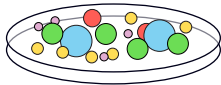


Biological sample

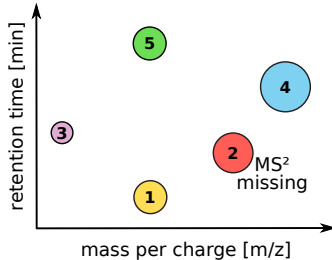
(containing multiple unknown small molecules)



LC-MS²

LC-MS Spectrum

(five MS features and MS²)



Input to our Framework

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

$$\begin{aligned} (x_5 &= \text{Intensity vs } [m/z] \text{ plot}, t_5 = 7.1, \mathcal{C}_5) \\ (x_4 &= \text{Intensity vs } [m/z] \text{ plot}, t_4 = 5.5, \mathcal{C}_4) \\ (x_3 &= \text{Intensity vs } [m/z] \text{ plot}, t_3 = 4.5, \mathcal{C}_3) \\ (x_2 &= \text{no MS}^2 \text{ plot}, t_2 = 4, \mathcal{C}_2) \\ (x_1 &= \text{Intensity vs } [m/z] \text{ plot}, t_1 = 2, \mathcal{C}_1) \end{aligned}$$