**Supplementary Table S3. Two-receptor, one-ligand (2R1L) model predictions.** Tabulated model predictions across system configurations. Predictions reported as % of total dimers formed at steady-state.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Input Parameter | | **Model Predictions** | | |
| [R1­]/[R2] | **kL1 /kL2** | **D11 (%)** | **D12 (%)** | **D22 (%)** |
| 0.1 | 1.00E-03 | 7.4 | 40.3 | 52.3 |
| 0.1 | 4.64E-03 | 7.4 | 40.2 | 52.4 |
| 0.1 | 2.15E-02 | 7.3 | 39.5 | 53.2 |
| 0.1 | 1.00E-01 | 6.6 | 36.0 | 57.4 |
| 0.1 | 4.64E-01 | 2.5 | 16.4 | 81.2 |
| 0.1 | 2.15E+00 | 0.5 | 7.0 | 92.5 |
| 0.1 | 1.00E+01 | 0.1 | 5.3 | 94.6 |
| 0.1 | 4.64E+01 | 0.0 | 4.9 | 95.1 |
| 0.1 | 2.15E+02 | 0.0 | 4.8 | 95.2 |
| 0.1 | 1.00E+03 | 0.0 | 4.8 | 95.2 |
| 0.2 | 1.00E-03 | 12.1 | 41.0 | 46.8 |
| 0.2 | 4.64E-03 | 12.1 | 40.9 | 47.0 |
| 0.2 | 2.15E-02 | 12.0 | 40.5 | 47.6 |
| 0.2 | 1.00E-01 | 11.2 | 38.0 | 50.9 |
| 0.2 | 4.64E-01 | 5.6 | 22.6 | 71.8 |
| 0.2 | 2.15E+00 | 1.3 | 11.1 | 87.6 |
| 0.2 | 1.00E+01 | 0.3 | 8.6 | 91.1 |
| 0.2 | 4.64E+01 | 0.1 | 7.9 | 92.0 |
| 0.2 | 2.15E+02 | 0.0 | 7.7 | 92.2 |
| 0.2 | 1.00E+03 | 0.0 | 7.7 | 92.3 |
| 0.3 | 1.00E-03 | 19.2 | 40.9 | 39.9 |
| 0.3 | 4.64E-03 | 19.2 | 40.8 | 40.0 |
| 0.3 | 2.15E-02 | 19.0 | 40.5 | 40.5 |
| 0.3 | 1.00E-01 | 18.2 | 38.9 | 42.9 |
| 0.3 | 4.64E-01 | 11.5 | 28.9 | 59.6 |
| 0.3 | 2.15E+00 | 3.3 | 17.1 | 79.6 |
| 0.3 | 1.00E+01 | 0.9 | 13.5 | 85.5 |
| 0.3 | 4.64E+01 | 0.2 | 12.5 | 87.3 |
| 0.3 | 2.15E+02 | 0.0 | 12.3 | 87.7 |
| 0.3 | 1.00E+03 | 0.0 | 12.2 | 87.8 |
| 0.5 | 1.00E-03 | 29.0 | 39.4 | 31.6 |
| 0.5 | 4.64E-03 | 29.0 | 39.3 | 31.7 |
| 0.5 | 2.15E-02 | 28.9 | 39.1 | 31.9 |
| 0.5 | 1.00E-01 | 28.1 | 38.3 | 33.6 |
| 0.5 | 4.64E-01 | 21.3 | 33.4 | 45.3 |
| 0.5 | 2.15E+00 | 8.2 | 24.4 | 67.4 |
| 0.5 | 1.00E+01 | 2.5 | 20.5 | 77.0 |
| 0.5 | 4.64E+01 | 0.6 | 19.2 | 80.2 |
| 0.5 | 2.15E+02 | 0.1 | 18.9 | 81.0 |
| 0.5 | 1.00E+03 | 0.0 | 18.9 | 81.1 |
| 0.8 | 1.00E-03 | 41.2 | 36.1 | 22.7 |
| 0.8 | 4.64E-03 | 41.2 | 36.1 | 22.7 |
| 0.8 | 2.15E-02 | 41.2 | 36.0 | 22.8 |
| 0.8 | 1.00E-01 | 40.6 | 35.6 | 23.8 |
| 0.8 | 4.64E-01 | 34.8 | 34.3 | 30.8 |
| 0.8 | 2.15E+00 | 18.1 | 31.3 | 50.7 |
| 0.8 | 1.00E+01 | 6.3 | 29.1 | 64.6 |
| 0.8 | 4.64E+01 | 1.5 | 28.2 | 70.3 |
| 0.8 | 2.15E+02 | 0.3 | 28.0 | 71.7 |
| 0.8 | 1.00E+03 | 0.1 | 27.9 | 72.0 |
| 1.3 | 1.00E-03 | 54.4 | 31.1 | 14.5 |
| 1.3 | 4.64E-03 | 54.4 | 31.1 | 14.5 |
| 1.3 | 2.15E-02 | 54.4 | 31.0 | 14.6 |

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Table S3 cont. | | | | |
| [R1­]/[R2] | **kL2 /kL1** | **D11 (%)** | **D12 (%)** | **D22 (%)** |
| 1.3 | 4.64E-01 | 50.2 | 31.3 | 18.5 |
| 1.3 | 2.15E+00 | 33.8 | 33.9 | 32.3 |
| 1.3 | 1.00E+01 | 14.5 | 37.0 | 48.5 |
| 1.3 | 4.64E+01 | 4.0 | 38.6 | 57.4 |
| 1.3 | 2.15E+02 | 0.9 | 39.1 | 60.0 |
| 1.3 | 1.00E+03 | 0.2 | 39.2 | 60.6 |
| 2.2 | 1.00E-03 | 66.8 | 24.9 | 8.3 |
| 2.2 | 4.64E-03 | 66.8 | 24.9 | 8.3 |
| 2.2 | 2.15E-02 | 67.0 | 24.8 | 8.2 |
| 2.2 | 1.00E-01 | 67.0 | 24.7 | 8.3 |
| 2.2 | 4.64E-01 | 64.8 | 25.5 | 9.8 |
| 2.2 | 2.15E+00 | 52.6 | 30.4 | 16.9 |
| 2.2 | 1.00E+01 | 29.4 | 39.9 | 30.7 |
| 2.2 | 4.64E+01 | 9.7 | 47.9 | 42.4 |
| 2.2 | 2.15E+02 | 2.3 | 50.9 | 46.7 |
| 2.2 | 1.00E+03 | 0.5 | 51.7 | 47.8 |
| 3.6 | 1.00E-03 | 77.0 | 18.7 | 4.2 |
| 3.6 | 4.64E-03 | 77.1 | 18.7 | 4.2 |
| 3.6 | 2.15E-02 | 77.2 | 18.6 | 4.2 |
| 3.6 | 1.00E-01 | 77.5 | 18.4 | 4.2 |
| 3.6 | 4.64E-01 | 76.5 | 18.9 | 4.6 |
| 3.6 | 2.15E+00 | 69.5 | 23.1 | 7.5 |
| 3.6 | 1.00E+01 | 49.8 | 34.7 | 15.5 |
| 3.6 | 4.64E+01 | 21.5 | 51.5 | 27.0 |
| 3.6 | 2.15E+02 | 5.9 | 60.7 | 33.3 |
| 3.6 | 1.00E+03 | 1.4 | 63.4 | 35.2 |
| 6.0 | 1.00E-03 | 84.7 | 13.3 | 2.0 |
| 6.0 | 4.64E-03 | 84.7 | 13.3 | 2.0 |
| 6.0 | 2.15E-02 | 84.9 | 13.1 | 2.0 |
| 6.0 | 1.00E-01 | 85.2 | 12.9 | 1.9 |
| 6.0 | 4.64E-01 | 84.9 | 13.1 | 2.0 |
| 6.0 | 2.15E+00 | 81.6 | 15.5 | 2.9 |
| 6.0 | 1.00E+01 | 69.5 | 24.3 | 6.2 |
| 6.0 | 4.64E+01 | 41.2 | 45.0 | 13.9 |
| 6.0 | 2.15E+02 | 14.2 | 64.6 | 21.2 |
| 6.0 | 1.00E+03 | 3.5 | 72.4 | 24.1 |
| 10.0 | 1.00E-03 | 90.1 | 9.0 | 0.9 |
| 10.0 | 4.64E-03 | 90.1 | 9.0 | 0.9 |
| 10.0 | 2.15E-02 | 90.3 | 8.9 | 0.9 |
| 10.0 | 1.00E-01 | 90.6 | 8.6 | 0.8 |
| 10.0 | 4.64E-01 | 90.6 | 8.6 | 0.8 |
| 10.0 | 2.15E+00 | 89.2 | 9.7 | 1.1 |
| 10.0 | 1.00E+01 | 83.4 | 14.5 | 2.1 |
| 10.0 | 4.64E+01 | 64.0 | 30.5 | 5.5 |
| 10.0 | 2.15E+02 | 30.8 | 57.9 | 11.3 |
| 10.0 | 1.00E+03 | 9.0 | 75.9 | 15.1 |

**Supplementary Table S4. Three-receptor, one-ligand (3R1L) model predictions.** Tabulated model predictions across system configurations. Predictions reported as % of total dimers formed at steady-state.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Input Parameter** | | | | | **Model Predictions** | | | | | | |
| **n1:n2:n3** | **kL1/kL2** | | **kL**2**/k**L3 | | **D11** | **D12** | **D13** | **D22** | **D23** | **D33** |
| 1:1:1 | 0.001 | | 0.1 | | 20.2% | 19.4% | 15.7% | 18.7% | 14.9% | 11.2% |
| 1:1:1 | 0.01 | | 0.1 | | 20.1% | 19.4% | 15.7% | 18.7% | 14.9% | 11.2% |
| 1:1:1 | 0.1 | | 0.1 | | 20.1% | 19.4% | 15.6% | 18.7% | 15.0% | 11.2% |
| 1:1:1 | 1 | | 0.1 | | 19.2% | 19.2% | 15.4% | 19.2% | 15.4% | 11.5% |
| 1:1:1 | 10 | | 0.1 | | 13.6% | 18.2% | 13.6% | 22.7% | 18.2% | 13.6% |
| 1:1:1 | 100 | | 0.1 | | 3.5% | 16.3% | 10.5% | 29.1% | 23.3% | 17.4% |
| 1:1:1 | 1000 | | 0.1 | | 0.4% | 15.7% | 9.5% | 31.0% | 24.8% | 18.6% |
| 1:1:1 | 0.001 | | 1 | | 23.7% | 18.4% | 18.4% | 13.2% | 13.2% | 13.2% |
| 1:1:1 | 0.01 | | 1 | | 23.6% | 18.4% | 18.4% | 13.2% | 13.2% | 13.2% |
| 1:1:1 | 0.1 | | 1 | | 22.7% | 18.2% | 18.2% | 13.6% | 13.6% | 13.6% |
| 1:1:1 | 1 | | 1 | | 16.7% | 16.7% | 16.7% | 16.7% | 16.7% | 16.7% |
| 1:1:1 | 10 | | 1 | | 4.5% | 13.6% | 13.6% | 22.7% | 22.7% | 22.7% |
| 1:1:1 | 100 | | 1 | | 0.5% | 12.6% | 12.6% | 24.7% | 24.7% | 24.7% |
| 1:1:1 | 1000 | | 1 | | 0.1% | 12.5% | 12.5% | 25.0% | 25.0% | 25.0% |
| 1:1:1 | 0.001 | | 10 | | 29.9% | 16.6% | 23.3% | 3.3% | 10.0% | 16.7% |
| 1:1:1 | 0.01 | | 10 | | 29.1% | 16.3% | 23.3% | 3.5% | 10.5% | 17.4% |
| 1:1:1 | 0.1 | | 10 | | 22.7% | 13.6% | 22.7% | 4.5% | 13.6% | 22.7% |
| 1:1:1 | 1 | | 10 | | 7.1% | 7.1% | 21.4% | 7.1% | 21.4% | 35.7% |
| 1:1:1 | 10 | | 10 | | 0.9% | 4.5% | 20.9% | 8.2% | 24.6% | 40.9% |
| 1:1:1 | 100 | | 10 | | 0.1% | 4.2% | 20.8% | 8.3% | 25.0% | 41.6% |
| 1:1:1 | 1000 | | 10 | | 0.0% | 4.2% | 20.8% | 8.3% | 25.0% | 41.7% |
| 1:2:1 | 0.001 | | 0.1 | | 10.3% | 20.0% | 8.4% | 38.8% | 16.1% | 6.4% |
| 1:2:1 | 0.01 | | 0.1 | | 10.3% | 20.0% | 8.4% | 38.8% | 16.1% | 6.4% |
| 1:2:1 | 0.1 | | 0.1 | | 10.2% | 20.0% | 8.3% | 38.9% | 16.2% | 6.4% |
| 1:2:1 | 1 | | 0.1 | | 9.8% | 19.7% | 8.2% | 39.4% | 16.4% | 6.5% |
| 1:2:1 | 10 | | 0.1 | | 7.1% | 17.9% | 7.1% | 43.0% | 17.9% | 7.1% |
| 1:2:1 | 100 | | 0.1 | | 1.9% | 14.3% | 5.1% | 49.8% | 20.7% | 8.2% |
| 1:2:1 | 1000 | | 0.1 | | 0.2% | 13.2% | 4.4% | 51.9% | 21.6% | 8.6% |
| 1:2:1 | 0.001 | | 1 | | 12.8% | 20.8% | 10.4% | 32.0% | 16.0% | 8.0% |
| 1:2:1 | 0.01 | | 1 | | 12.7% | 20.8% | 10.4% | 32.1% | 16.0% | 8.0% |
| 1:2:1 | 0.1 | | 1 | | 12.3% | 20.4% | 10.2% | 32.6% | 16.3% | 8.1% |
| 1:2:1 | 1 | | 1 | | 9.1% | 18.2% | 9.1% | 36.4% | 18.2% | 9.1% |
| 1:2:1 | | 10 | | 1 | 2.5% | 13.5% | 6.8% | 44.1% | 22.0% | 11.0% |
| 1:2:1 | | 100 | | 1 | 0.3% | 12.0% | 6.0% | 46.7% | 23.3% | 11.7% |
| 1:2:1 | | 1000 | | 1 | 0.0% | 11.8% | 5.9% | 47.0% | 23.5% | 11.8% |
| 1:2:1 | | 0.001 | | 10 | 20.3% | 23.2% | 16.5% | 11.6% | 15.7% | 12.7% |
| 1:2:1 | | 0.01 | | 10 | 19.7% | 22.7% | 16.4% | 12.0% | 16.1% | 13.1% |
| 1:2:1 | | 0.1 | | 10 | 15.7% | 19.3% | 15.7% | 14.3% | 19.3% | 15.7% |
| 1:2:1 | | 1 | | 10 | 5.1% | 10.3% | 13.8% | 20.6% | 27.7% | 22.5% |
| 1:2:1 | | 10 | | 10 | 0.7% | 6.5% | 13.0% | 23.2% | 31.2% | 25.4% |
| 1:2:1 | | 100 | | 10 | 0.1% | 6.0% | 12.9% | 23.6% | 31.7% | 25.8% |
| 1:2:1 | | 1000 | | 10 | 0.0% | 5.9% | 12.9% | 23.6% | 31.7% | 25.8% |
| 2:1:1 | | 0.001 | | 0.1 | 40.3% | 19.6% | 16.4% | 9.5% | 7.9% | 6.3% |
| 2:1:1 | | 0.01 | | 0.1 | 40.3% | 19.6% | 16.4% | 9.5% | 7.9% | 6.3% |
| 2:1:1 | | 0.1 | | 0.1 | 40.2% | 19.6% | 16.4% | 9.5% | 7.9% | 6.3% |
| 2:1:1 | | 1 | | 0.1 | 39.4% | 19.7% | 16.4% | 9.8% | 8.2% | 6.5% |
| 2:1:1 | | 10 | | 0.1 | 32.6% | 20.4% | 16.3% | 12.3% | 10.2% | 8.1% |
| 2:1:1 | | 100 | | 0.1 | 12.0% | 22.7% | 16.1% | 19.7% | 16.4% | 13.1% |
| 2:1:1 | | 1000 | | 0.1 | 1.6% | 23.9% | 16.0% | 23.5% | 19.5% | 15.5% |
| 2:1:1 | | 0.001 | | 1 | 43.8% | 17.8% | 17.8% | 6.9% | 6.9% | 6.9% |
| 2:1:1 | | 0.01 | | 1 | 43.7% | 17.8% | 17.8% | 6.9% | 6.9% | 6.9% |
| 2:1:1 | | 0.1 | | 1 | 43.0% | 17.9% | 17.9% | 7.1% | 7.1% | 7.1% |
| 2:1:1 | | 1 | | 1 | 36.4% | 18.2% | 18.2% | 9.1% | 9.1% | 9.1% |
| 2:1:1 | | 10 | | 1 | 14.3% | 19.3% | 19.3% | 15.7% | 15.7% | 15.7% |
| 2:1:1 | | 100 | | 1 | 2.0% | 19.9% | 19.9% | 19.4% | 19.4% | 19.4% |
| 2:1:1 | | 1000 | | 1 | 0.2% | 19.9% | 19.9% | 20.0% | 20.0% | 20.0% |
| 2:1:1 | | 0.001 | | 10 | 50.4% | 14.4% | 20.5% | 1.8% | 4.9% | 7.9% |
| 2:1:1 | | 0.01 | | 10 | 49.8% | 14.3% | 20.7% | 1.9% | 5.1% | 8.2% |
| 2:1:1 | | 0.1 | | 10 | 44.1% | 13.5% | 22.0% | 2.5% | 6.8% | 11.0% |
| 2:1:1 | | 1 | | 10 | 20.6% | 10.3% | 27.7% | 5.1% | 13.8% | 22.5% |
| 2:1:1 | | 10 | | 10 | 3.2% | 7.9% | 31.8% | 7.1% | 19.0% | 31.0% |
| 2:1:1 | | 100 | | 10 | 0.3% | 7.5% | 32.5% | 7.4% | 19.9% | 32.4% |
| 2:1:1 | | 1000 | | 10 | 0.0% | 7.4% | 32.6% | 7.4% | 20.0% | 32.5% |

**Supplementary Table S5. Four-receptor, one-ligand model (4R1L) predictions.** Tabulated model predictions across system configurations. Initial receptor concentrations (nR1, etc) expressed in receptors/cell. Predictions reported as % of total dimers formed at steady-state.

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Input Parameter | | | | | Model Predictions | | | | | | | | | |
| kL1/kL2 | **nR1** | **nR2** | **nR3** | **nR4** | **D11** | **D12** | **D13** | **D14** | **D22** | **D23** | **D24** | **D33** | **D34** | **D44** |
| 0.001 | 1000 | 1000 | 1000 | 1000 | 13.9% | 11.3% | 11.3% | 11.3% | 8.7% | 8.7% | 8.7% | 8.7% | 8.7% | 8.7% |
| 0.01 | 1000 | 1000 | 1000 | 1000 | 13.9% | 11.3% | 11.3% | 11.3% | 8.7% | 8.7% | 8.7% | 8.7% | 8.7% | 8.7% |
| 0.1 | 1000 | 1000 | 1000 | 1000 | 13.4% | 11.1% | 11.1% | 11.1% | 8.9% | 8.9% | 8.9% | 8.9% | 8.9% | 8.9% |
| 1 | 1000 | 1000 | 1000 | 1000 | 10.0% | 10.0% | 10.0% | 10.0% | 10.0% | 10.0% | 10.0% | 10.0% | 10.0% | 10.0% |
| 10 | 1000 | 1000 | 1000 | 1000 | 2.8% | 7.6% | 7.6% | 7.6% | 12.4% | 12.4% | 12.4% | 12.4% | 12.4% | 12.4% |
| 100 | 1000 | 1000 | 1000 | 1000 | 0.3% | 6.8% | 6.8% | 6.8% | 13.2% | 13.2% | 13.2% | 13.2% | 13.2% | 13.2% |
| 1000 | 1000 | 1000 | 1000 | 1000 | 0.0% | 6.7% | 6.7% | 6.7% | 13.3% | 13.3% | 13.3% | 13.3% | 13.3% | 13.3% |
| 0.001 | 2000 | 1000 | 1000 | 1000 | 30.6% | 12.8% | 12.8% | 12.8% | 5.2% | 5.2% | 5.2% | 5.2% | 5.2% | 5.2% |
| 0.01 | 2000 | 1000 | 1000 | 1000 | 30.5% | 12.8% | 12.8% | 12.8% | 5.2% | 5.2% | 5.2% | 5.2% | 5.2% | 5.2% |
| 0.1 | 2000 | 1000 | 1000 | 1000 | 29.9% | 12.8% | 12.8% | 12.8% | 5.3% | 5.3% | 5.3% | 5.3% | 5.3% | 5.3% |
| 1 | 2000 | 1000 | 1000 | 1000 | 25.0% | 12.5% | 12.5% | 12.5% | 6.3% | 6.3% | 6.3% | 6.3% | 6.3% | 6.3% |
| 10 | 2000 | 1000 | 1000 | 1000 | 9.5% | 11.6% | 11.6% | 11.6% | 9.3% | 9.3% | 9.3% | 9.3% | 9.3% | 9.3% |
| 100 | 2000 | 1000 | 1000 | 1000 | 1.3% | 11.2% | 11.2% | 11.2% | 10.9% | 10.9% | 10.9% | 10.9% | 10.9% | 10.9% |
| 1000 | 2000 | 1000 | 1000 | 1000 | 0.1% | 11.1% | 11.1% | 11.1% | 11.1% | 11.1% | 11.1% | 11.1% | 11.1% | 11.1% |
| 0.001 | 10000 | 1000 | 1000 | 1000 | 75.3% | 7.0% | 7.0% | 7.0% | 0.6% | 0.6% | 0.6% | 0.6% | 0.6% | 0.6% |
| 0.01 | 10000 | 1000 | 1000 | 1000 | 75.3% | 7.0% | 7.0% | 7.0% | 0.6% | 0.6% | 0.6% | 0.6% | 0.6% | 0.6% |
| 0.1 | 10000 | 1000 | 1000 | 1000 | 75.1% | 7.0% | 7.0% | 7.0% | 0.6% | 0.6% | 0.6% | 0.6% | 0.6% | 0.6% |
| 1 | 10000 | 1000 | 1000 | 1000 | 73.5% | 7.4% | 7.4% | 7.4% | 0.7% | 0.7% | 0.7% | 0.7% | 0.7% | 0.7% |
| 10 | 10000 | 1000 | 1000 | 1000 | 60.5% | 10.3% | 10.3% | 10.3% | 1.4% | 1.4% | 1.4% | 1.4% | 1.4% | 1.4% |
| 100 | 10000 | 1000 | 1000 | 1000 | 21.8% | 18.9% | 18.9% | 18.9% | 3.6% | 3.6% | 3.6% | 3.6% | 3.6% | 3.6% |
| 1000 | 10000 | 1000 | 1000 | 1000 | 3.0% | 23.1% | 23.1% | 23.1% | 4.6% | 4.6% | 4.6% | 4.6% | 4.6% | 4.6% |
| 0.001 | 1000 | 10000 | 1000 | 1000 | 0.9% | 8.0% | 0.8% | 0.8% | 72.8% | 7.3% | 7.3% | 0.7% | 0.7% | 0.7% |
| 0.01 | 1000 | 10000 | 1000 | 1000 | 0.9% | 7.9% | 0.8% | 0.8% | 72.9% | 7.3% | 7.3% | 0.7% | 0.7% | 0.7% |
| 0.1 | 1000 | 10000 | 1000 | 1000 | 0.8% | 7.9% | 0.8% | 0.8% | 72.9% | 7.3% | 7.3% | 0.7% | 0.7% | 0.7% |
| 1 | 1000 | 10000 | 1000 | 1000 | 0.7% | 7.4% | 0.7% | 0.7% | 73.5% | 7.4% | 7.4% | 0.7% | 0.7% | 0.7% |
| 10 | 1000 | 10000 | 1000 | 1000 | 0.3% | 5.4% | 0.5% | 0.5% | 75.8% | 7.6% | 7.6% | 0.8% | 0.8% | 0.8% |
| 100 | 1000 | 10000 | 1000 | 1000 | 0.0% | 4.1% | 0.4% | 0.4% | 77.3% | 7.7% | 7.7% | 0.8% | 0.8% | 0.8% |
| 1000 | 1000 | 10000 | 1000 | 1000 | 0.0% | 3.9% | 0.4% | 0.4% | 77.5% | 7.7% | 7.7% | 0.8% | 0.8% | 0.8% |
| 0.001 | 1000 | 2000 | 2000 | 2000 | 4.1% | 7.2% | 7.2% | 7.2% | 12.4% | 12.4% | 12.4% | 12.4% | 12.4% | 12.4% |
| 0.01 | 1000 | 2000 | 2000 | 2000 | 4.1% | 7.2% | 7.2% | 7.2% | 12.4% | 12.4% | 12.4% | 12.4% | 12.4% | 12.4% |
| 0.1 | 1000 | 2000 | 2000 | 2000 | 4.0% | 7.1% | 7.1% | 7.1% | 12.4% | 12.4% | 12.4% | 12.4% | 12.4% | 12.4% |
| 1 | 1000 | 2000 | 2000 | 2000 | 3.2% | 6.5% | 6.5% | 6.5% | 12.9% | 12.9% | 12.9% | 12.9% | 12.9% | 12.9% |
| 10 | 1000 | 2000 | 2000 | 2000 | 1.1% | 4.6% | 4.6% | 4.6% | 14.2% | 14.2% | 14.2% | 14.2% | 14.2% | 14.2% |
| 100 | 1000 | 2000 | 2000 | 2000 | 0.1% | 3.8% | 3.8% | 3.8% | 14.7% | 14.7% | 14.7% | 14.7% | 14.7% | 14.7% |
| 1000 | 1000 | 2000 | 2000 | 2000 | 0.0% | 3.7% | 3.7% | 3.7% | 14.8% | 14.8% | 14.8% | 14.8% | 14.8% | 14.8% |

**Supplementary Table S6. Two-ligand, one receptor (2L1R) model predictions.** Tabulated model predictions across system configurations. DA and DB are the % of total dimers bound to LA and LB, respectively, at steady-state.

|  |  |  |  |
| --- | --- | --- | --- |
| Input Parameters | | Model Predictions | |
| [LA]/[LB] | **kLA/kLB** | **DA** | **DB** |
| 0.01 | 0.001 | 0.0% | 100.0% |
| 0.01 | 0.01 | 0.0% | 100.0% |
| 0.01 | 0.1 | 0.1% | 99.9% |
| 0.01 | 1 | 1.0% | 99.0% |
| 0.01 | 10 | 9.1% | 90.9% |
| 0.01 | 100 | 49.5% | 50.5% |
| 0.01 | 1000 | 90.6% | 9.4% |
| 0.1 | 0.001 | 0.0% | 100.0% |
| 0.1 | 0.01 | 0.1% | 99.9% |
| 0.1 | 0.1 | 1.0% | 99.0% |
| 0.1 | 1 | 9.1% | 90.9% |
| 0.1 | 10 | 50.0% | 50.0% |
| 0.1 | 100 | 90.9% | 9.1% |
| 0.1 | 1000 | 99.0% | 1.0% |
| 1 | 0.001 | 0.1% | 99.9% |
| 1 | 0.01 | 1.0% | 99.0% |
| 1 | 0.1 | 9.1% | 90.9% |
| 1 | 1 | 50.0% | 50.0% |
| 1 | 10 | 90.9% | 9.1% |
| 1 | 100 | 99.0% | 1.0% |
| 1 | 1000 | 99.9% | 0.1% |
| 10 | 0.001 | 1.0% | 99.0% |
| 10 | 0.01 | 9.1% | 90.9% |
| 10 | 0.1 | 50.0% | 50.0% |
| 10 | 1 | 90.9% | 9.1% |
| 10 | 10 | 99.0% | 1.0% |
| 10 | 100 | 99.9% | 0.1% |
| 10 | 1000 | 100.0% | 0.0% |
| 100 | 0.001 | 9% | 91% |
| 100 | 0.01 | 50% | 50% |
| 100 | 0.1 | 91% | 9% |
| 100 | 1 | 99% | 1% |
| 100 | 10 | 100% | 0% |
| 100 | 100 | 100% | 0% |
| 100 | 1000 | 100% | 0% |

**Supplementary Table S7. Two-ligand, two-receptor, no-overlapping interactions (2L2R0X) model predictions.** Tabulated model predictions across system configurations. D11, D12, and D22 are % homo- and heterodimers of total formed dimers at steady-state. DA and DB are the % of all dimers bound to LA and LB, respectively, at steady-state.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Input Parameters | | **Model Predictions** | | | | |
| [LA]/[LB] | **kA1/kB2** | **D11** | **D12** | **D22** | **DA** | **DB** |
| 0.01 | 0.001 | 0.0% | 99.9% | 0.1% | 0.0% | 100.0% |
| 0.01 | 0.01 | 0.1% | 99.8% | 0.1% | 0.1% | 99.9% |
| 0.01 | 0.1 | 0.8% | 99.0% | 0.1% | 0.8% | 99.2% |
| 0.01 | 1 | 7.6% | 92.3% | 0.1% | 7.6% | 92.4% |
| 0.01 | 10 | 36.1% | 63.8% | 0.2% | 36.2% | 63.8% |
| 0.01 | 100 | 27.3% | 50.0% | 22.7% | 50.0% | 50.0% |
| 0.01 | 1000 | 4.2% | 50.0% | 45.7% | 50.0% | 50.0% |
| 0.1 | 0.001 | 0.1% | 99.8% | 0.1% | 0.1% | 99.9% |
| 0.1 | 0.01 | 0.8% | 99.0% | 0.1% | 0.9% | 99.2% |
| 0.1 | 0.1 | 7.6% | 92.3% | 0.1% | 7.6% | 92.4% |
| 0.1 | 1 | 36.4% | 63.4% | 0.2% | 36.5% | 63.5% |
| 0.1 | 10 | 25.2% | 50.0% | 24.8% | 50.0% | 50.0% |
| 0.1 | 100 | 3.9% | 50.0% | 46.0% | 50.0% | 50.0% |
| 0.1 | 1000 | 0.4% | 50.0% | 49.5% | 50.0% | 50.0% |
| 1 | 0.001 | 0.8% | 99.0% | 0.1% | 0.9% | 99.2% |
| 1 | 0.01 | 7.6% | 92.3% | 0.1% | 7.6% | 92.4% |
| 1 | 0.1 | 36.5% | 63.4% | 0.2% | 36.6% | 63.4% |
| 1 | 1 | 25.0% | 50.0% | 25.0% | 50.0% | 50.0% |
| 1 | 10 | 3.9% | 50.0% | 46.1% | 50.0% | 50.0% |
| 1 | 100 | 0.4% | 50.0% | 49.5% | 50.0% | 50.0% |
| 1 | 1000 | 0.0% | 50.0% | 49.9% | 50.0% | 50.0% |
| 10 | 0.001 | 7.6% | 92.3% | 0.1% | 7.6% | 92.4% |
| 10 | 0.01 | 36.5% | 63.4% | 0.2% | 36.6% | 63.4% |
| 10 | 0.1 | 25.0% | 50.0% | 25.0% | 50.0% | 50.0% |
| 10 | 1 | 3.9% | 50.0% | 46.1% | 50.0% | 50.0% |
| 10 | 10 | 0.4% | 50.0% | 49.6% | 50.0% | 50.0% |
| 10 | 100 | 0.0% | 50.0% | 49.9% | 50.0% | 50.0% |
| 10 | 1000 | 0.0% | 50.0% | 50.0% | 50.0% | 50.0% |
| 100 | 0.001 | 36.5% | 63.3% | 0.2% | 36.6% | 63.4% |
| 100 | 0.01 | 25.0% | 50.0% | 25.0% | 50.0% | 50.0% |
| 100 | 0.1 | 3.9% | 50.0% | 46.1% | 50.0% | 50.0% |
| 100 | 1 | 0.4% | 50.0% | 49.6% | 50.0% | 50.0% |
| 100 | 10 | 0.0% | 50.0% | 49.9% | 50.0% | 50.0% |
| 100 | 100 | 0.0% | 50.0% | 50.0% | 50.0% | 50.0% |
| 100 | 1000 | 0.0% | 50.0% | 50.0% | 50.0% | 50.0% |

**Supplementary Table S8. Two-ligand, two-receptor, one-overlap (2L2R1X) model predictions.** Tabulated model predictions across system configurations. D11, D12, and D22 are % homo- and heterodimers of total formed dimers at steady-state. DA and DB are the % of all dimers bound to LA and LB, respectively, at steady-state.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Input Parameters | | **Model Predictions** | | | | |
| [LA]/[LB] | **kA2/kB2** | **D11** | **D12** | **D22** | **DA** | **DB** |
| 0.01 | 0.001 | 7.6% | 92.3% | 0.1% | 7.6% | 92.4% |
| 0.01 | 0.01 | 7.6% | 92.3% | 0.1% | 7.6% | 92.4% |
| 0.01 | 0.1 | 7.7% | 92.2% | 0.1% | 7.7% | 92.3% |
| 0.01 | 1 | 8.4% | 91.5% | 0.1% | 8.4% | 91.6% |
| 0.01 | 10 | 14.8% | 85.0% | 0.2% | 14.8% | 85.2% |
| 0.01 | 100 | 44.6% | 52.2% | 3.2% | 48.2% | 51.8% |
| 0.01 | 1000 | 46.3% | 36.3% | 17.4% | 87.6% | 12.4% |
| 0.1 | 0.001 | 36.6% | 63.1% | 0.3% | 36.8% | 63.2% |
| 0.1 | 0.01 | 36.6% | 63.1% | 0.3% | 36.8% | 63.2% |
| 0.1 | 0.1 | 36.8% | 62.9% | 0.3% | 37.0% | 63.0% |
| 0.1 | 1 | 38.5% | 61.1% | 0.5% | 38.8% | 61.2% |
| 0.1 | 10 | 46.6% | 48.1% | 5.3% | 53.4% | 46.6% |
| 0.1 | 100 | 46.9% | 36.1% | 17.0% | 88.6% | 11.4% |
| 0.1 | 1000 | 61.5% | 33.7% | 4.7% | 98.7% | 1.3% |
| 1 | 0.001 | 42.4% | 43.8% | 13.8% | 58.3% | 41.7% |
| 1 | 0.01 | 42.3% | 43.8% | 13.9% | 58.4% | 41.6% |
| 1 | 0.1 | 42.1% | 43.5% | 14.4% | 59.2% | 40.8% |
| 1 | 1 | 40.7% | 41.0% | 18.3% | 66.9% | 33.1% |
| 1 | 10 | 45.4% | 35.6% | 19.0% | 90.3% | 9.7% |
| 1 | 100 | 61.2% | 33.7% | 5.1% | 98.8% | 1.2% |
| 1 | 1000 | 66.0% | 33.4% | 0.6% | 99.9% | 0.1% |
| 10 | 0.001 | 23.9% | 35.8% | 40.3% | 80.1% | 19.9% |
| 10 | 0.01 | 24.0% | 35.8% | 40.2% | 80.4% | 19.6% |
| 10 | 0.1 | 25.1% | 35.4% | 39.5% | 83.7% | 16.3% |
| 10 | 1 | 34.4% | 34.4% | 31.2% | 94.0% | 6.0% |
| 10 | 10 | 56.9% | 33.6% | 9.5% | 99.2% | 0.8% |
| 10 | 100 | 65.5% | 33.4% | 1.2% | 99.9% | 0.1% |
| 10 | 1000 | 66.5% | 33.3% | 0.1% | 100.0% | 0.0% |
| 100 | 0.001 | 5.4% | 33.7% | 60.9% | 86.5% | 13.5% |
| 100 | 0.01 | 5.8% | 33.7% | 60.5% | 88.5% | 11.5% |
| 100 | 0.1 | 10.1% | 33.6% | 56.3% | 95.4% | 4.6% |
| 100 | 1 | 33.4% | 33.4% | 33.1% | 99.3% | 0.7% |
| 100 | 10 | 60.2% | 33.4% | 6.5% | 99.9% | 0.1% |
| 100 | 100 | 66.0% | 33.3% | 0.7% | 100.0% | 0.0% |
| 100 | 1000 | 66.6% | 33.3% | 0.1% | 100.0% | 0.0% |

**Supplementary Table S9. Two-ligand, two-receptor, two-overlap (2L2R2X) model predictions.** Tabulated model predictions across system configurations. D11, D12, and D22 are % homo- and heterodimers of total formed dimers at steady-state. DA and DB are the % of all dimers bound to LA and LB, respectively, at steady-state.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Input Parameters | | **Model Predictions** | | | | |
| [LA]/[LB] | **kA2/kB2** | **D11** | **D12** | **D22** | **DA** | **DB** |
| 0.01 | 0.001 | 33.3% | 33.3% | 33.4% | 0.5% | 99.5% |
| 0.01 | 0.01 | 33.3% | 33.3% | 33.4% | 0.5% | 99.5% |
| 0.01 | 0.1 | 33.3% | 33.3% | 33.4% | 0.5% | 99.5% |
| 0.01 | 1 | 33.3% | 33.3% | 33.3% | 1.0% | 99.0% |
| 0.01 | 10 | 33.5% | 33.3% | 33.2% | 5.2% | 94.8% |
| 0.01 | 100 | 34.9% | 33.3% | 31.7% | 31.8% | 68.2% |
| 0.01 | 1000 | 44.0% | 33.3% | 22.7% | 74.7% | 25.3% |
| 0.1 | 0.001 | 33.2% | 33.3% | 33.5% | 4.7% | 95.3% |
| 0.1 | 0.01 | 33.2% | 33.3% | 33.5% | 4.8% | 95.2% |
| 0.1 | 0.1 | 33.2% | 33.3% | 33.5% | 5.2% | 94.8% |
| 0.1 | 1 | 33.3% | 33.3% | 33.3% | 9.1% | 90.9% |
| 0.1 | 10 | 34.8% | 33.3% | 31.8% | 34.5% | 65.5% |
| 0.1 | 100 | 44.7% | 33.3% | 21.9% | 75.8% | 24.2% |
| 0.1 | 1000 | 61.3% | 33.3% | 5.3% | 86.1% | 13.9% |
| 1 | 0.001 | 31.6% | 33.3% | 35.0% | 32.1% | 67.9% |
| 1 | 0.01 | 31.7% | 33.3% | 35.0% | 32.4% | 67.6% |
| 1 | 0.1 | 31.8% | 33.3% | 34.9% | 34.6% | 65.4% |
| 1 | 1 | 33.3% | 33.3% | 33.3% | 50.0% | 50.0% |
| 1 | 10 | 43.5% | 33.3% | 23.2% | 79.8% | 20.2% |
| 1 | 100 | 60.9% | 33.3% | 5.8% | 88.2% | 11.8% |
| 1 | 1000 | 66.0% | 33.3% | 0.7% | 89.1% | 10.9% |
| 10 | 0.001 | 21.7% | 33.3% | 45.0% | 75.4% | 24.6% |
| 10 | 0.01 | 21.8% | 33.3% | 44.8% | 75.9% | 24.1% |
| 10 | 0.1 | 23.2% | 33.3% | 43.5% | 79.8% | 20.2% |
| 10 | 1 | 33.3% | 33.3% | 33.3% | 90.9% | 9.1% |
| 10 | 10 | 56.7% | 33.3% | 10.0% | 95.2% | 4.8% |
| 10 | 100 | 65.4% | 33.3% | 1.3% | 95.6% | 4.4% |
| 10 | 1000 | 66.5% | 33.3% | 0.1% | 95.6% | 4.4% |
| 100 | 0.001 | 5.3% | 33.3% | 61.4% | 86.2% | 13.8% |
| 100 | 0.01 | 5.7% | 33.3% | 60.9% | 88.2% | 11.8% |
| 100 | 0.1 | 10.0% | 33.3% | 56.7% | 95.2% | 4.8% |
| 100 | 1 | 33.3% | 33.3% | 33.3% | 99.0% | 1.0% |
| 100 | 10 | 60.2% | 33.3% | 6.5% | 99.4% | 0.6% |
| 100 | 100 | 65.9% | 33.3% | 0.7% | 99.4% | 0.6% |
| 100 | 1000 | 66.6% | 33.3% | 0.1% | 99.4% | 0.6% |