Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Roles of Different Amino-acid Residues Towards Binding and Selective Transport of K^+-ion Through KcsA K^+ ion Channel

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Electronic Supporting Information

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Figure S5: Superimposition of the optimized geometries of the binding sites in the selectivity filter of K^+-ion channel with and without potassium ion. The blue colour indicates structure with the K^+-ion.

Figure S6: Optimized geometries for four binding sites with sodium ion at the ONIOM(B3LYP/6-31+g*:AMBER96) level of theory. Atoms in high layer are shown in ball and stick and those in low layer are in wire frame.

Table S7: Cartesian coordinates of the optimized geometries of the binding sites of the selectivity filter of KcsA, with K^+-ion and with Na^+-ion.

Table S1. Computational Details

All the geometries were optimized using the hybrid Quantum Mechanical/ Molecular Mechanical method B3LYP:AMBER96 with the 6-31+g* basis set using ONIOM method as implemented in Gaussian09 program package. The single-point calculations of optimized geometries were done at the B3LYP/6-31g* level of theory for natural population analysis by NBO.[S1] The quantitative analysis of electrostatic potential (ESP) on the molecular van der Waals surface was carried out with the Multiwfn[S2] program at the same level of theory. The hybrid QM/MM methods allow the combination of two computational techniques viz. higher level of theory is applied to the region where the chemical process takes place and lower level of theory is used for the remainder of the system. In a two-layer ONIOM(QM:MM) calculation, the total energy of the system is obtained from three independent calculations:

$$E_{\mathrm{ONIOM}} = E_{\mathrm{real,MM}} + E_{\mathrm{model,QM}} - E_{\mathrm{model,MM}}$$

The real system contains all the atoms and is calculated only at the MM level. The model system contains the part of the system that is treated at the QM level. Both QM and MM calculations need to be carried out for the model system.

Table S2: Binding energies of K+-ion at the binding sites of the selectivity filter of KcsA at the B3LYP/6-31+g*:AMBER96, B2PLYP-D3/6-31+g*:AMBER96 and M06/6-31+g*:AMBER96 level of theories.

Sl. No.	Binding site	Binding Energy (kcal/mol)		
		B3LYP	**B2PLYPD3**	**M06**
1	TYR_{CO}	-60.5	-61.5	-60.4
2	Center of S1	-39.5	-43.8	-30.2
3	Center of S2	-49.8	-54.0	-46.9
4	Center of S3	-63.9	-64.0	-60.8
5	Center of S4	*Not suitable for binding-*		

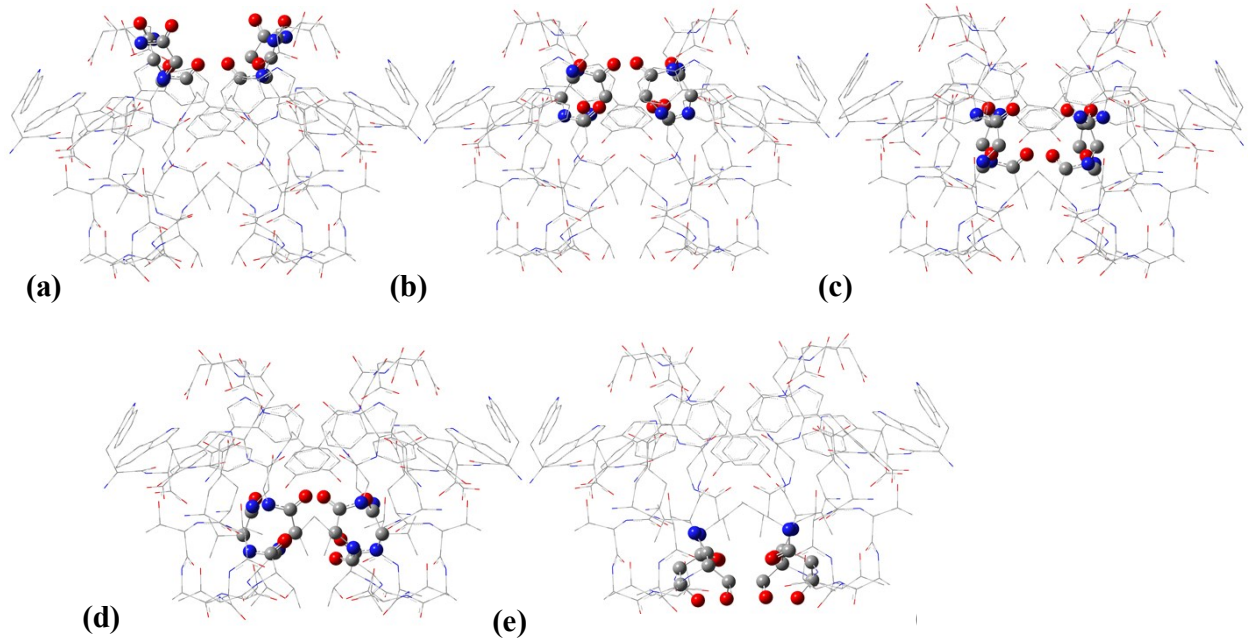


Figure S1: Optimized geometries of five binding sites in the selectivity filter of K^+-ion channel. (a) S0, (b) S1, (c) S2, (d) S3, (e) S4 at the ONIOM(B3LYP/6-31+g*:AMBER96) level of theory. Atoms in high layer are shown in ball and stick and those in low layer are shown in wire frame.

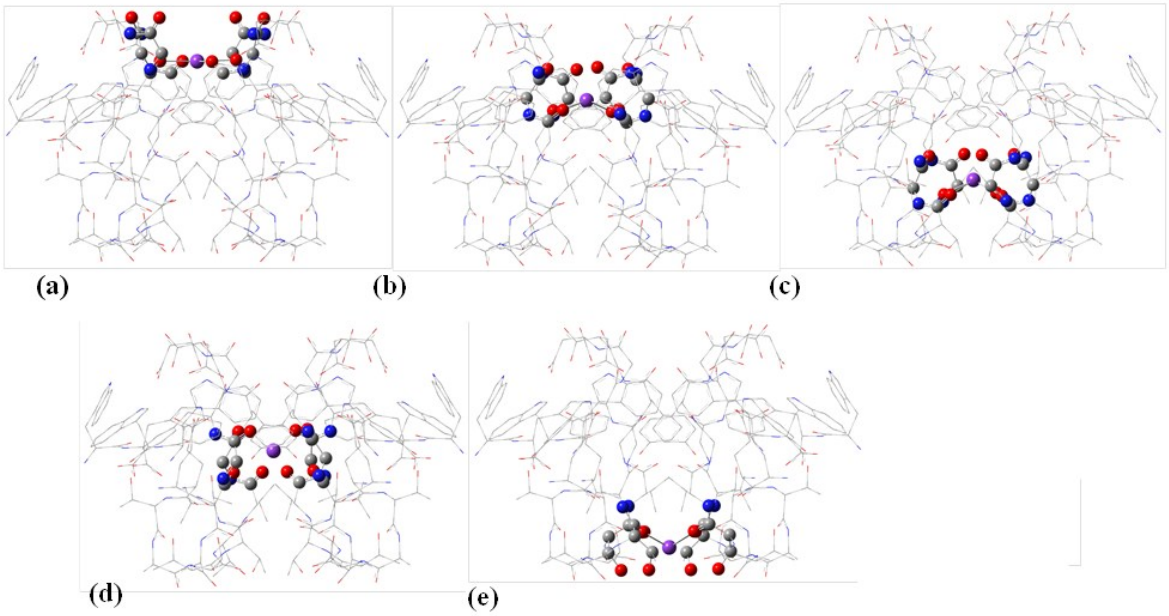


Figure S2: Optimized geometries of five binding sites in the selectivity filter of K^+-ion channel with potassium ion. (a) S0-K, (b) S1-K, (c) S2-K, (d) S3-K, (e) S4-K at ONIOM(B3LYP/6-31+g*:AMBER) level of theory. Atoms in high layer are shown in ball and stick and those in low layer are in wire frame. (f) Optimized geometry for $K(H_2O)_8^+$ at B3LYP/6-31+g* level of theory.

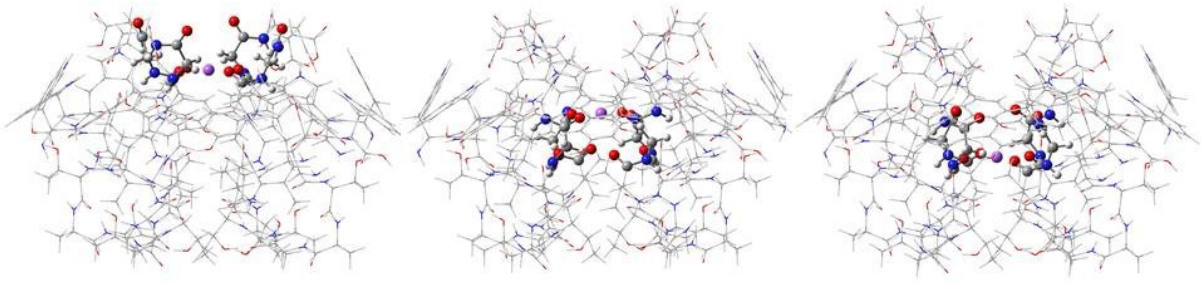
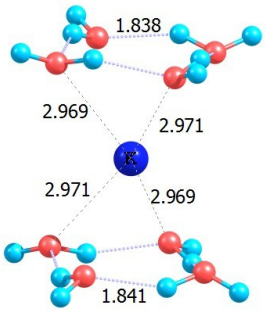


Figure S3: Optimized geometries of binding sites in the selectivity filter of K^+-ion channel with sodium ion. (a) TYR-Na, (b) GLY-Na, (c) VAL-Na at the ONIOM(B3LYP/6-31+g*:AMBER96) level of theory. Atoms in high layer are shown in ball and stick and those in low layer are in wire frame.

(a)



(b)

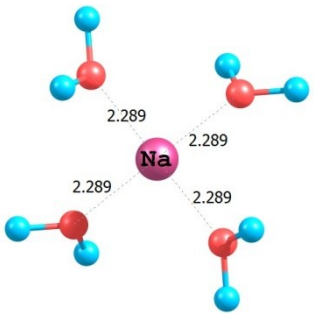


Figure S4: Optimized geometries of (a) $K(H_2O)_8^+$, (b) $Na(H_2O)_4^+$ at the B3LYP/6-31+g* level of theory.

Table S3: Atomic charge distribution (q) on the C- and O-atoms of the amino acids given by the Natural Population Analysis at the B3LYP/6-31+g* level of theory. The numbering of the O-atoms is according to Figure 2.

	q(C)		q(O)	
GLY	C1	0.789	O1	-0.615
TYR	C1	0.802	O1	-0.621
VAL	C1	0.799	O1	-0.619
THR	C1	0.803	O1	-0.612
THR	C3	0.067	O3	-0.778

Table S4: Atomic charge distribution (q) on the O-atoms of the binding sites (S0-S4) given by the Natural Population Analysis at the B3LYP/6-31+g* level of theory. The numbering of the O-atoms is according to Figure 1.

q(O)-S0			q(O)-S1			q(O)-S2			q(O)-S3			q(O)-S4		
G79	O1	-0.625	Y78	O2	-0.600	G77	O3	-0.628	V76	O4	-0.608	T75	O5	-0.603
	O1'	-0.623		O2'	-0.596		O3'	-0.628		O4'	-0.611		O5'	-0.603
	O1''	-0.625		O2''	-0.598		O3''	-0.630		O4''	-0.612		O5''	-0.606
	O1'''	-0.624		O2'''	-0.600		O3'''	-0.629		O4'''	-0.611		O5'''	-0.603
Y78	O2	-0.611	G77	O3	-0.596	V76	O4	-0.605	T75	O5	-0.595	T75	O6	-0.781
	O2'	-0.605		O3'	-0.608		O4'	-0.607		O5'	-0.595		O6'	-0.782
	O2''	-0.606		O3''	-0.608		O4''	-0.609		O5''	-0.593		O6''	-0.782
	O2'''	-0.612		O3'''	-0.603		O4'''	-0.610		O5'''	-0.593		O6'''	-0.782

Table S5: Atomic charge distribution (q) on the O-atoms of the binding sites (S0-S4) with K^+-ion given by the Natural Population Analysis at the B3LYP/6-31+g* level of theory. The numbering of the O-atoms is according to Figure 1.

	q(O)-S0			q(O)-S1			q(O)-S2			q(O)-S3			q(O)-S4[a]
G79	O1	-0.600	Y78	O2	-0.609	G77	O3	-0.633	V76	O4	-0.614	T75	O5
	O1'	-0.599		O2'	-0.612		O3'	-0.634		O4'	-0.616		O5'
	O1''	-0.601		O2''	-0.615		O3''	-0.635		O4''	-0.613		O5''
	O1'''	-0.602		O2'''	-0.613		O3'''	-0.633		O4'''	-0.615		O5'''
Y78	O2	-0.682	G77	O3	-0.657	V76	O4	-0.639	T75	O5	-0.672	T75	O6
	O2'	-0.694		O3'	-0.659		O4'	-0.638		O5'	-0.659		O6'
	O2''	-0.693		O3''	-0.659		O4''	-0.640		O5''	-0.665		O6''
	O2'''	-0.686		O3'''	-0.654		O4'''	-0.636		O5'''	-0.662		O6'''

[a]geometry can not be optimized.

Table S6: Atomic charge distribution (q) on the O-atoms of the binding sites with Na^+-ion given by the Natural Population Analysis at the B3LYP/6-31+g* level of theory. The numbering of the O-atoms is according to Figure 1.

Amino Acid	Atom	q(O)
TYR78	O2	-0.689
	O2'	-0.704
	O2''	-0.703
	O2'''	-0.691
GLY 77	O3	-0.686
	O3'	-0.687
	O3''	-0.687
	O3'''	-0.686
Val 76	O4	-0.687
	O4'	-0.687
	O4''	-0.684
	O4'''	-0.682

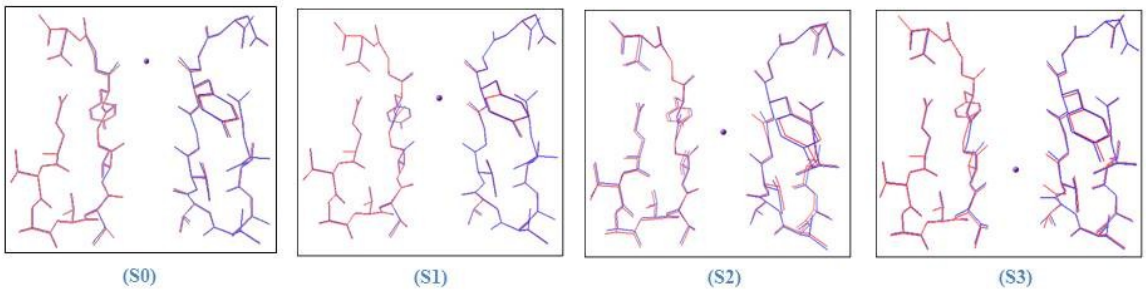


Figure S5: Superimposition of the optimized geometries of the binding sites in the selectivity filter of K^+-ion channel with and without potassium ion. The blue colour indicates structure with the K^+-ion.

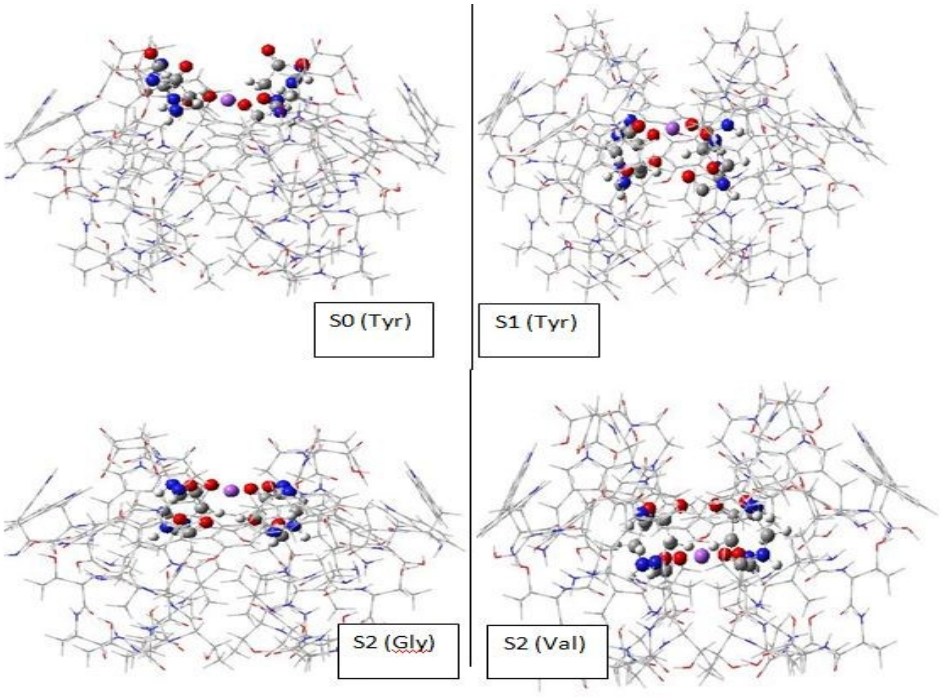


Figure S6: Optimized geometries for four binding sites with sodium ion at the ONIOM(B3LYP/6-31+g*:AMBER96) level of theory. Atoms in high layer are shown in ball and stick and those in low layer are in wire frame.

Table S7: Cartesian coordinates of the optimized geometries of the binding sites of the selectivity filter of KcsA, with K^+-ion and with Na^+-ion in the quantum mechanical region.

S4

1	-3.6399	-3.86256	-6.00688
6	-3.54253	-2.82581	-5.51272
6	-2.2308	-2.65749	-4.76911
8	-1.29228	-2.0055	-5.19528
6	-3.72918	-1.70678	-6.57074
8	-2.77665	-1.77474	-7.60621
1	-4.71025	-1.76898	-7.08642
7	-2.18352	-3.29983	-3.51332
1	-1.31251	-3.3169	-2.96038
1	3.58391	3.83583	-6.01759
6	3.4791	2.81416	-5.49208
6	2.16842	2.65914	-4.73874
8	1.25858	1.92881	-5.09927
6	3.66734	1.63962	-6.48501
8	2.66855	1.60016	-7.47373
1	4.62073	1.70144	-7.05005
7	2.10363	3.37863	-3.53288
1	1.23795	3.40222	-2.9755
1	-3.87062	3.58439	-5.99289
6	-2.84441	3.48719	-5.47372
6	-2.67951	2.18954	-4.70287
8	-2.00287	1.24898	-5.08695
6	-1.67491	3.66686	-6.47822
8	-1.62648	2.64943	-7.44606
1	-1.75099	4.60761	-7.06311
7	-3.31193	2.17612	-3.44001
1	-3.34464	1.30703	-2.88529
1	3.85204	-3.61774	-5.979
6	2.8231	-3.51229	-5.4689
6	2.65945	-2.20532	-4.71448
8	1.95351	-1.28655	-5.09635
6	1.66708	-3.68323	-6.48675
8	1.66708	-2.70036	-7.49198
1	1.72731	-4.64449	-7.03988
7	3.33107	-2.15633	-3.4751
1	3.36596	-1.27897	-2.93509
1	-2.80543	-4.08634	-3.30182
1	3.65931	0.68525	-5.87948
1	1.81785	1.53509	-6.9838
1	4.27508	2.8244	-4.72698
1	2.70614	4.19082	-3.37404
1	-0.7163	3.68084	-5.87665
1	-1.55843	1.81031	-6.93745
1	-2.85237	4.29581	-4.72316
1	-4.14192	2.75672	-3.28676
1	0.70618	-3.63979	-5.89912
1	1.63882	-1.83481	-7.02339
1	2.80823	-4.31349	-4.70886
1	4.15594	-2.74214	-3.31601
1	-4.35131	-2.80827	-4.76037
1	-3.66158	-0.71614	-6.04265
1	-1.91098	-1.579	-7.18698

S3

1	-3.88184	-0.98268	-2.51209
6	-3.46257	-0.16217	-1.86779
8	-2.2398	0.11155	-1.81195
7	-4.35298	0.50775	-1.12923
6	-3.94491	1.57261	-0.21441
6	-3.70464	1.04659	1.21378
8	-2.89906	1.62077	1.93765
1	-4.70997	2.39736	-0.21971
7	-4.49388	-0.00267	1.59556
1	-4.30698	-0.57629	2.43264
1	3.74581	0.88868	-2.33077
6	3.45103	0.13103	-1.54151
8	2.44942	0.25716	-0.84027
7	4.31563	-0.89554	-1.33426
6	3.99543	-1.93096	-0.35976
6	3.80794	-1.37104	1.05985
8	3.11052	-1.99085	1.85949
1	4.77032	-2.73981	-0.40763
7	4.45732	-0.20943	1.36999
1	4.01658	0.45675	2.01954
1	0.92663	-3.79126	-2.34165
6	0.23313	-3.46503	-1.5081
8	0.51886	-2.568	-0.71916
7	-0.89751	-4.19905	-1.34925
6	-1.90507	-3.81324	-0.37495
6	-1.29168	-3.57774	1.01347
8	-1.74435	-2.69041	1.72697
1	-2.71067	-4.59326	-0.35085
7	-0.31104	-4.44584	1.41572
1	0.39386	-4.10043	2.08209
1	-1.04453	3.90928	-2.32246
6	-0.33009	3.60122	-1.49876
8	-0.58903	2.71341	-0.6915
7	0.80562	4.33887	-1.37719
6	1.83206	3.98687	-0.40374
6	1.26611	3.81838	1.01586
8	1.81427	3.03674	1.78838
1	2.65029	4.75412	-0.43969
7	0.20947	4.61524	1.35521
1	-0.47472	4.29365	2.05476
1	-2.97852	1.9599	-0.5501
1	-5.32822	0.21766	-1.21957
1	-5.1119	-0.45561	0.91979
1	3.01609	-2.359	-0.60004
1	5.17232	-0.90739	-1.88162
1	5.02634	0.25962	0.65756
1	-2.34273	-2.84761	-0.65167
1	-1.0672	-4.91872	-2.04535
1	0.10603	-5.08284	0.72577
1	2.25076	3.00371	-0.64439
1	0.93013	5.09679	-2.04116
1	-0.22354	5.21005	0.64022

S2

1	0.86957	-3.85087	-2.67777
6	1.18677	-3.41627	-1.69037
8	0.44499	-2.80346	-0.93334
7	2.49657	-3.63646	-1.35181
6	3.11328	-2.82817	-0.31472
6	2.54929	-2.94294	1.09978
8	2.79988	-2.01575	1.86947
7	1.90029	-4.09152	1.44986
1	1.24546	-4.16883	2.24581
1	-0.78185	3.92884	-2.64418
6	-1.11171	3.49105	-1.65948
8	-0.37291	2.8929	-0.88629
7	-2.43124	3.67408	-1.35069
6	-3.06634	2.83089	-0.35222
6	-2.56449	2.92103	1.08833
8	-2.87792	1.99675	1.83997
7	-1.89974	4.04735	1.47367
1	-1.26824	4.10339	2.29046
1	3.95758	0.78294	-2.64964
6	3.51541	1.10653	-1.66471
8	2.91889	0.35997	-0.89728
7	3.68985	2.42489	-1.35195
6	2.84452	3.05131	-0.34939
6	2.94209	2.5452	1.0895
8	2.02098	2.855	1.84536
7	4.07128	1.88013	1.46769
1	4.12998	1.24306	2.27955
1	-3.98026	-0.78327	-2.65578
6	-3.54234	-1.11435	-1.67154
8	-2.94665	-0.37802	-0.89525
7	-3.71405	-2.4383	-1.36933
6	-2.8602	-3.06004	-0.37278
6	-2.96768	-2.5613	1.06804
8	-2.0366	-2.84989	1.82083
7	-4.11185	-1.924	1.45134
1	-4.17783	-1.28136	2.25859
1	4.17064	-3.11062	-0.25621
1	3.04895	-1.75922	-0.55338
1	3.11638	-4.0438	-2.05672
1	1.6309	-4.71116	0.69566
1	-4.12953	3.09765	-0.32885
1	-2.98411	1.76838	-0.61361
1	-3.04135	4.07175	-2.06968
1	-1.56117	4.64192	0.7265
1	3.10296	4.11636	-0.3233
1	1.78244	2.95956	-0.61025
1	4.08711	3.03667	-2.06973
1	4.66586	1.5482	0.71769
1	-3.10262	-4.12918	-0.35152
1	-1.7981	-2.94727	-0.62821
1	-4.10359	-3.048	-2.09264
1	-4.72402	-1.61585	0.70547

S1

1	1.01202	-3.9071	-2.53393
6	0.4562	-3.59667	-1.615
8	0.82866	-2.71794	-0.85356
7	-0.68353	-4.30484	-1.32585
6	-1.5718	-3.88212	-0.25467
6	-0.83278	-3.54302	1.04013
8	-1.26593	-2.68788	1.7959
1	-2.27579	-4.71104	0.00102
7	0.23194	-4.36965	1.36154
1	0.89891	-4.0613	2.08342
1	-0.92784	4.01057	-2.61453
6	-0.47486	3.72506	-1.62987
8	-0.99323	2.93568	-0.85073
7	0.69979	4.34829	-1.29708
6	1.54228	3.87633	-0.20132
6	0.78756	3.49697	1.07342
8	1.19847	2.57446	1.76283
1	2.25024	4.68767	0.098
7	-0.2272	4.34309	1.47047
1	-0.90215	4.01419	2.17618
1	3.97579	0.91718	-2.67331
6	3.70607	0.44706	-1.69151
8	2.90554	0.93184	-0.90501
7	4.36773	-0.71207	-1.36633
6	3.92595	-1.56281	-0.26668
6	3.57083	-0.81706	1.02129
8	2.67741	-1.24935	1.7379
1	4.74634	-2.27027	0.00848
7	4.40142	0.21693	1.38856
1	4.09135	0.87518	2.11788
1	-3.91625	-0.89933	-2.68709
6	-3.67753	-0.45142	-1.68778
8	-2.90658	-0.96316	-0.8859
7	-4.32682	0.7124	-1.36253
6	-3.87912	1.55014	-0.25353
6	-3.51728	0.78232	1.01705
8	-2.61769	1.18627	1.73533
1	-4.69794	2.24991	0.04762
7	-4.3743	-0.24756	1.38699
1	-4.03759	-0.93203	2.08113
1	-2.14398	-2.98584	-0.51723
1	-1.03373	-4.9422	-2.02996
1	0.64799	-4.9711	0.64731
1	2.10916	2.98298	-0.48506
1	1.17179	4.8057	-2.06899
1	-0.61853	5.04526	0.83545
1	3.02471	-2.12918	-0.52596
1	4.84871	-1.16569	-2.13455
1	5.09074	0.61083	0.74156
1	-2.98597	2.12774	-0.51477
1	-4.78275	1.18309	-2.13556
1	-4.99467	-0.66927	0.68911

S3-K

1	3.23772	2.22892	5.16045
6	2.47723	2.41971	4.34756
8	1.92284	1.50181	3.72137
7	2.245	3.69942	4.01747
6	1.23775	4.01453	3.0117

6	1.57071	3.34495	1.66304
8	0.66273	2.84954	0.99599
1	1.13673	5.12706	2.92683
7	2.87243	3.42216	1.26999
1	3.23668	2.84582	0.49736
1	-3.20855	-2.23179	5.12256
6	-2.46619	-2.43042	4.29177
8	-2.02704	-1.53001	3.55927
7	-2.14687	-3.7146	4.05795
6	-1.14498	-4.05555	3.05303
6	-1.50256	-3.43653	1.6899
8	-0.61336	-2.96391	0.98504
1	-1.03822	-5.17051	3.00165
7	-2.80966	-3.53168	1.31176
1	-3.18963	-2.90873	0.58524
1	2.21037	-3.2085	5.16092
6	2.3867	-2.47781	4.3138
8	1.48102	-2.11638	3.54791
7	3.65855	-2.09812	4.09876
6	3.98876	-1.11256	3.0731
6	3.33564	-1.48754	1.72899
8	2.77129	-0.62333	1.06059
1	5.10442	-1.02901	2.99457
7	3.51472	-2.77778	1.32204
1	2.91059	-3.17779	0.59002
1	-2.22254	3.2399	5.11658
6	-2.41767	2.50189	4.28123
8	-1.51958	2.08659	3.53398
7	-3.69903	2.1597	4.06012
6	-4.03666	1.16168	3.05086
6	-3.40203	1.51535	1.6931
8	-2.90951	0.62249	1.00539
1	-5.15217	1.06556	2.99102
7	-3.51096	2.81667	1.30206
1	-2.90276	3.19306	0.56137
1	0.27869	3.58049	3.31126
1	2.72902	4.40881	4.56044
1	3.59561	3.72979	1.93087
1	-0.18566	-3.60576	3.32661
1	-2.49963	-4.3916	4.73084
1	-3.52142	-3.80752	1.99927
1	3.56449	-0.13985	3.34038
1	4.31785	-2.35269	4.83376
1	3.83482	-3.48383	1.99528
1	-3.59968	0.19611	3.32451
1	-4.3737	2.48781	4.74759
1	-3.79911	3.532	1.97981
19	0.00451	0.02253	2.64541

S2-K

1	1.11603	3.69291	-2.68863
6	1.42066	3.19486	-1.7288
8	0.67637	2.5083	-1.03108
7	2.71115	3.41558	-1.33499
6	3.23376	2.61991	-0.2373
6	2.38107	2.67705	1.03745
8	2.13791	1.63331	1.64684
7	2.0185	3.91658	1.48503
1	1.34977	4.06571	2.25229
1	-1.01266	-3.79347	-2.6474
6	-1.33081	-3.29585	-1.68854
8	-0.59044	-2.61911	-0.97482
7	-2.63284	-3.48303	-1.32603
6	-3.17243	-2.63534	-0.27595
6	-2.37281	-2.65927	1.03319
8	-2.17372	-1.59861	1.63238
7	-2.0162	-3.88199	1.52312
1	-1.36179	-4.00739	2.30714
1	3.80333	-0.99732	-2.66711
6	3.30568	-1.31223	-1.7064
8	2.62656	-0.56933	-0.99782
7	3.49799	-2.6117	-1.33809
6	2.65436	-3.14984	-0.28345
6	2.68489	-2.34957	1.02575
8	1.62734	-2.15129	1.62929
7	3.90978	-1.98871	1.50798
1	4.03798	-1.3315	2.28921
1	-3.86027	1.00419	-2.66475
6	-3.36663	1.32439	-1.70431
8	-2.70265	0.5849	-0.97917
7	-3.53486	2.63492	-1.35859
6	-2.67761	3.17089	-0.3164
6	-2.71325	2.38429	1.00026
8	-1.6567	2.18393	1.60499
7	-3.94278	2.04168	1.4884
1	-4.07465	1.37966	2.26505
1	4.23901	2.97891	0.00376
1	3.27551	1.55592	-0.50197
1	3.3625	3.83149	-2.007
1	2.24451	4.74557	0.95394
1	-4.19355	-2.96503	-0.05982
1	-3.18794	-1.58165	-0.58096
1	-3.278	-3.87881	-2.01719
1	-2.16163	-4.71307	0.96714
1	2.98277	-4.17171	-0.06934
1	1.59921	-3.16119	-0.58438
1	3.89491	-3.25622	-2.02885
1	4.74008	-2.14049	0.95252
1	-2.98793	4.19999	-0.10894
1	-1.62255	3.16267	-0.62049
1	-3.91849	3.27628	-2.05943
1	-4.77094	2.19295	0.92938
19	-0.00679	0.00083	0.35159

S1-K

1	-1.97853	3.47527	-2.46145
6	-1.30453	3.31231	-1.58576
8	-1.27274	2.28897	-0.90812
7	-0.48087	4.34861	-1.25747
6	0.49551	4.19074	-0.19716
6	-0.13076	3.60083	1.07164
8	0.48866	2.80552	1.76469
1	0.94202	5.17851	0.0671
7	-1.36071	4.12159	1.41703
1	-1.92366	3.66833	2.15032
1	1.89902	-3.61515	-2.5443

6	1.31746	-3.41522	-1.60927
8	1.4023	-2.38406	-0.94345
7	0.48329	-4.4097	-1.19377
6	-0.46429	-4.17231	-0.11727
6	0.18964	-3.51998	1.10579
8	-0.39738	-2.62583	1.70687
1	-0.92015	-5.13733	0.20778
7	1.37005	-4.08023	1.52993
1	1.94094	-3.60493	2.24371
1	-3.5665	-1.87396	-2.60022
6	-3.38864	-1.27624	-1.66974
8	-2.36448	-1.32823	-0.99232
7	-4.40871	-0.46321	-1.26959
6	-4.21406	0.48287	-0.18453
6	-3.60298	-0.16363	1.06432
8	-2.75885	0.44516	1.7153
1	-5.19178	0.93596	0.10492
7	-4.13975	-1.36702	1.44517
1	-3.69047	-1.92487	2.1853
1	3.51264	1.84062	-2.62542
6	3.35916	1.27922	-1.66833
8	2.3509	1.36248	-0.96854
7	4.38093	0.46721	-1.26745
6	4.17026	-0.47605	-0.18105
6	3.53932	0.18673	1.04683
8	2.67877	-0.39754	1.69149
1	5.14319	-0.91969	0.14048
7	4.10496	1.38675	1.43802
1	3.62566	1.96581	2.14342
1	1.29617	3.49994	-0.48117
1	-0.48391	5.17862	-1.83529
1	-1.91217	4.65212	0.73777
1	-1.26054	-3.48601	-0.4259
1	0.29618	-5.15407	-1.85362
1	1.90329	-4.73473	0.94643
1	-3.51805	1.28119	-0.46427
1	-5.17045	-0.3183	-1.91973
1	-4.77396	-1.90185	0.84175
1	3.48594	-1.28131	-0.46842
1	5.10294	0.27144	-1.94942
1	4.66751	1.93465	0.77805
19	0.00612	-0.07715	-0.30479

TYR-K

1	1.3434	3.75356	-1.5591
6	1.69233	3.16498	-0.667
8	0.94258	2.5762	0.10882
7	3.04164	3.13656	-0.48418
6	3.65471	2.33466	0.553
6	3.93137	3.09565	1.84946
8	4.35502	2.52725	2.84787
7	3.73653	4.45962	1.77865
1	4.25138	5.08441	2.40194
1	-1.39915	-3.69158	-1.60845
6	-1.77134	-3.08592	-0.73617
8	-1.03518	-2.4456	0.01495
7	-3.1146	-3.09229	-0.54701
6	-3.75787	-2.32263	0.49287
6	-4.00331	-3.07269	1.80546
8	-4.44944	-2.47305	2.78679
7	-3.73391	-4.41082	1.77484
1	-4.2631	-5.03999	2.38326
1	3.72871	-1.37922	-1.59716
6	3.11457	-1.73484	-0.72369
8	2.48836	-0.97611	0.01984
7	3.09549	-3.07422	-0.52431
6	2.32484	-3.69739	0.52993
6	3.08485	-3.94018	1.83777
8	2.48984	-4.35395	2.83368
7	4.42969	-3.69965	1.78898
1	5.05277	-4.23092	2.40191
1	-3.73716	1.38783	-1.66046
6	-3.13975	1.74276	-0.7765
8	-2.50972	1.00207	-0.02778
7	-3.16178	3.0894	-0.5589
6	-2.35438	3.70733	0.46985
6	-3.0912	3.98748	1.78169
8	-2.5014	4.43858	2.75758
7	-4.45114	3.76862	1.7507
1	-5.0748	4.28304	2.37889
1	3.06499	1.44568	0.77998
1	4.63535	1.98608	0.20337
1	3.6415	3.53107	-1.21421
1	3.43289	4.87678	0.9073
1	-3.20907	-1.40619	0.71106
1	-4.75911	-2.03167	0.14407
1	-3.71592	-3.58537	-1.21245
1	-3.58369	-4.83447	0.86484
1	1.41804	-3.13376	0.75046
1	2.01325	-4.69562	0.19367
1	3.58113	-3.68585	-1.18599
1	4.84933	-3.58276	0.87224
1	-1.45892	3.12421	0.68795
1	-2.01888	4.69218	0.11582
1	-3.56909	3.69735	-1.27665
1	-4.88027	3.4437	0.8922
19	0.	0.	0.

VAL-Na

H	0.90665	-3.67488	-2.6284
C	1.25325	-3.15941	-1.69288
O	0.60476	-2.31415	-1.07754
N	2.47999	-3.55113	-1.2405
C	3.0781	-2.82777	-0.13389
C	2.28586	-2.86552	1.18231
O	2.2469	-1.84663	1.86642
N	1.74743	-4.06547	1.55322
H	1.09666	-4.18608	2.34371
H	-0.77614	3.74436	-2.59024
C	-1.14468	3.22885	-1.66014
O	-0.51127	2.37935	-1.03286
N	-2.38522	3.60639	-1.23992
C	-3.02328	2.84002	-0.18572
C	-2.31486	2.8502	1.17699
O	-2.37593	1.83135	1.86188
N	-1.75001	4.0229	1.58349

H	-1.12207	4.11524	2.397
H	3.75179	0.77845	-2.60518
C	3.23564	1.1422	-1.67262
O	2.37913	0.50973	-1.05528
N	3.62471	2.37519	-1.2388
C	2.8648	3.00857	-0.17693
C	2.87819	2.29048	1.18092
O	1.86432	2.35432	1.87156
N	4.04919	1.71303	1.57731
H	4.1398	1.07594	2.38396
H	-3.77211	-0.7679	-2.62015
C	-3.26217	-1.13637	-1.6867
O	-2.41488	-0.50704	-1.054
N	-3.64171	-2.38144	-1.27614
C	-2.88036	-3.02279	-0.22212
C	-2.91126	-2.32506	1.14508
O	-1.90073	-2.38618	1.84193
N	-4.09321	-1.76718	1.53872
H	-4.19662	-1.13157	2.34481
H	4.07035	-3.24766	0.05544
H	3.17142	-1.75967	-0.36577
H	3.0838	-4.07956	-1.87733
H	1.84724	-4.88017	0.96443
H	-4.03245	3.23669	-0.04089
H	-3.08792	1.77793	-0.45304
H	-2.9789	4.12641	-1.89372
H	-1.71624	4.80935	0.9494
H	3.26416	4.01583	-0.02709
H	1.80182	3.07613	-0.43972
H	4.1483	2.96932	-1.8889
H	4.83378	1.68143	0.94073
H	-3.26711	-4.03729	-0.08876
H	-1.8142	-3.07292	-0.47743
H	-4.15285	-2.97088	-1.93974
H	-4.87344	-1.74026	0.89664
Na	-0.00342	0.0154	-1.04038

GLY-Na

H	-1.79528	-3.5347	2.75913
C	-1.96918	-3.02663	1.77262
O	-1.07214	-2.61196	1.0431
N	-3.27169	-2.89537	1.37572
C	-3.55191	-1.97723	0.27776
C	-2.66123	-2.19843	-0.94991
O	-2.12569	-1.23635	-1.51448
N	-2.62758	-3.47103	-1.4477
H	-1.99791	-3.74809	-2.20847
H	1.74117	3.66294	2.71161
C	1.92496	3.15454	1.72459
O	1.02994	2.76383	0.97701
N	3.2257	2.96931	1.35786
C	3.49133	1.99423	0.30571
C	2.63336	2.18156	-0.95023
O	2.10643	1.20184	-1.49551
N	2.62311	3.43289	-1.496
H	1.99899	3.69032	-2.2681
H	-3.64836	1.71377	2.73749
C	-3.1385	1.89443	1.75009
O	-2.74132	0.99595	1.01001
N	-2.96202	3.19411	1.37746
C	-1.99493	3.46251	0.31796
C	-2.19444	2.60783	-0.93874
O	-1.21941	2.08455	-1.49468
N	-3.45251	2.59031	-1.46814
H	-3.7177	1.96558	-2.23735
H	3.72828	-1.73284	2.71977
C	3.21628	-1.92158	1.73524
O	2.83612	-1.03172	0.9771
N	3.00317	-3.22467	1.38784
C	2.00845	-3.48044	0.35279
C	2.20733	-2.64562	-0.91716
O	1.23331	-2.12086	-1.4725
N	3.4625	-2.65232	-1.46052
H	3.72793	-2.02094	-2.22464
H	-4.59358	-2.12017	-0.03152
H	-3.38924	-0.93611	0.57634
H	-4.01129	-3.10961	2.04915
H	-3.06576	-4.23372	-0.95092
H	4.5428	2.09069	0.01023
H	3.29911	0.9725	0.64821
H	3.95778	3.15945	2.04858
H	3.01655	4.21341	-0.98957
H	-2.09271	4.51487	0.02686
H	-0.97048	3.26662	0.65189
H	-3.1533	3.92495	2.0688
H	-4.22729	2.9933	-0.96043
H	2.07233	-4.53845	0.07138
H	0.99472	-3.25011	0.70117
H	3.18745	-3.94847	2.08806
H	4.23924	-3.03849	-0.94228
Na	-0.005	-0.01751	-1.59689

TYR-Na

H	-0.72603	-4.01125	2.56896
C	-0.21304	-3.63357	1.65217
O	-0.66756	-2.77142	0.90477
N	0.97855	-4.21509	1.33136
C	1.77882	-3.63975	0.26131
C	0.90069	-3.31014	-0.95095
O	1.03106	-2.25559	-1.57036
H	2.56637	-4.36859	-0.05376
N	0.09	-4.34484	-1.37645
H	-0.62936	-4.17828	-2.09358
H	0.56917	4.10857	2.67334
C	0.17342	3.76676	1.68362
O	0.77934	3.01656	0.91941
N	-1.04429	4.25341	1.30579
C	-1.75487	3.6302	0.19391
C	-0.82511	3.30023	-0.97872
O	-0.88745	2.19784	-1.53037
H	-2.55299	4.32402	-0.17052
N	-0.08514	4.34639	-1.47047
H	0.6566	4.18142	-2.16488
H	-4.08527	0.58521	2.72906
C	-3.75203	0.16225	1.74741
O	-2.99001	0.73412	0.9713

N	-4.27129	-1.04902	1.38706
C	-3.6838	-1.77858	0.26913
C	-3.3722	-0.86375	-0.92262
O	-2.28713	-0.94858	-1.50637
H	-4.39398	-2.57494	-0.06727
N	-4.41872	-0.10793	-1.38455
H	-4.2702	0.61211	-2.10487
H	4.0457	-0.57213	2.75663
C	3.75773	-0.18106	1.74751
O	3.0315	-0.78642	0.95921
N	4.26823	1.02965	1.37686
C	3.65529	1.74385	0.26017
C	3.32107	0.81468	-0.91003
O	2.23242	0.88725	-1.4769
H	4.35666	2.532	-0.11302
N	4.37825	0.06274	-1.39865
H	4.19516	-0.67757	-2.09187
H	2.25777	-2.70362	0.56295
H	1.42403	-4.80533	2.02205
H	-0.17264	-5.08336	-0.71563
H	-2.2142	2.68428	0.49635
H	-1.61372	4.61436	2.06311
H	0.10998	5.17341	-0.89168
H	-2.73053	-2.23903	0.54738
H	-4.67481	-1.59738	2.13761
H	-5.23363	0.09432	-0.79141
H	2.7141	2.21662	0.55681
H	4.60174	1.60062	2.14582
H	5.13912	-0.1969	-0.75874
Na	-0.04197	-0.01841	-1.21113