Supporting Information for

Supramolecularly cross-linked nanoassemblies of self-immolative polyurethane from recycled plastic waste: high encapsulation stability and triggered release of guest molecules

*Subrata Santra, Soumya Kolay, Sujauddin Sk, Debleena Ghosh, Kishor Sarkar, Anmol Mishra, Lisa Roy and Mijanur Rahaman Molla**

Materials and Methods. All the reagents were purchased from commercial sources and used without further purification unless mentioned. ^{1}HNMR spectra were recorded on a Bruker DPX-300 MHz NMR spectrometer using $CDCl_3$, and DMSO-d_6 as solvent. Chemical shifts (δ) were represented in ppm unit with trimethylsilane (TMS) as the internal standard. The IR and GPC measurements were done using PerkinElmer Spectrum 100 FT-IR spectrometer and Waters GPC equipped with a Waters 515 HPLC pump and a Waters 2414 refractive index (RI) detector using DMF solvent respectively. Molecular weight and PDI were calculated with respect to poly(methyl methacrylate) (PMMA) standards. The column temperature and flow rate were maintained at 35 °C and 1 mL/min, respectively. Mass spectra were recorded using a Qtof Micro YA263 mass spectrometer. The DLS measurements were carried out on a Malvern Nanozetasizer. UV−vis spectra were recorded in a Labtronics spectrometer (Model: LT-291). Photoluminescence spectra were recorded in a Fluoromax-3 spectrophotometer from HORIBA Jobin Yvon. The TEM images were collected using a 200 kV transmission electron microscope (model: JEOL JEM 2100 HR with EELS). Optical fluorescence microscopic images were taken on Olympus Fluorescence Microscope (BX51). ITC experiments were performed using a Microcal-200 ITC ultrasensitive isothermal titration micro-calorimeter

NMR Characterization. ^{1}H NMR spectra were recorded at room temperature on a Bruker DRX-300 (300 MHz). Unless stated otherwise, all spectra were recorded in $CDCl_3$ and DMSO-

d_6 purchased from Sigma-Aldrich. All chemical shifts are given in ppm (δ) units relative to tetramethylsilane (singlet δH = 0.00). Calibration was achieved using the residual solvent signal of chloroform at δH = 7.27. Analysis followed first-order and the following abbreviations were used throughout the text: s = singlet, br. s = broad singlet, d = doublet, t = triplet, q = quartet, quin = quintet,dd = doublet of doublets, dt = doublet of triplets, m = multiplet.

FT-IR Characterization. The sample was mixed with KBr and then a pellet was prepared and placed in the chamber inside the instruments, and the spectrum was recorded at room temperature.

Electrospray Ionization Mass Spectrometery Characterization. The samples were dissolved in appropriate solvents and then injected in the column for recording mass spectra at room temperature.

Gel Permeable Chromatography. A measured quantity (3 mg) of polymer sample was dissolved in 1 mL of DMF and sonicated for 3 min. Then the solution was kept at room temperature for a few hours to obtain a homogeneous solution. The polymer solution was then filtered using a membrane filter with 0.22 μm pore size. Next, the solution was injected into the GPC column to obtain the molecular weight of the polymer.

Fluorescence Microscopy Studies. In a typical fluorescence microscopic experiment, 50 μl of dye encapsulated polymer solution was placed on a cleaned cover glass, and then another cover glass was placed on it. Finally, images were taken on a fluorescence microscope (OLIMPUS BX-51) in 40 x magnification.

Isothermal Titration Calorimetric (ITC) Experiments. In a typical ITC experiment, the reference cell was filled with deionized water and the sample cell was filled with the aqueous solution of the compound (50 μM, 1 μL injection volume, and number of injections 40). The

sample was injected with a gap of 120 s between each addition with continuous stirring at 400 rpm. The data were analyzed by MicroCal Origin software package (ver. 7.0). Experimental temperature = 25^{o}C.

Determination of Critical Aggregation Concentration (CAC). At first, a measured amount of a solution of DiI dye in acetone (20 μL, 1 mM) was placed in various screw-capped vials. Solutions of various concentrations of **P1-Ar** polymer were added to vials that contained DiI, and the mixture was sonicated and allowed to stand for 6 h before spectroscopic analysis. The final concentration of DiI was maintained at 2×10^{-6} M. The absorption intensity of the encapsulated DiI at 580 nm was plotted against the concentration of **P1-Ar** solution, and the inflection point of such a plot was taken as the CAC of **P1-Ar**.

Transmission Electron Microscopy (TEM). A solution of the polymer samples (20 μL, 0.01 mM) was placed on a TEM grid (300-mesh carbon-coated Cu grid). The samples were allowed to dry in air at room temperature for a few hours before the measurements were recorded.

Dynamic Light Scattering (DLS). For the DLS measurements, 0.01 mM polymer samples were used. The measurements were carried out at room temperature.

Zeta-Potential Measurement. Here, a 0.01 mM polymer solution was used and the solution pH was maintained using phosphate buffer. The measurements were done at pH 7.4 and 6.6.

DiI Dye Release Study. Ten microliters of DiI stock solution (10^{-3} M) in acetone was transferred to a vial and to this a solution of **P1-Ar** (2 mL, 0.01 mM) was added, stirred for 4h at room temperature to evaporate the acetone and obtain a homogeneous solution. The solution was filtered using a membrane filter of 0.22 μm pore size to remove unencapsulated DiI. Next, this dye-encapsulated solution was used for absorption measurement to check the extent of dye encapsulation. After confirmation of DiI encapsulation, redox-responsive guest release was

tested. For release study, GSH was added to the solution and the concentration was maintained at 10 mM. Then time dependent UV−vis spectra were recorded to examine the DiI release.

The percentage of dye release was calculated from the change in absorption intensity of DiI at 520 nm by using the equation

% of DiI release = $\{(A - A0)/A0\} \times 100$ where A0 is the initial absorption intensity (before the addition of GSH) and A is the absorption intensity at different time intervals after the addition of GSH.

Calculation of dye loading capacity (DLC) and dye loading efficiency (DLE): The dye loading efficiency (DLE) and dye loading capacity (DLC) were calculated by absorption spectroscopy using the following equations:

DLE (%) = [weight of dye in micelles/weight of dye in feed] ×100%

DLC (%) = [weight of dye in micelles/weight of dye loaded vesicles] × 100%

Synthesis of monomers: The monomer **M1, M3** and **M5** were commercially available. Monomer **M2** and **M4** were synthesized in the laboratory. The procedure for **M2** is reported elsewhere[1] and **M4** is described below.

Compound M4 (**BHET**): BHET was synthesized by depolymerization of PET as reported earlier with minor modifications [2]. Briefly, 100 g of washed PET flakes with 5 × 5 $mm2$ dimension, 333 g of ethylene glycol and 1.0 g of zinc acetate as a catalyst were mixed in a three necked 1L round bottom flask equipped with a magnetic stirrer, a reflux condenser and a thermometer was put on an oil bath. After degassing of the flask with nitrogen gas for 30 min, the reaction was carried out under nitrogen atmosphere at 198 °C for 8 h with constant stirring. The reaction was stopped and the crude product was collected by addition of 1 lit of distilled water followed by filtering with Buchner funnel. The solid cake was re-suspended in 1 lit of

distilled water and boiled for 30 min to dissolve the BHET. After filtering the solution in hot condition, the supernatant was cooled down to room temperature followed and kept the solution at 4 °C overnight. The purified BHET crystals were obtained after the filtration of chilled solution followed by drying the BHET crystals at 60 °C for 24 h.

^{1}H-NMR (300 MHz, $CDCl_3$, TMS): δ (ppm) = 8.12 (s, 4H), 4.96 (t, 2H), 4.32 (t, 4H), 3.73 (q, 4H).

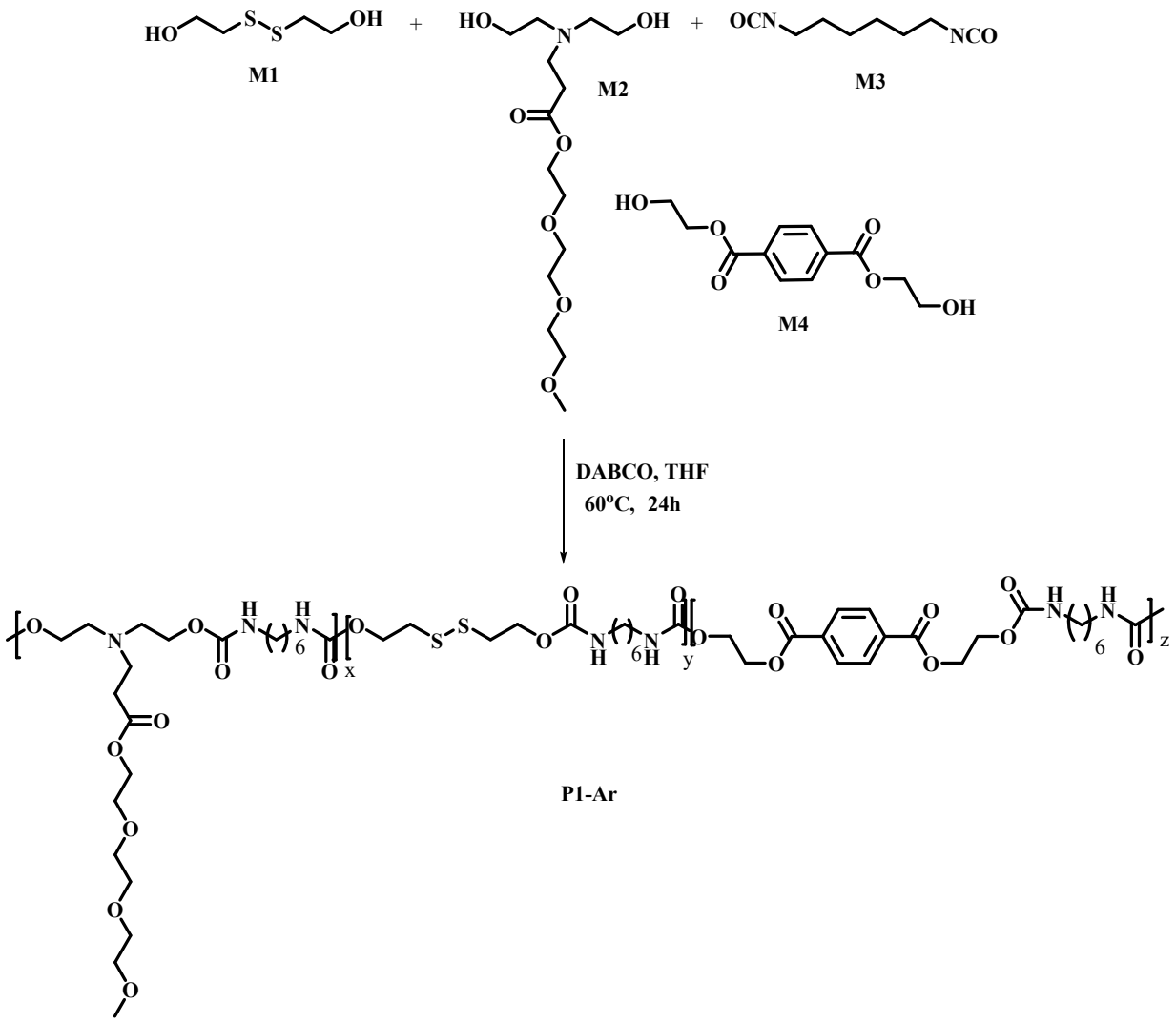
^{13}C-NMR: 165.55, 134, 129.8, 67.31, 59.27.

Synthesis of Polymer: Synthesis of polymer **P1** is described in the literature.[1] Synthesis of **P1-Ar** and **P2-Ar** explained below.

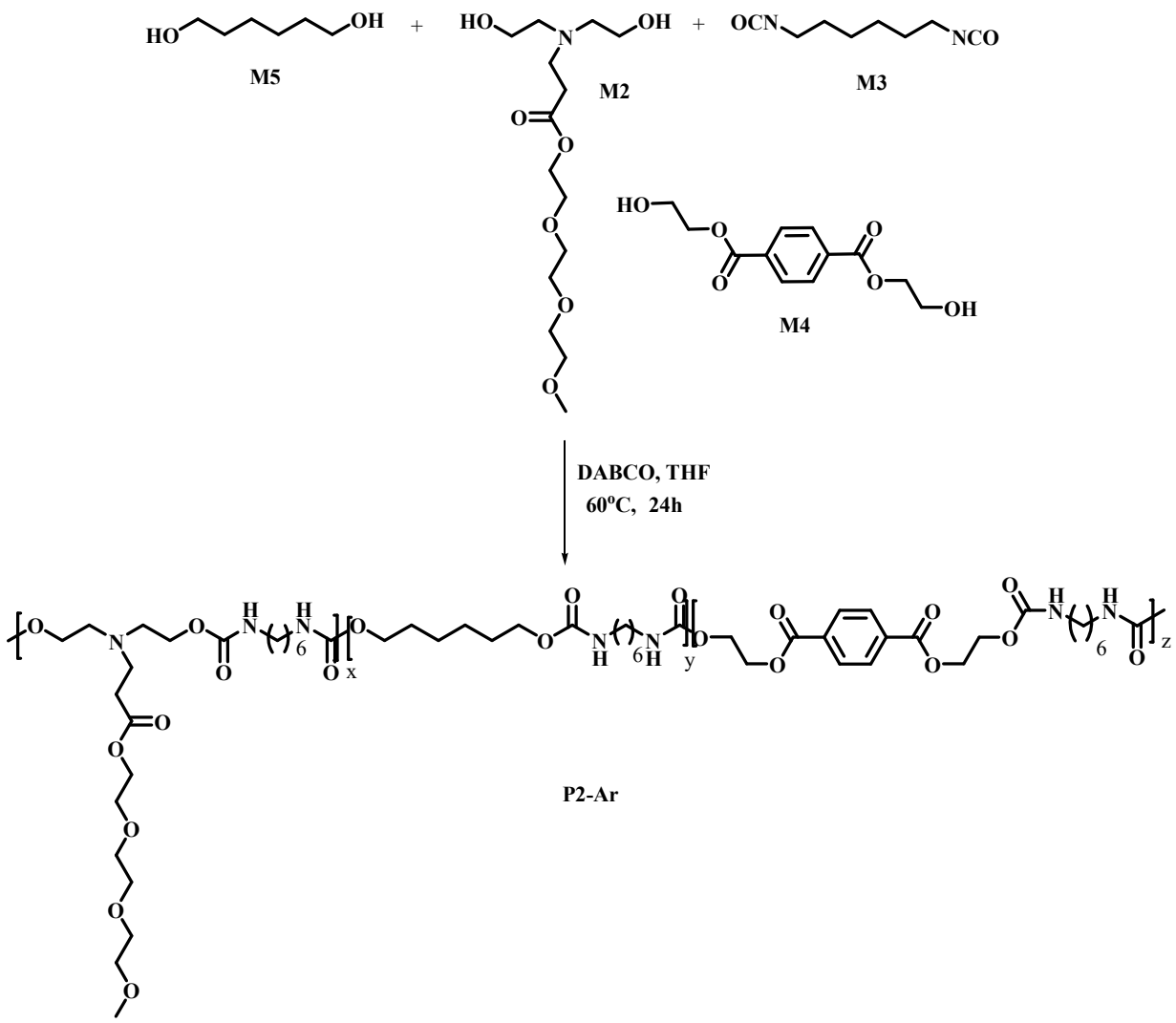
Synthesis of P1-Ar: Diethanol amine based monomer (2) (73 mg, 0.225 mmol), hexamethylene diisocyanate (3) (183 mg, 1.09 mmol), hydroxyethyl disulfide (1) (115 mg, 0.685 mmol), bis (2-hydroxyethyl) terephthalate (BHET) (57.5 mg, 0.225 mmol) and 1.0 ml of freshly dried tetrahydrofuran (THF) were placed in a reaction vial under a continuous flow of argon. To this mixture catalytic amount DABCO (4.0 mg, 4×10^{-5} mol) in 1.0 mL of dried THF was added, and the reaction mixture was stirred for 24 h at 60 °C. Heating was stopped, the reaction mixture was allowed to cool at room temperature, and then the polymer was precipitated out in excess of diethyl ether. It was washed and dried under vacuum to isolate the polymer as a white solid in 75% yield. Mn = 7715 g/mol (PDI = 1.49) from GPC. ^{1}H NMR (300 MHz, DMSO-d6, TMS): δ (ppm) = 1.21 (4H, broad peak), 1.35 (8H, broad peak), 2.40 (2H, broad peak), 2.64 (4H, broad peak), 2.80 (8H, broad peak), 3.30 (3H, S), 3.40-3.75 (10H, m), 4.20 (2H, t), 4.30 (4H, broad peak), 4.50 (4H, t), 7.10-7.40 (3H, multiple broad peak for -NH), 8.10 (4H, s). FT-IR (wavenumber/cm^{-1}: 3320 (N−H), 2931 (CH alkyl), 1726 (ester carbonyl), 1688 (Carbonyl of urethane), 1535 (-NH of urethane), 1260 (C-N).

Synthesis of P2-Ar: Diethanol amine based monomer (2) (73 mg, 0.225 mmol), hexamethylene diisocyanate (3) (115 mg, 0.685 mmol), 1,6 hexane diol (35 mg, 0.225 mmol), bis (2-hydroxyethyl) terephthalate (BHET) (57.5 mg, 0.225 mmol) and 1.0 mL of freshly dried tetrahydrofuran (THF) were placed in a reaction vial under a continuous flow of argon. To this mixture catalytic amount DABCO (4.0 mg, 4×10^{-5} mol) in 1.0 mL of dried THF was added, and the reaction mixture was stirred for 24 h at 60 °C. Heating was stopped, the reaction mixture was allowed to cool at room temperature, and then the polymer was precipitated out in excess of diethyl ether. It was washed and dried under vacuum to isolate the polymer as a white solid in 80% yield. Mn = 6451 g/mol (PDI = 1.54) from GPC. ^{1}H NMR (300 MHz, DMSO-d6, TMS): δ (ppm) = 1.10 (4H, broad peak), 1.41 (12H, broad peak), 1.50 (4H, broad peak) 2.40 (2H, broad peak), 2.64 (4H, broad peak), 2.80 (8H, broad peak), 3.30 (3H, S), 3.40-3.75 (10H, m), 4.10 (4H, t), 4.20 (2H, t), 4.40 (4H, broad peak), 4.50 (4H, t), 7.0-7.30 (2H, multiple broad peak for -NH), 8.10 (4H, s). FT-IR (wavenumber/cm^{-1}: 3322 (N−H), 2933 (CH alkyl), 1720 (ester carbonyl), 1685 (Carbonyl of urethane), 1534 (-NH of urethane), 1262 (C-N).

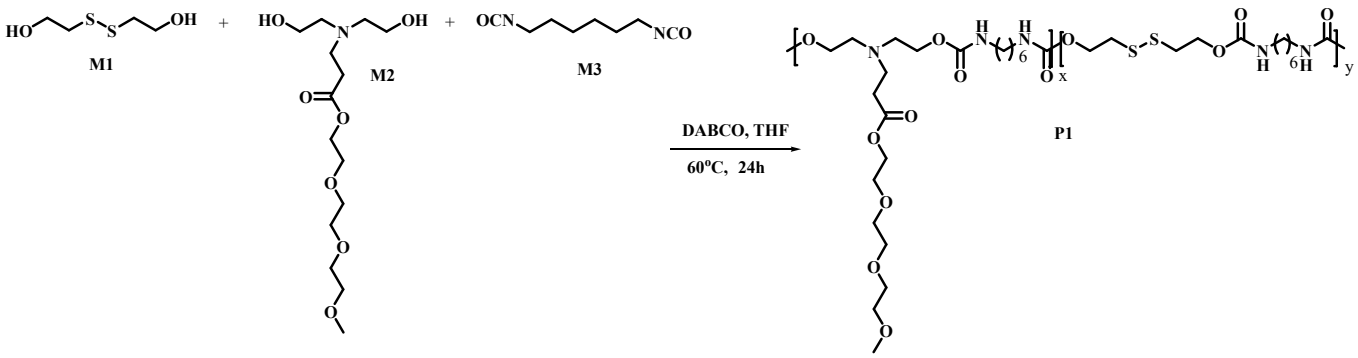
Synthesis of polymer **P1-Ar, P2-Ar** and **P1** are schematically presented below:



Scheme S1: Synthetic scheme of Polymer **P1-Ar**



Scheme S2: Synthetic scheme of Polymer **P2-Ar**



Scheme S3: Synthetic Scheme of Polymer **P1**

Additional Figures:

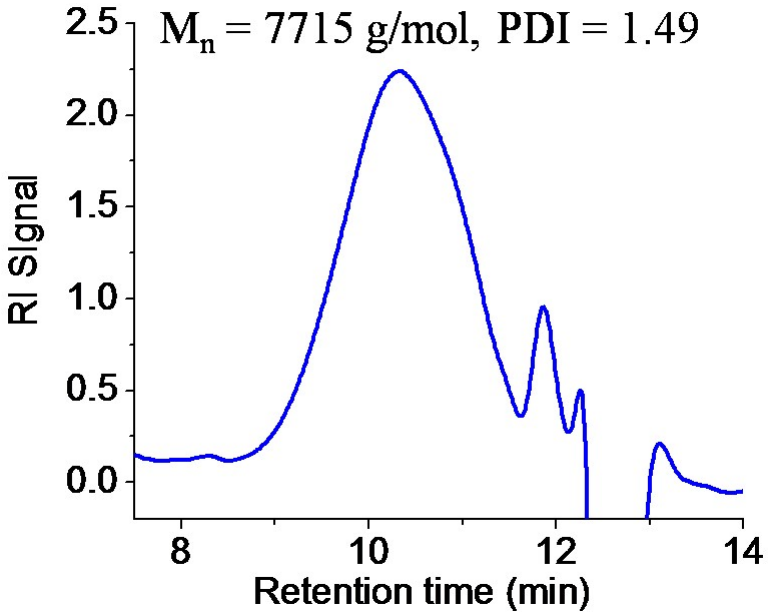


Figure S1: GPC chromatogram of polymer **P1-Ar.** Solvent = DMF; M_n = 7715 g/mol, PDI = 1.49.

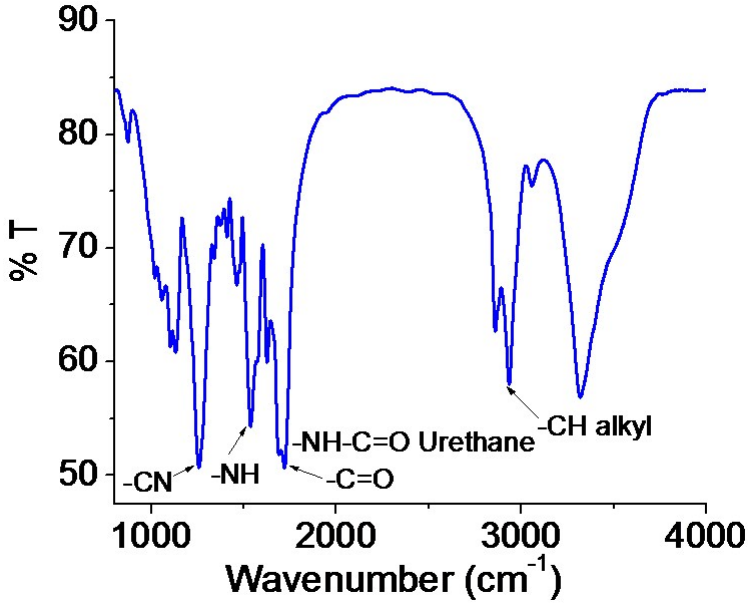


Figure S2: FTIR spectrum of polymer **P1-Ar**

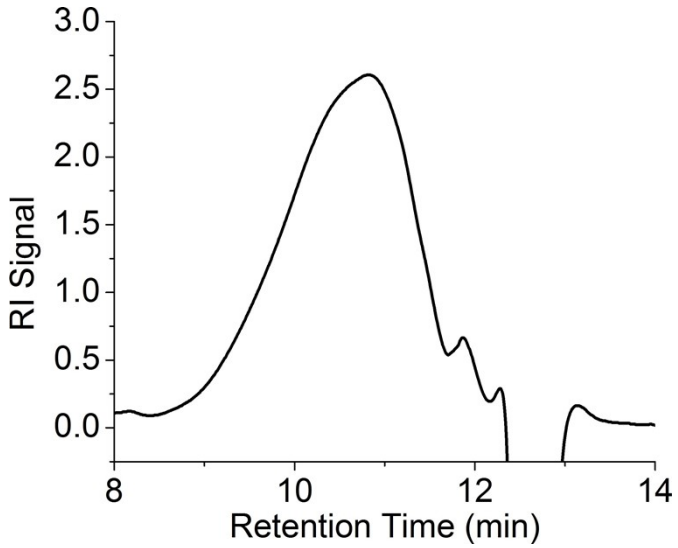


Figure S3: GPC chromatogram of control polymer **P2-Ar.** Solvent = DMF; M_n = 6451 g/mol, PDI = 1.52.

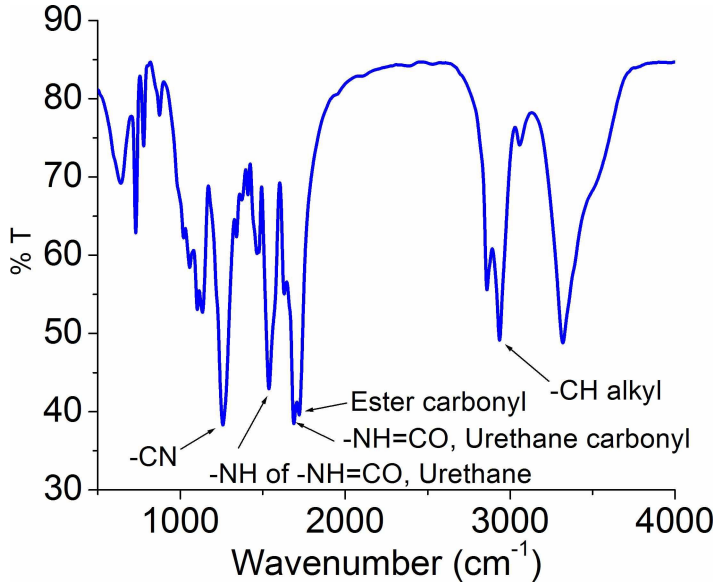


Figure S4: FTIR spectrum of control polymer **P2-Ar**

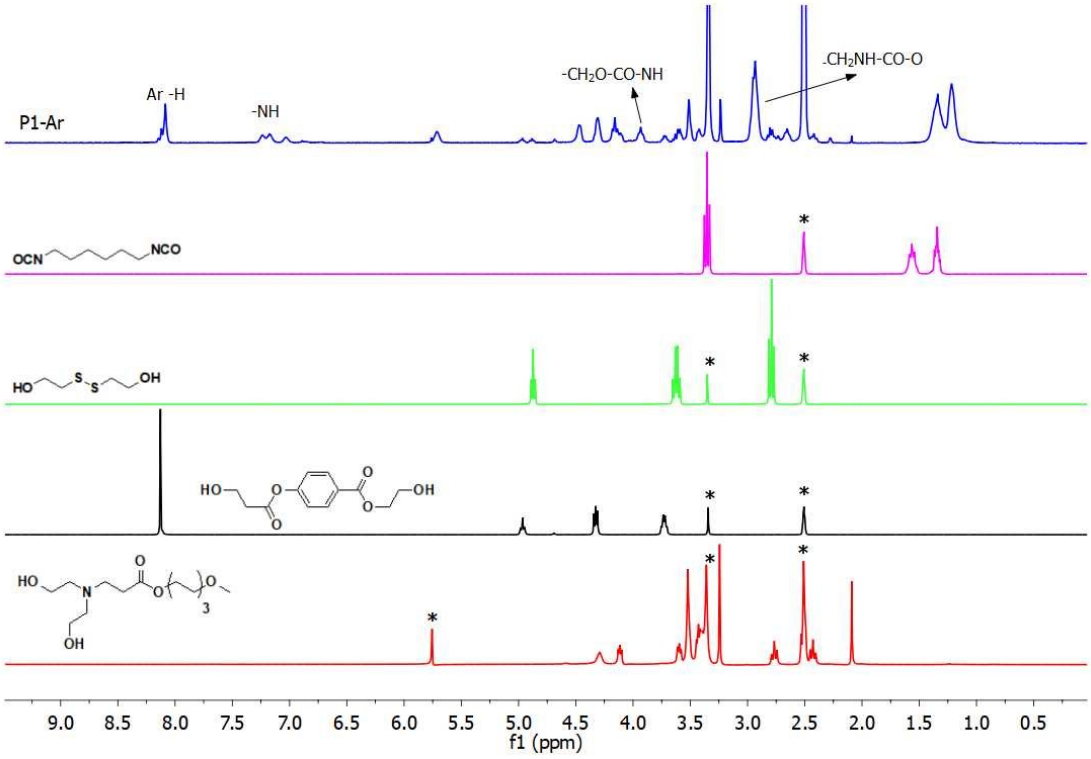
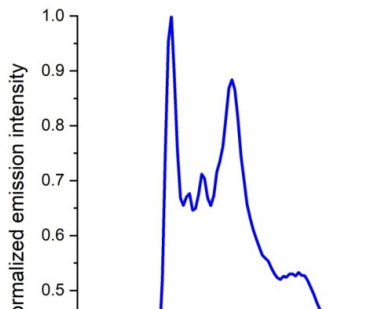


Figure S5. ^{1}H-NMR stack plot of monomers and polymer **P1-Ar**. Three new peaks for –NH as pointed out in polymer spectrum, indicate formation of polymer from monomers. Solvents: DMSO-d_6. Asterisk indicates peaks from solvents.



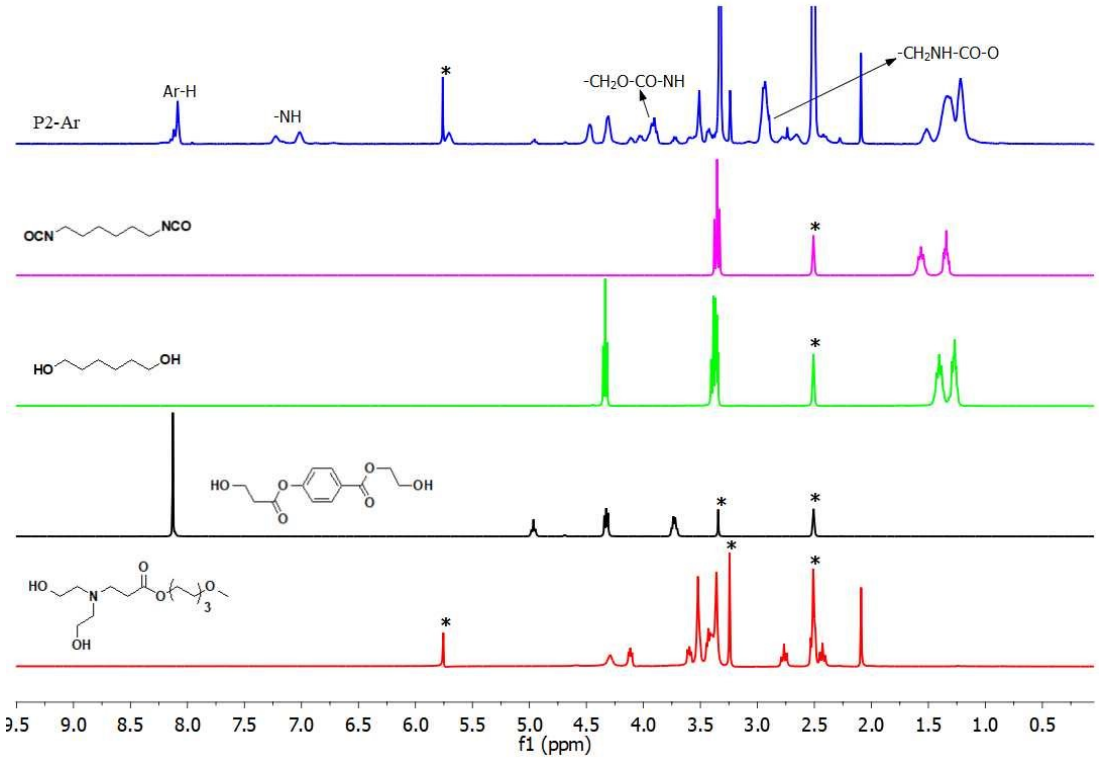


Figure S6. ^{1}H-NMR stack plot of monomers and polymer **P2-Ar**. Asterisk indicates peaks from solvents. Two new peaks for –NH as pointed out in polymer spectrum, indicate formation of polymer from monomers. Solvents: DMSO-d_6.

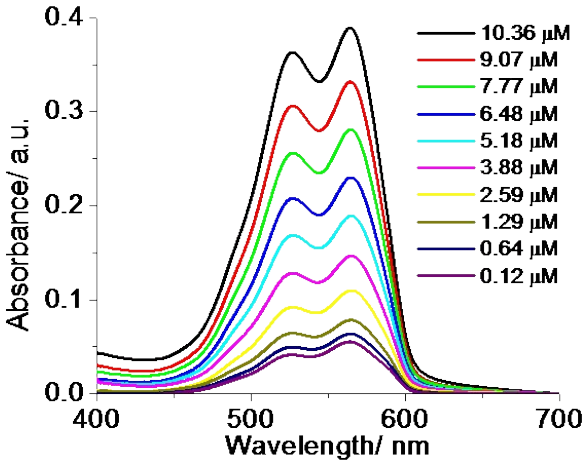


Figure S8: UV-Vis spectra of CMC determination of **P1-Ar** by using DiI as a hydrophobic guest molecule. The concentration of DiI = 10^{-5} M. Temperature = 25°C.

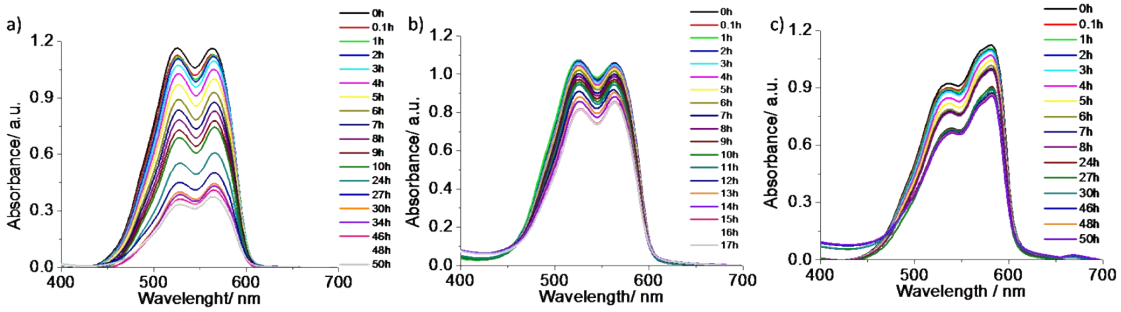


Figure S9. Guest release profile of polymer **P1-Ar** based nanoassemblies a) in presence of GSH (10 mM concentration), b) in absence of GSH; (c) Control polymer **P2-Ar** based nanoassemblies in presence of GSH (10 mM concentration). Temperature = 25°C

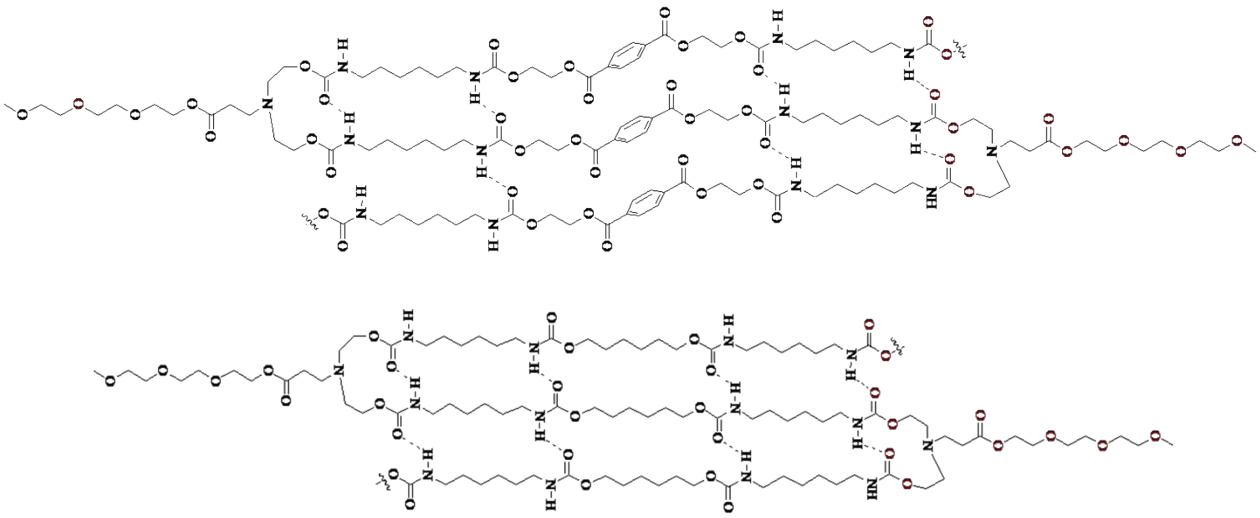


Figure S10: Segmental representation of polymer chain structure which shows core structure of the nanoassembly of Top: **P1-Ar** and Bottom: control polymer **P1**

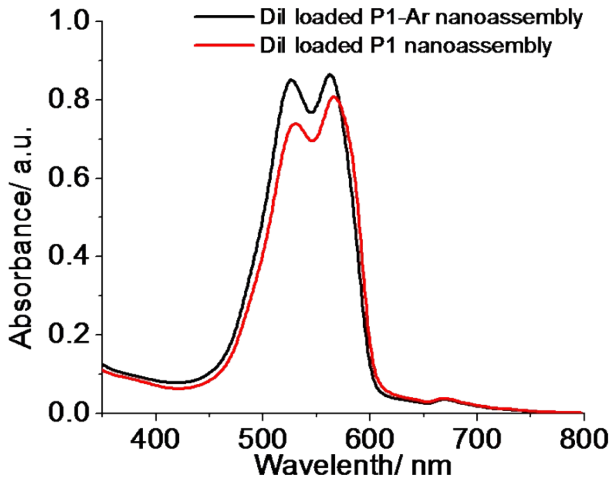


Figure S11: Determination of encapsulation efficiency and encapsulation capacity of **P1-Ar** and **P1** nanoassembly. DiI dye was used as a guest molecule.

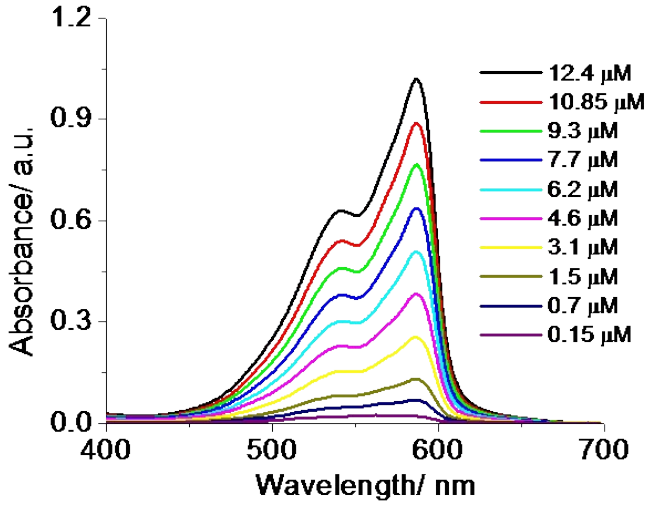


Figure S12: UV-Vis spectra of CMC determination of control polymer **P2-Ar** by using DiI as a hydrophobic guest molecule. The concentration of DiI = 10^{-5} M. Temperature = 25°C.

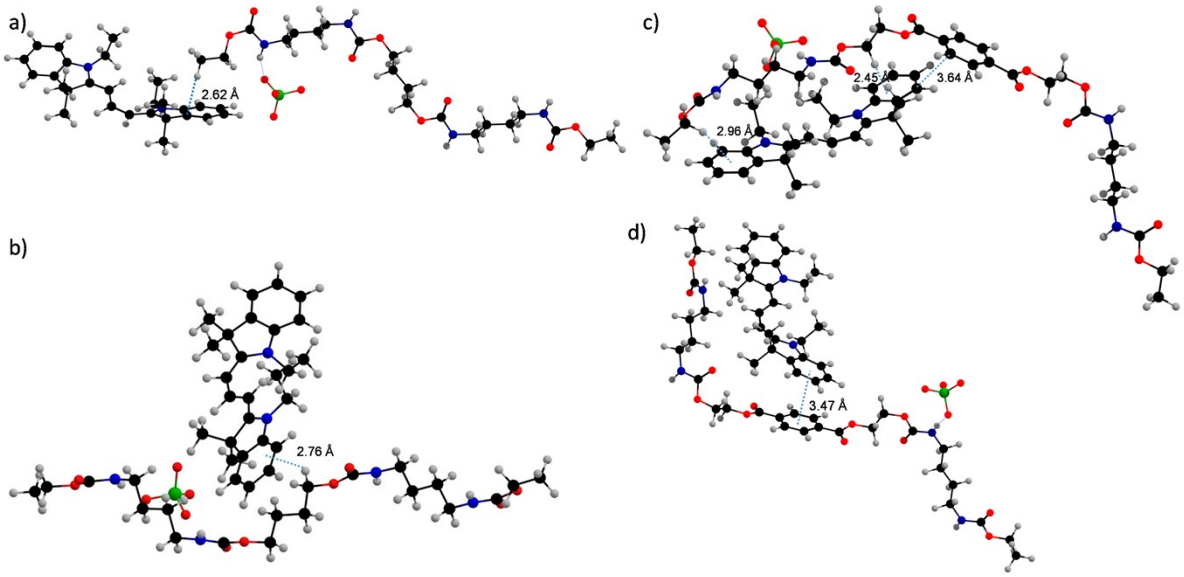


Figure S13: Interaction of DiI with the **P1** and **P1-Ar** nanoassembly by DFT calculation; a) **P1**-DiI_a (CH-π, peripheral), b) **P1**-DiI (CH-π, central), c) **P1-Ar**-DiI_a (CH-π, peripheral), d) **P1-Ar**-DiI (CH-π, central).

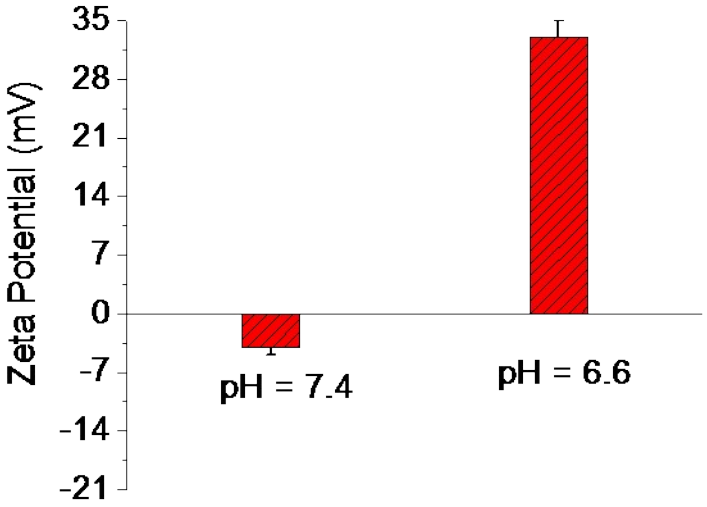


Figure S14: Zeta potential of **P1-Ar** nanoassemblies at tumor relevant pH and neutral pH

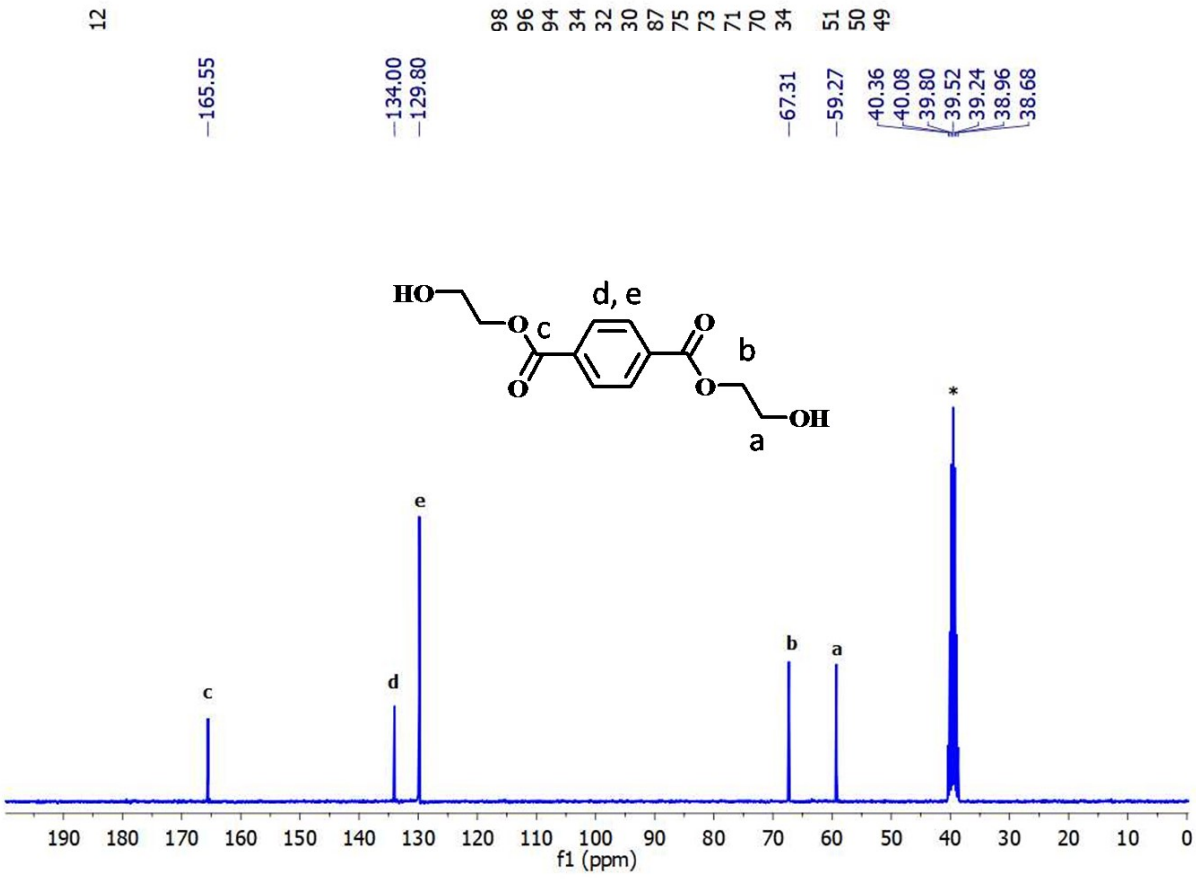


Figure S16: ^{13}C-NMR of BHET monomer. * indicates solvent peak. Solvent = DMSO-d_6.

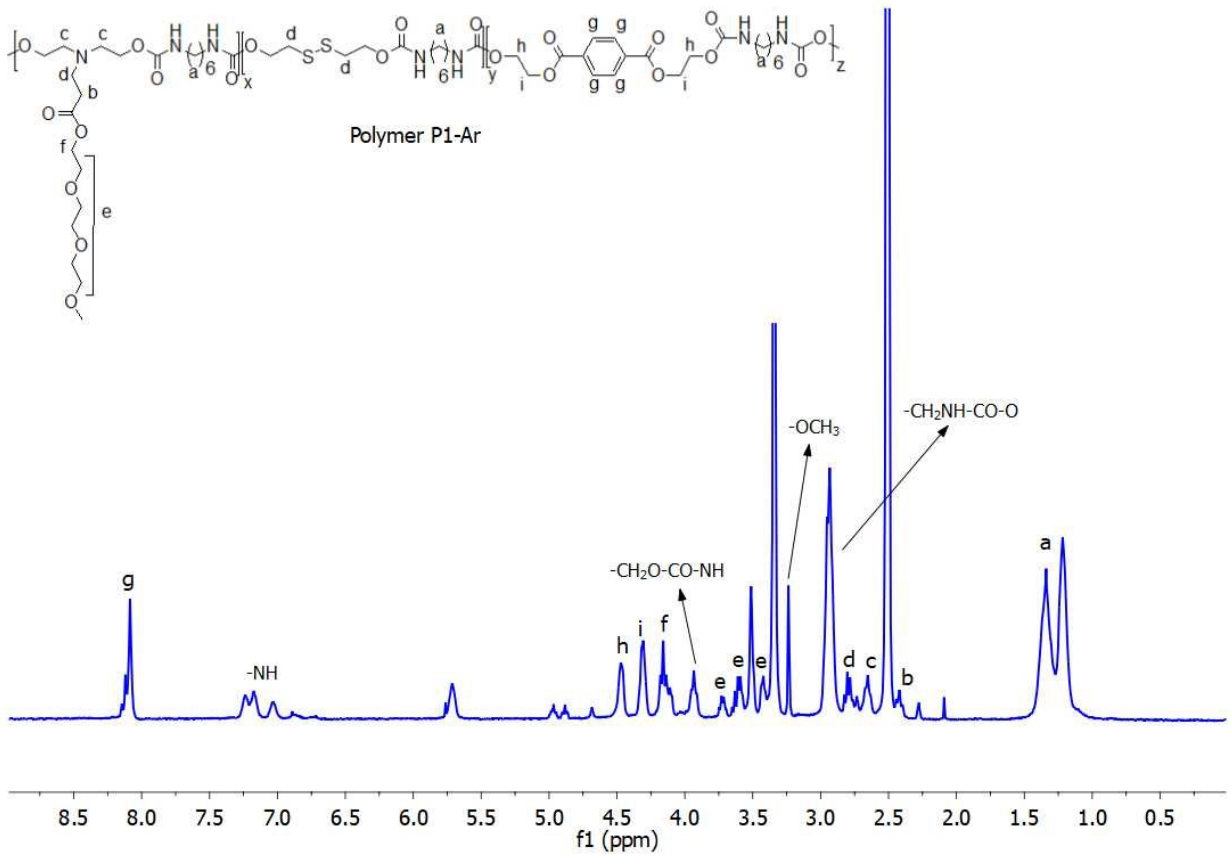


Figure S17: ^{1}H-NMR of **P1-Ar** polymer. * indicates solvent peak. Solvent = DMSO-d_6.

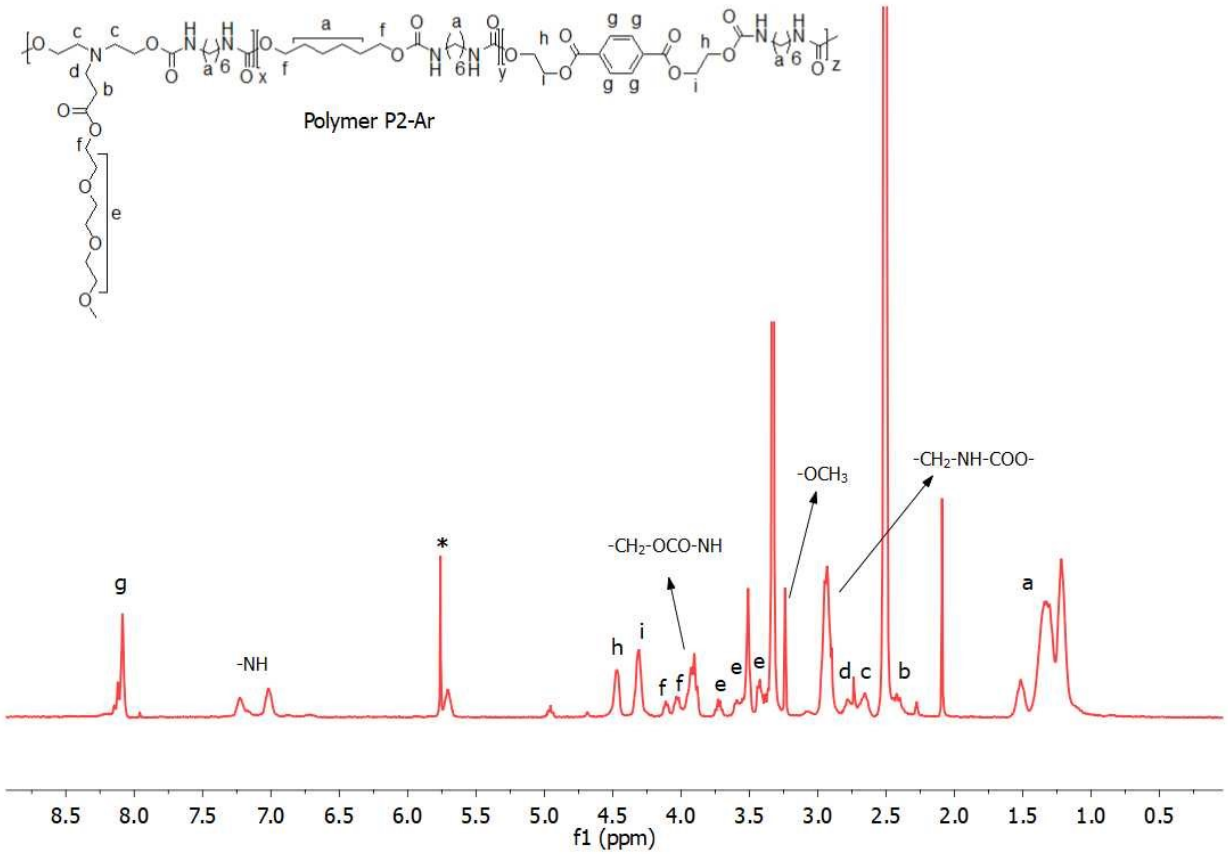


Figure S18: ^{1}H-NMR of polymer **P2-Ar**. * indicates solvent peak. Solvent = DMSO-d_6.

Computational Details

All the computational calculations were done using ORCA 4.2.1 software.[3] To reduce the cost of computation, the alkyl chain in the monomers were replaced by $(CH_2)_4$ units. The monomer was truncated by removing the tertiary amine from the actual position and retaining the carbon atoms, thus, making it an ethyl group. The long alkyl chains attached to the nitrogen of the DiI molecule were replaced by ethyl fragment. To neutralize the positive charge on the DiI molecule, perchlorate (ClO^{4-}) was used as a counter ion. Geometry optimizations were done using the generalized gradient approximated BP86 functional together with Pople's 6-31G(d) basis set.[4] Dispersion correction was accounted through the Becke-Johnson D3BJ damping.[5] The following thresholds were used for optimizations: energy change tolerance of 3×10^{-5} a.u., root mean square gradient of 5×10^{-4} a.u., maximum gradient of 2×10^{-3} a.u., root mean square displacement of 7×10^{-3} a.u., maximum displacement of 1×10^{-2} a.u. The self-consistent field (SCF) was set to a TightSCF convergence criteria with energy change tolerance = 1×10^{-8} a.u. The DFT integration grid was always set to Grid6. To further refine the calculated energies,

single-point energies were calculated using Head Gordon's ωb97x-D3BJ and M06-2X functionals in conjugation with def2-SVP basis set on all the atoms.[6-7] Solvent effect was introduced through the Conductor-like Polarizable Continuum model (CPCM) implicit solvent model[8] using the dielectric parameters of water (ε=80.4, η=1.33).

XYZ Coordinates of optimized geometries

P1

6	-11.184475000	-9.218772000	7.543504000
1	-10.461698000	-9.999355000	7.842360000
1	-11.230339000	-8.477136000	8.362671000
6	-12.570569000	-9.843168000	7.316170000
1	-12.517957000	-10.604354000	6.515707000
1	-13.286731000	-9.067719000	6.988967000
6	-10.673649000	-8.532335000	6.277954000
1	-10.579818000	-9.251095000	5.447516000
1	-11.339337000	-7.708969000	5.974377000
8	-9.387334000	-7.895067000	6.500641000
6	-8.300506000	-8.729559000	6.393493000
8	-8.361847000	-9.923234000	6.072932000
7	-7.151887000	-8.039841000	6.647708000
1	-7.244890000	-7.104623000	7.043414000
6	-13.103922000	-10.495272000	8.590665000
1	-12.434709000	-11.296610000	8.941715000
1	-13.232961000	-9.749716000	9.392212000
8	-14.373316000	-11.161504000	8.353321000
6	-15.475183000	-10.341555000	8.390359000
8	-15.441580000	-9.133401000	8.654600000
7	-16.606060000	-11.064601000	8.140146000
1	-16.477177000	-12.009652000	7.778089000
6	-17.876502000	-10.392244000	7.872704000
1	-17.951963000	-9.544242000	8.573099000
1	-18.688662000	-11.099642000	8.111880000
6	-18.003960000	-9.894034000	6.423882000
1	-17.896865000	-10.752845000	5.733699000
1	-17.163937000	-9.204965000	6.214313000
6	-5.875474000	-8.736418000	6.794474000
1	-5.821668000	-9.502309000	6.002696000
1	-5.073337000	-8.002904000	6.606590000
6	-5.692847000	-9.391862000	8.173240000
1	-5.760371000	-8.613801000	8.957611000
1	-6.529882000	-10.095204000	8.341801000
6	-4.353759000	-10.133474000	8.283865000
1	-4.292713000	-10.918299000	7.505602000
1	-3.516274000	-9.433409000	8.103280000
6	-19.340304000	-9.182812000	6.171001000
1	-20.182256000	-9.867371000	6.383580000
1	-19.442582000	-8.318066000	6.854171000
6	-4.162510000	-10.777408000	9.666815000
1	-4.980211000	-11.487145000	9.878678000
1	-4.180128000	-10.001648000	10.450277000
6	-19.461953000	-8.696241000	4.718464000
1	-18.644458000	-7.996570000	4.475823000
1	-19.392005000	-9.550715000	4.025166000
1	-2.828135000	-12.422031000	9.360740000
7	-2.901246000	-11.504451000	9.800747000
6	-1.731371000	-10.834332000	10.025271000
8	-1.639055000	-9.647473000	10.364229000
8	-0.662858000	-11.675451000	9.861692000
6	0.635239000	-11.071941000	10.122918000
1	0.762631000	-10.197039000	9.462705000
1	0.662583000	-10.718760000	11.168152000
6	1.686359000	-12.137601000	9.859091000
1	1.645225000	-12.482000000	8.811979000
1	1.543293000	-13.006924000	10.522832000
1	2.689147000	-11.718441000	10.047661000
7	-20.720962000	-8.001872000	4.440786000
1	-20.769249000	-7.016118000	4.692724000
6	-21.873302000	-8.711132000	4.256587000
8	-21.924700000	-9.943683000	4.155868000
8	-23.039060000	-8.000754000	4.136787000
6	-23.019489000	-6.545486000	4.180948000
1	-22.651361000	-6.214438000	5.169877000
1	-22.335957000	-6.168091000	3.398857000
6	-24.442952000	-6.067280000	3.944808000
1	-24.469635000	-4.965138000	3.974064000
1	-25.120118000	-6.453665000	4.724543000
1	-24.808528000	-6.399757000	2.959111000

$P1_{dim}$

6	-1.935543000	0.915402000	0.469125000
1	-1.301939000	0.018333000	0.343361000
1	-1.534205000	1.489704000	1.324615000
6	-3.388230000	0.491936000	0.736420000

1	-3.726940000	-0.178490000	-0.073535000
1	-4.046229000	1.378992000	0.732744000
6	-1.861333000	1.774290000	-0.790656000
1	-2.233805000	1.224974000	-1.669643000
1	-2.433513000	2.706993000	-0.668819000
8	-0.497732000	2.209172000	-1.049820000
6	0.223874000	1.419152000	-1.893854000
8	-0.222767000	0.405012000	-2.465372000
7	1.482968000	1.889743000	-2.074232000
6	-3.538258000	-0.219704000	2.079538000
1	-2.929325000	-1.136664000	2.118901000
8	-4.899052000	-0.682398000	2.287688000
6	-5.801601000	0.294258000	2.652616000
8	-5.485673000	1.464637000	2.906519000
7	-7.052252000	-0.237051000	2.737768000
1	-7.212130000	-1.157195000	2.302768000
6	-8.229042000	0.629188000	2.803180000
1	-7.928370000	1.561674000	3.307785000
1	-8.987660000	0.133410000	3.434611000
6	-8.811126000	0.922327000	1.411270000
1	-9.086343000	-0.040519000	0.941487000
1	-8.021132000	1.377169000	0.783331000
6	2.100503000	2.999948000	-1.339229000
1	3.031300000	3.235053000	-1.880446000
6	2.418540000	2.679328000	0.131941000
1	3.031893000	3.513845000	0.523249000
1	1.484421000	2.666162000	0.721294000
6	3.163778000	1.348031000	0.309716000
1	2.457637000	0.501842000	0.220315000
1	3.917549000	1.216940000	-0.486434000
6	-10.031628000	1.850722000	1.463373000
1	-10.816275000	1.417633000	2.110980000
1	-9.748016000	2.826614000	1.901136000
6	3.871256000	1.263682000	1.671133000
1	3.160090000	1.491667000	2.482481000
1	4.674520000	2.025491000	1.713780000
6	-10.619336000	2.074989000	0.062185000
1	-9.849708000	2.468914000	-0.621760000
1	-10.980613000	1.118895000	-0.351867000
6	-4.455890000	-3.245891000	-0.048331000
1	-3.736410000	-3.861237000	0.519553000
1	-4.501125000	-2.257978000	0.440885000
6	-5.854053000	-3.879640000	-0.013022000
1	-5.883163000	-4.807564000	-0.614002000
1	-6.590510000	-3.179370000	-0.445788000
6	-3.934419000	-3.082766000	-1.475080000
1	-3.740093000	-4.065459000	-1.937132000
1	-4.649092000	-2.524687000	-2.100531000
8	-2.721216000	-2.283499000	-1.527115000
6	-1.581247000	-2.931038000	-1.104666000
8	-1.553061000	-4.109507000	-0.720299000
7	-0.507043000	-2.107096000	-1.196024000
1	-0.617453000	-1.165672000	-1.599807000
6	-6.252405000	-4.194881000	1.427967000
1	-5.661427000	-5.029644000	1.834726000
1	-6.119790000	-3.312595000	2.075069000
8	-7.631232000	-4.652142000	1.519316000
6	-8.567785000	-3.656150000	1.518322000
8	-8.302550000	-2.441643000	1.516502000
7	-9.826161000	-4.161255000	1.545959000
1	-9.943256000	-5.165732000	1.418571000
6	-10.993545000	-3.284400000	1.472946000
1	-10.810985000	-2.427467000	2.143681000
1	-11.851588000	-3.849461000	1.873013000
6	-11.296164000	-2.775843000	0.054600000
1	-11.449497000	-3.638405000	-0.620974000
1	-10.412712000	-2.223383000	-0.316470000
6	0.794414000	-2.506102000	-0.668884000
1	1.025134000	-3.529518000	-1.015221000
1	1.544113000	-1.827433000	-1.109839000
6	0.846498000	-2.461594000	0.867180000
1	0.669190000	-1.424526000	1.211657000
1	0.007927000	-3.074239000	1.248151000
6	2.169400000	-2.984479000	1.442082000
1	2.419605000	-3.960782000	0.983282000
1	2.998865000	-2.292979000	1.210535000
6	-12.529828000	-1.864287000	0.040680000
1	-13.424820000	-2.429570000	0.363923000
1	-12.393531000	-1.036019000	0.761421000
6	2.072986000	-3.160073000	2.966016000
1	1.273206000	-3.881555000	3.211402000
1	1.819752000	-2.202024000	3.447441000
6	-12.798064000	-1.262243000	-1.346762000
1	-11.917564000	-0.684044000	-1.683156000
1	-12.983782000	-2.052468000	-2.090794000
1	4.148685000	-0.542808000	2.832131000
7	4.413222000	-0.060945000	1.959677000
6	5.408711000	-0.612545000	1.218233000
8	5.958847000	-0.100616000	0.232488000
8	5.710096000	-1.862704000	1.703128000
6	6.693715000	-2.611246000	0.943648000
1	6.498142000	-2.473226000	-0.132725000
1	7.698406000	-2.207478000	1.161707000
6	6.567106000	-4.067341000	1.360627000
1	5.556770000	-4.448593000	1.138191000
1	6.749699000	-4.186655000	2.440308000
1	7.302596000	-4.675268000	0.807153000
1	3.659954000	-4.553364000	3.349580000
7	3.316259000	-3.619976000	3.574827000
6	4.181226000	-2.758830000	4.168792000
8	3.952988000	-1.552692000	4.386064000
8	5.324481000	-3.391641000	4.551337000
6	6.376347000	-2.508311000	5.037399000
1	6.620780000	-1.789355000	4.237786000
1	6.000509000	-1.946654000	5.908704000
6	7.565501000	-3.382396000	5.398574000
1	7.932805000	-3.934682000	4.516906000
1	7.299998000	-4.109016000	6.184755000
1	8.385330000	-2.747327000	5.774235000
7	-13.961305000	-0.373338000	-1.351862000
1	-13.904865000	0.401246000	-0.673469000
6	-15.173166000	-0.819163000	-1.793729000
8	-15.371036000	-1.904900000	-2.357801000
8	-16.244367000	0.024807000	-1.636137000
6	-16.047873000	1.361650000	-1.091667000
1	-15.683681000	1.291350000	-0.052764000
1	-15.281591000	1.886138000	-1.690383000
6	-17.385743000	2.078555000	-1.157920000
1	-17.274265000	3.095342000	-0.745766000
1	-18.148184000	1.545813000	-0.565133000
1	-17.738742000	2.161370000	-2.199457000
7	-11.738140000	3.020662000	0.036623000
1	-11.509423000	4.012314000	-0.021801000
6	-12.983979000	2.640963000	0.418356000
8	-13.285669000	1.474008000	0.740092000
8	-13.970179000	3.580029000	0.419386000
6	-13.708564000	4.913460000	-0.111579000
1	-12.984631000	5.428607000	0.545820000
1	-13.272915000	4.818095000	-1.121730000
6	-15.035379000	5.652697000	-0.147908000
1	-14.874012000	6.673956000	-0.531100000
1	-15.472583000	5.723653000	0.861862000
1	-15.750462000	5.139321000	-0.811692000
1	2.081563000	1.287760000	-2.636643000
1	1.442259000	3.882042000	-1.406914000
1	-3.250092000	0.442358000	2.912727000

P2-Ar

6	1.126878000	0.619650000	-0.409993000
6	1.195712000	-0.498374000	0.447142000
6	-0.105424000	0.993735000	-0.982558000
1	2.150684000	-0.787552000	0.890875000
1	-0.140669000	1.862793000	-1.644572000
6	0.039826000	-1.231652000	0.724846000
6	-1.261303000	0.260288000	-0.705042000
1	0.075130000	-2.100993000	1.386473000
1	-2.216286000	0.549450000	-1.148796000
6	-1.192337000	-0.858056000	0.151644000
6	-2.392972000	-1.680936000	0.482202000
8	-2.383811000	-2.661867000	1.224191000
8	-3.513084000	-1.218204000	-0.129429000
6	2.328711000	1.439554000	-0.743798000
8	2.319623000	2.422793000	-1.482696000
8	3.447937000	0.976962000	-0.130596000
6	-4.724117000	-1.966741000	0.146588000
1	-4.913619000	-1.978158000	1.232034000
1	-4.605111000	-3.004021000	-0.206717000
6	4.659471000	1.726288000	-0.402604000
1	4.525569000	2.773355000	-0.086234000
1	4.873394000	1.703612000	-1.483563000
6	-5.828773000	-1.242292000	-0.609461000
1	-5.949477000	-0.208944000	-0.244620000
1	-5.614085000	-1.213998000	-1.691012000
8	-7.026820000	-2.006196000	-0.357349000
6	-8.164809000	-1.476086000	-0.921585000
8	-8.182799000	-0.431876000	-1.582051000
7	-9.232061000	-2.282532000	-0.670775000
1	-9.102217000	-3.044662000	-0.005967000
6	5.751280000	1.031257000	0.398339000
1	5.530292000	1.059742000	1.478305000
1	5.861479000	-0.020789000	0.086538000
8	6.960288000	1.766363000	0.114635000
6	8.079671000	1.277355000	0.748905000
8	8.071639000	0.293321000	1.496462000
7	9.161309000	2.050878000	0.459113000
1	9.058544000	2.752370000	-0.273611000
6	10.507424000	1.638085000	0.852280000
1	10.445095000	1.234565000	1.876713000
1	11.134885000	2.544365000	0.885542000
6	11.122440000	0.590393000	-0.089564000
1	11.161937000	1.002462000	-1.115825000
1	10.453910000	-0.290424000	-0.119697000
6	-10.591754000	-1.862271000	-0.999954000
1	-10.547446000	-1.329889000	-1.964443000
1	-11.196890000	-2.772968000	-1.145391000
6	-11.224962000	-0.960591000	0.071951000
1	-11.229009000	-1.494415000	1.041049000
1	-10.590762000	-0.063361000	0.198247000
6	-12.654666000	-0.546511000	-0.303007000
1	-12.641723000	-0.012575000	-1.273377000
1	-13.286385000	-1.444310000	-0.440067000
6	12.527262000	0.166744000	0.360204000
1	13.200008000	1.044569000	0.382063000
1	12.487546000	-0.236410000	1.390207000
6	-13.286930000	0.351953000	0.764357000
1	-12.659992000	1.251071000	0.928128000
1	-13.359370000	-0.176557000	1.728196000
6	13.135398000	-0.892167000	-0.573886000
1	12.491711000	-1.787287000	-0.612247000
1	13.214358000	-0.490879000	-1.597883000
7	-14.645414000	0.738462000	0.380875000
1	-14.790600000	1.009571000	-0.590755000
6	-15.590186000	1.030813000	1.319359000
8	-15.424564000	0.915125000	2.540275000
8	-16.815997000	1.447659000	0.868220000
6	-17.089482000	1.507084000	-0.560343000
1	-16.892824000	0.516143000	-1.007951000
1	-16.420982000	2.252328000	-1.030306000
6	-18.546253000	1.907679000	-0.725851000
1	-18.735095000	2.894126000	-0.270966000
1	-19.211522000	1.165179000	-0.254987000
1	-18.791556000	1.965853000	-1.799448000
7	14.471082000	-1.324854000	-0.170366000
1	14.554324000	-1.992640000	0.595757000
6	15.572410000	-0.575673000	-0.468700000
8	15.595308000	0.386532000	-1.246445000
8	16.671266000	-1.061942000	0.189682000
6	17.913578000	-0.358507000	-0.092209000
1	17.780617000	0.711059000	0.143124000
1	18.138269000	-0.446788000	-1.169122000
6	18.994708000	-0.997028000	0.763958000
1	19.111808000	-2.066421000	0.520526000
1	18.755703000	-0.903190000	1.836617000
1	19.957141000	-0.491577000	0.577127000

P2-Ar$_{Dim}$

6	0.205169000	1.103930000	-0.397311000
6	0.927139000	0.678104000	0.736812000
6	0.881754000	1.686998000	-1.486372000
1	0.401448000	0.213637000	1.573302000
1	0.306573000	1.998192000	-2.362086000
6	2.313029000	0.848301000	0.781392000
6	2.264964000	1.876234000	-1.434244000
1	2.888525000	0.515788000	1.648787000
1	2.790936000	2.341771000	-2.270676000
6	2.985049000	1.462939000	-0.294483000
6	4.460476000	1.656348000	-0.186995000
8	5.186512000	1.074017000	0.618801000
8	4.912256000	2.566006000	-1.082813000
6	-1.278664000	0.976445000	-0.488382000
8	-1.949577000	1.323002000	-1.460030000
8	-1.816052000	0.457335000	0.643304000
6	6.346748000	2.776208000	-1.093437000
1	6.854653000	1.810149000	-1.241903000
1	6.666735000	3.208612000	-0.131418000
6	-3.262519000	0.356668000	0.651206000
1	-3.601197000	-0.204424000	-0.233738000
1	-3.701784000	1.365197000	0.620882000
6	6.593777000	3.734358000	-2.254715000
1	6.211204000	3.307353000	-3.193678000
1	6.130314000	4.713504000	-2.066360000
8	8.011495000	3.992010000	-2.371843000
6	8.692252000	3.141318000	-3.202954000
8	8.158207000	2.204018000	-3.826230000
7	10.003346000	3.460627000	-3.282732000
6	-3.615388000	-0.362739000	1.949836000
1	-3.101493000	-1.332837000	2.003432000
1	-3.337469000	0.253047000	2.820046000
8	-5.021057000	-0.679322000	1.990081000
6	-5.849169000	0.382336000	2.316050000
8	-5.446802000	1.543776000	2.462913000
7	-7.119672000	-0.062223000	2.471360000
1	-7.332518000	-1.039573000	2.229943000
6	-8.251676000	0.856725000	2.537458000
1	-7.865543000	1.831806000	2.875761000
1	-8.958015000	0.488673000	3.303063000
6	-8.966820000	0.992488000	1.183569000
1	-9.300677000	-0.012291000	0.861113000
1	-8.237899000	1.347273000	0.430005000
6	10.679379000	4.540576000	-2.553741000
1	11.631556000	4.709873000	-3.082352000
6	10.954983000	4.217189000	-1.076299000
1	11.576251000	5.041821000	-0.676122000
1	10.007680000	4.229558000	-0.507907000
6	11.672510000	2.872563000	-0.876828000
1	10.948674000	2.038945000	-0.936436000

1	12.415771000	2.707970000	-1.676555000
6	-10.162822000	1.951032000	1.250179000
1	-10.897055000	1.594005000	1.995482000
1	-9.827410000	2.953970000	1.575647000
6	12.400276000	2.813014000	0.475486000
1	11.702969000	3.058544000	1.293930000
1	13.202859000	3.576640000	0.487031000
6	-10.864707000	2.070793000	-0.110195000
1	-10.164435000	2.438564000	-0.878039000
1	-11.230321000	1.082309000	-0.434095000
6	-2.319245000	-2.626093000	-0.690208000
6	-1.652516000	-3.080731000	0.466311000
6	-1.585746000	-2.050938000	-1.747879000
1	-2.220623000	-3.536990000	1.280028000
1	-2.120459000	-1.695057000	-2.631629000
6	-0.265580000	-2.946266000	0.564542000
6	-0.197691000	-1.929816000	-1.654566000
1	0.268081000	-3.283740000	1.456590000
1	0.373175000	-1.479320000	-2.468733000
6	0.467131000	-2.374714000	-0.493475000
6	1.946118000	-2.256659000	-0.332213000
8	2.562888000	-2.595352000	0.678188000
8	2.539714000	-1.741094000	-1.434433000
6	-3.801604000	-2.705291000	-0.834014000
8	-4.429645000	-2.289023000	-1.807975000
8	-4.392370000	-3.274592000	0.246053000
6	3.989573000	-1.638614000	-1.359955000
1	4.410893000	-2.630784000	-1.155866000
1	4.267177000	-0.961028000	-0.537529000
6	-5.838311000	-3.372047000	0.175543000
1	-6.122411000	-3.977663000	-0.700663000
1	-6.268885000	-2.364202000	0.077582000
6	4.427836000	-1.077431000	-2.715852000
1	4.550754000	-1.882278000	-3.459437000
1	3.669754000	-0.365469000	-3.074795000
8	5.639093000	-0.290612000	-2.644294000
6	6.760960000	-0.978927000	-2.234964000
8	6.732843000	-2.129401000	-1.776378000
7	7.869500000	-0.212181000	-2.382672000
1	7.824583000	0.646685000	-2.952476000
6	-6.272905000	-4.058075000	1.468185000
1	-5.659622000	-4.952914000	1.648488000
1	-6.198896000	-3.375936000	2.329040000
8	-7.623387000	-4.556813000	1.330901000
6	-8.621533000	-3.632295000	1.504396000
8	-8.431085000	-2.437858000	1.781125000
7	-9.840892000	-4.205611000	1.364902000
1	-9.880205000	-5.166658000	1.026711000
6	-11.062032000	-3.401327000	1.376190000
1	-10.931640000	-2.614798000	2.137665000
1	-11.886193000	-4.056241000	1.704481000
6	-11.386964000	-2.766574000	0.014916000
1	-11.499899000	-3.564098000	-0.743760000
1	-10.529693000	-2.140978000	-0.298647000
6	9.162727000	-0.668479000	-1.875963000
1	9.338961000	-1.709632000	-2.203189000
1	9.935081000	-0.035033000	-2.343006000
6	9.233527000	-0.589959000	-0.342446000
1	9.133567000	0.465263000	-0.023645000
1	8.356238000	-1.128640000	0.061170000
6	10.516418000	-1.199564000	0.238324000
1	10.681889000	-2.206052000	-0.192498000
1	11.397627000	-0.584950000	-0.019327000
6	-12.661991000	-1.915390000	0.081461000
1	-13.516519000	-2.534767000	0.414395000
1	-12.537165000	-1.109285000	0.829207000
6	10.416614000	-1.317743000	1.767487000
1	9.542772000	-1.937037000	2.039325000
1	10.276937000	-0.323473000	2.221354000
6	-13.011265000	-1.278918000	-1.272197000
1	-12.161924000	-0.669197000	-1.633198000
1	-13.214465000	-2.052308000	-2.029291000
1	12.699928000	1.032367000	1.671186000
7	12.951351000	1.497187000	0.784413000
6	13.936755000	0.933999000	0.038557000
8	14.440842000	1.410534000	-0.989065000
8	14.304926000	-0.274724000	0.583236000
6	15.221271000	-1.061221000	-0.221815000
1	14.682311000	-1.421619000	-1.116692000
1	16.051644000	-0.419500000	-0.559717000
6	15.707338000	-2.215116000	0.639114000
1	14.857758000	-2.787775000	1.045566000
1	16.314553000	-1.847446000	1.482862000
1	16.332410000	-2.891750000	0.031953000
1	11.833365000	-2.872249000	2.202667000
7	11.604497000	-1.895571000	2.385242000
6	12.536619000	-1.136513000	3.013833000
8	12.442301000	0.089551000	3.219070000
8	13.583723000	-1.896398000	3.437876000
6	14.685742000	-1.144328000	4.023491000
1	15.111827000	-0.495381000	3.239908000
1	14.293148000	-0.504239000	4.830455000
6	15.692841000	-2.155682000	4.542978000
1	16.069589000	-2.797138000	3.728880000
1	15.241411000	-2.798701000	5.317187000
1	16.549641000	-1.622999000	4.988965000
7	-14.194058000	-0.422677000	-1.194075000
1	-14.125889000	0.338144000	-0.501465000
6	-15.412467000	-0.880460000	-1.603214000
8	-15.610615000	-1.952276000	-2.193668000
8	-16.492789000	-0.064616000	-1.377937000
6	-16.298287000	1.259706000	-0.805304000
1	-15.884981000	1.169021000	0.213893000
1	-15.571387000	1.816490000	-1.423463000
6	-17.651034000	1.951194000	-0.788537000
1	-17.539362000	2.958678000	-0.353648000
1	-18.373763000	1.387187000	-0.175337000
1	-18.055450000	2.053954000	-1.809330000
7	-12.006483000	2.988317000	-0.097411000
1	-11.822608000	3.971752000	-0.289286000
6	-13.202505000	2.604944000	0.414642000
8	-13.439723000	1.451602000	0.827718000
8	-14.213439000	3.516120000	0.452661000
6	-14.019693000	4.848396000	-0.108294000
1	-13.243243000	5.375774000	0.475522000
1	-13.682705000	4.751183000	-1.155657000
6	-15.353854000	5.569523000	-0.021683000
1	-15.245625000	6.589988000	-0.425390000
1	-15.692860000	5.641554000	1.024871000
1	-16.122030000	5.041252000	-0.610287000
1	10.561302000	2.830314000	-3.855810000
1	10.076970000	5.459533000	-2.642709000

DiI

6	-6.619851000	1.187070000	0.436942000
6	-5.309044000	1.679849000	0.580628000
6	-4.292739000	0.982185000	-0.082518000
6	-4.542063000	-0.164640000	-0.856318000
6	-5.845038000	-0.640040000	-0.995113000
6	-6.889160000	0.045461000	-0.339329000
1	-7.440406000	1.704822000	0.942979000
1	-5.104847000	2.564394000	1.189534000
1	-6.057212000	-1.529468000	-1.597491000
1	-7.917316000	-0.316643000	-0.433287000
6	-3.227891000	-0.678583000	-1.427746000
7	-2.909665000	1.262865000	-0.117665000
6	-2.221935000	0.326660000	-0.837529000
6	-2.323624000	2.419848000	0.569424000

1	-3.071264000	3.227796000	0.527369000
1	-1.459838000	2.754073000	-0.024850000
6	-1.924874000	2.105971000	2.014910000
1	-1.495853000	3.009221000	2.479781000
1	-2.803833000	1.794109000	2.603020000
1	-1.185353000	1.291419000	2.045937000
6	-3.267166000	-0.612238000	-2.976130000
1	-4.082318000	-1.256646000	-3.346050000
1	-3.454501000	0.418376000	-3.319970000
1	-2.322701000	-0.963083000	-3.421195000
6	-2.957717000	-2.117426000	-0.921456000
1	-2.856305000	-2.126707000	0.174306000
1	-3.796448000	-2.768745000	-1.219741000
1	-2.028141000	-2.526337000	-1.345431000
6	-0.826551000	0.330211000	-0.921430000
1	-0.300192000	1.018236000	-0.264812000
6	-0.087297000	-0.592596000	-1.672796000
1	-0.668917000	-1.301125000	-2.268952000
6	1.290876000	-0.861457000	-1.722021000
6	6.029216000	-0.260077000	-0.037299000
6	4.694875000	-0.128183000	-0.419891000
6	4.064731000	1.125622000	-0.355990000
6	4.735636000	2.281909000	0.060826000
6	6.081297000	2.136619000	0.447405000
6	6.721285000	0.885076000	0.407219000
6	3.711354000	-1.141043000	-0.969134000
6	2.448570000	-0.283422000	-1.178800000
7	2.726227000	0.997698000	-0.812476000
1	6.532998000	-1.230917000	-0.085117000
1	4.252761000	3.261286000	0.084347000
1	6.634455000	3.018718000	0.783881000
1	7.767032000	0.800145000	0.717505000
1	1.513519000	-1.824968000	-2.192968000
6	1.874398000	2.183956000	-0.963213000
1	1.035071000	1.908036000	-1.615048000
1	2.470229000	2.941038000	-1.501634000
6	1.403372000	2.730719000	0.390803000
1	0.706403000	3.568928000	0.229535000
1	0.904487000	1.945682000	0.981834000
1	2.249601000	3.104522000	0.987996000
6	4.222452000	-1.729006000	-2.307760000
1	5.172121000	-2.261679000	-2.132437000
1	3.498567000	-2.449754000	-2.723251000
1	4.398769000	-0.933257000	-3.049954000
6	3.428786000	-2.268961000	0.051545000
1	4.362200000	-2.823283000	0.248805000
1	3.044440000	-1.856161000	0.996791000
1	2.674265000	-2.968434000	-0.341758000
17	-0.038979000	-1.638296000	1.940651000
8	-1.477481000	-1.172321000	2.057526000
8	0.862872000	-0.447051000	1.675132000
8	0.380830000	-2.283954000	3.250107000
8	0.080587000	-2.647117000	0.824280000

P1-DiI$_a$

6	-11.510962000	-9.757161000	7.619890000
1	-10.640970000	-10.429818000	7.729657000
1	-11.707472000	-9.305209000	8.610034000
6	-12.737664000	-10.553749000	7.147982000
1	-12.528781000	-11.032998000	6.173495000
1	-13.597469000	-9.874569000	7.004993000
6	-11.155755000	-8.650046000	6.628948000
1	-10.916943000	-9.067709000	5.637331000
1	-11.977315000	-7.923010000	6.530435000
8	-10.027075000	-7.862781000	7.094788000
6	-8.791944000	-8.382517000	6.791293000
8	-8.606971000	-9.411964000	6.129972000
7	-7.808629000	-7.575779000	7.285338000
1	-8.089341000	-6.851977000	7.946890000
6	-13.127966000	-11.629124000	8.160634000
1	-12.308454000	-12.347991000	8.318539000
1	-13.409230000	-11.178767000	9.126742000
8	-14.231041000	-12.439983000	7.674683000
6	-15.476815000	-11.885940000	7.847549000
8	-15.691306000	-10.812073000	8.421736000
7	-16.434703000	-12.720097000	7.343281000
1	-16.107202000	-13.487512000	6.755646000
6	-17.800812000	-12.238661000	7.136980000
1	-18.051461000	-11.598332000	7.998413000
1	-18.475512000	-13.111569000	7.157281000
6	-17.968946000	-11.453199000	5.827293000
1	-17.700544000	-12.106299000	4.974419000
1	-17.253785000	-10.609259000	5.829139000
6	-6.412928000	-8.009328000	7.279717000
1	-6.224428000	-8.499431000	6.310106000
1	-5.782716000	-7.105118000	7.327097000
6	-6.065379000	-8.968365000	8.429967000
1	-6.271971000	-8.469219000	9.396076000
1	-6.735119000	-9.846857000	8.369725000
6	-4.600162000	-9.422003000	8.375841000
1	-4.397753000	-9.925089000	7.410719000
1	-3.928839000	-8.544187000	8.429514000
6	-19.390773000	-10.906040000	5.651071000
1	-20.134196000	-11.724779000	5.689067000
1	-19.623429000	-10.211903000	6.479290000
6	-4.247849000	-10.378232000	9.527086000
1	-4.899759000	-11.268062000	9.502644000
1	-4.401200000	-9.875841000	10.496513000
6	-19.542436000	-10.148726000	4.322793000
1	-18.742739000	-9.393406000	4.232134000
1	-19.460899000	-10.839086000	3.468070000
1	-2.613597000	-11.557579000	8.807351000
7	-2.862652000	-10.843157000	9.491656000
6	-1.848951000	-10.054117000	9.957438000
8	-1.992304000	-9.030431000	10.638368000
8	-0.635647000	-10.577808000	9.597247000
6	0.518730000	-9.840046000	10.087848000
1	0.459728000	-8.799805000	9.724470000
1	0.488564000	-9.819353000	11.190877000
6	1.758170000	-10.550863000	9.569579000
1	1.771318000	-10.567749000	8.466706000
1	1.802168000	-11.589236000	9.939151000
1	2.659301000	-10.019355000	9.919306000
7	-20.816486000	-9.442896000	4.204733000
1	-20.927241000	-8.652786000	4.850956000
6	-21.912489000	-10.040852000	3.662531000
8	-21.927907000	-11.161587000	3.133161000
8	-23.077689000	-9.313152000	3.672512000
6	-23.056538000	-7.922378000	4.108504000
1	-22.891458000	-7.877096000	5.200286000
1	-22.219405000	-7.398349000	3.613799000
6	-24.387867000	-7.294916000	3.731742000
1	-24.351903000	-6.228741000	4.000965000
1	-25.225705000	-7.771454000	4.266898000
1	-24.563302000	-7.374174000	2.645816000
6	-35.347445000	-5.822420000	6.796459000
6	-33.975433000	-6.131008000	6.854008000
6	-33.094096000	-5.210314000	6.275430000
6	-33.533882000	-4.030167000	5.651370000
6	-34.895386000	-3.733837000	5.602549000
6	-35.805273000	-4.642088000	6.182504000
1	-36.067173000	-6.519125000	7.236798000
1	-33.627145000	-7.051882000	7.328633000
1	-35.254655000	-2.818492000	5.121257000
1	-36.877528000	-4.426634000	6.153553000
6	-32.331508000	-3.269306000	5.111961000
7	-31.682818000	-5.263580000	6.202349000
6	-31.170920000	-4.192447000	5.527578000
6	-30.900401000	-6.380001000	6.748159000

1	-31.481272000	-6.806589000	7.579204000
1	-29.981657000	-5.962237000	7.187013000
6	-30.591714000	-7.442089000	5.687725000
1	-30.011150000	-8.260203000	6.144416000
1	-31.523756000	-7.862224000	5.275065000
1	-30.004212000	-7.017270000	4.856766000
6	-32.230965000	-1.878665000	5.788021000
1	-33.140990000	-1.298698000	5.560709000
1	-32.146769000	-1.981792000	6.882243000
1	-31.360081000	-1.312391000	5.421888000
6	-32.445223000	-3.151336000	3.569667000
1	-32.502100000	-4.149479000	3.105477000
1	-33.364990000	-2.597178000	3.318885000
1	-31.590035000	-2.611228000	3.134791000
6	-29.797875000	-4.043987000	5.290639000
1	-29.149015000	-4.858663000	5.612254000
6	-29.230746000	-2.955875000	4.609932000
1	-29.931539000	-2.215550000	4.214370000
6	-27.902635000	-2.686512000	4.234676000
6	-22.968559000	-3.818645000	4.009563000
6	-24.313777000	-3.655412000	4.342282000
6	-24.802712000	-4.155226000	5.560731000
6	-23.979358000	-4.796533000	6.494549000
6	-22.625857000	-4.958650000	6.147189000
6	-22.125173000	-4.488235000	4.918834000
6	-25.447963000	-2.980982000	3.599786000
6	-26.635794000	-3.205144000	4.555236000
7	-26.193961000	-3.878577000	5.651979000
1	-22.576837000	-3.439268000	3.060355000
1	-24.355733000	-5.161016000	7.452890000
1	-21.950613000	-5.468272000	6.838581000
1	-21.072201000	-4.649706000	4.673970000
1	-27.830570000	-1.919122000	3.455587000
6	-26.939433000	-4.205157000	6.875098000
1	-27.876994000	-3.634484000	6.857004000
1	-26.343468000	-3.826644000	7.722896000
6	-27.178796000	-5.713319000	7.023640000
1	-27.769865000	-5.901874000	7.934310000
1	-27.714934000	-6.128384000	6.153473000
1	-26.230868000	-6.266121000	7.114062000
6	-25.153576000	-1.472717000	3.404598000
1	-24.249775000	-1.358742000	2.783130000
1	-25.989573000	-0.971032000	2.889470000
1	-24.980119000	-0.974626000	4.372461000
6	-25.729849000	-3.662440000	2.238490000
1	-24.846219000	-3.560307000	1.586445000
1	-25.947581000	-4.735542000	2.368792000
1	-26.591269000	-3.186393000	1.741450000
17	-19.233302000	-6.821224000	6.074846000
8	-20.475822000	-7.613810000	6.473555000
8	-17.998895000	-7.600620000	6.465583000
8	-19.247584000	-6.600995000	4.577300000
8	-19.249469000	-5.490575000	6.791626000

P1-DiI

6	-10.239011000	-9.277606000	7.728217000
1	-9.468986000	-10.064001000	7.823065000
1	-10.282522000	-8.737270000	8.690857000
6	-11.601500000	-9.919173000	7.435067000
1	-11.591209000	-10.419765000	6.449044000
1	-12.395858000	-9.151028000	7.411962000
6	-9.769697000	-8.303905000	6.651944000
1	-9.633940000	-8.812470000	5.683218000
1	-10.463391000	-7.457800000	6.527557000
8	-8.514150000	-7.687707000	7.050277000
6	-7.405212000	-8.487816000	6.891831000
8	-7.411134000	-9.587615000	6.326367000
7	-6.306972000	-7.869750000	7.412081000
1	-6.454031000	-7.021110000	7.957675000
6	-11.912532000	-10.945828000	8.521235000
1	-11.160811000	-11.746888000	8.526781000
1	-11.936386000	-10.467947000	9.514504000
8	-13.176759000	-11.619168000	8.294011000
6	-14.271732000	-10.999891000	8.844937000
8	-14.225982000	-9.966309000	9.524175000
7	-15.402425000	-11.713798000	8.573330000
1	-15.329273000	-12.451067000	7.872242000
6	-16.722619000	-11.158640000	8.864708000
1	-16.660872000	-10.664190000	9.848403000
1	-17.427710000	-12.002056000	8.956411000
6	-17.211993000	-10.158472000	7.804547000
1	-17.269856000	-10.666174000	6.822709000
1	-16.459755000	-9.352907000	7.708745000
6	-5.014207000	-8.543674000	7.483728000
1	-4.981968000	-9.261336000	6.648231000
1	-4.222941000	-7.791470000	7.318898000
6	-4.780771000	-9.285904000	8.807829000
1	-4.819238000	-8.568980000	9.650484000
1	-5.605773000	-10.008504000	8.950585000
6	-3.451260000	-10.049821000	8.800805000
1	-3.471526000	-10.783888000	7.975794000
1	-2.603923000	-9.363251000	8.612816000
6	-18.576566000	-9.557764000	8.168468000
1	-19.329787000	-10.359932000	8.279837000
1	-18.509366000	-9.037989000	9.143421000
6	-3.209408000	-10.808498000	10.116534000
1	-4.121997000	-11.357817000	10.399454000
1	-2.954823000	-10.113236000	10.932768000
6	-19.072582000	-8.567440000	7.103303000
1	-18.339234000	-7.756179000	6.958231000
1	-19.204165000	-9.081741000	6.137335000
1	-2.343898000	-12.621056000	9.437971000
7	-2.137347000	-11.794989000	10.013576000
6	-0.831980000	-11.440956000	10.178327000
8	-0.423456000	-10.372835000	10.655196000
8	-0.010108000	-12.463542000	9.772597000
6	1.410407000	-12.215025000	9.953335000
1	1.688188000	-11.297469000	9.406530000
1	1.613495000	-12.047363000	11.025370000
6	2.149275000	-13.433450000	9.423627000
1	1.935890000	-13.589399000	8.352619000
1	1.859159000	-14.342740000	9.976733000
1	3.235998000	-13.286373000	9.543278000
7	-20.350855000	-7.941998000	7.448138000
1	-20.317928000	-7.160607000	8.100879000
6	-21.522204000	-8.619999000	7.265585000
8	-21.619104000	-9.697402000	6.664075000
8	-22.666551000	-8.041972000	7.749721000
6	-22.609132000	-6.752453000	8.423254000
1	-21.991554000	-6.844588000	9.336340000
1	-22.144157000	-6.010468000	7.748981000
6	-24.035938000	-6.360554000	8.771676000
1	-24.033218000	-5.386427000	9.288758000
1	-24.495608000	-7.108626000	9.438728000
1	-24.650153000	-6.270790000	7.860370000
6	-9.819668000	-14.039748000	8.706677000
6	-10.398721000	-13.801801000	9.968321000
6	-9.851790000	-12.761018000	10.728042000
6	-8.759583000	-11.994146000	10.287931000
6	-8.202472000	-12.230372000	9.033098000
6	-8.744778000	-13.261803000	8.239313000
1	-10.221266000	-14.843006000	8.081593000
1	-11.238193000	-14.405330000	10.322393000
1	-7.352356000	-11.653473000	8.661486000
1	-8.307230000	-13.468832000	7.259484000
6	-8.359430000	-11.016966000	11.384302000
7	-10.254052000	-12.288215000	11.999415000
6	-9.438800000	-11.288715000	12.448396000
6	-11.390965000	-12.858386000	12.732761000

1	-12.085270000	-13.267843000	11.983470000
1	-11.918527000	-12.031372000	13.231084000
6	-10.954632000	-13.936843000	13.729613000
1	-11.840655000	-14.342827000	14.244497000
1	-10.442570000	-14.763317000	13.209811000
1	-10.267680000	-13.523658000	14.486824000
6	-8.384988000	-9.556705000	10.877464000
1	-7.732535000	-9.462956000	9.993529000
1	-9.404665000	-9.260518000	10.587099000
1	-8.023093000	-8.853351000	11.643328000
6	-6.952125000	-11.410168000	11.909281000
1	-6.955559000	-12.439653000	12.302491000
1	-6.235614000	-11.371537000	11.073897000
1	-6.608848000	-10.728798000	12.703390000
6	-9.620595000	-10.672938000	13.693582000
1	-10.434315000	-11.042860000	14.318645000
6	-8.776696000	-9.675635000	14.205686000
1	-7.891307000	-9.437321000	13.609572000
6	-8.798325000	-8.990768000	15.433653000
6	-10.851783000	-7.860431000	19.925793000
6	-10.577712000	-8.243097000	18.613027000
6	-11.630835000	-8.547328000	17.734164000
6	-12.975719000	-8.457990000	18.113615000
6	-13.240457000	-8.074330000	19.441564000
6	-12.197282000	-7.786222000	20.340185000
6	-9.265946000	-8.366420000	17.865586000
6	-9.734282000	-8.806163000	16.465557000
7	-11.092908000	-8.888773000	16.463433000
1	-10.041228000	-7.616332000	20.619980000
1	-13.794099000	-8.664308000	17.420502000
1	-14.280082000	-7.998825000	19.774109000
1	-12.432233000	-7.493434000	21.367816000
1	-7.839874000	-8.517281000	15.674777000
6	-11.978527000	-9.122137000	15.313626000
1	-11.368546000	-9.049542000	14.403885000
1	-12.699670000	-8.287264000	15.291486000
6	-12.716435000	-10.463530000	15.406638000
1	-13.315076000	-10.615346000	14.493897000
1	-12.013580000	-11.305837000	15.521099000
1	-13.399594000	-10.491229000	16.269371000
6	-8.536649000	-7.000626000	17.813362000
1	-8.296322000	-6.678527000	18.840265000
1	-7.592026000	-7.079060000	17.249832000
1	-9.169864000	-6.230736000	17.343072000
6	-8.349665000	-9.451778000	18.481004000
1	-8.068153000	-9.158569000	19.506348000
1	-8.864507000	-10.425696000	18.522608000
1	-7.430343000	-9.563017000	17.882263000
17	-4.903605000	-13.628463000	8.264429000
8	-5.543857000	-14.898814000	7.753552000
8	-5.377983000	-12.450718000	7.443648000
8	-5.253554000	-13.427968000	9.721186000
8	-3.387909000	-13.754448000	8.128393000

P2-Ar-DiI$_a$

6	-2.442125000	-2.878532000	-0.057958000
6	-2.053551000	-2.519426000	1.249302000
6	-1.553204000	-2.698480000	-1.135965000
1	-2.746158000	-2.658835000	2.082153000
1	-1.874166000	-2.980513000	-2.141600000
6	-0.780091000	-1.990747000	1.471134000
6	-0.287711000	-2.153633000	-0.915890000
1	-0.459898000	-1.706893000	2.476991000
1	0.396492000	-1.995418000	-1.751451000
6	0.103536000	-1.797382000	0.390789000
6	1.427009000	-1.172453000	0.673419000
8	1.880889000	-0.973004000	1.799529000
8	2.074778000	-0.824128000	-0.469650000
6	-3.776862000	-3.467362000	-0.356358000
8	-4.109088000	-3.914945000	-1.455047000
8	-4.607736000	-3.442151000	0.717296000
6	3.373209000	-0.199731000	-0.296915000
1	4.109538000	-0.970764000	-0.016112000
1	3.319300000	0.558170000	0.500001000
6	-5.941985000	-3.954348000	0.466808000
1	-5.889147000	-5.033494000	0.251060000
1	-6.367717000	-3.439081000	-0.409251000
6	3.723796000	0.423755000	-1.645212000
1	3.737209000	-0.342608000	-2.435952000
1	3.012675000	1.221699000	-1.906752000
8	5.009274000	1.064527000	-1.548395000
6	6.093077000	0.231962000	-1.763104000
8	5.993996000	-0.962931000	-2.073076000
7	7.244966000	0.935479000	-1.624167000
1	7.178131000	1.875688000	-1.204352000
6	-6.773265000	-3.651054000	1.711376000
1	-6.539340000	-4.328911000	2.544389000
1	-6.630284000	-2.604515000	2.021568000
8	-8.161016000	-3.884608000	1.384815000
6	-8.786063000	-2.806121000	0.782847000
8	-8.313963000	-1.664898000	0.742756000
7	-9.995045000	-3.181493000	0.285222000
1	-10.179053000	-4.182152000	0.213916000
6	-10.757227000	-2.269608000	-0.569918000
1	-10.856026000	-1.305995000	-0.041444000
1	-11.767344000	-2.696600000	-0.680144000
6	-10.104731000	-2.046428000	-1.944177000
1	-9.948211000	-3.022100000	-2.440678000
1	-9.104289000	-1.604311000	-1.778639000
6	8.535283000	0.252512000	-1.603568000
1	8.516110000	-0.530838000	-2.379881000
1	9.306390000	0.988532000	-1.889330000
6	8.868764000	-0.369521000	-0.237207000
1	8.863763000	0.424728000	0.533749000
1	8.065559000	-1.082390000	0.028948000
6	10.225509000	-1.086416000	-0.243379000
1	10.226333000	-1.884192000	-1.010804000
1	11.029078000	-0.376026000	-0.515005000
6	-10.939107000	-1.125691000	-2.844659000
1	-11.875758000	-1.629944000	-3.146677000
1	-11.227777000	-0.212629000	-2.289048000
6	10.559384000	-1.702208000	1.125247000
1	9.777780000	-2.420433000	1.426256000
1	10.603461000	-0.912783000	1.893878000
6	-10.159624000	-0.718817000	-4.103598000
1	-9.250063000	-0.162841000	-3.811142000
1	-9.848019000	-1.606521000	-4.676018000
1	11.886830000	-3.333293000	0.724337000
7	11.839665000	-2.407068000	1.149126000
6	13.014415000	-1.719253000	1.264368000
8	13.119277000	-0.526758000	1.579223000
8	14.076848000	-2.548215000	1.017783000
6	15.383646000	-1.923921000	1.159778000
1	15.446554000	-1.064704000	0.470144000
1	15.489343000	-1.543687000	2.190342000
6	16.424754000	-2.983725000	0.838734000
1	16.303832000	-3.356812000	-0.192253000
1	16.348280000	-3.836567000	1.534143000
1	17.433532000	-2.547653000	0.934009000
7	-10.933300000	0.121432000	-5.012299000
1	-11.193328000	1.048275000	-4.680191000
6	-11.469590000	-0.372575000	-6.165962000
8	-11.281869000	-1.517432000	-6.595100000
8	-12.245135000	0.478793000	-6.909976000
6	-12.542213000	1.821002000	-6.429358000
1	-13.084285000	1.750210000	-5.468605000
1	-11.597521000	2.373351000	-6.270941000
6	-13.390623000	2.499470000	-7.491860000
1	-13.645116000	3.520505000	-7.162172000

1	-14.326588000	1.941725000	-7.660113000
1	-12.841374000	2.567932000	-8.445746000
6	-7.500594000	2.142186000	-12.400788000
6	-6.482241000	2.187460000	-11.430239000
6	-6.795795000	1.688787000	-10.160727000
6	-8.062638000	1.170946000	-9.841852000
6	-9.062968000	1.128949000	-10.811854000
6	-8.772346000	1.619722000	-12.101626000
1	-7.293640000	2.523025000	-13.405423000
1	-5.497979000	2.599083000	-11.668027000
1	-10.054274000	0.725682000	-10.580680000
1	-9.544913000	1.596828000	-12.875886000
6	-8.078334000	0.749698000	-8.380449000
7	-5.969290000	1.601924000	-9.016062000
6	-6.639314000	1.080673000	-7.947204000
6	-4.580782000	2.079418000	-9.004526000
1	-4.188155000	1.955824000	-10.025143000
1	-3.999218000	1.405086000	-8.357817000
6	-4.479053000	3.538126000	-8.546551000
1	-3.423252000	3.854274000	-8.553170000
1	-5.046160000	4.198953000	-9.222621000
1	-4.876453000	3.664362000	-7.525456000
6	-8.416059000	-0.756365000	-8.258027000
1	-9.406054000	-0.942332000	-8.704759000
1	-7.666870000	-1.367840000	-8.786623000
1	-8.464303000	-1.085511000	-7.209129000
6	-9.092269000	1.631299000	-7.607714000
1	-8.855620000	2.700485000	-7.732258000
1	-10.102687000	1.444613000	-8.006368000
1	-9.097969000	1.395591000	-6.532196000
6	-6.045651000	0.947262000	-6.684288000
1	-5.046917000	1.364306000	-6.564513000
6	-6.676287000	0.357487000	-5.579354000
1	-7.703823000	0.019856000	-5.743699000
6	-6.271904000	0.182059000	-4.243965000
6	-3.141894000	0.778844000	-0.309291000
6	-3.739073000	0.629985000	-1.560757000
6	-2.947842000	0.614784000	-2.720479000
6	-1.553685000	0.734827000	-2.681799000
6	-0.965318000	0.905840000	-1.416166000
6	-1.743743000	0.932180000	-0.245735000
6	-5.190804000	0.458726000	-1.956526000
6	-5.097443000	0.364828000	-3.491740000
7	-3.789375000	0.437847000	-3.855005000
1	-3.744444000	0.777459000	0.604385000
1	-0.935969000	0.693446000	-3.581453000
1	0.122155000	0.994720000	-1.343573000
1	-1.256701000	1.055449000	0.725288000
1	-7.097760000	-0.126554000	-3.593399000
6	-3.205521000	0.217479000	-5.185745000
1	-3.975214000	-0.250232000	-5.813500000
1	-2.399010000	-0.524519000	-5.058095000
6	-2.649474000	1.506881000	-5.803099000
1	-2.237967000	1.287664000	-6.801592000
1	-3.427615000	2.282831000	-5.896979000
1	-1.840562000	1.929932000	-5.187956000
6	-5.774856000	-0.846579000	-1.366416000
1	-5.666360000	-0.838421000	-0.270266000
1	-6.850113000	-0.941498000	-1.589435000
1	-5.250533000	-1.725471000	-1.771674000
6	-6.044086000	1.679044000	-1.535925000
1	-6.060689000	1.753356000	-0.435716000
1	-5.627274000	2.613450000	-1.945952000
1	-7.081424000	1.567915000	-1.893754000
17	6.292217000	4.524903000	-1.072409000
8	4.925787000	4.439365000	-0.438789000
8	6.837582000	5.927695000	-0.927289000
8	7.242374000	3.563649000	-0.358859000
8	6.214967000	4.152232000	-2.531836000

P2-Ar-DiI

6	-2.169791000	-2.190575000	-2.343774000
6	-1.867494000	-0.987075000	-1.671343000
6	-1.130838000	-3.052684000	-2.745745000
1	-2.676164000	-0.320649000	-1.365167000
1	-1.382991000	-3.979379000	-3.267680000
6	-0.539402000	-0.664287000	-1.385026000
6	0.198583000	-2.731170000	-2.458890000
1	-0.288949000	0.259047000	-0.856645000
1	1.004363000	-3.403655000	-2.760598000
6	0.498882000	-1.537301000	-1.770401000
6	1.897942000	-1.154172000	-1.417493000
8	2.206105000	-0.131192000	-0.806960000
8	2.803142000	-2.069633000	-1.846024000
6	-3.576145000	-2.625111000	-2.586684000
8	-3.895062000	-3.675410000	-3.141873000
8	-4.466807000	-1.726493000	-2.092651000
6	4.186096000	-1.771926000	-1.521464000
1	4.295310000	-1.673804000	-0.429804000
1	4.483012000	-0.825899000	-2.002795000
6	-5.865549000	-2.119428000	-2.125330000
1	-6.114408000	-2.535711000	-3.113106000
1	-6.414992000	-1.185179000	-1.951498000
6	5.002009000	-2.949030000	-2.048237000
1	4.684538000	-3.886586000	-1.565867000
1	4.913224000	-3.039792000	-3.140686000
8	6.402819000	-2.707854000	-1.793202000
6	6.824928000	-3.047301000	-0.522368000
8	6.094671000	-3.548862000	0.339723000
7	8.153589000	-2.786007000	-0.387768000
1	8.596426000	-2.232318000	-1.121071000
6	-6.125027000	-3.113220000	-0.986263000
1	-5.886766000	-4.143605000	-1.280607000
1	-5.503940000	-2.827458000	-0.126723000
8	-7.511805000	-3.129348000	-0.600339000
6	-7.874733000	-2.102301000	0.248686000
8	-7.115337000	-1.187215000	0.594387000
7	-9.171778000	-2.241054000	0.617240000
1	-9.648343000	-3.131490000	0.405218000
6	-9.796917000	-1.340147000	1.581686000
1	-9.360127000	-0.337198000	1.447482000
1	-9.549795000	-1.652448000	2.616725000
6	-11.316808000	-1.324943000	1.383648000
1	-11.666108000	-2.362795000	1.223680000
1	-11.566089000	-0.767649000	0.461780000
6	8.798723000	-2.849833000	0.923330000
1	8.412000000	-3.744894000	1.438190000
1	9.878506000	-2.998744000	0.755202000
6	8.551267000	-1.598854000	1.781671000
1	8.931159000	-0.708304000	1.245350000
1	7.459382000	-1.464693000	1.899406000
6	9.215977000	-1.703730000	3.161124000
1	8.830219000	-2.591731000	3.697651000
1	10.307656000	-1.842848000	3.048207000
6	-12.068478000	-0.743224000	2.586962000
1	-11.809577000	-1.310134000	3.499979000
1	-11.776581000	0.308977000	2.764374000
6	8.966775000	-0.449596000	4.015066000
1	7.884190000	-0.283030000	4.147485000
1	9.383965000	0.438552000	3.511981000
6	-13.585978000	-0.839888000	2.371415000
1	-13.903124000	-0.161774000	1.559566000
1	-13.853110000	-1.867501000	2.077642000
1	9.101045000	-1.088972000	6.053317000
7	9.567751000	-0.522044000	5.345291000
6	10.900469000	-0.281307000	5.525856000
8	11.658622000	0.220912000	4.686097000
8	11.280472000	-0.640443000	6.791709000

6	12.676792000	-0.380383000	7.108220000
1	13.313763000	-0.927451000	6.392058000
1	12.876655000	0.698362000	6.989291000
6	12.905727000	-0.844046000	8.537413000
1	12.696686000	-1.922126000	8.641363000
1	12.260808000	-0.290090000	9.240278000
1	13.957737000	-0.665897000	8.817379000
7	-14.370954000	-0.535424000	3.562896000
1	-14.470522000	0.440379000	3.833123000
6	-14.944285000	-1.524461000	4.304318000
8	-14.845518000	-2.735499000	4.059343000
8	-15.711096000	-1.142534000	5.372147000
6	-15.789927000	0.258313000	5.750959000
1	-14.771502000	0.627368000	5.972023000
1	-16.217236000	0.841477000	4.914222000
6	-16.677993000	0.345689000	6.980846000
1	-16.769666000	1.398921000	7.294437000
1	-16.247492000	-0.230973000	7.816089000
1	-17.686267000	-0.044324000	6.764179000
6	-13.572655000	-1.839021000	7.448834000
6	-12.766880000	-2.662351000	6.642026000
6	-11.493472000	-2.180463000	6.323055000
6	-11.021939000	-0.932126000	6.761899000
6	-11.832315000	-0.120890000	7.554524000
6	-13.117453000	-0.586799000	7.900138000
1	-14.575694000	-2.180608000	7.715180000
1	-13.137381000	-3.621259000	6.274865000
1	-11.479416000	0.853041000	7.908590000
1	-13.766126000	0.032162000	8.527419000
6	-9.597030000	-0.732779000	6.268922000
7	-10.476154000	-2.812675000	5.568111000
6	-9.362627000	-2.028554000	5.468354000
6	-10.651916000	-4.163750000	5.013241000
1	-11.214127000	-4.740410000	5.765505000
1	-9.657847000	-4.628561000	4.935456000
6	-11.382149000	-4.157894000	3.668517000
1	-11.484813000	-5.187885000	3.293272000
1	-12.385436000	-3.708003000	3.762154000
1	-10.811505000	-3.598319000	2.912323000
6	-8.644551000	-0.628106000	7.489716000
1	-8.953810000	0.228439000	8.111514000
1	-8.695780000	-1.541724000	8.104175000
1	-7.598786000	-0.469371000	7.184297000
6	-9.512068000	0.523523000	5.367424000
1	-10.220881000	0.448897000	4.527368000
1	-9.774145000	1.414174000	5.962196000
1	-8.499822000	0.665356000	4.958033000
6	-8.237992000	-2.406811000	4.719447000
1	-8.334142000	-3.315578000	4.130280000
6	-7.042085000	-1.673802000	4.697335000
1	-7.050547000	-0.765141000	5.304943000
6	-5.811884000	-1.816576000	4.026984000
6	-2.662734000	-3.745796000	0.568773000
6	-3.653316000	-3.504022000	1.519278000
6	-4.643832000	-4.469893000	1.762438000
6	-4.686032000	-5.693655000	1.084724000
6	-3.693469000	-5.917642000	0.112211000
6	-2.698217000	-4.959361000	-0.148006000
6	-3.885013000	-2.325481000	2.442431000
6	-5.206536000	-2.719016000	3.137319000
7	-5.534408000	-3.984573000	2.756604000
1	-1.878781000	-3.008426000	0.374320000
1	-5.455878000	-6.443541000	1.280562000
1	-3.703868000	-6.855019000	-0.451674000
1	-1.941861000	-5.152751000	-0.913356000
1	-5.159083000	-0.953066000	4.192355000
6	-6.560319000	-4.871512000	3.321329000
1	-6.798353000	-4.500739000	4.327015000
1	-6.080514000	-5.855310000	3.456163000
6	-7.792291000	-4.999163000	2.421493000
1	-8.509255000	-5.712019000	2.857827000
1	-8.300084000	-4.030802000	2.285120000
1	-7.533326000	-5.360968000	1.415292000
6	-2.751158000	-2.258565000	3.503114000
1	-1.792613000	-2.060246000	2.994656000
1	-2.940389000	-1.443987000	4.222072000
1	-2.666132000	-3.208954000	4.055373000
6	-3.986658000	-0.986563000	1.680986000
1	-3.056766000	-0.820966000	1.111356000
1	-4.842824000	-0.987586000	0.989919000
1	-4.107278000	-0.148257000	2.387576000
17	-10.523078000	-5.971333000	0.019483000
8	-10.597791000	-6.629306000	1.377713000
8	-10.930595000	-4.503755000	0.136718000
8	-9.117582000	-6.056684000	-0.521279000
8	-11.483283000	-6.655681000	-0.927319000

References:

(1) S. Santra, S. M. Ali, A. Mondal, M. R. Molla, *Langmuir* 2020**, 36***,* 8282–8289.

(2) K. Ghosal, U. Bhattacharjee, K. Sarkar, *Eur. Polym. J.* 2020**, 122***,* 109338.

(3) F. Neese, Software update: the ORCA program system, version 4.0. WIREs *Comput. Mol. Sci.* 2018, **8**, e1327.

(4) A. D. Becke, *Phys. Rev. A*, 1988, **38**, 3098-3100.

(5) S. Grimme, J. Antony, S. Ehrlich, H. A. Krieg, *J. Chem. Phys.* 2010, **132,** 154104.

(6) J. D. Chai, M. Head-Gordon, *Phys. Chem. Chem. Phys*. 2008, **10,** 6615-6620.

(7) Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* 2008, **120**, 215–241.

(8) (a) M. Cossi, N. Rega, G. Scalmani, V. Barone, *J. Comput. Chem.* 2003, **24,** 669–681. (b) V. Borane, M. Cossi, *J. Phys. Chem. A.* 1998, **102**, 1995–2001.