Crystal structure of*N*-(1-deoxy-β-D-fructopyranos-1-yl)-L-proline—an Amadori compound.

Autorzy

M. Tarnawski

Katarzyna Ślepokura

Tadeusz Lis

R. Kuliś-Orzechowska

B. Szelepin

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Streszczenie

Here we report the crystal structure data on*N*-(1-deoxy-β-d-fructopyranos-1-yl)-l-proline (Fru-Pro)—an Amadori compound. X-ray crystal and molecular structures of its two isomorphous crystalline forms, (Fru-Pro)·MeOH, $C_{11}H_{19}NO_7{\cdot}CH_4O$ (**1a**) and (Fru-Pro)·$2H_2O$, $C_{11}H_{19}NO_7{\cdot}2H_2O$ (**1b**) were determined. In **1a** and **1b** the compound crystallizes as the β-anomer with the overall geometry of Fru-Pro zwitterions being very similar. Fructose ring adopts the chair $^2C_5$ conformation with the proline moiety bonded to equatorial C-1 atom and remaining in a *trans–gauche* (*tg*) orientation with respect to the sugar ring. The five-membered pyrrolidine ring adopts an envelope conformation, with the Cβ atom puckered. Fructosyl and carboxylate groups are in bisectional and axial positions of pyrrolidine ring, respectively. The overall molecular geometry of Fru-Pro zwitterions, especially the relative orientation of sugar and amino acid moieties, is stabilized by intramolecular, three-centred N–H···O_{Fru}/O_{Pro} hydrogen bonds (with bifurcated acceptor) formed between aminium and hydroxyl/carboxylate groups. The packing diagrams are very similar in both **1a** and **1b** with the adjacent zwitterions linked to each other by the extensive network of O–H···O and C–H···O hydrogen bonds to form channels along the *a*-axis, filled up with solvent molecules.

Słowa kluczowe

Amadori compound, Fructosyl-proline, Fru-Pro, X-ray crystal structure

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