Supporting Information

iTRAQ-based proteomic analysis reveals recovery of impaired mitochondrial function in ischemic myocardium by Shenmai formula

Yi Wang[1], Yu Zhao[1], Wei Jiang[1], Xiaoping Zhao[2*], Guanwei Fan[3], Han Zhang[3], Peiqiang Shen[4], Jiangmin He[4], Xiaohui Fan[1*]

[1]Pharmaceutical Informatics Institute, College of Pharmaceutical Sciences, Zhejiang University, Hangzhou, P.R. China;

[2]College of Preclinical Medicine, Zhejiang Chinese Medical University, Hangzhou 310053, P.R. China;

[3]Tianjin State Key Laboratory of Modern Chinese Medicine, Tianjin University of Traditional Chinese Medicine, Tianjin 300193, P.R. China;

[4] Chiatai Qingchunbao Pharmaceutical Co., Ltd. Hangzhou, 310023, P.R. China;

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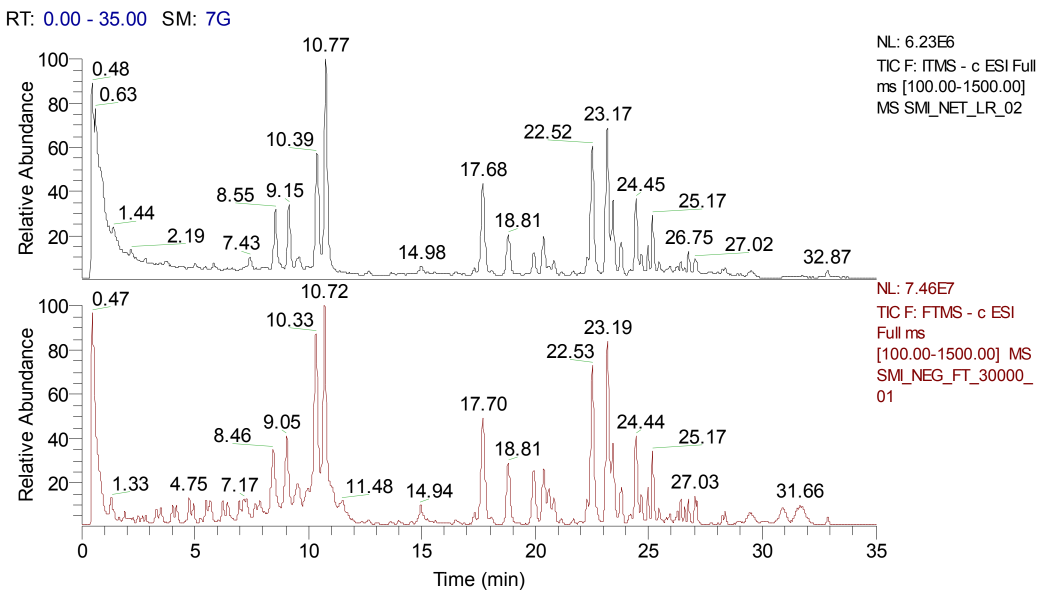
Supporting Information1.

Total ion chromatogram of SM, RG and OP were analyzed. Identification of each peak was listed in the following Table.

1) Total ion chromatogram of SM and peak analysis.



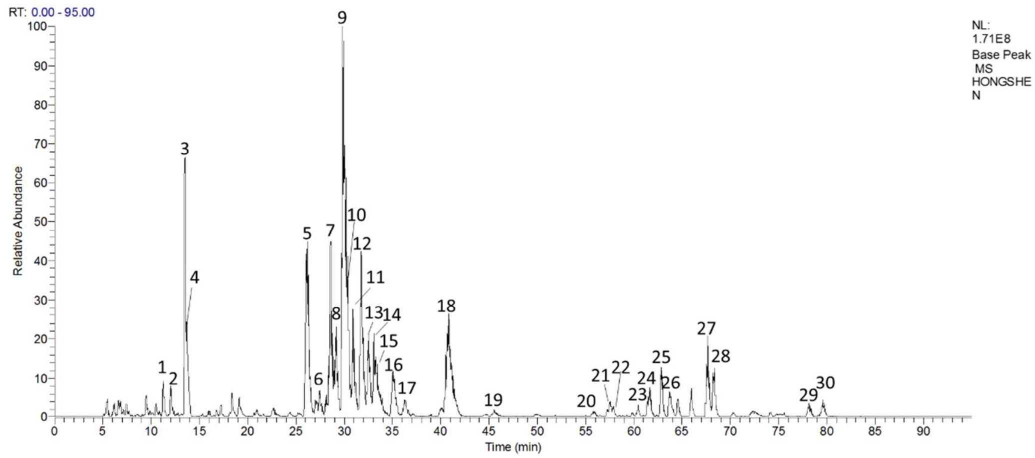
No.	t_R	Ions	Molecular Formula	RDB	Error /ppm	Resorces[1)]	Name of compounds
1	7.27	653.42628	$C_{36}H_{62}O_{10}$	6.5	-1.13	HS	Hydroxy-ginsenoside Rh1
2	7.29	961.53650	$C_{48}H_{82}O_{19}$	8.5	-1.30	HS	20glcRf iso
3	8.45	961.53668	$C_{48}H_{82}O_{19}$	8.5	-1.12	HS	20glcRf
4	9.06	931.52576	$C_{47}H_{80}O_{18}$	8.5	-1.53	HS	Ginsenoside R_1
	9.41	447.22321	$C_{21}H_{36}O_{10}$	4.5	-0.81	MD	Borneol
5	9.53	961.53650	$C_{48}H_{82}O_{19}$	8.5	-1.30	HS	20glcRf iso
6	10.03	961.53607	$C_{48}H_{82}O_{19}$	8.5	-1.75	HS	20glcRf iso
7	10.33	799.48480	$C_{42}H_{72}O_{14}$	7.5	-0.16	HS	Ginsenoside Rg1
8	10.72	945.54206	$C_{48}H_{82}O_{18}$	8.5	-0.82	HS	Ginsenoside Re
9	14.94	841.49597	$C_{44}H_{74}O_{15}$	8.5	0.57	HS	acetylated Ginsenoside Rg1
10	17.34	987.55194	$C_{50}H_{84}O_{19}$	9.5	-1.48	HS	acetylated Ginsenoside Re
11	17.70	799.48383	$C_{42}H_{72}O_{14}$	7.5	-1.38	HS	Ginsenoside Rf
12	18.82	769.47400	$C_{41}H_{70}O_{13}$	7.5	-0.48	HS	NR2

13	19.95	637.43182	$C_{36}H_{62}O_9$	6.5	-0.45	HS	Ginsenoside Rh_1
14	20.04	769.47357	$C_{41}H_{70}O_{13}$	7.5	-1.03	HS	NR2 iso
15	20.38	783.48926	$C_{42}H_{72}O_{13}$	7.5	-0.96	HS	Ginsenoside 20(R)-Rg2
16	20.61	637.43146	$C_{36}H_{62}O_9$	6.5	-1.01	HS	Ginsenoside F1
17	20.81	783.48895	$C_{42}H_{72}O_{13}$	7.5	-1.36	HS	Ginsenoside 20(S) Rg2
18	21.15	1,269.64624	$C_{60}H_{102}O_{28}$	10.5	-1.77	HS	Rb1+glc
19	21.68	1,105.57764	$C_{54}H_{90}O_{23}$	10.5	-2.15	HS	Rh4+3glc
20	22.28	1,209.62549	$C_{58}H_{98}O_{26}$	10.5	-1.53	HS	Ginsenoside Ra1
21	22.53	1,107.59351	$C_{54}H_{92}O_{23}$	9.5	-1.94	HS	Ginsenoside Rb1
22	23.19	955.48987	$C_{48}H_{76}O_{19}$	11.5	-0.98	HS	Ginsenoside Ro
23	23.29	1,047.49890	$C_{50}H_{80}O_{23}$	11.5	-2.73	MD	O3
24	23.42	1,077.58435	$C_{53}H_{90}O_{22}$	9.5	-0.69	HS	Ginsenoside Rc
25	23.66	1017.49084	$C_{49}H_{78}O_{22}$	11.5	-0.35	MD	O2+132
26	23.79	1,209.62549	$C_{58}H_{98}O_{26}$	10.5	-1.54	HS	Ginsenoside Ra2
27	24.17	915.45850	$C_{45}H_{72}O_{19}$	10.5	-1.10	MD	O1
28	24.20	1,209.62561	$C_{58}H_{98}O_{26}$	10.5	-1.44	HS	Ra_2 iso
29	24.44	1,077.58374	$C_{53}H_{90}O_{22}$	9.5	-1.26	HS	Ginsenoside Rb2
30	24.53	753.40564	$C_{39}H_{62}O_{14}$	9.5	-1.38	HS	O1-glc
31	24.67	1,077.58337	$C_{53}H_{90}O_{22}$	9.5	-1.60	HS	Ginsenoside Rb_3
32	24.71	885.44806	$C_{44}H_{70}O_{18}$	10.5	-0.99	MD	O2
33	24.96	793.43726	$C_{42}H_{66}O_{14}$	10.5	-0.91	HS	Ro-glc
34	24.97	1,149.60474	$C_{56}H_{94}O_{24}$	10.5	-1.29	HS	Rb1+Ac
35	25.17	945.54211	$C_{48}H_{82}O_{18}$	8.5	-0.77	HS	Ginsenoside Rd
36	25.23	1,119.59521	$C_{55}H_{92}O_{23}$	10.5	-0.40	HS	acetylated ginsenosideRb2
37	25.45	1,119.59460	$C_{55}H_{92}O_{23}$	10.5	-0.95	HS	acetylated ginsenosideRb3
38	25.75	781.47345	$C_{42}H_{70}O_{13}$	8.5	-1.17	HS	Rf-H2O
39	25.78	1031.50574	$C_{50}H_{80}O_{22}$	11.5	-1.07	MD	O3-O
40	25.89	987.55231	$C_{50}H_{84}O_{19}$	9.5	-1.11	HS	acetylated ginsenosideRd
41	25.95	781.47339	$C_{42}H_{70}O_{13}$	8.5	-1.25	HS	Rf-H2O
42	26.13	751.46271	$C_{41}H_{68}O_{12}$	8.5	-1.45	HS	NR2-H2O
43	26.19	987.55200	$C_{50}H_{84}O_{19}$	9.5	-1.42	HS	Rd+Ac
44	26.26	765.47852	$C_{42}H_{70}O_{12}$	8.5	-1.22	HS	ginsenosideRg6/Rg4
45	26.30	751.46271	$C_{41}H_{68}O_{12}$	8.5	-1.45	HS	NR2-H_2O
46	26.40	619.42151	$C_{36}H_{60}O_8$	7.5	-0.05	HS	ginsenosideRk3/Rh4
47	26.41	765.47894	$C_{42}H_{70}O_{12}$	8.5	-0.67	HS	ginsenosideRg6/Rg4
48	26.58	619.42151	$C_{36}H_{60}O_8$	7.5	-0.05	HS	ginsenosideRk3/Rh4
49	26.76	793.43726	$C_{42}H_{66}O_{14}$	10.5	-0.91	HS	Ro-glc
50	27.03	783.48932	$C_{42}H_{72}O_{13}$	7.5	-0.89	HS	20(R)-Rg_3
51	27.12	783.48926	$C_{42}H_{72}O_{13}$	7.5	-0.96	HS	20(S)-Rg_3
52	27.72	825.49994	$C_{44}H_{74}O_{14}$	8.5	-0.78	HS	Rs_3iso
53	27.78	825.50024	$C_{44}H_{74}O_{14}$	8.5	-0.41	HS	Rs_3iso
54	28.25	765.47833	$C_{42}H_{70}O_{12}$	8.5	-1.46	HS	Ginsenoside Rk1/Rg5

55	28.36	765.47839	$C_{42}H_{70}O_{12}$	8.5	-1.39	HS	Ginsenoside Rk1/Rg5

1) HS represents *Red Ginseng*; MD represents *Radix Ophiopogonis*.

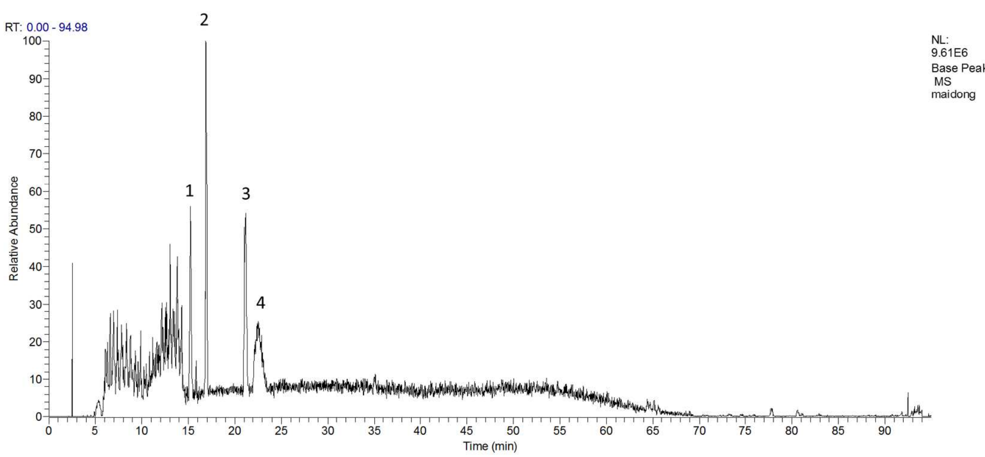
2) Total ion chromatogram of RG and peak analysis.



Peak	RT(min)	Observed m/z	Molecular formula	Error (ppm)	Compounds
1	11.21	961.5366	$C_{48}H_{82}O_{19}$	-1.12	20glcRf
2	12	931.5257	$C_{47}H_{80}O_{18}$	-1.53	Ginsenoside R1
3	13.47	945.5420	$C_{48}H_{82}O_{18}$	-0.82	Ginsenoside Re
4	13.72	799.4848	$C_{42}H_{72}O_{14}$	-0.16	Ginsenoside Rg1
5	26.19	799.4838	$C_{42}H_{72}O_{14}$	-1.38	Ginsenoside Rf
6	27.41	1209.63	$C_{58}H_{98}O_{26}$	-1.53	Ginsenoside Ra1
7	28.56	1107.59	$C_{54}H_{92}O_{23}$	-1.94	Ginsenoside Rb1
8	29.17	769.4740	$C_{41}H_{70}O_{13}$	-0.48	NR2
9	29.97	955.4898	$C_{48}H_{76}O_{19}$	-0.98	Ginsenoside Ro
10	30.71	1209.63	$C_{58}H_{98}O_{26}$	-1.54	Ginsenoside Ra2
11	30.96	1077.58	$C_{53}H_{90}O_{22}$	-0.69	Ginsenoside Rc
12	31.84	783.4892	$C_{42}H_{72}O_{13}$	-0.96	20(R)Rg2
13	32.57	783.4889	$C_{42}H_{72}O_{13}$	-1.36	20(S)Rg2
14	33.16	1077.58	$C_{53}H_{90}O_{22}$	-1.26	Ginsenoside Rb2
15	33.45	637.4318	$C_{36}H_{62}O_{9}$	-0.45	Ginsenoside Rh1
16	35.12	637.4314	$C_{36}H_{62}O_{9}$	-1.01	Ginsenoside F1
17	36.23	653.4262	$C_{36}H_{62}O_{10}$	-1.13	Hydroxy Ginsenoside Rh1
18	40.78	945.5421	$C_{48}H_{82}O_{18}$	-0.77	Ginsenoside Rd
19	45.56	1119.59	$C_{55}H_{92}O_{23}$	-0.95	Acetyl ginsenoside Rb3
20	55.82	781.4734	$C_{42}H_{70}O_{13}$	-1.17	Rf-H2O

21	57.23	961.5365	$C_{48}H_{82}O_{19}$	-1.3	20glcRf iso
22	57.53	987.5519	$C_{50}H_{84}O_{19}$	-1.48	Ginsenoside Re
23	60.4	751.4627	$C_{41}H_{68}O_{12}$	-1.45	NR2-H2O
24	61.67	765.4785	$C_{42}H_{70}O_{12}$	-1.22	Ginsenoside Rg6/Rg4
25	62.85	765.4789	$C_{42}H_{70}O_{12}$	-0.67	Ginsenoside Rg6/Rg4
26	63.74	793.4372	$C_{42}H_{66}O_{14}$	-0.91	Ro-glc
27	67.65	783.4893	$C_{42}H_{72}O_{13}$	-0.89	20(R)Rg3
28	68.21	783.4892	$C_{42}H_{72}O_{13}$	-0.96	20(S)Rg3
29	78.1	765.4783	$C_{42}H_{70}O_{12}$	-1.46	Ginsenoside Rk1/Rg5
30	79.58	765.4783	$C_{42}H_{70}O_{12}$	-1.39	Ginsenoside Rk1/Rg5

3) Total ion chromatogram of OP and peak analysis.



Peak	RT(min)	Observed m/z	Molecular	Error (ppm)	Compounds
1	15.14	187.36			
2	16.89	447.2232	$C_{21}H_{36}O_{10}$	-0.81	2-Bornanol, (1S,2R)-form,O-[α-l-arabinofuranosyl-(1 → 6)-β-d-glucopyranoside]
3	21.20	201.26			
4	22.54	233.30			

Supporting Information 2.xlsx/ All identified proteins

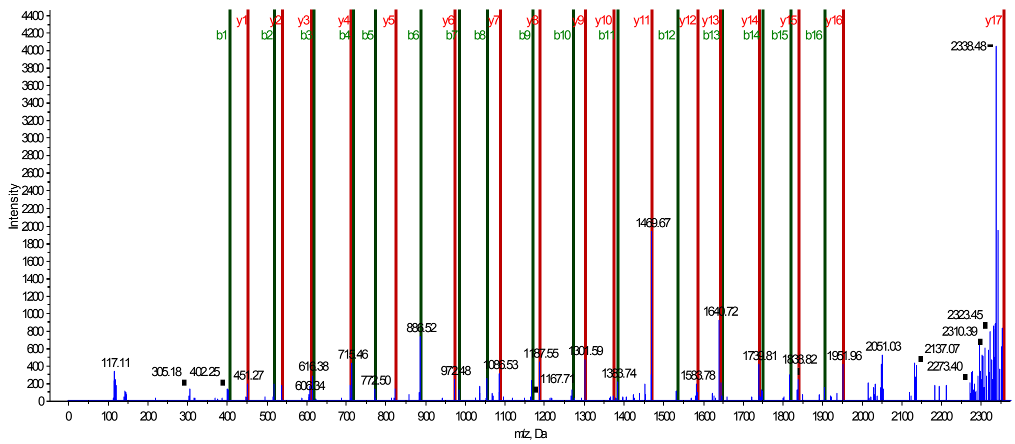
Supporting Information 3.xlsx/ 101 differentially expressed proteins

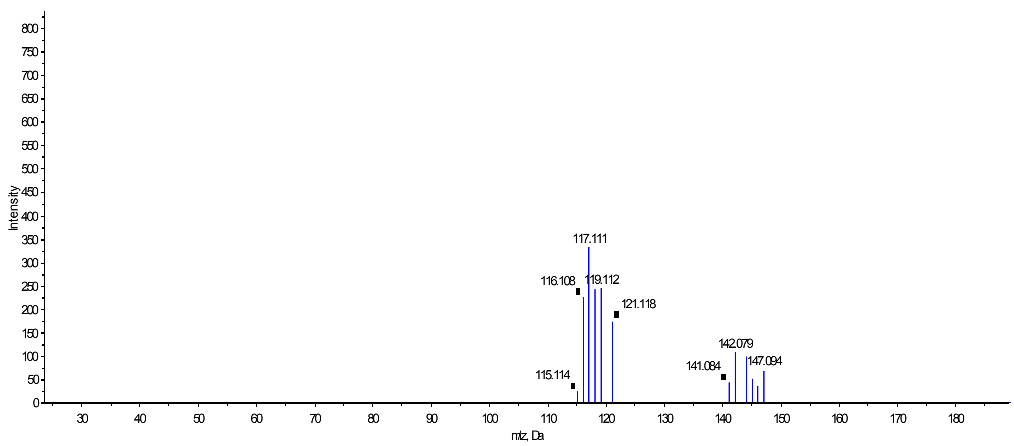
Supporting Information 4

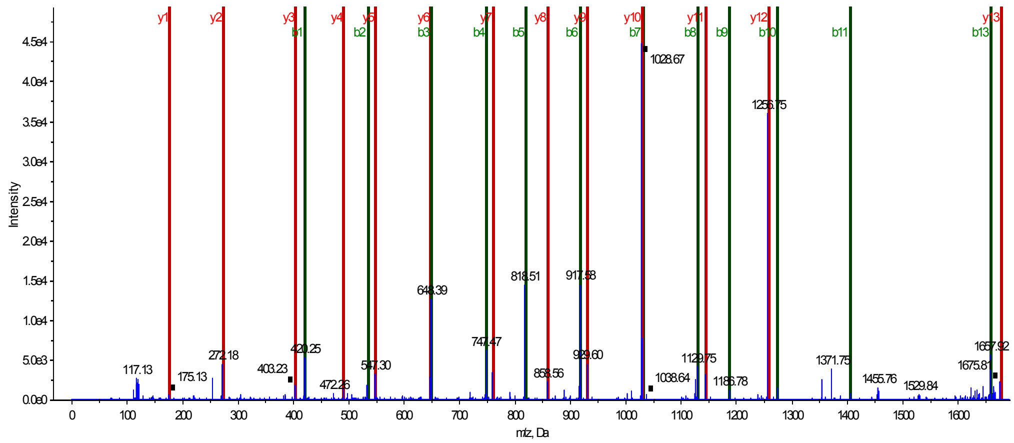
Peptide chromatograms for the identification of two representative proteins (ATP5D and MDH1)

Spectra was generated directly from ProteinPilot Software 4.5. The reporter ion region is shown below each peptide spectra.

IPI00198717.8	Mdh1 Malate dehydrogenase, cytoplasmic






y1
y2
y3
y4
y5
y6
y7
y8
y9
y10
y11
y12
y13
b1
b2
b3
b4
b5
b6
b7
b8
b9
b10
b11
b13
1028.67
1256.75
818.51
917.58
747.47
272.18
117.13
175.13
403.23
420.25
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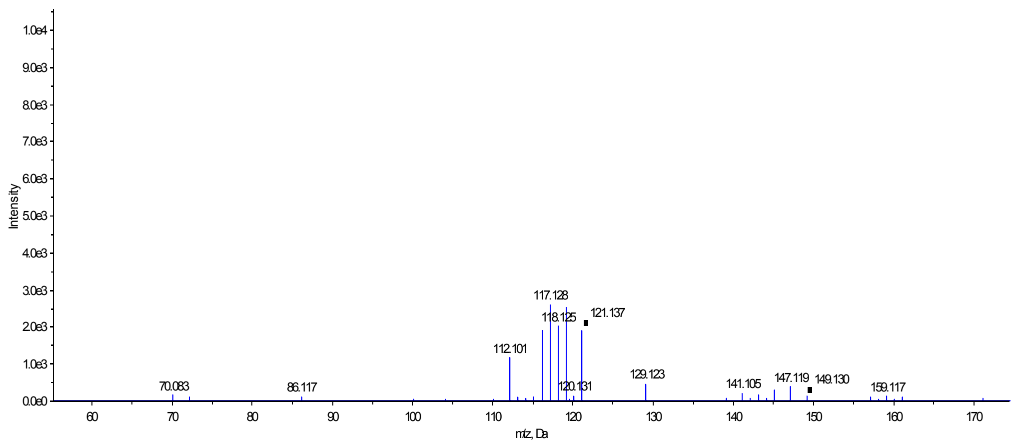
1038.64
1129.75
1371.75
1455.76
1529.84
1675.81
1657.92
Intensity
m/z, Da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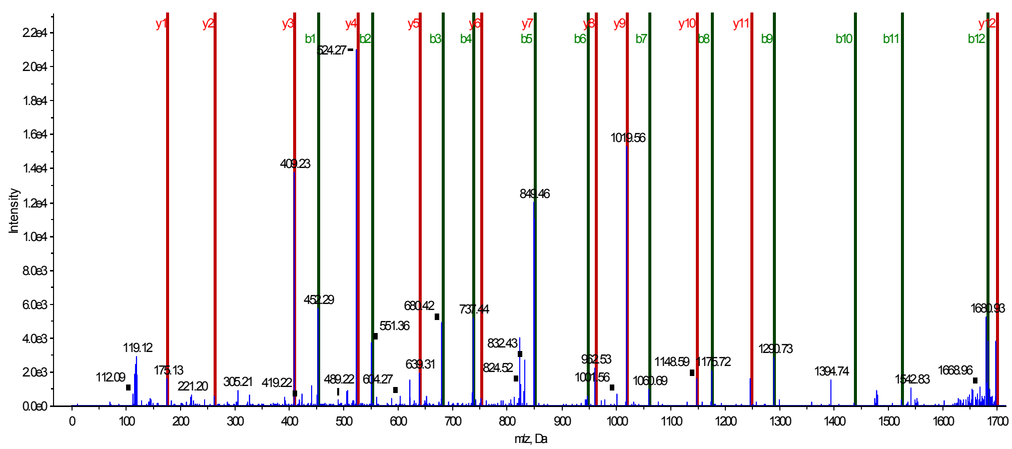
149.130
159.117
Intensity
m/z, Da


y1
y2
y3
y4
y5
y6
y7
y8
y9
y10
y11
y12
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b2
b3
b4
b5
b6
b7
b8
b9
b10
b11
b12
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1019.56
409.23
849.46
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551.36
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112.09
175.13
221.20
305.21
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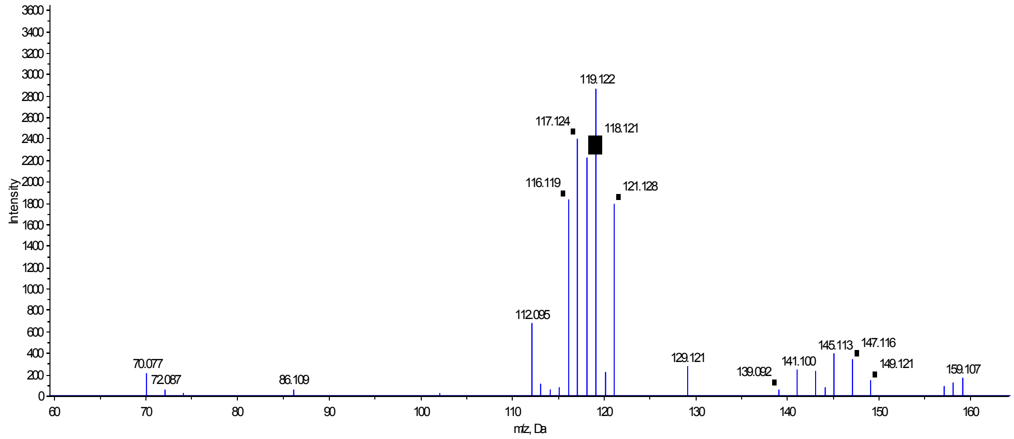
1680.93
Intensity
m/z, Da



Intensity
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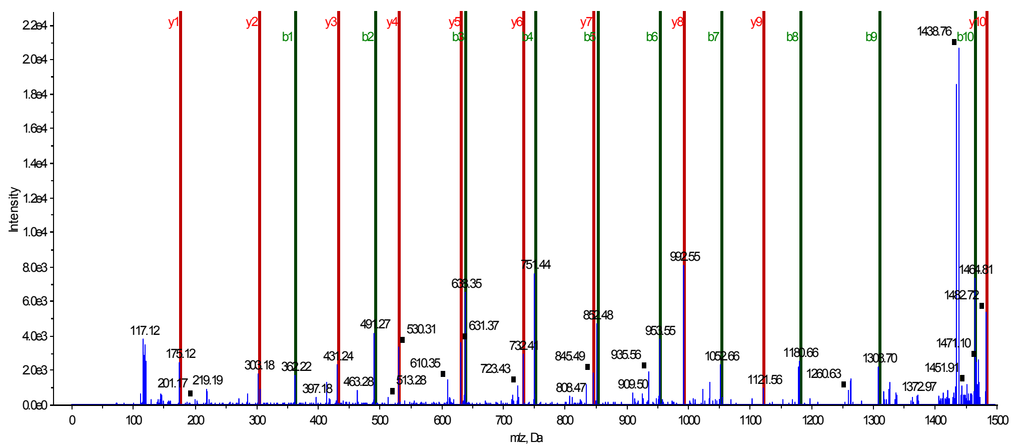

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m/z, Da
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751.44
1464.81
1482.72
4.0e3
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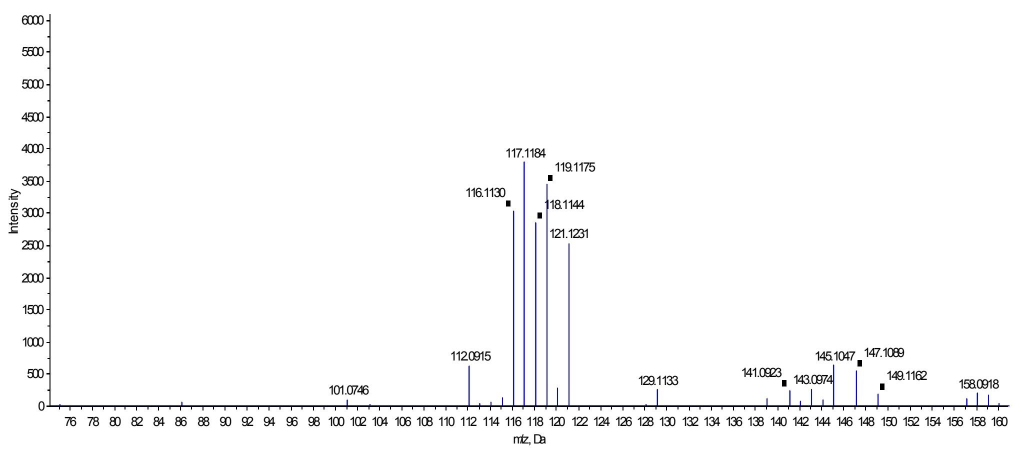

Intensity
m/z, Da
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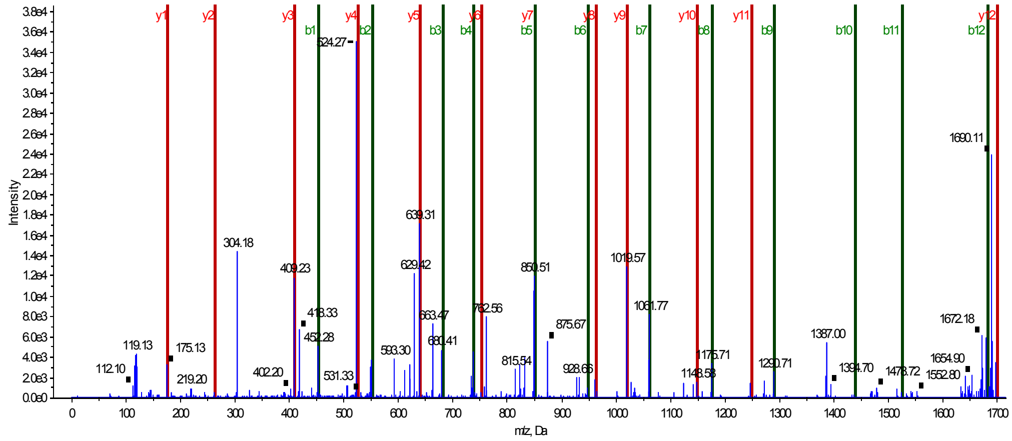

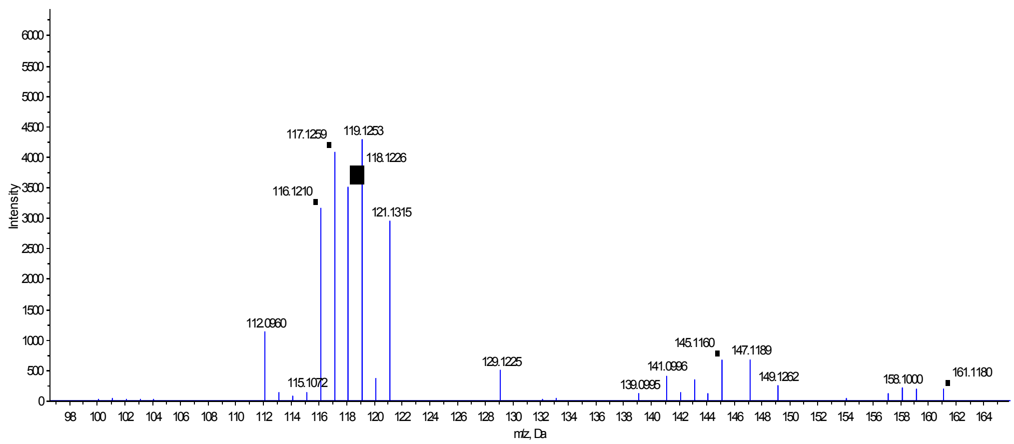

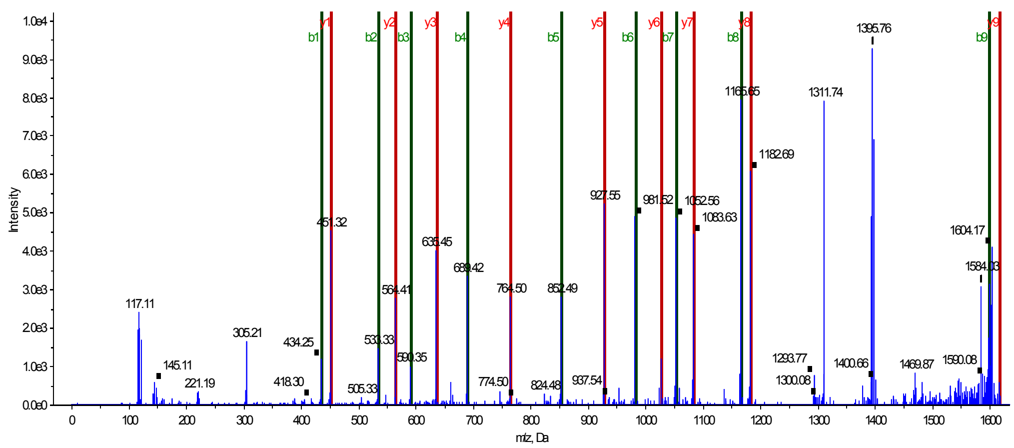

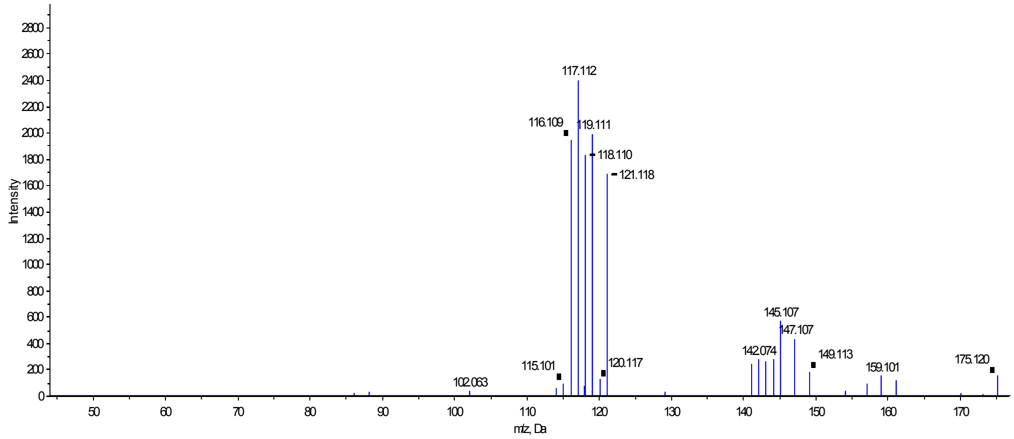
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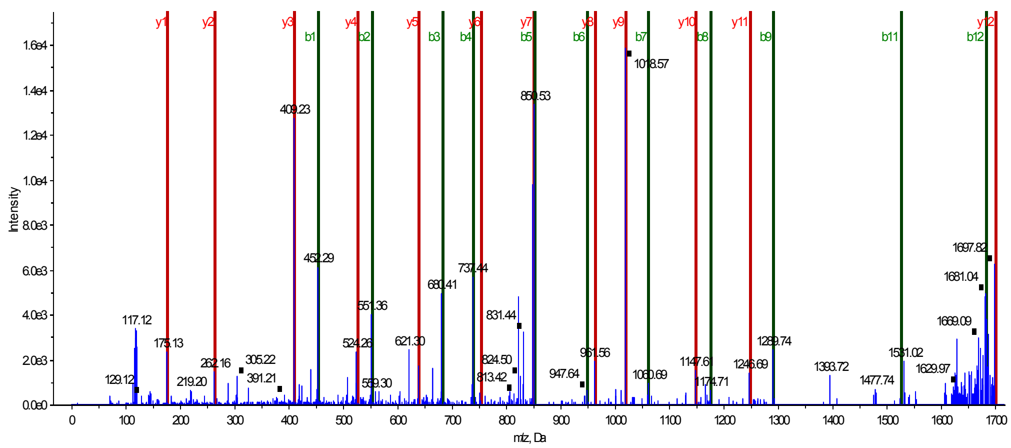
102.063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m/z, Da
y1
y2
y3
y4
y5
y6
y7
y8
y9
y10
y11
y12
b1
b2
b3
b4
b5
b6
b7
b8
b9
b11
b12
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409.23
850.53
452.29
1697.82
737.44
680.41
1681.04
551.36
831.44
117.12
1669.09
175.13
1289.74
305.22
262.16
961.56
824.50
1531.02
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1246.69
1393.72
621.30
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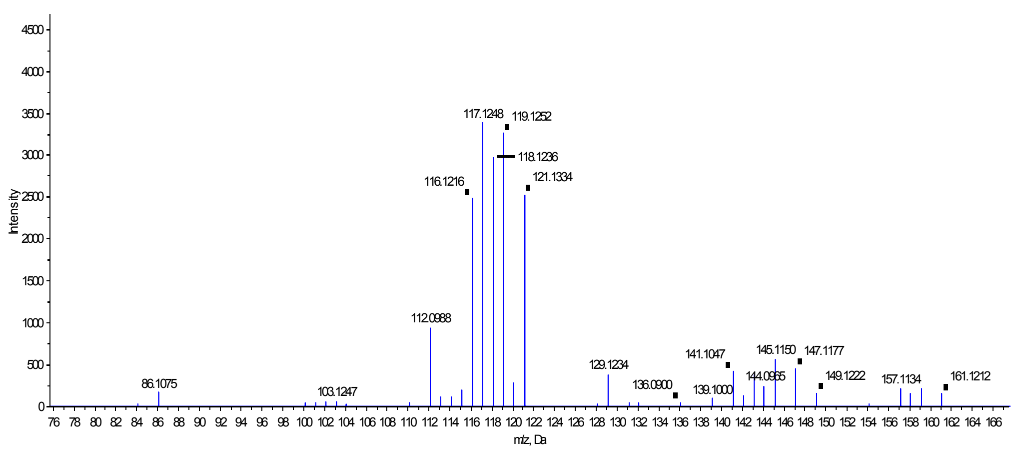
1477.74
1629.97
559.30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161.1212
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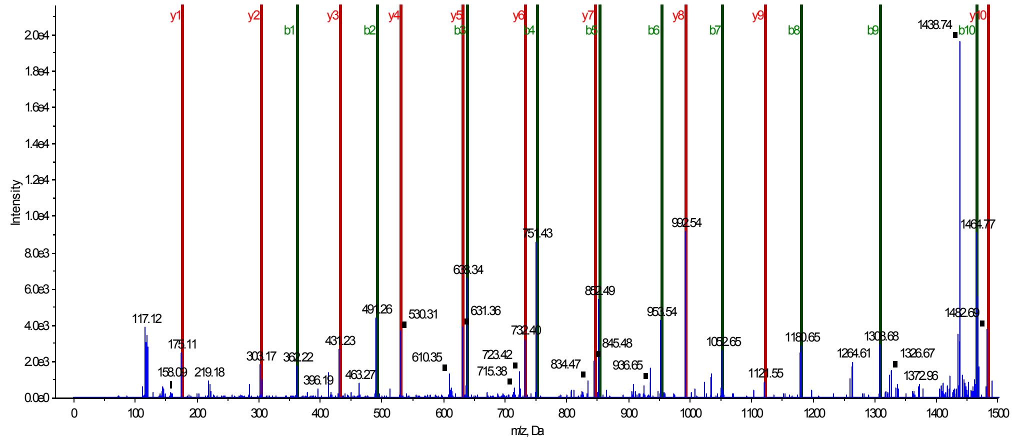
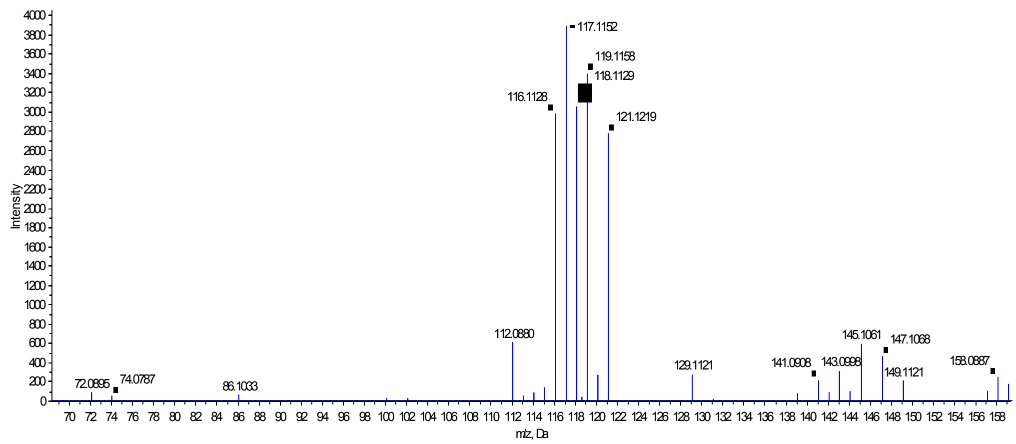
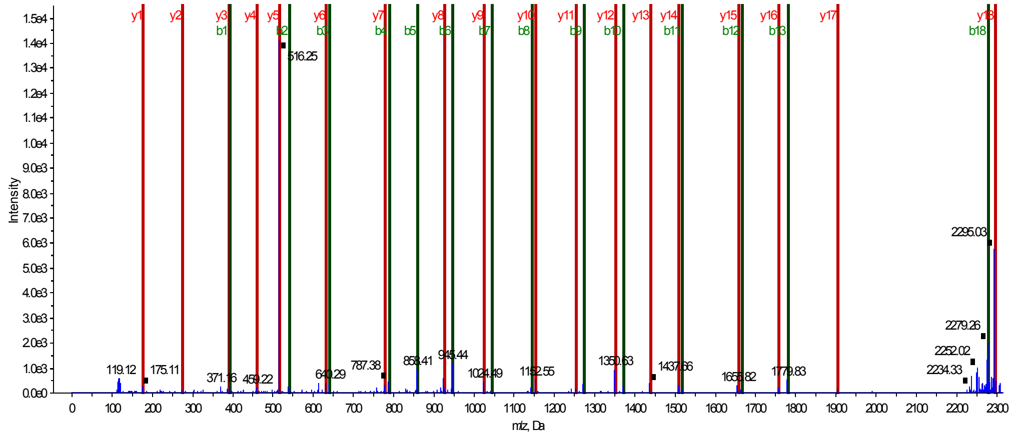
136.0900
139.1000
86.1075
103.1247





IPI00198620.1 Atp5d ATP synthase subunit delta, mitochondrial


Intensity
m/z, Da
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2279.26
2252.02
2234.33
119.12
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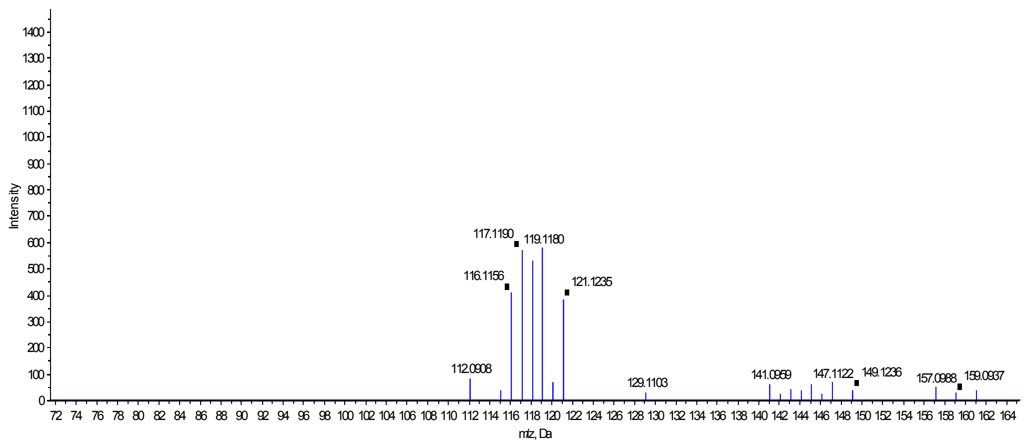
371.16
787.38
1437.66
1779.83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m/z, Da
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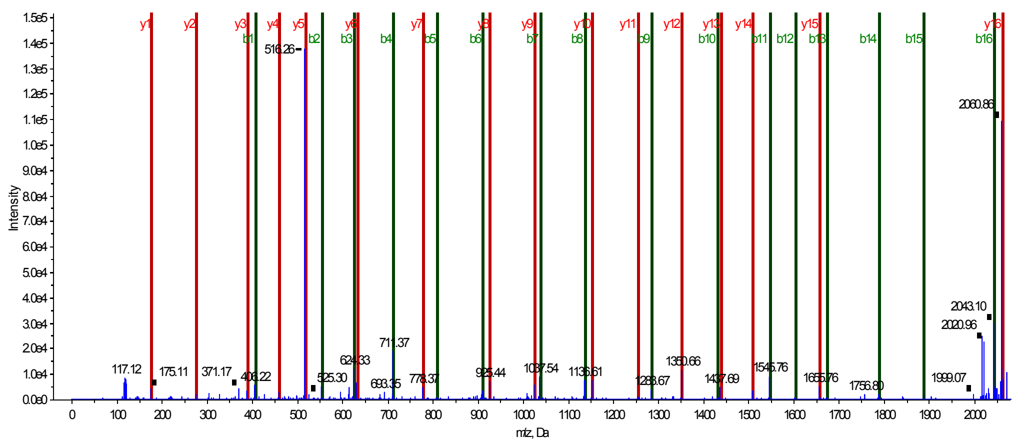
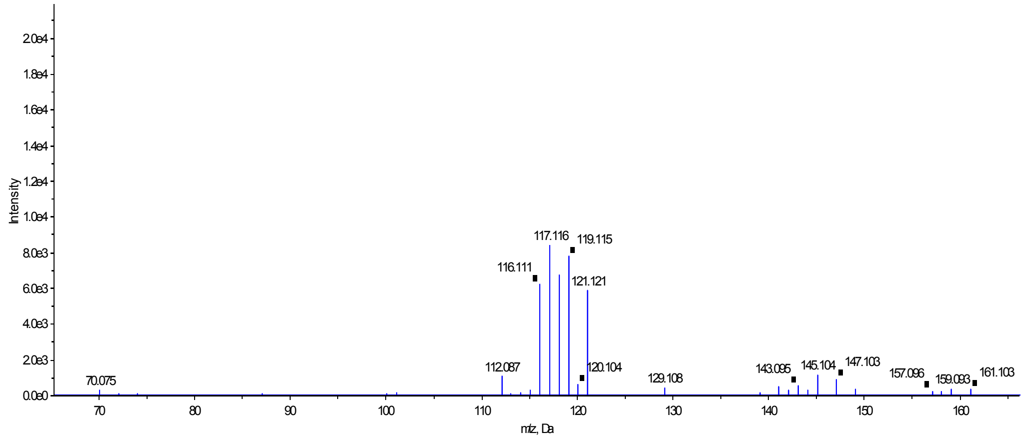
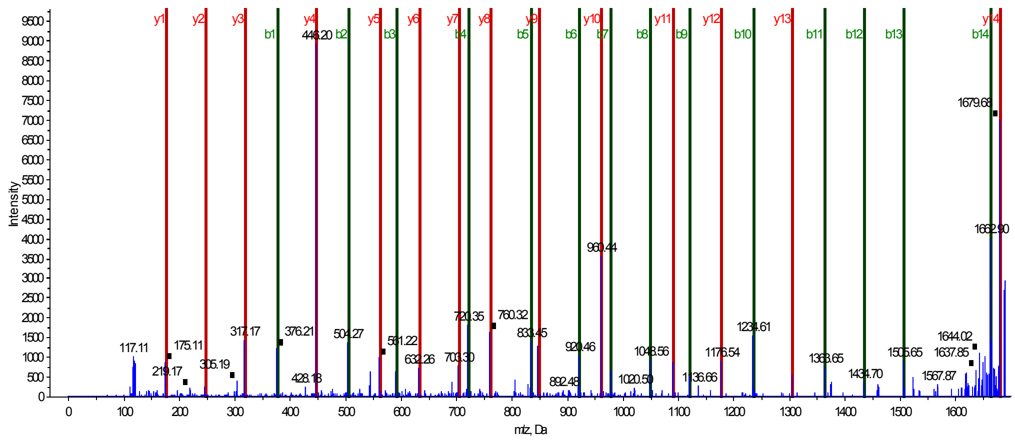
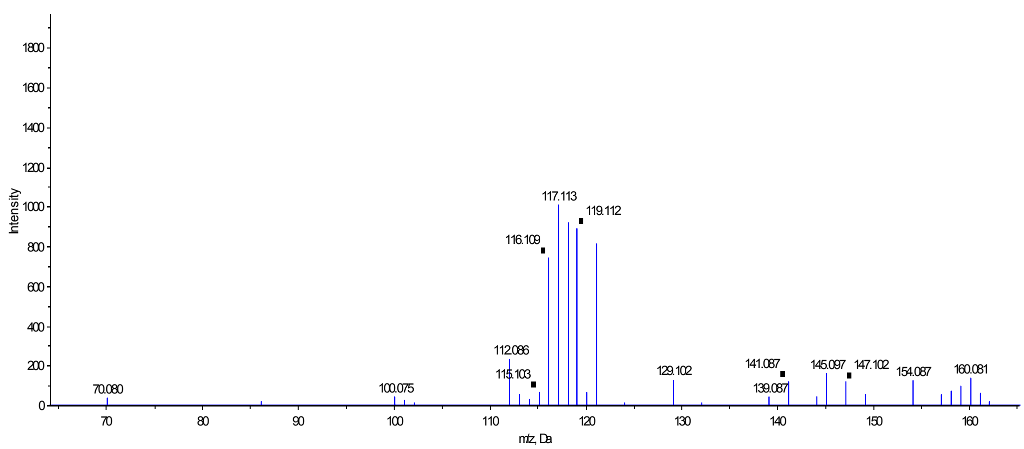
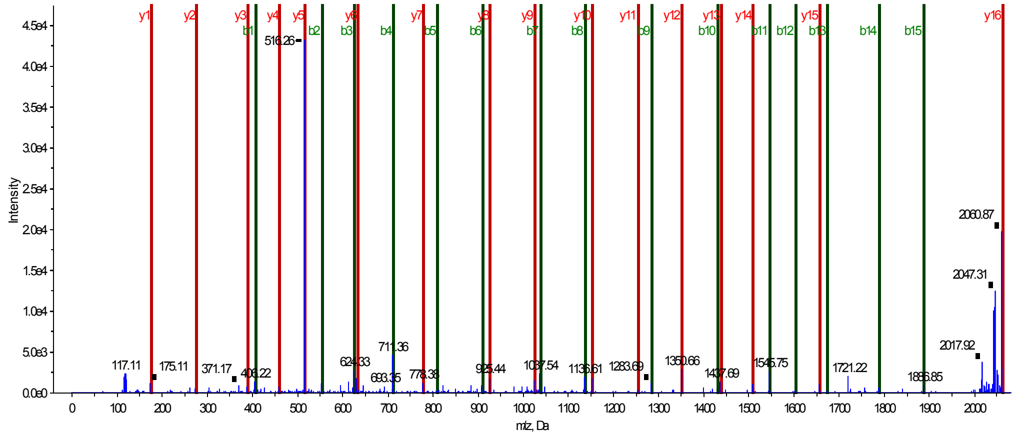
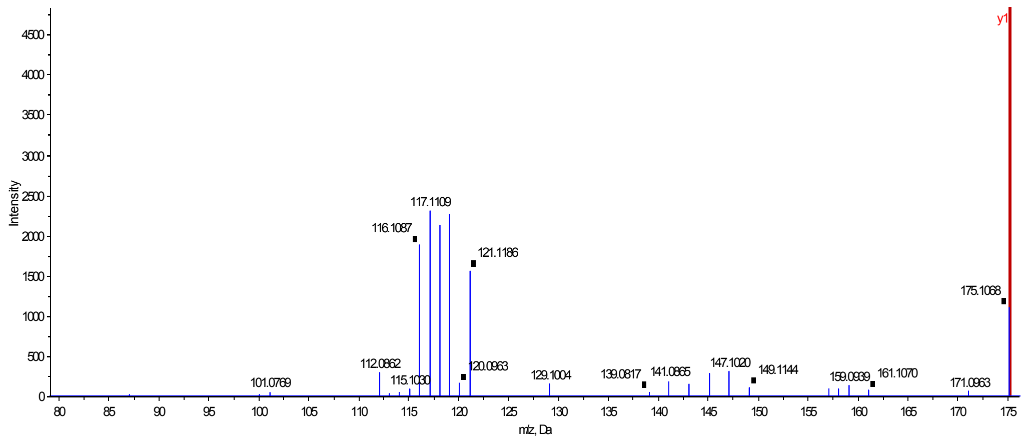

Intensity
m/z, Da
y1 y2 y3 y4 y5 y6 y7 y8 y9 y10 y11 y12 y13 y14 y15 y16
b1 b2 b3 b4 b5 b6 b7 b8 b9 b10 b11 b12 b13 b14 b15 b16
516.26
2060.86
2043.10
2020.96
711.37
624.33
117.12
175.11
371.17
525.30
693.35
778.37
925.44
1037.54
1135.61
1350.66
1437.69
1545.76
1655.76
1756.80
1999.07








y1
y2
y3
y4
y5
y6
y7
y8
y9
y10
y11
y12
y13
y14
y15
y16
b1
b2
b3
b4
b5
b6
b7
b8
b9
b10
b11
b12
b13
b14
b15
516.26
2060.87
2047.31
2017.92
117.11
175.11
371.17
406.22
624.33
711.36
693.35
778.38
925.44
1037.54
1136.61
1283.69
1350.66
1437.69
1545.75
1721.22
1885.85
Intensity
m/z, Da


y1
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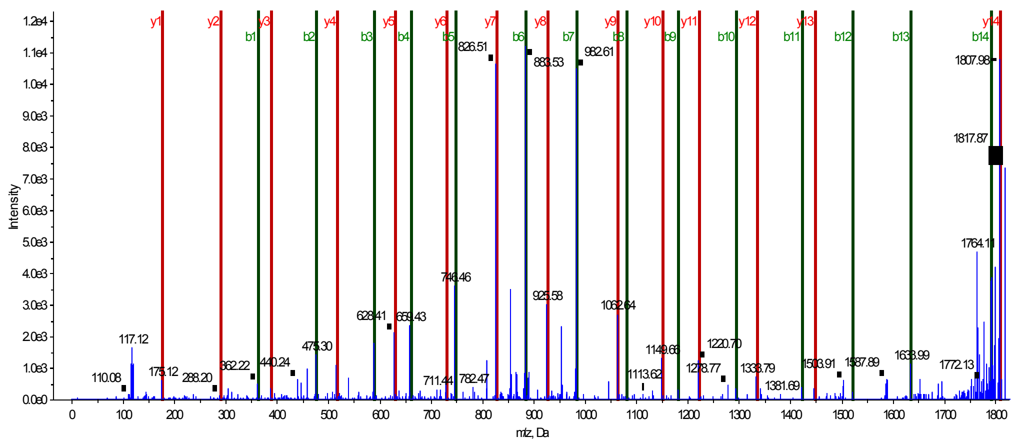
116.1087
121.1186
175.1068
112.0862
115.1030
120.0963
101.0769
129.1004
139.0817
141.0865
147.1020
149.1144
159.0939
161.1070
171.0963
Intensity
m/z, Da


y1
y2
y3
y4
y5
y6
y7
y8
y9
y10
y11
y12
y13
y14
b1
b2
b3
b4
b5
b6
b7
b8
b9
b10
b11
b12
b13
b14
826.51
883.53
982.61
1807.98
1817.87
1764.11
746.46
925.58
1062.64
628.41
659.43
475.30
117.12
110.08
175.12
288.20
362.22
440.24
711.44
782.47
1113.62
1149.66
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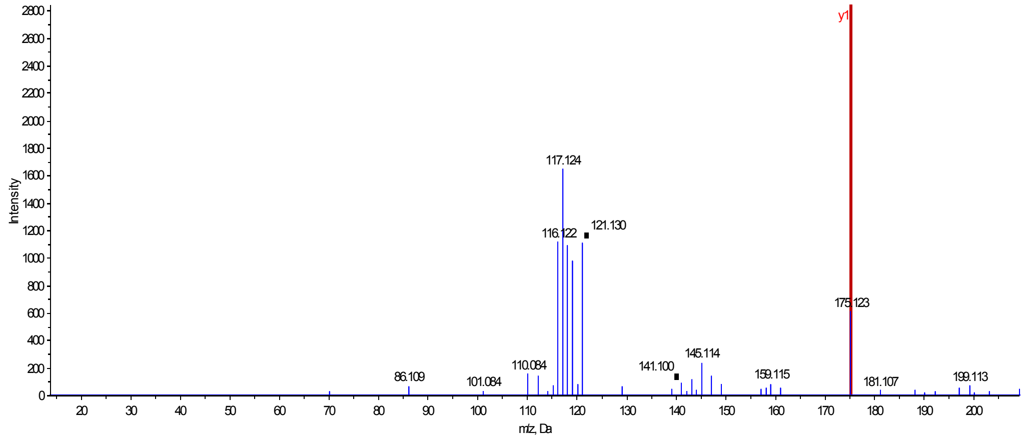
1587.89
1633.99
1772.13
Intensity
m/z, Da


Intensity
m/z, Da
y1
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175.123
145.114
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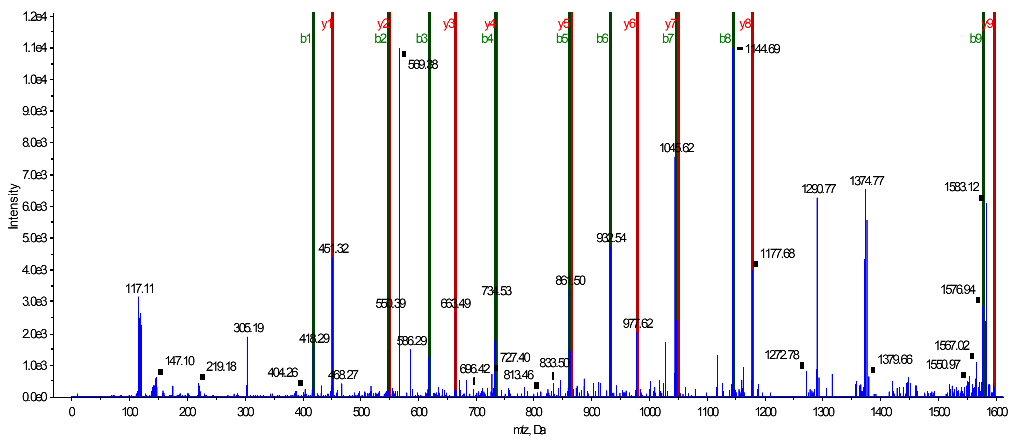
86.109
101.084
159.115
181.107
199.113


Intensity
m/z, Da
b1
y1
b2
y2
b3
y3
b4
y4
b5
y5
b6
y6
b7
y7
b8
y8
b9
y9
569.38
1144.69
1290.77
1374.77
1583.12
932.54
451.32
1177.68
117.11
861.50
734.53
550.39
663.49
1576.94
305.19
977.62
418.29
586.29
1272.78
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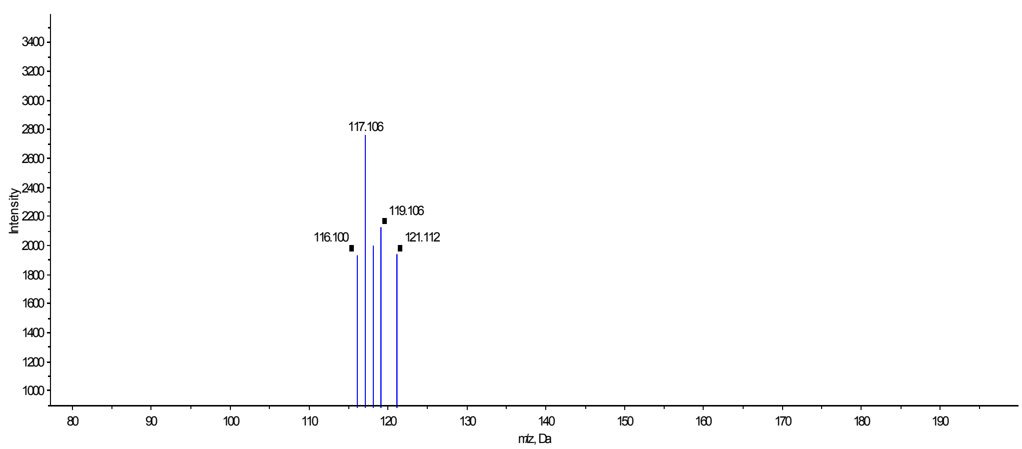
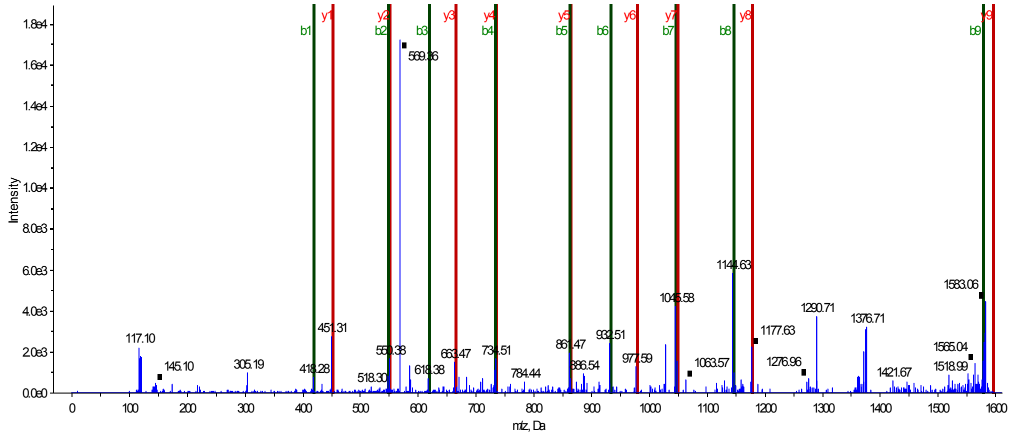
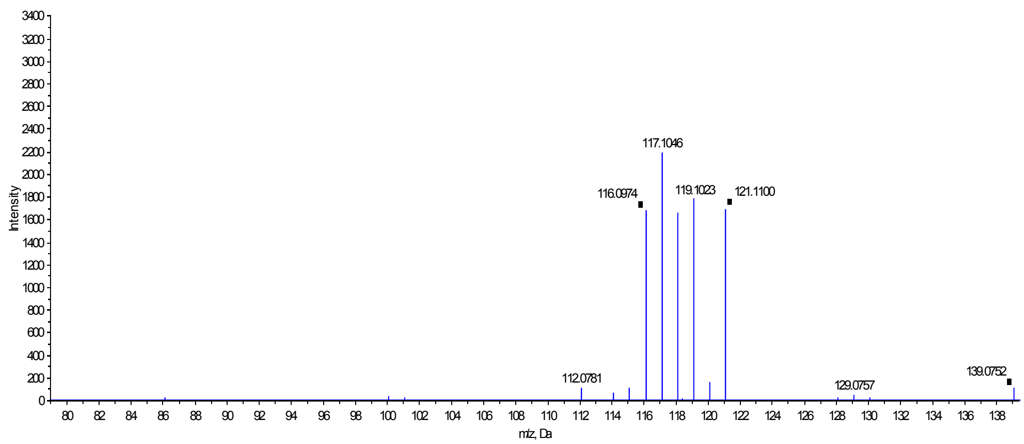
147.10
219.18
727.40
833.50
1550.97
696.42
404.26
468.27
813.46


Intensity
m/z, Da
117.106
119.106
116.100
121.112



Intensity
m/z, Da
b1
y1
y2
b2
b3
y3
y4
b4
y5
b5
b6
y6
y7
b7
b8
y8
y9
b9
569.36
451.31
117.10
145.10
305.19
418.28
518.30
550.38
618.38
663.47
734.51
784.44
861.47
886.54
932.51
977.59
1045.58
1063.57
1144.63
1177.63
1276.96
1290.71
1376.71
1421.67
1518.99
1565.04
1583.06



Intensity
m/z, Da
117.1046
116.0974
119.1023
121.1100
112.0781
129.0757
139.0752

Supporting Information 5

All significant pathways induced by MI, SM, RG and PO

Pathway	P-value	Ratio
MI group		
Oxidative Phosphorylation	2.99E-24	0.158
Mitochondrial Dysfunctin	1.39E-24	0.098
TCA Cycle II(Eukaryotic)	1.24E-13	0.2
Aspartate Degradation II	2.73E-06	0.231
Gluconeogenesis I	2.27E-04	0.064
SM group		
Oxidative Phosphorylation	6.14E-10	0.067
Mitochondrial Dysfunction	1.86E-08	0.037
RAN Signaling	1.38E-05	0.125
Protein Ubiquitination Pathway	7.24E-04	0.019
Acute Phase Response Signaling	1.28E-03	0.022
RG group		
Remodeling of Epithelial Adherens Junctions	2.30E-04	0.043
Actin Cytoskeleton Signaling	5.18E-04	0.017
Oxidative Phosphorylation	8.92E-04	0.025
Epithelial Adherens Junction Signaling	2.21E-03	0.019
Epithelial Adherens Junction Signaling	3.05E-03	0.014
OP group		
Mitochondrial Dysfunction	3.85E-07	0.033
Oxidative Phosphorylation	5.54E-07	0.05
Ketolysis	3.42E-04	0.105
Remodeling of Epithelial Adherens Junctions	9.17E-04	0.043
TCA Cycle II (Eukaryotic)	1.72E-03	0.05