# Available Models

# keras and torch models have slightly different interfaces. They also save their models differently. These two wrappers implement the same interface.

**ddm.pipeline.parameter\_parser.py:**

model\_wl = {**'AttentiveFPModel'**:dcm.AttentiveFPModel,

**'GCNModel'**:dcm.GCNModel,

**'MPNNModel'**:dcm.MPNNModel,

**'GraphConvModel'**:dcm.GraphConvModel,

**'PytorchMPNNModel'**:dcmt.MPNNModel}#, dcm.GCNModel, dcm.GATModel]

**ddm.pipeline.model\_wrapper.py:**

params.model\_type == 'NN/ RF/ xgboost/ hybrid

# Available Featurizers

featurizer\_wl = {**'MolGraphConvFeaturizer'**:dcf.MolGraphConvFeaturizer,

**'WeaveFeaturizer'**:dcf.WeaveFeaturizer,

**'ConvMolFeaturizer'**:dcf.ConvMolFeaturizer}

# Available Splitters

# List of splitter types that require SMILES strings as compound IDs

smiles\_splits = [**'scaffold'**, **'butina'**, **'fingerprint'**]

dc.splits -> **Index, Random**, **Scaffold**, **RandomStratified**, **Fingerprint**, **AVEMin**(metric=**jaccard**/**euclidean**), **Temporal**