Supplementary Data

This supplementary data is a part of paper entitled "Computational Evaluation of Intermolecular Interaction in Poly(Styrene-Maleic Acid)-Water Complexes Using Density Functional Theory".

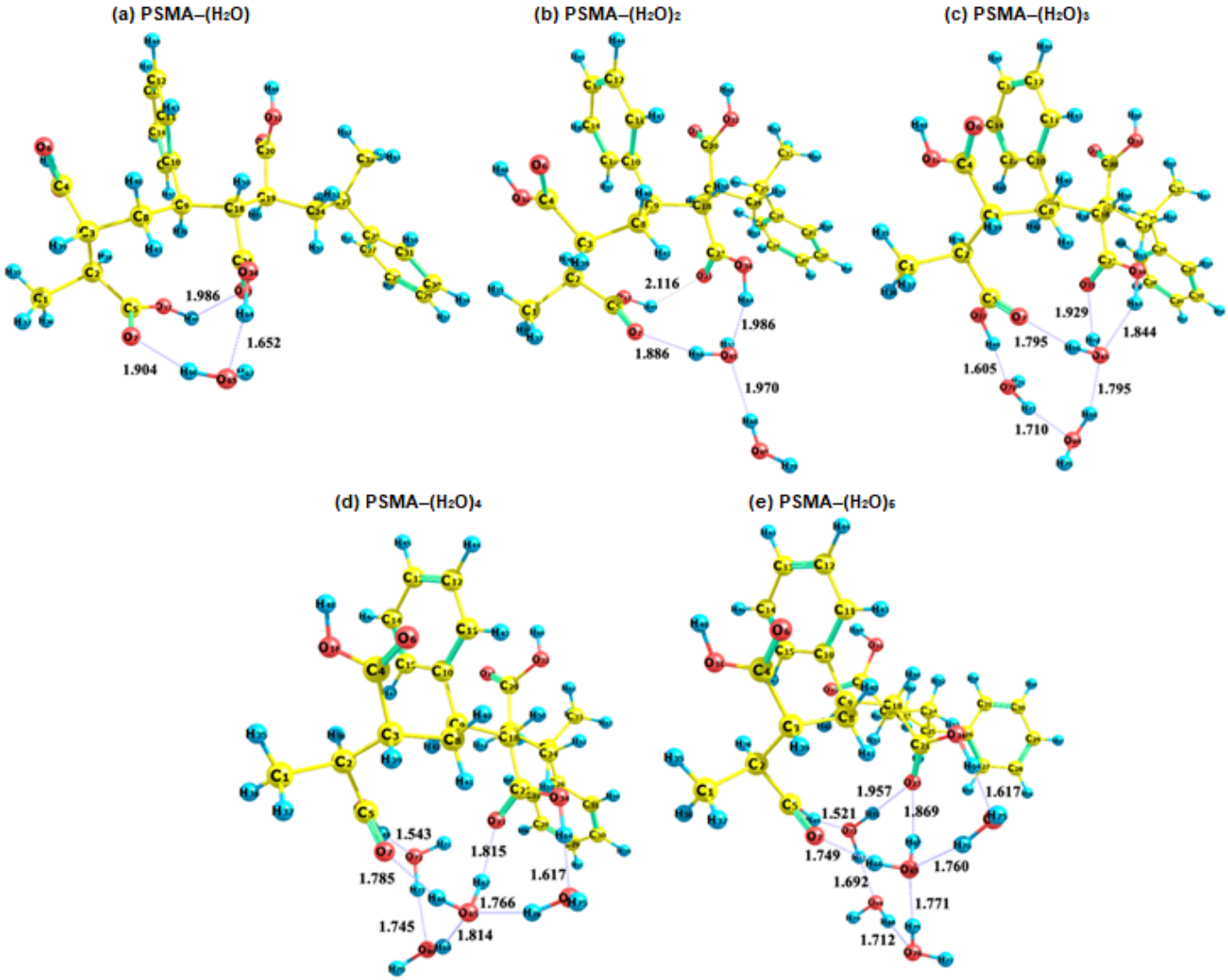

Fig S1. Optimized structures of PSMA–$(H_2O)_n$ complexes; n = 1–5

Table S1. Comparison of $E_{opt_{PSMA\cdots(H_2O)_1}}$ with DFT, HF, and MP2 methods

Method	Energy (kcal/mol)
DFT	–1058789.36
HF	–1052424.16
MP2	–1055764.52

Table S2. NBO analysis of PSMA–$(H_2O)_n$ complexes

Donor (i)	Acceptor (j)	$E^{(2)}$ (kcal/mol)	$E_{(i)} - E_{(j)}$ (a.u)	$F_{(i,j)}$ (a.u.)
PSMA–H_2O				
LP (1) O7	BD*(1) O65-H66	6.90	1.04	0.076
LP (2) O7	BD*(1) O65-H66	5.16	0.75	0.056
LP (2) O65	BD*(1) O34-H64	34.00	0.79	0.146
PSMA–$(H_2O)_2$				
LP (1) O7	BD*(1) O65-H66	7.87	1.03	0.080
LP (2) O7	BD*(1) O65-H66	6.43	0.75	0.062
LP (2) O65	BD*(1) O34-H64	24.38	0.76	0.122
LP (1) O65	BD*(1) H68-O69	7.77	1.05	0.081
PSMA–$(H_2O)_3$				
LP (1) O7	BD*(1) O65-H66	9.28	1.01	0.086
LP (2) O7	BD*(1) O65-H66	9.41	0.73	0.074
LP (1) O65	BD*(1) O34-H64	4.97	0.95	0.061
LP (2) O65	BD*(1) O34-H64	12.17	0.73	0.084
LP (2) O16	BD*(1) H47-O48	6.43	0.79	0.063
LP (1) O65	BD*(1) H68-O69	6.50	1.00	0.072
LP (2) O65	BD*(1) H68-O69	14.15	0.79	0.094
LP (1) O23	BD*(1) O65-H67	3.66	1.01	0.054
LP (2) O23	BD*(1) O65-H67	8.52	0.72	0.070
LP (2) O69	BD*(1) O72-H73	27.52	0.87	0.138
LP (2) O72	BD*(1) O17-H49	39.50	0.89	0.168
PSMA–$(H_2O)_4$				
LP (1) O7	BD*(1) O65-H66	10.77	1.02	0.094
LP (2) O7	BD*(1) O65-H66	8.75	0.74	0.072
LP (1) O23	BD*(1) O65-H67	8.22	1.03	0.082
LP (2) O23	BD*(1) O65-H67	9.12	0.75	0.074
LP (1) O23	BD*(1) H71-O72	4.38	1.06	0.061
PSMA–$(H_2O)_5$				
LP (1) O7	BD*(1) O65-H66	11.74	1.02	0.098
LP (2) O7	BD*(1) O65-H66	9.95	0.75	0.077
LP (1) O23	BD*(1) O65-H67	8.05	1.04	0.082
LP (2) O23	BD*(1) O65-H67	4.79	0.75	0.054
LP (1) O23	BD*(1) H71-O72	6.86	1.08	0.077
LP (2) O23	BD*(1) H71-O72	2.80	0.79	0.042
LP (1) O65	BD*(1) O74-H76	8.15	0.99	0.080
LP (2) O65	BD*(1) O74-H76	14.21	0.78	0.094
LP (1) O65	BD*(1) O78-H79	12.64	1.01	0.101
LP (2) O65	BD*(1) O78-H79	9.36	0.80	0.077
LP (2) O69	BD*(1) O72-H73	29.89	0.89	0.146
LP (2) O72	BD*(1) O17-H49	50.32	0.86	0.186
LP (2) O74	BD*(1) O34-H64	39.06	0.83	0.161

Table S3. QTAIM analysis of PSMA-water complexes

CP	BCP	$\rho_{(BCP)}$	$\nabla^2_{(BCP)}$	$G_{(BCP)}$	$H_{(BCP)}$	$V_{(BCP)}$	$\lvert V/G \rvert$	λ_1	λ_2	λ_3	$\varepsilon_{(BCP)}$	E_{HB}
PSMA–$(H_2O)_1$												
101	O7···H66	0.0252	0.0738	0.0187	-0.0002	-0.0189	1.0126	-0.0102	0.0708	0.0131	0.006252	-4.8890
120	O65···H64	0.0523	0.1366	0.0375	-0.0033	-0.0408	1.0884	0.2718	-0.0897	-0.0455	0.0319	-10.9296
PSMA–$(H_2O)_2$												
101	O23···H67	0.0138	0.0509	0.0118	0.0009	-0.0109	0.9223	0.0657	-0.0121	-0.0026	0.6129	-2.3407
110	O65···H68	0.0255	0.0674	0.0183	-0.0014	-0.0197	1.0770	0.1219	-0.0218	-0.0327	0.0156	-4.9535
114	O65···H64	0.0425	0.1146	0.0302	-0.0015	-0.0317	1.0497	0.1877	-0.0667	-0.0063	0.0312	-8.7310
130	O7···H66	0.0277	0.0815	0.0204	0.0000	-0.0205	1.0023	-0.0095	0.0890	0.0019	0.0099	-5.4324
PSMA–$(H_2O)_3$												
107	O23···H67	0.0293	0.0833	0.0221	-0.0013	-0.0233	1.0569	0.1305	-0.0333	-0.0139	0.0553	-5.7857
117	O65···H64	0.0343	0.0921	0.0244	-0.0014	-0.0257	1.0558	0.1368	-0.0388	-0.0059	0.0491	-6.9053
121	O7···H66	0.0377	0.1052	0.0275	-0.0012	-0.0287	1.0431	0.1927	-0.0545	-0.0331	0.0492	-7.6689
122	O69···H73	0.0455	0.1269	0.0332	-0.0015	-0.0347	1.0442	0.0136	-0.0395	0.1529	0.0307	-9.4090
130	O72···H49	0.0563	0.1543	0.0422	-0.0036	-0.0459	1.0862	0.2069	0.0471	-0.0997	0.0592	-11.8146
143	O7···H66	0.0348	0.1031	0.0258	0.0000	-0.0258	0.9998	-0.0134	0.1353	-0.0187	0.0261	-7.0111
PSMA–$(H_2O)_4$												
116	O7···H66	0.0348	0.1065	0.0262	0.0004	-0.0258	0.9846	-0.0076	0.1210	-0.0069	0.0226	-7.0289
126	O74···H64	0.0567	0.1458	0.0410	-0.0046	-0.0456	1.1110	0.3177	-0.1024	-0.0695	0.0447	-11.9100
129	O65···H76	0.0398	0.1129	0.0293	-0.0011	-0.0304	1.0371	-0.0486	-0.0544	0.2159	0.0435	-8.1279
136	O72···H49	0.0679	0.1615	0.0504	-0.0100	-0.0604	1.1988	-0.1114	0.4075	-0.1345	0.0340	-14.3956
139	O23···H67	0.0340	0.1001	0.0253	-0.0003	-0.0256	1.0119	0.1891	-0.0417	-0.0473	0.0090	-6.8437
142	O65···H68	0.0366	0.1008	0.0266	-0.0014	-0.0280	1.0522	0.0101	0.0031	0.0876	0.0493	-7.4139
143	O23···H71	0.0166	0.0540	0.0134	0.0001	-0.0132	0.9897	-0.0017	-0.0178	0.0735	0.0515	-2.9510
152	O69···H73	0.0423	0.1166	0.0305	-0.0014	-0.0319	1.0446	0.2035	-0.0516	-0.0353	0.0453	-8.6862
PSMA–$(H_2O)_5$												
118	O7···H66	0.0375	0.1161	0.0284	0.0006	-0.0278	0.9789	-0.0107	0.1341	-0.0073	-0.0107	-7.6309
130	O74···H64	0.0566	0.1464	0.0411	-0.0045	-0.0456	1.1090	0.2921	-0.0942	-0.0515	0.2921	-11.8894
131	O65···H76	0.0404	0.1138	0.0296	-0.0011	-0.0307	1.0378	-0.0310	-0.0586	0.2035	-0.0310	-8.2763
138	O72···H49	0.0703	0.1663	0.0531	-0.0116	-0.0647	1.2174	-0.1214	0.4307	-0.1429	-0.1214	-14.9458
144	O23···H67	0.0297	0.0885	0.0225	-0.0003	-0.0228	1.0150	0.1541	-0.0275	-0.0382	0.1541	-5.8784
145	O65···H79	0.0391	0.1105	0.0285	-0.0009	-0.0293	1.0301	0.1476	-0.0158	-0.0213	0.1476	-7.9731
148	O23···H71	0.0237	0.0738	0.0186	-0.0001	-0.0187	1.0077	-0.0038	-0.0297	0.1073	-0.0038	-4.5467
159	O69···H73	0.0471	0.1324	0.0345	-0.0014	-0.0359	1.0405	0.2032	0.0043	-0.0751	0.2032	-9.7638
160	O78···H68	0.0454	0.1278	0.0334	-0.0014	-0.0348	1.0432	0.0041	-0.0434	0.1672	0.0041	-9.3957

CP: critical point; BCP: Bond critical point); ρ : Electron density (a.u.); $\nabla^2\rho$: Laplacian of electron density (a.u); G: Lagrangian kinetic energy (a.u); H: Hamiltonian kinetic energy or electronic energy density (a.u); V: Potential energy density (a.u.); ε: Ellipticity of electron density (a.u); λ_1, λ_2, λ_3 : Components of Laplacian in x/y/z (a.u.); E_{HB}: Hydrogen bond energy (kcal/mol)

Table S4. Comparison of reported hydrogen bond energy

Siahaan [1]				Safia [2]				Bo Wang [3]		
Method	Functional	BCP	E_{HB}	Method	Functional	Interaction	E_{HB}	Method	Molecules	E_{HB}
		Chi-Cre				Orientation 1		DFT	Dimer H_2O	–4.76
		16	–8.3565			O151···H136	–0.998	HF		–3.60
		19	–0.8238			O150···H130	–2.225			
		27	–5.2382	DFT	WB97XD	O149···H137	–1.533			
		51	–8.0788							
DFT-D3	B3LYP					Orientation 2				
		Chi-Urea				O151···H118	–0.217			
		86	–0.7816			O149···H125	–0.373			
		91	–4.2357							
		110	–1.5222							
		119	–0.8928							

Chi: Chitosan, Cre: Creatinine, BCP: Bond critical point, and E_{HB}: Hydrogen bond energy (kcal/mol)

References of supporting information

[1] Siahaan, P., Sasongko, N.A., Lusiana, R.A., Prasasty, V.D., and Martoprawiro, M.A., 2021, The validation of molecular interaction among dimer chitosan with urea and creatinine using density functional theory: In application for hemodyalisis membrane, *Int. J. Biol. Macromol.*, 168, 339–349.

[2] Safia, H., Ismahan, L., Abdelkrim, G., Mouna, C., Leila, N., and Fatiha, M., 2019, Density functional theories study of the interactions between host β-cyclodextrin and guest 8-anilinonaphthalene-1-sulfonate: Molecular structure, HOMO, LUMO, NBO, QTAIM and NMR analyses, *J. Mol. Liq.*, 280, 218–229.

[3] Wang, B., Jiang, W., Dai, X., Gao, Y., Wang, Z., and Zhang, R.Q., 2016, Molecular orbital analysis of the hydrogen bonded water dimer, *Sci. Rep.*, 6 (1), 22099.