Protein interaction calculus

Introduction
Signaling pathways
Proteins, kinases...

\[ A + B \leftrightarrow A.B \rightarrow A^* + B \]
Model as a review...
OK I got it...
More facts

Activated RAF kinases phosphorylate and activate MEK1 and MEK2 (ref. 2). These are dual-specificity kinases that in turn phosphorylate and activate ERK1 and ERK2 in what constitutes the RAF-MEK-ERK signaling cascade (or classical MAPK cascade). Active ERK phosphorylates serine or threonine residues within the Ser/Thr-Pro motif in many cytoplasmic and nuclear proteins. 
Formal reasoning vs. formal languages

Eléments d’Euclide, Livre I, prop.48. R. Descartes (XVIe siècle)
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Systems biology 2.0

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Part II
Rule-based modeling
Kappa by example

“Kinase B is a highly efficient enzyme that phosphorylates A” (1)

“Kinase A phosphorylates C” (2)

“A has a closed and an open form” (3)

“Kinase B activates A” (4)
"Kinase $B$ is a highly efficient enzyme that phosphorylates $A$"

\[
\text{%agent: A(x1, x2{u phos})}
\]
\[
\text{%agent: B(y1)}
\]

\[
\text{'A.B' A(x1[ .], x2{u}), B(y1[ .]) } \leftrightarrow \text{ A(x1[1], x2{x} phos), B(y1[1]) } @ \text{ k_AB/ V, k_A.B}
\]

\[
\text{'B phos A' A(x1[1], x2{u}), B(y1[1]) } \rightarrow \text{ A(x1[ .], x2{phos}), B(y1[ .]) } @ \text{ k_phos}
\]
“Kinase A phosphorylates C”

\[
\text{%agent: } A(x1, x2\{u \text{ phos}\}, x4)
\]

\[
\text{%agent: } C(z1, z2\{u \text{ phos}\})
\]

\['A \text{ binds } C' \ A(x4[\cdot]), C(z1[\cdot]) \leftrightarrow A(x4[1]), C(z1[1]) @ \text{'k_{AC'/'V'}, 'k_{A..C'}}
\]

\['A \text{ phos } C' \ C(z1[x4.A], z2\{u\}) \rightarrow C(z1[x4.A], z2\{\text{phos}\}) @ \text{'k_{phos'}}
\]
"A has a closed and an open form"

\[
\text{\%agent: } A(x_1, x_2\{u \text{ phos}\}, x_3\{\text{close open}\}, x_4)
\]

'A folds' \( A(x_3\{\text{open}\}) \leftrightarrow A(x_3\{\text{close}\}) \) @ 'k_open', 'k_close'
Exercises