

Halogenated polycyclic aromatic hydrocarbons associated with drinking water disinfection

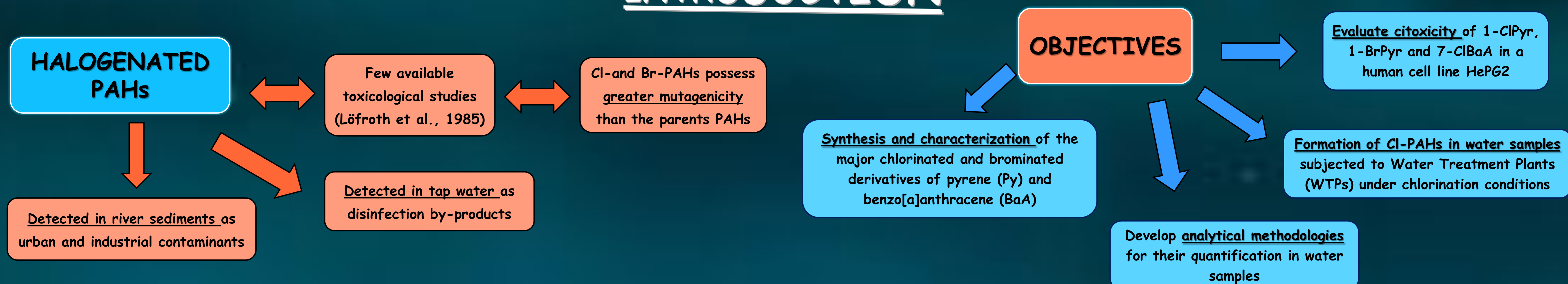
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INTRODUCTION



RESULTS AND DISCUSSION

1 SYNTHESIS and CHARACTERIZATION OF 1-ClPyr, 1-BrPyr AND 7-ClBaA

• 1-ClPyr and 7-ClBaA were prepared by adaptation of the method described by Mitchell et al.⁴, using N-chlorosuccinimide in DMF.
• 1-BrPyr was purchased from Sigma-Aldrich.

Characterized by ¹H-NMR (Fig. 2) and ¹³C-NMR, bidimensional NMR (COSY, HSQC, HMBC) and GC-MS (FAB)

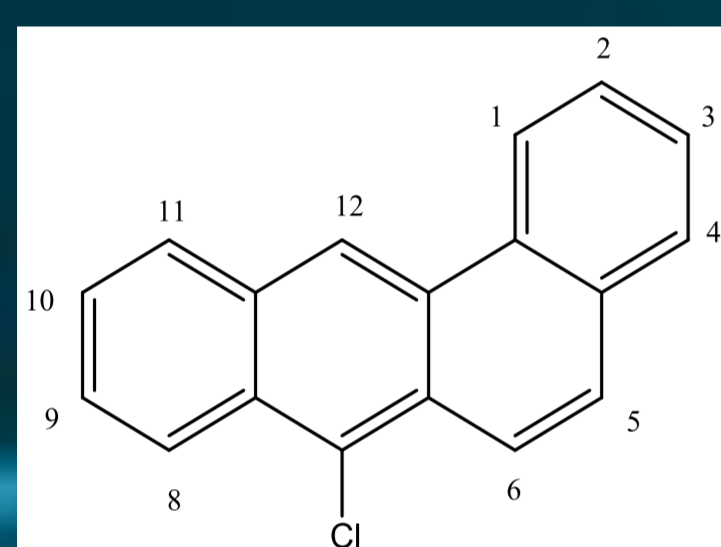


Figure 1: 7-ClBaA structure.

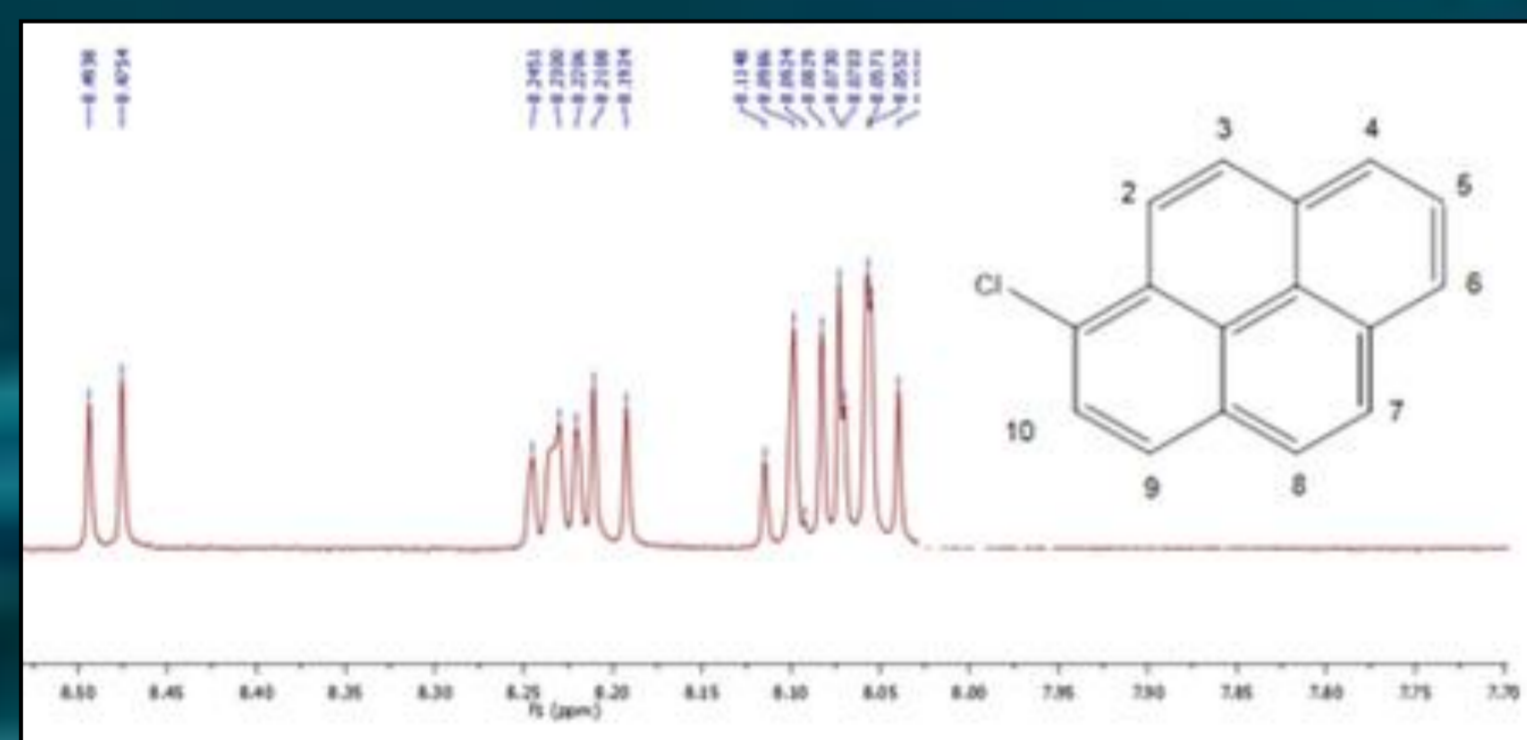


Figure 2: ¹H-NMR spectra of 1-ClPyr.

2 OPTIMIZATION OF SPME-GC-MS METHODOLOGY

- GC-MS conditions: Electronic impact (EI); Tinjector = 280°C.
- SPME conditions: 100 μm PDMS fiber, 70°C/50 min stirring
- Calibration curves: Concentration from 0.018 to 0.22 μg/L-1

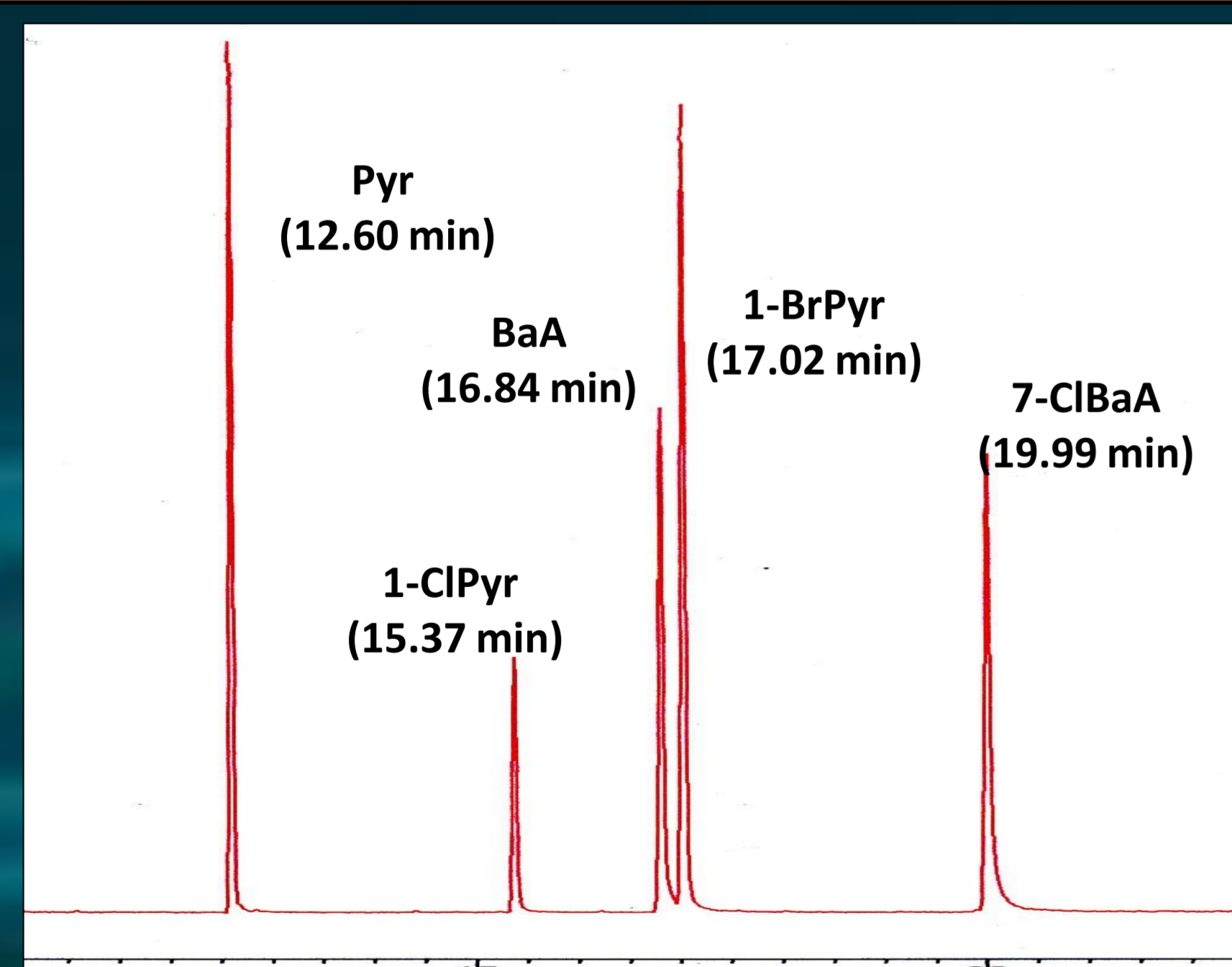
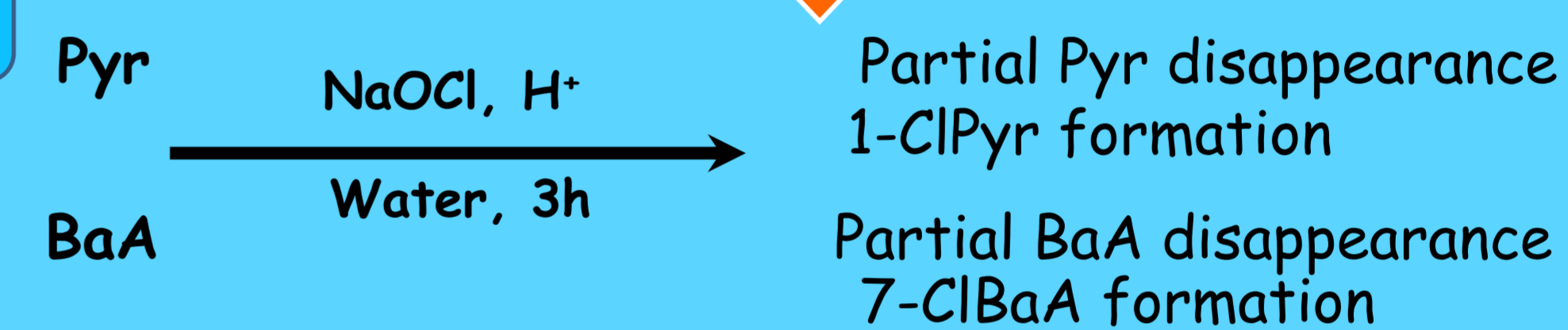


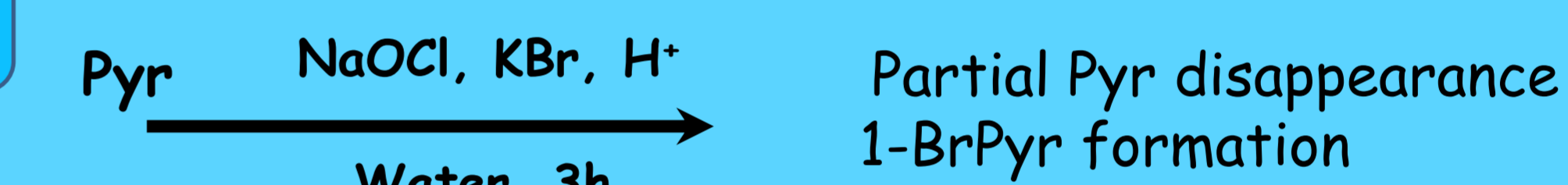
Figure 3: Chromatogram of a mixture of BaP, Pyr and their derivatives after SPME-GC-MS.

3 FORMATION OF HALOGENATED PAHs UNDER SIMILAR WATER TREATMENT PLANTS (WTP) DISINFECTION CONDITIONS:

Chlorination



Bromination



4 EVALUATION OF CITOTOXIC AND GENOTOXIC EFFECTS

Neutral Red Test

- Cell viability > 60% for Pyr and derivatives.
- Cell viability < 50% for BaA and 7-ClBaA;
- IC50= 3.37 μM and 12.63 μM, respectively.

Comet Assay

- 7-ClBaA exerted a significantly higher DNA damaging effect than its parent compound for 15 and 20 μM.
- Pyr, 1-ClPyr and 1-BrPyr showed no significant differences for all tested concentrations.

- **Cellular Line** > HepG2 (metabolic competent cell line)
- **Cytotoxicity** > Neutral Red test⁵
- **Genotoxicity** > Comet Assay⁶

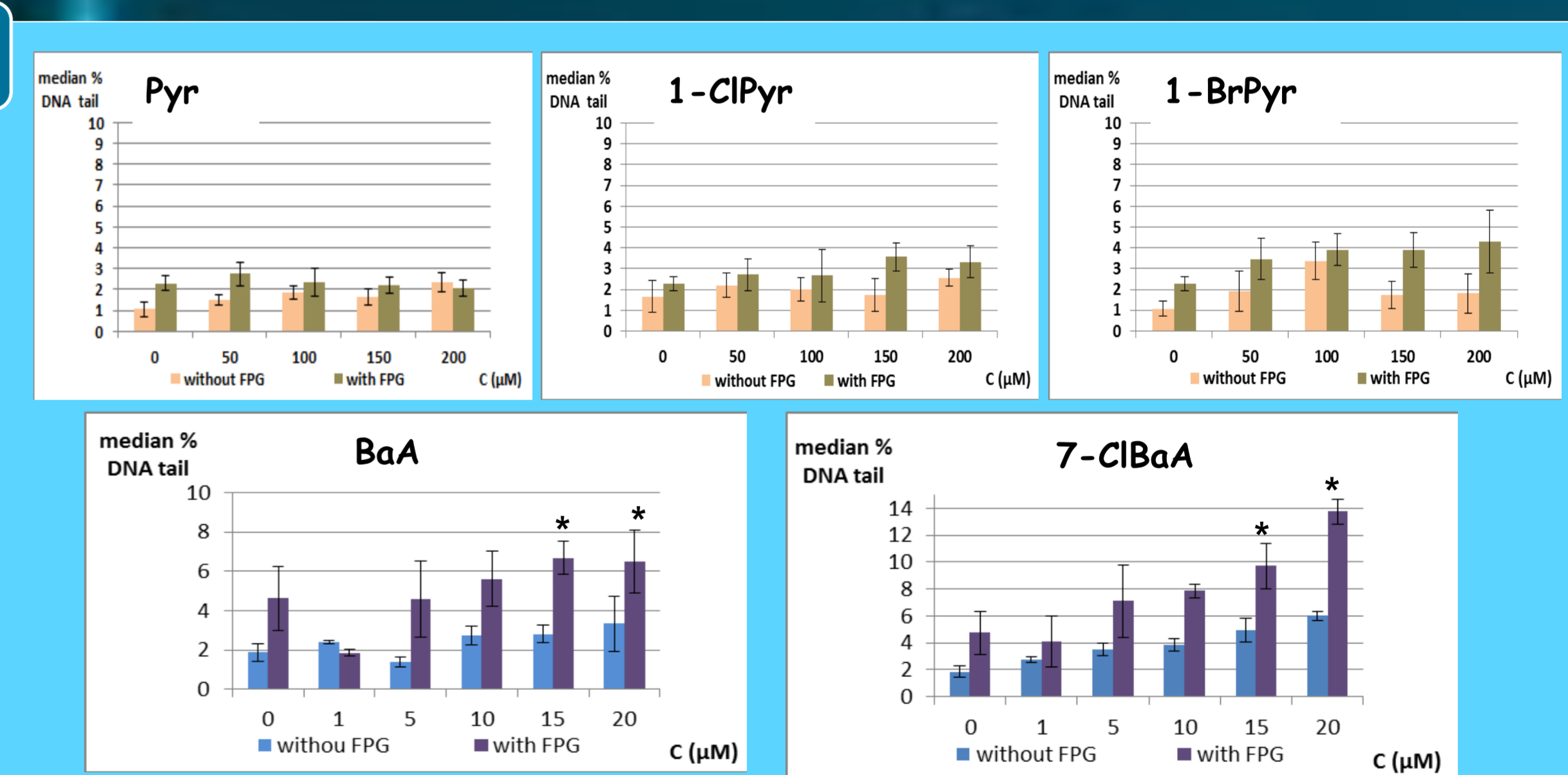


Figure 4- DNA breakage assessed by the Comet assay following 24h exposure to different concentrations of the studied compounds (*p<0.05 significantly values by Tukey's test).

CONCLUSIONS

• 1-ClPyr, 7-ClBaA and 1-BrPyr were formed under similar WTPs disinfection conditions

- BaA and 7-ClBaA showed cytotoxicity and genotoxic effects.
- Pyr, 1-ClPyr, 1-BrPyr were neither cytotoxic nor genotoxic.

FUTURE WORK

- > Application of the analytical methodology to real water samples - Monitor the formation of halogenated derivatives of PAHs
- > The formation of Cl- and Br-Pyr and BaA derivatives will be using different experimental conditions.
- > Human exposure to Cl- and Br-PAHs - contaminated water will be studied using the comet assay.