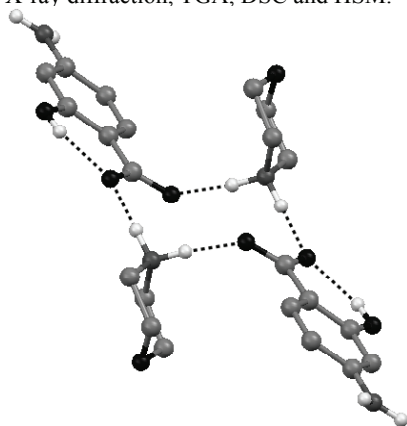


solvate that loses the solvent and transforms into the original form of ASA, all the others are stable until melting point ($>150^{\circ}\text{C}$). Also 2 new forms with 4,4'-bipyridine (one anhydrous and one hydrated) and 3 hydrated new forms with DABCO were obtained [3]. All new solid species were obtained both by the traditional method of slow evaporation from solution and also by the "green" processes of grinding and/or kneading together the starting materials. Also slurries induce the formation of these crystal forms. All the species were characterized by single-crystal and powder X-ray diffraction, TGA, DSC and HSM.



[1] (a) Schreiber, S.; Howaldt, S.; Raedler, A., *Gut*. **1994**, 33, 1081-1085; (b) Bailey, M. A.; Ingram, M. J.; Naughton, D. P.; Rutt, K. J.; Dodd, H. T., *Transition Met. Chem.* **2008**, 33, 195-202. [2] André, V.; Braga, D.; Grepioni, F.; Duarte, M. T., in submission to *Crystal Growth & Design*. [3] André, V.; Braga, D.; Grepioni, F.; Duarte, M. T., in preparation.

Keywords: solvates; salts; 4-aminosalicylic acid

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Crystal Structures and Theoretical Investigations on DPPH Radical-scavenging Mechanism of New Triazolymethyl Benzimidazole Derivatives. Arzu Karayel^a, Suheyla Ozbey^a, Gulgun Ayhan-Kilcigil^b, Cana Kus^b. ^a*Physics Engineering Department, Hacettepe University, 06800 Ankara, Turkey.* ^b*Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ankara University, 06100 Ankara, Turkey.*

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Free radicals, including superoxide radical ($\text{O}_2^{\cdot-}$), nitric oxide (NO), hydroxyl (OH) and peroxy (RO_2^{\cdot}) have been implicated in a number of disease processes, including atherosclerosis, rheumatoid arthritis and carcinogenesis [1]. It was also reported that pathogenesis and symptoms of inflammatory processes are accompanied and/or initiated by the production of reactive oxygen species (ROS) [2]. These ROS are produced as a normal consequence of biochemical processes in the body and as a result of increased exposure to environmental and dietary xenobiotics. Drugs possessing antioxidant and free radical scavenging properties are considered for preventing and/or treatment of such diseases which are directly related to the lack of the antioxidant

capacity of the organisms.

In our previous study we described synthesis and antioxidant properties of compounds 5-(2-(p-chlorophenylbenzimidazol-1-yl-methyl)-4-(3-methylphenyl)-2,4-dihydro-[1,2,4]-triazole-3 thione (A) and 5-(2-(p-chlorophenylbenzimidazol-1-yl-methyl)-4-(2-methylphenyl)-2,4-dihydro-[1,2,4]-triazole-3 thione (B)[3]. According to the biological activity results compounds A and B were found to interact with DPPH strongly (78% and 76%, respectively) at 10^{-3} M concentration. The aim of this study was to determine the structures of compounds A and B by X-ray diffraction method and was to clarify the DPPH radical scavenging mechanisms. This mechanism will be helpful to elucidate the structure activity relationships for the novel antioxidants and to design novel compounds with better antioxidant properties. The elucidation of radical-scavenging mechanisms and structure-activity relationships (SAR) for these compounds were established by density functional theory (DFT) calculations using the B3LYP/6-311+G (2D, 2P) method.

[1] Rice-Evans, C., Diplock, AT., **1991**, *Techniques in Free Radical Research*, p. 291, Elsevier, Amsterdam. [2] Graßmann, J., Hippeli, S., Dornisch, K., Rohnert, U., Beuscher, N., Elstner, EF., **2000**, *Arzneim.-Forsch./Drug Res.* 50(1), 135-139. [3] Ayhan-Kilcigil, G., Kus, C., Coban, T., Can-Eke, B., Iscan, M., **2004**, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 19(2), 129-135.

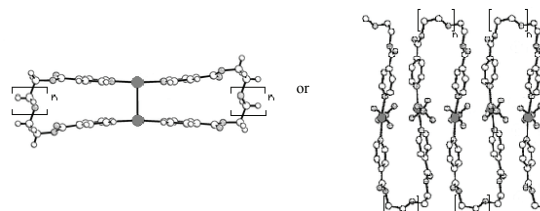
Keywords: antioxidants; density functional theory; pharmaceutical structure determination

FA4-MS09-P05

Synthesis of New Silver Compounds with Derivates of Nicotinate Acid. Chevrier Inès^a, Katharina M. Fromm^a. ^a*Department of Chemistry, University of Fribourg, Fribourg, Switzerland.*

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Silver ions have antibacterial properties, and complexes with this Ion have a great potential of applications in medical uses. Complexes of silver with several ligands derived from nicotinic acids and until three ethylene groups for spacer are already known. In our group we obtain metallacycles and in special conditions chain structures. We propose the development of complexes with longer spacers and to study the possible formation of solids, liquid crystals or polymers.



Keywords: silver compounds; coordination polymer; liquid crystals