SBML Model Report

Model name: "Begitt2014 - STAT1 cooperative DNA binding - single GAS polymer model"

May 5, 2016

1 General Overview

This is a document in SBML Level 2 Version 4 format. This model was created by the following three authors: Nick Juty[1], Vijayalakshmi Chelliah[2] and Michelle Baker[3] at January seventh 2014 at 4:30 p. m. and last time modified at October nineth 2014 at 4:07 p. m. Table 1 provides 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	14
events	0	constraints	0
reactions	18	function definitions	18
global parameters	7	unit definitions	0
rules	1	initial assignments	0

Model Notes

Begitt2014 - STAT1 cooperative DNA binding - single GAS polymer model

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The importance of STAT1-cooperative DNA binding in type 1 and type 2 interferon signalling has been studies using experimental and modelling approaches. The authors have developed two ODE models to describe STAT1 binding to short promoter regions of DNA, namely „single GAS polymer model„ and „double GAS polymer model„ considering binding to single or double GAS sites, respectively. The length of DNA in the single GAS model was three sites and four sites in double GAS model. This model correspond to the „single GAS polymer model„.

This model is described in the article:STAT1-cooperative DNA binding distinguishes type 1 from type 2 interferon signaling.Begitt A, Droescher M, Meyer T, Schmid CD, Baker M, Antunes F, Owen MR, Naumann R, Decker T, Vinkemeier UNat Immunol. 2014 Feb;15(2):168-76.

Abstract:

STAT1 is an indispensable component of a heterotrimer (ISGF3) and a STAT1 homodimer (GAF) that function as transcription regulators in type 1 and type 2 interferon signaling, respectively. To investigate the importance of STAT1-cooperative DNA binding, we generated gene-targeted mice expressing cooperativity-deficient STAT1 with alanine substituted for Phe77. Neither ISGF3 nor GAF bound DNA cooperatively in the STAT1F77A mouse strain, but type 1 and type 2 interferon responses were affected differently. Type 2 interferon-mediated transcription and antibacterial immunity essentially disappeared owing to defective promoter recruitment of GAF. In contrast, STAT1 recruitment to ISGF3 binding sites and type 1 interferon-dependent responses, including antiviral protection, remained intact. We conclude that STAT1 cooperativity is essential for its biological activity and underlies the cellular responses to type 2, but not type 1 interferon.

This model is hosted on BioModels Database and identifiedby: BIOMD0000000500 .

To cite BioModels Database, please use: BioModels Database: An enhanced, curated and annotated resourcefor published quantitative kinetic models .

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 l

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`	default		3	1	litre	☑	
`nucleus`	nucleus		3	1	litre	☑	

3.1 Compartment `default`

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

Name default

3.2 Compartment `nucleus`

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

Name nucleus

4 Species

This model contains 14 species. Section 9 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 Condition
S1	S1	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_000	DNA_000	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_100	DNA_100	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_010	DNA_010	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_001	DNA_001	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_110	DNA_110	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_101	DNA_101	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_011	DNA_011	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_111	DNA_111	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_1B10	DNA_1B10	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_01B1	DNA_01B1	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_1B11	DNA_1B11	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_11B1	DNA_11B1	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟
DNA_1B1B1	DNA_1B1B1	nucleus	$\mathrm{mol} \cdot \mathrm{l}^{-1}$	⊟	⊟

5 Parameters

This model contains seven global parameters.

Table 4: Properties of each parameter.

Id	Name	SBO	Value	Unit	Constant
Kon_P1	Kon_P1	0000341	60000.000		☑
Koff_P1	Koff_P1	0000338	100.000		☑
Kon_G1	Kon_G1	0000341	$2 \cdot 10^{10}$		☑
Koff_G1	Koff_G1	0000338	100.000		☑
Kon_NG1	Kon_NG1	0000341	$2 \cdot 10^{10}$		☑
Koff_NG1	Koff_NG1	0000338	20000.000		☑
parameter_1	GAS-_siteOccupancy	0000540	0.000		⊟

6 Function definitions

This is an overview of 18 function definitions.

6.1 Function definition function_4_DNA1

Name function_4_DNA1

Arguments [DNA_000], [DNA_100], Koff_NG1, Kon_NG1, [S1], vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_NG1} \cdot [\text{DNA\_000}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_100}]}{\text{vol}\,(\text{nucleus})} \tag{1}$$

6.2 Function definition function_4_DNA50

Name function_4_DNA50

Arguments [DNA_011], [DNA_01B1], Koff_P1, Kon_P1, vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_P1} \cdot [\text{DNA\_011}] - \text{Koff\_P1} \cdot [\text{DNA\_01B1}]}{\text{vol}\,(\text{nucleus})} \tag{2}$$

6.3 Function definition function_4_DNA3

Name function_4_DNA3

Arguments [DNA_000], [DNA_001], Koff_NG1, Kon_NG1, [S1], vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_NG1} \cdot [\text{DNA\_000}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_001}]}{\text{vol}\,(\text{nucleus})} \tag{3}$$

6.4 Function definition function_4_DNA53

Name function_4_DNA53

Arguments [DNA_11B1], [DNA_1B1B1], Koff_P1, Kon_P1, vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_P1} \cdot [\text{DNA\_11B1}] - \text{Koff\_P1} \cdot [\text{DNA\_1B1B1}]}{\text{vol}\,(\text{nucleus})} \tag{4}$$

6.5 Function definition function_4_DNA54

Name function_4_DNA54

Arguments [DNA_1B11], [DNA_1B1B1], Koff_P1, Kon_P1, vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_P1} \cdot [\text{DNA\_1B11}] - \text{Koff\_P1} \cdot [\text{DNA\_1B1B1}]}{\text{vol}\,(\text{nucleus})} \tag{5}$$

6.6 Function definition function_4_DNA2

Name function_4_DNA2

Arguments [DNA_000], [DNA_010], Koff_G1, Kon_G1, [S1], vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_G1} \cdot [\text{DNA\_000}] \cdot [\text{S1}] - \text{Koff\_G1} \cdot [\text{DNA\_010}]}{\text{vol}\,(\text{nucleus})} \tag{6}$$

6.7 Function definition function_4_DNA4

Name function_4_DNA4

Arguments [DNA_100], [DNA_110], Koff_G1, Kon_G1, [S1], vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_G1} \cdot [\text{DNA\_100}] \cdot [\text{S1}] - \text{Koff\_G1} \cdot [\text{DNA\_110}]}{\text{vol}\,(\text{nucleus})} \tag{7}$$

6.8 Function definition function_4_DNA51

Name function_4_DNA51

Arguments [DNA_111], [DNA_11B1], Koff_P1, Kon_P1, vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_P1} \cdot [\text{DNA\_111}] - \text{Koff\_P1} \cdot [\text{DNA\_11B1}]}{\text{vol}\,(\text{nucleus})} \tag{8}$$

6.9 Function definition function_4_DNA12

Name function_4_DNA12

Arguments [DNA_011], [DNA_111], Koff_NG1, Kon_NG1, [S1], vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_NG1} \cdot [\text{DNA\_011}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_111}]}{\text{vol}\,(\text{nucleus})} \tag{9}$$

6.10 Function definition function_4_DNA9

Name function_4_DNA9

Arguments [DNA_001], [DNA_011], Koff_G1, Kon_G1, [S1], vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_G1} \cdot [\text{DNA\_001}] \cdot [\text{S1}] - \text{Koff\_G1} \cdot [\text{DNA\_011}]}{\text{vol}\,(\text{nucleus})} \tag{10}$$

6.11 Function definition function_4_DNA52

Name function_4_DNA52

Arguments [DNA_111], [DNA_1B11], Koff_P1, Kon_P1, vol(nucleus)

Mathematical Expression

$$\frac{\text{Kon\_P1} \cdot [\text{DNA\_111}] - \text{Koff\_P1} \cdot [\text{DNA\_1B11}]}{\text{vol}(\text{nucleus})} \tag{11}$$

6.12 Function definition function_4_DNA6

Name function_4_DNA6

Arguments [DNA_010], [DNA_110], Koff_NG1, Kon_NG1, [S1], vol(nucleus)

Mathematical Expression

$$\frac{\text{Kon\_NG1} \cdot [\text{DNA\_010}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_110}]}{\text{vol}(\text{nucleus})} \tag{12}$$

6.13 Function definition function_4_DNA49

Name function_4_DNA49

Arguments [DNA_110], [DNA_1B10], Koff_P1, Kon_P1, vol(nucleus)

Mathematical Expression

$$\frac{\text{Kon\_P1} \cdot [\text{DNA\_110}] - \text{Koff\_P1} \cdot [\text{DNA\_1B10}]}{\text{vol}(\text{nucleus})} \tag{13}$$

6.14 Function definition function_4_DNA8

Name function_4_DNA8

Arguments [DNA_001], [DNA_101], Koff_NG1, Kon_NG1, [S1], vol(nucleus)

Mathematical Expression

$$\frac{\text{Kon\_NG1} \cdot [\text{DNA\_001}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_101}]}{\text{vol}(\text{nucleus})} \tag{14}$$

6.15 Function definition function_4_DNA7

Name function_4_DNA7

Arguments [DNA_010], [DNA_011], Koff_NG1, Kon_NG1, [S1], vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_NG1} \cdot [\text{DNA\_010}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_011}]}{\text{vol}\,(\text{nucleus})} \tag{15}$$

6.16 Function definition function_4_DNA10

Name function_4_DNA10

Arguments [DNA_110], [DNA_111], Koff_NG1, Kon_NG1, [S1], vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_NG1} \cdot [\text{DNA\_110}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_111}]}{\text{vol}\,(\text{nucleus})} \tag{16}$$

6.17 Function definition function_4_DNA11

Name function_4_DNA11

Arguments [DNA_101], [DNA_111], Koff_G1, Kon_G1, [S1], vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_G1} \cdot [\text{DNA\_101}] \cdot [\text{S1}] - \text{Koff\_G1} \cdot [\text{DNA\_111}]}{\text{vol}\,(\text{nucleus})} \tag{17}$$

6.18 Function definition function_4_DNA5

Name function_4_DNA5

Arguments [DNA_100], [DNA_101], Koff_NG1, Kon_NG1, [S1], vol (nucleus)

Mathematical Expression

$$\frac{\text{Kon\_NG1} \cdot [\text{DNA\_100}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_101}]}{\text{vol}\,(\text{nucleus})} \tag{18}$$

7 Rule

This is an overview of one rule.

7.1 Rule parameter_1

Rule parameter_1 is an assignment rule for parameter parameter_1:

$$\begin{aligned} \text{parameter\_1} = {} & [\text{DNA\_010}] + [\text{DNA\_011}] + [\text{DNA\_110}] + [\text{DNA\_111}] + [\text{DNA\_01B1}] \\ & + [\text{DNA\_1B10}] + [\text{DNA\_1B11}] + [\text{DNA\_11B1}] + [\text{DNA\_1B1B1}] \end{aligned} \tag{19}$$

Derived unit $\text{mol} \cdot \text{l}^{-1}$

8 Reactions

This model contains 18 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 5: Overview of all reactions

№	Id	Name	Reaction Equation	SBO
1	DNA1	DNA1	$\mathrm{DNA\_000} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_000,\ DNA\_100,\ S1}} \mathrm{DNA\_100}$	
2	DNA2	DNA2	$\mathrm{DNA\_000} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_000,\ DNA\_010,\ S1}} \mathrm{DNA\_010}$	
3	DNA3	DNA3	$\mathrm{DNA\_000} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_000,\ DNA\_001,\ S1}} \mathrm{DNA\_001}$	
4	DNA4	DNA4	$\mathrm{DNA\_100} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_100,\ DNA\_110,\ S1}} \mathrm{DNA\_110}$	
5	DNA5	DNA5	$\mathrm{DNA\_100} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_100,\ DNA\_101,\ S1}} \mathrm{DNA\_101}$	
6	DNA6	DNA6	$\mathrm{DNA\_010} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_010,\ DNA\_110,\ S1}} \mathrm{DNA\_110}$	
7	DNA7	DNA7	$\mathrm{DNA\_010} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_010,\ DNA\_011,\ S1}} \mathrm{DNA\_011}$	
8	DNA8	DNA8	$\mathrm{DNA\_001} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_001,\ DNA\_101,\ S1}} \mathrm{DNA\_101}$	
9	DNA9	DNA9	$\mathrm{DNA\_001} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_001,\ DNA\_011,\ S1}} \mathrm{DNA\_011}$	
10	DNA10	DNA10	$\mathrm{DNA\_110} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_110,\ DNA\_111,\ S1}} \mathrm{DNA\_111}$	
11	DNA11	DNA11	$\mathrm{DNA\_101} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_101,\ DNA\_111,\ S1}} \mathrm{DNA\_111}$	
12	DNA12	DNA12	$\mathrm{DNA\_011} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_011,\ DNA\_111,\ S1}} \mathrm{DNA\_111}$	
13	DNA49	DNA49	$\mathrm{DNA\_110} \xrightleftharpoons{\mathrm{DNA\_110,\ DNA\_1B10}} \mathrm{DNA\_1B10}$	
14	DNA50	DNA50	$\mathrm{DNA\_011} \xrightleftharpoons{\mathrm{DNA\_011,\ DNA\_01B1}} \mathrm{DNA\_01B1}$	
15	DNA51	DNA51	$\mathrm{DNA\_111} \xrightleftharpoons{\mathrm{DNA\_111,\ DNA\_11B1}} \mathrm{DNA\_11B1}$	

№	Id	Name	Reaction Equation	SBO
16	DNA52	DNA52	DNA_111 $\overset{\text{DNA\_111, DNA\_1B11}}{\rightleftharpoons}$ DNA_1B11	
17	DNA53	DNA53	DNA_11B1 $\overset{\text{DNA\_11B1, DNA\_1B1B1}}{\rightleftharpoons}$ DNA_1B1B1	
18	DNA54	DNA54	DNA_1B11 $\overset{\text{DNA\_1B11, DNA\_1B1B1}}{\rightleftharpoons}$ DNA_1B1B1	

8.1 Reaction DNA1

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA1

Reaction equation

$$\mathrm{DNA\_000} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_000,\ DNA\_100,\ S1}} \mathrm{DNA\_100} \tag{20}$$

Reactants

Table 6: Properties of each reactant.

Id	Name	SBO
DNA_000	DNA_000	
S1	S1	

Modifiers

Table 7: Properties of each modifier.

Id	Name	SBO
DNA_000	DNA_000	
DNA_100	DNA_100	
S1	S1	

Product

Table 8: Properties of each product.

Id	Name	SBO
DNA_100	DNA_100	

Kinetic Law

Derived unit contains undeclared units

$$v_1 = \mathrm{vol}\left(\mathrm{nucleus}\right) \cdot \mathrm{function\_4\_DNA1}\left(\left[\mathrm{DNA\_000}\right], \left[\mathrm{DNA\_100}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \tag{21}$$

$$\begin{aligned}&\text{function\_4\_DNA1}\left([\text{DNA\_000}], [\text{DNA\_100}], \text{Koff\_NG1}, \text{Kon\_NG1}, [\text{S1}], \text{vol}\left(\text{nucleus}\right)\right)\\ &= \frac{\text{Kon\_NG1} \cdot [\text{DNA\_000}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_100}]}{\text{vol}\left(\text{nucleus}\right)}\end{aligned} \tag{22}$$

$$\begin{aligned}&\text{function\_4\_DNA1}\left([\text{DNA\_000}], [\text{DNA\_100}], \text{Koff\_NG1}, \text{Kon\_NG1}, [\text{S1}], \text{vol}\left(\text{nucleus}\right)\right)\\ &= \frac{\text{Kon\_NG1} \cdot [\text{DNA\_000}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_100}]}{\text{vol}\left(\text{nucleus}\right)}\end{aligned} \tag{23}$$

8.2 Reaction DNA2

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA2

Reaction equation

$$\text{DNA\_000} + \text{S1} \xrightleftharpoons{\text{DNA\_000, DNA\_010, S1}} \text{DNA\_010} \tag{24}$$

Reactants

Table 9: Properties of each reactant.

Id	Name	SBO
DNA_000	DNA_000	
S1	S1	

Modifiers

Table 10: Properties of each modifier.

Id	Name	SBO
DNA_000	DNA_000	
DNA_010	DNA_010	
S1	S1	

Product

Table 11: Properties of each product.

Id	Name	SBO
DNA_010	DNA_010	

Kinetic Law

Derived unit contains undeclared units

$$v_2 = \mathrm{vol}\,(\mathrm{nucleus}) \cdot \mathrm{function\_4\_DNA2}\,([\mathrm{DNA\_000}], [\mathrm{DNA\_010}], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) \tag{25}$$

$$\mathrm{function\_4\_DNA2}\,([\mathrm{DNA\_000}], [\mathrm{DNA\_010}], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_G1} \cdot [\mathrm{DNA\_000}] \cdot [\mathrm{S1}] - \mathrm{Koff\_G1} \cdot [\mathrm{DNA\_010}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{26}$$

$$\mathrm{function\_4\_DNA2}\,([\mathrm{DNA\_000}], [\mathrm{DNA\_010}], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_G1} \cdot [\mathrm{DNA\_000}] \cdot [\mathrm{S1}] - \mathrm{Koff\_G1} \cdot [\mathrm{DNA\_010}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{27}$$

8.3 Reaction DNA3

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA3

Reaction equation

$$\mathrm{DNA\_000} + \mathrm{S1} \underset{}{\overset{\mathrm{DNA\_000,\ DNA\_001,\ S1}}{\rightleftharpoons}} \mathrm{DNA\_001} \tag{28}$$

Reactants

Table 12: Properties of each reactant.

Id	Name	SBO
DNA_000	DNA_000	
S1	S1	

Modifiers

Table 13: Properties of each modifier.

Id	Name	SBO
DNA_000	DNA_000	
DNA_001	DNA_001	
S1	S1	

Product

Table 14: Properties of each product.

Id	Name	SBO
DNA_001	DNA_001	

Kinetic Law

Derived unit contains undeclared units

$$v_3 = \mathrm{vol}\left(\mathrm{nucleus}\right) \cdot \mathrm{function\_4\_DNA3}\left(\left[\mathrm{DNA\_000}\right], \left[\mathrm{DNA\_001}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \tag{29}$$

$$\mathrm{function\_4\_DNA3}\left(\left[\mathrm{DNA\_000}\right], \left[\mathrm{DNA\_001}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) = \frac{\mathrm{Kon\_NG1} \cdot \left[\mathrm{DNA\_000}\right] \cdot \left[\mathrm{S1}\right] - \mathrm{Koff\_NG1} \cdot \left[\mathrm{DNA\_001}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \tag{30}$$

$$\mathrm{function\_4\_DNA3}\left(\left[\mathrm{DNA\_000}\right], \left[\mathrm{DNA\_001}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) = \frac{\mathrm{Kon\_NG1} \cdot \left[\mathrm{DNA\_000}\right] \cdot \left[\mathrm{S1}\right] - \mathrm{Koff\_NG1} \cdot \left[\mathrm{DNA\_001}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \tag{31}$$

8.4 Reaction DNA4

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA4

Reaction equation

$$\mathrm{DNA\_100} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_100,\ DNA\_110,\ S1}} \mathrm{DNA\_110} \tag{32}$$

Reactants

Table 15: Properties of each reactant.

Id	Name	SBO
DNA_100	DNA_100	
S1	S1	

Modifiers

Table 16: Properties of each modifier.

Id	Name	SBO
DNA_100	DNA_100	
DNA_110	DNA_110	
S1	S1	

Product

Table 17: Properties of each product.

Id	Name	SBO
DNA_110	DNA_110	

Kinetic Law

Derived unit contains undeclared units

$$v_4 = \mathrm{vol}\left(\mathrm{nucleus}\right) \cdot \mathrm{function\_4\_DNA4}\left(\left[\mathrm{DNA\_100}\right], \left[\mathrm{DNA\_110}\right], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \tag{33}$$

$$\mathrm{function\_4\_DNA4}\left(\left[\mathrm{DNA\_100}\right], \left[\mathrm{DNA\_110}\right], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) = \frac{\mathrm{Kon\_G1} \cdot \left[\mathrm{DNA\_100}\right] \cdot \left[\mathrm{S1}\right] - \mathrm{Koff\_G1} \cdot \left[\mathrm{DNA\_110}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \tag{34}$$

$$\mathrm{function\_4\_DNA4}\left(\left[\mathrm{DNA\_100}\right], \left[\mathrm{DNA\_110}\right], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) = \frac{\mathrm{Kon\_G1} \cdot \left[\mathrm{DNA\_100}\right] \cdot \left[\mathrm{S1}\right] - \mathrm{Koff\_G1} \cdot \left[\mathrm{DNA\_110}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \tag{35}$$

8.5 Reaction DNA5

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA5

Reaction equation

$$\mathrm{DNA\_100} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_100,\ DNA\_101,\ S1}} \mathrm{DNA\_101} \tag{36}$$

Reactants

Table 18: Properties of each reactant.

Id	Name	SBO
DNA_100	DNA_100	
S1	S1	

Modifiers

Table 19: Properties of each modifier.

Id	Name	SBO
DNA_100	DNA_100	
DNA_101	DNA_101	
S1	S1	

Product

Table 20: Properties of each product.

Id	Name	SBO
DNA_101	DNA_101	

Kinetic Law

Derived unit contains undeclared units

$$v_5 = \mathrm{vol}\left(\mathrm{nucleus}\right) \cdot \mathrm{function\_4\_DNA5}\left(\left[\mathrm{DNA\_100}\right], \left[\mathrm{DNA\_101}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \tag{37}$$

$$\begin{aligned} &\mathrm{function\_4\_DNA5}\left(\left[\mathrm{DNA\_100}\right], \left[\mathrm{DNA\_101}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \\ &= \frac{\mathrm{Kon\_NG1} \cdot \left[\mathrm{DNA\_100}\right] \cdot \left[\mathrm{S1}\right] - \mathrm{Koff\_NG1} \cdot \left[\mathrm{DNA\_101}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \end{aligned} \tag{38}$$

$$\begin{aligned}&\text{function\_4\_DNA5}\left([\text{DNA\_100}], [\text{DNA\_101}], \text{Koff\_NG1}, \text{Kon\_NG1}, [\text{S1}], \text{vol}\left(\text{nucleus}\right)\right)\\ &= \frac{\text{Kon\_NG1} \cdot [\text{DNA\_100}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_101}]}{\text{vol}\left(\text{nucleus}\right)}\end{aligned} \tag{39}$$

8.6 Reaction DNA6

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA6

Reaction equation

$$\text{DNA\_010} + \text{S1} \overset{\text{DNA\_010, DNA\_110, S1}}{\rightleftharpoons} \text{DNA\_110} \tag{40}$$

Reactants

Table 21: Properties of each reactant.

Id	Name	SBO
DNA_010	DNA_010	
S1	S1	

Modifiers

Table 22: Properties of each modifier.

Id	Name	SBO
DNA_010	DNA_010	
DNA_110	DNA_110	
S1	S1	

Product

Table 23: Properties of each product.

Id	Name	SBO
DNA_110	DNA_110	

Kinetic Law

Derived unit contains undeclared units

$$v_6 = \mathrm{vol}\,(\mathrm{nucleus}) \cdot \mathrm{function\_4\_DNA6}\,([\mathrm{DNA\_010}], [\mathrm{DNA\_110}], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) \tag{41}$$

$$\mathrm{function\_4\_DNA6}\,([\mathrm{DNA\_010}], [\mathrm{DNA\_110}], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_NG1} \cdot [\mathrm{DNA\_010}] \cdot [\mathrm{S1}] - \mathrm{Koff\_NG1} \cdot [\mathrm{DNA\_110}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{42}$$

$$\mathrm{function\_4\_DNA6}\,([\mathrm{DNA\_010}], [\mathrm{DNA\_110}], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_NG1} \cdot [\mathrm{DNA\_010}] \cdot [\mathrm{S1}] - \mathrm{Koff\_NG1} \cdot [\mathrm{DNA\_110}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{43}$$

8.7 Reaction DNA7

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA7

Reaction equation

$$\mathrm{DNA\_010} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_010,\ DNA\_011,\ S1}} \mathrm{DNA\_011} \tag{44}$$

Reactants

Table 24: Properties of each reactant.

Id	Name	SBO
DNA_010	DNA_010	
S1	S1	

Modifiers

Table 25: Properties of each modifier.

Id	Name	SBO
DNA_010	DNA_010	
DNA_011	DNA_011	
S1	S1	

Product

Table 26: Properties of each product.

Id	Name	SBO
DNA_011	DNA_011	

Kinetic Law

Derived unit contains undeclared units

$$v_7 = \mathrm{vol}\,(\mathrm{nucleus}) \cdot \mathrm{function\_4\_DNA7}\,([\mathrm{DNA\_010}], [\mathrm{DNA\_011}], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) \tag{45}$$

$$\mathrm{function\_4\_DNA7}\,([\mathrm{DNA\_010}], [\mathrm{DNA\_011}], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_NG1} \cdot [\mathrm{DNA\_010}] \cdot [\mathrm{S1}] - \mathrm{Koff\_NG1} \cdot [\mathrm{DNA\_011}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{46}$$

$$\mathrm{function\_4\_DNA7}\,([\mathrm{DNA\_010}], [\mathrm{DNA\_011}], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_NG1} \cdot [\mathrm{DNA\_010}] \cdot [\mathrm{S1}] - \mathrm{Koff\_NG1} \cdot [\mathrm{DNA\_011}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{47}$$

8.8 Reaction DNA8

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA8

Reaction equation

$$\mathrm{DNA\_001} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_001,\ DNA\_101,\ S1}} \mathrm{DNA\_101} \tag{48}$$

Reactants

Table 27: Properties of each reactant.

Id	Name	SBO
DNA_001	DNA_001	
S1	S1	

Modifiers

Table 28: Properties of each modifier.

Id	Name	SBO
DNA_001	DNA_001	
DNA_101	DNA_101	
S1	S1	

Product

Table 29: Properties of each product.

Id	Name	SBO
DNA_101	DNA_101	

Kinetic Law

Derived unit contains undeclared units

$$v_8 = \mathrm{vol}\left(\mathrm{nucleus}\right) \cdot \mathrm{function\_4\_DNA8}\left(\left[\mathrm{DNA\_001}\right], \left[\mathrm{DNA\_101}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \tag{49}$$

$$\mathrm{function\_4\_DNA8}\left(\left[\mathrm{DNA\_001}\right], \left[\mathrm{DNA\_101}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) = \frac{\mathrm{Kon\_NG1} \cdot \left[\mathrm{DNA\_001}\right] \cdot \left[\mathrm{S1}\right] - \mathrm{Koff\_NG1} \cdot \left[\mathrm{DNA\_101}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \tag{50}$$

$$\mathrm{function\_4\_DNA8}\left(\left[\mathrm{DNA\_001}\right], \left[\mathrm{DNA\_101}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) = \frac{\mathrm{Kon\_NG1} \cdot \left[\mathrm{DNA\_001}\right] \cdot \left[\mathrm{S1}\right] - \mathrm{Koff\_NG1} \cdot \left[\mathrm{DNA\_101}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \tag{51}$$

8.9 Reaction DNA9

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA9

Reaction equation

$$\mathrm{DNA\_001} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_001,\ DNA\_011,\ S1}} \mathrm{DNA\_011} \tag{52}$$

Reactants

Table 30: Properties of each reactant.

Id	Name	SBO
DNA_001	DNA_001	
S1	S1	

Modifiers

Table 31: Properties of each modifier.

Id	Name	SBO
DNA_001	DNA_001	
DNA_011	DNA_011	
S1	S1	

Product

Table 32: Properties of each product.

Id	Name	SBO
DNA_011	DNA_011	

Kinetic Law

Derived unit contains undeclared units

$$v_9 = \mathrm{vol}\left(\mathrm{nucleus}\right) \cdot \mathrm{function\_4\_DNA9}\left(\left[\mathrm{DNA\_001}\right], \left[\mathrm{DNA\_011}\right], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \tag{53}$$

$$\mathrm{function\_4\_DNA9}\left(\left[\mathrm{DNA\_001}\right], \left[\mathrm{DNA\_011}\right], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) = \frac{\mathrm{Kon\_G1} \cdot \left[\mathrm{DNA\_001}\right] \cdot \left[\mathrm{S1}\right] - \mathrm{Koff\_G1} \cdot \left[\mathrm{DNA\_011}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \tag{54}$$

$$\mathrm{function\_4\_DNA9}\left(\left[\mathrm{DNA\_001}\right], \left[\mathrm{DNA\_011}\right], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) = \frac{\mathrm{Kon\_G1} \cdot \left[\mathrm{DNA\_001}\right] \cdot \left[\mathrm{S1}\right] - \mathrm{Koff\_G1} \cdot \left[\mathrm{DNA\_011}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \tag{55}$$

8.10 Reaction DNA10

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA10

Reaction equation

$$\mathrm{DNA\_110} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_110,\ DNA\_111,\ S1}} \mathrm{DNA\_111} \tag{56}$$

Reactants

Table 33: Properties of each reactant.

Id	Name	SBO
DNA_110	DNA_110	
S1	S1	

Modifiers

Table 34: Properties of each modifier.

Id	Name	SBO
DNA_110	DNA_110	
DNA_111	DNA_111	
S1	S1	

Product

Table 35: Properties of each product.

Id	Name	SBO
DNA_111	DNA_111	

Kinetic Law

Derived unit contains undeclared units

$$v_{10} = \mathrm{vol}\left(\mathrm{nucleus}\right) \cdot \mathrm{function\_4\_DNA10}\left(\left[\mathrm{DNA\_110}\right], \left[\mathrm{DNA\_111}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \tag{57}$$

$$\begin{aligned} &\mathrm{function\_4\_DNA10}\left(\left[\mathrm{DNA\_110}\right], \left[\mathrm{DNA\_111}\right], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, \left[\mathrm{S1}\right], \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \\ &= \frac{\mathrm{Kon\_NG1} \cdot \left[\mathrm{DNA\_110}\right] \cdot \left[\mathrm{S1}\right] - \mathrm{Koff\_NG1} \cdot \left[\mathrm{DNA\_111}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \end{aligned} \tag{58}$$

$$\begin{aligned}&\text{function\_4\_DNA10}\left([\text{DNA\_110}], [\text{DNA\_111}], \text{Koff\_NG1}, \text{Kon\_NG1}, [\text{S1}], \text{vol}\left(\text{nucleus}\right)\right)\\ &= \frac{\text{Kon\_NG1} \cdot [\text{DNA\_110}] \cdot [\text{S1}] - \text{Koff\_NG1} \cdot [\text{DNA\_111}]}{\text{vol}\left(\text{nucleus}\right)}\end{aligned} \tag{59}$$

8.11 Reaction DNA11

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA11

Reaction equation

$$\text{DNA\_101} + \text{S1} \overset{\text{DNA\_101, DNA\_111, S1}}{\rightleftharpoons} \text{DNA\_111} \tag{60}$$

Reactants

Table 36: Properties of each reactant.

Id	Name	SBO
DNA_101	DNA_101	
S1	S1	

Modifiers

Table 37: Properties of each modifier.

Id	Name	SBO
DNA_101	DNA_101	
DNA_111	DNA_111	
S1	S1	

Product

Table 38: Properties of each product.

Id	Name	SBO
DNA_111	DNA_111	

Kinetic Law

Derived unit contains undeclared units

$$v_{11} = \mathrm{vol}\,(\mathrm{nucleus}) \cdot \mathrm{function\_4\_DNA11}\,([\mathrm{DNA\_101}], [\mathrm{DNA\_111}], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) \tag{61}$$

$$\mathrm{function\_4\_DNA11}\,([\mathrm{DNA\_101}], [\mathrm{DNA\_111}], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_G1} \cdot [\mathrm{DNA\_101}] \cdot [\mathrm{S1}] - \mathrm{Koff\_G1} \cdot [\mathrm{DNA\_111}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{62}$$

$$\mathrm{function\_4\_DNA11}\,([\mathrm{DNA\_101}], [\mathrm{DNA\_111}], \mathrm{Koff\_G1}, \mathrm{Kon\_G1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_G1} \cdot [\mathrm{DNA\_101}] \cdot [\mathrm{S1}] - \mathrm{Koff\_G1} \cdot [\mathrm{DNA\_111}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{63}$$

8.12 Reaction DNA12

This is a reversible reaction of two reactants forming one product influenced by three modifiers.

Name DNA12

Reaction equation

$$\mathrm{DNA\_011} + \mathrm{S1} \xrightleftharpoons{\mathrm{DNA\_011},\ \mathrm{DNA\_111},\ \mathrm{S1}} \mathrm{DNA\_111} \tag{64}$$

Reactants

Table 39: Properties of each reactant.

Id	Name	SBO
DNA_011	DNA_011	
S1	S1	

Modifiers

Table 40: Properties of each modifier.

Id	Name	SBO
DNA_011	DNA_011	
DNA_111	DNA_111	
S1	S1	

Product

Table 41: Properties of each product.

Id	Name	SBO
DNA_111	DNA_111	

Kinetic Law

Derived unit contains undeclared units

$$v_{12} = \mathrm{vol}\,(\mathrm{nucleus}) \cdot \mathrm{function\_4\_DNA12}\,([\mathrm{DNA\_011}], [\mathrm{DNA\_111}], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) \tag{65}$$

$$\mathrm{function\_4\_DNA12}\,([\mathrm{DNA\_011}], [\mathrm{DNA\_111}], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_NG1} \cdot [\mathrm{DNA\_011}] \cdot [\mathrm{S1}] - \mathrm{Koff\_NG1} \cdot [\mathrm{DNA\_111}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{66}$$

$$\mathrm{function\_4\_DNA12}\,([\mathrm{DNA\_011}], [\mathrm{DNA\_111}], \mathrm{Koff\_NG1}, \mathrm{Kon\_NG1}, [\mathrm{S1}], \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_NG1} \cdot [\mathrm{DNA\_011}] \cdot [\mathrm{S1}] - \mathrm{Koff\_NG1} \cdot [\mathrm{DNA\_111}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{67}$$

8.13 Reaction DNA49

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name DNA49

Reaction equation

$$\mathrm{DNA\_110} \underset{\text{DNA\_110, DNA\_1B10}}{\rightleftharpoons} \mathrm{DNA\_1B10} \tag{68}$$

Reactant

Table 42: Properties of each reactant.

Id	Name	SBO
DNA_110	DNA_110	

Modifiers

Table 43: Properties of each modifier.

Id	Name	SBO
DNA_110	DNA_110	
DNA_1B10	DNA_1B10	

Product

Table 44: Properties of each product.

Id	Name	SBO
DNA_1B10	DNA_1B10	

Kinetic Law

Derived unit contains undeclared units

$$v_{13} = \mathrm{vol}(\mathrm{nucleus}) \cdot \mathrm{function\_4\_DNA49}([\mathrm{DNA\_110}], [\mathrm{DNA\_1B10}], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}(\mathrm{nucleus})) \tag{69}$$

$$\mathrm{function\_4\_DNA49}([\mathrm{DNA\_110}], [\mathrm{DNA\_1B10}], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}(\mathrm{nucleus})) = \frac{\mathrm{Kon\_P1} \cdot [\mathrm{DNA\_110}] - \mathrm{Koff\_P1} \cdot [\mathrm{DNA\_1B10}]}{\mathrm{vol}(\mathrm{nucleus})} \tag{70}$$

$$\mathrm{function\_4\_DNA49}([\mathrm{DNA\_110}], [\mathrm{DNA\_1B10}], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}(\mathrm{nucleus})) = \frac{\mathrm{Kon\_P1} \cdot [\mathrm{DNA\_110}] - \mathrm{Koff\_P1} \cdot [\mathrm{DNA\_1B10}]}{\mathrm{vol}(\mathrm{nucleus})} \tag{71}$$

8.14 Reaction DNA50

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name DNA50

Reaction equation

$$\mathrm{DNA\_011} \xrightleftharpoons{\mathrm{DNA\_011,\ DNA\_01B1}} \mathrm{DNA\_01B1} \tag{72}$$

Reactant

Table 45: Properties of each reactant.

Id	Name	SBO
DNA_011	DNA_011	

Modifiers

Table 46: Properties of each modifier.

Id	Name	SBO
DNA_011	DNA_011	
DNA_01B1	DNA_01B1	

Product

Table 47: Properties of each product.

Id	Name	SBO
DNA_01B1	DNA_01B1	

Kinetic Law

Derived unit contains undeclared units

$$v_{14} = \mathrm{vol}(\mathrm{nucleus}) \cdot \mathrm{function\_4\_DNA50}([\mathrm{DNA\_011}], [\mathrm{DNA\_01B1}], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}(\mathrm{nucleus})) \tag{73}$$

$$\begin{aligned} &\mathrm{function\_4\_DNA50}([\mathrm{DNA\_011}], [\mathrm{DNA\_01B1}], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}(\mathrm{nucleus})) \\ &= \frac{\mathrm{Kon\_P1} \cdot [\mathrm{DNA\_011}] - \mathrm{Koff\_P1} \cdot [\mathrm{DNA\_01B1}]}{\mathrm{vol}(\mathrm{nucleus})} \end{aligned} \tag{74}$$

$$\begin{aligned} &\mathrm{function\_4\_DNA50}([\mathrm{DNA\_011}], [\mathrm{DNA\_01B1}], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}(\mathrm{nucleus})) \\ &= \frac{\mathrm{Kon\_P1} \cdot [\mathrm{DNA\_011}] - \mathrm{Koff\_P1} \cdot [\mathrm{DNA\_01B1}]}{\mathrm{vol}(\mathrm{nucleus})} \end{aligned} \tag{75}$$

8.15 Reaction DNA51

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name DNA51

Reaction equation

$$\mathrm{DNA\_111} \underset{}{\overset{\mathrm{DNA\_111,\ DNA\_11B1}}{\rightleftharpoons}} \mathrm{DNA\_11B1} \tag{76}$$

Reactant

Table 48: Properties of each reactant.

Id	Name	SBO
DNA_111	DNA_111	

Modifiers

Table 49: Properties of each modifier.

Id	Name	SBO
DNA_111	DNA_111	
DNA_11B1	DNA_11B1	

Product

Table 50: Properties of each product.

Id	Name	SBO
DNA_11B1	DNA_11B1	

Kinetic Law

Derived unit contains undeclared units

$$v_{15} = \mathrm{vol}\left(\mathrm{nucleus}\right) \cdot \mathrm{function\_4\_DNA51}\left(\left[\mathrm{DNA\_111}\right], \left[\mathrm{DNA\_11B1}\right], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \tag{77}$$

$$\begin{aligned} &\mathrm{function\_4\_DNA51}\left(\left[\mathrm{DNA\_111}\right], \left[\mathrm{DNA\_11B1}\right], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \\ &= \frac{\mathrm{Kon\_P1} \cdot \left[\mathrm{DNA\_111}\right] - \mathrm{Koff\_P1} \cdot \left[\mathrm{DNA\_11B1}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \end{aligned} \tag{78}$$

$$\begin{aligned} &\mathrm{function\_4\_DNA51}\left(\left[\mathrm{DNA\_111}\right], \left[\mathrm{DNA\_11B1}\right], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \\ &= \frac{\mathrm{Kon\_P1} \cdot \left[\mathrm{DNA\_111}\right] - \mathrm{Koff\_P1} \cdot \left[\mathrm{DNA\_11B1}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \end{aligned} \tag{79}$$

8.16 Reaction DNA52

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name DNA52

Reaction equation

$$\mathrm{DNA\_111} \xrightleftharpoons{\mathrm{DNA\_111},\ \mathrm{DNA\_1B11}} \mathrm{DNA\_1B11} \tag{80}$$

Reactant

Table 51: Properties of each reactant.

Id	Name	SBO
DNA_111	DNA_111	

Modifiers

Table 52: Properties of each modifier.

Id	Name	SBO
DNA_111	DNA_111	
DNA_1B11	DNA_1B11	

Product

Table 53: Properties of each product.

Id	Name	SBO
DNA_1B11	DNA_1B11	

Kinetic Law

Derived unit contains undeclared units

$$v_{16} = \mathrm{vol}\left(\mathrm{nucleus}\right) \cdot \mathrm{function\_4\_DNA52}\left(\left[\mathrm{DNA\_111}\right], \left[\mathrm{DNA\_1B11}\right], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \tag{81}$$

$$\begin{aligned} &\mathrm{function\_4\_DNA52}\left(\left[\mathrm{DNA\_111}\right], \left[\mathrm{DNA\_1B11}\right], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \\ &= \frac{\mathrm{Kon\_P1} \cdot \left[\mathrm{DNA\_111}\right] - \mathrm{Koff\_P1} \cdot \left[\mathrm{DNA\_1B11}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \end{aligned} \tag{82}$$

$$\begin{aligned}&\text{function\_4\_DNA52}\left(\left[\text{DNA\_111}\right],\left[\text{DNA\_1B11}\right],\text{Koff\_P1},\text{Kon\_P1},\text{vol}\left(\text{nucleus}\right)\right)\\&=\frac{\text{Kon\_P1}\cdot\left[\text{DNA\_111}\right]-\text{Koff\_P1}\cdot\left[\text{DNA\_1B11}\right]}{\text{vol}\left(\text{nucleus}\right)}\end{aligned}\tag{83}$$

8.17 Reaction DNA53

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name DNA53

Reaction equation

$$\text{DNA\_11B1}\ \underset{\text{DNA\_11B1, DNA\_1B1B1}}{\rightleftharpoons}\ \text{DNA\_1B1B1}\tag{84}$$

Reactant

Table 54: Properties of each reactant.

Id	Name	SBO
DNA_11B1	DNA_11B1	

Modifiers

Table 55: Properties of each modifier.

Id	Name	SBO
DNA_11B1	DNA_11B1	
DNA_1B1B1	DNA_1B1B1	

Product

Table 56: Properties of each product.

Id	Name	SBO
DNA_1B1B1	DNA_1B1B1	

Kinetic Law

Derived unit contains undeclared units

$$v_{17} = \mathrm{vol}\left(\mathrm{nucleus}\right) \cdot \mathrm{function\_4\_DNA53}\left(\left[\mathrm{DNA\_11B1}\right], \left[\mathrm{DNA\_1B1B1}\right], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\left(\mathrm{nucleus}\right)\right) \tag{85}$$

$$\mathrm{function\_4\_DNA53}\left(\left[\mathrm{DNA\_11B1}\right], \left[\mathrm{DNA\_1B1B1}\right], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\left(\mathrm{nucleus}\right)\right) = \frac{\mathrm{Kon\_P1} \cdot \left[\mathrm{DNA\_11B1}\right] - \mathrm{Koff\_P1} \cdot \left[\mathrm{DNA\_1B1B1}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \tag{86}$$

$$\mathrm{function\_4\_DNA53}\left(\left[\mathrm{DNA\_11B1}\right], \left[\mathrm{DNA\_1B1B1}\right], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\left(\mathrm{nucleus}\right)\right) = \frac{\mathrm{Kon\_P1} \cdot \left[\mathrm{DNA\_11B1}\right] - \mathrm{Koff\_P1} \cdot \left[\mathrm{DNA\_1B1B1}\right]}{\mathrm{vol}\left(\mathrm{nucleus}\right)} \tag{87}$$

8.18 Reaction DNA54

This is a reversible reaction of one reactant forming one product influenced by two modifiers.

Name DNA54

Reaction equation

$$\mathrm{DNA\_1B11} \underset{}{\overset{\mathrm{DNA\_1B11,\ DNA\_1B1B1}}{\rightleftharpoons}} \mathrm{DNA\_1B1B1} \tag{88}$$

Reactant

Table 57: Properties of each reactant.

Id	Name	SBO
DNA_1B11	DNA_1B11	

Modifiers

Table 58: Properties of each modifier.

Id	Name	SBO
DNA_1B11	DNA_1B11	
DNA_1B1B1	DNA_1B1B1	

Product

Table 59: Properties of each product.

Id	Name	SBO
DNA_1B1B1	DNA_1B1B1	

Kinetic Law

Derived unit contains undeclared units

$$v_{18} = \mathrm{vol}\,(\mathrm{nucleus}) \cdot \mathrm{function\_4\_DNA54}\,([\mathrm{DNA\_1B11}], [\mathrm{DNA\_1B1B1}], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\,(\mathrm{nucleus})) \tag{89}$$

$$\mathrm{function\_4\_DNA54}\,([\mathrm{DNA\_1B11}], [\mathrm{DNA\_1B1B1}], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_P1} \cdot [\mathrm{DNA\_1B11}] - \mathrm{Koff\_P1} \cdot [\mathrm{DNA\_1B1B1}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{90}$$

$$\mathrm{function\_4\_DNA54}\,([\mathrm{DNA\_1B11}], [\mathrm{DNA\_1B1B1}], \mathrm{Koff\_P1}, \mathrm{Kon\_P1}, \mathrm{vol}\,(\mathrm{nucleus})) = \frac{\mathrm{Kon\_P1} \cdot [\mathrm{DNA\_1B11}] - \mathrm{Koff\_P1} \cdot [\mathrm{DNA\_1B1B1}]}{\mathrm{vol}\,(\mathrm{nucleus})} \tag{91}$$

9 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.

9.1 Species S1

Name S1

SBO:0000608 homodimer

Initial concentration $10^{-10}\ \mathrm{mol} \cdot \mathrm{l}^{-1}$

This species takes part in 24 reactions (as a reactant in DNA1, DNA2, DNA3, DNA4, DNA5, DNA6, DNA7, DNA8, DNA9, DNA10, DNA11, DNA12 and as a modifier in DNA1, DNA2, DNA3, DNA4, DNA5, DNA6, DNA7, DNA8, DNA9, DNA10, DNA11, DNA12).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{S1} = -v_1 - v_2 - v_3 - v_4 - v_5 - v_6 - v_7 - v_8 - v_9 - v_{10} - v_{11} - v_{12} \tag{92}$$

9.2 Species DNA_000

Name DNA_000

SBO:0000354 informational molecule segment

Initial concentration $10^{-10}\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in DNA1, DNA2, DNA3 and as a modifier in DNA1, DNA2, DNA3).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_000} = -v_1 - v_2 - v_3 \tag{93}$$

9.3 Species DNA_100

Name DNA_100

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in DNA4, DNA5 and as a product in DNA1 and as a modifier in DNA1, DNA4, DNA5).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_100} = v_1 - v_4 - v_5 \tag{94}$$

9.4 Species DNA_010

Name DNA_010

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in DNA6, DNA7 and as a product in DNA2 and as a modifier in DNA2, DNA6, DNA7).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_010} = v_2 - v_6 - v_7 \tag{95}$$

9.5 Species DNA_001

Name DNA_001

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in DNA8, DNA9 and as a product in DNA3 and as a modifier in DNA3, DNA8, DNA9).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_001} = v_3 - v_8 - v_9 \tag{96}$$

9.6 Species DNA_110

Name DNA_110

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in DNA10, DNA49 and as a product in DNA4, DNA6 and as a modifier in DNA4, DNA6, DNA10, DNA49).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_110} = v_4 + v_6 - v_{10} - v_{13} \tag{97}$$

9.7 Species DNA_101

Name DNA_101

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in six reactions (as a reactant in DNA11 and as a product in DNA5, DNA8 and as a modifier in DNA5, DNA8, DNA11).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_101} = v_5 + v_8 - v_{11} \tag{98}$$

9.8 Species DNA_011

Name DNA_011

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in eight reactions (as a reactant in DNA12, DNA50 and as a product in DNA7, DNA9 and as a modifier in DNA7, DNA9, DNA12, DNA50).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_011} = v_7 + v_9 - v_{12} - v_{14} \tag{99}$$

9.9 Species DNA_111

Name DNA_111

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in ten reactions (as a reactant in DNA51, DNA52 and as a product in DNA10, DNA11, DNA12 and as a modifier in DNA10, DNA11, DNA12, DNA51, DNA52).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_111} = v_{10} + v_{11} + v_{12} - v_{15} - v_{16} \tag{100}$$

9.10 Species DNA_1B10

Name DNA_1B10

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a product in DNA49 and as a modifier in DNA49).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_1B10} = v_{13} \tag{101}$$

9.11 Species DNA_01B1

Name DNA_01B1

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in two reactions (as a product in DNA50 and as a modifier in DNA50).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_01B1} = v_{14} \tag{102}$$

9.12 Species DNA_1B11

Name DNA_1B11

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in DNA54 and as a product in DNA52 and as a modifier in DNA52, DNA54).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_1B11} = v_{16} - v_{18} \tag{103}$$

9.13 Species DNA_11B1

Name DNA_11B1

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a reactant in DNA53 and as a product in DNA51 and as a modifier in DNA51, DNA53).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_11B1} = v_{15} - v_{17} \tag{104}$$

9.14 Species DNA_1B1B1

Name DNA_1B1B1

SBO:0000354 informational molecule segment

Initial concentration $0\ \mathrm{mol}\cdot\mathrm{l}^{-1}$

This species takes part in four reactions (as a product in DNA53, DNA54 and as a modifier in DNA53, DNA54).

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{DNA\_1B1B1} = v_{17} + v_{18} \tag{105}$$

A Glossary of Systems Biology Ontology Terms

SBO:0000338 dissociation rate constant: Rate with which a complex dissociates into its components

SBO:0000341 association rate constant: Rate with which components associate into a complex

SBO:0000354 informational molecule segment: Fragment of a macromolecule that carries genetic information

SBO:0000540 fraction of an entity pool: A ratio that represents the quantity of a defined constituent entity over the total number of all constituent entities present.

SBO:0000608 homodimer: A macromolecular complex composed of precisely two identical monomeric units, which are usually non-covalently bound

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