Electronic Supplementary Information (ESI)

Impact of the chemical structure on the distribution of neuroprotective *N*-alkyl-9*H*-carbazoles at octanol/water Interfaces

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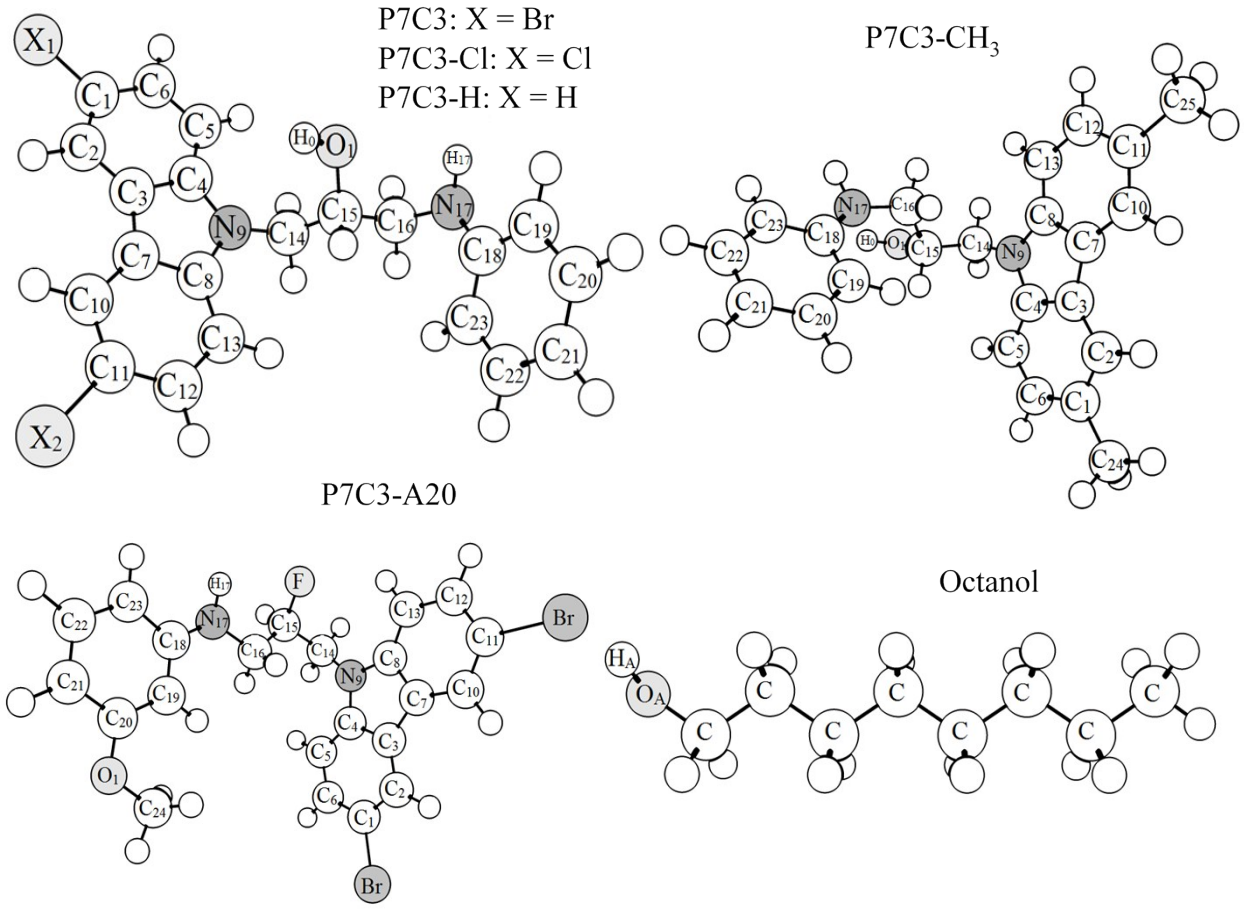

Fig. S1. *Ab initio* calculated optimised molecular structures and labelling of P7C3 derivatives and octanol.

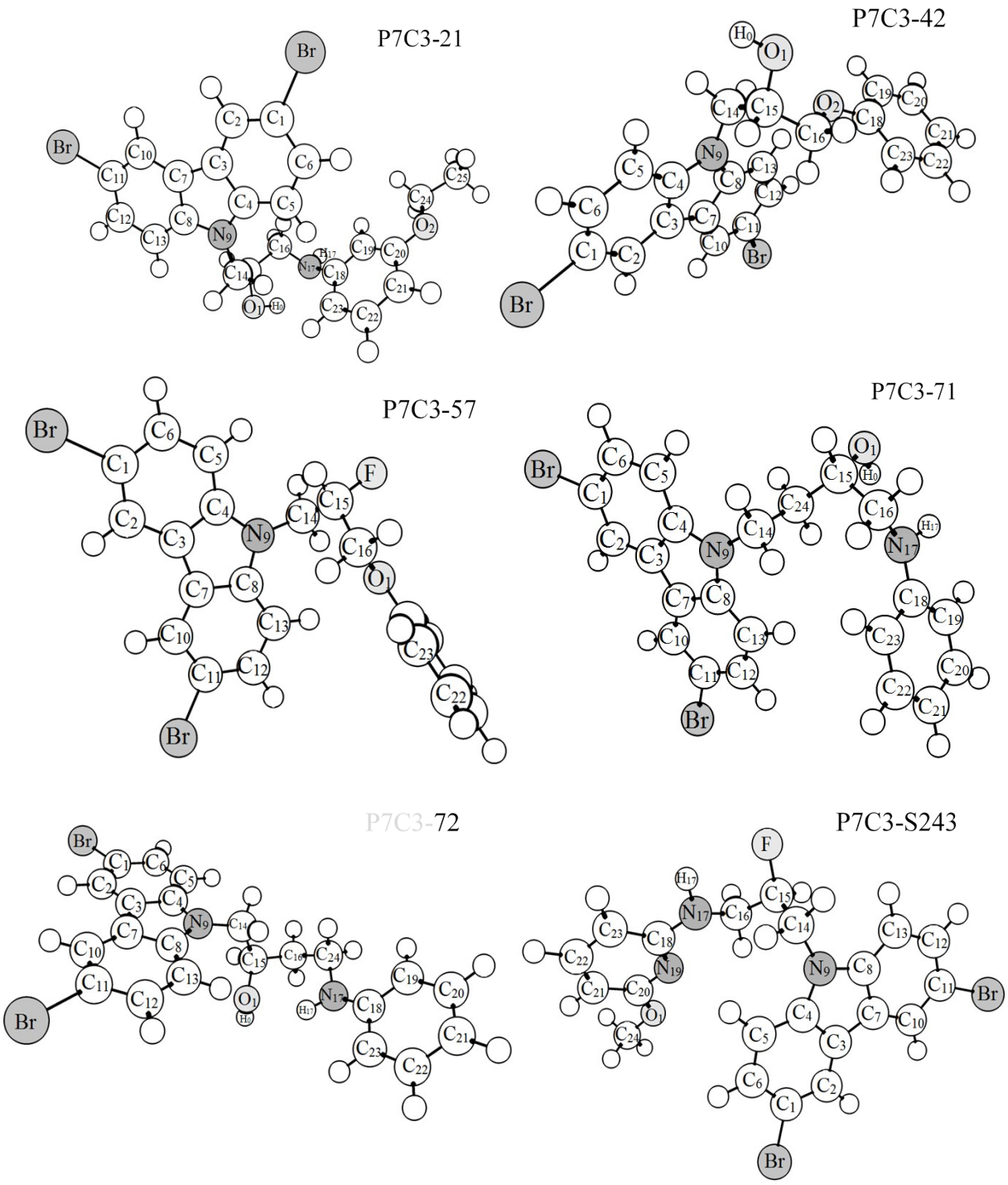

Fig. S2. *Ab initio* calculated optimised molecular structures and labelling of P7C3 derivatives.

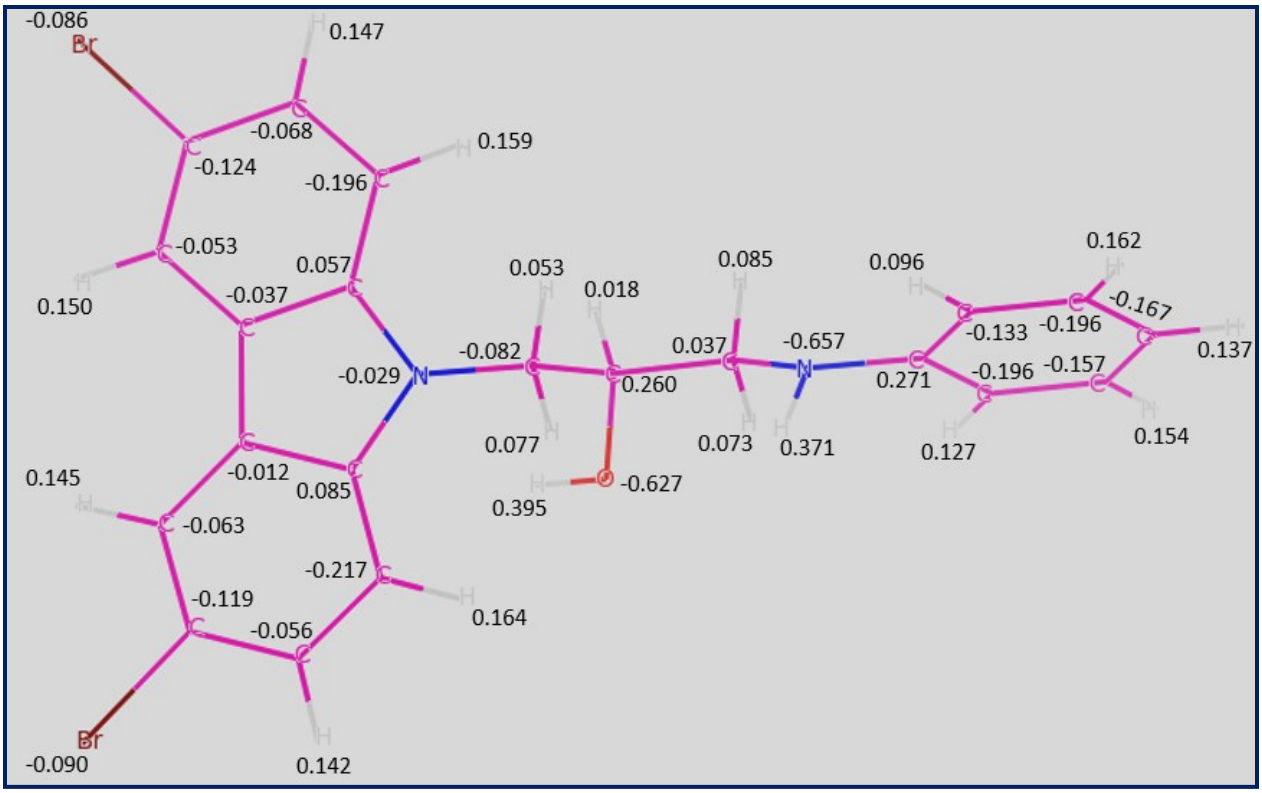

Fig. S3. *Ab initio* calculated atomic charges of P7C3 using the RESP (restrained electrostatic potential) method.

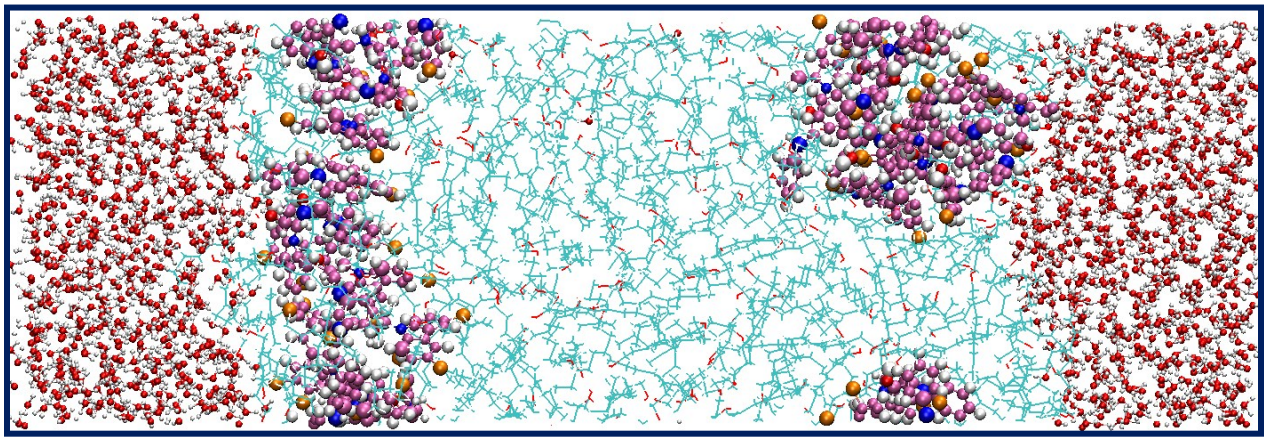

Fig. S4. MD simulation sample snapshots of the octanol/P7C3/water system after 20 ns simulation using RESP charges.

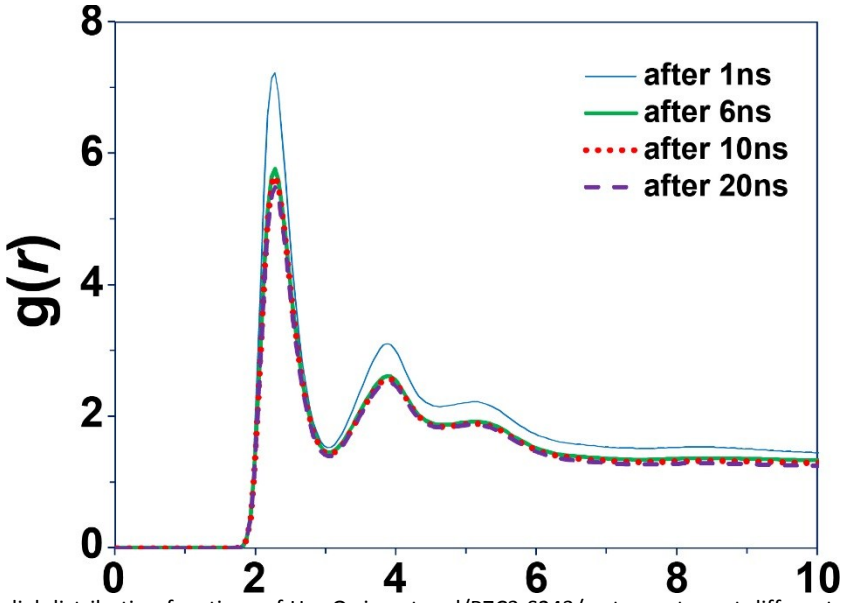

Fig. S5. Calculated radial distribution functions of $H_{17}\cdots O_A$ in octanol/P7C3-S243/water system at different simulation times. H_{17} and O_A are the amine H atom of the aminopyridine group of the drug and the octanol O atom, respectively.

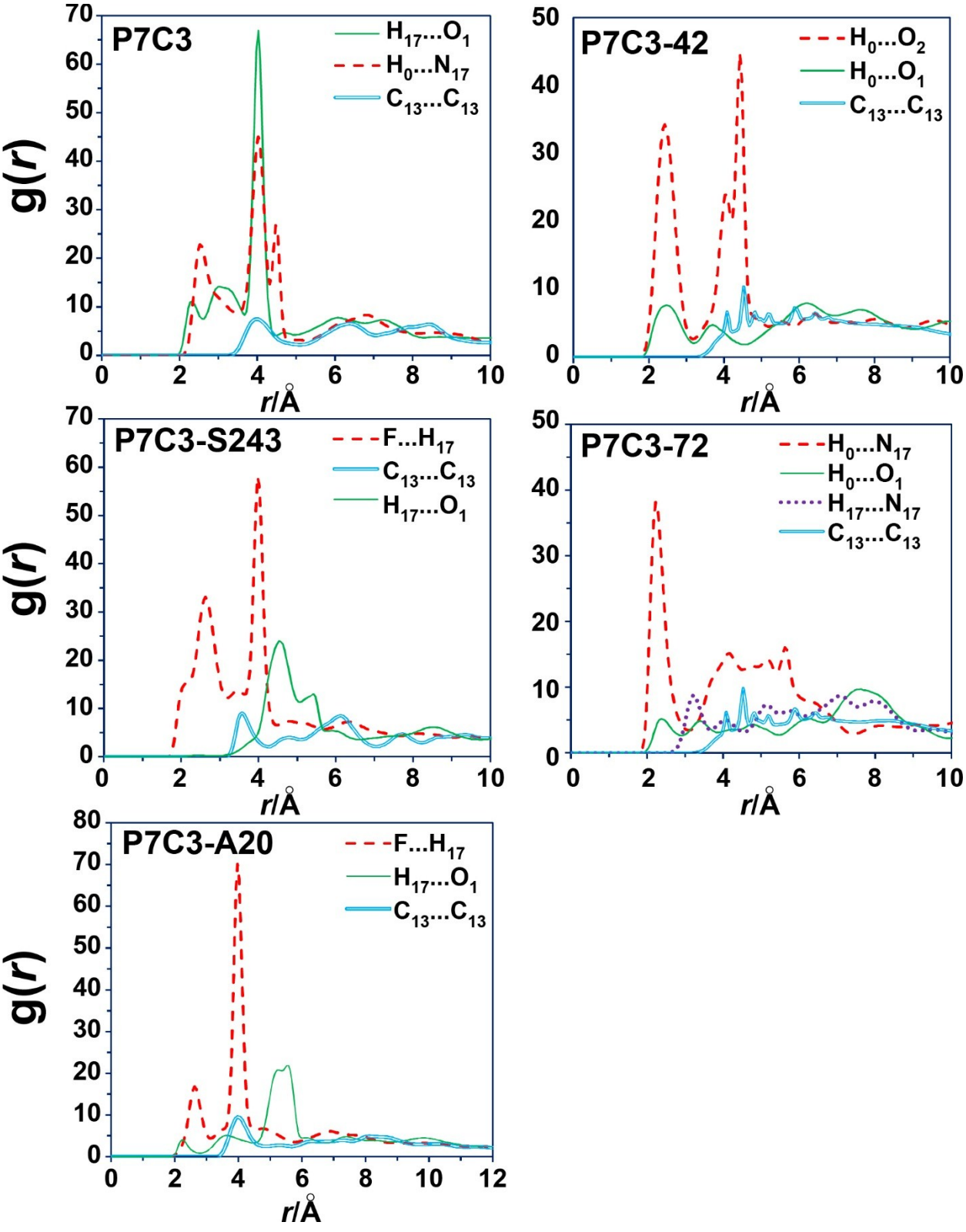

Fig. S6. Radial distribution functions between different sites of P7C3 derivatives.

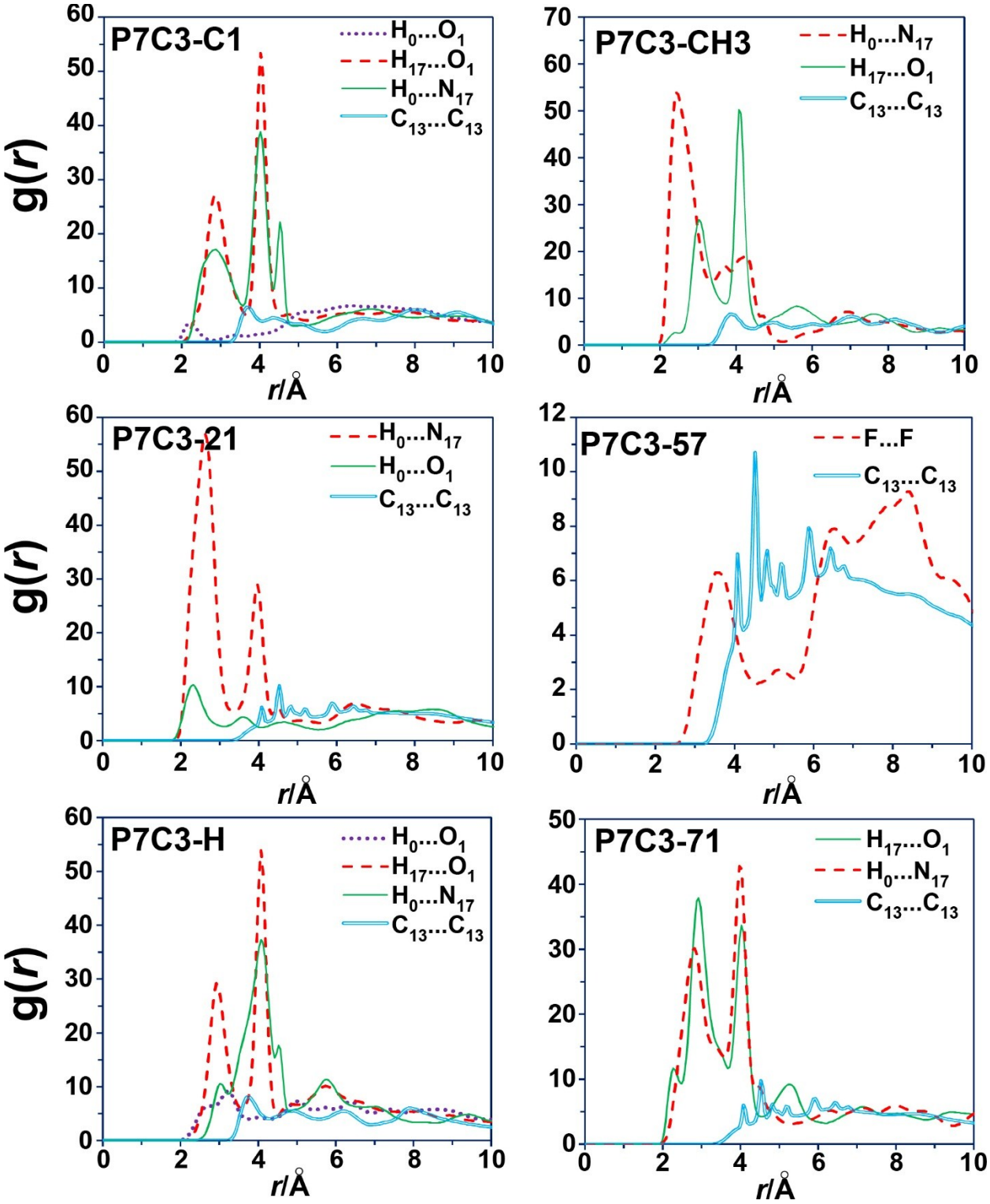

Fig. S7. Radial distribution functions between different sites of P7C3 derivatives.

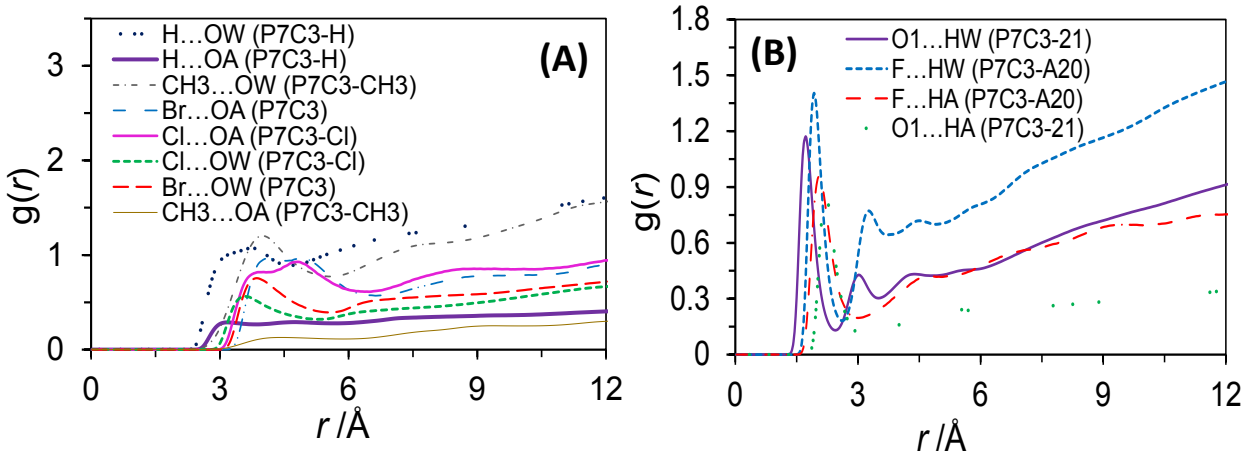

Fig. S8 Radial distribution functions of water oxygen atom (O_W), octanol oxygen atom (O_A), water hydrogen atom (H_W) and octanol hydrogen atom (H_A) with different atom sites of the drug molecules.

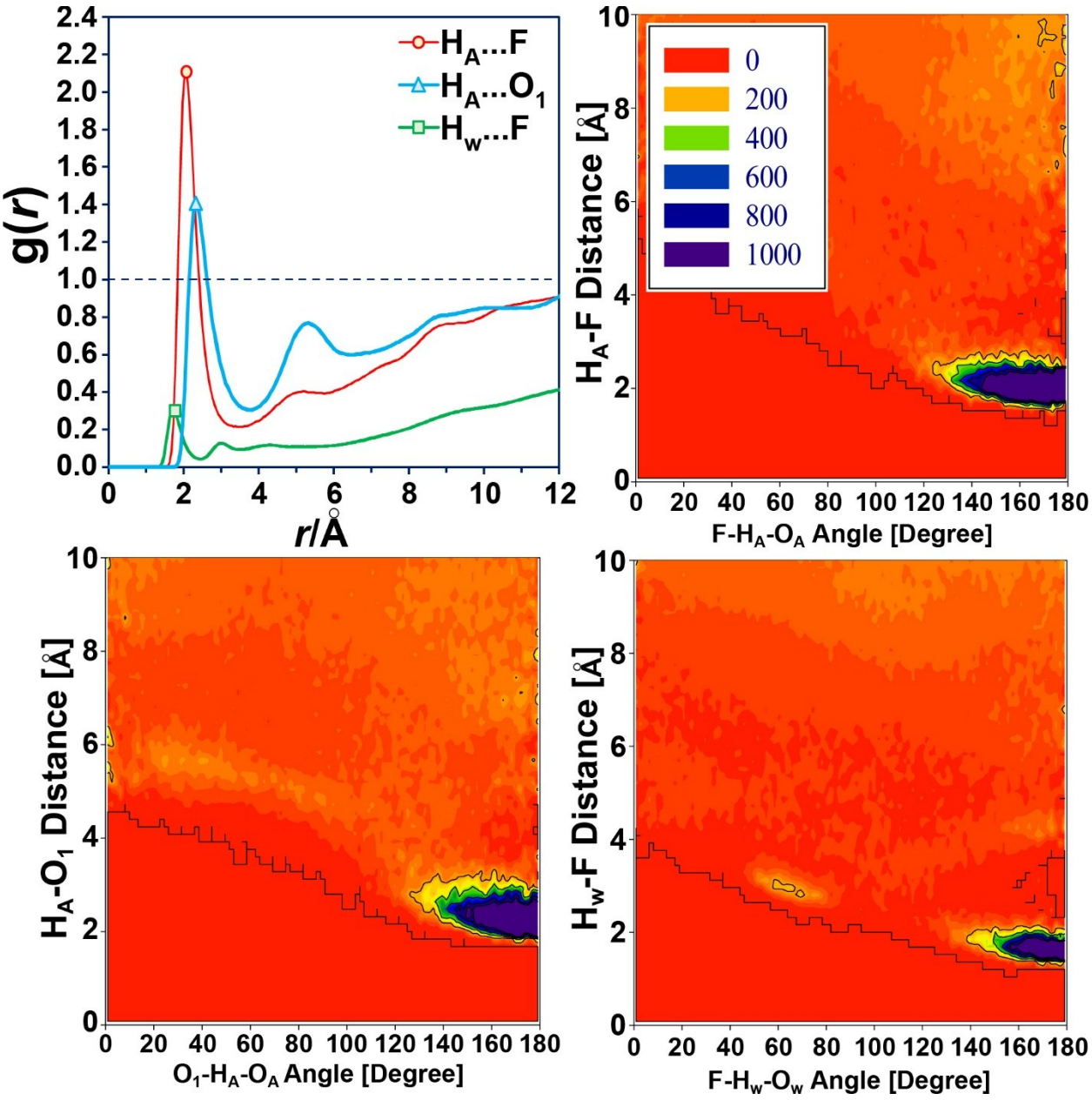

Fig. S9. Distribution functions of octanol/P7C3-S243/water. O_A and H_A are octanol hydroxyl atoms. Dark blue corresponds to high normalised probability and red corresponds to low probability.

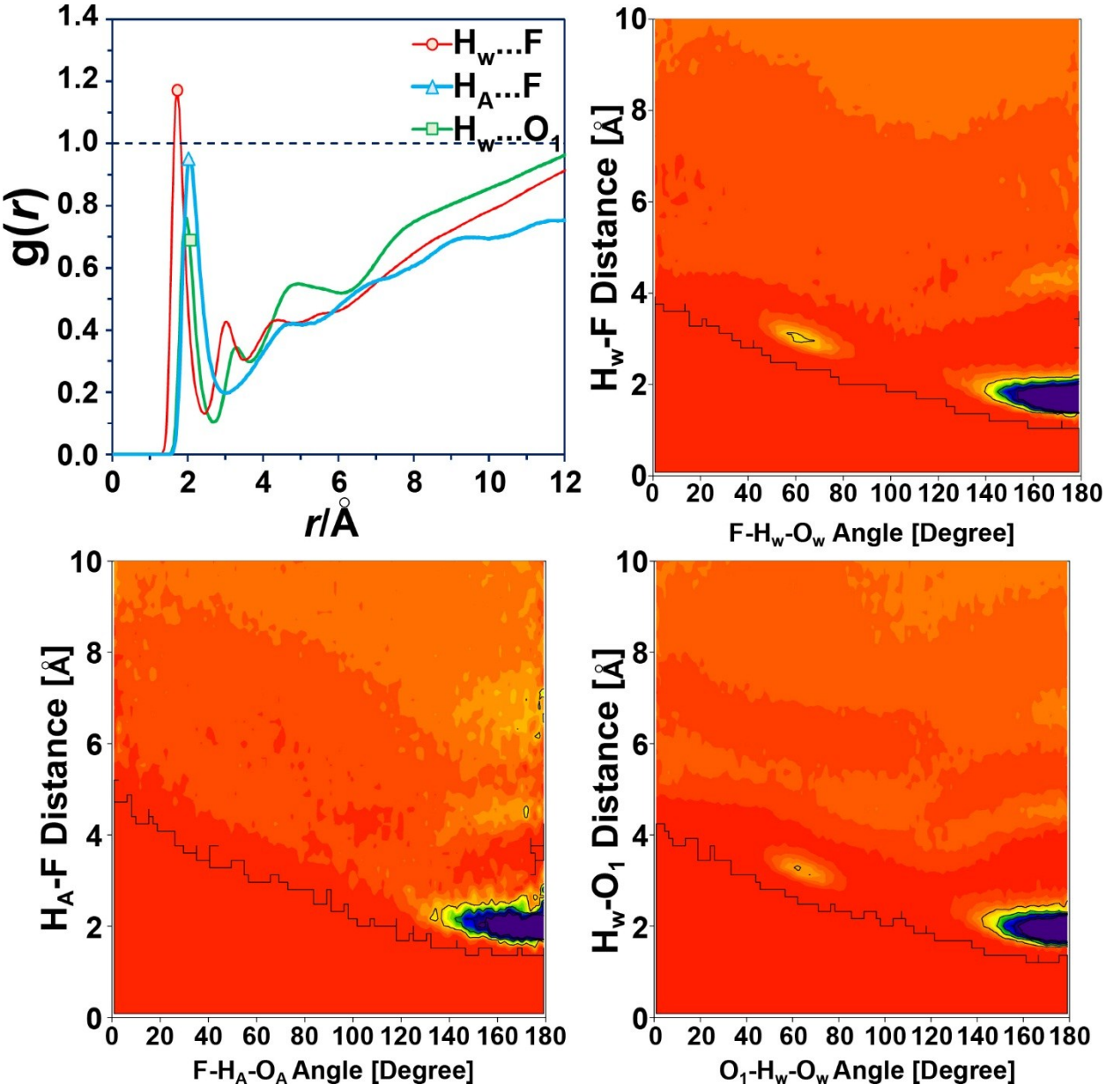

Fig. S10. Distribution functions of octanol/P7C3-A20/water. O_A and H_A are octanol hydroxyl atoms. Dark blue corresponds to high normalised probability and red corresponds to low probability.

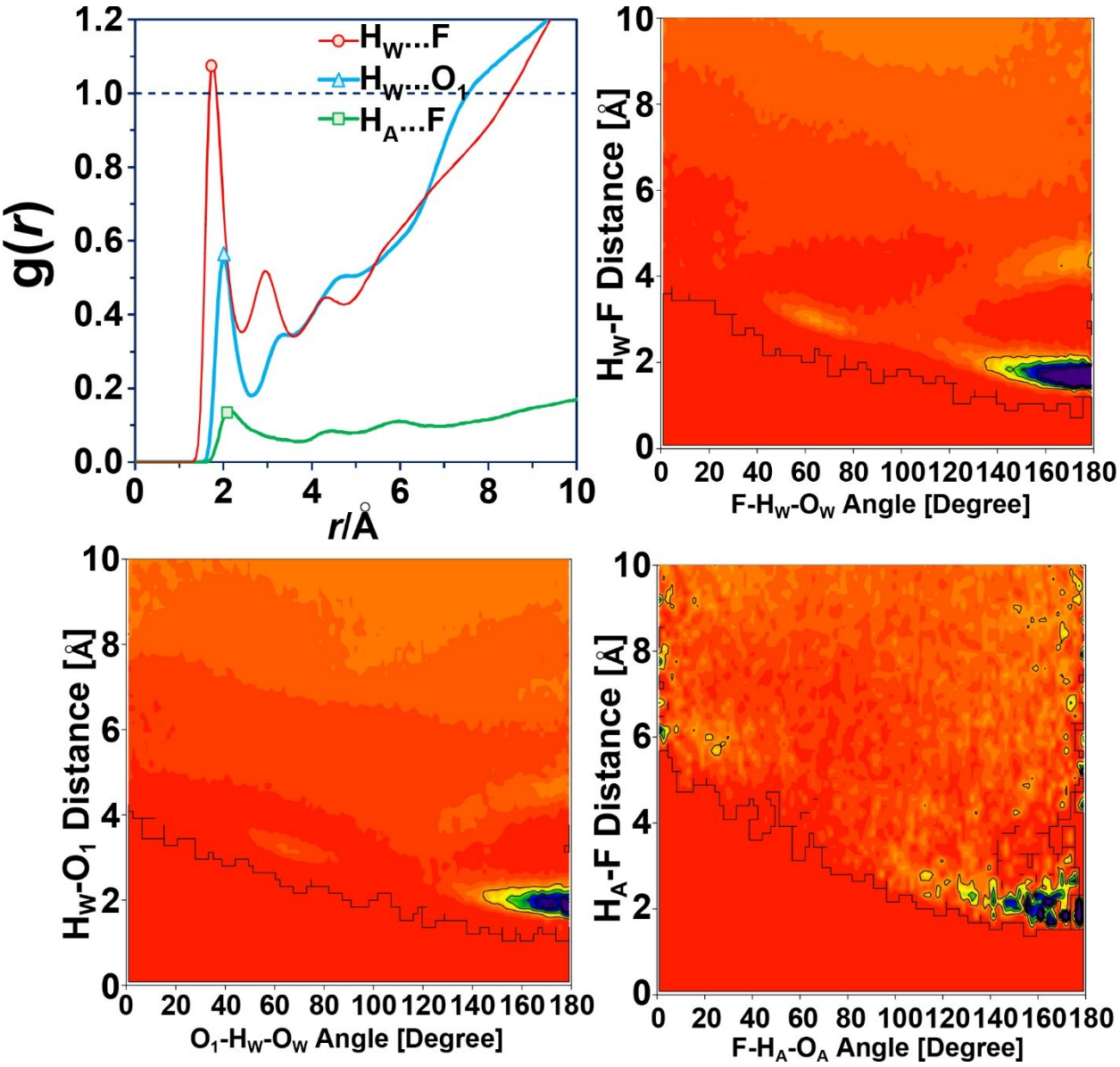

Fig. S11. Distribution functions of octanol/P7C3-57/water. O_A and H_A are octanol hydroxyl atoms. Dark blue corresponds to high normalised probability and red corresponds to low probability.

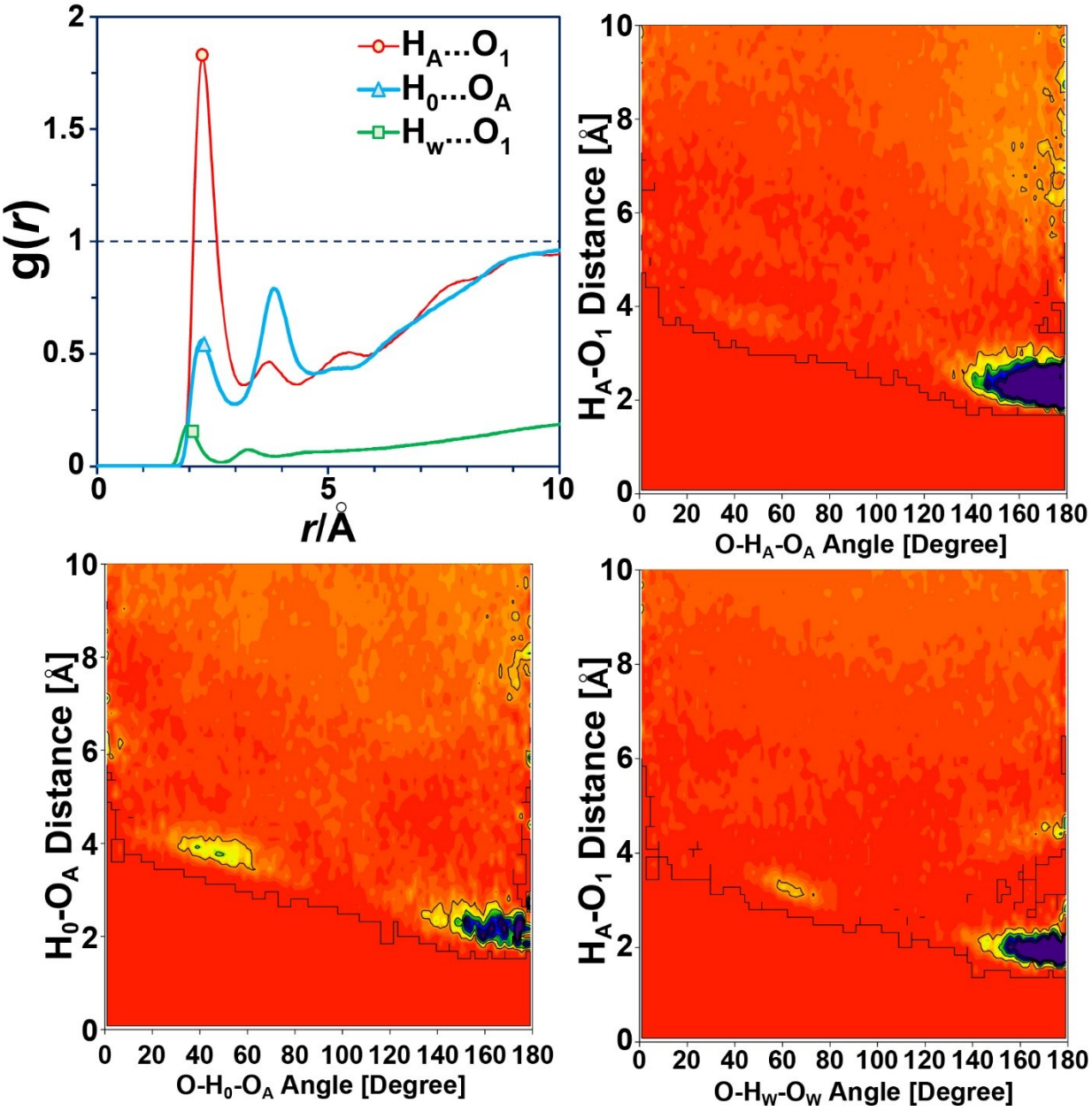

Fig. S12. Distribution functions of octanol/P7C3-42/water. O_A and H_A are octanol hydroxyl atoms. Dark blue corresponds to high normalised probability and red corresponds to low probability.

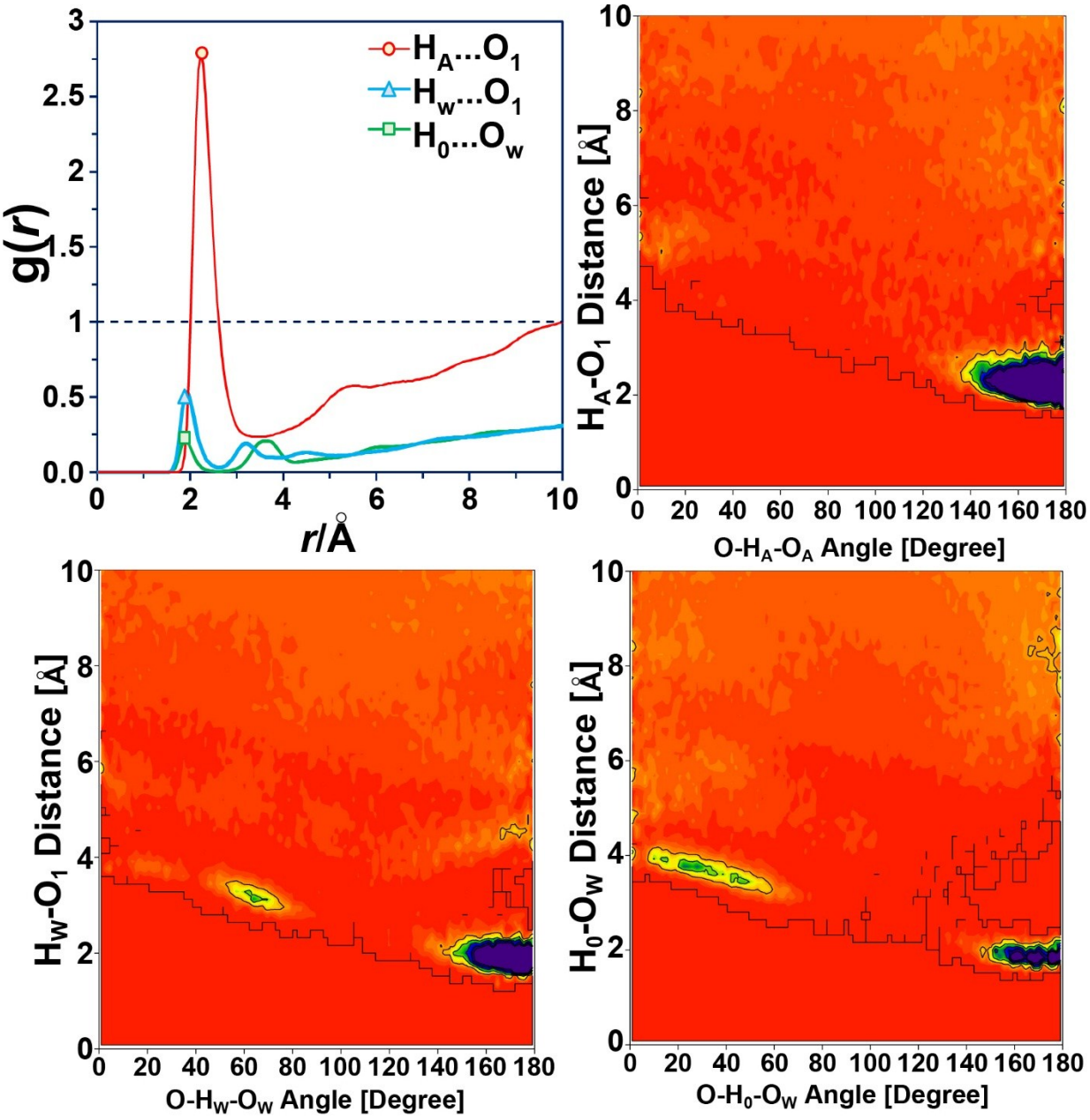

Fig. S13. Distribution functions of octanol/P7C3-72/water. O_A and H_A are octanol hydroxyl atoms. Dark blue corresponds to high normalised probability and red corresponds to low probability. The H_A…O_1 peak is located at 2.25 Å.

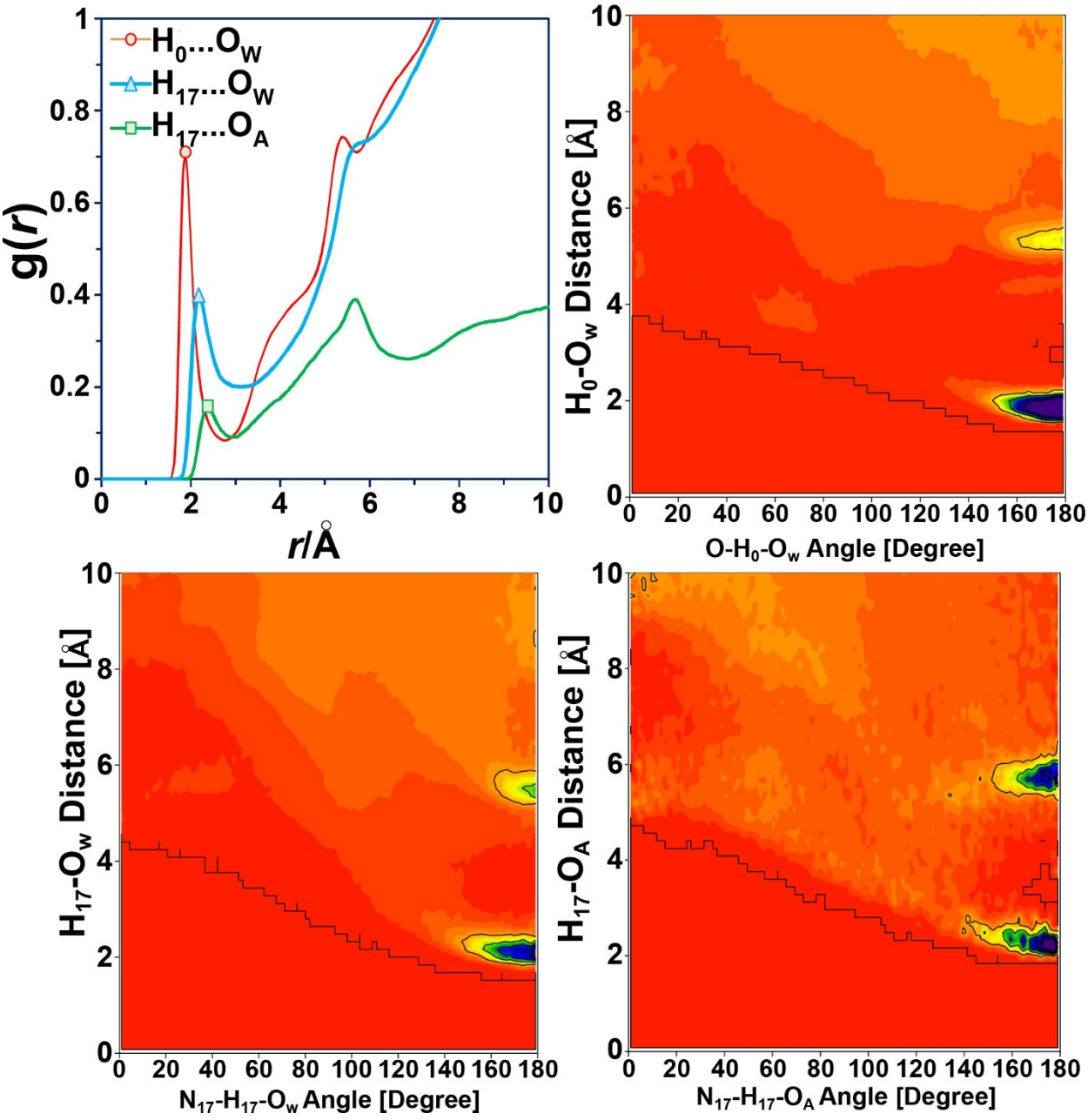

Fig. S14. Distribution functions of octanol/P7C3-H/water. O_A and H_A are octanol hydroxyl atoms. Dark blue corresponds to high normalised probability and red corresponds to low probability. The H_{17}…O_A peak is located at 2.37 Å.

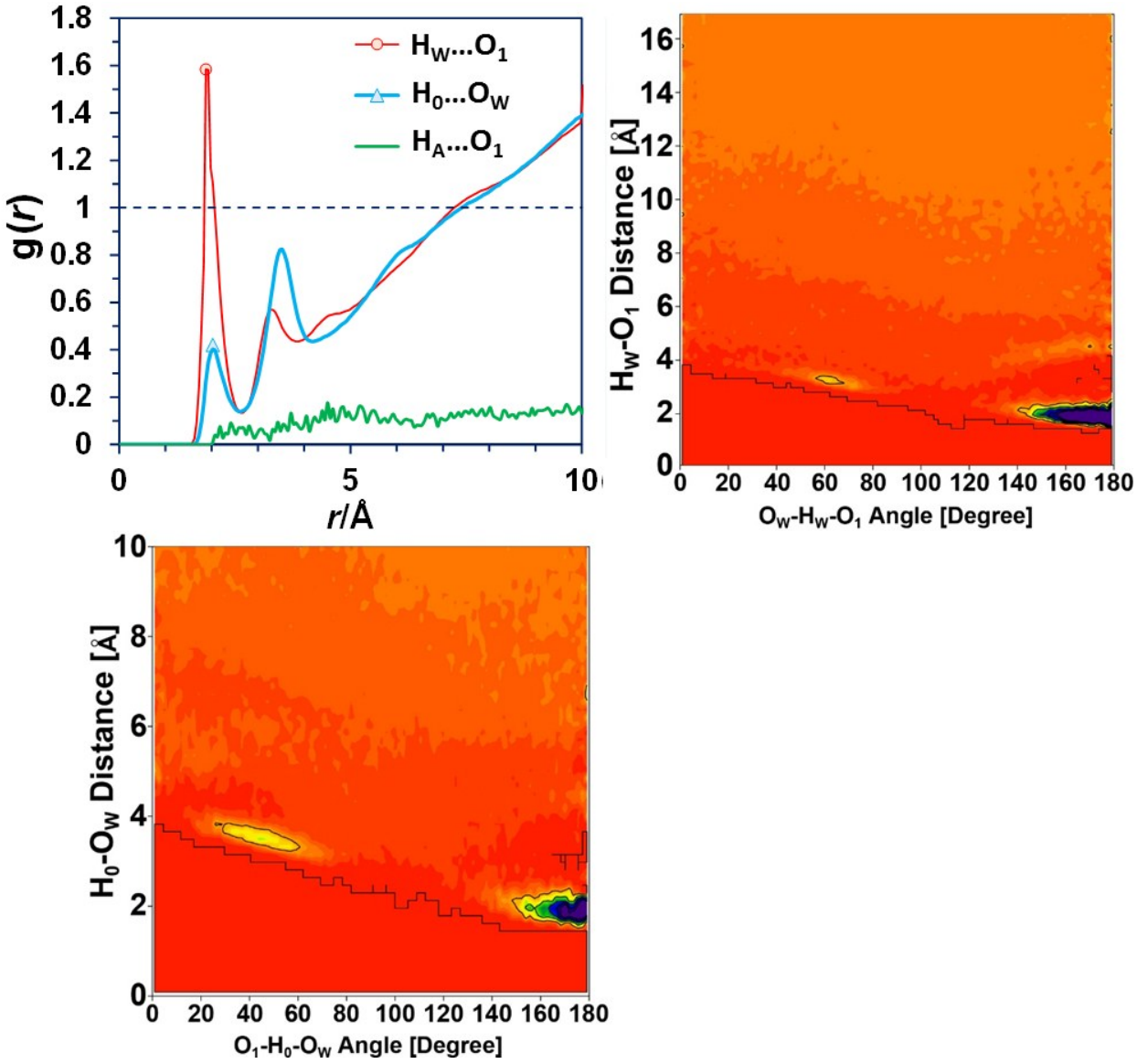

Fig. S15. Distribution functions of octanol/P7C3-CH_3/water. O_A and H_A are octanol hydroxyl atoms. Dark blue corresponds to high normalised probability and red corresponds to low probability. The H_A…O_1 peak should not be considered as hydrogen bonding.

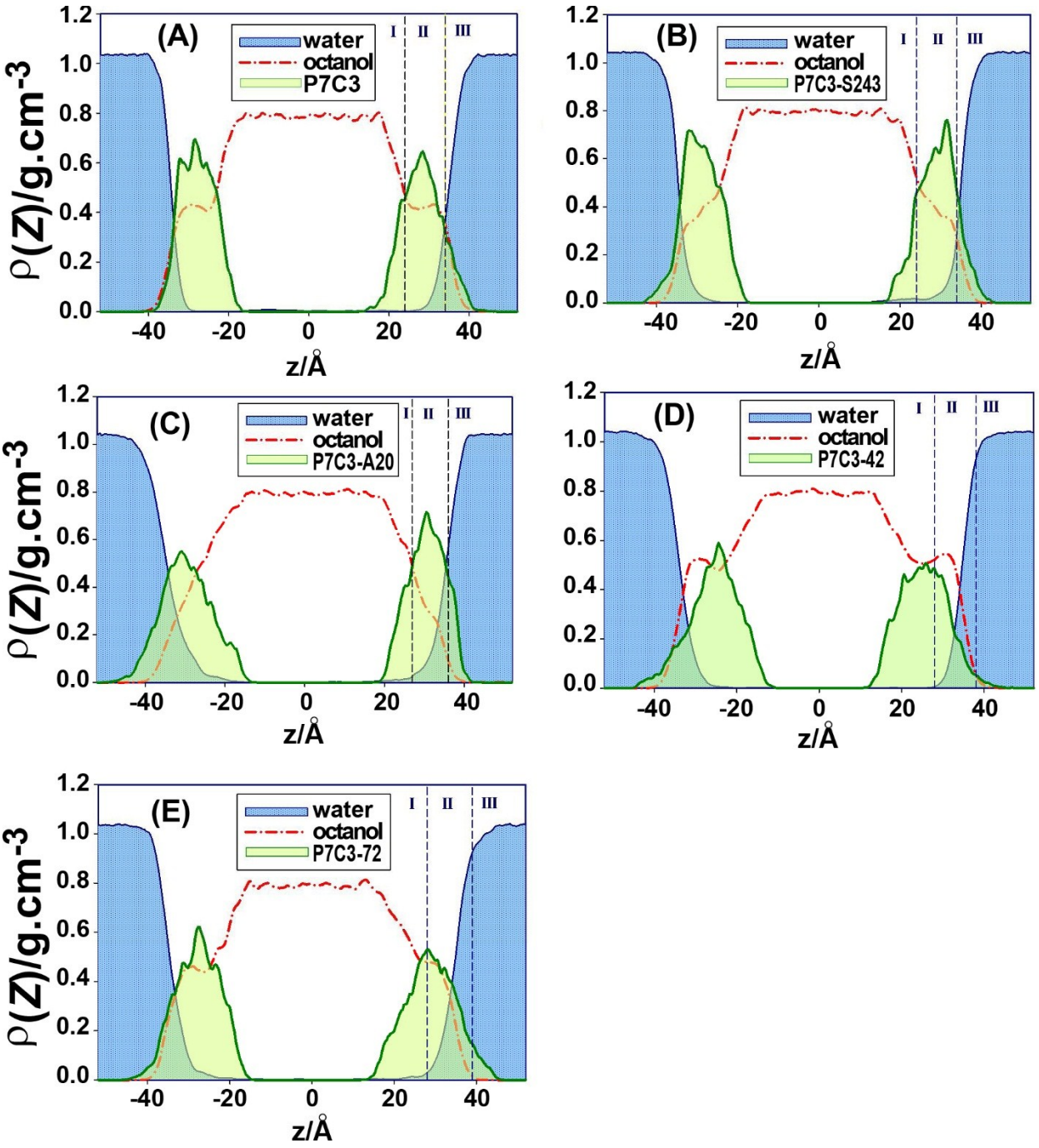

Fig. S16. Total density profiles of (A) octanol/P7C3/water, (B) octanol/P7C3-S243/water, (C) octanol/P7C3-A20/water, (D) octanol/P7C3-42/water, and (E) octanol/P7C3-72/water after 6 ns of simulation.

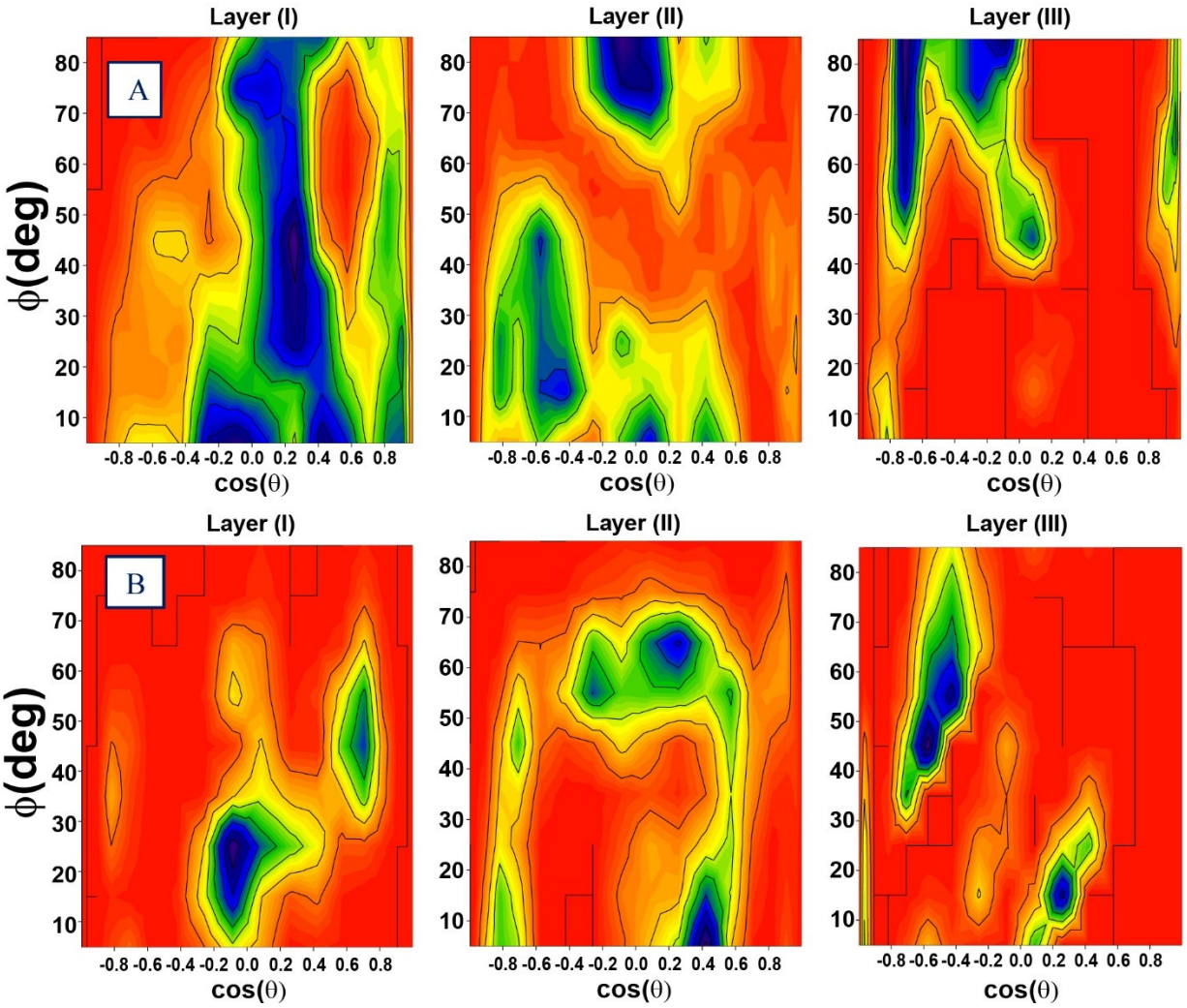

Fig. S17. Bivariate orientation distribution of drug molecules: (A) octanol/P7C3-42/water and (B) octanol/P7C3-72/water. Dark blue corresponds to high normalized probability and red corresponds to low probability.

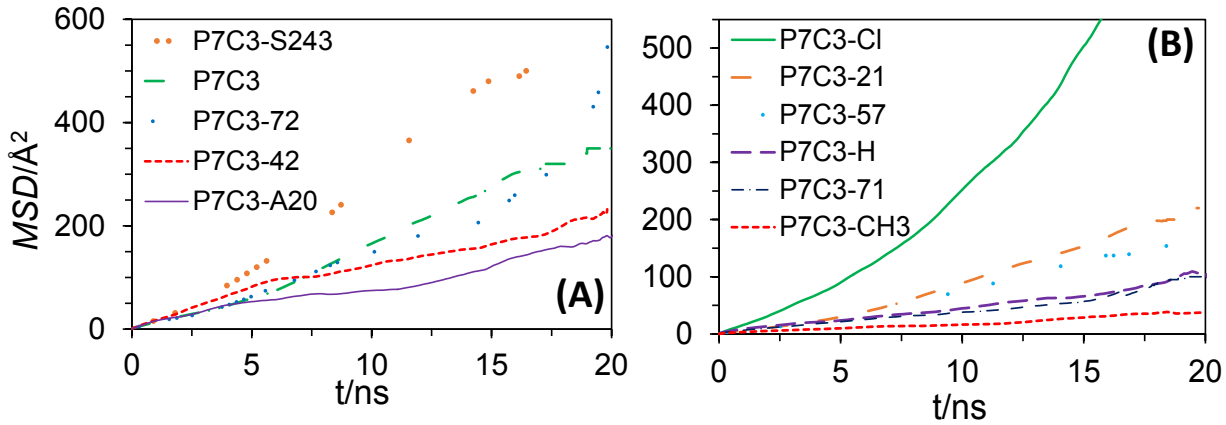

Fig. S18. Mean-squared displacements of the centre of mass of (A) active drug molecules (B) inactive drug molecules present at the octanol/water interface.

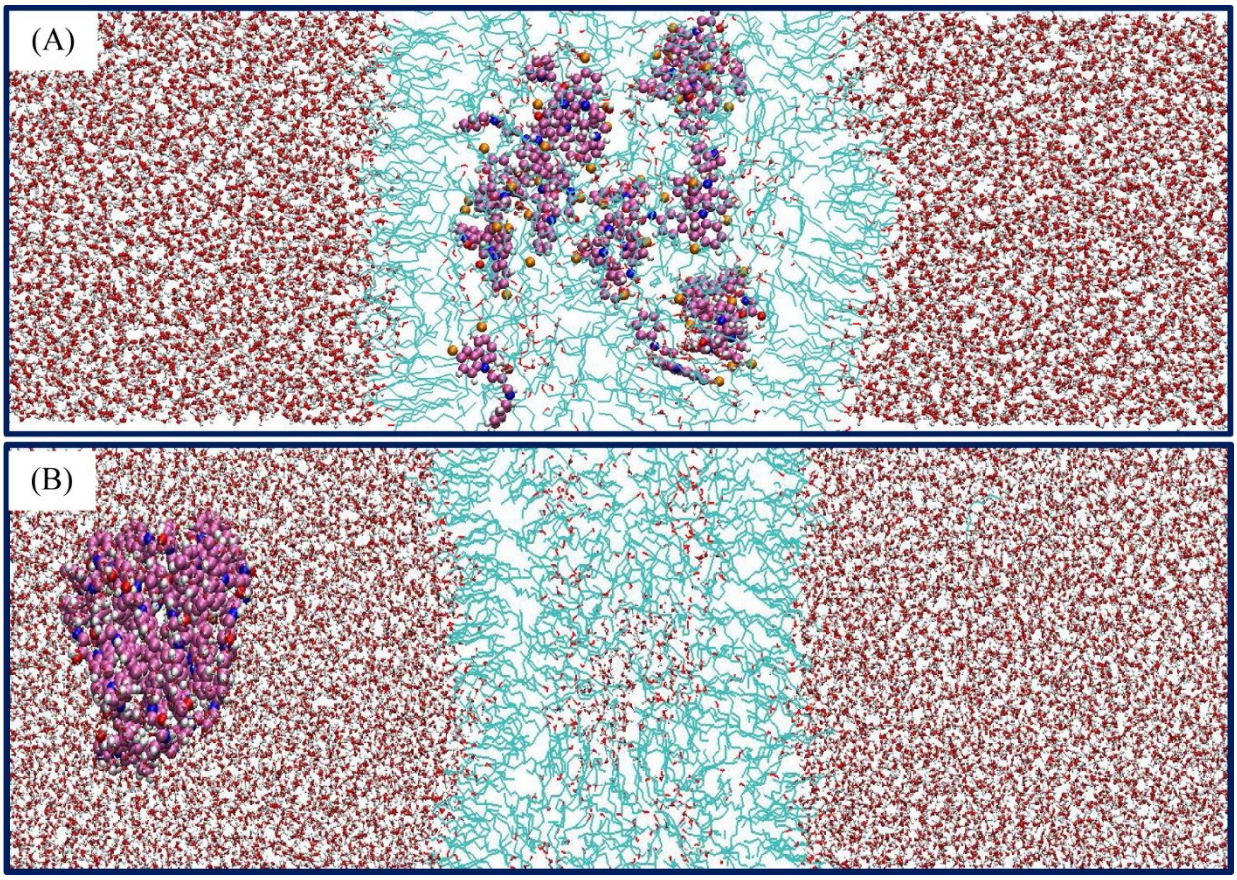

Fig. S19. MD simulation sample snapshot of (A) octanol/P7C3/water and (B) octanol/P7C3-CH_3/water after 100 ns simulation.

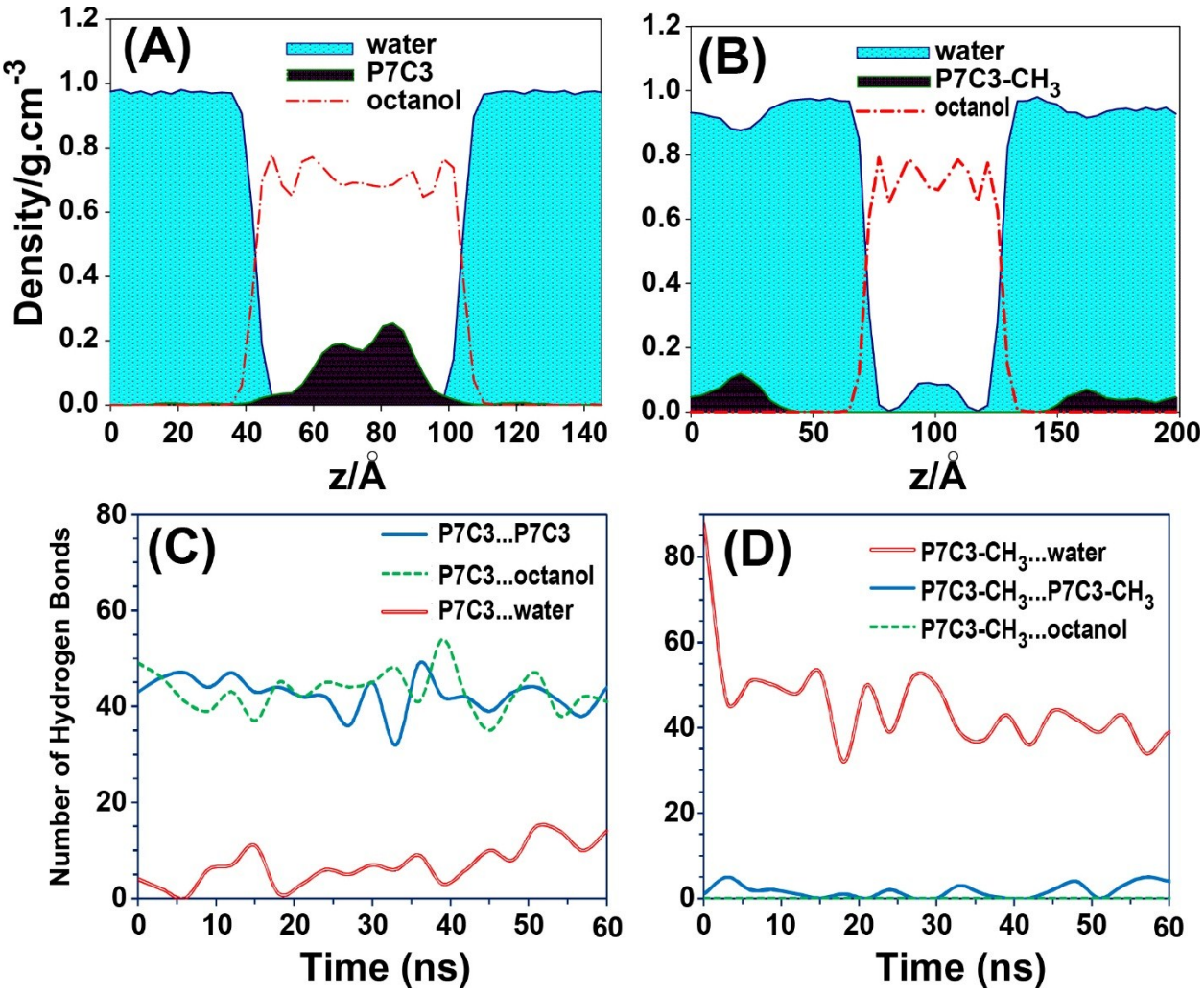

Fig. S20. Density profiles for (A) octanol/P7C3/water and (B) octanol/P7C3-CH_3/water systems. Number of hydrogen bonds for (C) octanol/P7C3/water and (D) octanol/P7C3-CH_3/water over the last 60 ns of simulations.

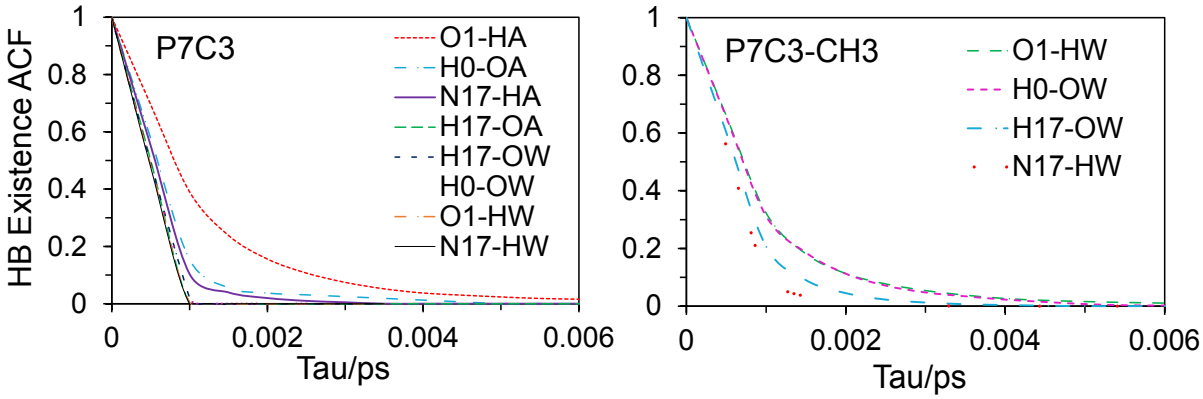

Fig. S21. Average HB existence ACFs of P7C3 and P7C3-CH_3 drugs with water oxygen atom (O_W), octanol oxygen atom (O_A), water hydrogen atom (H_W) and octanol hydrogen atom (H_A).

Supporting Tables:

Table S1. *Ab initio* calculated partial atomic charges of P7C3.

atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO
C_1	-0.124	C_{12}	-0.215	C_{23}	-0.241	H_{14}	0.214
C_2	-0.186	C_{13}	-0.222	Br_1	0.059	H_{15}	0.172
C_3	-0.061	C_{14}	-0.179	Br_2	0.060	H_{16}	0.196
C_4	0.185	C_{15}	0.111	O_1	-0.750	H_{16}	0.179
C_5	-0.220	C_{16}	-0.187	H_2	0.223	H_{17}	0.386
C_6	-0.215	N_{17}	-0.630	H_5	0.212	H_{19}	0.200
C_7	-0.084	C_{18}	0.180	H_6	0.222	H_{20}	0.203
C_8	0.192	C_{19}	-0.271	H_{10}	0.223	H_{21}	0.204
N_9	-0.446	C_{20}	-0.180	H_{12}	0.223	H_{22}	0.203
C_{10}	-0.186	C_{21}	-0.247	H_{13}	0.223	H_{23}	0.200
C_{11}	-0.124	C_{22}	-0.183	H_{14}	0.209	H_0	0.472

Table S2. *Ab initio* calculated partial atomic charges of P7C3-Cl.

atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO
C_1	-0.060	C_{12}	-0.215	C_{23}	-0.273	H_{14}	0.212
C_2	-0.185	C_{13}	-0.219	Cl_1	-0.006	H_{15}	0.174
C_3	-0.063	C_{14}	-0.180	Cl_2	-0.005	H_{16}	0.197
C_4	0.184	C_{15}	0.095	O_1	-0.748	H_{16}	0.206
C_5	-0.221	C_{16}	-0.188	H_2	0.225	H_{17}	0.378
C_6	-0.213	N_{17}	-0.623	H_5	0.211	H_{19}	0.200
C_7	-0.086	C_{18}	0.177	H_6	0.222	H_{20}	0.204
C_8	0.193	C_{19}	-0.244	H_{10}	0.223	H_{21}	0.205
N_9	-0.445	C_{20}	-0.180	H_{12}	0.222	H_{22}	0.201
C_{10}	-0.185	C_{21}	-0.247	H_{13}	0.222	H_{23}	0.197
C_{11}	-0.060	C_{22}	-0.247	H_{14}	0.206	H_0	0.471

Table S3. *Ab initio* calculated partial atomic charges of P7C3-H.

atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO
C_1	-0.233	C_{12}	-0.187	C_{23}	-0.270	H_{14}	0.224
C_2	-0.189	C_{13}	-0.254	H_1	0.206	H_{15}	0.170
C_3	-0.167	C_{14}	-0.192	H_{11}	0.199	H_{16}	0.188
C_4	-0.479	C_{15}	0.350	O_1	-0.518	H_{16}	0.195
C_5	-0.368	C_{16}	-0.186	H_2	0.205	H_{17}	0.385
C_6	-0.281	N_{17}	-0.640	H_3	0.209	H_{19}	0.199
C_7	0.645	C_{18}	0.413	H_6	0.205	H_{20}	0.202
C_8	0.124	C_{19}	-0.242	H_{10}	0.206	H_{21}	0.204
N_9	-0.465	C_{20}	-0.184	H_{12}	0.202	H_{22}	0.201
C_{10}	-0.490	C_{21}	-0.247	H_{13}	0.213	H_{23}	0.201
C_{11}	-0.254	C_{22}	-0.180	H_{14}	0.206	H_0	0.474

Table S4. *Ab initio* calculated partial atomic charges of P7C3-S243.

atom	*q*/*e* MP2 NBO	atom	*q*/*e* MP2 NBO	atom	*q*/*e* MP2 NBO	atom	*q*/*e* MP2 NBO
C_1	-0.207	C_{13}	-0.234	F	-0.414	H_{15}	0.177
C_2	-0.121	C_{14}	-0.196	Br_1	0.053	H_{16}	0.195
C_3	-0.187	C_{15}	0.226	Br_2	0.056	H_{16}	0.243
C_4	0.195	C_{16}	-0.219	O_1	-0.525	H_{17}	0.385
C_5	-0.220	N_{17}	-0.638	H_1	0.222	H_{21}	0.216
C_6	-0.059	C_{18}	0.417	H_3	0.222	H_{22}	0.206
C_7	-0.084	N_{19}	-0.545	H_6	0.223	H_{23}	0.209
C_8	0.190	C_{20}	0.557	H_{10}	0.223	H_{24}	0.171
N_9	-0.438	C_{21}	-0.367	H_{12}	0.222	H_{24}	0.170
C_{10}	-0.187	C_{22}	-0.133	H_{13}	0.215	H_{24}	0.195
C_{11}	-0.124	C_{23}	-0.311	H_{14}	0.222		
C_{12}	-0.211	C_{24}	-0.208	H_{14}	0.216		

Table S5. *Ab initio* calculated partial atomic charges of P7C3-A20.

atom	*q*/*e* MP2 NBO	atom	*q*/*e* MP2 NBO	atom	*q*/*e* MP2 NBO	atom	*q*/*e* MP2 NBO
C_1	-0.220	C_{14}	-0.269	H_1	0.232	H_{20}	0.236
C_2	-0.058	C_{15}	0.089	H_3	0.232	H_{21}	0.235
C_3	-0.201	C_{16}	-0.294	H_6	0.233	H_{22}	0.237
C_4	-0.077	N_{17}	-0.670	H_{10}	0.232	H_{23}	0.236
C_5	0.177	C_{18}	0.169	H_{12}	0.233	H_{24}	0.235
C_6	-0.271	C_{19}	-0.276	H_{13}	0.239	H_{24}	0.239
C_7	-0.077	C_{20}	-0.217	H_{14}	0.242	H_{24}	0.239
C_8	0.176	C_{21}	-0.268	H_{14}	0.253	H_{25}	0.239
N_9	-0.397	C_{22}	-0.212	H_{15}	0.209	H_{25}	0.235
C_{10}	-0.201	C_{23}	-0.290	H_{16}	0.238	H_{25}	0.239
C_{11}	-0.057	C_{24}	-0.684	H_{16}	0.233	H_0	0.485
C_{12}	-0.218	C_{25}	-0.684	H_{17}	0.409		
C_{13}	-0.271	O_1	-0.766	H_{19}	0.227		

Table S6. *Ab initio* calculated partial atomic charges of P7C3-42.

atom	*q*/*e* MP2 NBO	atom	*q*/*e* MP2 NBO	atom	*q*/*e* MP2 NBO	atom	*q*/*e* MP2 NBO
C_1	-0.233	C_{12}	-0.236	C_{23}	-0.316	H_{14}	0.235
C_2	-0.127	C_{13}	-0.266	Br_1	0.047	H_{15}	0.219
C_3	-0.216	C_{14}	-0.283	Br_2	0.049	H_{16}	0.230
C_4	-0.074	C_{15}	0.076	O_1	-0.745	H_{16}	0.222
C_5	0.181	C_{16}	-0.130	H_1	0.257	H_{19}	0.245
C_6	-0.261	O_2	-0.542	H_3	0.255	H_{20}	0.238
C_7	-0.070	C_{18}	0.317	H_6	0.255	H_{21}	0.237
C_8	0.181	C_{19}	-0.276	H_{10}	0.256	H_{22}	0.238
N_9	-0.395	C_{20}	-0.220	H_{12}	0.255	H_{23}	0.238
C_{10}	-0.214	C_{21}	-0.260	H_{13}	0.237	H_0	0.474
C_{11}	-0.128	C_{22}	-0.213	H_{14}	0.263		

Table S7. *Ab initio* calculated partial atomic charges of P7C3-72.

atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO
C_1	-0.237	C_{13}	-0.250	O_1	-0.772	H_{16}	0.244
C_2	-0.129	C_{14}	-0.272	Br_1	0.046	H_{16}	0.248
C_3	-0.214	C_{15}	0.086	Br_2	0.047	H_{17}	0.415
C_4	-0.070	C_{16}	-0.497	H_1	0.255	H_{18}	0.237
C_5	0.182	C_{18}	-0.263	H_3	0.256	H_{18}	0.205
C_6	-0.267	N_{17}	-0.653	H_6	0.239	H_{20}	0.227
C_7	-0.075	C_{19}	0.173	H_{10}	0.255	H_{21}	0.234
C_8	0.189	C_{20}	-0.277	H_{12}	0.255	H_{22}	0.233
N_9	-0.388	C_{21}	-0.219	H_{13}	0.250	H_{23}	0.233
C_{10}	-0.217	C_{22}	-0.275	H_{14}	0.246	H_{24}	0.230
C_{11}	-0.127	C_{23}	-0.214	H_{14}	0.253	H_0	0.488
C_{12}	-0.237	C_{24}	-0.300	H_{15}	0.227		

Table S8. *Ab initio* calculated partial atomic charges of P7C3-71.

atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO
C_1	-0.236	C_{13}	-0.262	O_1	-0.753	H_{15}	0.254
C_2	-0.129	C_{14}	-0.247	Br_1	0.046	H_{16}	0.228
C_3	-0.215	C_{15}	-0.509	Br_2	0.045	H_{17}	0.404
C_4	-0.072	C_{16}	0.093	H_1	0.255	H_{18}	0.234
C_5	0.183	C_{18}	-0.278	H_3	0.255	H_{18}	0.227
C_6	-0.263	N_{17}	-0.662	H_6	0.242	H_{20}	0.224
C_7	-0.073	C_{19}	0.177	H_{10}	0.255	H_{21}	0.237
C_8	0.183	C_{20}	-0.303	H_{12}	0.256	H_{22}	0.237
N_9	-0.386	C_{21}	-0.212	H_{13}	0.248	H_{23}	0.238
C_{10}	-0.216	C_{22}	-0.271	H_{14}	0.239	H_{24}	0.227
C_{11}	-0.128	C_{23}	-0.212	H_{14}	0.236	H_0	0.470
C_{12}	-0.232	C_{24}	-0.278	H_{15}	0.244		

Table S9. *Ab initio* calculated partial atomic charges of P7C3-21.

atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO
C_1	-0.238	C_{14}	-0.278	Br_2	0.045	H_{16}	0.230
C_2	-0.129	C_{15}	0.081	O_1	-0.772	H_{17}	0.407
C_3	-0.217	C_{16}	-0.288	O_2	-0.529	H_{19}	0.237
C_4	-0.074	N_{17}	-0.718	H_1	0.255	H_{21}	0.250
C_5	0.182	C_{18}	0.160	H_3	0.254	H_{22}	0.244
C_6	-0.263	C_{19}	-0.343	H_6	0.253	H_{23}	0.247
C_7	-0.073	C_{20}	-0.335	H_{10}	0.254	H_{24}	0.208
C_8	0.181	C_{21}	-0.281	H_{12}	0.255	H_{24}	0.210
N_9	-0.391	C_{22}	0.213	H_{13}	0.247	H_{25}	0.241
C_{10}	-0.216	C_{23}	-0.293	H_{14}	0.245	H_{25}	0.239
C_{11}	-0.128	C_{24}	-0.108	H_{14}	0.250	H_{25}	0.239
C_{12}	-0.236	C_{25}	-0.695	H_{15}	0.221	H_0	0.494
C_{13}	-0.263	Br_1	0.042	H_{16}	0.240		

Table S10. *Ab initio* calculated partial atomic charges of P7C3-57.

atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO
C_1	-0.233	C_{12}	-0.235	C_{23}	-0.316	H_{14}	0.253
C_2	-0.127	C_{13}	-0.266	Br_1	0.048	H_{15}	0.221
C_3	-0.216	C_{14}	-0.295	Br_2	0.050	H_{16}	0.229
C_4	-0.073	C_{15}	-0.295	F	-0.380	H_{16}	0.225
C_5	0.180	C_{16}	-0.150	H_1	0.257	H_{19}	0.246
C_6	-0.263	O_1	-0.545	H_3	0.255	H_{20}	0.240
C_7	-0.071	C_{18}	0.315	H_6	0.254	H_{21}	0.239
C_8	0.180	C_{19}	-0.275	H_{10}	0.256	H_{22}	0.239
N_9	-0.397	C_{20}	-0.219	H_{12}	0.256	H_{23}	0.239
C_{10}	-0.214	C_{21}	-0.258	H_{13}	0.244		
C_{11}	-0.128	C_{22}	-0.213	H_{14}	0.261		

Table S11. *Ab initio* calculated partial atomic charges of P7C3-CH_3.

atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO
C_1	-0.220	C_{14}	-0.269	H_1	0.232	H_{20}	0.236
C_2	-0.058	C_{15}	0.089	H_3	0.232	H_{21}	0.235
C_3	-0.201	C_{16}	-0.294	H_6	0.233	H_{22}	0.237
C_4	-0.077	N_{17}	-0.670	H_{10}	0.232	H_{23}	0.236
C_5	0.177	C_{18}	0.169	H_{12}	0.233	H_{24}	0.235
C_6	-0.271	C_{19}	-0.276	H_{13}	0.239	H_{24}	0.239
C_7	-0.077	C_{20}	-0.217	H_{14}	0.242	H_{24}	0.239
C_8	0.176	C_{21}	-0.268	H_{14}	0.253	H_{25}	0.239
N_9	-0.397	C_{22}	-0.212	H_{15}	0.209	H_{25}	0.235
C_{10}	-0.201	C_{23}	-0.290	H_{16}	0.238	H_{25}	0.239
C_{11}	-0.057	C_{24}	-0.684	H_{16}	0.233	H_0	0.485
C_{12}	-0.218	C_{25}	-0.684	H_{17}	0.409		
C_{13}	-0.271	O_1	-0.766	H_{19}	0.227		

Table S12. *Ab initio* calculated partial atomic charges of octanol.

atom	*q/e* MP2 NBO	atom	*q/e* MP2 NBO
C	-0.569	H	0.186
C	-0.377	H	0.186
C	-0.374	H	0.186
C	-0.372	H	0.187
C	-0.370	H	0.189
C	-0.376	H	0.187
C	-0.403	H	0.181
C	-0.015	H	0.198
H	0.190	H	0.171
H	0.192	H	0.147
H	0.185	H	0.199
H	0.185	H_A	0.449
H	0.185	O_A	-0.732
H	0.185		

Table S13. Self-diffusion coefficients ($1 \times 10^{-11}\, m^2/s$) of drug candidate molecules calculated by *MSD*–time curves.

Drug	Diffusion Coefficient	Drug	Diffusion Coefficient
P7C3-S243	17.60	P7C3-Cl	22.90
P7C3	10.02	P7C3-21	4.45
P7C3-72	9.61	P7C3-57	3.85
P7C3-42	6.50	P7C3-H	2.79
P7C3-A20	4.89	P7C3-71	2.62
		P7C3-CH_3	0.88

Table S14. Average hydrogen bond lifetimes, $\tau(HB)$, between hydrogen bond donor and acceptor atoms in each system.

Drug	Donor-Acceptor	$\tau(HB)/ps$
P7C3	**O_1-H_A**	**0.0025**
	O_A-H_0	**0.0014**
	N_{17}-H_A	**0.0012**
	O_A-H_{17}	**0.0010**
	O_W-H_{17}	**0.0010**
	O_W-H_0	**0.0010**
	O_1-H_W	**0.0009**
	N_{17}-H_W	**0.0008**
P7C3-CH_3	**O_1-H_W**	**0.0021**
	O_W-H_0	**0.0019**
	O_W-H_{17}	**0.0014**
	N_{17}-H_W	**0.0012**