Visualizing Rule-based models

MMBioS 2015
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A picture is worth a thousand words.

Show, don’t tell.

Rule-based models
specify systems
of kinetic interactions
between sites on
molecules and complexes

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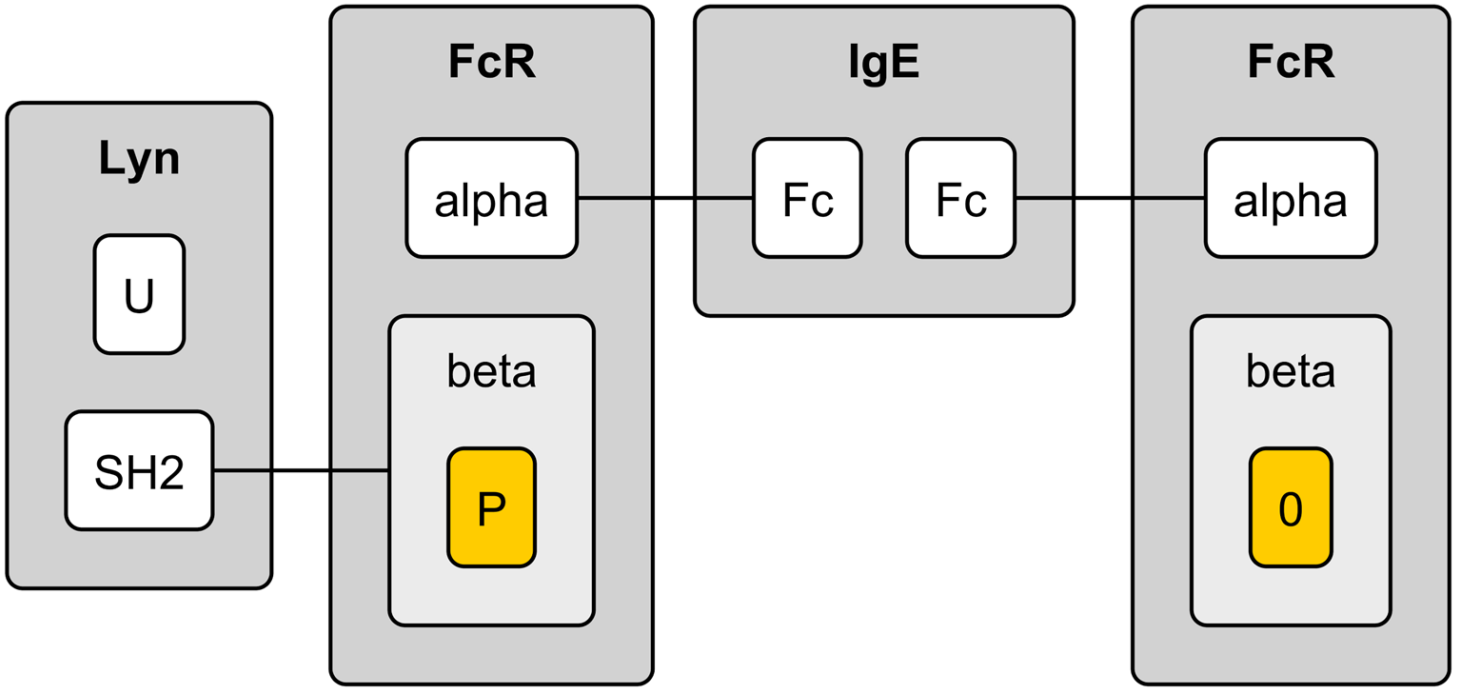
Complexes are structured graphs

IgE(Fc!1,Fc!2).
Lyn(U,SH2!3).
FcR(alpha!2,beta~P!3).
FcR(alpha!1,beta~0)

Complexes are structured graphs



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Reaction Rules are graph rewirings

R6:

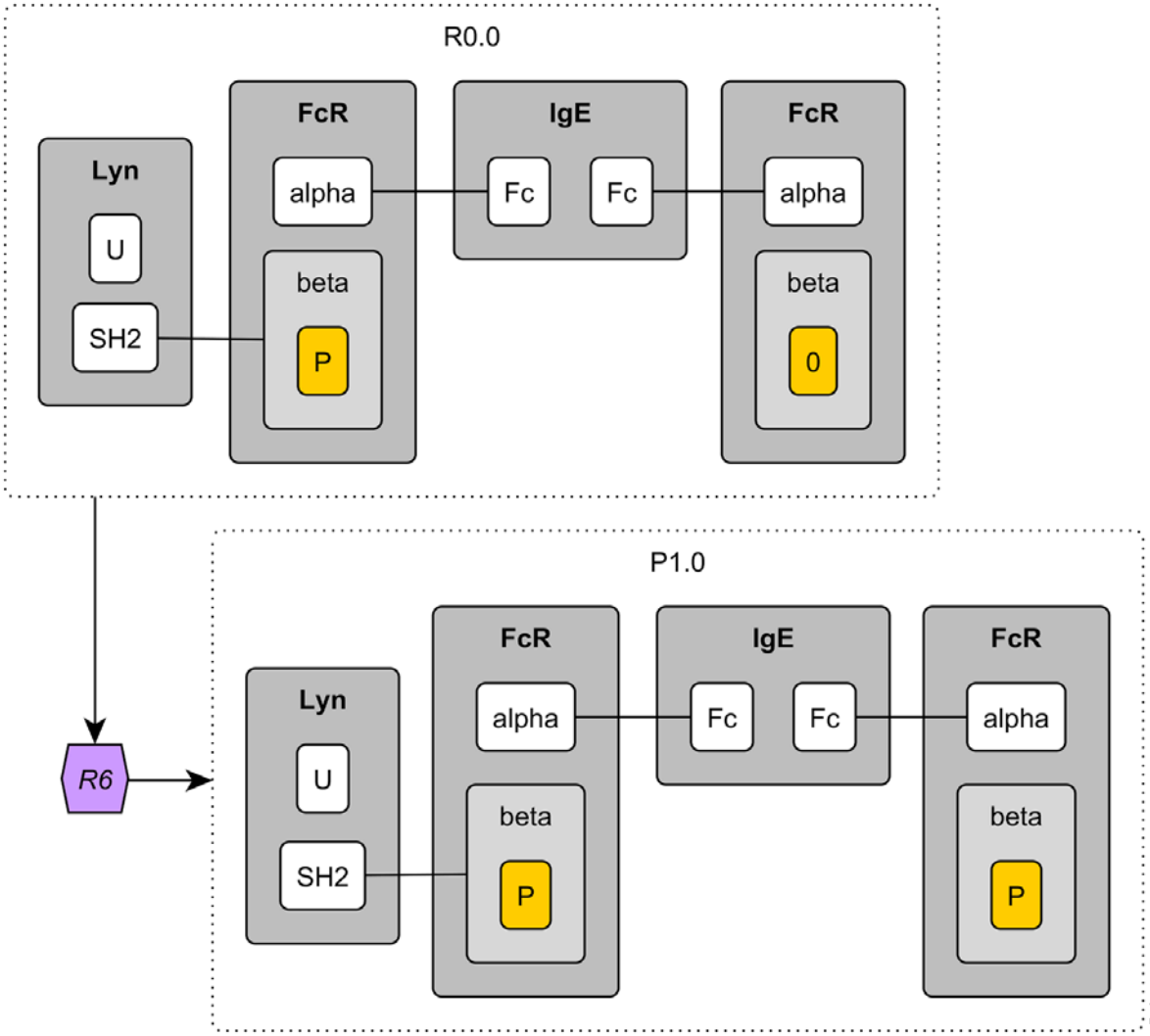
IgE(Fc!1,Fc!2).Lyn(U,SH2!3).
FcR(alpha!2,beta~P!3).FcR(alpha!1,beta~0)

->

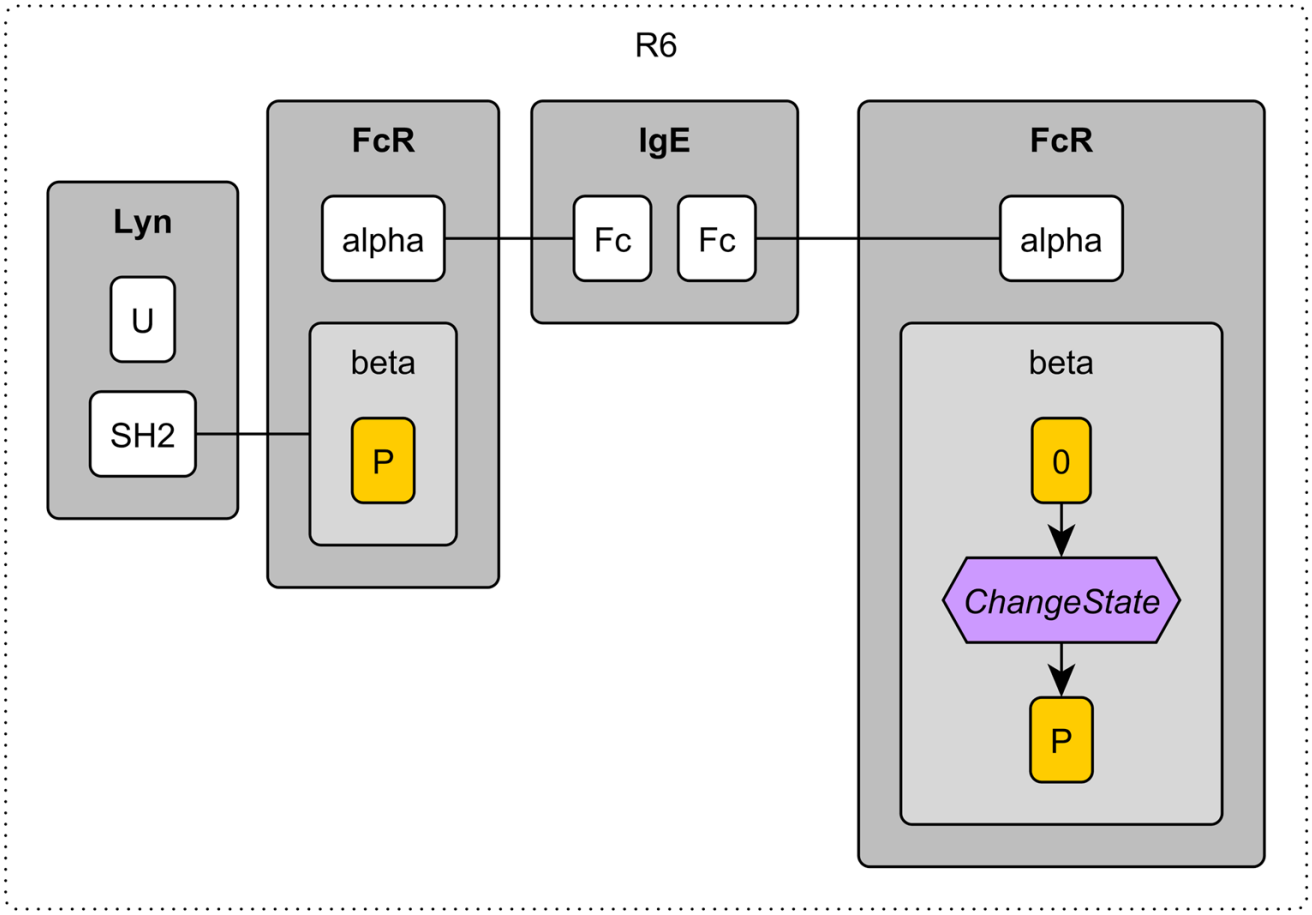
IgE(Fc!1,Fc!2).Lyn(U,SH2!3).
FcR(alpha!2,beta~P!3).FcR(alpha!1,beta~P)

pLbs

Reaction Rules are graph rewirings



Reaction Rules are graph rewirings

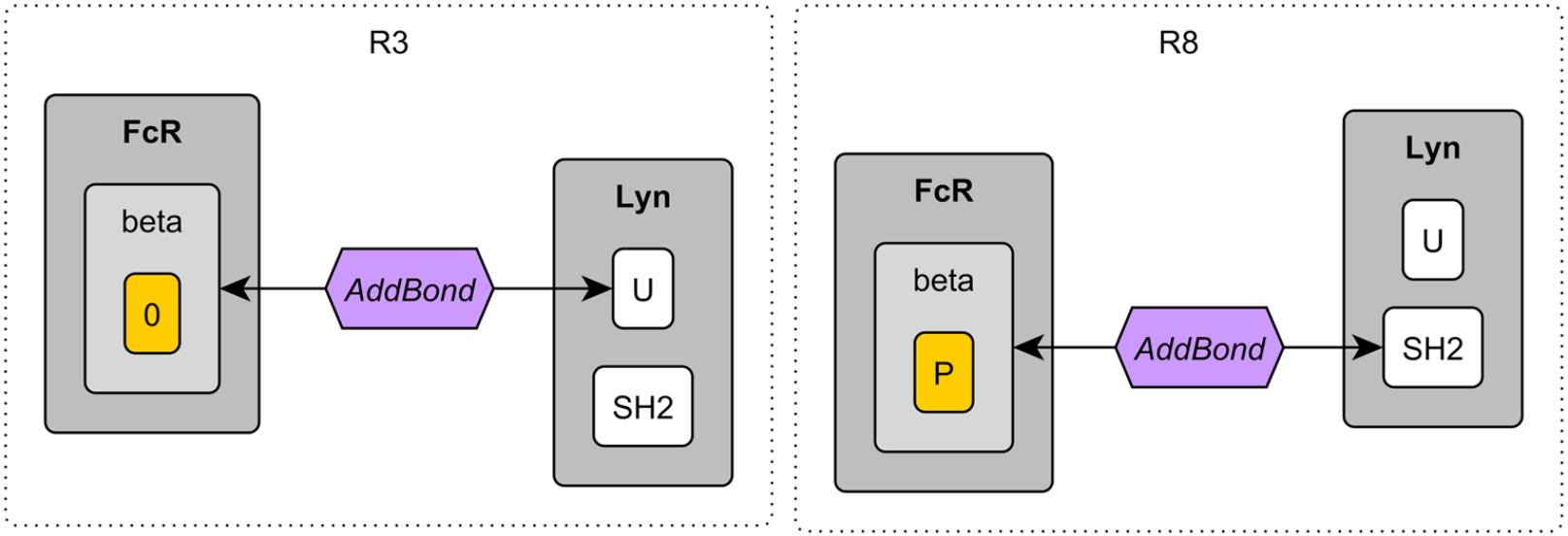


Reaction Rules can look very similar

R3: FcR(beta~0) + Lyn(U,SH2) <->
FcR(beta~0!1).Lyn(U!1,SH2)
kpL, kmL

R8: FcR(beta~P) + Lyn(U,SH2) <->
FcR(beta~P!1).Lyn(U,SH2!1)
kpLs, kmLs

Reaction Rules can look very similar



Reaction Rules can look very similar

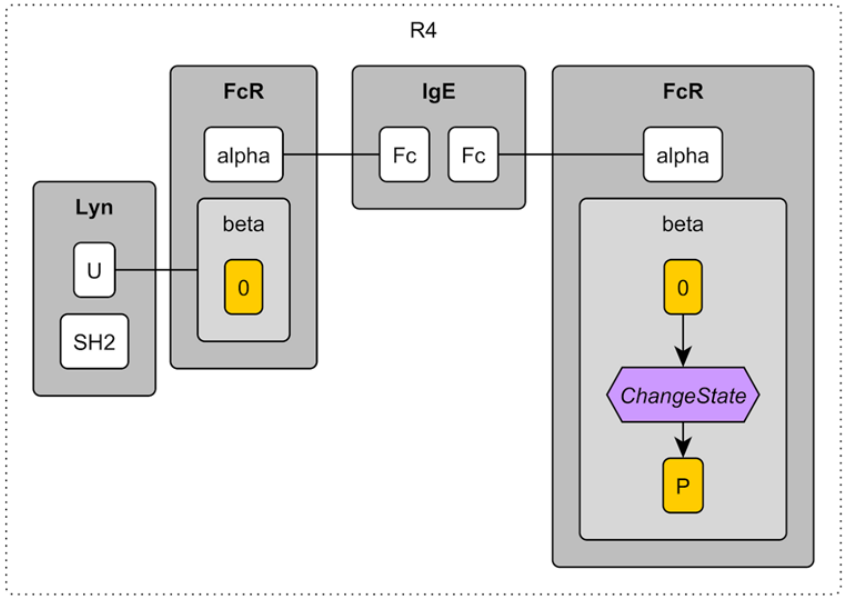
R4:

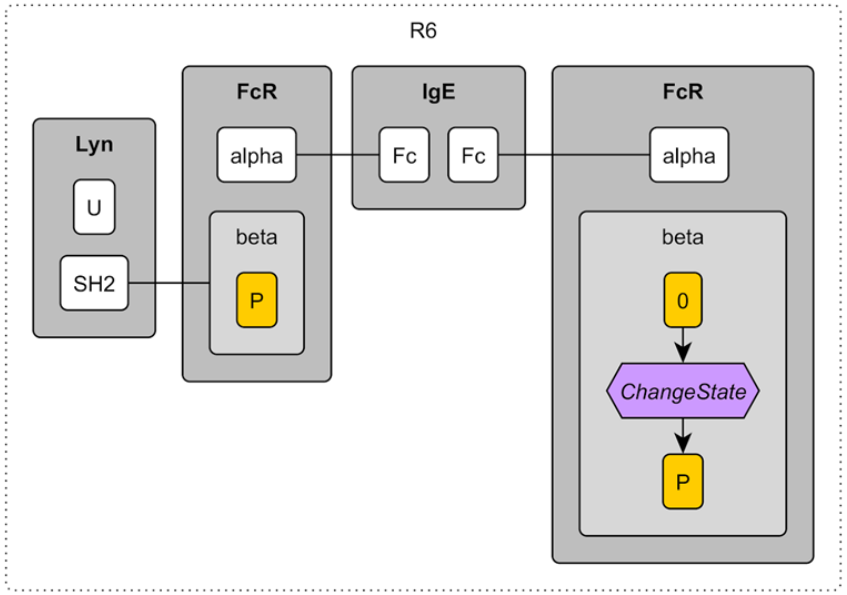
IgE(Fc!1,Fc!2).Lyn(U!3,SH2).
FcR(alpha!2,beta~0!3).FcR(alpha!1,beta~0)
-> IgE(Fc!1,Fc!2).Lyn(U!3,SH2).
FcR(alpha!2,beta~0!3).FcR(alpha!1,beta~P)
pLb

R6:

IgE(Fc!1,Fc!2).Lyn(U,SH2!3).
FcR(alpha!2,beta~P!3).FcR(alpha!1,beta~0)
-> IgE(Fc!1,Fc!2).Lyn(U,SH2!3).
FcR(alpha!2,beta~P!3).FcR(alpha!1,beta~P)
pLbs

Reaction Rules can look very similar





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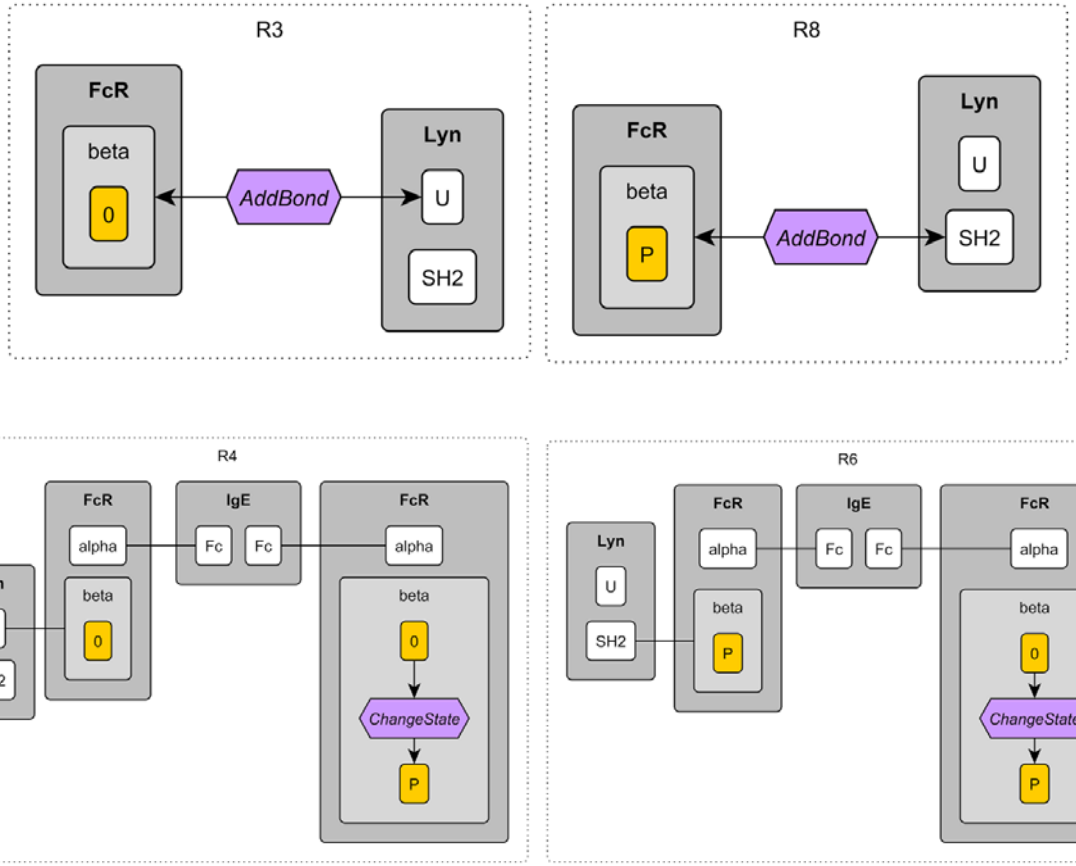
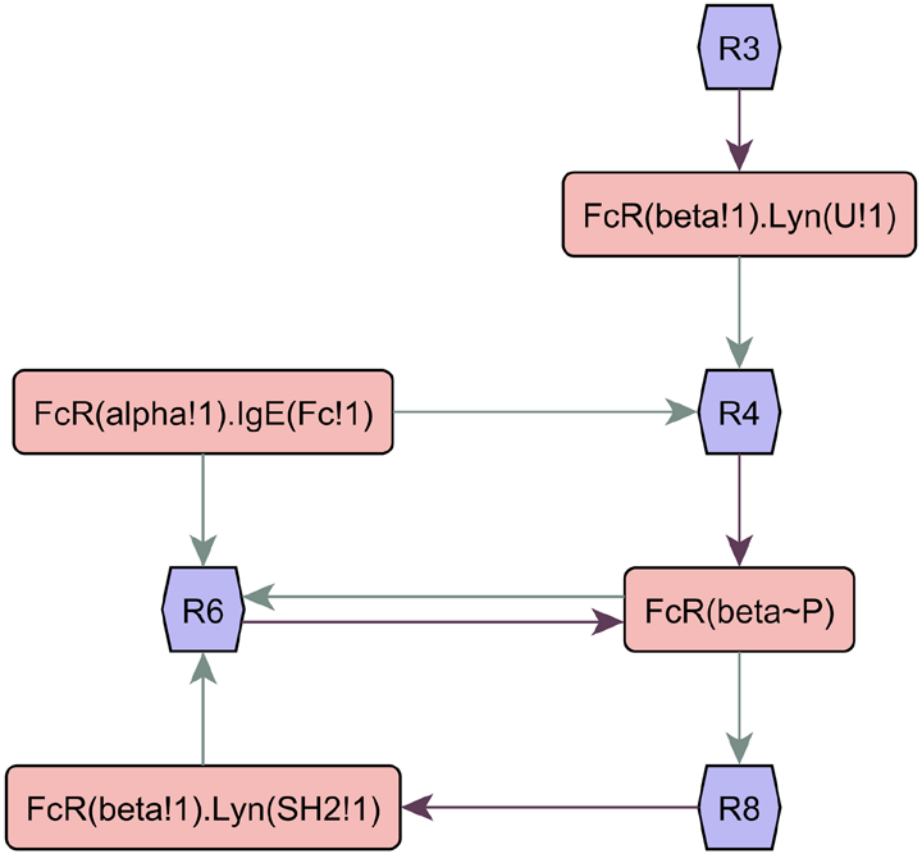
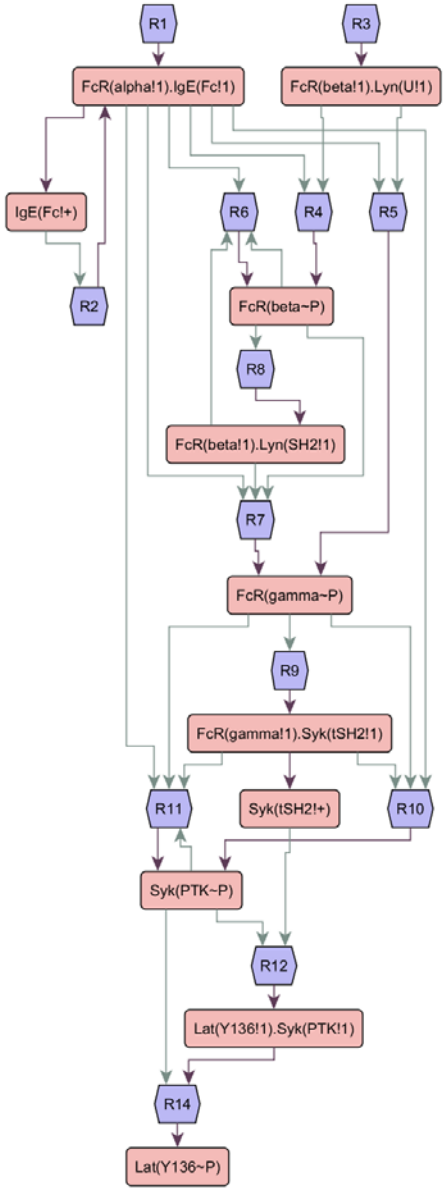
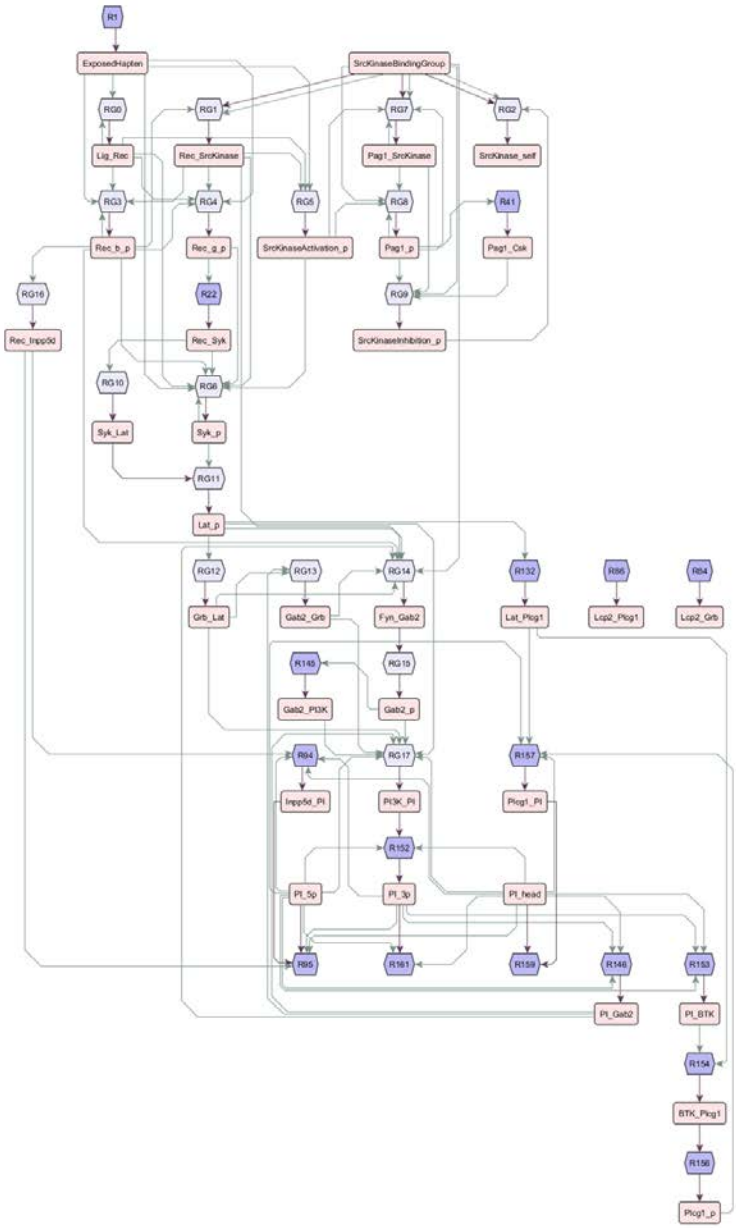
Reaction Rules overlap in complex ways



Reaction Rules overlap in complex ways




R1
R3
FcR(alpha!1).IgE(Fc!1)
FcR(beta!1).Lyn(U!1)
IgE(Fc!+)
R6
R4
R5
R2
FcR(beta~P)
R8
FcR(beta!1).Lyn(SH2!1)
R7
FcR(gamma~P)
R9
FcR(gamma!1).Syk(tSH2!1)
R11
Syk(tSH2!+)
R10
Syk(PTK~P)
R12
Lat(Y136!1).Syk(PTK!1)
R14
Lat(Y136~P)


R1
ExposedHapten
SrcKinaseBindingGroup
RG0
RG1
RG7
RG2
Lig_Rec
Rec_SrcKinase
Pag1_SrcKinase
SrcKinase_self
RG3
RG4
RG5
RG8
R41
Rec_b_p
Rec_g_p
SrcKinaseActivation_p
Pag1_p
Pag1_Csk
RG16
R22
RG9
Rec_Inpp5d
Rec_Syk
SrcKinaseInhibition_p
RG10
RG6
Syk_Lat
Syk_p
RG11
Lat_p
RG12
RG13
RG14
R132
R86
R84
Grb_Lat
Gab2_Grb
Fyn_Gab2
Lat_Plcg1
Lcp2_Plcg1
Lcp2_Grb
R145
RG15
Gab2_PI3K
Gab2_p
R94
RG17
R157
Inpp5d_PI
PI3K_PI
Plcg1_PI
R152
PI_5p
PI_3p
PI_head
R95
R161
R159
R146
R153
PI_Gab2
PI_BTK
R154
BTK_Plcg1
R156
Plcg1_p