***Information S2***

***Supporting Coordinates are provided in PDB format:***

The MD coordinates of Complex 14, extracted every 2 ns, are provided as Supporting Information in PDB format. The structures are aligned with regard to the backbone of the CCR5 transmembrane helical region. The correspondence of PDB files and time in the MD simulation is as follows:

|  |  |
| --- | --- |
| PDB file | Time (ns) |
| coordinates.s1.pdb | 2 |
| coordinates.s2.pdb | 4 |
| coordinates.s3.pdb | 6 |
| coordinates.s4.pdb | 8 |
| coordinates.s5.pdb | 10 |
| coordinates.s6.pdb | 12 |
| coordinates.s7.pdb | 14 |
| coordinates.s8.pdb | 16 |
| coordinates.s9.pdb | 18 |
| coordinates.s10.pdb | 20 |