

Evaluation of β -cyclodextrin as decontaminant agent by interaction with some polycyclic aromatic hydrocarbons.

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Polycyclic aromatic hydrocarbons, a part of the persistent organic pollutants, are characterised by a very low aqueous solubility and long shelf life that make very difficult their elimination from the environment. Solubility increase through different strategies, like the use of cyclodextrin complexation can improve their bioavailability and make possible their biotransformation and inactivation by microorganisms.

Experimental

Materials: Anthracene (ANT), Fluoranthene (FLT) and Pyrene (PYR) (Sigma-Aldrich, St. Louis, MI, USA); β -CD (Roquette Laboratories, Lestrem, France); DMSO-d₆ (Sigma-Aldrich, St. Louis, MI, USA).

Methods: Solubility studies were performed by the Higuchi method and the samples analysed by HPLC. ¹H NMR studies (Bruker AV-500 spectrometer, 500 MHz, 300 K) were carried out by dissolving samples in DMSO-d₆, in order to reach measurable analyte concentrations. Molecular modeling studies were performed by means Chem3DPro software (ChemBioOffice 2008 suite, CambridgeSoft). Binary systems were subjected to energy minimisation, continued by molecular dynamics (heating speed of 1 K·min⁻¹ with a final temperature of 300 K).

Results and discussion

All the resultant solubility curves were ascribed to A_L Higuchi type. The calculated stability constants of complexes as well the solubilising efficiency and other parameters are reported in table 1. From these data, only in the case of ANT a good solubility increase was registered.

| PAH | Slope | K _c (M ⁻¹) | R ² | Solubilising efficiency* |
|-----|--------|-----------------------------------|----------------|--------------------------|
| ANT | 0.0016 | 3922 | 0.9973 | 45,7 |
| FLT | 0.0001 | 208 | 0.9273 | 4,6 |
| PYR | 0.0004 | 249 | 0.9909 | 4,3 |

Table 1. Data from PAH- β -CD solubility curves. *Calculated at 12 mM of β -CD (1,6 % w/v).

From the NMR data unfortunately was not possible to appreciate clearly the liquid medium interaction. In our case, the solvation of DMSO-d₆ induces decomplexation in all systems, and only slight modifications of chemical shift of PAH and CD protons were observed.

The molecular modeling experiments of the three complexes indicate that ANT fits in the CD cavity, whereas FLT and PYR only interact partially. This fact can be explained by the better steric compatibility of ANT with this CD in comparison with the other polycyclic systems.