

Additional file 3. Description of prepared systems for molecular dynamics simulations.

| System | Model | Cell | POPC Lipid count | Sodium ion count | Chlorine ion count | TIP3P water count | System size, nm |
|---------------|-------------------|-------------|---------------------------------|---------------------------------|-----------------------------------|----------------------------------|-----------------------------|
| 1 | <i>m5HT7/CDK5</i> | hexagon | 400 | 137 | 156 | 50159 | 13.12* 11.36*15.378*6.56 |
| 2 | <i>h5HT7/CDK5</i> | hexagon | 478 | 154 | 171 | 56641 | 4.25 *12.34 *14.84*7.13 |