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Research Area: Computational Science / Computational Biology

The project aims to develop a "PTM-filter" program that would scan a large set of MS/MS spectra and separate those which are likely candidates for containing PTMs. The program will not identify peptides or verify the specific PTM - it will design a very fast intermediate filter, which can be adjusted to minimize "false negatives" or to minimize "false positives." The PTM-filter will be essentially a de novo program that looks only for b-ions connectable by modified residue mass and sets high restrictions on the probability of the adjacent ions.

Specific subtasks:

1. Implement modifications of the existing software to provide three parameters (database, Pb limit, type of connectors)
2. Design test sets that would allow determination of false positive/false negative values
3. Run program for various databases -- collect results for all combinations of parameters
4. Build sensitivity/specificity curves based on the collected combinations of the parameters.

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