```
function [GTest_pvalue] = GTest(Peptide_Vector,Groups)

    % Peptide_Vector is a list of observed and unobserved values for a specific peptide.
        % Unobserved values are represented as NaN values

    % Groups is a vector of class indices associated with each observation in Peptide_Vector.  This vector
        % is numeric and sequential, which means that if there are 4 classes, then each position in
        % Peptide_Vector will be represented in "Groups" as a 1,2,3 or a 4.  If the data are in another format,
        % such as a Cell structure it would need to be converted.

    % 1) determine how many samples are in each group (nk in paper)
    N = length(Groups);
    num_g = max(Groups);
    nk = zeros(num_g,1);
    for i = 1:num_g
        nk(i) = length(find(Groups == i));
    end

    % 2) Create the Observed Count Matrix (C_Ok and C_Ak in paper)
       Count_Matrix = zeros(num_g,2);
      % If there is a 0 in the Count_Matrix this will create problems with the log transformation.
      % G-test ignores 0's in the sum, they can be replaced with a NaN.
        for i = 1:num_g
        Number_Missing = sum(isnan(Peptide_Vector(Groups == i)));
        if Number_Missing == 0
            Count_Matrix(i,1) = NaN;
        else
            Count_Matrix(i,1) = Number_Missing;
        end
        if Number_Missing == nk(i)
            Count_Matrix(i,2) = NaN;
        else
            Count_Matrix(i,2) = nk(i) - Number_Missing;
        end
    end

    % 3) Create the Expected Count Matrix (E_Ok and E_Ak in paper)
      % All summations must be done ignoring the NaN values
    M_Values = nansum(Count_Matrix);
    Expected_Matrix = (nk * M_Values) ./ N;

    % 4) Compute the G statistic and associated significant value (Equation 2 in paper)
    G_Value = 2*nansum(nansum(Count_Matrix .* (log(Count_Matrix ./ Expected_Matrix))));
    GTest_pvalue = 1 - chi2cdf(G_Value,num_g - 1);
```

Figure S4. Generic MatLab® code for computing the G-value in Equation 2 and the associated significance value from a χ2 distribution.