Electronic Supplementary Information for

Room temperature synthesis of non-isocyanate polyurethanes (NIPUs) using highly reactive *N*-substituted 8-membered cyclic carbonates

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[6] Institute of Bioengineering and Nanotechnology, 31 Biopolis Way, Singapore 138669, Singapore

Content:

Part 1: ^{1}H and ^{13}C NMR Spectra

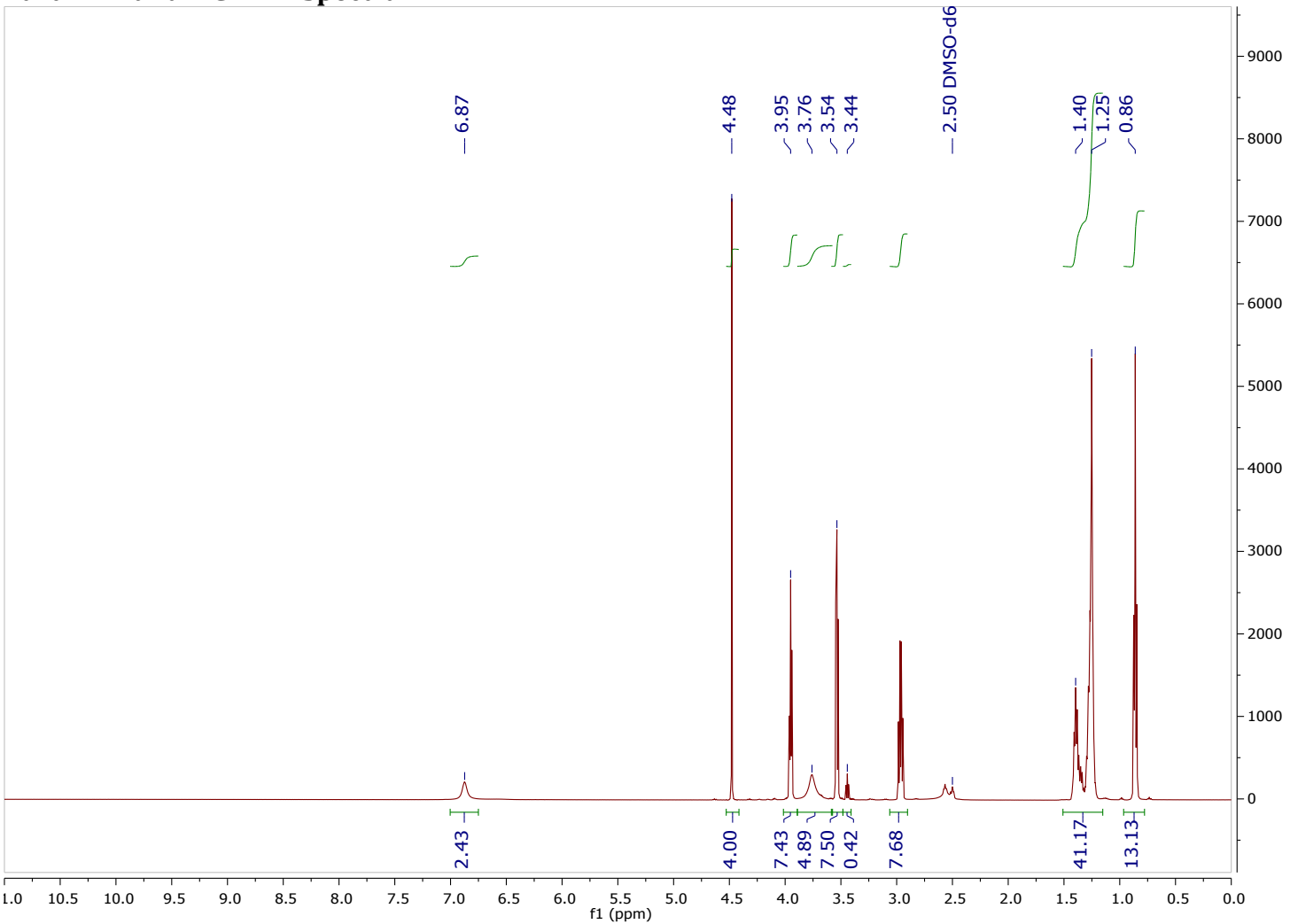


Figure 1S. ^{1}H NMR of ethylene carbonate (5-C) and hexylamine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (78.79% conversion)

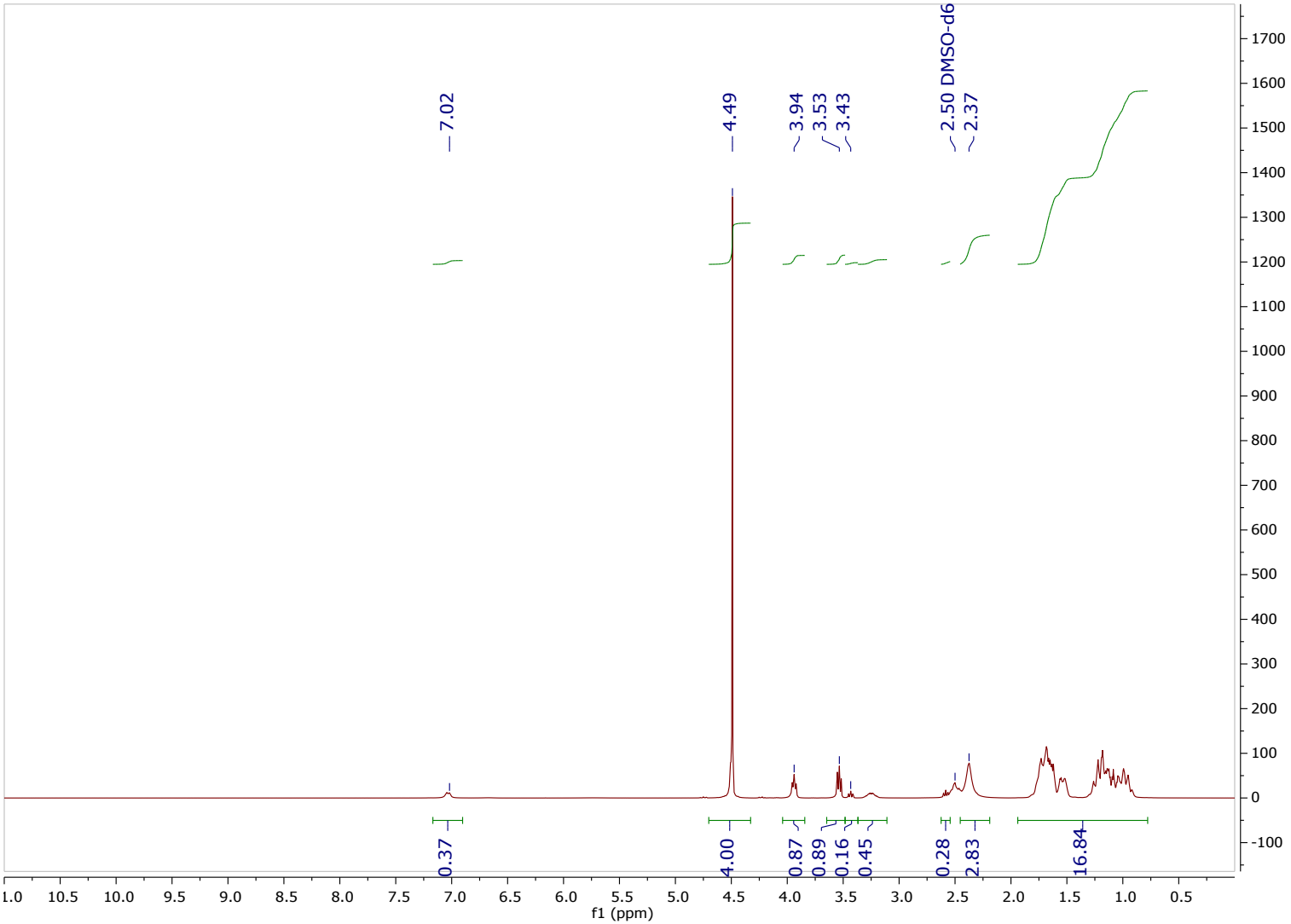


Figure 2S. ^{1}H NMR of 5-C and cyclohexylamine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (30.31% conversion)

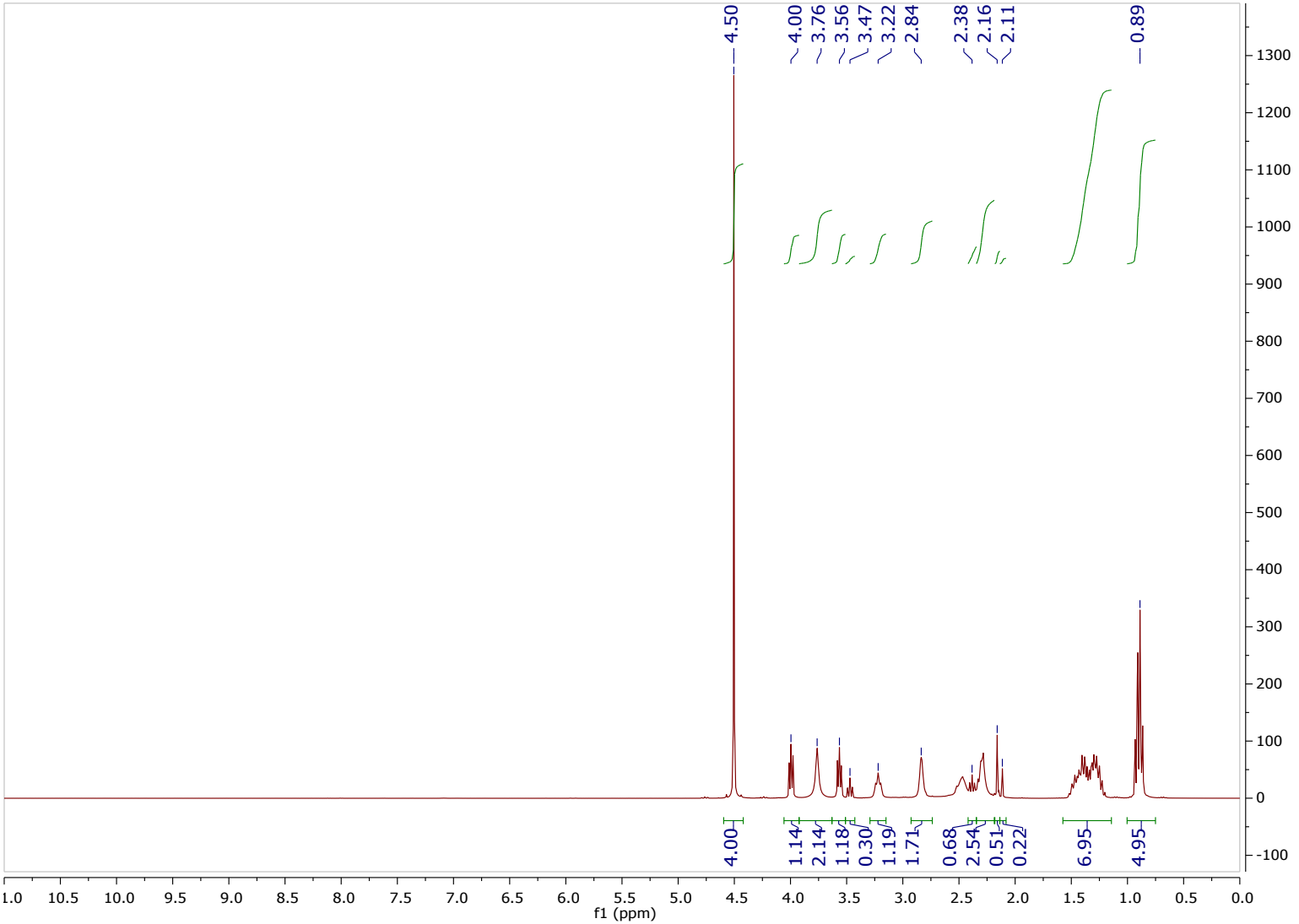


Figure 3S. ^{1}H NMR of 5-C and *N*-methylbutylamine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (36.31% conversion)

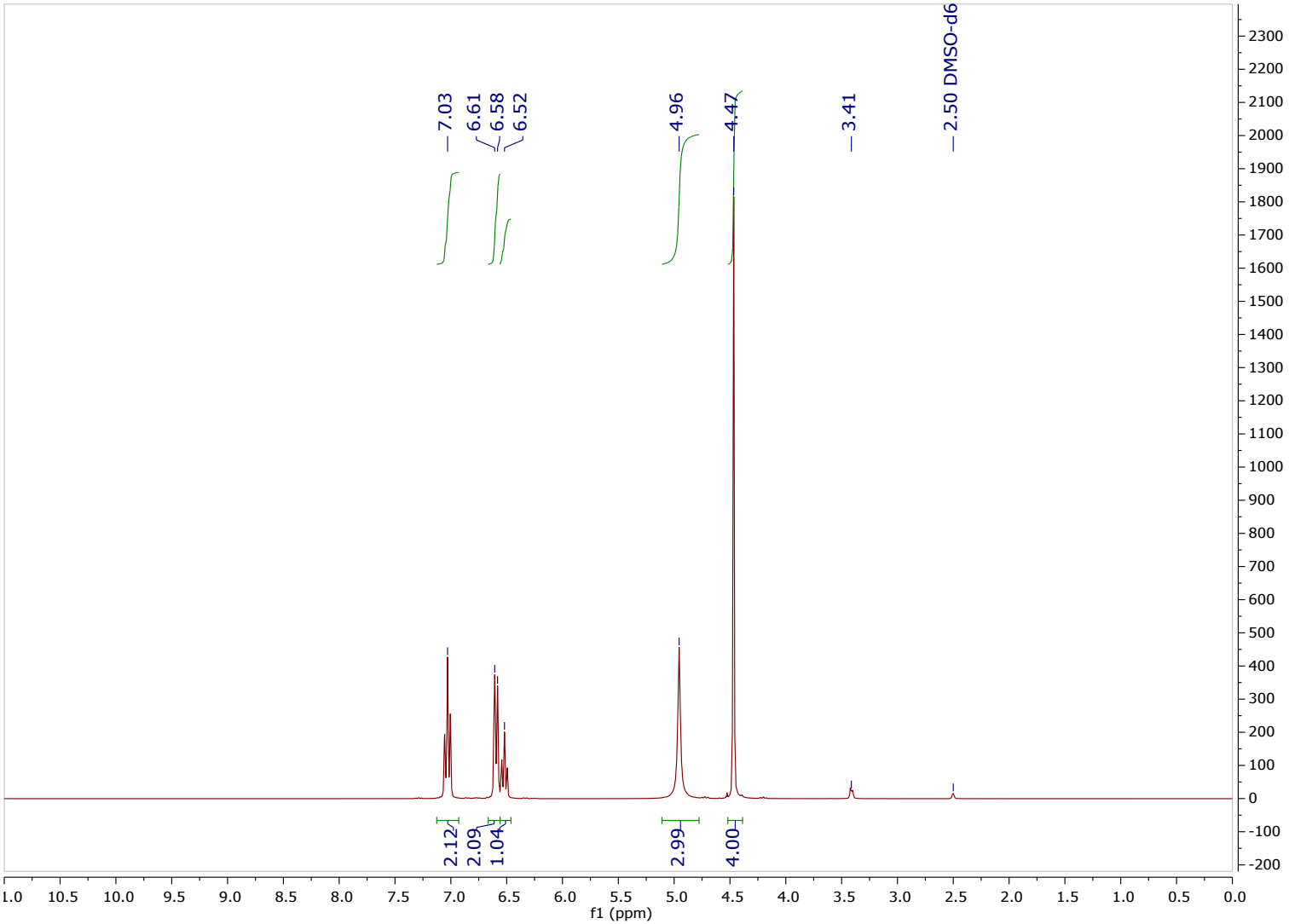


Figure 4S. ^{1}H NMR of ethylene carbonate (5-C) and aniline at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (0% conversion)

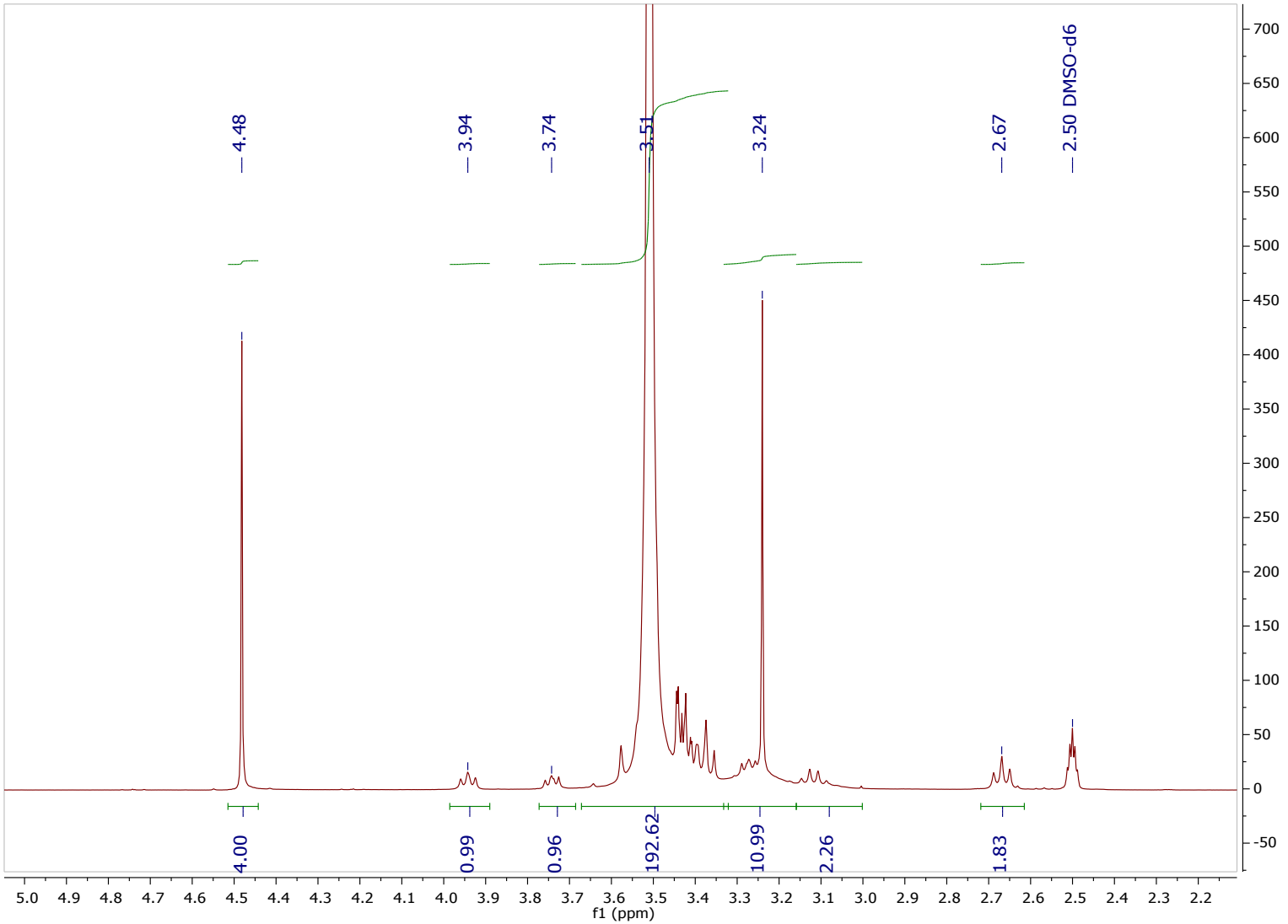


Figure 5S. ^{1}H NMR of ethylene carbonate (5-C) and PEG-amine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (33.33% conversion)

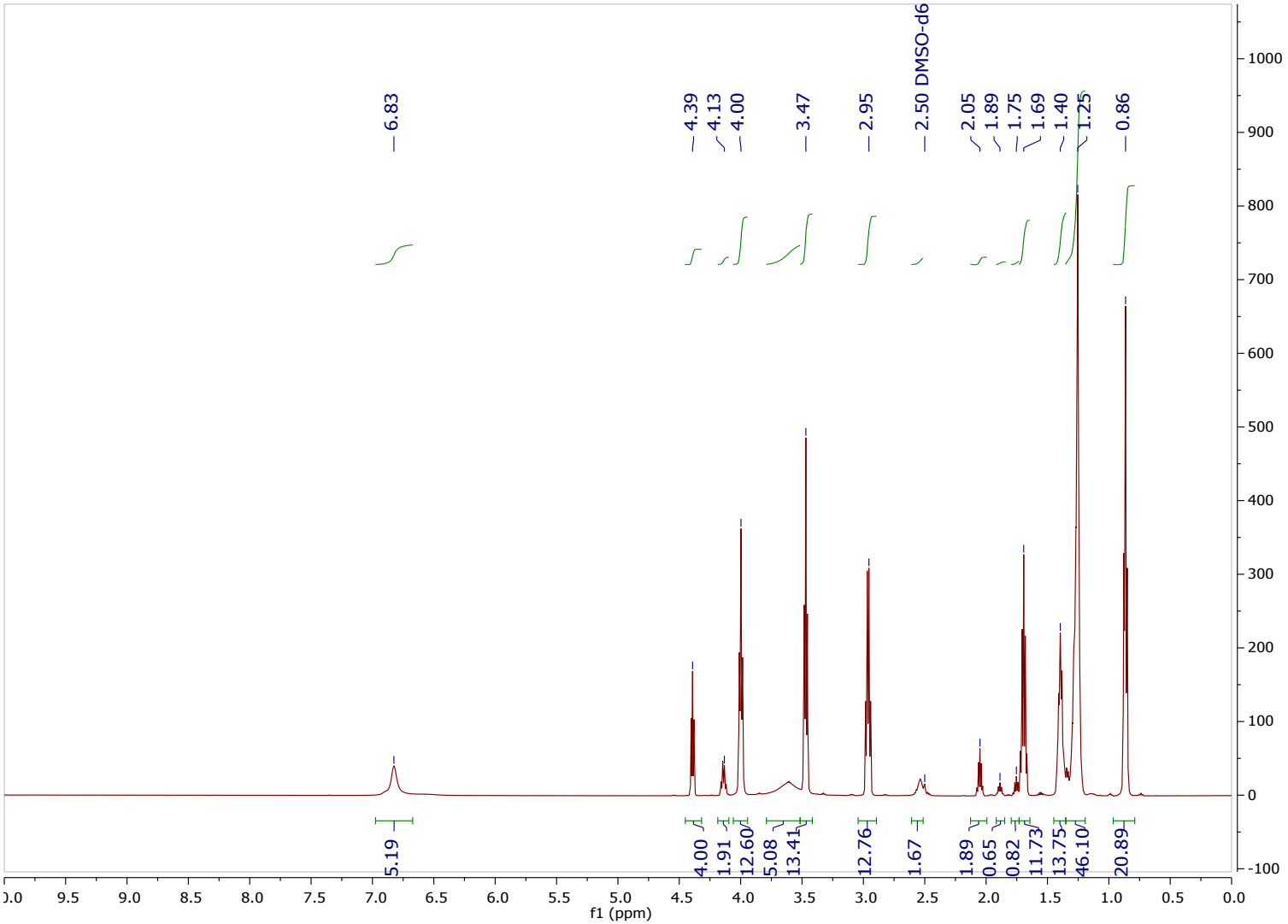


Figure 6S. ^{1}H NMR of 6-C and hexylamine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (86.30% conversion)

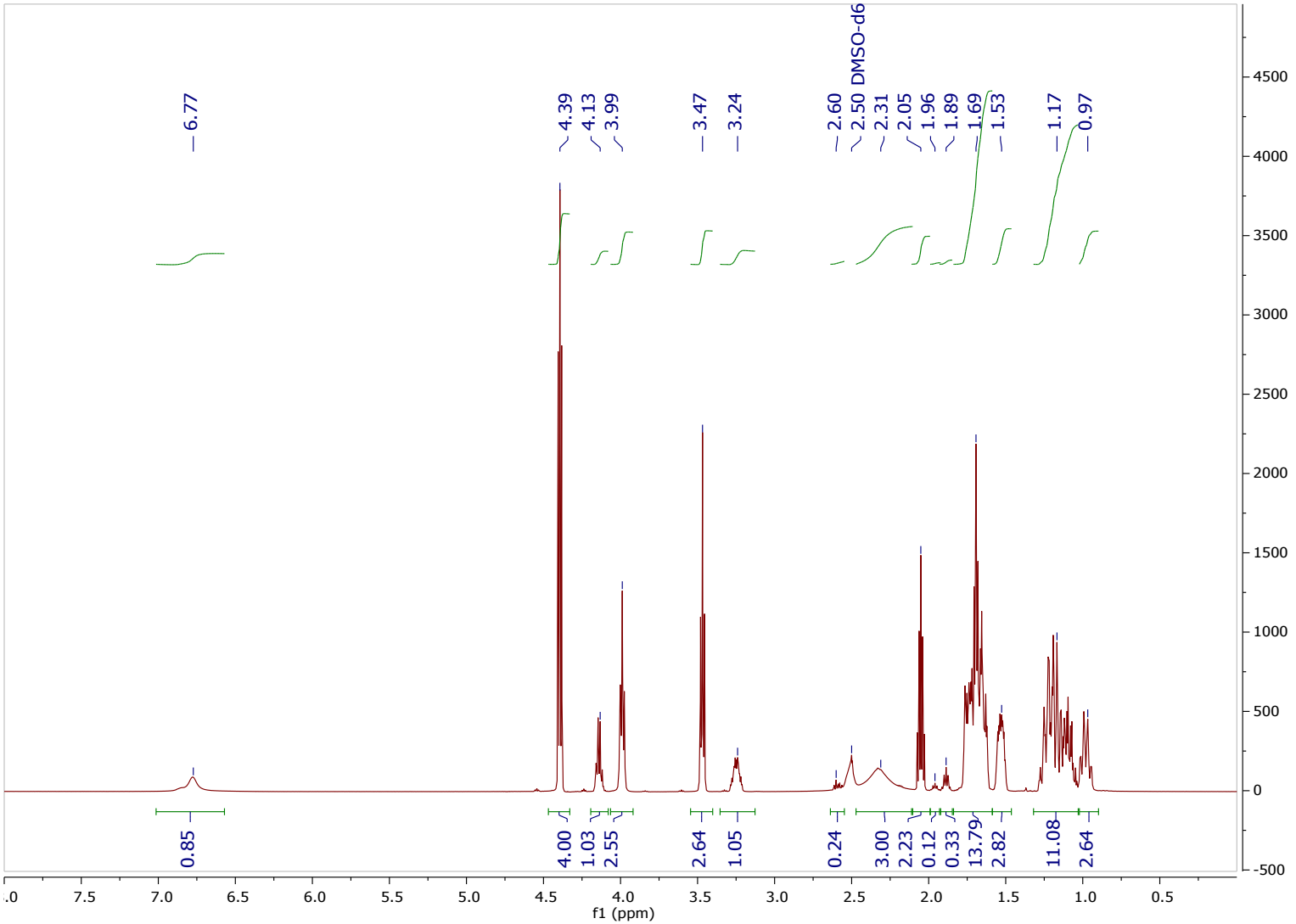


Figure 7S. ^{1}H NMR of 6-C and cyclohexylamine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (56.04% conversion)

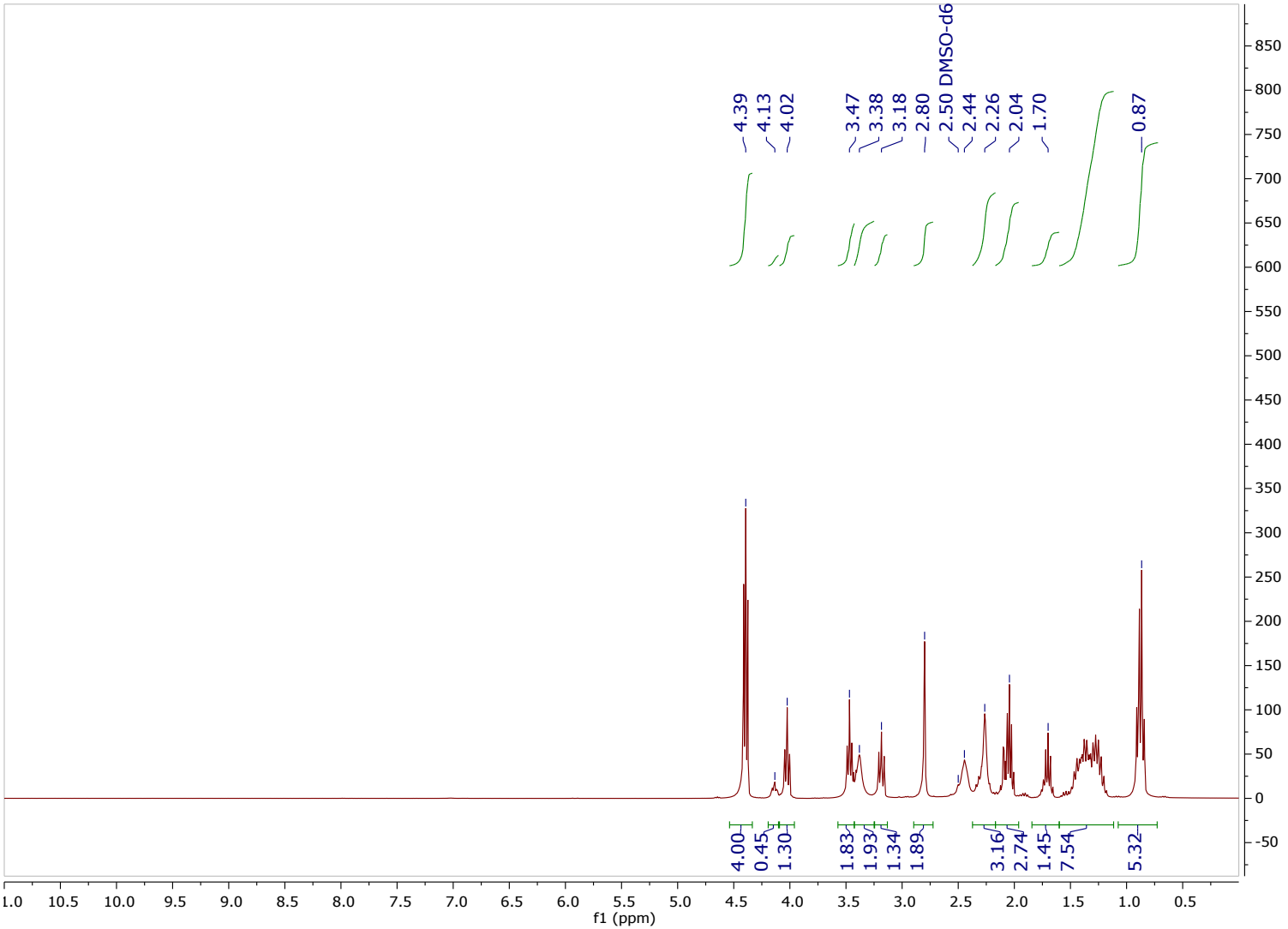


Figure 8S. ^{1}H NMR of 6-C and *N*-methylbutylamine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (39.39% conversion)

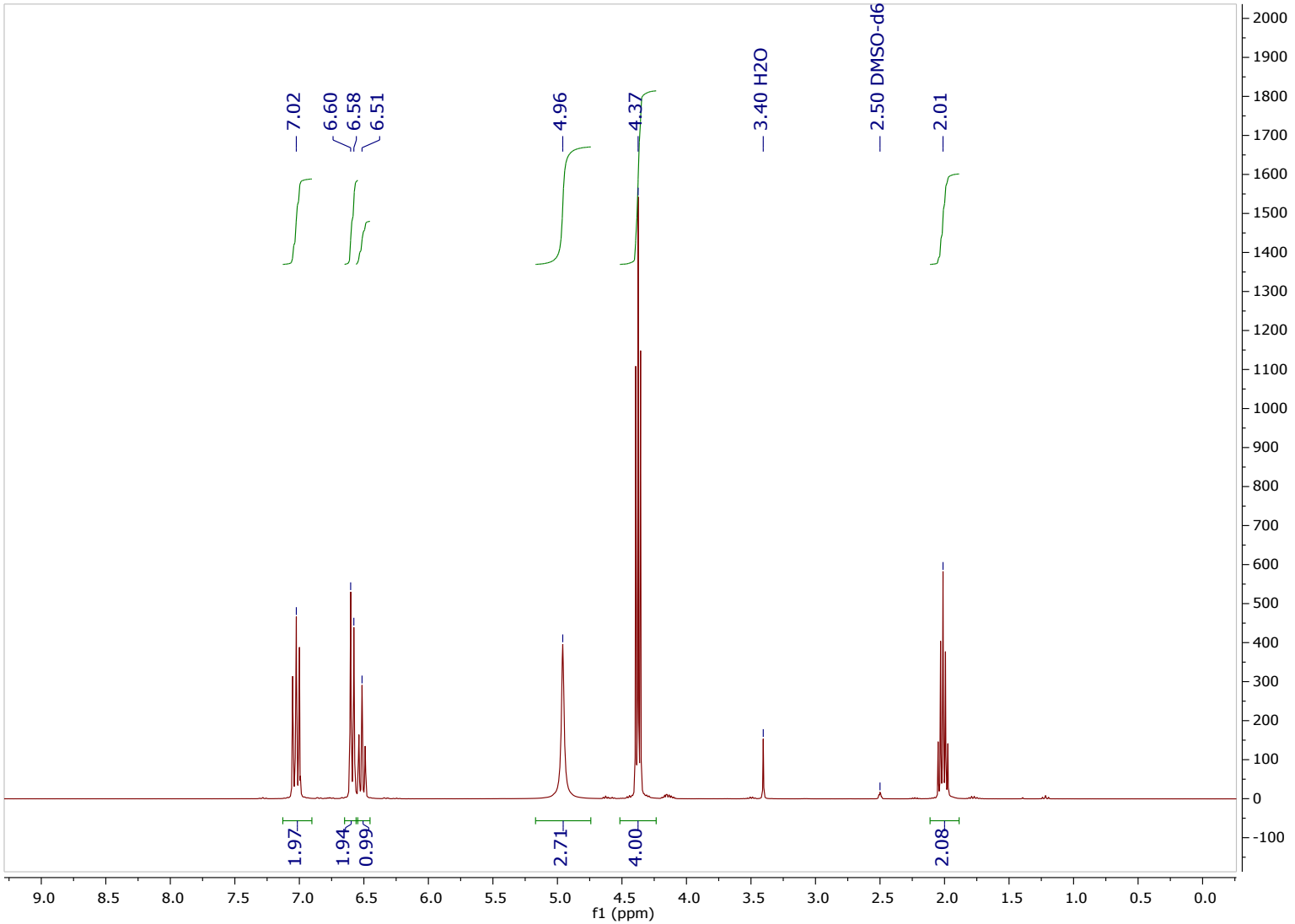


Figure 9S. ^{1}H NMR of 6-C and anilne at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (0% conversion)

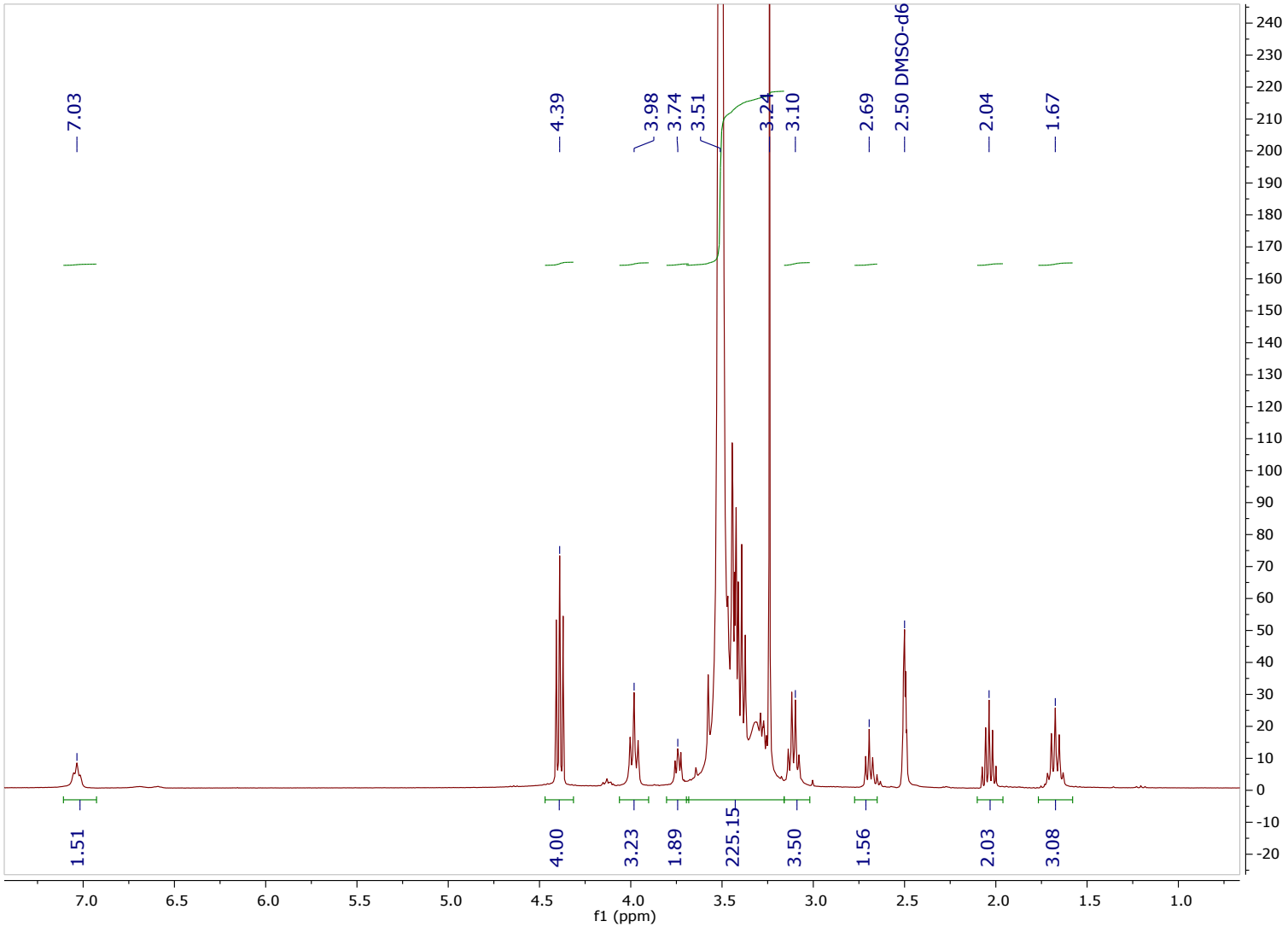


Figure 10S. ^{1}H NMR of 6-C and PEG-amine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (61.76% conversion)

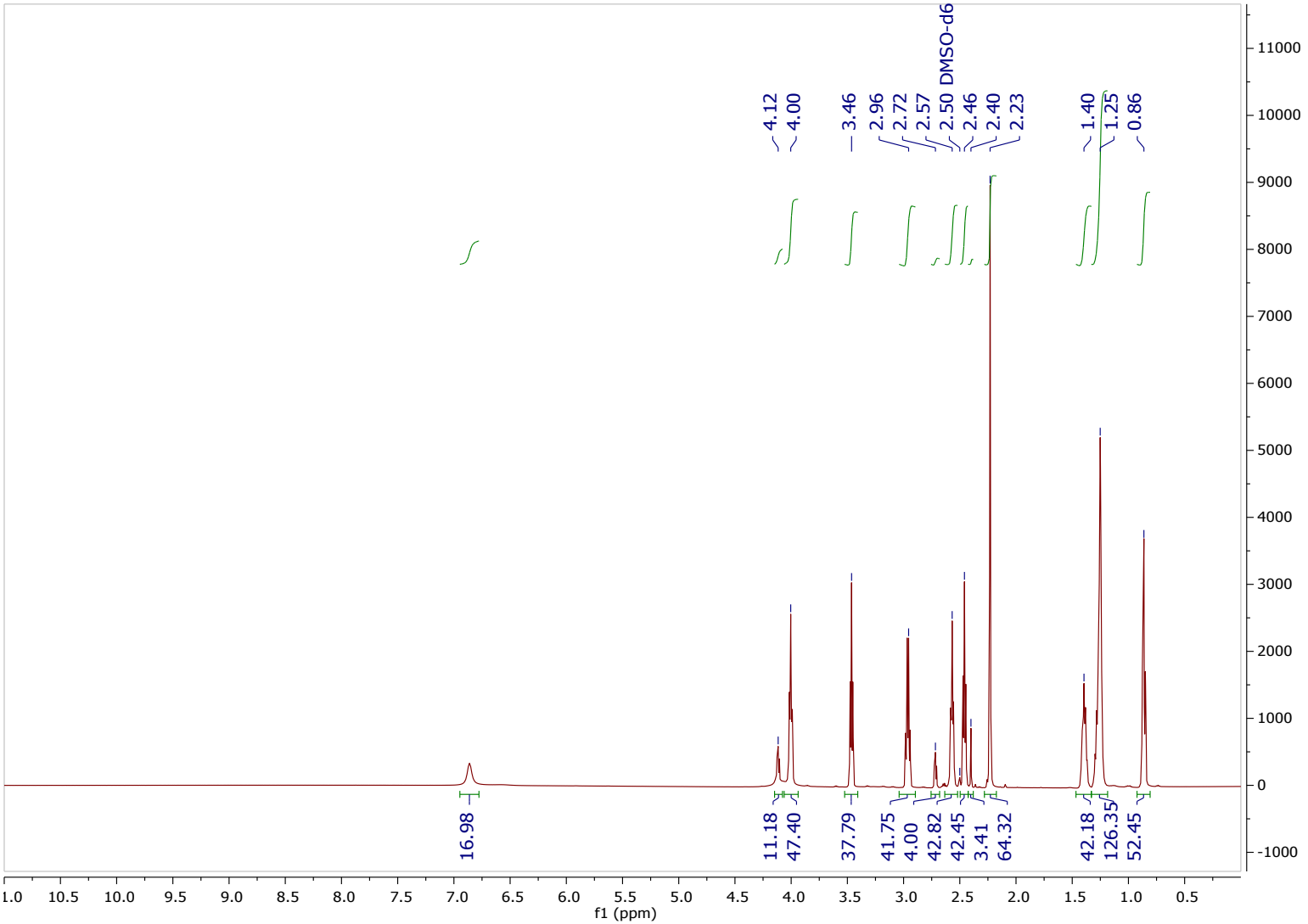


Figure 11S. ^{1}H NMR of *N*-8-C and hexylamine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (95.95% conversion)

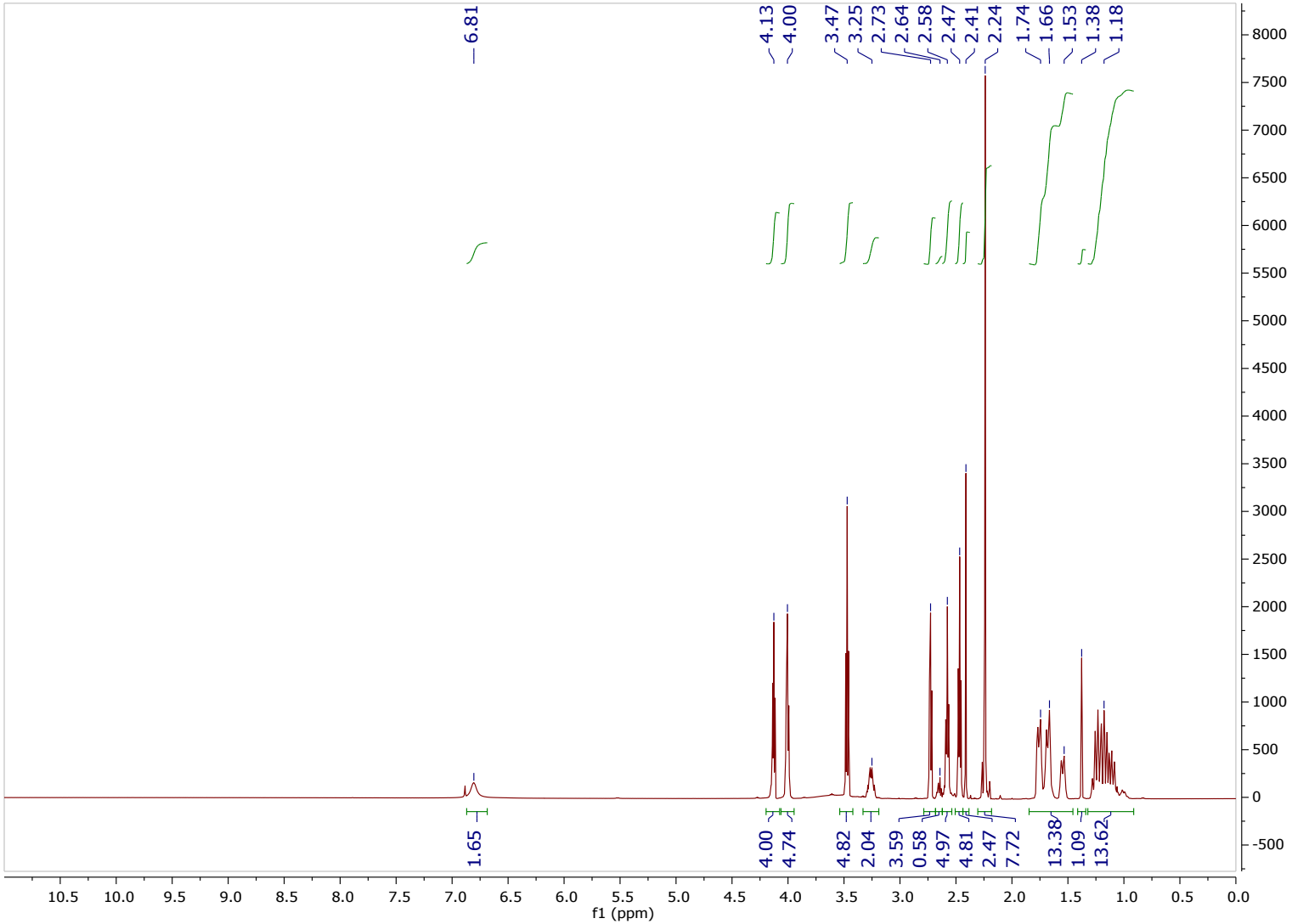


Figure 12S. ^{1}H NMR of *N*-8-C and cyclohexylamine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (70.33% conversion)

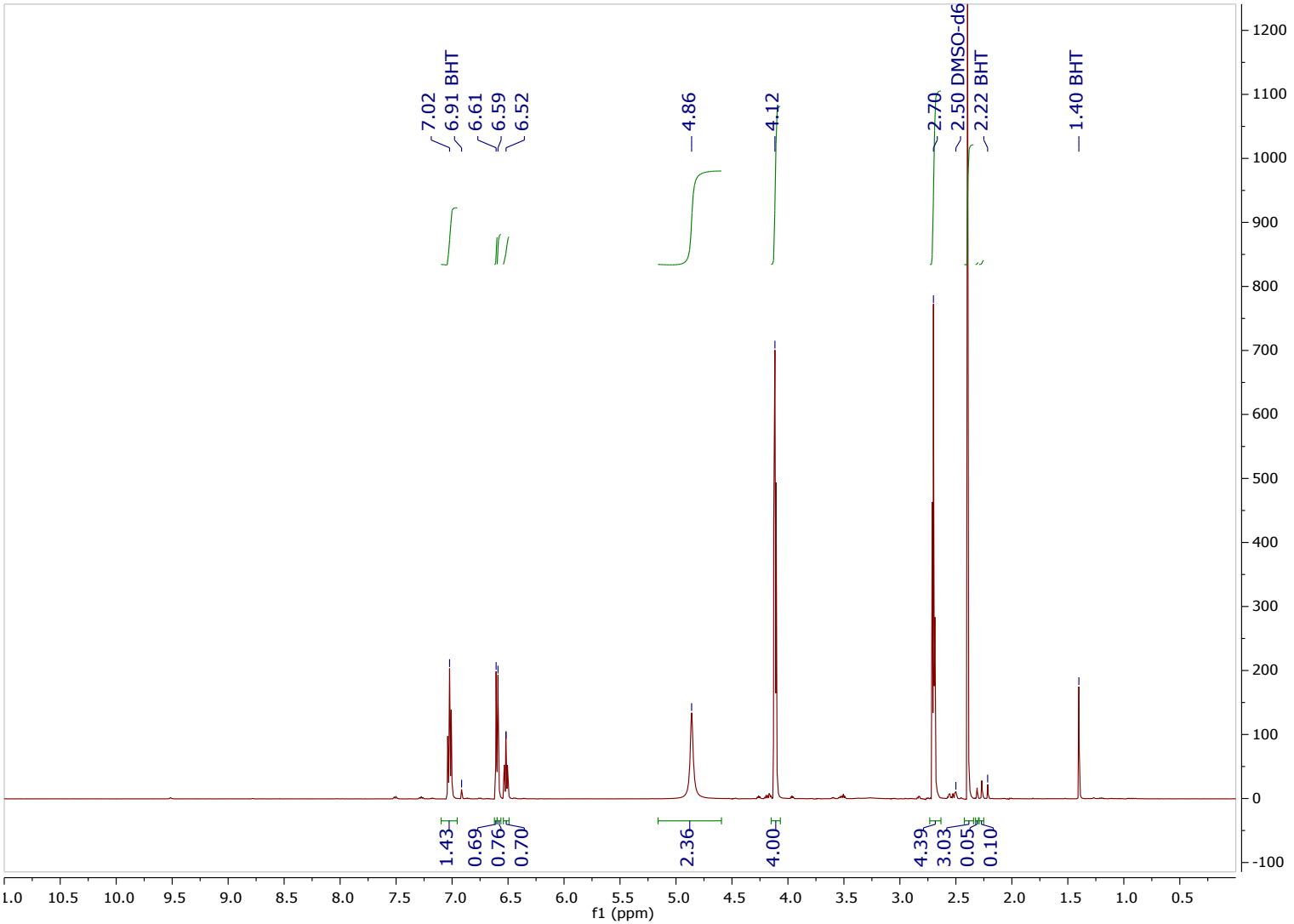


Figure 13S. ^{1}H NMR of *N*-8-C and aniline at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (0% conversion)

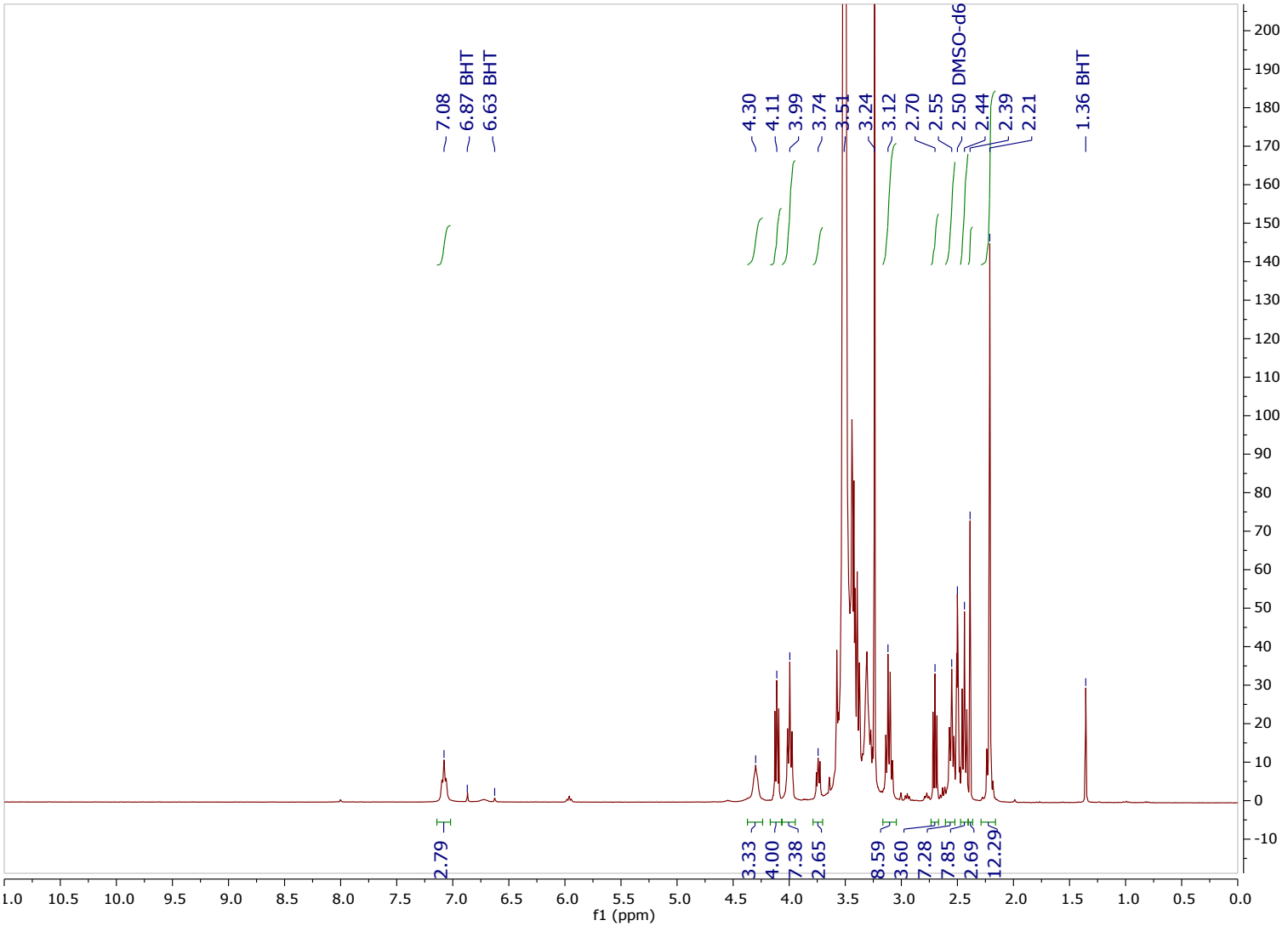


Figure 14S. ^{1}H NMR of *N*-8-C and PEG-amine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (78.67% conversion)

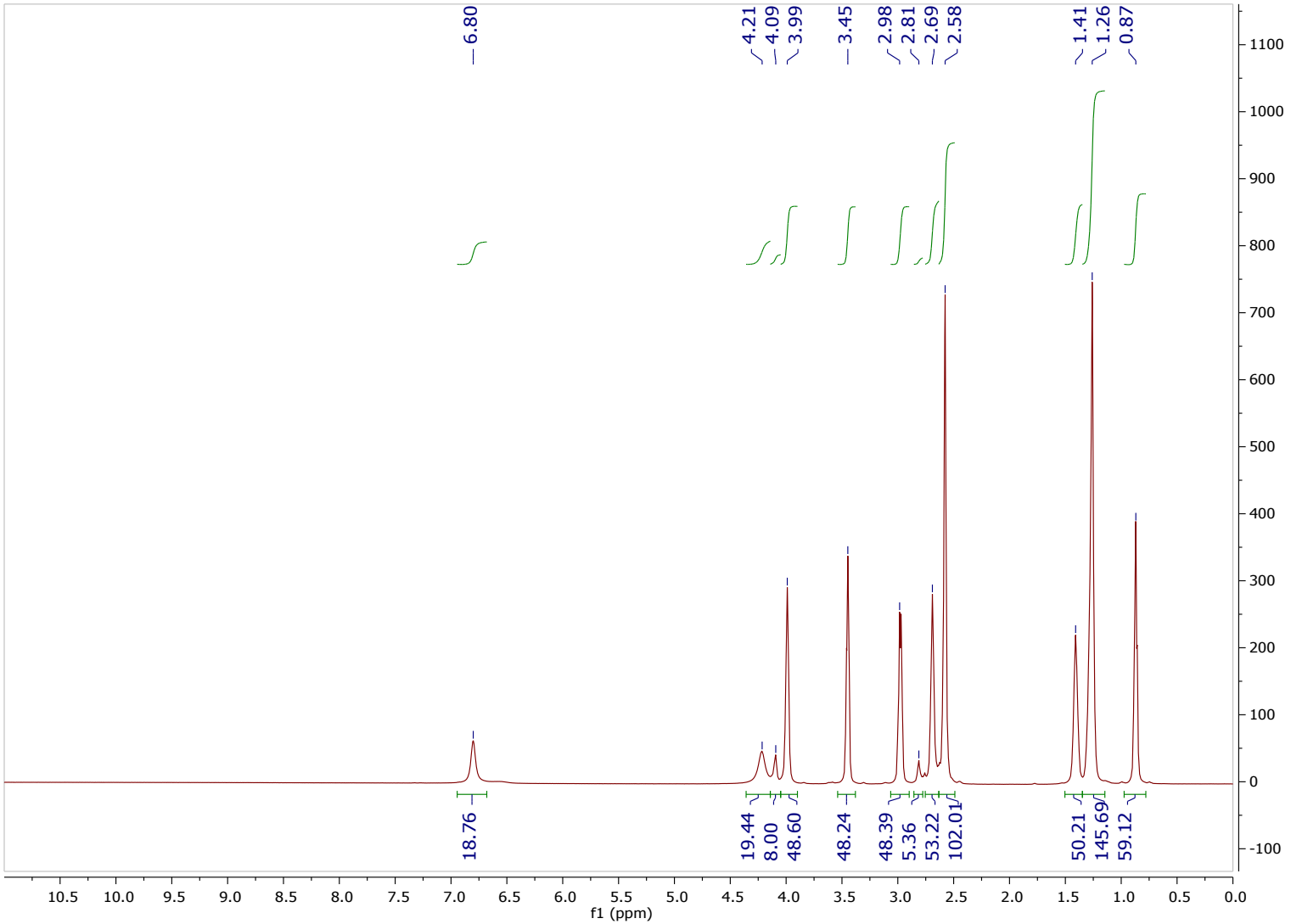


Figure 15S. ^{1}H NMR of (bis) *N*-8-C and hexylamine at 50 °C for 6 h. Solvent used in NMR: d_6-DMSO. (92.40% conversion)

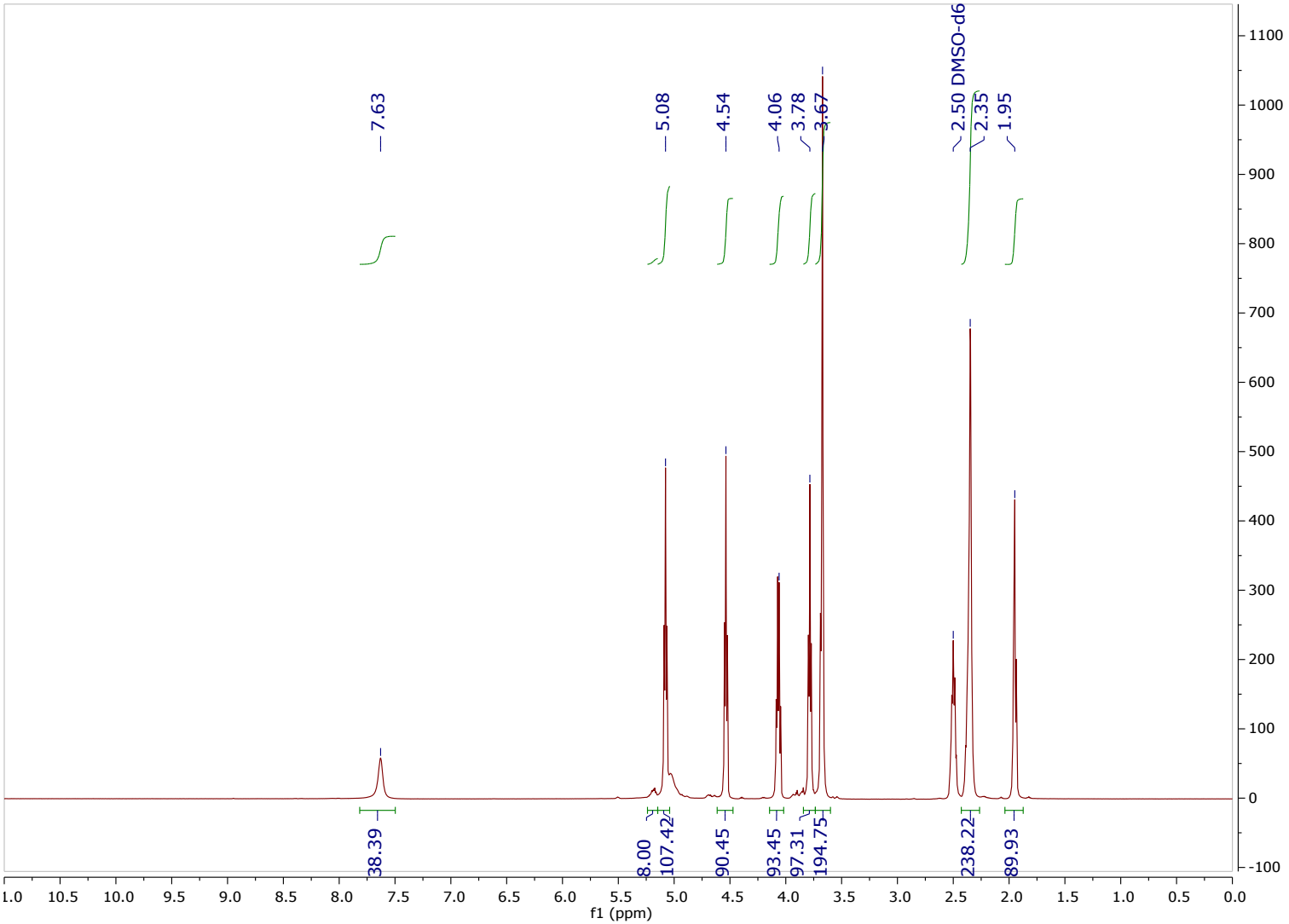


Figure 16S. ^{1}H NMR of (bis) *N*-8-C and hexylamine at 80 °C for 6 h. Solvent used in NMR: d_6-DMSO. (96.41% conversion)

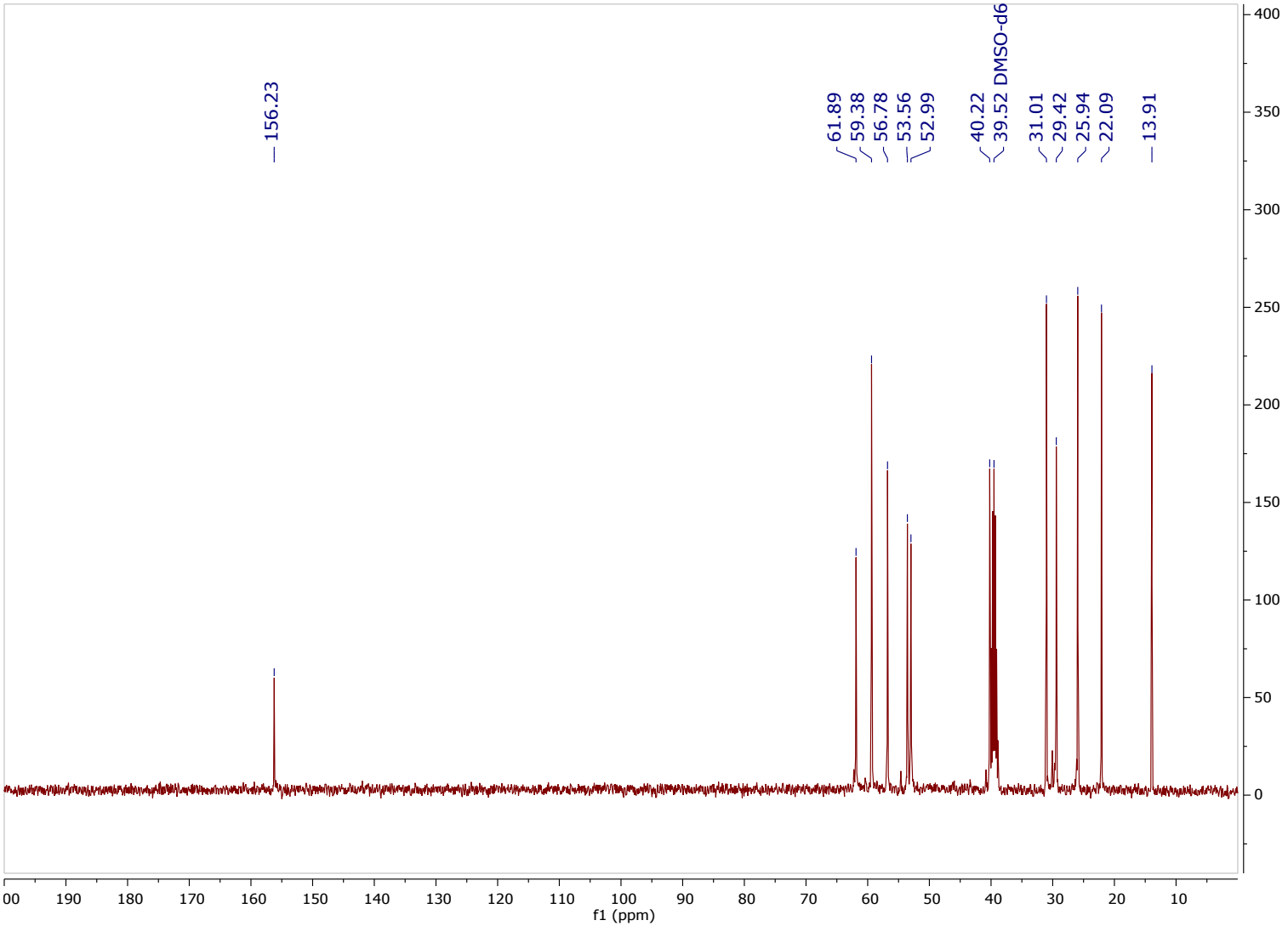


Figure 17S. ^{13}C NMR of (bis) *N*-8-C and hexylamine at 80 °C for 6 h. Solvent used in NMR: d_6-DMSO.

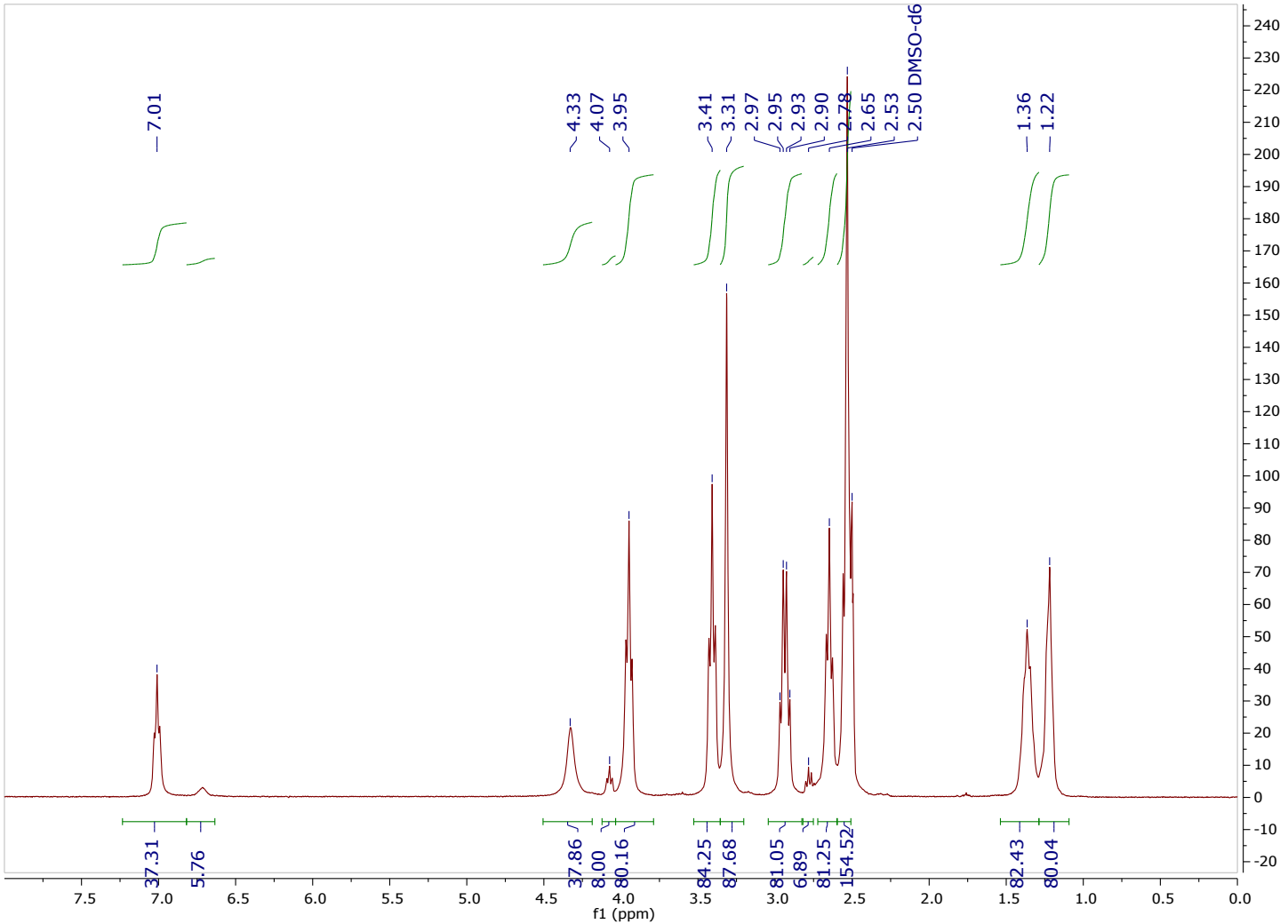


Figure 18S. Crude ^{1}H NMR of polymerization with (bis) *N*-8-C and hexamethylenediamine in d_6-DMSO at 25 °C for 24 h (95.25% conversion) (NIPU1).

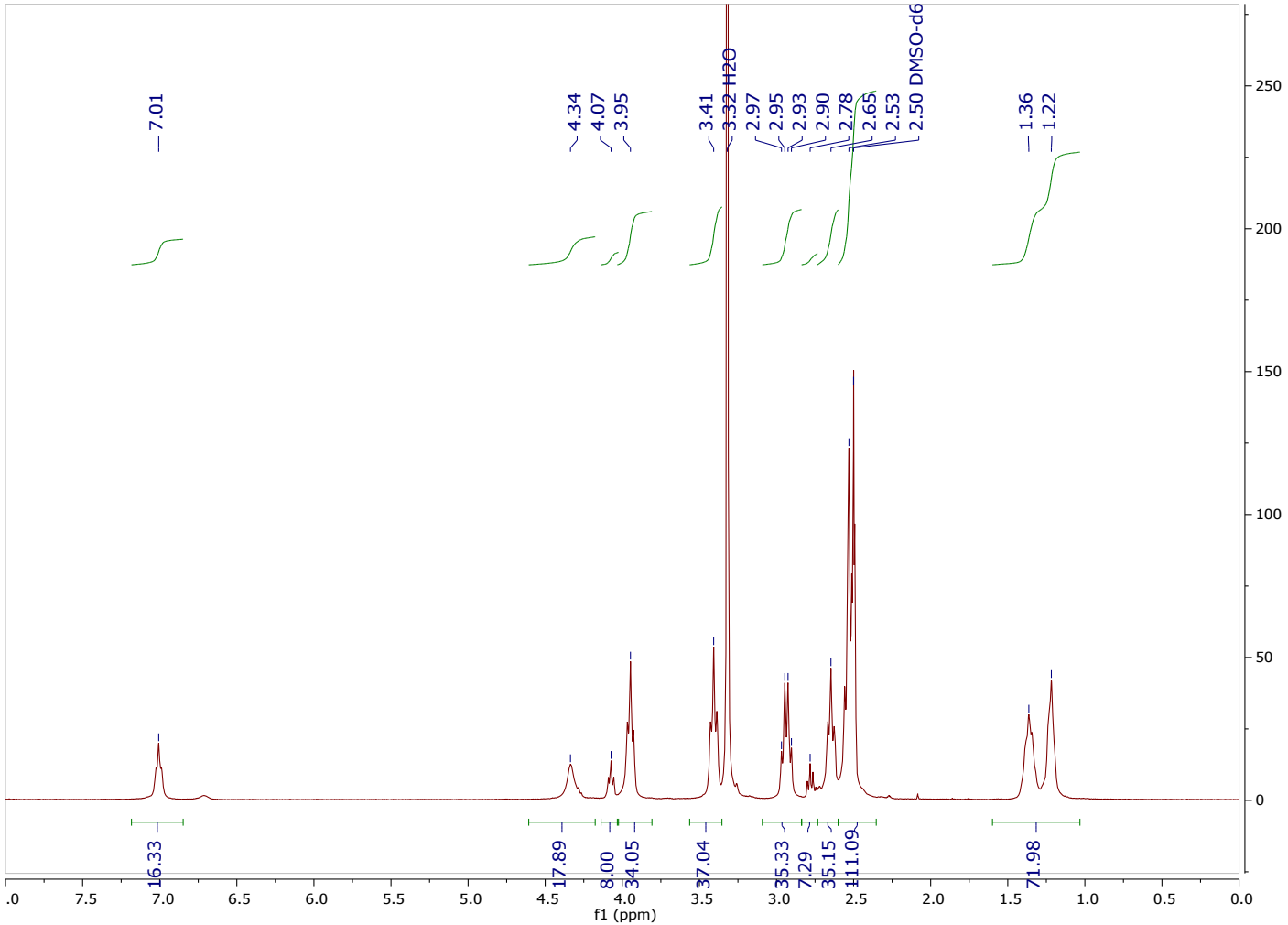


Figure 19S. Crude ^{1}H NMR of polymerization with (bis) *N*-8-C and hexamethylenediamine in d_6-DMSO at 50 °C for 24 h. (89.49% conversion)(NIPU2)

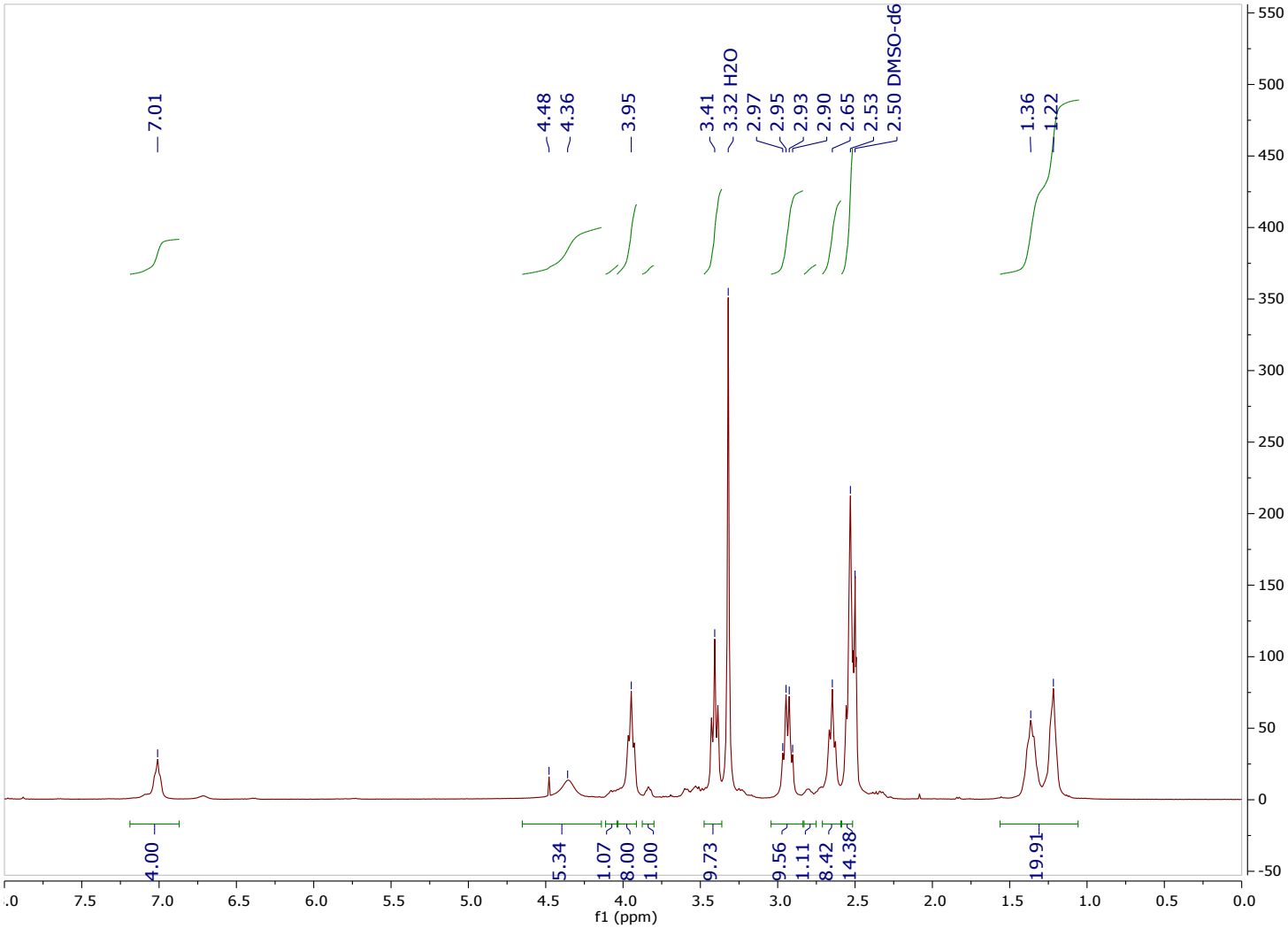


Figure 20S. Crude ^{1}H NMR of polymerization with (bis) *N*-8-C and hexamethylenediamine in d_6-DMSO at 80 °C for 24 h. (93.52% conversion)(NIPU3)

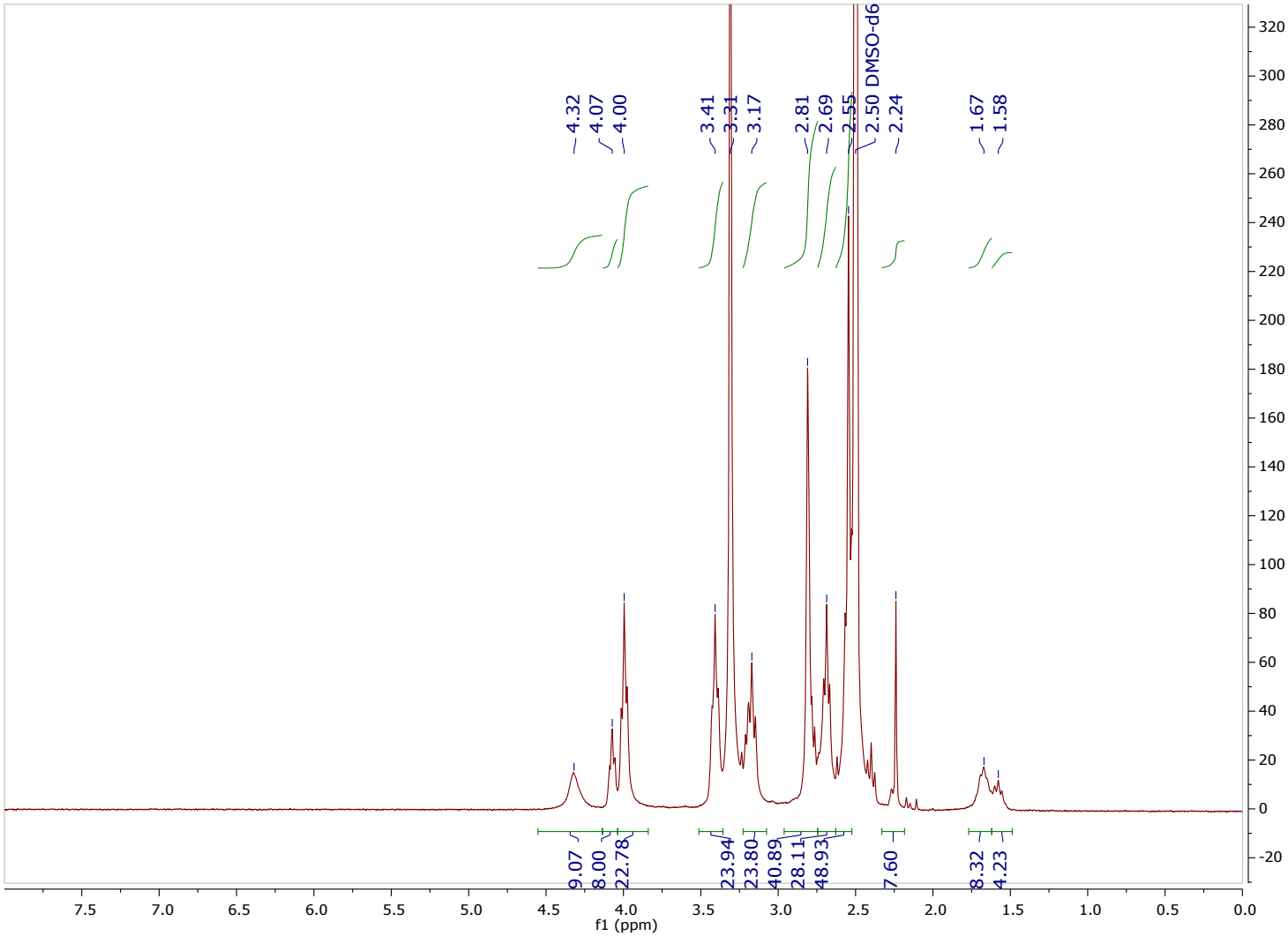


Figure 21S. Crude ^{1}H NMR of polymerization with (bis) *N*-8-C and *N,N'*-dimethyl-1,3-propanediamine in d_6-DMSO at 25 °C for 24 h. (85.06% conversion) (NIPU5)

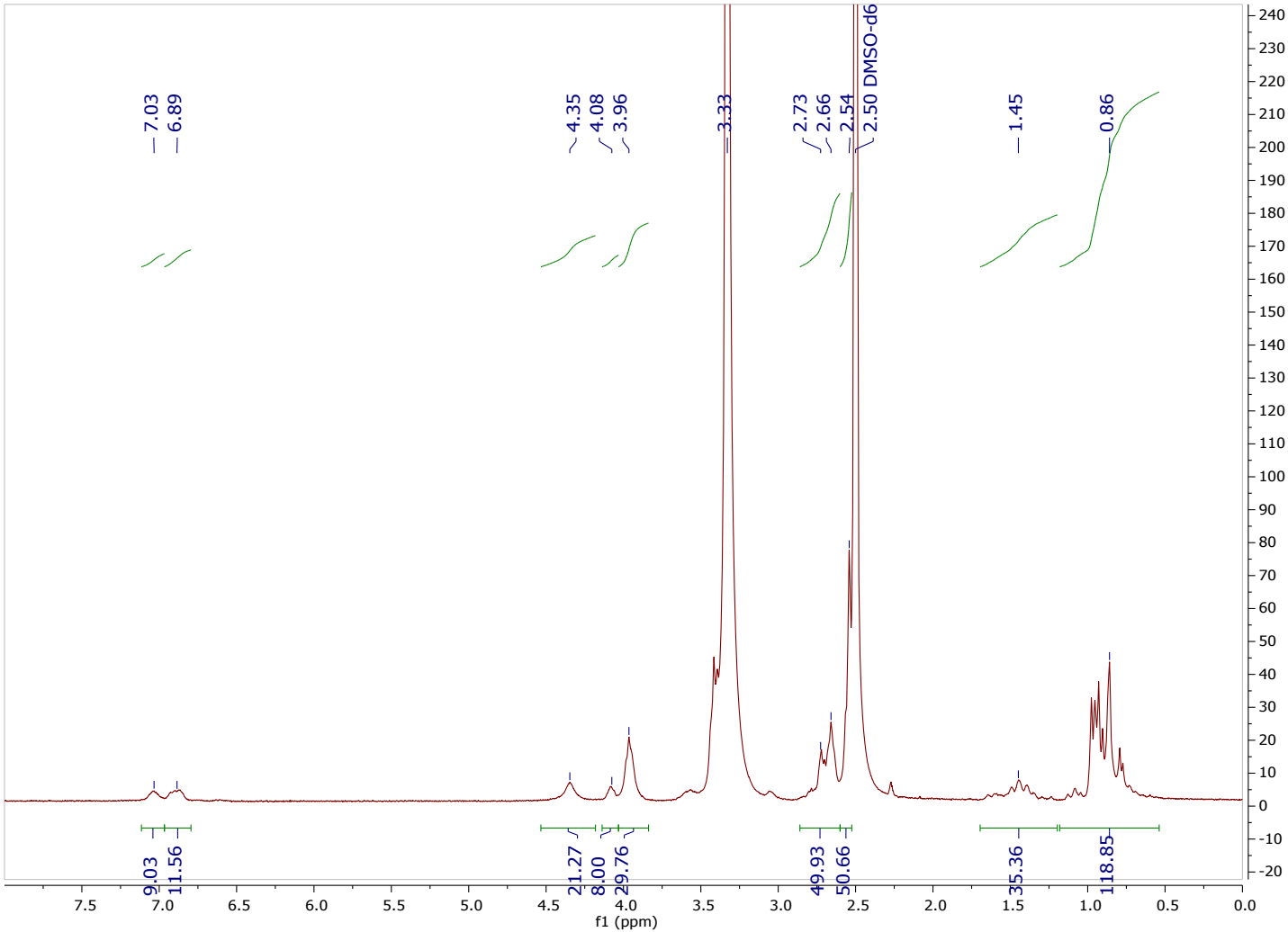


Figure 22S. Crude ^{1}H NMR of polymerization with *N*-8-C and 5-amino-1,3,3-trimethylcyclohexanemethylamine in d_6-DMSO at 25 °C for 24 h. (88.15% conversion)(NIPU6)

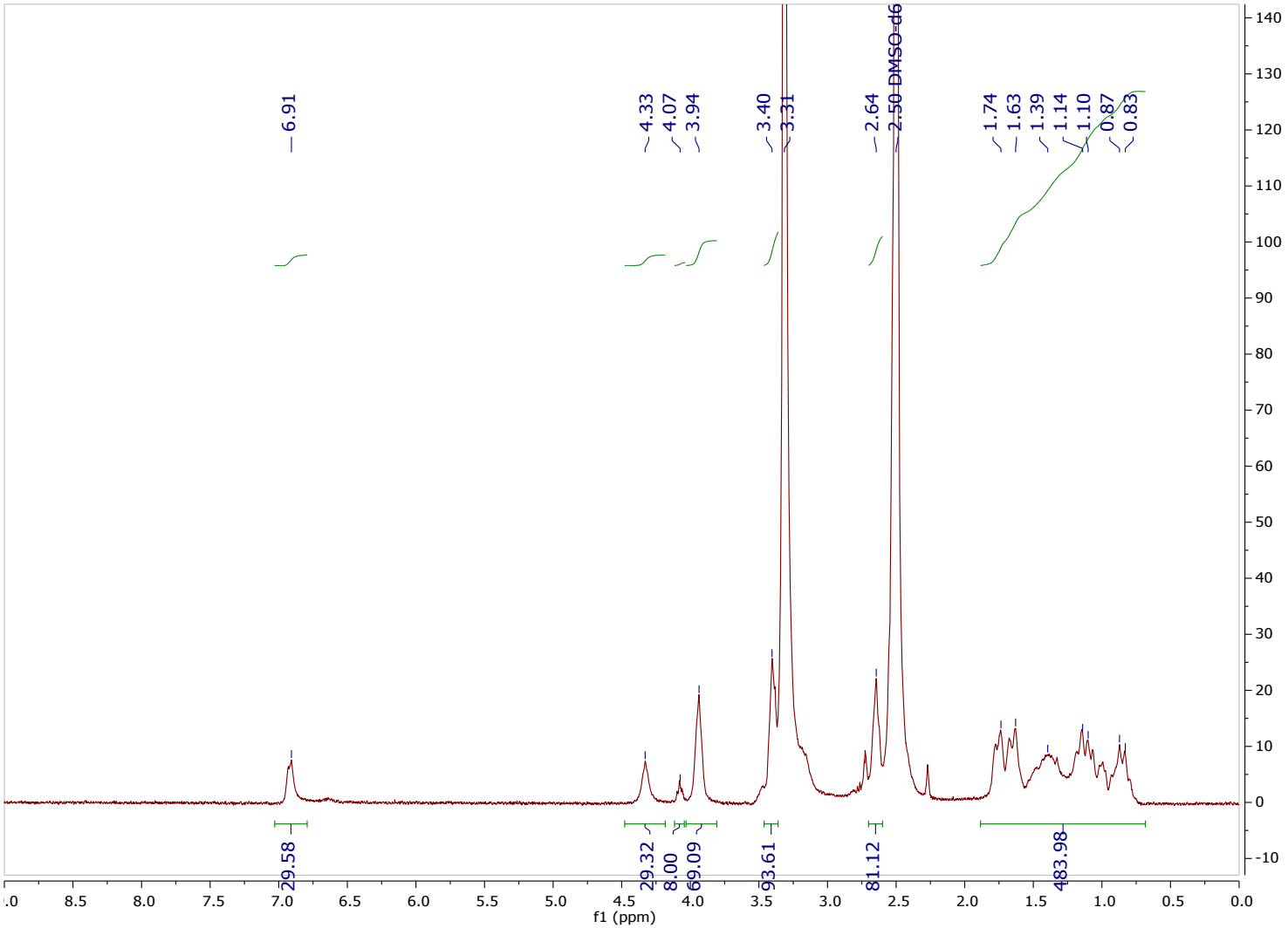


Figure 23S. Crude ^{1}H NMR of polymerization with (bis) *N*-8-C and 4,4-methylenebis(cyclohexylamine) in d_6-DMSO at 25 °C for 24 h. (94.53% conversion) (NIPU7)

Part 2. Kinetic study data

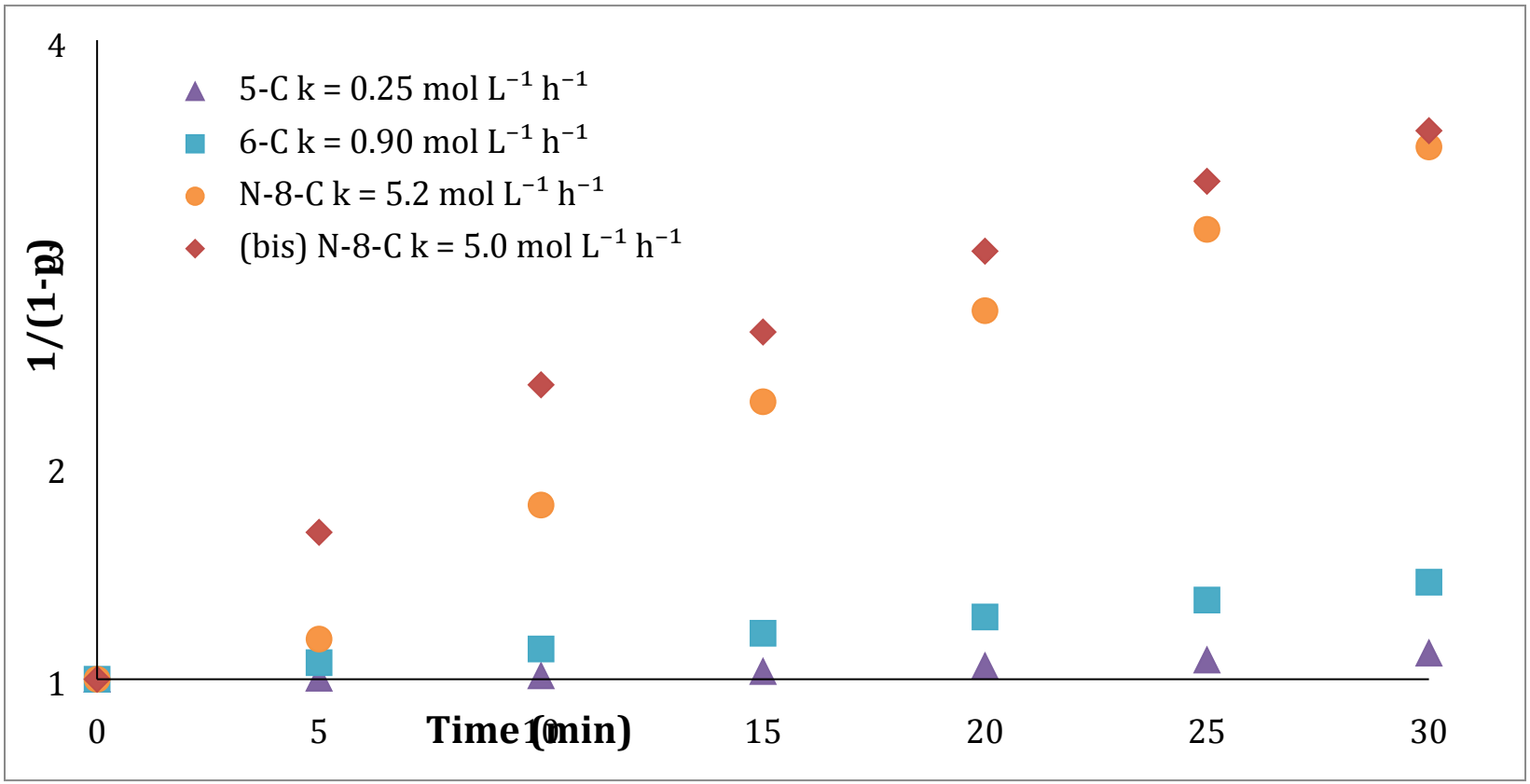


Figure 24S. Kinetic study of 5-C, 6-C, *N*-8-C, and (bis) *N*-8-C with hexylamine at 50 °C in d_6-DMSO.

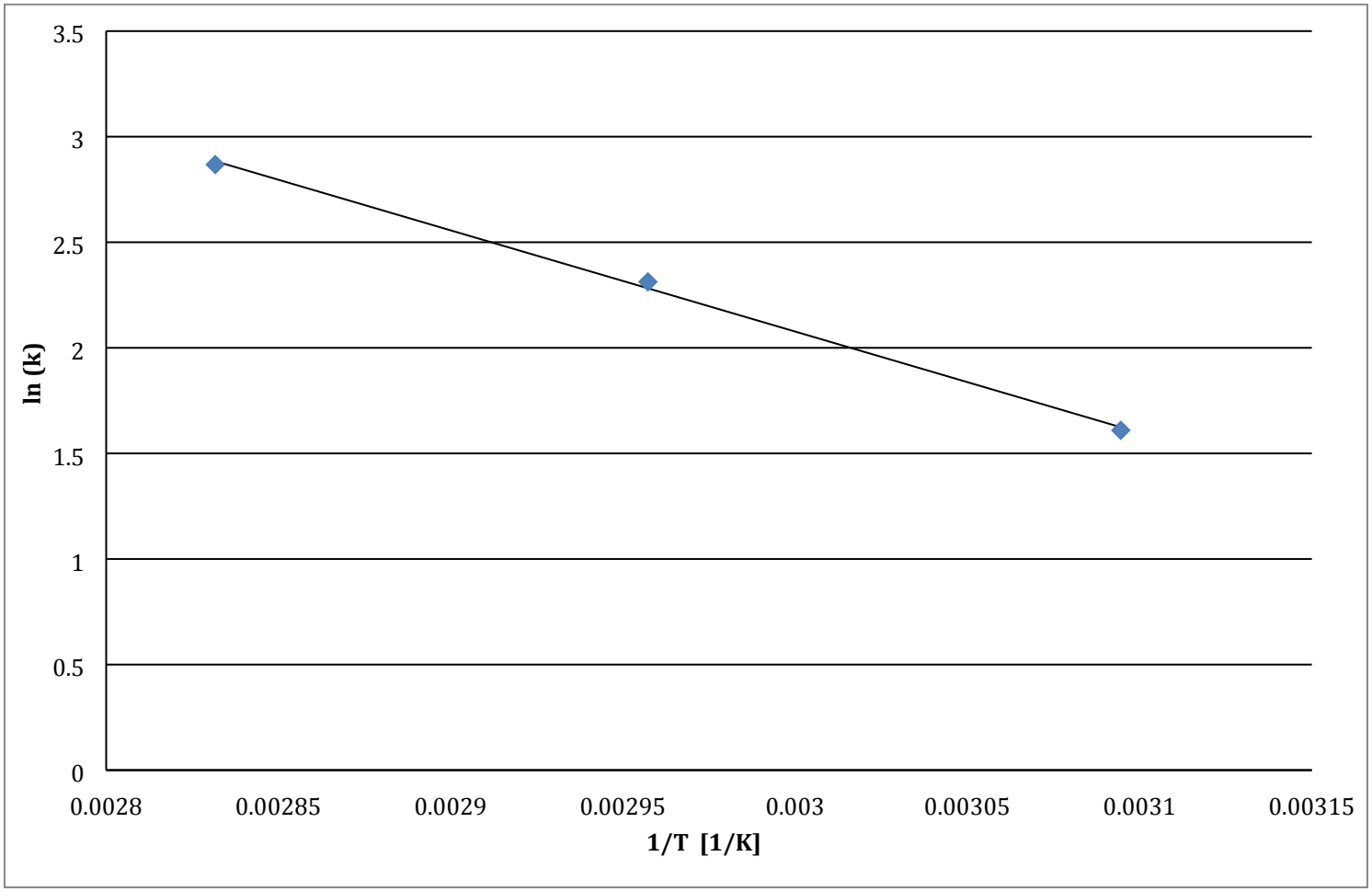


Figure 25S. Arrhenius plot used to determine the E_a (39.8 kJ mol^{-1}) of *N*-8-C.

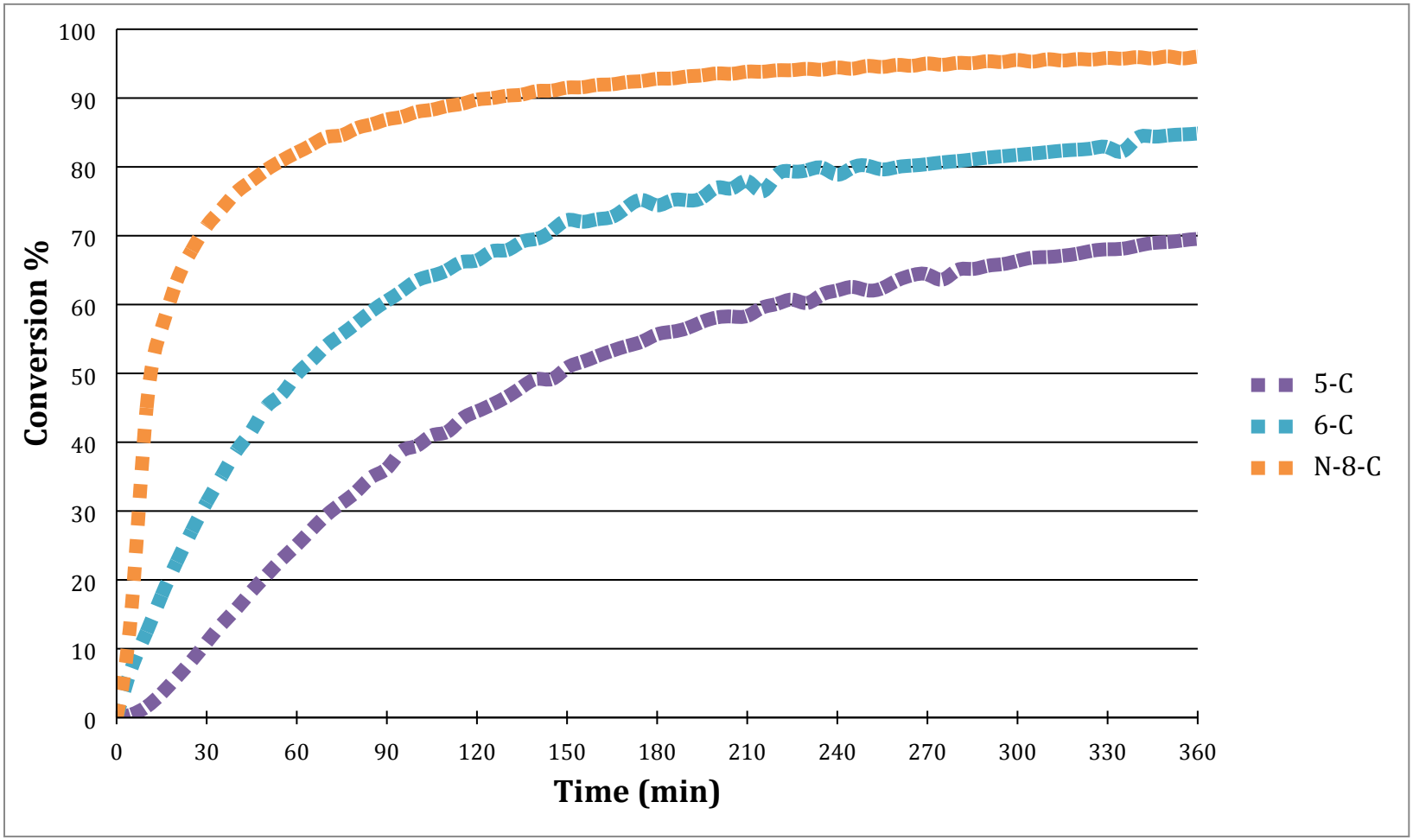


Figure 26S. Plot of conversion (%) vs. time (min) of the kinetic studies with different cyclic carbonates with hexylamine in d_6-DMSO at 50 °C.

Part 3: FTIR-ATR spectra

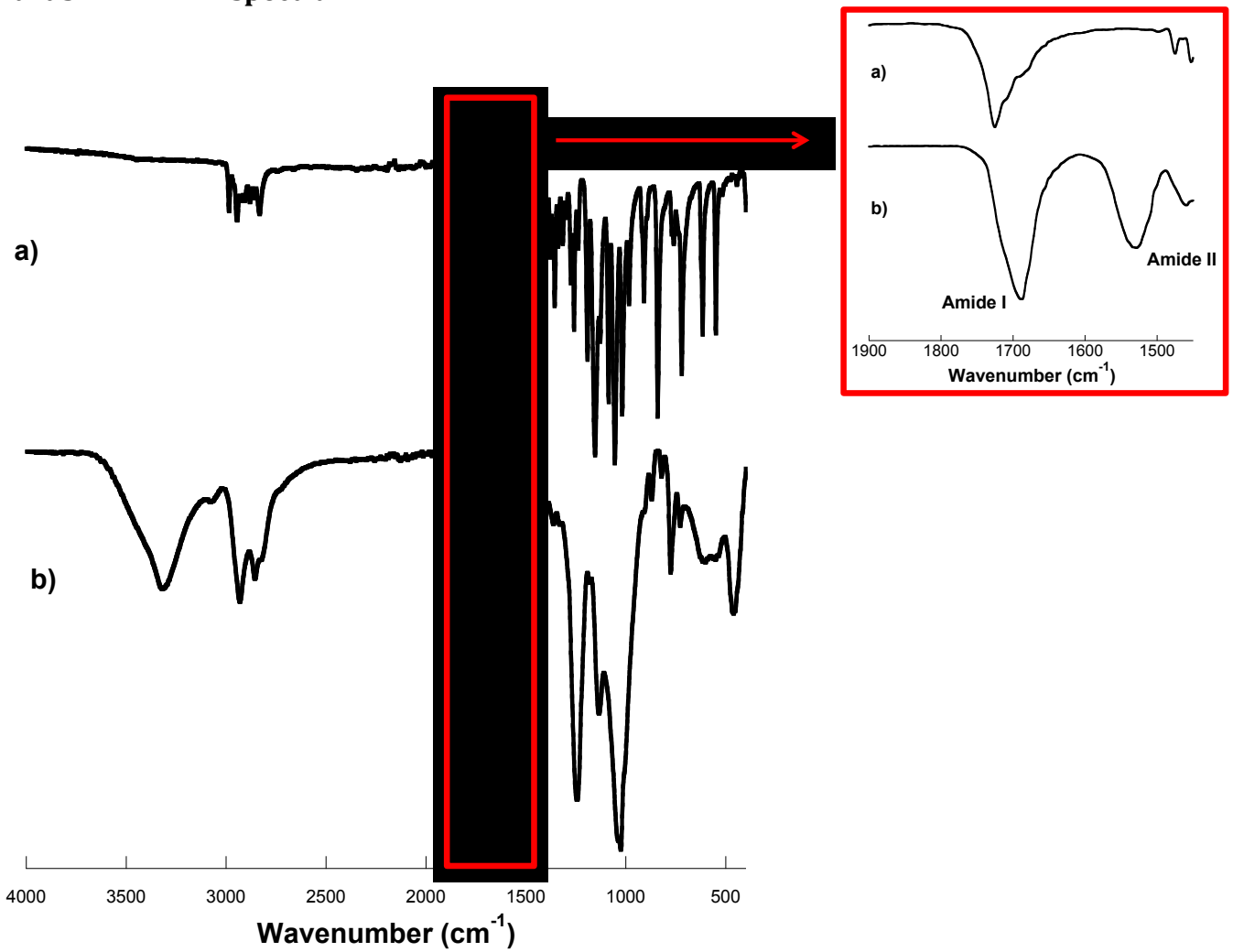


Figure 27S. FTIR-ATR spectra of (a) (bis) *N*-8-C monomer and (b) lyophilized NIPU1.

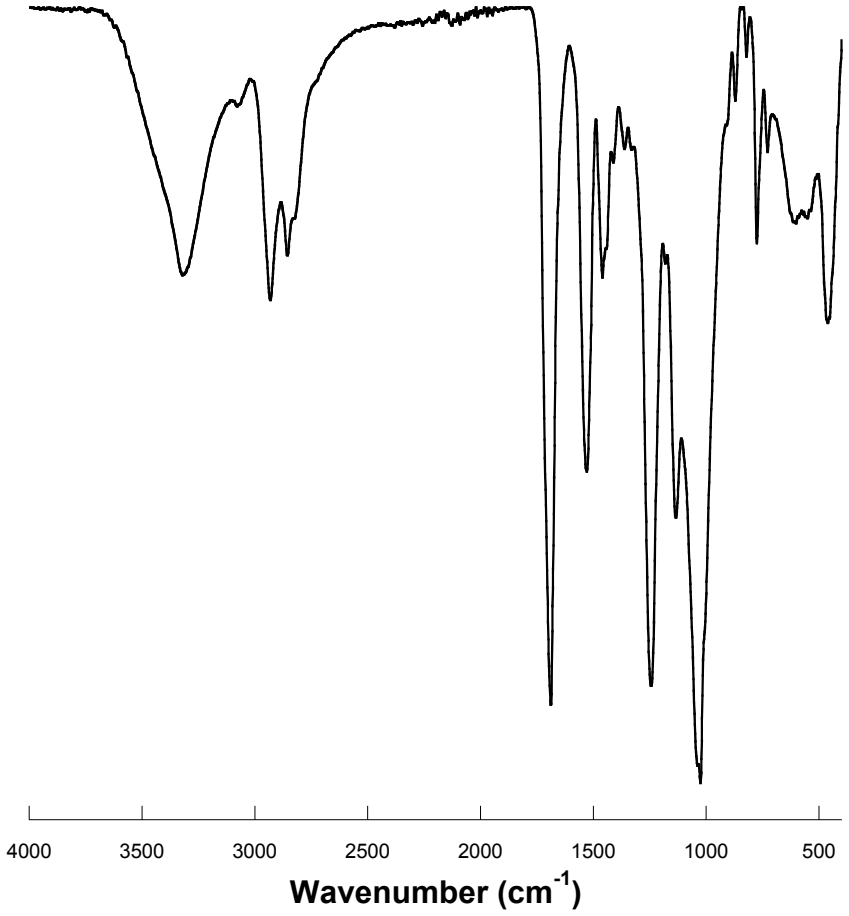


Figure 28S. FTIR-ATR spectra of (a) (bis) *N*-8-C monomer and (b) lyophilized NIPU4

Part 4: GPC data

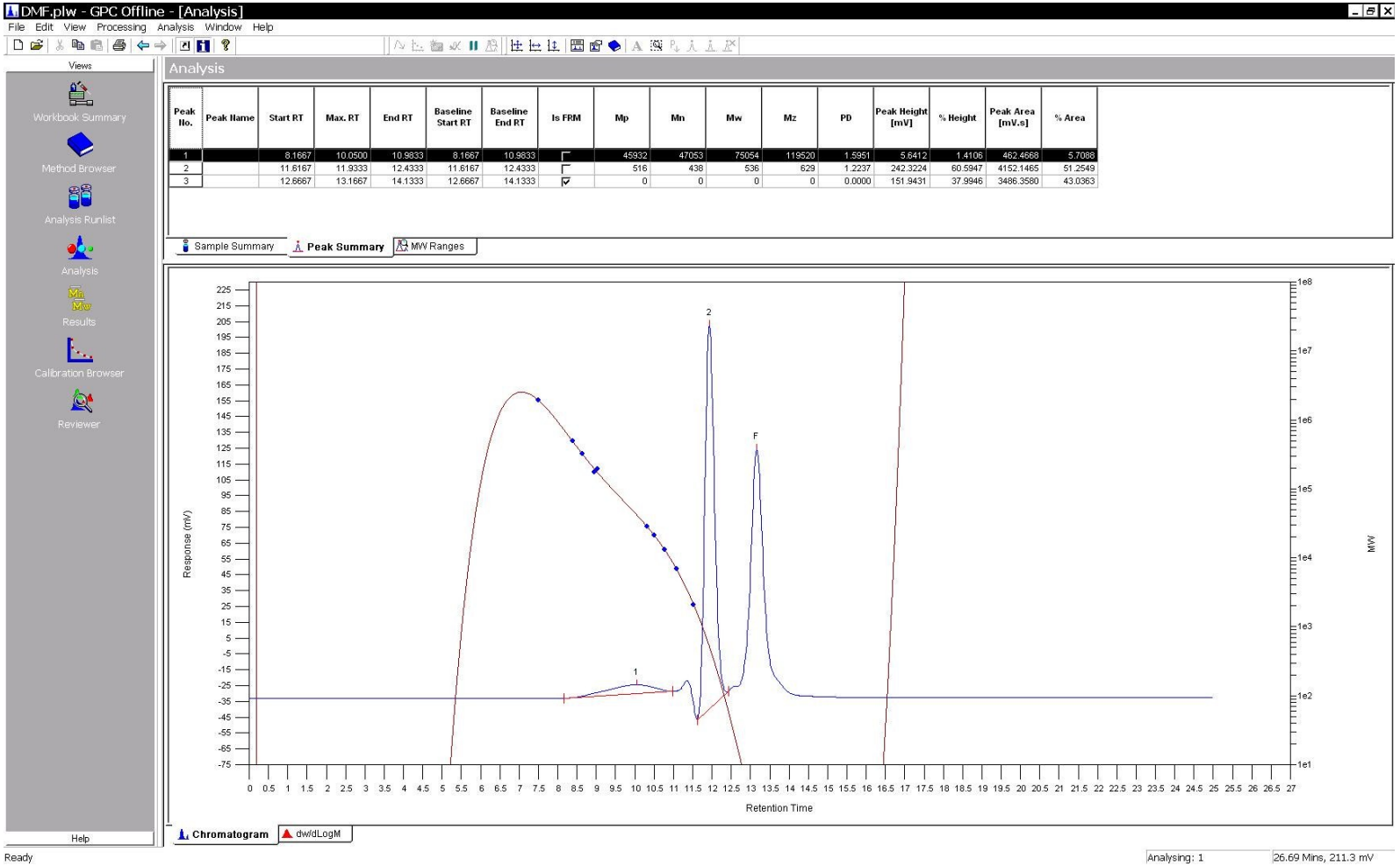
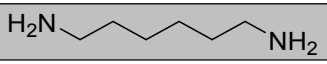
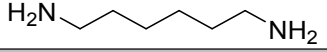
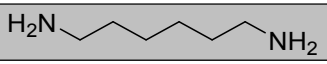
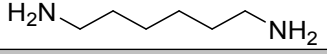
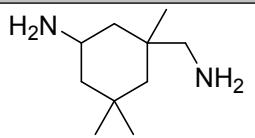
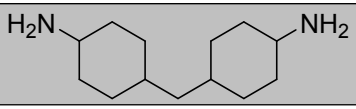


Figure 29S. Screenshot of the GPC analysis of the polymerization of (bis) *N*-8-C and hexamethylenediamine in d_6-DMSO at 25 °C for 24 h (NIPU1).

Part 5: Table of NIPUs

Table 1S. Table of synthesized NIPUs and their respective conditions and characterization results

NIPU	T (°C)	Co-monomer	Solvent	Time	Conversion [A]	M_n (g mol^{-1}) [B]	PDI [B]
1	25		d_6-DMSO	1 d	95%	47053	1.60
2	50		d_6-DMSO	1 d	89% [C]	38217 [C]	1.66 [C]
3	80		d_6-DMSO	1 d	93% [C]	27708 [C]	1.46 [C]
4	25		D_2O	1 d	- [D]	- [D]	- [D]
5	25		d_6-DMSO	1 d	85%	- [E]	- [E]
6	25		d_6-DMSO	1 d	88%	19534	1.22
7	25		d_6-DMSO	1 d	95%	22678	1.26

[a] Conversions were calculated by ^{1}H NMR. [B] M_n obtained by GPC in DMF. [C] Reactions were partially forming gels, results were not repeatable, and gels were obtained. [D] Resulting NIPUs were forming gels. [E] Products were below the detection limit of the GPC.

Part 6: Computational study data

1. Computational details:

All the density functional calculations (DFT) have been carried out with the Gaussian 09[1] suite of programs using the hybrid meta-GGA exchange-correlation functional M06-2X.[2] Structure optimizations were performed in gas phase and in DMSO by using the 6-31+G(d,p) basis set[3] and harmonic vibrational frequencies were obtained, at the same level of theory, by analytical differentiation of the gradients in order to determine whether the structures were minima or transition states. These frequencies were then used to evaluate the zero-point vibrational energy (ZPVE) and the thermal corrections, at T = 298 K, to the enthalpy and Gibbs free energy in the harmonic oscillator approximation. The integral equation formalism of the polarized continuum model (PCM) of Tomasi and co-workers[4,5] is used in order to estimate the effects of the solvent (dimethylsulfoxide).
As mentioned in the Main Text, the structures corresponding to TS1, INT1 and INT2, lacking the second molecule of amine, were not localizable, and they usually broke apart to the starting separate reactants (Figure S1) or did not converge properly.

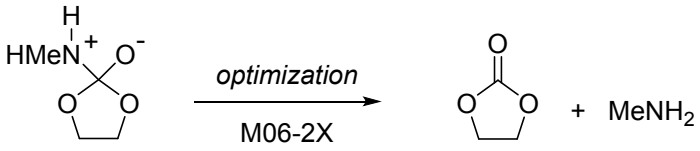


Figure S1

2. Energy profiles and Tables of energies for compounds 5-C, 6-C and *N*-8-C:

[1] Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, v. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian Inc., Wallingford CT, **2009**.
[2] Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.* **120**, 215 (2008)
[3] W. J. Hehre, R. Ditchfield and J. A. Pople, *J. Chem. Phys.* **56**, 2257 (1972)
[4] B. Menucci and J. Tomasi, *J. Chem. Phys.* **106**, 5151 (1997)
[5] J. Tomasi, B. Menucci and E. Cances, *J. Mol. Struct.: THEOCHEM* **464**, 211 (1999)

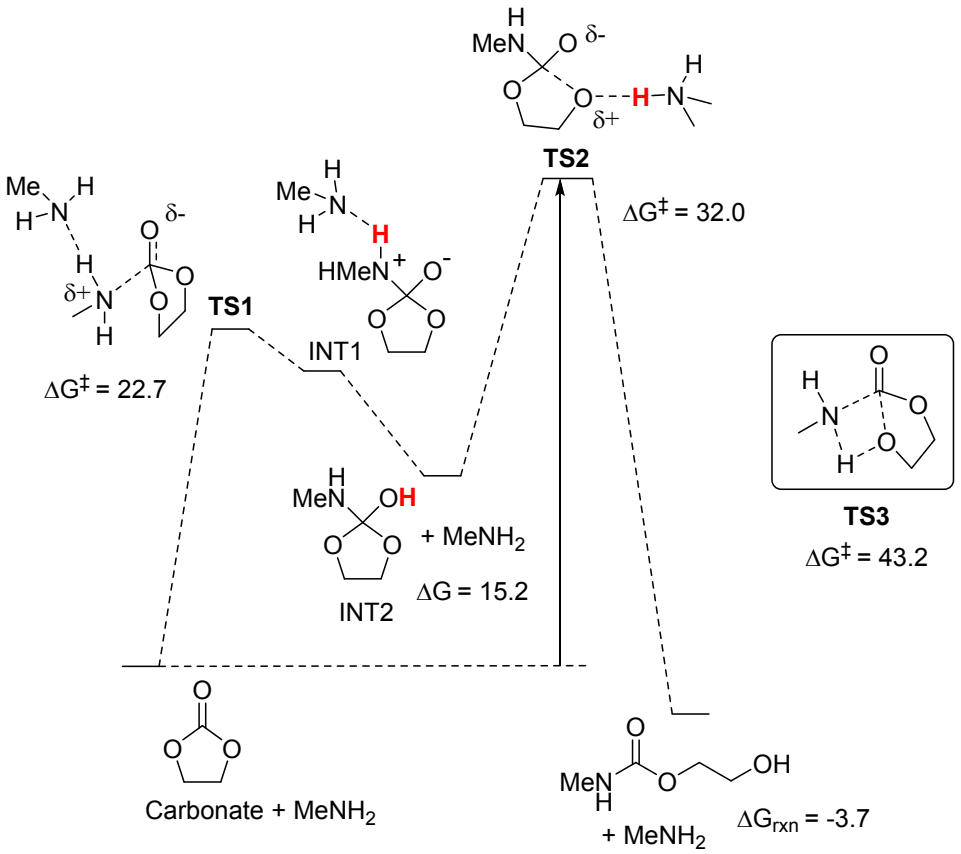


Figure S2. Reaction energy profile for substrate **5-C** and its Gibbs Free energies computed at m062x/6-31+G(d,p) (pcm, solvent =DMSO) level

Structure	G energy (M06-2x)	Relative G energies	Frequency
$MeNH_2$	-95.774170		
5-C	-342.244799	0	
TS1-5-C	-533.756916	22.7	-270.7
INT1-5-C	-533.757756	22.2	
INT2-5-C	-533.768993	15.2	
TS2-5-C	-533.742201	32.0	-357.0
Product	-438.024853	-3.7	
TS3-5-C	-437.950079	43.2	-663.8

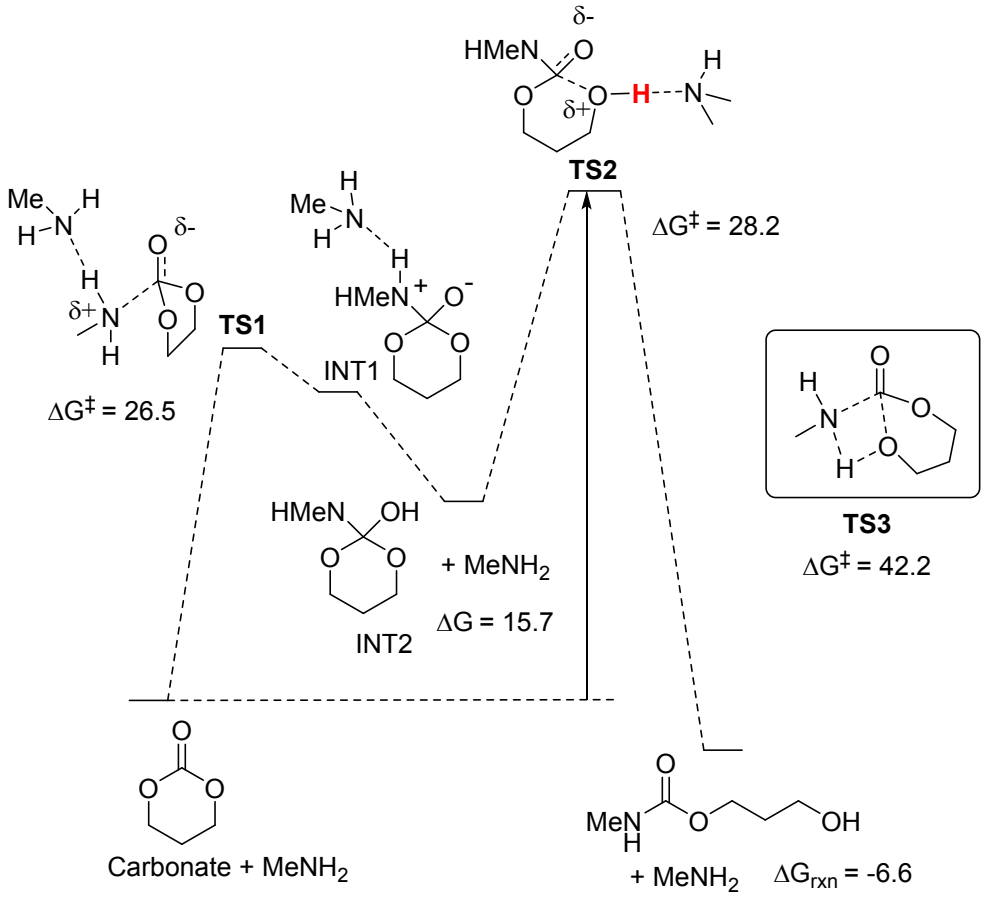


Figure S3. Reaction energy profile for substrate **6-C** and its Gibbs Free energies computed at m062x/6-31+G(d,p) (pcm, solvent =DMSO) level

Structure	G energy (M06-2x)	Relative G energies	Frequency
$MeNH_2$	-95.774170		
6-C	-381.512232	0	
TS1-6-C	-573.018302	26.5	-226.5
INT1-6-C	-573.021684	24.4	
INT2-6-C	-573.035536	15.7	
TS2-6-C	-573.015616	28.2	-277.1
Product	-477.296996	-6.6	
TS3-6-C	-477.219100	42.2	-654.4

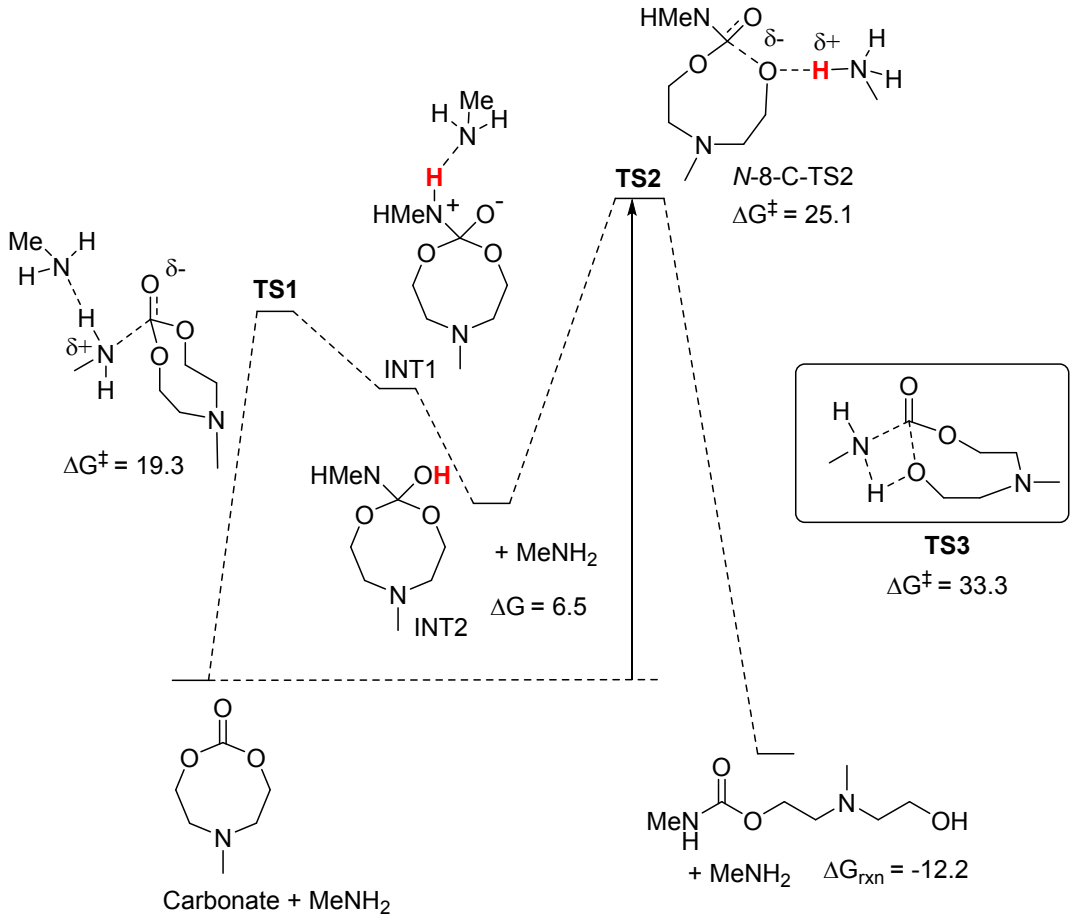


Figure S4. Reaction energy profile for substrate ***N*-8-C** and its Gibbs Free energies computed at m062x/6-31+G(d,p) (pcm, solvent =DMSO) level

Structure	G energy (M06-2x)	Relative G energies	Frequency
$MeNH_2$	-95.774170		
***N*-8-C**	-515.337872	0	
TS1- *N*-8-C	-706.855444	19.3	-174.5
INT1- *N*-8-C	-706.858790	17.2	
INT2- *N*-8-C	-706.875915	6.5	
TS2- *N*-8-C	-706.846157	25.1	-459.6
Product	-611.131462	-12.2	
TS3- *N*-8-C	-611.059017	33.3	-940.6

3. Cartesian coordinates:

Cartesian coordinates (in ångstrom, Å) of all the optimized structures at the M06-2X/6-31+G(d,p) level of theory, in DMSO:

$MeNH_2$

Standard orientation:

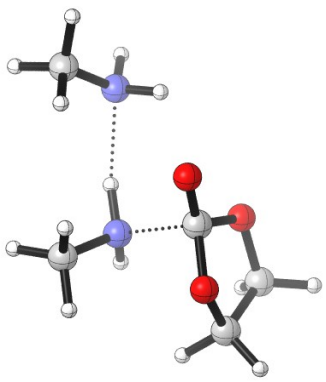
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.751032	0.000007	-0.125556
2	6	0	0.707990	-0.000005	0.017226
3	1	0	1.117932	-0.882126	-0.480594
4	1	0	-1.144203	-0.812114	0.340593
5	1	0	1.061729	0.000673	1.056705
6	1	0	1.118070	0.881448	-0.481692
7	1	0	-1.144244	0.812102	0.340521

5-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.301588	0.754689	-0.118521
2	6	0	1.301606	-0.754691	0.118453
3	6	0	-0.836366	-0.000001	0.000002
4	1	0	1.557520	1.021908	-1.145452
5	1	0	1.917016	-1.309021	-0.586977
6	8	0	-0.077861	1.101176	0.106650
7	8	0	-0.077887	-1.101175	-0.106493
8	1	0	1.557674	-1.021998	1.145319
9	8	0	-2.038040	0.000006	-0.000062
10	1	0	1.917129	1.309074	0.586746

TS1-5-C



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.554580	-0.264472	0.591520
2	6	0	-2.287654	-1.009731	-0.726947
3	6	0	-2.626875	0.362854	-0.110036
4	7	0	0.204183	0.775546	-0.772955
5	6	0	0.510506	2.118520	-0.270915
6	1	0	-3.616514	0.396437	0.345107
7	1	0	-2.991584	-1.788698	-0.427537
8	8	0	-1.653613	0.517394	0.914502
9	8	0	-1.008554	-1.329123	-0.179524
10	1	0	-2.229239	-0.972908	-1.817803
11	1	0	-0.414006	2.691550	-0.179080
12	8	0	0.347982	-0.430610	1.411218
13	1	0	-0.322689	0.820909	-1.644203
14	1	0	0.957429	2.012229	0.719998
15	1	0	-2.537784	1.177778	-0.837059
16	1	0	1.066989	0.231878	-0.949342
17	7	0	2.577028	-0.942324	-0.561957
18	1	0	3.055327	-1.635321	-1.129408
19	1	0	1.994172	-1.438234	0.110010
20	6	0	3.544476	-0.110719	0.161067
21	1	0	4.125190	0.479758	-0.552172
22	1	0	2.995802	0.580559	0.806607
23	1	0	4.242414	-0.679779	0.787956
24	1	0	1.204257	2.651288	-0.926402

INT1-5-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.533242	0.050395	0.498623
2	6	0	-2.299927	-1.276894	-0.275889
3	6	0	-2.674537	0.196559	-0.376365
4	7	0	0.310346	0.671004	-0.704022
5	6	0	0.797884	2.032648	-0.418093
6	1	0	-3.688232	0.417090	-0.039227
7	1	0	-2.792012	-1.754241	0.579574
8	8	0	-1.750403	0.801379	0.514935
9	8	0	-0.894077	-1.230078	-0.064413
10	1	0	-2.513203	-1.842718	-1.184771
11	1	0	-0.052240	2.709131	-0.328839

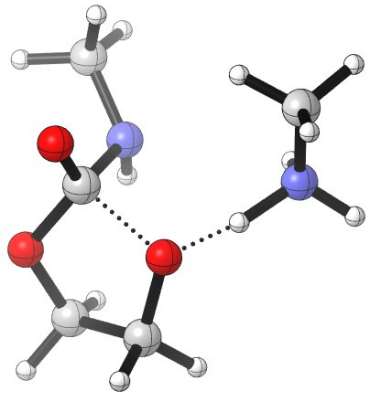
12	8	0	0.141886	0.058932	1.557612
13	1	0	-0.234872	0.651685	-1.566940
14	1	0	1.342972	1.995797	0.524458
15	1	0	-2.544231	0.581037	-1.397691
16	1	0	1.136974	0.009295	-0.820010
17	7	0	2.537845	-1.007170	-0.655166
18	1	0	3.087880	-1.217096	-1.483434
19	1	0	2.185219	-1.896201	-0.309101
20	6	0	3.372507	-0.363598	0.371030
21	1	0	3.778073	0.567018	-0.033485
22	1	0	2.736841	-0.118059	1.225437
23	1	0	4.206859	-0.987547	0.709602
24	1	0	1.457264	2.361458	-1.222170

INT2-5-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.640664	0.173430	0.047502
2	6	0	0.331382	-2.054417	0.452934
3	6	0	1.487242	-1.836348	-0.550601
4	7	0	0.891106	1.372146	0.777527
5	6	0	1.544512	2.425444	0.000047
6	1	0	1.163897	-2.015176	-1.580495
7	1	0	-0.549661	-2.487672	-0.030320
8	8	0	1.828934	-0.467312	-0.368315
9	8	0	0.038799	-0.744637	0.936856
10	1	0	0.618842	-2.671608	1.306044
11	1	0	2.508671	2.115243	-0.423580
12	8	0	-0.136212	0.389946	-1.065304
13	1	0	1.444320	1.130587	1.595014
14	1	0	1.707350	3.285721	0.651608
15	1	0	0.886829	2.730071	-0.815359
16	1	0	2.368192	-2.440213	-0.330423
17	7	0	-2.601201	0.906721	-0.175174
18	1	0	-3.189094	1.468792	-0.784973
19	1	0	-2.538203	1.409963	0.706163
20	6	0	-3.205159	-0.416658	0.041463
21	1	0	-4.202907	-0.370200	0.490315
22	1	0	-3.276854	-0.935450	-0.917240
23	1	0	-2.547263	-0.995424	0.693051
24	1	0	-1.067473	0.650615	-0.750234

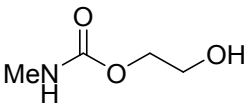
TS2-5-C



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.611466	0.600104	0.467362
2	6	0	-1.249665	-1.840758	-0.016556
3	6	0	-2.156912	-0.781926	-0.652172
4	7	0	0.160447	1.035019	-0.670992
5	6	0	0.416357	2.475366	-0.688417
6	7	0	2.105132	-1.181576	-0.563349
7	6	0	2.932035	-0.447189	0.421212
8	1	0	-0.928483	-2.589447	-0.751687
9	1	0	-3.214608	-1.049338	-0.637398
10	1	0	-1.770999	-2.350656	0.803255
11	8	0	-1.980003	0.359309	0.163118
12	8	0	-0.162226	-1.104465	0.483857
13	1	0	-1.862770	-0.577218	-1.692096
14	1	0	-0.499051	3.081961	-0.646253
15	8	0	-0.382782	1.129499	1.565344
16	1	0	-0.281090	0.744203	-1.538353
17	1	0	1.042260	2.740195	0.164819
18	1	0	2.489192	-2.104014	-0.761570
19	1	0	1.022963	-1.230797	-0.137721
20	1	0	2.449062	0.513229	0.602839
21	1	0	2.961858	-1.021824	1.346376
22	1	0	2.050582	-0.660097	-1.437211
23	1	0	0.956562	2.719840	-1.605545
24	1	0	3.943463	-0.298460	0.043811

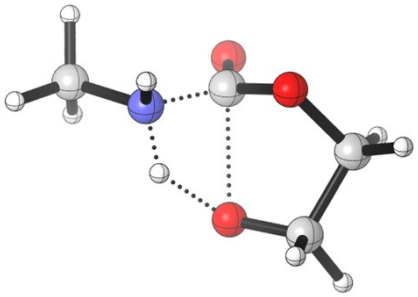
Product



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.812940	0.246206	-0.137902
2	6	0	-2.233585	0.262098	0.513529
3	6	0	-1.450193	0.656722	-0.722201
4	7	0	1.837052	-0.611502	-0.288847
5	6	0	3.115961	-0.371982	0.354899
6	1	0	-3.144047	0.864044	0.569559
7	1	0	-1.168917	1.711196	-0.691955
8	1	0	-1.633218	0.454591	1.411533
9	8	0	-0.274842	-0.161665	-0.837371
10	8	0	-2.640429	-1.096221	0.458567
11	1	0	-2.025570	0.445110	-1.625118
12	1	0	3.567294	0.556832	-0.004124
13	8	0	0.845480	1.264883	0.538262
14	1	0	1.707250	-1.411816	-0.889216
15	1	0	2.995724	-0.308397	1.439255
16	1	0	-1.848042	-1.641451	0.367262
17	1	0	3.777752	-1.203834	0.119118

TS3-5-C



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.963460	-0.542306	-0.186423
2	7	0	-1.258124	0.368147	-0.623995
3	6	0	1.862051	0.958235	0.113959
4	6	0	-2.615227	0.448701	-0.046144
5	6	0	-0.338188	-0.613439	0.040302
6	1	0	2.079216	-1.135905	0.726335
7	1	0	2.676291	1.241729	0.800208

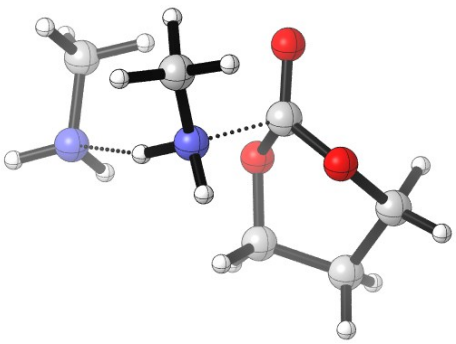
8	8	0	0.690732	-0.866933	-0.789791
9	8	0	0.601869	1.173333	0.652802
10	1	0	2.017068	1.510270	-0.830072
11	1	0	-3.118248	-0.510227	-0.161349
12	8	0	-0.700618	-1.271417	0.979865
13	1	0	-1.262439	0.223109	-1.635533
14	1	0	-3.160220	1.233014	-0.567917
15	1	0	-2.520744	0.693766	1.010054
16	1	0	2.728038	-0.813358	-0.914625
17	1	0	-0.600530	1.193554	-0.332310

6-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.016824	-1.215865	0.207671
2	6	0	-1.666860	-0.000179	-0.408998
3	6	0	-1.017085	1.215933	0.207114
4	6	0	1.085715	0.000017	-0.009701
5	1	0	-1.314004	-2.147882	-0.271521
6	1	0	-1.313909	2.147572	-0.273044
7	8	0	0.419104	-1.154137	0.039903
8	8	0	0.418983	1.154085	0.040540
9	1	0	-1.222462	1.279510	1.279767
10	1	0	-1.531764	-0.000475	-1.494933
11	1	0	-2.737831	-0.000193	-0.193028
12	8	0	2.290883	0.000125	-0.118478
13	1	0	-1.221456	-1.278565	1.280526

TS1-6-C



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.435620	0.566761	0.553099
2	6	0	-1.089213	-1.473266	-0.465783
3	6	0	-2.733515	0.243098	0.213148
4	6	0	-2.584445	-1.147136	-0.408062
5	7	0	0.756591	0.871151	-1.003558
6	6	0	1.526731	2.094957	-0.780616
7	1	0	-2.845457	0.177432	1.301225
8	1	0	-0.890026	-2.536675	-0.329041
9	8	0	-1.577619	1.041548	-0.087818
10	8	0	-0.394591	-0.809076	0.596189
11	1	0	-0.657473	-1.162033	-1.422987
12	1	0	-3.123352	-1.879684	0.198804
13	1	0	0.851964	2.953688	-0.784336
14	1	0	-3.001064	-1.174453	-1.418413
15	8	0	0.075260	1.190739	1.475652
16	1	0	0.204285	0.944456	-1.854387
17	1	0	1.993948	2.033871	0.203894
18	1	0	-3.585844	0.790299	-0.189446
19	1	0	1.375976	0.050113	-1.076345
20	7	0	2.445305	-1.512319	-0.445637
21	1	0	3.177155	-2.056272	-0.893111
22	1	0	1.723155	-2.169507	-0.162795
23	6	0	2.971496	-0.824269	0.740552
24	1	0	3.754405	-0.126414	0.430774
25	1	0	2.162567	-0.246693	1.198955
26	1	0	2.298368	2.241590	-1.542322
27	1	0	3.391110	-1.498099	1.497679

INT1-6-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.268608	0.190218	0.336850
2	6	0	-1.850320	-1.266975	-0.759825
3	6	0	-2.561391	0.624226	0.660045
4	6	0	-3.060478	-0.630218	-0.075459
5	7	0	0.684052	0.498446	-0.883869
6	6	0	1.244010	1.864312	-0.853495
7	1	0	-2.365083	0.407728	1.716503
8	1	0	-1.992102	-2.334439	-0.938175
9	8	0	-1.357905	1.081491	0.047989

10	8	0	-0.703778	-1.150575	0.080352
11	1	0	-1.665174	-0.786481	-1.729797
12	1	0	-3.509943	-1.329133	0.636150
13	1	0	0.448883	2.588024	-1.027763
14	1	0	-3.817116	-0.381662	-0.825871
15	8	0	0.335951	0.329025	1.435221
16	1	0	0.191150	0.335353	-1.762978
17	1	0	1.677495	2.018146	0.134215
18	1	0	-3.273144	1.449311	0.604737
19	1	0	1.477882	-0.205510	-0.792303
20	7	0	2.851683	-1.164152	-0.315510
21	1	0	3.472348	-1.525329	-1.034440
22	1	0	2.457262	-1.972930	0.158456
23	6	0	3.598073	-0.335621	0.644281
24	1	0	4.065917	0.494494	0.109220
25	1	0	2.886993	0.076422	1.364704
26	1	0	2.013796	1.956551	-1.620631
27	1	0	4.378847	-0.885784	1.180755

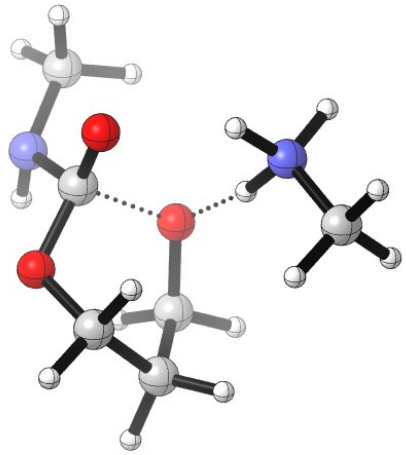
INT2-6-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.280051	0.489637	0.052295
2	6	0	-1.238511	-1.292379	-1.211714
3	6	0	-1.908564	-0.835420	1.120492
4	6	0	-2.070845	-1.823912	-0.043617
5	7	0	-0.143509	1.632986	-0.812351
6	6	0	-0.432053	2.914749	-0.167299
7	1	0	-1.116002	-1.156693	1.803834
8	1	0	-0.910907	-2.087372	-1.882999
9	8	0	-1.577239	0.453670	0.597767
10	8	0	-0.047607	-0.679473	-0.715860
11	1	0	-1.815548	-0.566640	-1.798316
12	1	0	-1.723471	-2.816013	0.259052
13	1	0	-1.456653	2.988286	0.217902
14	1	0	-3.117089	-1.912596	-0.350874
15	8	0	0.628756	0.529140	1.076783
16	1	0	-0.751414	1.500638	-1.617005
17	1	0	-0.269211	3.714227	-0.892835
18	1	0	0.263511	3.056073	0.661941
19	1	0	-2.830380	-0.706181	1.688988
20	7	0	3.036132	0.030139	0.024376
21	1	0	3.834406	0.487033	0.456988
22	1	0	3.027448	0.326290	-0.948356

23	6	0	3.173391	-1.431535	0.106916
24	1	0	4.067743	-1.813729	-0.396460
25	1	0	3.212628	-1.724854	1.158286
26	1	0	2.287583	-1.887472	-0.340125
27	1	0	1.557513	0.403584	0.683847

TS2-6-C

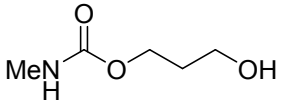


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.001810	-0.051465	-0.500509
2	6	0	0.243311	1.202744	1.424948
3	6	0	0.528180	1.688942	-0.987280
4	6	0	1.041079	2.037958	0.416728
5	7	0	-2.336476	-0.137667	-0.021205
6	6	0	-2.702932	-1.437048	0.524725
7	1	0	1.106085	0.870581	-1.433103
8	1	0	0.785292	1.089326	2.371053
9	8	0	-0.836438	1.294760	-0.912822
10	8	0	-0.027723	-0.077535	0.895683
11	1	0	-0.706865	1.707163	1.653103
12	1	0	2.112392	1.816544	0.488536
13	1	0	-2.640581	-2.188281	-0.264253
14	1	0	0.911685	3.103770	0.631958
15	8	0	-0.558330	-0.977547	-1.237192
16	1	0	-2.518114	0.612934	0.637826
17	1	0	-2.052630	-1.747844	1.353776
18	1	0	0.573754	2.542377	-1.666702
19	1	0	1.253243	-1.869561	-0.796821
20	7	0	1.738966	-1.722283	0.095631
21	1	0	1.727270	-2.597815	0.617024
22	6	0	3.116475	-1.211539	-0.075339

23	1	0	3.543106	-1.009463	0.906321
24	1	0	3.727968	-1.942727	-0.602276
25	1	0	1.051270	-0.982212	0.568061
26	1	0	3.076977	-0.287317	-0.651467
27	1	0	-3.734173	-1.392807	0.880988

Product



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.355831	-0.262187	0.034412
2	6	0	2.667124	0.779174	-0.282546
3	6	0	0.879094	-1.011258	-0.129107
4	6	0	2.169445	-0.569265	-0.790157
5	7	0	-2.227431	0.686127	-0.359350
6	6	0	-3.603936	0.674410	0.099692
7	1	0	0.978220	-1.036923	0.959661
8	1	0	3.569656	1.073524	-0.831396
9	8	0	-0.129119	-0.050710	-0.484339
10	8	0	2.913465	0.774546	1.119259
11	1	0	1.905526	1.545653	-0.446889
12	1	0	2.929208	-1.338175	-0.604498
13	1	0	-4.085500	-0.272175	-0.157551
14	1	0	2.026146	-0.513538	-1.875358
15	8	0	-1.634393	-1.204350	0.764860
16	1	0	-1.886527	1.439943	-0.936459
17	1	0	-3.661409	0.813914	1.182976
18	1	0	0.569136	-1.999931	-0.477990
19	1	0	3.648071	0.176179	1.303349
20	1	0	-4.135508	1.487511	-0.392397

TS3-6-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.701331	-1.130996	-0.323662
2	7	0	-1.621120	0.194004	-0.640587
3	6	0	2.211845	0.107300	0.412730
4	6	0	1.526743	1.382918	-0.100011
5	6	0	-2.906890	0.265279	0.083278
6	6	0	-0.530287	-0.529841	0.089202
7	1	0	1.695514	-2.025488	0.304433
8	1	0	2.050277	2.257148	0.319107
9	8	0	0.362364	-0.909760	-0.835190
10	8	0	0.181448	1.383309	0.272568
11	1	0	1.652858	1.437155	-1.197904
12	1	0	2.008483	0.025470	1.485393
13	1	0	-3.305640	-0.738405	0.222725
14	1	0	3.297292	0.165313	0.280750
15	8	0	-0.701710	-1.007245	1.185405
16	1	0	-1.718720	-0.171654	-1.589655
17	1	0	-3.593577	0.871567	-0.504383
18	1	0	-2.725752	0.730025	1.050500
19	1	0	2.280126	-1.330496	-1.226054
20	1	0	-1.046298	1.122945	-0.612284

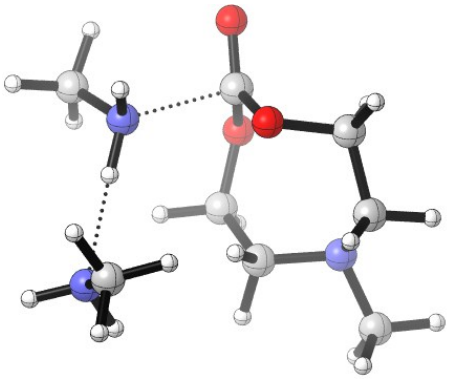
***N*-8-C**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.508671	-0.027964	-0.462512
2	6	0	-0.184755	1.465452	1.062241
3	6	0	-0.269108	-1.439434	1.072576
4	1	0	-0.355223	2.522694	1.267513
5	1	0	-0.347815	-2.499287	1.315039
6	1	0	-0.164551	0.944691	2.018412
7	1	0	-0.583854	-0.879437	1.951344
8	6	0	1.157947	-1.124908	0.592348
9	1	0	1.530845	-2.003268	0.059756
10	1	0	1.808522	-0.969206	1.470191
11	6	0	1.105078	1.300728	0.278504
12	1	0	1.137919	2.049126	-0.519470
13	1	0	1.944759	1.504079	0.968240
14	7	0	1.198707	-0.008411	-0.343543
15	6	0	2.356932	-0.081804	-1.227416
16	1	0	2.307137	0.730482	-1.956758
17	1	0	2.348210	-1.031276	-1.767242
18	1	0	3.309341	0.002233	-0.677671

19	8	0	-1.203144	-1.242614	0.008922
20	8	0	-1.339574	1.074115	0.293696
21	8	0	-2.116129	0.060450	-1.504992

TS1-*N*-8-C



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.548871	-1.654087	-0.172207
2	6	0	0.173868	-0.125673	1.602285
3	6	0	1.472483	-1.337079	-1.318081
4	8	0	0.098030	-0.932840	-1.146320
5	8	0	-0.112538	-1.431939	1.089092
6	1	0	-0.774851	0.388517	1.793867
7	1	0	1.594361	-1.623891	-2.366183
8	1	0	0.657419	-0.338263	2.558214
9	1	0	1.688833	-2.204836	-0.686812
10	6	0	2.408554	-0.195780	-0.982552
11	1	0	3.425812	-0.528460	-1.216524
12	6	0	1.074474	0.793134	0.787603
13	1	0	0.547260	1.170937	-0.096737
14	1	0	1.252497	1.654154	1.444196
15	8	0	-1.116232	-2.700965	-0.420917
16	1	0	-2.526631	-0.346454	-1.137120
17	7	0	-2.214332	-0.232108	-0.176333
18	6	0	-3.210242	-0.750989	0.757601
19	1	0	-4.202140	-0.300199	0.638786
20	1	0	-3.294919	-1.832723	0.619541
21	1	0	-2.038387	0.767006	-0.016928
22	7	0	-1.663249	2.771811	0.154810
23	1	0	-2.458080	3.309933	0.488445
24	1	0	-0.857529	3.104213	0.677659
25	6	0	-1.466641	3.006924	-1.280716

26	1	0	-0.625776	2.401463	-1.633339
27	1	0	-1.270078	4.053388	-1.542626
28	1	0	-2.869351	-0.568151	1.781049
29	1	0	-2.358197	2.678733	-1.821435
30	7	0	2.362872	0.194534	0.422252
31	1	0	2.181250	0.663213	-1.642725
32	6	0	3.473796	1.092065	0.728375
33	1	0	3.427397	2.032736	0.151500
34	1	0	3.464911	1.338593	1.792809
35	1	0	4.420565	0.595297	0.500587

INT1-*N*-8-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.894328	-1.269067	0.248741
2	6	0	-0.230114	-0.143642	-1.649502
3	6	0	-1.125951	-1.115587	1.496205
4	8	0	0.115248	-0.497591	1.166951
5	8	0	0.235191	-1.321932	-1.005263
6	1	0	0.613856	0.509353	-1.922951
7	1	0	-1.164329	-1.251080	2.582780
8	1	0	-0.669835	-0.515890	-2.579059
9	1	0	-1.185626	-2.100153	1.023239
10	6	0	-2.295345	-0.250208	1.063863
11	1	0	-3.212614	-0.735289	1.416652
12	6	0	-1.277449	0.701289	-0.922534
13	1	0	-0.815034	1.305402	-0.131784
14	1	0	-1.654280	1.401673	-1.678431
15	8	0	1.296773	-2.404782	0.630886
16	1	0	2.549526	-0.264083	0.997820
17	7	0	2.102550	-0.252127	0.079187
18	6	0	3.067631	-0.688785	-0.947768
19	1	0	3.938416	-0.033628	-0.930473
20	1	0	3.358152	-1.716101	-0.730984
21	1	0	1.796751	0.747597	-0.092362
22	7	0	1.550617	2.520681	-0.191621
23	1	0	2.406037	2.980984	-0.493182
24	1	0	0.822109	2.844341	-0.823386
25	6	0	1.231668	2.910273	1.191038
26	1	0	0.334918	2.374750	1.513821
27	1	0	1.067987	3.985750	1.315761
28	1	0	2.585638	-0.641874	-1.924123
29	1	0	2.053651	2.606054	1.843638

30	7	0	-2.399024	-0.074398	-0.382523
31	1	0	-2.225947	0.731870	1.572278
32	6	0	-3.679781	0.541608	-0.715441
33	1	0	-3.793927	1.546763	-0.270826
34	1	0	-3.775790	0.631812	-1.800351
35	1	0	-4.496267	-0.088202	-0.351581

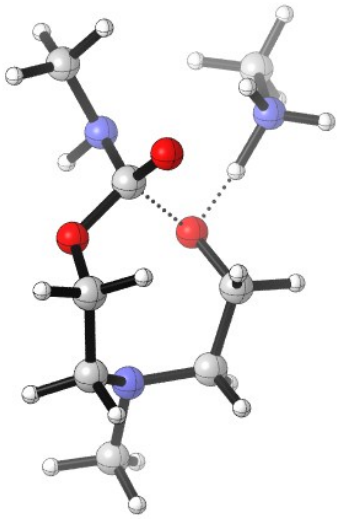
INT2-*N*-8-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.688973	0.789140	0.511205
2	6	0	-0.407656	0.054762	-1.536915
3	6	0	-1.190485	-0.016543	1.746264
4	8	0	-0.493131	1.101866	1.200689
5	8	0	0.443027	-0.237180	-0.439677
6	1	0	0.004907	0.878903	-2.136801
7	1	0	-1.353176	0.188849	2.809307
8	1	0	-0.375144	-0.853175	-2.145151
9	1	0	-0.585489	-0.923006	1.655053
10	6	0	-2.539473	-0.205201	1.075278
11	1	0	-3.081450	-0.969584	1.643517
12	6	0	-1.864374	0.362739	-1.194593
13	1	0	-1.968876	1.370606	-0.767790
14	1	0	-2.394975	0.370230	-2.153812
15	8	0	1.645922	0.283716	1.350779
16	7	0	1.118234	2.038679	-0.051322
17	6	0	2.296929	1.932402	-0.904324
18	1	0	2.536029	2.922112	-1.297443
19	1	0	3.140455	1.585931	-0.303191
20	1	0	0.341881	2.489228	-0.526488
21	1	0	2.169562	1.237339	-1.746597
22	7	0	-2.475684	-0.641624	-0.317667
23	1	0	-3.113415	0.737967	1.163779
24	6	0	-3.815135	-0.996727	-0.778327
25	1	0	-4.508850	-0.136869	-0.763384
26	1	0	-3.764492	-1.381646	-1.799832
27	1	0	-4.228011	-1.780430	-0.137343
28	1	0	1.966956	-0.634550	1.046372
29	7	0	2.563743	-2.070582	0.522608
30	1	0	3.159501	-2.582061	1.168056
31	6	0	3.281320	-1.792952	-0.729878
32	1	0	4.143905	-1.158763	-0.511924
33	1	0	3.630440	-2.696479	-1.240920
34	1	0	2.612002	-1.241667	-1.394214

35	1	0	1.757045	-2.661184	0.336897

TS2-*N*-8-C

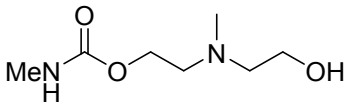


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.749090	-0.820042	0.185142
2	6	0	0.585505	1.384628	0.767731
3	6	0	1.460689	-1.512583	0.830528
4	1	0	0.258198	2.404226	1.024907
5	1	0	1.702040	-2.555082	1.068309
6	1	0	0.536990	0.811395	1.701290
7	1	0	1.101007	-1.051661	1.750044
8	6	0	2.730863	-0.852121	0.289229
9	1	0	3.230559	-1.568260	-0.372106
10	1	0	3.413625	-0.677648	1.146136
11	6	0	2.015869	1.507932	0.237781
12	1	0	2.042569	2.353005	-0.459037
13	1	0	2.673805	1.773840	1.091224
14	7	0	2.532028	0.359147	-0.494690
15	6	0	3.783533	0.722855	-1.146436
16	1	0	3.625201	1.587008	-1.797343
17	1	0	4.138825	-0.109926	-1.759474
18	1	0	4.578178	0.979558	-0.420426
19	1	0	-1.173552	-1.034367	-1.766142
20	7	0	-1.683318	-0.958938	-0.891196
21	6	0	-2.605789	-2.078963	-0.719115
22	1	0	-3.243947	-2.142575	-1.603162
23	1	0	-2.101503	-3.045635	-0.578184

24	1	0	-3.240406	-1.892185	0.149744
25	1	0	-1.537370	1.299766	0.114830
26	7	0	-2.626326	1.518514	0.492092
27	1	0	-2.825411	0.663142	1.018815
28	6	0	-3.592066	1.725275	-0.607562
29	1	0	-3.305906	2.616979	-1.164737
30	1	0	-3.539594	0.853647	-1.259014
31	1	0	-4.602203	1.846811	-0.215705
32	1	0	-2.640096	2.296852	1.149232
33	8	0	0.426045	-1.511145	-0.142003
34	8	0	-0.307485	0.833628	-0.172009
35	8	0	-1.171659	-0.860213	1.365709

Product



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.013056	-0.406956	0.129590
2	6	0	1.233547	1.649931	0.804682
3	6	0	0.037872	-1.451021	0.657134
4	1	0	1.366515	2.195436	1.748628
5	1	0	-0.364390	-2.425013	0.953347
6	1	0	0.217256	1.238102	0.782755
7	1	0	0.068185	-0.816470	1.546827
8	6	0	1.406264	-1.632142	0.033918
9	1	0	1.309273	-2.276994	-0.846113
10	1	0	2.026349	-2.176584	0.773293
11	6	0	2.268649	0.539633	0.726553
12	1	0	3.245260	1.019279	0.597613
13	1	0	2.305976	0.008570	1.692319
14	7	0	2.044342	-0.389723	-0.383226
15	6	0	3.276078	-0.683451	-1.105952
16	1	0	3.711745	0.245203	-1.482157
17	1	0	3.054361	-1.328228	-1.960831
18	1	0	4.027570	-1.192486	-0.475634
19	1	0	-2.368045	0.109406	-1.800939
20	7	0	-2.753088	0.110138	-0.868539
21	6	0	-4.066818	0.671082	-0.612692
22	1	0	-4.474620	1.030486	-1.556210
23	1	0	-4.738926	-0.084915	-0.198508

24	1	0	-4.003726	1.506549	0.089513
25	1	0	0.736007	3.181580	-0.311702
26	8	0	-0.825826	-0.862253	-0.322000
27	8	0	1.435143	2.517994	-0.304454
28	8	0	-2.360916	-0.455652	1.302798

TS3-*N*-8-C

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.436288	0.038963	-0.451623
2	6	0	-3.522032	0.275527	0.518282
3	6	0	-1.142656	-0.427178	0.139651
4	8	0	-0.642471	-1.395483	-0.641650
5	8	0	-0.482476	1.142517	-0.867354
6	1	0	-3.810085	-0.661027	0.995936
7	8	0	-0.916710	-0.260923	1.321280
8	1	0	-2.717534	-0.569778	-1.220872
9	1	0	-4.368812	0.701983	-0.017040
10	1	0	-3.162716	0.976901	1.268701
11	1	0	-1.872982	0.955756	-0.822573
12	6	0	1.865078	1.441159	-0.459724
13	1	0	2.568877	2.156400	-0.008897
14	1	0	2.001662	1.488925	-1.548049
15	6	0	1.841413	-1.058994	-0.756919
16	1	0	2.679062	-1.776051	-0.751289
17	1	0	1.666558	-0.773614	-1.799157
18	7	0	2.267100	0.114885	-0.018974
19	6	0	2.398857	-0.061036	1.413101
20	1	0	1.438928	-0.103907	1.949353
21	1	0	2.945053	-0.990710	1.614953
22	1	0	2.984287	0.769052	1.823734
23	6	0	0.438124	1.892608	-0.144261
24	1	0	0.355074	2.964834	-0.388017
25	1	0	0.252631	1.791690	0.941888
26	6	0	0.650969	-1.894422	-0.264087
27	1	0	0.676332	-2.026981	0.821574
28	1	0	0.702727	-2.875282	-0.740523