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ABSTRACTS

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CHEMOMETRIC CLASIFICATION AND STRUCTURE-ACTIVITY STUDY OF CHOLINESTERASE DUAL INHIBITORS

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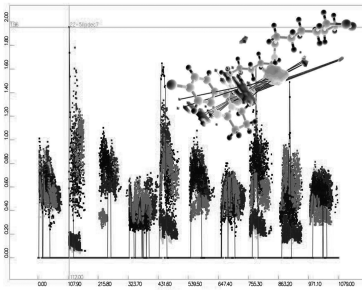
Set of eighty-eight structurally diverse, dual acetylcholineesterase (AChE) inhibitors are classified by principal component analysis (PCA) of 3D-dependent, alignment independent descriptors (GRIND)[1,2] derived from molecular interaction fields (MIF).[3] Conformations of all compounds studied are adjusted to ligand cocrystalized with the respective enzyme binding site (PDB entry 2CKM).[4] Tautomeric and protomeric states of compounds studied are ascribed in a way to fit experimental conditions under which determination of their potency were done. The first and second generation of GRIND descriptors are used and compared. First three PC's give good classification of compounds in respect to their structural properties, using both methods. Inclusion of potency data obtained under the exactly same conditions, spanning 4.2 p(IC_{50}) units, and subsequent structure-activity study by partial least square analysis (PLS) give good results. Fractional factorial design are used to obtain final models. X variable space is covered by 836 and 870 variables. Four latent variables (LV) models show r^2 0.91 and q^2 0.76 - 0.81 (validated by 5 randomly chosen subgroups of compounds). Very good external predictivity is proven using both external literature set, as well as potency values of compounds synthesized by our group. To the best of our knowledge this is the first reported PCA/PLS analysis on such number of AChE inhibitors so far. Along with this, statistical quality of models obtained significantly exceeds so far reported ones, using smaller set of compounds.



[1] *J.Med.Chem.* 43 (2000) 3233-3243; [2] *J.Chem.Inf.Model.* 48 (2008) 1813-1823; [3] *J.Med.Chem.* 28 (1985) 849-857; [4] *J.Med.Chem.* 49 (2006) 5491-5500.

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INFLUENCE OF PROTOLYTIC EQUILIBRIA ON ELECTRO-OXIDATION POTENTIALS OF ELLAGIC ACID IN AQUEOUS METHANOL MEDIUM

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Ellagic acid is plant-derived polyphenol found in a wide variety of fruits and nuts such as raspberries, strawberries, walnuts, grapes, and black currants. It is the major phenolic constituent present in distilled beverages. It exhibits antimutagenic, antioxidant, and anti-inflammatory activity in bacterial and mammalian systems. The protective effects of ellagic acid are often attributed to antioxidant activity. Electrochemistry provides powerful tool for the study of redox reactions. However, the voltammetric methods have not been used for the analysis of ellagic acid, so far. We studied the electro-oxidation of ellagic acid at various pH in methanol-water medium using cyclic voltammetry (CV) on the glassy carbon (GC) electrode. Acidity constants (pK_{a1} and pK_{a2}) were potentiometrically determined and UV/VIS spectrophotometry was used for pK_a values evaluation.
The cyclic voltammetry study of eallagic acid (0.2 mM) was carried out in pH range 2–9 (methanol:water=1:1, *v/v*) at t=25±1 ºC. In acidic media, the oxidation of ellagic acid is a two step process (two peaks), but peaks are almost completely overlapped. The separation of peaks 1 and 2 was much better in the second scan. The oxidation potentials of both peaks depend on pH. At higher pH values (>5) the peak 2 E_p value becomes pH independent, which implies that protons no longer participate in the oxidation process. This result is in accordance with potentiometrically determined acidity constants (pK_{a1}=5.42±0.01 and pK_{a2}=6.76±0.01). According to heat of formation and electron densities calculated on semiempirical level (MOPAC 2007, MNDO-RM1 Hamiltonian) dissociation scheme was proposed. The behavior of ellagic acid was also spectrophotometrically studied and obtained results are in a good agreement with experimentally determined pK_a values.

MODERNISATION OF POST-GRADUATE STUDIES IN CHEMISTRY - AN EXAMPLE OF TEMPUS PROJECT ACTIVITIES

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With the ever increasing progress and achievement in science and technology it is evident that higher education is under pressure to continue to produce new generations of highly skilled individuals who will be capable of contributing further intellectual and technical advances in the 21st century. Therefore, higher education (HE) systems around the globe are facing an enormous challenge to develop programmes that will help produce such scientific graduate leaders and the necessary new generations of scientists and technologists.

To further this aim of developing modern scientists who are competitive on a world stage we have created a joint-project, funded by the European Union's TEMPUS programme, which aims to respond to current societal needs to develop and modernise existing Chemistry programmes in Serbia with a view of making programme outcomes consistent with best practice in the rest of Europe. To achieve this aim the following objectives and work programmes have been formulated:

- Revisit current benchmarking statements and align them with 21st century needs.
- Modernisation of the HE quality assurance (QA) system.
- Staff development – both pedagogical and scientific.
- Implementation of modern technologies in teaching practice.
- Aligning assessment criteria and methodology with new teaching strategies.

Higher education modernisation is often driven by its desire to establish the most effective ways of delivering teaching and learning. When talking about modernisation of curricula in the 21st century we often think about the use of interactive boards, public response systems and virtual learning environments. Although, it is evident that computer aided teaching and learning processes are often dominant, implementation of new teaching strategies is often dictated by:

- An effective understanding of how learners learn (teaching theories).
- The desired learning outcomes (stake holders input)
- Available tools (technologies).
- Latest scientific discoveries (research informed teaching).