**Speed benchmarks**

All data and scripts required to run the speed benchmarks are available at [https://git.scicore.unibas.ch/schwede/promod3_pipeline_benchmark](https://git.scicore.unibas.ch/schwede/promod3_pipeline_benchmark).

For ProMod3 specific benchmarks we used a Singularity container built with instructions from the documentation ([ProMod3, version 3.1.0](https://salilab.org/modeller/)). Scripts calling external tools have been executed natively on a Linux system. Used Hardware:

- CPU: Intel i7-6600U 2.60GHz
- Memory: 16GB DDR4 2133 MHz
- HD: Dell NVMe LITEON 256GB SSD

**Sidechain modelling speed benchmark:** ProMod3 is compared to the binary of SCWRL4 as distributed by the Dunbrack lab. The corresponding scripts in the benchmark repository are `sidechain/reconstruct_sidechains_promod.py` and `sidechain/reconstruct_sidechains_scwrl.py`. Computation time is the average over three independent runs on the full test set used to measure sidechain modelling accuracy. The observed timings are:

- ProMod3 with subrotamers (FRM) and post-processing: 549 s
- ProMod3 no subrotamers (RRM): 253 s
- SCWRL4 with subrotamers (FRM): 1670 s
- SCWRL4 no subrotamers (RRM): 548 s

This gives the reported speedups of 3.0x in case of FRM and 2.2x in case of RRM.

**Homology modelling speed benchmark:** ProMod3 is compared to MODELLER (version 9.24) installed from the RPM package available from [https://salilab.org/modeller/](https://salilab.org/modeller/). The corresponding scripts in the benchmark repository are `modelling/build_promod_models.py` and `modelling/build_modeller_models.py`. Computation time is the average over three independent runs on the full test set used to measure homology modelling accuracy. The observed timings are:

- ProMod3: 1626 s
- MODELLER default settings: 2070 s

This gives the reported speedup of 1.3x.