Release Notes

Version 0.2.2

- Add the `sequest-rally` code variant. This is an adaptation of the greylag code to run the Yates' lab's SEQUEST binary. Although it may not be useful in itself, it contains a number of improvements that should be folded into the main greylag code.

Version 0.2.1

- New program `greylag-reannotate` takes a set of SQT files and a FASTA database and reannotates the found peptides as if the search had been done against the specified database. (This is usually much faster than redoing the search.)

  This command will work on SQT files produced by greylag or SEQUEST, and fixes some truncation problems in loci generated by the latter. It also produces better flanking residues and handles isobaric residues more correctly.

- `greylag-validate --prefer-closer-mass` now has better charge alias handling.

- `maximum_missed_cleavage_sites` now defaults to 1.

- Carriage return characters in ms2 files are now handled better.

Version 0.2

- Fix some subtle but significant bugs in peak scoring and validation. These were found by comparing greylag and MyriMatch results. Greylag's results are now more similar to those of MyriMatch.

- New program `greylag-call-proteins` takes the validated peptide list from `greylag-validate` and assigns them to specific protein groups using the parsimony criterion.

- New filter flags to `greylag-validate` to support high-accuracy spectra (e.g., Orbitrap). This should help greylag to more often correctly distinguish between, for example, trimethlyation, acetylation, and carbamylation.

  The new `-exact-ptms` flag supports validation of specific peptide modifications, as opposed to the peptide in general (with whatever modifications).

  The `--bootstrap` flag provides a rough estimation of validation variance.

- Better performance on single hosts.

- More documentation.

- Many other bug fixes and improvements.

Version 0.1.2

- Fix validation bugs.

- Better `greylag-chase` error reporting back to user.

- Add basic Markov shuffle to `greylag-shuffle-database`.

- Add `--mass-error-histogram` to `greylag-validate`.

- Add `greylag-flatten-fasta` utility.

- Reduce RAM and open file requirements of various programs. In particular, `greylag-chase` no longer requires RAM linear in the number of spectra searched.

Version 0.1.1

- Significant improvements to `greylag-validate`, including saturation and FDR adjustment. There is now no need to use DTASelect for further quality filtering.

- Search for basic terminal modifications now works.

- Better logging, modification tracking in output.

- Doc improvements.

Version 0.1

- Initial internal release. Based on the new "rally" master/slave parallel search architecture.

- Known issues:

  - `greylag-merge` is currently not working
  - some fields of the SQT output are not calculated
  - N15 is the only isotope currently supported.
  - N- and C-terminal modification handling may not be correct.

See also the TODO file.