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Tris(1-amino)triphosphonates based on tris(2-aminoethyl)amine: modeling complexes with proteinogenic amino acids

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Abstract

The modeling of complexes of tris(1-amino)triphosphonates based on tris(2-aminoethyl)amine was carried out. The regularities of the influence of substituents at the α-carbon on the energy of stabilization and geometry of the complexes formed was determined. The binding sites which responsible for the molecular recognition between tris(1-amino)triphosphonate and α-amino acids were identified.