

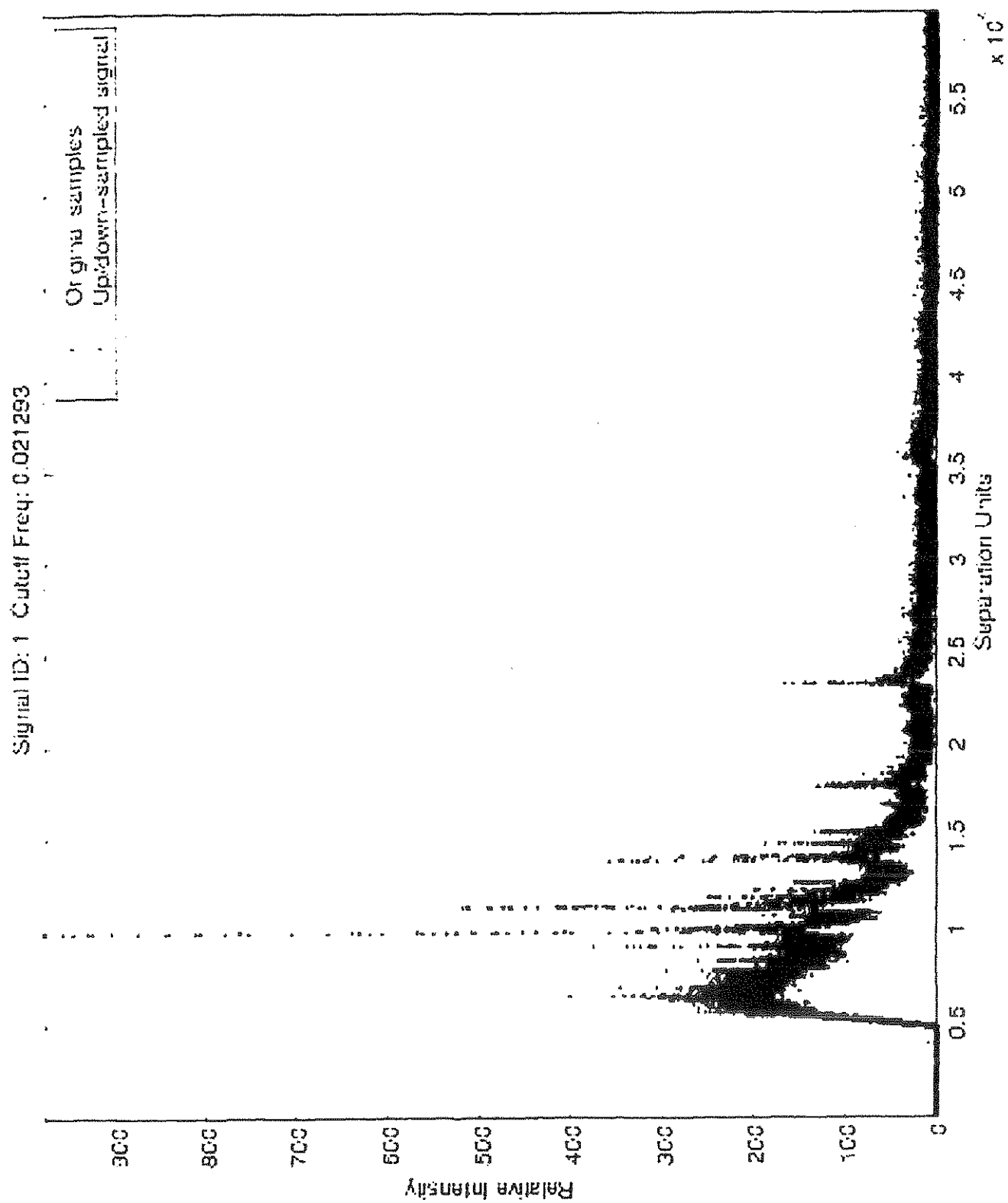


Fig. 1a

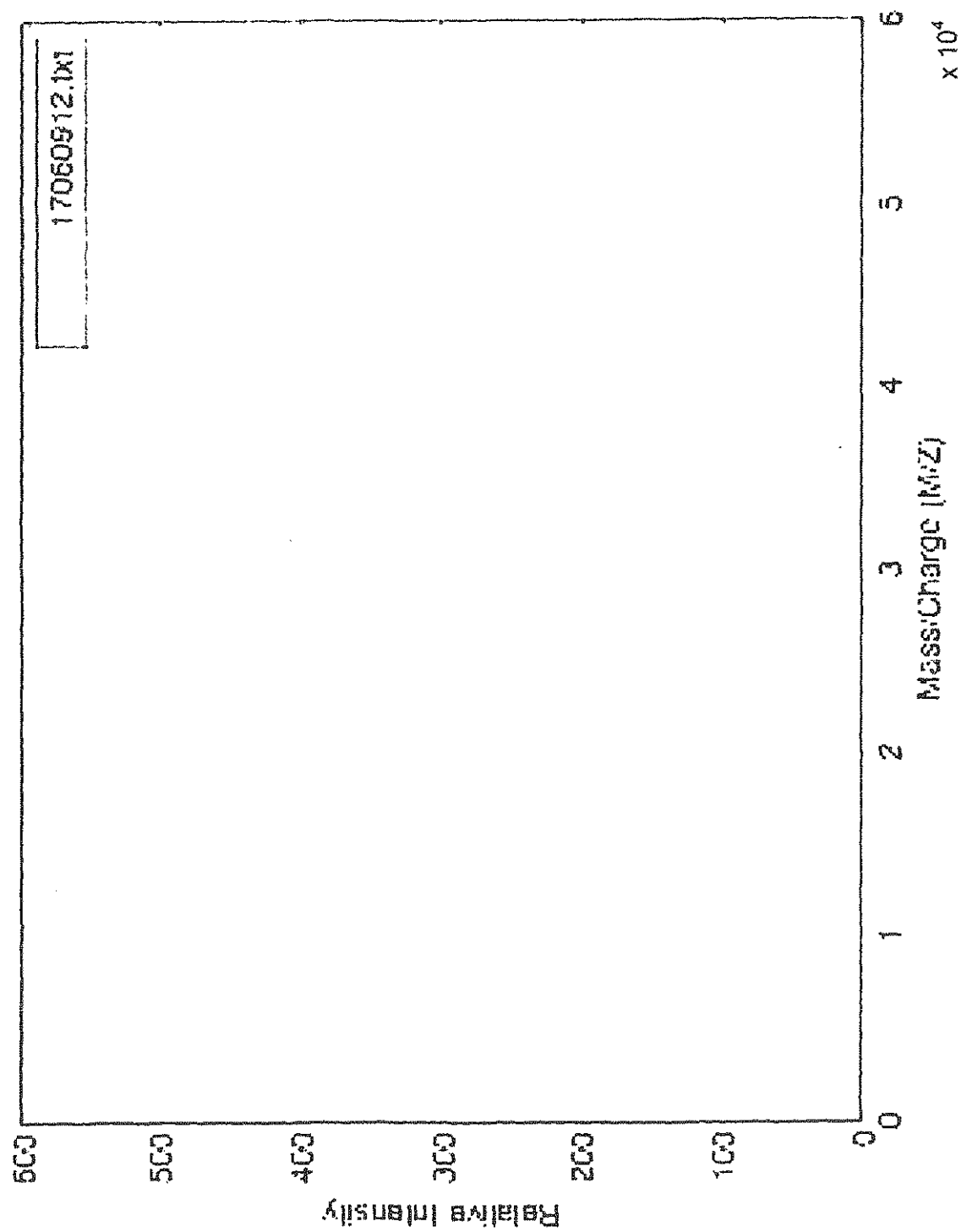


Fig. 1b

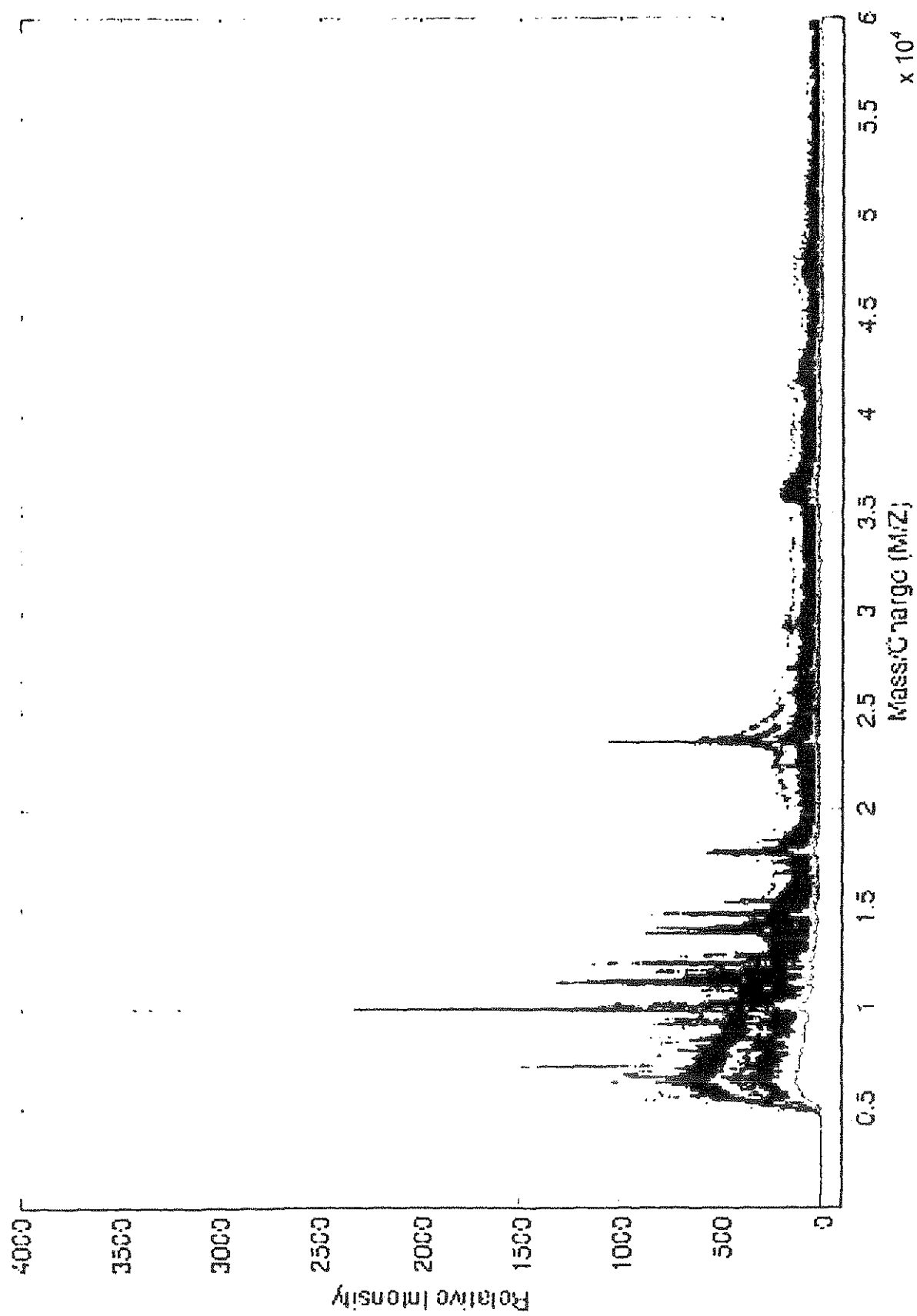


Fig. 2a

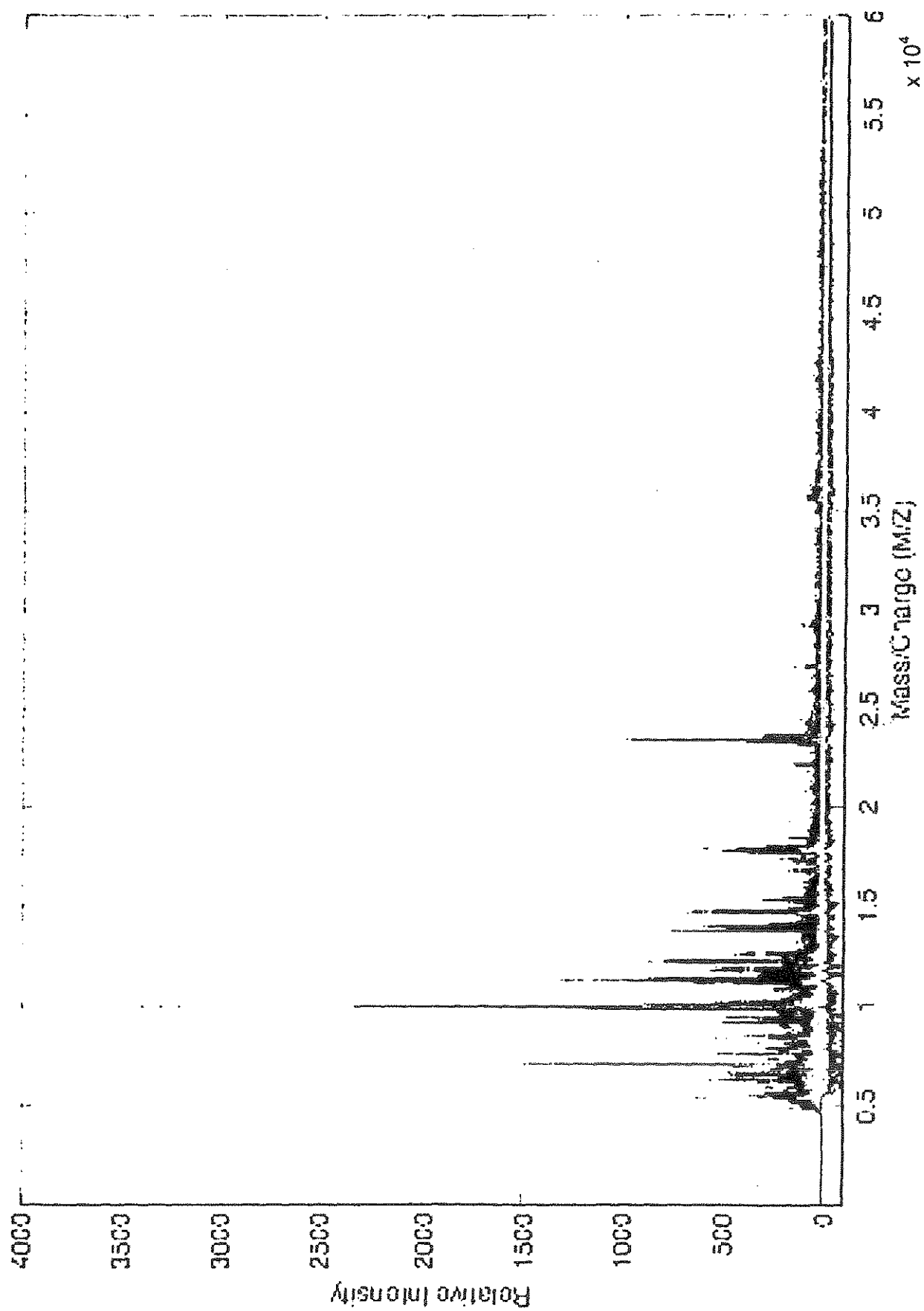


Fig. 2b

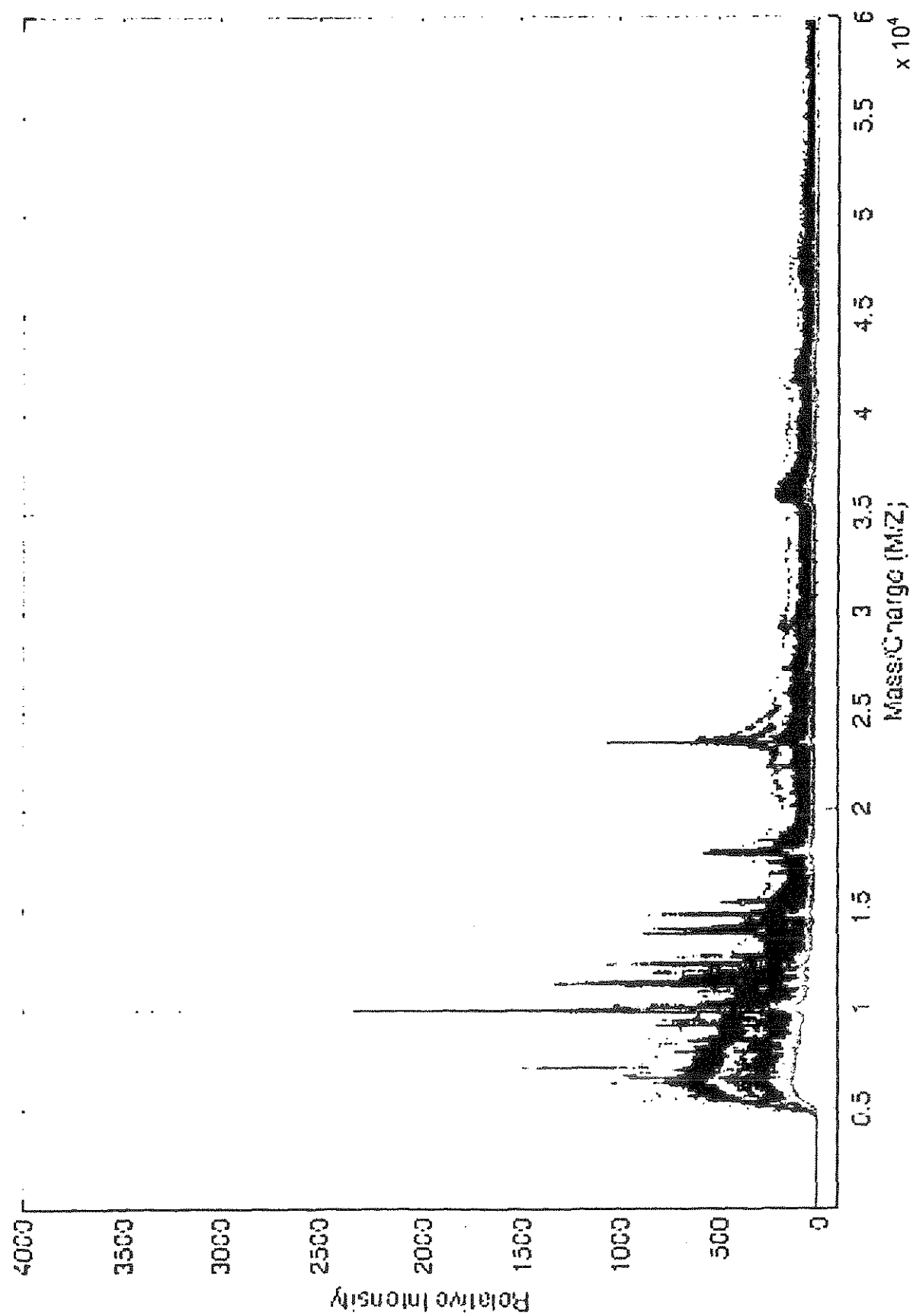


Fig. 3a

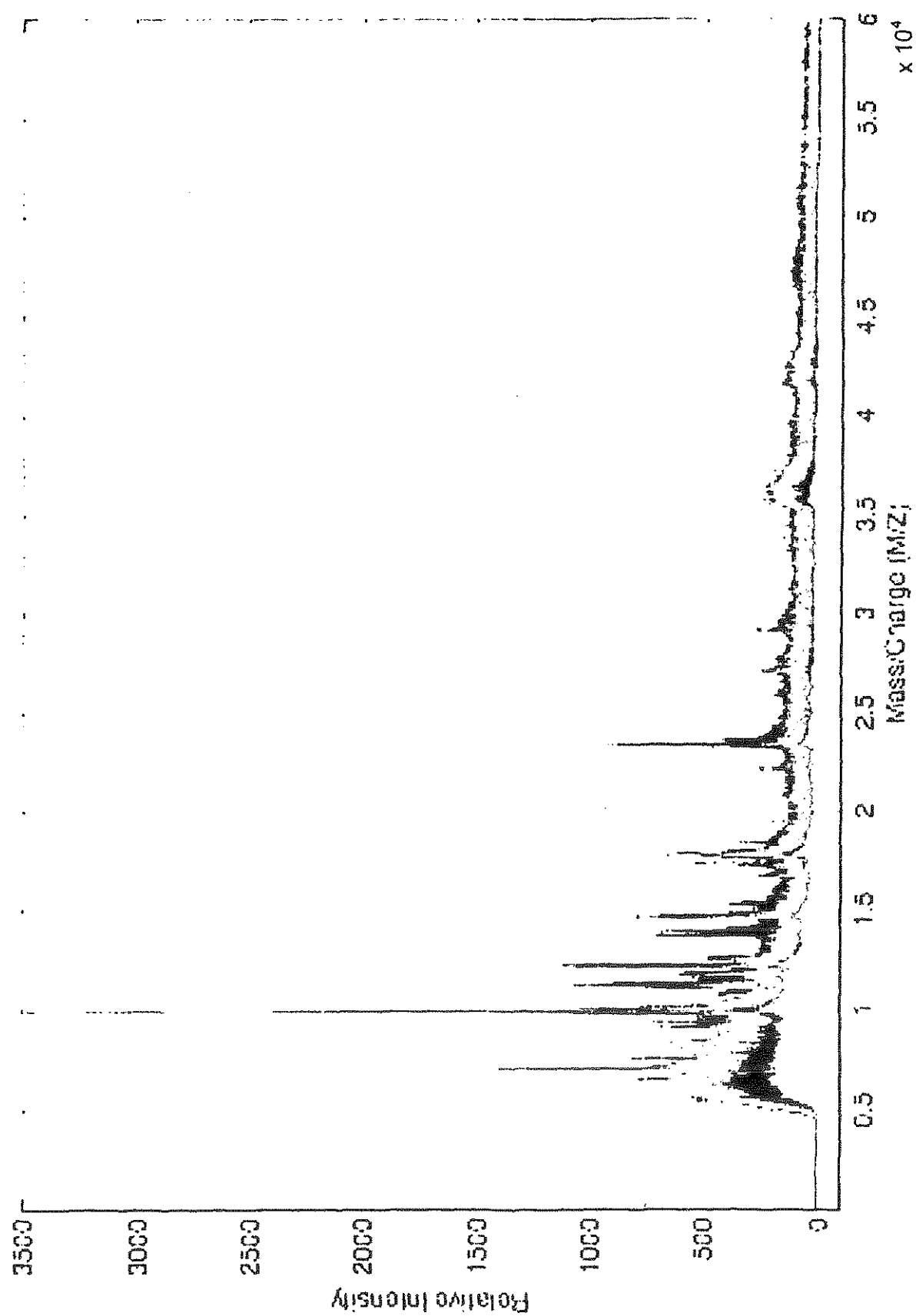


Fig. 3b

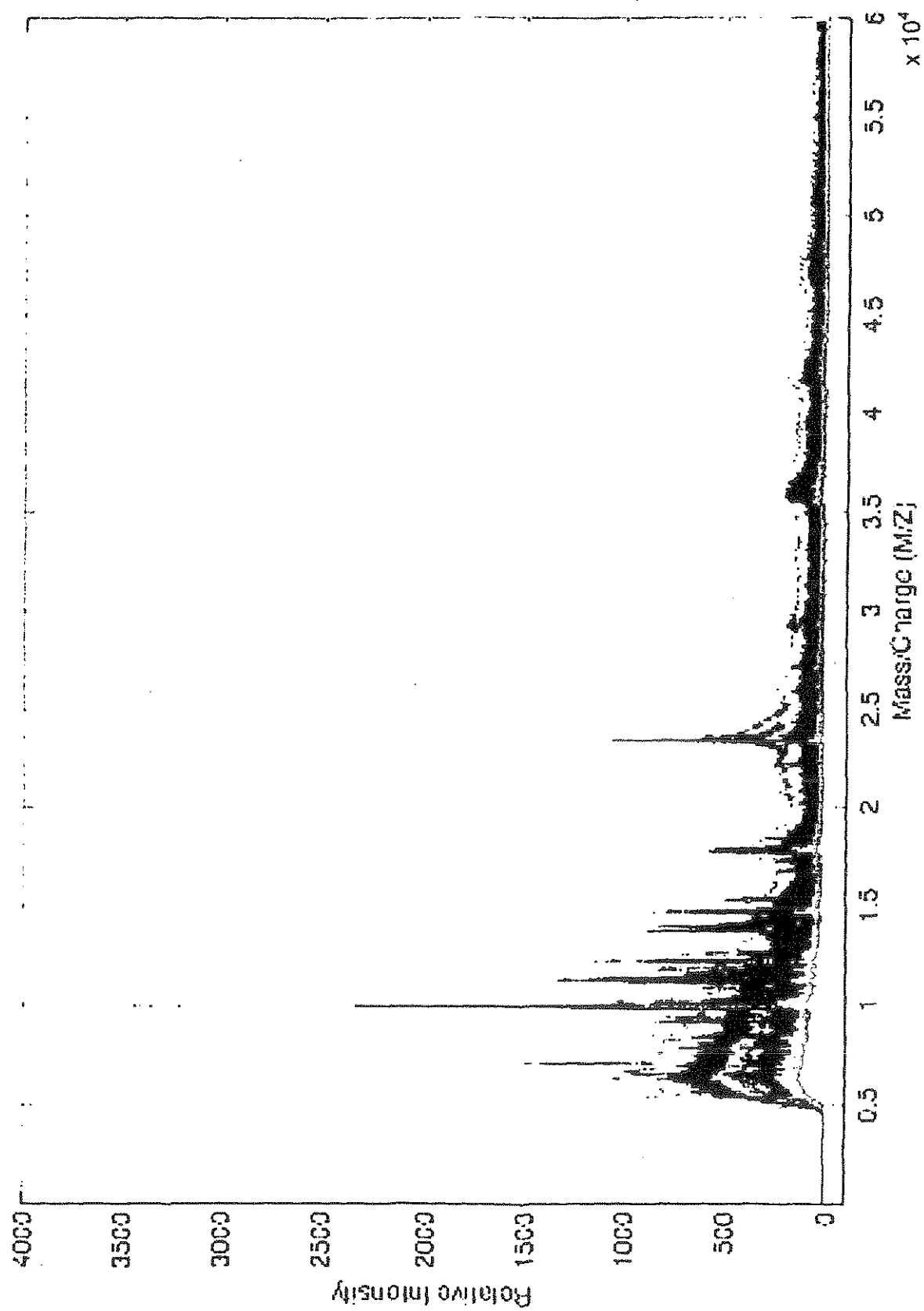


Fig. 4a

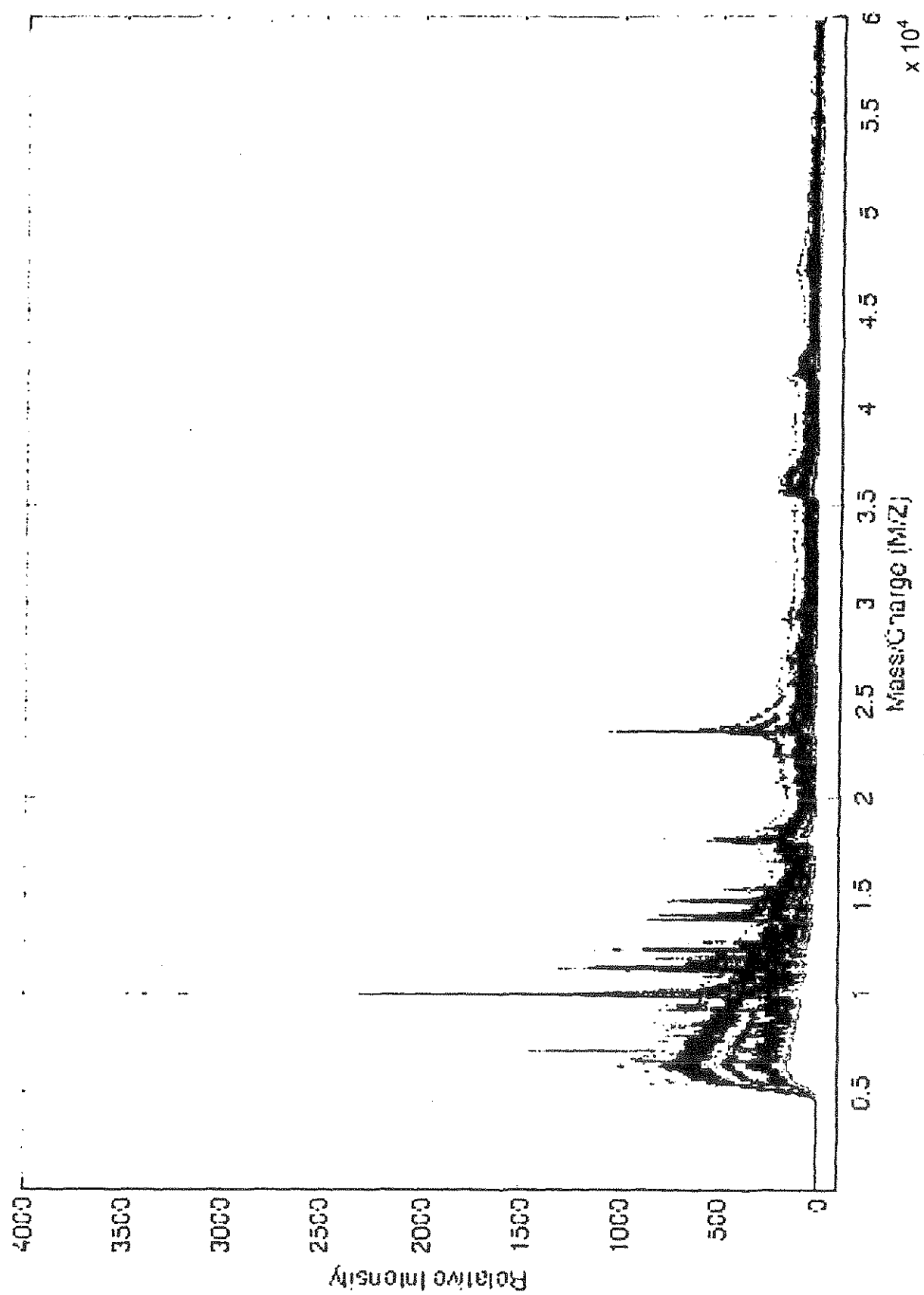


Fig. 4b

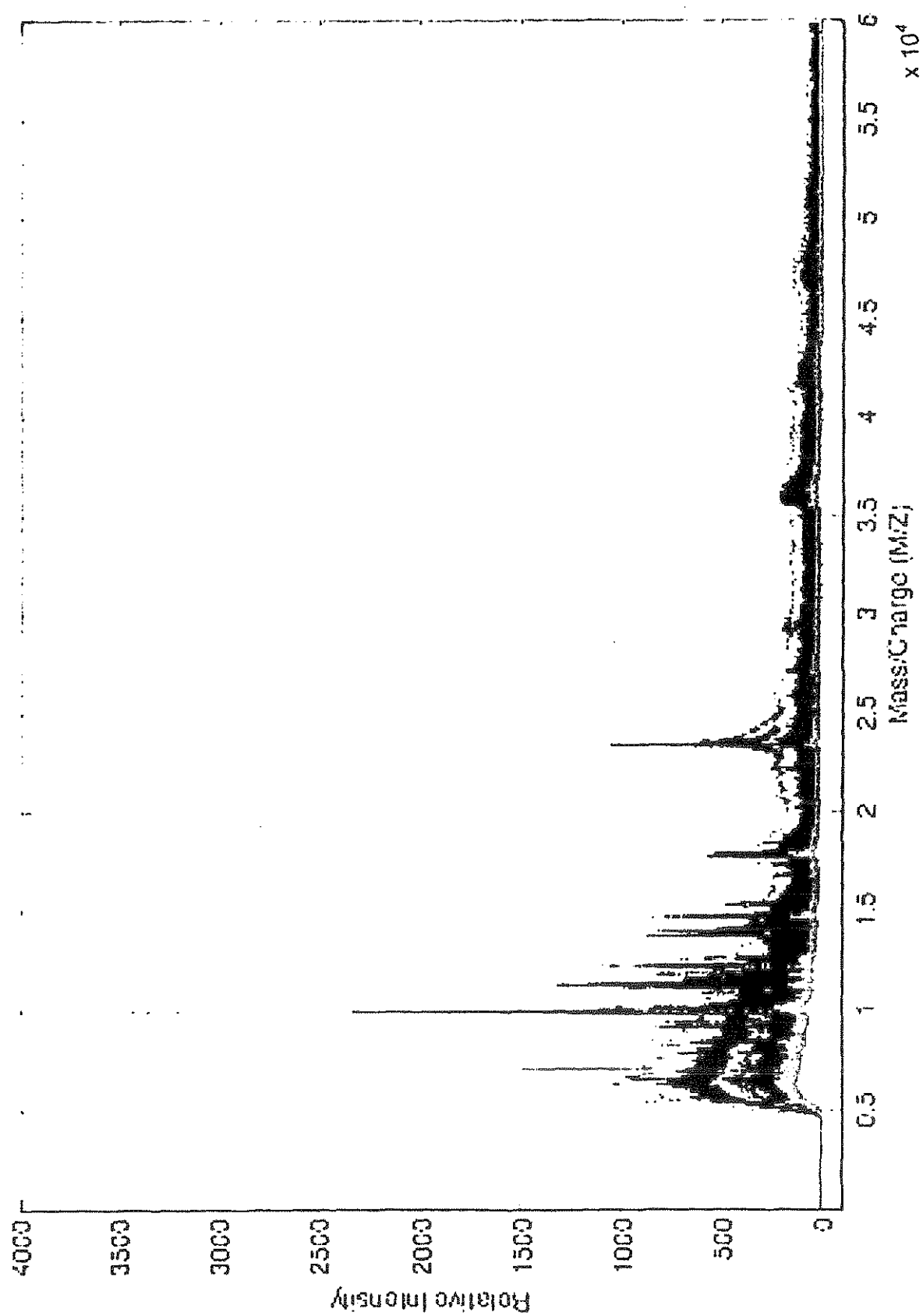


Fig. 5a

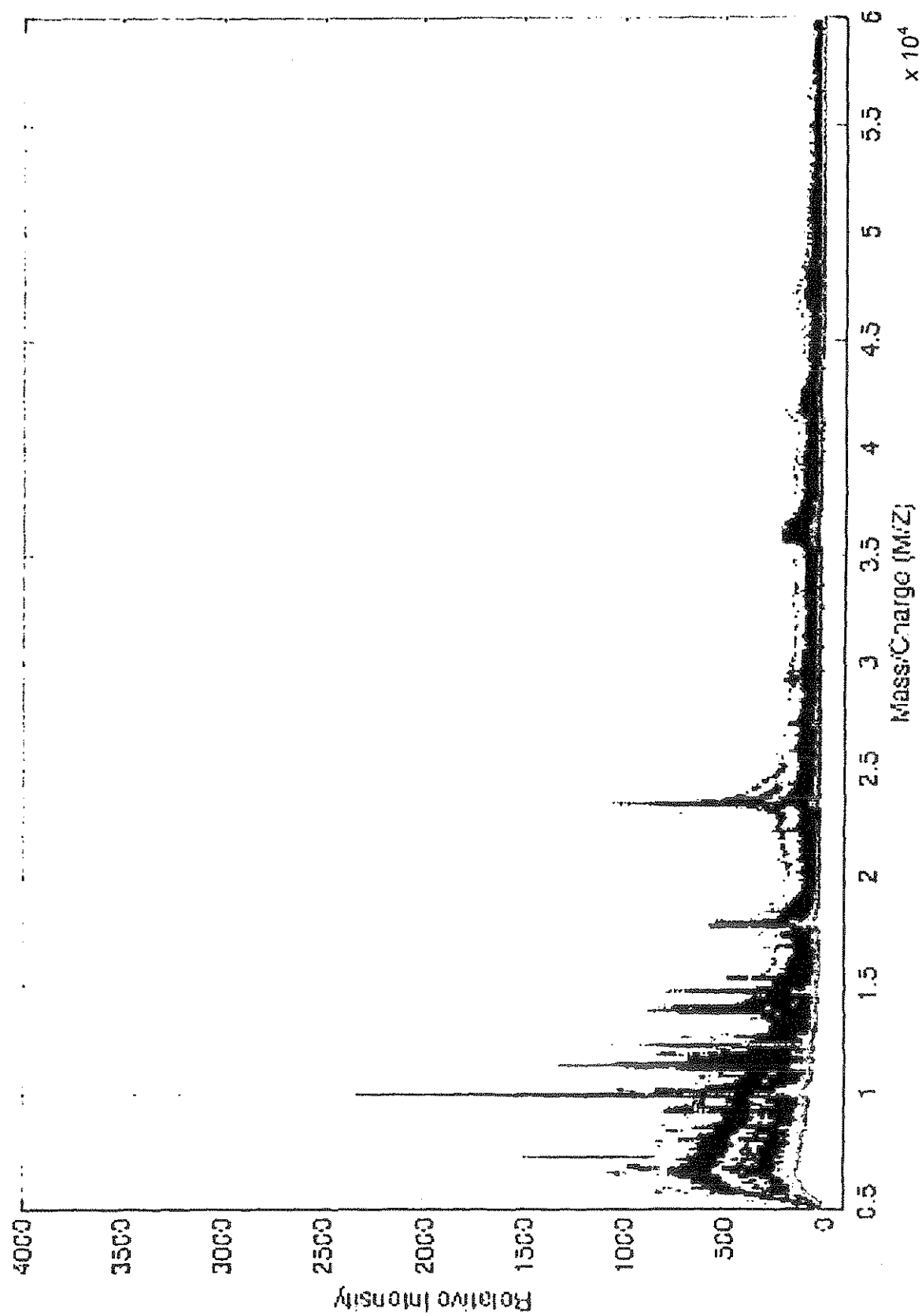


Fig. 5b

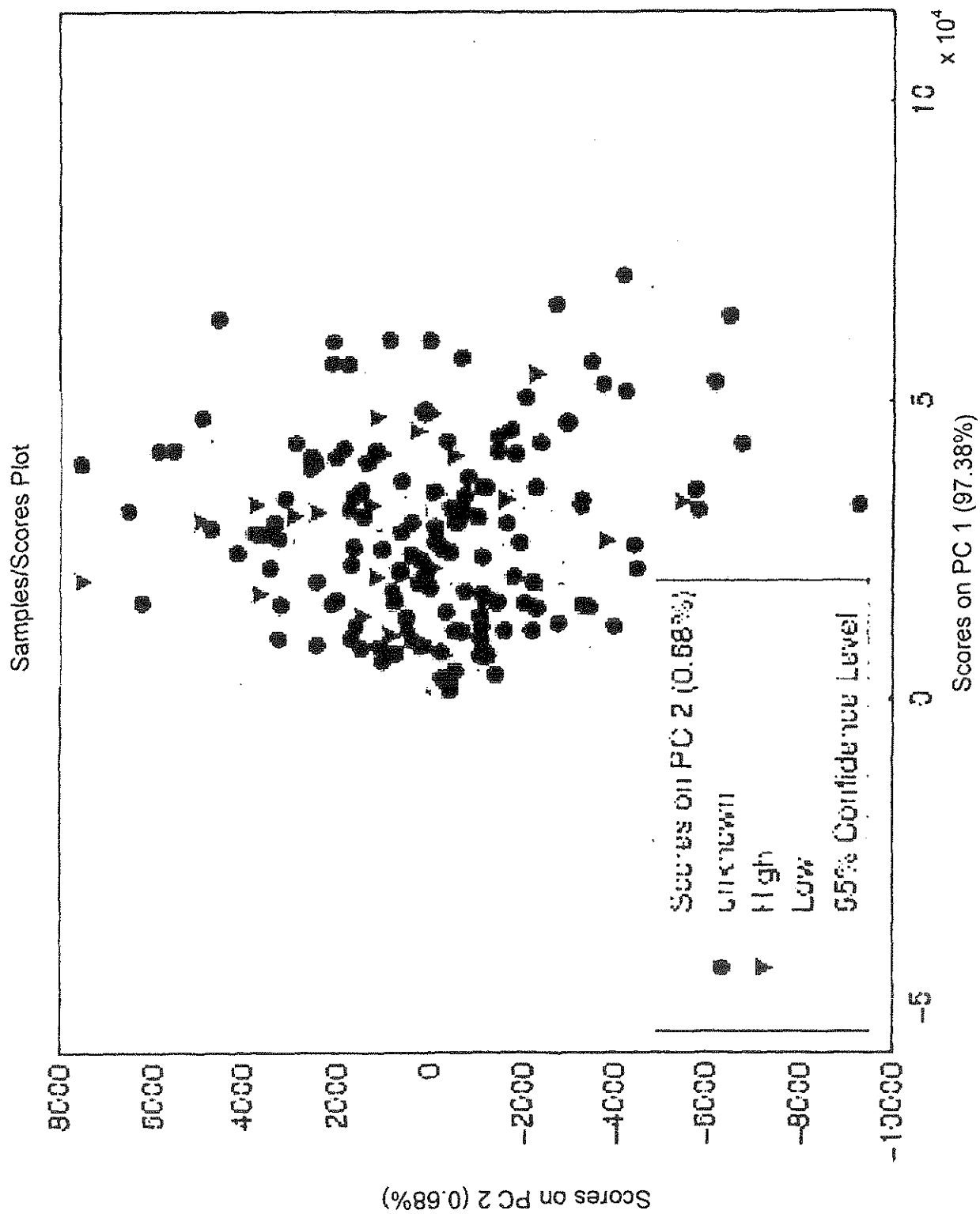


Fig. 6a

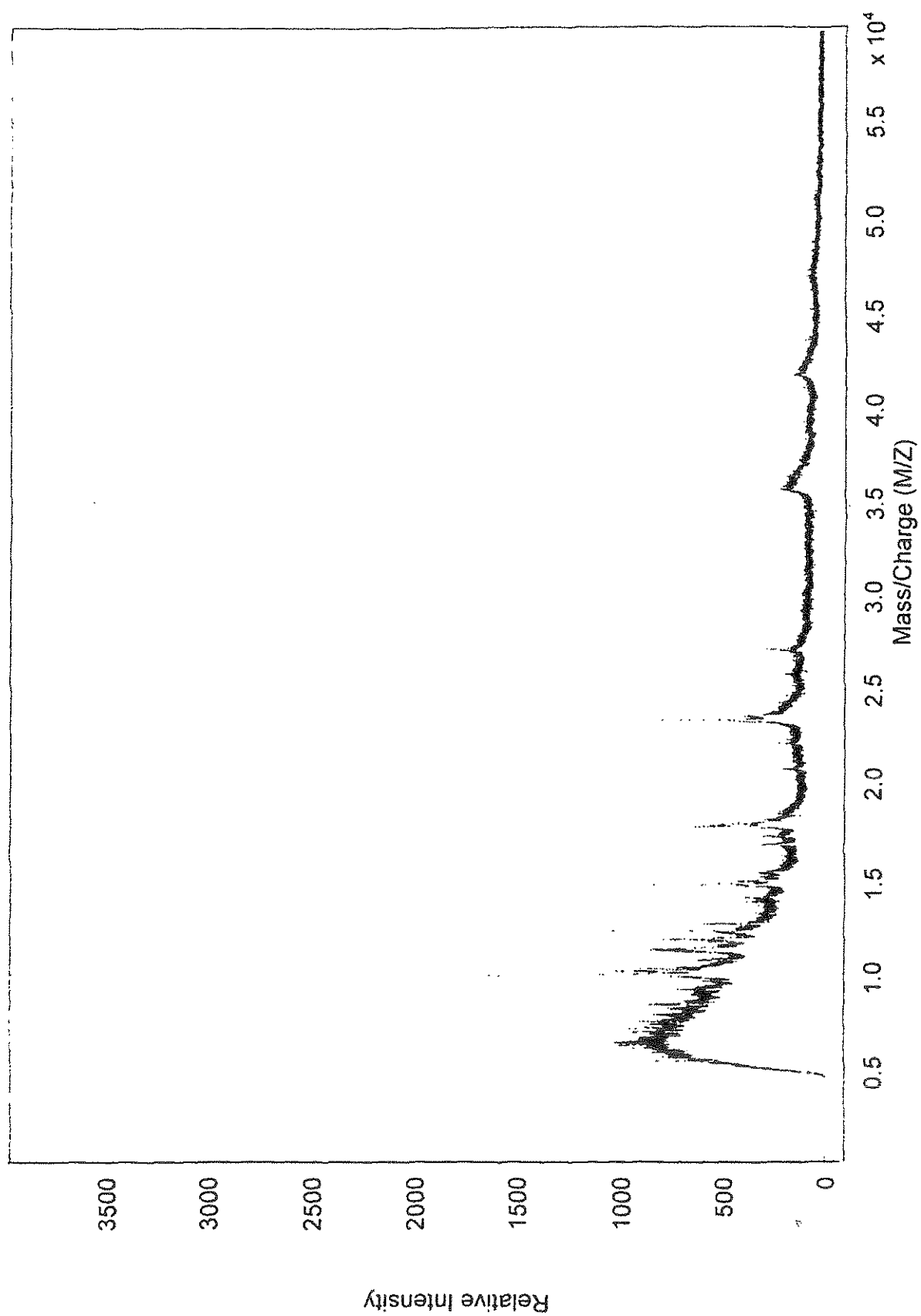


Fig. 6b

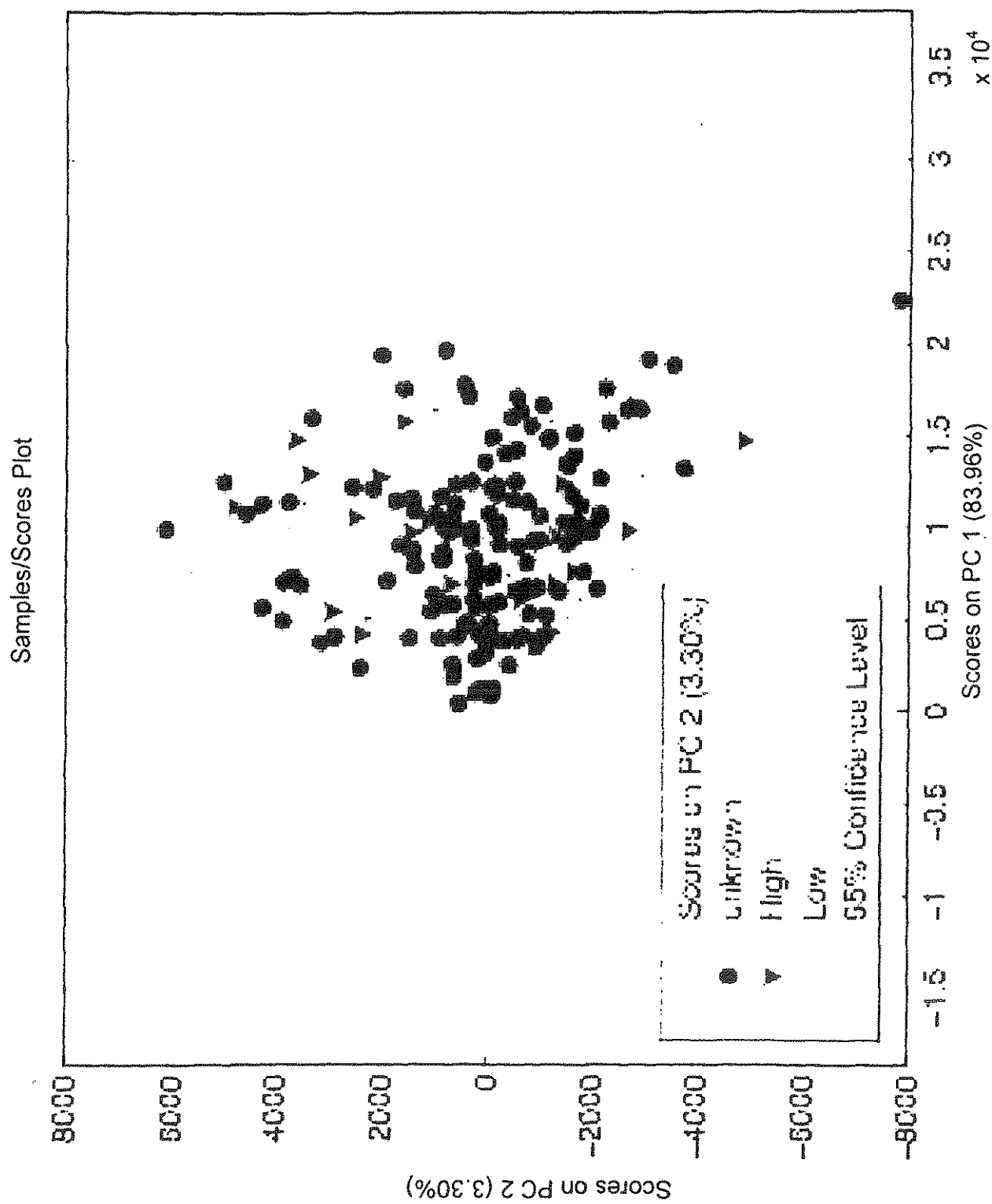


Fig. 7a

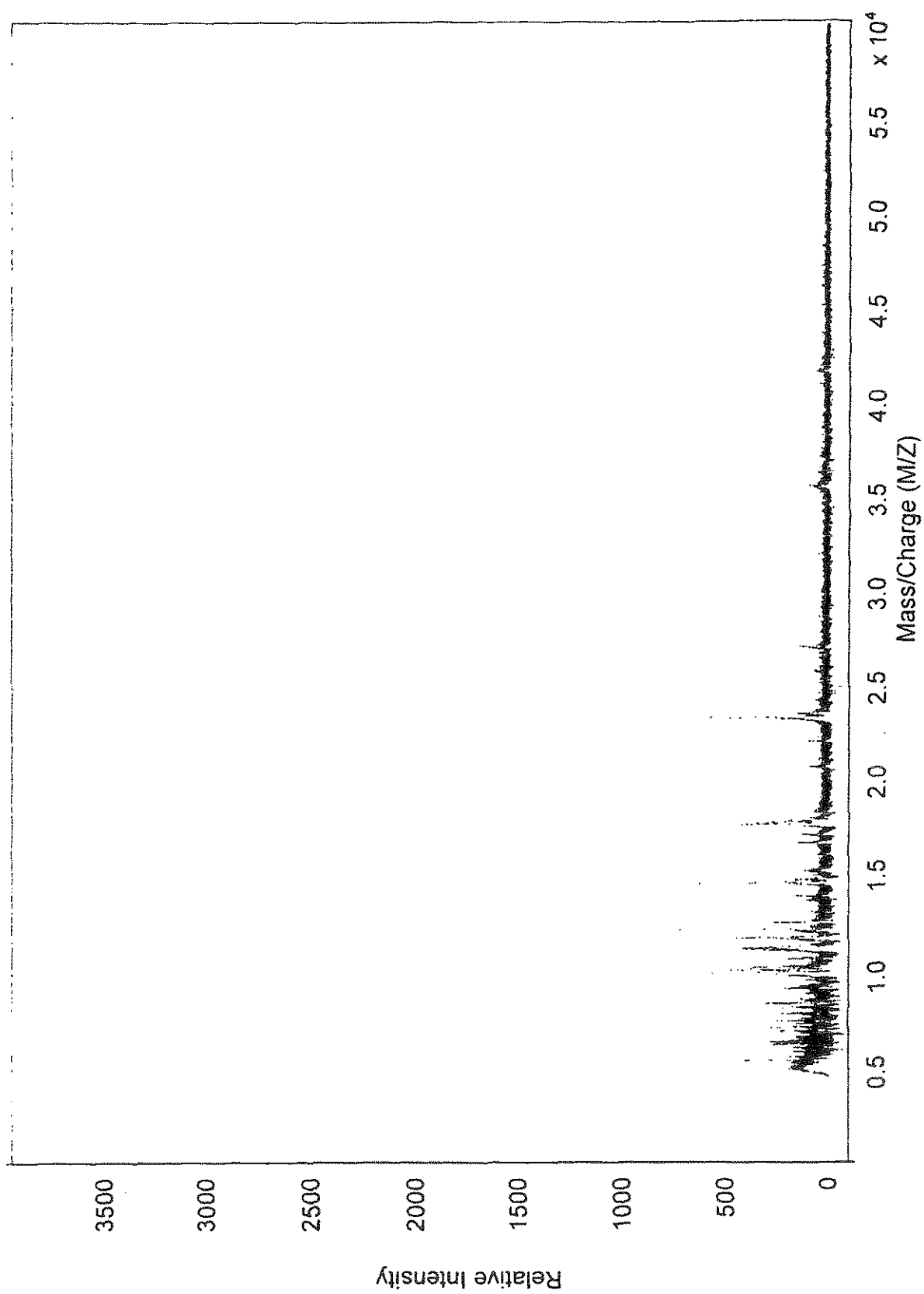


Fig. 7b

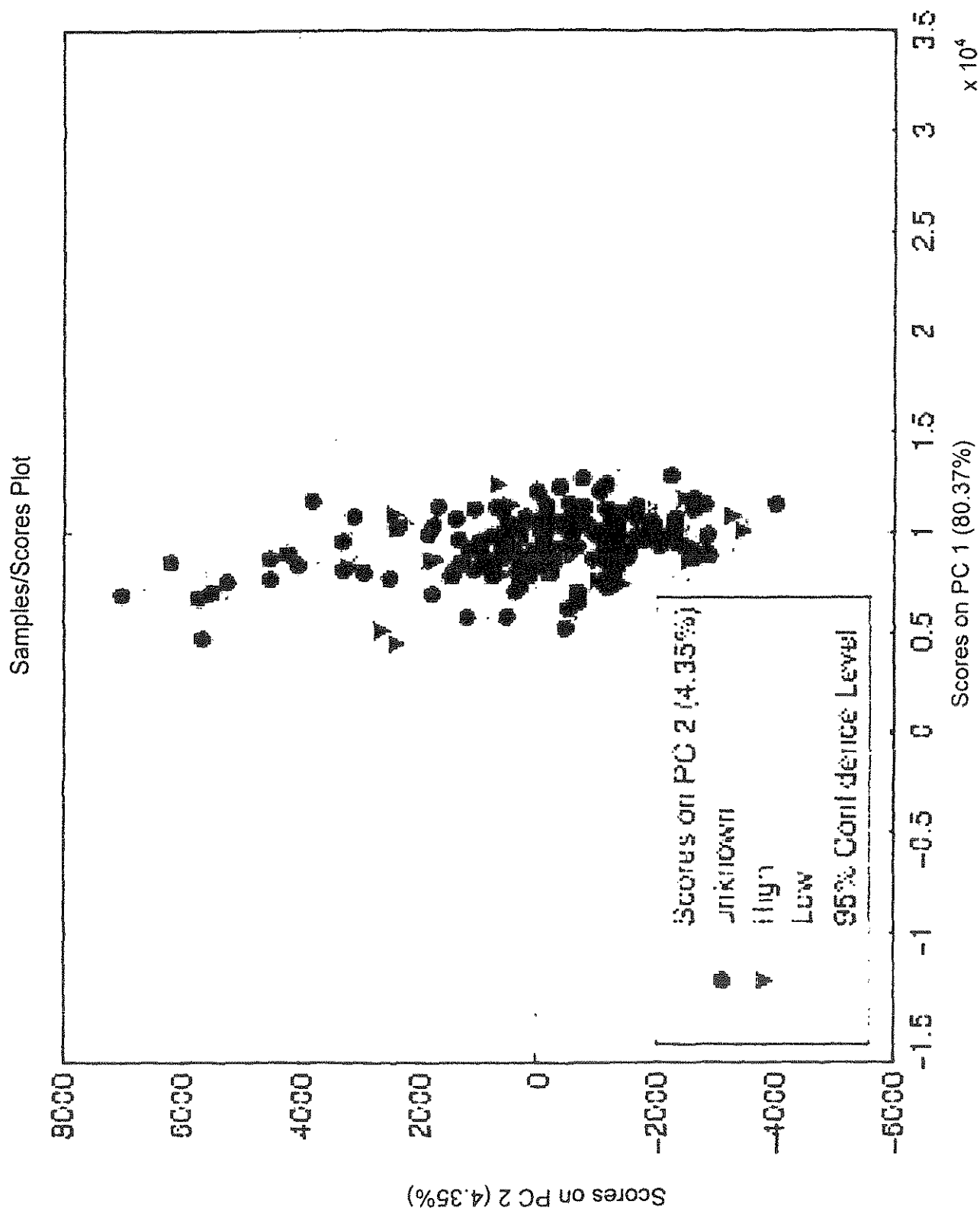


Fig. 8a

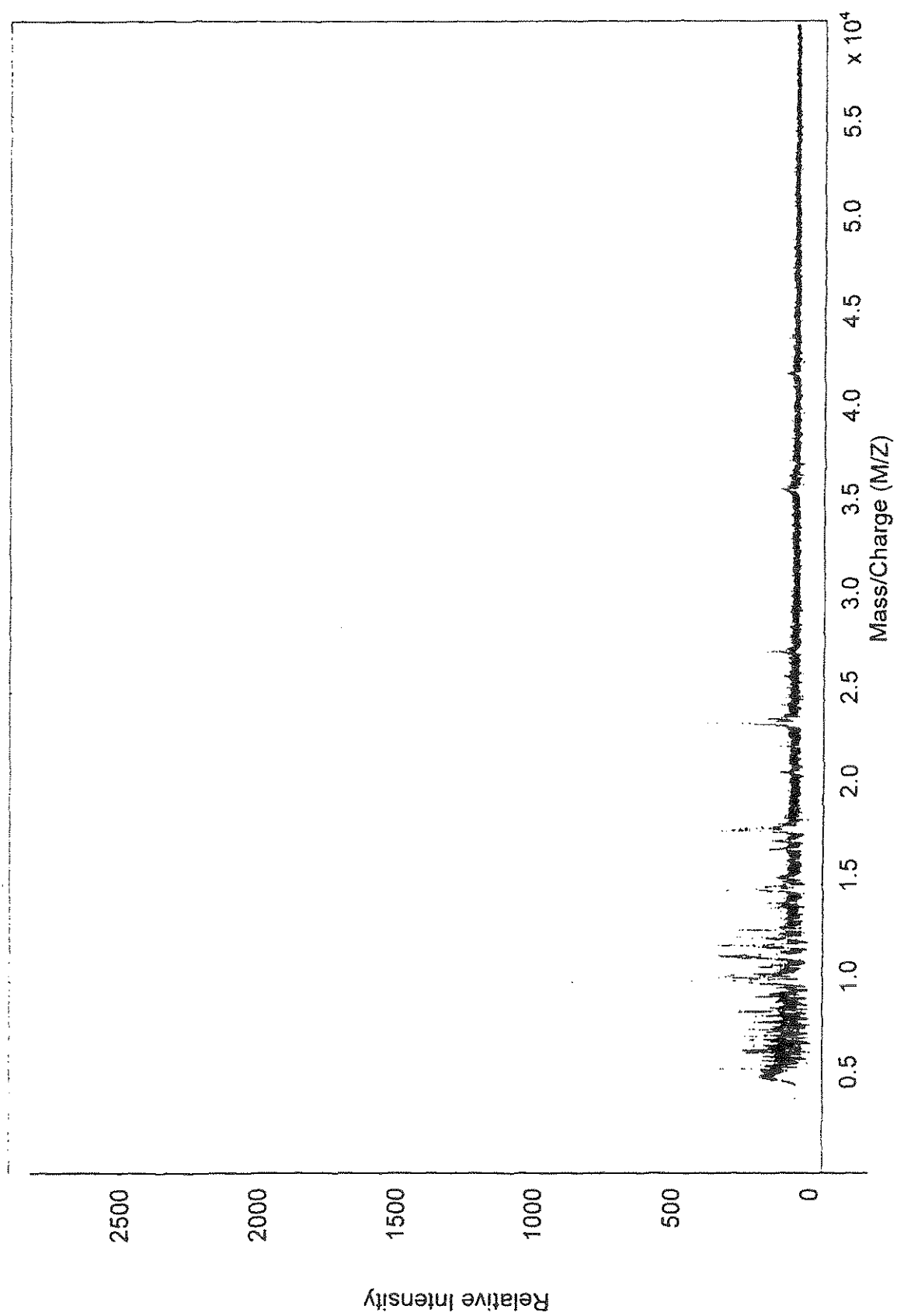


Fig. 8b

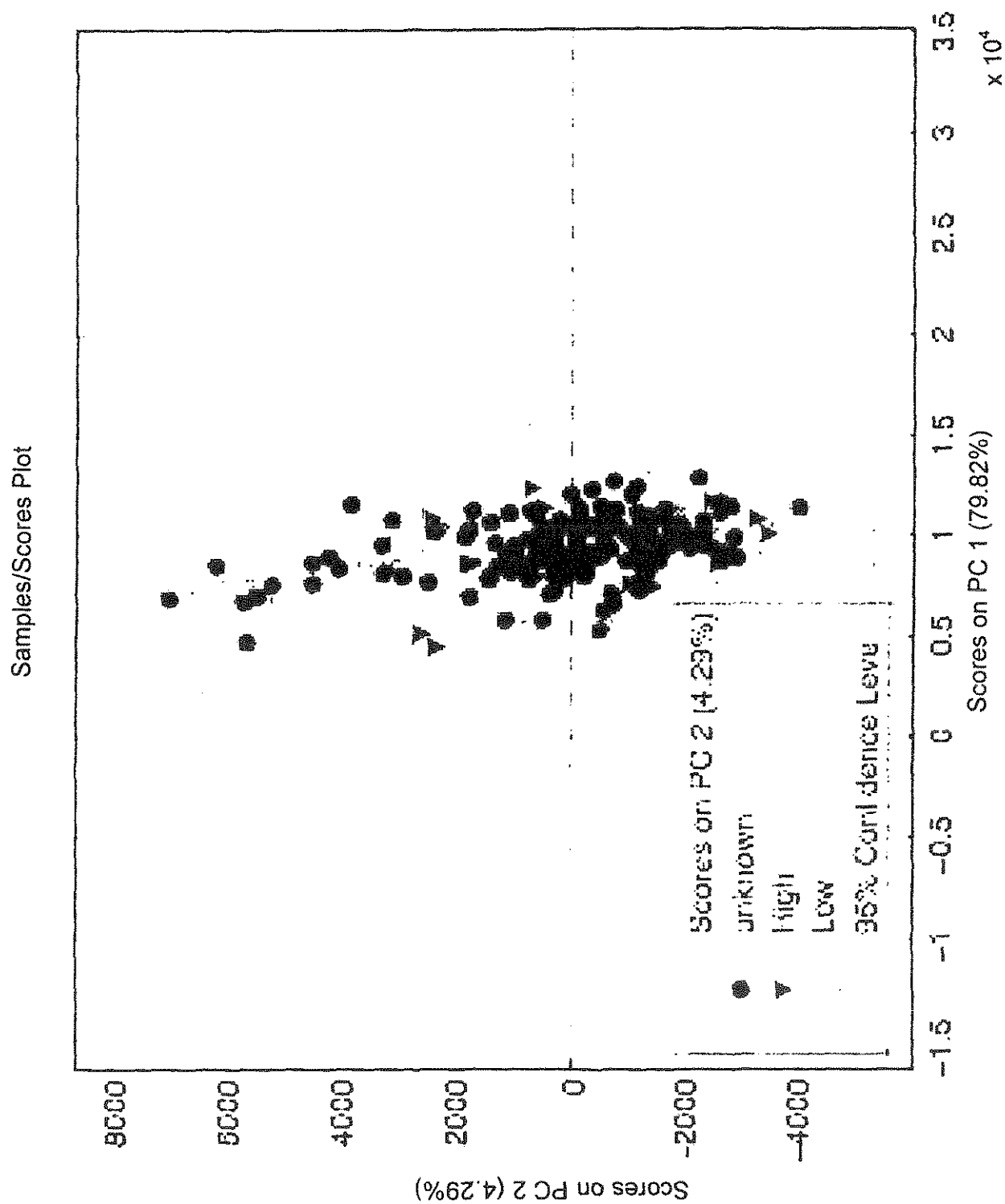


Fig. 9a

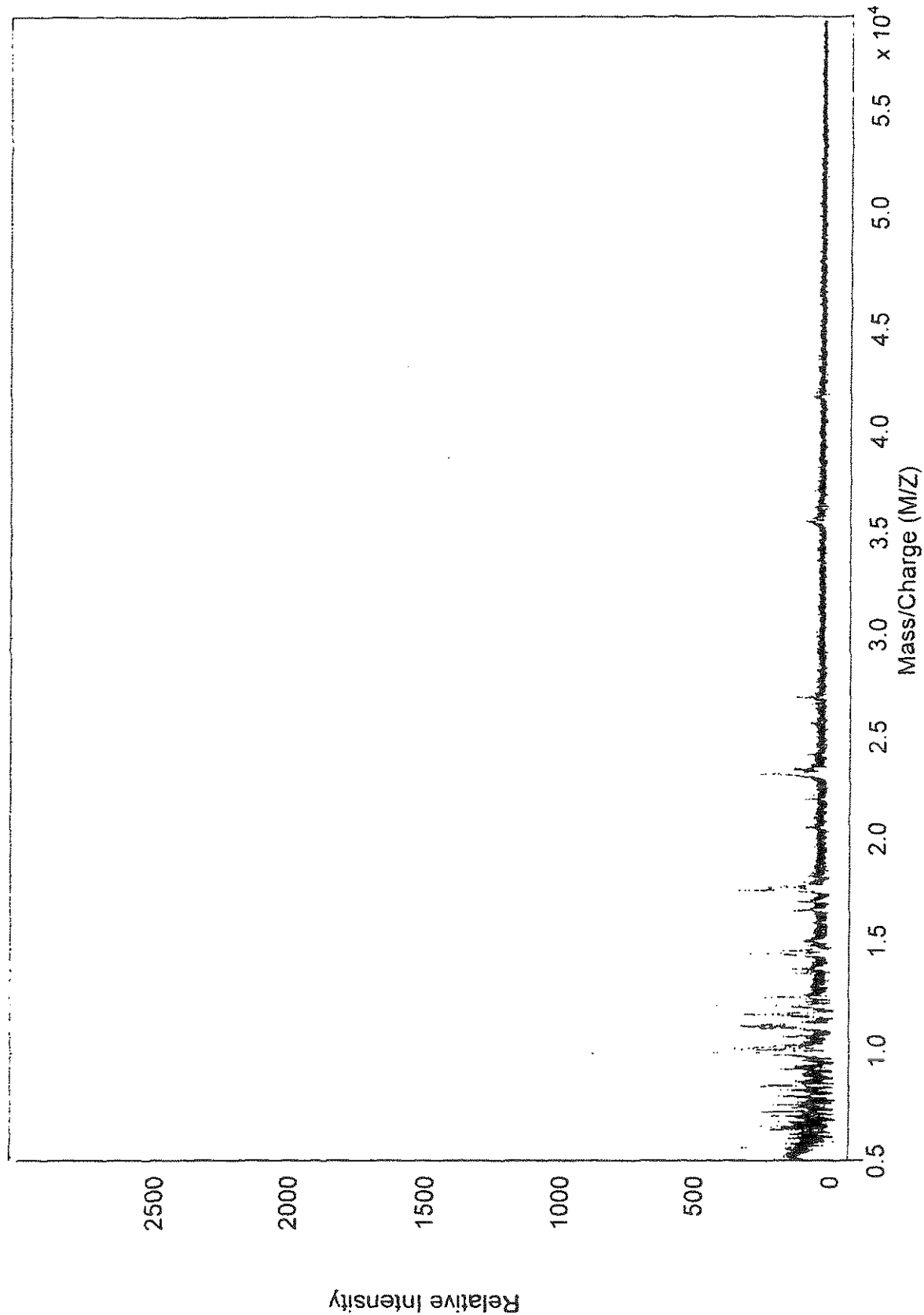


Fig. 9b

Fig. 10

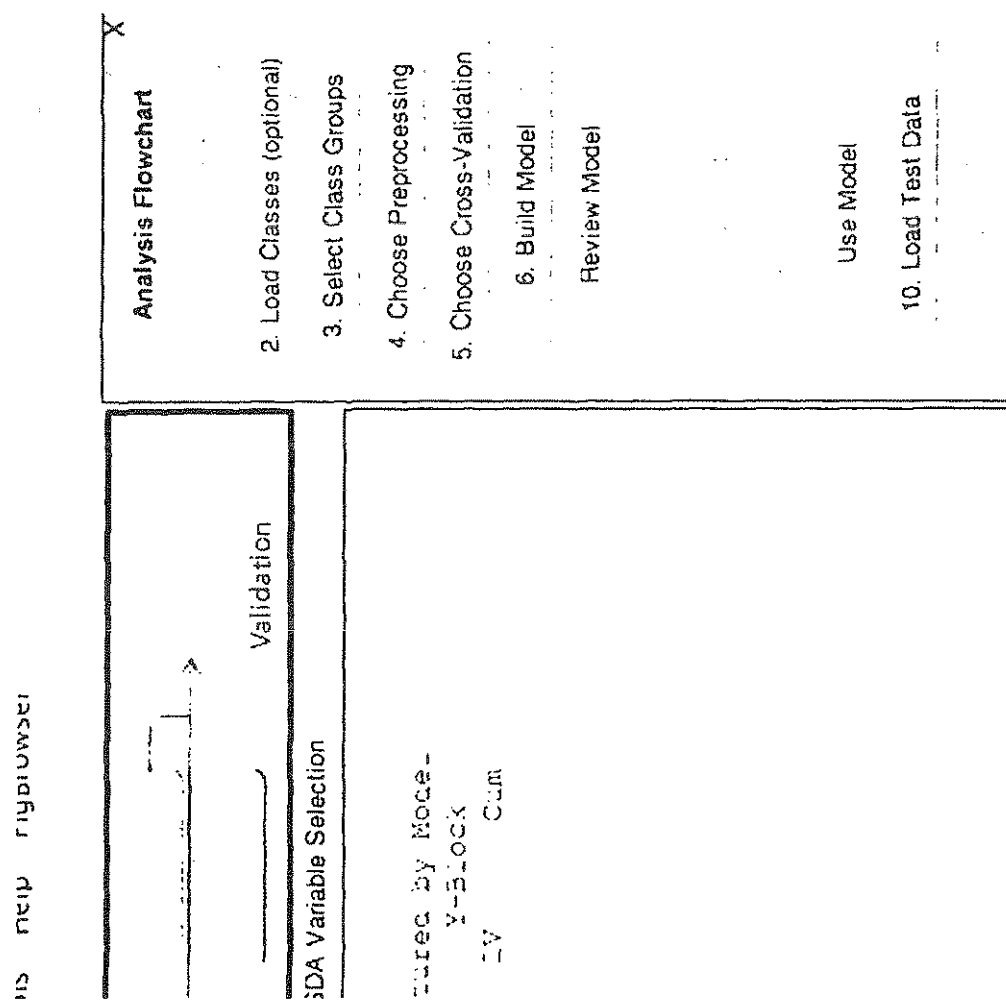


Fig. 12

PLSDA Class Groups

Help FigBrowser

Available Classes

Low

Model As Group

Class Groups

[Medium]

Remove Group

Default

OK

Cancel

Fig. 13

Preprocessing X-block

Available Methods	Selected Methods	Load	Save
--- Transformations --- Absolute Value Log10 Transmission to Absorbance ($\log(1/T)$) --- Filtering --- Baseline (Specified points) Baseline (Weighted Least Squares) Derivative (SavGol) Detrend EPO Filter GLS Weighting Kaiser HoloReact Method OSC (Orthogonal Signal Correction) Smoothing (SavGol) --- Normalization --- MSC (mean) Normalize SNV --- Scaling and Centering --- Autoscale Group Scale Log Decay Scaling Mean Center Median Center Multiway Center Multiway Scale Sqrt Mean Scale --- Other ---			
Show OK Cancel			
X Y			

Fig. 14

Cross-Validation

Cross-Val Method	Number of Subsets	Number of Features	Number of Trials
leave one out	1	1	1
venetian blinds	1	1	1
contiguous block	1	1	1
random subsets	1	1	1
custom	1	1	1

Close

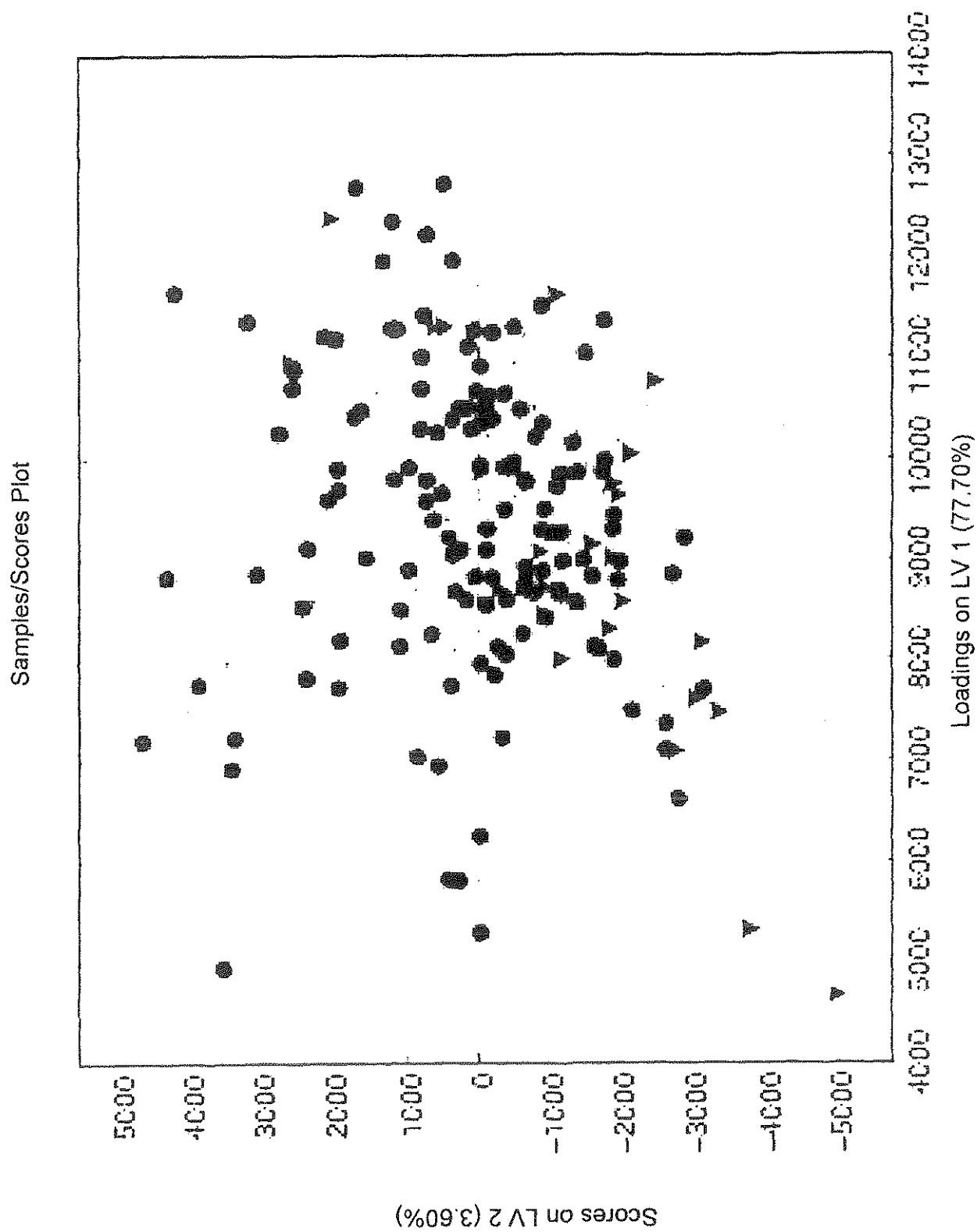


Fig. 15a

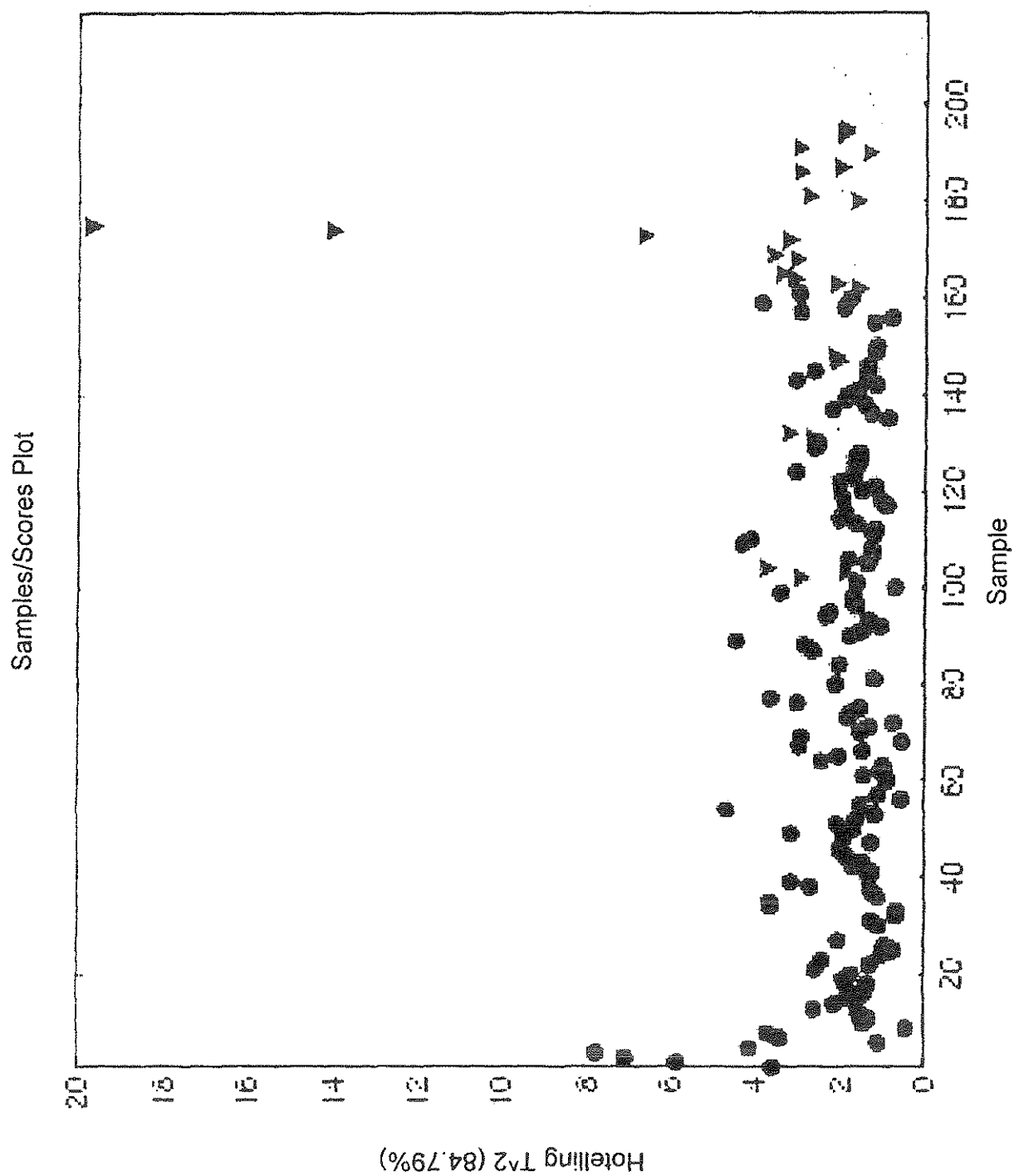


Fig. 15b

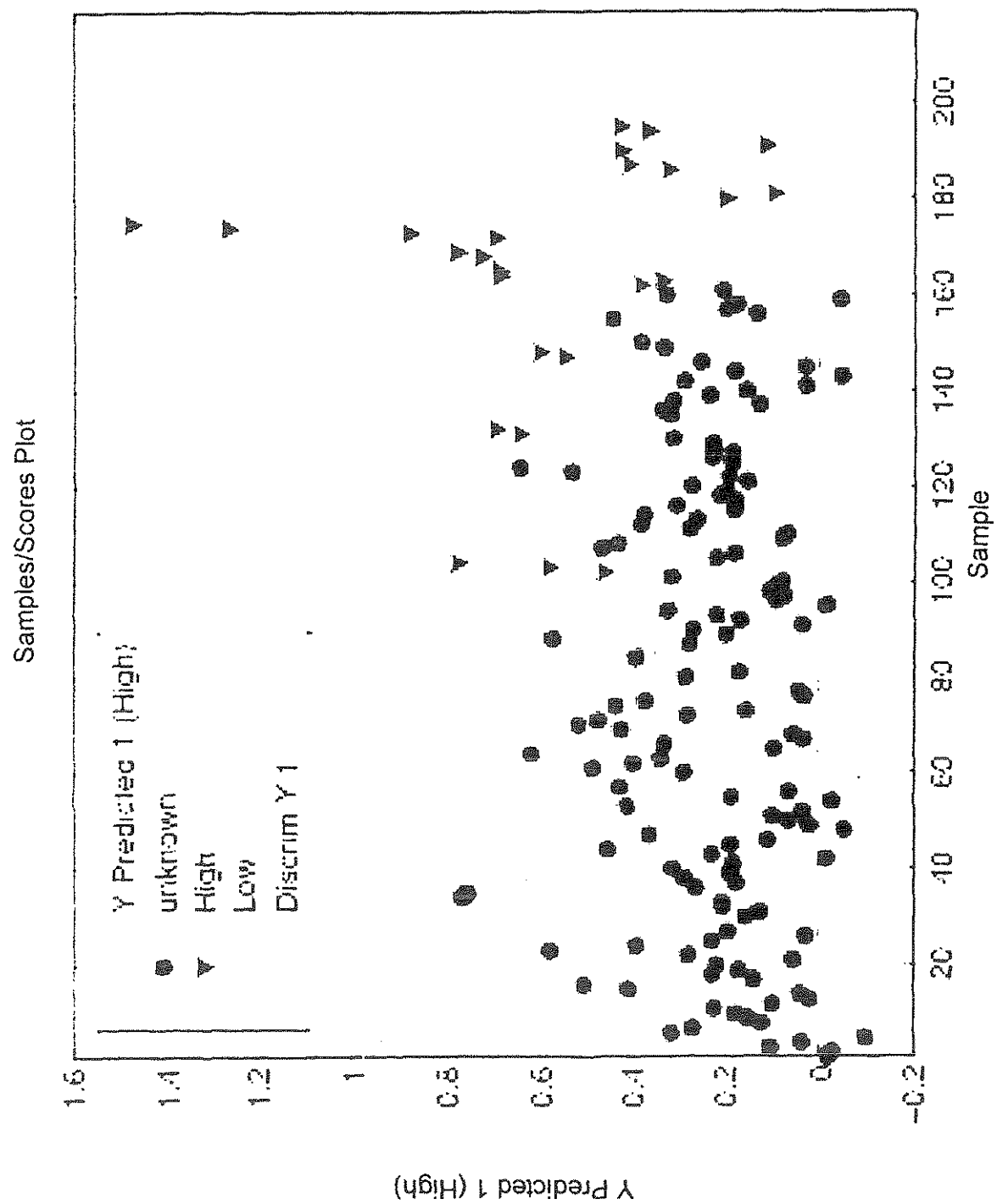


Fig. 15c

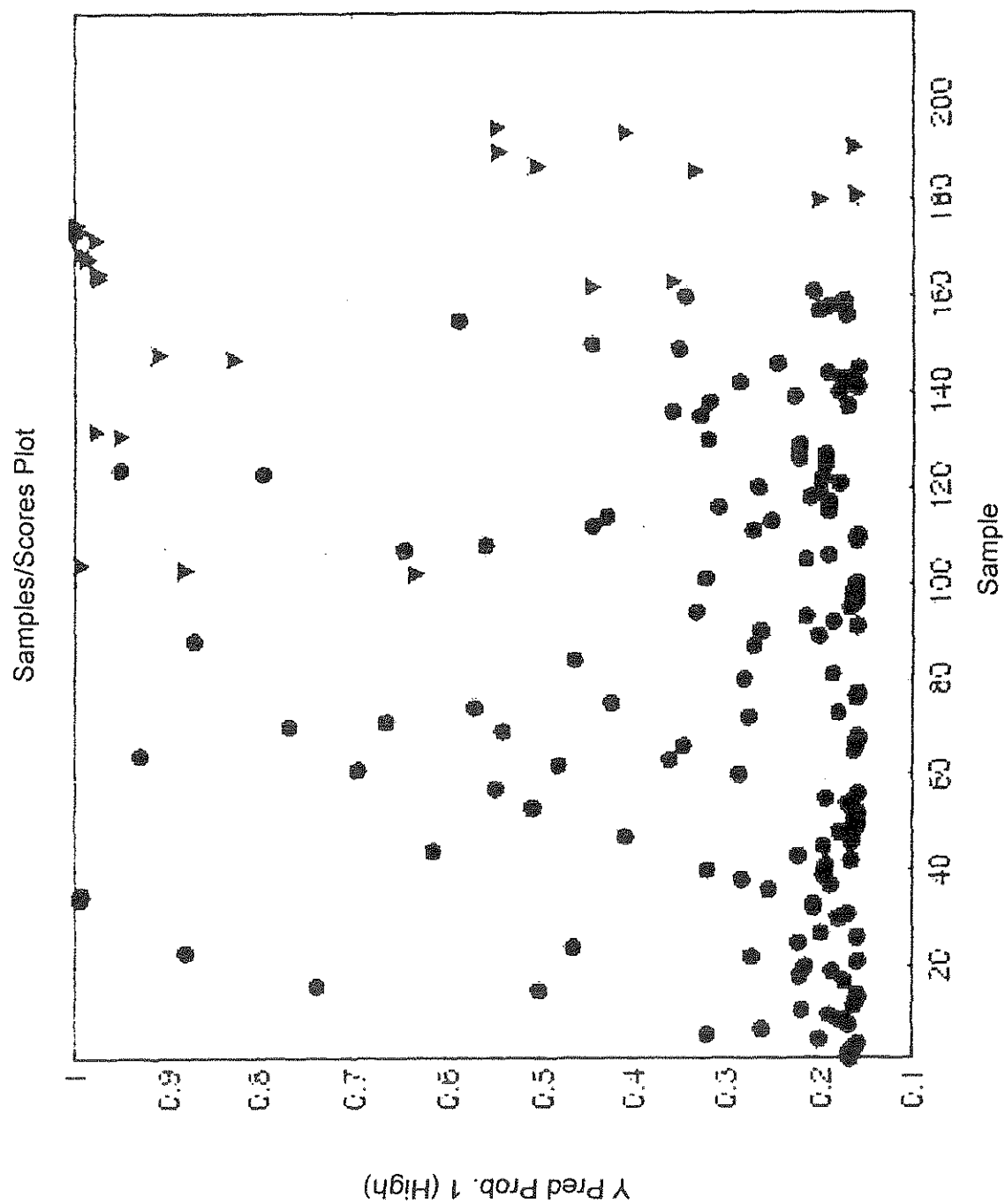


Fig. 15d

Variables/Loadings Plot

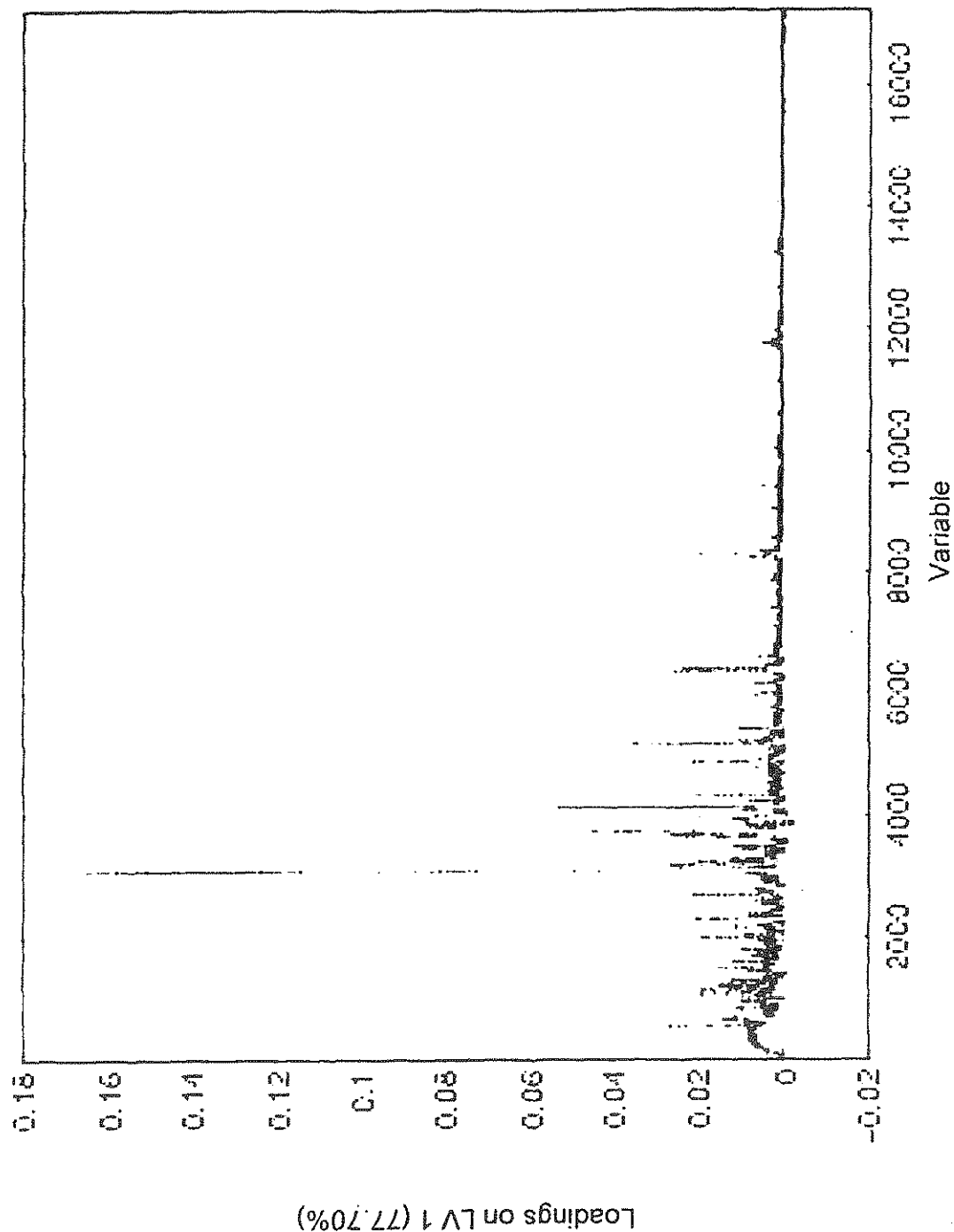


Fig. 16a

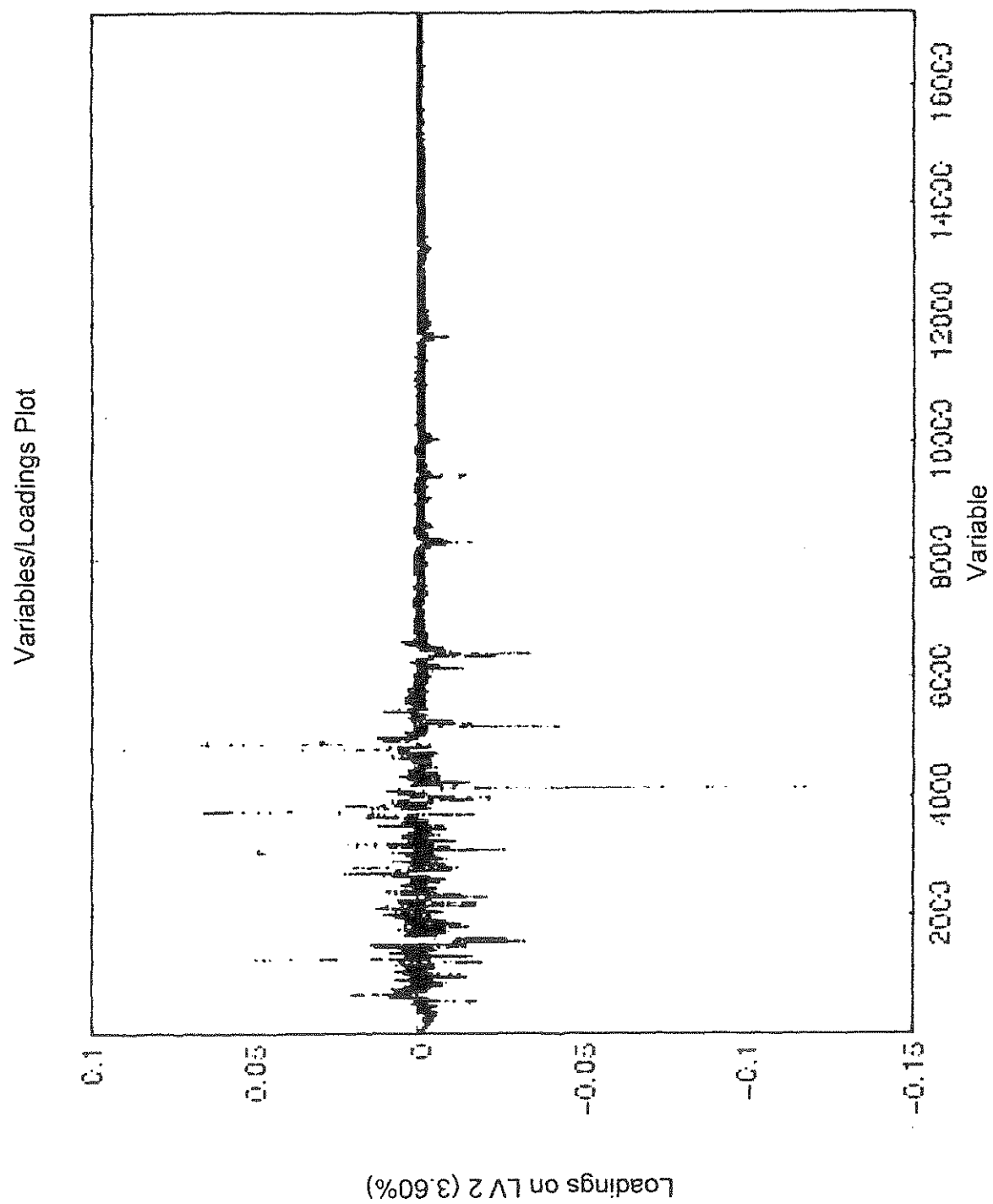


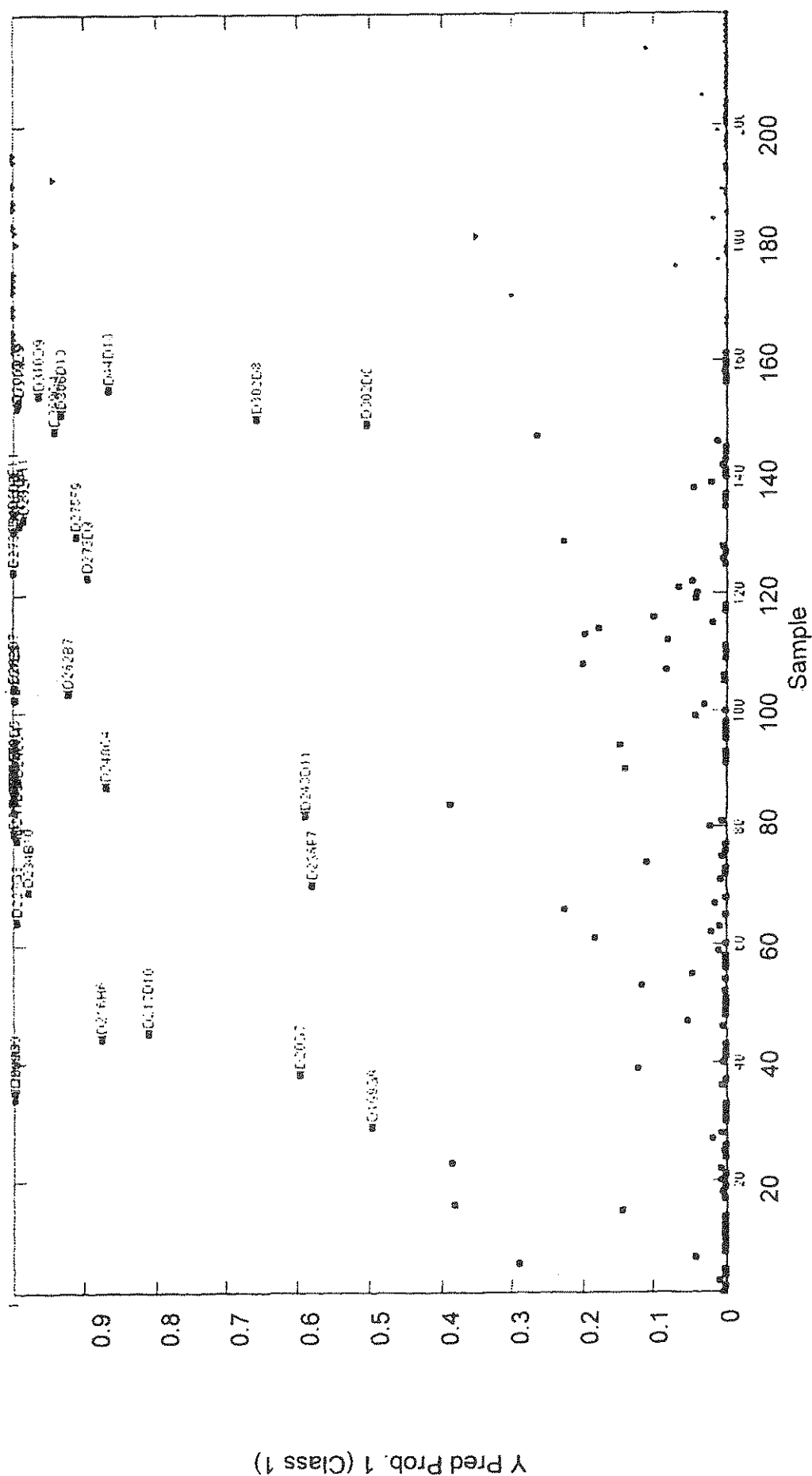
Fig. 16b

Fig. 18

Figure 1. Samples/Scores - PLSDA S LVs -

File Edit View Insert Tools Desktop Window Help FigBrowser PlotGUI

Samples/Scores Plot



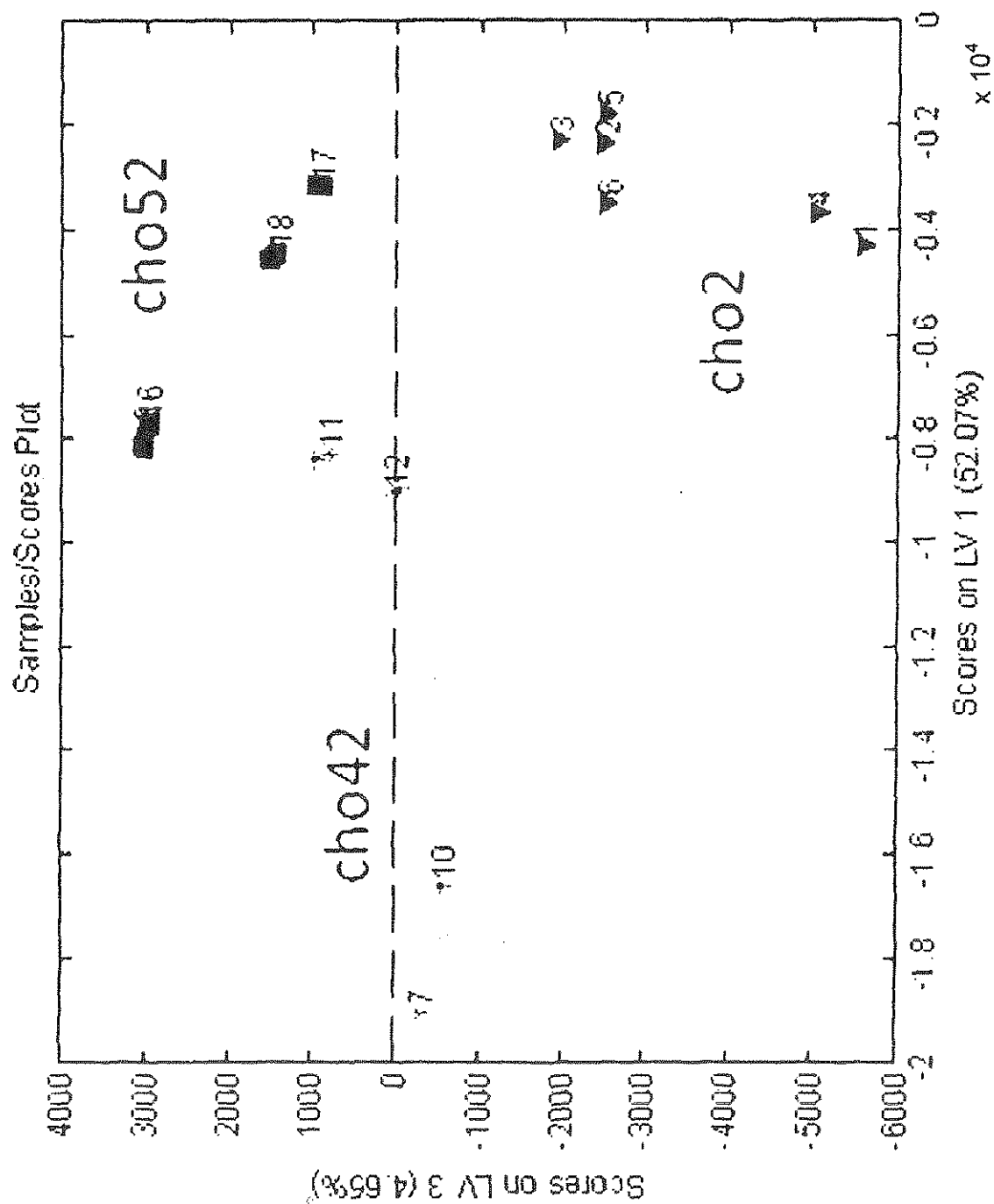


Fig. 19a

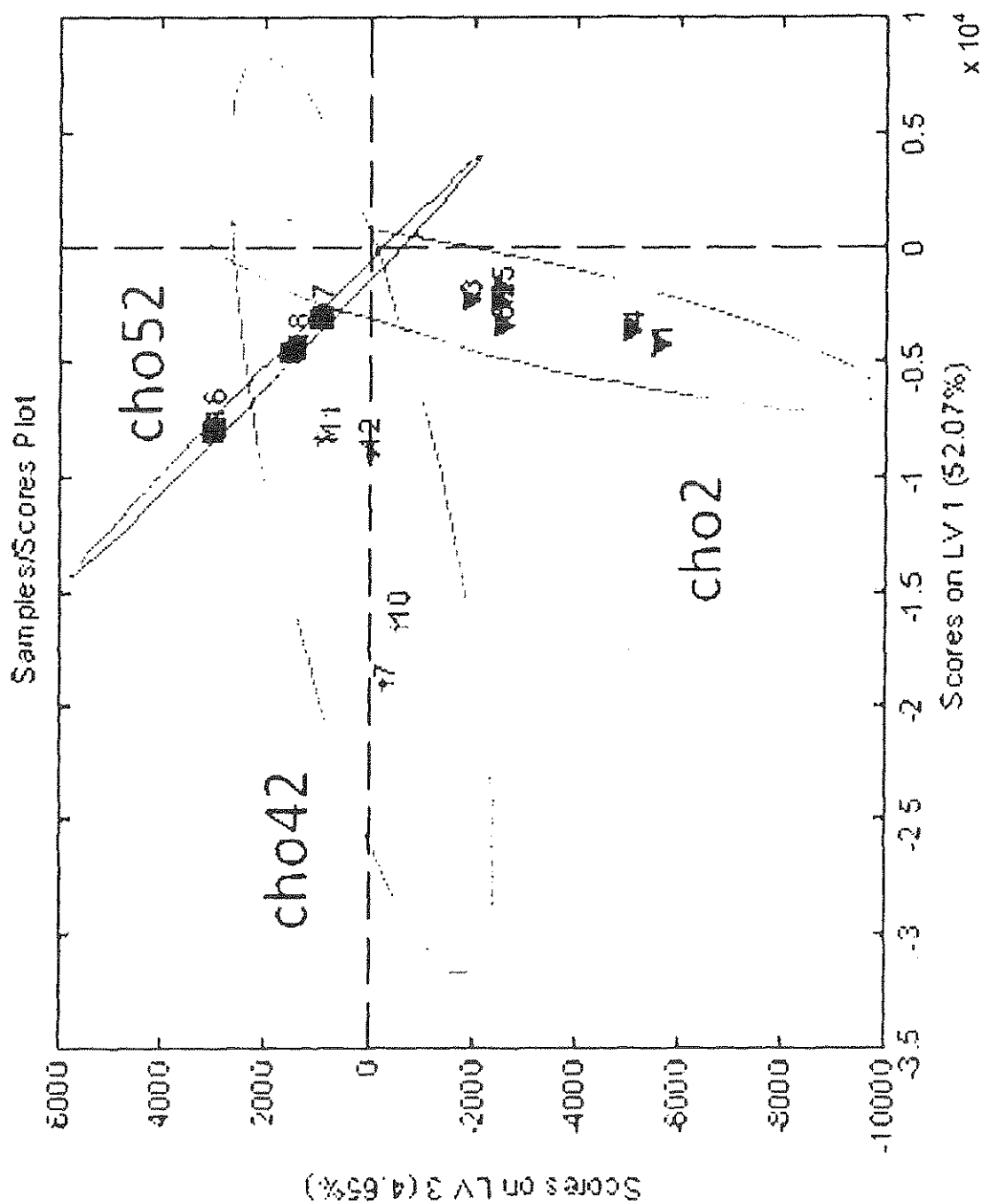


Fig. 19b

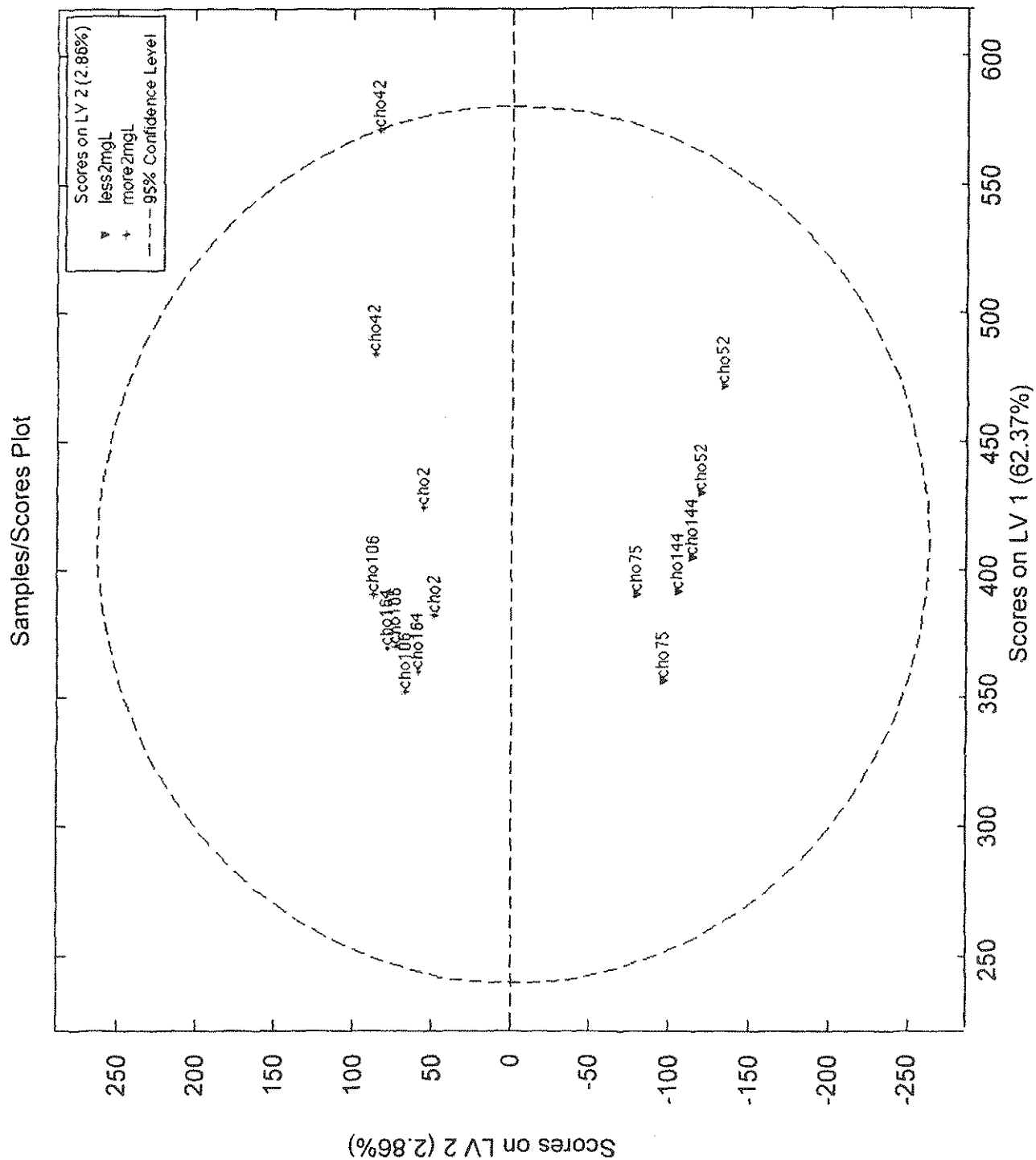


Fig. 20

Fig. 21a

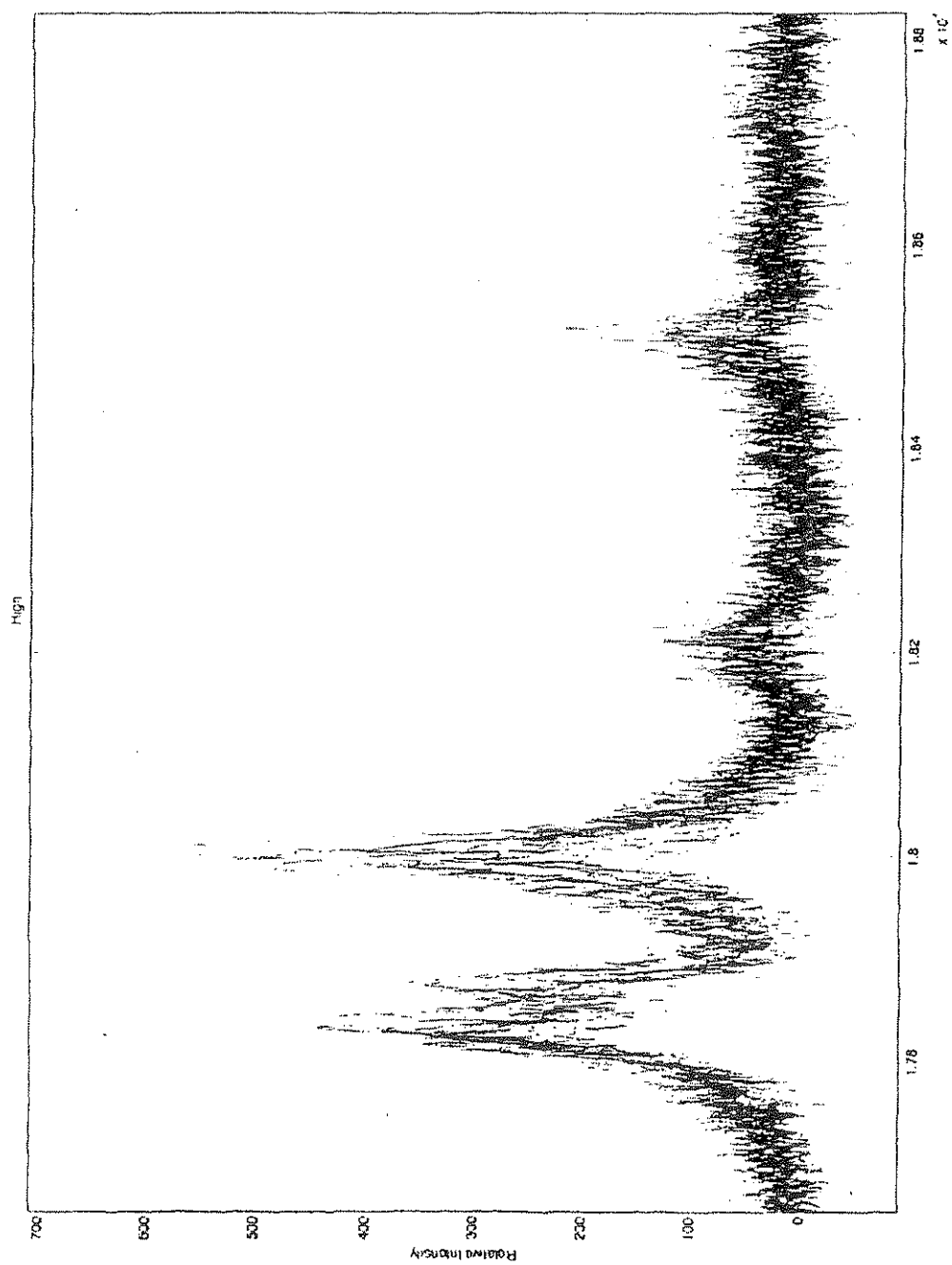


Fig. 21b

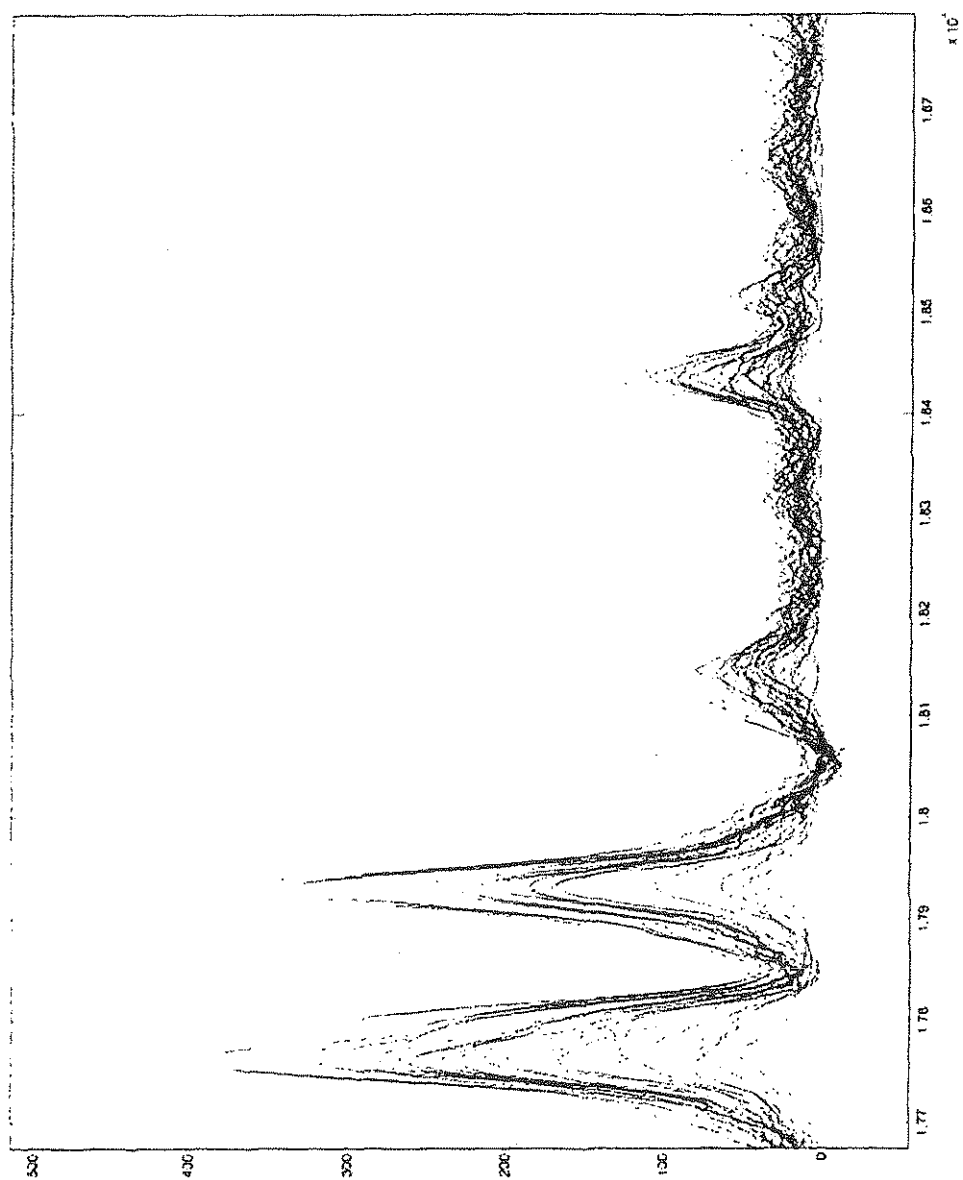


Fig. 22

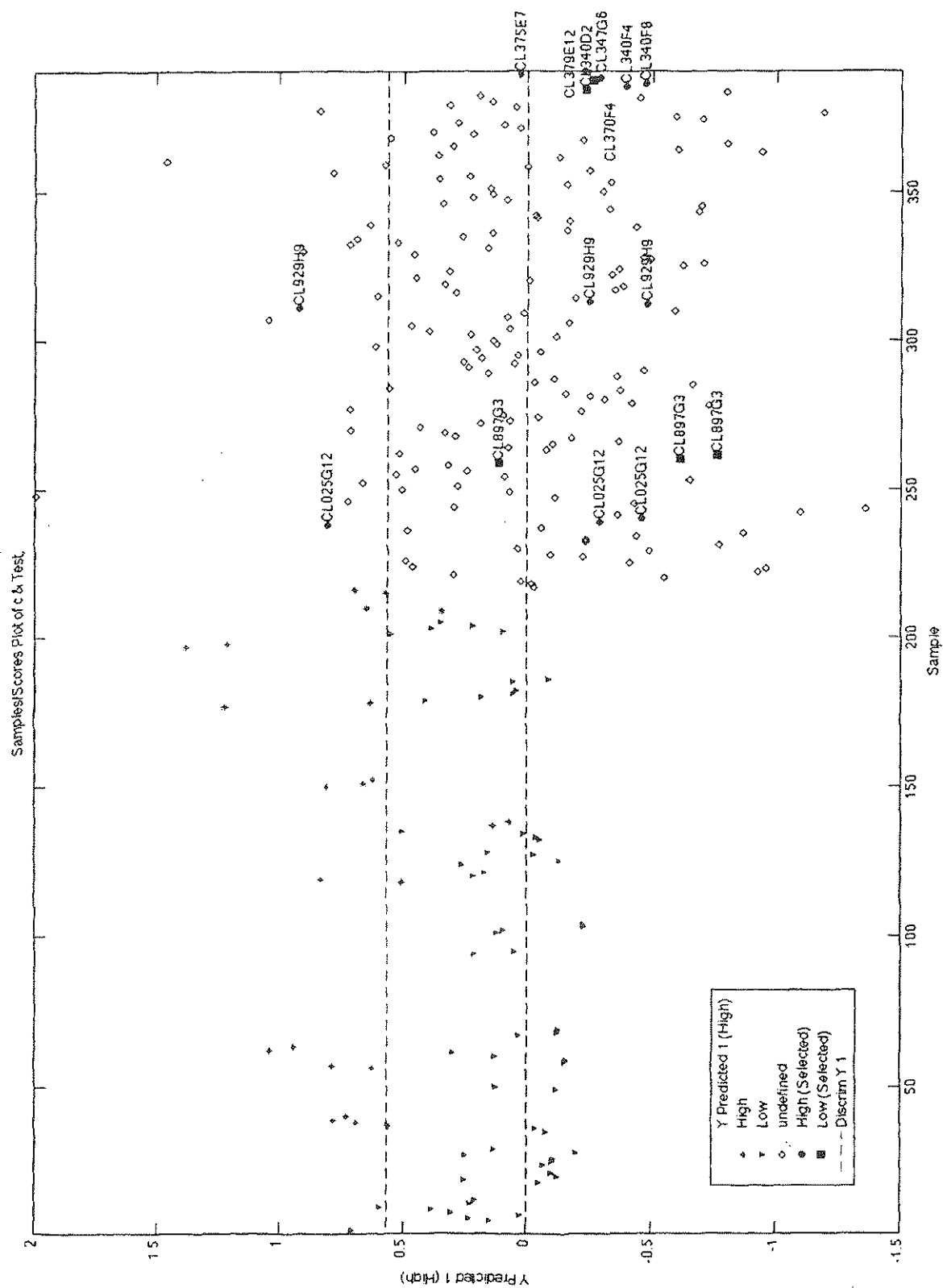


Fig. 23

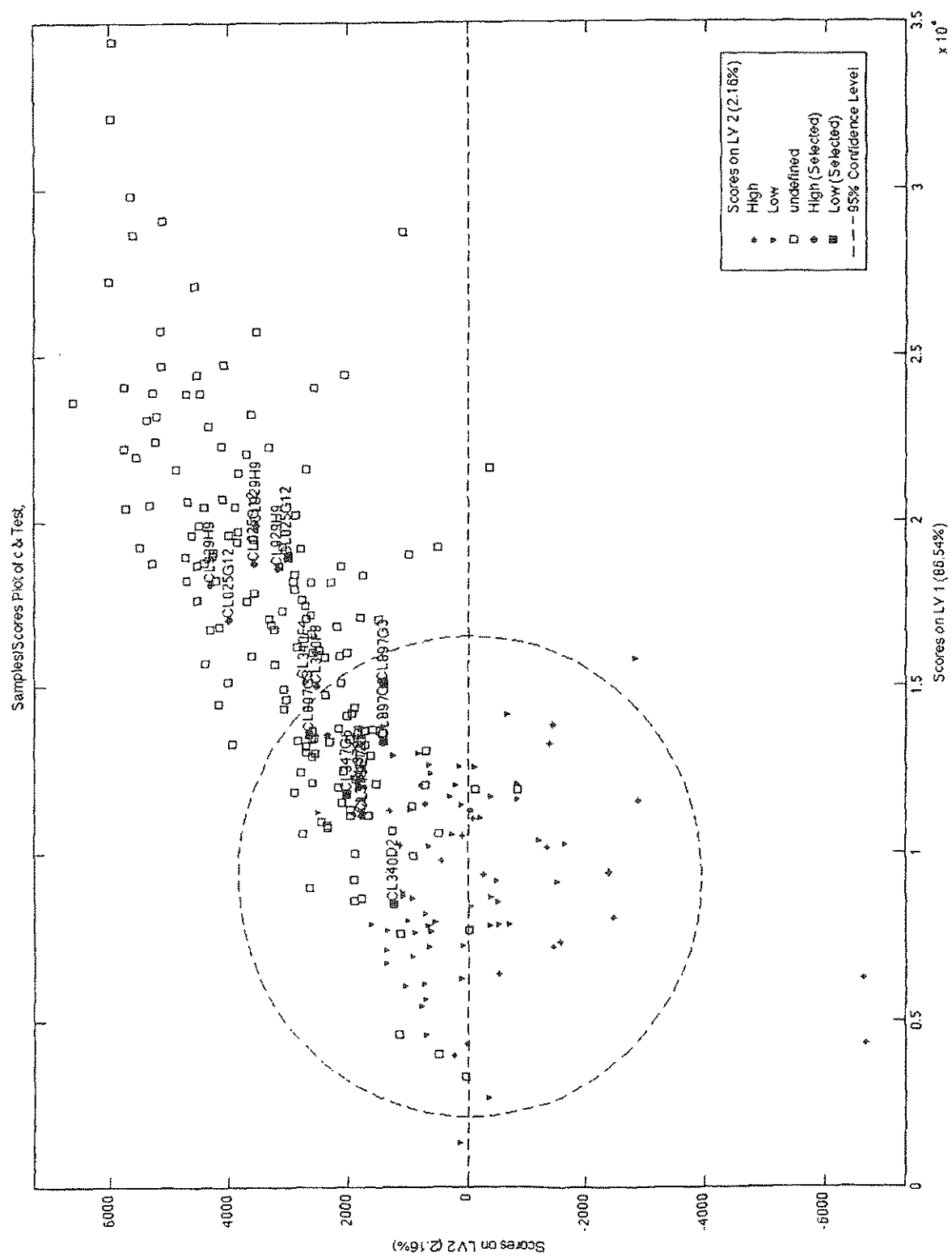


Fig. 24

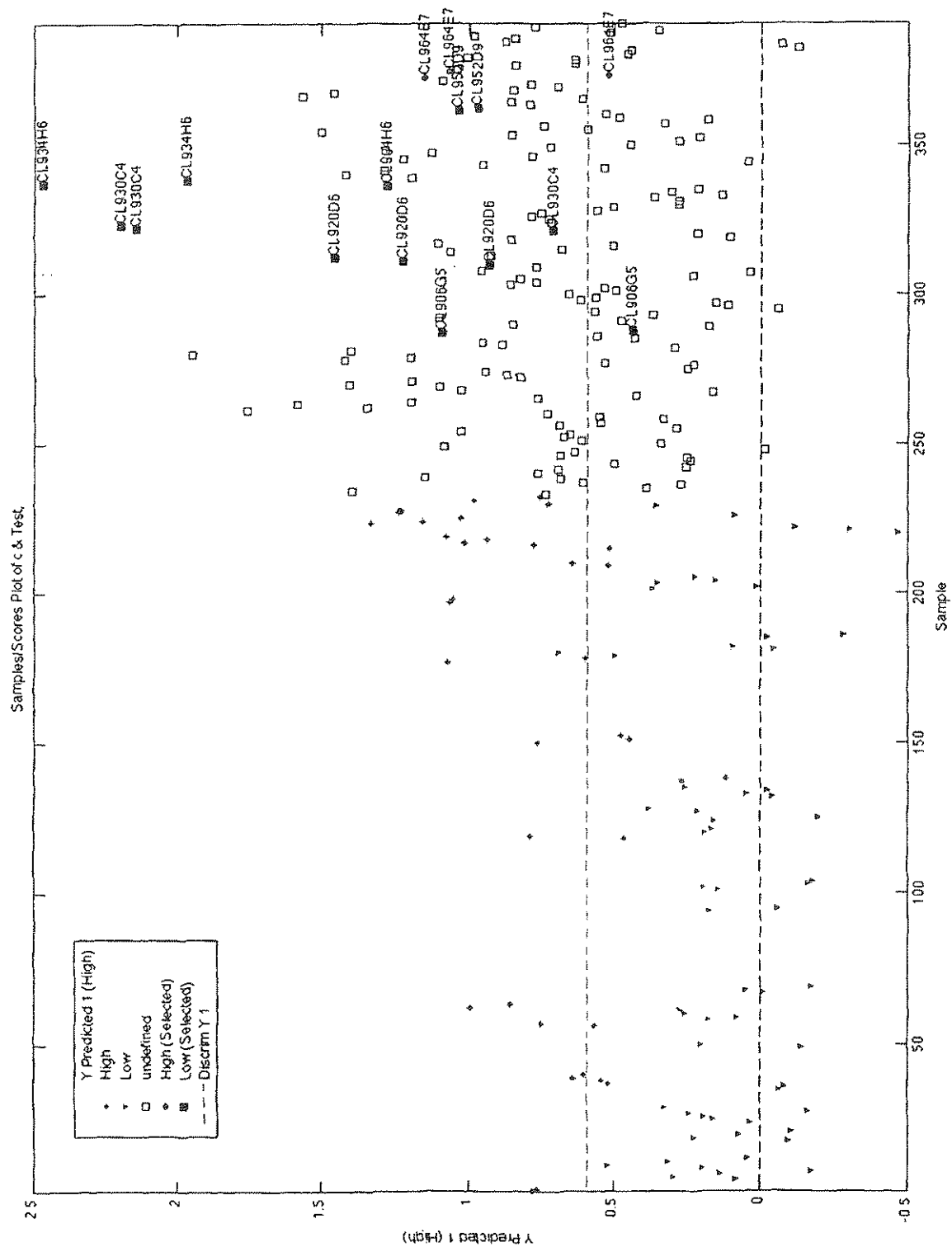


Fig. 25

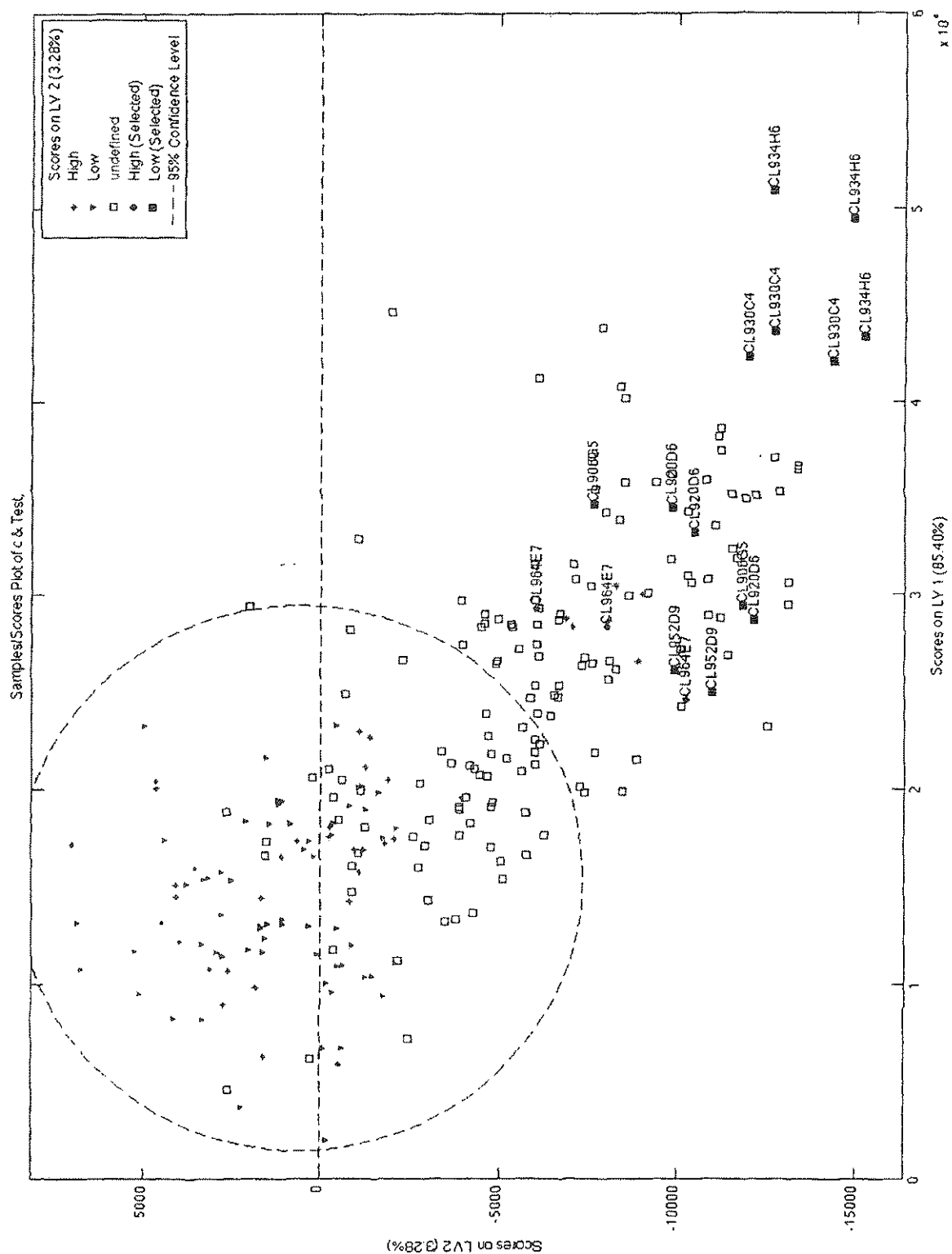


Fig. 26

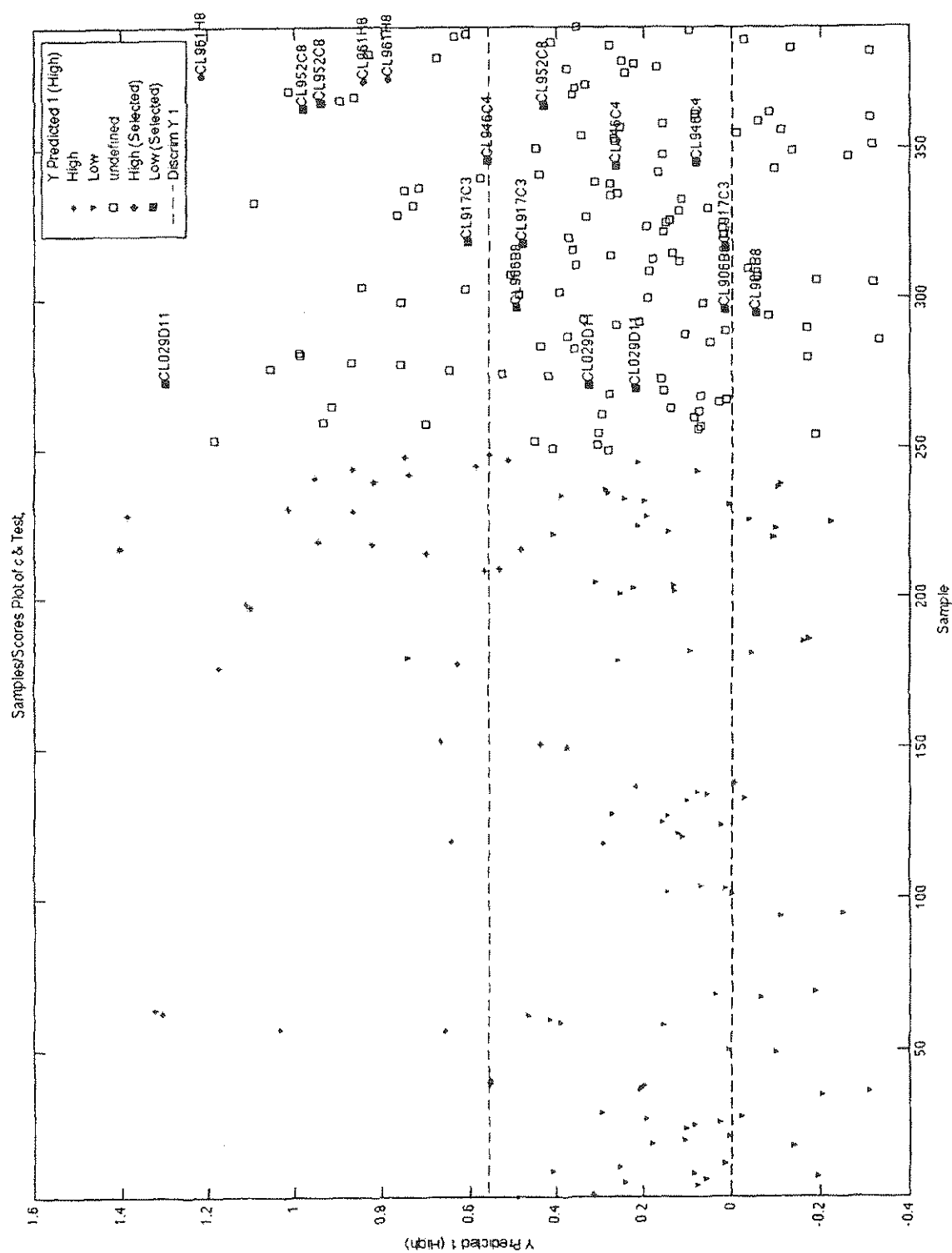


Fig. 27

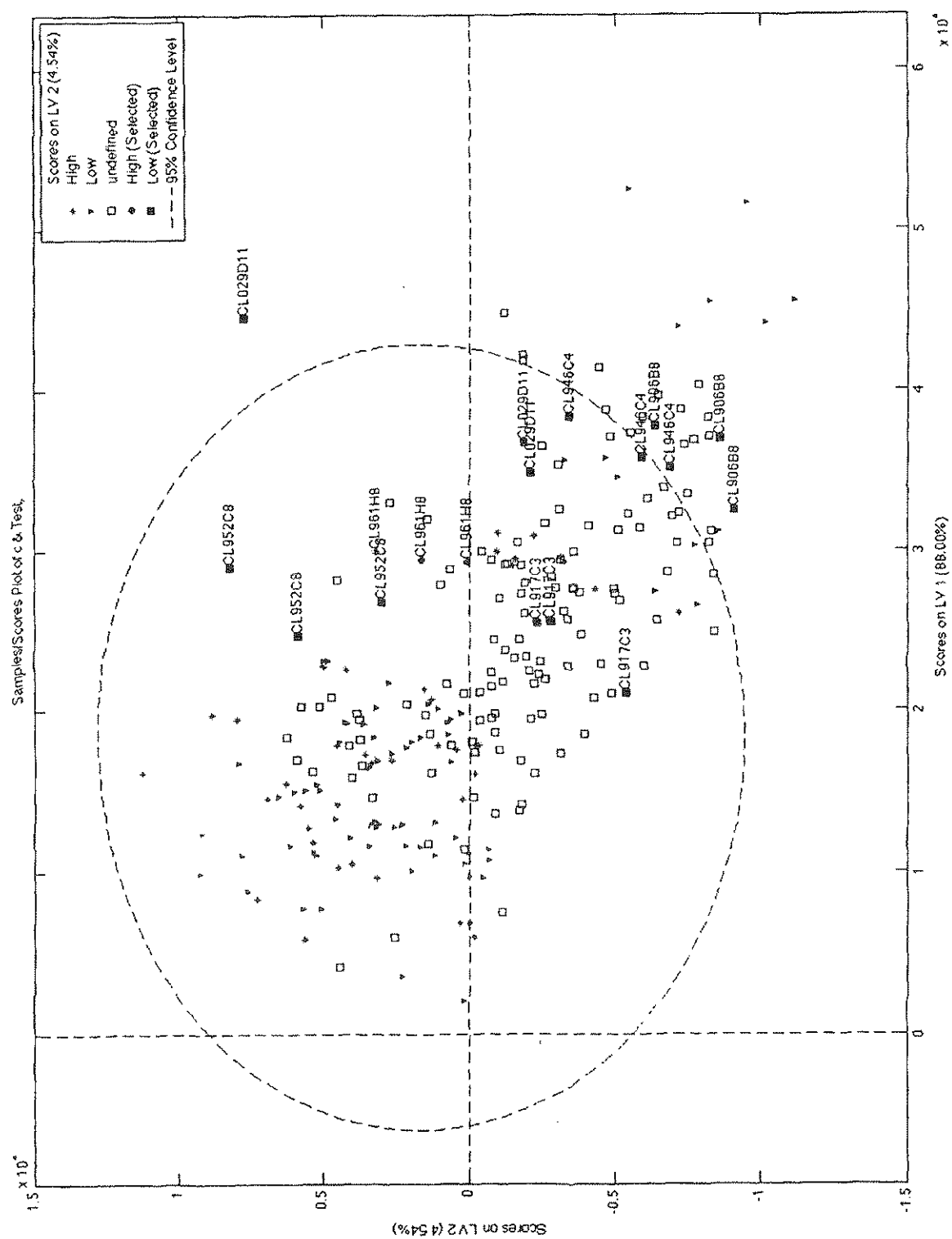


Fig. 29

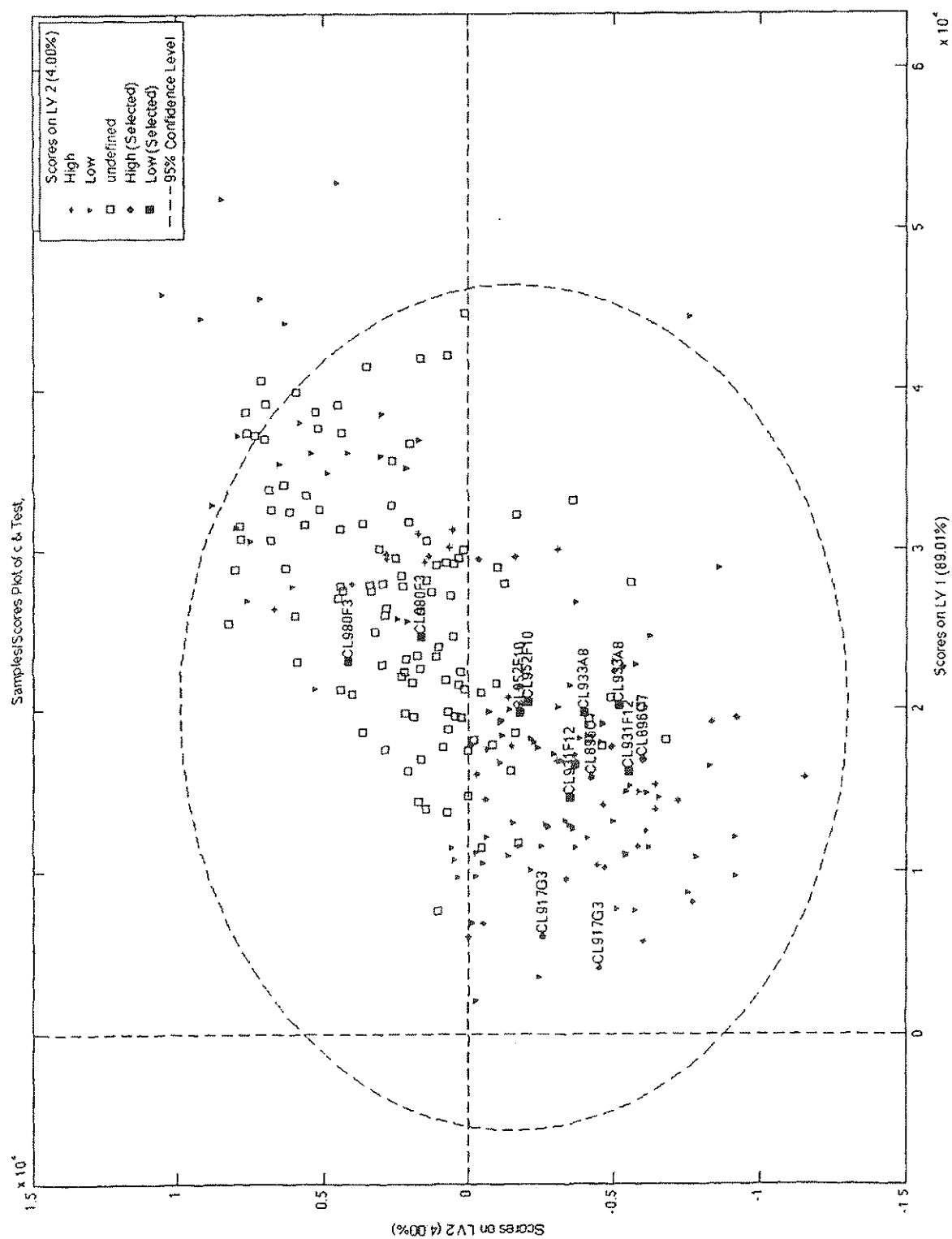


Fig. 30

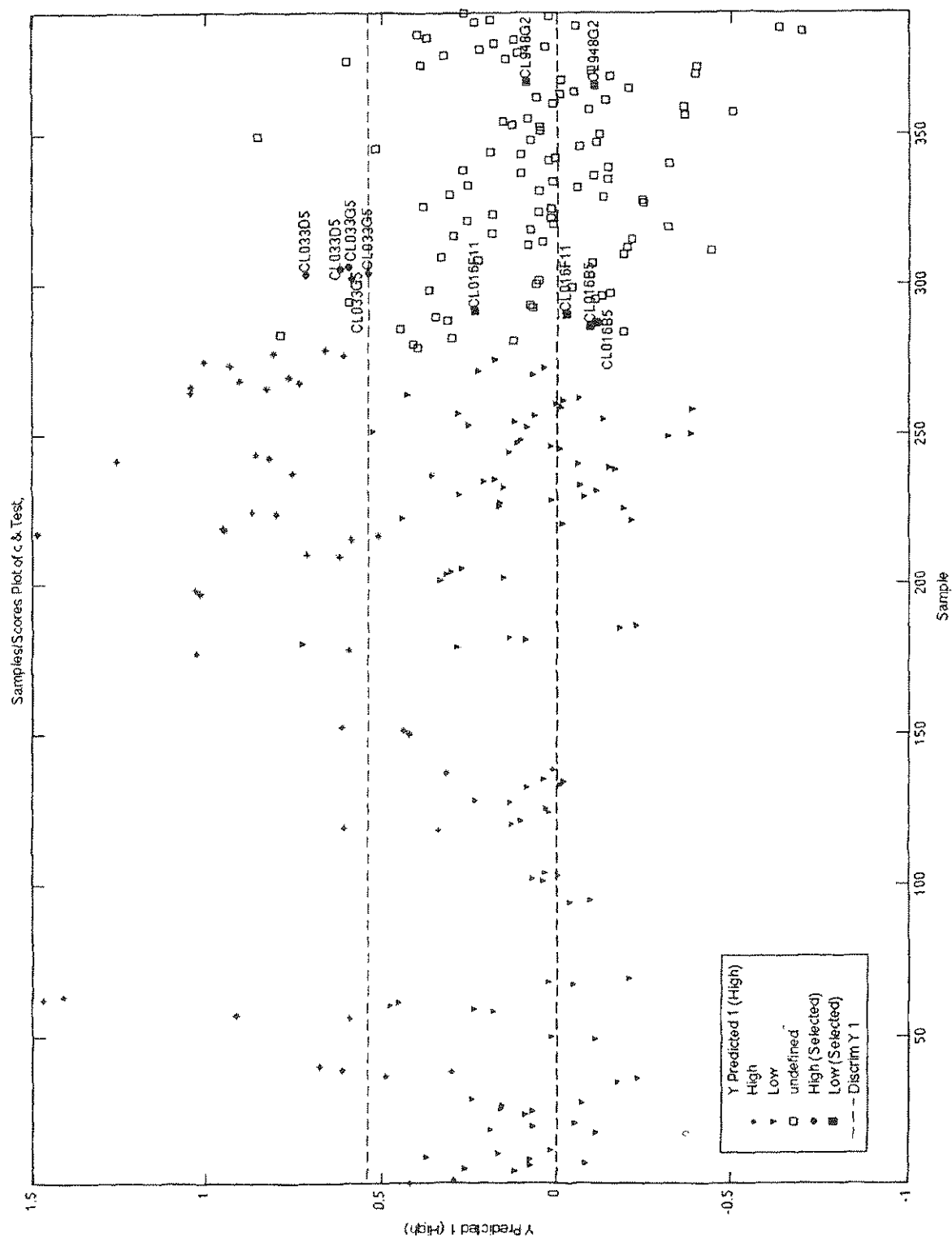


Fig. 31

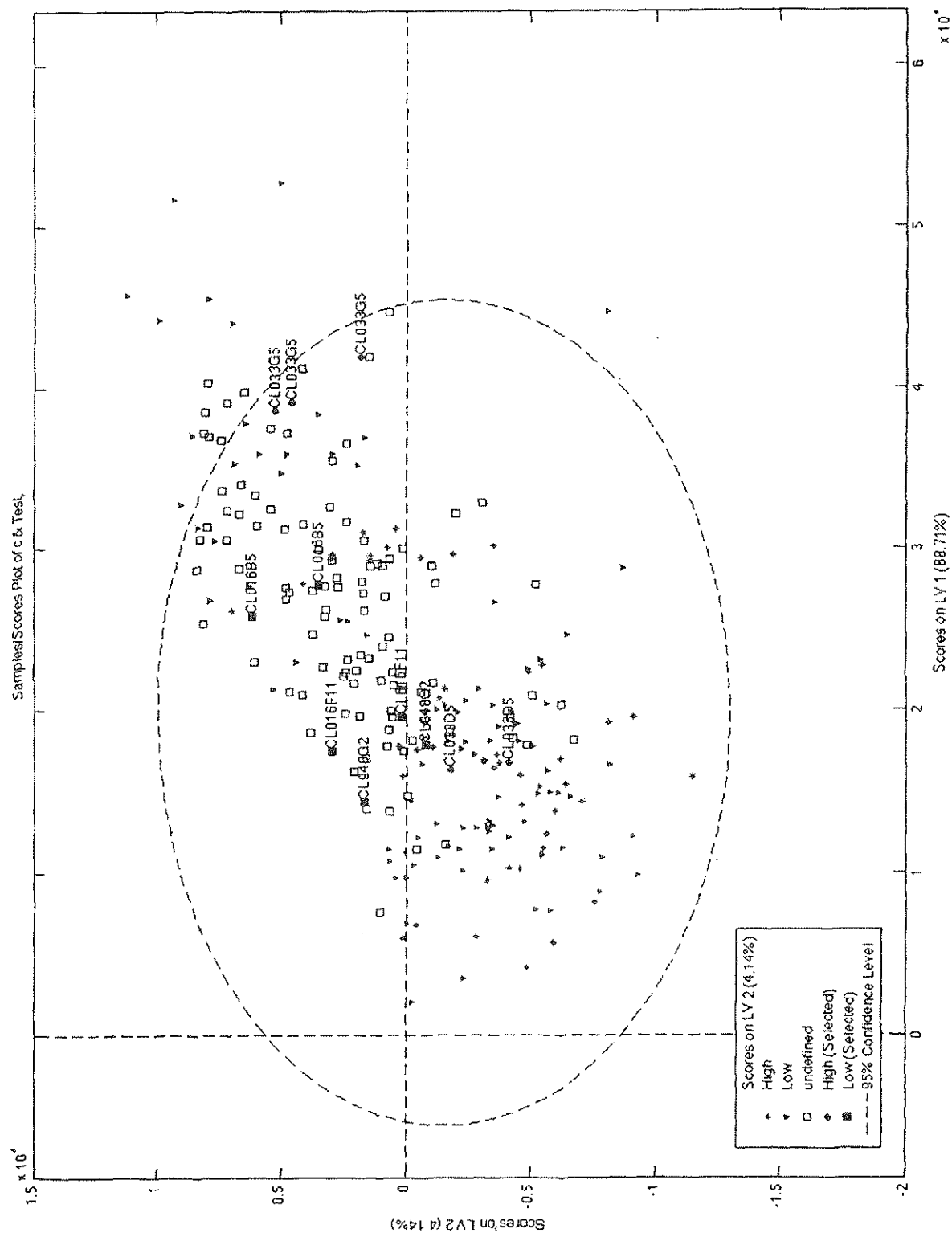


Fig. 32

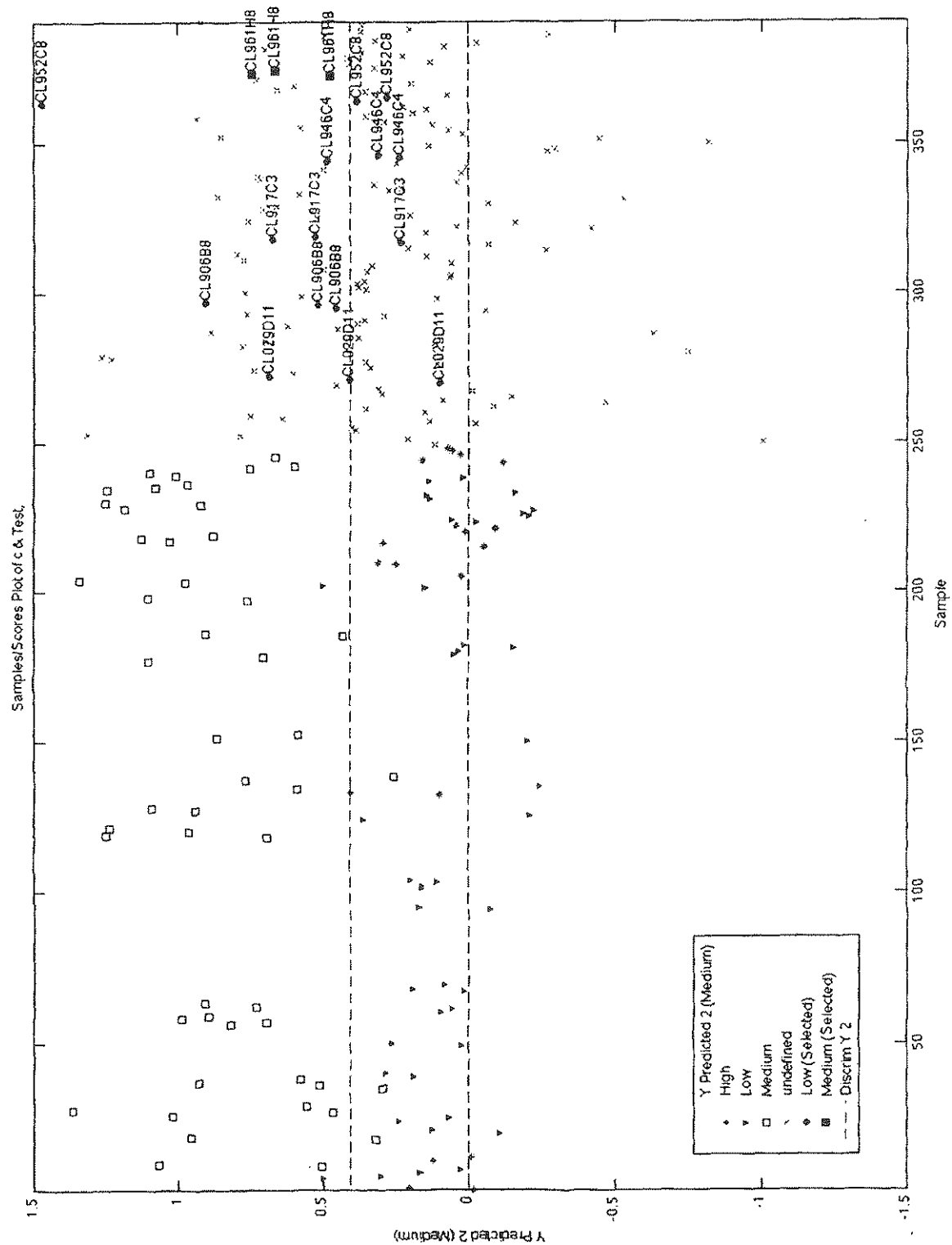


Fig. 33

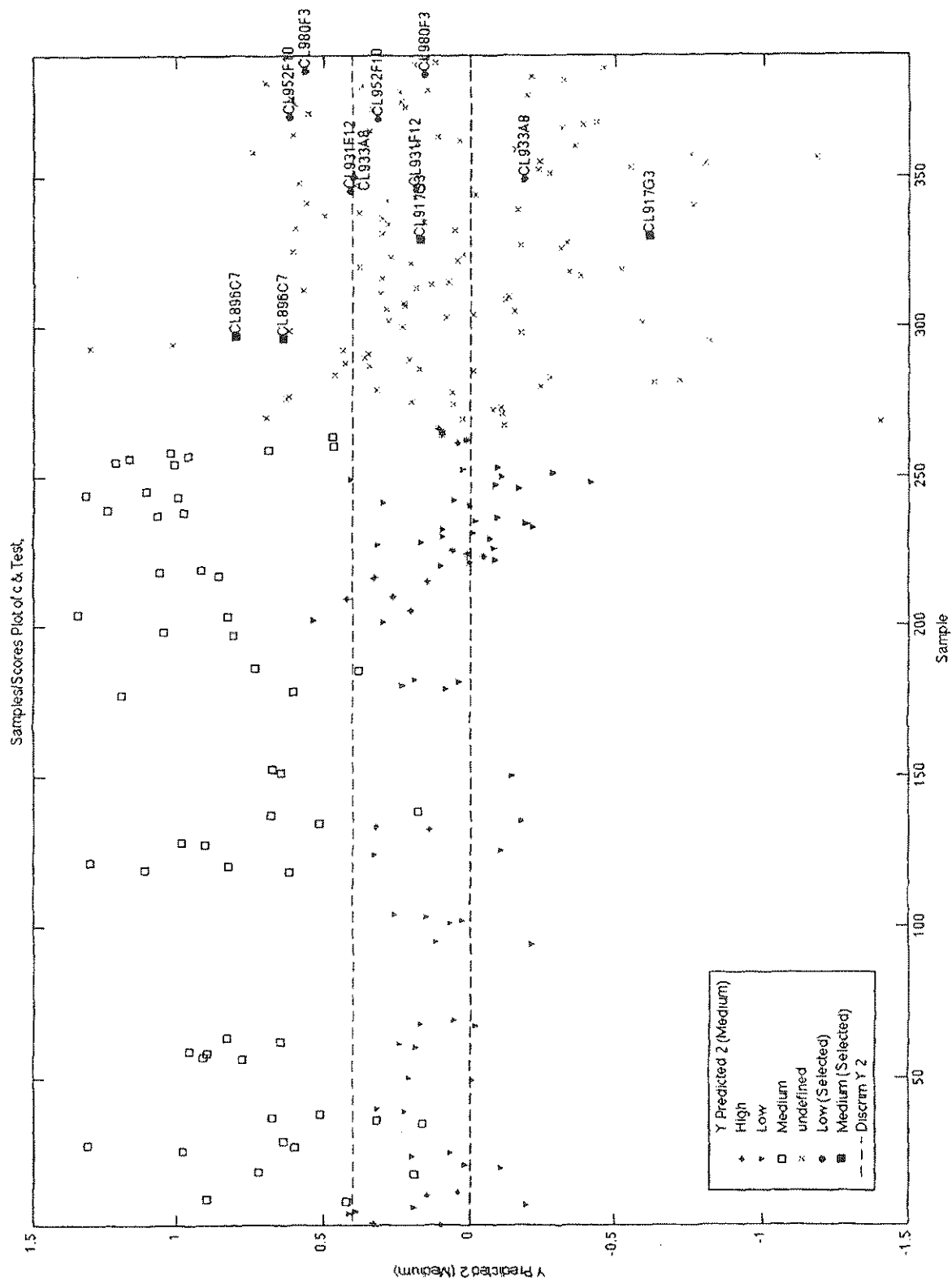


Fig. 34

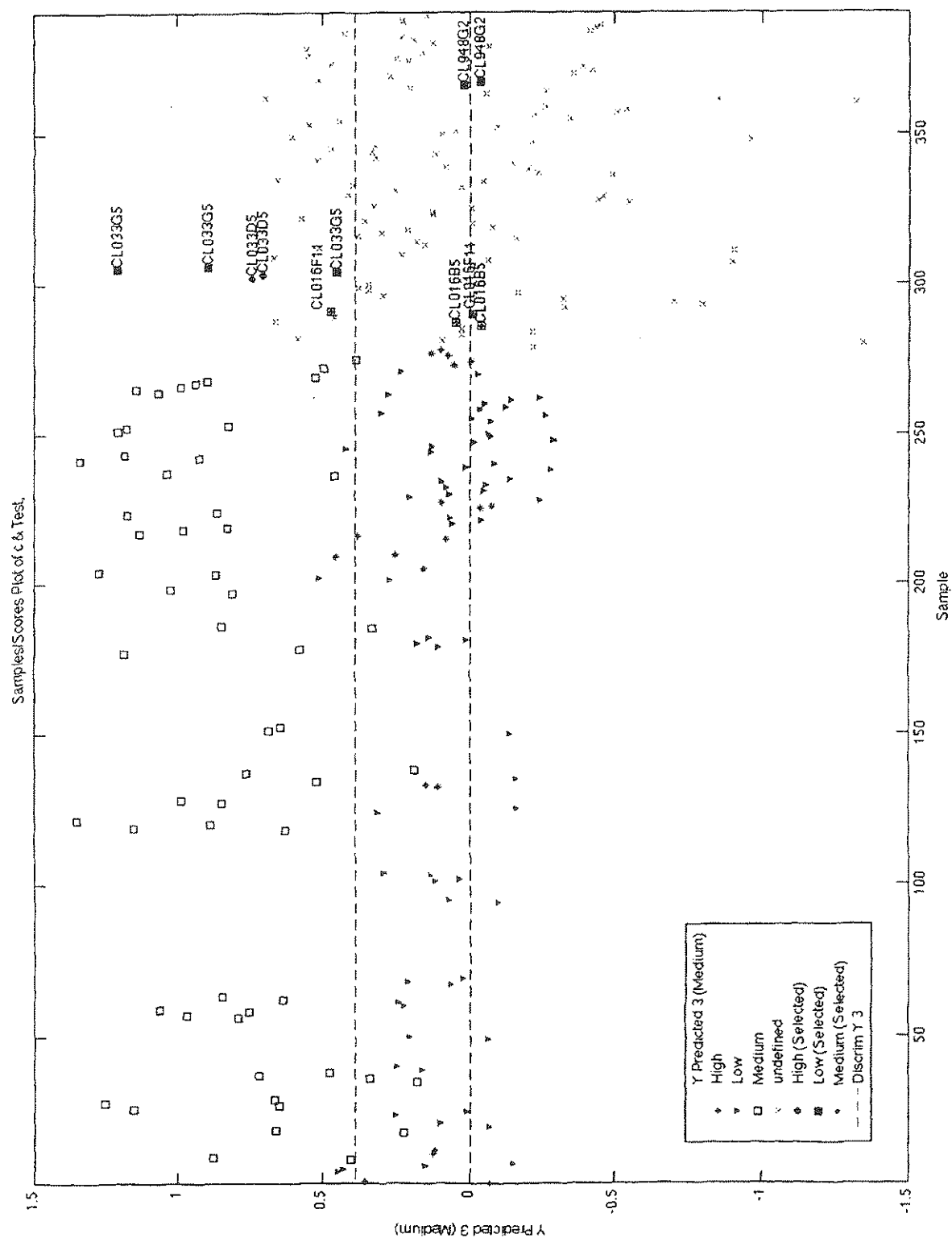


Fig. 35

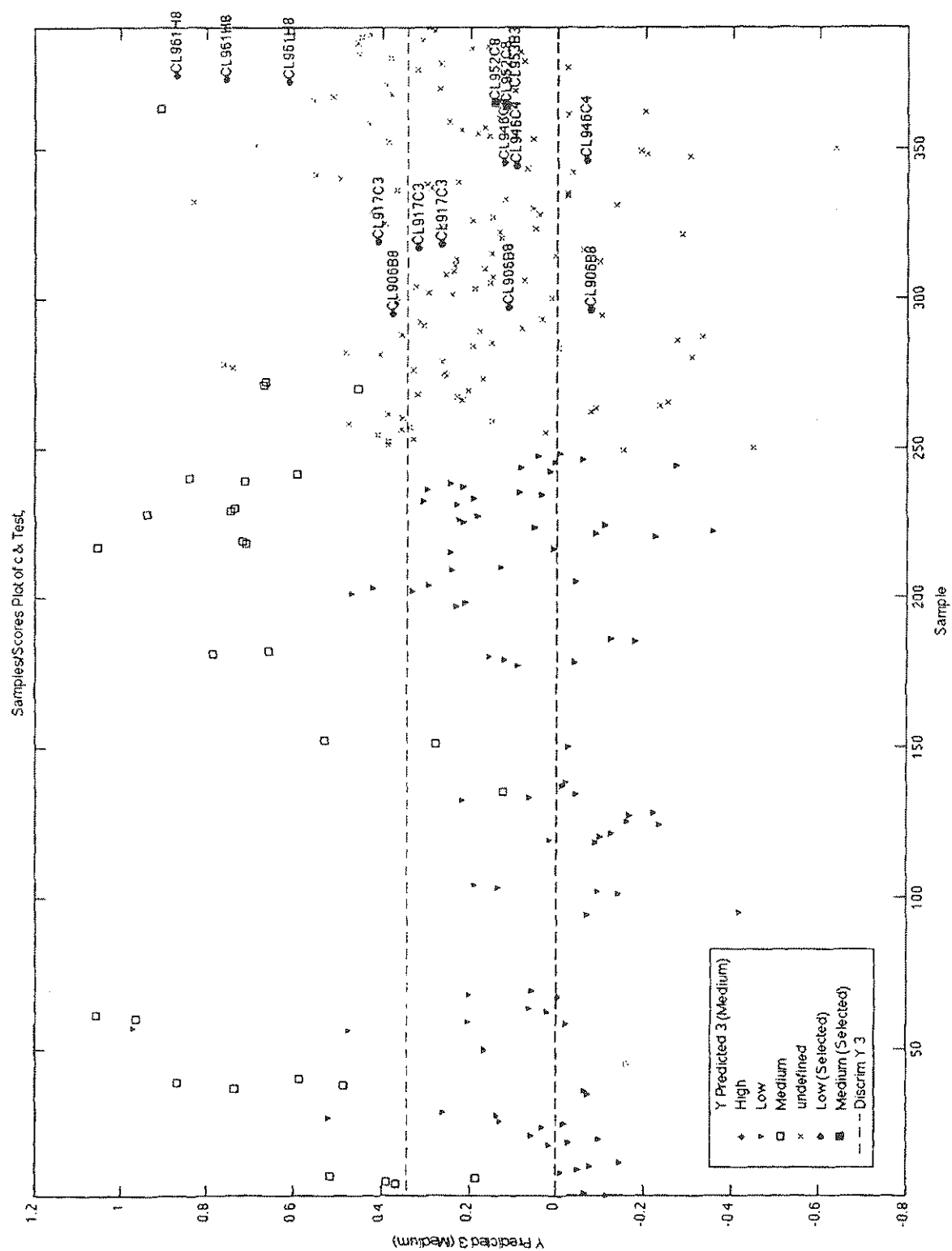
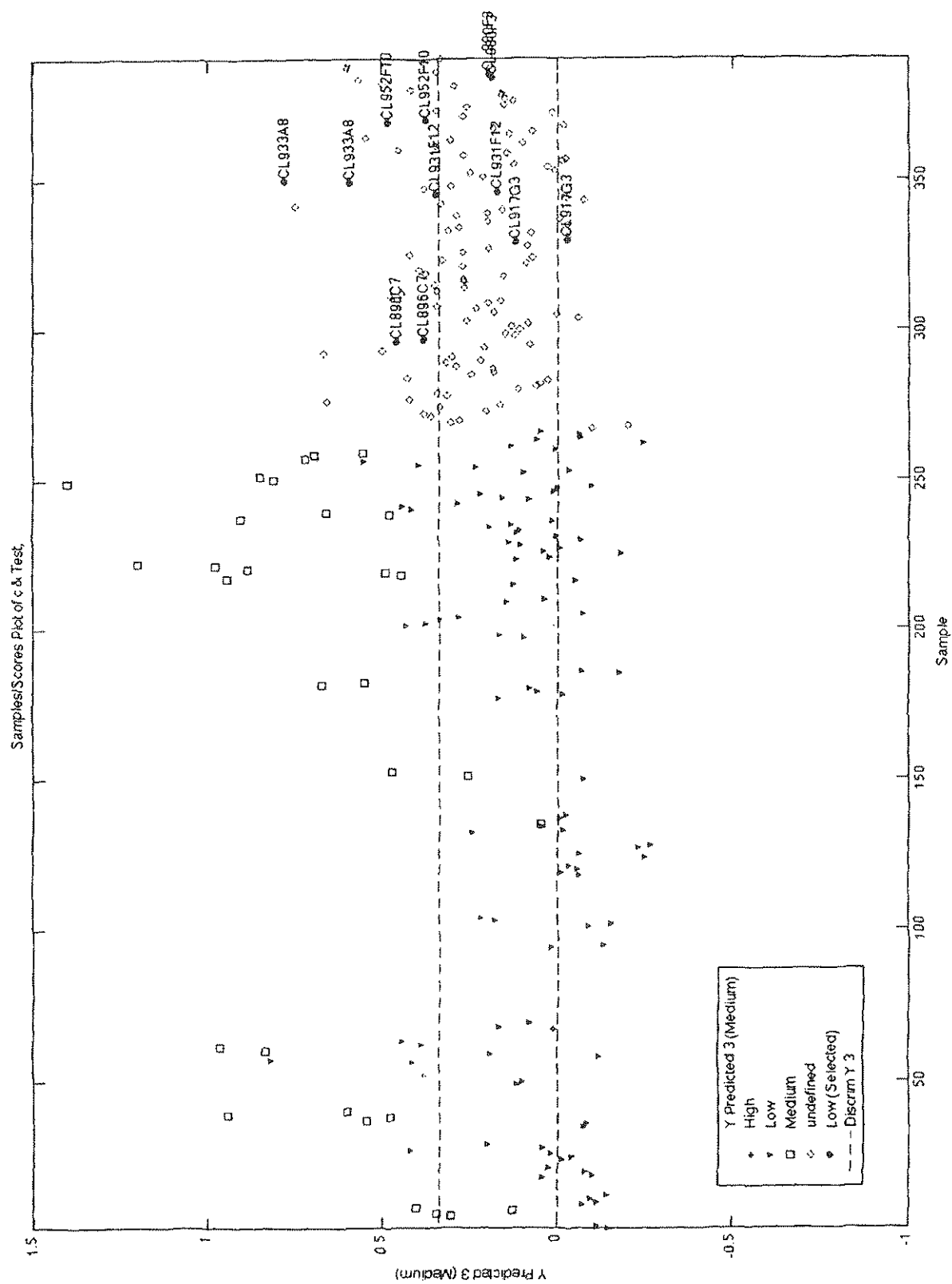


Fig. 36



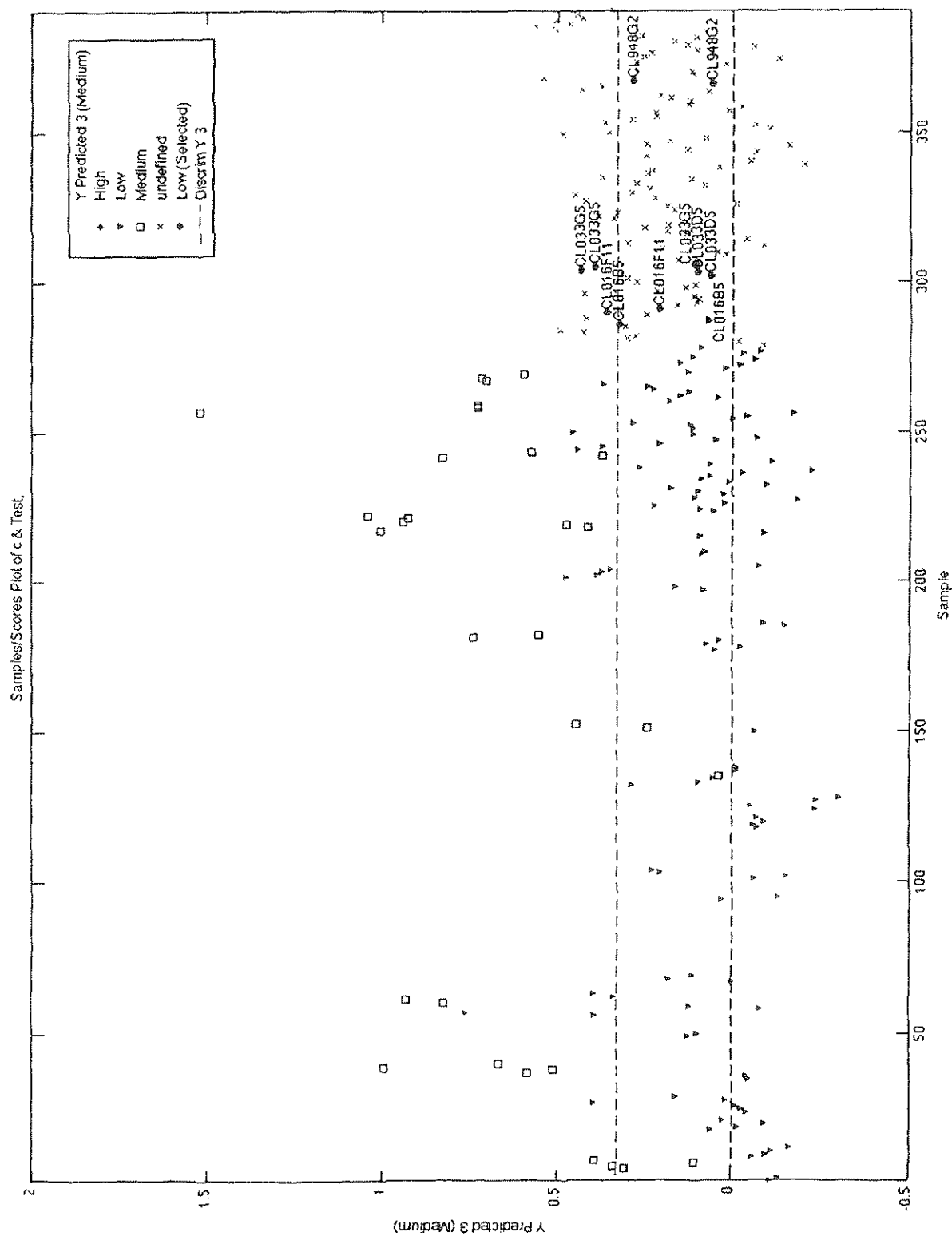
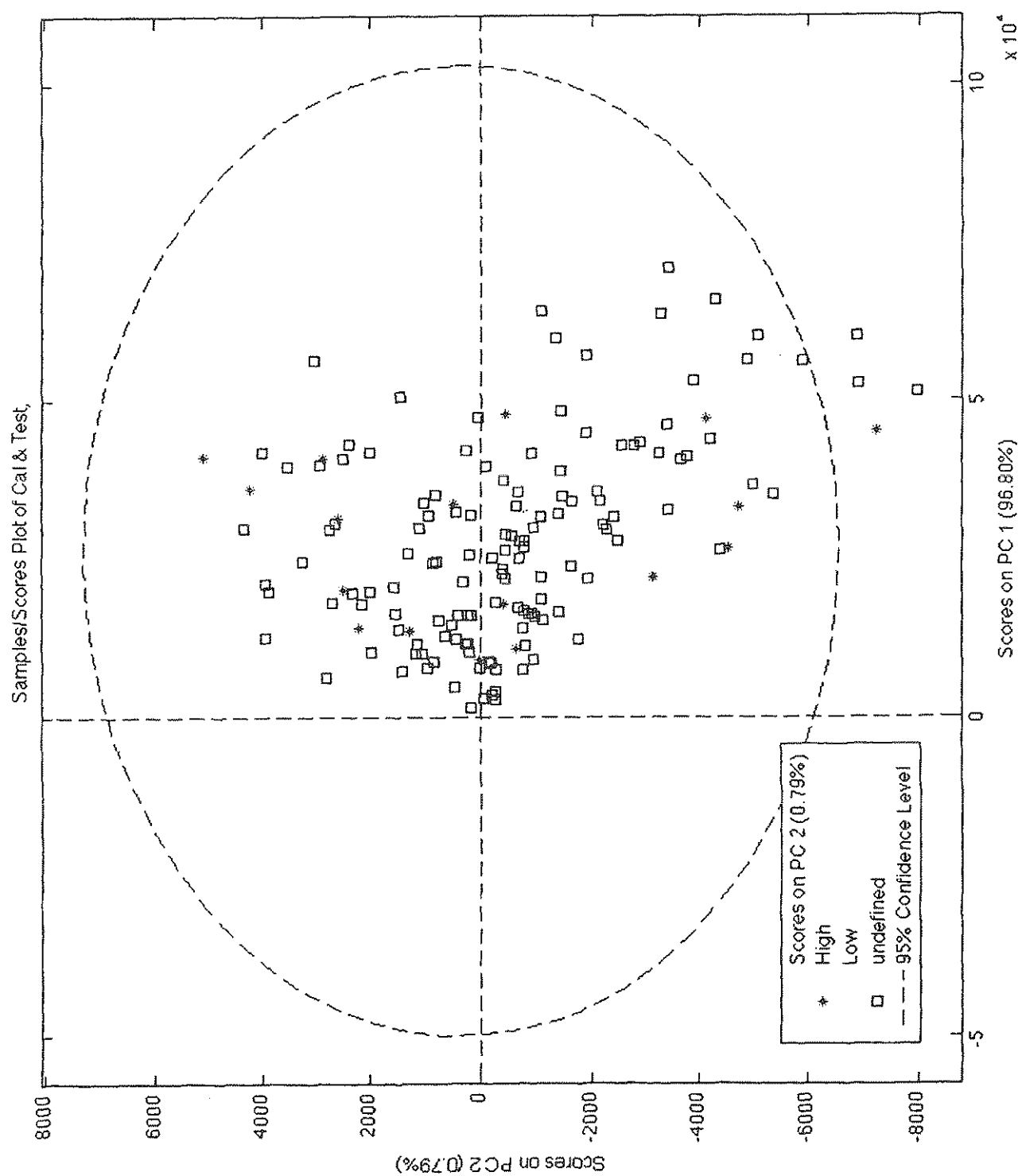


Fig. 37

Fig. 38



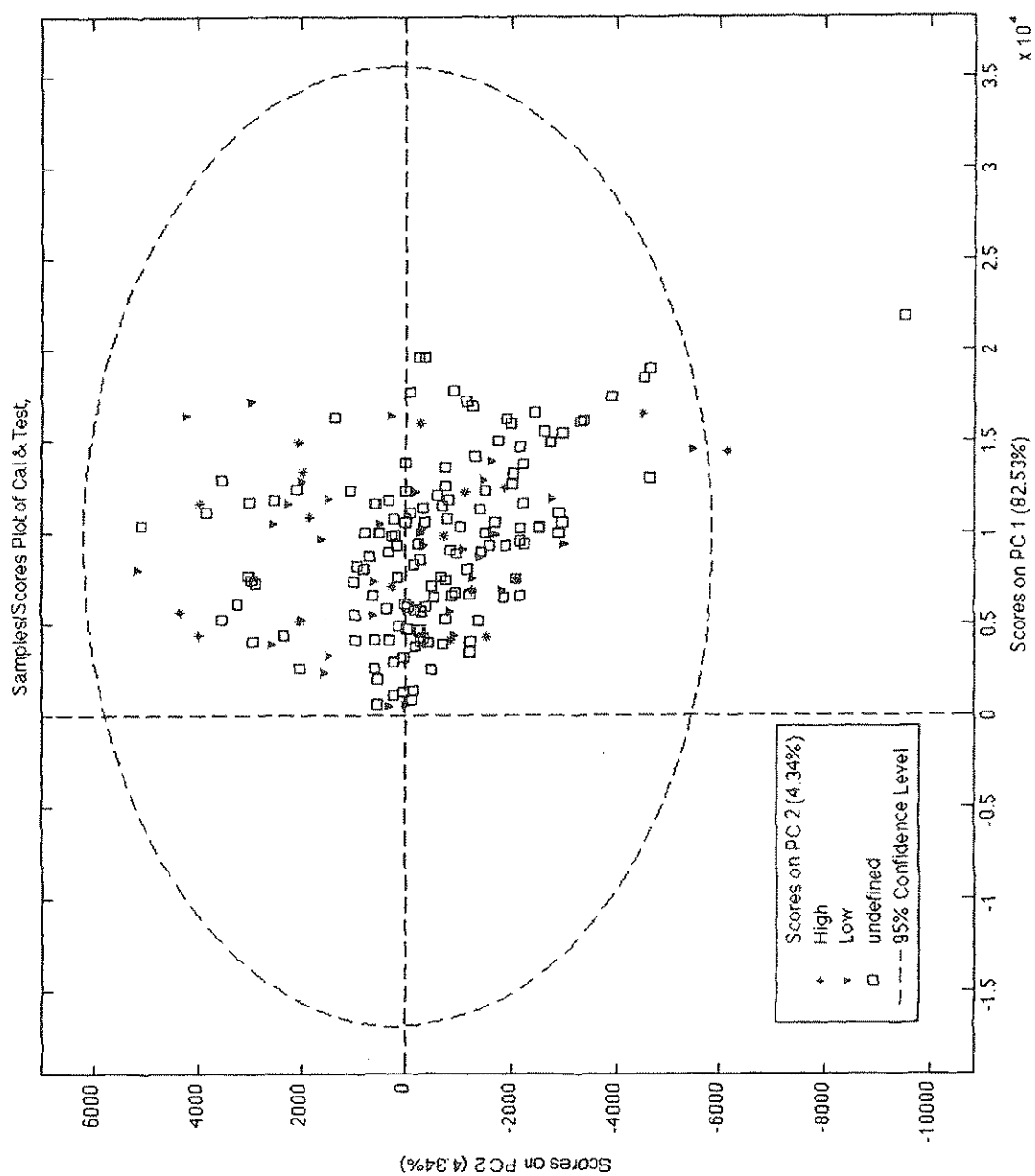


Fig. 39

Fig. 40

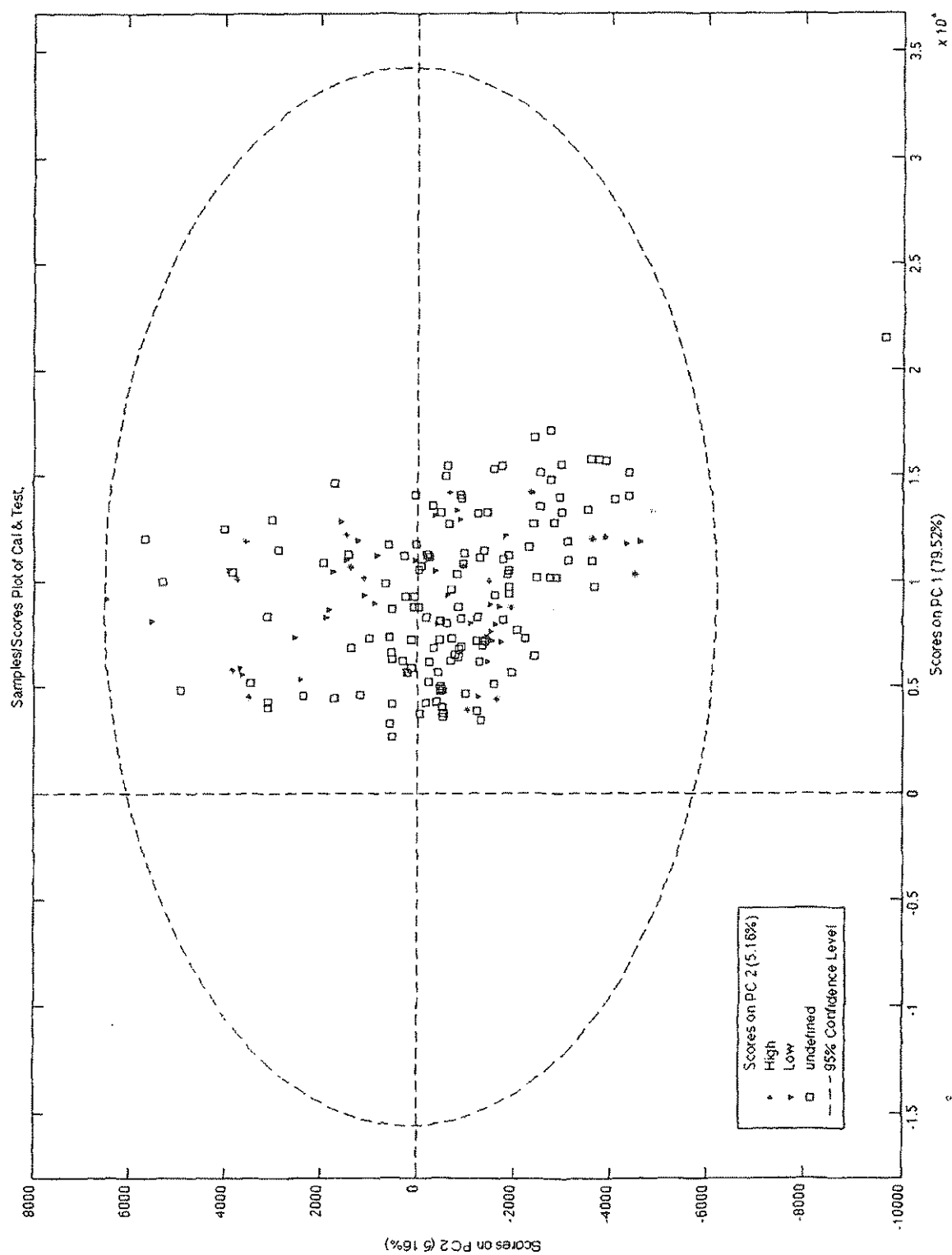


Fig. 41

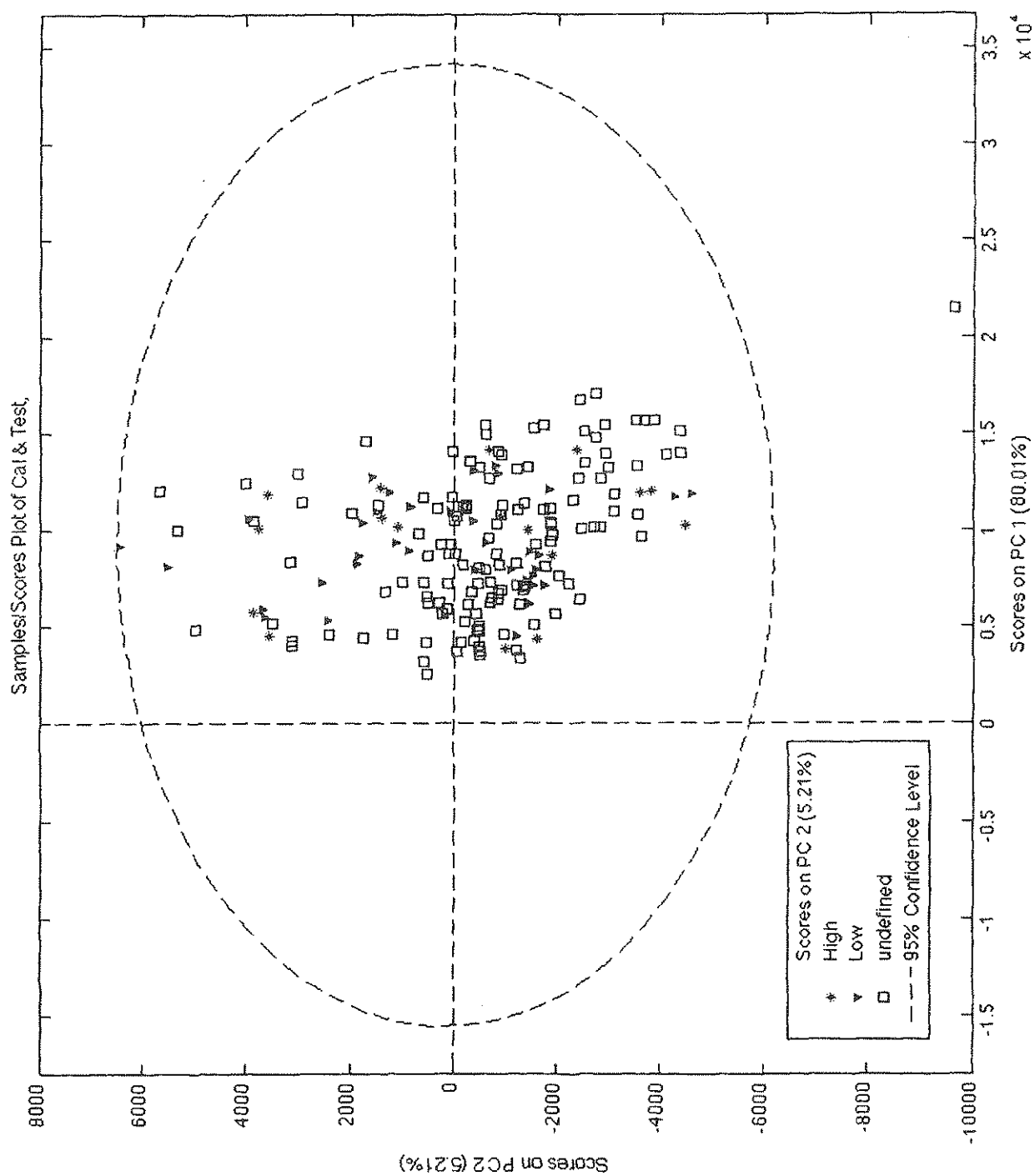
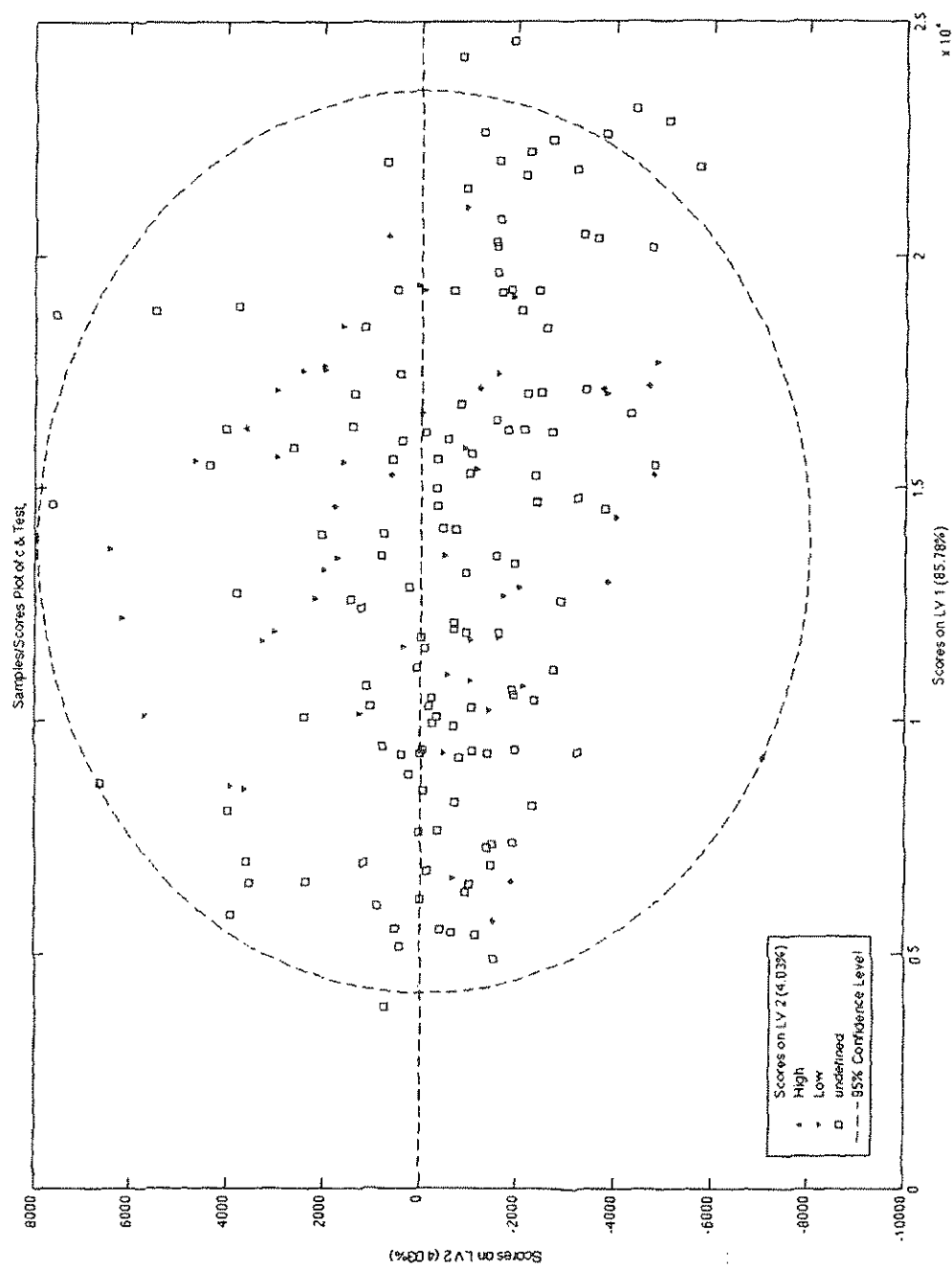


Fig. 42



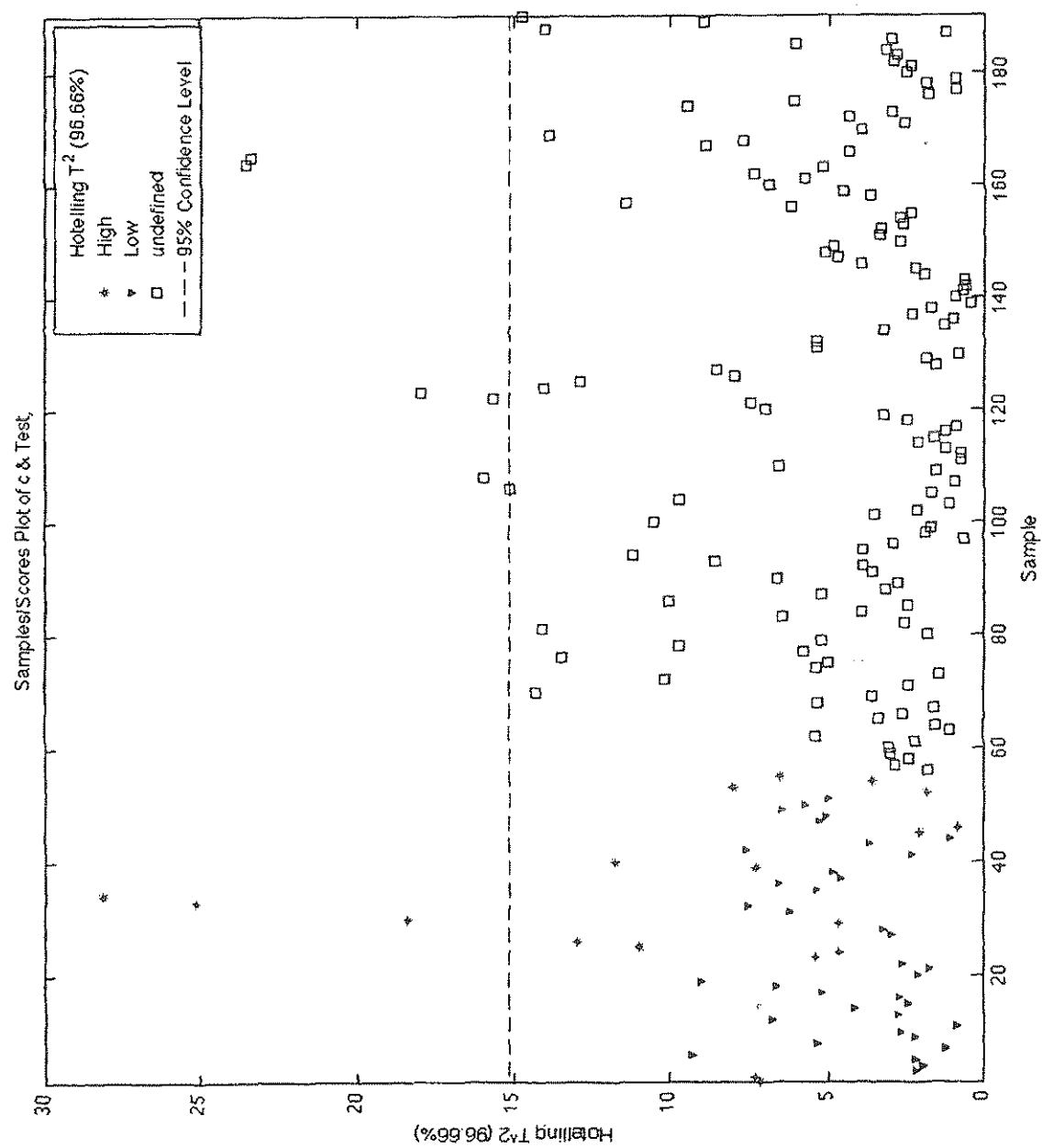


Fig. 43

Fig. 44

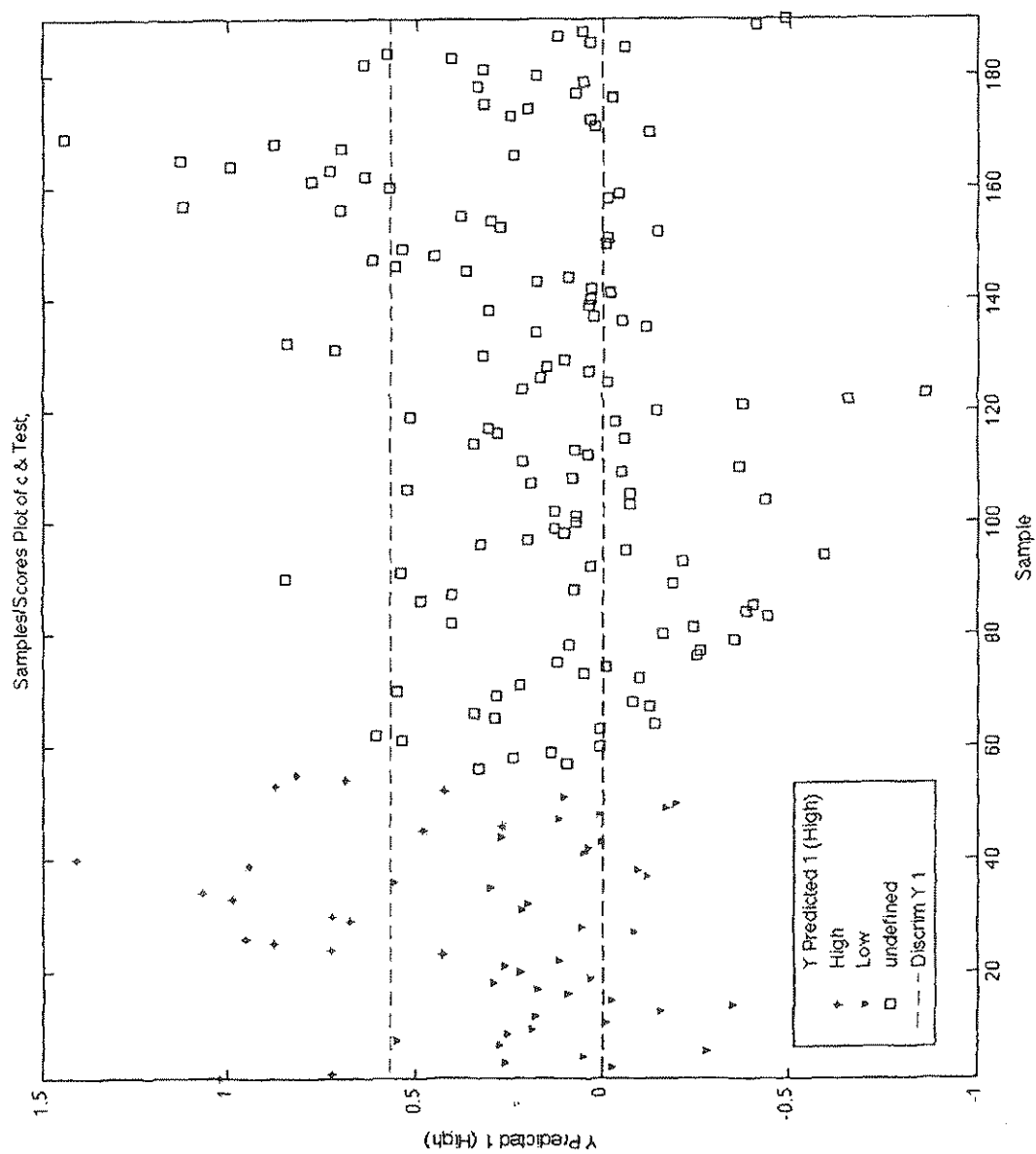


Fig. 45

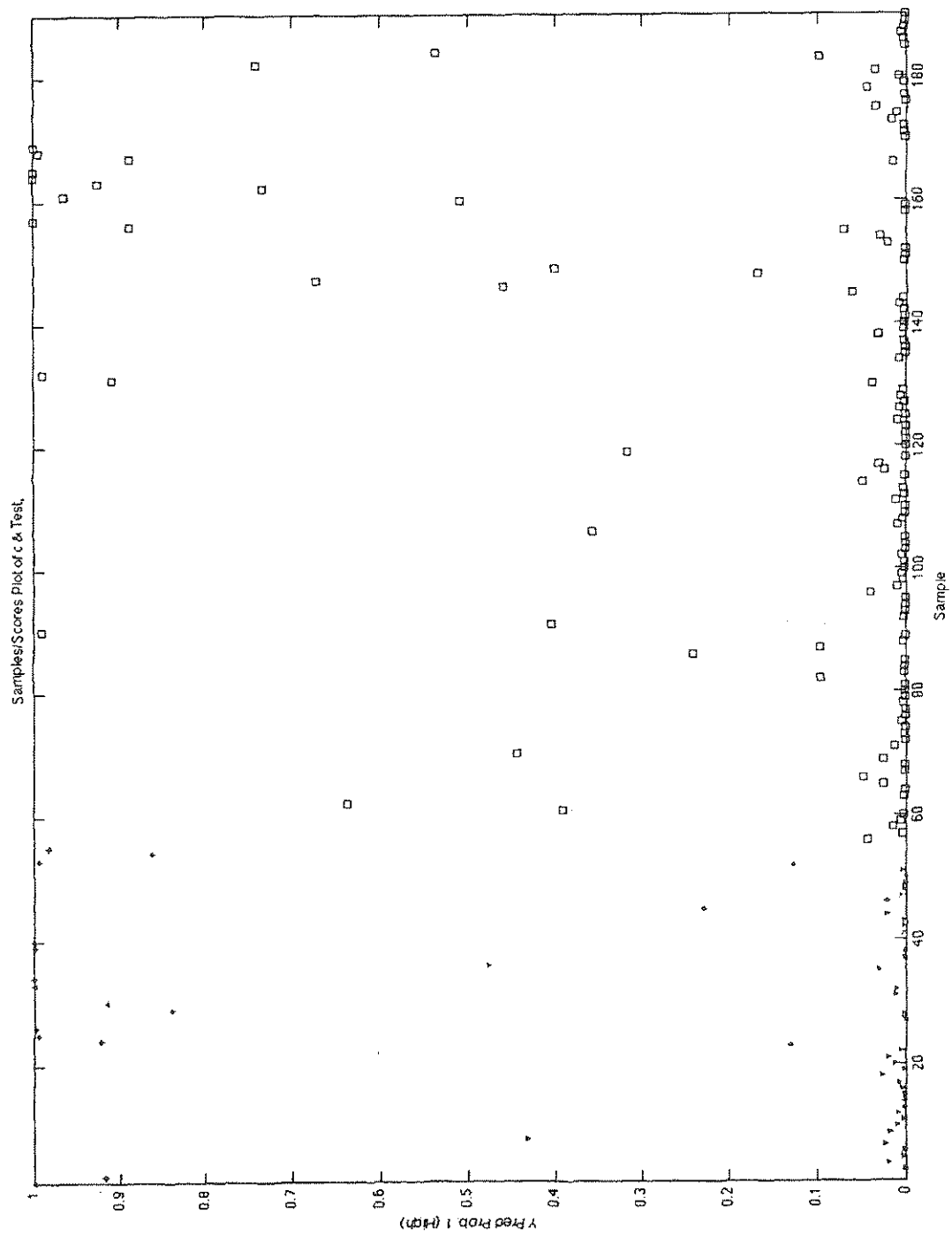


Fig. 46

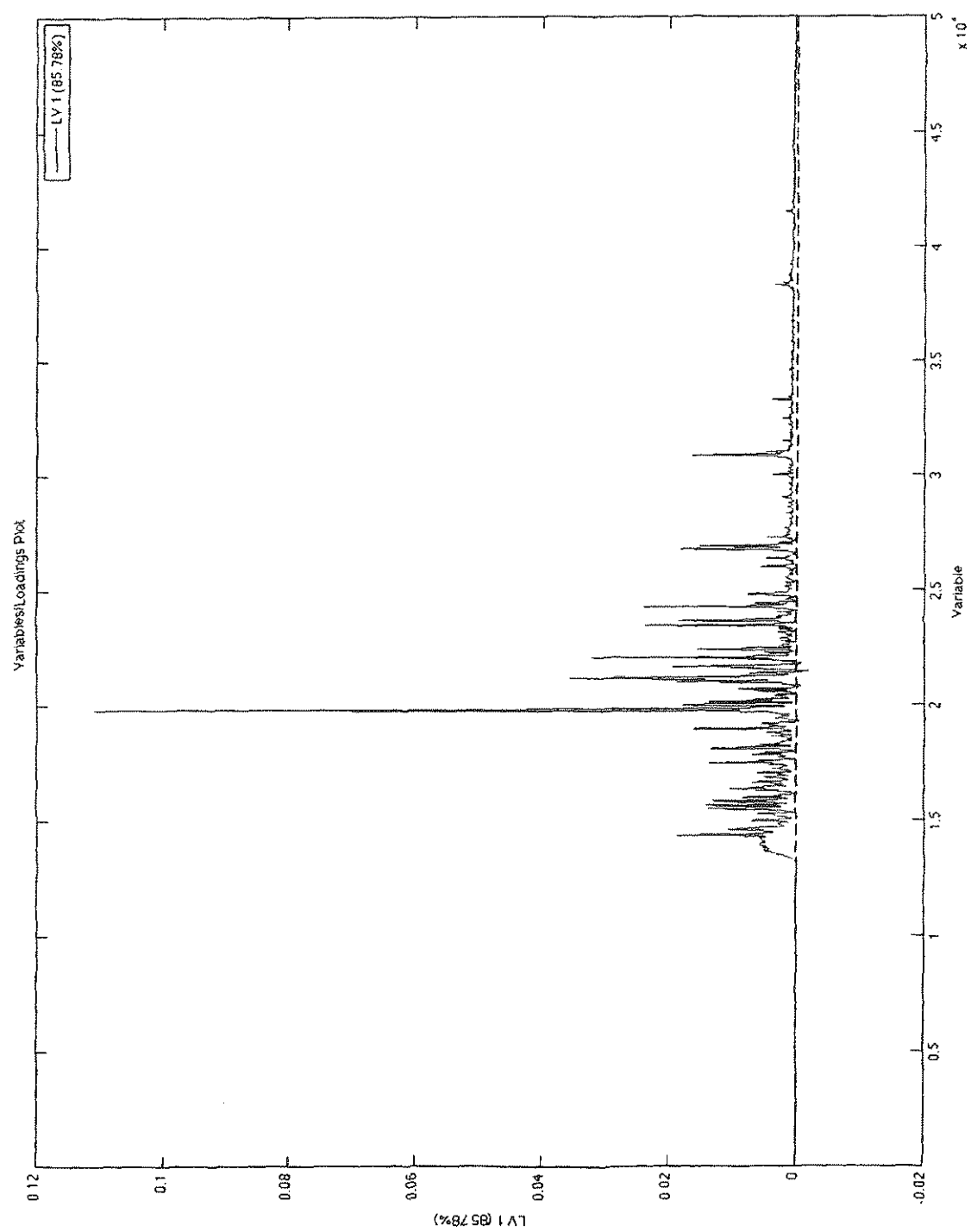


Fig. 47

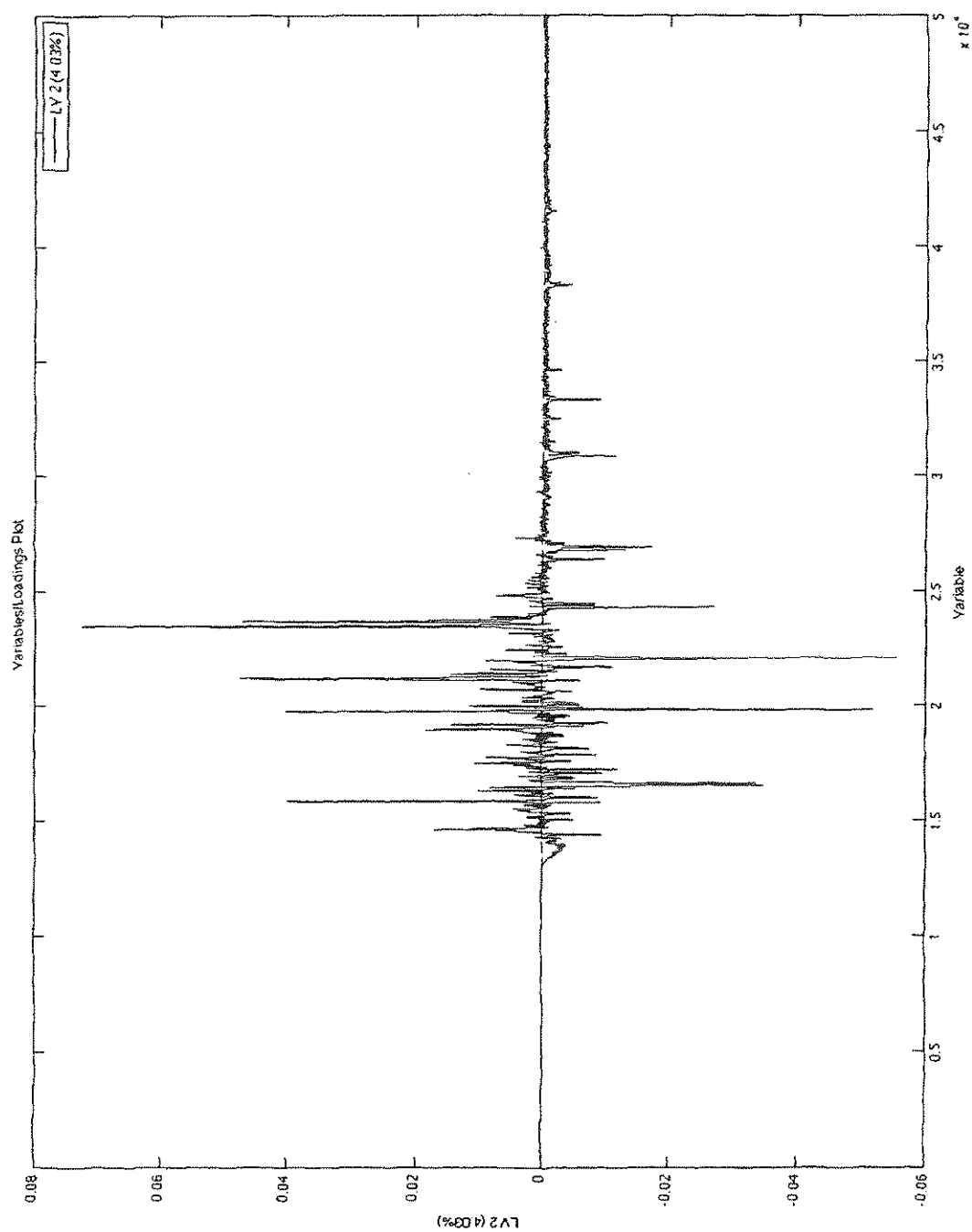


Fig. 48

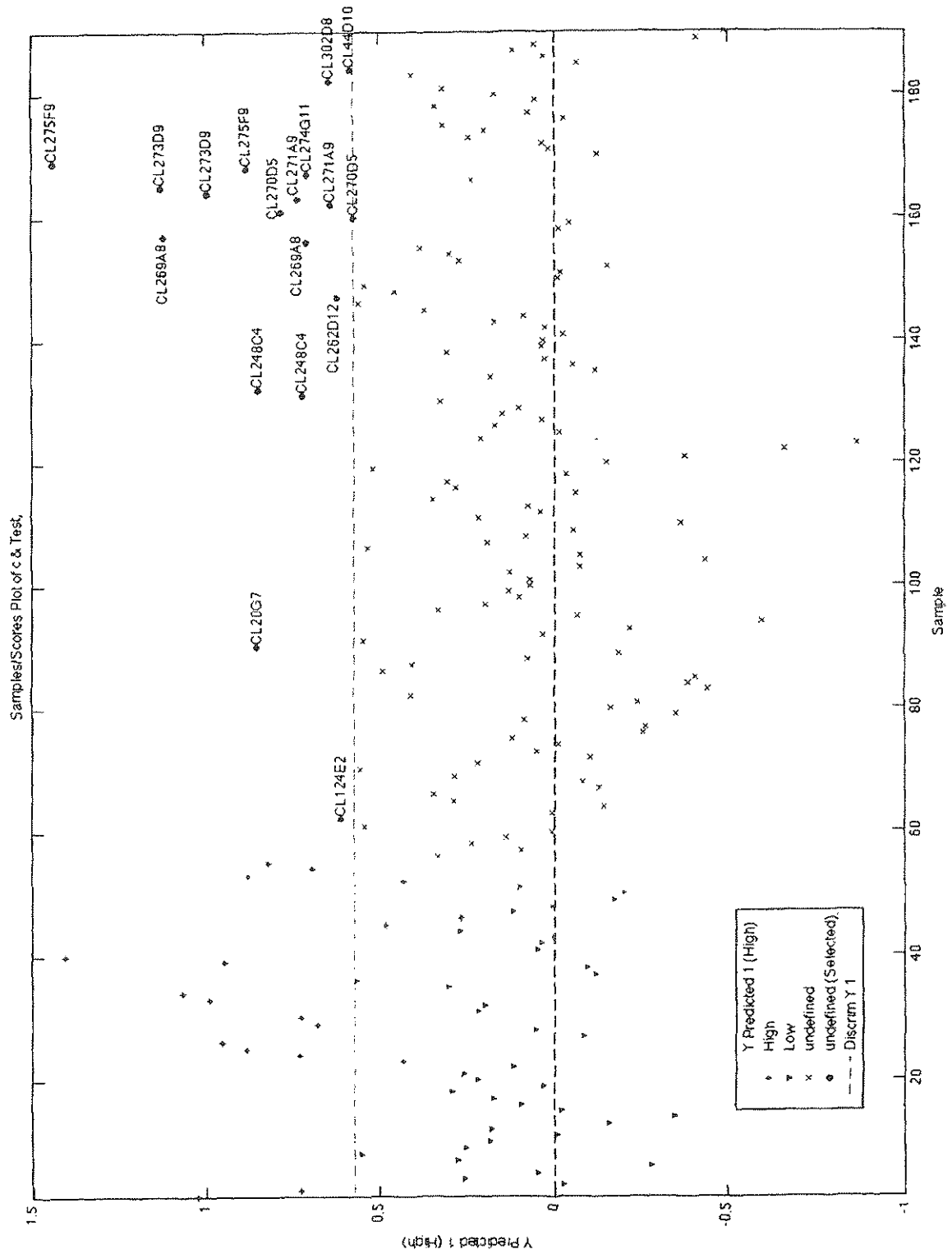


Fig. 49

