ON PHYSICO-CHEMICAL PROPERTIES OF PAHs

Márcia M. C. Ferreira (PQ) and Rudolf Kiralj (PQ), Instituto de Química, Universidade Estadual de Campinas, Campinas, SP, 13083-970, Brazil. marcia@iqm.unicamp.br

Many benzenoid polycyclic aromatic hydrocarbons (PAHs) are characterized by number of physical, chemical, biochemical and environmental properties. Some PAHs are toxic and even mutagens and cancerogens, while all of them are air, soil, water and food pollutants with tendency to accumulate in all media including living organisms. PAHs undergo chemical changes, especially if mediated by UV light; this can go up to enzymatic oxydation *via* mechanism of free radicals where PAHs turn into reactive epoxydes and polydiols,[1,2] which then easily bind to DNA and other biological macromolecules. There are various studies on PAHs in environmental science at QSPR/SPR or even QSAR/SAR level. This work continues a recent study on 48 PAHs[3] on several physico-chemical properties like boiling point, rentention index, *n*-octanol/water coefficient, solubility, *n*-octanol/air coefficient, soil sorption, Henry's law constant and bioconcentration factor. Various types of molecular descriptors were used as quantum-mechanical (semi-empirical ESP-PM3 charges, dipole moments), shape descriptors (number of rings, Conolly volumes and surfaces), aromaticity (PM3 resonance energy) and intermolecular interaction descriptors (crystal packing energy, water-PAH interaction energy). All physico-chemical properties showed high correlation with molecular descriptors. The full description of the properties is carried out by using Principal Component Analysis and the high-level prediction by Partial Least Squares Regression (r>0.9). The detailed analysis of all the data will be discussed.

1 A. F. Lehner, J. Horn, J. W. Flesher, *J. Mol. Struct. (Theochem)*, **366** (1996) 203-217.

2 J. Jacob, *Pure Appl. Chem*., **68** (1996) 301-308.

3 M. M. C. Ferreira, *Chemosphere*, **44** (2001) 125-146.

FAPESP