

## GROMACS - Feature #2491

### Allow constant bias AWH simulations

04/25/2018 04:01 PM - Viveca Lindahl

<b>Status:</b>	New
<b>Priority:</b>	Low
<b>Assignee:</b>	Viveca Lindahl
<b>Category:</b>	mdrun
<b>Target version:</b>	future
<b>Difficulty:</b>	uncategorized
<b>Description</b>	
Some users prefer to simulate in constant ensemble when applying a bias potential along a reaction coordinate. AWH can provide this feature simply by not performing updates of the bias potential (and free energy). To make this feature useful, one could e.g. perform a shorter AWH simulation to get a rough estimate of the free energy and corresponding bias potential. In a follow-up simulation, the AWH output data can be fed as input using the mdp-option awh1-user-data and setting awh-nsamples-update=0.	

### History

#### #1 - 04/25/2018 04:04 PM - Gerrit Code Review Bot

Gerrit received a related patchset '1' for Issue [#2491](#).  
Uploader: Viveca Lindahl ([vivecalindahl@gmail.com](mailto:vivecalindahl@gmail.com))  
Change-Id: gromacs~master~l23dbc80992e130a28af413754d12f8fd167e7bde  
Gerrit URL: <https://gerrit.gromacs.org/7794>

#### #2 - 06/05/2018 10:38 PM - Viveca Lindahl

- Priority changed from Normal to Low
- Target version changed from 2018.2 to future