S2 Table. File formats of M-models

|  |  |  |  |
| --- | --- | --- | --- |
| **Format** | **Description** | **Conversion tool** | **Reference** |
| JSON | Plain text format data structure | COBRApy  COBREXA.jl | (1,2) |
| mat | Matlab variable data structure | COBRA Toolbox  Systems Biology Format Converter (SBFC)  COBREXA.jl | (1,3) |
| sbml | Representation format based on XML | COBRApy  COBREXA.jl  KEGGtranslator  COBRA Toolbox | (4–6) |
| yaml | Human readable markup language | Raven 2.0 / Cobrapy | (7) |

**REFERENCES**

1. Heirendt L, Thiele I, Fleming RMT. DistributedFBA.jl: High-level, high-performance flux balance analysis in Julia. Bioinformatics. 2017 May 1;33(9):1421–3.

2. Ebrahim A, Lerman JA, Palsson BO, Hyduke DR. COBRApy: COnstraints-Based Reconstruction and Analysis for Python. BMC Syst Biol. 2013 Aug 8;7.

3. Heirendt L, Arreckx S, Pfau T, Mendoza SN, Richelle A, Heinken A, et al. Creation and analysis of biochemical constraint-based models using the COBRA Toolbox v.3.0. Nature Protocols 2019 14:3 [Internet]. 2019 Feb 20 [cited 2023 Jun 4];14(3):639–702. Available from: https://www.nature.com/articles/s41596-018-0098-2

4. Wrzodek C, Dräger A, Zell A. KEGGtranslator: Visualizing and converting the KEGG PATHWAY database to various formats. Bioinformatics. 2011 Aug;27(16):2314–5.

5. Hucka M, Bergmann FT, Chaouiya C, Dräger A, Hoops S, Keating SM, et al. The Systems Biology Markup Language (SBML): Language Specification for Level 3 Version 2 Core Release 2. J Integr Bioinform. 2019 Jun 20;16(2).

6. Olivier BG, Bergmann FT. SBML Level 3 Package: Flux Balance Constraints version 2. J Integr Bioinform. 2018 Mar 9;15(1).

7. Wang H, Marcišauskas S, Sánchez BJ, Domenzain I, Hermansson D, Agren R, et al. RAVEN 2.0: A versatile toolbox for metabolic network reconstruction and a case study on *Streptomyces* *coelicolor*. PLoS Comput Biol. 2018 Oct 1;14(10).