Implementation and validation of Amber force field, ff12SB and ff14SB, in Gomacs

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Abstract

This report shows the test result of old ff99SB, and two new ff12SB and ff14SB force fields implemented into gromacs

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Methods

The twenty tripeptides (each tripeptide contains three residues of a specific amino acid type) of twenty amino acids and eight trinucleotides (each trinucleotide contains three reisdues of a specific nucleic, DA, DC, DG, DT, RA, RC, RG or RU) were generated by Amber14 and undergone 1 ns simulations in tip3p explicit solvent with ff12SB and ff14SB force fields. From the last 500 ps of 1 ns simulation of each force field, 50 conformations of the models (tripeptides and trinucleotides) were taken. Therefore, for each model, there are 100 different structures which will be used for single-point simulations in AMBER14 (pmemd) and GROMACS-4.5.5 for checking energy differences.

Results

Table 1: The energy differences (%) of the simulations with the amber force fields in AMBER and GROMACS.

Error (%)	ff99SB		ff12SB		ff14SB	
	Amino	Nucleic	Amino	Nucleic	Amino	Nucleic
BOND	0.003	0.002	0.003	0.002	0.003	0.002
ANGLE	0.001	0.001	0.001	0.001	0.001	0.001
DIHEDRAL	0.134	0.000	0.085	0.003	0.107	0.003
1-4vdW	0.001	0.001	0.001	0.001	0.001	0.001
1-4QQ	0.001	0.001	0.001	0.001	0.001	0.001
vdW	0.001	0.000	0.001	0.000	0.001	0.000
QQ	0.004	0.004	0.004	0.004	0.004	0.004
Total Potetial	0.152	0.004	0.149	0.005	0.143	0.005