**Supplementary Information**

**Comparison study of stability and transport of molecules through cyclic peptide nanotube and aquaporin: A molecular dynamics simulation approach.**

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| Number | Atom | Residue | Residue ID | Chain | Accepts/donates | Atom | Residue | Residue ID | Chain | Atom | Distance (Å) | Energy (kJ/mol) |
| 1 | O | CYS | 1 | A | accepts | N | GLY | 4 | B, | O | 1.95 | 16.43 |
| 2 | O | MET | 3 | A | accepts | N | MET | 3 | B, | O | 2.02 | 19.55 |
| 3 | N | CYS | 5 | A | donates | O | CYS | 1 | B, | H | 1.8 | 24.43 |
| 4 | O | MET | 7 | A | accepts | N | MET | 7 | B, | O | 2.02 | 19.55 |
| 5 | O | CYS | 1 | B | accepts | N | CYS | 5 | A, | O | 1.8 | 24.43 |
| 6 | N | GLY | 2 | B | donates | O | GLY | 12 | B, | H | 2.13 | 20 |
| 7 | O | GLY | 2 | B | accepts | N | GLY | 12 | B, | O | 2.2 | 14.23 |
| 8 | N | MET | 3 | B | donates | O | MET | 3 | A, | H | 2.02 | 19.55 |
| 9 | O | MET | 3 | B | accepts | N | MET | 11 | B, | O | 2 | 19.93 |
| 10 | N | GLY | 4 | B | donates | O | CYS | 1 | A, | H | 1.95 | 16.43 |
| 11 | O | GLY | 4 | B | accepts | N | GLY | 10 | B, | O | 1.88 | 24.43 |
| 12 | N | GLY | 6 | B | donates | O | GLY | 16 | B, | H | 2.37 | 7.93 |
| 13 | N | MET | 7 | B | donates | O | MET | 7 | A, | H | 2.02 | 19.55 |
| 14 | N | GLY | 8 | B | donates | O | GLY | 14 | B, | H | 1.83 | 24.43 |
| 15 | O | GLY | 8 | B | accepts | N | GLY | 14 | B, | O | 2.24 | 14.43 |
| 16 | N | CYS | 9 | B | donates | O | CYS | 5 | C, | H | 1.74 | 25 |
| 17 | O | CYS | 9 | B | accepts | N | CYS | 5 | C, | O | 1.98 | 23.85 |
| 18 | N | GLY | 10 | B | donates | O | GLY | 4 | B, | H | 1.88 | 24.43 |
| 19 | N | MET | 11 | B | donates | O | MET | 3 | B, | H | 2 | 19.93 |
| 20 | O | MET | 11 | B | accepts | N | MET | 3 | C, | O | 2.14 | 20.15 |
| 21 | N | GLY | 12 | B | donates | O | GLY | 2 | B, | H | 2.2 | 14.23 |
| 22 | O | GLY | 12 | B | accepts | N | GLY | 2 | B, | O | 2.13 | 20 |
| 23 | N | CYS | 13 | B | donates | O | CYS | 1 | C, | H | 1.81 | 23.85 |
| 24 | O | CYS | 13 | B | accepts | N | CYS | 1 | C, | O | 2.16 | 22.1 |
| 25 | N | GLY | 14 | B | donates | O | GLY | 8 | B, | H | 2.24 | 14.43 |
| 26 | O | GLY | 14 | B | accepts | N | GLY | 8 | B, | O | 1.83 | 24.43 |
| 27 | N | MET | 15 | B | donates | O | MET | 7 | C, | H | 1.83 | 25 |
| 28 | O | MET | 15 | B | accepts | N | MET | 7 | C, | O | 1.87 | 25 |
| 29 | O | GLY | 16 | B | accepts | N | GLY | 6 | B, | O | 2.37 | 7.93 |
| 30 | N | CYS | 1 | C | donates | O | CYS | 13 | B, | H | 2.16 | 22.1 |
| 31 | SG | CYS | 1 | C | donates | O | GLY | 4 | D, | H | 1.73 | 19.93 |
| 32 | O | CYS | 1 | C | accepts | N | CYS | 13 | B, | O | 1.81 | 23.85 |
| 33 | N | GLY | 2 | C | donates | O | GLY | 4 | D, | H | 2.12 | 23.78 |
| 34 | O | GLY | 2 | C | accepts | N | GLY | 4 | D, | O | 2.17 | 18.35 |
| 35 | N | MET | 3 | C | donates | O | MET | 11 | B, | H | 2.14 | 20.15 |
| 36 | O | GLY | 4 | C | accepts | N | GLY | 2 | D, | O | 1.85 | 22.28 |
| 37 | N | CYS | 5 | C | donates | O | CYS | 9 | B, | H | 1.98 | 23.85 |
| 38 | O | CYS | 5 | C | accepts | N | CYS | 9 | B, | O | 1.74 | 25 |
| 39 | N | GLY | 6 | C | donates | O | GLY | 8 | D, | H | 1.84 | 25 |
| 40 | O | GLY | 6 | C | accepts | N | GLY | 8 | D, | O | 2.03 | 22.88 |
| 41 | N | MET | 7 | C | donates | O | MET | 15 | B, | H | 1.87 | 25 |
| 42 | O | MET | 7 | C | accepts | N | MET | 15 | B, | O | 1.83 | 25 |
| 43 | N | GLY | 8 | C | donates | O | GLY | 6 | D, | H | 1.8 | 25 |
| 44 | O | GLY | 8 | C | accepts | N | GLY | 6 | D, | O | 1.9 | 23.85 |
| 45 | N | CYS | 1 | D | donates | O | CYS | 5 | E, | H | 1.82 | 21.88 |
| 46 | O | CYS | 1 | D | accepts | N | CYS | 5 | E, | O | 2.08 | 22.88 |
| 47 | N | GLY | 2 | D | donates | O | GLY | 4 | C, | H | 1.85 | 22.28 |
| 48 | O | MET | 3 | D | accepts | N | MET | 3 | E, | O | 2.05 | 19.55 |
| 49 | N | GLY | 4 | D | donates | O | GLY | 2 | C, | H | 2.17 | 18.35 |
| 50 | O | GLY | 4 | D | accepts | SG | CYS | 1 | C, | O | 1.73 | 19.93 |
| 51 | O | GLY | 4 | D | accepts | N | GLY | 2 | C, | O | 2.12 | 23.78 |
| 52 | N | CYS | 5 | D | donates | O | CYS | 1 | E, | H | 1.91 | 25 |
| 53 | O | CYS | 5 | D | accepts | N | CYS | 1 | E, | O | 2.03 | 23.45 |
| 54 | N | GLY | 6 | D | donates | O | GLY | 8 | C, | H | 1.9 | 23.85 |
| 55 | O | GLY | 6 | D | accepts | N | GLY | 8 | C, | O | 1.8 | 25 |
| 56 | N | MET | 7 | D | donates | O | MET | 7 | E, | H | 1.92 | 25 |
| 57 | O | MET | 7 | D | accepts | N | MET | 7 | E, | O | 2.07 | 21.88 |
| 58 | N | GLY | 8 | D | donates | O | GLY | 6 | C, | H | 2.03 | 22.88 |
| 59 | O | GLY | 8 | D | accepts | N | GLY | 6 | C, | O | 1.84 | 25 |
| 60 | N | CYS | 1 | E | donates | O | CYS | 5 | D, | H | 2.03 | 23.45 |
| 61 | O | CYS | 1 | E | accepts | N | CYS | 5 | D, | O | 1.91 | 25 |
| 62 | O | GLY | 2 | E | accepts | N | GLY | 12 | E, | O | 1.88 | 20.33 |
| 63 | N | MET | 3 | E | donates | O | MET | 3 | D, | H | 2.05 | 19.55 |
| 64 | N | GLY | 4 | E | donates | O | GLY | 10 | E, | H | 1.82 | 25 |
| 65 | O | GLY | 4 | E | accepts | N | GLY | 10 | E, | O | 1.73 | 25 |
| 66 | N | CYS | 5 | E | donates | O | CYS | 1 | D, | H | 2.08 | 22.88 |
| 67 | O | CYS | 5 | E | accepts | N | CYS | 1 | D, | O | 1.82 | 21.88 |
| 68 | N | GLY | 6 | E | donates | O | GLY | 16 | E, | H | 2.06 | 17.78 |
| 69 | O | GLY | 6 | E | accepts | N | GLY | 16 | E, | O | 2.18 | 17.2 |
| 70 | N | MET | 7 | E | donates | O | MET | 7 | D, | H | 2.07 | 21.88 |
| 71 | O | MET | 7 | E | accepts | N | MET | 7 | D, | O | 1.92 | 25 |
| 72 | N | GLY | 8 | E | donates | O | GLY | 14 | E, | H | 1.84 | 24.43 |
| 73 | O | GLY | 8 | E | accepts | N | GLY | 14 | E, | O | 1.86 | 25 |
| 74 | N | CYS | 9 | E | donates | O | CYS | 5 | F, | H | 1.94 | 18.57 |
| 75 | O | CYS | 9 | E | accepts | N | CYS | 5 | F, | O | 1.87 | 25 |
| 76 | N | GLY | 10 | E | donates | O | GLY | 4 | E, | H | 1.73 | 25 |
| 77 | O | GLY | 10 | E | accepts | N | GLY | 4 | E, | O | 1.82 | 25 |
| 78 | N | MET | 11 | E | donates | O | MET | 3 | F, | H | 2.21 | 11.03 |
| 79 | N | GLY | 12 | E | donates | O | GLY | 2 | E, | H | 1.88 | 20.33 |
| 80 | O | CYS | 13 | E | accepts | N | CYS | 1 | F, | O | 1.8 | 21.1 |
| 81 | N | GLY | 14 | E | donates | O | GLY | 8 | E, | H | 1.86 | 25 |
| 82 | O | GLY | 14 | E | accepts | N | GLY | 8 | E, | O | 1.84 | 24.43 |
| 83 | N | MET | 15 | E | donates | O | MET | 7 | F, | H | 1.85 | 24.43 |
| 84 | O | MET | 15 | E | accepts | N | MET | 7 | F, | O | 1.96 | 23.85 |
| 85 | N | GLY | 16 | E | donates | O | GLY | 6 | E, | H | 2.18 | 17.2 |
| 86 | O | GLY | 16 | E | accepts | N | GLY | 6 | E, | O | 2.06 | 17.78 |
| 87 | N | CYS | 1 | F | donates | O | CYS | 13 | E, | H | 1.8 | 21.1 |
| 88 | O | MET | 3 | F | accepts | N | MET | 11 | E, | O | 2.21 | 11.03 |
| 89 | N | CYS | 5 | F | donates | O | CYS | 9 | E, | H | 1.87 | 25 |
| 90 | O | CYS | 5 | F | accepts | N | CYS | 9 | E, | O | 1.94 | 18.57 |
| 91 | N | MET | 7 | F | donates | O | MET | 15 | E, | H | 1.96 | 23.85 |
| 92 | O | MET | 7 | F | accepts | N | MET | 15 | E, | O | 1.85 | 24.43 |

Table 1. The details of the hydrogen bonds between the adjacent rings of the CPN.



**Figure 1.** Structure of (a) POPA, (b) POPC, (c)POPE, (d) POPG, (e) POPS lipids.



**Figure 2.** The number of hydrogen bonds and non-bonded interaction energies between the adjacent ring of the CPN in the water.

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**Figure 3.** PMF profiles for single (a) K+, (b) Na+ ions and (c)water along the z-direction of the CPN.

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**Figure 4.** The number of hydrogen bonds formed between urea- CPN and urea-water molecules.

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**Figure 5.** The number of hydrogen bonds formed between fluorouracil - CPN and fluorouracil -water molecules.

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**Figure 6.** The radial distribution function of urea with CPN C, Cα and N molecules.

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**Figure 7.** The electrostatic and van der Waals interaction energies of urea and fluorouracil at each gap/position of the CPN.

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**Figure 8.** The solvent accessible surface area of the CPN in different lipid bilayers.