

Supporting Information

Exclusivity and Compensation in NF κ B Dimer distributions and I κ B inhibition

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Supplementary Note 1

ODEs:

$$\frac{d}{dt} [A] = -2k_{a1}[A]^2 + 2kd_1[A:A] - k_{a2}[A][50] + k_{d2}[A:50]$$

$$\frac{d}{dt} [50] = -k_{a2}[A][50] + kd_2[A:50] - 2k_{a3}[50]^2 + 2k_{d3}[50:50]$$

$$\frac{d}{dt} [A:A] = k_{a1}[A]^2 - kd_1[A:A] - k_{a6}[A:A][\alpha] + k_{d6}[A:A:\alpha]$$

$$\frac{d}{dt} [A:50] = k_{a2}[A][50] - kd_2[A:50] - k_{a7}[A:50][\alpha] + k_{d7}[A:50:\alpha]$$

$$\frac{d}{dt} [50:50] = k_{a3}[50]^2 - kd_3[50:50]$$

$$\frac{d}{dt} [\alpha] = -k_{a6}[A:A][\alpha] + k_{d6}[A:A:\alpha] - k_{a7}[A:50][\alpha] + k_{d7}[A:50:\alpha]$$

$$\frac{d}{dt} [A:A:\alpha] = k_{a6}[A:A][\alpha] - k_{d6}[A:A:\alpha]$$

$$\frac{d}{dt} [A:50:\alpha] = k_{a7}[A:50][\alpha] - k_{d7}[A:50:\alpha]$$

Parameters:

$$k_{a1} = k_{a2} = k_{a3} = k_{a6} = k_{a7} = 10^9 \text{ M}^{-1}\text{s}^{-1}$$

$$k_{d1} = 18.6 \text{ s}^{-1}; k_{d2} = 0.3 \text{ s}^{-1}; k_{d3} = 0.4 \text{ s}^{-1}; k_{d6} = 0.047 \text{ s}^{-1}; k_{d7} = 0.041 \text{ s}^{-1}$$

Initial concentrations:

$$[A]_0 = [50]_0 = [A:A]_0 = [A:50]_0 = [50:50]_0 = [\alpha]_0 = [A:A:\alpha]_0 = 0$$

$$[A:50:\alpha]_0 = 350 \text{ nM}$$

Supplementary Note 2

ODEs:

$$\frac{d}{dt} [A] = -2k_{a1}[A]^2 + 2kd_1[A:A] - k_{a2}[A][50] + k_{d2}[A:50]$$

$$\frac{d}{dt} [50] = -k_{a2}[A][50] + kd_2[A:50] - 2k_{a3}[50]^2 + 2k_{d3}[50:50]$$

$$\frac{d}{dt} [A:A] = k_{a1}[A]^2 - kd_1[A:A] - k_{a4}[A:A][\beta] + k_{d4}[A:A:\beta] - k_{a6}[A:A][\alpha] + k_{d6}[A:A:\alpha]$$

$$\frac{d}{dt} [A:50] = k_{a2}[A][50] - kd_2[A:50] - k_{a5}[A:50][\beta] + k_{d5}[A:50:\beta] - k_{a7}[A:50][\alpha] + k_{d7}[A:50:\alpha]$$

$$\frac{d}{dt} [50:50] = k_{a3}[50]^2 - kd_3[50:50]$$

$$\frac{d}{dt} [\beta] = -k_{a4}[A:A][\beta] + k_{d4}[A:A:\beta] - k_{a5}[A:50][\beta] + k_{d5}[A:50:\beta]$$

$$\frac{d}{dt} [A:A:\beta] = k_{a4}[A:A][\beta] - k_{d4}[A:A:\beta]$$

$$\frac{d}{dt} [A:50:\beta] = k_{a5}[A:50][\beta] - k_{d5}[A:50:\beta]$$

$$\frac{d}{dt} [\alpha] = -k_{a6}[A:A][\alpha] + k_{d6}[A:A:\alpha] - k_{a7}[A:50][\alpha] + k_{d7}[A:50:\alpha]$$

$$\frac{d}{dt} [A:A:\alpha] = k_{a6}[A:A][\alpha] - k_{d6}[A:A:\alpha]$$

$$\frac{d}{dt} [A:50:\alpha] = k_{a7}[A:50][\alpha] - k_{d7}[A:50:\alpha]$$

Parameters:

$$k_{a1} = k_{a2} = k_{a3} = k_{a4} = k_{a5} = k_{a6} = k_{a7} = 10^9 \text{ M}^{-1}\text{s}^{-1}$$

$$k_{d1} = 18.6 \text{ s}^{-1}; k_{d2} = 0.3 \text{ s}^{-1}; k_{d3} = 0.4 \text{ s}^{-1}; k_{d4} = 0.024 \text{ s}^{-1}; k_{d5} = 0.895 \text{ s}^{-1};$$

$$k_{d6} = 0.047 \text{ s}^{-1}; k_{d7} = 0.041 \text{ s}^{-1}$$

Initial concentrations:

$$[A]_0 = [50]_0 = [A:A]_0 = [50:50]_0 = [A:A:\beta]_0 = [A:50:\beta]_0 = [A:A:\alpha]_0 = [A:50:\alpha]_0 = 0$$

$$[A:50]_0 = 350 \text{ nM}$$

$$[\beta]_0 = 0, 10, 20, 50, \text{ or } 80 \text{ nM}$$

$$[\alpha]_0 = 0 \text{ or } 350 \text{ nM}$$