

## GROMACS - Task #3014

### gmxapi example Python scripts

06/28/2019 11:07 AM - Eric Irrgang

<b>Status:</b>	In Progress	
<b>Priority:</b>	Normal	
<b>Assignee:</b>		
<b>Category:</b>	documentation	
<b>Target version:</b>	2021-infrastructure-stable	
<b>Difficulty:</b>	uncategorized	
<b>Description</b>		
<p>Complete functioning sample scripts serve as documentation by example. In addition to their possible "cook book" utility, they illustrate the idioms of the user interface, the scope of functionality, and use cases of note.</p> <p>They should be tested.</p> <p>Task: Small samples of script in documentation strings should be tested with a utility such as doctest</p> <p>Task: Complete sample scripts should be viewable and tested. The scripts should be discoverable, so a home needs to be found and hyperlinks added somewhere. Sample input also needs a home, and automated testing should occur regularly (perhaps once per patch release).</p>		
<b>Related issues:</b>		
Related to GROMACS - Feature #2896: Python packaging		<b>Feedback wanted</b>
Related to GROMACS - Task #2756: gmxapi integration testing		<b>In Progress</b>
Related to GROMACS - Feature #2961: How should Python package find GROMACS re...		<b>New</b>
Related to GROMACS - Feature #3295: Expand gmxapi.modify_input use cases.		<b>New</b>

### History

#### #1 - 12/11/2019 11:29 AM - Eric Irrgang

- Status changed from New to In Progress
- Target version changed from 2020 to 2021-infrastructure-stable

This is somewhat blocked by pending updates to automated infrastructure, as well as a few other tracked issues. I don't think there is anything blocking the 2020 release, though.

#### #2 - 12/11/2019 11:29 AM - Eric Irrgang

- Related to Feature #2896: Python packaging added

#### #3 - 12/11/2019 11:30 AM - Eric Irrgang

- Related to Task #2756: gmxapi integration testing added

#### #4 - 12/11/2019 11:31 AM - Eric Irrgang

- Related to Feature #2961: How should Python package find GROMACS resources under various circumstances? added

#### #5 - 01/03/2020 11:00 AM - Eric Irrgang

- Parent task deleted (#2985)

#### #6 - 01/13/2020 04:51 PM - Eric Irrgang

- Related to Feature #3295: Expand gmxapi.modify\_input use cases. added