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Conformation of FMN dimer obtained by molecular modelling methods

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The structure of flavomononucleotide (FMN) is obtained by molecular modelling methods. At the first stage the geometry of FMN molecule was optimized. The maximal dimension of FMN monomer was obtained equal d=15.82A. Then, the structure of dimer both in vacuum and in the vicinity of 302 water molecules was calculated in a periodic box. HyperChem software (version 5.02) was used to obtain the stacking structure of the dimer. We found that the isoalloxazine rings are almost parallel, shifted one to another by about 0.58A towards the short axis of the ring and slightly twisted one to another at an angle a=3.5^{o}. For the average distance between isoalloxazine rings the value of 3.57A has been obtained in vacuum compared to that of 3.70A in the vicinity of water.