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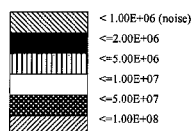
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(54) Title: METHOD OF VISUALIZING NON-TARGETED METABOLOMIC DATA GENERATED FROM FOURIER TRANS-
FORM ION CYCLOTRON RESONANCE MASS SPECTROMETERS

Absolute Intensity of Metabolite Peaks in Each Sample, Represented in Colour

Mean Mass	StdDev Mass	Mean Int	StdDev Int	N	Int 170	Int 171	Int 172	Int 173
300.057819	0.00E+00	7.188800E+06	0.00E+00	1				
300.205909	2.73E-05	2.359573E+07	1.41E+07	4				
301.139005	0.00E+00	1.092600E+07	0.00E+00	1				
326.072051	1.54E-04	1.147967E+07	4.22E+06	3				
328.236638	3.01E-05	5.578233E+07	2.05E+07	3				
329.138741	1.65E-06	1.059135E+07	2.00E+06	2				
348.134579	0.00E+00	1.028300E+07	0.00E+00	1				
348.177108	0.00E+00	8.421060E+06	0.00E+00	1				
356.005996	7.27E-05	8.992475E+06	2.11E+06	4				
367.345218	7.88E-05	1.936950E+07	4.21E+06	4				
374.243265	7.89E-05	3.368725E+07	1.67E+07	4				
374.315531	0.00E+00	5.983600E+06	0.00E+00	1				
378.144236	1.47E-04	2.072585E+07	1.34E+07	4				
378.310570	8.70E-05	1.456655E+07	6.06E+06	2				
379.147434	3.49E-05	8.096500E+06	8.30E+04	2				
380.189947	2.08E-05	8.381150E+06	2.86E+06	2				
380.290099	1.65E-04	1.756248E+07	1.32E+07	4				
388.258123	0.00E+00	8.673200E+06	0.00E+00	1				
388.331240	0.00E+00	6.048300E+06	0.00E+00	1				
390.143565	5.48E-04	1.609270E+07	1.25E+07	4				
390.156981	0.00E+00	1.335000E+07	0.00E+00	1				
390.310944	0.00E+00	5.616000E+06	0.00E+00	1				
392.289805	0.00E+00	8.319100E+06	0.00E+00	1				
392.326216	1.43E-04	2.210743E+07	2.02E+07	4				
394.138692	2.72E-04	7.325000E+06	1.62E+05	2				

Key : (absolute intensity level)



(57) Abstract: The invention can be summarized as follows. The present invention provides a method of displaying spectroscopic data comprising the steps of, i) obtaining spectroscopic data from a plurality of samples, each sample comprising one or more components wherein each component is characterized by an ordered pair (X,Y) of data comprising data element value X and data element value Y, wherein X is a data element value, equivalent or directly proportional to the mass of the component, and Y is a data element value equivalent or directly proportional to the amount of the component; ii) identifying all unique components comprising a common data element value X in said samples; computing the average of all X therefrom; and determining the average and optionally, the standard deviation for all Y values from all ordered data pairs comprising a common X; iii) generating a data structure comprising an array of codable cells, each cell assigned a color or other identifiable characteristic based on the relationship of the amount of each unique component present in each of said samples in relation to a predetermined value or other characteristic of the spectroscopic data. Also disclosed are data structures comprising spectroscopic data.

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