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## BOOK OF ABSTRACTS



**UNIVERSITY of  
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## Thermodynamic analysis of POPs interaction with biosubstrates

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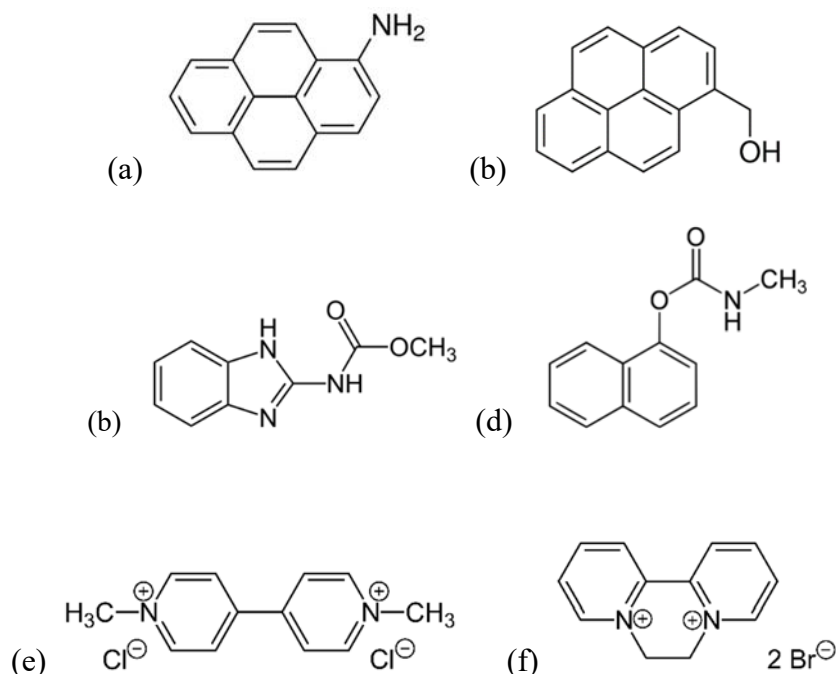
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Persistent organic pollutants (POPs) as polycyclic aromatic hydrocarbons (PAH), pesticides and herbicides are nowadays ubiquitous [1]. These species are highly lipophilic and all at least suspected of carcinogenic effects [2,3]. However, information on their toxic activity is often related to *in vitro/in vivo* studies, whereas a detailed analysis of the mechanistic/chemical aspects of the binding to biosubstrates is sometimes missing.

To contribute to this field and in the frame of our participation to PNRA (National Antarctic Research Program) we have done some tests on the binding of model targets (two PAHs, two pesticides and two herbicides, **Fig. 1**) to biosubstrates (natural DNA and bovine serum albumin - BSA). The interaction with micelles and liposomes was also tested, both as to scale the lipophilicity and to get information on the possible accumulation on membranes.



**Figure 1.** The target molecules used in this study. PAHs: 1-aminopyrene (a) and 1-hydroxymethylpyrene (b). Pesticides: carbendazim (c) and carbaryl (d). Herbicides: paraquat (e) and diquat (f).

The results collected show that the high hydrophobicity of these species turns into very high affinity for DNA. Absorbance and fluorescence titrations suggest complex binding modes that are discussed in relation with the different pollutant/DNA ratio. BSA binding is also found to occur.

Ultrafiltration coupled with absorbance spectroscopy enables the percentage of retention (R%) on the micelle/liposome be measured. R% dependence on the molecule and on the type of system (sodium dodecyl sulphate anionic micelles, TritonX-100 neutral micelles, dodecyl trimethyl ammonium chloride positive micelles and 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine liposomes) is discussed.

#### References:

- [1] A. Lo Giudice, P. Casella, V. Bruni, L. Michaud, *Ecotoxicology* **2013**, 22, 240-250.
- [2] H. Yu, *Journal of Environmental Science and Health* **2002**, 20, 149-183.
- [3] M.C.R. Alavanja, M.R. Bonner, *Journal of Toxicology and Environmental Health B* **2012**, 15, 238-263.