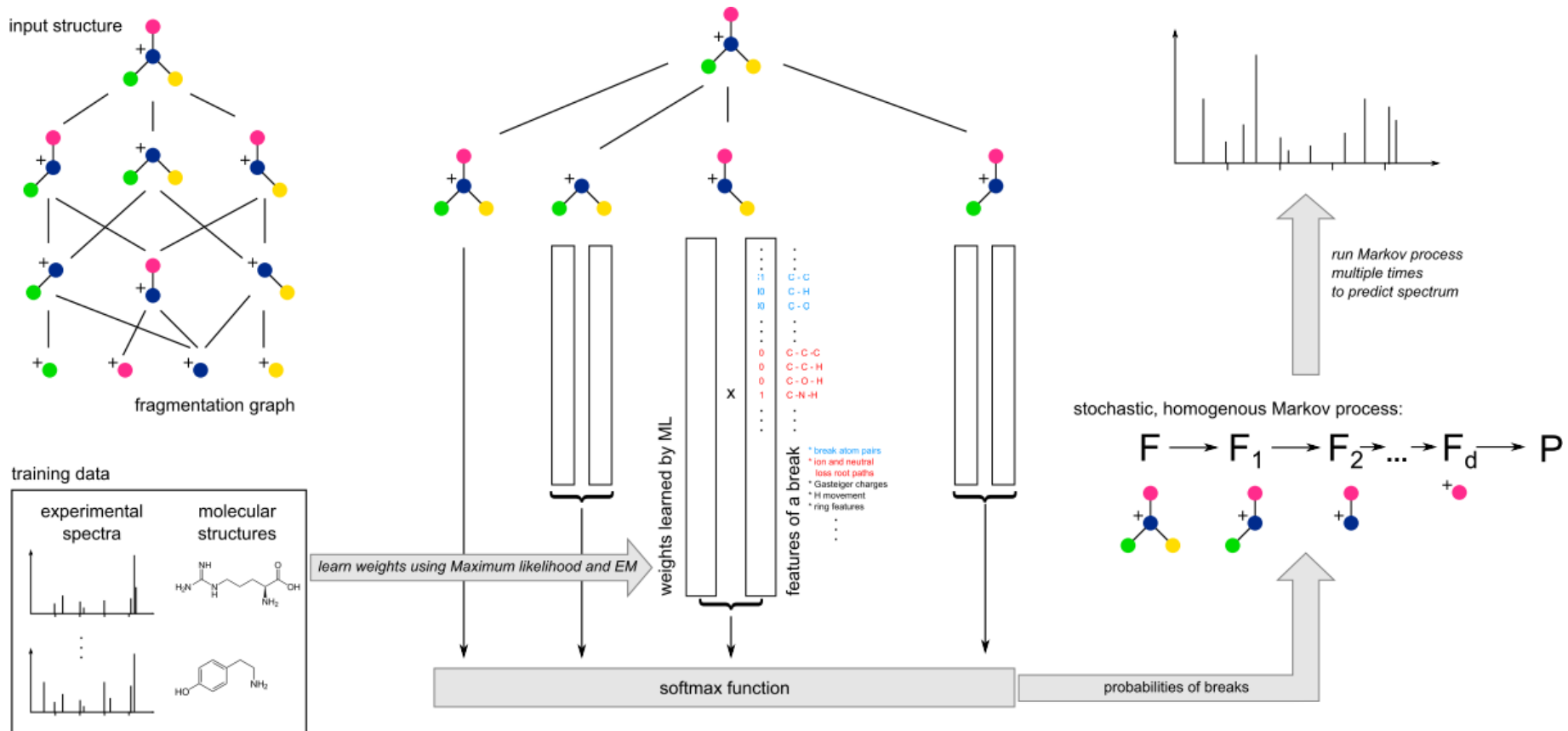
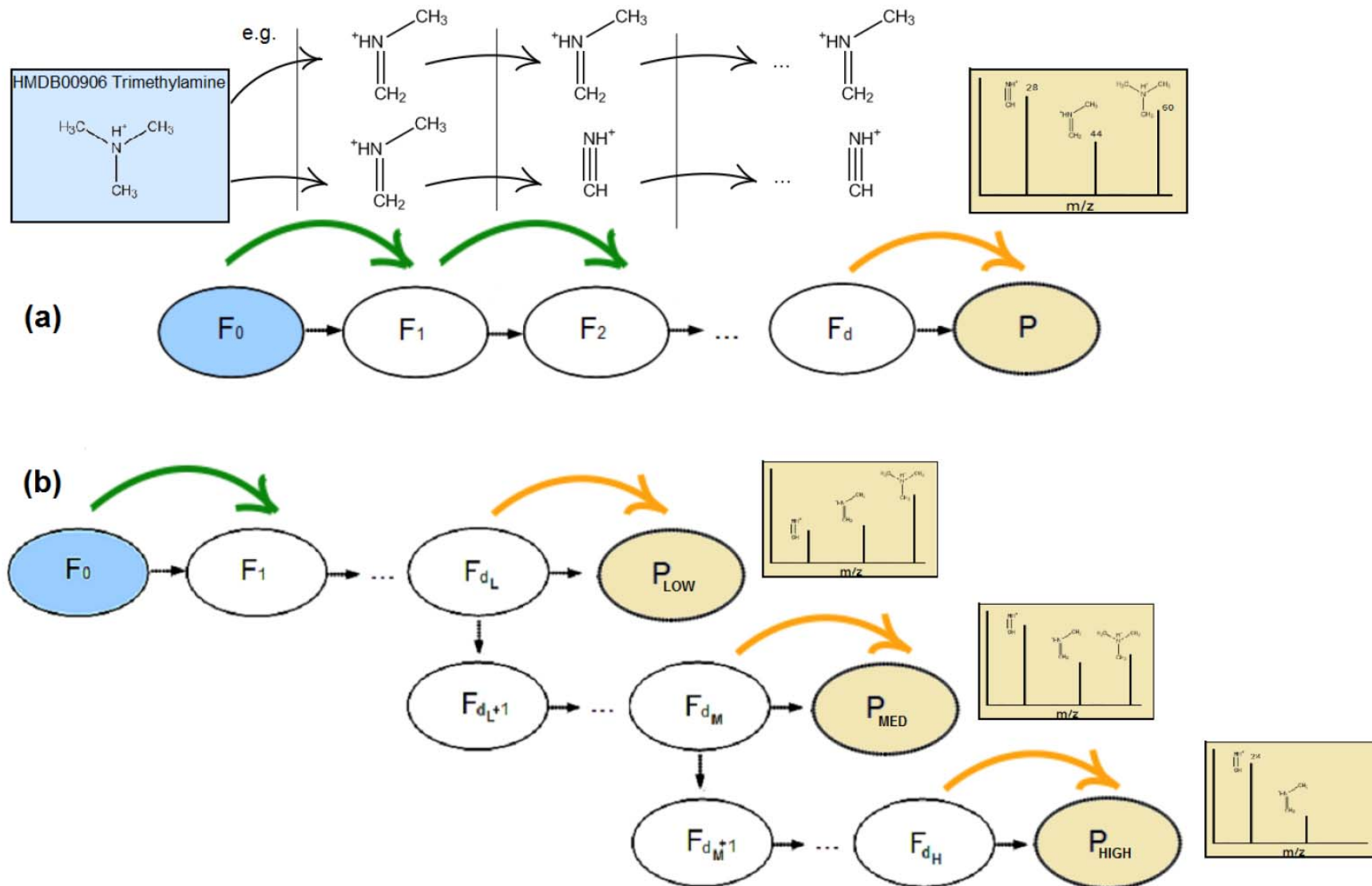


Competitive Fragmentation Modelling

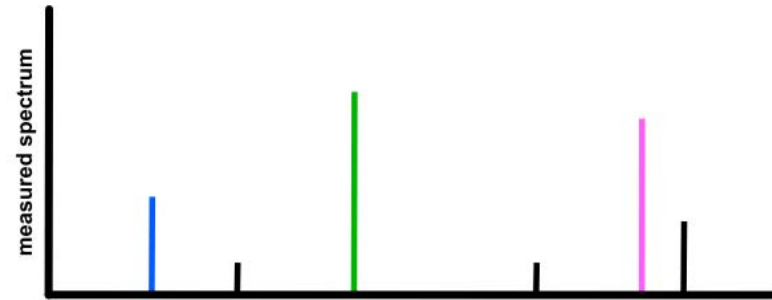
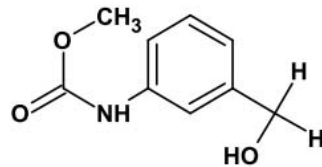
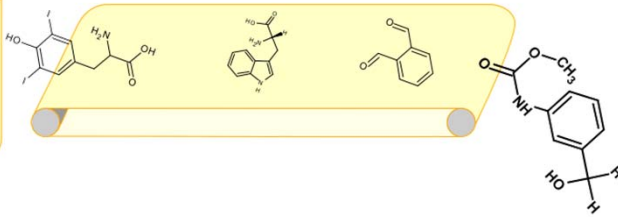
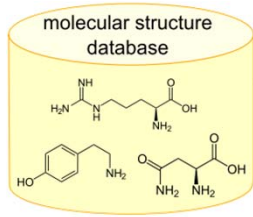


[Allen, Greiner, Wishart, *Metabolomics* 2014]

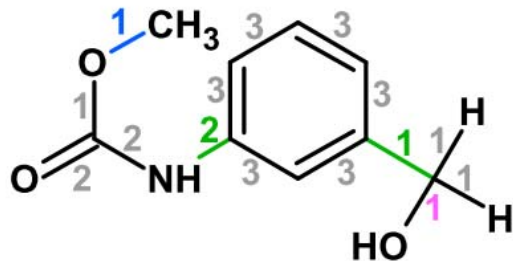
Competitive Fragmentation Modelling



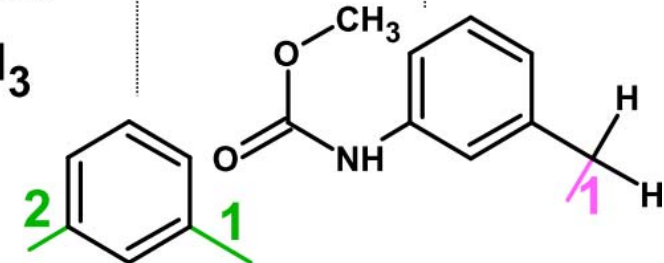
Kombinatorische Fragmentierung



score fragmentation of each bond



combinatorial optimization



no fragment found

no fragment found

McLafferty Umordnung

