

Supplement to Memote: A community driven effort towards a standardized genome-scale metabolic model test suite

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1 Supplemental figures from the comparative analysis of model collections

To simplify interpretation the following figures are grouped by the sections of their corresponding test cases as they appear in a snapshot report. The code that was used to generate the data and figures has been deposited on GitHub <https://github.com/biosustain/memote-meta-study>.

1.1 Tested models

In order to respect the limited resources on the DTU high performance computing infrastructure, we set a maximum time limit for running the memote test suite. This introduced a bias against large models. Additionally, certain models failed the testing procedure. In the following we tabulate the total size of the collections as well as the final number of tested models. The results are shown in Table S1.

1.2 Clustering

Explain which features were used and methods + parameters. Show all plots here.

Table S1: Number of tested models.

Collection	Number of Models	Tested Models	%
AGORA	818	801	97.9
CarveMe	5587	5511	98.6
Path2Models	2641	2641	100.0
KBase	1637	1632	99.7
BiGG*	36	36	100.0
Ebrahim <i>et al.</i> †	83	80	96.4
OptFlux Models†	100	79	79.0

* Please note that we removed the large number of Escherichia coli strain models from the BiGG collection and only included results from the models iJR904, iAF1260, iJO1366, and iML1515.

† 39 models from these two collections are likely identical based on a filename comparison.

1.3 Independent Section

1.3.1 Consistency

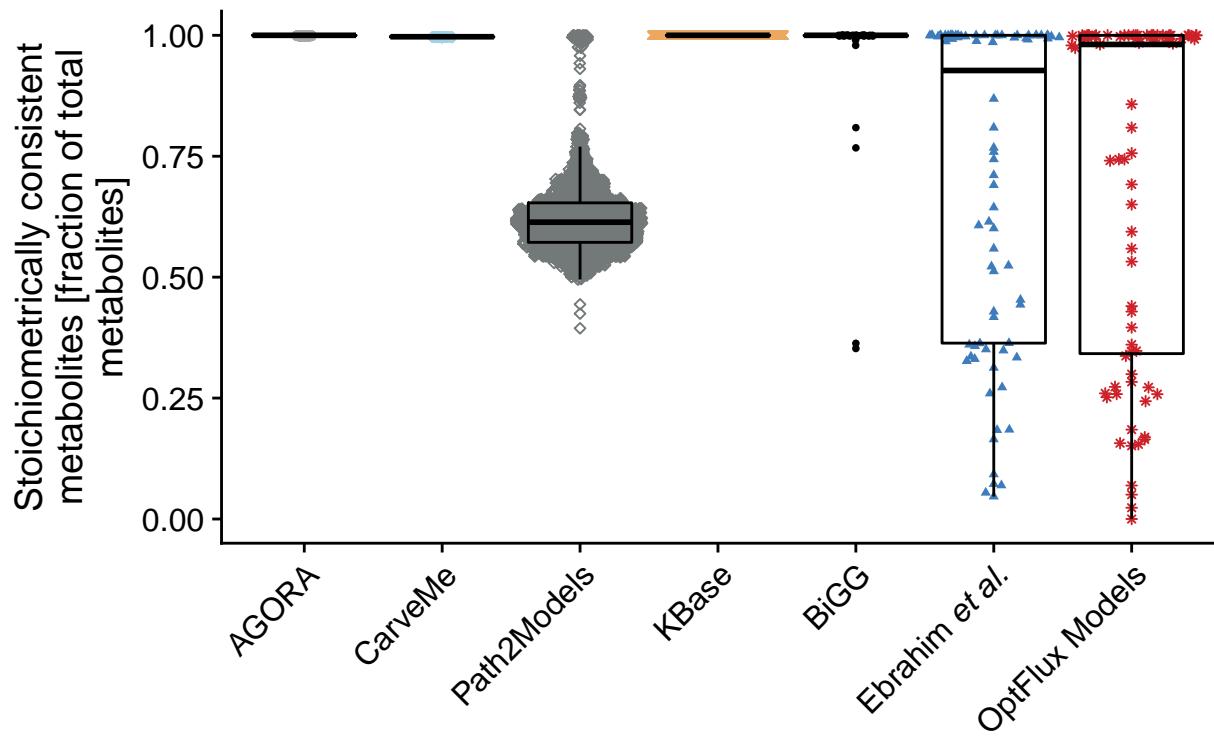


Figure S1: Stoichiometric consistency

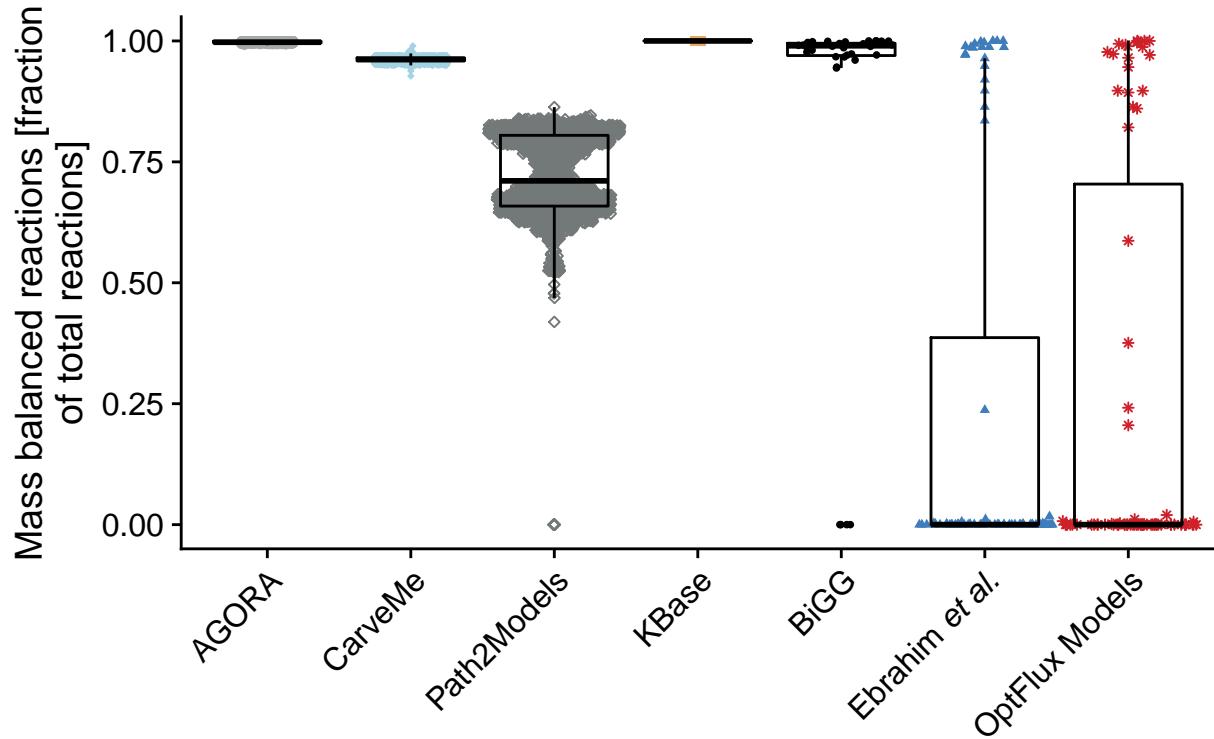


Figure S2: Mass Balance

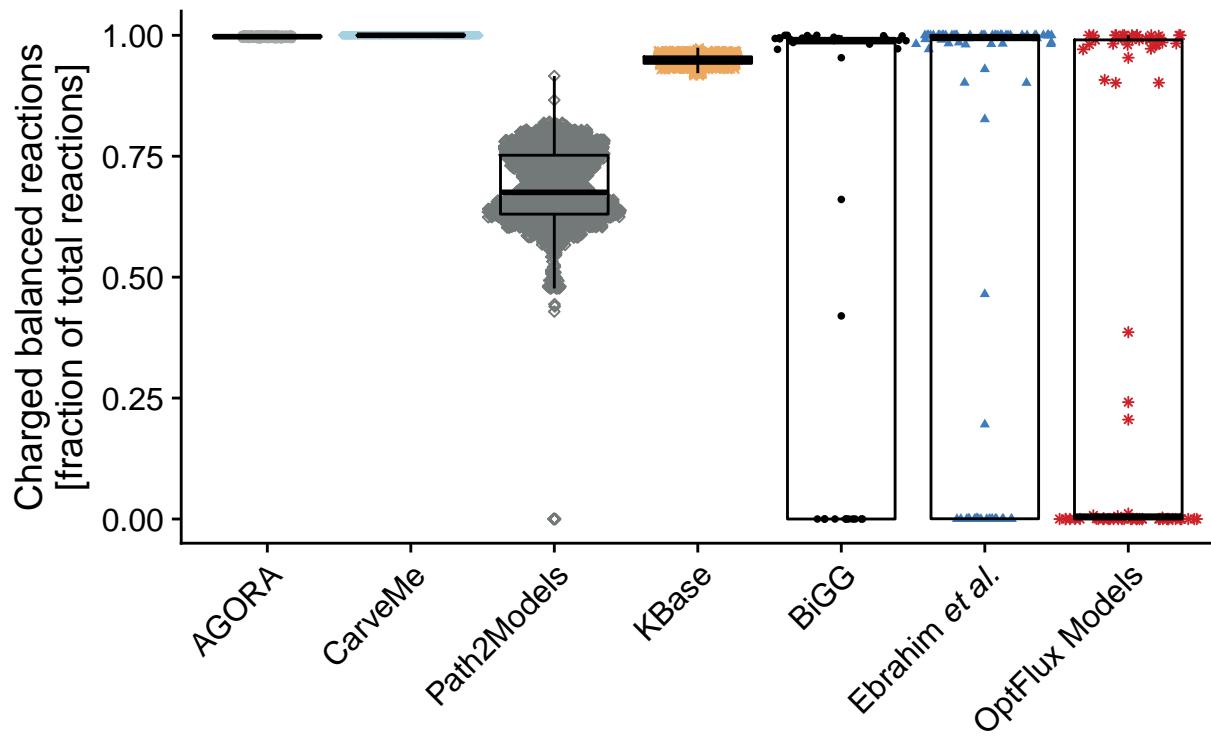


Figure S3: Charge Balance

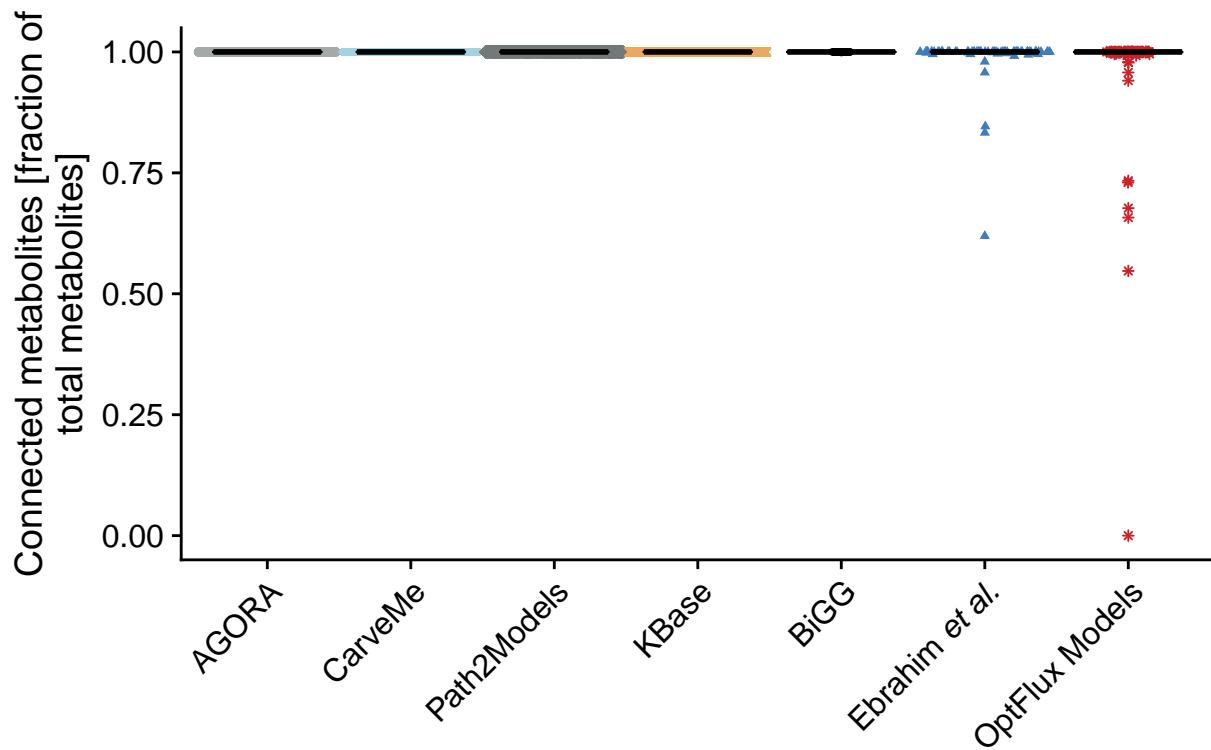


Figure S4: Metabolite Connectivity

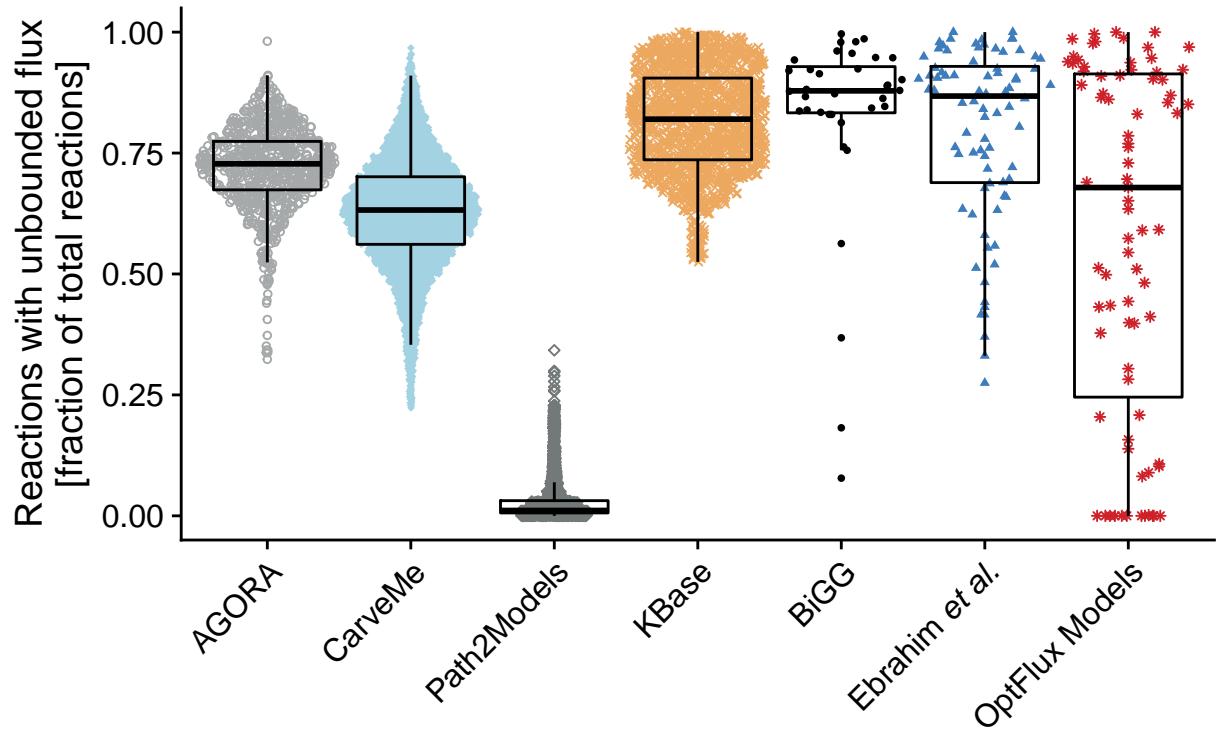


Figure S5: Unbounded Flux in Default Medium

1.3.2 Annotation - Metabolites

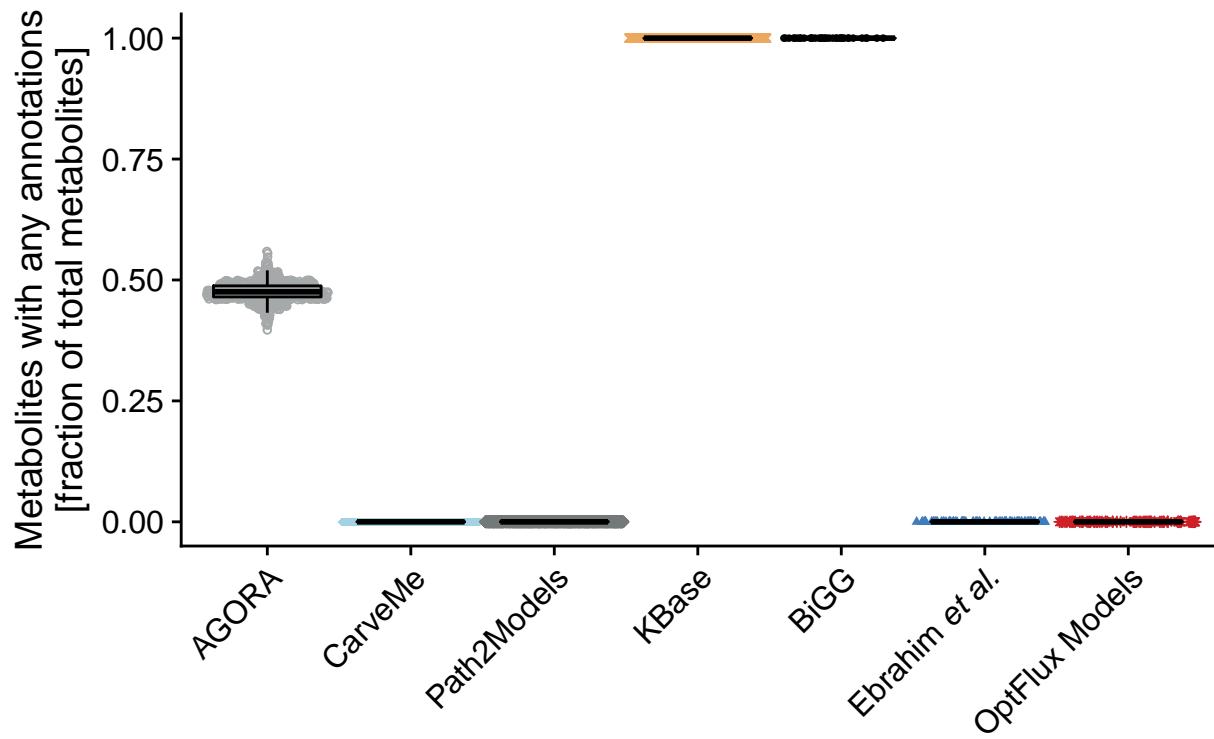


Figure S6: Presence of Metabolite Annotation

1.3.2.1 Metabolite Annotations Per Database

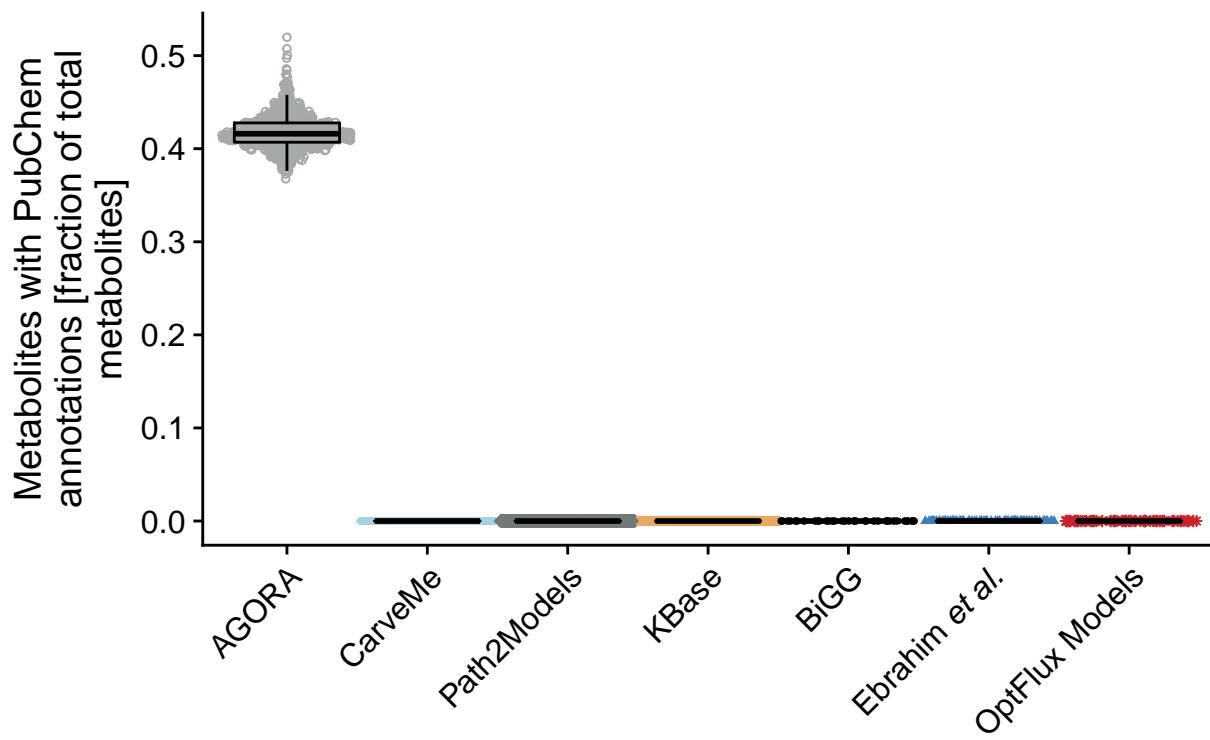


Figure S7: Metabolite Pubchem.compound Annotation

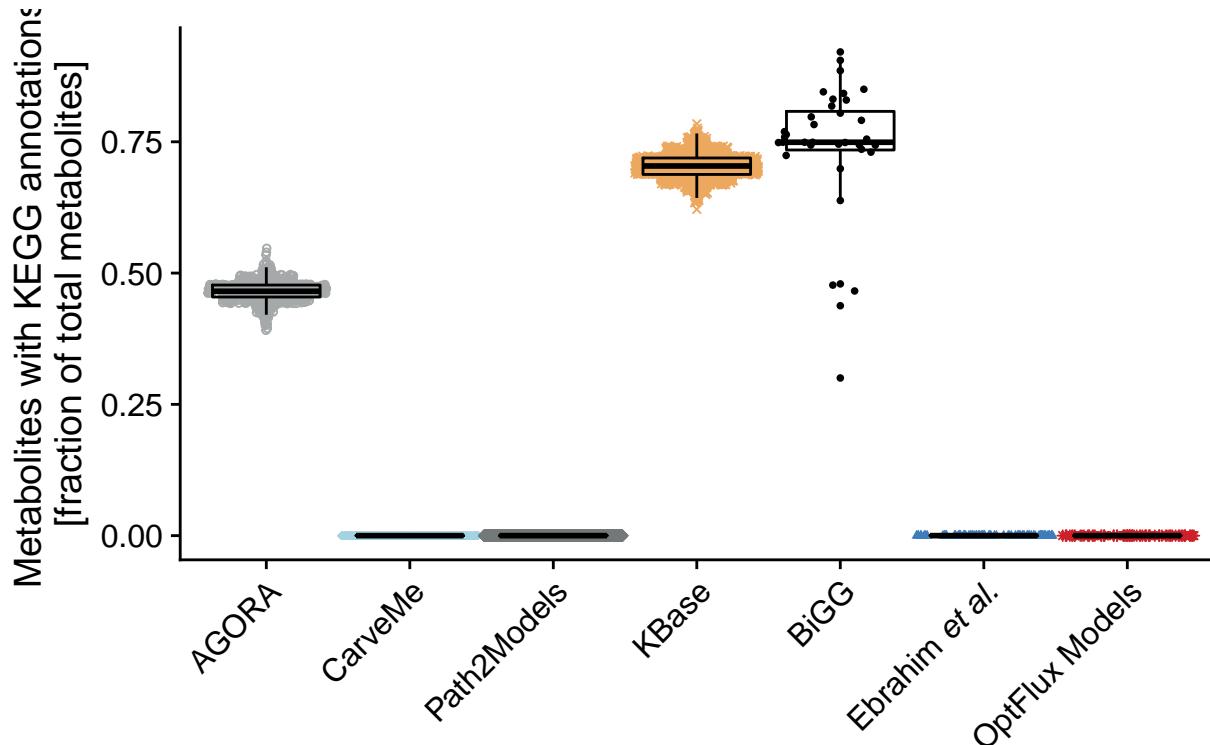


Figure S8: Metabolite KEGG.compound Annotation

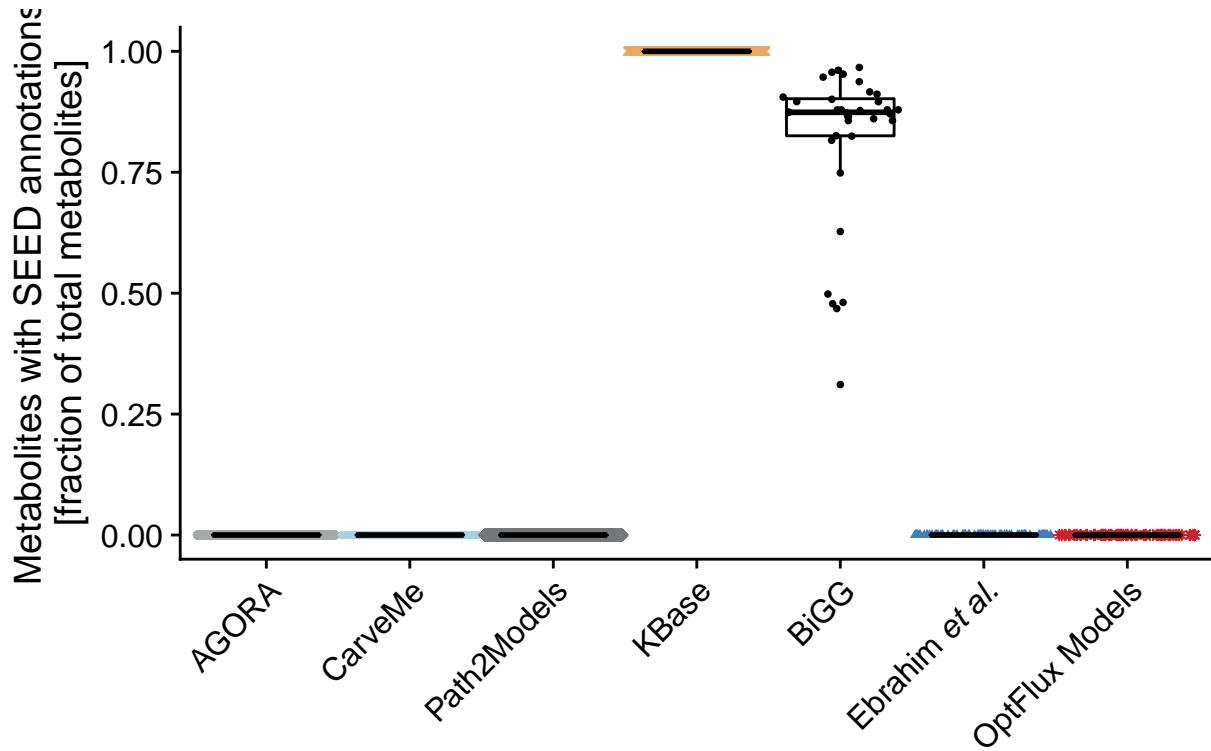


Figure S9: Metabolite SEED.compound Annotation

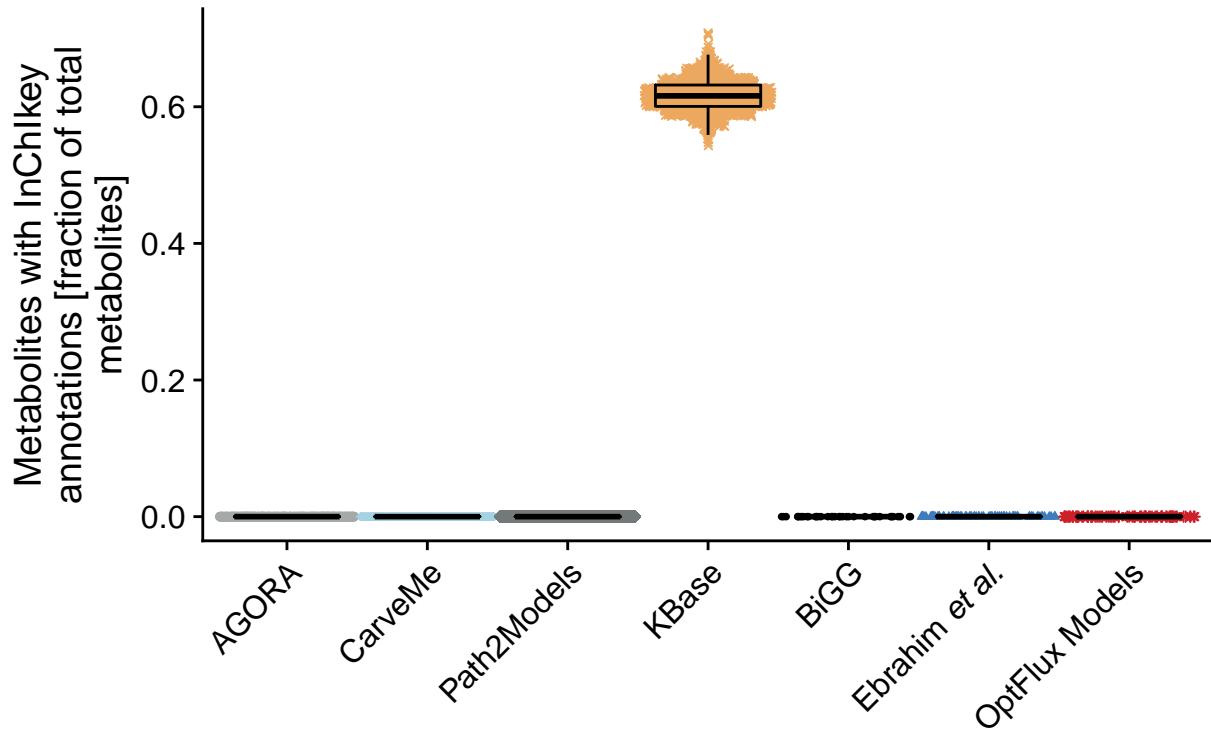


Figure S10: Metabolite InChIKey Annotation

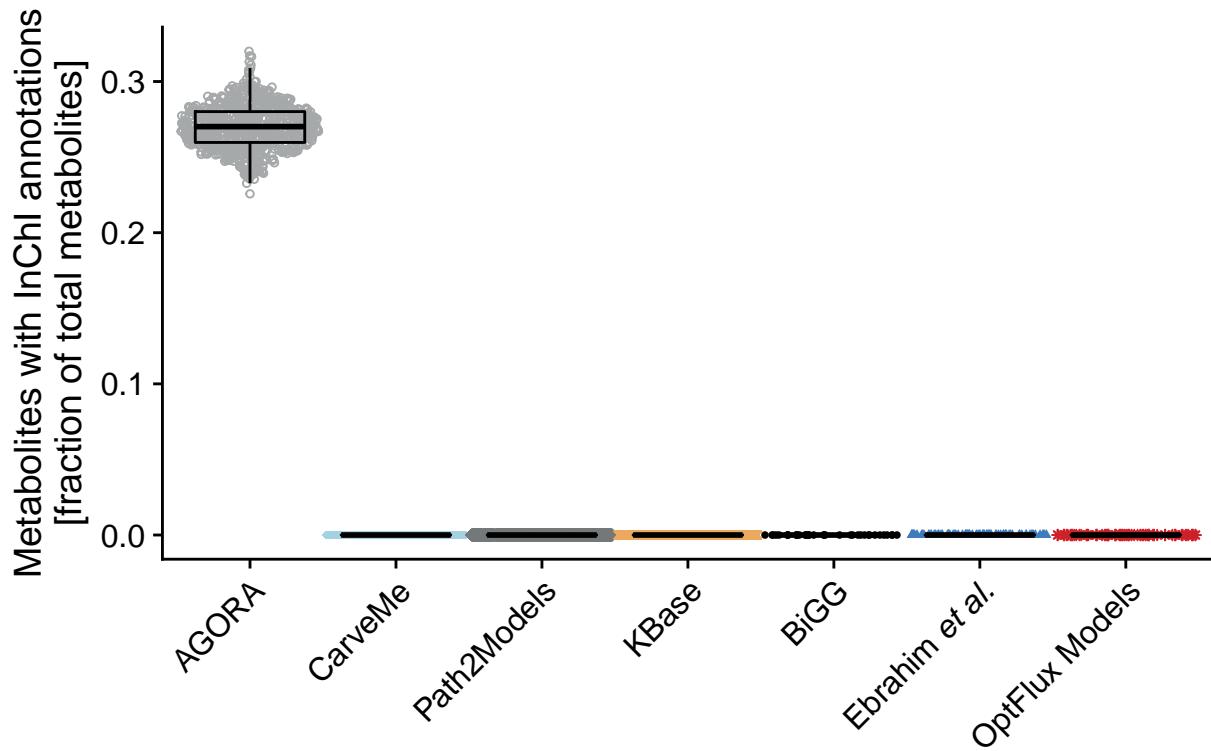


Figure S11: Metabolite InChI Annotation

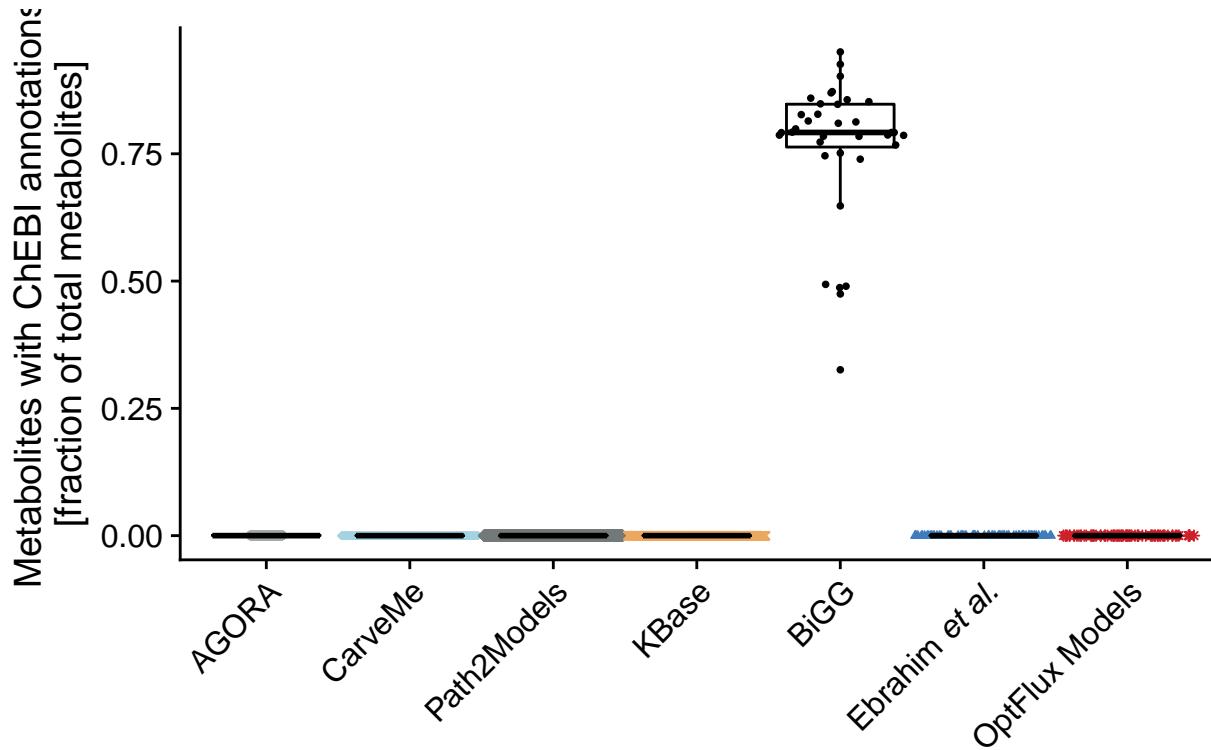


Figure S12: Metabolite ChEBI Annotation

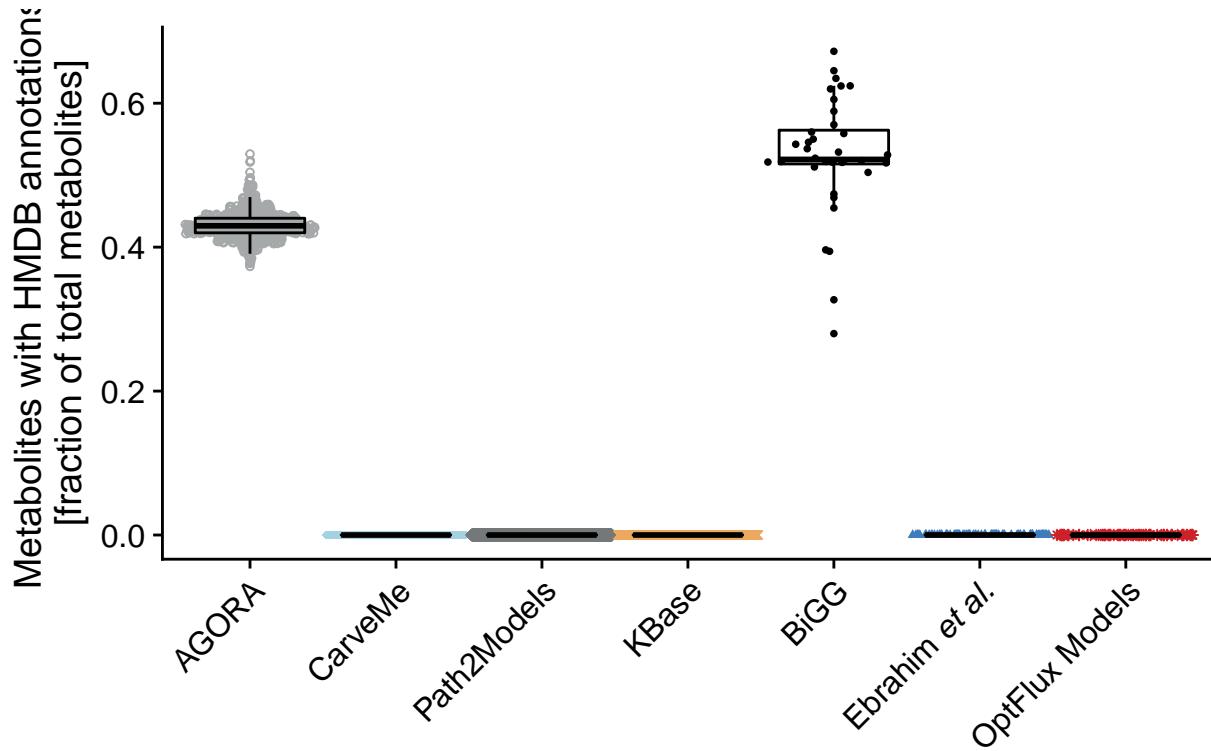


Figure S13: Metabolite HMDB Annotation

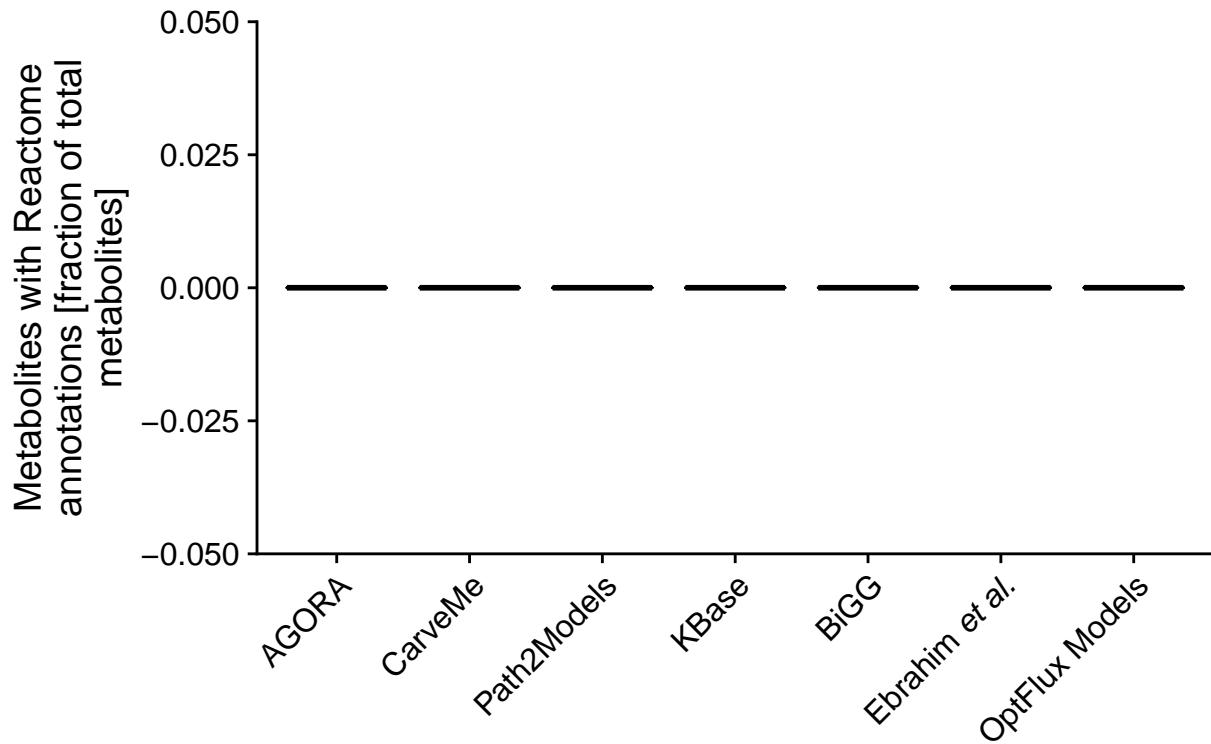


Figure S14: Metabolite Reactome Annotation

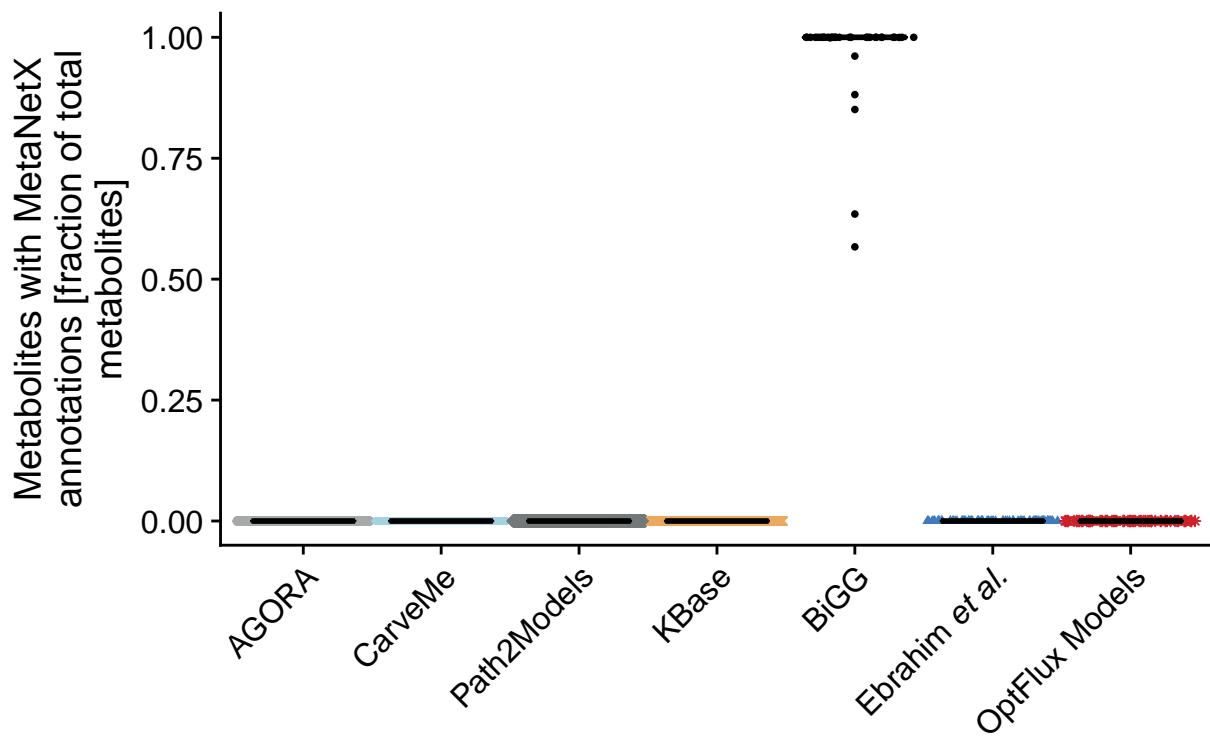


Figure S15: Metabolite MetaNetX.chemical Annotation

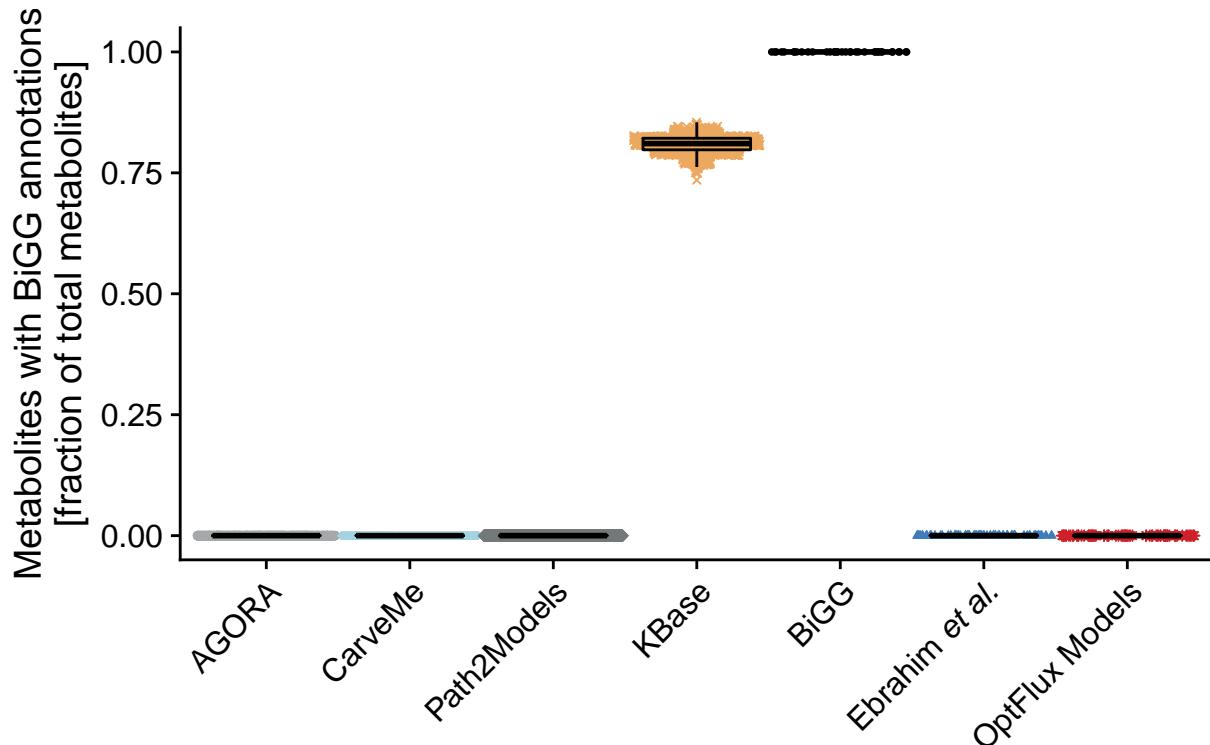


Figure S16: Metabolite BiGG.metabolite Annotation

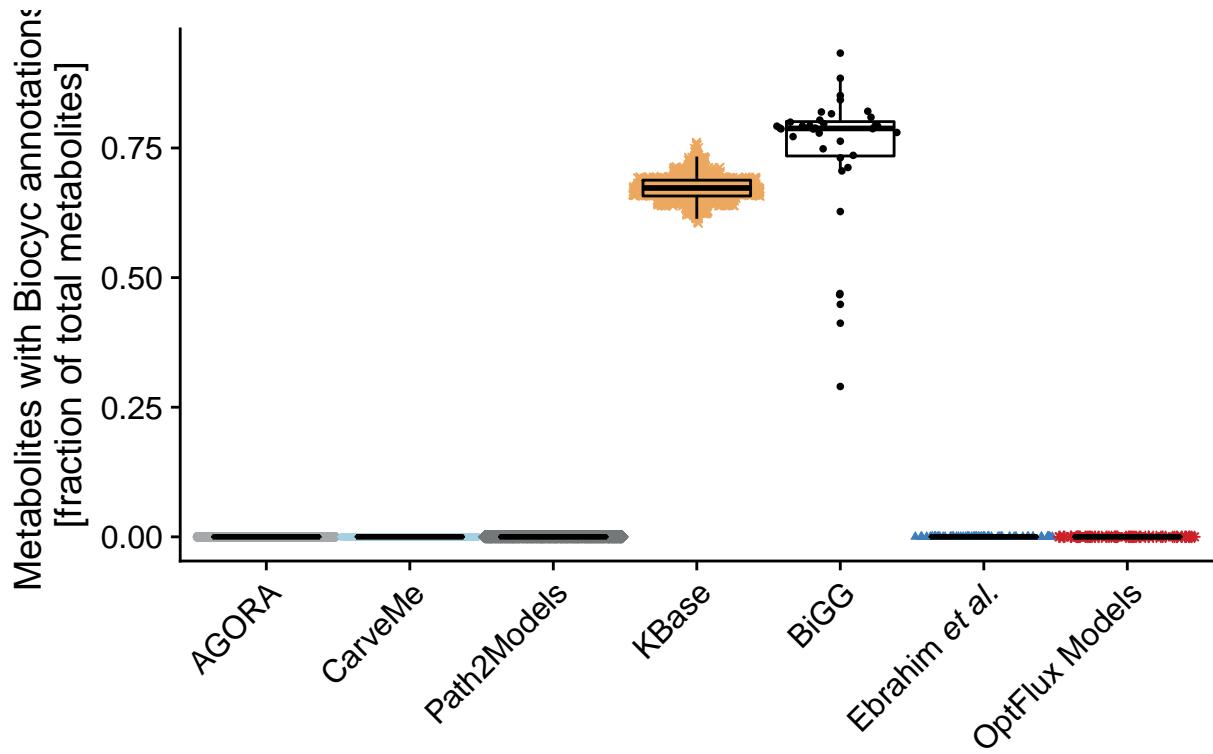


Figure S17: Metabolite BioCyc Annotation

1.3.2.2 Metabolite Annotation Conformity per Database

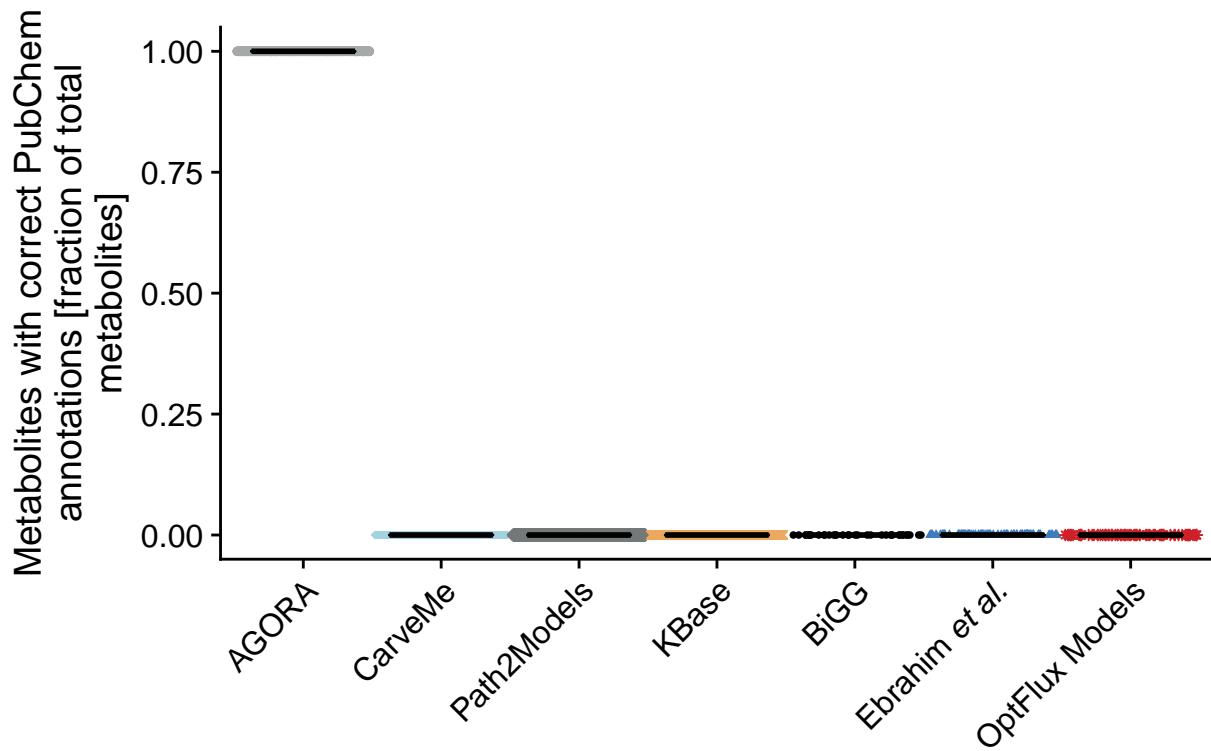


Figure S18: Correct Metabolite Pubchem.compound Annotation

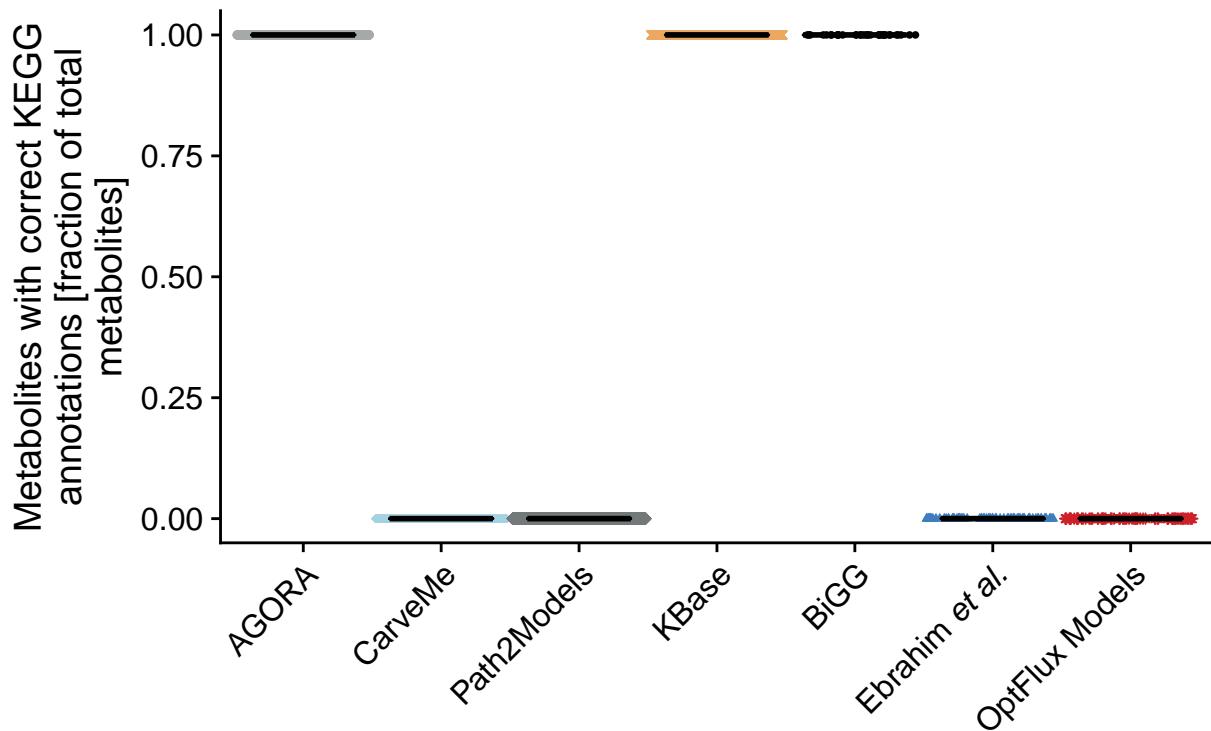


Figure S19: Correct Metabolite KEGG.compound Annotation

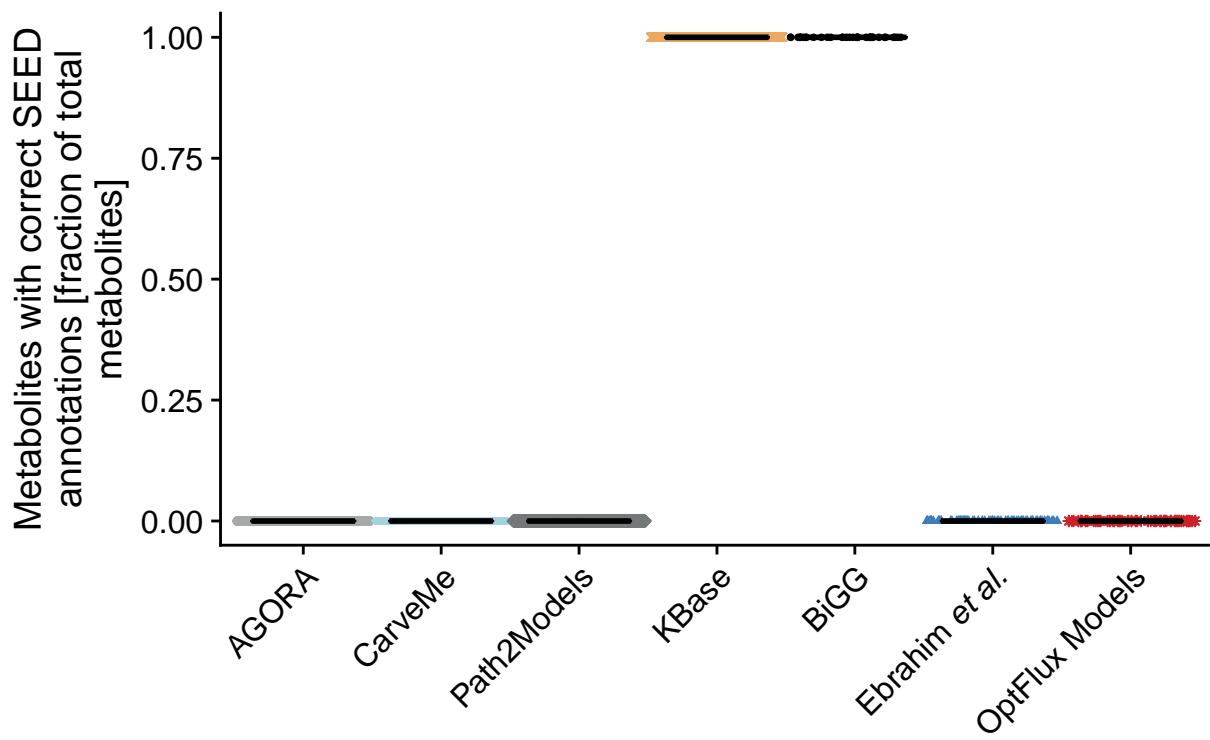


Figure S20: Correct Metabolite SEED.compound Annotation

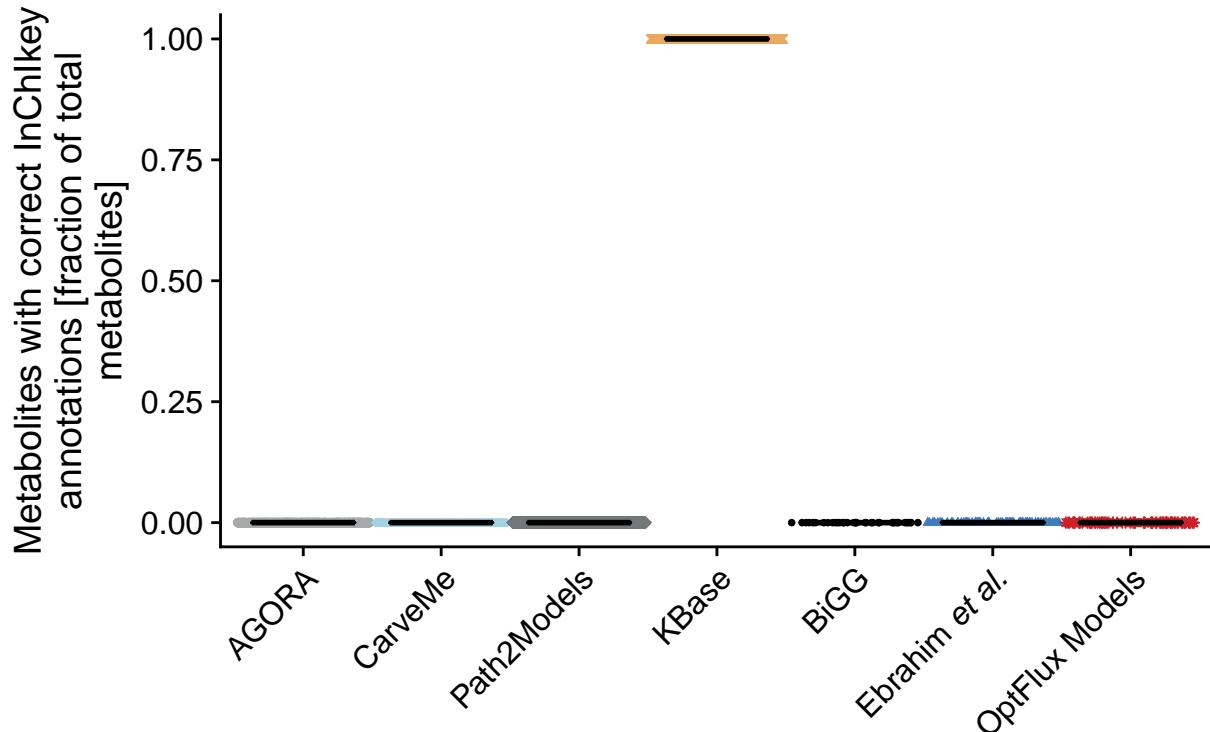


Figure S21: Correct Metabolite InChIKey Annotation

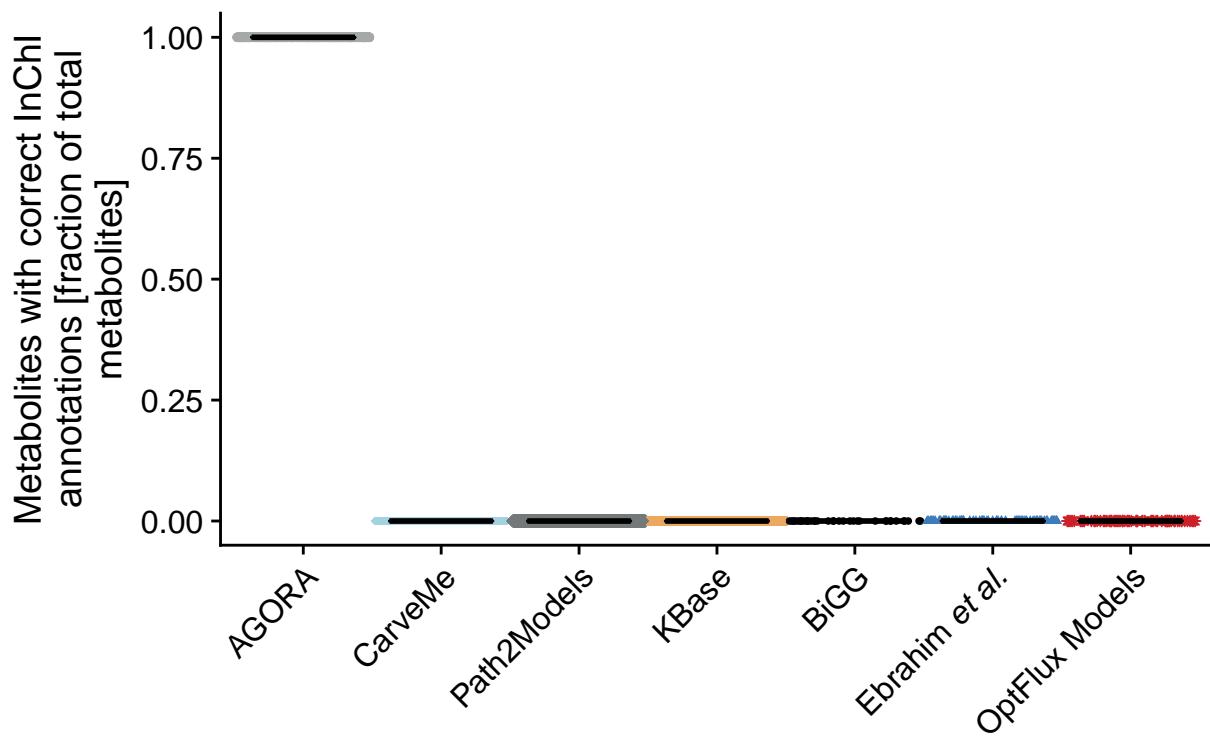


Figure S22: Correct Metabolite InChI Annotation

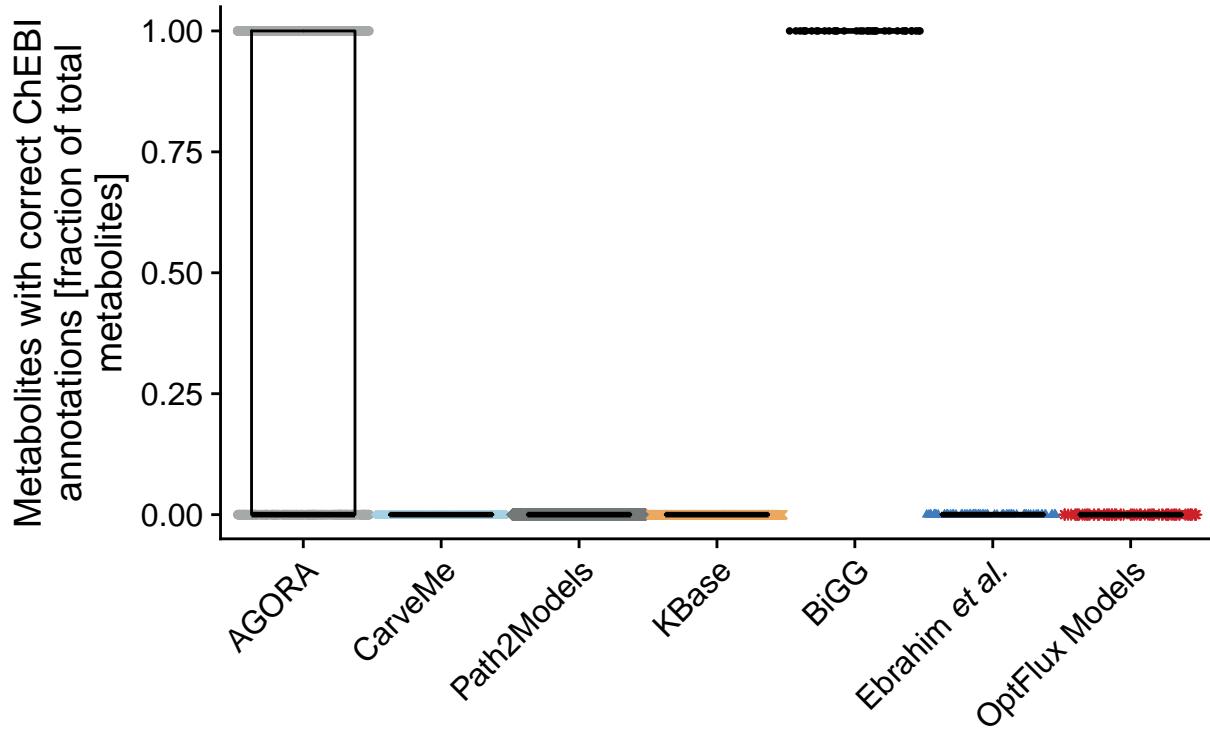


Figure S23: Correct Metabolite ChEBI Annotation

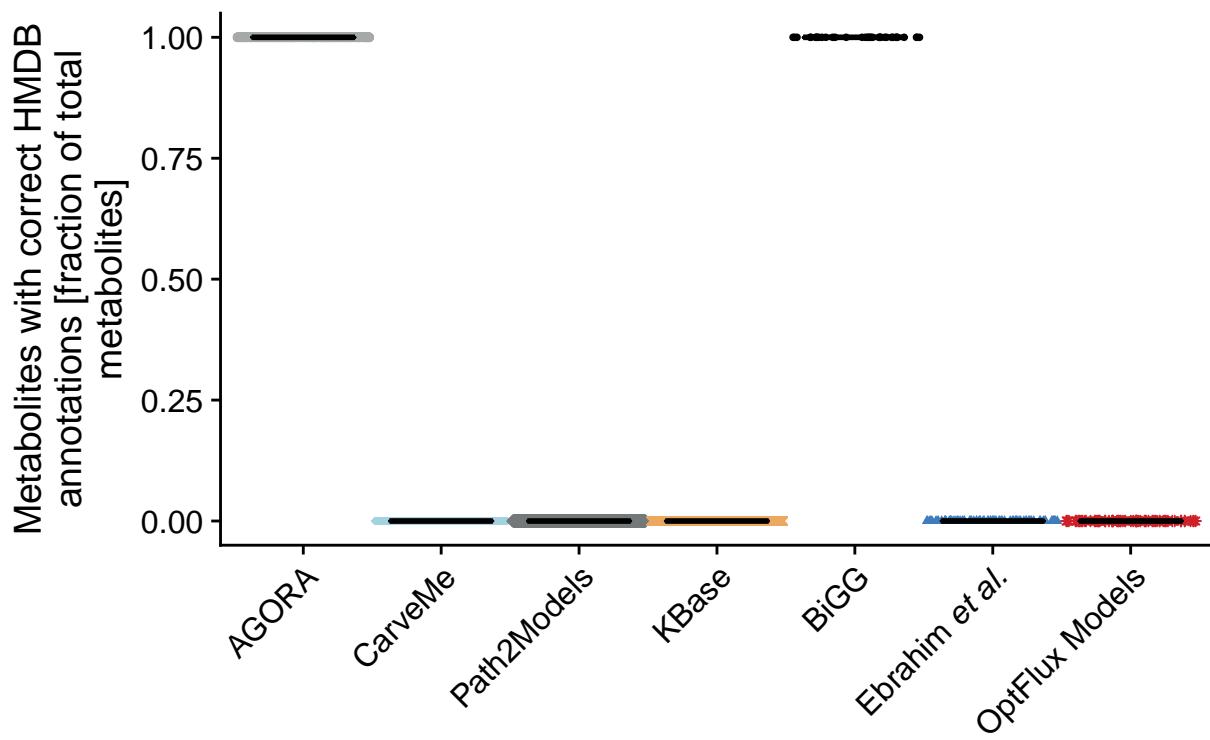


Figure S24: Correct Metabolite HMDB Annotation

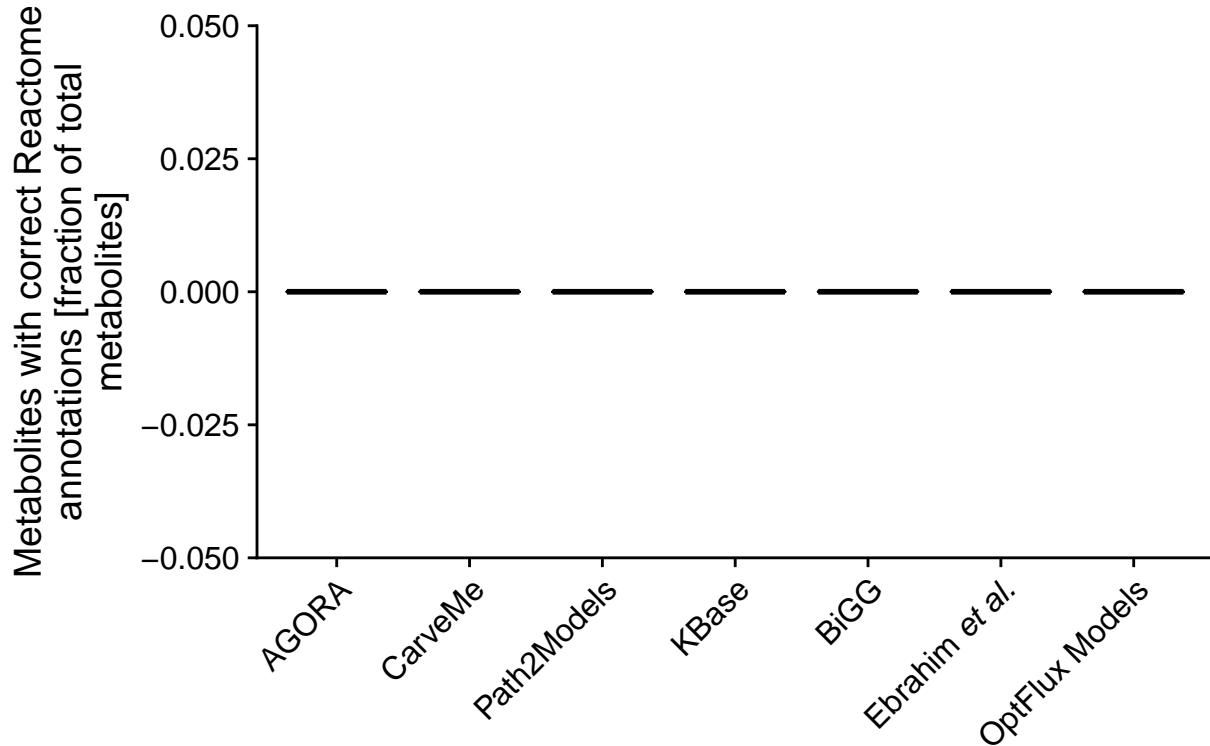


Figure S25: Correct Metabolite Reactome Annotation

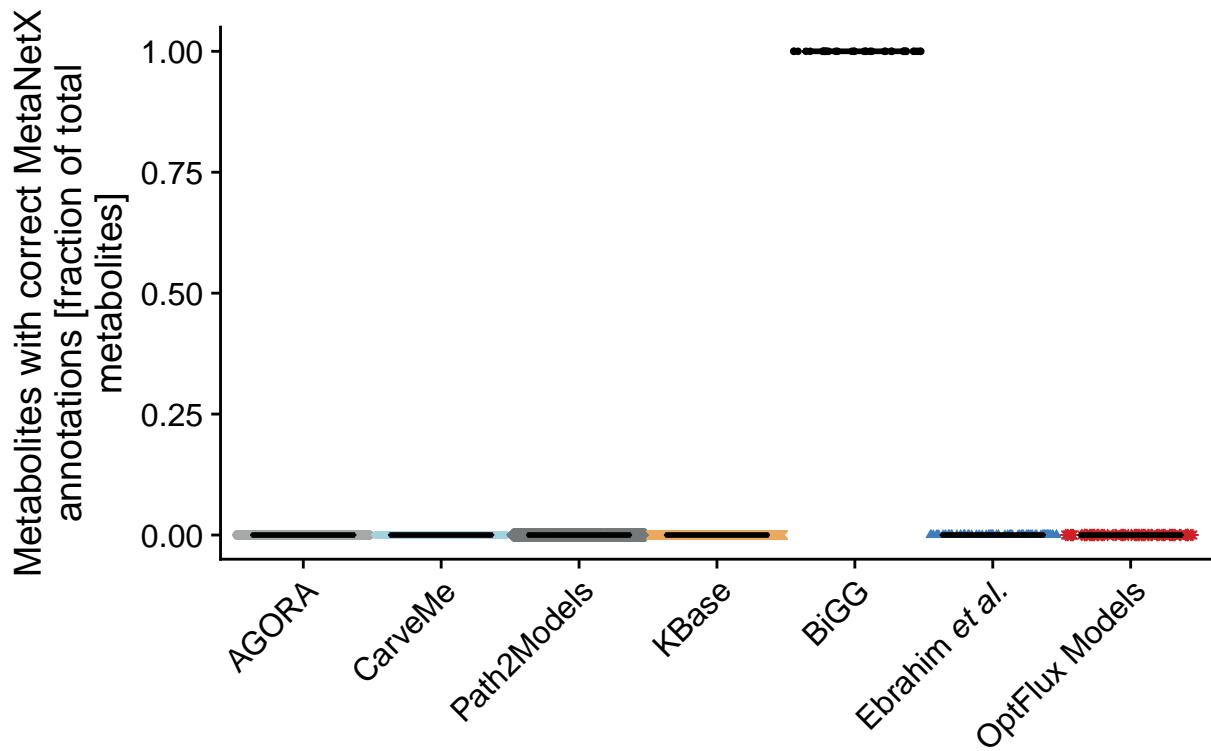


Figure S26: Correct Metabolite MetaNetX.chemical Annotation

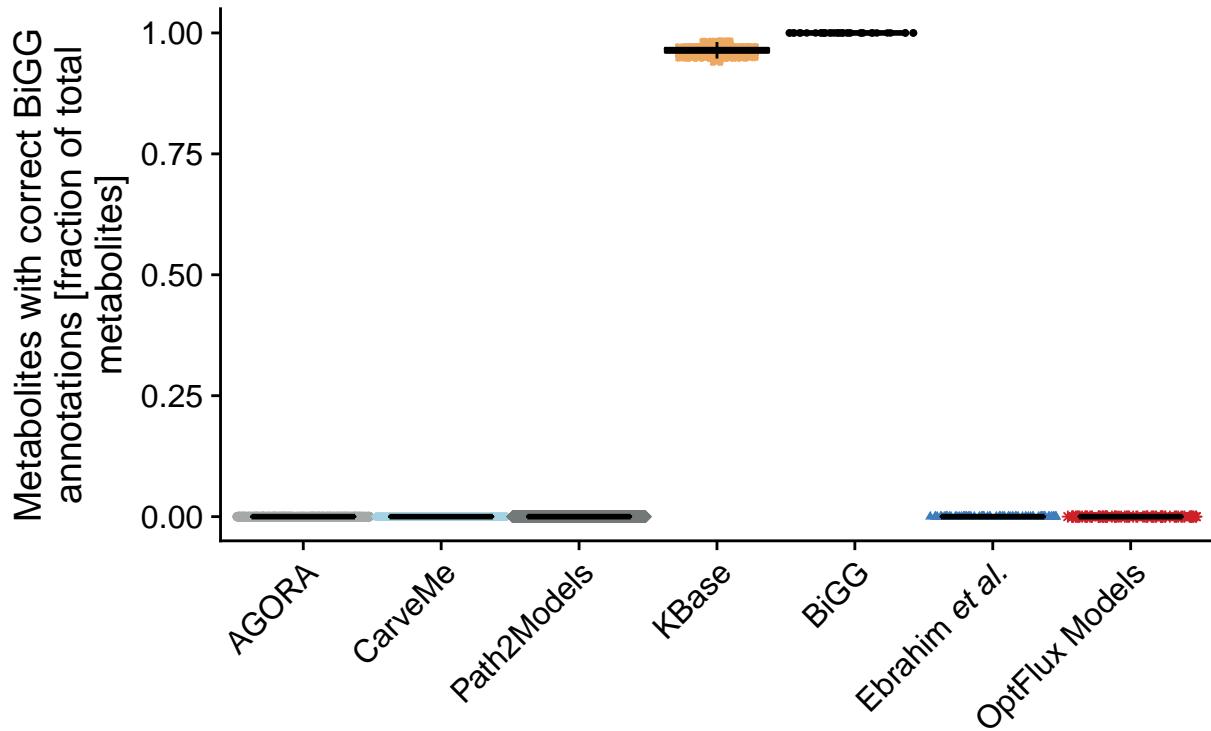


Figure S27: Correct Metabolite BiGG.metabolite Annotation

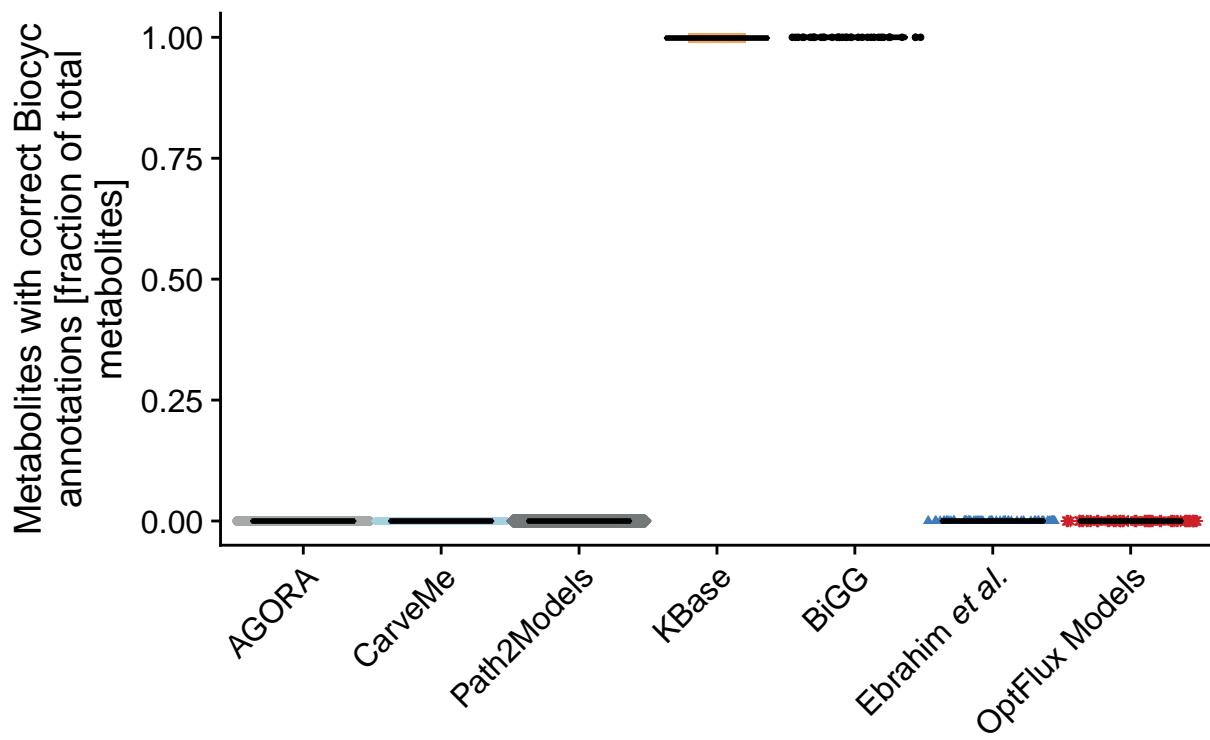


Figure S28: Correct Metabolite BioCyc Annotation

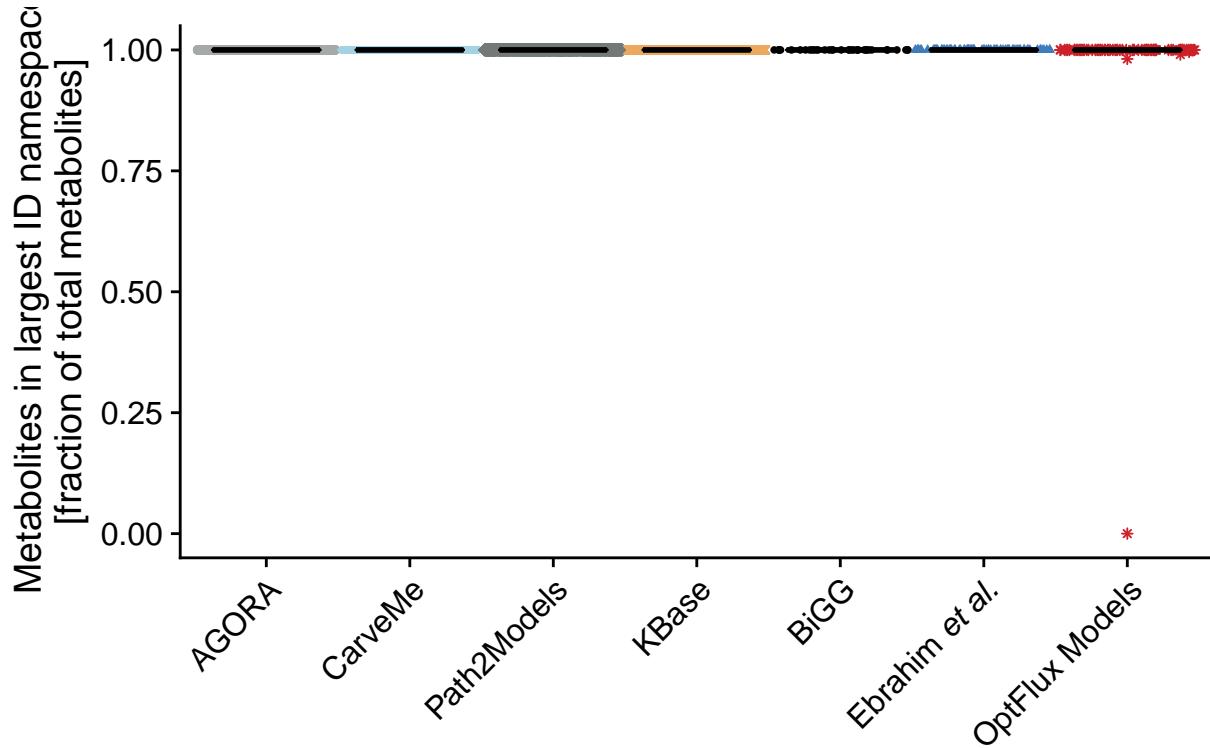


Figure S29: Uniform Metabolite Identifier Namespace

1.3.3 Annotation - Reactions

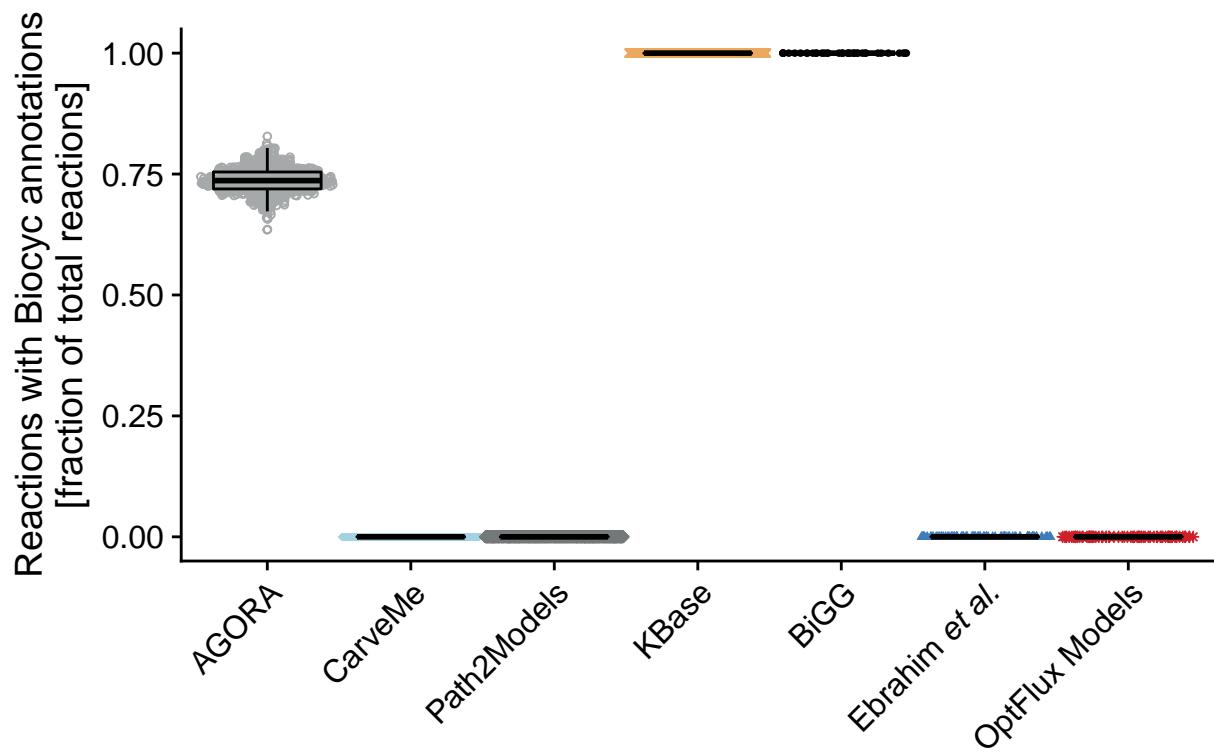


Figure S30: Presence of Reaction Annotation

1.3.3.1 Reaction Annotations Per Database

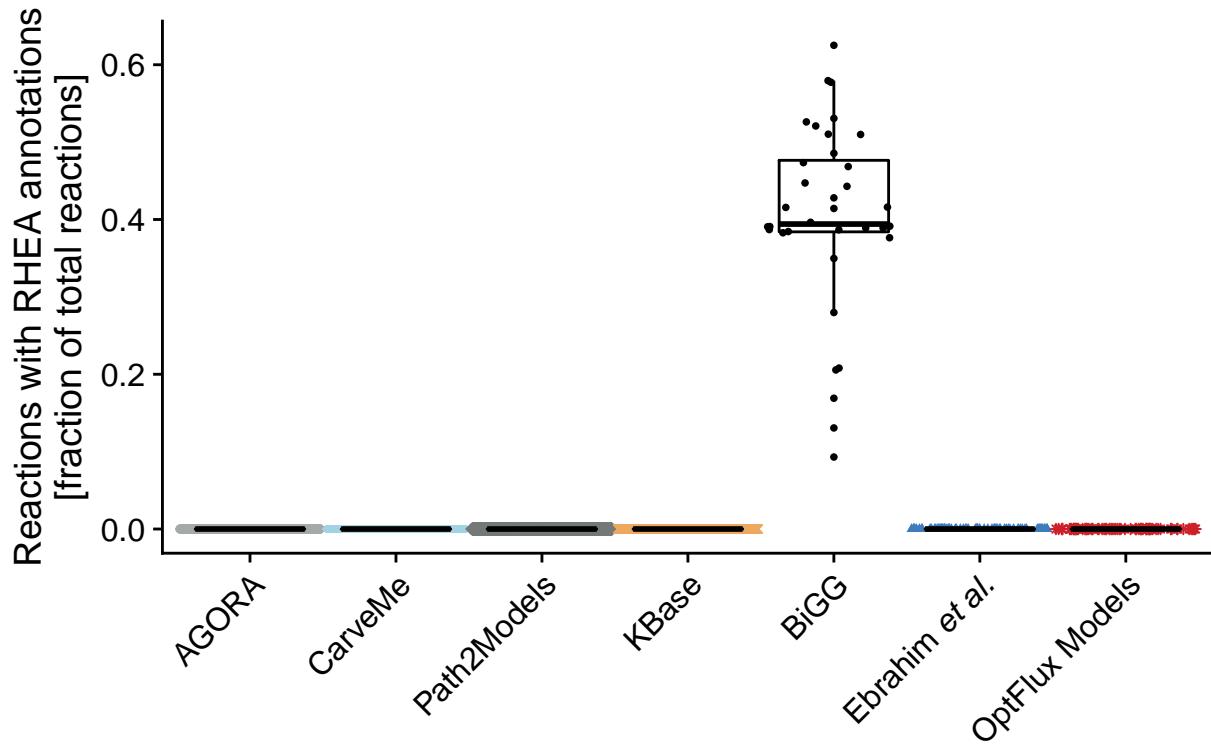


Figure S31: Reaction Rhea Annotation

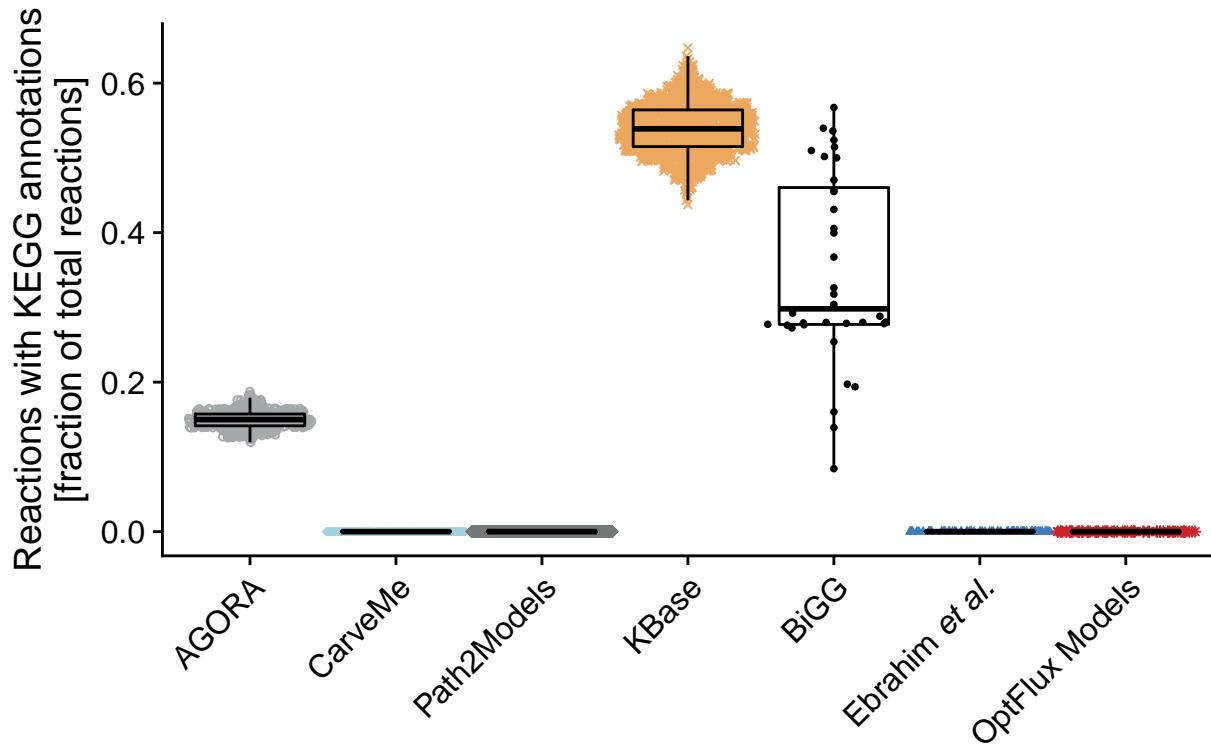


Figure S32: Reaction KEGG.reaction Annotation

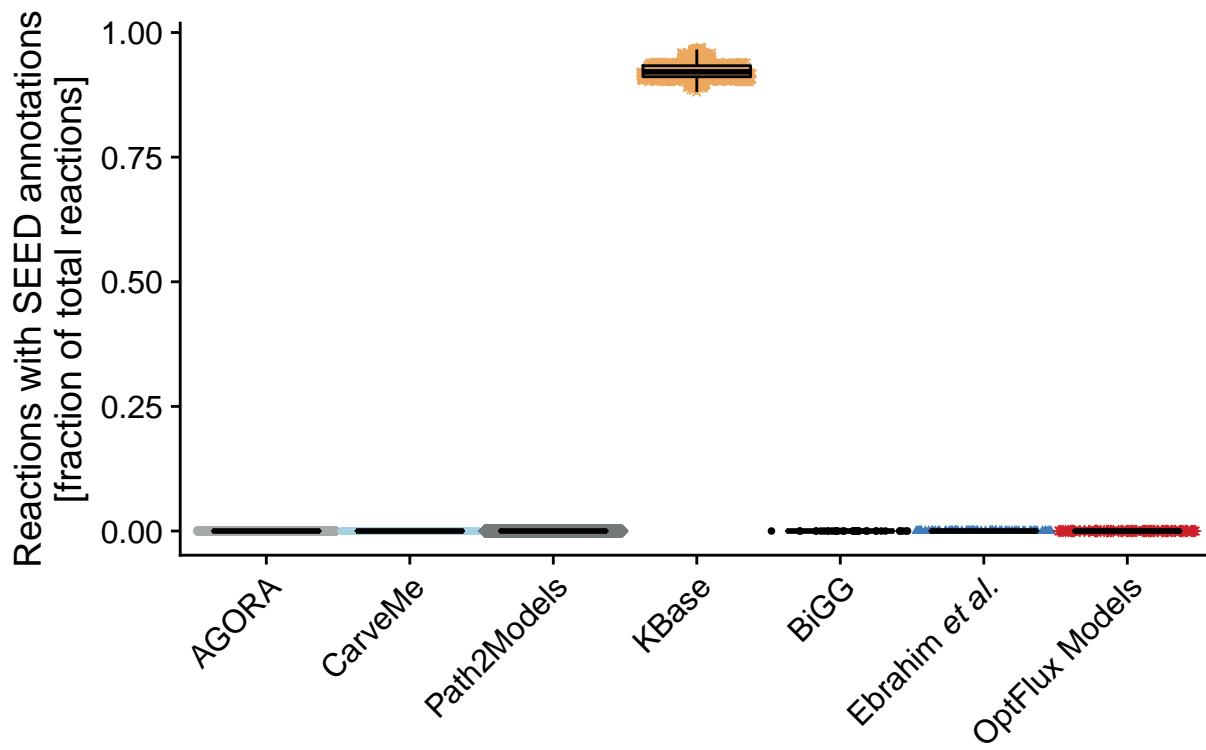


Figure S33: Reaction SEED.reaction Annotation

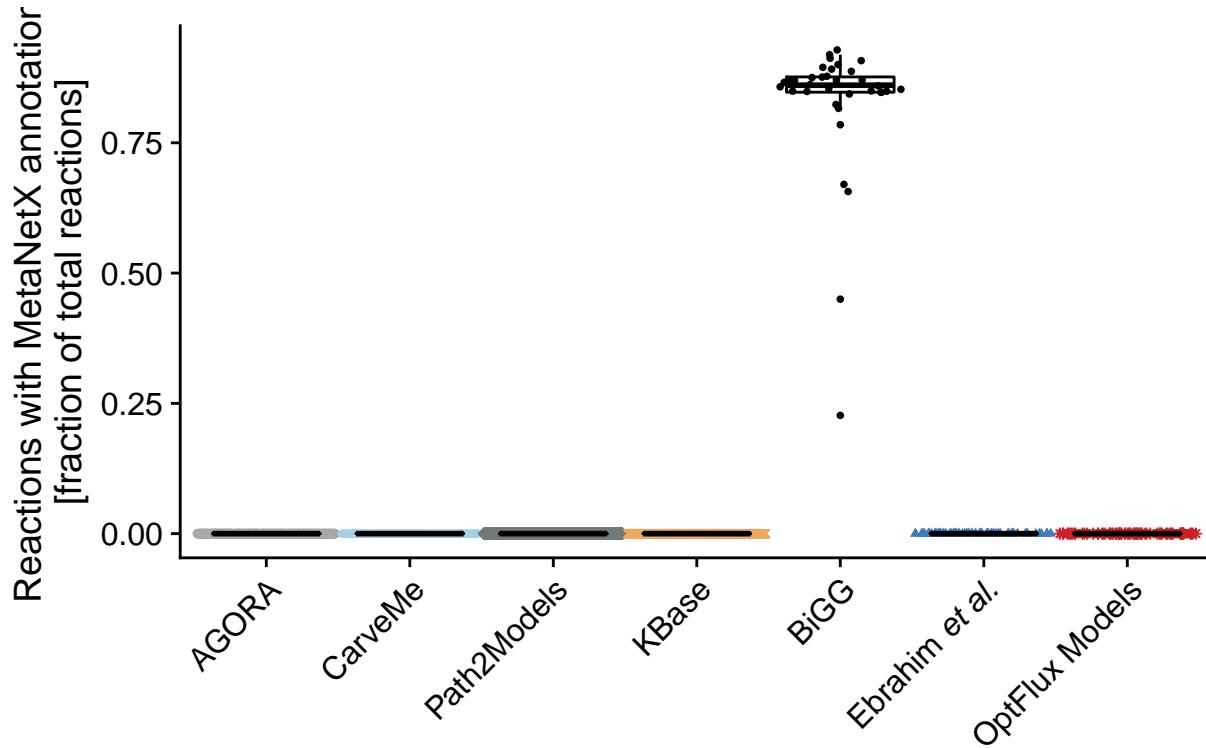


Figure S34: Reaction MetaNetX.reaction Annotation

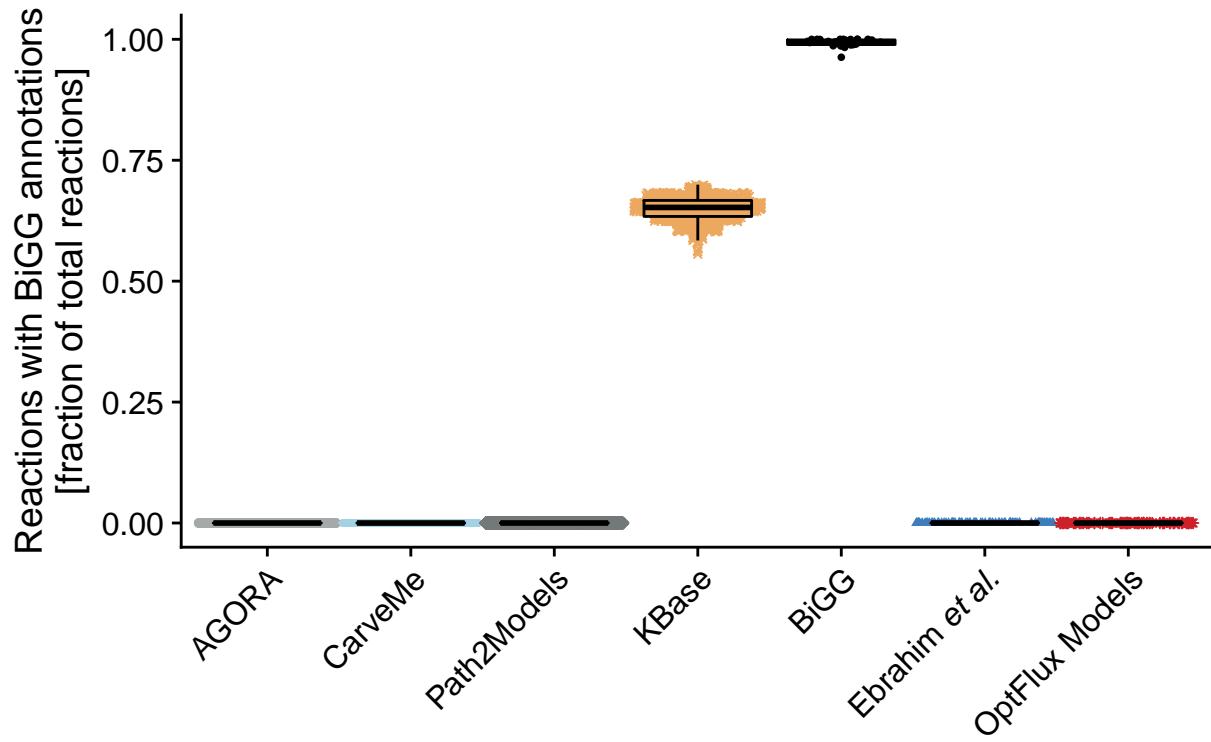


Figure S35: Reaction BiGG.reaction Annotation

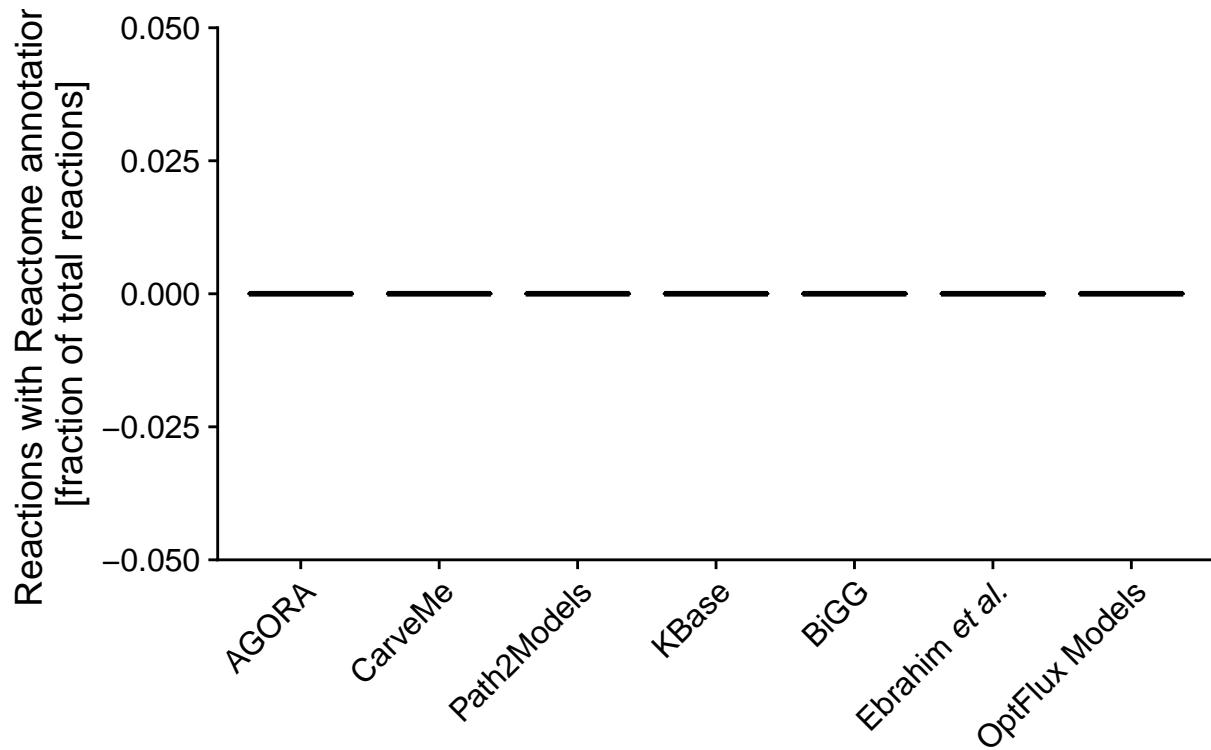


Figure S36: Reaction Reactome Annotation

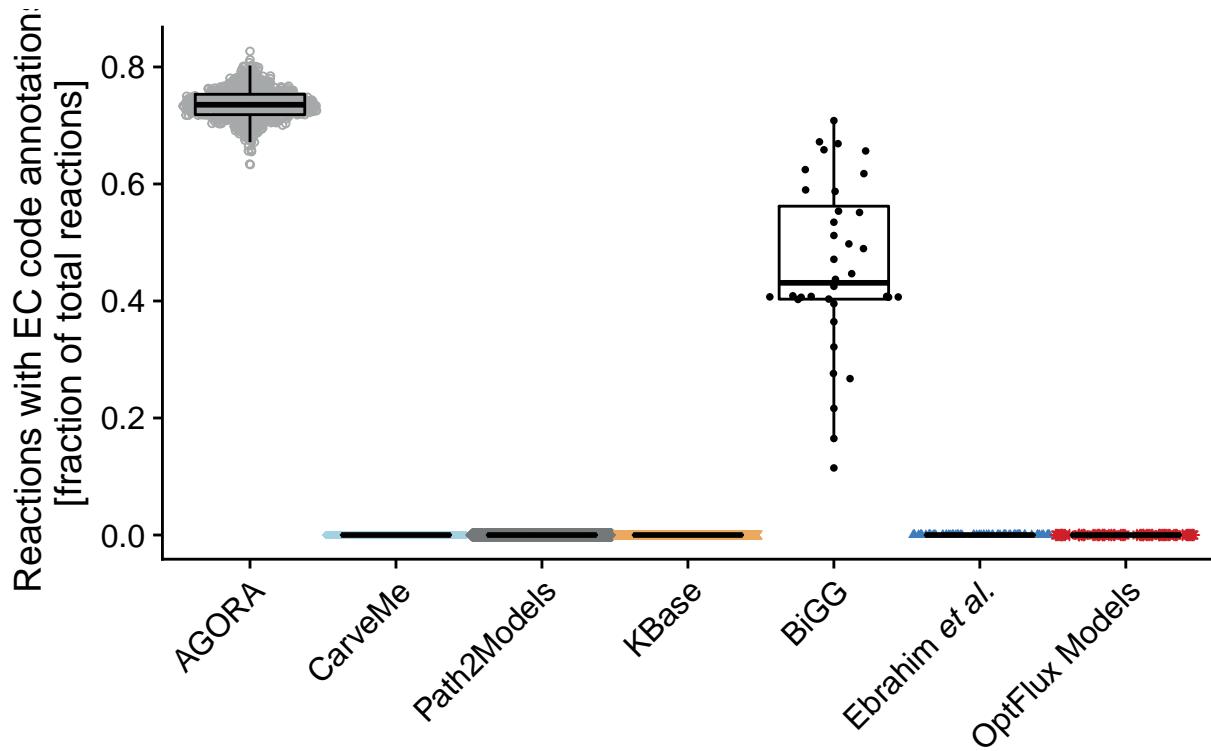


Figure S37: Reaction Enzyme Classification Annotation

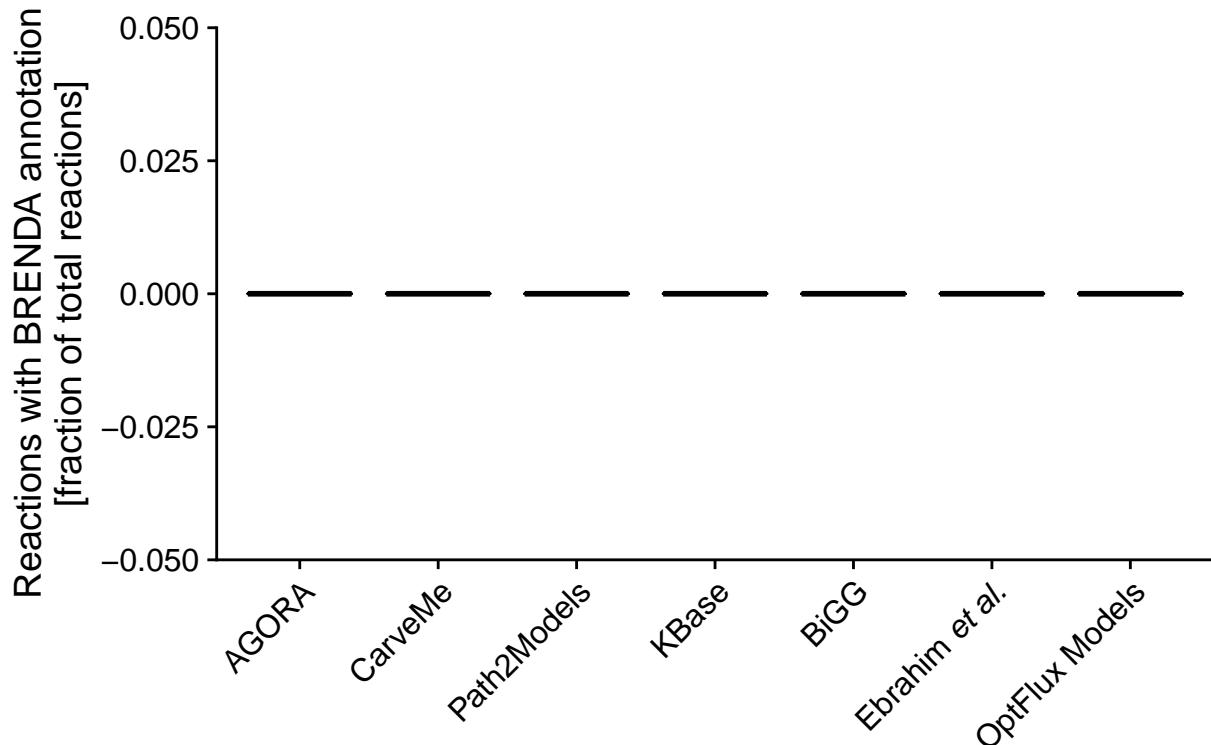


Figure S38: Reaction BRENDA Annotation

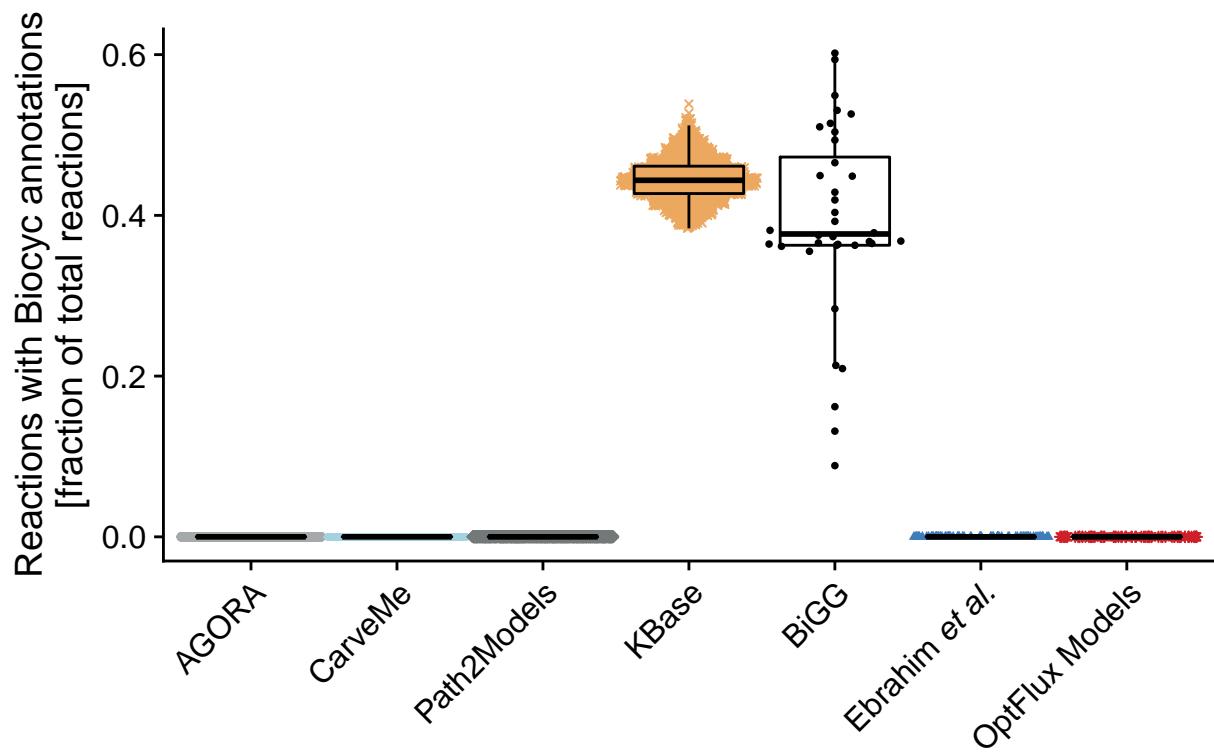


Figure S39: Reaction BioCyc Annotation

1.3.3.2 Reaction Annotation Conformity Per Database

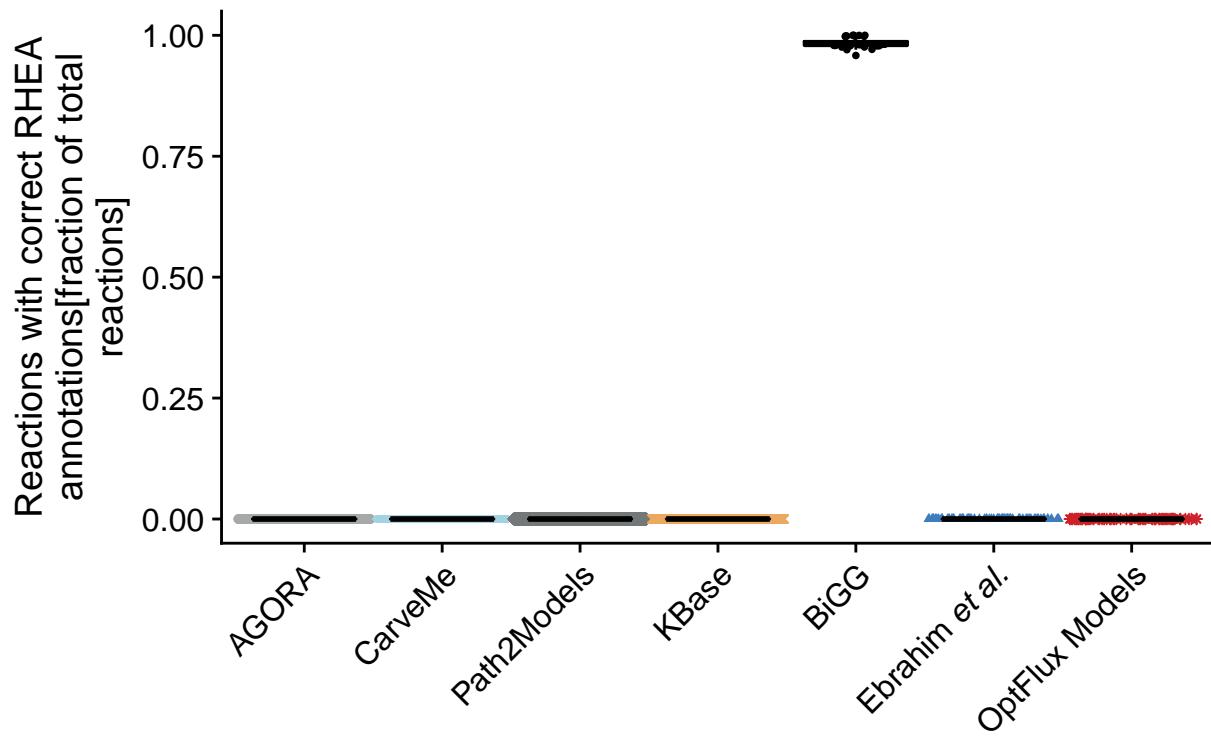


Figure S40: Correct Reaction Rhea Annotation

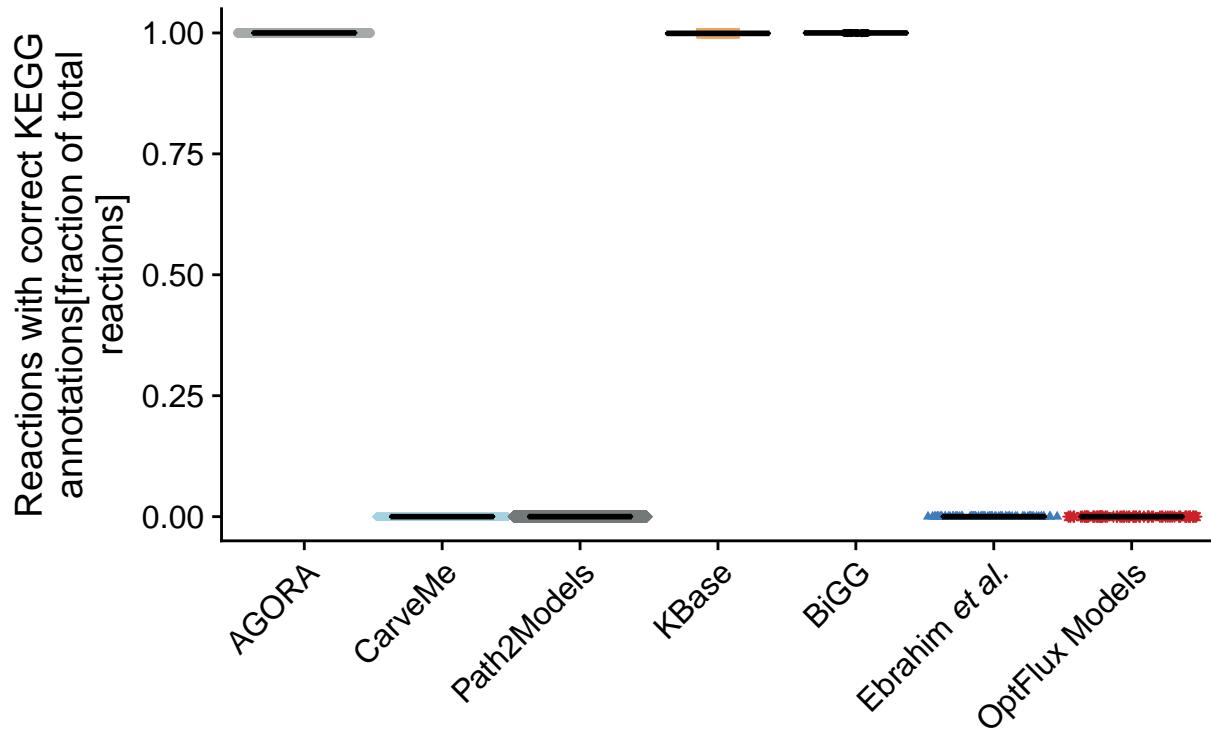


Figure S41: Correct Reaction KEGG.reaction Annotation

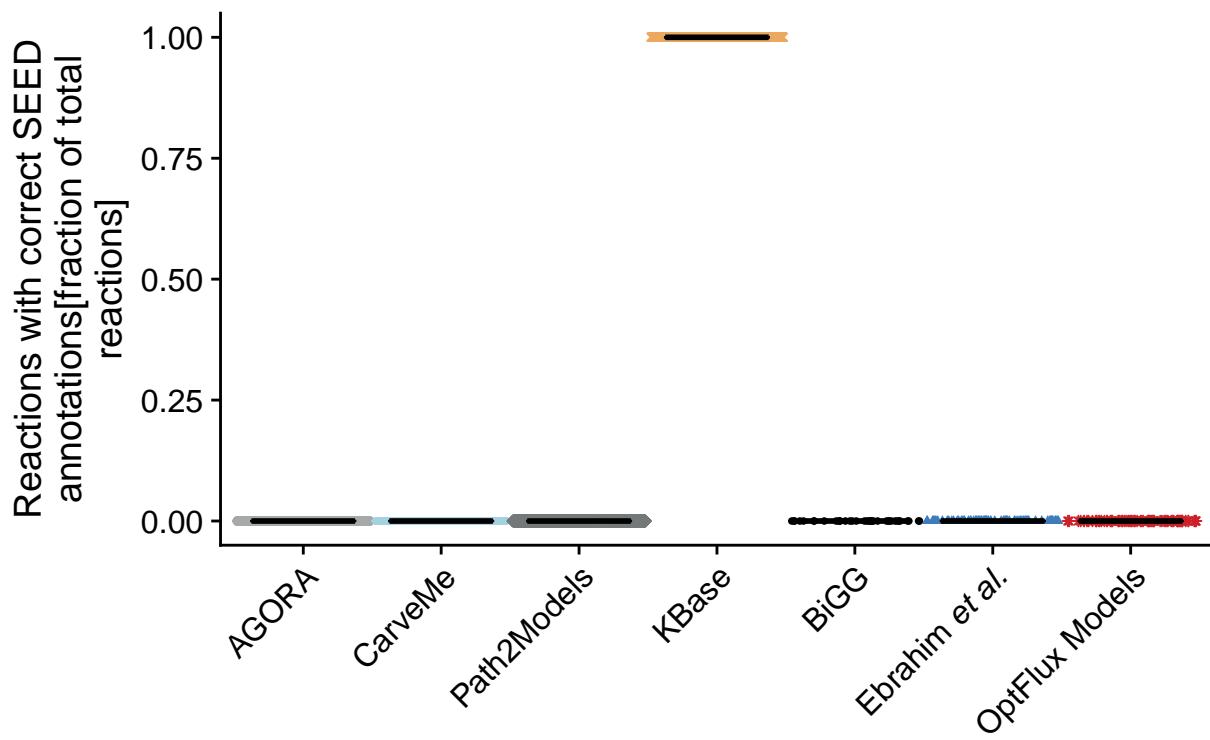


Figure S42: Correct Reaction SEED.reaction Annotation

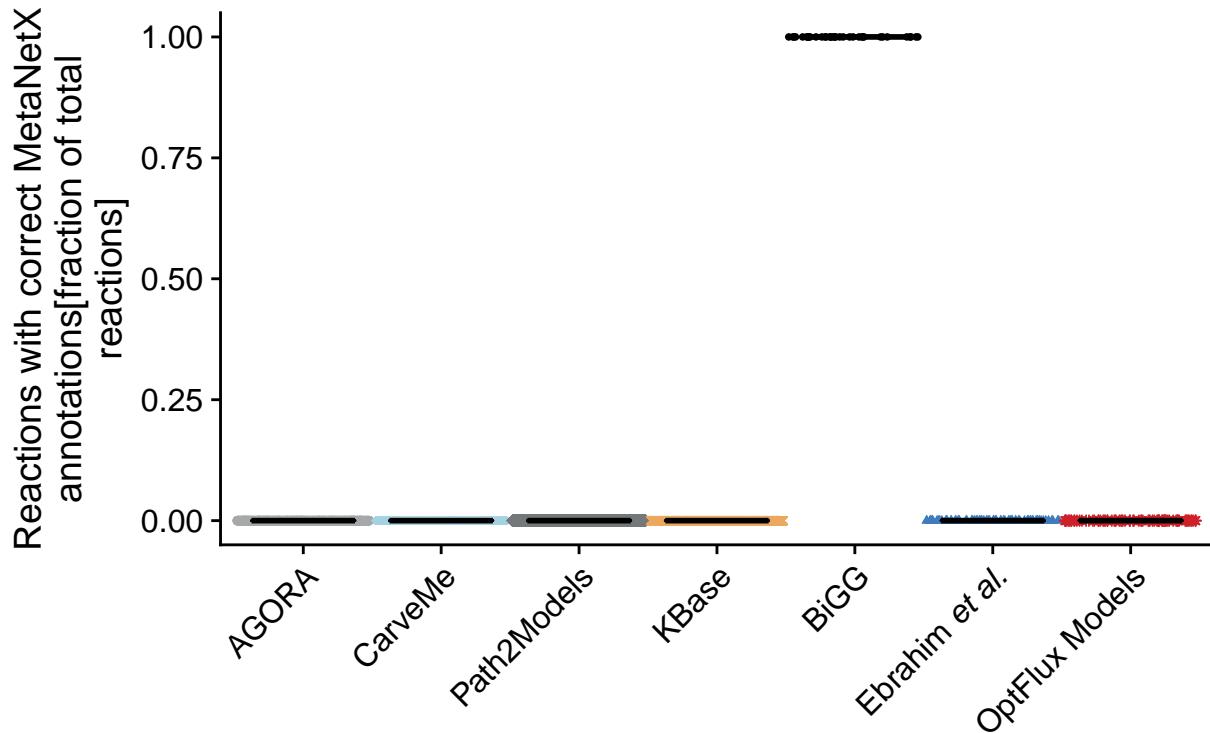


Figure S43: Correct Reaction MetaNetX.reaction Annotation

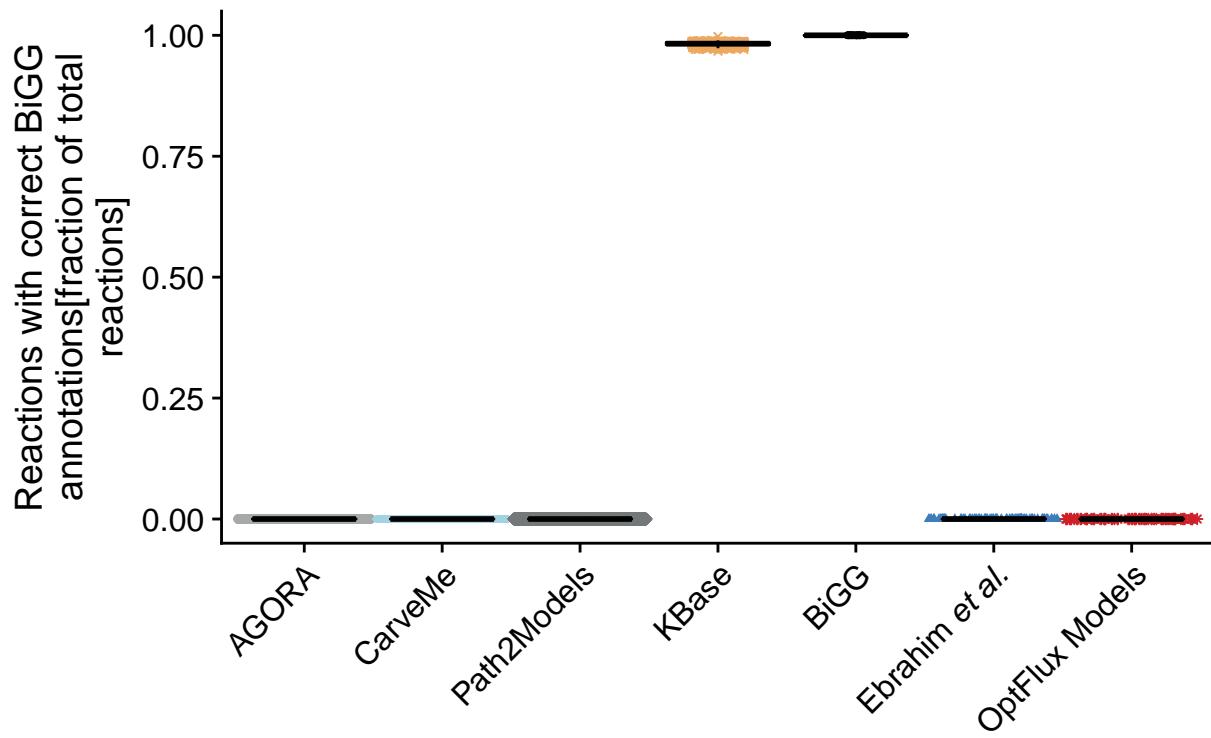


Figure S44: Correct Reaction BiGG.reaction Annotation

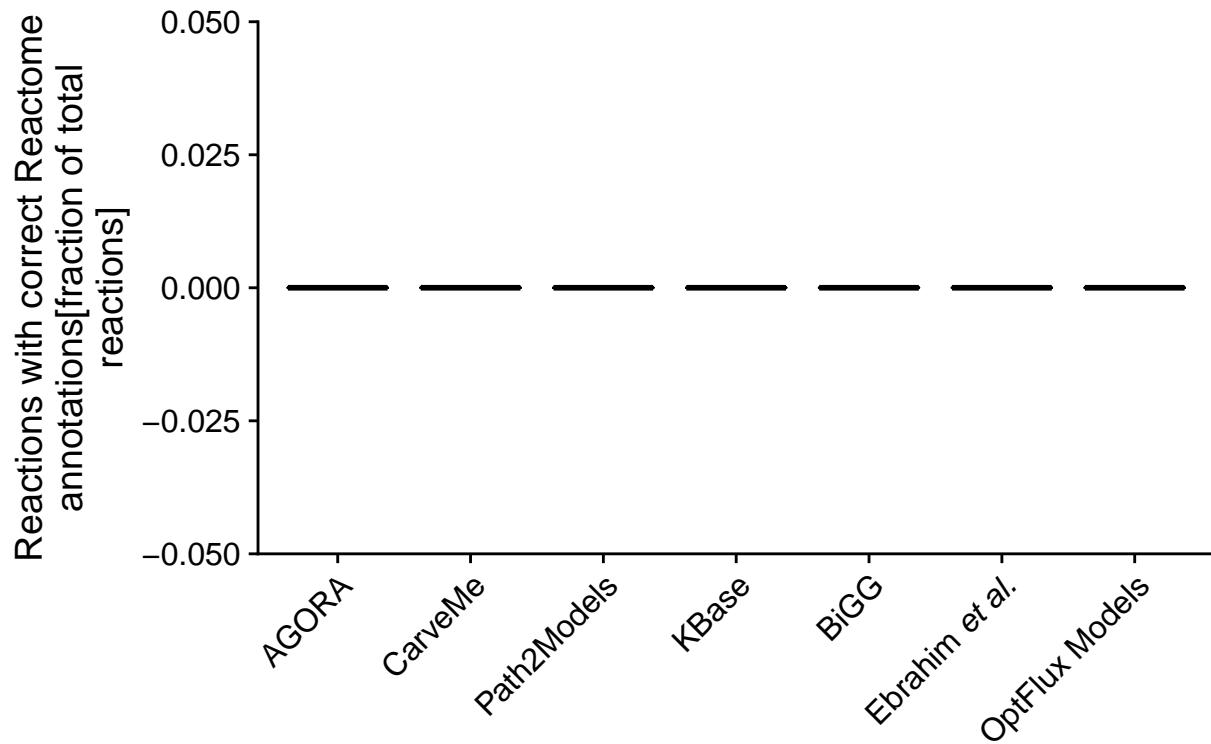


Figure S45: Correct Reaction Reactome Annotation

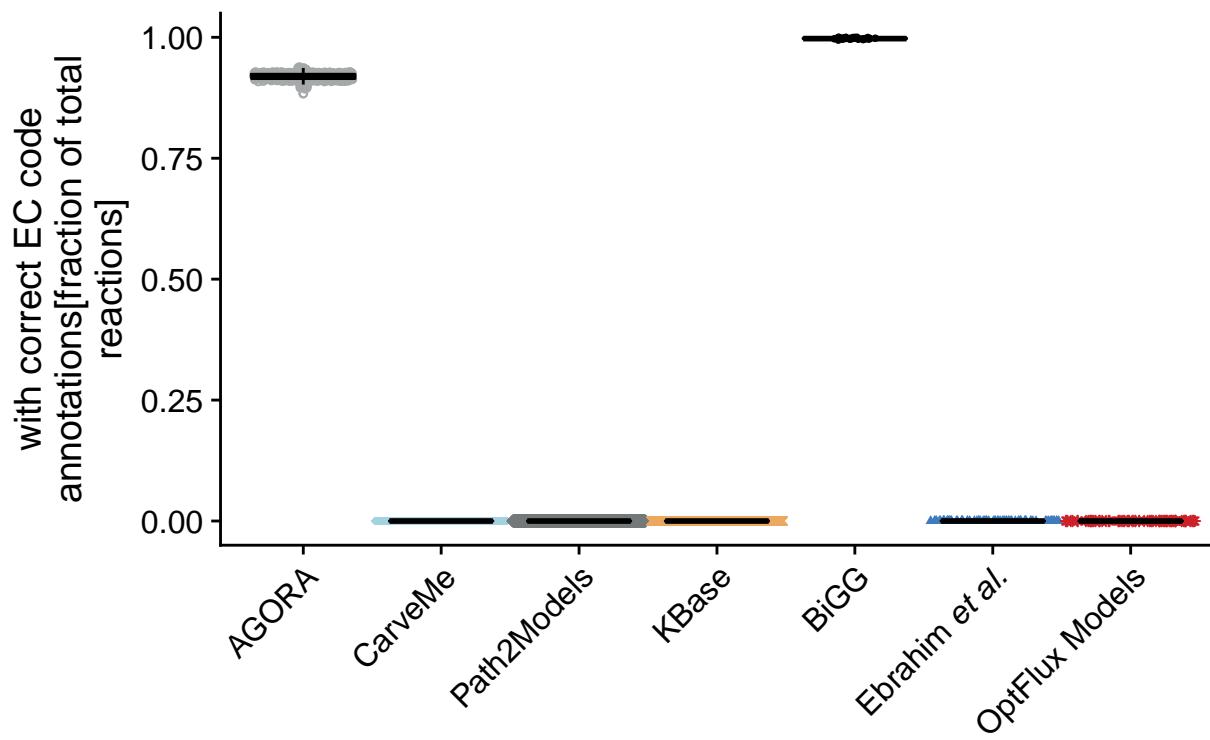


Figure S46: Correct Reaction Enzyme Classification Annotation

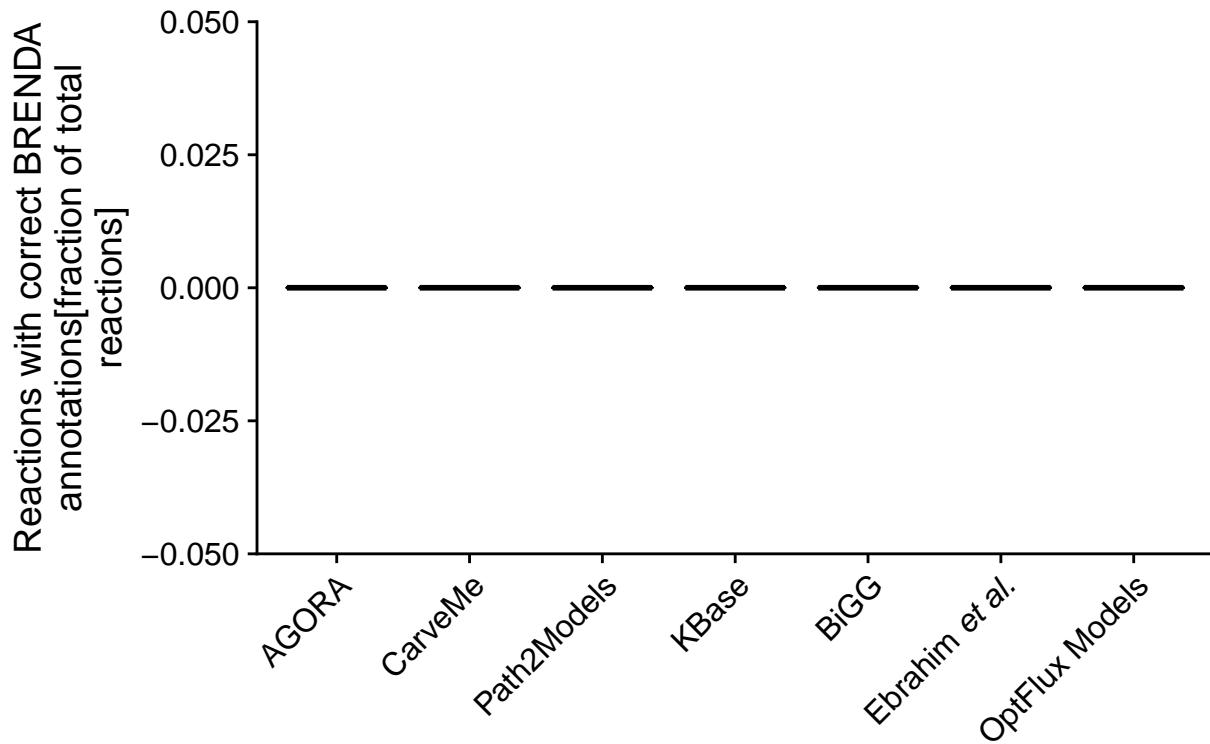


Figure S47: Correct Reaction BRENDA Annotation

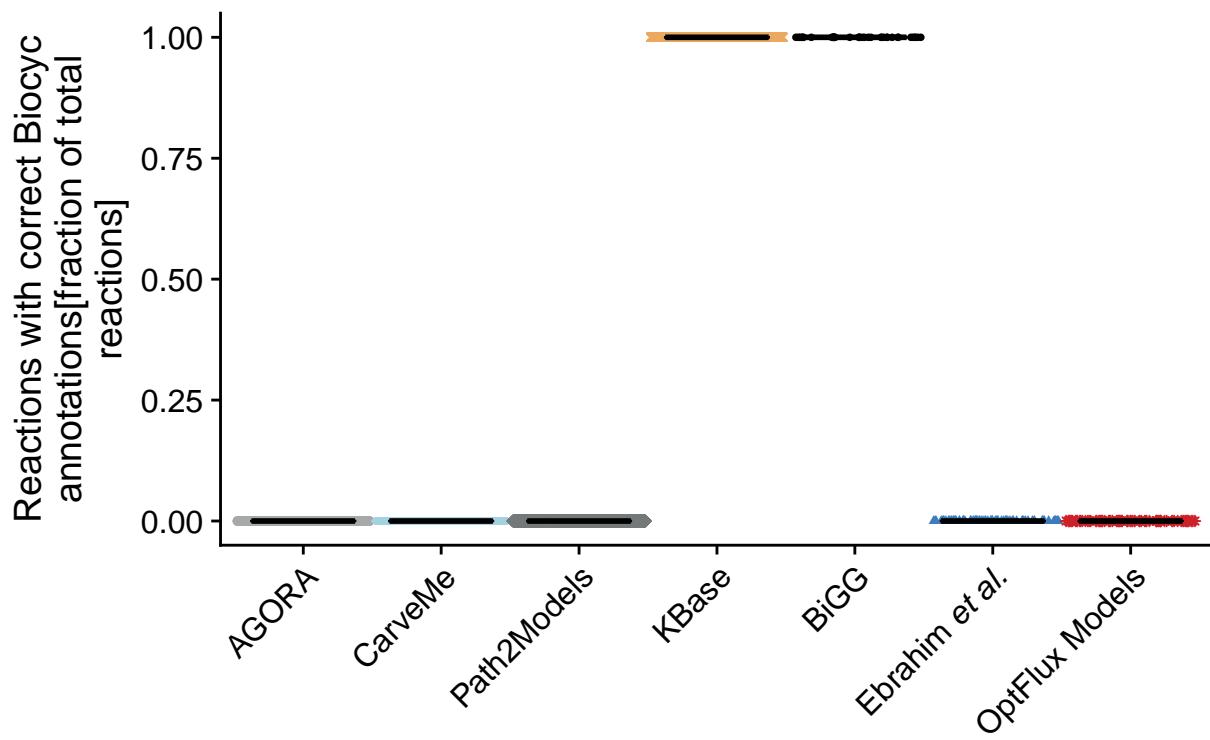


Figure S48: Correct Reaction BioCyc Annotation

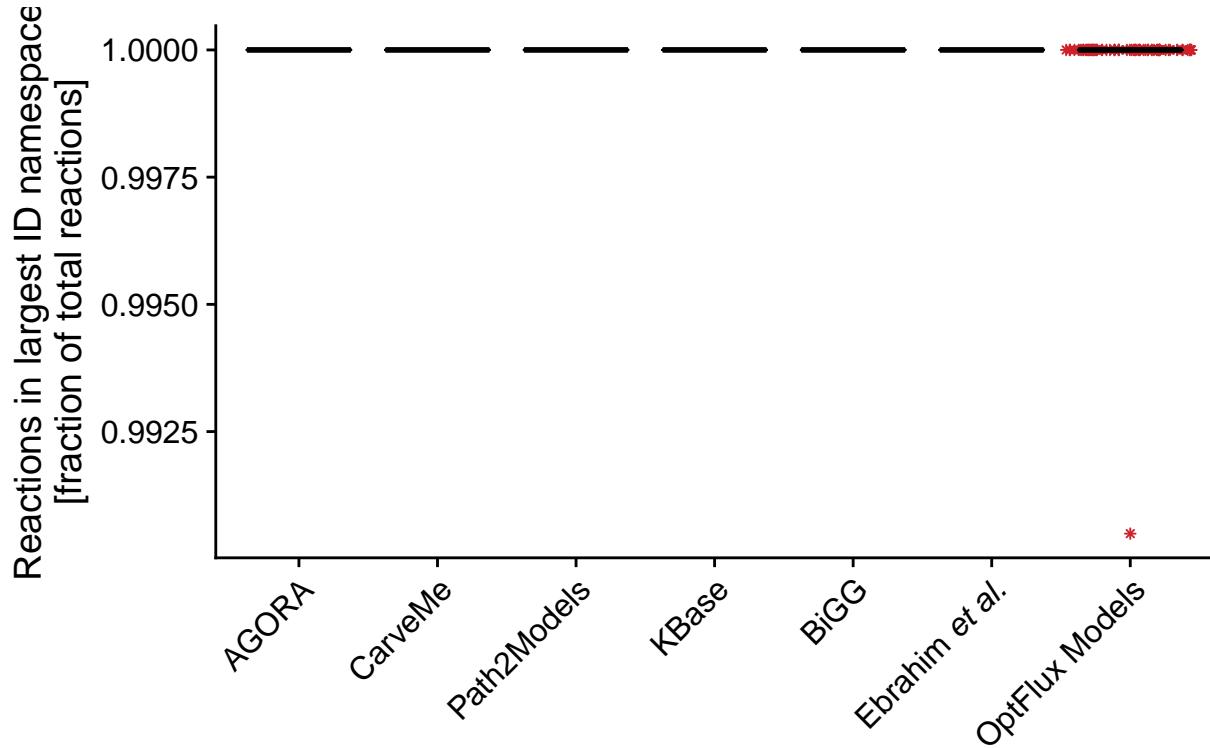


Figure S49: Uniform Reaction Identifier Namespace

1.3.4 Annotation - Genes

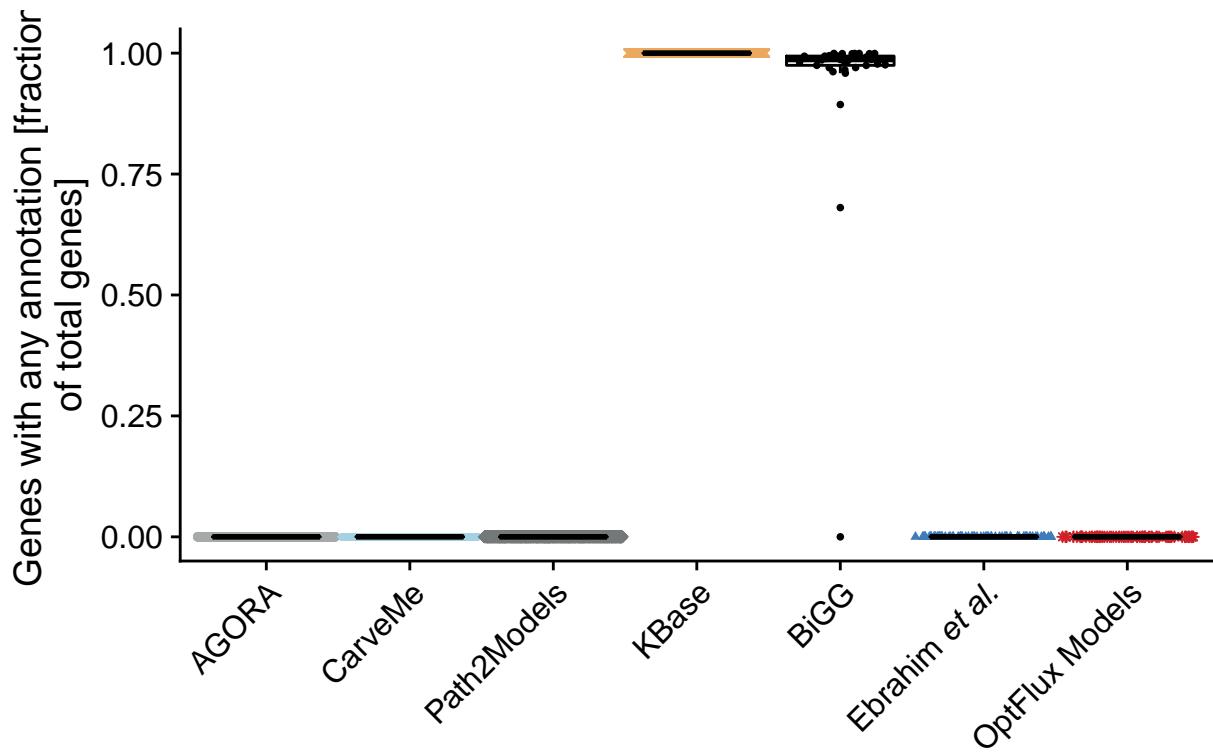


Figure S50: Presence of Gene Annotation

1.3.4.1 Gene Annotations Per Database

1.3.4.2 Gene Annotation Conformity Per Database

We're missing a test for uniform gene identifier namespace.

1.3.5 Annotation - SBO Terms

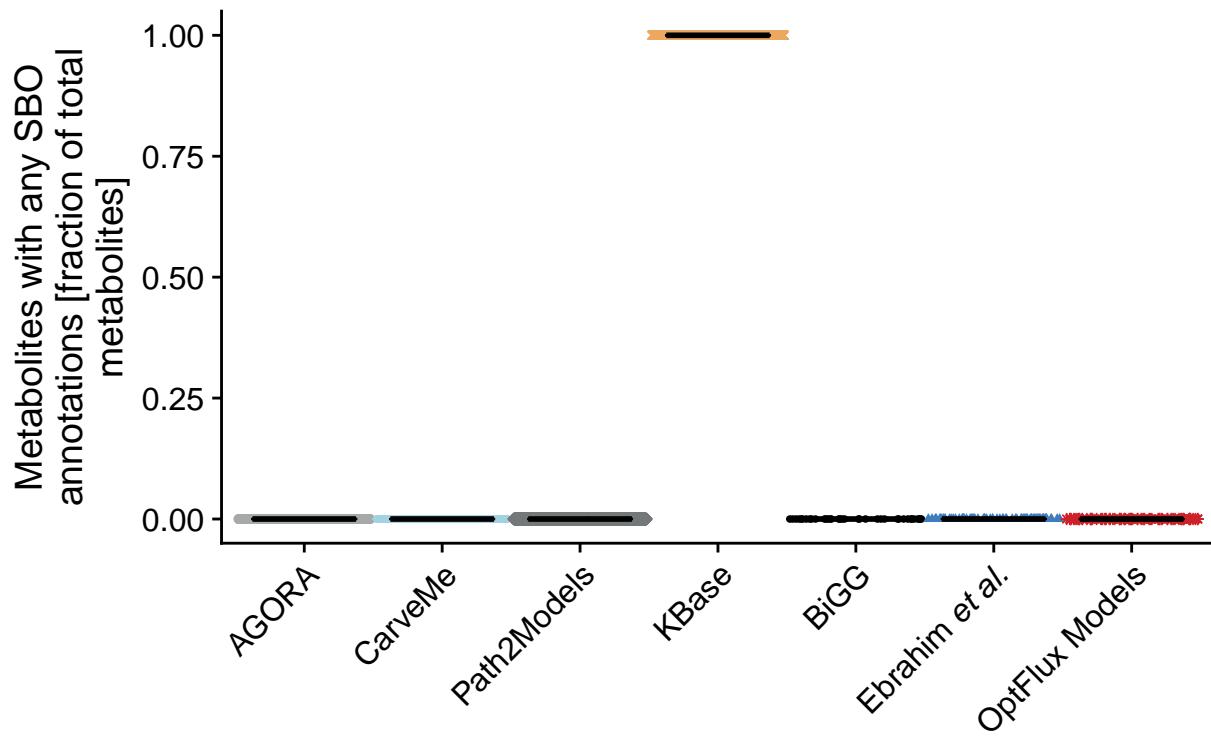


Figure S51: Metabolite General SBO Presence

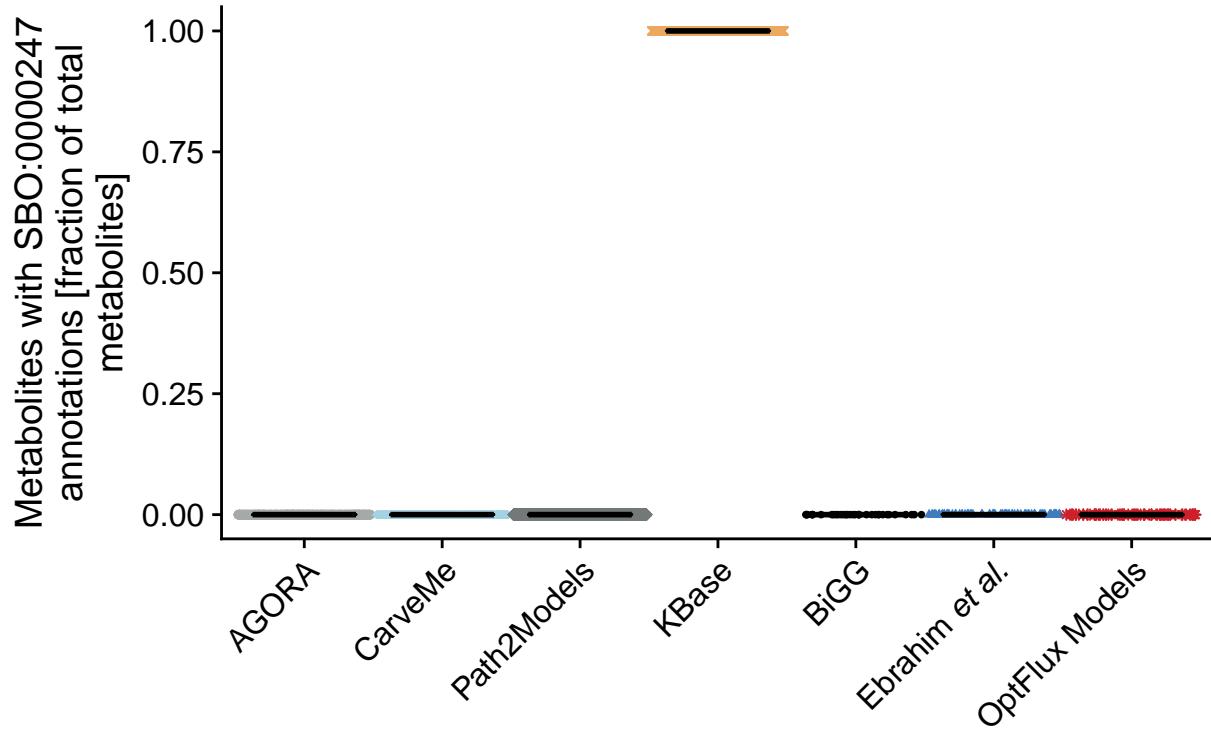


Figure S52: Metabolite SBO:0000247 Presence

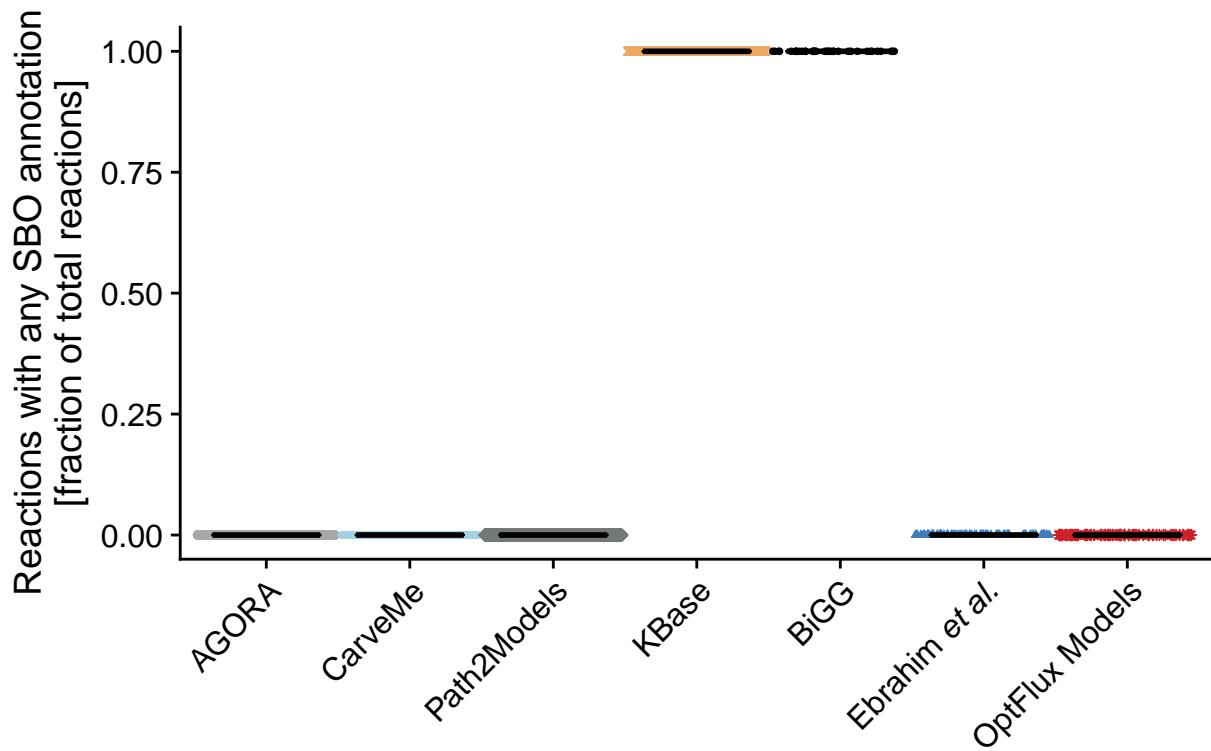


Figure S53: Reaction General SBO Presence

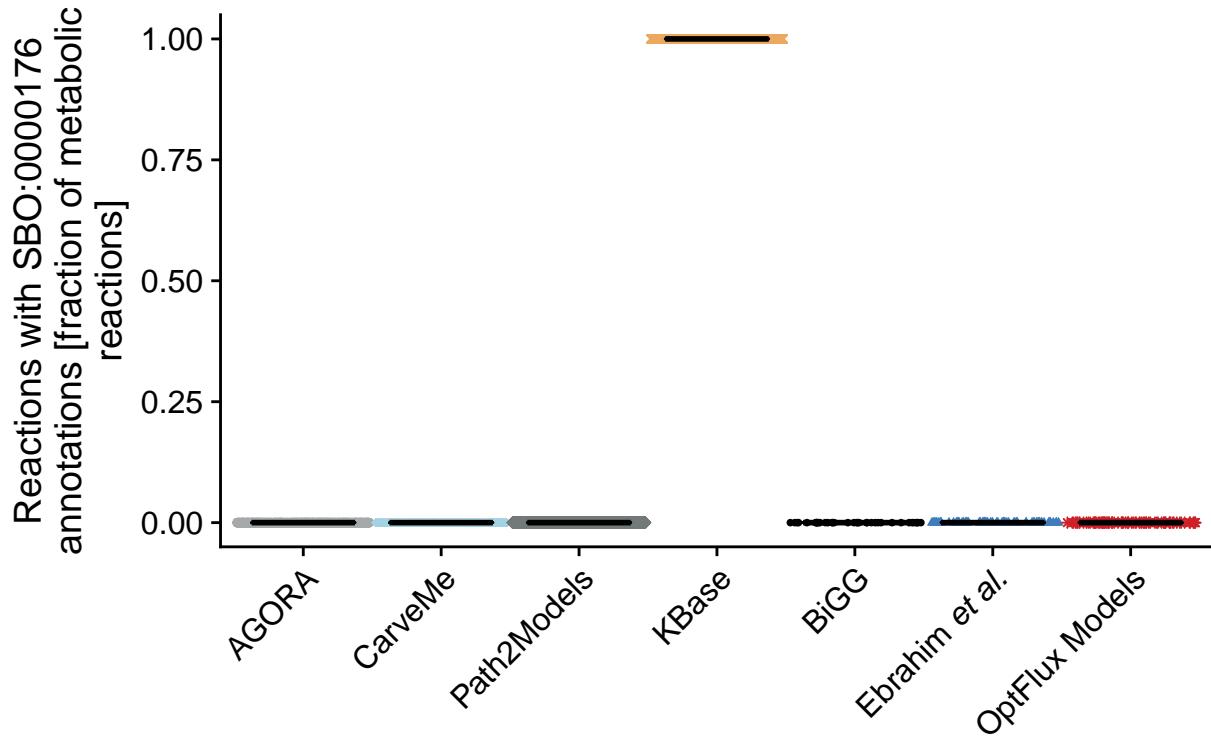


Figure S54: Metabolic Reaction SBO:0000176 Presence

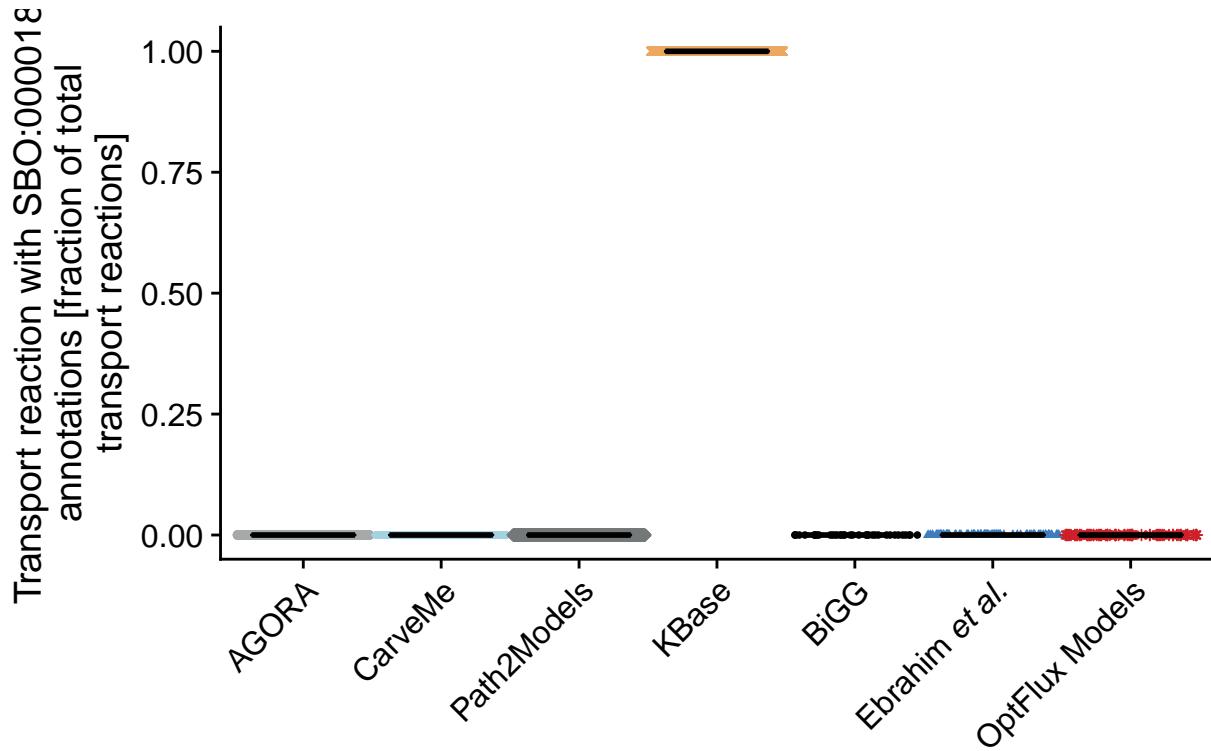


Figure S55: Transport Reaction SBO:0000185 Presence

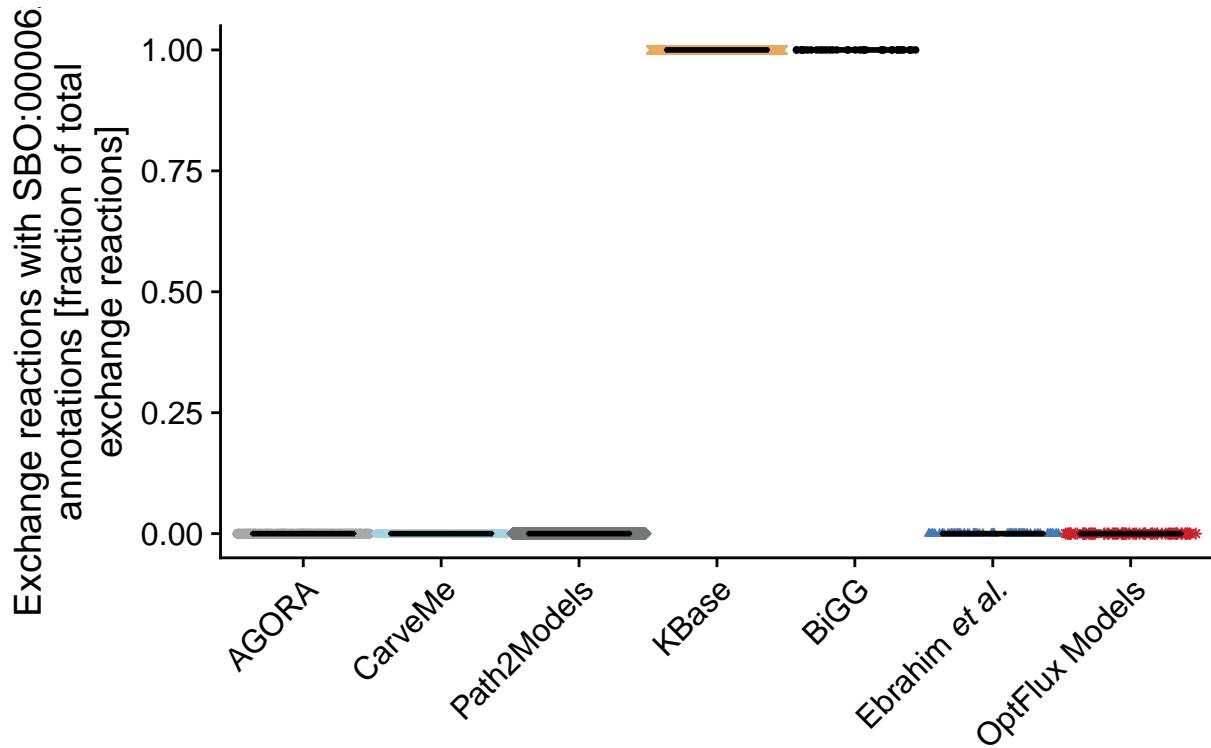


Figure S56: Exchange Reaction SBO:0000627 Presence

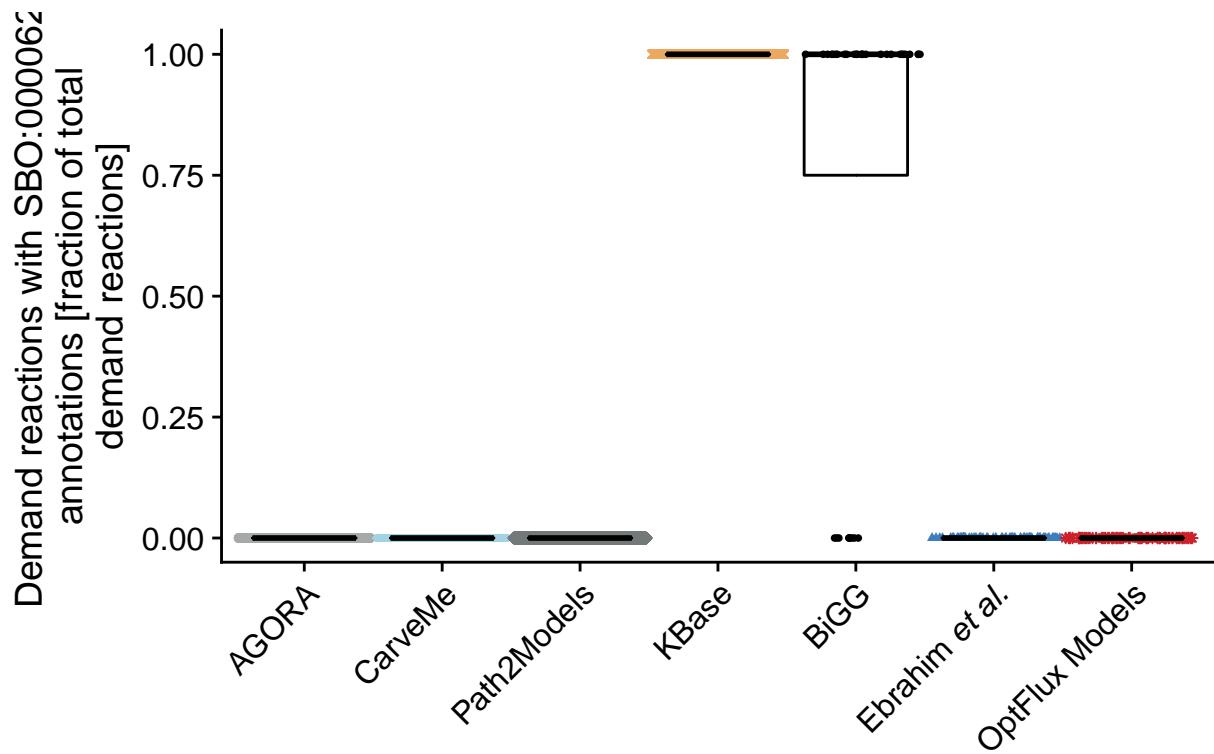


Figure S57: Demand Reaction SBO:0000628 Presence

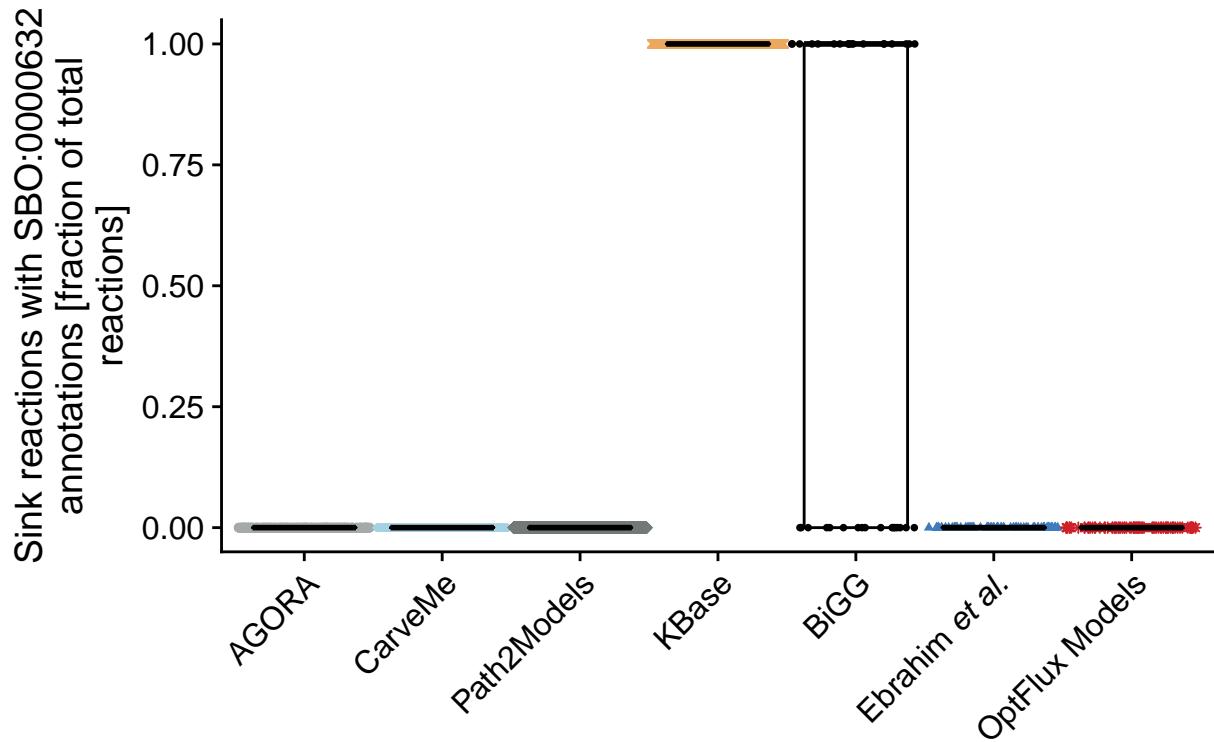


Figure S58: Sink Reaction SBO:0000632 Presence

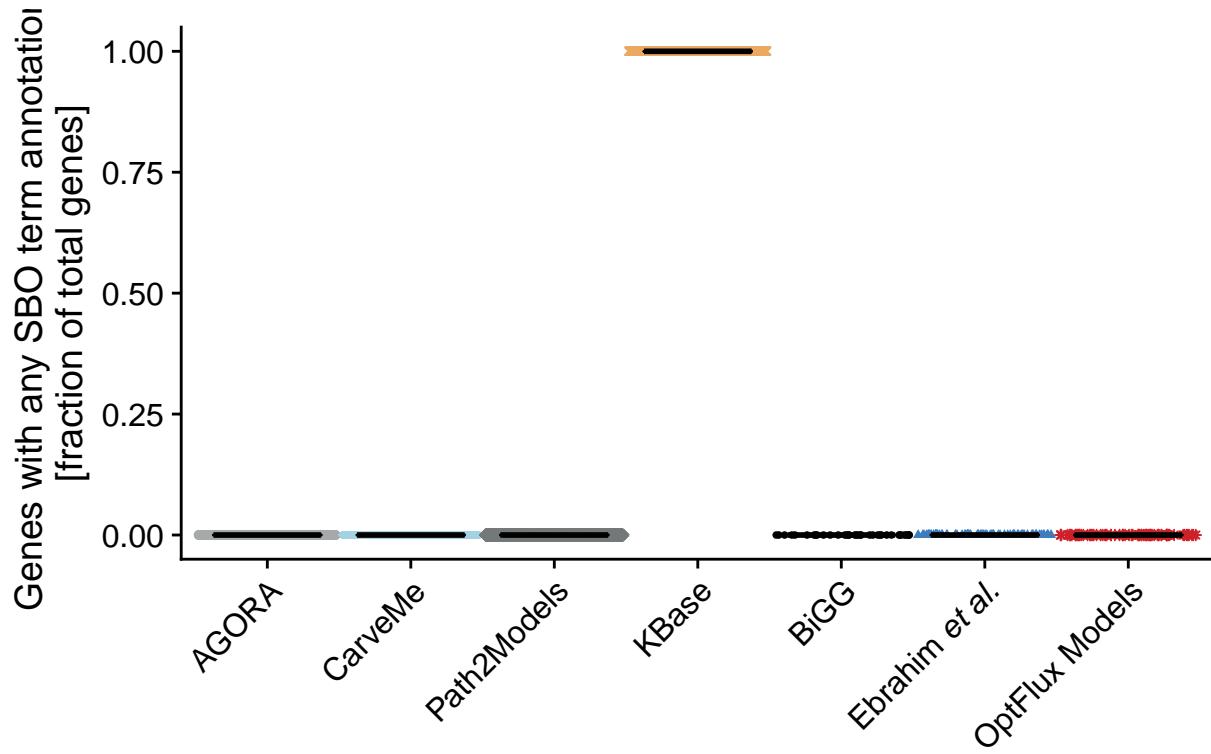


Figure S59: Gene General SBO Presence

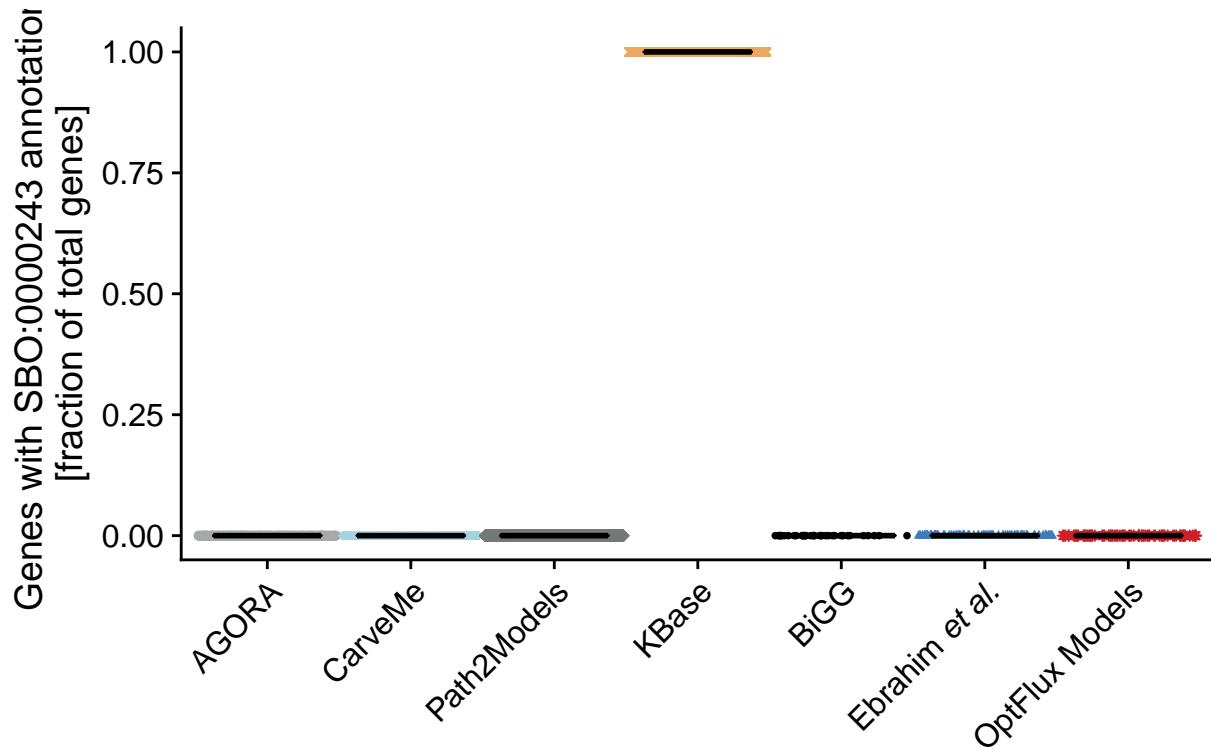


Figure S60: Gene SBO:0000243 Presence

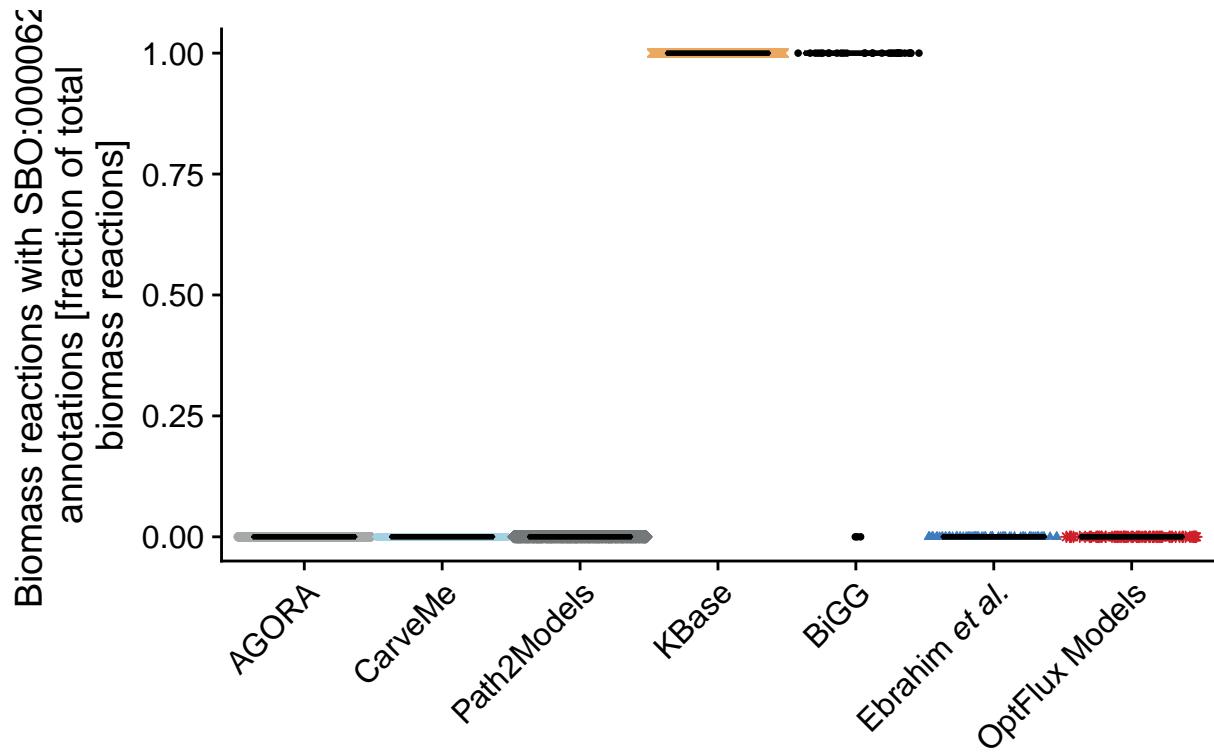


Figure S61: Biomass Reaction SBO:0000629 Presence

1.4 Specific Section

1.4.1 SBML

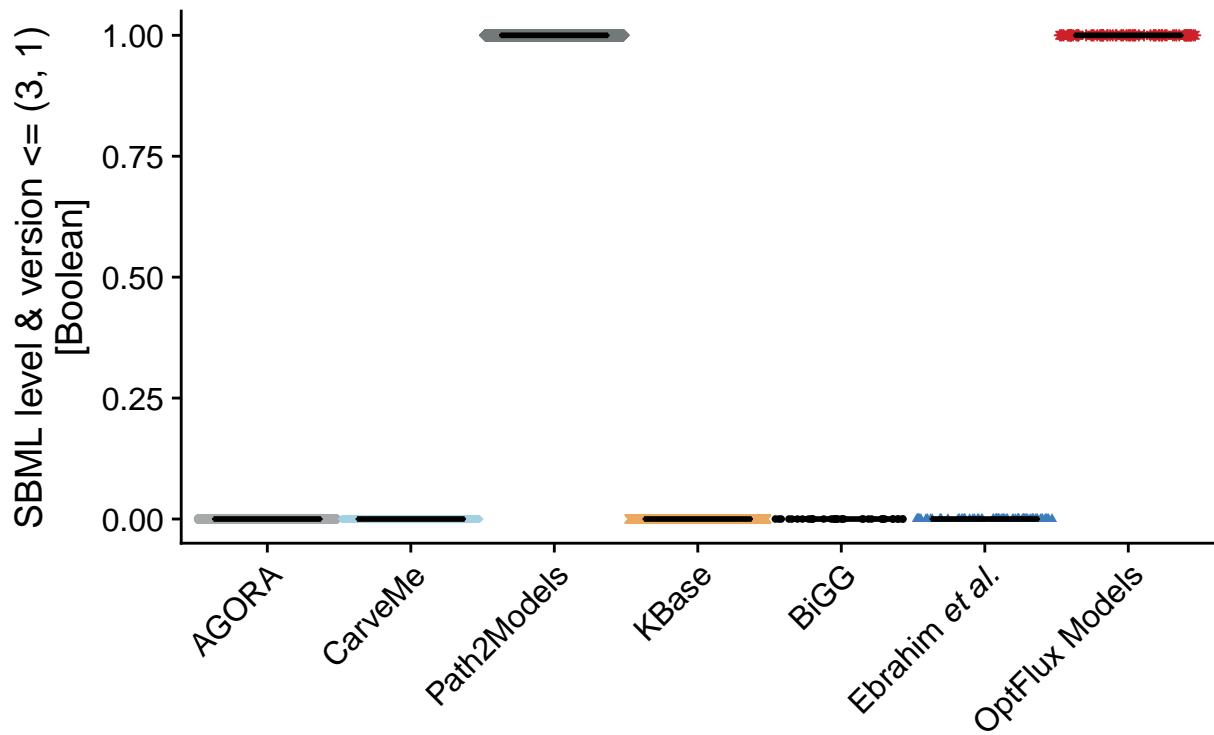


Figure S62: SBML Level and Version

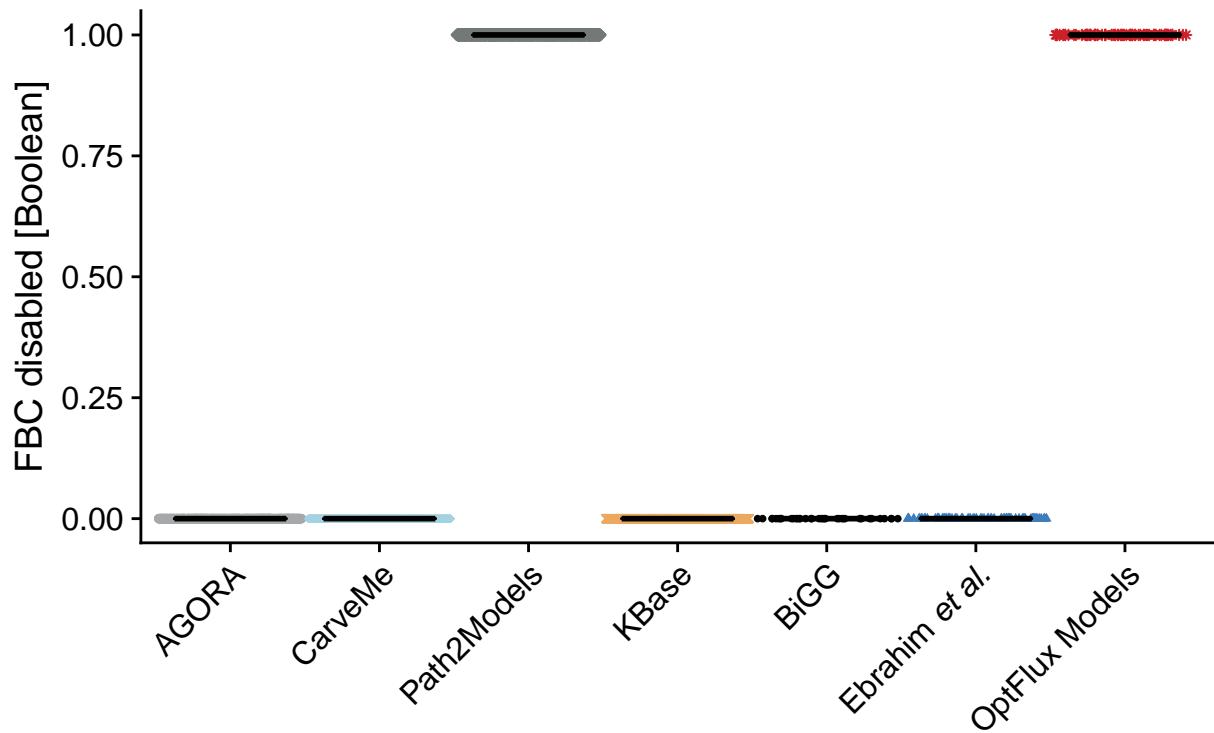


Figure S63: FBC Enabled