An automated coarse-grained mapping algorithm for the Martini force field and benchmarks for membrane–water partitioning

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This script can be used to automatically generate a coarse-grained model of an organic solute using the Martini forcefield parameters. The coarse-grained models are compatible with the Gromacs simulation package (recommended 2018 or newer). If you use this method, please cite the attached paper, DOI:10.1021/acs.jctc.1c00322.

The following files are included:

- *cg_param.py* – automatically generates a coarse-grained model of an organic solute
- *fragment_DGs.dat* – contains ΔG_{OW} values for organic fragments which could make up individual coarse-grained beads

The following external packages are required, all of which are freely available and open source:

- Python 3.7 or newer with the following packages:
  - numpy
  - scipy
  - RDKit, version 2020 or newer
  - requests

The easiest way to install the correct python packages is using the conda package manager, for example from: `https://docs.conda.io/en/latest/miniconda.html`. A working environment can be created using:

```
$ conda create -c rdkit -n cg_param rdkit numpy scipy requests
$ conda activate cg_param
```

The most recent version of Gromacs, and detailed installation instructions, can be found at: `https://manual.gromacs.org/documentation/current/download.html`.

The command used to parametrise, for example, an octane molecule would be:

```
$ cg_param.py "CCCCCCCC" octane.gro octane.itp
```