General workflow for running *ab initio* chemical shift calculations with `karminus`:

1. Decide on a set of reference compounds (from here on termed the training set) and add all geometries in the xyz/ directory. Delete all prior .xyz files in that directory.
2. Add the experimental chemical shifts for the compounds to `experiment/exp_chemical_shifts.py` according to the scheme described in the comments of that file.
3. Execute

   ```
   python actions/calibrate_chemical_shifts.py --method <method> \
     --basis_set <basis_set>
   ```

   which will perform all calculations necessary and will automatically save the generated output in `output\`.
4. Execute

   ```
   python actions/report_calibration.py --method <method> \
     --basis_set <basis_set> --nuclei_type <nucleus>
   ```

   which will extract the chemical shifts, average homotopic protons, perform a calibration and finally report the calibration and core statistics about the success of the chemical shift calibration. A plot is also generated, that can be saved in several graphics formats.
   The calibration is now done, and can be applied to new compounds via the formula $\delta(\sigma) = \sigma \cdot \text{slope} + \text{intercept}$. Alternatively, the following steps can be performed to automate the process of nmr calculation and calibration:
5. Run the chemical shift calculation jobs on which the calibration should be applied via

   ```
   actions/run_job.py --method <method> --basis_set <basis_set> \
     --xyz_file <absolute-path-to-xyzfile.xyz>
   ```

   which will generate output in `output/`.
6. Finally, the calibration can then be applied to the calculated chemical shifts:

   ```
   actions/apply_calibration.py --method <method> \
     --basis_set <basis_set> --job_name <jobname> \
     --nuclei_type <nucleus>
   ```

   Which will print out the calibrated chemical shifts.