Supplemental Table 8

DIALib-QC assessment report of the Mouse hybrid T6 spectral assay library.

library	Mouse-tissue- Project- specific_Lukas- Resource-Hybrid-T6- Library.xls	Name of library file being analyzed
format	Spectronaut	Library format, one of OpenSWATH, PeakView, or Spectronaut
pepions	455814	Number of peptide ions (i.e. precursor, sequence + modifications + charge)
fragments	9981770	Number of fragment (fragment ions) in library
ptp_percent	100	Percentage of proteotypic pepions (not shared)
shared_percent	0	Percentage of shared peptide ions (pepions)
shared_pepions	0	Number of shared pepions
peptides	175952	Number of distinct peptide sequences
mod_peps	332402	Number of distinct modified peptides (sequences + modifications)
mod_percent	60.6	percentage of distinct modified peptides with a mass modification
total_mods	366023	Number of mass modified amino acids
chg_2	23.1	Percentage of charge 2 precursors
chg_3	40.2	Percentage of charge 3 precursors
precursor_min	380	Minimum precursor <i>m/z</i> (mass/charge) in library
precursor_max	1251.2	Maximum precursor <i>m/z</i> in library

fragment_min	199.1	Minimum fragment <i>m/z</i> in library
fragment_max	1699.9	Maximum fragment <i>m/z</i> in library
avg_len	18.5	Average peptide Length
avg_num_frags	21.9	Average number of fragments per assay (precursor)
avg_frag_len	1.18	Average fragment sequence length
short_perc	100	Percentage of assays with 5 or fewer transitions
fragment_above_precursor	0.582	Percentage of fragment <i>m/z</i> above precursor <i>m/z</i>
y_perc	61.3	Percentage of y ions
b_perc	38.7	Percentage of b ions
t6_y_perc	61.7	Percentage of y ions considering only the top 6 fragments per assay
avg_intensity	0	Average Intensity
rt_min	-10790.2	Minimum RT (retention time) in library
rt_max	572.2	Maximum RT in library
rt_med	41.9	Median RT in library
rt_rsq	1	r-squared value of fit between RT of +2 and +3 charge states for the same modified peptide
rt_five	100	Percentage of +2/+3 charge pairs of the same mod pep within 5 RT units of each other
n_irt	11	Number of iRT peptides in library

irt_cnt	614	Number of iRT assays (precursor + fragment)
low_nr	0	Number of fragments annotated as y1,y2,b1, or b2
db_peps	0	Peptides in reference library, often 7-50 AA
seen_peps	0	Number of library peptides seen
mc_peps	75590	Number of Missed cleavage peptides
db_prots	0	Number of Proteins in reference library
lib_prots	10821	Number of proteins with at least one assay in ion library
seen_prots	N/A	Number of library proteins seen
ux_prots	N/A	Unexplained (not in reference library) proteins
decoy_pct	0	Percentage of decoy (optionally includes "alternative", non-db decoys) assays
mixed_pct	0	Percentage of mixed decoy/target (has both decoy and no-decoy annotations) assays
fwd_pct	100	Percentage of target (non-decoy) assays
med_ppp	18	Median number of pepions per protein
mean_ppp	42.1	Mean number of pepions per protein
stddev_ppp	96	Standard deviation of the number of pepions per protein
3_sigma_ppp	112	number of pepions per protein more than 3 standard deviations from the mean
max_intensity_idx	1	Average index of most intense fragment

precursor_ok	455814	Number of assays where precursor is within 5 ppm (parts per million <i>m/z</i>) of theoretical
precursor_bad	0	Number of assays where precursor is more than 5 ppm from theoretical
fragment_ok	9981770	Number of assays where fragment is within 1 ppm of theoretical
fragment_bad	0	Number of assays where fragment is more than 1 ppm from theoretical
fragment_na	0	Number of assays where peak annotation not found in expected b/y series
fragment_avg_mdiff	0	Average <i>m/z</i> difference between reported and theoretical fragment
problem_assays	0	Assays whose precursor or any fragment <i>m/z</i> values do not match SWATHs file or differ significantly from theoretical values
im_min	0.6155	Minimum ion mobility reported in library
im_max	1.5881	Maximum ion mobility reported in library

