

Reference Standards for PAH Analysis and Research

Jon E. Johansen¹, Huiling Liu¹, John Fetzer², Eirik Sundby³

¹Chiron AS

²Fetzpahs Consulting

³HIST

Chiron AS has been involved in supplying PAHs for the past 20 years. Chiron AS offer specific PAH compounds, solutions and mixtures for use within petroleum and basic research, environmental analysis and toxicological studies.

Petroleum PAHs and "Petroleum POPs"

The occurrence of alkylated PAHs in petroleum prompted us to synthesize a series of all the methylisomers of naphthalene, phenanthrene and dibenzothiophene, but also other common petroleum PAHs. This work was supported by the petroleum industry and the results are now available for the environmental community.

The alkyl PAHs are important biomarkers in a geochemical context, and examples will be shown. Alkyl PAHs are to be monitored in produced water from offshore production installations and they play an important role in the fingerprinting of petroleum spills and in air particulate monitoring. Certain dialkylated dibenzothiophenes are extremely slowly degraded, they are the major part of nondestructed sulfur in desulfurized diesel and may be regarded as potentially new "Petroleum POPs".

Naphthenic acids are a large part of crude petroleum. The naphthenic acids play an important role as natural surfactants for crude petroleum. However, relatively little has been done on the properties and use of this part of petroleum. Chiron has synthesized a series of model naphthenic acids, aromatics as well as hydrogenated acidic components for further studies.

The John Fetzer Collection of Large PAHs

Large PAHs are common constituents from downstream petroleum refining and production. However, relatively little has been done on the chemistry of these compounds compared to the smaller PAHs. In collaboration with Fetzpahs Consulting, Chiron now offers an extensive range of larger PAHs. The collection includes several partly and completely hydrogenated PAHs as well.

Toxicology and Metabolites

In an ongoing project Chiron AS and HIST Trondheim has for some time developed new methodology for the production of β -D-glucuronides from hydroxy-PAHs. Xenobiotic uptake in living organisms often requires biotransformation to facilitate excretion. Among the so-called Phase 2-biotransformation are the conjugation of a hydroxyl group in the foreign compound and glucuronic acid to produce the corresponding glucuronide. We have for some time produced enzymatic preparations for doing these syntheses *in vitro*, and have optimized parameters to increase the yields. Thus several PAHglucuronides will now be offered using this technology along with the primary metabolites hydroxyl- and aminoPAHs.

Internal Standards and Routine Analysis

Chiron has developed a range of internal standards for PAH analyses using now well documented technology including deuterated, monofluorinated and other nonnatural standards. We will present the application of fluorinated standards for dibenzothiophene analysis and fluorinated PAHs for metabolites monitoring in toxicological analysis. The result of new multicomponent PAH mixtures used in a multiclient round robin "isotope dilution testing" experiment will be presented.