

Electronic Supplementary Information

Entropy Driven Chain Effects on Ligation Chemistry

*Kai Pahnke,^{ab} Josef Brandt,^{cd} Ganna Gryn'ova,^e Peter Lindner,^f Ralf Schweins,^f Friedrich Georg Schmidt,^g Albena Lederer,^{*cd} Michelle L. Coote,^{*e} Christopher Barner-Kowollik^{*ab}*

^a Preparative Macromolecular Chemistry, Institut für Technische Chemie und Polymerchemie, Karlsruhe Institute of Technology (KIT), Engesserstr. 18, 76131 Karlsruhe, Germany. E-mail: christopher.barner-kowollik@kit.edu

^b Institut für Biologische Grenzflächen, Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany.

^c Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden, Germany.
E-Mail: lederer@ipfdd.de

^d Technische Universität Dresden, 01062 Dresden, Germany.

^e ARC Centre of Excellence for Electromaterials Science, Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia. E-mail: michelle.coote@anu.edu.au

^f Institut Laue-Langevin (ILL), 6 Rue Jules Horowitz, 38042 Grenoble, France.

^g Evonik Industries AG, Paul-Baumann-Strasse 1, 45764 Marl, Germany.

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1. List of Syntheses

Table S1. List of the ARGET ATRP synthetic conditions for the bromo functional polymethacrylates.

Polymer	m _{CuBr} [mg]	V _{Me6TREN*} [μL]	V _{Monomer} [mL]	M _{EBIB**} [μL]	V _{Sn(EH)2} [μL]	V _{Anisole} [mL]	t [min.]	Precip. in cold
BrPMMA	9.4	192.0	15.0	95.7	106	15.0	35	Hexane/Et ₂ O 1:1
BrP ⁱ BuMA	6.2	127.8	15.0	63.8	70	15.0	45	MeOH/H ₂ O 4:1
BrP ^t BuMA	6.2	126.2	15.0	63.0	70	15.0	56	MeOH/H ₂ O 4:1

*c = 0.34 mmol mL⁻¹; **ethyl α-bromo isobutyrate

Table S2. List of the ARGET ATRP synthetic conditions for the bromo difunctional polyacrylates.

Polymer	m_{CuBr} [mg]	V_{Me6TREN*} [μL]	V_{Monomer} [mL]	m_{BDBIB**} [mg]	V_{Sn(EH)2} [μL]	V_{Anisole} [mL]	t [min.]	Precip. in cold
Br ₂ P ⁿ BuA	272.5	412.9	20.0	272.5	227.4	20.0	55	MeOH/ H ₂ O 4:1
Br ₂ P ⁱ BuA	19.9	408.0	20.0	269.5	225.0	20.0	45	MeOH/ H ₂ O 4:1
Br ₂ P ^r BuA	21.4	439.0	20.0	289.5	242.0	20.0	40	MeOH/ H ₂ O 4:1
Br ₂ PMA _{large}	31.9	653.0	20.0	431.0	359.6	20.0	35	MeOH/ H ₂ O 7:3
Br ₂ P ⁱ BoA large	13.6	278.4	20.0	183.7	153.0	20.0	35	MeOH
Br ₂ PMA _{small}	95.6	1959	12.0	2586	1079	20.0	55	MeOH/ H ₂ O 7:3
Br ₂ P ⁱ BoA small	4.1	460.0	12.0	1102	575.0	20.0	55	MeOH

*c = 0.34 mmol mL⁻¹; **butylene bis(2-bromoisobutyrate)

Table S3. List of the reaction conditions for the Cp functionalization reactions of the bromo (di-) functional poly(meth-)acrylates.

Polymer	m_{Br(2)Polym.} [g]	m_{NaI} [mg]	m_{PPh3} [mg]	V_{THF} [mL]	m_{NiCp2} [mg]	t [h]
CpPMMA	0.86	138.1	80.6	4.0	58.0	12
CpP ⁱ BuMA	2.00	264.5	154.3	6.0	111.1	12
CpP ^t BuMA	1.37	170.7	99.6	5.0	71.8	12
Cp ₂ P ⁿ BuA	2.68	149.9	262.3	8.0	306.8	5
Cp ₂ P ⁱ BuA	2.45	648.0	378.0	7.0	275.0	5
Cp ₂ P ^t BuA	3.4	927.0	541.0	10.0	389.0	5
Cp ₂ PMA _{large}	3.23	1336	779.0	15.0	561.0	5
Cp ₂ P ⁱ BoA _{large}	2.99	549.0	320.0	6.0	231.0	5
Cp ₂ PMA _{small}	2.02	3050	1779	17.0	1281	5
Cp ₂ P ⁱ BoA _{small}	1.00	785.0	458.0	4.5	330.0	5

Table S4. List of the synthetic conditions for the DA linkage reactions.

Polymer	m_{Cp(2)Polymer} [mg]	m_{CDTE} [mg]	V_{Anisole} [μL]
b-PMMA	50.0	5.4	200.0
b-P ⁱ BuMA	50.0	3.3	200.0
b-P ^t BuMA	50.0	4.5	200.0
DA-P ⁿ BuA	50.0	8.5	200.0
DA-P ⁱ BuA	50.0	8.2	200.0
DA-P ^t BuA	50.0	11.5	200.0
DA-PMA _{large}	50.0	12.7	200.0
DA-P ⁱ BoA _{large}	50.0	4.0	200.0
DA-PMA _{small}	50.0	35.0	200.0
DA-P ⁱ BoA _{small}	49.0	29.0	200.0

2. Additional Offline SEC Elugrams

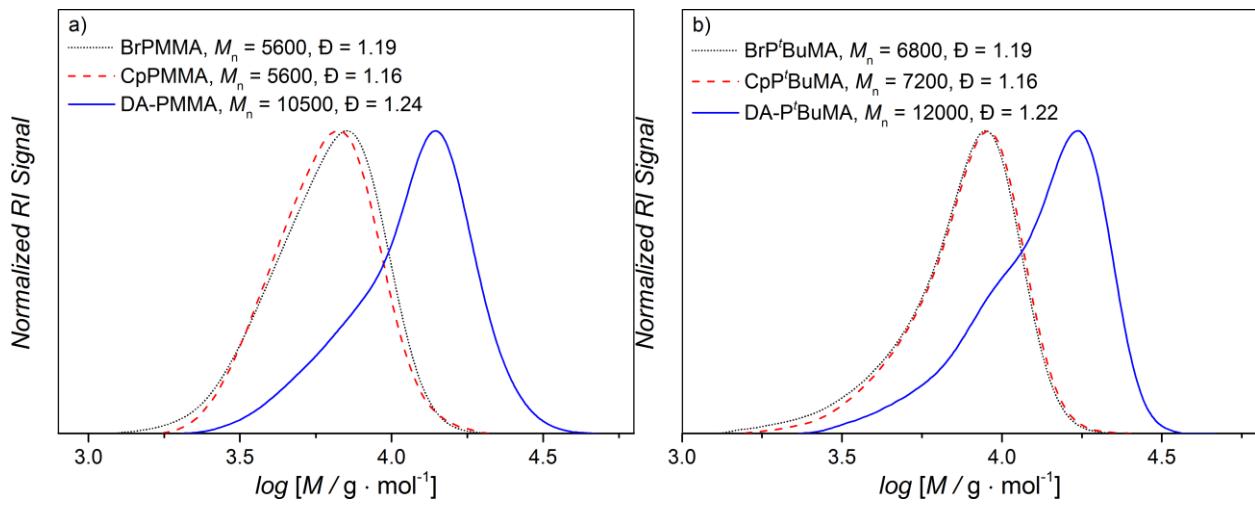


Figure S1. SEC elugrams of the bromo precursor polymer (···), Cp functional building block (---) and Diels–Alder diblock polymer (—) for 50 (a) methyl methacrylate and (b) *tert*-butyl methacrylate repeating units per building block.

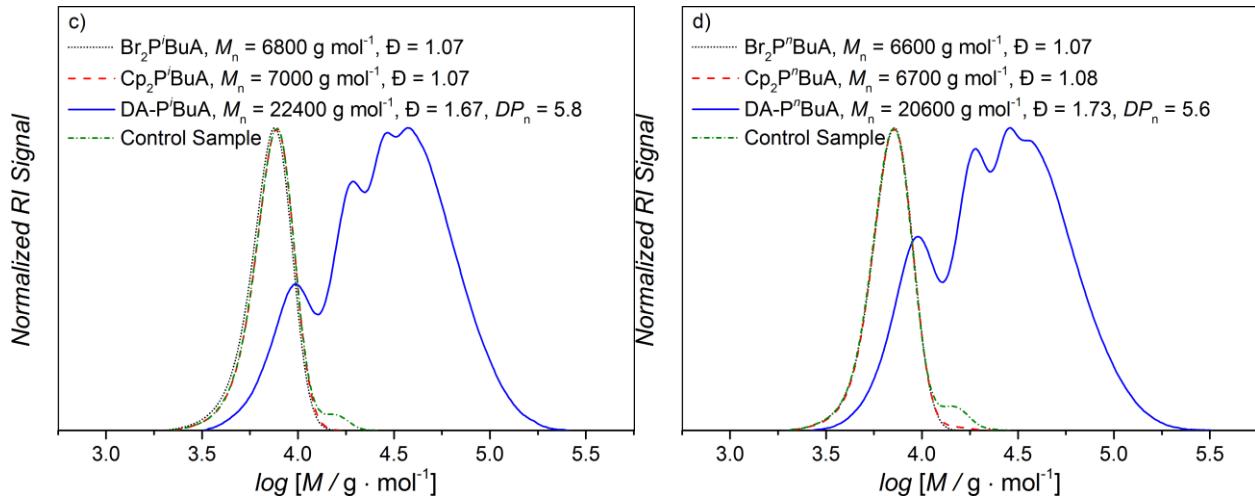


Figure S2. SEC elugrams of the dibromo precursor polymer (···), Cp functional building block (---), Diels–Alder polymer (—) and control sample of heated Cp difunctional macromonomer without CDTE dilinker (···) for 50 (c) *iso*-butyl acrylate and (d) *n*-butyl acrylate repeating units per building block.

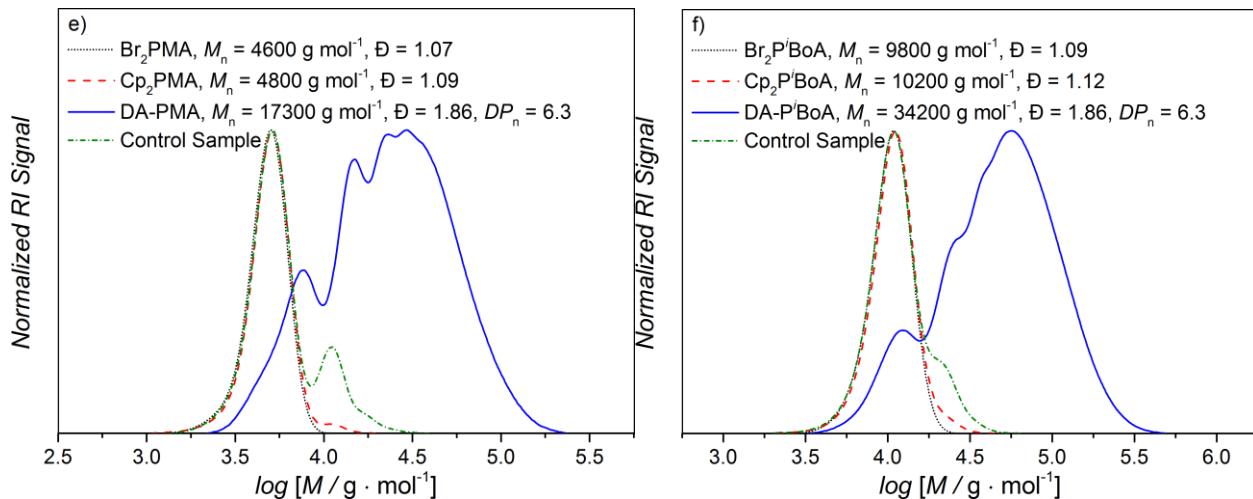


Figure S3. SEC elugrams of the dibromo precursor polymer (· · ·), Cp functional building block (— · —), Diels–Alder polymer (—) and control sample of heated Cp difunctional macromonomer without CDTE dilinker (— · —) for 50 (e) methyl acrylate and (f) isobornyl acrylate repeating units per building block.

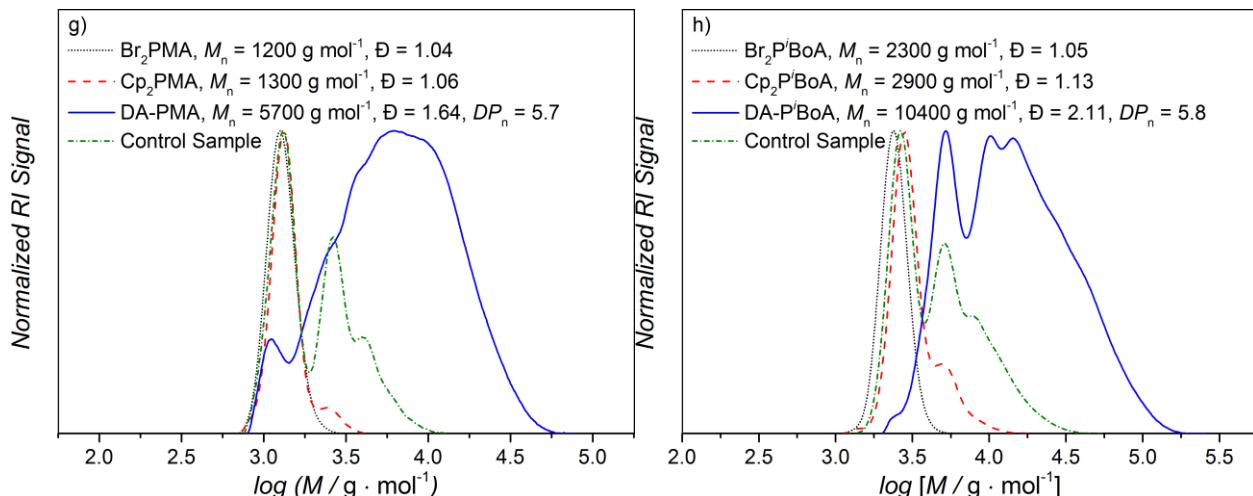


Figure S4. SEC elugrams of the dibromo precursor polymer (· · ·), Cp functional building block (— · —), Diels–Alder polymer (—) and control sample of heated Cp difunctional macromonomer without CDTE dilinker (— · —) for 10 (g) methyl acrylate and (h) isobornyl acrylate repeating units per building block.

3. Applied MHKS Parameters

Table S5. Applied Mark-Houwink-Kuhn-Sakurada parameters:

Polymer	K [10 ⁻³ mL·g ⁻¹]	α	Ref.
PMA	19.50	0.66	¹
P <i>t</i> BoA	5.00	0.745	²
PMMA	12.80	0.72	³
P <i>t</i> BuMA	5.84	0.76	⁴
P <i>i</i> BuMA	9.70	0.705	⁵
P <i>t</i> BuA	19.70	0.66	²
P <i>n</i> BuA	12.20	0.70	⁶
P <i>i</i> BuA	12.70	0.71	⁷

4. Calculation of the average DP_n

$$DP_n = \frac{M_n(DA - Polymer)}{(M_n(Macromonomer) + M(Dilinker))/2} \quad \text{Equation S1}$$

5. NMR Spectra

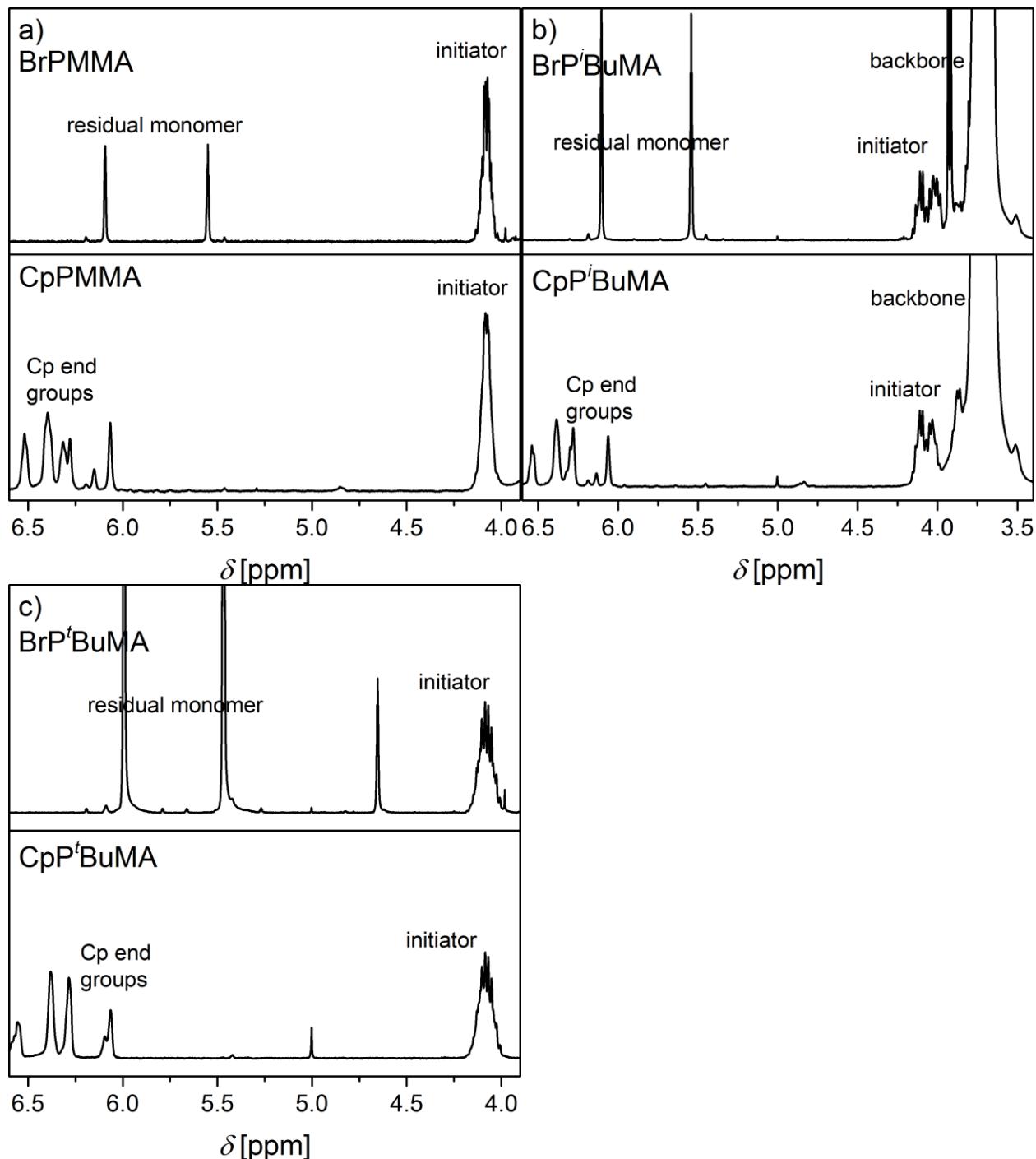


Figure S5. ¹H NMR spectra of the bromo precursor and Cp functionalized polymer building blocks with 50 (a) methyl methacrylate, (b) *iso*-butyl methacrylate and (c) *tert*-butyl methacrylate repeating units.

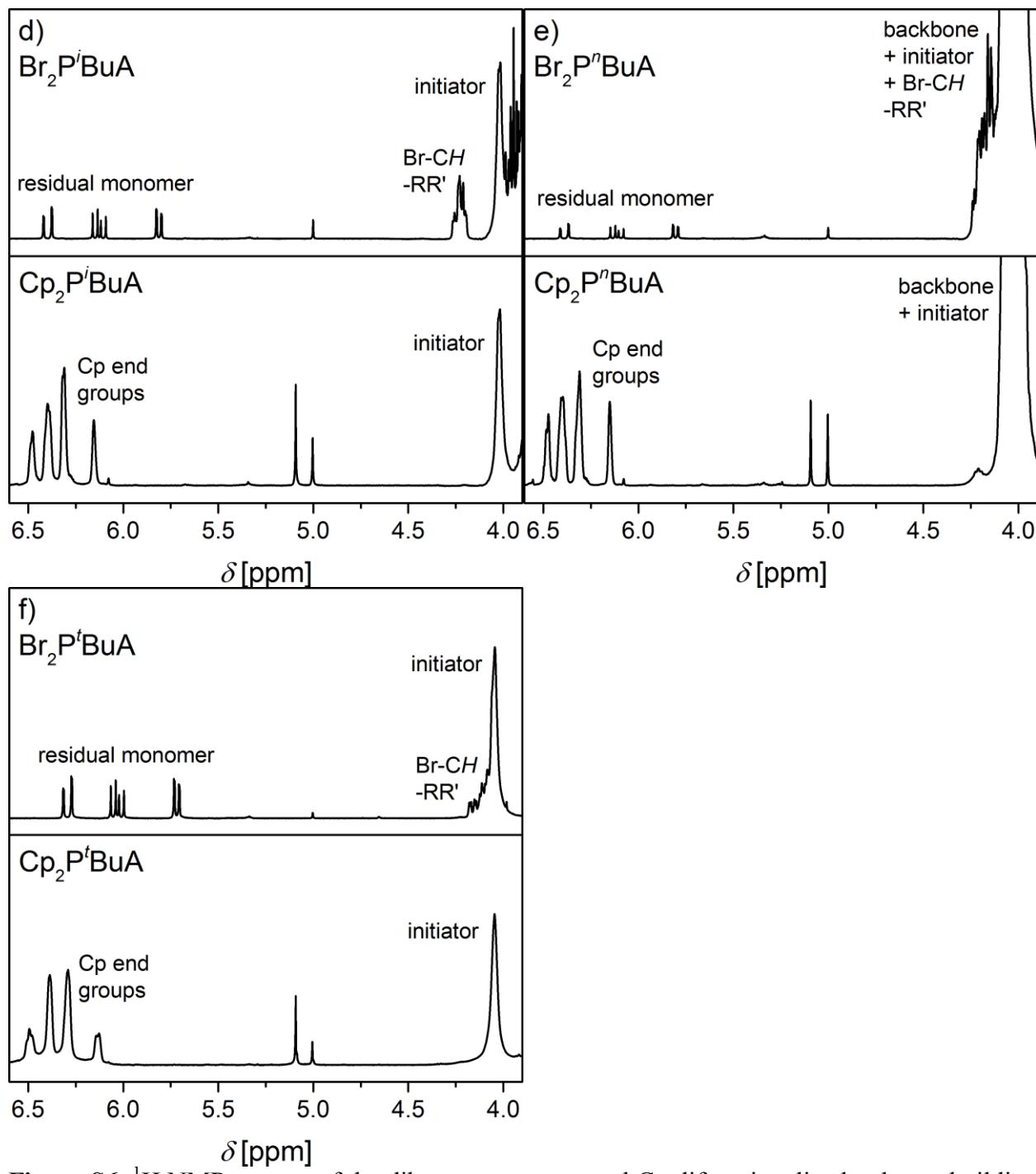


Figure S6. ^1H NMR spectra of the dibromo precursor and Cp difunctionalized polymer building blocks with 50 (d) *iso*-butyl acrylate, (e) *n*-butyl acrylate and (f) *tert*-butyl acrylate repeating units.

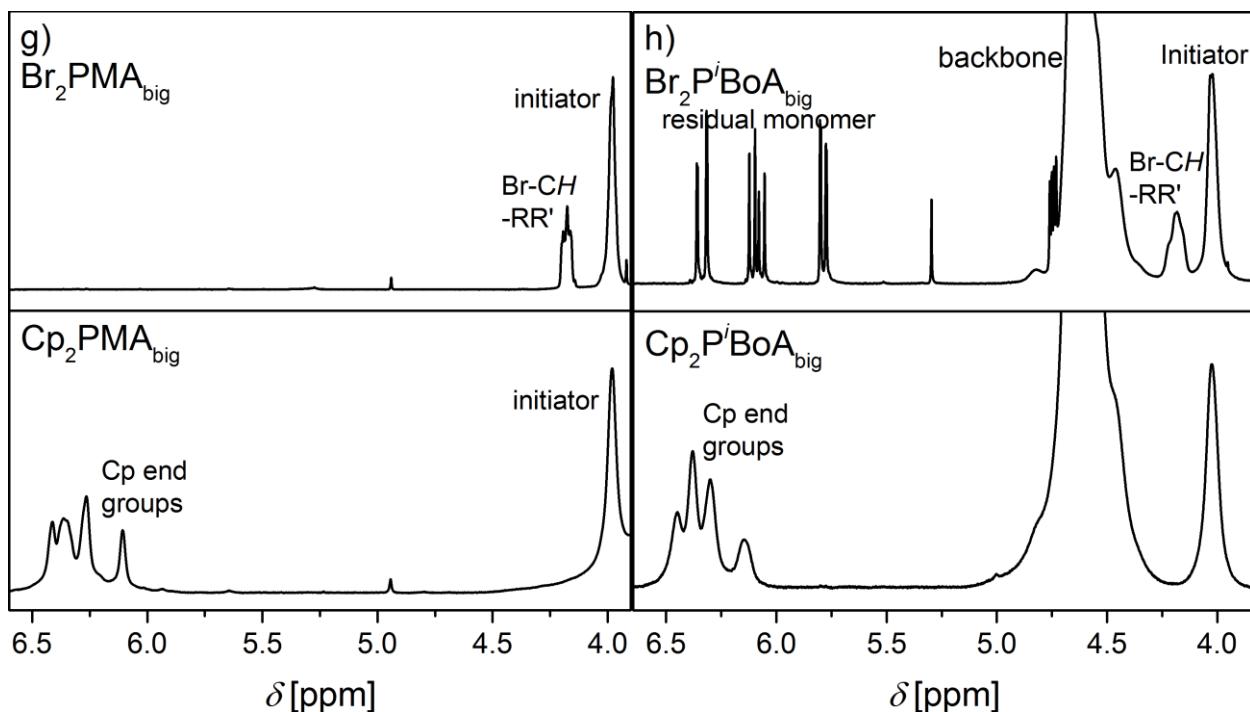


Figure S7. ^1H NMR spectra of the dibromo precursor and Cp difunctionalized polymer building blocks with 50 (g) methyl acrylate and (h) isobornyl butyl acrylate repeating units.

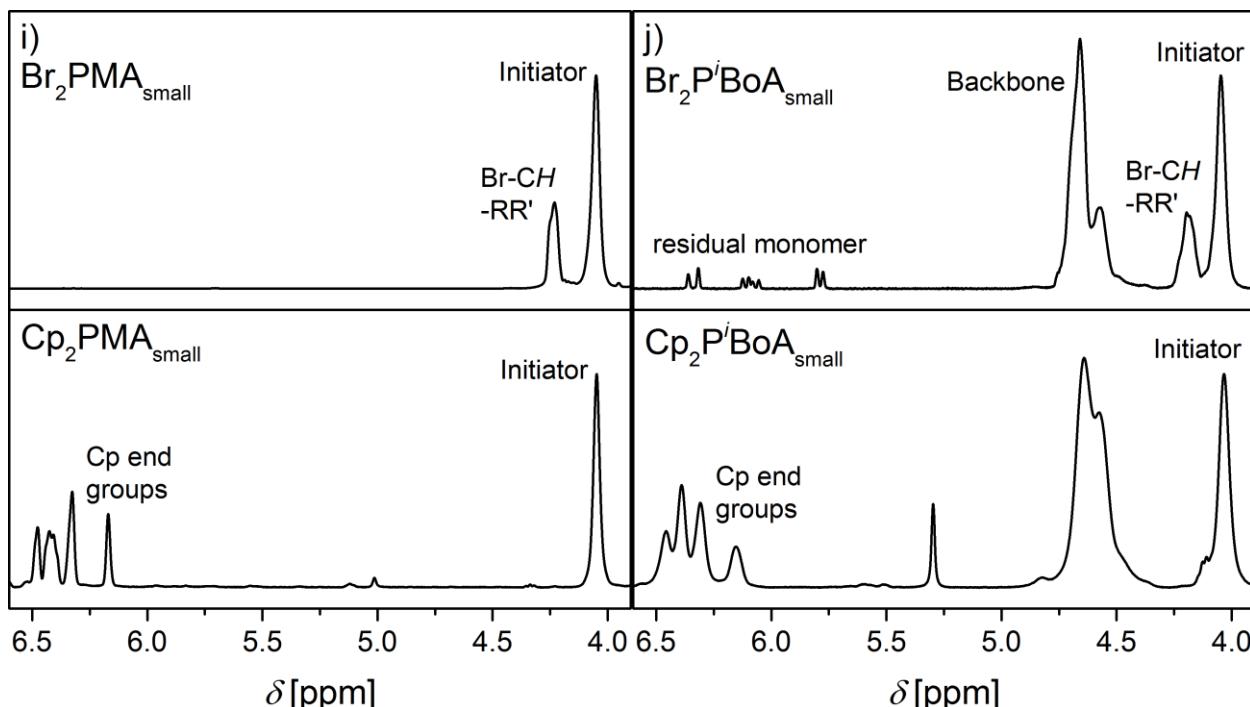


Figure S8. NMR spectra of the dibromo precursor and Cp difunctionalized polymer building blocks with 10 (i) methyl acrylate and (j) isobornyl butyl acrylate repeating units.

6. HT NMR Spectra

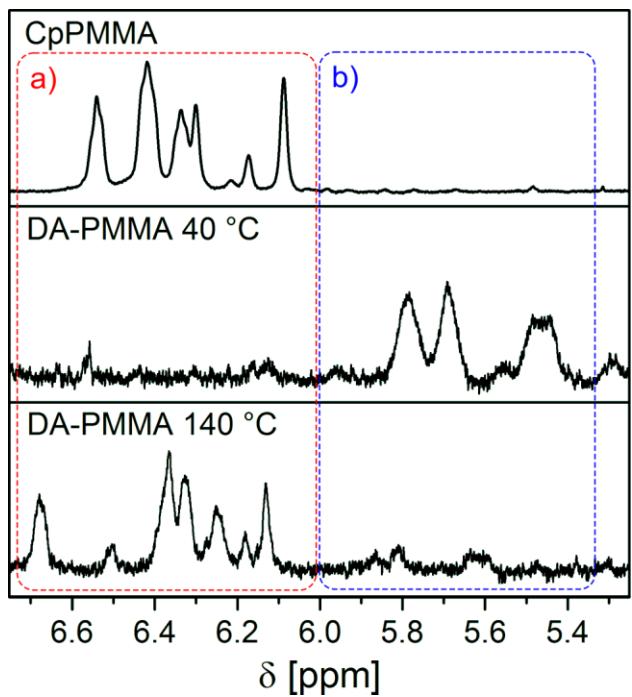


Figure S9. ^1H NMR of Cp functional PMMA (top), DA diblock PMMA at 40 °C (middle) and 140 °C (bottom) and the applied integration borders for (a) Cp and (b) DA adduct signal.

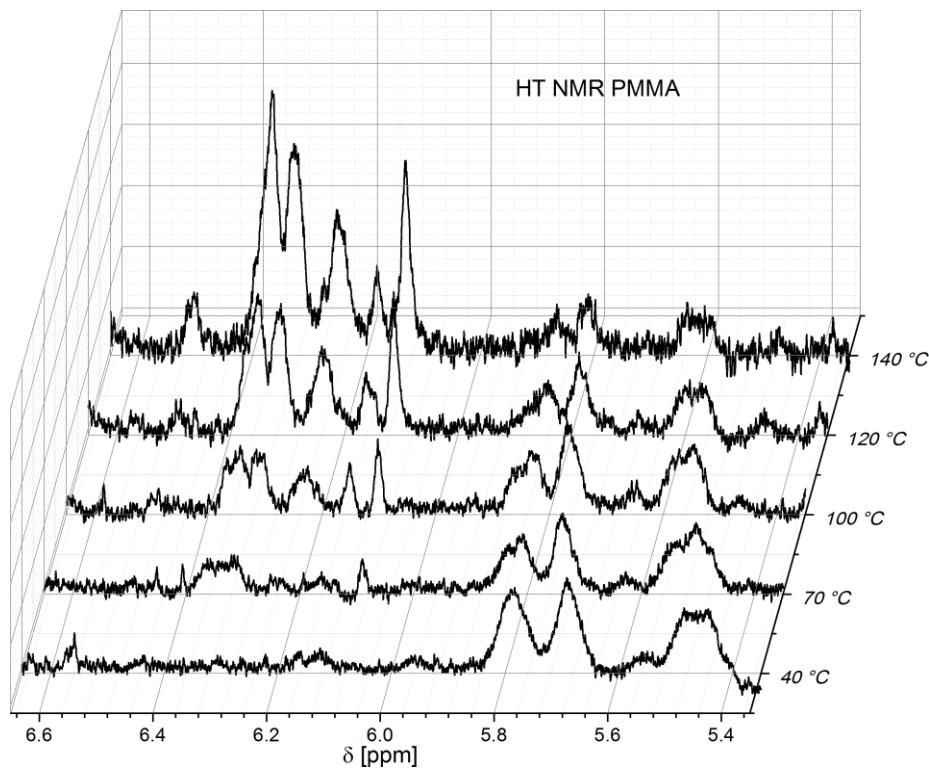


Figure S10. ^1H HT NMR spectra of the DA diblock polymer out of PMMA building blocks.

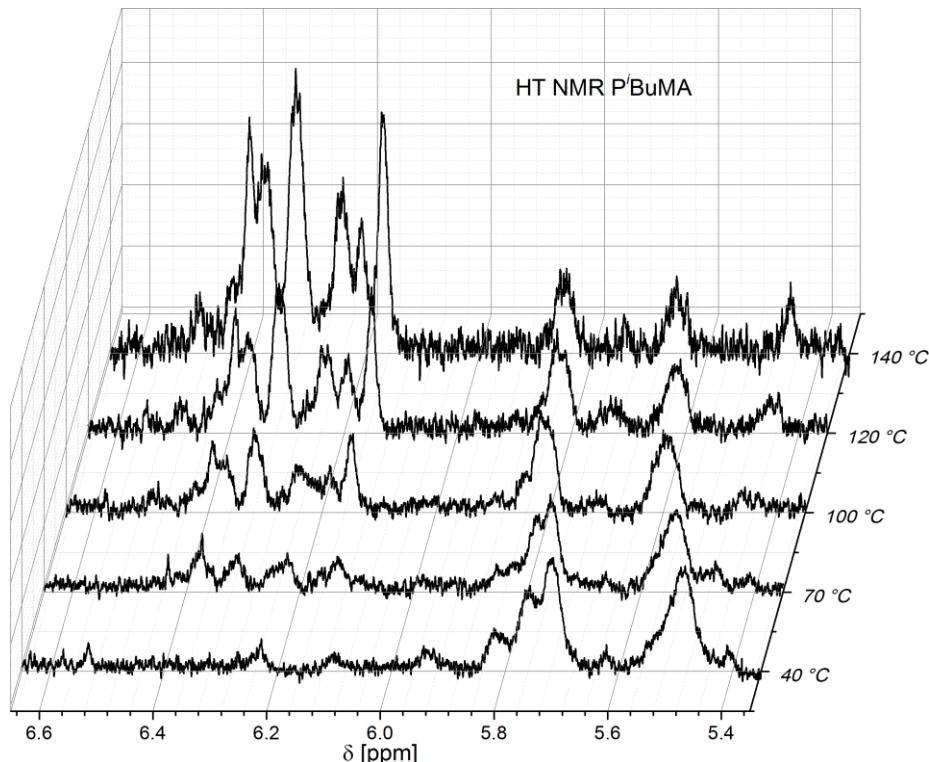


Figure S11. ^1H HT NMR spectra of the DA diblock polymer out of P^iBuMA building blocks.

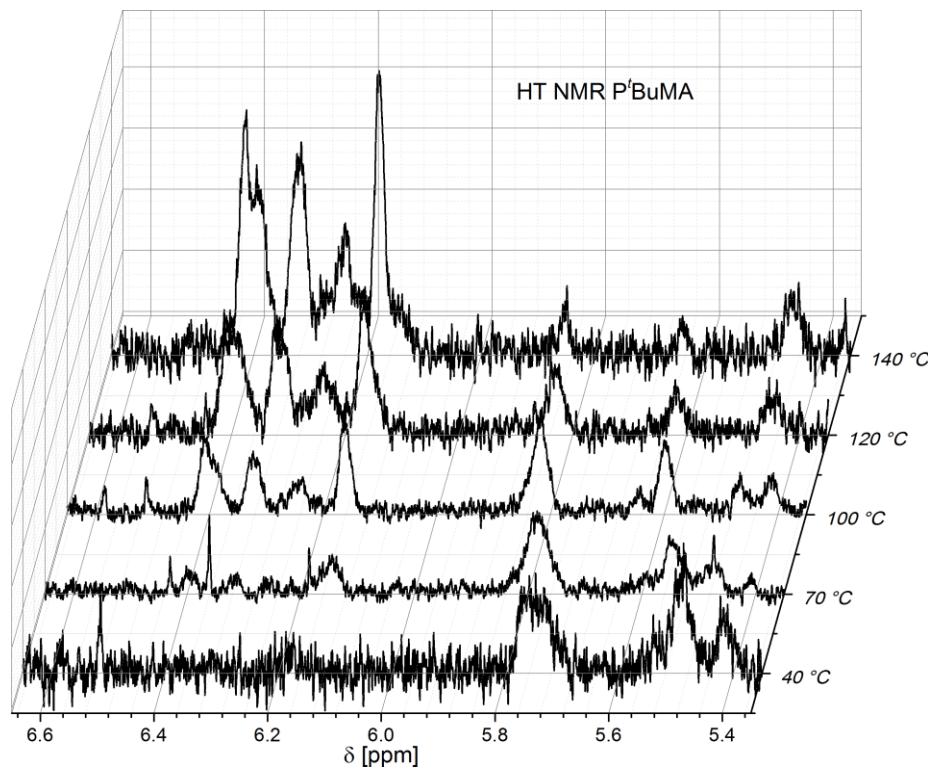


Figure S12. ¹H HT NMR spectra of the DA diblock polymer out of P'BuMA building blocks.

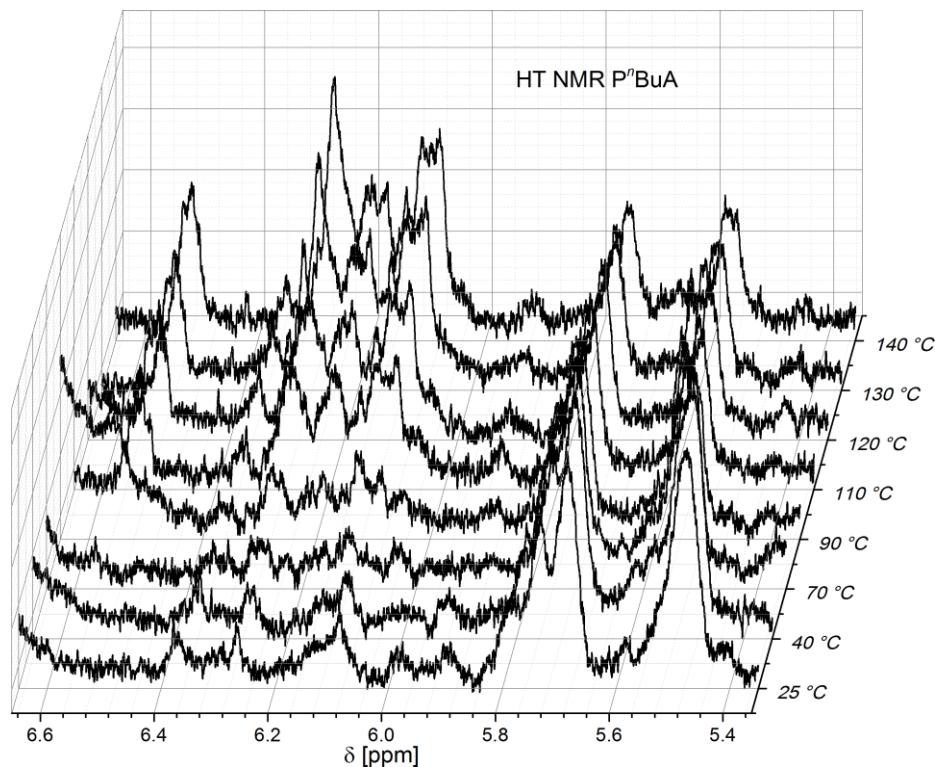


Figure S13. ¹H HT NMR spectra of the DA polymer out of P"BuA building blocks.

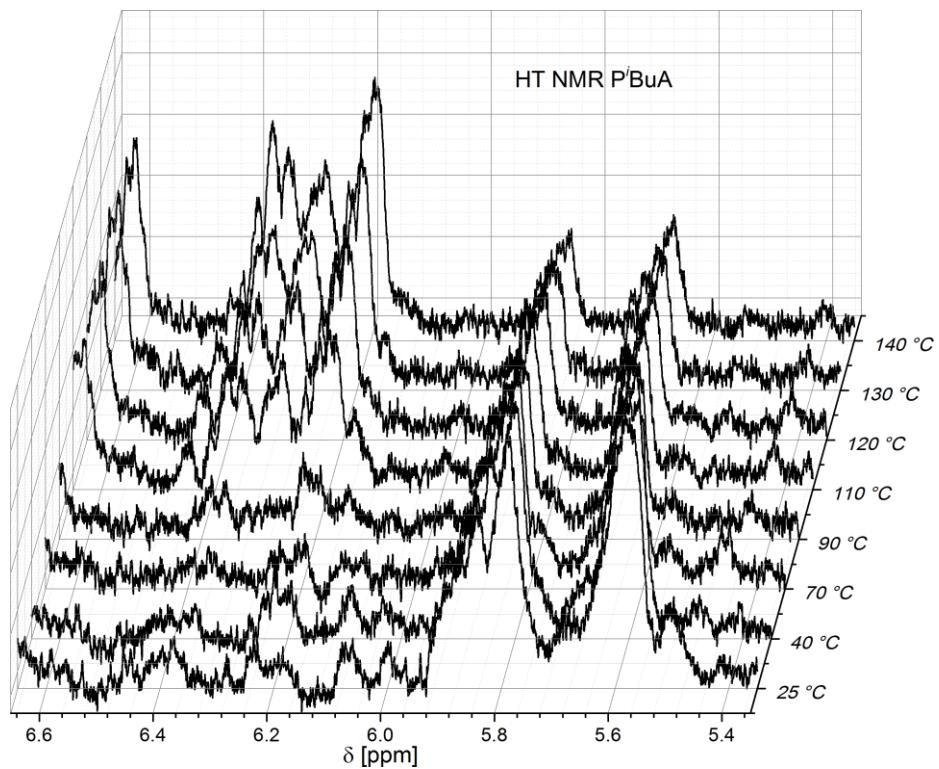


Figure S14. ^1H HT NMR spectra of the DA polymer out of P*i*BuA building blocks.

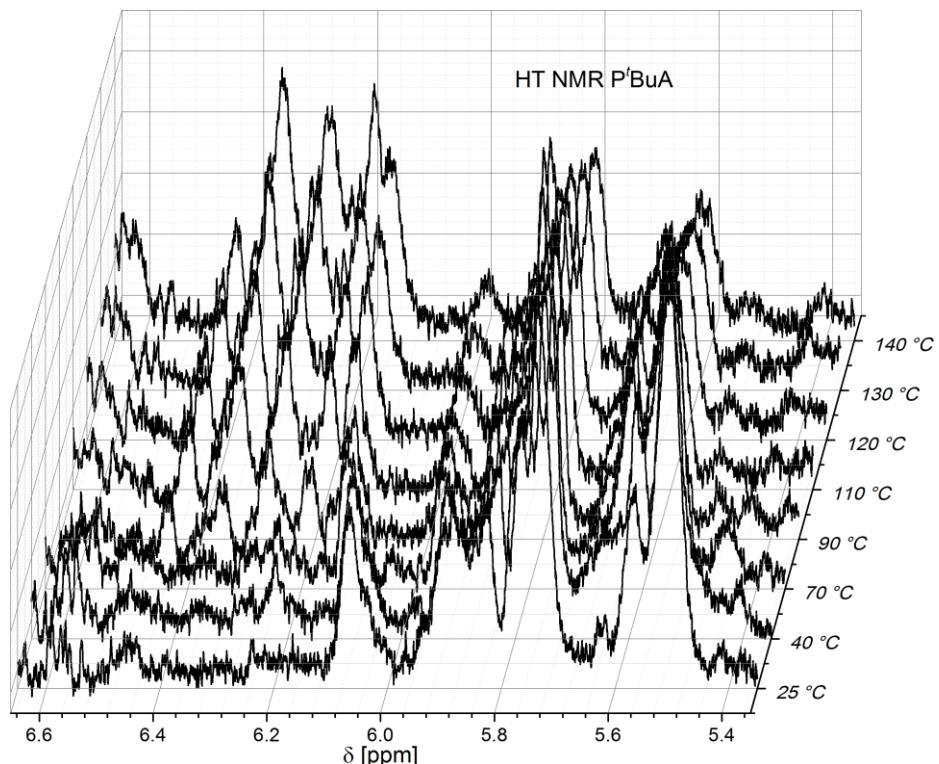


Figure S15. ^1H HT NMR spectra of the DA polymer out of P*i*BuA building blocks.

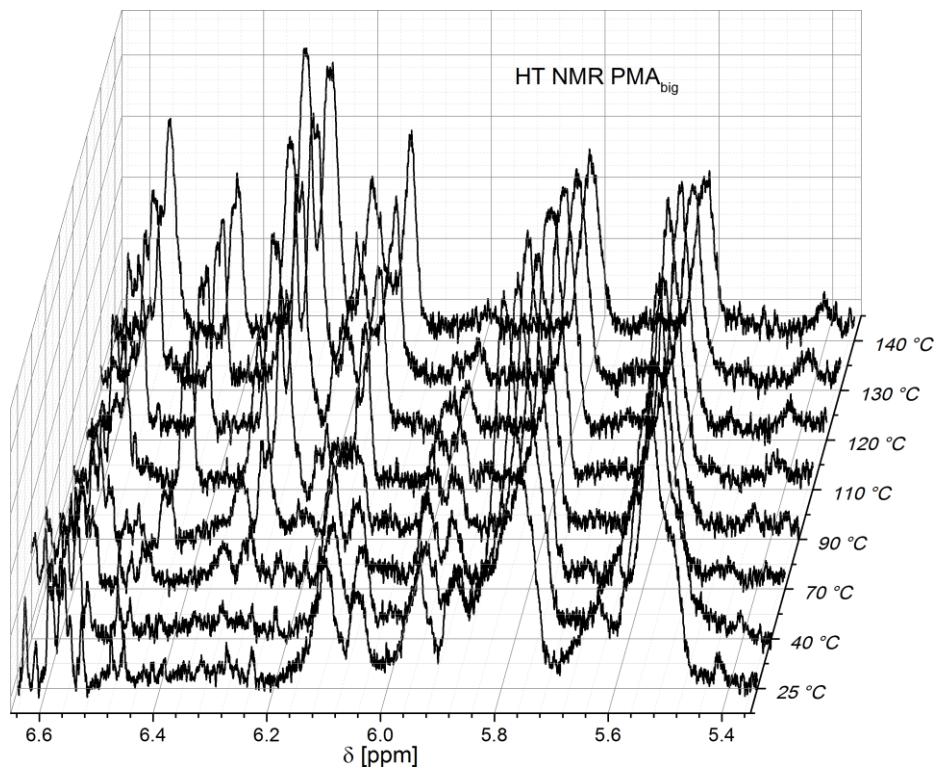


Figure S16. ^1H HT NMR spectra of the DA polymer out of $\text{PMA}_{\text{large}}$ building blocks.

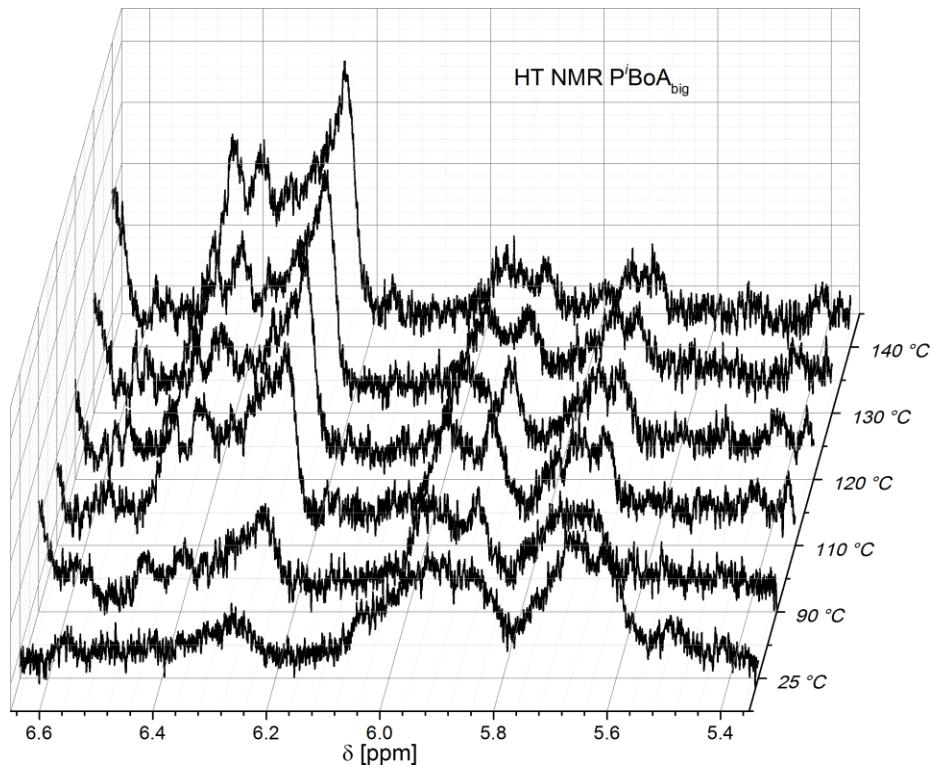


Figure S17. ^1H HT NMR spectra of the DA polymer out of $\text{P}'\text{BoA}_{\text{large}}$ building blocks.

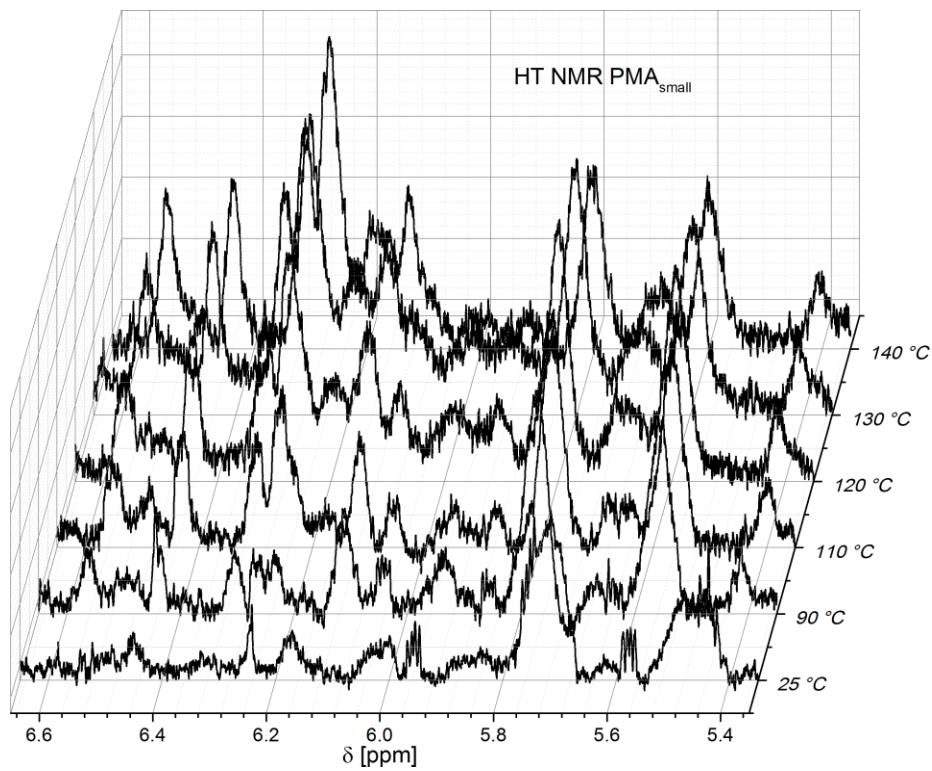


Figure S18. ¹H HT NMR spectra of the DA polymer out of PMA_{small} building blocks.

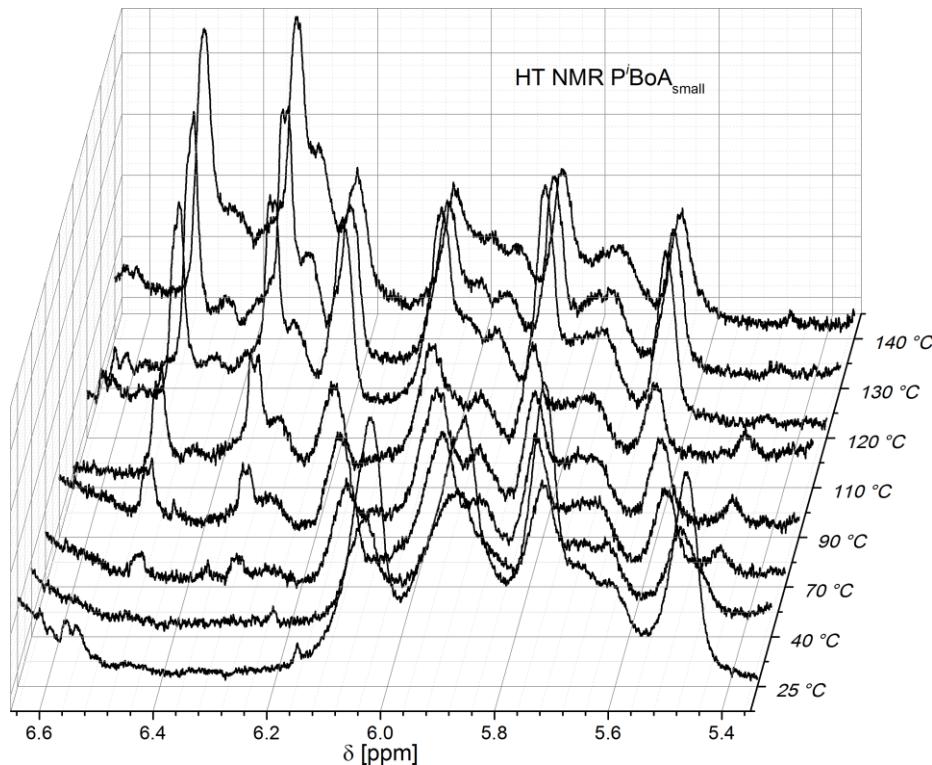


Figure S19. ¹H HT NMR spectra of the DA polymer out of P'ⁱBoA_{small} building blocks.

7. Experimental Debonding Values (HT NMR)

Polymer	Degree of Debonding [%]								
	25 °C	40 °C	70 °C	90 °C	100 °C	110 °C	120 °C	130 °C	140 °C
PMMA	n.d.	7.4	17.1	n.d.	30.2	n.d.	46.0	n.d.	67.5
P <i>t</i> BuMA	n.d.	9.6	22.3	n.d.	42.3	n.d.	61.5	n.d.	81.0
P <i>t</i> BuMA	n.d.	8.5	19.3	n.d.	35.9	n.d.	53.0	n.d.	74.2
P <i>n</i> BuA	2.0	3.9	12.8	23.5	n.d.	40.0	47.7	56.9	65.5
P <i>i</i> BuA	5.1	6.8	16.7	28.6	n.d.	42.7	52.7	61.1	72.6
P <i>t</i> BuA	1.3	2.0	8.0	18.0	n.d.	30.9	38.5	46.2	55.1
PMA _{large}	2.6	3.9	8.5	21.1	n.d.	36.7	46.2	53.9	62.3
P <i>i</i> BoA _{large}	1.3	n.d.	n.d.	28.9	n.d.	45.9	53.7	64.0	73.4
PMA _{small}	2.6	n.d.	n.d.	18.5	n.d.	30.6	39.3	47.0	55.5
P <i>i</i> BoA _{small}	0.6	0.7	2.0	8.5	n.d.	21.5	30.2	38.8	46.4

8. TD SEC evaluation

The TD SEC experiments were carried out in a mixture of 60 % TCB and 40 % DMF to minimize enthalpic interactions of the DA polymers with the column material. Although the polyacrylate building blocks are rather unpolar, the DA polymers become more polar due to the incorporation of the rather polar linker molecule. Working in only TCB leads to significant shifts to higher elution volumes of the DA polymer peaks in comparison to the individual building blocks. Increasing the polarity of the solvent reduces the enthalpic interactions; the ratio of 60/40 TCB/DMF has been found as an optimum.

Calculation of molar mass averages relative to standards is not possible due to the different refractive index increments (dn/dc) of the acrylate building blocks and the linker in the employed

solvent mixture in the investigated temperature range. Actually, all PBuA isomers and PMA exhibit a negative dn/dc , and PⁱBoA and the linker a positive one, while, in addition, the magnitude of the dn/dc of the linker is much higher than of all polymers. As a consequence, the overlaying peaks contribute to the dRI signal with different magnitudes so that the resulting signal is not representative of the relative concentrations. Moreover, the building block peak in the middle of the chromatogram does not cover only the building block but partially also building blocks with one or two linkers attached. A block with a linker and a block without linker have virtually identical elution volumes but significantly differing dn/dc values. As the amount of linker still present in this region of the chromatogram is unknown it is not possible to evaluate this peak with respect to concentrations.

It is, however, possible to evaluate the area of the DA polymer and of the linker because their composition is constant. The dn/dc of the linker and the DA polymer can be estimated by injecting samples of pure linker and building block of known concentration and calculating the peak areas. Dividing the peak area by the concentration gives a dn/dc related contrast value in units of mV s mg^{-1} . Unfortunately, the contrast for the DA polymers cannot be measured directly because the DA polymer would undergo rDA reaction in the column. However, the contrast value for the DA polymer can be calculated from the contrast from the linker and the building block, as shown in Equation S2 and Equation S3:

$$contrast_{DA\ Polymer}$$

$$= X \cdot contrast_{dilinker} + (X - 1) \cdot contrast_{building\ block} \quad \text{Equation S2}$$

with

$$X = \frac{M(\text{CDTE dilinker})}{M(\text{CDTE dilinker}) + M_n(\text{building block})} \quad \text{Equation S3}$$

It must be noted that the contrast values are unique for every polymer at any temperature in any particular solvent and have to be determined for each experiment individually.

With these values in hand it is now possible to deconvolute the chromatograms by using multiple Gauss functions, as shown in Equation S4

$$y = y_0 + \frac{A}{w\sqrt{\pi/2}} \cdot e^{-2\frac{(x-x_c)^2}{w^2}} \quad \text{Equation S4}$$

where y_0 is an offset (usually $y_0 = 0$), A the peak area, w the peak width and x_c the position of the peak center. Multiple Gauss functions can be overlaid for fitting asymmetrical peaks and the necessary peak parameters are gained by fitting the functions to chromatograms of the individual building blocks and the CDTE linker.

It is now possible to calculate the remaining concentration of the DA polymer in the reaction mixture according to Equation S5. The calculated concentration needs to be related to the initial concentration of the DA polymer, which can be calculated by using Equation S6.

$$c(\text{DA polymer}) = \frac{\text{Peak area (DA polymer)}}{\text{contrast (DA polymer)}} \quad \text{Equation S5}$$

$$c_0(\text{DA polymer}) = \text{weighed mass} \cdot \text{DA polymer content} \quad \text{Equation S6}$$

The “DA polymer content” gives the percentage of DA polymer in the investigated systems at ambient temperature, so before any rDA reaction, and has been determined by deconvoluting

chromatograms acquired at ambient temperature in THF. Eventually, the DA polymer decrease can be calculated according to Equation S7:

$$DA\ polymer\ decrease = 100\% - \frac{c\ (DA\ polymer)}{c_0(DA\ polymer)} \cdot 100\% \quad \text{Equation S7}$$

A similar procedure could be performed for calculating and tracking the concentration of the released linker. However, as a consequence of the proximity of linker and solvent peak, it is very difficult to define a good base line and precise integration borders. Both facts complicate the data processing and further optimization is needed for the exact evaluation of the peak area of the linker.

Figure S20 shows an example chromatogram (DA-PⁿBuA at 110 °C in 60 % TCB, 40 % DMF) with the calculated peaks for the DA polymer, the building block and the released CDTE dilinker.

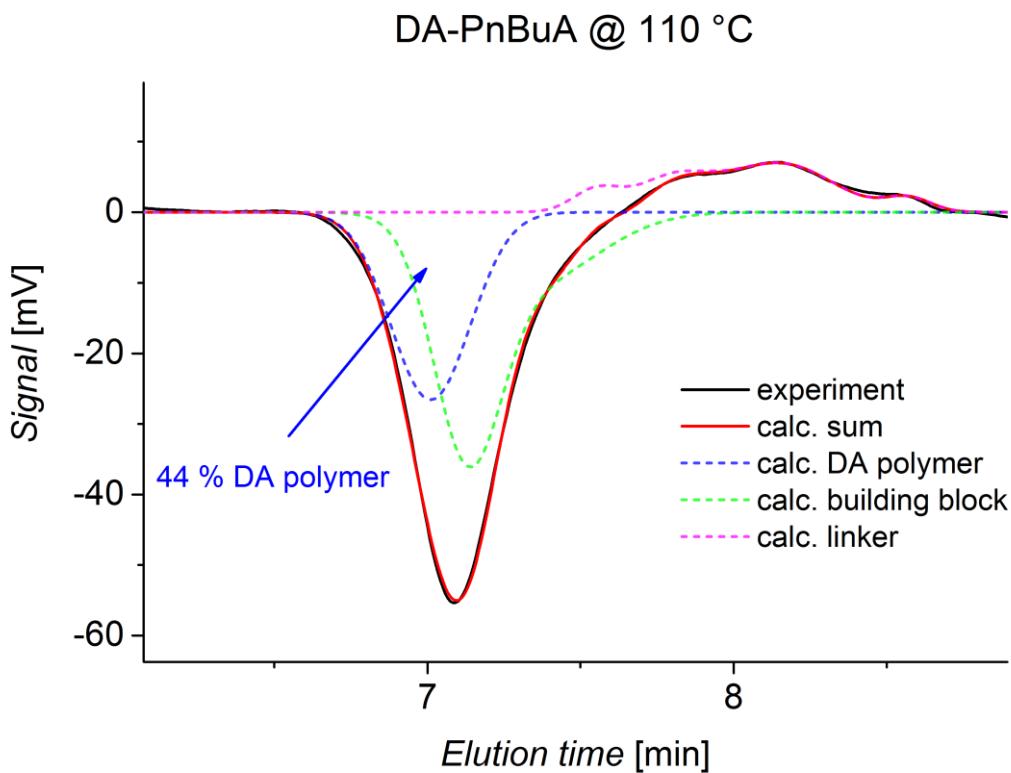


Figure S20. Chromatogram of DA-PⁿBuA at 110 °C in 60 % TCB, 40 % DMF, deconvoluted into the DA polymer, the building block and the CDTE dilinker.

The peak of the linker is much broader than it would be expected for an organic molecule. This can be assigned to the surface modifications of the employed SEC column (Agilent ResiPore). It is known (and it has been observed by the authors as well) that enthalpic interactions occur with rather polar substances like the linker. In their case the separation mechanism of SEC and HPLC begin to overlap and the peak position is a function of both size and polarity. The CDTE dilinker on the other hand has been shown to be a very reactive molecule that might undergo dimerization/multimerization as well, which would lead to multiple peaks. In addition the linker molecules are expected to be affine to the DMF in the solvent mixture so that the effective hydrodynamic volume could increase due to attached DMF molecules. Degradation or

conversion of the linker in DMF at high temperatures can be neglected. Heating the CDTE linker to 120 °C in pure DMF for more than two hours led to insignificant changes of the ^1H NMR spectrum.

9. SANS Measurements

Polymer samples were synthesized *via* ARGET ATRP. First, the absolute scattering intensities (extrapolated to zero concentration) were normalized to the molar mass averages of the investigated polymer samples (determined by static light scattering; $\text{P}''\text{BuA}$: 37400 g mol $^{-1}$, $\text{P}'\text{BuA}$: 41600 g mol $^{-1}$, $\text{P}'\text{BuA}$: 46500 g mol $^{-1}$), multiplied with the momentum transfer q , divided by π and then plotted over q . The resulting plots were fitted with two linear regressions in the middle and the high q -range, respectively. The point of intersection of these two fits (q^*) represents the coil-to-rod transition and, thus, corresponds to the persistence length of the investigated polymer.^{8,9} **Figure S21** shows exemplary plots for the $\text{P}''\text{BuA}$ specimen.

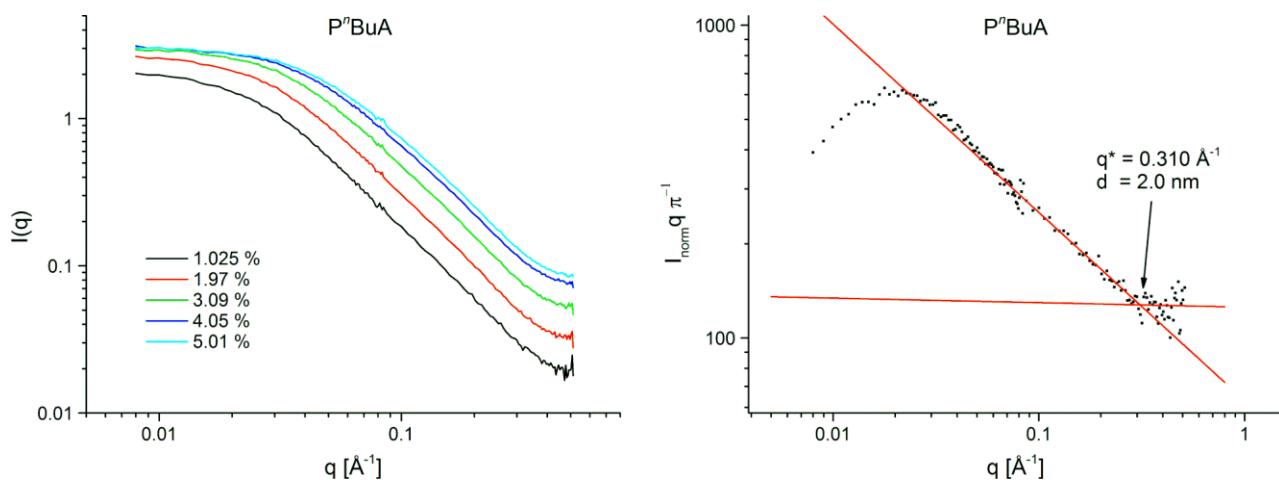


Figure S21. Left: scattering curves of $\text{P}''\text{BuA}$ at concentrations from 1 to 5 weight-%. Right: Resulting Casassa-Holtzer-plot of $\text{P}''\text{BuA}$.

10. Computational data

Table S6. Calculated entropies, enthalpies and free energies of DA reactions in the gas phase and in toluene solution at 25 °C.

n=m=	R	ΔS _{trans}	ΔS _{rot}	ΔS _{vib}	ΔS _{tot}	-TΔS	ΔE _{DFT}	ΔE _{ONIOM}	ΔH ^{0K}	ΔH ^{298K}	ΔG _{gas}	ΔG _{soln}
		J mol ⁻¹ K ⁻¹		kJ mol ⁻¹								
Extended chain conformers												
0	n/a	-176.7	-140.9	27.3	-290.4	86.6	-119.4	-119.3	-106.8	-112.2	-25.6	-27.0
1	MA	-179.7	-147.9	49.2	-278.4	83.0	-118.4	-118.3	-106.3	-111.3	-28.3	-29.9
	^t BuA	-180.7	-150.1	41.3	-289.6	86.3	-125.1	-125.0	-112.3	-117.8	-31.4	-30.8
	ⁱ BuA	-180.7	-150.5	29.0	-302.2	90.1	-120.8	-120.7	-107.4	-113.0	-22.9	-24.9
	ⁱ BoA	-182.1	-152.2	50.6	-283.7	84.6	-119.8	-119.6	-106.9	-111.9	-27.4	-29.1
2	MA	-181.5	-151.5	75.4	-257.6	76.8	-109.8	-109.7	-98.4	-102.7	-25.9	-29.9
	^t BuA	-182.8	-153.5	48.2	-288.1	85.9	-115.0	-114.9	-102.4	-107.2	-21.3	-24.7
	ⁱ BuA	-182.8	-153.9	44.9	-291.8	87.0	-116.9	-116.8	-103.8	-109.5	-22.5	-22.5
	ⁱ BoA	-184.3	-155.8	82.8	-257.2	76.7	-104.7	-104.6	-91.3	-94.0	-17.4	-16.9
Lowest energy conformers												
0	n/a	-176.7	-139.9	64.3	-252.4	75.2	-119.8	-119.7	-106.8	-109.9	-34.6	-32.1
1	MA	-179.7	-147.3	29.6	-297.4	88.7	-172.4	-172.3	-157.0	-162.0	-73.3	-63.9
	^t BuA	-180.7	-148.0	7.3	-321.4	95.8	-173.5	-173.4	-156.6	-163.0	-67.1	-54.8

	ⁱ BuA	-180.7	-146.4	56.9	-270.2	80.6	-137.7	-137.6	-122.3	-126.3	-45.7	-45.9
	ⁱ BoA	-182.1	-149.0	60.4	-270.7	80.7	-137.3	-137.2	-122.0	-126.4	-45.7	-48.8
2	MA	-181.5	-152.1	-6.1	-339.7	101.3	-159.4	-159.3	-143.8	-150.5	-49.2	-26.2
	^t BuA	-182.8	-152.0	-23.2	-358.0	106.7	-150.6	-150.5	-132.4	-140.2	-33.5	-13.9
	ⁱ BuA	-182.8	-152.5	1.0	-334.3	99.7	-153.0	-152.9	-132.4	-139.3	-39.7	-20.5
	ⁱ BoA	-184.3	-155.2	52.3	-287.2	85.6	-151.8	-151.7	-136.7	-140.3	-54.7	-24.6

Table S7. Contributions to the free energies of all species at 25 °C.^a

n=m=	R	Species	ZPVE (kJ/mol)	TC ^{298K} (kJ/mol)	ΔS _{trans} (J/mol/K)	ΔS _{rot} (J/mol/K)	ΔS _{vib} (J/mol/K)	E _{DFT} (Hartree)	ΔG _{solv} (kcal/mol)
Extended chain conformers									
0	n/a	CDTE	1631.6414	125.6937	189.8686	172.6474	899.7482	-3352.88164	-25.18
		Cp ₂ R _{nm}	1230.4532	77.0501	182.0938	153.5117	493.9101	-1156.76869	-15.65
1	MA	DA	2874.6165	197.3387	195.2222	185.2170	1420.9089	-4509.69581	-39.27
		Cp ₂ R _{nm}	1747.3673	114.3286	186.9863	164.5139	773.3666	-1769.51907	-21.11
	^t BuA	DA	3391.0211	234.9987	197.1553	189.2908	1722.2989	-5122.44581	-44.77
		Cp ₂ R _{nm}	2175.9329	136.0542	188.8221	168.3404	929.3106	-2005.30301	-23.54
	ⁱ BuA	DA	3820.2958	256.2532	198.0010	190.8449	1870.3272	-5358.23231	-46.66
	ⁱ BoA	Cp ₂ R _{nm}	2182.0835	135.7107	188.8221	168.1402	942.5430	-2005.29037	-24.07

		DA	3827.0276	255.8036	198.0010	190.2962	1871.2812	-5358.21803	-47.83
	ⁱ BoA	Cp ₂ R _{nm}	2836.8834	161.2541	191.7106	173.1194	1107.3776	-2472.01821	-28.11
		DA	4481.2816	281.9043	199.4683	193.5855	2057.7479	-5824.94546	-51.82
2	MA	Cp ₂ R _{nm}	2263.1802	151.0864	190.4912	172.2773	1055.7870	-2382.27614	-26.77
		DA	3906.1582	272.4673	198.8285	193.4364	2030.9266	-5735.19961	-51.01
	^t BuA	Cp ₂ R _{nm}	3121.4899	194.0171	193.1686	177.3284	1349.2083	-2853.83932	-30.43
		DA	4765.5947	314.9215	200.2721	196.5071	2297.1203	-6206.76474	-54.53
	ⁱ BuA	Cp ₂ R _{nm}	3134.6214	193.8876	193.1686	177.9135	1379.6645	-2853.81577	-32.31
		DA	4779.2142	313.9018	200.2721	196.6235	2324.3575	-6206.74192	-55.60
	ⁱ BoA	Cp ₂ R _{nm}	4446.5582	243.7436	197.0754	184.8147	1685.5159	-3787.26716	-39.37
		DA	6091.4842	366.6700	202.6302	201.6869	2668.1104	-7140.18867	-62.55

Lowest energy conformers

0	n/a	Cp ₂ R _{nm}	1636.4399	122.4521	189.8686	164.7263	789.9214	-3352.90249	-22.08
		DA	1232.5235	74.6264	182.0938	147.3629	425.6339	-1156.77903	-13.28
1	MA	Cp ₂ R _{nm}	2881.8795	193.9691	195.2222	172.2027	1279.8073	-4509.72714	-32.86
		DA	1750.1724	111.3840	186.9863	157.4583	704.1694	-1769.53529	-17.95
	^t BuA	Cp ₂ R _{nm}	3401.9044	228.8460	197.1553	174.9131	1523.6806	-5122.50343	-35.90
		DA	2179.5628	132.8813	188.8221	159.6643	839.2074	-2005.32394	-18.52

	ⁱ BuA	Cp ₂ R _{nm}	3832.7661	249.0228	198.0010	176.4008	1636.3850	-5358.29251	-35.77
		DA	2186.0904	131.2480	188.8221	158.5328	812.4027	-2005.32110	-17.28
	ⁱ BoA	Cp ₂ R _{nm}	3837.8255	249.6885	198.0010	176.8598	1659.1784	-5358.27603	-37.50
		DA	2843.0628	156.1613	191.7106	163.9197	962.2787	-2472.05114	-20.08
2	MA	Cp ₂ R _{nm}	4494.7328	274.2276	199.4683	179.6939	1812.5741	-5825.00594	-41.01
		DA	2267.1863	147.5858	190.4912	163.6835	948.0688	-2382.29937	-21.09
	^t BuA	Cp ₂ R _{nm}	3919.1827	263.3122	198.8285	176.3090	1731.8758	-5735.26258	-35.78
		DA	3126.0584	190.6702	193.1686	167.1302	1244.5727	-2853.87288	-23.41
	ⁱ BuA	Cp ₂ R _{nm}	4780.5524	305.3181	200.2721	179.8408	2011.3248	-6206.83272	-38.90
		DA	3136.2416	190.2279	193.1686	167.9530	1257.8938	-2853.84793	-27.24
	ⁱ BoA	Cp ₂ R _{nm}	4793.1644	305.7227	200.2721	180.1388	2048.8095	-6206.80868	-42.85
		DA	6102.3206	357.6053	202.6302	183.5647	2369.4788	-7140.27142	-42.82

^a ONIOM electronic energy correction from the core-layer reaction is equal to 0.111 kJ mol⁻¹.

M06-2X/6-31G(d) optimized geometries of all species in the form of Gaussian archive entries

CDTE.ext

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kp_11_r2.ext

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 62,2.079253319\c,-4.7026956275,-15.7879721703,5.9819204937\c,-3.403896
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 54O8)]\\@

kda_11_r2.ext

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kp_11_r3.ext

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kda_11_r3.ext

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kda_22_r2.ext

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kda_22_r3.ext

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kp_00

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 , 2.3304782036, -0.8219684704\H, 1.1674253646, 2.8292955973, -2.4480557395\
 H, 0.0192666752, 0.6472650901, 3.0068665095\H, 0.8433467537, 2.1239439219, 0
 .9820339011\H, -2.6468992443, 0.8607603997, 2.6710077926\H, 2.6582621603, 4
 .2280292424, -0.77925705\H, 2.441189675, 0.4487430085, -2.3768448757\\Vers
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 834e-06\Dipole=0.1791329, 0.4445925, 0.0425238\Quadrupole=-3.886301, 1.16
 89064, 2.7173947, 0.9845302, 5.775317, -1.3679873\PG=C01 [X(C22H30O4)]\\@

kda_00

1\1\GINC-R3525\FOpt\RM062X\Gen\C54H66N4O8S4\ROOT\23-Mar-2014\0\\#M062X
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 28\kda_00.freq\0, 1\C, 6.0664864486, 1.1647013864, 0.3578219456\C, 4.8030
 536568, 0.9338434088, -0.4756976239\C, 5.0062969564, -0.2127598736, -1.4625
 213676\C, 5.4536159889, -1.5315294348, -0.8092366616\C, 6.6265856018, -1.27
 12180946, 0.1584944657\C, 6.5082137527, -0.0839044621, 1.1376591263\C, 6.01
 36199546, -2.4564349069, -1.9136798969\N, 4.4369765655, 2.1249877645, -1.23
 50126979\N, 5.0471570557, -2.8516525415, -2.9150926912\C, 4.4396721128, -4.
 0638122206, -2.8597699643\C, 3.9771659088, 3.2386898272, -0.6128959797\O, 3
 .9509741099, 4.28245109, -1.4787027648\O, 3.631957376, 3.3041385979, 0.5498
 74718\O, 3.4563058056, -4.1352367743, -3.7849271038\O, 4.7407691438, -4.963
 7021883, -2.0998888489\C, 4.2638651725, -2.2331761427, -0.1414466875\C, 7.8
 979880888, 0.1702278723, 1.7355939347\C, 5.5483530065, -0.3560541178, 2.306
 6881798\C, 3.435895865, 5.5031620324, -0.9358086639\C, 2.692308605, -5.3492
 968853, -3.790843554\C, 1.9286811143, 5.5160668508, -0.9400504124\C, 1.4971
 248748, -5.2646279421, -2.8747311354\C, 1.2092242679, 5.1968098624, 0.21464
 99804\C, -0.1797091743, 5.1877683182, 0.1925529864\C, -0.8723932682, 5.4860
 508722, -0.9852593641\C, -0.1532083463, 5.7949223904, -2.1390874496\C, 1.23
 73324445, 5.8145006217, -2.1129566323\C, 0.2073364072, -5.2805014326, -3.39
 54460828\C, -0.9019057101, -5.2183045333, -2.5520186269\C, -0.7318094826, -
 5.121418913, -1.1727249273\C, 0.5650868022, -5.1045487876, -0.6501158519\C
 , 1.6672063701, -5.1858248252, -1.4856165052\C, -1.9222044333, -4.999858857
 2, -0.2618008744\S, -2.0640925619, -3.3710322124, 0.5585253875\C, -2.377906
 4315, 5.483954825, -1.000775138\S, -2.9689631699, 3.7868848669, -0.68279384

36\C,-4.672163548,4.0591458568,-0.4756002008\C,-2.1565947324,-2.225553
 9493,-0.8795539749\S,-5.514870086,5.4457770915,-0.6620733759\S,-3.3472
 425341,-2.7681266314,-2.1820520391\C,-5.3492071363,2.8486113497,-0.067
 4531349\N,-5.8983134601,1.8931177625,0.2857890015\C,-0.8157987842,-2.0
 151809555,-1.4405574687\N,0.2545998169,-1.8222184539,-1.8358918487\H,5
 .895904208,2.0009267503,1.046559938\H,6.8719093236,1.4632075829,-0.330
 798503\H,3.9563791518,0.7171581945,0.1843150358\H,5.7776304243,0.10506
 52488,-2.185393647\H,4.0778002445,-0.37815876,-2.0226649739\H,7.519299
 8278,-1.0804239337,-0.4578664767\H,6.8365211935,-2.1905181876,0.723025
 5785\H,6.8537534394,-1.9565185285,-2.4116710302\H,6.3898518943,-3.3802
 722529,-1.4655589094\H,4.8270944154,2.2522558867,-2.1597837201\H,4.645
 9627896,-2.1655512741,-3.540467756\H,4.5829245784,-3.1727121534,0.3229
 256355\H,3.7918937543,-1.6162014743,0.6249822077\H,3.4905696884,-2.466
 0383199,-0.8824326524\H,8.6364852369,0.370330463,0.9514221244\H,7.8767
 78122,1.0328791539,2.4106235551\H,8.2392466963,-0.6991796084,2.3092926
 192\H,5.6671215853,0.4204215934,3.0703535743\H,4.4968700838,-0.3573522
 243,2.0142146477\H,5.7690383069,-1.3235064289,2.7715421652\H,3.8254048
 731,5.640409286,0.0752928838\H,3.832739327,6.2811861899,-1.5910252522
 \H,2.3725446537,-5.4763339995,-4.8269724106\H,3.3492776479,-6.174535705
 5,-3.50659983\H,1.7488105449,4.9376397547,1.1198686097\H,-0.7346081624
 ,4.9431821311,1.0953302632\H,-0.6824588923,6.0196178963,-3.061297827\H
 ,1.7916600995,6.051694504,-3.0171880193\H,0.0625763409,-5.3463259246,-
 4.471337979\H,-1.9055604022,-5.2443175987,-2.9714006421\H,0.7047577956
 ,-5.0184136065,0.4247666696\H,2.6707735042,-5.193403817,-1.072016345\H
 ,-2.8548931938,-5.1994967389,-0.7957944783\H,-1.854406124,-5.697905089
 9,0.5791198798\H,-2.8018162987,6.120320998,-0.2169581009\H,-2.78073419
 36,5.8197172696,-1.9599123193\C,-2.7583552134,-0.8647544362,-0.3361975
 509\C,-4.269547852,-1.1299464733,-0.3112831147\C,-4.4477067439,-1.2522
 338924,-1.8316683938\C,-3.6412992587,-0.0629546547,-2.3114578475\C,-2.
 6561083162,0.1695450751,-1.435535618\H,-2.2873252982,-0.6030617307,0.6
 140845591\H,-4.8114703103,-0.2640737583,0.0793938912\H,-4.5463574721,-
 2.0327035616,0.2357020645\H,-3.7953685284,0.4223851111,-3.268454447\H,
 -1.8360606204,0.8716258604,-1.5486390661\C,-1.2015554569,-2.4252508951
 ,-5.3428580691\C,-2.4462111615,-1.5795955431,-5.5439722513\C,-3.643299
 4459,-2.4216028884,-5.9765129155\O,-0.1117627475,-1.6199405487,-4.8836
 520056\H,-0.9104481168,-2.9351712848,-6.267175639\H,-1.3585195156,-3.1
 555185966,-4.5449622432\H,-2.2402309202,-0.8058022282,-6.2930730537\H,
 -2.6671815893,-1.0870606926,-4.5908045423\H,-3.4853524134,-2.816728463
 1,-6.9876376936\C,-4.9363545781,-1.6204361416,-5.9729997634\H,-3.76781
 75402,-3.284262678,-5.3104856307\O,-5.224235089,-1.1310769779,-4.65039
 84182\C,0.5033040131,-0.8697375651,-5.8055158574\H,-5.7804227733,-2.22
 08960717,-6.3182421943\H,-4.8480027359,-0.7203493546,-6.5860307302\C,-
 5.7582344384,-2.0286421601,-3.8009937042\C,1.5856620196,0.0046619751,-
 5.1739322167\C,-5.8739663339,-1.4752699501,-2.3801948431\O,0.222242875
 6,-0.8842978152,-6.9813677789\O,-6.078412427,-3.1441899776,-4.13032583
 5\C,2.592538514,-0.9004676276,-4.4495985687\C,0.9226308612,0.965335726
 6,-4.212424149\C,2.285314758,0.7856765395,-6.2953919207\C,-6.637327825
 7,-2.4915117332,-1.5281071905\C,-6.6382598892,-0.1416194158,-2.4049295
 379\H,2.1267329798,-1.4103868573,-3.6006166784\H,3.4248882748,-0.28000
 42092,-4.0948007889\H,2.9927357962,-1.6531491998,-5.1385798193\C,-0.36
 63674112,1.6802929782,-4.5348760554\C,1.3568535709,1.3822252318,-3.007
 5470303\H,2.7507907973,0.0978052397,-7.0072063986\H,3.0541043814,1.432
 0186805,-5.8624335705\H,1.5748905489,1.4036869035,-6.8495136438\H,-7.5
 969402554,-2.7226869711,-1.9965093991\H,-6.8264996493,-2.074890458,-0.
 5348538514\H,-6.0804057005,-3.4260297769,-1.4254854058\H,-7.6503780109
 ,-0.3037458663,-2.7895146024\H,-6.1460392141,0.5980485353,-3.039584874
 5\H,-6.7193919526,0.2624281237,-1.3922735755\C,0.4378543354,2.39999663

84,-2.4788452011\c,-0.5649889136,2.5901560255,-3.3559737855\h,-1.19148
 64563,0.9557504111,-4.6197412719\h,2.2426633128,1.0385765116,-2.484625
 5587\h,-1.3995773988,3.2750715374,-3.2534133436\h,0.5722050902,2.91266
 31147,-1.5299147053\h,-0.3256274535,2.2221674474,-5.4895350129\Versio
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 9407,-4.5372824,8.453204,3.7718576,-4.1564119\PG=C01 [X(C54H66N4O8S4)]
 \\\@

kp_11_r1

1\1\GINC-R2410\FOpt\RM062X\Gen\C30H42O8\ROOT\10-Mar-2014\0\#\M062X/gen
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 38764,3.4558114095,-0.0555450882\c,-1.3925101022,4.0332267849,1.231087
 0619\c,-2.9122095308,3.9619727275,1.2661419313\o,1.239516767,2.5290286
 062,-1.0345504455\o,-3.3397043754,2.5923784745,1.2516371817\h,1.022338
 5993,2.8957776437,0.9768128401\h,1.2022979111,4.3081067363,-0.09145640
 57\h,-1.2112590799,2.4526521759,-0.2051431847\h,-1.100474743,4.0579116
 243,-0.9219492181\h,-1.0910442009,5.0800063817,1.3649436325\h,-1.00299
 37317,3.4730703604,2.0906265356\h,-3.3590156533,4.4847455013,0.4176958
 173\h,-3.3002213555,4.3774400766,2.1990072602\c,1.0463555702,1.2147274
 552,-0.8922978542\c,-3.7597924556,2.0858946517,0.0731564434\c,1.772719
 071,0.3860252887,-1.9442833581\c,-4.1362757056,0.6115156873,0.19817123
 33\o,0.3929114662,0.7420371936,0.014930768\o,-3.8109384855,2.729709813
 7,-0.9460601577\c,3.2795030467,0.370691393,-1.5814274694\c,1.614632446
 1,1.0434103958,-3.3222979175\c,1.1776655343,-1.0234724943,-1.957509215
 3\c,-2.8154104617,-0.1687119621,0.4355355232\c,-4.8279808313,0.1937911
 678,-1.1018544512\c,-5.094423824,0.4413802917,1.3875694272\h,3.8219257
 255,-0.0714181262,-2.4262204984\c,3.6743539952,-0.4159707059,-0.315766
 4277\h,3.6243238351,1.4054863397,-1.4727340327\h,2.0750982203,2.033841
 744,-3.3455729981\h,0.5572956338,1.1480433237,-3.5844551825\h,2.092504
 4352,0.415152453,-4.0807386701\h,1.2287846155,-1.4936049942,-0.9724091
 733\h,1.7264509263,-1.6459070585,-2.6729399539\h,0.1226265827,-1.00179
 63277,-2.2472980706\h,-2.0672935363,0.1202006459,-0.3129511791\c,-2.97
 59029815,-1.6937692923,0.3732123055\h,-2.4114769361,0.10881221,1.41450
 97718\h,-4.1563187613,0.2958887291,-1.9567492269\h,-5.7057160893,0.820
 7679459,-1.2816647561\h,-5.1643150795,-0.8472212678,-1.0359636308\h,-4
 .612005384,0.7214630357,2.3267052408\h,-5.4323542633,-0.5966987626,1.4
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 01637984,-0.3853520498\c,3.0406311256,0.2184420805,0.9138145922\c,5.16
 81865507,-0.4284666051,-0.1269505354\c,-2.9783375906,-2.1735343107,-1.
 073710914\h,-3.9276127019,-2.008418328,0.8172408663\c,-1.8606381782,-2
 .4519575253,1.0531285957\c,5.9606950868,-1.5101082037,-0.0016907707\c,
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 .192246849\c,-2.0339876972,-3.8442861518,1.6036045741\o,3.1286451831,1
 .3954240442,1.1836816102\o,2.3837060154,-0.6684805176,1.6679270775\c,1
 .6960307663,-0.1097285378,2.7910045247\o,-2.3506888181,-1.6827702461,-
 1.9794579654\o,-3.7461181645,-3.2682619332,-1.2237519582\c,-3.75523461
 72,-3.8144247373,-2.5430003973\c,7.3523778166,-1.0803915181,0.18085579
 41\c,7.4031484386,0.2627764682,0.1715292457\c,0.1746355048,-3.16956320
 22,1.8347852152\c,-0.6548397359,-4.1984907325,2.0828525934\h,5.6280156
 898,-2.5426538049,-0.0254447708\h,5.6904488748,1.4603988427,0.79274219
 81\h,5.9568846468,1.4213063138,-0.9414785018\h,-0.1428450111,-1.138731
 9167,0.8669380505\h,-2.4006949097,-4.5381790586,0.8340650244\h,-2.7741
 668316,-3.8693595994,2.4160970575\h,8.1913971687,-1.7554536865,0.30408
 99347\h,8.2865792993,0.8797662113,0.2808058711\h,1.2364744085,-3.12533
 19058,2.0537077156\h,-0.4012988893,-5.1414017678,2.5518419194\h,1.2301

345429, -0.9518469593, 3.3013621347\H, 0.9365593698, 0.5915170069, 2.436573
 9699\H, 2.4004734573, 0.4054372722, 3.4471746899\H, -4.4111384541, -4.68247
 38319, -2.5009090236\H, -2.745824163, -4.105793973, -2.8409930748\H, -4.13
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 4433233, 0.4168529\Quadrupole=-1.7818044, 6.0074701, -4.2256657, 5.5633672
 , -4.6626754, 6.5301966\PG=C01 [X(C30H42O8)]\\@

kda_11_r1

1\1\GINC-R2549\FOpt\RM062X\Gen\C62H78N4O12S4\ROOT\15-Apr-2014\0\#M062
 X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1677721
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 0.4158594278,2.9126181923,5.9733454102\C,-0.2963991482,4.2477655022,5.
 2490421055\C,1.12780951,4.6296508815,4.8345381097\C,2.0667482322,4.483
 5686413,6.0478236184\C,1.9671398053,3.1758970363,6.8647031545\C,1.1040
 868093,6.1238323995,4.4412742709\N, -1.8234698594,2.7479509992,6.323048
 6872\N,0.1298744374,6.4394417545,3.41423887\C,0.5069711023,6.940864333
 6,2.2146317553\C,-2.3237059494,1.6220084812,6.8745534797\O,-3.63160030
 26,1.8209468858,7.2247558844\O,-1.7287229479,0.5803378054,7.0569820235
 \O,-0.5833401968,7.2773513706,1.4792214584\O,1.6539857191,7.0873382961
 ,1.8357377859\C,1.5836067934,3.8272164688,3.6080438317\C,2.7430836741,
 3.3780399825,8.1724269091\C,2.5926996551,1.9740587875,6.1406345708\C,-
 4.276116066,0.6755509458,7.7868535266\C,-0.3140130774,7.8813755298,0.2
 053427526\C,-4.7384745552,-0.2667557379,6.7046531346\C,-0.2482092865,6
 .8574961499,-0.8990521673\C,-4.1395765283,-1.5125661475,6.524316327\C,
 -4.5382457331,-2.3385986003,5.4766548576\C,-5.528970362,-1.9209375025,
 4.5862433241\C,-6.1328273881,-0.6747639921,4.7709845935\C,-5.746653578
 3,0.1387848269,5.8278805897\C,-1.3183768956,6.69866807,-1.7737557332\C
 ,-1.3075276322,5.6905019362,-2.7358868378\C,-0.2115415201,4.8380634077
 ,-2.8440061359\C,0.8920091179,5.0392162678,-2.0077179714\C,0.875784270
 7,6.0336288356,-1.0427897048\C,-0.2596606251,3.659133419,-3.7761055946
 \S,-0.2527624046,2.0521874571,-2.8996040794\C,-5.9030954142,-2.7683387
 399,3.4016045705\S,-4.8171149478,-2.292304112,2.0103726155\C,-5.384585
 524,-3.3617446968,0.762844967\C,-1.7241717091,2.1884666424,-1.80864257
 51\S,-6.616269423,-4.4335239243,0.8189288284\S,-3.2872285151,2.6644942
 646,-2.678277705\C,-4.5977178693,-3.2282826425,-0.4425928216\N,-3.965
 6608301,-3.1410015704,-1.4085373918\C,-1.4701046201,3.1159753635,-0.70
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 16318933,7.7204634606\H,0.1301183393,3.6731605444,7.8958799675\H,-0.15
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 778193\H,-0.939691241,4.2404269124,4.3674427758\H,1.8329631714,5.30629
 41739,6.7413395768\H,3.1077969907,4.636430855,5.7294958837\H,0.8848541
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 .7588358169,3.6982207131\H,1.0656094592,4.190094819,2.7128988812\H,2.3
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 762218\H,3.8027576573,3.572215608,7.970004418\H,2.646035733,1.11710114
 69,6.8213400426\H,2.0267493021,1.6556966684,5.2634903698\H,3.611907092
 ,2.2093410632,5.8133645337\H,-3.5947810004,0.1742179338,8.4773169002\H
 ,-5.1257789454,1.0823073191,8.3403423682\H,-1.1496585375,8.5658589859,
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 ,-6.9045383556,-0.3436306877,4.0801464467\H,-6.2132436442,1.111824579
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 1,5.5515382925,-3.388108227\H,1.7487477688,4.3744589036,-2.0876119935\H
 ,1.7163958089,6.1671526038,-0.3687325892\H,-1.1392545322,3.6969015851

$, -4.4251728821\text{H}, 0.630950429, 3.6000921569, -4.4106299843\text{H}, -5.757133730$
 $7, -3.8365140137, 3.5853971916\text{H}, -6.9391054602, -2.6138503328, 3.088372022$
 $2\text{C}, -1.9976636645, 0.7257593208, -1.2600057907\text{C}, -2.7863499397, 0.0688044$
 $127, -2.3991387105\text{C}, -4.0283937587, 0.9642169564, -2.2724653981\text{C}, -4.2368$
 $667692, 0.9694309415, -0.7756497565\text{C}, -3.051406603, 0.81136906, -0.1759115$
 $185\text{H}, -1.05447126, 0.2543316935, -0.9754520854\text{H}, -3.020635226, -0.9694254$
 $088, -2.1501551105\text{H}, -2.3088196425, 0.1243564958, -3.3777510752\text{H}, -5.1868$
 $429418, 1.1847064532, -0.2965453222\text{H}, -2.8385602267, 0.8601289756, 0.88712$
 $74161\text{C}, -6.7743397129, 4.0573016733, -1.7223035501\text{C}, -7.6493382306, 2.929$
 $947789, -1.2024600218\text{C}, -8.746631846, 2.5616076632, -2.2005089426\text{O}, -5.74$
 $01448472, 4.3840074552, -0.7908286609\text{H}, -7.3726387168, 4.9506402531, -1.92$
 $53777278\text{H}, -6.2500808885, 3.7585054487, -2.6360035134\text{H}, -8.0910574236, 3.$
 $2310439249, -0.2465896303\text{H}, -7.0202180839, 2.0523754265, -1.0131872645\text{H},$
 $-9.5517480481, 3.3046031775, -2.1697621082\text{C}, -9.3282417366, 1.184389689, -$
 $1.9180217359\text{H}, -8.3578340913, 2.5597562991, -3.227027214\text{O}, -8.3321954272$
 $, 0.1700389329, -2.1340688488\text{C}, -6.0936788506, 5.1885088811, 0.2289459698\text{H},$
 $-10.1893132079, 0.9763275, -2.5558338555\text{H}, -9.6121795563, 1.0790509314,$
 $-0.8679302627\text{C}, -8.1369503253, -0.1742725422, -3.4257281029\text{C}, -4.9071175$
 $504, 5.4993854657, 1.139478763\text{C}, -7.0373078228, -1.216125119, -3.582248834$
 $4\text{O}, -7.2190859928, 5.6018796957, 0.380436623\text{O}, -8.7795568591, 0.294701211$
 $3, -4.3330109405\text{C}, -3.7917024788, 6.1189037649, 0.2848470601\text{C}, -2.8238100$
 $6, 2.770722527, 3.0474519081\text{C}, -5.3888724148, 6.4932598746, 2.1998088471\text{C}$
 $, -6.8303325546, -1.4689070243, -5.0789238453\text{C}, -7.4986438522, -2.51641132$
 $13, -2.8985798631\text{H}, -3.4467516599, 5.4153029826, -0.477403184\text{H}, -2.931954$
 $273, 6.3976700047, 0.9039935631\text{H}, -4.1579450718, 7.0257421803, -0.21167524$
 $66\text{C}, -3.7341696884, 1.7518596714, 3.6829381323\text{C}, -1.6120813211, 2.2076025$
 $238, 2.8588039225\text{H}, -5.8607654946, 7.3521582431, 1.7159512791\text{H}, -4.548518$
 $1188, 6.8627287975, 2.7936735977\text{H}, -6.1312760895, 6.0385162887, 2.86256829$
 $52\text{H}, -7.7162559719, -1.950863277, -5.5009943987\text{H}, -5.9619293862, -2.11482$
 $18665, -5.2346603447\text{H}, -6.6818926295, -0.5390028135, -5.6317687483\text{H}, -8.4$
 $091834921, -2.9027794344, -3.367109674\text{H}, -7.6958774526, -2.3535728325, -1.$
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 $-4.6159708596, 1.5377693391, 3.059093408\text{H}, -0.7594013353, 2.6982811919, 2.$
 $4039732023\text{H}, -3.1774281332, -0.3854223569, 4.2864408325\text{H}, -0.7773973185,$
 $0.1559847439, 3.3348219628\text{H}, -4.121232125, 2.0928220941, 4.6521541683\text{C}, -$
 $5.247637237, 0.6651397514, -3.151006512\text{C}, -4.4512234217, 4.1451570232, 1.7$
 $332669114\text{C}, -5.7453051511, -0.760029242, -2.8694736551\text{C}, -3.2307179369, 4$
 $.1775671465, 2.6762941917\text{C}, -4.8589231741, 0.8441484454, -4.6053858271\text{H},$
 $-6.037295854, 1.3887720692, -2.914554764\text{H}, -4.9562313271, -1.4694681224, -$
 $3.1407181485\text{H}, -5.8958783935, -0.8441581806, -1.7863012342\text{O}, -4.07451183$
 $59, 0.143719229, -5.1956977286\text{O}, -5.4907485123, 1.890472965, -5.1581962843$
 $\text{C}, -5.1384880127, 2.1478434703, -6.519022105\text{H}, -5.372758751, 1.2799736485$
 $, -7.1393531018\text{H}, -4.0703556375, 2.363231019, -6.5936552497\text{H}, -5.73122364$
 $62, 3.0091459198, -6.8210949364\text{H}, -5.2946155088, 3.688761789, 2.2681848669$
 $\text{H}, -4.1829398758, 3.4799413539, 0.9038091439\text{H}, -2.3814633133, 4.655523765$
 $4, 2.1786448178\text{C}, -3.4855905802, 4.9773048407, 3.9393978738\text{O}, -2.78784635$
 $03, 5.8778161835, 4.3581823849\text{O}, -4.5849518425, 4.5703472376, 4.5933877146$
 $\text{C}, -4.9221904139, 5.3244707254, 5.7575805735\text{H}, -5.8177200065, 4.857536641$
 $, 6.1635711345\text{H}, -5.1159590855, 6.3650011789, 5.4859296506\text{H}, -4.111010235$
 $2, 5.295169113, 6.4889138074\text{Version=EM64L-G09RevC.01\State=1-A\HF=-512}$
 $2.5034339\text{RMSD}=4.652e-09\text{RMSF}=2.792e-06\text{Dipole}=-1.8812303, -0.5520617, 1$
 $.6459023\text{Quadrupole}=-7.3579445, -8.5078027, 15.8657472, -2.735958, -13.025$
 $0507, -14.004116\text{PG=C01 [X(C62H78N4012S4)]}\backslash\backslash@$

kp_11_r2

1\1\GINC-R3398\FOpt\RM062X\Gen\C36H5408\ROOT\02-Apr-2014\0\#M062X/gen

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 742\C,1.8827202071,5.2936866068,0.3035432772\O,-1.0304520767,2.6516000
 509,-2.7718596318\O,2.245614851,4.1294668109,1.0608818526\H,0.90479716
 91,3.0599010673,-3.0944730577\H,-0.1852841365,4.4671856001,-3.27004120
 89\H,0.4858480673,3.076307318,-0.635909384\H,-0.5472809256,4.489952163
 4,-0.8098776502\H,1.3928453861,5.8134177348,-1.7071136533\H,2.43247666
 7,4.3945218182,-1.5641806481\H,1.0333807633,5.7836016751,0.7847515986\H,
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 -2.6212492457\C,1.3069247083,3.5802106034,1.8597650287\C,-3.3273159303
 ,2.0655783247,-2.9125819002\C,1.7403702646,2.2219845411,2.4036548263\O
 ,-2.5142802487,4.2918731074,-2.3684774125\O,0.2341925297,4.0927178841,
 2.0714035764\C,-3.1124150694,0.8070888713,-2.042992346\C,-3.1396529,1.
 663279952,-4.3876184442\C,-4.715157806,2.6760161904,-2.7150928106\C,1.
 4893887096,1.1907741461,1.2704549496\C,0.8287820918,1.8632400445,3.579
 1436912\C,3.2044801988,2.2469980314,2.8595034108\H,-3.6290312274,-0.03
 26069655,-2.5248779854\C,-3.6388707529,0.8806938786,-0.6004755451\H,-2
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 0.971469565,-4.6825569035\H,-4.8383669833,3.0815877975,-1.7070298088\H
 ,-5.4837425026,1.91419623,-2.8862942932\H,-4.8730798835,3.4959257473,-
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 6102\H,1.1621661279,0.9201247913,4.0228315706\H,3.8805781475,2.5343870
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 \C,-3.0142418451,2.0404451265,0.1689179526\C,-3.3630192759,-0.391050645
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 \C,-4.2736006357,-1.1889091,0.7484255943\C,-1.9903847827,-0.9695344928,
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 0.0373065655,-2.2367671279\O,-1.8161538995,2.2280765023,0.2379419807\O
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 \H,-1.3391320115,-0.2611682304,0.9238800681\H,-1.4712318573,-1.20731886
 47,-0.5477994572\H,-0.1764977034,0.8615708416,-1.0182985615\H,3.436423
 6771,-0.8362791568,-1.8828449534\H,3.614696163,0.775462823,-2.5618878
 116\H,-4.1001985478,-3.1100366861,1.9353366773\H,-1.4997139189,-2.8822
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 547240762,2.8806273421\C,7.0951401374,1.2956189482,-0.5506440749\C,6.2
 196987868,-1.0488848768,-0.3973391938\C,6.5090650063,0.3506274892,1.69
 64055945\H,-5.531116042,4.7784174727,1.1153886571\H,-4.9203049293,5.25
 19735934,2.715945017\H,-5.6202023416,3.6354553767,2.4742730025\H,-3.22
 70984041,5.1255349665,-0.0794401291\H,-1.7734218837,4.6374833442,0.834
 522866\H,-2.8539558184,5.8787122139,1.4900804854\H,-1.9109870944,3.004
 3333212,2.6133439319\H,-3.484917869,2.5458752773,3.3413907788\H,-2.794
 6687741,4.1625168159,3.6103727558\H,6.8154544084,1.3342462651,-1.60752
 07826\H,8.1297417755,0.949309659,-0.4739154382\H,7.0307407488,2.305817
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29108, -1.4395592995, -0.3224160766\H, 5.9478569093, -1.0091885466, -1.4572
 487419\H, 5.8774108165, -0.3465086236, 2.2476343911\H, 6.379121865, 1.35610
 41986, 2.1097802259\H, 7.5562485171, 0.0601358788, 1.8271255744\\Version=E
 M64L-G09RevC.01\\State=1-A\\HF=-2005.3239372\\RMSD=4.892e-09\\RMSF=3.656e-
 06\\Dipole=0.8952057, 0.1072099, -0.542041\\Quadrupole=11.8676782, -8.70783
 93, -3.1598389, 5.133318, -2.3689051, 3.029712\\PG=C01 [X(C36H54O8)]\\@

kda_11_r2

1\\1\\GINC-R2142\\FOpt\\RM062X\\Gen\\C68H90N4O1S4\\ROOT\\30-Apr-2014\\0\\#M062
 X/gen 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1677721
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 169093,5.7912476909\C,2.2574631196,3.2198999956,6.5117588309\C,0.91842
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 48\N,-0.0926770577,6.5298016369,3.4096136091\C,0.2463425116,7.07408709
 55,2.2179392896\C,-1.835031978,1.2284473792,6.7424711245\O,-3.09706665
 71,1.2678434447,7.2745127019\O,-1.1439409148,0.2316977288,6.7296179391
 \O,-0.8602602401,7.3299331277,1.4749994802\O,1.3805094707,7.3206509391
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 9787329041,-0.906962085\C,-3.4761285184,-2.0122269832,6.2767381317\C,-
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 8,-3.4619339831,0.5412389061\C,-1.5797210795,2.2623802283,-1.910222239
 7\S,-6.2644009885,-4.524442611,0.5530320089\S,-3.1481314479,2.69469457
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 481328511, 0.9228218964, -0.9350412402\C, -2.8628995254, 0.791705571, -0.32
 84669399\H, -0.8389707216, 0.3330930932, -1.1254404788\H, -2.7429492579, -0
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 , -5.0111226696, 1.1021749035, -0.4654375631\H, -2.6611225774, 0.8274697212
 , 0.7371247135\C, -6.5759258917, 3.8872439491, -2.0037241936\C, -7.60911807
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kp_11_r3

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kda_11_r3

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kp_11_r4

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kp_22_r1

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 22604535,-2.0095585984,4.9302147785\H,-4.0164211486,-0.9330485822,5.12
 87824182\H,-3.3900868873,-2.4373816406,5.8569159257\C,0.3315742716,0.2
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 $073\backslash H, -2.5872393877, -1.8188275313, -4.5424827261\backslash C, -2.4864152529, -3.333$
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 $5139, -2.9323019283\backslash H, -5.6542327387, -4.3697071249, -3.1032151391\backslash H, -4.43$
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 $91219081, -1.195930889\backslash H, 5.2545828047, -0.4051737626, 0.387682459\backslash H, 4.979$
 $6499386, 1.2489323862, 0.954024432\backslash H, 4.4443353058, 1.9598217353, -1.377009$
 $8456\backslash C, 4.4865466761, -0.0093666454, -2.1871254555\backslash O, 3.2927192148, 0.33557$
 $0982, -2.6870282194\backslash O, 5.0480473558, -1.0477730063, -2.4417753039\backslash C, 2.6534$
 $605788, -0.6630357054, -3.4947583997\backslash H, 1.73921338, -0.2076839149, -3.86934$
 $0326\backslash H, 2.4043492679, -1.5320167012, -2.8807935152\backslash H, 3.3153315246, -0.9623$
 $106061, -4.310200651\backslash Version=EM64L-G09RevC.01\backslash State=1-A\HF=-2382.29936$
 $7\backslash RMSD=7.002e-09\RMSF=7.181e-06\backslash Dipole=-0.6057888, -1.1457887, 0.0758541$
 $\backslash Quadrupole=-7.7938344, -2.7075881, 10.5014225, 8.6836552, 9.9964715, -0.64$
 $9639\backslash PG=C01 [X(C38H54O12)] \backslash @$

kda_22_r1

$1\backslash 1\backslash GINC-R2406\backslash FOpt\backslash RM062X\backslash Gen\backslash C70H90N4O16S4\backslash ROOT\backslash 12-Jun-2014\backslash 0\backslash \#M062$
 $X/gen 6D SCF=Tight INT(grid=ultrafine) OPT=(GEDIIS,maxstep=10) IOP(2/1$
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 $0144051556\backslash C, -6.3253940312, 0.4949335456, 0.3521862497\backslash C, -7.3538994328, 1$
 $.6111157545, 0.6326738899\backslash C, -6.9176710489, 3.0713969422, 0.3969792585\backslash C, -$
 $6.9236419358, -0.7718376824, 1.0104462462\backslash N, -3.2638114373, 2.5177995641, 1$
 $.4320086168\backslash N, -6.2371624004, -2.0183301062, 0.7284061858\backslash C, -6.6591112138$
 $, -2.8377317189, -0.2665812387\backslash C, -2.5162011841, 3.6148676934, 1.171749693\backslash$
 $O, -1.6365128869, 3.8299025415, 2.2004595673\backslash O, -2.5762128422, 4.3261543675$
 $, 0.1906997791\backslash O, -5.8801850384, -3.9495475408, -0.3365566516\backslash O, -7.6039500$
 $551, -2.6217106071, -0.9983069515\backslash C, -6.1440540558, 0.2339032052, -1.146277$
 $4697\backslash C, -7.968668772, 3.9810531592, 1.0466479862\backslash C, -6.8295352556, 3.453074$
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 $706\backslash C, -4.9153223102, -3.9892138383, -2.5364795623\backslash C, 0.4429737776, 5.19251$
 $51842, -0.1096242945\backslash C, 1.5820551203, 5.0020645761, -0.883722165\backslash C, 2.69924$
 $56883, 4.3473193263, -0.3552644754\backslash C, 2.6568161974, 3.8976099793, 0.9646854$
 $383\backslash C, 1.5255970543, 4.1115730386, 1.7487973601\backslash C, -3.6567641924, -4.554693$
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 $, -1.9044502689, -4.7498195588\backslash S, -2.0246365251, -0.1233227512, -5.04321963$
 $38\backslash C, 3.9553252185, 4.1461116338, -1.1654226561\backslash S, 3.5439499988, 3.38250647$
 $58, -2.7678679145\backslash C, 5.1237618584, 3.1281806903, -3.4436458769\backslash C, -1.675769$
 $6469, 0.6835200574, -3.3979361777\backslash S, 6.5808455506, 3.4553995085, -2.7785174$
 $708\backslash S, -1.1954668909, -0.4461114339, -2.0270895228\backslash C, 5.0240472988, 2.53098$
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kp_22_r3

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kda_22_r3

1\\1\\GINC-R3294\\FOpt\\RM062X\\Gen\\C82H114N4O16S4\\ROOT\\11-May-2014\\0\\#M062X/gen 6D SCF=Tight INT(grid=ultrafine) OPT=(MaxStep=10,GEDIIS) IOP(2/17=4) maxdisk=23488102400\\kda_22_r3.freq\\0,1\c, -6.3501403858, -4.0007002883, -1.7415108184\c, -5.208246987, -3.1333799719, -1.2087707758\c, -5.7753020613, -1.8580325796, -0.5955788468\c, -6.7667784535, -2.0971476703, 0.5489121114\c, -7.8547104139, -3.0738029571, 0.0622147431\c, -7.3746601134, -4.3599426198, -0.6466869681\c, -7.4409985563, -0.7434145633, 0.8712125914\N, -4.2918991079, -2.7182470236, -2.2703257045\N, -6.487606755, 0.3349523087, 1.0337428249\c, -6.4277503185, 1.1073698242, 2.1494723614\c, -3.5220138302, -3.5941975988, -2.9570366153\o, -2.6790014509, -2.9066659783, -3.7868897502\o, -3.5728841355, -4.8052906373, -2.9084080286\o, -5.645241793, 2.1814971177, 1.8919110598\o, -6.9817419445, 0.8884236685, 3.2089314142\c, -6.050008285, -2.5615918537, 1.8271190492\c, -8.5908394857, -5.0126838847, -1.3156362549\c, -6.7848218647, -5.3847542064, 0.3339135427\c, -1.7687751815, -3.7179683159, -4.5358124434\c, -5.5851740928, 3.1934234393, 2.8986620188\c, -0.5902280222, -4.1261752272, -3.6897119266\c, -4.3418532216, 3.0646985866, 3.7393890517\c, -0.5237520935, -5.4041513595, -3.136411898\c, 0.525165974, -5.7452507261, -2.2878531227\c, 1.5106056606, -4.8098831939, -1.9724187047\c, 1.4496077965, -3.5262942093, -2.5271924528\c, 0.4103404272, -3.1976785017, -3.3902967051\c, -3.176826068, 3.7214733666, 3.3514024714\c, -2.003513107, 3.5664127533, 4.0833357721\c, -1.9839805265, 2.764058235, 5.2216251462\c, -3.1627843868, 2.1356085607, 5.6336703325\c, -4.3296478471, 2.2771074679, 4.8943069056\c, -0.6783235764, 2.5232563256, 5.9276314451\s, -0.1318601259, 0.7797809693, 5.8906404627\c, 2.5895029326, -5.1561040693, -0.9834648209\s, 2.175519408, -4.3188543233, 0.5853204165\c, 3.4979088825, -4.798762743, 1.5924818795\c, -0.0506527812, 0.3790495341, 4.1012841307\s, 4.8103638318, -5.6947559989, 1.1985705141\s, 1.0876363458, 1.4449343056, 3.0855896988\

C, 3.3350174991, -4.3280385763, 2.9499566346\N, 3.2172177267, -3.9899638114
 , 4.0509486909\C, -1.382489169, 0.3777046466, 3.4916941516\N, -2.4322846129
 , 0.3507039974, 3.0063752507\H, -5.9495903539, -4.9135430617, -2.1944338261
 \H, -6.8548259442, -3.4314387614, -2.5359641422\H, -4.6340592567, -3.695527
 6166, -0.4593577178\H, -6.279423097, -1.2979177219, -1.4006609728\H, -4.958
 076425, -1.2324551823, -0.2309038447\H, -8.480637338, -2.5289920966, -0.661
 2243312\H, -8.5146124103, -3.3429475683, 0.8995114581\H, -8.137251526, -0.4
 855469691, 0.0611769312\H, -8.013766749, -0.8149716336, 1.8010097191\H, -3.
 9374716059, -1.7685970957, -2.2359567607\H, -6.0295563899, 0.7237353006, 0.
 2138919348\H, -6.7571731062, -3.0359458753, 2.5164840233\H, -5.2408568158,
 -3.2710005111, 1.6329591467\H, -5.6150938081, -1.6964009465, 2.34005223\H,
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 478, -6.3248056666, -0.1896675122\H, -5.8515025772, -5.0549981156, 0.793780
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 084009, -4.9224044022\H, -1.4544349726, -3.0810332397, -5.3663154224\H, -5.
 5705655366, 4.1339410805, 2.3443622724\H, -6.4841262046, 3.1335824076, 3.51
 62208054\H, -1.319117989, -6.1133603035, -3.3424913358\H, 0.5658174815, -6.
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 4504277562\H, -1.0870565994, 4.0592188018, 3.7665476498\H, -3.1488265801, 1
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 388473\O, 2.0083506588, 5.3148387063, -0.0840290126\H, 3.1870179978, 6.9364
 733585, -0.5896839932\H, 3.97996084, 5.5654088729, 0.2298762419\H, 2.906529
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 633\H, 5.0099534293, 6.8010758038, -2.599937862\C, 5.5882600353, 4.93827212
 57, -3.4860972242\H, 5.7515028325, 5.6584250962, -1.4835397128\O, 5.6289034
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 91\H, 6.5907628409, 5.2704919458, -3.7642688816\H, 4.9262204955, 4.99317582
 38, -4.3531317179\C, 6.6202021309, 3.1677602175, -2.3166300066\C, -0.378061
 5631, 5.2784797932, -0.0597595339\C, 6.4065509663, 1.744777121, -1.81035099
 67\O, 0.9627364784, 6.7067574238, -1.4999132584\O, 7.525122203, 3.896515104
 1, -1.9909129161\C, -0.3152963726, 5.4051575549, 1.4689025565\C, -2.2494250
 994, -0.8960995175, -0.0530462132\C, -1.5353710077, 6.1203638389, -0.606635
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 80814\H, 8.5372076076, 1.4596392946, -1.5586580627\H, 7.5380058371, 0.30218
 29364, -0.6538469648\H, 7.7193496665, 1.9834189854, -0.0871756218\H, 7.1275
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 ,-0.3414061109\C,3.6146162087,0.9991085013,0.9031437842\C,-2.640886791
 9,0.5586988118,-0.1731994445\C,4.4521270632,-0.908127856,2.3740804958\
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 3291562048,-1.9312475952,3.370306872\H,5.7666539913,-2.8582893478,3.23
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 ,-3.1924859545,3.349844202\H,9.1125177002,-2.9881651911,1.6259772284\H
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 762\H,-4.4734413512,0.0404642338,-6.2832257753\H,-2.9397079079,0.48811
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 4344\H,5.7419197408,0.5796295572,0.6933499126\H,5.1456997933,2.7450726
 259,-0.3665250978\H,4.2427156499,1.8998604942,-1.623627948\O,3.6121829
 441,-0.9671339598,-1.2097960522\O,5.7341603391,-1.4340936424,-0.606355
 3264\C,5.5553899293,-2.8537659849,-0.7587897889\H,6.0891883837,-3.2870
 383952,0.0935600288\C,6.1229007839,-3.3836832705,-2.0673252222\H,4.489
 3757746,-3.0694822459,-0.6501809838\C,7.5806502053,-2.9547062348,-2.24
 17199446\C,5.2613193754,-3.0035984848,-3.2717796123\H,6.0998072084,-4.
 4788505572,-1.9608107197\H,7.6565481393,-1.8700178281,-2.3707681746\H,
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 1.3671802748\H,5.1445170143,-1.9187741288,-3.354677093\H,4.2566502467,
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 9943\H,-4.3527467562,5.0640707621,-1.9087733963\H,-4.9994439389,3.4430
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 4138599391,-5.2509029738\H,-1.8297730924,4.8486723499,-3.7607688498\H,
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 09RevC.01\\State=1-A\\HF=-6206.8086775\\RMSD=3.153e-09\\RMSF=3.441e-06\\Dip
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 .0245611,-5.570798,16.0109015,4.191804\\PG=C01 [X(C82H114N4O16S4)]\\@

kp_22_r4

1\1\GINC-R2703\FOpt\RM062X\Gen\C74H110O12\ROOT\16-May-2014\0\\#M062X/g
 en 6D SCF=Tight INT(grid=ultrafine) OPT IOP(2/17=4) maxdisk=1006632960
 0\\kp_22_r4.freq\\0,1\c,2.9268803124,-3.2112314473,4.0978885027\c,4.08
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 9832,2.6286905756\h,5.6296027314,-3.0627792396,4.8682749437\h,4.705603
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 09,-3.0431557301,2.2076705467\h,1.042399482,-4.4220777967,0.8800754494
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