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Uloga vode u procesu konverzije kreatina u kreatinin

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U ovom radu ispitan je uticaj strukturne organizacije molekula vode na konverziju biološki aktivnog molekula kreatina u njegov biološki neaktivan oblik, kreatinin. Kreatin je esencijalna, neproteinska aminokiselina koja se u organizmu metaboliše do fosfokreatina, glavnog oblika skladištenja energije. Dodatna suplementacija kreatinom, kojom se dobija više energije tokom vežbanja, ograničena je njegovom slabom rastvorljivošću u vodi i spontanom konverzijom u kreatinin. Na osnovu volumetrijskih i viskozimetrijskih merenja vodenih rastvora ispitivanih supstanci različitih molaliteta u temperaturnom opsegu od 293,15 do 313,15 K, kao i računarskih simulacija (molekulske dinamike I DFT proračuna) proučavane su interakcije između kreatina/kreatinina i vode, njihove *structure making/breaking osobine*, kao i uticaj temperature na njih. Dobijeni rezultati ukazuju na to da je brža konverzija kreatina u kreatinin na povišenim temperaturama posledica smanjenja broja molekula vode u hidratacionoj sferi kreatina, što može da dovede do olakšanog formiranja neutralne forme kreatina i zatim do njegove ciklizacije.

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The water role in the conversion process of creatine into creatinine

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In this paper, the influence of the structural organization of the water molecule on the conversion of biologically active creatine into its inactive form, creatinine, was examined. Creatine is an essential, non-proteinaceous amino acid that is metabolized to the phosphocreatine, the main energy storage form in the organism. Additional creatine supplementation, which generates more energy during exercises, is limited by its low solubility in water and spontaneous conversion into creatinine. Based on volumetric and viscometric measurements of creatine/creatinine aqueous solutions at different molalities in the temperature range from 293.15 to 313.15 K, as well as on the results of computational simulations (molecular dynamics and DFT calculations), interactions between creatine/creatinine and water, their *structure making/breaking* properties were studied, as well as the temperature influence on them. The obtained results suggest that a faster conversion of creatine into creatinine at a higher temperature can be explained by a decrease of the number of water molecules in the hydration shell of creatine, which may lead to the more favourable formation of creatine neutral form and further cyclization.