

Supporting Information

Rigidification of Poly(*p*-phenylene)s through *ortho*-Phenyl Substitution

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General information

Methods

All reactions dealing with air or moisture sensitive compounds have been carried out in a flame-dried reaction vessel under argon atmosphere. Reagents were purchased at reagent grade from commercial sources and used without further purification. Preparative column chromatography has been performed on silica gel from Merck with a grain size of 0.063-0.200 mm. For the polymer separation, a Shimadzu Recycling GPC system, equipped with a LC-20 AD pump, a SPD-20 A UV detector and a set of two preparative columns from JAI (1 HH, 2 H, 20 x 600 mm) was employed. The system was operated at a flow rate of 1.5 mL/min. UV-visible spectra were measured on a Perkin Elmer Lambda 9 spectrophotometer at room temperature. NMR spectra have been measured on a Bruker Avance 300 MHz spectrometer, and referenced to residual signals of the deuterated solvent. For MALDI-ToF-MS measurements, the samples were analyzed with a SYNAPT G2 Si high-resolution time-of-flight mass spectrometer (Waters Corp., Manchester, UK) by matrix-assisted laser desorption/ionization. All Gel permeation chromatography (GPC) measurements were done using a PSS SECcurity Agilent 1260 Infinity Setup (Polymer Standards Service GmbH (PSS)). A column combination from PSS (SDV 10^6 , 10^4 , 500 Å, 300 × 8 mm) was connected and maintained at 30 °C. Tetrahydrofuran (THF) was used as eluent with a flow rate of 1 mL/min. The relative molecular weights were calculated based on a universal poly-*para*-phenylene (PPP) calibration using the signal recorded by a PSS SECcurity UV detector (254 nm). For absolute molecular weight determinations measurements were performed with the same conditions, using a DAWN (Wyatt Technology) multiangle laser light scattering (MALLS) detector (wavelength 685 nm) in combination with an RI-101 (ERC) detector. The refractive index increment dn/dc was calculated assuming complete elution of the polymer samples.

Light Scattering (LS)

All light scattering experiments were performed on a commercially available instrument from ALV GmbH (Langen, Germany) consisting of an electronically controlled goniometer and an ALV-5000 multiple tau full-digital correlators with 320 channels (resolution of $10^{-7} \text{ s} \leq t \leq 10^3 \text{ s}$). A HeNe laser with a wavelength of 632.8 nm and an output power of 25 mW (JDS Uniphase, Milpitas, USA, Type 1145P) was utilized as the light source.

The samples were diluted to concentrations of 0.844 g/L, 0.984 g/L and 0.584 g/L for **PPP 2-3**, **PPP 2-2** and **PPP 2-1**, respectively. The solutions were then filtered through Millex LS filters with a pore size of 5 µm (Merck Millipore, Billerica, USA) into dust-free quartz light scattering cuvettes (inner diameter 18 mm, Hellma, Müllheim), which were cleaned before with acetone in a Thurmont-apparatus.

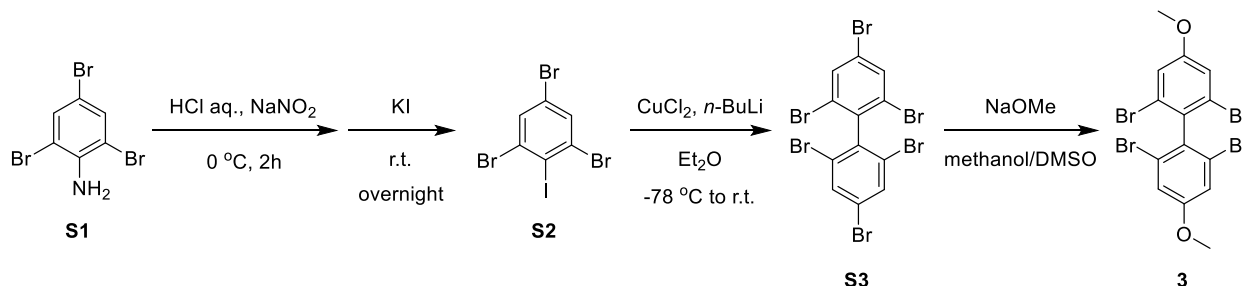
Dynamic light scattering light (DLS)

The DLS technique records the autocorrelation function $G(q, t) = \langle I(q, t)I(q, 0) \rangle / \langle I(q, 0) \rangle^2$ of the light scattering intensity $I(q, t)$ at a scattering wave vector $q = [(4\pi n_s / \lambda) \sin(\theta/2)]$ with λ , θ and n_s being, respectively, the laser wavelength in vacuum, the scattering angle (between incident and scattered light) and the refractive index of the solvent. The desired relaxation function, $C(q, t) = [G(q, t) - 1]^{1/2} / f^*$ is computed from the experimental $G(q, t)$ where the instrumental factor $f^* \leq 1$ is the amplitude $C(q, t = 0.1 \mu s) = 1$ for a dilute suspension of latex spheres dilution at the shortest time ($\sim 0.1 \mu s$) of the ALV-5000/E correlator. The complexity of $C(q, t)$ depends on the number of processes of the solution dynamics probed by DLS. A sensitive method to resolve these dynamic modes is the inverse-Laplace transformation (ILT) of $C(q, t)$. In the simple case of a single relaxation process, $C(q, t) = \alpha(q) \exp\{-[\Gamma(q)t]^\beta\}$ where $\alpha(q)$ is the amplitude, $\Gamma(q)$ is the decay (relaxation) rate and the exponent $\beta \leq 1$ accounts for possible deviations from the single ($\beta=1$) exponential decay. In the case of dilute solutions of a polymer with $qR_g \ll 1$, with R_g being the radius of gyration, the $C(q, t)$ represents its center-of-mass translation diffusion with $\Gamma(q) = Dq^2$, where D is the corresponding diffusion coefficient and β is a measure of the size polydispersity. In this case, $\alpha(q) = [I(q) - I_s] / I_s$, where $I(q)$ is the full light scattered intensity by the solution and I_s is the (q -independent) light scattering intensity of the solvent and the excess Rayleigh ratio $R(q) = [(I(q) - I_s) / I_T] R_T (n_s / n_T)^2$, where T stands for the standard toluene. For more than one relaxation process in $C(q, t)$, the time average total light scattering intensity, $\langle I(q) \rangle$, measured by static light scattering (SLS), includes more than one contributions and hence cannot be used to compute $R(q)$. Instead, $R(q) = \alpha(q) [\langle I(q) \rangle / I_T] R_T (n_s / n_T)^2$ where the amplitude $\alpha(q)$ is accessible only by DLS. At very dilute solutions, $R(q \rightarrow 0)$ is related to the weight-average molar mass, $M_w = R(q \rightarrow 0) / Kc$, where c is the solute concentration and $K = [2\pi n_s (dn/dc)]^2 / (N_A \lambda_0^4)$ is the optical contrast with N_A being the Avogadro's number and dn/dc the refractive index increment in the solvent that can be obtained experimentally.

Synthetic procedures

Synthetic route towards tetra-*ortho*-bromo-biphenyl 3

The NMR data of **S2**, **S3**, and **3** were consistent with the literature,^{1, 2} and thus not listed below.



1,3,5-Tribromo-2-iodobenzene (**S2**)¹

To a suspension of 2,4,6-tribromo-aniline (15.0 g, 45.5 mmol) in concentrated hydrochloric acid (25 mL) was added dropwise a solution of NaNO₂ (4.1 g, 59.1 mmol) in 10 mL water at 0 °C. After vigorously stirring for 2 hours at 0 °C, the diazonium salt was added to a solution of KI (60.4 g, 364.0 mmol) in water (90 mL) and stirred at room temperature overnight. The reaction was quenched by the addition of a saturated aqueous solution of Na₂SO₃ and the mixture was extracted three times with dichloromethane. The combined organic phases were then dried over MgSO₄, filtered, and the solvents were evaporated in vacuo. The residue was subjected to silica gel column chromatography (eluent: *n*-hexane) yielding 1,3,5-tribromo-2-iodobenzene (**S2**) as white crystalline solid (16.5 g, 82 % yield).

2,2',4,4',6,6'-Hexabromo-1,1'-biphenyl (**S3**)²

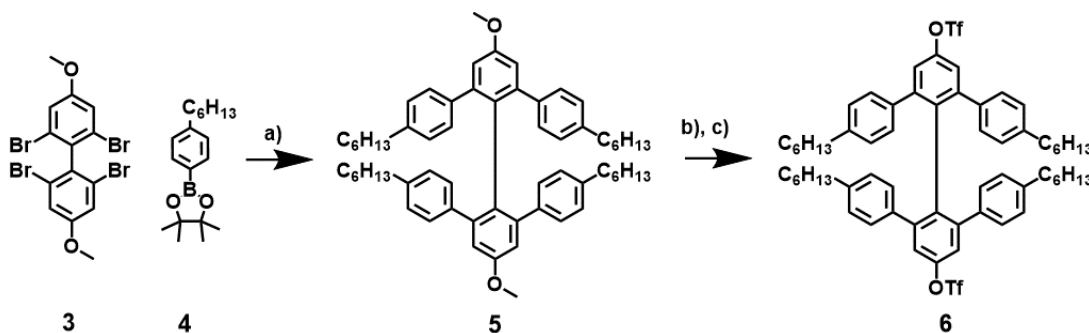
1,3,5-Tribromo-2-iodobenzene (**S2**) (10.0 g, 22.7 mmol) and anhydrous CuCl₂ (18.3 g, 136.0 mmol) were added to a flame-dried 250-mL Schlenk flask and suspended in 100 mL of anhydrous Et₂O under argon atmosphere. The resulting mixture was cooled to -78 °C and *n*-BuLi (14.9 mL, 24.0 mmol, 1.6 M in hexane) was added dropwise over 2 hours and then the reaction mixture was allowed to warm up to room temperature overnight. The reaction was then quenched with a saturated aqueous solution of NH₄Cl, and extracted three time with dichloromethane. The combined organic phases were dried over MgSO₄ and the solvents were evaporated in vacuo. The

residue was subjected to silica gel column chromatography (eluent: *n*-hexane) yielding 2,2',4,4',6,6'-hexabromo-1,1'-biphenyl (**S3**) as white crystalline solid (3.6 g, 50 % yield).

2,2',6,6'-Tetrabromo-4,4'-dimethoxy-1,1'-biphenyl (**3**)²

2,2',4,4',6,6'-Hexabromo-1,1'-biphenyl (**S3**) (3.0 g, 4.8 mmol) was added to a flame-dried 100-mL Schlenk flask and dissolved in 10 mL of anhydrous methanol and 20 mL of anhydrous dimethyl sulfoxide (DMSO). The solution was heated to 180 °C and a solution of NaOMe (5.3 mL, 28.7 mmol, 5.4 M in methanol) was added dropwise. After stirring for 1.5 hours at 180 °C, the reaction mixture was allowed to cool to room temperature and carefully quenched with water. The mixture was extracted three times with ethyl acetate, and the combined organic phases were dried over MgSO₄ and dried in vacuo. The residue was subjected to silica gel column chromatography (eluent: *n*-hexane/Et₂O = 9:1) yielding 2,2',6,6'-tetrabromo-4,4'-dimethoxy-1,1'-biphenyl (**3**) as white crystalline solid (2.2 g, 87 % yield).

Synthetic route towards tetra-*ortho*-phenylated monomer **6**



4,4'-Dimethoxy-2,2',6,6'-tetra-(4-hexylphenyl)-1,1'-biphenyl (**5**)

To a 250-mL Schlenk flask was added 2,2',6,6'-tetrabromo-4,4'-dimethoxy-1,1'-biphenyl (**3**) (0.5 g, 0.9 mmol), 1-(4-hexylphenyl)pinacolboronic ester (**4**) (2.7 g, 9.4 mmol, 10 eq.) and K₂CO₃ (5.2 g, 38.0 mmol, 40 eq.) followed by evacuating and backfilling with argon for three times. After the addition of 60 mL of dioxane and 20 mL of water, the resulting mixture was degassed by argon bubbling for 1 hour. Pd(PPh₃)₄ (218.0 mg, 0.2 mmol, 20 mol%) was added and the mixture was stirred under argon atmosphere at 100 °C for 24 hours. After cooling down to room temperature,

the mixture was extracted three times with dichloromethane, and the combined organic phases were dried over MgSO_4 . The solvents were evaporated in vacuo, and the residue was subjected to silica gel column chromatography (eluent: *n*-hexane/ diethylether 30 :1). Finally, the product fraction was crystallized from methanol, yielding 4,4'-dimethoxy-2,2',6,6'-tetra-(4-hexylphenyl)-1,1'-biphenyl (**5**) as a colorless, crystalline solid (420.0 mg, 52 % yield).

^1H NMR (300 MHz, CD_2Cl_2) δ 6.78 (d, J = 8.0 Hz, 8H), 6.66 (s, 4H), 6.52 (d, J = 8.2 Hz, 8H), 3.79 (s, 6H), 2.53 (t, J = 7.5 Hz, 8H), 1.70 – 1.55 (m, 8H), 1.42 – 1.24 (m, 24H), 1.00 – 0.85 (m, 12H).

^{13}C NMR (300 MHz, CD_2Cl_2) δ 158.9, 143.9, 140.9, 139.3, 129.3, 128.8, 127.6, 115.0, 55.5, 35.7, 32.3, 32.1, 30.1, 30.0, 29.8, 29.6, 23.1, 14.3.

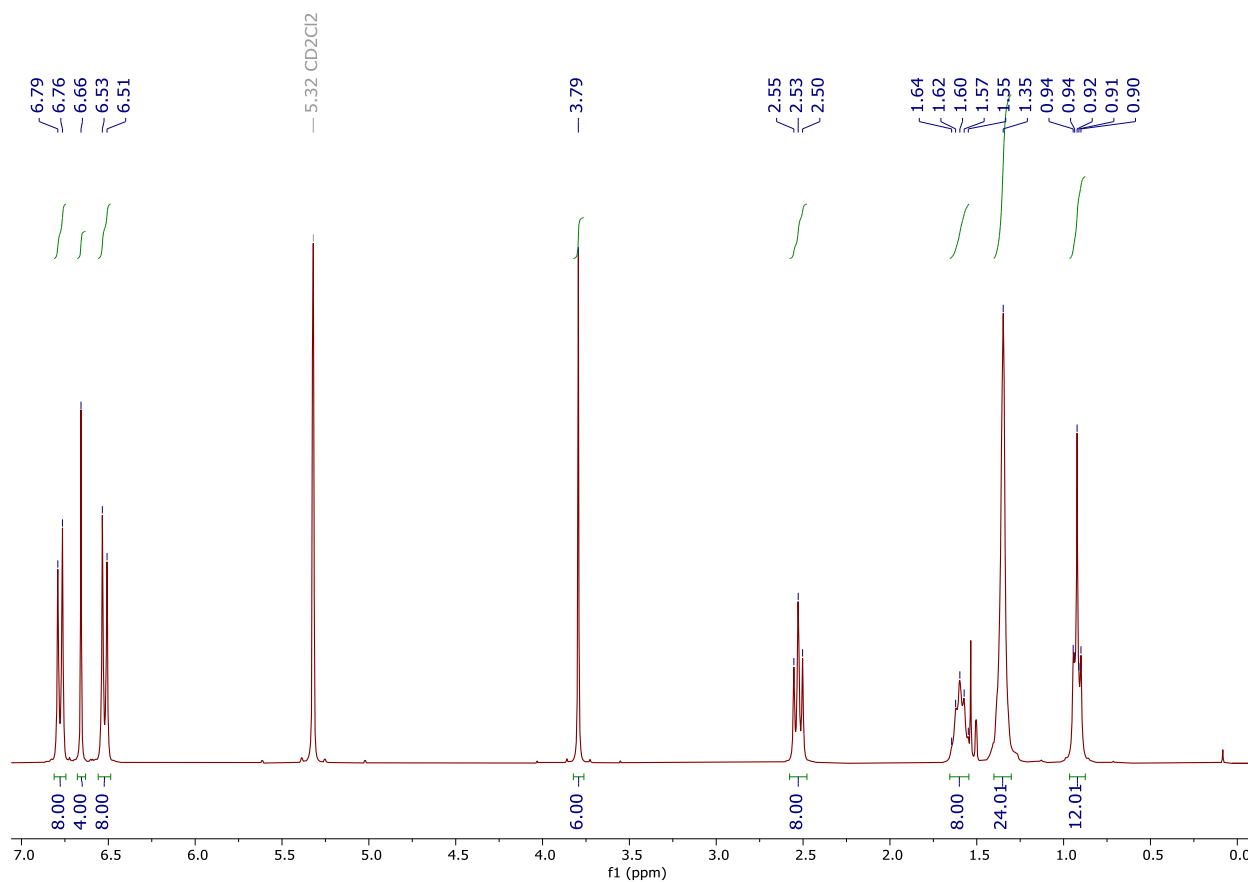


Figure S1. ^1H NMR spectrum of **5** in CD_2Cl_2 (300 MHz).

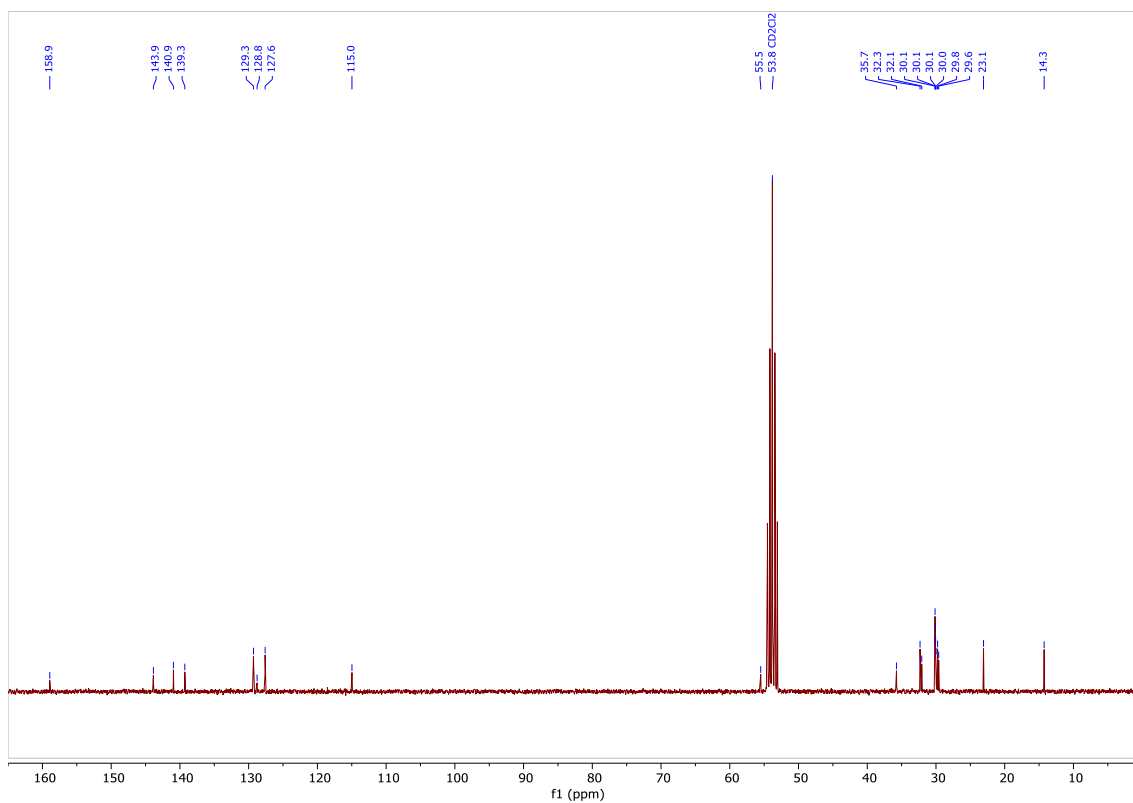


Figure S2. ^{13}C NMR spectrum of **5** in CD_2Cl_2 (300 MHz).

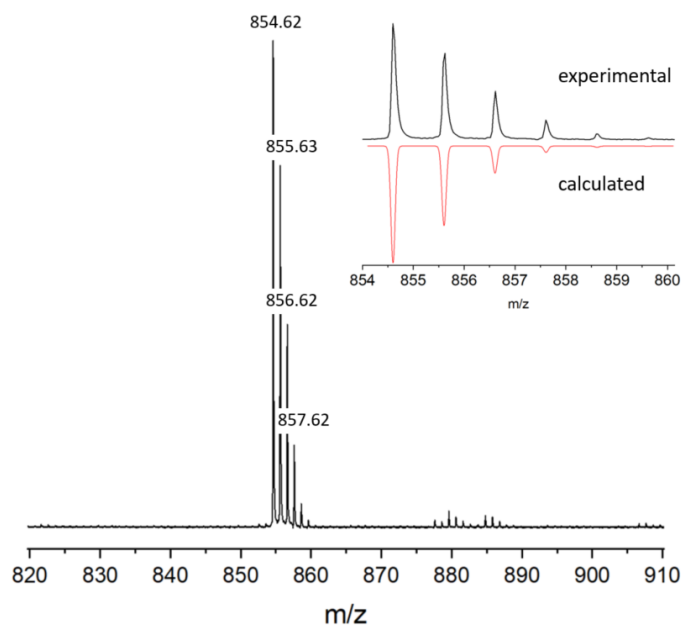


Figure S3. MALDI-TOF MS spectrum of **5**; inset: the isotopic distribution in agreement with the calculated result.

4,4'-Bistriflat-2,2',6,6'-tetra-(4-hexylphenyl)-1,1'-biphenyl (6)

Compound 5 (400.0 mg, 0.5 mmol) was dissolved in 30 mL of dry dichloromethane in a 100-mL Schlenk flask at 0 °C. Boron tribromide (2.3 mL, 2.3 mmol, 1 M in dichloromethane) was then added to the solution at this temperature. After stirring for 12 hours at room temperature, water was added and the reaction mixture was extracted with dichloromethane. The combined organic phases were dried over MgSO₄, and removal of the solvent gave a diol intermediate as brown oil (382.0 mg, 99% crude yield), which was used without further purification.

The diol was dissolved in 5 mL of dry dichloromethane in a 50-mL Schlenk flask under argon. After addition of pyridine (2 mL), the solution was cooled to 0 °C, and then trifluoromethanesulfonic anhydride (1.4 mL, 1.4 mmol, 1 M in dichloromethane) was added dropwise, when white fumes evolved. After stirring for 2 hours at room temperature, water was added and the mixture was extracted three times with dichloromethane. The combined organic phases were dried over MgSO₄ and the solvents were evaporated in vacuo. The residue was subjected to silica gel column chromatography (eluent: *n*-hexane/dichloromethane 2:1) yielding 4,4'-bistriflat-2,2',6,6'-tetra-(4-hexylphenyl)-1,1'-biphenyl (**6**) as a colorless oil (490.0 mg, 0.45 mmol, 98 % yield).

¹H NMR (300 MHz, CD₂Cl₂) δ 7.10 (s, 4H), 6.82 (d, *J* = 8.2 Hz, 8H), 6.48 (d, *J* = 8.3 Hz, 8H), 2.54 (t, *J* = 7.5 Hz, 8H), 1.65 – 1.53 (m, 8H), 1.44 – 1.28 (m, 24H), 0.96 – 0.88 (m, 12H).

¹³C NMR (126 MHz, CD₂Cl₂) δ 149.8, 145.0, 142.6, 136.7, 135.4, 129.2, 128.2, 123.1, 121.8, 120.6, 118.0, 115.5, 35.8, 32.2, 32.0, 30.1, 29.2, 23.1, 14.3.

MS (MALDI-TOF) *m/z*: Calcd for C₆₂H₇₂F₆O₆S₂: 1090.46; Found: 1090.46 (M⁺).

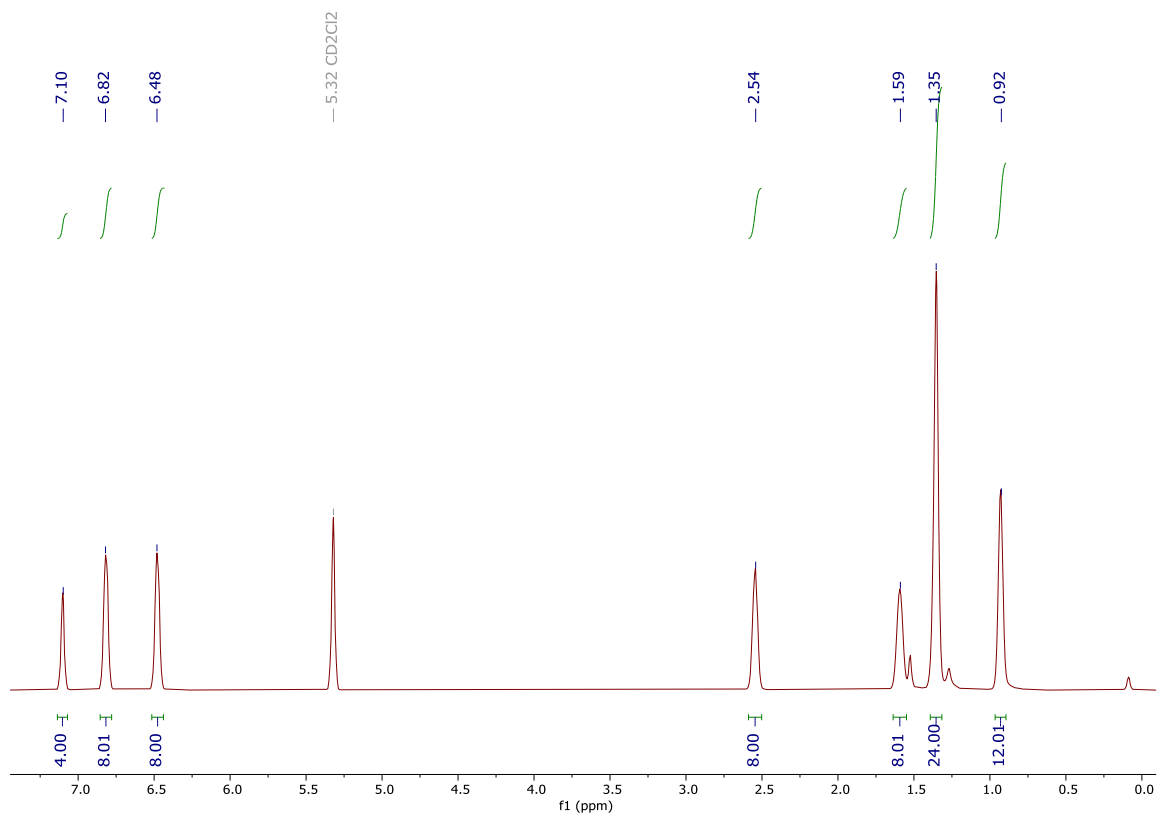


Figure S4. ¹H NMR spectrum of **6** in CD₂Cl₂ (300 MHz).

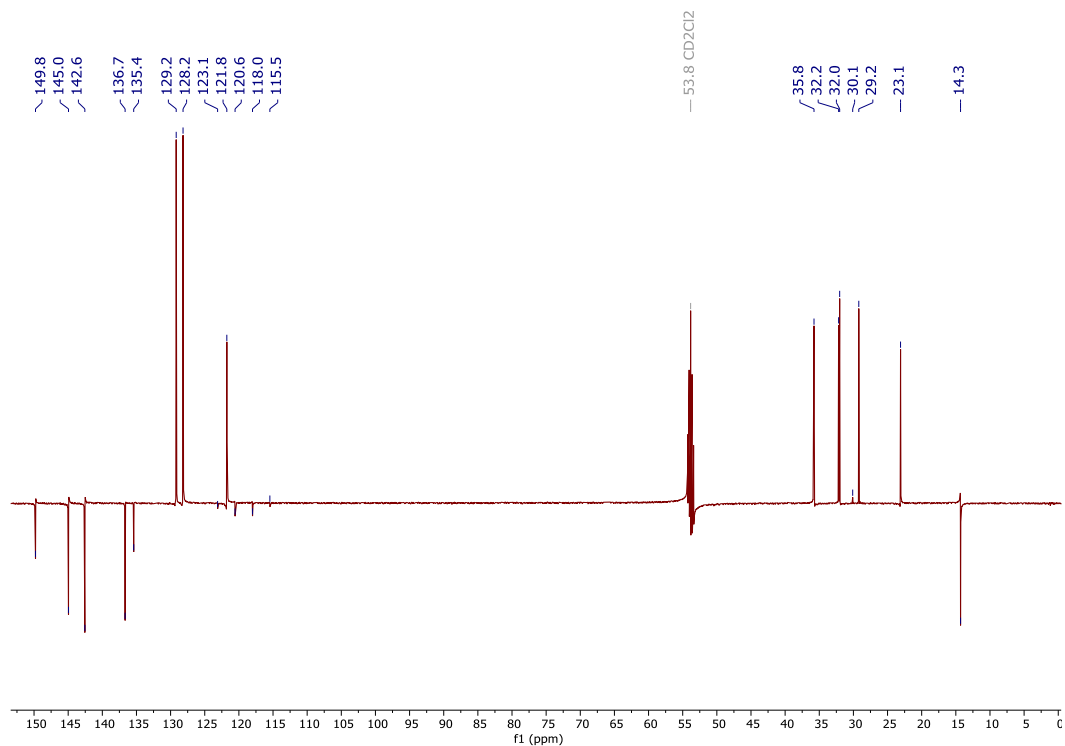


Figure S5. ¹³C NMR spectrum of **6** in CD₂Cl₂ (300 MHz).

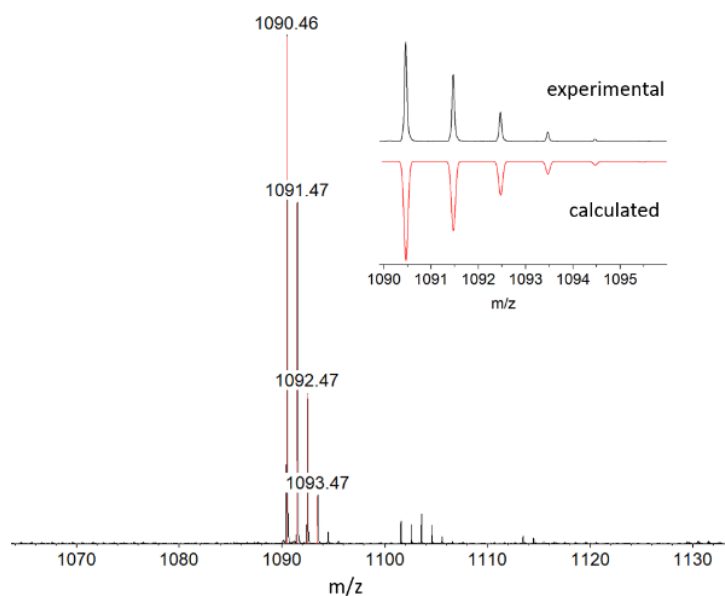
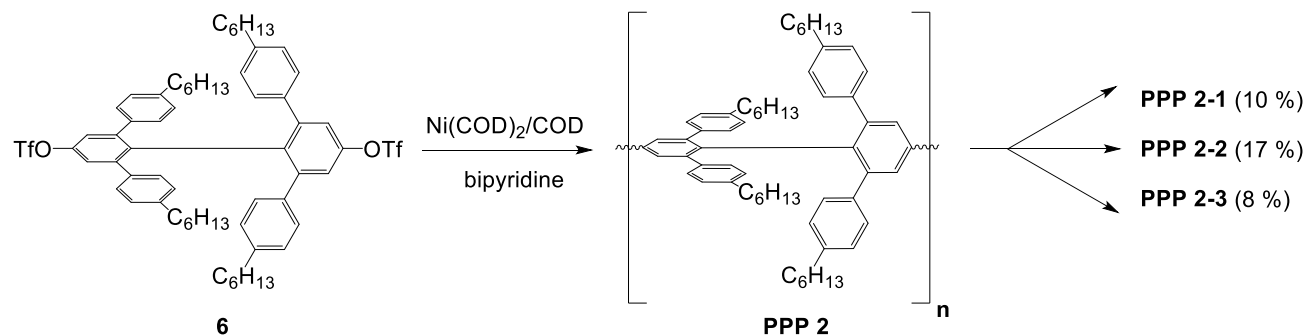


Figure S6. MALDI-TOF MS spectrum of monomer **6**; inset: the isotopic distribution in agreement with the calculated result.

Polymerization



To a freshly prepared solution of bis(1,5-cyclooctadiene)nickel(0) (63.6 mg, 0.2 mmol), 2,2′-bipyridine (36.1 mg, 0.2 mmol), and 1,5-cyclooctadiene (0.03 mL, 0.2 mmol) in 0.9 mL of anhydrous THF in a flame-dried 7-mL microwave vial was added dropwise a solution of compound **6** (101.0 mg, 0.1 mmol) in 1.0 mL of THF in a glove box. The reaction vial was sealed, placed in a microwave reactor and heated to 90 °C with maximum irradiation at 300 W for 3 hours. After cooling, the reaction mixture was added to a stirred 1:1 mixture of methanol and concentrated

hydrochloric acid, in order to remove the nickel salts. The resulting precipitate was collected by filtration and washed with methanol, yielding **PPP 2** as a colorless solid (73.0 mg, 72 % yield). The **PPP 2** was fractionated by preparative recycling GPC (eluent: chloroform) and provide **PPP 2-1**, **PPP 2-2**, and **PPP 2-3**. Analytical SEC profiles of the isolated polymer fractions are shown in Figure S7. The absence of residual triflate end groups was determined via MALDI-TOF MS.

^1H NMR (700 MHz, CD_2Cl_2) δ 7.46 (s), 6.82 (d), 6.62 (d), 2.54 (t), 1.60 – 1.58 (m), 1.34 – 1.31 (m), 0.87 (m).

^{13}C NMR (126 MHz, CD_2Cl_2) δ 149.8, 145.0, 142.6, 136.7, 135.4, 129.2, 128.2, 123.1, 121.8, 120.6, 118.0, 115.5, 35.8, 32.2, 32.0, 30.1, 29.2, 23.1, 14.3.

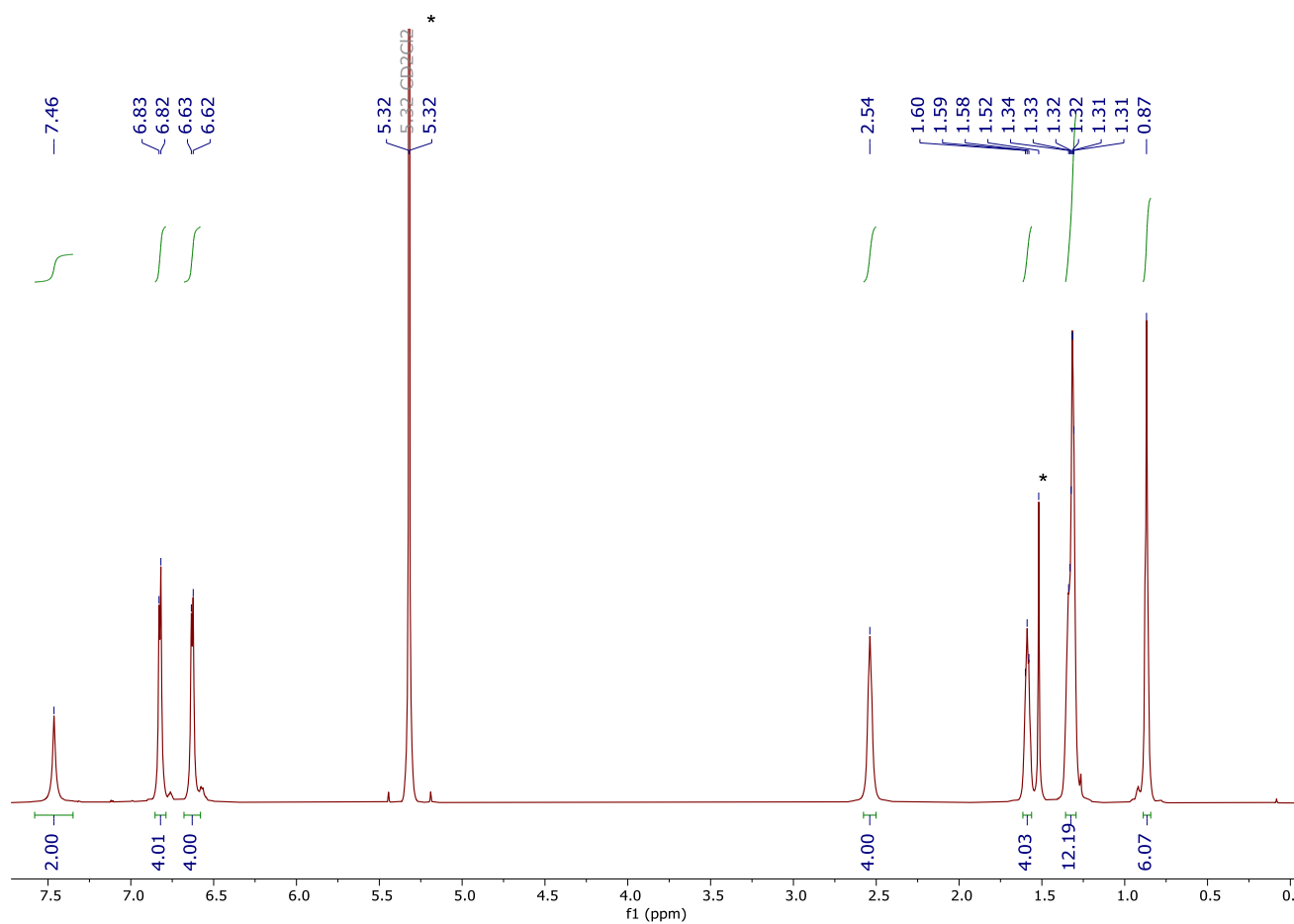


Figure S7. ^1H NMR spectrum of **PPP 2** in CD_2Cl_2 (300 MHz). The solvent peaks were marked with asterisks.

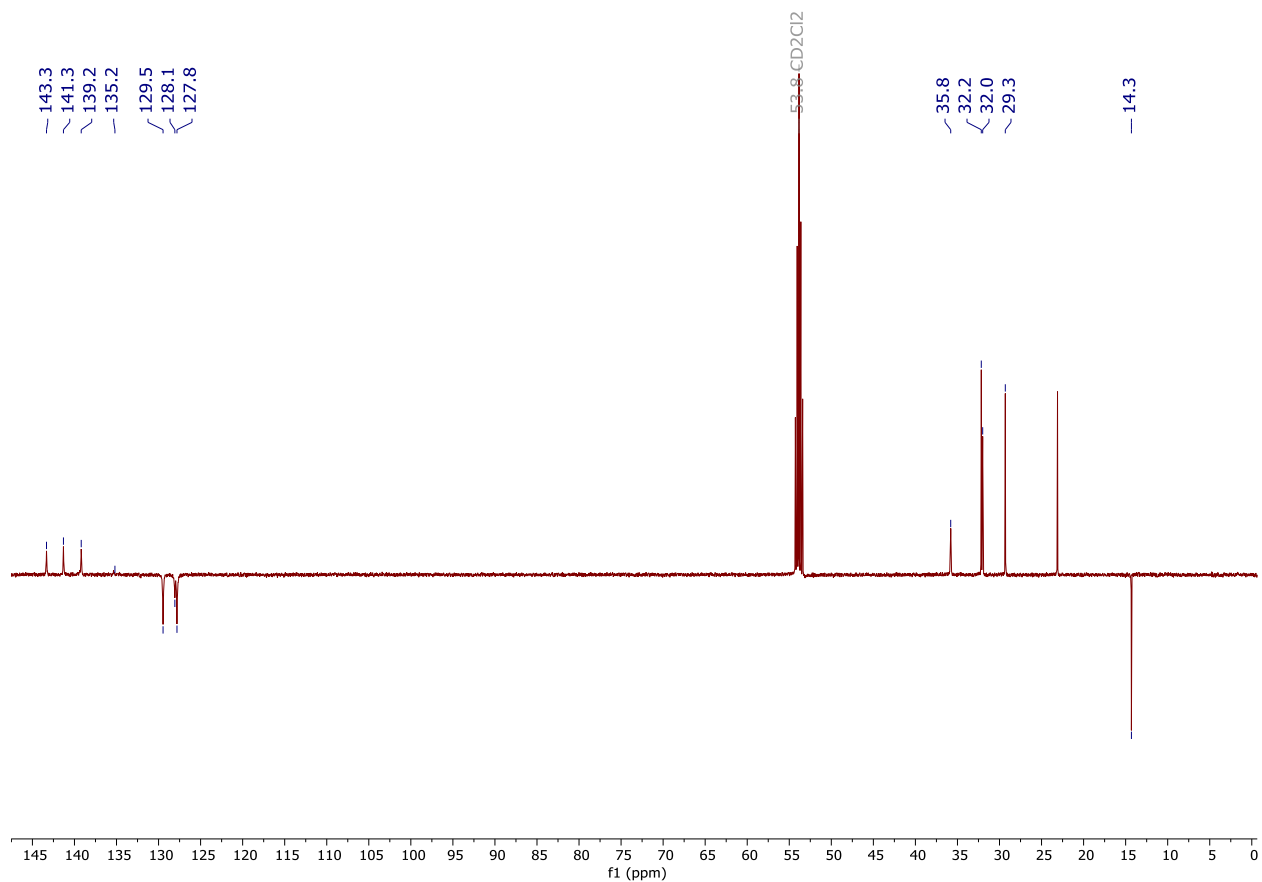


Figure S8. ^{13}C NMR spectrum of **PPP 2** in CD_2Cl_2 (300 MHz).

Table S1. GPC-MALLS and SEC analysis of polymer **PPP 2**.

#	Absolute M_w [g/mol] ¹	dn/dc ¹ [mL/g]	M_w [g/mol] ²	PDI
PPP 2	-	-	18900	1.9
PPP 2-3	8800	0.284	11100	1.1
PPP 2-2	15250	0.288	20400	1.1
PPP 2-1	29400	0.285	36500	1.1

¹ Data obtained from GPC-MALLS;

² Data obtained from SEC calibrated with PPP standard in THF;

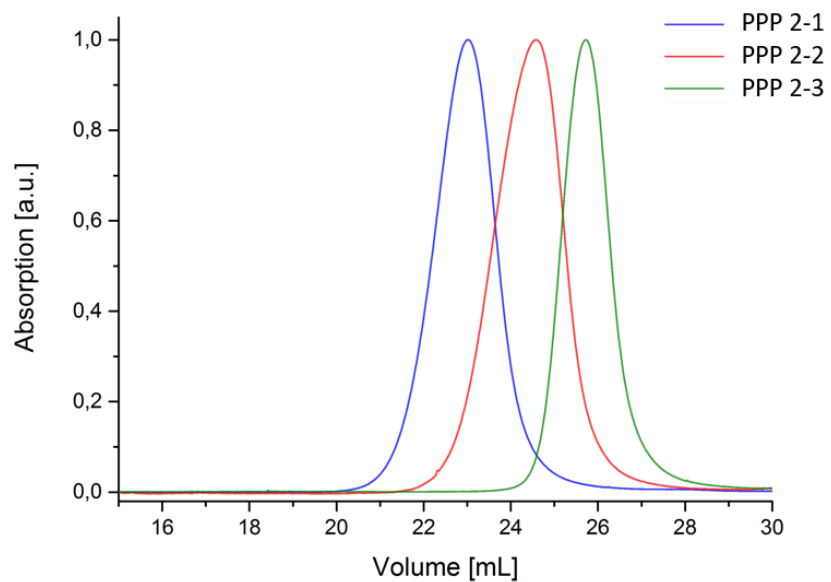


Figure S9. SEC analysis of the polymer fractions **PPP 2-1**, **PPP 2-2**, **PPP 2-3**.

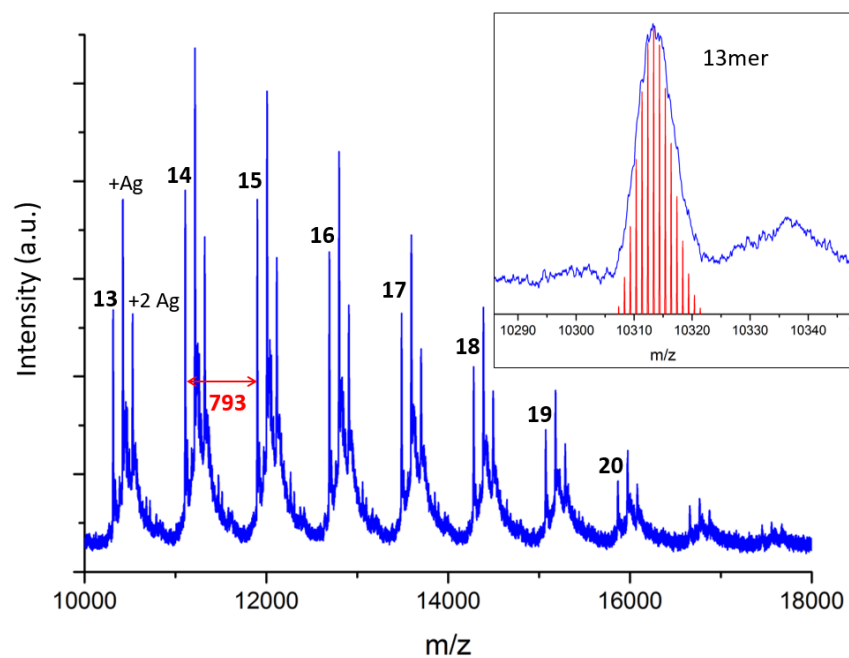


Figure S10. Reflection-mode MALDI-TOF MS analysis of **PPP 2-3**; inset: zoomed spectrum and calculated m/z of 13 mer.

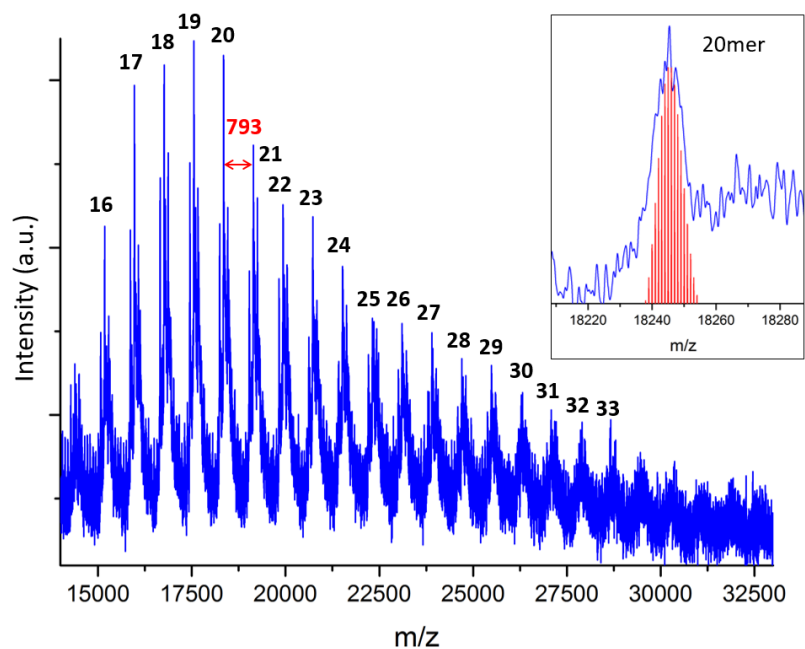


Figure S11. Reflection mode MALDI-TOF MS analysis of **PPP 2-2**; inset: zoomed spectrum and calculated m/z of 20 mer.

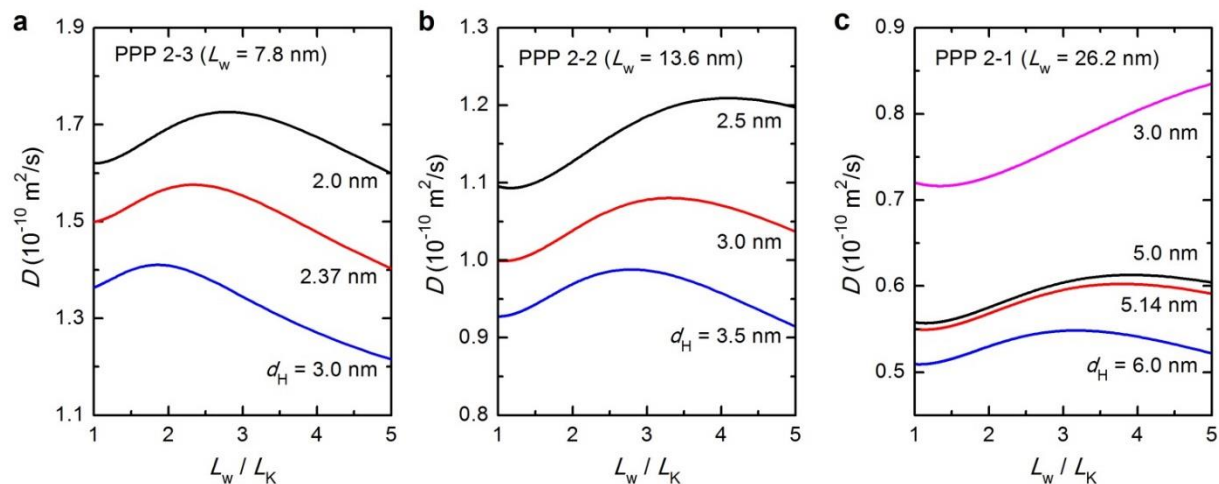


Figure S12: Predicted translational diffusion coefficients (Eq. (S1)) of the three **PPP 2** fractions as a function of chain flexibility L_w/L_K . (a) **PPP 2-3** (b) **PPP 2-2** (c) **PPP 2-1**.

Semi-rigid chain model:

$$D = \frac{k_B T}{3\pi\eta L_w} \left[1 + \frac{\sqrt{6}}{\sqrt{\pi} L_w} \int_{d_H}^{L_K/2} \frac{L_w - s}{s} \exp\left(-\frac{3d_H^2}{2s^2}\right) ds + \frac{\sqrt{6}}{\sqrt{\pi} L_w} \int_{L_K/2}^{L_w} \frac{L_w - s}{\sqrt{s} L_K} \exp\left(-\frac{3d_H^2}{2sL_K}\right) ds \right] \quad (S1)$$

Where

D : Translational diffusion coefficient of polymer, [m²/s]

k_B : Boltzmann constant, = 1.38 x 10⁻²³ [J/K]

T : Temperature, = 293 [K]

η : Shear viscosity of the solvent (THF), = 4.9 x 10⁻⁴ [Pa.s]

L_w : Contour length of the semi-rigid chain, [m]

d_H : Hydrodynamic diameter of the monomer for the semi-rigid chain, [m]

L_K : Kuhn segment length of the semi-rigid chain, [m]

In the limit of rigid chain (small L_w/l_p), and assuming Schulz-Zimm-like size polydispersity,

Eq.(S1) can be approximated by Eq. (S2),

$$\langle D \rangle_z = \frac{k_B T}{3\pi\eta L_w} \left\{ 1 + \sqrt{\frac{6}{\pi}} \left[\Psi(1+m) - 1 - \ln\left(\frac{(m+1)d_H}{L_w}\right) \right] \right\} \quad (S2)$$

Here $m = 1/(M_w/M_n - 1)$ and Ψ the digamma function, i.e., the logarithmic derivative of the gamma

function given by $\Psi(z) = \frac{d}{dz} \ln[\Gamma(z)]$.

Rod-like chain model (or Garcia de la Torre model):

$$D = \frac{k_B T}{3\pi\eta L} (\ln p + \delta) \quad (S3)$$

$$\delta = 0.312 + \frac{0.565}{p} - \frac{0.100}{p^2}$$

Where

D : Translational diffusion coefficient of polymer, [m²/s]

k_B : Boltzmann constant, = 1.38 x 10⁻²³ [J/K]

T : Temperature, = 293 [K]

η : Dynamic viscosity of the solvent (THF), = 4.9×10^{-4} [Pa.s]

δ : Correction factors accounting for end effects of the rigid rod

p : Aspect ratio of the rigid rod, = L_{RR}/d_{RR}

L_{RR} : Length of the rigid rod, [m]

d_{RR} : Diameter of the rigid rod, [m]

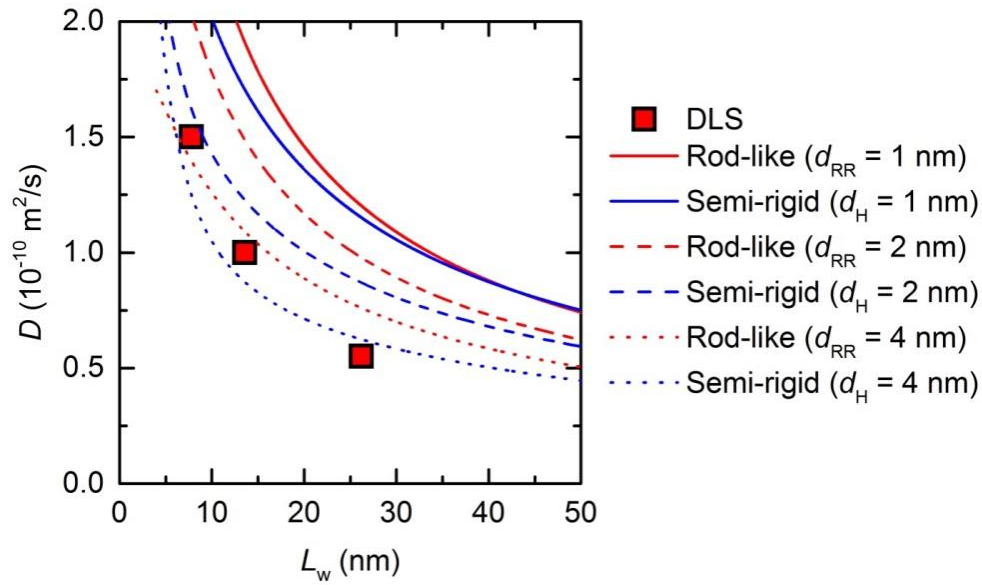


Figure S 13. Comparison of the rod-like (red lines) and semi-rigid chain (blue lines) using three different diameters d_{RR} (eq. (S3)) and d_H (eq. (S1)). For thin rods ($d_{RR} = 1 \text{ nm}$), the rate of decrease of the translational diffusion, D , becomes stronger than for the semi-rigid chains ($d_H = 1 \text{ nm}$) in the rigid rod limit.

The structural of **PPP 2** trimer was optimized by Universal Force Field (UFF) calculations using the Gaussian 09 software package.^[2]

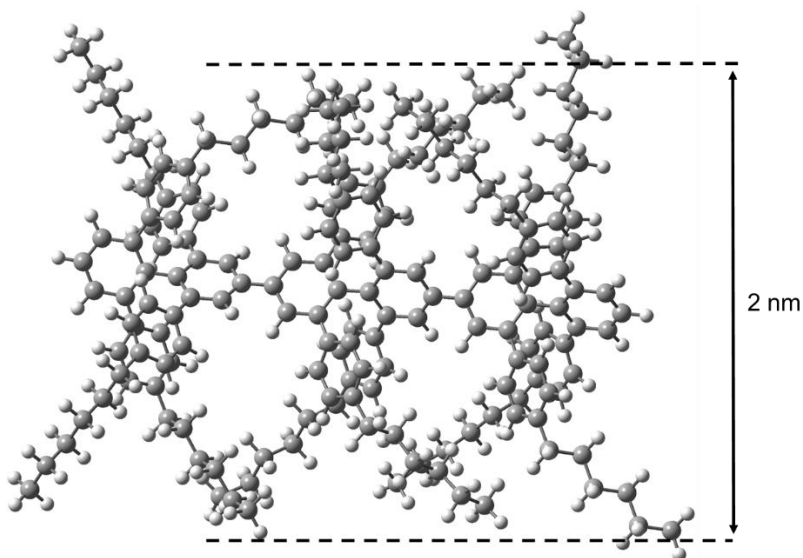


Figure S14. Optimized **PPP 2** trimer calculated by UFF. The monomer diameter was by analyzing the conformation of middle repeating unit.

The Cartesian coordinates of the optimized **PPP 2** trimer are listed as follows:

	X	Y	Z		X	Y	Z
C	1.426549	1.109555	0.780115	H	-2.069898	-3.60201	0.985304
C	2.788523	1.11346	0.733612	H	-4.796727	-2.167136	-0.383155
C	3.520506	0.052286	0.302045	H	-4.976832	1.908275	0.436218
C	2.843388	-1.047916	-0.118923	H	5.087419	-1.141612	-1.408774
C	1.484141	-1.099183	-0.189939	H	5.063387	1.333741	1.971278
C	0.743481	-0.006043	0.279212	H	-8.698991	-1.85812	-2.116097
C	0.921314	-2.224677	-0.76352	H	-9.606163	-3.975236	-2.664918
C	0.802248	2.211929	1.341162	H	-6.867379	-5.862318	-0.063623
C	-0.641044	-0.024998	0.238801	H	-5.982385	-3.761601	0.565999
C	-0.108544	-2.141538	-1.659799	H	-6.164744	3.404313	-0.686018
C	-0.726402	-3.249091	-2.115368	H	-7.205135	5.460562	-0.133178
C	-0.32664	-4.474278	-1.70675	H	-10.054263	3.428612	2.230511
C	0.734277	-4.582371	-0.87443	H	-8.999278	1.362894	1.765387

C	1.360511	-3.476875	-0.419141	H	6.091932	3.356447	1.92193
C	-0.27976	2.091189	2.17186	H	7.096198	4.762006	3.553134
C	-0.949534	3.176998	2.608237	H	10.128129	1.892312	4.207933
C	-0.548011	4.416952	2.252333	H	9.115314	0.436119	2.642706
C	0.558755	4.561851	1.491761	H	8.961199	0.16535	-2.408052
C	1.230669	3.481326	1.047602	H	10.028809	-1.241465	-3.980183
C	-1.34852	0.973165	-0.452795	H	7.369282	-4.384277	-3.028945
C	-2.710117	0.930048	-0.440233	H	6.328575	-3.03179	-1.383245
C	-3.401787	-0.085109	0.118198	H	-12.7236	-0.487229	-0.314382
C	-2.717474	-1.061782	0.75053	H	-11.603595	1.024641	-1.730928
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C	-0.764003	1.979171	-1.206079	H	-10.199362	-3.684708	1.222024
C	-0.796589	-2.023148	1.688354	H	-9.036909	-5.108979	2.732119
C	-1.286519	3.247773	-1.191652	H	-6.532293	-1.904792	3.877776
C	-0.718774	4.24588	-1.894763	H	-7.705805	-0.443901	2.430609
C	0.380584	4.016718	-2.645125	H	-7.499603	0.07358	-2.619068
C	0.898403	2.768788	-2.697156	H	-6.392989	1.685775	-3.958128
C	0.332318	1.762586	-1.997378	H	-9.373268	4.537752	-3.047038
C	0.242944	-1.762826	2.541189	H	-10.466821	2.974667	-1.634533
C	0.804505	-2.743733	3.27848	H	12.841959	0.855308	0.011555
C	0.339988	-4.010927	3.202082	H	11.461608	2.742528	-0.290009
C	-0.706208	-4.284479	2.394051	H	11.955976	-1.303676	0.337601
C	-1.272727	-3.310066	1.657122	H	10.031874	4.114849	0.821919
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C	4.90549	0.100108	0.277527	H	6.226996	3.796196	-2.192672
C	-5.409474	-1.295595	-0.172632	H	7.536559	1.870631	-1.805824
C	-6.762079	-1.379595	-0.308774	H	7.983958	-1.473277	1.982563
C	-7.528796	-0.219834	-0.103537	H	7.135486	-3.666915	2.220777
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C	-5.504227	0.997052	0.169709	H	10.861723	-2.918021	-0.814468
C	5.621229	-0.611634	-0.629547	H	-6.754981	-9.690866	-0.017967
C	6.982352	-0.564119	-0.715176	H	-5.377591	-9.533008	1.137334
C	7.678068	0.265783	0.173823	H	-6.468035	-8.122326	0.82407
C	6.955004	0.983379	1.134864	H	-5.694708	-8.085367	-1.57241
C	5.598214	0.872633	1.149751	H	-4.586024	-9.466966	-1.226602
C	-7.277106	-2.606609	-0.696954	H	-4.492629	-6.676152	0.101023
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C	-8.292385	-2.718795	-1.607928	H	-2.703041	-5.17857	-0.734974
C	-8.798068	-3.923779	-1.94453	H	-1.539508	-6.406994	-0.104926
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C	-7.605879	4.545171	0.284935	H	-1.162091	8.439004	-8.682286
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C	-8.595558	2.243071	1.289373	H	-0.978487	6.925591	-6.639922
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C	7.547096	3.798534	3.345686	H	0.647797	7.523098	-4.801737
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C	9.227025	2.217898	3.701664	H	-0.812841	5.525168	-4.537304
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C	9.616015	1.673027	-0.128915	H	-1.883459	6.020233	0.544452
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C	5.108272	6.099895	-0.588079	H	-6.626372	3.803597	-5.290267
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H	-1.082785	-5.295286	2.309657	H	8.737367	-6.663606	1.122294

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