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# **NistDataSelection Documentation**

**nistdataselection**

**Apr 22, 2020**



**USER GUIDE**

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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.

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## 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
```