

Interactions between Artificial Channel Protein, Water Molecules and Ions based on Theoretical Approaches

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Supplementary Material – Table S1

Table S1. Atomic coordinates of the interaction models used in the SAPT and AIM study.

The XYZ format is used throughout. The structures with water were optimized at the ω B97XD/6-311++G(d,p) level of theory in the gas phase or with PCM implicit solvent (water). A first series of models with Na⁺ and Cl⁻ ions was obtained with atom replacement scheme, i.e. the ions were placed at the water oxygen atom coordinates (and the water protons were removed). These models are not shown below. A second series of models containing the Na⁺ and Cl⁻ ions was obtained through optimization of the atom replacement models at the ω B97XD/6-311++G(d,p) level of theory in the gas phase or with PCM implicit solvent (water). The coordinates of the water molecule or small ions are labeled with blue color.

Asp-Lys-Water model, gas phase:

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45
ASP_LYS_GAS.log   Energy: -656440.7064657
C      3.14696      -1.00365      -0.84544
C      2.50730      -1.96283       0.15555
N      2.86113      -3.37658       0.04297
C      2.95823       0.45548      -0.42876
O      2.88850       0.69272       0.79676
O      2.88901       1.31314      -1.35256
C      0.98285      -1.82023       0.17012
N      0.32783      -2.73604       0.89793
O      0.40463      -0.90201      -0.41552
N      1.17410       3.06228      -0.65356
C     -0.07043       2.36183      -1.08487
C     -1.15867       2.36474      -0.02297
C     -2.43405       1.71262      -0.57189
C     -3.39907       1.16387       0.49156
C     -3.18313      -0.32151       0.86232
C     -3.48432      -1.18134      -0.37131
N     -2.42398      -1.69654      -1.03992
N     -1.90015      -0.65553       1.47872
O     -4.63591      -1.35028      -0.73186
H      2.74379      -3.70724      -0.90871
H      2.81533      -1.62848       1.15163
H      4.22398      -1.20172      -0.87700
H      2.75262      -1.14077      -1.85432
H     -1.11737      -0.29761       0.93776
H     -3.96608      -0.59642       1.57303
H     -4.42810       1.25204       0.13364
H     -3.32893       1.76361       1.40671
H     -2.15468       0.90400      -1.25654
H     -2.95885       2.44672      -1.19098
H     -1.37525       3.38732       0.30839
H     -0.78491       1.83275       0.85607
H      0.21698       1.33234      -1.30717
H     -0.41731       2.82413      -2.01198
H      1.24402       3.11180       0.38107
H      2.03475       2.44157      -0.97220
H      1.23861       4.00299      -1.02688
H      3.83108      -3.51952       0.29444
H      0.84867      -3.50405       1.29013
H     -0.64864      -2.57748       1.12303
H     -1.46152      -1.44884      -0.83313
H     -2.62411      -2.19248      -1.89301
H     -1.84018      -0.23589       2.39892
O      1.62539       2.62405       2.03611
H      2.18288       1.88460       1.67861
H      2.13366       3.04868       2.72624
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Asp-Lys-Water model, PCM water solvation:

45

ASP_LYS_PCM.log Energy: -656460.0719475

C	-1.23551	-2.54271	-0.64316
C	-2.62644	-2.19112	-0.10963
N	-3.72049	-2.63348	-0.98248
C	-0.05955	-2.16386	0.26139
O	-0.22956	-1.28732	1.13312
O	1.02424	-2.77251	0.02563
C	-2.78086	-0.68226	0.04453
N	-3.24957	-0.22235	1.21864
O	-2.55083	0.06388	-0.90692
H	-3.58111	-2.24917	-1.91240
H	-2.77122	-2.66787	0.86315
H	-1.19377	-3.61599	-0.84536
H	-1.08714	-2.03487	-1.60336
H	-3.68724	-3.64263	-1.08011
H	-3.23004	-0.82797	2.02279
H	-3.11494	0.76689	1.39254
N	4.37157	-1.18793	-0.88295
C	3.17172	-0.35648	-1.20179
C	2.94352	0.67539	-0.11035
C	1.58786	1.35778	-0.26028
C	1.34999	2.39928	0.83393
C	-0.12078	2.84238	0.95287
C	-0.57327	3.43822	-0.38206
N	-1.50569	2.76801	-1.07150
N	-1.01393	1.79911	1.45350
O	-0.06157	4.48262	-0.78982
H	-1.89717	1.88110	-0.76190
H	-1.76992	3.12040	-1.97804
H	-0.98043	1.79518	2.46598
H	-0.71184	0.86830	1.16542
H	-0.16285	3.68037	1.65357
H	1.98054	3.27473	0.65434
H	1.64041	1.98636	1.80618
H	0.81442	0.58356	-0.21946
H	1.51433	1.83262	-1.24519
H	3.74873	1.41848	-0.12536
H	2.98068	0.17700	0.86434
H	2.33151	-1.05052	-1.26145
H	3.32896	0.10644	-2.17574
H	4.16116	-1.74333	-0.01396
H	4.58915	-1.83850	-1.63542
H	5.19759	-0.61268	-0.72555
O	3.33094	-2.57543	1.19973
H	3.29195	-2.20594	2.08375
H	2.38909	-2.61522	0.85796

Lys-Water model, gas phase:

29

LYS_GAS.log Energy: -347640.6582735

C	0.83806	0.85262	0.72837
C	2.32174	0.93149	0.35403
N	2.51748	1.63470	-0.91321
C	-0.01188	0.06640	-0.27060
C	-1.43329	-0.14765	0.25016
C	-2.25484	-0.98021	-0.71781
N	-3.62617	-1.24701	-0.15407
C	2.88044	-0.49970	0.31506
N	3.32584	-0.92026	-0.88916
O	2.87554	-1.18635	1.31838
H	1.90452	2.43833	-0.97861
H	2.83982	1.41503	1.19156
H	0.78364	0.37433	1.70985
H	0.44375	1.86963	0.84184
H	-0.03753	0.58087	-1.23658
H	0.45197	-0.91002	-0.44755
H	-1.38196	-0.65919	1.21953
H	-1.92660	0.81703	0.41445
H	-2.40341	-0.46890	-1.66990
H	-1.79129	-1.94913	-0.90977
H	-4.14044	-0.35192	0.01166
H	-4.18716	-1.82597	-0.77914
H	-3.55698	-1.73779	0.73848
H	3.46441	1.98920	-0.98638
H	3.24976	-0.31344	-1.68996
H	3.73819	-1.83512	-0.96631
O	-4.93812	1.15097	0.25233
H	-5.02586	1.61479	1.08865
H	-5.48571	1.62568	-0.37778

Lys-Water model, PCM water solvation:

29

LYS_PCM.log Energy: -347702.3876300

C	0.81306	0.71498	0.79702
C	2.26133	0.93665	0.33728
N	2.30465	1.65634	-0.93466
C	-0.04528	-0.09432	-0.17393
C	-1.47353	-0.26054	0.34017
C	-2.31307	-1.07520	-0.62863
N	-3.70671	-1.24269	-0.11542
C	2.97293	-0.41682	0.24002
N	3.23721	-0.84284	-1.00405
O	3.25088	-1.05355	1.25271
H	1.58434	2.36839	-0.96098
H	2.77873	1.47471	1.14095
H	0.84071	0.21534	1.76939
H	0.35783	1.69823	0.96159
H	-0.06333	0.39383	-1.15334
H	0.40072	-1.08369	-0.32515
H	-1.45685	-0.75574	1.31743
H	-1.93399	0.72278	0.48334
H	-2.39419	-0.58237	-1.59754
H	-1.89928	-2.07234	-0.77856
H	-4.16157	-0.31361	0.01992
H	-4.27823	-1.78348	-0.76270
H	-3.71523	-1.73265	0.77859
H	3.19103	2.13542	-1.04473
H	2.95489	-0.26531	-1.78231
H	3.67847	-1.73529	-1.15388
O	-4.83246	1.28148	0.17845
H	-4.75822	1.72442	1.02754
H	-4.61195	1.94380	-0.48146

Lys-Lys-Water model, gas phase:

55

LYS_LYS_GAS.log Energy: -647309.0929525

C	2.31010	-1.56357	0.16304
C	3.48556	-1.08810	-0.70415
N	4.73713	-1.80060	-0.51214
C	1.89750	-3.00341	-0.14611
C	0.73771	-3.52460	0.71215
C	-0.52751	-2.71123	0.49288
N	-1.72907	-3.26675	1.18925
C	3.69301	0.42773	-0.54178
N	4.95869	0.82509	-0.50074
O	2.71990	1.19215	-0.48909
O	-3.46286	-1.30742	1.02705
C	-4.01619	-0.41988	0.35926
N	-4.90768	0.41402	0.87420
C	-3.67382	-0.22153	-1.12111
N	-4.59413	0.71339	-1.74676
C	-2.21412	0.24150	-1.23859
C	-1.92768	1.67321	-0.77176
C	-0.43449	1.85338	-0.48040
C	-0.01897	3.31706	-0.47607
N	1.37616	3.47742	0.04972
H	4.85813	-2.14105	0.43400
H	3.19833	-1.19870	-1.75733
H	2.58880	-1.47475	1.22162
H	1.48125	-0.87037	-0.00467
H	1.62572	-3.08641	-1.20570
H	2.74966	-3.67169	0.00208
H	0.55133	-4.57235	0.45427
H	1.01654	-3.49904	1.77194
H	-0.42196	-1.69101	0.86310
H	-0.78412	-2.66118	-0.56751
H	-1.56114	-3.38404	2.18878
H	-2.52613	-2.57231	1.06865
H	-1.99863	-4.17664	0.81591
H	-4.17398	1.20059	-2.52731
H	-3.72949	-1.22860	-1.55721
H	-1.60511	-0.45246	-0.65452
H	-1.89740	0.12774	-2.28055
H	-2.25170	2.38489	-1.53776
H	-2.50535	1.91072	0.12739
H	-0.19601	1.40123	0.48929
H	0.16854	1.32313	-1.22401
H	-0.04282	3.72611	-1.48695
H	-0.67460	3.92367	0.15138
H	1.99270	2.68045	-0.23951
H	1.79347	4.34843	-0.27354
H	1.36991	3.51010	1.08685
H	5.67413	0.11114	-0.57298
H	5.19878	1.80228	-0.46847
H	4.86177	-2.57042	-1.15371
H	-5.20525	0.31621	1.83251
H	-5.31463	1.11076	0.26256
H	-5.42795	0.25349	-2.09246
O	1.22233	3.72704	2.84773
H	0.76805	4.44513	3.29547
H	1.82982	3.35951	3.49399

Lys-Lys-Water model, PCM water solvation:

55

LYS_LYS_PCM.log Energy: -647436.5799725

C	-2.51884	0.36829	-0.72167
C	-3.25729	-0.85656	-1.27857
N	-4.59200	-0.96775	-0.69780
C	-2.97557	1.69295	-1.33550
C	-2.49821	2.91347	-0.54490
C	-0.98852	2.92974	-0.37113
N	-0.54448	4.19378	0.30125
C	-2.42005	-2.09812	-0.96235
N	-2.76255	-2.75189	0.18447
O	-1.46434	-2.41576	-1.65142
H	-4.98667	-0.05613	-0.50338
H	-3.27113	-0.78794	-2.37306
H	-2.66246	0.39343	0.36477
H	-1.44905	0.23489	-0.90278
H	-2.61599	1.75513	-2.36777
H	-4.06728	1.73823	-1.38567
H	-2.81861	3.82211	-1.06312
H	-2.97295	2.91608	0.44233
H	-0.65053	2.11568	0.26768
H	-0.46401	2.88152	-1.32543
H	-0.98987	4.30628	1.21292
H	0.46449	4.20066	0.45174
H	-0.77593	5.01656	-0.25687
H	-3.70297	-2.56407	0.51507
H	-2.40639	-3.69085	0.29776
H	-5.22893	-1.43646	-1.33085
N	-1.11400	-1.57061	2.56310
C	0.33435	-1.68074	2.21328
C	0.61002	-0.95996	0.90565
C	2.08823	-0.97630	0.53141
C	2.32207	-0.25380	-0.79520
C	3.78158	-0.23743	-1.27014
N	4.28809	-1.59579	-1.45849
C	4.62973	0.54377	-0.26154
N	5.46910	-0.19240	0.48142
O	4.50930	1.76116	-0.15104
H	6.04233	0.24334	1.18508
H	5.48983	-1.19162	0.33987
H	5.06125	-1.60171	-2.11385
H	3.56751	-2.18875	-1.85331
H	3.81644	0.35475	-2.19279
H	1.98246	0.78289	-0.71507
H	1.71718	-0.72178	-1.58024
H	2.43940	-2.01055	0.46246
H	2.67207	-0.49744	1.32532
H	0.26651	0.07637	0.99251
H	0.03112	-1.43007	0.10396
H	0.57643	-2.74144	2.14806
H	0.89546	-1.24371	3.03949
H	-1.70238	-1.97501	1.81896
H	-1.32934	-2.05788	3.43111
H	-1.37635	-0.57156	2.67284
O	-1.55352	1.22151	2.62554
H	-0.92099	1.71233	3.15742
H	-2.41643	1.56218	2.87647

Ser-Lys-Water model, gas phase:

44

SER_LYS_GAS.log Energy: -585563.4592658

C	4.02633	0.78521	1.19586
C	3.09522	-0.44456	1.33628
N	3.69526	-1.36840	2.29320
C	3.42324	2.11857	0.73839
C	2.89274	2.16698	-0.70400
C	1.38294	1.94579	-0.78013
N	0.97614	1.29904	-2.05704
C	2.93924	-1.17451	-0.00404
N	3.85915	-2.10556	-0.25024
O	2.03648	-0.89671	-0.80313
O	-1.48244	0.51236	-1.66765
C	-1.80437	-0.51715	-1.05147
N	-0.93944	-1.37421	-0.51613
C	-3.27580	-0.84421	-0.84064
C	-3.85072	0.15657	0.16723
O	-5.19716	-0.18699	0.35844
N	-3.44808	-2.20130	-0.34040
H	4.03031	-0.88590	3.11697
H	2.08965	-0.10885	1.62432
H	4.45290	0.96102	2.18820
H	4.87249	0.52015	0.55315
H	2.63325	2.42306	1.43488
H	4.21256	2.86580	0.84706
H	3.13912	3.12943	-1.15971
H	3.40581	1.40587	-1.30123
H	1.04287	1.26919	0.00205
H	0.82605	2.87877	-0.68536
H	1.51809	0.43265	-2.14616
H	-0.05506	1.00073	-1.98801
H	1.13153	1.89329	-2.86775
H	-4.29110	-2.23309	0.22375
H	-3.77441	-0.66765	-1.80108
H	-3.28397	0.08405	1.10827
H	-3.73225	1.16836	-0.23513
H	-5.59496	0.41520	1.00555
H	-1.35058	-2.17748	-0.05225
H	0.06475	-1.25868	-0.60211
H	-3.58145	-2.85591	-1.10180
H	3.83095	-2.62844	-1.11068
H	4.51366	-2.33892	0.48492
H	3.03890	-2.07781	2.59845
O	-6.29896	1.61264	2.19912
H	-6.94490	2.24202	1.87297
H	-6.63173	1.30957	3.04580

Ser-Lys-Water model, PCM water solvation:

44

SER_LYS_PCM.log Energy: -585607.1933714

C	-1.85416	1.11264	0.10464
C	-0.47770	1.78273	0.20207
N	-0.45308	2.82329	1.22367
C	-2.09585	0.11965	1.24257
C	-3.47909	-0.53272	1.20813
C	-3.64646	-1.46149	0.01631
N	-4.99251	-2.12122	0.04552
C	-0.09156	2.34142	-1.16725
N	-0.14681	3.66605	-1.29599
O	0.23137	1.57657	-2.08320
N	0.32870	-1.26647	-1.49195
C	1.34593	-2.01755	-1.04066
O	1.28004	-3.24352	-0.97492
C	2.62744	-1.32892	-0.57852
C	2.90707	-1.78499	0.86633
O	4.04874	-1.15370	1.41021
N	2.60587	0.13683	-0.62612
H	-1.07654	2.60158	1.98937
H	0.25648	0.99055	0.39057
H	-2.62949	1.88785	0.10208
H	-1.91280	0.59830	-0.85752
H	-1.32241	-0.65672	1.21103
H	-1.99085	0.62058	2.20906
H	-3.62463	-1.10545	2.12884
H	-4.25223	0.24297	1.18307
H	-3.58690	-0.93590	-0.93534
H	-2.90696	-2.26210	0.02383
H	-5.74499	-1.43211	0.01885
H	-5.12080	-2.74425	-0.75203
H	-5.11773	-2.67719	0.89249
H	3.56734	0.46339	-0.63649
H	3.41756	-1.73601	-1.22227
H	2.02338	-1.58165	1.48443
H	3.08431	-2.85977	0.87111
H	3.76626	-0.30199	1.77125
H	0.35802	-0.25805	-1.63918
H	-0.48679	-1.75815	-1.82434
H	2.19462	0.49063	-1.48463
H	0.08832	4.10809	-2.16976
H	-0.39367	4.21243	-0.48271
H	0.47747	2.91685	1.61669
O	2.45483	1.23016	1.95940
H	2.28609	0.94660	1.03360
H	1.71812	0.89942	2.47848

Asp-Lys-Cl⁻ model, gas phase:

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alwg_cl.log Energy: -897331.6270907

C	1.84239	2.49912	-0.76592
C	3.00141	2.27730	0.21761
N	4.30530	2.67243	-0.32319
C	0.43875	2.15114	-0.24805
O	0.35165	1.33103	0.69035
O	-0.51987	2.70380	-0.84526
C	3.11394	0.79964	0.58830
N	2.84825	0.45673	1.87237
O	3.47426	-0.01586	-0.25277
N	-2.96058	1.64605	-0.82915
C	-2.70223	0.26444	-1.29737
C	-2.22281	-0.60527	-0.14513
C	-1.75138	-1.97023	-0.64734
C	-1.27227	-2.92880	0.45330
C	0.22937	-2.85488	0.79097
C	1.04804	-3.32732	-0.41817
N	2.08055	-2.55421	-0.80626
N	0.71304	-1.59233	1.34096
O	0.75216	-4.36797	-0.99041
H	4.57448	1.99007	-1.02623
H	2.81935	2.86007	1.12576
H	1.84395	3.54284	-1.09426
H	2.02307	1.88523	-1.65663
H	0.52584	-0.79295	0.73526
H	0.42106	-3.62331	1.54983
H	-1.47369	-3.95884	0.15087
H	-1.84131	-2.74533	1.37240
H	-0.95143	-1.83574	-1.38758
H	-2.57707	-2.44728	-1.18755
H	-3.04796	-0.72461	0.56509
H	-1.41931	-0.07371	0.37159
H	-1.94394	0.31892	-2.08373
H	-3.63143	-0.12669	-1.71937
H	-3.70504	1.62180	-0.06604
H	-2.03663	2.10291	-0.57886
H	-3.36460	2.20535	-1.57536
H	4.22194	3.56804	-0.79096
H	2.18985	1.07455	2.32530
H	2.58854	-0.52178	1.96960
H	2.39694	-1.72010	-0.32402
H	2.62204	-2.87613	-1.59086
H	0.20248	-1.38539	2.19264
Cl	-5.42117	1.30721	0.82092

Asp-Lys-Cl⁻ model, PCM water solvation:

43

alwp_cl_rest.log Energy: -897390.2263973

C	2.93979	-1.71718	-0.71286
C	2.22285	-2.43310	0.43294
N	2.61879	-3.82247	0.66329
C	2.98652	-0.19035	-0.57600
O	2.91340	0.31113	0.56141
O	3.12912	0.46751	-1.65162
C	0.70120	-2.33836	0.30399
N	0.01902	-3.29863	0.93808
O	0.15124	-1.41519	-0.30641
N	1.49480	2.52765	-1.17260
C	0.24916	1.77536	-1.48990
C	-0.95536	2.25943	-0.70317
C	-2.21911	1.51649	-1.15575
C	-3.31424	1.42914	-0.08317
C	-3.26785	0.15109	0.78921
C	-3.70912	-1.04362	-0.05830
N	-2.74930	-1.84202	-0.56306
N	-2.01894	-0.10508	1.50336
O	-4.90295	-1.23053	-0.28423
H	2.66905	-4.32943	-0.21462
H	2.44768	-1.87298	1.34722
H	3.98139	-2.05728	-0.71697
H	2.51312	-1.98457	-1.68229
H	-1.22003	-0.17475	0.87839
H	-4.05360	0.24973	1.54205
H	-4.30351	1.47129	-0.54759
H	-3.24841	2.29523	0.58412
H	-1.94512	0.50735	-1.48422
H	-2.61586	2.01159	-2.04612
H	-1.09201	3.33906	-0.82575
H	-0.76662	2.09092	0.36059
H	0.44683	0.72878	-1.25194
H	0.08465	1.85427	-2.56594
H	1.53049	2.81349	-0.17617
H	2.31479	1.88582	-1.37254
H	1.57108	3.37895	-1.72348
H	3.54438	-3.85415	1.07268
H	0.53945	-4.05329	1.36090
H	-0.98847	-3.28735	0.95964
H	-1.75418	-1.64052	-0.48208
H	-3.03394	-2.57450	-1.19497
H	-1.82931	0.66461	2.13524
Cl	1.50165	3.92970	1.73089

Lys-Cl⁻ model, gas phase:

27

lwg_cl.log Energy: -588608.5377517

C	1.14742	0.41846	1.01079
C	2.51942	0.88968	0.51339
N	2.38185	1.89188	-0.54523
C	0.28509	-0.25399	-0.05659
C	-1.09632	-0.61527	0.48067
C	-1.94406	-1.32241	-0.56526
N	-3.32908	-1.49800	-0.06716
C	3.32112	-0.33059	0.03917
N	3.52953	-0.39505	-1.29518
O	3.70581	-1.17081	0.83052
H	1.56990	2.47647	-0.38893
H	3.06804	1.27026	1.38342
H	1.31728	-0.27555	1.83831
H	0.61513	1.28368	1.42435
H	0.17336	0.40897	-0.92106
H	0.79256	-1.15654	-0.41696
H	-0.99112	-1.25937	1.36346
H	-1.62237	0.29141	0.79695
H	-2.01975	-0.70941	-1.46660
H	-1.51575	-2.29154	-0.83587
H	-3.82526	-0.39806	-0.00400
H	-3.89663	-2.05602	-0.69840
H	-3.34672	-1.93420	0.85103
H	3.18916	2.50235	-0.57773
H	3.13523	0.32349	-1.88282
H	4.02492	-1.18189	-1.67808
Cl	-4.34039	1.13914	-0.03596

Lys-Cl⁻ model, PCM water solvation:

27

lwp_cl.log Energy: -588638.7004414

C	1.14575	0.59281	0.86918
C	2.55160	0.98037	0.38819
N	2.48610	1.78724	-0.82943
C	0.33358	-0.22722	-0.13208
C	-1.06696	-0.53088	0.39428
C	-1.86137	-1.36002	-0.60016
N	-3.24040	-1.61942	-0.09219
C	3.38081	-0.29007	0.17415
N	3.63716	-0.60346	-1.10454
O	3.75311	-0.96513	1.13020
H	1.70042	2.42568	-0.78755
H	3.04403	1.50787	1.21426
H	1.24967	0.03551	1.80441
H	0.60797	1.51632	1.11198
H	0.25772	0.31170	-1.08171
H	0.85258	-1.16838	-0.34641
H	-0.99391	-1.07052	1.34529
H	-1.60194	0.40394	0.59190
H	-1.97429	-0.83823	-1.55112
H	-1.38994	-2.32531	-0.78565
H	-3.76579	-0.71159	0.01317
H	-3.76736	-2.21151	-0.73188
H	-3.22249	-2.08743	0.81302
H	3.31894	2.35658	-0.92667
H	3.27505	-0.00182	-1.82977
H	4.15185	-1.43843	-1.33151
Cl	-4.63810	1.12213	0.06225

Lys-Lys-Cl⁻ model, gas phase:

53

llwg_cl.log Energy: -888337.9033365

C	2.66390	-0.88787	-0.31284
C	3.63256	-0.07856	-1.18069
N	4.91026	-0.71893	-1.47083
C	2.29799	-2.24245	-0.92212
C	1.19639	-2.95760	-0.13137
C	-0.18236	-2.38536	-0.44484
N	-1.15124	-2.63145	0.65700
C	3.86090	1.32020	-0.58734
N	5.08252	1.82124	-0.76553
O	2.95721	1.94397	-0.02459
O	-3.32930	-1.39053	-0.38358
C	-4.16389	-0.49766	-0.54362
N	-5.35661	-0.48973	0.05060
C	-3.88821	0.67699	-1.49564
N	-4.89153	1.72148	-1.33040
C	-2.42357	1.11835	-1.37961
C	-2.07256	1.75904	-0.03329
C	-0.57212	1.70901	0.23852
C	-0.18978	2.39838	1.54160
N	1.13242	1.89212	2.00486
H	5.25582	-1.24181	-0.67361
H	3.14626	0.12018	-2.14464
H	3.10151	-1.04478	0.68079
H	1.76580	-0.28734	-0.15149
H	1.98193	-2.11156	-1.96597
H	3.18337	-2.88308	-0.95110
H	1.20509	-4.02852	-0.35492
H	1.39804	-2.84236	0.93835
H	-0.14309	-1.30143	-0.55592
H	-0.59918	-2.79854	-1.36461
H	-0.80639	-2.10502	1.50514
H	-2.08267	-2.25841	0.39275
H	-1.22784	-3.62002	0.88568
H	-4.62336	2.40210	-0.62969
H	-4.03123	0.24404	-2.49203
H	-1.79984	0.23387	-1.53551
H	-2.20070	1.81277	-2.19534
H	-2.42390	2.79705	-0.00156
H	-2.58145	1.22715	0.78048
H	-0.28023	0.65798	0.32146
H	-0.00578	2.14206	-0.59223
H	-0.13003	3.48181	1.42806
H	-0.90763	2.16142	2.32933
H	1.84242	1.92007	1.24379
H	1.48127	2.41205	2.80631
H	0.99118	0.88769	2.29919
H	5.76833	1.24955	-1.23955
H	5.29416	2.75396	-0.45128
H	4.84725	-1.35373	-2.25471
H	-5.63517	-1.25956	0.63657
H	-5.99155	0.26508	-0.17148
H	-5.06479	2.21636	-2.19455
Cl	0.18900	-0.88438	2.73089

Lys-Lys-Cl⁻ model, PCM water solvation:

53

llwp_cl.log Energy: -888379.1329363

C	-2.36754	0.05191	-1.03707
C	-3.24132	-1.19052	-1.25289
N	-4.57105	-1.00487	-0.68028
C	-2.74677	1.25122	-1.91158
C	-2.20908	2.56748	-1.34682
C	-0.68712	2.61247	-1.29530
N	-0.23205	3.65996	-0.33257
C	-2.52411	-2.36733	-0.58669
N	-2.90952	-2.61812	0.69707
O	-1.61357	-2.96144	-1.14054
H	-4.86796	-0.03908	-0.73826
H	-3.26418	-1.42288	-2.32419
H	-2.42943	0.33756	0.02134
H	-1.33170	-0.23252	-1.23434
H	-2.38477	1.09103	-2.93234
H	-3.83398	1.34593	-1.98406
H	-2.57566	3.40865	-1.94146
H	-2.59995	2.69004	-0.33133
H	-0.26342	1.67831	-0.92986
H	-0.24862	2.83289	-2.26769
H	-0.52301	3.37392	0.62891
H	0.78183	3.76222	-0.33850
H	-0.63717	4.57158	-0.54300
H	-3.82808	-2.26219	0.94015
H	-2.62714	-3.50229	1.09632
H	-5.26242	-1.55697	-1.17341
N	-1.22343	-0.86821	2.65595
C	0.21752	-1.16030	2.39748
C	0.55198	-0.85919	0.94775
C	2.04404	-0.97693	0.65711
C	2.33906	-0.66282	-0.80921
C	3.82269	-0.72867	-1.19649
N	4.37550	-2.05751	-0.94092
C	4.58935	0.35569	-0.43196
N	5.40733	-0.08734	0.53399
O	4.42691	1.54377	-0.69782
H	5.92546	0.56330	1.10127
H	5.46230	-1.08151	0.70058
H	5.18174	-2.22906	-1.53064
H	3.69360	-2.77242	-1.16557
H	3.89580	-0.44008	-2.25220
H	1.97657	0.34090	-1.04966
H	1.78836	-1.35788	-1.45317
H	2.39278	-1.98440	0.90422
H	2.59427	-0.28526	1.30468
H	0.21816	0.15905	0.72058
H	-0.00250	-1.54336	0.29647
H	0.39539	-2.20615	2.64721
H	0.79270	-0.53225	3.07849
H	-1.82915	-1.39593	2.00964
H	-1.49425	-1.11413	3.60674
H	-1.39341	0.15269	2.52763
Cl	-1.22755	2.26272	2.29257

Ser-Lys-Cl⁻ model, gas phase:

42

slwg_cl.log Energy: -826527.8397606

C	3.19633	-0.52484	0.23176
C	2.21237	0.66078	0.20560
N	2.68054	1.81444	-0.54626
C	3.02976	-1.47122	-0.96330
C	2.04360	-2.62670	-0.74436
C	0.57884	-2.26564	-0.49734
N	0.24100	-2.01029	0.93809
C	1.76733	1.01658	1.61562
N	1.93915	2.28243	1.98748
O	1.24758	0.14815	2.33021
O	-2.43640	-1.68675	1.06050
C	-3.15691	-0.82559	0.53889
N	-4.47330	-0.76709	0.74623
C	-2.58724	0.25804	-0.36023
C	-1.72346	1.20311	0.50318
O	-1.23343	2.28228	-0.23754
N	-3.63700	1.01937	-1.02780
H	3.64732	1.71479	-0.82674
H	1.28498	0.33961	-0.28463
H	4.21283	-0.11608	0.25078
H	3.08846	-1.08388	1.16700
H	2.71513	-0.89737	-1.84150
H	3.99715	-1.92040	-1.20731
H	2.05784	-3.24636	-1.64543
H	2.40383	-3.27374	0.06819
H	0.28667	-1.38216	-1.07434
H	-0.06826	-3.08952	-0.80387
H	0.72562	-1.19207	1.38562
H	-0.79584	-1.83551	1.01405
H	0.45815	-2.82442	1.50885
H	-3.31846	1.97988	-1.11671
H	-1.91454	-0.22899	-1.07658
H	-2.33723	1.62165	1.30827
H	-0.92033	0.62135	0.97084
H	-0.72356	1.92161	-0.99372
H	-4.97661	-0.02324	0.27834
H	-4.92083	-1.43092	1.35496
H	-3.76493	0.68033	-1.97381
H	1.54246	2.61156	2.85136
H	2.25151	2.91774	1.26247
H	2.11573	1.90989	-1.38837
Cl	0.17144	0.66810	-2.48684

Ser-Lys-Cl⁻ model, PCM water solvation:

42

slwp_cl_rest.log Energy: -826543.2477536

C	-1.27607	-1.52763	-0.19611
C	0.23550	-1.71385	-0.01653
N	0.84388	-2.47891	-1.10182
C	-1.61814	-0.50313	-1.27673
C	-3.11458	-0.38463	-1.56899
C	-3.88128	0.17639	-0.38231
N	-5.32734	0.37301	-0.72821
C	0.50457	-2.34642	1.35313
N	1.09417	-3.54646	1.32793
O	0.18809	-1.75800	2.38863
N	-0.58132	1.15766	1.92580
C	-0.14844	2.26348	1.30623
O	-0.84752	3.26276	1.13700
C	1.29170	2.23148	0.78148
C	1.24184	2.25601	-0.75338
O	2.50560	2.50772	-1.32815
N	2.03252	1.07772	1.26726
H	0.20525	-2.60126	-1.87679
H	0.69889	-0.72352	0.06212
H	-1.72799	-2.49824	-0.43881
H	-1.69142	-1.21235	0.76325
H	-1.23534	0.47724	-0.97299
H	-1.11028	-0.75810	-2.21132
H	-3.25661	0.27572	-2.42990
H	-3.51919	-1.36552	-1.84093
H	-3.86187	-0.48868	0.47952
H	-3.49677	1.15147	-0.08289
H	-5.76979	-0.50777	-0.99345
H	-5.85285	0.75359	0.05904
H	-5.43948	1.01804	-1.51148
H	2.70485	0.74568	0.58211
H	1.73556	3.18436	1.09729
H	0.84281	1.30161	-1.11978
H	0.56473	3.05284	-1.06467
H	2.95064	1.65231	-1.46081
H	0.00860	0.33713	2.03001
H	-1.52915	1.13080	2.26571
H	2.53788	1.29156	2.11733
H	1.32865	-4.02374	2.18254
H	1.33835	-3.92560	0.42324
H	1.67103	-2.00028	-1.44966
Cl	3.60531	-0.42109	-1.55918

Asp-Lys-Na⁺ model, gas phase:

43

alwg_na.log Energy: -710227.6240059

C	3.40482	0.14112	-0.74612
C	3.48084	-1.06419	0.20419
N	4.52385	-1.96361	-0.26590
C	2.42504	1.22513	-0.35325
O	2.14919	1.48476	0.81451
O	1.93562	1.86141	-1.37003
C	2.13188	-1.79391	0.21227
N	2.03358	-2.83499	-0.60478
O	1.19318	-1.39619	0.91641
N	0.20015	3.71076	-0.72719
C	-1.16119	3.14537	-0.66658
C	-1.21931	1.95199	0.27880
C	-2.62162	1.35757	0.40649
C	-2.67644	0.06503	1.23511
C	-2.65779	-1.22996	0.40881
C	-4.00140	-1.37936	-0.33242
N	-3.94590	-2.11704	-1.46363
N	-1.53343	-1.42142	-0.50275
O	-5.01898	-0.87744	0.09992
H	5.32049	-1.46371	-0.63888
H	3.63826	-0.69578	1.22457
H	4.38888	0.62406	-0.76770
H	3.19106	-0.18528	-1.76574
H	-1.46619	-0.66590	-1.17577
H	-2.63777	-2.07149	1.11182
H	-3.58608	0.05029	1.83650
H	-1.84094	0.03388	1.95268
H	-3.03064	1.16709	-0.59248
H	-3.28346	2.10535	0.85046
H	-0.88063	2.28476	1.27334
H	-0.51491	1.18984	-0.07640
H	-1.43037	2.82167	-1.67527
H	-1.89733	3.89657	-0.35962
H	0.45232	4.11909	0.16872
H	1.27739	2.61863	-1.08330
H	0.23498	4.46738	-1.40394
H	4.85920	-2.57258	0.47075
H	2.86151	-3.12150	-1.11162
H	1.16733	-3.34596	-0.67712
H	-3.07868	-2.54700	-1.74003
H	-4.80472	-2.33148	-1.94291
H	-0.65591	-1.47937	0.00386
Na	0.73340	0.39931	2.13614

Asp-Lys-Na⁺ model, PCM water solvation:

43

alwp_na.log Energy: -710295.2266866

C	3.18764	-0.62072	-0.96117
C	2.66622	-1.77131	-0.10495
N	2.90998	-3.10292	-0.66926
C	2.89450	0.77020	-0.41053
O	2.43900	0.87720	0.75351
O	3.10871	1.74554	-1.18158
C	1.15805	-1.64935	0.11857
N	0.68837	-2.12520	1.28152
O	0.41558	-1.16011	-0.73746
N	1.09924	3.23807	-0.31323
C	-0.03289	2.46727	-0.90246
C	-1.26208	2.45837	-0.01186
C	-2.40692	1.68881	-0.68660
C	-3.45185	1.12817	0.29147
C	-3.18343	-0.33001	0.72784
C	-3.47549	-1.26713	-0.44708
N	-2.42914	-1.83147	-1.07195
N	-1.86587	-0.56873	1.31603
O	-4.63836	-1.45515	-0.80078
H	2.59511	-3.13196	-1.63428
H	3.15129	-1.73801	0.87333
H	4.27192	-0.72376	-1.07138
H	2.76281	-0.67982	-1.96668
H	-1.13382	-0.18959	0.72032
H	-3.92904	-0.59532	1.48093
H	-4.44713	1.16131	-0.15790
H	-3.49336	1.75245	1.19009
H	-1.98792	0.86938	-1.28386
H	-2.89337	2.35210	-1.40584
H	-1.58325	3.48001	0.21396
H	-0.99834	1.99604	0.94529
H	0.32909	1.44750	-1.04791
H	-0.24270	2.89927	-1.88120
H	1.17545	3.05945	0.68736
H	2.01159	2.86843	-0.71876
H	1.00393	4.24044	-0.45635
H	3.90691	-3.28725	-0.68556
H	1.29668	-2.58540	1.93797
H	-0.30940	-2.07341	1.46942
H	-1.45862	-1.63279	-0.83994
H	-2.61712	-2.40423	-1.87991
H	-1.80136	-0.07602	2.20028
Na	1.31005	0.58340	2.68727

Lys-Na⁺ model, gas phase: divergent optimization

Lys-Na⁺ model, PCM water solvation:

27

lwp_na_rest.log Energy: -401530.8551764

C	0.98439	-1.01120	0.33345
C	2.50465	-0.88572	0.50969
N	2.82998	-0.16920	1.74189
C	0.24472	0.32321	0.25536
C	-1.26495	0.12560	0.13190
C	-1.97772	1.46308	0.05661
N	-3.46190	1.27936	-0.06165
C	3.10226	-0.18871	-0.71706
N	3.53127	1.06633	-0.51585
O	3.14983	-0.76053	-1.80247
H	2.19573	-0.44002	2.48422
H	2.91893	-1.90108	0.49288
H	0.79365	-1.59364	-0.57217
H	0.59810	-1.59941	1.17341
H	0.46281	0.92327	1.14435
H	0.60523	0.89594	-0.60622
H	-1.48936	-0.46216	-0.76492
H	-1.63286	-0.44057	0.99429
H	-1.80986	2.06215	0.95075
H	-1.66594	2.03670	-0.81552
H	-3.83813	0.76580	0.73647
H	-3.94587	2.17667	-0.10494
H	-3.70614	0.75762	-0.90425
H	3.76397	-0.40529	2.05711
H	3.43862	1.46713	0.40594
H	3.91420	1.60213	-1.27738
Na	-6.15067	-1.26855	-0.23133

Lys-Lys-Na⁺ model, gas phase: divergent optimization

Lys-Lys-Na⁺ model, PCM water solvation:

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llwp_na_rest.log Energy: -701265.6699016

C	-2.05803	0.88313	-0.65575
C	-3.22312	0.03424	-1.18880
N	-4.38019	-0.03721	-0.30213
C	-2.41166	2.35774	-0.48623
C	-1.30767	3.16729	0.19811
C	-0.03627	3.22449	-0.63268
N	0.98864	4.10247	0.02097
C	-2.69427	-1.36162	-1.54086
N	-3.24533	-2.39342	-0.83541
O	-1.79965	-1.51794	-2.35501
H	-4.12572	0.14512	0.66141
H	-3.54753	0.45420	-2.14640
H	-1.73832	0.47379	0.31052
H	-1.21671	0.76365	-1.34312
H	-2.64178	2.79697	-1.46336
H	-3.31713	2.45189	0.11959
H	-1.66896	4.18500	0.37350
H	-1.08430	2.72732	1.17649
H	0.42963	2.24733	-0.74593
H	-0.22010	3.64238	-1.62200
H	1.21973	3.77288	0.95939
H	1.85659	4.12745	-0.51490
H	0.65594	5.06379	0.10756
H	-4.14684	-2.18159	-0.42024
H	-3.12084	-3.31807	-1.22506
H	-5.08414	0.64081	-0.55978
N	-1.52515	-2.82103	1.67466
C	-0.07383	-2.84023	1.30223
C	0.30829	-1.54208	0.61683
C	1.78509	-1.48747	0.23838
C	2.10672	-0.15940	-0.44648
C	3.56569	0.01139	-0.88826
N	3.95742	-1.03705	-1.82754
C	4.46612	0.02399	0.35142
N	5.23876	-1.05921	0.51611
O	4.44063	0.97118	1.13294
H	5.84303	-1.13713	1.31767
H	5.18338	-1.80112	-0.16615
H	4.73367	-0.73022	-2.40266
H	3.19380	-1.24872	-2.45890
H	3.65777	1.01654	-1.31809
H	1.86607	0.66337	0.23333
H	1.47006	-0.04099	-1.33152
H	2.02839	-2.32298	-0.42472
H	2.40148	-1.60422	1.13620
H	0.07428	-0.69839	1.27643
H	-0.29186	-1.42485	-0.29055
H	0.07026	-3.69938	0.64765
H	0.48843	-2.99981	2.22194
H	-2.12464	-2.67629	0.84285
H	-1.81070	-3.69485	2.11563
H	-1.72804	-2.06691	2.33167
Na	-2.56674	0.88150	3.31309

Ser-Lys-Na⁺ model, gas phase:

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slwg_na.log Energy: -639277.9760594

C	4.53148	0.41254	0.87338
C	3.55000	-0.78163	0.97687
N	4.29791	-1.94260	1.44180
C	3.97497	1.84036	0.90233
C	3.14818	2.27445	-0.32020
C	1.64159	2.18882	-0.07529
N	0.91045	1.84232	-1.33099
C	2.94089	-1.12611	-0.38818
N	3.64861	-1.97257	-1.12499
O	1.86942	-0.62835	-0.77849
O	-1.60961	0.95875	-0.74458
C	-1.88929	-0.23271	-0.57786
N	-1.00491	-1.21229	-0.42446
C	-3.36966	-0.64120	-0.51207
C	-3.90268	-0.14019	0.82983
O	-5.33421	-0.30569	0.94132
N	-3.52602	-2.07905	-0.63267
H	4.93581	-1.70750	2.19093
H	2.70998	-0.50490	1.62928
H	5.20103	0.32612	1.73429
H	5.16546	0.27725	-0.00923
H	3.39533	1.99310	1.82004
H	4.83833	2.50291	0.99075
H	3.40847	3.29705	-0.60341
H	3.41780	1.64533	-1.17565
H	1.39871	1.39037	0.62355
H	1.23144	3.12413	0.30663
H	1.31113	0.95413	-1.66381
H	-0.09949	1.64072	-1.13820
H	1.00281	2.55946	-2.04786
H	-4.44893	-2.38899	-0.35641
H	-3.86201	-0.06851	-1.31042
H	-3.41799	-0.66910	1.65460
H	-3.69281	0.92528	0.92371
H	-5.51533	-1.13253	1.39346
H	-1.35814	-2.14902	-0.28056
H	-0.00125	-1.04156	-0.47699
H	-3.39909	-2.38697	-1.59056
H	3.33256	-2.24375	-2.04250
H	4.46480	-2.40143	-0.70528
H	3.69367	-2.68627	1.77092
Na	-7.01384	1.21184	0.66029

Ser-Lys-Na⁺ model, PCM water solvation:

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slwp_na.log Energy: -639438.9955350

C	-2.50733	0.77206	-0.07322
C	-1.40982	1.74553	0.37929
N	-1.97837	2.93968	0.99456
C	-3.15276	0.01458	1.08787
C	-4.34726	-0.84548	0.67034
C	-3.95445	-1.96246	-0.28326
N	-5.13678	-2.83136	-0.59334
C	-0.55832	2.10418	-0.84050
N	-0.71245	3.33801	-1.31826
O	0.19794	1.26599	-1.34166
N	0.86638	-1.23096	0.00235
C	2.05563	-1.85412	-0.04479
O	2.20054	-3.02754	0.29084
C	3.26469	-1.06121	-0.53964
C	4.41982	-1.27387	0.44686
O	5.59629	-0.60933	0.01235
N	3.02067	0.37140	-0.69589
H	-2.85378	2.73567	1.45899
H	-0.73468	1.20545	1.05697
H	-3.26751	1.33686	-0.62662
H	-2.05884	0.06606	-0.77627
H	-2.39935	-0.61377	1.57567
H	-3.50647	0.71536	1.84939
H	-4.79675	-1.28227	1.56717
H	-5.10830	-0.21296	0.20110
H	-3.59584	-1.58734	-1.24066
H	-3.19320	-2.61235	0.14816
H	-5.88480	-2.29739	-1.03798
H	-4.88617	-3.59095	-1.22646
H	-5.52375	-3.25278	0.25207
H	3.85972	0.79190	-1.08295
H	3.54983	-1.53549	-1.48988
H	4.12594	-0.92734	1.44376
H	4.64318	-2.33807	0.50631
H	5.64361	0.25169	0.43006
H	0.68674	-0.31163	-0.39891
H	0.06902	-1.79171	0.26154
H	2.28559	0.56086	-1.37171
H	-0.20311	3.64071	-2.13255
H	-1.35037	3.95691	-0.83747
H	-1.35556	3.32565	1.69373
Na	2.41994	1.70831	1.32188