

## GROMACS - Feature #2547

### Add option of averaging and obtaining error bars for AWH PMFs

06/06/2018 11:31 AM - Viveca Lindahl

<b>Status:</b>	New	
<b>Priority:</b>	Low	
<b>Assignee:</b>	Viveca Lindahl	
<b>Category:</b>	analysis tools	
<b>Target version:</b>	future	
<b>Difficulty:</b>	uncategorized	
<b>Description</b>		
Statistical errors in the PMF calculated with AWH can be estimated by running multiple independent simulations. Currently, the procedure has to be implemented by the user. This feature could either be added to gmx awh or contributed as a python script.		

#### History

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#1 - 06/06/2018 11:31 AM - Viveca Lindahl

- Description updated