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The influence of the peptide 1B03 on micelle formation in magnesium hexanoate solution

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For computer simulations, the OPLS-AA, CHARMM, AMBER potentials are widely used, in which the charge of the divalent magnesium ion is +2e and the charge of the acid residue of hexanoic acid is -1e. Earlier it was published [1] that the electric charges of ions, specified in the standard file of potentials of atom-atom interactions OPLS-AA, are not acceptable for simulation of concentrated ionic systems. As a result of simulation of micelle formation in an aqueous solution of magnesium hexanoate, the charges calculated by the Mulliken method turned out to be the best suitable: +1.4e for the magnesium ion and -0.7e for the acid residue.

In continuation of that work, the influence of the 1B03 peptide molecule (Fig. 1) to the micelle formation process in an aqueous solution of magnesium hexanoate was investigated. Two model systems were created with different charges on ions: taken from OPLS-AA (system I) and calculated by the Mulliken method (system II). The charge of peptide 1B03 in the second system was scaled 0.7 times.

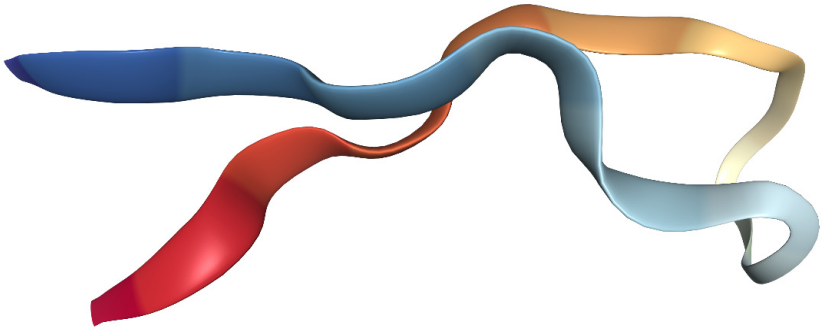

Fig. 1. Schematic representation of the structure of a peptide 1B03.

References

1. N.A. Antonova, A.M. Ryzhkov, A.V. Komolkin. Computer simulation of micelle formation in magnesium hexanoate solution // Magnetic resonance and its applications: Proceedings 16th International School-Conference, Saint-Petersburg, March 31–April 5, 2019. — Saint Petersburg, VVM Publisher, 2019. P. 130-132.