GmadeStudio 质谱相关交流

Gmade Studio

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A novel workflow for HRMS metabolomics

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Typical workflow for HRMS metabolomics/NTA

1. Collect samples
2. Acquire data (peaks) using mass spectrometry
3. Annotate peaks for identification with compound name
4. Build links between compounds using pathway/network analysis

New idea: Reactions

Mass spectrum could directly measure relationship (reactions), Small molecule combination is a chemical reaction or paired mass distance, which is unique for reactions.

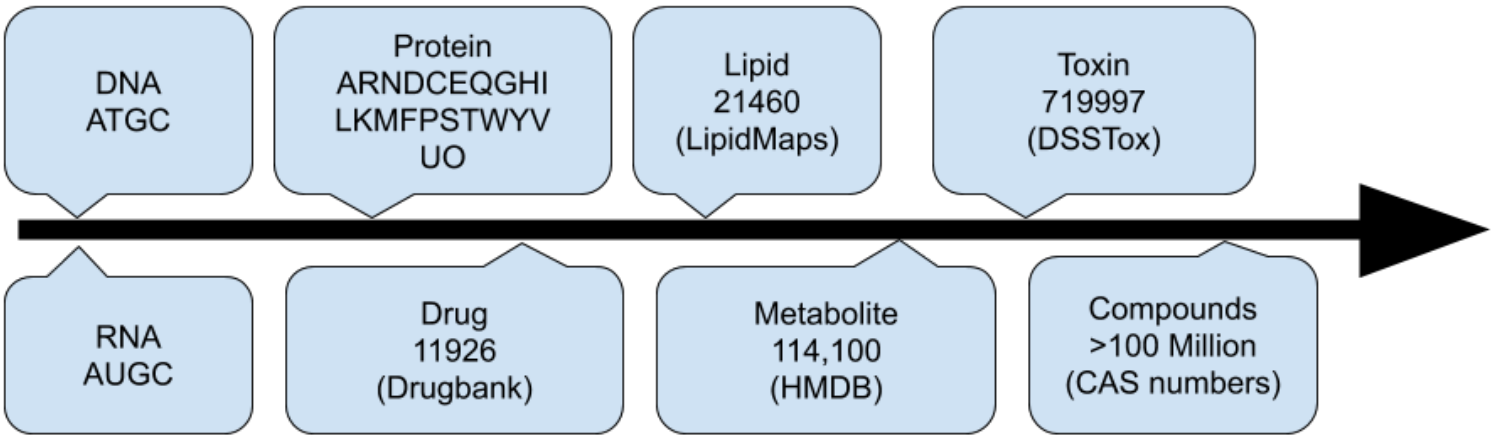

Figure: reaction scales

Gap between features and compounds

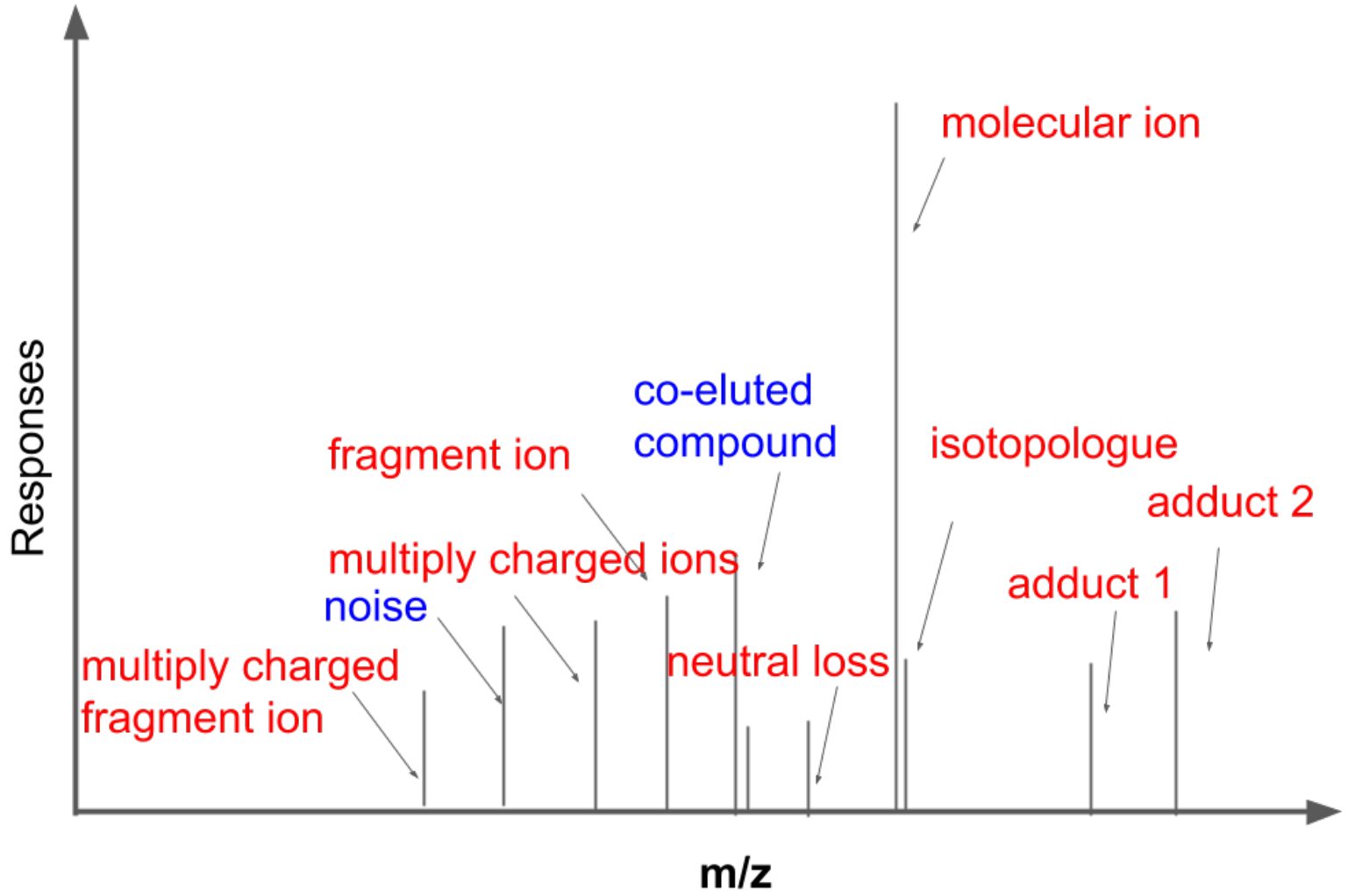

Figure: The Gaps

Expected results: PMD Network

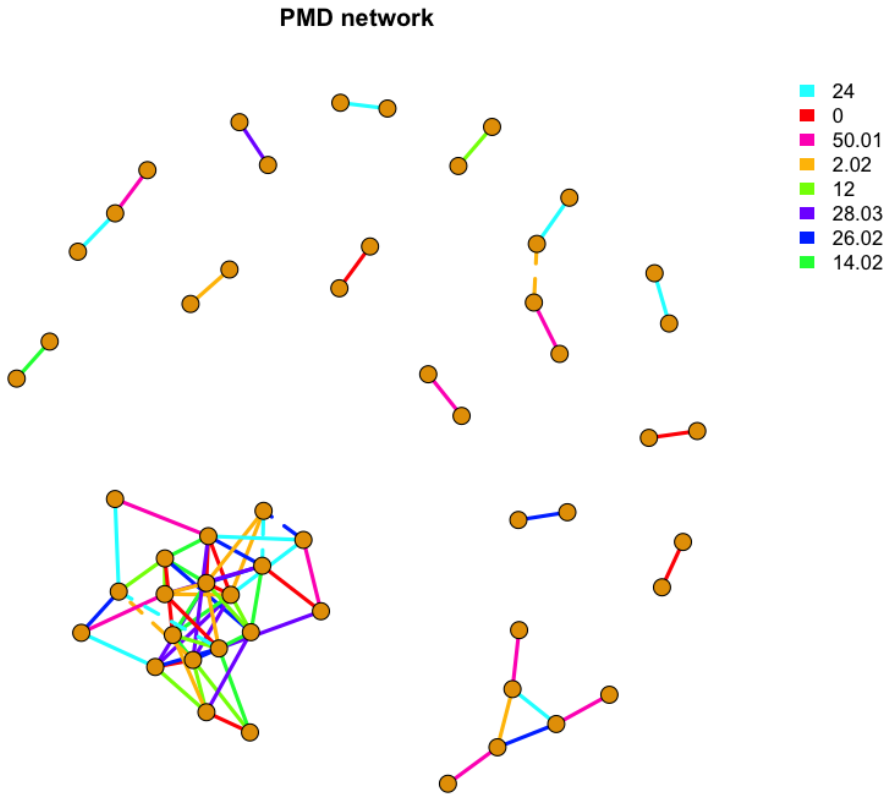

Figure: PMD Network

Methods: Materials

1. HRMS
2. Bio-samples
3. Data analysis codes
4. Road-map: Downstream analysis