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MetExpert: An Expert System to Enhance Gas Chromatography–Mass Spectrometry-Based Metabolite Identifications

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Highlights

- MetExpert assists users with limited expertise in informatics to interpret GCMS data for metabolite identification without querying spectral databases
- MetExpert performs in silico derivatization to increase the searchable chemical space of existing molecular structure databases
- MetExpert employs machine learning techniques for the prediction of retention indices and molecular substructures
- MetExpert prioritizes the candidate molecules using orthogonal dataset through a streamlined, automated pipeline
- MetExpert outperformed current state-of-the-art methods for ranking the correct identifications

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