

Supplementary Table 1. Tools and formats used to execute each stage of the biochemical modeling workflow shown in Figure 1. Hyperlinks to the homepage for each tool or format is provided to readily access the tool or browse documentation.

Aggregate data	Management resources: Pathway Tools , PROV , Quilt , RightField , SEPIO Data sources: BioCyc , BRENDA , ChEBI , GenBank , KEGG , KEGG Pathway , PDB , Pub-Chem , SABIO-RK , UniMod , UniProt
Construct model	Formats: CellML , SBML , SBtab Languages: Antimony , BioNetGen , BioPAX , C/C++ , Java , MATLAB , PySB , Python Ontologies: BcForms , BpForms , InChI , MIRIAM , SBO Versioning tools: Git , mercurial , SVN
Estimate parameters	Software: COPASI , Data2Dynamics , PyBioNetFit , PyDREAM , SBML-PET , SciPy Optimize
Simulate model	Formats: SED-ML , SESSL Ontologies: KiSAO , MIASE Simulators: COBRApy , COPASI , libRoadRunner , OpenCOR , SimPy , StochSS , Sundials , Tellurium , VCell Languages: C/C++ , Java , MATLAB , Python
Store & analyze results	Formats: HDF , SBRML , SEEK Simulators: COPASI , JWS Online , Tellurium Software: Excel , R , RightField Visualization packages: D3 , matplotlib , Vega
Verify & validate model	Packages: BioLab , CircleCI , JUnit , LoLA , memote , NuSMV , PRISM , pytest , SBML2Prism , SciUnit , Travis
Document artifacts	Ontologies: BcForms , BpForms , InChI , KiSAO , MIASE , MIRIAM , SBGN , SBO Software: RightField , SEEK
Package artifacts & documentation	Format: COMBINE archive Software: AMI , Docker , Parallels , Singularity , Virtual box , VMware

Publish & disseminate	<p>Preprint server: bioRxiv</p> <p>Repositories: BioModels, Bitbucket, DockerHub, FAIRDOMHub, FigShare, GitHub, JWS Online, Physiome, PubMed, SimTK, Zenodo</p>
-----------------------	---