Crystal Structures of 8-Styrylxanthine Analogs from Powder Diffractin Data

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Adenosine modulates several physiological functions acting via specific G-protein-coupled receptor subtypes identified as A1, A2a, A2b and A3. Since the discovery that xanthines are the most important class of potent and selective antagonist at adenosine receptors (AR), the interest in this class of compounds has significantly increased. A novel classes of A2aAR antagonists [1] were investigated by means of X-ray powder diffractometry and the crystal structures of some analogs of 8-styrylxanthines: $C_{14}H_{13}N_6O_2Cl$, $C_{14}H_{14}N_6O_2$ (azo-analogs) and $C_{15}H_{14}N_5O_2Br$ (imine-anlog) were solved from laboratory diffractometer data. The results can be useful for the development of more potent and selective A2aAR antagonists which are important for the treatment of Morbus Parkinson. Complexity of the investigated compounds solved by global optimization technique [2] ranges from 22 to 46 atoms in an asymmetric unit. Powder diffraction data were recorded both using Bragg-Brentano and DSH geometry (to reduce texture). It was astonishing that in the case of very strong texture one can encounter problems even in the indexing procedure. In such cases crystal structure solution process from powder data verifies the indexing and space group determination results.

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