

GROMACS - Bug #2526

Bug of gmx hbond

05/28/2018 03:57 AM - Lang Li

Status: New	
Priority: Normal	
Assignee:	
Category:	
Target version:	
Affected version - extra info:	Difficulty: uncategorized
Affected version: 2016.5	
Description	
<p>I found the generated hbond index were wrong. For example</p> <p>Hbonds between resid 583 and DNA [hbonds_r_583-DNA] 5443 5444 343 5443 5444 346 5443 5444 377 5443 5444 583 5443 5444 596 5443 5444 599</p> <p>Line1 is wrong the correct ndx is 343 345 5443 but other lines are right</p> <p>Other samples in gmx hbond are similar. Their first several lines are wrong(not only line 1), and others are right.</p> <p>Please fix the bug Thanks~</p>	

History

#1 - 05/29/2018 04:45 PM - Paul Bauer

Hello, could you please also upload the tpr file, a small trajectory and give us the exact command you used to run gmx hbond?
Thank you!

#2 - 05/30/2018 03:12 PM - Lang Li

- File Bug of gmx hbond.7z added

Hello, I attach those files.
Command is local in readme.sh.

Files

hbondMOL.ndx	7.47 KB	05/28/2018	Lang Li
Bug of gmx hbond.7z	31.8 MB	05/30/2018	Lang Li