Electronic Supplementary Information

Connecting Energetic Nitropyrazole and Aminotetrazole Moieties with N,N'-Ethylene Bridges: A Promising Approach for Fine Tuning Energetic Properties of Compounds

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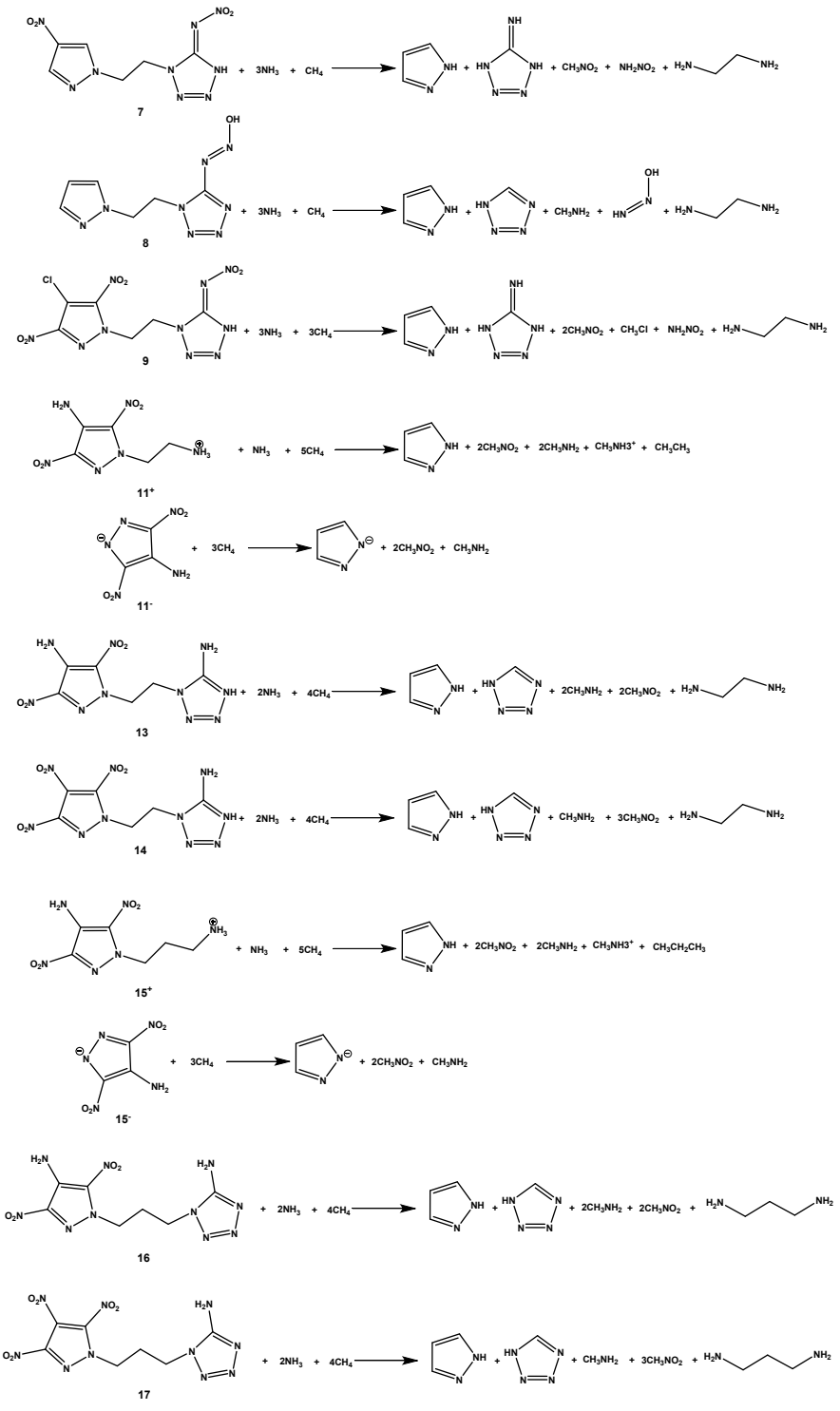
1. Isodesmic Reactions



Scheme S1: Isodesmic reactions for the synthesized compounds

2. Crystal Structures of compounds 5, 9·H_2O and 12

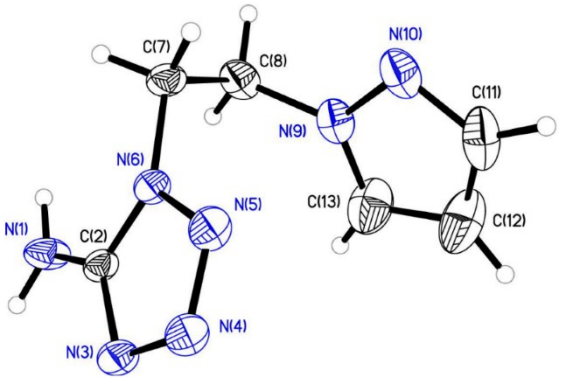


Figure S1. Thermal ellipsoid plot (50%) and labeling scheme for **5**

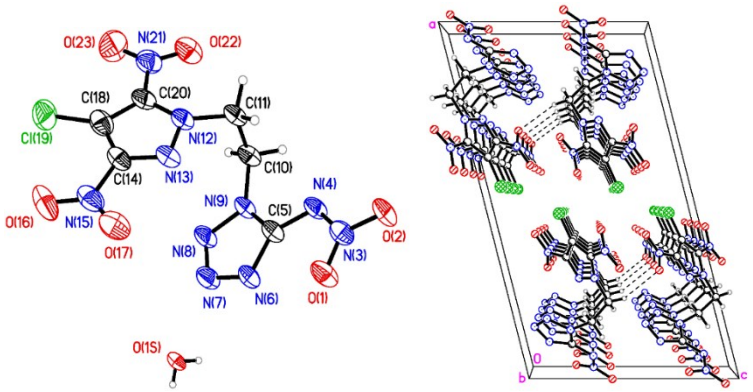


Figure S2. (a) Thermal ellipsoid plot (50%) and labeling scheme for **9**·H_2O. (b) Ball-and-stick packing diagram of **9**·H_2O viewed down the *b* axis. Dashed lines indicate strong hydrogen bonding.

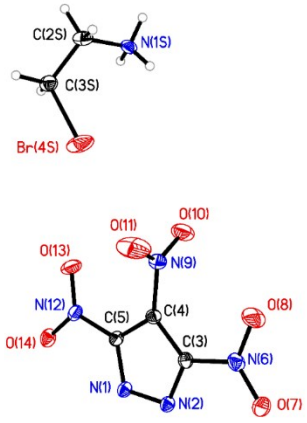


Figure S3. Thermal ellipsoid plot (50%) and labeling scheme for **12.**

3. Crystal Structure Data

Table S1. X-ray crystal structure parameters of compounds **5**, **7** **9**, **12** and **13**.

Parameters	**5**	**7·H_2O**	**8**	**9·H_2O**	**12**	**13**
CCDC number	1454188	1454189	1454190	1454191	1454192	1454193
Formula	$C_6H_9N_7$	$C_6H_9N_9O_5$	$C_6H_8N_8O$	$C_6H_6ClN_{10}O_7$	$C_5H_7BrN_6O_6$	$C_6H_8N_{10}O_4$
MW	179.20	287.22	208.20	365.66	327.08	284.22
cryst syst	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	triclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	*P***Error!**
a /Å	5.388(3)	13.624(4)	6.794(3)	20.688(4)	8.668(2)	7.105(2)
b /Å	29.349(2)	8.667(3)	16.520(7)	5.487(1)	9.223(2)	9.063(3)
c /Å	5.948(2)	10.397(3)	8.397(4)	12.004(2)	14.411(3)	17.442(5)
α (°)	90.00	90.00	90.00	90.00	90.00	93.227(2)
β (°)	113.925(2)	109.82(1)	98.104(2)	104.552(1)	103.053(2)	100.858(2)
γ (°)	90.00	90.00	90.00	90.00	90.00	92.641(2)
V /Å^3	859.68(8)	1155.00(6)	932.96(7)	1318.8(4)	1122.30(4)	1099.42(6)
Z	4	4	4	4	4	2
T /K	296(2)	296(2)	296(2)	150(2)	150(2)	150(2)
λ /Å	0.71073	0.71073	0.71073	1.54178	0.71073	1.54178
ρ_c (g/cm3)	1.385	1.652	1.482	1.784	1.889	1675
μ (mm-1)	0.099	0.143	0.113	3.228	3.698	1.270
Goodness of fit	1.054	0.972	1.049	1.136	1.086	1.020
θ range	3.81 - 26.52	2.83 - 26.54	3.03 - 27.59	2.21 – 66.97	3.27 - 27.52	2.58 – 66.61
Total reflections	8071	10873	9660	5815	10798	6472
Unique reflections	1767	2372	2152	2141	2579	3385
Observed data[$I > 2\sigma(I)$]	1262	1859	1386	1574	2374	2246
R_{int}	0.0406	0.0254	0.0335	0.0639	0.0203	0.0397
R_1, wR_2 [$(I > 2\sigma(I)$]	0.0492, 0.1102	0.0363, 0.1040	0.0371, 0.0891	0.0743, 0.1752	0.0228, 0.0538	0.0571, 0.1364
R_1, wR_2 (all data)	0.0778, 0.1209	0.0501, 0.1149	0.0726, 0.1011	0.1011, 0.1893	0.0256, 0.0551	0.0958, 0.1620

$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = \Sigma\,(|F_o|^2 - |F_c|^2)^2]\}^{½}$

Table S2. Bond lengths [Å] and angles [°] for compound **5**.

N(1)-C(2)	1.338(2)	(1)-H(1A)	0.85(2)
N(1)-H(1B)	0.88(2) C(2)-N(3)	1.327(2)	
C(2)-N(6)	1.343(2)	N(3)-N(4)	1.369(2)
N(4)-N(5)	1.281(2)	N(5)-N(6)	1.369(2)
N(6)-C(7)	1.453(2)	C(7)-C(8)	1.508(3)
C(7)-H(7A)	0.9700 C(7)-H(7B)	0.9700	
C(8)-N(9)	1.447(3)	C(8)-H(8A)	0.9700
C(8)-H(8B)	0.9700 N(9)-C(13)	1.332(3)	
N(9)-N(10)	1.347(2)	N(10)-C(11)	1.324(3)
C(11)-C(12)	1.364(4)	C(11)-H(11)	0.9300
C(12)-C(13)	1.358(4)	C(12)-H(12)	0.9300
C(13)-H(13)	0.9300		

C(2)-N(1)-H(1A)	118.8(16)	C(2)-N(1)-H(1B)	117.9(15)
H(1A)-N(1)-H(1B)	123(2)	N(3)-C(2)-N(1)	126.21(18)
N(3)-C(2)-N(6)	108.82(15)	N(1)-C(2)-N(6)	124.97(17)
C(2)-N(3)-N(4)	105.11(15)	N(5)-N(4)-N(3)	111.94(15)
N(4)-N(5)-N(6)	106.03(15)	C(2)-N(6)-N(5)	108.09(14)
C(2)-N(6)-C(7)	130.14(15)	N(5)-N(6)-C(7)	121.27(15)
N(6)-C(7)-C(8)	111.40(15)	N(6)-C(7)-H(7A)	109.3
C(8)-C(7)-H(7A)	109.3	N(6)-C(7)-H(7B)	109.3
C(8)-C(7)-H(7B)	109.3	H(7A)-C(7)-H(7B)	108.0
N(9)-C(8)-C(7)	111.63(16)	N(9)-C(8)-H(8A)	109.3
C(7)-C(8)-H(8A)	109.3	N(9)-C(8)-H(8B)	109.3
C(7)-C(8)-H(8B)	109.3	H(8A)-C(8)-H(8B)	108.0
C(13)-N(9)-N(10)	112.0(2)	C(13)-N(9)-C(8)	127.9(2)
N(10)-N(9)-C(8)	119.68(18)	C(11)-N(10)-N(9)	103.7(2)
N(10)-C(11)-C(12)	112.2(2)	N(10)-C(11)-H(11)	123.9
C(12)-C(11)-H(11)	123.9	C(13)-C(12)-C(11)	105.2(3)
C(13)-C(12)-H(12)	127.4	C(11)-C(12)-H(12)	127.4
N(9)-C(13)-C(12)	106.8(3)	N(9)-C(13)-H(13)	126.6
C(12)-C(13)-H(13)	126.6		

Table S3. Hydrogen bonds for compound **5** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)	
N(1)-H(1A)...N(4)#1		0.85(2)	2.12(3)	2.964(2)	169(2)
N(1)-H(1B)...N(3)#2		0.88(2)	2.12(3)	2.994(2)	172(2)

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z-1 #2 -x+1,-y,-z+2

Table S4. Bond lengths [Å] and angles [°] for compound **7**.

O(1)-N(3)	1.2272(18)	O(2)-N(3)	1.230(2)
N(3)-C(4)	1.422(2)	C(4)-C(8)	1.372(2)
C(4)-C(5)	1.392(2)	C(5)-N(6)	1.323(2)
C(5)-H(5)	0.9300	N(6)-N(7)	1.3712(18)
N(7)-C(8)	1.326(2)	N(7)-C(9)	1.4584(19)
C(8)-H(8)	0.9300	C(9)-C(10)	1.515(3)
C(9)-H(9A)	0.9700	C(9)-H(9B)	0.9700
C(10)-N(11)	1.459(2)	C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700	N(11)-C(15)	1.347(2)
N(11)-N(12)	1.358(2)	N(12)-N(13)	1.277(2)
N(13)-N(14)	1.361(2)	N(14)-C(15)	1.338(2)
N(14)-H(14)	0.98(2)	C(15)-N(16)	1.336(2)
N(16)-N(17)	1.3413(19)	N(17)-O(19)	1.2318(18)
N(17)-O(18)	1.2372(19)	O(1S)-H(1S)	0.823(10)
O(1S)-H(2S)	0.817(10)		
O(1)-N(3)-O(2)	123.51(15)	O(1)-N(3)-C(4)	118.06(15)
O(2)-N(3)-C(4)	118.42(14)	C(8)-C(4)-C(5)	106.39(13)
C(8)-C(4)-N(3)	125.61(15)	C(5)-C(4)-N(3)	127.89(14)
N(6)-C(5)-C(4)	110.64(13)	N(6)-C(5)-H(5)	124.7
C(4)-C(5)-H(5)	124.7	C(5)-N(6)-N(7)	104.29(13)
C(8)-N(7)-N(6)	112.83(13)	C(8)-N(7)-C(9)	127.39(14)
N(6)-N(7)-C(9)	119.74(13)	N(7)-C(8)-C(4)	105.84(14)
N(7)-C(8)-H(8)	127.1	C(4)-C(8)-H(8)	127.1
N(7)-C(9)-C(10)	113.02(14)	N(7)-C(9)-H(9A)	109.0
C(10)-C(9)-H(9A)	109.0	N(7)-C(9)-H(9B)	109.0
C(10)-C(9)-H(9B)	109.0	H(9A)-C(9)-H(9B)	107.8
N(11)-C(10)-C(9)	112.37(13)	N(11)-C(10)-H(10A)	109.1
C(9)-C(10)-H(10A)	109.1	N(11)-C(10)-H(10B)	109.1
C(9)-C(10)-H(10B)	109.1	H(10A)-C(10)-H(10B)	107.9
C(15)-N(11)-N(12)	110.17(14)	C(15)-N(11)-C(10)	127.76(14)
N(12)-N(11)-C(10)	122.03(13)	N(13)-N(12)-N(11)	107.65(13)
N(12)-N(13)-N(14)	108.27(14)	C(15)-N(14)-N(13)	109.94(15)
C(15)-N(14)-H(14)	129.8(11)	N(13)-N(14)-H(14)	120.2(11)
N(16)-C(15)-N(14)	136.59(15)	N(16)-C(15)-N(11)	119.40(15)
N(14)-C(15)-N(11)	103.95(14)	C(15)-N(16)-N(17)	115.53(14)
O(19)-N(17)-O(18)	121.55(14)	O(19)-N(17)-N(16)	116.44(15)
O(18)-N(17)-N(16)	122.00(14)	H(1S)-O(1S)-H(2S)	91.0(13)

Table S5. Hydrogen bonds for compound **7** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(9)-H(9B)...O(1)#1	0.97	2.56	3.108(2)	115.5
C(10)-H(10B)...N(13)#2	0.97	2.55	3.519(2)	173.4
N(14)-H(14)...O(1S)#3	0.98(2)	1.69(2)	2.646(2)	163.0(17)
O(1S)-H(1S)...O(18)#4	0.823(10)	2.115(10)	2.9239(19)	167(2)
O(1S)-H(2S)...O(19)#5	0.817(10)	2.165(10)	2.977(2)	173(3)

Symmetry transformations used to generate equivalent atoms:
#1 x,y-1,z #2 x,-y+1/2,z+1/2 #3 -x+1,y-1/2,-z+1/2
#4 x+1,y+1,z+1 #5 -x+1,-y,-z+1

Table S6. Bond lengths [Å] and angles [°] for compound **8**.

N(1)-C(2)	1.327(2)	N(1)-N(5)	1.3527(17)
C(2)-C(3)	1.377(2)	C(2)-H(2)	0.9300
C(3)-C(4)	1.355(2)	C(3)-H(3)	0.9300
C(4)-N(5)	1.343(2)	C(4)-H(4)	0.9300
N(5)-C(6)	1.441(2)	C(6)-C(7)	1.508(2)
C(6)-H(6A)	0.9700	C(6)-H(6B)	0.9700
C(7)-N(8)	1.4622(18)	C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700	N(8)-C(12)	1.339(2)
N(8)-N(9)	1.3464(19)	N(9)-N(10)	1.302(2)
N(10)-N(11)	1.365(2)	N(11)-C(12)	1.315(2)
C(12)-N(13)	1.395(2)	N(13)-N(14)	1.2504(17)
N(14)-O(15)	1.3386(19)	O(15)-H(15)	0.853(9)
C(2)-N(1)-N(5)	104.94(13)	N(1)-C(2)-C(3)	111.58(15)
N(1)-C(2)-H(2)	124.2	C(3)-C(2)-H(2)	124.2
C(4)-C(3)-C(2)	104.94(15)	C(4)-C(3)-H(3)	127.5
C(2)-C(3)-H(3)	127.5	N(5)-C(4)-C(3)	107.98(14)
N(5)-C(4)-H(4)	126.0	C(3)-C(4)-H(4)	126.0
C(4)-N(5)-N(1)	110.56(13)	C(4)-N(5)-C(6)	128.55(13)
N(1)-N(5)-C(6)	120.71(12)	N(5)-C(6)-C(7)	112.63(13)
N(5)-C(6)-H(6A)	109.1	C(7)-C(6)-H(6A)	109.1
N(5)-C(6)-H(6B)	109.1	C(7)-C(6)-H(6B)	109.1
H(6A)-C(6)-H(6B)	107.8	N(8)-C(7)-C(6)	112.17(12)
N(8)-C(7)-H(7A)	109.2	C(6)-C(7)-H(7A)	109.2
N(8)-C(7)-H(7B)	109.2	C(6)-C(7)-H(7B)	109.2
H(7A)-C(7)-H(7B)	107.9	C(12)-N(8)-N(9)	108.30(13)
C(12)-N(8)-C(7)	128.76(14)	N(9)-N(8)-C(7)	122.86(14)
N(10)-N(9)-N(8)	105.86(15)	N(9)-N(10)-N(11)	111.43(14)
C(12)-N(11)-N(10)	104.74(15)	N(11)-C(12)-N(8)	109.66(16)

N(11)-C(12)-N(13)	132.12(16)	N(8)-C(12)-N(13)	118.21(13)
N(14)-N(13)-C(12)	112.69(13)	N(13)-N(14)-O(15)	109.26(13)
N(14)-O(15)-H(15)	102.3(15)		

Table S7. Hydrogen bonds for compound **8** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(2)-H(2)...N(13)#1	0.93	2.60	3.526(2)	176.6
O(15)-H(15)...N(1)#2	0.853(9)	1.772(10)	2.6200(17)	172(2)

Symmetry transformations used to generate equivalent atoms:
#1 x,y,z+1 #2 -x+1,-y+1,-z+1

Table S8. Bond lengths [Å] and angles [°] for compound **9**.

O(1)-N(3)	1.241(5)	O(2)-N(3)	1.243(5)
N(3)-N(4)	1.348(6)	N(4)-C(5)	1.344(6)
C(5)-N(9)	1.344(6)	C(5)-N(6)	1.346(6)
N(6)-N(7)	1.367(5)	N(7)-N(8)	1.279(6)
N(8)-N(9)	1.372(5)	N(9)-C(10)	1.463(6)
C(10)-C(11)	1.523(7)	C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900	C(11)-N(12)	1.462(6)
C(11)-H(11A)	0.9900	C(11)-H(11B)	0.9900
N(12)-N(13)	1.335(5)	N(12)-C(20)	1.357(6)
N(13)-C(14)	1.319(6)	C(14)-C(18)	1.399(8)
C(14)-N(15)	1.459(7)	N(15)-O(16)	1.211(6)
N(15)-O(17)	1.225(6)	C(18)-C(20)	1.384(7)
C(18)-Cl(19)	1.684(5)	C(20)-N(21)	1.443(7)
N(21)-O(23)	1.210(6)	N(21)-O(22)	1.219(6)
O(1S)-H(1S)	0.92(6)	O(1S)-H(2S)	0.82(6)
O(1)-N(3)-O(2)	122.2(4)	O(1)-N(3)-N(4)	121.6(4)
O(2)-N(3)-N(4)	116.2(4)	C(5)-N(4)-N(3)	115.7(4)
N(9)-C(5)-N(4)	119.2(4)	N(9)-C(5)-N(6)	105.4(4)
N(4)-C(5)-N(6)	135.4(5)	C(5)-N(6)-N(7)	108.4(4)
N(8)-N(7)-N(6)	109.5(4)	N(7)-N(8)-N(9)	107.1(4)
C(5)-N(9)-N(8)	109.6(4)	C(5)-N(9)-C(10)	127.8(4)
N(8)-N(9)-C(10)	121.5(4)	N(9)-C(10)-C(11)	110.7(4)
N(9)-C(10)-H(10A)	109.5	C(11)-C(10)-H(10A)	109.5
N(9)-C(10)-H(10B)	109.5	C(11)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	108.1	N(12)-C(11)-C(10)	109.7(4)
N(12)-C(11)-H(11A)	109.7	C(10)-C(11)-H(11A)	109.7
N(12)-C(11)-H(11B)	109.7	C(10)-C(11)-H(11B)	109.7

H(11A)-C(11)-H(11B)	108.2	N(13)-N(12)-C(20)	110.8(4)
N(13)-N(12)-C(11)	116.0(4)	C(20)-N(12)-C(11)	132.3(4)
C(14)-N(13)-N(12)	105.1(4)	N(13)-C(14)-C(18)	113.5(4)
N(13)-C(14)-N(15)	117.8(5)	C(18)-C(14)-N(15)	128.7(5)
O(16)-N(15)-O(17)	125.4(5)	O(16)-N(15)-C(14)	117.9(5)
O(17)-N(15)-C(14)	116.7(5)	C(20)-C(18)-C(14)	101.9(5)
C(20)-C(18)-Cl(19)	129.0(5)	C(14)-C(18)-Cl(19)	128.9(4)
N(12)-C(20)-C(18)	108.6(5)	N(12)-C(20)-N(21)	123.0(4)
C(18)-C(20)-N(21)	128.4(5)	O(23)-N(21)-O(22)	125.1(5)
O(23)-N(21)-C(20)	116.8(5)	O(22)-N(21)-C(20)	118.1(5)
H(1S)-O(1S)-H(2S)	103(5)		

Table S9. Hydrogen bonds for compound **9** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(10)-H(10B)...O(1S)#1	0.99	2.60	3.393(6)	136.6
C(11)-H(11B)...O(17)#2	0.99	2.47	3.163(6)	126.4
C(11)-H(11B)...O(22)	0.99	2.25	2.815(7)	114.8
O(1S)-H(1S)...O(2)#3	0.92(6)	2.01(6)	2.891(5)	161(5)
O(1S)-H(2S)...N(4)#4	0.82(6)	2.08(6)	2.803(5)	147(6)

Symmetry transformations used to generate equivalent atoms:
#1 x,y+2,z+1 #2 x,-y+3/2,z+1/2 #3 -x,-y-1,-z+1
#4 x,y-2,z-1

Table S10. Bond lengths [Å] and angles [°] for compound **12**.

N(1)-C(5)	1.3447(18)	N(1)-N(2)	1.3453(16)
N(2)-C(3)	1.3439(18)	C(3)-C(4)	1.3849(19)
C(3)-N(6)	1.4352(18)	C(4)-C(5)	1.3832(19)
C(4)-N(9)	1.4536(17)	C(5)-N(12)	1.4409(17)
N(6)-O(7)	1.2252(17)	N(6)-O(8)	1.2353(17)
N(9)-O(10)	1.2131(17)	N(9)-O(11)	1.2165(18)
N(12)-O(14)	1.2261(16)	N(12)-O(13)	1.2268(16)
N(1S)-C(2S)	1.492(2)	N(1S)-H(1S)	0.884(19)
N(1S)-H(2S)	0.86(2)	N(1S)-H(3S)	0.899(19)
C(2S)-C(3S)	1.503(2)	C(2S)-H(5S)	0.9900
C(2S)-H(4S)	0.9900	C(3S)-Br(4S)	1.9495(15)
C(3S)-H(7S)	0.9900	C(3S)-H(6S)	0.9900
C(5)-N(1)-N(2)	107.73(11)	C(3)-N(2)-N(1)	107.09(11)
N(2)-C(3)-C(4)	111.83(12)	N(2)-C(3)-N(6)	120.19(12)

C(4)-C(3)-N(6)	127.91(12)	C(5)-C(4)-C(3)	101.91(12)
C(5)-C(4)-N(9)	128.67(12)	C(3)-C(4)-N(9)	129.38(12)
N(1)-C(5)-C(4)	111.45(12)	N(1)-C(5)-N(12)	121.35(12)
C(4)-C(5)-N(12)	127.21(12)	O(7)-N(6)-O(8)	124.27(12)
O(7)-N(6)-C(3)	118.52(12)	O(8)-N(6)-C(3)	117.19(12)
O(10)-N(9)-O(11)	124.88(13)	O(10)-N(9)-C(4)	118.15(12)
O(11)-N(9)-C(4)	116.97(12)	O(14)-N(12)-O(13)	125.28(12)
O(14)-N(12)-C(5)	118.40(12)	O(13)-N(12)-C(5)	116.32(12)
C(2S)-N(1S)-H(1S)	109.5(12)	C(2S)-N(1S)-H(2S)	110.7(12)
H(1S)-N(1S)-H(2S)	108.6(17)	C(2S)-N(1S)-H(3S)	109.7(12)
H(1S)-N(1S)-H(3S)	107.2(17)	H(2S)-N(1S)-H(3S)	111.2(17)
N(1S)-C(2S)-C(3S)	112.81(12)	N(1S)-C(2S)-H(5S)	109.0
C(3S)-C(2S)-H(5S)	109.0	N(1S)-C(2S)-H(4S)	109.0
C(3S)-C(2S)-H(4S)	109.0	H(5S)-C(2S)-H(4S)	107.8
C(2S)-C(3S)-Br(4S)	111.31(11)	C(2S)-C(3S)-H(7S)	109.4
Br(4S)-C(3S)-H(7S)	109.4	C(2S)-C(3S)-H(6S)	109.4
Br(4S)-C(3S)-H(6S)	109.4	H(7S)-C(3S)-H(6S)	108.0

Table S11. Hydrogen bonds for compound **12** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1S)-H(1S)...N(1)#1	0.884(19)	2.06(2)	2.9110(17)	162.4(18)
N(1S)-H(2S)...O(8)#2	0.86(2)	2.47(2)	3.2644(18)	152.4(16)
N(1S)-H(3S)...N(2)#3	0.899(19)	2.117(19)	2.9637(17)	156.8(16)
C(2S)-H(4S)...O(13)#4	0.99	2.55	3.3265(19)	135.2
C(3S)-H(6S)...O(10)#5	0.99	2.52	3.267(2)	132.5

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z #2 -x+1,-y+2,-z #3 x-1,-y+3/2,z+1/2
#4 -x+1,y+1/2,-z+1/2 #5 x,-y+3/2,z+1/2

Table S12. Bond lengths [Å] and angles [°] for compound **13**.

N(1A)-C(2A)	1.334(5)	N(1A)-H(1A)	0.92(4)
N(1A)-H(2A)	0.83(5)	C(2A)-N(3A)	1.335(4)
C(2A)-N(6A)	1.342(5)	N(3A)-N(4A)	1.366(4)
N(4A)-N(5A)	1.288(4)	N(5A)-N(6A)	1.369(4)
N(6A)-C(7A)	1.463(4)	C(7A)-C(8A)	1.508(5)
C(7A)-H(7A1)	0.9900	C(7A)-H(7A2)	0.9900
C(8A)-N(9A)	1.467(4)	C(8A)-H(8A1)	0.9900
C(8A)-H(8A2)	0.9900	N(9A)-N(10A)	1.320(4)
N(9A)-C(17A)	1.382(5)	N(10A)-C(11A)	1.337(4)
C(11A)-C(15A)	1.407(5)	C(11A)-N(12A)	1.419(5)
N(12A)-O(14A)	1.229(4)	N(12A)-O(13A)	1.244(4)

C(15A)-N(16A)	1.349(5)	C(15A)-C(17A)	1.397(5)
N(16A)-H(16A)	0.92(2)	N(16A)-H(17A)	0.92(2)
C(17A)-N(18A)	1.392(5)	N(18A)-O(20A)	1.235(4)
N(18A)-O(19A)	1.243(4)	N(1B)-C(2B)	1.341(4)
N(1B)-H(1B)	0.91(4)	N(1B)-H(2B)	0.88(4)
C(2B)-N(3B)	1.328(4)	C(2B)-N(6B)	1.352(4)
N(3B)-N(4B)	1.361(4)	N(4B)-N(5B)	1.285(4)
N(5B)-N(6B)	1.365(4)	N(6B)-C(7B)	1.454(4)
C(7B)-C(8B)	1.525(5)	C(7B)-H(7B1)	0.9900
C(7B)-H(7B2)	0.9900	C(8B)-N(9B)	1.473(4)
C(8B)-H(8B1)	0.9900	C(8B)-H(8B2)	0.9900
N(9B)-N(10B)	1.327(4)	N(9B)-C(17B)	1.385(4)
N(10B)-C(11B)	1.333(5)	C(11B)-C(15B)	1.399(5)
C(11B)-N(12B)	1.428(5)	N(12B)-O(13B)	1.226(4)
N(12B)-O(14B)	1.239(4)	C(15B)-N(16B)	1.347(5)
C(15B)-C(17B)	1.396(5)	N(16B)-H(16B)	0.92(2)
N(16B)-H(17B)	0.92(2)	C(17B)-N(18B)	1.401(5)
N(18B)-O(20B)	1.230(4)	N(18B)-O(19B)	1.239(4)
C(2A)-N(1A)-H(1A)	118(3)	C(2A)-N(1A)-H(2A)	121(3)
H(1A)-N(1A)-H(2A)	119(4)	N(1A)-C(2A)-N(3A)	126.1(3)
N(1A)-C(2A)-N(6A)	125.3(3)	N(3A)-C(2A)-N(6A)	108.6(3)
C(2A)-N(3A)-N(4A)	104.9(3)	N(5A)-N(4A)-N(3A)	112.3(3)
N(4A)-N(5A)-N(6A)	105.5(3)	C(2A)-N(6A)-N(5A)	108.6(3)
C(2A)-N(6A)-C(7A)	130.6(3)	N(5A)-N(6A)-C(7A)	120.8(3)
N(6A)-C(7A)-C(8A)	113.8(3)	N(6A)-C(7A)-H(7A1)	108.8
C(8A)-C(7A)-H(7A1)	108.8	N(6A)-C(7A)-H(7A2)	108.8
C(8A)-C(7A)-H(7A2)	108.8	H(7A1)-C(7A)-H(7A2)	107.7
N(9A)-C(8A)-C(7A)	111.8(3)	N(9A)-C(8A)-H(8A1)	109.3
C(7A)-C(8A)-H(8A1)	109.3	N(9A)-C(8A)-H(8A2)	109.3
C(7A)-C(8A)-H(8A2)	109.3	H(8A1)-C(8A)-H(8A2)	107.9
N(10A)-N(9A)-C(17A)	111.2(3)	N(10A)-N(9A)-C(8A)	117.5(3)

Table S13. Hydrogen bonds for compound **13** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8A)-H(8A1)...O(19A)#1	0.99	2.58	3.417(4)	142.4
C(8A)-H(8A2)...O(20A)	0.99	2.31	2.877(5)	115.1
C(8B)-H(8B1)...O(20B)	0.99	2.33	2.895(4)	115.6
C(8B)-H(8B2)...O(19B)#2	0.99	2.52	3.184(5)	123.9
N(16A)-H(16A)...O(13A)	0.92(2)	2.32(4)	2.859(4)	117(3)
N(16A)-H(16A)...O(14B)#3	0.92(2)	2.24(2)	3.150(4)	170(3)
N(1B)-H(1B)...N(3A)	0.91(4)	2.07(4)	2.966(5)	168(3)
N(1A)-H(1A)...N(3B)	0.92(4)	2.07(5)	2.976(5)	167(4)

N(16A)-H(17A)...O(14A)#20.92(2)	2.38(4)	2.957(4)	120(4)
N(16A)-H(17A)...O(19A)0.92(2)	2.16(4)	2.810(4)	127(4)
N(16B)-H(16B)...O(13B)#10.92(2)	2.56(3)	3.077(4)	117(3)
N(16B)-H(16B)...O(19B)0.92(2)	2.19(3)	2.785(5)	122(3)
N(16B)-H(17B)...O(13A)#40.92(2)	2.41(3)	3.274(5)	157(5)
N(16B)-H(17B)...O(14B)0.92(2)	2.26(6)	2.841(5)	121(5)

Symmetry transformations used to generate equivalent atoms:
#1 x+1,y,z #2 x-1,y,z #3 x,y+1,z-1 #4 x,y-1,z+1

4. NMR spectra

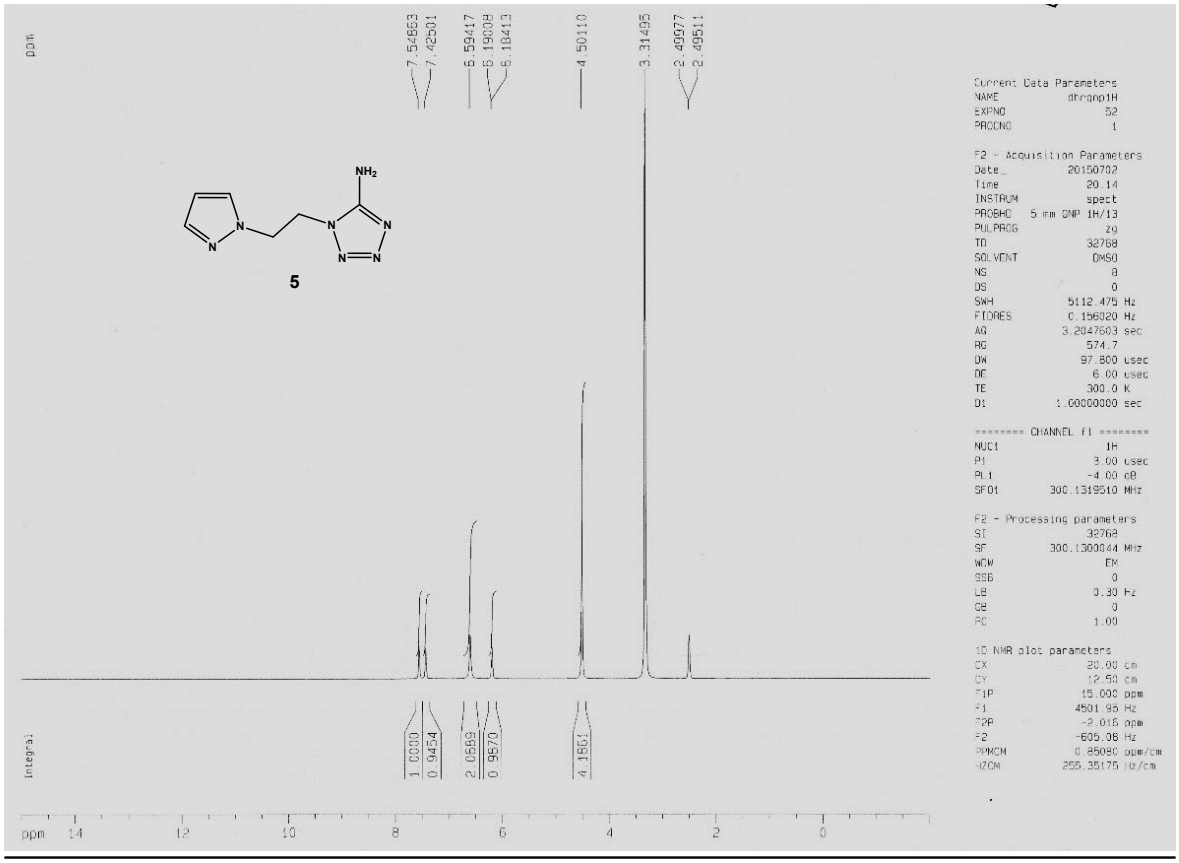


Fig S4: ^{1}H NMR Spectrum of compound **5**

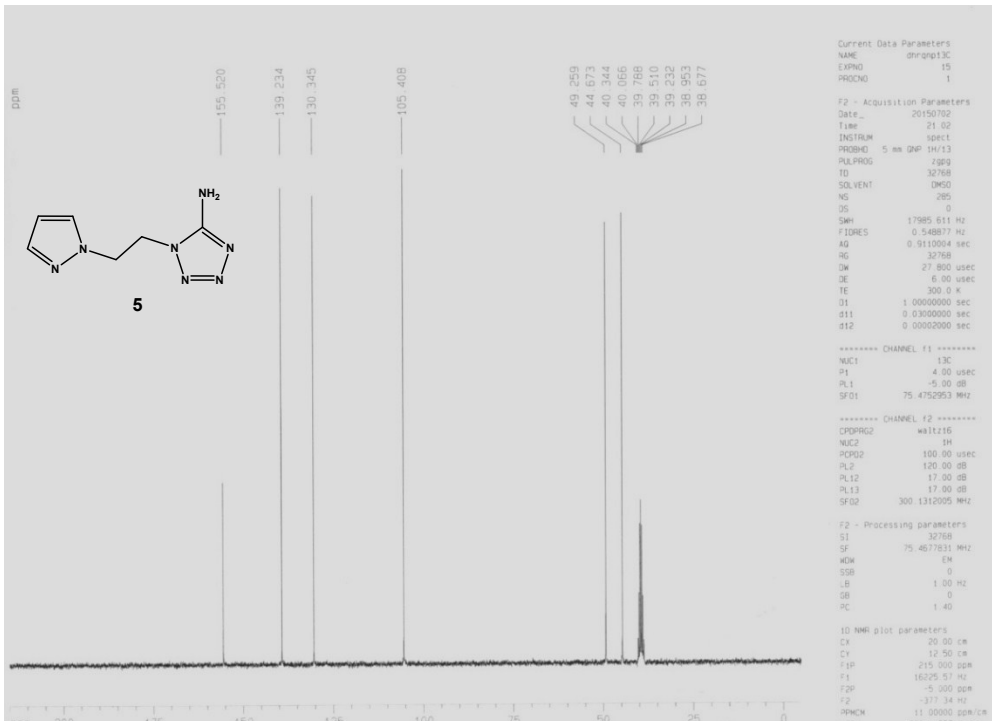


Fig S5: $^{13}C\{^{1}H\}$ NMR Spectrum of compound **5**

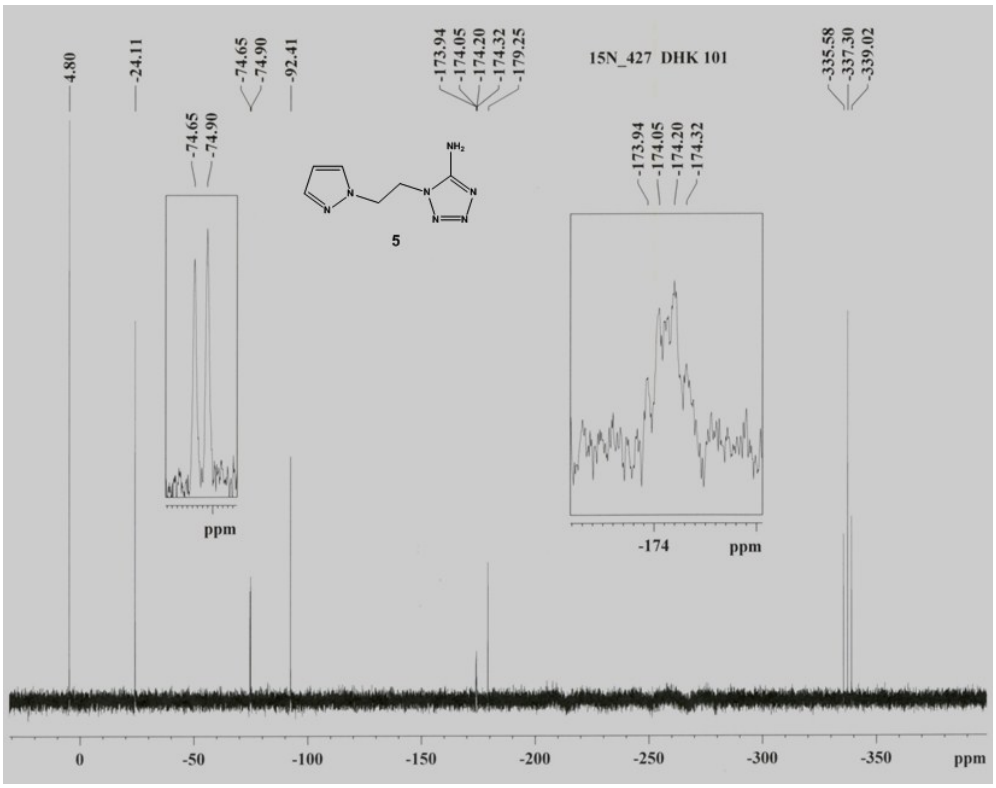


Fig S6: ^{15}N NMR Spectrum of compound **5**

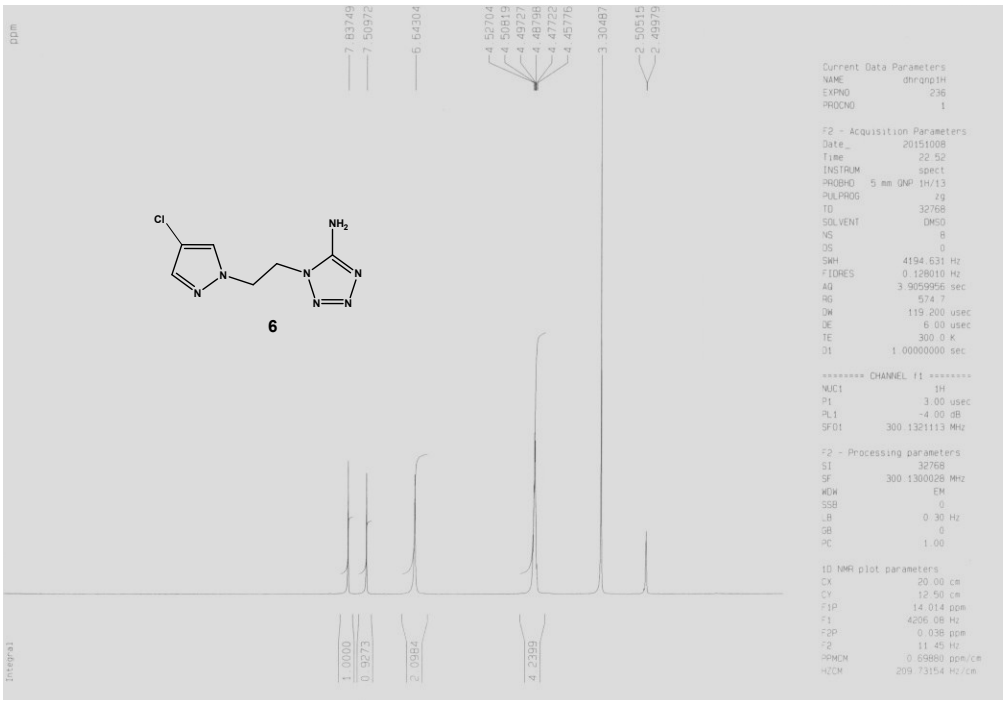


Fig S7: ^{1}H NMR Spectrum of compound **6**

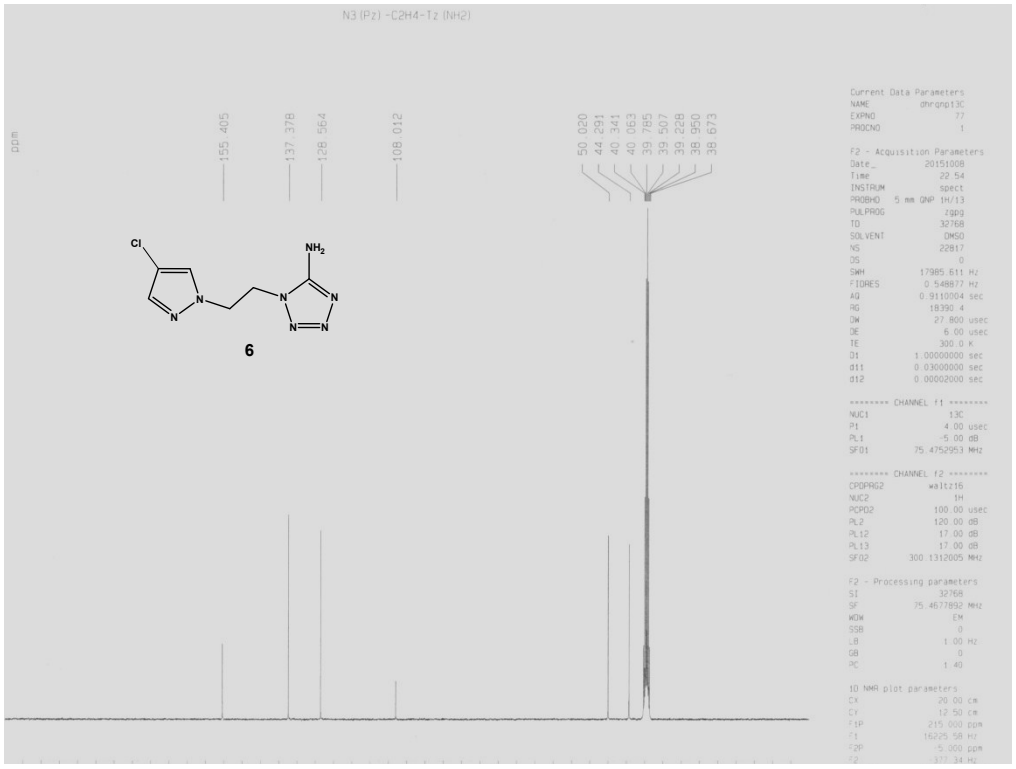


Fig S8: ^{13}C{^{1}H} NMR Spectrum of compound **6**

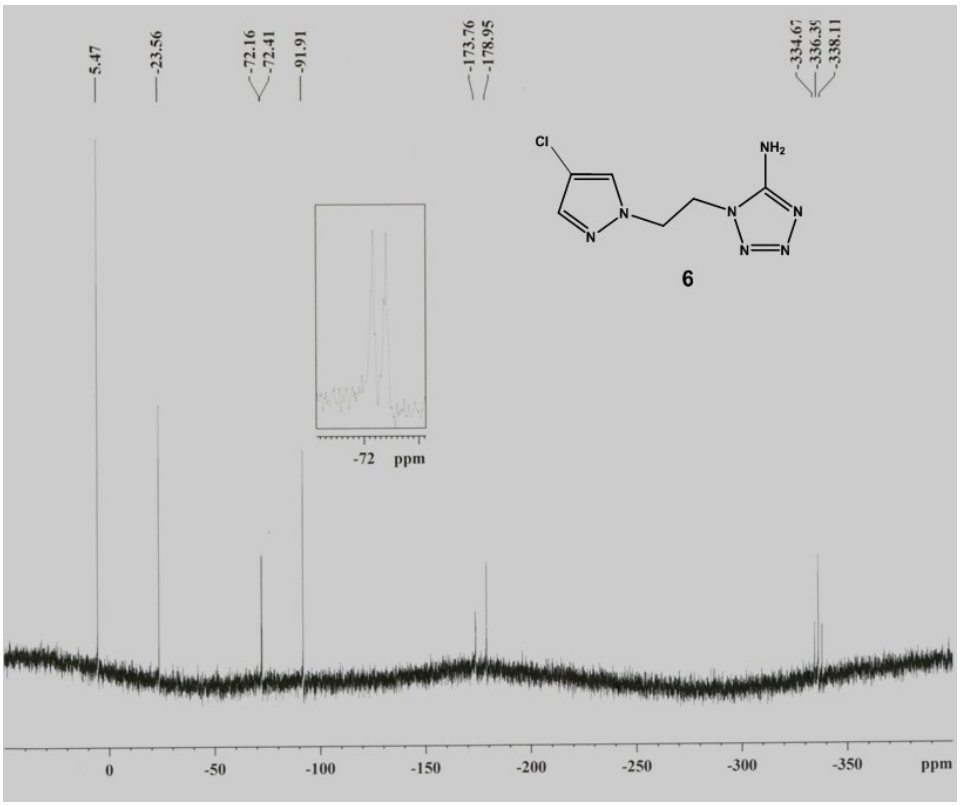


Fig S9: ^{15}N NMR Spectrum of compound **6**

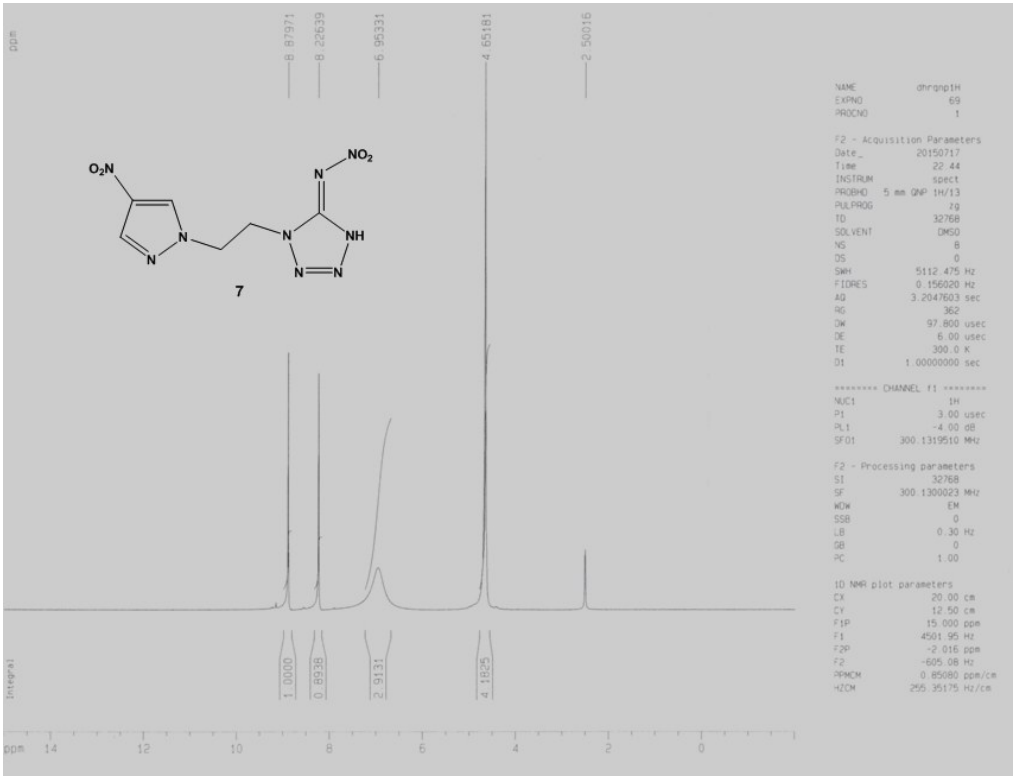


Fig S10: ^{1}H NMR Spectrum of compound **7**

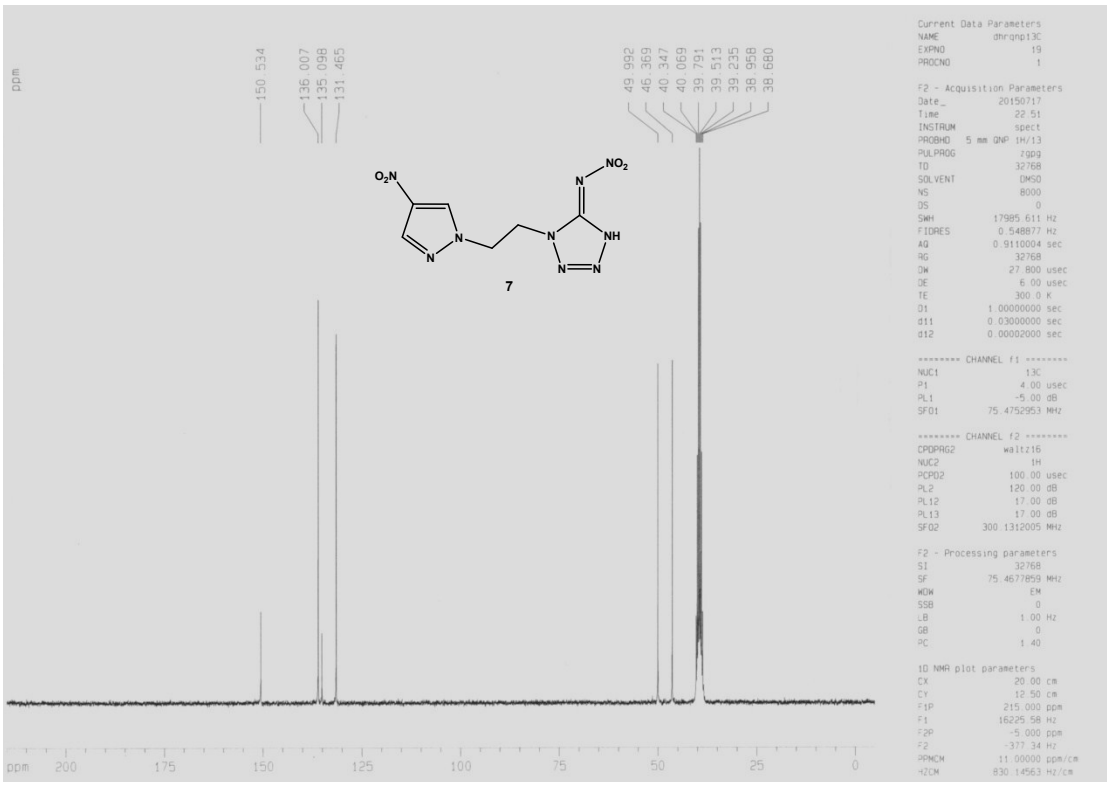


Fig S11: $^{13}C\{^{1}H\}$ NMR Spectrum of compound **7**

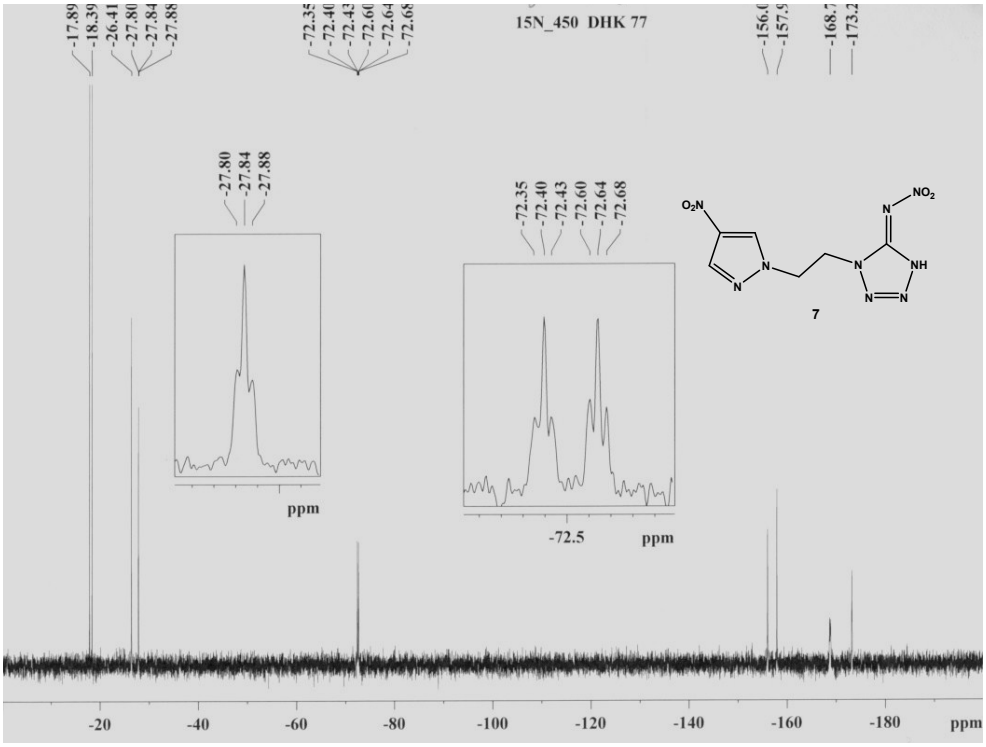


Fig S12: ^{15}N NMR Spectrum of compound **7**

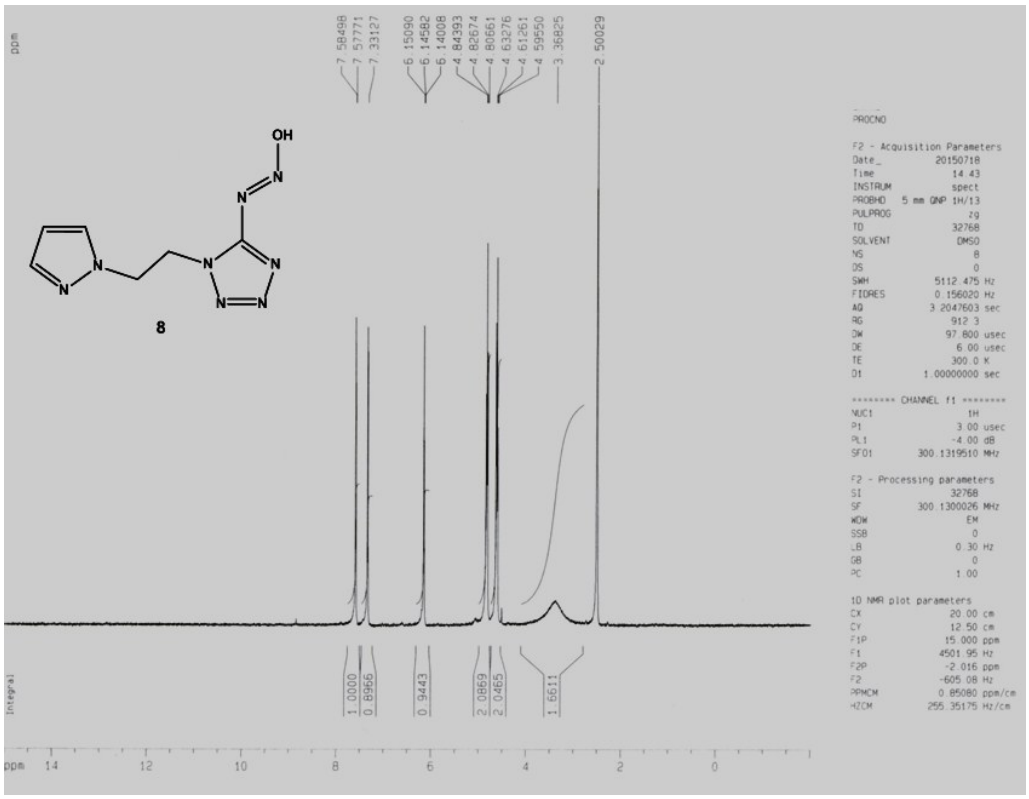


Fig S13: ^{1}H NMR Spectrum of compound **8**

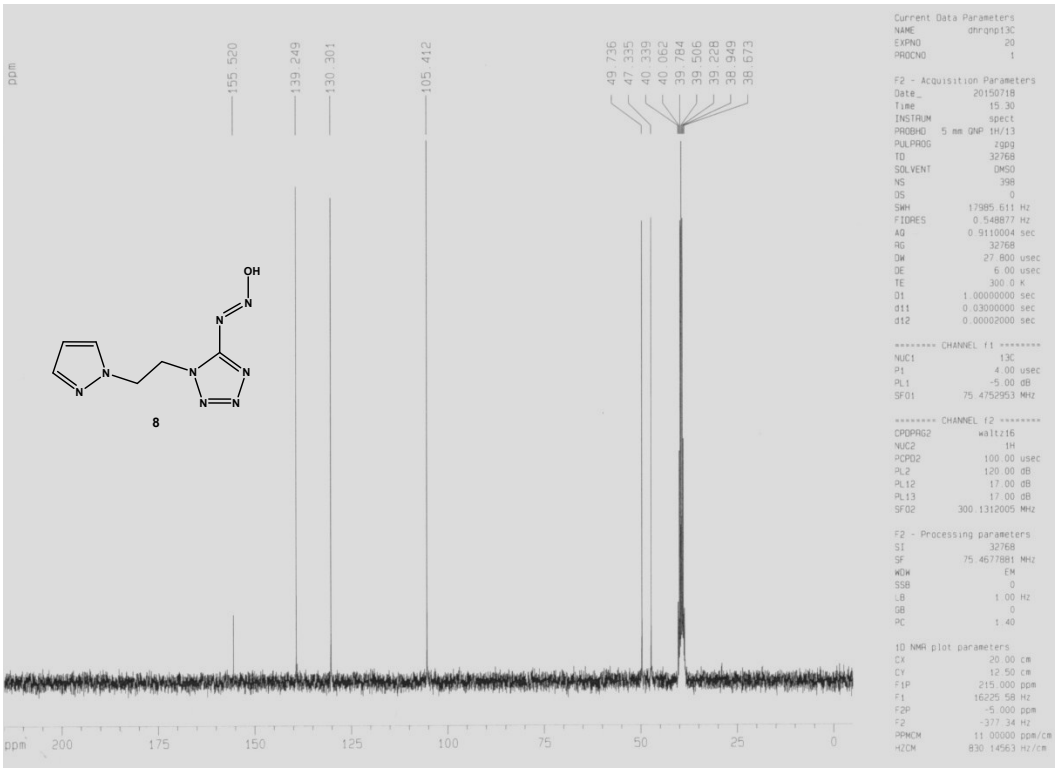


Fig S14: ^{13}C{^{1}H} NMR Spectrum of compound **8**

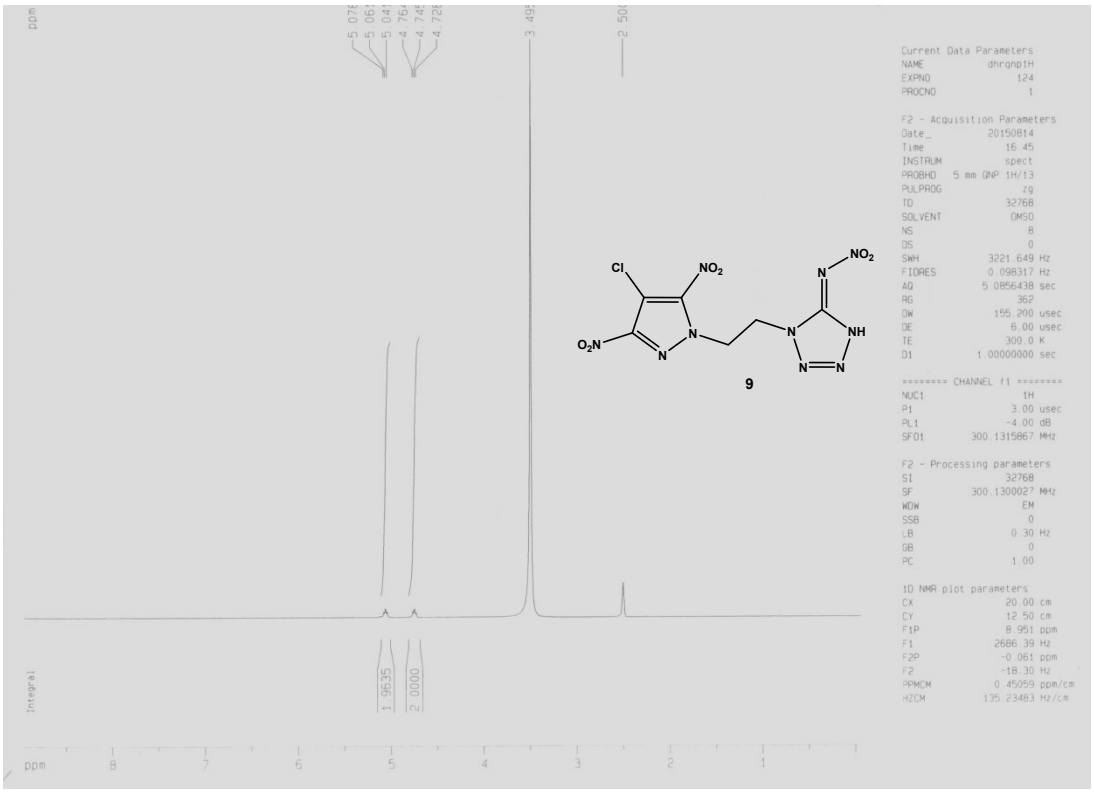


Fig S15: ^{1}H NMR Spectrum of compound **9**

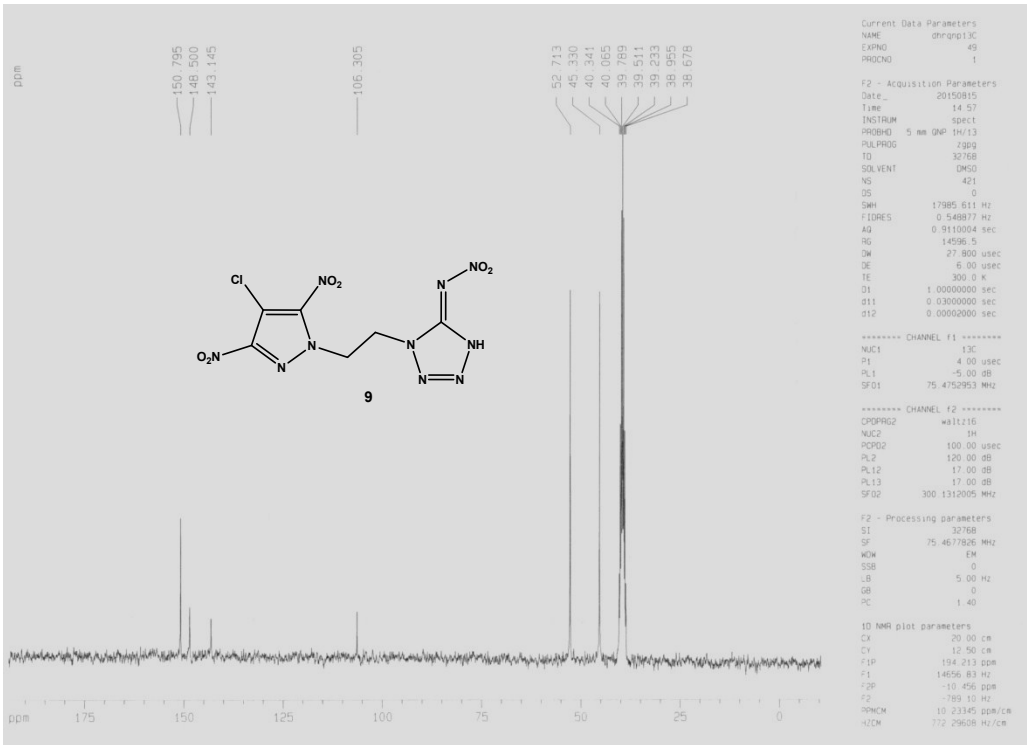


Fig S16: ^{13}C{^{1}H} NMR Spectrum of compound **9**

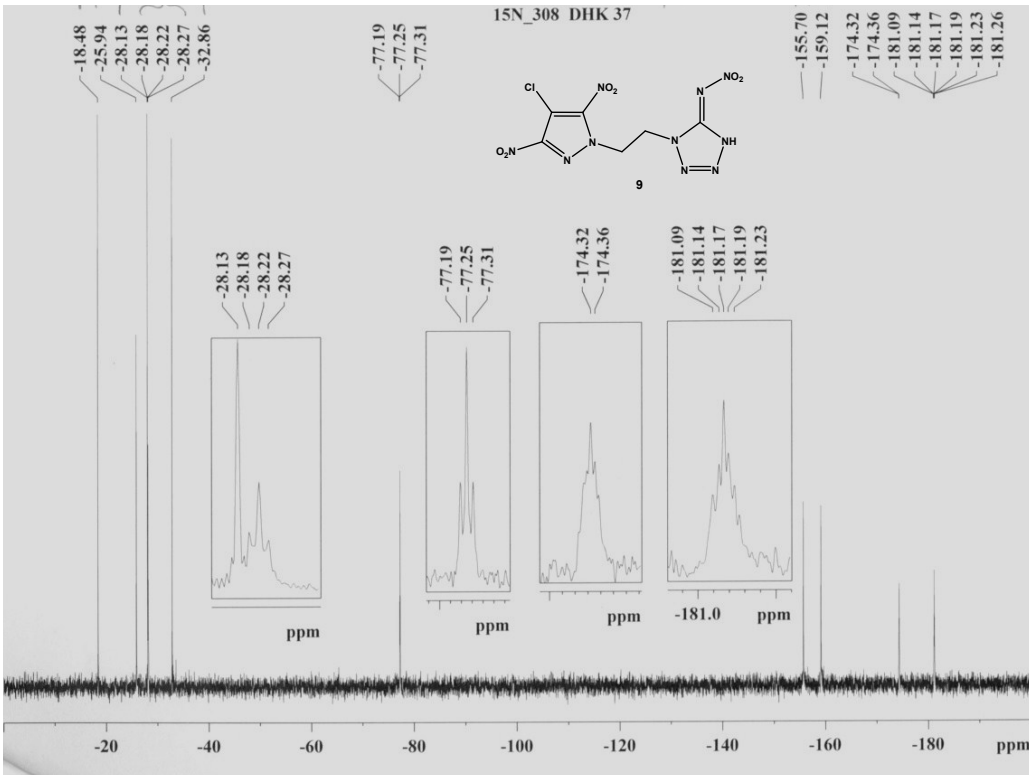


Fig S17: ^{15}N NMR Spectrum of compound **9**

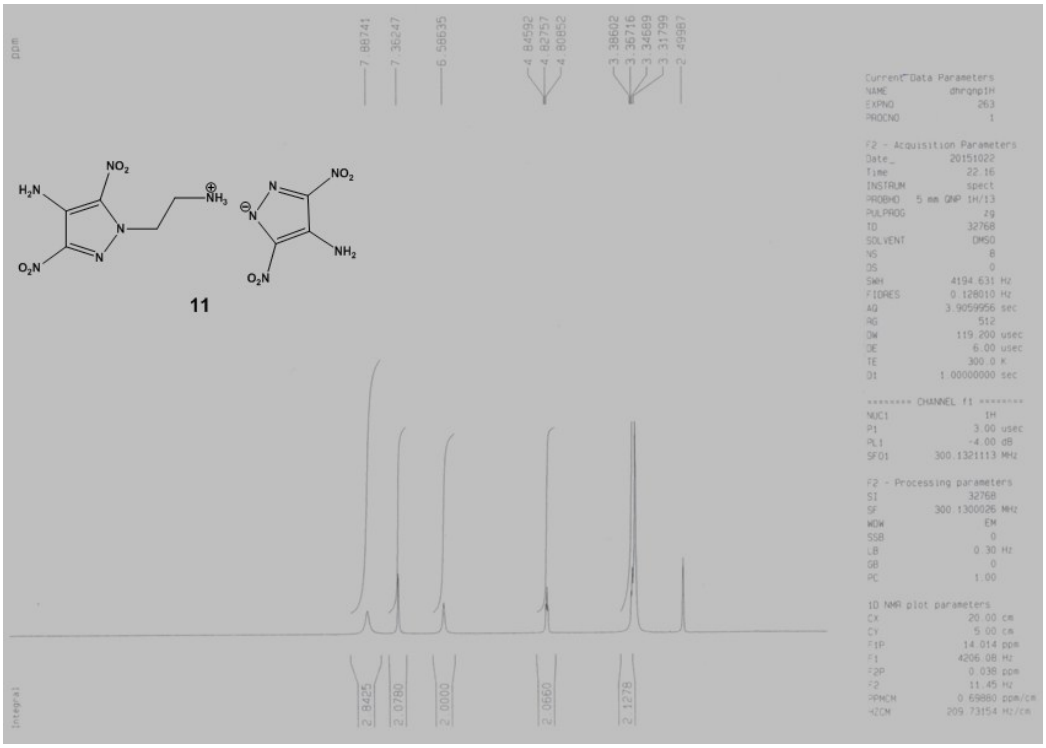


Fig S18: ^{1}H NMR Spectrum of compound **11**

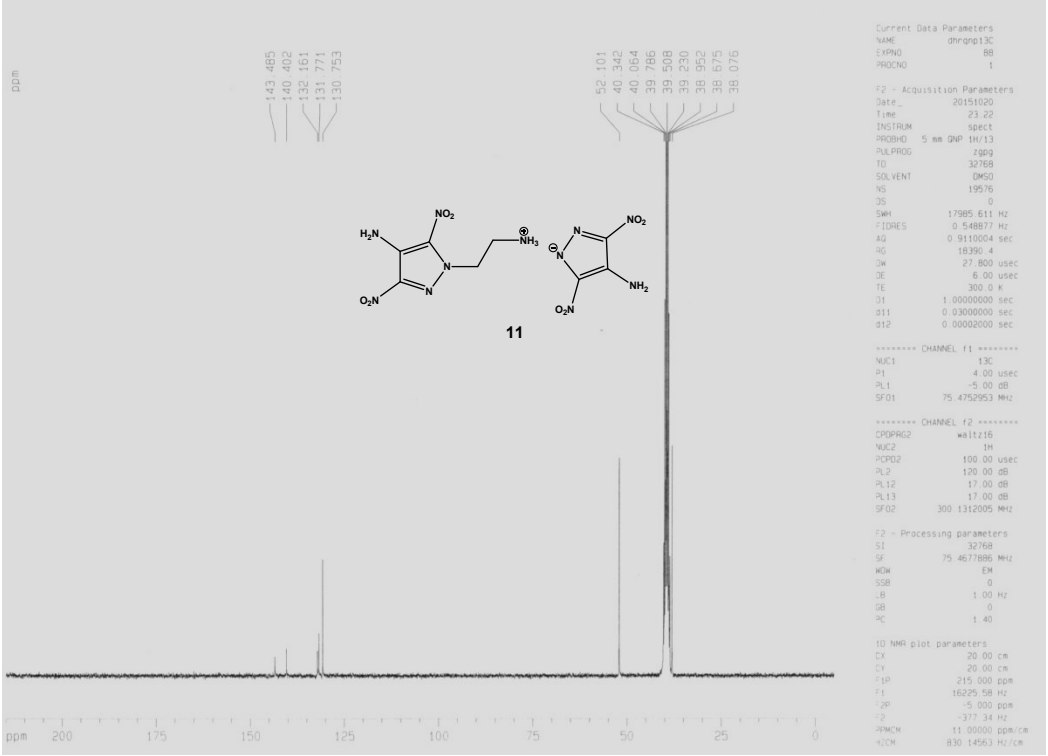


Fig S19: $^{13}C\{^{1}H\}$ NMR Spectrum of compound **11**

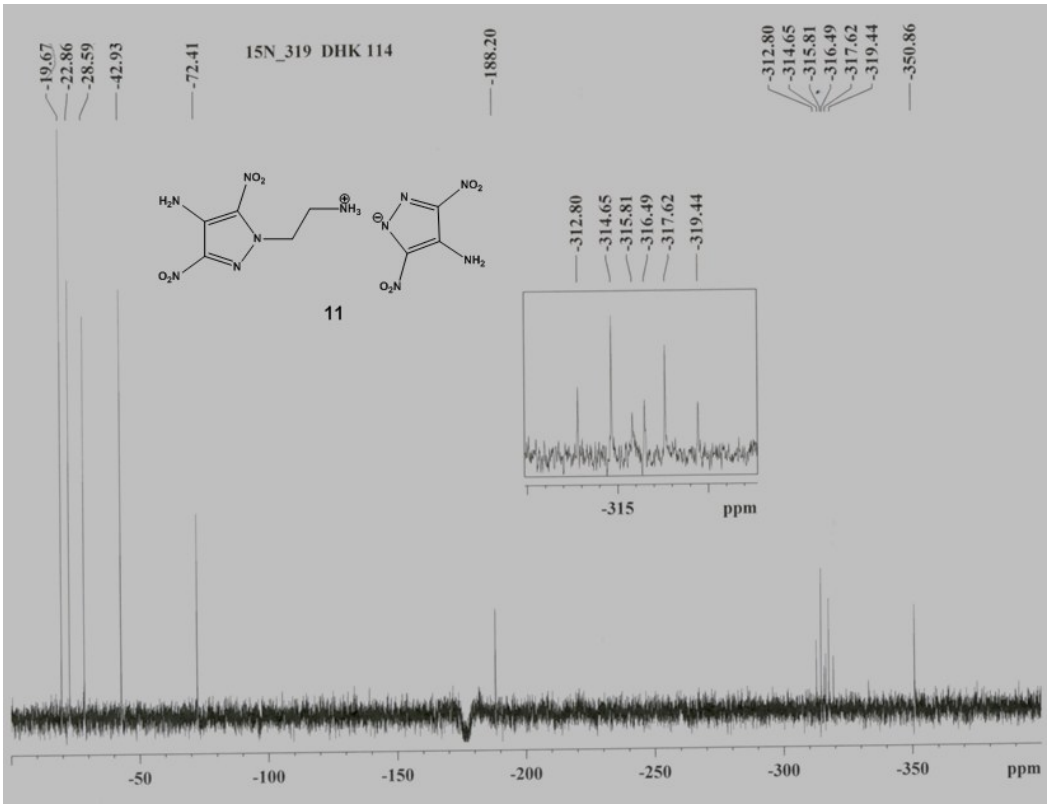


Fig S20: ^{15}N NMR Spectrum of compound **11**

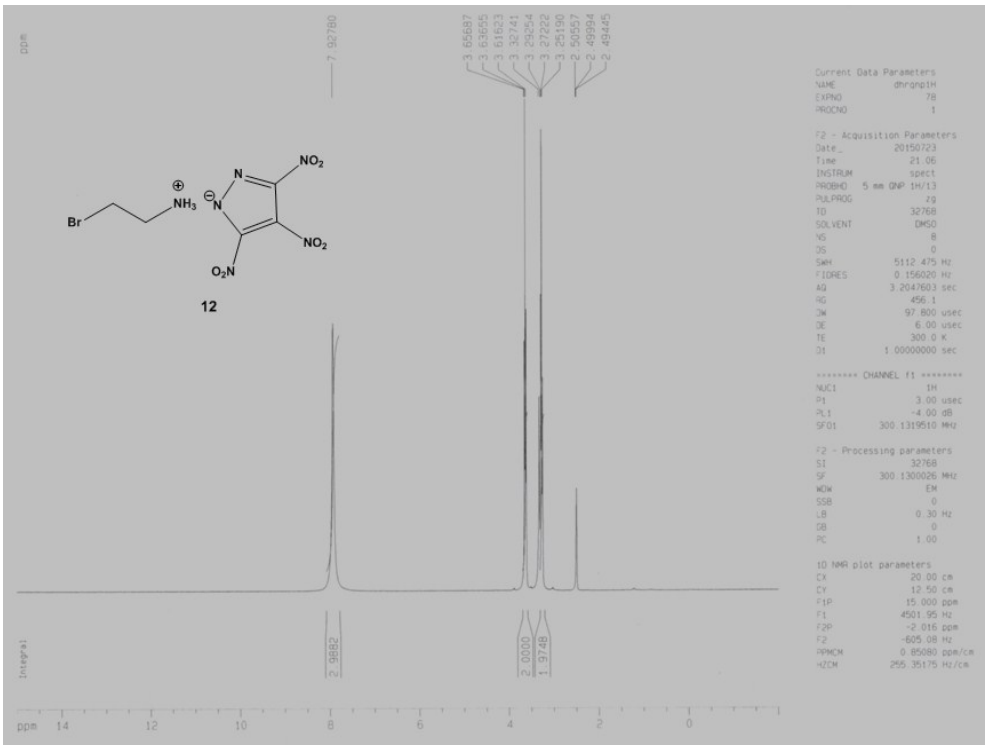


Fig S21: ^{1}H NMR Spectrum of compound **12**

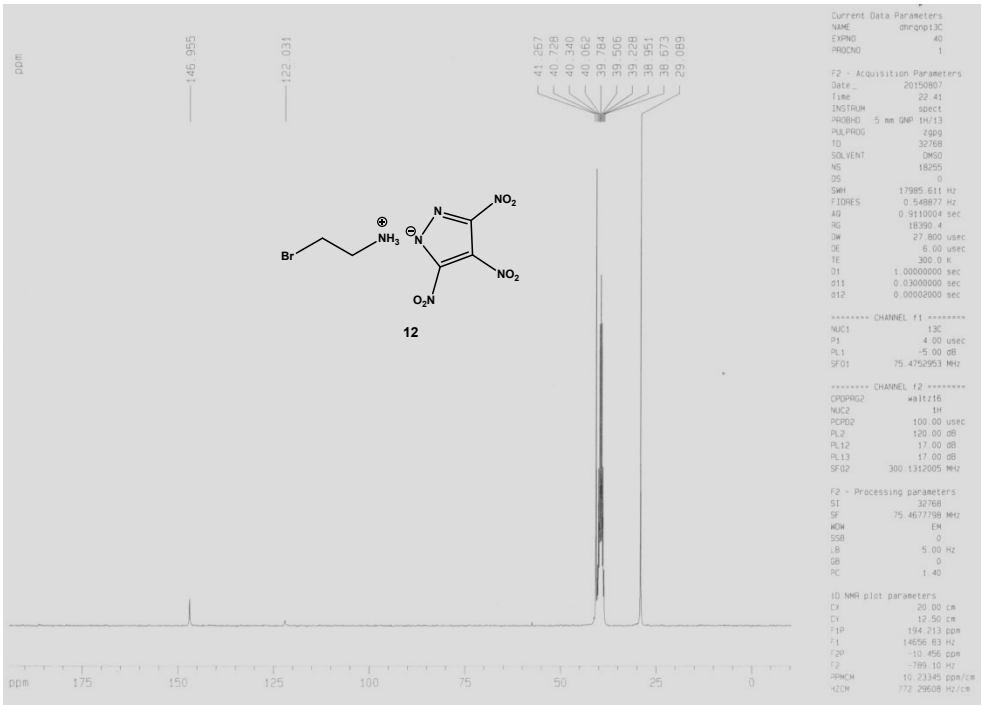


Fig S22: ^{13}C{^{1}H} NMR Spectrum of compound **12**

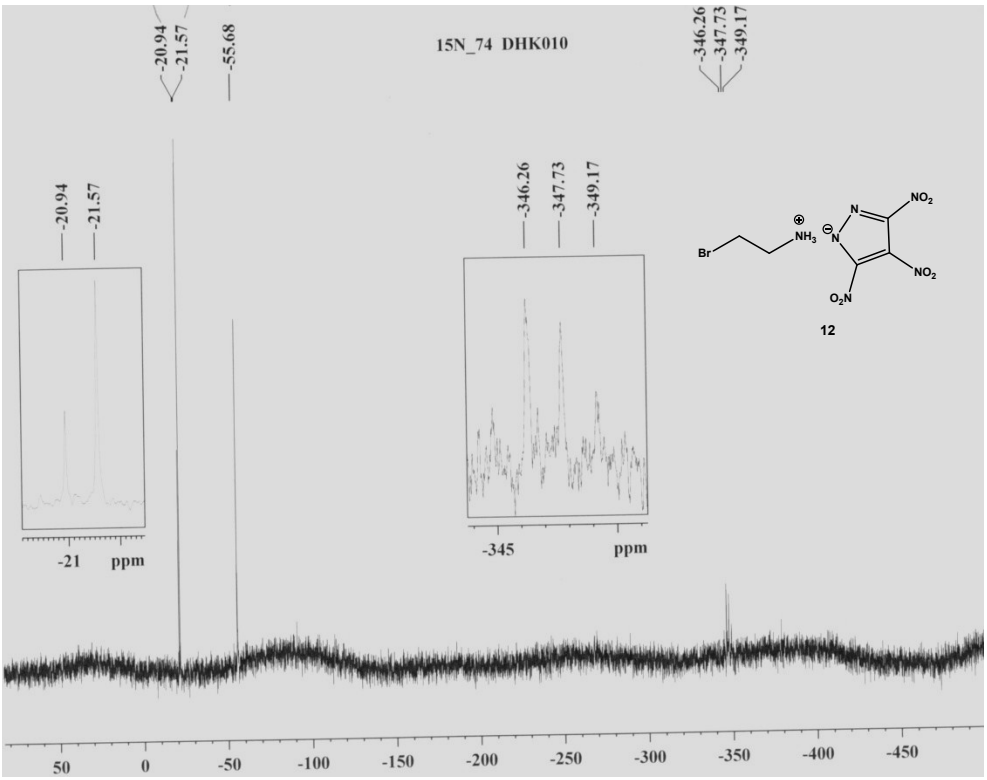


Fig S23: ^{15}N NMR Spectrum of compound **12**

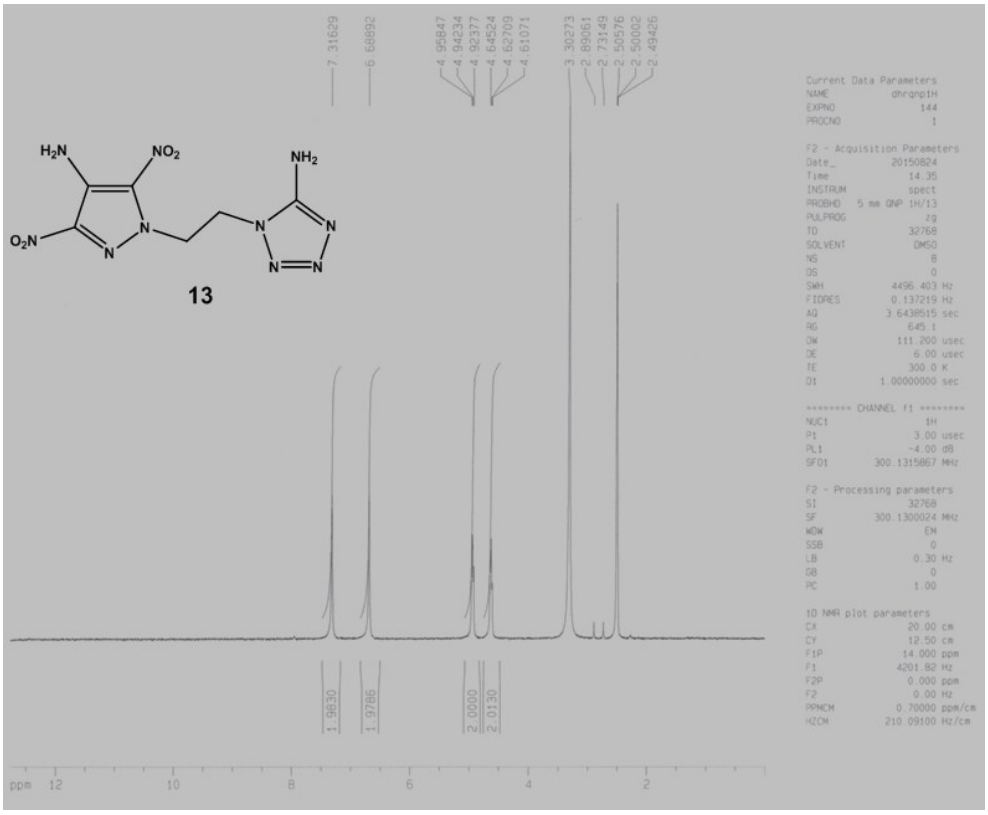


Fig S24: ^{1}H NMR Spectrum of compound **13**

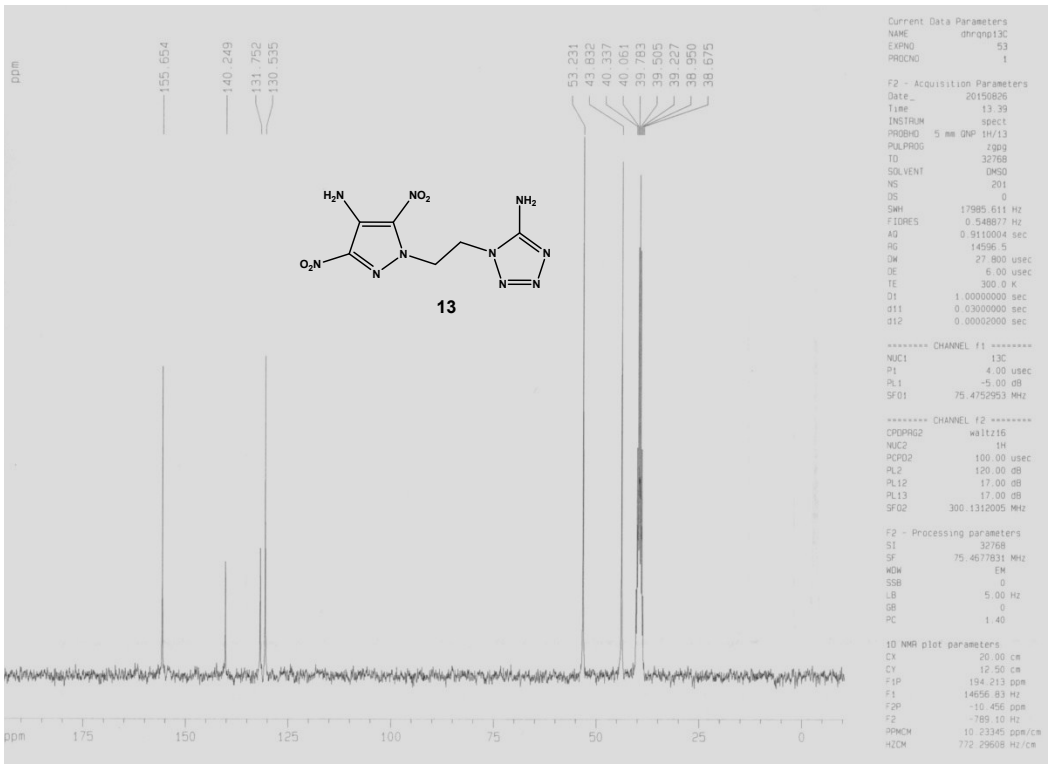


Fig S25: $^{13}C\{^{1}H\}$ NMR Spectrum of compound **13**

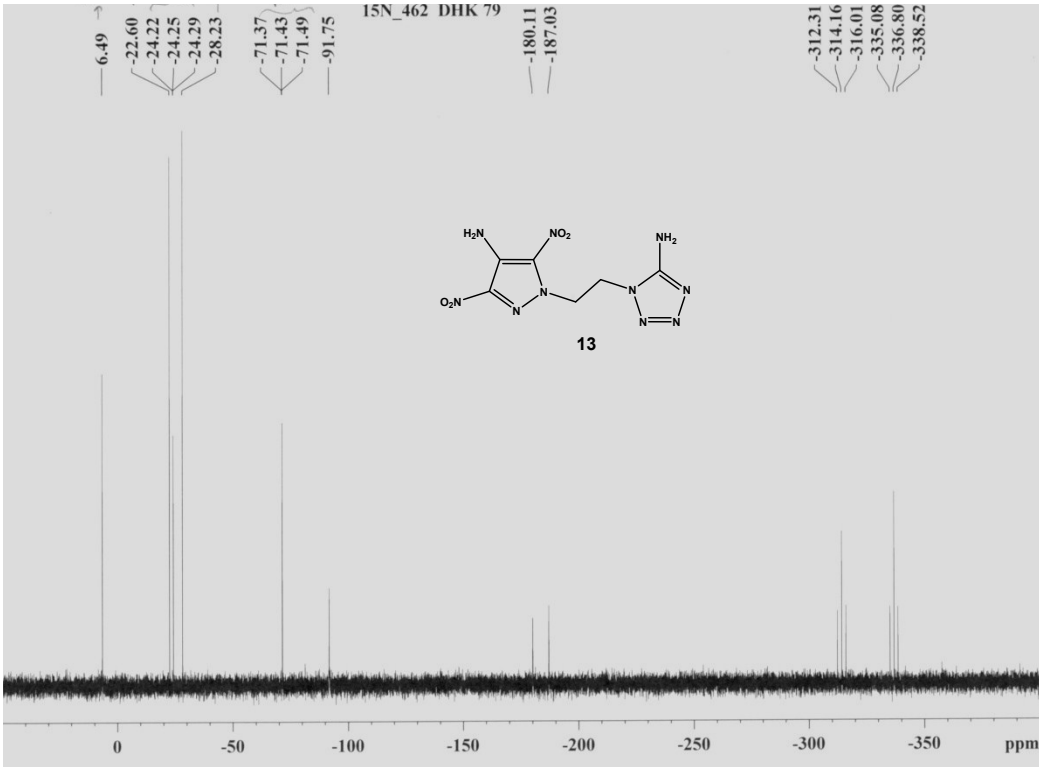


Fig S26: ^{15}N NMR Spectrum of compound **13**

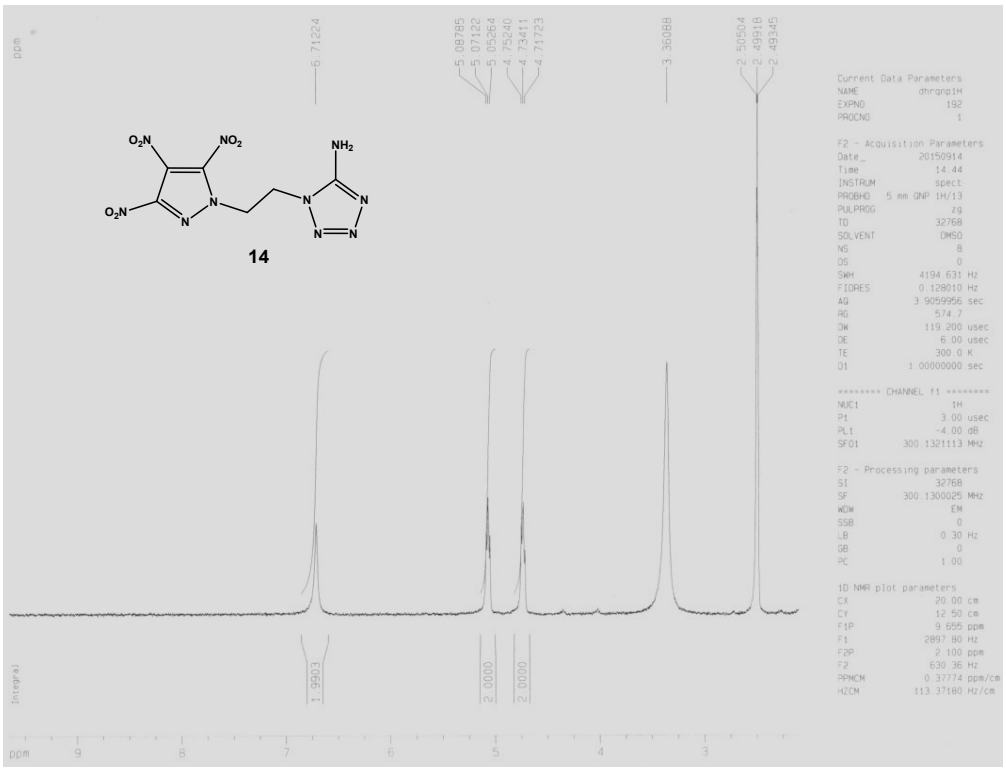


Fig S27: ^{1}H NMR Spectrum of compound **14**

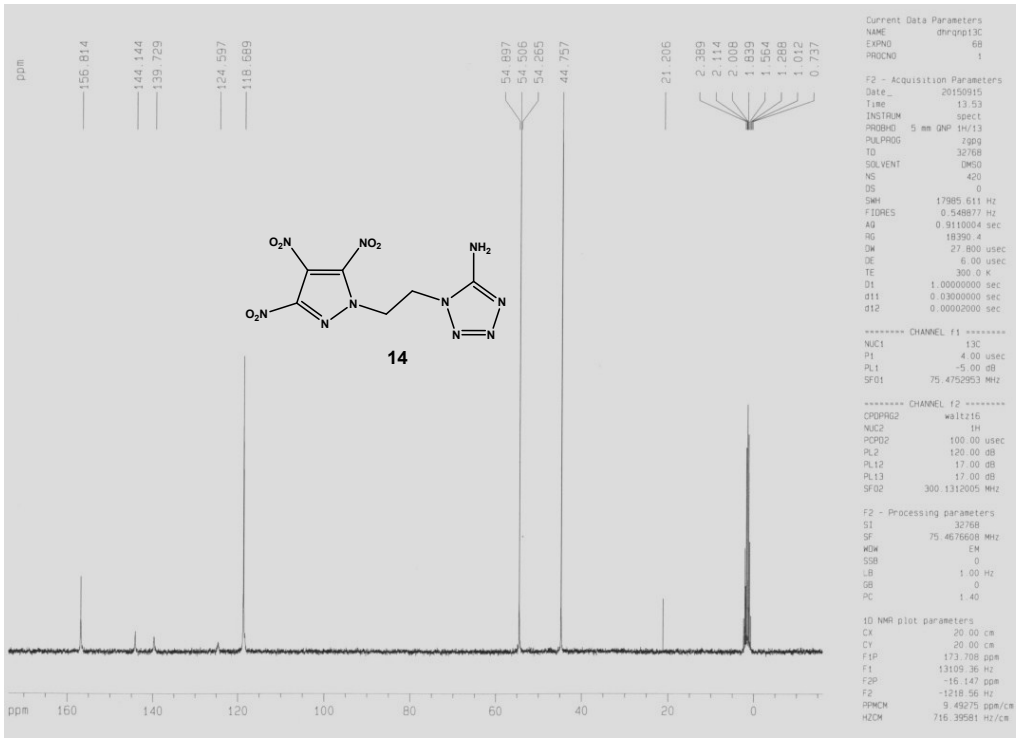


Fig S28: $^{13}C\{^{1}H\}$ NMR Spectrum of compound **14**

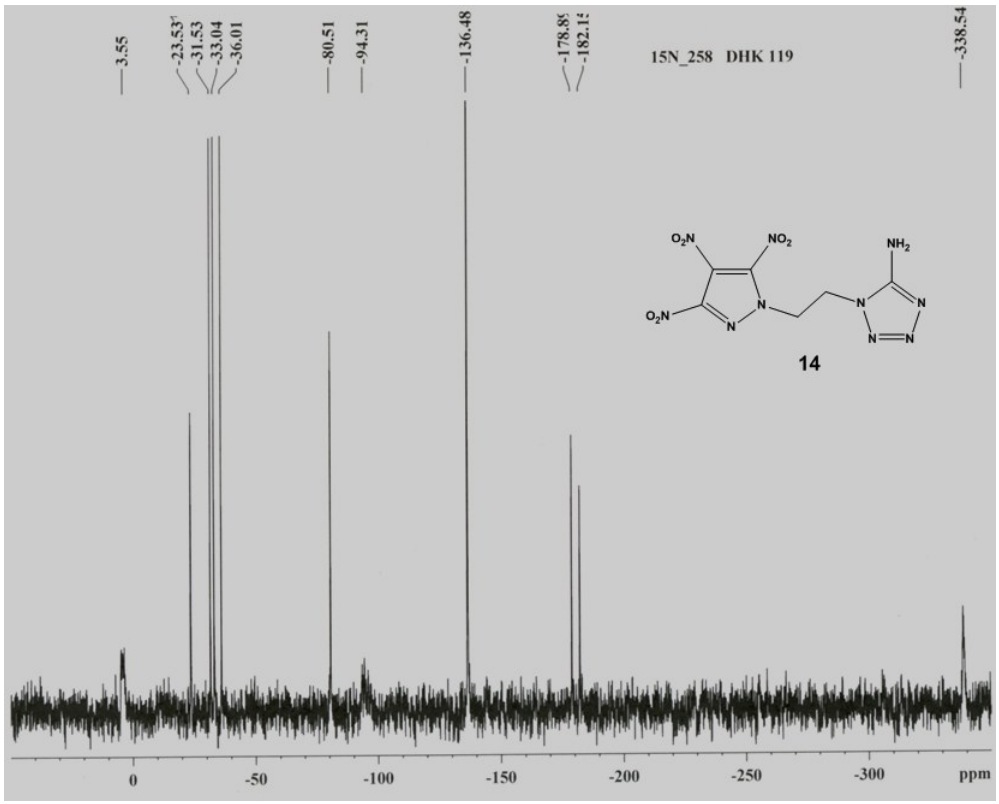


Fig S29: ^{15}N NMR Spectrum of compound **14**

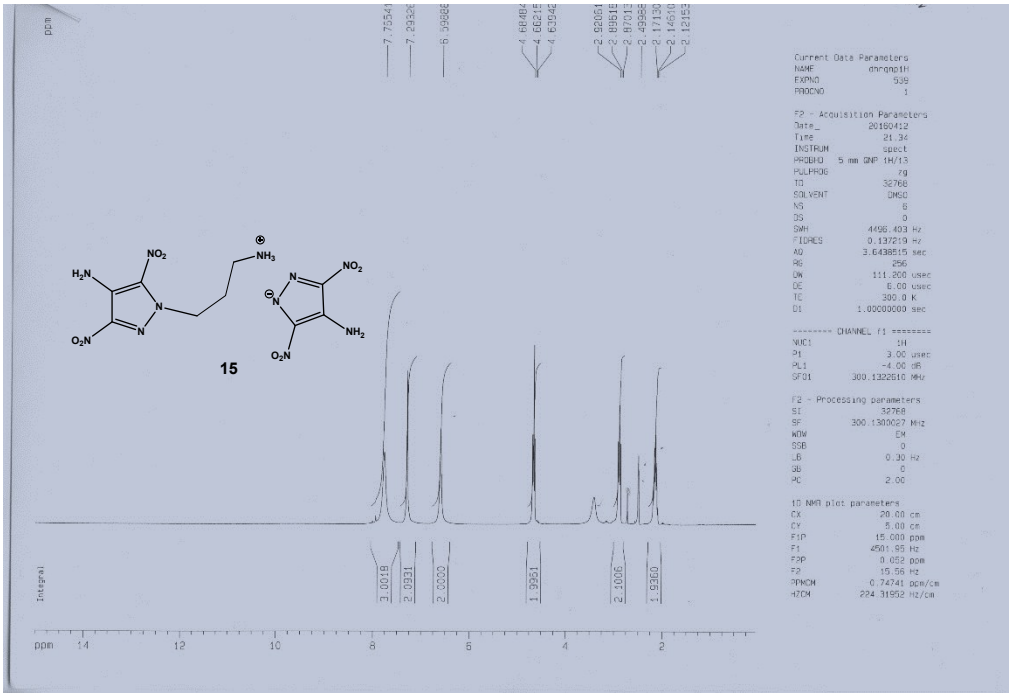


Fig S30: ^{1}H NMR Spectrum of compound **15**

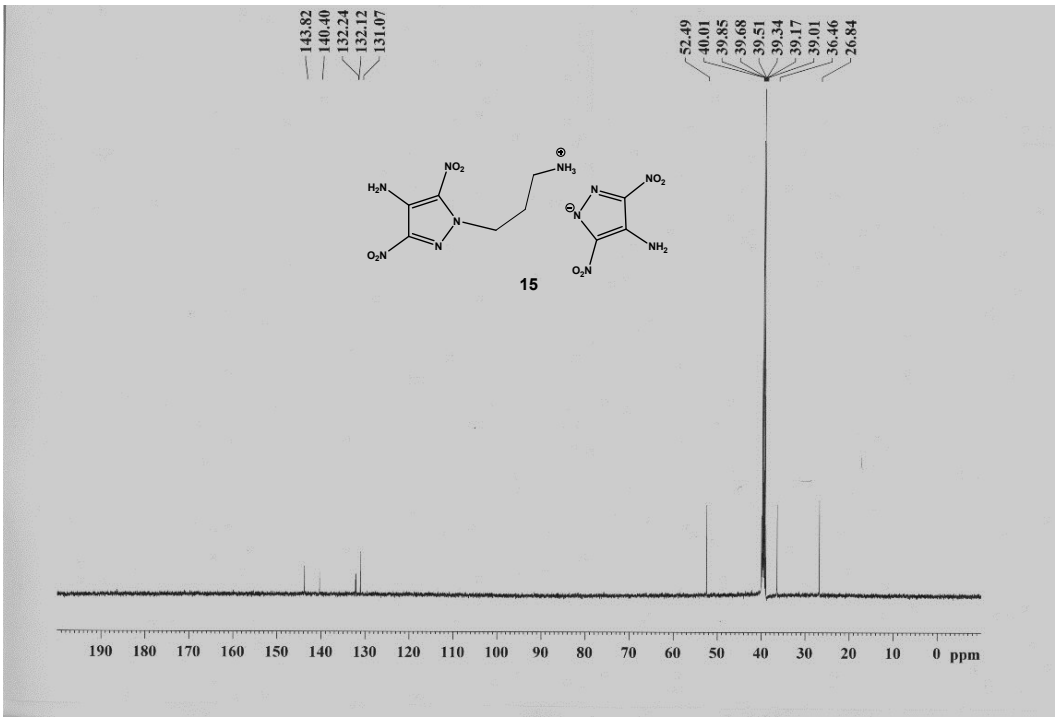


Fig S31: $^{13}C\{^{1}H\}$ NMR Spectrum of compound **15**

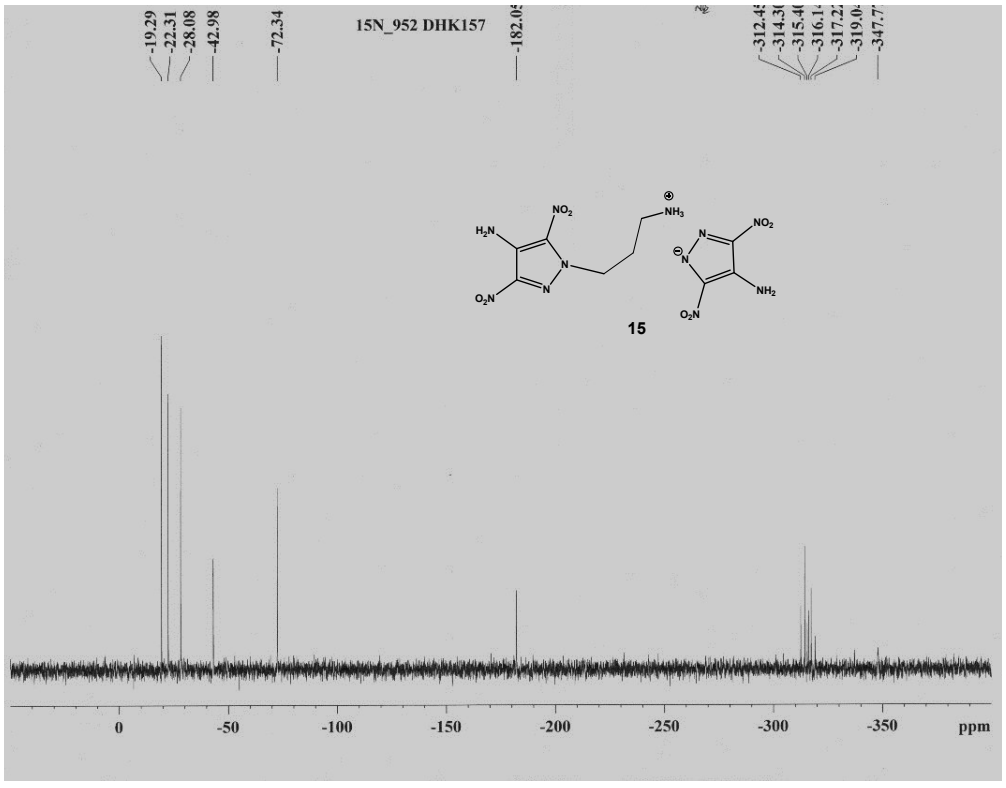


Fig S32: ^{15}N NMR Spectrum of compound **15**

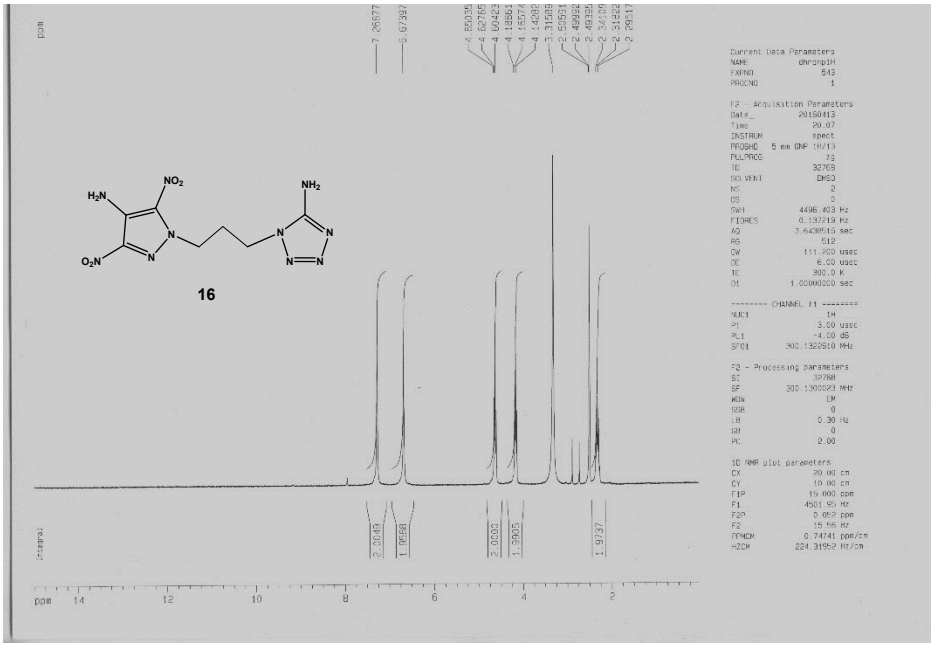


Fig S33: ^{1}H NMR Spectrum of compound **16**

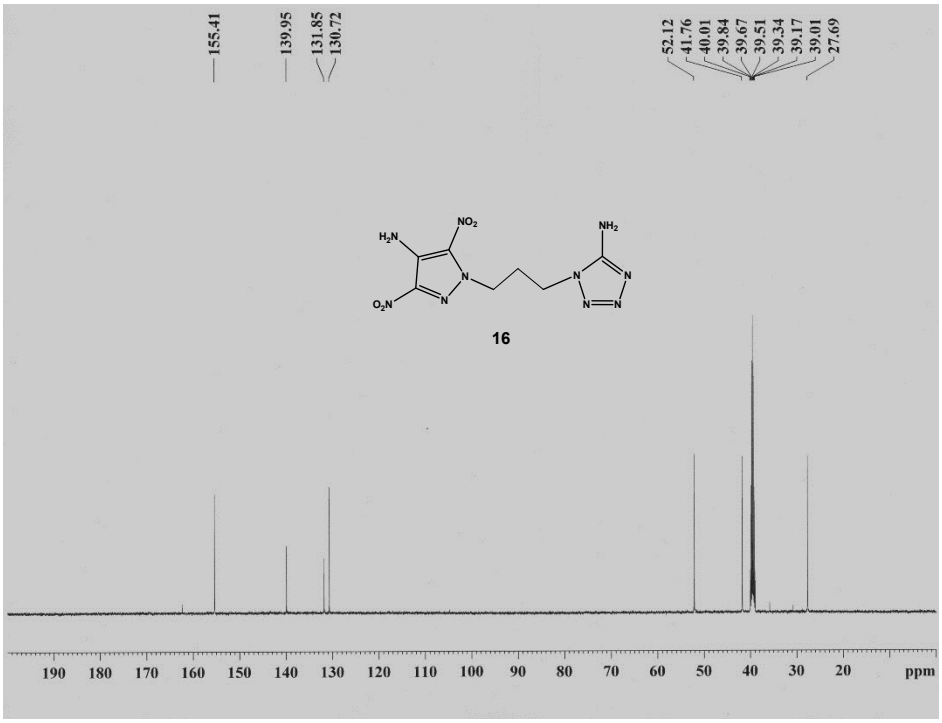


Fig S34: $^{13}C\{^{1}H\}$ NMR Spectrum of compound **16**

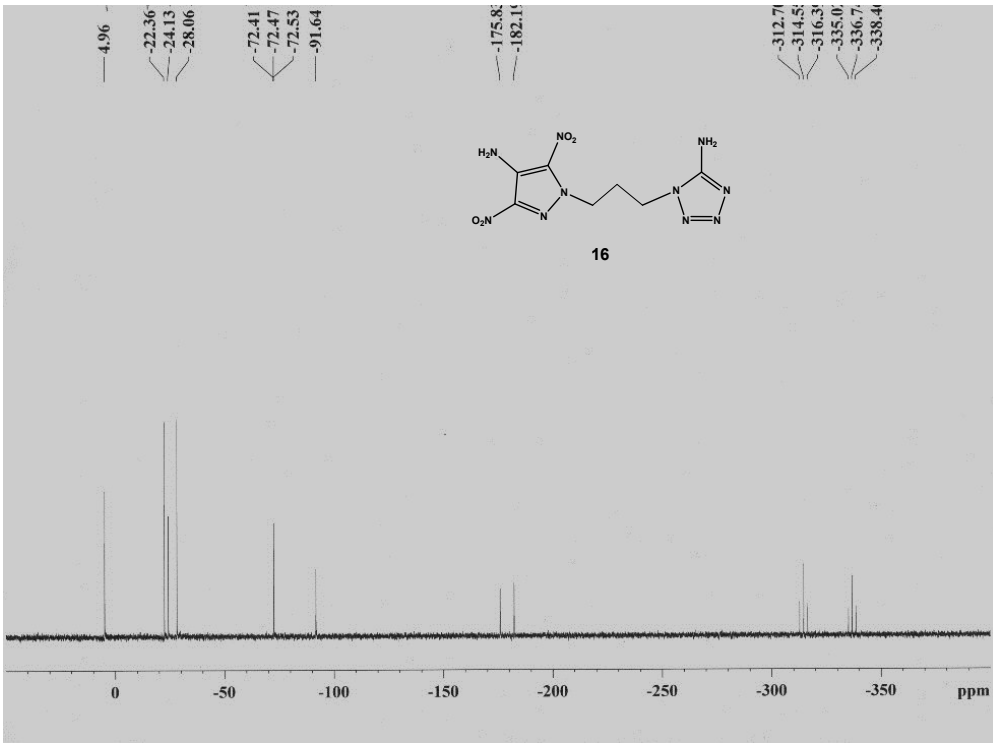


Fig S35: ^{15}N NMR Spectrum of compound **16**

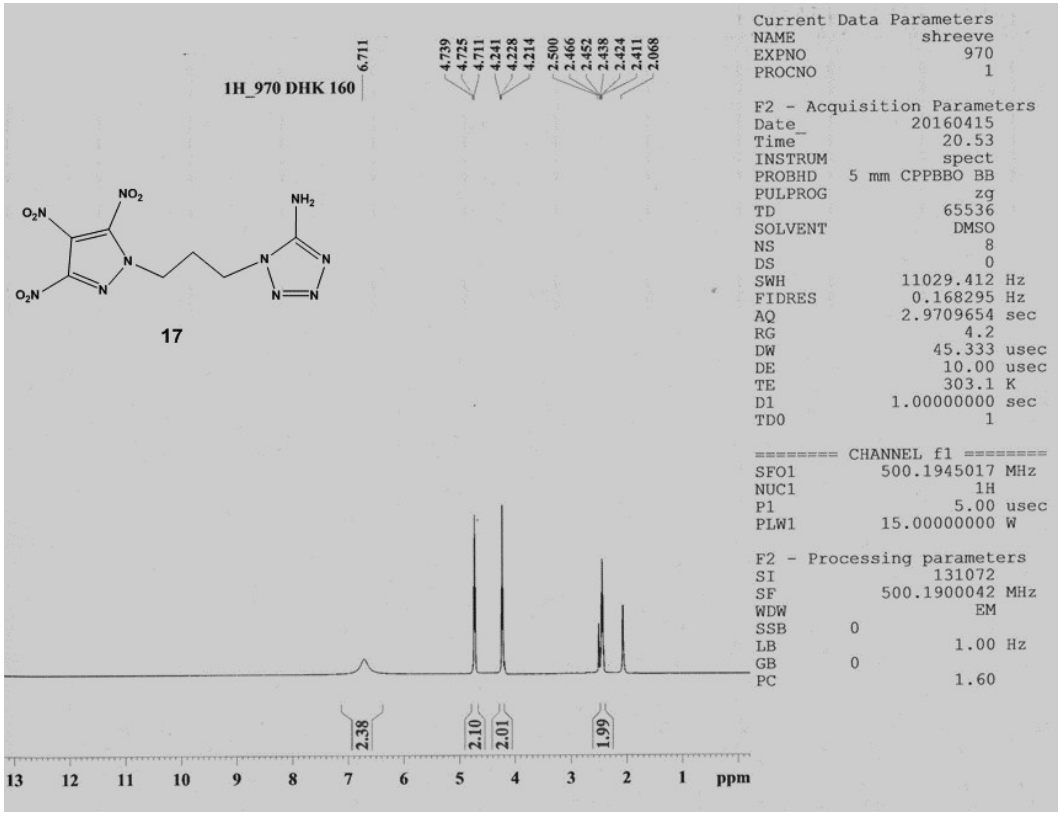


Fig S36: ^{1}H NMR Spectrum of compound **17**

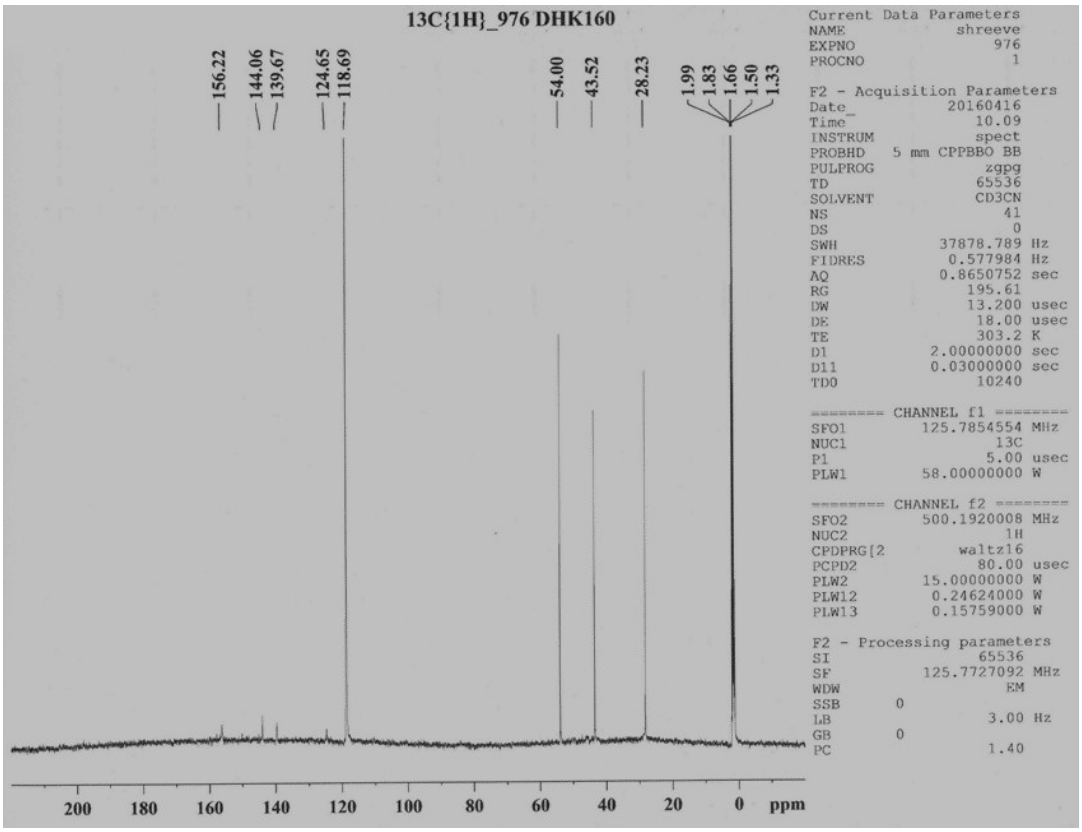


Fig S37: $^{13}C\{^{1}H\}$ NMR Spectrum of compound **17**