

100 – method for analysing
LC-ESI-MS data

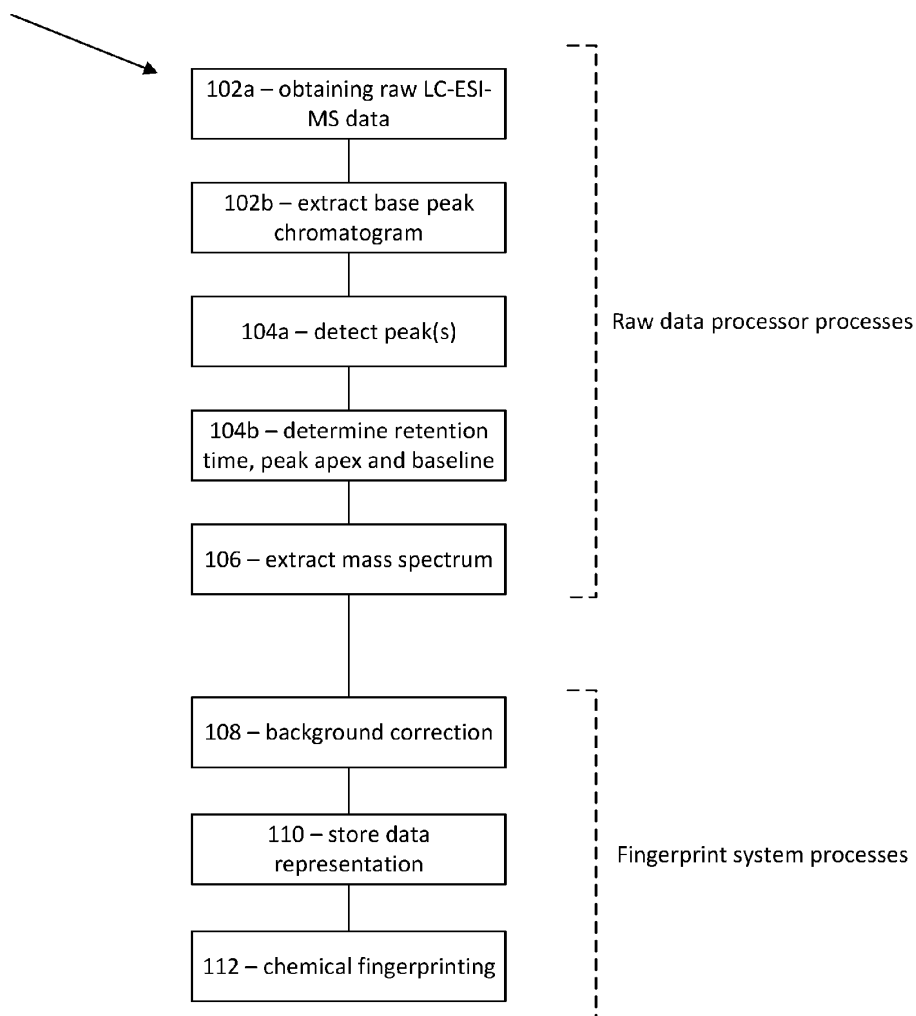
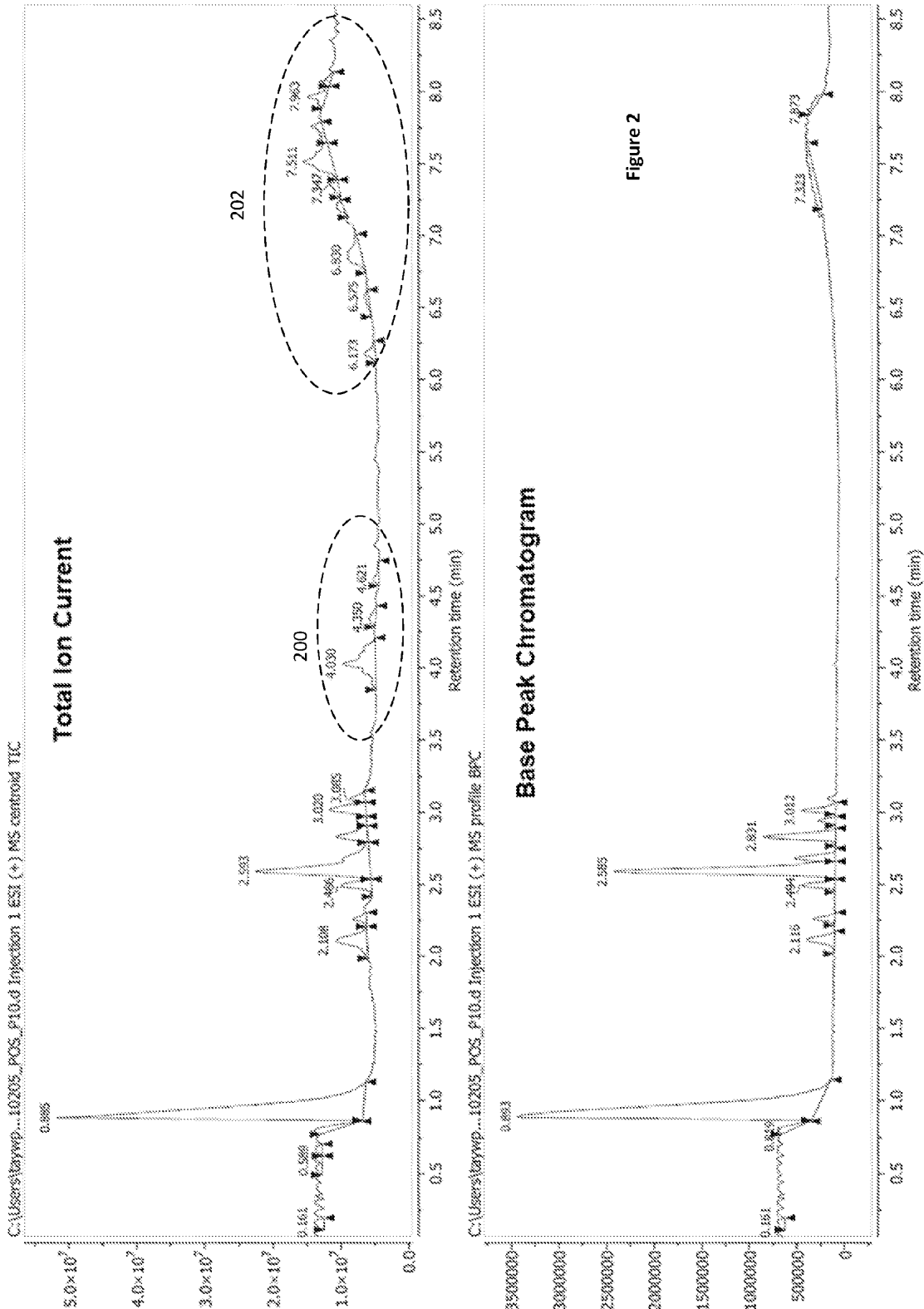
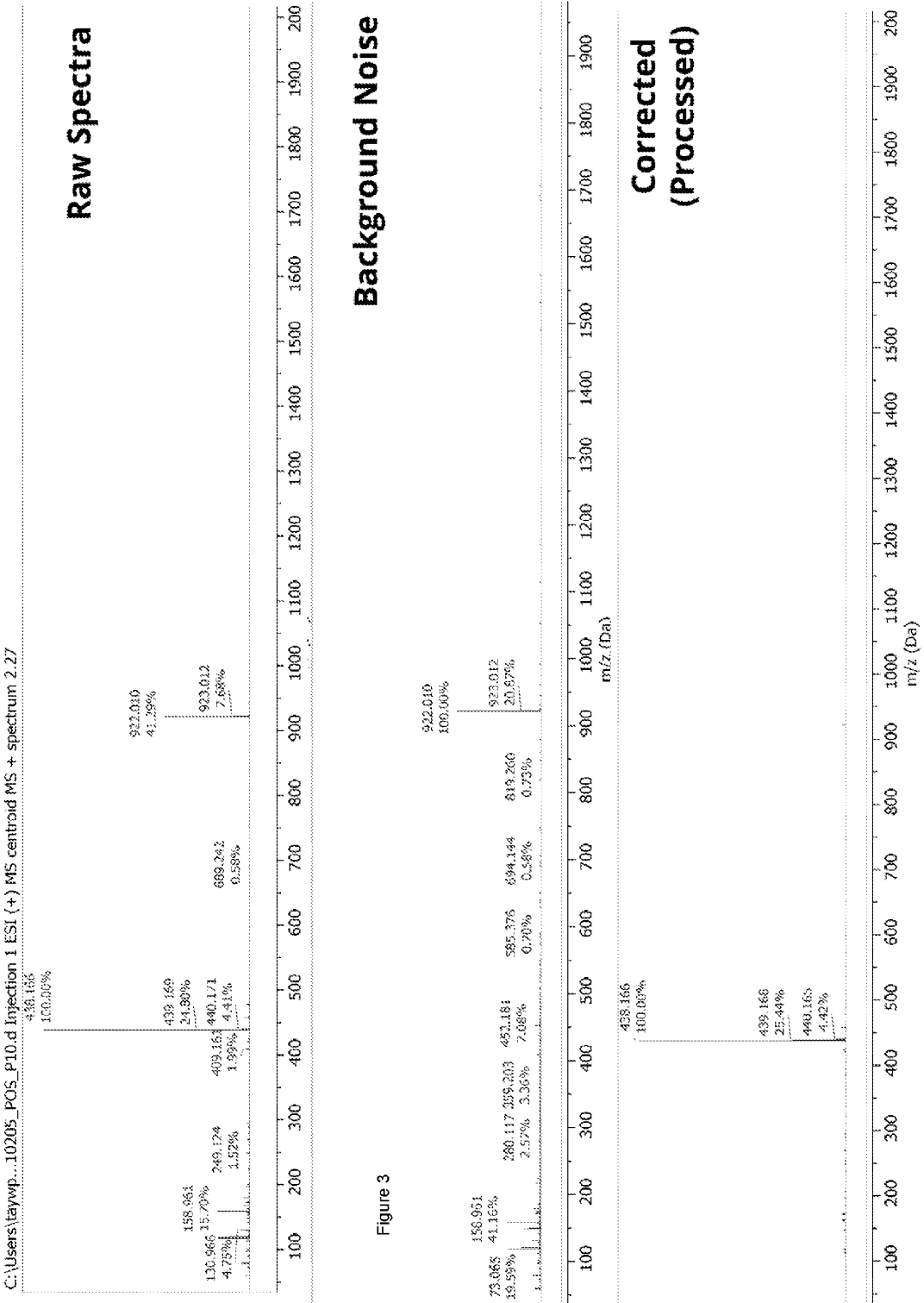
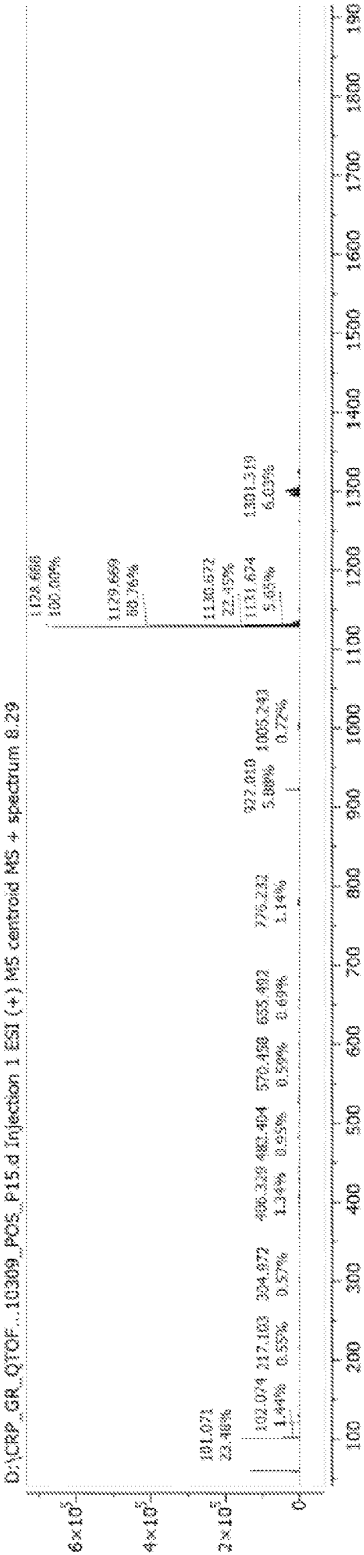


Figure 1







Sample	RT (min)
C ₅₃ theory	1.608
Sample-1	1.604
Sample-2	1.597
C ₅₄ theory	1.578
Sample-3	1.561
C ₅₅ theory	1.549

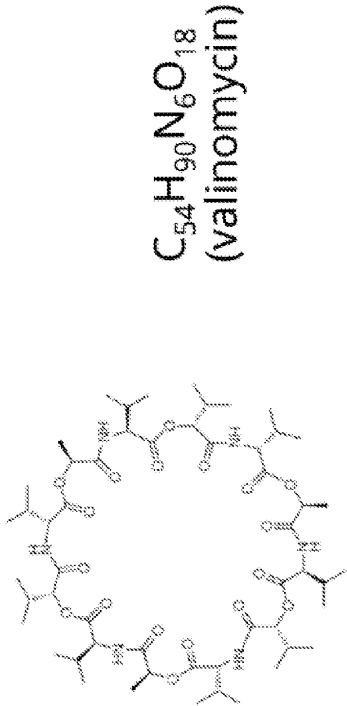


Figure 4

A

abundance	{Alt}																		
Max of abundance		Column Labels																	
Row Labels	v	2	17	25	28	30	31	32	33	34	36	37	38	39 Grand Total					
A100055		1.90E+06	1.80E+05	3.90E+05	4.50E+05	1.80E+05								1.90E+06					
CA021.B		3.00E+05												3.00E+05					
CA071.B		1.80E+05												1.80E+05					
CA091.B			3.90E+05											3.90E+05					
CA101.B		1.90E+06			4.50E+05	1.80E+05								1.90E+06					
A100056		2.50E+06			1.90E+05	2.70E+05	2.10E+05	2.90E+05						2.50E+06					
A100058		1.30E+06	1.90E+05			2.00E+05			1.60E+05					1.30E+06					
A100060		1.10E+06			1.70E+05									1.10E+06					
A100061		1.30E+06			1.70E+05					2.20E+05				1.30E+06					
A100196		4.00E+05					3.00E+05		2.80E+05			2.20E+05	1.80E+05	4.00E+05					
Grand Total		2.50E+06	1.90E+05	3.90E+05	4.50E+05	2.00E+05	2.70E+05	2.10E+05	2.90E+05	2.00E+05	2.20E+05	2.20E+05	1.80E+05	2.50E+06					

B

PivotTable Fields

Choose fields to add to reports

Search

☐ Sample

☐ RT

☐ peaks

☐ largest m/z

☐ most abundant m/z

☒ abundance

☒ compound no.

☒ strain

☒ media

☐ GR

More Tables...

C

Drag fields between areas below

Filters

abundance

Columns

compound no.

Rows

strain

media

Values

Max of abundance

Figure 5

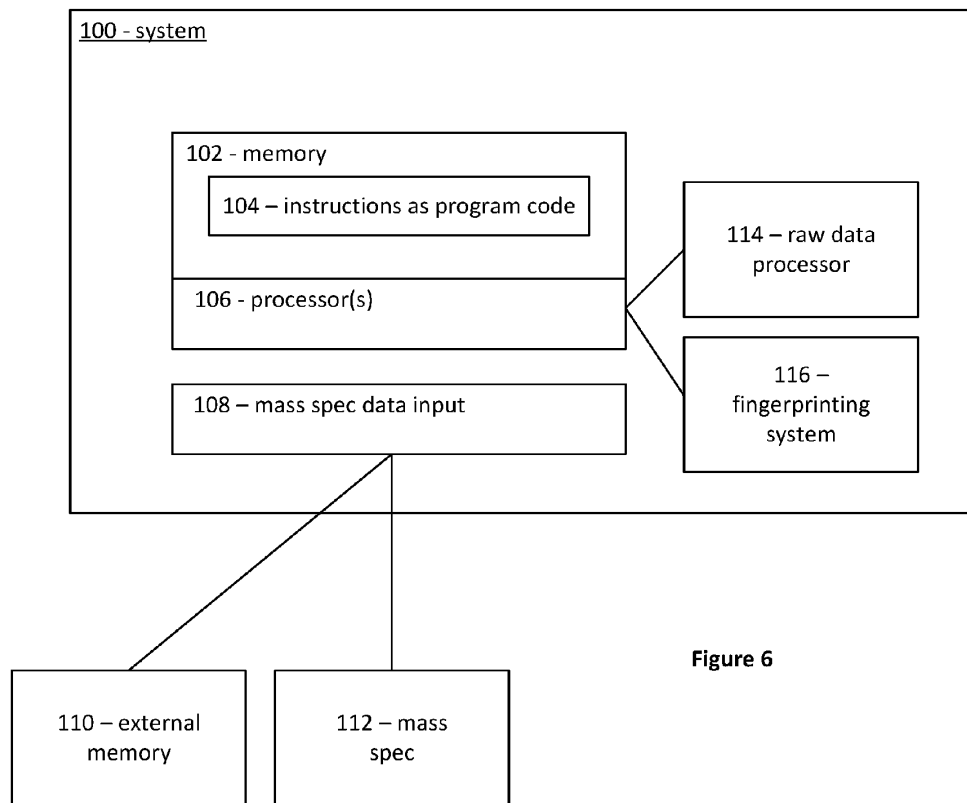


Figure 6