

Table S2: Notation summary (Scores)

$S_{MetFrag}^c$	MetFrag score of a candidate c
S_{Peak}^c	statistical score evaluating fragment - m/z peak assignments of a candidate c
S_{Loss}^c	statistical score evaluating loss fragment - m/z loss assignments of a candidate c
$S_{RawPeak}^c$	non-normalized statistical score evaluating fragment - m/z peak assignments of a candidate c
$\omega_1, \omega_2, \omega_3$	score weights
S_{Fin}^c	final/consensus score of a candidate c