Description of the comment fields of the library spectra.

- Pep= can be “Tryptic”, “N-Semitryptic”, “C-Semitryptic”, “Non-Tryptic” (reflects the tryptic properties of the termini).
- Peptype= shows the location of the peptide relative to the protein. For example,
  - <Protein><Peptide><Protein>: the peptide is in the middle of the protein;
  - <Protein_start><Peptide><Protein>: the peptide is at the beginning of the protein;
  - <Protein><Peptide><Protein_end>: the peptide is at the end of the protein;
  - <Signal_peptide><Peptide><Protein>: the peptide is adjacent to a signal peptide (the left terminus is regarded as tryptic);
  - <Protein><Peptide><Propeptide>: the peptide is adjacent to a propeptide (the right terminus is regarded as tryptic).

- Mods=: the list of modifications.
- Fullname=: the peptide name with adjacent amino acids.
- Charge=: the precursor charge.
- Parent=: the theoretical value of precursor.
- CE=: the average (among replicate spectra) collision energy.
- NCE=: the average (among replicate spectra) normalized collision energy.
- Q-value=: the average Q-value (among replicate spectra) returned by MS-GF+ for the peptide identification.
- Nprot=: the number of proteins containing the peptide.
- Protein=: the protein name.
- Nrep=: the average number of replicate spectra contributed to the consensus (averaged over all peaks).
- Theo_mz_diff=: the difference between the experimental and theoretical precursor values.
- Quality=: defines the number of quality criteria satisfied for the given spectrum; 7/7 corresponds to the best quality spectra.
- MC=: the number of missed cleavages
- MCtype=: a type of the missed cleavage: “Normal” or “Exception”. Some missed cleavages can be disregarded. We set “MCtype=Exception” if one of the missed cleavages
  - is flanked by the amino acids D, E, P in the combinations KD, RD, KE, RE, KP, RP, DK, DR inside the peptide;
  - occurs at the distance 1 or 2 amino acids from the N-terminus as follows: K.K…, K.R…, R.K…, R.R…, K.xK…, K.xR…, R.xK…, R.xR…, where x is any amino acid.

The fields Unassigned_all_20ppm=, Unassigned_20ppm=, num_unassigned_peaks_20ppm=, max_unassigned_ab_20ppm=, top_20_num_unassigned_peaks_20ppm= are related to peaks annotation. For example, top_20_num_unassigned_peaks_20ppm= is the number of unassigned peaks among the largest 20 peaks of the spectrum.