

Initial Conditions:

	CD3ζ	LCK	Phosphatase
molecules/μm ²	1	1000	10-100000

Parameter Values:

	k _{cat} (min ⁻¹)	K _{M,A1} (μm ⁻²)	K _{M,A2} (μm ⁻²)	K _{M,B1} (μm ⁻²)	K _{M,B2} (μm ⁻²)	K _{M,C1} (μm ⁻²)	K _{M,C2} (μm ⁻²)	X _i
LCK parameters	360	97	332	270	154	485	405	0.115
Phosphatase parameters	360	11	36	32	18	67	57	0.1

Equations:

$$\frac{dpY_{A1}}{dt} = \frac{\left(\frac{K_{cat}}{K_{M,A1}}\right)(Y_{A1})(LCK)}{1 + \frac{Y_{A1}}{K_{M,A1}} + \frac{Y_{A2}}{K_{M,A2}} + \frac{Y_{B1}}{K_{M,B1}} + \frac{Y_{B2}}{K_{M,B2}} + \frac{Y_{C1}}{K_{M,C1}} + \frac{Y_{C2}}{K_{M,C2}} + \frac{pY_{A1}}{K_{I,A1}} + \frac{pY_{A2}}{K_{I,A2}} + \frac{pY_{B1}}{K_{I,B1}} + \frac{pY_{B2}}{K_{I,B2}} + \frac{pY_{C1}}{K_{I,C1}} + \frac{pY_{C2}}{K_{I,C2}}} - \frac{\left(\frac{P_{cat}}{P_{M,A1}}\right)(pY_{A1})(Phos)}{1 + \frac{pY_{A1}}{P_{M,A1}} + \frac{pY_{A2}}{P_{M,A2}} + \frac{pY_{B1}}{P_{M,B1}} + \frac{pY_{B2}}{P_{M,B2}} + \frac{pY_{C1}}{P_{M,C1}} + \frac{pY_{C2}}{P_{M,C2}} + \frac{Y_{A1}}{P_{I,A1}} + \frac{Y_{A2}}{P_{I,A2}} + \frac{Y_{B1}}{P_{I,B1}} + \frac{Y_{B2}}{P_{I,B2}} + \frac{Y_{C1}}{P_{I,C1}} + \frac{Y_{C2}}{P_{I,C2}}}$$

$$\frac{dY_{A1}}{dt} = - \frac{\left(\frac{K_{cat}}{K_{M,A1}}\right)(Y_{A1})(LCK)}{1 + \frac{Y_{A1}}{K_{M,A1}} + \frac{Y_{A2}}{K_{M,A2}} + \frac{Y_{B1}}{K_{M,B1}} + \frac{Y_{B2}}{K_{M,B2}} + \frac{Y_{C1}}{K_{M,C1}} + \frac{Y_{C2}}{K_{M,C2}} + \frac{pY_{A1}}{K_{I,A1}} + \frac{pY_{A2}}{K_{I,A2}} + \frac{pY_{B1}}{K_{I,B1}} + \frac{pY_{B2}}{K_{I,B2}} + \frac{pY_{C1}}{K_{I,C1}} + \frac{pY_{C2}}{K_{I,C2}}} + \frac{\left(\frac{P_{cat}}{P_{M,A1}}\right)(pY_{A1})(Phos)}{1 + \frac{pY_{A1}}{P_{M,A1}} + \frac{pY_{A2}}{P_{M,A2}} + \frac{pY_{B1}}{P_{M,B1}} + \frac{pY_{B2}}{P_{M,B2}} + \frac{pY_{C1}}{P_{M,C1}} + \frac{pY_{C2}}{P_{M,C2}} + \frac{Y_{A1}}{P_{I,A1}} + \frac{Y_{A2}}{P_{I,A2}} + \frac{Y_{B1}}{P_{I,B1}} + \frac{Y_{B2}}{P_{I,B2}} + \frac{Y_{C1}}{P_{I,C1}} + \frac{Y_{C2}}{P_{I,C2}}}$$

$$\frac{dpY_{A2}}{dt} = \frac{\left(\frac{K_{cat}}{K_{M,A2}}\right)(Y_{A2})(LCK)}{1 + \frac{Y_{A1}}{K_{M,A1}} + \frac{Y_{A2}}{K_{M,A2}} + \frac{Y_{B1}}{K_{M,B1}} + \frac{Y_{B2}}{K_{M,B2}} + \frac{Y_{C1}}{K_{M,C1}} + \frac{Y_{C2}}{K_{M,C2}} + \frac{pY_{A1}}{K_{I,A1}} + \frac{pY_{A2}}{K_{I,A2}} + \frac{pY_{B1}}{K_{I,B1}} + \frac{pY_{B2}}{K_{I,B2}} + \frac{pY_{C1}}{K_{I,C1}} + \frac{pY_{C2}}{K_{I,C2}}} - \frac{\left(\frac{P_{cat}}{P_{M,A2}}\right)(pY_{A2})(Phos)}{1 + \frac{pY_{A1}}{P_{M,A1}} + \frac{pY_{A2}}{P_{M,A2}} + \frac{pY_{B1}}{P_{M,B1}} + \frac{pY_{B2}}{P_{M,B2}} + \frac{pY_{C1}}{P_{M,C1}} + \frac{pY_{C2}}{P_{M,C2}} + \frac{Y_{A1}}{P_{I,A1}} + \frac{Y_{A2}}{P_{I,A2}} + \frac{Y_{B1}}{P_{I,B1}} + \frac{Y_{B2}}{P_{I,B2}} + \frac{Y_{C1}}{P_{I,C1}} + \frac{Y_{C2}}{P_{I,C2}}}$$

