**Simulation of metabolic processes of polycyclic aromatic hydrocarbons using electrochemistry/mass spectrometry**

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**Introduction**

- Polycyclic aromatic hydrocarbons (PAHs) are a group of ubiquitous environmental contaminants.
- Responsible for their toxic effects are reactive metabolites: epoxides, radical cations and quinones.
- Pyrene was investigated as a PAH model compound (Figure 1).
- Electrochemistry in combination with liquid chromatography and mass spectrometry (EC-LC-MS) was used to study the generation of metabolites and their reactivity towards thiol groups (SH groups).

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**Results and Discussion**

**A: Identification and characterization of oxidation products**

- Quinones are the major oxidation products of pyrene (Figure 4).
- Two different quinone isomers are formed as can be seen in Figure 6.
- Possible structures are shown in Figure 5.

**B: Reactivity of pyrene quinones towards thiol groups**

- Pyrene quinones show high reactivity towards SH groups.
- Formation of adducts was observed with glutathione as well as with β-lactoglobulin (Figures 7 and 9).
- Initial glutathione diol adducts undergo further oxidation to rebuild the quinoid structure (Figure 8). [2]

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**Summary and Conclusion**

- EC/MS is a prompting tool for simulating metabolic processes of PAHs.
- Quinones were found to be the major oxidation products of pyrene. Distinction between two different isomers was achieved by means of HPLC separation.
- Adduct formation of pyrene quinones with glutathione and β-lactoglobulin A was observed. This may play a role in the toxicity of PAHs.

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**Literature**


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