Simulation details about BBA5 in NaF solution

We also performed simulations of BBA5 in NaF solutions. The molar ratio of electrolyte/water in NaF solutions is exactly the same as that in NaI solutions. The concentration of NaF is ~4.9 mol/L. Force field parameters of F^- were also taken from Joung and Cheatham [1]. Comparison between the three salt systems is given in the supplementary information.

We used the same simulation procedure that described in the simulation details to simulate BBA5 in NaF solution.

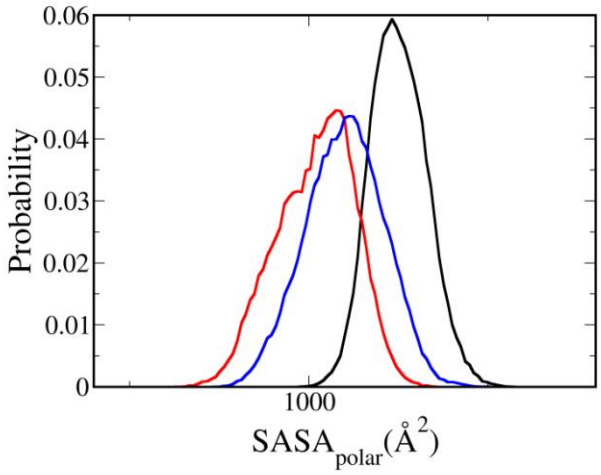
Results on the simulation of BBA5 in NaF solution.

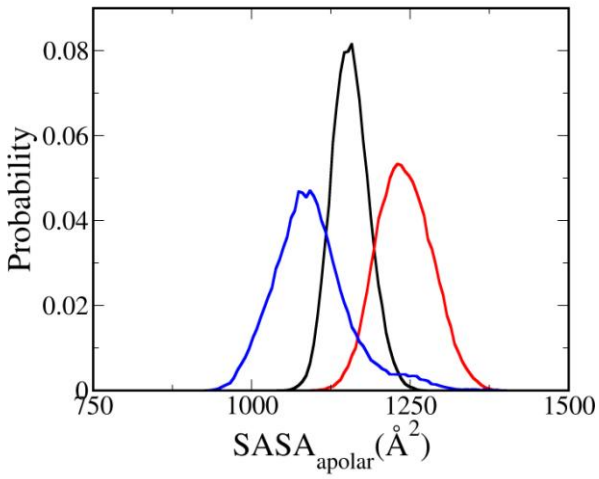
1.Hydrogen bond number

Backbone HB	In NaI solution	In NaF solution	In Na_2SO_3 solution	In Water
F8O-Y1H	0.00	0.00	0.00	0.00
Y1O-F8H	*0.00*	*0.00*	*0.00*	0.68
Y6O-V3H	*0.00*	0.96	0.96	0.96
V3O-Y6H	*0.00*	**0.48**	**0.75**	0.27
R10O-L14H	**0.27**	0.07	**0.89**	0.07
S11O-A15H	*0.00*	**0.68**	**0.62**	0.19
D12O-K16	0.00	0.00	0.10	0.09
E13O-L17H	0.00	0.00	0.00	0.07
L14O-L18H	0.41	**0.84**	**0.96**	0.35
A15O-R19	**0.40**	*0.00*	**0.38**	0.27
K16O-Q20	*0.00*	*0.00*	*0.00*	0.12
L17O-H21H	**0.45**	*0.19*	*0.00*	0.30
L18O-A22H	*0.19*	*0.03*	0.28	0.36
R19O-G23	0.00	0.00	0.00	0.00

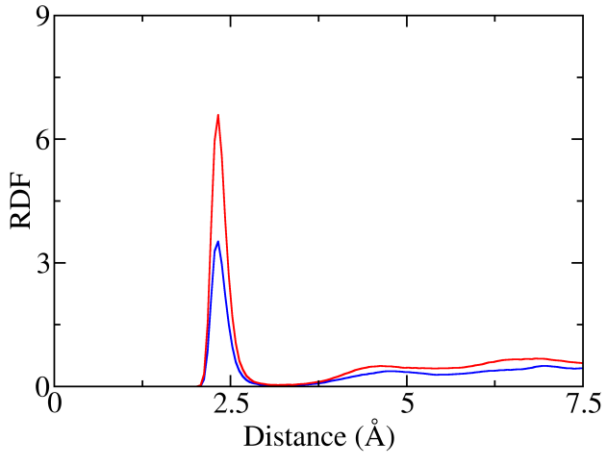
Table 1. The average number of backbone hydrogen bonds of BBA5 formed in NaI solution, NaF solution ,Na_2SO_3 solution, and pure water, respectively. The average is over the last 50 ns of the simulations. Overall, hydrogen bonds are strengthened (**bold**) in the Na_2SO_3 solution and weakened (*italic*) in the NaI solution, compared to those in pure water. The strengthening of hydrogen bond in the Na_2SO_3 solution is seen where strong hydrophobic contacts are formed between the alpha and the beta domains (residues 3,6 and 10-15).

2.Comparison between of polar and apolar SASA distribution functions for the three salt systems (black Na_2SO_3, red, NaI, and blue, NaF).

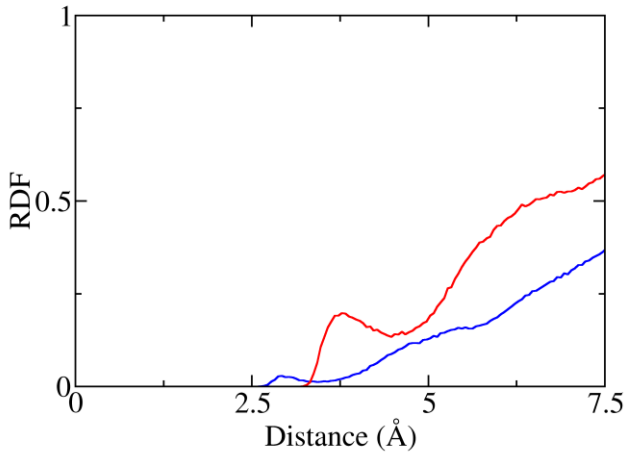




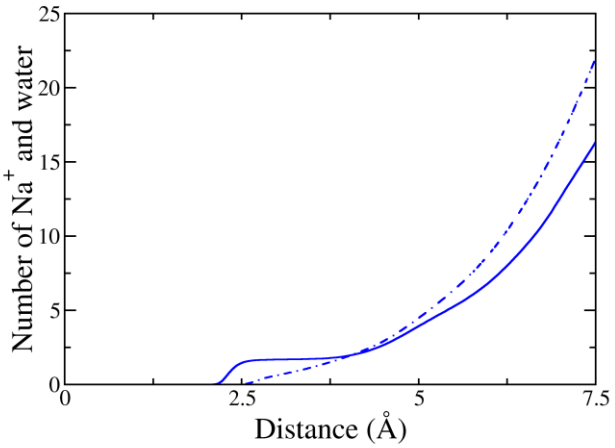
3.The RDF of Na^+ around the carbonyl oxygen averaged for all residues in NaF (blue) and NaI (red) solutions.



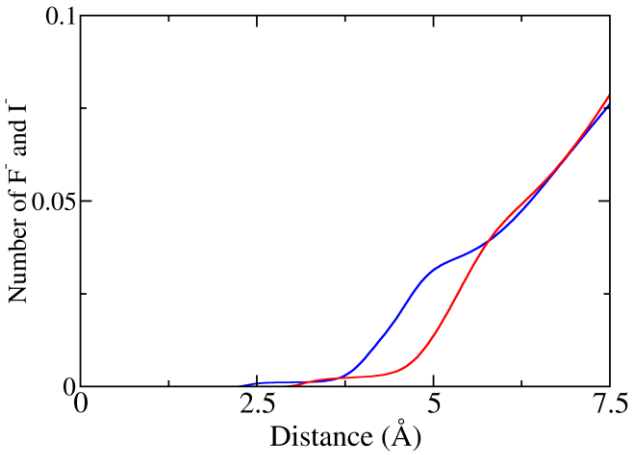
4.The RDF of F^- (blue) and I^- (red) around the polypeptide backbone NH groups.



5.The number of Na^+ (line)and water molecules(dash dot) around the BBA5 backbone carbonyl oxygen as a function of center-to-center distances in NaF solution



6. The averaged number of F^- (blue) and I^- (red) around Na^+ as a function of center-to-center distances between the ions.



Reference

1. In Suk Joung; T. E. Cheatham III. J. Phys. Chem. B, 2008, 112, 9020.