Supplementary file 1

**Substrate transport and anion permeation proceed through distinct pathways in glutamate transporters**

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**Table 1. Summary of MD simulations**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | *Run #* | Run Identifier | Duration (ns) | Initial conformation | Voltage  kcal/(mol.Å.e) |
| GltPh | *1* | cMD\_iOFS | 100 | 3V8G | 0.0 |
| *2* | tMD1\_*i*OFS→IFS | 10 | 6 ns of *run* 1 | 0.1 |
| *3* | tMD2\_*i*OFS→IFS | 10 | 6 ns of *run 1* | -0.1 |
| *4* | tMD3\_*i*OFS→IFS | 10 | 6 ns of *run* 1 | 0.3 |
| *5* | tMD4\_*i*OFS→IFS | 10 | 6 ns of *run* 1 | -0.3 |
| *6* | tMD5\_*i*OFS→IFS | 10 | 6 ns of *run* 1 | 0.0 |
| *7* | tMD6\_iOFS→IFS | 10 | 6 ns of *run* 1 | 0.0 |
| *8* | cMD1\_*iCh*S | 100 | 7.5 ns of *run 6* | 0.0 |
| *9* | cMD2\_*iCh*S | 100 | 7.5 ns of *run 6* | 0.0 |
| *10* | cMD3\_*iCh*S | 100 | 6 ns of *run* 8 | -0.1 |
| *11* | cMD4\_*iCh*S | 100 | 6 ns of *run* 8 | -0.3 |
| *12* | cMD5\_*iCh*S | 100 | 6 ns of *run* 8 | 0.1 |
| *13* | cMD6\_*iCh*S | 100 | 6 ns of *run* 8 | 0.3 |
| *14* | Meta\_*iCh*S | 20 | 6 ns of *run* 8 | 0.0 |
| *15* | Meta\_S65 | 20 | 100 ns of *run*1 | 0.0 |
| *16* | ABF\_*iCh*S | 100 | 100 ns of *run*10 | 0.0 |
| EAAT1 | *17* | cMD1\_EAAT1\_*i*OFS | 100 | EAAT1\_*i*OFS | -0.1 |
| *18* | cMD2\_EAAT1\_*i*OFS | 100 | 0.1 |
| *19* | cMD1\_EAAT1\_*iCh*S | 100 | EAAT1\_*iCh*S | -0.1 |
| *20* | cMD2\_EAAT1\_*iCh*S | 100 | 0.1 |
| R477C | *21* | cMD1\_R477C\_*iCh*S | 50 | R477C of EAAT1\_*iChS* | -0.1 |
| *22* | cMD2\_R477C\_*iCh*S | 50 | 0.1 |

cMD: conventional MD simulation tMD: targeted MD simulations

Meta: Metadynamics simulations ABF: adaptive biasing force calculations

*i*OFS: intermediate outward-facing state *iCh*S: intermediate channeling state