**Table S1.** Summary of atomistic simulation systems of HER2 homodimers and heterodimers.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **HER dimers** | **Ligand** | **Trastuzumab Binding** | **Conformation of HER2** | **Time (ns)** |
| HER2+HER2 | n/a | no | receiver | 500 |
| HER2+HER2 | n/a | no | activator | 500 |
| HER2+HER2 | n/a | yes | receiver | 300 |
| HER2+HER2 | n/a | yes | activator | 500 |
| HER1+HER2 | yes | no | receiver | 500 |
| HER1+HER2 | yes | no | activator | 500 |
| HER1+HER2 | yes | yes | receiver | 300 |
| HER1+HER2 | yes | yes | activator | 500 |
| HER3+HER2 | yes | no | receiver | 500 |
| HER3+HER2 | yes | yes | receiver | 300 |