Tuning and Validating Rosetta

H-Bonds with OH Donors

Rosetta Con 2010

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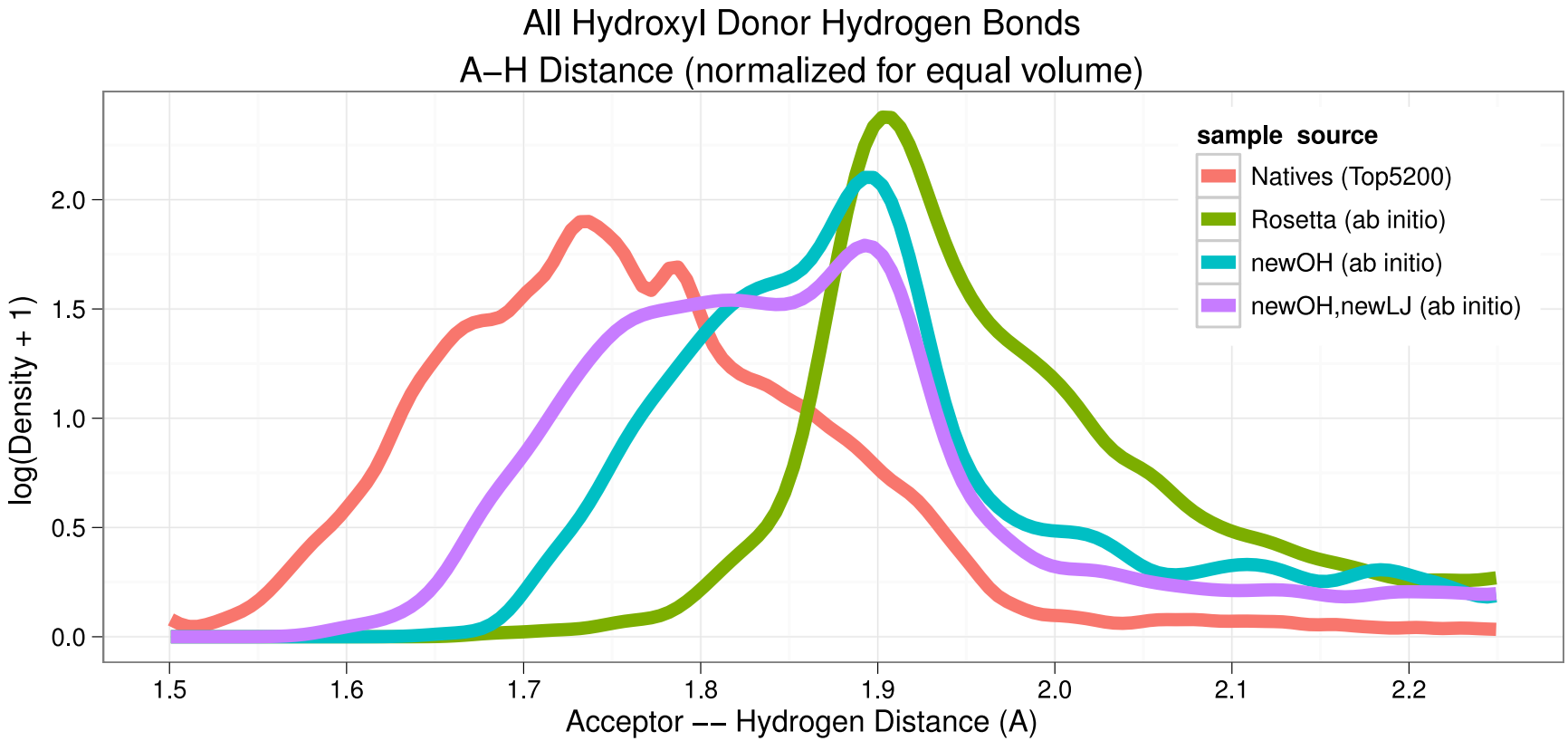
HBond Potential Correction

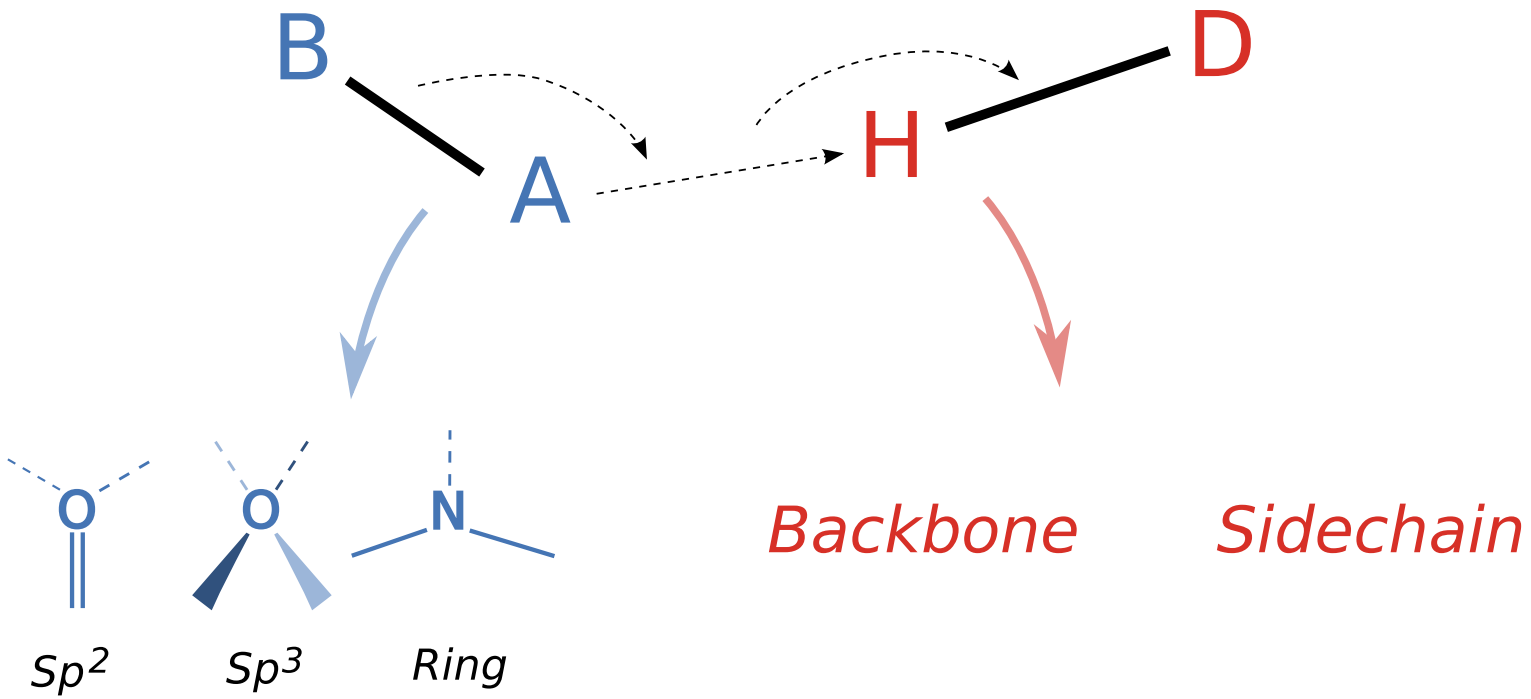


To use:

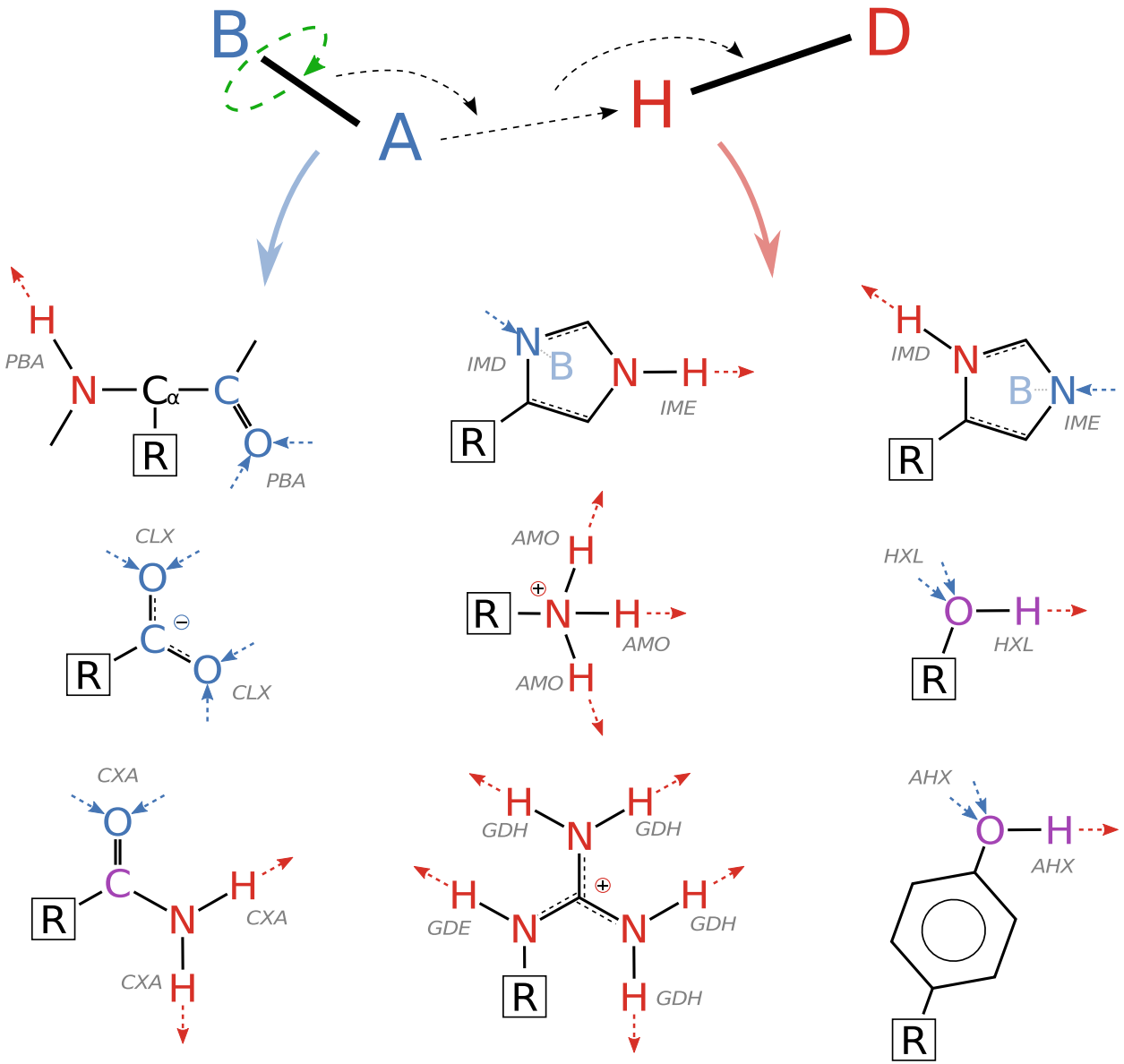
-hbond_params newOH_params -lj_hbond_hdis 1.75 -lj_hbond_OH_donor_dis 2.6

patch weights: ref_SER -= 0.1; ref_THR -= 0.1;

Classic Model



Refined Model

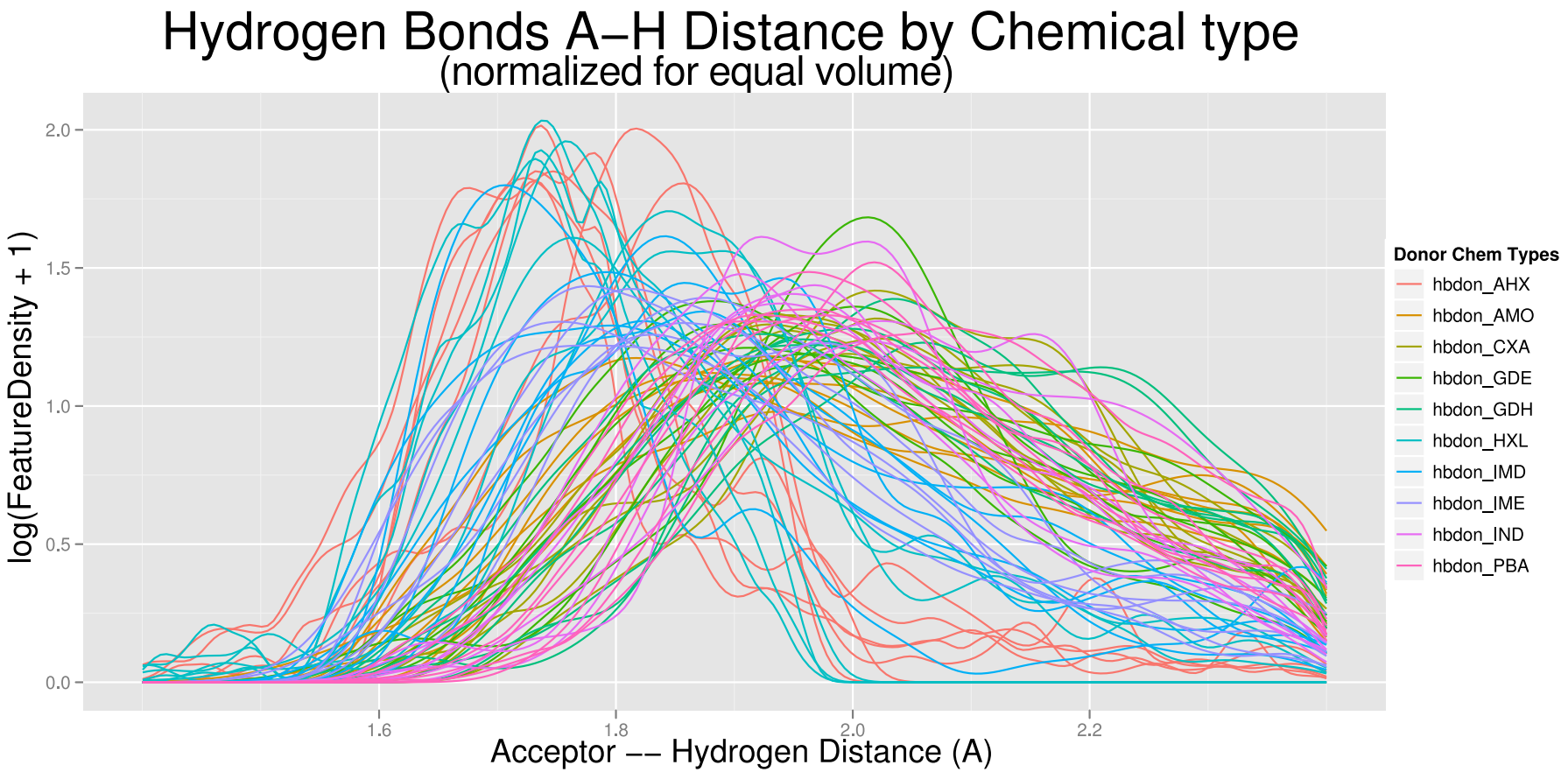


Organize Model Parameters

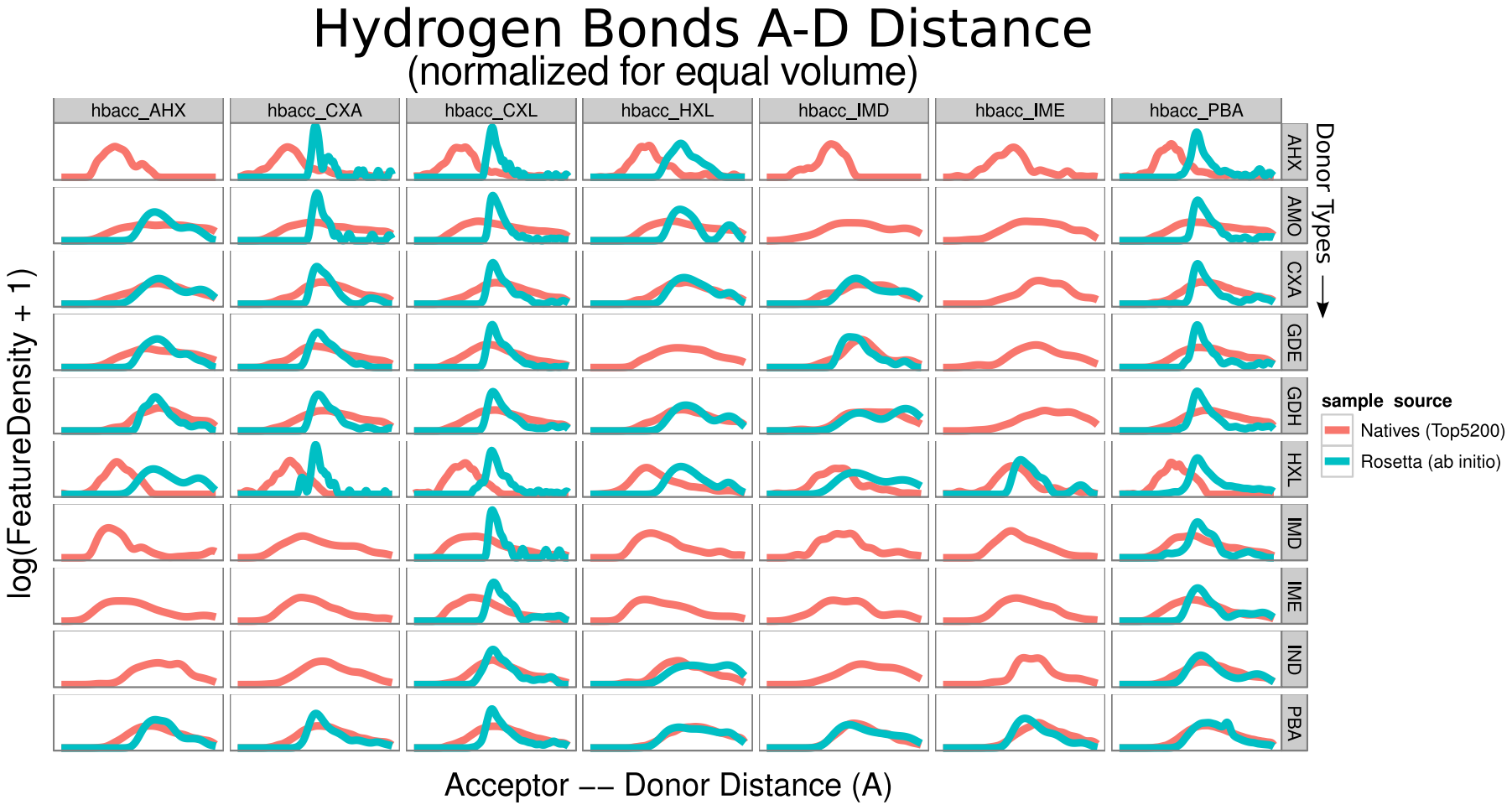
I have moved the HBond model parameters to minirosetta_database:

- Clearer model specification
- Parameters are adjustable without recompiling
- Parameters are accessable to external model validation code
- No loss of performance

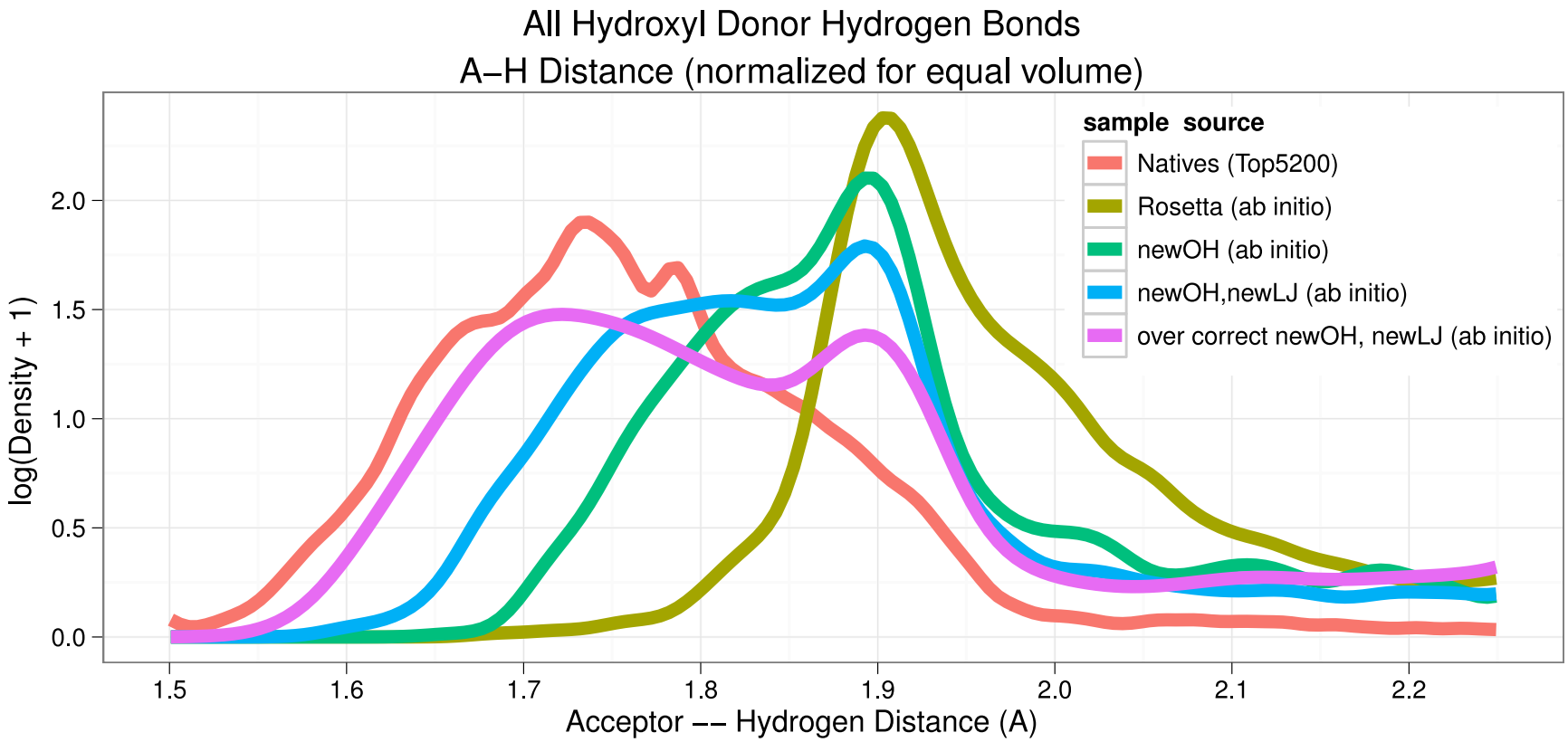
Native vs. Native



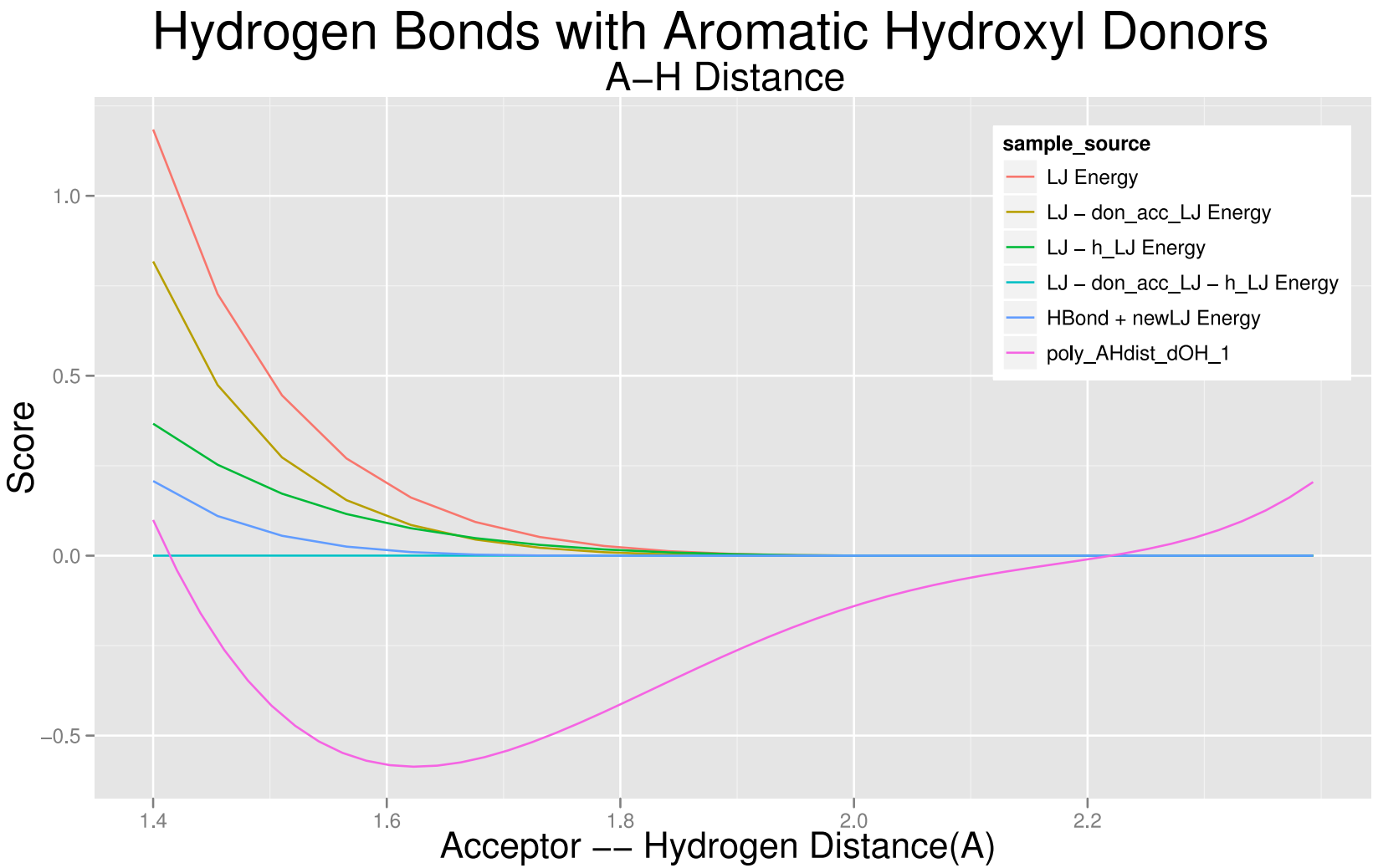
Native vs. Rosetta



Rosetta vs. Rosetta



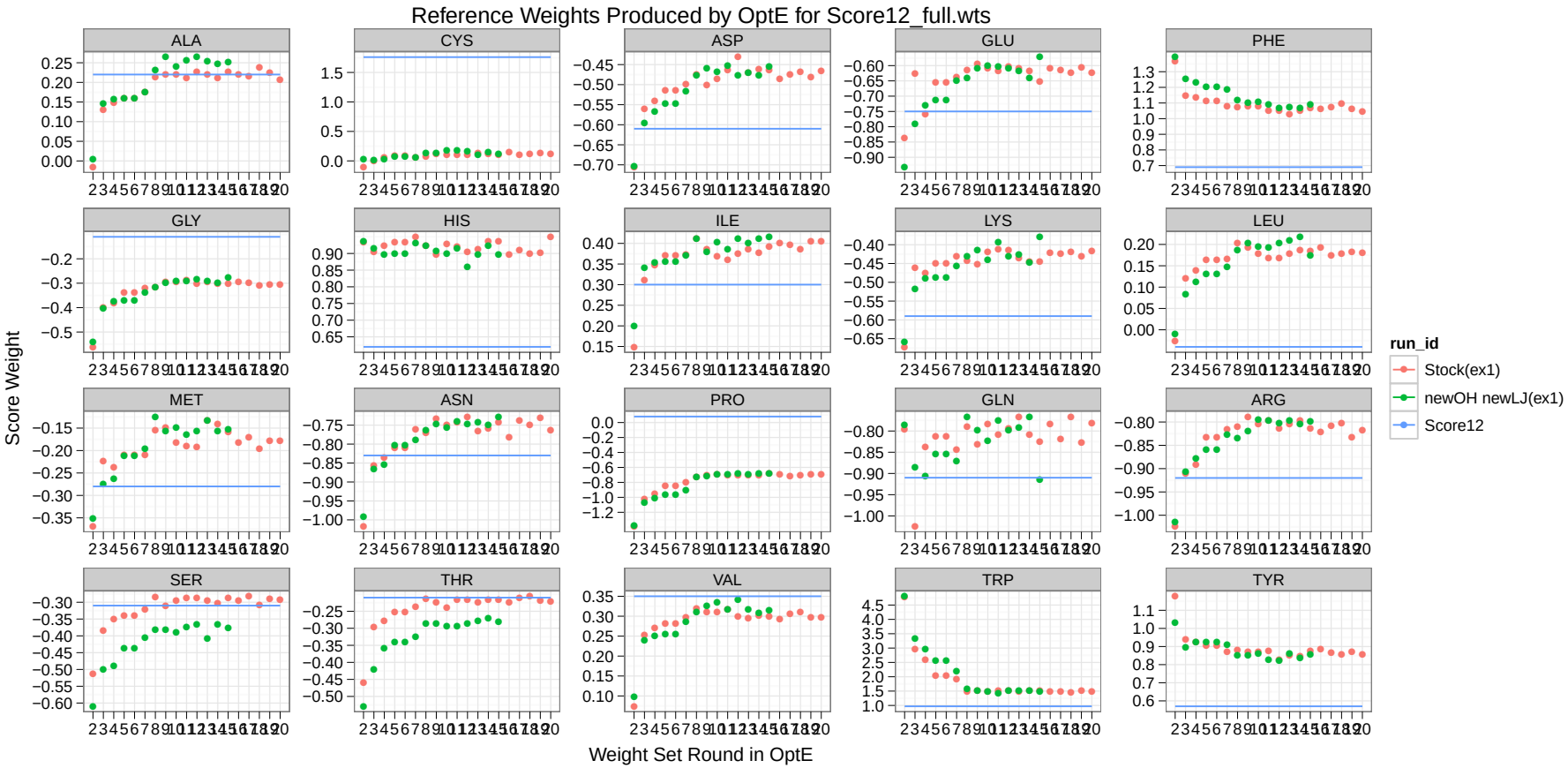
Assess Score Term Dependence



Optimize score term weights

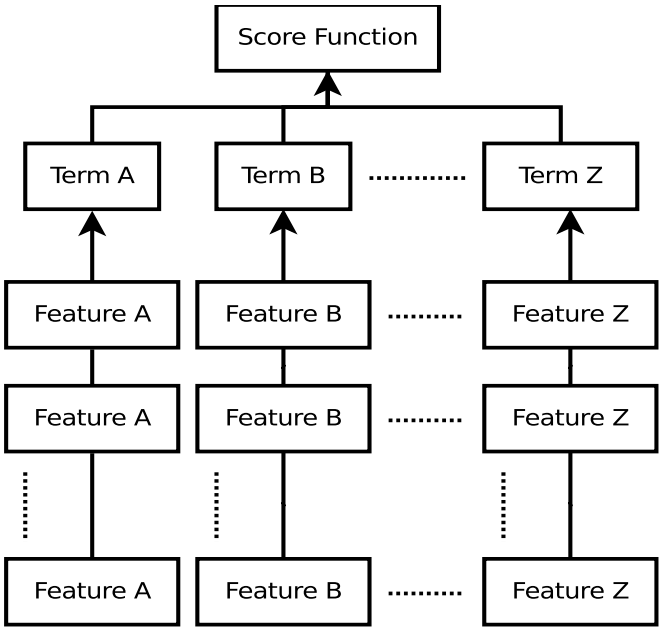
OptE with only reference weights free:

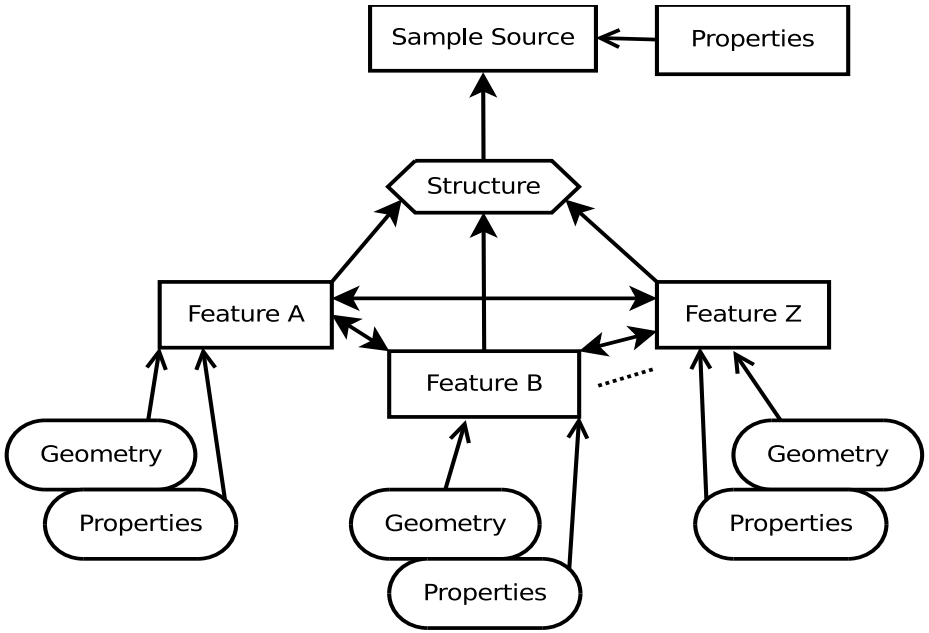
Optimized for sequence recovery, rotamer recovery, and sequence entropy; w/Ex1 flag



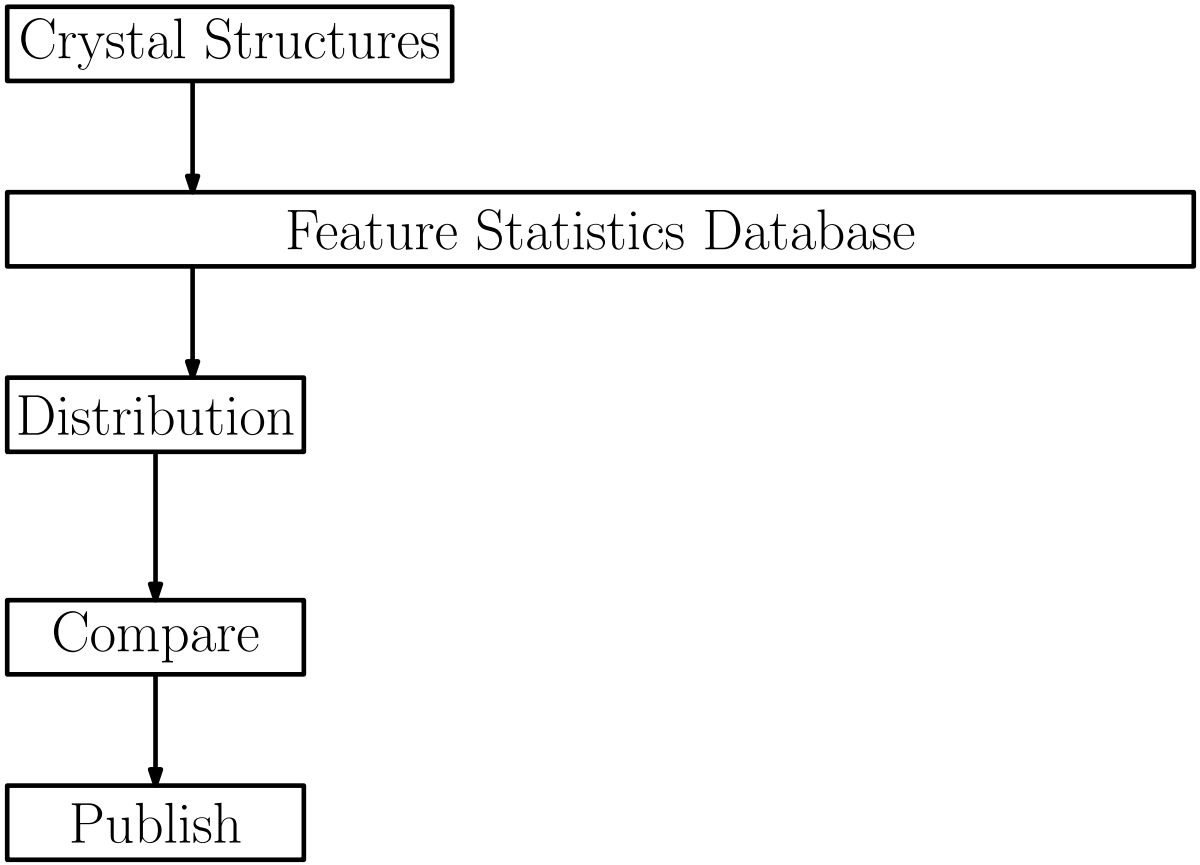
Feature Database

Build Feature Database:

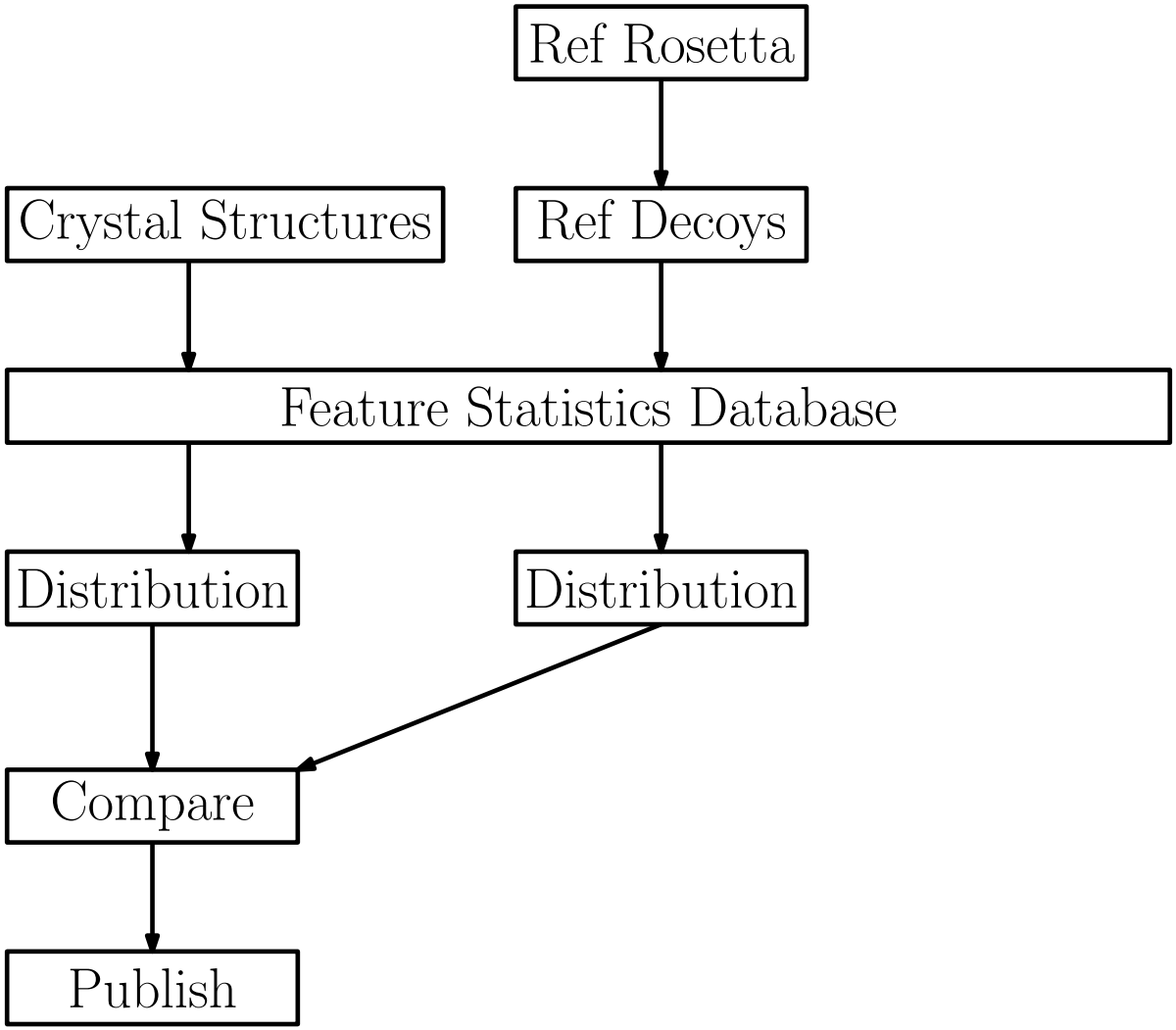




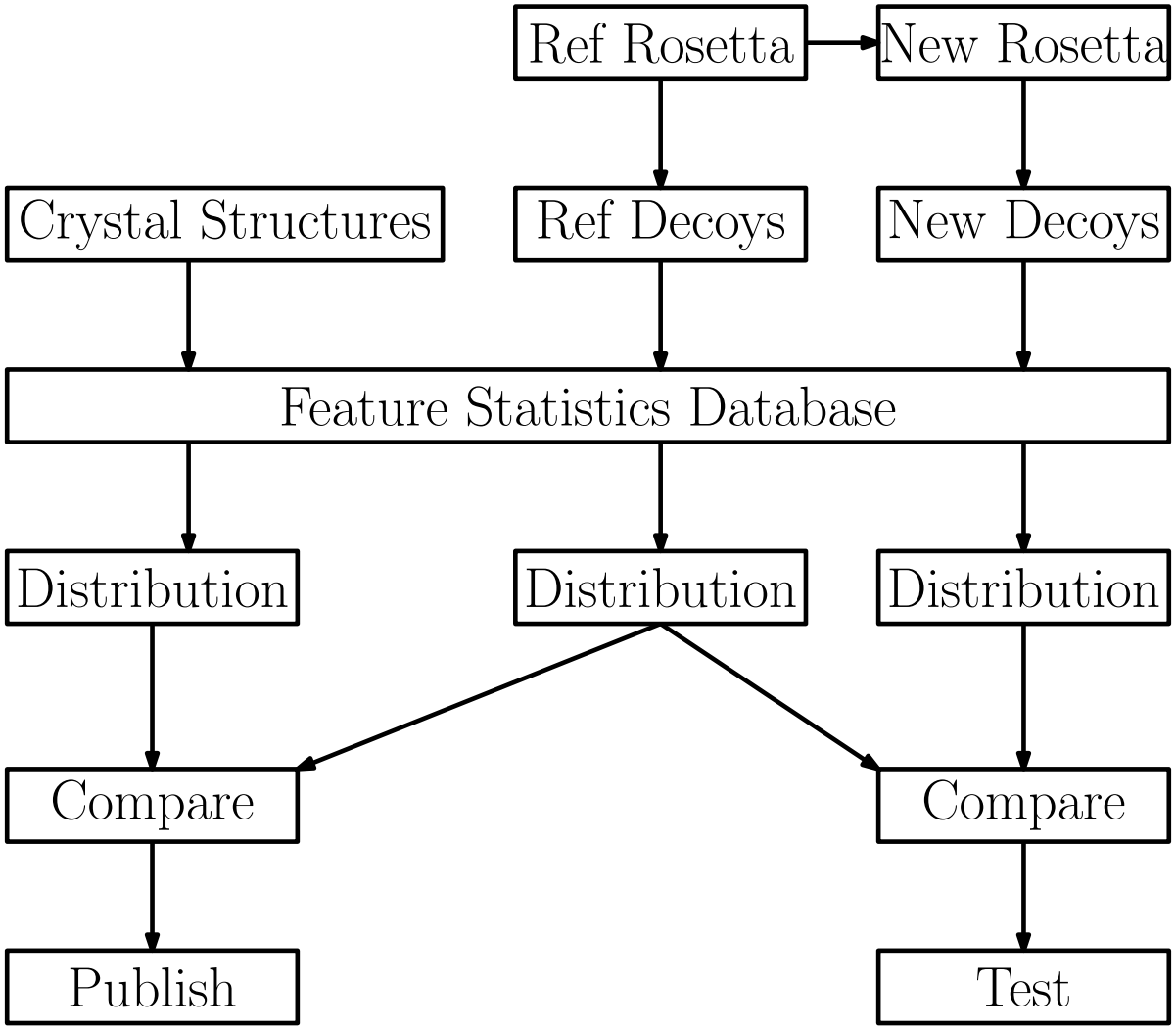
Score Term Tuning Workflow



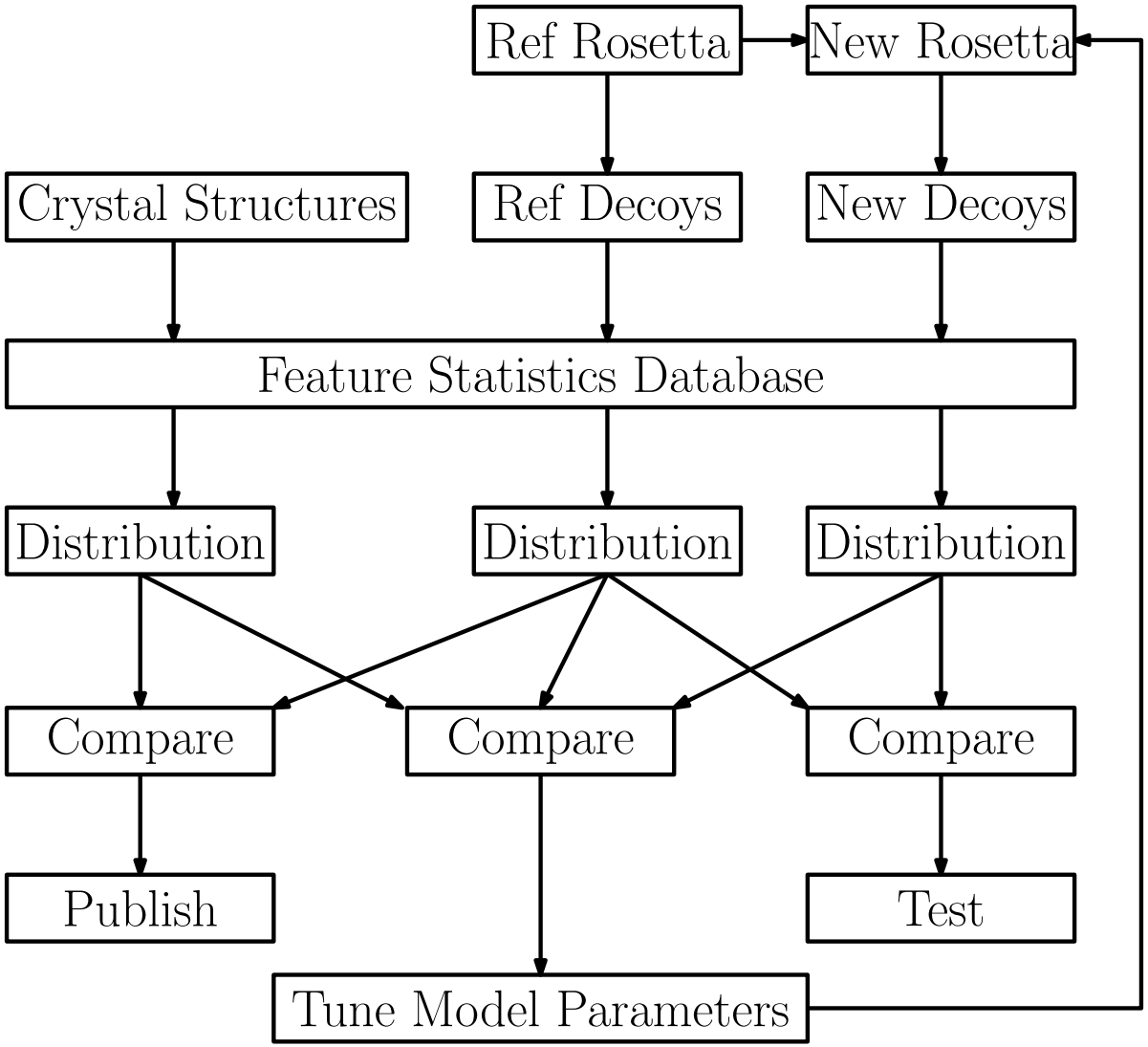
Score Term Tuning Workflow



Score Term Tuning Workflow



Score Term Tuning Workflow



Next Steps

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- Correct further distribution problems
- Identify hbond chemical types in Residue 'params' files
- Add χ term to model
- Address Backbone-Sidechain exclusion rule

Thanks!

Thanks to

- Jack Snoeyink
- Brian Kuhlman and the Kuhlman Lab
- UNC Computer Science Department
- NIH

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- Mike Tyka (Decoy Generation)
- Rosetta Community (Opportunity and support)