Supporting Information

Synthetic approach to novel azido esters and their utility as energetic plasticizers

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Contents

NMR (^{1}H, ^{13}C, ^{19}F, COSY, DEPT and HMBC) spectra

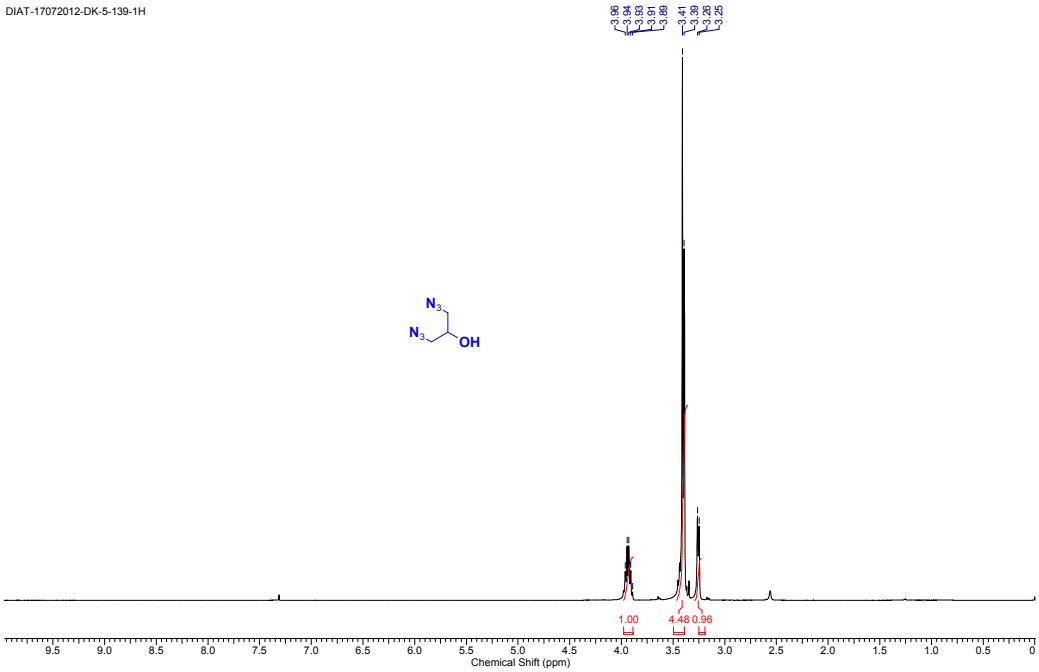


Figure S1: ^{1}H NMR (300MHz, $CDCl_3$) of 1,3-diazidopropan-2-ol **(2)**

^{1}H NMR (300MHz, $CDCl_3$) δ 3.26 (1H, d, J = 4.8 Hz), 3.41 (4H, d, J = 6.2 Hz), 3.93 (1H, quin, J_1 = 10.5 Hz J_2 = 5.2 Hz).

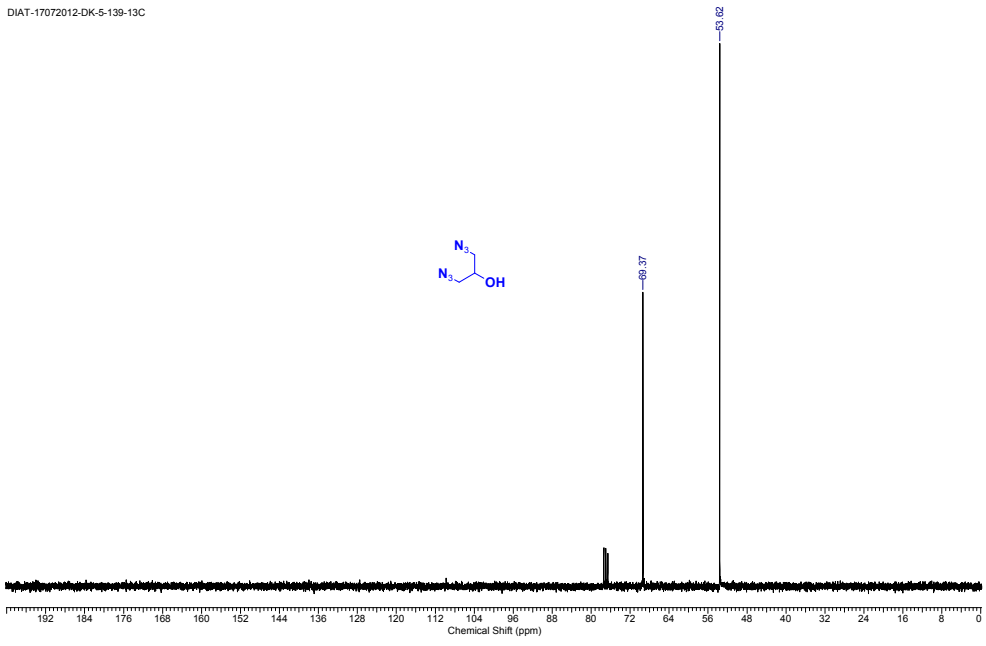


Figure S2: ^{13}C NMR (75MHz, $CDCl_3$) of 1,3-diazidopropan-2-ol **(2)**
^{13}C NMR ($CDCl_3$, 75 MHz) δ 53.6, 69.4 ppm.

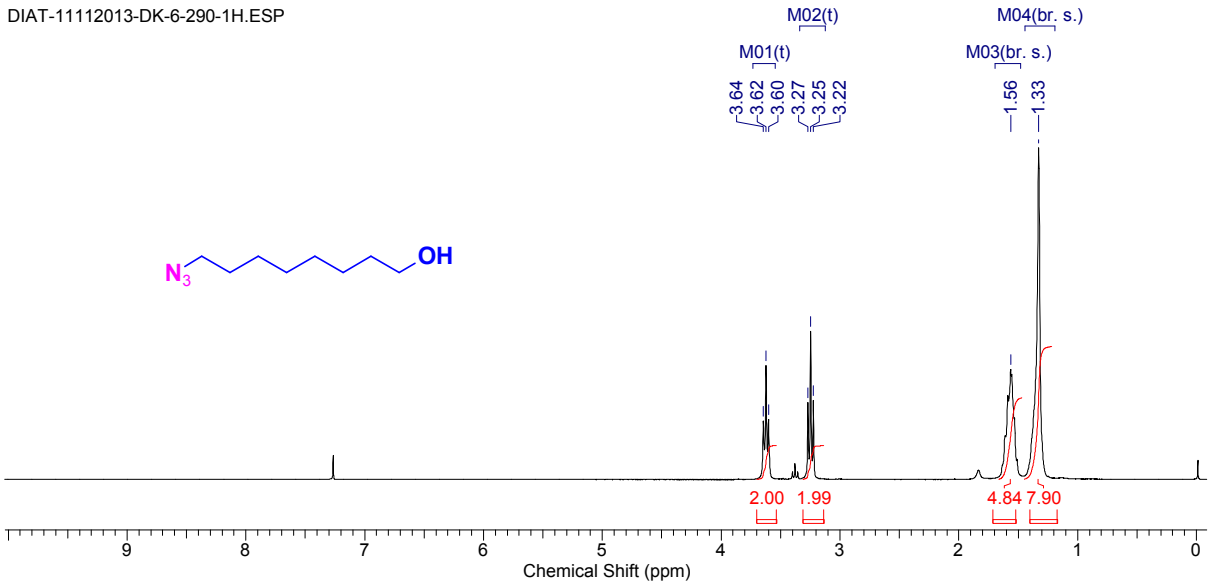


Figure S3: ^{1}H NMR (300MHz, $CDCl_3$) 8-azidooctan-1-ol **(4)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 1.33 (8H, m), 1.56 (4H, m), 3.25 (2H, t, J = 6.7 Hz), 3.62 (2H, t, J = 6.7 Hz).

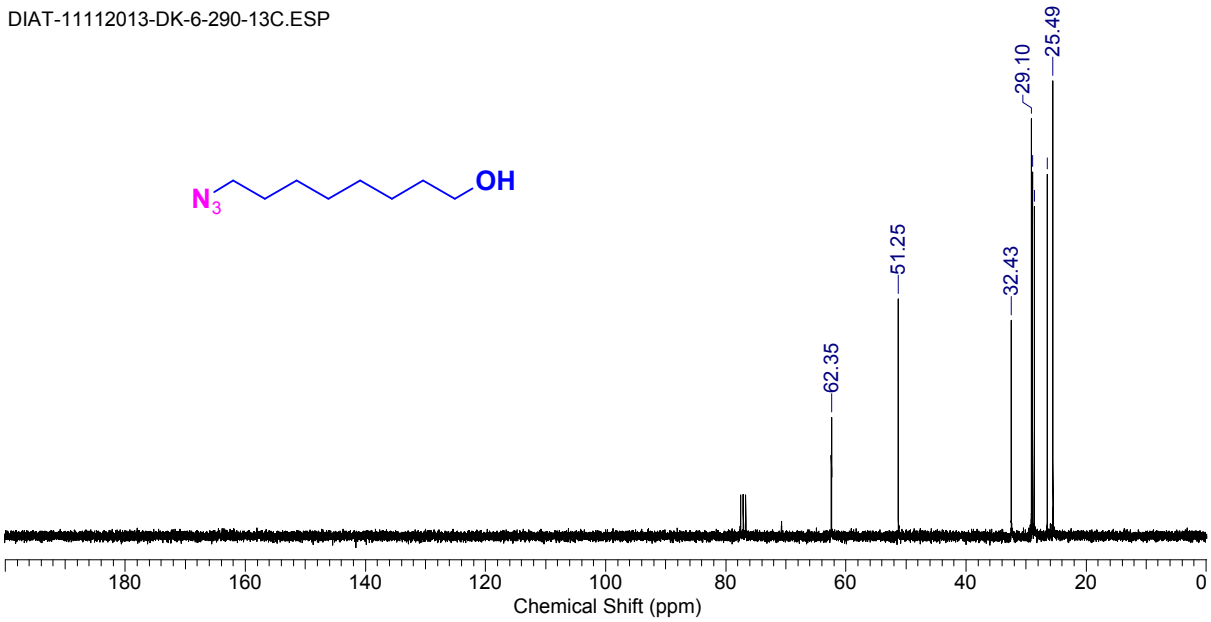


Figure S4: ^{13}C NMR (75MHz, $CDCl_3$) 8-azidooctan-1-ol **(4)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 25.5, 26.4, 28.6, 28.9, 29.1, 32.4, 51.3, 62.6 ppm.

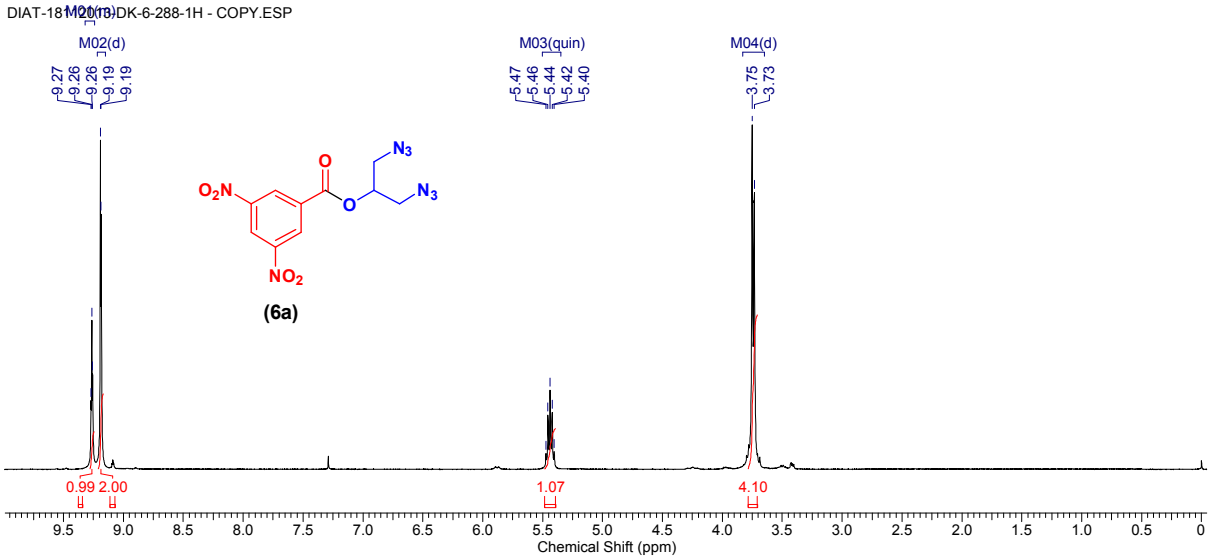


Figure S5: ^{1}H NMR (300MHz, $CDCl_3$) of **(6a)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 3.74 (4H, d, J = 5.7 Hz), 5.44 (1H, quin, J_1 = 10.5 Hz J_2 = 5.2 Hz), 9.19 (1H, d, J = 1.9 Hz), 9.26 (2H, t, J = 1.9 Hz).

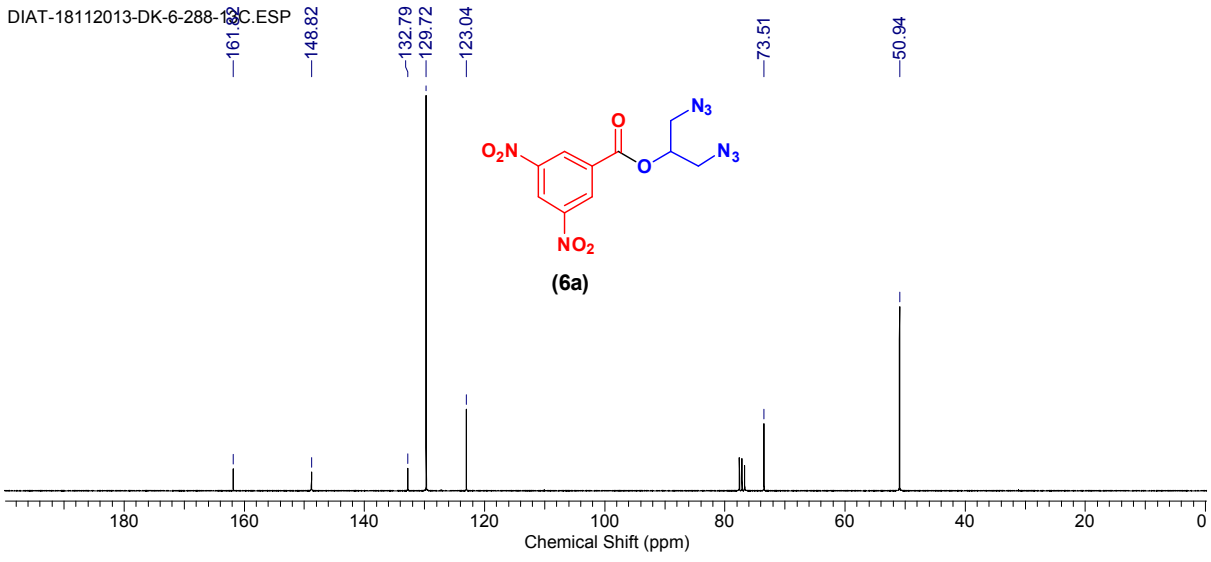


Figure S6: ^{13}C NMR (75MHz, $CDCl_3$) of **(6a)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 50.9, 73.5, 123.0, 129.7, 132.8, 148.8, 161.8 ppm.

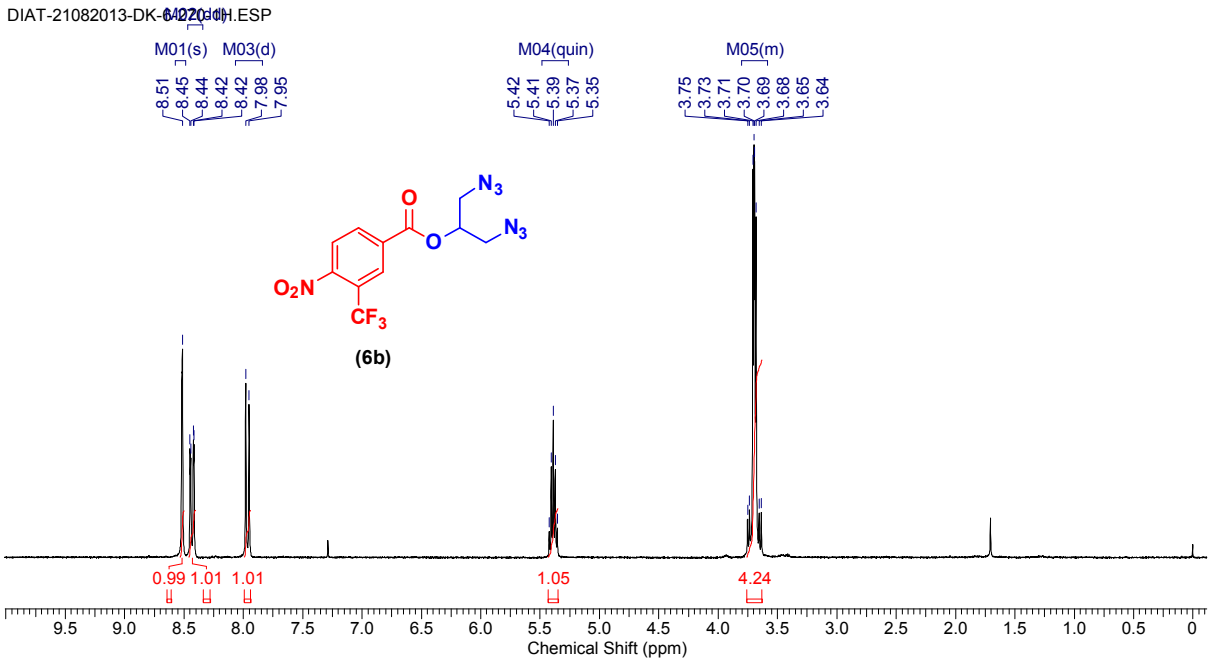


Figure S7: ^{1}H NMR (300MHz, $CDCl_3$) of **(6b)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 3.58-3.80 (4H, m), 5.39 (1H, quin, J_1 = 10.1 Hz J_2 = 4.8 Hz), 7.97 (1H, d, J = 8.4 Hz), 8.43 (1H, dd, J = 8.4, 1.76Hz), 8.51 (1H, s).

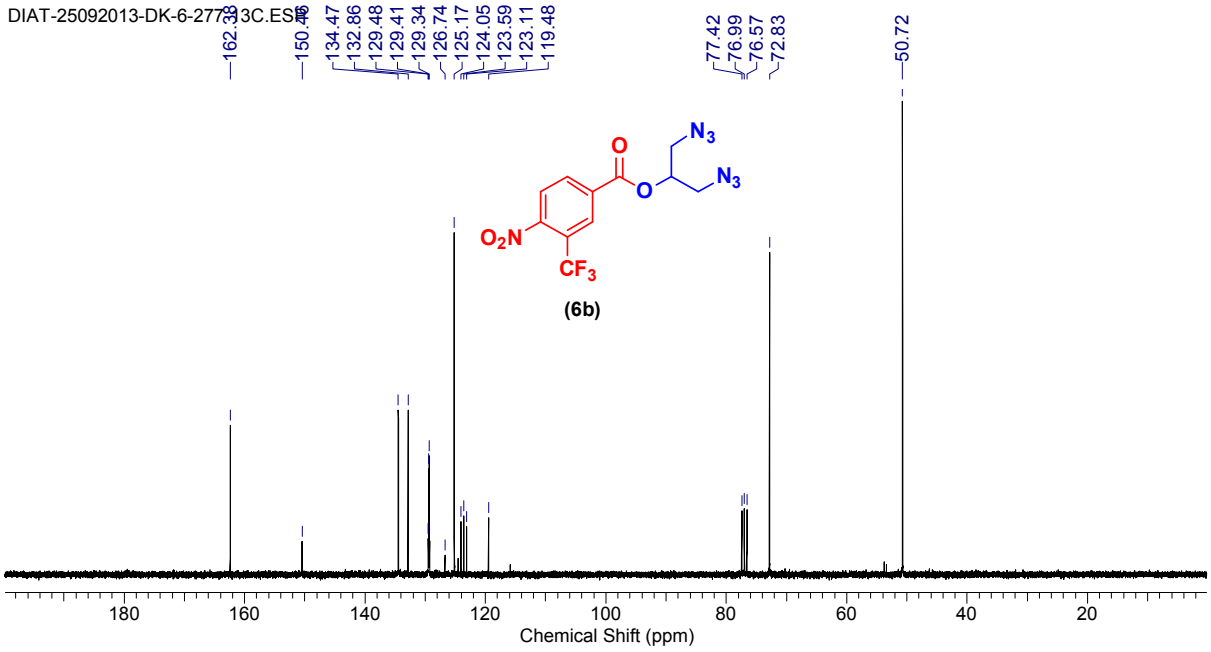


Figure S8: ^{13}C NMR (75MHz, $CDCl_3$) of **(6b)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 50.7, 72.8, 119.5, 123.1, 123.6, 124.1, 125.2, 126.7, 129.2, 129.3, 129.4, 129.5, 132.9, 134.5, 150.5, 162.4 ppm.

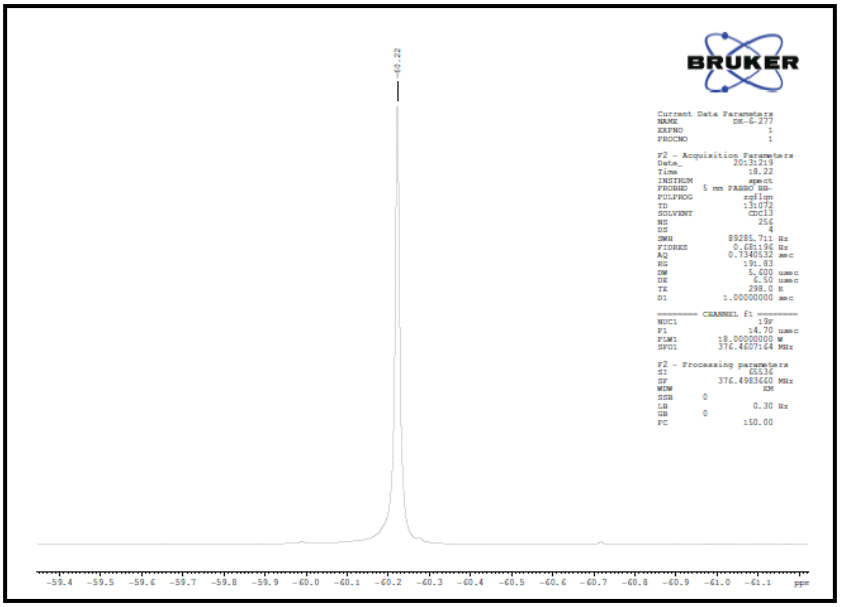


Figure S9: ^{19}F NMR (376 MHz, $CDCl_3$) of **(6b)**

^{19}F NMR ($CDCl_3$, 376 MHz) δ -60.2 (3F,s, CF_3).

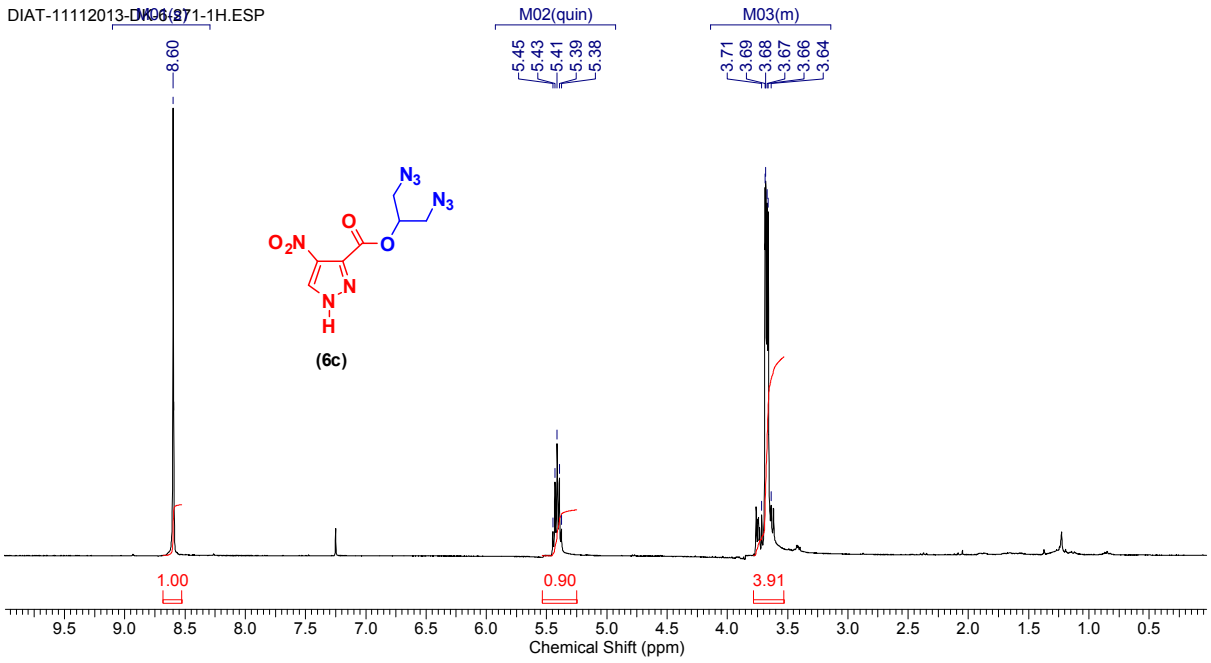


Figure S10: ^{1}H NMR (300MHz, $CDCl_3$) of **(6c)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 3.41-4.14 (4H, m), 5.41 (1H, quin, J_1 = 10.5 Hz J_2 = 5.7 Hz), 8.60 (1H, s).

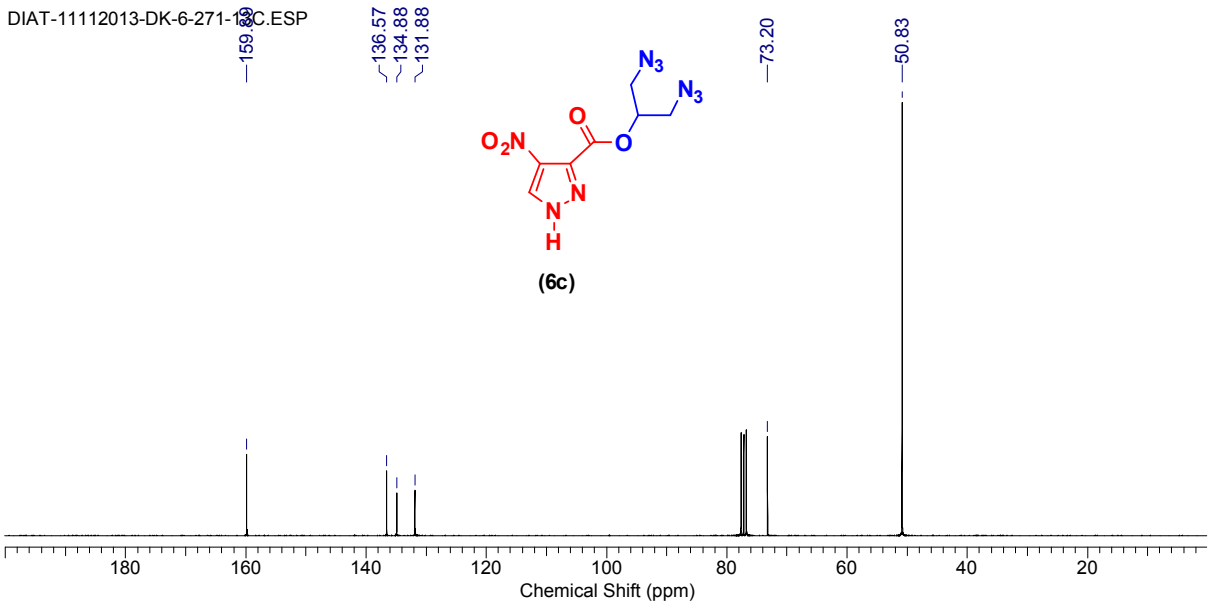


Figure S11: ^{13}C NMR (75MHz, $CDCl_3$) of **(6c)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 50.8, 73.2, 131.9, 134.9, 136.6, 159.9 ppm.

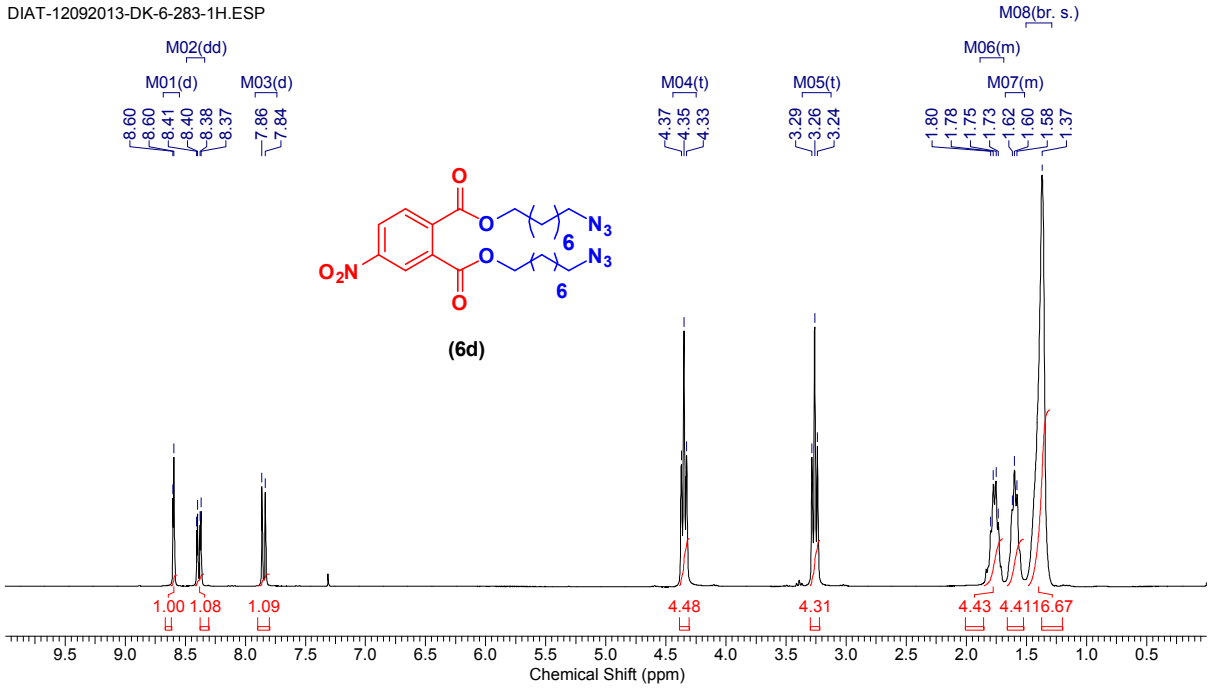


Figure S12: ^{1}H NMR, 300MHz, $CDCl_3$ **(6d)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 1.37 (16H, m), 1.52 - 1.69 (4H, m), 1.69 - 1.89 (4H, m), 3.26 (4H, t, J = 6.7 Hz), 4.35 (4H, t, J = 6.7 Hz), 7.84 (1H, d, J = 8.1 Hz), 8.39 (1H, dd, J = 8.7 Hz, 2.38Hz), 8.60 (1H, d, J = 2.4 Hz).

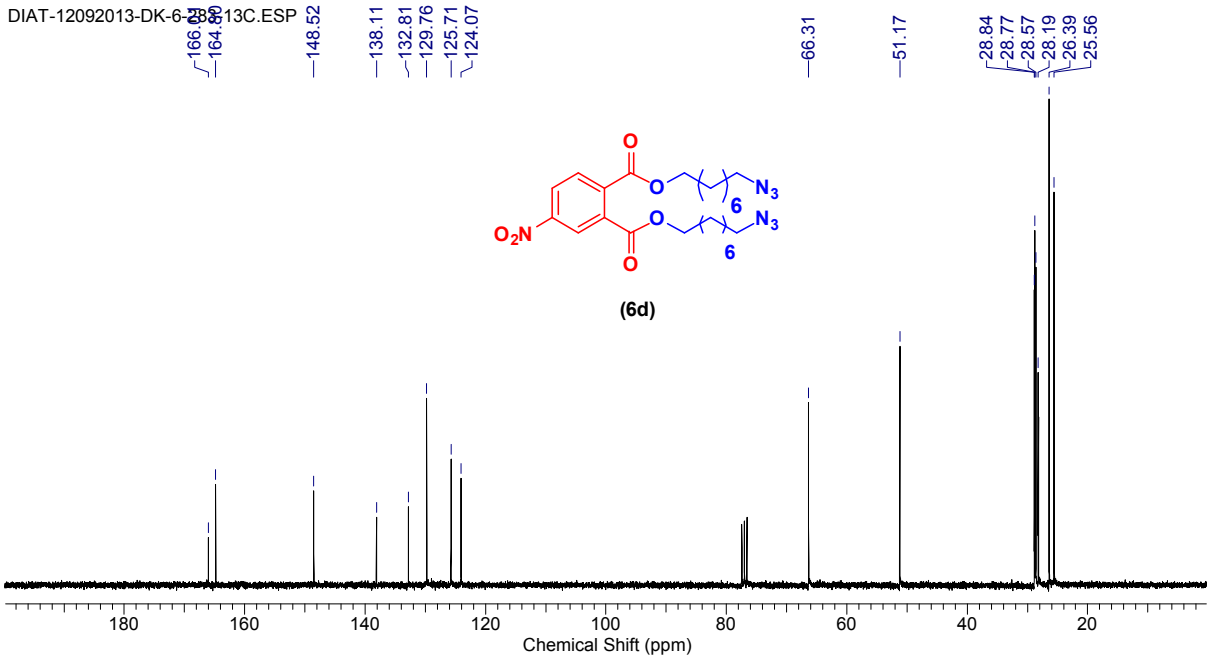


Figure S13: ^{13}C NMR, 75MHz, $CDCl_3$ **(6d)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 25.6, 26.4, 28.2, 28.6, 28.8, 28.9, 51.2, 66.3, 124.1, 125.7, 129.7, 132.8, 138.1, 148.5, 164.8, 166.0 ppm.

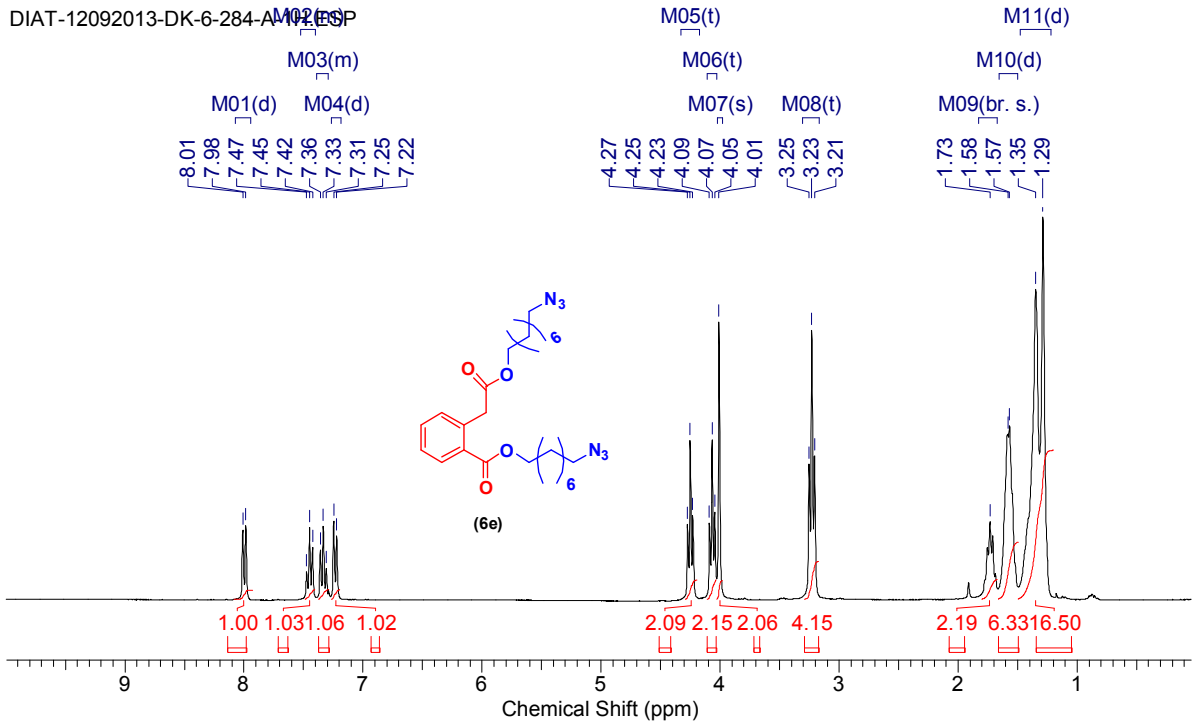


Figure S14: ^{1}H NMR, 300MHz, $CDCl_3$ of **(6e)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 1.32 (16H, m), 1.58 (6H, m), 1.73 (2H, m), 3.23 (4H, m), 4.01 (2H, s), 4.07 (2H, t, J = 6.7 Hz), 4.25 (2H, t, J = 6.7 Hz), 7.23 (1H, d, J = 7.6 Hz), 7.34 (1H, t, J = 7.6 Hz), 7.46 (1H, t, J = 7.1 Hz), 8.00 (1H, d, J = 7.6 Hz).

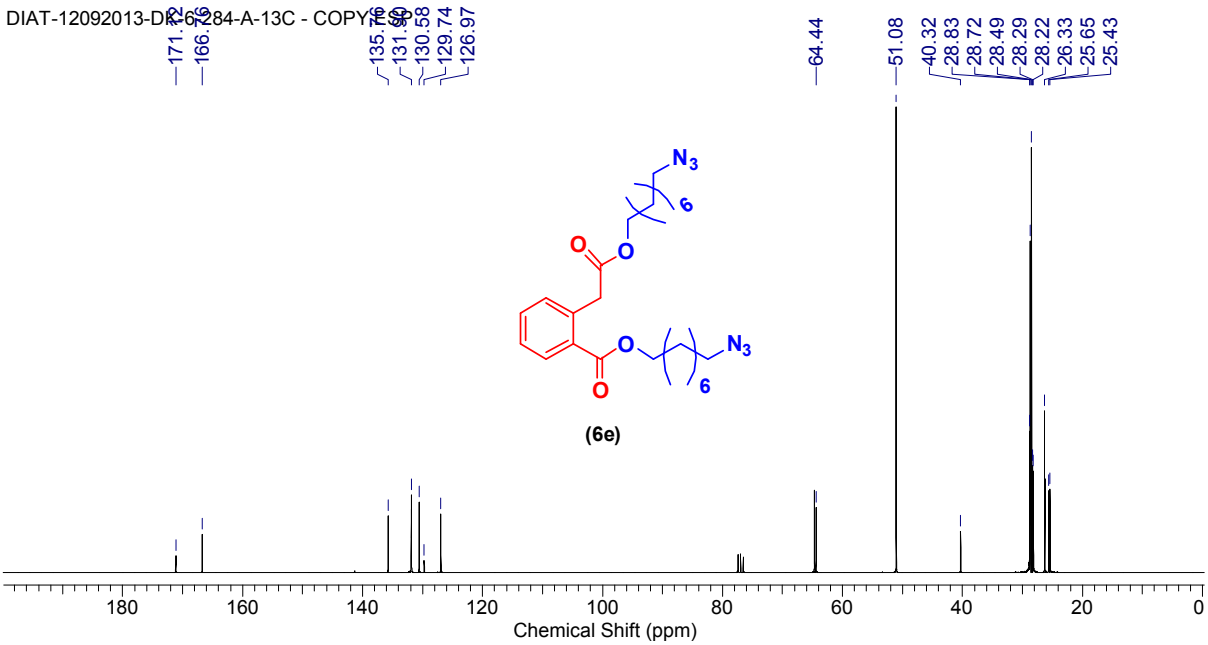


Figure S15: ^{13}C NMR, 75MHz, $CDCl_3$ of **(6e)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 25.4, 25.6, 26.2, 26.3, 28.2, 28.3, 28.5, 28.7, 28.8, 40.3, 51.1, 64.4, 64.7, 126.9, 129.7, 130.6, 131.8, 131.9, 135.8, 166.8, 171.1 ppm.

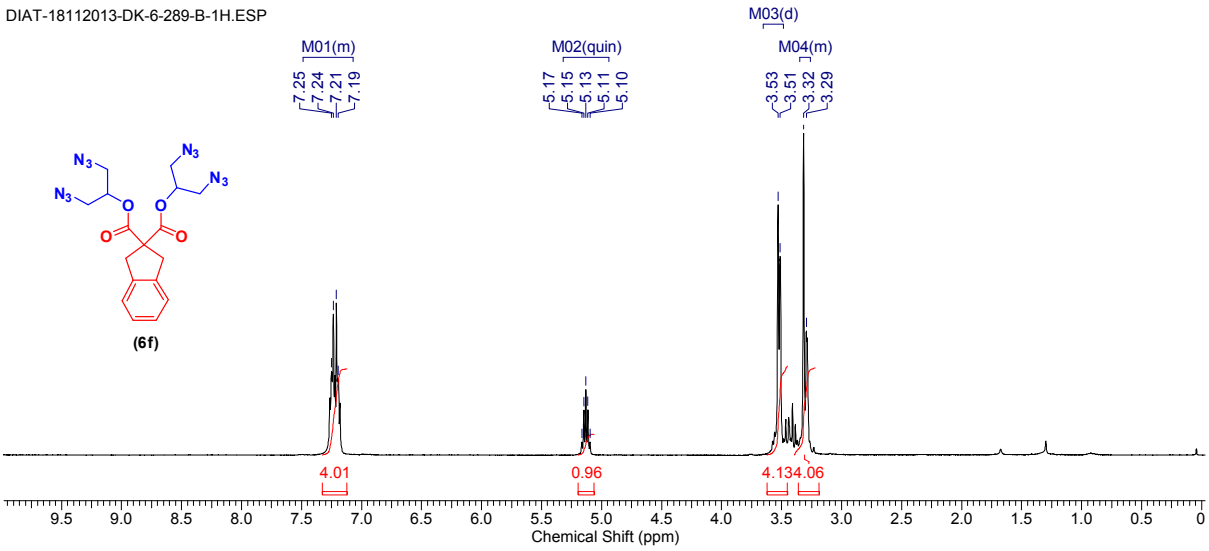


Figure S16: ^{1}H NMR, 300MHz, $CDCl_3$ of **(6f)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 3.30 (8H, d, J = 7.2 Hz), 3.52 (4H, d, J = 4.3 Hz), 5.13 (2H, quin, J_1 = 10.0 Hz J_2 = 5.3 Hz), 7.28 (4H, dd, J_1 = 8.1 Hz J_2 = 3.8 Hz).

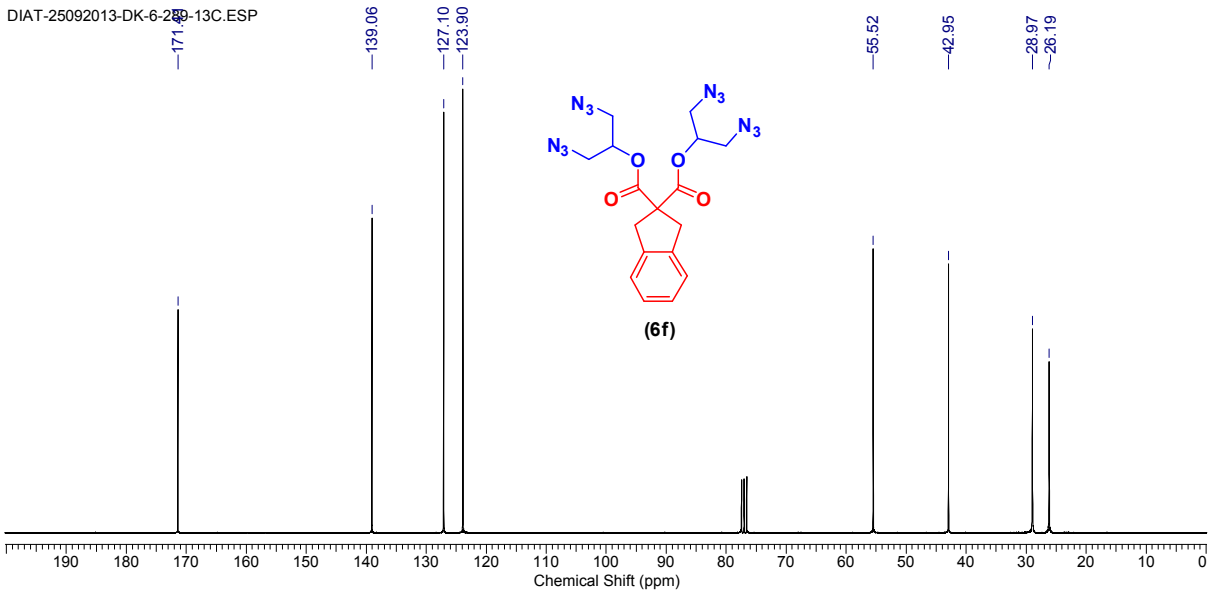


Figure S17: ^{13}C NMR, 75MHz, $CDCl_3$ of **(6f)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 26.2, 28.9, 42.9, 55.5, 123.9, 127.1, 139.1, 171.4 ppm.

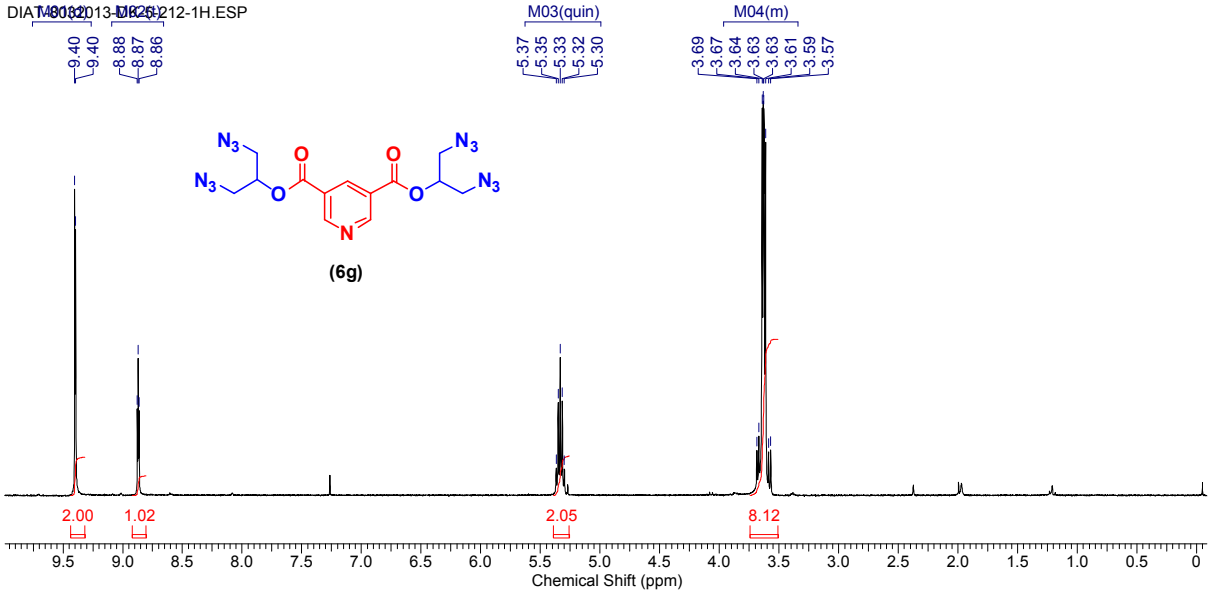


Figure S18: ^{1}H NMR, 300MHz, $CDCl_3$ of **(6g)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 3.34 - 3.97 (8H, m), 5.33 (2H, quin, J_1 = 10.3 Hz J_2 = 5.1 Hz), 8.87 (1H, t, J = 2.4 Hz), 9.40 (2H, d, J = 1.9 Hz).

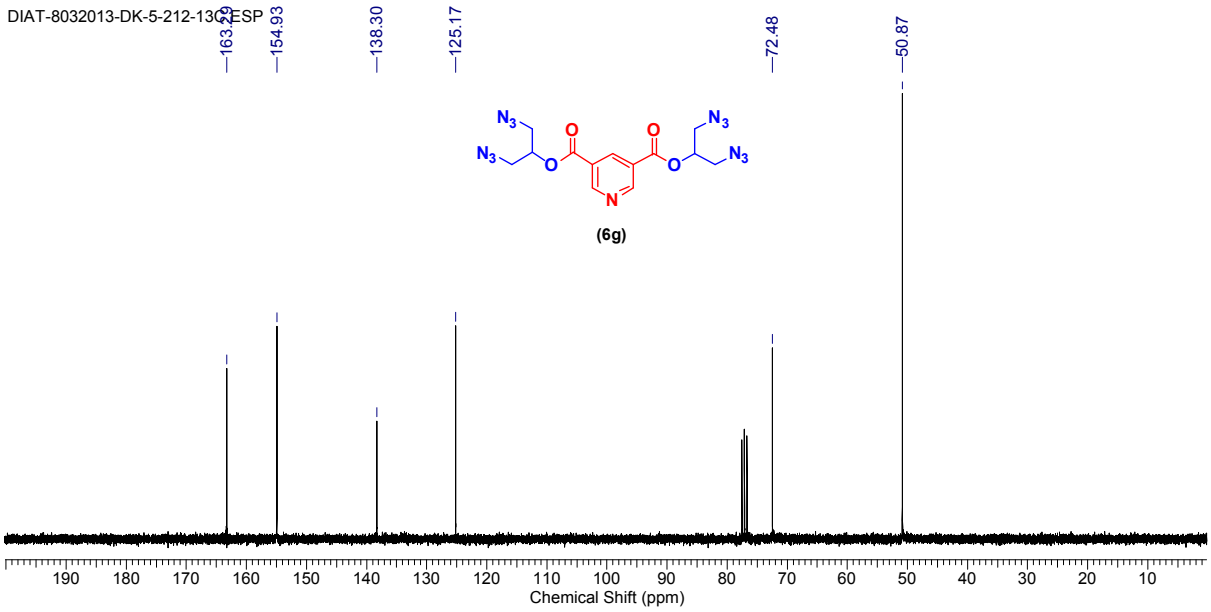


Figure S19: ^{13}C NMR, 75MHz, $CDCl_3$ of **(6g)**

^{13}C ($CDCl_3$, 75 MHz) NMR δ 50.8, 72.5, 125.2, 138.3, 154.9, 163.3 ppm.

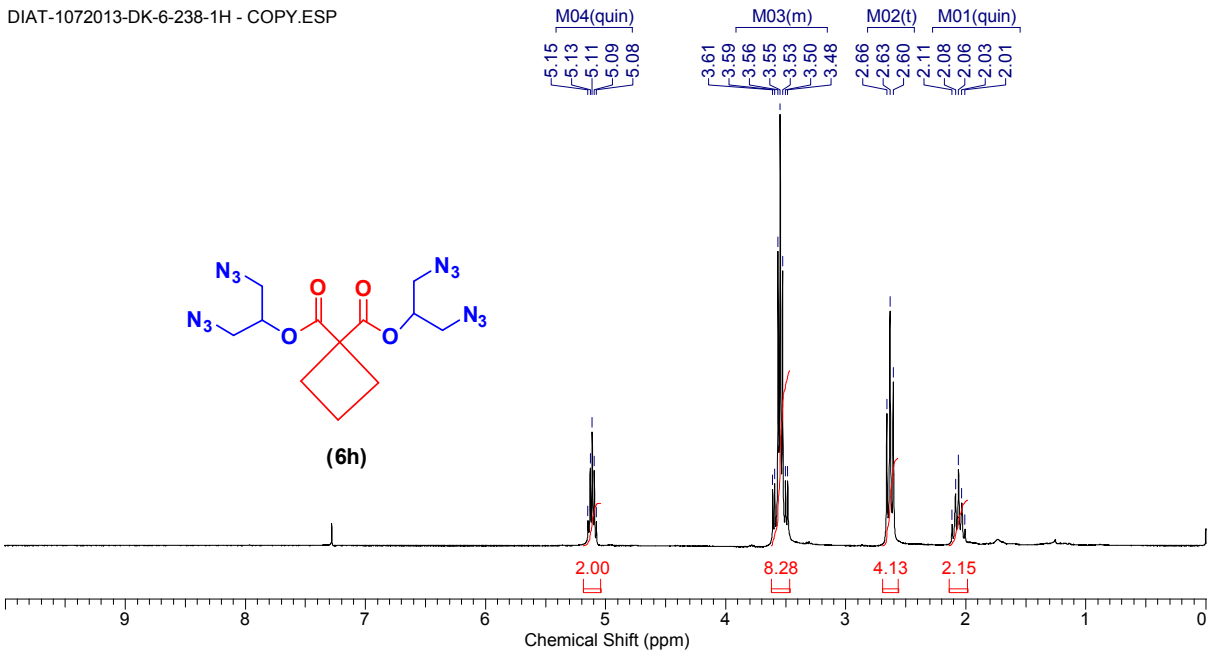


Figure S20: ^{1}H NMR, 300MHz, $CDCl_3$ of **(6h)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 2.06 (2H, quin, $J_1 = 6.1$ Hz $J_2 = 7.9$ Hz), 2.63(4H, t, $J = 8.2$ Hz), 3.91-3.15 (8H, m), 5.11 (2H, q, $J_1 = 10.2$ Hz $J_2 = 4.98$ Hz).

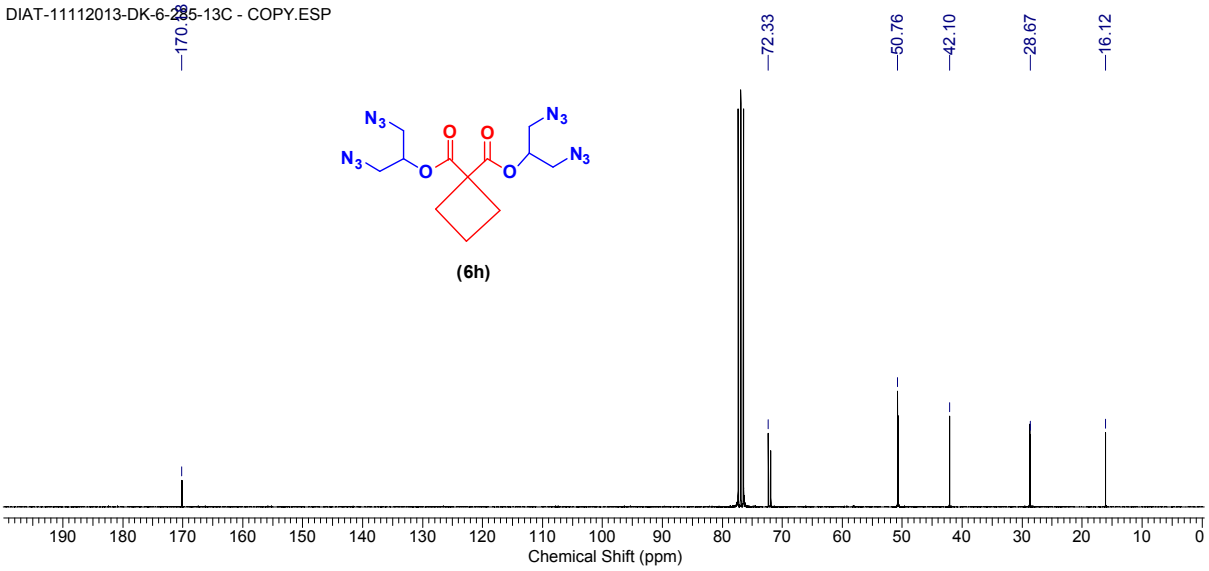


Figure S21: ^{13}C NMR, 75MHz, $CDCl_3$ of **(6h)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 16.1, 28.7, 42.1, 50.8, 72.3, 170.2 ppm.

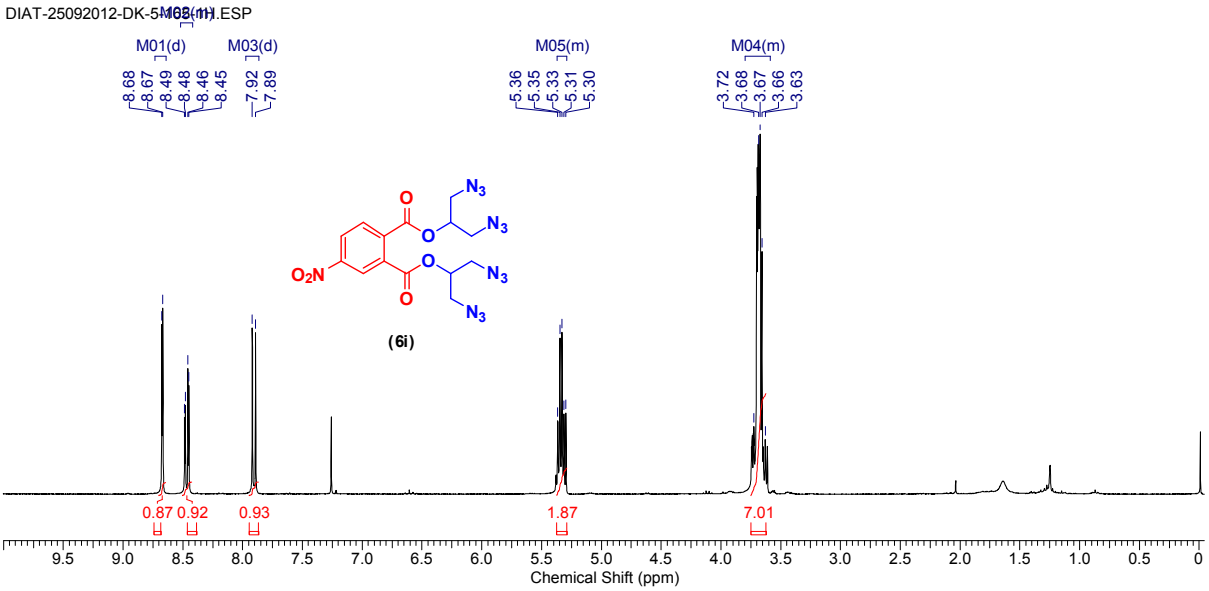


Figure S22: ^{1}H NMR, 300MHz, $CDCl_3$ of **(6i)**

NMR ($CDCl_3$, 300MHz) δ 3.59 - 3.80 (8H, m), 5.33 (2H, quin, J_1 = 10.5 Hz J_2 = 5.2 Hz), 7.91 (1H, d J = 8.8 Hz), 8.42 - 8.52 (1H, dd, J_1 = 8.7 J_2= 2.4 Hz), 8.67 (1H, d, J = 2.4 Hz).

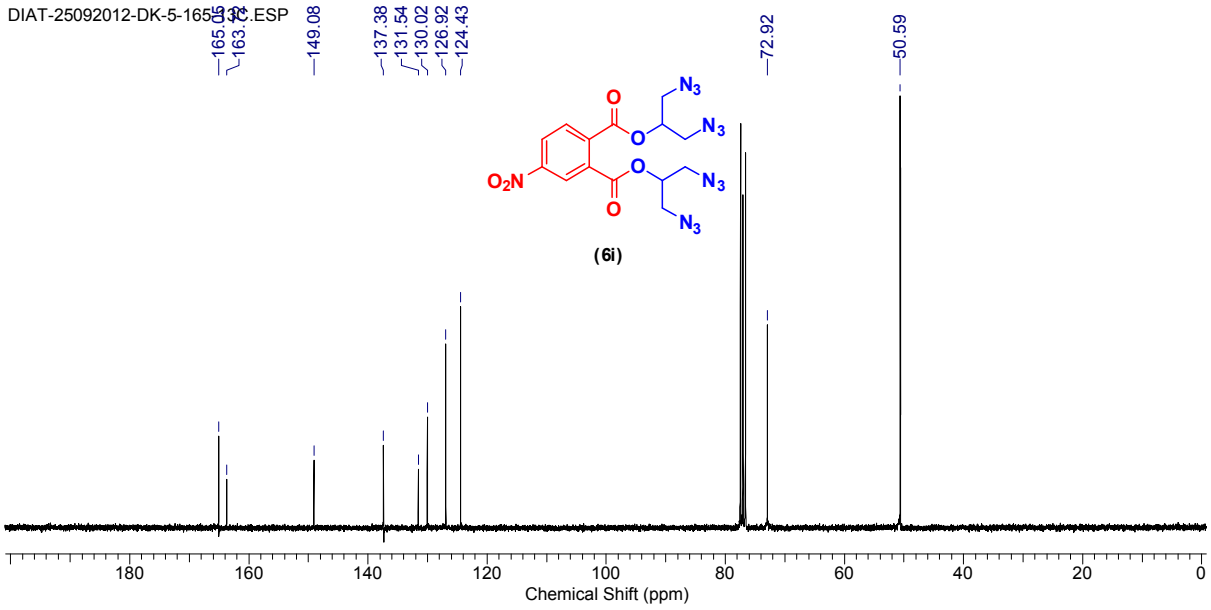


Figure S23: ^{13}C NMR, 75MHz, $CDCl_3$ of **(6i)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 50.6, 72.9, 124.4, 126.9, 130.0, 131.5, 137.4, 149.1, 163.7, 165.1 ppm.

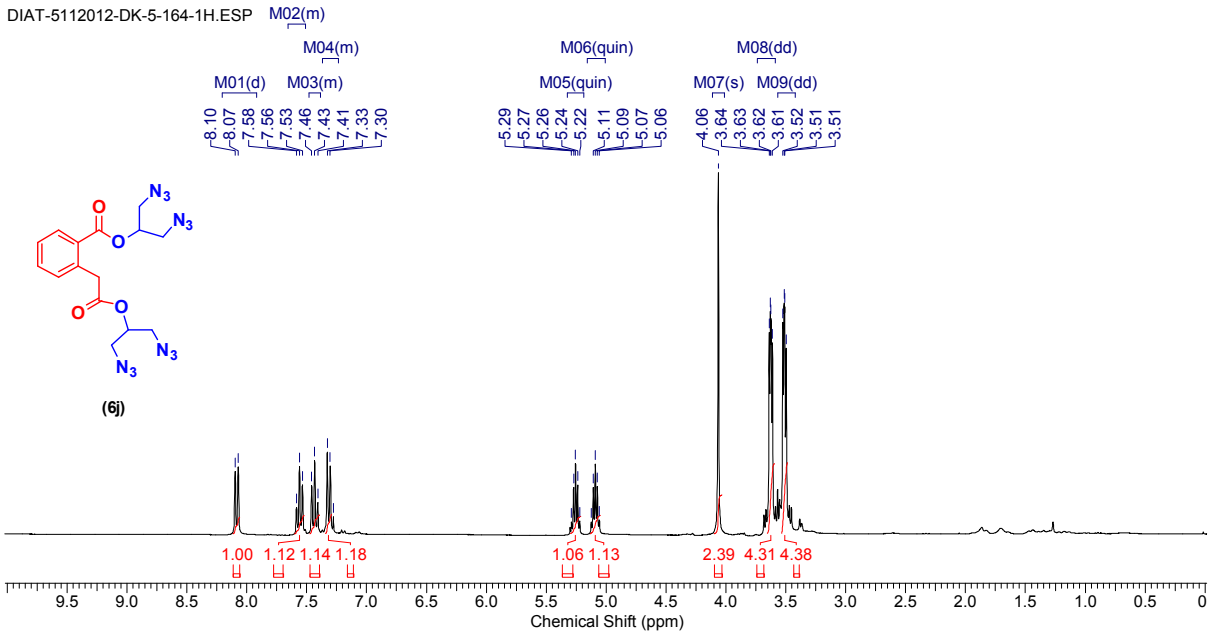


Figure S24: ^{1}H NMR, 300MHz, $CDCl_3$ of **(6j)**

^{1}H NMR δ 3.51 (4H, m), 3.63 (4H, m) 4.06 (2H, s), 5.09 (1H, quin, J_1 = 10.5 Hz J_2 = 5.2 Hz), 5.26 (1H, quin, J_1 = 10.5 Hz J_2 = 5.2 Hz), 7.33 (1H, d, J = 7.2 Hz) ,7.43 (1H, t, J = 7.6Hz), 7.58 (1H, t, J = 7.6 Hz), 8.08 (1H, d, J = 7.6 Hz).

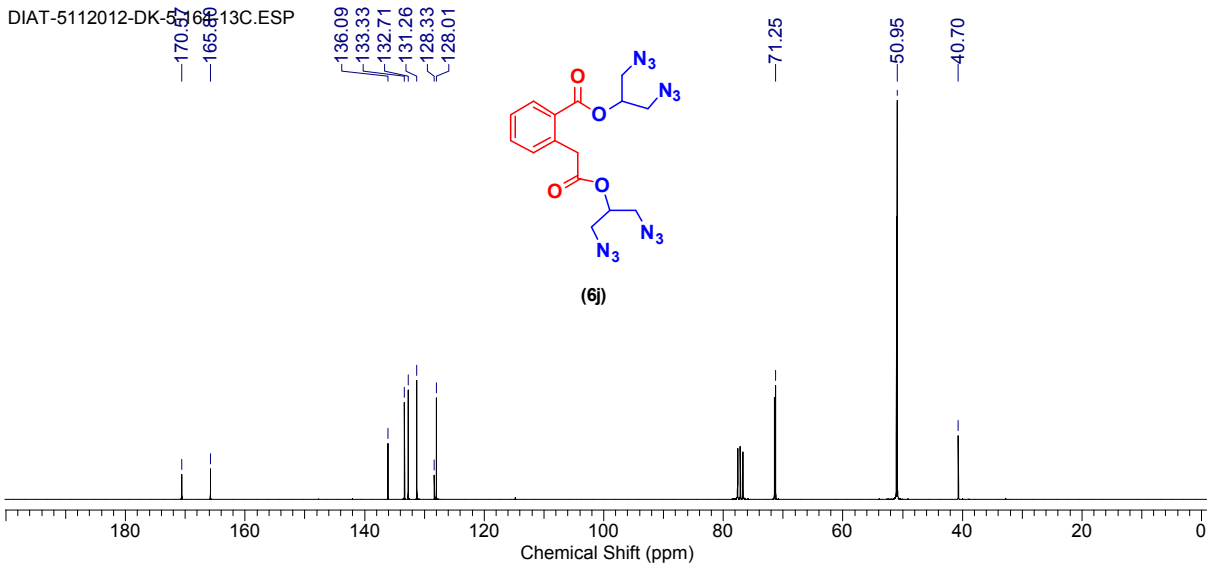


Figure S25: ^{13}C NMR, 75MHz, $CDCl_3$ of **(6j)**

^{13}C NMR δ 40.7, 50.9, 71.3, 128.0, 128.3, 131.3, 132.7, 133.3, 136.1, 165.8, 170.6 ppm.

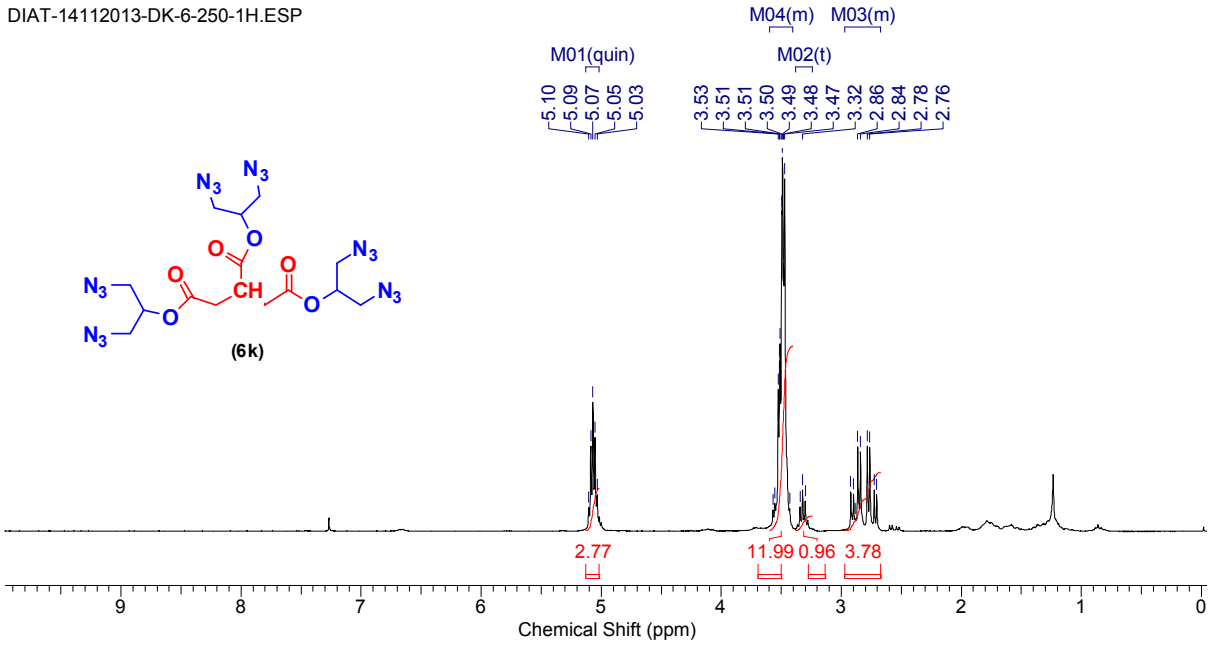


Figure S26: ^{1}H NMR, 300MHz, $CDCl_3$ of **(6k)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 2.67-2.97 (4H, m), 3.32 (1H, q, J_1 = 12.9 Hz J_2=6.7 Hz) 3.40 - 3.60 (12H, m), 5.07 (3H, quin, J_1 = 10.5 Hz J_2 =5.3 Hz).

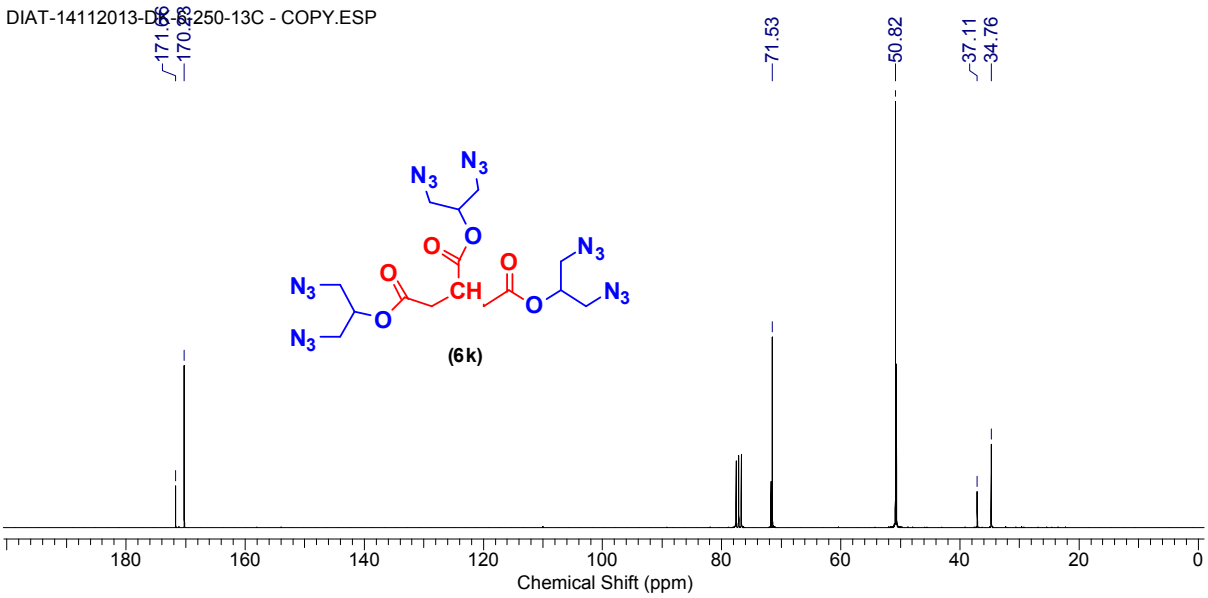


Figure S27: ^{13}C NMR, 75MHz, $CDCl_3$ of **(6k)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 34.8, 37.1, 50.8, 71.5, 170.2, 171.7 ppm.

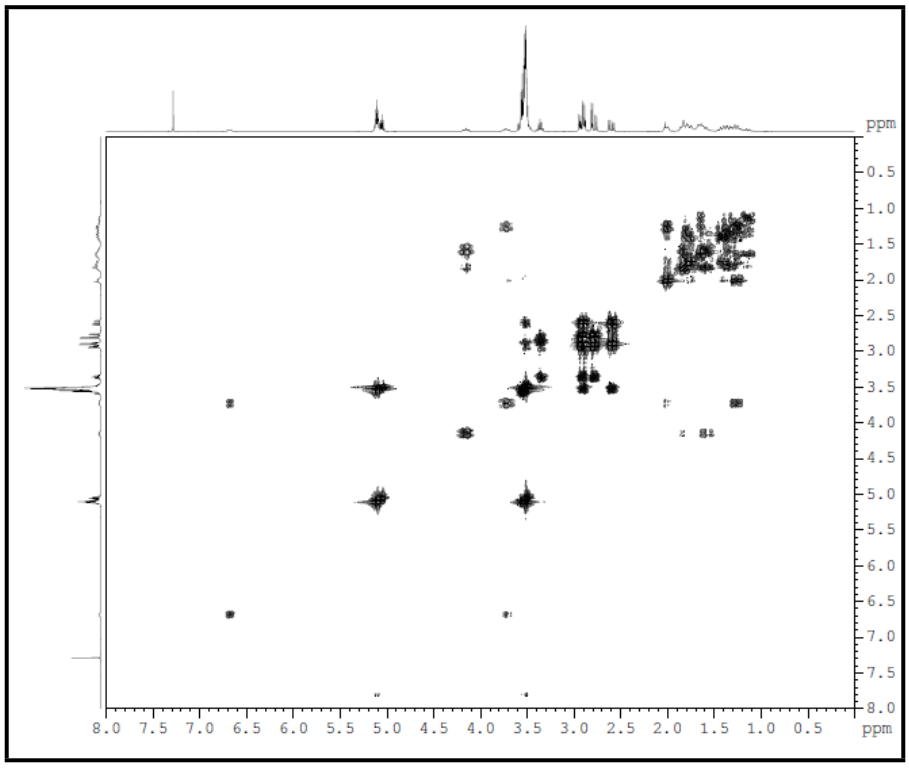


Figure S28: COSY (^{1}H-NMR) of **(6k)**

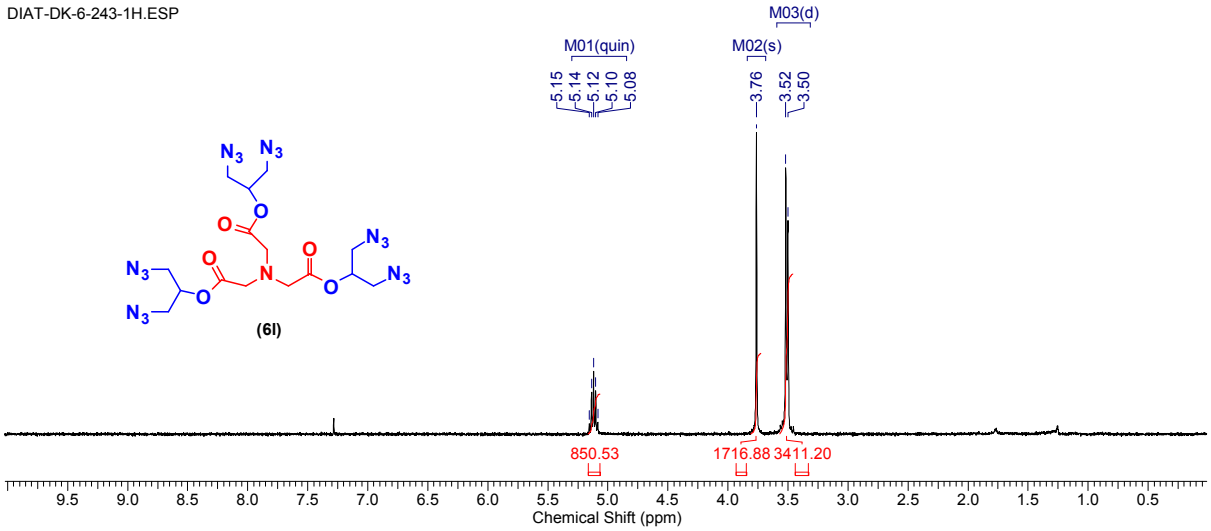


Figure S29: ^{1}H NMR, 300MHz, $CDCl_3$ of **(6l)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 3.51 (12H, d, J = 6.7 Hz), 3.76 (6H, s), 5.12 (3H, quin, J_1 = 10.4 Hz J_2 = 6.2 Hz).

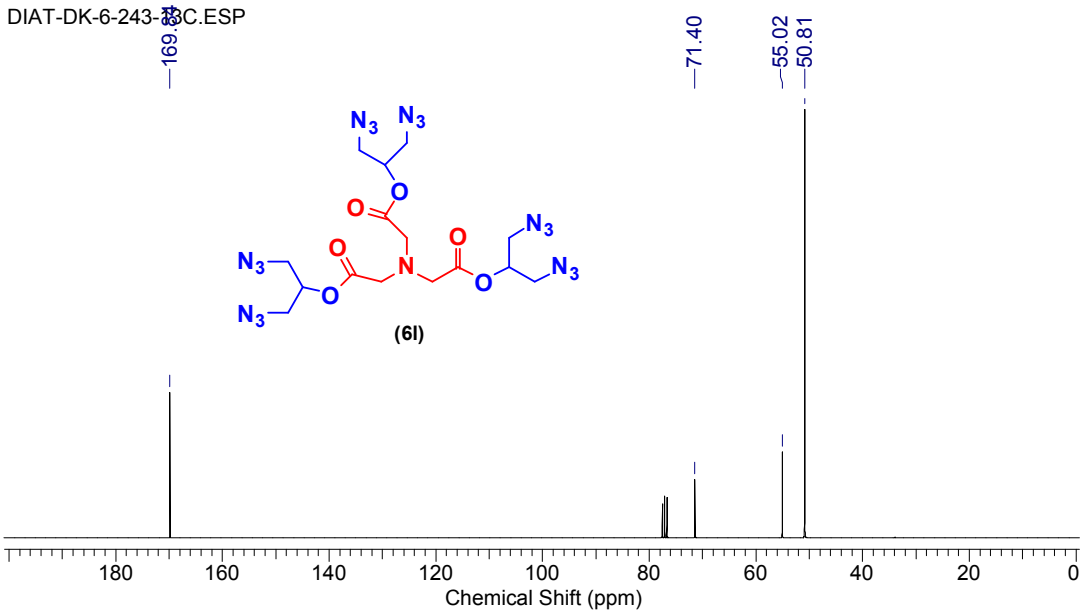


Figure S30: ^{13}C NMR, 75MHz, $CDCl_3$ of **(6l)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 50.8, 55.0, 71.4, 169.8 ppm.

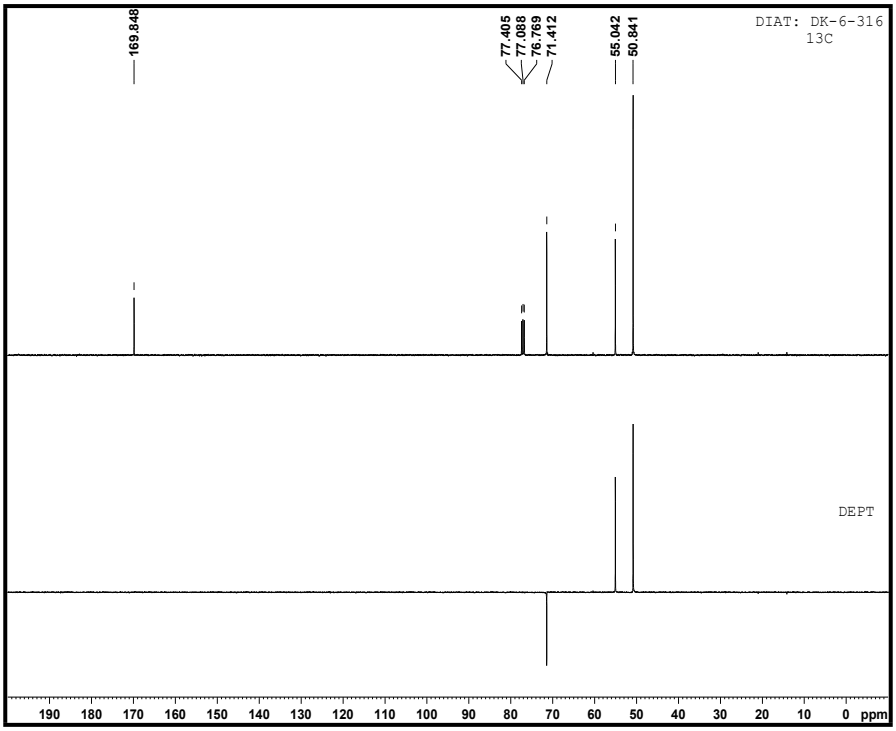


Figure S31: DEPT of **(6l)**

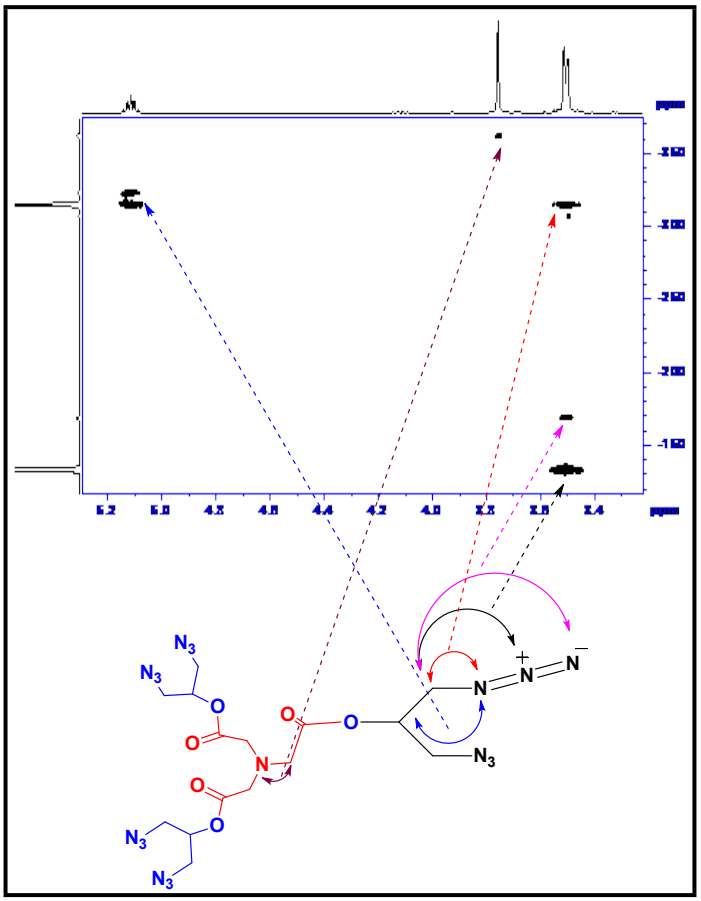


Figure S32(a): 1H-15N HMBC of **(6l)**

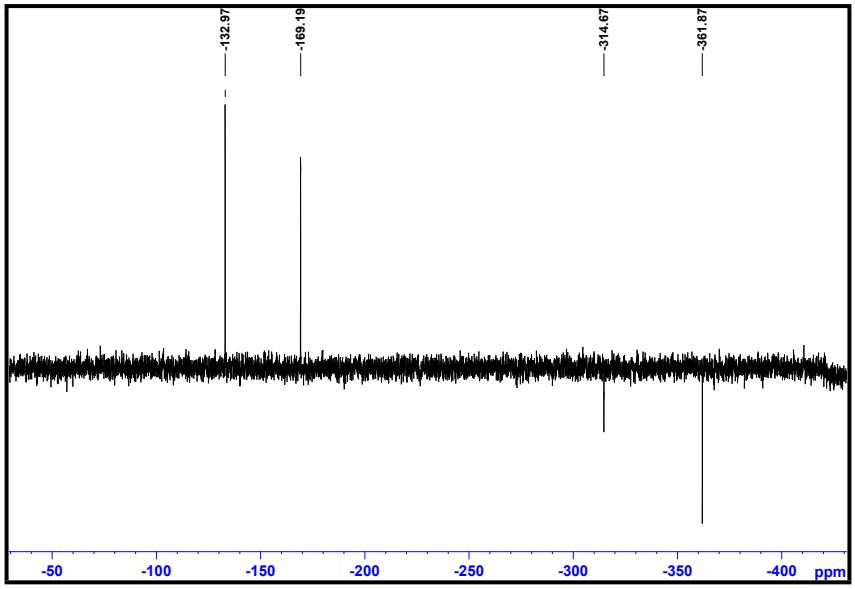


Figure S32(b): 15N: BB decoupling; with NOE of **(6l)**

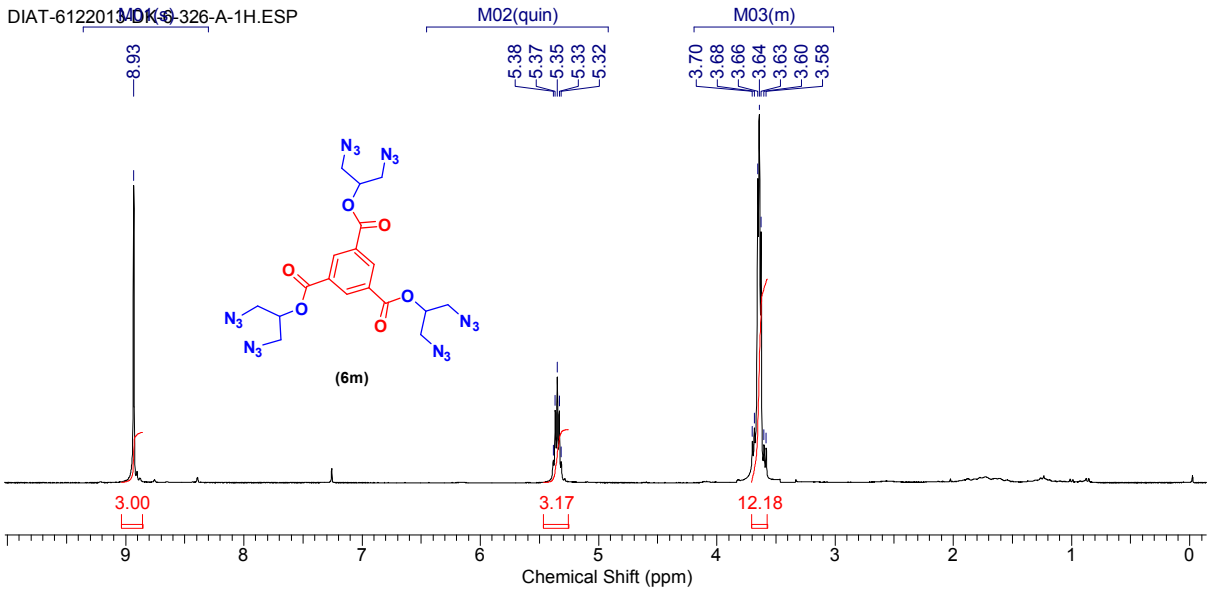


Figure S33: ^{1}H NMR, 300MHz, $CDCl_3$ of **(6m)**

^{1}H NMR ($CDCl_3$, 300MHz) δ 3.01 – 4.20 (12H, m), 5.35 (3H, quin, J_1 = 10.5 Hz J_2 = 5.2 Hz) 8.93 (3H, s).

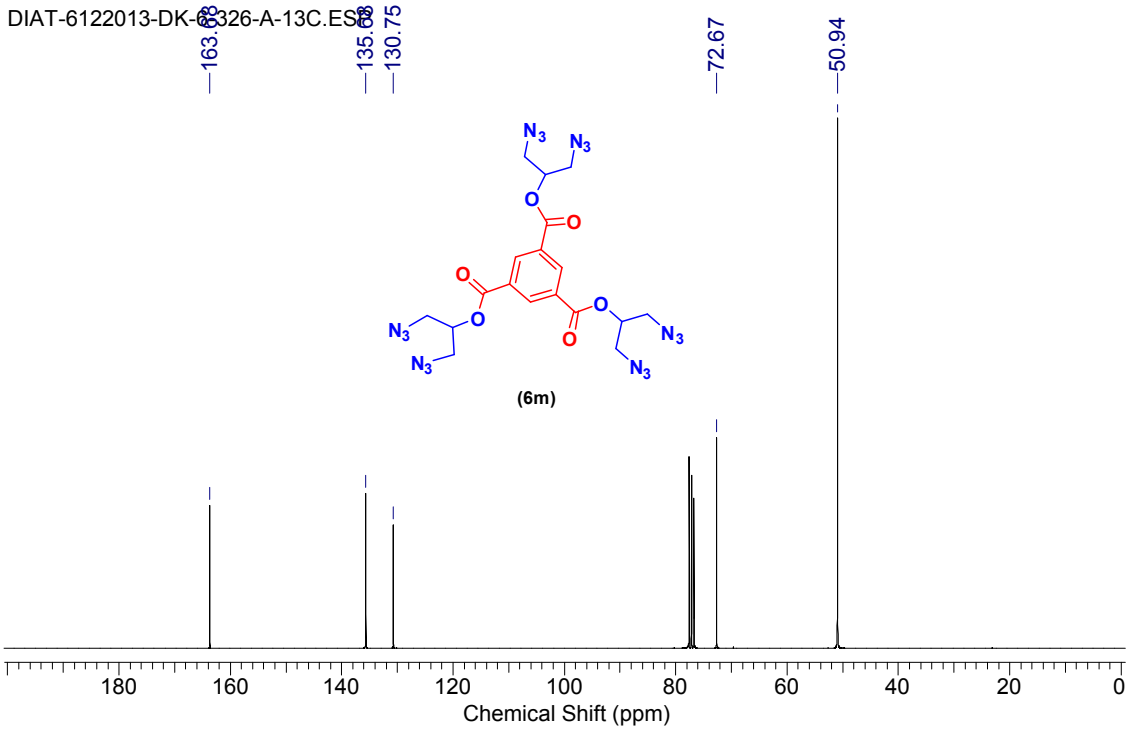
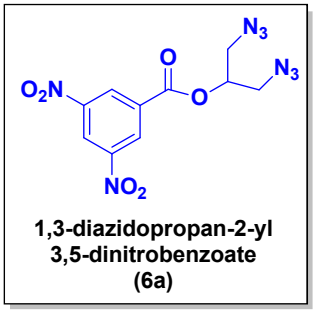


Figure S34: ^{13}C NMR, 75MHz, $CDCl_3$ of **(6m)**

^{13}C NMR ($CDCl_3$, 75 MHz) δ 50.9, 72.7, 130.8, 135.7, 163.7 ppm.

DSC & TGA Curves



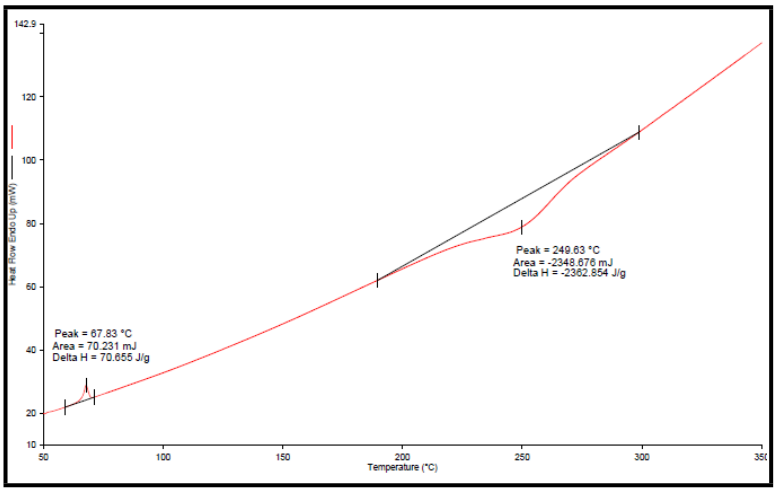


Figure S35: DSC curve of **(6a)**

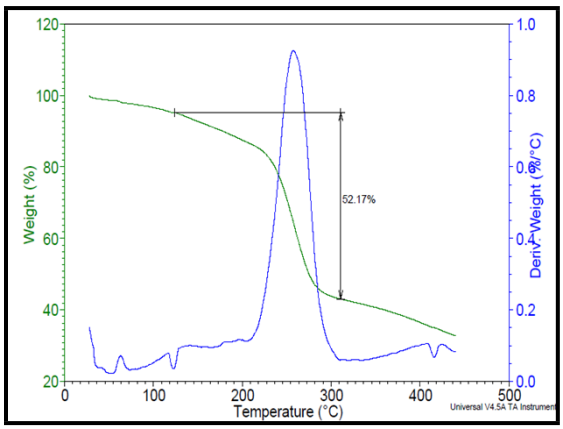


Figure S36: TGA curve of **(6a)**

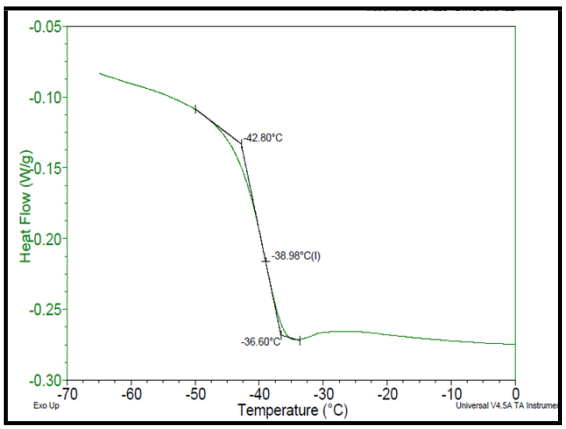
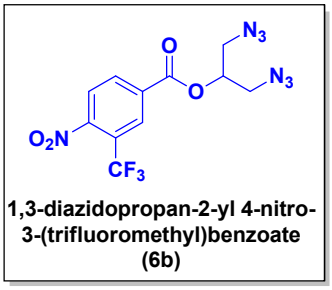


Figure S37: T_g curve of **(6a)**



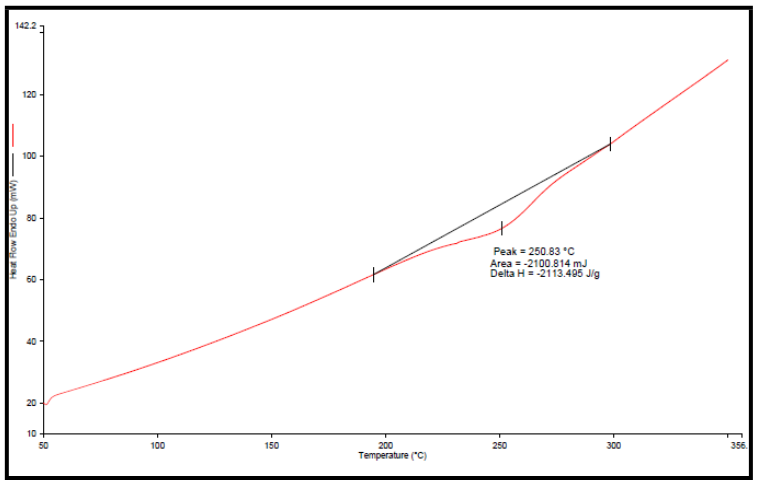


Figure S38: DSC curve of **(6b)**

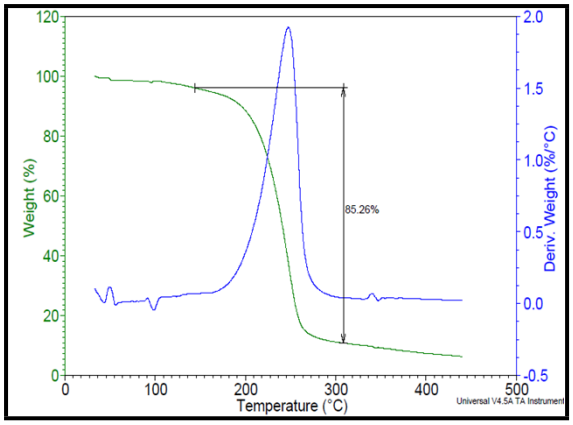


Figure S39: TGA curve of **(6b)**

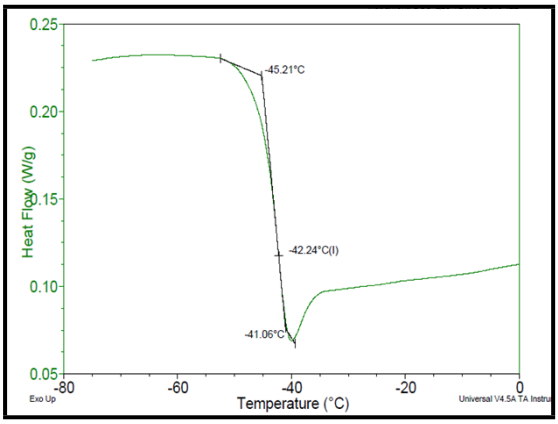


Figure S40: T_g curve of **(6b)**

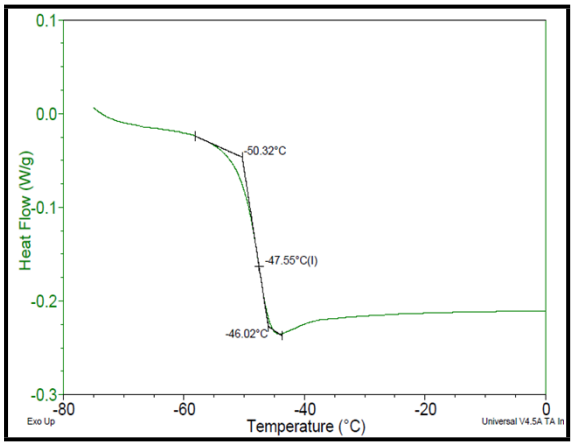


Figure S41: T_g of **(6b)** + GAP

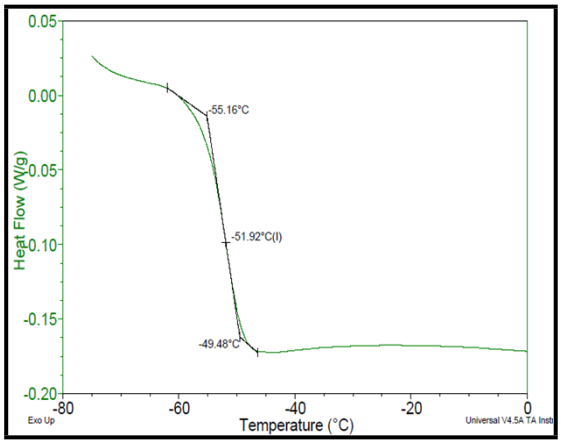
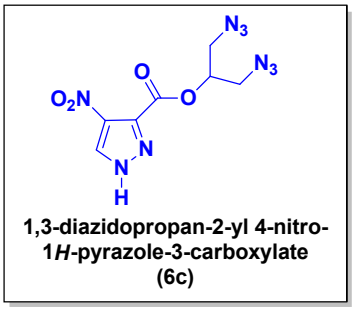


Figure S42: T_g of **(6b)** + BAMO



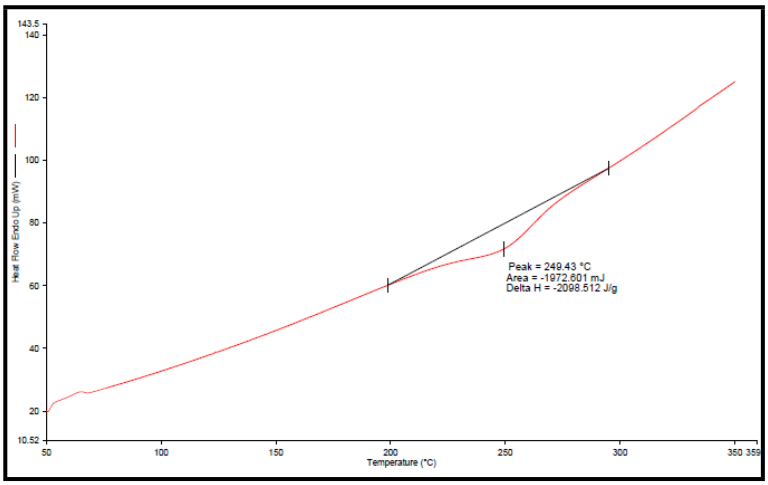


Figure S43: DSC curve of **(6c)**

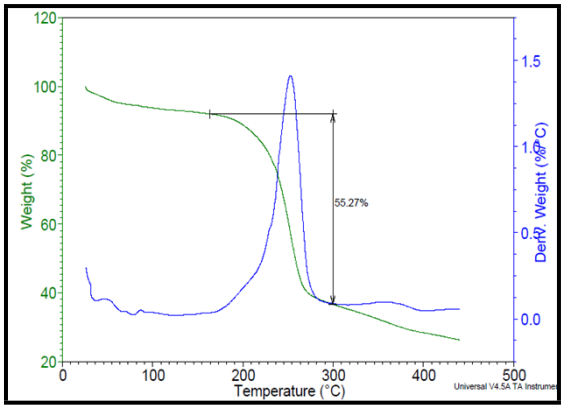


Figure S44: TGA curve of **(6c)**

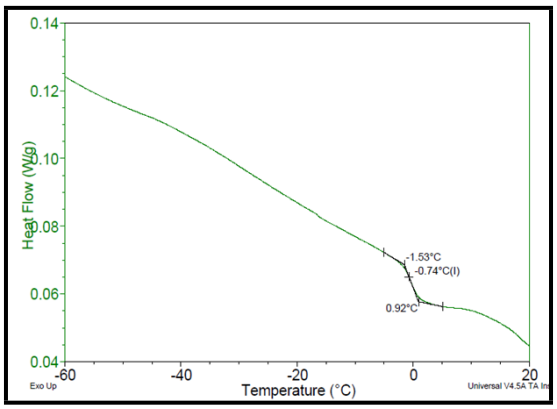
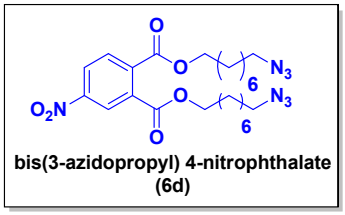


Figure S45: T_g curve of **(6c)**



bis(3-azidopropyl) 4-nitrophthalate (6d)

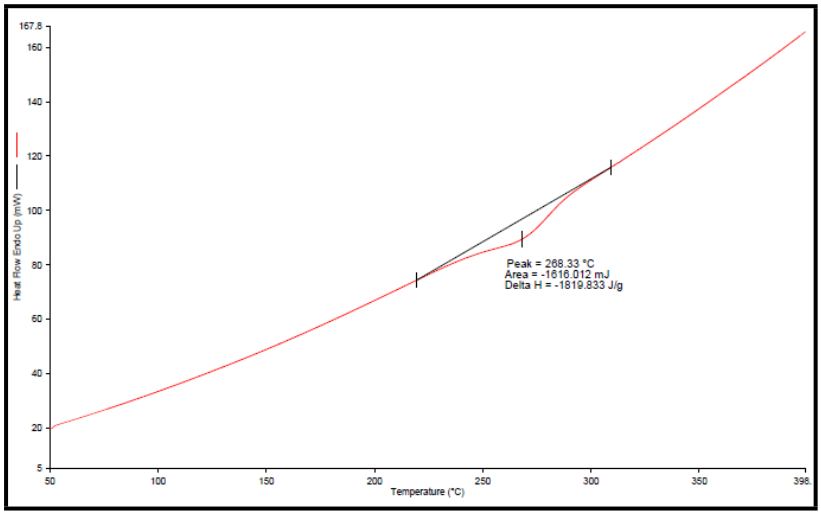


Figure S46: DSC curve of **(6d)**

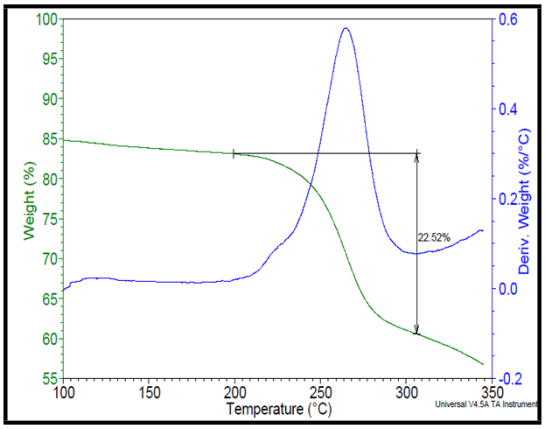


Figure S47: TGA of **(6d)**

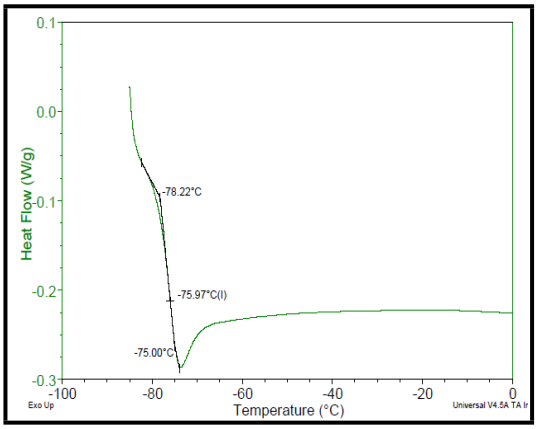


Figure S48: T_g of **(6d)**

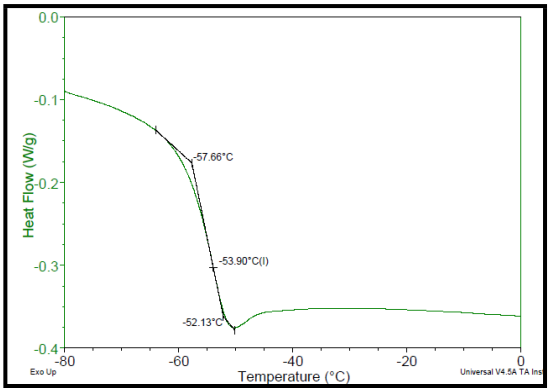


Figure S49: T_g of **(6d)** + GAP

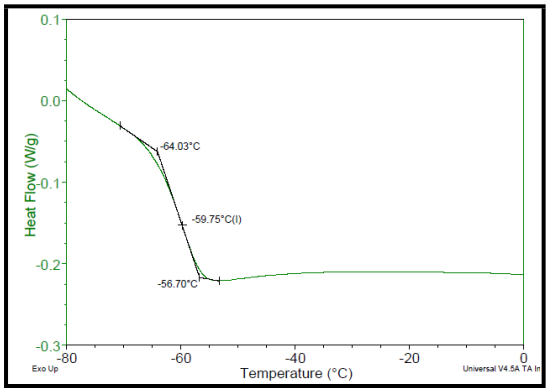
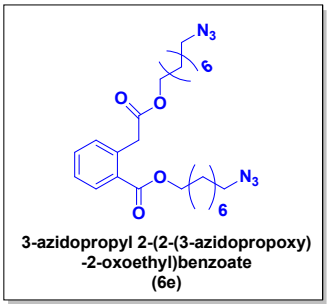


Figure S50: T_g of **(6d)** + BAMO



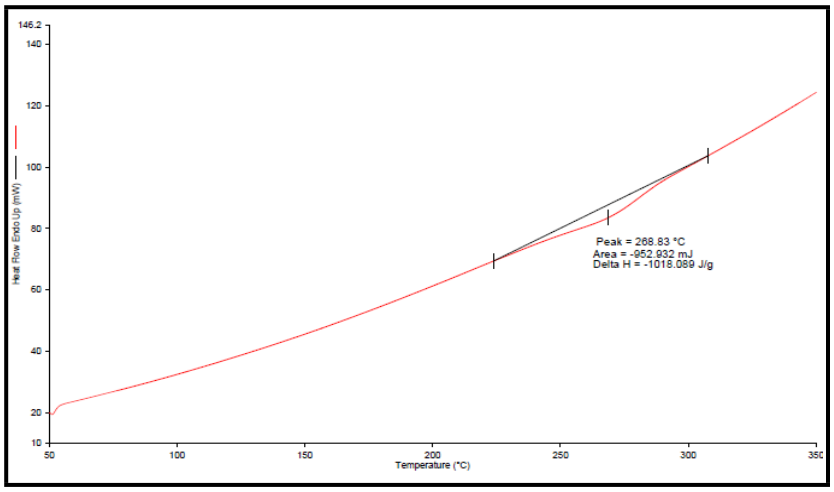


Figure S51: DSC curve of **(6e)**

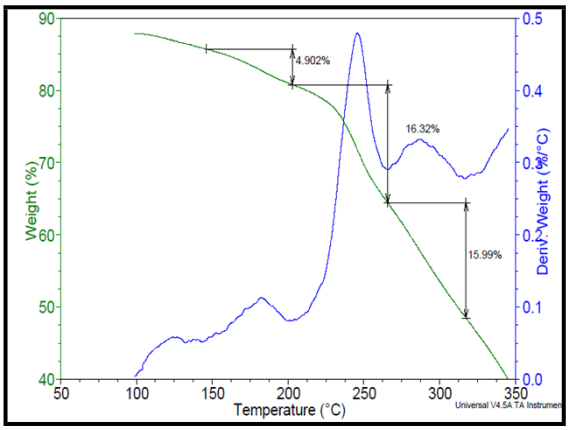


Figure S52: TGA curve of **(6e)**

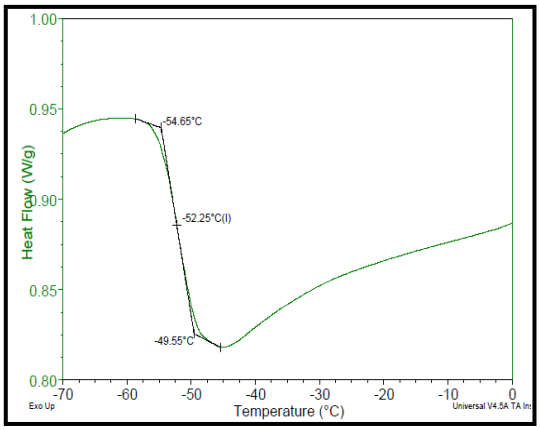


Figure S53: T_g curve of **(6e)**

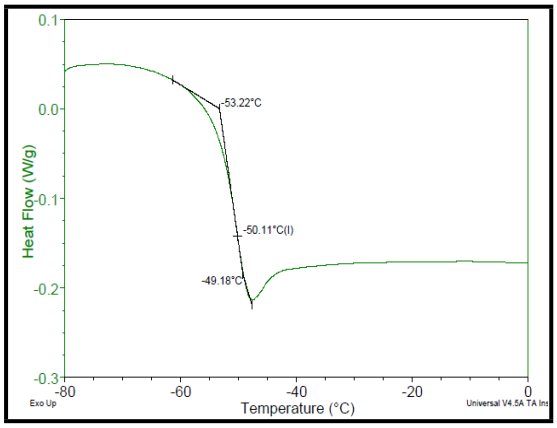


Figure S54: T_g of GAP + **(6e)**

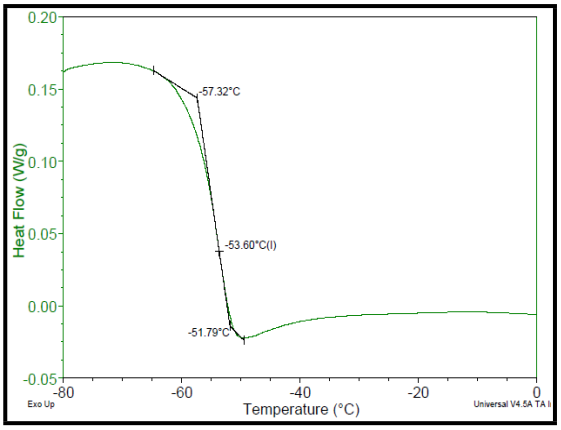
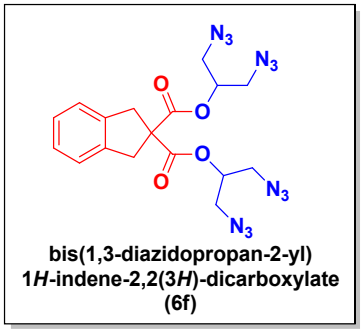


Figure S55: T_g of BAMO + **(6e)**



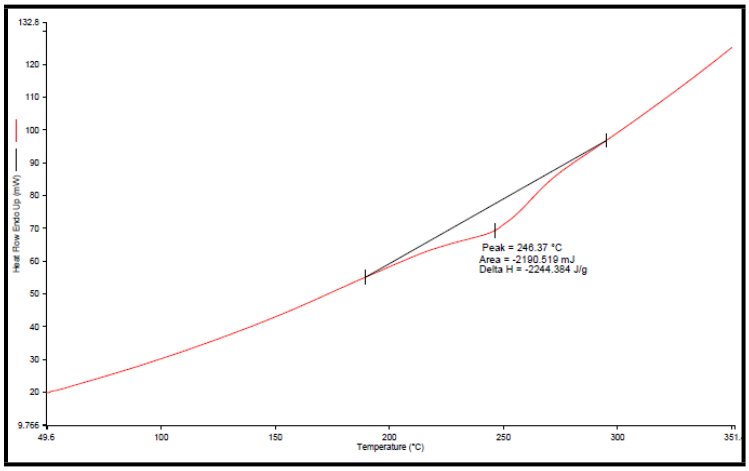


Figure S56: DSC curve of **(6f)**

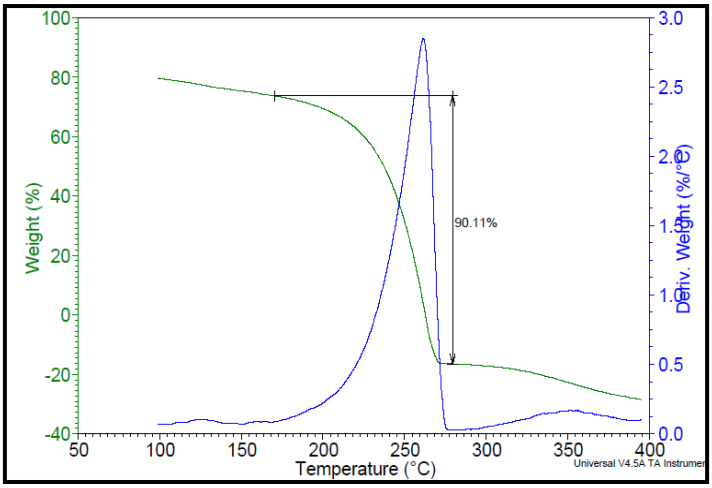
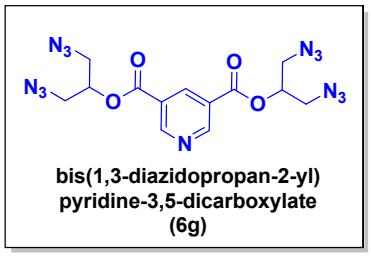


Figure S57: TGA curve of **(6f)**



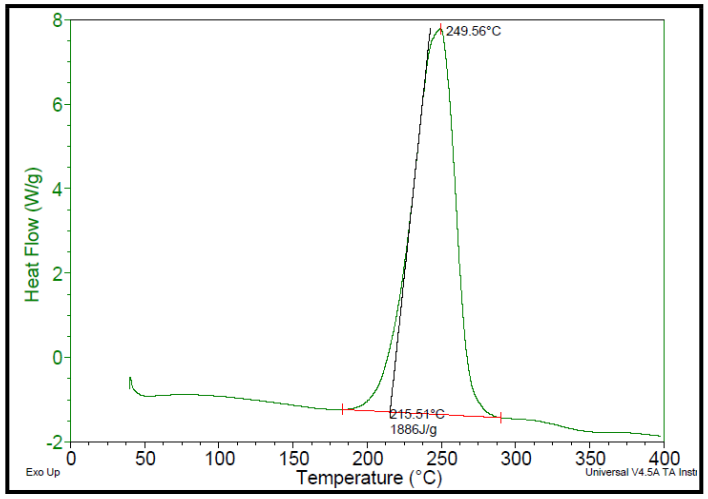


Figure S58: DSC curve of **(6g)**

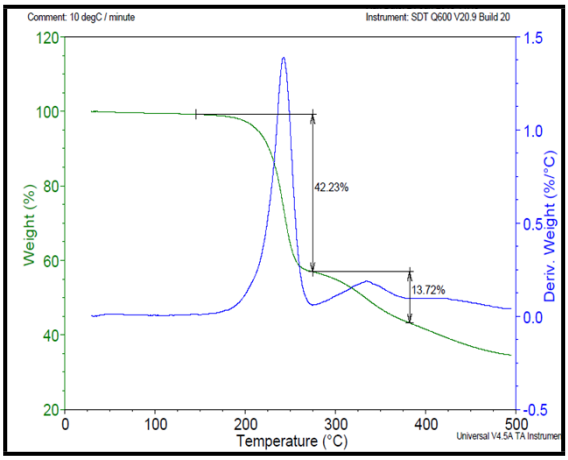


Figure S59: TGA curve of **(6g)**

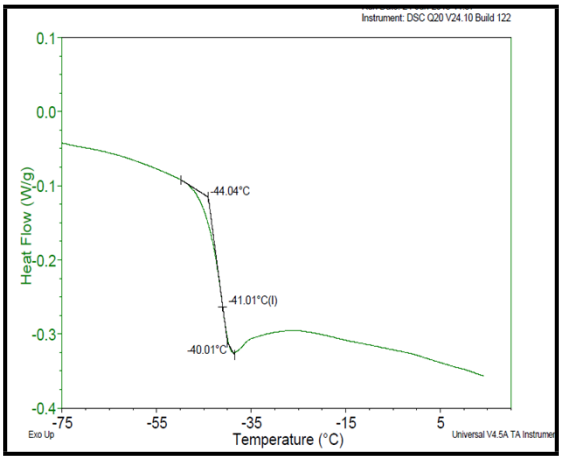


Figure S60: T_g curve of **(6g)**

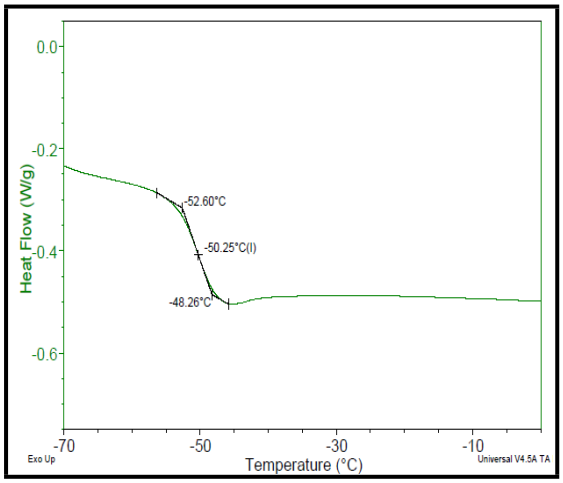


Figure S61: T_g of **(6g)** + GAP

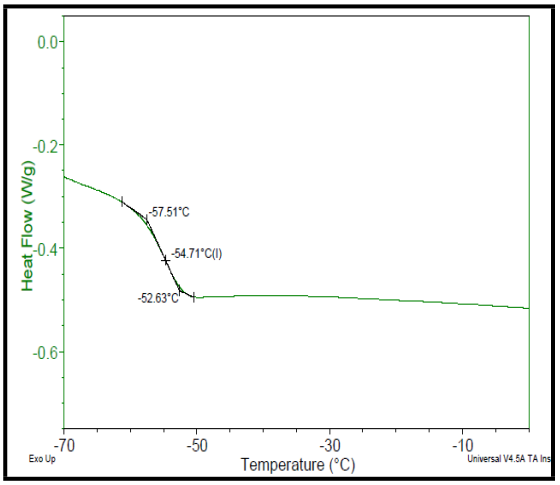


Figure S62: T_g of **(6g)** + BAMO

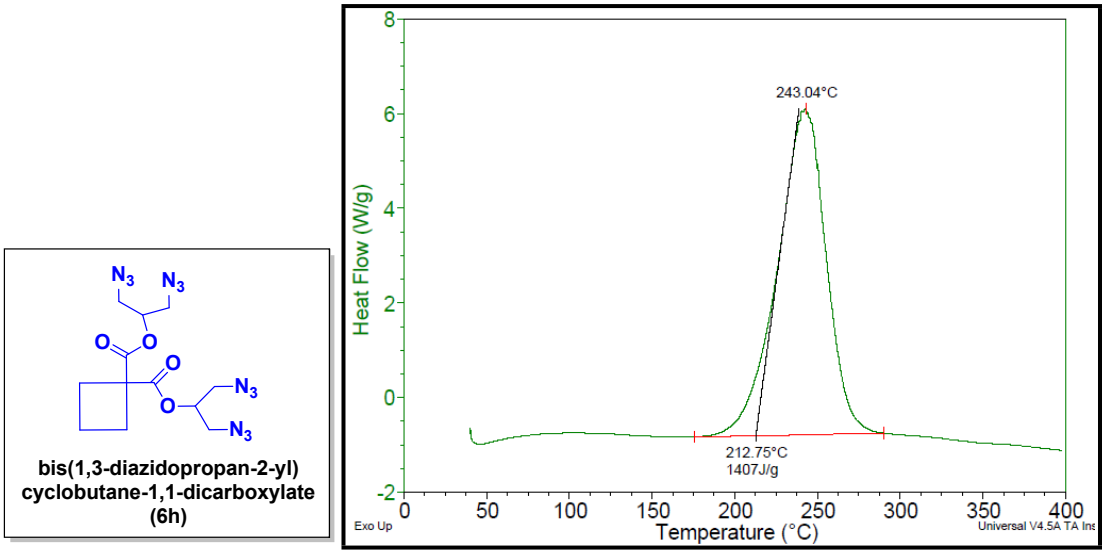


Figure S63: DSC curve of **(6h)**

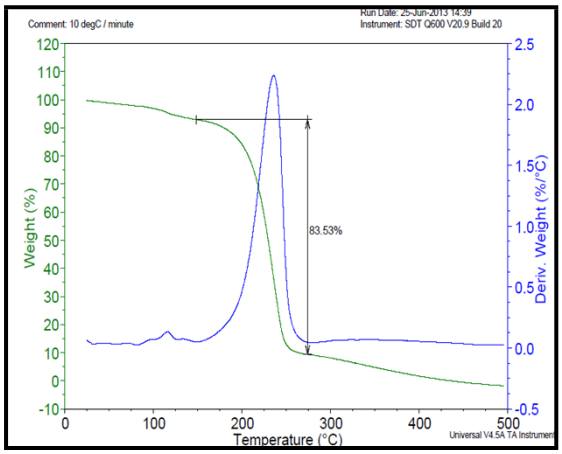


Figure S64: TGA curve of **(6h)**

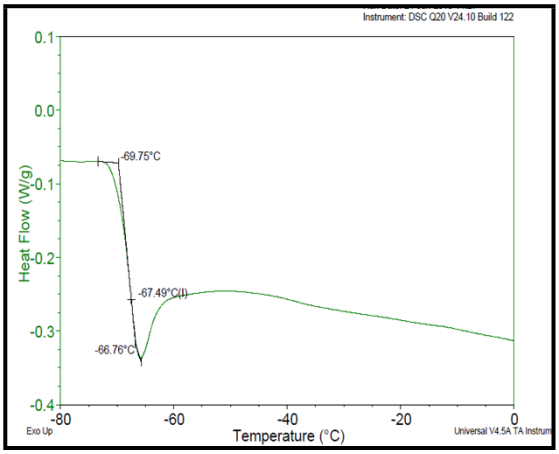


Figure S65: T_g curve of **(6h)**

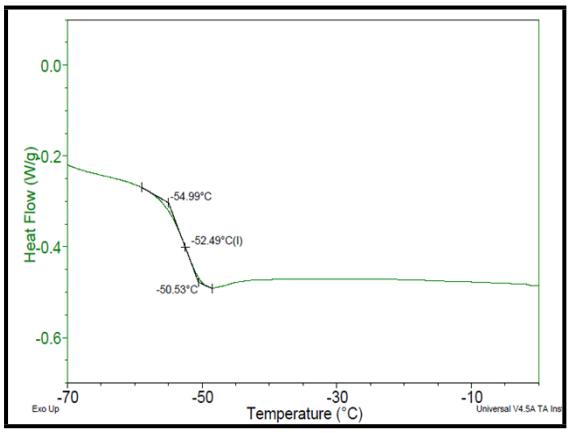


Figure S66: T_g of **(6h)** + GAP

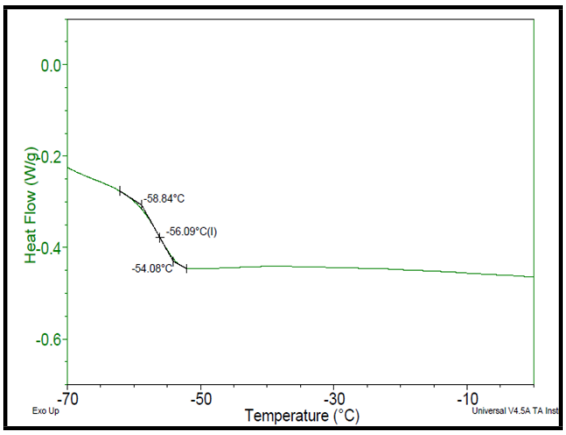


Figure S67: T_g of **(6h)** + BAMO

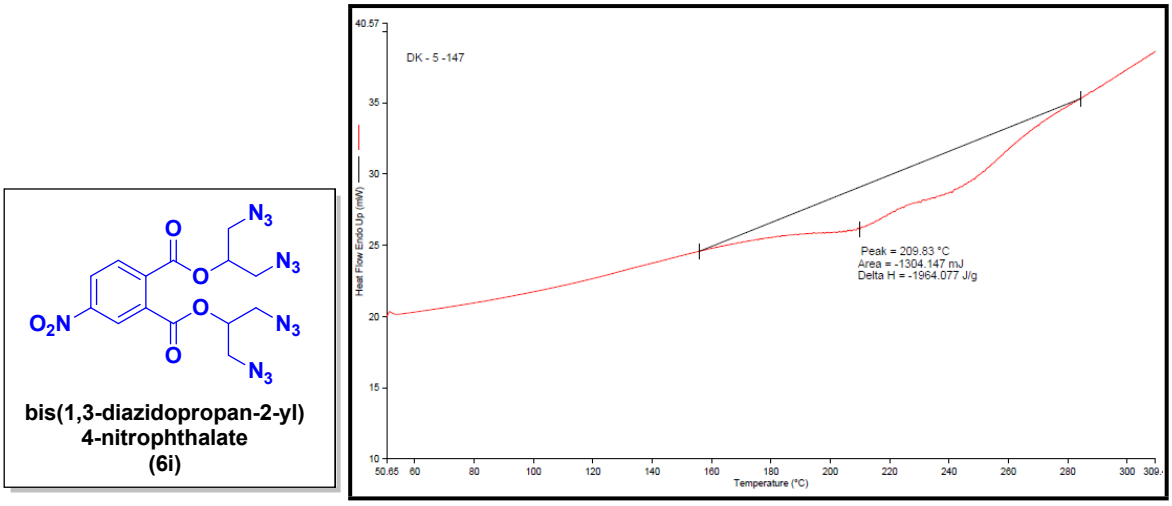


Figure S68: DSC curve of **(6i)**

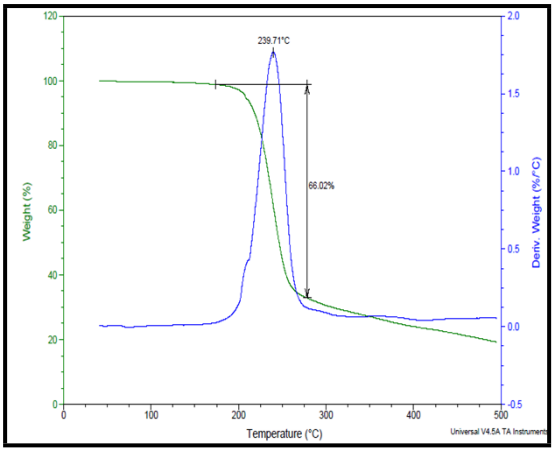


Figure S69: TGA curve of **(6i)**

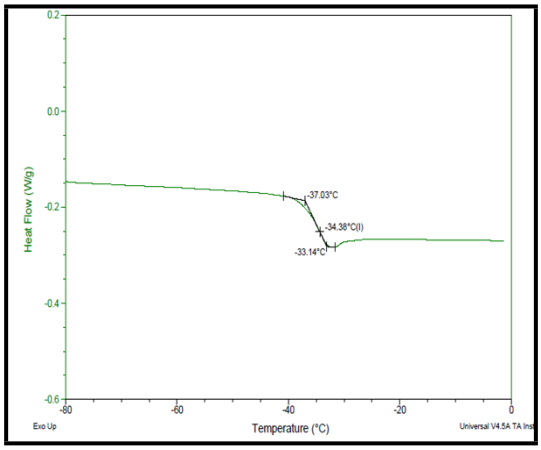


Figure S70: T_g curve of **(6i)**

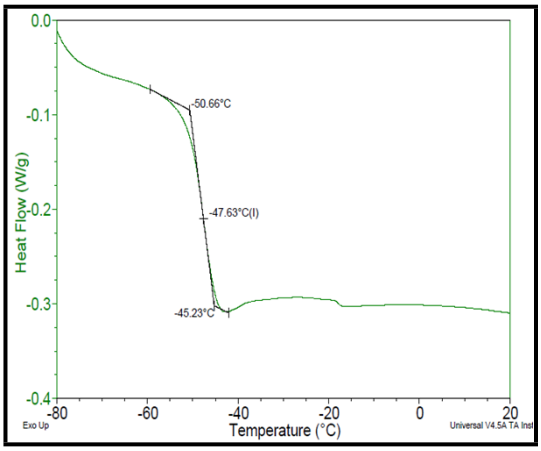


Figure S71: T_g of **(6i)** + GAP

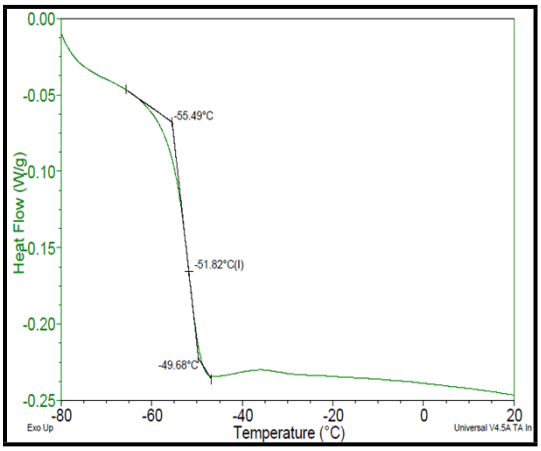


Figure S72: T_g of **(6i)** + BAMO

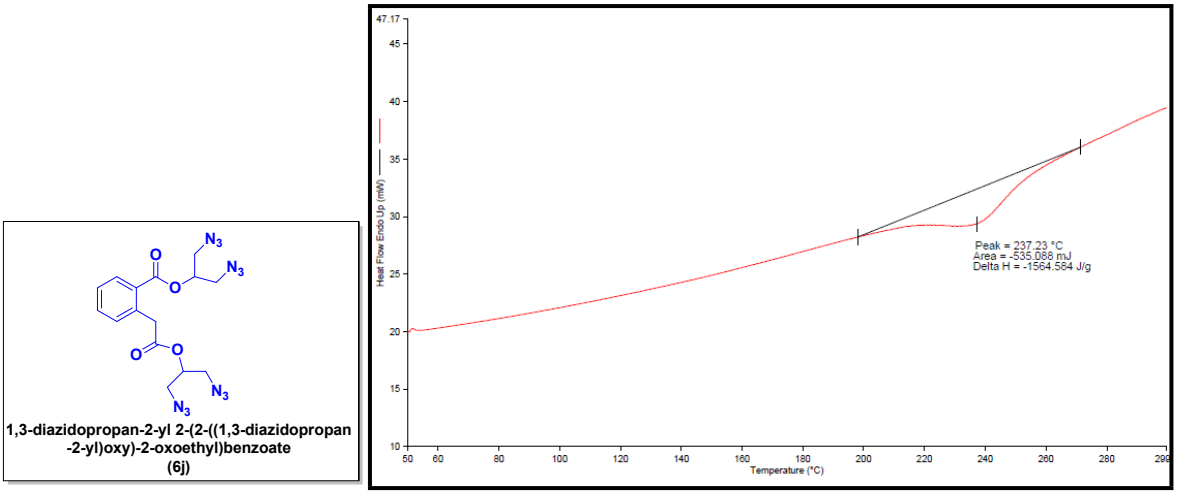


Figure S73: DSC curve of **(6j)**

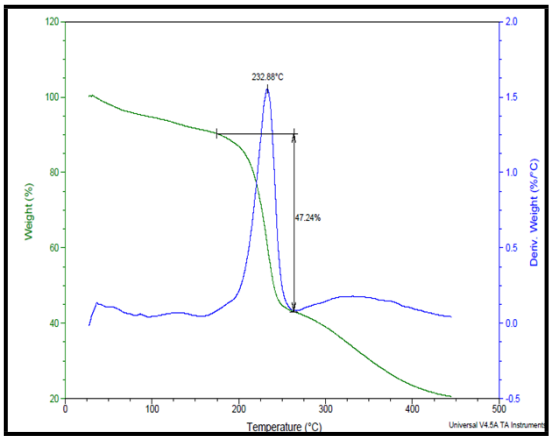


Figure S74: TGA curve of **(6j)**

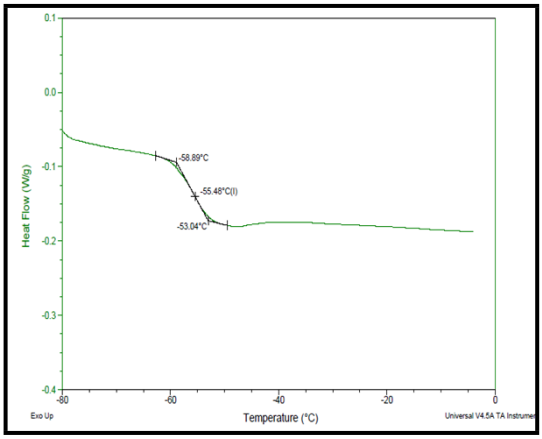


Figure S75: T_g curve of **(6j)**

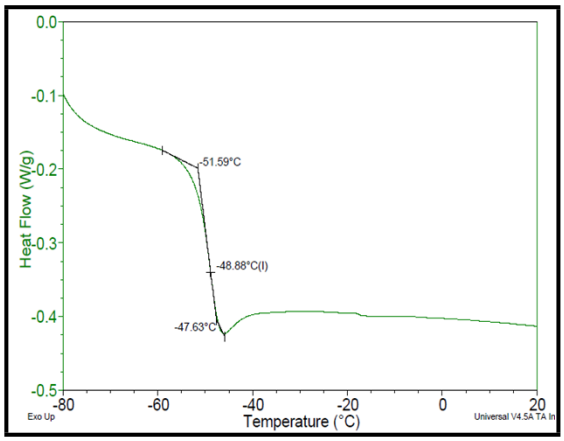


Figure S76: T_g of **(6j)** + GAP

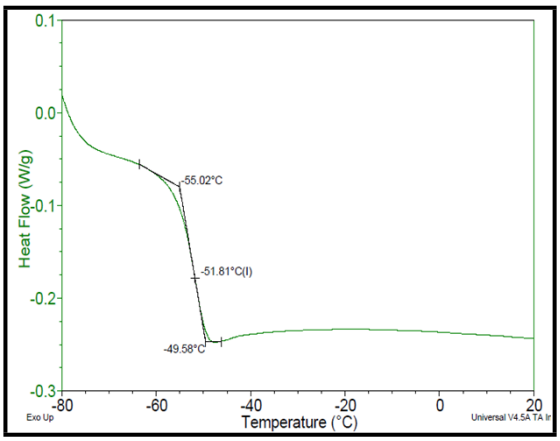
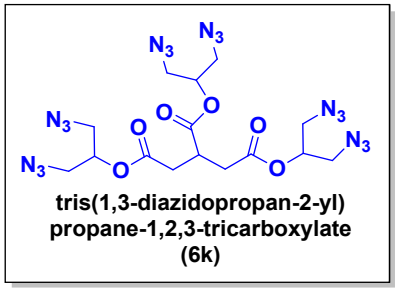


Figure S77: T_g of **(6j)** + BAMO



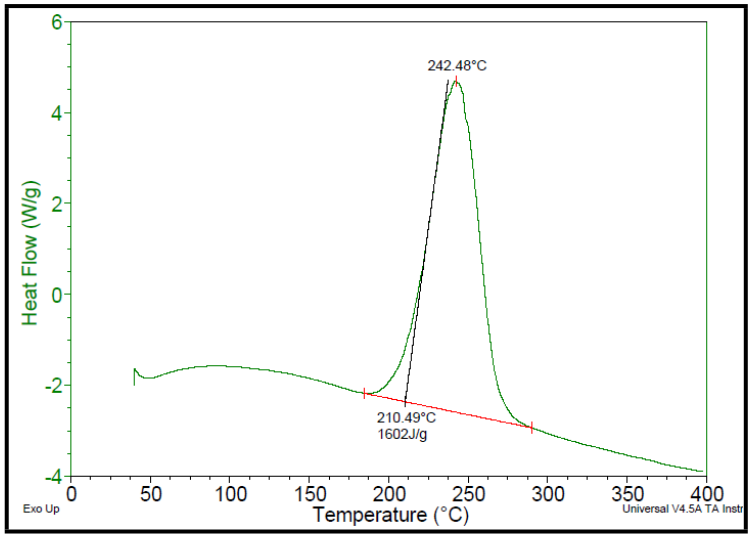


Figure S78: DSC curve of **(6k)**

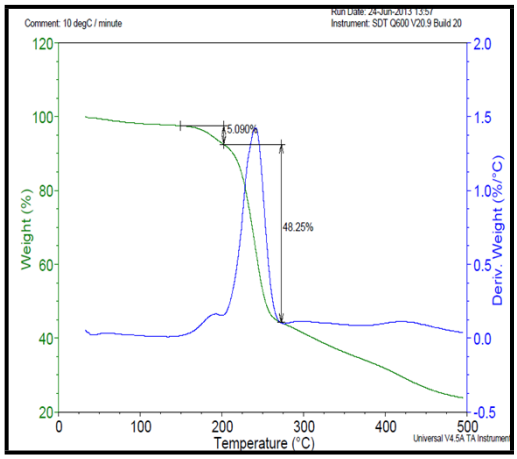


Figure S79: TGA curve of **(6k)**

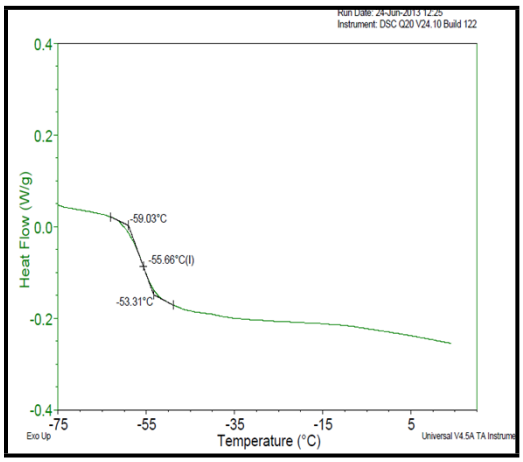


Figure S80: T_g curve of **(6k)**

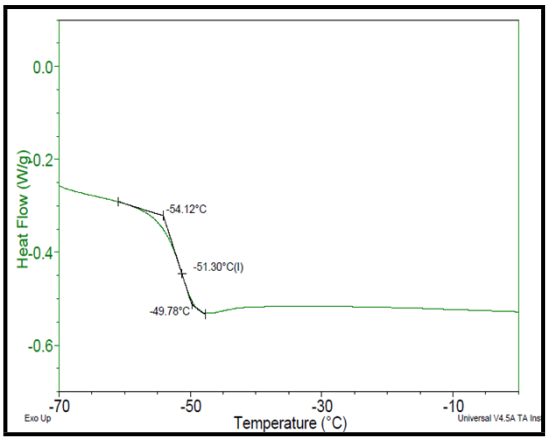


Figure S81: T_g of **(6k)** + GAP

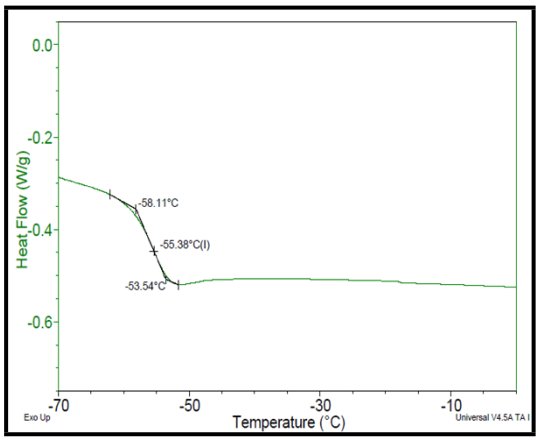


Figure S82: T_g of **(6k)** + BAMO

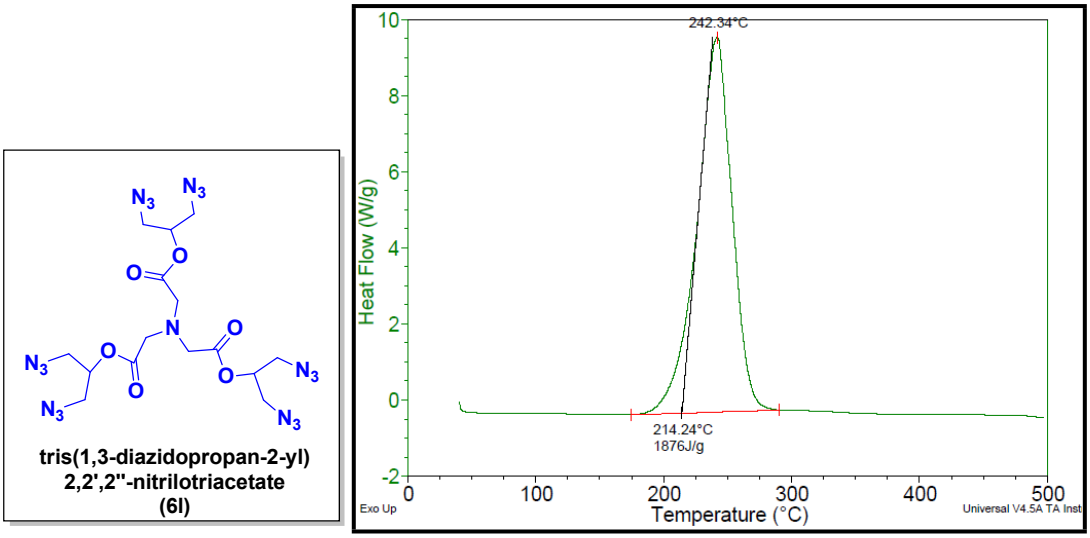


Figure S83: DSC curve of **(6l)**

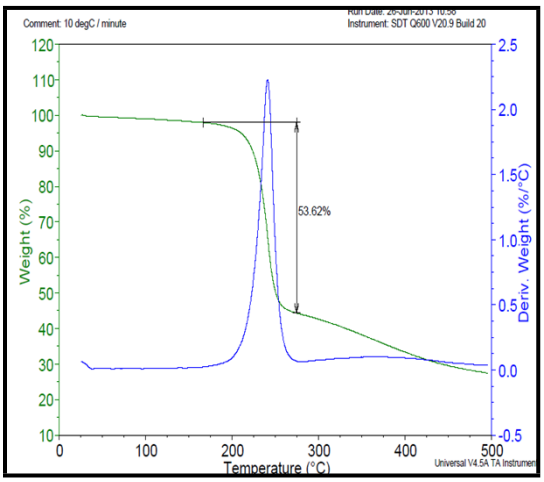


Figure S84:TGA curve of **(6l)**

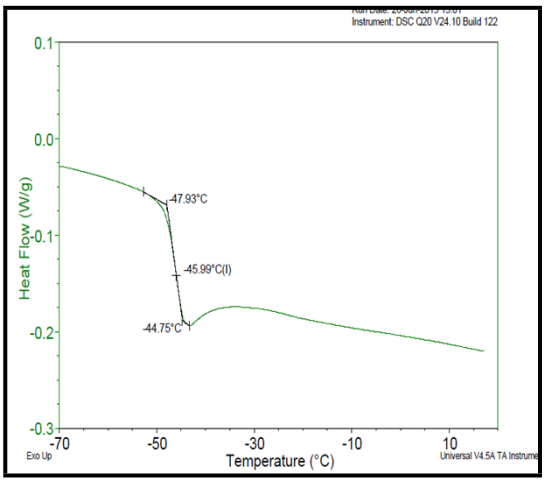


Figure S85: T_g curve of **(6l)**

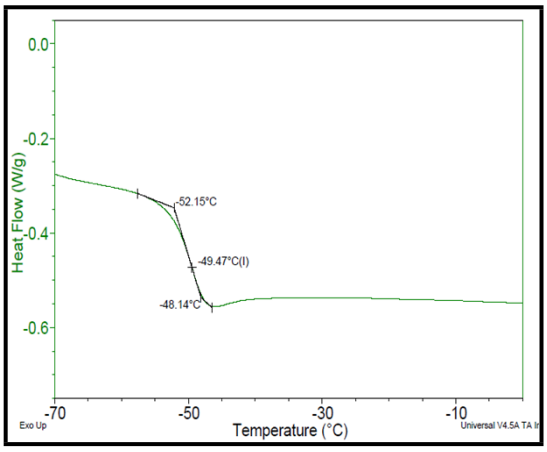


Figure S86:T_g of **(6l)** + GAP

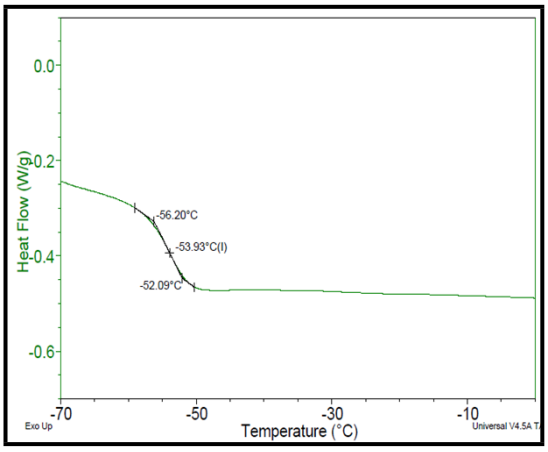


Figure S87: T_g of **(6l)** +BAMO

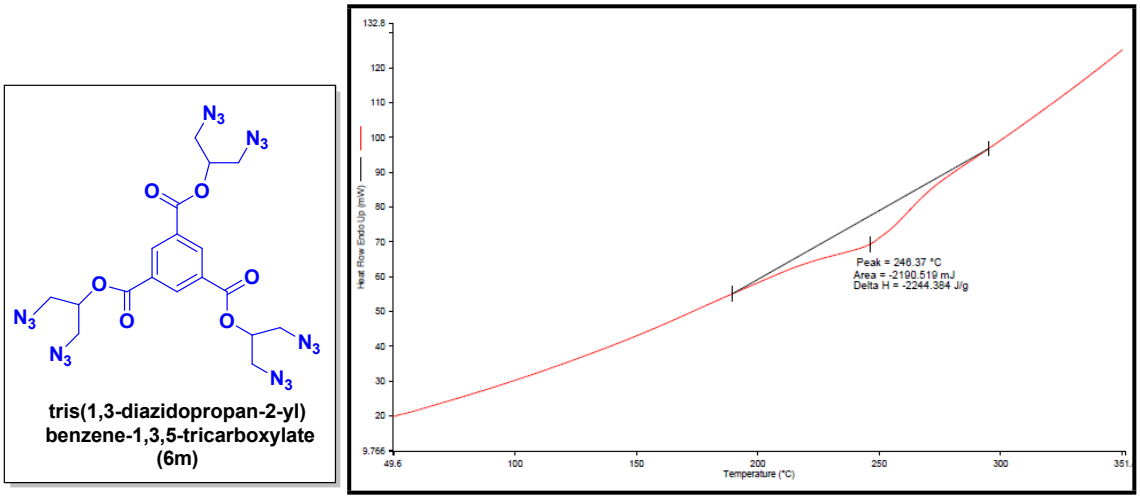


Figure S88: DSC curve of **(6m)**

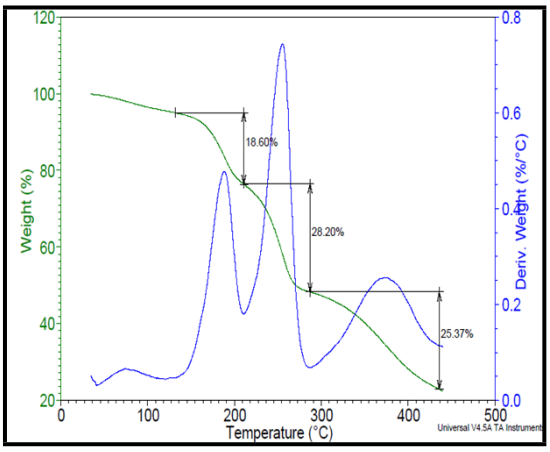


Figure S89: TGA curve of **(6m)**

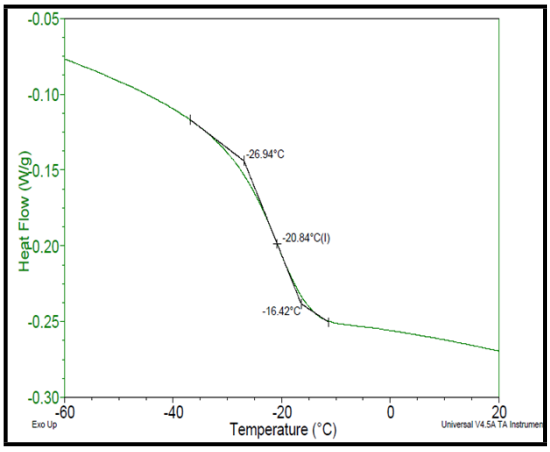


Figure S90: T_g curve of **(6m)**

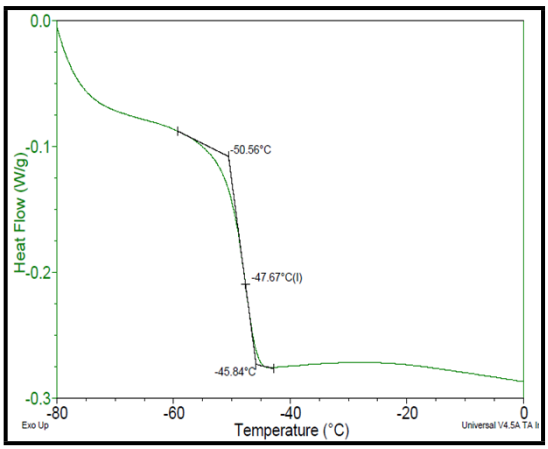


Figure S91: T_g of **(6m)** + GAP

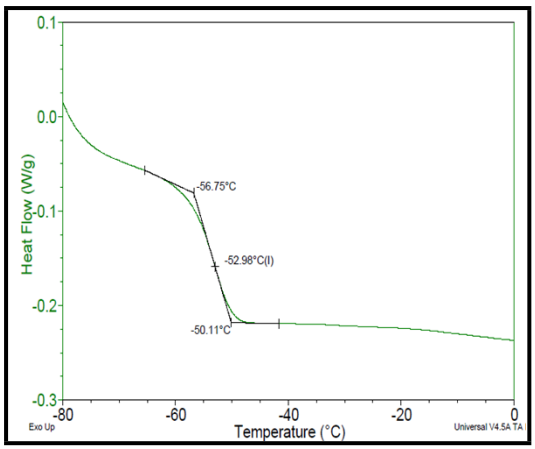


Figure S92: T_g of **(6m)** + BAMO

Computational Studies

Table S1. Enthalpies (including ZPE and thermal correction to enthalpy) computed at the M06/6-31G* level of theory.

Compound	Enthalpy in atomic unit	Compound	Enthalpy in atomic unit
cyclobutane	-157.004938	water	-76.348059
benzene	-232.02955	trimethylamine	-174.246421
ethanoic acid	-228.913934	Benzoic acid	-420.521967
isopropanol	-194.134125	Trifluromethyl benzene	-568.960289
methane	-40.432534	Pyrazole	-226.025102
methaneazide	-203.941776	Octane	-315.266675
nitrobenzene	-436.451707	Methanol	-115.598255
propanoic acid	-268.175778	Toluene	-271.296679
pyridine	-248.076657	P1	-865.5736531

Table S2. Heats of formation of compounds taken from the literature.

Compound	Enthalpy of formation(KJ/mol)	Compound	Enthalpy of formation(KJ/mol)
cyclobutane	3	water	-285.8
benzene	49.0	trimethylamine	23
ethanoic acid	-277.7	Benzoic acid	-385.2
isopropanol	-317.9	Trifluromethyl benzene	108
methane	-74.8	Pyrazole	105.4
methaneazide	304.3	Octane	-250.3
nitrobenzene	12.4	Methanol	-238.4
propanoic acid	-510.7	Toluene	12

pyridine 101.2

Table S3. Optimized geometries (M06-2X/6-31G*, Cartesian coordinates in Å) of Azido-esters. Notation: E = total electronic energy in a. u.; Tc = thermal correction at 298K to obtain the enthalpy; Nimag = number of imaginary frequencies.

6a			
E =-1274.416412			
Tc =0.239569			
Nimag = 0			
C	-1.20928400	0.76677600	-0.02024400
C	-2.53436700	1.09325400	0.23116800
C	-3.55289600	0.15405100	0.25309700
C	-3.19393900	-1.16205500	0.00559800
C	-1.88901700	-1.54763200	-0.25389700
C	-0.89504600	-0.56968500	-0.26449000
H	-0.45268500	1.54462600	-0.02033600
H	-4.57956900	0.43423200	0.45431000
H	-1.64276000	-2.58602000	-0.44579900
N	-4.25083400	-2.19197700	0.01984100
O	-3.91391700	-3.33380200	-0.22032600
O	-5.38029200	-1.82221100	0.27091100
N	-2.87957200	2.50614300	0.48606500
O	-4.04722500	2.75835500	0.70830500
O	-1.97123000	3.31107000	0.45338900
C	0.50142300	-1.02266100	-0.54805700
O	0.80125900	-2.17133500	-0.75302900
O	1.37575500	-0.00220500	-0.55115800
C	2.74698300	-0.32838900	-0.83858200
H	2.77894300	-1.10537100	-1.60879400
C	3.40378100	-0.84773800	0.43406400
H	2.86608500	-1.73744000	0.78026100
H	3.36163800	-0.06862600	1.20453900
C	3.38487900	0.95159400	-1.35865100
H	4.43650900	0.75662300	-1.57158600
H	2.88361500	1.26219500	-2.28272200
N	4.79148000	-1.17739700	0.07320300
N	5.50867000	-1.47826300	1.03146400
N	6.24648800	-1.76538500	1.83673300
N	3.35526200	2.02043700	-0.34671400
N	2.28367400	2.63203600	-0.29633100
N	1.35316500	3.26236500	-0.17778400
6b			
E =-1406.929423			
Tc = 0.242906			
Nimag = 0			

0 1			
C	-1.20865200	0.57657900	-0.05136700
C	-2.52081600	0.98396500	0.17947700
C	-3.56565500	0.06986600	0.15729600
C	-3.26248300	-1.26125600	-0.09724000
C	-1.97217200	-1.70471700	-0.32647000
C	-0.94022500	-0.76764000	-0.30268100
H	-0.39691000	1.29740000	-0.03753200
H	-4.59268200	0.36985900	0.32794700
H	-1.76546500	-2.75075300	-0.52252800
N	-4.36583700	-2.23930900	-0.12770400
O	-4.07664700	-3.39811900	-0.34931000
O	-5.48824900	-1.81623200	0.07084200
C	0.44654000	-1.26290400	-0.55519500
O	0.72473800	-2.42113900	-0.74161700
O	1.34021100	-0.26116200	-0.55024400
C	2.70826000	-0.61556400	-0.79057500
H	2.74657600	-1.40972500	-1.54264000
C	3.31664600	-1.11904600	0.51228500
H	2.77689300	-2.01604500	0.83574500
H	3.22417200	-0.33715500	1.27482900
C	3.39336100	0.62504700	-1.32753800
H	4.42726200	0.36627000	-1.58118800
H	2.87237700	0.95813800	-2.23317700
N	4.72832600	-1.42096400	0.22298600
N	5.35621800	-1.87513800	1.18310300
N	6.01646400	-2.29527800	1.99754800
N	3.34238000	1.66661300	-0.28657600
N	4.04009100	2.65438800	-0.52920800
N	4.64565600	3.59941100	-0.65894700
C	-2.78536700	2.43310100	0.49258400
F	-2.38874400	2.73696600	1.73476900
F	-2.11404000	3.23566800	-0.34309300
F	-4.08525500	2.72987600	0.39602400

6c
E =-1063.947463
Tc = 0.204232
Nimag = 0

C	1.88201700	0.21935700	-0.90047800
C	2.43447400	0.87791200	0.22047300
C	3.80096000	0.77123300	0.09160100
N	3.98100900	0.08484700	-1.04913400
H	4.85806000	-0.19394600	-1.46679400
H	4.60402600	1.14134500	0.71011100
N	2.84345400	-0.26039100	-1.66820100
N	1.75837200	1.61665400	1.24634100
O	2.41888300	1.95378200	2.21271600
O	0.57936400	1.87154900	1.06758300

C	0.44742100	-0.00913700	-1.24778700
O	-0.04412000	0.21955900	-2.31798300
O	-0.19605000	-0.52472400	-0.18932200
C	-1.61210700	-0.71236400	-0.31654100
C	-2.29345400	0.62870000	-0.07445800
C	-1.98140900	-1.75320200	0.72843900
H	-1.83938300	-1.08024900	-1.32101000
H	-2.00984200	1.00810800	0.91565900
H	-1.95570500	1.34586200	-0.83163000
H	-1.71946200	-1.37699800	1.72644800
H	-3.05675400	-1.92867400	0.69121100
N	-1.33441000	-3.04420500	0.45433700
N	-3.74358100	0.38907000	-0.16317200
N	-0.14748900	-3.10111700	0.79168700
N	-4.43075300	1.41330800	-0.16575100
N	0.93389500	-3.27156500	1.07114900
N	-5.14806300	2.28600300	-0.17660700

6e
E =-1604.163628
Tc = 0.670205
Nimag = 0

C	-5.10018000	-2.96874100	-2.09695900
C	-4.23918600	-1.87707900	-2.03855700
C	-4.42392400	-0.88355900	-1.07885800
C	-5.47980000	-0.96769000	-0.15799300
C	-6.31759700	-2.07854900	-0.21488000
C	-6.13756900	-3.07059700	-1.17696900
H	-3.42981500	-1.77625300	-2.75593000
H	-7.12763900	-2.16693200	0.50416000
H	-6.80995800	-3.92233600	-1.20491700
C	-3.54660300	0.33180100	-1.09469400
O	-3.99719700	1.44922300	-1.02258600
O	-2.22379000	0.15930400	-1.27224700
C	-1.52017400	-0.94404300	-0.67724300
H	-0.89693100	-0.50475300	0.11020900
H	-2.22228800	-1.63123600	-0.19720900
C	-0.67047700	-1.63063000	-1.73654300
H	-0.28018500	-0.85937600	-2.41271200
H	-1.30525600	-2.29000500	-2.33872000
C	0.49898000	-2.41777200	-1.13419500
H	0.85671900	-3.15247600	-1.86514400
H	0.15520100	-2.99399400	-0.26356200
C	1.66424700	-1.51387900	-0.73268900
H	1.32003500	-0.75489300	-0.01585700
H	2.00383700	-0.96004300	-1.61902300
C	2.85216000	-2.26346700	-0.13603700
H	2.53155300	-2.82350300	0.75319700
H	3.21284600	-3.00864900	-0.85839700

C	3.99667000	-1.32208700	0.23474500
H	3.63932100	-0.60304900	0.98686300
H	4.28101900	-0.72967300	-0.64649800
C	5.22601800	-2.04842200	0.77443000
H	4.95426300	-2.63119000	1.66555400
H	5.60170300	-2.76120000	0.03087900
C	6.34422600	-1.07253600	1.12648300
H	5.99904100	-0.35216600	1.88104700
H	6.64626300	-0.50632500	0.24302600
N	7.57356000	-1.74793500	1.59344900
N	7.45235200	-2.29546100	2.69029800
N	7.44173500	-2.82405800	3.69149500
H	-4.95940900	-3.73311000	-2.85422300
C	-5.71212300	0.11421900	0.86546600
H	-6.04044400	1.04304300	0.39170500
H	-6.49703600	-0.19008700	1.56725800
C	-4.47277500	0.43312600	1.68262800
O	-3.48412300	-0.26115100	1.74053900
O	-4.63469500	1.57868400	2.34982800
C	-3.58705300	1.98477100	3.24903700
H	-4.10974800	2.50909600	4.05190300
H	-3.10298700	1.09061100	3.65221000
C	-2.57286500	2.89794500	2.57562100
H	-1.94571200	3.32061500	3.37291900
H	-3.10280900	3.73768900	2.10971500
C	-1.68969400	2.18988900	1.55099600
H	-2.29900100	1.86763700	0.70001500
H	-1.28027100	1.27801700	2.00786900
C	-0.53954100	3.04766500	1.02859100
H	-0.93452700	3.89073700	0.44611900
H	0.02080300	3.48139600	1.86963200
C	0.40549800	2.21398800	0.16671400
H	-0.16690100	1.74960600	-0.64928700
H	0.79340900	1.38807000	0.78236800
C	1.59015600	2.98441400	-0.41108800
H	1.22906800	3.75414600	-1.10647300
H	2.11292000	3.51402200	0.39776100
C	2.56457500	2.04812700	-1.12005100
H	2.05098500	1.51332100	-1.92882700
H	2.91632500	1.28411300	-0.41554700
C	3.77717300	2.76066800	-1.69084500
H	4.28750600	3.33375900	-0.90476600
H	3.47955100	3.46403200	-2.48004600
N	4.69424800	1.73310900	-2.23550400
N	5.65511200	2.19284900	-2.85561500
N	6.56530000	2.51827900	-3.44329400

6g
E =-1423.98821585
Th = 0.360851

Nimag = 0

0 1

C	0.96547400	2.89381700	-0.70363000
C	0.61627200	1.45565400	-0.23392000
C	-0.05117900	2.09198400	1.01933600
C	-0.13889000	3.42403200	0.23078800
H	1.96102000	3.17310200	-0.34867900
H	0.88337000	3.09984600	-1.77228400
H	-0.12104000	0.96626300	-0.87203800
H	0.65138900	2.14526000	1.85317600
H	0.05794400	4.34043800	0.78939700
H	-1.09937400	3.50447200	-0.28389900
C	-1.32526300	1.44474000	1.48501000
O	-1.57642300	1.08130300	2.60390600
C	1.79854300	0.56553200	0.02398400
O	2.68509000	0.83765500	0.79681900
O	1.75595100	-0.55571300	-0.72838100
O	-2.17902000	1.28125600	0.44318800
C	-3.22314100	0.32690400	0.62129800
C	-2.62691000	-1.07486000	0.67966900
C	-4.13860500	0.52817100	-0.57555100
H	-3.76255800	0.52245100	1.55340400
H	-2.05256400	-1.19111200	1.60359400
H	-3.44228900	-1.80727400	0.66034700
H	-4.45965600	1.57592400	-0.60821100
H	-3.58681700	0.29699400	-1.49474400
C	2.83051900	-1.51954300	-0.73493400
C	3.33152800	-1.93849000	0.64743800
C	3.96312900	-1.08104200	-1.66344100
H	2.35131300	-2.39048900	-1.19347000
H	4.06373800	-2.73543300	0.50050700
H	3.81711700	-1.10917200	1.16216500
H	3.52746800	-0.70055500	-2.59522200
H	4.56130700	-1.96331300	-1.90519200
N	-5.29028600	-0.37085900	-0.39500300
N	-1.76071900	-1.22737900	-0.50648200
N	-0.95550600	-2.15555800	-0.46236400
N	-6.02078800	-0.46417200	-1.38374200
N	4.89921500	-0.11636600	-1.06835700
N	4.59922000	1.06626300	-1.24680600
N	2.27000100	-2.54205000	1.46831000
N	1.34975400	-1.79153700	1.78389000
N	4.41888100	2.17529400	-1.36361100
N	0.44282300	-1.20399900	2.12397000
N	-0.18092800	-2.97706200	-0.53754300
N	-6.74938300	-0.61897500	-2.23360300

6h

E =--1703.419131

Tc = 0.355151
Nimag = 0

0 1

C	1.70300400	3.17044100	0.45086400
C	1.81400900	1.79410200	0.33843100
C	0.68181600	1.06643800	-0.01623700
C	-0.53123100	1.72796700	-0.24663100
C	-0.60760200	3.11393700	-0.14057600
C	0.51642600	3.85044700	0.21548400
H	2.76359700	1.30682800	0.51841000
H	-1.55173800	3.61301700	-0.33299300
H	0.48825700	4.92902400	0.31214200
N	2.89928800	3.94277600	0.83053700
O	2.77928700	5.14946900	0.91885700
O	3.92568100	3.32211300	1.03126900
C	0.74008100	-0.41331800	-0.20531500
O	-0.16420600	-1.06380200	-0.66475200
O	1.91570700	-0.92870400	0.19909300
C	-1.77495700	0.97105900	-0.62659200
O	-2.22381500	0.93645300	-1.73899800
O	-2.31871300	0.40009500	0.46005300
C	-3.39741100	-0.50717600	0.23202500
C	-4.73490200	0.22925000	0.33973100
C	-3.31330400	-1.57225600	1.32373200
H	-3.27088000	-0.95074000	-0.76321000
H	-5.55250700	-0.49029200	0.19329300
H	-4.82513400	0.64500400	1.34594700
H	-3.45075400	-1.09428300	2.29642200
H	-4.12603700	-2.29724400	1.18168800
C	2.12670200	-2.33605900	0.00896200
C	2.13369700	-2.98782100	1.38638300
C	3.44795700	-2.49681500	-0.71769800
H	1.30590500	-2.73736900	-0.59154900
H	2.32434800	-4.05825800	1.28512200
H	2.92864100	-2.54754900	2.00343100
H	4.24553100	-1.99554700	-0.15335900
H	3.69065900	-3.56523600	-0.79132700
N	3.28573600	-1.90438800	-2.05299500
N	4.34315400	-1.75549800	-2.67192600
N	5.25154600	-1.57539600	-3.31896900
N	0.82076900	-2.87126800	2.03202200
N	0.59214500	-1.75600500	2.51709600
N	0.27785700	-0.78244100	2.99329400
N	-2.01125800	-2.23552300	1.41140400
N	-1.76277500	-3.04109500	0.50889400
N	-1.42157600	-3.80250900	-0.25097400
N	-4.86764200	1.38047200	-0.55968100
N	-5.00151200	1.07353100	-1.75177100
N	-5.13532400	0.90684000	-2.85887000

6i
E =-1538.28243624
Tc = 0.38011
Nimag = 0

C	1.34334500	-2.79146700	0.06251400
C	2.23955800	-2.11466600	-0.77921000
C	3.05345800	-2.82690400	-1.66285000
C	2.95938500	-4.20895200	-1.75379300
C	2.05762400	-4.88665800	-0.93926500
C	1.26998100	-4.18035300	-0.03593400
H	3.75656200	-2.27164600	-2.27504700
H	3.58665900	-4.75334500	-2.45199800
H	1.97295200	-5.96739300	-0.99749800
H	0.58441400	-4.71767100	0.61392000
C	0.49299600	-2.08786300	1.09024500
H	1.03620000	-1.28748500	1.59919400
H	0.18511400	-2.80194400	1.86412400
C	2.42866900	-0.63291200	-0.78853600
O	3.46493100	-0.09820000	-1.08910500
C	-0.78109600	-1.52661800	0.49709200
O	-1.28146300	-1.86655100	-0.54300800
C	-2.62879700	-0.09333700	0.99429200
C	-3.67708300	-1.18895700	0.73439900
C	-2.47696200	0.90056600	-0.15358900
H	-2.93898000	0.44169600	1.89528400
H	-3.37982100	-2.08772200	1.28160000
H	-3.73724700	-1.43861200	-0.32813900
H	-1.81409100	1.71617000	0.16425100
H	-2.03773000	0.39493500	-1.02159800
C	1.27292400	1.42590300	-0.17860700
C	2.31631400	2.29929300	-0.87875300
C	1.31322300	1.56515800	1.33746500
H	0.29515900	1.77440100	-0.52408500
H	3.30230000	2.18530800	-0.42261300
H	2.38743800	2.03343000	-1.93749100
H	0.42145100	1.09185000	1.76712100
H	1.31890700	2.63067000	1.59591500
N	1.79484600	3.67486100	-0.71710800
N	2.60893100	4.55822400	-0.99782800
N	3.28050400	5.43669400	-1.22906800
N	2.52594400	0.87470300	1.81269400
N	2.90880100	1.22058400	2.93330600
N	3.34117300	1.47081400	3.94645200
N	-4.97943900	-0.77570000	1.28291800
N	-5.80435800	-0.41164000	0.44223000
N	-6.63117800	-0.06632700	-0.24481700
N	-3.82148000	1.41785300	-0.45185400
N	-3.89079000	2.09723500	-1.48026900
N	-4.05843100	2.73017700	-2.40001400

O	-1.33666200	-0.62214800	1.33583800
O	1.28292100	0.03085100	-0.50025800

6j
E =-1515.0210647
Tc =0.337441
Nimag = 0

C	0.99988900	1.49326300	0.17753500
C	-0.22362200	2.06230700	0.51532400
C	-1.40651800	1.36965800	0.27627900
C	-1.36195200	0.09616400	-0.29728400
C	1.03868300	0.21877200	-0.39448100
H	1.92820200	2.02431500	0.35915500
H	-2.36391700	1.80423300	0.54437900
C	2.32290800	-0.43777700	-0.76794300
O	2.41587000	-1.54890200	-1.22986400
O	3.38403600	0.35996700	-0.53026900
C	4.66969600	-0.17003400	-0.86235700
H	4.56213649	-0.90179858	-1.66917010
C	5.24792775	-0.85422344	0.36957529
H	4.59585029	-1.68777496	0.65275291
H	5.29670439	-0.12778062	1.18889203
C	5.51429612	0.99222089	-1.34754556
H	5.06657096	1.92315140	-0.98321112
H	6.52608007	0.89343151	-0.93700122
N	6.59284610	-1.32660292	-0.00180906
N	7.15061260	-2.00566392	0.86296401
N	7.74665512	-2.63641605	1.58658727
N	5.55822496	0.95855862	-2.82094904
N	5.88178344	2.02773171	-3.34165632
N	6.16565090	2.96186236	-3.91158966
H	-0.25681600	3.04748400	0.96845800
C	-2.59708200	-0.69344900	-0.55210400
O	-2.62240800	-1.85590100	-0.86898200
O	-3.71618300	0.05121800	-0.39318600
C	-4.94960400	-0.66475200	-0.43556700
H	-4.95371636	-1.34047014	-1.29630230
C	-5.14026024	-1.50134138	0.84418425
H	-4.16395702	-1.88522516	1.16342141
H	-5.54193037	-0.87396157	1.63801512
C	-6.01402570	0.40747363	-0.63766823
H	-6.04926448	1.09036678	0.22060254
H	-5.75667518	0.99234766	-1.52875569
N	-7.29464016	-0.29551927	-0.80986474
N	-8.25967775	0.45100042	-0.99582794
N	-9.18416534	1.04584460	-1.25421276
N	-6.11436945	-2.59804449	0.71183325
N	-6.05009494	-3.27226804	-0.31526643

N	-6.09912826	-3.95069731	-1.22095951
N	-0.14003400	-0.48507800	-0.62566600

6k
E =-2019.365045
Tc = 0.475569
Nimag = 0

0 1

C	-0.00870200	-0.14901100	-1.75093200
H	0.64100800	0.14589500	-2.58526900
C	-0.32166100	1.14688400	-1.01554900
O	-1.11418600	1.96217500	-1.42454500
O	0.39291100	1.30738400	0.10818800
C	0.13576600	2.50094900	0.86431900
C	0.70256400	3.72331000	0.13963300
C	0.81462800	2.30047100	2.20987000
H	-0.94702600	2.60669400	0.98850800
H	0.08285400	3.96078300	-0.72881800
H	0.69213000	4.57865500	0.82128300
H	1.89438700	2.19495200	2.06679200
H	0.61671300	3.17591400	2.83229900
N	2.10736000	3.49290800	-0.24070100
N	0.25833300	1.15340400	2.93975200
N	2.23580200	3.11900200	-1.41362300
N	0.74925300	0.06284200	2.65299800
N	1.11938900	-0.99555800	2.49656700
N	2.44791000	2.80253100	-2.47574100
C	-1.31918100	-0.68788300	-2.32529800
H	-1.75118900	0.03246300	-3.02735100
C	0.73539400	-1.17399800	-0.90209500
H	0.72828400	-2.15517100	-1.39532100
H	0.26862000	-1.30963400	0.07774200
C	2.18297900	-0.80182600	-0.70328000
O	2.76157000	0.10396300	-1.24694200
C	-2.34888700	-0.88005100	-1.23883700
O	-2.17813100	-0.57298300	-0.08168500
O	2.77350700	-1.67329200	0.14233900
H	-1.16973500	-1.62809600	-2.86538500
O	-3.47860100	-1.43016200	-1.71928800
C	-4.71159300	-1.20577800	-1.03011300
C	-5.24281900	0.18579700	-1.41437000
C	-4.67843000	-1.45928700	0.48116300
H	-5.39059800	-1.95347000	-1.44908900
H	-5.62736600	0.15007400	-2.43413200
H	-6.06847700	0.45048600	-0.74249000
H	-4.07194100	-2.34666000	0.69390100
H	-4.25781800	-0.61876100	1.03850900
C	4.15780900	-1.48875200	0.43621100
C	4.72288900	-2.88995400	0.63017400

C	4.29820500	-0.64130000	1.69825100
H	4.64153600	-1.00310900	-0.41868600
H	5.78181800	-2.83389300	0.88884700
H	4.18788800	-3.38940800	1.44826800
H	3.74569100	-1.11300600	2.51363100
H	5.35815600	-0.57801000	1.98052800
N	3.70884900	0.70020100	1.55570800
N	4.65478100	-3.67501000	-0.61010000
N	3.52443000	-4.07792100	-0.90284100
N	4.30034700	1.40358500	0.72215200
N	-4.19380900	1.21447800	-1.44980500
N	-6.09257600	-1.69141200	0.84375200
N	-6.32735700	-1.60006200	2.05172600
N	-3.87101800	1.69720200	-0.36014000
N	-3.48811700	2.21052200	0.56907100
N	-6.64433100	-1.53598900	3.13411600
N	4.77425500	2.11197400	-0.01461000
N	2.54717600	-4.50995700	-1.27016600

6l

E =-2074.662483

Th = 0.494313

Nimag = 0

0 1

N	-0.18056200	-0.73590900	-0.32739200
C	-1.40948500	-0.12898200	-0.78127800
H	-1.50735400	0.87481400	-0.35516100
H	-1.39023600	-0.00712300	-1.87083100
C	0.17603400	-1.97015500	-1.00415300
H	-0.23051100	-1.95813800	-2.01824300
H	-0.23457100	-2.86559600	-0.51228500
C	-0.05100400	-0.76052700	1.13314700
H	0.45500400	-1.66852700	1.46056700
H	-1.02891500	-0.70051400	1.63092500
C	-2.64392600	-0.93809500	-0.40808600
O	-2.61852600	-2.05974800	0.03454600
C	1.67269500	-2.17853200	-1.16093500
O	2.16755200	-2.80160600	-2.06620000
C	0.80697600	0.42637300	1.52336600
O	1.90200800	0.38770100	2.02462400
O	2.37646500	-1.65100300	-0.14235100
O	-3.76917800	-0.23499400	-0.64052000
O	0.19172100	1.56945100	1.15611800
C	1.02350100	2.72094500	0.99209300
C	0.12475000	3.94587100	1.06935100
C	1.70755100	2.56943600	-0.36460900
H	1.76724600	2.76105200	1.79364400
H	-0.42970800	3.91971000	2.00954900

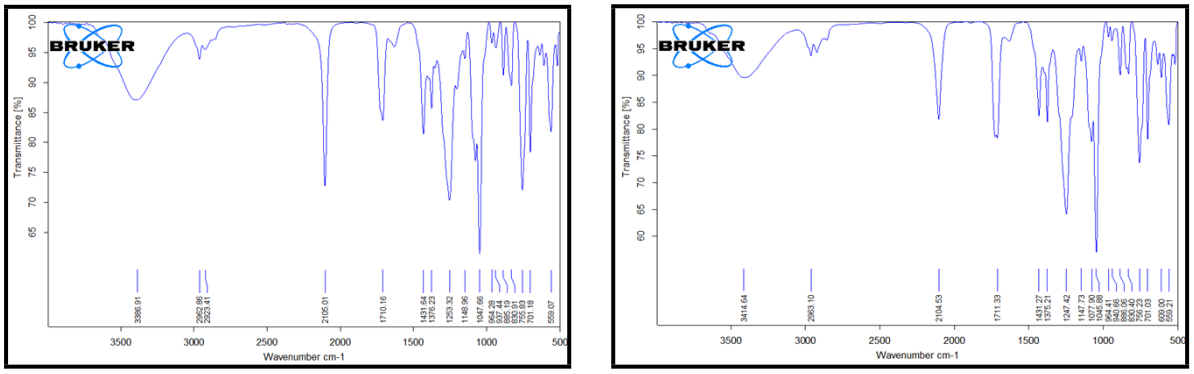
H	0.75066900	4.84368900	1.04712800
H	2.33282700	1.66927100	-0.37088400
H	0.93272300	2.44394200	-1.13060100
C	-4.99227500	-0.79041400	-0.14986700
C	-6.07059200	-0.34721300	-1.12561100
C	-5.23692800	-0.25387800	1.26003500
H	-4.91750300	-1.88233400	-0.13831500
H	-6.09673600	0.74997300	-1.16881500
H	-5.83014700	-0.72618100	-2.12616400
H	-5.31963300	0.83468800	1.21869700
H	-6.17789100	-0.66202100	1.64549100
C	3.79358100	-1.87722900	-0.16006100
C	4.07374700	-3.32266900	0.26602800
C	4.41530600	-0.89333300	0.80911300
H	4.16572100	-1.70859800	-1.17648900
H	3.78310600	-3.45974300	1.31069100
H	3.48817000	-4.00509500	-0.35745900
H	3.86304800	-0.92236300	1.75426300
H	5.45719800	-1.18875200	0.97824100
N	-4.10784400	-0.52359700	2.16587300
N	-7.34560900	-0.89255800	-0.63405300
N	-8.31012200	-0.66916400	-1.37154800
N	-4.00991800	-1.71082000	2.50491000
N	4.36756800	0.45299700	0.21329600
N	5.51188600	-3.62551400	0.19561400
N	5.90211300	-3.94270300	-0.93543100
N	4.37741300	1.37863300	1.02535600
N	-0.88056300	3.95878800	-0.01011900
N	-0.56021900	4.63641600	-0.99293700
N	2.47565900	3.79510800	-0.63994000
N	3.62318900	3.60068500	-1.04835800
N	6.36456100	-4.25298600	-1.91761000
N	4.36806500	2.31230600	1.66334000
N	4.68782400	3.52115300	-1.41766800
N	-0.37324800	5.22991500	-1.93586200
N	-3.82484600	-2.76060600	2.87387700
N	-9.25283800	-0.51931200	-1.97490400

6m
E =-2132.4419214
Tc =0.471425
Nimag = 0

C	-0.73607700	-1.49263600	0.56922800
C	-1.13461200	-0.23334000	0.12732100
C	-0.17491800	0.72318100	-0.18844700
C	1.18072200	0.42399500	-0.07966700
C	1.57206700	-0.83219400	0.38301100
C	0.61605400	-1.79253900	0.71371900
H	-2.18696100	0.00048000	0.03018400

H	1.91347000	1.17927000	-0.34151000
H	0.92573600	-2.76882800	1.07455700
C	-0.56856500	2.08283900	-0.65100200
O	0.17418900	2.86713000	-1.18361400
C	-1.74188000	-2.53972400	0.89805800
O	-1.51364800	-3.54781100	1.51265500
C	3.00820400	-1.18920800	0.55909500
O	3.40330500	-2.24242900	0.99294900
O	-2.95551400	-2.22537600	0.37758500
O	3.82768200	-0.18608300	0.17787600
O	-1.87606200	2.32013800	-0.40150200
C	-4.05156300	-3.10554700	0.64454600
C	-4.27018000	-4.00648100	-0.56769100
C	-5.26984600	-2.21605200	0.87315600
H	-3.82007300	-3.70010200	1.53194400
H	-5.17399700	-4.60202000	-0.41928400
H	-4.40931700	-3.37688500	-1.45727900
H	-5.52069800	-1.68656700	-0.05454100
H	-6.12062300	-2.83502100	1.16609500
C	5.22900400	-0.36958300	0.41370200
C	5.82804400	1.02874300	0.44814000
C	5.81189600	-1.22679000	-0.70314900
H	5.36704500	-0.86717900	1.37782400
H	6.90237300	0.95043400	0.61645800
H	5.65833600	1.52503300	-0.51694300
H	5.34309200	-2.21624900	-0.67738300
H	5.59760100	-0.75520000	-1.67180500
C	-2.39893200	3.59068800	-0.78251700
C	-2.30272700	4.55589300	0.39910300
C	-3.85812500	3.35325100	-1.15853000
H	-1.83420000	3.96012000	-1.64494200
H	-2.75298000	5.51778300	0.11594200
H	-2.86927400	4.14394000	1.23756100
H	-4.41812000	3.02914200	-0.27269000
H	-4.29539000	4.28160900	-1.53193700
N	-5.04205100	-1.26937400	1.97476900
N	-4.56931000	-0.19013900	1.61949900
N	-3.18394200	-4.97380700	-0.76299900
N	-2.15885200	-4.49560400	-1.25718900
N	-0.93801300	4.72846800	0.90809200
N	-0.18621600	5.34139600	0.13806500
N	-3.97842200	2.37054100	-2.24602300
N	-4.03368600	1.20141500	-1.86617200
N	7.26339700	-1.30923600	-0.46991700
N	7.83921000	-2.16791000	-1.14292600
N	5.28166800	1.81672700	1.56141200
N	4.18084700	2.32761900	1.33204800
N	3.18680700	2.85571100	1.22963300
N	-4.11399400	0.09750200	-1.62864900
N	0.58018500	5.88864100	-0.48220500

N	8.45884400	-2.92316600	-1.71008900
N	-4.15778900	0.84091500	1.39829000
N	-1.17397300	-4.16702600	-1.70396600



(a) **(b)**

Figure S93: FTIR spectrum of 1,3-diazidopropan-2-ol (2), **(a)** by **method (b) and (b) by method (c)**

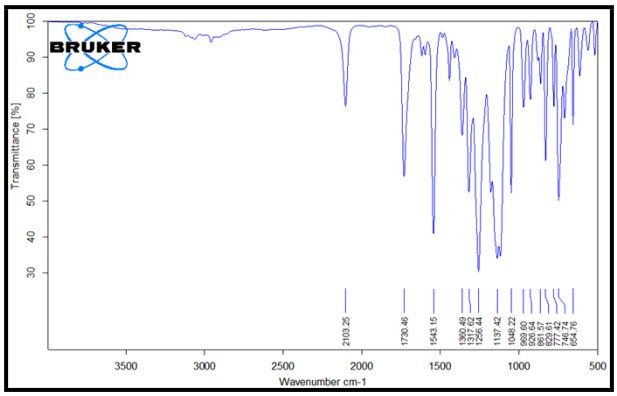


Figure S94: FTIR spectrum of (6b) formed by using EDC. HCl