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Supporting information for article:

REGALS: a general method to deconvolve X-ray scattering data from evolving mixtures

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Supporting Information

REGALS: a general method to deconvolve X-ray scattering data from evolving mixtures

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Contents

Supplementary Tables

	B1 (salt gradient)	**B2** (salt gradient)	**C1** (dimer)	**C2** (monomer)
Concentration basis				
Model	*smooth*	*smooth*	*smooth*	*smooth*
Range ($x_{\min}$–$x_{\max}$)[a]	1–1737	201–1737	730–1270	1150–1600
Control points	50	50	50	50
Zero boundary conditions	none	$x_{\min}$	$x_{\min}$, $x_{\max}$	$x_{\min}$, $x_{\max}$
Regularization parameter (λ')[b]	7.8×10^8	4.5×10^8	0	0
SAXS basis				
Model	*simple*	*simple*	*simple*	*simple*

[a] x = frame number
[b] Estimated using $n_g = 8$ (see Methods in the Main Text)

Table S1: REGALS model for *Bs*RNR AEX-SAXS dataset

	C1 (resting tetramer)	**C2** (activated tetramer)	**C3** (unknown oligomer)
Concentration basis			
Model	*smooth*	*smooth*	*smooth*
Range ($x_{\min}$–$x_{\max}$)[a]	1–5	1–3.5	1–5
Control points	31	21	31
Zero boundary conditions	$x_{\min}$	$x_{\max}$	none
Regularization parameter (λ')	10	10	10
SAXS basis			
Model	*real-space*	*real-space*	*real-space*
$d_{\max}$ (Å)	130	130	300
Control points	101	101	101
Zero boundary conditions	$r = 0$, $d_{\max}$	$r = 0$, $d_{\max}$	$r = 0$, $d_{\max}$
Regularization parameter (λ)	1×10^{12}	1×10^{12}	1×10^{12}

[a] $x = \log_{10} c$ for $c > 0$ and $x = 1$ for $c = 0$, where c is the ligand concentration in μM

Table S2: REGALS model for PheH titration dataset

	C1 (dimer)	**C2** (monomer)
Concentration basis		
Model	*smooth*	*smooth*
Range ($x_{\min}$–$x_{\max}$)[a]	1.3–5.1	1.3–5.1
Control points	31	31
Zero boundary conditions	$x_{\max}$	none
Regularization parameter (λ')	1×10^{-3}	1×10^{-3}
SAXS basis		
Model	*real-space*	*real-space*
$d_{\max}$ (Å)	70	62
Control points	101	101
Zero boundary conditions	$r = 0$, $d_{\max}$	$r = 0$, $d_{\max}$
Regularization parameter (λ)	1×10^{11}	1×10^{11}

[a] $x = \log_{10}(t)$ where t is the delay time in ms

Table S3: REGALS model for MsbA NDB time-resolved dataset

	C1 (transient)	**C2** (intraparticle)	**C3** (interparticle)
Concentration basis			
Model	*smooth*	*smooth*	*smooth*
Range ($x_{\min}$–$x_{\max}$)[a]	2.75–6	2.75–6	2.75–6
Control points	31	31	31
Zero boundary conditions	$x_{\min}$, $x_{\max}$	none	none
Regularization parameter (λ')	10	10	10
SAXS basis			
Model	*real-space*	*real-space*	*real-space*
$d_{\max}$ (Å)	59	46	150
Control points	101	101	101
Zero boundary conditions	$r = 0$, $d_{\max}$	$r = 0$, $d_{\max}$	$r = 0$, $d_{\max}$
Regularization parameter (λ)	1×10^{11}	1×10^{11}	1×10^{11}

[a] $x = \log_{10}(t)$ where t is the time delay in ns

Table S4: REGALS model for CypA T-jump dataset