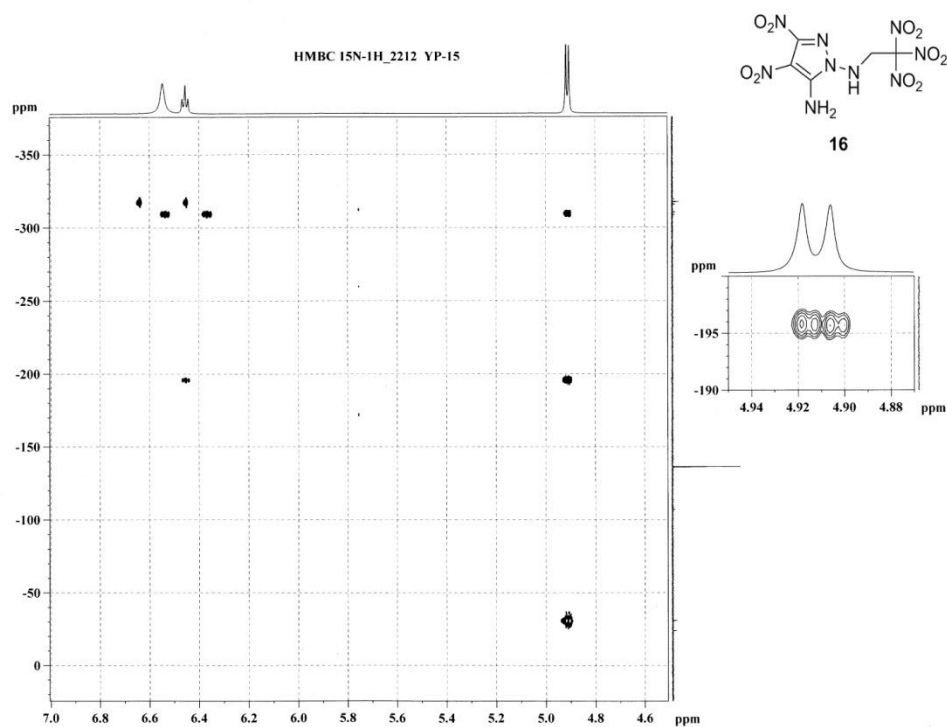
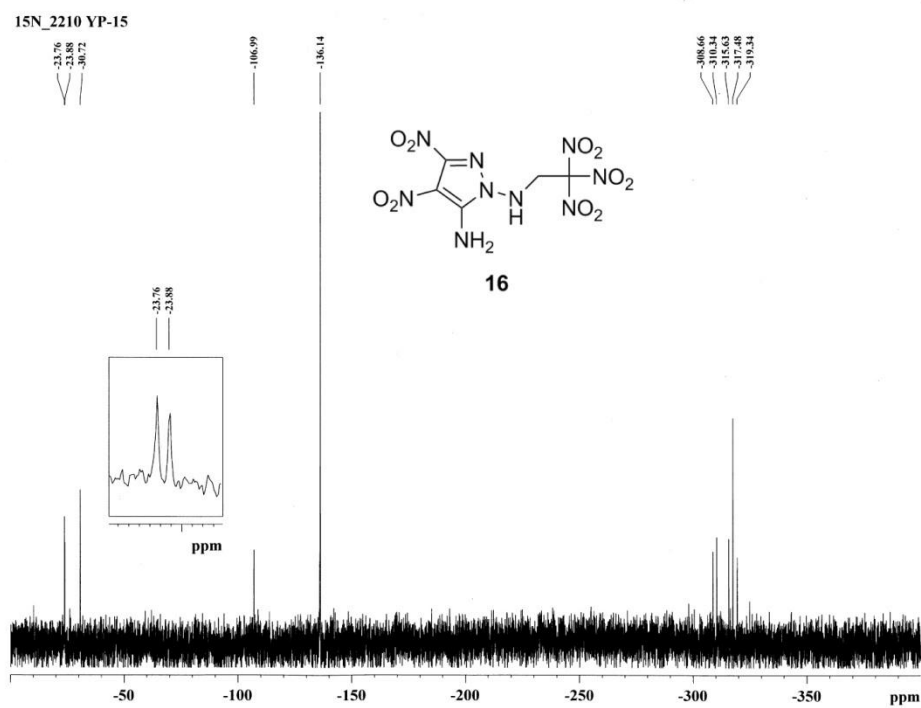
Sample: 015 EA 1,5 diNH2 3,4 diNO2 pyra
Size: 0.6000 mg
Method: Ramp

DSC

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Operator: ping
Run Date: 04-May-2013 10:45
Instrument: DSC Q10 V9.9 Build 303



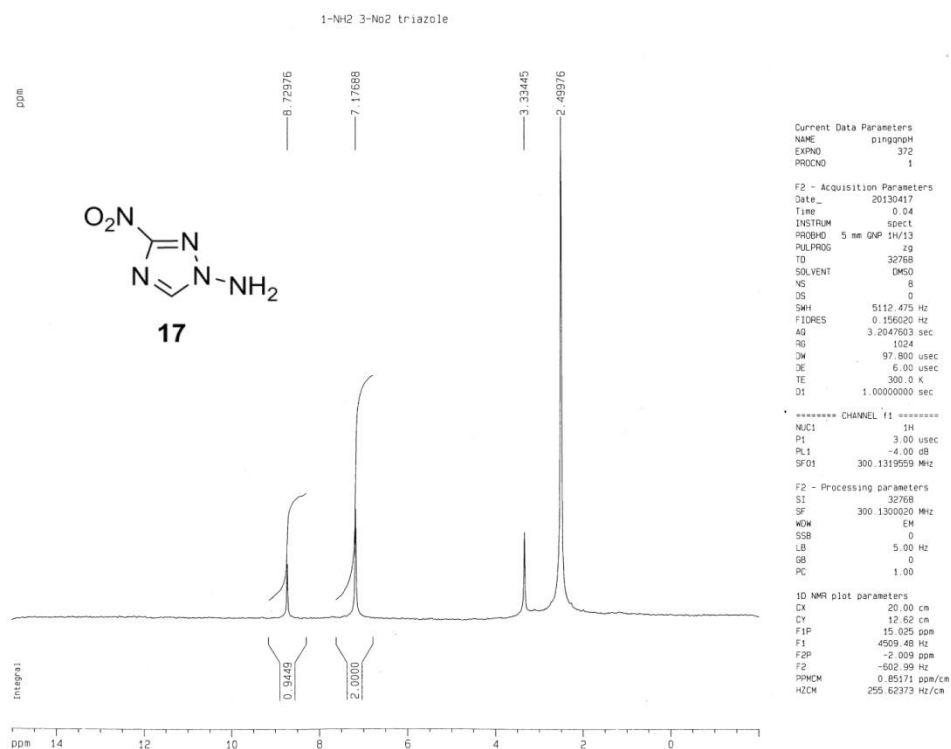
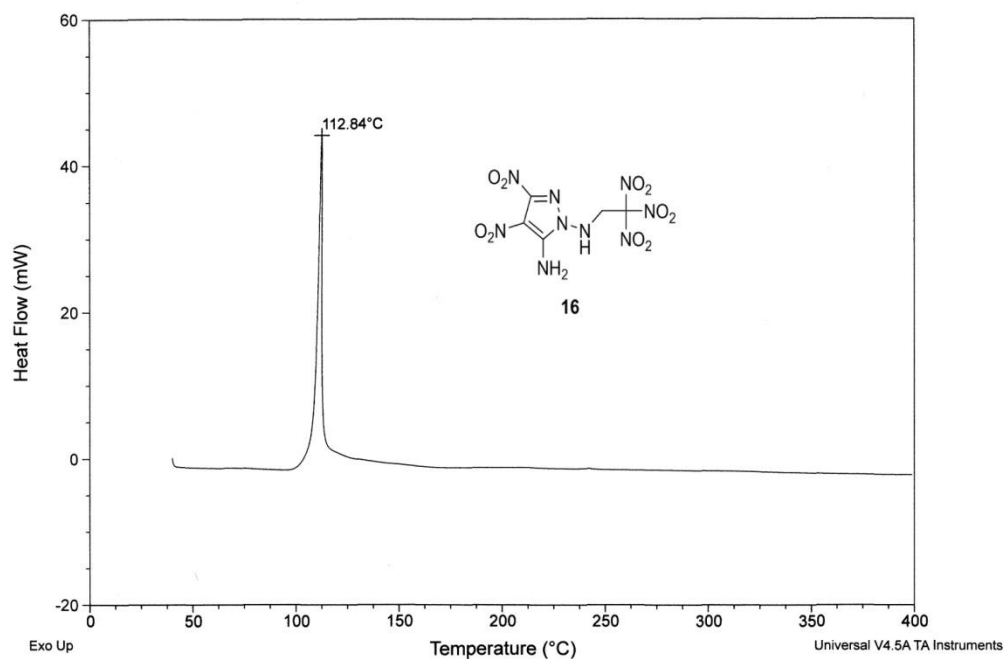


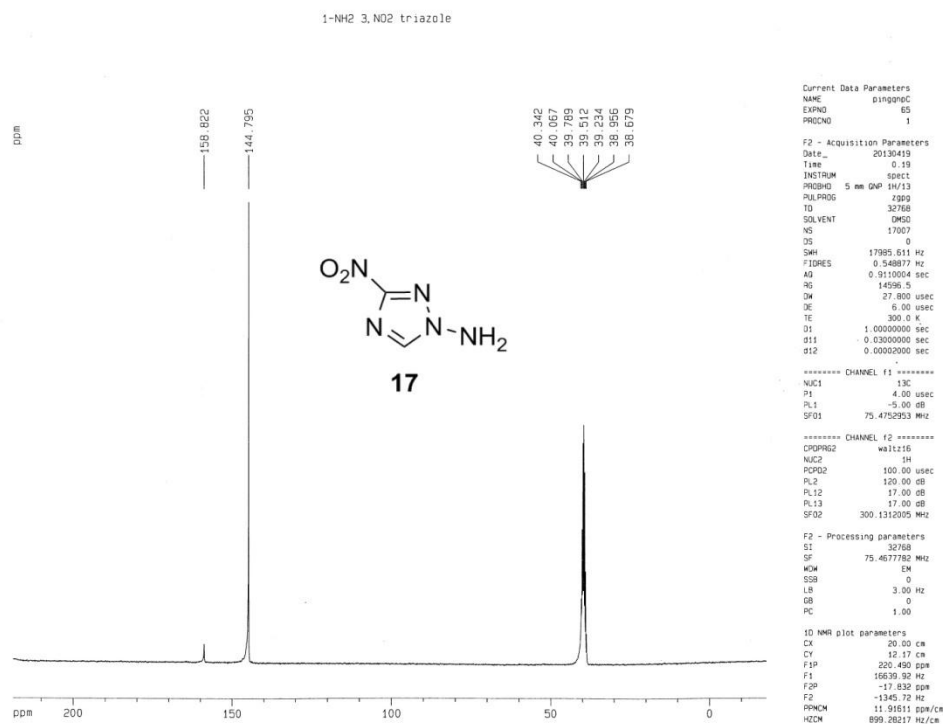


Sample: 1,5 diNH2 pyrazole TNE
Size: 0.0000 mg
Method: Ramp

DSC

File: C:\...011 1,5 diNH2 pyrazole TNE.001
Operator: ping
Run Date: 20-Apr-2013 13:10
Instrument: DSC Q10 V9.9 Build 303

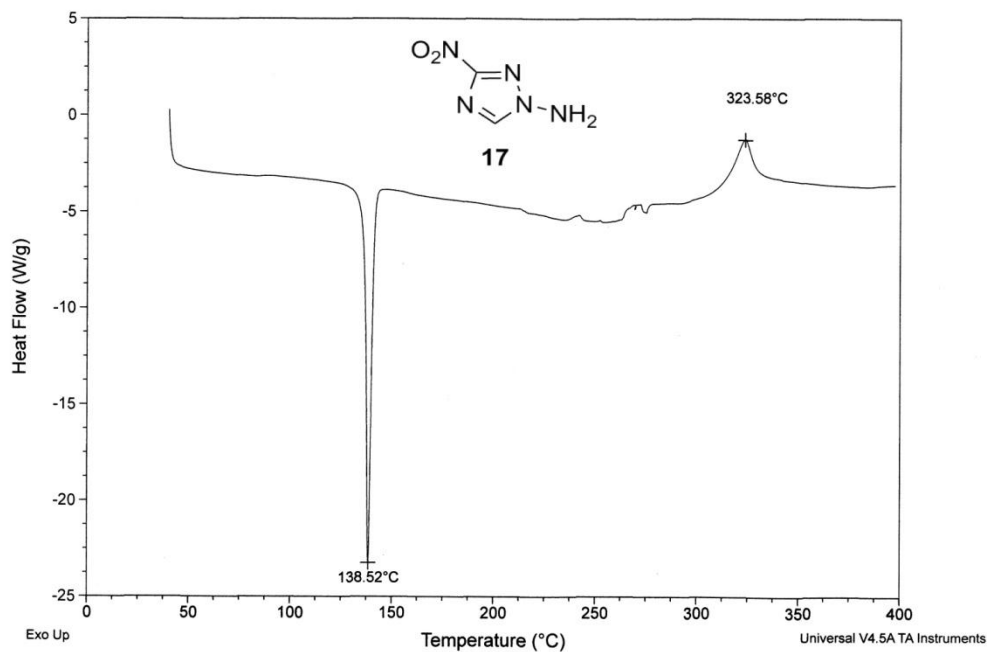


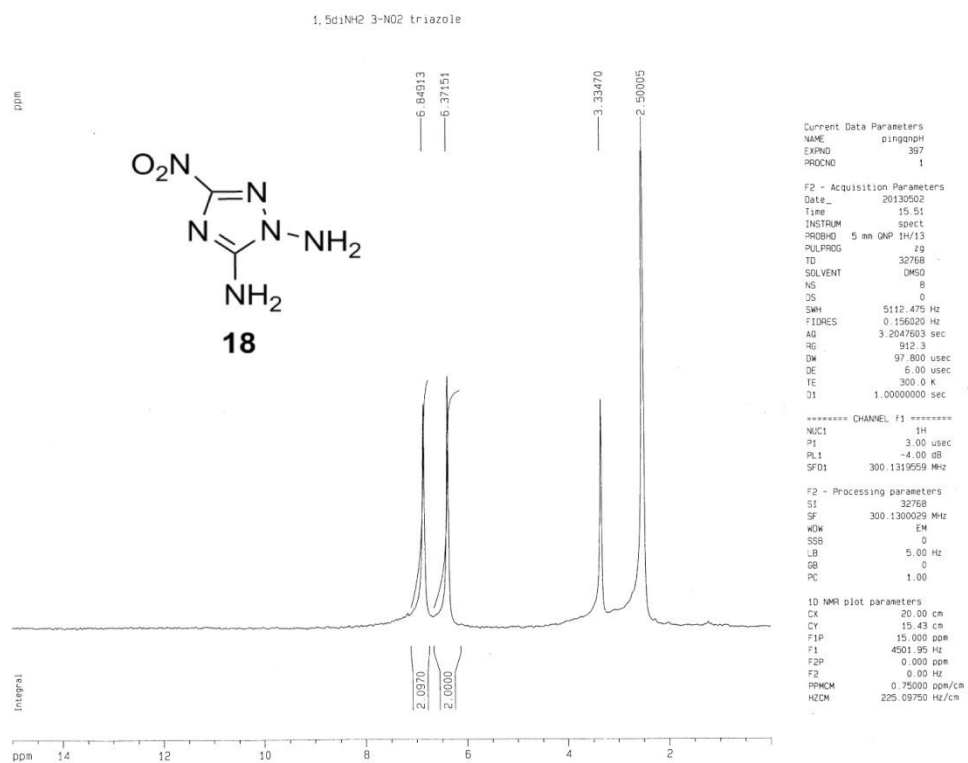


Sample: 001 3-NO2 1NH2 tria
Size: 1.1000 mg
Method: Ramp

DSC

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Operator: ping
Run Date: 17-Apr-2013 11:02
Instrument: DSC Q10 V9.9 Build 303

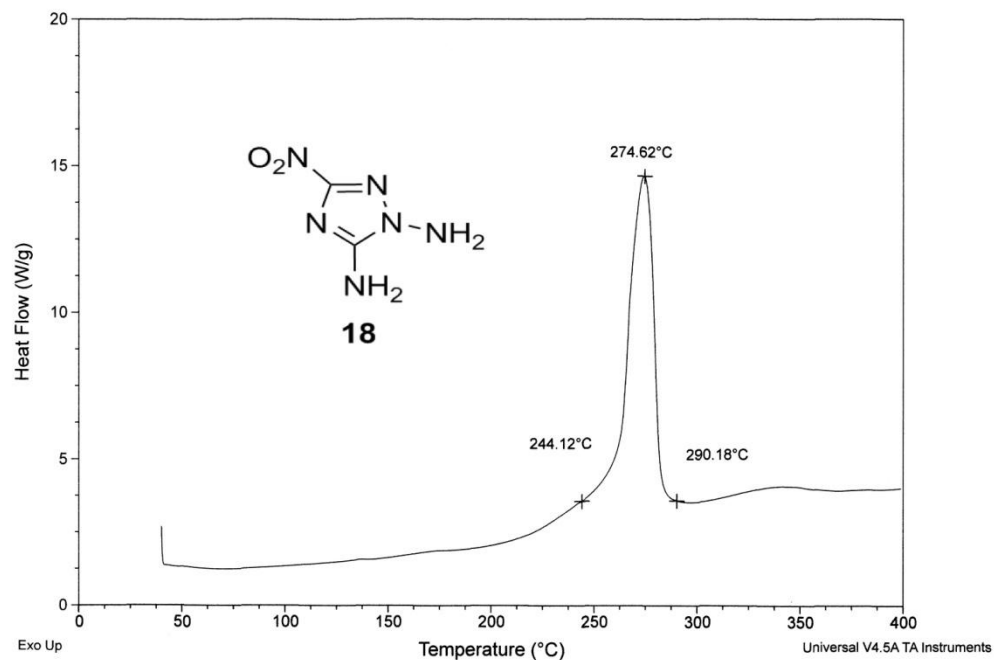


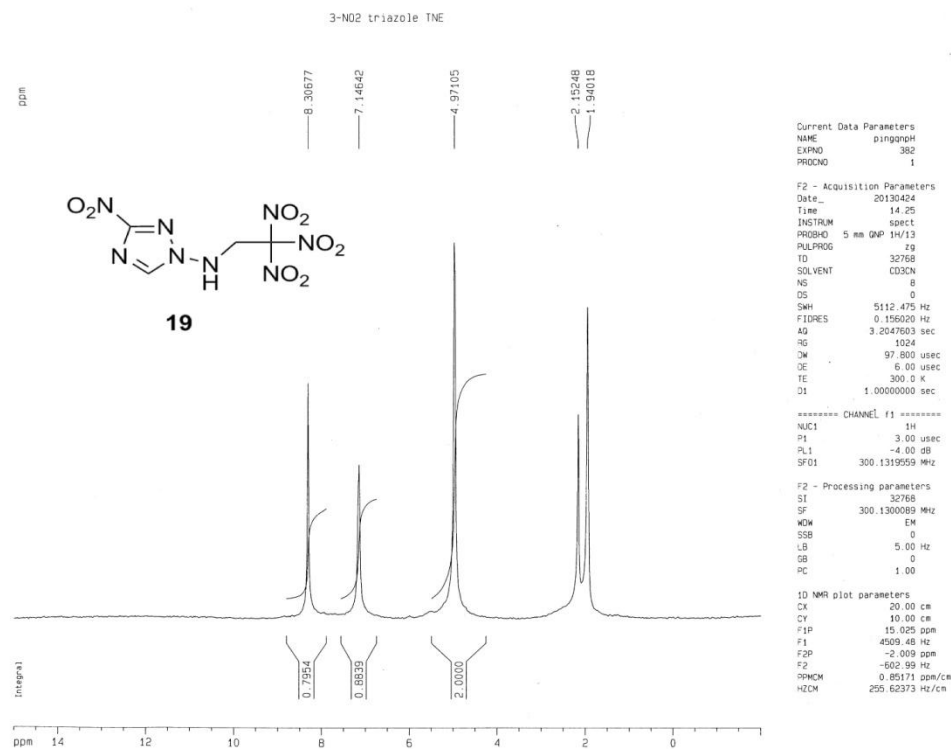
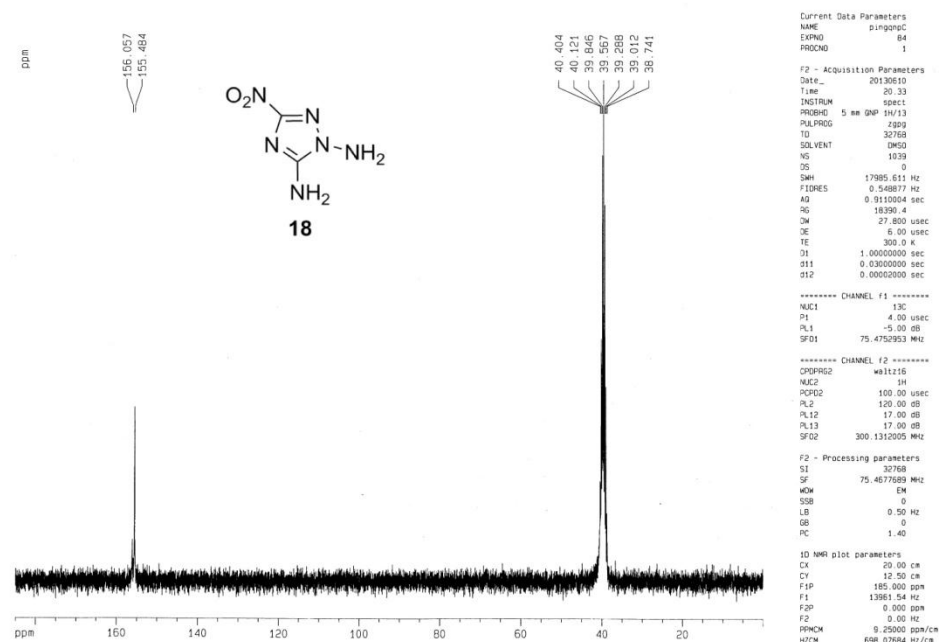


Sample: 003 3-NO₂ 1,5 diNH₂ triazole
Size: 1.2000 mg
Method: Ramp

DSC

File: C:\...003 3-NO₂ 1,5 diNH₂ triazole.001
Operator: ping
Run Date: 02-May-2013 20:42
Instrument: DSC Q10 V9.9 Build 303





Sample: 002 3-NO₂ triazole TNE
Size: 1.0000 mg
Method: Ramp

DSC

File: C:\...002 3-NO₂ triazole TNE.001
Operator: ping
Run Date: 25-Apr-2013 10:53
Instrument: DSC Q10 V9.9 Build 303

