



Differential Equation System

Cell Death

1 Global Parameters

| Parameter | Value | Value Units |
|----------------------|---------------------------|-------------|
| vol | 7e-016 | |
| N | 6022999999999999800000000 | |
| k_{B0032} | 0.16667 | |
| $translation_{LuxR}$ | 0.038889 | |

2 Rate Laws

2.1 Reaction 1

| Species | Reactants | Products |
|---------|-----------|-------------------------|
| | mRNA_LuxR | C0062_LuxR mRNA_LuxR |

Reaction Rate

$$v_1 = mRNA_{LuxR} \cdot translation_{LuxR} \quad (1)$$

| Parameters | Parameter | Value | Value Units |
|------------|-----------|-------|-------------|
| | | | |

2.2 Reaction 2

| Species | Reactants | Products |
|---------|------------|---------------|
| | C0062_LuxR | sa38_degraded |

Reaction Rate

$$v_2 = C0062_{LuxR} \cdot d_{LuxR} \quad (2)$$

| Parameters | Parameter | Value | Value Units |
|------------|------------|------------|-------------|
| | d_{LuxR} | 9.627e-005 | |

2.3 Reaction 3

| Species | Reactants | Products |
|---------|------------------|----------|
| | HSL_LuxR_complex | HSL |

Reaction Rate

$$v_3 = HSL_{LuxR_complex} \cdot d_{complex} \quad (3)$$

| Parameters | Parameter | Value | Value Units |
|------------|---------------|------------|-------------|
| | $d_{complex}$ | 9.627e-005 | |

2.4 Reaction 4

| Species | Reactants | Products |
|---------|------------------|----------------------------|
| | Gene_LuxR | mRNA_LuxR |
| | CIIP22 | Gene_LuxR |
| | HSL_LuxR_complex | CIIP22 HSL_LuxR_complex |

Reaction Rate

$$v_4 = k_{transcr} \cdot Gene_{LuxR} \cdot \frac{Km_{CIIP22}^2}{(Km_{CIIP22}^2 + CIIP22^2)} \cdot \left(\frac{(\frac{HSL_{LuxR.complex}}{vol \cdot N})^{hill}}{(Km_{LuxR}^{hill} + (\frac{HSL_{LuxR.complex}}{vol \cdot N})^{hill})} + \frac{k_l}{k_{transcr}} \right) \quad (4)$$

| Parameter | Value | Value Units |
|---------------|-----------|-------------|
| $k_{transcr}$ | 0.003 | |
| Km | 0.1099 | |
| Km_{CIIP22} | 0.1099 | |
| Km_{LuxR} | 4.05e-006 | |
| $hill$ | 2.08 | |
| k_l | 0.0005 | |

2.5 Reaction 5

| Species | Reactants | Products |
|---------|------------------|---------------|
| | HSL lactonase | EnzymeComplex |

Reaction Rate

$$v_5 = HSL \cdot lactonase \cdot k_{a1} \quad (5)$$

| Parameter | Value | Value Units |
|-----------|-------|-------------|
| k_{a1} | 0.1 | |

2.6 Reaction 6

| Species | Reactants | Products |
|---------|---------------|--------------------------|
| | EnzymeComplex | hydroxyacid lactonase |

Reaction Rate

$$v_6 = EnzymeComplex \cdot k_{cat} \quad (6)$$

| Parameter | Value | Value Units |
|-----------|-------|-------------|
| k_{cat} | 29 | |

2.7 Reaction 7

| Species | Reactants | Products |
|---------|---------------|------------------|
| | EnzymeComplex | HSL lactonase |

Reaction Rate

$$v_7 = EnzymeComplex \cdot k_{d1} \quad (7)$$

| Parameter | Value | Value Units |
|-----------|----------|-------------|
| k_{d1} | 188428.3 | |

2.8 Reaction 8

| Species | Reactants | Products |
|---------|-----------|---------------|
| | HSL | sa72_degraded |

Reaction Rate

$$v_8 = d_{HSL} \cdot HSL \quad (8)$$

| Parameter | Value | Value Units |
|-----------|-----------|-------------|
| d_{HSL} | 1.02e-006 | |

2.9 Reaction 9

| Species | Reactants | Products |
|---------|-----------|---------------|
| | mRNA_LuxR | sa64_degraded |

Reaction Rate

$$v_9 = d_{mRNA_LuxR} \cdot mRNA_{LuxR} \quad (9)$$

| Parameter | Value | Value Units |
|------------------|---------|-------------|
| d_{mRNA_LuxR} | 0.00227 | |

2.10 Reaction 10

| Species | Reactants | Products |
|---------|------------------|------------------|
| | Gene_ccdB | mRNA_ccdB |
| | HSL_LuxR_complex | Gene_ccdB |
| | CIIP22 | HSL_LuxR_complex |
| | | CIIP22 |

Reaction Rate

$$v_{10} = f_{stop} \cdot k_{transcr} \cdot Gene_{ccdB} \cdot \frac{Km_{CIIP22}^2}{(Km_{CIIP22}^2 + CIIP22^2)} \cdot \left(\frac{\left(\frac{HSL_{LuxR_complex}}{(vol \cdot N)} \right)^{hill}}{(Km_{LuxR}^{hill} + \left(\frac{HSL_{LuxR_complex}}{(vol \cdot N)} \right)^{hill})} + \frac{k_l}{k_{transcr}} \right) \quad (10)$$

| Parameter | Value | Value Units |
|---------------|-----------|-------------|
| Km | 4.05e-006 | |
| k_1 | 0.0025 | |
| $hill$ | 2.08 | |
| Km_{CIIP22} | 0.1099 | |
| Km_{LuxR} | 4.05e-006 | |
| k_l | 0.000504 | |
| $k_{transcr}$ | 0.003 | |
| f_{stop} | 0.4 | |

2.11 Reaction 11

| Species | Reactants | Products |
|---------|-----------|------------|
| | mRNA_ccdB | P1010_ccdB |
| | | mRNA_ccdB |

Reaction Rate

$$v_{11} = mRNA_{ccdB} \cdot k_{Cdb} \quad (11)$$

| Parameter | Value | Value Units |
|-----------|-------|-------------|
| k_{Cdb} | 0.038 | |

2.12 Reaction 12

| Species | Reactants | Products |
|---------|-----------|---------------|
| | mRNA_ccdB | sa44_degraded |

Reaction Rate

$$v_{12} = mRNA_{ccdB} \cdot d_{mRNA_{ccdB}} \quad (12)$$

| Parameters | Parameter | Value | Value Units |
|------------|-------------------|---------|-------------|
| | $d_{mRNA_{ccdB}}$ | 0.00231 | |

2.13 Reaction 13

| Species | Reactants | Products |
|---------|------------|---------------|
| | P1010_ccdB | sa45_degraded |

Reaction Rate

$$v_{13} = P1010_{ccdB} \cdot d_{CdB} \quad (13)$$

| Parameters | Parameter | Value | Value Units |
|------------|-----------|----------|-------------|
| | d_{CdB} | 0.000289 | |

2.14 Reaction 14

| Species | Reactants | Products |
|---------|-----------|-------------------|
| | HSL | extracellular HSL |

Reaction Rate

$$v_{14} = (HSL - [extracellularHSL]) \cdot diff_{rate} \quad (14)$$

| Parameters | Parameter | Value | Value Units |
|------------|---------------|-------|-------------|
| | $diff_{rate}$ | 0.4 | |

2.15 Reaction 15

| Species | Reactants | Products |
|---------|-------------------|------------------|
| | C0062_LuxR HSL | HSL_LuxR_complex |

Reaction Rate

$$v_{15} = C0062_{LuxR} \cdot HSL \cdot k_a - HSL_{LuxR_complex} \cdot k_d \quad (15)$$

| Parameters | Parameter | Value | Value Units |
|------------|-----------|-------|-------------|
| | k_a | 100 | |
| | k_d | 42100 | |

2.16 Reaction 16

| Species | Reactants | Products |
|---------|-------------------|---------------|
| | extracellular HSL | sa70_degraded |

Reaction Rate

$$v_{16} = [extracellularHSL] \cdot d_{HSL_{ex}} \quad (16)$$

| Parameters | Parameter | Value | Value Units |
|------------|----------------|--------|-------------|
| | $d_{HSL_{ex}}$ | 0.0025 | |

3 Equations

3.1 Species: Gene_LuxR

$$\frac{d[Gene_{LuxR}]}{dt} = +v_4 - v_4 \quad (17)$$

3.2 Species: sa64_degraded

$$\frac{d[sa64_{degraded}]}{dt} = +v_9 \quad (18)$$

3.3 Species: mRNA_LuxR

$$\frac{d[mRNA_{LuxR}]}{dt} = +v_1 - v_1 + v_4 - v_9 \quad (19)$$

3.4 Species: C0062_LuxR

$$\frac{d[C0062_{LuxR}]}{dt} = +v_1 - v_2 - v_{15} \quad (20)$$

3.5 Species: sa38_degraded

$$\frac{d[sa38_{degraded}]}{dt} = +v_2 \quad (21)$$

3.6 Species: Gene_ccdB

$$\frac{d[Gene_{ccdB}]}{dt} = +v_{10} - v_{10} \quad (22)$$

3.7 Species: mRNA_ccdB

$$\frac{d[mRNA_{ccdB}]}{dt} = +v_{10} + v_{11} - v_{11} - v_{12} \quad (23)$$

3.8 Species: sa44_degraded

$$\frac{d[sa44_{degraded}]}{dt} = +v_{12} \quad (24)$$

3.9 Species: sa72_degraded

$$\frac{d[sa72_{degraded}]}{dt} = +v_8 \quad (25)$$

3.10 Species: HSL

$$\frac{d[HSL]}{dt} = +v_3 - v_5 + v_7 - v_8 - v_{14} - v_{15} \quad (26)$$

3.11 Species: P1010_ccdB

$$\frac{d[P1010_{ccdB}]}{dt} = +v_{11} - v_{13} \quad (27)$$

3.12 Species: sa45_degraded

$$\frac{d[sa45_{degraded}]}{dt} = +v_{13} \quad (28)$$

3.13 Species: EnzymeComplex

$$\frac{d[EnzymeComplex]}{dt} = +v_5 - v_6 - v_7 \quad (29)$$

3.14 Species: extracellular HSL

$$\frac{d[extracellularHSL]}{dt} = +v_{14} - v_{16} \quad (30)$$

3.15 Species: hydroxyacid

$$\frac{d[hydroxyacid]}{dt} = +v_6 \quad (31)$$

3.16 Species: sa70_degraded

$$\frac{d[sa70_{degraded}]}{dt} = +v_{16} \quad (32)$$

3.17 Species: lactonase

$$\frac{d[lactonase]}{dt} = -v_5 + v_6 + v_7 \quad (33)$$

3.18 Species: CIIP22

$$\frac{d[CIIP22]}{dt} = +v_4 - v_4 + v_{10} - v_{10} \quad (34)$$

3.19 Species: HSL_LuxR_complex

$$\frac{d[HSL_{LuxR.complex}]}{dt} = -v_3 + v_4 - v_4 + v_{10} - v_{10} + v_{15} \quad (35)$$

4 Compartments

4.1 Cell Death

| Species | Initial Amount | Initial Amount Units |
|-------------------|----------------|----------------------|
| Gene_LuxR | 0 | |
| sa64_degraded | 0 | |
| mRNA_LuxR | 0 | |
| C0062_LuxR | 0 | |
| sa38_degraded | 0 | |
| Gene_ccdB | 0 | |
| mRNA_ccdB | 0 | |
| sa44_degraded | 0 | |
| sa72_degraded | 0 | |
| HSL | 0 | |
| P1010_ccdB | 0 | |
| sa45_degraded | 0 | |
| EnzymeComplex | 0 | |
| extracellular HSL | 0 | |
| hydroxyacid | 0 | |
| sa70_degraded | 0 | |
| lactonase | 0 | |
| CIIP22 | 0 | |
| HSL_LuxR_complex | 0 | |