Supporting Information for:

AtomNet PoseRanker: Enriching Ligand Pose Quality for Dynamic Proteins in Virtual High Throughput Screens

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Rosetta Protocols

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    <ScoreFunction name="r15" weights="ref2015">
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    <ScoreFunction name="cen" weights="cen_std"/>
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Table S1. AtomNet PoseRanker model hyperparameters

| Parameter description                                      | Value                |
|-----------------------------------------------------------|----------------------|
| Minibatch size                                            | 64                   |
| Optimizer                                                 | adam                 |
| Learning rate                                             | 0.001                |
| Activation function                                       | LeakyReLU            |
| Radial thresholds                                         | 10Å (l→l, r→l), 5Å (l→r) |
| Radial filter resolution (δ_{l})                          | 0.15625              |
| Atom dropout                                              | 0.15                 |
| Edge dropout                                              | 0.15                 |
| Atom embedding initial embedding dimension                 | 32                   |
| Message passing output filters                            | 256                  |
| Atom update hidden layer sizes                            | 256                  |
| Readout layer hidden layer sizes                          | 512                  |

We trained the model by sampling a 1:1 ratio of positive to negative examples for a total of 1 million iterations, sufficient to ensure convergence for all models.
Modifications to smina

We exposed the number of Monte Carlo steps as a user parameter by adding the following changes to the file src/main/main.cpp:

Line 67:
double steps_fraction;
int mc_steps;

Line 76:
steps_fraction(1), score_only(false), randomize_only(false), local_only(false),
dominimize(false), include_atom_info(false), mc_steps(-1)

Line 418:
par.mc.num_steps = unsigned(par.mc.num_steps * settings.steps_fraction);
if (settings.mc_steps > -1)  // if present, --mc_steps overrides --steps_fraction
    par.mc.num_steps = (unsigned) settings.mc_steps;

Line 994:
("steps_fraction", value<double>(&settings.steps_fraction)->default_value(1.0),
    "fraction of mc steps to perform (i.e. 1 is normal length)"
("mc_steps", value<int>(&settings.mc_steps)->default_value(-1),
    "number of mc steps to take (if >= 0 then overrides steps_fraction)"