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Development and Application of Retention Time Prediction Models in the Suspect and Non-target Screening of Emerging Contaminants

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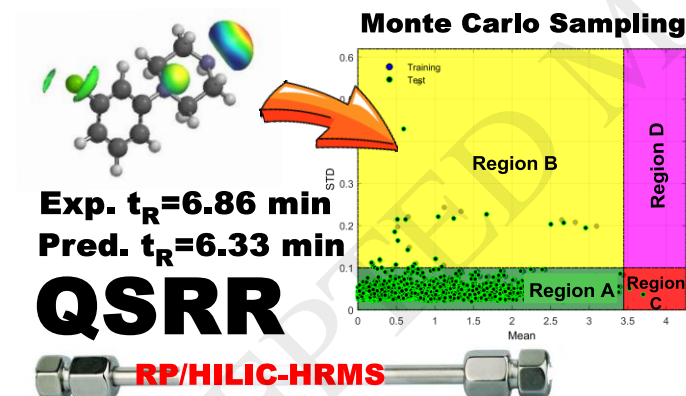
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Graphical abstract



Highlights

- Three new t_R prediction models were developed for RPLC and HILIC platforms
- Monte Carlo sampling method was developed to facilitate suspect and non-target screening
- t_R prediction was useful in the identification of 10 new TPs of emerging contaminants
- A comprehensive database of 273 biocides was built and used for this study
- 28 biocides in total were detected in treated wastewater and sludge of Athens

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