Webmetabase 3.2.0. Release notes

- New Features:
  - Metabolite Identification tools
    - Fragmentation Pathway: Representation of the fragmentation tree for the parent.
    - Manual edition of Markush.
  - New Analysis tool:
    - Metabolic pathway kinetic analysis: Being able to check if a metabolic scheme makes kinetic “sense”
  - Peptide mode:
    - Approval process: Chemical aware peptides in the database.
    - Peptide frequency analysis: Automatic analysis of which are the most common amide bonds that get metabolite in a series of experiments.
  - Data sharing and database manager:
    - Export/Import of experiments. Now, one can share experiments between different WebMetabase servers.
    - Import data from external sources (xml).
    - Consolidation tool: A new tool to consolidate the nomenclature of units, properties, protocols and more.
- Improvements compared to the 3.1.9 version
  - Metabolite Identification tools:
    - Chromatogram time scale need to shows the entire range of experiment
    - Manual edited metabolite need to keep original MS/MSMS spectra
    - Manual edition of fragments:
    - Isomorphism create complete MSomSpot data
    - Show current prediction number in the ranking chart
  - Analysis tools:
    - Simplify report pop-up window: Report window has been simplified to make it easier to follow.
  - Information management:
    - Makush system:
      - Revise the rules to render markush structures to allow ring openings in oxanes
      - Change the rules that enable/disable markush rendering of a molecule
    - New category to control user access to Notebook and Experiment settings
    - Assign a different owner to an experiment
    - Improve the IT manual with some advanced sections
  - Algorithms:
    - Speedup kinetic calculation process
    - Improve internal scheduler to coordinate application tasks
- Bug fixing
  - Mass shift review in the Chroma tab
  - The browser screen appears to be cut on the left part
  - No mechanism showed in the FA
  - Clustering process should take into account multiple charges
  - Calibration line experiment needs to check if the peaks of the different points can be clustered

- Kinetic analysis fail to select right substrate if there are more than one
- Kinetic analysis don't work after a merge until you save the experiment
- No Reaction mechanism in peaks from Chromatogram browser and MMSITE calculation
- % Area does not recalculate until you exit an experiment
- Manual Fragment edition
- Edit and already edited metabolite
- JSDraw license expire on August 26, 2016