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Validation of polarizable force field parameters for nucleic acids by inter-molecular interactions

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Supplementary Information

Interaction energy calculation test between B3LYP/6-311++g** and RI-MP2/6-311++g** levels.

16 structures was chosen to make sure the interaction energies calculated at B3LYP/6-311++g** level are reliable, and can be used as references to do the comparison with the results of force fields. All the 16 structures chosen for this test contain an RNA fragment which have two joint uracils. And in 8 of these structures, the RNA fragment is cooperated with a water molecule, while in the others, the RNA fragment is cooperated with one sodium ion. All the calculations were done using orca-3.0.2 software package at RI-MP2/6-311++g** levels.

Interaction energies of these 16 structures are compared with the ones calculated at B3LYP//6-311++g** level. All the data are listed in Table S1 and S2, R^2-analysis are performed (Fig. S1 and S2).

Table S1 Interaction energies of two joint uracils with a water molecule

Structure Num.	MP2/6-311++g** /(kcal·mol^{-1})	B3LYP/6-311++g**/(kcal·mol^{-1})
1	2.435	2.335
2	–2.087	–2.794
3	1.832	1.816
4	–0.484	–0.530
5	–1.429	–1.476
6	–0.189	–0.201
7	–1.683	–1.890
8	1.335	1.274

Table S2 Interaction energies of two joint uracils with one sodium ion

Structure Num.	MP2/6-311++g**/(kcal·mol^{-1})	B3LYP/6-311++g**/(kcal·mol^{-1})
1	–29.837	–30.646
2	–36.805	–37.345
3	–44.693	–48.223
4	–47.638	–49.761
5	–26.635	–28.161
6	–55.934	–59.886
7	–40.854	–41.958
8	–77.890	–84.453

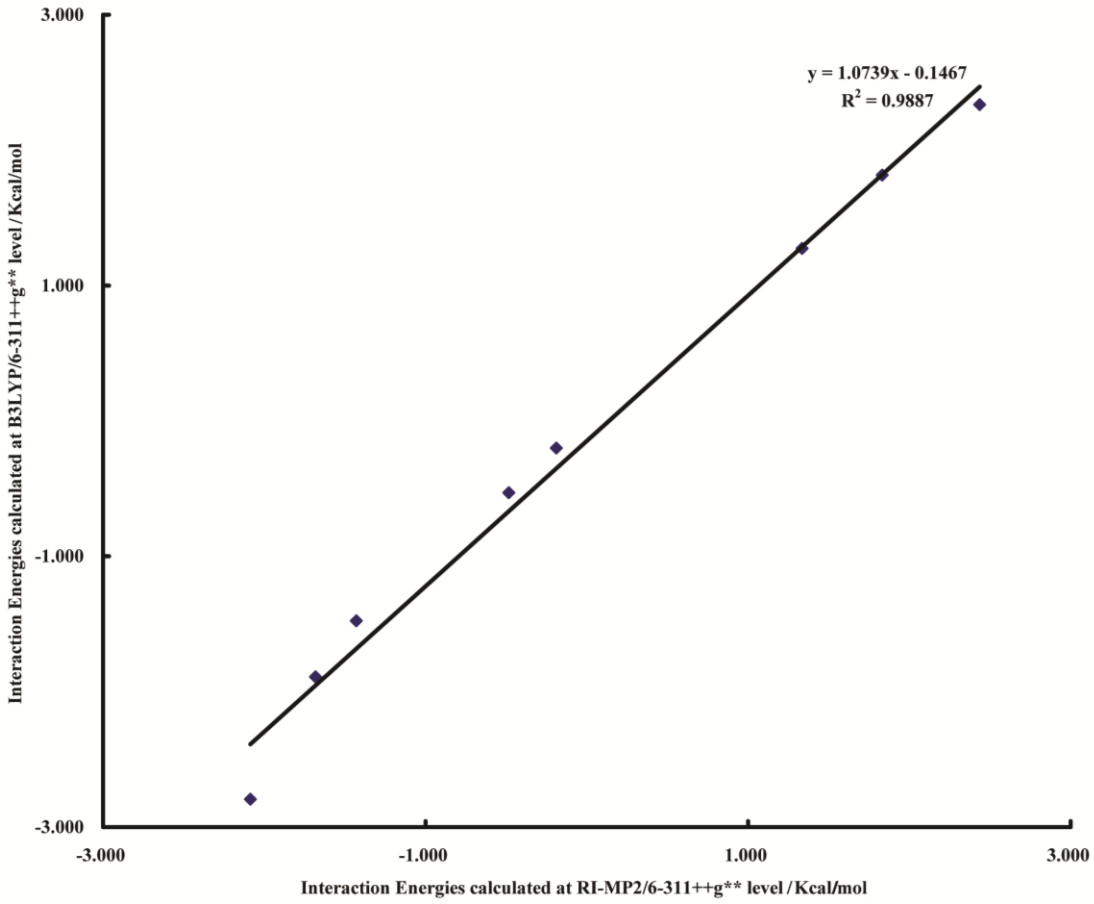

Fig. S1 Linear fit curve for the interaction energies between two joint uracils and a water molecule, data corresponding to Table S1.

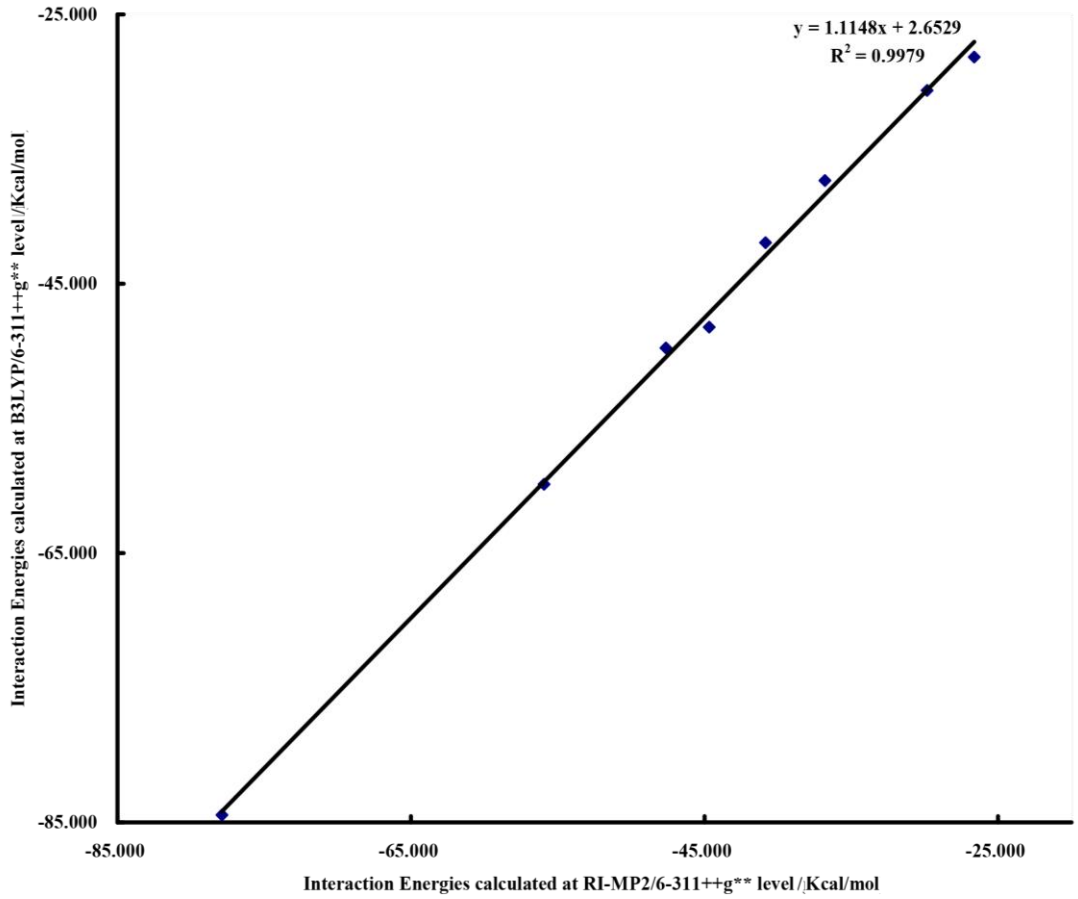

Fig. S2 Linear fit curve for the interaction energies between two joint uracils and one sodium ion, data corresponding to Table S2.