Supplementary Material for "Stoichiometries and affinities of interacting proteins from concentration series of solution scattering data: Decomposition by least squares and quadratic optimization"

H. Chandola, T.E. Williamson, B.A. Craig, A.M. Friedman, and C. Bailey-Kellogg

The supplementary material includes tables for the initial concentrations (one-stage in Tab. 1 and two-stage in Tab. 2), the complete results for the association model searches (Tab. 3: bovine IFN-gama; Tab. 4: BAF-Emerin complex; Tab. 5: human calcineurin; Tab. 6: HGH-receptor complex), and the results of running our contaminant-free searches on data containing a simulated contaminant (Tab. 7 and Tab. 8).

Table 1: Initial concentrations and fractional masses for one-stage simulations ($A + B \rightarrow AB$).

Init Conc A (mg/ml)	Init Conc B (mg/ml)	Fractional Masses					
		1AUI			1D9G		
		A	B	AB	A	B	AB
0.5	1.0	0.108	0.610	0.282	0.001	0.357	0.642
1.0	1.0	0.182	0.396	0.422	0.010	0.043	0.947
2.0	1.0	0.281	0.207	0.512	0.310	0.001	0.689
3.0	1.0	0.360	0.123	0.517	0.483	0.000	0.517
4.0	1.0	0.429	0.079	0.493	0.586	0.000	0.414
4.5	1.0	0.458	0.065	0.477	0.624	0.000	0.376
0.5	0.0	1.000	0.000	0.000	1.000	0.000	0.000
0.0	1.0	0.000	1.000	0.000	0.000	1.000	0.000

Table 2: Initial concentrations and fractional masses for two-stage simulations ($A + B \rightarrow AB$, $AB + B \rightarrow AB_2$).

Init Conc A (mg/ml)	Init Conc B (mg/ml)	Fractional Masses							
		3HHR				2ODG			
		A	B	AB	AB_2	A	B	AB	AB_2
1.0	1.0	0.115	0.017	0.661	0.206	0.294	0.004	0.359	0.343
3.0	1.0	0.525	0.001	0.453	0.021	0.629	0.001	0.276	0.095
1.0	3.0	0.000	0.253	0.073	0.674	0.016	0.012	0.132	0.839
1.0	5.0	0.000	0.486	0.019	0.496	0.000	0.249	0.004	0.747
5.0	1.0	0.681	0.001	0.311	0.008	0.749	0.000	0.207	0.045
5.0	5.0	0.108	0.004	0.666	0.223	0.293	0.001	0.360	0.346
5.0	0.0	1.000	0.000	0.000	0.000	1.000	0.000	0.000	0.000
0.0	5.0	0.000	1.000	0.000	0.000	0.000	1.000	0.000	0.000

Table 3: Bovine IFN-gamma association model searches, over 10 sets of simulated noise. Pathways are abbreviated by the reaction products; e.g., (AB) means $A + B \rightarrow AB$, while (AB, AB_2) means $A + B \rightarrow AB$, $AB + B \rightarrow AB_2$. The bolded entries obtain the best scores, and are for the correct pathway. The simulated association constant was $K_1 = 3.43e6$.

	χ^2			MSMRD		
Pathway	$K_1 \pm$ SD	$K_2 \pm$ SD	Score $\pm$ SD	$K_1 \pm$ SD	$K_2 \pm$ SD	Score $\pm$ SD
(AB)	**3.30e06 $\pm$ 4.8e05**	-	**1.53e0 $\pm$ 1.1e-1**	**3.70e06 $\pm$ 4.8e5**	-	**3.74e-07 $\pm$ 3.0e-07**
(AB) **Fine**	**3.40e06 $\pm$ 7.1e04**	-	**1.49e0 $\pm$ 1.2e-1**	**3.64e06 $\pm$ 5.2e5**	-	**1.82e-11 $\pm$ 1.8e-11**
(AB_2)	8.00e07 $\pm$ 0.0e00	-	8.81e2 $\pm$ 2.1e0	8.00e07 $\pm$ 0.0e0	-	1.97e-05 $\pm$ 1.0e-05
(A_2B)	8.00e22 $\pm$ 1.8e07	-	1.82e3 $\pm$ 3.2e0	3.00e05 $\pm$ 0.0e0	-	2.69e-03 $\pm$ 3.6e-04
(A_2)	1.00e19 $\pm$ 0.0e00	-	7.32e3 $\pm$ 6.4e0	1.00e04 $\pm$ 0.0e0	-	1.07e-04 $\pm$ 1.3e-05
(B_2)	1.00e-06 $\pm$ 2.2e-22	-	2.86e3 $\pm$ 2.9e0	3.00e14 $\pm$ 0.0e0	-	1.36e-02 $\pm$ 2.4e-04
(AB, AB_2)	1.38e11 $\pm$ 1.7e11	3.30e08 $\pm$ 4.0e08	1.62e0 $\pm$ 1.2e-1	1.07e08 $\pm$ 3.1e8	9.01e04 $\pm$ 2.5e5	1.19e-03 $\pm$ 1.2e-03
(B_2, AB_2)	5.60e06 $\pm$ 5.2e05	8.30e14 $\pm$ 1.2e14	1.05e2 $\pm$ 1.0e1	5.00e04 $\pm$ 0.0e0	2.00e10 $\pm$ 0.0e0	4.41e-04 $\pm$ 4.1e-05
(AB, A_2B)	7.50e06 $\pm$ 4.8e06	7.29e03 $\pm$ 8.8e03	1.55e0 $\pm$ 2.0e-1	1.20e09 $\pm$ 1.3e9	1.40e01 $\pm$ 5.2e0	8.21e-04 $\pm$ 1.8e-03
(A_2, A_2B)	9.00e06 $\pm$ 0.0e00	7.00e14 $\pm$ 0.0e00	3.94e2 $\pm$ 1.6e0	1.20e09 $\pm$ 1.3e9	1.40e01 $\pm$ 5.2e0	8.21e-04 $\pm$ 0.0e00

Table 4: BAF-Emerin complex association model searches, over 10 sets of simulated noise. Pathways are abbreviated by the reaction products; e.g., (AB, AB_2) means $A + B \rightarrow AB$, $AB + B \rightarrow AB_2$. The bolded entries obtain the best scores, and are for the correct pathway. The simulated association constants were $K_1 = 3.21e5$, $K_2 = 4.23e5$.

	χ^2				MSMRD			
Pathway	$K_1 \pm$ SD	$K_2 \pm$ SD	$K_3 \pm$ SD	Score $\pm$ SD	$K_1 \pm$ SD	$K_2 \pm$ SD	$K_3 \pm$ SD	Score $\pm$ SD
(AB)	1.48e10 $\pm$ 3.0e10	-	-	3.98e4 $\pm$ 1.3e2	1.00e19 $\pm$ 0.0e00	-	-	6.23e-4 $\pm$ 1.9e-05
(AB_2)	3.00e18 $\pm$ 0.0e00	-	-	8.20e3 $\pm$ 5.9e0	1.00e09 $\pm$ 0.0e00	-	-	1.09e-5 $\pm$ 3.1e-06
(A_2B)	5.00e18 $\pm$ 0.0e00	-	-	5.56e4 $\pm$ 1.2e1	9.00e04 $\pm$ 0.0e00	-	-	8.75e-5 $\pm$ 1.1e-05
(A_2)	3.00e14 $\pm$ 0.0e00	-	-	4.37e4 $\pm$ 6.0e0	1.00e02 $\pm$ 0.0e00	-	-	1.20e-1 $\pm$ 5.2e-04
(B_2)	4.00e03 $\pm$ 0.0e00	-	-	5.25e3 $\pm$ 6.2e0	7.00e03 $\pm$ 0.0e00	-	-	4.62e-6 $\pm$ 2.0e-06
(AB, AB_2)	**3.00e05 $\pm$ 0.0e00**	**4.00e05 $\pm$ 0.0e0**	-	**1.17e0 $\pm$ 2.4e-1**	**3.00e05 $\pm$ 0.0e00**	**4.00e05 $\pm$ 0.0e0**	-	**1.33e-6 $\pm$ 6.8e-07**
(AB, AB_2) Fine	**3.21e05 $\pm$ 4.5e03**	**4.24e05 $\pm$ 6.9e3**	-	**1.12e0 $\pm$ 2.4e-1**	**3.24e05 $\pm$ 1.3e04**	**4.29e05 $\pm$ 1.9e4**	-	**1.03e-9 $\pm$ 6.6e-10**
(B_2, AB_2)	1.00e07 $\pm$ 0.0e00	6.00e14 $\pm$ 0.0e0	-	4.88e3 $\pm$ 7.4e0	9.00e03 $\pm$ 0.0e00	4.00e10 $\pm$ 0.0e0	-	4.53e-4 $\pm$ 2.7e-05
(AB, A_2B)	6.00e15 $\pm$ 0.0e00	3.00e13 $\pm$ 0.0e0	-	1.39e3 $\pm$ 3.0e0	5.00e04 $\pm$ 0.0e00	2.00e15 $\pm$ 0.0e0	-	1.42e-2 $\pm$ 2.0e-05
(A_2, A_2B)	4.00e07 $\pm$ 0.0e00	9.00e15 $\pm$ 0.0e0	-	2.25e4 $\pm$ 6.0e0	6.00e01 $\pm$ 0.0e00	4.00e05 $\pm$ 0.0e0	-	3.40e-3 $\pm$ 2.4e-04
(A_2, B_2, A_2B_2)	9.00e01 $\pm$ 0.0e00	9.00e10 $\pm$ 0.0e0	2.23e8 $\pm$ 6.2e8	2.62e3 $\pm$ 5.0e0	8.00e01 $\pm$ 0.0e00	9.00e10 $\pm$ 0.0e0	2.00e5 $\pm$ 0.0e0	1.27e-1 $\pm$ 3.7e-04
(AB, AB_2, A_2B_2)	2.00e05 $\pm$ 0.0e00	3.00e05 $\pm$ 0.0e0	1.00e1 $\pm$ 0.0e0	4.49e0 $\pm$ 3.9e-1	8.00e02 $\pm$ 0.0e00	8.00e02 $\pm$ 0.0e0	5.00e1 $\pm$ 0.0e0	2.50e-3 $\pm$ 2.5e-06
(AB, A_2B, A_2B_2)	4.50e10 $\pm$ 1.4e10	1.09e10 $\pm$ 5.0e9	8.90e3 $\pm$ 7.4e2	2.18e3 $\pm$ 3.8e1	6.20e10 $\pm$ 1.8e10	7.50e08 $\pm$ 1.4e8	7.90e6 $\pm$ 9.9e5	4.85e-2 $\pm$ 5.2e-05
(AB, AB_2, AB_3)	3.80e05 $\pm$ 4.2e04	4.80e04 $\pm$ 4.2e4	1.60e3 $\pm$ 8.4e2	1.28e0 $\pm$ 3.8e-1	1.07e07 $\pm$ 1.4e07	1.60e07 $\pm$ 2.1e7	3.10e1 $\pm$ 1.7e1	6.09e-5 $\pm$ 2.7e-05

Table 5: Human Calcineurin association model searches, over 10 sets of simulated noise. Pathways are abbreviated by the reaction products; e.g., (AB) means $A + B \rightarrow AB$, while (AB, AB_2) means $A + B \rightarrow AB$, $AB + B \rightarrow AB_2$. The bolded entries obtain the best scores, and are for the correct pathway. The simulated association constant was $K_1 = 4.24e4$.

	χ^2			MSMRD		
Pathway	$K_1 \pm$ SD	$K_2 \pm$ SD	Score $\pm$ SD	$K_1 \pm$ SD	$K_2 \pm$ SD	Score $\pm$ SD
(AB)	**4.00e04 $\pm$ 0.0e00**	-	**1.10e00 $\pm$ 5.0e-2**	**4.00e04 $\pm$ 0.0e00**	-	**5.03e-5 $\pm$ 2.4e-5**
(AB) **Fine**	**4.24e04 $\pm$ 9.7e02**	-	**1.08e00 $\pm$ 5.0e-2**	**4.24e04 $\pm$ 5.9e02**	-	**6.96e-9 $\pm$ 7.1e-9**
(AB_2)	6.00e07 $\pm$ 0.0e00	-	2.91e00 $\pm$ 1.0e-1	3.00e08 $\pm$ 0.0e00	-	3.55e-4 $\pm$ 8.4e-5
(A_2B)	3.20e18 $\pm$ 4.2e17	-	1.20e02 $\pm$ 9.0e-1	3.00e07 $\pm$ 0.0e00	-	1.00e-3 $\pm$ 1.6e-4
(A_2)	3.00e14 $\pm$ 0.0e00	-	3.27e02 $\pm$ 2.8e0	3.00e03 $\pm$ 0.0e00	-	1.88e-4 $\pm$ 5.1e-5
(B_2)	7.00e03 $\pm$ 0.0e00	-	7.71e02 $\pm$ 3.6e0	6.70e17 $\pm$ 1.2e18	-	4.57e-2 $\pm$ 1.3e-3
(AB, AB_2)	4.30e04 $\pm$ 4.8e03	5.35e02 $\pm$ 7.8e02	1.28e00 $\pm$ 8.0e-2	3.00e04 $\pm$ 0.0e00	5.10e2 $\pm$ 7.4e1	1.06e-3 $\pm$ 3.3e-4
(B_2, AB_2)	6.30e02 $\pm$ 4.8e01	1.00e08 $\pm$ 0.0e00	1.920e0 $\pm$ 9.0e-2	3.00e03 $\pm$ 0.0e00	1.00e9 $\pm$ 0.0e0	4.52e-3 $\pm$ 3.4e-4
(AB, A_2B)	7.30e04 $\pm$ 4.7e04	9.41e03 $\pm$ 1.5e04	1.29e00 $\pm$ 1.0e-1	5.60e04 $\pm$ 7.0e03	7.50e1 $\pm$ 1.8e1	8.15e-4 $\pm$ 2.9e-4
(A_2, A_2B)	8.20e05 $\pm$ 1.9e05	5.27e12 $\pm$ 1.7e12	1.31e00 $\pm$ 1.0e-1	5.80e03 $\pm$ 1.9e03	2.24e8 $\pm$ 1.8e8	2.79e-2 $\pm$ 3.1e-3

Table 6: HGH-receptor complex association model searches, over 10 sets of simulated noise. Pathways are abbreviated by the reaction products; e.g., (AB, AB_2) means $A + B \rightarrow AB$, $AB + B \rightarrow AB_2$. The bolded entries obtain the best scores, and are for the correct pathway. The simulated association constants were $K_1 = 8.43e5$ and $K_2 = 6.26e4$.

	χ^2				MSMRD			
Pathway	$K_1 \pm$ SD	$K_2 \pm$ SD	$K_3 \pm$ SD	Score $\pm$ SD	$K_1 \pm$ SD	$K_2 \pm$ SD	$K_3 \pm$ SD	Score $\pm$ SD
(AB)	6.00e04 $\pm$ 0.0e0	-	-	1.19e4 $\pm$ 9.2e0	2.20e06 $\pm$ 4.2e05	-	-	5.25e-06 $\pm$ 1.9e-06
(AB_2)	9.00e09 $\pm$ 0.0e0	-	-	1.01e3 $\pm$ 3.3e0	2.00e08 $\pm$ 0.0e00	-	-	1.57e-05 $\pm$ 3.9e-06
(A_2B)	5.00e17 $\pm$ 0.0e0	-	-	2.62e4 $\pm$ 1.5e1	1.00e06 $\pm$ 0.0e00	-	-	4.60e-03 $\pm$ 8.3e-05
(A_2)	6.00e02 $\pm$ 0.0e0	-	-	1.00e4 $\pm$ 2.9e0	1.00e-06 $\pm$ 2.2e-22	-	-	2.50e-01 $\pm$ 0.0e00
(B_2)	1.00e19 $\pm$ 0.0e0	-	-	4.56e4 $\pm$ 1.0e1	1.00e19 $\pm$ 0.0e00	-	-	2.97e-02 $\pm$ 1.1e-04
(AB, AB_2)	**8.00e05 $\pm$ 0.0e0**	**6.00e04 $\pm$ 0.0e0**	-	**1.14e0 $\pm$ 0.0e0**	**8.00e05 $\pm$ 0.0e00**	**6.00e4 $\pm$ 0.0e0**	-	**3.22e-06 $\pm$ 1.7e-06**
(AB, AB_2) Fine	**8.43e05 $\pm$ 9.1e3**	**6.26e04 $\pm$ 3.1e2**	-	**9.8e-1 $\pm$ 1.5e-1**	**8.45e05 $\pm$ 2.2e04**	**6.27e4 $\pm$ 8.4e2**	-	**3.37e-10 $\pm$ 3.4e-10**
(B_2, AB_2)	4.00e06 $\pm$ 0.0e0	9.00e15 $\pm$ 0.0e0	-	4.40e2 $\pm$ 2.6e0	9.10e02 $\pm$ 1.5e02	4.70e8 $\pm$ 4.8e7	-	7.14e-06 $\pm$ 3.3e-06
(AB, A_2B)	2.00e04 $\pm$ 0.0e0	9.00e04 $\pm$ 0.0e0	-	2.19e3 $\pm$ 4.5e0	1.00e11 $\pm$ 0.0e00	3.00e2 $\pm$ 0.0e0	-	1.91e-02 $\pm$ 7.4e-05
(A_2, A_2B)	3.00e06 $\pm$ 0.0e0	6.00e13 $\pm$ 0.0e0	-	1.11e4 $\pm$ 7.2e0	5.00e02 $\pm$ 0.0e00	9.00e6 $\pm$ 0.0e0	-	8.92e-04 $\pm$ 8.5e-05
(A_2, B_2, A_2B_2)	9.00e10 $\pm$ 0.0e0	4.00e04 $\pm$ 0.0e0	2.00e6 $\pm$ 0.0e0	2.62e3 $\pm$ 4.8e1	9.00e10 $\pm$ 0.0e00	1.60e5 $\pm$ 5.2e4	6.00e2 $\pm$ 0.0e0	7.47e-02 $\pm$ 2.3e-04
(AB, AB_2, A_2B_2)	8.00e05 $\pm$ 0.0e0	6.00e04 $\pm$ 0.0e0	1.10e1 $\pm$ 3.2e0	1.38e0 $\pm$ 1.9e-1	2.30e04 $\pm$ 4.8e03	1.00e3 $\pm$ 0.0e0	1.00e1 $\pm$ 0.0e0	1.27e-02 $\pm$ 3.6e-05
(AB, A_2B, A_2B_2)	9.70e03 $\pm$ 4.8e2	8.00e03 $\pm$ 1.3e3	2.00e3 $\pm$ 0.0e0	2.34e3 $\pm$ 1.4e1	9.00e10 $\pm$ 0.0e00	9.00e6 $\pm$ 0.0e0	5.00e7 $\pm$ 0.0e0	2.39e-01 $\pm$ 4.4e-04
(AB, AB_2, AB_3)	8.80e05 $\pm$ 4.2e4	5.00e04 $\pm$ 1.6e4	6.81e4 $\pm$ 1.5e5	1.33e0 $\pm$ 3.0e-1	8.3e05 $\pm$ 1.1e05	7.20e4 $\pm$ 4.2e3	3.40e1 $\pm$ 1.5e1	7.71e-05 $\pm$ 5.1e-05

Table 7: Contaminant-free search results for varying levels of contaminant.

	χ^2			MSMRD		
Contam	$K_1 \pm$ SD	$K_2 \pm$ SD	Score $\pm$ SD	$K_1 \pm$ SD	$K_2 \pm$ SD	Score $\pm$ SD
Bovine IFN-gamma, $A + B \rightarrow AB$						
.0000	3.40e06 $\pm$ 7.1e04	-	1.49e0 $\pm$ 1.2e-1	3.64e6 $\pm$ 5.2e5	-	1.82e-11 $\pm$ 1.8e-11
.0047	2.81e06 $\pm$ 6.2e04	-	1.48e0 $\pm$ 9.0e-2	2.36e6 $\pm$ 2.4e5	-	1.65e-10 $\pm$ 1.4e-10
.0113	2.22e06 $\pm$ 3.4e04	-	1.93e0 $\pm$ 7.0e-2	1.57e6 $\pm$ 1.8e5	-	4.81e-10 $\pm$ 5.9e-10
.0231	1.52e06 $\pm$ 2.6e04	-	3.56e0 $\pm$ 3.5e-1	9.19e5 $\pm$ 7.4e4	-	1.98e-10 $\pm$ 4.6e-10
BAF-Emerin complex, $A + B \rightarrow AB$, $AB + B \rightarrow AB_2$						
.0000	3.21e05 $\pm$ 4.5e03	4.24e05 $\pm$ 6.9e03	1.12e0 $\pm$ 2.4e-1	3.24e5 $\pm$ 1.3e4	4.29e5 $\pm$ 1.9e4	1.03e-09 $\pm$ 6.6e-10
.0047	4.23e05 $\pm$ 6.0e03	5.98e05 $\pm$ 8.2e03	1.60e0 $\pm$ 8.0e-2	3.14e5 $\pm$ 2.7e4	3.90e5 $\pm$ 3.1e4	4.07e-05 $\pm$ 1.1e-05
.0113	6.53e05 $\pm$ 2.4e04	1.02e06 $\pm$ 4.8e04	2.10e0 $\pm$ 9.0e-2	1.00e5 $\pm$ 0.0e0	1.10e5 $\pm$ 1.5e3	1.09e-06 $\pm$ 7.3e-07
.0231	3.57e15 $\pm$ 7.2e14	6.23e15 $\pm$ 1.2e15	2.68e0 $\pm$ 1.6e-1	6.35e4 $\pm$ 1.1e3	5.75e4 $\pm$ 8.1e2	1.64e-09 $\pm$ 9.1e-10

Table 8: Mean MARDs (%) for the best fine grid points resulting from contaminant-free searches for varying levels of contaminant.

Contam	I_A	I_B	I_{AB}	I_{AB_2}
Bovine IFN-gamma, $A + B \rightarrow AB$				
.0000	0.24	0.16	0.22	-
.0047	0.23	8.10	3.77	-
.0113	0.45	8.10	3.77	-
.0231	0.94	7.90	3.74	-
BAF-Emerin complex, $A + B \rightarrow AB,\ AB + B \rightarrow AB_2$				
.0000	0.08	0.08	0.15	0.06
.0047	1.33	33.13	23.94	27.93
.0113	3.25	33.15	23.92	28.02
.0231	6.57	33.13	23.83	27.98