Materials for Supporting Information

Reduction-Alkylation Strategies for the Modification of Specific Monoclonal Antibody Disulfides

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Figure S1. Mechanism used for the simulation of cAC10 partial reduction.

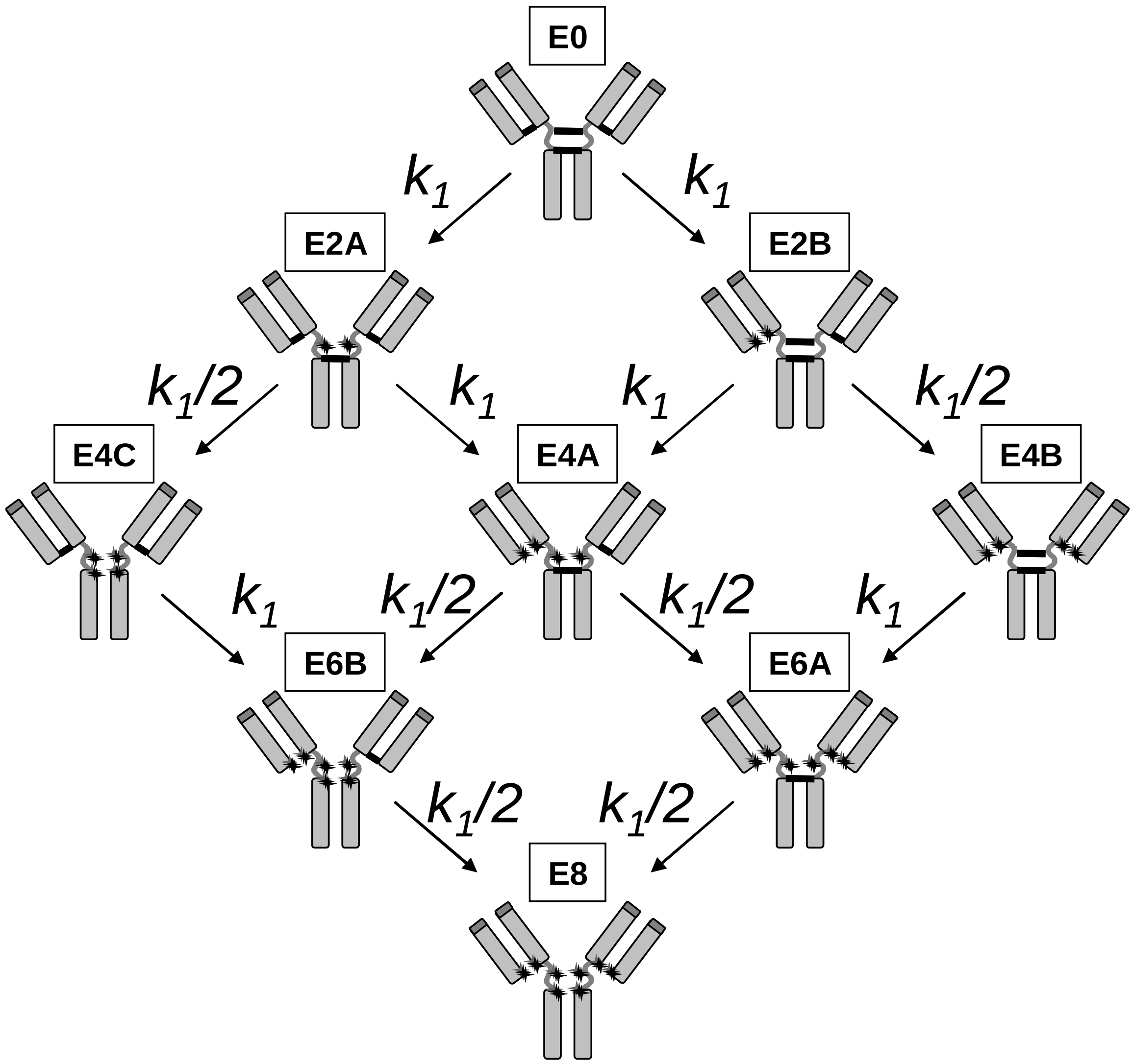

Figure S2. Rate equations used for the simulation of cAC10 partial reduction. The concentration of reductant is [R].

$$\frac{d[E0]}{dt} = -2(k_1[R][E0])$$

$$\frac{d[E2B]}{dt} = k_1[R][E0] - k_1[R][E2B] - \frac{k_1}{2}[R][E2B]$$

$$\frac{d[E2A]}{dt} = k_1[R][E0] - k_1[R][E2A] - \frac{k_1}{2}[R][E2A]$$

$$\frac{d[E4C]}{dt} = \frac{k_1}{2}[R][E2A] - k_1[R][E4C]$$

$$\frac{d[E4B]}{dt} = \frac{k_1}{2}[R][E2B] - k_1[R][E4B]$$

$$\frac{d[E4A]}{dt} = (k_1[R][E2B] + k_1[R][E2A]) - 2(\frac{k_1}{2}[R][E4A])$$

$$\frac{d[E6B]}{dt} = \frac{k_1}{2}[R][E4A] + k_1[R][E4C] - \frac{k_1}{2}[R][E6B]$$

$$\frac{d[E6A]}{dt} = \frac{k_1}{2}[R][E4A] + k_1[R][E4B] - \frac{k_1}{2}[R][E6A]$$

$$\frac{d[E8]}{dt} = \frac{k_1}{2}[R][E6A] + \frac{k_1}{2}[R][E6B]$$

$$\frac{d[R]}{dt} = -2(k_1[R][E0]) - k_1[R][E2B] - \frac{k_1}{2}[R][E2B] - k_1[R][E2A] - \frac{k_1}{2}[R][E2A]$$

$$- k_1[R][E4C] - k_1[R][E4B] - 2(\frac{k_1}{2}[R][E4A]) - \frac{k_1}{2}[R][E6B] - \frac{k_1}{2}[R][E6A]$$