**Table S1.** **Root mean square distances among docking solutions.**

|  |  |  |  |
| --- | --- | --- | --- |
| **Morphinan core RMSD (Å)** | **MedusaDock** | **Previous Docking\*** | **-FNA** |
| **MedusaDock** | 0 | 5.7 | 3.8 |
| **Previous Docking** | 5.7 | 0 | 4.7 |
| **-FNA** | 3.8 | 4.7 | 0 |

Values are computed over the morphinan core’s heavy atoms of the MedusaDock solution, the previously published docking solutions for morphine,\* and the crystallographic conformation of -FNA covalently bound to 7TM-mOR. \*Ref. [7] in the main text.