Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information: Probing the Potential of Ureasil-Poly(ethylene oxide) as a Glyphosate Scavenger in Aqueous Milieu: Force-Field Parameterization and MD Simulations

Alechania Misturini,[†,‡] Germano Heinzelmann,[¶] Renato L. T. Parreira,[§] Eduardo F. Molina,[§] and Giovanni Finoto Caramori*[,†]

†*Departamento de Química, Universidade Federal de Santa Catarina, Campus Universitário Trindade, CP 476, Florianópolis, SC, 88040-900, Brazil*

‡*Polytechnic University of Valencia, Institute of Chemical Tecnology Avenida de los Naranjos, s/n Valencia, Valencia, ES 46022*

¶*Departamento de Física, Universidade Federal de Santa Catarina, Campus Universitário Trindade, CP 476, Florianópolis, SC, 88040-900, Brazil*

§*Núcleo de Pesquisa em Ciências Exatas e Tecnológicas, Universidade de Franca, Franca, SP, 14404-600, Brazil.*

E-mail: giovanni.caramori@ufsc.br

Phone: +55 (48)3721 3644

Section S1 – Parameterization

During the parameterization of the polymer fragment, a few considerations needed to be done, and are further explained below. Concerning the sampling procedure, an adequate amount of samples describing the term of interest is mandatory. In order to give a better description for bonds and bends, the oscillation sampled was restricted to ranges where the main displacements take place during simulations in solution – normally, $r_{eq} \pm 0.4$ Å and $\theta_{eq} \pm 20°$.

Due to steric effects, the sampling of torsional barriers and bends can be challenging, once some spatial configurations can be highly prohibited energetically. An approach to overcome these difficulties was simplifying our model, breaking it into 3 fragments (illustrated by top and bottom molecules in Fig. S1, respectively) containing all terms desired, but minimizing repulsive interaction between bulky groups.[S1] Thus, the description of sterically hindered configurations was also improved by sampling and fitting each term individually, despite Paramfit's capability to treat them simultaneously.

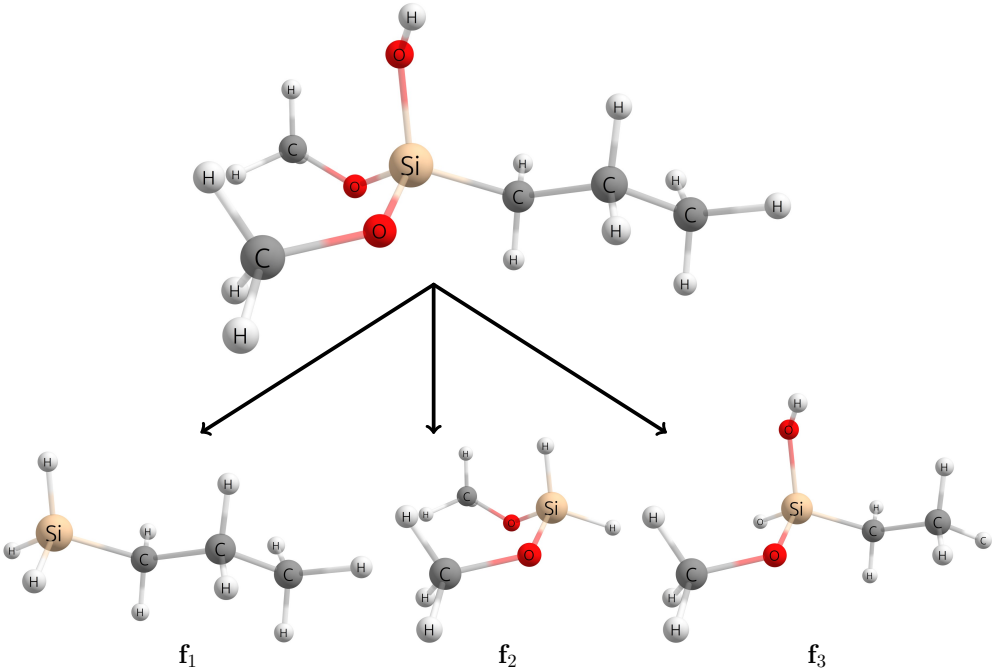


Figure S1: Polymer portion and the 3 fragments considered for the parameterization procedure.

Regarding the fitting procedure, the parameters of GAFF atom type c3 (carbon sp^3) for the terms involving Silicon atom have been used as an initial guess. Furthermore, only the torsional barrier was fitted, conserving n and γ parameters of c3 AT, and consequently, its torsional energy profiles. Lastly, k_r and k_θ parameters for bonded terms not containing the silicon atom, already described by GAFF force field, could be refined by Parmcal (from Ambertools package) considering the new equilibrium values from QM calculation on PBE0/def2-TZVP level of theory.

Section S2 – Supplementary Data

Table S1: Composition, time simulated (ns), and total number of atoms for simulations between polymer and pesticide.

composition	**time**	**number of atoms**
1 U-PEO : 10 GLY	300	200112
10 U-PEO : 10 GLY	300	200094
50 U-PEO : 10 GLY	410	200103
100 U-PEO : 10 GLY	460	200199
1 U-PEO : 10 $[GLY]^{2-}$	300	200085
10 U-PEO : 10 $[GLY]^{2-}$	300	200298
50 U-PEO : 10 $[GLY]^{2-}$	300	200586
100 U-PEO : 10 $[GLY]^{2-}$	300	200001
50 $[U\text{-}PEO]^{4+}$: 10 $[GLY]^{2-}$	300	200340
50 $[U\text{-}PEO]^{4+}$: 10 $[GLY]^{-}$	300	200126

Table S2: Geometrical parameters of YIBFEV at its crystallographic structure and calculated models. Absolute value of average deviation for bond lengths ($|\ \overline{\mathbf{D_{bond}}}\ |$, in Å), angles ($|\ \overline{\mathbf{D_{ang}}}\ |$, in degrees) and tosions ($|\ \overline{\mathbf{D_{tors}}}\ |$, in degrees) when compared with reference geometry. Calculation time (day:hour:min:sec) from Gaussian g09 geometry optimization output, using 8 cores in the same CPU.

		MP2				**B3LYP**				**PBE0**			
Term	**YIBFEV**	**6-31G***	**6-311G***	**def2-TZVP**	**cc-pVTZ**	**6-31G***	**6-311G***	**def2-TZVP**	**cc-pVTZ**	**6-31G***	**6-311G***	**def2-TZVP**	**cc-pVTZ**
J3-SI	1.841	1.858	1.852	1.851	1.855	1.865	1.862	1.859	1.863	1.858	1.853	1.851	1.856
SI-QH	1.637	1.675	1.661	1.656	1.662	1.670	1.666	1.656	1.663	1.665	1.659	1.650	1.657
SI-QS	1.619	1.659	1.649	1.641	1.647	1.654	1.650	1.638	1.646	1.650	1.645	1.635	1.642
QS-c3	1.445	1.430	1.423	1.421	1.420	1.421	1.420	1.418	1.418	1.411	1.409	1.407	1.408
	$\lvert\ \overline{\mathbf{D_{bond}}}\ \rvert$	0.028	0.022	0.019	0.023	0.029	0.027	0.021	0.026	0.028	0.024	0.019	0.024
J3-SI-QH	111.27	114.06	114.11	113.97	114.16	114.00	114.06	113.96	114.20	114.30	114.38	114.16	114.37
J3-SI-QS	105.79	107.55	107.62	107.70	107.60	107.44	107.72	107.53	107.49	107.51	107.74	107.52	107.51
SI-QS-c3	132.50	123.03	123.83	124.14	123.85	125.78	127.60	127.98	127.38	124.40	126.20	126.47	125.95
QH-SI-QS	111.48	107.51	107.48	107.34	107.29	107.64	107.46	107.54	107.46	107.41	107.22	107.38	107.30
	$\lvert\ \overline{\mathbf{D_{ang}}}\ \rvert$	4.50	4.34	4.28	4.39	3.73	3.41	3.22	3.44	4.23	3.91	3.69	3.89
J3-SI-QS-c3	167.60	158.18	158.44	161.34	162.90	158.07	156.28	159.80	160.34	159.85	158.92	162.19	162.59
QH-SI-QS-c3	55.63	48.43	50.07	48.14	47.98	48.69	44.81	45.00	44.92	49.07	46.94	46.56	45.99
	$\lvert\ \overline{\mathbf{D_{tors}}}\ \rvert$	8.31	7.36	6.88	6.17	8.23	11.07	9.21	8.99	7.16	8.68	7.24	7.32
Calculation time	opt	0:03:03:10	0:05:23:50	2:08:22:28	4:06:30:50	0:00:37:39	0:00:53:42	0:17:21:29	0:12:09:53	0:00:32:47	0:00:50:35	0:16:32:03	0:15:38:28

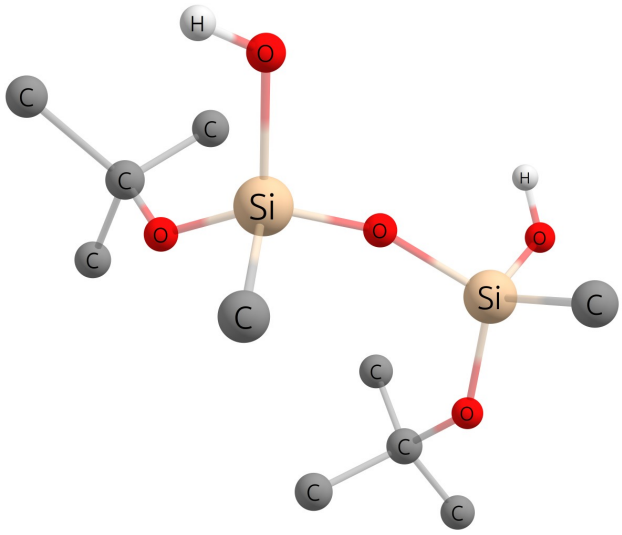
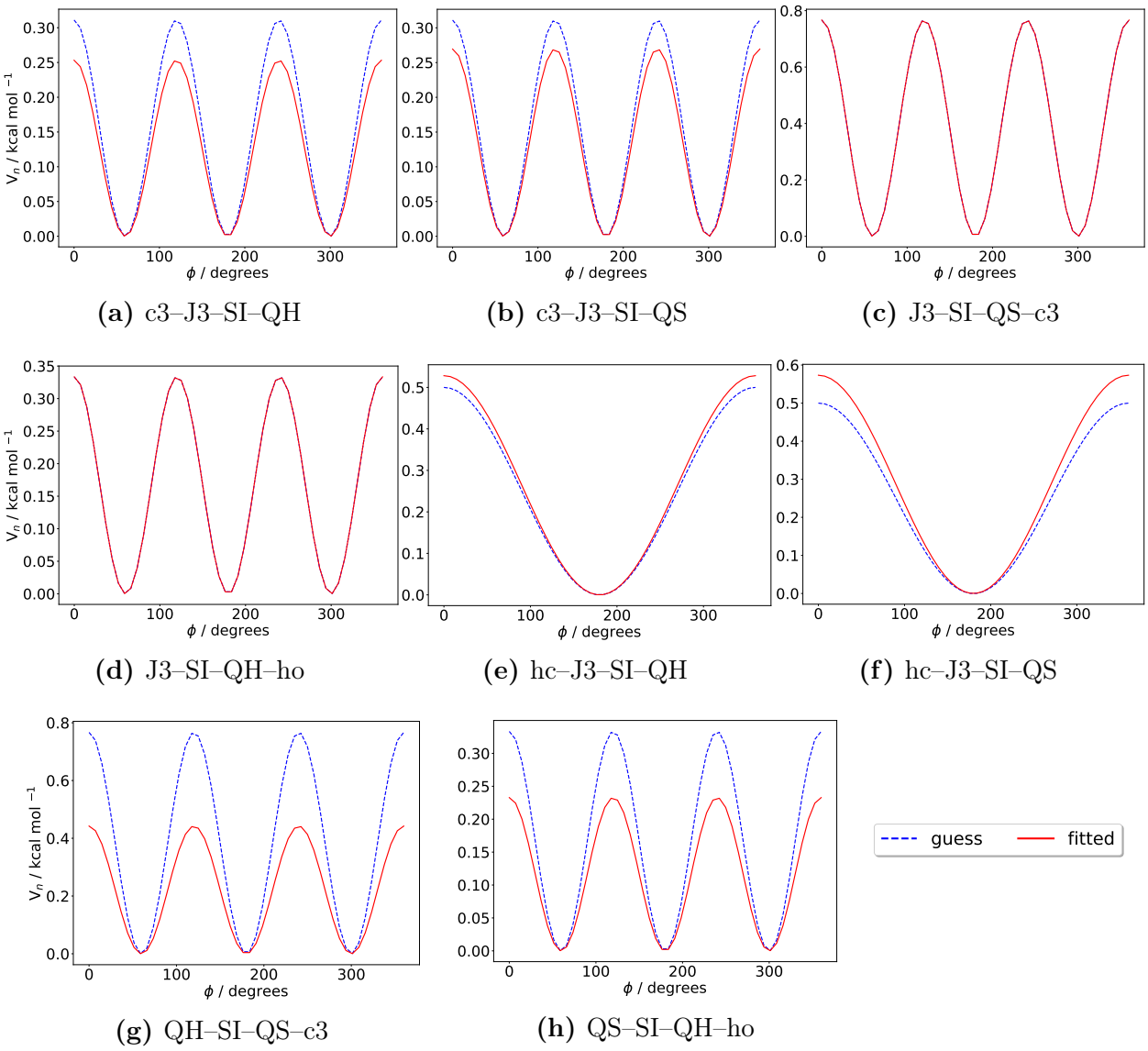


Figure S2: Geometry of 1,3-di-t-butoxy-1,3-dimethyldisiloxane-1,3-diol (crystallographic code YIBFEV),[S2] used as reference on benchmark procedure. Aliphatic hydrogens omitted for better visualization.

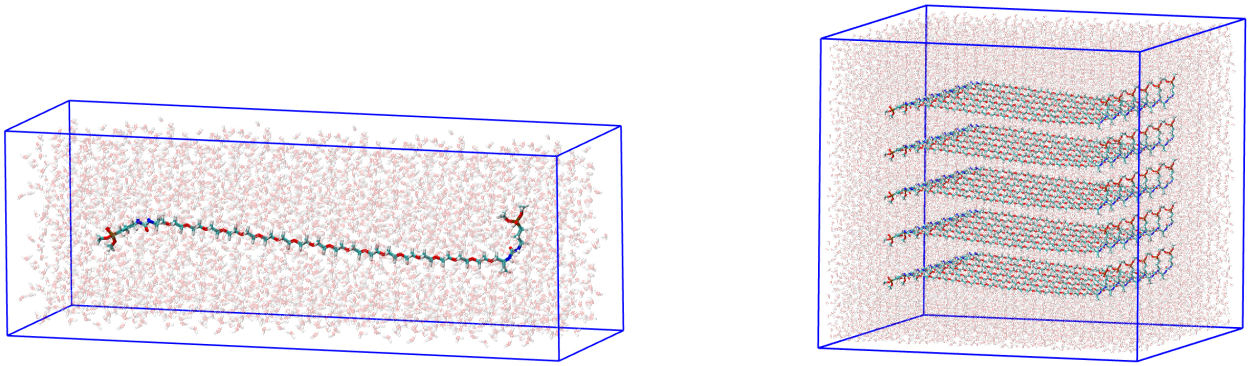


(a) c3–J3–SI–QH **(b)** c3–J3–SI–QS **(c)** J3–SI–QS–c3

(d) J3–SI–QH–ho **(e)** hc–J3–SI–QH **(f)** hc–J3–SI–QS

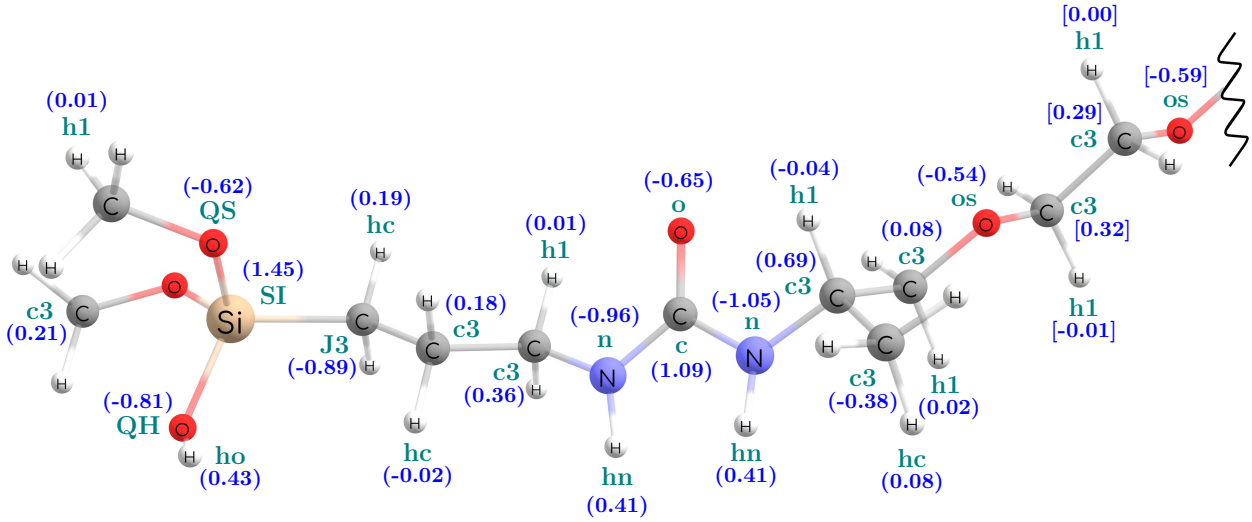
(g) QH–SI–QS–c3 **(h)** QS–SI–QH–ho

Figure S3: Torsional barrier for dihedral angles parameterized. Dashed blue lines refer to initial parameters (guess, GAFF torsional terms considering SI as c3 atom type) and continue red lines to fitted parameters.

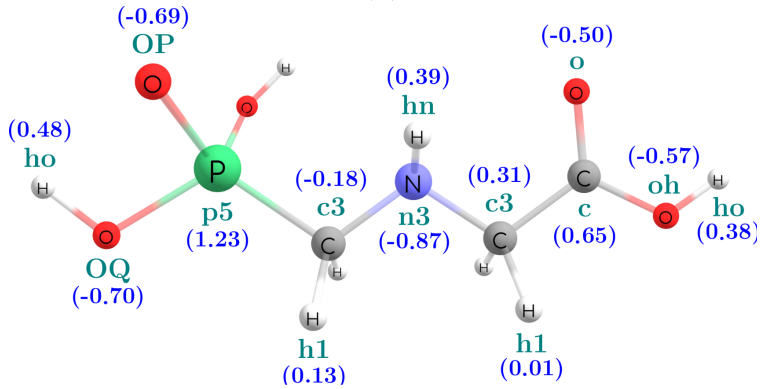


(a) 1 U-PEO : 3 298 WAT **(b)** 30 U-PEO : 40 035 WAT

Figure S4: Initial configuration of simulation boxes containing (a) 1 U-PEO [10 095 atoms, 144.1 nm^3] and (b) 30 U-PEO [126 135 atoms, 1543.6 nm^3] molecules, in aqueous media.



(a)



(b)

Figure S5: U-PEO (a) and GLY (b) geometries (net charge = 0), with atom types in teal and RESP charges in blue (absolute values in parentheses and average values in brackets). Repeated U-PEO portions were omitted for better visualization.

(a) 1 U-PEO (300 ns)

(b) 30 U-PEO (333 ns)

(c) 1 U-PEO : 10 GLY (300 ns)

(d) 10 U-PEO : 10 GLY (300 ns)

(e) 50 U-PEO : 10 GLY (410 ns)

(f) 100 U-PEO : 10 GLY (460 ns)

(g) 1 U-PEO : 10 $[GLY]^{2-}$(300 ns)

(h) 10 U-PEO : 10 $[GLY]^{2-}$(300 ns)

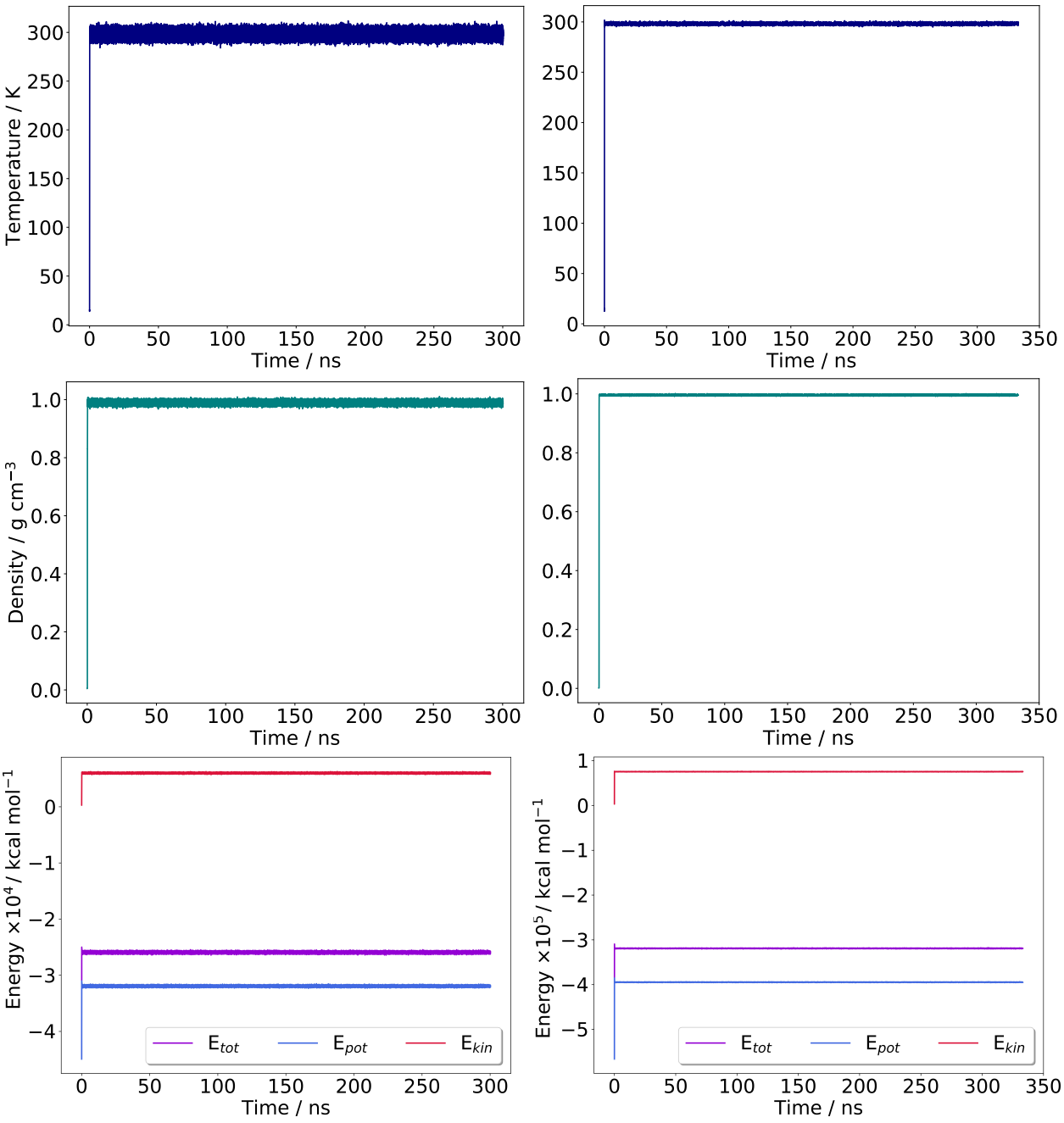
(i) 50 U-PEO : 10 $[GLY]^{2-}$(300 ns)

(j) 100 U-PEO : 10 $[GLY]^{2-}$(300 ns)

(k) 50 $[U\text{-}PEO]^{4+}$: 10 $[GLY]^{2-}$(300 ns)

(l) 100 $[U\text{-}PEO]^{4+}$: 10 $[GLY]^{-}$(300 ns)

Figure S6: QR codes with links embedded to all simulation movies.



(a) 1 U-PEO **(b)** 30 U-PEO

Figure S7: Plots of temperature (K), density (g cm^{-3}) and system energy (total in purple, kinetic in red, and potential in blue, kcal/mol) during simulations with (a) 1 and (b) 30 U-PEO in water.

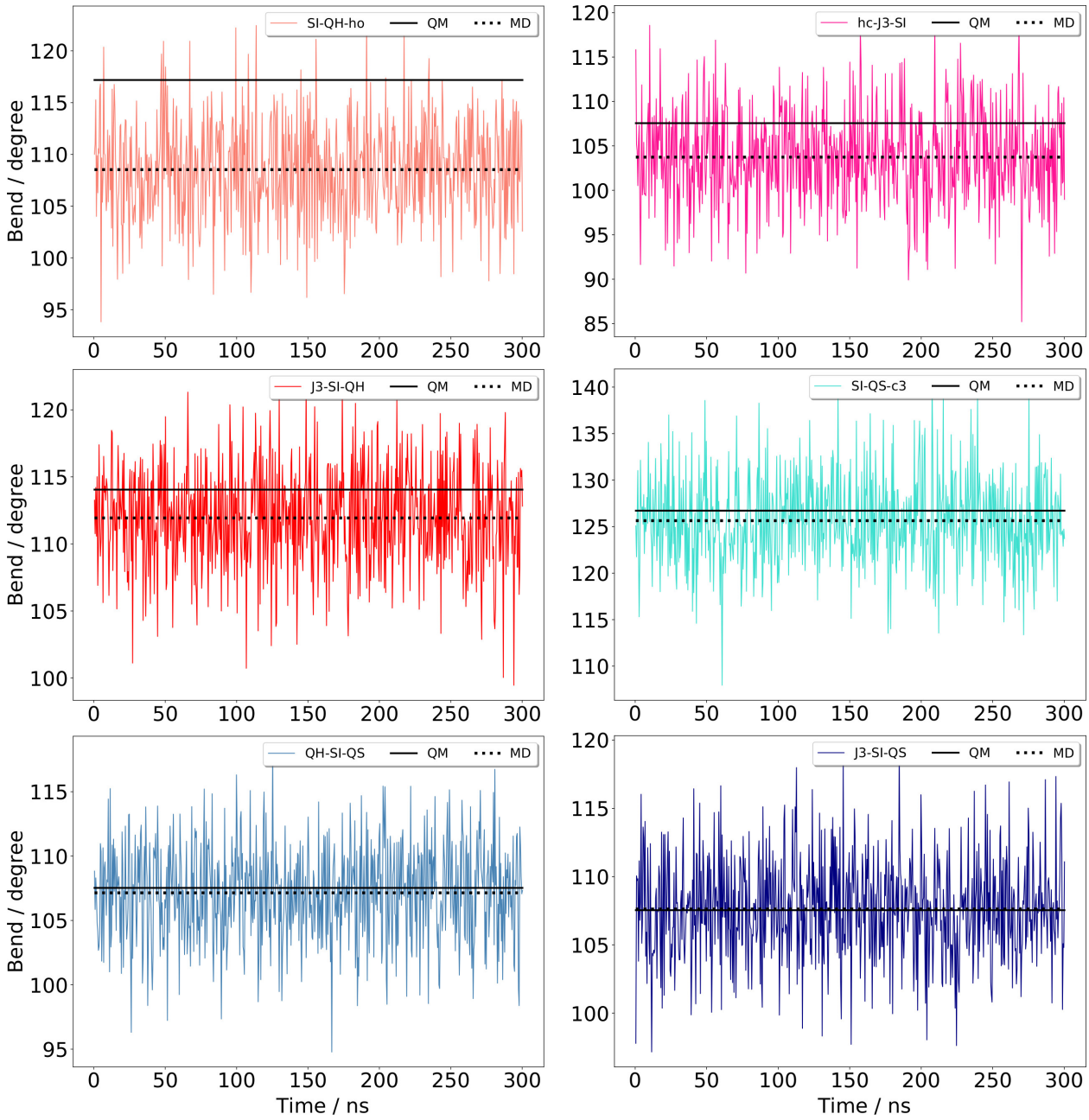


Figure S8: Examples of bond angle oscillations during simulation with 1 U-PEO molecule in water, for one edge of the polymer. Solid lines represent bond angle equilibrium value (θ_{eq}) stemming from QM calculations, and dashed lines to its average value during simulation ($\overline{\theta_{\mathrm{MD}}}$). Angle values in degree and time in ns.

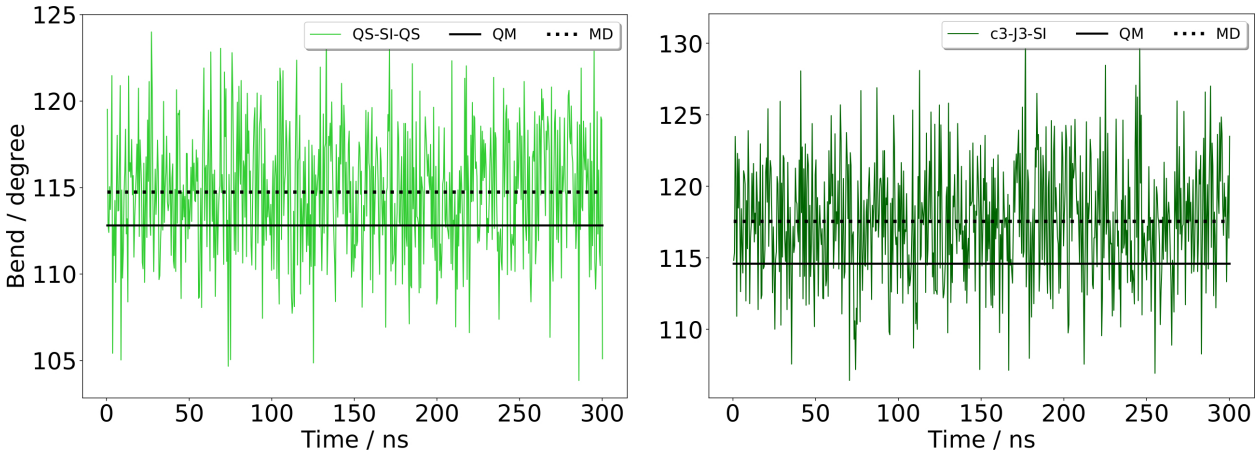
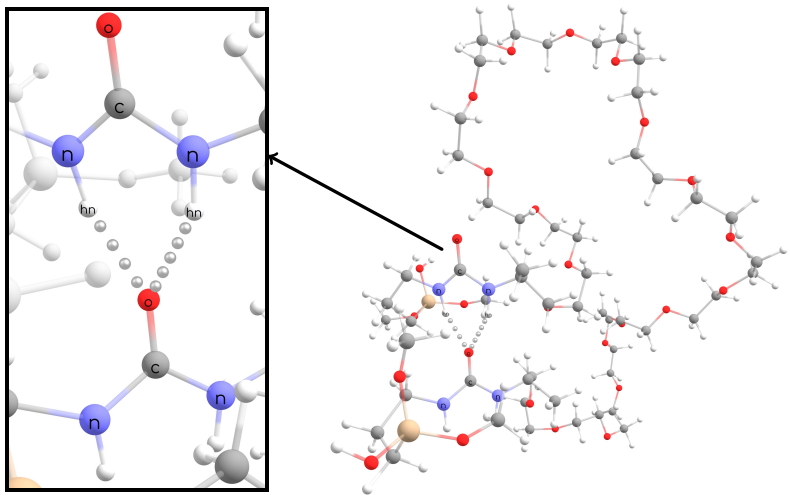
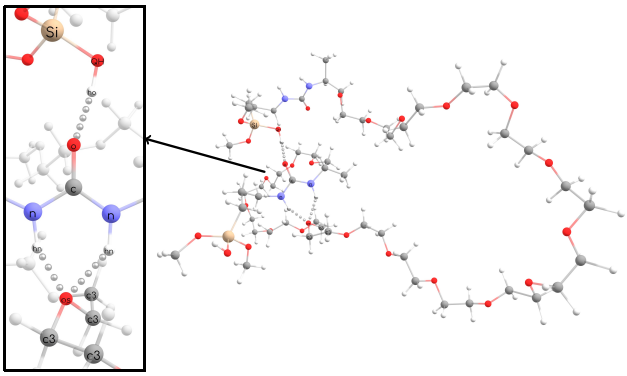


Figure S8: (continued) Examples of bond angle oscillations during simulation with 1 U-PEO molecule in water, for one edge of the polymer. Solid lines represent bond angle equilibrium value (θ_{eq}) from QM calculations, and dashed lines to its average value during simulation ($\overline{\theta_{\mathrm{MD}}}$). Angle values in degree and time in ns.



(a)



(b)

Figure S9: U-PEO intramolecular hydrogen bonds **o**$\cdots$**hn–n** (a), **o**$\cdots$**ho–QH** and **os**$\cdots$**hn–n** (b), observed during simulation with 1 U-PEO in water.

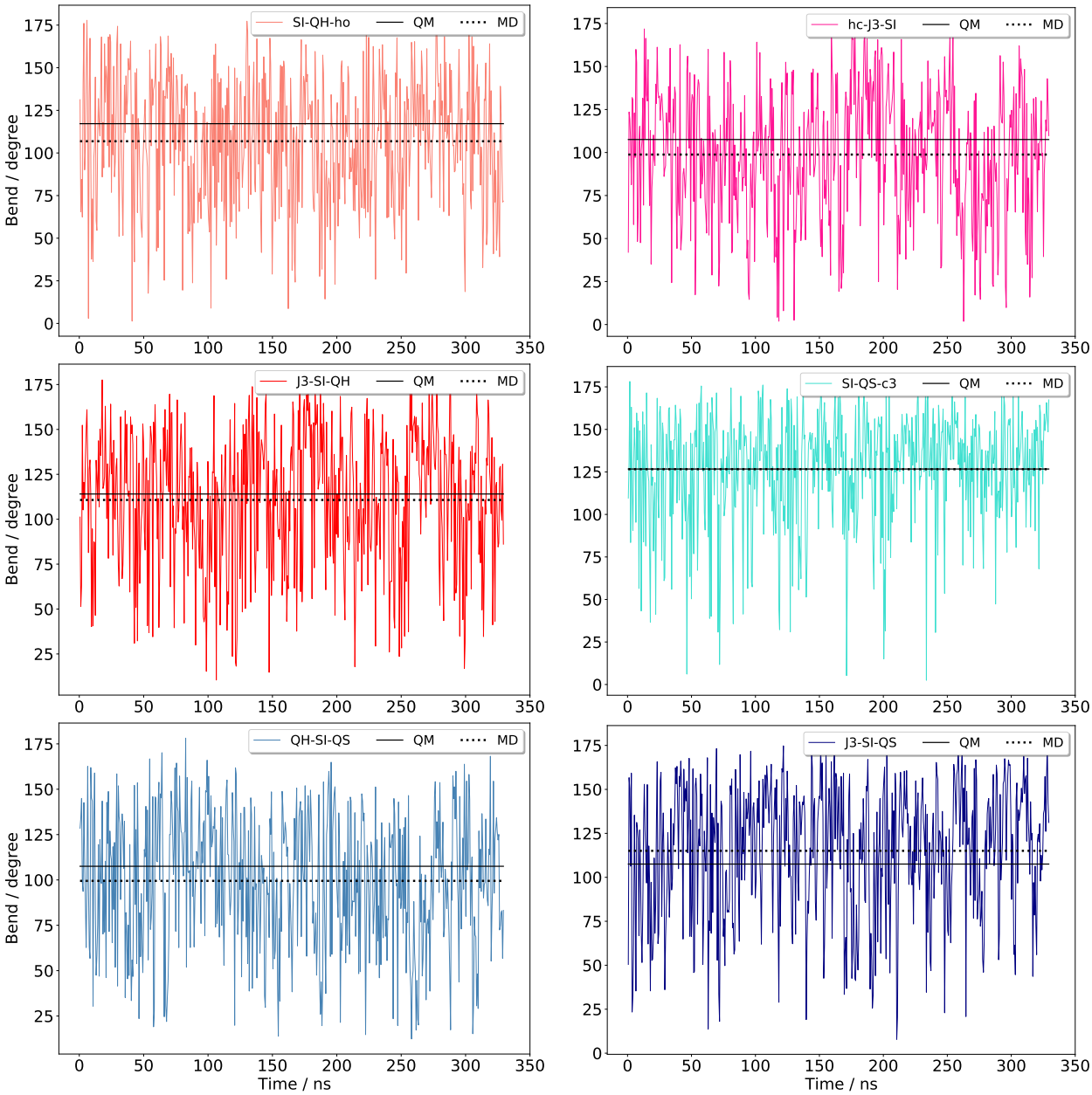


Figure S10: Examples of bond angle oscillations during simulation with 30 U-PEO molecules in water, for one edge of the polymer. Solid lines represent bond angle equilibrium value (θ_{eq}) from QM calculations, and dashed lines to its average value during simulation ($\overline{\theta_{\mathrm{MD}}}$). Angle values in degree and time in ns.

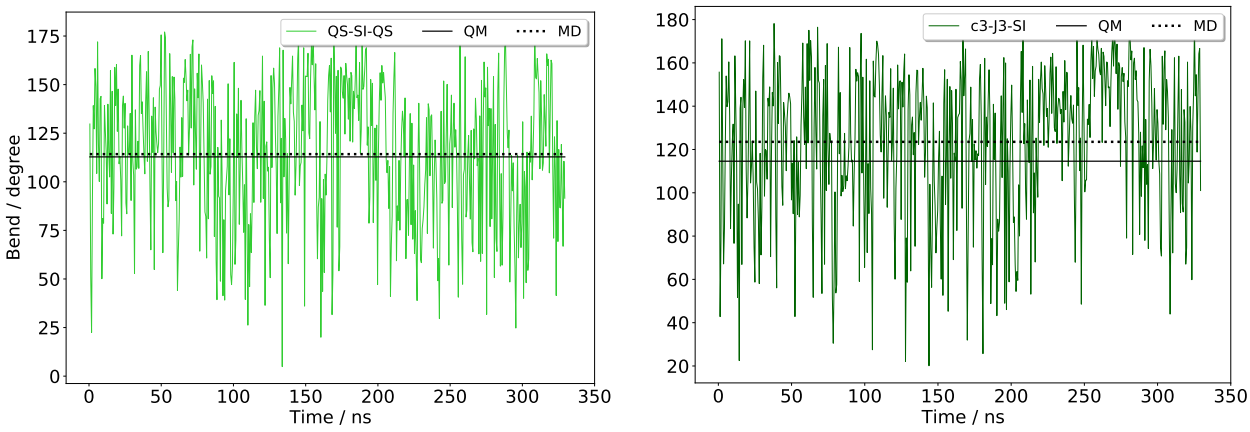
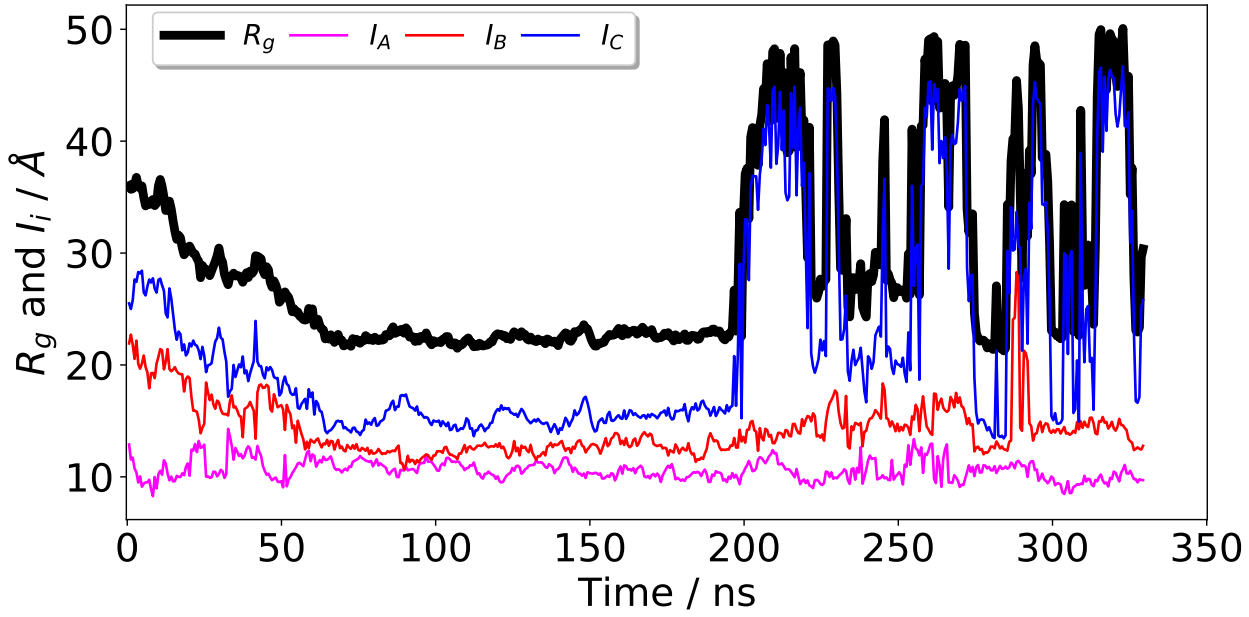
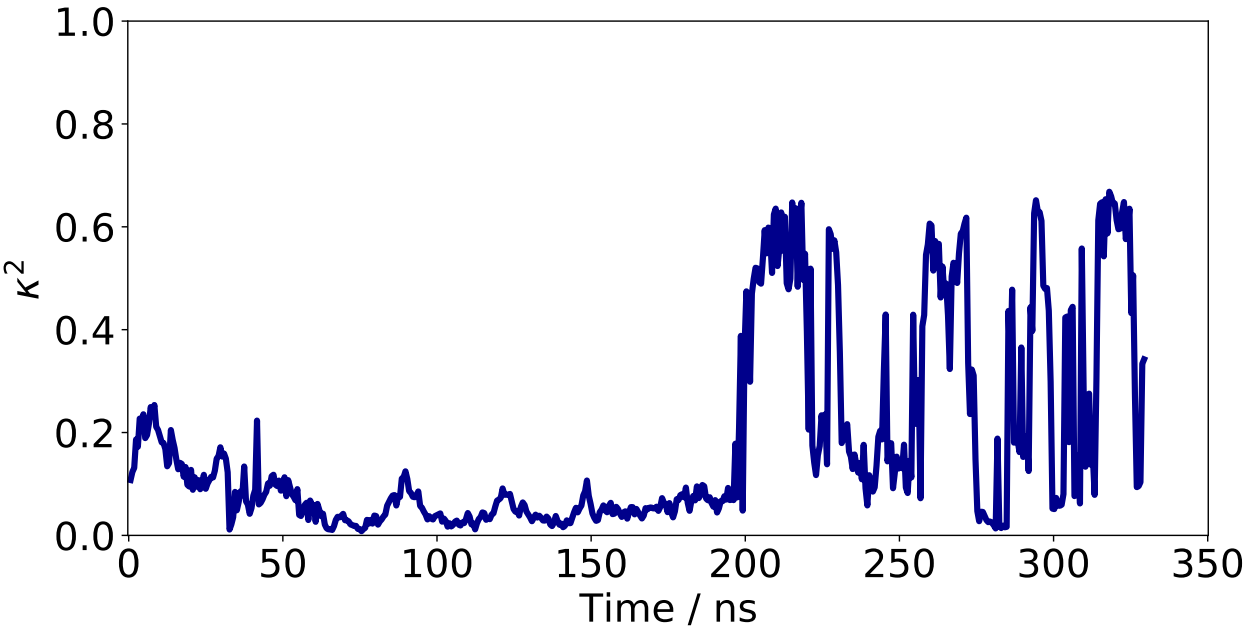


Figure S10: (continued) Examples of bond angle oscillations during simulation with 30 U-PEO molecules in water, for one edge of the polymer. Solid lines represent bond angle equilibrium value (θ_{eq}) from QM calculations, and dashed lines to its average value during simulation ($\overline{\theta_{\mathrm{MD}}}$). Angle values in degree and time in ns.

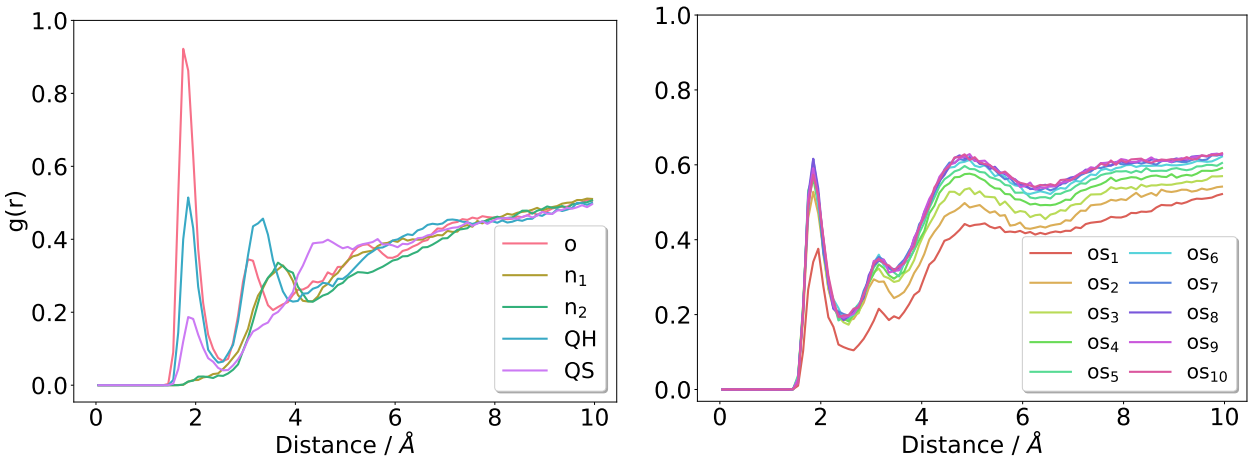


(a)



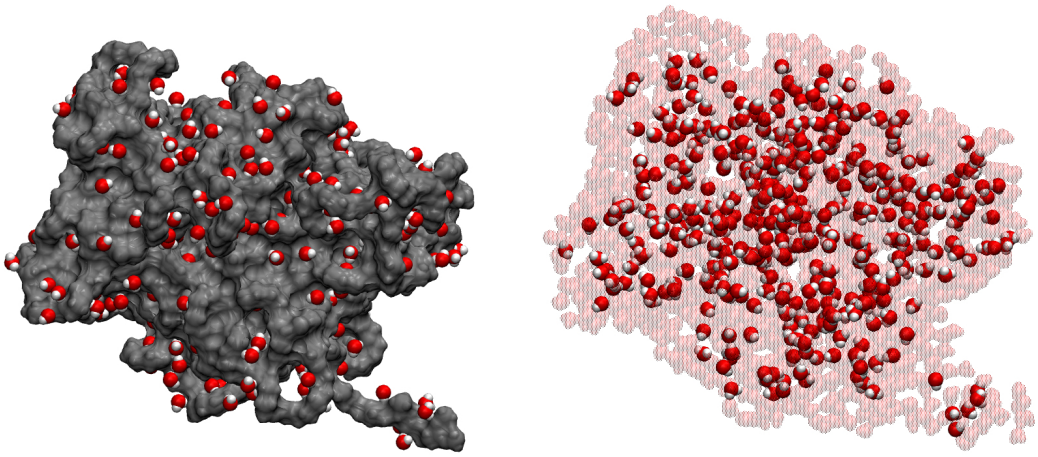
(b)

Figure S11: (a) Radius of Gyration (R_g) and principal moments of inertia (I_i, with i = A, B or C), and (b) Relative shape anisotropy (κ^2), during the simulation of 30 U-PEO molecules in water. Distance values expressed in Å and time in ns.



(a) **(b)**

Figure S12: Radial distribution function (g(r)) between the hydrogens of water and the atoms (a) of the ends and (b) of the monomeric units of U-PEO, throughout the simulation with 30 PEO in water (single representation of equivalent atoms, reported by their atom types). In (b), the increasing numbering of equal atomic types corresponds to an increasing distance from the Silicon atom. Distance values in Å.

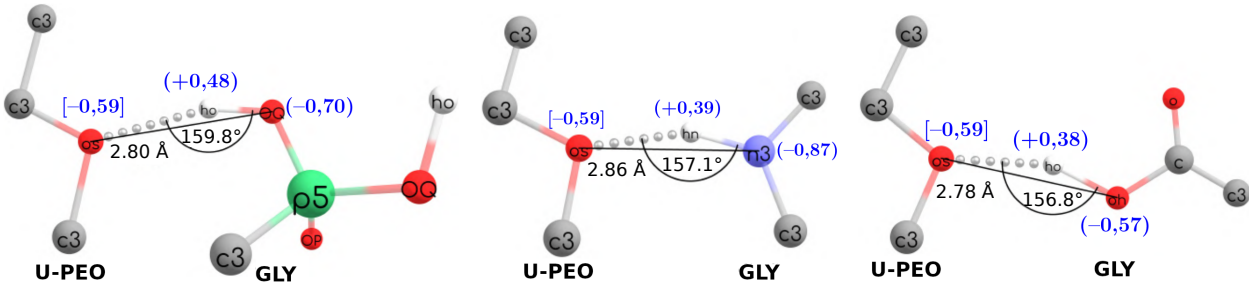


(a) **(b)**

Figure S13: Conformation of average RMSD and adsorbed water in the simulation with 30 U-PEO molecules. (a) Representation of the U-PEO surface, in gray, and first solvation sphere. (b) waters of the first (solid color) and second solvation sphere (transparent), omitting the polymer surface for better visualization.

Table S3: Intra and intermolecular Hydrogen bonds for simulations with 1 and 30 U-PEO molecules in water, at the final 200 ns simulated. Atom types for Hydrogen bond (HB) acceptor (A), donor (D) and Hydrogen (H) atoms, and number of occurrences (N_{HB}). Average distance between A–D ($\overline{d_{\text{A-D}}}$) and standard deviation (σ_d), average angle A–H–D ($\overline{A_{\text{A-H-D}}}$) and standard deviation (σ_A). Average lifetime ($\bar{t}$) and standard deviation (σ_t), maximum (t_{max}) and total lifetimes (t_{tot}, adding up all the occurrences). Distance values in Å, angles in degree and time in ns.

	1 U-PEO											
	A	H	D	N_{HB}	$\overline{d_{\text{A-D}}}$	σ_d	$\overline{A_{\text{A-H-D}}}$	σ_A	$\bar{t}$	σ_t	t_{max}	t_{tot}
U-PEO–U-PEO$_{intra}$	os	hn	n	109	2.890	0.060	155.35	9.20	0.65	0.28	2.29	50.00
	o	hn	n	46	2.882	0.036	158.58	1.29	1.30	0.48	3.67	21.10
	os	ho	QH	34	2.770	0.110	156.76	8.67	0.48	0.09	0.92	15.60
	o	ho	QH	27	2.756	0.061	165.03	3.87	0.50	0.05	0.92	12.39
	QS	hn	n	20	2.861	0.091	156.12	5.90	0.47	0.03	0.92	9.17
	QH	hn	n	9	2.875	0.078	157.66	11.35	0.48	0.05	0.92	4.13
	QS	ho	QH	3	2.842	0.00	163.44	5.90	0.46	0.00	0.46	1.38
	QH	ho	QH	2	2.719	0.00	172.37	11.35	0.46	0.00	0.46	0.92
	n	hn	n	1	2.941	0.00	140.90	5.90	0.46	0.00	0.46	0.46
	30 U-PEO											
	A	H	D	N_{HB}	$\overline{d_{\text{A-D}}}$	σ_d	$\overline{A_{\text{A-H-D}}}$	σ_A	$\bar{t}$	σ_t	t_{max}	t_{tot}
U-PEO–U-PEO$_{intra}$	os	hn	n	978	2.888	0.056	156.34	7.55	0.81	0.37	5.97	583.88
	o	ho	QH	571	2.727	0.075	163.07	5.21	1.55	1.71	9.55	340.89
	os	ho	QH	433	2.781	0.105	159.59	8.81	0.76	0.39	5.37	258.51
	QH	hn	n	339	2.883	0.052	155.67	7.48	0.85	0.48	6.57	202.39
	QS	hn	n	199	2.840	0.073	154.89	7.30	0.79	0.45	3.58	118.80
	o	hn	n	128	2.898	0.042	156.56	6.55	1.08	0.51	7.16	76.42
	QH	ho	QH	82	2.749	0.072	163.65	4.20	1.30	1.08	7.16	48.95
	n	ho	QH	41	2.873	0.089	157.41	11.13	0.67	0.18	1.19	24.48
	QS	ho	QH	24	2.754	0.068	159.74	8.97	0.74	0.25	1.79	14.33
U-PEO–U-PEO$_{inter}$	os	hn	n	3612	2.890	0.055	157.11	7.06	0.87	0.41	8.36	2156.40
	o	hn	n	3388	2.877	0.040	158.13	5.00	1.28	0.55	9.55	2022.67
	o	ho	QH	2586	2.729	0.083	163.82	6.13	1.84	2.26	9.55	1543.87
	os	ho	QH	1974	2.777	0.099	160.49	8.52	0.86	0.63	8.96	1178.50
	QH	ho	QH	1094	2.776	0.085	163.64	5.98	1.19	0.77	7.76	653.13
	QH	hn	n	1055	2.890	0.056	158.19	6.67	0.89	0.46	7.16	629.85
	QS	hn	n	520	2.866	0.072	156.98	8.76	0.78	0.38	3.58	310.45
	QS	ho	QH	299	2.804	0.104	159.44	9.25	0.74	0.47	5.37	178.51
	n	ho	QH	50	2.870	0.084	157.27	11.30	0.65	0.16	1.19	29.85
	n	hn	n	5	2.932	0.036	163.11	14.00	0.75	0.30	1.19	2.99



(a) **os···ho–OQ** (b) **os···hn–n3** (c) **os···ho–oh**

Figure S14: Simplified representation of the main hydrogen bonds between PEO–GLY, with mean distances between HB donor (D) and acceptor (A) atom, in Å, mean angle between D–H–A, in degrees, and RESP charges of such atoms in blue parentheses (in square brackets for average value). Average values considering all simulations 10 GLY : x U-PEO, where x = 1, 10, 50 and 100.

Table S4: Hydrogen bonds observed in the simulation with 10 GLY : x U-PEO (x = 1, 10, 50 or 100), at the final 200 ns simulated. Atom types for Hydrogen bond (HB) acceptor (A), donor (D) and Hydrogen (H) atoms, and number of occurrences (N_{HB}). Average distance between A–D ($\overline{d_{\text{A-D}}}$) and standard deviation (σ_d), average angle A–H–D ($\overline{A_{\text{A-H-D}}}$) and standard deviation (σ_A). Average lifetime ($\bar{t}$) and standard deviation (σ_t), maximum (t_{max}) and total lifetimes (t_{tot}, adding up all the occurrences). Distance values in Å, angles in degree and time in ns.

10 GLY : 1 U-PEO												
A···D	A	H	D	N_{HB}	$\overline{d_{\text{A-D}}}$	σ_d	$\overline{A_{\text{A-H-D}}}$	σ_A	$\bar{t}$	σ_t	t_{max}	t_{tot}
U-PEO···GLY	os	ho	oh	3	2.766	0.156	161.57	8.95	0.54	0.00	0.54	1.63
	os	hn	n3	2	2.809	0.009	152.28	6.61	0.54	0.00	0.54	1.09
	QS	ho	OQ	1	2.944	0.00	160.07	8.95	0.54	0.00	0.54	0.54
	QH	ho	OQ	1	2.853	0.00	172.46	8.95	0.54	0.00	0.54	0.54
	o	ho	OQ	1	2.821	0.00	158.84	6.29	0.54	0.00	0.54	0.54
	o	ho	oh	1	2.911	0.00	171.02	6.29	0.54	0.00	0.54	0.54
G···U	OP	ho	QH	1	2.705	0.00	148.68	3.33	0.54	0.00	0.54	0.54
	oh	ho	QH	1	2.862	0.00	166.17	3.33	0.54	0.00	0.54	0.54
	n3	ho	QH	1	2.931	0.00	174.53	3.33	0.54	0.00	0.54	0.54
10 GLY : 10 U-PEO												
A···D	A	H	D	N_{HB}	$\overline{d_{\text{A-D}}}$	σ_d	$\overline{A_{\text{A-H-D}}}$	σ_A	$\bar{t}$	σ_t	t_{max}	t_{tot}
U-PEO···GLY	os	ho	OQ	169	2.807	0.090	159.61	7.66	0.57	0.26	1.83	77.52
	os	ho	oh	123	2.767	0.097	154.44	8.77	0.54	0.16	2.29	56.42
	os	hn	n3	122	2.869	0.073	159.65	8.08	0.58	0.30	1.83	55.96
	o	ho	OQ	44	2.780	0.071	161.57	9.63	0.84	0.68	2.29	20.18
	QH	ho	OQ	24	2.801	0.104	161.87	8.44	0.56	0.20	1.83	11.01
	o	hn	n3	12	2.909	0.074	160.31	11.10	0.48	0.05	0.92	5.50
	QS	ho	OQ	7	2.863	0.090	162.18	9.36	0.46	0.00	0.46	3.21
	QH	ho	oh	7	2.838	0.129	162.41	7.56	0.46	0.00	0.46	3.21
	o	ho	oh	7	2.798	0.134	159.34	5.24	0.46	0.00	0.46	3.21
	QH	hn	n3	5	2.848	0.073	157.38	6.03	0.46	0.00	0.46	2.29
	QS	hn	n3	3	2.906	0.074	153.34	8.32	0.46	0.00	0.46	1.38
	QS	ho	oh	2	2.871	0.093	153.32	2.88	0.46	0.00	0.46	0.92
GLY···U-PEO	o	hn	n	42	2.924	0.042	157.71	7.20	0.65	0.30	2.29	19.27
	OP	ho	QH	35	2.804	0.077	160.83	6.74	0.72	0.70	3.21	16.05
	OP	hn	n	13	2.912	0.043	163.60	6.37	0.56	0.31	1.38	5.96
	o	ho	QH	9	2.753	0.077	162.04	8.56	0.54	0.19	0.92	4.13
	oh	ho	QH	7	2.840	0.097	163.53	7.67	0.54	0.19	0.92	3.21
	oh	hn	n	6	2.908	0.081	157.02	6.06	0.46	0.00	0.46	2.75
	n3	ho	QH	6	2.834	0.019	158.33	1.70	0.69	0.23	0.92	2.75
	OQ	ho	QH	2	2.904	0.057	154.64	19.24	0.46	0.00	0.46	0.92
	OQ	hn	n	2	2.893	0.013	155.85	21.05	0.46	0.00	0.46	0.92
	n3	hn	n	1	2.992	0.00	159.23	7.90	0.46	0.00	0.46	0.46

Table S4: (Continued) Hydrogen bonds observed in the simulation with 10 GLY : x U-PEO (x = 1, 10, 50 or 100), at the final 200 ns simulated. Atom types for Hydrogen bond (HB) acceptor (A), donor (D) and Hydrogen (H) atoms, and number of occurrences (N_{HB}). Average distance between A–D ($\overline{d_{\text{A-D}}}$) and standard deviation (σ_d), average angle A–H–D ($\overline{A_{\text{A-H-D}}}$) and standard deviation (σ_A). Average lifetime ($\bar{t}$) and standard deviation (σ_t), maximum (t_{max}) and total lifetimes (t_{tot}, adding up all the occurrences). Distance values in Å, angles in degree and time in ns.

10 GLY : 50 U-PEO												
A$\cdots$D	A	H	D	N_{HB}	$\overline{d_{\text{A-D}}}$	σ_d	$\overline{A_{\text{A-H-D}}}$	σ_A	$\bar{t}$	σ_t	t_{max}	t_{tot}
U-PEO$\cdots$GLY	os	ho	OQ	1189	2.803	0.086	159.90	8.70	0.68	0.61	9.13	542.92
	os	hn	n3	769	2.885	0.059	157.79	9.01	0.63	0.31	5.94	351.14
	os	ho	oh	752	2.778	0.090	154.95	8.42	0.61	0.27	4.57	343.38
	o	ho	OQ	556	2.771	0.087	162.45	7.44	1.21	1.64	8.22	253.88
	QH	ho	OQ	287	2.815	0.078	161.59	7.64	0.87	0.83	9.13	131.05
	o	hn	n3	134	2.860	0.057	156.82	8.27	0.73	0.46	3.65	61.19
	o	ho	oh	99	2.709	0.083	160.85	7.87	0.85	0.54	3.20	45.21
	QS	ho	OQ	61	2.843	0.093	162.04	9.27	0.57	0.22	3.20	27.85
	QH	ho	oh	53	2.816	0.082	157.42	7.77	0.96	1.54	7.31	24.20
	QS	ho	oh	34	2.838	0.089	152.17	12.65	0.65	0.50	4.57	15.53
	QS	hn	n3	28	2.886	0.072	156.73	7.69	0.58	0.30	1.83	12.79
	QH	hn	n3	28	2.891	0.060	154.77	8.12	0.55	0.25	1.37	12.79
	n	ho	oh	7	2.902	0.055	153.99	6.22	0.51	0.11	0.91	3.20
	n	hn	n3	3	2.943	0.00	157.42	8.30	0.46	0.00	0.46	1.37
	n	ho	OQ	2	2.913	0.055	160.35	17.02	0.46	0.00	0.46	0.91
GLY$\cdots$U-PEO	OP	hn	n	559	2.897	0.044	158.56	3.05	0.87	0.38	4.11	255.25
	OP	ho	QH	120	2.814	0.072	162.50	8.50	0.88	0.93	5.48	54.79
	n3	ho	QH	120	2.802	0.063	158.49	7.29	0.95	0.47	6.85	54.79
	o	ho	QH	100	2.787	0.093	160.40	10.08	0.59	0.36	7.76	45.66
	o	hn	n	99	2.903	0.051	157.94	5.65	0.63	0.21	2.28	45.21
	n3	hn	n	63	2.922	0.038	161.22	3.83	0.59	0.17	1.83	28.77
	OQ	ho	QH	26	2.874	0.068	157.82	9.13	0.51	0.17	1.83	11.87
	oh	hn	n	25	2.890	0.055	157.57	9.30	0.50	0.07	1.37	11.42
	OQ	hn	n	21	2.925	0.043	156.87	11.71	0.47	0.03	0.91	9.59
	oh	ho	QH	21	2.868	0.087	155.21	12.02	0.58	0.20	1.83	9.59

Table S4: (Continued) Hydrogen bonds observed in the simulation with 10 GLY : x U-PEO (x = 1, 10, 50 or 100), at the final 200 ns simulated. Atom types for Hydrogen bond (HB) acceptor (A), donor (D) and Hydrogen (H) atoms, and number of occurrences (N_{HB}). Average distance between A–D ($\overline{d_{\text{A-D}}}$) and standard deviation (σ_d), average angle A–H–D ($\overline{A_{\text{A-H-D}}}$) and standard deviation (σ_A). Average lifetime ($\bar{t}$) and standard deviation (σ_t), maximum (t_{max}) and total lifetimes (t_{tot}, adding up all the occurrences). Distance values in Å, angles in degree and time in ns.

10 GLY : 100 U-PEO												
A···D	A	H	D	N_{HB}	$\overline{d_{\text{A-D}}}$	σ_d	$\overline{A_{\text{A-H-D}}}$	σ_A	$\bar{t}$	σ_t	t_{max}	t_{tot}
U-PEO···GLY	os	ho	OQ	1121	2.800	0.092	159.98	8.98	0.66	0.45	5.98	515.40
	os	ho	oh	762	2.796	0.088	156.04	8.11	0.64	0.31	5.52	350.34
	os	hn	n3	672	2.874	0.066	158.51	8.35	0.62	0.22	4.14	308.97
	o	ho	OQ	266	2.738	0.096	164.20	7.20	1.05	1.26	5.98	122.30
	QH	ho	OQ	87	2.798	0.092	163.95	6.94	0.72	0.64	4.14	40.00
	o	hn	n3	63	2.856	0.072	157.18	8.52	0.72	0.44	2.30	28.97
	o	ho	oh	48	2.733	0.072	158.87	10.29	0.76	0.65	3.22	22.07
	QS	hn	n3	41	2.885	0.079	159.53	8.97	0.56	0.24	2.30	18.85
	QH	ho	oh	35	2.763	0.089	161.43	7.30	0.66	0.50	4.14	16.09
	QS	ho	OQ	27	2.832	0.084	161.76	7.37	0.50	0.14	0.92	12.41
	QH	hn	n3	23	2.910	0.046	158.40	10.42	0.48	0.05	0.92	10.57
	QS	ho	oh	6	2.860	0.097	151.07	13.43	0.46	0.00	0.46	2.76
	n	ho	oh	6	2.855	0.135	152.42	4.45	0.46	0.00	0.46	2.76
	n	ho	OQ	3	2.925	0.020	158.20	3.36	0.46	0.00	0.46	1.38
	n	hn	n3	2	2.921	0.028	158.33	1.93	0.46	0.00	0.46	0.92
GLY···U-PEO	o	hn	n	235	2.886	0.044	158.36	5.82	0.63	0.22	3.22	108.05
	OP	hn	n	166	2.907	0.047	158.44	5.27	0.63	0.18	1.84	76.32
	OP	ho	QH	130	2.803	0.079	163.23	8.05	0.85	0.89	8.74	59.77
	o	ho	QH	104	2.776	0.096	163.12	5.38	0.66	0.36	4.60	47.82
	n3	ho	QH	96	2.820	0.086	159.50	8.28	1.02	0.70	5.52	44.14
	n3	hn	n	71	2.927	0.054	160.88	6.82	0.54	0.14	2.30	32.64
	oh	hn	n	37	2.887	0.089	155.86	6.78	0.51	0.13	1.84	17.01
	oh	ho	QH	29	2.793	0.103	158.85	10.53	0.51	0.19	2.30	13.33
	OQ	hn	n	11	2.953	0.045	165.48	6.19	0.51	0.15	0.92	5.06
	OQ	ho	QH	9	2.876	0.128	169.37	4.11	0.48	0.05	0.92	4.14

References

(S1) Hopfinger, A. J.; Pearlstein, R. A. Molecular mechanics force-field parameterization procedures. *Journal of Computational Chemistry* **1984**, *5*, 486–499.

(S2) ichi Suyama, K.; Nakatsuka, T.; Gunji, T.; Abe, Y. Synthesis and crystal structure of disiloxane-1, 3-diols and disiloxane-1, 1, 3, 3-tetraol. *Journal of Organometallic Chemistry* **2007**, *692*, 2028–2035.