# Supporting Information for: Selective Permeability of Truncated Aquaporin 1 *in Silico*

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**Table S1**. Summary of structures studied using the MD method.

| Structure | Residues in each AQP monomer | Channel length (A) | Number of atoms in each lipid molecule |
|---|---|---|---|
| **WT** | All 1-249 | 15 | 125 |
| **H182A** | All 1-249, but histidine 182 replaced with alanine | 15 | 125 |
| **R197V** | All 1-249, but histidine 182 replaced with alanine and arginine 197 replaced with valine | 15 | 125 |
| **T1** | 13-32, 50-88, 93-94, 96-117, 127-129, 138-159, 167-204, 211-234 | 15 | 101 |
| **T2** | 14-32, 50-69, 75-84, 96-98, 100-117, 127-129, 138-155, 171-204, 211-228 | 15 | 83 |
| **T3** | 14-31, 51-66, 75-84, 97-114 139-155, 171-186, 190-204, 211-225 | 15 | 73 |
| **T4** | 18-31, 50-65, 77-80, 100-117, 127-129, 138-151 175-204, 211-224 | 13 | 73 |
| **T5** | 25-31, 50-58, 106-117, 127-129, 138-147, 179-204, 211-218 | 7 | 67 |
| **T5-H182A** | 25-31, 50-58, 106-117, 127-129, 138-147, 179-204, 211-218, but histidine 182 replaced with alanine | 7 | 67 |
| **T5-R197V** | 25-31, 50-58, 106-117, 127-129, 138-147, 179-204, 211-218, but histidine 182 replaced with alanine, arginine 197 replaced with valine | 7 | 67 |
| **T6** | 21, 24-25, 28-29, 54-55, 57-59, 61-62, 77-78, 103, 107, 127-129, 151, 175, 178-179, 181-182, 186, 190-198, 201 | 13 | 73 |
| **T7** | 1-78, 81-249 | 15 | 125 |

**Table S2**. The number of atoms and the height of the simulated systems.

| Structure | Description | Number of atoms | Height (Å) |
|---|---|---|---|
| **WT** | Unmodified AQP | 65,497 | 79.9 |
| **H182A** | Selectivity filter mutant | 65,433 | 78.5 |
| **R197V** | Selectivity filter mutant | 65,469 | 79.6 |
| **T1** | Removed outer loops | 57,105 | 69.7 |
| **T2** | As T1, and truncated cytoplasmic vestibule | 53,065 | 67.0 |
| **T3** | As T2, and truncated extracellular vestibule | 50,613 | 66.9 |
| **T4** | As T2, and removed cytoplasmic vestibule | 49,885 | 65.3 |
| **T5** | As T4, and truncated NPA motif | 46,713 | 60.8 |
| **HAT5** | As T5, with filter mutation as H182A | 45,555 | 60.8 |
| **RVT5** | As T5, with filter mutation as R197V | 45,515 | 60.8 |
| **T6** | As T4, and residues far from channel removed | 32,338 | 57.9 |
| **T7** | Truncated NPA motif | 65,401 | 79.9 |

**Table S3**. Duration of MD simulations.

| Structure | NaCl concentration and bias condition | Duration of equilibration simulation (ns) | Duration of production simulation (ns) |
|---|---|---|---|
| **WT** | 0 M, 0 V | 1 | 130 |
| | 1 M, 1 V | 1 | 51 |
| | 1 M, -1 V | 1 | 62 |
| **H182A** | 0 M, 0 V | 1 | 67 |
| | 1 M, 1 V | 1 | 51 |
| **R197V** | 0 M, 0 V | 1 | 67 |
| | 1 M, 1 V | 1 | 51 |
| **T1** | 0 M, 0 V | 1 | 51 |
| | 1 M, 1 V | 1 | 70 |
| **T2** | 0 M, 0 V | 1 | 55 |
| | 1 M, 1 V | 1 | 65 |
| **T3** | 0 M, 0 V | 1 | 170 |
| | 1 M, 1 V | 1 | 67 |
| | 1 M, -1 V | 1 | 69 |
| **T4** | 0 M, 0 V | 1 | 68 |
| | 1 M, 1 V | 1 | 70 |
| | 1 M, -1 V | 1 | 59 |
| **T5** | 0 M, 0 V | 1 | 55 |
| | 1 M, 1 V | 1 | 400 |
| | 1 M, -1 V | 1 | 400 |
| **T5-H182A** | 0 M, 0 V | 1 | 40 |
| | 1 M, 1 V | 1 | 55 |
| | 1 M, -1 V | 1 | 47 |
| **T5-R197V** | 0 M, 0 V | 1 | 64 |
| | 1 M, 1 V | 1 | 76 |
| | 1 M, -1 V | 1 | 58 |
| **T6** | 0 M, 0 V | 1 | 51 |
| **T7** | 0 M, 0 V | 1 | 30 |
| | 1 M, 1 V | 1 | 51 |
| | 1 M, -1 V | 1 | 56 |