

```

close; clear all;
mass_spec_data;

% Creates the matrix A describing how the concentration of each species
% effects a particular mass in the total mass spectrum
M = length(total_spectrum);
N = length(ion_masses);
A = zeros(M,N);
for i = 1:M
    for j = 1:N
        indx = find(ion_masses{j} == masses(i));
        if(~isempty(indx))
            imass = ion_masses{j};
            ispec = ion_spectra{j};
            A(i,j) = imass(indx)*ispec(indx);
        end
    end
end

% Gets the indexes of the columns of A that are all 0
for i = 1:275
    if(sum(A(:,i)) == 0)
        Iempty(i) = i;
    end
end
Iempty(:,find(sum(Iempty,1) == 0)) = [];

% Removes the columns of A that are 0
A(:, find(sum(abs(A)) == 0)) = [];
C = (A'*A)\A'*total_spectrum;
[sorted, I] = sort(C, 'descend');

% Removes the species that don't contribute to the total mass spectrum
ion_masses(Iempty) = [];
ion_names(Iempty) = [];
ion_spectra(Iempty) = [];

disp(['The top 10 species with the greatest concentration are']);
for i = 1:10
    disp(['Species #' num2str(I(i)) ' with name: ' ion_names{I(i)} ' and concentration ' nu
m2str(sorted(i))]);
end

```

Warning: Matrix is close to singular or badly scaled. Results may be inaccurate.

RCOND = 2.576646e-22.

The top 10 species with the greatest concentration are

Species #12 with name: C38H70NO7P and concentration 8337415569.5539

Species #52 with name: C38H76NO10P and concentration 227743786.1004

Species #6 with name: C36H64NO8P and concentration 108308369.6705

Species #31 with name: C36H72NO10P and concentration 25396261.2155

Species #16 with name: C37H70NO8P and concentration 12668499.7409

Species #32 with name: C40H75N2O6P and concentration 7167006.7473

Species #15 with name: C38H75N2O6P and concentration 4027622.8695

Species #54 with name: C40H70NO9P and concentration 3987486.0978

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Species #43 with name: C40H72NO8P and concentration 180926.1186

Species #8 with name: C36H68NO8P and concentration 164275.123

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