Hands-On

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Modello 1

$$\mathcal{S} = \{A,\ R_A,\ P_A\}$$

Dove:

- A: gene A
- R_A: mRNA per A
- P_A: proteina A

#	**Reagenti**	**Prodotti**	**Costanti**
r_1	A	$A + R_A$	-
r_2	R_A	$R_A + P_A$	-
r_3	R_A	$\emptyset$	-
r_4	P_A	$\emptyset$	-

Modello 2

$$\mathcal{S} = \{A,\ R_A,\ P_A,\ B,\ R_B,\ P_B,\ A \cdot P_B,\ B \cdot P_A\}$$

Dove:

- A: gene A
- R_A: mRNA per A
- P_A: proteina A
- B: gene B
- R_B: mRNA per B
- P_B: proteina B
- $A \cdot P_B$: composto di A e P_B
- $B \cdot P_A$: composto di B e P_A

#	**Reagenti**	**Prodotti**	**Costanti**
r_1	A	$A + R_A$	-
r_2	B	$B + R_B$	k_1
r_3	R_A	$R_A + P_A$	-
r_4	R_B	$R_B + P_B$	-
r_5	$A + P_B$	$A \cdot P_B$	-
r_6	$B + P_A$	$B \cdot P_A$	-
r_7	$B \cdot P_A$	$R_B + B \cdot P_A$	k_2
r_8	$A \cdot P_B$	$A + P_B$	-
r_9	$B \cdot P_A$	$B + P_A$	-
r_{10}	R_A	$\emptyset$	-
r_{11}	R_B	$\emptyset$	-
r_{12}	P_A	$\emptyset$	-
r_{13}	P_B	$\emptyset$	-

Assunzioni:

- $k_2 > k_1$

Modello 3

$\mathcal{S} = \{A,\ R_A,\ P_A,\ B,\ R_B,\ P_B,\ C,\ R_C,\ P_C,\ A{\cdot}P_B,\ B{\cdot}P_A,\ P_B^P,\ C{\cdot}P_B^P,\ C{\cdot}2P_B^P,\ K,\ F\}$

Dove:

- A: gene A
- R_A: mRNA per A
- P_A: proteina A
- B: gene B
- R_B: mRNA per B
- P_B: proteina B
- C: gene C
- R_C: mRNA per C
- P_C: proteina C
- $A \cdot P_B$: composto di A e P_B
- $B \cdot P_A$: composto di B e P_A
- P_B^P: P_B fosforilata
- $C \cdot P_B^P$: composto di C e P_B^P
- $C \cdot 2P_B^P$: composto di $C \cdot P_B^P$ e P_B^P
- K: chinasi
- F: fosfatasi

#	**Reagenti**	**Prodotti**	**Costanti**
r_1	A	$A + R_A$	-
r_2	B	$B + R_B$	k_1
r_3	C	$C + R_C$	k_2
r_4	R_A	$R_A + P_A$	-
r_5	R_B	$R_B + P_B$	-
r_6	R_C	$R_C + P_C$	-
r_7	$A + P_B$	$A \cdot P_B$	-
r_8	$B + P_A$	$B \cdot P_A$	-
r_9	$B \cdot P_A$	$R_B + B \cdot P_A$	k_3
r_{10}	$P_B + K$	$P_B^P + K$	-
r_{11}	$P_B^P + C$	$C \cdot P_B^P$	-
r_{12}	$C \cdot P_B^P$	$R_C + C \cdot P_B^P$	k_4
r_{13}	$C \cdot P_B^P + P_B^P$	$C \cdot 2P_B^P$	-
r_{14}	$C \cdot 2P_B^P$	$C \cdot P_B^P + P_B^P$	-
r_{15}	$C \cdot P_B^P$	$P_B^P + C$	-
r_{16}	$P_B^P + F$	$P_B + F$	-
r_{17}	$A \cdot P_B$	$A + P_B$	-
r_{18}	$B \cdot P_A$	$B + P_A$	-
r_{19}	R_A	$\emptyset$	-
r_{20}	R_B	$\emptyset$	-
r_{21}	R_C	$\emptyset$	-
r_{22}	P_A	$\emptyset$	-
r_{23}	P_B	$\emptyset$	-
r_{24}	P_C	$\emptyset$	-

Assunzioni:

- $k_3 > k_1$
- $k_4 < k_2$

Equazioni differenziali ottenute con COPASI (con i *reaction rate* "a caso" con il solo mantenimento "a spanne" delle due assunzioni):

$$
\begin{aligned}
\frac{\mathrm{d}\left([\mathrm{A}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= -V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{A}] \cdot [\mathrm{PB}] - 0.1 \cdot [\mathrm{APB}])) \\
\frac{\mathrm{d}\left([\mathrm{B}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= -V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{B}] \cdot [\mathrm{PA}] - 0.1 \cdot [\mathrm{BPA}])) \\
\frac{\mathrm{d}\left([\mathrm{RA}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= +V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{A}]) \\
&\quad -V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{RA}]) \\
\frac{\mathrm{d}\left([\mathrm{RB}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= +V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{B}]) \\
&\quad -V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{RB}]) \\
&\quad +V_{\mathrm{compartment}} \cdot (0.2 \cdot [\mathrm{BPA}]) \\
\frac{\mathrm{d}\left([\mathrm{PA}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= -V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{PA}]) \\
&\quad +V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{RA}]) \\
&\quad -V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{B}] \cdot [\mathrm{PA}] - 0.1 \cdot [\mathrm{BPA}])) \\
\frac{\mathrm{d}\left([\mathrm{PB}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= +V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{PBP}] \cdot [\mathrm{F}]) \\
&\quad -V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{PB}]) \\
&\quad +V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{RB}]) \\
&\quad -V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{A}] \cdot [\mathrm{PB}] - 0.1 \cdot [\mathrm{APB}])) \\
&\quad -V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{PB}] \cdot [\mathrm{K}]) \\
\frac{\mathrm{d}\left([\mathrm{APB}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= +V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{A}] \cdot [\mathrm{PB}] - 0.1 \cdot [\mathrm{APB}])) \\
\frac{\mathrm{d}\left([\mathrm{BPA}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= +V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{B}] \cdot [\mathrm{PA}] - 0.1 \cdot [\mathrm{BPA}])) \\
\frac{\mathrm{d}\left([\mathrm{PBP}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= -V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{PBP}] \cdot [\mathrm{C}] - 0.1 \cdot [\mathrm{CPBP}])) \\
&\quad -V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{CPBP}] \cdot [\mathrm{PBP}] - 0.1 \cdot [\mathrm{C2PBP}])) \\
&\quad -V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{PBP}] \cdot [\mathrm{F}]) \\
&\quad +V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{PB}] \cdot [\mathrm{K}]) \\
\frac{\mathrm{d}\left([\mathrm{C}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= -V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{PBP}] \cdot [\mathrm{C}] - 0.1 \cdot [\mathrm{CPBP}])) \\
\frac{\mathrm{d}\left([\mathrm{RC}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= +V_{\mathrm{compartment}} \cdot (0.05 \cdot [\mathrm{CPBP}]) \\
&\quad -V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{RC}]) \\
&\quad +V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{C}]) \\
\frac{\mathrm{d}\left([\mathrm{PC}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= -V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{PC}]) \\
&\quad +V_{\mathrm{compartment}} \cdot (0.1 \cdot [\mathrm{RC}]) \\
\frac{\mathrm{d}\left([\mathrm{CPBP}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= +V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{PBP}] \cdot [\mathrm{C}] - 0.1 \cdot [\mathrm{CPBP}])) \\
&\quad -V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{CPBP}] \cdot [\mathrm{PBP}] - 0.1 \cdot [\mathrm{C2PBP}])) \\
\frac{\mathrm{d}\left([\mathrm{C2PBP}] \cdot V_{\mathrm{compartment}}\right)}{\mathrm{d}t} &= +V_{\mathrm{compartment}} \cdot ((0.1 \cdot [\mathrm{CPBP}] \cdot [\mathrm{PBP}] - 0.1 \cdot [\mathrm{C2PBP}]))
\end{aligned}
$$

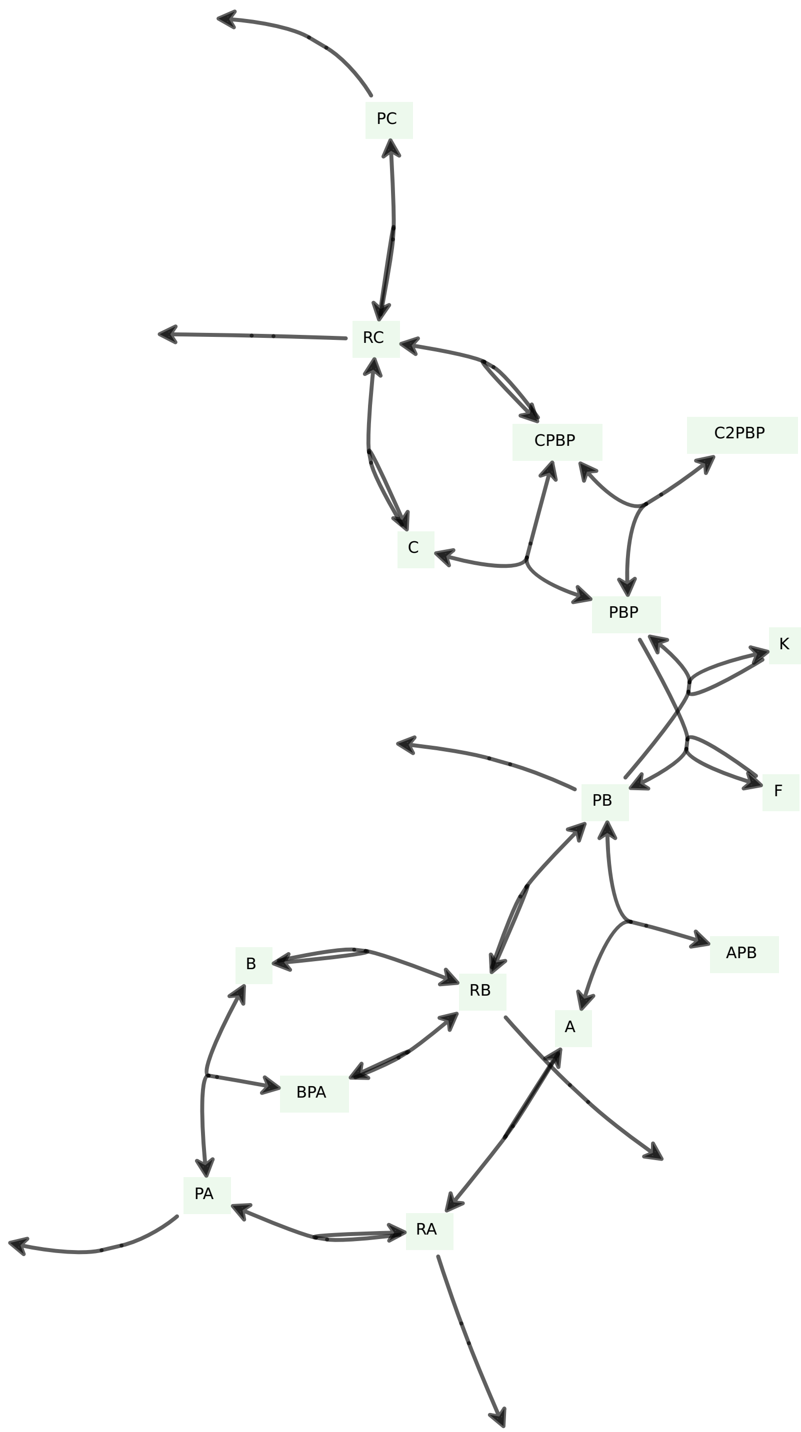

Figura 1: Modello3 rappresentato graficamente con COPASI