Figure S1: **Weight Parameter Scan for the test dataset.** The plots show the distribution of the number of Top1 rankings for the 1000 combinations of the weight parameters $\omega_1$ (MetFrag), $\omega_2$ (Peak), $\omega_3$ (Loss) for (a) the negative and (b) the positive mode test dataset. The shown Top1 rankings result for the optimum $\alpha$, $\beta$, $\alpha^L$, $\beta^L$ parameter set for negative and positive mode as highlighted in Table 7. The circles mark specific quantiles (0.1%, 25%, 50%, 75%, 100%) and their Top1 ranking values.