

Alkylated PAHs – The overlooked blow-out?

Malmquist, Linus Mattias Valdemar; Christensen, Jan Henning; Selck, Henriette

Publication date:
2010

Document Version
Peer reviewed version

Citation for published version (APA):
Malmquist, L. M. V., Christensen, J. H., & Selck, H. (2010). Alkylated PAHs – The overlooked blow-out?. Poster session presented at EnviroSymp 2010, København, Denmark.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain.
- You may freely distribute the URL identifying the publication in the public portal.

Take down policy

If you believe that this document breaches copyright please contact rucforsk@kb.dk providing details, and we will remove access to the work immediately and investigate your claim.



Alkylated PAHs – The overlooked blow-out?

Linus Malmquist^{1,2}, Jan H. Christensen² and Henriette Selck¹

¹Department of Environmental, Social and Spatial Change, Roskilde University, Universitetsvej 1, 4000 Roskilde, Denmark (lmvm@ruc.dk);

²Department of Basic Sciences and Environment, Faculty of Life Sciences, Copenhagen University, Thorvaldsensvej 40, 1871 Frederiksberg C, Denmark



Introduction

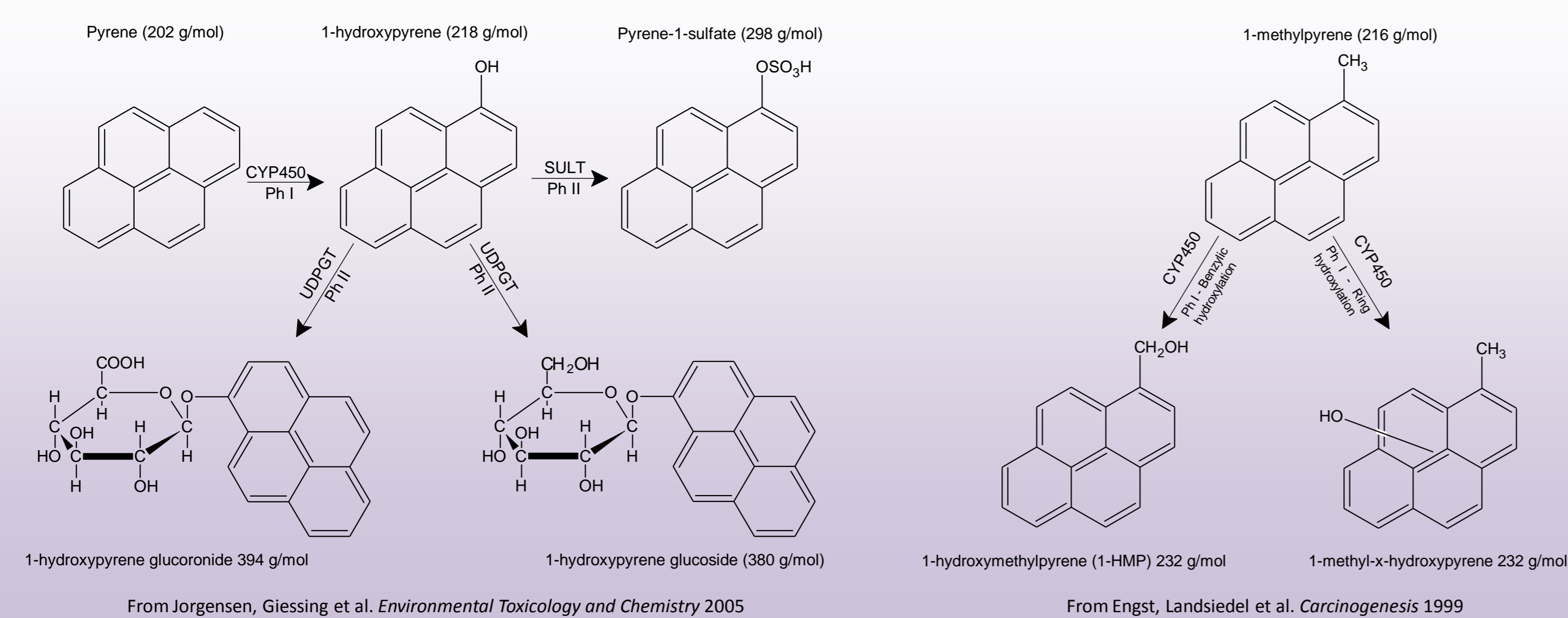
PAHs are widespread compounds originating mostly from anthropogenic input such as pyrogenic and petrogenic sources. Assessments of contaminations are often limited to consider the “16 USEPA priority PAHs”, which are all **non alkylated PAHs**. However, it is commonly known that oils from spills (petrogenic input) **contain magnitudes higher proportions of alkylated PAHs**. Despite this, fate and effects of alkylated PAHs has, to our knowledge, **never been examined** with respect to ecotoxicology.

Hypothesis

Pyrene metabolism is well described, and 1-hydroxypyrene (1OH-P) is reported as the primarily phase I product (>99%). 1-sulfate-, 1-glucuronide- and 1-glucoside are reported as the existing phase II conjugates.

For 1-methylpyrene (1MP) only little literature is on the field. This shows that 1MP can either be hydroxylated on the methyl group (benzylic hydroxylation) or on the ring structure to form different hydroxymethylpyrenes (HMP). There is to our knowledge no information on phase II metabolism. We expect that cytochrome P450 enzymes will further metabolize HMP to either sulfate, glucuronide or glucoside conjugates, following the same routes as pyrene. (Engst, Landsiedel et al. *Carcinogenesis* 1999.)

Documented cytochrome P450 pathways



Expected results from mass analysis

mass	Method	Groups or compounds	Examples of structure
202	GC-MS or UPLC-F/qTOF	Pyrene	
216	GC-MS or UPLC-F/qTOF	Methylpyrenes	
218	GC-MS or UPLC-F/qTOF	Hydroxypyrenes	
232	GC-MS or UPLC-F/qTOF	Hydroxymethylpyrenes	
246	GC-MS or UPLC-F/qTOF	1-pyrenecarboxylic acid	
298	UPLC-F/qTOF	Pyrene-1-sulfate	
312	UPLC-F/qTOF	Methylpyrene sulfates	
381	UPLC-F/qTOF	Pyrene-1-glucoside	
394	UPLC-F/qTOF	Pyrene-1-glucuronide	
395	UPLC-F/qTOF	Methylpyrene glucosides	
408	UPLC-F/qTOF	Methylpyrene glucuronides	

Experimental setup

Setup:

For each replicate: 100 g dw 500µm-sieved, prefrozen and thawed sediment, 650 ml 17 % sterile filtered seawater, covered with alumina foil and wetted paper towels to prevent evaporation. Exposure at 17°C in the dark, continuously aerated through glass Pasteur pipette.

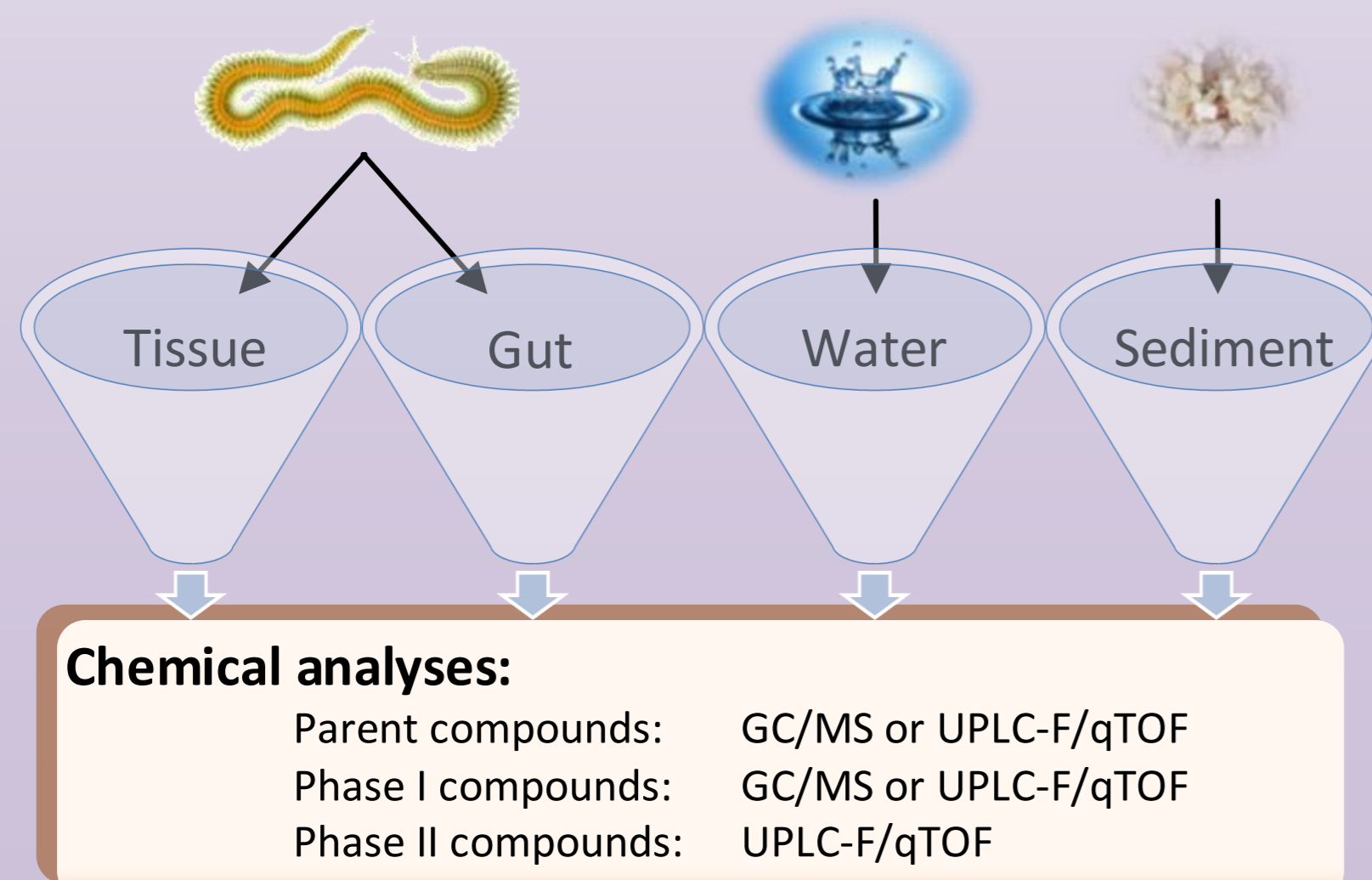
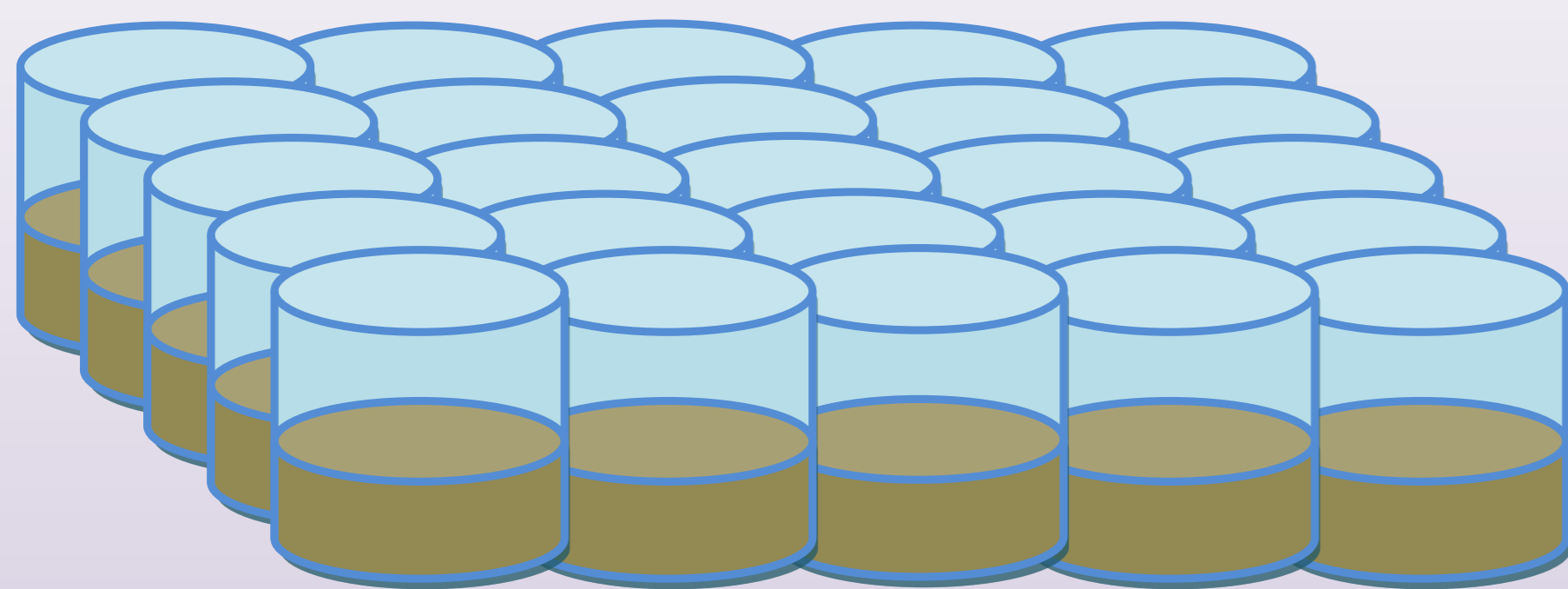
Exposure:

5 replicates of each exposure:

Pyrene	1MP	Pyrene	1MP	None
Worms	Worms	No worms	No worms	Worms



Sampling site



Results

None yet. Worms are in culture, experiments are starting June 15th 2010.

Perspectives

To develop an experiment suitcase that includes exposure, extraction, fractionation and analysis of toxic compounds and their metabolites. This suitcase will be used in future studies with the final perspective to couple conventional toxicological endpoints (e.g. mortality) with studies of sub-lethal endpoints (such as metabolism).

Cited references:

Engst, W., R. Landsiedel, et al. (1999). "Benzylic hydroxylation of 1-methylpyrene and 1-ethylpyrene by human and rat cytochromes P450 individually expressed in V79 Chinese hamster cells." *Carcinogenesis* **20**(9): 1777-1785.

Jørgensen, A., A. M. B. Giessing, et al. (2005). "Biotransformation of the polycyclic aromatic hydrocarbon pyrene in the marine polychaete *Nereis virens*." *Environmental Toxicology and Chemistry* **24**(11): 2796-2805.