

Biological sample

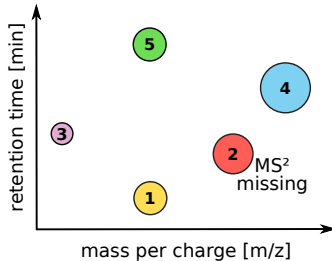
(containing multiple unknown small molecules)



LC-MS²

LC-MS Spectrum

(five MS features and MS²)



Input to our Framework

Set of (MS², RT, Candidate Set)-tuples

