GROMACS - Bug #2011

gmx clustsize -mol ignores index file

07/21/2016 11:57 AM - David van der Spoel

Status:	Closed		
Priority:	Low		
Assignee:	David van der Spoel		
Category:	analysis tools		
Target version:			
Affected version - extra info:		**Difficulty:**	uncategorized
Affected version:	5.1		

Description

When running gmx clustsize -mol the index file is ignored, meaning all water is taken into account as well when doing the analysis on a bunch of solute molecules.

Problem be circumvented by making a subset of the trajectory first.

History

#1 - 07/21/2016 11:59 AM - David van der Spoel

- Status changed from New to Accepted

#2 - 12/21/2017 03:22 PM - Mark Abraham

- Target version deleted (2018)

#3 - 12/31/2017 04:59 PM - Erik Lindahl

- Status changed from Accepted to Rejected

The output of gmx clustsize clearly states "Using molecules rather than atoms. Not reading index file" in this case, so this is not a bug but rather functionality that was never implemented.

The only way for a generic tool to automatically handle the combination of indices and molecule-based properties would be for the tool to first check that the index file corresponds to only molecules, and then go through the entire topology to create a subset consisting of only the molecules you are interested in.

#4 - 12/31/2017 05:00 PM - Erik Lindahl

- Status changed from Rejected to Closed