Crystal structures of (2*R*, 4*R*)-2-(polyhydroxyalkyl)-1,3-thiazolidine-4-carboxylic acids: condensation products of L-cysteine with D-hexoses.

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Streszczenie

We report herein the first crystal structures of (4-carboxy-1,3-thiazolidin-2-yl)pentitols [2-(polyhydroxyalkyl)thiazolidine-4-carboxylic acids], condensation products of l-cysteine with d-galactose and d-mannose: 2-(d-*galacto*-pentahydroxypentyl)thiazolidine-4-carboxylic acid hydrate, Gal-Cys·H_2O (**1**), and 2-(d-*manno*-pentahydroxypentyl)thiazolidine-4-carboxylic acid hydrate, Man-Cys·H_2O (**2**). In **1** and **2** the compounds crystallize as zwitterions, with the carboxylic groups deprotonated and the thiazolidine N atoms protonated. The sugar moiety and carboxylate group are in a *cis* configuration relative to the thiazolidinium ring, which adopts different conformation: twisted (*T*) on C^{β}–S in **1**, and S-puckered envelope (*E*) in **2**. The carbon chain of the galactosyl/mannosyl moiety remains in an extended zig-zag conformation. The orientation of the sugar O2 atom with respect to the thiazolidinium S and N atoms is trans–gauche in **1** and gauche–gauche in **2**. The molecular conformation is stabilized by the intramolecular N–H···O_{Cys} contacts in both **1** and **2** and by the additional N–H···O_{Man} interaction in **2**. The crystal packing of orthorhombic **1** and monoclinic **2** is determined mainly by N/O/C–H···O hydrogen bonds forming ribbons linked to each other by direct and water-mediated O/C–H···O/S contacts.

Słowa kluczowe

cysteine, galactose, mannose, X-ray crystal structure

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