Crystal Structure of the Trihydrate of the Neuraminidase Inhibitor $C_{15}H_{28}N_4O_4$ (Peramivir), a Potential Influenza A/B and Avian-influenza (H5N1) Drug

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The crystal structure of the trihydrate of peramivir ($C_{15}H_{28}N_4O_4$), a potential influenza A/B and avian-influenza drug, has been determined. The structure, belonging to the tetragonal space group $P4_22_12$ with Z = 32, a = 27.216(4), c = 23.084(5) Å, V = 17098(5) Å³, contains four organic molecules plus 12 partially disordered water molecules per asymmetric unit. 16 Organic molecules per unit cell form a kind of 1D infinite micelle separated from vicinal micelles by approximately planar water layers. During exposure to X-rays or under long-time storage on air peramivir trihydrate undergoes a phase transition to a structurally closely related phase with reduced water contents.

Key words: Crystal Structure, Peramivir, Neuraminidase Inhibitor