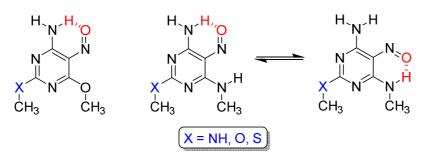
## Novel 5-nitrosopyrimidines and their physicochemical properties

Lucie Cechova<sup>1,2</sup>, Eliska Prochazkova<sup>1</sup>, Zlatko Janeba<sup>1</sup>, Martin Dracinsky<sup>1</sup>

<sup>1</sup>IOCB AS CR, v.v.i., Prague, Czech Republic, <sup>2</sup>UCT Prague, Prague, Czech Republic

5-Nitrosopyrimidine derivatives are not naturally occuring compounds, but their interesting physicochemical and biological properties have been reported. The cytostatic, antifungal or antibacterial effects of these compounds are well known.

2,4,6-Triamino-5-nitrosopyrimidines can form strong intramolecular hydrogen bonds between the 5-nitroso group and amino groups in positions C-4 and C-6, and so, two rotamers can be observed. In our previous work we have reported separation of such rotamers, as planamers, by chromatography at room temperature. The rotational barrier of the nitroso group is unusually high (more than 20 kcal/mol) and thus, resonance-assisted hydrogen bonding is expected to play a key role in the stability of the rotamers. To further study the described phenomenon, novel series of 5-nitrosopyrimidines with different substituents in position C-2 (namely methylamino, methoxy and methylthio group) was prepared and influence of these substituents on the rotational barrier of the 5-nitroso group was studied.



Acknowledgments. The study was supported by IOCB AS CR (RVO61388963), by the

Ministry of Interior of the Czech Republic (VG20102015046) and by the Czech Science Foundation (grant no. 15-11223S).