
qmdesc

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qmdesc is a package for QM atomic/bond descriptors prediction

At its core, qmdesc contains a derived ChemProp model that was trained on QM descriptors including hirshfeld partial charges, nucleophilicity/electrophilicity Fukui indices, NMR shielding constants, bond lengths, and bond indices calculated under B3LYP/def2svp level of theory. This work was first presented in [Regio-Selectivity Prediction with a Machine-Learned Reaction Representation and On-the-Fly Quantum Mechanical Descriptors](#).

qmdesc can be used through either [python module](#) or [command line](#)

Prerequisite: [RDKit](#)

INDICES AND TABLES

- `genindex`
- `modindex`
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