

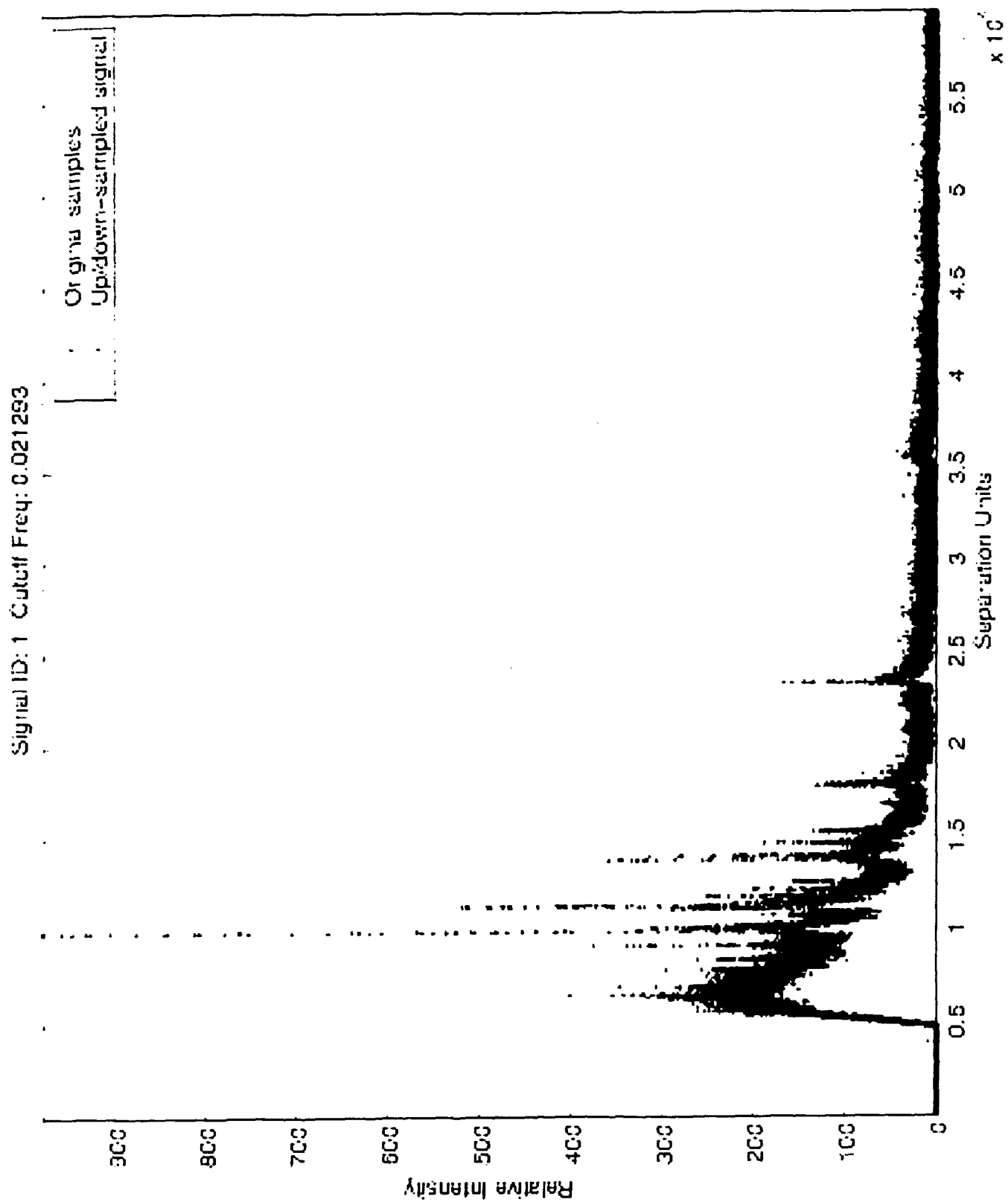


Fig. 1a

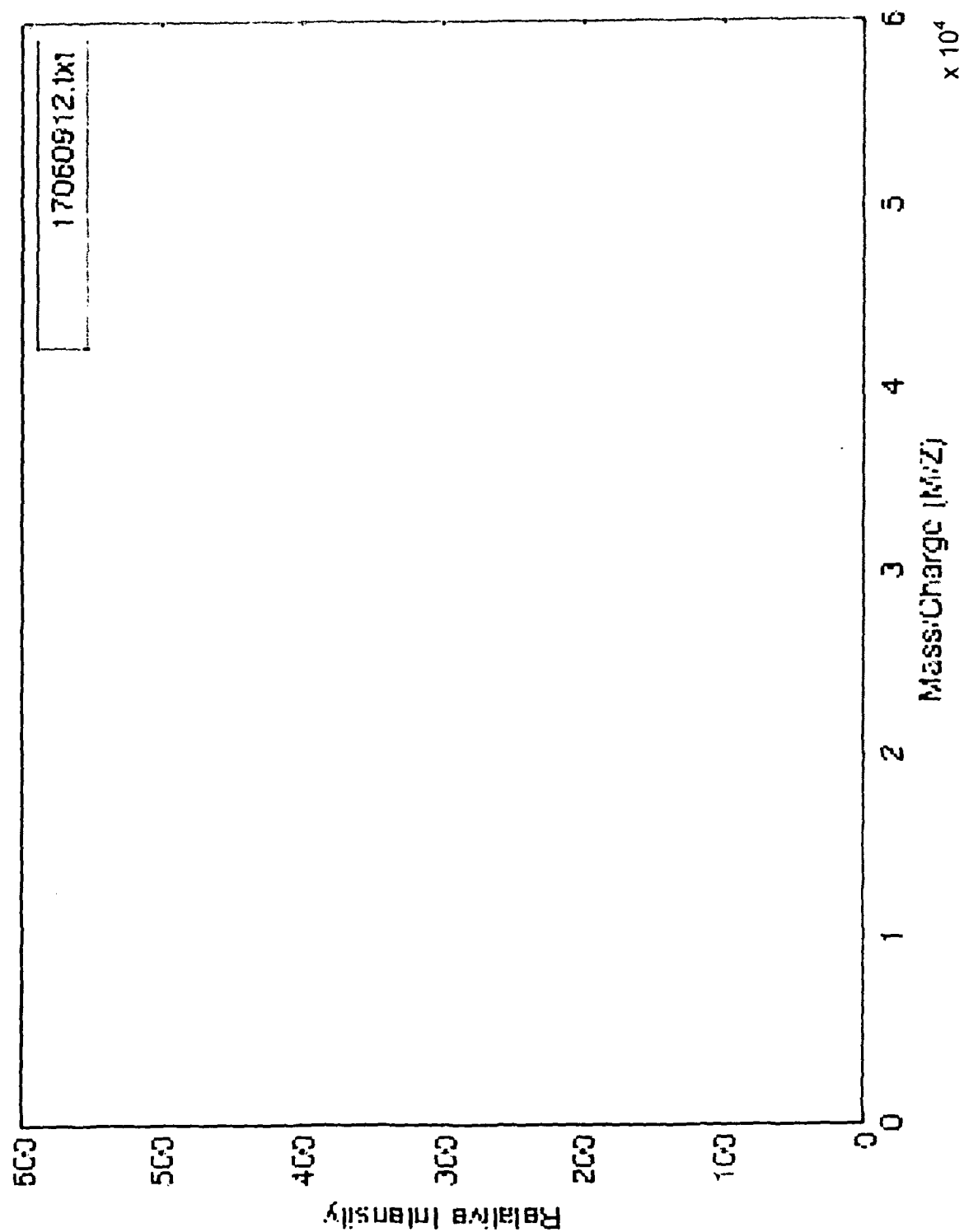


Fig. 1b

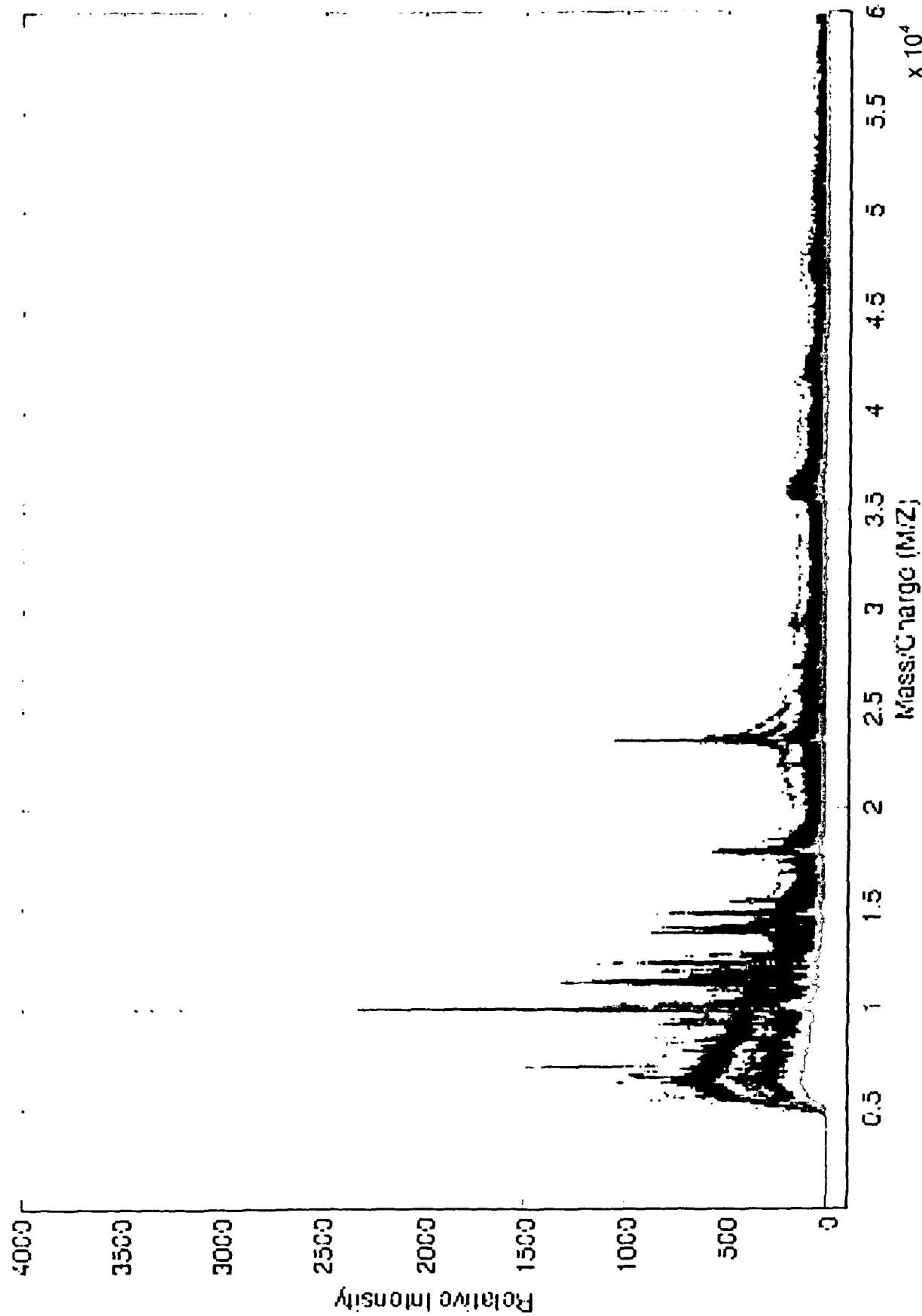


Fig. 2a

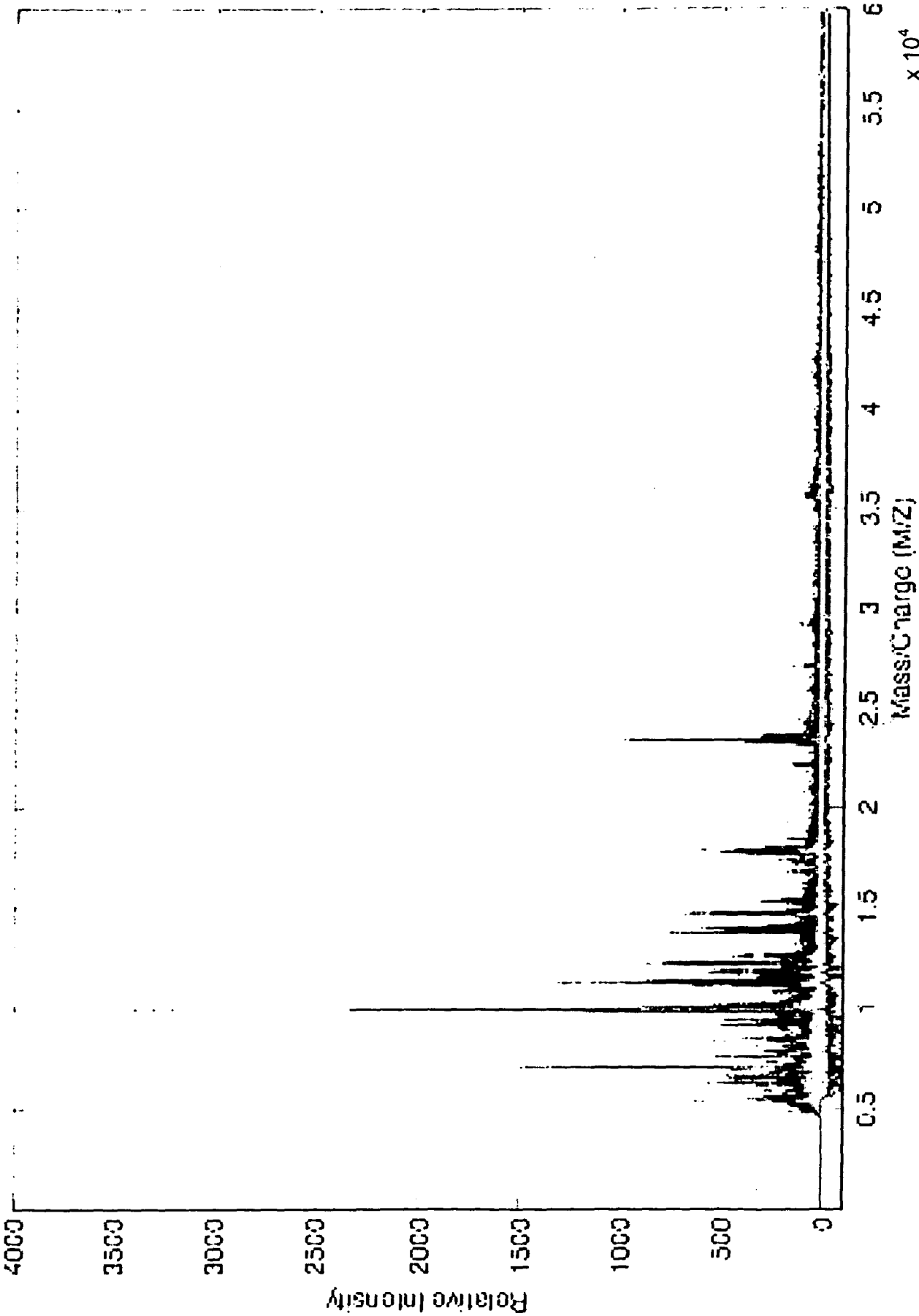


Fig. 2b

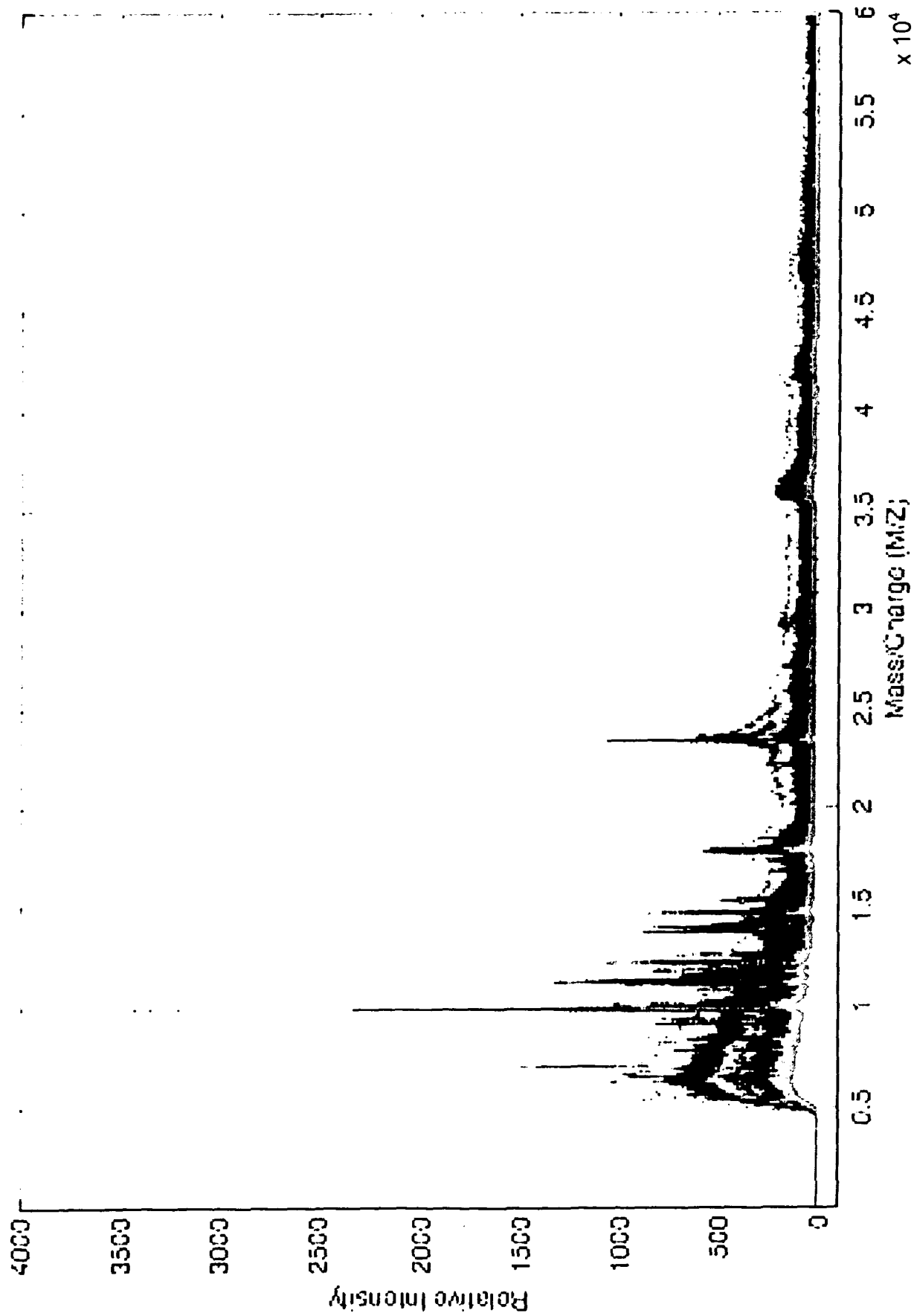


Fig. 3a

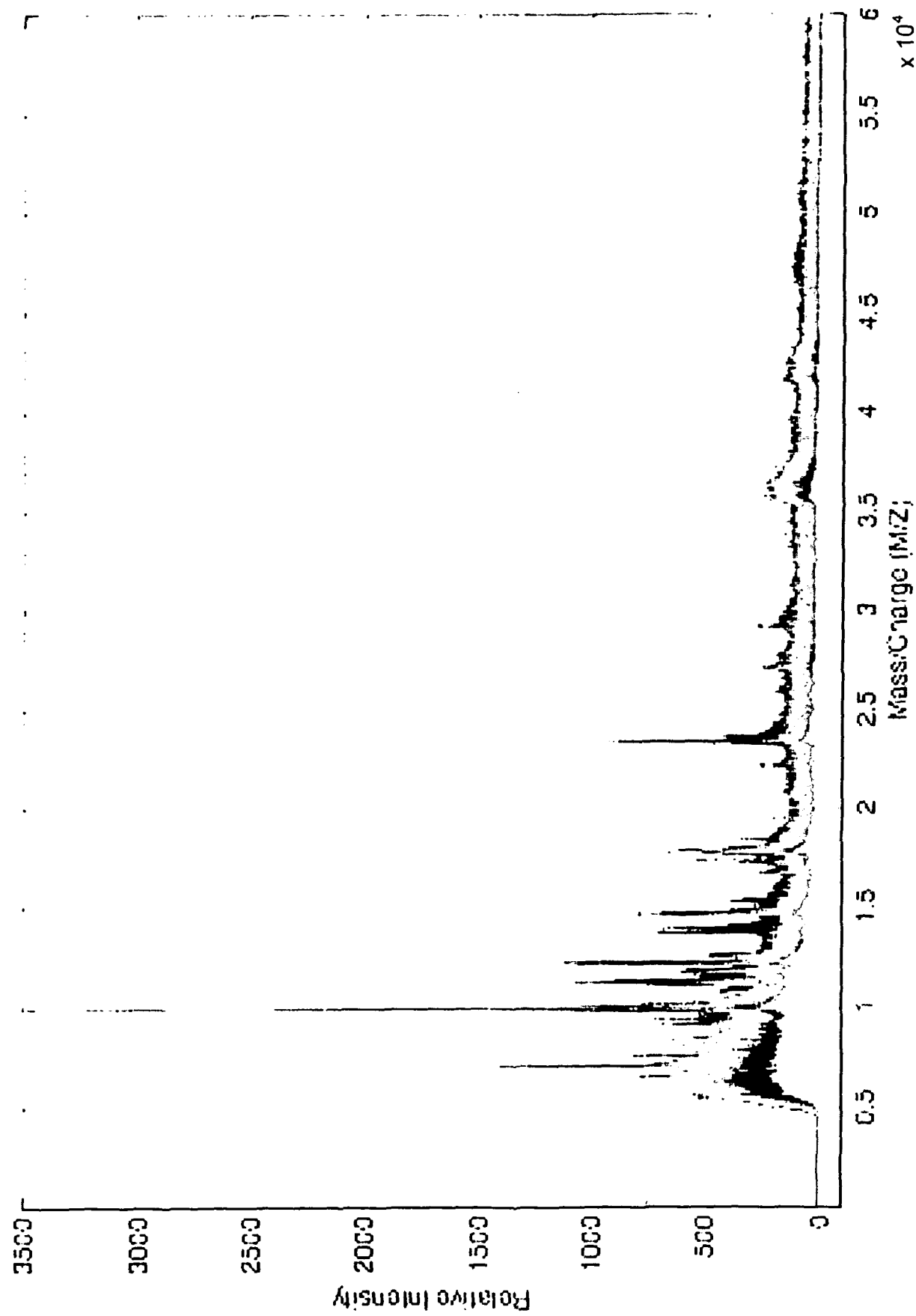


Fig. 3b

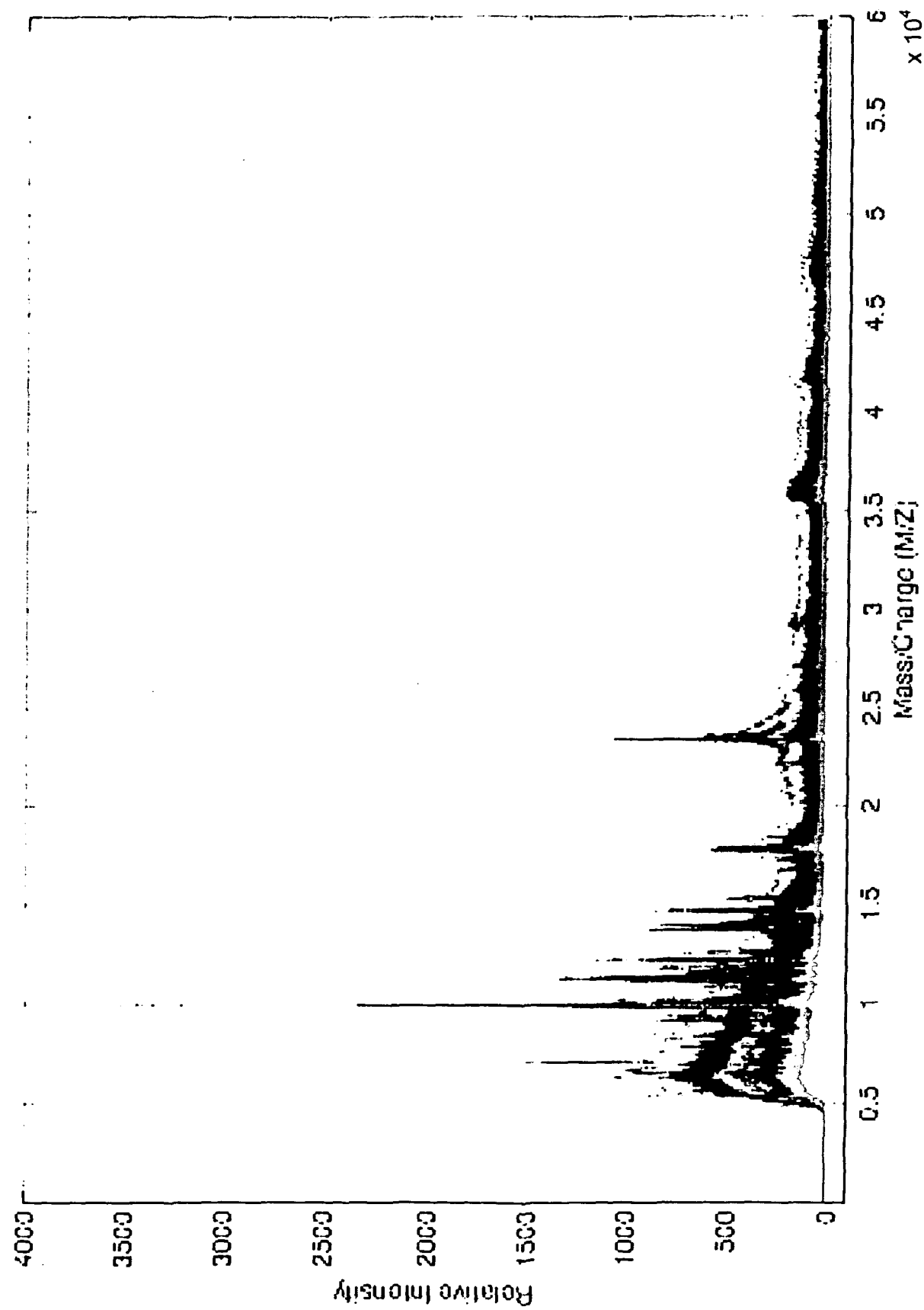


Fig. 4a

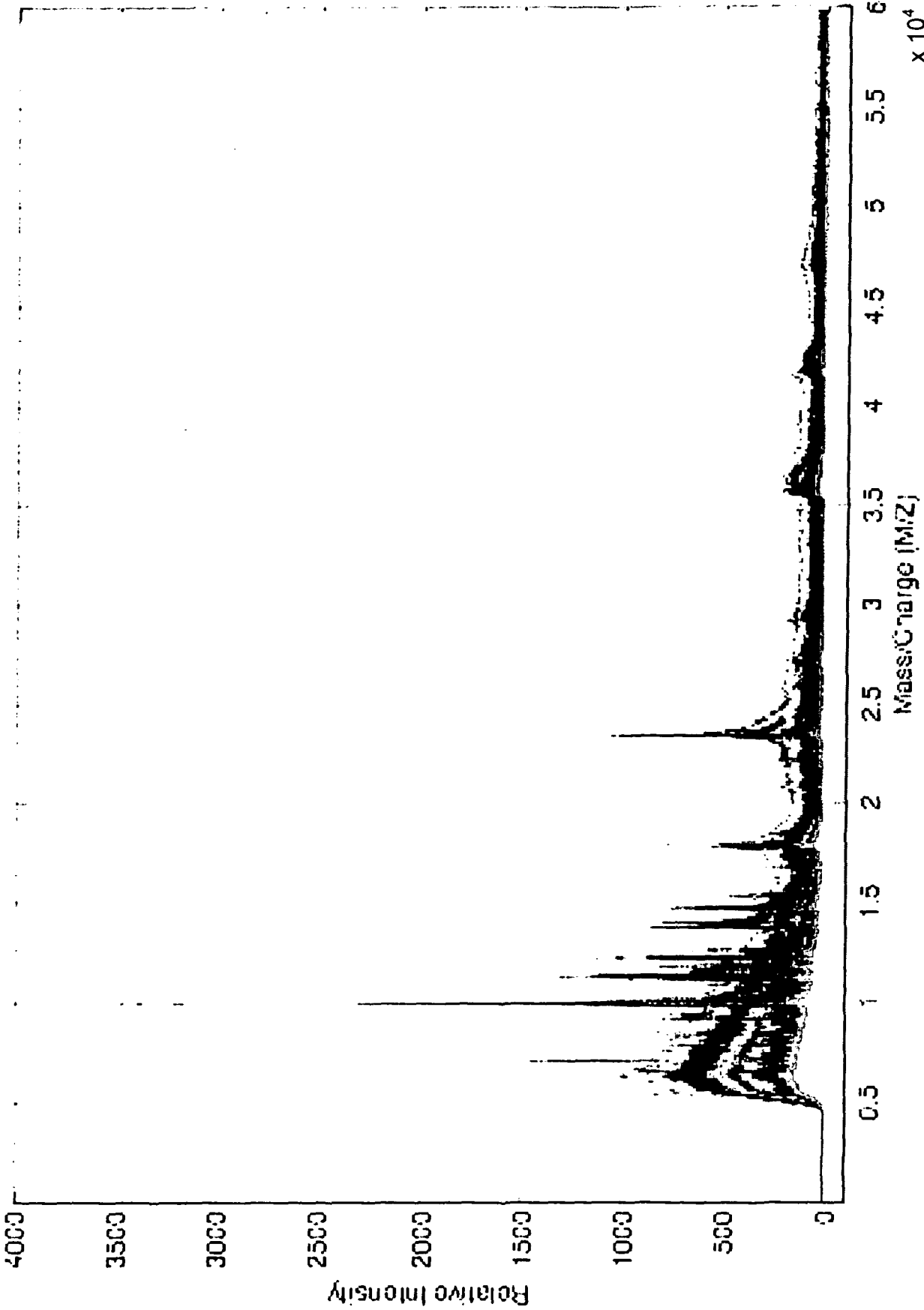


Fig. 4b

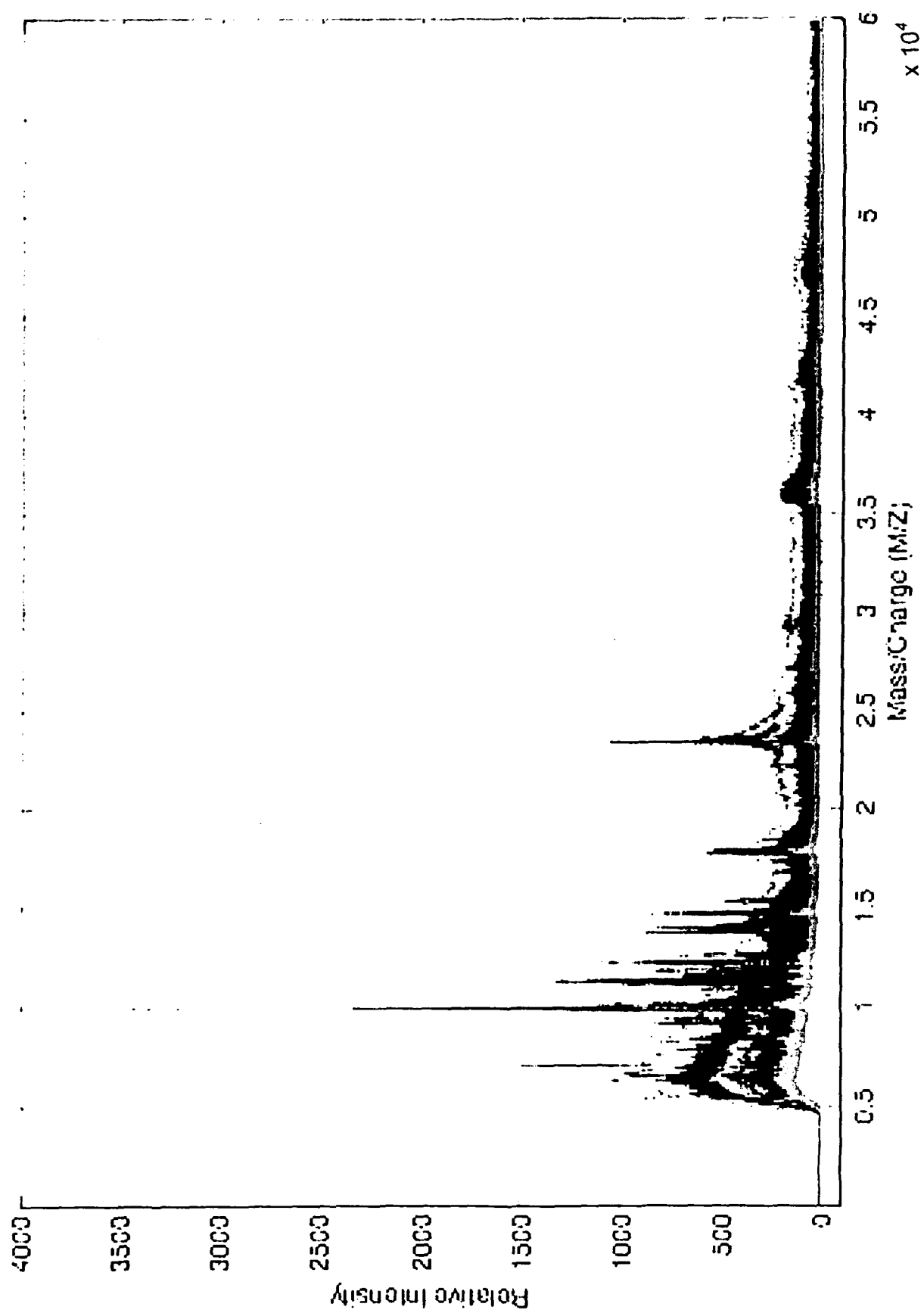


Fig. 5a

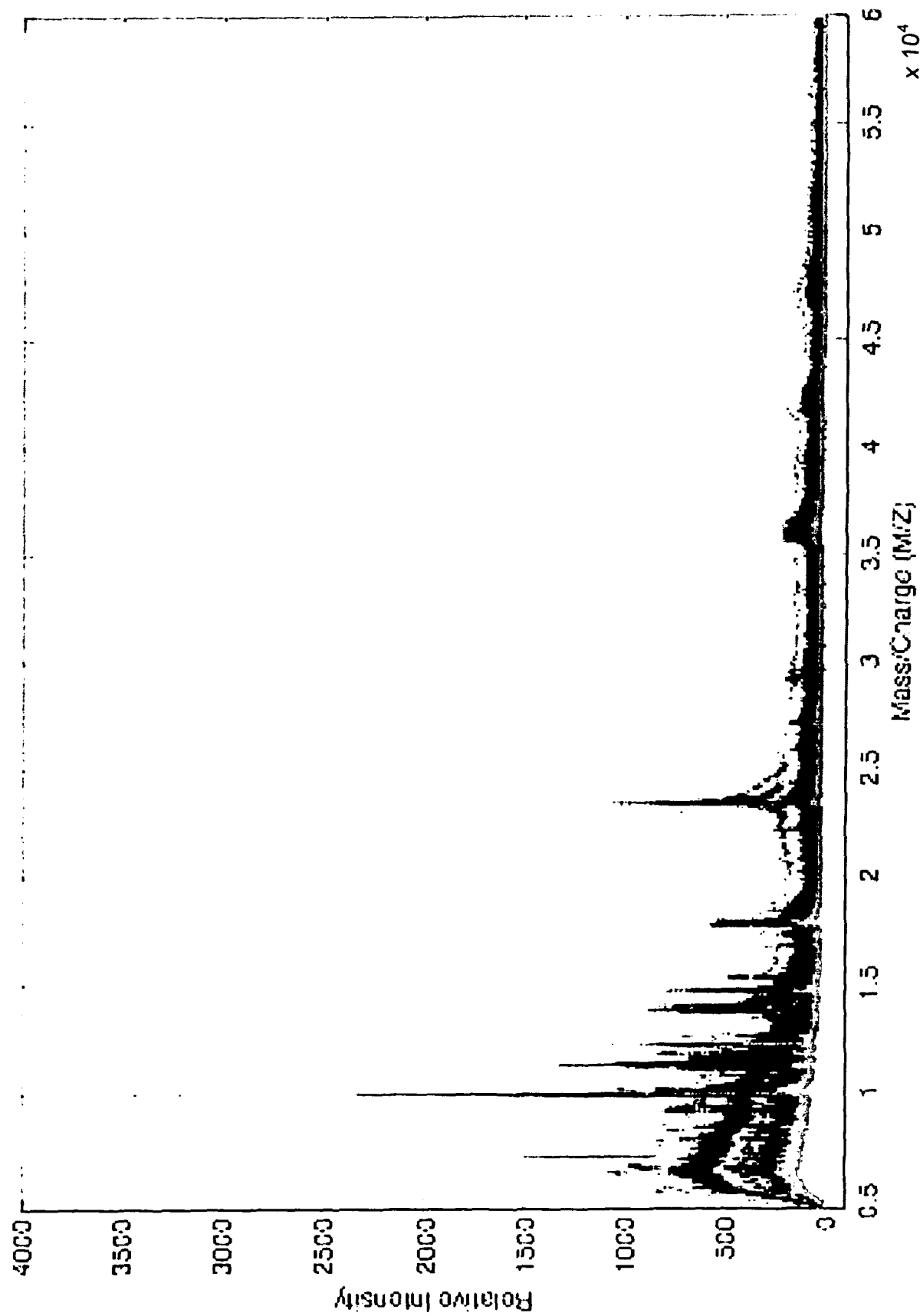


Fig. 5b

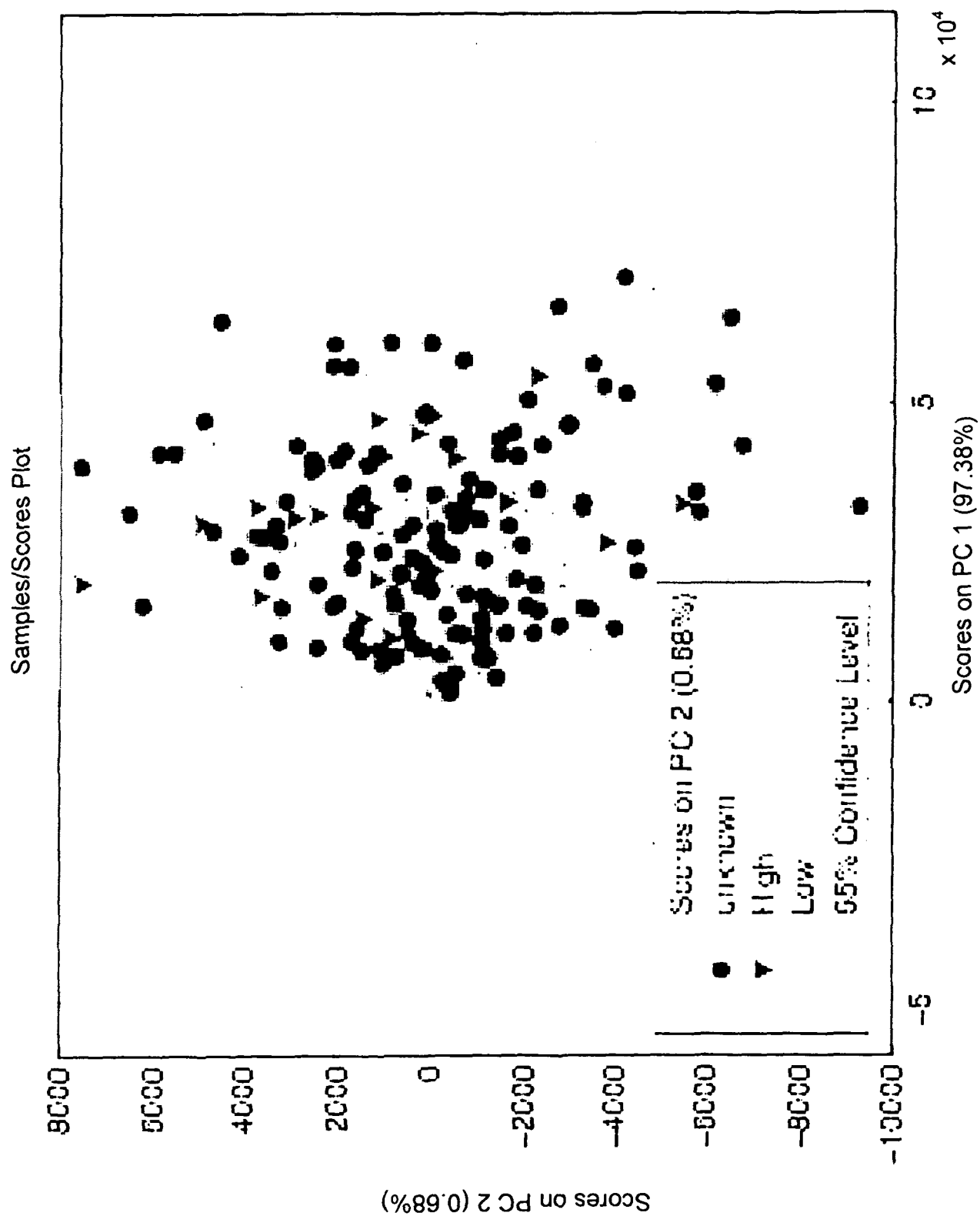


Fig. 6a

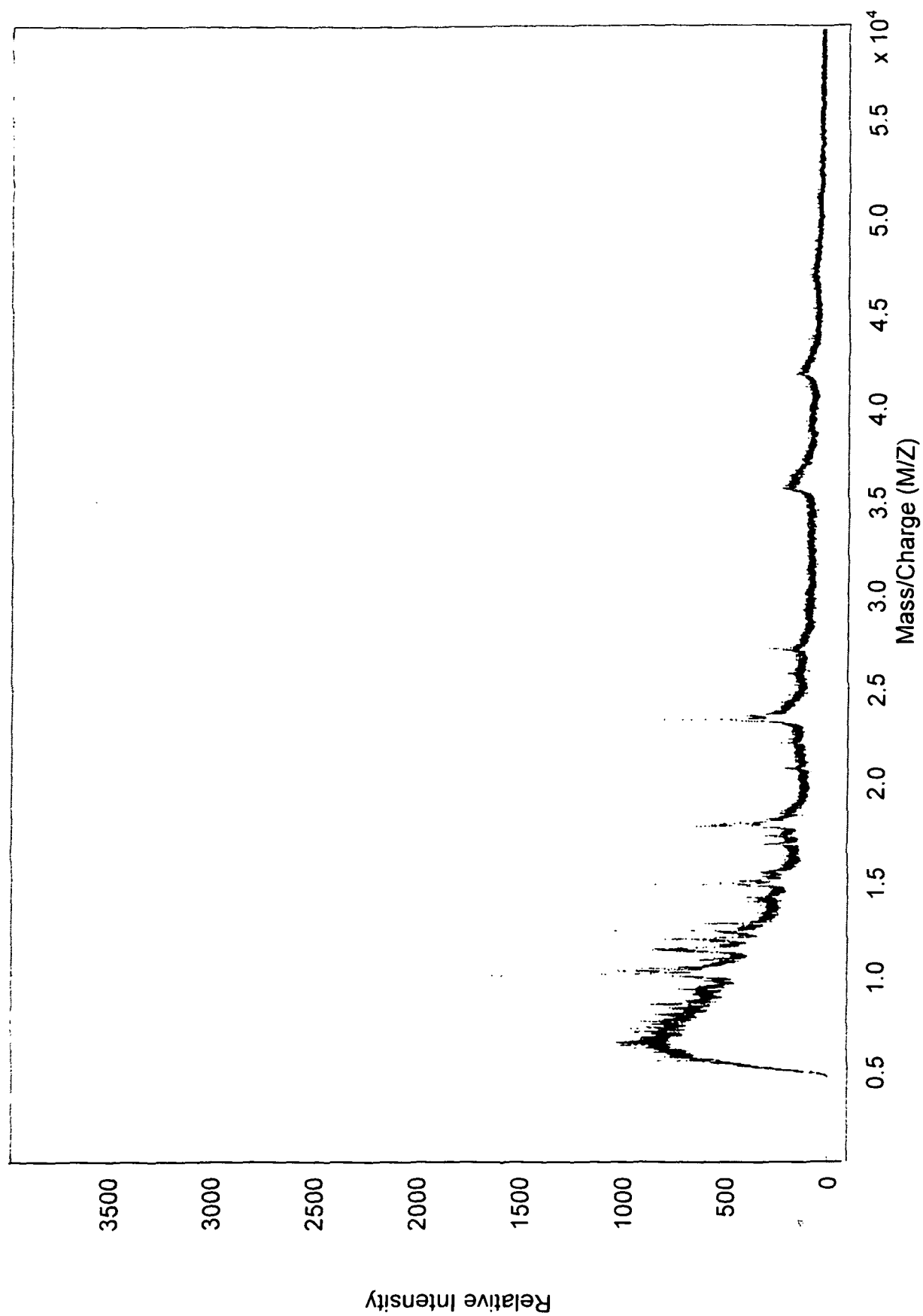


Fig. 6b

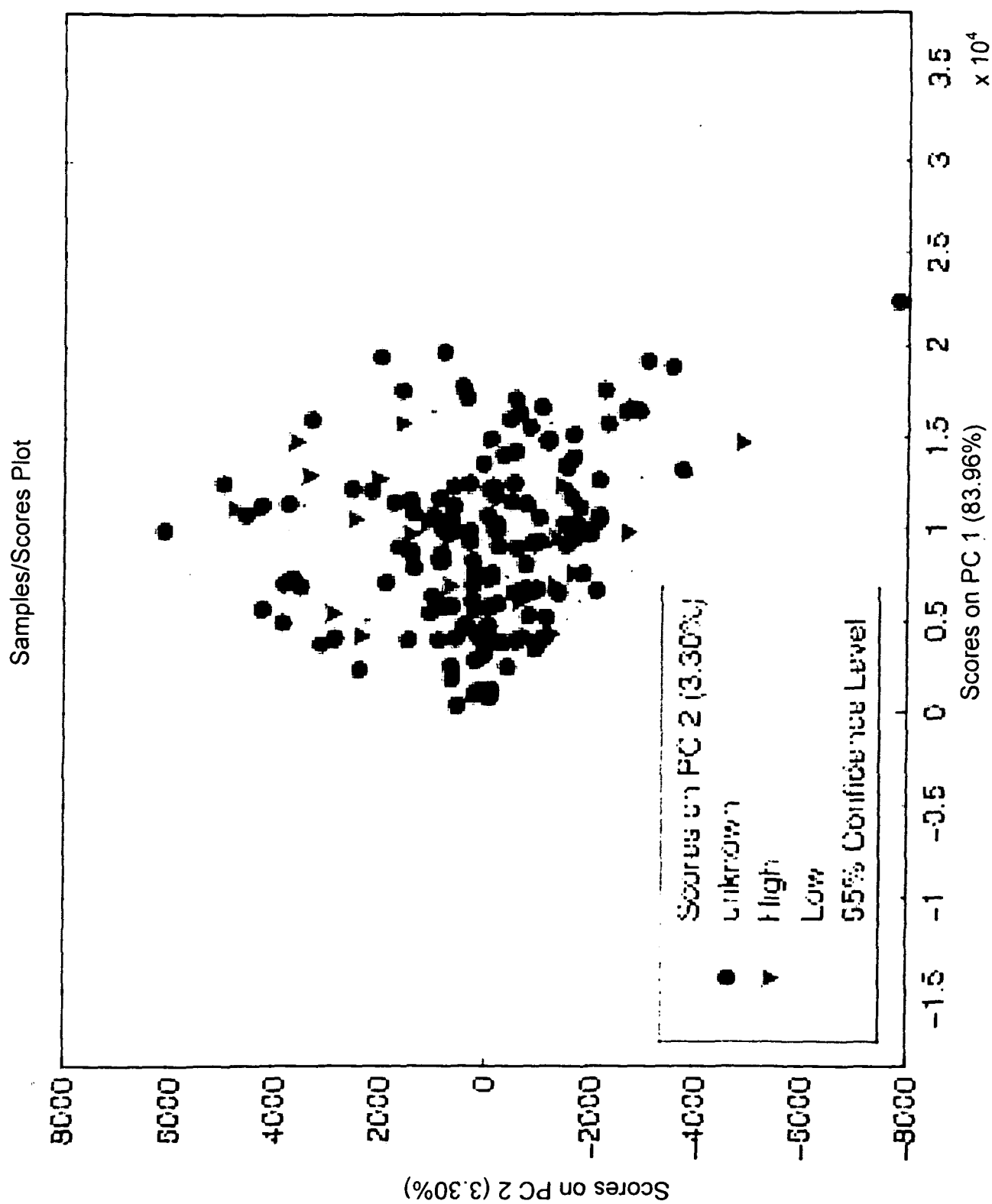


Fig. 7a

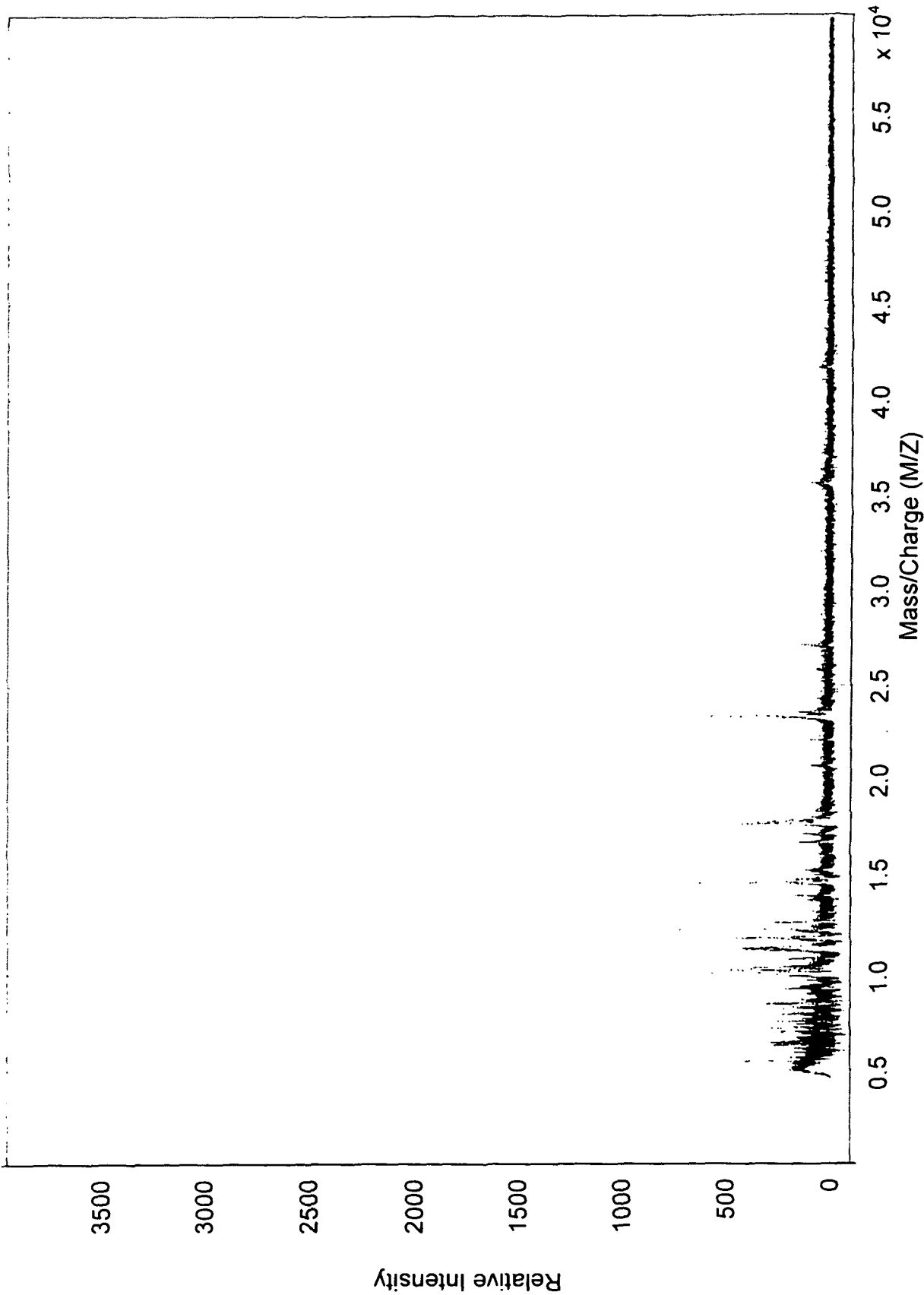


Fig. 7b

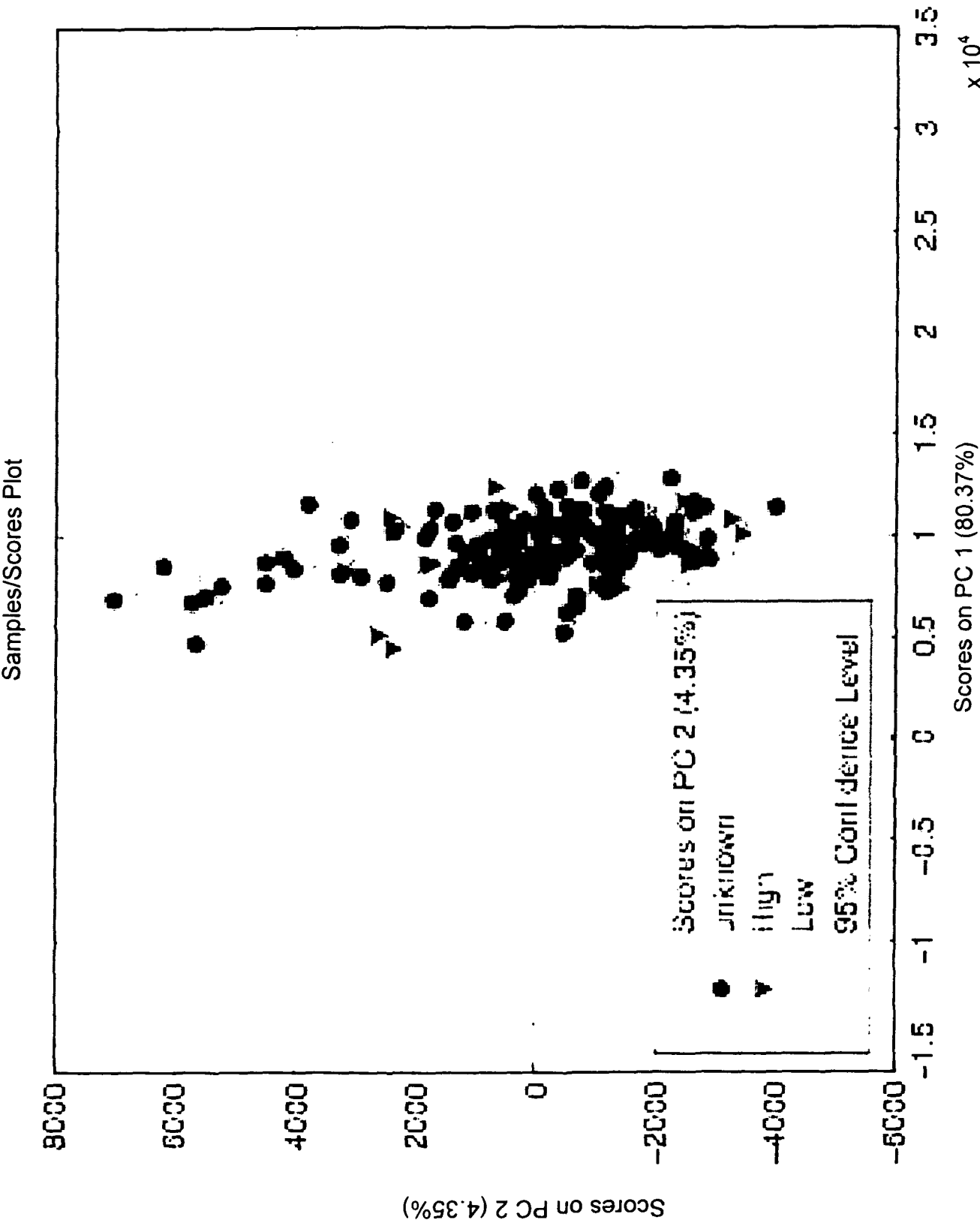


Fig. 8a

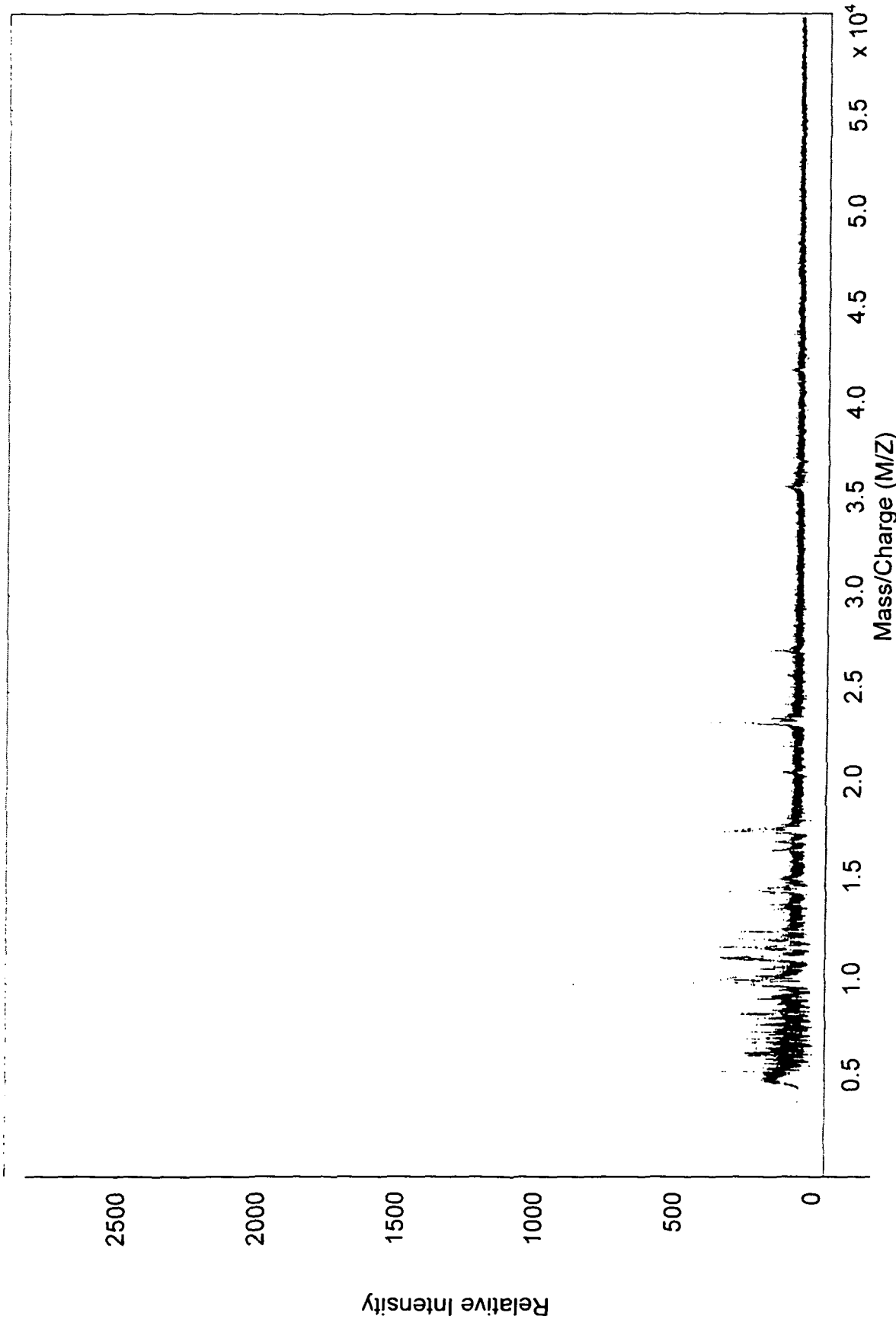


Fig. 8b

Samples/Scores Plot

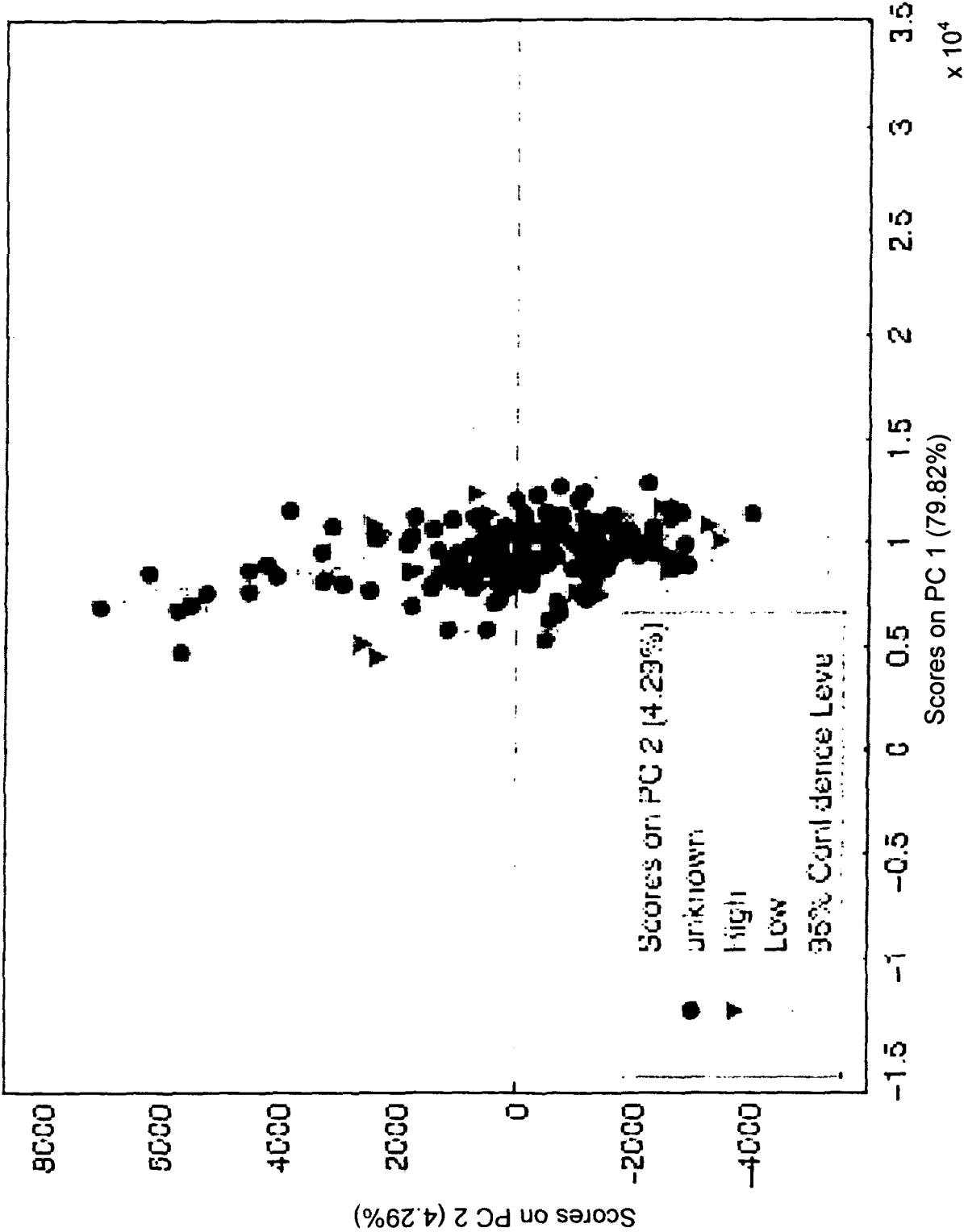


Fig. 9a

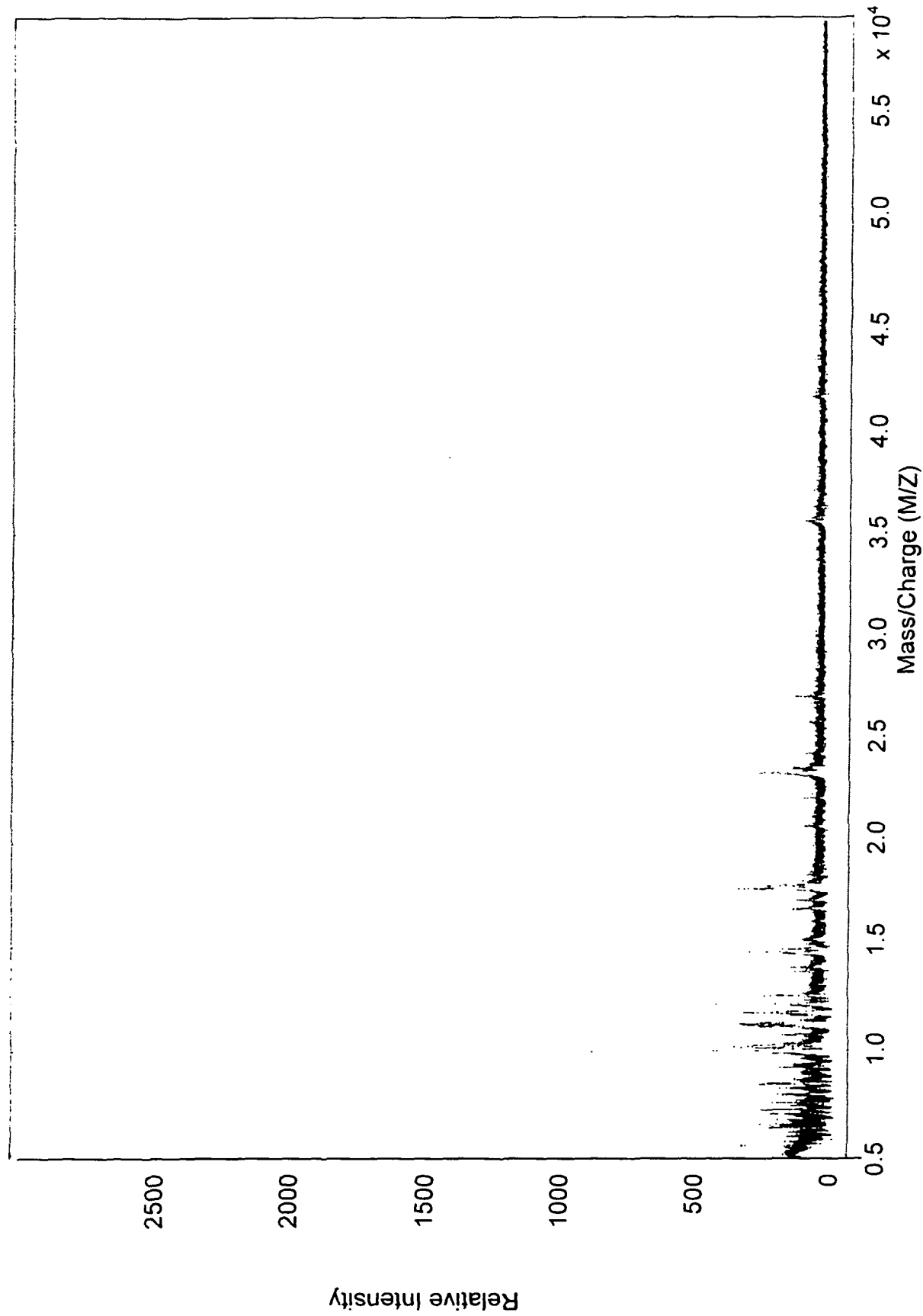


Fig. 9b

Fig. 10

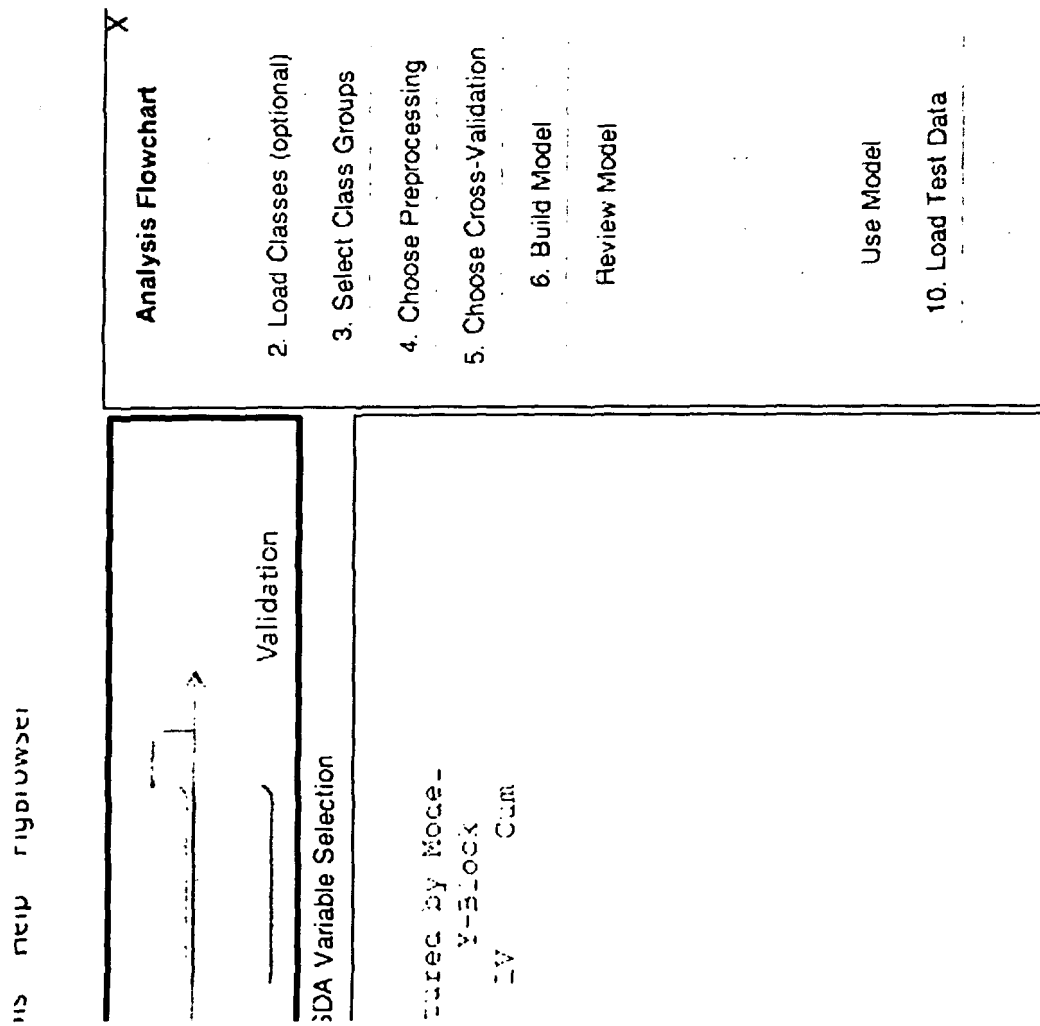


Fig. 12

PLSDA Class Groups

Help FigBrowser

Available Classes

Low

Class Groups

[Medium]

Model As Group

Remove Group

Default

OK

Cancel

Preprocessing X-block

Available Methods	All	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. 13

Fig. 14

Cross-Val Method	Cross-Validation
☐ leave one out	
☐ venetian blinds	
☐ contiguous block	
☐ random subsets	
☐ custom	

Close

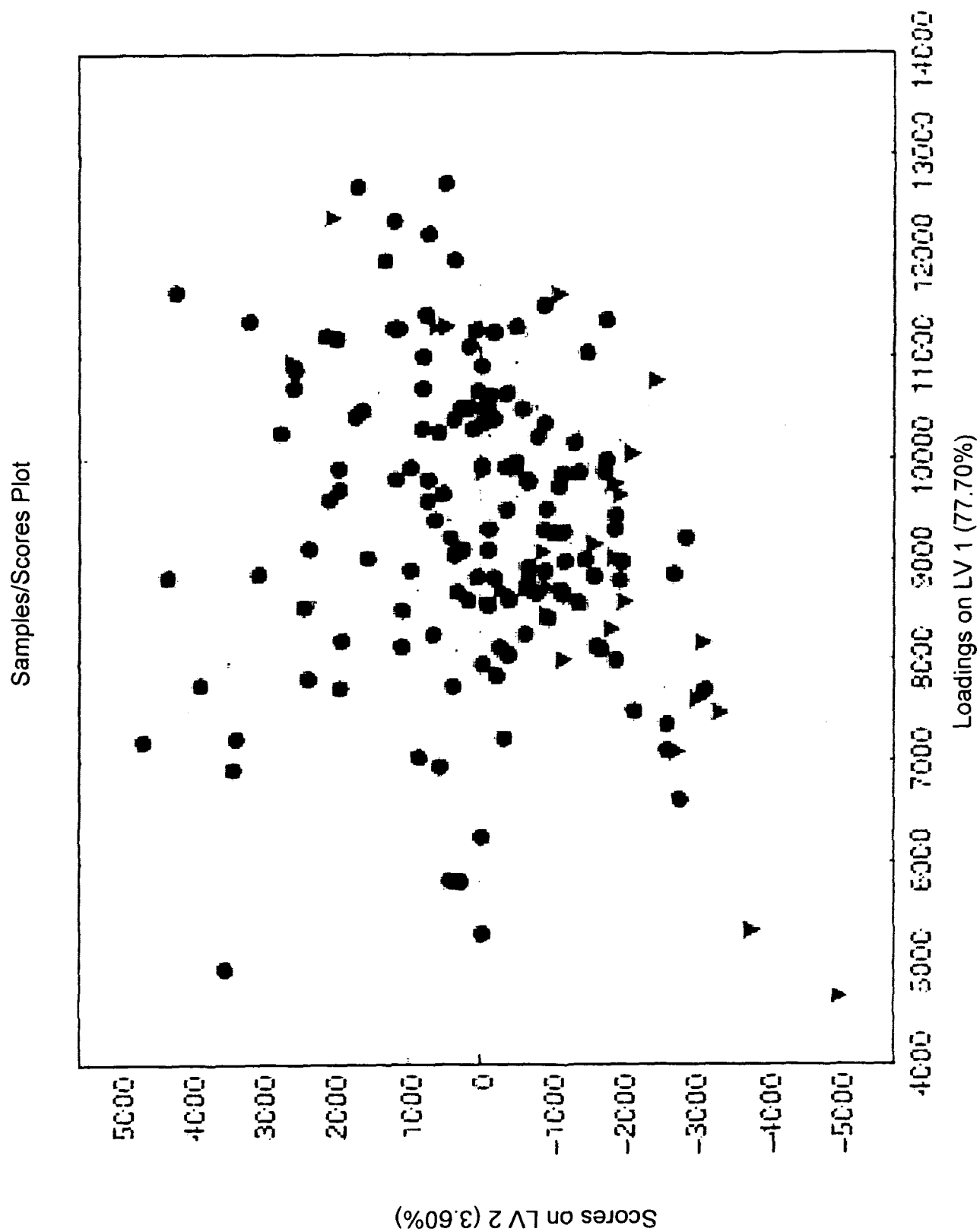


Fig. 15a

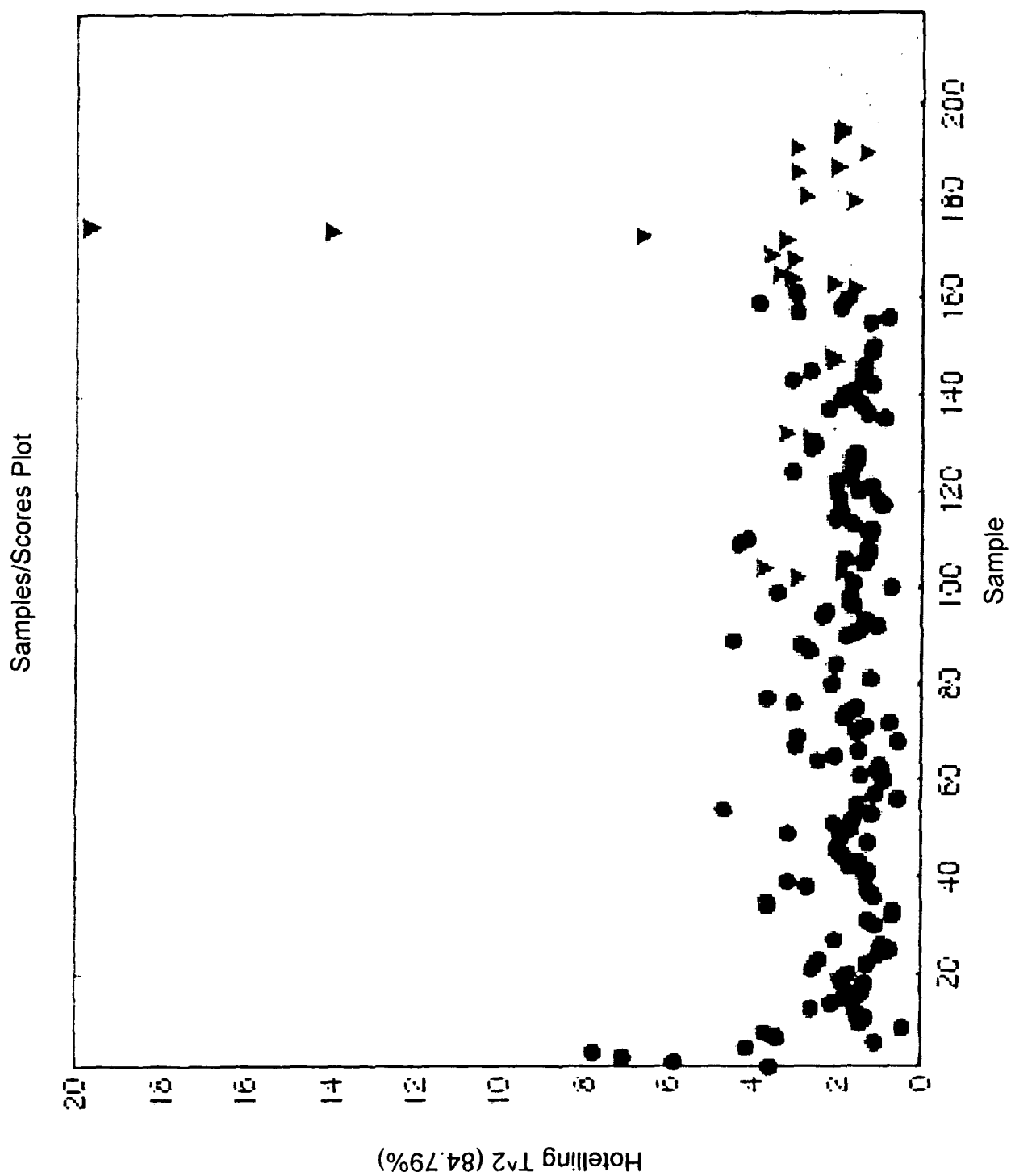


Fig. 15b

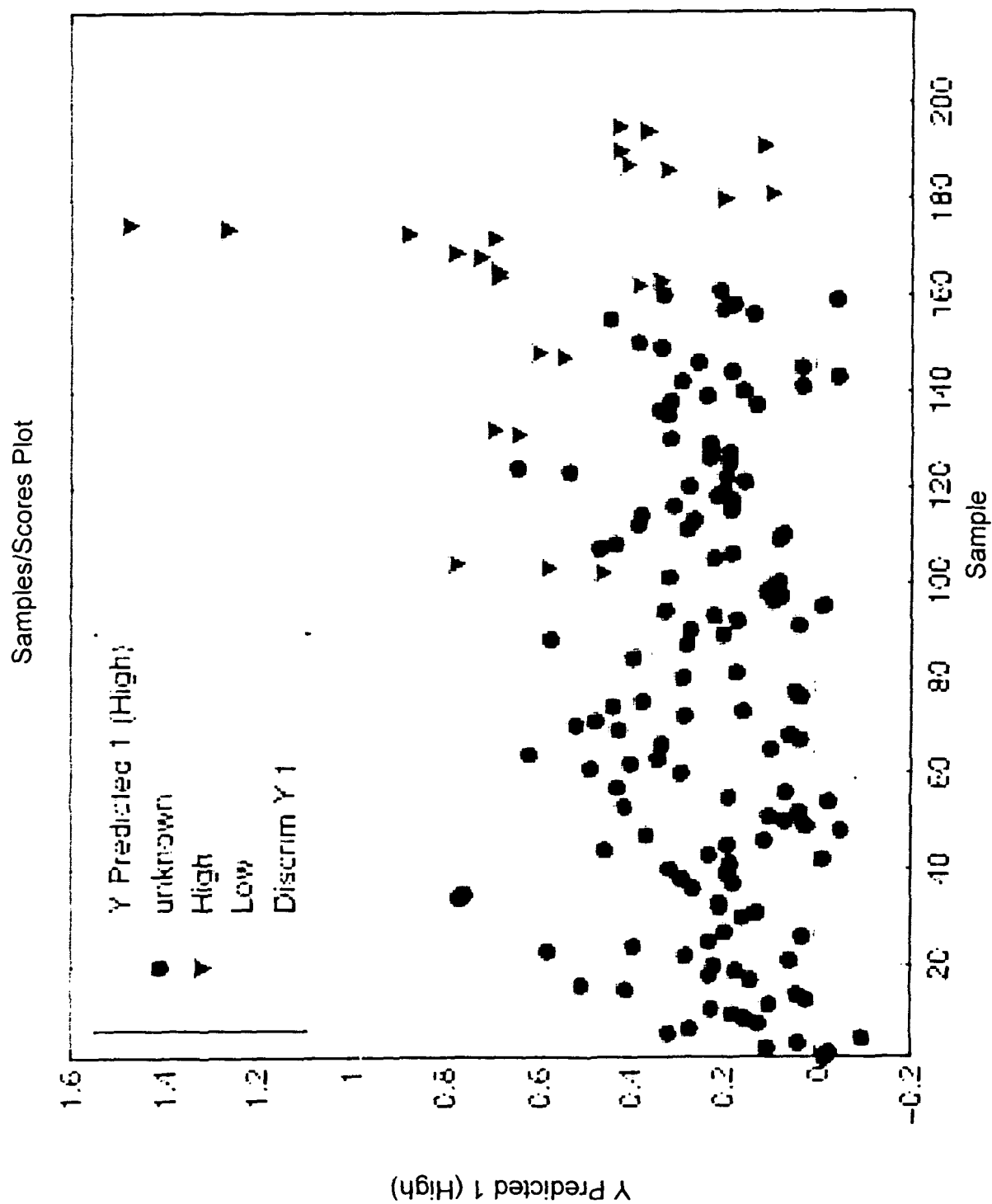


Fig. 15c

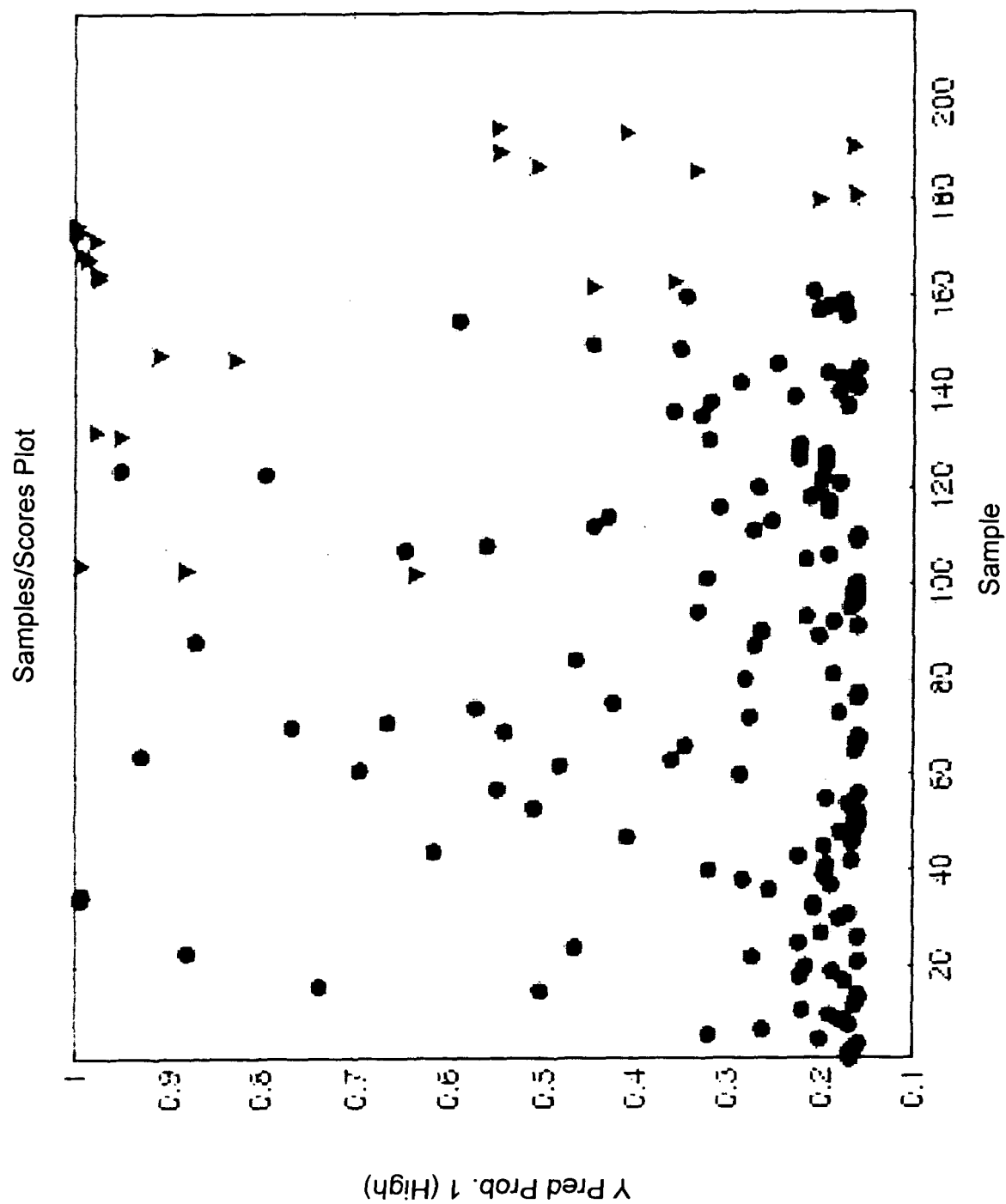


Fig. 15d

Variables/Loadings Plot

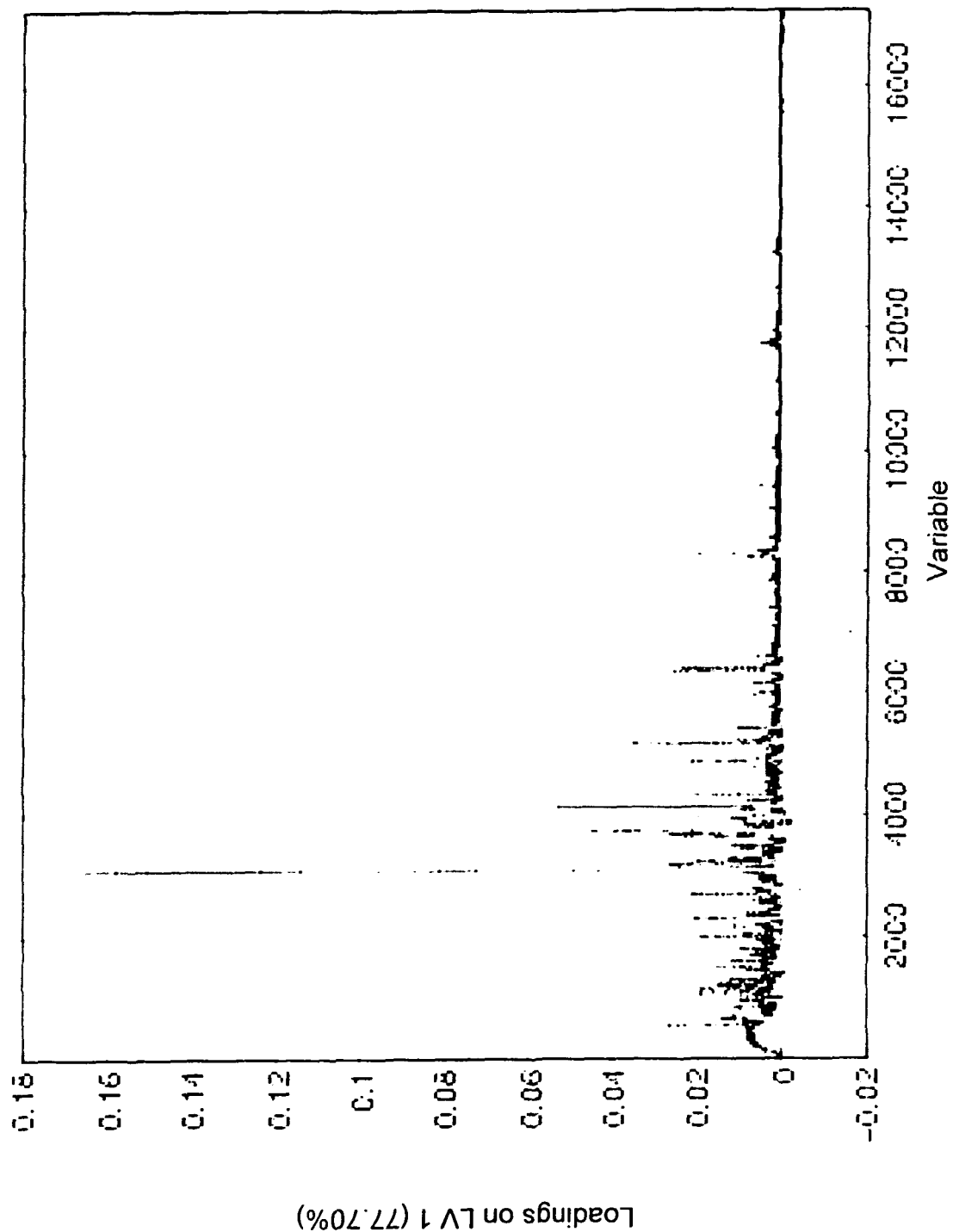


Fig. 16a

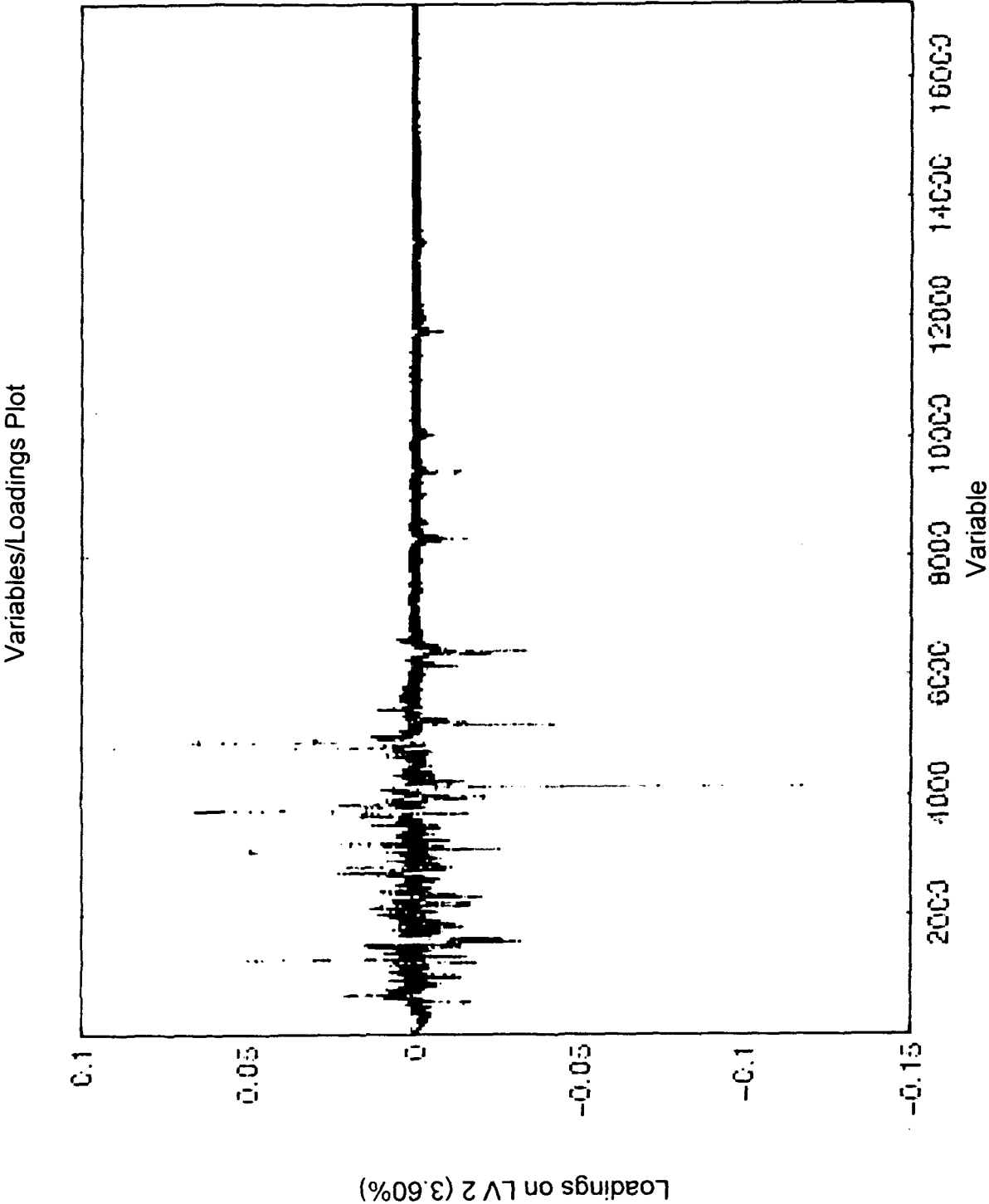


Fig. 16b

Fig. 17

Figure 1. Samples/Scores - PLSDA S LVs - data

PlotGUI

FigBrowser

Help

Window

Desktop

Tools

Insert

View

Edit

File

Samples/Scores Plot

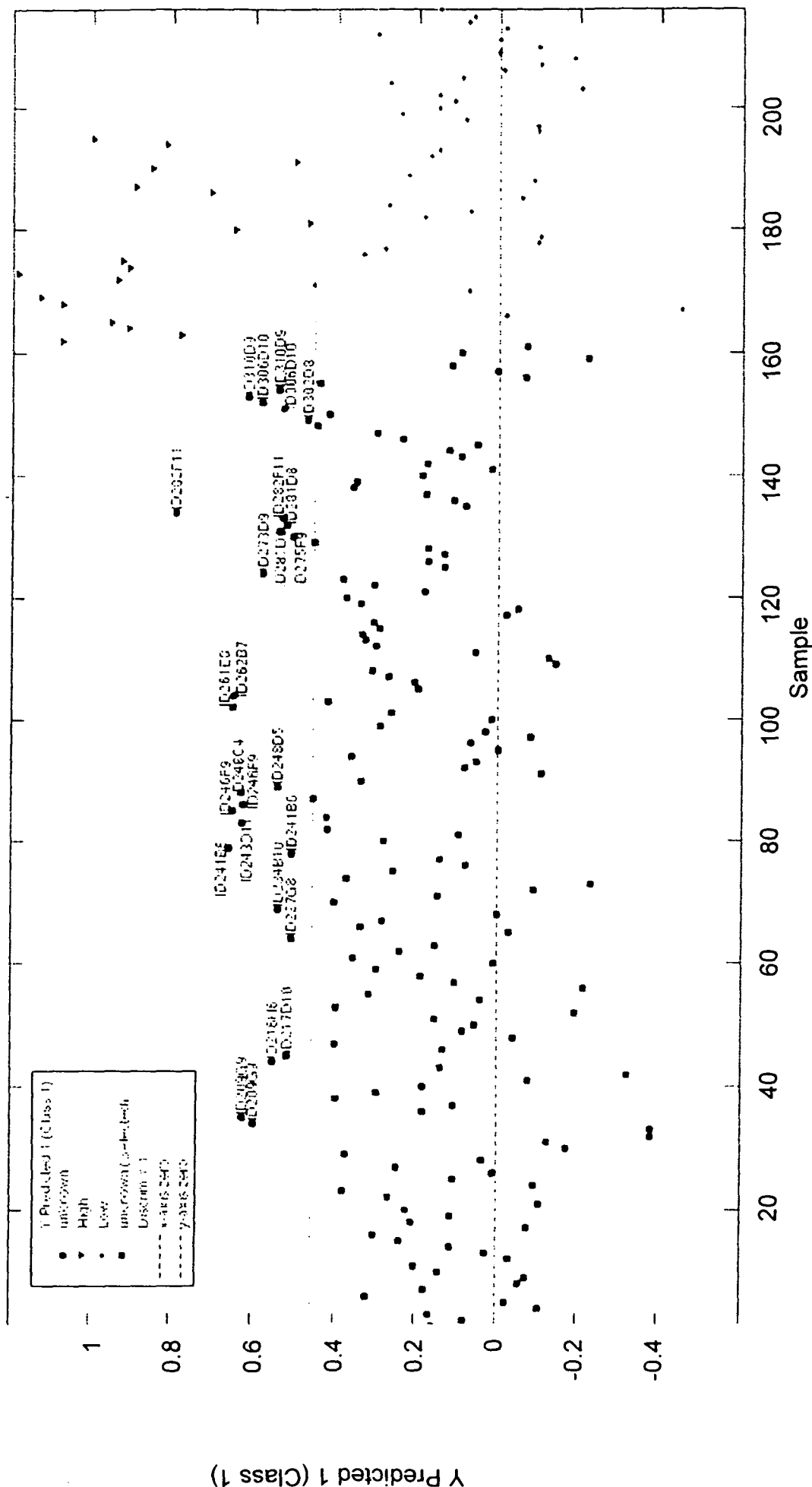


Fig. 18

Figure 1. Samples/Scores - PLSDA 5 LVs -

File Edit View Insert Tools Desktop Window Help FigBrowser PlotGUI



Samples/Scores Plot

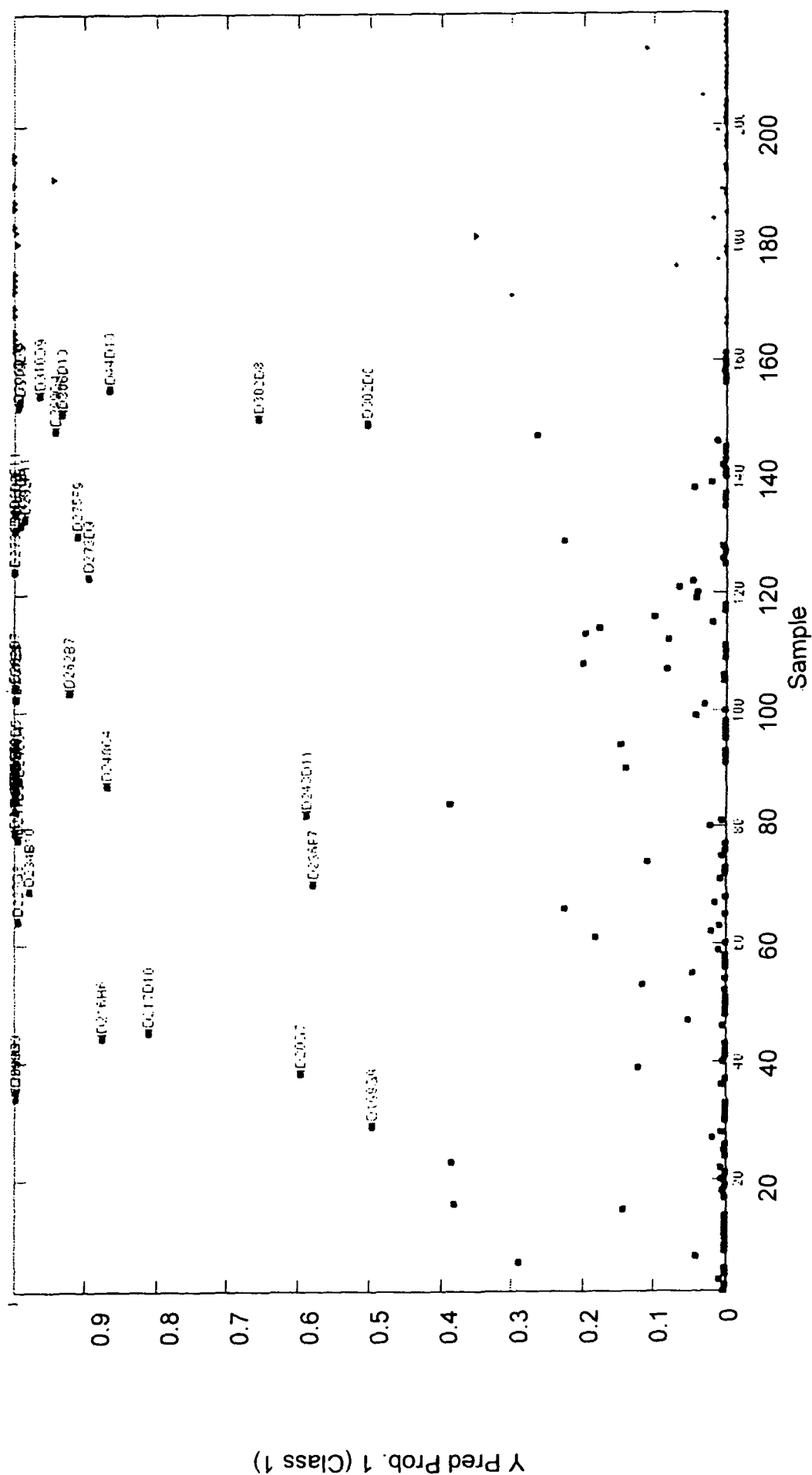
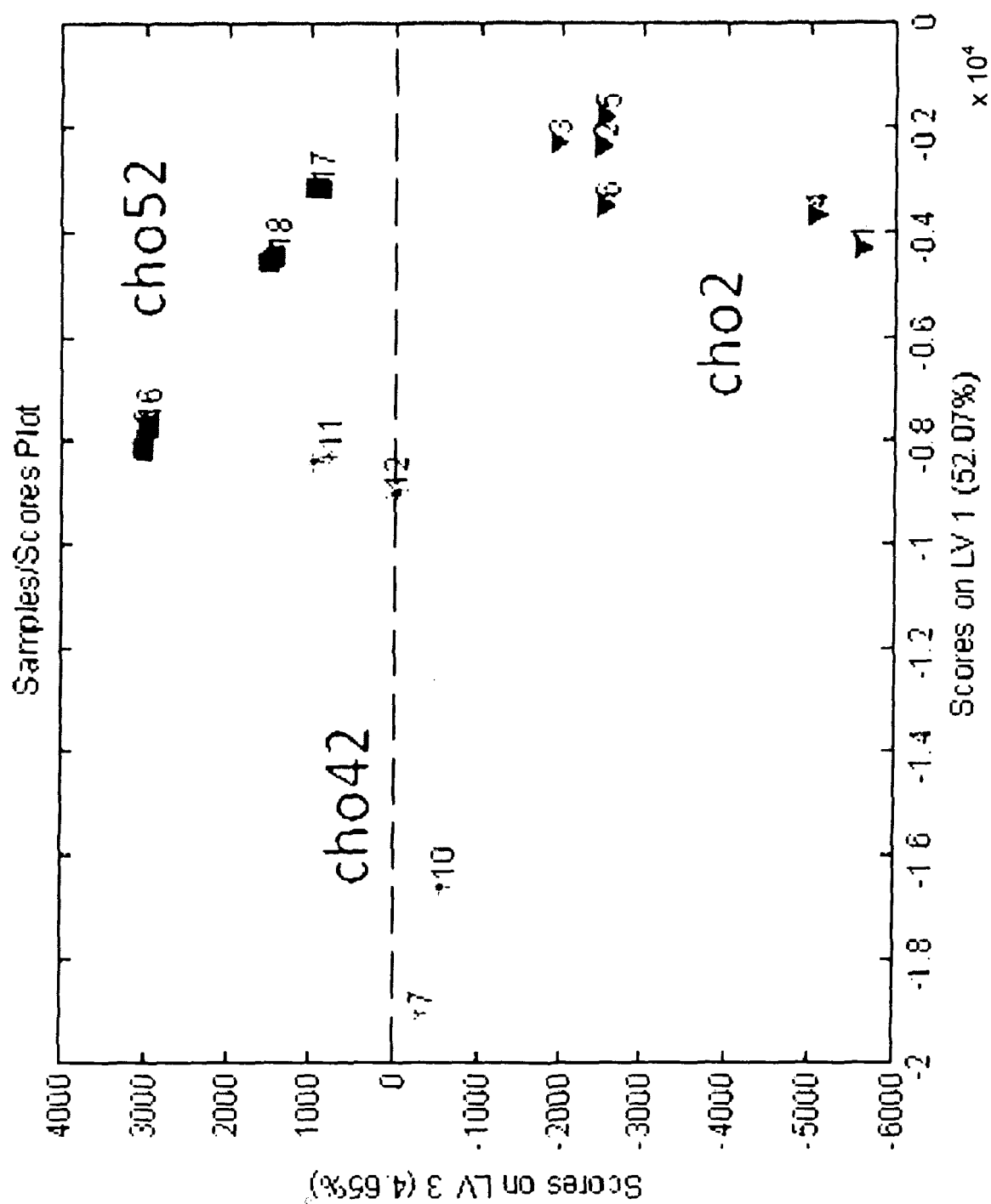


Fig. 19a



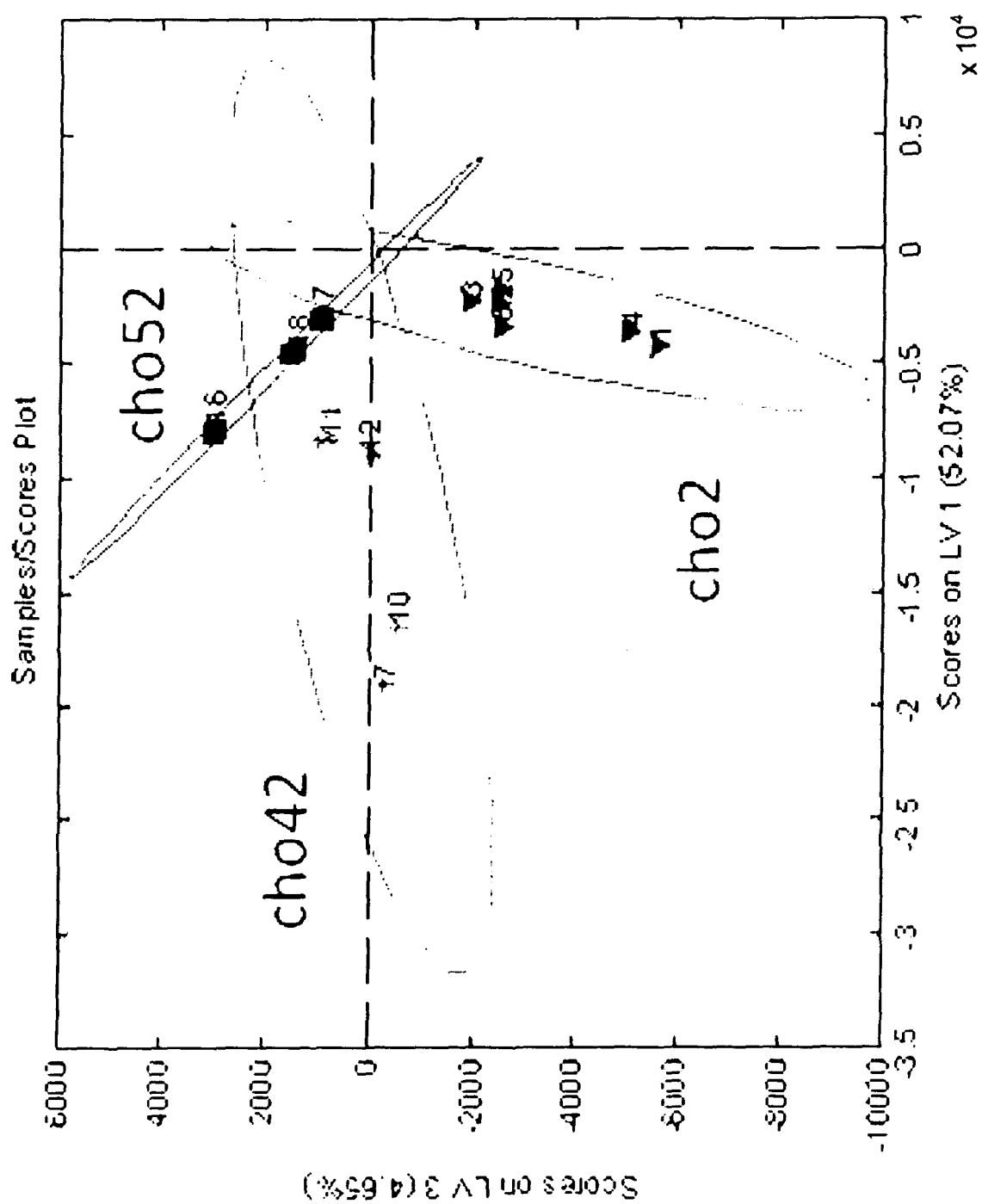


Fig. 19b

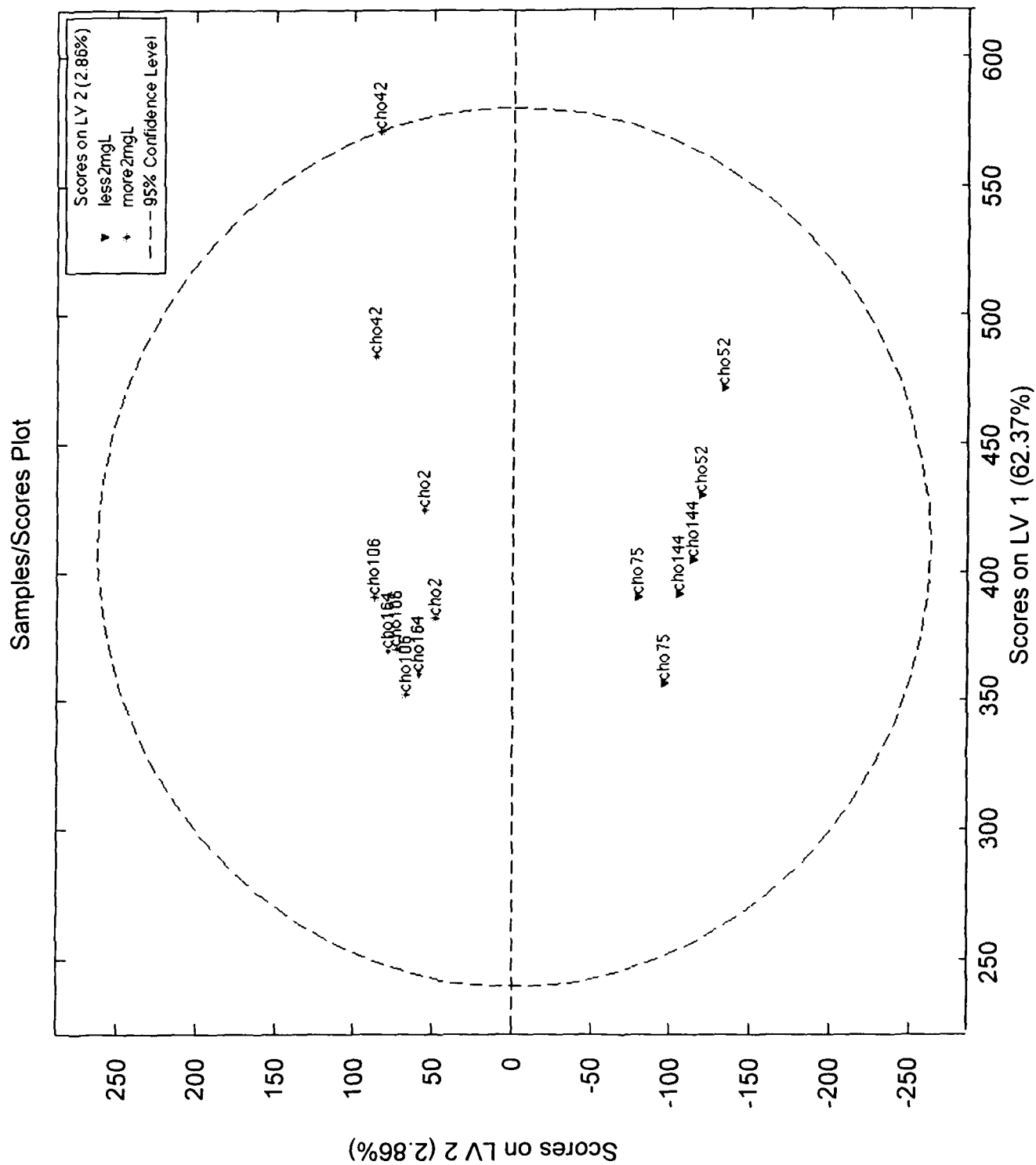


Fig. 20

Fig. 21a

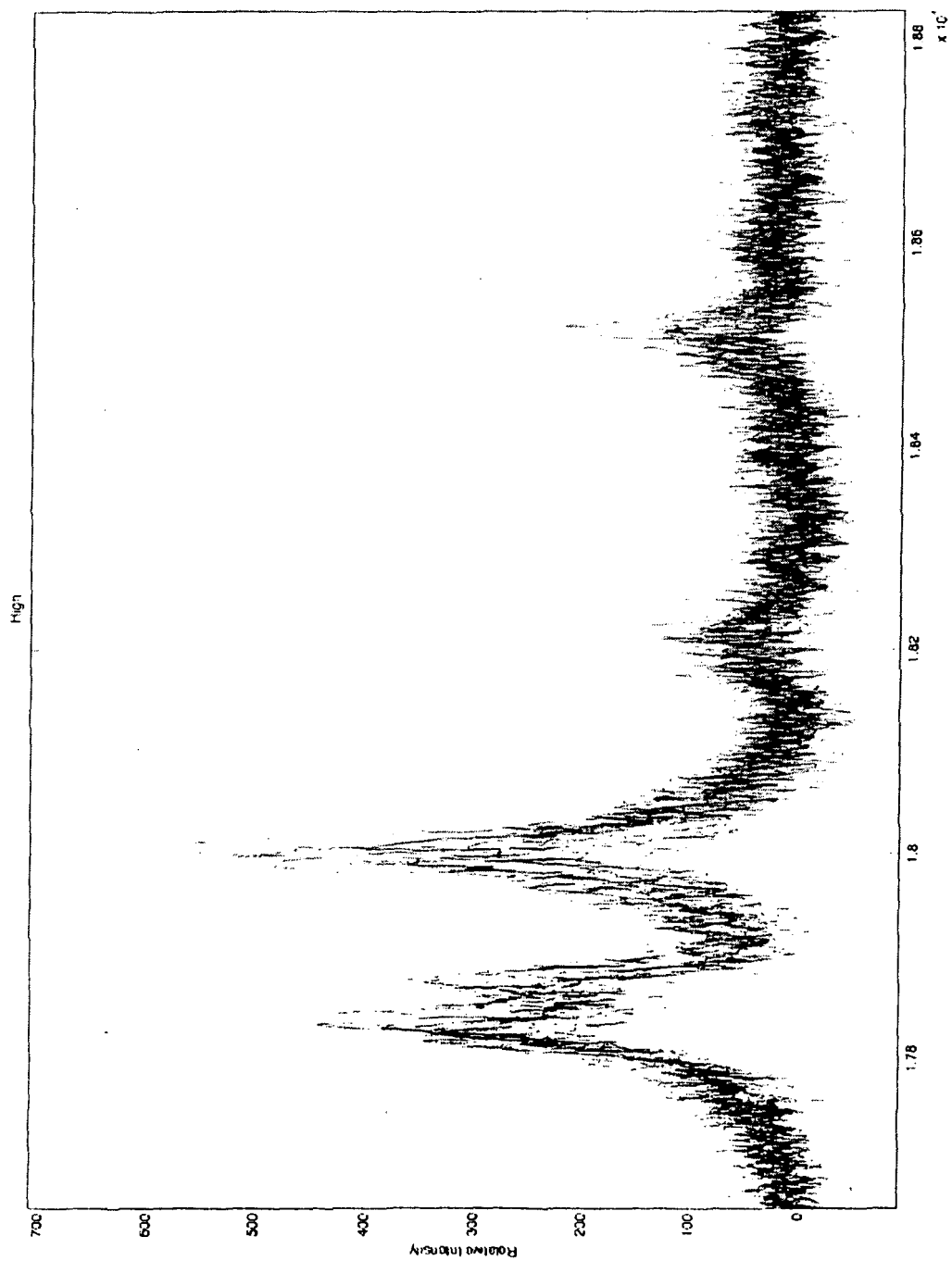


Fig. 21b

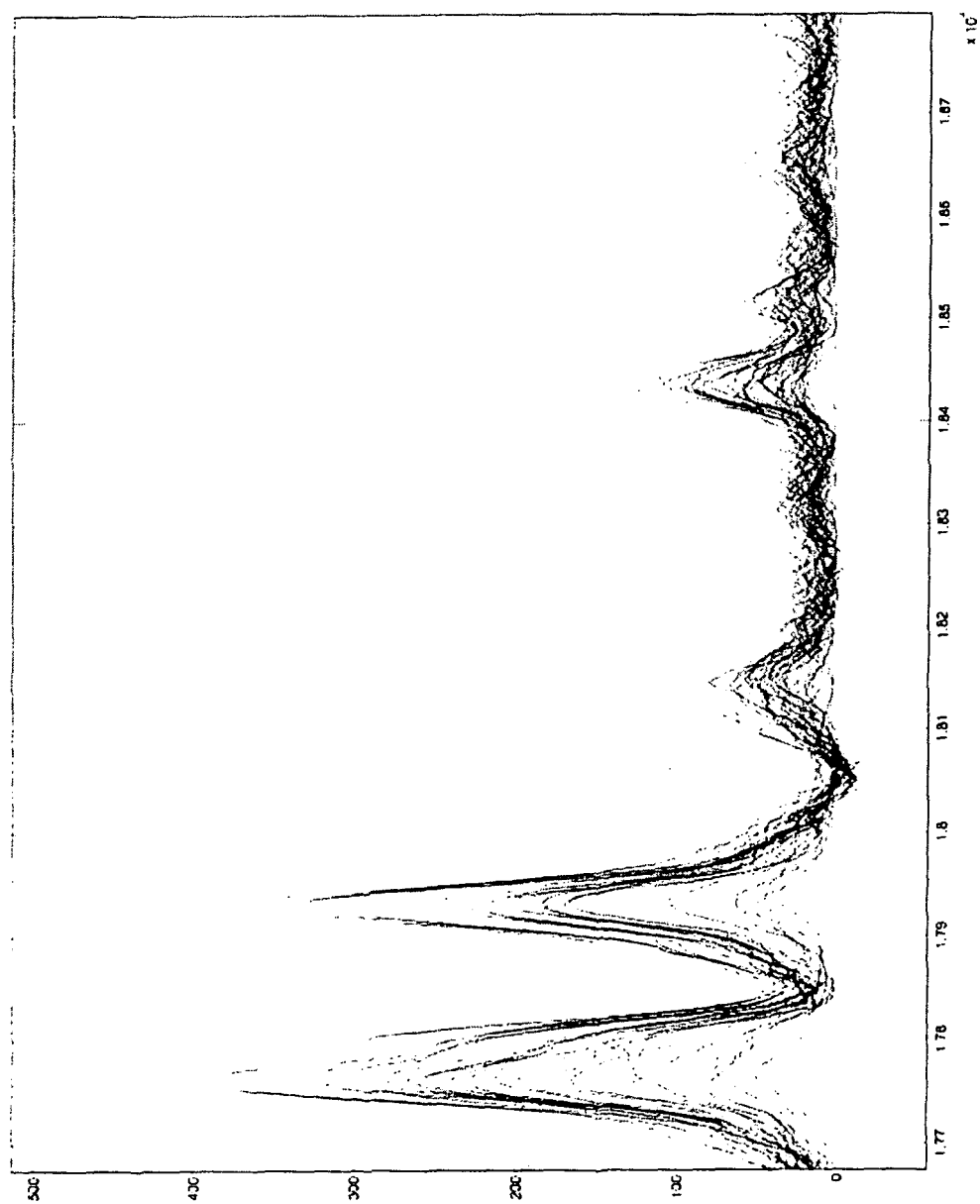


Fig. 22

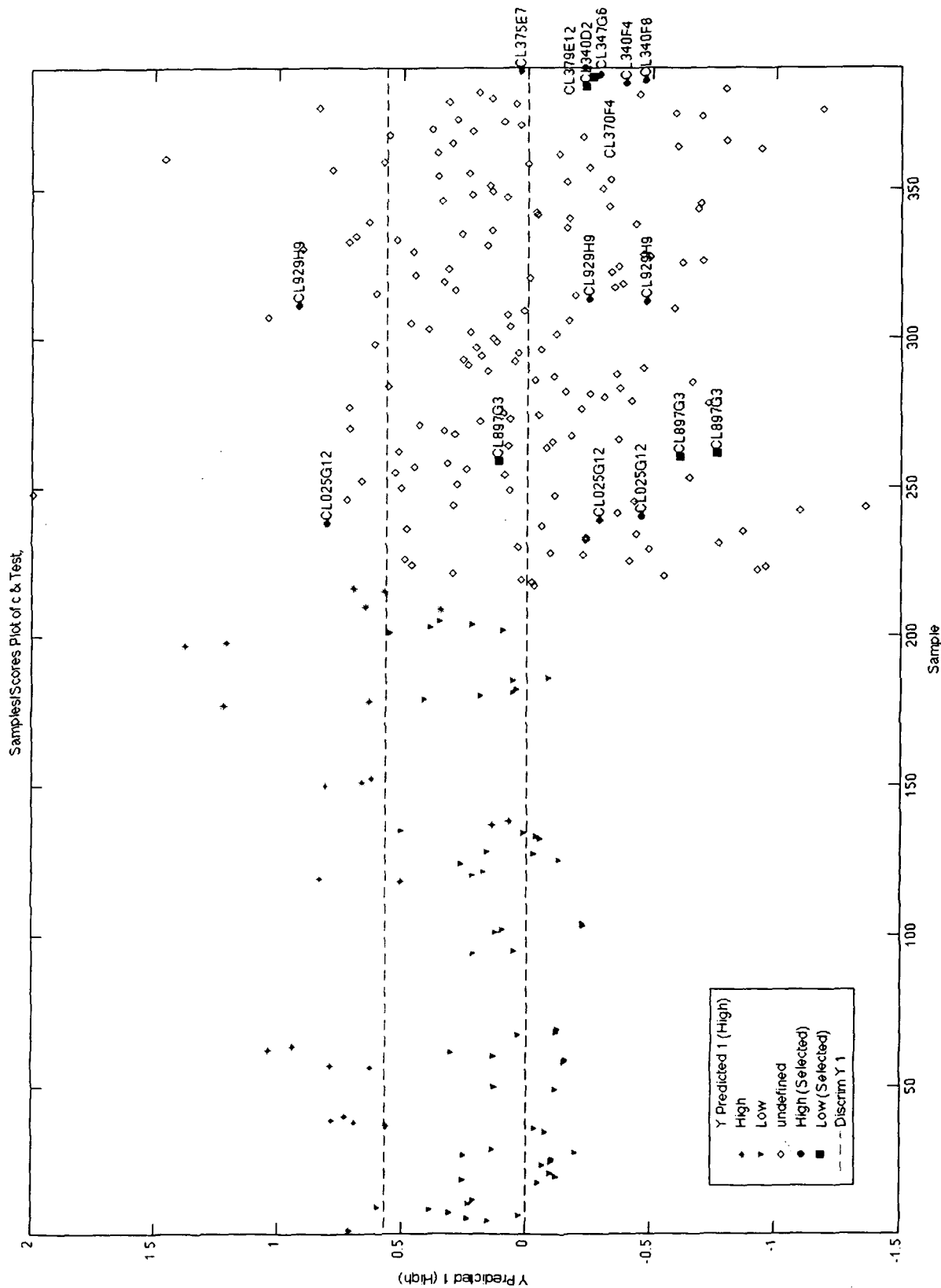


Fig. 23

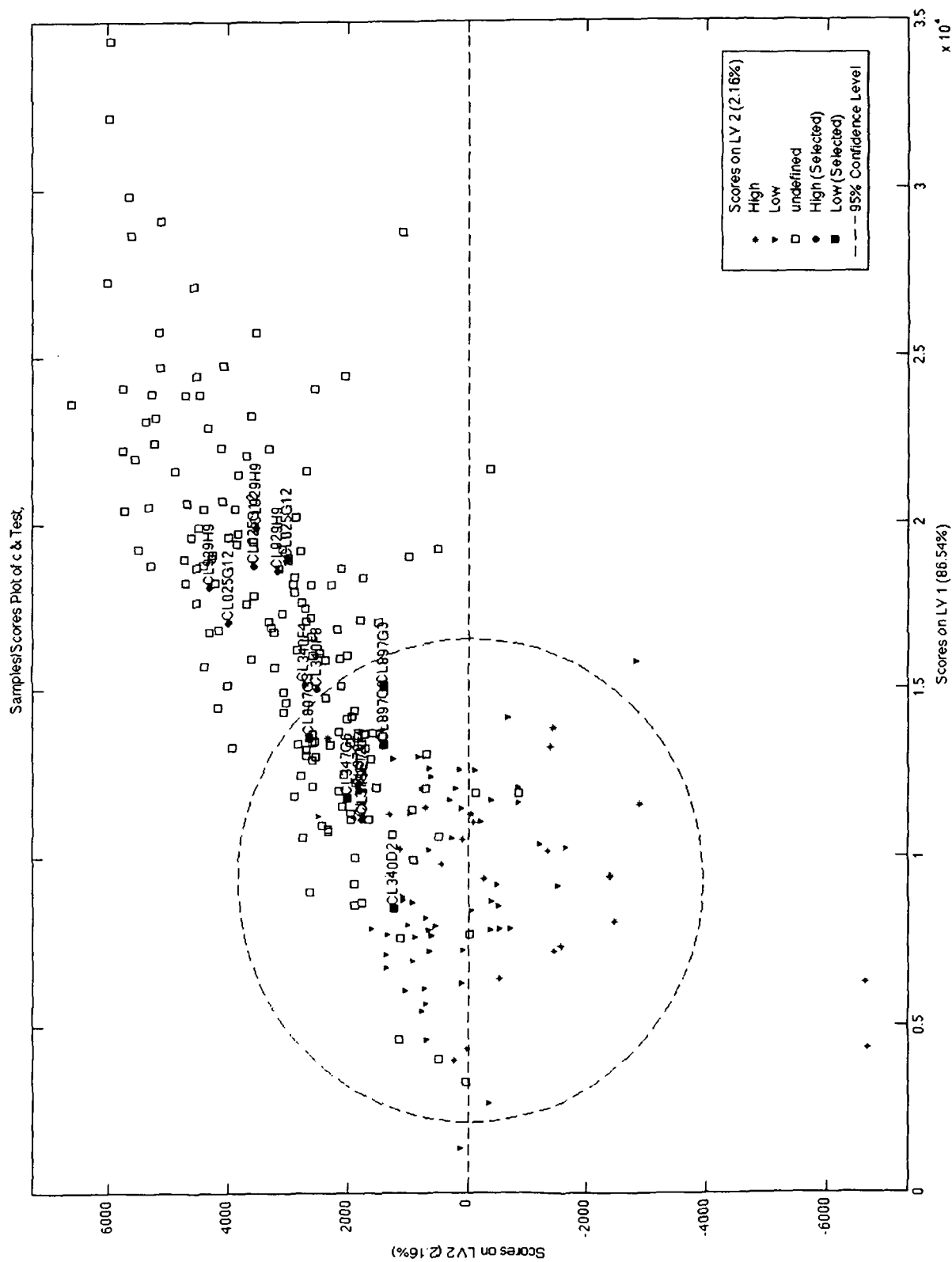


Fig. 24

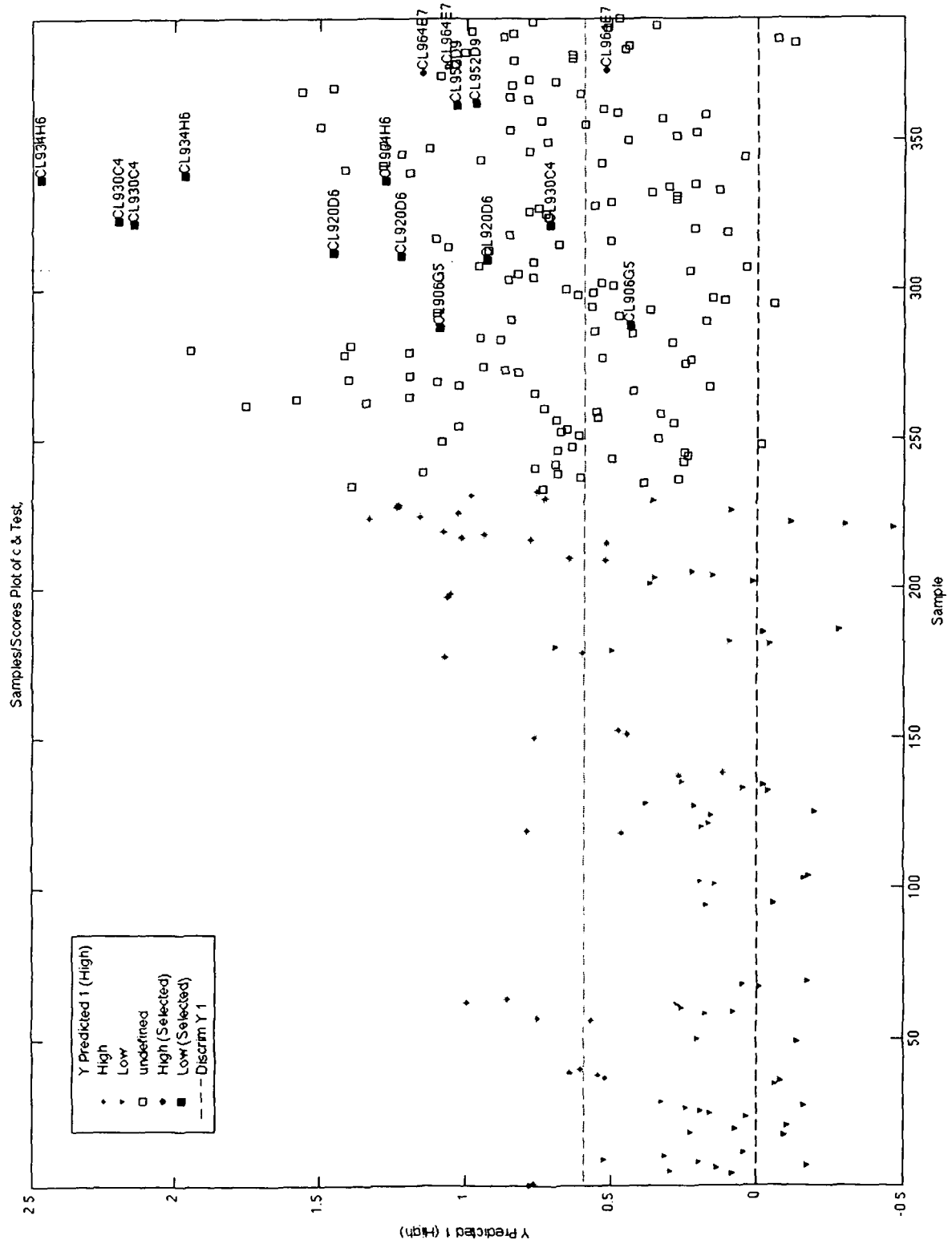


Fig. 25

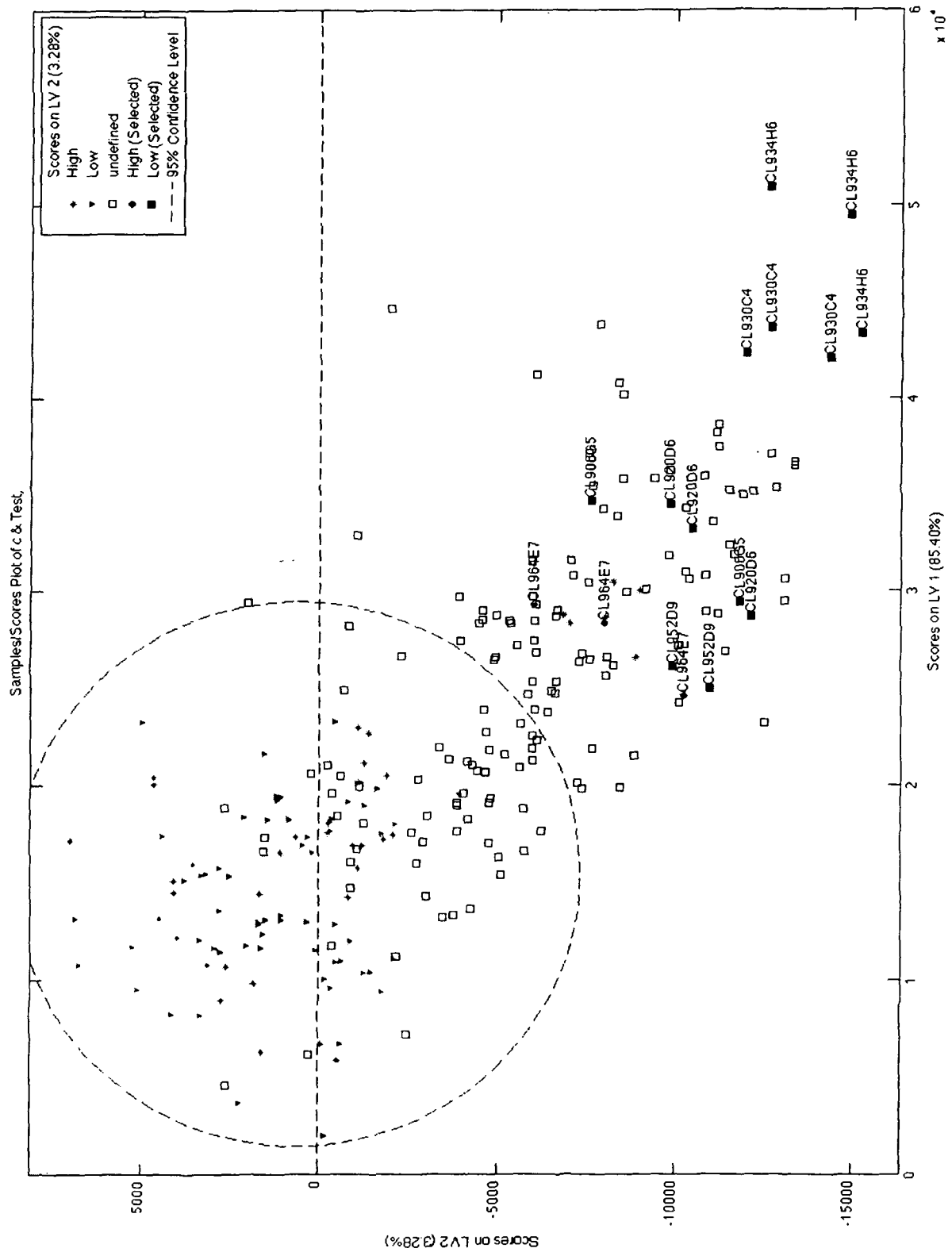


Fig. 26

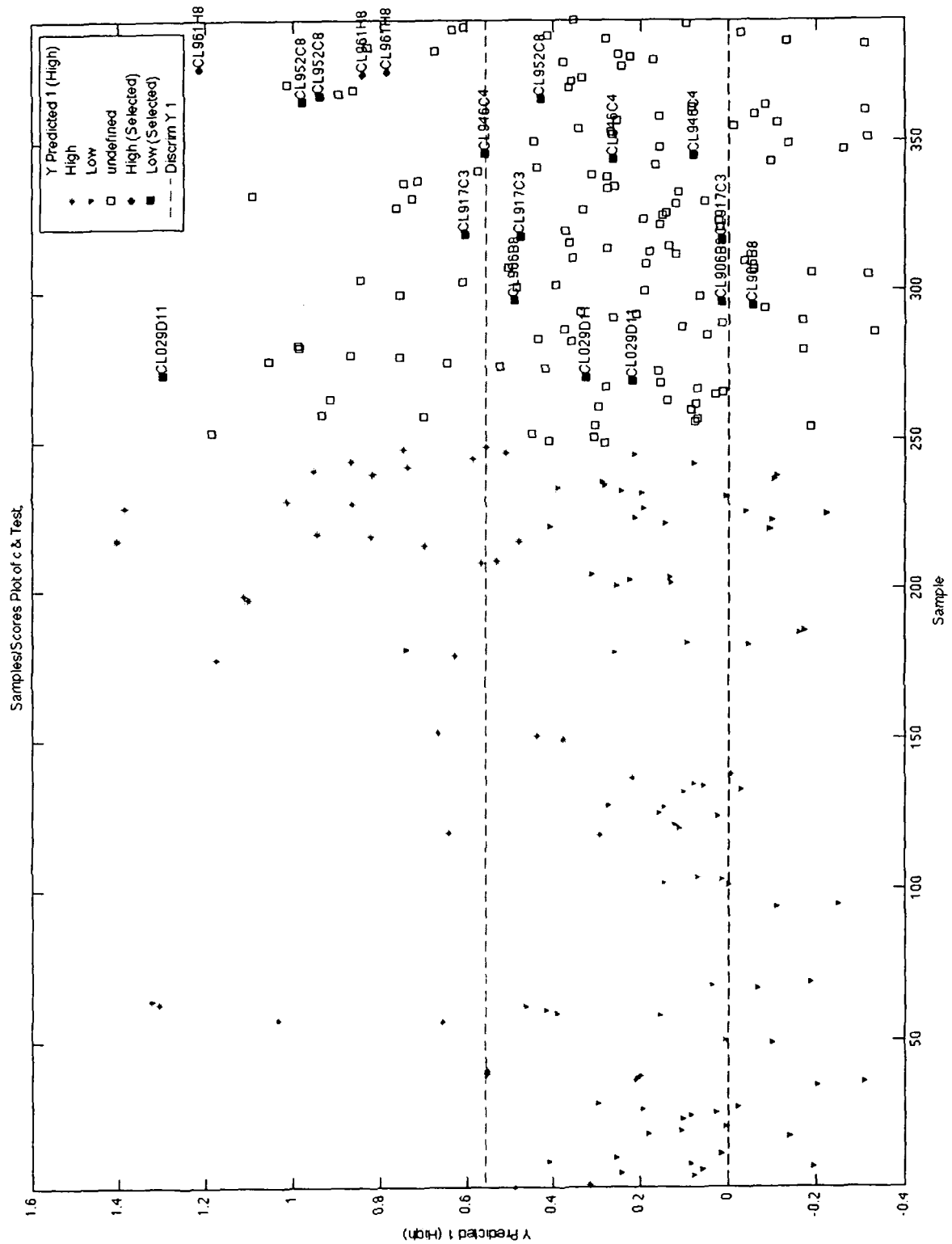


Fig. 27

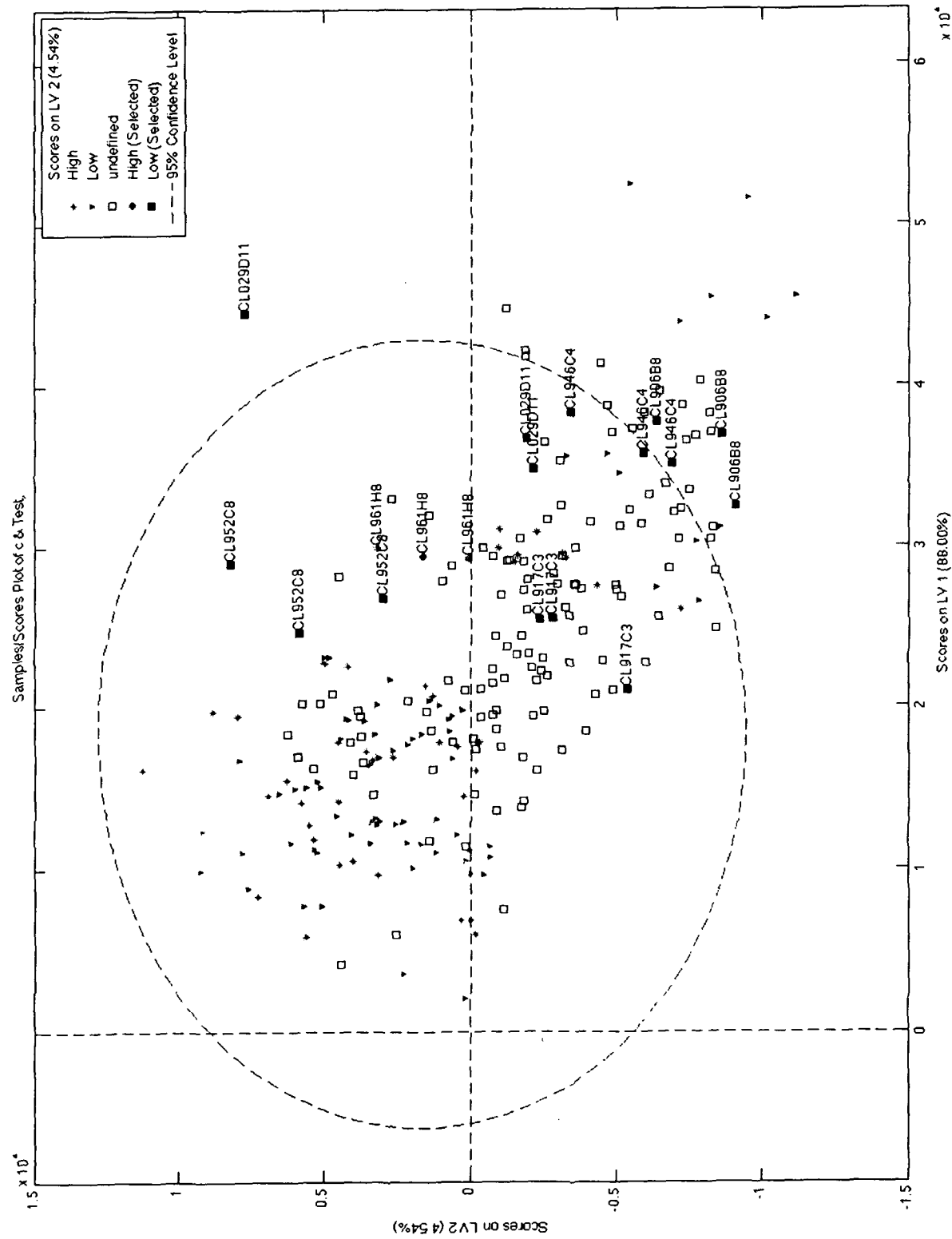


Fig. 28

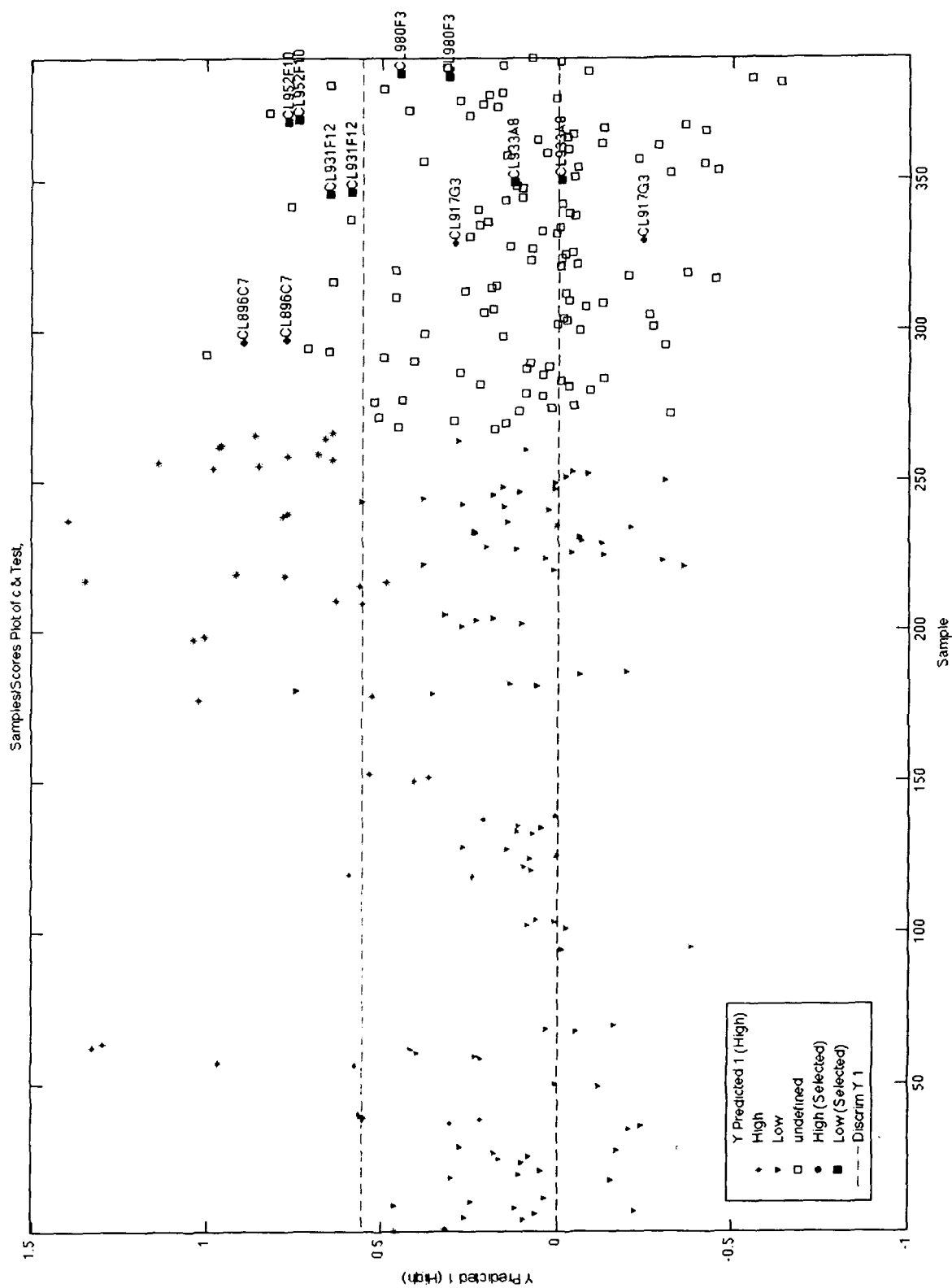


Fig. 30

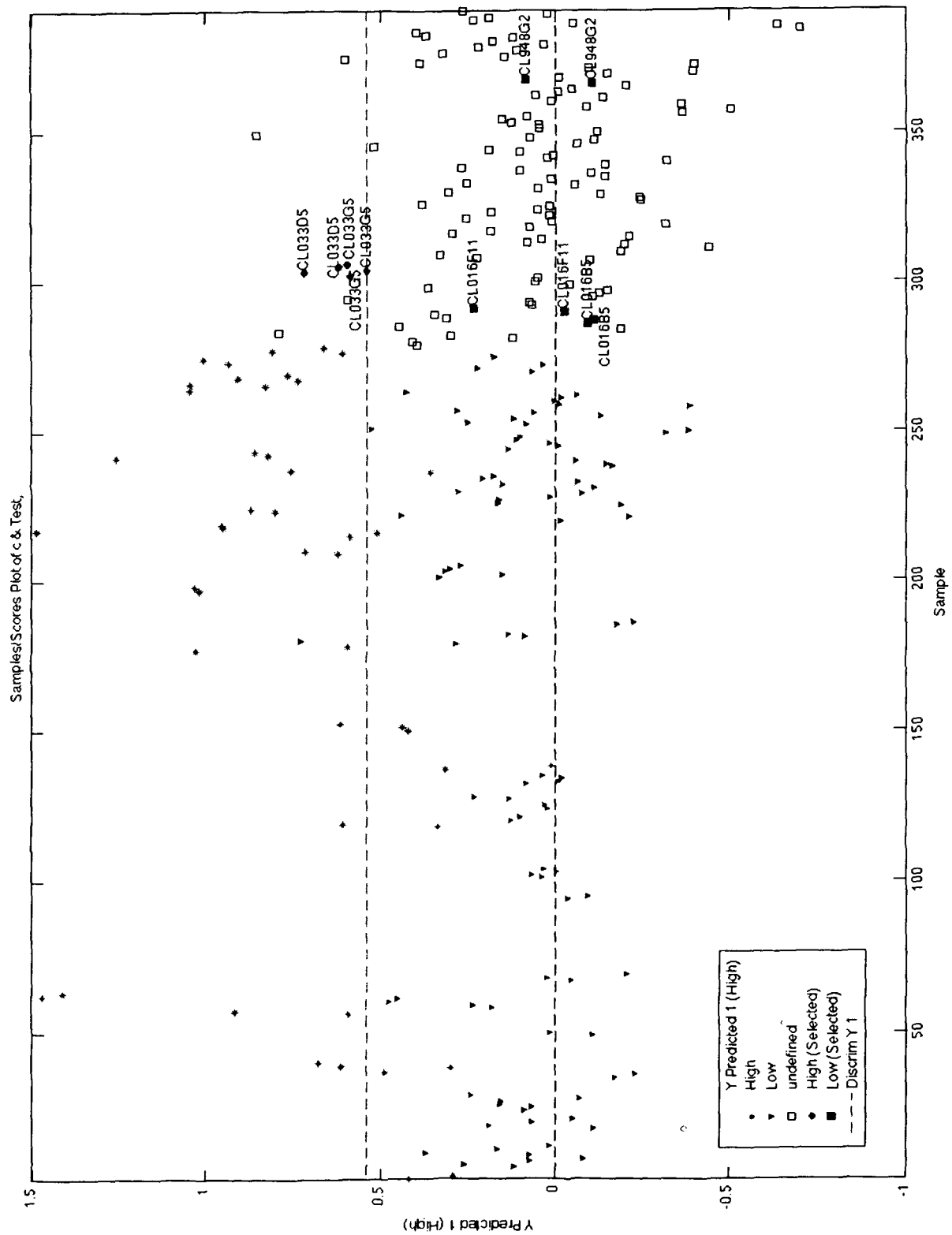


Fig. 32

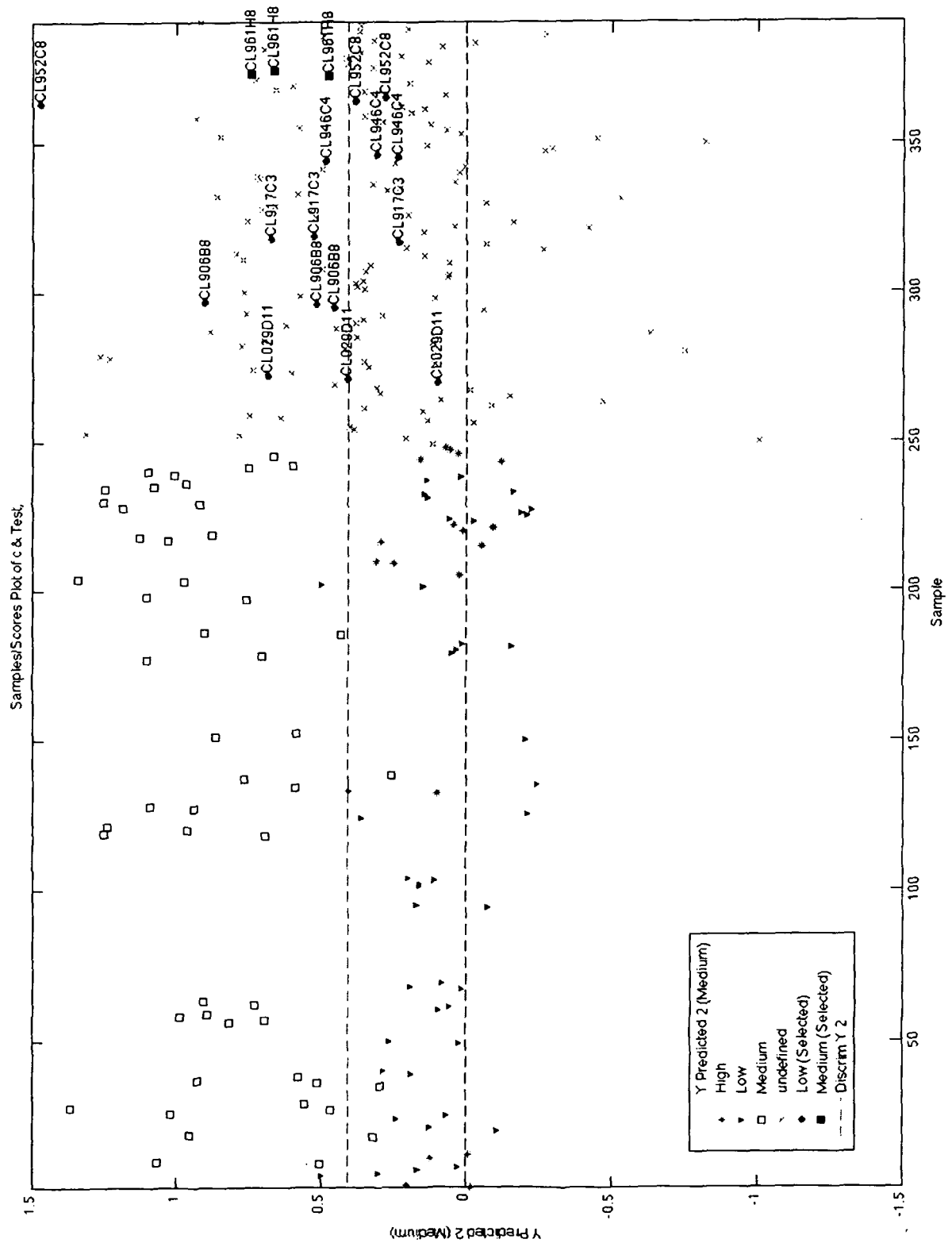


Fig. 33

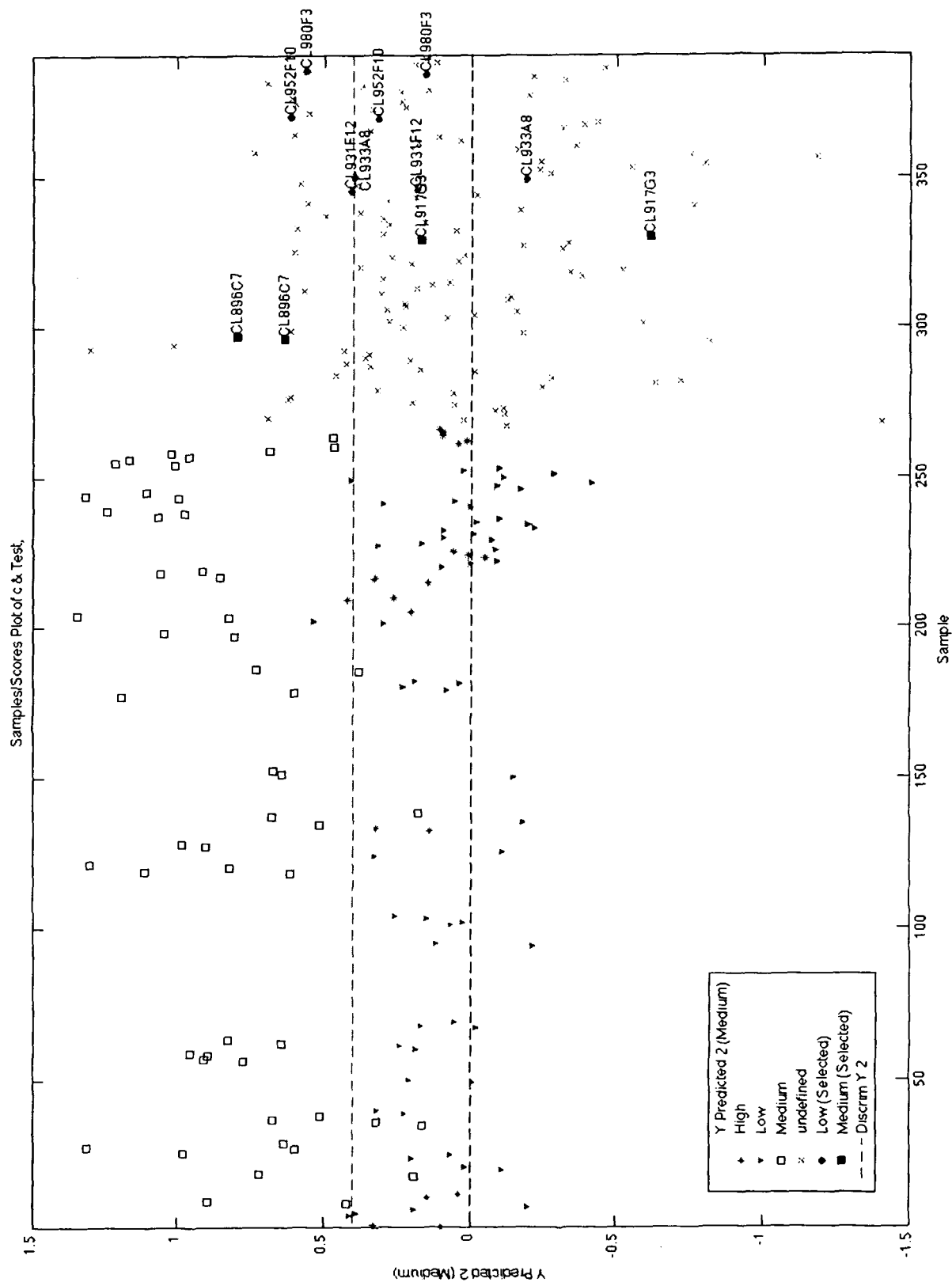


Fig. 34

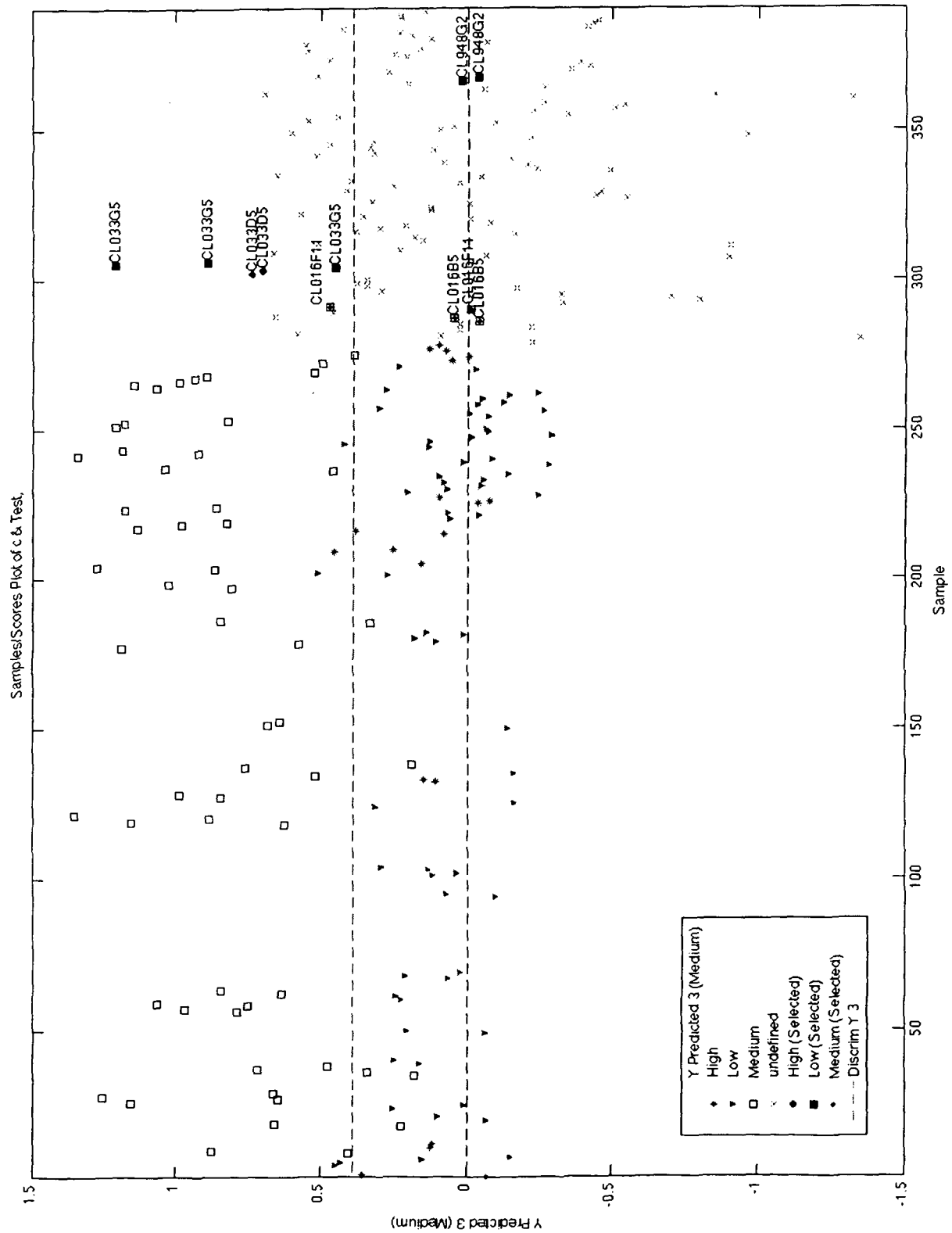


Fig. 35

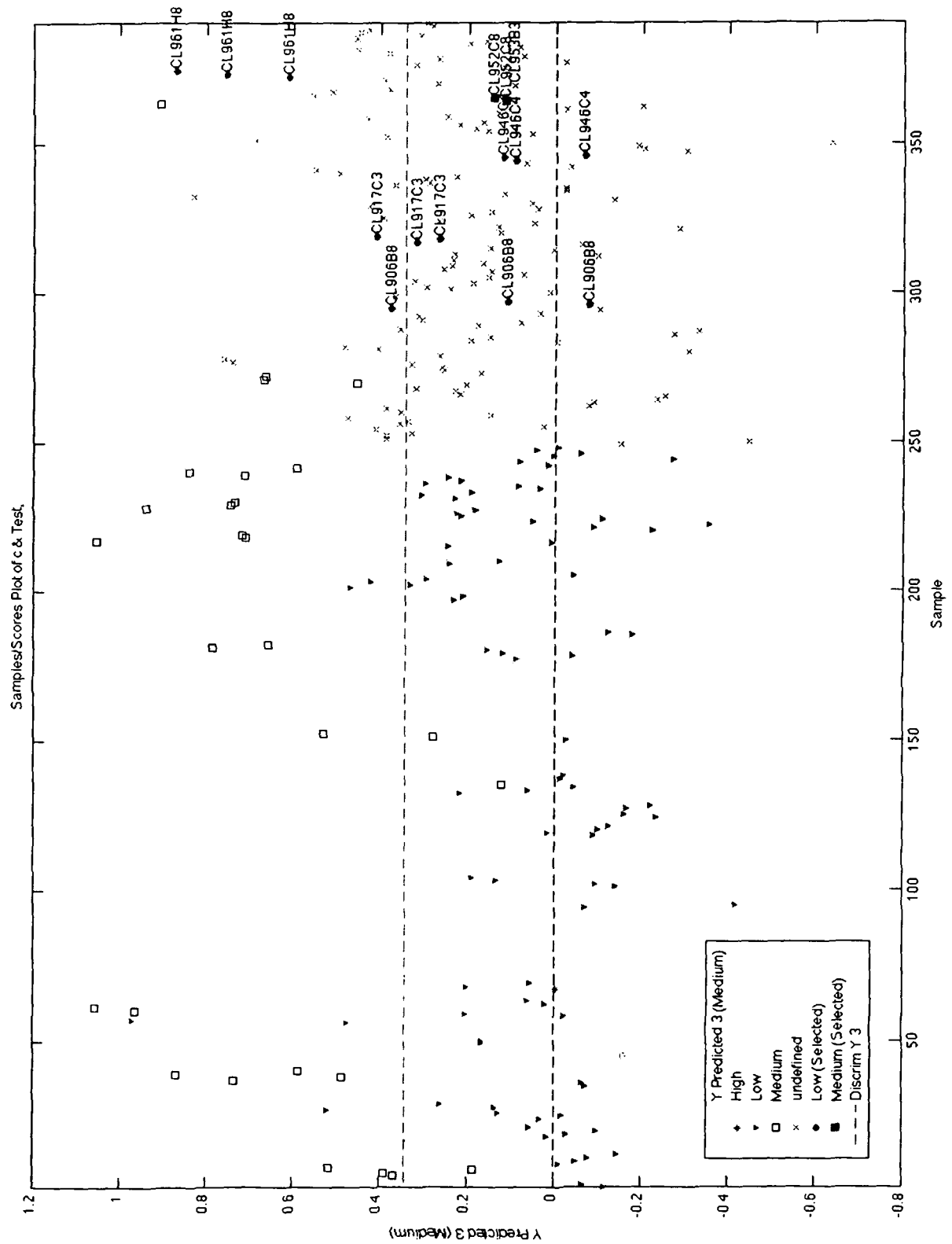
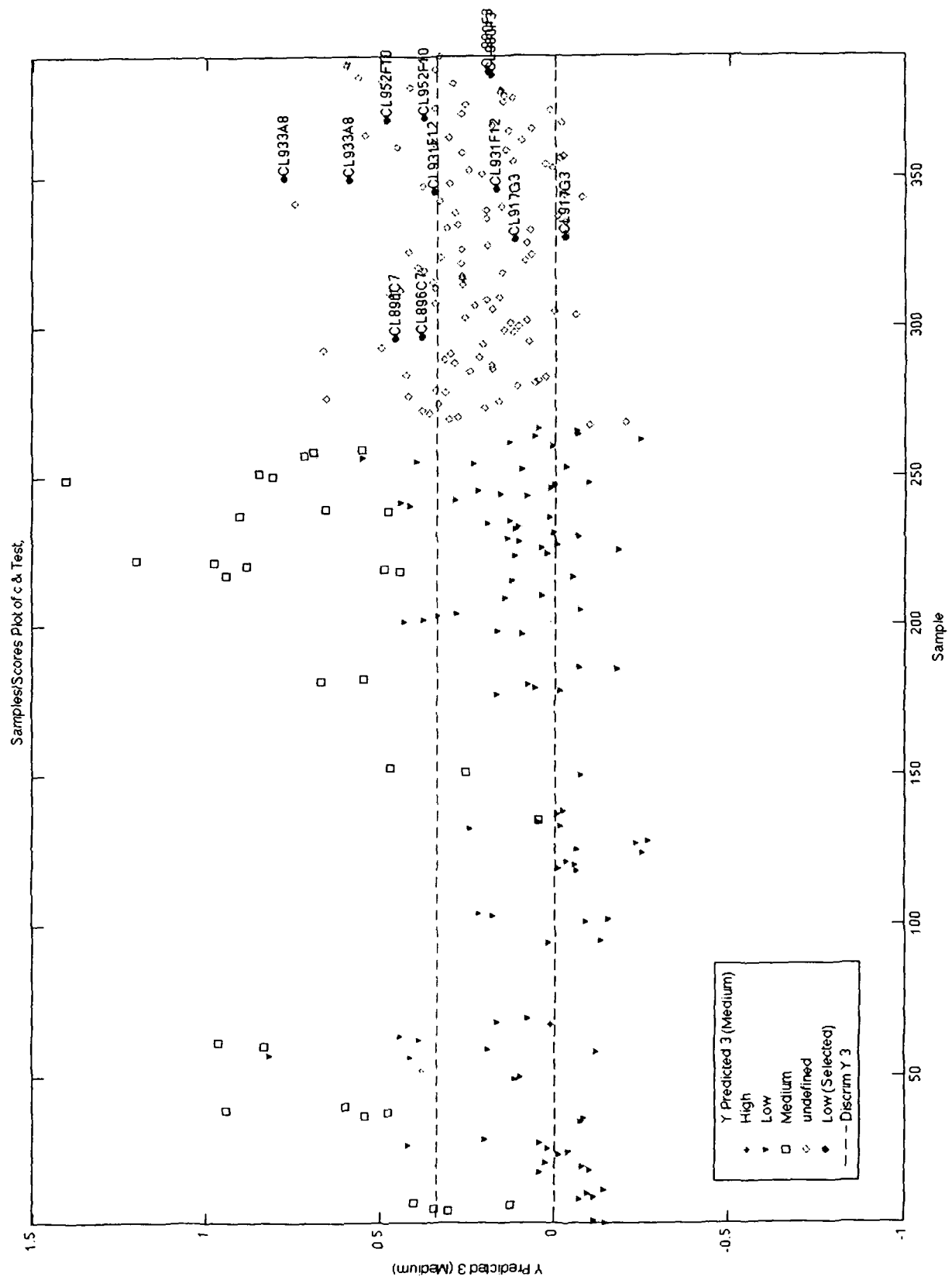


Fig. 36



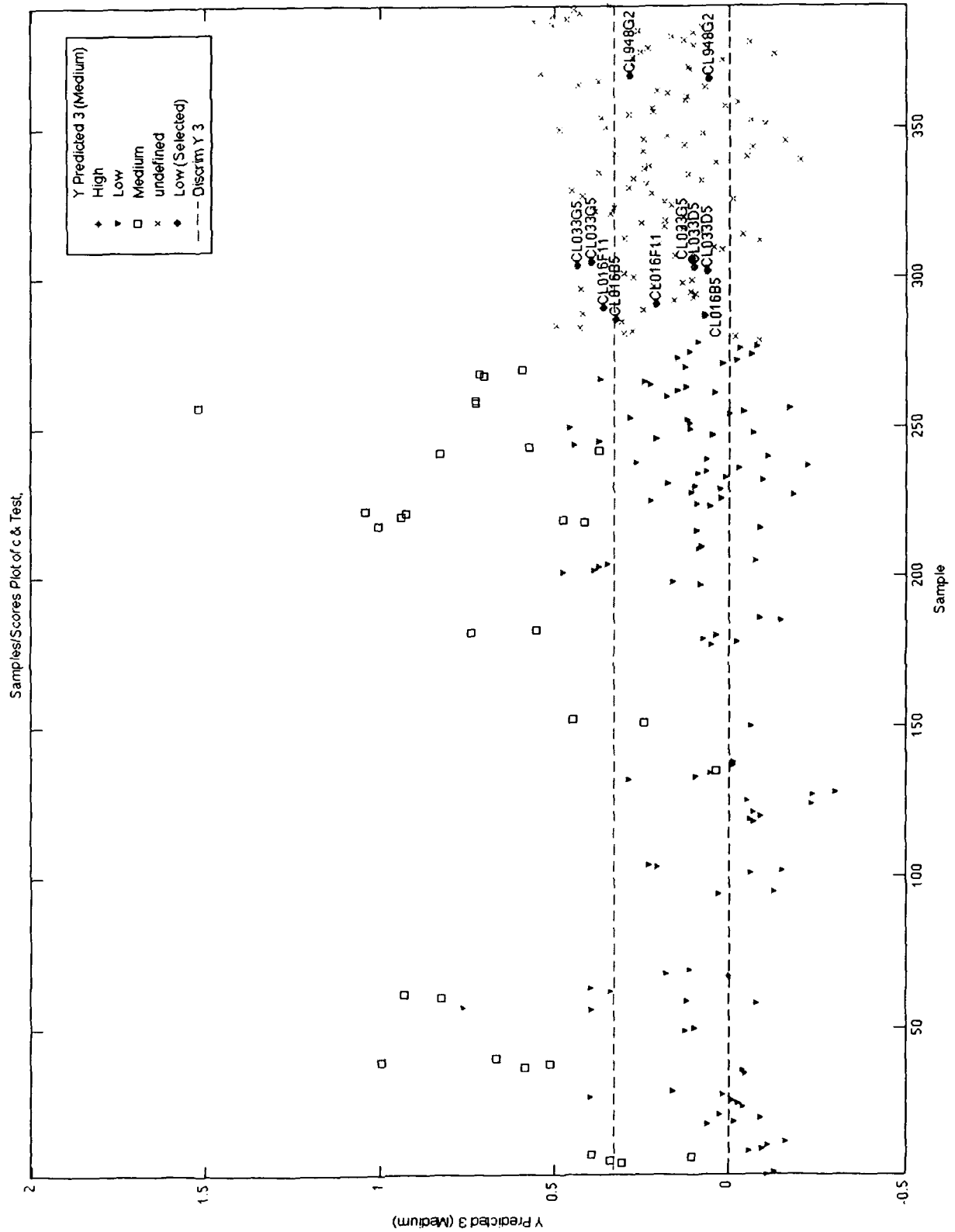


Fig. 37

Fig. 38

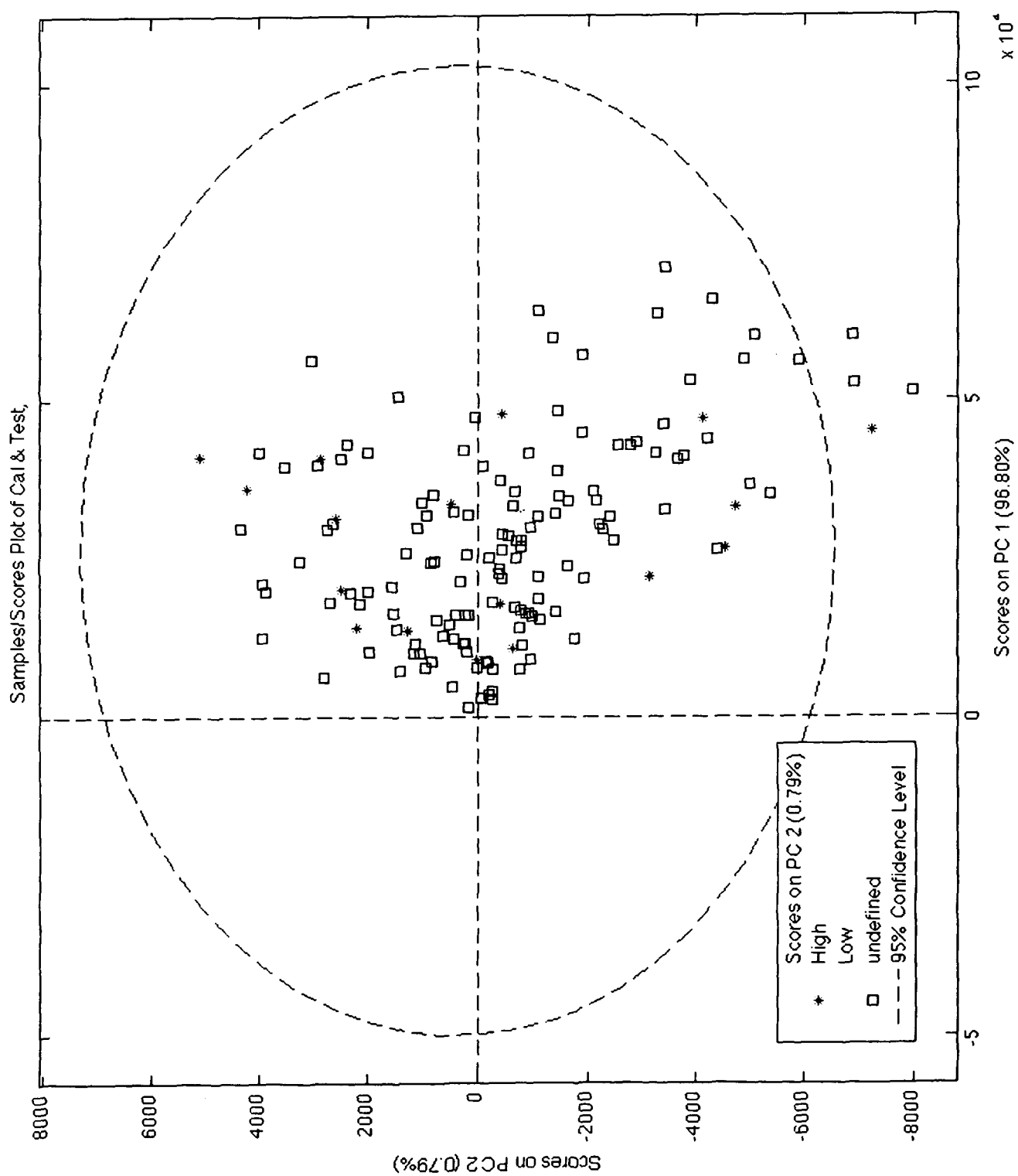


Fig. 39

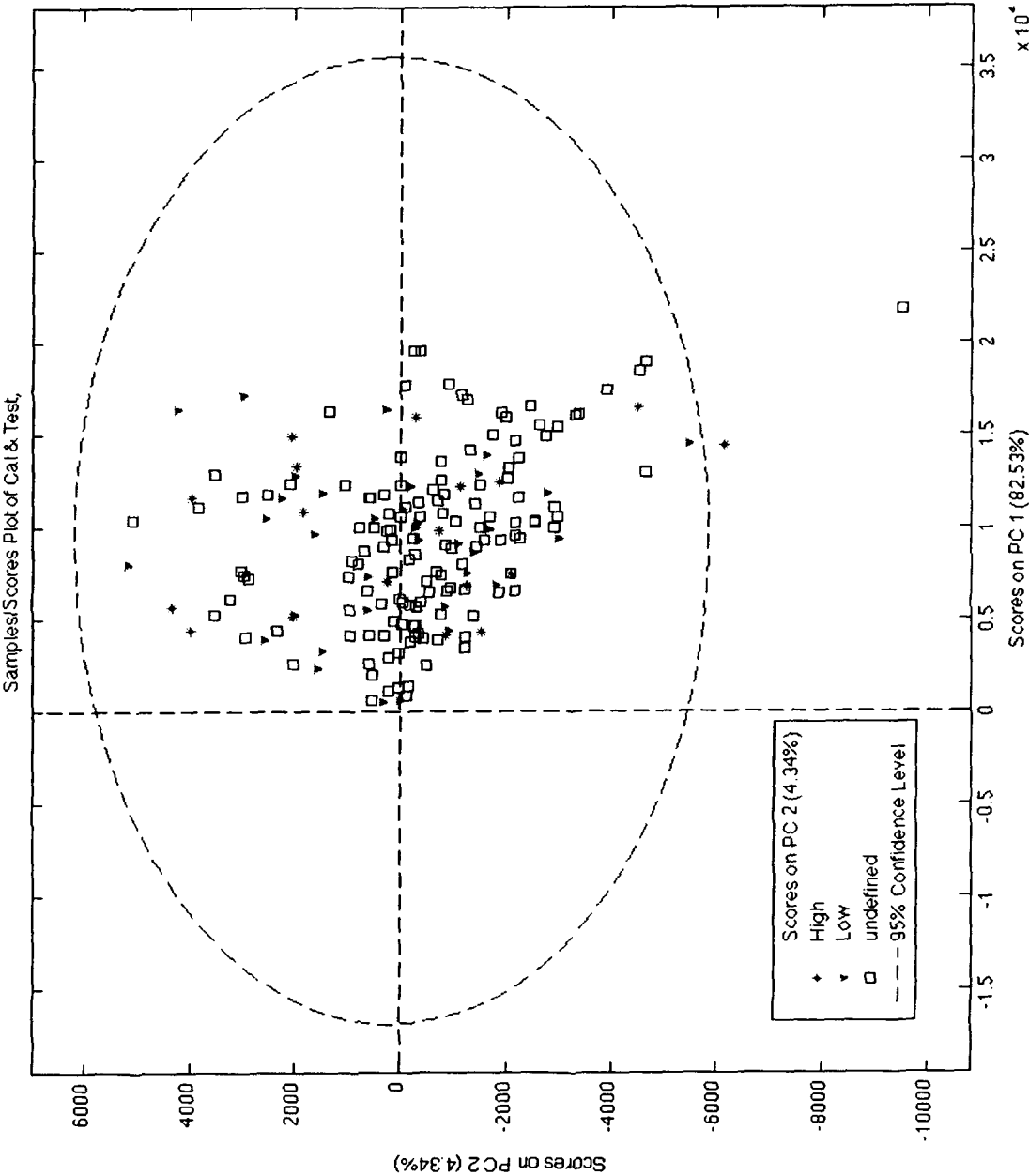


Fig. 40

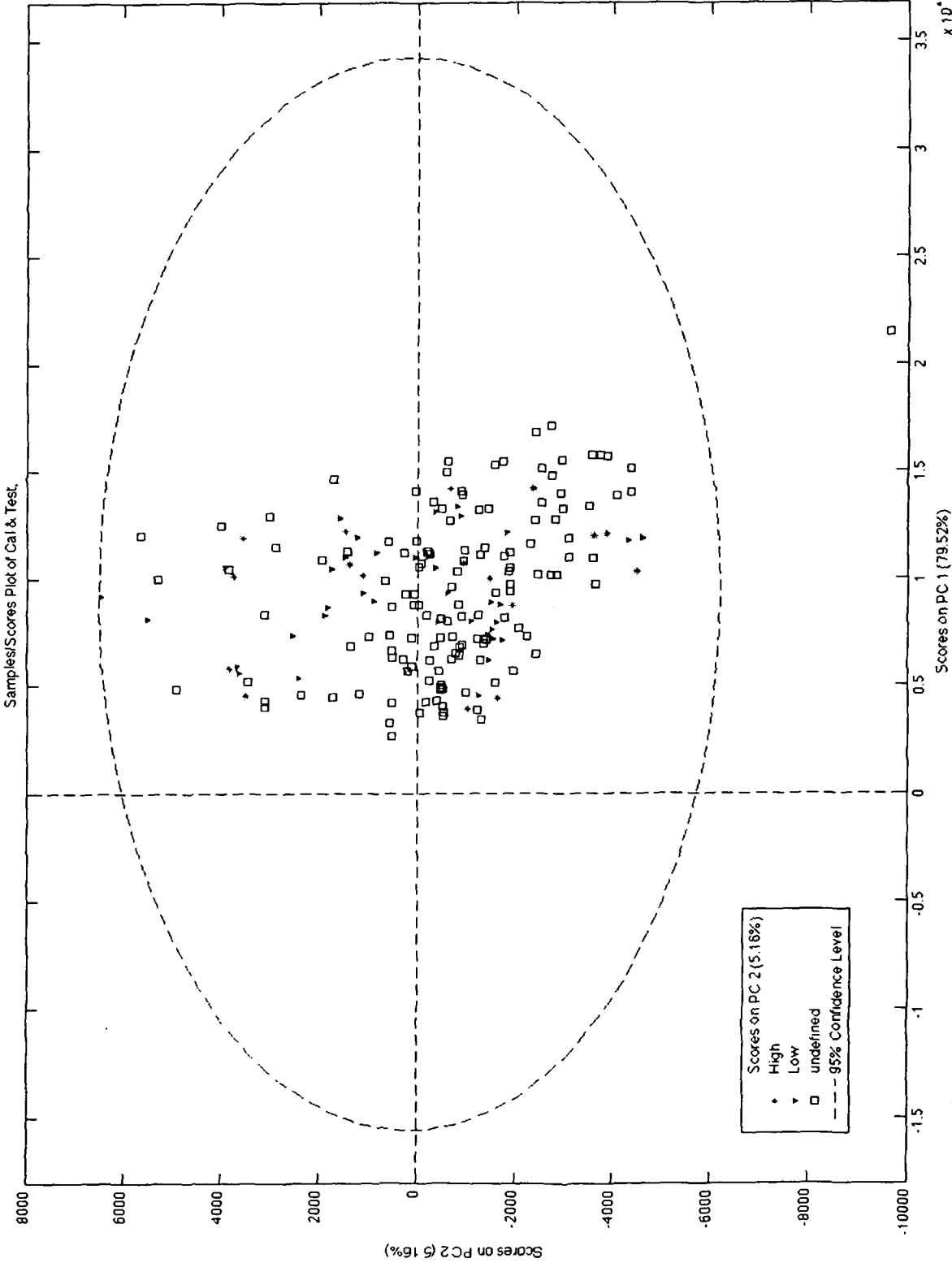


Fig. 41

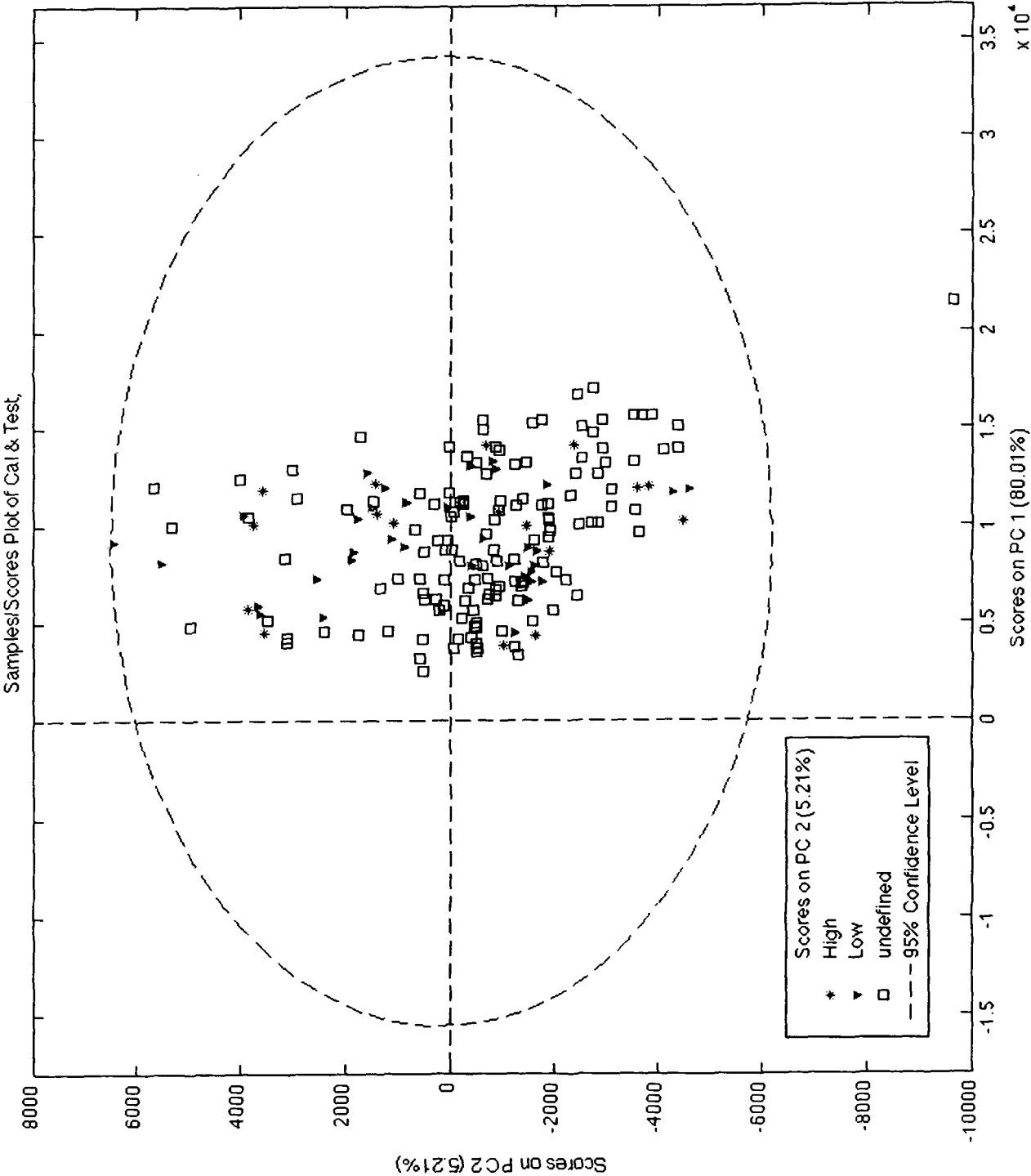
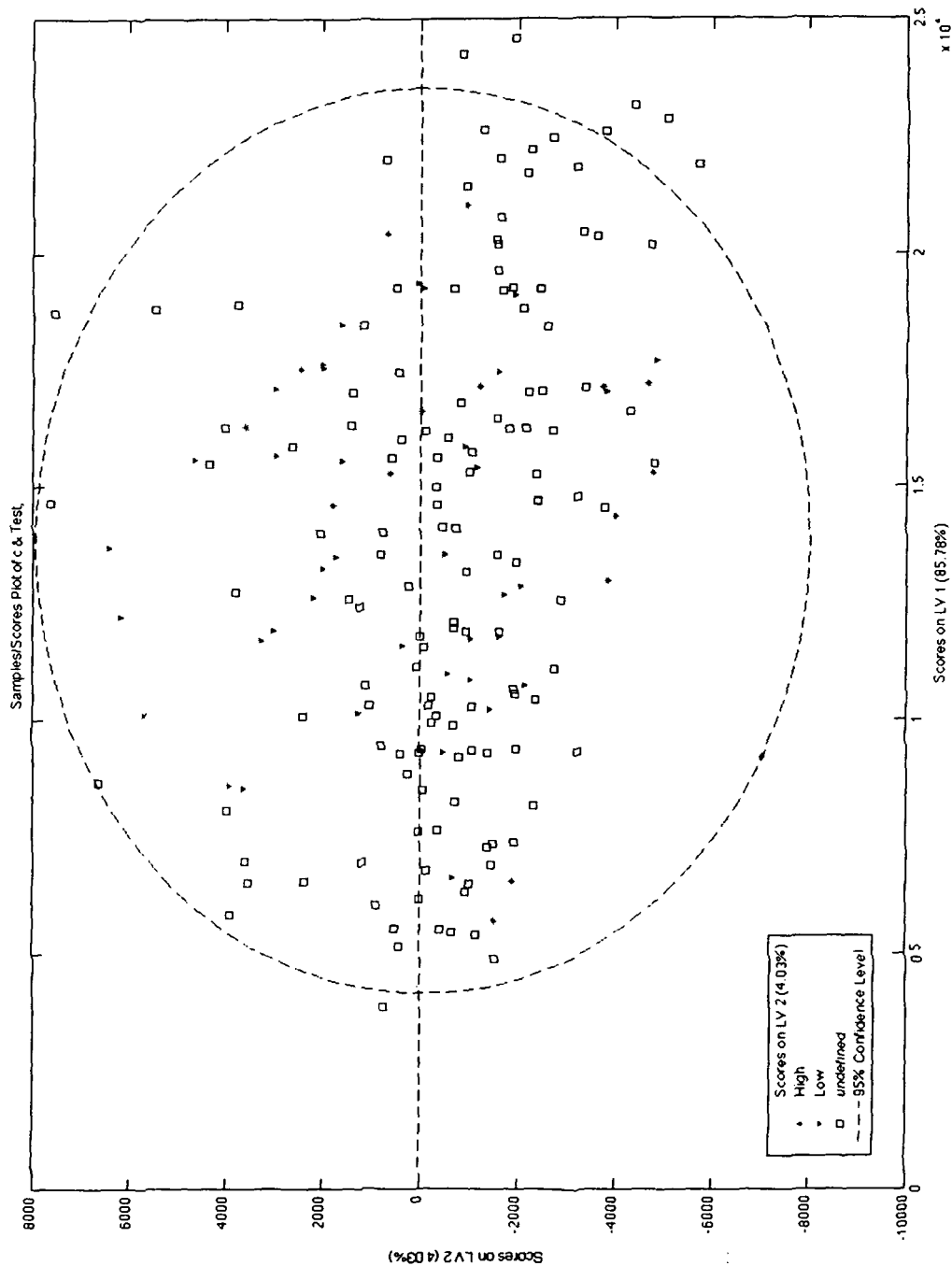


Fig. 42



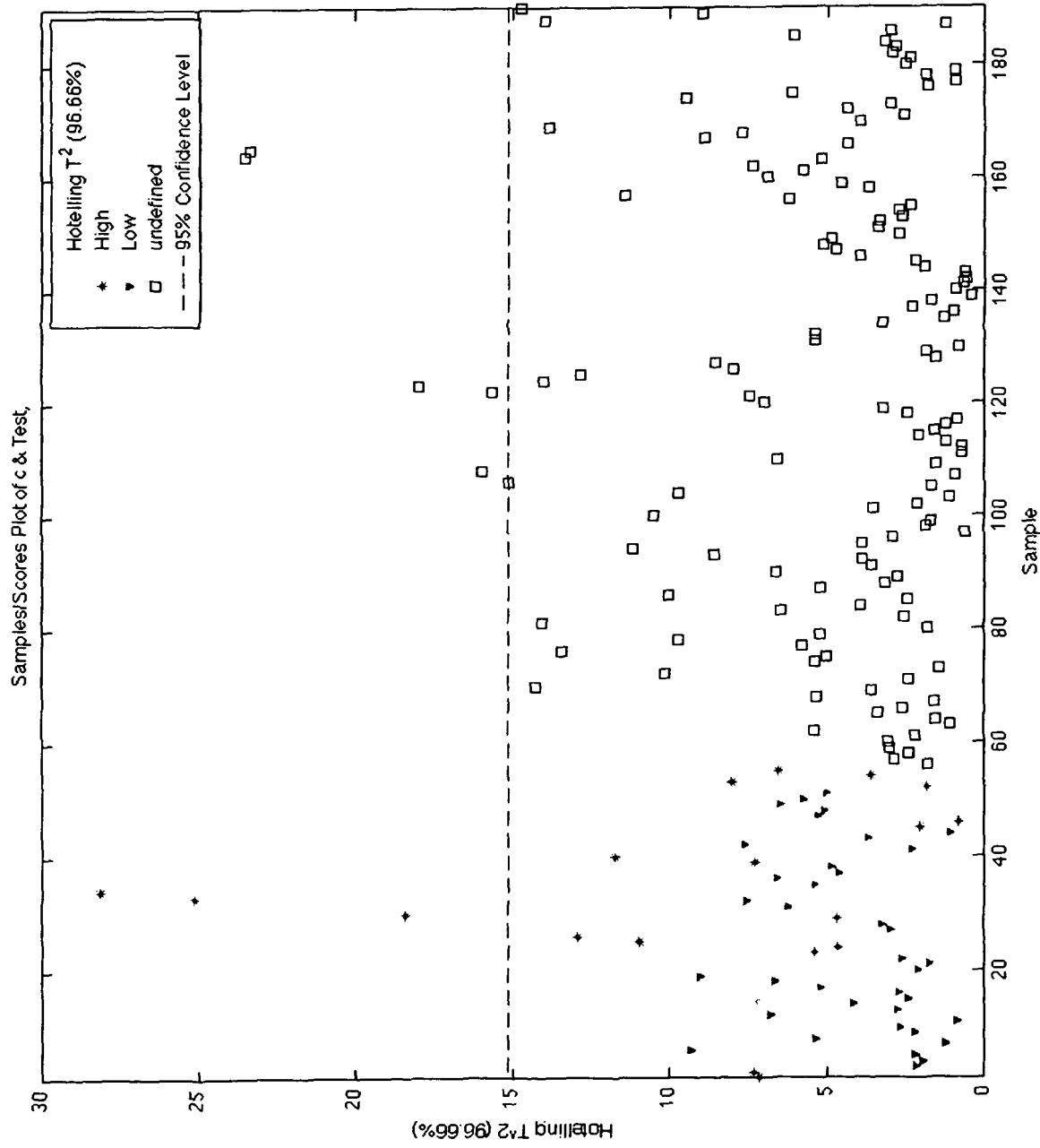


Fig. 43

Fig. 44

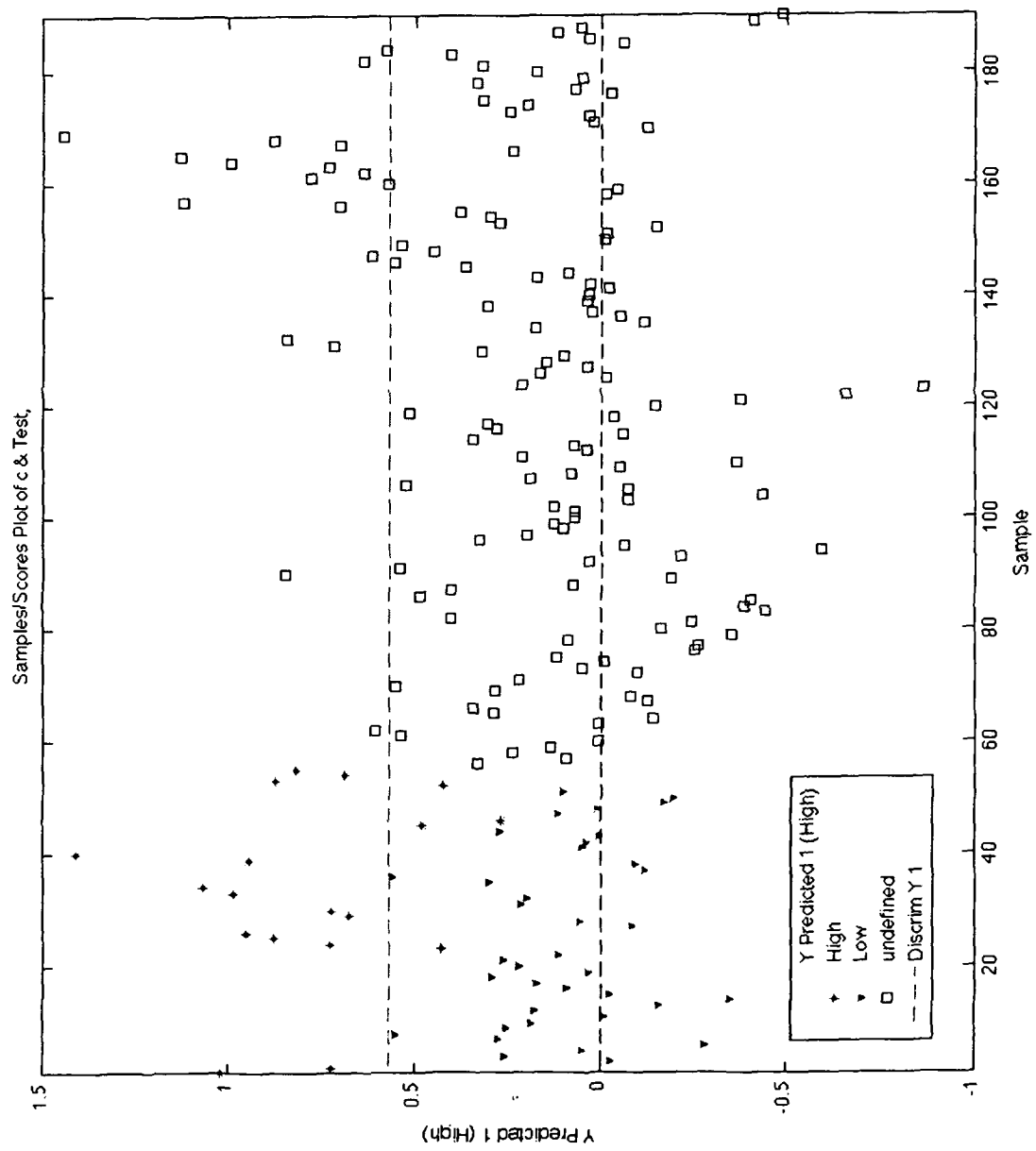


Fig. 45

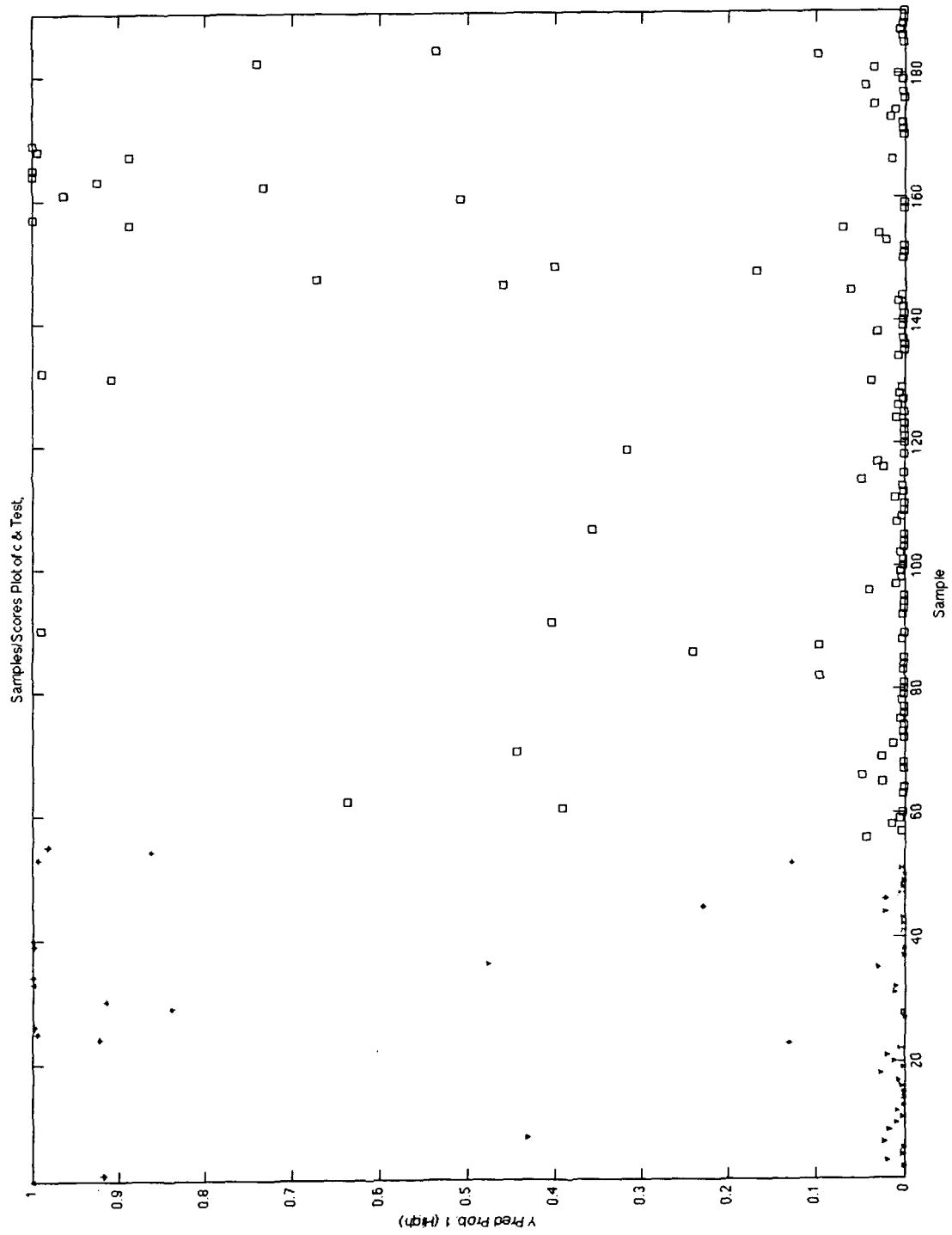


Fig. 46

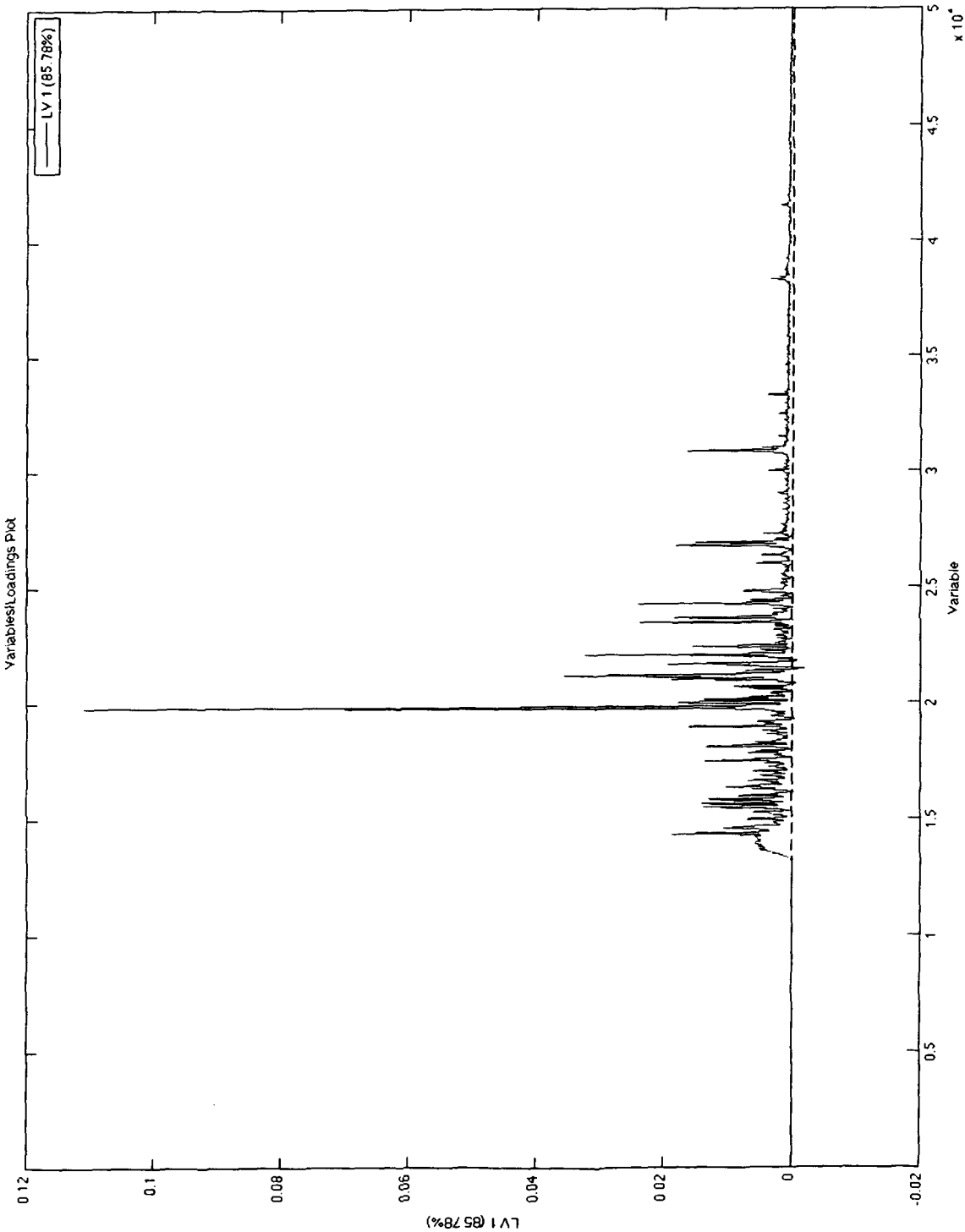


Fig. 47

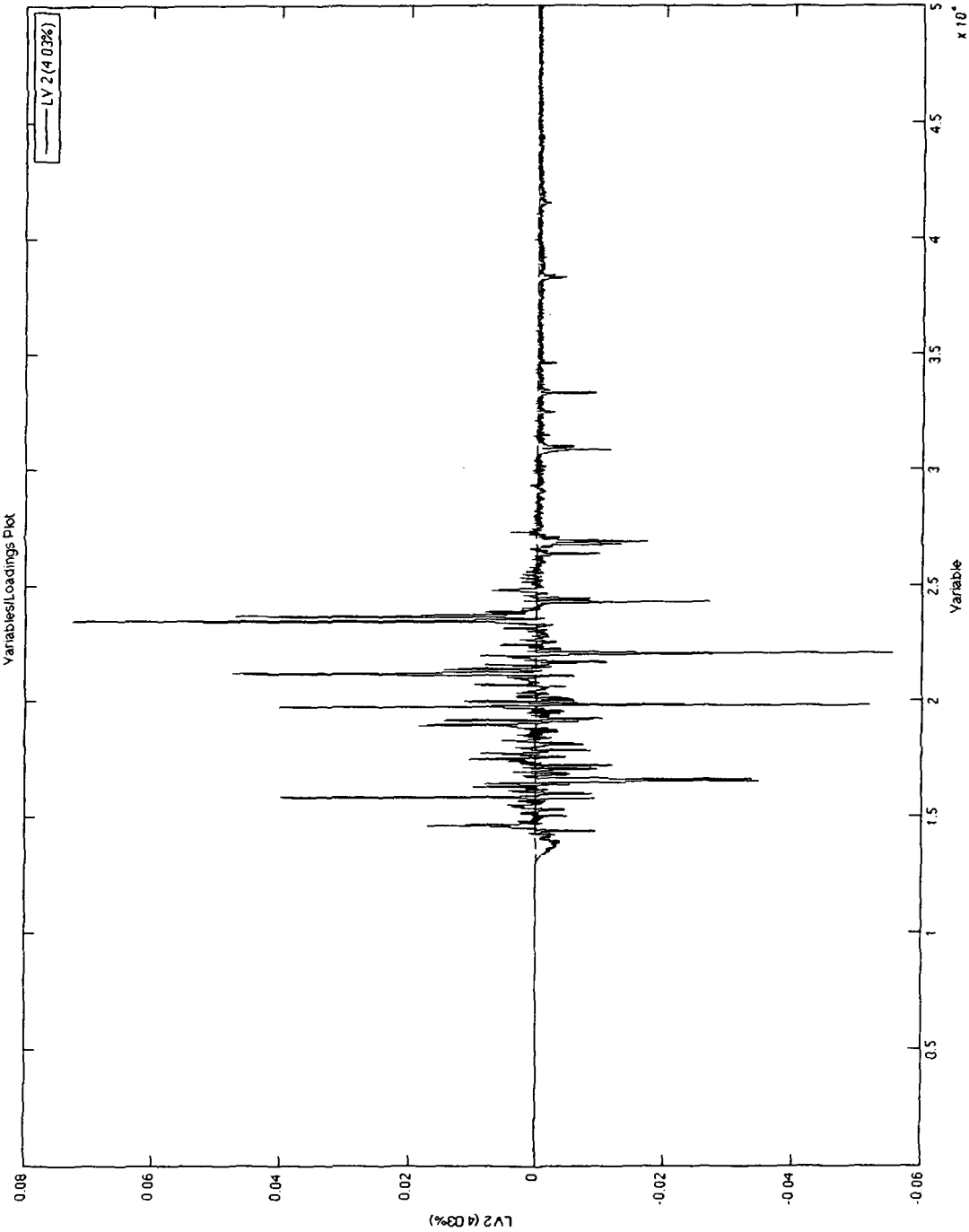


Fig. 48

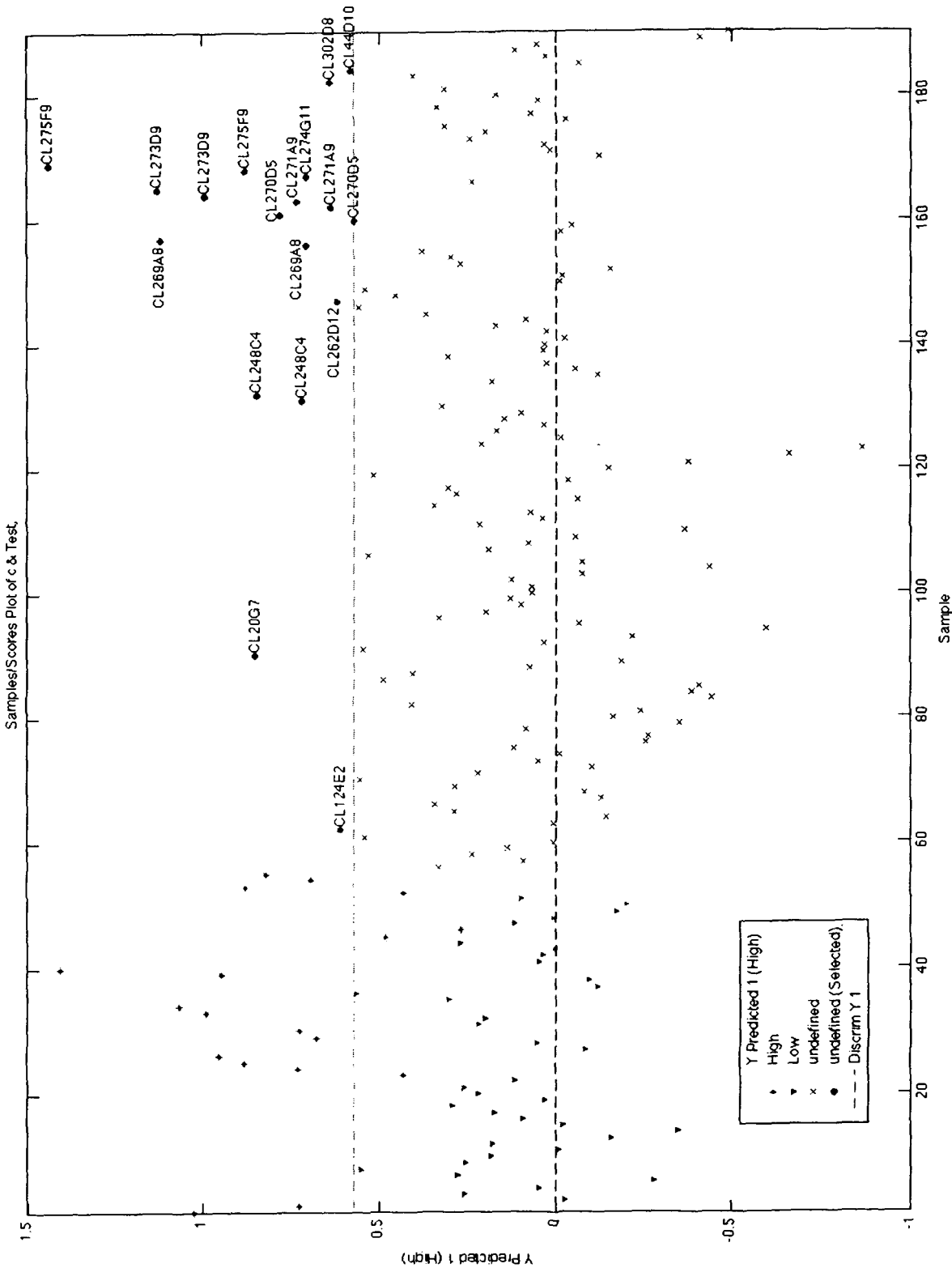


Fig. 49

