

Tunable Dimroth rearrangement of versatile 1,2,3-triazoles towards high-performance energetic materials

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Electronic Supplementary Information

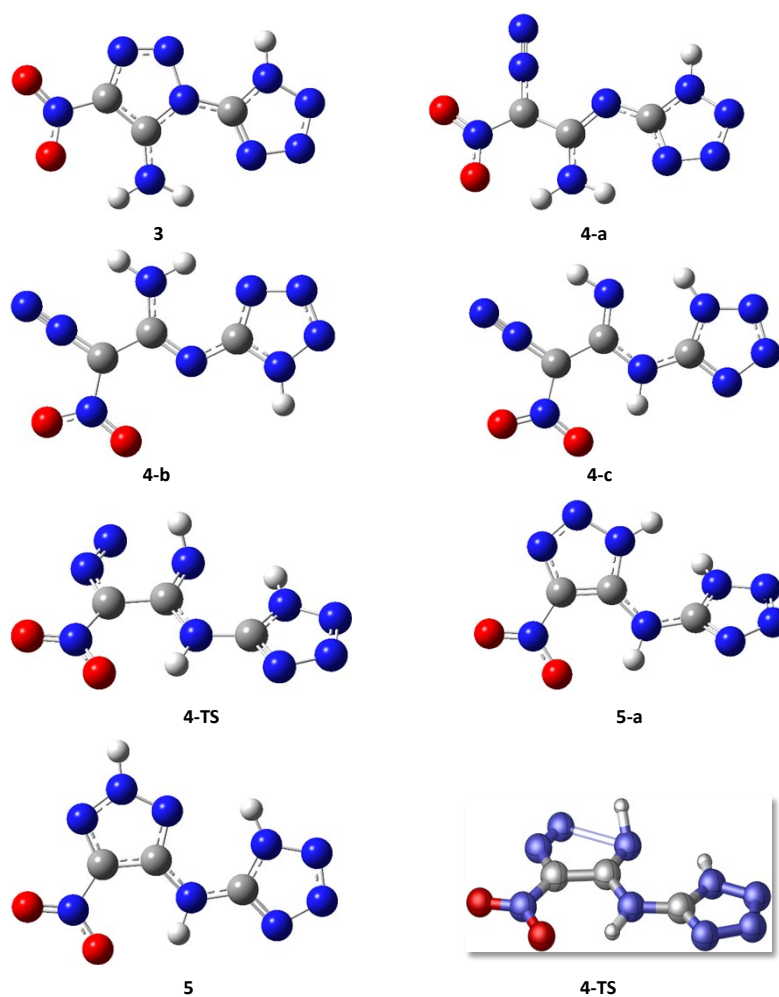
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1. DFT Calculations of Mechanism of Dimroth Rearrangement

All the DFT calculations of Mechanism were performed with Gaussian 09 package.¹ The geometry optimization of Dimroth rearrangement in this study were performed using M062X/6-31G(d,p). Frequency calculations at the same level of theory were also performed to identify all the stationary points as minima (zero imaginary frequencies) or transition states (one imaginary frequency) and to obtain the thermodynamic corrections to Gibbs free energy at 298.15 K. Intrinsic reaction coordinate (IRC) was carried out to confirm the connection between the transition state and the right reactant/product. The single-point energy calculations of key intermediates and transition states were performed with M062X/6-311++G(d,p) level. The reported Gibbs free energy of all species in this study was calculated in the gas-phase of 298.15 K, 1atm.

1.1 The geometry structures of key intermediates and transition states.



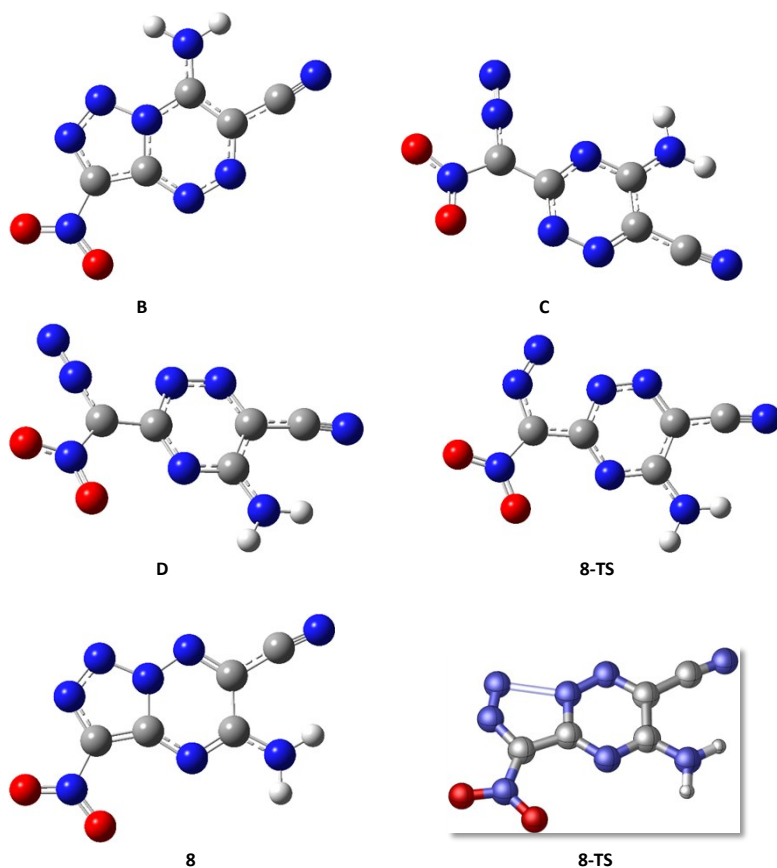


Table 1. The calculated Gibbs free energy of all species in this study.

Species	E(M062x/6-311++g**)(a.u.)	TCG(a.u.)	G(a.u.)	del-G(kcal/mol)
3	-759.071641	0.071121	-759.00052	0
4-a	-759.0654581	0.068049	-758.9974091	2.0
4-b	-759.0467914	0.067688	-758.9791034	13.4
4-c	-759.0446338	0.066855	-758.9777788	14.3
4-TS	-758.9990084	0.067017	-758.9319914	41.0
5-a	-759.0565911	0.070083	-758.9865081	8.8
5	-759.0761675	0.072554	-759.0036135	-1.9
B	-779.898656	0.062686	-779.83597	0
C	-779.9028067	0.057339	-779.8454677	-6.0
D	-779.9073867	0.057921	-779.8494657	-8.5
8-TS	-779.8819959	0.059921	-779.8220749	8.7
8	-779.9127022	0.062676	-779.8500262	-8.8

Cartesian coordinates of all the species:

3

O	3.92185400	-0.75622900	0.00043200
O	3.22474300	1.30174200	0.00087500
N	-2.33891100	1.10829200	-0.00068900

N	-3.67653500	0.87763000	0.00017500
N	-3.93394800	-0.37279100	0.00103600
N	-0.44139500	-0.35347900	-0.00077500
N	0.01126400	-1.66788900	-0.00070700
N	1.28063200	-1.62214700	-0.00044200
N	3.04873700	0.08146200	0.00036300
N	0.46560000	1.85566800	-0.00046100
H	-0.45536400	2.27562100	-0.00067900
H	1.32009300	2.39359900	0.00049700
C	-1.79059700	-0.08034700	-0.00028200
C	1.69017300	-0.32992500	-0.00035700
C	0.59296700	0.53202400	-0.00041500
N	-2.74774000	-1.01287600	0.00073000
H	-2.66669800	-2.02090800	0.00144900

4-a

O	3.91680100	0.14022400	-0.00029300
O	2.85197500	-1.75054700	-0.00007200
N	-2.50782000	-1.01060900	-0.00004700
N	-3.84268500	-0.80783700	-0.00018600
N	-4.12165800	0.44124300	0.00002000
N	-0.63254100	0.57074700	-0.00008000
N	1.90909200	2.59857000	0.00016300
N	1.79681400	1.48766900	0.00010400
N	2.89581600	-0.52633500	-0.00010500
N	0.11566900	-1.68306600	0.00041600
H	-0.84053600	-2.03330600	-0.00006100
H	0.92349000	-2.28829300	0.00031500
C	-1.94154000	0.18988700	-0.00001800
C	1.65614000	0.17036100	0.00011500
C	0.28481200	-0.36164700	0.00010900
N	-2.94593700	1.08911500	-0.00008100
H	-2.89687500	2.09609400	0.00000300

4-b

O	3.54904900	-1.18751000	-0.00002800
O	1.60668800	-2.14999300	-0.00002900
N	-2.55266100	0.97897100	-0.00001200
N	-3.86862000	0.68402100	-0.00001400
N	-4.05760200	-0.58383100	0.00000100
N	-0.57255900	-0.48065800	0.00001500
N	3.38754100	1.91217300	0.00000500

N	2.62129600	1.09019200	0.00000800
N	2.32440000	-1.17947400	0.00003600
N	0.00582700	1.80819800	-0.00001100
H	-0.97852600	2.07576600	-0.00001900
H	0.71397500	2.52192100	-0.00002000
C	-1.90287700	-0.17856800	0.00000500
C	1.71692400	0.13392300	0.00001800
C	0.28755100	0.48743400	0.00000700
N	-2.84150200	-1.14507700	0.00001300
H	-2.71376700	-2.14601400	0.00002700

4-c

O	3.52978800	-1.22251800	-0.00020200
O	1.54864600	-2.10160700	0.00037500
N	-2.82715700	-1.23317700	-0.00036700
N	-4.03593100	-0.62925000	-0.00029200
N	-3.92783500	0.64731200	0.00003700
N	3.43924200	1.91733000	-0.00039800
N	2.66349800	1.10851600	-0.00016200
N	2.31480600	-1.14958600	0.00011300
N	-0.06922400	1.80846100	0.00026900
H	0.68765800	2.48438200	0.00005600
C	-1.95313700	-0.25151900	-0.00004200
C	1.74037900	0.16452000	0.00011700
C	0.31846000	0.58798800	0.00030400
N	-2.60947500	0.91616600	0.00020500
H	-2.20620900	1.84456100	0.00048300
N	-0.58787800	-0.43528800	0.00002700
H	-0.26345100	-1.39528400	-0.00020800

4-TS

N	2.71122300	-1.33031100	0.04980100
N	3.92769100	-0.74228100	0.02499900
N	3.83372700	0.53371000	-0.04454900
N	0.47979100	-0.51160100	-0.03497900
H	0.13273800	-1.46570700	-0.11894700
N	-0.06945000	1.75700400	0.04823500
N	-2.13242500	2.36397600	-0.11770600
H	-0.35764200	2.33212900	0.83980000
N	-2.55020600	1.28606100	-0.02790600
N	-2.47043600	-1.10698700	0.00859700
O	-1.72487000	-2.08694700	-0.02857900

O	-3.68268000	-1.14652600	-0.00509100
C	-1.83407600	0.15430000	0.07186900
C	-0.41819500	0.48364100	0.07718300
C	1.85246300	-0.34168600	-0.00947300
N	2.51967700	0.81791800	-0.06911900
H	2.13700500	1.75141600	-0.15056800

5-a

N	-2.75023800	-1.15423800	-0.64162400
N	-3.92867300	-0.58704500	-0.28575600
N	-3.76006200	0.42024000	0.47952600
N	-0.46997700	-0.68099100	-0.06999200
H	-0.12794400	-1.62750800	-0.20198100
N	0.25657400	1.62241000	-0.23749100
N	1.43379400	2.32154100	-0.23960900
H	-0.60592300	2.10684100	-0.44579800
N	2.38330700	1.47874800	-0.10506000
N	2.61986800	-0.96210100	0.11116700
O	1.96332900	-2.00509800	0.08430700
O	3.81827600	-0.88597500	0.23643900
C	1.85606700	0.23443300	-0.01844100
C	0.47552200	0.29855000	-0.10765800
C	-1.82737200	-0.45094600	-0.03647700
N	-2.42558900	0.53887400	0.66072000
H	-2.05729900	1.17495600	1.35409800

5

N	2.76193400	-1.38012500	0.00030700
N	3.94816800	-0.72959000	-0.00046500
N	3.79531400	0.53905100	0.00048100
N	0.49498700	-0.65208900	0.00008700
H	0.16978200	-1.61112600	0.00041800
N	-0.16564400	1.63356700	-0.00031300
N	-1.37162000	2.20566000	-0.00016200
H	-1.47374400	3.21046700	-0.00012100
N	-2.40395400	1.41900100	-0.00063500
N	-2.62481700	-0.99406900	0.00010900
O	-1.96316700	-2.02773700	0.00060600
O	-3.83043700	-0.91818200	0.00001000
C	-1.85410700	0.21385500	-0.00014600
C	-0.44531800	0.33211200	-0.00011100
C	1.85111500	-0.43432800	0.00011200

N	2.46313000	0.76022700	-0.00001900
H	2.06017900	1.68673800	-0.00009200

B

O	4.07954700	0.23315500	-0.00128500
O	3.02264900	-1.66561500	0.00115100
N	3.07878200	-0.45033400	-0.00007100
N	1.71908100	1.56970400	0.00019100
N	0.47826000	1.93512200	0.00025900
N	-0.25161700	0.79375900	0.00014500
N	0.00799600	-1.58724800	-0.00003300
N	-4.66117800	-0.80323800	-0.00031500
C	-2.08469300	-0.59094700	-0.00012300
C	0.53221500	-0.33445000	0.00005500
C	1.80673500	0.23220600	0.00000900
C	-3.50403000	-0.77862000	-0.00028700
N	-1.27794700	-1.68446000	-0.00012200
C	-1.61000300	0.72462300	0.00006100
N	-2.30986200	1.85313400	0.00001800
H	-1.82445700	2.73988600	0.00131300
H	-3.31905300	1.81784600	0.00096100

C

O	-3.96018700	-0.34647100	-0.00230700
O	-2.56377000	-2.00941300	0.00203900
N	-2.83518100	-0.83158500	-0.00008500
N	-2.16703400	1.36982900	-0.00091500
N	-2.51785500	2.43172500	0.00153400
N	0.41526800	1.01527700	0.00024300
N	0.14237400	-1.37140100	-0.00020000
N	4.82898400	-0.70988900	-0.00024200
C	2.24937000	-0.48152900	-0.00010700
C	-0.30964500	-0.11231100	0.00018000
C	-1.74937800	0.11367200	0.00037600
C	3.67208700	-0.67834900	-0.00013700
N	1.45209000	-1.53455600	-0.00026900
C	1.73190000	0.84941600	0.00002800
N	2.53418300	1.92195100	-0.00012700
H	2.11832700	2.83961500	0.00040400
H	3.53752200	1.82261200	0.00012400

D

O	-3.86765500	0.64369100	0.00012100
O	-2.20971300	2.04612700	-0.00038100
N	-2.67666600	0.92748100	-0.00009000
N	-2.37854800	-1.35519600	0.00024800
N	-2.89607300	-2.34497000	-0.00098100
N	0.35292300	0.97348400	-0.00001300
N	0.21214600	-1.42162500	0.00077000
N	4.85242500	-0.54645700	-0.00078000
C	2.26567400	-0.44062900	0.00014700
C	-0.30838500	-0.17531500	0.00037900
C	-1.76399800	-0.17931700	0.00007000
C	3.69519600	-0.56909900	-0.00029700
N	1.51815900	-1.53449000	0.00061200
C	1.68098800	0.85986000	0.00007800
N	2.42012300	1.97438800	0.00009300
H	1.94308200	2.86292100	0.00041400
H	3.42758100	1.93723100	0.00038200

8-TS

N	0.23638700	1.06271800	-0.00241700
N	0.17009100	-1.31979700	0.00018200
N	-1.52634200	-2.47044500	-0.00080200
N	-2.19734500	-1.52730600	-0.00103200
N	-2.86234900	0.76528100	0.00115100
O	-2.49208100	1.92615100	0.00475000
O	-4.01961200	0.37866700	-0.00114200
C	-1.84634500	-0.22794500	-0.00056400
C	-0.42464300	-0.09754600	-0.00078200
C	1.56038600	0.95994200	-0.00134000
N	1.46432500	-1.43979800	0.00079300
N	2.29130400	2.07751000	-0.00301000
H	1.80577400	2.96206500	-0.00471700
H	3.29923900	2.05097500	0.00079900
C	2.18518600	-0.33624300	0.00067300
C	3.61653300	-0.43190000	0.00119400
N	4.77276100	-0.38379500	0.00227400

8

O	-4.09174400	0.08868600	0.00002800
O	-2.73847900	1.78766000	-0.00002100
N	-2.98966600	0.59374500	0.00002700
N	-1.97456600	-1.62813700	0.00001500

N	-0.82159400	-2.19141900	0.00004300
N	0.08939200	-1.17617200	-0.00004100
N	1.39027900	-1.39583000	-0.00000900
N	0.21684600	1.19963000	0.00003300
N	2.33089100	2.09826500	-0.00031100
H	1.90834200	3.01444400	0.00063000
H	3.33471100	2.00765900	0.00143900
N	4.69612800	-0.41956900	0.00002400
C	1.51923900	1.03290800	0.00000500
C	2.10734900	-0.31206700	0.00001400
C	-0.51081400	0.07046700	-0.00005000
C	-1.85014800	-0.28197000	-0.00002800
C	3.54016700	-0.44208000	-0.00003900

Reference:

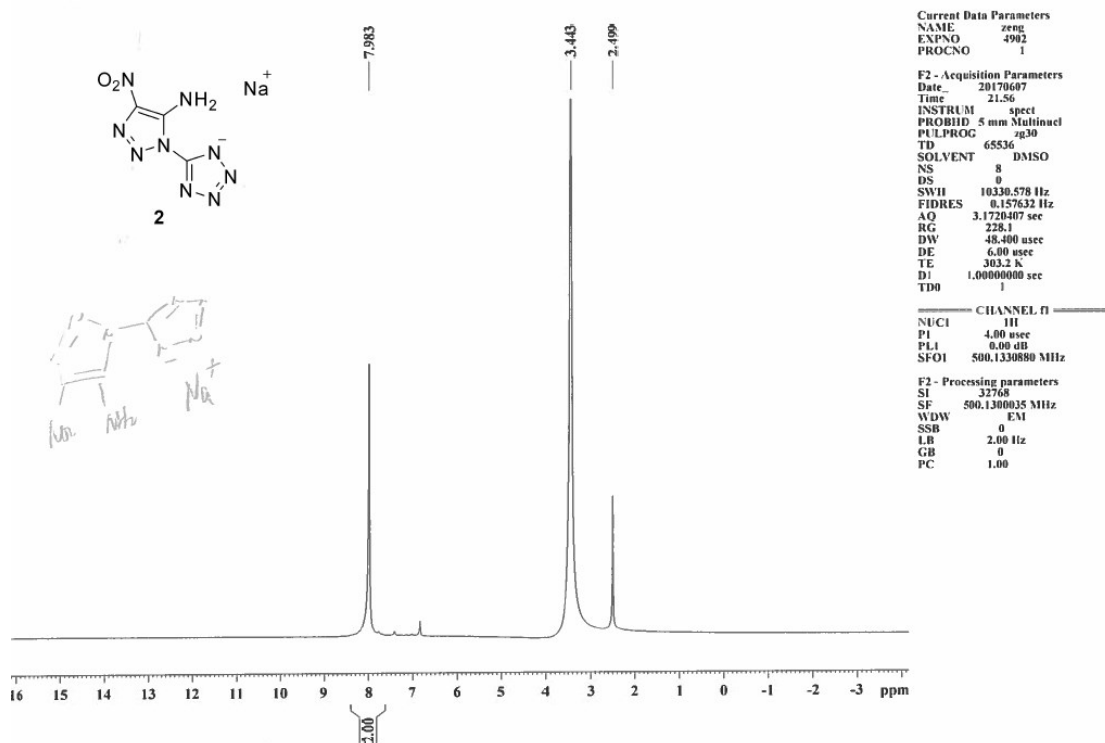
1. M. J. Frisch, et al. Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.

2. X-ray Crystallography

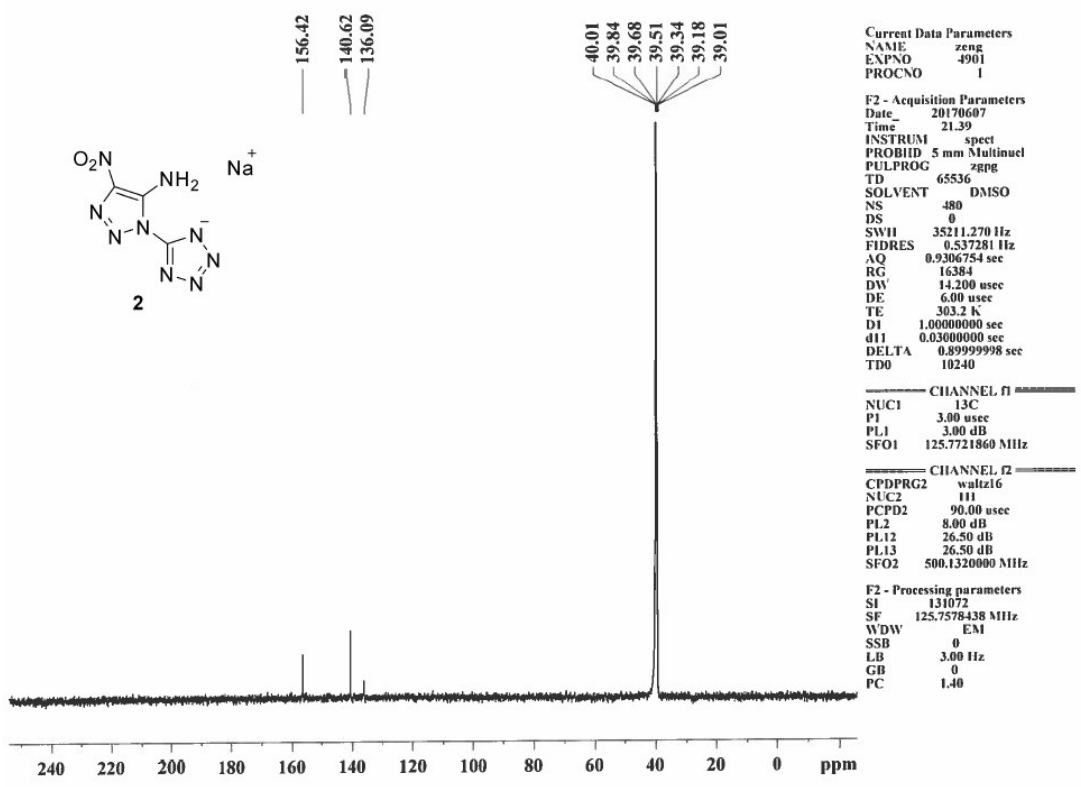
Compound	2	5	8
CCDC No.	2033555	2033556	2033557
Empirical formula	C ₆ H ₂₀ N ₁₈ Na ₂ O ₁₂	C ₅ H ₉ N ₉ O ₃ S	C ₃ H ₂ N ₈ O ₂
Formula weight	582.38	275.27	206.15
Temperature	170 K	170(2) K	296 K
Crystal system	Orthorhombic	Triclinic	Orthorhombic
Space group	Pbca	P ₁	P2 ₁ 2 ₁
Unit cell dimensions	$a = 11.5770(6) \text{ \AA}$ $\alpha = 90^\circ$. $b = 12.9948(8) \text{ \AA}$ $\beta = 90^\circ$. $c = 30.5442(18) \text{ \AA}$ $\gamma = 90^\circ$.	$a = 9.5017(5) \text{ \AA}$ $\alpha = 72.499(2)^\circ$. $b = 10.4256(6) \text{ \AA}$ $\beta = 84.501(2)^\circ$. $c = 12.9711(7) \text{ \AA}$ $\gamma = 65.426(2)^\circ$.	$a = 5.348(10) \text{ \AA}$ $\alpha = 90^\circ$. $b = 9.841(19) \text{ \AA}$ $\beta = 90^\circ$. $c = 14.02(3) \text{ \AA}$ $\gamma = 90^\circ$.
Volume	4595.1(5) Å ³	1113.82(11) Å ³	738(3) Å ³
Z	8	4	4
Density (calculated)	1.684 g cm ⁻³ (170 K)	1.642 g cm ⁻³ (293 K)	1.856 g cm ⁻³ (296 K)
Crystal size	0.190 x 0.080 x 0.040 mm ³	0.120 x 0.100 x 0.080 mm ³	0.120 x 0.100 x 0.060 mm ³
Theta range for data collection	2.207 to 27.106°	2.243 to 26.429°	2.906 to 27.526°
Completeness	99.8 % ($\theta = 25.242^\circ$)	96.7 % ($\theta = 25.242^\circ$)	99.1 % ($\theta = 25.242^\circ$)
F000	2400.0	568.0	416.0
Goodness-of-fit on F ²	1.061	1.080	0.907
R (reflections)	0.0387(4310)	0.0538(2907)	0.0738(662)
wR ₂ (reflections)	0.1029(5608)	0.1393(4428)	0.1942(1675)

Compound	9	10	16
CCDC No.	1997519	1997520	2033570
Empirical formula	C ₇ H ₁₀ N ₁₁ O ₃ S	C ₇ H ₁₂ N ₁₂ O ₄	C ₅ H ₅ N ₇ O ₃
Formula weight	328.32	328.29	211.16
Temperature	296(2) K	296(2)K	140 K
Crystal system	Monoclinic	Monoclinic	Orthorhombic
Space group	P2 ₁	P2 ₁ /c	Pbca
Unit cell dimensions	$a = 6.423(7) \text{ \AA}$ $\alpha = 90^\circ$. $b = 9.662(10) \text{ \AA}$ $\beta = 94.020(15)^\circ$. $c = 10.780 \text{ \AA}$ $\gamma = 90^\circ$.	$a = 10.869 \text{ \AA}$ $\alpha = 90^\circ$. $b = 17.502(6) \text{ \AA}$ $\beta = 102.927(6)^\circ$. $c = 7.255(2) \text{ \AA}$ $\gamma = 90^\circ$.	$a = 15.886(4) \text{ \AA}$ $\alpha = 90^\circ$. $b = 6.0794(15) \text{ \AA}$ $\beta = 90^\circ$. $c = 16.529(4) \text{ \AA}$ $\gamma = 90^\circ$.
Volume	667.4(12) Å ³	1345.1(8) Å ³	1596.4(7) Å ³
Z	2	4	8
Density (calculated)	1.634 g cm ⁻³ (296 K)	1.621 g cm ⁻³ (296 K)	1.766 g cm ⁻³ (296 K)
Crystal size	0.15 x 0.12 x 0.04 mm ³	0.12 x 0.11 x 0.08 mm ³	0.100 x 0.070 x 0.050 mm ³
Theta range for data collection	2.834 to 27.641°	1.922 to 27.563°	2.464 to 26.455°
Completeness	97.2 % ($\theta = 25.242^\circ$)	98.6% ($\theta = 25.242^\circ$)	99.9% ($\theta = 25.242^\circ$)
F000	338.0	680.0	872.0
Goodness-of-fit on F ²	0.946	0.889	0.990
R (reflections)	0.0734(1352)	0.0624(1465)	0.0578(954)
wR ₂ (reflections)	0.2153(2795)	0.2068(3069)	0.1781(1647)

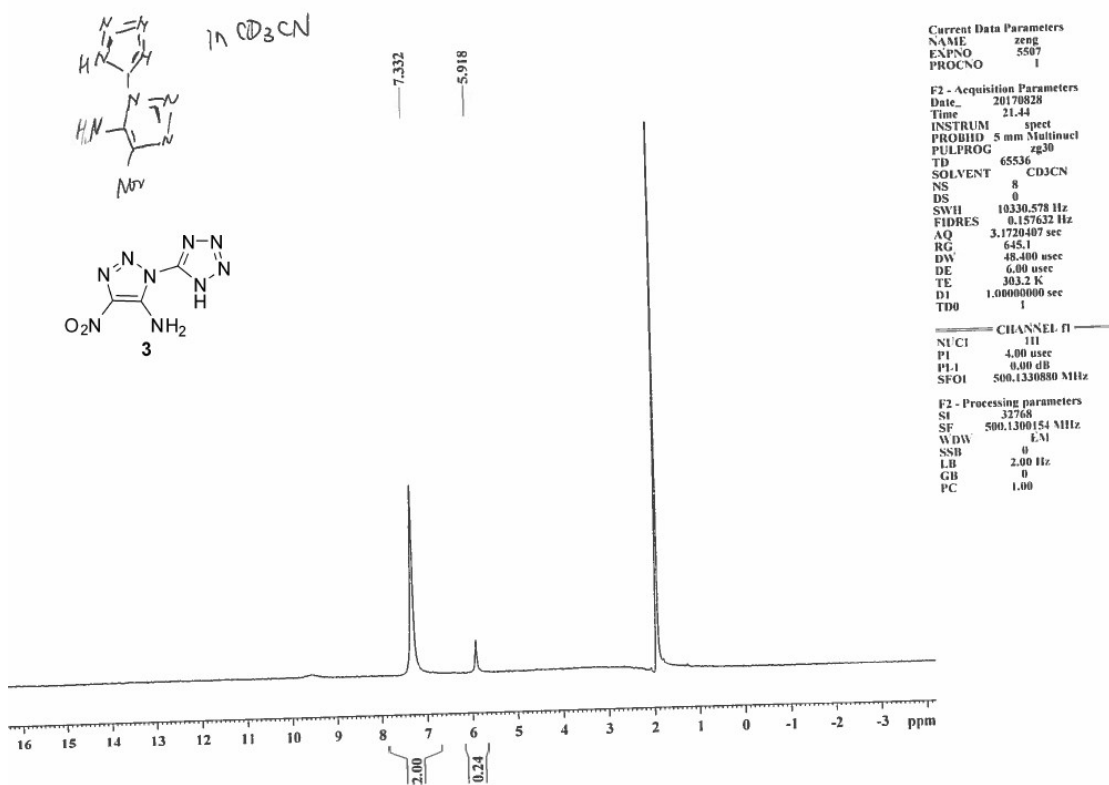
Compound	17	18
CCDC No.	2033571	2013573
Empirical formula	C ₄ H ₂ ClN ₇ O ₂	C ₄ H ₂ N ₁₀ O ₂
Formula weight	215.58	222.16
Temperature	296 K	296 K
Crystal system	Monoclinic	Monoclinic
Space group	P2 ₁ /c	P2 ₁ /n
Unit cell dimensions	$a = 5.6820(19) \text{ \AA}$ $\alpha = 90^\circ$. $b = 8.178(3) \text{ \AA}$ $\beta = 95.565(4)^\circ$. $c = 16.188(5) \text{ \AA}$ $\gamma = 90^\circ$.	$a = 13.700(5) \text{ \AA}$ $\alpha = 90^\circ$. $b = 4.2254(16) \text{ \AA}$ $\beta =$ $94.885(5)^\circ$. $c = 14.004(5) \text{ \AA}$ $\gamma = 90^\circ$.
Volume	748.6(4) Å ³	807.7(5) Å ³
Z	4	4
Density (calculated)	1.913 g cm ⁻³ (296 K)	1.827 g cm ⁻³ (293 K)
Crystal size	0.120 x 0.100 x 0.080 mm ³	0.120 x 0.100 x 0.090 mm ³
Theta range for data collection	2.528 to 27.135°	1.966 to 27.489°
Completeness	99.3 % ($\theta = 25.242^\circ$)	99.1 % ($\theta = 25.242^\circ$)
F000	432.0	448.0
Goodness-of-fit on F ²	1.048	1.013
R (reflections)	0.0350(1367)	0.0551(1274)
wR ₂ (reflections)	0.1034(1648)	0.1601(1845)



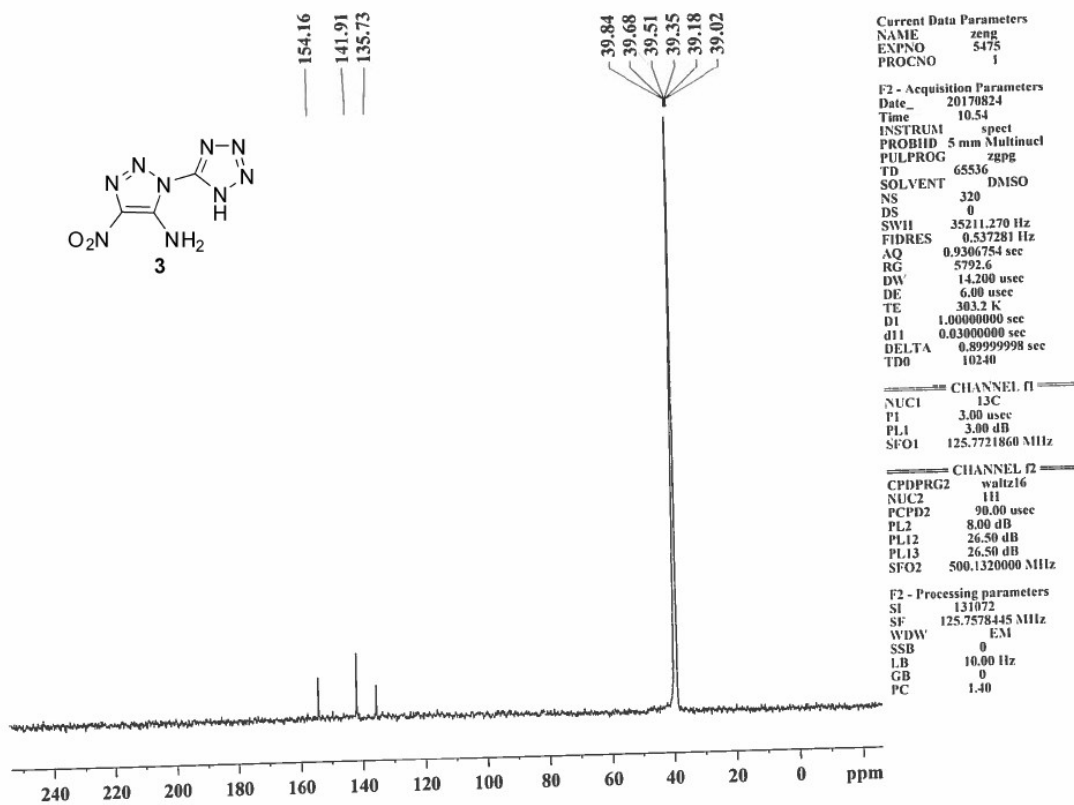
¹H NMR of compound 2



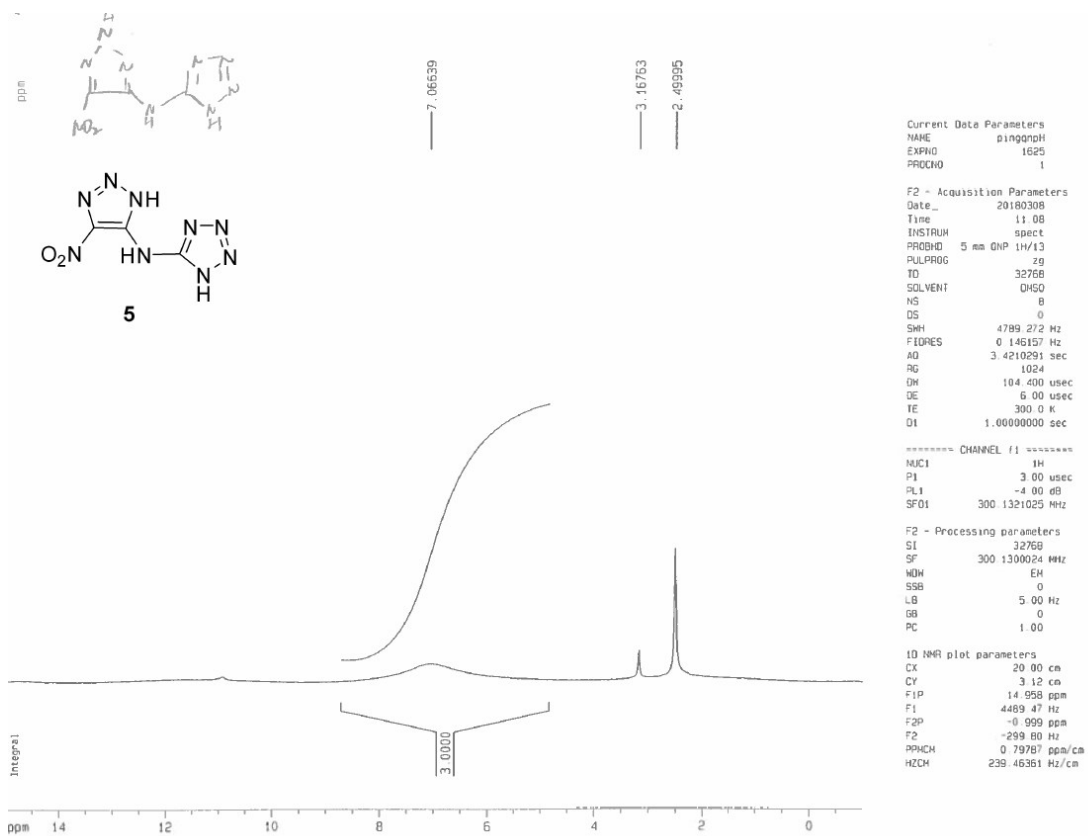
¹³C NMR of compound 2



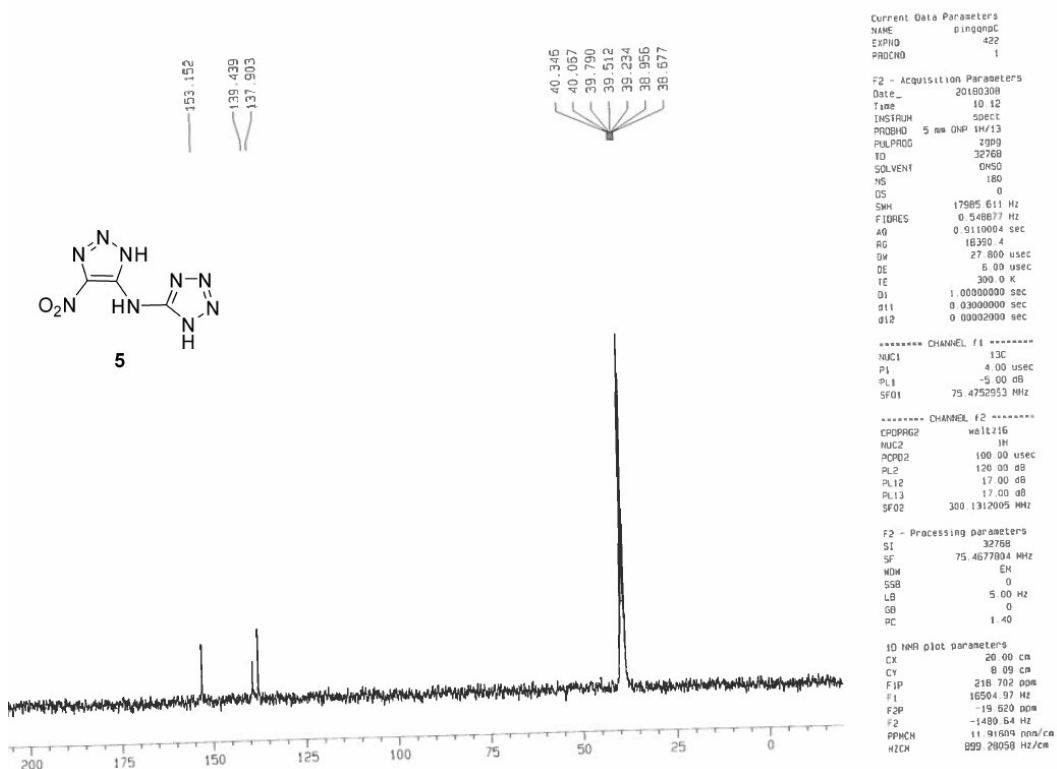
¹H NMR of compound 3



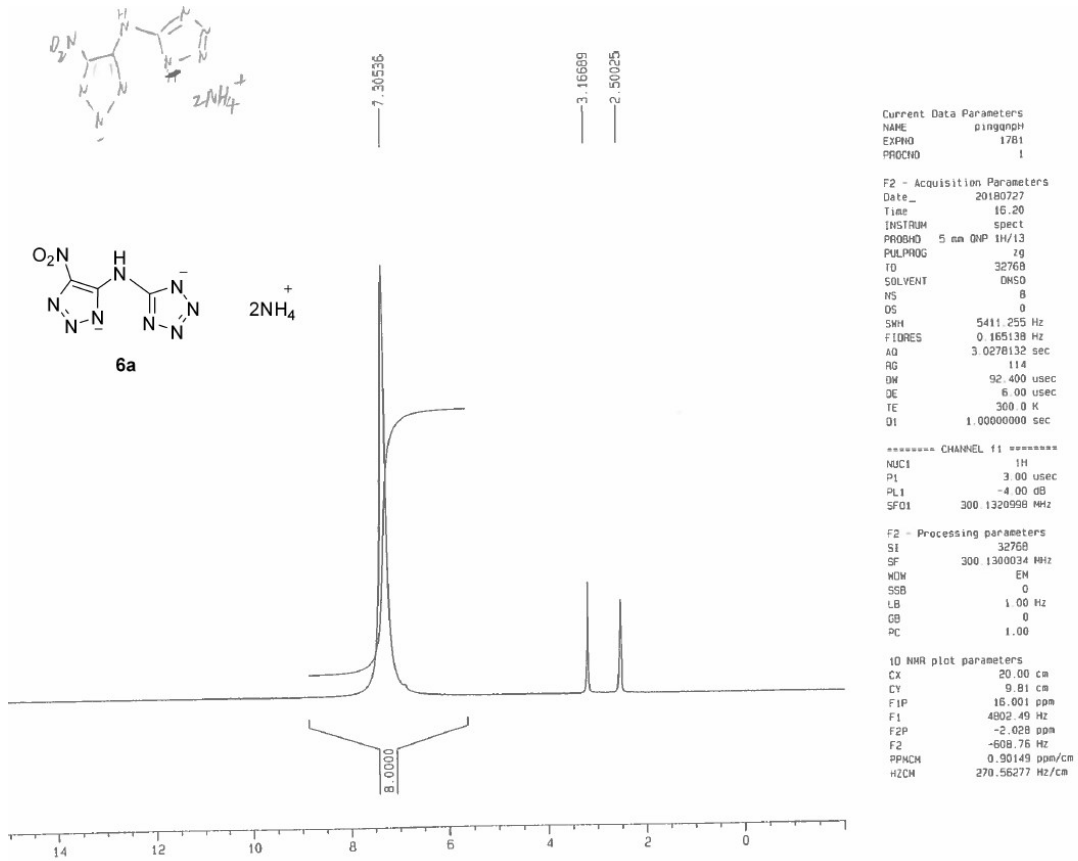
¹³C NMR of compound 3



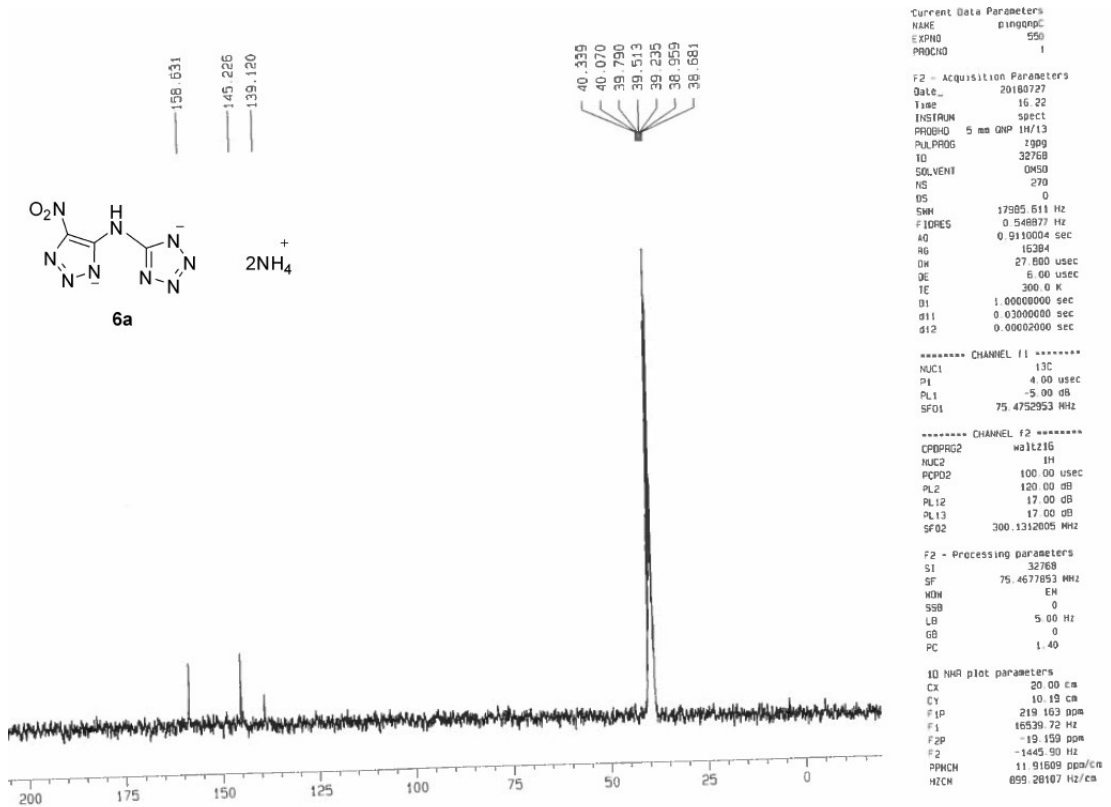
¹H NMR of compound 5



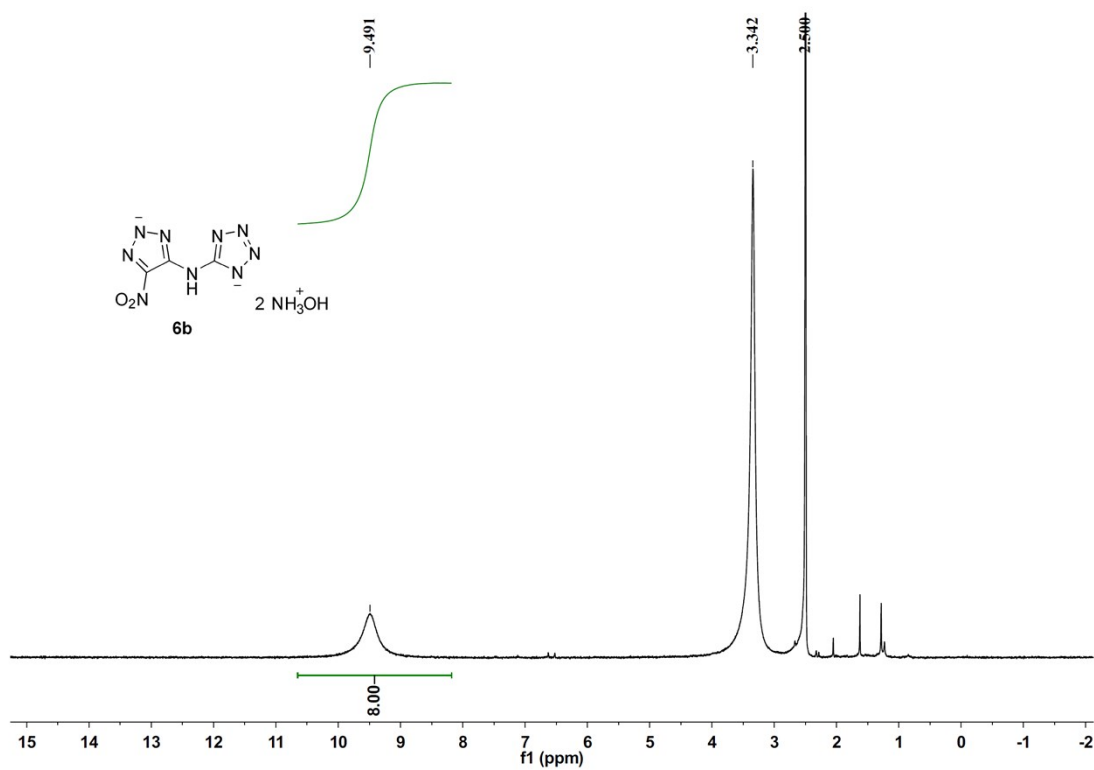
¹³C NMR of compound 5



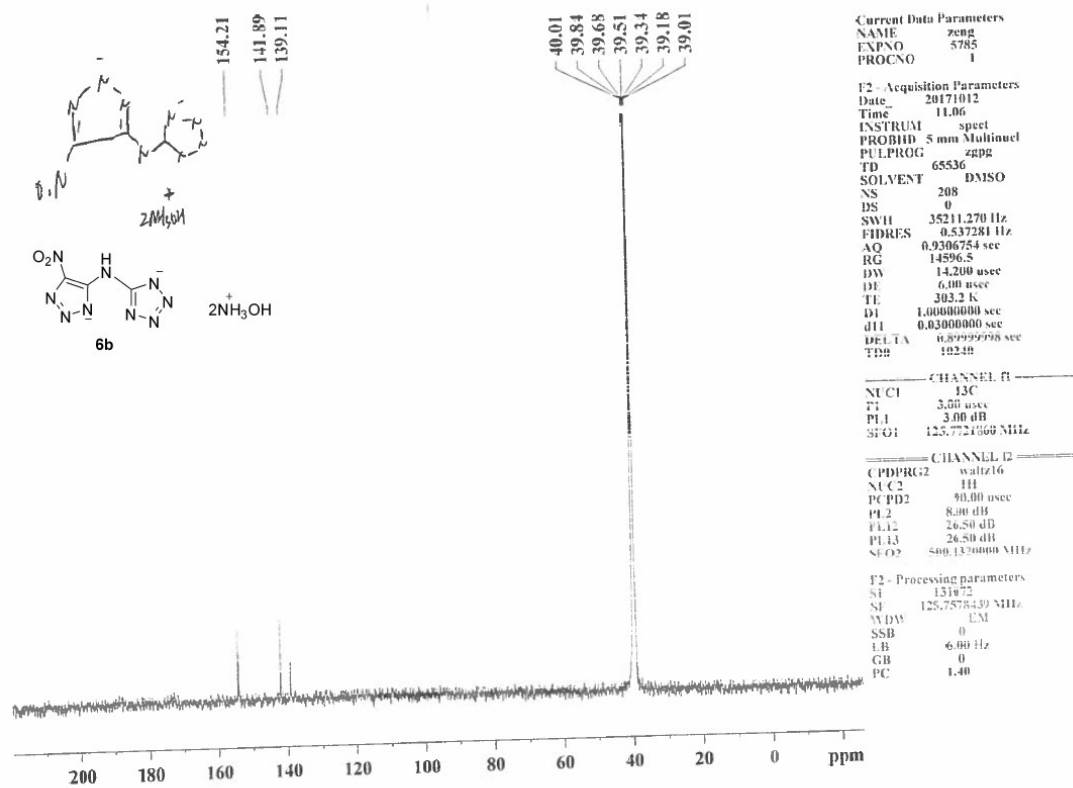
¹H NMR of compound 6a



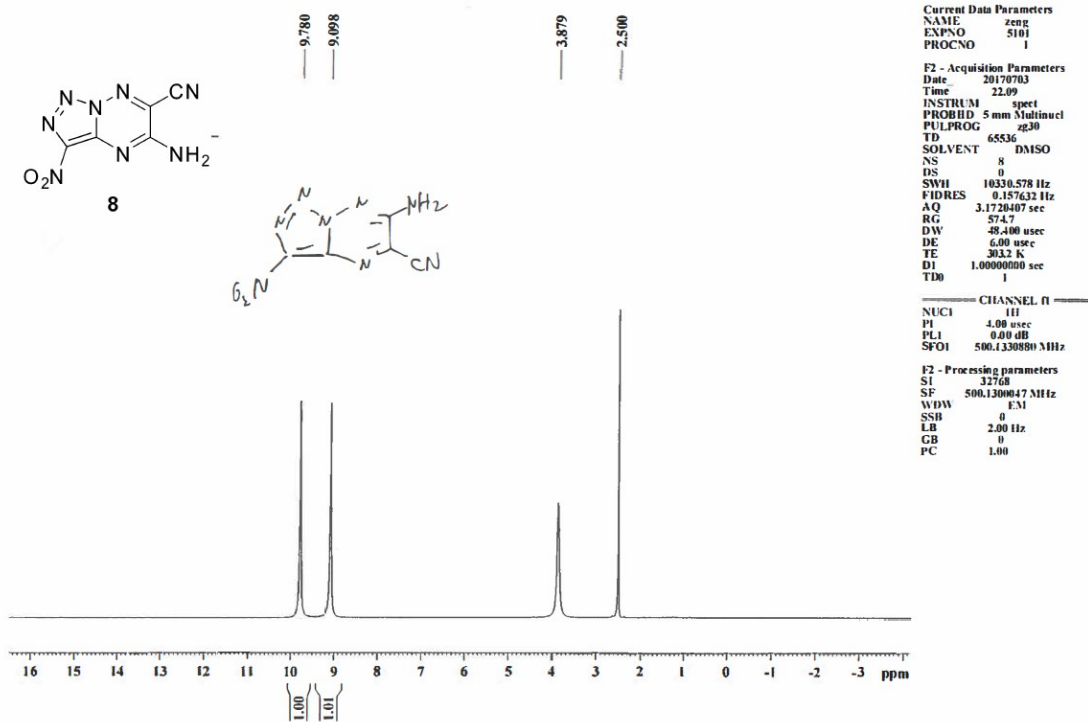
¹³C NMR of compound 6a



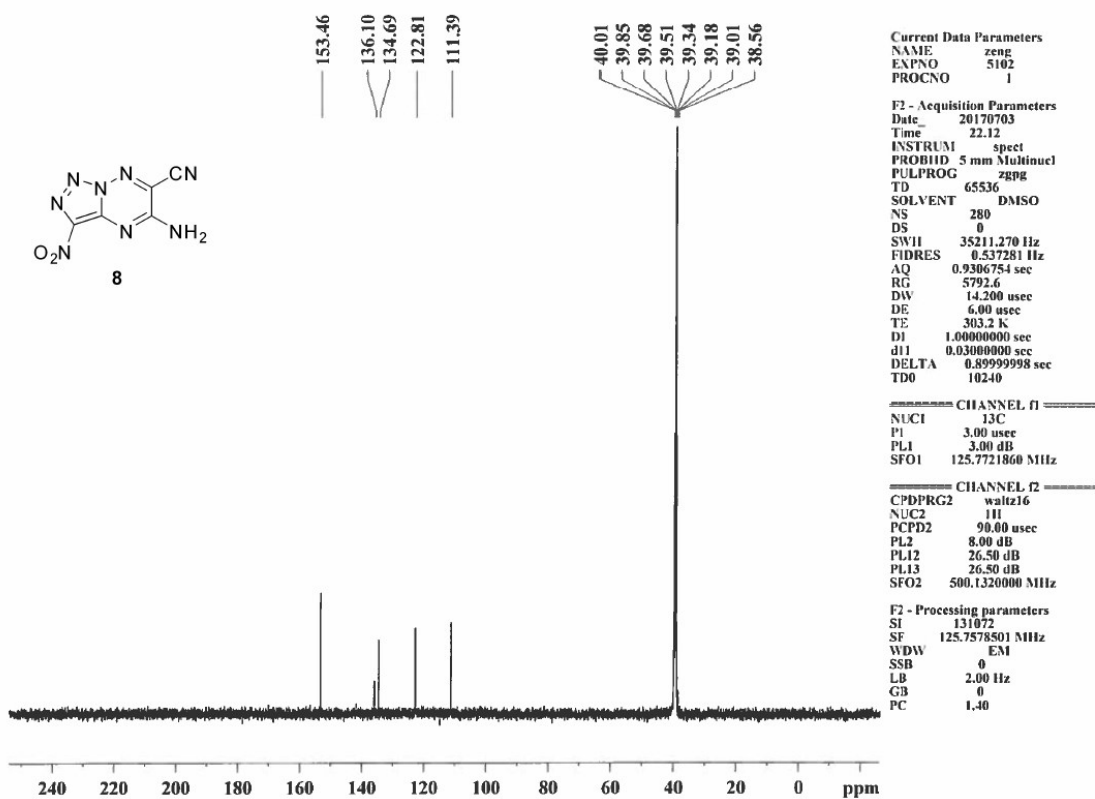
¹H NMR of compound **6b**



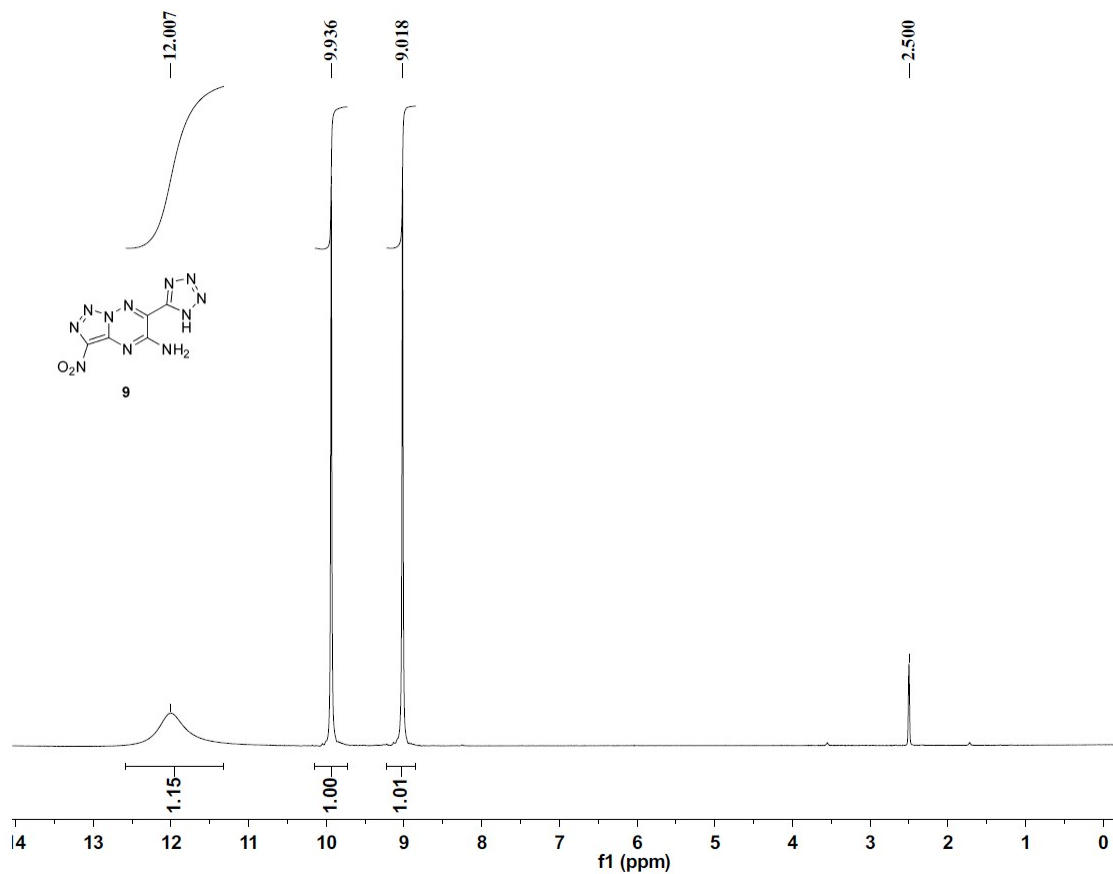
¹³C NMR of compound **6b**



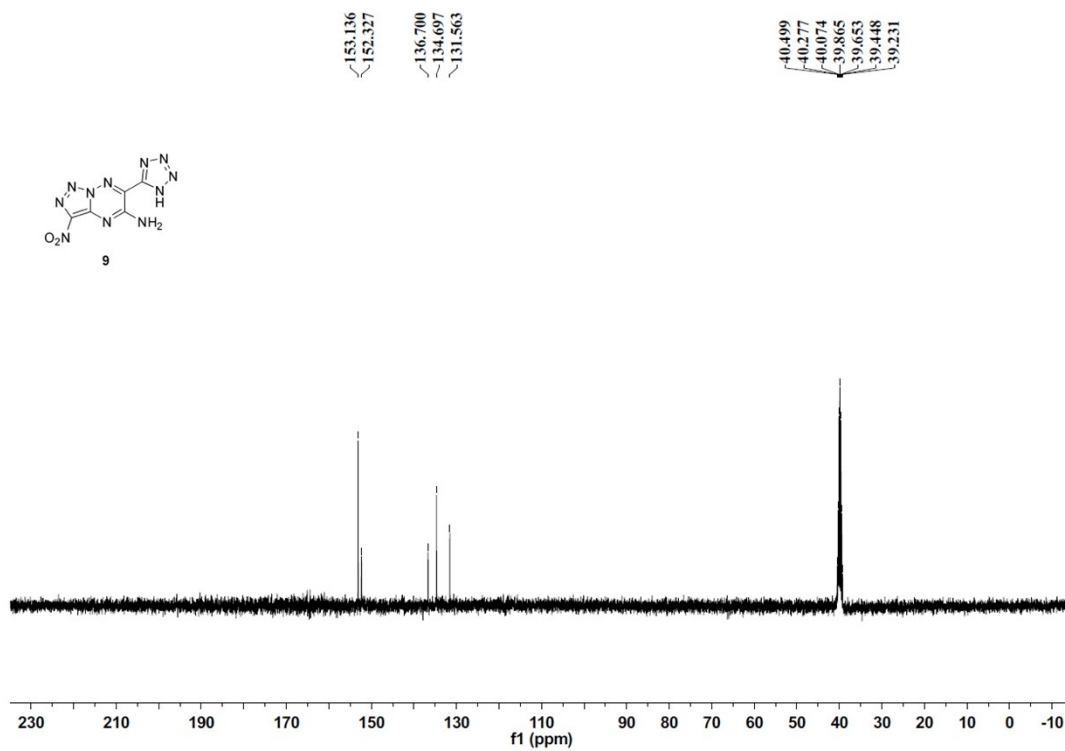
¹H NMR of compound 8



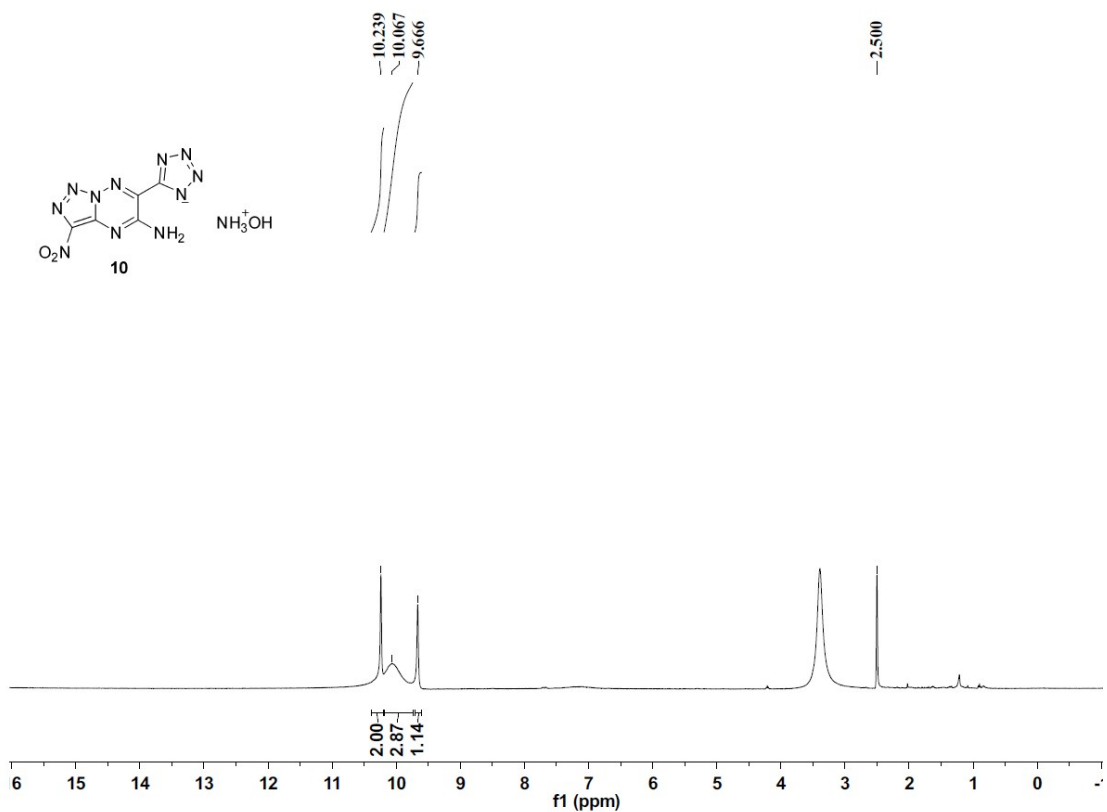
¹³C NMR of compound 8



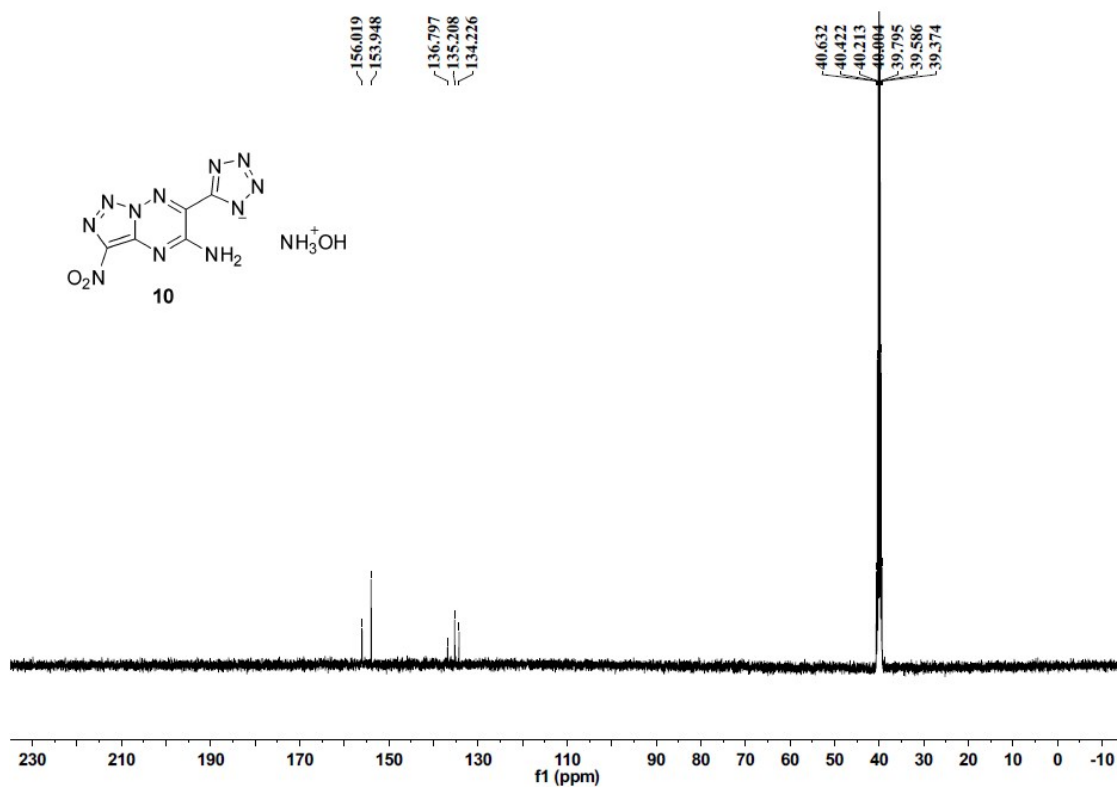
¹H NMR of compound 9



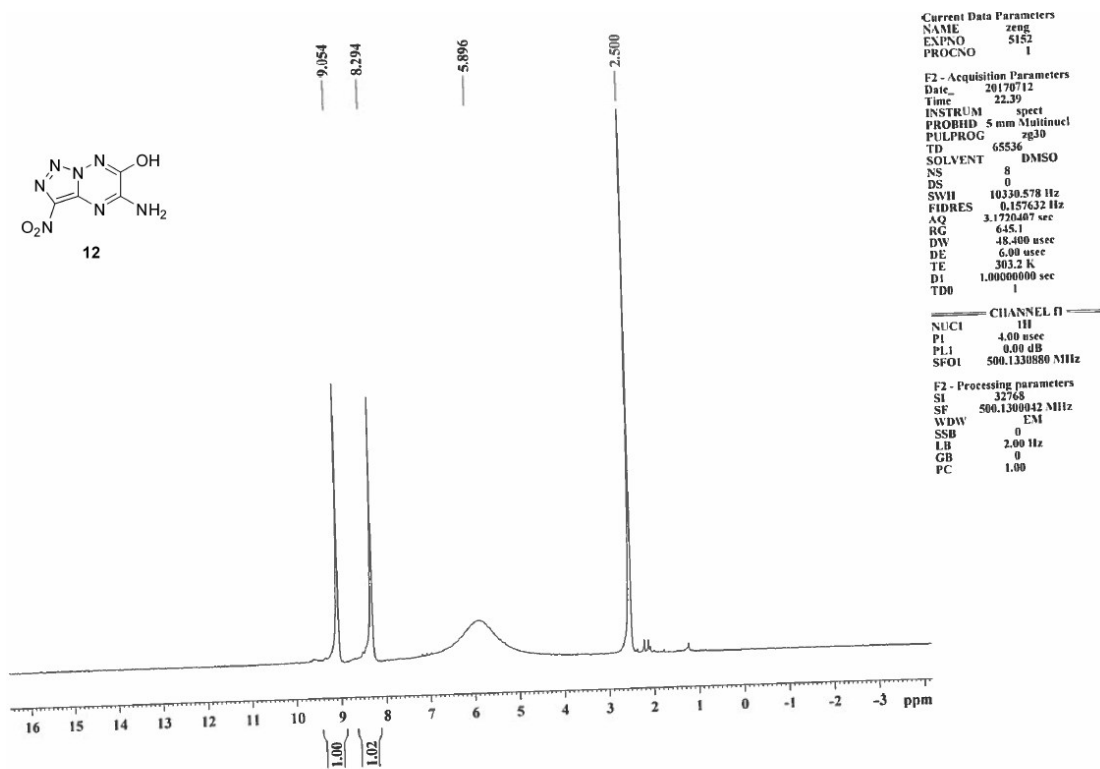
¹³C NMR of compound 9



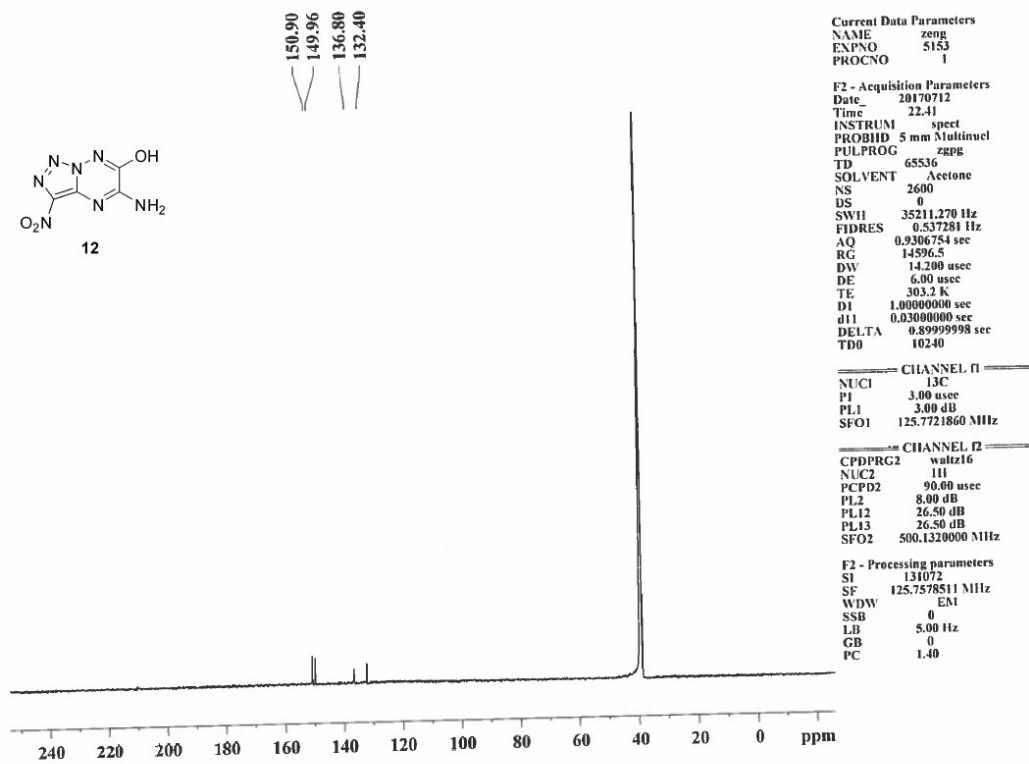
^1H NMR of compound 10



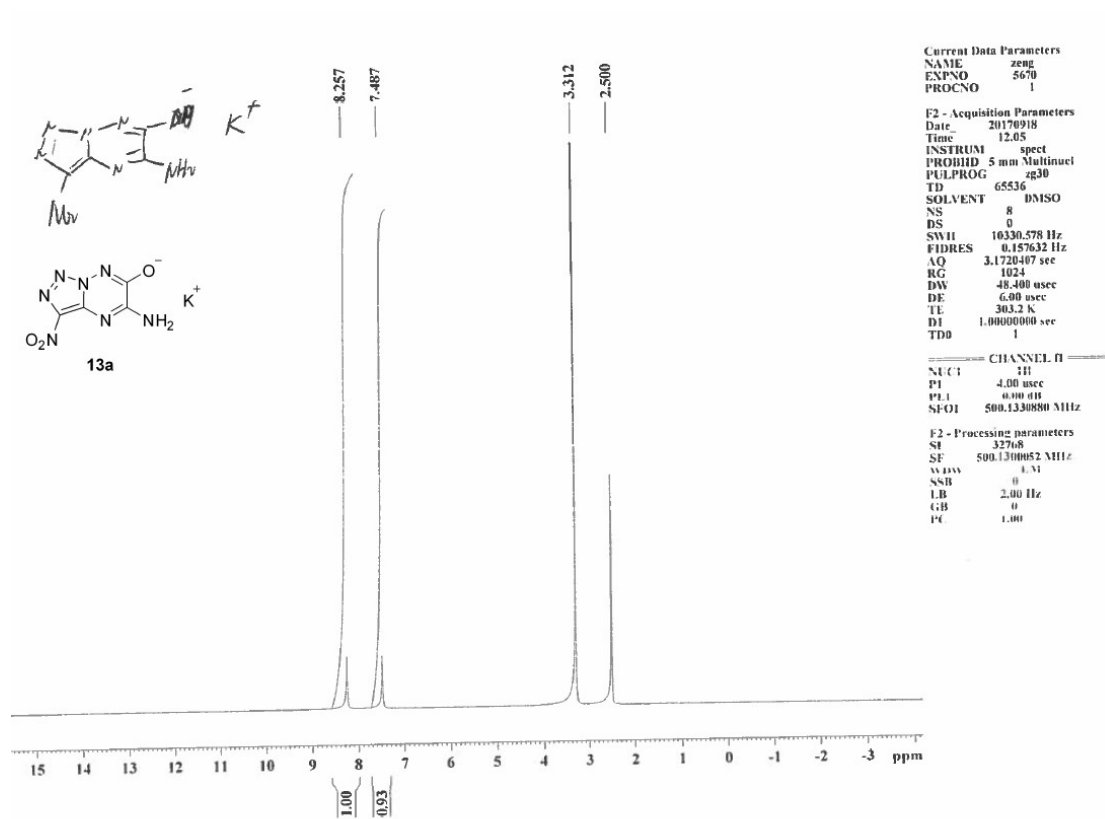
^{13}C NMR of compound 10



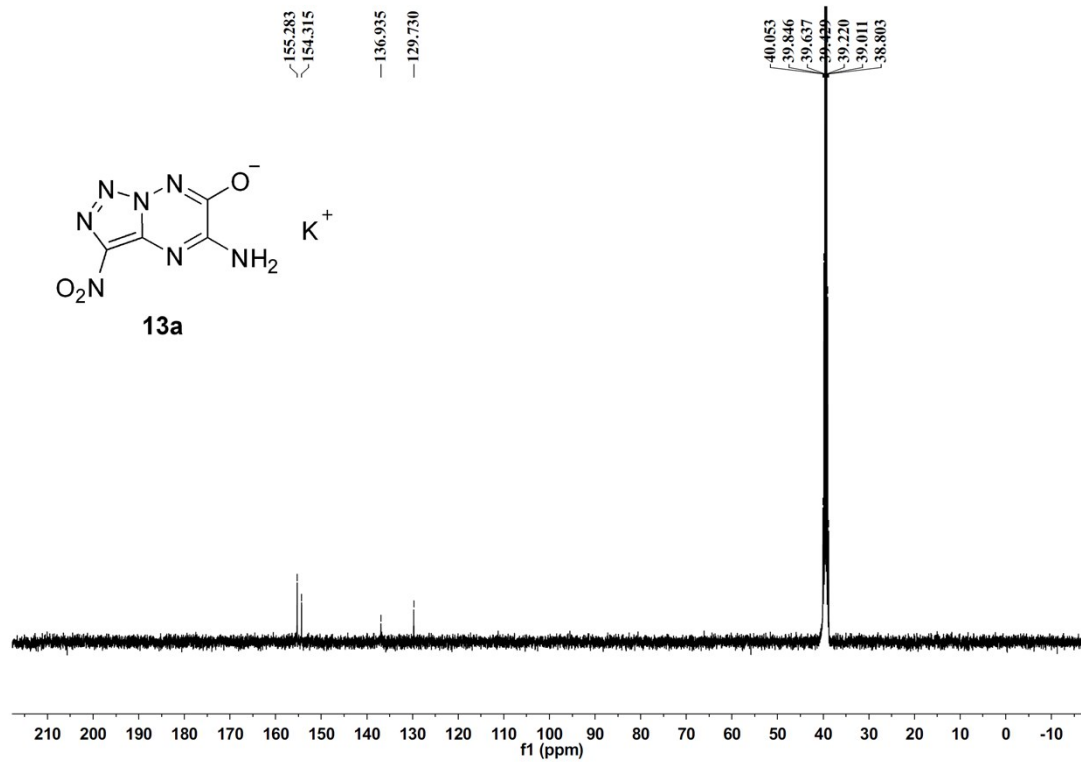
¹H NMR of compound 12



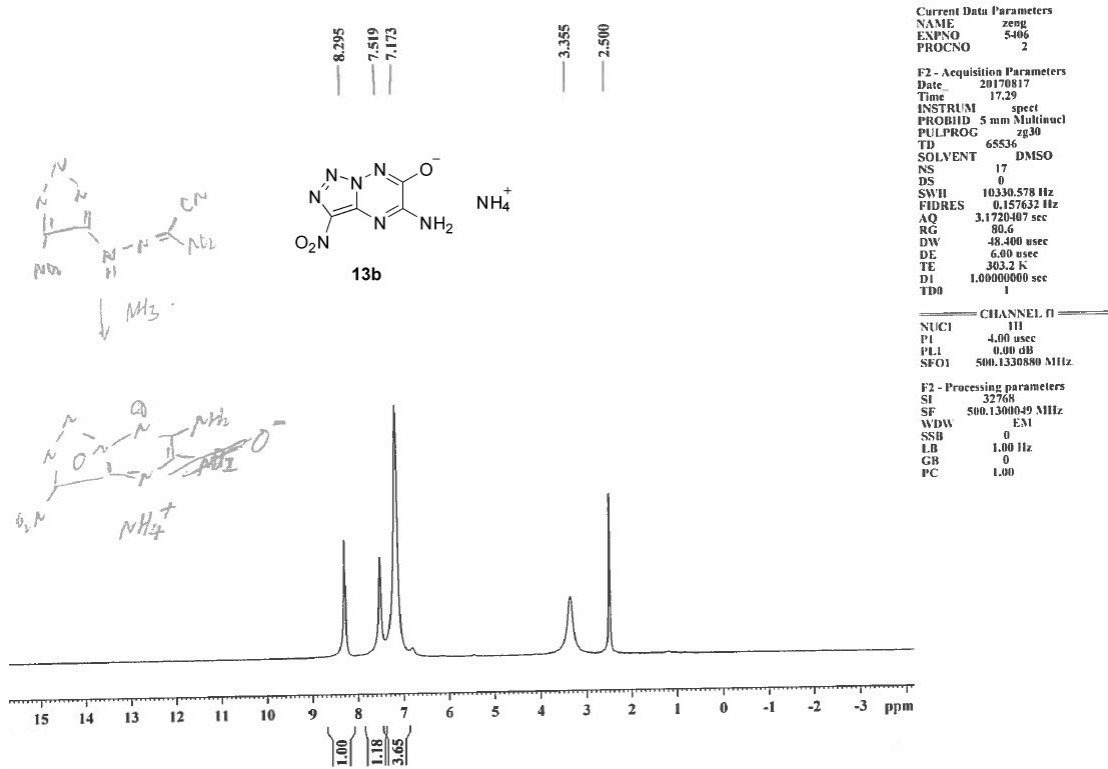
¹³C NMR of compound 12



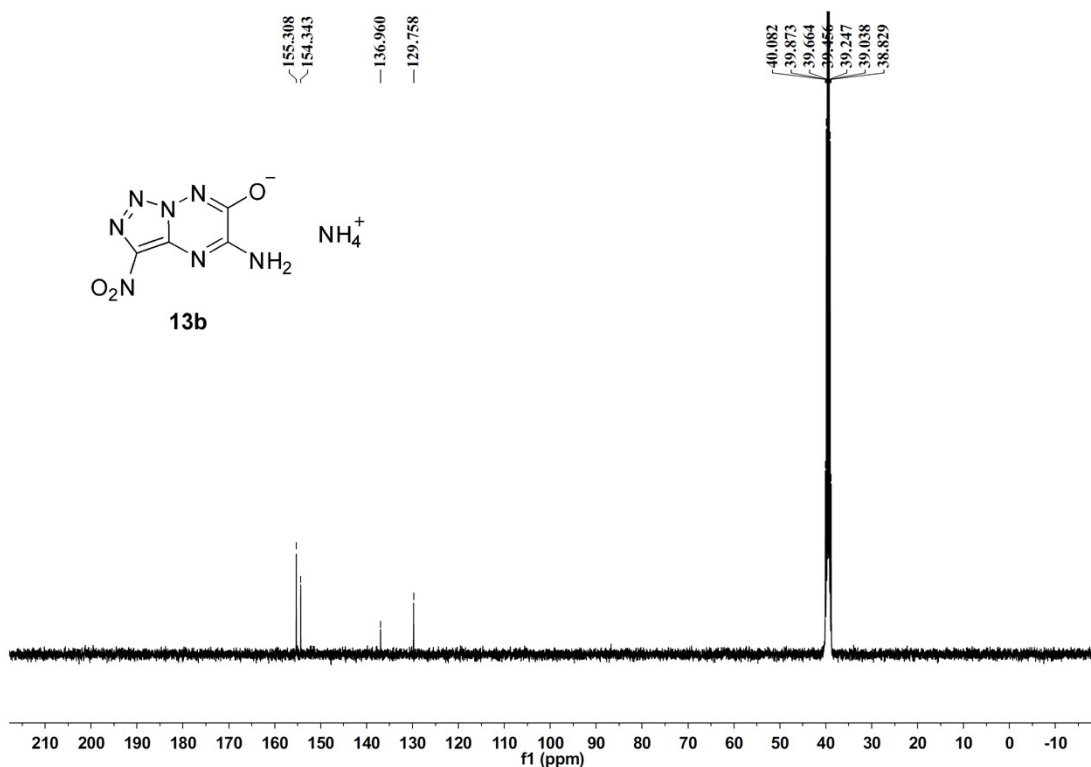
¹H NMR of compound 13a



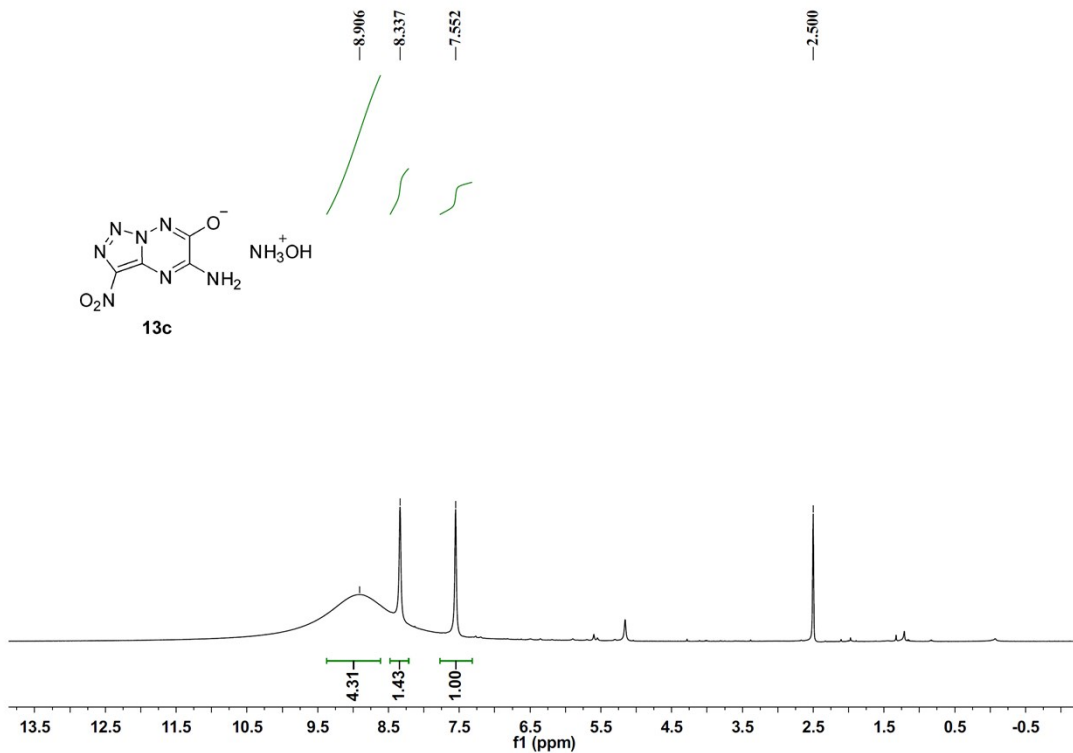
¹³C NMR of compound 13a



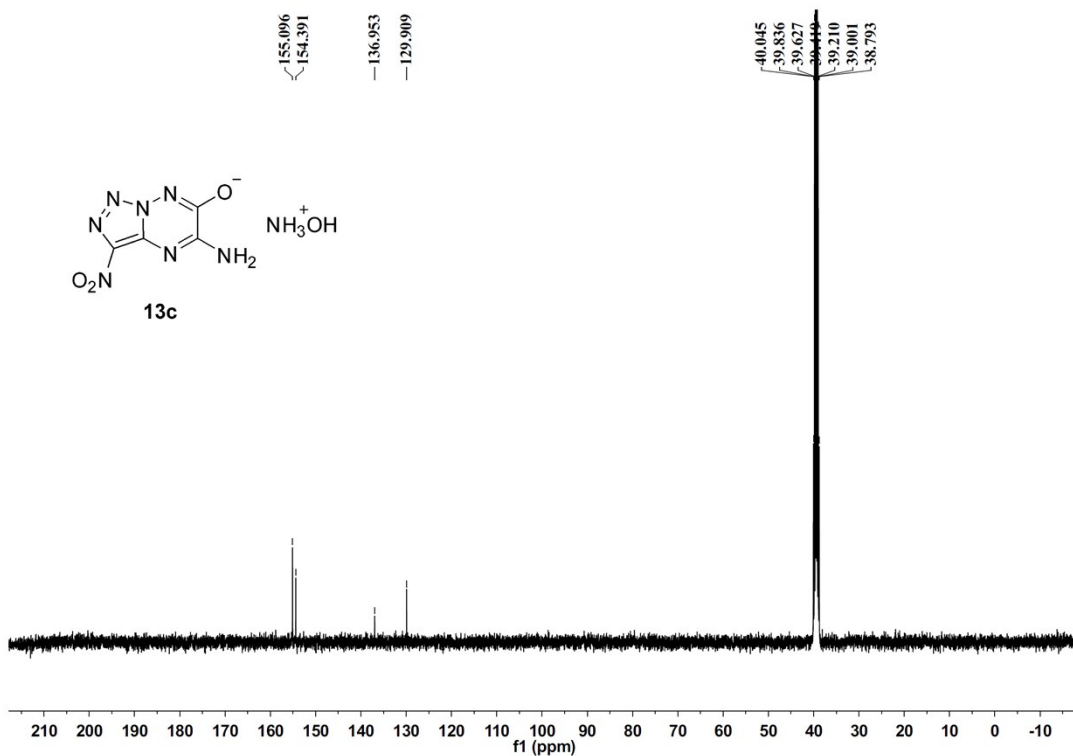
¹H NMR of compound 13b



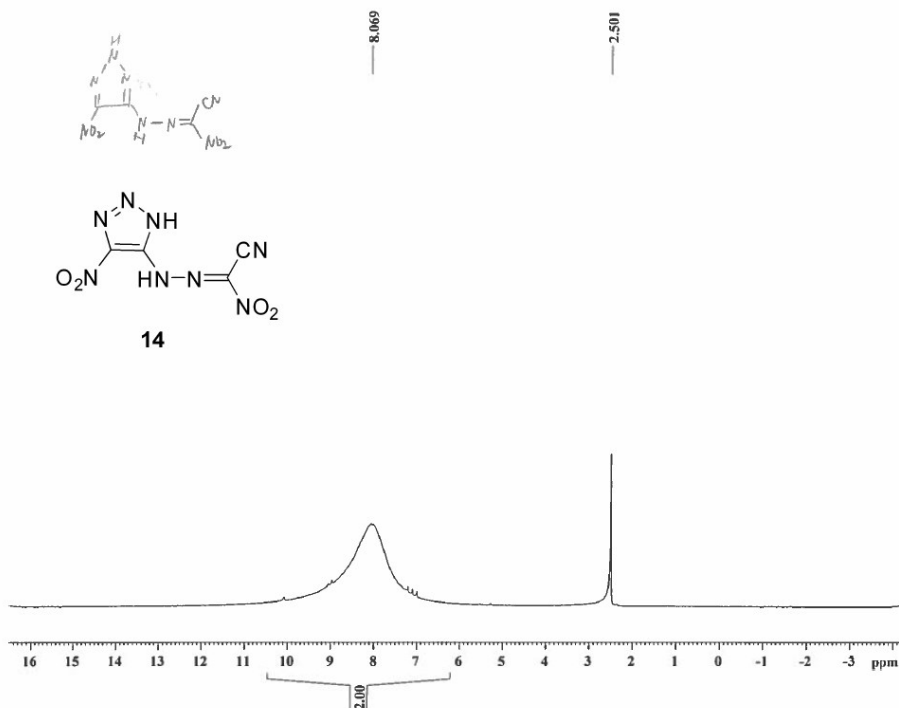
¹³C NMR of compound 13b



^1H NMR of compound **13c**



^{13}C NMR of compound **13c**



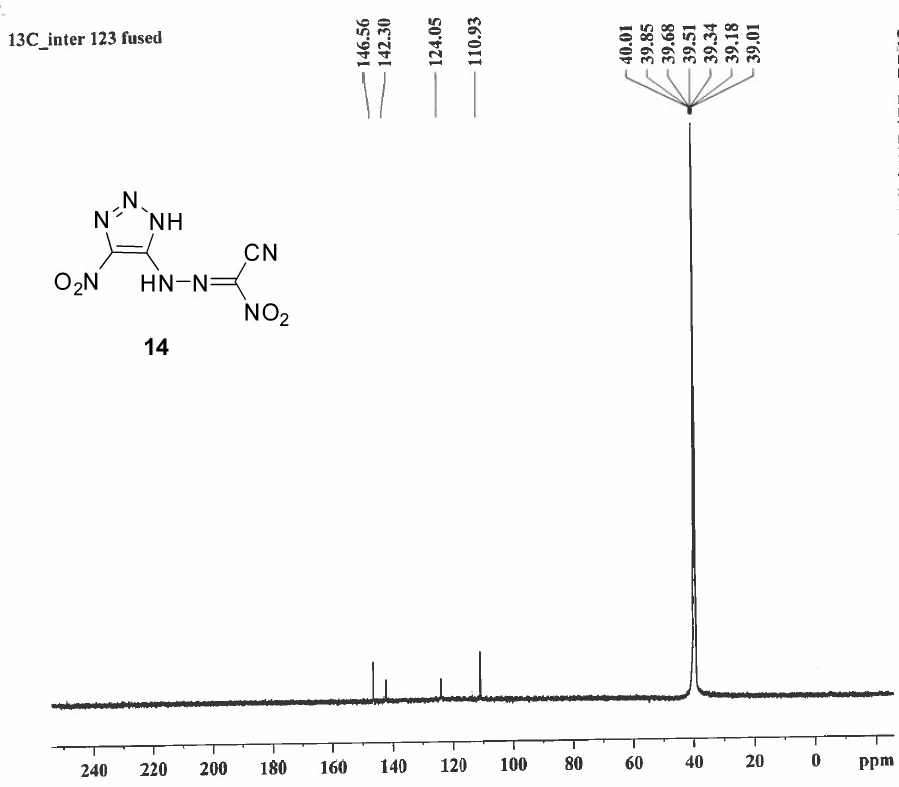
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 EXPNO 4835
 PROCNO 1

F2 - Acquisition Parameters
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 Time 11.52
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 PROBHID 5 mm Multinucl
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 0
 SWH 10330.578 Hz
 FIDRES 0.157632 Hz
 AQ 3.1720407 sec
 RG 322.5
 DW -48.400 usec
 DE 6.00 usec
 TE 303.2 K
 D1 1.00000000 sec
 TDD 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 4.00 usec
 PL1 0.00 dB
 SFO1 500.1330880 MHz

F2 - Processing parameters
 SI 32768
 SF 500.1330833 MHz
 WDW EM1
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.00

¹H NMR of compound 14



Current Data Parameters
 NAME zeng
 EXPNO 4835
 PROCNO 1

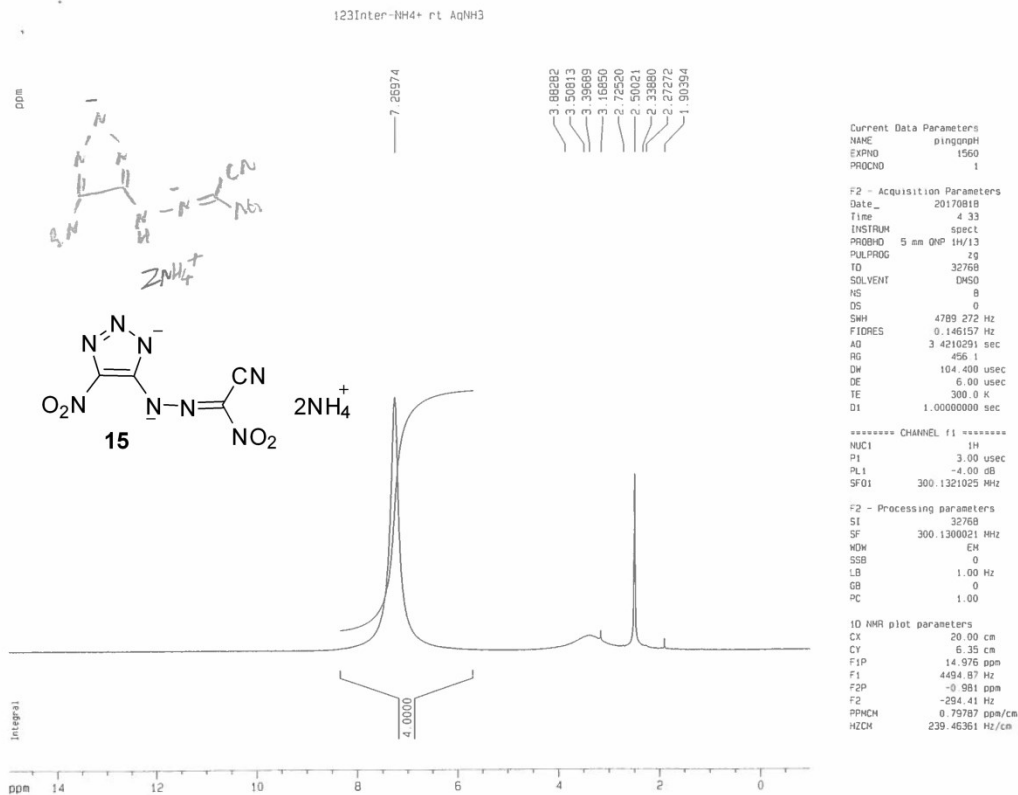
F2 - Acquisition Parameters
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 Time 11.58
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 PROBHID 5 mm Multinucl
 PULPROG zgpg
 TD 65536
 SOLVENT DMSO
 NS 4720
 DS 0
 SWH 35211.270 Hz
 FIDRES 0.537281 Hz
 AQ 0.9306754 sec
 RG 9195.2
 DW 14.200 usec
 DE 6.00 usec
 TE 303.2 K
 D1 1.00000000 sec
 d11 0.03000000 sec
 DELTA 0.89999998 sec
 TDD 10240

===== CHANNEL f1 =====
 NUC1 13C
 P1 3.00 usec
 PL1 3.00 dB
 SFO1 125.7721860 MHz

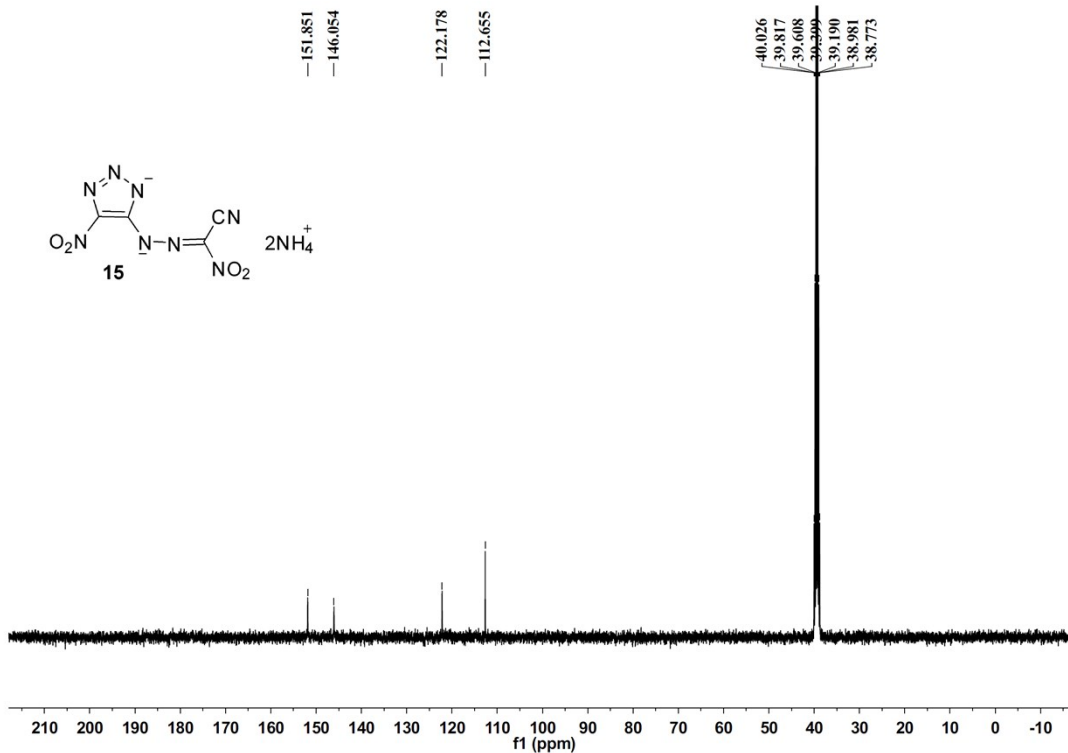
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL2 8.00 dB
 PL12 26.50 dB
 PL13 26.50 dB
 SFO2 500.1320000 MHz

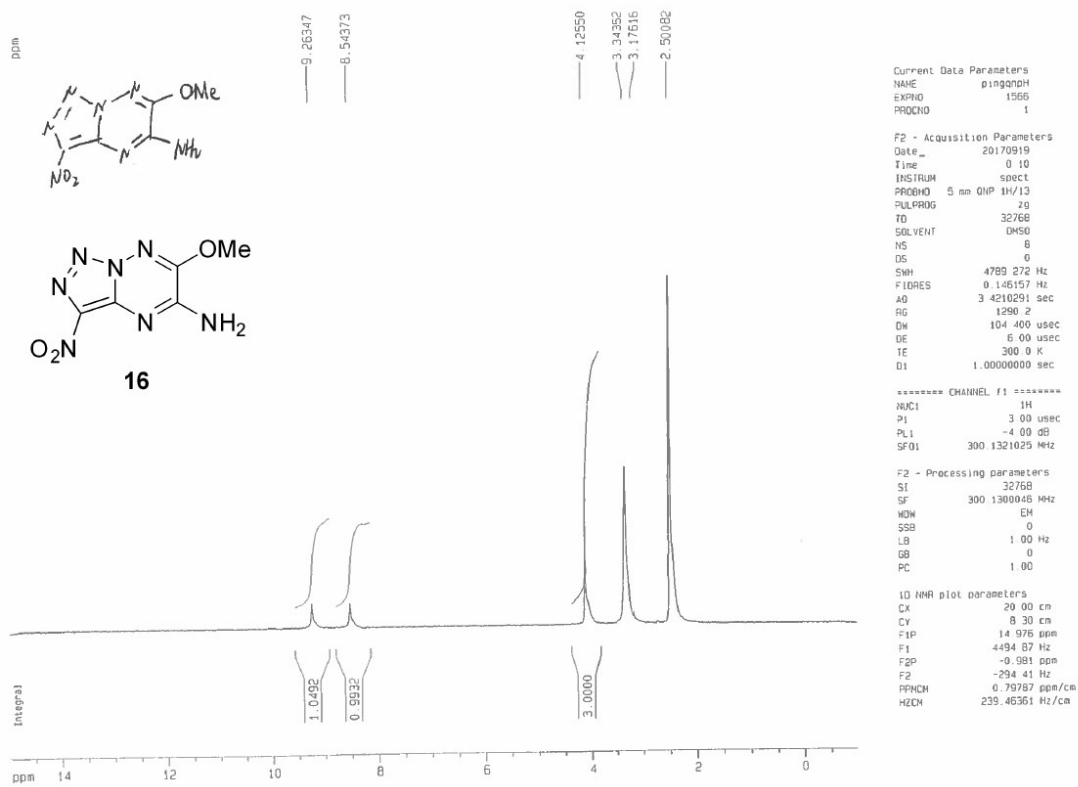
F2 - Processing parameters
 SI 131072
 SF 125.7578275 MHz
 WDVV EM1
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹³C NMR of compound 14

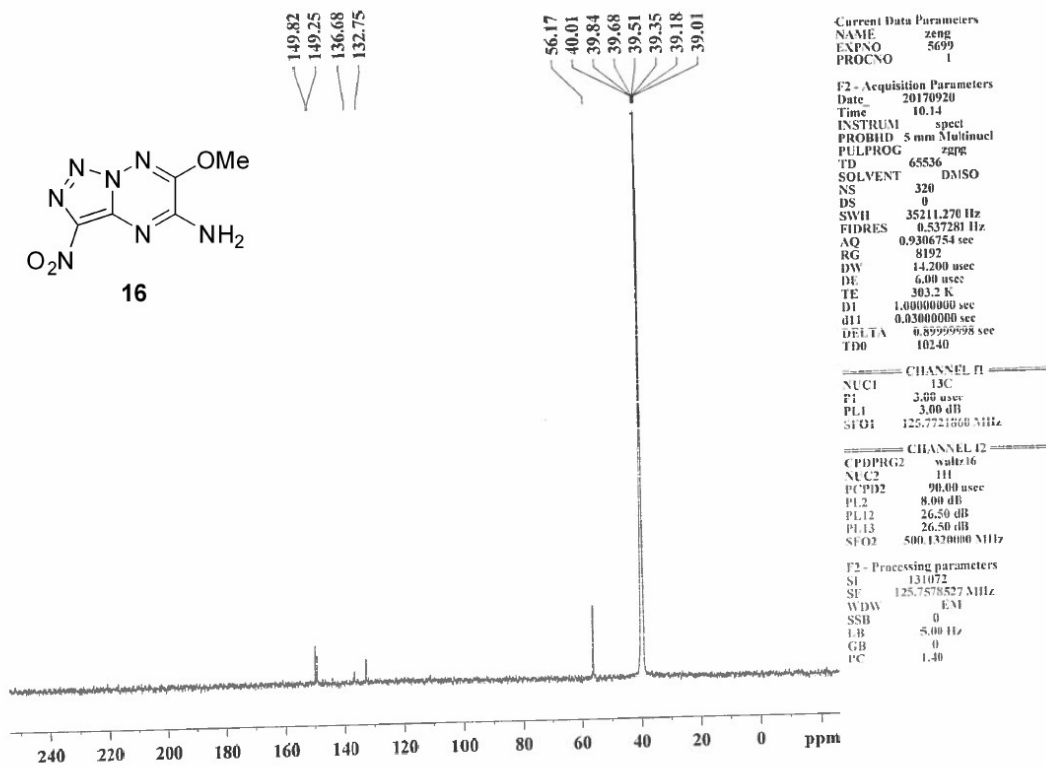


¹H NMR of compound 15

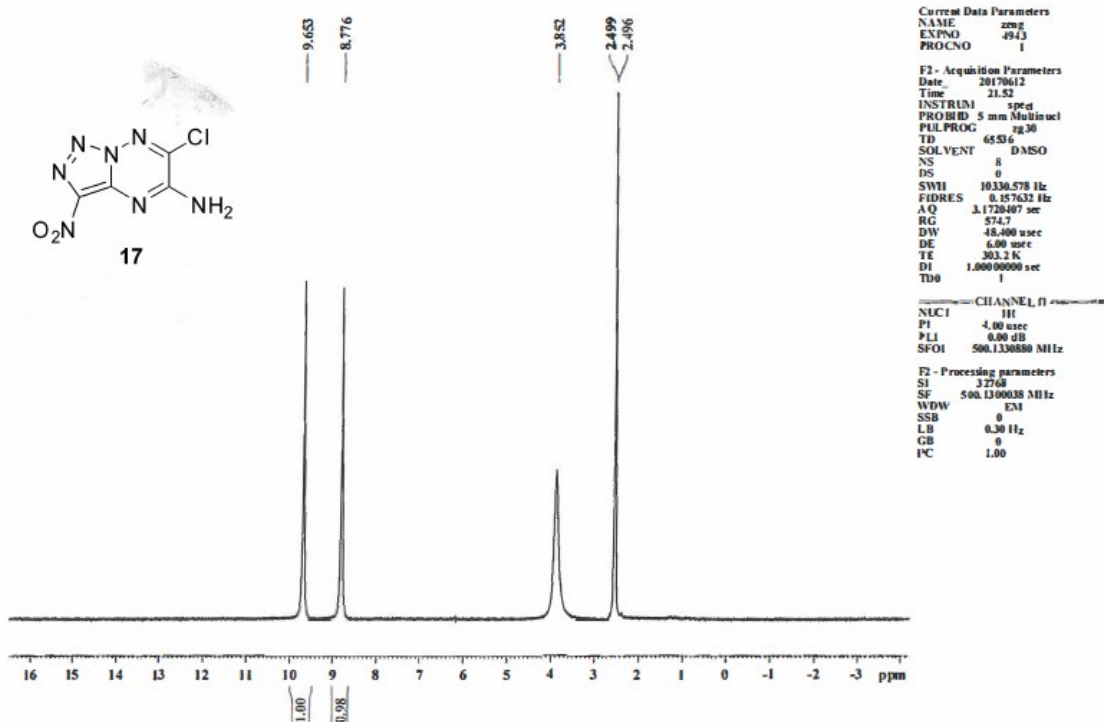




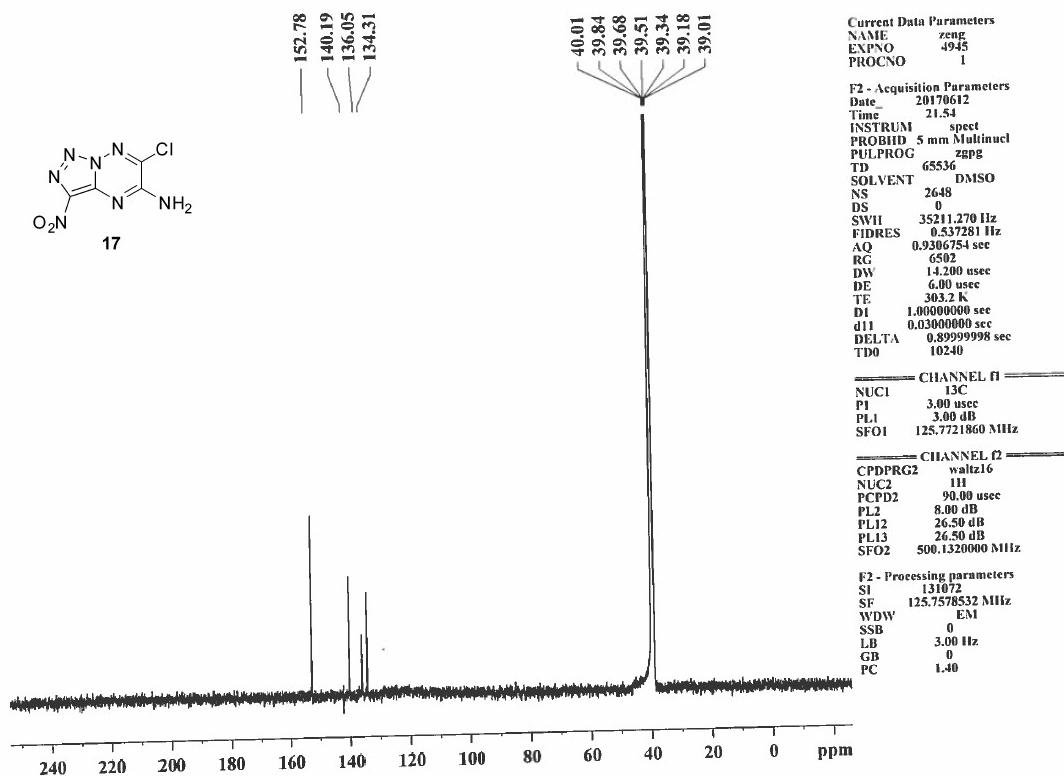
¹H NMR of compound 16



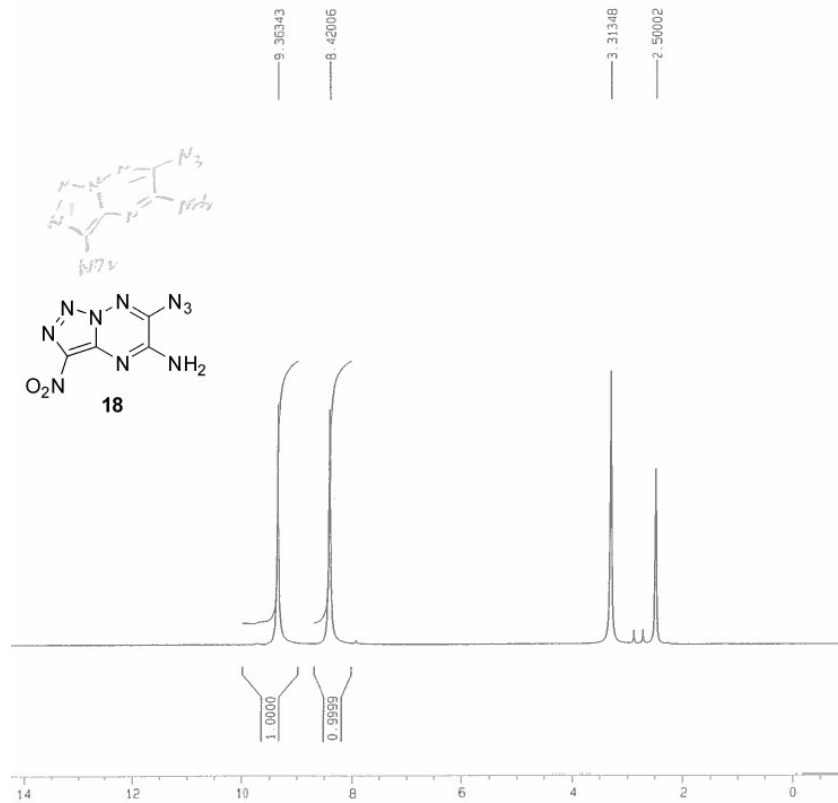
¹³C NMR of compound 16



¹H NMR of compound 17



¹³C NMR of compound 17



Current Date Parameters
NAME pingqinH
EXPNO 1572
PROCNO 1

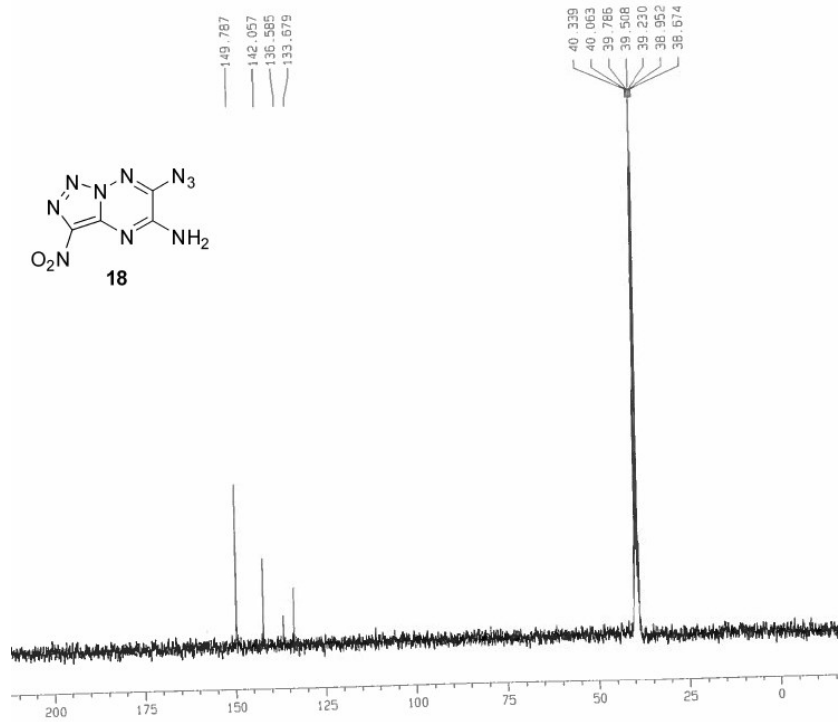
F2 - Acquisition Parameters
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Time 15.59
INSTRUM spect
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PULPROG zg
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 4789.272 Hz
FIDRES 0.146157 Hz
AQ 3.4210291 sec
RG 512
DH 104.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec

----- CHANNEL f1 -----
NUC1 1H
P1 3.00 usec
PL1 -4.00 dB
SFO1 300.1321025 MHz

F2 - Processing parameters
SI 32768
SF 300.1300030 MHz
WDW EH
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 6.27 cm
F1P 14.976 ppm
F1 4494.87 Hz
F2P -0.981 ppm
F2 -294.41 Hz
PRNCH 0.75787 ppm/cm
HZCH 239.46351 Hz/cm

¹H NMR of compound 18



Current Date Parameters
NAME pingqinC
EXPNO 405
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170925
Time 16.01
INSTRUM spect
PROBHD 5 mm QNP 1H/13
PULPROG zgpg
TD 32768
SOLVENT CD3CN
NS 382
DS 0
SWH 17985.611 Hz
FIDRES 0.548877 Hz
AQ 0.9110004 sec
RG 10390.4
DH 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
S11 0.03000000 sec
d12 0.0002000 sec

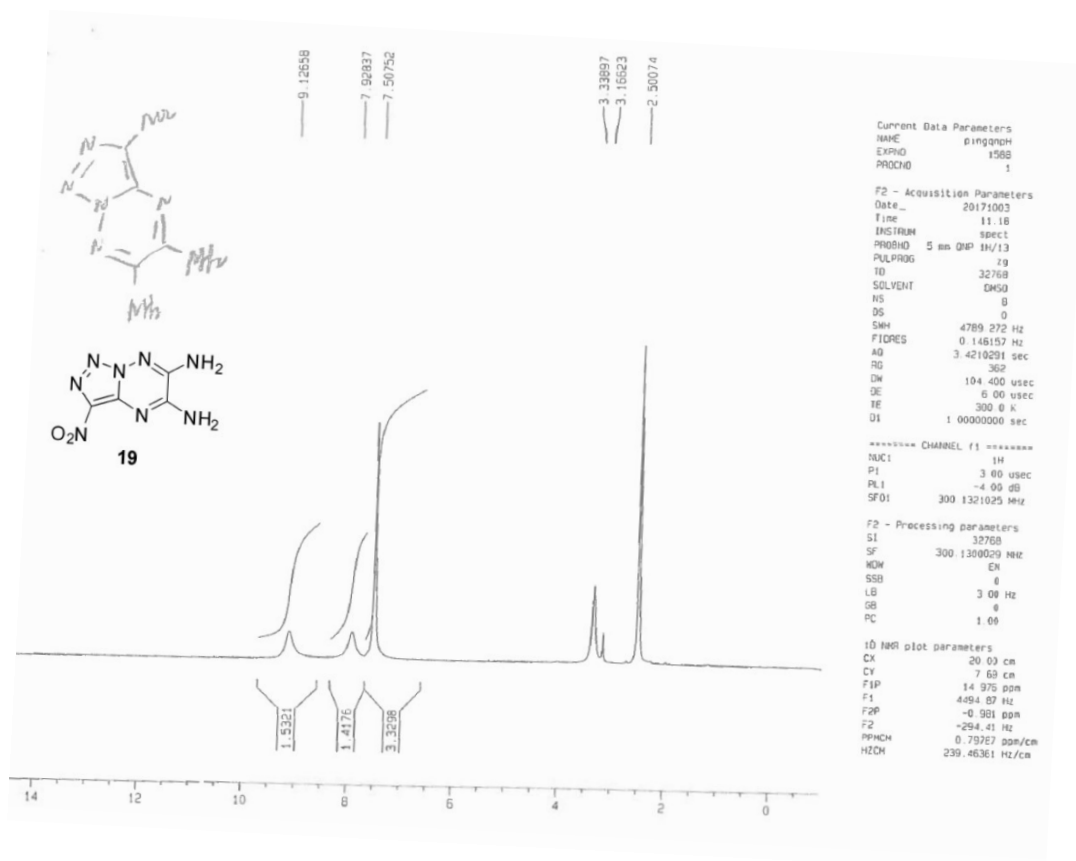
----- CHANNEL f1 -----
NUC1 13C
P1 4.00 usec
PL1 -5.00 dB
SFO1 75.4752953 MHz

----- CHANNEL f2 -----
CPRPRG2 waltz16
NUC2 1H
PCPD2 190.00 usec
PL2 120.00 dB
PL12 17.00 dB
PL13 17.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677881 MHz
WDW EH
SSB 0
LB 3.00 Hz
GB 6
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 12.83 cm
F1P 219.702 ppm
F1 16504.97 Hz
F2P -19.520 ppm
F2 -1480.64 Hz
PRNCH 11.91609 ppm/cm
HZCH 899.26864 Hz/cm

¹³C NMR of compound 18



¹H NMR of compound 19

¹³C NMR of compound 19