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 (%)	ff99	ff99SB		ff12SB		ff14SB	
	Amino	Amino	Nucleic	Amino	Nucleic	Amino	Nucleic
BOND	0.003	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	0.001
DIHEDRAL	0.139	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	0.001
1-4QQ	0.001	0.001	0.001	0.001	0.001	0.001	0.001
vdW	0.001	0.001	0.000	0.001	0.000	0.001	0.000
QQ	0.004	0.001	0.004	0.004	0.004	0.004	0.004
Total Potetial	0.204	0.152	0.004	0.149	0.005	0.143	0.005

Table 2: The dihedral energy difference (%) of the amino acids of the simulations with the amber force fields in AMBER and GROMACS.

Amino-FF	ff99	ff99SB	ff12SB	ff14SB
ARG	0.08131	0.07772	0.03977	0.07777
LYS	0.12403	0.11652	0.08061	0.11591
ASP	0.15641	0.14384	0.04203	0.07021
GLU	0.13793	0.12819	0.06064	0.06897
ASN	0.06801	0.06166	0.03994	0.04976
GLN	0.06984	0.06533	0.03285	0.05067
HIE	0.13709	0.12591	0.06336	0.09312
SER	0.14136	0.12614	0.07730	0.08557
THR	0.17146	0.15773	0.05722	0.09808
TYR	0.05721	0.05803	0.03273	0.05732
GLY	0.26945	0.38971	0.38971	0.38971
PRO	0.11043	0.08836	0.08974	0.08974
CYS	0.10454	0.08839	0.04469	0.06005
ALA	0.26464	0.21140	0.20826	0.20826
TRP	0.07430	0.06704	0.02684	0.05619
MET	0.25817	0.23366	0.14780	0.16821
PHE	0.08953	0.08377	0.04006	0.07408
VAL	0.23410	0.22289	0.09322	0.15738
ILE	0.09679	0.09450	0.03428	0.06998
LEU	0.13805	0.13054	0.10346	0.10648