```
## Activate environment ##

WARNING: No ICDs were found. Either,

- Install a conda package providing a OpenCL implementation (pocl, oclgrind, intel-compute-runtime, beigne
t) or

- Make your system-wide implementation visible by installing ocl-icd-system conda package.

## Execute Scripts ##

15:14:12 step0_reduce_remove_hydrogens: Removing Hydrogens

15:14:12     Not using any container

15:14:12     Executing: reduce -Trim path/to/data/inputs/files/m...

15:14:12     Exit code 0

15:14:12 step1_extract_molecule: Extracting Protein

15:14:14     Executing: check_structure -i path/to/data/outputs/...

15:14:14     Exit code 0

15:14:14     Not using any container

15:14:14     Executing: ...

15:14:14     Exit code 0

15:14:14 step00_cat_pdb: Concatenating protein with included ions

15:14:14 step2_fix_side_chain: Modeling the missing heavy atoms in the structure side chains

15:14:14     Not using any container

15:14:16     Executing: check_structure -i path/to/data/outputs/...

15:14:16     Exit code 0

15:14:16 step4_pdb2gmx: Generate the topology

15:14:16     Not using any container

15:14:19     Executing: gmx -nobackup -nocopyright pdb2gmx -f path/to/data/biobb/Web/projects/BBB654...

15:14:19     Exit code 0

15:14:19     Compressing topology to: path/to/data/outputs/wf_setup/step4_pdb2gmx/pdb2gmx_top.zip

15:14:19 step5_editconf: Create the solvent box

15:14:19     Centering molecule in the box.

15:14:19     Distance of the box to molecule:   0.80

15:14:19     Box type: octahedron

15:14:19     Not using any container

15:14:19     Executing: gmx -nobackup -nocopyright editconf -f path/to/data/biobb/Web/projects/BBB65...

15:14:19     Exit code 0

15:14:19 step6_solvate: Fill the solvent box with water molecules

15:14:19     Not using any container

15:14:22     Executing: gmx -nobackup -nocopyright solvate -cp path/to/data/biobb/Web/projects/BBB65...

15:14:22     Exit code 0

15:14:22     Compressing topology to: path/to/data/outputs/wf_setup/step6_solvate/solvate_top.zip

15:14:22 step7_grompp_genion: Preprocess ion generation
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15:14:22     Not using any container
15:14:24     Executing: gmx -nobackup -nocopyright grompp -f 899e2048-68e3-4b92-8ec8-705729bae249/grompp..
.
15:14:24     Exit code 0
15:14:24 step8_genion: Ion generation
15:14:25     To reach up 0.05 mol/litre concentration
15:14:25     Not using any container
15:14:25     Executing: echo "SOL" | gmx -nobackup -nocopyright genion -s path/to/data/biobb/Web/pro...
15:14:25     Exit code 0
15:14:25     Compressing topology to: path/to/data/outputs/wf_setup/step8_genion/genion_top.zip
15:14:25 step9_grompp_min: Preprocess energy minimization
15:14:26     Not using any container
15:14:27     Executing: gmx -nobackup -nocopyright grompp -f 41f7b097-8747-424b-b4d8-9c275016a2e3/grompp..
.
15:14:27     Exit code 0
15:14:28 step10_mdrun_min: Execute energy minimization
15:14:28     Not using any container
15:25:45     Executing: gmx -nobackup -nocopyright mdrun -s path/to/data/biobb/Web/projects/BBB6543b...
15:25:45     Exit code 0
15:25:45 step100_make_ndx: Creating an index file for the whole system
15:25:45     Not using any container
15:25:46     Executing: echo -e 'System\nq' | gmx -nobackup -nocopyright make_ndx -f path/to/data/bi...
15:25:46     Exit code 0
15:25:46 step11_grompp_nvt: Preprocess system temperature equilibration
15:25:46     Not using any container
15:25:48     Executing: gmx -nobackup -nocopyright grompp -f 66ba6e14-3061-4562-8157-e8fe1f4aeba8/grompp..
.
15:25:48     Exit code 0
15:25:48 step12_mdrun_nvt: Execute system temperature equilibration
15:25:49     Not using any container
16:16:16     Executing: gmx -nobackup -nocopyright mdrun -s path/to/data/biobb/Web/projects/BBB6543b...
16:16:16     Exit code 0
16:16:16 step13_grompp_npt: Preprocess system pressure equilibration
16:16:16     Not using any container
16:16:19     Executing: gmx -nobackup -nocopyright grompp -f f6c40599-1d5c-47fc-9cf8-c23266c074da/grompp..
.
16:16:19     Exit code 0
16:16:19 step14_mdrun_npt: Execute system pressure equilibration
16:16:19     Not using any container
17:07:39     Executing: gmx -nobackup -nocopyright mdrun -s path/to/data/biobb/Web/projects/BBB6543b...
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17:07:39     Exit code 0

17:07:39 step15_grompp_md: Preprocess free dynamics

17:07:39     Not using any container

17:07:40     Executing: gmx -nobackup -nocopyright grompp -f 19c611e6-9336-45d2-8c04-4249930cb6a8/grompp..
.

17:07:40     Exit code 0

17:07:40 step16_mdrun_md: Execute free molecular dynamics simulation

17:07:41     Not using any container

21:23:16     Executing: gmx -nobackup -nocopyright mdrun -s path/to/data/biobb/Web/projects/BBB6543b...

21:23:16     Exit code 0

21:23:16 step17_gmx_image1: Image Trajectory, step1, moving ligand to center of the water box

21:23:17     Not using any container

21:23:23     Executing: echo "Protein" "System" | gmx trjconv -f path/to/data/biobb/Web/projects/BBB...

21:23:23     Exit code 0

21:23:23 step18_gmx_image2: Image Trajectory, step2, removing rotation

21:23:24     Not using any container

21:23:29     Executing: echo "Protein" "System" "System" | gmx trjconv -f path/to/data/biobb/Web/pro...

21:23:29     Exit code 0

21:23:29 step19_gmx_trjconv_str: Convert final structure from GRO to PDB

21:23:29     Not using any container

21:23:31     Executing: echo "System" | gmx trjconv -f path/to/data/biobb/Web/projects/BBB6543bc5ada...

21:23:31     Exit code 0

21:23:31 step20_gmx_energy: Generate energy plot from minimization/equilibration

21:23:31     Not using any container

21:23:31     Executing: gmx energy -f path/to/data/outputs/wf_se...

21:23:31     Exit code 0

21:23:31 step21_gmx_rgyr: Generate Radius of Gyration plot for the resulting setup trajectory from the fre
e md step

21:23:31     Not using any container

21:23:33     Executing: echo "Protein-H" | gmx gyrate -s path/to/data/biobb/Web/projects/BBB6543bc5a...

21:23:33     Exit code 0

21:23:33 step22_rmsd_first: Generate RMSd (against 1st snp.) plot for the resulting setup trajectory from
the free md step

21:23:33     Not using any container

21:23:34     Executing: echo 'Protein-H Protein-H' | gmx rms -s path/to/data/biobb/Web/projects/BBB6...

21:23:34     Exit code 0

21:23:34 step23_rmsd_exp: Generate RMSd (against exp.) plot for the resulting setup trajectory from the fr
ee md step

21:23:35     Not using any container

21:23:36     Executing: echo 'Protein-H Protein-H' | gmx rms -s path/to/data/biobb/Web/projects/BBB6...
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21:23:36     Exit code 0

21:23:36 step24_grompp_md: Preprocess long MD simulation after setup

21:23:37     Not using any container

21:23:38     Executing: gmx -nobackup -nocopyright grompp -f 28838d3b-70fc-4903-b599-dbe282c2b737/grompp..
.

21:23:38     Exit code 0

21:23:38

21:23:38

21:23:38 Execution successful:

21:23:38   Workflow_path: path/to/data/outputs/wf_setup

21:23:38   Config File: path/to/data/inputs/.conf/setup.yml

21:23:38

21:23:38 Elapsed time: 369.4 minutes

21:23:38

## Quality check ##

## Generate results file ##

1814c5c6-0afd-49ac-a2b2-36fe5268d918 directory successfully created

Adding:

['path/to/data/biobb/Conf/structure/setup.outputs.md', '1814c5c6-0afd-49ac-a2b2-36fe5268d918/biobb.MDsetup
.cpt', '1814c5c6-0afd-49ac-a2b2-36fe5268d918/biobb.MDsetup.energy.xvg', '1814c5c6-0afd-49ac-a2b2-36fe5268d
918/biobb.MDsetup.gro', '1814c5c6-0afd-49ac-a2b2-36fe5268d918/biobb.MDsetup.prod.tpr', '1814c5c6-0afd-49ac
-a2b2-36fe5268d918/biobb.MDsetup.rgyr.xvg', '1814c5c6-0afd-49ac-a2b2-36fe5268d918/biobb.MDsetup.rmsd_exp.x
vg', '1814c5c6-0afd-49ac-a2b2-36fe5268d918/biobb.MDsetup.rmsd_first.xvg', '1814c5c6-0afd-49ac-a2b2-36fe526
8d918/biobb.MDsetup.top.pdb', '1814c5c6-0afd-49ac-a2b2-36fe5268d918/biobb.MDsetup.top.zip', '1814c5c6-0afd
-49ac-a2b2-36fe5268d918/biobb.MDsetup.tpr', '1814c5c6-0afd-49ac-a2b2-36fe5268d918/biobb.MDsetup.xtc']

to: path/to/data/downloads/workflow.results.zip

Removed temporary folder: 1814c5c6-0afd-49ac-a2b2-36fe5268d918

## Execute end-of-work routines ##

## Deactivate environment ##

## End of job ##
```