

Non-target Analysis Using High Resolution Mass Spectrometry to Characterize Urban Waters

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Goals

- Establish a non-targeted screening workflow for the tentative identification of “unknown” compounds based on HPLC-ESI/HRMS and Compound Discoverer
- Evaluate the developed workflow using the EPA’s ENTACT project samples
- To shed light onto the water quality of different water bodies



Figure 1. Thermo Q-Exactive Orbitrap.

Research Methodology

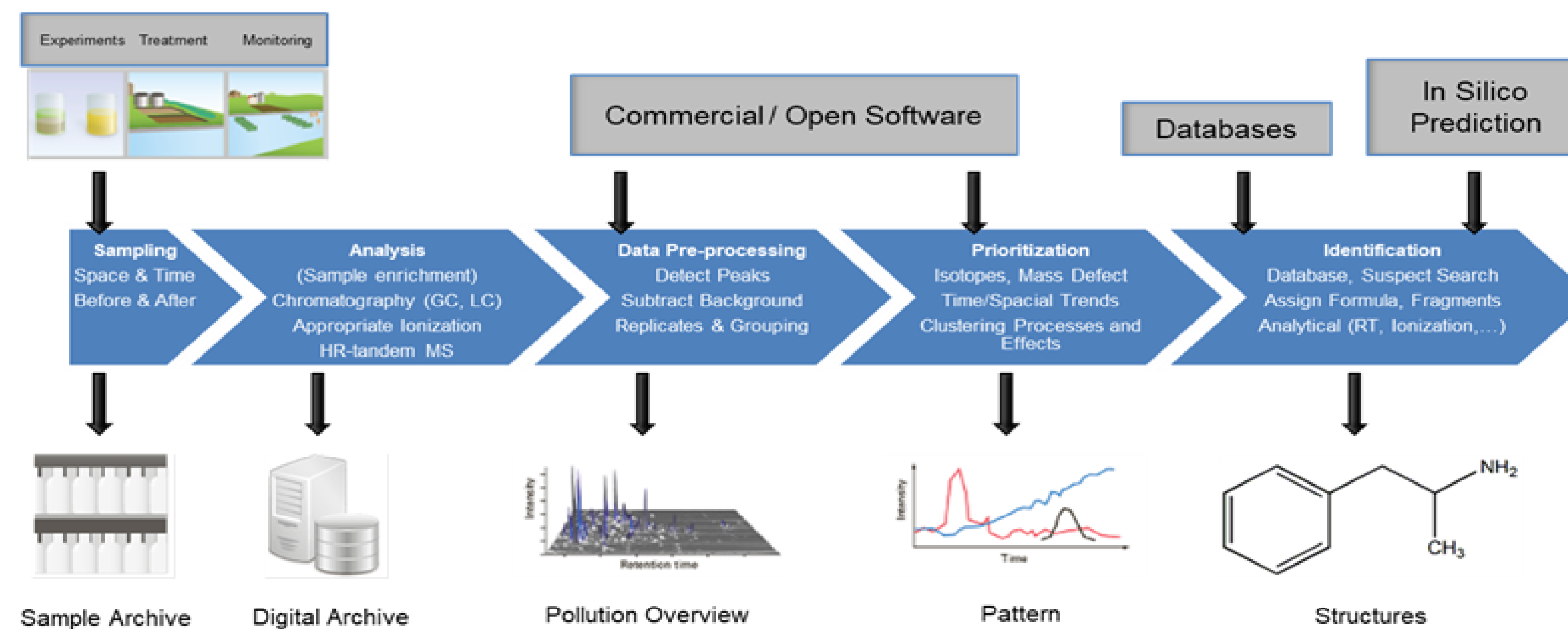


Figure 2. Non-target analysis workflow for environmental analysis adopted from Hollender *et. al.*

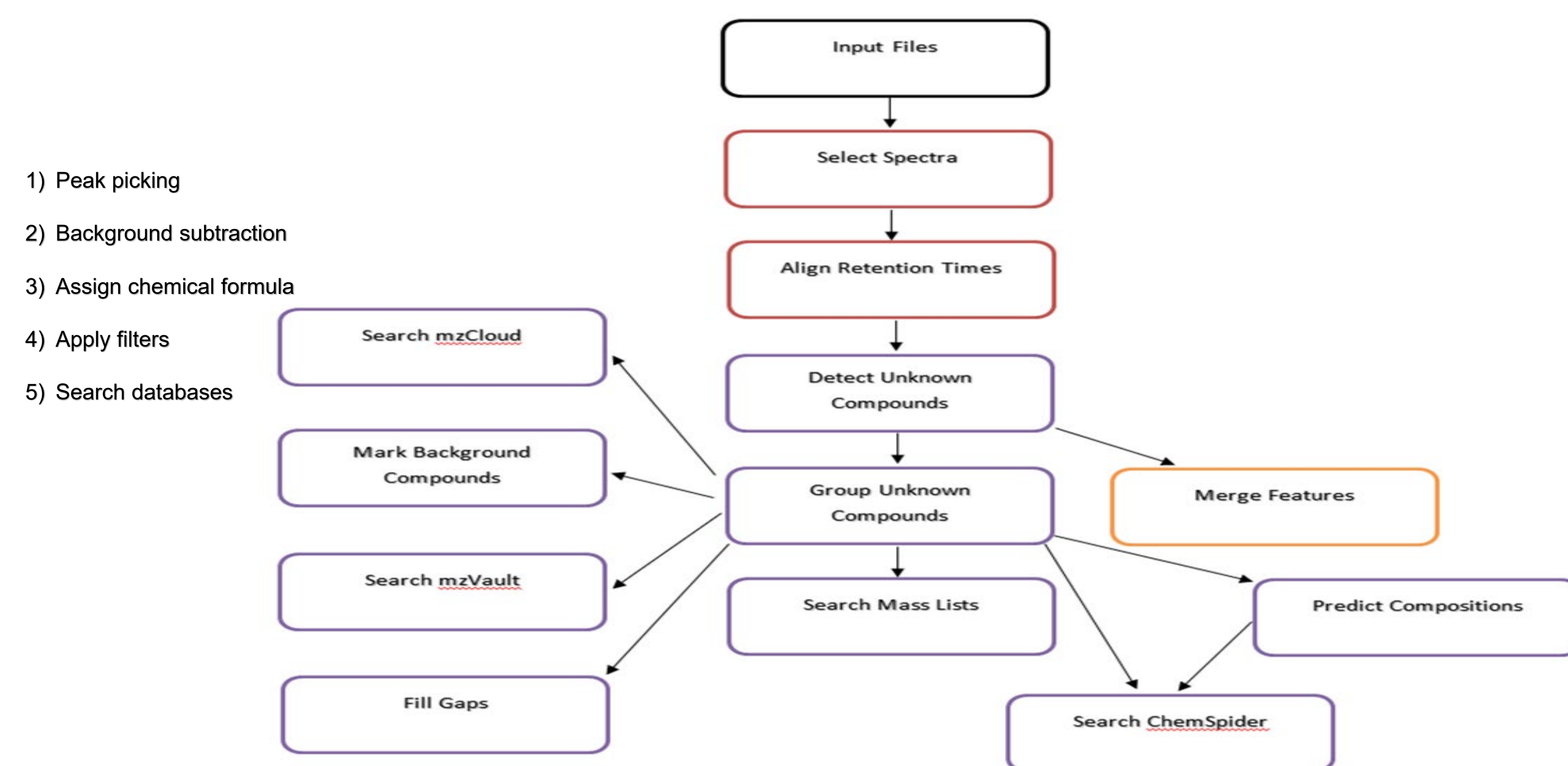


Figure 3. Compound Discoverer non-target screening workflow

Results

Quality Control

Log K_{ow} VS Retention Time

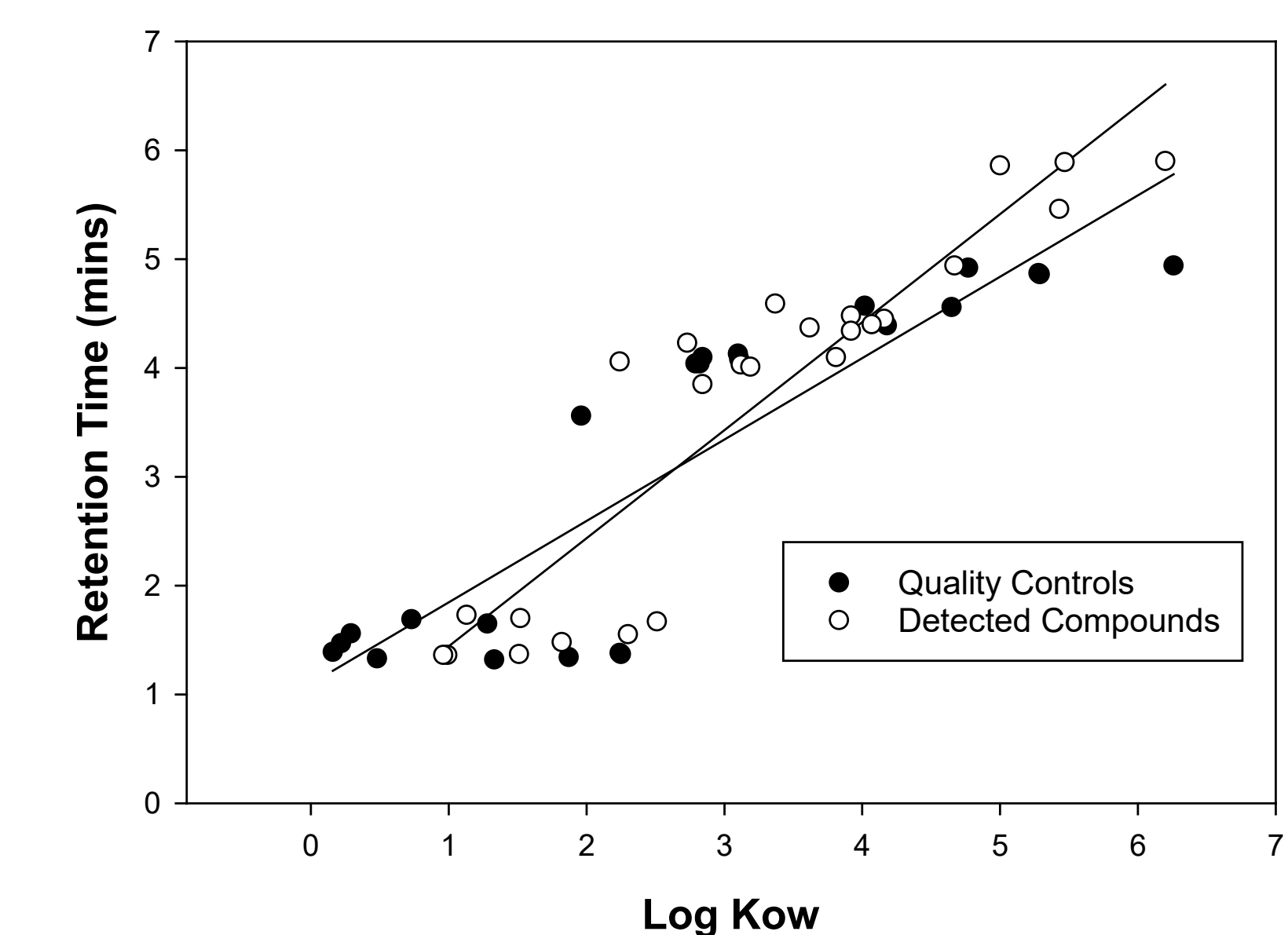


Figure 3. Correlation between Log K_{ow} and retention time in QC samples

ENTACT Samples

Blinded

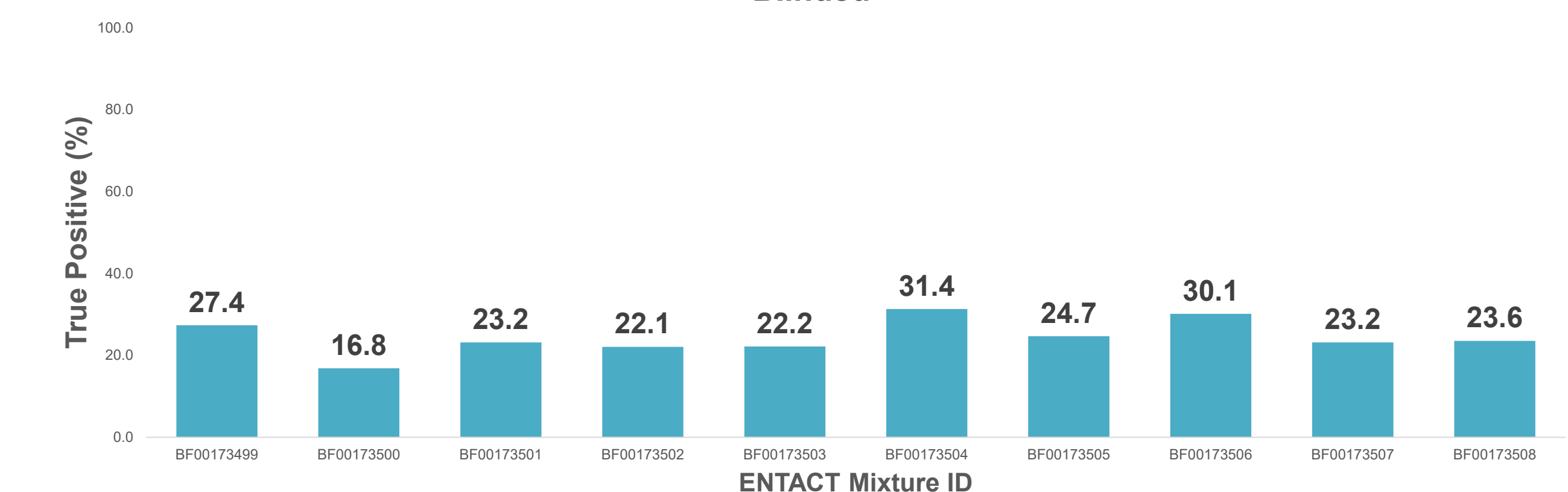


Table 1. Results of the 10 unknown liquid mixtures (blinded)

Unblinded

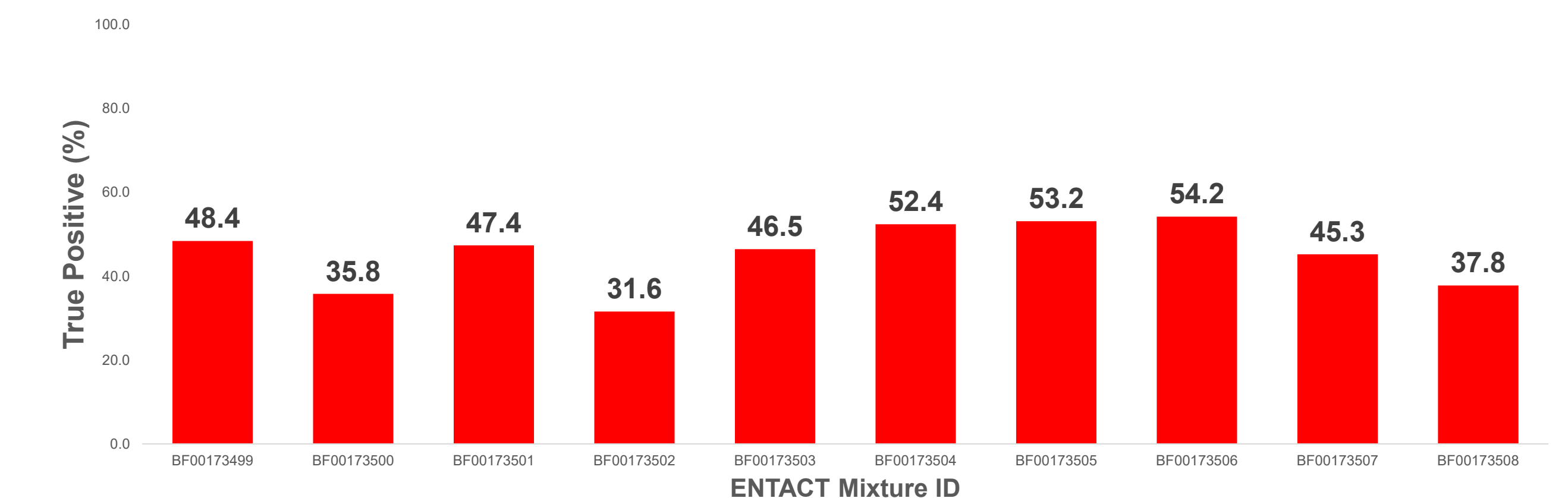


Table 2. Results of the 10 unknown liquid mixtures (unblinded)



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