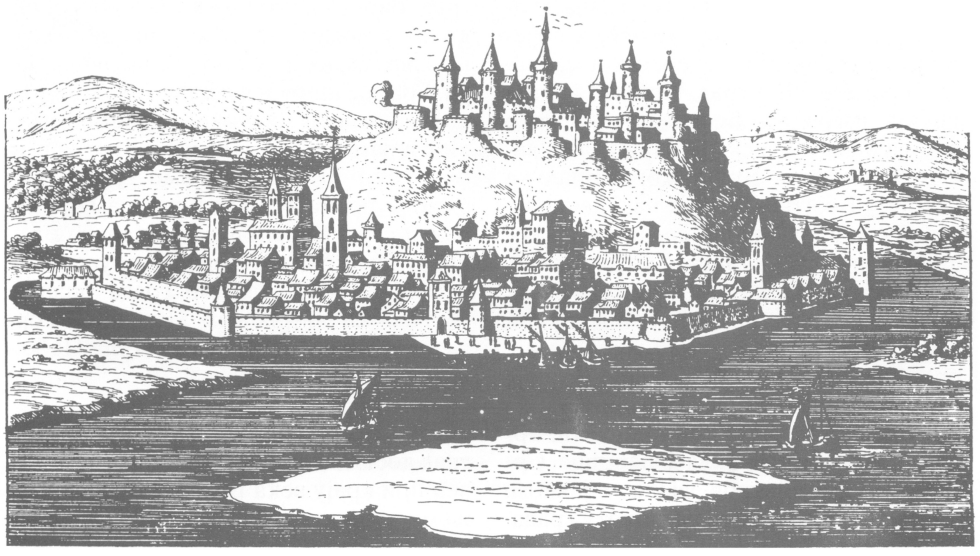
The Sixth European Meeting on Environmental Chemistry

(EMEC6)

PROGRAMME AND THE BOOK OF ABSTRACTS



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Poster No. 52:

A QSAR STUDY OF ACUTE TOXICITY OF *N*-ARYL-SUBSTITUTED FLOUOROACETAMIDES TOWARD RATS. CLASSICAL AND MOLECULAR PROPERTY SPACES APPROACH

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In our previous paper a QSAR study of acute toxicity of set of 19 *N*-alkyl-substituted flouoroacetamides toward rats was described. Main factors that influence the biological action of studied set of compounds were: atomic charges on the amide moiety, sterical bulkiness of nearest vicinity of amide N and overall lipofilicity of compounds. Possible mode of action was suggested.

In the present communication, as an extension of previous work, we study relation between acute toxicity of five *N*-aryl-substituted flouoroacetamides comparing classical and novel (literature) approach which includes range and sensitivities of chosen molecular descriptors for number of possible conformations of each compound. Assessed results are in excellent agreement with results obtained in previous work. Main factors which influence the acute toxicity of *N*-aryl-substituted flouoroacetamides toward rats are the atomic charges on an amide moiety, derived by the semiempirical MNDO-PM3 MO calculations, and range of polar surface area (PSA, which encoded polarity and H-bonding capacity). Obtained two-parameter correlations have very good statistics ($r = 0.999$ and 0.998; $F = 455$ and 347; $Q^2 = 0.998$ and 0.939 for 99% confidence interval). Consis−tency of data derived in previous work and in this communication are additional proof of validity of a suggested mechanism of action for studied class of compounds.

Poster No. 66:

ANTIBACTERIAL ACTIVITY OF 4-ARYL-4-OXO-2-BUTENOIC ACIDS AGAINST *Escherichia coli*. A QSAR STUDY

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Diverse groups of biological active, natural and synthetic molecules comprise common structural fragment: 4-aryl-4-oxo-2-buten. In our previous articles quantitative structure-activity and structure-reactivity relationships of alkyl, alkoxy, nitro and halo-phenyl substituted 4-phenyl-4-oxo-2-butenoic acids were reported.

Present study describes the antibacterial assay and quantitative correlation between structure and antibacterial activity of nineteen 4-aryl-4-oxo-2-butenoic acids against *Escherichia coli* (ATCC 35210), a bacterial species widespread in the nature. Studied compounds exert activities in a range of concentrations $1.32 \cdot 10^{-3}$ to $3.8 \cdot 10^{-5}$ M/L. Four compounds act in markedly lower concentrations than the control (streptomycin hydrochloride). Main factors influencing the antibacterial activity of studied set of compounds are virtual log *P* (conformation dependent property), and an indicator variable that describes steric demand in position 4 of the phenyl ring. One parabolic, one bilinear and one two-parameter equation were obtained for sixteen compounds, having good statistics. The reason for exclusion of the three compounds (outliners) from correlations was offered.

Poster No. 82:

ADSORPTION OF PESTICIDES ON FUNCTIONALIZED SYNTHETIC ZEOLITES

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The extent of pesticide contamination of the water environment has recently raised much concern because of the entry of these compounds into the food chain of humans and animals. A number of different methods for the removal of pesticides from waste water have been used including membrane technology, solid phase extraction, ozone and chemical oxidation, photocatalysis and adsorption on different solid substrates. Particularly, the adsorption techniques have been studied on various substrates such as soil and organic adsorbents, inorganic adsorbents, sediment fractions, silica gel, dissolved organic carbon organoclays and zeolites.

In this work, we have studied the effective behavior of synthetic zeolites (FAU and ZSM) functionalized by cationic surfactant (distearyl-dimethyl-ammonium chloride) for the removal of organophosphorus insecticides (malathion and fenitrothion), pyrethroid ester insecticides (delta–methrin) and herbicides (glyphosate) from water solutions. Comparison with natural zeolite (Clino–ptilolite) functionalized by the same cationic surfactant has been made. The batchwise adsorption method was applied to obtain the adsorption isotherms. When equilibrium is attained, the mixtures, containing fixed amounts of zeolites and aqueous solution with varying amounts of pesticides, were measured by GC-MS chromatograph after separation of the supernatant. Obtained results have shown that the adsorption efficiency of pesticides depends on the zeolite type and hydrophobicity of these molecules.

In addition, the optimized structures of the pesticide molecules have been obtained at B3LYP/6-31+G (d, p) level of theory. The calculated values of molecular sizes and dipole moments are relevant for achieving better understanding of the adsorption mechanism.

Poster No. 150:

β-HYDROXY-β-ARYLALKANOIC ACIDS SELECTIVELY SUPPRESS PROLIFERATION OF FOUR HUMAN TUMOR CELL LINES *IN VITRO*. A QSAR STUDY OF ANTIPROLIFERATIVE ACTIVITY TOWARD HeLa CELLS

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In our previous communication we have reported antiproliferative activity of six β-hydroxy-β-arylalkanoic acids against human cervix carcinoma (HeLa) cells. Present work describe syntheses and determination of antiproliferative activity of eight novel congeners. Compounds were synthesized by modified Reformatsky reaction, starting from aromatic or cikloalkyl aldehydes or ketones, as described previously. Antiproliferative activity were assess using Kenacid Blue R dye binding method, as described in literature. Examined compounds influence proliferation of HeLa, Fem-X, K562 and LS174 cells in concentration range 62-154 μM/L. Seven of eight examined compounds didn't affect proliferation of healthy human peripheral mononuclear blood cells (PBMC and PBMC+PHA). A QSAR study of antiproliferative activity toward HeLa cells, against which all 14 compounds exert activity, results with two-parameter correlation (r=0.941, F=42.5, Q^2=0.810). The highest weight descriptor in correlation is the estimate log *P*, while indicator variable that describes the steric demands for the activity has a less weight. Arrangement of H-bond donor, H-bond acceptor and hydrophobic areas within receptor is discussed.

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