Distribution of ammonia and carbon dioxide in aquaporins investigated by 3D-RISM

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Aquaporins (AQPs), known as a water channel, are membrane proteins that facilitate the transportation of water through the cell membrane. The AQPs are not permeable to only water, but also several members in the aquaporin family can conduct other molecules, such as glycerol and urea. Recently there were reports of the evidences that AQP1 can transport the CO_2 and NH_3. However, it is still controversial. In this study, we have applied the 3D-RISM, the statistical mechanics theory of liquids, to calculate the distribution function and potential of mean forces (PMFs) of CO_2 and NH_3 in AQP1 and GlpF. From the results, the distribution functions of water in AQP1 and Glpf are continuous, and the PMFs of water are negative throughout the channels. In AQP1, the distribution function of CO_2 is discontinuous; it is interrupted by a gap. The corresponding PMFs show a very high positive potential barrier at the gap area. The distributions of NH_3 and water inside the water channel are similar. However, the PMFs are different at selective filter area. At this area, PMF of NH_3 rises up to the sharp peak, ~2.5 kJ/mol, whereas that of water falls down to the minimum. On the other hand, the PMFs of both CO_2 and NH_3 are negative throughout the GlpF channel, and there is no barrier. These results reveal that CO_2 can not transport through AQP1 due to the steric effect, whereas NH_3 has a possibility to permeate through the channel. However, GlpF is permeable to the both molecules because of the larger pore size than AQP1.