Electronic Supplementary Information

Molecular engineering of high-performance nanofiltration membranes from intrinsically microporous poly(ether-ether-ketone)

Mahmoud A. Abdulhamid,[a] Sang-Hee Park,[a] Hakkim Vovusha,[b] Faheem Hassan Akhtar,[c] Kim Choon Ng,[c] Udo Schwingenschlögl[b] and Gyorgy Szekely [*a]

[a] Advanced Membranes and Porous Materials Center, Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal, 23955-6900, Saudi Arabia. E-mail: gyorgy.szekely@kaust.edu.sa; Web: www.szekelygroup.com, @SzekelyGroup

[b] Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal, 23955-6900, Saudi Arabia.

[c] Water Desalination and Reuse Center, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia.

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1. Experimental section

1.1. Materials

4,4′-Isopropylidenediphenol (Bisphenol A, 97%), *p*-anisidine (99%), anthracene, 1,4-benzoquinone (98%), 4,4'-difluorobenzophenone (**1**, 99%), paraformaldehyde (powder, 95%), methanesulfonic acid (MSA), trifluoroacetic acid (CF_3COOH), boron tribromide (99%), glacial acetic acid, hydrobromic acid (33%), anhydrous *N*,*N*-dimethylacetamide (DMAc, 99.8%), anhydrous potassium carbonate (K_2CO_3), estradiol (98%), valsartan (98%), oleuropein (98%), methyl orange (85%), rose bengal (95%) were obtained from Sigma-Aldrich. Losartan (95%) and acid fuchsine was purchased from TCI. Roximthromycin (98%) was provided by Hovione PharmaScience. All chemicals and solvents were used as received unless otherwise stated.

1.2. Membrane filtration experiments

The separation performance of the iPEEK membranes were tested in a typical crossflow nanofiltration apparatus shown in Fig. S1. A micro annular gear pump, i.e. recirculation pump, supplied by Michael-Smith-Engineers Ltd (GD-M35JF5S6 ATEX) was used for ensuring homogeneous concentration in the retentate loop, and to mitigate concentration polarization at the membrane surface. The recirculation of the retentate was performed at 1.2 L min^{-1}. The membranes were washed with and soaked in acetonitrile, followed by their conditioning under 30 bar applied pressure for 24 h prior to the measurement of the membrane performance. Once the system reached steady-state, the rejection and flux were measured. The flux was determined by measuring the volume of the solvent permeating through the membrane (V) within a given time (t) over a given membrane surface area (A). Equation S1 and S2 were used to calculate the flux and permeance, respectively.

$$Flux\ [L\ m^{-2}\ h^{-1}] = \frac{V}{A \cdot t} \quad \text{(S1)}$$

$$Permeance\ [L\ m^{-2}\ h^{-1}\ bar^{-1}] = \frac{J}{\Delta P} = \frac{V}{\Delta P \cdot A \cdot t} \quad \text{(S2)}$$

The active membrane area was 52 cm^2. The solute rejection was obtained from the ratio of the permeate ($c_{permeate}$) and retentate ($c_{retentate}$) concentrations of the solutes. Standard polystyrene markers containing 1 g L^{-1} PS580 and PS1300 and 0.1 g L^{-1} methyl styrene dimer (236 g mol^{-1}) were used for the filtrations.[1,2] The feed concentrations for dyes and active pharmaceutical ingredients (API) were 10 µM and 100 µM, respectively. Molecular weight cut-off (MWCO) is defined as the lowest molecular weight solute in which 90% of it is retained by the membrane, and was estimated from the rejections curve in this study by linear interpolation. Two independent measurements were performed on independently prepared membranes from independently prepared polymer batches, and the standard deviations are reported in the manuscript.

$$Rejection\ [\%] = \left(1 - \frac{c_{permeate}}{c_{retentate}}\right) \cdot 100 \qquad \text{(S3)}$$

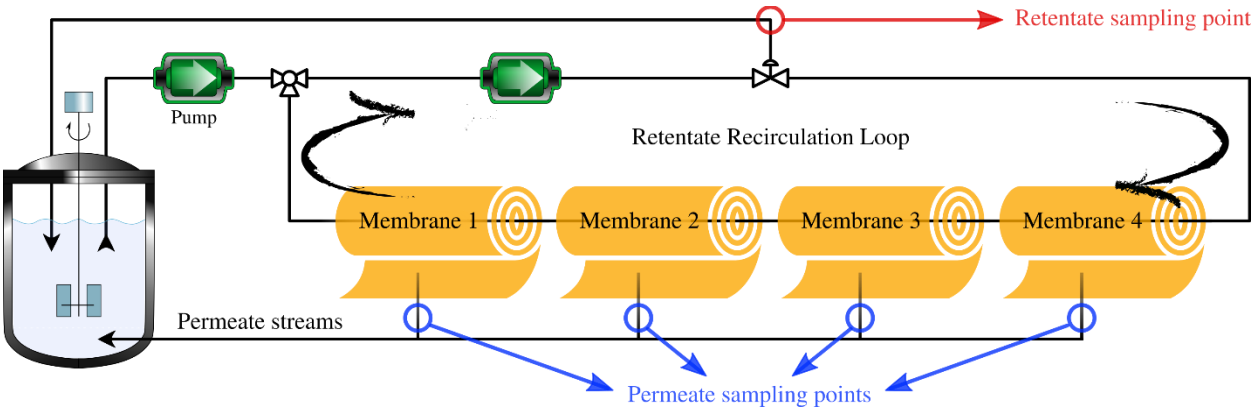


Fig. S1 Schematic of the multistage crossflow nanofiltration apparatus used for membrane testing.

2. Pore size distribution

Table S1 Physical properties of acetonitrile.

Solvent	MW (Da)	dm (nm)	H (mPa.s)	V_m (cm^3 mol^{-1})	Density (g ml^{-1})	δ_d ($MPa^{0.5}$)	δ_P ($MPa^{0.5}$)	δ_h ($MPa^{0.5}$)	δ_t ($MPa^{0.5}$)	Ref
MeCN	41.05	0.55	0.343	52.5	0.786	15.3	18	6.1	24.4	[3]

Solvent permeance can be correlated to its physical properties, as suggested by Livingston *et al*.[4] The solute diameter was obtained using the following equation.

$$d_{\mathrm{m}} = 2 \cdot \left(\frac{3V_m}{4\pi N_A}\right)^{\frac{1}{3}} \tag{S4}$$

where V_{m} is the molar volume calculated from solvent density, and N_A is the Avogardo's number. To correlate the MWCO data with pore size distribution, the styrene rejection values were used as input data into the pore flow model. The Hagen–Poiseuille equation describes the volumetric flux (J_v) through a membrane comprising uniform capillaries:

$$J_{v,i} = \frac{r_i^2 \Delta P \varepsilon}{8\mu_0 l} \tag{S5}$$

where ε is porosity, ΔP is transmembrane pressure, l is capillary length, μ_0 is solvent bulk viscosity, and r_i is capillary radius. Next, the pore flow rate ($Q_{p,i}$) allows for calculations of the flow through a pore with radius r_i:

$$Q_{p,i} = \frac{\pi r_i^4 \Delta P}{8\mu_0 l} \tag{S6}$$

The overall solute rejection can be calculated using the following set of equations:

$$R_{ij} = 1 - \frac{\Phi_{ij} K_{c,ij}}{1 - \left(1 - \Phi_{ij} K_{c,ij}\right)\left(\exp(-P_{e,ij})\right)} \tag{S7}$$

where Φ_{ij} is a partition coefficient, and λ_{ij} is a ratio between the solute radius $r_{s,j}$ (sub-index for a solute is j) and pore radius r_i (sub-index for a pore-size-class in the discrete method is i):

$$\Phi_{ij} = \left(1 - \lambda_{ij}\right)^2 \tag{S8}$$

$$\lambda_{ij} = \frac{r_{s,j}}{r_i} \tag{S9}$$

Therefore, it is assumed that the steric behavior between the solute and pore wall occurs. Then, the solute convective $K_{c,ij}$ and diffusive $K_{d,ij}$ hindrance factors are expressed as following:

$$K_{c,ij} = \left(2 - \Phi_{ij}\right)\left(1 + 0.054\lambda_{ij} - 0.988\lambda_{ij}^2 + 0.44\lambda_{ij}^3\right) \tag{S10}$$

$$K_{d,ij} = 1 - 2.3\lambda_{ij} + 1.154\lambda_{ij}^2 + 0.224\lambda_{ij}^3 \tag{S11}$$

The Peclet number ($P_{e,ij}$) characterizing the pore flow is defined as:

$$P_{e,ij} = \frac{K_{c,ij}}{K_{d,ij} D_{s,j}} \left(\frac{r_i^2 \Delta P}{8\mu_{p,i}} \right) \tag{S12}$$

Diffusivity $D_{s,ij}$ of a solute with the radius $r_{s,j}$ is calculated using the Stokes–Einstein equation:

$$D_{s,ij} = \frac{kT}{6\pi\mu_{p,i} r_{s,j}} \tag{S13}$$

where k is the Boltzmann constant and T is temperature. To solve the above equation, the Wilke–Chang formula can be used to estimate the solute diffusivity:

$$D_{s,ij} = 7.4 \times 10^{-8} \frac{T\sqrt{\phi M_{solv}}}{\mu_{p,i} V_{m,j}^{0.6}} \tag{S14}$$

where M_{solv} is the molecular weight (MW) of the solvent molecule, ϕ is a dimensionless solvent parameter and $V_{m,j}$ is the solute molar volume (in cm^3 g mol^{-1}). If rejection $R(r)$ is a continuous function of the pore radius r, PDF $f_R(r)$ is introduced to describe the pore size distribution:

$$f(r) = \frac{1}{r\sqrt{2\pi b}} \exp\left[-\frac{\left(\log(r/r^*) + b/2\right)^2}{2b} \right] \tag{S15}$$

$$b = \log\left[1 + \left(\frac{\sigma}{r^*} \right)^2 \right] \tag{S16}$$

To calculate the function $f(r)$, the mean pore radius (r^*) and the standard deviation (σ) need to be estimated. For simplification, the distribution function is truncated to r_{max}:

$$\frac{f'_R(r)}{f_R(r)} = \frac{1}{\int_0^{r_{max}} f_R(r)dr} \tag{S17}$$

The overall rejection over the pore radii $0 < r < r_{max}$ can now be calculated using the following expression:

$$R_j = \frac{\int_0^{r_{max}} f'_R(r) r^4 R(r)/\mu(r) dr}{\int_0^{r_{max}} f'_R(r) r^4/\mu(r) dr} \tag{S18}$$

Implementing the above models, the mean pore size and the standard deviation can be fitted by minimizing the error.

3. Molecular dynamics (MD) simulations

Molecular dynamics (MD) simulations were performed using the Materials Studio 8.0 software and COMPASS (Condensed-phase Optimized Molecular Potentials for Atomistic Simulation Studies) force field. Energy-minimized amorphous cells of the four PEEK polymers were constructed using five chains of five repeat units each; the experimental geometric density of each polymer at the temperature of 298 K were used as simulation constraints.[5,6] Long-range Coulombic interactions were taken into account with the Ewald sum method, and the nonbonded energy was calculated with a cutoff distance of 9.5 Å. A probe radius of 1.65 Å was used to calculate the fractional free volume:

$$FFV = \frac{V_f}{V_f + V_o} \quad \text{(S19)}$$

where V_f and V_o, respectively, are the free volume and occupied volume of the polymer chains in a cell.

Interaction of monomers of iPEEK-SBI, iPEEK-TB, and iPEEK-Trip with acetonitrile, acetone, ethanol, methyl-ethyl-ketone, and n-hexane solvents were studied with density functional theory using the M062X/6-31G* level of theory (Gaussian 09 program). The binding energy between the polymer and solvent was calculated for the relaxed geometry. To understand the conformational changes of the iPEEK-SBI, iPEEK-TB, and iPEEK-Trip polymers in the above mentioned solvents, classical molecular dynamics simulations were performed with a single chain (consists of five repeat units) of each polymer using the COMPASS force field and Forcite module of the Materials Studio 2019 software. Throughout the simulations, 298 K were maintained by Nose-Hover thermostat. Employing a time step of 1 fs, the simulations were continued for 2000 ps in a NVT ensemble.

4. Characterization

4.1. Monomer characterization (^{1}H & ^{13}C NMR)

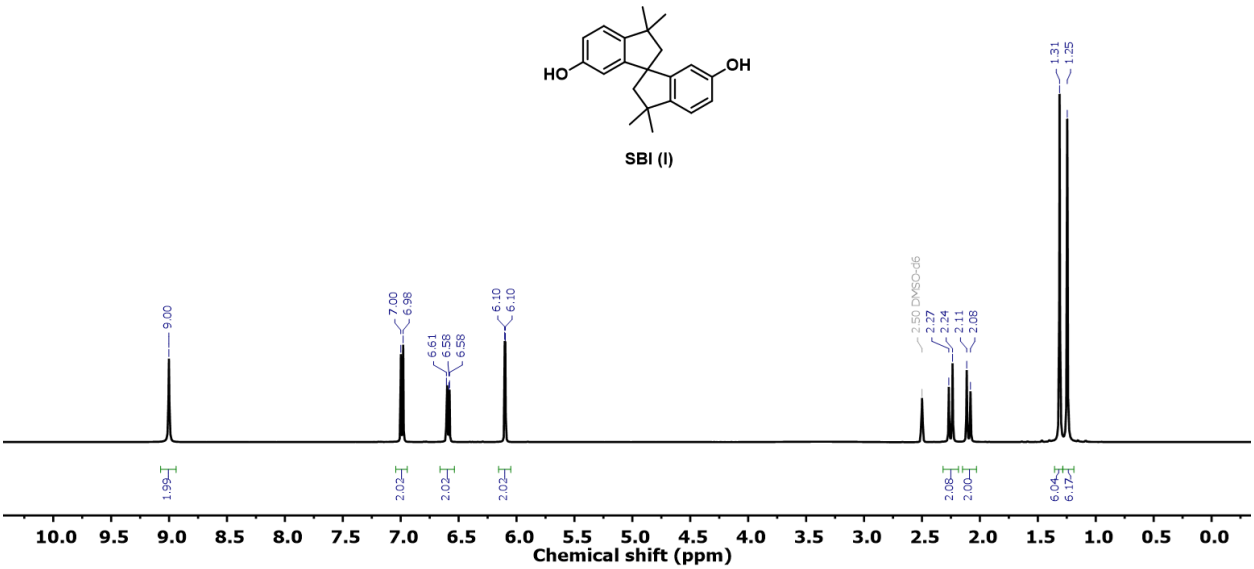


Fig. S2 ^{1}H NMR spectrum of 3,3,3',3'-tetramethyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-6,6'-diol (SBI) (I) in DMSO-d_6

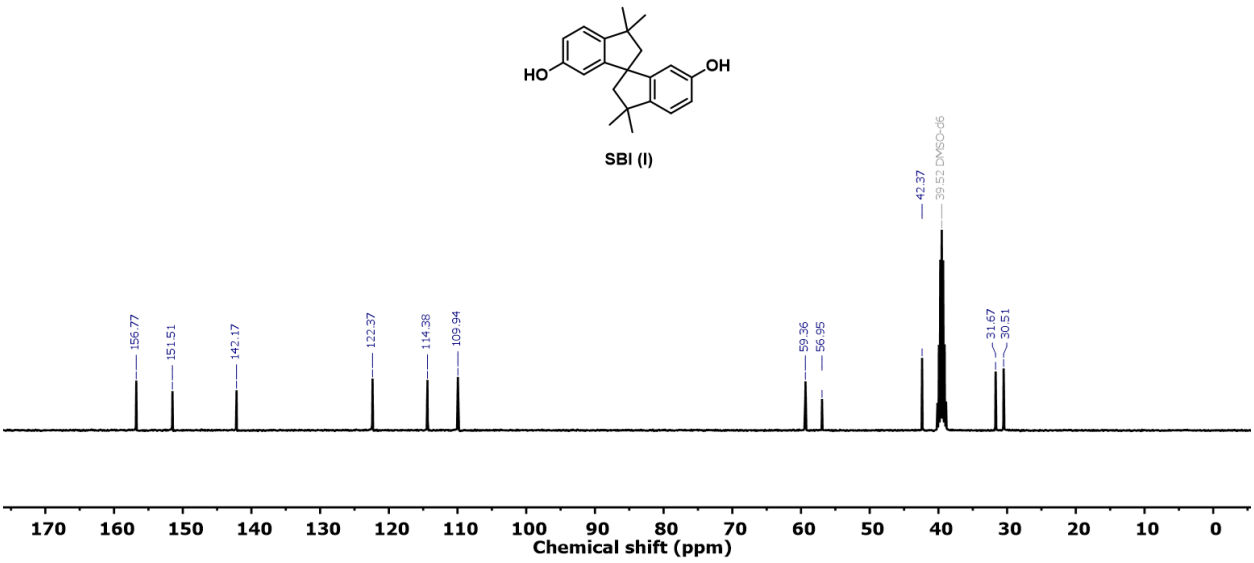


Fig. S3 ^{13}C NMR spectrum of 3,3,3',3'-tetramethyl-2,2',3,3'-tetrahydro-1,1'-spirobi[indene]-6,6'-diol (SBI) (I) in DMSO-d_6

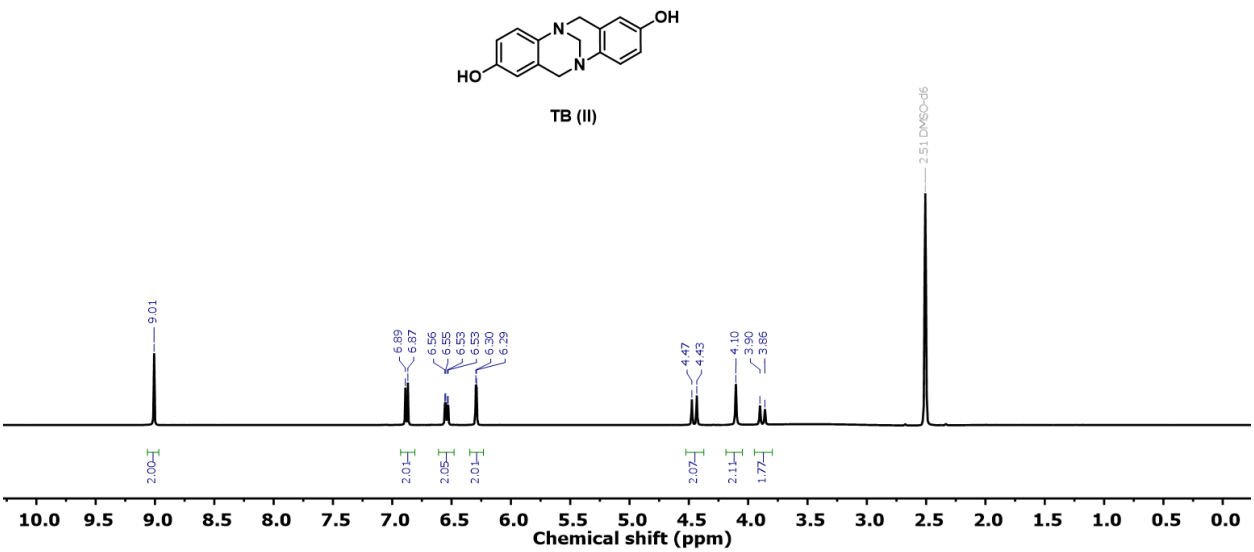


Fig. S4 1H NMR spectrum of 6H,12H-5,11-methanodibenzo[b,f][1,5]diazocine-2,8-diol (TB) (II) in DMSO-d_6

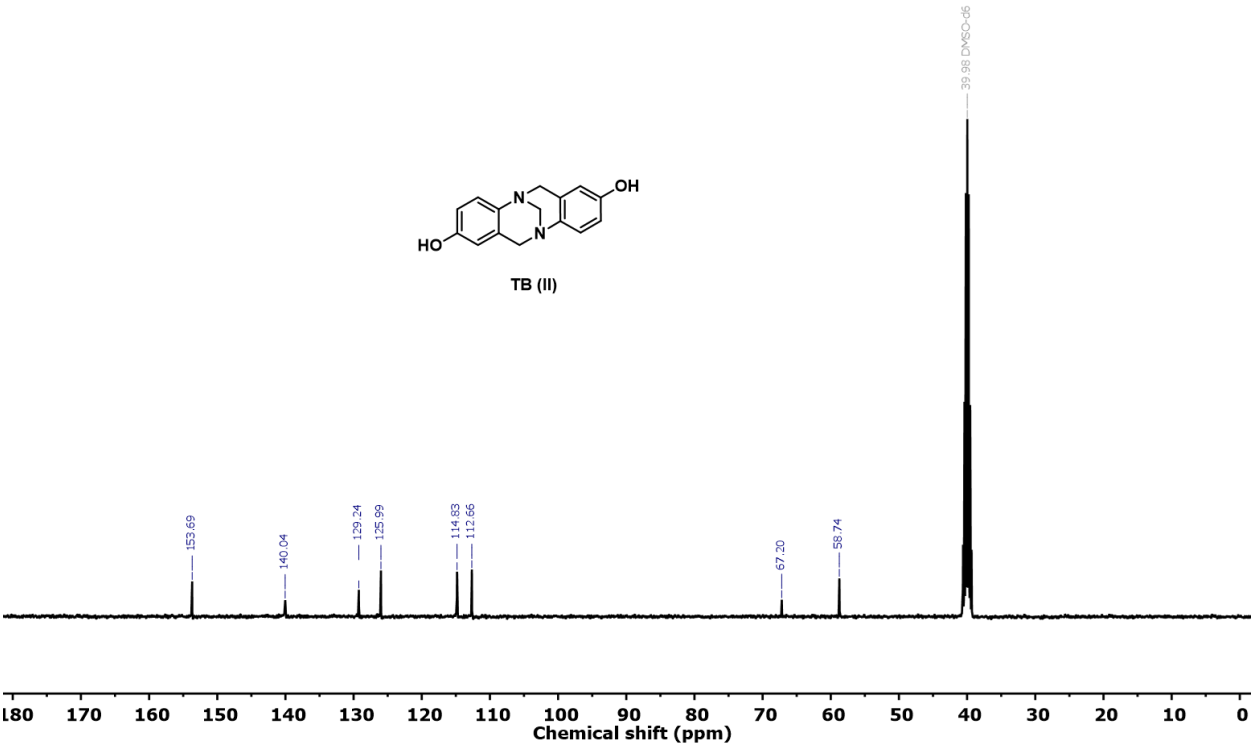


Fig. S5 ^{13}C NMR spectrum of 6H,12H-5,11-methanodibenzo[b,f][1,5]diazocine-2,8-diol (TB) (II) in DMSO-d_6

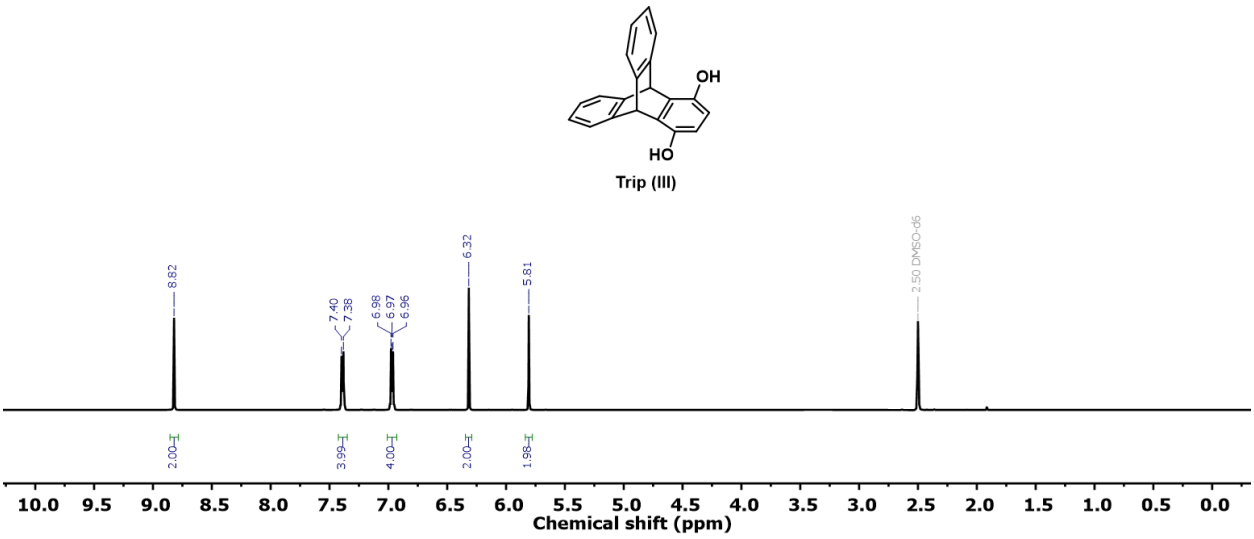


Fig. S6 ^{1}H NMR of (9s,10s)-9,10-dihydro-9,10-[1,2]benzenoanthracene-1,4-diol in DMSO-d_6.

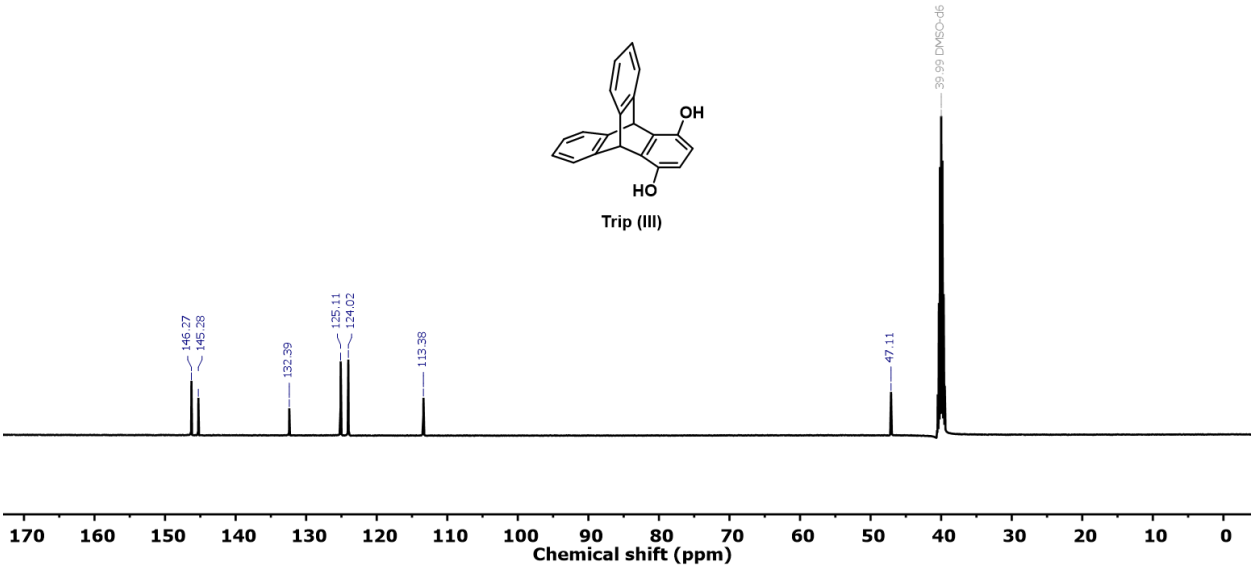


Fig. S7 ^{13}C NMR of (9s,10s)-9,10-dihydro-9,10-[1,2]benzenoanthracene-1,4-diol in DMSO-d_6.

4.2. Polymer characterization

4.2.1. ^{1}H & ^{13}C NMR spectra

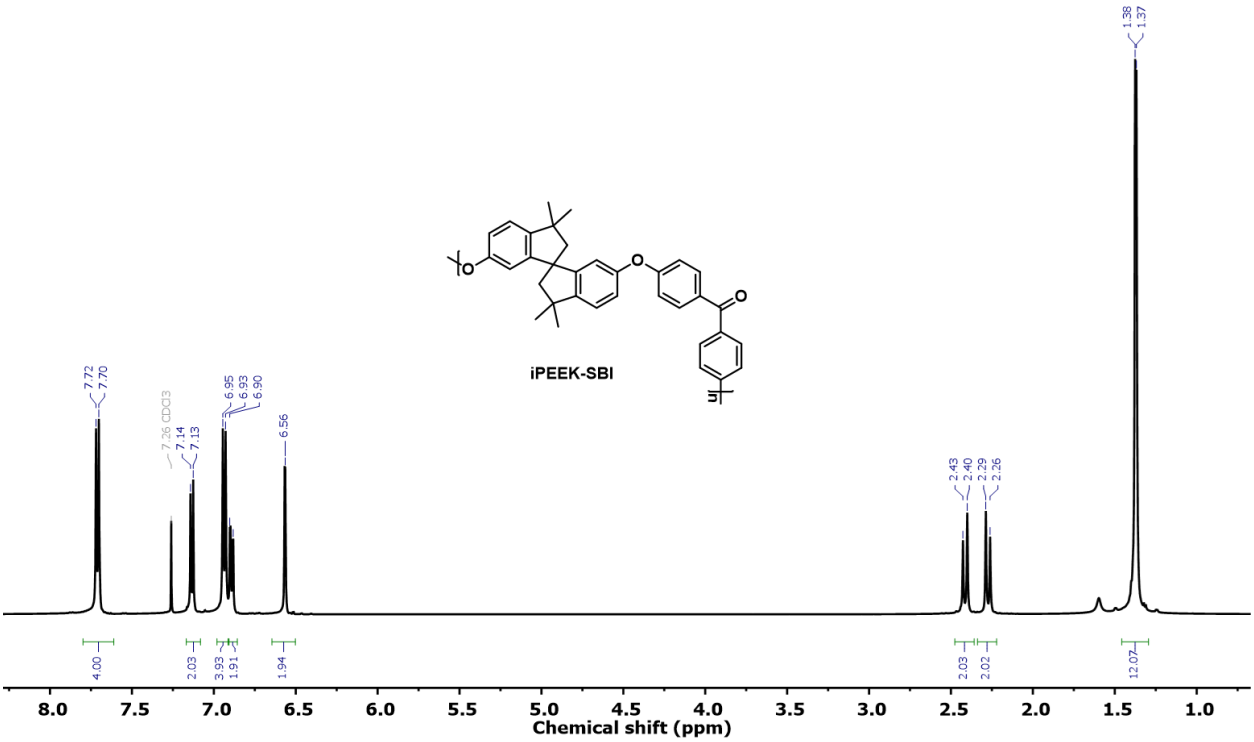


Fig. S8 ^{1}H NMR spectrum of iPEEK-SBI in $CDCl_3$.

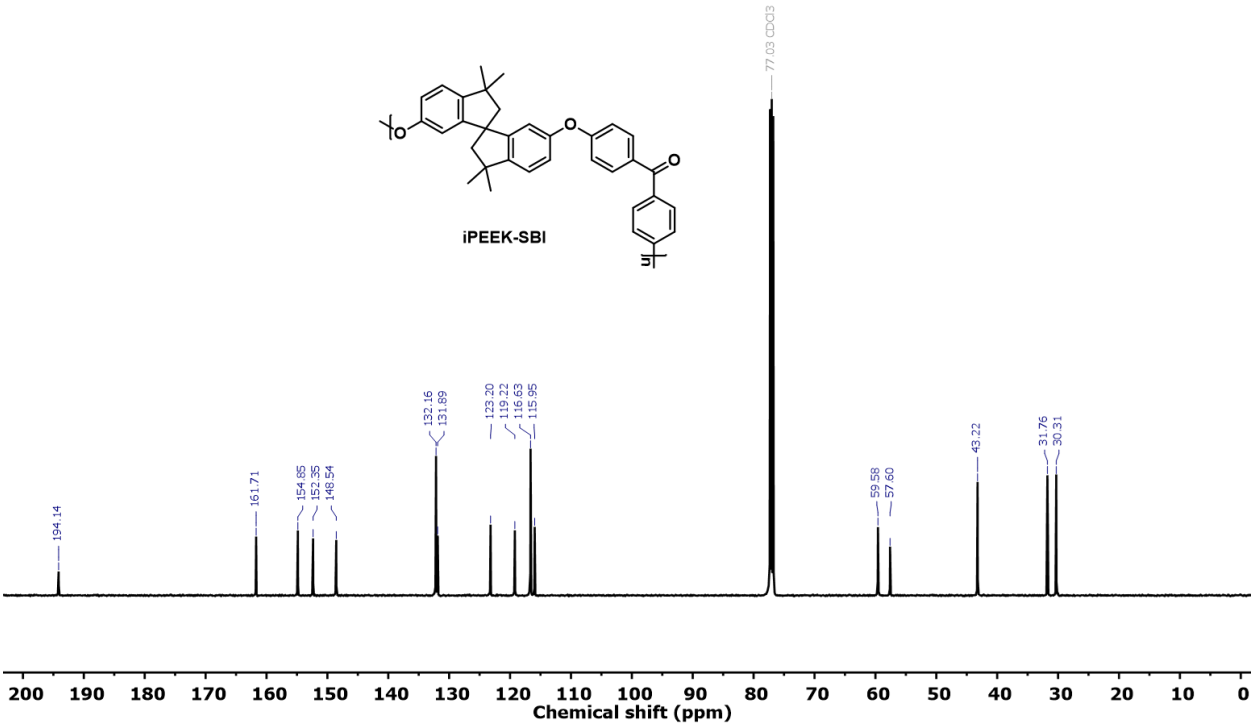


Fig. S9 ^{13}C NMR spectrum of iPEEK-SBI in $CDCl_3$.

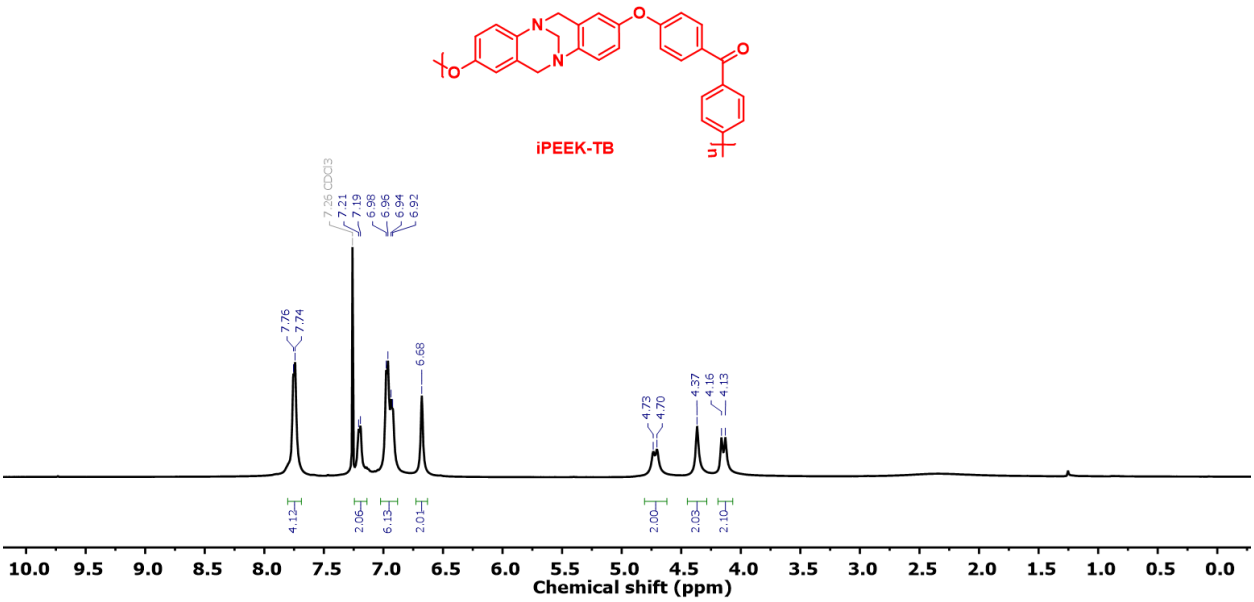


Fig. S10 ^{1}H NMR spectrum of iPEEK-TB in $CDCl_3$.

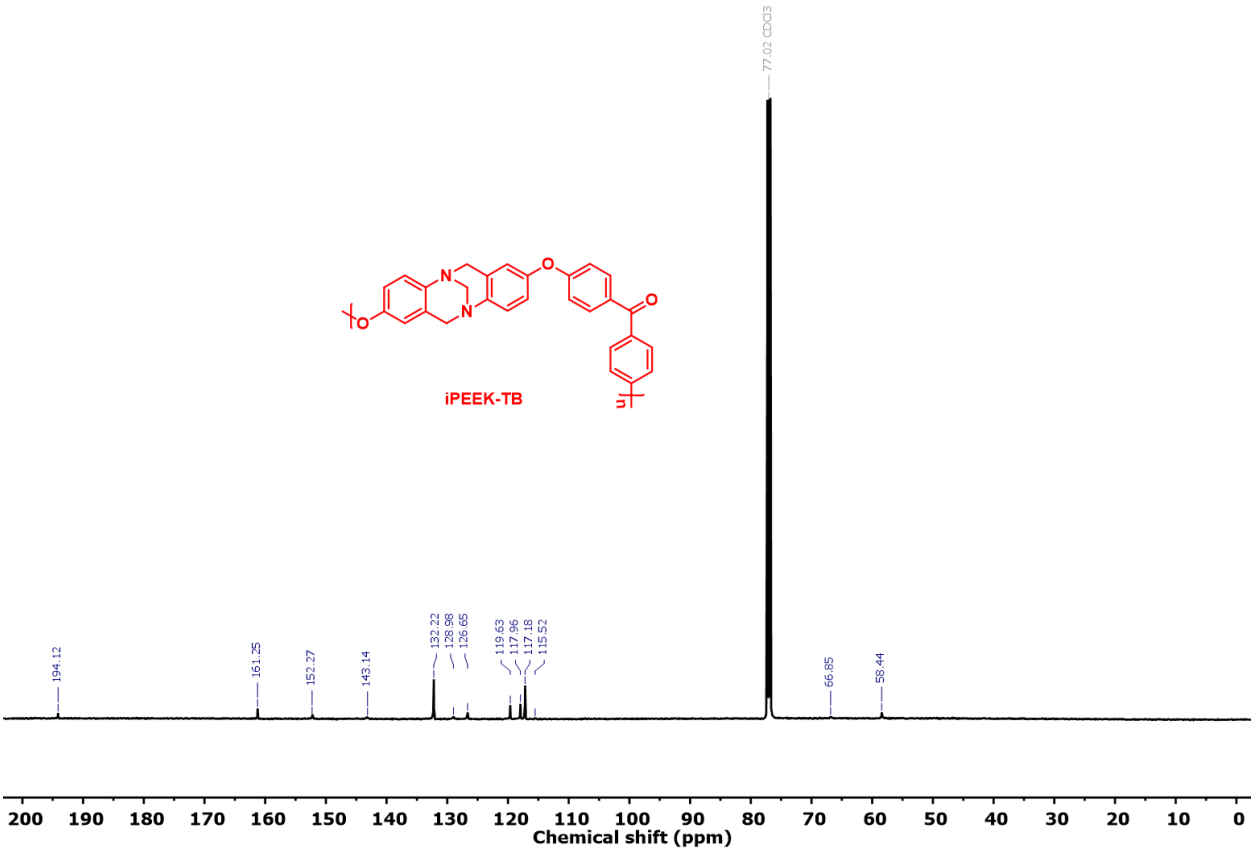


Fig. S11 ^{13}C NMR spectrum of iPEEK-TB in $CDCl_3$.

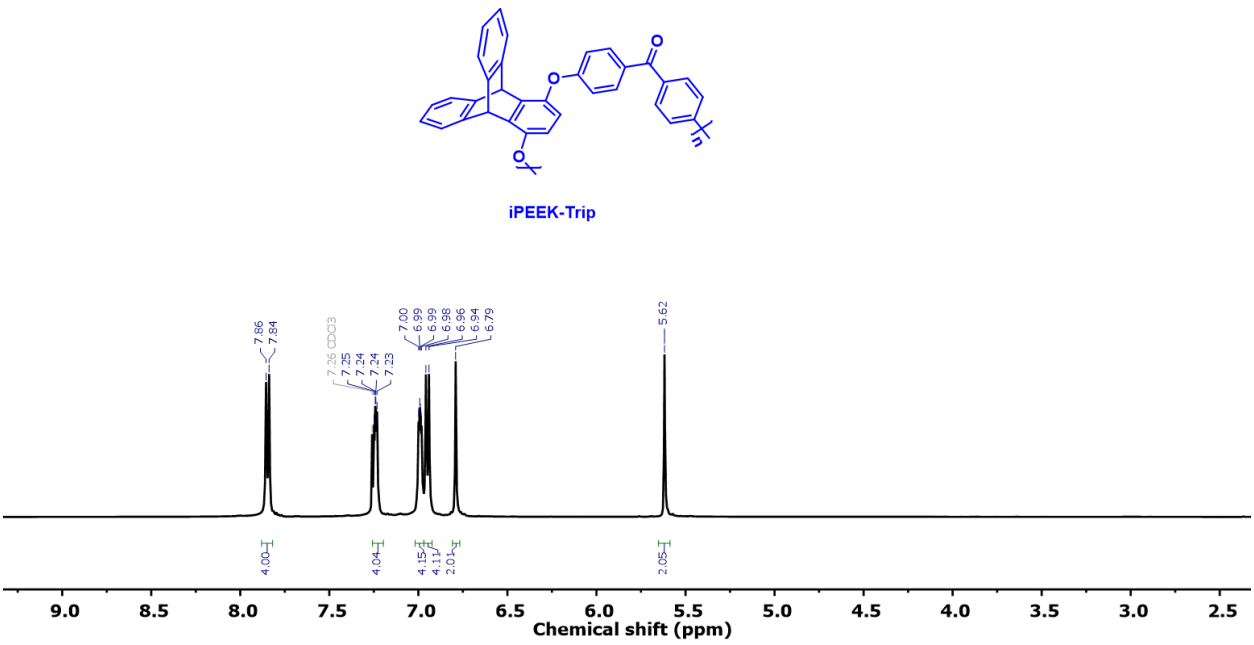


Fig. S12 ^{1}H NMR spectrum of iPEEK-Trip in $CDCl_3$.

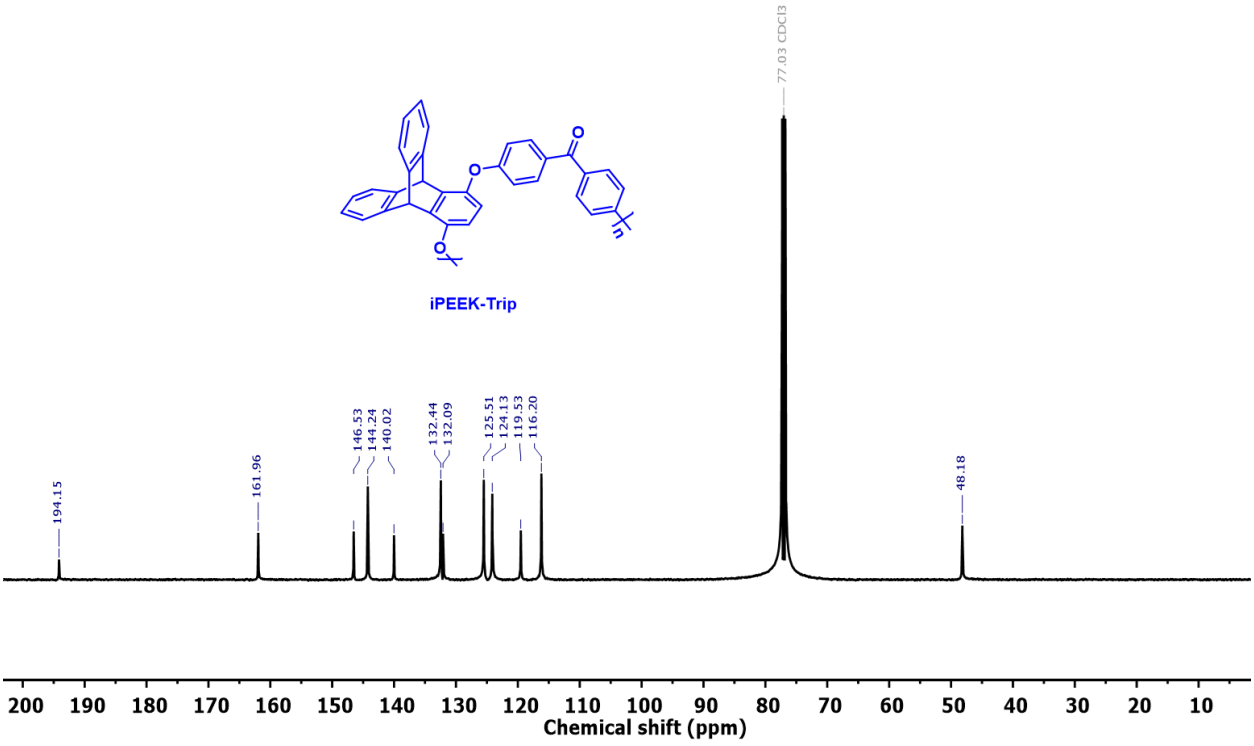


Fig. S13 ^{13}C NMR spectrum of iPEEK-Trip in $CDCl_3$.

4.2.2. Solubility tests

Table S2 iPEEK solubility in esters

Polymer	EtOAc	γ-Valerolactone	Butyl acetate	Propylene carbonate	Dimethyl carbonate	Ethyl lactate
iPEEK-SBI	--	--	++	--	--	--
iPEEK-TB	--	--	--	--	--	--
iPEEK-Trip	--	--	--	--	--	--

Table S3 iPEEK solubility in ethers

Polymer	CPME	DEE	Dioxane	Eucalyptol	Cyrene	MeTHF	THF
iPEEK-SBI	++	--	++	--	++	++	++
iPEEK-TB	--	--	++	--	--	--	--
iPEEK-Trip	--	--	++	--	--	++	++

Table S4 iPEEK solubility in alcohols

Polymer	MeOH	EtOH	IPA	Glycerol	Cyclohexanol	n-Butanol	Ethyl lactate
iPEEK-SBI	--	--	--	--	--	--	--
iPEEK-TB	--	--	--	--	--	--	--
iPEEK-Trip	--	--	--	--	--	--	--

Table S5 iPEEK solubility in ketones

Polymer	MEK	Acetone	Cyclohexanone	Cyclopentanone
iPEEK-SBI	--	--	++	++
iPEEK-TB	--	--	--	--
iPEEK-Trip	--	--	++	++

Table S6 iPEEK solubility in chlorinated solvents

Polymer	Dichlorobenzene	Trichlorobenzene	CH_3Cl	DCM
iPEEK-SBI	++	++	++	++
iPEEK-TB	++	++	++	--
iPEEK-Trip	++	++	++	++

Table S7 iPEEK solubility in polar aprotic solvents (PAS)

Polymer	NMP	DMAc	DMF	DMSO	Sulfolane	MeCN	Polarclean
iPEEK-SBI	++	++	--	--	--	--	++
iPEEK-TB	++	--	--	--	--	--	--
iPEEK-Trip	++	++	++	--	--	--	++

Table S8 iPEEK solubility in hydrocarbons

Polymer	Heptane	Hexane	Toluene	Iso-octane	Cyclohxane	α-Pinene
iPEEK-SBI	--	--	++	--	--	--
iPEEK-TB	--	--	--	--	--	--
iPEEK-Trip	--	--	--	--	--	--

Table S9 iPEEK solubility in acids

Polymer	H_2SO_4	MSA
iPEEK-SBI	++	++
iPEEK-TB	++	++
iPEEK-Trip	++	++

4.2.3. Thermal glass transition temperature (T_g)

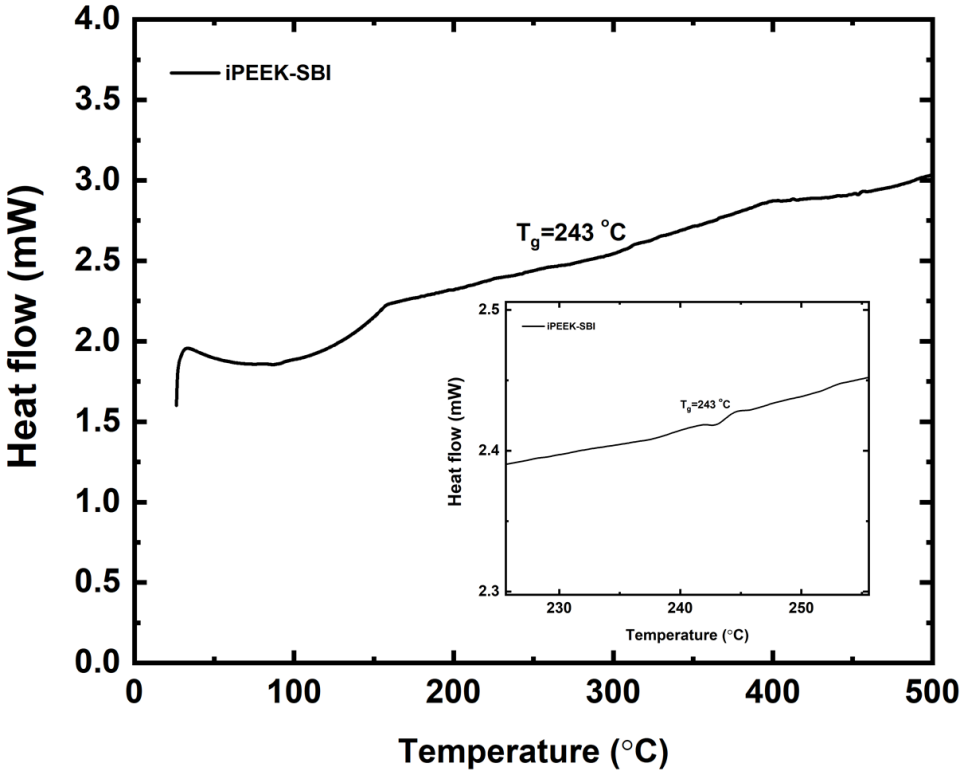


Fig. S14 DSC scan of iPEEK-SBI for T_g determination.

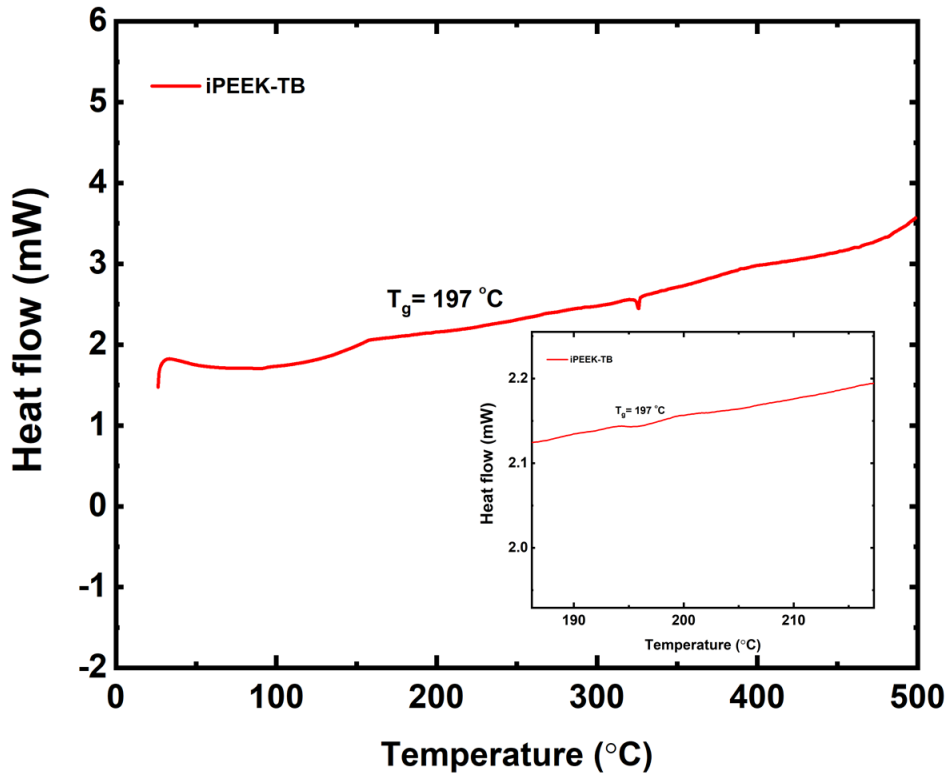


Fig. S15 DSC scan of iPEEK-TB for T_g determination.

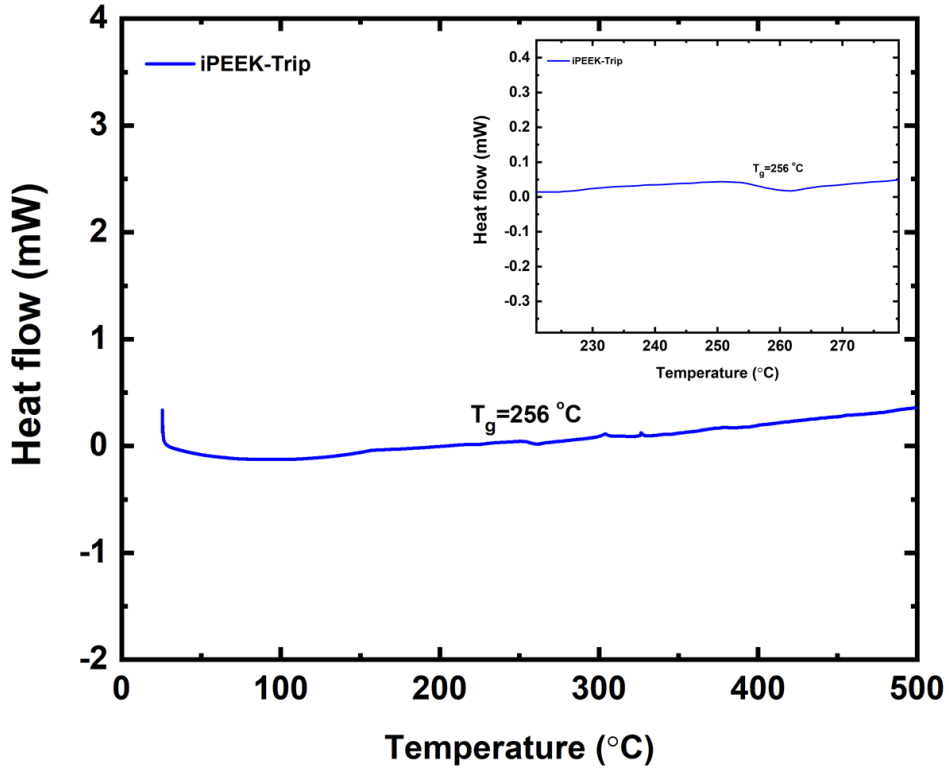


Fig. S16 DSC scan of iPEEK-Trip for T_g determination.

4.2.4. Wide-angle X-ray diffraction

Table S10 2θ and d-spacing measurements obtained from WXRD taking into consideration peak deconvolution using 2nd derivative with Quadratic Savitzky-Golay method, for the four polymers.

Polymer	2θ (degree)	d-spacing (Å)[a]
iPEEK-SBI	12.16	7.3
	17.8	5.0
	20.1	4.4
iPEEK-TB	10.9	8.1
	18.05	4.9
	27.2	3.3
iPEEK-Trip	11.9	7.4
	13.14	6.7
	19.9	4.5
PEEK	19.26	4.6
	21.28	4.2
	23.32	3.8
	26.41	3.4
	29.35	3.0
	33.47	2.7
	39.32	2.3
	41.49	2.2
	47.88	1.9

[a] Calculated from $n\lambda=2d\sin\theta$.

4.2.5. BET surface area analysis

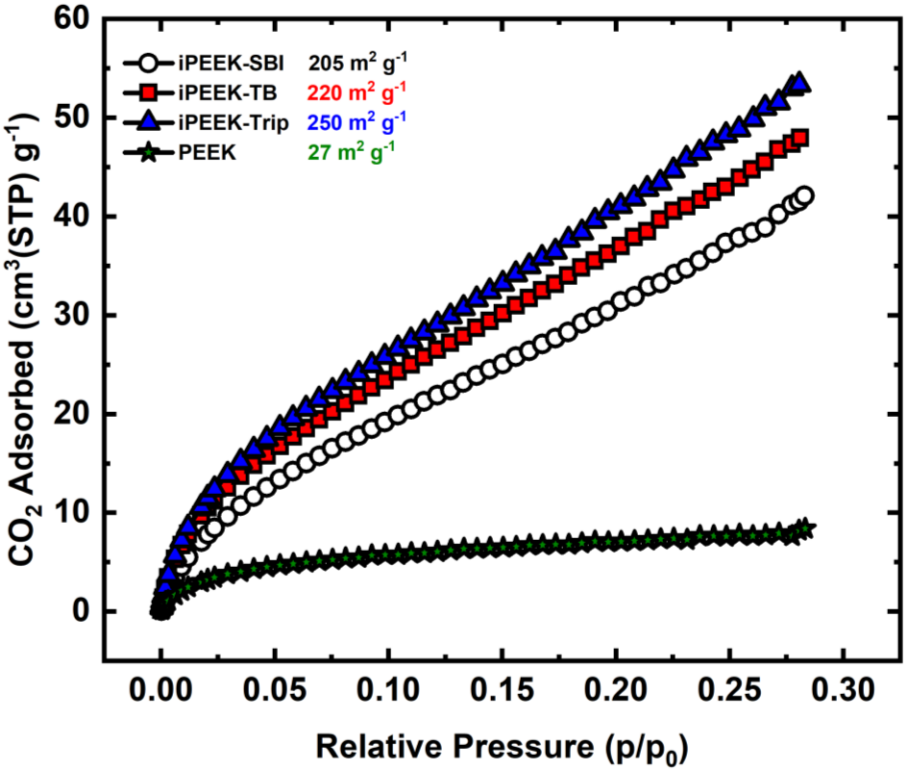


Fig. S17 CO_2 physisorption isotherms (at 0 °C) of iPEEK polymers and conventional PEEK (measured at relative pressure in the range of 0-0.3 with CO_2 pressure up to 10 bar.

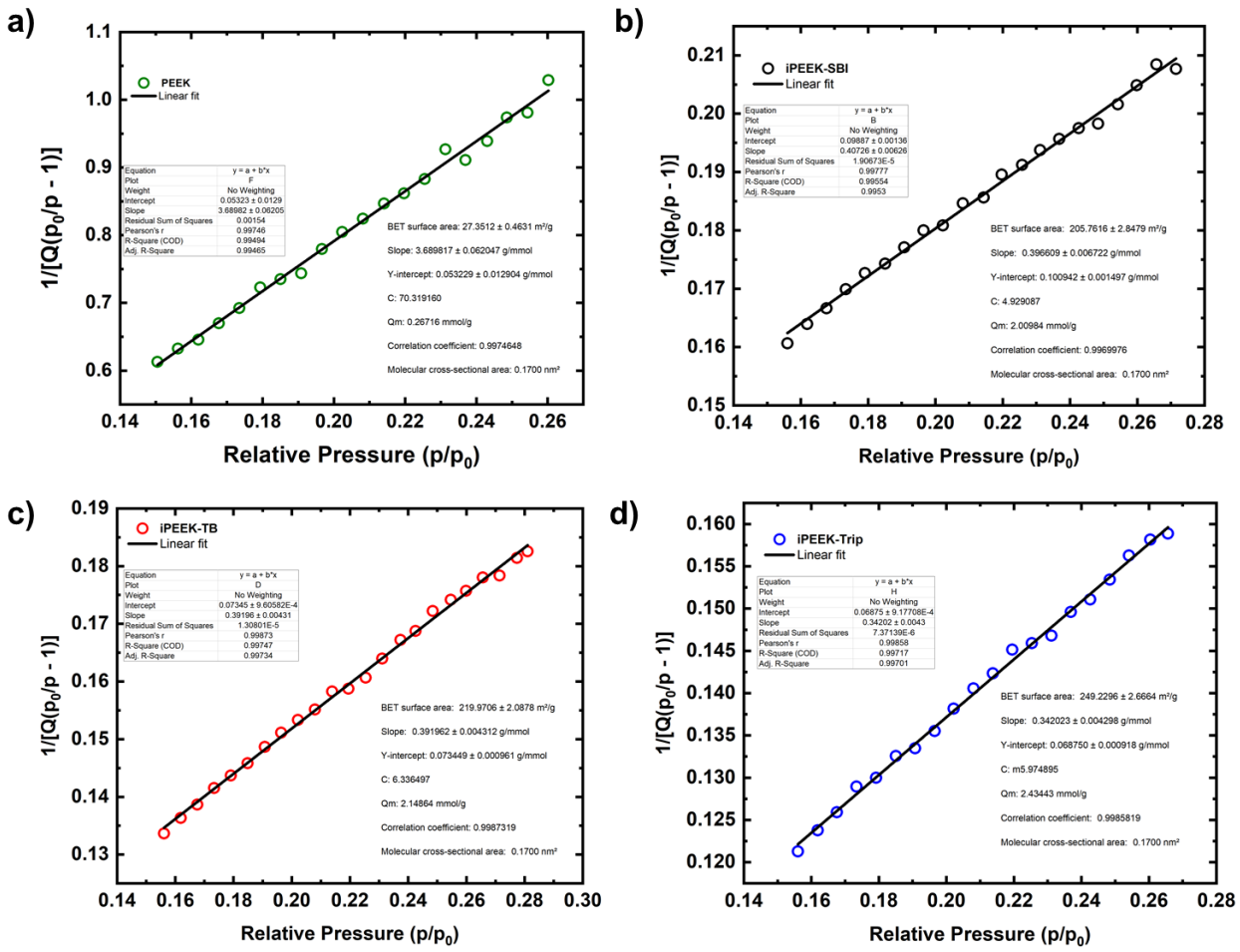


Fig. S18 BET surface area plots with linear fitting using a relative pressure range from 0.15 to 0.28 for BET calculation of a) PEEK; b) iPEEK-SBI; c) iPEEK-TB; and d) iPEEK-Trip.

4.3. Membrane characterization

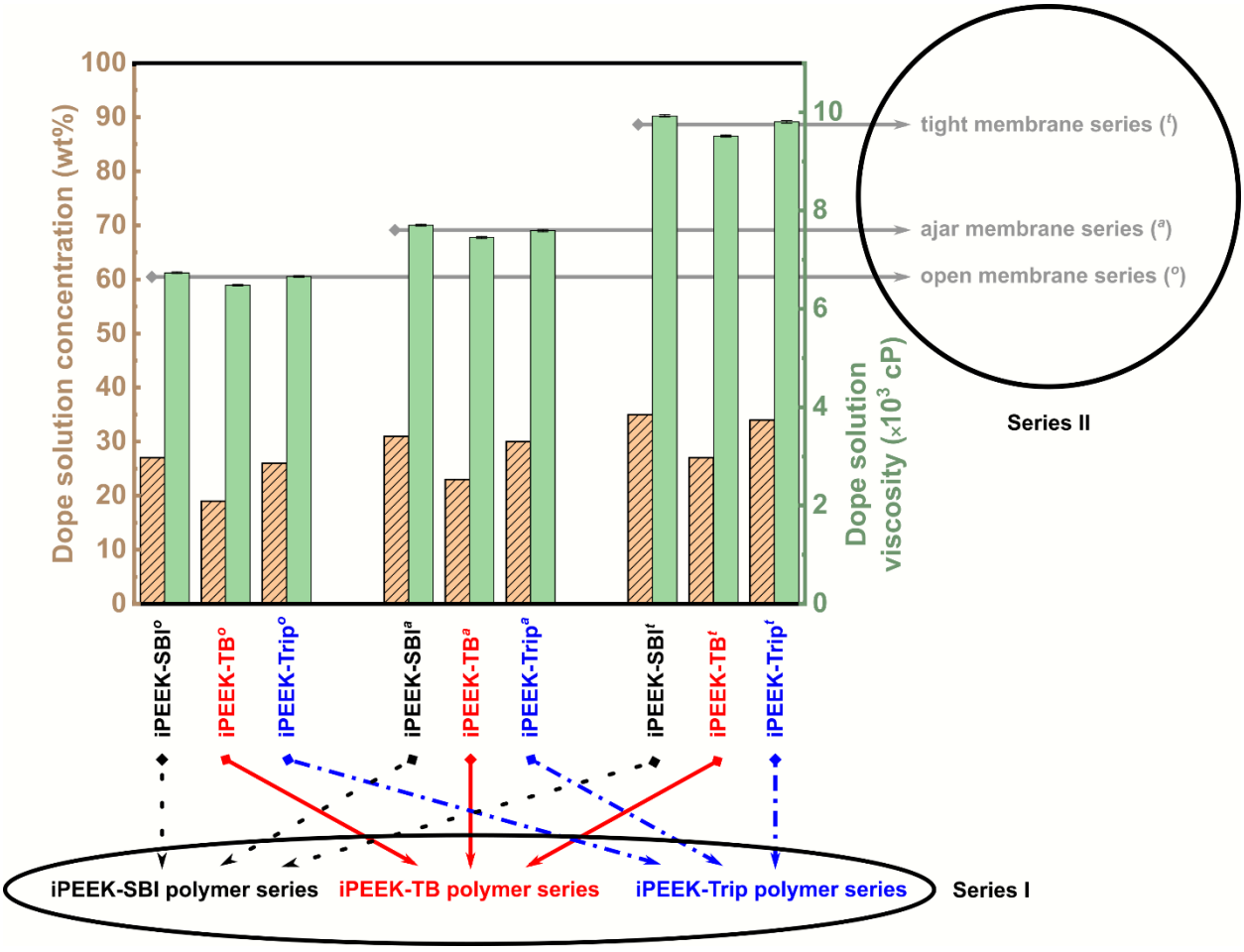


Fig. S19 Representation of the two types of membrane series. Series I is based on the polymer used to fabricate the membranes, while Series II is based on the tightness of the membranes. The latter series was achieved by having similar dope solution viscosities resulting in clusters named as open (obtained from lower viscosity dope solutions), ajar (obtained from medium viscosity dope solutions) and tight (obtained from higher viscosity dope solutions). Refer to **Table 2** for the actual values.

4.3.1. FT-IR

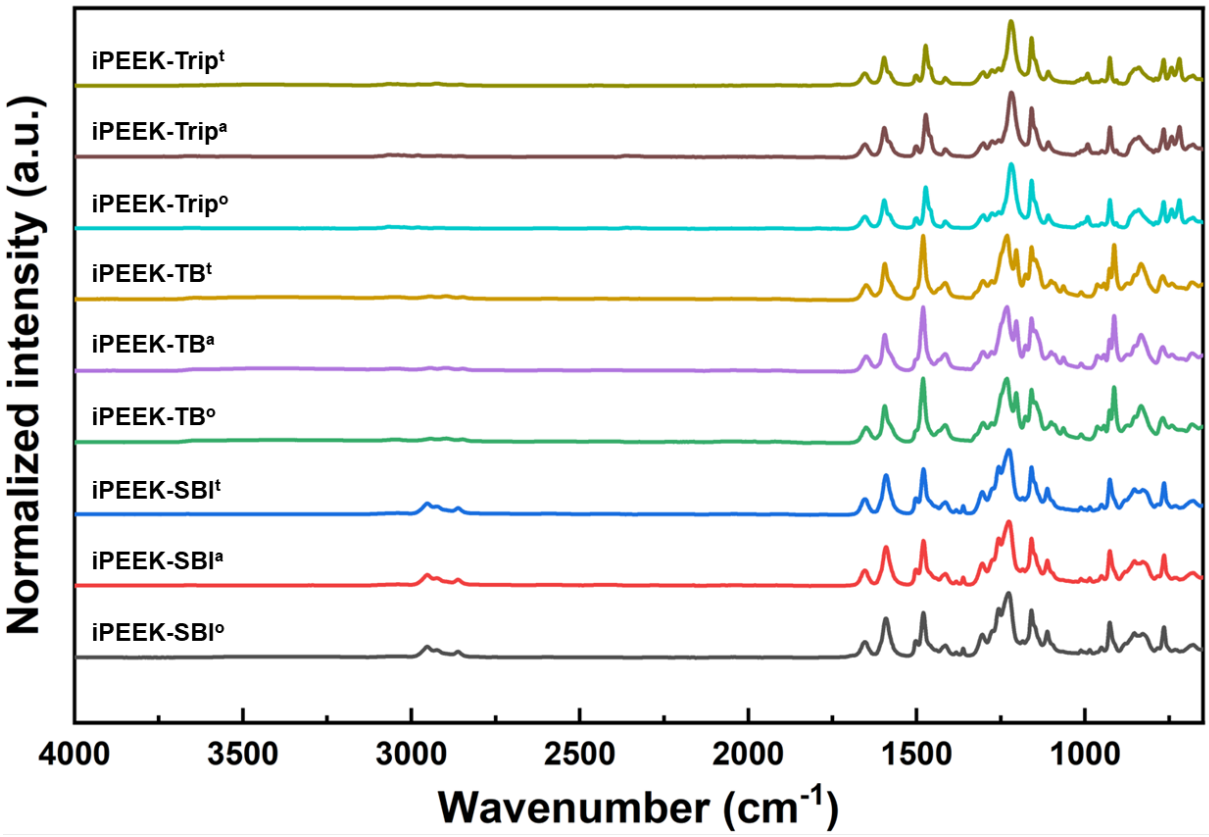


Fig. S20 FTIR spectra of the iPEEK membranes with different dope solution concentrations.

4.3.2. Nanoindentation

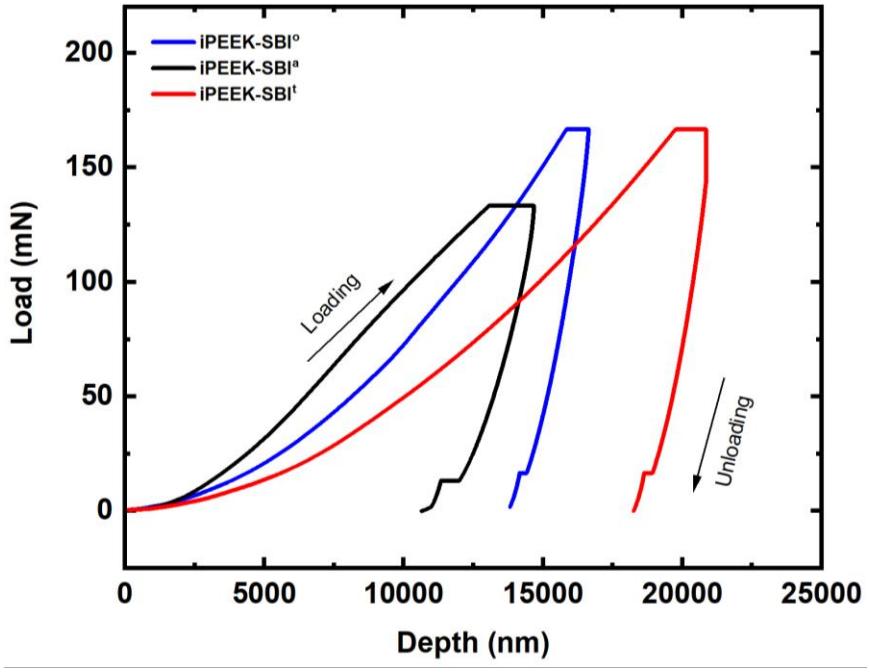


Fig. S21 Mechanical properties of the three iPEEK-SBI membranes obtained by Nanoindentation technique.

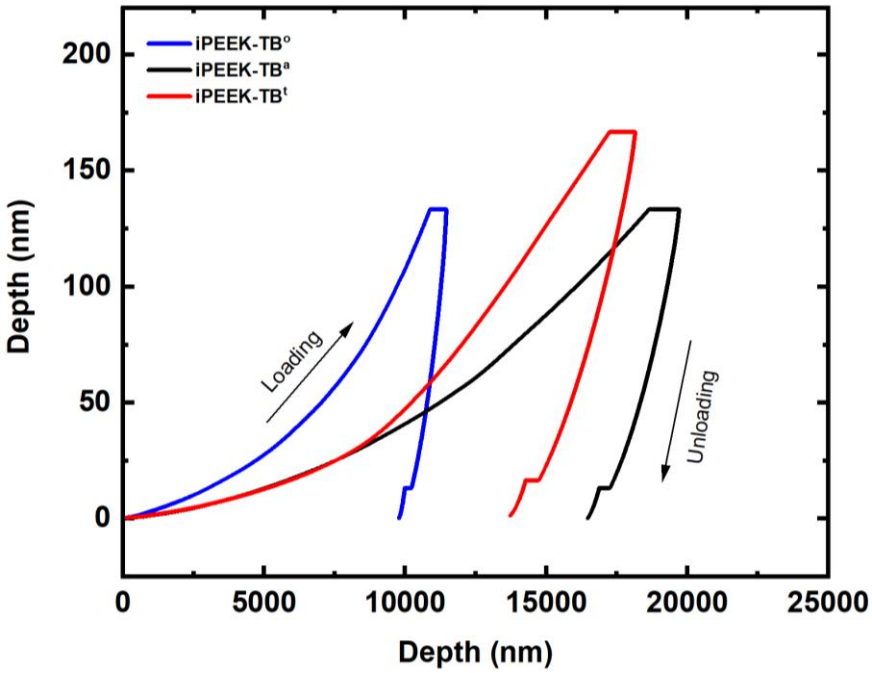


Fig. S22. Mechanical properties of the three iPEEK-TB membranes obtained by Nanoindentation technique.

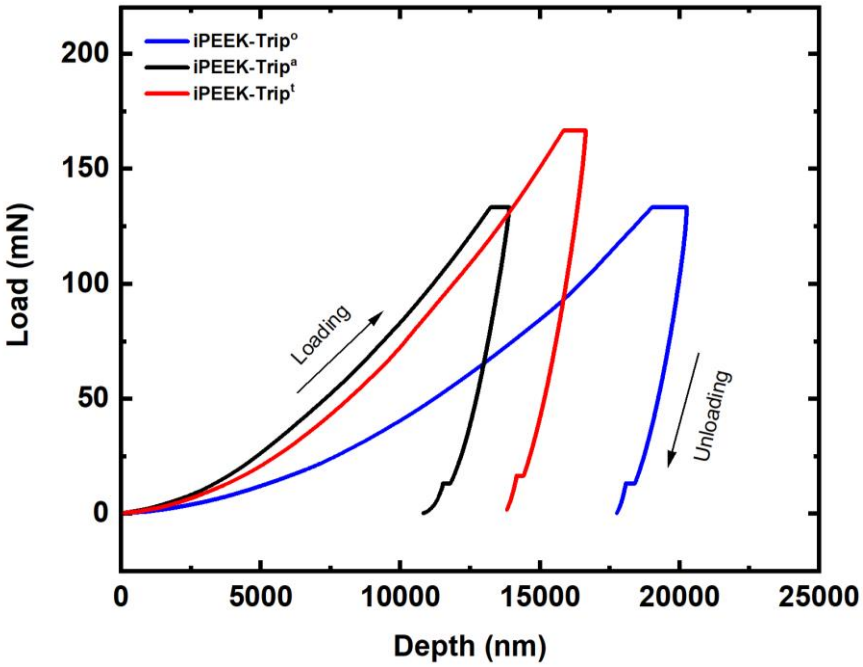


Fig. S23 Mechanical properties of the three iPEEK-Trip membranes obtained by Nanoindentation technique.

Fig. S24 Photos of iPEEK phase inversion membranes with high flexibility.

4.3.3. Atomic force microscopy (AFM)

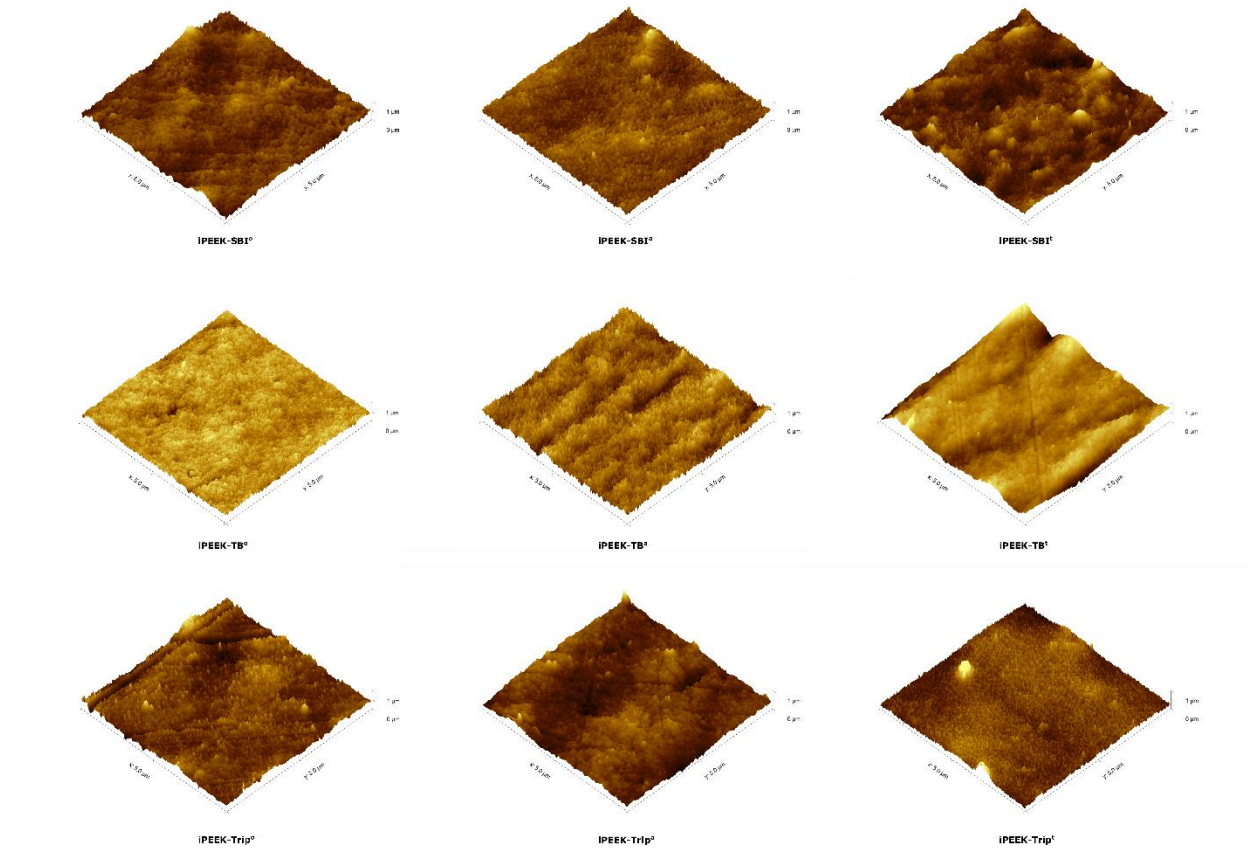


Fig. S25 5x5 µm AFM images for the nine iPEEK membranes.

4.3.4. Scanning electron microscopy (SEM)

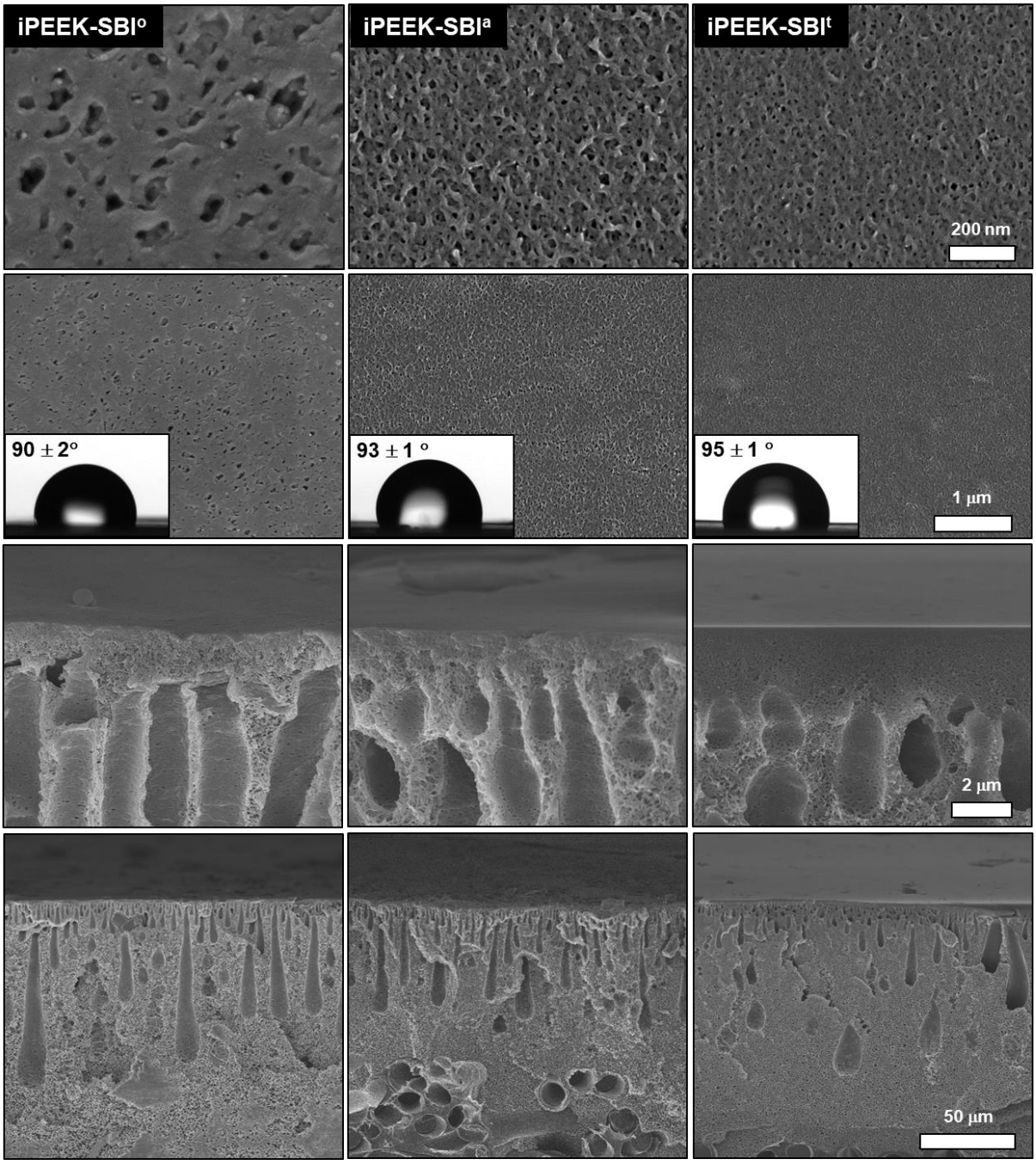


Fig. S26 The SEM surface and cross-sectional images of iPEEK-SBI membrane. Inset image is water contact angle of the

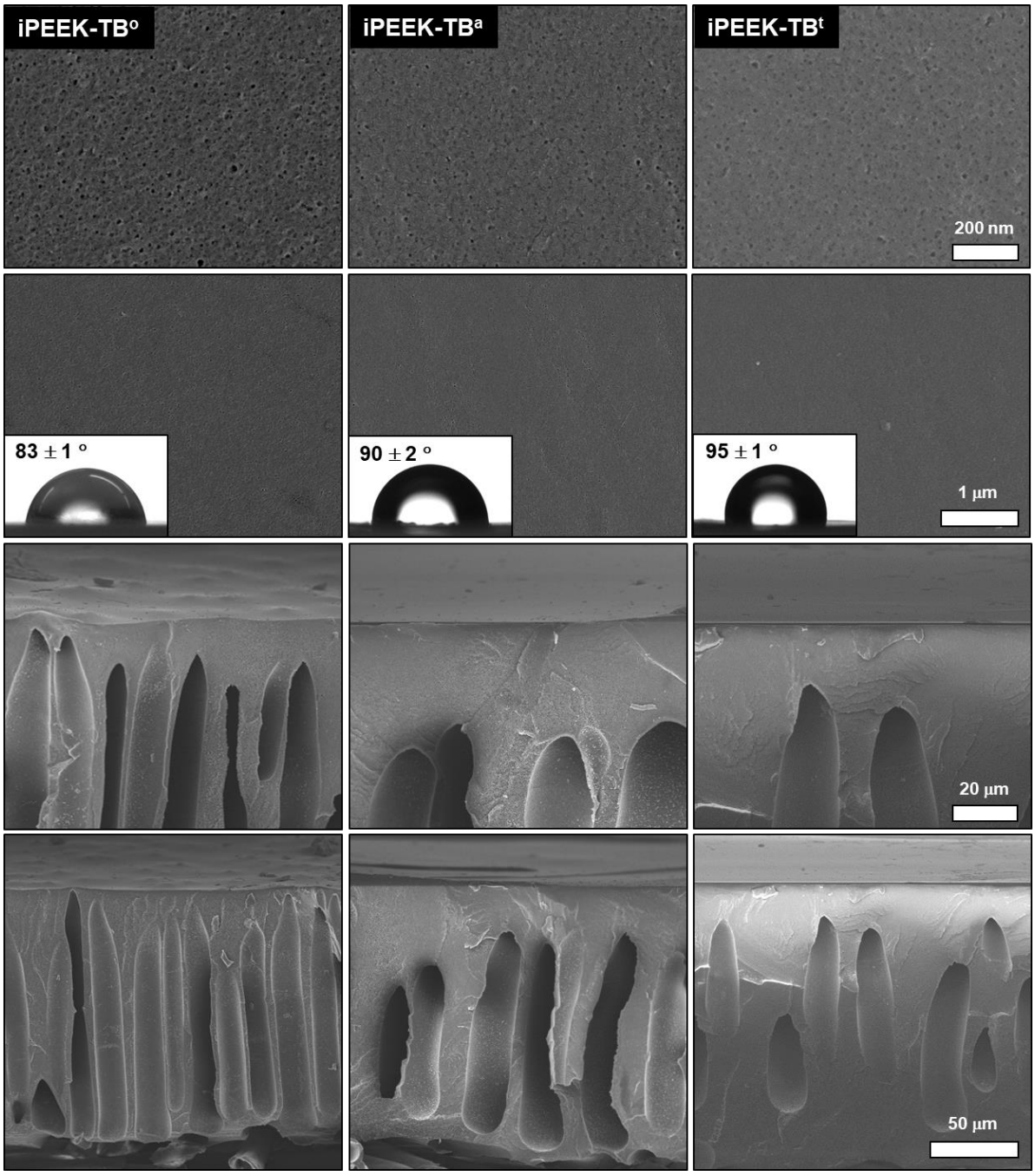


Fig. S27 The SEM surface and cross-sectional images of iPEEK-TB membrane. Inset image is water contact angle of the membrane surface.

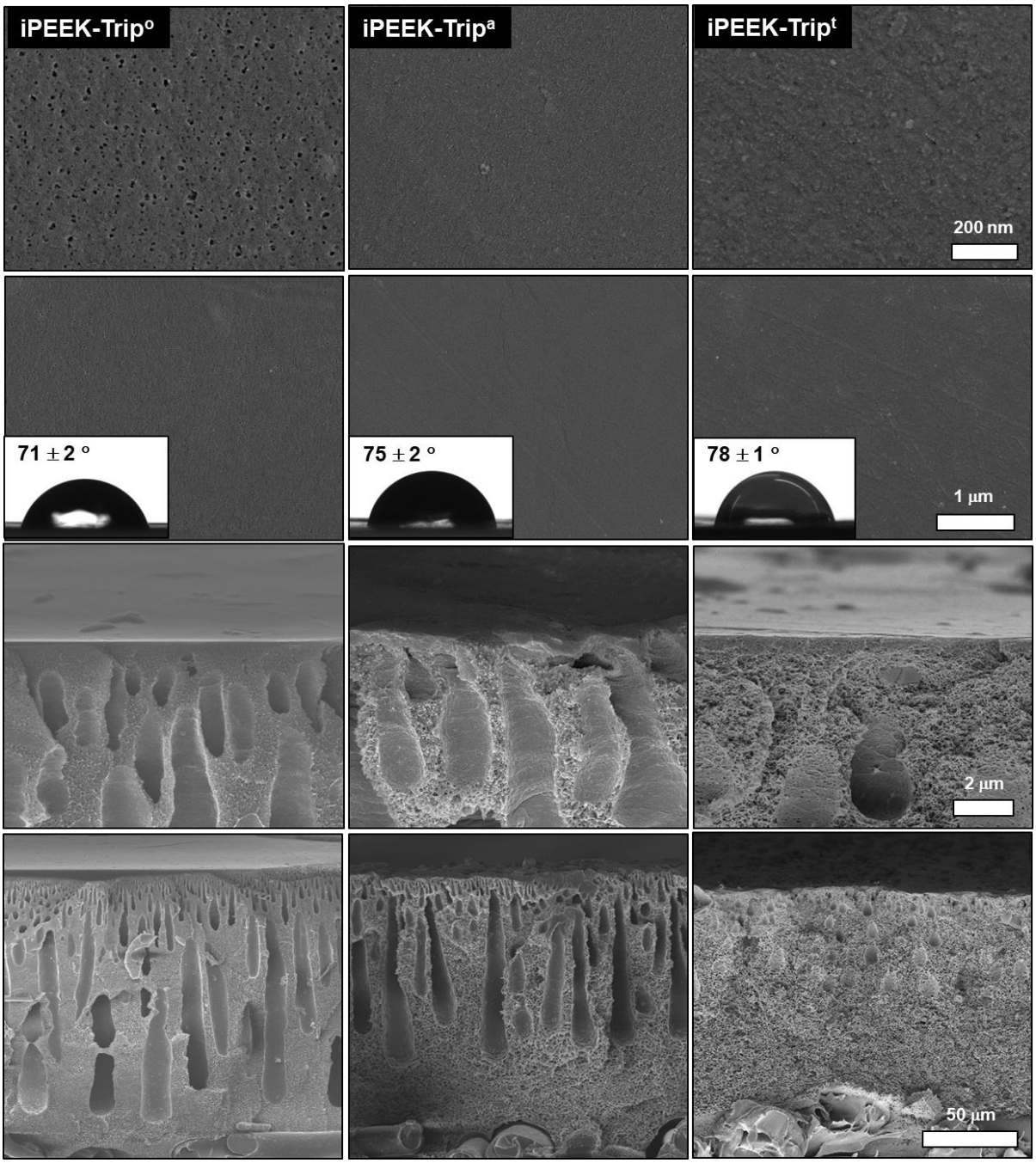


Fig. S28 The SEM surface and cross-sectional images of iPEEK-Trip membrane. Inset image is water contact angle of the membrane surface.

4.4. Membrane performance

4.4.1. Rejection profile

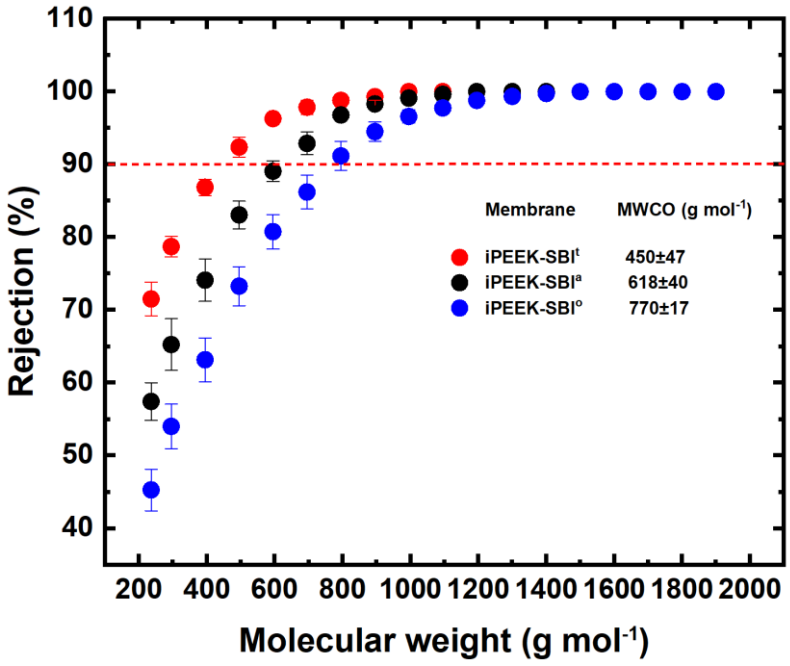


Fig. S29 The rejection profile of the iPEEK-SBI membranes obtained from acetonitrile using styrene oligomers.

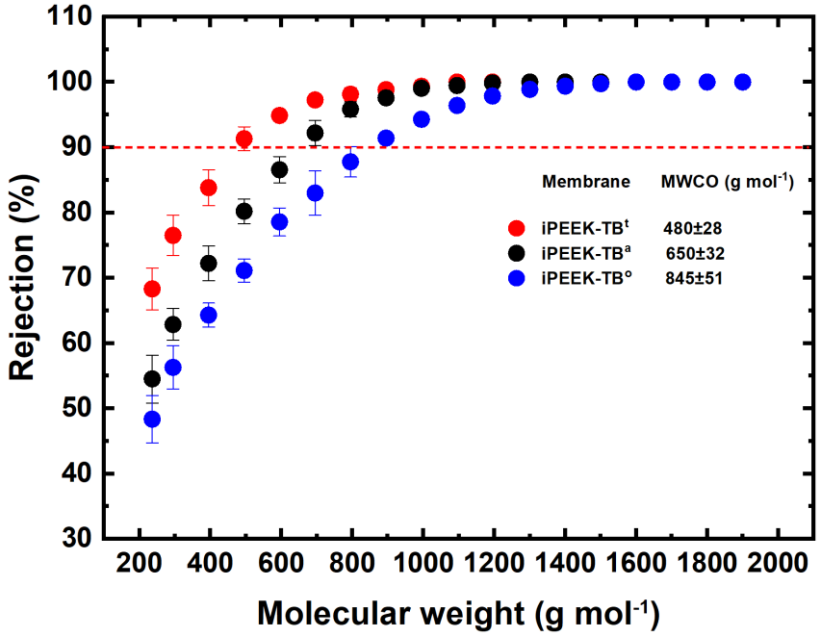


Fig. S30 The rejection profile of the iPEEK-TB membranes obtained from acetonitrile using styrene oligomers.

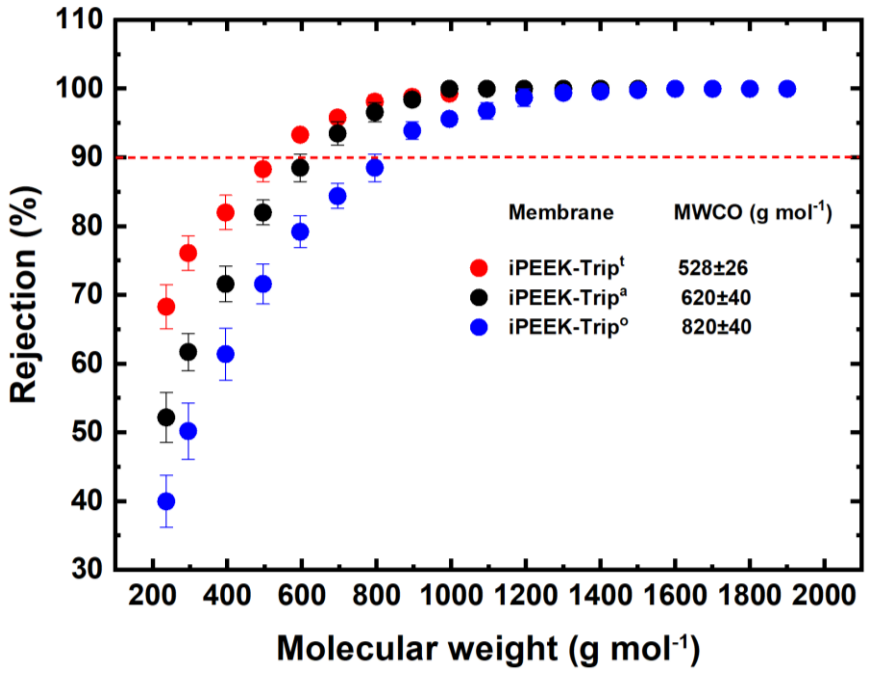


Fig. S31 The rejection profile of the iPEEK-Trip membranes obtained from acetonitrile using styrene oligomers.

4.4.2. Membrane permeance

Table S11 Permeances of the nine membranes prepared from three iPEEK polymers and tested with five different solvents.

	Permeance (L m^{-2} h^{-1} bar^{-1})				
Membrane code	**Acetonitrile (MeCN)**	**Hexane (Hex)**	**Methylethyl ketone (MEK)**	**Ethanol (EtOH)**	**Acetone (AcMe)**
iPEEK-SBI^{o}	7.81±0.25	3.36±0.13	5.38±0.18	6.87±0.21	8.14±0.25
iPEEK-SBI^{a}	5.51±0.28	2.41±0.13	4.58±0.25	5.26±0.31	6.36±0.31
iPEEK-SBI^{t}	3.57±0.25	1.83±0.16	3.14±0.15	3.5±0.21	4.04±0.27
iPEEK-TB^{o}	9.13±0.21	4.03±0.20	7.69±0.25	7.2±0.28	6.60±0.32
iPEEK-TB^{a}	6.10±0.25	3.06±0.21	5.00±0.29	4.67±0.25	4.42±0.25
iPEEK-TB^{t}	3.91±0.18	2.43±0.17	3.42±0.15	2.96±0.06	2.71±0.13
iPEEK-Trip^{o}	11.09±0.42	4.87±0.23	7.47±0.36	8.17±0.37	7.03±0.25
iPEEK-Trip^{a}	7.22±0.34	3.52±0.21	4.83±0.31	5.32±0.29	4.73±0.22
iPEEK-Trip^{t}	4.92±0.30	2.67±0.20	3.24±0.09	3.53±0.16	2.91±0.09

Table S12. Permeance and rejection of 3 dyes and five APIs for iPEEK-Trip^{t} (34% dope solution) in acetonitrile at 30 bar.

Name	**Mw (g mol^{-1})**	**Permeance (L m^2 h bar^{-1})**	**Rejection (%)**
Estradiol	272.38	4.995±0.305	76.5±1.20
Methyl orange	327.33	5.195±0.435	75.65±2.45
Losartan	422.92	5.035±0.325	87.05±1.25
Valsartan	435.52	5.155±0.425	84.75±2.25
Oleuropein	540.51	5.045±0.395	97±0.80
Acid fuchsin	585.54	5.115±0.395	99.05±0.55
Roxithromycin	837.05	4.965±0.325	99.6±0.20
Rose Bengal	1017.65	4.98±0.320	99.75±0.25

Table S13 Binding energies (BEs) calculated from Material Studio and the permeances of the most lose membrane from each polymer.

Solvents	**Binding energy (kJ mol^{-1})**			**Permeance (L m^{-2} h^{-1} bar^{-1})**		
	iPEEK-SBI	iPEEK-TB	iPEEK-Trip	iPEEK-SBI^{o}	iPEEK-TB^{o}	iPEEK-Trip^{o}
Hexane	-5.46	-6.73	-2.93	3.36±0.13	4.03±0.2	4.87±0.23
Acetone	-20.32	-15.55	-11.28	8.14±0.25	6.6±0.32	7.03±0.25
Ethanol	-15.14	-16.80	-14.08	6.87±0.21	7.29±0.28	8.17±0.37
Methyethylketone	-11.18	-17.64	-12.84	5.38±0.18	7.69±0.25	7.47±0.36
Acetonitrile	-19.52	-25.70	-30.59	7.81±0.25	9.13±0.21	11.09±0.42

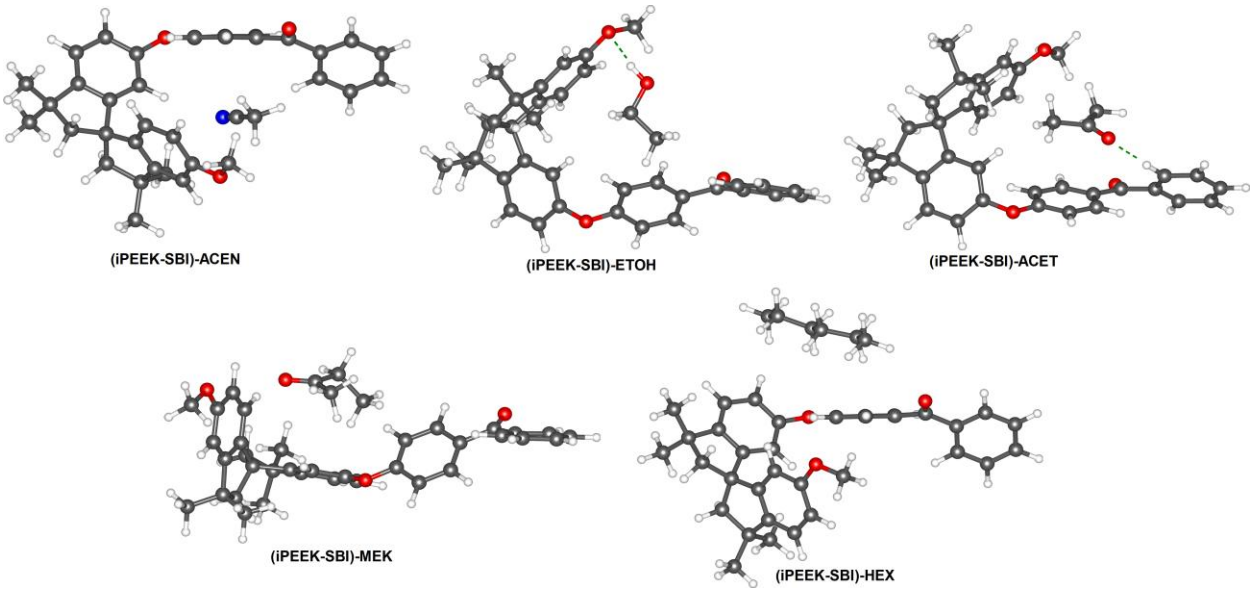


Fig. S32 Interaction of the iPEEK-SBI repeating unit with different solvents obtained from MD.

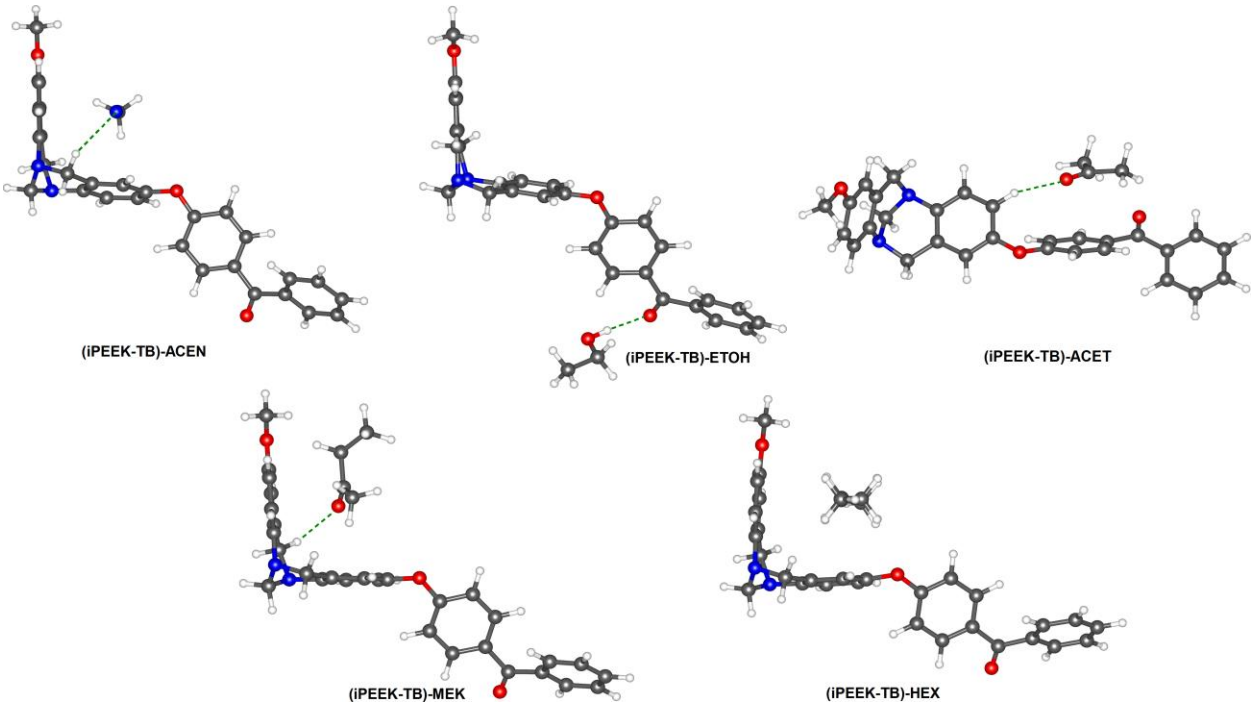


Fig. S33 Interaction of the iPEEK-TB repeating unit with different solvents obtained from MD.

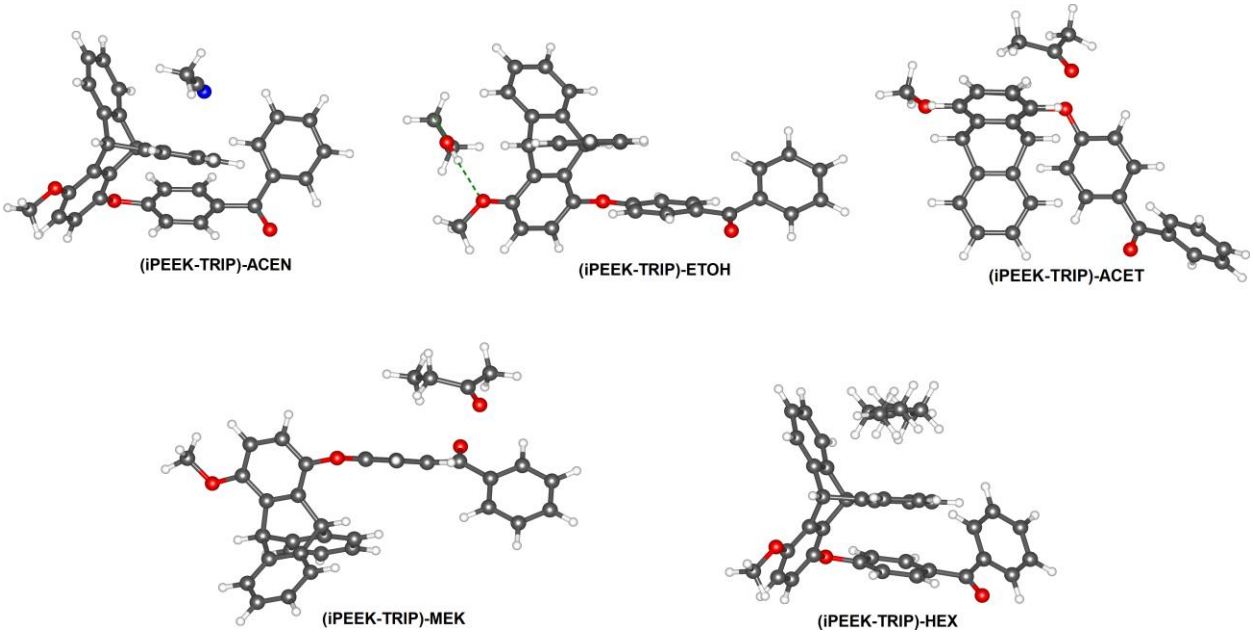
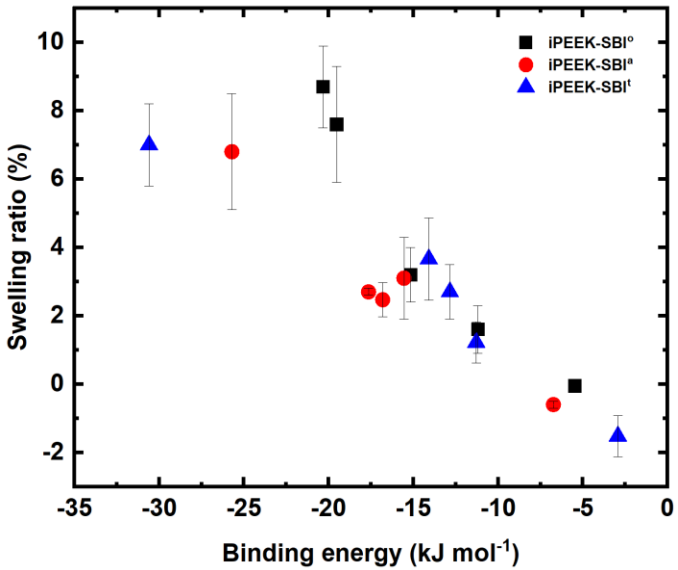


Fig. S34 Interaction of the iPEEK-Trip repeating unit with different solvents obtained from MD.

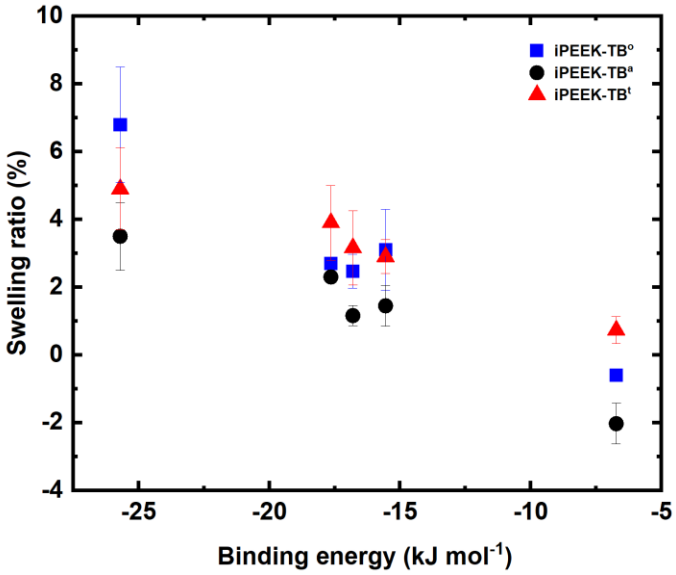
4.4.3. Swelling ratio and binding energy



	Swelling ratio (%)		
	iPEEK-SBIº	**iPEEK-SBIª**	**iPEEK-SBIᵗ**
Acetonitrile	7.6±1.7	4.9±1.2	1.35±0.5
Acetone	8.73±1.4	5.9±1.1	2.4±0.8
Ethanol	3.2±0.8	2.4±0.8	1.08±0.05
Methyl ethyl ketone	1.6±0.7	0.16±0.07	0.27±0.09
Hexane	-0.05±0.01	-1.4±0.06	-0.27±0.01
Linear fit (R^2)	n.l[a]	n.l[a]	0.984
Slope	-	-	-0.137±0.008

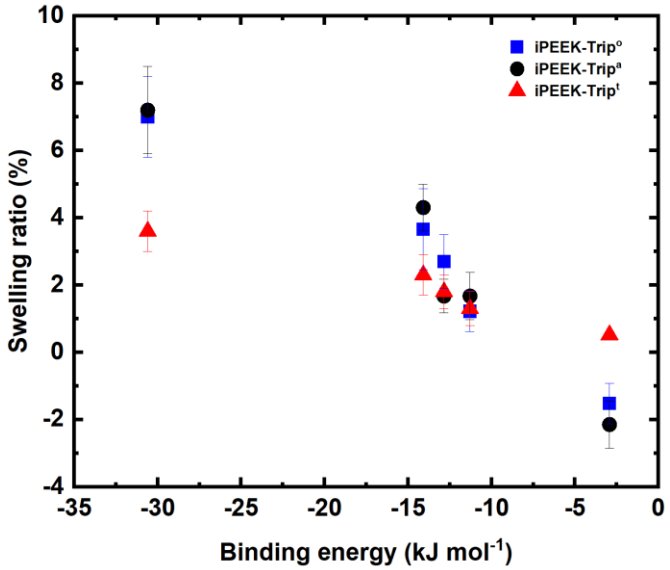
[a] non-linear fit

Figure S 35. Swelling ratio graph of iPEEK-SBI membranes with five different solvents versus binding energies obtained from MD (left) and values in the table (right).



	Swelling ratio (%)		
	iPEEK-TB°	**iPEEK-TBª**	**iPEEK-TBᵗ**
Acetonitrile	7.4±1.3	3.5±1.0	4.9±1.2
Acetone	3.1±1.2	1.45±0.6	2.9±0.5
Ethanol	2.47±0.5	1.16±0.3	3.16±1.1
Methyl ethyl ketone	2.7±0. 1	2.6 ±0.07	3.9±1.1
Hexane	-0.6±0.1	-2.03±0.6	0.73±0.4
Linear fit (R^2)	0.995	0.844	0.979
Slope	-0.304±0.009	-0.37±0.09	-0.24±0.02

Fig. S36 Swelling ratio graph of iPEEK-TB membranes with five different solvents versus binding energies obtained from MD (left) and values in the table (right).



	Swelling ratio (%)		
	iPEEK-Trip^{o}	**iPEEK-Trip^{a}**	**iPEEK-Trip^{t}**
Acetonitrile	7.01±1.2	7.16±1.3	3.6±0.6
Acetone	1.22±0.6	1.67±0.7	1.3±0.5
Ethanol	3.66±1.2	5.5±0.7	2.3±0.6
Methyl ethyl ketone	2.7±0.8	1.67±0.5	1.8±0.5
Hexane	-1.52±0.6	-2.15±0.7	0.52±0.1
Linear fit (R^2)	0.947	0.855	0.977
Slope	-0.32±0.04	-0.37±0.08	-0.117±0.01

Fig. S37 Swelling ratio graph of iPEEK-Trip membranes with five different solvents versus binding energies obtained from MD (left) and values (right).

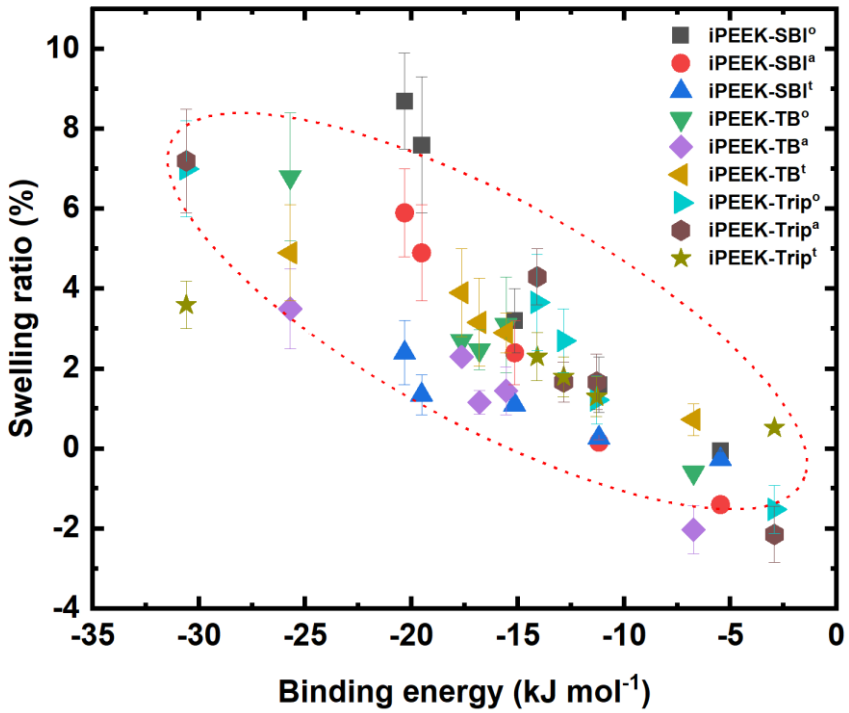


Fig. S38 Swelling ratio versus binding energy for the nine iPEEK membranes with five different solvents.

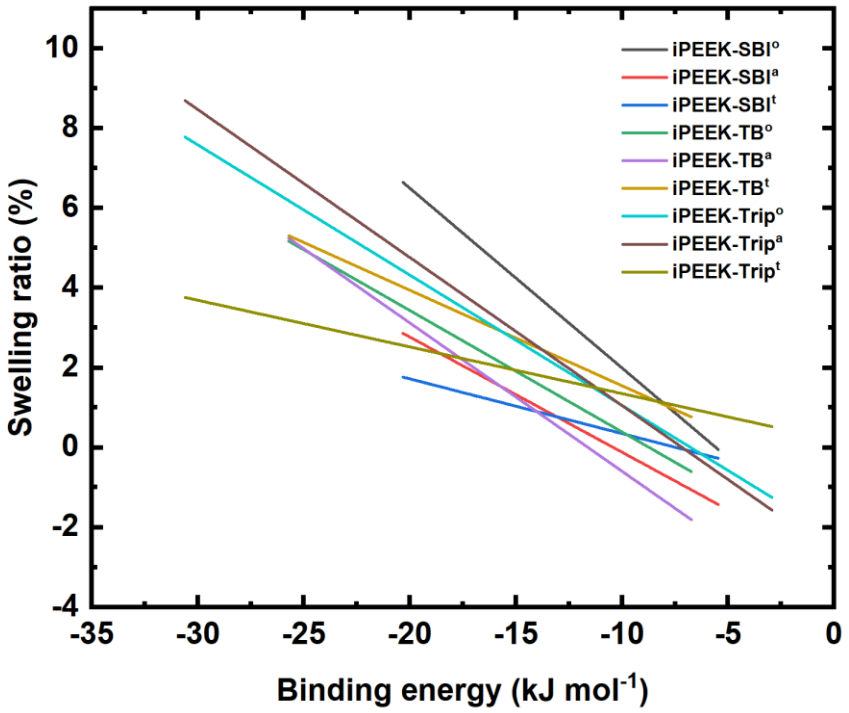


Fig. S39. Linear fitting for the swelling ratio versus binding energy for the nine iPEEK membranes. R^2 and slope are reported in tables in Figures S35–S37.

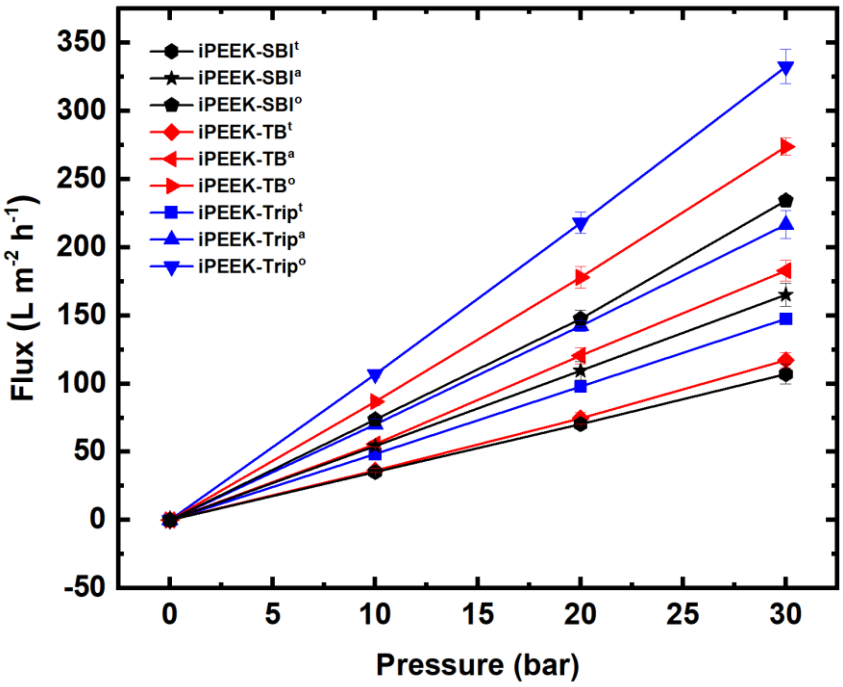


Fig. S40 Variation of flux versus pressure for the nine iPEEK membranes.

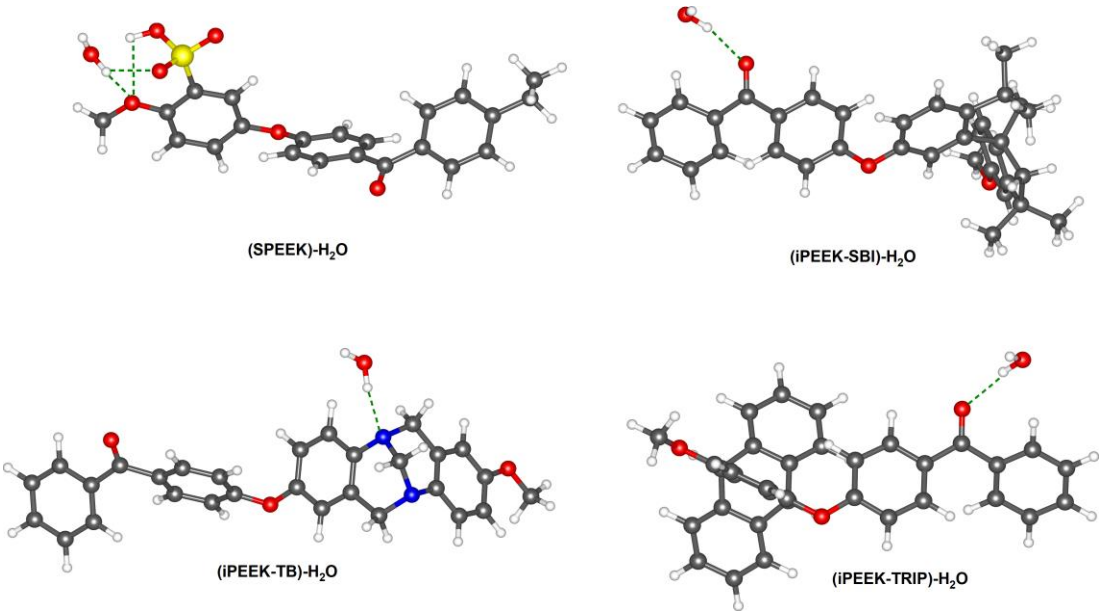


Fig. S41 Interaction of iPEEK and SPEEK repeating units with H_2O obtained from MD. (dotted green line: hydrogen bond)

Table S14 Binding energies for water-polymer obtained from MD simulations for iPEEK polymers compared to SPEEK.

Solvent	**Binding energy (kJ mol^{-1})**			
	iPEEK-SBI	iPEEK-TB	iPEEK-Trip	SPEEK
Water	-15.04	-17.87	-15.12	-54.17

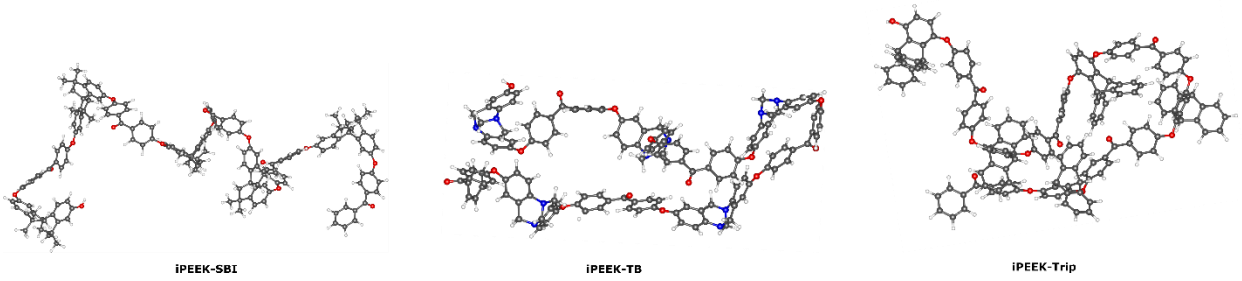


Fig. S42 MD snapshots of iPEEK-SBI, iPEEK-TB, and iPEEK-Trip polymer chains in the gas phase.

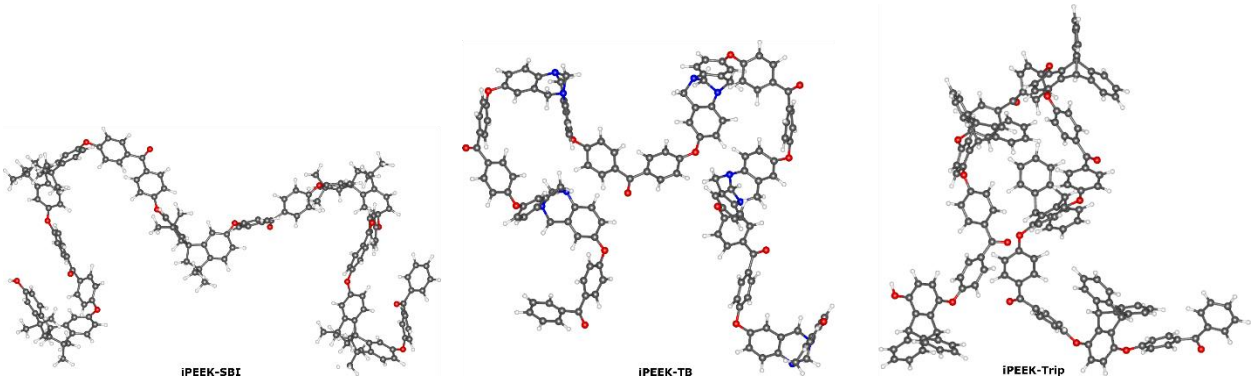


Fig. S43 MD snapshots of iPEEK-SBI, iPEEK-TB, and iPEEK-Trip polymer chains in acetonitrile.

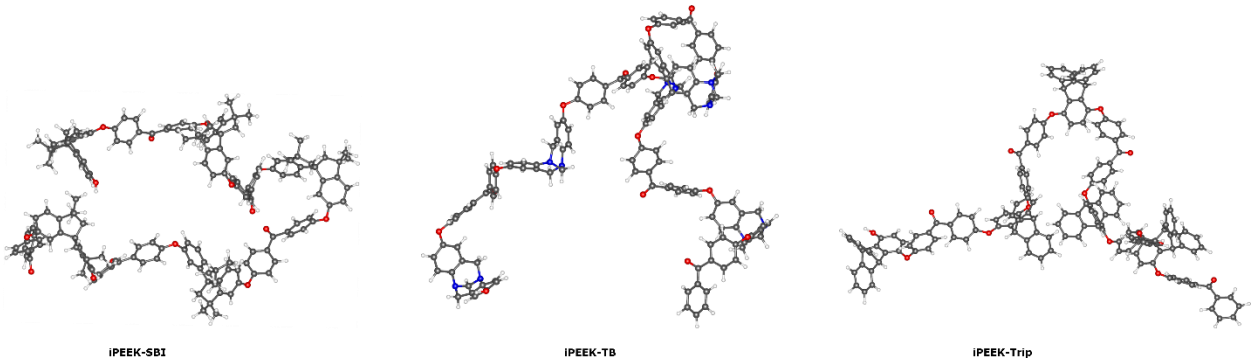


Fig. S44 MD snapshots of iPEEK-SBI, iPEEK-TB, and iPEEK-Trip polymer chains in acetone.

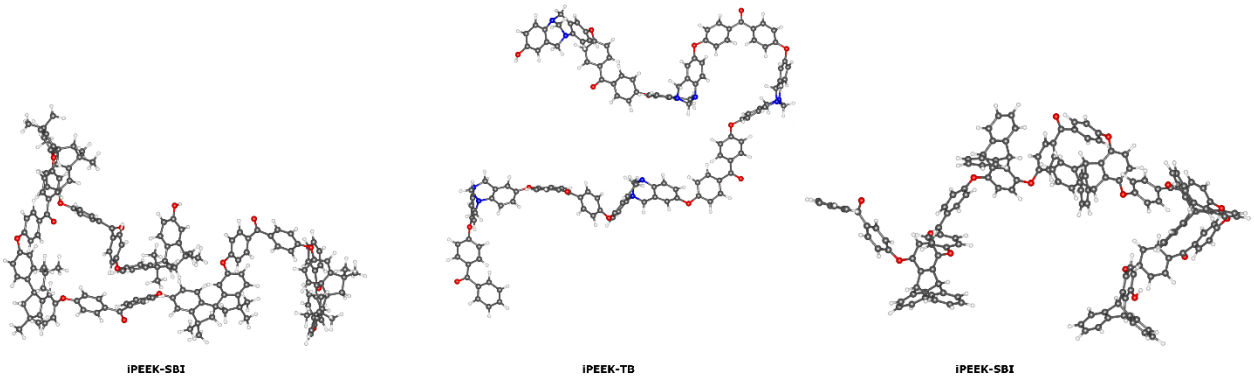


Fig. S45 MD snapshots of iPEEK-SBI, iPEEK-TB, and iPEEK-Trip polymer chains in ethanol.

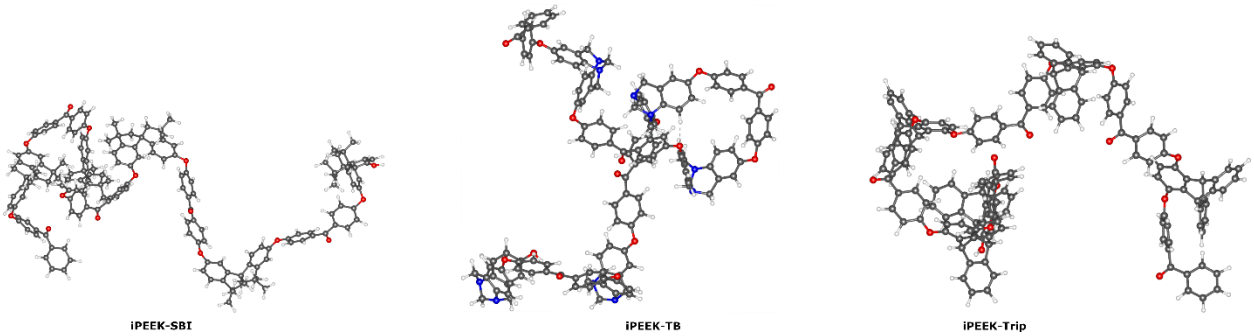


Fig. S46 MD snapshots of iPEEK-SBI, iPEEK-TB, and iPEEK-Trip polymer chains in methyl ethyl ketone.

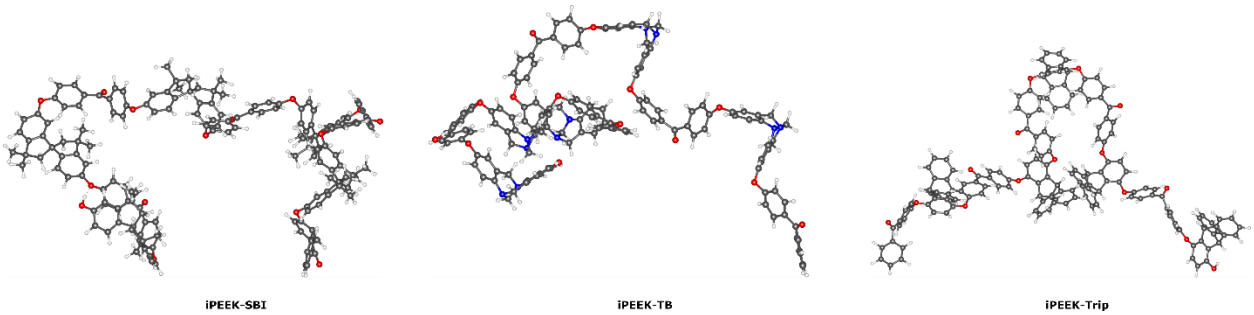


Fig. S47 MD snapshots of iPEEK-SBI, iPEEK-TB, and iPEEK-Trip polymer chains in hexane.

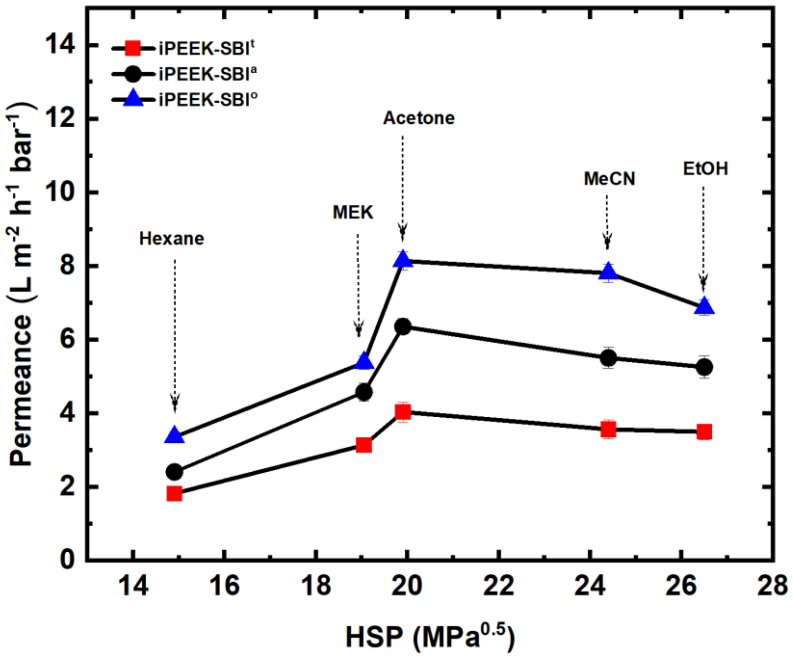


Fig. S48 Permeance versus HSP for iPEEK-SBI membranes.

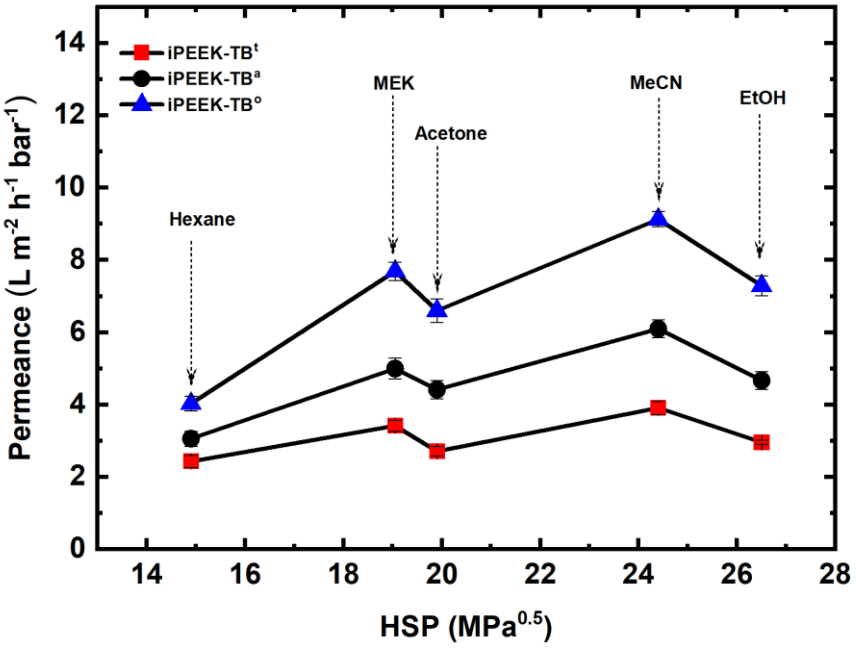


Fig. S49 Permeance versus HSP for iPEEK-TB membranes.

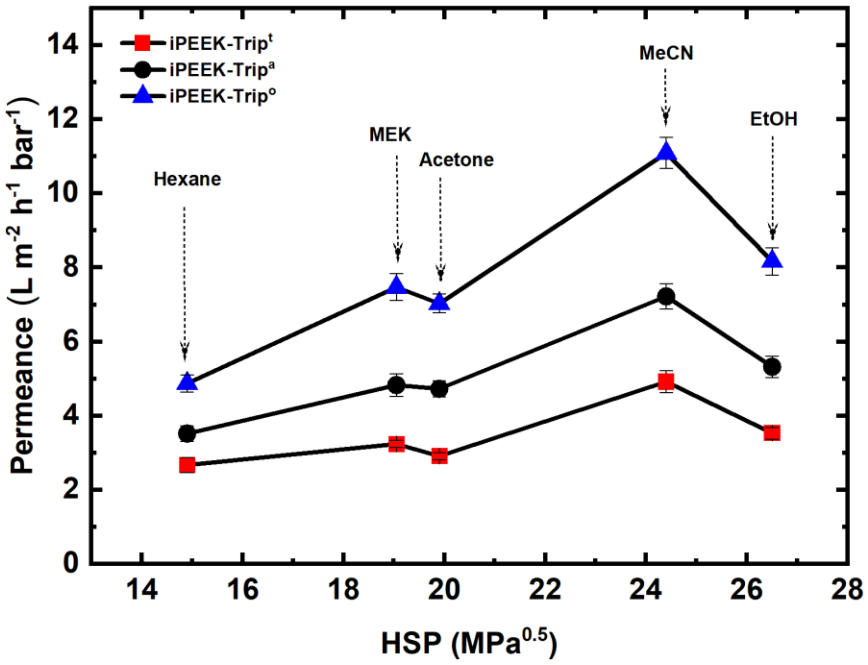


Fig. S50 Permeance versus HSP for iPEEK-Trip membranes.

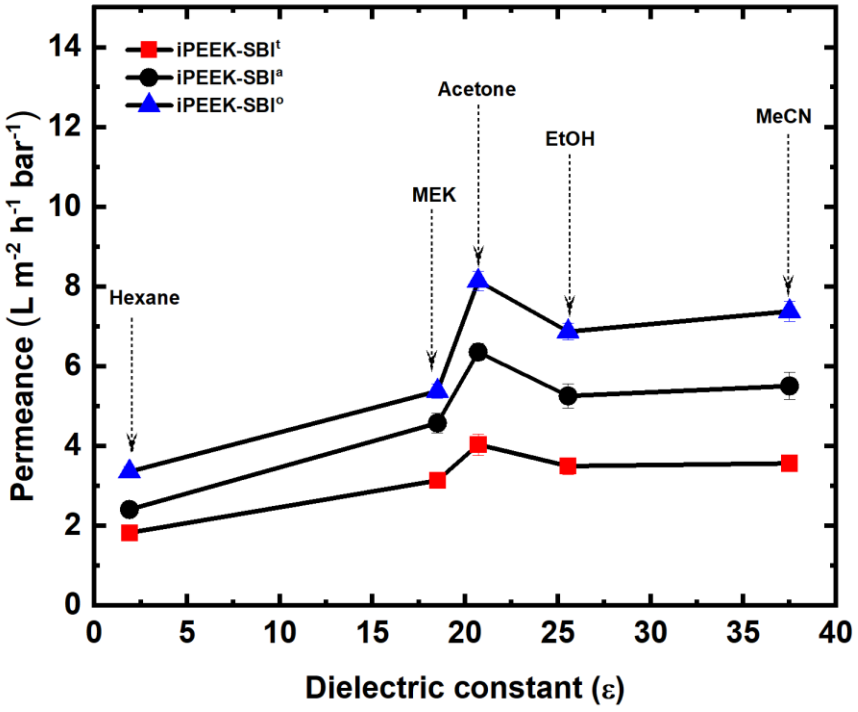


Fig. S51 Permeance versus dielectric constant for iPEEK-SBI membranes.

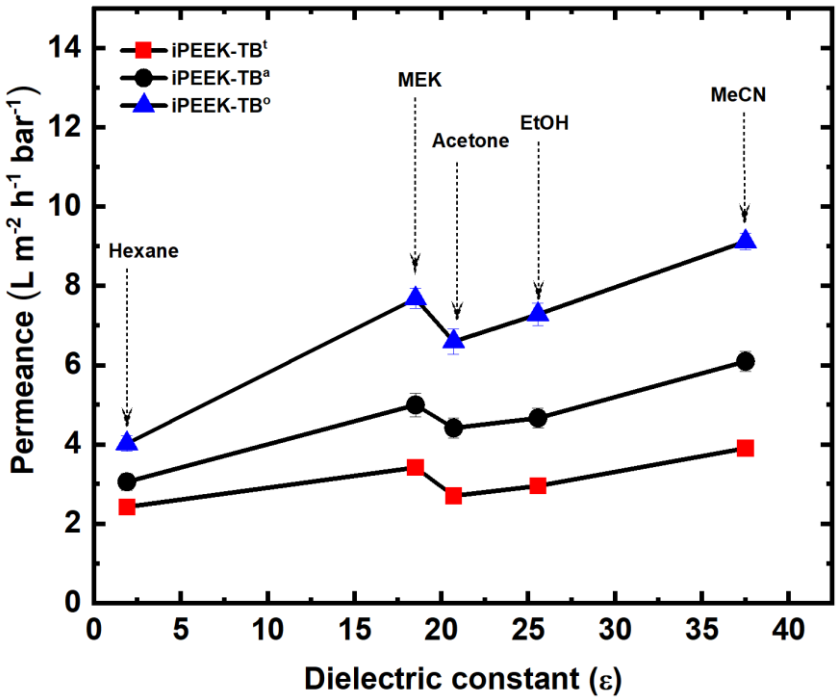


Fig. S52 Permeance versus dielectric constant for iPEEK-TB membranes.

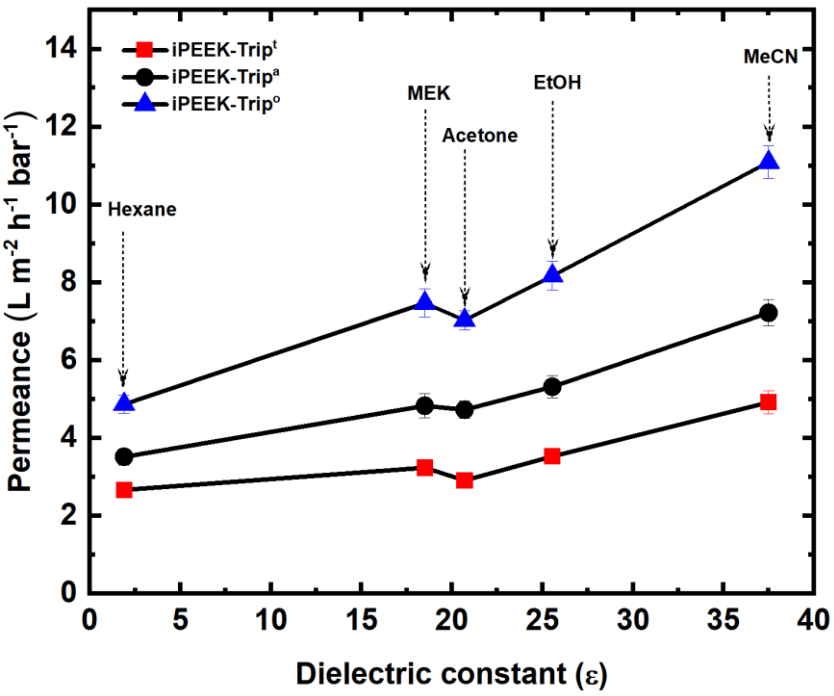


Fig. S53 Permeance versus dielectric constant for iPEEK-Trip membranes

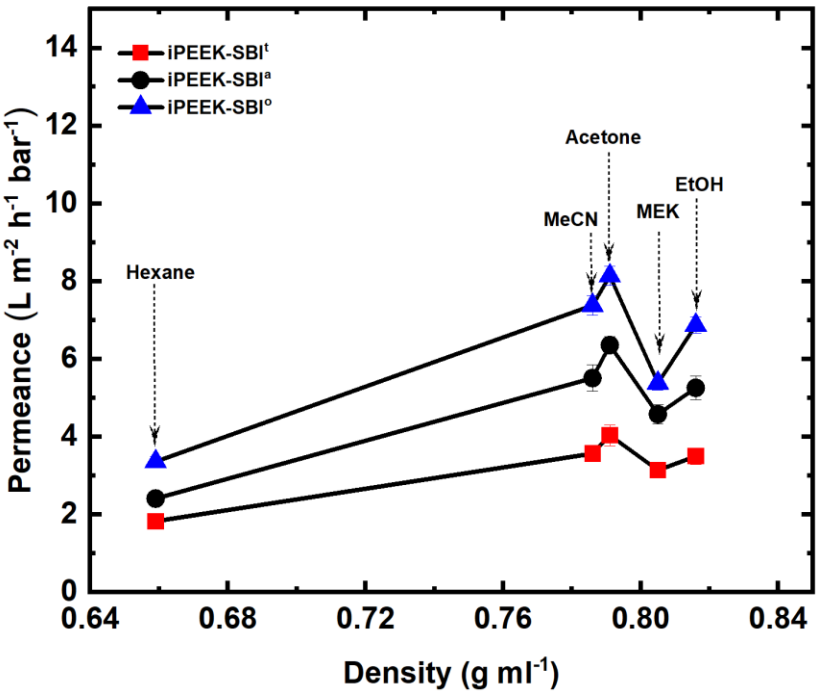


Fig. S54 Permeance versus solvents densities for iPEEK-SBI membranes.

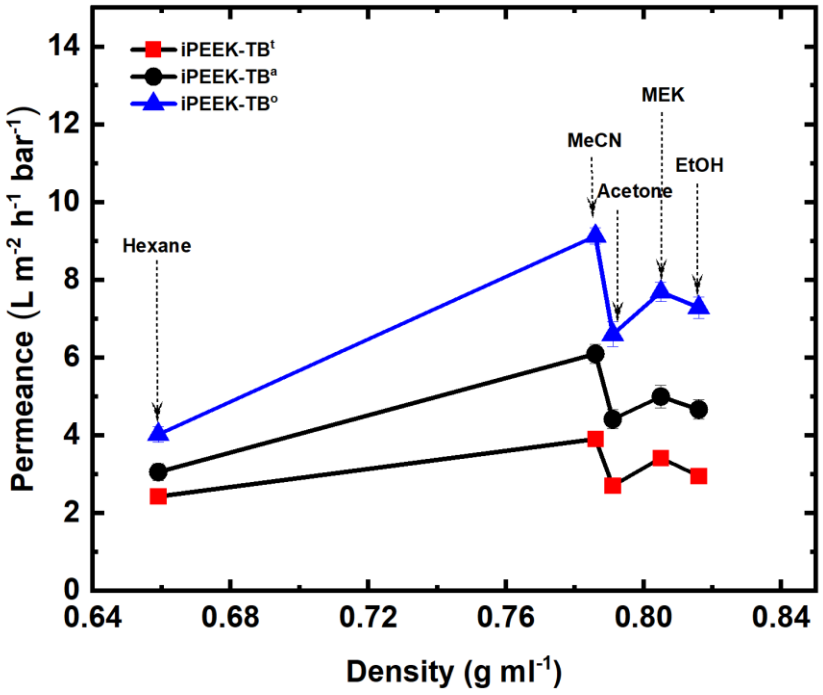


Fig. S55 Permeance versus solvents densities for iPEEK-TB membranes.

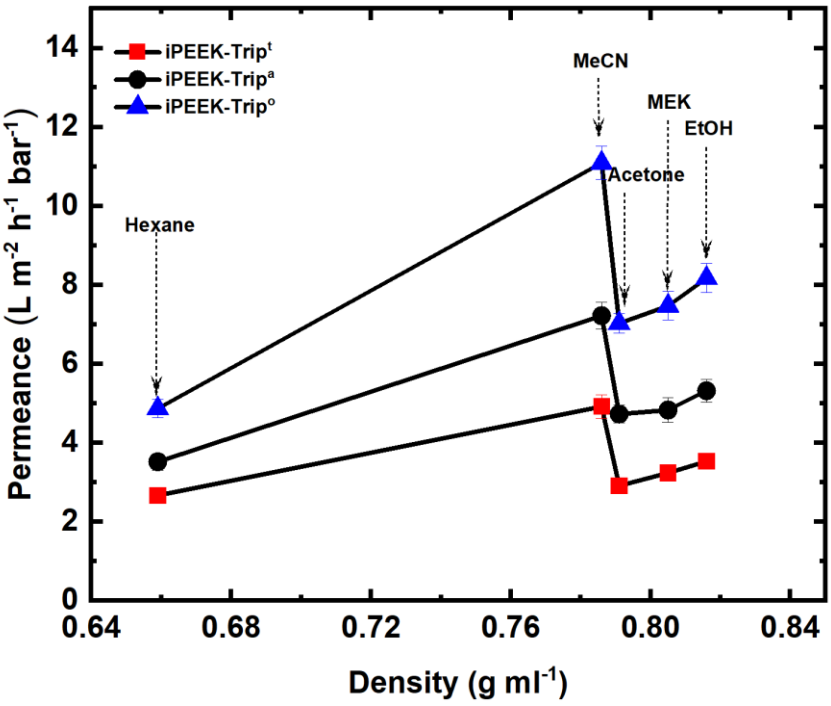


Fig. S56 Permeance versus solvents densities for iPEEK-Trip membranes.

5. XYZ coordinates and total energies

Table S15 XYZ coordinates and total energies of iPEEK polymer unit with solvents

iPEEK-SBI-MeCN (-1711.940)				iPEEK-SBI-EtOH (-1734.199)				iPEEK-SBI-AcMe (-1772.305)			
C	1.842	1.472	1.662	C	-2.240	1.280	-1.702	C	-1.906	1.144	-1.681
C	2.417	1.418	0.400	C	-2.938	1.131	-0.510	C	-2.754	1.209	-0.582
C	1.979	2.284	-0.603	C	-2.902	2.142	0.449	C	-2.636	2.262	0.323
C	0.996	3.228	-0.345	C	-2.200	3.315	0.215	C	-1.709	3.274	0.119
C	0.446	3.303	0.938	C	-1.511	3.467	-0.992	C	-0.866	3.215	-0.995
C	0.855	2.419	1.941	C	-1.523	2.450	-1.951	C	-0.957	2.146	-1.894
H	2.157	0.783	2.443	H	-2.242	0.486	-2.446	H	-1.968	0.311	-2.378
H	0.640	3.918	-1.105	H	-2.158	4.122	0.943	H	-1.602	4.110	0.807
H	0.425	2.465	2.934	H	-0.976	2.557	-2.880	H	-0.302	2.087	-2.756
C	2.685	2.029	-1.921	C	-3.656	1.759	1.707	C	-3.570	2.100	1.507
C	3.271	3.317	-2.508	C	-4.661	2.839	2.120	C	-4.423	3.351	1.738
H	3.852	3.094	-3.410	H	-5.249	2.506	2.983	H	-5.139	3.182	2.550
H	2.477	4.018	-2.788	H	-4.149	3.766	2.403	H	-3.799	4.207	2.014
H	3.927	3.814	-1.787	H	-5.349	3.067	1.300	H	-4.982	3.615	0.835
C	1.716	1.401	-2.933	C	-2.669	1.514	2.857	C	-2.759	1.794	2.774
H	2.231	1.225	-3.885	H	-3.208	1.221	3.766	H	-3.427	1.658	3.632
H	1.316	0.450	-2.572	H	-1.963	0.715	2.608	H	-2.169	0.879	2.655
H	0.864	2.063	-3.119	H	-2.094	2.420	3.078	H	-2.071	2.615	3.005
C	3.807	1.031	-1.518	C	-4.375	0.444	1.289	C	-4.445	0.880	1.096
H	3.908	0.230	-2.258	H	-4.301	-0.313	2.077	H	-4.558	0.179	1.930
H	4.766	1.560	-1.479	H	-5.441	0.646	1.134	H	-5.450	1.224	0.826
C	3.489	0.468	-0.093	C	-3.755	-0.060	-0.057	C	-3.793	0.193	-0.149
C	4.739	0.370	0.821	C	-4.820	-0.533	-1.081	C	-4.817	-0.212	-1.243
H	5.473	1.156	0.612	H	-5.754	0.034	-1.004	H	-5.680	0.462	-1.279

H	4.419	0.487	1.864	H	-4.424	-0.376	-2.093	H	-4.322	-0.163	-2.221
C	5.319	-1.055	0.645	C	-5.018	-2.052	-0.861	C	-5.218	-1.685	-0.970
C	5.993	-1.554	1.924	C	-5.379	-2.771	-2.161	C	-5.576	-2.423	-2.259
H	6.401	-2.562	1.789	H	-5.512	-3.846	-1.996	H	-5.858	-3.462	-2.055
H	6.824	-0.895	2.201	H	-6.320	-2.379	-2.565	H	-6.427	-1.940	-2.753
H	5.283	-1.582	2.756	H	-4.597	-2.635	-2.915	H	-4.732	-2.428	-2.956
C	6.322	-1.118	-0.518	C	-6.096	-2.335	0.197	C	-6.391	-1.775	0.019
H	5.879	-0.751	-1.449	H	-5.877	-1.825	1.140	H	-6.172	-1.242	0.949
H	7.207	-0.513	-0.294	H	-7.077	-1.999	-0.157	H	-7.298	-1.345	-0.421
H	6.647	-2.151	-0.687	H	-6.156	-3.409	0.404	H	-6.597	-2.821	0.273
C	3.033	-0.985	-0.104	C	-2.934	-1.332	0.105	C	-3.161	-1.159	0.149
C	4.064	-1.838	0.300	C	-3.650	-2.449	-0.333	C	-3.947	-2.211	-0.323
C	1.780	-1.478	-0.437	C	-1.646	-1.461	0.609	C	-1.927	-1.396	0.732
C	3.854	-3.211	0.348	C	-3.090	-3.718	-0.250	C	-3.503	-3.522	-0.193
C	1.579	-2.855	-0.353	C	-1.093	-2.740	0.673	C	-1.468	-2.708	0.802
H	0.959	-0.821	-0.720	H	-1.061	-0.597	0.917	H	-1.287	-0.582	1.058
C	2.598	-3.724	0.025	C	-1.799	-3.863	0.254	C	-2.247	-3.773	0.362
H	4.647	-3.884	0.662	H	-3.640	-4.592	-0.589	H	-4.104	-4.352	-0.558
H	2.386	-4.787	0.074	H	-1.320	-4.834	0.325	H	-1.847	-4.779	0.434
O	0.359	-3.417	-0.684	O	0.163	-2.941	1.214	O	-0.208	-2.973	1.310
C	-0.782	-2.837	-0.206	C	1.264	-2.424	0.592	C	0.873	-2.412	0.682
C	-0.839	-2.195	1.035	C	1.242	-1.811	-0.664	C	0.813	-1.826	-0.587
C	-1.925	-2.968	-0.992	C	2.467	-2.578	1.285	C	2.088	-2.488	1.364
C	-2.039	-1.645	1.453	C	2.434	-1.355	-1.209	C	1.973	-1.318	-1.150
H	0.052	-2.124	1.649	H	0.309	-1.703	-1.206	H	-0.125	-1.778	-1.128
C	-3.116	-2.400	-0.568	C	3.645	-2.098	0.734	C	3.241	-1.974	0.785
H	-1.850	-3.497	-1.935	H	2.451	-3.080	2.246	H	2.108	-2.956	2.342
C	-3.182	-1.706	0.646	C	3.642	-1.471	-0.517	C	3.198	-1.370	-0.476
H	-2.116	-1.153	2.418	H	2.445	-0.891	-2.191	H	1.953	-0.880	-2.144

H	-4.003	-2.500	-1.185	H	4.579	-2.232	1.271	H	4.181	-2.054	1.321
C	-4.420	-1.043	1.144	C	4.879	-0.963	-1.183	C	4.396	-0.845	-1.204
O	-4.578	-0.831	2.334	O	4.946	-0.916	-2.399	O	4.331	-0.636	-2.404
C	-5.467	-0.588	0.168	C	6.037	-0.497	-0.352	C	5.689	-0.597	-0.487
C	-5.153	-0.146	-1.122	C	5.876	0.062	0.919	C	5.751	-0.064	0.804
C	-6.789	-0.524	0.617	C	7.313	-0.557	-0.922	C	6.871	-0.836	-1.197
C	-6.158	0.341	-1.955	C	6.981	0.542	1.616	C	6.990	0.209	1.379
H	-4.122	-0.163	-1.469	H	4.883	0.148	1.353	H	4.839	0.177	1.345
C	-7.793	-0.059	-0.223	C	8.417	-0.094	-0.218	C	8.103	-0.584	-0.610
H	-7.007	-0.842	1.632	H	7.414	-0.969	-1.921	H	6.799	-1.220	-2.210
C	-7.477	0.375	-1.511	C	8.251	0.455	1.053	C	8.164	-0.060	0.681
H	-5.908	0.693	-2.951	H	6.849	0.988	2.597	H	7.035	0.637	2.376
H	-8.820	-0.026	0.125	H	9.406	-0.156	-0.660	H	9.018	-0.787	-1.159
H	-8.260	0.745	-2.166	H	9.114	0.823	1.602	H	9.128	0.144	1.139
O	-0.512	4.264	1.114	O	-0.823	4.639	-1.126	O	0.029	4.236	-1.114
C	-1.006	4.459	2.421	C	0.073	4.749	-2.219	C	0.797	4.297	-2.298
H	-0.195	4.695	3.121	H	-0.464	4.721	-3.174	H	0.154	4.336	-3.185
H	-1.694	5.302	2.363	H	0.562	5.716	-2.106	H	1.381	5.215	-2.231
H	-1.547	3.575	2.784	H	0.823	3.951	-2.177	H	1.478	3.442	-2.381
C	-1.635	0.949	-0.547	C	2.259	1.315	1.091	C	2.519	2.072	0.058
N	-1.076	0.368	-1.375	H	2.798	1.828	1.893	H	1.989	3.032	0.017
C	-2.368	1.680	0.486	H	2.894	1.307	0.201	H	2.219	1.499	-0.828
H	-2.058	1.322	1.471	H	2.067	0.278	1.390	H	3.599	2.229	0.045
H	-2.150	2.749	0.406	C	0.965	2.043	0.786	C	0.624	1.126	1.504
H	-3.442	1.513	0.368	H	0.396	1.498	0.015	H	0.120	0.912	0.554
				H	0.333	2.087	1.686	H	0.456	0.325	2.228
				O	1.310	3.343	0.342	H	0.195	2.059	1.889
				H	0.504	3.874	0.262	C	2.108	1.313	1.299
								O	2.912	0.893	2.104

iPEEK-SBI-MEK (-1811.592)				iPEEK-SBI-Hex (-1816.181)			
C	3.661	0.692	1.701	C	-2.1	-1.914	1.643
C	3.889	0.744	0.324	C	-2.903	-2.024	0.518
C	4.308	1.928	-0.268	C	-2.824	-3.137	-0.317
C	4.495	3.088	0.486	C	-1.946	-4.167	-0.005
C	4.258	3.035	1.859	C	-1.138	-4.081	1.128
C	3.848	1.836	2.462	C	-1.21	-2.949	1.948
H	3.354	-0.236	2.179	H	-2.123	-1.04	2.289
H	4.825	4.004	0.005	H	-1.873	-5.044	-0.644
H	3.690	1.835	3.535	H	-0.453	-4.889	1.358
C	4.523	1.779	-1.762	C	-3.722	-3.012	-1.533
C	5.922	2.247	-2.176	C	-4.663	-4.214	-1.669
H	6.097	2.039	-3.238	H	-5.357	-4.068	-2.505
H	6.039	3.326	-2.024	H	-4.099	-5.134	-1.859
H	6.693	1.736	-1.592	H	-5.247	-4.356	-0.754
C	3.474	2.574	-2.553	C	-2.883	-2.878	-2.812
H	3.651	2.473	-3.630	H	-3.534	-2.788	-3.689
H	2.461	2.219	-2.343	H	-2.241	-1.992	-2.773
H	3.521	3.639	-2.299	H	-2.243	-3.756	-2.951
C	4.360	0.247	-1.972	C	-4.515	-1.704	-1.24
H	3.784	0.030	-2.878	H	-4.561	-1.065	-2.128
H	5.349	-0.208	-2.100	H	-5.547	-1.954	-0.968
C	3.696	-0.362	-0.693	C	-3.839	-0.97	-0.037
C	4.270	-1.743	-0.289	C	-4.849	-0.368	0.974
H	5.338	-1.830	-0.515	H	-5.772	-0.954	1.042
H	4.143	-1.871	0.793	H	-4.387	-0.363	1.97

C	3.417	-2.817	-1.010	C	-5.102	1.1	0.543
C	3.320	-4.108	-0.196	C	-5.413	1.995	1.742
H	2.660	-4.836	-0.684	H	-5.591	3.03	1.429
H	4.309	-4.571	-0.100	H	-6.315	1.645	2.257
H	2.943	-3.910	0.812	H	-4.585	1.993	2.458
C	3.968	-3.143	-2.408	C	-6.245	1.198	-0.48
H	4.058	-2.246	-3.028	H	-6.067	0.551	-1.344
H	4.957	-3.607	-2.329	H	-7.197	0.907	-0.021
H	3.304	-3.843	-2.928	H	-6.342	2.226	-0.846
C	2.235	-0.720	-0.934	C	-3.07	0.28	-0.441
C	2.086	-2.094	-1.137	C	-3.777	1.44	-0.117
C	1.140	0.134	-1.004	C	-1.805	0.341	-1.005
C	0.839	-2.617	-1.463	C	-3.227	2.687	-0.391
C	-0.103	-0.404	-1.332	C	-1.247	1.598	-1.226
H	1.224	1.197	-0.799	H	-1.229	-0.559	-1.21
C	-0.264	-1.769	-1.572	C	-1.949	2.766	-0.946
H	0.714	-3.682	-1.648	H	-3.765	3.6	-0.149
H	-1.241	-2.158	-1.841	H	-1.475	3.72	-1.151
O	-1.143	0.492	-1.491	O	0.02	1.73	-1.765
C	-2.396	0.208	-1.029	C	1.083	1.127	-1.153
C	-2.648	-0.625	0.065	C	1.035	0.534	0.113
C	-3.447	0.854	-1.681	C	2.283	1.172	-1.867
C	-3.955	-0.806	0.490	C	2.192	-0.022	0.641
H	-1.826	-1.119	0.570	H	0.112	0.509	0.681
C	-4.748	0.682	-1.231	C	3.429	0.607	-1.328
H	-3.218	1.482	-2.536	H	2.292	1.664	-2.834
C	-5.017	-0.147	-0.137	C	3.396	-0.005	-0.068
H	-4.178	-1.462	1.325	H	2.176	-0.47	1.629
H	-5.562	1.175	-1.753	H	4.362	0.666	-1.879

C	-6.400	-0.432	0.354	C	4.611	-0.559	0.6
O	-6.645	-1.482	0.919	O	4.69	-0.571	1.816
C	-7.489	0.580	0.153	C	5.738	-1.105	-0.225
C	-7.244	1.956	0.138	C	5.54	-1.688	-1.479
C	-8.803	0.112	0.058	C	7.019	-1.092	0.335
C	-8.302	2.852	0.015	C	6.615	-2.239	-2.171
H	-6.229	2.327	0.249	H	4.541	-1.734	-1.903
C	-9.856	1.007	-0.085	C	8.094	-1.626	-0.364
H	-8.976	-0.958	0.102	H	7.147	-0.659	1.322
C	-9.606	2.379	-0.107	C	7.893	-2.2	-1.619
H	-8.108	3.920	0.017	H	6.455	-2.701	-3.14
H	-10.873	0.638	-0.172	H	9.089	-1.601	0.07
H	-10.429	3.079	-0.213	H	8.732	-2.623	-2.163
O	4.407	4.092	2.704	O	-0.445	-2.757	3.057
C	4.819	5.317	2.143	C	0.502	-3.752	3.378
H	4.100	5.677	1.397	H	1.233	-3.881	2.571
H	4.870	6.027	2.969	H	1.013	-3.404	4.276
H	5.807	5.230	1.676	H	0.018	-4.714	3.584
C	0.498	-1.346	2.171	C	2.962	2.529	2.595
H	0.997	-0.390	2.337	H	2.109	1.871	2.794
H	-0.473	-1.366	2.676	H	3.084	3.182	3.467
H	0.322	-1.457	1.094	H	3.848	1.894	2.51
C	0.706	-3.832	2.838	C	2.72	3.349	1.33
H	1.492	-4.564	3.040	H	3.528	4.082	1.201
H	0.090	-3.744	3.743	H	2.756	2.695	0.45
C	1.378	-2.490	2.612	C	1.379	4.079	1.354
O	2.577	-2.355	2.758	H	1.354	4.766	2.213
C	-0.173	-4.268	1.661	H	0.573	3.348	1.521
H	-0.623	-5.243	1.863	C	1.087	4.853	0.071

H	-0.984	-3.556	1.476	H	0.954	4.14	-0.757
H	0.418	-4.347	0.744	H	1.957	5.47	-0.194
				C	-0.144	5.752	0.181
				H	0.025	6.497	0.969
				H	-1.003	5.153	0.512
				C	-0.474	6.462	-1.13
				H	-0.67	5.741	-1.933
				H	-1.354	7.105	-1.034
				H	0.365	7.086	-1.453

iPEEK-TB-MeCN (-1586.8148)

				iPEEK-TB-EtOH (-1609.074)				iPEEK-TB-AcMe (-1647.180)			
C	-6.023	-0.276	-1.232	C	6.923	-0.454	-1.013	C	-6.536	0.471	1.26
C	-5.163	-1.005	-0.417	C	5.948	0.449	-0.607	C	-5.802	0.717	0.106
C	-4.99	-0.626	0.927	C	5.733	0.665	0.764	C	-5.863	-0.197	-0.96
C	-5.63	0.523	1.39	C	6.488	-0.052	1.689	C	-6.637	-1.346	-0.823
C	-6.46	1.274	0.565	C	7.448	-0.973	1.285	C	-7.353	-1.605	0.341
C	-6.68	0.857	-0.752	C	7.673	-1.17	-0.08	C	-7.309	-0.683	1.389
H	-6.18	-0.561	-2.269	H	7.108	-0.636	-2.068	H	-6.505	1.164	2.096
H	-5.475	0.827	2.421	H	6.324	0.135	2.747	H	-6.687	-2.039	-1.659
H	-6.937	2.162	0.962	H	8.018	-1.51	2.034	H	-7.946	-2.51	0.411
C	-4.382	-2.181	-0.978	C	5.124	1.207	-1.634	C	-4.939	1.962	-0.01
H	-5.044	-3.038	-1.156	H	5.741	1.97	-2.126	H	-5.572	2.851	-0.136
H	-3.941	-1.908	-1.942	H	4.773	0.524	-2.413	H	-4.36	2.105	0.907
N	-4.191	-1.4	1.831	N	4.766	1.613	1.236	N	-5.155	0.027	-2.187
N	-3.315	-2.606	-0.065	N	3.966	1.875	-1.029	N	-4.018	1.892	-1.15
C	-3.899	-2.712	1.27	C	4.414	2.557	0.182	C	-4.771	1.429	-2.311
H	-3.201	-3.228	1.936	H	3.617	3.21	0.547	H	-4.159	1.543	-3.211

H	-4.82	-3.298	1.197	H	5.287	3.166	-0.069	H	-5.669	2.045	-2.409
C	-2.913	-0.765	2.166	C	3.529	0.982	1.709	C	-3.938	-0.785	-2.299
H	-3.083	0.283	2.426	H	3.788	0.123	2.335	H	-4.17	-1.811	-2.001
H	-2.506	-1.262	3.055	H	2.999	1.701	2.347	H	-3.643	-0.813	-3.356
C	-2.193	-1.719	-0.066	C	2.892	0.976	-0.741	C	-2.89	1.046	-0.901
C	-1.935	-0.854	1.009	C	2.633	0.539	0.565	C	-2.803	-0.239	-1.452
C	-1.331	-1.725	-1.169	C	2.081	0.536	-1.793	C	-1.852	1.523	-0.092
C	-0.793	-0.05	0.982	C	1.545	-0.304	0.8	C	-1.664	-1.009	-1.209
C	-0.22	-0.895	-1.21	C	1.018	-0.322	-1.56	C	-0.733	0.75	0.175
H	-1.54	-2.404	-1.99	H	2.291	0.896	-2.796	H	-1.937	2.525	0.319
C	0.051	-0.069	-0.117	C	0.754	-0.731	-0.253	C	-0.651	-0.519	-0.402
H	-0.584	0.64	1.796	H	1.321	-0.656	1.804	H	-1.568	-2.009	-1.624
H	0.448	-0.893	-2.065	H	0.381	-0.666	-2.368	H	0.077	1.111	0.805
O	1.113	0.814	-0.142	O	-0.274	-1.623	0.003	O	0.41	-1.365	-0.125
C	2.39	0.332	-0.215	C	-1.562	-1.199	-0.149	C	1.683	-0.902	-0.26
C	3.376	1.281	-0.49	C	-2.533	-2.202	-0.186	C	2.654	-1.535	0.518
C	2.73	-1.006	-0.006	C	-1.926	0.147	-0.239	C	2.035	0.113	-1.153
C	4.706	0.896	-0.538	C	-3.87	-1.856	-0.299	C	3.979	-1.144	0.412
H	3.074	2.309	-0.661	H	-2.214	-3.237	-0.134	H	2.34	-2.307	1.211
C	4.065	-1.38	-0.083	C	-3.267	0.48	-0.37	C	3.36	0.509	-1.234
H	1.962	-1.74	0.211	H	-1.169	0.922	-0.21	H	1.272	0.589	-1.76
C	5.068	-0.44	-0.33	C	-4.256	-0.511	-0.387	C	4.347	-0.109	-0.459
H	5.468	1.637	-0.764	H	-4.618	-2.641	-0.353	H	4.728	-1.614	1.042
H	4.353	-2.418	0.058	H	-3.552	1.526	-0.459	H	3.653	1.312	-1.904
C	6.477	-0.929	-0.43	C	-5.673	-0.101	-0.578	C	5.73	0.442	-0.511
O	6.707	-2.08	-0.757	O	-5.953	0.956	-1.129	O	5.91	1.625	-0.76
C	7.613	0	-0.119	C	-6.787	-0.982	-0.104	C	6.904	-0.444	-0.227
C	7.505	1.027	0.823	C	-6.677	-1.794	1.029	C	6.892	-1.816	-0.495
C	8.841	-0.237	-0.743	C	-8.004	-0.914	-0.789	C	8.067	0.154	0.268

C	8.612	1.816	1.125	C	-7.771	-2.54	1.461	C	8.03	-2.582	-0.256
H	6.564	1.192	1.339	H	-5.746	-1.821	1.587	H	6.001	-2.278	-0.91
C	9.938	0.564	-0.456	C	-9.087	-1.674	-0.369	C	9.195	-0.615	0.522
H	8.912	-1.059	-1.45	H	-8.078	-0.257	-1.65	H	8.064	1.225	0.443
C	9.824	1.592	0.479	C	-8.971	-2.489	0.757	C	9.176	-1.985	0.261
H	8.526	2.604	1.867	H	-7.686	-3.159	2.348	H	8.021	-3.645	-0.476
H	10.887	0.384	-0.953	H	-10.026	-1.629	0 -0.913	H	10.091	-0.149	0.919
H	10.684	2.213	0.711	H	-9.82	-3.079	1.089	H	10.06	-2.585	0.456
O	-7.492	1.497	-1.637	O	8.592	-2.034	-0.592	O	-7.978	-0.821	2.567
C	-8.169	2.646	-1.18	C	9.365	-2.775	0.324	C	-8.763	-1.979	2.734
H	-8.767	3	-2.02	H	10.023	-3.404	-0.275	H	-9.209	-1.902	3.725
H	-8.829	2.412	-0.336	H	9.97	-2.119	0.961	H	-9.559	-2.036	1.981
H	-7.465	3.432	-0.879	H	8.734	-3.411	0.958	H	-8.151	-2.888	2.679
C	-2.929	2.332	0.5	C	-4.582	4.512	1.453	C	4.378	1.614	2.509
N	-2.832	2.683	1.598	H	-4.732	5.485	0.976	H	4.494	2.356	3.308
C	-3.063	1.874	-0.881	H	-3.506	4.32	1.502	H	5.271	1.674	1.879
H	-4.097	1.569	-1.062	H	-4.979	4.553	2.471	H	4.282	0.624	2.955
H	-2.795	2.68	-1.567	C	-5.267	3.427	0.645	C	3.229	3.108	0.762
H	-2.401	1.019	-1.052	H	-5.115	2.447	1.127	H	4.056	2.944	0.062
				H	-6.352	3.605	0.61	H	2.288	3.231	0.222
				O	-4.713	3.439	-0.655	H	3.452	4.023	1.324
				H	-5.142	2.718	-1.147	C	3.127	1.943	1.718
								O	2.097	1.324	1.886

iPEEK-TB-MEK (-1686.472)				iPEEK-TB-Hex (-1691.061)			
C	-5.683	0.01	-0.709	C	-5.346	-0.367	1.249
C	-4.818	-1.062	-0.517	C	-4.86	0.854	0.8
C	-4.654	-1.595	0.774	C	-4.953	1.179	-0.565
C	-5.329	-1.005	1.841	C	-5.522	0.256	-1.439
C	-6.167	0.09	1.655	C	-5.988	-0.977	-0.994
C	-6.357	0.592	0.365	C	-5.899	-1.292	0.364
H	-5.82	0.435	-1.7	H	-5.264	-0.644	2.297
H	-5.206	-1.432	2.833	H	-5.599	0.515	-2.492
H	-6.677	0.522	2.508	H	-6.412	-1.673	-1.707
C	-4.026	-1.626	-1.683	C	-4.172	1.809	1.757
H	-4.679	-2.201	-2.351	H	-4.904	2.381	2.341
H	-3.596	-0.802	-2.259	H	-3.559	1.249	2.469
N	-3.827	-2.741	1.018	N	-4.444	2.417	-1.088
N	-2.949	-2.511	-1.219	N	-3.325	2.763	1.029
C	-3.512	-3.425	-0.233	C	-4.153	3.363	-0.015
H	-2.796	-4.224	-0.02	H	-3.635	4.224	-0.445
H	-4.423	-3.864	-0.649	H	-5.086	3.703	0.441
C	-2.555	-2.407	1.667	C	-3.194	2.217	-1.831
H	-2.749	-1.728	2.503	H	-3.339	1.427	-2.574
H	-2.134	-3.329	2.089	H	-2.974	3.14	-2.383
C	-1.839	-1.791	-0.681	C	-2.169	2.123	0.475
C	-1.581	-1.762	0.698	C	-2.054	1.857	-0.897
C	-1.003	-1.082	-1.553	C	-1.147	1.718	1.34

C	-0.458	-1.08	1.172	C	-0.918	1.204	-1.377
C	0.087	-0.375	-1.074	C	-0.035	1.04	0.867
H	-1.232	-1.086	-2.614	H	-1.243	1.936	2.401
C	0.364	-0.395	0.294	C	0.072	0.787	-0.502
H	-0.237	-1.044	2.236	H	-0.818	0.967	-2.434
H	0.729	0.187	-1.745	H	0.746	0.706	1.543
O	1.411	0.342	0.818	O	1.102	0.025	-1.018
C	2.685	0.09	0.393	C	2.388	0.274	-0.617
C	3.623	1.089	0.657	C	3.251	-0.819	-0.579
C	3.068	-1.096	-0.238	C	2.846	1.557	-0.307
C	4.95	0.895	0.305	C	4.584	-0.628	-0.239
H	3.287	2.005	1.131	H	2.855	-1.802	-0.808
C	4.396	-1.266	-0.603	C	4.174	1.73	0.048
H	2.334	-1.869	-0.438	H	2.162	2.399	-0.341
C	5.355	-0.288	-0.325	C	5.061	0.649	0.075
H	5.673	1.683	0.495	H	5.247	-1.486	-0.185
H	4.714	-2.171	-1.111	H	4.552	2.713	0.313
C	6.753	-0.527	-0.792	C	6.461	0.913	0.53
O	6.97	-1.275	-1.727	O	6.703	1.885	1.223
C	7.899	0.157	-0.104	C	7.571	-0.02	0.147
C	7.886	0.461	1.26	C	7.595	-0.713	-1.066
C	9.047	0.42	-0.858	C	8.654	-0.126	1.024
C	9.004	1.035	1.858	C	8.685	-1.518	-1.388
H	7.01	0.224	1.858	H	6.775	-0.605	-1.769
C	10.154	1.011	-0.264	C	9.732	-0.944	0.71
H	9.049	0.149	-1.909	H	8.631	0.445	1.947
C	10.133	1.319	1.096	C	9.748	-1.642	-0.497
H	8.993	1.257	2.921	H	8.706	-2.045	-2.336
H	11.038	1.227	-0.856	H	10.564	-1.033	1.402

H	11.001	1.776	1.563	H	10.593	-2.276	-0.746
O	-7.157	1.654	0.06	O	-6.294	-2.475	0.91
C	-7.788	2.32	1.131	C	-6.756	-3.47	0.025
H	-8.345	3.146	0.688	H	-6.974	-4.345	0.637
H	-8.481	1.657	1.662	H	-7.67	-3.154	-0.494
H	-7.052	2.717	1.842	H	-5.99	-3.725	-0.72
C	-4.313	3.255	-1.214	C	-2.686	-1.826	-2.851
H	-5.307	2.88	-0.931	H	-2.893	-0.75	-2.818
H	-4.369	3.563	-2.262	H	-3.652	-2.339	-2.787
C	-2.843	1.669	0.215	H	-2.239	-2.058	-3.823
H	-3.671	1.591	0.931	C	-1.78	-2.226	-1.691
H	-2.325	0.713	0.142	H	-1.56	-3.301	-1.745
H	-2.148	2.43	0.589	H	-0.813	-1.711	-1.776
C	-3.365	2.068	-1.147	C	-2.404	-1.9	-0.338
O	-3.064	1.458	-2.153	H	-2.651	-0.828	-0.303
C	-3.933	4.424	-0.305	H	-3.361	-2.434	-0.236
H	-4.634	5.252	-0.439	C	-1.502	-2.246	0.843
H	-3.958	4.136	0.751	H	-0.527	-1.754	0.709
H	-2.929	4.797	-0.529	H	-1.301	-3.327	0.854
				C	-2.101	-1.826	2.182
				H	-3.059	-2.344	2.328
				H	-2.335	-0.754	2.136
				C	-1.168	-2.099	3.358
				H	-0.228	-1.547	3.241
				H	-1.616	-1.801	4.311
				H	-0.919	-3.164	3.423

iPEEK-Trip-MeCN (-1667.838)				iPEEK-Trip-EtOH (-1690.098)				iPEEK-Trip-AcMe (-1728.201)			
C	2.921	-1.775	-0.313	C	-3.099	1.605	0.126	C	-3.181	0.946	-1.662
C	1.776	-1.478	-1.063	C	-1.903	1.84	-0.561	C	-2.027	0.192	-1.899
C	1.391	-2.292	-2.116	C	-1.805	2.886	-1.464	C	-1.871	-0.496	-3.093
C	2.152	-3.428	-2.412	C	-2.917	3.704	-1.68	C	-2.892	-0.442	-4.046
C	3.283	-3.731	-1.66	C	-4.106	3.469	-0.998	C	-4.051	0.289	-3.8
C	3.676	-2.901	-0.605	C	-4.206	2.413	-0.086	C	-4.2	0.992	-2.601
H	0.495	-2.061	-2.685	H	-0.875	3.065	-1.998	H	-0.982	-1.094	-3.264
H	1.855	-4.075	-3.231	H	-2.851	4.526	-2.386	H	-2.782	-0.981	-4.982
H	3.868	-4.615	-1.895	H	-4.967	4.107	-1.176	H	-4.841	0.32	-4.544
H	4.562	-3.135	-0.02	H	-5.138	2.199	0.429	H	-5.098	1.571	-2.407
C	1.036	-0.241	-0.57	C	-0.801	0.848	-0.202	C	-1.024	0.246	-0.75
C	3.169	-0.771	0.808	C	-3.019	0.411	1.072	C	-3.158	1.66	-0.317
C	4.141	2.739	-0.443	C	-2.697	-2.976	-0.76	C	-3.439	-0.732	2.688
C	2.983	3.039	-1.159	C	-1.497	-2.739	-1.426	C	-2.251	-1.439	2.503
C	1.942	2.124	-1.235	C	-0.843	-1.522	-1.283	C	-1.423	-1.161	1.422
C	2.058	0.894	-0.592	C	-1.387	-0.533	-0.473	C	-1.783	-0.177	0.505
C	3.205	0.601	0.141	C	-2.58	-0.77	0.209	C	-2.942	0.565	0.721
C	4.256	1.514	0.221	C	-3.238	-1.99	0.07	C	-3.784	0.292	1.8
C	1.896	-0.788	1.65	C	-1.84	0.689	2	C	-1.875	2.49	-0.305
C	1.799	-1.078	3.002	C	-1.87	0.723	3.385	C	-1.777	3.855	-0.089
C	0.542	-1.061	3.616	C	-0.691	0.991	4.087	C	-0.516	4.459	-0.103
C	-0.598	-0.751	2.879	C	0.499	1.219	3.405	C	0.627	3.7	-0.329
C	-0.5	-0.461	1.515	C	0.529	1.186	2.007	C	0.528	2.323	-0.549
C	0.746	-0.489	0.907	C	-0.642	0.924	1.313	C	-0.723	1.726	-0.537

H	2.69	-1.313	3.577	H	-2.801	0.543	3.916	H	-2.671	4.446	0.092
H	0.457	-1.285	4.675	H	-0.707	1.019	5.172	H	-0.43	5.528	0.066
H	-1.57	-0.735	3.363	H	1.41	1.424	3.957	H	1.602	4.177	-0.336
H	-1.388	-0.232	0.931	H	1.458	1.357	1.469	H	1.418	1.722	-0.718
H	4.071	-0.98	1.385	H	-3.952	0.233	1.607	H	-4.055	2.249	-0.123
H	0.132	-0.042	-1.146	H	0.13	1.031	-0.742	H	-0.139	-0.362	-0.943
H	2.878	3.991	-1.669	H	-1.06	-3.497	-2.068	H	-1.951	-2.214	3.201
H	4.939	3.471	-0.404	H	-3.19	-3.932	-0.886	H	-4.069	-0.97	3.537
O	5.336	1.132	0.958	O	-4.4	-2.144	0.781	O	-4.899	1.065	1.907
O	0.83	2.44	-1.996	O	0.32	-1.301	-2	O	-0.286	-1.927	1.257
C	-0.39	2.379	-1.371	C	1.505	-1.222	-1.323	C	0.928	-1.298	1.24
C	-1.469	1.941	-2.14	C	2.618	-0.878	-2.095	C	1.959	-1.975	0.587
C	-0.558	2.715	-0.028	C	1.639	-1.469	0.045	C	1.158	-0.068	1.86
C	-2.703	1.754	-1.535	C	3.861	-0.76	-1.494	C	3.228	-1.416	0.554
H	-1.303	1.707	-3.186	H	2.481	-0.714	-3.158	H	1.732	-2.92	0.106
C	-1.811	2.567	0.553	C	2.894	-1.357	0.63	C	2.436	0.471	1.83
H	0.292	3.059	0.553	H	0.777	-1.743	0.643	H	0.346	0.455	2.355
C	-2.88	2.044	-0.178	C	4.013	-0.986	-0.12	C	3.481	-0.184	1.17
H	-3.535	1.369	-2.118	H	4.724	-0.509	-2.103	H	4.033	-1.952	0.06
H	-1.968	2.818	1.598	H	3.023	-1.557	1.689	H	2.644	1.416	2.321
C	-4.178	1.812	0.528	C	5.336	-0.932	0.574	C	4.841	0.434	1.237
O	-4.545	2.562	1.413	O	5.526	-1.579	1.588	O	5.127	1.189	2.148
C	-4.993	0.609	0.16	C	6.437	-0.076	0.02	C	5.861	0.12	0.183
C	-4.413	-0.551	-0.363	C	6.193	1.123	-0.656	C	5.516	-0.14	-1.146
C	-6.363	0.63	0.442	C	7.755	-0.471	0.268	C	7.209	0.172	0.548
C	-5.197	-1.675	-0.61	C	7.256	1.908	-1.092	C	6.511	-0.361	-2.095
H	-3.347	-0.604	-0.563	H	5.172	1.454	-0.819	H	4.471	-0.145	-1.444
C	-7.148	-0.483	0.173	C	8.815	0.304	-0.184	C	8.2	-0.068	-0.395
H	-6.789	1.53	0.873	H	7.925	-1.39	0.82	H	7.457	0.405	1.579

C	-6.565	-1.637	-0.352	C	8.566	1.495	-0.867	C	7.851	-0.336	-1.719
H	-4.726	-2.572	-0.998	H	7.061	2.845	-1.606	H	6.239	-0.551	-3.129
H	-8.214	-0.459	0.379	H	9.837	-0.014	-0.001	H	9.245	-0.041	-0.103
H	-7.179	-2.51	-0.555	H	9.395	2.104	-1.215	H	8.625	-0.517	-2.458
C	6.407	2.044	1.057	C	-5.137	-3.336	0.586	C	-5.751	0.826	3.005
H	6.088	2.983	1.525	H	-4.573	-4.208	0.936	H	-5.228	0.979	3.957
H	7.158	1.563	1.685	H	-6.046	-3.228	1.177	H	-6.565	1.546	2.919
H	6.839	2.259	0.073	H	-5.4	-3.468	-0.47	H	-6.161	-0.191	2.976
C	-0.966	-3.157	-0.097	C	-6.881	0.771	-1.88	C	-1.946	-4.368	0.359
N	-1.76	-2.647	-0.766	H	-6.641	1.8	-1.599	H	-2.422	-5.302	0.039
C	0.044	-3.795	0.746	H	-7.929	0.581	-1.635	H	-2.441	-4.047	1.282
H	-0.288	-4.797	1.028	H	-6.744	0.667	-2.96	H	-0.885	-4.537	0.545
H	0.987	-3.864	0.195	C	-5.986	-0.196	-1.13	C	-3.525	-2.792	-0.912
H	0.197	-3.193	1.648	H	-6.197	-1.228	-1.454	H	-3.79	-2.167	-0.049
				H	-4.931	0.013	-1.362	H	-3.592	-2.194	-1.823
				O	-6.241	-0.046	0.256	H	-4.243	-3.619	-0.946
				H	-5.674	-0.692	0.707	C	-2.12	-3.321	-0.722
								O	-1.182	-2.942	-1.39

iPEEK-Trip-MEK (-1767.493)				iPEEK-Trip-Hex (-1772.081)			
C	-4.587	-1.463	0.249	C	-3.237	-0.082	1.045
C	-3.403	-1.776	0.93	C	-1.982	-0.176	1.659
C	-3.394	-2.758	1.906	C	-1.838	-0.843	2.865
C	-4.581	-3.434	2.205	C	-2.961	-1.426	3.461
C	-5.756	-3.123	1.53	C	-4.207	-1.335	2.85
C	-5.763	-2.131	0.545	C	-4.351	-0.659	1.635
H	-2.475	-2.999	2.434	H	-0.861	-0.923	3.334
H	-4.584	-4.206	2.969	H	-2.856	-1.954	4.404
H	-6.674	-3.652	1.768	H	-5.074	-1.793	3.316
H	-6.68	-1.885	0.015	H	-5.322	-0.593	1.151
C	-2.21	-0.945	0.471	C	-0.862	0.449	0.834
C	-4.402	-0.36	-0.787	C	-3.188	0.634	-0.301
C	-3.673	3.09	0.768	C	-2.352	4.385	-0.063
C	-2.475	2.783	1.412	C	-1.088	4.283	0.516
C	-1.953	1.498	1.348	C	-0.555	3.04	0.828
C	-2.63	0.511	0.641	C	-1.286	1.888	0.563
C	-3.812	0.821	-0.026	C	-2.539	1.985	-0.037
C	-4.347	2.108	0.034	C	-3.085	3.229	-0.351
C	-3.289	-0.842	-1.715	C	-2.178	-0.153	-1.133
C	-3.362	-0.978	-3.092	C	-2.413	-0.765	-2.354
C	-2.24	-1.429	-3.794	C	-1.383	-1.487	-2.966
C	-1.064	-1.737	-3.12	C	-0.137	-1.588	-2.357
C	-0.99	-1.602	-1.73	C	0.102	-0.968	-1.125
C	-2.104	-1.157	-1.036	C	-0.921	-0.254	-0.52
H	-4.281	-0.735	-3.618	H	-3.39	-0.689	-2.825
H	-2.289	-1.537	-4.873	H	-1.56	-1.971	-3.921
H	-0.196	-2.082	-3.673	H	0.658	-2.15	-2.838

H	-0.071	-1.832	-1.197	H	1.076	-1.04	-0.648
H	-5.322	-0.103	-1.315	H	-4.165	0.721	-0.779
H	-1.289	-1.192	1.004	H	0.116	0.369	1.314
H	-1.938	3.54	1.973	H	-0.506	5.172	0.736
H	-4.063	4.098	0.839	H	-2.749	5.367	-0.291
O	-5.51	2.312	-0.643	O	-4.316	3.219	-0.932
O	-0.783	1.21	2.031	O	0.684	2.975	1.443
C	0.322	0.865	1.304	C	1.719	2.398	0.76
C	1.371	0.29	2.028	C	2.863	2.124	1.513
C	0.436	1.069	-0.073	C	1.677	2.095	-0.603
C	2.526	-0.104	1.372	C	3.955	1.519	0.91
H	1.255	0.167	3.1	H	2.869	2.392	2.564
C	1.605	0.681	-0.716	C	2.784	1.503	-1.196
H	-0.381	1.514	-0.632	H	0.79	2.316	-1.188
C	2.651	0.082	-0.012	C	3.924	1.188	-0.451
H	3.358	-0.514	1.936	H	4.845	1.318	1.497
H	1.716	0.838	-1.785	H	2.777	1.269	-2.256
C	3.917	-0.222	-0.739	C	5.084	0.582	-1.172
O	4.253	0.457	-1.697	O	5.229	0.766	-2.367
C	4.778	-1.357	-0.285	C	6.073	-0.264	-0.424
C	4.243	-2.507	0.3	C	5.716	-1.044	0.68
C	6.153	-1.272	-0.516	C	7.379	-0.325	-0.917
C	5.079	-3.564	0.65	C	6.661	-1.863	1.291
H	3.172	-2.583	0.463	H	4.693	-1.03	1.045
C	6.988	-2.319	-0.15	C	8.326	-1.128	-0.295
H	6.546	-0.371	-0.976	H	7.629	0.265	-1.793
C	6.45	-3.468	0.431	C	7.967	-1.899	0.811
H	4.659	-4.463	1.091	H	6.376	-2.476	2.141
H	8.058	-2.245	-0.317	H	9.342	-1.163	-0.675

H	7.102	-4.289	0.713	H	8.705	-2.532	1.293
C	-6.069	3.606	-0.596	C	-4.887	4.467	-1.259
H	-5.386	4.351	-1.023	H	-5.856	4.249	-1.707
H	-6.98	3.566	-1.193	H	-5.029	5.086	-0.365
H	-6.319	3.894	0.433	H	-4.266	5.012	-1.981
C	6.291	2.676	-0.419	C	-0.046	-3.663	1.516
H	6.463	3.757	-0.452	H	0.09	-2.583	1.384
H	5.984	2.355	-1.421	H	-0.539	-3.814	2.483
H	7.207	2.155	-0.136	H	0.943	-4.129	1.56
C	3.937	3.177	0.54	C	-0.892	-4.229	0.378
H	3.152	2.623	1.064	H	-0.973	-5.32	0.476
H	4.162	4.067	1.146	H	-0.391	-4.036	-0.579
C	5.188	2.316	0.552	C	-2.286	-3.608	0.338
O	5.302	1.374	1.308	H	-2.182	-2.517	0.309
C	3.484	3.606	-0.858	H	-2.822	-3.837	1.27
H	2.513	4.105	-0.804	C	-3.116	-4.048	-0.864
H	4.194	4.304	-1.313	H	-3.261	-5.138	-0.847
H	3.393	2.738	-1.516	H	-2.555	-3.823	-1.782
				C	-4.474	-3.353	-0.93
				H	-4.315	-2.267	-0.867
				H	-5.068	-3.624	-0.047
				C	-5.241	-3.688	-2.206
				H	-5.409	-4.767	-2.291
				H	-6.217	-3.193	-2.238
				H	-4.673	-3.373	-3.089

T**able S16**. XYZ coordinates of iPEEK polymers in gas phase and solvents (from MD snapshot) in gas phase

iPEEK-SBI				iPEEK-TB				iPEEK-Trip			
O	4.582	24.015	10.815	O	2.13	4.23	1.256	O	3.456	4.603	12.331
C	4.002	25.239	10.783	C	1.366	5.057	0.495	C	3.632	5.818	13.012
C	4.496	26.269	11.595	C	1.851	6.216	-0.059	C	2.638	6.762	12.969
C	2.765	25.502	10.21	C	0.019	4.733	0.218	C	4.691	5.975	13.906
C	4.002	27.556	11.619	C	1.082	7.044	-0.867	C	2.815	7.946	13.641
H	5.384	26.025	12.162	H	2.918	6.515	0.065	H	1.900	6.596	12.214
C	2.3	26.8	10.045	C	-0.783	5.558	-0.537	C	4.811	7.130	14.698
H	2.287	24.669	9.676	H	-0.346	3.76	0.565	C	5.706	4.928	14.224
C	2.93	27.837	10.744	C	-0.248	6.706	-1.127	C	3.884	8.158	14.522
C	4.559	28.906	12.195	C	1.671	8.386	-1.415	H	2.113	8.703	13.453
H	1.498	27.019	9.332	H	-1.784	5.27	-0.812	C	6.026	7.041	15.688
C	2.689	29.292	10.537	N	-0.994	7.588	-1.956	C	5.585	4.635	15.723
C	5.862	29.234	11.397	H	1.647	9.133	-0.633	C	7.036	5.673	14.095
C	3.396	29.77	11.801	H	2.751	8.298	-1.715	H	5.707	4.030	13.609
C	4.993	28.808	13.68	N	0.907	8.942	-2.511	O	3.969	9.350	15.175
C	1.214	29.721	10.372	C	-0.452	8.941	-2.048	C	5.700	5.771	16.532
C	3.214	29.833	9.222	C	-1.144	7.063	-3.335	C	7.321	6.748	14.967
H	5.633	29.443	10.352	C	1.091	8.205	-3.73	H	6.101	7.887	16.329
H	6.381	30.193	11.747	H	-1.089	9.489	-2.768	C	5.169	3.475	16.287
H	6.655	28.385	11.544	H	-0.644	9.437	-1.125	C	8.108	5.194	13.307
H	2.706	29.649	12.674	H	-1.394	5.971	-3.293	C	3.452	10.613	14.830
H	3.506	30.906	11.846	H	-2.012	7.508	-3.873	C	5.390	5.658	17.882
H	5.97	28.293	13.581	C	0.197	7.214	-4.098	C	8.570	7.245	15.124
H	5.278	29.722	14.329	C	2.184	8.5	-4.555	C	4.966	3.296	17.630
H	4.234	28.278	14.214	C	0.448	6.386	-5.192	H	5.157	2.551	15.692

C	1.041	30.728	9.348	C	2.488	7.631	-5.578	C	9.373	5.698	13.451
C	0.126	29.356	11.134	H	2.923	9.249	-4.199	H	8.053	4.423	12.534
H	4.32	30.012	9.133	C	1.611	6.613	-5.927	C	3.129	10.983	13.542
H	2.988	29.169	8.387	H	-0.239	5.524	-5.406	C	3.371	11.554	15.848
C	2.395	31.096	8.765	H	3.429	7.772	-6.157	C	5.136	4.404	18.460
C	-0.194	31.264	9.093	O	2.012	5.741	-6.977	H	5.483	6.391	18.707
C	-1.1	29.852	10.814	C	1.597	4.452	-6.966	C	9.600	6.655	14.443
H	0.136	28.7	11.936	C	1.391	3.865	-8.237	H	8.783	8.010	15.912
C	2.19	31.207	7.252	C	1.382	3.616	-5.824	H	4.613	2.304	18.063
C	2.793	32.549	9.342	C	1.105	2.499	-8.427	H	10.150	5.385	12.770
C	-1.251	30.79	9.851	H	1.622	4.531	-9.121	C	2.710	12.215	13.212
H	-0.236	32.183	8.437	C	1.023	2.319	-5.986	H	3.271	10.205	12.773
O	-2.117	29.536	11.693	H	1.495	3.99	-4.828	C	2.971	12.847	15.533
H	3.107	31.344	6.651	C	0.929	1.725	-7.29	H	3.632	11.145	16.836
H	1.861	30.24	6.833	H	1.097	1.981	-9.374	H	5.005	4.285	19.500
H	1.43	32.027	7.067	H	0.966	1.736	-5.098	H	10.630	6.943	14.680
H	3.824	32.822	9.214	C	0.562	0.279	-7.418	C	2.620	13.173	14.240
H	2.122	33.353	8.866	O	-0.013	-0.157	-8.396	H	2.519	12.380	12.134
H	2.612	32.602	10.419	C	0.867	-0.684	-6.255	H	2.616	13.560	16.310
H	-2.263	31.214	9.78	C	-0.172	-1.201	-5.408	C	2.142	14.540	13.885
C	-2.997	28.517	11.395	C	2.131	-1.084	-6.016	O	2.357	14.933	12.740
C	-2.718	27.579	10.366	C	0.088	-2.104	-4.418	C	1.381	15.490	14.815
C	-4.193	28.533	12.042	H	-1.287	-0.989	-5.607	C	0.435	15.053	15.697
C	-3.65	26.66	10.001	C	2.423	-1.911	-4.901	C	1.660	16.889	14.738
H	-1.82	27.772	9.744	H	2.92	-0.76	-6.664	C	-0.371	15.936	16.341
C	-5.16	27.565	11.698	C	1.382	-2.414	-4.113	H	0.084	13.983	15.696
H	-4.374	29.405	12.763	H	-0.745	-2.414	-3.747	C	0.903	17.809	15.413
C	-4.858	26.603	10.715	H	3.503	-2.136	-4.737	H	2.377	17.269	14.028
H	-3.393	26.014	9.156	H	1.589	-2.991	-3.202	C	-0.074	17.291	16.256

H	-6.139	27.786	12.136	O	11.936	9.622	15.377	H	-1.193	15.614	16.957
C	-5.938	25.655	10.366	C	11.143	8.513	15.455	H	1.044	18.896	15.284
O	-7.007	26.158	10	C	9.769	8.684	15.338	H	-0.738	17.956	16.818
C	-5.833	24.158	10.546	C	11.645	7.222	15.35	O	13.395	-2.649	4.008
C	-6.968	23.4	10.284	C	8.905	7.587	15.347	C	12.267	-2.601	4.790
C	-4.627	23.508	10.894	H	9.394	9.733	15.383	C	11.054	-2.147	4.270
C	-6.841	21.971	10.171	C	10.777	6.066	15.432	C	12.330	-2.839	6.121
H	-7.976	23.769	10.231	H	12.704	6.924	15.267	C	9.967	-1.971	5.087
C	-4.501	22.126	10.779	C	9.405	6.281	15.543	H	11.051	-1.996	3.216
H	-3.747	24.113	11.041	C	7.464	7.93	15.398	C	11.215	-2.566	6.972
C	-5.618	21.326	10.409	H	11.17	5.014	15.186	C	13.557	-3.301	6.839
H	-7.792	21.448	10.198	N	8.525	5.205	15.692	C	9.931	-2.362	6.428
H	-3.545	21.642	10.803	H	7.244	8.374	16.349	H	8.959	-1.930	4.711
H	-5.602	20.249	10.251	H	7.124	8.526	14.568	C	11.498	-2.885	8.406
O	4.831	19.427	-2.731	N	6.719	6.679	15.255	C	13.043	-4.554	7.515
C	3.914	18.731	-2.025	C	7.203	5.653	16.171	C	13.825	-2.267	7.902
C	2.599	18.958	-2.254	C	8.474	4.447	14.497	H	14.384	-3.482	6.134
C	4.331	17.87	-1.045	C	6.578	6.186	13.94	O	8.770	-2.280	7.186
C	1.655	18.099	-1.694	H	6.442	4.789	16.25	C	11.862	-4.355	8.259
H	2.402	19.74	-3.037	H	7.353	6.003	17.198	C	12.718	-2.118	8.800
C	3.401	17.033	-0.452	H	9.501	4.397	13.951	H	10.685	-2.678	9.070
H	5.487	17.632	-0.88	H	8.23	3.376	14.616	C	13.568	-5.841	7.459
C	2.084	17.168	-0.751	C	7.45	5.148	13.542	C	15.000	-1.562	8.091
C	0.156	18.199	-1.919	C	5.643	6.639	13.086	C	8.267	-0.982	7.280
H	3.63	16.152	0.186	C	7.247	4.557	12.318	C	11.194	-5.407	8.839
C	0.975	16.232	-0.415	C	5.512	6.026	11.861	C	12.843	-1.206	9.866
C	-0.084	18.386	-3.36	H	5.182	7.661	13.42	C	12.939	-6.881	8.121
C	-0.143	16.793	-1.338	C	6.262	4.958	11.456	H	14.531	-5.968	6.997
C	-0.276	19.402	-1.118	H	7.837	3.684	11.937	C	15.055	-0.589	9.109

C	0.636	16.297	0.989	H	4.627	6.354	11.29	H	15.804	-1.686	7.263
C	1.219	14.733	-0.517	O	5.999	4.181	10.421	C	8.996	0.250	7.203
H	0.37	19.319	-3.7	C	5.819	4.827	9.293	C	6.868	-0.908	7.756
H	0.385	17.549	-4.033	C	6.4	6.064	8.958	C	11.687	-6.721	8.711
H	-1.104	18.516	-3.644	C	5.032	4.193	8.309	H	10.244	-5.066	9.348
H	-1.081	16.816	-0.742	C	5.977	6.719	7.819	C	13.987	-0.410	9.942
H	-0.337	16.032	-2.119	H	7.064	6.654	9.639	H	12.205	-1.147	10.800
H	0.348	20.312	-1.244	C	4.695	4.76	7.122	H	13.387	-7.887	8.089
H	-1.333	19.573	-1.341	H	4.534	3.256	8.561	H	15.937	0.102	9.323
H	-0.352	19.142	-0.12	C	5.259	6.042	6.824	C	8.304	1.436	7.369
C	0.219	15.104	1.489	H	6.387	7.707	7.532	H	10.055	0.213	6.947
C	0.461	17.408	1.767	H	4.074	4.318	6.337	C	6.223	0.315	7.916
H	1.138	14.341	-1.502	C	5.05	6.71	5.462	H	6.331	-1.858	7.922
H	2.336	14.61	-0.273	O	5.3	7.882	5.375	H	11.149	-7.574	9.126
C	0.43	13.911	0.602	C	4.24	6.038	4.407	H	14.139	0.265	10.739
C	-0.316	15.009	2.83	C	4.533	4.773	3.92	C	6.963	1.465	7.653
C	-0.049	17.333	3.083	C	3.243	6.732	3.693	H	8.838	2.405	7.239
H	0.803	18.366	1.517	C	3.882	4.154	2.851	H	5.182	0.316	8.213
C	1.334	12.846	1.297	H	5.213	4.026	4.44	C	6.267	2.801	7.745
C	-0.798	13.181	0.163	C	2.441	6.096	2.717	O	6.249	3.517	6.739
C	-0.398	16.141	3.601	H	2.958	7.772	4.097	C	5.554	3.378	8.938
H	-0.605	13.964	3.192	C	2.852	4.865	2.245	C	4.584	4.378	8.828
O	-0.162	18.502	3.826	H	4.085	3.104	2.528	C	5.887	2.866	10.174
H	2.363	13.098	1.487	H	1.445	6.645	2.247	C	3.894	4.866	9.962
H	0.977	12.518	2.3	O	12.165	17.395	11.053	H	4.211	4.724	7.808
H	1.537	12.077	0.549	C	13.305	16.588	11.291	C	5.270	3.380	11.282
H	-0.594	12.09	-0.12	C	14.589	17.141	11.524	H	6.572	2.023	10.393
H	-1.414	13.132	1.086	C	13.176	15.203	11.427	C	4.268	4.332	11.219
H	-1.475	13.709	-0.653	C	15.716	16.303	11.678	H	3.132	5.633	9.825

H	-0.766	16.026	4.593	H	14.811	18.254	11.486	H	5.439	2.871	12.244
C	0.87	18.776	4.668	C	14.24	14.377	11.682	O	9.796	8.541	3.699
C	2.126	18.361	4.331	H	12.183	14.844	11.162	C	11.012	7.899	4.034
C	0.694	19.474	5.881	C	15.518	14.906	11.693	C	12.211	8.544	3.761
C	3.234	18.716	5.129	C	17.057	16.946	11.857	C	11.053	6.602	4.617
H	2.385	17.864	3.364	H	14.136	13.292	11.689	C	13.350	8.119	4.412
C	1.762	19.83	6.666	N	16.684	14.028	11.502	H	12.280	9.395	2.996
H	-0.356	19.758	6.193	H	17.203	17.754	11.121	C	12.186	6.144	5.125
C	3.059	19.44	6.331	H	17.111	17.457	12.829	C	9.881	5.700	4.888
H	4.24	18.395	4.929	N	18.079	15.866	11.7	C	13.350	6.880	5.085
H	1.6	20.372	7.623	C	17.741	14.742	10.821	H	14.283	8.695	4.406
C	4.231	19.632	7.256	C	17.038	13.314	12.769	C	12.073	4.740	5.850
O	5.163	18.877	7.201	C	18.502	15.444	12.96	C	9.761	5.446	6.353
C	4.292	20.758	8.213	H	18.62	14.012	10.836	C	10.173	4.301	4.347
C	4.797	20.602	9.521	H	17.361	15.047	9.829	H	9.019	6.061	4.427
C	3.93	21.99	7.763	H	16.236	13.359	13.486	O	14.586	6.569	5.693
C	4.784	21.704	10.374	H	17.268	12.211	12.625	C	10.985	5.009	6.882
H	5.234	19.666	9.883	C	18.189	14.135	13.445	C	11.344	3.779	4.904
C	3.989	23.098	8.568	C	19.355	16.28	13.744	H	12.944	4.341	6.399
H	3.613	22.112	6.684	C	18.685	13.785	14.632	C	8.670	5.464	7.191
C	4.411	22.995	9.856	C	20.023	15.775	14.856	C	9.353	3.625	3.487
H	5.311	21.707	11.315	H	19.306	17.38	13.437	C	15.192	5.334	5.637
H	3.53	24.045	8.317	C	19.637	14.508	15.299	C	11.055	4.512	8.177
O	11.431	10.641	-1.864	H	18.434	12.7	14.942	C	11.710	2.515	4.488
C	11.135	11.011	-0.584	H	20.672	16.449	15.431	C	8.788	5.129	8.506
C	9.897	11.578	-0.395	O	20.233	13.965	16.461	H	7.677	5.750	6.733
C	12.039	10.834	0.454	C	19.424	13.155	17.184	C	9.720	2.321	3.144
C	9.594	12.065	0.895	C	19.861	11.823	17.382	H	8.380	4.019	3.147
H	9.2	11.817	-1.124	C	18.117	13.454	17.543	C	15.482	4.732	4.478

C	11.723	11.367	1.742	C	18.976	10.846	17.751	C	15.644	4.762	6.814
H	13.061	10.491	0.229	H	20.908	11.453	17.234	C	9.998	4.624	9.049
C	10.502	11.96	1.944	C	17.297	12.476	18.071	H	11.944	3.951	8.444
C	8.34	12.834	1.286	H	17.692	14.437	17.326	C	10.925	1.866	3.546
H	12.475	11.325	2.523	C	17.664	11.141	18.072	H	12.686	2.154	4.820
C	9.891	12.501	3.223	H	19.309	9.847	17.972	H	7.944	5.229	9.320
C	7.222	11.89	0.861	H	16.254	12.771	18.345	H	9.051	1.703	2.457
C	8.452	12.911	2.845	C	16.652	10.164	18.464	C	16.174	3.512	4.448
C	8.241	14.148	0.575	O	16.697	9.753	19.562	H	15.066	5.192	3.595
C	10.557	13.761	3.834	C	15.596	9.795	17.52	C	16.152	3.499	6.857
C	9.968	11.596	4.461	C	15.324	10.629	16.373	H	15.530	5.353	7.713
H	6.242	12.298	1.243	C	14.611	8.814	17.869	H	10.062	4.309	10.112
H	7.24	11.594	-0.193	C	14.164	10.454	15.679	H	11.308	0.874	3.237
H	7.317	10.939	1.346	H	16.044	11.41	16.026	C	16.495	2.866	5.647
H	8.095	13.873	3.256	C	13.414	8.728	17.088	H	16.510	3.047	3.496
H	7.684	12.237	3.218	H	14.736	8.042	18.688	H	16.355	2.889	7.778
H	9.169	14.693	0.654	C	13.141	9.581	16.041	C	17.054	1.472	5.686
H	8.019	13.931	-0.463	H	14.123	11.246	14.817	O	18.191	1.306	6.144
H	7.439	14.812	0.892	H	12.658	8.089	17.511	C	16.107	0.356	5.228
C	10.9	13.62	5.16	O	12.562	2.93	2.596	C	16.558	-0.921	4.735
C	10.857	14.985	3.13	C	11.778	3.705	3.389	C	14.722	0.583	5.297
H	8.925	11.393	4.737	C	12.335	4.639	4.224	C	15.550	-1.821	4.224
H	10.33	10.578	4.12	C	10.404	3.495	3.542	H	17.594	-1.218	4.638
C	10.682	12.285	5.723	C	11.592	5.396	5.127	C	13.770	-0.381	4.915
C	11.468	14.681	5.887	H	13.411	4.718	4.251	H	14.430	1.506	5.729
C	11.454	16.03	3.82	C	9.581	4.318	4.406	C	14.212	-1.593	4.361
H	10.607	15.005	2.07	H	9.85	2.765	2.897	H	15.933	-2.763	3.803
C	12.062	11.611	6.042	C	10.19	5.266	5.152	H	12.740	-0.102	4.986
C	9.914	12.315	7.053	C	12.39	6.424	6.01	O	6.756	15.875	13.649

C	11.625	15.877	5.237	H	8.502	4.404	4.378	C	6.407	14.540	13.555
H	11.78	14.527	6.879	N	9.539	6.148	6.021	C	5.760	14.032	12.427
O	11.623	17.29	3.217	H	12.942	5.8	6.702	C	6.907	13.611	14.462
H	12.721	11.397	5.184	H	13.092	7.085	5.433	C	5.716	12.628	12.253
H	12.656	12.228	6.755	N	11.569	7.276	6.913	H	5.321	14.773	11.711
H	11.86	10.627	6.514	C	10.332	6.596	7.258	C	6.716	12.246	14.363
H	8.851	12.722	6.896	C	8.944	7.251	5.282	C	7.718	14.015	15.593
H	9.837	11.258	7.422	C	11.092	8.466	6.099	C	6.225	11.741	13.152
H	10.539	12.893	7.789	H	9.7	7.222	7.952	H	5.204	12.300	11.385
H	12.091	16.791	5.639	H	10.625	5.746	7.878	C	7.292	11.393	15.503
C	11.259	17.346	1.903	H	8.884	6.931	4.232	C	8.954	13.169	15.507
C	9.941	17.094	1.494	H	7.98	7.543	5.81	C	7.007	13.386	16.863
C	12.233	17.67	0.969	C	9.927	8.442	5.317	H	7.839	15.097	15.646
C	9.6	17.08	0.149	C	11.977	9.504	5.963	O	6.465	10.464	12.885
H	9.203	16.939	2.281	C	9.679	9.528	4.471	C	8.720	11.773	15.416
C	11.859	17.61	-0.334	C	11.727	10.55	4.977	C	6.820	11.962	16.818
H	13.23	17.826	1.329	H	12.988	9.563	6.521	H	7.122	10.310	15.341
C	10.549	17.422	-0.799	C	10.515	10.652	4.332	C	10.268	13.675	15.372
H	8.586	16.835	-0.113	H	8.698	9.617	3.899	C	6.437	14.150	17.906
H	12.576	17.681	-1.138	H	12.522	11.288	4.793	C	6.263	10.030	11.620
C	10.181	17.624	-2.294	O	10.253	11.694	3.521	C	9.795	10.956	15.143
O	10.973	17.239	-3.095	C	10.033	12.901	4.225	C	6.088	11.338	17.835
C	8.801	18.2	-2.58	C	10.786	13.243	5.411	C	11.321	12.804	15.171
C	8.407	19.47	-2.112	C	8.955	13.744	3.893	H	10.396	14.783	15.500
C	7.897	17.461	-3.327	C	10.348	14.344	6.121	C	5.828	13.426	18.950
C	7.061	19.817	-2.274	H	11.618	12.646	5.754	H	6.442	15.219	17.929
H	9.153	20.08	-1.567	C	8.592	14.865	4.616	C	5.468	8.905	11.323
C	6.575	17.83	-3.426	H	8.523	13.506	2.962	C	6.950	10.596	10.511
H	8.131	16.435	-3.776	C	9.219	15.129	5.828	C	11.099	11.420	15.028

C	6.129	18.968	-2.811	H	10.816	14.459	7.093	H	9.793	9.923	14.900
H	6.829	20.734	-1.772	H	7.695	15.563	4.369	C	5.690	12.073	18.929
H	5.839	17.287	-4.028	C	8.701	16.105	6.801	H	6.016	10.243	17.783
O	20.717	2.048	3.301	O	7.563	16.503	6.739	H	12.336	13.146	15.026
C	21.563	3.121	3.218	C	9.59	16.612	7.888	H	5.380	14.042	19.738
C	22.096	3.788	4.302	C	9.108	16.8	9.222	C	5.334	8.405	10.035
C	21.993	3.546	1.935	C	10.973	16.787	7.683	H	4.955	8.368	12.117
C	23.082	4.756	4.238	C	9.965	16.991	10.274	C	6.683	10.180	9.252
H	21.698	3.503	5.301	H	8.035	16.82	9.39	H	7.638	11.440	10.740
C	22.905	4.592	1.893	C	11.828	17.056	8.737	H	11.935	10.710	14.998
H	21.634	2.96	1.122	H	11.456	16.721	6.724	H	5.220	11.649	19.777
C	23.445	5.212	3.022	C	11.359	17.157	10.015	C	5.928	9.048	9.008
C	23.949	5.399	5.315	H	9.676	17.004	11.372	H	4.612	7.590	9.923
H	23.459	4.886	0.978	H	12.852	17.302	8.536	H	7.229	10.621	8.423
C	24.338	6.328	3.051	H	11.351	-5.173	-5.303	C	5.718	8.506	7.621
C	25.133	4.479	5.664	O	11.187	-4.449	-4.64	O	4.669	7.950	7.350
C	24.334	6.683	4.535	C	10.292	-3.487	-5.182	C	6.832	8.568	6.591
C	23.027	5.552	6.528	C	9.226	-3.849	-6.007	C	8.192	8.492	6.986
C	23.863	7.287	2.01	C	10.468	-2.128	-4.853	C	6.543	8.501	5.253
C	25.802	5.926	2.593	C	8.296	-2.954	-6.463	C	9.175	8.652	6.034
H	25.584	3.921	4.809	H	8.962	-4.832	-6.126	H	8.524	8.485	8.018
H	25.885	5.127	6.088	C	9.458	-1.24	-5.204	C	7.570	8.629	4.279
H	24.958	3.757	6.532	H	11.294	-1.908	-4.2	H	5.550	8.527	4.832
H	23.484	7.373	4.748	C	8.391	-1.643	-6.001	C	8.866	8.525	4.649
H	25.313	7.122	4.874	C	7.19	-3.465	-7.334	H	10.223	8.767	6.342
H	22.101	6.048	6.179	H	9.537	-0.162	-4.858	H	7.325	8.577	3.208
H	22.763	4.611	7.008	N	7.32	-0.696	-6.234	H	15.135	26.364	9.921
H	23.5	6.152	7.311	H	7.413	-3.376	-8.42	O	15.733	25.946	10.482
C	24.734	7.422	0.982	H	6.955	-4.511	-7.108	C	15.467	24.579	10.382

C	22.587	7.84	1.942	N	6.024	-2.677	-6.908	C	16.157	23.808	9.456
H	26.535	6.262	3.345	C	6.429	-1.306	-7.223	C	14.582	23.946	11.205
H	25.983	4.798	2.507	C	6.522	-0.504	-4.998	C	15.950	22.442	9.382
C	26.048	6.772	1.316	C	5.77	-2.839	-5.496	H	16.910	24.287	8.830
C	24.328	8.102	-0.162	H	5.546	-0.614	-7.36	C	14.384	22.560	11.161
C	22.16	8.55	0.789	H	7.002	-1.244	-8.16	C	13.831	24.733	12.347
H	21.813	7.646	2.679	H	7.162	0.002	-4.26	C	15.028	21.811	10.202
C	26.563	5.867	0.263	H	5.67	0.14	-5.209	H	16.518	21.861	8.560
C	27.082	7.812	1.625	C	6.119	-1.921	-4.535	C	13.384	22.190	12.215
C	23.073	8.628	-0.274	C	5.429	-4.125	-5.042	C	14.199	24.001	13.632
H	25.034	8.146	-0.971	C	6.304	-2.335	-3.227	C	12.369	24.443	12.233
O	20.983	9.157	0.834	C	5.467	-4.429	-3.696	H	14.111	25.807	12.397
H	25.969	4.914	0.177	H	5.045	-4.932	-5.712	O	14.757	20.510	9.833
H	26.811	6.232	-0.769	C	5.959	-3.553	-2.686	C	14.007	22.624	13.529
H	27.505	5.529	0.722	H	6.858	-1.518	-2.614	C	12.082	23.065	12.156
H	27.373	8.31	0.71	H	5.002	-5.423	-3.345	H	13.129	21.147	12.257
H	26.673	8.556	2.304	O	6.147	-3.941	-1.411	C	14.782	24.501	14.749
H	28.015	7.308	2.09	C	7.375	-3.448	-1.053	C	11.351	25.367	12.231
H	22.834	9.149	-1.233	C	7.584	-2.403	-0.119	C	14.197	19.503	10.576
C	20.041	9.004	-0.195	C	8.478	-3.83	-1.84	C	14.296	21.773	14.537
C	19.934	7.791	-0.835	C	8.822	-1.92	0.116	C	10.814	22.643	11.835
C	19.096	10.021	-0.315	H	6.804	-2.105	0.668	C	15.041	23.724	15.860
C	18.88	7.56	-1.678	C	9.744	-3.237	-1.707	H	15.057	25.623	14.692
H	20.704	7.028	-0.594	H	8.374	-4.673	-2.566	C	10.073	24.931	12.183
C	18.057	9.737	-1.143	C	9.919	-2.305	-0.688	H	11.653	26.411	12.529
H	19.104	11.025	0.222	H	8.947	-1.25	0.931	C	14.943	18.391	11.136
C	17.893	8.55	-1.804	H	10.59	-3.476	-2.334	C	12.834	19.559	10.789
H	18.798	6.615	-2.252	C	11.226	-1.618	-0.386	C	14.808	22.324	15.767
H	17.358	10.605	-1.118	O	12.231	-2.062	-0.949	H	14.064	20.692	14.441

C	16.555	8.199	-2.527	C	11.404	-0.356	0.446	C	9.816	23.615	11.844
O	16.519	7.171	-3.145	C	11.985	-0.536	1.698	H	10.434	21.658	11.644
C	15.191	8.881	-2.328	C	11.12	0.871	-0.133	H	15.351	24.319	16.736
C	15.009	10.221	-2.614	C	12.34	0.566	2.454	H	9.225	25.594	12.497
C	14.076	8.107	-2.234	H	12.266	-1.531	2.011	C	14.295	17.542	12.004
C	13.747	10.847	-2.4	C	11.548	1.977	0.578	H	16.029	18.391	11.132
H	15.832	10.874	-2.899	H	10.587	0.9	-1.061	C	12.147	18.520	11.473
C	12.814	8.667	-2.059	C	12.057	1.824	1.889	H	12.203	20.400	10.426
H	14.152	6.973	-2.277	H	12.765	0.418	3.473	H	15.172	21.622	16.531
C	12.655	10.031	-2.121	H	11.503	2.874	-0.05	H	8.734	23.321	11.815
H	13.702	11.908	-2.496					C	12.924	17.556	12.162
H	11.911	7.939	-1.992					H	14.899	16.887	12.609
H	15.452	-1.025	7.092					H	11.077	18.505	11.532
O	15.239	-1.793	7.634					C	12.264	16.567	13.095
C	15.491	-2.864	6.856					O	12.927	15.877	13.808
C	14.937	-4.071	7.296					C	10.767	16.435	13.169
C	16.044	-2.783	5.566					C	10.057	17.095	14.188
C	15.086	-5.209	6.487					C	10.072	15.608	12.235
H	14.397	-4.125	8.206					C	8.714	17.008	14.322
C	16.174	-3.956	4.828					H	10.703	17.764	14.826
H	16.471	-1.875	5.24					C	8.777	15.450	12.398
C	15.738	-5.184	5.28					H	10.546	15.105	11.307
C	14.576	-6.629	6.849					C	8.061	16.127	13.449
H	16.699	-3.889	3.87					H	8.118	17.551	15.062
C	15.747	-6.499	4.562					H	8.372	14.853	11.563
C	13.082	-6.924	6.773								
C	15.302	-7.4	5.742								
C	15.085	-7.103	8.209								
C	17.063	-6.92	4.041								

C	14.966	-6.391	3.271		
H	12.443	-6.475	7.567		
H	12.75	-6.512	5.777		
H	12.729	-7.996	6.833		
H	16.243	-7.873	6.135		
H	14.609	-8.164	5.257		
H	16.204	-6.95	8.268		
H	14.609	-6.529	8.984		
H	15.01	-8.173	8.336		
C	16.961	-7.543	2.76		
C	18.294	-6.775	4.711		
H	13.861	-6.374	3.455		
H	15.231	-5.421	2.903		
C	15.562	-7.474	2.219		
C	18.101	-8.071	2.179		
C	19.403	-7.383	4.137		
H	18.37	-6.399	5.711		
C	15.552	-6.876	0.828		
C	15.136	-8.943	2.4		
C	19.326	-8.022	2.851		
H	18.034	-8.539	1.186		
O	20.613	-7.352	4.776		
H	14.619	-7.1	0.346		
H	15.754	-5.838	0.814		
H	16.261	-7.352	0.139		
H	15.033	-9.274	3.514		
H	14.166	-9.224	2.024		
H	15.752	-9.804	1.96		
H	20.145	-8.517	2.317		

C	20.94	-6.101	5.29								
C	20.67	-4.979	4.551								
C	21.447	-5.972	6.591								
C	20.873	-3.712	5.097								
H	20.41	-5.177	3.495								
C	21.563	-4.702	7.141								
H	21.736	-6.757	7.217								
C	21.242	-3.568	6.441								
H	20.631	-2.888	4.371								
H	21.878	-4.768	8.205								
C	21.394	-2.2	6.983								
O	21.714	-1.987	8.131								
C	21.193	-0.978	6.069								
C	22.186	-0.055	5.988								
C	19.947	-0.883	5.442								
C	22.09	0.909	5.029								
H	23.137	-0.133	6.544								
C	19.841	0.084	4.471								
H	19.122	-1.672	5.418								
C	20.863	1.032	4.288								
H	22.82	1.651	4.889								
H	18.914	0.406	3.951								

In MeCN

iPEEK-SBI

O	8.629	5.818	16.983
C	8.159	7.098	16.749
C	9.158	8.011	16.336

iPEEK-TB

O	18.637	-2.167	8.135
C	17.373	-1.610	8.103
C	17.033	-0.384	8.701

iPEEK-Trip

O	29.660	5.656	11.865
C	30.067	4.467	11.288
C	30.773	4.464	10.108

C	6.791	7.447	16.982	C	16.356	-2.076	7.246	C	29.808	3.217	11.884
C	8.799	9.287	16.187	C	15.734	0.181	8.754	C	31.192	3.281	9.533
H	10.207	7.652	16.257	H	17.918	0.132	9.143	H	30.932	5.426	9.593
C	6.475	8.725	16.598	C	15.105	-1.542	7.240	C	30.290	2.048	11.336
H	6.085	6.691	17.277	H	16.454	-3.052	6.711	C	29.136	3.002	13.229
C	7.449	9.647	16.129	C	14.763	-0.491	8.020	C	30.982	2.056	10.175
C	9.675	10.492	15.823	C	15.416	1.384	9.620	H	31.745	3.305	8.625
H	5.405	9.022	16.738	H	14.310	-2.143	6.770	C	29.964	0.789	12.085
C	7.276	11.102	15.817	N	13.389	-0.122	8.104	C	30.252	2.322	14.018
C	10.176	10.316	14.424	H	15.583	1.275	10.741	C	28.032	2.034	13.013
C	8.709	11.678	15.931	H	16.089	2.245	9.305	H	28.757	3.962	13.673
C	10.918	10.678	16.723	N	14.087	1.864	9.275	O	31.444	0.875	9.542
C	6.399	11.999	16.665	C	13.062	0.722	9.213	C	30.642	1.134	13.375
C	6.587	11.351	14.459	C	12.946	0.563	6.847	C	28.453	0.790	12.396
H	10.727	9.326	14.442	C	14.064	2.532	8.028	H	30.358	-0.098	11.534
H	9.395	10.356	13.692	H	12.009	1.086	9.203	C	30.767	2.705	15.233
H	10.924	11.152	14.149	H	13.086	0.092	10.123	C	26.736	2.147	13.231
H	8.962	12.192	16.871	H	13.164	-0.008	5.975	C	32.182	0.014	10.254
H	8.946	12.414	15.102	H	11.836	0.652	6.859	C	31.606	0.381	13.981
H	11.328	11.538	16.340	C	13.533	1.983	6.875	C	27.568	-0.217	12.191
H	10.834	10.790	17.845	C	14.463	3.866	7.985	C	31.660	1.913	15.873
H	11.580	9.815	16.631	C	13.457	2.749	5.709	H	30.299	3.580	15.733
C	5.597	12.907	15.964	C	14.306	4.668	6.836	C	25.780	1.167	12.923
C	6.394	12.047	18.069	H	14.779	4.318	8.951	H	26.394	3.079	13.659
H	7.338	11.257	13.619	C	13.825	4.114	5.640	C	33.206	0.375	11.180
H	5.807	10.558	14.446	H	13.123	2.349	4.755	C	32.104	-1.362	9.919
C	5.836	12.773	14.398	H	14.691	5.669	6.818	C	32.148	0.775	15.214
C	4.752	13.781	16.626	O	13.636	4.914	4.581	H	31.921	-0.549	13.510
C	5.501	12.893	18.768	C	14.053	4.493	3.402	C	26.225	-0.062	12.465

H	7.248	11.504	18.621	C	13.426	4.768	2.237	H	27.956	-1.058	11.660
C	4.519	12.727	13.659	C	15.253	3.738	3.320	H	32.274	2.249	16.728
C	6.721	13.953	14.032	C	13.800	4.159	1.081	H	24.722	1.326	13.204
C	4.663	13.781	18.014	H	12.517	5.376	2.321	C	34.060	-0.559	11.785
H	3.939	14.340	16.020	C	15.757	3.220	2.178	H	33.263	1.440	11.455
O	5.548	12.973	20.170	H	15.804	3.624	4.240	C	32.880	-2.285	10.590
H	3.931	13.629	13.895	C	14.993	3.385	0.983	H	31.402	-1.733	9.161
H	4.494	12.626	12.542	H	13.214	4.471	0.125	H	32.996	0.200	15.542
H	3.865	11.958	14.131	H	16.719	2.698	2.066	H	25.464	-0.811	12.031
H	7.552	14.078	14.770	C	15.374	2.825	-0.296	C	33.919	-1.890	11.449
H	7.212	13.946	12.933	O	15.073	3.329	-1.347	H	34.908	-0.245	12.366
H	6.075	14.864	14.238	C	16.020	1.490	-0.223	H	32.825	-3.380	10.285
H	3.994	14.493	18.533	C	15.334	0.484	0.385	C	34.887	-2.867	11.870
C	5.831	11.891	20.909	C	17.164	1.229	-1.059	O	36.001	-2.336	12.003
C	5.485	10.567	20.482	C	15.900	-0.811	0.433	C	34.769	-4.322	12.175
C	6.517	12.014	22.110	H	14.455	0.611	0.965	C	35.825	-5.241	12.125
C	5.909	9.510	21.280	C	17.710	-0.035	-1.034	C	33.464	-4.825	12.331
H	4.882	10.368	19.556	H	17.664	2.036	-1.664	C	35.588	-6.587	12.376
C	7.146	10.983	22.747	C	17.054	-1.080	-0.338	H	36.892	-4.765	12.117
H	6.636	13.038	22.503	H	15.307	-1.479	0.960	C	33.220	-6.148	12.440
C	6.888	9.702	22.319	H	18.577	-0.332	-1.633	H	32.609	-4.159	12.450
H	5.872	8.484	20.737	H	17.424	-2.104	-0.345	C	34.284	-7.052	12.463
H	7.838	11.215	23.579	O	12.835	2.345	13.383	H	36.408	-7.275	12.428
C	7.511	8.492	22.894	C	13.837	2.041	14.243	H	32.204	-6.351	12.535
O	8.723	8.418	23.128	C	13.602	1.836	15.592	H	34.003	-8.103	12.636
C	6.608	7.351	23.308	C	15.183	2.080	13.824	O	23.100	1.293	19.933
C	7.045	6.045	23.499	C	14.597	1.638	16.503	C	22.658	2.531	19.483
C	5.244	7.581	23.477	H	12.656	1.807	16.081	C	22.276	2.751	18.099
C	6.185	5.040	23.955	C	16.223	1.941	14.759	C	22.658	3.665	20.266

H	8.155	5.881	23.506	H	15.321	2.331	12.745	C	21.822	3.976	17.602
C	4.349	6.606	23.868	C	15.941	1.758	16.103	H	22.129	1.812	17.520
H	4.711	8.535	23.381	C	14.222	1.395	17.986	C	22.340	4.929	19.752
C	4.819	5.285	24.017	H	17.289	2.054	14.560	C	23.008	3.577	21.753
H	6.392	3.975	23.995	N	16.938	1.594	17.092	C	22.012	5.110	18.381
H	3.354	6.821	24.053	H	13.837	2.301	18.444	H	21.447	4.058	16.529
H	4.168	4.457	24.338	H	13.430	0.552	18.000	C	22.362	5.994	20.827
O	6.002	-3.492	12.564	N	15.404	0.946	18.735	C	21.706	4.159	22.343
C	4.675	-3.380	12.257	C	16.540	1.822	18.472	C	24.065	4.623	22.070
C	4.209	-3.260	10.958	C	17.685	0.370	16.952	H	23.218	2.629	22.043
C	3.813	-3.370	13.356	C	15.741	-0.390	18.410	O	21.877	6.341	17.803
C	2.814	-3.113	10.879	H	17.351	1.586	19.266	C	21.358	5.388	21.826
H	4.825	-3.187	10.024	H	16.249	2.855	18.568	C	23.711	5.854	21.541
C	2.397	-3.152	13.180	H	18.068	0.277	15.904	H	22.281	7.042	20.500
H	4.117	-3.549	14.375	H	18.687	0.299	17.437	C	20.906	3.596	23.299
C	1.888	-3.161	11.897	C	16.770	-0.709	17.453	C	25.149	4.504	22.921
C	2.077	-2.998	9.613	C	15.064	-1.427	19.021	C	22.403	6.525	16.557
H	1.830	-3.102	14.079	C	17.030	-2.061	17.137	C	20.184	5.990	22.143
C	0.481	-2.916	11.524	C	15.263	-2.754	18.588	C	24.534	6.977	21.795
C	2.196	-4.297	8.721	H	14.266	-1.166	19.709	C	19.689	4.205	23.634
C	0.672	-2.593	10.066	C	16.242	-3.063	17.669	H	21.259	2.668	23.757
C	2.694	-1.812	8.926	H	17.864	-2.292	16.441	C	25.984	5.608	23.116
C	-0.190	-1.850	12.312	H	14.674	-3.633	18.935	H	25.523	3.542	23.299
C	-0.417	-4.116	11.826	O	16.388	-4.395	17.266	C	22.037	7.488	15.672
H	3.243	-4.476	8.424	C	17.161	-4.561	16.130	C	23.493	5.741	16.139
H	1.912	-5.156	9.288	C	16.638	-4.459	14.907	C	19.337	5.429	23.113
H	1.558	-4.186	7.867	C	18.584	-4.778	16.373	H	19.891	6.858	21.576
H	0.534	-1.528	9.866	C	17.448	-4.697	13.802	C	25.666	6.803	22.584
H	-0.145	-3.031	9.544	H	15.586	-4.338	14.676	H	24.215	7.975	21.609

H	2.232	-1.466	7.972	C	19.346	-5.111	15.267	H	19.124	3.642	24.331
H	2.726	-0.876	9.514	H	19.013	-4.942	17.349	H	26.857	5.540	23.772
H	3.739	-2.012	8.708	C	18.775	-5.052	13.968	C	22.504	7.544	14.371
C	-1.475	-2.198	12.644	H	17.018	-4.563	12.815	H	21.241	8.139	16.035
C	0.394	-0.667	12.801	H	20.390	-5.353	15.450	C	24.048	5.875	14.904
H	-0.373	-4.926	11.120	C	19.619	-5.303	12.742	H	23.909	4.833	16.628
H	-0.017	-4.490	12.816	O	20.486	-6.178	12.732	H	18.521	5.967	23.570
C	-1.858	-3.607	12.067	C	19.396	-4.408	11.548	H	26.323	7.694	22.831
C	-2.221	-1.296	13.409	C	18.685	-3.227	11.566	C	23.553	6.812	13.929
C	-0.447	0.185	13.656	C	19.923	-4.738	10.332	H	22.005	8.260	13.649
H	1.328	-0.301	12.397	C	18.381	-2.434	10.446	H	24.854	5.219	14.546
C	-2.555	-4.469	13.136	H	18.287	-2.947	12.542	C	24.133	6.811	12.604
C	-2.800	-3.411	10.875	C	19.650	-4.033	9.181	O	23.403	6.926	11.622
C	-1.771	-0.160	13.969	H	20.509	-5.671	10.265	C	25.565	6.419	12.536
H	-3.358	-1.519	13.519	C	18.897	-2.838	9.223	C	25.972	5.400	11.643
O	0.128	1.378	14.093	H	17.762	-1.539	10.562	C	26.588	7.175	13.108
H	-2.533	-5.533	12.803	H	20.009	-4.437	8.174	C	27.329	5.144	11.472
H	-1.831	-4.456	14.017	O	15.951	14.967	20.147	H	25.227	4.853	11.020
H	-3.570	-4.170	13.506	C	14.945	14.308	19.618	C	27.927	6.821	13.074
H	-2.848	-4.356	10.210	C	13.882	14.964	18.962	H	26.299	8.018	13.798
H	-3.803	-3.246	11.306	C	14.913	12.957	19.742	C	28.325	5.842	12.146
H	-2.520	-2.466	10.297	C	12.785	14.221	18.461	H	27.572	4.484	10.637
H	-2.303	0.507	14.613	H	13.811	16.064	18.816	H	28.654	7.488	13.576
C	1.307	1.301	14.844	C	13.895	12.275	19.187	O	14.878	-1.334	26.524
C	1.910	2.533	15.084	H	15.722	12.373	20.247	C	14.819	-1.773	25.226
C	1.958	0.166	15.304	C	12.767	12.786	18.608	C	14.420	-0.921	24.187
C	3.064	2.669	15.818	C	11.514	14.931	17.990	C	15.051	-3.145	24.921
H	1.433	3.386	14.596	H	13.796	11.129	19.215	C	14.331	-1.450	22.912
C	3.154	0.311	15.905	N	11.699	12.032	18.280	H	14.257	0.145	24.300

H	1.508	-0.879	15.255	H	10.890	15.156	18.802	C	14.991	-3.573	23.626
C	3.745	1.516	16.237	H	11.715	15.816	17.396	C	15.424	-4.117	25.935
H	3.433	3.720	16.075	N	10.768	13.936	17.152	C	14.680	-2.749	22.621
H	3.482	-0.674	16.290	C	10.476	12.823	18.113	H	14.187	-0.791	22.104
C	4.911	1.546	17.158	C	11.944	11.219	17.091	C	15.357	-5.011	23.520
O	5.014	0.638	17.889	C	11.551	13.459	16.039	C	16.723	-4.679	25.475
C	5.882	2.691	17.127	H	9.734	12.109	17.717	C	14.374	-5.167	25.753
C	5.981	3.527	16.022	H	10.094	13.192	19.038	H	15.349	-3.778	27.008
C	6.788	2.866	18.219	H	12.895	10.716	17.219	O	14.570	-3.191	21.341
C	6.903	4.561	15.993	H	11.169	10.428	17.075	C	16.752	-5.107	24.157
H	5.449	3.357	15.059	C	12.026	12.164	15.942	C	14.408	-5.723	24.440
C	7.671	3.947	18.158	C	11.716	14.337	14.910	H	15.232	-5.341	22.524
H	6.772	2.233	19.161	C	12.612	11.694	14.755	C	17.959	-4.696	26.151
C	7.743	4.735	17.022	C	12.285	13.819	13.724	C	13.552	-5.695	26.720
H	6.841	5.166	15.077	H	11.311	15.383	15.012	C	15.788	-3.275	20.674
H	8.428	4.173	18.951	C	12.745	12.522	13.609	C	17.929	-5.526	23.509
O	17.456	-3.354	1.692	H	12.986	10.674	14.795	C	13.539	-6.823	24.208
C	17.548	-2.448	2.743	H	12.404	14.456	12.844	C	19.178	-5.019	25.568
C	18.563	-2.588	3.754	O	13.236	12.165	12.394	H	18.007	-4.221	27.135
C	16.653	-1.383	2.966	C	13.319	10.904	11.897	C	12.643	-6.704	26.337
C	18.741	-1.613	4.690	C	14.122	10.668	10.714	H	13.653	-5.363	27.807
H	19.292	-3.416	3.818	C	12.714	9.763	12.424	C	16.208	-4.418	20.031
C	16.849	-0.442	3.965	C	14.235	9.370	10.225	C	16.591	-2.220	20.764
H	15.788	-1.370	2.360	H	14.758	11.510	10.332	C	19.116	-5.471	24.215
C	17.880	-0.540	4.821	C	12.956	8.494	11.948	H	17.920	-5.920	22.477
C	19.849	-1.636	5.690	H	12.041	9.845	13.268	C	12.619	-7.280	25.098
H	16.281	0.500	3.977	C	13.715	8.290	10.851	H	13.452	-7.262	23.173
C	18.281	0.313	5.965	H	15.016	9.172	9.462	H	20.173	-5.125	26.082
C	21.195	-1.847	5.067	H	12.476	7.626	12.403	H	11.910	-7.012	27.104

C	19.719	-0.263	6.406	C	13.813	6.932	10.285	C	17.500	-4.396	19.459
C	19.522	-2.827	6.602	O	14.220	6.756	9.154	H	15.509	-5.343	20.009
C	17.367	0.452	7.145	C	13.600	5.745	11.098	C	17.862	-2.178	20.350
C	18.456	1.830	5.574	C	12.866	4.694	10.615	H	16.285	-1.362	21.389
H	21.447	-2.928	4.828	C	14.101	5.673	12.367	H	19.994	-5.610	23.635
H	21.267	-1.379	4.060	C	12.677	3.567	11.357	H	12.051	-8.172	24.964
H	21.975	-1.393	5.633	H	12.504	4.796	9.559	C	18.355	-3.249	19.589
H	19.990	-0.456	7.500	C	13.815	4.623	13.254	H	17.878	-5.242	18.831
H	20.519	0.459	5.996	H	14.645	6.394	12.894	H	18.547	-1.407	20.631
H	20.246	-3.067	7.402	C	13.101	3.515	12.745	C	19.766	-3.249	18.994
H	18.544	-2.726	7.126	H	12.285	2.625	10.991	O	20.226	-4.189	18.410
H	19.454	-3.817	6.074	H	14.264	4.544	14.253	C	20.666	-2.093	19.270
C	17.290	1.788	7.618	O	17.912	13.925	8.084	C	21.994	-2.262	19.612
C	16.673	-0.553	7.753	C	16.596	14.323	7.982	C	20.153	-0.831	18.954
H	19.517	1.846	5.133	C	15.702	13.773	8.926	C	22.838	-1.104	19.829
H	17.765	2.091	4.766	C	16.160	15.309	7.103	H	22.444	-3.218	19.828
C	18.200	2.683	6.844	C	14.432	14.264	9.089	C	20.992	0.299	19.145
C	16.490	2.077	8.706	H	16.042	13.007	9.580	H	19.162	-0.621	18.544
C	15.689	-0.228	8.723	C	14.830	15.737	7.255	C	22.297	0.223	19.622
H	16.675	-1.609	7.405	H	16.799	15.808	6.296	H	23.886	-1.244	20.162
C	17.498	4.026	6.659	C	13.972	15.267	8.245	H	20.586	1.317	19.048
C	19.550	2.904	7.487	C	13.632	13.773	10.310	O	14.578	5.172	17.257
C	15.697	1.091	9.233	H	14.493	16.564	6.596	C	14.530	5.644	18.550
H	16.543	3.125	9.097	N	12.656	15.760	8.438	C	14.910	6.917	18.910
O	15.000	-1.182	9.308	H	13.101	12.860	10.036	C	14.140	4.852	19.618
H	18.114	4.743	6.061	H	14.395	13.490	10.996	C	14.927	7.342	20.206
H	16.579	3.905	6.091	N	12.775	14.887	10.621	H	15.243	7.566	18.113
H	17.263	4.506	7.680	C	11.879	15.013	9.445	C	14.010	5.294	20.906
H	19.486	3.441	8.479	C	12.725	17.096	8.855	C	13.786	3.413	19.451

H	19.967	1.972	7.845	C	13.582	16.081	10.920	C	14.381	6.591	21.202
H	20.260	3.324	6.763	H	10.952	15.667	9.729	H	15.114	8.367	20.417
H	14.996	1.293	10.100	H	11.496	14.085	9.008	C	13.456	4.184	21.860
C	13.624	-1.019	9.191	H	13.300	17.677	8.051	C	12.407	3.201	19.994
C	13.078	-0.665	7.952	H	11.654	17.593	8.849	C	14.756	2.705	20.439
C	12.828	-1.172	10.360	C	13.486	17.208	10.115	H	13.792	3.011	18.468
C	11.697	-0.575	7.899	C	14.329	16.145	12.067	O	14.164	7.212	22.472
H	13.708	-0.332	7.067	C	14.211	18.385	10.509	C	12.172	3.642	21.267
C	11.494	-0.922	10.281	C	15.042	17.265	12.503	C	14.550	3.069	21.731
H	13.316	-1.074	11.294	H	14.584	15.229	12.639	H	13.303	4.679	22.866
C	10.903	-0.789	9.014	C	14.913	18.444	11.700	C	11.318	2.567	19.328
H	11.226	-0.497	6.931	H	14.214	19.240	9.832	C	15.741	1.792	20.135
H	10.784	-1.025	11.095	H	15.629	17.263	13.407	C	14.625	6.469	23.535
C	9.448	-0.774	8.907	O	15.652	19.631	11.945	C	10.954	3.529	21.872
O	8.881	-0.141	8.076	C	16.088	19.698	13.251	C	15.258	2.569	22.821
C	8.522	-1.417	9.943	C	15.279	19.941	14.336	C	10.097	2.465	19.959
C	8.848	-2.670	10.424	C	17.402	19.338	13.518	H	11.585	2.065	18.385
C	7.292	-0.858	10.311	C	15.659	19.806	15.651	C	16.580	1.369	21.164
C	8.013	-3.337	11.316	H	14.181	20.093	14.112	H	16.092	1.591	19.133
H	9.804	-3.175	10.140	C	17.935	19.434	14.769	C	13.830	6.396	24.670
C	6.513	-1.527	11.293	H	18.072	19.149	12.584	C	15.896	5.857	23.588
H	7.083	0.120	9.785	C	17.023	19.675	15.844	C	9.894	2.961	21.190
C	6.844	-2.759	11.800	H	14.919	20.014	16.401	H	10.953	3.968	22.926
H	8.254	-4.359	11.639	H	18.997	19.293	14.864	C	16.299	1.700	22.478
H	5.610	-1.036	11.800	C	17.502	19.578	17.233	H	15.099	2.976	23.826
O	25.749	-3.766	-5.035	O	18.081	20.507	17.732	H	9.268	1.931	19.539
C	25.916	-4.992	-4.507	C	17.158	18.354	17.956	H	17.354	0.552	21.037
C	26.404	-5.953	-5.329	C	16.956	17.120	17.361	C	14.221	5.620	25.693
C	25.644	-5.224	-3.179	C	16.965	18.374	19.360	H	12.941	7.016	24.676

C	26.765	-7.192	-4.788	C	16.626	15.931	18.067	C	16.272	5.036	24.674
H	26.439	-5.975	-6.421	H	17.100	17.088	16.236	H	16.528	5.916	22.738
C	26.132	-6.419	-2.613	C	16.512	17.268	20.061	H	8.886	2.840	21.738
H	25.199	-4.499	-2.481	H	17.225	19.302	19.928	H	16.845	1.268	23.336
C	26.729	-7.366	-3.381	C	16.373	16.017	19.452	C	15.359	4.863	25.663
C	27.277	-8.478	-5.424	H	16.556	14.942	17.578	H	13.695	5.643	26.638
H	25.884	-6.691	-1.564	H	16.258	17.296	21.135	H	17.182	4.408	24.541
C	27.343	-8.658	-2.985	H	27.799	21.903	-1.617	C	15.915	4.087	26.854
C	28.655	-8.212	-6.044	O	27.158	22.418	-1.079	O	16.561	4.651	27.719
C	27.197	-9.425	-4.269	C	25.907	21.987	-1.503	C	15.681	2.667	26.800
C	26.311	-8.856	-6.526	C	25.662	21.322	-2.680	C	16.576	1.845	26.196
C	26.674	-9.263	-1.782	C	24.853	22.471	-0.752	C	14.624	2.135	27.567
C	28.779	-8.461	-2.371	C	24.363	21.003	-3.061	C	16.393	0.448	26.185
H	29.058	-9.152	-6.598	H	26.476	20.893	-3.296	H	17.383	2.187	25.545
H	28.694	-7.302	-6.668	C	23.541	22.246	-1.157	C	14.276	0.833	27.363
H	29.276	-7.892	-5.183	H	25.068	23.088	0.160	H	14.009	2.786	28.143
H	26.247	-10.037	-4.303	C	23.302	21.489	-2.301	C	15.158	-0.006	26.707
H	28.010	-10.167	-4.361	C	24.141	20.172	-4.312	H	17.069	-0.187	25.572
H	25.293	-9.026	-6.107	H	22.711	22.644	-0.604	H	13.276	0.440	27.686
H	26.273	-8.120	-7.350	N	21.923	21.389	-2.638	H	14.982	10.852	8.114
H	26.726	-9.773	-7.036	H	24.502	20.719	-5.203	O	15.665	10.944	7.428
C	27.378	-9.196	-0.532	H	24.725	19.358	-4.186	C	16.793	10.649	8.092
C	25.411	-9.853	-1.841	N	22.695	19.913	-4.430	C	16.735	9.951	9.256
H	29.315	-9.392	-2.611	C	21.855	21.055	-4.027	C	18.043	11.002	7.604
H	29.424	-7.729	-2.820	C	21.254	20.335	-1.805	C	17.843	9.704	10.071
C	28.792	-8.506	-0.832	C	22.412	18.769	-3.582	H	15.743	9.724	9.677
C	26.715	-9.626	0.676	H	20.779	20.896	-4.187	C	19.196	10.730	8.352
C	24.813	-10.272	-0.642	H	22.115	21.966	-4.521	C	18.412	11.781	6.396
H	24.881	-9.805	-2.808	H	21.485	20.572	-0.781	C	19.095	10.085	9.643

C	28.672	-7.069	-0.346	H	20.174	20.311	-2.005	H	17.637	9.200	10.976
C	29.932	-9.282	-0.214	C	21.735	19.003	-2.315	C	20.518	11.156	7.817
C	25.462	-10.174	0.560	C	22.884	17.520	-3.961	C	19.348	10.782	5.689
H	27.256	-9.518	1.674	C	21.458	17.840	-1.590	C	19.250	12.945	6.838
O	23.503	-10.781	-0.678	C	22.620	16.456	-3.169	H	17.657	12.127	5.721
H	29.620	-6.545	-0.585	H	23.407	17.478	-4.962	O	20.218	9.923	10.419
H	27.853	-6.496	-0.786	C	21.886	16.559	-1.965	C	20.460	10.478	6.418
H	28.638	-6.953	0.752	H	21.025	17.909	-0.585	C	20.383	12.598	7.550
H	30.885	-8.873	-0.496	H	22.912	15.524	-3.516	H	21.278	10.894	8.534
H	30.016	-9.312	0.924	O	21.603	15.416	-1.253	C	19.171	10.002	4.538
H	29.794	-10.339	-0.379	C	21.424	15.692	0.080	C	19.071	14.228	6.379
H	24.977	-10.321	1.463	C	20.206	15.508	0.712	C	20.096	8.966	11.328
C	22.542	-10.133	0.073	C	22.429	16.340	0.821	C	21.320	9.530	5.975
C	21.307	-10.814	0.176	C	20.039	15.825	2.043	C	21.231	13.614	7.966
C	22.724	-8.910	0.809	H	19.417	14.938	0.146	C	20.150	9.104	3.996
C	20.217	-10.250	0.950	C	22.288	16.627	2.136	H	18.289	10.218	3.926
H	21.203	-11.790	-0.357	H	23.452	16.501	0.403	C	19.993	15.219	6.740
C	21.708	-8.469	1.591	C	21.031	16.399	2.820	H	18.179	14.548	5.735
H	23.621	-8.263	0.706	H	19.084	15.631	2.479	C	20.321	7.632	11.062
C	20.495	-9.062	1.641	H	23.068	17.179	2.746	C	19.804	9.320	12.608
H	19.271	-10.797	1.080	C	20.927	16.787	4.296	C	21.308	8.874	4.764
H	21.809	-7.564	2.218	O	21.526	17.811	4.608	H	22.173	9.394	6.802
C	19.475	-8.520	2.583	C	20.183	15.971	5.281	C	21.112	14.886	7.523
O	19.193	-9.268	3.477	C	19.937	16.508	6.516	H	22.175	13.480	8.521
C	18.915	-7.174	2.356	C	19.678	14.708	4.946	H	20.197	8.679	2.970
C	19.196	-6.475	1.191	C	19.278	15.722	7.478	H	19.839	16.255	6.369
C	17.979	-6.644	3.241	H	20.395	17.455	6.770	C	20.070	6.668	12.088
C	18.673	-5.204	0.951	C	18.990	13.976	5.875	H	20.763	7.361	10.088
H	19.875	-6.859	0.453	H	19.941	14.110	4.035	C	19.516	8.389	13.578

C	17.573	-5.302	3.096	C	18.752	14.475	7.153	H	19.802	10.379	12.954
H	17.774	-7.105	4.178	H	19.186	16.144	8.530	H	22.136	8.268	4.345
C	17.878	-4.613	1.940	H	18.684	12.891	5.734	H	21.855	15.639	7.764
H	18.982	-4.649	0.053					C	19.611	6.982	13.340
H	16.833	-4.761	3.740					H	20.283	5.663	11.780
H	26.481	1.562	-10.330					H	19.390	8.831	14.591
O	26.546	1.631	-9.361					C	19.482	5.922	14.411
C	25.894	2.786	-9.005					O	20.341	5.078	14.631
C	26.643	3.726	-8.285					C	18.239	5.808	15.243
C	24.633	3.111	-9.437					C	17.025	6.252	14.712
C	26.113	4.918	-7.963					C	18.192	5.194	16.521
H	27.563	3.458	-7.776					C	15.814	6.104	15.416
C	24.091	4.351	-9.108					H	16.907	6.778	13.740
H	23.999	2.511	-10.002					C	16.992	4.987	17.190
C	24.864	5.283	-8.395					H	19.109	5.048	17.118
C	26.673	5.962	-7.004					C	15.810	5.408	16.623
H	23.042	4.711	-9.295					H	14.893	6.495	14.977
C	24.397	6.565	-7.847					H	16.988	4.620	18.209
C	28.132	6.219	-7.529								
C	25.740	7.172	-7.450								
C	26.621	5.586	-5.515								
C	23.494	6.491	-6.611								
C	23.632	7.418	-8.869								
H	28.769	5.317	-7.421								
H	28.138	6.472	-8.655								
H	28.677	6.938	-6.954								
H	25.791	8.002	-6.651								
H	26.124	7.620	-8.402								
H	26.052	4.697	-5.270								

H	27.659	5.444	-5.233
H	26.232	6.411	-4.927
C	22.465	7.375	-6.876
C	23.480	5.829	-5.387
H	24.297	8.055	-9.427
H	23.063	6.872	-9.662
C	22.647	8.317	-8.039
C	21.449	7.656	-5.941
C	22.422	5.974	-4.474
H	24.211	5.060	-5.217
C	21.284	8.383	-8.732
C	23.357	9.658	-7.734
C	21.363	6.820	-4.814
H	20.665	8.420	-6.138
O	22.385	5.379	-3.274
H	21.522	8.894	-9.696
H	21.004	7.342	-9.057
H	20.454	8.842	-8.189
H	23.552	10.200	-8.731
H	22.816	10.345	-7.081
H	24.347	9.419	-7.203
H	20.539	7.022	-4.176
C	23.279	4.372	-2.964
C	24.627	4.627	-2.791
C	22.844	3.097	-2.674
C	25.542	3.547	-2.652
H	25.037	5.590	-2.903
C	23.710	2.099	-2.383
H	21.760	2.914	-2.705

C	25.083	2.298	-2.471								
H	26.625	3.681	-2.776								
H	23.304	1.095	-2.298								
C	26.127	1.169	-2.279								
O	27.129	1.445	-1.677								
C	26.021	-0.195	-2.894								
C	25.250	-0.351	-4.015								
C	26.799	-1.301	-2.516								
C	25.116	-1.518	-4.731								
H	24.629	0.499	-4.379								
C	26.547	-2.513	-3.083								
H	27.464	-1.196	-1.685								
C	25.773	-2.587	-4.287								
H	24.639	-1.564	-5.693								
H	27.120	-3.353	-2.865								

In EtOH

iPEEK-SBI				iPEEK-TB				iPEEK-Trip			
O	9.020	-2.164	-0.803	O	8.864	25.033	21.438	O	26.353	1.883	3.695
C	7.666	-2.220	-1.177	C	9.576	25.457	20.259	C	26.796	1.073	2.662
C	7.333	-3.073	-2.242	C	8.936	26.308	19.413	C	25.870	0.246	2.009
C	6.693	-1.527	-0.485	C	10.948	25.118	20.096	C	28.089	0.962	2.317
C	6.013	-3.214	-2.601	C	9.577	26.603	18.232	C	26.240	-0.574	0.950
H	7.998	-3.796	-2.698	H	7.844	26.395	19.415	H	24.846	0.389	2.178
C	5.387	-1.552	-0.965	C	11.622	25.556	19.006	C	28.514	0.077	1.325
H	6.920	-1.001	0.380	H	11.571	24.472	20.728	C	29.191	1.693	2.955
C	5.017	-2.496	-1.936	C	10.892	26.190	18.000	C	27.593	-0.663	0.509

C	5.407	-3.963	-3.757	C	8.817	27.182	17.091	H	25.573	-1.288	0.387
H	4.661	-0.864	-0.601	H	12.675	25.353	18.869	C	29.995	0.057	1.115
C	3.636	-2.761	-2.484	N	11.548	26.413	16.717	C	29.926	2.377	1.839
C	5.350	-5.411	-3.287	H	8.069	26.464	16.611	C	30.128	0.626	3.471
C	4.027	-3.310	-3.850	H	8.157	27.931	17.436	H	28.836	2.366	3.724
C	6.299	-3.801	-4.932	N	9.726	27.658	16.114	O	27.996	-1.309	-0.600
C	2.777	-1.533	-2.535	C	10.569	26.555	15.672	C	30.353	1.502	0.854
C	2.750	-3.598	-1.604	C	12.529	27.478	16.869	C	30.577	-0.270	2.502
H	6.375	-5.791	-3.202	C	10.437	28.802	16.549	H	30.379	-0.531	0.334
H	4.891	-5.366	-2.334	H	10.968	26.762	14.630	C	30.195	3.730	1.852
H	4.908	-6.142	-4.055	H	10.014	25.596	15.410	C	30.398	0.422	4.801
H	4.098	-2.387	-4.525	H	13.201	27.325	17.676	C	27.170	-1.376	-1.655
H	3.337	-4.060	-4.355	H	13.275	27.384	16.054	C	31.067	2.034	-0.192
H	5.899	-4.291	-5.822	C	11.753	28.778	16.957	C	31.184	-1.456	2.875
H	6.543	-2.794	-5.116	C	9.688	29.945	16.803	C	30.807	4.238	0.726
H	7.329	-4.147	-4.737	C	12.377	29.904	17.483	H	29.866	4.262	2.697
C	1.508	-1.691	-1.994	C	10.348	31.105	17.111	C	31.060	-0.745	5.188
C	3.176	-0.279	-2.900	H	8.587	29.923	16.666	H	29.886	1.166	5.495
H	2.751	-4.677	-1.823	C	11.670	31.131	17.511	C	27.347	-2.464	-2.542
H	3.092	-3.560	-0.538	H	13.398	29.856	17.787	C	26.210	-0.406	-2.020
C	1.314	-3.103	-1.668	H	9.824	32.058	17.055	C	31.293	3.391	-0.317
C	0.640	-0.627	-1.864	O	12.237	32.373	17.752	H	31.383	1.399	-0.980
C	2.334	0.819	-2.686	C	13.553	32.495	17.992	C	31.465	-1.661	4.241
H	4.179	-0.193	-3.304	C	14.422	32.675	16.977	H	31.513	-2.199	2.106
C	0.467	-3.271	-0.341	C	14.018	32.466	19.265	H	30.981	5.302	0.674
C	0.510	-3.740	-2.800	C	15.773	32.790	17.288	H	31.254	-1.039	6.219
C	1.041	0.616	-2.273	H	14.162	32.798	15.934	C	26.409	-2.648	-3.529
H	-0.337	-0.896	-1.511	C	15.363	32.495	19.587	H	28.121	-3.184	-2.371
O	2.761	2.088	-3.090	H	13.293	32.518	20.109	C	25.241	-0.653	-2.966

H	-0.584	-2.936	-0.413	C	16.309	32.561	18.569	H	26.160	0.550	-1.481
H	0.501	-4.379	-0.025	H	16.428	32.925	16.387	H	31.867	3.876	-1.068
H	0.812	-2.686	0.584	H	15.784	32.409	20.545	H	31.886	-2.569	4.495
H	1.147	-3.945	-3.708	C	17.744	32.655	18.792	C	25.316	-1.797	-3.743
H	0.044	-4.623	-2.346	O	18.504	32.800	17.853	H	26.477	-3.552	-4.150
H	-0.353	-3.107	-2.989	C	18.408	32.502	20.180	H	24.466	0.121	-3.051
H	0.286	1.372	-2.122	C	19.482	33.235	20.593	C	24.213	-2.124	-4.649
C	4.127	2.357	-3.167	C	18.027	31.382	20.953	O	23.105	-1.666	-4.468
C	4.631	3.194	-4.239	C	20.059	32.970	21.883	C	24.235	-2.963	-5.861
C	5.044	1.837	-2.282	H	19.881	34.185	20.094	C	24.441	-4.266	-5.618
C	5.985	3.426	-4.294	C	18.642	31.037	22.191	C	23.967	-2.404	-7.107
H	3.932	3.590	-4.968	H	17.170	30.764	20.627	C	24.428	-5.115	-6.695
C	6.409	2.024	-2.407	C	19.606	31.853	22.662	H	24.640	-4.709	-4.670
H	4.681	1.217	-1.445	H	20.827	33.590	22.318	C	23.843	-3.327	-8.167
C	6.920	2.854	-3.439	H	18.294	30.171	22.768	H	23.772	-1.338	-7.199
H	6.412	3.947	-5.242	H	20.135	31.579	23.594	C	24.199	-4.674	-8.019
H	7.059	1.640	-1.628	O	5.958	22.588	38.316	H	24.558	-6.232	-6.608
C	8.416	3.157	-3.558	C	5.802	22.476	36.929	H	23.736	-3.006	-9.165
O	8.789	4.143	-4.141	C	6.022	23.669	36.208	H	24.151	-5.491	-8.776
C	9.437	2.258	-2.972	C	5.373	21.337	36.308	O	18.819	5.413	9.954
C	10.595	2.747	-2.412	C	5.973	23.697	34.823	C	18.623	5.862	8.658
C	9.303	0.902	-3.015	H	6.535	24.438	36.817	C	19.317	7.017	8.302
C	11.660	1.880	-2.075	C	5.103	21.412	34.932	C	17.805	5.192	7.724
H	10.677	3.879	-2.350	H	5.249	20.413	36.913	C	19.194	7.600	7.085
C	10.296	0.025	-2.509	C	5.340	22.616	34.230	H	19.981	7.486	9.100
H	8.384	0.412	-3.381	C	6.389	24.922	34.077	C	17.750	5.769	6.437
C	11.515	0.561	-2.052	H	4.564	20.606	34.401	C	16.993	3.889	7.867
H	12.643	2.191	-1.675	N	4.988	22.645	32.790	C	18.471	6.878	6.113
H	10.120	-1.020	-2.563	H	5.788	25.840	34.301	H	19.759	8.442	6.785

H	12.260	-0.066	-1.610	H	7.453	25.187	34.318	C	16.824	5.063	5.523
O	8.651	11.726	9.637	N	6.231	24.704	32.646	C	17.547	3.042	6.733
C	8.320	11.323	8.351	C	4.986	23.997	32.291	C	15.548	4.214	7.389
C	7.030	11.010	7.927	C	6.013	21.887	32.067	H	17.043	3.507	8.838
C	9.359	11.144	7.428	C	7.323	24.098	31.957	O	18.515	7.450	4.840
C	6.822	10.625	6.578	H	4.719	24.105	31.237	C	17.369	3.670	5.484
H	6.131	11.163	8.537	H	4.130	24.544	32.646	C	15.513	4.977	6.226
C	9.116	10.503	6.162	H	6.281	21.021	32.648	H	16.764	5.537	4.565
H	10.362	11.333	7.789	H	5.579	21.564	31.129	C	18.092	1.807	6.799
C	7.868	10.281	5.734	C	7.272	22.702	31.648	C	14.383	3.895	8.107
C	5.489	10.371	5.973	C	8.384	24.854	31.550	C	19.654	7.102	4.145
H	9.946	10.347	5.408	C	8.401	22.152	31.149	C	17.709	3.025	4.310
C	7.368	9.547	4.510	C	9.498	24.246	30.957	C	14.366	5.523	5.749
C	5.028	11.650	5.321	H	8.374	25.938	31.710	C	18.441	1.158	5.665
C	5.913	9.315	4.896	C	9.491	22.886	30.741	H	18.358	1.435	7.790
C	4.343	9.955	6.903	H	8.311	21.039	30.922	C	13.168	4.496	7.628
C	8.115	8.316	4.122	H	10.347	24.874	30.627	H	14.343	3.232	8.952
C	7.684	10.359	3.195	O	10.523	22.264	30.095	C	20.371	5.886	4.369
H	5.838	12.229	4.885	C	10.229	21.696	28.837	C	20.134	7.967	3.165
H	4.281	11.454	4.525	C	11.303	21.138	28.094	C	18.285	1.760	4.424
H	4.563	12.181	6.087	C	8.965	21.789	28.249	H	17.612	3.509	3.384
H	5.778	8.340	5.321	C	11.074	20.694	26.808	C	13.191	5.353	6.480
H	5.248	9.343	4.021	H	12.293	21.051	28.571	H	14.309	6.149	4.791
H	4.184	10.665	7.733	C	8.774	21.340	26.993	H	18.863	0.136	5.771
H	3.398	10.001	6.359	H	8.127	22.240	28.764	H	12.229	4.167	8.150
H	4.559	8.940	7.304	C	9.831	20.936	26.239	C	21.511	5.637	3.667
C	8.427	8.236	2.733	H	11.996	20.326	26.282	H	20.003	5.107	5.092
C	8.479	7.376	5.037	H	7.784	21.563	26.583	C	21.339	7.767	2.562
H	6.891	11.065	2.861	C	9.826	20.611	24.777	H	19.539	8.884	2.922

H	8.588	10.903	3.397	O	10.263	19.541	24.362	H	18.665	1.149	3.564
C	7.889	9.435	2.057	C	9.427	21.734	23.911	H	12.256	5.805	6.130
C	9.123	7.146	2.287	C	8.718	22.829	24.421	C	22.054	6.643	2.880
C	9.326	6.340	4.604	C	9.860	21.664	22.612	H	22.051	4.742	3.939
H	8.315	7.530	6.122	C	8.564	23.873	23.523	H	21.857	8.523	1.983
C	8.978	9.887	1.112	H	8.277	23.020	25.439	C	23.411	6.528	2.285
C	6.549	9.004	1.401	C	9.775	22.753	21.759	O	23.848	7.471	1.617
C	9.554	6.208	3.228	H	10.289	20.682	22.293	C	24.216	5.284	2.515
H	9.262	7.122	1.122	C	9.077	23.870	22.214	C	24.451	5.058	3.888
O	9.873	5.493	5.470	H	8.046	24.717	23.966	C	24.721	4.445	1.531
H	9.904	10.010	1.647	H	10.104	22.755	20.708	C	25.133	3.871	4.261
H	9.201	9.182	0.237	O	-10.281	12.403	42.657	H	24.035	5.542	4.778
H	8.763	10.910	0.655	C	-9.140	13.107	42.939	C	25.491	3.373	1.936
H	6.705	8.145	0.795	C	-7.956	12.490	42.538	H	24.568	4.682	0.449
H	5.737	8.798	2.100	C	-9.110	14.271	43.681	C	25.675	3.009	3.259
H	6.136	9.866	0.821	C	-6.778	13.019	42.884	H	25.167	3.689	5.357
H	10.138	5.309	2.913	H	-7.961	11.495	42.091	H	26.109	2.863	1.141
C	10.135	4.149	5.139	C	-7.925	14.957	43.799	O	20.124	-1.310	18.317
C	11.415	3.623	5.321	H	-9.967	14.719	44.049	C	18.868	-1.005	17.820
C	9.150	3.302	4.703	C	-6.769	14.343	43.385	C	17.732	-1.120	18.628
C	11.673	2.271	5.056	C	-5.513	12.303	42.452	C	18.636	-0.488	16.595
H	12.207	4.138	5.804	H	-7.714	15.872	44.379	C	16.483	-0.787	18.110
C	9.420	2.020	4.341	N	-5.483	14.914	43.659	H	17.661	-1.611	19.702
H	8.108	3.736	4.652	H	-5.523	11.221	42.692	C	17.350	-0.132	16.074
C	10.683	1.482	4.446	H	-5.452	12.415	41.373	C	19.740	-0.208	15.660
H	12.709	1.908	5.360	N	-4.356	12.938	43.038	C	16.242	-0.369	16.837
H	8.606	1.425	3.969	C	-4.553	13.912	44.089	H	15.654	-1.015	18.796
C	11.000	0.141	4.032	C	-4.861	15.784	42.681	C	17.436	0.444	14.687
O	11.710	-0.573	4.695	C	-3.600	13.593	42.036	C	19.618	1.223	15.148

C	10.327	-0.474	2.825	H	-3.546	14.224	44.365	C	19.403	-0.984	14.392
C	9.848	0.295	1.752	H	-4.964	13.403	44.942	H	20.729	-0.509	15.979
C	10.298	-1.854	2.666	H	-5.577	16.217	42.011	O	14.959	-0.134	16.455
C	9.346	-0.217	0.548	H	-4.354	16.537	43.240	C	18.347	1.639	14.754
H	9.880	1.384	1.912	C	-3.835	14.968	41.847	C	18.205	-0.576	13.807
C	9.838	-2.434	1.470	C	-2.634	12.872	41.296	H	16.504	0.759	14.117
H	10.748	-2.512	3.395	C	-3.090	15.550	40.887	C	20.666	2.127	15.149
C	9.415	-1.591	0.388	C	-1.786	13.589	40.445	C	20.138	-1.983	13.786
H	8.899	0.468	-0.197	H	-2.357	11.838	41.498	C	14.580	0.788	15.511
H	9.793	-3.505	1.350	C	-2.022	14.950	40.234	C	18.113	3.009	14.421
O	8.793	8.530	25.908	H	-3.334	16.642	40.608	C	17.826	-1.001	12.552
C	7.497	8.843	25.422	H	-0.985	13.035	39.951	C	20.525	3.444	14.678
C	6.795	7.843	24.774	O	-1.274	15.653	39.330	H	21.606	1.730	15.498
C	6.879	10.148	25.623	C	-0.371	16.512	39.825	C	19.787	-2.472	12.549
C	5.603	8.117	24.214	C	0.587	17.069	38.994	H	21.051	-2.318	14.272
H	7.380	6.944	24.518	C	-0.373	16.955	41.143	C	13.913	0.340	14.385
C	5.631	10.316	25.051	C	1.497	17.926	39.441	C	14.978	2.065	15.576
H	7.468	10.856	26.217	H	0.542	16.763	37.915	C	19.243	3.909	14.423
C	4.973	9.329	24.323	C	0.511	17.900	41.609	H	17.110	3.392	14.282
C	4.772	7.188	23.300	H	-1.123	16.571	41.906	C	18.650	-1.918	11.926
H	5.079	11.317	25.158	C	1.478	18.401	40.768	H	16.957	-0.707	11.954
C	3.746	9.445	23.497	H	2.340	18.255	38.772	H	21.433	4.046	14.482
C	4.486	5.881	23.938	H	0.527	18.147	42.712	H	20.262	-3.294	12.076
C	3.513	7.987	23.139	C	2.474	19.299	41.331	C	13.755	1.173	13.303
C	5.623	7.052	22.037	O	2.724	19.333	42.553	H	13.521	-0.679	14.250
C	3.650	10.385	22.269	C	3.301	20.230	40.495	C	14.764	2.949	14.555
C	2.525	10.054	24.378	C	2.904	20.707	39.256	H	15.353	2.353	16.526
H	3.763	5.241	23.296	C	4.495	20.694	41.052	H	19.162	5.008	14.199
H	5.371	5.161	24.172	C	3.786	21.478	38.517	H	18.392	-2.343	10.921

H	3.816	6.005	24.784	H	1.929	20.416	38.815	C	14.189	2.496	13.341
H	3.130	7.861	22.134	C	5.434	21.446	40.320	H	13.286	0.705	12.422
H	2.753	7.540	23.850	H	4.816	20.405	42.085	H	14.975	4.033	14.606
H	6.718	6.649	22.122	C	5.075	21.816	39.017	C	14.155	3.224	12.142
H	5.146	6.391	21.341	H	3.392	21.762	37.507	O	13.074	3.314	11.581
H	5.709	8.062	21.450	H	6.447	21.698	40.654	C	15.370	3.771	11.572
C	2.414	11.071	22.218	O	-4.460	22.446	31.353	C	15.303	4.995	10.873
C	4.736	10.645	21.464	C	-4.143	21.239	31.839	C	16.630	3.181	11.834
H	1.993	9.286	24.973	C	-4.332	20.959	33.167	C	16.420	5.468	10.315
H	2.973	10.927	24.931	C	-3.621	20.233	30.958	H	14.325	5.489	10.715
C	1.509	10.688	23.349	C	-3.995	19.713	33.732	C	17.744	3.818	11.442
C	2.295	12.081	21.265	H	-4.789	21.860	33.676	H	16.767	2.213	12.357
C	4.522	11.595	20.462	C	-3.336	19.014	31.434	C	17.662	4.956	10.545
H	5.664	10.052	21.635	H	-3.350	20.419	29.895	H	16.283	6.338	9.588
C	0.758	11.880	23.965	C	-3.466	18.751	32.810	H	18.691	3.550	11.778
C	0.551	9.597	22.870	C	-4.235	19.421	35.208	O	20.503	3.370	27.477
C	3.291	12.253	20.345	H	-3.062	18.259	30.662	C	20.559	2.003	27.282
H	1.329	12.601	21.370	N	-3.088	17.486	33.358	C	20.597	1.175	28.356
O	5.550	11.925	19.560	H	-3.561	19.772	35.959	C	20.374	1.375	26.008
H	1.415	12.474	24.599	H	-5.235	19.765	35.566	C	20.565	-0.170	28.194
H	0.370	12.558	23.177	N	-4.081	18.010	35.379	H	20.593	1.598	29.400
H	-0.098	11.555	24.621	C	-2.888	17.530	34.752	C	20.533	-0.008	25.875
H	0.151	9.036	23.711	C	-3.950	16.392	32.992	C	20.357	2.172	24.687
H	-0.300	10.116	22.304	C	-5.254	17.370	34.924	C	20.577	-0.816	27.027
H	0.980	8.965	22.137	H	-2.722	16.565	35.086	H	20.589	-0.827	29.141
H	3.137	13.005	19.592	H	-1.952	18.073	35.059	C	20.707	-0.407	24.464
C	5.444	11.637	18.211	H	-4.263	16.399	31.916	C	19.333	1.503	23.883
C	4.251	11.111	17.684	H	-3.474	15.419	33.008	C	21.587	1.823	23.802
C	6.460	11.906	17.316	C	-5.233	16.586	33.756	H	20.260	3.276	24.819

C	4.171	10.892	16.333	C	-6.472	17.631	35.529	O	20.587	-2.198	27.068
H	3.368	10.872	18.360	C	-6.404	16.047	33.331	C	19.526	0.134	23.721
C	6.356	11.712	15.908	C	-7.687	17.131	35.044	C	21.800	0.448	23.757
H	7.433	12.201	17.689	H	-6.464	18.303	36.378	H	21.083	-1.431	24.355
C	5.178	11.194	15.422	C	-7.573	16.272	33.940	C	18.225	2.181	23.444
H	3.165	10.537	15.941	H	-6.372	15.394	32.428	C	22.305	2.714	23.044
H	7.203	11.904	15.268	H	-8.655	17.466	35.410	C	20.246	-2.971	26.028
C	4.971	10.904	13.965	O	-8.690	15.565	33.432	C	18.594	-0.489	22.934
O	3.892	10.546	13.581	C	-9.466	15.107	34.441	C	22.792	-0.011	22.949
C	6.019	11.019	12.868	C	-10.811	15.418	34.417	C	17.286	1.514	22.680
C	6.201	10.022	11.879	C	-8.894	14.400	35.529	H	18.101	3.237	23.763
C	6.852	12.128	12.853	C	-11.684	14.795	35.359	C	23.410	2.245	22.258
C	7.069	10.299	10.847	H	-11.258	15.941	33.600	H	22.075	3.774	23.048
H	5.639	9.027	11.890	C	-9.749	13.911	36.434	C	19.082	-2.798	25.298
C	7.710	12.329	11.811	H	-7.844	14.135	35.657	C	21.090	-4.069	25.778
H	6.774	12.967	13.582	C	-11.133	14.100	36.414	C	17.524	0.196	22.388
C	7.790	11.474	10.741	H	-12.715	15.187	35.372	H	18.776	-1.601	22.714
H	7.161	9.650	9.984	H	-9.419	13.312	37.243	C	23.611	0.850	22.223
H	8.139	13.310	11.631	C	-12.055	13.456	37.376	H	22.958	-1.081	22.783
O	17.984	14.525	19.397	O	-13.160	13.074	37.024	H	16.304	1.917	22.377
C	18.735	13.495	20.018	C	-11.618	13.165	38.777	H	24.030	3.001	21.755
C	19.634	12.763	19.223	C	-10.760	14.063	39.360	C	18.804	-3.598	24.226
C	18.531	13.112	21.393	C	-12.088	12.092	39.437	H	18.471	-1.875	25.615
C	20.383	11.773	19.735	C	-10.313	13.789	40.641	C	20.803	-4.823	24.672
H	19.749	12.989	18.152	H	-10.401	14.958	38.833	H	21.972	-4.338	26.439
C	19.395	12.106	21.921	C	-11.576	11.739	40.704	H	16.771	-0.355	21.722
H	17.879	13.727	21.978	H	-12.849	11.431	39.046	H	24.416	0.455	21.583
C	20.285	11.435	21.093	C	-10.708	12.654	41.372	C	19.759	-4.498	23.812
C	21.406	10.954	18.972	H	-9.572	14.439	41.083	H	17.910	-3.344	23.626

H	19.209	11.772	22.905	H	-11.795	10.787	41.172	H	21.541	-5.542	24.355
C	21.343	10.421	21.437	H	-2.516	20.023	15.795	C	19.735	-5.152	22.512
C	22.644	11.753	18.455	O	-3.386	20.357	15.930	O	19.707	-6.353	22.308
C	21.732	9.874	20.055	C	-4.304	19.570	16.549	C	19.800	-4.143	21.389
C	20.678	10.165	17.874	C	-3.856	18.713	17.572	C	20.686	-3.085	21.547
C	20.823	9.346	22.347	C	-5.648	19.558	16.100	C	19.196	-4.319	20.156
C	22.389	11.006	22.407	C	-4.696	17.712	18.079	C	20.769	-2.105	20.537
H	23.296	11.137	17.914	H	-2.835	18.749	17.955	H	21.393	-3.056	22.425
H	22.513	12.692	17.795	C	-6.527	18.593	16.688	C	19.254	-3.383	19.117
H	23.179	12.127	19.345	H	-5.905	20.186	15.284	H	18.482	-5.213	20.148
H	21.106	9.014	19.789	C	-5.954	17.636	17.565	C	20.014	-2.260	19.349
H	22.829	9.559	20.015	C	-4.183	16.677	19.076	H	21.335	-1.171	20.719
H	20.497	10.865	17.060	H	-7.574	18.507	16.446	H	18.737	-3.640	18.139
H	21.351	9.381	17.592	N	-6.796	16.576	17.886	H	28.245	-0.331	20.726
H	19.664	9.848	18.336	H	-3.426	16.130	18.499	O	28.869	0.240	20.252
C	21.778	8.979	23.312	H	-3.640	17.067	19.890	C	28.068	1.298	19.808
C	19.600	8.813	22.297	N	-5.329	15.961	19.558	C	26.642	1.257	19.885
H	23.102	11.525	21.786	C	-6.039	15.435	18.444	C	28.614	2.509	19.364
H	21.875	11.787	23.088	C	-7.922	16.930	18.732	C	25.892	2.352	19.534
C	22.974	9.897	23.267	C	-6.158	16.795	20.445	H	26.155	0.328	20.205
C	21.470	8.038	24.250	H	-5.378	15.099	17.689	C	27.922	3.639	19.060
C	19.305	7.801	23.183	H	-6.621	14.580	18.815	C	30.134	2.727	19.406
H	18.782	9.220	21.636	H	-8.487	17.749	18.370	C	26.485	3.551	19.190
C	23.350	10.402	24.680	H	-8.605	16.149	18.805	H	24.822	2.207	19.566
C	24.205	9.274	22.588	C	-7.388	17.293	20.078	C	28.761	4.864	18.720
C	20.239	7.363	24.108	C	-5.714	16.998	21.741	C	30.456	3.989	20.209
H	22.108	7.842	25.119	C	-8.073	18.097	20.937	C	30.381	3.267	18.019
O	18.070	7.104	23.086	C	-6.437	17.774	22.623	H	30.718	1.844	19.647
H	22.442	10.621	25.168	H	-4.815	16.538	22.042	O	25.690	4.679	19.038

H	23.776	9.555	25.207	C	-7.551	18.470	22.178	C	29.676	5.148	19.830
H	24.066	11.220	24.782	H	-8.985	18.656	20.620	C	29.719	4.413	17.658
H	24.703	8.439	23.111	H	-6.119	17.961	23.672	H	28.173	5.736	18.448
H	23.930	8.789	21.637	O	-8.275	19.303	22.925	C	31.216	4.138	21.348
H	24.951	10.094	22.394	C	-7.480	20.078	23.685	C	31.397	2.778	17.281
H	19.967	6.565	24.795	C	-6.715	21.094	23.135	C	25.156	5.156	20.212
C	16.880	7.700	22.937	C	-7.322	19.843	25.078	C	29.750	6.371	20.449
C	15.787	7.002	22.413	C	-5.609	21.654	23.798	C	29.968	5.074	16.471
C	16.737	9.019	23.218	H	-6.939	21.375	22.071	C	31.285	5.348	22.012
C	14.585	7.606	22.303	C	-6.380	20.505	25.789	H	31.823	3.297	21.675
H	15.813	5.921	22.092	H	-7.903	19.069	25.424	C	31.691	3.467	16.152
C	15.568	9.728	23.079	C	-5.451	21.300	25.171	H	31.886	1.857	17.649
H	17.574	9.483	23.776	H	-4.949	22.391	23.229	C	23.712	5.256	20.378
C	14.486	9.010	22.688	H	-6.173	20.347	26.826	C	25.957	5.501	21.288
H	13.719	7.081	22.045	C	-4.274	21.889	25.834	C	30.561	6.471	21.570
H	15.500	10.769	23.276	O	-3.273	22.104	25.152	H	29.229	7.234	19.984
C	13.155	9.723	22.512	C	-4.333	22.120	27.267	C	30.989	4.579	15.683
O	12.956	10.372	21.525	C	-5.557	22.255	27.948	H	29.332	5.920	16.192
C	11.993	9.385	23.378	C	-3.209	22.296	27.972	H	31.772	5.456	23.006
C	10.776	10.046	23.231	C	-5.635	22.486	29.285	H	32.506	3.171	15.560
C	12.117	8.418	24.402	H	-6.549	22.257	27.394	C	23.280	5.687	21.621
C	9.726	9.767	24.040	C	-3.178	22.482	29.379	H	23.054	4.989	19.550
H	10.661	10.866	22.485	H	-2.200	22.108	27.451	C	25.454	5.984	22.509
C	11.053	8.112	25.186	C	-4.434	22.554	30.001	H	27.057	5.440	21.186
H	13.189	7.943	24.608	H	-6.590	22.557	29.826	H	30.537	7.295	22.281
C	9.867	8.806	25.084	H	-2.281	22.714	29.958	H	31.193	4.978	14.696
H	8.798	10.367	23.976					C	24.080	6.029	22.675
H	11.144	7.317	25.962					H	22.228	5.941	21.603
H	15.808	6.284	9.977					H	26.134	6.359	23.324

O	15.250	5.899	10.656		C	23.415	6.645	23.850
C	14.019	6.403	10.550		O	23.503	7.858	23.992
C	13.452	7.001	9.425		C	22.686	5.790	24.838
C	13.181	6.081	11.636		C	23.210	4.583	25.240
C	12.120	7.404	9.464		C	21.524	6.231	25.491
H	14.125	7.324	8.638		C	22.542	3.766	26.116
C	11.904	6.686	11.712		H	24.189	4.269	24.870
H	13.639	5.551	12.477		C	20.802	5.422	26.351
C	11.368	7.355	10.665		H	20.978	7.170	25.268
C	11.326	8.179	8.426		C	21.286	4.136	26.634
H	11.383	6.738	12.670		H	23.000	2.797	26.525
C	10.113	8.071	10.570		H	19.873	5.847	26.785
C	10.774	7.105	7.512					
C	10.186	8.884	9.246					
C	12.317	9.066	7.633					
C	9.675	8.781	11.826					
C	8.945	7.028	10.484					
H	11.303	6.124	7.584					
H	9.747	6.874	7.743					
H	10.733	7.495	6.503					
H	10.532	9.952	9.238					
H	9.225	8.907	8.676					
H	11.750	9.739	6.891					
H	12.798	9.756	8.260					
H	12.965	8.461	7.037					
C	8.818	8.029	12.575					
C	10.246	9.967	12.415					
H	8.211	7.587	9.865					
H	9.141	6.061	9.965					

C	8.339	6.721	11.835		
C	8.445	8.464	13.814		
C	9.849	10.449	13.643		
H	11.139	10.521	12.006		
C	8.795	5.513	12.676		
C	6.810	6.753	11.737		
C	8.875	9.685	14.320		
H	7.783	7.820	14.481		
O	10.297	11.662	14.172		
H	8.206	4.684	12.285		
H	9.830	5.242	12.565		
H	8.557	5.684	13.750		
H	6.637	7.505	11.024		
H	6.540	5.775	11.296		
H	6.376	7.033	12.678		
H	8.449	9.901	15.343		
C	11.650	11.989	14.210		
C	12.653	10.972	14.105		
C	11.977	13.324	14.108		
C	13.997	11.398	14.222		
H	12.392	9.924	14.010		
C	13.336	13.669	14.352		
H	11.122	14.044	14.102		
C	14.363	12.701	14.398		
H	14.753	10.637	14.252		
H	13.569	14.743	14.486		
C	15.763	13.277	14.357		
O	16.271	13.497	13.285		
C	16.472	13.644	15.607		

C	17.265	14.798	15.856								
C	16.256	12.801	16.686								
C	17.711	15.073	17.061								
H	17.647	15.407	15.028								
C	16.816	13.062	17.896								
H	15.717	11.852	16.555								
C	17.573	14.213	18.110								
H	18.321	15.911	17.201								
H	16.767	12.278	18.653								

In AcMe

iPEEK-SBI				iPEEK-TB				iPEEK-Trip			
O	5.588	23.707	6.474	O	29.975	31.323	-0.391	O	12.281	22.925	35.774
C	5.351	22.390	6.018	C	29.586	31.576	-1.690	C	11.672	22.703	36.958
C	4.340	22.102	5.113	C	30.357	31.028	-2.697	C	12.047	23.450	38.077
C	5.973	21.318	6.689	C	28.566	32.432	-2.064	C	10.593	21.821	37.130
C	3.974	20.747	4.874	C	30.153	31.237	-4.017	C	11.356	23.420	39.265
H	3.948	22.918	4.562	H	31.186	30.363	-2.505	H	12.907	24.145	37.853
C	5.655	20.016	6.402	C	28.333	32.590	-3.386	C	9.851	21.832	38.295
H	6.721	21.492	7.461	H	27.923	32.875	-1.366	C	9.984	21.023	36.034
C	4.648	19.712	5.526	C	29.068	31.999	-4.393	C	10.202	22.646	39.373
C	2.917	20.172	3.928	C	31.013	30.616	-5.097	H	11.663	24.019	40.070
H	6.156	19.239	6.997	H	27.492	33.220	-3.691	C	8.697	20.830	38.337
C	4.202	18.368	5.059	N	28.711	32.159	-5.765	C	8.472	21.372	36.016
C	3.317	20.427	2.470	H	31.800	31.346	-5.200	C	10.027	19.580	36.586
C	2.844	18.645	4.326	H	31.483	29.652	-4.914	H	10.462	21.032	35.093
C	1.667	20.910	4.154	N	30.343	30.578	-6.388	O	9.427	22.716	40.486
C	4.028	17.447	6.251	C	29.817	31.884	-6.666	C	7.818	21.283	37.257
C	5.268	17.533	4.252	C	27.529	31.327	-6.072	C	9.317	19.502	37.832

H	3.523	21.464	2.118	C	29.291	29.549	-6.407	H	8.332	20.772	39.331
H	4.182	19.865	2.350	H	29.513	32.095	-7.727	C	7.847	21.764	34.838
H	2.459	20.123	1.864	H	30.528	32.698	-6.473	C	10.369	18.423	35.979
H	2.094	18.413	5.021	H	26.707	31.475	-5.357	C	8.133	23.064	40.336
H	2.639	17.951	3.546	H	27.153	31.692	-7.003	C	6.467	21.615	37.219
H	1.743	21.940	3.820	C	27.950	29.911	-6.147	C	9.033	18.270	38.389
H	0.821	20.331	3.720	C	29.654	28.250	-6.649	C	6.520	22.131	34.851
H	1.364	20.993	5.193	C	26.979	28.940	-6.090	H	8.370	21.826	33.842
C	4.439	16.159	5.944	C	28.693	27.264	-6.541	C	10.056	17.203	36.567
C	3.732	17.809	7.538	H	30.655	27.980	-6.842	H	10.730	18.496	35.023
H	5.192	17.767	3.161	C	27.334	27.626	-6.268	C	7.726	24.000	39.339
H	6.266	17.684	4.648	H	25.862	29.221	-5.819	C	7.162	22.344	41.049
C	4.947	16.107	4.514	H	28.856	26.243	-6.611	C	5.814	22.031	36.059
C	4.386	15.175	6.829	O	26.500	26.548	-6.149	H	5.923	21.502	38.164
C	3.729	16.770	8.442	C	25.265	26.783	-5.727	C	9.417	17.109	37.801
H	3.344	18.801	7.768	C	24.248	27.190	-6.623	H	8.477	18.318	39.356
C	6.168	15.277	4.427	C	24.866	26.446	-4.439	H	6.116	22.695	34.043
C	3.935	15.554	3.558	C	22.921	27.312	-6.254	H	10.316	16.305	36.001
C	4.030	15.420	8.170	H	24.457	27.523	-7.689	C	6.374	24.090	39.119
H	4.657	14.125	6.576	C	23.557	26.520	-3.994	H	8.482	24.454	38.697
O	3.407	16.991	9.730	H	25.515	26.047	-3.730	C	5.765	22.564	40.837
H	6.950	15.717	5.023	C	22.574	27.033	-4.947	H	7.457	21.598	41.796
H	5.854	14.261	4.800	H	22.180	27.870	-6.926	H	4.769	22.336	36.107
H	6.540	15.118	3.412	H	23.297	26.221	-2.977	H	9.207	16.193	38.262
H	2.945	15.899	3.838	C	21.155	27.065	-4.499	C	5.395	23.483	39.886
H	4.191	15.825	2.518	O	20.883	26.720	-3.356	H	6.006	24.797	38.364
H	3.774	14.474	3.554	C	20.138	27.632	-5.367	H	4.955	21.996	41.370
H	3.980	14.769	9.014	C	19.743	26.861	-6.477	C	3.963	23.613	39.514
C	4.134	17.802	10.507	C	19.473	28.841	-5.062	O	3.655	23.745	38.342

C	3.712	18.090	11.797	C	18.701	27.356	-7.263	C	2.877	23.729	40.529
C	5.258	18.462	10.040	H	20.317	26.018	-6.810	C	1.548	23.574	40.137
C	4.380	18.907	12.705	C	18.419	29.289	-5.900	C	3.089	24.092	41.879
H	2.830	17.503	12.144	H	19.868	29.601	-4.404	C	0.505	23.491	41.043
C	5.926	19.363	10.817	C	18.039	28.532	-7.030	H	1.317	23.330	39.110
H	5.651	18.382	9.015	H	18.447	26.834	-8.211	C	2.077	24.185	42.763
C	5.466	19.584	12.146	H	17.772	30.181	-5.585	H	4.125	24.315	42.251
H	3.933	19.109	13.637	H	17.279	28.772	-7.749	C	0.784	23.843	42.365
H	6.775	19.879	10.483	O	39.172	32.044	13.585	H	-0.417	23.155	40.633
C	6.079	20.749	12.863	C	38.569	32.842	12.636	H	2.293	24.367	43.824
O	5.492	21.856	12.959	C	38.051	32.275	11.530	H	-0.003	23.768	43.114
C	7.469	20.599	13.391	C	38.632	34.178	12.690	O	18.463	29.423	27.041
C	7.795	21.352	14.510	C	37.654	32.972	10.398	C	17.590	29.797	28.124
C	8.347	19.581	12.964	H	37.994	31.166	11.419	C	16.833	30.975	27.890
C	8.959	21.107	15.221	C	38.249	34.933	11.576	C	17.349	29.115	29.319
H	7.027	22.092	14.807	H	39.022	34.676	13.547	C	15.869	31.407	28.837
C	9.514	19.381	13.644	C	37.847	34.368	10.385	H	17.035	31.521	26.977
H	8.187	18.964	12.047	C	36.998	32.210	9.237	C	16.435	29.602	30.194
C	9.789	20.053	14.804	H	38.500	35.966	11.663	C	18.102	27.846	29.701
H	9.164	21.728	16.104	N	37.558	35.088	9.225	C	15.696	30.733	29.959
H	10.235	18.650	13.317	H	37.656	31.398	8.936	H	15.389	32.394	28.688
H	10.795	19.931	15.254	H	36.031	31.696	9.520	C	16.303	28.706	31.414
O	17.281	33.467	-0.476	N	36.699	33.184	8.207	C	16.948	26.834	30.011
C	16.286	32.534	-0.442	C	37.647	34.237	8.047	C	18.639	28.191	31.054
C	15.084	32.967	0.098	C	36.353	35.871	9.253	H	18.922	27.536	29.101
C	16.440	31.248	-0.915	C	35.367	33.691	8.388	O	14.671	31.171	30.854
C	14.038	32.067	0.318	H	37.499	34.767	7.136	C	15.945	27.346	30.834
H	15.118	33.934	0.615	H	38.706	33.853	7.885	C	17.694	28.716	31.914
C	15.359	30.446	-0.810	H	36.171	36.244	10.255	H	15.564	28.987	32.189

H	17.445	30.898	-1.053	H	36.471	36.842	8.676	C	16.946	25.485	29.672
C	14.162	30.815	-0.216	C	35.190	35.022	8.790	C	19.968	28.154	31.483
C	12.741	32.354	0.978	C	34.269	32.903	8.147	C	13.775	30.224	31.329
H	15.505	29.359	-0.988	C	33.886	35.569	8.729	C	14.842	26.578	31.135
C	12.891	30.053	0.055	C	32.977	33.416	8.104	C	17.974	29.076	33.228
C	11.765	33.012	0.053	H	34.430	31.797	7.942	C	15.964	24.678	30.046
C	12.308	30.905	1.262	C	32.824	34.826	8.296	H	17.877	25.173	29.097
C	13.001	33.113	2.314	H	33.737	36.619	8.812	C	20.342	28.585	32.755
C	13.078	28.594	0.333	H	32.106	32.689	7.878	H	20.819	27.931	30.804
C	12.048	30.020	-1.283	O	31.642	35.516	8.179	C	13.070	29.396	30.470
H	11.237	32.385	-0.609	C	30.781	35.165	7.167	C	13.522	30.073	32.686
H	10.962	33.565	0.581	C	29.462	35.681	7.135	C	14.894	25.200	30.770
H	12.202	33.822	-0.530	C	31.226	34.590	5.961	H	13.911	26.979	31.653
H	12.711	30.538	2.201	C	28.549	35.167	6.212	C	19.310	29.083	33.637
H	11.212	30.887	1.301	H	29.155	36.306	7.946	H	17.106	29.298	33.875
H	12.013	33.066	2.942	C	30.347	34.128	5.069	H	15.811	23.738	29.418
H	13.864	32.527	2.868	H	32.286	34.392	5.833	H	21.364	28.731	33.050
H	13.238	34.178	2.164	C	28.967	34.331	5.164	C	12.166	28.456	30.949
C	12.706	27.796	-0.761	H	27.442	35.491	6.275	H	13.341	29.426	29.402
C	13.565	28.013	1.471	H	30.885	33.765	4.176	C	12.634	29.122	33.158
H	10.963	30.097	-1.057	C	27.935	33.987	4.088	H	14.023	30.704	33.440
H	12.206	30.828	-1.902	O	26.740	34.175	4.240	H	14.003	24.633	30.991
C	12.246	28.646	-1.972	C	28.415	33.248	2.833	H	19.569	29.310	34.605
C	12.810	26.388	-0.702	C	28.094	31.875	2.654	C	11.920	28.276	32.328
C	13.764	26.665	1.574	C	29.119	33.983	1.920	H	11.582	27.903	30.193
H	13.883	28.662	2.300	C	28.526	31.272	1.494	H	12.511	29.060	34.270
C	13.325	28.652	-3.055	H	27.512	31.388	3.425	C	10.782	27.493	32.832
C	10.834	28.049	-2.237	C	29.595	33.362	0.769	O	9.695	27.528	32.335
C	13.352	25.792	0.510	H	29.178	35.091	1.949	C	11.114	26.414	33.776

H	12.645	25.578	-1.461	C	29.337	31.992	0.624	C	12.469	26.227	34.113
O	14.269	26.161	2.730	H	28.259	30.183	1.333	C	10.167	25.568	34.292
H	12.837	28.964	-4.026	H	30.199	34.044	0.152	C	12.863	25.072	34.779
H	14.242	29.252	-2.978	O	31.704	23.557	9.862	H	13.197	26.976	33.972
H	13.715	27.606	-3.197	C	32.474	23.488	8.739	C	10.551	24.448	34.978
H	10.713	27.185	-2.828	C	32.042	24.174	7.603	H	9.052	25.717	33.997
H	10.332	27.686	-1.285	C	33.657	22.794	8.797	C	11.903	24.132	35.196
H	10.282	28.813	-2.880	C	32.866	24.108	6.460	H	13.885	24.881	35.163
H	13.602	24.727	0.689	H	31.099	24.789	7.611	H	9.728	23.743	35.181
C	13.394	25.923	3.751	C	34.479	22.795	7.689	O	24.147	20.560	25.657
C	12.001	26.197	3.699	H	33.889	22.405	9.792	C	22.953	20.675	24.993
C	13.990	25.455	4.937	C	33.972	23.249	6.456	C	21.955	21.460	25.431
C	11.240	25.929	4.824	C	32.508	24.801	5.181	C	22.759	19.871	23.877
H	11.575	26.579	2.746	H	35.358	22.232	7.836	C	20.787	21.588	24.688
C	13.229	25.267	6.091	N	34.724	22.951	5.353	H	22.057	22.113	26.346
H	15.017	25.300	4.792	H	31.681	24.297	4.631	C	21.633	19.987	23.133
C	11.859	25.552	6.082	H	32.222	25.807	5.215	C	23.701	18.832	23.341
H	10.182	26.191	4.778	N	33.673	24.727	4.211	C	20.633	20.848	23.510
H	13.735	24.821	6.988	C	34.064	23.314	4.119	H	19.979	22.148	25.077
C	10.981	25.323	7.304	C	36.063	23.501	5.391	C	21.618	19.115	21.899
O	11.508	25.448	8.375	C	34.789	25.480	4.628	C	24.054	19.308	21.939
C	9.544	24.939	7.165	H	34.711	23.229	3.219	C	22.948	17.500	23.184
C	8.606	25.142	8.145	H	33.199	22.666	3.889	H	24.581	18.682	23.925
C	9.124	24.157	5.997	H	36.369	23.208	6.434	O	19.407	20.838	22.881
C	7.222	24.809	7.905	H	36.611	22.841	4.699	C	22.889	19.548	21.198
H	8.790	25.648	9.096	C	35.949	24.991	5.212	C	21.797	17.670	22.346
C	7.771	23.814	5.808	C	34.748	26.861	4.503	H	20.721	19.152	21.269
H	9.750	24.091	5.196	C	37.063	25.802	5.527	C	25.231	19.668	21.366
C	6.854	24.100	6.757	C	35.811	27.648	4.822	C	23.286	16.265	23.656

H	6.485	25.156	8.693	H	33.871	27.389	4.086	C	18.607	21.958	23.065
H	7.469	23.495	4.772	C	36.978	27.143	5.403	C	22.920	20.085	19.916
O	22.701	24.232	-3.790	H	38.051	25.456	5.800	C	21.086	16.591	21.979
C	23.571	24.858	-4.608	H	35.763	28.725	4.884	C	25.356	20.201	20.087
C	24.953	24.850	-4.397	O	38.076	27.975	5.769	H	26.167	19.436	21.853
C	23.112	25.471	-5.745	C	38.717	27.713	6.922	C	22.484	15.164	23.328
C	25.833	25.481	-5.196	C	38.451	28.591	7.977	H	24.243	16.160	24.253
H	25.261	24.302	-3.448	C	39.644	26.685	7.176	C	17.218	21.764	23.343
C	23.982	26.114	-6.609	C	38.985	28.458	9.224	C	19.197	23.255	22.961
H	22.049	25.387	-6.066	H	37.756	29.498	7.888	C	24.149	20.483	19.396
C	25.315	26.095	-6.337	C	40.166	26.565	8.450	H	21.977	20.239	19.400
C	27.264	25.950	-4.942	H	39.932	26.079	6.346	C	21.427	15.337	22.435
H	23.567	26.618	-7.537	C	39.823	27.392	9.484	H	20.332	16.617	21.215
C	26.361	26.915	-7.071	H	38.764	29.249	9.984	H	26.295	20.502	19.650
C	28.126	24.760	-5.465	H	40.900	25.735	8.713	H	22.619	14.187	23.732
C	27.382	27.066	-5.976	C	40.327	27.275	10.884	C	16.479	22.915	23.627
C	27.562	26.338	-3.526	O	40.860	26.280	11.347	H	16.796	20.760	23.516
C	25.888	28.254	-7.574	C	40.162	28.495	11.696	C	18.367	24.340	23.168
C	26.693	26.248	-8.422	C	40.787	29.638	11.361	H	20.316	23.428	22.695
H	29.169	25.066	-5.570	C	39.417	28.472	12.910	H	24.285	21.007	18.464
H	28.223	23.987	-4.677	C	40.490	30.858	11.963	H	20.847	14.465	22.149
H	27.800	24.384	-6.458	H	41.431	29.723	10.445	C	16.989	24.190	23.489
H	27.330	28.011	-5.490	C	39.142	29.611	13.618	H	15.382	22.627	23.820
H	28.409	26.976	-6.314	H	39.044	27.485	13.315	H	18.804	25.286	23.055
H	26.834	27.024	-3.159	C	39.620	30.852	13.089	C	16.237	25.416	23.866
H	27.635	25.458	-2.827	H	40.897	31.835	11.707	O	15.109	25.541	23.408
H	28.512	26.861	-3.468	H	38.499	29.676	14.448	C	16.856	26.387	24.777
C	26.527	28.501	-8.813	O	19.472	34.045	16.052	C	17.842	26.041	25.702
C	25.176	29.260	-6.962	C	20.122	33.201	15.191	C	16.340	27.668	24.661

H	27.438	25.473	-8.347	C	21.004	33.663	14.204	C	18.414	27.036	26.449
H	25.756	25.750	-8.752	C	19.740	31.829	15.253	H	18.250	25.036	25.804
C	27.244	27.251	-9.343	C	21.399	32.813	13.176	C	16.900	28.655	25.369
C	26.342	29.698	-9.476	H	21.277	34.763	14.153	H	15.436	27.851	24.068
C	24.992	30.516	-7.650	C	20.271	31.004	14.317	C	17.982	28.378	26.322
H	24.680	29.183	-6.001	H	18.981	31.411	15.901	H	19.131	26.777	27.284
C	26.853	26.868	-10.774	C	21.093	31.437	13.314	H	16.543	29.657	25.383
C	28.771	27.213	-9.274	C	22.196	33.303	12.024	O	27.009	28.681	36.464
C	25.601	30.703	-8.879	H	19.992	29.968	14.402	C	26.232	28.516	35.344
H	26.757	29.705	-10.477	N	21.698	30.442	12.464	C	26.602	29.054	34.139
O	24.285	31.562	-7.088	H	21.534	33.832	11.294	C	25.051	27.833	35.394
H	27.477	25.960	-11.101	H	22.867	34.092	12.396	C	25.801	28.925	33.027
H	25.784	26.591	-11.019	N	22.984	32.206	11.533	H	27.545	29.614	34.007
H	27.106	27.730	-11.395	C	22.140	31.000	11.194	C	24.204	27.692	34.346
H	29.160	27.326	-8.249	C	22.832	29.790	13.136	C	24.520	27.197	36.644
H	29.159	26.242	-9.618	C	24.141	31.796	12.408	C	24.552	28.281	33.187
H	29.213	28.009	-9.884	H	22.662	30.254	10.563	H	26.256	29.278	32.017
H	25.501	31.644	-9.309	H	21.338	31.366	10.553	C	23.022	26.772	34.558
C	23.887	31.364	-5.805	H	22.509	29.473	14.157	C	24.569	25.760	36.176
C	24.858	31.471	-4.791	H	23.043	28.856	12.679	C	23.099	27.604	36.890
C	22.511	31.312	-5.462	C	24.033	30.733	13.288	H	25.217	27.398	37.473
C	24.416	31.584	-3.486	C	25.274	32.614	12.350	O	23.734	28.092	32.100
H	25.943	31.426	-5.035	C	25.102	30.450	14.132	C	23.748	25.530	35.075
C	22.114	31.401	-4.139	C	26.313	32.381	13.223	C	22.335	27.292	35.771
H	21.777	31.219	-6.249	H	25.362	33.445	11.631	H	22.447	26.619	33.656
C	23.051	31.576	-3.103	C	26.225	31.285	14.063	C	25.307	24.706	36.723
H	25.135	31.365	-2.715	H	25.008	29.735	14.982	C	22.552	27.999	38.097
H	21.013	31.316	-3.873	H	27.135	33.033	13.286	C	24.291	27.481	31.039
C	22.523	31.548	-1.639	O	27.255	30.938	14.941	C	23.595	24.257	34.613

O	23.169	30.936	-0.783	C	28.401	30.392	14.252	C	20.995	27.442	35.828
C	21.166	32.182	-1.364	C	29.571	30.258	14.931	C	25.234	23.426	36.166
C	20.549	33.196	-2.094	C	28.412	30.039	12.891	H	25.915	24.889	37.623
C	20.484	31.694	-0.266	C	30.658	29.623	14.341	C	21.207	28.383	38.014
C	19.307	33.648	-1.802	H	29.631	30.661	15.956	H	23.241	28.327	38.875
H	21.053	33.581	-2.975	C	29.542	29.548	12.266	C	24.244	27.995	29.734
C	19.223	32.136	0.039	H	27.460	30.095	12.402	C	24.968	26.316	31.251
H	20.926	31.062	0.524	C	30.680	29.301	12.987	C	24.276	23.168	35.183
C	18.523	33.038	-0.781	H	31.499	29.576	15.010	H	23.044	24.058	33.696
H	18.895	34.390	-2.483	H	29.400	29.203	11.225	C	20.418	28.031	36.965
H	18.684	31.600	0.818	C	31.876	28.659	12.333	H	20.320	27.192	34.985
O	19.829	16.846	-3.047	O	32.950	29.261	12.348	H	25.777	22.662	36.717
C	18.832	16.701	-3.986	C	31.805	27.266	11.807	H	20.787	28.767	38.945
C	19.218	16.315	-5.285	C	32.971	26.568	11.510	C	24.815	27.317	28.618
C	17.525	17.073	-3.760	C	30.609	26.570	11.571	H	23.707	28.919	29.622
C	18.233	16.207	-6.228	C	32.984	25.308	10.926	C	25.538	25.620	30.231
H	20.273	16.004	-5.512	H	33.929	27.026	11.583	H	24.976	25.763	32.230
C	16.561	16.855	-4.768	C	30.615	25.367	10.908	H	24.109	22.242	34.680
H	17.316	17.700	-2.899	H	29.689	26.955	11.926	H	19.389	28.358	36.955
C	16.890	16.359	-5.945	C	31.779	24.747	10.558	C	25.485	26.167	28.929
C	18.376	15.871	-7.657	H	33.959	24.700	10.736	H	24.728	27.758	27.633
H	15.534	17.132	-4.523	H	29.664	24.839	10.851	H	26.060	24.648	30.388
C	16.008	16.162	-7.150	H	11.323	40.319	10.535	C	26.167	25.451	27.790
C	18.535	14.325	-7.792	O	12.072	40.399	9.959	O	27.031	26.102	27.181
C	17.017	16.268	-8.321	C	12.683	41.613	10.063	C	25.652	24.132	27.218
C	19.623	16.581	-8.313	C	12.014	42.678	10.583	C	26.054	23.700	25.953
C	14.839	17.083	-7.201	C	14.077	41.738	9.875	C	24.753	23.270	27.966
C	15.339	14.793	-6.937	C	12.632	43.858	11.039	C	25.572	22.518	25.409
H	17.639	13.742	-7.376	H	10.961	42.617	10.908	H	26.748	24.330	25.297

H	18.940	13.950	-8.816	C	14.628	42.994	10.077	C	24.260	22.119	27.388
H	19.364	13.984	-7.174	H	14.576	40.855	9.340	H	24.248	23.729	28.802
H	16.976	17.250	-8.707	C	13.967	43.989	10.799	C	24.687	21.714	26.147
H	16.727	15.545	-9.096	C	11.918	44.914	11.883	H	25.938	21.988	24.494
H	19.385	16.745	-9.367	H	15.732	42.953	10.054	H	23.508	21.474	27.885
H	19.791	17.619	-7.817	N	14.805	45.012	11.397	H	39.023	36.783	33.541
H	20.536	16.027	-8.151	H	11.535	45.802	11.329	O	38.119	37.210	33.402
C	13.669	16.428	-6.732	H	11.104	44.468	12.528	C	37.245	36.627	34.294
C	14.785	18.435	-7.480	N	12.907	45.622	12.765	C	36.030	36.240	33.825
H	15.205	14.460	-8.007	C	13.981	46.099	11.872	C	37.472	36.477	35.656
H	15.909	13.952	-6.415	C	15.600	44.444	12.537	C	34.982	35.891	34.659
C	13.924	14.991	-6.378	C	13.406	44.775	13.769	H	35.681	36.427	32.805
C	12.490	17.132	-6.667	H	14.606	46.886	12.397	C	36.477	36.054	36.525
C	13.625	19.174	-7.330	H	13.541	46.651	10.961	C	38.767	36.869	36.346
H	15.702	18.872	-7.917	H	16.036	43.464	12.212	C	35.188	35.752	36.057
C	13.719	14.870	-4.869	H	16.435	45.154	12.765	H	34.021	35.670	34.313
C	12.946	14.208	-7.163	C	14.689	44.196	13.685	C	36.856	36.118	37.947
C	12.453	18.532	-6.949	C	12.545	44.615	14.852	C	39.109	35.625	37.148
H	11.693	16.561	-6.212	C	15.081	43.374	14.781	C	38.371	37.930	37.339
O	13.676	20.548	-7.420	C	13.017	43.809	15.876	H	39.604	37.206	35.716
H	13.728	13.789	-4.569	H	11.512	44.970	14.778	O	34.198	35.438	36.917
H	14.447	15.389	-4.216	C	14.285	43.188	15.911	C	38.019	35.149	37.881
H	12.745	15.300	-4.622	H	16.011	42.821	14.745	C	37.321	37.526	38.163
H	13.065	13.164	-6.859	H	12.332	43.522	16.716	H	36.092	35.823	38.607
H	11.915	14.600	-7.016	O	14.697	42.375	16.940	C	40.357	35.008	37.076
H	13.154	14.330	-8.187	C	15.857	41.768	16.670	C	38.892	39.240	37.511
H	11.520	19.096	-6.712	C	15.828	40.365	16.418	C	33.610	34.276	36.728
C	14.687	21.309	-7.061	C	17.079	42.465	16.625	C	38.265	34.056	38.643
C	15.725	20.994	-6.158	C	16.974	39.687	16.159	C	36.845	38.396	39.191

C	14.664	22.633	-7.513	H	14.873	39.798	16.619	C	40.547	33.896	37.777
C	16.663	21.964	-5.708	C	18.191	41.762	16.205	H	41.104	35.378	36.402
H	15.811	19.884	-5.829	H	17.203	43.465	16.941	C	38.321	40.120	38.355
C	15.497	23.630	-7.059	C	18.211	40.359	16.090	H	39.664	39.592	36.824
H	13.806	22.939	-8.132	H	16.965	38.655	16.164	C	34.340	33.183	37.199
C	16.537	23.307	-6.101	H	19.052	42.432	16.094	C	32.390	34.029	36.149
H	17.487	21.861	-5.052	C	19.460	39.671	15.739	C	39.519	33.442	38.643
H	15.330	24.651	-7.475	O	20.373	40.345	15.284	H	37.441	33.593	39.251
C	17.391	24.377	-5.637	C	19.510	38.189	15.735	C	37.367	39.664	39.278
O	16.922	25.475	-5.510	C	20.368	37.530	16.608	H	36.081	38.035	39.905
C	18.783	24.144	-5.052	C	18.682	37.438	14.894	H	41.551	33.396	37.635
C	19.724	23.350	-5.630	C	20.483	36.152	16.659	H	38.772	41.185	38.451
C	19.175	24.839	-3.920	H	20.988	38.163	17.270	C	34.018	31.892	36.786
C	21.050	23.243	-5.178	C	18.713	36.108	15.000	H	35.222	33.211	37.860
H	19.470	22.665	-6.479	H	17.839	37.906	14.356	C	32.020	32.710	35.811
C	20.431	24.758	-3.443	C	19.600	35.410	15.866	H	31.789	34.883	35.848
H	18.453	25.322	-3.305	H	21.071	35.621	17.399	H	39.638	32.545	39.207
C	21.380	24.085	-4.149	H	18.109	35.568	14.258	H	37.042	40.346	40.097
H	21.825	22.639	-5.639					C	32.835	31.644	36.103
H	20.683	25.319	-2.505					H	34.699	31.114	37.148
H	14.849	19.433	9.028					H	31.052	32.638	35.214
O	15.572	18.893	9.179					C	32.402	30.245	35.749
C	15.197	17.618	9.025					O	33.189	29.598	35.101
C	15.980	16.631	9.646					C	31.010	29.785	35.850
C	14.059	17.226	8.332					C	30.308	30.271	36.960
C	15.643	15.301	9.619					C	30.380	28.836	35.048
H	16.779	17.039	10.260					C	29.058	29.756	37.212
C	13.714	15.893	8.226					H	30.798	31.092	37.600
H	13.369	17.970	7.789					C	29.120	28.358	35.289

C	14.542	14.960	8.861		H	30.880	28.435	34.165
C	16.262	14.096	10.379		C	28.386	28.918	36.353
H	12.763	15.616	7.639		H	28.458	30.223	37.982
C	14.208	13.508	9.047		H	28.590	27.696	34.605
C	15.788	14.149	11.853					
C	15.548	12.984	9.572					
C	17.807	14.251	10.263					
C	13.745	12.893	7.718					
C	12.971	13.217	9.955					
H	16.153	15.073	12.391					
H	14.713	14.074	11.868					
H	16.176	13.318	12.500					
H	16.070	12.578	8.684					
H	15.514	12.091	10.262					
H	18.310	13.370	10.609					
H	18.081	14.415	9.202					
H	18.121	15.126	10.858					
C	12.421	12.434	7.818					
C	14.443	12.947	6.534					
H	13.297	12.571	10.742					
H	12.522	14.217	10.306					
C	11.829	12.511	9.157					
C	11.703	12.019	6.722					
C	13.781	12.525	5.417					
H	15.485	13.282	6.569					
C	10.507	13.286	9.018					
C	11.481	11.185	9.745					
C	12.476	11.949	5.533					
H	10.725	11.512	6.893					

O	14.373	12.445	4.176		
H	10.509	14.396	8.771		
H	9.819	12.820	8.245		
H	9.953	13.189	9.975		
H	10.787	10.602	9.134		
H	12.341	10.541	9.925		
H	10.902	11.310	10.651		
H	11.959	11.759	4.589		
C	15.365	13.368	3.801		
C	16.388	12.936	2.993		
C	15.332	14.676	4.227		
C	17.358	13.800	2.581		
H	16.296	11.954	2.480		
C	16.317	15.596	3.785		
H	14.512	14.929	4.908		
C	17.254	15.151	2.881		
H	18.153	13.418	1.877		
H	16.279	16.648	4.136		
C	18.299	16.104	2.379		
O	18.786	16.877	3.149		
C	18.743	16.178	0.910		
C	19.797	16.995	0.577		
C	18.000	15.558	-0.097		
C	20.116	17.203	-0.758		
H	20.551	17.550	1.284		
C	18.496	15.628	-1.449		
H	17.195	14.806	0.139		
C	19.478	16.582	-1.778		
H	20.900	17.880	-1.085		

H 17.991 15.155 -2.291		

In MEK

iPEEK-SBI				iPEEK-TB				iPEEK-Trip			
O	19.230	13.398	34.725	O	-3.366	5.848	23.260	O	-0.008	34.371	9.634
C	19.519	12.705	33.578	C	-3.584	4.644	22.650	C	0.313	35.698	9.957
C	20.475	13.127	32.627	C	-3.451	3.505	23.428	C	0.858	36.047	11.199
C	18.764	11.552	33.339	C	-3.857	4.542	21.293	C	0.207	36.684	8.969
C	20.655	12.353	31.526	C	-3.332	2.207	22.878	C	1.161	37.352	11.450
H	20.918	14.136	32.712	H	-3.386	3.556	24.510	H	0.937	35.249	11.903
C	19.066	10.674	32.274	C	-3.969	3.238	20.753	C	0.577	38.002	9.248
H	17.947	11.219	34.109	H	-4.037	5.486	20.745	C	-0.318	36.412	7.600
C	20.020	11.166	31.320	C	-3.659	2.122	21.484	C	1.115	38.389	10.487
C	21.492	12.839	30.341	C	-3.081	0.974	23.678	H	1.466	37.584	12.535
H	18.422	9.805	32.031	H	-4.186	3.043	19.715	C	0.363	38.916	8.073
C	20.311	10.631	29.948	N	-3.659	0.866	20.829	C	0.719	36.915	6.719
C	22.938	12.709	30.759	H	-1.996	0.885	23.926	C	-1.429	37.398	7.417
C	21.003	11.857	29.307	H	-3.552	1.044	24.670	H	-0.447	35.325	7.498
C	21.136	14.289	29.899	N	-3.536	-0.187	22.971	O	1.532	39.608	10.834
C	19.119	10.067	29.211	C	-3.102	-0.206	21.602	C	1.111	38.229	6.968
C	21.233	9.323	30.083	C	-4.989	0.533	20.515	C	-1.086	38.767	7.655
H	23.115	13.324	31.632	C	-4.964	-0.115	22.905	H	0.561	39.960	8.224
H	23.248	11.649	31.031	H	-3.430	-1.186	21.117	C	1.311	36.178	5.718
H	23.699	13.128	30.009	H	-2.013	-0.082	21.510	C	-2.712	37.115	7.052
H	20.329	12.396	28.588	H	-5.363	1.324	19.799	C	2.543	40.207	10.114
H	21.827	11.583	28.625	H	-5.094	-0.317	19.811	C	2.089	38.872	6.228
H	20.075	14.514	29.808	C	-5.657	0.311	21.780	C	-2.016	39.716	7.558
H	21.444	14.995	30.678	C	-5.647	-0.485	24.051	C	2.324	36.750	5.026
H	21.632	14.638	28.953	C	-6.991	0.374	21.788	H	0.964	35.088	5.585
C	19.224	8.696	28.976	C	-7.048	-0.372	24.105	C	-3.688	38.138	6.999
C	18.042	10.735	28.636	H	-4.986	-0.808	24.865	H	-3.014	36.021	6.840

H	22.077	9.339	29.385	C	-7.728	0.131	22.931	C	2.541	41.593	10.049
H	21.619	9.223	31.084	H	-7.487	0.847	20.908	C	3.404	39.480	9.293
C	20.388	8.105	29.671	H	-7.635	-0.574	25.020	C	2.734	38.081	5.262
C	18.260	7.979	28.281	O	-9.091	0.141	22.877	H	2.103	39.935	6.328
C	17.109	10.048	27.803	C	-9.565	1.131	22.109	C	-3.342	39.449	7.340
H	17.844	11.806	28.743	C	-10.223	0.768	20.913	H	-1.692	40.796	7.724
C	19.755	7.245	30.819	C	-9.222	2.483	22.344	H	2.785	36.069	4.271
C	21.052	7.126	28.670	C	-10.457	1.648	19.961	H	-4.761	38.041	6.811
C	17.246	8.670	27.635	H	-10.357	-0.270	20.685	C	3.420	42.283	9.228
H	18.338	6.885	28.115	C	-9.519	3.398	21.400	H	1.941	42.185	10.712
O	16.047	10.716	27.252	H	-8.650	2.817	23.282	C	4.360	40.111	8.545
H	19.133	6.470	30.295	C	-10.158	3.012	20.201	H	3.525	38.383	9.473
H	20.481	6.623	31.429	H	-10.960	1.391	19.023	H	3.598	38.441	4.607
H	19.085	7.768	31.482	H	-9.231	4.458	21.510	H	-4.041	40.274	7.129
H	21.616	7.762	27.884	C	-10.447	4.085	19.111	C	4.238	41.541	8.375
H	21.837	6.633	29.223	O	-11.032	5.075	19.445	H	3.383	43.336	9.183
H	20.380	6.387	28.189	C	-9.872	3.893	17.787	H	5.126	39.506	7.974
H	16.618	8.069	26.936	C	-10.317	4.734	16.748	C	5.183	42.239	7.454
C	16.191	11.956	26.754	C	-8.897	2.911	17.557	O	6.387	42.238	7.601
C	16.772	12.126	25.472	C	-9.802	4.515	15.521	C	4.560	43.063	6.354
C	15.742	13.087	27.441	H	-11.030	5.555	16.893	C	3.328	42.728	5.709
C	16.999	13.381	24.926	C	-8.395	2.728	16.325	C	5.263	44.116	5.812
H	16.913	11.263	24.900	H	-8.577	2.239	18.370	C	2.891	43.470	4.626
C	16.035	14.367	26.930	C	-8.748	3.612	15.293	H	2.730	41.925	6.054
H	15.316	12.835	28.435	H	-10.112	5.102	14.660	C	4.748	44.942	4.825
C	16.684	14.460	25.727	H	-7.739	1.874	16.289	H	6.266	44.240	6.067
H	17.533	13.526	23.928	H	-8.300	3.494	14.325	C	3.557	44.601	4.215
H	15.803	15.251	27.533	O	11.481	-0.977	25.271	H	1.921	43.353	4.100
C	16.917	15.943	25.208	C	10.423	-0.663	26.013	H	5.260	45.822	4.475

O	17.047	16.842	26.010	C	10.459	0.514	26.717	H	3.151	45.201	3.436
C	16.997	16.204	23.727	C	9.258	-1.457	26.005	O	4.099	22.612	17.512
C	16.287	15.516	22.763	C	9.380	0.784	27.546	C	3.089	23.357	16.961
C	17.961	17.170	23.295	H	11.315	1.151	26.743	C	2.436	22.885	15.801
C	16.466	15.704	21.403	C	8.164	-1.151	26.726	C	2.793	24.694	17.352
H	15.572	14.799	23.070	H	9.166	-2.314	25.283	C	1.431	23.633	15.159
C	18.049	17.466	21.951	C	8.196	-0.083	27.565	H	2.674	21.969	15.228
H	18.538	17.556	24.070	C	9.281	2.074	28.369	C	1.717	25.359	16.822
C	17.306	16.733	21.012	H	7.396	-1.872	26.571	C	3.601	25.488	18.395
H	15.901	15.102	20.681	N	7.058	0.212	28.423	C	1.085	24.879	15.682
H	18.784	18.204	21.563	H	9.762	2.007	29.329	H	0.968	23.451	14.211
H	17.513	16.827	19.934	H	9.761	2.871	27.790	C	1.521	26.801	17.358
O	19.074	18.537	29.264	N	7.893	2.491	28.532	C	2.584	25.976	19.381
C	19.476	19.758	29.877	C	7.296	1.386	29.306	C	4.022	26.777	17.652
C	20.533	20.495	29.424	C	5.957	0.592	27.552	H	4.426	24.982	18.907
C	18.629	20.320	30.855	C	7.251	2.709	27.286	O	0.236	25.681	14.928
C	20.832	21.681	30.059	H	6.319	1.783	29.667	C	1.506	26.680	18.853
H	21.156	20.304	28.552	H	7.926	1.048	30.134	C	2.878	27.443	17.139
C	18.977	21.450	31.523	H	5.551	-0.260	26.839	H	0.637	27.304	16.863
H	17.895	19.627	31.246	H	5.005	0.799	28.110	C	2.678	25.778	20.717
C	20.054	22.189	31.081	C	6.341	1.751	26.766	C	5.287	27.275	17.381
C	21.905	22.736	29.826	C	7.543	3.758	26.441	C	0.804	26.790	14.421
H	18.354	21.856	32.282	C	5.747	1.909	25.485	C	0.652	27.353	19.684
C	20.645	23.489	31.650	C	7.034	3.914	25.170	C	2.965	28.690	16.532
C	21.493	23.333	28.541	H	8.404	4.367	26.821	C	1.752	26.255	21.607
C	22.012	23.652	31.015	C	6.107	3.008	24.675	H	3.532	25.225	21.060
C	23.218	22.030	29.612	H	5.110	1.081	25.091	C	5.347	28.403	16.571
C	20.876	23.409	33.115	H	7.478	4.729	24.584	H	6.194	26.880	17.814
C	19.765	24.705	31.491	O	5.677	3.184	23.423	C	2.172	26.871	14.022

H	20.503	23.735	28.461	C	4.719	4.109	23.165	C	-0.028	27.936	14.134
H	22.155	24.210	28.312	C	4.067	4.696	24.267	C	0.687	27.075	21.093
H	21.755	22.513	27.787	C	4.349	4.482	21.878	H	0.022	28.060	19.291
H	22.923	23.397	31.676	C	3.208	5.748	24.107	C	4.235	29.100	16.089
H	22.336	24.648	30.748	H	4.356	4.353	25.254	H	1.989	29.153	16.158
H	23.477	21.485	30.519	C	3.497	5.566	21.749	H	1.874	26.091	22.668
H	23.170	21.264	28.735	H	4.758	3.846	21.026	H	6.331	28.834	16.379
H	24.084	22.665	29.329	C	2.927	6.230	22.874	C	2.714	28.018	13.495
C	20.137	24.359	33.709	H	2.753	6.094	25.085	H	2.844	25.997	14.162
C	21.763	22.671	33.891	H	3.224	5.975	20.795	C	0.545	29.108	13.695
H	20.194	25.328	30.713	C	1.953	7.283	22.712	H	-1.142	27.825	14.366
H	18.863	24.369	31.008	O	2.268	8.446	22.574	H	0.080	27.711	21.743
C	19.370	25.287	32.838	C	0.576	6.984	22.826	H	4.401	29.988	15.442
C	20.200	24.608	35.080	C	0.246	5.692	22.644	C	1.890	29.098	13.276
C	21.882	22.932	35.297	C	-0.399	7.975	22.937	H	3.813	28.044	13.318
H	22.510	22.071	33.375	C	-1.115	5.400	22.705	H	-0.030	30.032	13.736
C	17.818	25.224	33.138	H	1.006	4.881	22.370	C	2.603	30.344	12.739
C	19.857	26.722	32.999	C	-1.745	7.645	23.156	O	3.787	30.427	13.040
C	21.084	23.911	35.887	H	-0.157	9.016	23.009	C	1.921	31.407	11.968
H	19.636	25.415	35.550	C	-2.088	6.320	23.059	C	2.616	32.566	11.562
O	22.863	22.403	36.058	H	-1.417	4.354	22.544	C	0.672	31.261	11.438
H	17.598	25.570	34.152	H	-2.528	8.372	23.400	C	2.050	33.538	10.775
H	17.095	25.772	32.546	O	2.319	-1.663	27.221	H	3.638	32.705	11.963
H	17.395	24.243	33.029	C	1.880	-0.984	26.099	C	0.121	32.211	10.673
H	20.939	26.612	32.742	C	2.478	0.161	25.632	H	-0.049	30.457	11.668
H	19.370	27.342	32.274	C	0.810	-1.432	25.401	C	0.753	33.413	10.303
H	19.757	27.119	33.997	C	1.870	0.856	24.595	H	2.613	34.541	10.699
H	21.056	23.956	36.962	H	3.308	0.588	26.194	H	-0.826	31.930	10.205
C	22.994	21.037	36.154	C	0.226	-0.875	24.301	O	13.361	26.351	25.215

C	23.980	20.467	37.024	H	0.265	-2.349	25.735	C	13.304	25.763	23.976
C	22.109	20.103	35.589	C	0.732	0.319	23.916	C	12.408	26.075	23.013
C	24.010	19.106	37.272	C	2.594	2.044	24.043	C	14.318	24.891	23.688
H	24.676	21.162	37.522	H	-0.648	-1.267	23.818	C	12.433	25.559	21.724
C	22.225	18.734	35.763	N	0.152	0.948	22.711	H	11.605	26.730	23.208
H	21.317	20.438	34.941	H	2.381	3.010	24.582	C	14.382	24.333	22.434
C	23.195	18.199	36.599	H	3.678	1.892	24.074	C	15.360	24.386	24.645
H	24.892	18.815	37.813	N	2.280	2.173	22.601	C	13.422	24.608	21.460
H	21.545	18.197	35.090	C	0.765	2.284	22.523	H	11.671	25.866	21.012
C	23.330	16.721	36.747	C	0.481	0.148	21.522	C	15.589	23.422	22.177
O	24.316	16.246	37.236	C	2.850	1.164	21.834	C	16.641	24.746	23.921
C	22.274	15.771	36.199	H	0.469	2.640	21.507	C	15.318	22.869	24.517
C	20.954	16.043	36.477	H	0.352	2.992	23.255	H	15.190	24.720	25.702
C	22.611	14.584	35.534	H	0.035	-0.818	21.785	O	13.540	23.986	20.241
C	19.919	15.229	36.106	H	0.024	0.552	20.597	C	16.774	24.181	22.659
H	20.769	16.969	37.097	C	1.978	0.182	21.314	C	15.451	22.358	23.186
C	21.562	13.727	35.168	C	4.245	0.950	21.751	H	15.548	23.054	21.208
H	23.673	14.345	35.121	C	2.545	-0.889	20.638	C	17.620	25.572	24.414
C	20.233	14.080	35.392	C	4.771	-0.081	20.913	C	15.053	21.979	25.504
H	18.915	15.503	36.264	H	4.832	1.768	22.214	C	12.510	24.032	19.336
H	21.911	12.789	34.709	C	3.891	-1.042	20.414	C	17.927	24.437	21.911
O	31.054	25.770	29.070	H	1.932	-1.699	20.213	C	15.431	20.998	22.897
C	30.353	25.020	29.967	H	5.828	-0.183	20.803	C	18.830	25.669	23.730
C	31.033	24.005	30.658	O	4.283	-2.163	19.728	H	17.599	25.935	25.466
C	28.960	25.016	30.092	C	5.591	-2.579	19.979	C	15.017	20.573	25.252
C	30.417	23.159	31.496	C	6.502	-2.731	18.960	H	14.734	22.429	26.491
H	32.124	23.758	30.475	C	5.966	-2.928	21.269	C	12.849	23.967	18.015
C	28.346	24.154	31.018	C	7.767	-3.196	19.138	C	11.181	24.070	19.742
H	28.317	25.690	29.435	H	6.149	-2.710	17.865	C	18.979	25.137	22.460

C	29.022	23.172	31.632	C	7.252	-3.322	21.520	H	17.913	24.143	20.878
C	31.022	22.015	32.266	H	5.290	-2.928	22.141	C	15.165	20.117	23.904
H	27.244	24.179	31.113	C	8.169	-3.394	20.467	H	15.357	20.785	21.800
C	28.570	22.077	32.476	H	8.325	-3.354	18.192	H	19.574	26.394	24.182
C	32.241	22.481	33.041	H	7.484	-3.507	22.611	H	14.587	19.974	26.076
C	29.871	21.486	33.086	C	9.586	-3.739	20.756	C	11.933	23.792	16.980
C	31.551	20.897	31.360	O	10.202	-4.569	20.135	H	13.901	23.771	17.724
C	27.878	21.144	31.512	C	10.050	-3.116	21.957	C	10.221	24.039	18.731
C	27.344	22.422	33.424	C	10.945	-3.736	22.927	H	10.747	24.114	20.706
H	33.007	22.833	32.371	C	9.842	-1.737	22.108	H	19.839	25.180	21.853
H	32.038	23.306	33.742	C	11.440	-3.036	24.023	H	14.901	19.064	23.725
H	32.626	21.619	33.547	H	11.204	-4.821	22.807	C	10.594	23.873	17.390
H	29.849	20.384	33.111	C	10.426	-1.026	23.144	H	12.135	23.628	15.901
H	29.931	21.764	34.165	H	9.274	-1.133	21.370	H	9.198	24.219	19.063
H	32.466	21.138	30.762	C	11.146	-1.697	24.122	C	9.515	23.982	16.384
H	31.918	20.077	32.043	H	12.032	-3.564	24.774	O	9.788	24.217	15.211
H	30.836	20.431	30.634	H	10.319	0.063	23.252	C	8.069	23.602	16.724
C	26.783	20.586	32.128	O	5.934	13.082	30.754	C	7.729	22.622	17.598
C	28.069	20.837	30.218	C	5.899	12.443	31.969	C	7.017	24.340	16.161
H	27.707	22.752	34.396	C	4.773	12.141	32.739	C	6.432	22.300	17.922
H	26.836	23.311	33.109	C	7.104	12.066	32.619	H	8.516	21.955	17.998
C	26.432	21.220	33.499	C	4.775	11.623	34.008	C	5.707	23.993	16.355
C	26.015	19.640	31.459	H	3.791	12.304	32.200	H	7.135	25.150	15.469
C	27.220	19.988	29.473	C	7.132	11.463	33.829	C	5.407	22.960	17.280
H	28.996	21.198	29.733	H	8.114	12.297	32.137	H	6.070	21.457	18.608
C	24.966	21.524	33.535	C	5.976	11.348	34.605	H	4.938	24.618	15.902
C	26.884	20.215	34.576	C	3.410	11.442	34.724	O	15.127	32.377	16.512
C	26.273	19.263	30.152	H	8.098	11.182	34.090	C	15.818	32.854	17.608
H	25.130	19.138	31.875	N	6.015	10.839	35.961	C	16.465	31.954	18.435

O	27.515	19.778	28.158	H	3.082	12.358	35.164	C	15.806	34.175	18.020
H	24.661	22.086	34.438	H	2.737	10.944	34.001	C	17.068	32.315	19.585
H	24.638	22.085	32.649	N	3.699	10.423	35.748	H	16.306	30.931	18.195
H	24.411	20.605	33.689	C	4.765	10.921	36.616	C	16.546	34.638	19.159
H	26.583	20.704	35.502	C	6.476	9.429	35.907	C	15.235	35.318	17.212
H	26.392	19.315	34.512	C	4.026	9.158	35.236	C	17.091	33.659	20.019
H	28.002	20.030	34.606	H	4.796	10.376	37.571	H	17.562	31.534	20.165
H	25.688	18.453	29.648	H	4.520	11.947	36.871	C	16.488	36.117	19.276
C	26.510	19.196	27.484	H	7.317	9.250	35.170	C	16.340	36.255	16.837
C	26.735	18.077	26.716	H	6.761	9.067	36.897	C	14.335	36.131	18.160
C	25.236	19.748	27.482	C	5.339	8.639	35.337	H	14.646	34.939	16.361
C	25.652	17.424	26.166	C	3.115	8.408	34.537	O	17.795	33.995	21.192
H	27.736	17.664	26.830	C	5.646	7.391	35.000	C	17.040	36.584	17.974
C	24.127	19.144	26.881	C	3.431	7.051	34.291	C	15.006	36.475	19.354
H	25.192	20.662	28.060	H	2.104	8.822	34.389	H	16.991	36.372	20.216
C	24.330	17.881	26.264	C	4.682	6.514	34.609	C	16.760	36.623	15.571
H	25.833	16.411	25.678	H	6.652	6.939	35.188	C	12.966	36.445	18.073
H	23.185	19.646	26.807	H	2.696	6.415	33.860	C	17.651	33.097	22.218
C	23.155	17.145	25.709	O	5.030	5.215	34.359	C	18.150	37.346	17.851
O	23.134	16.529	24.641	C	4.144	4.345	33.712	C	14.403	37.136	20.431
C	21.970	17.282	26.540	C	2.869	4.105	34.254	C	17.859	37.355	15.452
C	20.692	17.555	26.091	C	4.511	3.666	32.562	H	16.130	36.316	14.786
C	22.206	17.203	27.898	C	2.044	3.115	33.668	C	12.406	37.082	19.167
C	19.755	18.055	27.038	H	2.468	4.545	35.121	H	12.347	36.279	17.172
H	20.365	17.613	25.052	C	3.699	2.711	32.004	C	18.711	33.000	23.118
C	21.290	17.633	28.829	H	5.591	3.820	32.188	C	16.480	32.364	22.463
H	23.127	16.745	28.262	C	2.523	2.360	32.581	C	18.592	37.758	16.587
C	20.042	18.084	28.414	H	1.107	2.905	34.184	H	18.572	37.639	18.806
H	18.820	18.511	26.665	H	4.091	2.208	31.084	C	13.065	37.530	20.322

H	21.513	17.647	29.937	C	1.816	1.223	32.022	H	15.099	37.520	21.256
O	35.135	33.032	18.781	O	0.961	0.634	32.708	H	18.108	37.751	14.417
C	34.165	32.334	18.134	C	2.105	0.568	30.701	H	11.336	37.402	19.071
C	33.208	33.012	17.380	C	1.342	0.886	29.579	C	18.680	32.068	24.181
C	34.027	30.972	18.239	C	2.926	-0.553	30.627	H	19.733	33.495	23.055
C	32.200	32.298	16.804	C	1.391	0.251	28.367	C	16.451	31.480	23.493
H	33.215	34.107	17.465	H	0.495	1.567	29.787	H	15.664	32.435	21.807
C	32.972	30.193	17.675	C	2.930	-1.305	29.482	H	19.362	38.572	16.497
H	34.820	30.392	18.838	H	3.436	-0.959	31.544	H	12.534	38.088	21.124
C	32.060	30.900	16.975	C	2.210	-0.912	28.312	C	17.539	31.269	24.348
C	31.203	32.838	15.790	H	0.747	0.544	27.523	H	19.410	31.952	25.016
H	32.995	29.139	17.905	H	3.472	-2.253	29.309	H	15.433	31.045	23.731
C	30.899	30.408	16.104	H	-1.253	9.928	36.615	C	17.414	30.300	25.443
C	31.987	32.993	14.469	O	-2.090	9.861	36.211	O	18.167	30.447	26.432
C	30.165	31.713	15.758	C	-2.739	10.964	36.618	C	16.267	29.370	25.449
C	30.764	34.261	16.241	C	-2.087	12.127	37.021	C	15.451	29.039	26.517
C	29.972	29.409	16.782	C	-4.141	10.907	36.605	C	16.104	28.591	24.302
C	31.365	29.586	14.909	C	-2.772	13.302	37.392	C	14.545	27.965	26.428
H	31.263	33.464	13.715	H	-0.965	12.126	37.123	H	15.816	29.499	27.458
H	32.763	33.685	14.696	C	-4.787	12.103	36.930	C	15.165	27.576	24.201
H	32.451	32.125	14.061	H	-4.660	10.063	36.033	H	16.697	28.783	23.405
H	29.342	31.817	16.416	C	-4.176	13.303	37.324	C	14.322	27.256	25.278
H	29.643	31.766	14.810	C	-1.946	14.526	37.547	H	14.072	27.778	27.374
H	31.583	34.918	15.895	H	-5.868	12.178	36.863	H	15.097	27.052	23.262
H	29.902	34.671	15.712	N	-4.924	14.480	37.441	H	20.565	25.740	11.812
H	30.512	34.433	17.310	H	-1.503	14.634	38.554	O	20.264	25.036	11.320
C	29.591	28.448	15.876	H	-1.127	14.522	36.887	C	19.127	24.693	11.969
C	29.439	29.454	18.066	N	-2.832	15.661	37.337	C	18.144	25.642	12.285
H	31.760	30.125	14.019	C	-4.054	15.505	38.063	C	18.813	23.353	12.165

H	32.176	28.895	15.175	C	-5.450	15.029	36.145	C	16.894	25.300	12.880
C	30.228	28.579	14.497	C	-3.036	15.877	35.983	H	18.369	26.699	11.984
C	28.668	27.500	16.280	H	-4.614	16.448	38.189	C	17.621	22.978	12.801
C	28.526	28.433	18.495	H	-3.877	15.211	39.099	C	19.722	22.179	11.833
H	29.702	30.271	18.682	H	-6.160	14.259	35.756	C	16.669	23.931	13.179
C	30.813	27.282	13.949	H	-6.108	15.916	36.333	H	16.170	26.156	13.120
C	29.127	29.133	13.598	C	-4.289	15.582	35.373	C	17.440	21.493	13.026
C	28.158	27.485	17.543	C	-1.936	16.302	35.262	C	18.864	21.277	11.052
H	28.266	26.778	15.545	C	-4.285	15.614	33.988	C	19.900	21.557	13.190
O	28.051	28.432	19.763	C	-2.067	16.357	33.906	H	20.695	22.453	11.337
H	31.538	26.879	14.566	H	-0.986	16.508	35.676	O	15.428	23.468	13.651
H	29.943	26.627	13.891	C	-3.186	16.003	33.233	C	17.666	20.911	11.661
H	31.370	27.305	13.006	H	-5.259	15.460	33.421	C	18.719	21.062	13.770
H	28.212	28.529	13.544	H	-1.169	16.706	33.336	H	16.451	21.225	13.498
H	28.776	30.049	14.113	O	-3.211	16.072	31.857	C	19.214	20.731	9.842
H	29.427	29.220	12.464	C	-1.989	16.213	31.203	C	21.177	21.210	13.671
H	27.590	26.629	17.782	C	-1.665	17.434	30.655	C	14.832	24.343	14.516
C	28.606	27.598	20.714	C	-0.978	15.223	31.296	C	16.792	20.221	10.879
C	28.025	27.391	21.993	C	-0.388	17.609	30.196	C	18.857	20.229	14.939
C	29.664	26.786	20.331	H	-2.293	18.293	30.636	C	18.377	19.913	9.200
C	28.602	26.580	22.967	C	0.274	15.393	30.806	H	20.209	20.997	9.579
H	27.175	28.058	22.189	H	-1.299	14.262	31.594	C	21.314	20.503	14.865
C	30.181	25.958	21.345	C	0.611	16.620	30.296	H	22.127	21.504	13.232
H	30.090	26.863	19.379	H	-0.099	18.602	29.817	C	15.514	24.935	15.594
C	29.679	25.824	22.649	H	1.063	14.569	30.854	C	13.569	24.863	14.060
H	28.266	26.560	23.993	C	1.934	16.868	29.636	C	17.157	19.633	9.678
H	31.067	25.299	21.060	O	2.013	17.782	28.859	H	15.770	20.007	11.180
C	30.219	24.771	23.541	C	3.091	16.055	30.034	C	20.167	20.017	15.467
O	30.629	23.734	23.065	C	3.244	15.717	31.341	H	17.881	20.121	15.481

C	30.337	25.019	25.015	C	3.995	15.641	29.069	H	18.653	19.502	8.225
C	30.525	23.940	25.889	C	4.268	14.768	31.653	H	22.230	20.348	15.303
C	30.405	26.319	25.536	H	2.638	16.104	32.251	C	14.837	25.879	16.312
C	30.722	24.173	27.261	C	4.896	14.684	29.359	H	16.557	24.635	15.807
H	30.412	22.919	25.539	H	3.887	15.965	28.026	C	12.872	25.755	14.877
C	30.512	26.538	26.920	C	5.051	14.161	30.612	H	13.143	24.418	13.115
H	30.349	27.183	24.865	H	4.313	14.523	32.695	H	16.355	19.066	9.133
C	30.770	25.474	27.746	H	5.604	14.336	28.624	H	20.363	19.445	16.390
H	30.974	23.332	27.889					C	13.535	26.298	15.990
H	30.409	27.494	27.430					H	15.316	26.472	17.068
H	50.984	30.481	20.632					H	11.875	25.995	14.528
O	50.222	29.894	20.802					C	12.915	27.352	16.887
C	49.268	30.503	21.580					O	12.038	26.981	17.712
C	47.986	29.906	21.506					C	13.566	28.670	16.805
C	49.398	31.778	22.086					C	14.431	28.907	15.750
C	46.909	30.539	22.118					C	13.256	29.558	17.768
H	47.786	28.932	21.073					C	15.053	30.127	15.693
C	48.268	32.437	22.645					H	14.435	28.192	14.898
H	50.401	32.297	22.029					C	13.776	30.842	17.650
C	46.981	31.836	22.619					H	12.480	29.323	18.523
C	45.471	30.021	21.987					C	14.647	31.155	16.596
H	48.321	33.521	22.978					H	15.758	30.413	14.848
C	45.609	32.378	22.936					H	13.579	31.657	18.377
C	45.185	29.183	23.241								
C	44.771	31.369	22.134								
C	45.269	29.332	20.593								
C	45.374	33.777	22.507								
C	45.365	32.472	24.469								
H	44.153	28.787	23.203								

H	45.840	28.293	23.310		
H	45.412	29.825	24.105		
H	44.547	31.860	21.154		
H	43.828	31.328	22.668		
H	45.726	29.864	19.733		
H	45.773	28.362	20.581		
H	44.218	29.155	20.391		
C	45.361	34.636	23.583		
C	45.208	34.318	21.233		
H	44.340	32.142	24.634		
H	46.161	31.877	24.996		
C	45.431	33.953	24.924		
C	45.144	36.002	23.388		
C	45.100	35.688	21.008		
H	45.207	33.629	20.363		
C	46.715	34.333	25.571		
C	44.225	34.498	25.680		
C	45.025	36.542	22.135		
H	45.112	36.673	24.241		
O	44.925	36.185	19.776		
H	47.653	33.893	25.155		
H	46.784	35.442	25.554		
H	46.747	33.999	26.657		
H	43.232	34.325	25.227		
H	44.258	33.932	26.637		
H	44.263	35.601	25.920		
H	44.830	37.622	21.980		
C	43.755	35.680	19.181		
C	43.781	35.421	17.806		

C	42.582	35.284	19.934					
C	42.755	34.730	17.223					
H	44.419	35.889	16.986					
C	41.581	34.526	19.316					
H	42.497	35.431	21.043					
C	41.668	34.296	17.947					
H	42.920	34.479	16.202					
H	40.859	34.001	19.924					
C	40.651	33.390	17.261					
O	41.019	32.865	16.252					
C	39.198	33.250	17.626					
C	38.354	32.194	17.278					
C	38.565	34.249	18.329					
C	37.037	32.060	17.615					
H	38.816	31.364	16.705					
C	37.236	34.140	18.735					
H	39.208	35.080	18.632					
C	36.418	33.035	18.397					
H	36.475	31.110	17.450					
H	36.856	34.852	19.431					

In Hex

iPEEK-SBI iPEEK-TB iPEEK-Trip

O	17.766	9.008	-7.566	O	9.185	22.324	26.484	O	8.574	40.555	8.401
C	19.101	8.626	-7.210	C	10.191	23.193	26.341	C	8.179	41.446	7.439
C	19.370	7.271	-6.958	C	10.445	24.019	27.392	C	7.507	41.056	6.368
C	20.061	9.558	-6.959	C	10.863	23.360	25.184	C	8.308	42.788	7.602
C	20.689	6.929	-6.769	C	11.400	24.985	27.359	C	6.931	41.940	5.455

H	18.586	6.547	-7.247	H	9.734	23.988	28.221	H	7.123	40.040	6.316
C	21.277	9.198	-6.416	C	11.845	24.337	25.099	C	7.827	43.744	6.751
H	19.868	10.619	-7.038	H	10.552	22.755	24.305	C	8.811	43.427	8.797
C	21.648	7.861	-6.390	C	12.243	25.130	26.184	C	7.026	43.312	5.702
C	21.299	5.561	-6.715	C	11.733	25.849	28.587	H	6.255	41.516	4.757
H	22.067	9.931	-6.242	H	12.348	24.381	24.046	C	8.061	45.200	7.105
C	22.954	7.229	-6.166	N	13.460	25.850	26.251	C	7.695	44.195	9.241
C	21.649	5.152	-8.094	H	11.027	26.788	28.829	C	9.921	44.245	8.240
C	22.497	5.840	-5.862	H	11.481	25.307	29.545	H	9.102	42.710	9.548
C	20.255	4.613	-6.149	N	13.135	26.123	28.598	O	6.321	44.142	4.956
C	23.593	7.944	-5.026	C	13.460	26.827	27.362	C	7.370	45.309	8.415
C	23.962	7.466	-7.330	C	14.460	24.850	26.412	C	9.479	45.275	7.533
H	21.911	4.104	-8.069	C	13.782	24.909	28.831	H	7.856	46.034	6.431
H	20.726	5.241	-8.768	H	14.404	27.360	27.410	C	6.926	43.940	10.402
H	22.390	5.744	-8.491	H	12.704	27.617	27.285	C	11.279	43.991	8.406
H	22.171	5.701	-4.825	H	14.383	23.973	25.692	C	5.519	43.577	4.036
H	23.319	5.123	-5.987	H	15.475	25.259	26.251	C	6.510	46.310	8.837
H	19.454	4.582	-6.848	C	14.508	24.280	27.808	C	10.326	46.279	7.095
H	20.616	3.573	-6.101	C	13.672	24.215	30.033	C	6.070	44.962	10.764
H	19.814	4.881	-5.162	C	15.127	23.112	28.059	H	7.137	43.045	10.899
C	24.863	8.323	-5.299	C	14.412	23.046	30.283	C	12.152	44.997	8.000
C	23.020	8.150	-3.839	H	13.005	24.607	30.743	H	11.615	43.185	9.003
H	24.136	6.479	-7.664	C	15.247	22.514	29.309	C	5.986	43.623	2.715
H	23.507	8.085	-8.102	H	15.785	22.630	27.278	C	4.254	43.124	4.347
C	25.198	8.113	-6.769	H	14.452	22.580	31.202	C	5.769	46.079	9.990
C	25.634	8.900	-4.291	O	16.108	21.538	29.578	H	6.258	47.061	8.150
C	23.724	8.743	-2.799	C	17.280	21.907	30.227	C	11.646	46.160	7.437
H	21.907	7.854	-3.658	C	18.423	21.490	29.539	H	9.868	47.201	6.638
C	25.543	9.569	-7.227	C	17.349	22.627	31.385	H	5.482	44.824	11.699

C	26.451	7.250	-6.897	C	19.642	21.524	30.184	H	13.249	44.854	8.254
C	25.108	9.167	-3.029	H	18.300	21.125	28.595	C	5.283	43.019	1.737
H	26.679	9.128	-4.547	C	18.581	22.874	31.890	H	7.062	43.987	2.459
O	23.102	8.994	-1.553	H	16.458	23.187	31.767	C	3.470	42.592	3.335
H	26.503	9.900	-6.926	C	19.713	22.366	31.316	H	3.833	43.193	5.353
H	25.695	9.556	-8.354	H	20.524	21.177	29.687	H	5.087	46.840	10.276
H	24.723	10.266	-6.921	H	18.699	23.504	32.793	H	12.332	46.924	7.227
H	26.277	6.319	-6.365	C	21.006	22.682	32.031	C	4.003	42.497	2.064
H	26.576	6.915	-7.957	O	20.909	23.159	33.109	H	5.702	42.795	0.754
H	27.370	7.647	-6.501	C	22.319	22.348	31.501	H	2.464	42.192	3.503
H	25.762	9.562	-2.271	C	23.290	21.856	32.357	C	3.182	41.977	0.921
C	22.844	7.869	-0.847	C	22.434	22.467	30.153	O	1.988	42.125	0.953
C	23.829	6.884	-0.966	C	24.527	21.564	31.812	C	3.854	41.229	-0.196
C	21.703	7.725	-0.076	H	23.076	21.883	33.407	C	4.954	40.404	0.075
C	23.662	5.750	-0.212	C	23.692	22.159	29.611	C	3.392	41.389	-1.531
H	24.633	7.016	-1.648	H	21.637	22.900	29.558	C	5.810	40.087	-0.953
C	21.544	6.529	0.619	C	24.728	21.749	30.462	H	5.219	40.267	1.123
H	20.949	8.541	0.006	H	25.325	21.382	32.479	C	4.220	41.010	-2.519
C	22.533	5.554	0.590	H	23.934	22.178	28.543	H	2.642	42.182	-1.759
H	24.478	5.046	-0.212	H	25.572	21.462	29.944	C	5.454	40.367	-2.256
H	20.657	6.428	1.291	O	-2.071	16.210	22.046	H	6.673	39.404	-0.721
C	22.513	4.441	1.588	C	-1.334	17.254	21.491	H	3.909	41.254	-3.531
O	23.527	3.926	1.953	C	-0.984	18.323	22.271	H	6.205	40.178	-2.936
C	21.220	4.065	2.255	C	-0.972	17.328	20.157	O	6.244	34.418	18.691
C	21.164	3.636	3.575	C	-0.438	19.484	21.809	C	5.476	34.192	17.604
C	20.060	4.085	1.509	H	-1.225	18.349	23.305	C	4.466	35.068	17.261
C	19.976	3.133	4.088	C	-0.304	18.453	19.672	C	5.768	33.203	16.655
H	22.122	3.616	4.144	H	-1.282	16.579	19.484	C	3.778	34.959	16.051
C	18.839	3.699	1.999	C	-0.021	19.511	20.499	H	4.073	35.801	17.974

H	20.055	4.433	0.462	C	-0.032	20.495	22.871	C	5.133	33.110	15.443
C	18.818	3.207	3.307	H	0.018	18.379	18.633	C	6.902	32.238	16.749
H	19.893	2.715	5.122	N	0.856	20.559	20.109	C	4.076	33.974	15.139
H	17.887	3.631	1.426	H	-0.621	21.368	22.934	H	3.012	35.644	15.820
H	17.922	2.859	3.687	H	-0.126	19.965	23.820	C	5.622	32.101	14.489
O	12.449	10.784	-7.247	N	1.304	20.896	22.459	C	7.812	32.477	15.591
C	12.523	9.458	-6.780	C	1.050	21.543	21.154	C	6.218	30.884	16.461
C	13.401	9.012	-5.807	C	2.171	20.045	19.828	H	7.270	32.465	17.748
C	11.509	8.662	-7.297	C	2.203	19.816	22.345	O	3.313	34.031	14.048
C	13.005	7.849	-5.136	H	1.953	22.123	20.922	C	7.182	32.383	14.372
H	14.116	9.681	-5.390	H	0.099	22.176	21.186	C	5.515	30.780	15.235
C	11.088	7.538	-6.590	H	2.246	19.336	18.995	H	5.184	32.153	13.487
H	10.916	8.982	-8.156	H	2.753	20.867	19.435	C	9.158	32.650	15.563
C	11.825	7.218	-5.478	C	2.723	19.409	21.087	C	6.216	29.816	17.354
C	13.800	7.049	-4.205	C	2.227	18.960	23.411	C	3.544	35.210	13.461
H	10.189	6.993	-6.975	C	3.587	18.332	21.077	C	7.710	32.557	13.090
C	11.615	6.059	-4.586	C	3.007	17.850	23.308	C	4.869	29.573	14.907
C	13.877	7.708	-2.782	H	1.710	19.164	24.314	C	9.806	32.840	14.321
C	13.077	5.739	-4.266	C	3.740	17.515	22.180	H	9.635	32.753	16.551
C	15.203	6.982	-4.823	H	4.015	18.019	20.098	C	5.744	28.590	16.939
C	10.803	4.977	-5.283	H	3.082	17.158	24.132	H	6.817	30.089	18.224
C	10.653	6.428	-3.398	O	4.550	16.436	22.276	C	2.516	36.126	13.328
H	14.220	6.960	-2.116	C	5.881	16.722	22.260	C	4.800	35.470	12.958
H	14.559	8.521	-2.807	C	6.455	17.388	21.218	C	9.058	32.803	13.152
H	12.904	8.082	-2.436	C	6.582	16.415	23.468	H	7.133	32.410	12.115
H	13.438	5.125	-5.156	C	7.744	17.830	21.403	C	5.055	28.464	15.716
H	13.075	5.188	-3.348	H	5.851	17.541	20.358	H	4.456	29.552	13.932
H	15.841	6.385	-4.119	C	7.870	16.791	23.576	H	10.868	33.073	14.196
H	15.346	6.539	-5.853	H	6.150	15.660	24.148	H	5.874	27.645	17.568

H	15.711	7.954	-4.840	C	8.454	17.533	22.575	C	2.769	37.312	12.714
C	9.702	4.582	-4.518	H	8.313	18.501	20.760	H	1.576	35.845	13.731
C	11.007	4.568	-6.563	H	8.478	16.719	24.505	C	4.975	36.626	12.251
H	11.137	6.941	-2.520	C	9.763	18.167	22.878	H	5.565	34.701	12.977
H	10.001	7.267	-3.773	O	10.747	17.850	22.251	H	9.699	32.929	12.260
C	9.751	5.202	-3.121	C	9.811	19.259	23.868	H	4.691	27.443	15.420
C	8.818	3.688	-5.023	C	10.590	19.236	25.015	C	4.040	37.646	12.259
C	10.082	3.592	-7.047	C	8.925	20.286	23.533	H	1.958	38.075	12.582
H	11.867	4.906	-7.197	C	10.355	20.266	25.968	H	5.944	36.780	11.758
C	8.341	5.527	-2.569	H	11.412	18.576	25.162	C	4.178	39.020	11.573
C	10.512	4.255	-2.247	C	8.730	21.299	24.422	O	3.233	39.719	11.488
C	8.914	3.309	-6.308	H	8.414	20.172	22.616	C	5.424	39.535	11.017
H	8.034	3.412	-4.334	C	9.464	21.308	25.670	C	6.682	39.123	11.371
O	10.179	3.135	-8.356	H	10.791	20.237	26.955	C	5.263	40.437	9.946
H	7.809	6.198	-3.310	H	8.106	22.194	24.197	C	7.732	39.544	10.578
H	7.611	4.736	-2.467	O	6.694	13.730	22.978	H	6.901	38.354	12.242
H	8.324	6.097	-1.626	C	6.145	13.014	21.960	C	6.317	40.786	9.180
H	10.821	4.756	-1.295	C	6.555	11.713	21.753	H	4.189	40.755	9.717
H	10.010	3.293	-2.013	C	5.143	13.499	21.140	C	7.547	40.320	9.373
H	11.539	4.119	-2.688	C	6.093	10.838	20.820	H	8.780	39.155	10.705
H	8.117	2.745	-6.782	H	7.350	11.293	22.305	H	6.169	41.619	8.500
C	11.352	3.497	-8.885	C	4.695	12.687	20.162	O	5.451	39.886	28.048
C	12.486	2.712	-8.487	H	4.813	14.472	21.379	C	5.123	40.731	27.027
C	11.593	4.662	-9.610	C	5.193	11.361	19.965	C	3.951	40.439	26.311
C	13.777	3.076	-8.837	C	6.352	9.375	20.874	C	5.926	41.829	26.610
H	12.337	1.804	-7.905	H	4.022	13.035	19.372	C	3.630	41.204	25.223
C	12.885	5.030	-9.952	N	4.999	10.676	18.743	H	3.285	39.621	26.521
H	10.751	5.407	-9.757	H	7.412	9.089	20.813	C	5.592	42.511	25.504
C	13.975	4.206	-9.568	H	5.968	8.856	21.700	C	7.376	41.966	27.057

H	14.607	2.400	-8.641	N	5.639	8.759	19.782	C	4.442	42.258	24.781
H	13.020	6.060	-10.456	C	5.753	9.494	18.553	H	2.741	41.061	24.639
C	15.326	4.584	-9.954	C	3.586	10.395	18.500	C	6.632	43.391	24.898
O	16.028	3.845	-10.638	C	4.271	8.408	19.894	C	7.734	43.397	27.068
C	15.929	5.804	-9.429	H	5.380	8.944	17.659	C	8.124	41.583	25.788
C	15.287	6.488	-8.419	H	6.783	9.818	18.325	H	7.634	41.327	27.876
C	17.108	6.265	-9.854	H	3.016	11.251	18.793	O	4.162	42.845	23.586
C	15.804	7.659	-7.877	H	3.419	10.193	17.419	C	7.201	44.153	26.049
H	14.354	6.168	-7.935	C	3.238	9.143	19.298	C	7.652	42.297	24.638
C	17.702	7.348	-9.297	C	3.968	7.299	20.634	H	6.296	43.844	23.992
H	17.713	5.931	-10.744	C	1.965	8.653	19.274	C	8.465	43.985	28.052
C	17.077	8.049	-8.268	C	2.641	6.812	20.599	C	9.076	40.548	25.585
H	15.303	8.309	-7.172	H	4.750	6.854	21.237	C	4.653	42.107	22.570
H	18.681	7.688	-9.573	C	1.663	7.461	19.832	C	7.191	45.513	26.201
O	14.367	24.738	0.133	H	1.201	9.180	18.635	C	8.061	42.012	23.381
C	14.510	23.975	-0.995	H	2.343	6.045	21.237	C	8.634	45.344	28.057
C	13.428	23.470	-1.715	O	0.358	7.038	19.703	H	9.066	43.399	28.713
C	15.784	23.513	-1.224	C	-0.599	8.037	19.659	C	9.502	40.315	24.308
C	13.748	22.601	-2.751	C	-0.790	8.842	20.751	H	9.482	39.937	26.449
H	12.361	23.589	-1.462	C	-1.237	8.250	18.476	C	4.242	42.382	21.260
C	16.036	22.609	-2.225	C	-1.527	10.029	20.585	C	5.392	40.982	22.756
H	16.532	23.987	-0.638	H	-0.262	8.657	21.694	C	7.949	46.145	27.183
C	15.073	22.274	-3.094	C	-2.007	9.381	18.249	H	6.601	45.993	25.430
C	12.698	21.982	-3.708	H	-1.193	7.402	17.784	C	8.891	40.901	23.216
H	17.098	22.364	-2.435	C	-2.028	10.332	19.295	H	7.726	42.549	22.559
C	15.024	21.369	-4.360	H	-1.768	10.740	21.378	H	9.217	45.803	28.862
C	11.675	23.095	-4.163	H	-2.531	9.463	17.237	H	10.207	39.519	24.117
C	13.587	21.469	-4.800	C	-2.796	11.582	19.080	C	4.609	41.631	20.226
C	12.025	20.881	-2.871	O	-3.487	11.539	18.094	H	3.515	43.212	21.127

C	15.342	19.988	-3.869	C	-2.597	12.805	19.861	C	5.932	40.301	21.730
C	16.130	21.511	-5.481	C	-1.341	13.251	20.232	H	5.593	40.615	23.734
H	11.687	24.017	-3.623	C	-3.666	13.653	20.098	H	8.038	47.235	27.203
H	11.983	23.359	-5.165	C	-1.140	14.394	20.925	H	9.158	40.482	22.235
H	10.697	22.632	-4.285	H	-0.544	12.675	19.983	C	5.546	40.561	20.403
H	13.120	20.545	-5.127	C	-3.551	14.784	20.865	H	4.173	41.765	19.252
H	13.568	22.203	-5.594	H	-4.628	13.403	19.689	H	6.672	39.559	22.072
H	12.613	20.033	-2.617	C	-2.259	15.143	21.341	C	6.138	39.887	19.244
H	11.636	21.258	-1.942	H	-0.135	14.669	21.153	O	6.292	40.528	18.235
H	11.262	20.323	-3.439	H	-4.392	15.491	20.835	C	6.436	38.483	19.254
C	16.307	19.457	-4.775	O	-2.861	3.121	29.136	C	7.007	37.888	18.164
C	15.098	19.358	-2.671	C	-1.778	3.620	29.692	C	5.852	37.721	20.259
H	15.859	22.264	-6.240	C	-0.495	3.439	29.129	C	6.859	36.489	18.041
H	16.964	21.965	-4.954	C	-1.890	4.263	30.939	H	7.490	38.442	17.421
C	16.437	20.149	-6.047	C	0.585	4.007	29.775	C	5.838	36.305	20.182
C	17.045	18.330	-4.455	H	-0.389	2.940	28.174	H	5.609	38.174	21.209
C	15.839	18.241	-2.321	C	-0.763	4.788	31.489	C	6.250	35.709	18.988
H	14.471	19.886	-1.947	H	-2.877	4.370	31.346	H	7.389	35.843	17.329
C	17.832	19.902	-6.707	C	0.521	4.540	31.023	H	5.531	35.662	21.043
C	15.323	19.651	-6.867	C	1.906	3.874	29.089	O	14.150	29.936	21.533
C	16.835	17.781	-3.194	H	-0.817	5.440	32.395	C	13.869	31.218	21.997
H	17.710	17.862	-5.131	N	1.695	5.053	31.616	C	13.948	31.531	23.405
O	15.453	17.476	-1.257	H	2.419	2.943	29.272	C	13.337	32.168	21.154
H	17.964	20.549	-7.560	H	1.836	3.963	28.031	C	13.590	32.797	23.800
H	18.646	20.081	-5.964	N	2.867	4.862	29.509	H	14.220	30.752	24.116
H	17.940	18.897	-7.100	C	2.985	4.685	30.961	C	13.163	33.433	21.457
H	14.314	19.453	-6.457	C	1.723	6.495	31.666	C	13.177	31.883	19.705
H	15.259	20.211	-7.824	C	2.216	6.074	29.266	C	13.327	33.774	22.857
H	15.606	18.581	-7.103	H	3.741	5.435	31.266	H	13.645	33.071	24.818

H	17.284	16.827	-2.922	H	3.319	3.673	31.146	C	12.860	34.365	20.318
C	14.436	16.625	-1.590	H	0.786	6.745	32.121	C	14.223	32.815	19.137
C	14.790	15.420	-2.282	H	2.562	6.953	32.206	C	11.824	32.370	19.425
C	13.084	16.883	-1.288	C	1.707	6.874	30.247	H	13.351	30.821	19.456
C	13.780	14.563	-2.592	C	2.001	6.468	27.907	O	13.145	35.079	23.165
H	15.818	15.164	-2.525	C	1.075	8.030	29.928	C	14.022	34.183	19.403
C	12.102	16.003	-1.583	C	1.375	7.662	27.577	C	11.649	33.696	19.762
H	12.841	17.861	-0.769	H	2.372	5.847	27.073	H	12.638	35.433	20.591
C	12.419	14.836	-2.282	C	0.928	8.475	28.650	C	15.388	32.436	18.571
H	14.124	13.681	-3.161	H	0.670	8.737	30.705	C	10.797	31.580	19.008
H	11.071	16.141	-1.200	H	1.241	7.992	26.566	C	12.280	35.295	24.186
C	11.405	13.762	-2.598	O	0.366	9.732	28.373	C	14.915	35.114	19.076
O	10.512	13.570	-1.845	C	1.464	10.558	28.292	C	10.380	34.235	19.544
C	11.648	13.066	-3.893	C	1.807	11.204	27.126	C	16.336	33.373	18.188
C	12.474	13.553	-4.916	C	2.313	10.694	29.392	H	15.678	31.424	18.404
C	11.007	11.811	-4.044	C	2.967	11.951	27.035	C	9.547	32.121	18.828
C	12.794	12.770	-5.985	H	1.114	11.034	26.282	H	10.900	30.510	18.821
H	12.895	14.596	-4.948	C	3.405	11.432	29.312	C	10.922	35.246	23.894
C	11.281	10.999	-5.139	H	2.083	10.250	30.351	C	12.708	35.664	25.457
H	10.400	11.463	-3.175	C	3.822	11.990	28.105	C	16.089	34.695	18.478
C	12.201	11.493	-6.078	H	3.165	12.690	26.275	H	14.979	36.170	19.339
H	13.474	13.030	-6.784	H	3.974	11.591	30.230	C	9.325	33.509	18.964
H	10.727	10.097	-5.282	C	5.037	12.763	28.071	H	10.162	35.289	19.777
O	14.282	23.385	8.965	O	5.348	13.407	29.034	H	17.291	33.067	17.754
C	13.184	24.215	8.906	C	5.771	12.772	26.748	H	8.818	31.408	18.372
C	12.054	24.024	8.163	C	5.428	11.886	25.732	C	10.015	35.611	24.878
C	13.233	25.327	9.658	C	6.665	13.782	26.529	H	10.565	34.923	22.906
C	11.042	24.914	8.104	C	5.708	12.187	24.447	C	11.766	35.855	26.465
H	12.013	23.172	7.460	H	4.956	10.942	25.907	H	13.825	35.818	25.561

C	12.150	26.184	9.768	C	7.107	13.981	25.268	H	16.899	35.365	18.127
H	14.085	25.508	10.362	H	6.915	14.526	27.286	H	8.474	34.144	18.776
C	11.021	25.989	8.965	C	6.526	13.260	24.195	C	10.384	35.899	26.185
C	9.679	24.847	7.453	H	5.253	11.487	23.737	H	8.978	35.531	24.705
H	12.247	26.916	10.636	H	7.913	14.654	25.204	H	11.999	35.992	27.502
C	9.728	26.699	9.148	H	6.309	6.974	25.701	C	9.417	35.973	27.310
C	9.317	23.340	7.479	O	6.559	7.305	24.866	O	9.625	35.217	28.213
C	8.891	25.656	8.470	C	6.730	6.294	24.001	C	8.296	36.962	27.409
C	9.986	25.352	6.074	C	6.711	5.003	24.382	C	7.459	36.965	28.433
C	9.531	28.103	8.596	C	7.113	6.613	22.712	C	8.096	37.837	26.348
C	9.524	26.941	10.682	C	6.961	3.960	23.467	C	6.587	37.975	28.676
H	8.247	23.332	7.560	H	6.187	4.846	25.332	H	7.595	36.237	29.244
H	9.691	22.751	6.701	C	7.297	5.620	21.794	C	7.072	38.844	26.475
H	9.591	22.935	8.432	H	7.377	7.616	22.386	H	8.912	37.943	25.645
H	7.900	26.060	8.028	C	7.203	4.293	22.116	C	6.375	38.929	27.668
H	8.547	24.969	9.272	C	7.013	2.524	23.921	H	6.099	38.082	29.643
H	9.014	25.435	5.503	H	7.907	5.993	20.916	H	6.828	39.470	25.645
H	10.480	26.328	6.066	N	7.477	3.330	21.153	H	20.925	18.837	22.773
H	10.577	24.641	5.564	H	7.996	2.489	24.513	O	20.423	18.399	22.066
C	9.592	29.045	9.633	H	6.202	2.263	24.584	C	19.162	18.955	22.101
C	9.382	28.452	7.283	N	6.965	1.615	22.784	C	18.350	18.816	20.961
H	8.535	26.620	10.849	C	7.831	1.986	21.681	C	18.707	19.599	23.230
H	10.178	26.292	11.284	C	6.194	3.215	20.472	C	17.031	19.143	21.169
C	9.725	28.454	11.025	C	5.616	1.635	22.297	H	18.652	18.267	20.075
C	9.659	30.384	9.247	H	7.678	1.203	20.889	C	17.483	20.183	23.254
C	9.330	29.816	6.919	H	8.836	2.044	22.039	C	19.509	19.643	24.540
H	9.025	27.687	6.542	H	5.700	4.249	20.395	C	16.596	19.909	22.250
C	11.123	28.850	11.526	H	6.450	2.760	19.537	H	16.352	18.785	20.434
C	8.564	29.091	11.847	C	5.247	2.356	21.141	C	17.281	20.910	24.523

C	9.556	30.775	7.941	C	4.682	0.831	22.893	C	18.457	19.133	25.507
H	9.864	31.026	10.079	C	3.883	2.241	20.737	C	19.637	21.065	24.916
O	9.199	30.357	5.641	C	3.381	0.738	22.471	H	20.428	19.136	24.448
H	11.160	29.861	11.926	H	4.988	0.211	23.690	O	15.242	20.227	22.198
H	11.539	28.222	12.319	C	3.009	1.463	21.349	C	17.338	19.883	25.605
H	11.813	28.853	10.640	H	3.425	2.813	19.865	C	18.458	21.816	24.756
H	8.437	30.113	11.648	H	2.706	-0.068	22.847	H	16.317	21.443	24.492
H	8.580	28.840	12.883	O	1.779	1.317	20.736	C	18.561	18.045	26.335
H	7.616	28.702	11.450	C	0.926	0.861	21.661	C	20.739	21.662	25.484
H	9.674	31.844	7.681	C	0.530	-0.445	21.772	C	14.743	21.469	22.458
C	9.130	29.290	4.788	C	0.517	1.798	22.628	C	16.221	19.496	26.362
C	10.293	28.553	4.644	C	-0.163	-0.902	22.867	C	18.481	23.142	25.159
C	8.142	29.124	3.877	H	0.858	-1.043	20.944	C	17.580	17.732	27.234
C	10.335	27.409	3.901	C	-0.129	1.352	23.734	H	19.340	17.382	26.246
H	11.129	28.807	5.311	H	0.962	2.825	22.554	C	20.787	23.053	25.777
C	8.109	27.887	3.164	C	-0.455	0.024	23.881	H	21.697	21.106	25.616
H	7.250	29.805	4.096	H	-0.535	-1.885	22.899	C	13.401	21.558	22.570
C	9.265	27.058	3.130	H	-0.293	1.995	24.588	C	15.525	22.599	22.545
H	11.211	26.734	4.029	C	-1.065	-0.462	25.147	C	16.361	18.494	27.312
H	7.195	27.567	2.654	O	-1.104	-1.643	25.287	H	15.335	20.178	26.341
C	9.283	25.760	2.489	C	-1.647	0.404	26.222	C	19.587	23.801	25.614
O	8.305	25.026	2.386	C	-1.767	0.019	27.514	H	17.543	23.601	25.025
C	10.594	25.379	1.787	C	-2.046	1.688	25.936	H	17.798	16.855	27.881
C	11.618	24.715	2.431	C	-2.144	0.898	28.550	H	21.689	23.584	26.104
C	10.855	25.716	0.476	H	-1.701	-1.064	27.728	C	12.848	22.680	23.107
C	12.807	24.331	1.838	C	-2.402	2.576	26.930	H	12.684	20.697	22.475
H	11.361	24.224	3.361	H	-2.120	2.128	24.995	C	14.901	23.797	22.929
C	12.074	25.476	-0.106	C	-2.526	2.182	28.228	H	16.523	22.658	22.103
H	10.126	26.128	-0.167	H	-2.104	0.527	29.611	H	15.570	18.281	28.025

C	13.103	24.854	0.599	H	-2.391	3.559	26.506	H	19.521	24.886	25.729
H	13.524	23.788	2.417					C	13.571	23.873	23.266
H	12.257	25.836	-1.133					H	11.762	22.750	23.409
H	15.402	23.821	9.795					H	15.468	24.746	22.938
O	16.145	23.907	10.420					C	12.889	24.987	23.872
C	17.025	23.044	9.966					O	12.185	24.793	24.850
C	17.084	22.668	8.682					C	13.200	26.288	23.277
C	17.894	22.436	10.898					C	14.046	27.149	23.991
C	17.866	21.616	8.317					C	12.588	26.715	22.083
H	16.412	23.050	8.046					C	14.382	28.389	23.452
C	18.817	21.459	10.531					H	14.448	26.822	24.930
H	17.952	22.744	11.928					C	12.906	27.988	21.595
C	18.693	21.067	9.226					H	11.783	26.217	21.520
C	17.901	20.902	6.990					C	13.848	28.806	22.229
H	19.443	20.908	11.194					H	15.264	28.991	23.792
C	19.622	20.062	8.548					H	12.441	28.313	20.632
C	18.494	21.826	5.954								
C	18.824	19.726	7.301								
C	16.497	20.352	6.682								
C	20.061	18.859	9.344								
C	21.033	20.773	8.319								
H	18.407	21.411	4.910								
H	17.977	22.812	6.054								
H	19.606	21.888	6.098								
H	18.192	18.795	7.504								
H	19.356	19.245	6.473								
H	16.131	19.865	7.585								
H	15.805	21.176	6.564								
H	16.575	19.653	5.880								

C	21.458	18.675	9.281		
C	19.200	18.012	9.940		
H	20.944	21.253	7.303		
H	21.128	21.533	9.138		
C	22.105	19.689	8.423		
C	21.942	17.532	9.886		
C	19.712	16.833	10.445		
H	18.182	18.282	10.054		
C	23.325	20.183	9.156		
C	22.471	19.000	7.123		
C	21.082	16.580	10.336		
H	23.003	17.360	9.929		
O	18.885	15.835	10.882		
H	23.091	20.584	10.136		
H	24.150	19.439	9.251		
H	23.659	21.056	8.583		
H	23.087	19.653	6.490		
H	23.047	18.086	7.369		
H	21.572	18.720	6.594		
H	21.507	15.683	10.796		
C	17.579	15.976	10.399		
C	17.400	16.165	9.074		
C	16.487	16.069	11.253		
C	16.182	16.624	8.540		
H	18.312	16.210	8.440		
C	15.259	16.579	10.769		
H	16.609	15.803	12.314		
C	15.132	16.923	9.456		
H	16.110	16.856	7.455		

H	14.404	16.808	11.399					
C	13.961	17.659	8.893					
O	12.979	17.055	8.563					
C	14.070	19.138	8.772					
C	14.750	19.828	9.710					
C	13.131	19.884	8.024					
C	14.681	21.213	9.818					
H	15.429	19.225	10.364					
C	13.272	21.249	7.978					
H	12.472	19.446	7.274					
C	14.062	21.995	8.841					
H	15.144	21.581	10.767					
H	12.839	21.723	7.089					

Table S17. XYZ coordinates and total energies of peek polymer unit with water

SPEEK-H_2O			(iPEEK-SBI)-H_2O			(iPEEK-TB)-H_2O		
(-1775.682)			(-1655.616)			(-1530.495)		
C	8.997	2.597	-0.364	C	3.036	1.288	1.695	6.046	-0.362	-1.285
H	8.198	3.337	-0.472	C	3.761	0.829	0.604	5.301	0.374	-0.372
H	9.157	2.434	0.706	C	4.311	1.743	-0.296	5.270	-0.024	0.975
H	-7.932	-0.611	0.638	C	4.160	3.107	-0.107	5.969	-1.164	1.362
C	-7.074	-1.227	0.373	C	3.442	3.567	1.002	6.696	-1.915	0.445
O	-5.981	-0.330	0.291	C	2.876	2.658	1.904	6.741	-1.505	-0.890
H	-6.900	-1.984	1.146	H	2.584	0.587	2.393	6.085	-0.073	-2.331
H	-7.247	-1.717	-0.591	H	4.579	3.839	-0.792	5.951	-1.453	2.410
C	-4.782	-0.805	-0.111	H	2.313	3.003	2.763	7.231	-2.796	0.781
C	-3.774	0.153	-0.305	C	5.015	1.050	-1.448	4.535	1.601	-0.824
C	-4.490	-2.145	-0.352	C	6.436	1.585	-1.651	5.220	2.431	-1.036
C	-2.504	-0.203	-0.724	H	6.954	1.011	-2.427	3.988	1.402	-1.749
C	-3.207	-2.511	-0.760	H	6.419	2.634	-1.967	4.541	0.720	1.963

H	-5.247	-2.909	-0.219	H	7.015	1.518	-0.725	3.576	2.061	0.199
C	-2.224	-1.550	-0.945	C	4.215	1.231	-2.747	4.263	2.068	1.493
H	-1.752	0.565	-0.879	H	4.724	0.731	-3.579	3.635	2.575	2.232
H	-2.962	-3.551	-0.948	H	3.212	0.803	-2.658	5.201	2.619	1.380
O	-0.998	-1.952	-1.426	H	4.112	2.292	-2.995	3.267	0.090	2.325
C	0.133	-1.643	-0.713	C	5.028	-0.436	-0.993	3.434	-0.979	2.483
C	0.123	-1.353	0.653	H	4.797	-1.108	-1.826	2.935	0.512	3.283
C	1.331	-1.687	-1.424	H	6.031	-0.696	-0.634	2.393	1.243	0.249
C	1.327	-1.099	1.295	C	4.015	-0.604	0.188	2.201	0.299	1.264
H	-0.811	-1.337	1.204	C	4.538	-1.532	1.315	1.424	1.406	-0.747
C	2.525	-1.416	-0.771	H	5.623	-1.462	1.443	1.021	-0.445	1.286
H	1.303	-1.937	-2.479	H	4.075	-1.226	2.262	0.267	0.642	-0.737
C	2.536	-1.108	0.594	C	4.064	-2.968	0.978	1.596	2.149	-1.523
H	1.349	-0.892	2.360	C	3.798	-3.787	2.242	0.069	-0.277	0.294
H	3.458	-1.465	-1.324	H	3.463	-4.800	1.994	0.844	-1.185	2.062
C	3.795	-0.874	1.369	H	4.714	-3.877	2.837	-0.486	0.759	-1.510
C	5.009	-0.336	0.678	H	3.029	-3.315	2.862	-1.031	-1.111	0.318
O	3.831	-1.125	2.560	C	5.078	-3.709	0.094	-2.285	-0.587	0.172
C	4.939	0.528	-0.418	H	5.317	-3.141	-0.810	-3.263	-1.462	-0.300
C	6.261	-0.661	1.210	H	6.009	-3.885	0.645	-2.613	0.728	0.515
C	6.104	1.040	-0.980	H	4.677	-4.680	-0.217	-4.575	-1.029	-0.416
H	3.973	0.820	-0.819	C	2.751	-1.347	-0.223	-2.970	-2.470	-0.572
C	7.419	-0.161	0.632	C	2.794	-2.678	0.196	-3.926	1.153	0.374
H	6.301	-1.310	2.079	C	1.649	-0.851	-0.912	-1.848	1.401	0.885
C	7.358	0.695	-0.473	C	1.750	-3.545	-0.111	-4.924	0.283	-0.076
H	6.040	1.720	-1.827	C	0.612	-1.729	-1.206	-5.328	-1.709	-0.803
H	8.389	-0.433	1.041	H	1.569	0.194	-1.198	-4.203	2.174	0.616
C	8.616	1.285	-1.059	C	0.651	-3.069	-0.824	-6.303	0.835	-0.245
H	8.474	1.465	-2.131	H	1.777	-4.584	0.209	-6.468	2.028	-0.426
H	9.438	0.567	-0.963	H	-0.185	-3.713	-1.076	-7.489	-0.082	-0.193
S	-4.125	1.865	0.006	O	-0.473	-1.255	-1.928	-7.519	-1.234	0.598
O	-2.993	2.634	-0.452	C	-1.650	-1.043	-1.273	-8.630	0.291	-0.911
O	-4.596	1.999	1.382	C	-1.785	-1.097	0.117	-8.672	-2.012	0.656
O	-5.346	2.163	-0.963	C	-2.749	-0.741	-2.081	-6.649	-1.508	1.188
H	-6.202	2.047	-0.449	C	-3.027	-0.851	0.683	-9.773	-0.497	-0.867
H	9.914	3.016	-0.789	H	-0.929	-1.331	0.741	-8.597	1.204	-1.496
O	-7.331	1.951	0.815	C	-3.978	-0.477	-1.499	-9.795	-1.650	-0.084
H	-7.543	2.847	1.116	H	-2.612	-0.724	-3.157	-8.693	-2.899	1.282
H	-6.605	1.661	1.400	C	-4.132	-0.523	-0.107	-10.651	-0.211	-1.438
				H	-3.159	-0.905	1.759	-10.690	-2.263	-0.045
				H	-4.832	-0.259	-2.133	7.427	-2.151	-1.872
				C	-5.443	-0.321	0.572	8.111	-3.331	-1.519
				O	-5.644	-0.846	1.659	8.568	-3.702	-2.437
				C	-6.499	0.522	-0.068	8.893	-3.135	-0.776
				C	-6.179	1.625	-0.866	7.422	-4.089	-1.125
				C	-7.840	0.229	0.208	3.052	4.072	-1.733

	C	-7.190	2.422	-1.393	3.157	3.636	-0.864
	H	-5.138	1.874	-1.053	2.460	4.818	-1.575
	C	-8.846	1.018	-0.337			
	H	-8.085	-0.609	0.855			
	C	-8.524	2.113	-1.138			
	H	-6.936	3.285	-2.000			
	H	-9.885	0.783	-0.129			
	H	-9.312	2.731	-1.556			
	O	3.342	4.919	1.119			
	C	2.615	5.429	2.213			
	H	3.066	5.129	3.168			
	H	2.652	6.514	2.122			
	H	1.570	5.096	2.189			
	O	-8.063	-1.855	2.788			
	H	-7.256	-1.327	2.657			
	H	-7.782	-2.746	2.542			

(iPEEK-Trip)-H_2O

(-1611.516)

C	-4.217	1.452	0.254
C	-3.030	1.957	-0.293
C	-3.009	3.202	-0.900
C	-4.188	3.951	-0.959
C	-5.366	3.451	-0.417
C	-5.385	2.194	0.195
H	-2.086	3.589	-1.324
H	-4.181	4.928	-1.433
H	-6.277	4.038	-0.466
H	-6.306	1.800	0.618
C	-1.847	1.006	-0.139
C	-4.045	0.068	0.874
C	-3.354	-2.703	-1.715
C	-2.166	-2.204	-2.245
C	-1.634	-1.010	-1.777
C	-2.290	-0.306	-0.775
C	-3.470	-0.808	-0.233
C	-4.014	-2.006	-0.697
C	-2.924	0.209	1.902
C	-2.994	-0.110	3.248
C	-1.865	0.074	4.053
C	-0.686	0.571	3.508
C	-0.616	0.893	2.150
C	-1.737	0.713	1.354
H	-3.915	-0.501	3.671
H	-1.911	-0.174	5.109

H	0.186	0.709	4.140
H	0.305	1.277	1.719
H	-4.967	-0.336	1.293
H	-0.924	1.400	-0.569
H	-1.644	-2.737	-3.032
H	-3.751	-3.635	-2.099
O	-5.172	-2.412	-0.108
O	-0.481	-0.515	-2.366
C	0.690	-0.559	-1.668
C	1.809	-0.061	-2.342
C	0.810	-1.058	-0.367
C	3.043	-0.048	-1.714
H	1.683	0.299	-3.357
C	2.056	-1.046	0.245
H	-0.056	-1.446	0.158
C	3.181	-0.532	-0.406
H	3.912	0.315	-2.254
H	2.172	-1.441	1.249
C	4.493	-0.612	0.298
O	4.651	-1.443	1.182
C	5.606	0.314	-0.077
C	5.365	1.623	-0.508
C	6.922	-0.136	0.076
C	6.431	2.470	-0.798
H	4.346	1.987	-0.593
C	7.982	0.709	-0.233
H	7.107	-1.142	0.445
C	7.739	2.009	-0.671
H	6.239	3.489	-1.119
H	9.002	0.352	-0.124
H	8.570	2.668	-0.905
C	-5.733	-3.628	-0.551
H	-5.047	-4.467	-0.385
H	-6.637	-3.777	0.040
H	-5.997	-3.580	-1.614
O	6.996	-2.871	1.955
H	6.652	-3.648	1.495
H	6.226	-2.279	1.991

6. References

1 Y. S. Toh, X. Loh, K. Li, A. Bismarck and A.G. Livingston, *J. Membr. Sci.*, 2007, **291**, 120. https://doi.org/10.1016/j.memsci.2006.12.053

2 F. Fei, L. Cseri, G. Szekely and C. F. Blanford, *ACS Appl. Mater. Interfaces*, 2018, **10**,16140. https://doi.org/10.1021/acsami.8b03591

3 J. R. Reimers, Khan and L. E. Hall, *J. Am. Chem. Soc.*,1999, **121**, 3730. https://doi.org/10.1021/ja983878n

4 S. Karan, Z. Jiang and A. G. Livingston, *Science*, 2015, **348**, 1347. https://doi.org/10.1126/science.aaa5058

5 M. A. Abdulhamid, G. Genduso, Y. Wang, X. Ma and I. Pinnau, *Ind. Eng. Chem. Res.* 2020, **59**, 5247–5256. https://doi.org/10.1021/acs.iecr.9b04994

6 M. A. Abdulhamid, H.W.H. Lai, Y.Wang, Z. Jin, Y. C. Teo, X. Ma, I. Pinnau and Y. Xia, *Chem. Mater.* 2019, **31**, 1767–1774. https://doi.org/10.1021/acs.chemmater.8b05359