Electronic Supplementary Material (ESI) for Polymer Chemistry.

Supporting Information

Catalyst-free, aza-Michael polymerization of hydrazides: polymerizability, kinetics, and mechanistic origin of an α-effect

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1) Hydrazide-Michael polymerizations

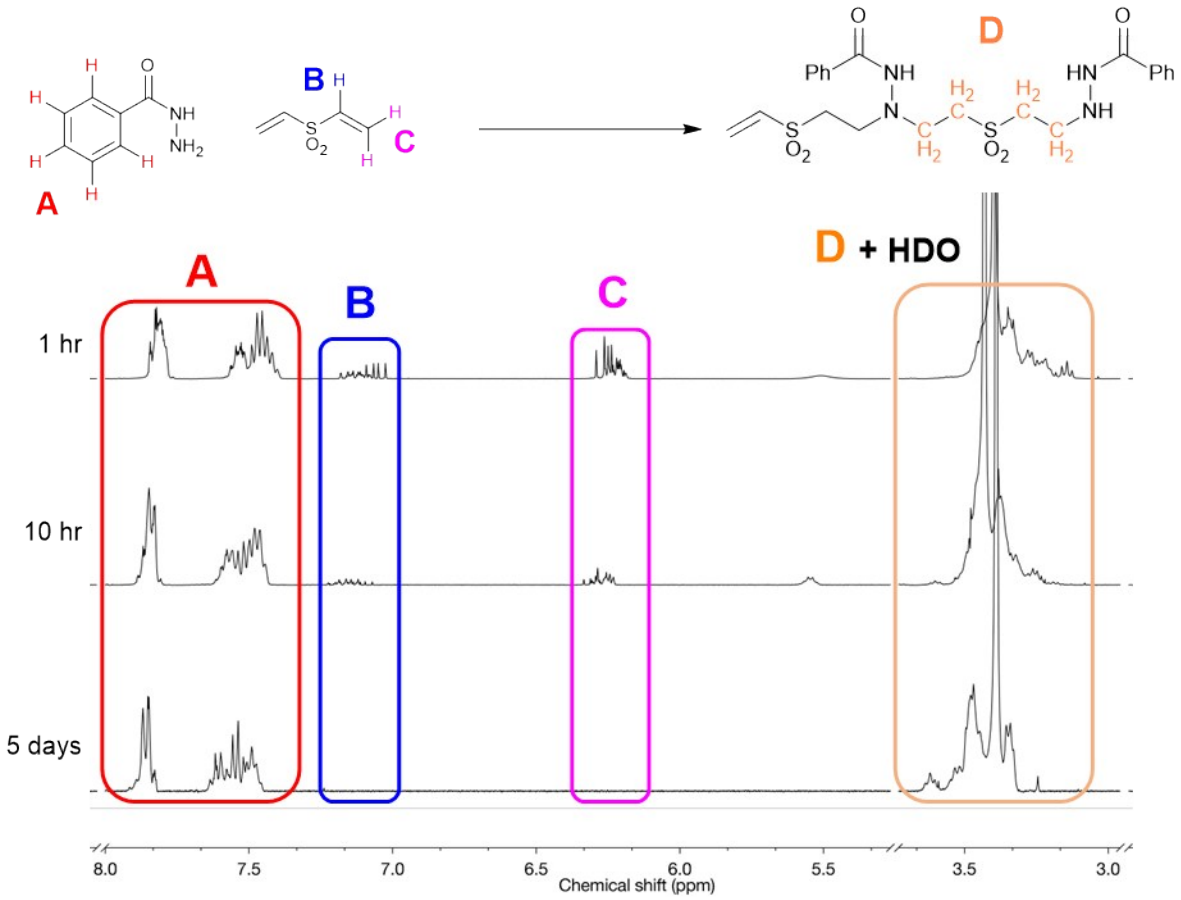

Figure S1. ^{1}H NMR spectrum of the crude reaction mixture for the polymerization of **H6** with divinyl sulfone after reaction times of 1 hour, 10 hours, and 5 days. Reaction was performed in DMSO at 75 °C, $[\text{hydrazide}]_0 = [\text{DVS}]_0 = 2.0$ M.

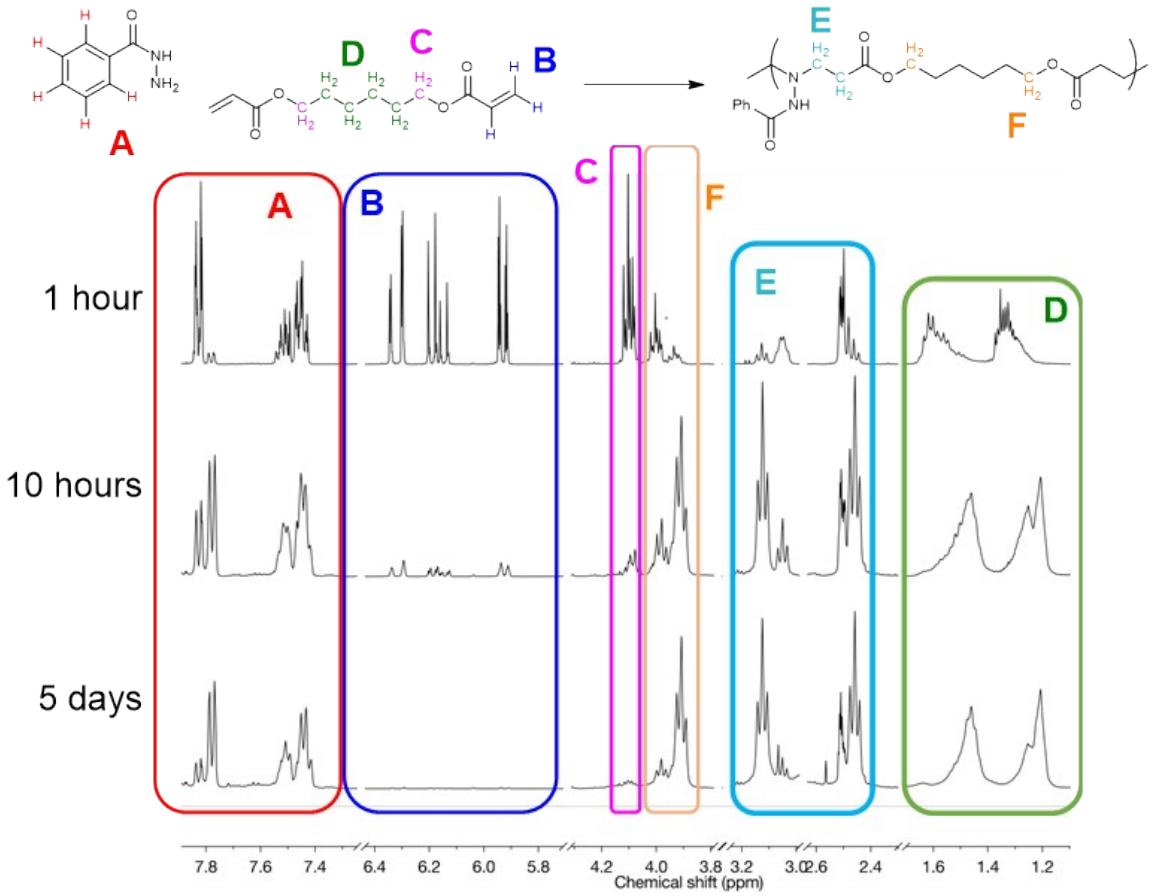

Figure S2. ^{1}H NMR spectrum of the crude reaction mixture for the polymerization of **H6** with 1,6-hexanediol diacrylate after reaction times of 1 hour, 10 hours, and 5 days. Reaction was performed in DMSO at 75 °C, $[\text{hydrazide}]_0 = [\text{HDA}]_0 = 2.0$ M.

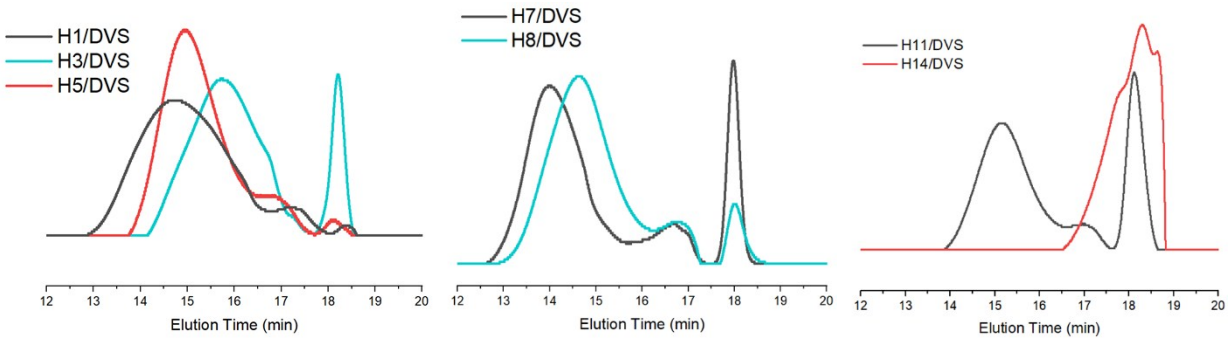

Figure S3. GPC traces of the crude hydrazide/DVS polymers after reacting for 5 days in DMSO at 75°C.

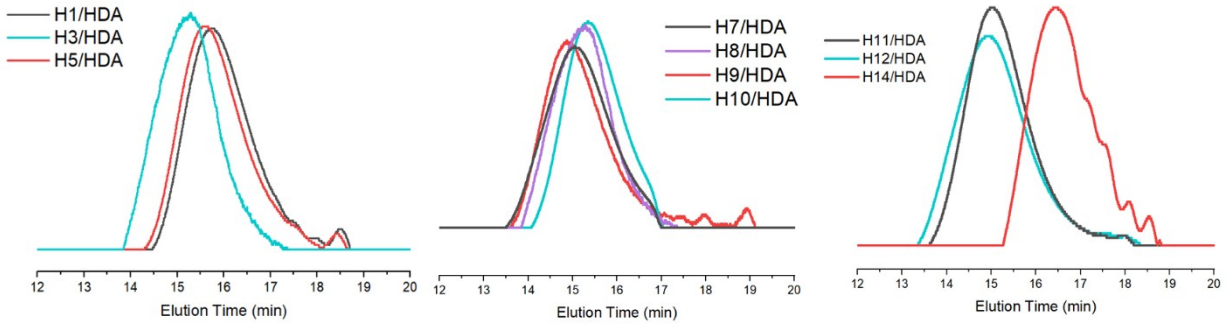

Figure S4. GPC traces of the crude hydrazide/HDA polymers after reacting for 5 days in DMSO at 75°C.

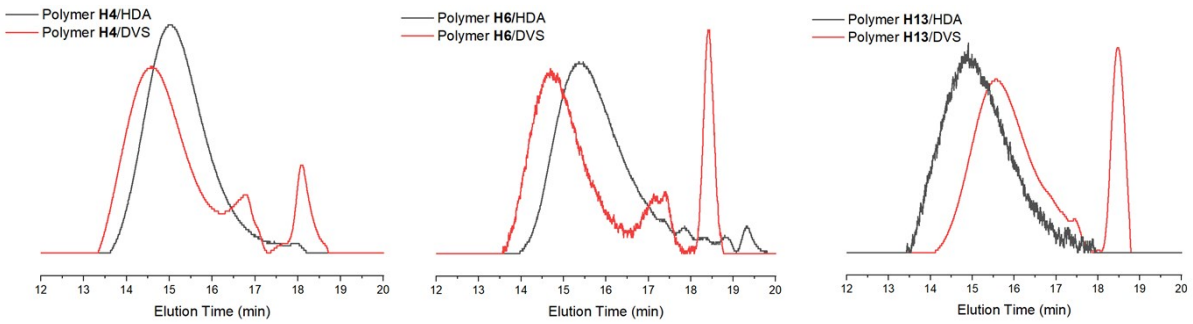

Figure S5. GPC traces of the crude polymerizations between **H4**, **H6** and **H13** with DVS and HDA carried out at 120 °C for 7 days. Reactions were formulated in DMSO, $[\text{hydrazide}]_0 = [\text{DVS}]_0$ or $[\text{HDA}]_0 = 2.0$ M.

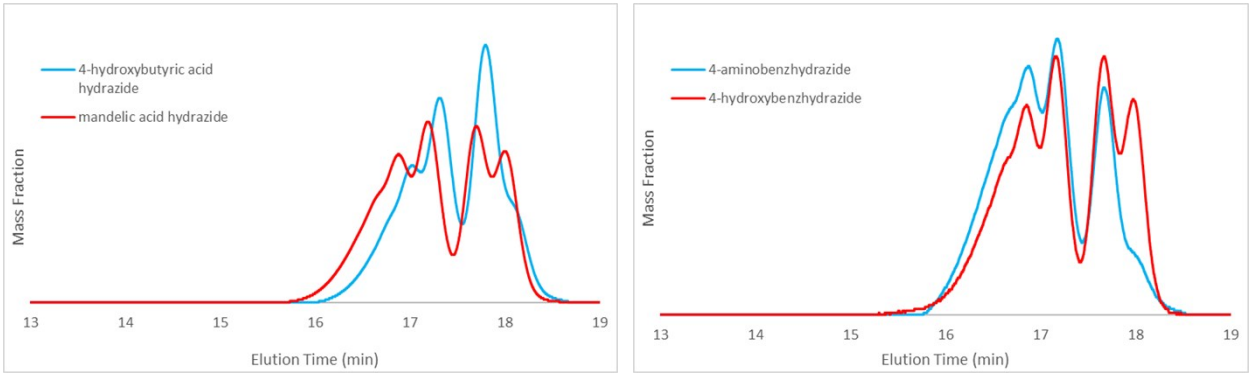

Figure S6. GPC traces of the crude, off-stoichiometric reactions of (left) 4-hydroxybutyric hydrazide (**H3**), mandelic acid hydrazide (**H5**), (right) 4-aminobenzhydrazide (**H8**), and 4-hydroxybenzhydrazide (**H7**) with DVS. Reactions were formulated in DMSO at 75 °C for 5 days, $[\text{hydrazide}]_0 = 1.33$ M, $[\text{DVS}]_0 = 2.0$ M.

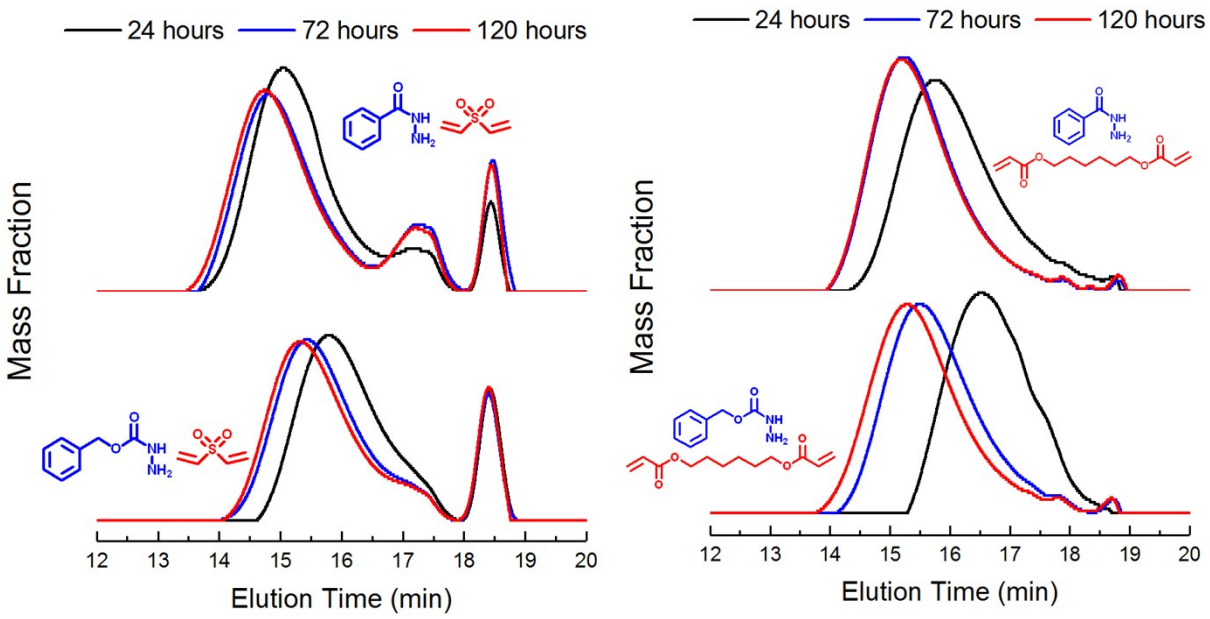

Figure S7. GPC traces for the polymerizations of **H6** and **H13** with (left) DVS and (right) HDA taken at 24, 72, and 120 h. Reactions were formulated in DMSO, $[\text{hydrazide}]_0 = [\text{DVS}]_0$ or $[\text{HDA}]_0 = 2.0$ M.

2) Reaction order modeling of hydrazide-Michael polymerizations

2A) Determination of the reaction order of the 1st addition step

In order to determine the reaction rate dependence on the 1° hydrazide (RNH_2) and vinyl functional group concentration during the 1st addition step of the hydrazide-Michael polymerization to form the mono-adduct, the conversion versus time data were analyzed using multiple analytical reaction order models and assessing the models accuracy based on the degree to which the data is linearized by the model. The model reaction of **H6** with DVS in DMSO, $[vinyl]_0 = [hydrazide]_0 = 2$ M, was performed at several temperatures and vinyl conversion was monitored by ^{1}H NMR and GPC of crude reaction mixture over the course of 1 hour. Identical reactions with **H12** replacing **H6** were also conducted to affirm the reaction order with another hydrazide.

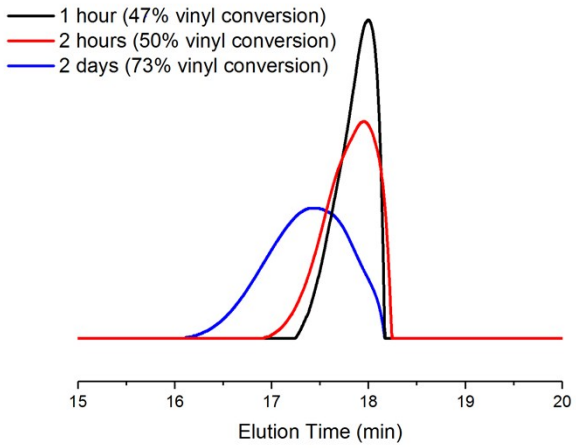

Figure S8. GPC curves of the crude reaction mixture during the reaction of **H6** and DVS in DMSO at 22°C, $[hydrazide]_0 = [divinyl\ sulfone]_0 = 2$ M. Samples were taken after 1 h, 2 h, and 2 days of reaction time.

1st order hydrazide dependence: $\frac{d[vinyl]}{dt} = -k_1[RNH_2]$; $[RNH_2] = [vinyl] - [RNH_2]_0$ **1**

1st order solution: $ln([RNH_2]) = -k_1 t + ln([RNH_2]_0)$ **2**

2nd order hydrazide dependence: $\frac{d[vinyl]}{dt} = -k_1[RNH_2]^2$; $[RNH_2] = [vinyl] - [RNH_2]_0$ **3**

2nd order solution: $^1/_{[RNH_2]} = k_1 t + {}^1/_{[RNH_2]_0}$ **4**

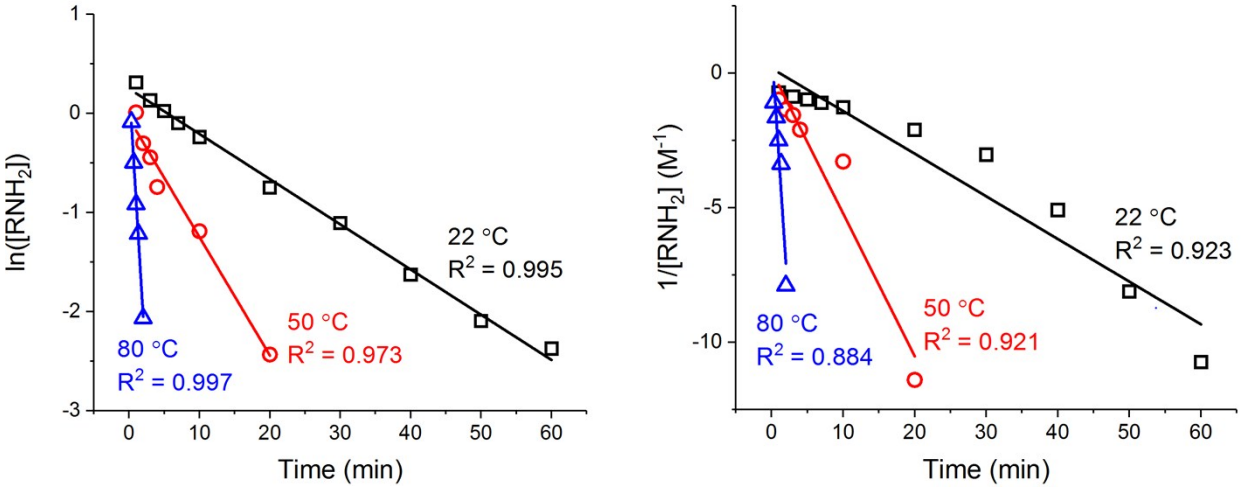

Figure S9. Results of fitting vinyl sulfone conversion data to a (left) 1st order overall, 1st order in hydrazide and a (right) 2nd order overall, 2nd order in hydrazide rate models based on equations **S2** and **S4**, respectively, for the stoichiometric reaction of **H6** and DVS at three temperatures.

1st order vinyl dependence: $$\frac{d[vinyl]}{dt} = -k_1[vinyl]$$ **5**

1st order solution: $$ln([vinyl]) = -k_1 t + ln([vinyl]_0)$$ **6**

2nd order vinyl dependence: $$\frac{d[vinyl]}{dt} = -k_1[vinyl]^2$$ **7**

2nd order solution: $$^1/_{[vinyl]} = k_1 t + {}^1/_{[vinyl]_0}$$ **8**

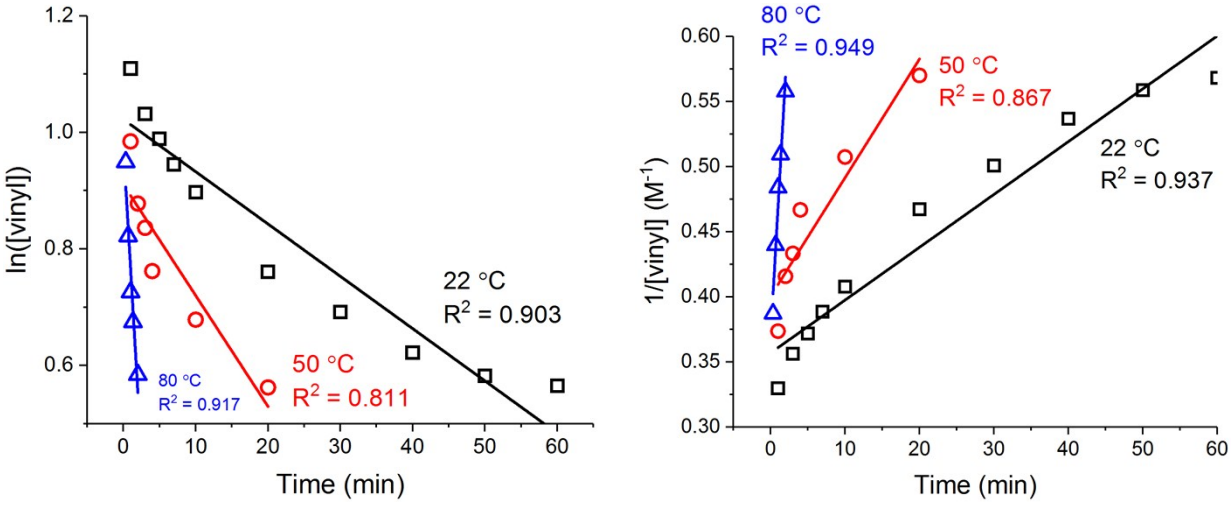

Figure S10. Results of fitting vinyl sulfone conversion data to a (left) 1st order overall, 1st order in vinyl and a (right) 2nd order overall, 2nd order in vinyl rate models based on equations **S6** and **S8**, respectively, for the stoichiometric reaction of **H6** and DVS at three temperatures.

A + 2B → C + B; A : vinyl, B: 1° hydrazide

1st order vinyl dependence; 2nd order hydrazide dependence:

$$\frac{d[vinyl]}{dt} = -k_1[vinyl][RNH_2]^2 \quad ; \quad [RNH_2] = [vinyl] - [RNH_2]_0 \qquad \textbf{9}$$

3rd order overall solution:

$$\ln\left[\frac{[vinyl]}{[vinyl]-[RNH_2]_0}\right] - \frac{[RNH_2]_0}{[vinyl]-[RNH_2]_0} = -k_1[RNH_2]_0{}^2 t - \ln\left[\frac{[vinyl]_0}{[vinyl]_0-[RNH_2]_0}\right] - \frac{[RNH_2]_0}{[vinyl]_0-[RNH_2]_0} \qquad \textbf{10}$$

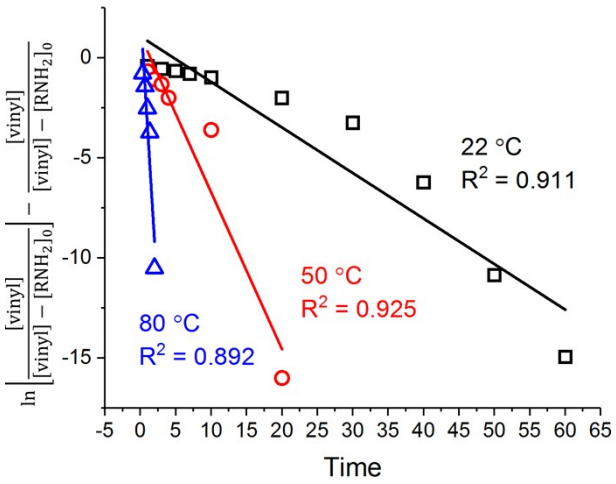

Figure S11. Results of fitting vinyl sulfone conversion data to a 3rd order overall, 1st order in vinyl, 2nd order in hydrazide rate model based on equation **S10** for the stoichiometric reaction of **H6** and DVS at three temperatures.

A + 2B → C + B; A : 1° hydrazide, B: vinyl

1st order hydrazide dependence; 2nd order vinyl dependence:

$$\frac{d[vinyl]}{dt} = -k_1[vinyl]^2[RNH_2] \quad ; \quad [RNH_2] = [vinyl] - [RNH_2]_0 \qquad \textbf{11}$$

3rd order overall solution:

$$\ln\left[\frac{[vinyl] - [RNH_2]_0}{[vinyl]}\right] + \frac{[RNH_2]_0}{[vinyl]} = -k_1[RNH_2]_0{}^2 t - \ln\left[\frac{[vinyl]_0 - [RNH_2]_0}{[vinyl]_0}\right] - \frac{[RNH_2]_0}{[vinyl]_0}$$

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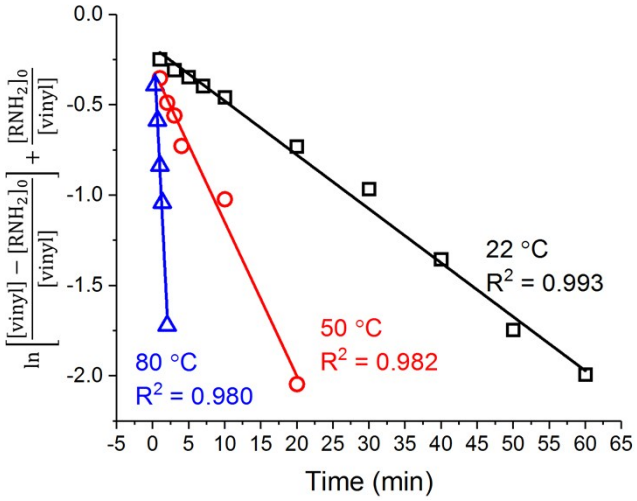

Figure S12. Results of fitting vinyl sulfone conversion data to a 3rd order overall, 1st order in vinyl, 2nd order in hydrazide rate model based on equation **S12** for the stoichiometric reaction of **H6** and DVS at three temperatures.

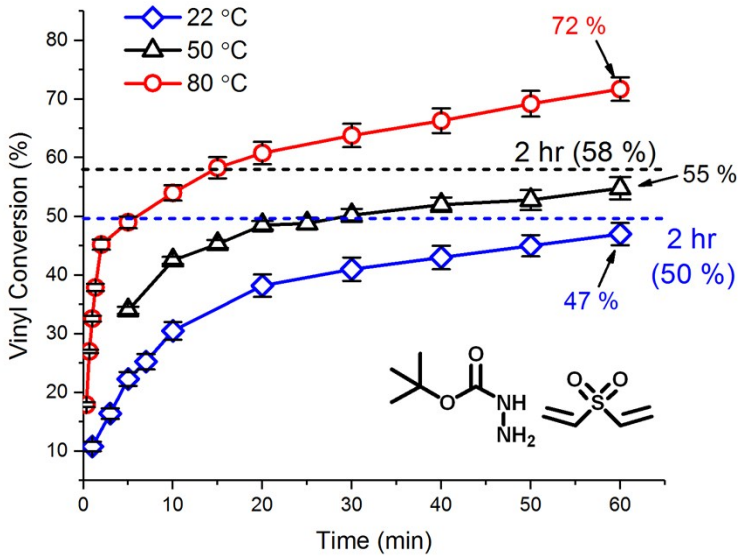

Figure S13. Vinyl conversion versus time during the reaction of **H13**, 2 M, and DVS, 2 M, in DMSO at three different temperatures. Vinyl conversions were determined by ^{1}H NMR of the crude reaction mixture.

A + B → C; A : 1° hydrazide, B: vinyl

1st order hydrazide dependence; 1st order vinyl dependence:

$$\frac{d[vinyl]}{dt} = -k_1[vinyl][RNH_2] \quad ; \quad [RNH_2] = [vinyl] - [RNH_2]_0 \qquad \textbf{13}$$

2nd order overall solution:

$$\ln\left[\frac{[vinyl]-[RNH_2]_0}{[vinyl]}\right] = -k_1[RNH_2]_0 t - \ln\left[\frac{[vinyl]_0-[RNH_2]_0}{[vinyl]_0}\right]$$

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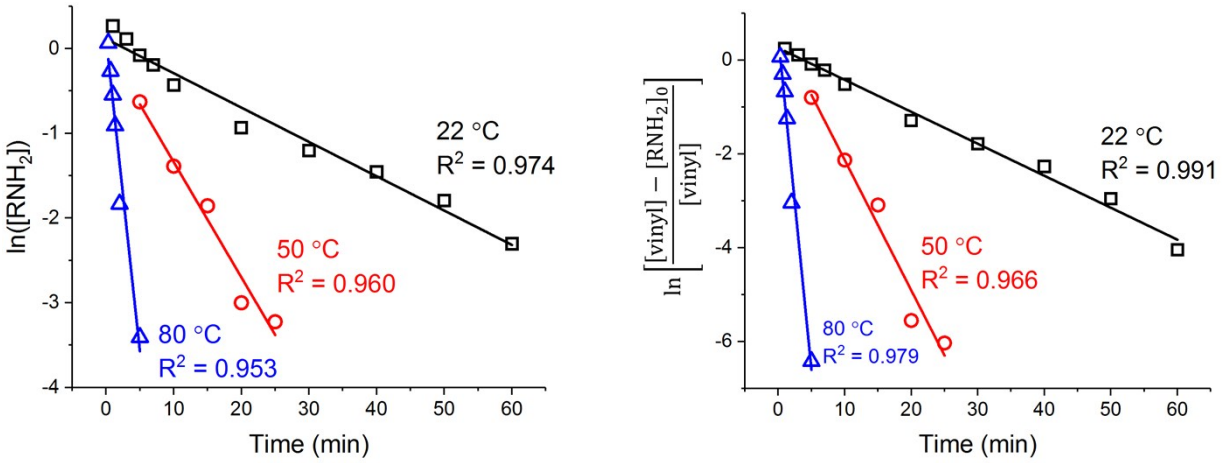


Figure S14. Results of fitting vinyl sulfone conversion data to a (left) 1st order overall, 1st order in hydrazide or hydrazide and a (right) 2nd order overall, 1st order in vinyl, 1st order in hydrazide rate models based on equations **S2** and **S14**, respectively, for the stoichiometric reaction of **H13** and DVS at three temperatures.

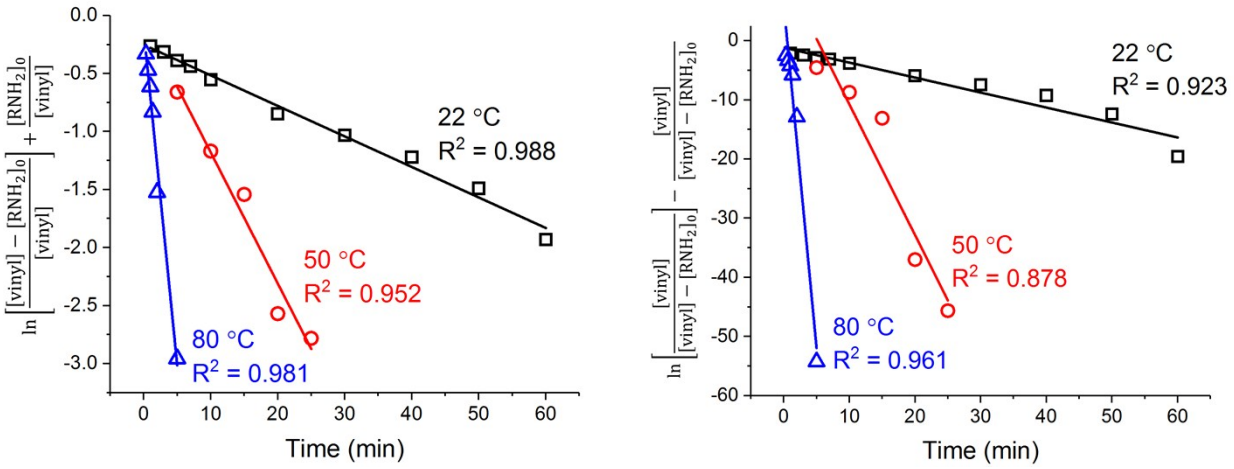


Figure S15. Results of fitting vinyl sulfone conversion data to a (left) 3rd order overall, 1st order in hydrazide, 2nd order in vinyl and a (right) 3rd order overall, 1st order in vinyl, 2nd order in hydrazide rate models based on equations **S12** and **S10**, respectively, for the stoichiometric reaction of **H13** and DVS at three temperatures.

2B) Determination of the reaction order of the 2nd addition step

In order to determine the reaction rate dependence on the 2° hydrazide (R_2NH) and vinyl functional group concentration during the 2nd addition step of the hydrazide-Michael polymerization to form the bis-adduct, the conversion versus time data were analyzed using multiple analytical reaction order models and assessing the models accuracy based on the degree to which the data is linearized by the model. The model reaction of **H6** with DVS in DMSO, $[vinyl]_0 = [hydrazide]_0 = 2$ M, was performed at several temperatures and vinyl conversion was monitored by ^{1}H NMR of crude reaction mixture over the course of 1 hour. Identical reactions with **H12** replacing **H6** were also conducted to affirm the reaction order with another hydrazide. Only vinyl conversions ≥ 50% were used for studying the 2nd addition kinetics as it was assumed that the 2nd addition is insignificant while 1° hydrazide persists in the reaction mixture.

3rd order overall, 3rd order in hydrazide or vinyl:

$$\frac{d[vinyl]}{dt} = -k_2[vinyl]^3 \quad ; \ [vinyl] = [R_2NH] \qquad \textbf{15}$$

3rd order overall solution:

$$1/_{2*[vinyl]^2} = k_2 t + 1/_{2*[vinyl]_0^2} \qquad \textbf{16}$$

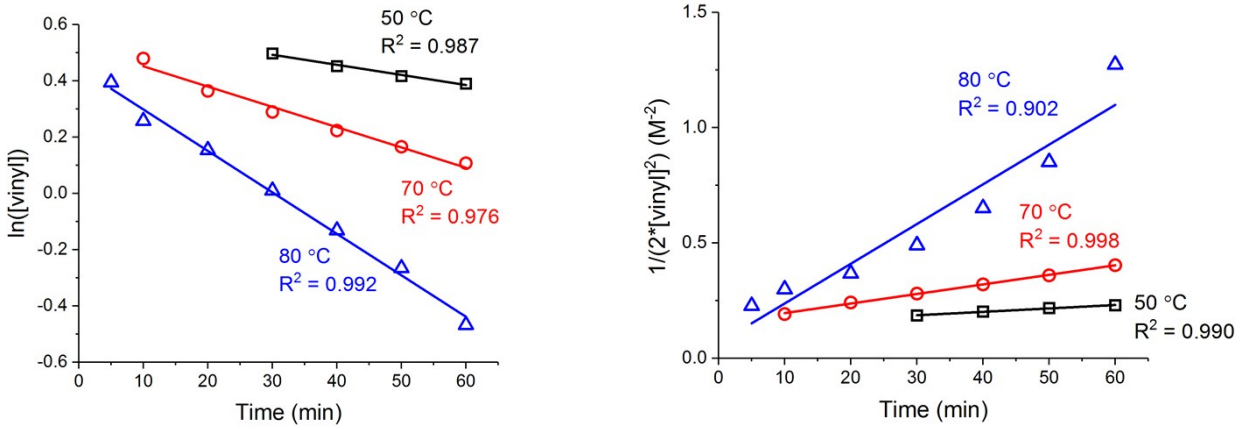


Figure S16. Results of fitting vinyl sulfone conversion data to a (left) 1st order overall, 1st order in hydrazide or vinyl and a (right) 3rd order overall, 3rd order in hydrazide or vinyl rate models based on equations **S2** and **S16**, respectively, for the stoichiometric reaction of **H6** and divinyl sulfone at three temperatures.

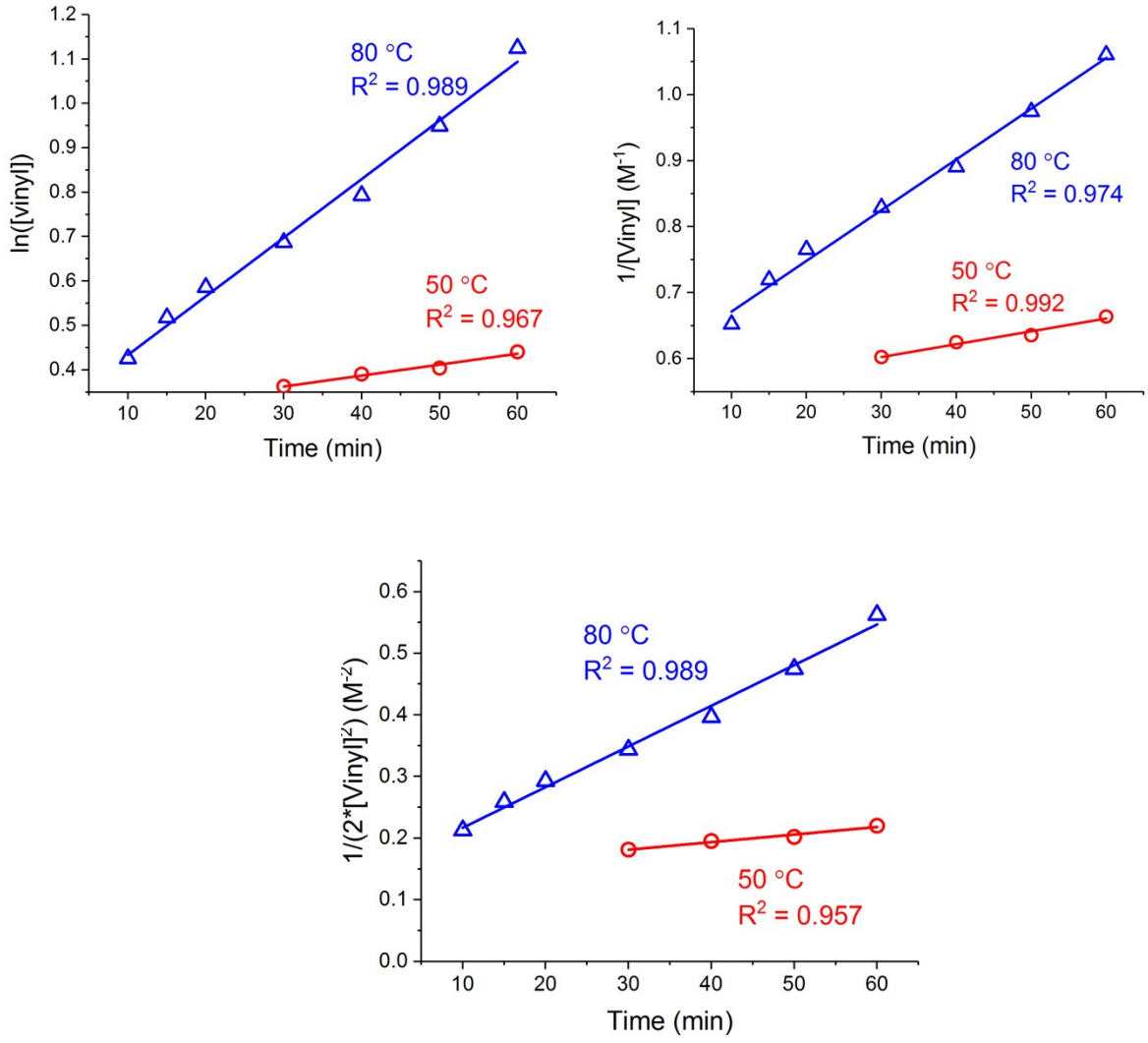


Figure S17. Results of fitting vinyl sulfone conversion data to a (top left) 1st order overall, 1st order in hydrazide or vinyl, a (top right) 2nd order overall, 2nd order in hydrazide or vinyl, and a (bottom) 3rd order overall, 3rd order in hydrazide or vinyl rate models based on equations **S6**, **S8**, and **S16**, respectively, for the stoichiometric reaction of **H12** and divinyl sulfone at three temperatures.

3) Evaluation of kinetic rate constants and activation energy for the 1st and 2nd addition steps

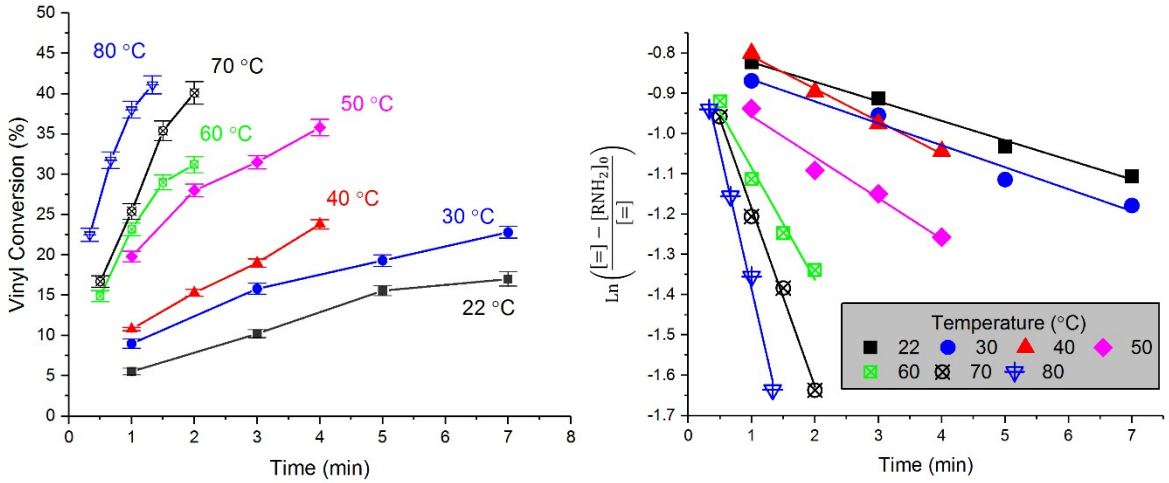


Figure S18. Stoichiometric reaction of **H6** and divinyl sulfone in DMSO, [hydrazide] = [DVS] = 2.0 M, at multiple temperatures. (left) Vinyl group conversion versus time; conversions determined by ^{1}H NMR spectrums of the crude reaction mixture. (right) Linear fitting of the vinyl conversion data to the 2nd order overall, 1st order in hydrazide, and 1st order in vinyl rate model based on equation **S14**.

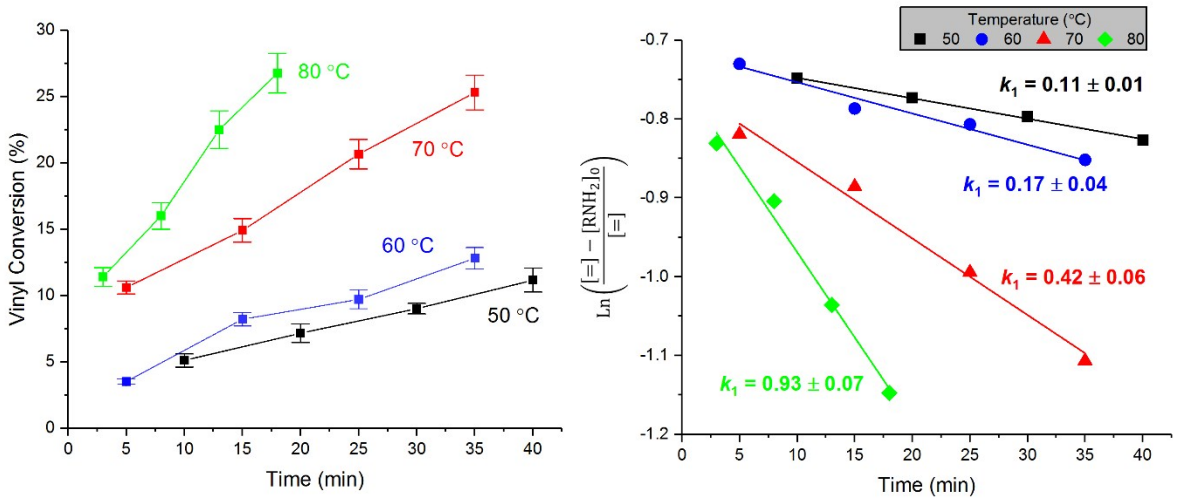
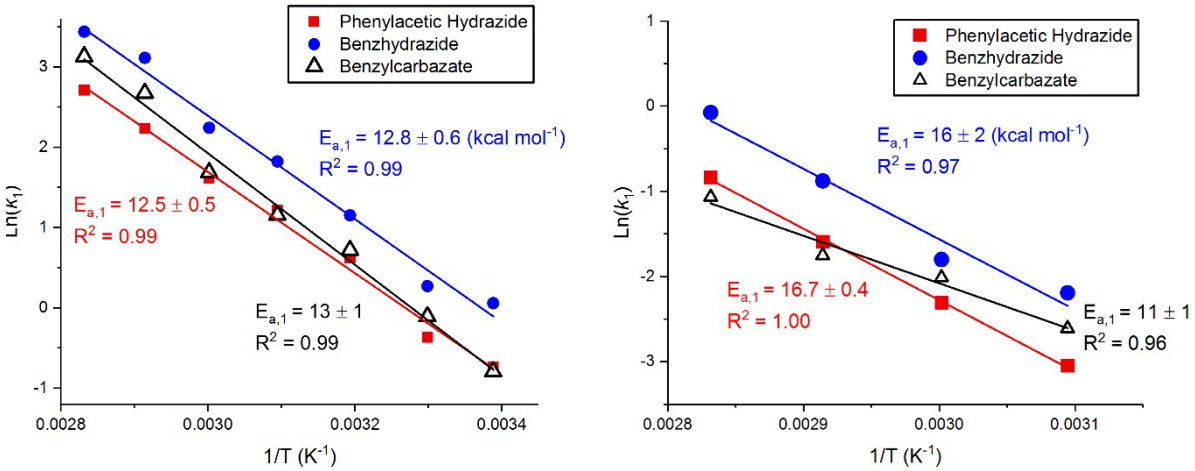


Figure S19. Stoichiometric reaction of **H6** and HDAA in DMSO, [hydrazide] = [HDA] = 2.0 M, at multiple temperatures. (left) Vinyl group conversion versus time; conversions determined by ^{1}H NMR spectrums of the crude reaction mixture. (right) Linear fitting of the vinyl conversion data to the 2nd order overall, 1st order in hydrazide, and 1st order in vinyl rate model based on equation **S14**.



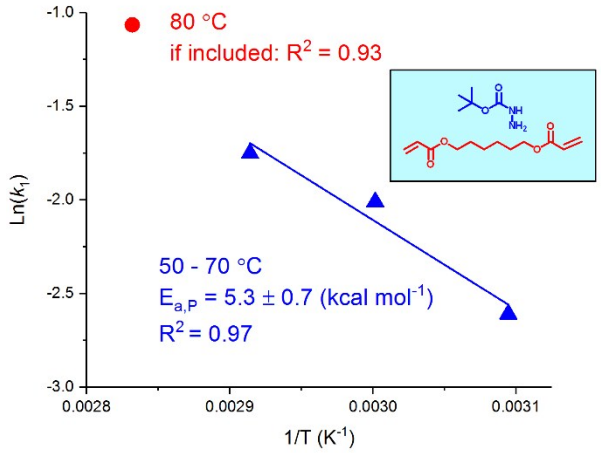


Figure S20. Determination of the apparent activation energy of the mono-addition step during the hydrazide-Michael polymerization using the Arrhenius relationship by linear fitting ln(k_1) versus 1/T for the stoichiometric reactions of (top left) benzhydrazide (**H6**), phenylacetichydrazide (**H4**), and benzylcarbazate (**H13**) with divinyl sulfone, (top right) benzhydrazide (**H6**), phenylacetichydrazide (**H4**), and benzylcarbazate (**H13**) with 1,6-hexanediol diacrylate, and (bottom) *t*-butyl carbazate (**H12**) with 1,6-hexanediol diacrylate in DMSO, [hydrazide] = [DVS] or [HDA] = 2.0 M.

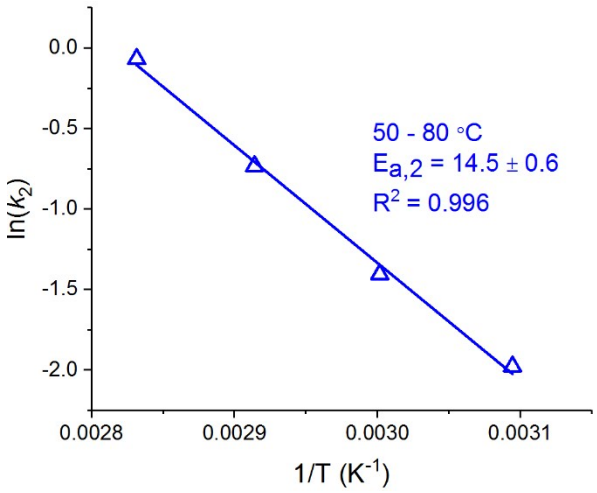


Figure S21. Determination of the apparent activation energy of the bis-addition step during the **H6**-DVS polymerization using the Arrhenius relationship by linear fitting ln(k_2) versus 1/T for the stoichiometric reaction of **H6** and divinyl sulfone in DMSO, $[\text{hydrazide}]_0 = [\text{DVS}]_0 = 2.0$ M.

4) Simulation of hydrazide-Michael reaction kinetics

Simulations of the hydrazide-Michael reaction were carried out using the experimentally determined rate equations (**Eq 1** and **Eq 2** from the main text, for the mono-addition and bis-addition reactions, respectively) and kinetic parameters for the reactions of benzhydrazide (**H6**) and tert-butyl carbazate (**H12**) with DVS in DMSO at 22, 30, 50, and 80 °C. The model reaction kinetics were simulated using the ODE45 differential equation solver in MATLAB R2019a and then plotted with the experimental conversion data to compare the model's accuracy. For the **H12**/DVS reaction model, the experimentally determined kinetic parameters were directly used. For the **H6**/DVS reaction model, the kinetic rate constants used for the mono-addition reaction were based off of the experimentally measured kinetic rate constant at 22 °C and 80 °C for the mono- and bis-addition steps respectively. The kinetic rate constants used for the simulation were extrapolated using the standard Arrhenius relationship and the experimentally determined 1st and 2nd addition activation energies. Additionally, the simulations were used to predict the concentration profiles of each species and their rates of consumption as a function of reaction time and 1° hydrazide conversion.

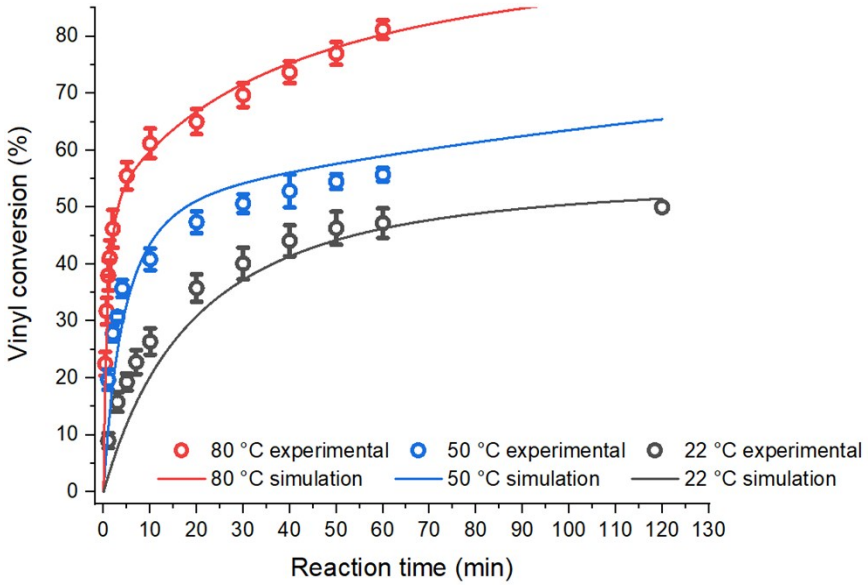


Figure S22. Model predicted and experimental vinyl functional group conversions versus time for the reaction of benzhydrazide (**H6**) with DVS at 22, 50, and 80 °C in DMSO, where hydrazide and DVS concentrations are 2 M. Kinetic parameters used for modeling are (80 °C) [k_1 = 25.35 L mol^{-1} hr^{-1}; k_2 = 0.941 L mol^{-1} hr^{-1}], (50 °C) [k_1 = 4.787 L mol^{-1} hr^{-1}; k_2 = 0.138 L mol^{-1} hr^{-1}], and (22 °C) [k_1 = 1.062 L mol^{-1} hr^{-1}; k_2 = 0.0162 L mol^{-1} hr^{-1}].

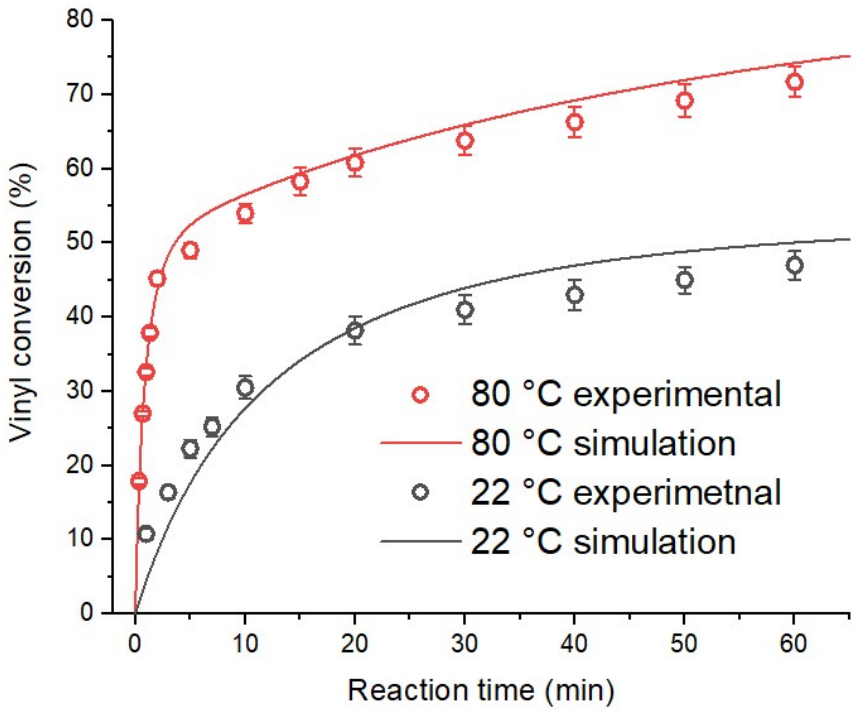


Figure S23. Model predicted and experimental vinyl functional group conversions versus time for the reaction of tert-butyl carbazate (**H12**) with DVS at 22, 50, and 80 °C in DMSO, where hydrazide and DVS concentrations are 2 M. Kinetic parameters used for modeling are (80 °C) [k_1 = 24.72 L mol^{-1} hr^{-1}; k_2 = 0.5749 L mol^{-1} hr^{-1}] and (22 °C) [k_1 = 1.746 L mol^{-1} hr^{-1}; k_2 = 0.0291 L mol^{-1} hr^{-1}].

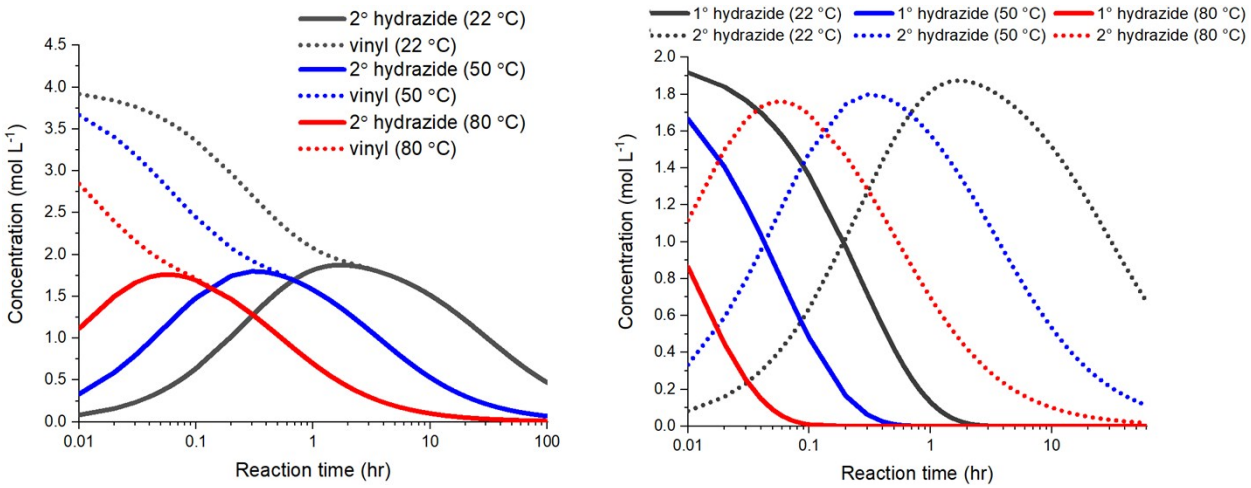


Figure S24. Simulated concentration profiles of (left) 2° hydrazide and vinyl functional groups and (right) 1° and 2° hydrazide functional groups versus time during the reaction of benzhydrazide (**H6**) with DVS in DMSO at 22, 50, and 80 °C, where the initial hydrazide and DVS concentrations are 2 M. Kinetic parameters used for modeling are (80 °C) [k_1 = 25.35 L mol^{-1} hr^{-1}; k_2 = 0.941 L mol^{-1} hr^{-1}], (50 °C) [k_1 = 4.787 L mol^{-1} hr^{-1}; k_2 = 0.138 L mol^{-1} hr^{-1}], and (22 °C) [k_1 = 1.062 L mol^{-1} hr^{-1}; k_2 = 0.0162 L mol^{-1} hr^{-1}].

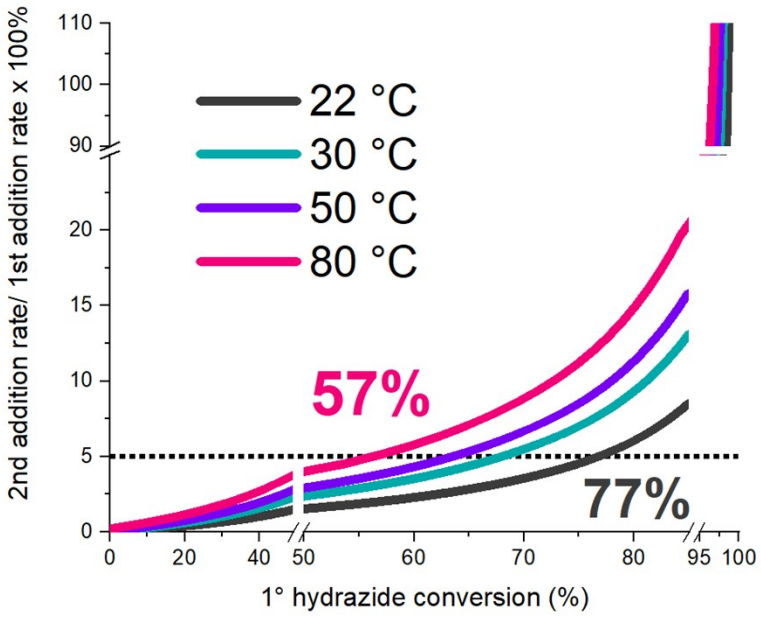


Figure S25. Model predictions for the ratio of the bis-addition to mono-addition reaction rate versus 1° hydrazide conversion for the reaction of benzhydrazide (**H6**) with DVS in DMSO at 22, 30, 50, and 80 °C, where the initial hydrazide and DVS concentrations are 2 M. The dotted line denotes where the rate of the bis-addition rate is 5% of the rate of the mono-addition reaction. Kinetic rate constants corresponding to (22 °C) [k_1 = 1.062 L mol^{-1} hr^{-1}; k_2 = 0.0162 L mol^{-1} hr^{-1}], (30 °C) [k_1 = 1.312 L mol^{-1} hr^{-1}; k_2 = 0.0312 L mol^{-1} hr^{-1}], (50 °C) [k_1 = 4.787 L mol^{-1} hr^{-1}; k_2 = 0.138 L mol^{-1} hr^{-1}], and (80 °C) [k_1 = 25.35 L mol^{-1} hr^{-1}; k_2 = 0.941 L mol^{-1} hr^{-1}].

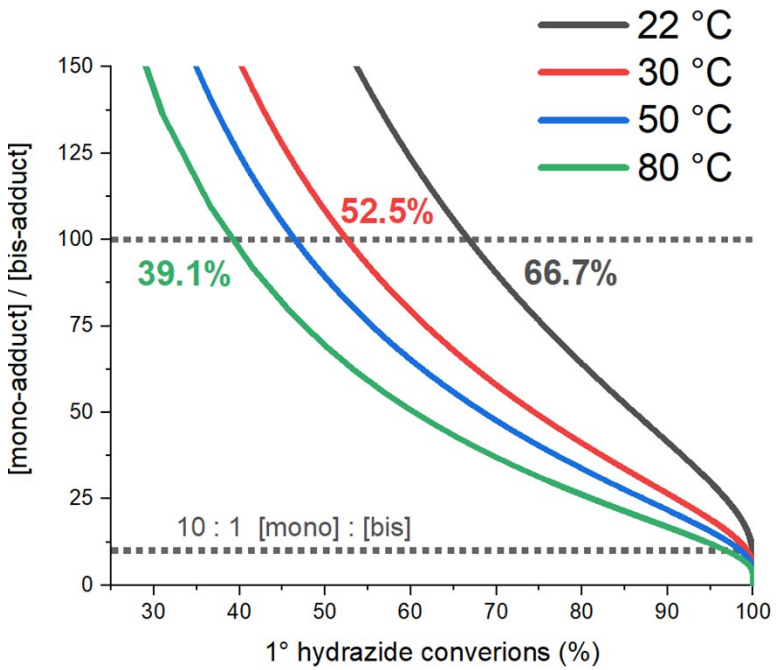


Figure S26. Model predictions of the selectivity of the mono-addition product relative to the bis-addition product versus 1° hydrazide conversion for the reaction between benzhydrazide (**H6**) and DVS in DMSO at at 22, 30, 50, and 80 °C, where the initial hydrazide and DVS concentrations are 2 M. The dotted lines indicate the predicted 1° hydrazide conversions where bis-addition product concentration is 1% and 10% of the mono-addition product concentration. Kinetic rate constants corresponding to (22 °C) [k_1 = 1.062 L mol^{-1} hr^{-1}; k_2 = 0.0162 L mol^{-1} hr^{-1}], (30 °C) [k_1 = 1.312 L mol^{-1} hr^{-1}; k_2 = 0.0312 L mol^{-1} hr^{-1}], (50 °C) [k_1 = 4.787 L mol^{-1} hr^{-1}; k_2 = 0.138 L mol^{-1} hr^{-1}], and (80 °C) [k_1 = 25.35 L mol^{-1} hr^{-1}; k_2 = 0.941 L mol^{-1} hr^{-1}].

5) Computational energetics and thermodynamics

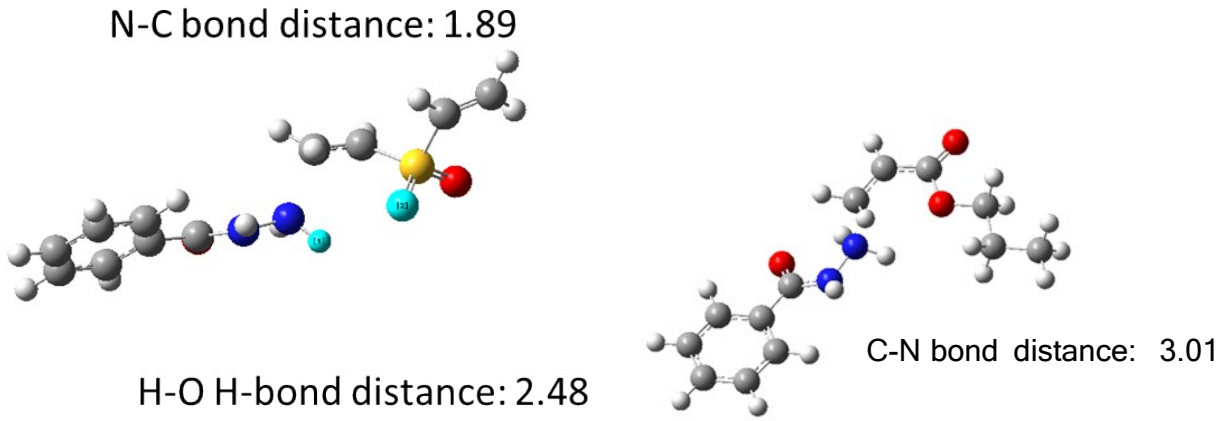


Figure S27. Optimized transition state structure for the formation of **Z1** in the (left) **H6**/DVS and (right) **H6**/HDA reaction. Distances are reported in angstroms. Color code: grey = C, white = H, blue = N, red = O, yellow = S.

Table S1. Enthalpy and Gibb's free energy of transition states, zwitterion intermediates, and mono- and bis-adducts of hydrazide-Michael reactions at 75 °C. All values reported in kcal mol^{-1}.

Acceptor	Hydrazide	TS1[a]		Z1[a]		Mono-adduct[a]		TS2[b]		Z2[b]		Bis-adduct[b]	
		H	G	H	G	H	G	H	G	H	G	H	G
DVS	Benzhydrazide (**H6**)	14.7	15.6	14.3	15.1	-19.8	-18.9	11.0	13.9	10.7	13.3	-21.7	-18.8
	Valerichydrazide (**H2**)			13.6	18.2								
	Phenylacetic hydrazide (**H4**)			14.0	19.6								
	Tert-butyl carbazate (**H12**)			13.5	17.7								
	Benzylcarbazate (**H13**)			12.9	17.9								
nPA	Benzhydrazide (**H6**)	16.4	17.5	15.2	16.8	-18.5	-17.4	*c*	*c*	4.60	9.66	-17.5	-12.3
	Phenylacetic hydrazide (**H4**)			14.3	19.0								
	Tert-butyl carbazate (**H12**)			14.1	21.2								
	Benzylcarbazate (**H13**)			13.4	20.9								

[a] Energies relative to hydrazide and DVS or nPA. [b] Energies relative to mono-addition adduct and DVS or nPA. [c] TS did not converge.

6) Michael reactivity comparison of benzhydrazide and hexyl amine

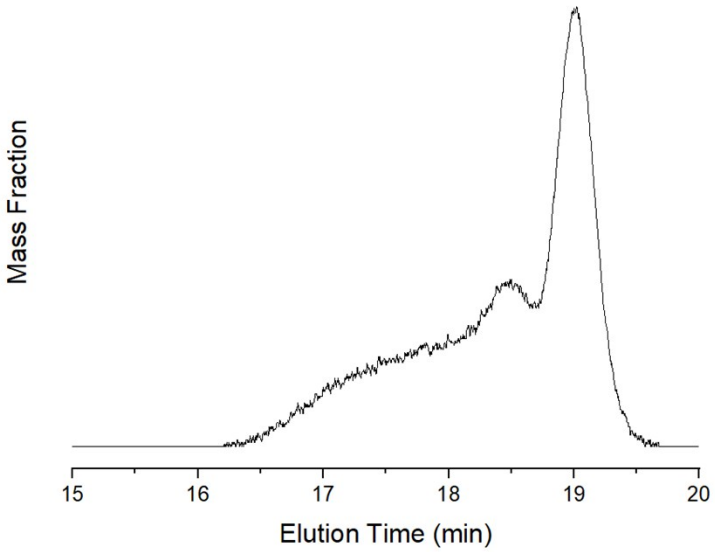


Figure S28. GPC curves of the crude reaction product for the reaction of hexyl amine with DVS in DMSO at 75 °C, $[\text{hexyl amine}]_0 = [\text{divinyl sulfone}]_0 = 2$ M. Final conversion vinyl conversion was 98% after 5 days.

7) IR of polymers

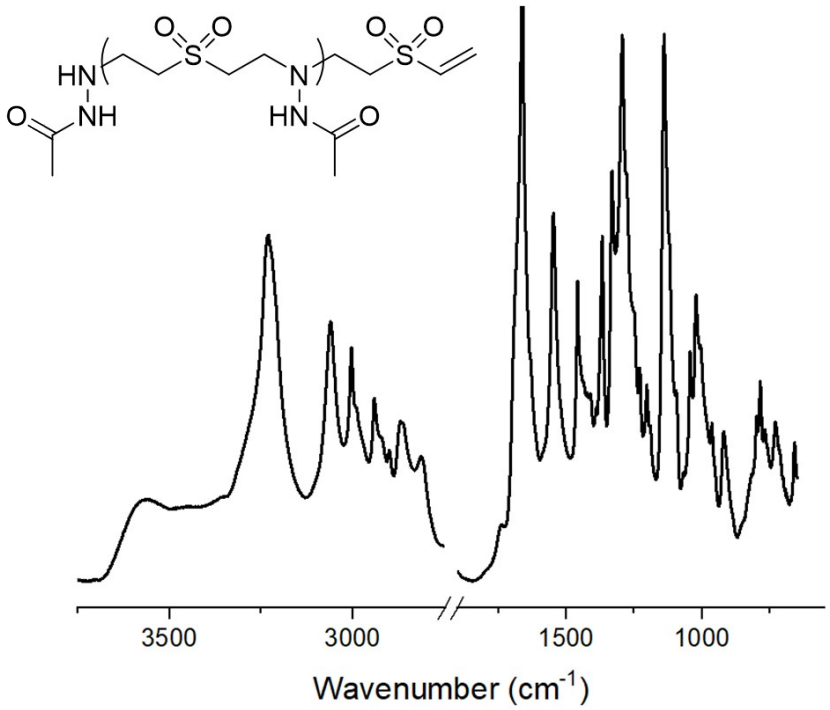


Figure S29: FTIR spectrum and structural assignment of the purified **H1**/DVS polymer.

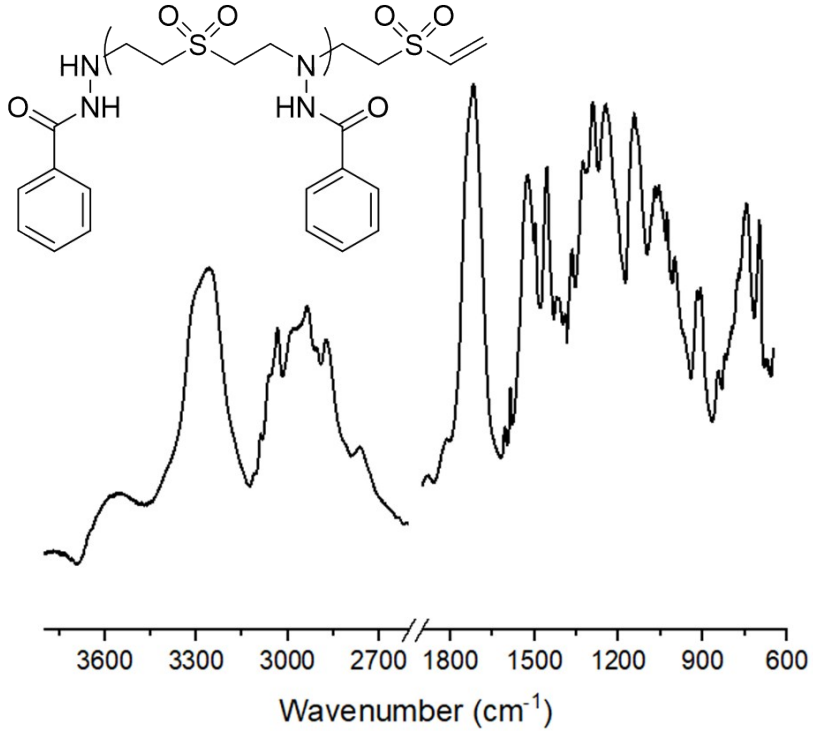


Figure S30: FTIR spectrum and structural assignment of the purified **H6**/DVS polymer.

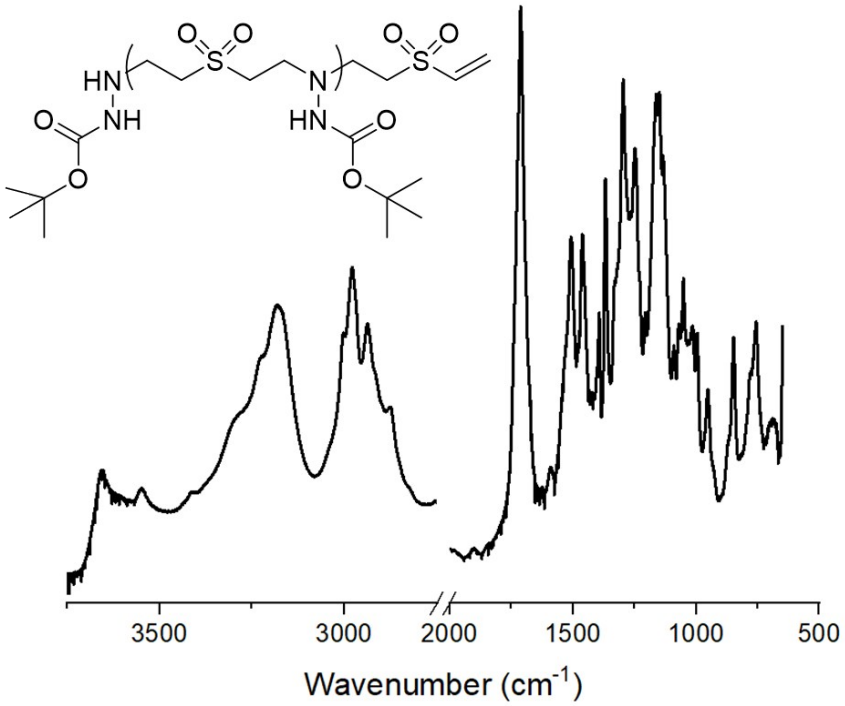


Figure S31: FTIR spectrum and structural assignment of the purified **H12**/DVS polymer.

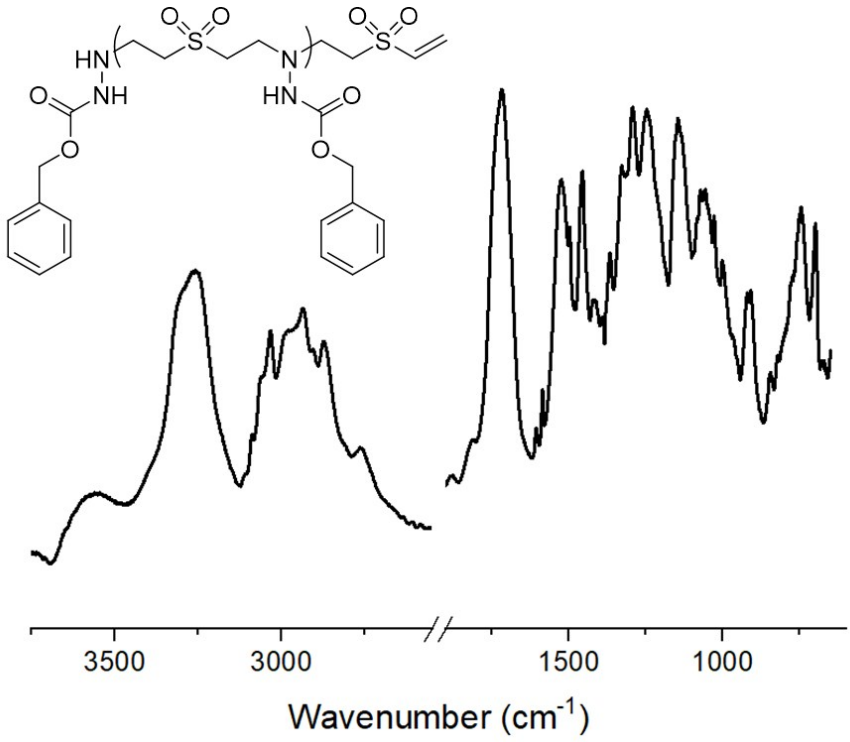


Figure S32: FTIR spectrum and structural assignment of the purified **H13**/DVS polymer.

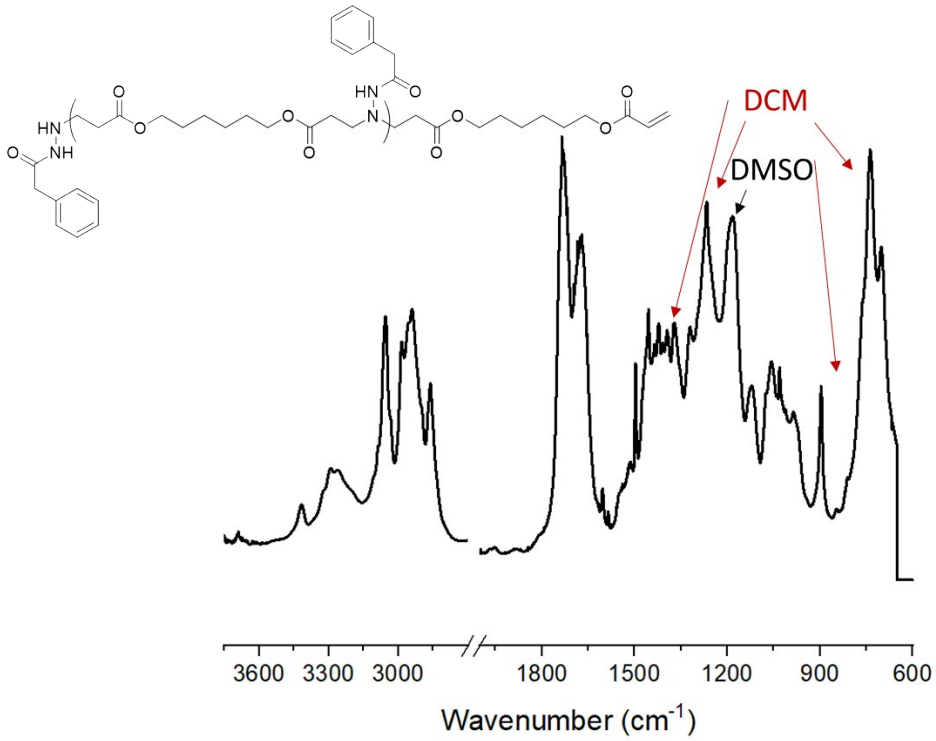


Figure S33: FTIR spectrum and structural assignment of the crude **H4**/HDA polymer.

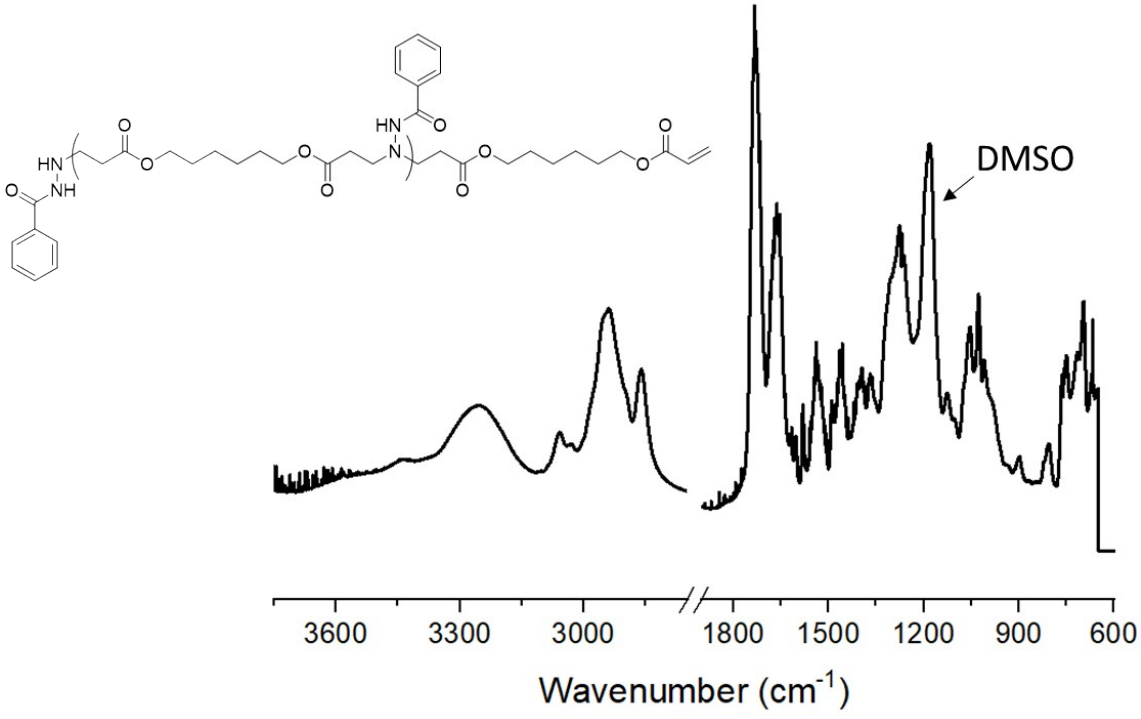


Figure S34: FTIR spectrum and structural assignment of the crude **H6**/HDA polymer.

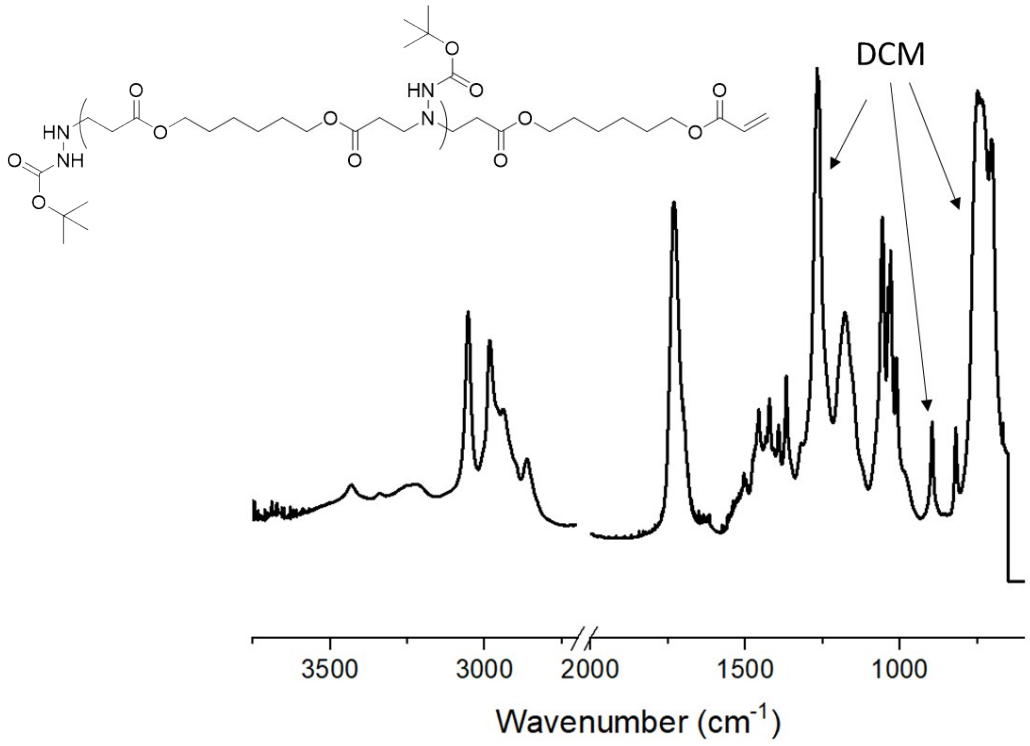


Figure S35: FTIR spectrum and structural assignment of the purified **H12**/HDA polymer.

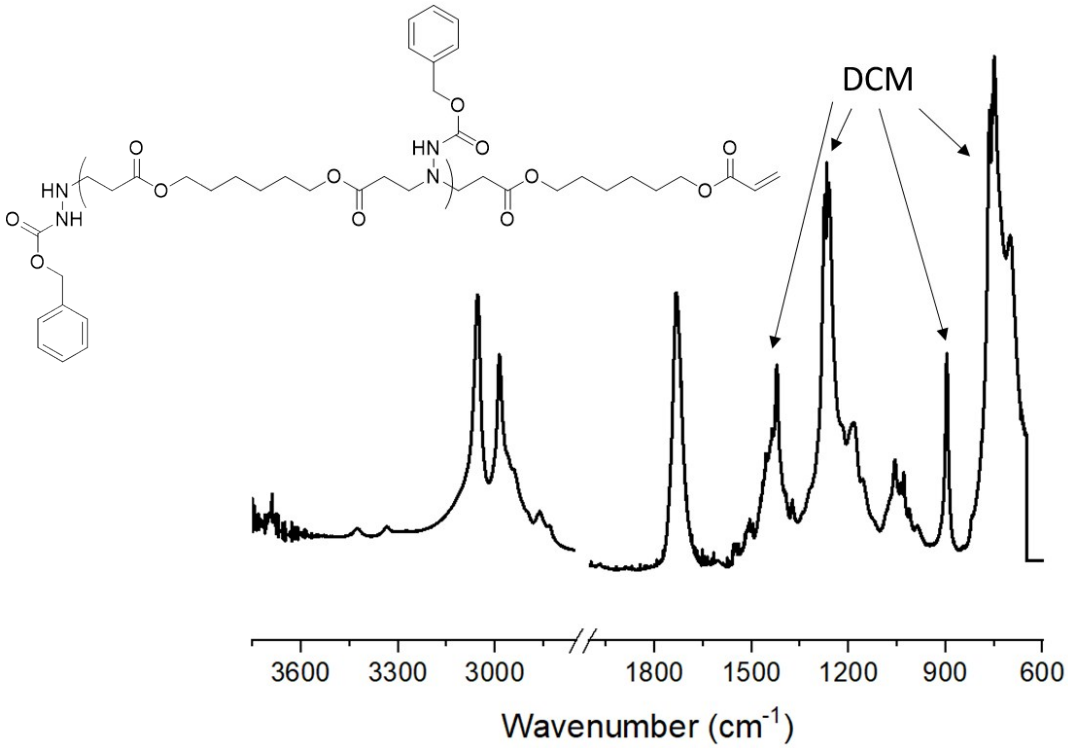


Figure S36: FTIR spectrum and structural assignment of the purified **H13**/HDA polymer.

10) NMR of polymers

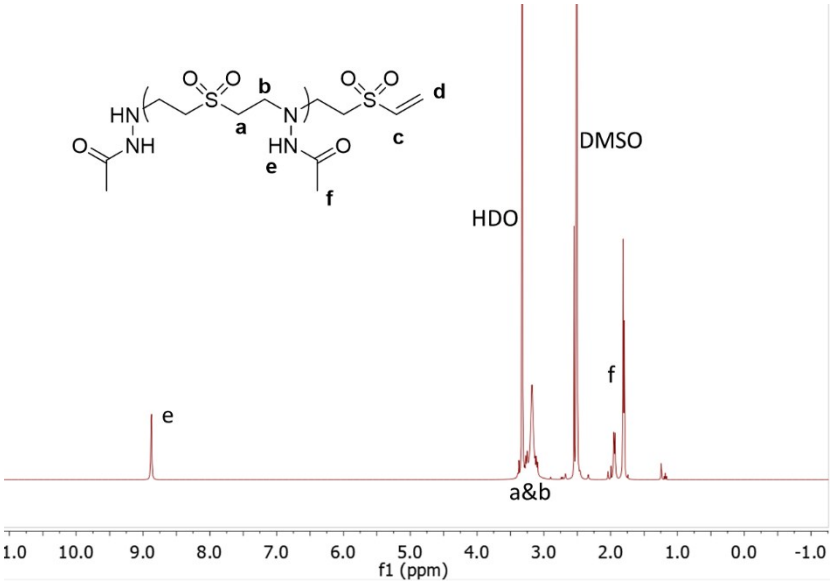


Figure S37: [1]H NMR spectrum and structural assignment of the crude product of the **H1**/DVS polymerization.

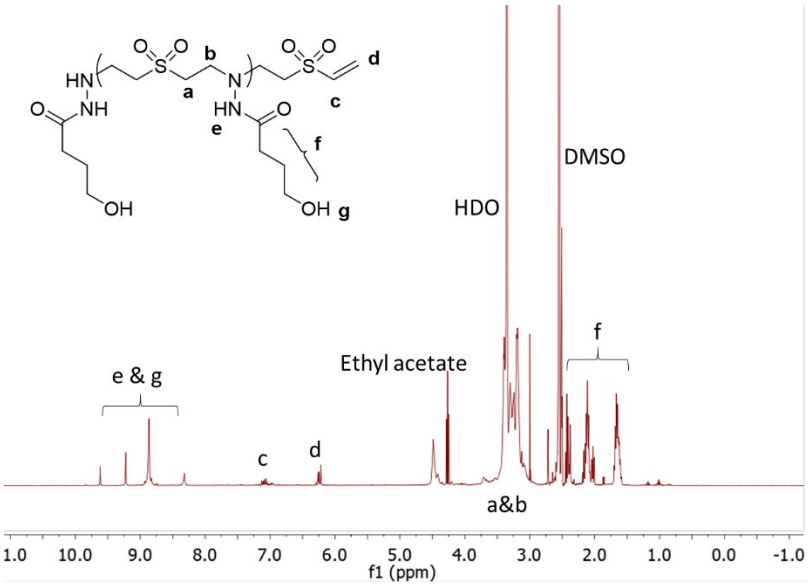


Figure S38: [1]H NMR spectrum and structural assignment of the **H3**/DVS polymerization.

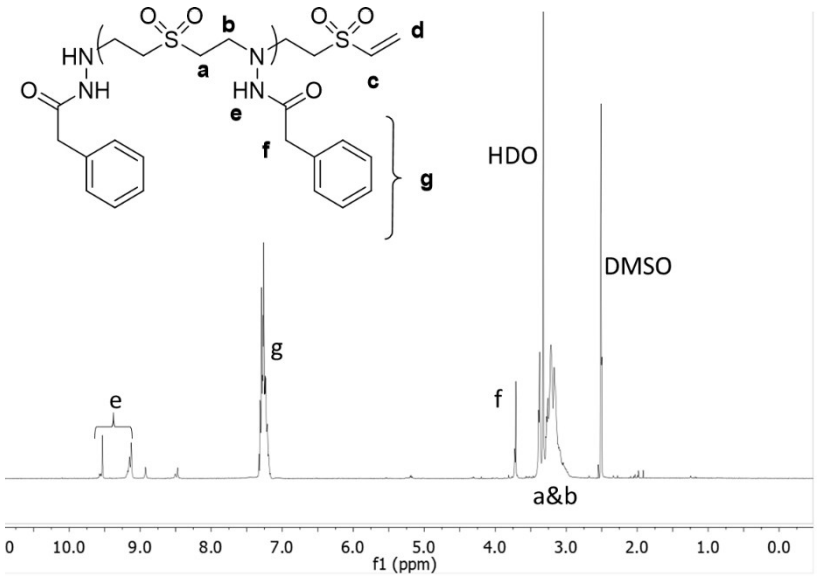


Figure S39: [1]H NMR spectrum and structural assignment of the crude product of the **H4**/DVS polymerization.

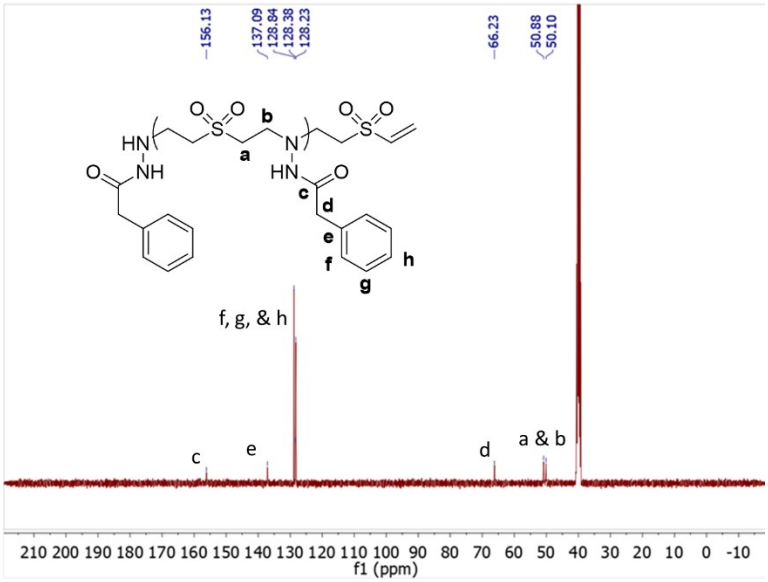


Figure S40: [13]C NMR spectrum and structural assignment of the crude product of the **H4**/DVS polymerization.

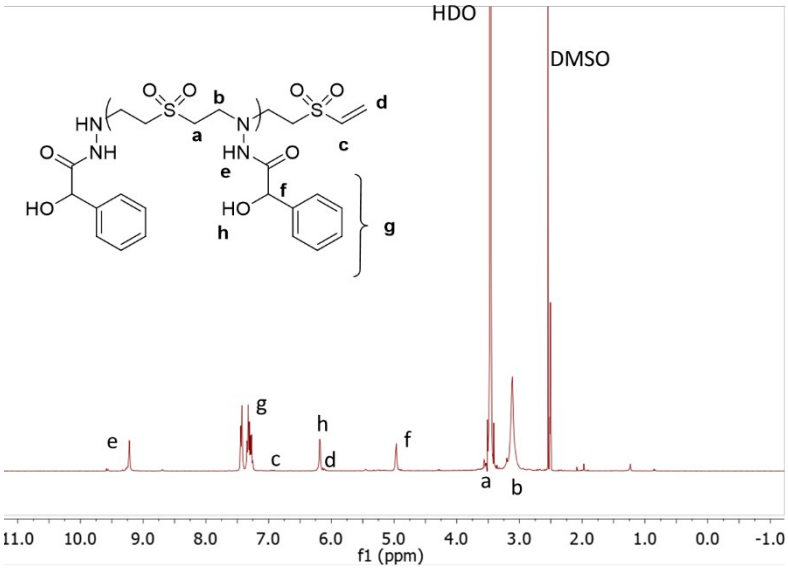


Figure S41: [1]H NMR spectrum and structural assignment of the crude product of the **H5**/DVS polymerization.

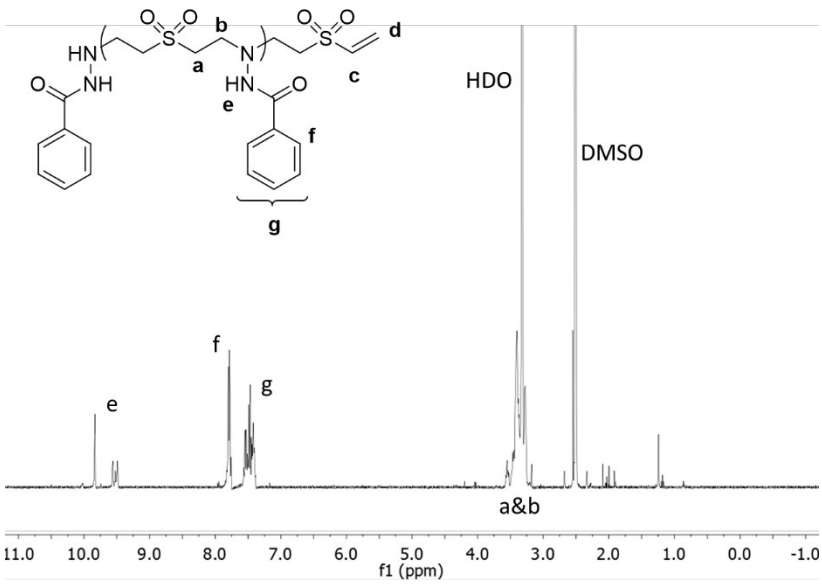


Figure S42: [1]H NMR spectrum and structural assignment of the crude product of the **H6**/DVS polymerization.

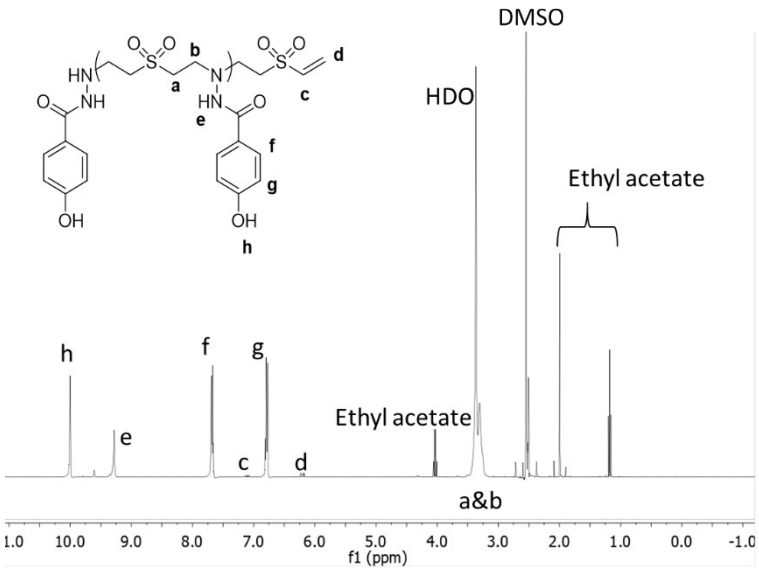


Figure S43: [1]H NMR spectrum and structural assignment of the **H7**/DVS polymerization.

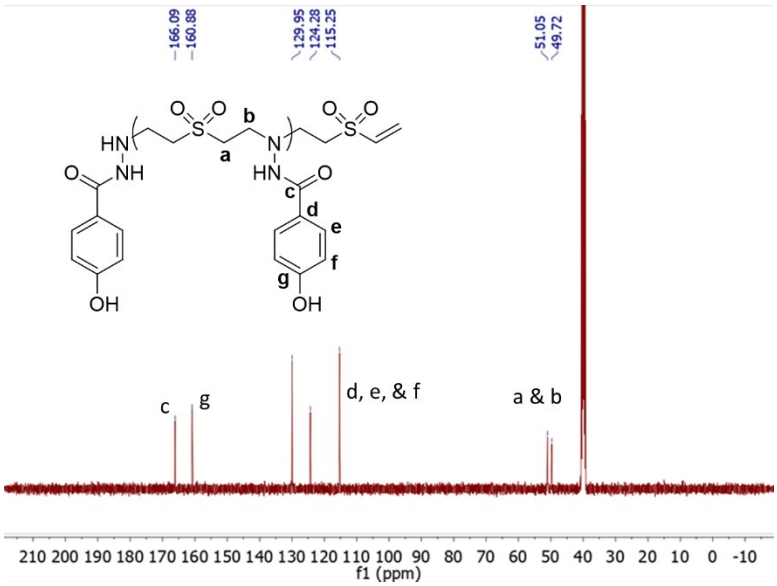


Figure S44: [13]C NMR spectrum and structural assignment of the crude product of the **H7**/DVS polymerization.

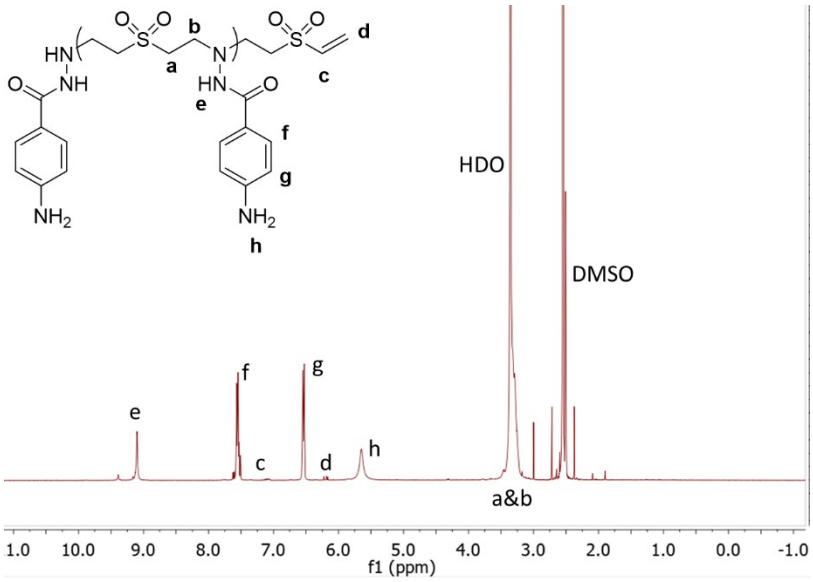


Figure S45: [1]H NMR spectrum and structural assignment of the crude product of the **H8**/DVS polymerization.

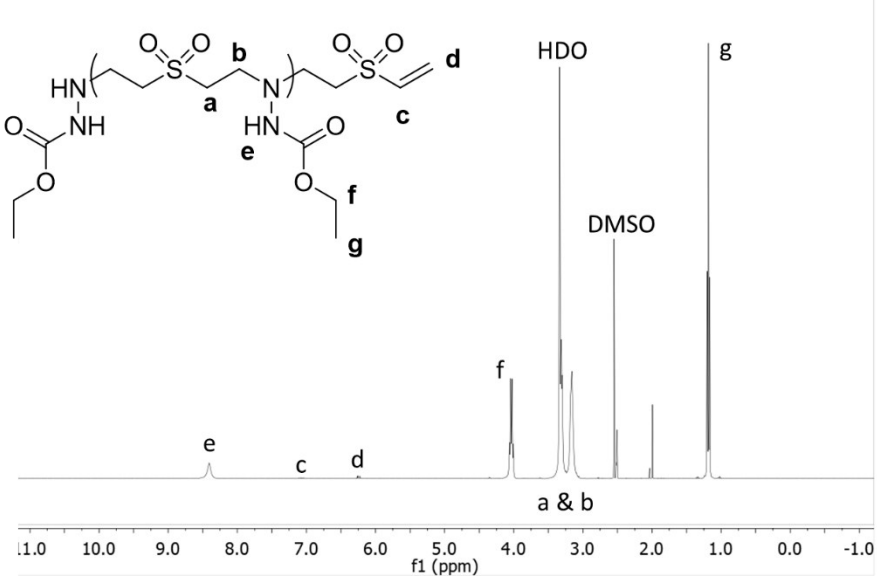


Figure S46: [1]H NMR spectrum and structural assignment of the crude product of the **H11**/DVS polymerization.

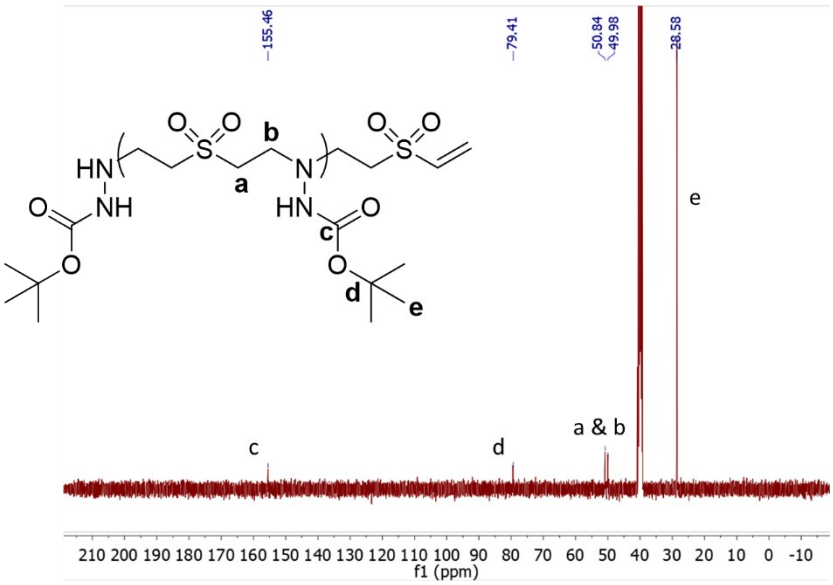


Figure S47: ^{13}C NMR spectrum and structural assignment of the crude product of the **H12**/DVS polymerization.

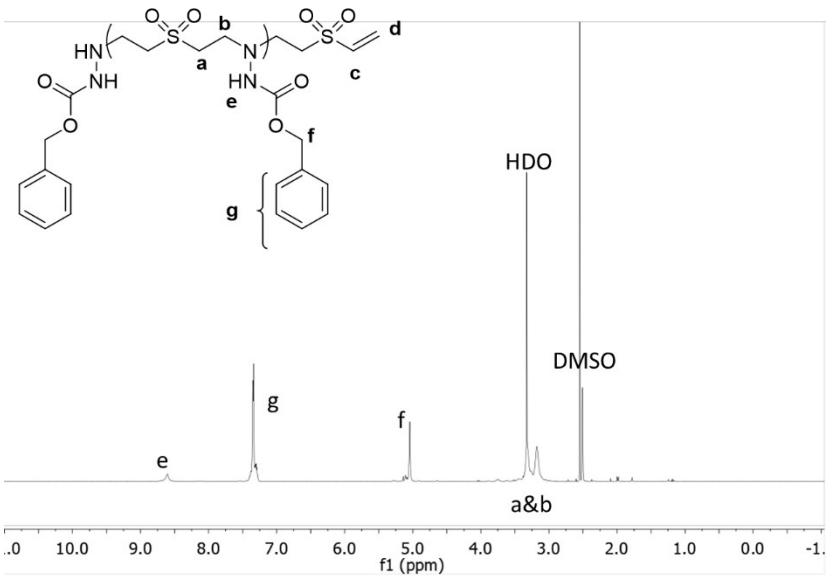


Figure S48: ^{1}H NMR spectrum and structural assignment of the crude product of the **H13**/DVS polymerization.

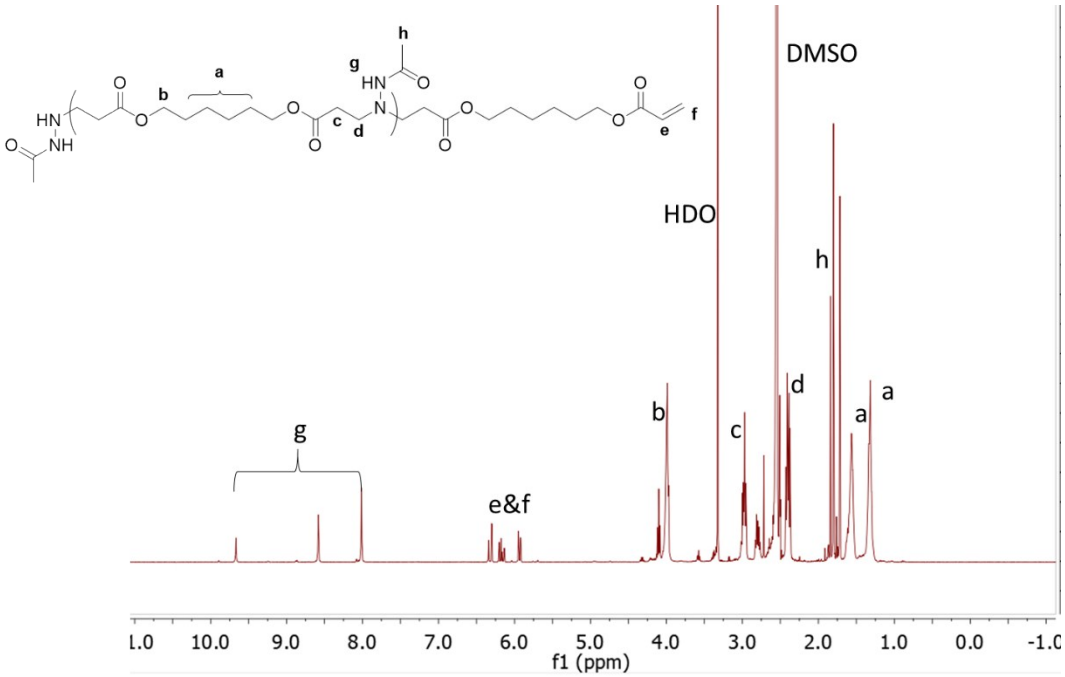


Figure S49: [1]H NMR spectrum and structural assignment of the crude product of the **H1**/HDA polymerization.

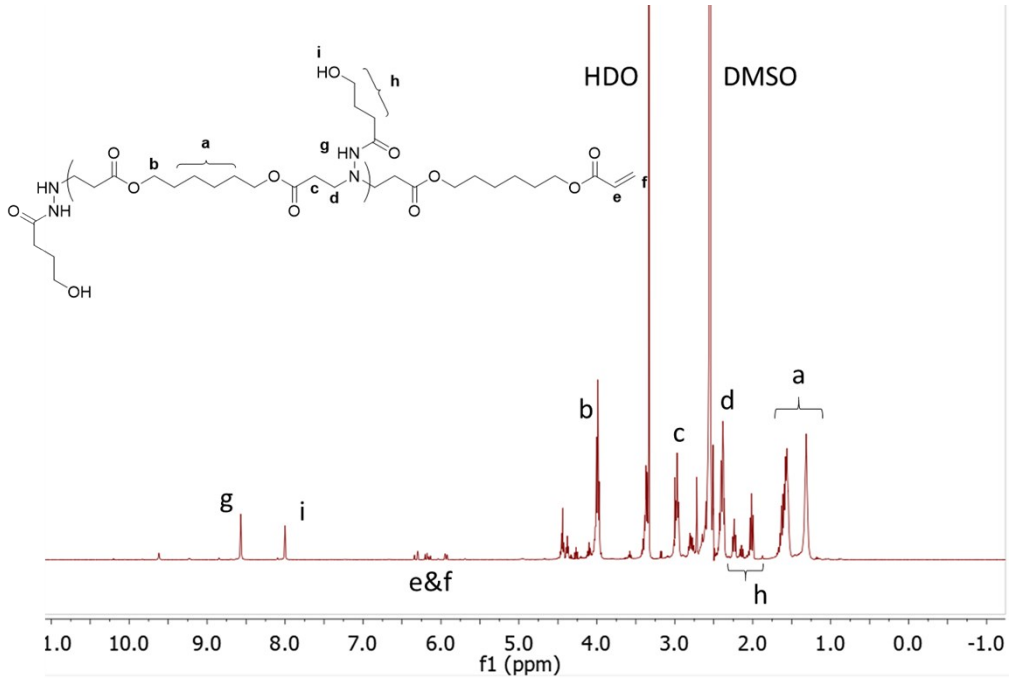


Figure S50: [1]H NMR spectrum and structural assignment of the crude product of the **H3**/HDA polymerization.

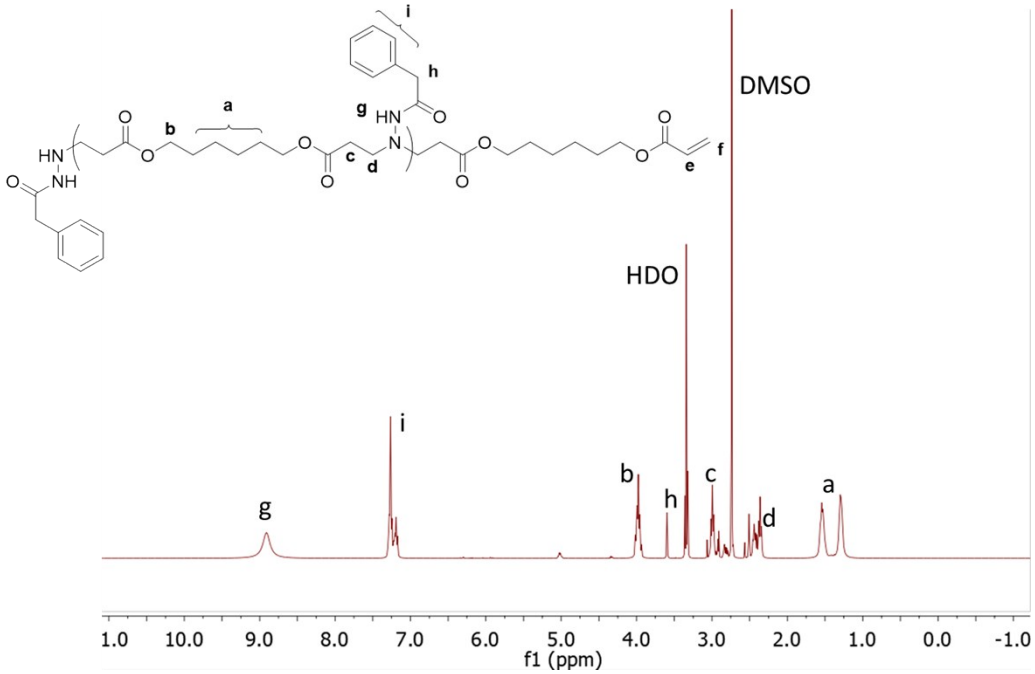


Figure S51: [1]H NMR spectrum and structural assignment of the crude product of the **H4**/HDA polymerization.

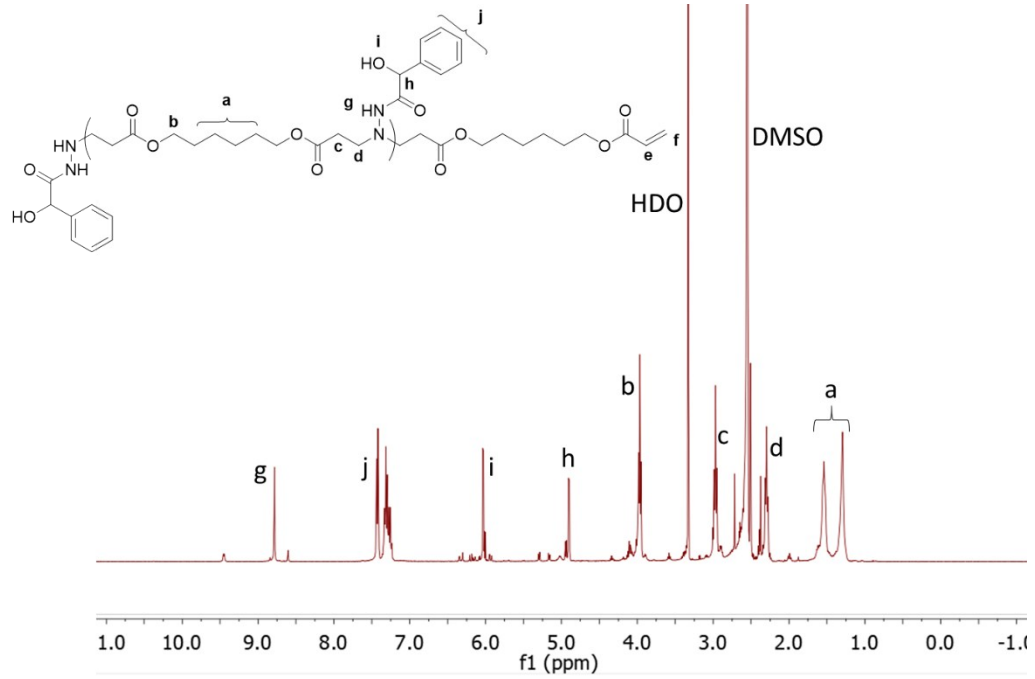


Figure S52: [1]H NMR spectrum and structural assignment of the crude product of the **H5**/HDA polymerization.

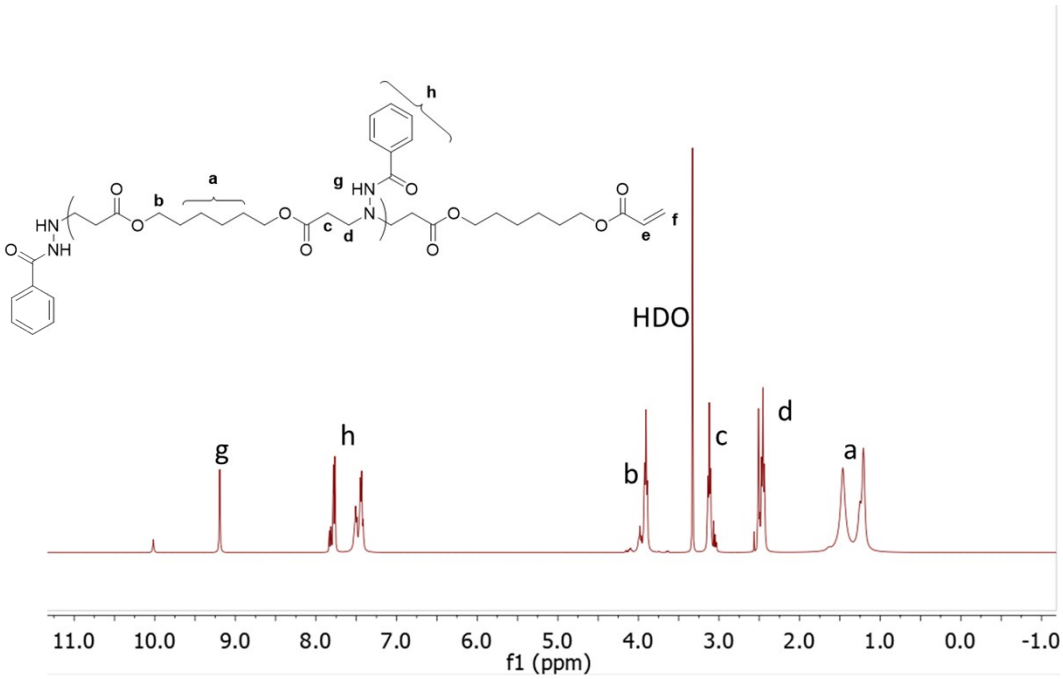


Figure S53: [1]H NMR spectrum and structural assignment of the crude product of the **H6**/HDA polymerization.

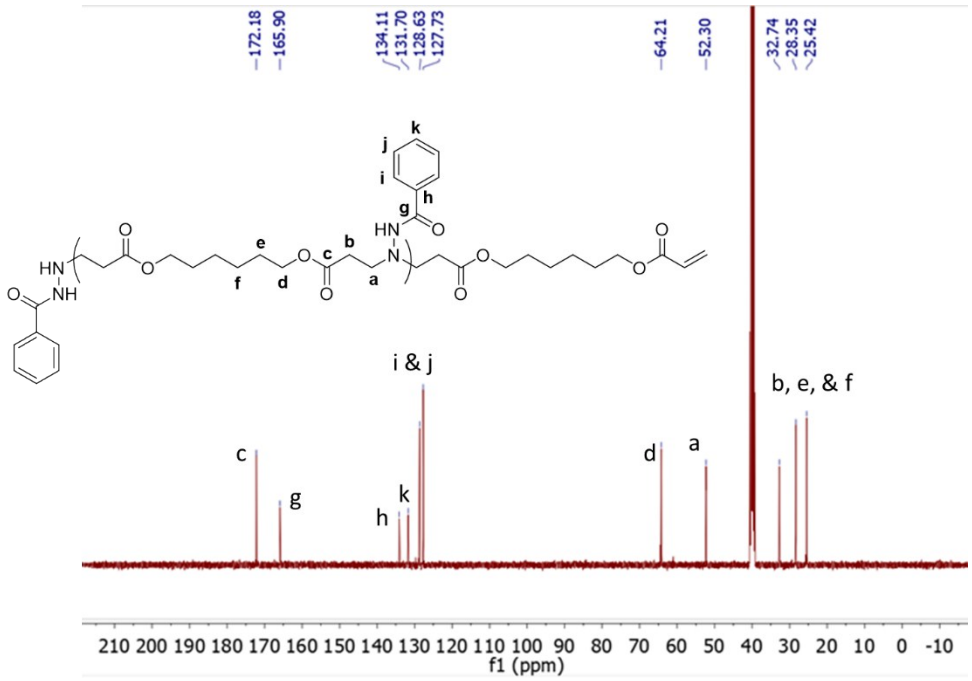


Figure S54: [13]C NMR spectrum and structural assignment of the crude product of the **H6**/HDA polymerization.

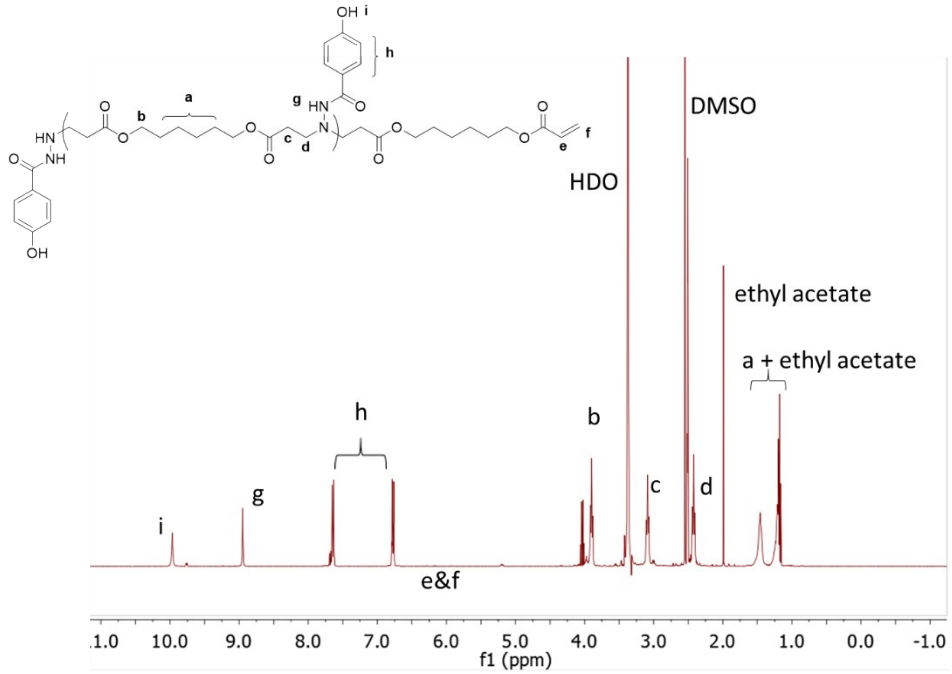


Figure S55: [1]H NMR spectrum and structural assignment of the **H7**/HDA polymerization.

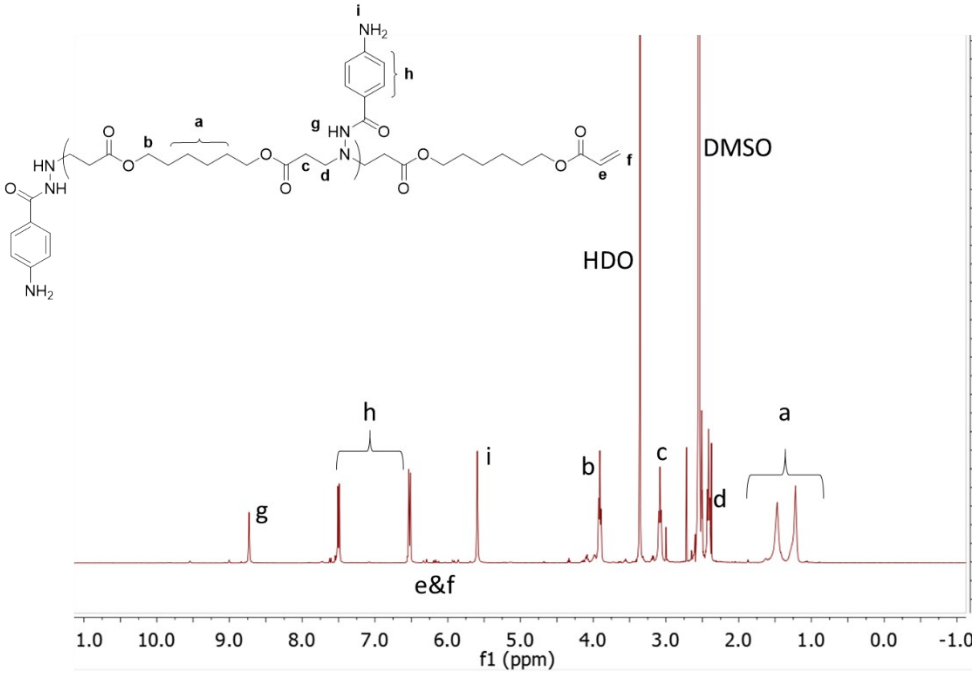


Figure S56: [1]H NMR spectrum and structural assignment of the crude product of the **H8**/HDA polymerization.

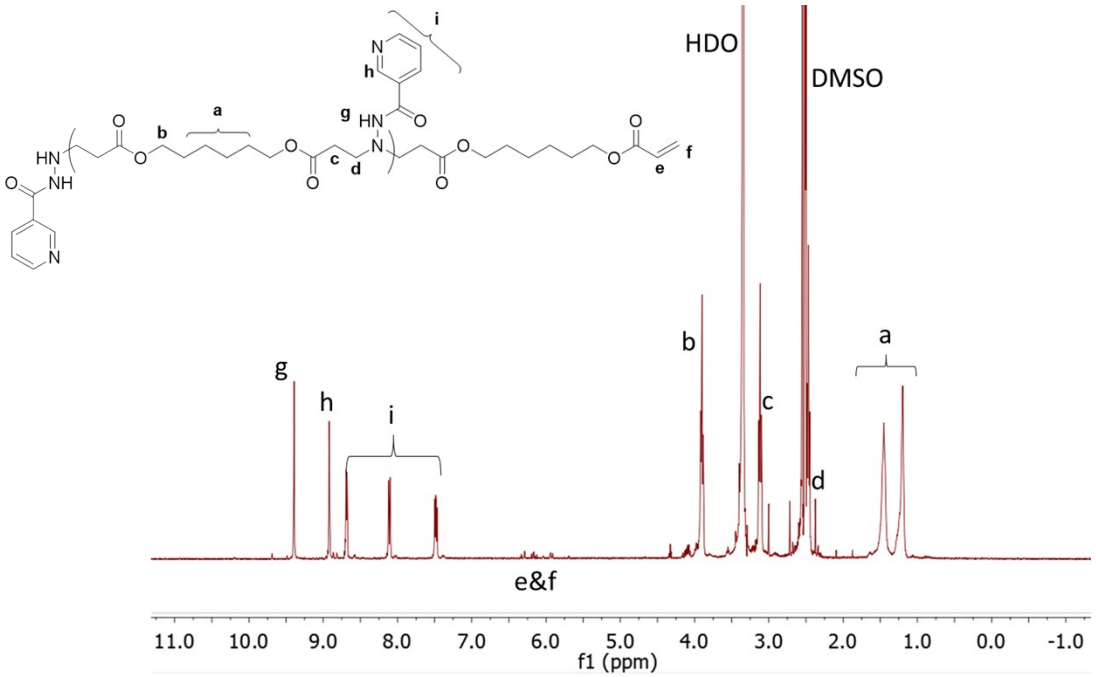


Figure S57: [1]H NMR spectrum and structural assignment of the crude product of the **H9**/HDA polymerization.

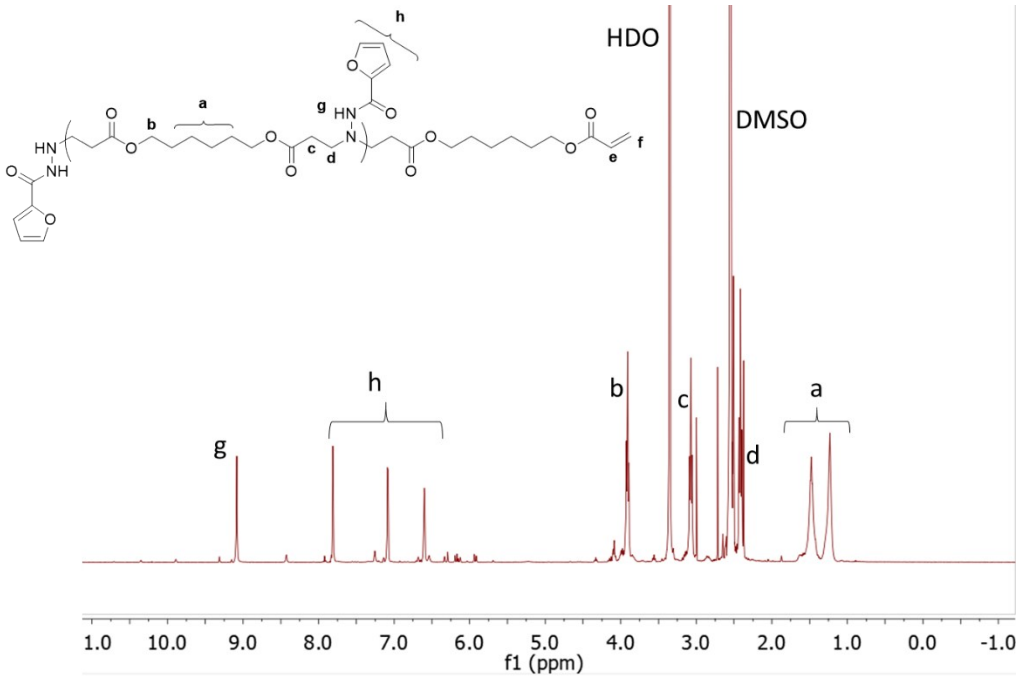


Figure S58: [1]H NMR spectrum and structural assignment of the crude product of the **H10**/HDA polymerization.

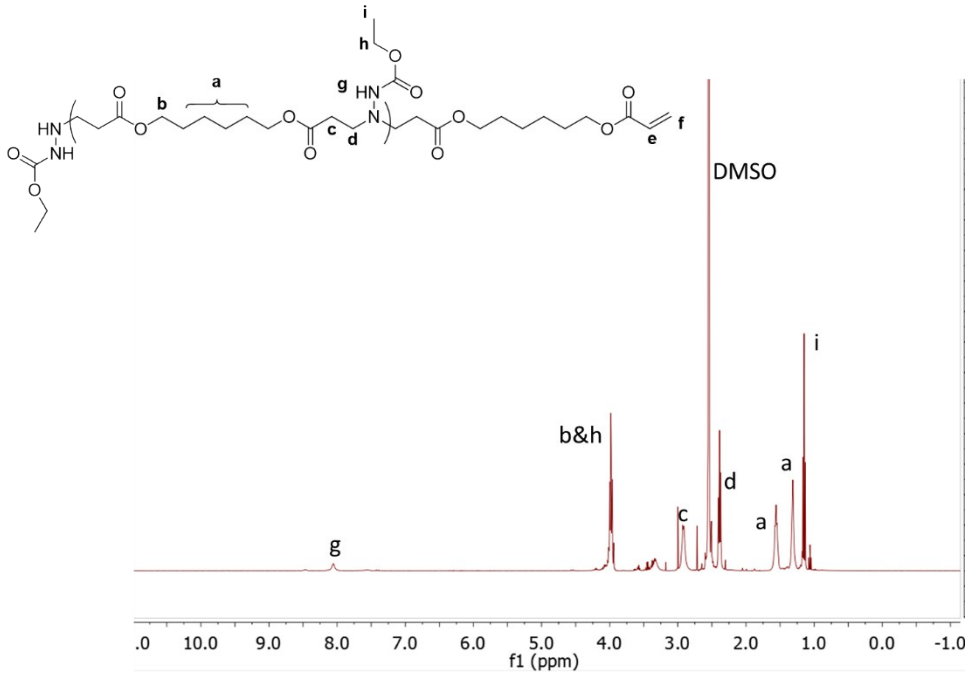


Figure S59: [1]H NMR spectrum and structural assignment of the crude product of the **H11**/HDA polymerization.

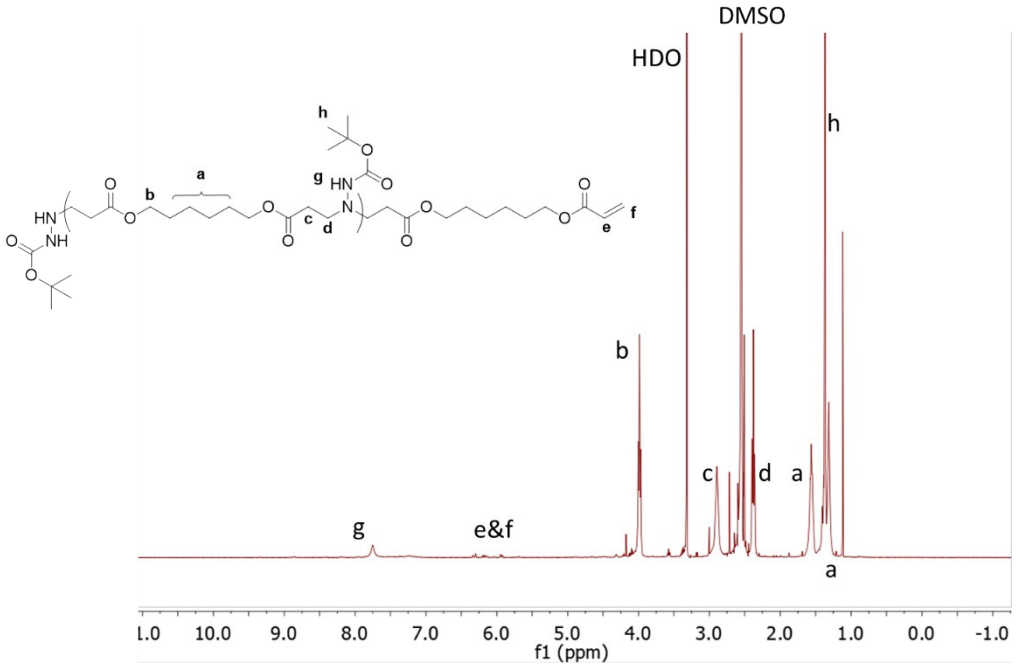


Figure S60: [1]H NMR spectrum and structural assignment of the crude product of the **H12**/HDA polymerization.

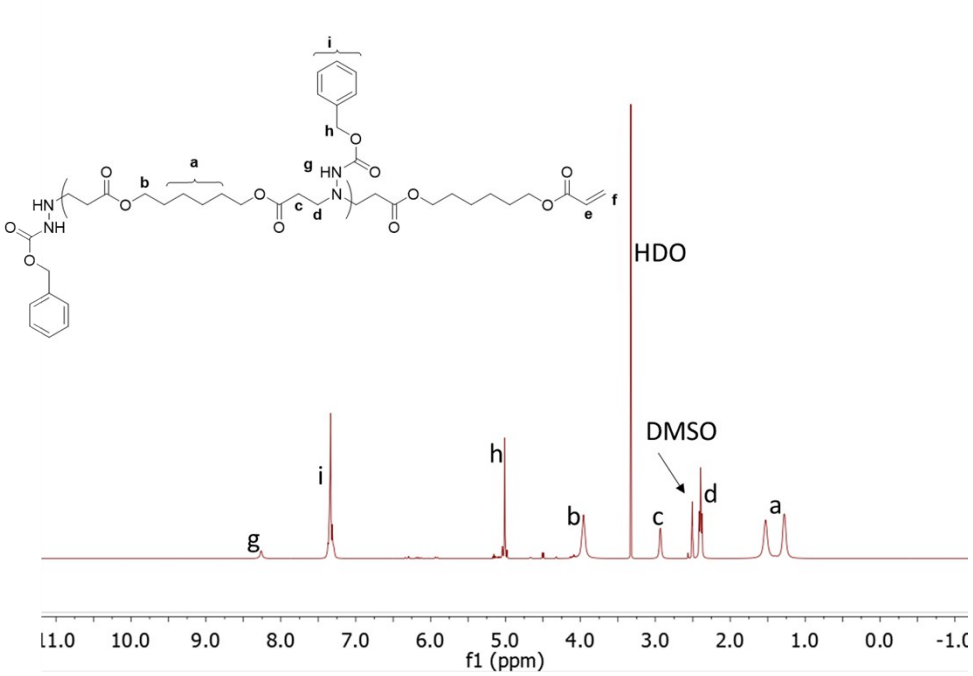


Figure S61: [1]H NMR spectrum and structural assignment of the crude product of the **H13**/HDA polymerization.

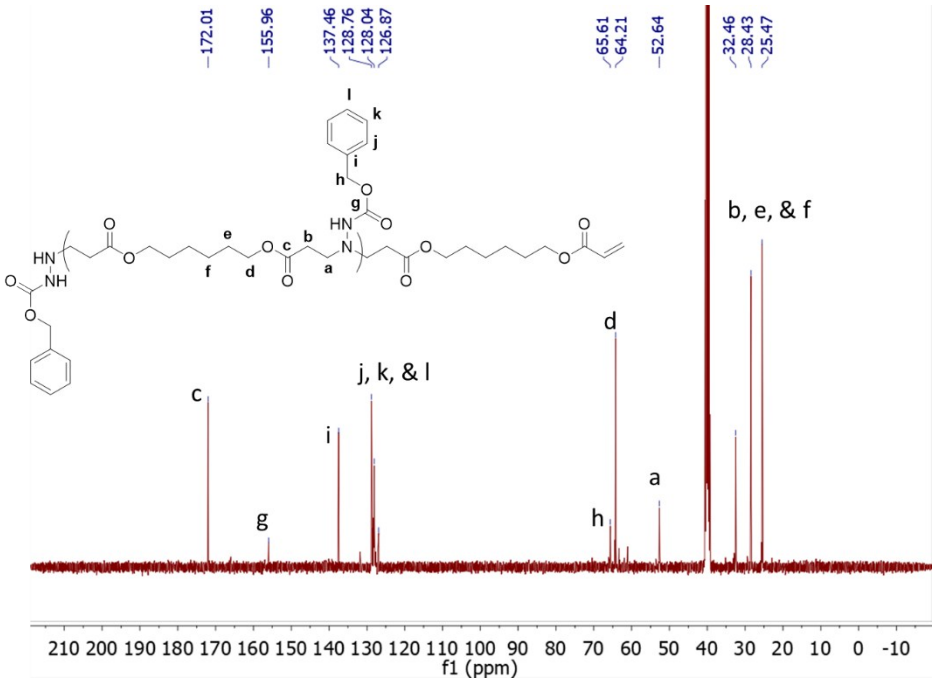


Figure S62: [13]C NMR spectrum and structural assignment of the crude product of the **H13**/HDA polymerization.1

8) Coordinates of molecular structures

Figure11_A

ZPE = -970.60

C	-0.0194	-0.3227	1.2075
H	-0.0723	-1.1626	1.9064
H	0.1730	0.5985	1.7655
H	0.8200	-0.4813	0.5228
C	-1.2796	-0.1406	0.3920
O	-1.4094	0.8027	-0.3925
N	-2.2247	-1.0958	0.6027
H	-2.0364	-1.8734	1.2402
N	-3.4425	-1.1169	-0.0880
H	-4.1865	-1.1924	0.6090
C	-3.5134	-2.2506	-1.0190
H	-4.5607	-2.3316	-1.3330
H	-3.2446	-3.1938	-0.5115
C	-2.6093	-2.0359	-2.2225
H	-1.5638	-1.9267	-1.9097
H	-2.6680	-2.8901	-2.9061
H	-2.8996	-1.1307	-2.7675
S	-4.3172	-3.5351	2.5919
C	-5.0396	-4.8763	1.6928
H	-6.0953	-4.9559	1.9637
H	-4.9337	-4.6352	0.6306
H	-4.5005	-5.7959	1.9336
C	-4.5385	-3.9651	4.2928
H	-4.0212	-4.9074	4.4892
H	-4.0988	-3.1565	4.8834
H	-5.6081	-4.0525	4.4986
O	-5.0847	-2.3104	2.3090
O	-2.8722	-3.5022	2.3009

Figure11_B

ZPE = -841.34

N	-4.9419	-1.4175	-0.5350
H	-5.7762	-1.0787	-0.0582
C	-4.5816	-2.7214	0.0228
H	-5.5056	-3.3043	0.1212
H	-4.1557	-2.6200	1.0388
C	-3.5916	-3.4753	-0.8558
H	-2.6310	-2.9499	-0.9180
H	-3.3975	-4.4741	-0.4480
H	-3.9866	-3.5861	-1.8744
C	-3.8728	-0.4119	-0.4888
H	-4.2881	0.5291	-0.1076
H	-3.0922	-0.7215	0.2275
C	-3.2457	-0.1571	-1.8568
H	-2.4431	0.5879	-1.7894
H	-2.8232	-1.0770	-2.2773
H	-4.0022	0.2167	-2.5574
S	-8.4221	-2.2159	-1.3154
C	-7.3311	-3.3095	-2.1825
H	-7.7082	-3.4446	-3.1995
H	-6.3519	-2.8195	-2.1937
H	-7.2834	-4.2642	-1.6523
C	-9.9924	-3.0344	-1.3719
H	-9.9090	-3.9994	-0.8659
H	-10.7047	-2.3894	-0.8495
H	-10.2887	-3.1623	-2.4160
O	-8.5220	-0.9611	-2.0754
O	-7.9964	-2.1316	0.0913

Figure11_C

ZPE = -1863.66

C	-1.3416	2.8954	-0.6844
H	-0.8828	2.9061	-1.6806
O	-2.6797	1.4548	1.6725
C	-0.4458	0.2279	2.4008
C	-1.1639	-0.8694	2.6257
S	-1.2365	1.6869	1.8066
O	-0.7904	2.8100	2.6550
C	-0.5480	1.9140	0.1667
H	-0.5707	0.9286	-0.3116
H	-2.3879	2.5977	-0.7829
H	-0.6899	-1.7645	3.0199
H	-2.2333	-0.8982	2.4274
H	0.6227	0.3373	2.5734
N	-1.3103	4.2956	-0.2157
H	-0.3549	4.5716	0.0736
N	-2.1800	4.6092	0.8461
H	-1.7900	4.4640	1.7795
C	-3.5370	4.5646	0.6498
O	-4.0319	4.3364	-0.4543
C	-4.3643	4.8181	1.8689
C	-5.6746	4.3220	1.8688
C	-3.8879	5.5371	2.9748
C	-6.5005	4.5300	2.9723
H	-6.0305	3.7720	1.0016
C	-4.7209	5.7495	4.0744
H	-2.8841	5.9563	2.9776
C	-6.0238	5.2439	4.0762
H	-7.5137	4.1370	2.9721
H	-4.3537	6.3154	4.9262
H	-6.6687	5.4103	4.9353
H	0.4950	2.2230	0.3009

C	-1.4146	5.4828	-1.5912
H	-2.3883	5.2134	-1.9950
O	2.2793	5.2092	-2.6927
C	1.3422	7.6036	-2.1968
C	2.2793	8.1186	-2.9899
S	1.2051	5.8581	-1.9202
O	1.2332	5.7306	-0.4344
C	-0.3158	5.3381	-2.4608
H	-0.3274	4.7712	-3.3851
H	-1.4576	6.3461	-0.9211
H	3.0010	7.4784	-3.4929
H	2.3420	9.1918	-3.1526
H	0.5898	8.1859	-1.6666

Figure8_IntA

ZPE = -930.13

C	-0.3944	0.1739	-4.0796
H	-0.6122	-0.4281	-4.9662
H	0.6907	0.2994	-4.0119
H	-0.8673	1.1542	-4.1754
C	-0.8631	-0.5737	-2.8691
O	-0.5265	-1.7237	-2.5859
N	-1.6934	0.1227	-2.0255
H	-2.1696	0.9823	-2.2942
N	-2.2835	-0.6005	-0.9726
H	-1.7499	-1.4885	-0.9213
C	-3.8298	-0.9202	-1.1658
H	-3.8402	-1.5080	-2.0886
H	-4.2390	0.0773	-1.3521
C	-4.4325	-1.5950	-0.0279
H	-4.6425	-1.0700	0.9010
H	-2.1544	-0.1063	-0.0778

S	-4.3597	-3.2707	0.1102
O	-5.3885	-3.7331	1.0726
O	-4.3540	-3.8816	-1.2435
C	-2.8182	-3.8242	0.8420
H	-1.9874	-3.5440	0.1868
H	-2.7063	-3.3519	1.8220
H	-2.8569	-4.9129	0.9489

Figure8_IntB

ZPE = -930.17

C	-0.0828	-0.0027	0.8925
H	0.3026	-0.8309	1.4930
H	-0.0584	0.9187	1.4838
H	0.5625	0.1450	0.0199
C	-1.4931	-0.2593	0.4289
O	-2.1030	0.5949	-0.2730
N	-2.0097	-1.4356	0.8202
N	-3.3495	-1.5249	0.2889
H	-4.0072	-1.6989	1.0585
C	-3.4995	-2.6028	-0.7249
H	-4.5619	-2.6632	-0.9772
H	-3.1783	-3.5349	-0.2534
C	-2.6430	-2.2797	-1.9389
H	-1.5874	-2.1704	-1.6617
H	-3.5646	-0.5907	-0.1329
H	-2.9743	-1.3740	-2.4585
S	-2.6491	-3.6000	-3.1430
C	-4.3036	-3.6363	-3.7740
H	-4.5472	-2.6560	-4.1913
H	-4.3190	-4.3988	-4.5584
H	-4.9930	-3.9083	-2.9710
O	-1.7444	-3.2025	-4.2278

O	-2.3876	-4.8635	-2.4405

Figure8_IntC

ZPE = -930.17

C	0.0287	-0.0464	1.0074
H	0.4161	-0.9342	1.5105
H	0.0341	0.8011	1.7007
H	0.6748	0.2086	0.1608
C	-1.3564	-0.2955	0.5245
O	-1.9322	0.7252	-0.1193
N	-1.9547	-1.4262	0.7153
N	-3.2767	-1.3932	0.1384
H	-3.9366	-1.5059	0.9110
C	-3.4441	-2.5231	-0.7787
H	-4.5149	-2.6237	-0.9823
H	-3.0777	-3.4571	-0.3279
C	-2.6795	-2.2335	-2.0661
H	-1.6203	-2.0293	-1.8602
H	-3.1054	-1.3861	-2.6150
H	-2.8261	0.3661	-0.3644
S	-2.6329	-3.6112	-3.1976
C	-4.3254	-3.9098	-3.6280
H	-4.8736	-4.2332	-2.7399
H	-4.7544	-2.9964	-4.0478
H	-4.3186	-4.7065	-4.3777
O	-2.1220	-4.7894	-2.4818
O	-1.9174	-3.1703	-4.4030

Figure8_IntD

ZPE = -930.19

C	-0.2039	-0.9699	1.4011
H	-0.6122	-1.7143	2.0901
H	0.1855	-0.1241	1.9759
H	0.6300	-1.4119	0.8472
C	-1.2209	-0.4530	0.4122
O	-0.9400	0.4023	-0.4282
N	-2.4601	-1.0135	0.5353
N	-3.5097	-0.6785	-0.3219
H	-4.3165	-0.3986	0.2355
C	-3.8579	-1.7737	-1.2247
H	-4.8147	-1.5246	-1.6928
H	-3.9774	-2.7243	-0.6797
C	-2.7772	-1.8996	-2.2933
H	-1.7885	-2.0987	-1.8633
H	-2.7180	-0.9911	-2.9039
H	-2.6023	-1.7730	1.2013
S	-3.0909	-3.2123	-3.4601
C	-2.8838	-4.7136	-2.5407
H	-3.6424	-4.7710	-1.7563
H	-3.0158	-5.5321	-3.2544
H	-1.8758	-4.7356	-2.1190
O	-2.0406	-3.1567	-4.4868
O	-4.4927	-3.1227	-3.8955

Figure8_TS1

ZPE = -930.13

C	0.3810	-1.0616	0.2407
H	0.4156	-1.9671	-0.3705
H	0.6166	-1.3014	1.2810
H	1.1362	-0.3576	-0.1249
C	-0.9643	-0.3997	0.1802
O	-1.3059	0.5213	0.9309

N	-1.7851	-0.8799	-0.8132
H	-2.0485	-2.0208	-0.9079
N	-3.1056	-0.3764	-0.7301
H	-3.1532	0.2860	0.0659
C	-4.0981	-1.5886	-0.5270
H	-4.9698	-1.3400	-1.1381
H	-4.3655	-1.5481	0.5295
C	-3.3796	-2.8409	-0.8757
H	-3.3762	-3.6274	-0.1212
H	-3.3425	0.1405	-1.5858
S	-3.7650	-3.5363	-2.4092
C	-2.8494	-2.5845	-3.6030
H	-3.0944	-2.9762	-4.5945
H	-3.1562	-1.5352	-3.5338
H	-1.7802	-2.6856	-3.4010
O	-3.2364	-4.9162	-2.4358
O	-5.1883	-3.3636	-2.7863

Figure8_TS2

ZPE = -930.17

C	-0.0694	-0.0297	0.9462
H	0.3319	-0.8639	1.5264
H	-0.0690	0.8777	1.5588
H	0.5700	0.1539	0.0764
C	-1.4571	-0.3257	0.4909
O	-2.1152	0.5401	-0.2199
N	-2.0296	-1.4750	0.8048
N	-3.3359	-1.3983	0.1882
H	-4.0551	-1.4291	0.9162
C	-3.5633	-2.4851	-0.7800
H	-4.6208	-2.4570	-1.0585
H	-3.3407	-3.4458	-0.3016

C	-2.6698	-2.2768	-1.9962
H	-1.6166	-2.1780	-1.7028
H	-3.0951	-0.2340	-0.2621
H	-2.9621	-1.4019	-2.5869
S	-2.6768	-3.6717	-3.1105
C	-4.3439	-3.7738	-3.6997
H	-4.6143	-2.8249	-4.1697
H	-4.3647	-4.5833	-4.4352
H	-5.0091	-4.0067	-2.8646
O	-2.3796	-4.8859	-2.3378
O	-1.8013	-3.3339	-4.2397

FigureS20_Left

ZPE = -1159.62

N	-1.6002	4.6109	-0.3416
H	-0.6550	4.2669	-0.1300
N	-2.3636	4.7262	0.8244
H	-1.9956	5.3559	1.5319
C	-3.6432	4.2584	0.8102
O	-4.0449	3.5756	-0.1396
C	-4.4946	4.5805	1.9932
C	-5.5924	3.7445	2.2378
C	-4.2517	5.6758	2.8342
C	-6.4314	3.9901	3.3236
H	-5.7735	2.9049	1.5723
C	-5.0982	5.9226	3.9158
H	-3.4269	6.3590	2.6456
C	-6.1845	5.0795	4.1646
H	-7.2767	3.3340	3.5136
H	-4.9116	6.7778	4.5597
H	-6.8405	5.2745	5.0091
C	-1.2990	6.1879	-1.3412

H	-2.3460	6.3841	-1.5668
O	1.8810	4.9775	-3.1158
C	1.9265	7.4563	-2.2847
C	2.8350	7.7342	-3.2173
S	1.2361	5.8335	-2.1032
O	1.4321	5.5022	-0.6707
C	-0.4380	5.9379	-2.4092
H	-0.7555	5.6425	-3.4039
H	-0.9263	6.7314	-0.4728
H	3.1864	6.9652	-3.9023
H	3.2442	8.7368	-3.3142
H	1.5294	8.1775	-1.5718
H	-2.0819	3.9426	-0.9586

FigureS20_RIght

ZPE = -840.14

N	-1.2926	4.9050	-0.2937
H	-0.3000	4.8674	-0.0360
N	-2.0901	5.0933	0.8444
H	-2.0676	6.0406	1.2181
C	-3.2058	4.3061	0.9639
O	-3.3819	3.3545	0.1975
C	-4.1503	4.6476	2.0663
C	-5.4528	4.1389	1.9779
C	-3.7764	5.4256	3.1715
C	-6.3815	4.4181	2.9793
H	-5.7246	3.5316	1.1187
C	-4.7074	5.6976	4.1745
H	-2.7609	5.8008	3.2736
C	-6.0095	5.1984	4.0782
H	-7.3930	4.0282	2.9036
H	-4.4134	6.2932	5.0345

H	-6.7317	5.4133	4.8616
C	-1.4759	6.1751	-1.6255
H	-2.5371	5.9913	-1.7948
H	-1.2843	7.0211	-0.9656
H	-1.5663	4.0047	-0.7121
C	-0.5866	5.9495	-2.6905
H	-0.8740	5.3215	-3.5292
C	0.7662	6.4062	-2.6745
O	1.6059	6.2566	-3.5745
O	1.1099	7.0674	-1.5222
C	2.4307	7.6084	-1.4654
H	2.5753	8.3172	-2.2916
H	3.1658	6.8024	-1.5886
C	2.6059	8.2985	-0.1258
H	2.4339	7.5703	0.6774
H	1.8425	9.0804	-0.0227
C	4.0020	8.9031	-0.0010
H	4.1814	9.6456	-0.7883
H	4.1344	9.4014	0.9651
H	4.7756	8.1302	-0.0883

Table4_DVS

ZPE = -704.00

C	-2.4949	0.8321	-0.5290
H	-3.2505	1.2343	-1.1990
O	0.6456	-1.1661	-0.6099
C	1.0771	1.2432	0.3670
C	2.3087	1.1881	-0.1343
S	-0.0476	-0.0934	0.1137
O	-0.6797	-0.3970	1.4034
C	-1.2626	0.5893	-0.9695
H	-0.9050	0.7670	-1.9815

H	-2.7753	0.6318	0.5030
H	2.6417	0.3335	-0.7196
H	3.0111	1.9998	0.0371
H	0.6677	2.0615	0.9558

Table4_nPA

ZPE = -384.53

C	3.0888	1.6432	-0.0000
H	2.1568	2.2030	-0.0000
H	4.0161	2.2104	-0.0000
C	3.1035	0.3064	-0.0000
C	1.8822	-0.5340	0.0000
O	1.9150	-1.7569	0.0000
O	0.7414	0.1640	-0.0000
C	-0.4814	-0.5973	0.0000
H	-0.4977	-1.2408	-0.8879
H	-0.4977	-1.2408	0.8879
C	-1.6445	0.3735	-0.0000
H	-1.5728	1.0196	0.8837
H	-1.5728	1.0196	-0.8838
H	4.0319	-0.2592	0.0000
C	-2.9725	-0.3794	0.0000
H	-3.8185	0.3151	-0.0000
H	-3.0629	-1.0191	-0.8861
H	-3.0629	-1.0191	0.8861

Table5_H13

ZPE = -570.03

N	-2.4906	2.6272	-0.0390
H	-2.3276	3.0918	-0.9329

H	-3.4941	2.4723	0.0651
N	-2.0178	3.4256	1.0087
H	-1.3040	3.0275	1.6092
C	-2.4500	4.6820	1.2983
O	-2.0215	5.3549	2.2306
O	-3.3993	5.0980	0.4422
C	-3.9152	6.4250	0.6859
H	-3.0913	7.1426	0.6199
H	-4.3322	6.4578	1.6976
C	-4.9671	6.7046	-0.3510
C	-4.6406	7.3968	-1.5230
C	-6.2808	6.2563	-0.1615
C	-5.6131	7.6350	-2.4977
H	-3.6214	7.7513	-1.6673
C	-7.2540	6.4900	-1.1349
H	-6.5375	5.7254	0.7538
C	-6.9205	7.1804	-2.3047
H	-5.3517	8.1766	-3.4034
H	-8.2717	6.1401	-0.9799
H	-7.6788	7.3667	-3.0613

Table5_H2

ZPE = -381.88

N	-2.1213	3.9619	-0.6004
H	-1.2313	3.5544	-0.3059
H	-1.8989	4.7749	-1.1786
N	-2.8201	4.3929	0.5362
H	-3.7369	3.9826	0.6756
C	-2.3055	5.3113	1.3943
O	-1.1883	5.8090	1.2102
C	-3.1569	5.6970	2.5867
H	-3.2441	6.7910	2.5528

H	-2.5522	5.4696	3.4749
C	-4.5416	5.0665	2.7229
H	-5.1499	5.2926	1.8345
H	-4.4561	3.9715	2.7841
C	-5.2711	5.5741	3.9668
H	-4.6618	5.3531	4.8545
H	-5.3558	6.6686	3.9116
C	-6.6564	4.9527	4.1200
H	-6.5888	3.8603	4.1992
H	-7.1683	5.3224	5.0156
H	-7.2877	5.1850	3.2530

Table5_H4

ZPE = -494.88

N	-2.1059	3.8944	-0.5373
H	-1.2445	3.4565	-0.2044
H	-1.8326	4.6767	-1.1356
N	-2.8172	4.3919	0.5628
H	-3.7557	4.0282	0.6958
C	-2.2914	5.3181	1.4020
O	-1.1541	5.7726	1.2452
C	-3.1708	5.7834	2.5554
H	-3.2737	6.8682	2.4334
H	-2.5804	5.6188	3.4643
C	-4.5272	5.1342	2.6795
C	-4.6859	3.9508	3.4145
C	-5.6443	5.6870	2.0380
C	-5.9345	3.3311	3.5058
H	-3.8228	3.5170	3.9173
C	-6.8948	5.0701	2.1275
H	-5.5291	6.6073	1.4675
C	-7.0426	3.8901	2.8622

H	-6.0427	2.4153	4.0818
H	-7.7529	5.5126	1.6275
H	-8.0156	3.4106	2.9354

Table5_H6

ZPE = -455.64

N	-1.8596	3.6192	-0.0701
H	-0.8883	3.9328	-0.1194
H	-2.3388	3.9955	-0.8914
N	-2.4510	4.1513	1.0831
H	-2.8632	3.4787	1.7210
C	-2.6647	5.4865	1.2254
O	-2.3348	6.2946	0.3506
C	-3.3262	5.9178	2.4997
C	-3.2310	5.1801	3.6881
C	-4.0433	7.1210	2.4842
C	-3.8579	5.6424	4.8469
H	-2.6503	4.2613	3.7265
C	-4.6755	7.5761	3.6408
H	-4.0995	7.6876	1.5583
C	-4.5837	6.8362	4.8240
H	-3.7732	5.0729	5.7688
H	-5.2381	8.5058	3.6209
H	-5.0724	7.1924	5.7274

Table5_Hexylamine

ZPE = -291.86

N	-2.1923	2.5295	0.0507
H	-1.8387	1.5843	0.2067
H	-1.6775	2.9055	-0.7455

C	-1.9689	3.3497	1.2463
H	-2.2869	4.3763	1.0223
H	-0.9057	3.4009	1.5368
C	-2.7763	2.8196	2.4248
H	-2.4918	1.7721	2.6110
H	-3.8421	2.8130	2.1529
C	-2.5718	3.6357	3.6993
H	-2.8439	4.6850	3.5071
H	-1.5038	3.6362	3.9660
C	-3.3852	3.1136	4.8823
H	-4.4541	3.1132	4.6177
H	-3.1144	2.0639	5.0754
C	-3.1838	3.9281	6.1592
H	-3.4539	4.9759	5.9635
H	-2.1159	3.9275	6.4214
C	-4.0034	3.3939	7.3312
H	-3.8494	3.9873	8.2398
H	-5.0759	3.4104	7.0984
H	-3.7298	2.3558	7.5590

TableS1_DVS

ZPE = -704.00

C	-2.4949	0.8321	-0.5290
H	-3.2505	1.2343	-1.1990
O	0.6456	-1.1661	-0.6099
C	1.0771	1.2432	0.3670
C	2.3087	1.1881	-0.1343
S	-0.0476	-0.0934	0.1137
O	-0.6797	-0.3970	1.4034
C	-1.2626	0.5893	-0.9695
H	-0.9050	0.7670	-1.9815
H	-2.7753	0.6318	0.5030

H	2.6417	0.3335	-0.7196
H	3.0111	1.9998	0.0371
H	0.6677	2.0615	0.9558

TableS1_DVS_75C

ZPE = -704.00

C	-2.4949	0.8321	-0.5290
H	-3.2505	1.2343	-1.1990
O	0.6456	-1.1661	-0.6099
C	1.0771	1.2432	0.3670
C	2.3087	1.1881	-0.1343
S	-0.0476	-0.0934	0.1137
O	-0.6797	-0.3970	1.4034
C	-1.2626	0.5893	-0.9695
H	-0.9050	0.7670	-1.9815
H	-2.7753	0.6318	0.5030
H	2.6417	0.3335	-0.7196
H	3.0111	1.9998	0.0371
H	0.6677	2.0615	0.9558

TableS1_H12-DVS_Z1_75C

ZPE = -1161.03

N	-1.8193	2.7417	-0.1764
H	-2.5358	3.2734	-0.6951
H	-2.2827	1.8987	0.2240
N	-1.2648	3.5791	0.8206
H	-0.6278	3.0991	1.4548
C	-1.9958	4.6366	1.3412
O	-1.6392	5.2187	2.3490
O	-3.0444	4.9074	0.5698

C	-3.9494	6.0452	0.8393
C	-3.1631	7.3465	0.7658
H	-3.8691	8.1829	0.8145
H	-2.4564	7.4400	1.5943
H	-2.6202	7.4115	-0.1843
C	-4.6319	5.8425	2.1846
H	-5.4036	6.6113	2.3028
H	-5.1179	4.8608	2.2218
H	-3.9250	5.9288	3.0136
C	-4.9539	5.9521	-0.2994
H	-5.6872	6.7591	-0.2012
H	-4.4509	6.0529	-1.2676
H	-5.4836	4.9935	-0.2700
C	-0.7895	2.2013	-1.1805
C	-1.4893	1.2970	-2.1194
H	-0.3682	3.0776	-1.6770
S	-1.7817	-0.2506	-1.5556
H	-1.3813	1.4116	-3.1932
O	-2.7331	-0.9772	-2.4192
C	-0.2958	-1.2282	-1.5397
O	-2.1032	-0.1200	-0.0999
C	-0.1485	-2.3332	-2.2698
H	0.4861	-0.8108	-0.9055
H	-0.9628	-2.7077	-2.8866
H	0.7883	-2.8860	-2.2645
H	-0.0200	1.7544	-0.5343

TableS1_H12-nPA_Z1_75C

ZPE = -841.55

N	-2.1072	2.4056	0.5042
H	-2.8813	2.6670	-0.1368
H	-2.5161	1.9640	1.3431

N	-1.3918	3.5856	0.8114
H	-0.5611	3.4361	1.3818
C	-2.0781	4.7795	0.9862
O	-1.5427	5.7601	1.4694
O	-3.3195	4.6736	0.5185
C	-4.2886	5.7875	0.5746
C	-3.8091	6.9240	-0.3169
H	-4.5759	7.7068	-0.3256
H	-2.8757	7.3572	0.0532
H	-3.6657	6.5742	-1.3463
C	-4.4875	6.2203	2.0212
H	-5.3384	6.9093	2.0624
H	-4.7195	5.3526	2.6498
H	-3.6067	6.7303	2.4187
C	-5.5582	5.1555	0.0229
H	-6.3535	5.9077	-0.0062
H	-5.3944	4.7811	-0.9944
H	-5.8842	4.3254	0.6597
C	-1.3098	1.3510	-0.2992
H	-0.5514	0.9628	0.3840
C	-2.2451	0.3196	-0.7901
C	-3.2562	0.6665	-1.6939
H	-2.2278	-0.6820	-0.3737
O	-4.1552	-0.0272	-2.2095
O	-3.2014	2.0395	-2.0012
C	-4.2069	2.5819	-2.8527
H	-4.3543	1.9294	-3.7211
H	-5.1627	2.6350	-2.3090
C	-3.7499	3.9680	-3.2732
H	-3.4531	4.5230	-2.3725
H	-2.8529	3.8736	-3.8987
C	-4.8450	4.7234	-4.0197
H	-4.5028	5.7174	-4.3276
H	-5.1556	4.1819	-4.9220

H	-5.7333	4.8549	-3.3882
H	-0.8285	1.9672	-1.0683

TableS1_H12

ZPE = -457.04

N	-2.1903	2.6553	-0.0554
H	-2.0250	3.1870	-0.9109
H	-3.1878	2.4456	-0.0000
N	-1.7992	3.4096	1.0567
H	-1.0819	3.0142	1.6546
C	-2.2983	4.6301	1.4076
O	-1.9100	5.2416	2.3994
O	-3.2350	5.0399	0.5426
C	-3.9231	6.3226	0.7038
C	-2.9237	7.4703	0.6162
H	-3.4748	8.4170	0.5784
H	-2.2554	7.4877	1.4807
H	-2.3272	7.3850	-0.2999
C	-4.7100	6.3351	2.0093
H	-5.3375	7.2334	2.0361
H	-5.3657	5.4580	2.0651
H	-4.0468	6.3445	2.8778
C	-4.8717	6.3530	-0.4877
H	-5.4524	7.2815	-0.4718
H	-4.3102	6.3075	-1.4277
H	-5.5656	5.5056	-0.4486

TableS1_H12_75C

ZPE = -457.04

N	-2.1898	2.6561	-0.0559

H	-2.0216	3.1886	-0.9103
H	-3.1874	2.4467	-0.0033
N	-1.8011	3.4084	1.0585
H	-1.0833	3.0131	1.6560
C	-2.2995	4.6293	1.4088
O	-1.9126	5.2401	2.4016
O	-3.2338	5.0407	0.5419
C	-3.9229	6.3228	0.7035
C	-2.9236	7.4705	0.6153
H	-3.4743	8.4176	0.5824
H	-2.2520	7.4850	1.4773
H	-2.3305	7.3874	-0.3032
C	-4.7093	6.3354	2.0093
H	-5.3392	7.2321	2.0347
H	-5.3628	5.4567	2.0667
H	-4.0461	6.3479	2.8778
C	-4.8721	6.3527	-0.4875
H	-5.4520	7.2817	-0.4723
H	-4.3110	6.3058	-1.4278
H	-5.5666	5.5059	-0.4472

TableS1_H13-DVS_Z1_75C

ZPE = -1274.01

N	-2.6661	2.2202	0.7550
H	-3.6652	2.4125	0.5790
H	-2.6003	1.2092	0.9952
N	-2.2154	2.9981	1.8483
H	-1.3332	2.6808	2.2486
C	-2.4433	4.3628	1.8229
O	-1.8483	5.1539	2.5285
O	-3.4291	4.6558	0.9723
C	-3.7486	6.0576	0.7950

H	-2.8154	6.5912	0.5859
H	-4.1806	6.4451	1.7221
C	-4.7191	6.1538	-0.3489
C	-4.3643	5.6604	-1.6127
C	-5.9765	6.7351	-0.1643
C	-5.2621	5.7440	-2.6768
H	-3.3831	5.2103	-1.7595
C	-6.8733	6.8298	-1.2335
H	-6.2533	7.1117	0.8186
C	-6.5185	6.3321	-2.4887
H	-4.9822	5.3570	-3.6534
H	-7.8488	7.2851	-1.0821
H	-7.2168	6.4001	-3.3191
C	-1.8990	2.3661	-0.5758
C	-2.5484	1.4969	-1.5766
H	-1.9599	3.4228	-0.8482
S	-2.1862	-0.1322	-1.4750
H	-2.8613	1.8759	-2.5439
O	-3.1260	-0.9545	-2.2614
C	-0.5702	-0.4806	-2.1309
O	-2.0224	-0.4387	-0.0186
C	-0.3724	-1.2764	-3.1812
H	0.2275	0.0498	-1.6113
H	-1.2062	-1.7826	-3.6632
H	0.6268	-1.4375	-3.5795
H	-0.8652	2.1291	-0.2867

TableS1_H13-nPA_Z1_75C

ZPE = -954.53

N	-1.6221	3.0473	0.1679
H	-0.7079	3.5283	0.1835
H	-2.2186	3.5299	-0.5312

N	-2.2643	3.0975	1.4281
H	-1.7263	2.6753	2.1835
C	-3.0636	4.1785	1.7490
O	-3.4152	4.4347	2.8842
O	-3.4221	4.8428	0.6487
C	-4.2488	6.0190	0.8259
H	-3.6696	6.7531	1.3965
H	-5.1414	5.7480	1.3963
C	-4.6042	6.5153	-0.5476
C	-3.5953	6.7693	-1.4873
C	-5.9428	6.6969	-0.9069
C	-3.9256	7.1918	-2.7755
H	-2.5521	6.6247	-1.2114
C	-6.2746	7.1326	-2.1938
H	-6.7258	6.4883	-0.1804
C	-5.2672	7.3769	-3.1297
H	-3.1389	7.3787	-3.5024
H	-7.3182	7.2697	-2.4661
H	-5.5244	7.7047	-4.1340
C	-1.4257	1.6218	-0.4054
H	-2.4486	1.2273	-0.3980
C	-0.7743	1.7181	-1.7232
C	-1.4294	2.3139	-2.8074
H	0.2653	1.4286	-1.8375
O	-1.0424	2.4747	-3.9825
O	-2.6969	2.8036	-2.4456
C	-3.5270	3.2679	-3.5094
H	-3.1208	4.2036	-3.9209
H	-3.5299	2.5266	-4.3188
C	-4.9326	3.4830	-2.9792
H	-5.2804	2.5559	-2.5050
H	-4.9138	4.2579	-2.2011
C	-5.8814	3.8845	-4.1068
H	-6.8807	4.1190	-3.7231

H	-5.5115	4.7713	-4.6374
H	-5.9834	3.0754	-4.8407
H	-0.8236	1.0917	0.3360

TableS1_H13

ZPE = -570.03

N	-2.4906	2.6272	-0.0390
H	-2.3276	3.0918	-0.9329
H	-3.4941	2.4723	0.0651
N	-2.0178	3.4256	1.0087
H	-1.3040	3.0275	1.6092
C	-2.4500	4.6820	1.2983
O	-2.0215	5.3549	2.2306
O	-3.3993	5.0980	0.4422
C	-3.9152	6.4250	0.6859
H	-3.0913	7.1426	0.6199
H	-4.3322	6.4578	1.6976
C	-4.9671	6.7046	-0.3510
C	-4.6406	7.3968	-1.5230
C	-6.2808	6.2563	-0.1615
C	-5.6131	7.6350	-2.4977
H	-3.6214	7.7513	-1.6673
C	-7.2540	6.4900	-1.1349
H	-6.5375	5.7254	0.7538
C	-6.9205	7.1804	-2.3047
H	-5.3517	8.1766	-3.4034
H	-8.2717	6.1401	-0.9799
H	-7.6788	7.3667	-3.0613

TableS1_H13_75C

ZPE = -570.03

N	-2.4906	2.6272	-0.0390
H	-2.3276	3.0918	-0.9329
H	-3.4941	2.4723	0.0651
N	-2.0178	3.4256	1.0087
H	-1.3040	3.0275	1.6092
C	-2.4500	4.6820	1.2983
O	-2.0215	5.3549	2.2306
O	-3.3993	5.0980	0.4422
C	-3.9152	6.4250	0.6859
H	-3.0913	7.1426	0.6199
H	-4.3322	6.4578	1.6976
C	-4.9671	6.7046	-0.3510
C	-4.6406	7.3968	-1.5230
C	-6.2808	6.2563	-0.1615
C	-5.6131	7.6350	-2.4977
H	-3.6214	7.7513	-1.6673
C	-7.2540	6.4900	-1.1349
H	-6.5375	5.7254	0.7538
C	-6.9205	7.1804	-2.3047
H	-5.3517	8.1766	-3.4034
H	-8.2717	6.1401	-0.9799
H	-7.6788	7.3667	-3.0613

TableS1_H2

ZPE = -381.88

N	-2.1213	3.9619	-0.6004
H	-1.2313	3.5544	-0.3059
H	-1.8989	4.7749	-1.1786
N	-2.8201	4.3929	0.5362
H	-3.7369	3.9826	0.6756
C	-2.3055	5.3113	1.3943

O	-1.1883	5.8090	1.2102
C	-3.1569	5.6970	2.5867
H	-3.2441	6.7910	2.5528
H	-2.5522	5.4696	3.4749
C	-4.5416	5.0665	2.7229
H	-5.1499	5.2926	1.8345
H	-4.4561	3.9715	2.7841
C	-5.2711	5.5741	3.9668
H	-4.6618	5.3531	4.8545
H	-5.3558	6.6686	3.9116
C	-6.6564	4.9527	4.1200
H	-6.5888	3.8603	4.1992
H	-7.1683	5.3224	5.0156
H	-7.2877	5.1850	3.2530

TableS1_H4-DVS_Z1_75C

ZPE = -1198.86

N	-3.3447	3.4219	-1.0395
H	-2.3458	3.1410	-1.0385
H	-3.4578	4.1639	-1.7457
N	-3.5922	3.9315	0.2485
H	-4.5612	4.1765	0.4514
C	-2.6679	3.6258	1.2143
O	-1.6009	3.0996	0.9008
C	-3.0144	4.0029	2.6381
H	-2.2315	4.7000	2.9597
H	-2.8872	3.0868	3.2262
C	-4.3860	4.5956	2.8489
C	-5.4776	3.7699	3.1490
C	-4.5921	5.9751	2.7110
C	-6.7545	4.3137	3.3108
H	-5.3213	2.6980	3.2582

C	-5.8677	6.5209	2.8722
H	-3.7460	6.6198	2.4784
C	-6.9516	5.6905	3.1722
H	-7.5929	3.6635	3.5478
H	-6.0146	7.5930	2.7667
H	-7.9443	6.1147	3.3006
C	-4.2436	2.1833	-1.4449
C	-3.9879	1.7017	-2.7950
H	-4.0203	1.4487	-0.6652
S	-2.8046	0.5458	-3.0828
H	-4.3021	2.2617	-3.6722
O	-3.0187	-0.0688	-4.4107
C	-1.1903	1.2966	-3.1744
O	-2.6875	-0.3472	-1.9036
C	-0.4788	1.3611	-4.2995
H	-0.8540	1.7113	-2.2228
H	-0.8561	0.9233	-5.2215
H	0.4922	1.8507	-4.3215
H	-5.2528	2.5822	-1.3036

TableS1_H4-nPA_Z1_75C

ZPE = -879.38

N	-2.2224	2.7736	-0.1506
H	-2.1204	1.7830	0.1166
H	-1.2687	3.1733	-0.2794
N	-2.8319	3.5089	0.8815
H	-3.8254	3.3331	1.0252
C	-2.1793	4.6245	1.3341
O	-1.0346	4.8679	0.9573
C	-2.9184	5.4880	2.3350
H	-2.8042	6.5174	1.9772
H	-2.3513	5.4098	3.2705

C	-4.3721	5.1488	2.5600
C	-4.7529	4.2993	3.6070
C	-5.3581	5.6559	1.7016
C	-6.0961	3.9632	3.7956
H	-3.9909	3.9043	4.2769
C	-6.7010	5.3205	1.8874
H	-5.0672	6.3176	0.8872
C	-7.0725	4.4729	2.9357
H	-6.3790	3.3069	4.6150
H	-7.4565	5.7231	1.2173
H	-8.1181	4.2143	3.0830
C	-2.9225	2.8581	-1.5369
H	-2.8926	3.9356	-1.7406
C	-2.2345	1.9959	-2.5095
C	-0.9347	2.2882	-2.9427
H	-2.6947	1.0669	-2.8309
O	-0.2165	1.6830	-3.7653
O	-0.4169	3.4214	-2.3046
C	0.8624	3.8732	-2.7405
H	1.6079	3.0800	-2.5954
H	0.8292	4.1002	-3.8151
C	1.2322	5.1097	-1.9423
H	0.4559	5.8729	-2.0853
H	1.2366	4.8575	-0.8744
C	2.5936	5.6519	-2.3703
H	2.8656	6.5442	-1.7966
H	3.3815	4.9036	-2.2187
H	2.5932	5.9246	-3.4331
H	-3.9544	2.5520	-1.3465

TableS1_H4

ZPE = -494.88

N	-2.1059	3.8944	-0.5373
H	-1.2445	3.4565	-0.2044
H	-1.8326	4.6767	-1.1356
N	-2.8172	4.3919	0.5628
H	-3.7557	4.0282	0.6958
C	-2.2914	5.3181	1.4020
O	-1.1541	5.7726	1.2452
C	-3.1708	5.7834	2.5554
H	-3.2737	6.8682	2.4334
H	-2.5804	5.6188	3.4643
C	-4.5272	5.1342	2.6795
C	-4.6859	3.9508	3.4145
C	-5.6443	5.6870	2.0380
C	-5.9345	3.3311	3.5058
H	-3.8228	3.5170	3.9173
C	-6.8948	5.0701	2.1275
H	-5.5291	6.6073	1.4675
C	-7.0426	3.8901	2.8622
H	-6.0427	2.4153	4.0818
H	-7.7529	5.5126	1.6275
H	-8.0156	3.4106	2.9354

TableS1_H4_75C

ZPE = -494.88

N	-2.1059	3.8944	-0.5373
H	-1.2445	3.4565	-0.2044
H	-1.8326	4.6767	-1.1356
N	-2.8172	4.3919	0.5628
H	-3.7557	4.0282	0.6958
C	-2.2914	5.3181	1.4020
O	-1.1541	5.7726	1.2452
C	-3.1708	5.7834	2.5554

H	-3.2737	6.8682	2.4334
H	-2.5804	5.6188	3.4643
C	-4.5272	5.1342	2.6795
C	-4.6859	3.9508	3.4145
C	-5.6443	5.6870	2.0380
C	-5.9345	3.3311	3.5058
H	-3.8228	3.5170	3.9173
C	-6.8948	5.0701	2.1275
H	-5.5291	6.6073	1.4675
C	-7.0426	3.8901	2.8622
H	-6.0427	2.4153	4.0818
H	-7.7529	5.5126	1.6275
H	-8.0156	3.4106	2.9354

TableS1_H6-DVS_BisAdduct

ZPE = -1863.71

C	-3.9599	2.7762	0.6132
H	-4.0977	2.7660	-0.4724
O	-4.3011	-0.5237	2.7797
C	-2.6134	1.2597	3.7057
C	-1.5314	0.4962	3.5713
S	-4.0768	0.9305	2.7564
O	-5.1293	1.8207	3.2664
C	-3.7475	1.3309	1.0326
H	-4.4730	0.6881	0.5191
H	-4.8822	3.1745	1.0596
H	-0.6444	0.6863	4.1706
H	-1.4971	-0.3350	2.8684
H	-2.7105	2.0962	4.3958
N	-2.8120	3.6382	0.8979
N	-2.7224	3.9713	2.2494
H	-1.9256	3.5903	2.7505

C	-3.6310	4.7807	2.8697
O	-4.5810	5.2811	2.2623
C	-3.4100	5.0070	4.3348
C	-2.1416	4.9552	4.9308
C	-4.5351	5.2931	5.1189
C	-2.0061	5.1836	6.3017
H	-1.2518	4.7657	4.3342
C	-4.3980	5.5106	6.4896
H	-5.5109	5.3357	4.6419
C	-3.1327	5.4558	7.0825
H	-1.0199	5.1539	6.7574
H	-5.2756	5.7231	7.0946
H	-3.0242	5.6300	8.1500
H	-2.7379	0.9752	0.7985
C	-2.6473	4.7792	-0.0085
H	-3.5903	5.0274	-0.5135
O	-3.2263	3.6159	-2.8423
C	-0.6555	3.4536	-3.4401
C	-0.9515	3.8682	-4.6693
S	-1.9318	3.2794	-2.2307
O	-1.7836	1.9514	-1.6165
C	-1.5390	4.5537	-1.0353
H	-0.5987	4.2585	-0.5577
H	-2.3567	5.6549	0.5790
H	-0.1756	3.9489	-5.4263
H	-1.9703	4.1313	-4.9465
H	0.3352	3.1727	-3.0884
H	-1.3799	5.4626	-1.6271

TableS1_H6-DVS_MonoAdduct

ZPE = -1159.67

C	-2.3134	3.0414	0.0624

H	-2.8629	3.6619	-0.6531
O	-1.3778	-0.0793	0.1844
C	1.0252	0.6382	-0.6451
C	1.1111	-0.5239	-1.2878
S	-0.4423	1.0507	0.2427
O	-0.0458	1.5531	1.5707
C	-1.1339	2.4197	-0.6761
H	-1.4380	2.0089	-1.6438
H	-3.0001	2.2570	0.4212
H	2.0207	-0.7942	-1.8180
H	0.2818	-1.2283	-1.2954
H	1.8075	1.3924	-0.5923
N	-1.8484	3.9153	1.1434
H	-1.3128	3.3904	1.8367
N	-2.9172	4.5398	1.7921
H	-3.5463	3.9574	2.3450
C	-3.3346	5.7768	1.3922
O	-2.7972	6.4136	0.4846
C	-4.5141	6.3230	2.1448
C	-4.8036	5.9571	3.4669
C	-5.3260	7.2578	1.4898
C	-5.9023	6.5176	4.1212
H	-4.1631	5.2566	3.9982
C	-6.4279	7.8099	2.1423
H	-5.0835	7.5407	0.4687
C	-6.7175	7.4398	3.4595
H	-6.1165	6.2390	5.1497
H	-7.0595	8.5284	1.6262
H	-7.5735	7.8732	3.9707
H	-0.3296	3.1495	-0.8248

TableS1_H6-DVS_TS1

ZPE = -1159.62

N	-1.6002	4.6109	-0.3416
H	-0.6550	4.2669	-0.1300
N	-2.3636	4.7262	0.8244
H	-1.9956	5.3559	1.5319
C	-3.6432	4.2584	0.8102
O	-4.0449	3.5756	-0.1396
C	-4.4946	4.5805	1.9932
C	-5.5924	3.7445	2.2378
C	-4.2517	5.6758	2.8342
C	-6.4314	3.9901	3.3236
H	-5.7735	2.9049	1.5723
C	-5.0982	5.9226	3.9158
H	-3.4269	6.3590	2.6456
C	-6.1845	5.0795	4.1646
H	-7.2767	3.3340	3.5136
H	-4.9116	6.7778	4.5597
H	-6.8405	5.2745	5.0091
C	-1.2990	6.1879	-1.3412
H	-2.3460	6.3841	-1.5668
O	1.8810	4.9775	-3.1158
C	1.9265	7.4563	-2.2847
C	2.8350	7.7342	-3.2173
S	1.2361	5.8335	-2.1032
O	1.4321	5.5022	-0.6707
C	-0.4380	5.9379	-2.4092
H	-0.7555	5.6425	-3.4039
H	-0.9263	6.7314	-0.4728
H	3.1864	6.9652	-3.9023
H	3.2442	8.7368	-3.3142
H	1.5294	8.1775	-1.5718
H	-2.0819	3.9426	-0.9586

TableS1_H6-DVS_TS2

ZPE = -1863.66

C	-1.3416	2.8954	-0.6844
H	-0.8828	2.9061	-1.6806
O	-2.6797	1.4548	1.6725
C	-0.4458	0.2279	2.4008
C	-1.1639	-0.8694	2.6257
S	-1.2365	1.6869	1.8066
O	-0.7904	2.8100	2.6550
C	-0.5480	1.9140	0.1667
H	-0.5707	0.9286	-0.3116
H	-2.3879	2.5977	-0.7829
H	-0.6899	-1.7645	3.0199
H	-2.2333	-0.8982	2.4274
H	0.6227	0.3373	2.5734
N	-1.3103	4.2956	-0.2157
H	-0.3549	4.5716	0.0736
N	-2.1800	4.6092	0.8461
H	-1.7900	4.4640	1.7795
C	-3.5370	4.5646	0.6498
O	-4.0319	4.3364	-0.4543
C	-4.3643	4.8181	1.8689
C	-5.6746	4.3220	1.8688
C	-3.8879	5.5371	2.9748
C	-6.5005	4.5300	2.9723
H	-6.0305	3.7720	1.0016
C	-4.7209	5.7495	4.0744
H	-2.8841	5.9563	2.9776
C	-6.0238	5.2439	4.0762
H	-7.5137	4.1370	2.9721
H	-4.3537	6.3154	4.9262
H	-6.6687	5.4103	4.9353
H	0.4950	2.2230	0.3009

C	-1.4146	5.4828	-1.5912
H	-2.3883	5.2134	-1.9950
O	2.2793	5.2092	-2.6927
C	1.3422	7.6036	-2.1968
C	2.2793	8.1186	-2.9899
S	1.2051	5.8581	-1.9202
O	1.2332	5.7306	-0.4344
C	-0.3158	5.3381	-2.4608
H	-0.3274	4.7712	-3.3851
H	-1.4576	6.3461	-0.9211
H	3.0010	7.4784	-3.4929
H	2.3420	9.1918	-3.1526
H	0.5898	8.1859	-1.6666

TableS1_H6-DVS_Z1

ZPE = -1159.62

C	-2.7882	2.4127	0.1487
H	-3.6929	2.9026	-0.2262
O	-0.6325	-0.2863	-1.7082
C	0.6047	1.1406	0.0696
C	1.7368	1.0176	-0.6230
S	-0.9580	0.4948	-0.4956
O	-1.4720	-0.2316	0.6917
C	-2.0110	1.7432	-0.8850
H	-1.8165	2.2172	-1.8443
H	-3.0359	1.7707	0.9985
H	1.7543	0.4791	-1.5683
H	2.6660	1.4509	-0.2596
H	0.5349	1.6645	1.0239
N	-2.0237	3.6280	0.8170
H	-1.1799	3.2951	1.3050
H	-1.7188	4.2598	0.0553

N	-2.7959	4.4113	1.6982
H	-3.2058	3.8906	2.4732
C	-3.4178	5.5038	1.1287
O	-3.1427	5.8287	-0.0267
C	-4.3711	6.2497	1.9914
C	-4.3518	6.1537	3.3900
C	-5.2989	7.0851	1.3550
C	-5.2670	6.8872	4.1449
H	-3.6151	5.5348	3.8962
C	-6.2157	7.8100	2.1139
H	-5.2958	7.1517	0.2705
C	-6.2004	7.7106	3.5087
H	-5.2469	6.8204	5.2291
H	-6.9407	8.4510	1.6199
H	-6.9135	8.2785	4.1007

TableS1_H6-DVS_Z1_75C

ZPE = -1159.62

N	-2.5337	3.1382	-0.0932
H	-2.5833	3.8594	-0.8348
H	-3.1075	2.3231	-0.3956
N	-3.0363	3.6943	1.0950
H	-3.5259	3.0625	1.7228
C	-2.9397	5.0542	1.2356
O	-2.4677	5.7298	0.3194
C	-3.4353	5.6341	2.5143
C	-3.5664	4.8815	3.6903
C	-3.7570	6.9980	2.5130
C	-4.0243	5.4964	4.8558
H	-3.2881	3.8305	3.7193
C	-4.2207	7.6053	3.6782
H	-3.6431	7.5671	1.5944

C	-4.3551	6.8543	4.8501
H	-4.1156	4.9161	5.7698
H	-4.4759	8.6615	3.6735
H	-4.7128	7.3286	5.7604
C	-1.0879	2.6099	-0.0240
C	-0.7482	2.0202	-1.3360
H	-0.4635	3.4733	0.2175
S	-1.3646	0.4933	-1.6254
H	0.1611	2.2908	-1.8625
O	-1.2509	0.1134	-3.0468
C	-0.4783	-0.7522	-0.7162
O	-2.7204	0.4574	-0.9893
C	0.1865	-1.7441	-1.3077
H	-0.5055	-0.5976	0.3623
H	0.1802	-1.8531	-2.3903
H	0.7491	-2.4672	-0.7215
H	-1.1173	1.9371	0.8449

TableS1_H6-DVS_Z2

ZPE = -1863.66

C	-4.4235	2.4819	0.6604
H	-4.6541	2.3723	-0.4036
O	-4.9112	-0.4003	3.2940
C	-2.8250	1.1112	3.7884
C	-1.9837	0.0803	3.7487
S	-4.4372	0.9708	3.0625
O	-5.2379	2.1028	3.5464
C	-4.2690	1.1025	1.2677
H	-5.0982	0.4791	0.9142
H	-5.2096	3.0640	1.1475
H	-2.2452	-0.8556	3.2575
H	-1.0046	0.1511	4.2156

H	-2.6298	2.0630	4.2781
N	-3.1722	3.2942	0.7017
H	-2.3748	2.7266	0.3266
N	-2.8098	3.6640	2.0161
H	-1.9097	3.3102	2.3339
C	-3.5400	4.6053	2.7043
O	-4.5732	5.0797	2.2397
C	-3.0149	4.9627	4.0554
C	-1.6551	4.8963	4.3904
C	-3.9518	5.3890	5.0062
C	-1.2402	5.2535	5.6743
H	-0.9090	4.6007	3.6564
C	-3.5337	5.7348	6.2901
H	-5.0013	5.4357	4.7283
C	-2.1776	5.6663	6.6249
H	-0.1847	5.2131	5.9290
H	-4.2630	6.0560	7.0288
H	-1.8510	5.9393	7.6251
H	-3.3316	0.6084	0.9854
C	-3.1744	4.4839	-0.3382
H	-4.1133	5.0170	-0.1855
O	-1.6185	2.5295	-3.3570
C	-0.4189	4.6848	-2.5192
C	0.1488	4.8305	-3.7157
S	-1.5489	3.3653	-2.1434
O	-0.9421	2.7681	-0.9064
C	-3.0459	3.9476	-1.6972
H	-3.7720	4.1313	-2.4801
H	-2.3436	5.0938	0.0456
H	-0.0338	4.1120	-4.5121
H	0.8070	5.6712	-3.9227
H	-0.2721	5.3725	-1.6868

TableS1_H6-nPA_BisAdduct

ZPE = -1224.75

C	-2.1324	2.8616	-0.4042
H	-2.4499	2.6082	-1.4254
C	-0.8641	2.0852	-0.0601
H	-1.0386	1.0011	-0.1161
H	-2.9429	2.5750	0.2727
N	-1.9075	4.3100	-0.2852
N	-2.7177	4.9332	0.6640
H	-2.3033	5.0009	1.5907
C	-4.0686	5.0278	0.5021
O	-4.6392	4.6186	-0.5145
C	-4.8211	5.6753	1.6265
C	-6.1801	5.3623	1.7607
C	-4.2256	6.5807	2.5166
C	-6.9348	5.9338	2.7845
H	-6.6307	4.6669	1.0572
C	-4.9853	7.1573	3.5364
H	-3.1800	6.8584	2.4053
C	-6.3373	6.8322	3.6744
H	-7.9868	5.6810	2.8884
H	-4.5220	7.8656	4.2184
H	-6.9255	7.2820	4.4704
H	-0.0738	2.3059	-0.7861
C	-1.8097	5.0634	-1.5350
H	-2.6669	4.8715	-2.1975
C	-0.5180	4.7238	-2.2688
H	-0.4495	5.3300	-3.1816
H	-1.8081	6.1249	-1.2690
C	0.6986	5.0335	-1.4294
C	-0.3786	2.4159	1.3317
O	0.8124	6.0003	-0.6958
O	1.6769	4.1332	-1.6089

C	2.9104	4.3375	-0.8909
H	2.7412	4.0970	0.1683
H	3.1957	5.3929	-0.9586
C	3.9617	3.4361	-1.5078
H	3.5799	2.4075	-1.5349
H	4.1265	3.7439	-2.5480
C	5.2694	3.4946	-0.7230
H	6.0258	2.8430	-1.1729
H	5.6735	4.5141	-0.7030
H	5.1231	3.1722	0.3157
O	-1.0670	2.9739	2.1708
O	0.8747	2.0712	1.6671
C	1.7007	1.2547	0.8140
H	1.2102	0.2856	0.6569
H	1.8356	1.7409	-0.1598
C	3.0372	1.0836	1.5097
H	2.8645	0.6658	2.5092
H	3.4897	2.0752	1.6458
C	3.9693	0.1755	0.7120
H	4.9395	0.0788	1.2101
H	3.5442	-0.8301	0.6073
H	4.1484	0.5690	-0.2961
H	-0.4914	3.6751	-2.5836

TableS1_H6-nPA_MonoAdduct

ZPE = -840.19

N	-1.2906	5.2413	-0.3693
N	-2.1763	5.3423	0.7122
H	-1.7726	5.6440	1.5942
C	-3.4036	4.7529	0.6566
O	-3.7783	4.1405	-0.3500
C	-4.2603	4.8731	1.8789

C	-5.2474	3.8990	2.0765
C	-4.1235	5.9227	2.7977
C	-6.0815	3.9626	3.1920
H	-5.3479	3.0969	1.3500
C	-4.9648	5.9880	3.9100
H	-3.3826	6.7030	2.6398
C	-5.9402	5.0074	4.1107
H	-6.8409	3.2002	3.3450
H	-4.8623	6.8082	4.6157
H	-6.5926	5.0602	4.9787
C	-1.5778	6.2543	-1.3950
H	-2.6285	6.2208	-1.7155
H	-1.3768	7.2399	-0.9631
H	-1.4150	4.3084	-0.7764
C	-0.6705	6.0019	-2.5937
H	-0.8386	6.7801	-3.3469
C	0.7910	6.0081	-2.2178
O	1.5787	5.1096	-2.4664
O	1.1476	7.1338	-1.5886
C	2.5249	7.2389	-1.1799
H	3.1642	7.1689	-2.0682
H	2.7630	6.3952	-0.5210
C	2.7102	8.5642	-0.4696
H	2.0330	8.6071	0.3925
H	2.4268	9.3780	-1.1486
C	4.1578	8.7328	-0.0153
H	4.8448	8.7063	-0.8700
H	4.3003	9.6883	0.4997
H	4.4503	7.9322	0.6749
H	-0.8909	5.0320	-3.0506

TableS1_H6-nPA_TS1

ZPE = -840.14

N	-1.2926	4.9050	-0.2937
H	-0.3000	4.8674	-0.0360
N	-2.0901	5.0933	0.8444
H	-2.0676	6.0406	1.2181
C	-3.2058	4.3061	0.9639
O	-3.3819	3.3545	0.1975
C	-4.1503	4.6476	2.0663
C	-5.4528	4.1389	1.9779
C	-3.7764	5.4256	3.1715
C	-6.3815	4.4181	2.9793
H	-5.7246	3.5316	1.1187
C	-4.7074	5.6976	4.1745
H	-2.7609	5.8008	3.2736
C	-6.0095	5.1984	4.0782
H	-7.3930	4.0282	2.9036
H	-4.4134	6.2932	5.0345
H	-6.7317	5.4133	4.8616
C	-1.4759	6.1751	-1.6255
H	-2.5371	5.9913	-1.7948
H	-1.2843	7.0211	-0.9656
H	-1.5663	4.0047	-0.7121
C	-0.5866	5.9495	-2.6905
H	-0.8740	5.3215	-3.5292
C	0.7662	6.4062	-2.6745
O	1.6059	6.2566	-3.5745
O	1.1099	7.0674	-1.5222
C	2.4307	7.6084	-1.4654
H	2.5753	8.3172	-2.2916
H	3.1658	6.8024	-1.5886
C	2.6059	8.2985	-0.1258
H	2.4339	7.5703	0.6774
H	1.8425	9.0804	-0.0227
C	4.0020	8.9031	-0.0010

H	4.1814	9.6456	-0.7883
H	4.1344	9.4014	0.9651
H	4.7756	8.1302	-0.0883

TableS1_H6-nPA_Z1

ZPE = -840.14

N	-1.2324	5.2736	-0.5060
H	-0.2301	5.4343	-0.3105
N	-1.9813	5.4296	0.6767
H	-1.8729	6.3300	1.1367
C	-3.0745	4.6081	0.8163
O	-3.2170	3.6569	0.0457
C	-4.0066	4.8939	1.9424
C	-4.9344	3.8930	2.2627
C	-3.9983	6.0958	2.6655
C	-5.8413	4.0860	3.3025
H	-4.9312	2.9694	1.6908
C	-4.9113	6.2862	3.7027
H	-3.3064	6.9003	2.4291
C	-5.8300	5.2834	4.0242
H	-6.5552	3.3051	3.5497
H	-4.9062	7.2204	4.2574
H	-6.5382	5.4364	4.8344
C	-1.6154	6.2121	-1.6890
H	-2.6590	5.9690	-1.9051
H	-1.5592	7.2031	-1.2239
H	-1.3515	4.2916	-0.8102
C	-0.7083	5.9893	-2.8245
H	-1.0510	5.4425	-3.6971
C	0.6421	6.3545	-2.7452
O	1.5461	6.2526	-3.5994
O	0.9627	6.8828	-1.4871

C	2.2961	7.3517	-1.3053
H	2.5065	8.1611	-2.0178
H	3.0081	6.5409	-1.5079
C	2.4359	7.8455	0.1232
H	2.1954	7.0230	0.8101
H	1.6999	8.6404	0.3013
C	3.8468	8.3621	0.3926
H	4.0959	9.1944	-0.2773
H	3.9500	8.7197	1.4225
H	4.5922	7.5726	0.2357

TableS1_H6-nPA_Z1_75C

ZPE = -840.14

N	-1.2353	2.9281	0.7099
H	-0.4872	2.3684	1.1454
H	-0.7895	3.6443	0.0982
N	-1.9619	3.6328	1.6897
H	-2.6535	3.0736	2.1868
C	-2.0944	4.9903	1.4976
O	-1.4646	5.5458	0.5974
C	-2.9898	5.7126	2.4413
C	-3.3996	5.1629	3.6643
C	-3.4064	6.9990	2.0737
C	-4.2306	5.8989	4.5088
H	-3.0591	4.1784	3.9763
C	-4.2412	7.7279	2.9184
H	-3.0737	7.4118	1.1253
C	-4.6541	7.1776	4.1358
H	-4.5419	5.4762	5.4601
H	-4.5690	8.7227	2.6293
H	-5.3026	7.7472	4.7965
C	-2.0750	2.0129	-0.2282

H	-2.7665	2.7298	-0.6877
C	-1.1935	1.2815	-1.1498
C	-0.4837	1.9496	-2.1566
H	-1.0060	0.2237	-0.9945
O	0.2894	1.4884	-3.0216
O	-0.6999	3.3308	-2.1156
C	-0.1033	4.1045	-3.1527
H	0.9862	3.9667	-3.1418
H	-0.4681	3.7595	-4.1300
C	-0.4617	5.5622	-2.9300
H	-1.5549	5.6642	-2.9203
H	-0.1053	5.8697	-1.9390
C	0.1440	6.4482	-4.0157
H	-0.1104	7.5017	-3.8583
H	1.2381	6.3663	-4.0263
H	-0.2212	6.1605	-5.0095
H	-2.6266	1.3550	0.4483

TableS1_H6-nPA_Z2

ZPE = -1224.71

C	-1.9405	2.9552	-0.2904
H	-2.2462	2.7863	-1.3310
C	-0.6100	2.2530	-0.0409
H	-0.7101	1.1784	-0.2470
H	-2.7112	2.5291	0.3581
N	-1.8706	4.4087	-0.0214
H	-0.2435	4.9240	0.5212
N	-2.8267	4.8481	0.9012
H	-2.5002	4.8830	1.8642
C	-4.1619	4.8061	0.6180
O	-4.5842	4.4297	-0.4790
C	-5.0797	5.2582	1.7130

C	-6.4029	4.7992	1.6781
C	-4.6693	6.1214	2.7389
C	-7.3054	5.1848	2.6685
H	-6.7090	4.1384	0.8713
C	-5.5770	6.5114	3.7252
H	-3.6552	6.5134	2.7609
C	-6.8926	6.0411	3.6943
H	-8.3288	4.8197	2.6410
H	-5.2576	7.1877	4.5138
H	-7.5961	6.3455	4.4650
H	0.1519	2.6267	-0.7363
C	-1.7861	5.2710	-1.2238
H	-2.5519	4.9890	-1.9573
C	-0.4128	5.1970	-1.8439
H	-0.3053	5.1512	-2.9226
H	-2.0189	6.2873	-0.8757
C	0.6997	5.2196	-1.0834
C	-0.1218	2.4306	1.3769
O	0.6808	5.2057	0.2658
O	1.9426	5.2747	-1.6073
C	2.9112	4.3790	-1.0327
H	2.5695	3.3434	-1.1894
H	2.9918	4.5590	0.0458
C	4.2434	4.6119	-1.7161
H	4.1266	4.4548	-2.7957
H	4.5365	5.6591	-1.5690
C	5.3136	3.6777	-1.1567
H	6.2809	3.8532	-1.6386
H	5.4446	3.8274	-0.0775
H	5.0447	2.6266	-1.3204
O	-0.7708	2.9981	2.2426
O	1.0886	1.9533	1.6959
C	1.8459	1.1100	0.8061
H	1.4478	0.0893	0.8741

H	1.7504	1.4526	-0.2288
C	3.3006	1.1596	1.2287
H	3.3834	0.8711	2.2836
H	3.6549	2.1961	1.1433
C	4.1423	0.2343	0.3538
H	5.2053	0.3141	0.6038
H	3.8424	-0.8124	0.4849
H	4.0277	0.4841	-0.7087

TableS1_H6

ZPE = -455.64

N	-1.8596	3.6192	-0.0701
H	-0.8883	3.9328	-0.1194
H	-2.3388	3.9955	-0.8914
N	-2.4510	4.1513	1.0831
H	-2.8632	3.4787	1.7210
C	-2.6647	5.4865	1.2254
O	-2.3348	6.2946	0.3506
C	-3.3262	5.9178	2.4997
C	-3.2310	5.1801	3.6881
C	-4.0433	7.1210	2.4842
C	-3.8579	5.6424	4.8469
H	-2.6503	4.2613	3.7265
C	-4.6755	7.5761	3.6408
H	-4.0995	7.6876	1.5583
C	-4.5837	6.8362	4.8240
H	-3.7732	5.0729	5.7688
H	-5.2381	8.5058	3.6209
H	-5.0724	7.1924	5.7274

TableS1_H6_75C

ZPE = -455.64

N	-1.8596	3.6192	-0.0701
H	-0.8883	3.9328	-0.1194
H	-2.3388	3.9955	-0.8914
N	-2.4510	4.1513	1.0831
H	-2.8632	3.4787	1.7210
C	-2.6647	5.4865	1.2254
O	-2.3348	6.2946	0.3506
C	-3.3262	5.9178	2.4997
C	-3.2310	5.1801	3.6881
C	-4.0433	7.1210	2.4842
C	-3.8579	5.6424	4.8469
H	-2.6503	4.2613	3.7265
C	-4.6755	7.5761	3.6408
H	-4.0995	7.6876	1.5583
C	-4.5837	6.8362	4.8240
H	-3.7732	5.0729	5.7688
H	-5.2381	8.5058	3.6209
H	-5.0724	7.1924	5.7274

TableS1_nPA

ZPE = -384.53

C	3.0888	1.6432	-0.0000
H	2.1568	2.2030	-0.0000
H	4.0161	2.2104	-0.0000
C	3.1035	0.3064	-0.0000
C	1.8822	-0.5340	0.0000
O	1.9150	-1.7569	0.0000
O	0.7414	0.1640	-0.0000
C	-0.4814	-0.5973	0.0000
H	-0.4977	-1.2408	-0.8879

H	-0.4977	-1.2408	0.8879
C	-1.6445	0.3735	-0.0000
H	-1.5728	1.0196	0.8837
H	-1.5728	1.0196	-0.8838
H	4.0319	-0.2592	0.0000
C	-2.9725	-0.3794	0.0000
H	-3.8185	0.3151	-0.0000
H	-3.0629	-1.0191	-0.8861
H	-3.0629	-1.0191	0.8861

TableS1_nPA_75C

ZPE = -384.53

C	3.0888	1.6432	-0.0000
H	2.1568	2.2030	-0.0000
H	4.0161	2.2104	-0.0000
C	3.1035	0.3064	-0.0000
C	1.8822	-0.5340	0.0000
O	1.9150	-1.7569	0.0000
O	0.7414	0.1640	0.0000
C	-0.4814	-0.5973	0.0000
H	-0.4977	-1.2408	-0.8879
H	-0.4977	-1.2408	0.8879
C	-1.6445	0.3735	-0.0000
H	-1.5728	1.0196	0.8837
H	-1.5728	1.0196	-0.8838
H	4.0319	-0.2592	0.0000
C	-2.9725	-0.3794	0.0000
H	-3.8185	0.3151	-0.0000
H	-3.0629	-1.0191	-0.8861
H	-3.0629	-1.0191	0.8861