

Goldenseal (*Hydrastis canadensis* L.) MS/MS data

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Table 2. Inclusion list for MS/MS experiment of goldenseal. MS/MS experiment was acquired on Acquity Ultra Performance Liquid Chromatography® (Waters Corporation, USA) coupled to Q Exactive™ Plus Hybrid Quadrupole-Orbitrap™ Mass Spectrometer (ThermoFisher Scientifics, USA) with such parameters: *dd-MS2* resolution 35,000; *automatic gain control (ACG)* 2×10^5 ion count; *maximum inject time (max IT)* 50 ms; *loop count* 3; *normalized collision energy (NCE)* 30eV. † indicates that the annotation had been corrected.

	Mass [<i>m/z</i>]	Polarity	Start [min]	End [min]	Tentative Annotation/ Putative Compound
A	300.1594	Positive	0.35	0.75	Unknown 3
B	342.1701	Positive	0.9	1.3	Corypalmine or Isocorypalmine
C	355.1024	Positive	0.5	0.9	Chlorogenic or Neochlorogenic acid
D	340.1544	Positive	3.35	3.75	S-canadine
E	342.1701	Positive	2.1	2.5	Corypalmine or Isocorypalmine
F	355.1024	Positive	0.65	1.05	Chlorogenic or Neochlorogenic acid
G	356.1857	Positive	3.1	3.4	Tetrahydropalmitine
H	370.165	Positive	3.4	3.8	S-canadoline
I	384.1441	Positive	2.25	2.65	beta-Hydrastine
J	400.1391	Positive	2.4	2.8	
K	445.2947	Positive	2.2	2.6	Unknown 2 – 2(H ₂ O) †
L	463.3057	Positive	2.2	2.6	Unknown 2 – H ₂ O †
M	481.316	Positive	2.2	2.6	Unknown 2 †
N	354.17	Positive	3.45	3.85	Unknown 5
O	340.1181	Positive	5.8	6.2	Oxotetrahydratalifendine
P	354.1337	Positive	6.25	6.65	Oxocanadine
Q	352.118	Positive	6.3	6.7	Berberastine or Oxyberberine
R	336.123	Positive	3.7	4.2	Berberine
S	352.118	Positive	2.35	2.75	Berberastine or Oxyberberine

Table Legends:

[Table 2A](#). Mass [m/z] 300.1549

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2B](#). Mass [m/z] 342.1701 (at 0.9 – 1.3)

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2E](#). Mass [m/z] 342.1701 (at 2.1 – 2.5)

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2C](#). Mass [m/z] 355.1024 (at 0.5 – 0.9)

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2F](#). Mass [m/z] 355.1024 (at 0.65 – 1.1)

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#) at 0.7

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#) at 0.9

[Table 2D](#). Mass [m/z] 340.1544

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2G](#). Mass [m/z] 356.1857

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2H](#). Mass [m/z] 370.1650

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2I](#). Mass [m/z] 384.1441

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2J](#). Mass [m/z] 400.1391

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2K](#). Mass [m/z] 445.2947

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2L](#). Mass [m/z] 463.3057

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2M](#). Mass [m/z] 481.3160

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2N](#). Mass [m/z] 354.1700

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2O](#). Mass [m/z] 340.1181

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2P](#). Mass [m/z] 354.1337

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2Q](#). Mass [m/z] 352.1180 at 2.4 – 2.8

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2S](#). Mass [m/z] 352.1180 at 6.3 – 6.7

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

[Table 2R](#). Mass [m/z] 336.1230

[GS_0315.raw](#) | [GS_0625.raw](#) | [GS_125.raw](#) | [GS_250.raw](#) | [GS_500.raw](#)

Mass [m/z] 300.1594

[GS_03125.raw](#)

FTMS + c ESI d Full ms2 300.1596@hcd30.00 [50.0000-325.0000]

Scan #: 90

RT: 0.54

m/z	Intensity	Relative
89.0597	11862.5	18.65
107.0491	25292.2	39.77
121.0648	28388.8	44.64
133.0859	6764.2	10.64
137.0595	5474.9	8.61
140.0818	8432	13.26
143.0315	5528.7	8.69
175.0752	8811.5	13.86
192.9785	6107.5	9.6
194.9574	6222.5	9.79
212.9679	8550.5	13.45
269.117	30134	47.39
270.1201	5722.4	9
282.1335	33692.5	52.98
283.1367	5390	8.48
299.0047	5701.9	8.97
300.105	9761.1	15.35
300.159	63590.5	100
301.1628	12403	19.5
302.1347	6758.8	10.63

[GS_0625.raw](#)

FTMS + c ESI d Full ms2 300.1588@hcd30.00 [50.0000-325.0000]

Scan #: 90

RT: 0.54

m/z	Intensity	Relative
89.0597	10344.3	8.69
101.0597	12209.7	10.26
107.0491	54419.3	45.72
121.0648	69440.9	58.34
137.0595	12217.5	10.26
140.0818	15461.4	12.99
150.0913	11452.7	9.62
162.0759	11214.5	9.42

175.0752	17193.4	14.45
237.091	12420.7	10.44
269.117	61096.9	51.33
270.12	12598.6	10.59
280.1175	8805.9	7.4
282.1333	85867.5	72.14
283.1369	12229.6	10.28
298.1281	11546	9.7
300.1052	18027.9	15.15
300.1591	119022.2	100
301.1626	26335	22.13
302.135	12820.6	10.77

[GS_125.raw](#)

FTMS + c ESI d Full ms2 300.1594@hcd30.00 [50.0000-325.0000]

Scan #: 90

RT: 0.53

<i>m/z</i>	Intensity	Relative
101.0598	18354.4	8.66
104.107	16209.5	7.65
107.0491	85817.8	40.5
121.0648	117228	55.32
137.0597	31693.7	14.96
140.0818	22334.4	10.54
150.0914	18156.1	8.57
162.0761	18052.9	8.52
175.0754	35278.3	16.65
237.0907	22275.8	10.51
269.1171	123845.8	58.44
270.1206	19583.8	9.24
280.118	15728.9	7.42
282.1335	133248.3	62.88
283.1367	20517	9.68
298.1284	17949.4	8.47
300.1054	15392.3	7.26
300.1593	211904.4	100
301.1628	40017.1	18.88
302.1347	24340.7	11.49

GS_250.raw

FTMS + c ESI d Full ms2 300.1592@hcd30.00 [50.0000-325.0000]

Scan #: 90

RT: 0.53

<i>m/z</i>	Intensity	Relative
101.0597	28732.2	8.48
104.107	21065.5	6.22
107.0491	134207	39.63
121.0648	196563.1	58.04
137.0597	44295.9	13.08
140.0818	27675.4	8.17
150.0913	35229.9	10.4
162.076	30378.6	8.97
175.0753	48588.6	14.35
237.091	22705.8	6.7
264.1229	23637.7	6.98
269.117	180246.6	53.22
270.1203	28207.9	8.33
280.1178	28915.3	8.54
282.1334	247513.3	73.08
283.1368	32883.4	9.71
298.1283	37826.9	11.17
300.1591	338689.9	100
301.1626	63145.8	18.64
302.1349	31448.7	9.29

GS_500.raw

FTMS + c ESI d Full ms2 300.1590@hcd30.00 [50.0000-325.0000]

Scan #: 92

RT: 0.54

<i>m/z</i>	Intensity	Relative
101.0598	46600	6.76
107.0492	85767.5	12.45
121.0648	486467.7	70.62
122.0679	34580.9	5.02
137.0598	55685.5	8.08
140.0818	57438.2	8.34
150.0913	80466.9	11.68
162.076	79485.4	11.54
164.0705	56691.9	8.23
175.0754	35199.4	5.11
264.123	56488.4	8.2
269.117	114304.4	16.59

280.1179	67626.3	9.82
282.1335	688843.9	100
283.1369	101153.2	14.68
298.1284	93871	13.63
299.1317	47725	6.93
300.1591	220615.4	32.03
301.1626	41557.9	6.03
302.1345	62708.4	9.1

Mass [m/z] 342.1701

GS_03125.raw

FTMS + c ESI d Full ms2 342.1697@hcd30.00 [50.0000-370.0000]

Scan #: 204

RT: 1.19

m/z	Intensity	Relative
58.0654	189758.9	88.21
59.0687	6929.8	3.22
89.0596	1959.1	0.91
237.0907	8695.5	4.04
238.0946	1676.9	0.78
265.0856	120310.3	55.93
266.089	21424.2	9.96
267.1014	1823	0.85
279.1009	8324.1	3.87
282.0886	22203.7	10.32
283.0924	3943	1.83
284.1039	3209.8	1.49
297.1117	215121.7	100
298.1152	35965.1	16.72
299.1278	26833	12.47
300.1305	4025.8	1.87
311.1272	5328.8	2.48
342.1696	175875.7	81.76
343.1729	35859.9	16.67
344.1764	1952.8	0.91

GS_0625.raw

FTMS + c ESI d Full ms2 342.1696@hcd30.00 [50.0000-370.0000]

Scan #: 202

RT: 1.17

<i>m/z</i>	Intensity	Relative
58.0655	538630.3	85.9
59.0688	13876.2	2.21
89.0597	8739	1.39
237.0908	31192.9	4.97
265.0857	366748.1	58.49
266.0891	63487.7	10.12
267.1025	6704.4	1.07
269.1164	8553.4	1.36
279.1012	20556	3.28
282.0884	51618	8.23
283.0919	9924	1.58
284.1044	9116.3	1.45
297.1118	627079.5	100
298.1152	129637.2	20.67
299.1277	80276.2	12.8
300.1307	14600.4	2.33
311.1274	14099.1	2.25
342.1697	541419.1	86.34
343.173	117247.8	18.7
344.1754	6508	1.04

GS_125.raw

FTMS + c ESI d Full ms2 342.1697@hcd30.00 [50.0000-370.0000]

Scan #: 202

RT: 1.15

<i>m/z</i>	Intensity	Relative
58.0655	1182061	82.02
59.0688	32056.7	2.22
237.0909	73521.7	5.1
238.0943	12239.8	0.85
265.0857	857153.4	59.47
266.0891	136316.5	9.46
267.1023	17583.9	1.22
269.1174	19408.9	1.35
279.1014	45219.1	3.14
282.0884	135025.9	9.37
283.0919	22363	1.55
284.1041	24450.5	1.7

297.1119	1441225	100
298.1153	252820.6	17.54
299.128	184157.4	12.78
300.1309	33660.5	2.34
311.1279	37119.4	2.58
342.1698	1197667	83.1
343.1731	237434.6	16.47
344.1764	15519.2	1.08

GS_250.raw

FTMS + c ESI d Full ms2 342.1699@hcd30.00 [50.0000-370.0000]

Scan #: 194

RT: 1.09

<i>m/z</i>	Intensity	Relative
58.0655	1637030	82.16
59.0688	41588.8	2.09
237.0907	84637.2	4.25
238.0944	16735.5	0.84
265.0857	1107071	55.57
266.0891	217705.2	10.93
267.1016	14189.5	0.71
269.1169	20488.6	1.03
279.1013	52731.5	2.65
282.0884	158480.8	7.95
283.0921	27326.5	1.37
284.1041	30058.6	1.51
297.1119	1992374	100
298.1153	382922.2	19.22
299.128	239480.3	12.02
300.1306	44593.7	2.24
311.1274	37955	1.91
342.1697	1757089	88.19
343.1731	369333.4	18.54
344.1746	22446.9	1.13

GS_500.raw

FTMS + c ESI d Full ms2 342.1698@hcd30.00 [50.0000-370.0000]

Scan #: 204

RT: 1.13

<i>m/z</i>	Intensity	Relative
58.0655	4184435	79.69
59.0688	100086.1	1.91
237.091	245920.3	4.68
238.0943	43297.8	0.82
265.0858	2973698	56.63
266.0891	508247.1	9.68
267.1025	68452.8	1.3
269.1173	64368.6	1.23
279.1012	163638.3	3.12
282.0886	421476.6	8.03
283.0917	85410.8	1.63
284.1044	95640.2	1.82
297.112	5251056	100
298.1154	885028.1	16.85
299.128	633818.4	12.07
300.1307	122092.4	2.33
311.1278	119462.4	2.28
342.1699	4599544	87.59
343.1732	1036711	19.74
344.1765	45363.6	0.86

GS_03125.raw

FTMS + c ESI d Full ms2 342.1697@hcd30.00 [50.0000-370.0000]

Scan #: 392

RT: 2.33

<i>m/z</i>	Intensity	Relative
50.2619	762.3	2.16
58.0655	861.8	2.45
59.5753	3291.9	9.34
59.577	6704	19.02
59.5782	1235	3.5
72.9337	793.9	2.25
76.1791	833.8	2.37
80.9478	3282.2	9.31
89.0597	1903.8	5.4
96.9173	3033.4	8.61
120.3216	775.6	2.2
151.0753	1277.5	3.62

165.0906	872.8	2.48
165.8063	1130.2	3.21
178.0862	35242.2	100
179.0895	3153.6	8.95
251.1839	775.3	2.2
340.5811	780.6	2.21
342.17	30279.7	85.92
343.1726	5212.2	14.79

GS_0625.raw

FTMS + c ESI d Full ms2 342.1696@hcd30.00 [50.0000-370.0000]

Scan #: 393

RT: 2.32

<i>m/z</i>	Intensity	Relative
59.577	1157.7	4.48
59.5793	10553.1	40.8
59.5808	2454.8	9.49
64.9776	1217.3	4.71
69.4022	862.1	3.33
80.948	1074	4.15
82.9449	1005.6	3.89
87.044	975.8	3.77
89.0597	1793.9	6.93
90.9767	970.9	3.75
105.6242	888.4	3.43
106.6142	814.1	3.15
133.0856	1175.5	4.54
151.0756	898.3	3.47
178.0862	25757.3	99.57
179.0894	2925.4	11.31
265.0857	1042.8	4.03
297.1114	981.9	3.8
342.1695	25868	100
343.1739	6692.8	25.87

GS_125.raw

FTMS + c ESI d Full ms2 342.1699@hcd30.00 [50.0000-370.0000]

Scan #: 393

RT: 2.29

<i>m/z</i>	Intensity	Relative
58.0654	4459.1	56.41
61.9864	908.4	11.49
69.8589	783.7	9.91
80.9478	823.8	10.42
85.0284	781.1	9.88
86.1988	766.7	9.7
87.0441	889.3	11.25
89.0597	2840.6	35.93
91.0573	822.9	10.41
97.4591	765.7	9.69
130.0791	896.3	11.34
133.0861	2861.2	36.19
141.152	776.2	9.82
168.8689	755	9.55
178.0862	5698.8	72.09
232.9276	994.6	12.58
265.0854	857	10.84
297.1124	5279	66.78
342.1395	830.5	10.5
342.1705	7905.5	100

GS_250.raw

FTMS + c ESI d Full ms2 342.1698@hcd30.00 [50.0000-370.0000]

Scan #: 402

RT: 2.30

<i>m/z</i>	Intensity	Relative
58.0655	6692.8	18.26
61.9857	1636.7	4.46
80.9479	1117.5	3.05
89.0596	1504.8	4.1
97.0249	882.2	2.41
133.086	1563.7	4.27
151.0754	1565.3	4.27
176.0705	1118.4	3.05
178.0862	30544.7	83.32
179.0897	3740.5	10.2
192.1025	902	2.46
265.0852	4345.1	11.85

297.1119	9688.6	26.43
298.1147	1039.4	2.84
340.1551	1300.3	3.55
341.1566	1494.5	4.08
342.1491	1840.5	5.02
342.1696	36661.5	100
343.1725	9978.8	27.22
344.1469	1065.1	2.91

GS_500.raw

FTMS + c ESI d Full ms2 342.1696@hcd30.00 [50.0000-370.0000]

Scan #: 407

RT: 2.29

<i>m/z</i>	Intensity	Relative
58.0654	11185.7	56.61
61.9831	988	5
64.9775	906.1	4.59
80.9479	1057.5	5.35
85.0284	1268.6	6.42
85.5281	962.5	4.87
89.0597	3365.6	17.03
127.0391	922.6	4.67
137.0596	913.9	4.62
178.0862	10756.9	54.44
265.0857	7544.6	38.18
282.0881	1389.6	7.03
297.112	11989.5	60.67
298.1148	1184.6	5.99
340.1541	1781.9	9.02
341.1203	1155.4	5.85
341.157	1780	9.01
342.17	19760.6	100
343.1725	5553.2	28.1
344.1482	1391.3	7.04

Mass [*m/z*] 355.1024

GS_03125.raw

FTMS + c ESI d Full ms2 355.1023@hcd30.00 [50.0000-380.0000]

Scan #: 89

RT: 0.53

<i>m/z</i>	Intensity	Relative
58.0655	1399.9	0.72
60.1274	4799.5	2.47
85.0284	1550	0.8
90.9767	15930.3	8.2
95.0492	1183.3	0.61
111.0438	1469.8	0.76
135.044	4476.6	2.3
139.039	1925.4	0.99
145.0284	3015.6	1.55
150.9978	1526.7	0.79
153.0546	1234	0.63
157.0493	1149.9	0.59
163.0389	194335.8	100
164.0423	18149.6	9.34
192.0248	1205.8	0.62
206.9551	4168.6	2.15
220.9344	5258.1	2.71
234.9498	5553.2	2.86
308.8994	3003.3	1.55
355.0996	3952.6	2.03

GS_0625.raw

FTMS + c ESI d Full ms2 355.1018@hcd30.00 [50.0000-380.0000]

Scan #: 89

RT: 0.53

<i>m/z</i>	Intensity	Relative
58.0655	5538.7	1.63
60.1272	4451.2	1.31
85.0283	4183.8	1.23
90.9765	3662.2	1.08
95.0491	3197.4	0.94
111.0441	5707.7	1.68
129.0546	4082.1	1.2
135.0441	8567.9	2.52
139.039	4018.5	1.18
145.0282	9173	2.7
153.0544	1824.8	0.54

157.0496	3024	0.89
163.0388	339686.5	100
164.0421	28774.2	8.47
179.0341	1967.5	0.58
206.9549	3392.6	1
234.9501	3521.3	1.04
308.8996	3364.3	0.99
354.1163	1967.6	0.58
355.0991	6358.5	1.87

GS_125.raw

FTMS + c ESI d Full ms2 355.1019@hcd30.00 [50.0000-380.0000]

Scan #: 89

RT: 0.53

<i>m/z</i>	Intensity	Relative
58.0655	15823.8	2.66
60.1248	6020.5	1.01
69.0336	5087.7	0.85
85.0285	12068.6	2.03
95.0491	3775.7	0.63
97.0285	4227.9	0.71
111.0441	6143.4	1.03
127.039	7096	1.19
129.0546	3762.6	0.63
135.0441	9887.6	1.66
139.0389	7339.5	1.23
145.0285	14689.4	2.46
145.0496	3742.4	0.63
153.0546	5850.6	0.98
157.0495	4417.3	0.74
163.0389	595964.1	100
164.0423	53120.3	8.91
245.0507	6110.6	1.03
353.084	5237	0.88
355.0995	5518.6	0.93

GS_250.raw

FTMS + c ESI d Full ms2 355.1018@hcd30.00 [50.0000-380.0000]

Scan #: 89

RT: 0.53

<i>m/z</i>	Intensity	Relative
58.0655	28554.9	2.81
69.0336	17594.5	1.73
73.0285	10139.6	1
85.0285	59255.1	5.82
97.0285	19854.3	1.95
111.0442	11671	1.15
127.039	36534.4	3.59
129.0545	8368.1	0.82
135.0441	20272.4	1.99
139.039	13390.5	1.32
145.0284	31841.9	3.13
145.0495	18721.6	1.84
163.0389	1017810	100
164.0423	91397.2	8.98
183.05	14759.2	1.45
203.04	16724.8	1.64
245.0505	44436.5	4.37
246.0524	8245.1	0.81
263.0612	15548.5	1.53
275.0616	8667.7	0.85

GS_500.raw

FTMS + c ESI d Full ms2 355.1011@hcd30.00 [50.0000-380.0000]

Scan #: 91

RT: 0.54

<i>m/z</i>	Intensity	Relative
58.0655	79584.4	5.45
69.0337	45010.8	3.09
73.0284	22209	1.52
85.0285	171948.5	11.79
97.0285	53433.1	3.66
111.0441	19464.2	1.33
127.039	93391.9	6.4
135.044	31449.4	2.16
145.0284	44665.5	3.06
145.0496	39703.4	2.72
163.0389	1458946	100
164.0423	138842.1	9.52

174.0449	28049.9	1.92
183.0501	31683.6	2.17
203.04	40999.7	2.81
245.0505	120169.6	8.24
246.0524	22032.6	1.51
263.0609	38519.8	2.64
275.0609	25286.1	1.73
365.0923	22616.8	1.55

GS_03125.raw

FTMS + c ESI d Full ms2 355.1020@hcd30.00 [50.0000-380.0000]

Scan #: 123

RT: 0.72

<i>m/z</i>	Intensity	Relative
83.0491	5068.3	0.29
89.0385	5167.6	0.29
95.0491	10278.2	0.58
107.0491	5685.9	0.32
111.0441	15208.4	0.86
117.0333	4566.3	0.26
129.0546	7868.9	0.44
133.0284	8329.7	0.47
134.0363	13687.3	0.77
135.044	27752.1	1.56
139.0388	11620.5	0.65
145.0283	55430.6	3.12
151.0387	8447.8	0.48
157.0494	4997	0.28
161.0237	7414.4	0.42
162.0311	4754	0.27
163.0388	1776555	100
164.0421	163769	9.22
179.0337	25332.1	1.43
355.0996	4985.1	0.28

GS_0625.raw

FTMS + c ESI d Full ms2 355.1020@hcd30.00 [50.0000-380.0000]

Scan #: 123

RT: 0.72

<i>m/z</i>	Intensity	Relative
83.0491	9271.3	0.31
95.0491	31385.6	1.06
107.0492	17218.9	0.58

111.044	28737.9	0.97
117.0334	11547.2	0.39
129.0545	15547.6	0.52
133.0283	15112	0.51
134.0362	21770.3	0.73
135.0439	52510.7	1.77
139.0388	25039	0.84
145.0283	100162.8	3.37
146.0316	9799.2	0.33
151.039	14969.9	0.5
157.0493	12590	0.42
161.0233	16864.1	0.57
163.0388	2972336	100
164.0421	279645.4	9.41
179.0338	65245.2	2.2
180.037	12664.2	0.43
355.0996	17357.4	0.58

GS_125.raw

FTMS + c ESI d Full ms2 355.1020@hcd30.00 [50.0000-380.0000]

Scan #: 123

RT: 0.71

<i>m/z</i>	Intensity	Relative
83.0492	14318.2	0.24
89.0384	18364.1	0.31
95.0491	31387	0.52
107.0492	17930.9	0.3
111.0441	44213.8	0.74
117.0335	21956.1	0.37
133.0285	17521.7	0.29
134.0363	40686.3	0.68
135.044	88269.9	1.47
139.0388	36070.5	0.6
145.0284	168055.1	2.81
151.0392	17648.3	0.29
153.0546	21470.2	0.36
157.0495	15342.6	0.26
162.0311	17941.8	0.3
163.0389	5988543	100
164.0422	542753.1	9.06
179.034	58104.8	0.97
181.0494	21820.9	0.36
355.0991	25165.4	0.42

GS_250.raw

FTMS + c ESI d Full ms2 355.1020@hcd30.00 [50.0000-380.0000]

Scan #: 125

RT: 0.72

<i>m/z</i>	Intensity	Relative
63.0229	15960.9	0.12
83.0491	15267.2	0.12
95.0493	55232.9	0.43
107.0491	14508.1	0.11
111.0441	70980.8	0.55
117.0335	53600.4	0.42
133.0284	36699.5	0.29
134.0363	60417.2	0.47
135.044	142520.6	1.11
139.0389	61086.8	0.48
145.0284	424601.4	3.31
146.0317	16456.1	0.13
151.0389	43528.1	0.34
162.0314	18451.3	0.14
163.0389	12843093	100
164.0422	1176082	9.16
165.0444	44146.1	0.34
179.0341	86689.4	0.67
181.0496	40681.1	0.32
355.0993	15473.5	0.12

GS_500.raw

FTMS + c ESI d Full ms2 355.1021@hcd30.00 [50.0000-380.0000]

Scan #: 127

RT: 0.72

<i>m/z</i>	Intensity	Relative
83.0491	63341	0.29
89.0384	71082.2	0.33
95.0491	71215.1	0.33
111.0441	108255.3	0.5
117.0334	57290.2	0.26
123.044	29412.1	0.13
129.0546	56179.8	0.26
133.0284	30527.5	0.14
134.0361	60717.7	0.28
135.044	259500	1.19
139.039	76639.8	0.35

145.0284	650540.8	2.98
146.0318	53160	0.24
151.039	60867.8	0.28
153.0543	30358.9	0.14
163.0389	21864120	100
164.0423	2070980	9.47
165.0442	79732.7	0.36
179.0338	71253.3	0.33
181.0494	28642.4	0.13

GS_03125.raw

FTMS + c ESI d Full ms2 355.1020@hcd30.00 [50.0000-380.0000]

Scan #: 154

RT: 0.90

<i>m/z</i>	Intensity	Relative
58.0653	3179.6	0.32
83.049	1681.4	0.17
89.0383	3351.7	0.33
90.9767	2085.7	0.21
95.0491	3304.5	0.33
107.0493	1735.8	0.17
111.044	6067.4	0.6
117.0334	1611.9	0.16
129.0546	1460.9	0.15
134.0363	10385.4	1.04
135.0439	11668.8	1.16
139.0389	1811.8	0.18
145.0283	24295	2.42
162.0312	4315.3	0.43
163.0388	1003119	100
164.0422	93466.3	9.32
165.0438	4136.5	0.41
179.0339	6060.5	0.6
181.0494	6143.8	0.61
308.8991	1773.6	0.18

GS_0625.raw

FTMS + c ESI d Full ms2 355.1021@hcd30.00 [50.0000-380.0000]

Scan #: 156

RT: 0.90

<i>m/z</i>	Intensity	Relative
58.0655	10736	0.74
83.0492	3667.5	0.25

89.0383	2413.5	0.17
95.0492	4259.8	0.29
111.044	10141.4	0.7
129.0545	6315.5	0.44
133.0284	2470.1	0.17
134.0363	15686	1.08
135.044	20049.8	1.38
139.039	5845.3	0.4
145.0284	33007.8	2.28
146.0318	4766	0.33
162.0314	7403.3	0.51
163.0389	1448023	100
164.0422	115915.4	8.01
165.0441	5066.3	0.35
179.0339	19675.9	1.36
181.0496	7270.2	0.5
308.8999	2479.4	0.17
356.0765	4427.5	0.31

GS_125.raw

FTMS + c ESI d Full ms2 355.1021@hcd30.00 [50.0000-380.0000]

Scan #: 156

RT: 0.89

<i>m/z</i>	Intensity	Relative
58.0655	39187	0.82
83.0491	5213.6	0.11
89.0383	13307.1	0.28
93.0336	4758.4	0.1
111.044	28559.9	0.6
117.0335	14386.2	0.3
129.0544	11099.3	0.23
133.0284	5173.2	0.11
134.0363	40514.4	0.85
135.044	45089.7	0.94
139.039	18483.9	0.39
145.0284	106699.5	2.23
146.0317	12742.9	0.27
161.0235	6639.3	0.14
162.0311	18752	0.39
163.0389	4777323	100
164.0423	436643.8	9.14
165.0438	14424.3	0.3
179.0339	25110.6	0.53

181.0494 19032.2 0.4

GS_250.raw

FTMS + c ESI d Full ms2 355.1021@hcd30.00 [50.0000-380.0000]

Scan #: 160

RT: 0.90

<i>m/z</i>	Intensity	Relative
58.0655	80653.4	1.17
59.9495	43365.1	0.63
83.0491	10527.4	0.15
89.0384	10292.3	0.15
95.0491	9491.4	0.14
96.9207	10998.7	0.16
111.044	45482.7	0.66
117.0334	8704.5	0.13
129.0547	11259.6	0.16
134.0363	58094.5	0.84
135.0441	67618.4	0.98
139.0388	7942	0.11
145.0284	154384.7	2.23
146.0315	9629.6	0.14
162.0311	23937.8	0.35
163.0388	6917875	100
164.0422	585099.1	8.46
165.0433	9627.2	0.14
179.0336	20725	0.3
181.0496	35319.9	0.51

GS_500.raw

FTMS + c ESI d Full ms2 355.1021@hcd30.00 [50.0000-380.0000]

Scan #: 162

RT: 0.91

<i>m/z</i>	Intensity	Relative
58.0654	235316	1.61
83.0491	23033.2	0.16
89.0384	43446.9	0.3
111.0441	93605.5	0.64
117.0334	43749.5	0.3
123.044	24541	0.17
129.0545	45723.2	0.31
133.028	18588.4	0.13
134.0361	65927.4	0.45
135.044	124366	0.85

139.039	35967.8	0.25
145.0283	351219.5	2.41
146.0316	48008.4	0.33
162.031	24423	0.17
163.0388	14602905	100
164.0421	1312955	8.99
165.0443	51502.9	0.35
179.034	44011.2	0.3
181.0495	82080.1	0.56
356.1493	19823.7	0.14

Mass [m/z] 340.1544

GS_03125.raw

FTMS + c ESI d Full ms2 340.1543@hcd30.00 [50.0000-365.0000]

Scan #: 609

RT: 3.58

m/z	Intensity	Relative
61.9901	1397	0.53
80.9479	1120.3	0.42
149.0596	14672	5.55
165.0908	7926.1	3
171.1164	947.6	0.36
174.0549	6764.9	2.56
176.0705	229392.4	86.82
177.0738	20520.8	7.77
189.0776	1054.3	0.4
199.1115	1984.2	0.75
203.1071	1213.5	0.46
204.1017	998.7	0.38
245.1168	1031.2	0.39
315.8853	1034.7	0.39
323.1276	1869.5	0.71
325.1312	1686.7	0.64
339.1415	5117.2	1.94
340.154	264218.9	100
341.1575	59734.3	22.61
342.1607	4162.5	1.58

GS_0625.raw

FTMS + c ESI d Full ms2 340.1541@hcd30.00 [50.0000-365.0000]

Scan #: 614

RT: 3.57

<i>m/z</i>	Intensity	Relative
80.9479	1145.8	0.93
131.0856	1780	1.45
145.101	1546	1.26
147.0802	1499.3	1.22
149.0596	7538.6	6.12
157.1012	1110.6	0.9
165.091	6350.2	5.16
171.1165	3070.9	2.49
174.0547	1874.7	1.52
175.0753	1174.3	0.95
176.0705	112957.3	91.74
177.0738	10476.9	8.51
199.1117	5096.7	4.14
203.106	1321	1.07
217.1224	3392.6	2.76
245.1169	3548.7	2.88
315.8855	1889.8	1.53
339.1415	4023.5	3.27
340.154	123132.9	100
341.1574	26106.7	21.2

GS_125.raw

FTMS + c ESI d Full ms2 340.1543@hcd30.00 [50.0000-365.0000]

Scan #: 623

RT: 3.58

<i>m/z</i>	Intensity	Relative
145.101	4555.8	0.69
147.0803	5089.9	0.77
149.0597	40081.4	6.03
151.0753	5554.7	0.84
157.101	4075	0.61
165.091	17278.6	2.6
171.1166	5752.7	0.87
174.055	20722.7	3.12
176.0705	563854.8	84.81
177.0739	54562.5	8.21
181.101	5804.7	0.87
199.1114	9584.7	1.44

245.117	4789.8	0.72
323.1277	4938.4	0.74
325.1304	5725.6	0.86
338.1375	4827	0.73
339.1406	6545.5	0.98
340.1541	664846.9	100
341.1574	136790.6	20.57
342.1598	8573.3	1.29

GS_250.raw

FTMS + c ESI d Full ms2 340.1543@hcd30.00 [50.0000-365.0000]

Scan #: 633

RT: 3.56

<i>m/z</i>	Intensity	Relative
131.0856	6343.2	2.01
145.1012	9637.2	3.06
149.0597	21932.1	6.96
157.1011	14289.9	4.53
165.0909	16493.8	5.23
171.1167	12717.5	4.03
174.055	10757.7	3.41
175.0753	8383.5	2.66
176.0706	303535	96.28
177.0738	25157.4	7.98
181.1009	8157	2.59
199.1116	20816.5	6.6
203.1065	7713.7	2.45
217.1223	10219.9	3.24
227.1063	7655	2.43
245.1173	14351.6	4.55
338.1396	7863.2	2.49
339.1418	8889.5	2.82
340.1541	315275.8	100
341.1575	72876.2	23.12

GS_500.raw

FTMS + c ESI d Full ms2 340.1545@hcd30.00 [50.0000-365.0000]

Scan #: 643

RT: 3.57

<i>m/z</i>	Intensity	Relative
131.0855	11891.6	2.01
143.0856	10850	1.83
145.1011	12450	2.1

147.0804	12715.9	2.15
149.0598	42017.2	7.1
157.1013	19370	3.27
165.091	26359.3	4.46
171.1169	22341.9	3.78
174.0548	12732.7	2.15
175.0754	14719.5	2.49
176.0706	534367.9	90.32
177.0739	52991	8.96
181.1011	14735.3	2.49
199.1117	29286.9	4.95
203.1065	13698.2	2.32
217.1222	16319.3	2.76
227.1066	14256.2	2.41
245.1169	21492.9	3.63
340.1541	591661.7	100
341.1576	131992.8	22.31

Mass [*m/z*] 356.1857

GS_03125.raw

FTMS + c ESI d Full ms2 356.1851@hcd30.00 [50.0000-385.0000]

Scan #: 560

RT: 3.29

<i>m/z</i>	Intensity	Relative
56.6515	859.3	6.11
73.0468	1752.9	12.47
75.448	812.5	5.78
87.044	1176.4	8.37
89.0597	3405.5	24.22
90.9767	4679.8	33.29
91.0573	1566.5	11.14
95.4885	785.4	5.59
102.0677	839.3	5.97
133.0857	1018.3	7.24
163.0388	1811.7	12.89
165.0905	2602.9	18.52
192.1018	14058.2	100
193.105	1236.7	8.8
220.9341	1830.6	13.02
256.1949	820.5	5.84
285.5766	896.9	6.38
308.8987	1867.5	13.28

356.1854	9833	69.95
357.1881	3281.2	23.34

[GS_0625.raw](#)

FTMS + c ESI d Full ms2 356.1854@hcd30.00 [50.0000-385.0000]

Scan #: 565

RT: 3.28

<i>m/z</i>	Intensity	Relative
59.9296	812.8	4.06
61.9903	1218	6.09
89.0596	1281.6	6.41
90.9767	6524.5	32.61
94.5575	839.6	4.2
133.0858	1181	5.9
163.0389	3540.9	17.7
165.0908	4077.9	20.38
190.0862	841.7	4.21
192.1018	20006.7	100
193.1053	1596.9	7.98
193.2147	810.3	4.05
198.8403	880.1	4.4
215.1023	930.8	4.65
220.9342	1374.2	6.87
246.8077	957	4.78
308.8999	3126.4	15.63
348.1893	866.8	4.33
356.1854	18191.6	90.93
357.1884	5197.5	25.98

[GS_125.raw](#)

FTMS + c ESI d Full ms2 356.1852@hcd30.00 [50.0000-385.0000]

Scan #: 572

RT: 3.27

<i>m/z</i>	Intensity	Relative
73.0469	884.6	3.25
87.6694	886.1	3.26
89.0597	2898.3	10.65
90.9766	5231.9	19.22
91.0573	952.8	3.5
133.086	1295.7	4.76
163.0388	5781.4	21.24
165.0908	4997.2	18.36
190.0858	1386.5	5.09

192.1018	27222.9	100
193.1052	1894.4	6.96
204.0653	1195.4	4.39
218.8109	833.6	3.06
220.9348	2769.5	10.17
252.0871	2790.6	10.25
258.8635	919.7	3.38
308.899	1568.8	5.76
340.1537	1076.4	3.95
356.185	26634.5	97.84
357.1881	5584.9	20.52

[GS_250.raw](#)

FTMS + c ESI d Full ms2 356.1855@hcd30.00 [50.0000-385.0000]

Scan #: 583

RT: 3.27

<i>m/z</i>	Intensity	Relative
73.0468	1078.1	1.67
89.0597	5300.3	8.2
90.9767	6285.7	9.73
133.0858	1167.6	1.81
163.0389	16328.7	25.28
165.091	13809.4	21.38
174.1728	969.4	1.5
190.0861	8032.4	12.43
192.1018	64599	100
193.1057	5973.8	9.25
204.0656	5349.7	8.28
220.9346	3806.7	5.89
252.0856	2772.8	4.29
293.1331	3151.4	4.88
308.8997	4091.3	6.33
356.1492	3397.5	5.26
356.1854	62549.8	96.83
357.1518	1182.6	1.83
357.1887	12800.6	19.82
358.1649	1734.3	2.68

GS_500.raw

FTMS + c ESI d Full ms2 356.1854@hcd30.00 [50.0000-385.0000]

Scan #: 589

RT: 3.25

<i>m/z</i>	Intensity	Relative
89.0597	4567.8	21.06
90.9767	6429.2	29.64
91.0573	1305.1	6.02
136.0758	1280.4	5.9
163.039	21690.4	100
165.091	3701.1	17.06
190.086	7181.1	33.11
192.0652	4238.1	19.54
192.1018	18183.8	83.83
193.1055	1343.7	6.2
204.0656	14870.8	68.56
252.0864	7230.1	33.33
293.1336	1452	6.69
308.8994	3630.6	16.74
338.1381	3883.1	17.9
340.154	1375.9	6.34
356.1495	8227.3	37.93
356.1852	17627.1	81.27
357.1885	4887.5	22.53
358.1646	5019.1	23.14

Mass [*m/z*] 370.1650

GS_03125.raw

FTMS + c ESI d Full ms2 370.1655@hcd30.00 [50.0000-395.0000]

Scan #: 623

RT: 3.66

<i>m/z</i>	Intensity	Relative
73.0284	3065	4.95
87.0443	978.6	1.58
89.0596	4369.8	7.05
90.9767	1557.8	2.51
91.4911	865.8	1.4
106.1459	775.5	1.25
124.0868	1165.3	1.88
133.0858	1190.2	1.92
161.0595	1234.7	1.99
186.2779	875.6	1.41

190.0862	61968.9	100
191.0703	1180.4	1.9
191.0898	6965.1	11.24
204.4969	801.4	1.29
290.093	1791.6	2.89
335.5732	910	1.47
352.154	1569.7	2.53
370.1646	18090.3	29.19
371.1669	3363.7	5.43
380.8224	804.5	1.3

[GS_0625.raw](#)

FTMS + c ESI d Full ms2 370.1654@hcd30.00 [50.0000-395.0000]

Scan #: 628

RT: 3.65

<i>m/z</i>	Intensity	Relative
73.0285	3016.6	3.81
85.3297	830.7	1.05
89.0598	3653	4.62
90.9768	1214.5	1.53
91.0575	1153.7	1.46
122.7876	787.5	0.99
128.0273	807.9	1.02
140.2922	920.3	1.16
177.2746	828.1	1.05
188.0705	1258	1.59
190.0861	79154.7	100
191.0707	1249	1.58
191.0894	6370.1	8.05
270.8444	837.3	1.06
290.0929	4155.2	5.25
291.0979	1517.8	1.92
306.0882	1098.1	1.39
352.1539	3921.5	4.95
370.1646	24958.3	31.53
371.1676	4463.2	5.64

GS_125.raw

FTMS + c ESI d Full ms2 370.1653@hcd30.00 [50.0000-395.0000]

Scan #: 635

RT: 3.64

<i>m/z</i>	Intensity	Relative
61.9879	820.3	0.75
73.0284	3665.7	3.34
89.0597	5027.3	4.59
100.0351	843	0.77
133.0858	3397.9	3.1
188.0705	1609.2	1.47
190.0862	109632.2	100
191.0894	10443.8	9.53
199.1114	3178	2.9
212.0833	942.9	0.86
212.6466	818	0.75
227.1066	1060.6	0.97
285.0095	915.2	0.83
290.0934	5850.9	5.34
306.0874	1514.5	1.38
321.1115	1235.8	1.13
352.1181	1319.9	1.2
352.1538	3342.8	3.05
370.1649	29458.8	26.87
371.1681	6710.3	6.12

GS_250.raw

FTMS + c ESI d Full ms2 370.1649@hcd30.00 [50.0000-395.0000]

Scan #: 645

RT: 3.62

<i>m/z</i>	Intensity	Relative
73.0285	1854.3	2.07
89.0597	5394.1	6.02
133.0858	1768.9	1.97
135.0802	1385.7	1.55
164.0706	1047.2	1.17
190.0862	89671.5	100
191.0704	1507.9	1.68
191.0893	7135.5	7.96
199.1116	5467	6.1
227.1062	1724.2	1.92
290.0935	5497.5	6.13
291.0982	1206.2	1.35

337.0895	1008.8	1.13
352.1179	3703.2	4.13
352.1537	4772.2	5.32
354.1703	1057.6	1.18
370.129	1740.3	1.94
370.1647	20741.2	23.13
370.2003	1331.6	1.49
371.1677	3430.7	3.83

GS_500.raw

FTMS + c ESI d Full ms2 370.1649@hcd30.00 [50.0000-395.0000]

Scan #: 651

RT: 3.61

<i>m/z</i>	Intensity	Relative
73.0285	4408.9	35.25
89.0597	8923.3	71.35
90.9767	1807.4	14.45
97.0285	1581.8	12.65
123.0803	3131.7	25.04
133.0859	3614.2	28.9
164.0706	1601.4	12.8
176.0705	1841.5	14.72
190.0862	12506.6	100
199.1117	7422.1	59.35
227.1063	5566.4	44.51
245.1172	1585.1	12.67
336.0861	3239.5	25.9
337.0894	2662.7	21.29
337.1069	4276.1	34.19
352.1172	5993	47.92
370.128	6560.8	52.46
370.1638	5439.4	43.49
371.2217	5128.6	41.01
372.1084	1756.5	14.04

Mass [*m/z*] 384.1441

GS_03125.raw

FTMS + c ESI d Full ms2 384.1439@hcd30.00 [50.0000-410.0000]

Scan #: 412

RT: 2.44

<i>m/z</i>	Intensity	Relative
149.0597	10823.5	6.01
176.071	3779.8	2.1
189.0785	5101.9	2.84
190.0861	109806	61.02
191.089	10068.9	5.6
282.0884	3307.8	1.84
293.0803	16748.7	9.31
294.0866	7308.1	4.06
295.0959	8961	4.98
297.1119	5239	2.91
320.0677	4351.3	2.42
322.0828	5195.7	2.89
323.091	179955	100
324.0945	39763.9	22.1
335.0911	26104.2	14.51
336.0934	3854.3	2.14
353.1016	3981.5	2.21
366.0973	14301.4	7.95
384.1437	57711.1	32.07
385.1473	12224.4	6.79

GS_0625.raw

FTMS + c ESI d Full ms2 384.1439@hcd30.00 [50.0000-410.0000]

Scan #: 416

RT: 2.44

<i>m/z</i>	Intensity	Relative
149.0597	26072	6.57
176.0706	11582.4	2.92
190.0862	209693.5	52.87
191.0888	20358.7	5.13
282.0889	9084.7	2.29
293.0805	41527.1	10.47
294.0869	12097.3	3.05
295.0958	13157.5	3.32
297.1116	11700.6	2.95
305.0802	8348.5	2.1
320.0677	11658.1	2.94

322.0834	10994.7	2.77
323.0911	396655.1	100
324.0946	76179.9	19.21
335.0911	54558.2	13.75
336.0949	10743.7	2.71
366.0972	34251.6	8.64
366.1324	9705.8	2.45
384.1438	116778.8	29.44
385.1474	24128.4	6.08

GS_125.raw

FTMS + c ESI d Full ms2 384.1439@hcd30.00 [50.0000-410.0000]

Scan #: 422

RT: 2.44

<i>m/z</i>	Intensity	Relative
149.0597	112695.7	5.82
176.0706	67604.8	3.49
190.0862	1101582	56.91
191.0888	105295.2	5.44
282.0884	51645.7	2.67
293.0805	193431.1	9.99
294.0873	67683.1	3.5
295.0963	59170.7	3.06
297.1119	56881.7	2.94
305.0804	35879.8	1.85
320.0679	62144	3.21
322.0834	55512.6	2.87
323.0911	1935556	100
324.0945	415656	21.47
335.091	299359.8	15.47
336.0948	60134.9	3.11
366.0972	103092.1	5.33
366.1328	46734	2.41
384.1439	558424.9	28.85
385.1472	130346.8	6.73

GS_250.raw

FTMS + c ESI d Full ms2 384.1438@hcd30.00 [50.0000-410.0000]

Scan #: 430

RT: 2.44

<i>m/z</i>	Intensity	Relative
149.0597	319894.6	6.52
176.0705	131239	2.67

190.0861	2841749	57.9
191.0889	279477.8	5.69
282.0884	121882.4	2.48
293.0804	450337.8	9.18
294.0872	182924.9	3.73
295.0962	166000.6	3.38
297.1118	134687.2	2.74
320.0677	151236.9	3.08
322.0832	129848.2	2.65
323.091	4907864	100
324.0944	1011703	20.61
335.091	705794.1	14.38
336.0947	154723.8	3.15
353.1014	95424.8	1.94
366.0971	260373.2	5.31
366.1326	138485.7	2.82
384.1437	1486921	30.3
385.1471	350067.8	7.13

GS_500.raw

FTMS + c ESI d Full ms2 384.1437@hcd30.00 [50.0000-410.0000]

Scan #: 437

RT: 2.44

<i>m/z</i>	Intensity	Relative
149.0597	300023	6.19
176.0705	152740.1	3.15
190.0862	2820454	58.14
191.0888	262487.8	5.41
282.0884	134290.3	2.77
293.0804	459877	9.48
294.0869	167837.8	3.46
295.0962	160046.2	3.3
297.1118	154958.7	3.19
320.0679	145417.9	3
322.0837	131217.5	2.71
323.091	4850735	100
324.0945	972755	20.05
335.091	746634.6	15.39
336.0948	162427.6	3.35
366.097	574952.3	11.85
366.1319	129661.6	2.67
367.1003	111648.6	2.3
384.1438	1489509	30.71

385.1472 344252.5 7.1

Mass [*m/z*] 400.1391

GS_03125.raw

FTMS + c ESI d Full ms2 400.1376@hcd30.00 [50.0000-430.0000]

Scan #: 442

RT: 2.59

<i>m/z</i>	Intensity	Relative
71.0856	3871.3	11.47
111.0441	1573.4	4.66
190.0862	33763.8	100
191.0893	5440	16.11
193.0496	5649.9	16.73
293.0806	3707.1	10.98
295.0961	1822.4	5.4
311.0914	11713.5	34.69
320.068	1924.2	5.7
322.0837	1386.2	4.11
323.0913	17931.3	53.11
324.0942	1811.9	5.37
325.1056	3291	9.75
335.0912	11269.9	33.38
336.095	1932.1	5.72
339.0863	4285	12.69
340.0935	1697.7	5.03
349.0941	1523.9	4.51
353.1013	5101.2	15.11
400.1387	5179.2	15.34

GS_0625.raw

FTMS + c ESI d Full ms2 400.1376@hcd30.00 [50.0000-430.0000]

Scan #: 447

RT: 2.59

<i>m/z</i>	Intensity	Relative
57.0702	4462.8	7.45
58.0655	6682.7	11.16
111.044	3376.8	5.64
188.0704	3500	5.84
190.0861	59898.3	100
191.0896	7492.1	12.51
193.0494	11220.5	18.73
293.0801	5263.8	8.79

311.0908	15246.5	25.45
320.0678	4528.2	7.56
322.0833	3927.5	6.56
323.091	27011.5	45.1
324.0943	5508.2	9.2
325.1067	3996.3	6.67
335.0911	20841.7	34.8
336.0939	4023.4	6.72
339.0858	9803.6	16.37
340.0923	4713.2	7.87
353.1024	9588	16.01
400.1389	11663.6	19.47

GS_125.raw

FTMS + c ESI d Full ms2 400.1381@hcd30.00 [50.0000-430.0000]

Scan #: 456

RT: 2.61

<i>m/z</i>	Intensity	Relative
58.0654	17607	3.79
190.0861	464156.1	100
191.0895	52379.2	11.28
193.0494	51984.4	11.2
293.0804	37898.6	8.17
295.0965	20834.6	4.49
296.0676	17365.3	3.74
311.091	137027.8	29.52
312.0946	21192.6	4.57
320.0675	27507	5.93
323.091	218262.9	47.02
324.0946	43761.9	9.43
325.1071	28278.5	6.09
335.091	147953.5	31.88
336.0945	31112.2	6.7
339.0861	70760	15.24
340.0925	28292.4	6.1
353.1015	45058.9	9.71
400.1388	76879.4	16.56
401.1418	18572.8	4

GS_250.raw

FTMS + c ESI d Full ms2 400.1374@hcd30.00 [50.0000-430.0000]

Scan #: 462

RT: 2.59

<i>m/z</i>	Intensity	Relative
58.0655	38900.8	6
190.0862	648767.8	100
191.0896	69419.4	10.7
193.0495	80218.7	12.36
293.0805	47217.5	7.28
295.0964	34175.4	5.27
296.0677	26046.1	4.01
311.0911	193062.8	29.76
312.0944	33399.3	5.15
320.0678	44900.1	6.92
322.0833	32477.6	5.01
323.0912	312041.8	48.1
324.0945	65558.5	10.11
325.1075	38622.7	5.95
335.0911	229489.5	35.37
336.0946	45962.5	7.08
339.0861	90795.9	14
340.0928	46387.7	7.15
353.1016	81645.9	12.58
400.1389	121642.9	18.75

GS_500.raw

FTMS + c ESI d Full ms2 400.1373@hcd30.00 [50.0000-430.0000]

Scan #: 470

RT: 2.60

<i>m/z</i>	Intensity	Relative
58.0655	71096.5	8
188.0705	36160.1	4.07
190.0861	888165.7	100
191.0895	105869.9	11.92
193.0494	122234.8	13.76
293.0804	78277.1	8.81
295.0964	39447.7	4.44
296.0677	37721.5	4.25
311.091	263629	29.68
312.0944	51696.8	5.82
320.0676	64497.6	7.26
323.091	427984.3	48.19

324.0945	86108.2	9.7
325.1074	57327.9	6.45
335.091	291166.5	32.78
336.0945	63590	7.16
339.0859	132769.9	14.95
340.0923	61090.4	6.88
353.1015	126461.9	14.24
400.1387	155874	17.55

Mass [m/z] 445.2947

GS_03125.raw

FTMS + c ESI d Full ms2 445.2945@hcd30.00 [50.0000-475.0000]

Scan #: 396

RT: 2.35

m/z	Intensity	Relative
69.07	15330.8	33.3
81.07	5054.9	10.98
97.0649	9008.6	19.57
99.0804	6052.1	13.15
123.0804	5992.7	13.02
125.0962	4453	9.67
165.1274	19817.6	43.05
249.1484	6638.3	14.42
283.169	6245.3	13.57
301.1796	11091.6	24.09
313.2159	4389.8	9.54
329.211	5033.2	10.93
331.2258	5959	12.94
353.2104	5201	11.3
371.2216	46034.4	100
372.2252	10480.1	22.77
409.274	6088.4	13.23
427.2839	12199.6	26.5
445.295	16157.2	35.1
446.298	5289.4	11.49

GS_0625.raw

FTMS + c ESI d Full ms2 445.2947@hcd30.00 [50.0000-475.0000]

Scan #: 397

RT: 2.34

m/z	Intensity	Relative
61.9907	1486.3	4.85

69.0701	7861.4	25.67
81.0698	3971.2	12.97
97.0648	1895	6.19
99.0805	5934.9	19.38
117.0698	1675.2	5.47
123.0804	3142.6	10.26
125.0959	1648.6	5.38
165.1273	12908.4	42.15
247.1318	1851.5	6.05
249.1483	3915.8	12.79
265.1584	1699.8	5.55
283.1682	1911	6.24
301.1796	5598.1	18.28
331.2256	3688.4	12.04
371.2212	30625.9	100
372.2252	7537.8	24.61
427.2841	5321.9	17.38
445.2951	8835.7	28.85
446.2965	1901.2	6.21

GS_125.raw

FTMS + c ESI d Full ms2 445.2946@hcd30.00 [50.0000-475.0000]

Scan #: 401

RT: 2.33

<i>m/z</i>	Intensity	Relative
69.07	10097.2	25.56
81.0699	5464.9	13.84
97.0649	9043.5	22.9
99.0805	7642.3	19.35
123.0805	4194.6	10.62
165.1274	16008.4	40.53
173.0962	3636.8	9.21
249.1483	4734.2	11.99
255.1742	4370	11.06
265.1583	3475.4	8.8
283.1693	4135.5	10.47
301.1797	11118.8	28.15
313.2156	3639	9.21
331.2262	4310.6	10.91
353.2107	3948.2	10
371.2214	39499.1	100
372.225	11727.1	29.69
427.2844	7005.5	17.74

445.2958	10153.6	25.71
446.2984	3513.8	8.9

[GS_250.raw](#)

FTMS + c ESI d Full ms2 445.2946@hcd30.00 [50.0000-475.0000]

Scan #: 423

RT: 2.41

<i>m/z</i>	Intensity	Relative
69.07	764645.9	33.66
81.0699	294998.1	12.99
97.0648	457116.6	20.12
99.0804	431024.5	18.97
123.0804	333816.6	14.69
165.1274	1014053	44.64
173.0961	221098.9	9.73
249.1484	294997.3	12.99
283.1691	305246.9	13.44
301.1795	715485.3	31.49
313.2159	203842.9	8.97
329.2106	208224.8	9.17
331.2264	369181.8	16.25
353.2107	196676.5	8.66
371.2214	2271772	100
372.2248	535562.5	23.57
409.2734	313968.8	13.82
427.284	574843.2	25.3
445.2945	793734.6	34.94
446.2981	230265.4	10.14

[GS_500.raw](#)

FTMS + c ESI d Full ms2 445.2946@hcd30.00 [50.0000-475.0000]

Scan #: 434

RT: 2.43

<i>m/z</i>	Intensity	Relative
69.07	1083479	25.52
81.0699	446190.7	10.51
97.0648	608629.8	14.34
99.0804	676237.8	15.93
123.0804	534234	12.58
125.0961	295321	6.96
165.1273	1828319	43.06
249.1485	500390.9	11.79
283.169	462137.6	10.88

301.1795	1115222	26.27
313.2159	300586.3	7.08
329.2108	389652.3	9.18
331.2264	557198.1	13.12
353.2107	317063.7	7.47
371.2214	4245653	100
372.2248	1033933	24.35
409.2733	465974.3	10.98
427.2841	1002837	23.62
445.2946	1298930	30.59
446.2978	384570.2	9.06

Mass [*m/z*] 463.3057

GS_03125.raw

FTMS + c ESI d Full ms2 463.3049@hcd30.00 [50.0000-490.0000]

Scan #: 399

RT: 2.37

<i>m/z</i>	Intensity	Relative
69.07	9105.8	37.21
81.0699	6104.6	24.94
97.0649	3837.6	15.68
99.0805	7688	31.41
107.0856	4015.6	16.41
109.1012	3255.1	13.3
125.0961	5108.8	20.87
147.1165	1852.9	7.57
165.1273	24474	100
173.0963	5761.9	23.54
249.1484	1984.3	8.11
283.1693	2985.2	12.2
301.1798	8392.2	34.29
303.0493	11022	45.04
303.1951	4324.2	17.67
329.2106	1907.1	7.79
371.2213	5952.8	24.32
409.2733	4770.2	19.49
427.284	7985.4	32.63
445.2945	9724.3	39.73

GS_0625.raw

FTMS + c ESI d Full ms2 463.3046@hcd30.00 [50.0000-490.0000]

Scan #: 400

RT: 2.35

<i>m/z</i>	Intensity	Relative
69.07	5981.7	24.2
81.0699	4859.3	19.66
97.0649	1294.4	5.24
99.0805	5897	23.86
107.0854	1684.8	6.82
123.0803	1607.8	6.51
125.0961	5279.9	21.36
165.1273	15464.7	62.58
247.1327	1197.7	4.85
249.1482	1383.3	5.6
283.169	3617.5	14.64
295.205	1802.5	7.29
301.1791	8599.2	34.8
303.0496	24713.2	100
329.2108	1338.1	5.41
353.2098	1324.1	5.36
371.2211	3757	15.2
409.2731	1465.9	5.93
427.2835	4608.3	18.65
445.2953	9218	37.3

GS_125.raw

FTMS + c ESI d Full ms2 463.3053@hcd30.00 [50.0000-490.0000]

Scan #: 404

RT: 2.35

<i>m/z</i>	Intensity	Relative
69.07	7327.4	16.15
81.0699	5390	11.88
85.0284	3704.4	8.16
99.0804	10789.7	23.78
107.0854	4002.3	8.82
123.0803	3682.6	8.12
125.096	7809.7	17.21
127.1116	3512.9	7.74
165.1274	26702	58.85
166.1306	3830.7	8.44
173.0959	3349.3	7.38
249.1481	3920.7	8.64

283.1689	4262.3	9.39
301.1797	11096.8	24.45
303.0496	45376.8	100
329.2102	3857	8.5
371.2211	5699.7	12.56
409.2731	5125.1	11.29
427.2838	6559.3	14.46
445.2948	11331.8	24.97

[GS_250.raw](#)

FTMS + c ESI d Full ms2 463.3052@hcd30.00 [50.0000-490.0000]

Scan #: 407

RT: 2.33

<i>m/z</i>	Intensity	Relative
61.0287	3344	3.5
61.9872	1243.1	1.3
69.07	3468.7	3.64
85.0284	6795.7	7.12
91.0389	1808.8	1.9
97.0284	3168.7	3.32
97.0647	1405	1.47
99.0803	5064.4	5.31
109.1009	1104.2	1.16
125.096	1695.1	1.78
127.0387	1093.8	1.15
165.1274	11950.4	12.52
265.1584	1137.5	1.19
283.1689	1088.6	1.14
301.1792	5679.7	5.95
302.1829	1099.9	1.15
303.0496	95416.5	100
371.2214	1694.9	1.78
427.2846	1945	2.04
445.294	5260.1	5.51

[GS_500.raw](#)

FTMS + c ESI d Full ms2 463.3051@hcd30.00 [50.0000-490.0000]

Scan #: 414

RT: 2.33

<i>m/z</i>	Intensity	Relative
61.0287	4761.3	3.03
69.07	6153.4	3.92
81.0699	4506.5	2.87

85.0284	13904.2	8.86
91.039	6065	3.87
97.0285	3542	2.26
97.0648	3190.3	2.03
99.0805	3732.3	2.38
107.0855	1655.8	1.06
125.096	4169.4	2.66
127.039	1742.1	1.11
145.0493	1866	1.19
165.1273	15043.1	9.59
173.0962	1511.3	0.96
283.1687	3196.3	2.04
301.1792	6258.8	3.99
303.0496	156901	100
371.2216	3589.2	2.29
427.2845	1800.7	1.15
445.2945	4780.4	3.05

Mass [*m/z*] 481.3160

GS_03125.raw

FTMS + c ESI d Full ms2 481.3155@hcd30.00 [50.0000-510.0000]

Scan #: 427

RT: 2.52

<i>m/z</i>	Intensity	Relative
69.07	7458	43.23
81.0699	4425.2	25.65
97.0647	4209.2	24.4
99.0803	5550.7	32.17
107.0855	1493.3	8.66
123.0802	3345.3	19.39
125.0961	5298.2	30.71
135.1167	1484	8.6
165.1274	17252.3	100
173.0961	1945	11.27
249.1478	1368.3	7.93
265.1583	3642.1	21.11
283.1686	3317	19.23
295.2047	3019.4	17.5
301.1791	3699.4	21.44
371.2213	11968.4	69.37
372.2237	1479.9	8.58
427.2834	4627.2	26.82

428.287	1435.2	8.32
445.2941	3522	20.41

[GS_0625.raw](#)

FTMS + c ESI d Full ms2 481.3156@hcd30.00 [50.0000-510.0000]

Scan #: 430

RT: 2.51

<i>m/z</i>	Intensity	Relative
69.07	13763.5	28.35
81.0699	12335.8	25.41
97.0648	9316.2	19.19
99.0804	11760.3	24.22
107.0855	7530.2	15.51
123.0806	7028.9	14.48
125.096	15340.7	31.59
165.1273	48555.4	100
166.1307	6439.7	13.26
173.0963	7467.5	15.38
249.1484	5498.8	11.32
283.169	7023	14.46
295.2054	5320.3	10.96
301.18	10070.2	20.74
313.2161	4501.9	9.27
371.2213	29605.7	60.97
372.2248	5651	11.64
409.2725	4798.7	9.88
427.2838	7606.6	15.67
445.2948	12494.4	25.73

[GS_125.raw](#)

FTMS + c ESI d Full ms2 481.3155@hcd30.00 [50.0000-510.0000]

Scan #: 431

RT: 2.48

<i>m/z</i>	Intensity	Relative
69.07	54856.7	31.94
81.0699	33013.4	19.22
97.0648	34633.9	20.16
99.0804	41732.4	24.3
107.0855	31022.9	18.06
123.0804	21789.8	12.69
125.096	52974.2	30.84
165.1273	171759.8	100
166.1307	16785.4	9.77

173.096	21194.4	12.34
187.1116	15228.3	8.87
265.1584	19374.8	11.28
283.169	27834.8	16.21
301.1794	22867.7	13.31
319.1898	15431.6	8.98
371.2213	95942.7	55.86
372.2245	18609.3	10.83
409.2734	22235.3	12.95
427.2841	33439	19.47
445.2946	35813.2	20.85

GS_250.raw

FTMS + c ESI d Full ms2 481.3157@hcd30.00 [50.0000-510.0000]

Scan #: 420

RT: 2.40

<i>m/z</i>	Intensity	Relative
69.07	902136.8	29.34
81.0699	645726.9	21
97.0648	559664.6	18.2
99.0805	753278.6	24.5
107.0855	542488.8	17.64
123.0804	432566.5	14.07
125.0961	812269.3	26.42
165.1274	3074644	100
166.1307	326650.8	10.62
173.0961	343822.7	11.18
191.1066	280958.4	9.14
249.1486	290207.5	9.44
265.1585	278470.4	9.06
283.1692	485767.2	15.8
301.1797	506145.3	16.46
371.2215	1640313	53.35
372.2249	416838.5	13.56
409.2736	367014.4	11.94
427.284	582882.6	18.96
445.2946	713141.9	23.19

GS_500.raw

FTMS + c ESI d Full ms2 481.3158@hcd30.00 [50.0000-510.0000]

Scan #: 427

RT: 2.40

<i>m/z</i>	Intensity	Relative
69.07	1928508	32.6
81.0699	1362068	23.02
97.0648	995372.2	16.82
99.0804	1437660	24.3
107.0855	925861.9	15.65
123.0804	638973.8	10.8
125.0961	1702848	28.78
143.1067	541722.9	9.16
165.1274	5916076	100
166.1307	623102.8	10.53
173.0961	782649.3	13.23
191.1065	581766.8	9.83
265.1584	612547.3	10.35
283.169	1048091	17.72
301.1796	906514.8	15.32
371.2214	3264021	55.17
372.2248	830733.5	14.04
409.2732	672415.5	11.37
427.284	1304867	22.06
445.2946	1430360	24.18

Mass [*m/z*] 354.1700

GS_03125.raw

FTMS + c ESI d Full ms2 354.1697@hcd30.00 [50.0000-380.0000]

Scan #: 646

RT: 3.79

<i>m/z</i>	Intensity	Relative
59.0494	1480.4	0.11
61.9904	1704	0.13
63.3209	2248.9	0.17
80.6952	1426.7	0.11
90.9768	1664.9	0.12
165.091	3718.5	0.28
176.0704	9443.4	0.7
188.0704	33566.5	2.49
189.0729	1333.1	0.1
189.0795	1443.3	0.11

190.0861	1346596	100
191.0895	138619.6	10.29
192.0923	5968.6	0.44
308.8995	1831	0.14
323.1266	2395.3	0.18
339.1465	4071.8	0.3
353.1573	1217.8	0.09
354.1695	1116729	82.93
355.1729	251293.8	18.66
356.1758	19316.1	1.43

GS_0625.raw

FTMS + c ESI d Full ms2 354.1698@hcd30.00 [50.0000-380.0000]

Scan #: 652

RT: 3.78

<i>m/z</i>	Intensity	Relative
63.3209	8719.3	0.19
118.3393	3792.9	0.08
165.0913	11200.2	0.24
165.8623	3364.9	0.07
176.0707	33705.5	0.72
188.0706	114120.9	2.45
188.4378	3197.5	0.07
189.0787	15069.7	0.32
190.0862	4660558	100
191.0896	503403.2	10.8
191.0988	6841.4	0.15
192.0917	20492.3	0.44
205.446	3193.2	0.07
308.9005	5798	0.12
323.1271	13765.4	0.3
338.1388	3885.7	0.08
339.1466	6948.8	0.15
354.1697	4243861	91.06
355.173	935694.9	20.08
356.1755	75383.3	1.62

GS_125.raw

FTMS + c ESI d Full ms2 354.1696@hcd30.00 [50.0000-380.0000]

Scan #: 663

RT: 3.79

<i>m/z</i>	Intensity	Relative
63.3208	14088.1	0.16
86.0962	7289	0.08
118.339	8680.5	0.1
165.0907	30283.9	0.35
176.0706	77438.5	0.89
179.1067	8126.8	0.09
180.2673	7452.7	0.09
188.0704	214953.6	2.46
189.0784	10428	0.12
190.0861	8741601	100
191.0894	989573.3	11.32
192.0909	11384.6	0.13
271.7413	7225.7	0.08
292.109	9578	0.11
339.1467	12595.3	0.14
352.1172	10311.1	0.12
354.1695	8016200	91.7
355.1728	1779421	20.36
356.1756	111846.4	1.28
357.4907	9302.4	0.11

GS_250.raw

FTMS + c ESI d Full ms2 354.1696@hcd30.00 [50.0000-380.0000]

Scan #: 672

RT: 3.76

<i>m/z</i>	Intensity	Relative
58.0654	20561.5	0.08
63.3208	52382.7	0.19
165.0908	71095.4	0.26
176.0706	236876.5	0.87
176.0771	25744	0.09
177.0741	20368.4	0.07
179.1066	27485.4	0.1
188.0705	635127.9	2.32
189.0728	21912.2	0.08
189.0791	33301.7	0.12
190.0861	27353292	100
191.0895	2838455	10.38

192.0929	129214.5	0.47
202.0858	20991	0.08
323.1279	33520.2	0.12
339.1457	70126.1	0.26
352.1178	21236.7	0.08
354.1696	24662602	90.16
355.1729	5692965	20.81
356.1758	539883.5	1.97

[GS_500.raw](#)

FTMS + c ESI d Full ms2 354.1695@hcd30.00 [50.0000-380.0000]

Scan #: 682

RT: 3.76

<i>m/z</i>	Intensity	Relative
63.3208	94195.2	0.2
66.5606	30210.4	0.06
82.5674	30802.8	0.06
165.0909	138309.7	0.29
174.0637	32882.4	0.07
176.0707	269073.4	0.56
188.0704	925692.1	1.92
189.0789	50505.6	0.1
190.0861	48295300	100
191.0895	5119071	10.6
191.099	37313.1	0.08
192.0923	162635.3	0.34
214.7129	32020.5	0.07
281.9102	33702	0.07
292.1091	40139.9	0.08
323.128	74380.6	0.15
339.1463	133561.6	0.28
354.1696	43169916	89.39
355.1728	9989258	20.68
356.1761	637673.9	1.32

Mass [*m/z*] 340.1181

[GS_03125.raw](#)

FTMS + c ESI d Full ms2 340.1181@hcd30.00 [50.0000-365.0000]

Scan #: 1006

RT: 5.97

<i>m/z</i>	Intensity	Relative
59.0494	1236.3	0.23

67.0544	1385.8	0.25
80.9478	1230.5	0.22
81.07	1339.1	0.24
122.0356	1293.4	0.24
123.0802	1368.1	0.25
149.0595	1718	0.31
150.0309	3340.5	0.61
175.0628	3793.7	0.69
176.0705	56639.3	10.31
177.074	4570.5	0.83
295.0833	1249.9	0.23
310.071	3457.1	0.63
324.0865	12366.4	2.25
325.0943	142061.8	25.86
326.0976	26831.7	4.88
327.1017	1469.9	0.27
340.1178	549392.9	100
341.1211	115501.9	21.02
342.1233	8288.1	1.51

GS_0625.raw

FTMS + c ESI d Full ms2 340.1180@hcd30.00 [50.0000-365.0000]

Scan #: 1017

RT: 5.96

<i>m/z</i>	Intensity	Relative
67.0545	1200.9	0.16
80.9478	1242.1	0.17
87.0439	1521.2	0.21
122.0357	1178.4	0.16
149.0598	2025.4	0.27
150.0313	4871	0.66
175.063	4646.8	0.63
176.0705	69933	9.46
177.0741	7069.6	0.96
295.0841	1436.7	0.19
310.0709	5655.7	0.77
324.0862	13471	1.82
325.0943	191223.4	25.87
326.0977	34397.9	4.65
327.0996	1670.8	0.23
338.1296	1700.8	0.23
339.1414	1445.4	0.2
340.1178	739092.6	100

341.1212	149031.8	20.16
342.1243	12735.4	1.72

[GS_125.raw](#)

FTMS + c ESI d Full ms2 340.1179@hcd30.00 [50.0000-365.0000]

Scan #: 1030

RT: 5.96

<i>m/z</i>	Intensity	Relative
80.9479	2154.6	0.15
149.0598	4282.1	0.31
150.0312	7468.4	0.53
175.0628	8315.5	0.59
176.0704	152975.3	10.92
177.0739	14266.6	1.02
295.0839	5164.2	0.37
296.0901	2165.7	0.15
308.0916	1761.9	0.13
310.0706	11127.6	0.79
324.0864	29004.7	2.07
325.0941	377342.3	26.94
326.0974	68804.4	4.91
326.1174	1918.5	0.14
327.0999	2342	0.17
338.1283	4492.8	0.32
339.1424	2072.7	0.15
340.1176	1400530	100
341.1209	306002	21.85
342.1236	21440.7	1.53

[GS_250.raw](#)

FTMS + c ESI d Full ms2 340.1179@hcd30.00 [50.0000-365.0000]

Scan #: 1047

RT: 5.95

<i>m/z</i>	Intensity	Relative
122.0359	2213.5	0.13
149.0598	9364.8	0.54
150.0304	8987.7	0.52
151.0392	2084.4	0.12
175.0628	9940.6	0.57
176.0705	170451	9.82
177.0738	18324.9	1.06
295.0834	8692.8	0.5
296.0908	3963.6	0.23

310.0703	14747.1	0.85
311.074	1950.2	0.11
324.0865	36986.5	2.13
325.0942	459816.8	26.49
326.0975	89632.7	5.16
326.1175	2123.9	0.12
327.1007	6022.6	0.35
338.1266	7582.4	0.44
340.1177	1736084	100
341.121	363737.1	20.95
342.1233	27821.9	1.6

GS_500.raw

FTMS + c ESI d Full ms2 340.1178@hcd30.00 [50.0000-365.0000]

Scan #: 1062

RT: 5.95

<i>m/z</i>	Intensity	Relative
58.0655	2035.7	0.23
149.0598	5957.2	0.66
150.031	4137.7	0.46
175.0626	4567.6	0.51
176.0705	97427.1	10.86
177.0737	8250.4	0.92
204.0655	1905.3	0.21
295.083	1863.5	0.21
310.0703	9453.8	1.05
323.1051	5557.1	0.62
324.0866	16150.2	1.8
325.0941	226819.3	25.28
326.0976	42348	4.72
338.1299	14829.7	1.65
339.1407	5738.5	0.64
340.1177	897070.3	100
340.153	31731.1	3.54
341.121	188718	21.04
341.1566	8541.4	0.95
342.1236	14749.4	1.64

Mass [*m/z*] 354.1337

GS_03125.raw

FTMS + c ESI d Full ms2 354.1335@hcd30.00 [50.0000-380.0000]

Scan #: 1085

RT: 6.43

<i>m/z</i>	Intensity	Relative
164.0465	8504.3	1.86
174.055	14537.7	3.19
176.0705	28079.8	6.15
185.0122	2040.3	0.45
203.0226	9000.5	1.97
221.0331	4939.6	1.08
245.1058	3369.6	0.74
308.9001	3881.1	0.85
324.0873	1543.8	0.34
338.1016	4218.2	0.92
339.1099	52701.4	11.55
340.1132	8995.2	1.97
352.1182	4223.1	0.93
353.0657	3514.5	0.77
353.121	1681	0.37
353.2298	1590.5	0.35
354.1332	456414.9	100
355.1366	96986.4	21.25
356.1373	6768.9	1.48
373.1526	4236.8	0.93

[GS_0625.raw](#)

FTMS + c ESI d Full ms2 354.1335@hcd30.00 [50.0000-380.0000]

Scan #: 1096

RT: 6.42

<i>m/z</i>	Intensity	Relative
100.112	3275	0.69
164.0466	6815.6	1.44
174.0549	14761.7	3.12
176.0705	37183.3	7.87
177.0738	3684.3	0.78
203.0228	11165.6	2.36
221.0332	3893.8	0.82
297.0752	3550.6	0.75
308.9002	6277.4	1.33
324.086	4520.2	0.96
338.1015	5946.8	1.26
339.1098	58707.1	12.43
340.1134	9979.3	2.11
352.1189	7429.1	1.57
353.0655	5830.7	1.23

353.1213	4000.5	0.85
354.1332	472397.5	100
355.1367	103944.8	22
356.1394	7803.6	1.65
373.1532	3398.9	0.72

GS_125.raw

FTMS + c ESI d Full ms2 354.1335@hcd30.00 [50.0000-380.0000]

Scan #: 1107

RT: 6.41

<i>m/z</i>	Intensity	Relative
95.0854	3013.7	1.81
164.0468	3480.6	2.1
174.055	4423.8	2.66
176.0704	15105.1	9.09
203.0226	15475.8	9.32
221.0327	5803.8	3.49
269.0804	5687.6	3.42
282.0515	3118.7	1.88
297.0753	12966.7	7.81
308.9	3798.9	2.29
325.0707	3683.4	2.22
338.0417	4574.5	2.75
339.1099	20741.1	12.49
340.1133	3250.6	1.96
352.117	8638.4	5.2
353.0654	18744.3	11.28
353.1212	7128.6	4.29
354.069	4291	2.58
354.1333	166125.9	100
355.1369	38323.1	23.07

GS_250.raw

FTMS + c ESI d Full ms2 354.1335@hcd30.00 [50.0000-380.0000]

Scan #: 1126

RT: 6.41

<i>m/z</i>	Intensity	Relative
164.0466	8730.4	1.51
174.0551	18690.2	3.24
176.0705	42780.8	7.42
203.0226	9876.2	1.71
221.0332	6325	1.1
269.0804	9832.6	1.71

282.0515	5749.1	1
297.0756	30635.4	5.32
298.0792	6817.6	1.18
325.0705	4998.5	0.87
338.0416	11365.4	1.97
338.101	5714.8	0.99
339.1098	68581.5	11.9
340.1135	12852	2.23
352.1177	14812.1	2.57
353.0652	35819.3	6.22
353.1204	8700	1.51
354.1333	576320.9	100
355.1366	127642	22.15
356.1387	12116	2.1

GS_500.raw

FTMS + c ESI d Full ms2 354.1340@hcd30.00 [50.0000-380.0000]

Scan #: 1139

RT: 6.39

<i>m/z</i>	Intensity	Relative
163.0389	11444.5	18.09
190.0497	17333.1	27.39
190.086	7713.2	12.19
191.0943	6027.4	9.53
203.0227	9558.6	15.11
237.0547	8240.4	13.02
254.0566	7053.2	11.15
269.0806	22716.1	35.9
282.0517	7880.1	12.45
297.0754	52037.8	82.24
298.0791	10518.9	16.62
325.0708	8268.5	13.07
336.1224	9385.9	14.83
338.0414	19606.6	30.98
352.1178	11652.1	18.41
353.0652	63279.1	100
353.1203	9495.8	15.01
354.0692	15034.6	23.76
354.1337	18714.1	29.57
354.1682	8054.4	12.73

Mass [*m/z*] 352.1180

GS_03125.raw

FTMS + c ESI d Full ms2 352.1172@hcd30.00 [50.0000-380.0000]

Scan #: 445

RT: 2.61

<i>m/z</i>	Intensity	Relative
61.9911	1182.9	2.09
90.9737	1136.2	2.01
90.9766	11749.9	20.76
193.0495	3546	6.26
232.9275	1347.7	2.38
294.0882	1676.5	2.96
305.0804	1376.8	2.43
308.0916	1195.9	2.11
320.0674	1519.9	2.69
322.0834	5856	10.35
322.1062	1599	2.83
323.09	2718	4.8
325.1062	2903.9	5.13
335.091	6618.1	11.69
336.0874	1489.4	2.63
337.0938	11886.1	21
338.0972	1661	2.93
352.1176	56602.1	100
353.1012	5410	9.56
353.1211	10517.2	18.58

GS_0625.raw

FTMS + c ESI d Full ms2 352.1182@hcd30.00 [50.0000-380.0000]

Scan #: 450

RT: 2.60

<i>m/z</i>	Intensity	Relative
90.9767	11016.7	5.85
193.0492	5692.6	3.02
277.0855	3184.6	1.69
294.0878	3854.2	2.05
305.0804	5370	2.85
308.0914	7277.3	3.87
320.0688	7275.6	3.87
321.0755	3385.7	1.8
322.0835	8041.8	4.27
322.107	3632.9	1.93
323.0908	3812.8	2.03

325.107	5230.6	2.78
335.0914	13478.7	7.16
336.0851	8935.1	4.75
337.094	36968.4	19.64
338.0786	3039.5	1.61
338.0974	5724.1	3.04
352.1176	188208.4	100
353.101	6447.4	3.43
353.1207	46287.7	24.59

GS_125.raw

FTMS + c ESI d Full ms2 352.1177@hcd30.00 [50.0000-380.0000]

Scan #: 462

RT: 2.63

<i>m/z</i>	Intensity	Relative
90.9766	11980.2	0.95
193.0493	7806.2	0.62
305.0806	5839.6	0.46
308.0914	48312.3	3.84
309.0945	8165.9	0.65
320.0675	5238	0.42
322.0703	9104	0.72
322.0839	8735.7	0.7
322.1074	5085.8	0.4
323.0902	4851.7	0.39
325.1072	8206.6	0.65
334.1069	5033.7	0.4
335.0911	13853.1	1.1
336.0861	52741.4	4.2
337.0941	272881.2	21.71
338.0973	49232.2	3.92
352.1176	1256872	100
353.1045	9778.5	0.78
353.121	273736.9	21.78
354.1231	21627.1	1.72

GS_250.raw

FTMS + c ESI d Full ms2 352.1176@hcd30.00 [50.0000-380.0000]

Scan #: 466

RT: 2.61

<i>m/z</i>	Intensity	Relative
193.0494	18482.1	0.84
294.0885	15460.2	0.71

305.0807	14516.3	0.66
308.0914	67574.4	3.08
309.0951	11438.6	0.52
320.0679	17605.3	0.8
320.089	8929.9	0.41
322.0696	9142.5	0.42
322.0836	19799.9	0.9
322.106	10576.5	0.48
323.0908	11845.7	0.54
325.1066	12551.7	0.57
335.0911	39079.5	1.78
336.086	90125	4.11
337.094	431764.2	19.69
338.0973	84467.3	3.85
352.1176	2192580	100
353.1028	23607.5	1.08
353.1209	478774.8	21.84
354.1234	41114.4	1.88

GS_500.raw

FTMS + c ESI d Full ms2 352.1177@hcd30.00 [50.0000-380.0000]

Scan #: 469

RT: 2.59

<i>m/z</i>	Intensity	Relative
193.0495	30601.1	1.39
277.0855	13498.5	0.61
294.088	19491.2	0.88
305.0805	27881.3	1.26
308.0911	84181.4	3.81
320.0678	29562.9	1.34
322.0836	32674.5	1.48
322.1068	21480.3	0.97
323.0906	20743.9	0.94
325.1065	22190.7	1.01
335.0911	63945.5	2.9
336.0859	110487.1	5.01
337.0939	482263.4	21.85
338.0782	11616.6	0.53
338.0973	89213.8	4.04
351.1095	15087.5	0.68
352.1175	2207074	100
353.1021	28840.4	1.31
353.1208	476405.4	21.59

354.1234 37550.6 1.7

GS_03125.raw

FTMS + c ESI d Full ms2 352.1178@hcd30.00 [50.0000-380.0000]

Scan #: 1114

RT: 6.60

<i>m/z</i>	Intensity	Relative
90.9762	5169.6	3.3
93.0695	1311	0.84
121.1008	1800.9	1.15
133.1043	2708.2	1.73
143.0883	1674.3	1.07
171.1204	5577	3.56
308.0911	3789.9	2.42
322.0705	18328	11.69
322.107	1381.7	0.88
323.0734	4414.3	2.81
336.0858	3161.3	2.02
337.0941	156831.5	100
338.0975	32852.6	20.95
339.0998	1304.8	0.83
351.1776	3311.3	2.11
351.2132	3152.2	2.01
352.1176	147092.1	93.79
353.1208	30912.2	19.71
353.1936	4091.1	2.61
354.1333	1283.7	0.82

GS_0625.raw

FTMS + c ESI d Full ms2 352.1176@hcd30.00 [50.0000-380.0000]

Scan #: 1123

RT: 6.58

<i>m/z</i>	Intensity	Relative
90.9767	6420.5	0.72
95.0854	1803.9	0.2
101.0597	1997.8	0.23
147.1167	1967.8	0.22
171.1196	5901.2	0.66
308.0913	14350.3	1.62
319.0836	10626.8	1.2
320.0905	5455	0.61
321.0989	2159.7	0.24
322.0705	100422.1	11.31

322.1057	9585.1	1.08
323.0736	20410.7	2.3
336.086	13386.6	1.51
337.094	845778.1	95.28
338.0974	169230.5	19.06
339.0991	11623.9	1.31
352.1175	887702.6	100
353.1208	194883.7	21.95
353.1924	4468.9	0.5
354.1252	11135.6	1.25

GS_125.raw

FTMS + c ESI d Full ms2 352.1177@hcd30.00 [50.0000-380.0000]

Scan #: 1140

RT: 6.60

<i>m/z</i>	Intensity	Relative
59.9105	5081.6	0.79
90.9766	4352.4	0.68
95.0854	4936.8	0.77
121.101	3735	0.58
147.1168	3818	0.59
171.1203	6553.9	1.02
259.2053	6192.4	0.96
308.0915	12010.7	1.87
319.0834	7517.6	1.17
320.0899	3885.2	0.6
322.0707	77335.3	12.04
322.1074	6800.7	1.06
323.0739	15107.9	2.35
336.086	10045.3	1.56
337.0941	642460.3	100
338.0974	119072.6	18.53
339.0995	11184.8	1.74
352.1176	614274.3	95.61
353.1209	126170.4	19.64
354.13	10254.2	1.6

GS_250.raw

FTMS + c ESI d Full ms2 352.1177@hcd30.00 [50.0000-380.0000]

Scan #: 1121

RT: 6.39

<i>m/z</i>	Intensity	Relative
90.9767	6647.4	17.15
101.0598	3779.2	9.75
133.1011	3592.9	9.27
135.1169	4155.1	10.72
157.1224	3691.7	9.52
190.0498	7265.7	18.74
237.0542	5705.3	14.72
259.2057	9459.8	24.4
269.0808	8501	21.93
282.0519	4364.8	11.26
292.0965	4068.5	10.49
297.0754	29118.1	75.1
325.0705	4634.1	11.95
337.0936	6754.9	17.42
338.0418	9630.1	24.84
352.1178	28598.5	73.76
353.0652	38770.6	100
353.1215	6940.5	17.9
354.0686	4667.3	12.04
354.1335	6950.7	17.93

GS_500.raw

FTMS + c ESI d Full ms2 352.1176@hcd30.00 [50.0000-380.0000]

Scan #: 1138

RT: 6.39

<i>m/z</i>	Intensity	Relative
59.908	6243.7	8.33
133.1007	7137.7	9.52
147.1169	9076.3	12.11
161.1326	8898.5	11.87
190.0499	10247.9	13.67
237.0547	6358.5	8.48
259.2052	14765.4	19.7
269.0807	22479.6	30
282.0524	6754.8	9.01
297.0755	58339.5	77.85
298.0792	6640.8	8.86
325.0706	9409.1	12.56

336.1223	6555.2	8.75
337.0943	8056.4	10.75
338.0414	19137.7	25.54
352.1177	46889.2	62.57
353.0653	74940.1	100
353.1205	8734.7	11.66
354.0685	11216.1	14.97
354.1336	11889.4	15.87

Mass [m/z] 336.1230

GS_03125.raw

FTMS + c ESI d Full ms2 336.1226@hcd30.00 [50.0000-360.0000]

Scan #: 685

RT: 4.03

m/z	Intensity	Relative
52.0649	829.2	0.56
61.9904	983.9	0.67
73.8433	838.9	0.57
85.1011	913.6	0.62
139.7907	829.1	0.56
149.0235	3131	2.12
204.4725	856.7	0.58
253.6291	857.8	0.58
271.0566	820.6	0.56
286.0576	944.7	0.64
292.0958	5569.5	3.78
293.1011	854	0.58
320.0911	5480.9	3.72
321.0992	31431.1	21.32
322.1034	6202.1	4.21
335.1826	3476	2.36
336.1226	147398.1	100
337.1258	30426.2	20.64
337.1975	960.5	0.65
338.1389	10655.8	7.23

GS_0625.raw

FTMS + c ESI d Full ms2 336.1215@hcd30.00 [50.0000-360.0000]

Scan #: 663

RT: 3.84

<i>m/z</i>	Intensity	Relative
53.5348	746.6	5.07
58.2657	735.8	5
59.9557	734.3	4.99
61.9896	898.6	6.11
62.9052	733.9	4.99
75.0087	725.9	4.93
85.1013	1285	8.73
87.9643	860.4	5.85
89.0596	870.6	5.92
90.9768	1068.3	7.26
92.2813	802.4	5.45
126.5633	746.1	5.07
134.4005	846.4	5.75
149.0234	1148	7.8
321.0992	1725.4	11.72
335.182	2956.6	20.09
336.123	14718.4	100
337.1257	3579.3	24.32
337.1975	852.6	5.79
338.138	1728	11.74

GS_125.raw

FTMS + c ESI d Full ms2 336.1214@hcd30.00 [50.0000-360.0000]

Scan #: 688

RT: 3.94

<i>m/z</i>	Intensity	Relative
53.5683	775.9	3.21
77.2764	771.2	3.19
78.4662	764.5	3.16
83.0645	829.5	3.43
85.1013	931.5	3.85
89.0599	785	3.24
90.9766	1607.1	6.64
99.0439	815.8	3.37
149.0233	1857.5	7.68
231.7607	913.1	3.77
250.5358	912.7	3.77
304.4357	828.8	3.43

321.0996	6267.3	25.9
322.1031	1524.1	6.3
335.1822	1894.4	7.83
336.1225	24194	100
336.1855	850.7	3.52
337.126	6796.4	28.09
337.1982	1429.2	5.91
338.1386	5421.9	22.41

GS_250.raw

FTMS + c ESI d Full ms2 336.1222@hcd30.00 [50.0000-360.0000]

Scan #: 662

RT: 3.71

<i>m/z</i>	Intensity	Relative
51.9411	922.3	2.03
52.9769	795	1.75
149.0233	3284.8	7.23
187.5407	794	1.75
232.9277	1605.8	3.54
234.1483	852	1.88
306.0756	837.8	1.84
315.7481	762.6	1.68
320.0901	3107.2	6.84
321.0989	13278.4	29.23
322.1029	2971.2	6.54
334.1072	1262.8	2.78
335.0894	958.7	2.11
335.1822	1241.7	2.73
335.2023	941.9	2.07
336.0866	3641.4	8.02
336.1226	45420.6	100
337.1267	11239.2	24.74
337.1608	1812.9	3.99
338.1384	19738.1	43.46

GS_500.raw

FTMS + c ESI d Full ms2 336.1223@hcd30.00 [50.0000-360.0000]

Scan #: 672

RT: 3.71

<i>m/z</i>	Intensity	Relative
68.1702	855.2	0.9
86.2802	848.6	0.89
89.26	870.9	0.91
149.0232	3193.7	3.35
164.07	861.6	0.9
292.0964	3934.4	4.13
320.0908	3024.7	3.17
321.0992	24268.6	25.45
322.104	3727.7	3.91
323.115	3636.3	3.81
334.1073	3302.5	3.46
335.1103	935.8	0.98
335.1822	4626	4.85
336.0874	4996.3	5.24
336.1226	95347.2	100
337.1264	21631.2	22.69
337.1615	1165.2	1.22
337.1982	1036	1.09
338.1385	29835.2	31.29
353.8969	912.2	0.96