Salvinorin A and B are potent κ selective opioid receptor agonists from *Salvia divinorum*. An infusion prepared from fresh or dried leaves is used by the Mazatec Indians to stop diarrhea, relieve headache and rheumatism, and is also used in traditional spiritual practices to produce “mystical” or hallucinogenic experiences.[1] Young adults and adolescents have begun to smoke the leaves and leaf extracts of the plants to induce powerful hallucinations.[2] The stereochemistry of Salvinorin has not previously been determined. In an effort to determine the stereochemistry of this opioid agonist a 3,4-dichlorobenzoyl derivative was prepared. Single crystal x-ray diffraction was able to unambiguously determine the absolute configuration of this dichloro derivative and by extension that of Salvinorin A.


Keywords: κ-opioid receptor, structure, stereochemistry

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Crystal Structures of Cholesterol Derivatives

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We have undertaken a series of crystal structures of the esters, carbonates and ethers of cholesterol. These are cholesteryl formate, pentanoate, hexanoate, heptanoate, crotonate, isobutyrate, aniline, 2,4-dichlorobenzoate and hemisuccinate, cholesteryl phenyl acetate, methyl carbonate, ethyl carbonate, propyl carbonate, butyl carbonate, isobutyl carbonate, isopropyl carbonate, pentyl carbonate, hexyl carbonate, crotyl carbonate, cholesteryl ethyl ether, isopropyl ether and methyl ether.

Among these structures, (1) cholesteryl ethyl carbonate, propyl carbonate, crotyl carbonate, crotonate are isostructure each other, (2) cholesteryl pentyl carbonate, hexyl carbonate, hexanoate, heptanoate are also isostructural.

These structures are remarkable in forming layer structures in which the central region of the layers, composed largely of semi-rigid cholesteryl groups is closely packed and the packing of the flexible fatty acid or carbonate chains and the isoprenoid tail of the cholesterol form the interface region between layers. Some of the crystals show the liquid crystalline states. Typical packing modes will be discussed.

Keywords: cholesteryl ester, cholesteryl carbonate, cholesteryl ether

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Structure and Tautomomer of Mercapto-1,2,4-triazole Derivatives in the Solid State

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Molecular and crystal structures and tautomomer of new mercapto-1,2,4-triazole derivatives, which are structurally labile compounds capable to exist in different tautomeric forms, are discussed. X-Ray single crystal diffraction experiments show the existence of only 1H-triazole tautomer in crystal. As a result of our investigations it can be concluded, that for 3,5-substituted 1,2,4-triazoles usually crystallizes the tautomer, where hydrogen atom is bonded with the nitrogen (one of two neighbouring) situated near the electron donor group. For 3-phenyl-5-mercapto-1,2,4-triazole two thion-thiolic tautomers were found in one crystal: two molecules of four symmetrically independent ones are 3-phenyl-4,5-dihydro-(1H)-1,2,4-triazole-5-tautomers, and the rest are 3-phenyl-5-mercapto-(1H)-1,2,4-triazole. The asymmetric part of the unit cell of 3(5)-2-(hydroxyethylthio)-1,2,4-triazolium oxalate consists of two cation-anion pairs. The two cations are the endocyclic tautomers: one of them is 3-(2-hydroxyethylthio)-(1H)-1,2,4-triazolium cation and the other is 5-(2-hydroxyethylthio)-(1H)-1,2,4-triazolium cation. The