

Electronic Supplementary Information

***N*-Trinitroethylamino Functionalization of Nitroimidazoles: A New Strategy for High Performance Energetic Materials**

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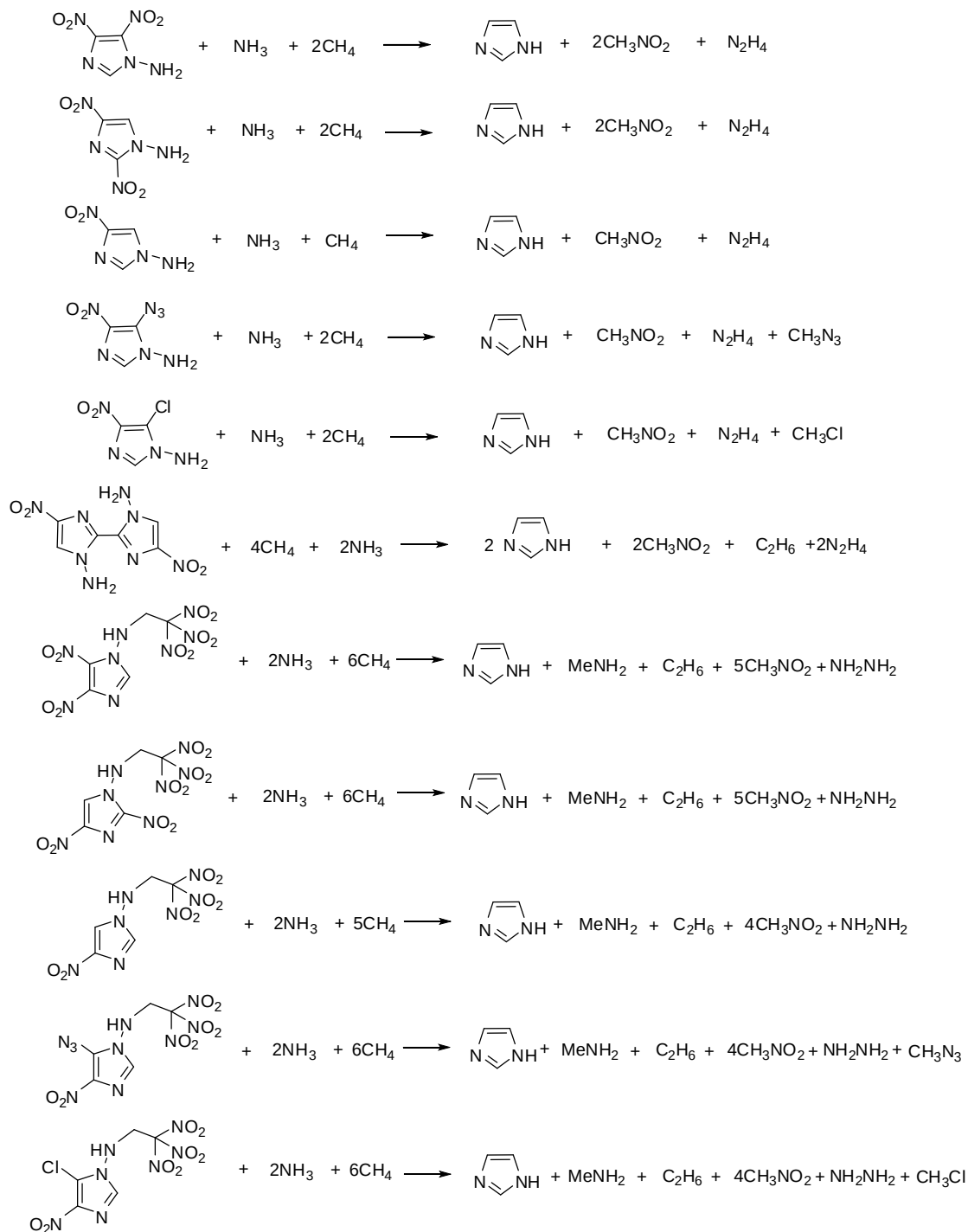
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Computational Data

S-1 Scheme 1s. Isodesmic reactions for the derivatives of *N*-aminonitroimidazoles and *N*-trinitroethylaminonitroimidazoles.

S-2 Table 1s. Calculated (MP2/6-311++G** // B3LYP/6-31+G**) total energy (E0), zero-point energy (ZPE), values of thermal correction (HT), and heats of formation (HoF) of derivatives of *N*-aminonitroimidazoles and *N*-trinitroethylaminonitroimidazoles.

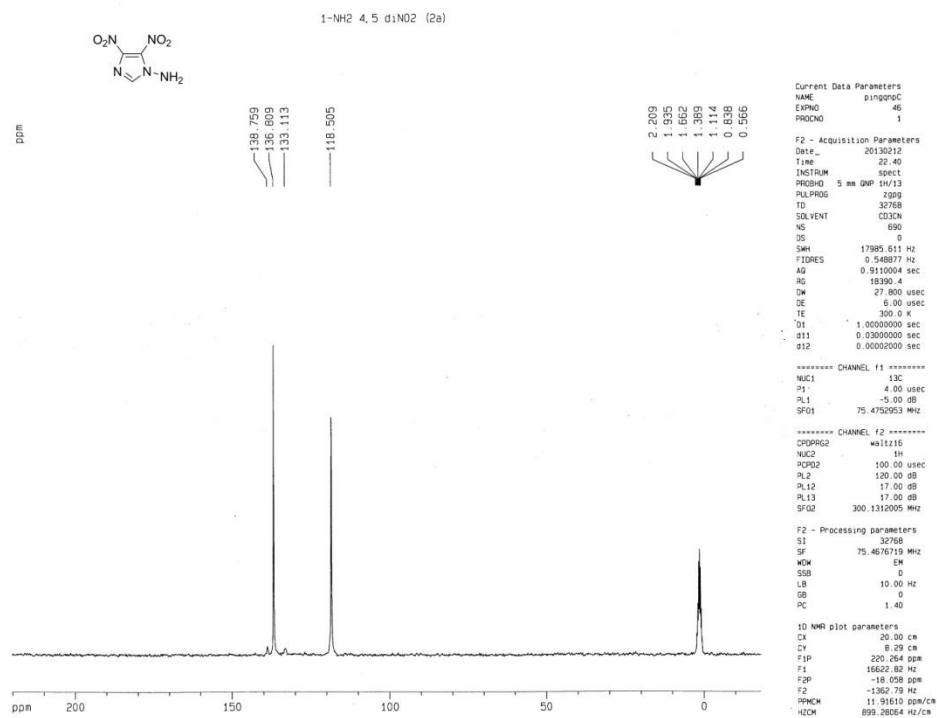
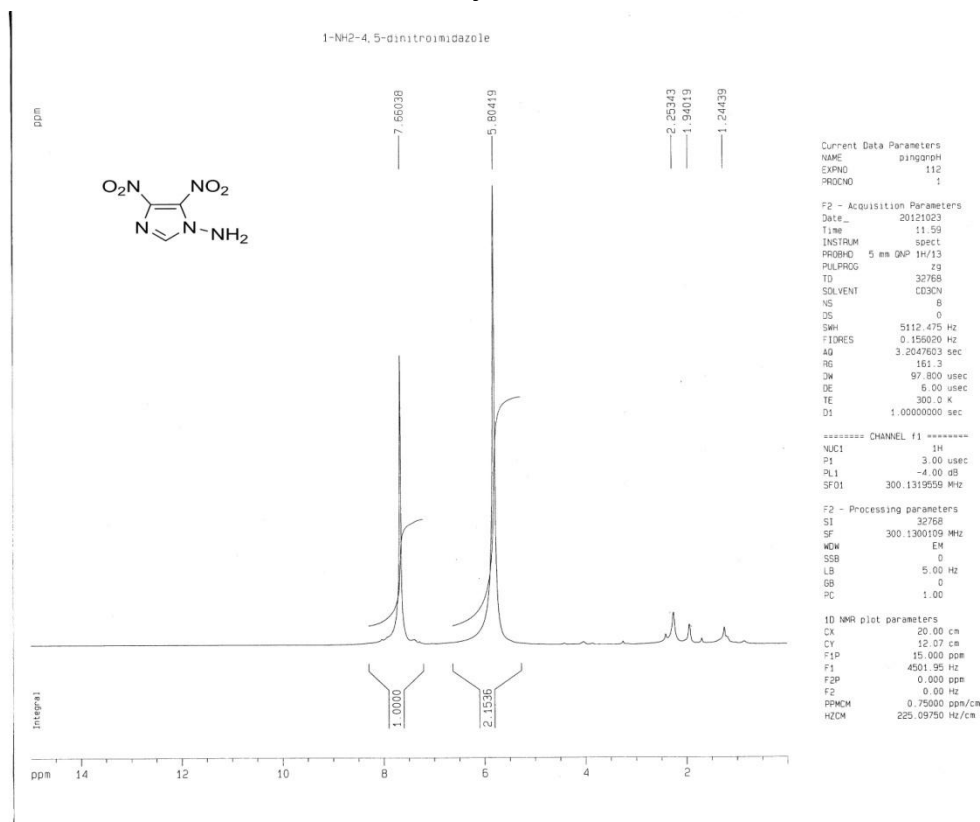


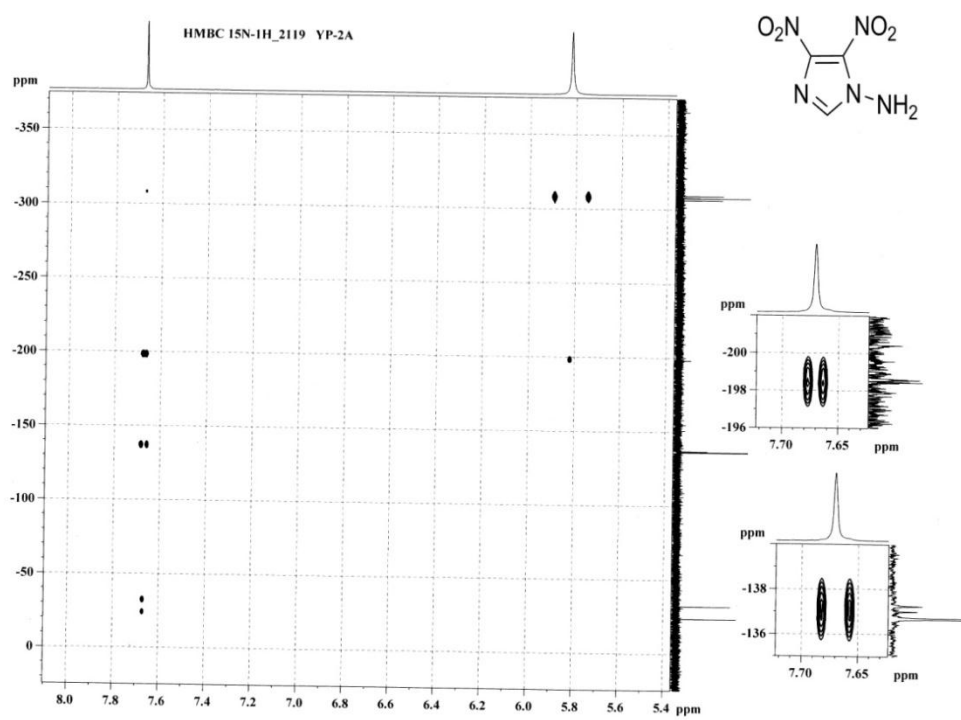
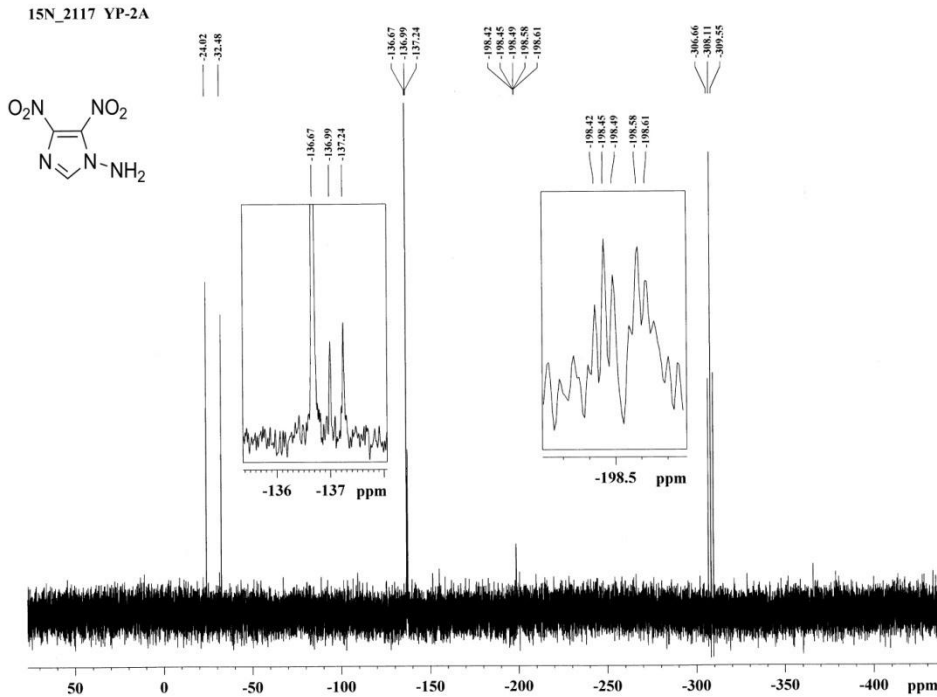
S-1 Scheme 1s. Isodesmic reactions for the derivatives of *N*-aminonitroimidazoles and *N*-trinitroethylaminonitroimidazoles.

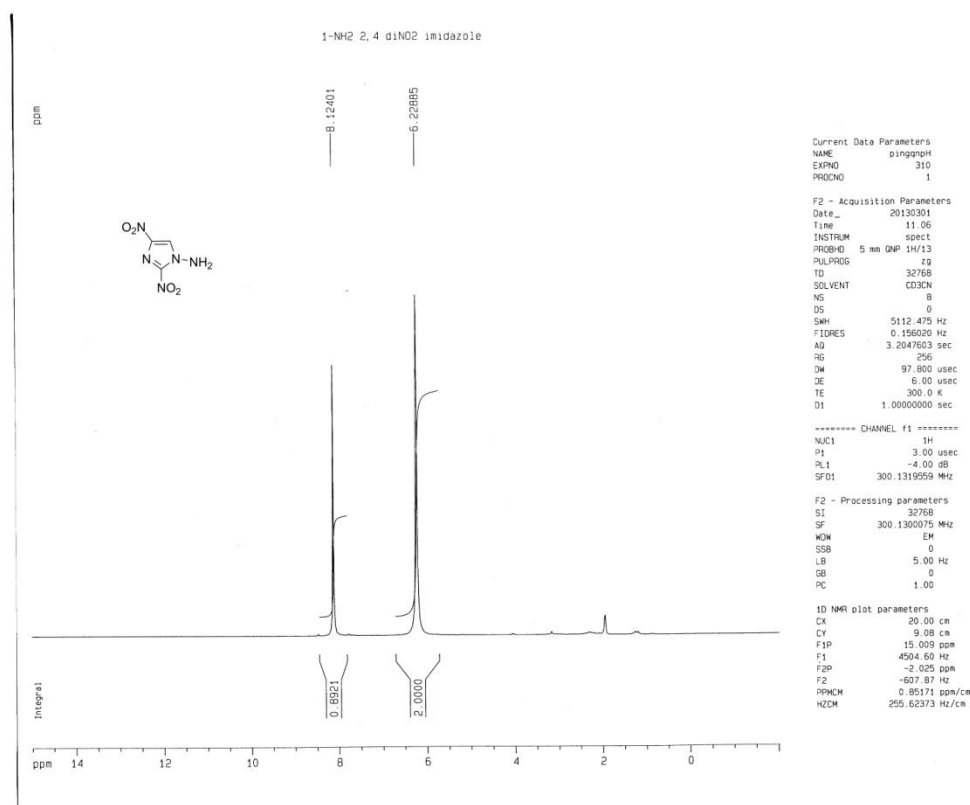
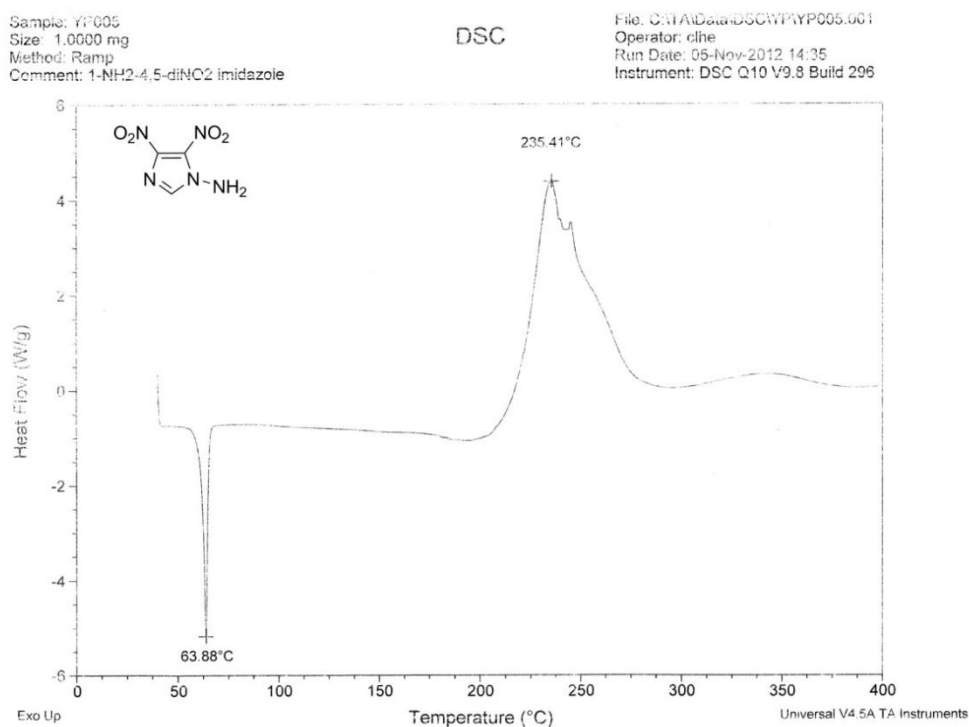
S-2 Table 1s. Calculated (MP2/6-311++G** // B3LYP/6-31+G**) total energy (E₀), zero-point energy (ZPE), values of thermal correction (HT), and heats of formation (HoF) of derivatives of *N*-aminonitroimidazoles and *N*-trinitroethylaminonitroimidazoles.

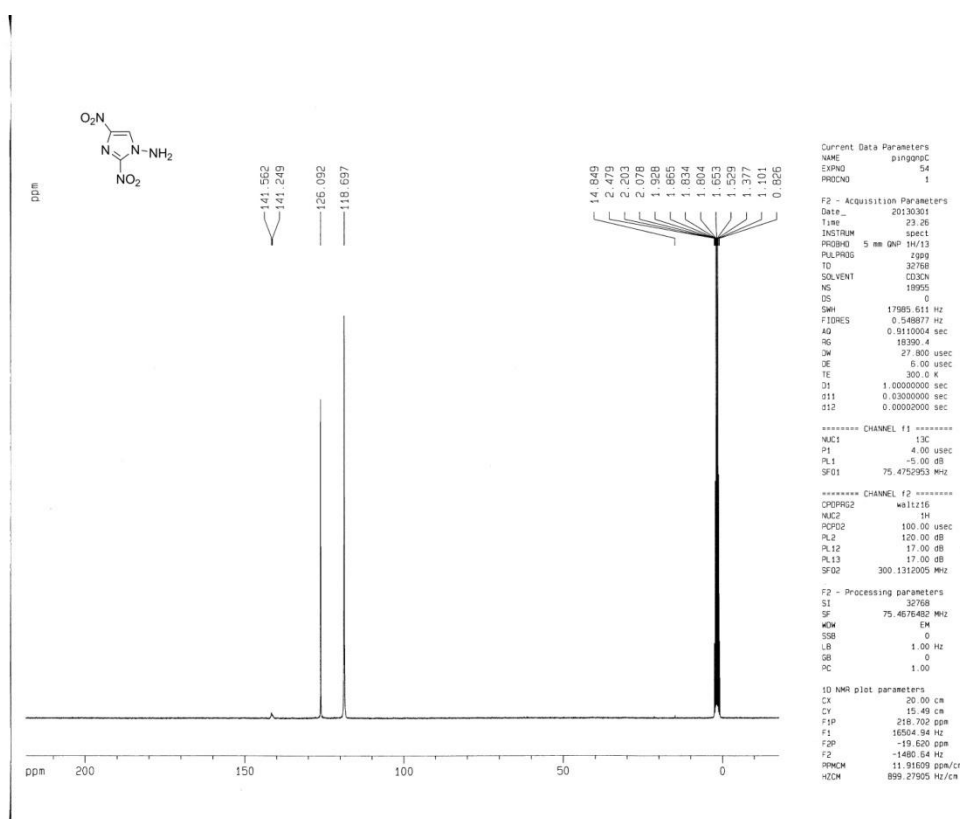
Compounds	E₀ [Hartree/Particle]	ZPE [Hartree/Particle]	H_T [Hartree/Particle]	HoF(gas) [kJ mol ⁻¹]
4a	-689.0210145	0.092826	0.103901	209.9
4b	-689.0243019	0.092659	0.103694	200.8
4c	-484.9316133	0.090549	0.098947	195.3
4d	-648.1700351	0.093554	0.104704	536.1
4g	-968.6946431	0.160924	0.177371	400.3
6a	-1379.6870028	0.155182	0.177582	190.4
6b	-1379.6915101	0.155144	0.176231	175.0
6c	-1175.601235	0.153288	0.171887	164.3
6d	-1338.8436338	0.156301	0.177622	494.6
6e	-1634.6527486	0.143672	0.163537	144.5

^1H , ^{13}C , ^{15}N NMR, ^{15}N - ^1H HMBC, and DSC for derivatives of
N-aminonitroimidazoles and *N*-trinitroethylaminonitroimidazoles.





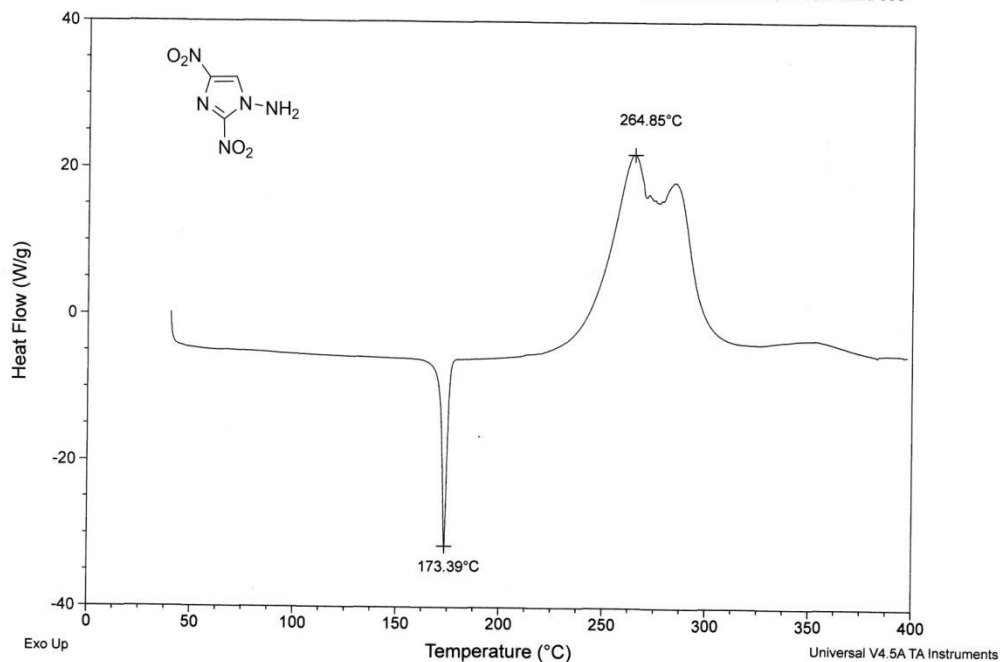


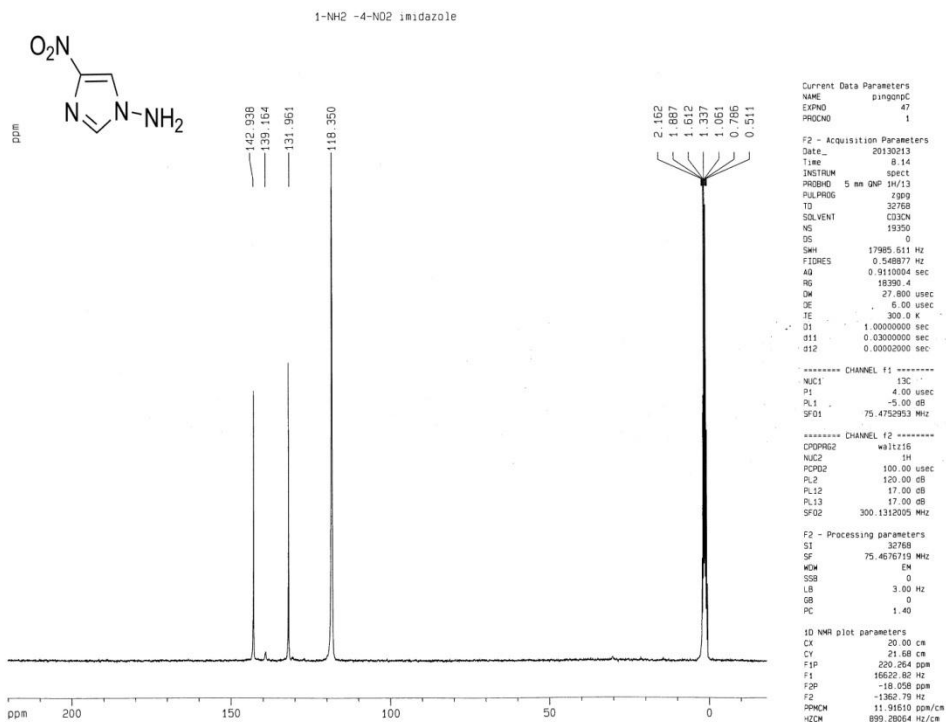
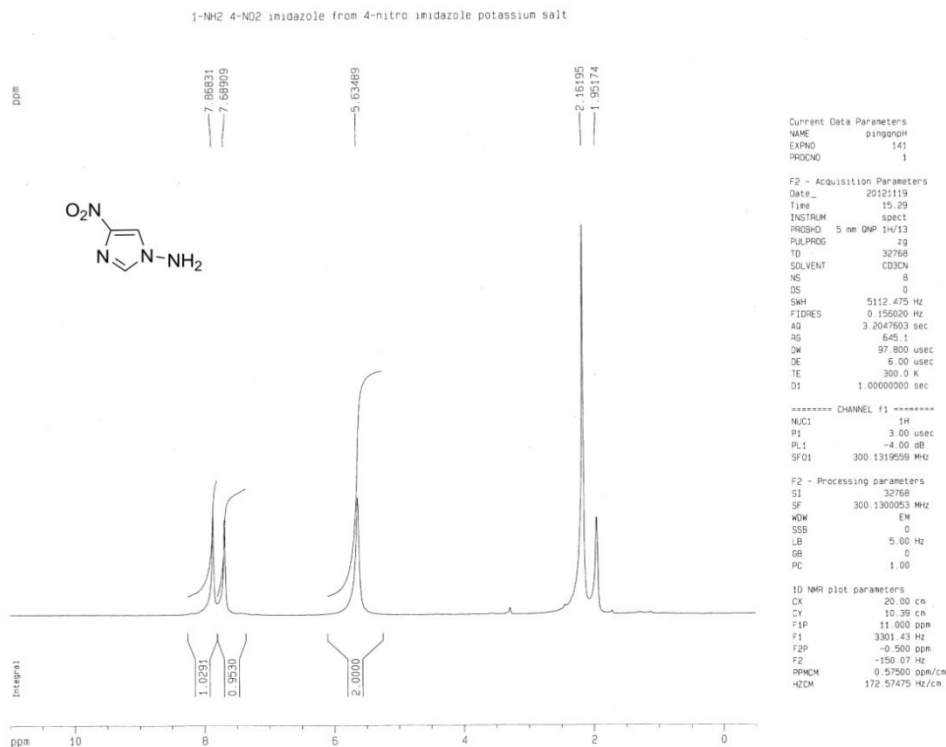


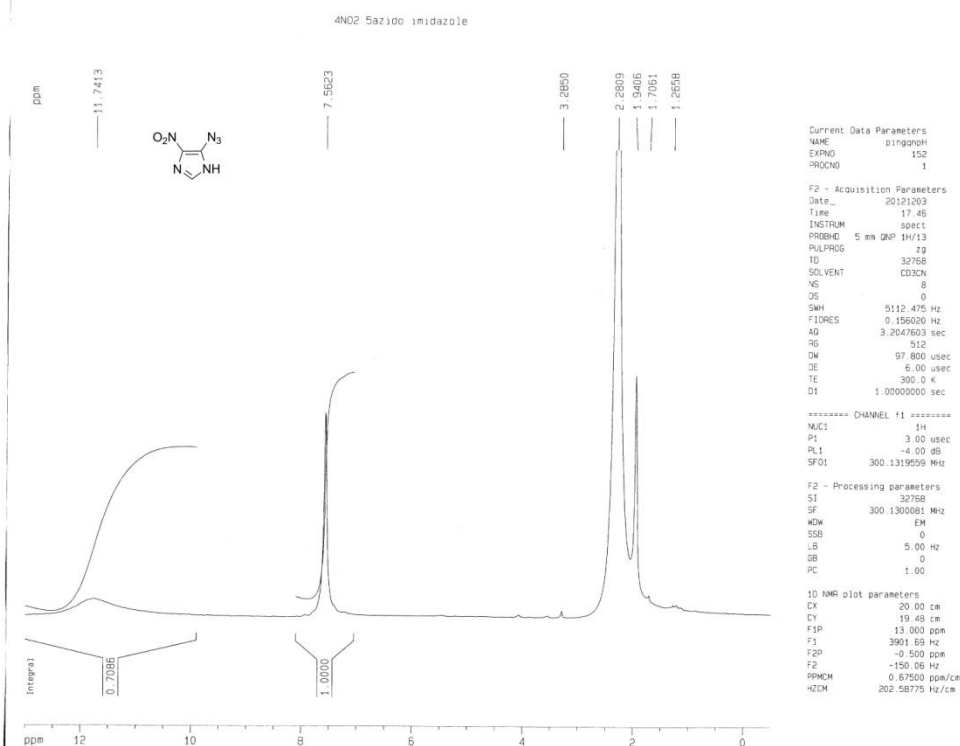
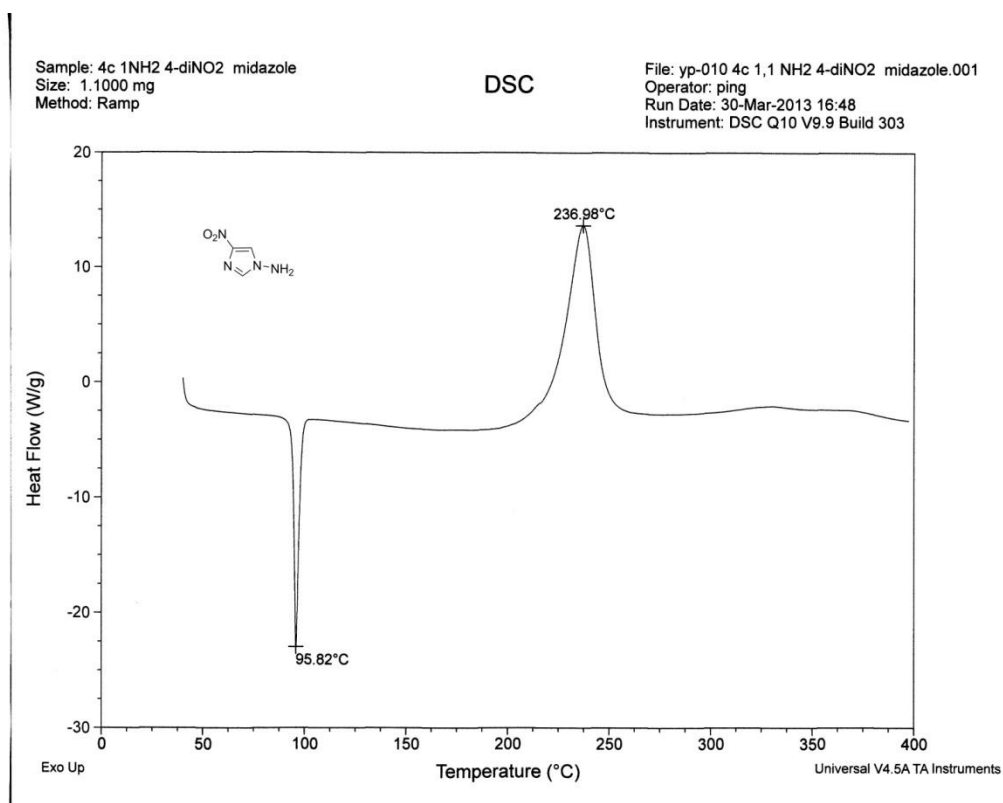
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Size: 0.6000 mg
Method: Ramp

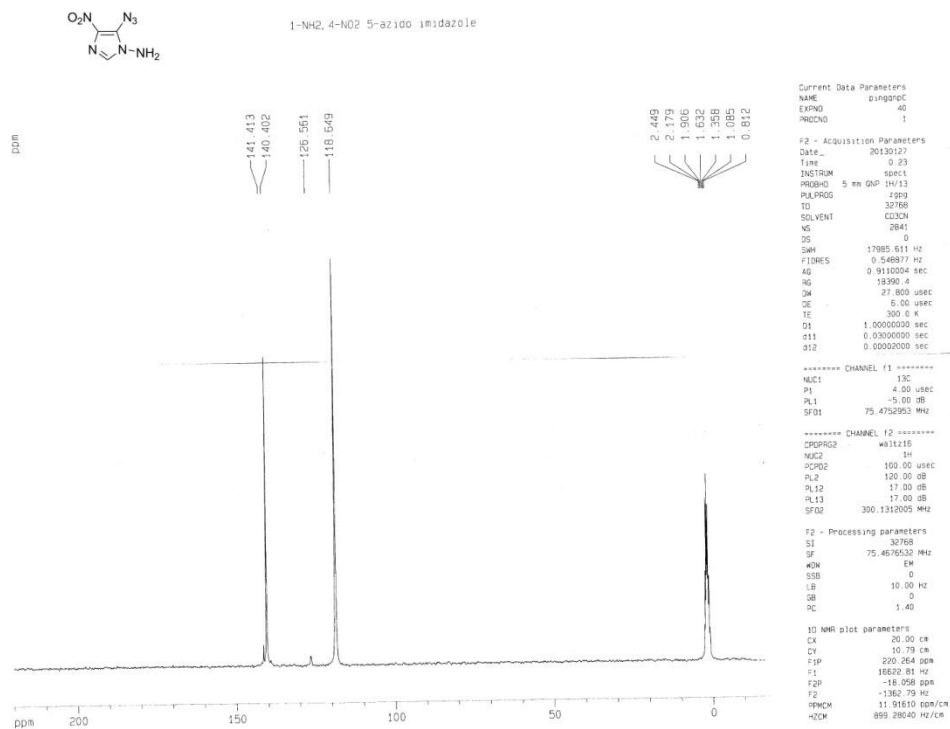
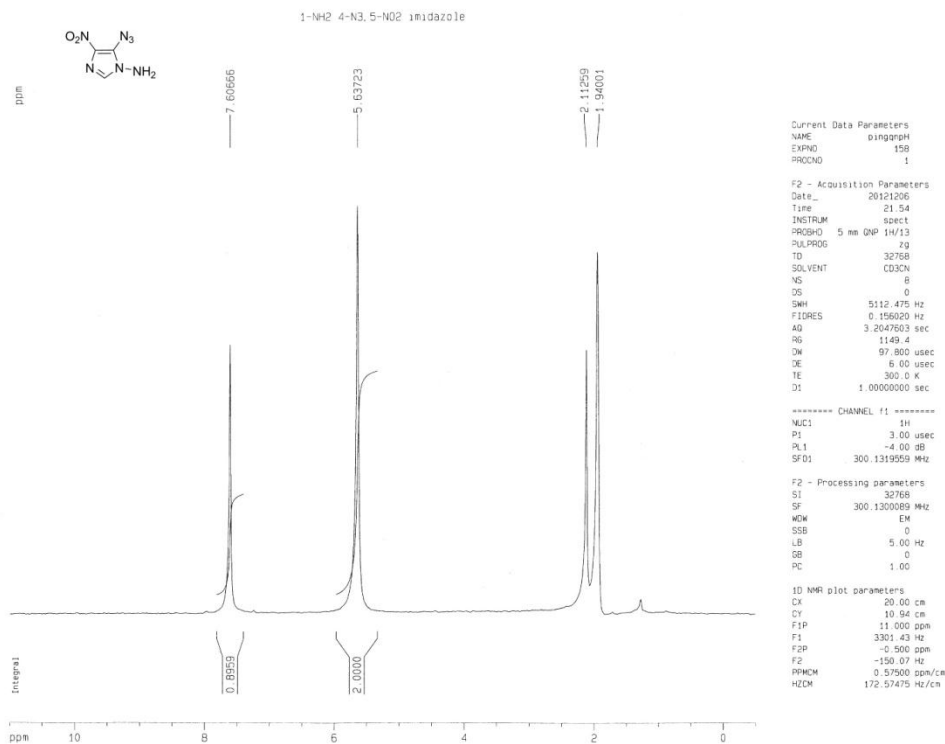
DSC

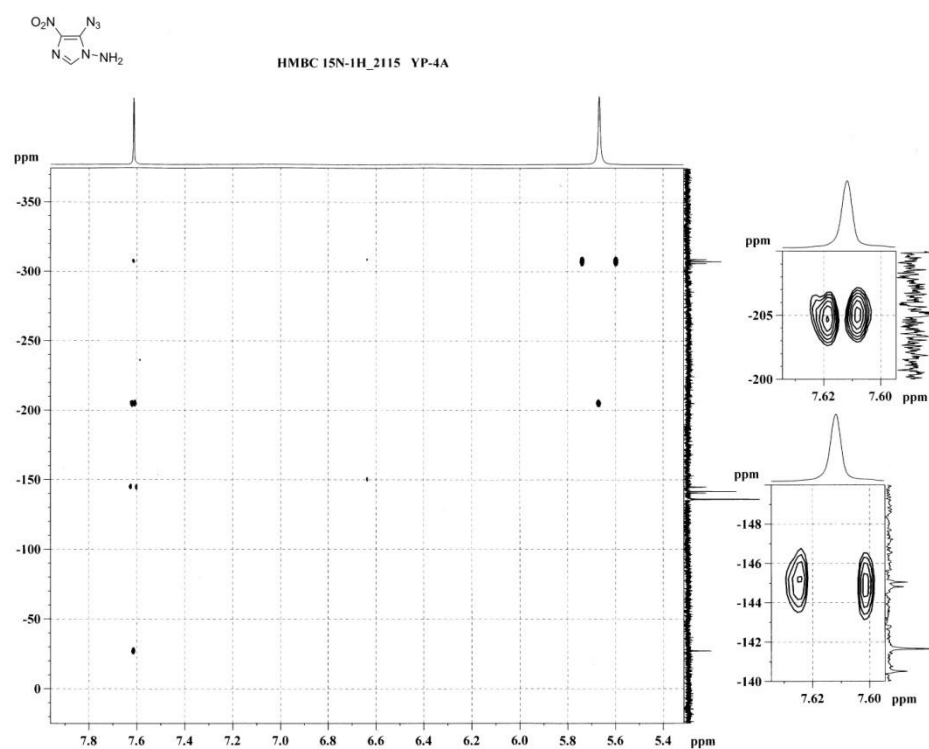
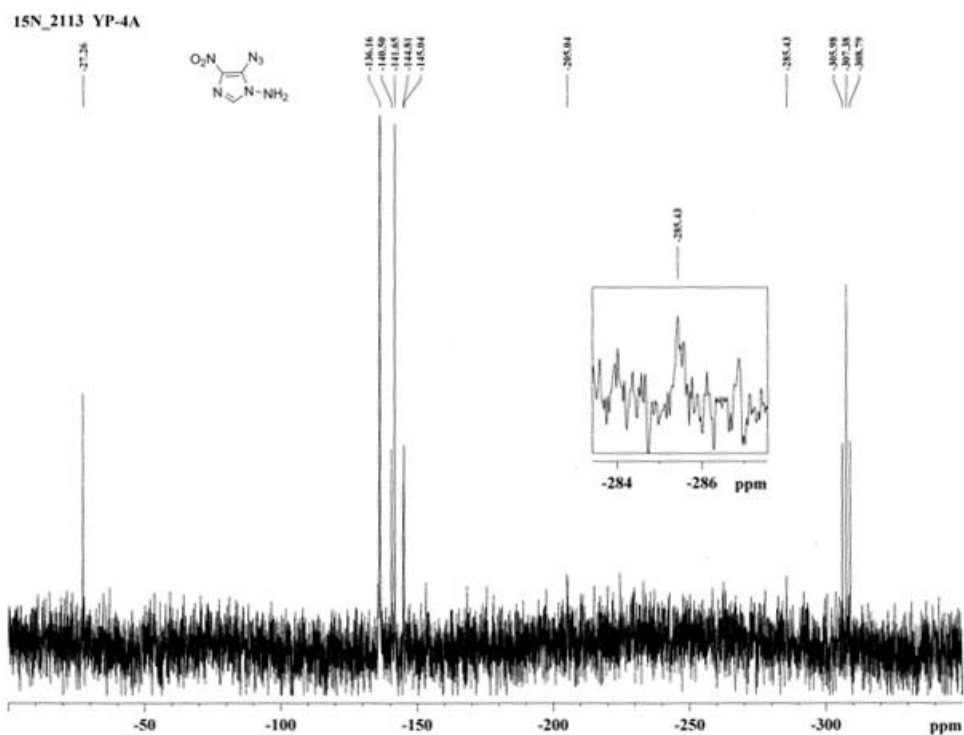
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Instrument: DSC Q10 V9.9 Build 303

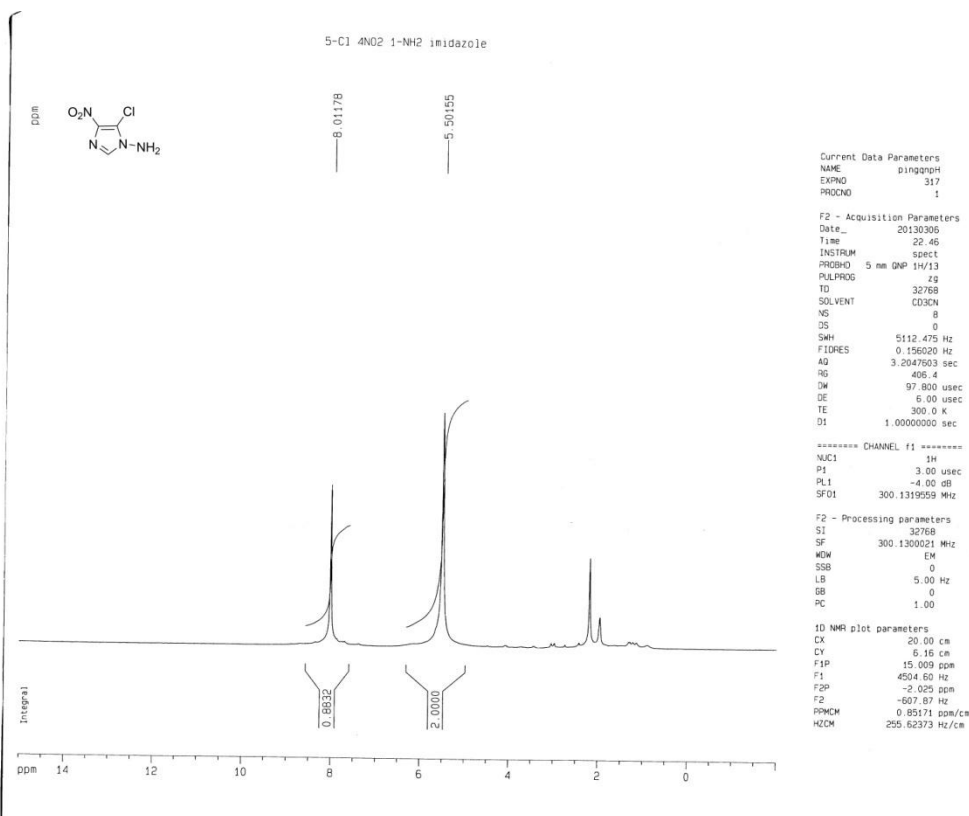
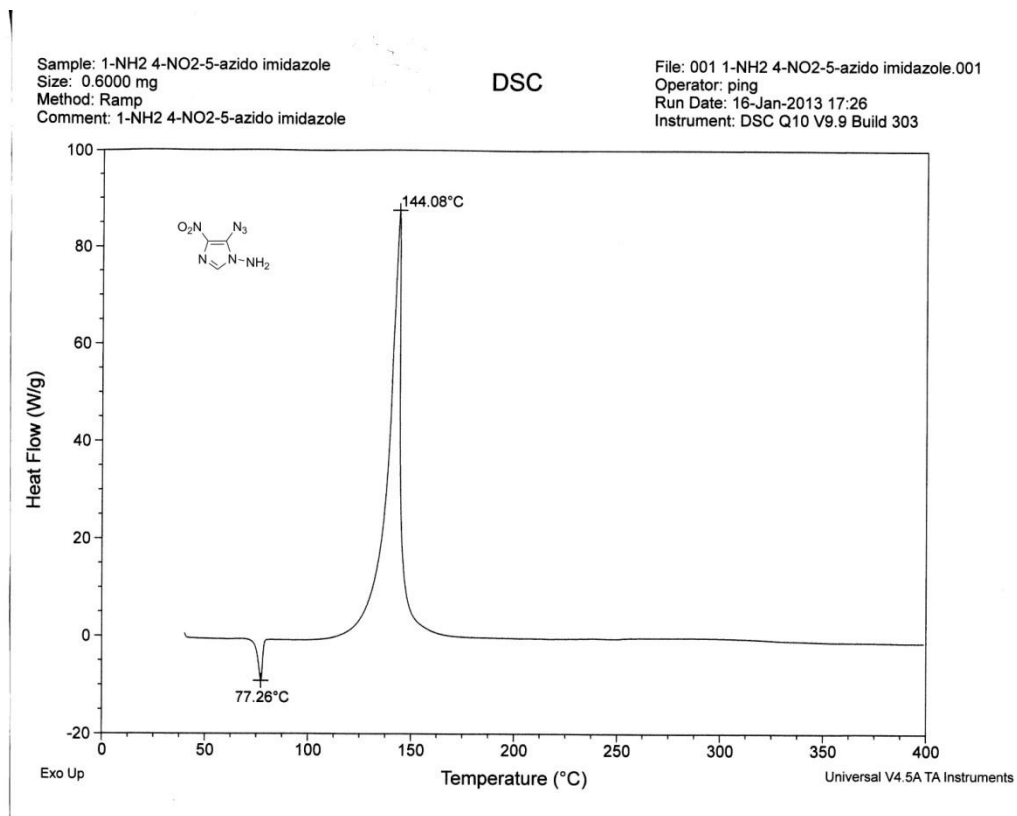


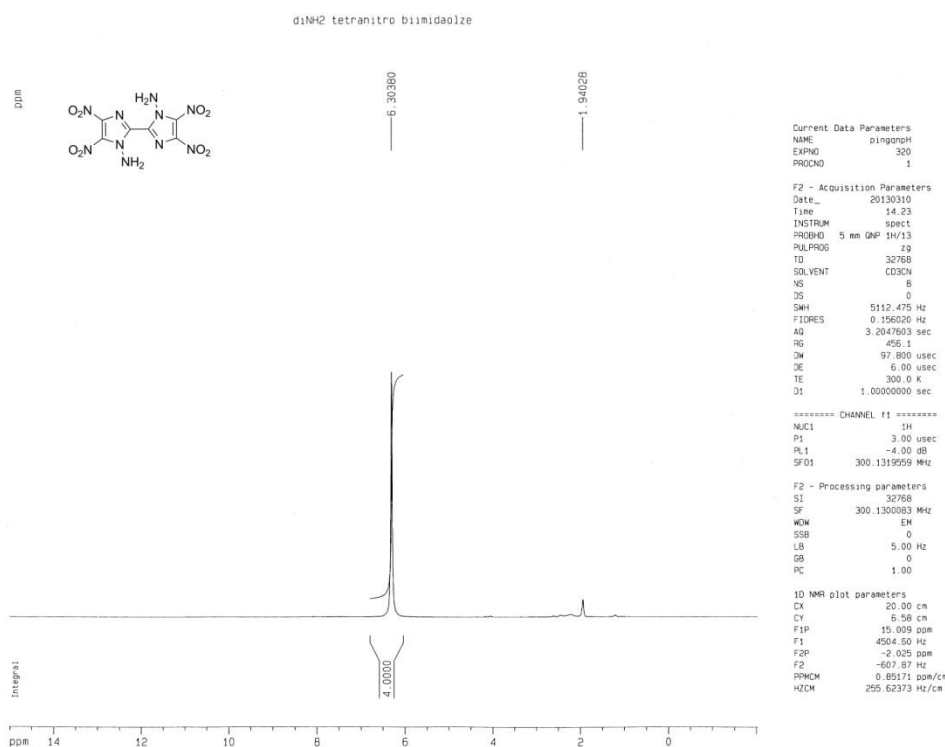
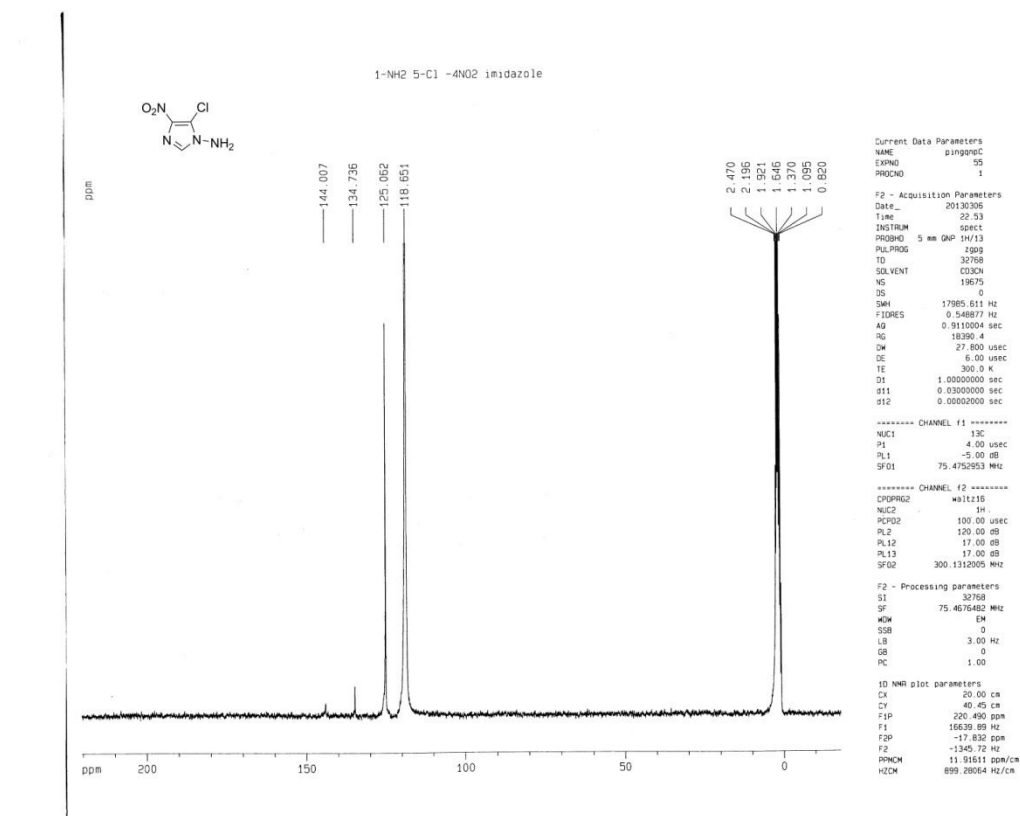


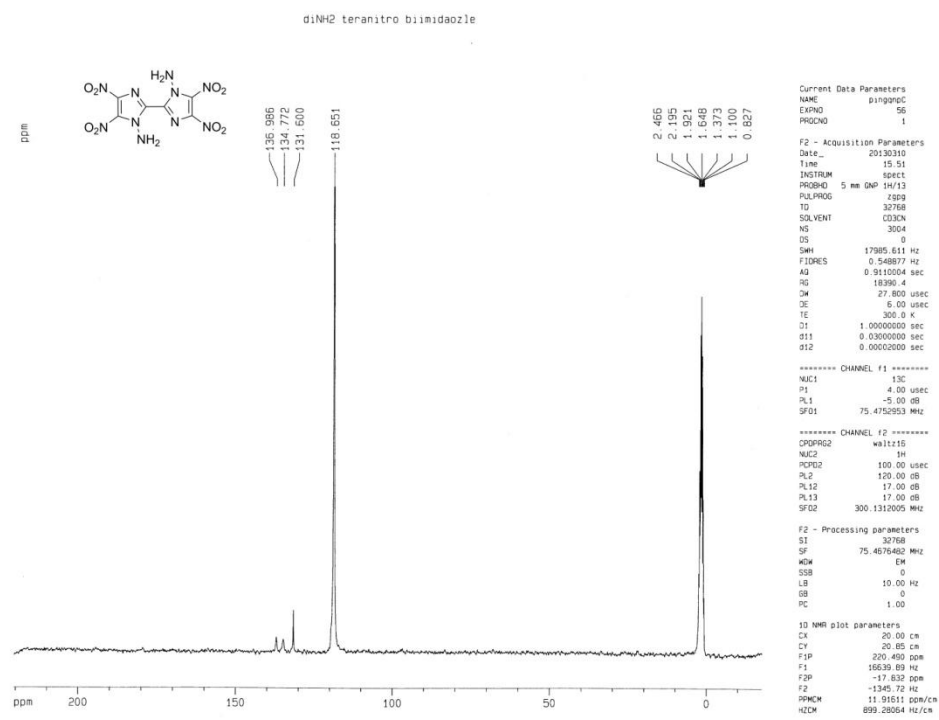








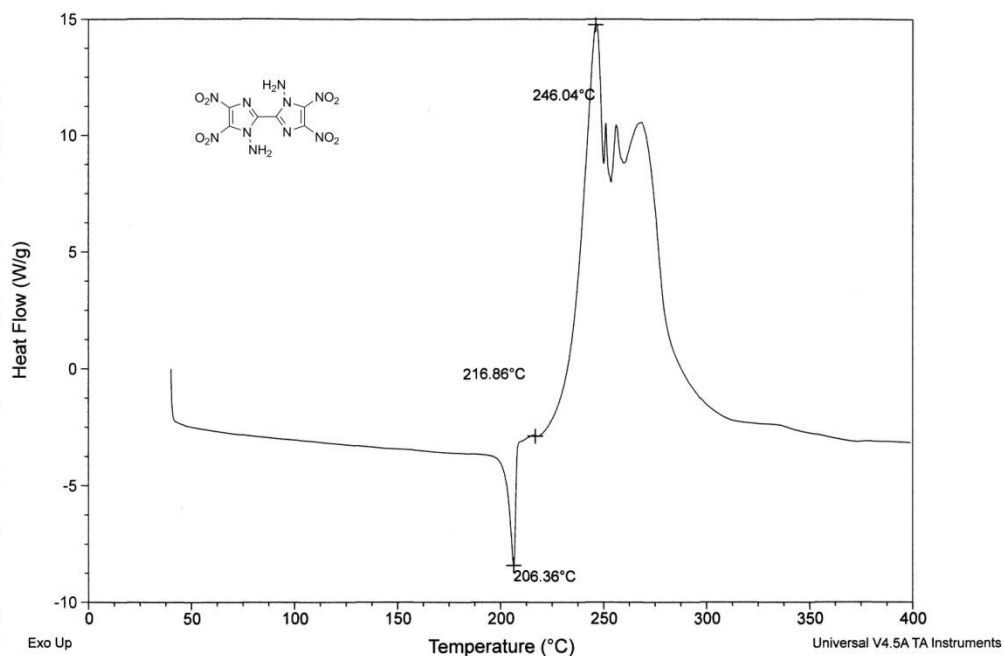


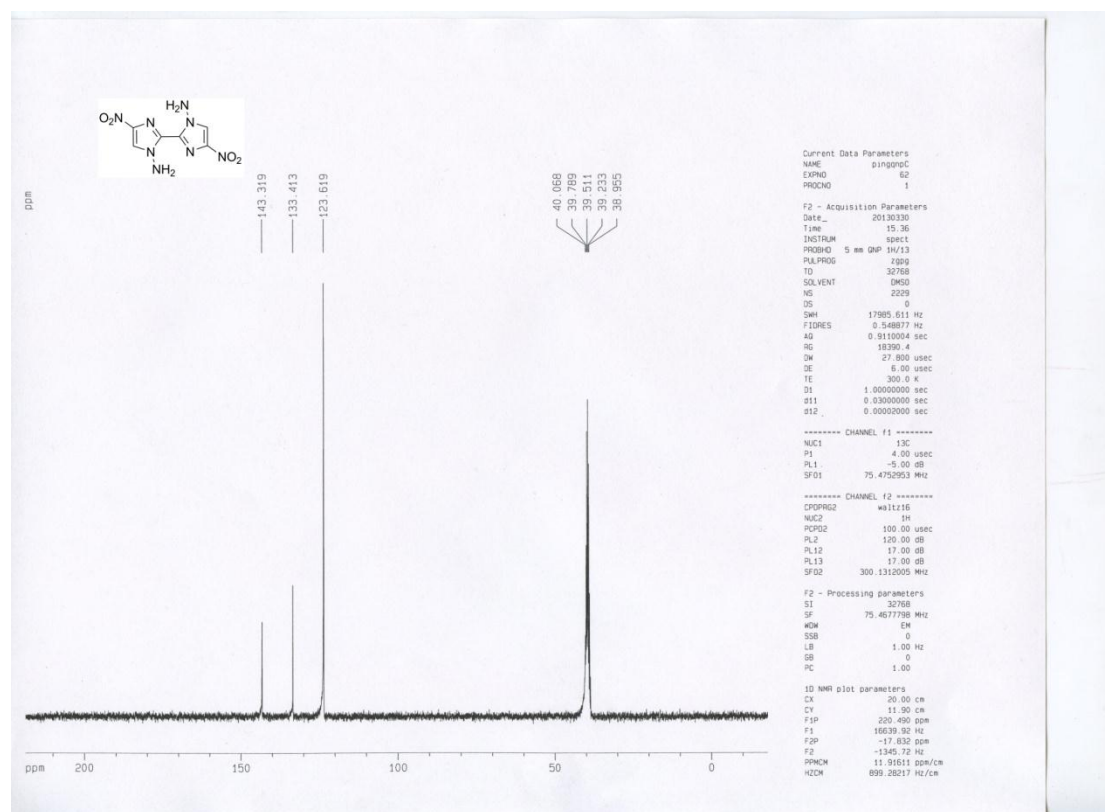
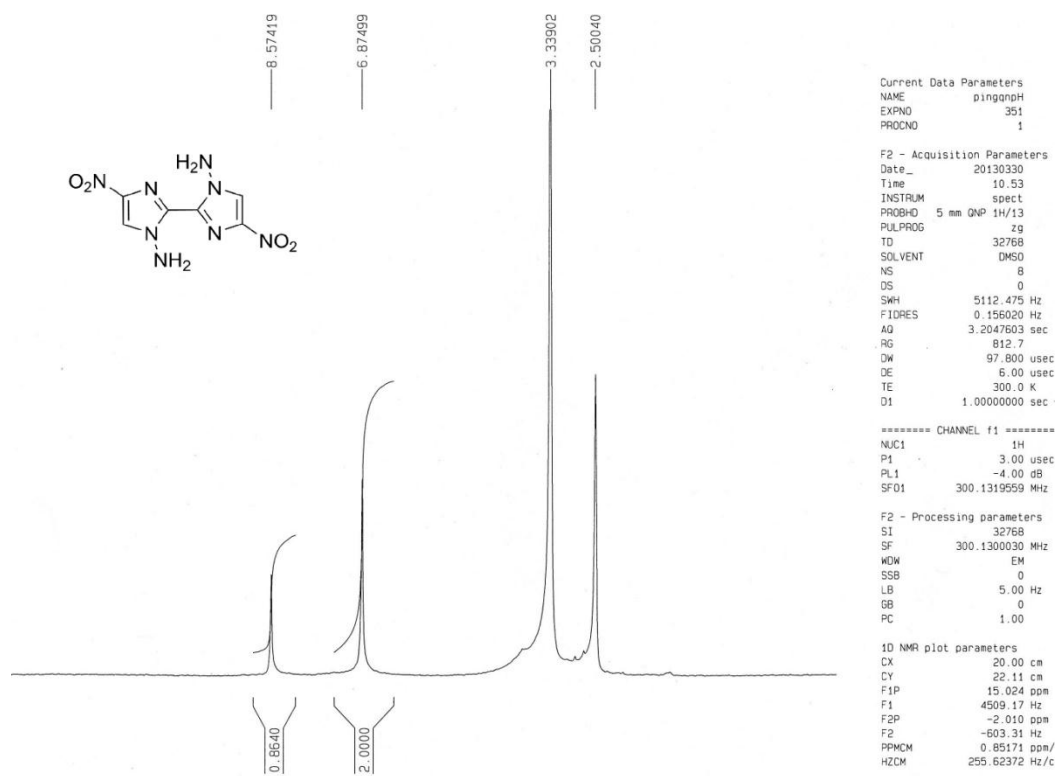


Sample: YP4F TERA no2BIIMI 5 C
Size: 0.6000 mg
Method: Ramp

DSC

File: C:\...\005YP4F TERA no2BIIMI.001
Operator: ping
Run Date: 10-Mar-2013 15:10
Instrument: DSC Q10 V9.9 Build 303

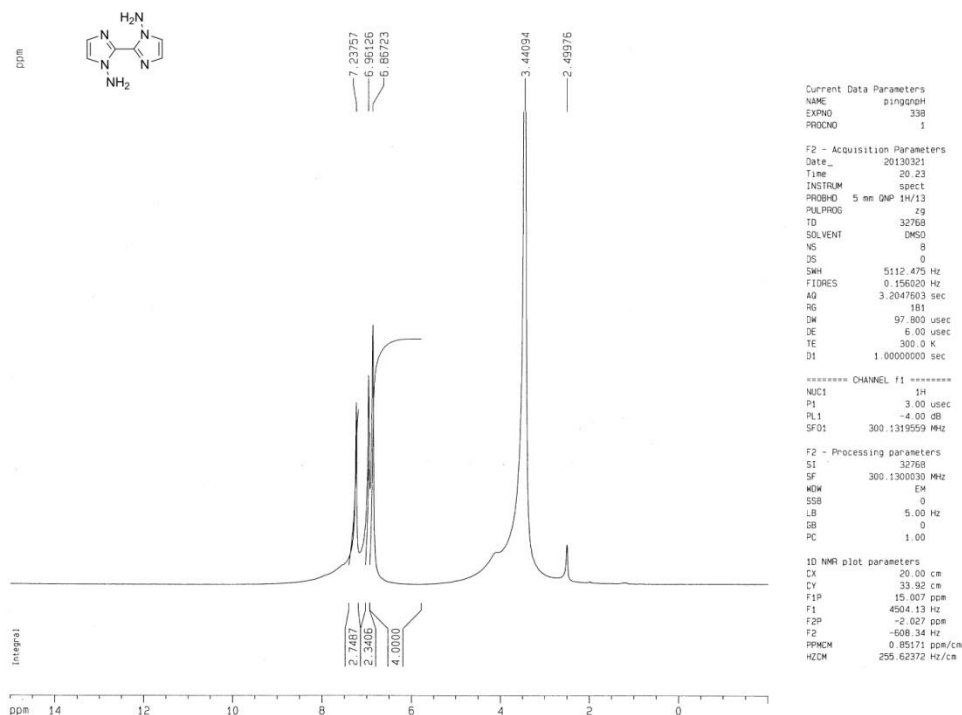
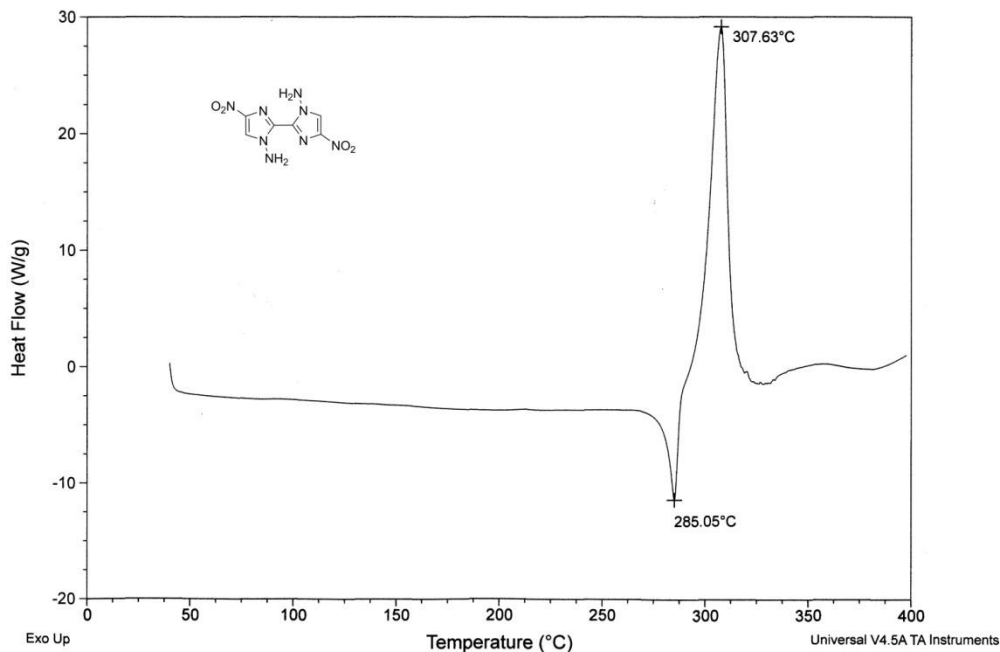


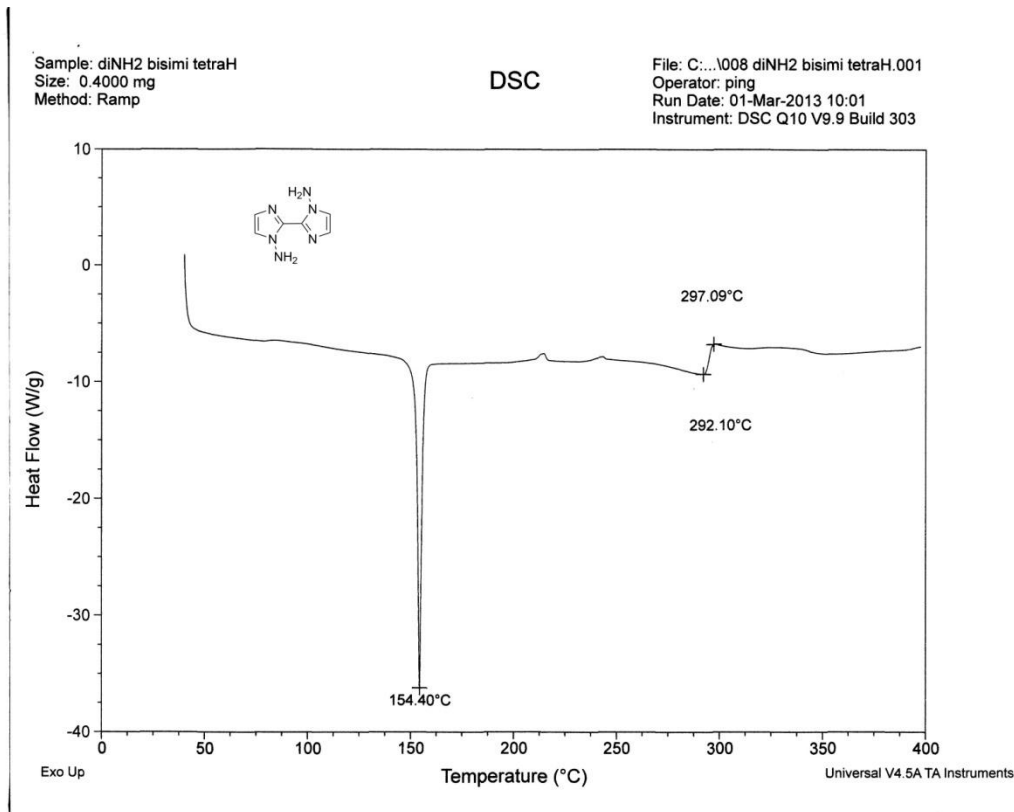
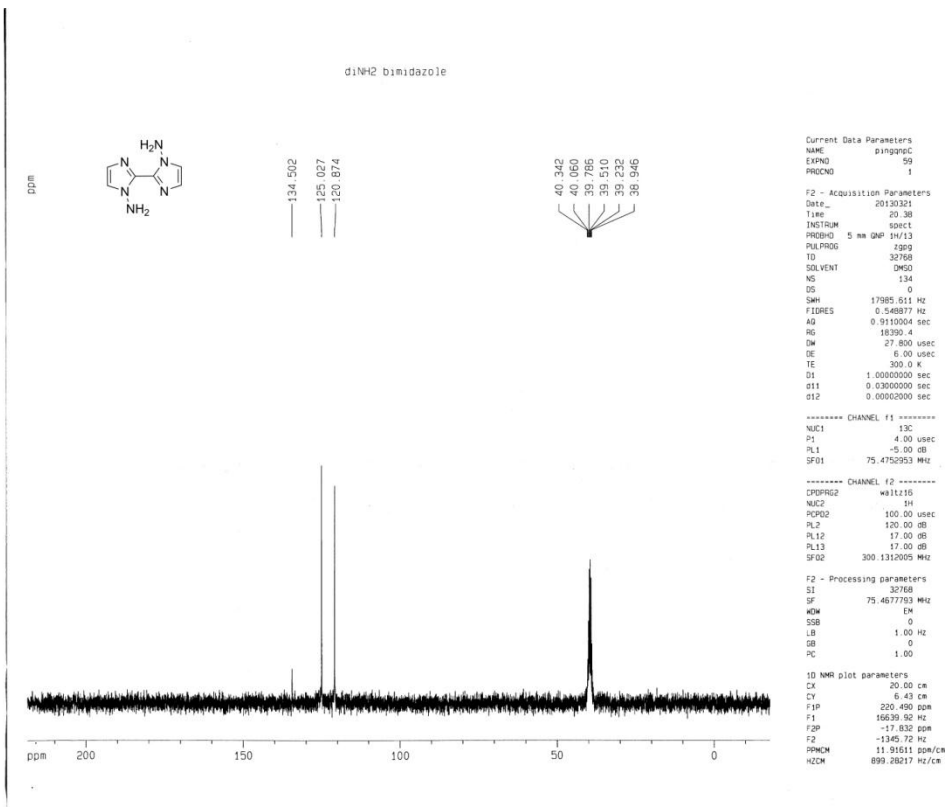


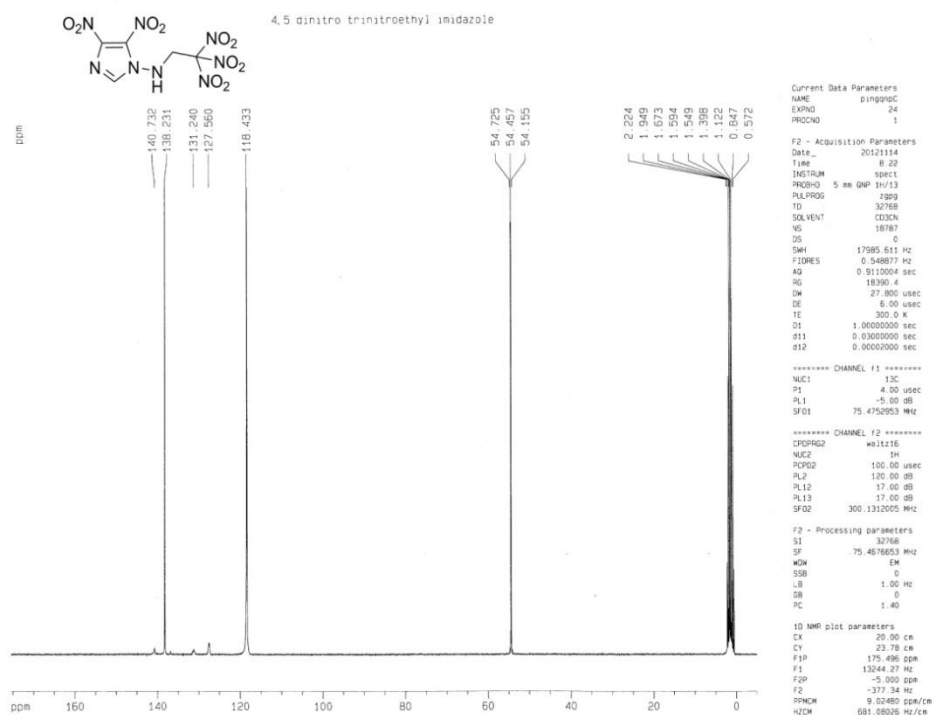
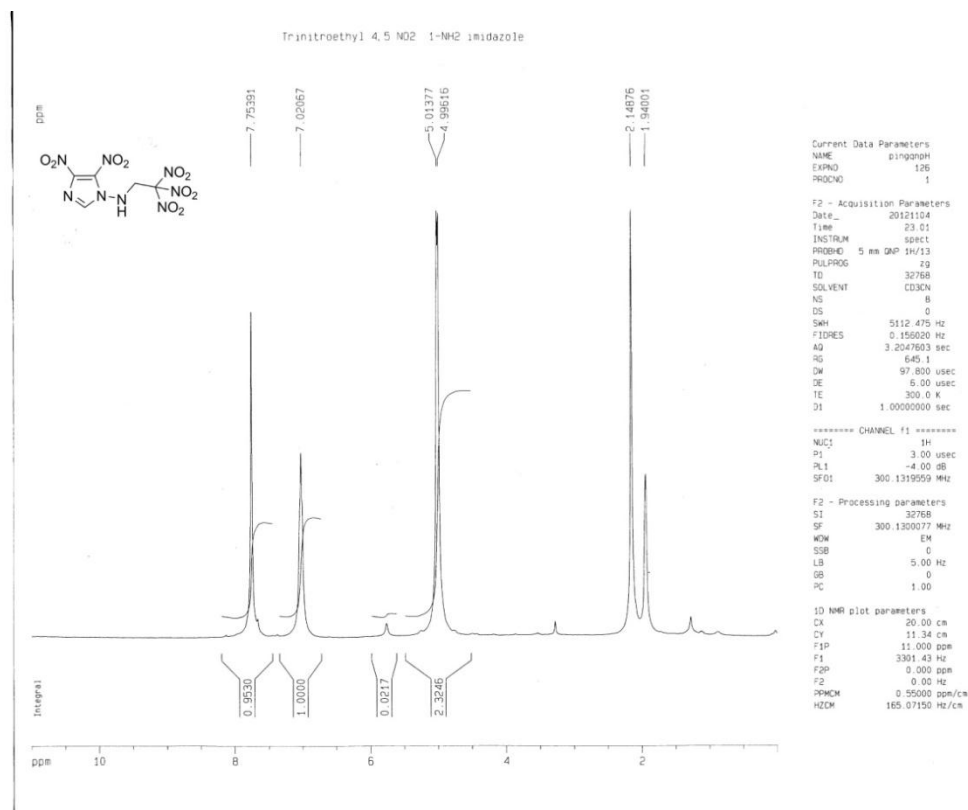
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Method: Ramp

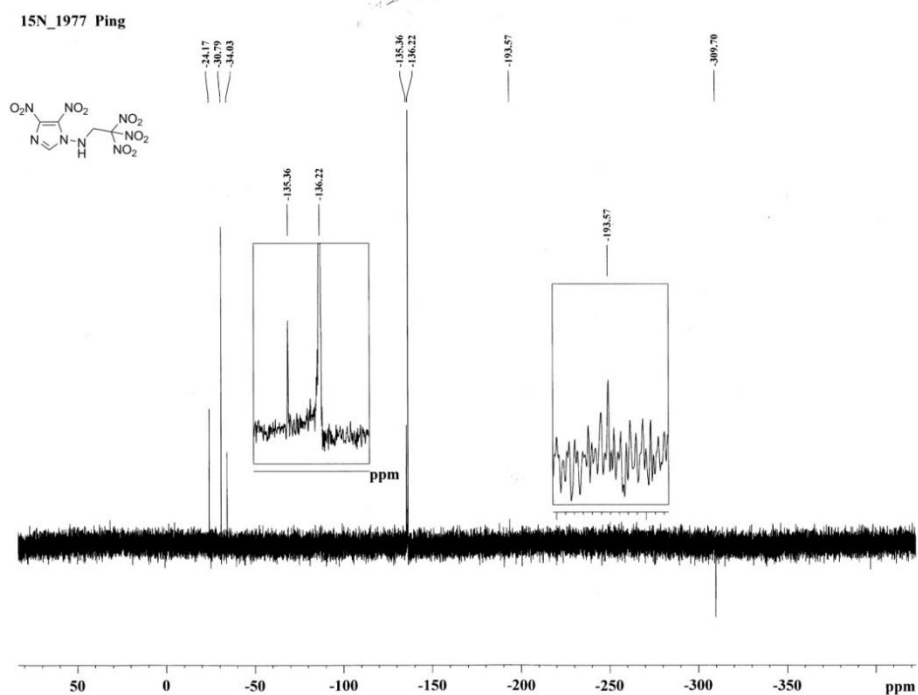
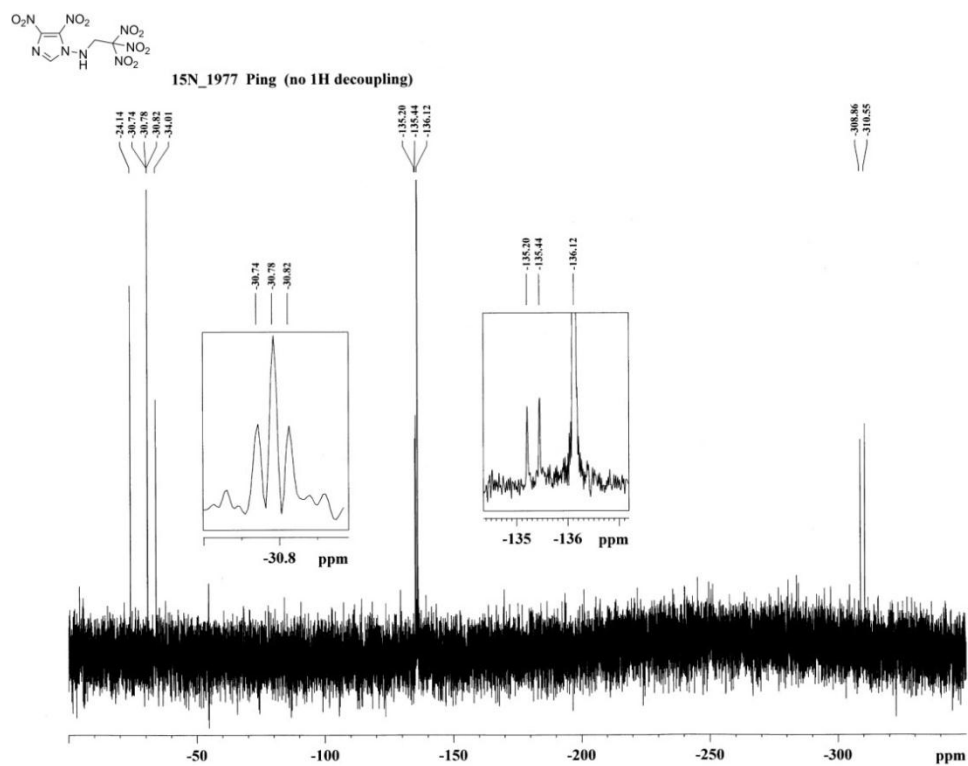
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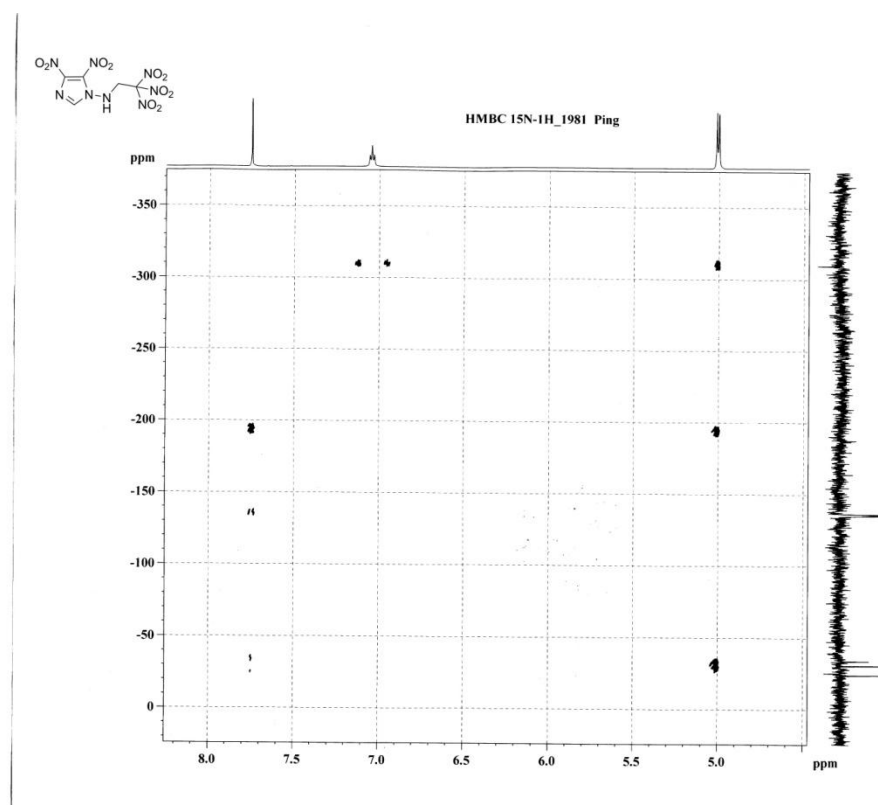
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Instrument: DSC Q10 V9.9 Build 303







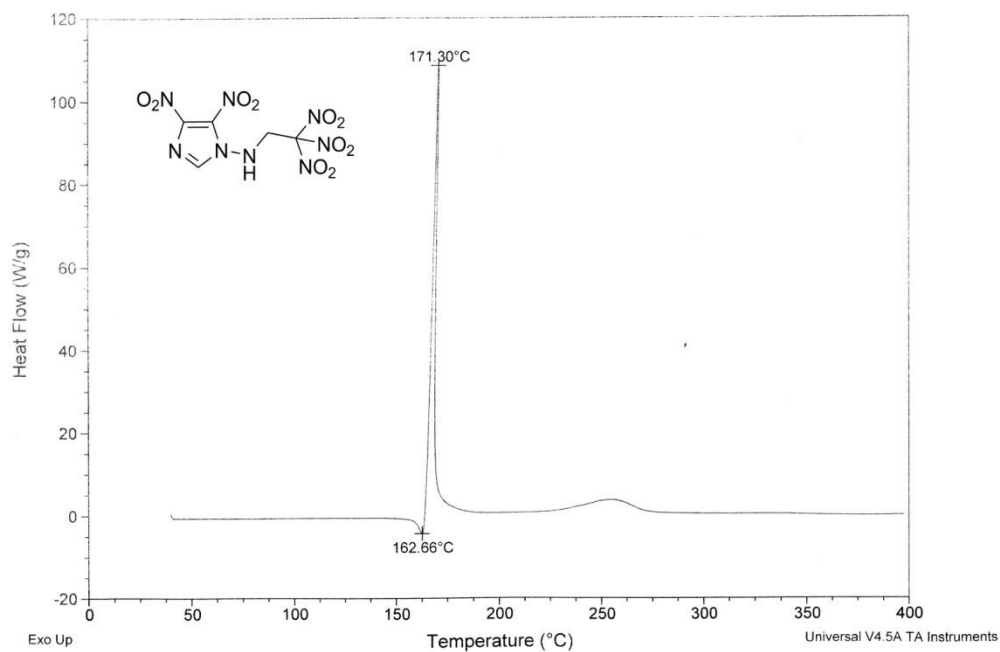


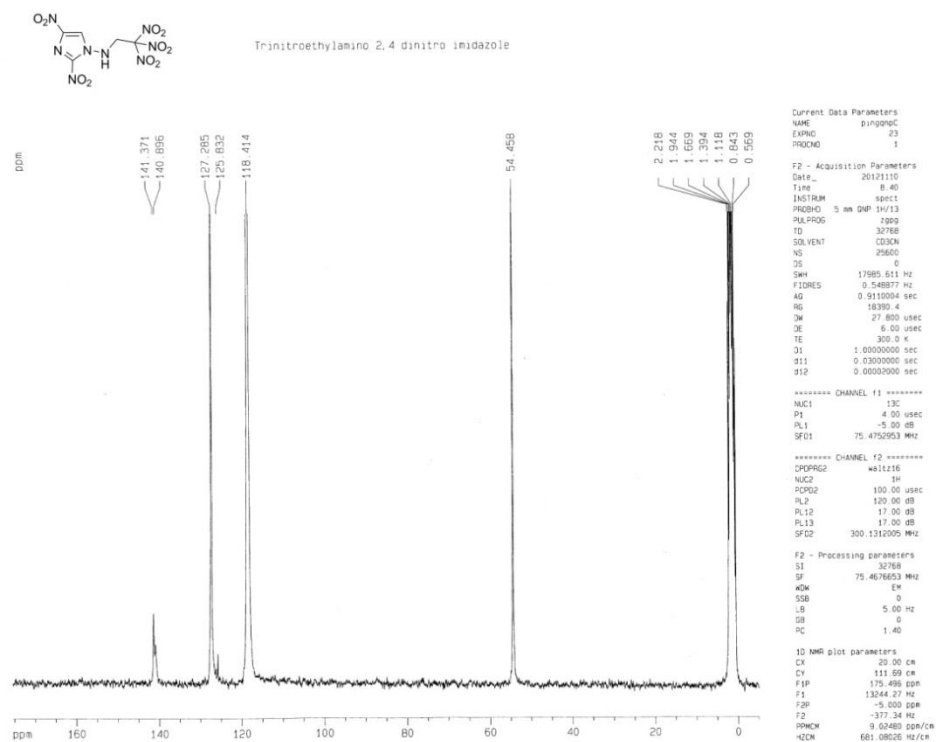
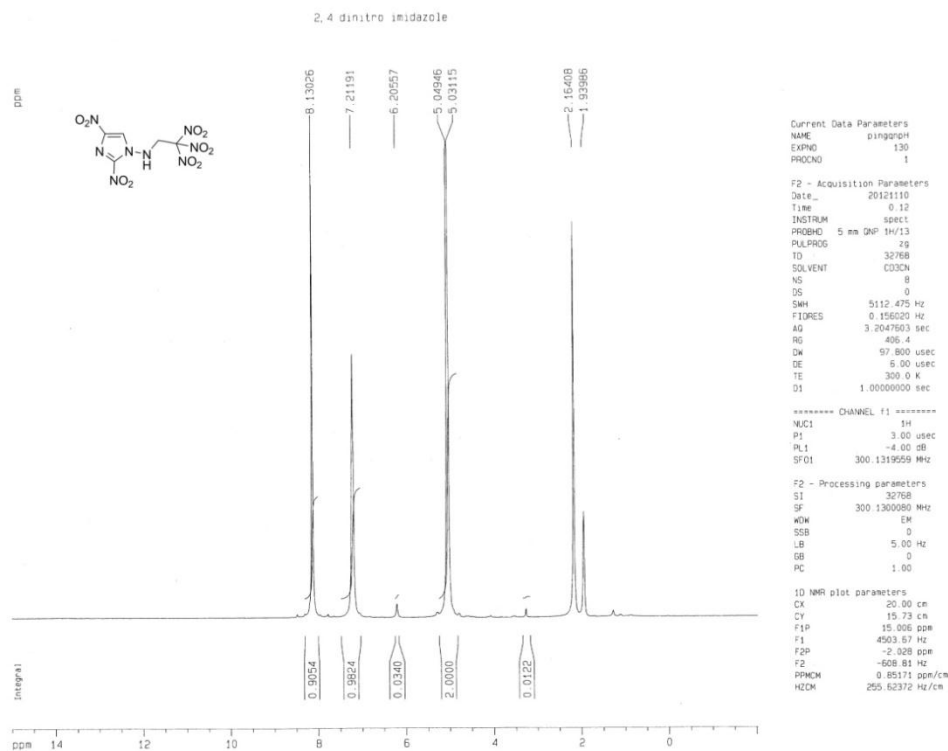


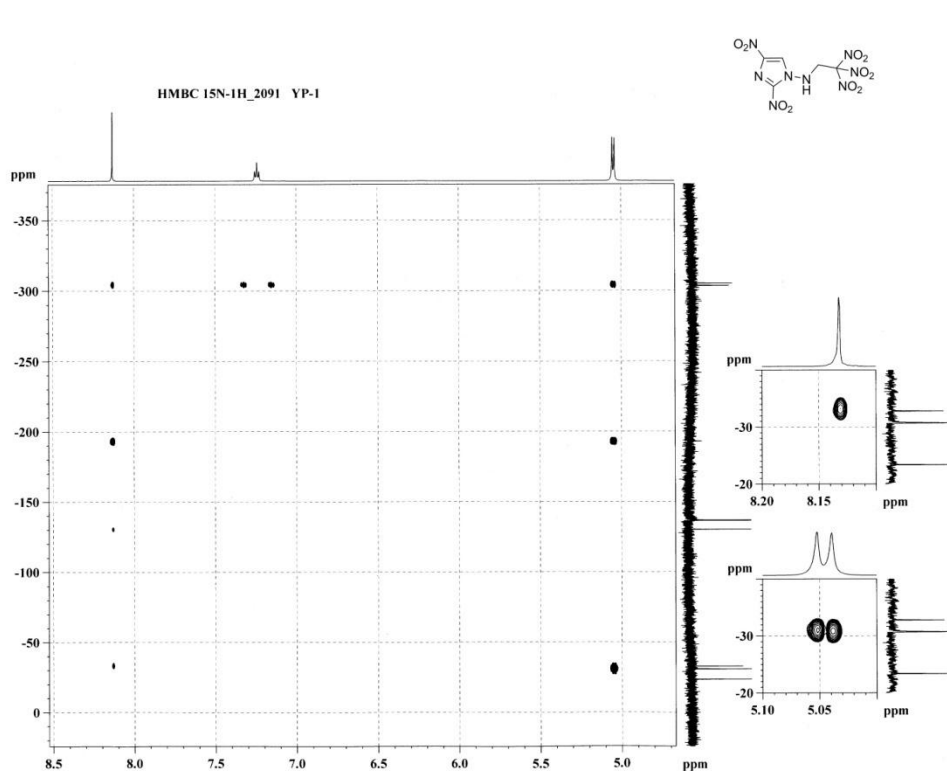
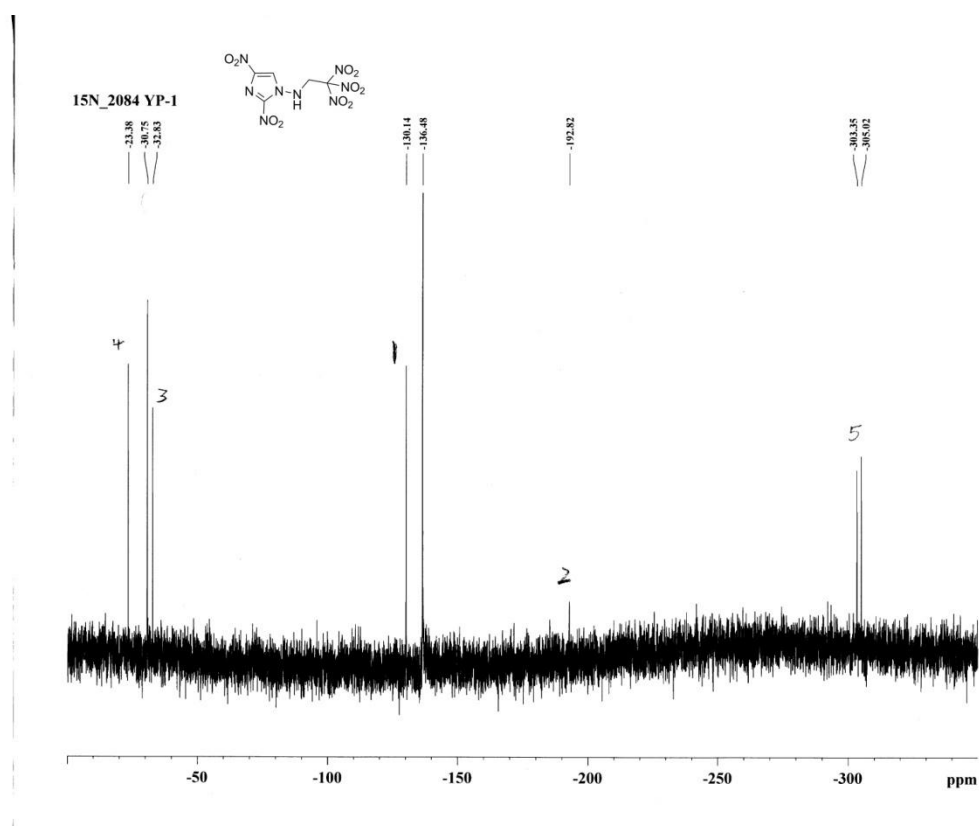
Sample: YP004
Size: 1.0000 mg
Method: Ramp
Comment: Trinitroethyl 4,5-diNO₂ imidazole

DSC

File: C:\TA\Data\DSC\YPI\YP004.001
Operator: clhe
Run Date: 05-Nov-2012 10:54
Instrument: DSC Q10 V9.8 Build 296



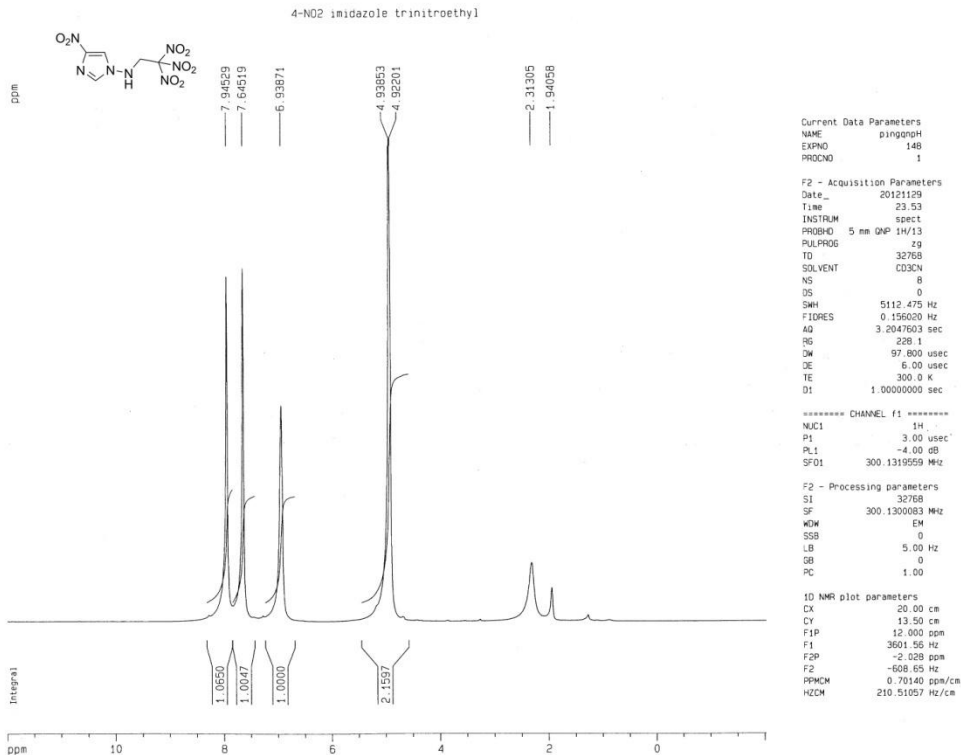
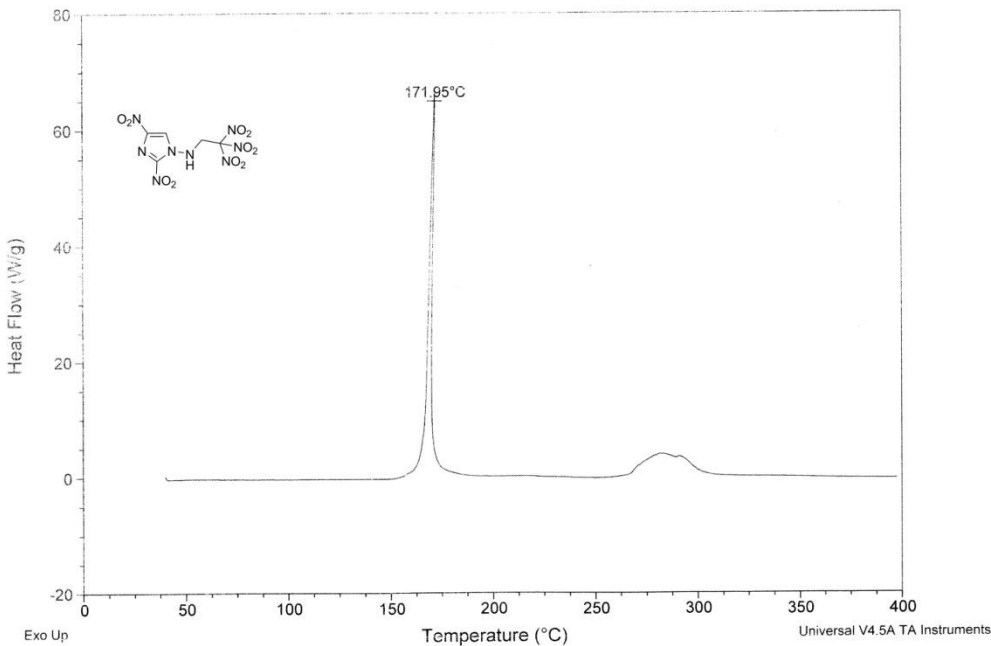


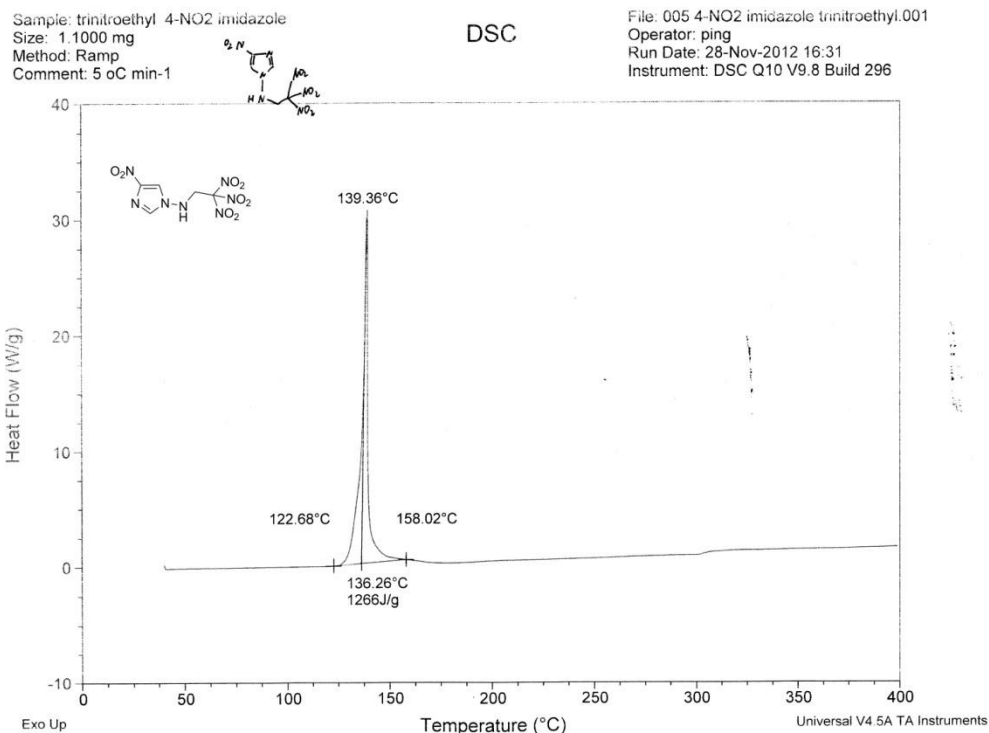
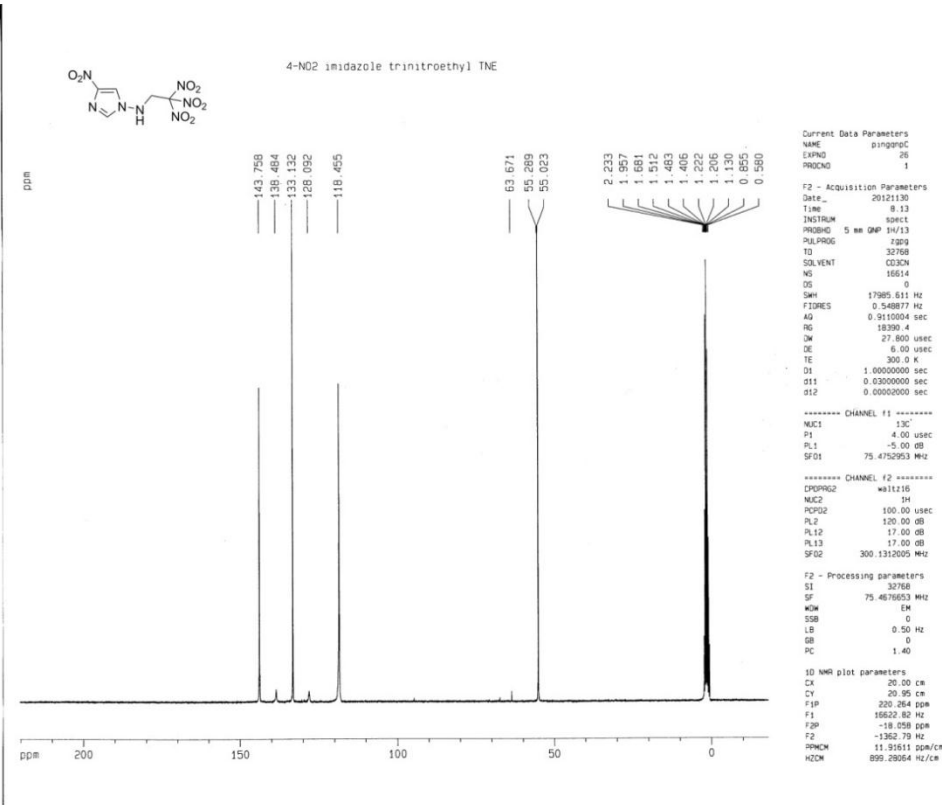


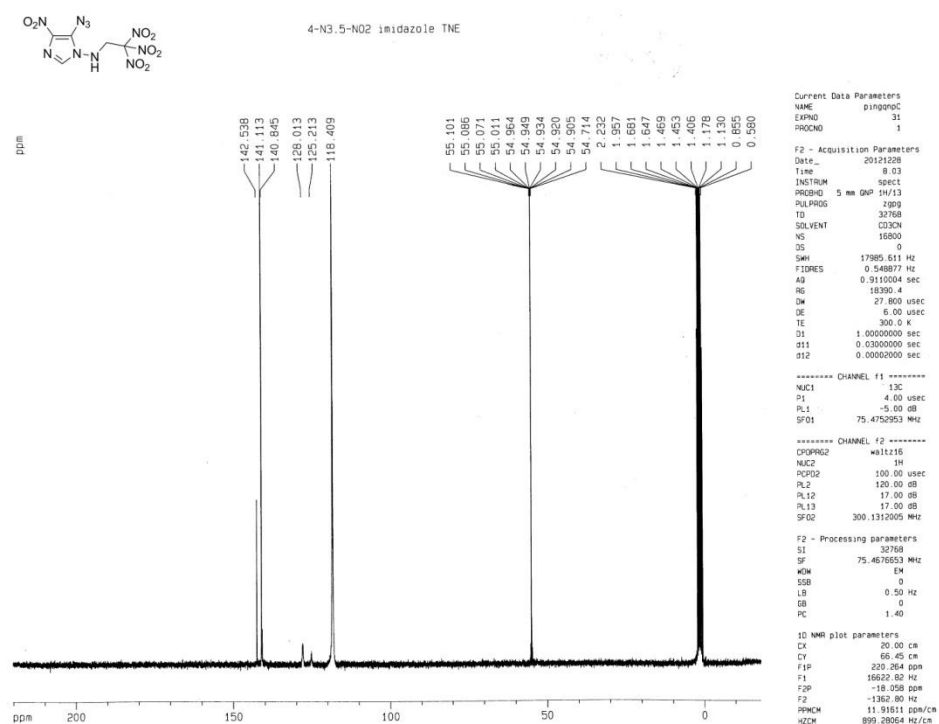
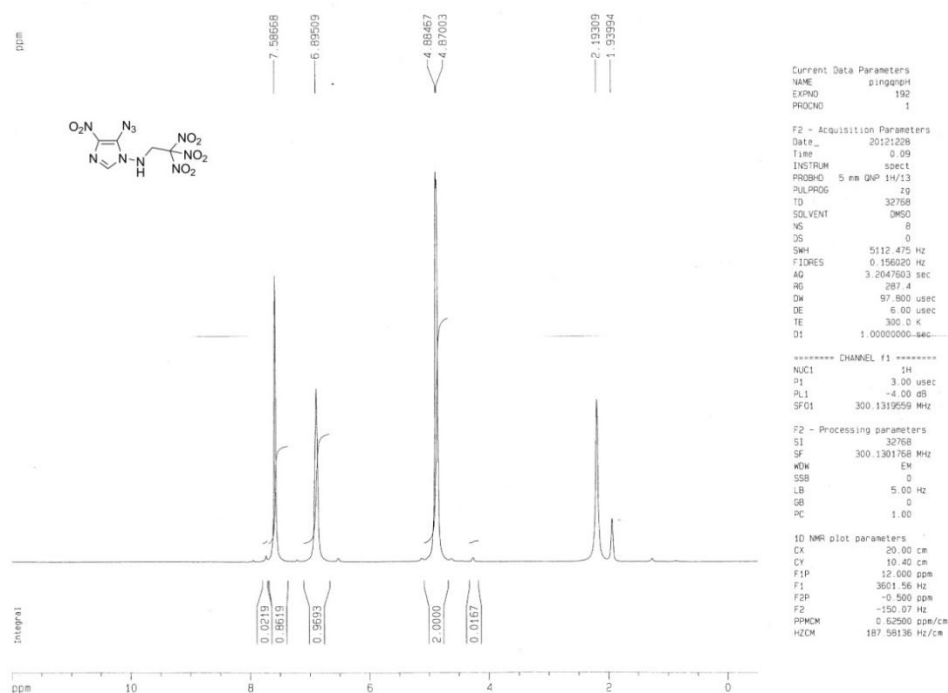
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Method: Ramp
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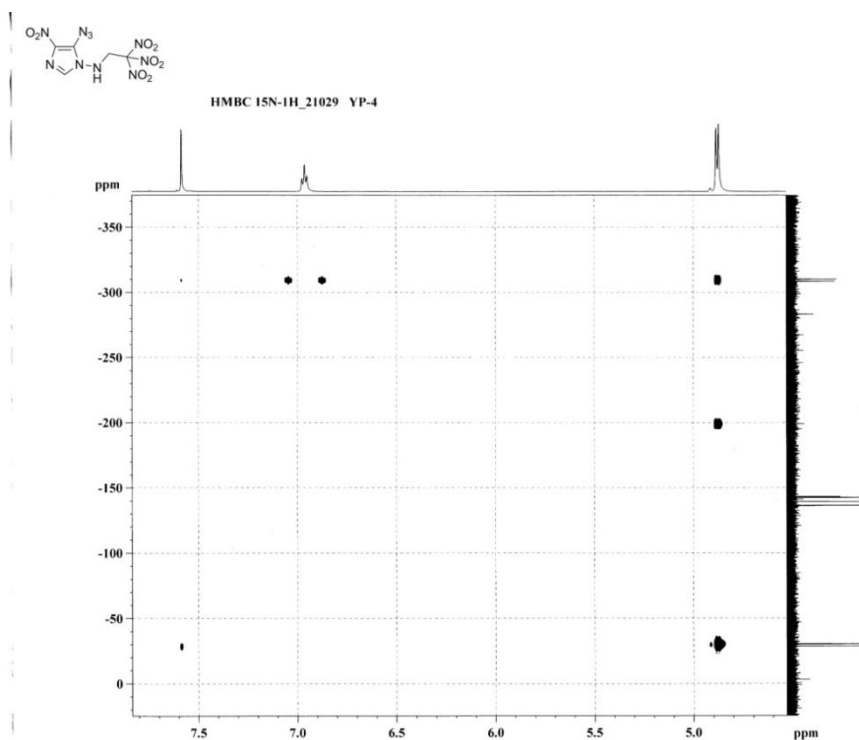
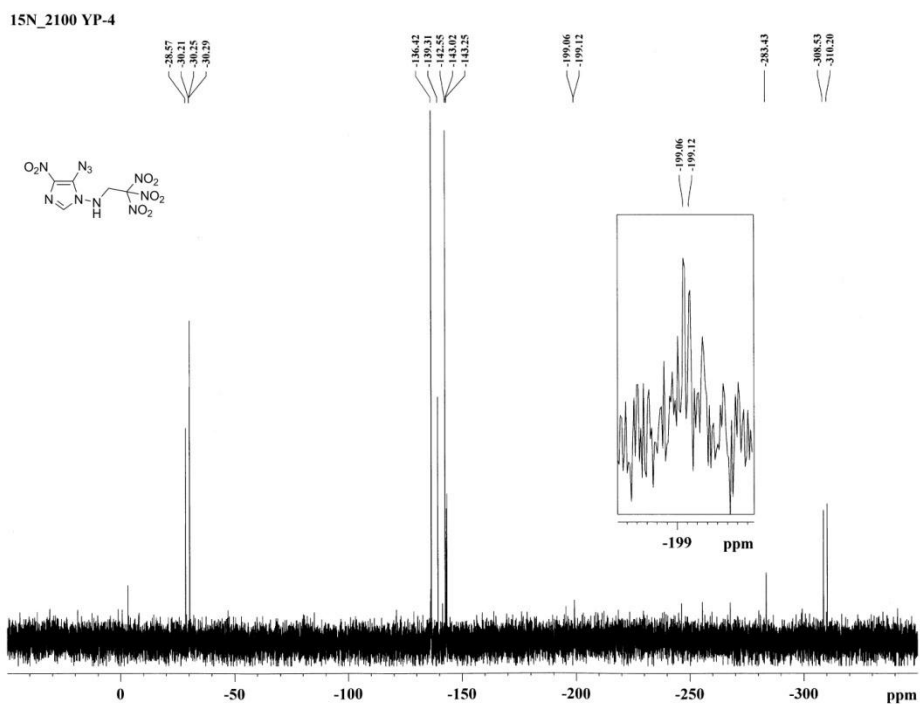
DSC

File: 002 1-NH2 Trinitroethyl 2 -4 NO2...
Operator: thao
Run Date: 09-Nov-2012 17:45
Instrument: DSC Q10 V9.8 Build 296









Sample: 06 1-NH2 5-N3 4-NO2 imi TNE
Size: 0.5000 mg
Method: Ramp
Comment: 06 1-NH2 5-N3 4-NO2 imidazole +TNE.001

DSC

File: 006 1-NH2 5-N3 4-NO2 imidazole +TNE.001
Operator: thao
Run Date: 15-Feb-2013 20:51
Instrument: DSC Q10 V9.9 Build 303

