

Supplementary Materials for

Fluorinated Polymer Surfactants Bearing Alternating Peptide Skeleton Prepared by Three-Component Polycondensation

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General methods:

Materials. Compound **1** was prepared according to the literature.¹ Trifluoromethanesulfonic acid (TfOH, Kanto chemicals), isobutyraldehyde (TCI), benzaldehyde (Kanto), biphenyl-4-carboxaldehyde (TCI), 1H,1H-heptafluorobutylamine (TCI), 1H,1H-pentadecafluorooctylamine (Wako), *i*-propylalcohol (Taiyo), chloroform (Kanto), and hexane (Kanto) were used as obtained. PANAM dendrimer generation 4 (core type: ethylenediamine, sigma-aldrich) MeOH solution was used as obtained for the DOSY measurement.²

Measurements. ¹H NMR (400 MHz), ¹³C NMR (100 MHz), and ¹⁹F NMR (376 MHz) spectra were recorded on a Bruker AVANCE II 400 spectrometer using CDCl₃, DMSO-*d*₆, and CD₃OD as the solvent. ¹H- and ¹³C NMR spectra were calibrated using residual undeuterated solvent and tetramethylsilane as the internal standard, while ¹⁹F spectra were calibrated using CF₃COOH as a standard. DOSY measurements were carried out using 3.0 mg of compound in 600 μL of CDCl₃ to estimate the diffusion coefficients. DOSY spectra were recorded on a Bruker AVANCE II 400 spectrometer. All experiments were run without spinning to avoid convection. The standard Bruker pulse program, ledbpgp2s, employing simulated echo and longitudinal eddy delay with bipolar gradients and two spoil gradients, was utilized. The obtained DOSY spectra were processed by Topspin 3.2 software. Diffusion dimension was generated using the inversion of Laplace transform driven by the CONTIN method.³ Diffusion coefficients of a chosen narrow chemical shift in the spectra of the compounds were extracted by using Dynamics center software (ver. 2.4.8, Bruker). FT-IR spectra using a KBr pellet were measured using a Thermo Fischer Scientific Nexus 870 spectrometer. FT-IR spectra via an attenuated total reflection (ATR) method were measured using a Perkin Elmer spectrum 100 spectrometer. SEC analyses were carried out using a chromatographic system consisting of a Shimadzu LC-20AT pump with a Shimadzu SPD-20A (UV detector) equipped with two consecutive linear polystyrene gel columns (Tosoh TSKgel GMH_{HR}-H and TSKgel G3000H_{HR}) at room temperature according to polystyrene standards using DMF as an eluent (flow rate: 1.0 mL/min). Differential scanning calorimetry analyses (DSC) were carried out on DSC7020 EXSTAR (Seiko Instruments Inc.) for **P1**, **P2**, **P3**, and **P6** and DSC-60 plus (Shimadzu Co. Ltd.) for **P4** and **P5** under N₂ atmosphere (flow rate: 150 mL/min). Thermogravimetric analyses (TGA) were carried out on TG/DTA 7300 EXSTAR (Seiko Instruments Inc.) under N₂ atmosphere (flow rate: 50 mL/min). The surface tensions of the surfactant solutions were determined by the Wilhelmy plate method at 25 °C using a DY-500 surface tension meter (Kyowa Kaimen Kagaku Co. Ltd.), the accuracy of which was intermittently checked with ultrapure water. The Pt plate was cleaned by flaming, and glassware was rinsed sequentially with ultrapure water and organic solvents. The size distribution of the assemblies of the **P6** solution was measured with a DLS instrument (DLS-7000, Otsuka Electronics Co. Ltd.) using an Ar laser with a wavelength of 488 nm as the source at 75 mW

at 25 °C. The time-dependent correlation function of the scattered light intensity was measured at a scattering angle of 90°. The size distributions were determined using the software provided with the instrument. The critical micelle concentration of **P6** was determined by UV spectra using a UV-3600 Plus UV-VIS-NIR spectrophotometer (Shimadzu Co. Ltd, Japan).

Synthetic procedures to give alternating peptides

Synthesis of **P1**

To a mixture of 1H,1H-heptafluorobutylamine (1.07 mL, 8.00 mmol) in *i*-PrOH (4.0 mL) was added TfOH (708 µL, 8.00 mmol) at 0 °C, which was followed by the addition of **1** (985 mg, 8.00 mmol). After the dissolution of **1**, isobutylaldehyde (730 µL, 8.00 mmol) was added to the mixture at the same temperature. The mixture was warmed to room temperature, stirred for 4 d, and concentrated in vacuo. The resulting crude was further stirred for 2.5 d at room temperature and diluted with CHCl₃. The reaction was quenched by the addition of water. The products were extracted with CHCl₃. The combined organic layer was dried over MgSO₄, filtered, and concentrated in vacuo. The crude was diluted with a small amount of CHCl₃ and the solution was reprecipitated in hexane to give hexane-insoluble part (**P1**, 2.30 g, 85%) as a pale yellow oil and hexane-soluble part (534 mg, 18%) as a pale yellow oil: M_w 7,400 Da (estimated by DOSY); M_w/M_n 1.5 (estimated by SEC on the basis of polystyrene standards); T_g -23.6 °C; T_{d5} 203.6 °C; T_{d10} 221.9 °C; ¹H NMR (400 MHz, 293 K, CDCl₃) δ 7.63 (brd, NH), 7.40 (brd, NH), 6.97 (brd, NH), 4.16–3.94 (m, 3H, CH, CH₂), 3.33–3.10 (m, 2H, CH₂), 2.16 (brd, 1H, CH), 1.03–0.90 (m, 6H, CH₃) ppm; ¹³C NMR (100 MHz, 293 K, CDCl₃) δ 174.8, 174.0, 172.2, 169.9, 116.0 (m), 68.3, 68.2, 47.9 (td, J_{CF} = 22, 7.1 Hz), 43.0, 41.0, 38.7 (t, J_{CF} = 22 Hz), 31.6, 31.5, 19.3, 17.4 ppm; ¹⁹F NMR (376 MHz, 293 K, CDCl₃) δ -81.37, -81.29, -81.41, -81.45, -81.48, -81.72, -81.74, -81.77, -117.73, -117.89, -120.00, -128.47, -128.54, -128.72 ppm; IR (KBr) ν 3315, 3086, 2969, 2939, 2880, 2615, 2536, 1733, 1655, 1538, 1471, 1394, 1376, 1354, 1222, 1119, 1030, 994, 958, 914, 787, 759, 739, 668, 639 cm⁻¹.

Synthesis of **P2**

To a mixture of 1H,1H-heptafluorobutylamine (1.07 mL, 8.00 mmol) in *i*-PrOH (4.0 mL) was added TfOH (708 µL, 8.00 mmol) at 0 °C, which was followed by the addition of **1** (985 mg, 8.00 mmol). After the dissolution of **1**, benzaldehyde (816 µL, 8.00 mmol) was added to the mixture at the same temperature. The mixture was warmed to room temperature, stirred for 4 d, and concentrated in vacuo. The resulting crude was further stirred for 2.5 d at room temperature and diluted with CHCl₃. The reaction was quenched by the addition of water. The products were extracted with CHCl₃. The combined organic layer was dried over MgSO₄, filtered, and concentrated in vacuo. The crude was diluted with a small amount of CHCl₃ and the solution was reprecipitated in hexane to give hexane-insoluble part (**P2**, 2.45 g, 82%) as an orange oil and hexane-soluble part (510 mg, 17%) as an orange oil: M_w 7,300 Da (estimated by DOSY); M_w/M_n 1.8 (estimated by SEC on the basis of polystyrene

standards); T_g -13.3 °C; T_{d5} 217.2 °C; T_{d10} 246.5 °C; ^1H NMR (400 MHz, 293 K, CDCl_3) δ 7.49 (brd, NH), 7.37 (brd, Ar, 5H), 6.73 (brd, NH), 4.40 (s, CH), 4.39 (s, CH), 4.13–3.85 (m, CH_2), 3.36–3.16 (m, CH_2) ppm; ^{13}C NMR (100 MHz, 293 K, CDCl_3) δ 172.8, 172.3, 172.0, 169.6, 137.3, 137.2, 129.2, 129.1, 128.9, 128.3, 127.5, 127.4, 119.0 (m), 116.1 (m), 66.4, 66.3, 46.5 (td, $J_{\text{CF}} = 22.5$, 13 Hz), 42.9, 41.2, 38.6 (t, $J_{\text{CF}} = 23.5$ Hz) ppm; ^{19}F NMR (376 MHz, 293 K, CDCl_3) δ -81.31 , -81.33 , -81.35 , -81.38 , -81.40 , -81.69 , -81.71 , -81.74 , -117.51 , -120.09 , -128.32 , -128.41 , -128.73 ppm; IR (KBr) ν 3310, 3071, 3032, 2941, 1655, 1528, 1498, 1455, 1422, 1393, 1354, 1221, 1174, 1118, 1058, 1030, 1003, 989, 960, 916, 739, 756, 668, 653 cm^{-1} .

Synthesis of P3

To a mixture of 1H,1H-heptafluorobutylamine (1.07 mL, 8.00 mmol) in *i*-PrOH (4.0 mL) was added TfOH (708 μL , 8.00 mmol) at 0 °C, which was followed by the addition of **1** (985 mg, 8.00 mmol). After the dissolution of **1**, biphenyl-4-carboxaldehyde (1.46 mg, 8.00 mmol) was added to the mixture at the same temperature. The mixture was warmed to room temperature, stirred for 4 d, and concentrated in vacuo. The resulting crude was further stirred for 2.5 d at room temperature and diluted with CHCl_3 . The reaction was quenched by the addition of water. The products were extracted with CHCl_3 . The combined organic layer was dried over MgSO_4 , filtered, and concentrated in vacuo. The crude was diluted with a small amount of CHCl_3 and the solution was reprecipitated in hexane to give hexane-insoluble part (**P3**, 2.25 g, 63%) as a yellow solid and hexane-soluble part (1.39 g, 38%) as a yellow solid: M_w 7,100 Da (estimated by DOSY); M_w/M_n 1.5 (estimated by SEC on the basis of polystyrene standards); T_g 31.4 °C; T_{d5} 234.6 °C; T_{d10} 264.0 °C; ^1H NMR (400 MHz, 293 K, CDCl_3) δ 7.47–7.33 (m, Ar, NH), 6.65 (brd, NH), 4.45 (s, CH), 4.44 (s, CH), 4.20–3.89 (m, CH_2), 3.39–3.23 (m, CH_2) ppm; ^{13}C NMR (100 MHz, 293 K, CDCl_3) δ 172.8, 172.3, 169.5, 141.9, 141.8, 140.2, 136.1, 135.9, 128.8, 127.94, 127.89, 127.79, 127.65, 127.61, 127.07, 127.01, 126.95, 66.0, 46.5 (t, $J_{\text{CF}} = 20.5$ Hz), 43.0, 41.2, 38.6 (t, $J_{\text{CF}} = 25$ Hz) ppm; ^{19}F NMR (376 MHz, 293 K, CDCl_3) δ -81.29 , -81.31 , -81.34 , -81.36 , -81.38 , -81.71 , -81.73 , -81.76 , -117.45 , -120.05 , -128.22 , -129.32 , -128.73 ppm; IR (KBr) ν 3319, 2970, 1667, 1523, 1227, 1119, 1008, 951, 817, 761, 739, 699, 642, 562, 533, 514 cm^{-1} .

Synthesis of P4

To a mixture of 1H,1H-pentadecafluorooctylamine (582 μL , 2.50 mmol) in *i*-PrOH (1.25 mL) was added TfOH (221 μL , 2.50 mmol) at 0 °C, which was followed by the addition of **1** (308 mg, 2.50 mmol). After the dissolution of **1**, isobutylaldehyde (228 μL , 2.50 mmol) was added to the mixture at the same temperature. The mixture was warmed to room temperature, stirred for 4 d, and concentrated in vacuo. The resulting crude was further stirred for 3 d at room temperature and diluted with CHCl_3 . The reaction was quenched by the addition of water. The products were extracted with CHCl_3 . The

combined organic layer was dried over MgSO₄, filtered, and concentrated in vacuo. The crude was diluted with a small amount of CHCl₃ and the solution was reprecipitated in hexane to give hexane-insoluble part (**P4**, 583 mg, 43%) as a white solid and hexane-soluble part (848 mg, 63%) as a white solid: M_w 7,600 Da (estimated by DOSY); M_w/M_n 1.2 (estimated by SEC on the basis of polystyrene standards); T_g -1.3 °C; T_{d5} 217.3 °C; T_{d10} 236.5 °C; ¹H NMR (400 MHz, 293 K, CDCl₃) δ ppm; ¹³C NMR (100 MHz, 293 K, CD₃OD) δ 177.0, 171.8, 70.03, 69.99, 42.97, 32.84, 19.83, 18.83, 18.73 ppm; ¹⁹F NMR (376 MHz, 293 K, CDCl₃) δ -81.58, -81.60, -81.64, -81.67, -81.69, -81.73, -81.75, -117.06, -122.59, -122.90, -123.67, -124.16, -124.25, -127.04 ppm; IR (KBr) ν 3319, 2988, 1692, 1653, 1525, 1204, 1148, 1104, 1020, 790, 701, 668, 567, 531 cm⁻¹.

Synthesis of P5

To a mixture of 1H,1H-pentadecafluorooctylamine (582 μ L, 2.50 mmol) in *i*-PrOH (1.25 mL) was added TfOH (221 μ L, 2.50 mmol) at 0 °C, which was followed by the addition of **1** (308 mg, 2.50 mmol). After the dissolution of **1**, benzaldehyde (255 μ L, 2.50 mmol) was added to the mixture at the same temperature. The mixture was warmed to room temperature, stirred for 4 d, and concentrated in vacuo. The resulting crude was further stirred for 3 d at room temperature and diluted with CHCl₃. The reaction was quenched by the addition of water. The products were extracted with CHCl₃. The combined organic layer was dried over MgSO₄, filtered, and concentrated in vacuo. The crude was diluted with a small amount of CHCl₃ and the solution was reprecipitated in hexane to give hexane-insoluble part (**P5**, 956 mg, 67%) as a yellow solid and hexane-soluble part (651 mg, 45%) as a yellow solid: M_w 7,400 Da (estimated by DOSY); M_w/M_n 1.3 (estimated by SEC on the basis of polystyrene standards); T_g 0.7 °C; T_{d5} 231.7 °C; T_{d10} 254.9 °C; ¹H NMR (400 MHz, 293 K, CDCl₃) δ ppm; ¹³C NMR (100 MHz, 293 K, CD₃OD) δ 175.0, 172.8, 171.9, 139.5, 139.4, 130.5, 130.3, 129.8, 129.7, 129.41, 129.35, 128.9, 127.8, 67.5, 45.3, 43.2, 41.9 ppm; ¹⁹F NMR (376 MHz, 293 K, CDCl₃) δ -81.51, -81.54, -81.59, -81.62, -81.65, -81.67, -116.50, -119.08, -122.62, -122.94, -123.65, -124.06, -124.36, -127.04 ppm; IR (KBr) ν 3315, 2960, 1651, 1524, 1143, 1053, 1020, 884, 736, 700, 665, 567, 531 cm⁻¹.

Synthesis of P6

To a mixture of 1H,1H-pentadecafluorooctylamine (582 μ L, 2.50 mmol) in *i*-PrOH (1.25 mL) was added TfOH (221 μ L, 2.50 mmol) at 0 °C, which was followed by the addition of **1** (308 mg, 2.50 mmol). After the dissolution of **1**, biphenyl-4-carboxaldehyde (456 mg, 2.50 mmol) was added to the mixture at the same temperature. The mixture was warmed to room temperature, stirred for 4 d, and concentrated in vacuo. The resulting crude was further stirred for 3 d at room temperature and diluted with CHCl₃. The reaction was quenched by the addition of water. The products were extracted with CHCl₃. The combined organic layer was dried over MgSO₄, filtered, and concentrated in vacuo. The

crude was diluted with a small amount of CHCl_3 and the solution was reprecipitated in hexane to give hexane-insoluble part (**P6**, 1.04 g, 64%) as a white solid and hexane-soluble part (0.95 mg, 41%) as a white solid: M_w 8,800 Da (estimated by DOSY); M_w/M_n 1.2 (estimated by SEC on the basis of polystyrene standards); T_g 45.5 °C; T_{d5} 199.8 °C; T_{d10} 235.4 °C; ^1H NMR (400 MHz, 293 K, CDCl_3) δ 7.46–7.32 (m, Ar, NH), 6.80 (brd, NH), 4.46 (s, CH), 4.45 (s, CH), 4.19–3.88 (m, CH_2), 3.39–3.24 (m, CH_2) ppm; ^{13}C NMR (100 MHz, 293 K, CDCl_3) δ 172.8, 172.30, 172.27, 169.5, 141.9, 141.8, 140.2, 140.1, 136.1, 136.0, 128.8, 128.0, 127.9, 127.81, 127.79, 127.65, 127.61, 127.0, 66.1, 46.8 (t, $J_{\text{CF}} = 22.5$ Hz), 43.1, 41.2 ppm; ^{19}F NMR (376 MHz, 293 K, CDCl_3) δ -81.44, -81.55, -81.58, -81.61, -81.64, -116.51, -119.18, -122.57, -122.86, -123.63, -123.92, -124.37, -127.03 ppm; IR (KBr) ν 3318, 3033, 1662, 1533, 1488, 1413, 1217, 1146, 1009, 882, 837, 808, 763, 735, 721, 699, 661, 565 cm^{-1} .

^1H NMR, ^{13}C NMR, ^{19}F NMR, DOSY, and IR spectra

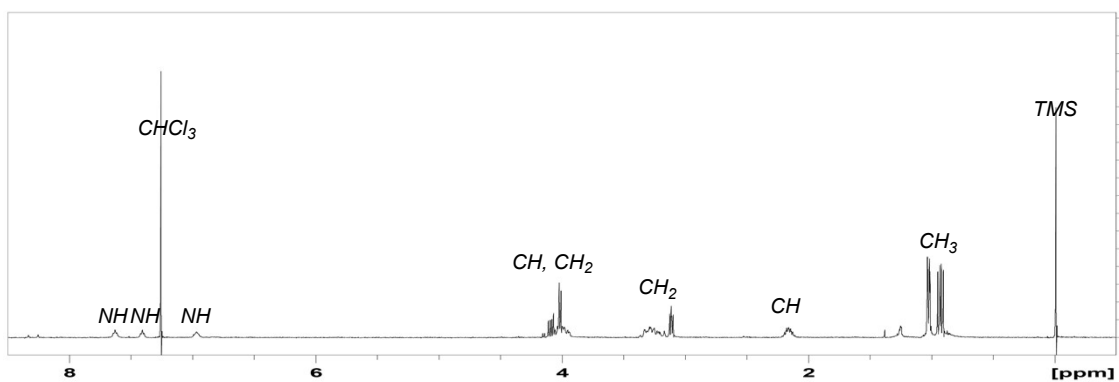


Figure S1. ^1H NMR spectrum of P1 (400 MHz, CDCl_3 , 298 K).

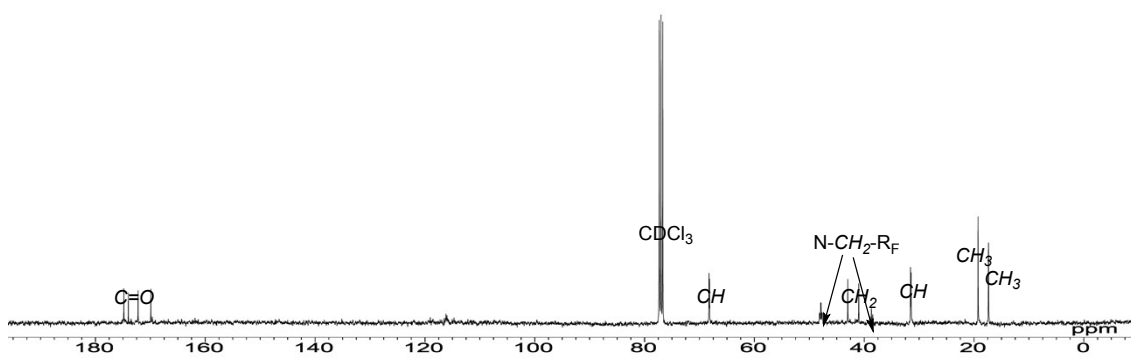


Figure S2. ^{13}C NMR spectrum of P1 (100 MHz, CDCl_3 , 298 K).

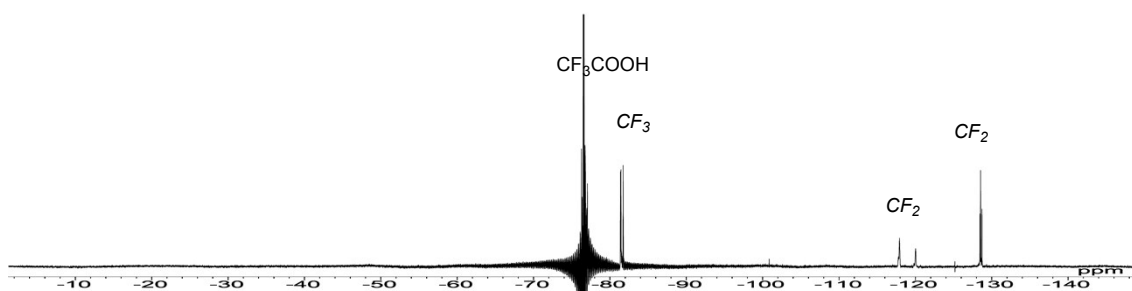


Figure S3. ^{19}F NMR spectrum of P1 (376 MHz, CDCl_3 , 298 K).

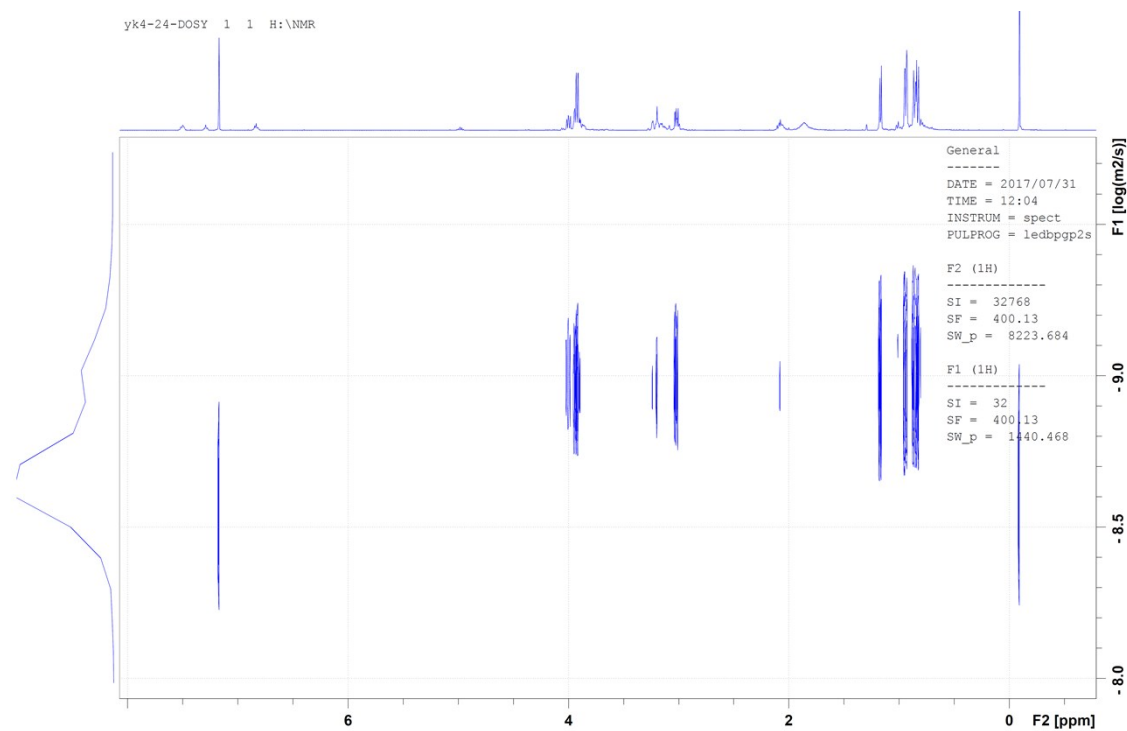


Figure S4. DOSY correlations of **P1** (400 MHz, CDCl₃, 298 K).

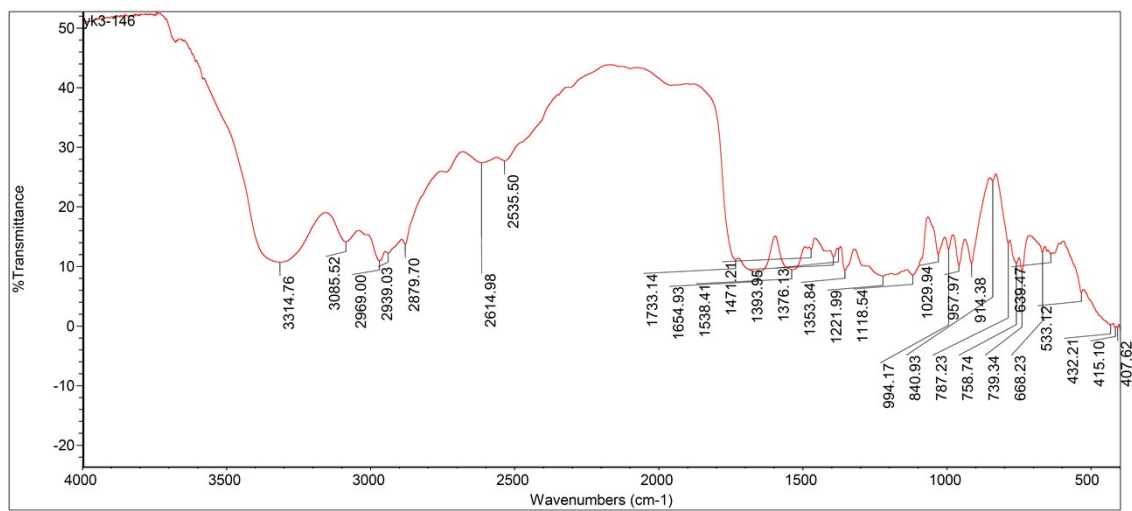


Figure S5. IR spectrum of **P1** (KBr).

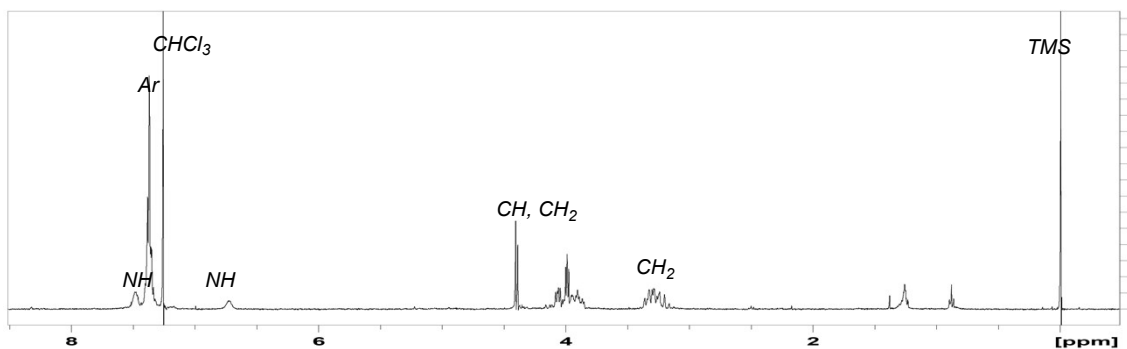


Figure S6. ^1H NMR spectrum of **P2** (400 MHz, CDCl_3 , 298 K).

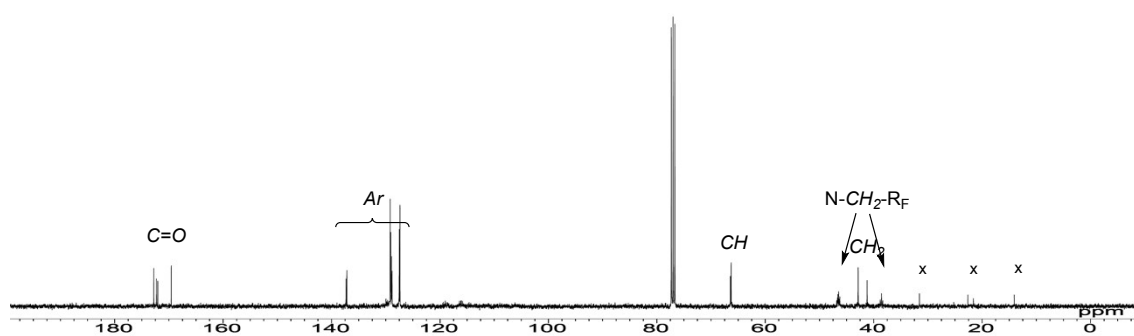


Figure S7. ^{13}C NMR spectrum of **P2** (100 MHz, CDCl_3 , 298 K).

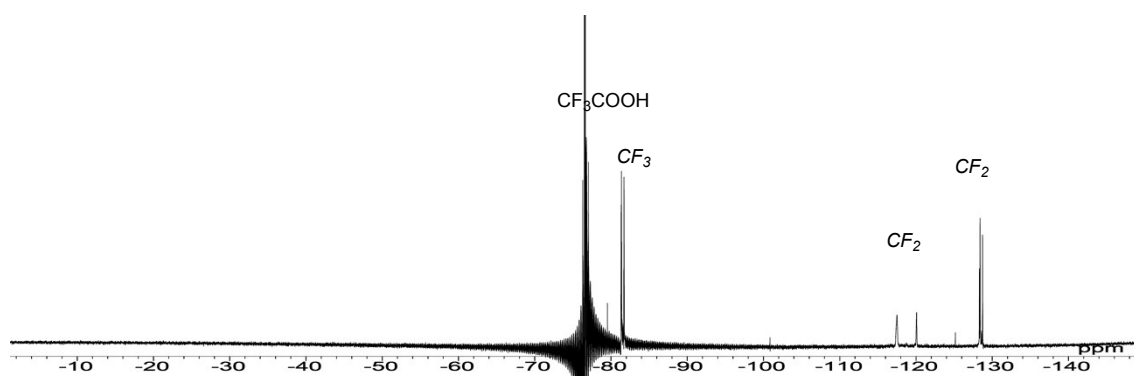


Figure S8. ^{19}F NMR spectrum of **P2** (376 MHz, CDCl_3 , 298 K).

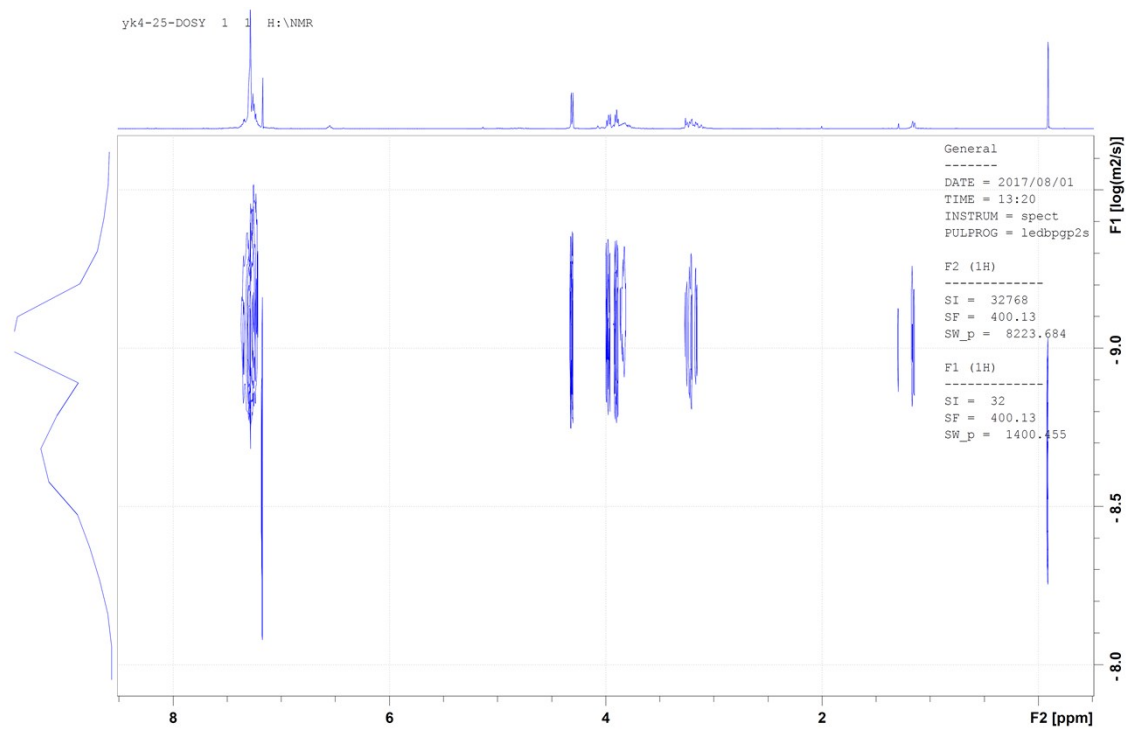


Figure S9. DOSY correlations of **P2** (400 MHz, CDCl₃, 298 K).

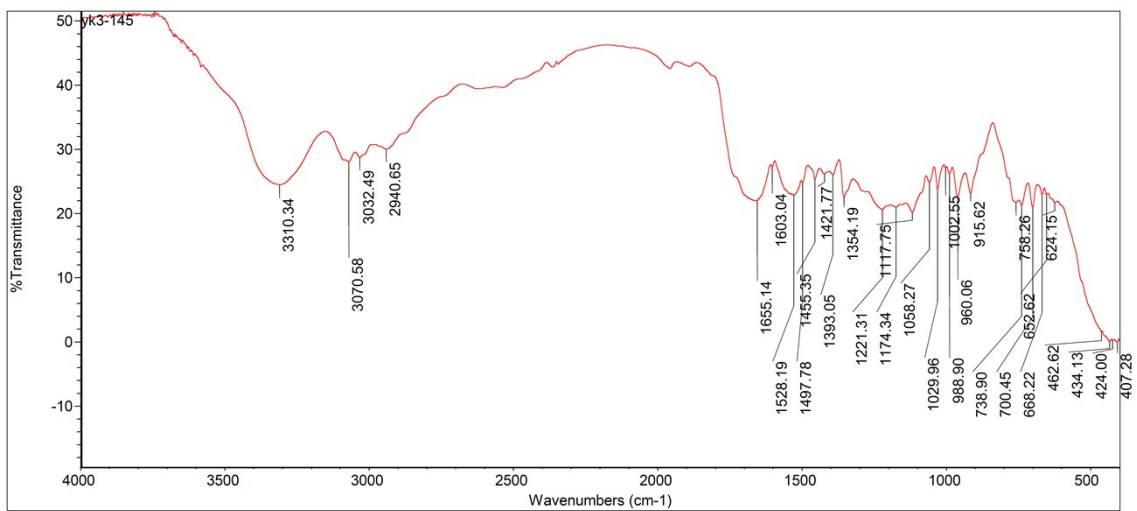


Figure S10. IR spectrum of **P2** (KBr).

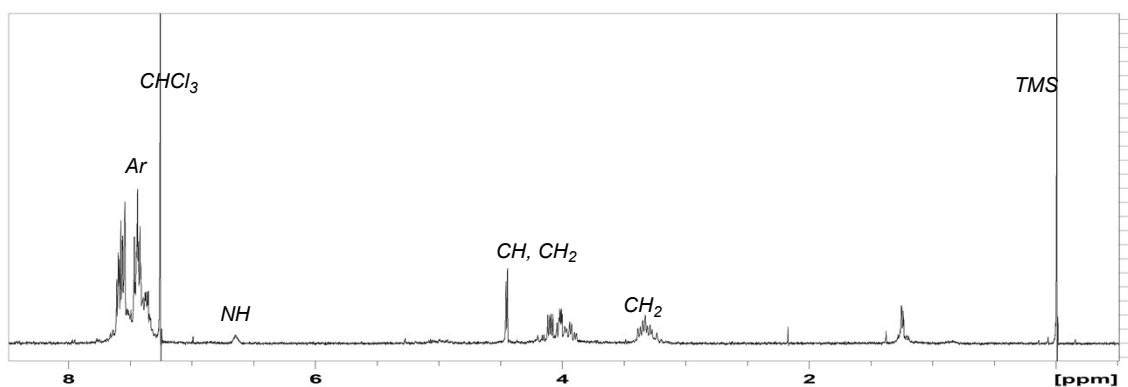


Figure S11. ^1H NMR spectrum of **P3** (400 MHz, CDCl_3 , 298 K).

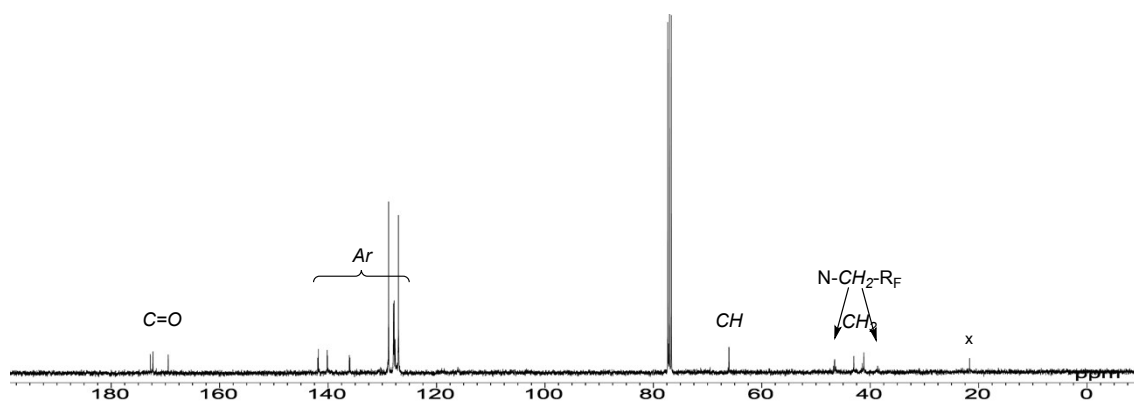


Figure S12. ^{13}C NMR spectrum of **P3** (100 MHz, CDCl_3 , 298 K).

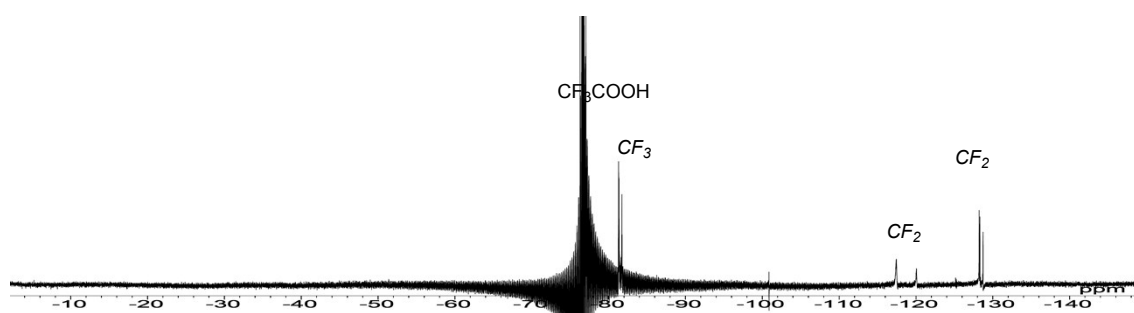


Figure S13. ^{19}F NMR spectrum of **P3** (376 MHz, CDCl_3 , 298 K).

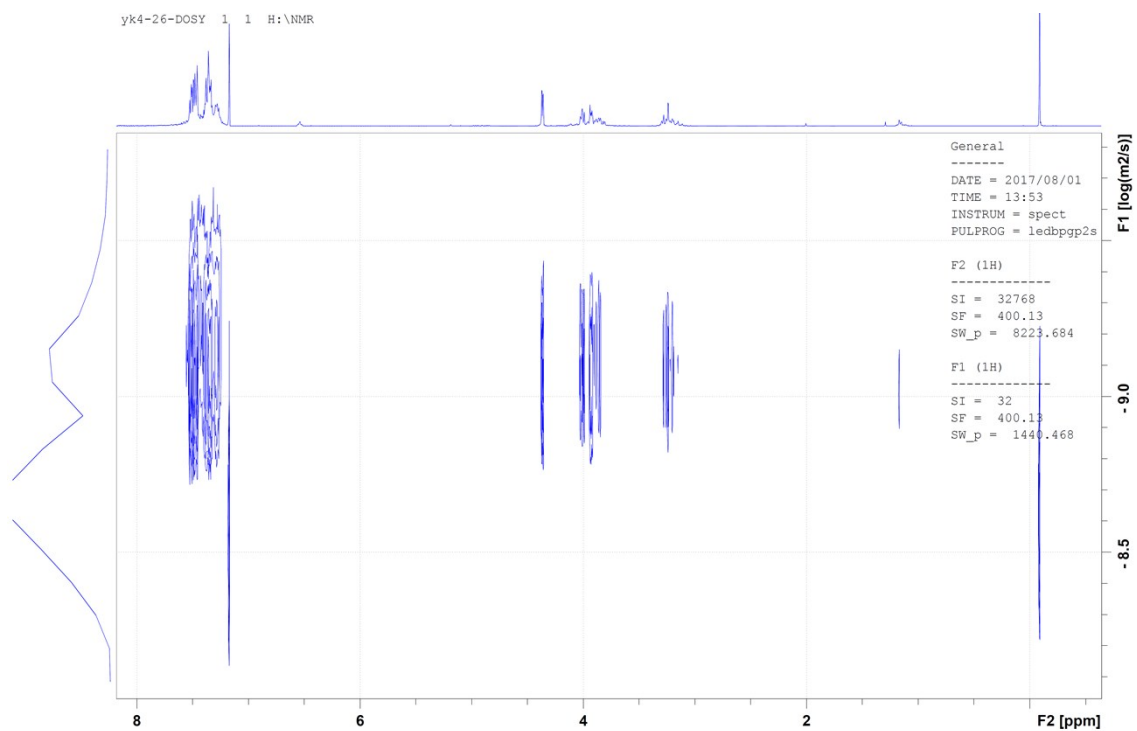


Figure S14. DOSY correlations of **P3** (400 MHz, CDCl₃, 298 K).

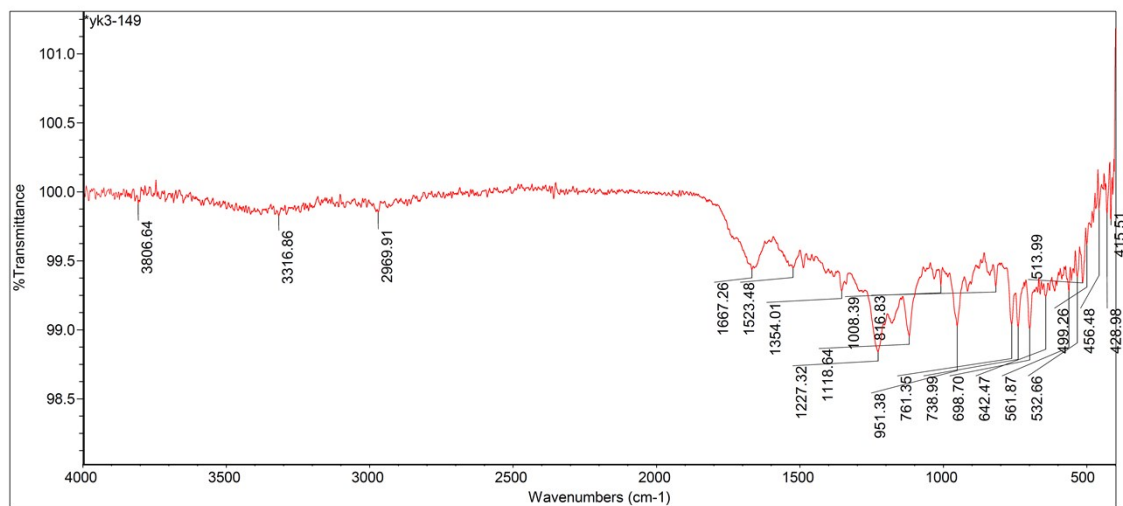


Figure S15. IR spectrum of **P3** (KBr).

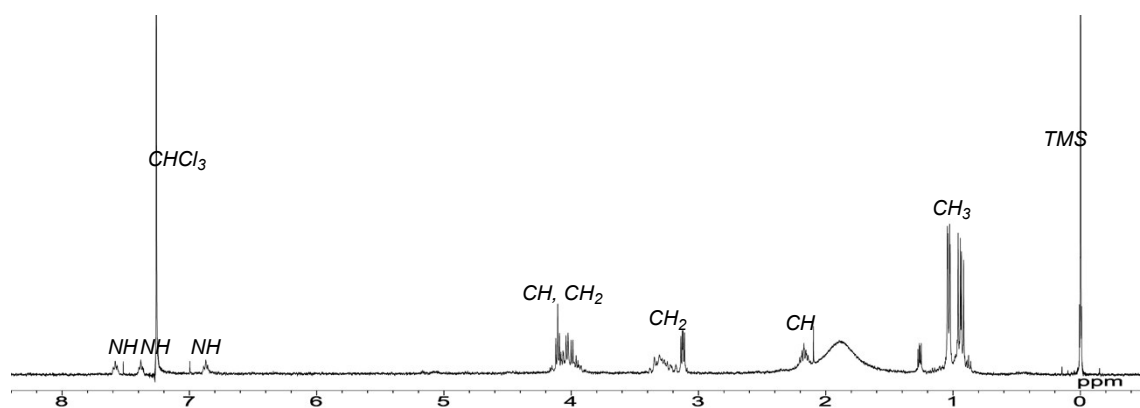


Figure S16. ^1H NMR spectrum of **P4** (400 MHz, CDCl_3 , 298 K).

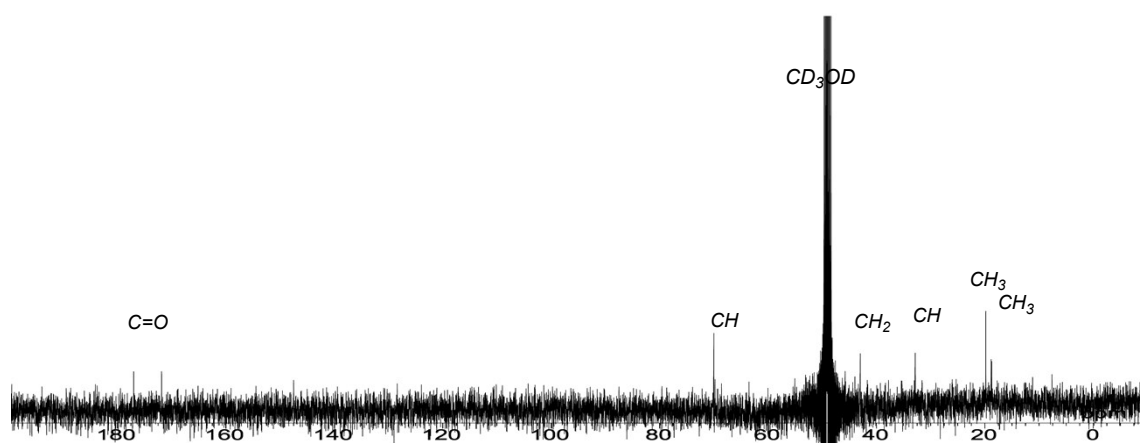


Figure S17. ^{13}C NMR spectrum of **P4** (100 MHz, CD_3OD , 298 K).

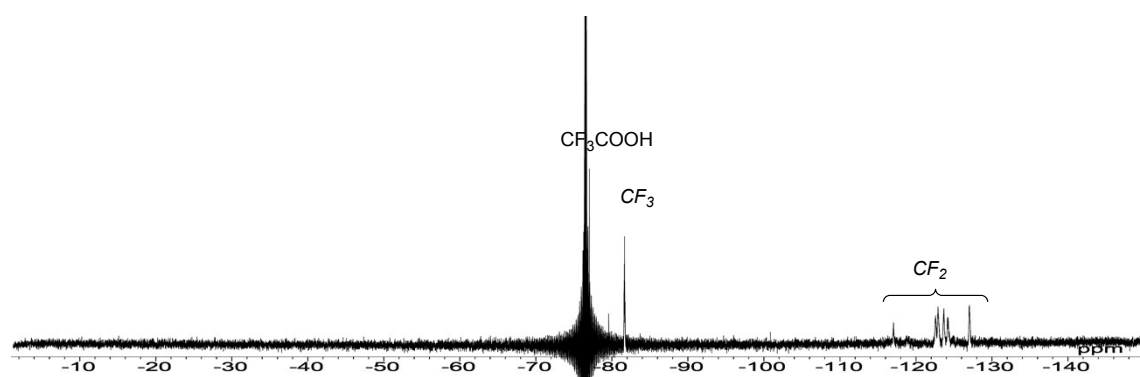


Figure S18. ^{19}F NMR spectrum of **P4** (376 MHz, CDCl_3 , 298 K).

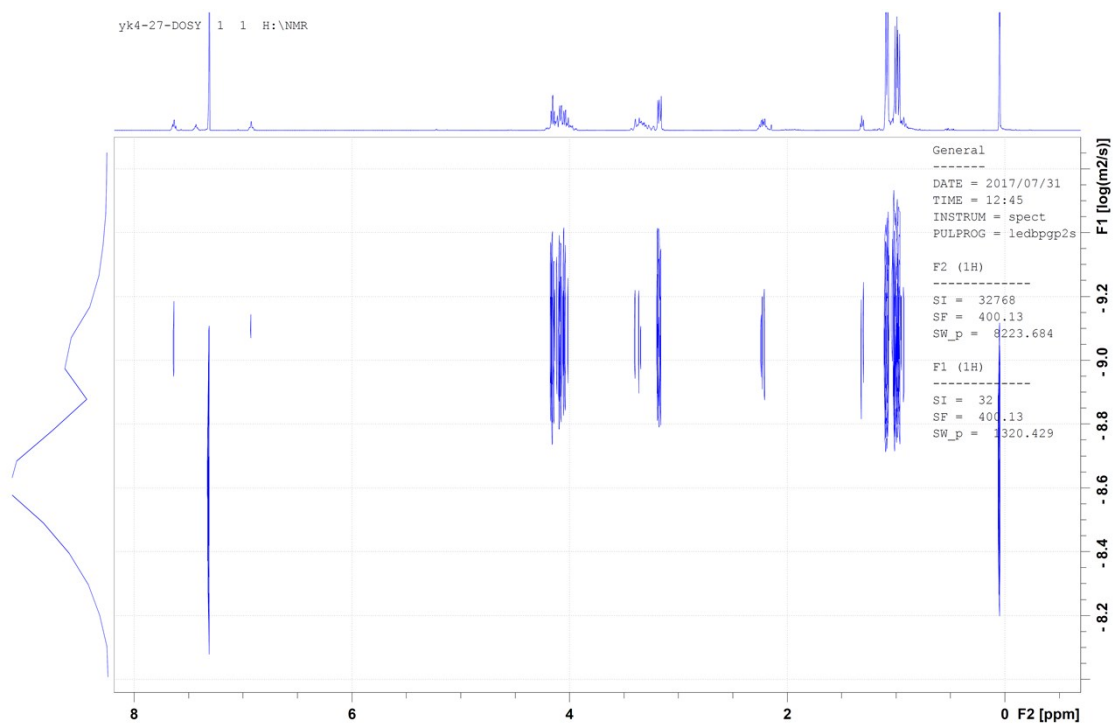


Figure S19. DOSY correlations of **P4** (400 MHz, CDCl₃, 298 K).

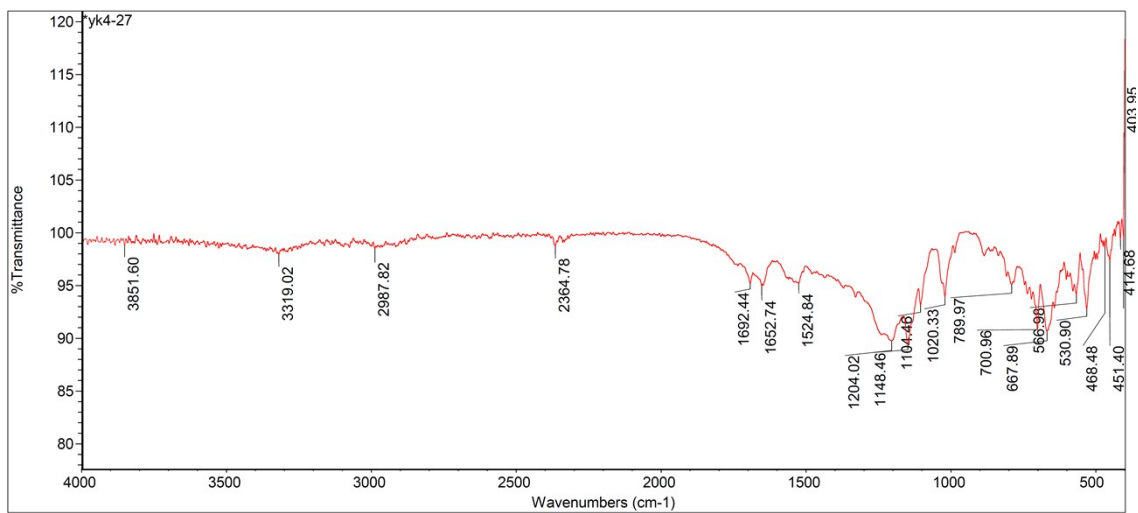


Figure S20. IR spectrum of **P4** (KBr).

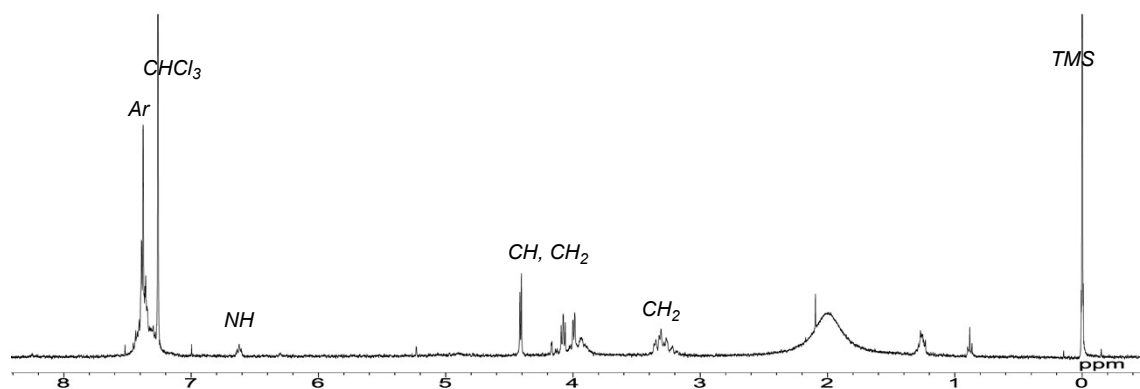


Figure S21. ^1H NMR spectrum of **P5** (400 MHz, CDCl_3 , 298 K).

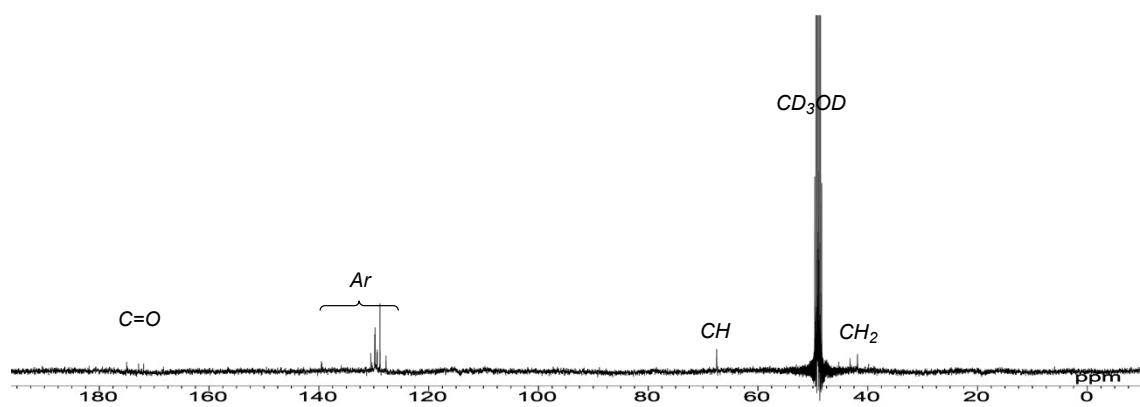


Figure S22. ^{13}C NMR spectrum of **P5** (100 MHz, CD_3OD , 298 K).

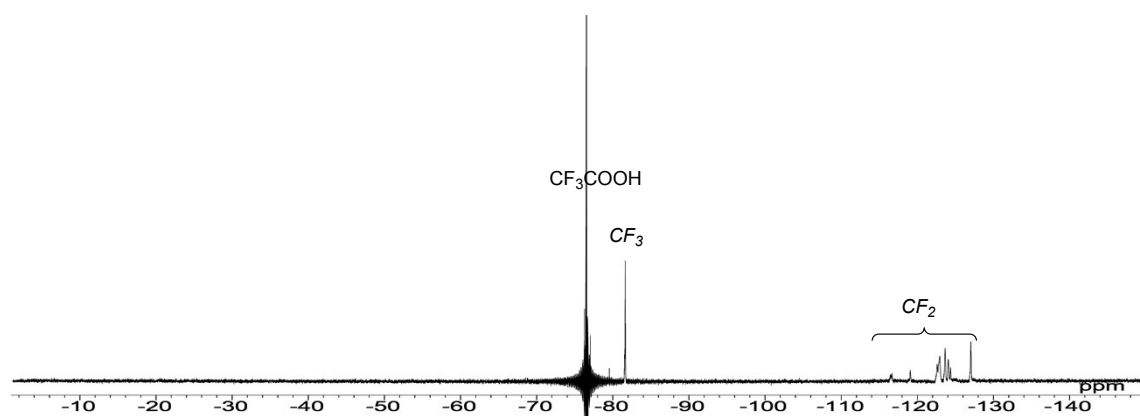


Figure S23. ^{19}F NMR spectrum of **P5** (376 MHz, CDCl_3 , 298 K).

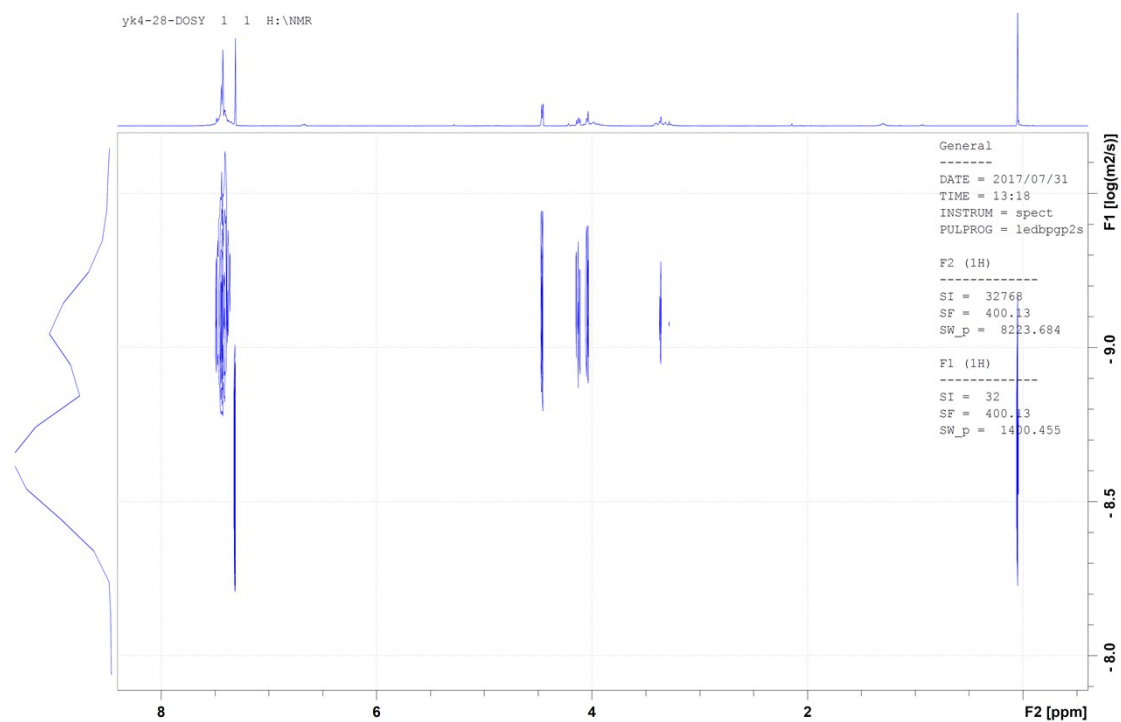


Figure S24. DOSY correlations of **P5** (400 MHz, CDCl_3 , 298 K).

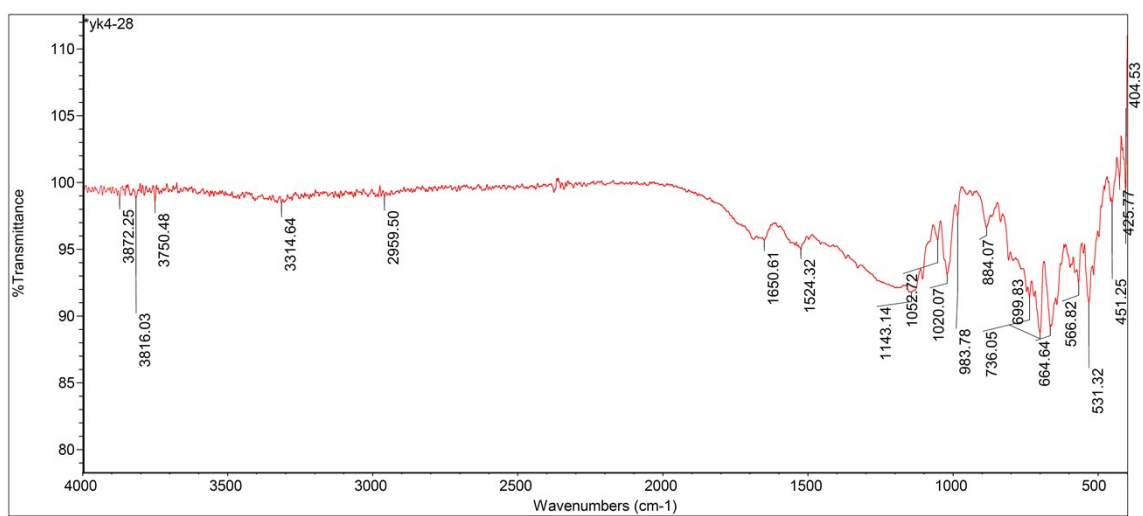


Figure S25. IR spectrum of **P5** (KBr).

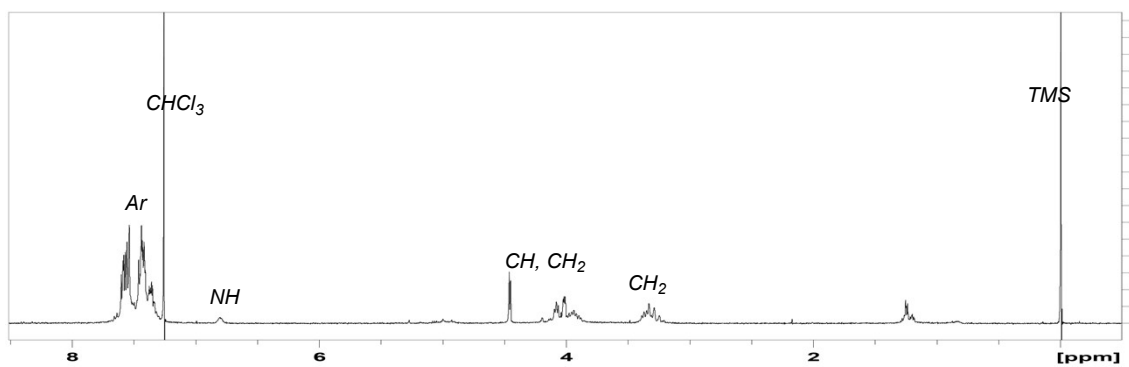


Figure S26. ^1H NMR spectrum of **P6** (400 MHz, CDCl_3 , 298 K).

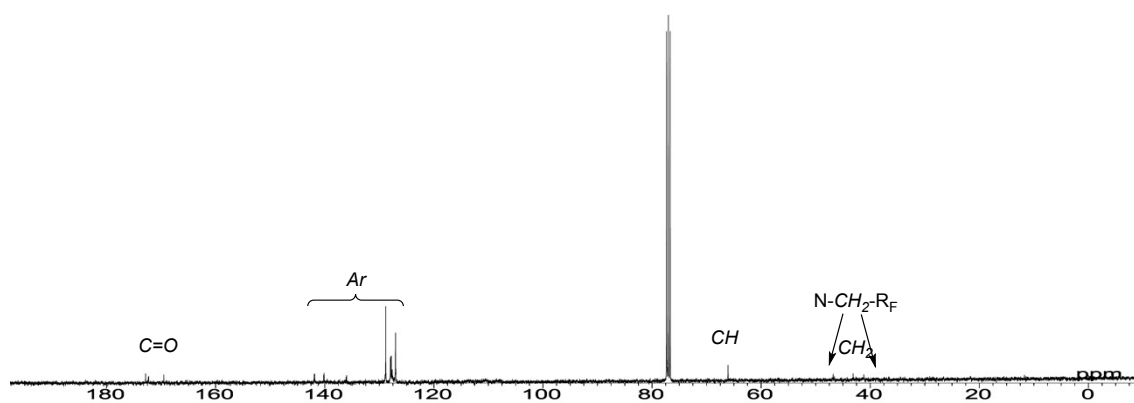


Figure S27. ^{13}C NMR spectrum of **P6** (100 MHz, CDCl_3 , 298 K).

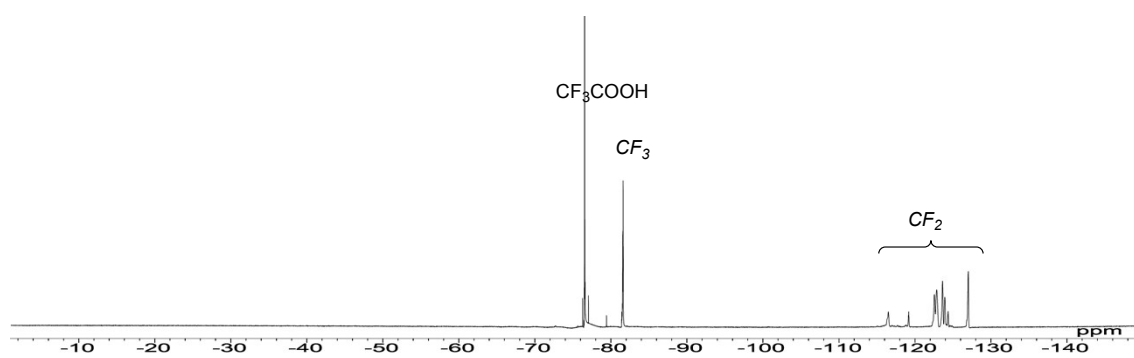


Figure S28. ^{19}F NMR spectrum of **P6** (376 MHz, CDCl_3 , 298 K).

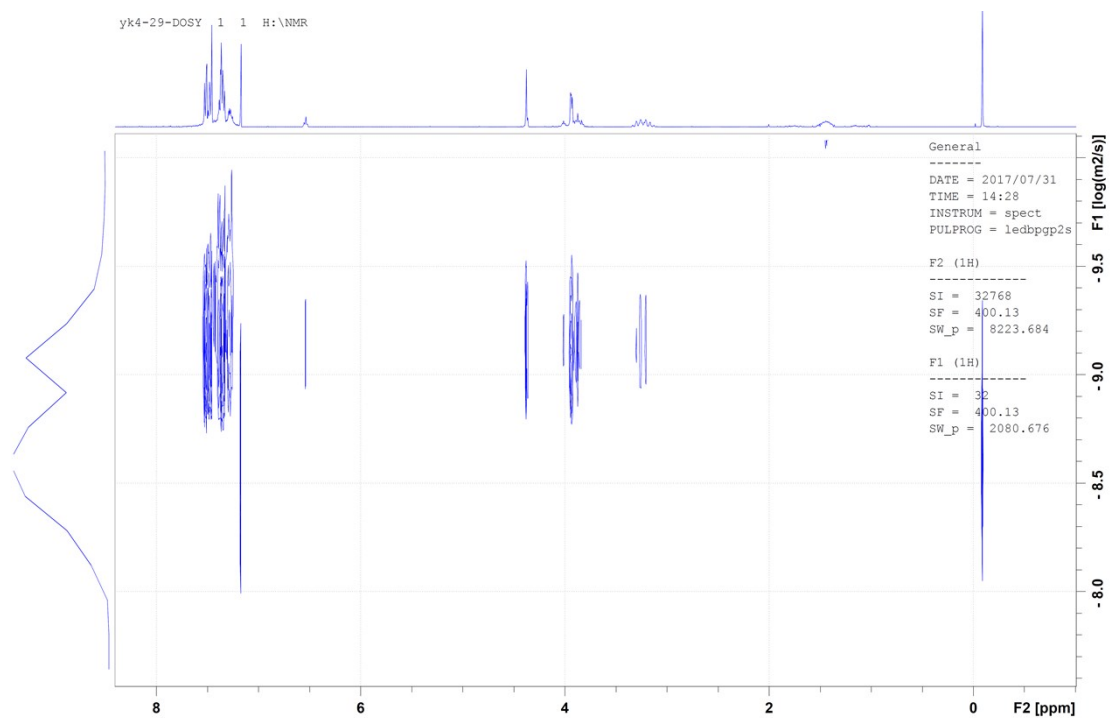


Figure S29. DOSY correlations of **P6** (400 MHz, CDCl₃, 298 K).

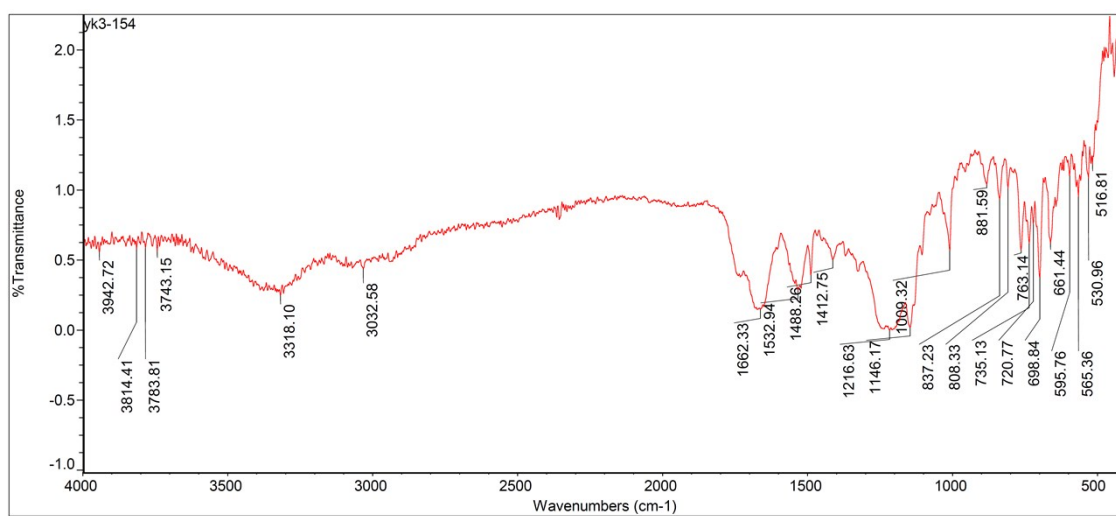


Figure S30. IR spectrum of **P6** (KBr).

Calibration curve in CDCl₃ for M_w prediction

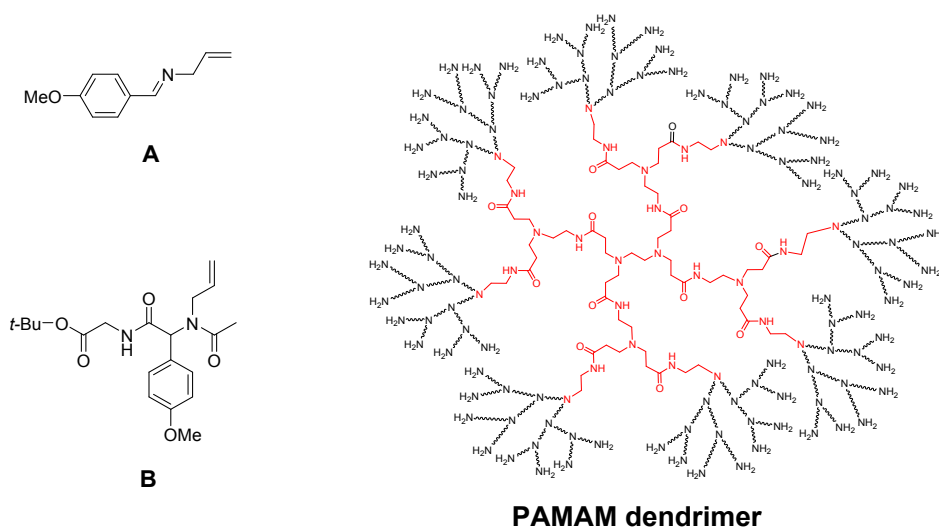
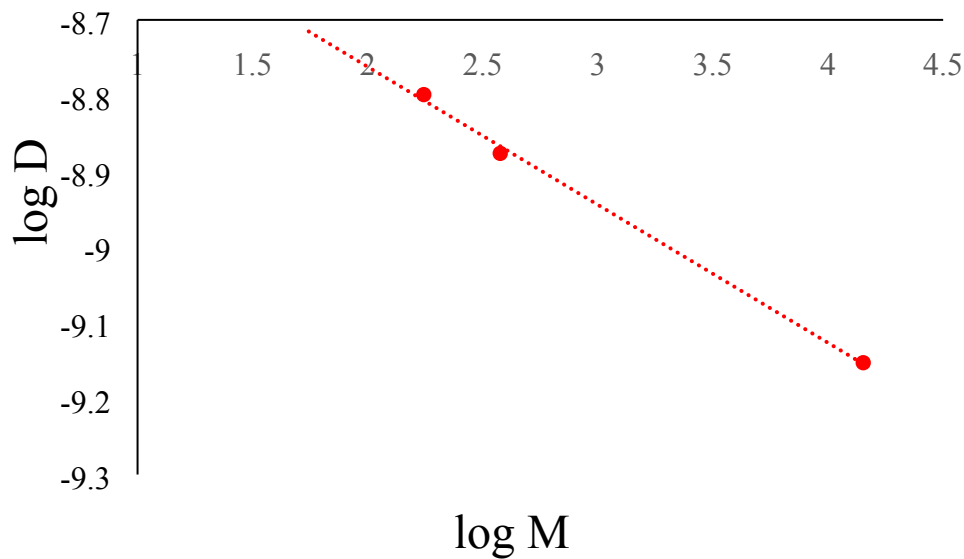


Figure S31. Calibration curve in CDCl₃ for M_w prediction using imine **A** (MW: 175.23, log D: -8.55), unit model **B** (MW: 376.45, log D: -8.70), and PAMAM dendrimer (MW: 14214.17, log D: -9.15) as standards. Imine **A** and unit model **B** were prepared according to the literature.^{1a}

DSC profiles

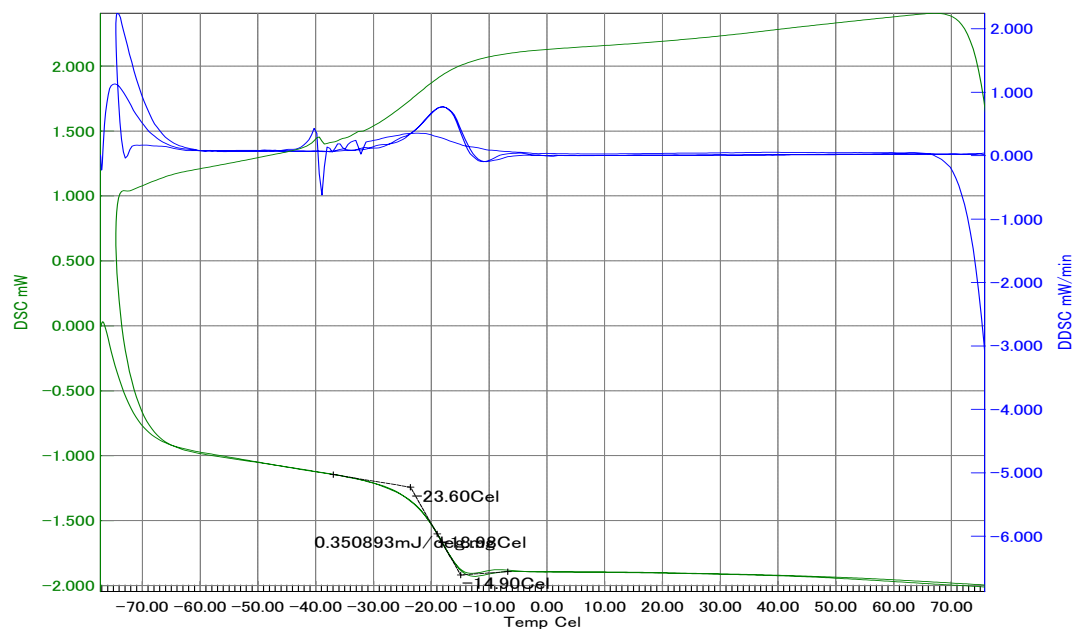


Figure S32. DSC profile of P1.

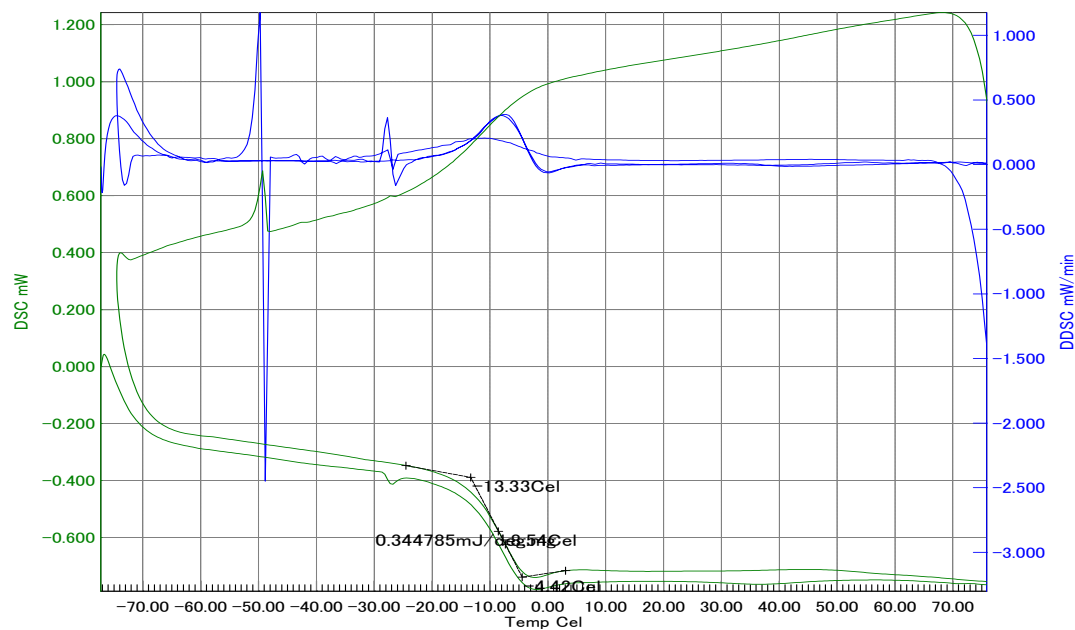


Figure S33. DSC profile of P2.

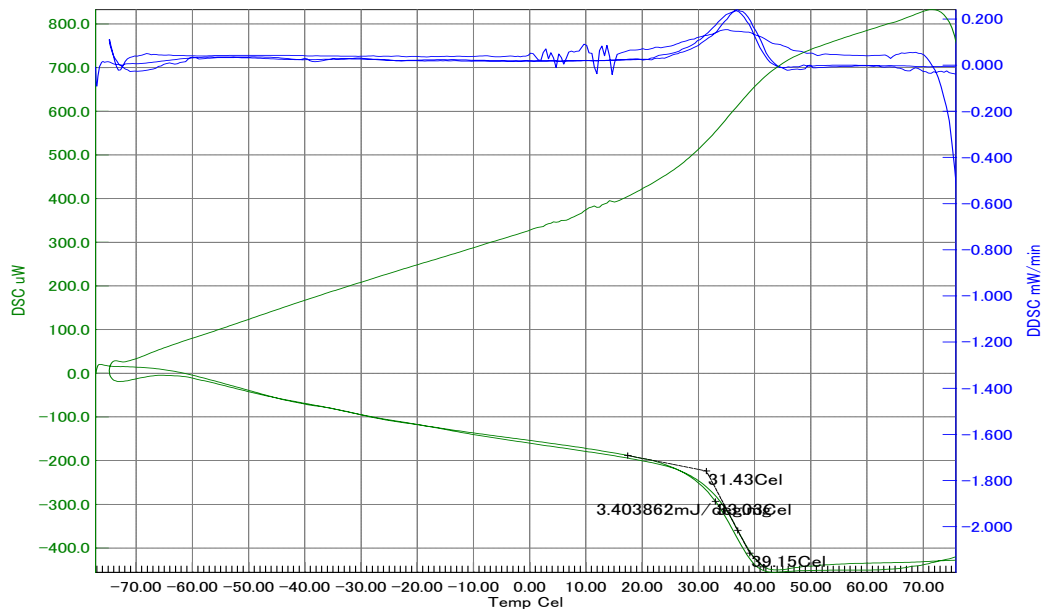


Figure S34. DSC profile of P3.

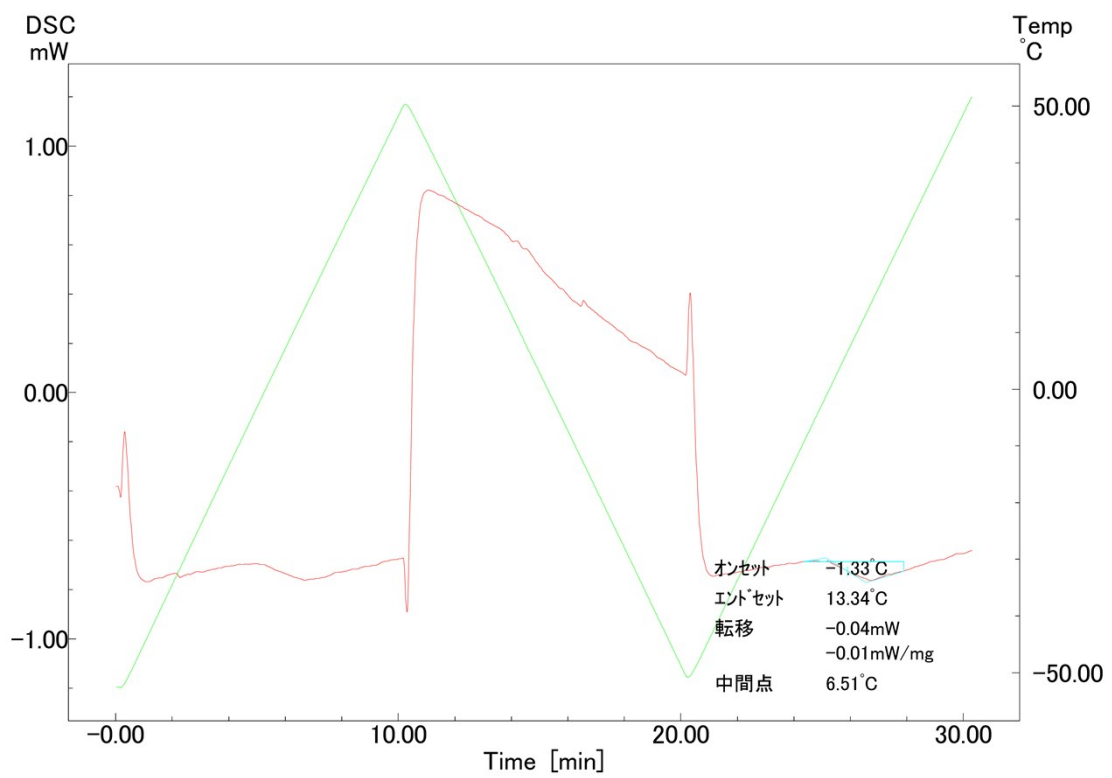


Figure S35. DSC profile of P4.

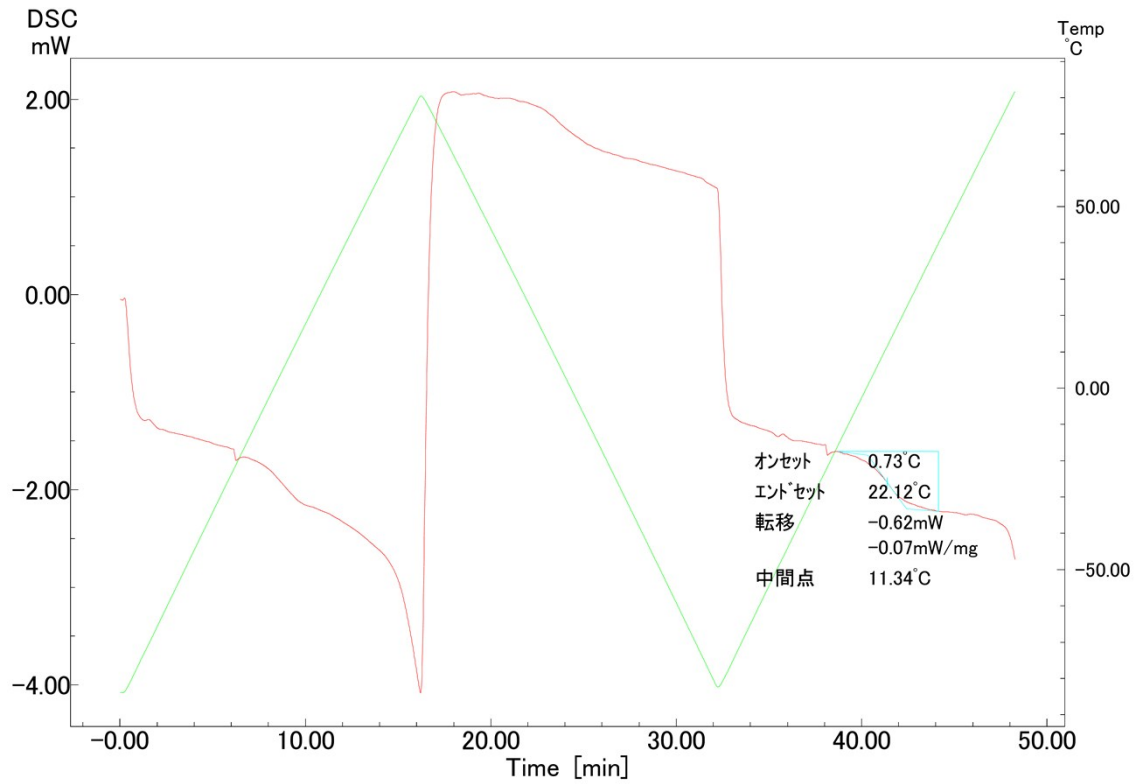


Figure S36. DSC profile of P5.

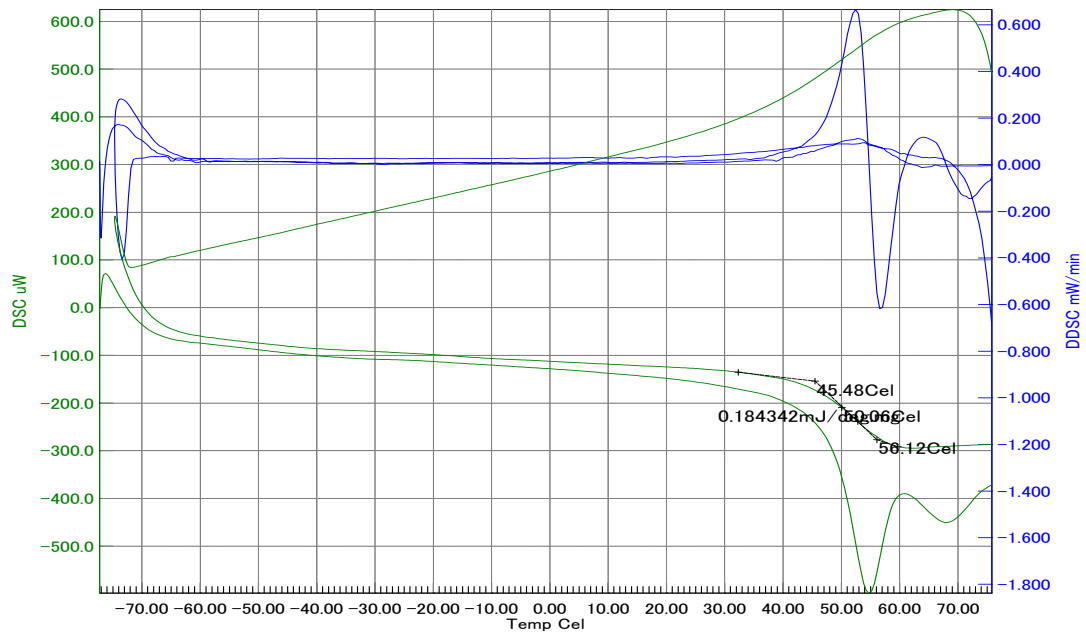


Figure S37. DSC profile of P6.

Comparison of IR spectra of cotton gauze before and after modification.

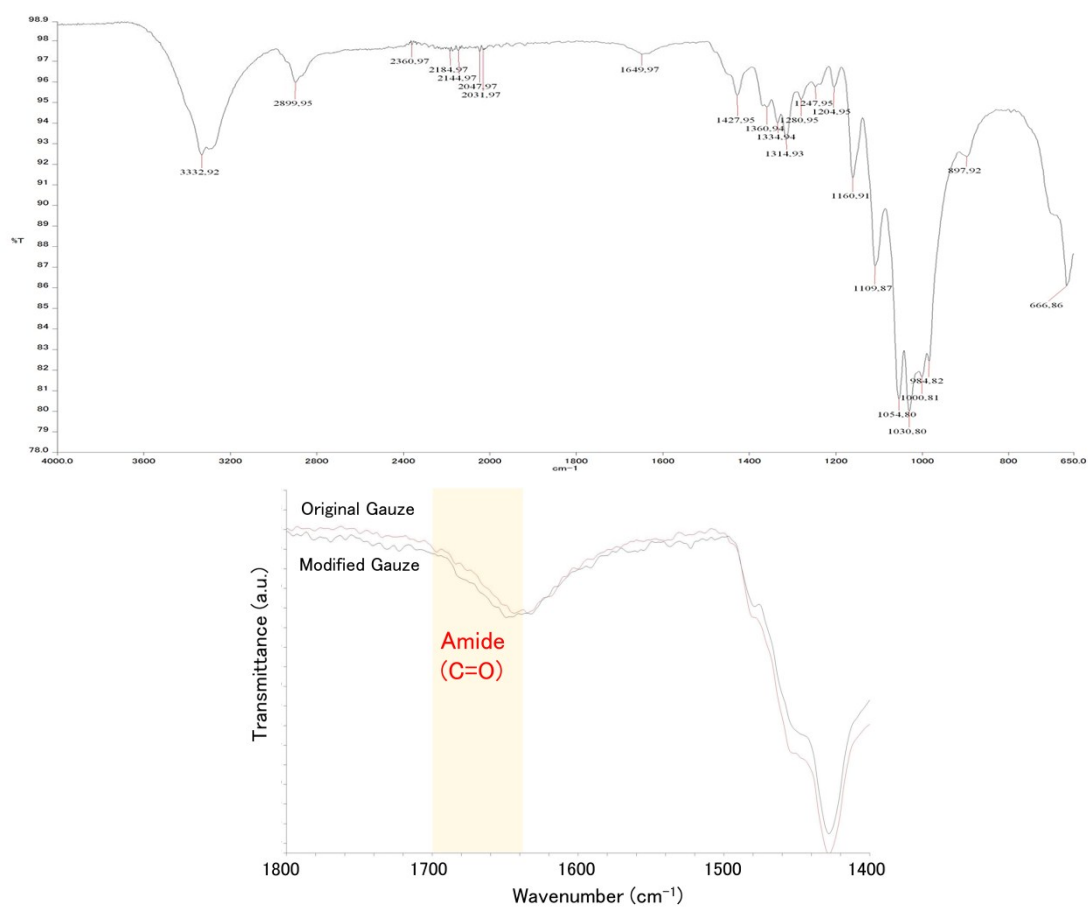


Figure S38. IR spectrum of modified gauze (ATR).

UV spectra of P6

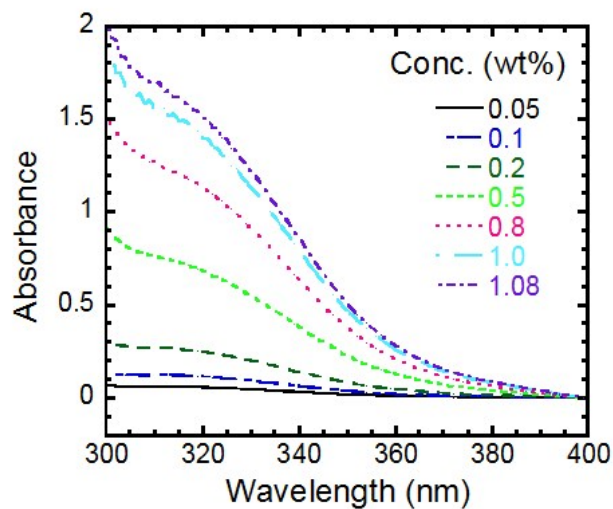


Figure S39. UV spectra of P6 at various concentrations (CHCl₃, room temperatures).

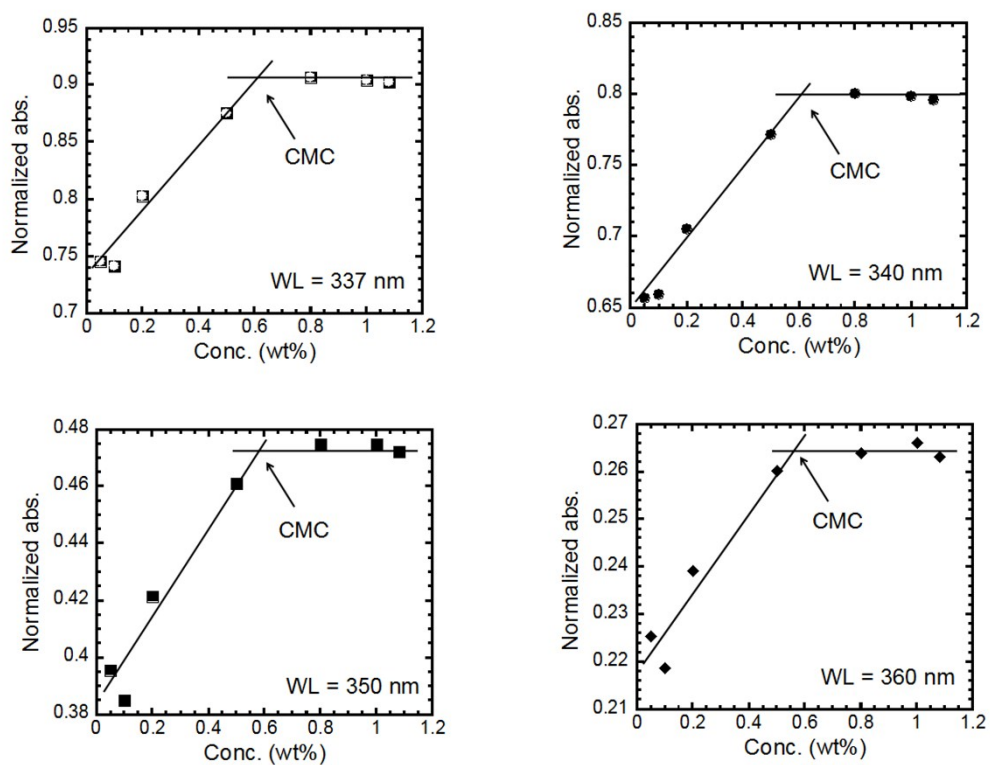


Figure S40. Normalized absorbance of P6 at 337, 340, 350, and 360 nm as a function of concentration (wt%).

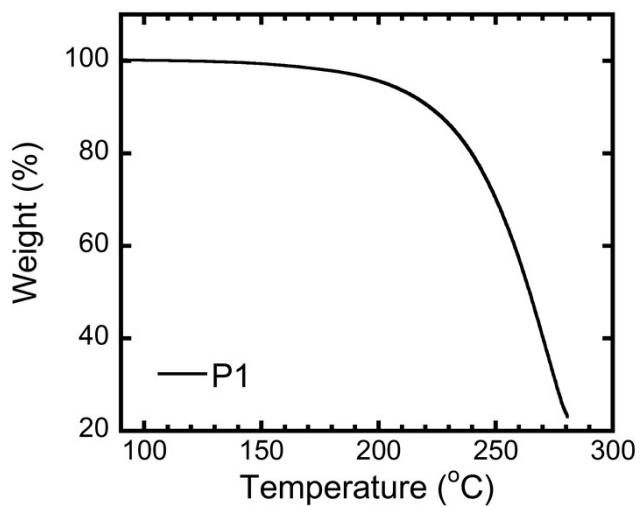


Figure S41. TGA profile of **P1**.

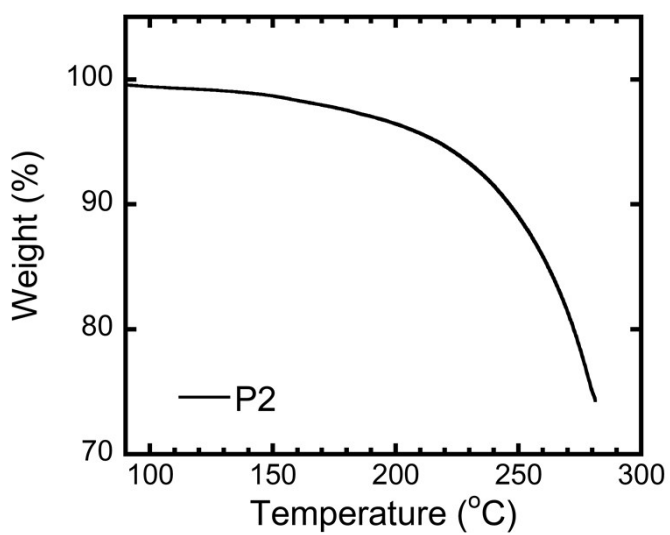


Figure S42. TGA profile of **P2**.

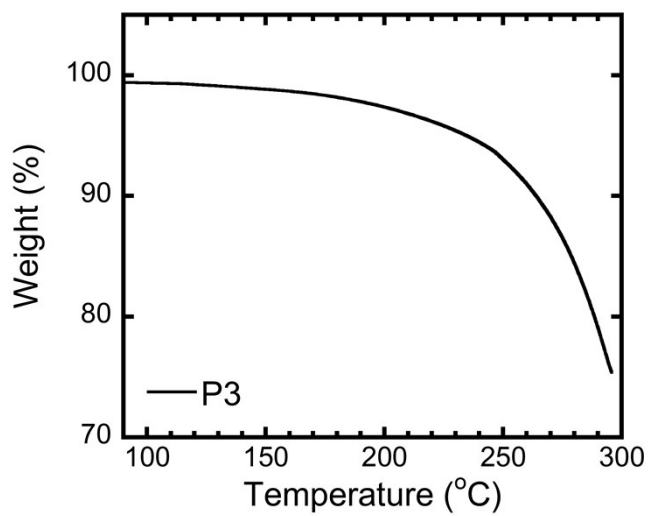


Figure S43. TGA profile of **P3**.

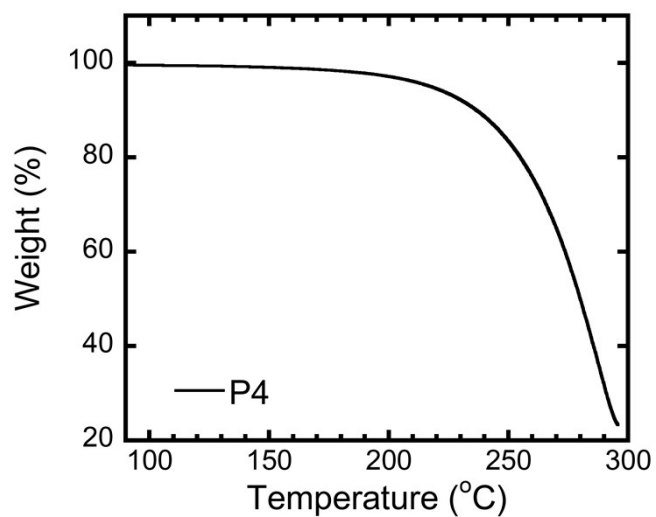


Figure S44. TGA profile of **P4**.

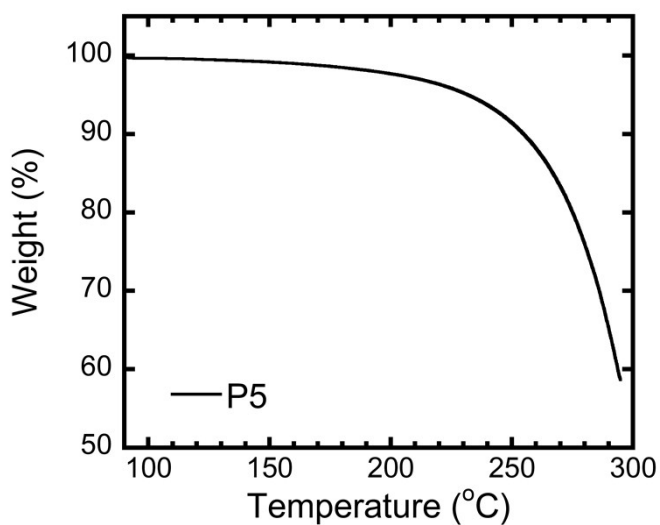


Figure S45. TGA profile of **P5**.

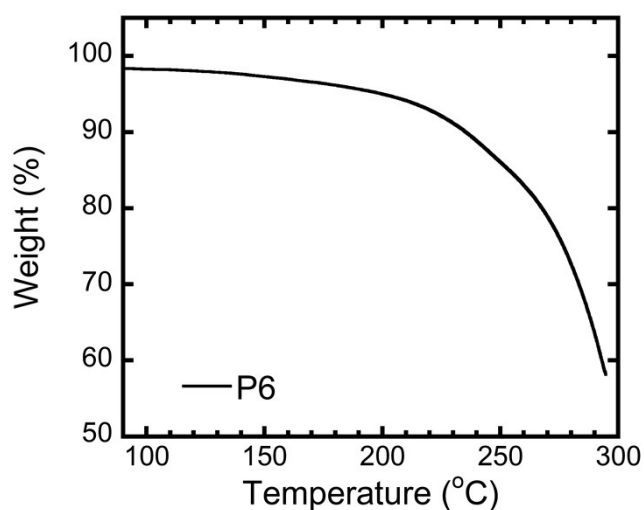


Figure S46. TGA profile of **P6**.

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