

## Additional materials – solvate and grompp commands

### Terminal commands

1. **cd Documents/firstmd** and press **Enter**.
2. **vmd box-added.gro** and press **Enter**.
3. Windows users must open VMD first. Then open the box-added.gro file via **VMD**.
4. Type **pbx box** in the **VMD terminal**.
5. **gmx solvate -cp box-added.gro -cs tip4p.gro -p topol.top -o solvated.gro** and press **Enter**.
6. Press **Ctrl+L** (Only to clear the screen for clarity in the video).
7. Type **pbx box** in the **VMD terminal**.
8. **gmx grompp -f ions.mdp -c solvated.gro -p topol.top -o input1.tpr -maxwarn 1** and press **Enter**.
9. **gmx dump -s input1.tpr** and press **Enter**.
10. **gmx genion -s input1.tpr -o ions-added.gro -p topol.top -pname NA -nname CL -nn 8** and press **Enter**.
11. Type **13** to replace the solvent.