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The best metabolite identification method is powered by machine learning

Title of the dissertation	Machine learning for small molecule identification
Contents of the dissertation	Metabolites are small molecules, such as sugars, fatty acids and amino acids that serve as sources of energy in the cells and as building materials for cell walls. Accurate identification of the metabolites of a biological sample is a requisite step for subsequent analyses such as anti-doping, drug control or other medical diagnostics.

In this dissertation, a series of machine learning methods are proposed to automatically identify metabolites. A special family of the machine learning algorithms, known as kernel methods, are used to handle the non-tabular nature of the data in this application. These methods are currently the most accurate ones as demonstrated in a recent small molecule identification challenge (CASMI 2016). |
Field of the dissertation	Machine learning and computational biology
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A doctoral dissertation is a public document and shall be available at Aalto University, School of Science's notice board in Konemiehentie 2, Espoo at the latest 10 days prior to public defence.