Supplementary Figure 1. The relationship between the first and second best C-score in a given search. If C corresponds to the best C-score and S be the second best C-score. Let $P_C$ be the posterior probability corresponding to C and likewise $P_S$ for S. The C-score is defined as $C = \frac{-10 \log_{10}(1-P_C)}{10}$, and $S = \frac{-10 \log_{10}(1-P_S)}{10}$. If $S$ is maximal, then $P_S = 1 - P_C$.

Solving for $P_C$ in the first equation: $P_C = 1 - 10^{-C/10}$. Therefore $P_S = 10^{-C/10}$. Therefore, as the best (highest) C-score returned from a search increases, the second highest possible score decreases non-linearly. This figure shows the relationship between these two values. Using the derivation above, it can be shown that this relationship is $S = -10 \log_{10} \left(1 - 10^{-C/10}\right)$. 
Supplementary Figure 2. Receiver Operating Characteristic curves comparing C-scores on the 295 experiments in the manually-curated test data set as a function of MS/MS mass tolerance. The area under the curve for the Blue 10 ppm tolerance is 0.99 compared to 0.85 for the Orange 30 ppm tolerance and 0.80 for the Green 100 ppm tolerance. As tolerance increases, the discriminative power of the score decreases as more fragment ions will match by chance.