

Poster Presentation

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Crystal structure of salts luminol with Li, Na and K

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The molecular and crystal structures of new drugs Tamerit® (A) and Galavit® (B) which possess high effective immunomodulator, anti-inflammatory and anti-oxidant properties, were studied by single crystal and powder X-ray diffraction methods. As shown, A and B are aminodihydroptalazindion (luminol) sodium salts, but A - is a dihydrate form and B anhydrous one, moreover it is a mixture two different crystal phases B1 and B2. The phase transition B1 <---> B2 is not registered by DSC method [1]. Crystal data for A: monoclinic system with $a = 8.3429(4)$, $b = 22.0562(11)$, $c = 5.2825(2)$ Å, $\beta = 99.893(3)^\circ$, $V = 957.59(8)$ Å³, $Z = 4$, sp.gr. P21/c. Crystal data for B1: monoclinic system with $a = 14.7157(18)$, $b = 3.7029(19)$, $c = 16.0233(15)$ Å, $\beta = 116.682(13)^\circ$, $V = 780.1(4)$ Å³, $Z = 4$, sp.gr. P21/c. Crystal data for B2: orthorhombic system with $a = 27.7765(15)$, $b = 3.3980(19)$, $c = 8.1692(19)$ Å, $V = 771.0(5)$ Å³, $Z = 4$, sp.gr. Pna21. As a continuation of this work, we studied by the same methods other luminol salts: with Li - monohydrate (C1) and anhydrous (C2) and with K - trihydrate (D1) and anhydrous (D2). Crystal data for C1: monoclinic system with $a = 13.0311(15)$, $b = 9.6002(7)$, $c = 7.3227(7)$ Å, $\beta = 101.320(9)^\circ$, $V = 898.26(15)$ Å³, $Z = 4$, sp.gr. P21/c. Crystal data for C2: monoclinic system with $a = 13.0979(14)$, $b = 8.7537(12)$, $c = 14.5358(17)$ Å, $\beta = 107.061(16)^\circ$, $V = 1593.3(4)$ Å³, $Z = 8$, sp.gr. C2/c. Crystal data for D1: monoclinic system with $a = 10.6760(6)$, $b = 14.2905(8)$, $c = 7.4902(5)$ Å, $\beta = 99.246(5)^\circ$, $V = 1127.90(12)$ Å³, $Z = 4$, sp.gr. P21/c. Crystal data for D2: orthorhombic system with $a = 27.3961(19)$, $b = 3.6811(14)$, $c = 8.6672(12)$ Å, $V = 874.1(4)$ Å³, $Z = 4$, sp.gr. Pna21 [2]. All X-ray experiments were made at $T = 295$ K. The features of molecular and crystal structures are discussed.

[1] V.B. Rybakov, V.V. Chernyshev, K.A. Paseshnikchenko, et al., *Crystallography Reports*, 2014, 59(2), 259-269, [2] V.B. Rybakov, V.V. Chernyshev, K.A. Paseshnikchenko, et al., *Crystallography Reports*, 2014, 59 (in press)

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