Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

Methodology

Stability analysis of molecules during molecular dynamics simulations

A sample of the zwitterion chemistries underwent stability analysis, where the root mean-squared displacement (RMSD) during NVT simulation is observed as shown in **Figure S1**. As can be seen that the molecule rapidly enters a steady-state condition with the RMSD leveling off followed by a sudden drop on the far right. This indicates the 10 ns length of NVT simulation is sufficient to achieve molecular stability.

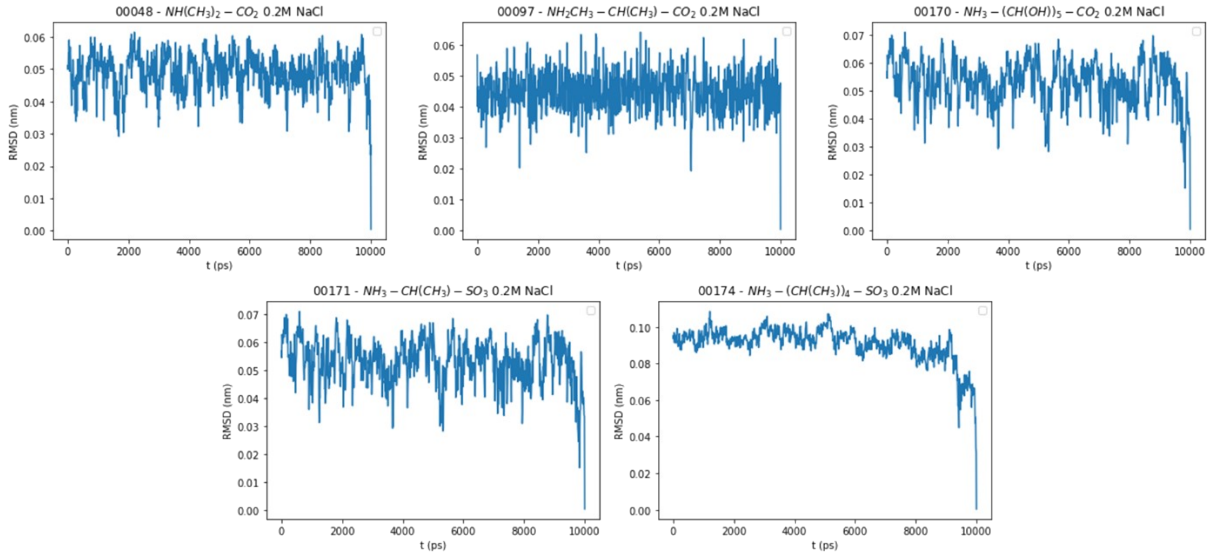


Figure S1. Root mean-squared displacement of five sample zwitterions, showing the stability of the molecules during the NVT simulation.

Lag time selection for effective residence time calculation

Selecting the maximum lag time for calculating the effective residence time, τ, is an important task. If the value is too large, then the lack of accuracy of residence time correlation function, $\overline{C}(t)$, considerably affects the linear model fit to $ln(\overline{C}(t))$ vs t, thus affecting the calculation of τ. If the maximum lag time is too short, it will not capture linear trend of $\ln(\overline{C}(t)) vs\ t$. Figure S2 illustrates a sample of the residence time correlation function, $\overline{C}(t)$, for zwitterion labeled 00239 in Table S1.

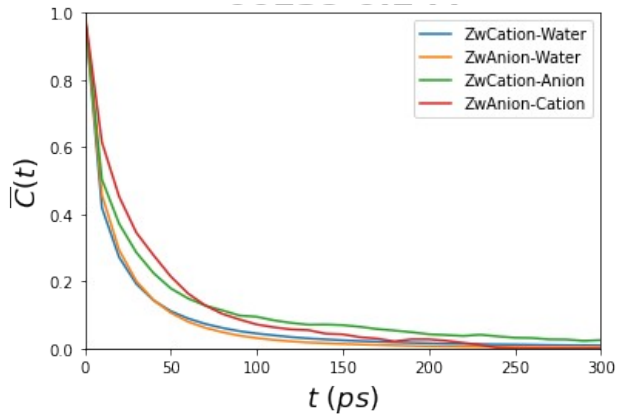


Figure S2. A sample residence time correlation function, $\overline{C}(t)$, as a function of t, for zwitterion labeled 00239 in Table S1, in four possible interactions shown in the legend.

Cheminformatic descriptor calculations

Volume, Surface Area: The built-in GROMACS[1] function, *gmx sasa*, is used to calculate the van der Waals surface area (nm^2) and volume (nm^3) during a simulation. These two descriptors will be used to describe the steric effects on association properties.

Charge: Electrostatic interactions are believed to be the predominant influence on zwitterion hydration and ion association.[2] Moiety charges are calculated by summing the partial charges from the topology of all atoms in the respective moiety.

HBondDonors/Acceptors: This feature is the number of hydrogen bond donating and accepting sites, and is manually calculated according to the chemistry of the charged moiety.

Table S1. Molecule SMILES input to LigParGen.[3] * indicates the molecule was unstable during simulation and is not included in the data for analysis.

Molecule	Cation	Spacer	Anion	SMILES
00000	$N(CH_3)_3$		CO_2	C[N+](C)(C)C(=O)[O-]
00001	$N(CH_3)_3$	CH_2	CO_2	C[N+](C)(C)CC(=O)[O-]
00002	$N(CH_3)_3$	$(CH_2)_2$	CO_2	C[N+](C)(C)CCC(=O)[O-]
00003	$N(CH_3)_3$	$(CH_2)_3$	CO_2	C[N+](C)(C)CCCC(=O)[O-]
00004	$N(CH_3)_3$	$(CH_2)_4$	CO_2	C[N+](C)(C)CCCCC(=O)[O-]
00005	$N(CH_3)_3$	$(CH_2)_5$	CO_2	C[N+](C)(C)CCCCCC(=O)[O-]
00006	$N(CH_3)_3$	CH(OH)	CO_2	C[N+](C)(C)C(O)C(=O)[O-]
00007	$N(CH_3)_3$	$(CH(OH))_2$	CO_2	C[N+](C)(C)C(O)C(O)C(=O)[O-]
00008	$N(CH_3)_3$	$(CH(OH))_3$	CO_2	C[N+](C)(C)C(O)C(O)C(O)C(=O)[O-]
00009	$N(CH_3)_3$	$(CH(OH))_4$	CO_2	C[N+](C)(C)C(O)C(O)C(O)C(O)C(=O)[O-]
00010	$N(CH_3)_3$	$(CH(OH))_5$	CO_2	C[N+](C)(C)C(O)C(O)C(O)C(O)C(O)C(=O)[O-]
00011	$N(CH_3)_3$	CH(CH3)	CO_2	C[N+](C)(C)C(C)C(=O)[O-]
00012	$N(CH_3)_3$	$(CH(CH3))_2$	CO_2	C[N+](C)(C)C(C)C(C)C(=O)[O-]
00013	$N(CH_3)_3$	$(CH(CH3))_3$	CO_2	C[N+](C)(C)C(C)C(C)C(C)C(=O)[O-]
00014	$N(CH_3)_3$	$(CH(CH3))_4$	CO_2	C[N+](C)(C)C(C)C(C)C(C)C(C)C(=O)[O-]
00015	$N(CH_3)_3$	$(CH(CH3))_5$	CO_2	C[N+](C)(C)C(C)C(C)C(C)C(C)C(C)C(=O)[O-]
00016	$N(CH_3)_3$		SO_3	C[N+](C)(C)S(=O)(=O)[O-]
00017	$N(CH_3)_3$	CH_2	SO_3	C[N+](C)(C)CS(=O)(=O)[O-]
00018	$N(CH_3)_3$	$(CH_2)_2$	SO_3	C[N+](C)(C)CCS(=O)(=O)[O-]
00019	$N(CH_3)_3$	$(CH_2)_3$	SO_3	C[N+](C)(C)CCCS(=O)(=O)[O-]
00020	$N(CH_3)_3$	$(CH_2)_4$	SO_3	C[N+](C)(C)CCCCS(=O)(=O)[O-]
00021	$N(CH_3)_3$	$(CH_2)_5$	SO_3	C[N+](C)(C)CCCCCS(=O)(=O)[O-]
00022	$N(CH_3)_3$	CH(OH)	SO_3	C[N+](C)(C)C(O)S(=O)(=O)[O-]
00023	$N(CH_3)_3$	$(CH(OH))_2$	SO_3	C[N+](C)(C)C(O)C(O)S(=O)(=O)[O-]
00024	$N(CH_3)_3$	$(CH(OH))_3$	SO_3	C[N+](C)(C)C(O)C(O)C(O)S(=O)(=O)[O-]
00025	$N(CH_3)_3$	$(CH(OH))_4$	SO_3	C[N+](C)(C)C(O)C(O)C(O)C(O)S(=O)(=O)[O-]
00026	$N(CH_3)_3$	$(CH(OH))_5$	SO_3	C[N+](C)(C)C(O)C(O)C(O)C(O)C(O)S(=O)(=O)[O-]
00027	$N(CH_3)_3$	CH(CH3)	SO_3	C[N+](C)(C)C(C)S(=O)(=O)[O-]
00028	$N(CH_3)_3$	$(CH(CH3))_2$	SO_3	C[N+](C)(C)C(C)C(C)S(=O)(=O)[O-]
00029	$N(CH_3)_3$	$(CH(CH3))_3$	SO_3	C[N+](C)(C)C(C)C(C)C(C)S(=O)(=O)[O-]
00030	$N(CH_3)_3$	$(CH(CH3))_4$	SO_3	C[N+](C)(C)C(C)C(C)C(C)C(C)S(=O)(=O)[O-]
00031	$N(CH_3)_3$	$(CH(CH3))_5$	SO_3	C[N+](C)(C)C(C)C(C)C(C)C(C)C(C)C(C)S(=O)(=O)[O-]
00032	$N(CH_3)_3$		OPO_3H	C[N+](C)(C)OP(=O)(O)[O-]
00033	$N(CH_3)_3$	CH_2	OPO_3H	C[N+](C)(C)COP(=O)(O)[O-]
00034	$N(CH_3)_3$	$(CH_2)_2$	OPO_3H	C[N+](C)(C)CCOP(=O)(O)[O-]
00035	$N(CH_3)_3$	$(CH_2)_3$	OPO_3H	C[N+](C)(C)CCCOP(=O)(O)[O-]
00036	$N(CH_3)_3$	$(CH_2)_4$	OPO_3H	C[N+](C)(C)CCCCOP(=O)(O)[O-]
00037	$N(CH_3)_3$	$(CH_2)_5$	OPO_3H	C[N+](C)(C)CCCCCOP(=O)(O)[O-]

00038	$N(CH_3)_3$	CH(OH)	OPO_3H	C[N+](C)(C)C(O)OP(=O)(O)[O-]
00039	$N(CH_3)_3$	$(CH(OH))_2$	OPO_3H	C[N+](C)(C)C(O)C(O)OP(=O)(O)[O-]
00040	$N(CH_3)_3$	$(CH(OH))_3$	OPO_3H	C[N+](C)(C)C(O)C(O)C(O)OP(=O)(O)[O-]
00041	$N(CH_3)_3$	$(CH(OH))_4$	OPO_3H	C[N+](C)(C)C(O)C(O)C(O)C(O)OP(=O)(O)[O-]
00042	$N(CH_3)_3$	$(CH(OH))_5$	OPO_3H	C[N+](C)(C)C(O)C(O)C(O)C(O)C(O)OP(=O)(O)[O-]
00043	$N(CH_3)_3$	CH(CH3)	OPO_3H	C[N+](C)(C)C(C)OP(=O)(O)[O-]
00044	$N(CH_3)_3$	$(CH(CH3))_2$	OPO_3H	C[N+](C)(C)C(C)C(C)OP(=O)(O)[O-]
00045	$N(CH_3)_3$	$(CH(CH3))_3$	OPO_3H	C[N+](C)(C)C(C)C(C)C(C)OP(=O)(O)[O-]
00046	$N(CH_3)_3$	$(CH(CH3))_4$	OPO_3H	C[N+](C)(C)C(C)C(C)C(C)C(C)OP(=O)(O)[O-]
00047	$N(CH_3)_3$	$(CH(CH3))_5$	OPO_3H	C[N+](C)(C)C(C)C(C)C(C)C(C)C(C)C(C)OP(=O)(O)[O-]
00048	$NH(CH_3)_2$		CO_2	C[NH+](C)C(=O)[O-]
00049	$NH(CH_3)_2$	CH_2	CO_2	C[NH+](C)CC(=O)[O-]
00050	$NH(CH_3)_2$	$(CH_2)_2$	CO_2	C[NH+](C)CCC(=O)[O-]
00051	$NH(CH_3)_2$	$(CH_2)_3$	CO_2	C[NH+](C)CCCC(=O)[O-]
00052	$NH(CH_3)_2$	$(CH_2)_4$	CO_2	C[NH+](C)CCCCC(=O)[O-]
00053	$NH(CH_3)_2$	$(CH_2)_5$	CO_2	C[NH+](C)CCCCCC(=O)[O-]
00054	$NH(CH_3)_2$	CH(OH)	CO_2	C[NH+](C)C(O)C(=O)[O-]
00055	$NH(CH_3)_2$	$(CH(OH))_2$	CO_2	C[NH+](C)C(O)C(O)C(=O)[O-]
00056	$NH(CH_3)_2$	$(CH(OH))_3$	CO_2	C[NH+](C)C(O)C(O)C(O)C(=O)[O-]
00057	$NH(CH_3)_2$	$(CH(OH))_4$	CO_2	C[NH+](C)C(O)C(O)C(O)C(O)C(=O)[O-]
00058	$NH(CH_3)_2$	$(CH(OH))_5$	CO_2	C[NH+](C)C(O)C(O)C(O)C(O)C(O)C(=O)[O-]
00059	$NH(CH_3)_2$	CH(CH3)	CO_2	C[NH+](C)C(C)C(=O)[O-]
00060	$NH(CH_3)_2$	$(CH(CH3))_2$	CO_2	C[NH+](C)C(C)C(C)C(=O)[O-]
00061	$NH(CH_3)_2$	$(CH(CH3))_3$	CO_2	C[NH+](C)C(C)C(C)C(C)C(=O)[O-]
00062	$NH(CH_3)_2$	$(CH(CH3))_4$	CO_2	C[NH+](C)C(C)C(C)C(C)C(C)C(=O)[O-]
00063	$NH(CH_3)_2$	$(CH(CH3))_5$	CO_2	C[NH+](C)C(C)C(C)C(C)C(C)C(C)C(=O)[O-]
00064	$NH(CH_3)_2$		SO_3	C[NH+](C)S(=O)(=O)[O-]
00065	$NH(CH_3)_2$	CH_2	SO_3	C[NH+](C)CS(=O)(=O)[O-]
00066	$NH(CH_3)_2$	$(CH_2)_2$	SO_3	C[NH+](C)CCS(=O)(=O)[O-]
00067	$NH(CH_3)_2$	$(CH_2)_3$	SO_3	C[NH+](C)CCCS(=O)(=O)[O-]
00068	$NH(CH_3)_2$	$(CH_2)_4$	SO_3	C[NH+](C)CCCCS(=O)(=O)[O-]
00069	$NH(CH_3)_2$	$(CH_2)_5$	SO_3	C[NH+](C)CCCCCS(=O)(=O)[O-]
00070	$NH(CH_3)_2$	CH(OH)	SO_3	C[NH+](C)C(O)S(=O)(=O)[O-]
00071	$NH(CH_3)_2$	$(CH(OH))_2$	SO_3	C[NH+](C)C(O)C(O)S(=O)(=O)[O-]
00072	$NH(CH_3)_2$	$(CH(OH))_3$	SO_3	C[NH+](C)C(O)C(O)C(O)S(=O)(=O)[O-]
00073	$NH(CH_3)_2$	$(CH(OH))_4$	SO_3	C[NH+](C)C(O)C(O)C(O)C(O)S(=O)(=O)[O-]
00074	$NH(CH_3)_2$	$(CH(OH))_5$	SO_3	C[NH+](C)C(O)C(O)C(O)C(O)C(O)S(=O)(=O)[O-]
00075	$NH(CH_3)_2$	CH(CH3)	SO_3	C[NH+](C)C(C)S(=O)(=O)[O-]
00076	$NH(CH_3)_2$	$(CH(CH3))_2$	SO_3	C[NH+](C)C(C)C(C)S(=O)(=O)[O-]
00077	$NH(CH_3)_2$	$(CH(CH3))_3$	SO_3	C[NH+](C)C(C)C(C)C(C)S(=O)(=O)[O-]
00078	$NH(CH_3)_2$	$(CH(CH3))_4$	SO_3	C[NH+](C)C(C)C(C)C(C)C(C)C(C)S(=O)(=O)[O-]

00079	$NH(CH_3)_2$	$(CH(CH3))_5$	SO_3	C[NH+](C)C(C)C(C)C(C)C(C)C(C)C(C)S(=O)(=O)[O-]
00080	$NH(CH_3)_2$		OPO_3H	C[NH+](C)OP(=O)(O)[O-]
00081	$NH(CH_3)_2$	CH_2	OPO_3H	C[NH+](C)COP(=O)(O)[O-]
00082	$NH(CH_3)_2$	$(CH_2)_2$	OPO_3H	C[NH+](C)CCOP(=O)(O)[O-]
00083	$NH(CH_3)_2$	$(CH_2)_3$	OPO_3H	C[NH+](C)CCCOP(=O)(O)[O-]
00084	$NH(CH_3)_2$	$(CH_2)_4$	OPO_3H	C[NH+](C)CCCCOP(=O)(O)[O-]
00085	$NH(CH_3)_2$	$(CH_2)_5$	OPO_3H	C[NH+](C)CCCCCOP(=O)(O)[O-]
00086	$NH(CH_3)_2$	CH(OH)	OPO_3H	C[NH+](C)C(O)OP(=O)(O)[O-]
00087	$NH(CH_3)_2$	$(CH(OH))_2$	OPO_3H	C[NH+](C)C(O)C(O)OP(=O)(O)[O-]
00088	$NH(CH_3)_2$	$(CH(OH))_3$	OPO_3H	C[NH+](C)C(O)C(O)C(O)OP(=O)(O)[O-]
00089	$NH(CH_3)_2$	$(CH(OH))_4$	OPO_3H	C[NH+](C)C(O)C(O)C(O)C(O)OP(=O)(O)[O-]
00090	$NH(CH_3)_2$	$(CH(OH))_5$	OPO_3H	C[NH+](C)C(O)C(O)C(O)C(O)C(O)OP(=O)(O)[O-]
00091	$NH(CH_3)_2$	CH(CH3)	OPO_3H	C[NH+](C)C(C)OP(=O)(O)[O-]
00092	$NH(CH_3)_2$	$(CH(CH3))_2$	OPO_3H	C[NH+](C)C(C)C(C)OP(=O)(O)[O-]
00093	$NH(CH_3)_2$	$(CH(CH3))_3$	OPO_3H	C[NH+](C)C(C)C(C)C(C)OP(=O)(O)[O-]
00094	$NH(CH_3)_2$	$(CH(CH3))_4$	OPO_3H	C[NH+](C)C(C)C(C)C(C)C(C)OP(=O)(O)[O-]
00095	$NH(CH_3)_2$	$(CH(CH3))_5$	OPO_3H	C[NH+](C)C(C)C(C)C(C)C(C)C(C)OP(=O)(O)[O-]
00096	$NH_2(CH_3)$		CO_2	C[NH2+]C(=O)[O-]
00097	$NH_2(CH_3)$	CH_2	CO_2	C[NH2+]CC(=O)[O-]
00098	$NH_2(CH_3)$	$(CH_2)_2$	CO_2	C[NH2+]CCC(=O)[O-]
00099	$NH_2(CH_3)$	$(CH_2)_3$	CO_2	C[NH2+]CCCC(=O)[O-]
00100	$NH_2(CH_3)$	$(CH_2)_4$	CO_2	C[NH2+]CCCCC(=O)[O-]
00101	$NH_2(CH_3)$	$(CH_2)_5$	CO_2	C[NH2+]CCCCCC(=O)[O-]
00102	$NH_2(CH_3)$	CH(OH)	CO_2	C[NH2+]C(O)C(=O)[O-]
00103	$NH_2(CH_3)$	$(CH(OH))_2$	CO_2	C[NH2+]C(O)C(O)C(=O)[O-]
00104	$NH_2(CH_3)$	$(CH(OH))_3$	CO_2	C[NH2+]C(O)C(O)C(O)C(=O)[O-]
00105	$NH_2(CH_3)$	$(CH(OH))_4$	CO_2	C[NH2+]C(O)C(O)C(O)C(O)C(=O)[O-]
00106	$NH_2(CH_3)$	$(CH(OH))_5$	CO_2	C[NH2+]C(O)C(O)C(O)C(O)C(O)C(=O)[O-]
00107	$NH_2(CH_3)$	CH(CH3)	CO_2	C[NH2+]C(C)C(=O)[O-]
00108	$NH_2(CH_3)$	$(CH(CH3))_2$	CO_2	C[NH2+]C(C)C(C)C(=O)[O-]
00109	$NH_2(CH_3)$	$(CH(CH3))_3$	CO_2	C[NH2+]C(C)C(C)C(C)C(=O)[O-]
00110	$NH_2(CH_3)$	$(CH(CH3))_4$	CO_2	C[NH2+]C(C)C(C)C(C)C(C)C(=O)[O-]
00111	$NH_2(CH_3)$	$(CH(CH3))_5$	CO_2	C[NH2+]C(C)C(C)C(C)C(C)C(C)C(=O)[O-]
00112	$NH_2(CH_3)$		SO_3	C[NH2+]S(=O)(=O)[O-]
00113	$NH_2(CH_3)$	CH_2	SO_3	C[NH2+]CS(=O)(=O)[O-]
00114	$NH_2(CH_3)$	$(CH_2)_2$	SO_3	C[NH2+]CCS(=O)(=O)[O-]
00115	$NH_2(CH_3)$	$(CH_2)_3$	SO_3	C[NH2+]CCCS(=O)(=O)[O-]
00116	$NH_2(CH_3)$	$(CH_2)_4$	SO_3	C[NH2+]CCCCS(=O)(=O)[O-]
00117	$NH_2(CH_3)$	$(CH_2)_5$	SO_3	C[NH2+]CCCCCS(=O)(=O)[O-]
00118	$NH_2(CH_3)$	CH(OH)	SO_3	C[NH2+]C(O)S(=O)(=O)[O-]
00119	$NH_2(CH_3)$	$(CH(OH))_2$	SO_3	C[NH2+]C(O)C(O)S(=O)(=O)[O-]

00120	$NH_2(CH_3)$	$(CH(OH))_3$	SO_3	C[NH2+]C(O)C(O)C(O)S(=O)(=O)[O-]
00121	$NH_2(CH_3)$	$(CH(OH))_4$	SO_3	C[NH2+]C(O)C(O)C(O)C(O)S(=O)(=O)[O-]
00122	$NH_2(CH_3)$	$(CH(OH))_5$	SO_3	C[NH2+]C(O)C(O)C(O)C(O)C(O)S(=O)(=O)[O-]
00123	$NH_2(CH_3)$	CH(CH3)	SO_3	C[NH2+]C(C)S(=O)(=O)[O-]
00124	$NH_2(CH_3)$	$(CH(CH3))_2$	SO_3	C[NH2+]C(C)C(C)S(=O)(=O)[O-]
00125	$NH_2(CH_3)$	$(CH(CH3))_3$	SO_3	C[NH2+]C(C)C(C)C(C)S(=O)(=O)[O-]
00126	$NH_2(CH_3)$	$(CH(CH3))_4$	SO_3	C[NH2+]C(C)C(C)C(C)C(C)S(=O)(=O)[O-]
00127	$NH_2(CH_3)$	$(CH(CH3))_5$	SO_3	C[NH2+]C(C)C(C)C(C)C(C)C(C)S(=O)(=O)[O-]
*00128	$NH_2(CH_3)$		OPO_3H	C[NH2+]OP(=O)(O)[O-]
00129	$NH_2(CH_3)$	CH_2	OPO_3H	C[NH2+]COP(=O)(O)[O-]
00130	$NH_2(CH_3)$	$(CH_2)_2$	OPO_3H	C[NH2+]CCOP(=O)(O)[O-]
00131	$NH_2(CH_3)$	$(CH_2)_3$	OPO_3H	C[NH2+]CCCOP(=O)(O)[O-]
00132	$NH_2(CH_3)$	$(CH_2)_4$	OPO_3H	C[NH2+]CCCCOP(=O)(O)[O-]
00133	$NH_2(CH_3)$	$(CH_2)_5$	OPO_3H	C[NH2+]CCCCCOP(=O)(O)[O-]
00134	$NH_2(CH_3)$	CH(OH)	OPO_3H	C[NH2+]C(O)OP(=O)(O)[O-]
00135	$NH_2(CH_3)$	$(CH(OH))_2$	OPO_3H	C[NH2+]C(O)C(O)OP(=O)(O)[O-]
00136	$NH_2(CH_3)$	$(CH(OH))_3$	OPO_3H	C[NH2+]C(O)C(O)C(O)OP(=O)(O)[O-]
00137	$NH_2(CH_3)$	$(CH(OH))_4$	OPO_3H	C[NH2+]C(O)C(O)C(O)C(O)OP(=O)(O)[O-]
00138	$NH_2(CH_3)$	$(CH(OH))_5$	OPO_3H	C[NH2+]C(O)C(O)C(O)C(O)C(O)OP(=O)(O)[O-]
00139	$NH_2(CH_3)$	CH(CH3)	OPO_3H	C[NH2+]C(C)OP(=O)(O)[O-]
00140	$NH_2(CH_3)$	$(CH(CH3))_2$	OPO_3H	C[NH2+]C(C)C(C)OP(=O)(O)[O-]
00141	$NH_2(CH_3)$	$(CH(CH3))_3$	OPO_3H	C[NH2+]C(C)C(C)C(C)OP(=O)(O)[O-]
00142	$NH_2(CH_3)$	$(CH(CH3))_4$	OPO_3H	C[NH2+]C(C)C(C)C(C)C(C)OP(=O)(O)[O-]
00143	$NH_2(CH_3)$	$(CH(CH3))_5$	OPO_3H	C[NH2+]C(C)C(C)C(C)C(C)C(C)OP(=O)(O)[O-]
00144	NH_3		CO_2	[NH3+]C(=O)[O-]
00145	NH_3	CH_2	CO_2	[NH3+]CC(=O)[O-]
00146	NH_3	$(CH_2)_2$	CO_2	[NH3+]CCC(=O)[O-]
00147	NH_3	$(CH_2)_3$	CO_2	[NH3+]CCCC(=O)[O-]
00148	NH_3	$(CH_2)_4$	CO_2	[NH3+]CCCCC(=O)[O-]
00149	NH_3	$(CH_2)_5$	CO_2	[NH3+]CCCCCC(=O)[O-]
00150	NH_3	CH(OH)	CO_2	[NH3+]C(O)C(=O)[O-]
00151	NH_3	$(CH(OH))_2$	CO_2	[NH3+]C(O)C(O)C(=O)[O-]
00152	NH_3	$(CH(OH))_3$	CO_2	[NH3+]C(O)C(O)C(O)C(=O)[O-]
00153	NH_3	$(CH(OH))_4$	CO_2	[NH3+]C(O)C(O)C(O)C(O)C(=O)[O-]
00154	NH_3	$(CH(OH))_5$	CO_2	[NH3+]C(O)C(O)C(O)C(O)C(O)C(=O)[O-]
00155	NH_3	CH(CH3)	CO_2	[NH3+]C(C)C(=O)[O-]
00156	NH_3	$(CH(CH3))_2$	CO_2	[NH3+]C(C)C(C)C(=O)[O-]
00157	NH_3	$(CH(CH3))_3$	CO_2	[NH3+]C(C)C(C)C(C)C(=O)[O-]
00158	NH_3	$(CH(CH3))_4$	CO_2	[NH3+]C(C)C(C)C(C)C(C)C(=O)[O-]
00159	NH_3	$(CH(CH3))_5$	CO_2	[NH3+]C(C)C(C)C(C)C(C)C(C)C(=O)[O-]
*00160	NH_3		SO_3	[NH3+]S(=O)(=O)[O-]

00161	NH_3	CH_2	SO_3	[NH3+]CS(=O)(=O)[O-]
00162	NH_3	$(CH_2)_2$	SO_3	[NH3+]CCS(=O)(=O)[O-]
00163	NH_3	$(CH_2)_3$	SO_3	[NH3+]CCCS(=O)(=O)[O-]
00164	NH_3	$(CH_2)_4$	SO_3	[NH3+]CCCCS(=O)(=O)[O-]
00165	NH_3	$(CH_2)_5$	SO_3	[NH3+]CCCCCS(=O)(=O)[O-]
00166	NH_3	CH(OH)	SO_3	[NH3+]C(O)S(=O)(=O)[O-]
00167	NH_3	$(CH(OH))_2$	SO_3	[NH3+]C(O)C(O)S(=O)(=O)[O-]
00168	NH_3	$(CH(OH))_3$	SO_3	[NH3+]C(O)C(O)C(O)S(=O)(=O)[O-]
00169	NH_3	$(CH(OH))_4$	SO_3	[NH3+]C(O)C(O)C(O)C(O)S(=O)(=O)[O-]
00170	NH_3	$(CH(OH))_5$	SO_3	[NH3+]C(O)C(O)C(O)C(O)C(O)S(=O)(=O)[O-]
00171	NH_3	CH(CH3)	SO_3	[NH3+]C(C)S(=O)(=O)[O-]
00172	NH_3	$(CH(CH3))_2$	SO_3	[NH3+]C(C)C(C)S(=O)(=O)[O-]
00173	NH_3	$(CH(CH3))_3$	SO_3	[NH3+]C(C)C(C)C(C)S(=O)(=O)[O-]
00174	NH_3	$(CH(CH3))_4$	SO_3	[NH3+]C(C)C(C)C(C)C(C)S(=O)(=O)[O-]
00175	NH_3	$(CH(CH3))_5$	SO_3	[NH3+]C(C)C(C)C(C)C(C)C(C)S(=O)(=O)[O-]
00176	NH_3		OPO_3H	[NH3+]OP(=O)(O)[O-]
00177	NH_3	CH_2	OPO_3H	[NH3+]COP(=O)(O)[O-]
00178	NH_3	$(CH_2)_2$	OPO_3H	[NH3+]CCOP(=O)(O)[O-]
00179	NH_3	$(CH_2)_3$	OPO_3H	[NH3+]CCCOP(=O)(O)[O-]
00180	NH_3	$(CH_2)_4$	OPO_3H	[NH3+]CCCCOP(=O)(O)[O-]
00181	NH_3	$(CH_2)_5$	OPO_3H	[NH3+]CCCCCOP(=O)(O)[O-]
00182	NH_3	CH(OH)	OPO_3H	[NH3+]C(O)OP(=O)(O)[O-]
00183	NH_3	$(CH(OH))_2$	OPO_3H	[NH3+]C(O)C(O)OP(=O)(O)[O-]
00184	NH_3	$(CH(OH))_3$	OPO_3H	[NH3+]C(O)C(O)C(O)OP(=O)(O)[O-]
00185	NH_3	$(CH(OH))_4$	OPO_3H	[NH3+]C(O)C(O)C(O)C(O)OP(=O)(O)[O-]
00186	NH_3	$(CH(OH))_5$	OPO_3H	[NH3+]C(O)C(O)C(O)C(O)C(O)OP(=O)(O)[O-]
00187	NH_3	CH(CH3)	OPO_3H	[NH3+]C(C)OP(=O)(O)[O-]
00188	NH_3	$(CH(CH3))_2$	OPO_3H	[NH3+]C(C)C(C)OP(=O)(O)[O-]
00189	NH_3	$(CH(CH3))_3$	OPO_3H	[NH3+]C(C)C(C)C(C)OP(=O)(O)[O-]
00190	NH_3	$(CH(CH3))_4$	OPO_3H	[NH3+]C(C)C(C)C(C)C(C)OP(=O)(O)[O-]
00191	NH_3	$(CH(CH3))_5$	OPO_3H	[NH3+]C(C)C(C)C(C)C(C)C(C)OP(=O)(O)[O-]
00192	$S(CH_3)_2$		CO_2	C[S+](C)C(=O)[O-]
00193	$S(CH_3)_2$	CH_2	CO_2	C[S+](C)CC(=O)[O-]
00194	$S(CH_3)_2$	$(CH_2)_2$	CO_2	C[S+](C)CCC(=O)[O-]
00195	$S(CH_3)_2$	$(CH_2)_3$	CO_2	C[S+](C)CCCC(=O)[O-]
00196	$S(CH_3)_2$	$(CH_2)_4$	CO_2	C[S+](C)CCCCC(=O)[O-]
00197	$S(CH_3)_2$	$(CH_2)_5$	CO_2	C[S+](C)CCCCCC(=O)[O-]
00198	$S(CH_3)_2$	CH(OH)	CO_2	C[S+](C)C(O)C(=O)[O-]
00199	$S(CH_3)_2$	$(CH(OH))_2$	CO_2	C[S+](C)C(O)C(O)C(=O)[O-]
00200	$S(CH_3)_2$	$(CH(OH))_3$	CO_2	C[S+](C)C(O)C(O)C(O)C(=O)[O-]
00201	$S(CH_3)_2$	$(CH(OH))_4$	CO_2	C[S+](C)C(O)C(O)C(O)C(O)C(=O)[O-]

00202	$S(CH_3)_2$	$(CH(OH))_5$	CO_2	C[S+](C)C(O)C(O)C(O)C(O)C(O)C(O)C(=O)[O-]
00203	$S(CH_3)_2$	CH(CH3)	CO_2	C[S+](C)C(C)C(=O)[O-]
00204	$S(CH_3)_2$	$(CH(CH3))_2$	CO_2	C[S+](C)C(C)C(C)C(=O)[O-]
00205	$S(CH_3)_2$	$(CH(CH3))_3$	CO_2	C[S+](C)C(C)C(C)C(C)C(C)C(=O)[O-]
00206	$S(CH_3)_2$	$(CH(CH3))_4$	CO_2	C[S+](C)C(C)C(C)C(C)C(C)C(C)C(C)C(=O)[O-]
00207	$S(CH_3)_2$	$(CH(CH3))_5$	CO_2	C[S+](C)C(C)C(C)C(C)C(C)C(C)C(C)C(C)C(C)C(=O)[O-]
00208	$S(CH_3)_2$		SO_3	C[S+](C)S(=O)(=O)[O-]
00209	$S(CH_3)_2$	CH_2	SO_3	C[S+](C)CS(=O)(=O)[O-]
00210	$S(CH_3)_2$	$(CH_2)_2$	SO_3	C[S+](C)CCS(=O)(=O)[O-]
00211	$S(CH_3)_2$	$(CH_2)_3$	SO_3	C[S+](C)CCCS(=O)(=O)[O-]
00212	$S(CH_3)_2$	$(CH_2)_4$	SO_3	C[S+](C)CCCCS(=O)(=O)[O-]
00213	$S(CH_3)_2$	$(CH_2)_5$	SO_3	C[S+](C)CCCCCS(=O)(=O)[O-]
00214	$S(CH_3)_2$	CH(OH)	SO_3	C[S+](C)C(O)S(=O)(=O)[O-]
00215	$S(CH_3)_2$	$(CH(OH))_2$	SO_3	C[S+](C)C(O)C(O)S(=O)(=O)[O-]
00216	$S(CH_3)_2$	$(CH(OH))_3$	SO_3	C[S+](C)C(O)C(O)C(O)S(=O)(=O)[O-]
00217	$S(CH_3)_2$	$(CH(OH))_4$	SO_3	C[S+](C)C(O)C(O)C(O)C(O)S(=O)(=O)[O-]
00218	$S(CH_3)_2$	$(CH(OH))_5$	SO_3	C[S+](C)C(O)C(O)C(O)C(O)C(O)S(=O)(=O)[O-]
00219	$S(CH_3)_2$	CH(CH3)	SO_3	C[S+](C)C(C)S(=O)(=O)[O-]
00220	$S(CH_3)_2$	$(CH(CH3))_2$	SO_3	C[S+](C)C(C)C(C)S(=O)(=O)[O-]
00221	$S(CH_3)_2$	$(CH(CH3))_3$	SO_3	C[S+](C)C(C)C(C)C(C)S(=O)(=O)[O-]
00222	$S(CH_3)_2$	$(CH(CH3))_4$	SO_3	C[S+](C)C(C)C(C)C(C)C(C)C(C)S(=O)(=O)[O-]
00223	$S(CH_3)_2$	$(CH(CH3))_5$	SO_3	C[S+](C)C(C)C(C)C(C)C(C)C(C)C(C)S(=O)(=O)[O-]
00224	$S(CH_3)_2$		OPO_3H	C[S+](C)OP(=O)(O)[O-]
00225	$S(CH_3)_2$	CH_2	OPO_3H	C[S+](C)COP(=O)(O)[O-]
00226	$S(CH_3)_2$	$(CH_2)_2$	OPO_3H	C[S+](C)CCOP(=O)(O)[O-]
00227	$S(CH_3)_2$	$(CH_2)_3$	OPO_3H	C[S+](C)CCCOP(=O)(O)[O-]
00228	$S(CH_3)_2$	$(CH_2)_4$	OPO_3H	C[S+](C)CCCCOP(=O)(O)[O-]
00229	$S(CH_3)_2$	$(CH_2)_5$	OPO_3H	C[S+](C)CCCCCOP(=O)(O)[O-]
00230	$S(CH_3)_2$	CH(OH)	OPO_3H	C[S+](C)C(O)OP(=O)(O)[O-]
00231	$S(CH_3)_2$	$(CH(OH))_2$	OPO_3H	C[S+](C)C(O)C(O)OP(=O)(O)[O-]
00232	$S(CH_3)_2$	$(CH(OH))_3$	OPO_3H	C[S+](C)C(O)C(O)C(O)OP(=O)(O)[O-]
00233	$S(CH_3)_2$	$(CH(OH))_4$	OPO_3H	C[S+](C)C(O)C(O)C(O)C(O)OP(=O)(O)[O-]
00234	$S(CH_3)_2$	$(CH(OH))_5$	OPO_3H	C[S+](C)C(O)C(O)C(O)C(O)C(O)OP(=O)(O)[O-]
00235	$S(CH_3)_2$	CH(CH3)	OPO_3H	C[S+](C)C(C)OP(=O)(O)[O-]
00236	$S(CH_3)_2$	$(CH(CH3))_2$	OPO_3H	C[S+](C)C(C)C(C)OP(=O)(O)[O-]
00237	$S(CH_3)_2$	$(CH(CH3))_3$	OPO_3H	C[S+](C)C(C)C(C)C(C)OP(=O)(O)[O-]
00238	$S(CH_3)_2$	$(CH(CH3))_4$	OPO_3H	C[S+](C)C(C)C(C)C(C)C(C)OP(=O)(O)[O-]
00239	$S(CH_3)_2$	$(CH(CH3))_5$	OPO_3H	C[S+](C)C(C)C(C)C(C)C(C)C(C)OP(=O)(O)[O-]

Table S2. Sample OPLS-AA compatible structure file (.gro) for molecule 00002 with chemical formula $N(CH_3)_3(CH_2)_2CO_2$.

```
00002
   22
    100002  C00    1   0.708   0.524   0.518
    100002  N01    2   0.559   0.524   0.518
    100002  C02    3   0.512   0.524   0.659
    100002  C03    4   0.515   0.650   0.450
    100002  C04    5   0.516   0.398   0.447
    100002  C05    6   0.367   0.359   0.457
    100002  C06    7   0.275   0.472   0.420
    100002  O07    8   0.287   0.516   0.304
    100002  O08    9   0.211   0.525   0.513
    100002  H09   10   0.749   0.610   0.569
    100002  H0A   11   0.747   0.524   0.416
    100002  H0B   12   0.749   0.435   0.568
    100002  H0C   13   0.551   0.608   0.716
    100002  H0D   14   0.539   0.431   0.711
    100002  H0E   15   0.403   0.530   0.665
    100002  H0F   16   0.573   0.738   0.479
    100002  H0G   17   0.412   0.674   0.472
    100002  H0H   18   0.519   0.640   0.341
    100002  H0I   19   0.574   0.312   0.482
    100002  H0J   20   0.539   0.407   0.341
    100002  H0K   21   0.341   0.324   0.557
    100002  H0M   22   0.345   0.276   0.390
   1.00000   1.00000   1.00000
```

Table S3. Sample OPLS-AA[4] compatible topology file (.itp) for molecule 00002 with chemical formula $N(CH_3)_3(CH_2)_2CO_2$.

```
[ atomtypes ]
  opls_807  O807    15.9990     0.000    A    2.96000E-01   8.78640E-01
  opls_818  H818     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_808  O808    15.9990     0.000    A    2.96000E-01   8.78640E-01
  opls_813  H813     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_802  C802    12.0110     0.000    A    3.50000E-01   2.76144E-01
  opls_815  H815     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_801  N801    14.0070     0.000    A    3.25000E-01   7.11280E-01
  opls_803  C803    12.0110     0.000    A    3.50000E-01   2.76144E-01
  opls_814  H814     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_821  H821     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_820  H820     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_811  H811     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_810  H810     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_816  H816     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_800  C800    12.0110     0.000    A    3.50000E-01   2.76144E-01
  opls_805  C805    12.0110     0.000    A    3.50000E-01   2.76144E-01
  opls_806  C806    12.0110     0.000    A    3.55000E-01   2.92880E-01
  opls_819  H819     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_804  C804    12.0110     0.000    A    3.50000E-01   2.76144E-01
  opls_817  H817     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_812  H812     1.0080     0.000    A    2.50000E-01   1.25520E-01
  opls_809  H809     1.0080     0.000    A    2.50000E-01   1.25520E-01
[ moleculetype ]
; Name               nrexcl
00002                   3
[ atoms ]
     1   opls_800      1  00002   C00      1  -0.142484    12.0110
     2   opls_801      1  00002   N01      1   0.300727    14.0070
     3   opls_802      1  00002   C02      1  -0.108037    12.0110
     4   opls_803      1  00002   C03      1   0.035732    12.0110
     5   opls_804      1  00002   C04      1   0.268680    12.0110
     6   opls_805      1  00002   C05      1  -0.234254    12.0110
     7   opls_806      1  00002   C06      1   0.752400    12.0110
     8   opls_807      1  00002   O07      1  -0.671895    15.9990
     9   opls_808      1  00002   O08      1  -0.692406    15.9990
    10   opls_809      1  00002   H09      1   0.079946     1.0080
    11   opls_810      1  00002   H0A      1   0.049012     1.0080
    12   opls_811      1  00002   H0B      1   0.080555     1.0080
    13   opls_812      1  00002   H0C      1   0.037719     1.0080
    14   opls_813      1  00002   H0D      1   0.041116     1.0080
    15   opls_814      1  00002   H0E      1   0.112866     1.0080
    16   opls_815      1  00002   H0F      1   0.024096     1.0080
    17   opls_816      1  00002   H0G      1   0.049359     1.0080
    18   opls_817      1  00002   H0H      1   0.026839     1.0080
    19   opls_818      1  00002   H0I      1  -0.036574     1.0080
    20   opls_819      1  00002   H0J      1  -0.023940     1.0080
    21   opls_820      1  00002   H0K      1   0.011666     1.0080
    22   opls_821      1  00002   H0M      1   0.038878     1.0080
[ bonds ]
    2     1     1      0.1471 307105.600
    3     2     1      0.1471 307105.600
    4     2     1      0.1471 307105.600
    5     2     1      0.1471 307105.600
    6     5     1      0.1529 224262.400
    7     6     1      0.1522 265265.600
    8     7     1      0.1250 548940.800
    9     7     1      0.1250 548940.800
   10     1     1      0.1090 284512.000
```

```
   11     1     1      0.1090 284512.000
   12     1     1      0.1090 284512.000
   13     3     1      0.1090 284512.000
   14     3     1      0.1090 284512.000
   15     3     1      0.1090 284512.000
   16     4     1      0.1090 284512.000
   17     4     1      0.1090 284512.000
   18     4     1      0.1090 284512.000
   19     5     1      0.1090 284512.000
   20     5     1      0.1090 284512.000
   21     6     1      0.1090 284512.000
   22     6     1      0.1090 284512.000
[ angles ]
;  ai    aj    ak funct            c0            c1            c2            c3
    1     2     3     1    113.000    418.400
    1     2     4     1    113.000    418.400
    1     2     5     1    113.000    418.400
    2     5     6     1    111.200    669.440
    5     6     7     1    111.100    527.184
    6     7     8     1    117.000    585.760
    6     7     9     1    117.000    585.760
    2     1    10     1    109.500    292.880
    2     1    11     1    109.500    292.880
    2     1    12     1    109.500    292.880
    2     3    13     1    109.500    292.880
    2     3    14     1    109.500    292.880
    2     3    15     1    109.500    292.880
    2     4    16     1    109.500    292.880
    2     4    17     1    109.500    292.880
    2     4    18     1    109.500    292.880
    2     5    19     1    109.500    292.880
    2     5    20     1    109.500    292.880
    5     6    21     1    110.700    313.800
    5     6    22     1    110.700    313.800
   13     3    15     1    107.800    276.144
    7     6    22     1    109.500    292.880
   21     6    22     1    107.800    276.144
    6     5    19     1    110.700    313.800
    8     7     9     1    126.000    669.440
   17     4    18     1    107.800    276.144
   16     4    17     1    107.800    276.144
    6     5    20     1    110.700    313.800
   19     5    20     1    107.800    276.144
   11     1    12     1    107.800    276.144
    3     2     4     1    113.000    418.400
   13     3    14     1    107.800    276.144
    3     2     5     1    113.000    418.400
    4     2     5     1    113.000    418.400
   16     4    18     1    107.800    276.144
   10     1    12     1    107.800    276.144
   10     1    11     1    107.800    276.144
   14     3    15     1    107.800    276.144
    7     6    21     1    109.500    292.880
[ dihedrals ]
; IMPROPER DIHEDRAL ANGLES
;  ai    aj    ak    al funct            c0            c1            c2            c3
c4            c5
     8     7     9     6    4        180.000     43.932     2
[ dihedrals ]
; PROPER DIHEDRAL ANGLES
;  ai    aj    ak    al funct            c0            c1            c2            c3
c4            c5
    7    6    5    2        3      -8.786  23.849  -8.368  -6.694  -0.000   0.000
```

```
     6     5     2     1         3        3.042  -1.351   0.519  -2.209  -0.000   0.000
     6     5     2     4         3        3.042  -1.351   0.519  -2.209  -0.000   0.000
     6     5     2     3         3        3.042  -1.351   0.519  -2.209  -0.000   0.000
    21     6     7     8         3        0.000   0.000   0.000  -0.000  -0.000   0.000
    22     6     7     8         3        0.000   0.000   0.000  -0.000  -0.000   0.000
    21     6     7     9         3        0.000   0.000   0.000  -0.000  -0.000   0.000
    22     6     7     9         3        0.000   0.000   0.000  -0.000  -0.000   0.000
    20     5     6     7         3       -0.209  -0.628   0.000   0.837  -0.000   0.000
    19     5     6     7         3       -0.209  -0.628   0.000   0.837  -0.000   0.000
    22     6     5    19         3        0.628   1.883   0.000  -2.510  -0.000   0.000
    21     6     5    20         3        0.628   1.883   0.000  -2.510  -0.000   0.000
    22     6     5    20         3        0.628   1.883   0.000  -2.510  -0.000   0.000
    21     6     5    19         3        0.628   1.883   0.000  -2.510  -0.000   0.000
    21     6     5     2         3        0.803   2.410   0.000  -3.213  -0.000   0.000
    22     6     5     2         3        0.803   2.410   0.000  -3.213  -0.000   0.000
    13     3     2     5         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    17     4     2     5         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    12     1     2     5         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    14     3     2     5         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    12     1     2     4         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    11     1     2     5         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    10     1     2     5         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    18     4     2     5         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    11     1     2     4         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    20     5     2     4         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    19     5     2     3         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    20     5     2     3         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    16     4     2     3         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    13     3     2     4         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    16     4     2     5         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    14     3     2     4         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    10     1     2     3         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    11     1     2     3         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    12     1     2     3         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    13     3     2     1         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    14     3     2     1         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    15     3     2     1         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    17     4     2     3         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    17     4     2     1         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    16     4     2     1         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    19     5     2     1         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    20     5     2     1         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    15     3     2     5         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    15     3     2     4         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    10     1     2     4         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    18     4     2     3         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    19     5     2     4         3        0.632   1.895   0.000  -2.527  -0.000   0.000
    18     4     2     1         3        0.632   1.895   0.000  -2.527  -0.000   0.000
     9     7     6     5         3        7.008   8.473  -4.184  -11.297  -0.000   0.000
     8     7     6     5         3        7.008   8.473  -4.184  -11.297  -0.000   0.000
[ pairs ]
     1     6     1
     3     6     1
     2     7     1
     4     6     1
     5     8     1
     3    10     1
     5     9     1
     4    10     1
     3    11     1
     1    13     1
     5    10     1
     4    11     1
```

```
 3    12    1
 1    14    1
 5    11    1
 4    12    1
 1    15    1
 5    12    1
 4    13    1
 1    16    1
 5    13    1
 4    14    1
 1    17    1
 5    14    1
 4    15    1
 3    16    1
 1    18    1
 5    15    1
 3    17    1
 1    19    1
 5    16    1
 3    18    1
 1    20    1
 5    17    1
 3    19    1
 5    18    1
 4    19    1
 3    20    1
 2    21    1
 4    20    1
 2    22    1
 7    19    1
 7    20    1
 8    21    1
 9    21    1
 8    22    1
 9    22    1
19    21    1
20    21    1
19    22    1
20    22    1
```

Table S4. Minimization simulation parameters. All unstated parameters are left as default GROMACS *mdrun* values.

Description	Parameter value(s)	Units
Run control		
integrator	steep	
emtol	0.01	kJ/mol/nm
emstep	0.001	nm
nsteps	10000000	steps

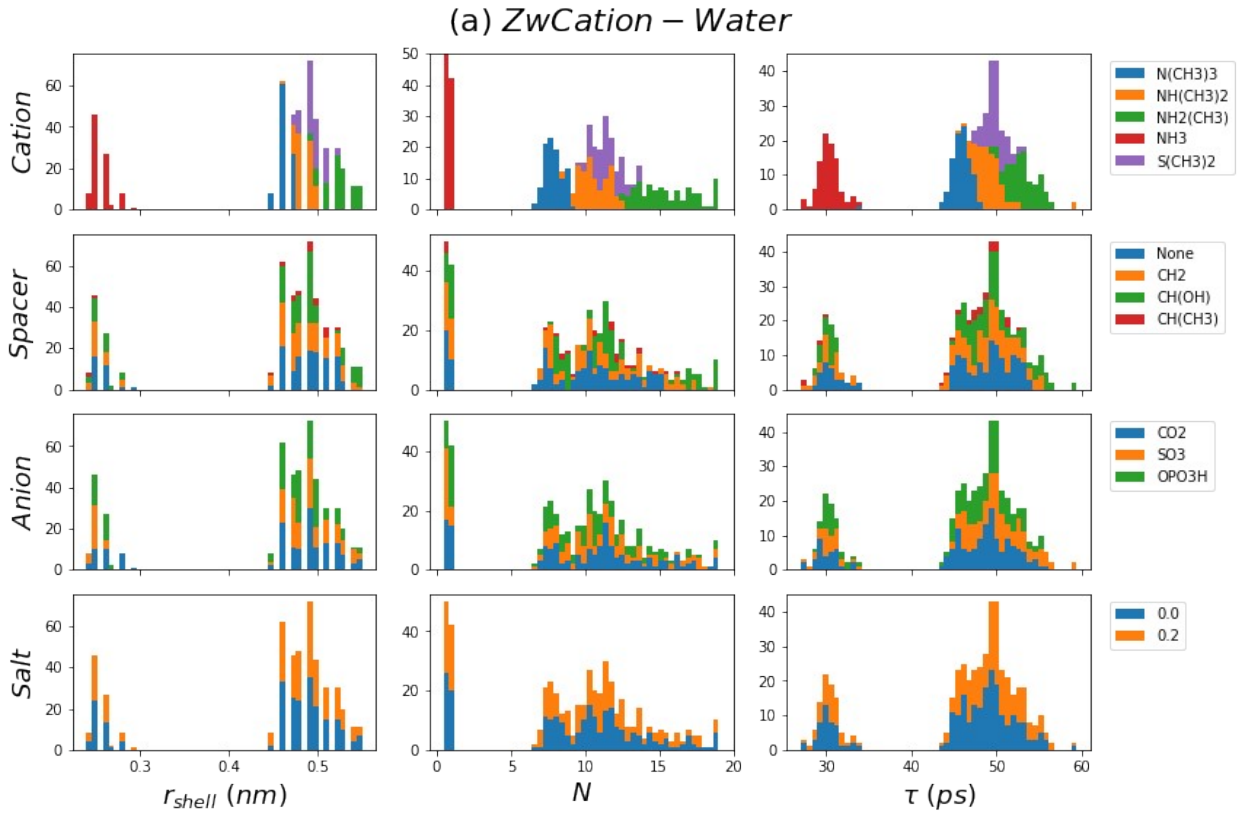
Table S5. Isothermal-isobaric (NPT) ensemble simulation parameters. All unstated parameters are left as default GROMACS *mdrun* values.

Description	Parameter value(s)	Units
Run control		
integrator	md	
dt	0.0001	ps
nsteps	5000000	steps
Output control		
nstxout	10000	steps
nstvout	10000	steps
nstenergy	10000	steps
nstlog	10000	steps
Bonds		
constraint_algorithm	lincs	
Neighbor searching		
cutoff-scheme	Verlet	
ns_type	grid	
nstlist	10	steps
rlist	1.0	nm
Velocity generation		
gen-vel	yes	
gen-temp	298	K
Van der Waals		
rvdw	1.1	nm
Electrostatics		
coulombtype	PME	
rcoulomb	1.1	nm
Pressure coupling		
pcoupl	Berendsen	
pcoupltype	isotropic	
tau_p	0.5	ps
ref_p	1.0	bar
compressibility	4.5e-5	bar^{-1}
refcoord_scaling	all	
Temperature coupling		
tcoupl	Berendsen	
tc-grps	System	
tau_t	0.1	ps
ref_t	298	bar

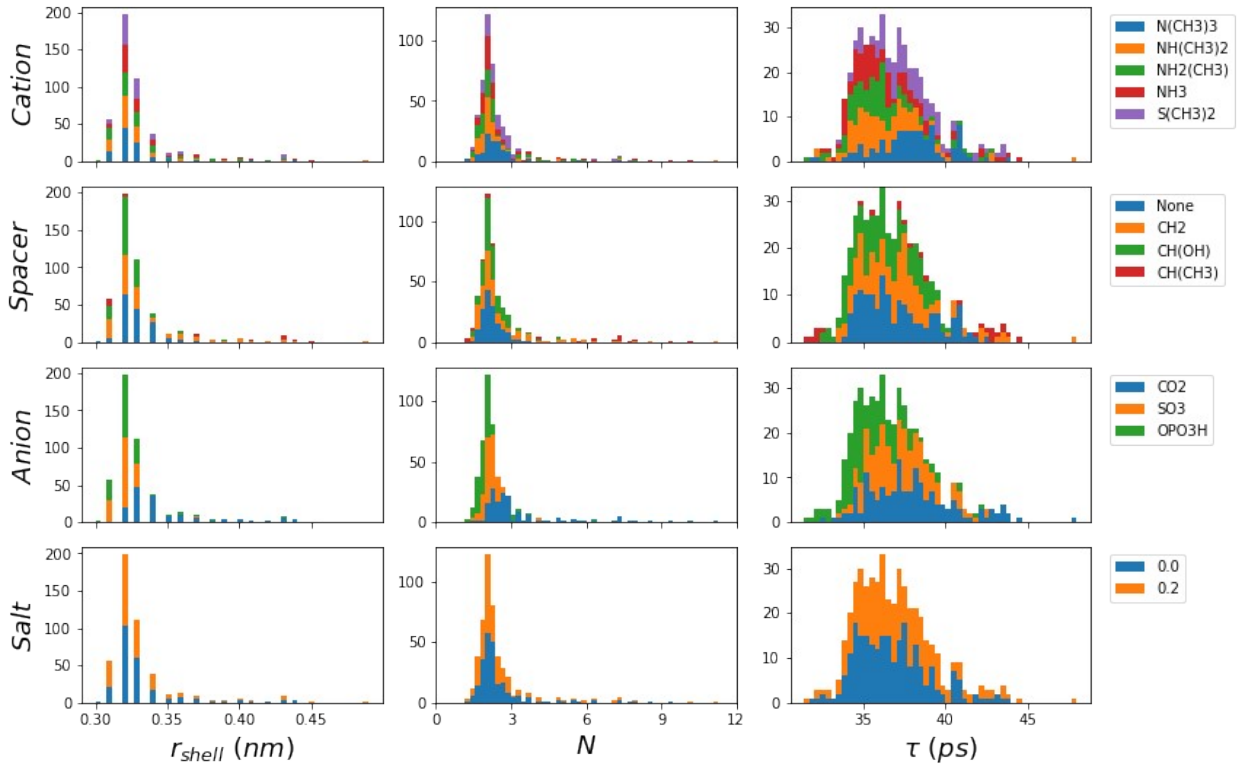
Table S6. Canonical (NVT) ensemble simulation parameters. All unstated parameters are left as default GROMACS *mdrun* values.

Description	Parameter value(s)	Units
Run control		
integrator	md	
dt	0.0005	ps
nsteps	20000000	steps
Output control		
nstxout	20000	steps
nstvout	200000	steps
nstenergy	200000	steps
nstlog	200000	steps
nstxout-compressed	20000	
Bonds		
constraint_algorithm	lincs	
Neighbor searching		
cutoff-scheme	Verlet	
ns_type	grid	
nstlist	10	steps
rlist	1.0	nm
Velocity generation		
gen-vel	yes	
gen-temp	298	K
Van der Waals		
rvdw	1.1	nm
Electrostatics		
coulombtype	PME	
fourierspacing	0.16	nm
rcoulomb	1.1	nm
Pressure coupling		
pcoupl	no	
Temperature coupling		
tcoupl	V-rescale	
tc-grps	System	
tau_t	0.1	ps
ref_t	298	bar

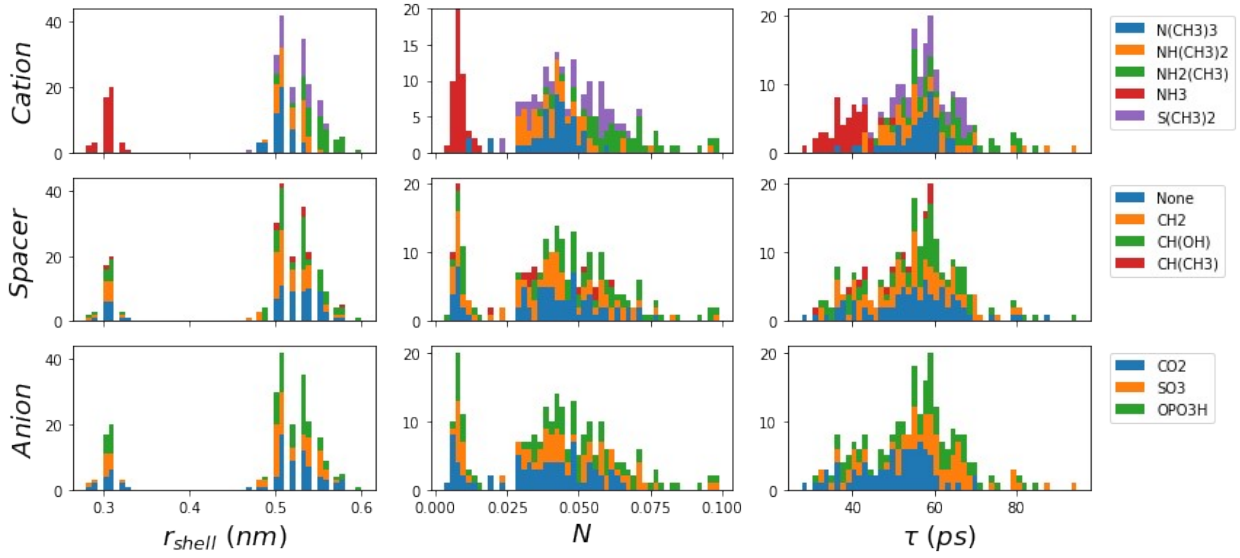
Figure S3. Distribution of association properties with changing zwitterion cation (a, c) and anion (b, d) subunit chemistries for interactions with water (a, b) and salt ions (c, d).



(b) *ZwAnion − Water*



(c) *ZwCation − Cl^-*



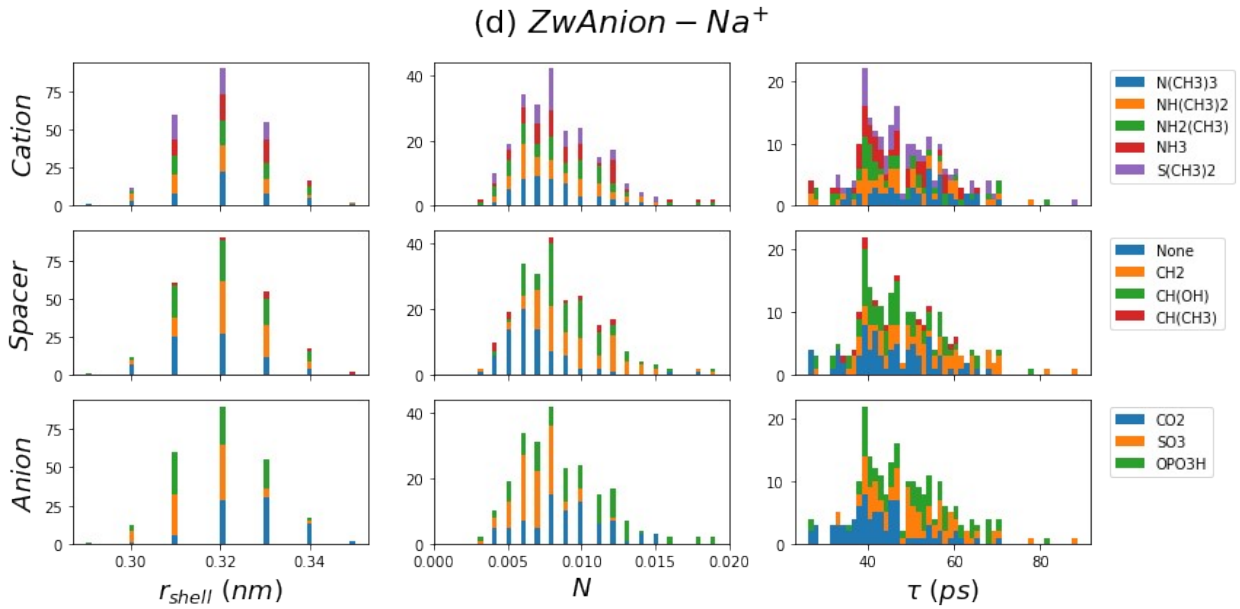

(d) ZwAnion − Na+
Cation
Spacer
Anion
N(CH3)3
NH(CH3)2
NH2(CH3)
NH3
S(CH3)2
None
CH2
CH(OH)
CH(CH3)
CO2
SO3
OPO3H
r_shell (nm)
N
τ (ps)

Figure S4. Correlation plots between the coordination shell radius and number of species within the coordination shell. The correlation coefficient, ρ, close to 1 implies a strong correlation.

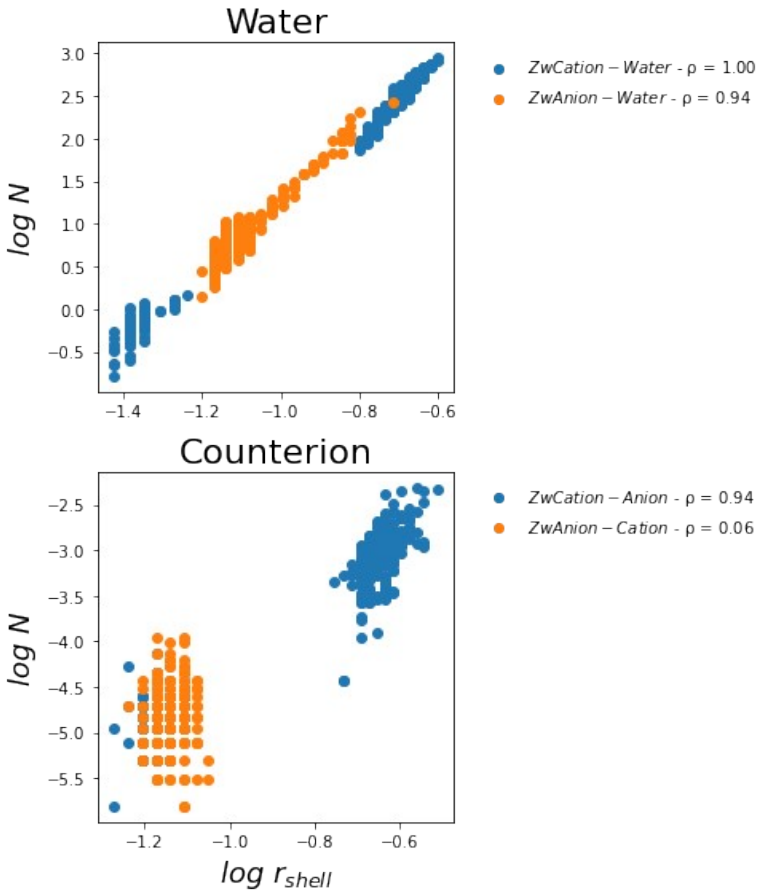


Table S7. p-values from MANOVA evaluated by Pillai's trace. α-level of 0.05 used to determine statistical significance.

Factor	ZwCation-Water	ZwAnion-Water	ZwCation-Cl^-	ZwAnion-Na^+
Cation	0.0000	0.0000	0.0000	0.0000
Spacer	0.0000	0.0000	0.0000	0.0000
Anion	0.0000	0.0000	0.0000	0.0000
CSL	0.0000	0.0000	0.0000	0.0000
Salt	0.0015	0.0144	0.0000	0.0000

References

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