

Calculation of protein expectation value from peptide expectation values in X! Tandem:

Assume that an experiment has generated s mass spectra. If a protein sequence is being inferred from the observation of n unique peptide sequences, each of which has been assigned an expectation value e_j , then the expectation value for the protein, E_{pro} , is given by:

$$E_{pro} = \left(\frac{\beta^n (1 - \beta)^{s-n}}{sN^{n-1}} \right) \times \left(\prod_{j=1}^n e_j \right) \times \left(\prod_{i=0}^{n-1} \frac{(s-i)}{(n-i)} \right)$$

where

N = peptide sequences scored in to find the n unique peptides

β = N /(total number of peptides in the proteome considered)

In the exceptional case that only one peptide has been observed, $E_{pro} = e_1$

The following page shows the code used by X! Tandem to implement this equation.

```

/*
 * expect_protein is used to assign the expectation value for a
 protein, if more than one peptide has been found for that
 protein. the expectation values for the peptides are combined
 with a simple Bayesian model for the probability of having two
 peptides from the same protein having the best score in
 different spectra.
 */

double mprocess::expect_protein(
    const unsigned long _c, // number of peptides found
    const unsigned long _t, // number of total spectra
    const unsigned long _n, // number of peptides considered
    const double _d // sum of log peptide expectation values
)
{
    double dValue = _d+log10((double)m_tProteinCount);
    if(_c == 1 && _d < 0.0) {
        return _d;
    }
    else if(_c == 1) {
        return 1.0;
    }
    if(_c == 0) {
        return 1.0;
    }
    double dN = _n;
    double dK = _c;
    double dV = _t;
    unsigned long a = 0;
    while(a < _c) {
        dValue += log10((dV - a)/(dK - a));
        a++;
    }
    dValue -= log10(dV);
    dValue -= (dK-1.0)*log10(dN);
    double dP = dN/(double)m_tPeptideCount;
    if(dP >= 1.0)
        dP = 0.9999999;
    double dLog = dK*log10(dP)+(dV-dK)*log10(1.0-dP);
    dValue += dLog;
    return dValue;
}

```