
NistDataSelection Documentation

nistdataselection

Jan 27, 2020

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This tool aims to automate the process of curating data sets of condensed phase physical properties from the NIST ThermoML archive for optimizing and benchmarking molecular force fields against.

User Guide

- *Installation*

1.1 Installation

The data selection tools are currently only installable from source. It is recommended to install the tools within a conda environment, and allow the conda package manager to install the required dependencies.

More information about conda and instructions to perform a lightweight miniconda installation [can be found here](#). It will be assumed that these have been followed and conda is available on your machine.

1.1.1 Installation from Source

To install the tools from source, clone the repository from [github](#):

```
git clone https://github.com/openforcefield/nistdataselection
cd nistdataselection
```

Create a custom conda environment which contains the required dependencies and activate it:

```
conda env create --name nistdataselection --file devtools/conda-envs/test_env.yaml
conda activate nistdataselection
```

The final step is to install the tools themselves:

```
python setup.py develop
```