SBML Model Report

Model name: "Tiago2010_FeMetabolism_FeAdequate"



May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 1 format. This model was created by the following two authors: Vijayalakshmi Chelliah¹ and Tiago Jose da Silva Lopes² at August 19th 2010 at 10:30 a.m. and last time modified at April fourth 2014 at 2:36 p.m. Table 1 gives an overview of the quantities of all components of this model.

Table 1: Number of components in this model, which are described in the following sections.

Element	Quantity	Element	Quantity
compartment types	0	compartments	2
species types	0	species	17
events	0	constraints	0
reactions	29	function definitions	0
global parameters	0	unit definitions	0
rules	0	initial assignments	0

Model Notes

This a model from the article:

Systems analysis of iron metabolism: the network of iron pools and fluxes

Tiago JS Lopes, Tatyana Luganskaja, Maja Vujic-Spasic, Matthias W Hentze, Martina U Muckenthaler, Klaus Schumann and Jens G Reich BMC Systems Biology2010, Aug 13;4(1):112.

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Abstract:

Background

Every cell of the mammalian organism needs iron in numerous oxido-reductive processes as well as for transport and storage of oxygen. The versatility of ionic iron makes it a toxic entity which cancatalyze the production of radicals that damage vital membranous and macromolecular assemblies in the cell. The mammalian organism maintains therefore a complex regulatory network of iron uptake, excretion and intra-body distribution. Intracellular regulation in different cell types is intertwined with a global hormonal signaling structure. Iron deficiency as well as excess of iron are frequent and serious human disorders. They can affect every cell, but also the organism as a whole.

Results

Here, we present a kinematic model of the dynamic system of iron pools and fluxes. It is based on ferrokinetic data and chemical measurements in C57BL6 wild-type mice maintained on iron-deficient, iron-adequate, or iron-loaded diet. The tracer iron levels in major tissues and organs (16 compartment) were followed for 28 days. The evaluation resulted in a whole-body model of fractional clearance rates. The analysis permits calculation of absolute flux rates in the steady-state, of iron distribution into different organs, of tracer-accessible pool sizes and of residence times of iron in the different compartments in response to three states of iron-repletion induced by the dietary regime.

Conclusions

This mathematical model presents a comprehensive physiological picture of mice under three different diets with varying iron contents. The quantitative results reflect systemic properties of iron metabolism: dynamic closedness, hierarchy of time scales, switch-over response and dynamics of iron storage in parenchymal organs. Therefore, we could assess which parameters will change under dietary perturbations and study in quantitative terms when those changes take place.

This model corresponds to the Iron Adequate condition - Mice

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To cite BioModels Database, please use Le Novre N., Bornstein B., Broicher A., Courtot M., Donizelli M., Dharuri H., Li L., Sauro H., Schilstra M., Shapiro B., Snoep J.L., Hucka M. (2006) BioModels Database: A Free, Centralized Database of Curated, Published, Quantitative Kinetic Models of Biochemical and Cellular Systems Nucleic Acids Res., 34: D689-D691.

2 Unit Definitions

This is an overview of five unit definitions which are all predefined by SBML and not mentioned in the model.

2.1 Unit substance

Notes Mole is the predefined SBML unit for substance.

Definition mol

2.2 Unit volume

Notes Litre is the predefined SBML unit for volume.

Definition 1

2.3 Unit area

Notes Square metre is the predefined SBML unit for area since SBML Level 2 Version 1.

Definition m^2

2.4 Unit length

Notes Metre is the predefined SBML unit for length since SBML Level 2 Version 1.

Definition m

2.5 Unit time

Notes Second is the predefined SBML unit for time.

Definition s

3 Compartments

This model contains two compartments.

Table 2: Properties of all compartments.

Id	Name	SBO	Spatial Dimensions	Size	Unit	Constant	Outside
default	Environment		3	1	litre	Ø	
c1	Organism		3	1	litre		default

3.1 Compartment default

This is a three dimensional compartment with a constant size of one litre.

Name Environment

3.2 Compartment c1

This is a three dimensional compartment with a constant size of one litre, which is surrounded by default (Environment).

Name Organism

4 Species

This model contains 17 species. Section 6 provides further details and the derived rates of change of each species.

Table 3: Properties of each species.

Id	Name	Compartment	Derived Unit	Constant	Boundary Condi- tion
s1	iron_in_Plasma	c1	$\text{mol} \cdot 1^{-1}$	⊣	
s2	iron_in_Bone Marrow	c1	$\text{mol} \cdot l^{-1}$		
s3	iron_in_RBC	c1	$\text{mol} \cdot 1^{-1}$		
s4	iron_in_Spleen	c1	$\operatorname{mol} \cdot 1^{-1}$		
s 5	iron_in_Liver	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
s 6	iron_in_Muscle	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
s 7	iron_in_Duodenum	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
s 8	iron_in_Integument	c1	$\operatorname{mol} \cdot 1^{-1}$		
ສ9	iron_in_Intestine	c1	$\operatorname{mol} \cdot 1^{-1}$		
s10	iron_ions_Outside	default	$\operatorname{mol} \cdot 1^{-1}$		\Box
s11	iron_in_Heart	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
s12	iron_in_Lungs	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
s13	iron_in_Kidneys	c1	$\operatorname{mol} \cdot 1^{-1}$		\Box
s14	iron_in_Testes	c1	$\operatorname{mol} \cdot 1^{-1}$		
s15	iron_in_Stomach	c1	$\mathrm{mol}\cdot \mathrm{l}^{-1}$		
s16	iron_in_Fat	c1	$\text{mol} \cdot 1^{-1}$		
s17	iron_in_Brain	c1	$\operatorname{mol} \cdot 1^{-1}$		

5 Reactions

This model contains 29 reactions. All reactions are listed in the following table and are subsequently described in detail. If a reaction is affected by a modifier, the identifier of this species is written above the reaction arrow.

Table 4: Overview of all reactions

$N_{\bar{0}}$	Id	Name	Reaction Equation	SBO
1	re1		s1 s2	
2	re2		$s2 \longrightarrow s3$	
3	re3		$s3 \longrightarrow s4$	
4	re4		$s4 \longrightarrow s1$	
5	re5		$s2 \longrightarrow s4$	
6	re6		$s1 \longrightarrow s5$	
7	re7		$s5 \longrightarrow s1$	
8	re8		$s1 \longrightarrow s6$	
9	re9		$s6 \longrightarrow s1$	
10	re10		$s1 \longrightarrow s7$	
11	re11		$s1 \longrightarrow s9$	
12	re12		$s1 \longrightarrow s8$	
13	re14		$s9 \longrightarrow s10$	
14	re15		$s8 \longrightarrow s10$	
15	re16		$s1 \longrightarrow s11$	
16	re17		$s11 \longrightarrow s1$	
17	re18		$s1 \longrightarrow s12$	
18	re19		$s12 \longrightarrow s1$	
19	re22		$s1 \longrightarrow s13$	
20	re23		$s13 \longrightarrow s1$	
21	re24		$s1 \longrightarrow s14$	
22	re25		$s14 \longrightarrow s1$	
23	re26		$s1 \longrightarrow s15$	

N⁰	Id	Name	Reaction Equation	SBO
24	re28		$s1 \longrightarrow s16$	
25	re29		$s16 \longrightarrow s1$	
26	re30		$s1 \longrightarrow s17$	
27	re31		$s17 \longrightarrow s1$	
28	re32		$s7 \longrightarrow s1$	
29	re33		$s15 \longrightarrow s10$	

5.1 Reaction re1

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s2$$
 (1)

Reactant

Table 5: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 6: Properties of each product.

Id	Name	SBO
s2	iron_in_Bone Marrow	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = [\mathbf{s}1] \cdot \mathbf{k}1 \tag{2}$$

Table 7: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	1kp_bon	12.670	Ø

5.2 Reaction re2

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s2 \longrightarrow s3$$
 (3)

Reactant

Table 8: Properties of each reactant.

1401	e or reperior or each re	
Id	Name	SBO
s2	iron_in_Bone Marrow	

Product

Table 9: Properties of each product.

Id	Name	SBO
s3	iron_in_RBC	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = [s2] \cdot k1 \tag{4}$$

Table 10: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	27kbon_rbc	1.067	

5.3 Reaction re3

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s3 \longrightarrow s4$$
 (5)

Reactant

Table 11: Properties of each reactant.

Id	Name	SBO
s3	iron_in_RBC	

Product

Table 12: Properties of each product.

Id	Name	SBO
s4	iron_in_Spleen	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = [s3] \cdot k1 \tag{6}$$

Table 13: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	29krbc_spl	0.061	

5.4 Reaction re4

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s4 \longrightarrow s1$$
 (7)

Reactant

Table 14: Properties of each reactant.

Id	Name	SBO
s4	iron_in_Spleen	

Product

Table 15: Properties of each product.

Id	Name	SBO
s1	iron_in_Plasma	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = [s4] \cdot k1 \tag{8}$$

Table 16: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	$23kspl_p$	7.277	

5.5 Reaction re5

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s2 \longrightarrow s4$$
 (9)

Reactant

Table 17: Properties of each reactant.

Id	Name	SBO
s2	iron_in_Bone Marrow	

Product

Table 18: Properties of each product.

Id	Name	SBO
s4	iron_in_Spleen	

Kinetic Law

$$v_5 = [s2] \cdot k1 \tag{10}$$

Table 19: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	28kbon_spl	0.101	

5.6 Reaction re6

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s5$$
 (11)

Reactant

Table 20: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 21: Properties of each product.

Id	Name	SBO
s 5	iron_in_Liver	

Kinetic Law

$$v_6 = [\mathbf{s}1] \cdot \mathbf{k}1 \tag{12}$$

Table 22: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	4kp_liv	2.613	

5.7 Reaction re7

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s5 \longrightarrow s1$$
 (13)

Reactant

Table 23: Properties of each reactant.

Id	Name	SBO
s5	iron_in_Liver	

Product

Table 24: Properties of each product.

Id	Name	SBO
s1	iron_in_Plasma	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = [s5] \cdot k1 \tag{14}$$

Table 25: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	15kliv_p	0.138	Ø

5.8 Reaction re8

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s6$$
 (15)

Reactant

Table 26: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 27: Properties of each product.

Id	Name	SBO
s6	iron_in_Muscle	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = [\mathbf{s}1] \cdot \mathbf{k}1 \tag{16}$$

Table 28: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	8kp_mus	1.493	Ø

5.9 Reaction re9

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s6 \longrightarrow s1$$
 (17)

Reactant

Table 29: Properties of each reactant.

Id	Name	SBO
s6	iron_in_Muscle	

Product

Table 30: Properties of each product.

Id	Name	SBO
s1	iron_in_Plasma	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = [\mathbf{s6}] \cdot \mathbf{k1} \tag{18}$$

Table 31: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	18kmus_p	0.154	

5.10 Reaction re10

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s7$$
 (19)

Reactant

Table 32: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 33: Properties of each product.

Id	Name	SBO
s7	iron_in_Duodenum	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = [s1] \cdot k1 \tag{20}$$

Table 34: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	10kp_duo	0.043	Ø

5.11 Reaction re11

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s9$$
 (21)

Reactant

Table 35: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 36: Properties of each product.

Id	Name	SBO
s 9	iron_in_Intestine	

Kinetic Law

$$v_{11} = [\mathbf{s}1] \cdot \mathbf{k}1 \tag{22}$$

Table 37: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	3kp_int	0.899	

5.12 Reaction re12

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s8$$
 (23)

Reactant

Table 38: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 39: Properties of each product.

Id	Name	SBO
s 8	iron_in_Integument	

Kinetic Law

$$v_{12} = [\mathbf{s}1] \cdot \mathbf{k}1 \tag{24}$$

Table 40: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	6kp_intg	1.144	Ø

5.13 Reaction re14

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s9 \longrightarrow s10$$
 (25)

Reactant

Table 41: Properties of each reactant.

Id	Name	SBO
s9	iron_in_Intestine	

Product

Table 42: Properties of each product.

Id	Name	SBO
s10	iron_ions_Outside	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = [\mathbf{s}9] \cdot \mathbf{k}1 \tag{26}$$

Table 43: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	25kint_out	0.355	Ø

5.14 Reaction re15

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s8 \longrightarrow s10$$
 (27)

Reactant

Table 44: Properties of each reactant.

Id	Name	SBO
s8	iron_in_Integument	

Product

Table 45: Properties of each product.

Id	Name	SBO
s10	iron_ions_Outside	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = [88] \cdot k1 \tag{28}$$

Table 46: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	24_kintg_out	0.044	

5.15 Reaction re16

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s11$$
 (29)

Reactant

Table 47: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 48: Properties of each product.

Id	Name	SBO
s11	iron_in_Heart	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = [\mathbf{s}1] \cdot \mathbf{k}1 \tag{30}$$

Table 49: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	12kp_hea	0.134	

5.16 Reaction re17

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s11 \longrightarrow s1$$
 (31)

Reactant

Table 50: Properties of each reactant.

Id	Name	SBO
s11	iron_in_Heart	

Product

Table 51: Properties of each product.

Id	Name	SBO
s1	iron_in_Plasma	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = [s11] \cdot k1 \tag{32}$$

Table 52: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	21khea_p	0.077	

5.17 Reaction re18

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s12$$
 (33)

Reactant

Table 53: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 54: Properties of each product.

Id	Name	SBO
s12	iron_in_Lungs	

Kinetic Law

$$v_{17} = [\mathbf{s}1] \cdot \mathbf{k}1 \tag{34}$$

Table 55: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	9kp_lun	0.305	

5.18 Reaction re19

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s12 \longrightarrow s1$$
 (35)

Reactant

Table 56: Properties of each reactant.

Id	Name	SBO
s12	iron_in_Lungs	

Product

Table 57: Properties of each product.

Id	Name	SBO
s1	iron_in_Plasma	

Kinetic Law

$$v_{18} = [s12] \cdot k1 \tag{36}$$

Table 58: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	19klung_p	0.192	Ø

5.19 Reaction re22

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s13$$
 (37)

Reactant

Table 59: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 60: Properties of each product.

Id	Name	SBO
s13	iron_in_Kidneys	

Kinetic Law

Derived unit contains undeclared units

$$v_{19} = [s1] \cdot k1 \tag{38}$$

Table 61: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	2kp_kid	0.446	\square

5.20 Reaction re23

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s13 \longrightarrow s1$$
 (39)

Reactant

Table 62: Properties of each reactant.

Id	Name	SBO
s13	iron_in_Kidneys	

Product

Table 63: Properties of each product.

Id	Name	SBO
s1	iron_in_Plasma	

Kinetic Law

Derived unit contains undeclared units

$$v_{20} = [s13] \cdot k1 \tag{40}$$

Table 64: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	14kkid_p	0.201	

5.21 Reaction re24

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s14$$
 (41)

Reactant

Table 65: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 66: Properties of each product.

Id	Name	SBO
s14	iron_in_Testes	

Kinetic Law

Derived unit contains undeclared units

$$v_{21} = [s1] \cdot k1 \tag{42}$$

Table 67: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	13kp_tes	0.055	

5.22 Reaction re25

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s14 \longrightarrow s1$$
 (43)

Reactant

Table 68: Properties of each reactant.

Id	Name	SBO
s14	iron_in_Testes	

Product

Table 69: Properties of each product.

Id	Name	SBO
s1	iron_in_Plasma	

Kinetic Law

Derived unit contains undeclared units

$$v_{22} = [s14] \cdot k1 \tag{44}$$

Table 70: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	22ktes_p	0.093	Ø

5.23 Reaction re26

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s15$$
 (45)

Reactant

Table 71: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 72: Properties of each product.

Id	Name	SBO
s15	iron_in_Stomach	

Kinetic Law

$$v_{23} = [\mathbf{s}1] \cdot \mathbf{k}1 \tag{46}$$

Table 73: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	5kp_sto	0.121	

5.24 Reaction re28

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s16$$
 (47)

Reactant

Table 74: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 75: Properties of each product.

Id	Name	SBO
s16	iron_in_Fat	

Kinetic Law

$$v_{24} = [s1] \cdot k1 \tag{48}$$

Table 76: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	7kp_fat	0.045	

5.25 Reaction re29

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s16 \longrightarrow s1$$
 (49)

Reactant

Table 77: Properties of each reactant.

Id	Name	SBO
s16	iron_in_Fat	

Product

Table 78: Properties of each product.

Id	Name	SBO
s1	iron_in_Plasma	

Kinetic Law

Derived unit contains undeclared units

$$v_{25} = [s16] \cdot k1 \tag{50}$$

Table 79: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	17kfat₋p	0.126	

5.26 Reaction re30

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s1 \longrightarrow s17$$
 (51)

Reactant

Table 80: Properties of each reactant.

Id	Name	SBO
s1	iron_in_Plasma	

Product

Table 81: Properties of each product.

Id	Name	SBO
s17	iron_in_Brain	

Kinetic Law

Derived unit contains undeclared units

$$v_{26} = [\mathbf{s}1] \cdot \mathbf{k}1 \tag{52}$$

Table 82: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	11kp_bra	0.032	

5.27 Reaction re31

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s17 \longrightarrow s1$$
 (53)

Reactant

Table 83: Properties of each reactant.

Id	Name	SBO
s17	iron_in_Brain	

Product

Table 84: Properties of each product.

Id	Name	SBO
s1	iron_in_Plasma	

Kinetic Law

Derived unit contains undeclared units

$$v_{27} = [s17] \cdot k1 \tag{54}$$

Table 85: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	20kbra_p	0.061	

5.28 Reaction re32

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s7 \longrightarrow s1$$
 (55)

Reactant

Table 86: Properties of each reactant.

Id	Name	SBO
s7	iron_in_Duodenum	

Product

Table 87: Properties of each product.

Id	Name	SBO
s1	iron_in_Plasma	

Kinetic Law

Derived unit contains undeclared units

$$v_{28} = \mathbf{k}1 \cdot [\mathbf{s}7] \tag{56}$$

Table 88: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	26kduo_p	0.42	Ø

5.29 Reaction re33

This is an irreversible reaction of one reactant forming one product.

Reaction equation

$$s15 \longrightarrow s10$$
 (57)

Reactant

Table 89: Properties of each reactant.

Id	Name	SBO
s15	iron_in_Stomach	

Product

Table 90: Properties of each product.

Id	Name	SBO
s10	iron_ions_Outside	

Kinetic Law

$$v_{29} = k1 \cdot [s15] \tag{58}$$

Table 91: Properties of each parameter.

Id	Name	SBO Value Unit	Constant
k1	16ksto_out	0.37	

6 Derived Rate Equations

When interpreted as an ordinary differential equation framework, this model implies the following set of equations for the rates of change of each species.

Identifiers for kinetic laws highlighted in gray cannot be verified to evaluate to units of SBML substance per time. As a result, some SBML interpreters may not be able to verify the consistency of the units on quantities in the model. Please check if

- parameters without an unit definition are involved or
- volume correction is necessary because the hasOnlySubstanceUnits flag may be set to false and spacialDimensions > 0 for certain species.

6.1 Species s1

Name iron_in_Plasma

Initial amount 100 mol

Charge 0

This species takes part in 23 reactions (as a reactant in re1, re6, re8, re10, re11, re12, re16, re18, re22, re24, re26, re28, re30 and as a product in re4, re7, re9, re17, re19, re23, re25, re29, re31, re32).

$$\frac{d}{dt}s1 = v_4 + v_7 + v_9 + v_{16} + v_{18} + v_{20} + v_{22} + v_{25} + v_{27} + v_{28} - v_1 - v_6 - v_8 - v_{10} - v_{11} - v_{12} - v_{15} - v_{17} - v_{19} - v_{21} - v_{23} - v_{24} - v_{26}$$
(59)

6.2 Species s2

Name iron_in_Bone Marrow

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re2, re5 and as a product in re1).

$$\frac{\mathrm{d}}{\mathrm{d}t}s2 = |v_1| - |v_2| - |v_5| \tag{60}$$

6.3 Species s3

Name iron_in_RBC

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re3 and as a product in re2).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}3 = |v_2| - |v_3| \tag{61}$$

6.4 Species s4

Name iron_in_Spleen

Initial amount 0 mol

This species takes part in three reactions (as a reactant in re4 and as a product in re3, re5).

$$\frac{\mathrm{d}}{\mathrm{d}t}s4 = |v_3| + |v_5| - |v_4| \tag{62}$$

6.5 Species s5

Name iron_in_Liver

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re7 and as a product in re6).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}5 = |v_6| - |v_7| \tag{63}$$

6.6 Species s6

Name iron_in_Muscle

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re9 and as a product in re8).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{s}6 = |v_8| - |v_9| \tag{64}$$

6.7 Species s7

Name iron_in_Duodenum

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re32 and as a product in re10).

$$\frac{d}{dt}s7 = |v_{10}| - |v_{28}| \tag{65}$$

6.8 Species s8

Name iron_in_Integument

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re15 and as a product in re12).

$$\frac{d}{dt}s8 = |v_{12}| - |v_{14}| \tag{66}$$

6.9 Species s9

Name iron_in_Intestine

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re14 and as a product in re11).

$$\frac{d}{dt}s9 = |v_{11}| - |v_{13}| \tag{67}$$

6.10 Species s10

Name iron_ions_Outside

Initial amount 0 mol

This species takes part in three reactions (as a product in re14, re15, re33).

$$\frac{\mathrm{d}}{\mathrm{d}t}s10 = |v_{13}| + |v_{14}| + |v_{29}| \tag{68}$$

6.11 Species s11

Name iron_in_Heart

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re17 and as a product in re16).

$$\frac{d}{dt}s11 = |v_{15}| - |v_{16}| \tag{69}$$

6.12 Species s12

Name iron_in_Lungs

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re19 and as a product in re18).

$$\frac{d}{dt}s12 = |v_{17}| - |v_{18}| \tag{70}$$

6.13 Species s13

Name iron_in_Kidneys

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re23 and as a product in re22).

$$\frac{d}{dt}s13 = |v_{19}| - |v_{20}| \tag{71}$$

6.14 Species s14

Name iron_in_Testes

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re25 and as a product in re24).

$$\frac{\mathrm{d}}{\mathrm{d}t}s14 = |v_{21}| - |v_{22}| \tag{72}$$

6.15 Species s15

Name iron_in_Stomach

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re33 and as a product in re26).

$$\frac{\mathrm{d}}{\mathrm{d}t}s15 = |v_{23}| - |v_{29}| \tag{73}$$

6.16 Species s16

Name iron_in_Fat

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re29 and as a product in re28).

$$\frac{\mathrm{d}}{\mathrm{d}t}s16 = |v_{24}| - |v_{25}| \tag{74}$$

6.17 Species s17

Name iron_in_Brain

Initial amount 0 mol

This species takes part in two reactions (as a reactant in re31 and as a product in re30).

$$\frac{\mathrm{d}}{\mathrm{d}t}s17 = |v_{26}| - |v_{27}| \tag{75}$$

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