

MS10-P6 Inside “false tobacco”Agata E. Owczarzak¹, Maciej Kubicki¹**Keywords:** cytosine, charge distribution, electron density, topological analysis, hydrogen bond , weak interactions

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Tobacco smoking kills around 6 million people each year and it's one of the main public health threats. Smoking cessation with Cytisine is healthy and very effective . Cytisine is natural alkaloid obtained from *Laburnum anagyroides*, during the Second World War the levels of this plants were called "false tobacco". It's a partial agonist at the $\alpha 4\beta 2$ nAChR (nicotinic acetylcholine receptors) and plays the part of nicotine substitute. Nicotine and cytosine have similar a mechanism action, but cytosine substance has low toxicity in contrast to nicotine. Therefore, cytosine has been applied in nicotine replacement therapy in the form of Tabex® Desmoxan® Chantix® etc. Moreover, cytosine derivatives have been explored as potential drugs Alzheimer's and Parkinson's diseases[1].It is important to note that still, a thorough understanding of structural requirements of $\alpha 4\beta 2$ agonists is lacking. High resolution X-ray crystallography can be used as main tool in analysis of structure relationships-activity. In this work will be present the analyse charge density distribution and intermolecular interactions in the cytosine and some of its new derivatives. The structures have been refined using Hansen-Coppens multipolar model [2] implemented in MoPro software [3], using several different strategies to obtain the best model of crystals. We will concentrated on a comparison of the multipole parameters and topological analyses in free base, protonated form and N-substituted cytosine.

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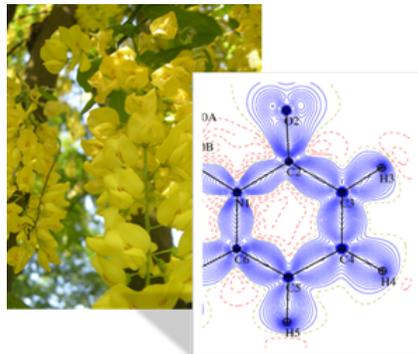


Figure 1. Schematic illustration: *Laburnum anagyroides* "false tobacco" and static deformation density map of cytosine drawn in ring A.