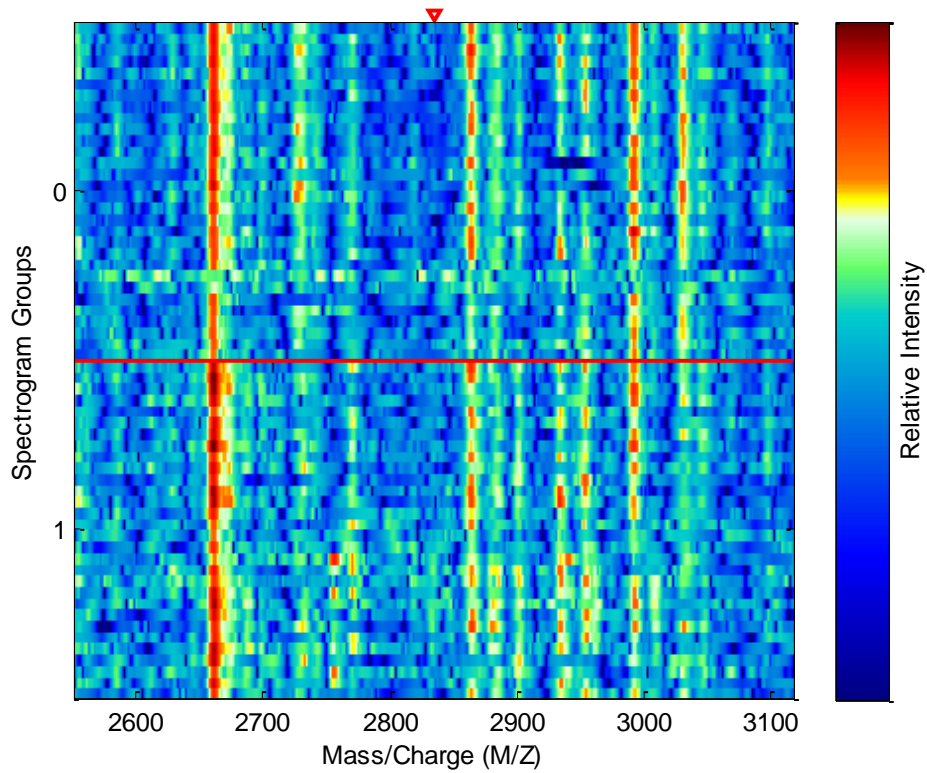
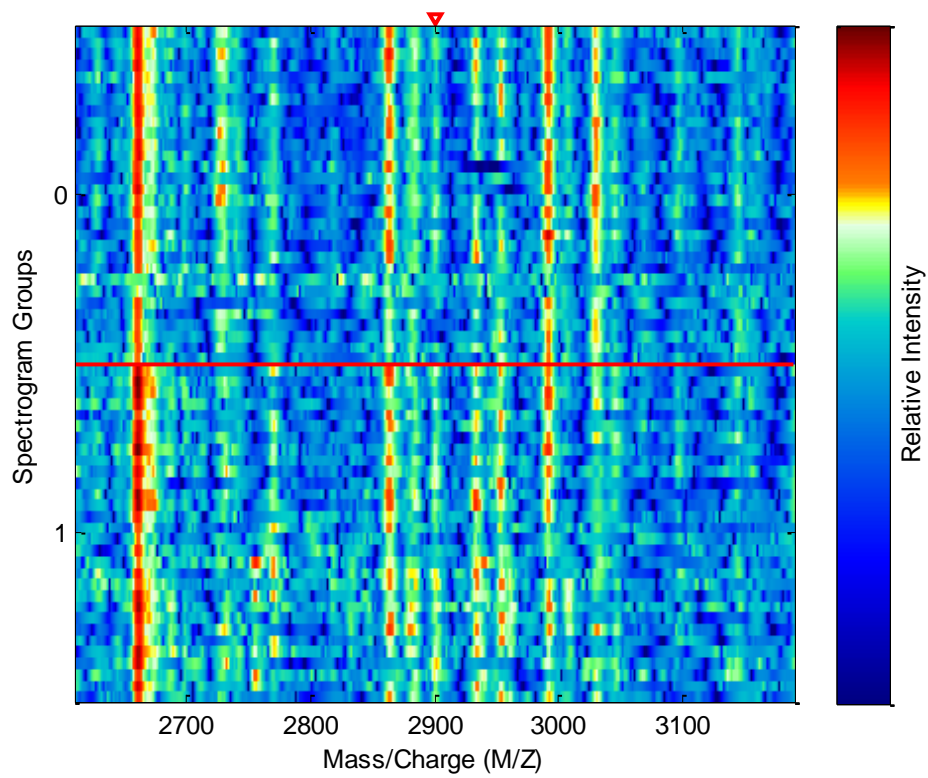


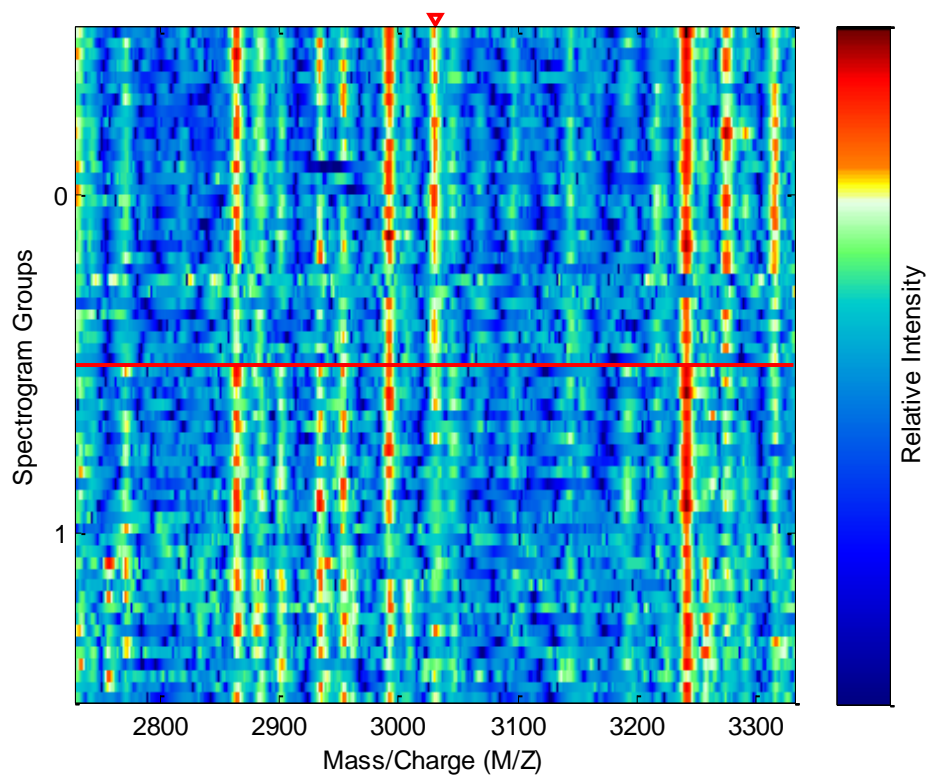
Biomarkers Principal Component Scatter Plot
Group 1: Crohn's disease patients, group 0: Healthy controls.



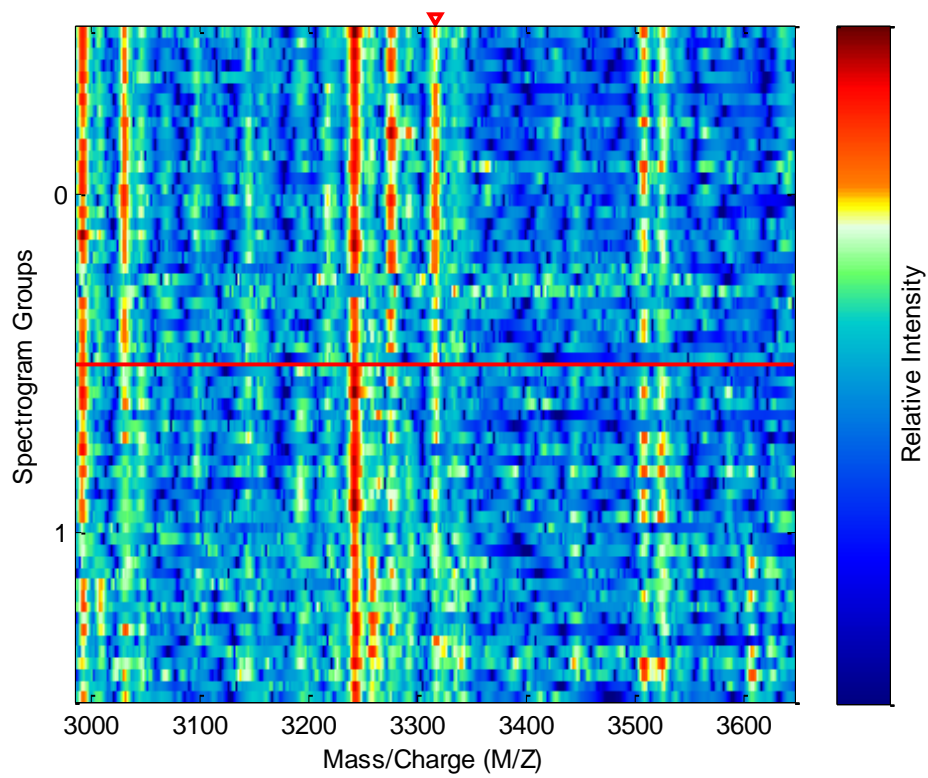
Gel figure: M/Z 2833



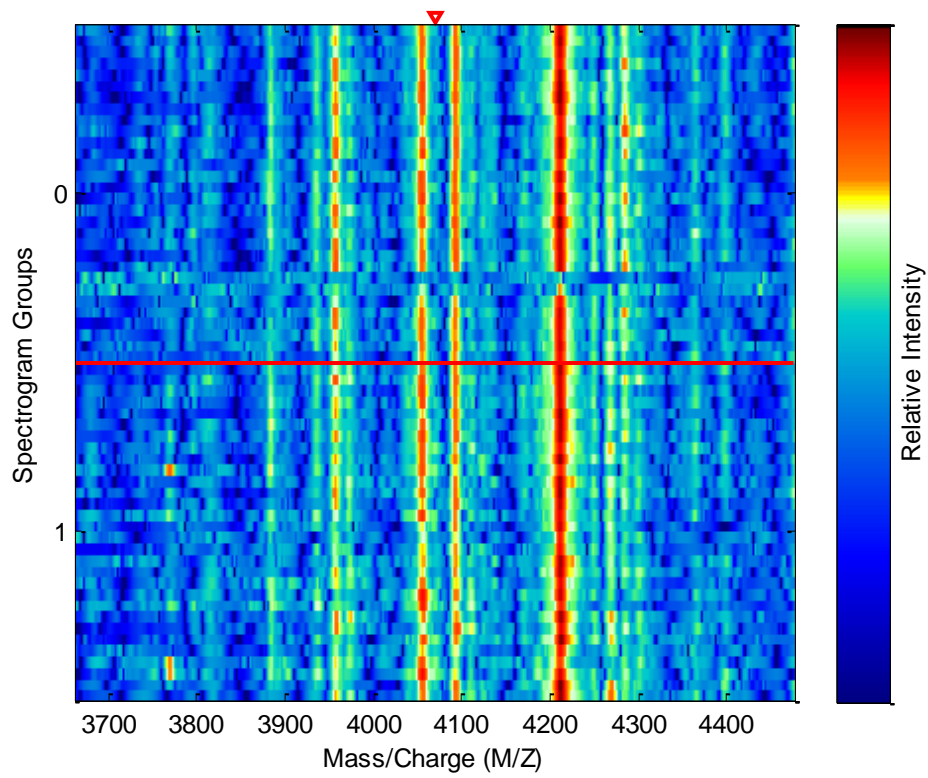
Gel figure: M/Z 2900



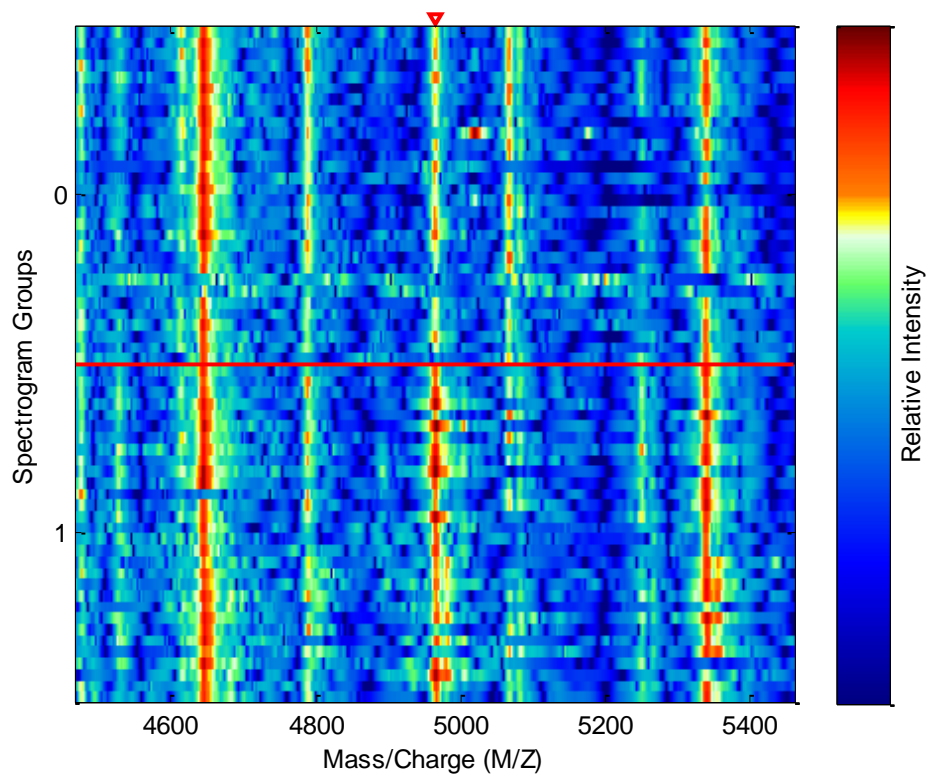
Gel figure: M/Z 3029



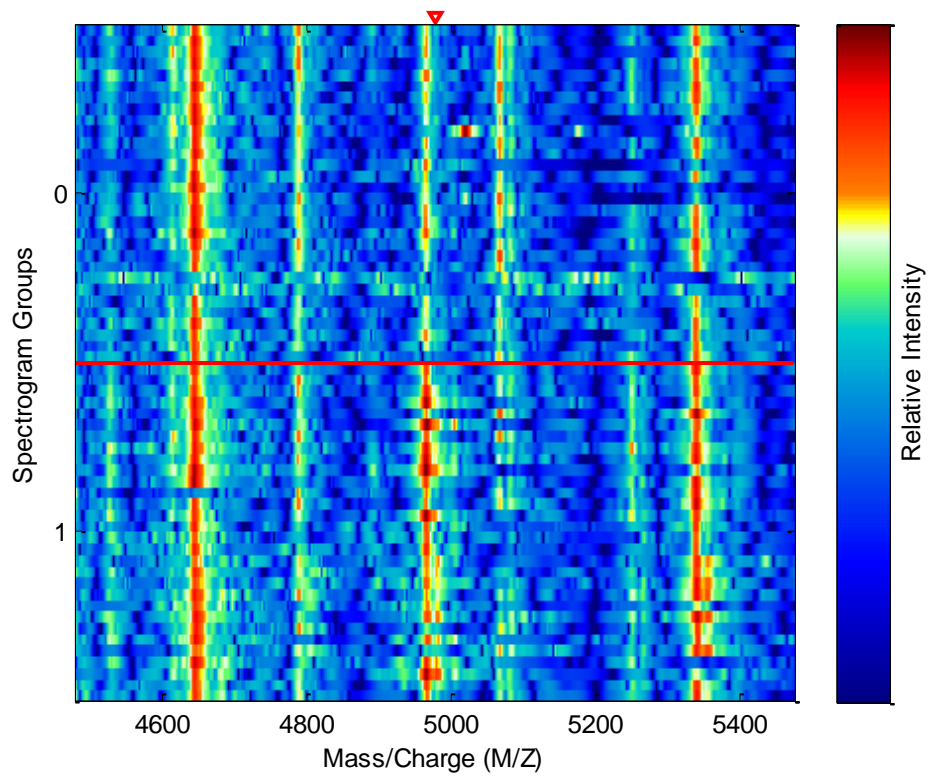
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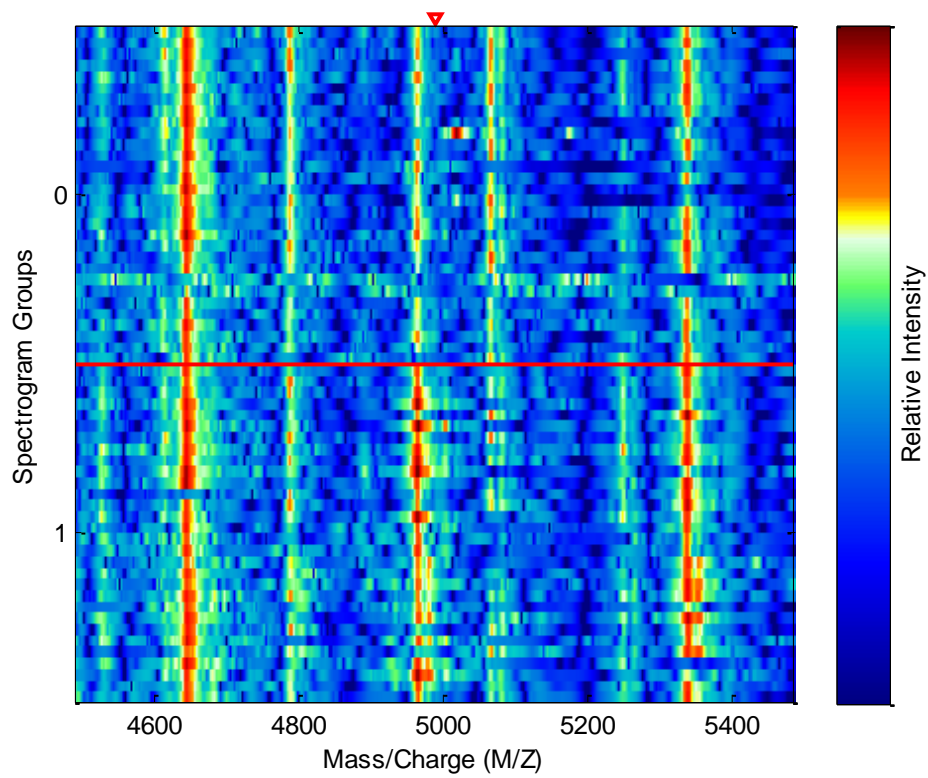
Gel figure: M/Z 4069



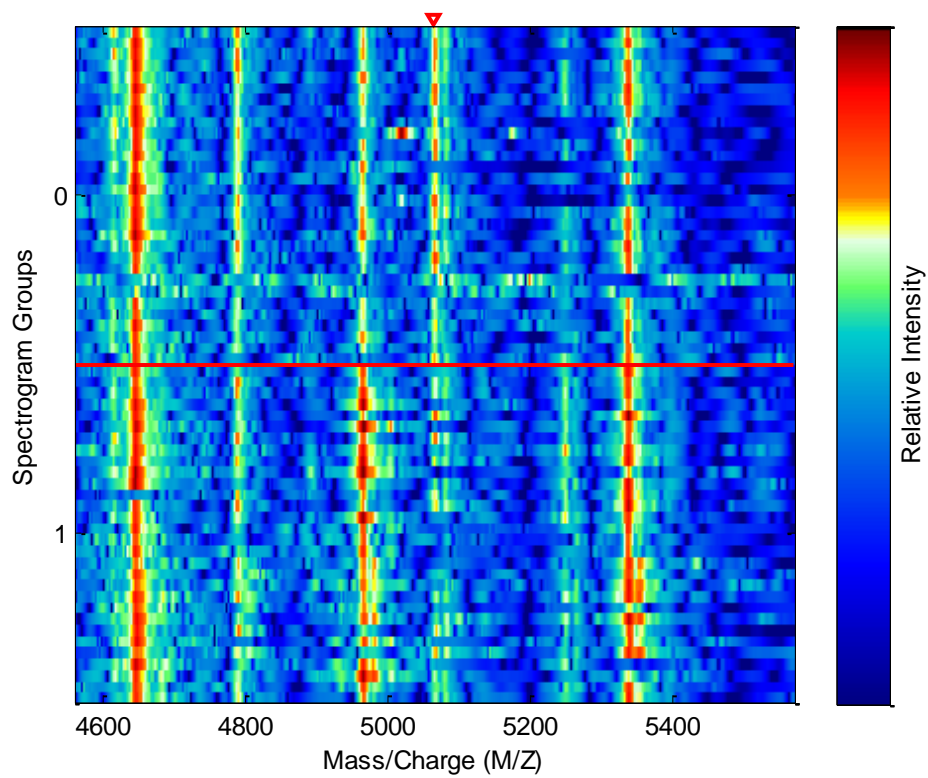
Gel figure: M/Z 4964



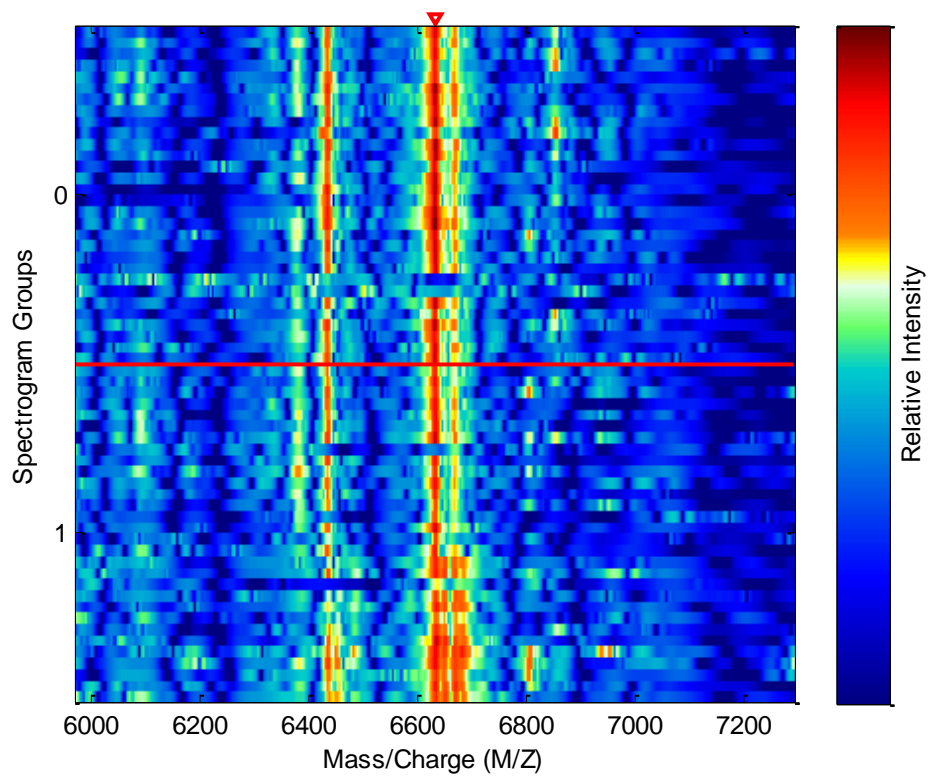
Gel figure: M/Z 4976



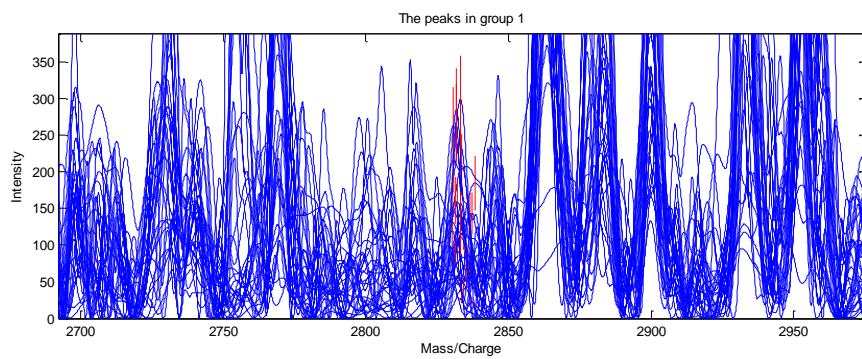
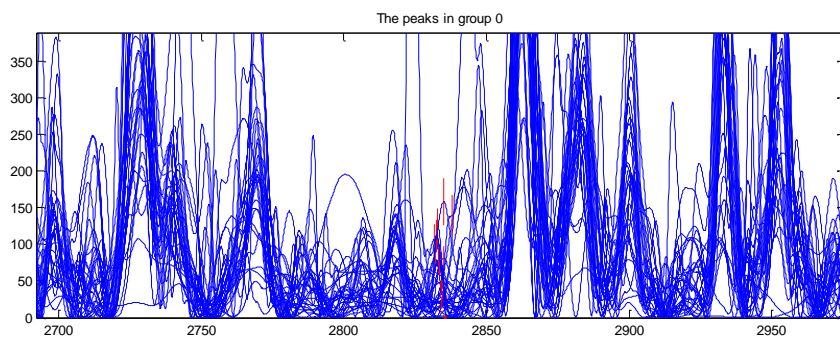
Gel figure: M/Z 4988



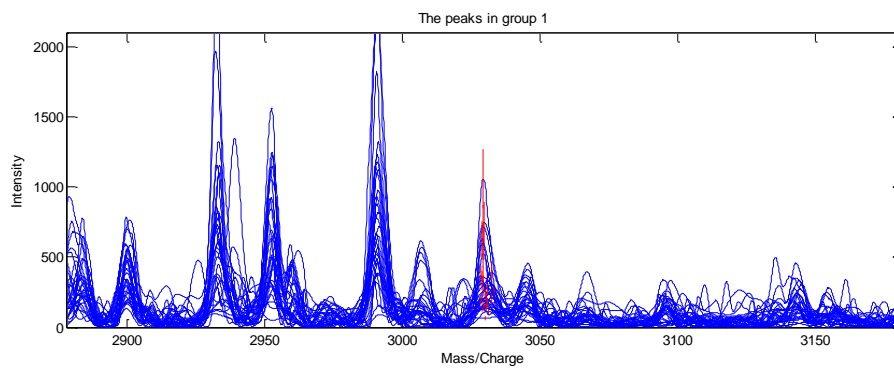
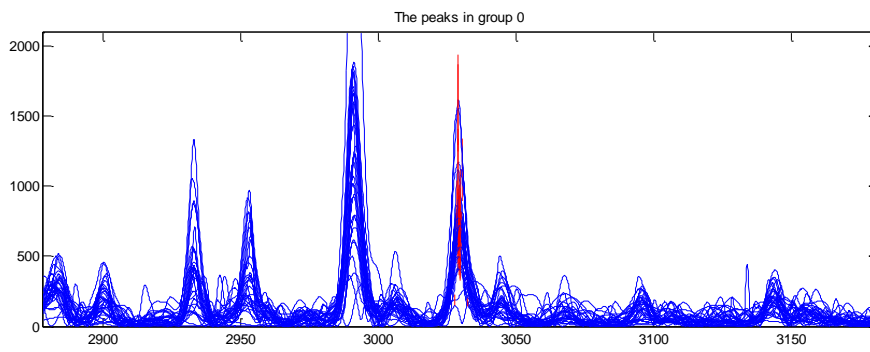
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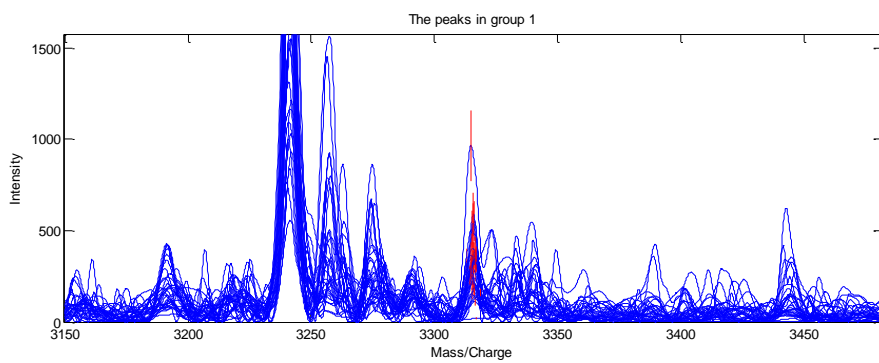
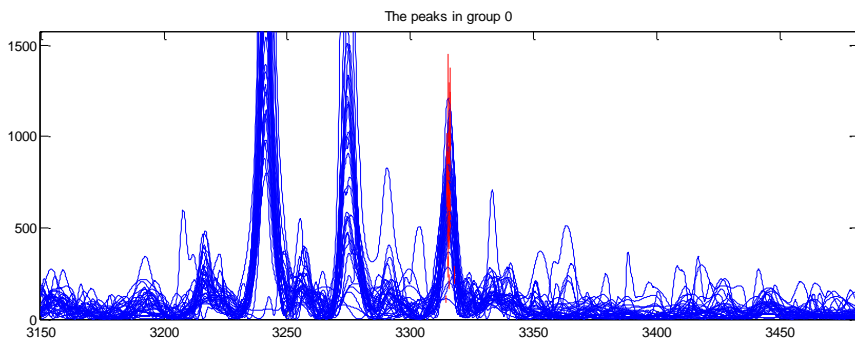
Gel figure: M/Z 6630



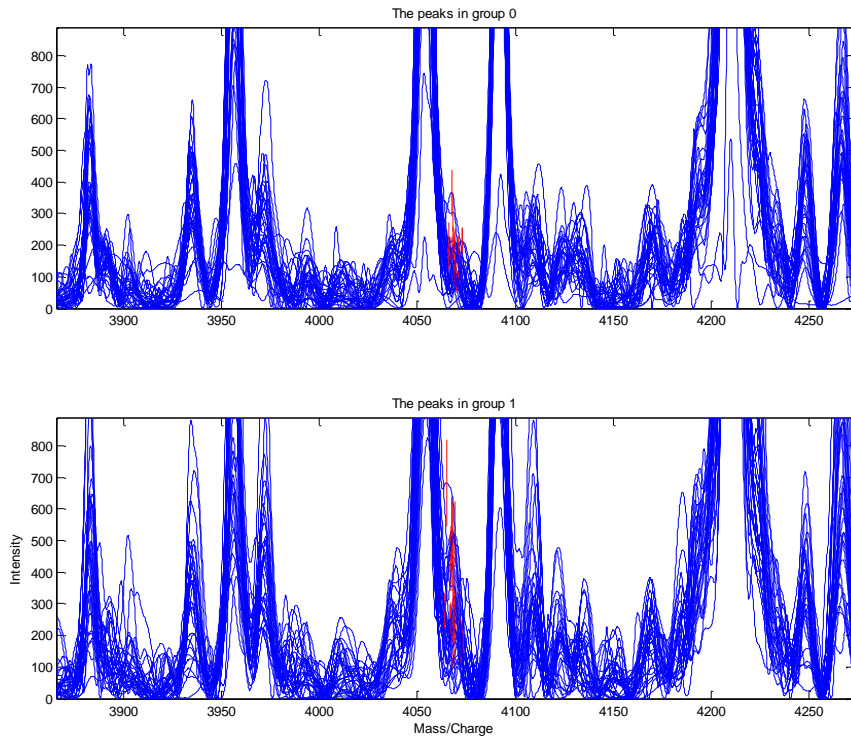
Peak figure: M/Z 2833



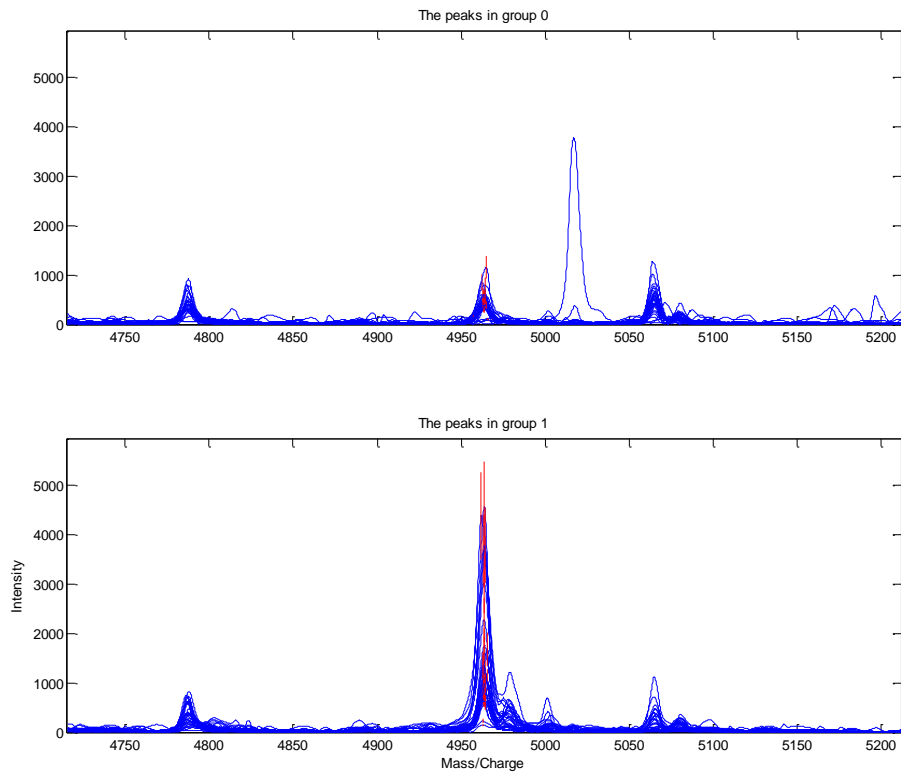
Peak figure: M/Z 3029



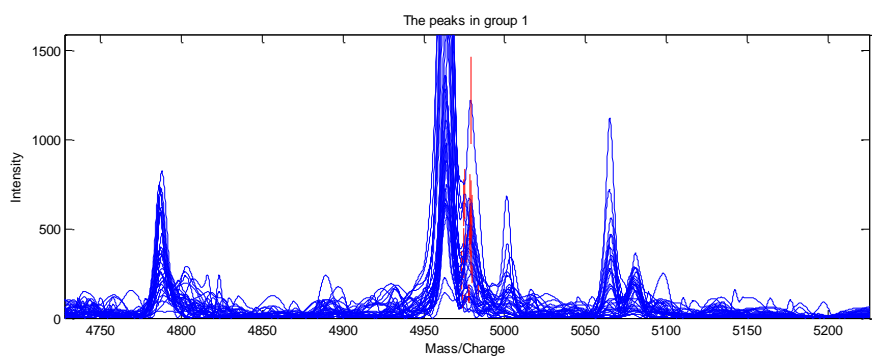
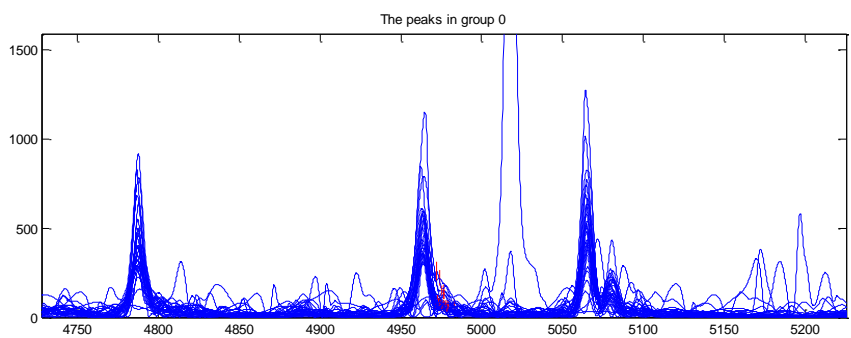
Peak figure: M/Z 3115



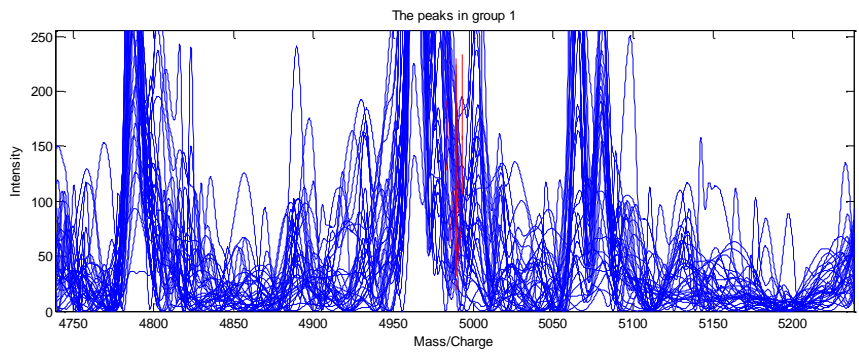
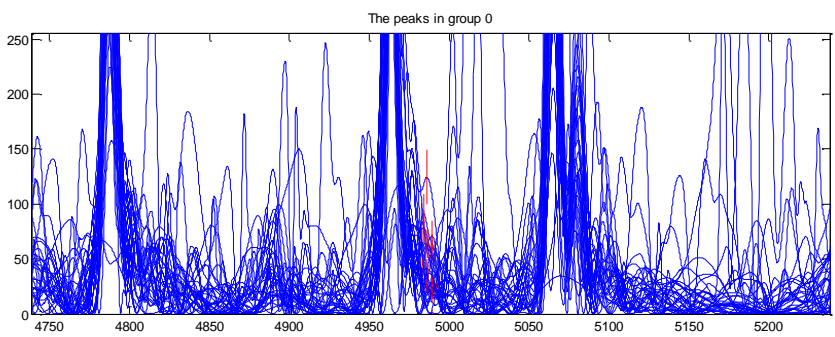
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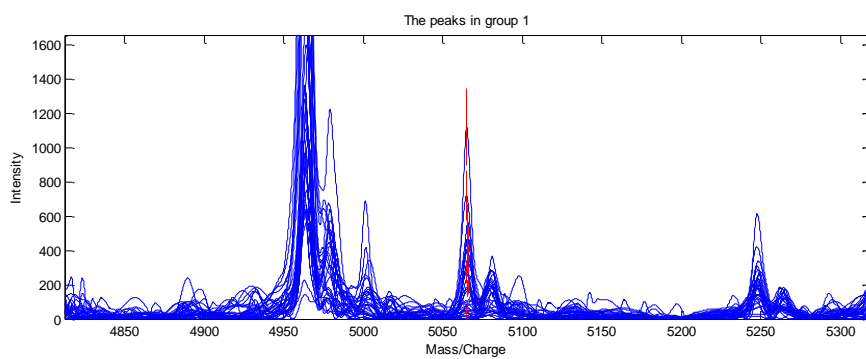
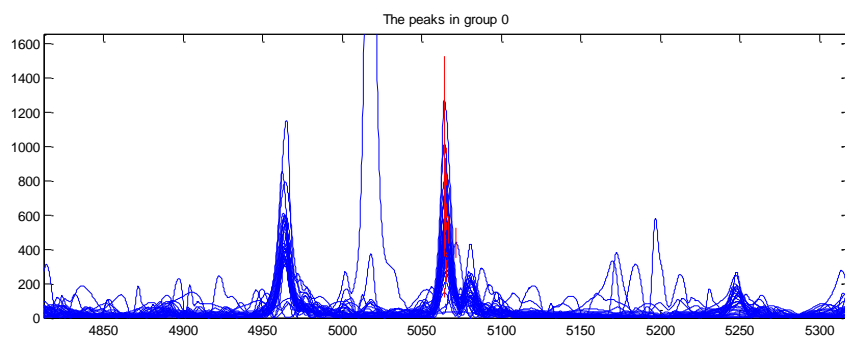
Peak figure: M/Z 4964



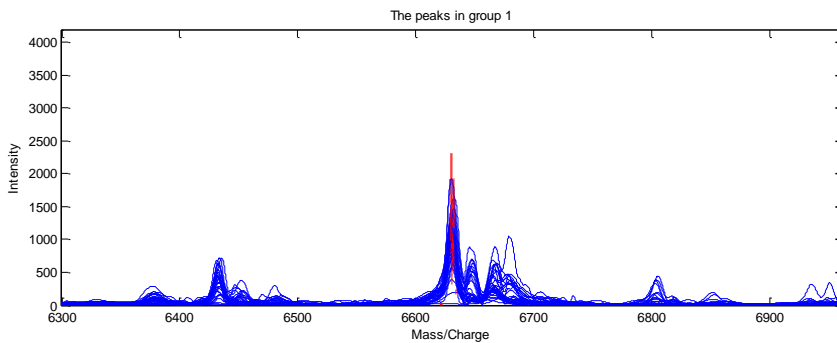
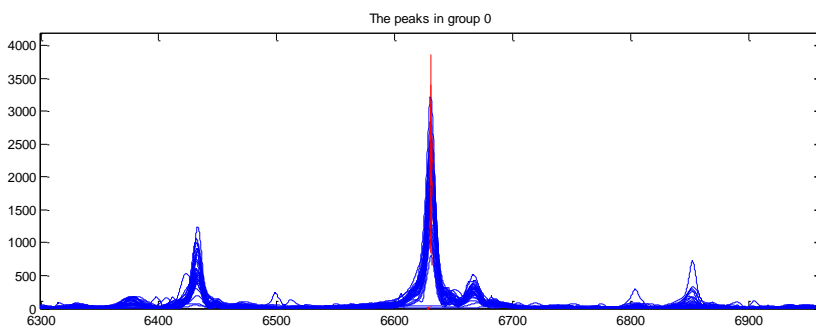
Peak figure: M/Z 4976



Peak figure: M/Z 4988



Peak figure: M/Z 5065



Peak figure: M/Z 6630

User Name zy2016 Peaks filtering factor Wilcoxon
 Repeat Sample 0 Small Size Sample No
 Test sample percent 0.3 Batch Analyze 1
 Wavelet threshold 100 Smoothing window 100
 Calibration coefficient (%)0.03 Minimal M/Z (%) 1000
 Cluster factor (%) 0.003 Minimal peak threshold (%) 0.1
 Excluded spectra threshold (%) 0.2 Minimal sinal/noise ratio (%) 2
 Minimal intensity 300 P value or Number of peaks 10
 Algorithm 1 Evaluation 1
 GA population 50 GA generation 20

Training result

| | Predicted Class 0 | Predicted Class 1 | Sum | Accuracy (%) | Error(%) |
|---------|-------------------|-------------------|-----|--------------|----------|
| Class 0 | 30 | 0 | 30 | 100 | 0 |
| Class 1 | 0 | 30 | 30 | 100 | 0 |

Validation result

| | Predicted Class 0 | Predicted Class 1 | Sum | Accuracy (%) | Error (%) |
|---------|-------------------|-------------------|-----|--------------|-----------|
| Class 0 | 29 | 1 | 30 | 96.6667 | 3.3333 |
| Class 1 | 1 | 29 | 30 | 96.6667 | 3.3333 |

selected markers is

4964.719 3029.7033 2833.9187 2900.1248

Biomarker M/Z

4976.5679 4964.719 3029.7033 4988.552 3315.7248
 2833.9187 6630.6521 4069.1778 2900.1248 5065.4939

P value or Weight

1.3111e-008 7.695e-008 7.043e-007 8.1975e-007 3.8349e-006
 1.0188e-005 1.5292e-005 2.7726e-005 3.5923e-005 3.5923e-005

Mean in Class0

91.5586 446.2517 747.9188 42.3675 666.6498
 50.7423 1746.3756 160.363 207.4617 505.9153

Mean in Class1

369.9864 1585.3402 321.625 108.3447 325.6311
 135.6622 1019.3287 299.7414 399.2346 232.4073

Std in Class0

49.6683 225.4799 327.0184 28.542 275.9018

43.03 721.7627 71.6869 114.6405 262.6943

Std in Class1

252.5572 1255.3035 228.6694 51.7756 180.4535

81.0189 436.1463 151.9196 183.067 251.7712