

## Enhanced Solubility of PAHs by Using Cyclodextrins

M.A. Sánchez-Trujillo<sup>1</sup>, E. Morillo<sup>1</sup>, M.E. Gómez-Pantoja<sup>2</sup>, J. Villaverde<sup>1</sup>, J.I. Pérez-Martínez<sup>2</sup>, J.R. Moyano<sup>2</sup>

1. *Instituto de Recursos Naturales y Agrobiología de Sevilla (IRNAS-CSIC), Apdo. 1052, 41080 Sevilla Spain*

2. *Department of Pharmacy and Pharmaceutical Technology. Faculty of Pharmacy. University of Seville, Spain*  
[morillo@irnase.csic.es](mailto:morillo@irnase.csic.es)

Contamination of soils, groundwater and surface waters by hydrophobic compounds is currently a significant concern throughout the world. Many of these compounds are a threat to both human health and the environment. The traditional techniques to recover the soils affected by this pollution are based in the use of different chemical agents such as cosolvents or surfactants, but it has been demonstrated that some of them could cause detrimental consequences for the environment. As an alternative to the use of these chemicals, cyclodextrins may have potential for use as solubility-enhancement agents. Hydrosolubility studies have been carried out using six polycyclic aromatic hydrocarbons (PAHs) and four different cyclodextrins, one natural cyclodextrin ( $\beta$ -cyclodextrin,  $\beta$ -CD), and three synthetic cyclodextrins (hydroxypropyl- $\beta$ -cyclodextrin, HPBCD; randomly methylated- $\beta$ -cyclodextrin, RAMEB; and hydroxypropyl- $\gamma$ -cyclodextrin, HPGCD). BCD enhanced the individual solubility of Anthracene, Fluoranthene, Pyrene and Phenanthrene and the inclusion complexes formed showed an unlimited solubility. In the case of Acenaphthene and Fluorene the inclusion complexes obtained showed a limited hydrosolubility what allowed obtaining a precipitated complex.

Phenanthrene molecules showed the best adaptation to HPBCD hydrophobic cavity due to aspects related to molecular size and structure and for this reason its water solubility was increased more than 1000-fold. When PMBCD was used, anthracene was the PAH that showed the highest solubility increase, because its complexation with the CD would be facilitated by the interactions between the outer methyl groups of the PMBCD, and the benzene rings of the anthracene not included in the cavity. Pyrene was the PAH that showed the highest solubility increase when an inclusion complex was formed with HPGCD due to the fact that the dimensions of its hydrophobic cavity were similar to pyrene molecular size, and therefore more interactions and contact points with the active centres of this cavity would be possible.