

Supplemental material: MSⁿ peak lists

Structural Characterization by MSⁿ of Human Milk Glycans Recognized by Human Rotaviruses

David J. Ashline¹, Ying Yu², Yi Lasanajak², Xuezheng Song², Liya Hu³, Sasirekha Ramani⁴, Venkataram Prasad^{3,4}, Mary K. Estes⁴, Richard D. Cummings², David F. Smith²,
and Vernon N. Reinhold¹

¹Glycomics Center, University of New Hampshire, Durham, NH, ²Department of Biochemistry and the National Center for Functional Glycomics, Emory University School of Medicine, Atlanta, GA, ³Verna and Marris McLean Department of Biochemistry and Molecular Biology and ⁴Department of Molecular Virology and Microbiology, Baylor College of Medicine, Houston, TX

Peak lists for mass spectra

Peak lists are the 50 most intense peaks. Spectra were collected in profile mode, then converted to centroid in Thermo Xcalibur 2.0 using their valley detection algorithm. Peaks are listed in order of m/z. Scan headers indicate actual precursor m/z settings and number of scans. Microscan count, maximum injection time, and AGC target values were modified depending on anticipated signal intensity.

HMG 13 Mass spectral peak lists

Mass spectra were acquired in profile mode, then centroided using the valley detection algorithm. The top 50 peaks are shown. Isolation mass and width are adjusted to capture an entire isotopic envelope, where possible.

SPECTRUM - MS

7-1-13_HMG13_837_MS2_01.raw

ITMS + p ESI E Full ms2 838.00@cid35.00 [230.00-2000.00]

Scan #: 1-20

RT: 0.00-1.70

AV: 20

m/z	Intensity	Relative
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259.14	3922.3	7.70
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260.15	495.8	0.97
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406.20	449.0	0.88
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412.27	2341.7	4.60
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413.28	574.7	1.13	
472.31	928.3	1.82	
486.32	32794.3		64.40
487.33	8833.7		17.35
488.34	1477.2		2.90
581.40	572.2	1.12	
581.90	514.6	1.01	
605.42	4632.9		9.10
605.93	4132.7		8.12
606.43	1659.9		3.26
606.92	440.6	0.87	
681.97	8610.9		16.91
682.47	8917.3		17.51
682.97	3982.5		7.82
683.47	1162.7		2.28
718.43	533.9	1.05	
718.97	13502.4		26.52
719.47	14519.2		28.51
719.96	6699.9		13.16
720.48	2331.9		4.58
721.00	415.5	0.82	
738.51	8563.1		16.82
739.52	4245.7		8.34
740.52	1065.0		2.09
760.44	529.9	1.04	
809.04	821.9	1.61	
837.10	10414.9		20.45
837.57	11023.1		21.65
838.06	5326.2		10.46
838.55	2349.2		4.61
839.08	350.3	0.69	
935.57	2100.4		4.12
936.58	1324.5		2.60
937.59	354.4	0.70	
983.66	416.8	0.82	
1079.62		1261.8	2.48
1080.63		891.5	1.75
1167.60		401.7	0.79
1187.75		50921.3	100.00
1188.76		41443.1	81.39
1189.76		15318.7	30.08
1190.77		3546.4	6.96
1414.88		11038.6	21.68
1415.89		11471.1	22.53
1416.89		4940.9	9.70
1417.90		1383.8	2.72

SPECTRUM - MS

7-1-13_HMG13_837_MS3_935_01.raw

ITMS + p ESI E Full ms3 838.00@cid35.00 936.00@cid35.00 [255.00-1000.00]

Scan #: 1-50

RT: 0.00-3.52

AV: 50

m/z Intensity Relative

268.14	1.7	0.32
315.19	2.7	0.50
398.24	0.9	0.17
412.26	7.6	1.41
413.21	0.8	0.15
413.40	0.5	0.10
424.24	7.1	1.32
425.25	1.3	0.24
430.30	1.2	0.21
440.23	2.4	0.44
441.28	0.5	0.09
442.31	0.7	0.14
444.30	1.3	0.24
454.28	1.3	0.24
472.30	538.5	100.00
473.31	97.6	18.12
486.31	172.1	31.96
487.32	31.7	5.89
542.39	1.1	0.21
543.36	0.5	0.10
625.37	53.5	9.93
626.38	15.1	2.81
628.41	0.6	0.11
657.45	2.0	0.37
658.46	0.8	0.15
690.53	0.9	0.16
699.44	353.8	65.70
700.44	111.2	20.65
701.53	1.1	0.20
702.43	0.5	0.09
708.37	1.7	0.32
708.55	0.9	0.18
709.44	0.6	0.11
717.44	3.6	0.66
738.50	7.6	1.42
739.54	2.7	0.50
766.49	5.3	0.98
767.52	2.5	0.47
778.48	8.6	1.59
779.56	2.3	0.43
861.55	0.5	0.10
864.55	0.6	0.12
893.55	4.5	0.83
894.57	1.1	0.21
903.54	0.8	0.15
905.46	1.3	0.25
905.63	0.9	0.17

906.52	0.8	0.15
935.56	37.4	6.95
936.56	21.6	4.00

SPECTRUM - MS

7-1-13_HMG13_837_MS4_935_486_01.raw

ITMS + p ESI E Full ms4 838.00@cid35.00 936.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-3.38

AV: 50

m/z	Intensity	Relative
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177.01	0.1	0.50
178.03	0.1	0.82
208.11	0.9	7.72
209.03	0.1	0.90
209.22	0.0	0.30
211.20	0.0	0.38
218.14	0.1	1.02
222.05	0.1	0.52
241.08	0.4	3.73
241.21	0.3	2.50
249.86	0.1	0.78
250.11	0.8	6.64
251.12	0.0	0.42
251.77	0.1	0.72
252.14	1.5	12.55
252.99	0.0	0.33
253.17	0.1	0.85
257.11	0.1	0.61
257.24	0.0	0.30
259.13	11.3	95.10
260.07	0.8	7.05
260.26	0.3	2.76
268.15	0.5	4.49
300.92	0.0	0.36
320.16	0.0	0.33
341.08	0.1	0.59
341.29	0.2	1.45
351.97	0.0	0.41
353.33	0.0	0.39
356.22	0.1	0.50
357.24	0.1	0.65
366.07	0.0	0.40
366.24	0.0	0.35
380.31	0.0	0.30
382.27	0.2	1.63
384.22	0.2	1.96
385.01	0.0	0.35
394.09	0.0	0.30
394.40	0.0	0.41

398.30	0.0	0.34
410.16	0.1	1.09
412.27	11.8	100.00
413.02	0.3	2.75
413.28	1.7	14.38
415.18	0.1	1.26
415.36	0.1	0.79
444.29	8.3	69.82
445.31	1.1	8.90
486.30	2.8	23.66
487.31	0.4	3.39

SPECTRUM - MS

7-1-13_HMG13_837_MS4_935_472_01.raw

ITMS + p ESI E Full ms4 838.00@cid35.00 936.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-3.34

AV: 50

m/z Intensity Relative

149.01	0.7	2.56
170.93	0.3	1.08
171.06	0.2	0.90
178.04	0.2	0.58
180.04	1.0	3.85
188.09	0.4	1.66
194.05	0.4	1.68
199.14	0.1	0.47
204.00	0.8	3.16
218.07	0.3	0.96
220.09	2.9	10.79
221.09	0.4	1.46
227.10	16.2	61.05
228.11	1.3	4.91
229.19	0.1	0.48
232.08	0.1	0.50
236.09	3.5	13.20
237.01	0.1	0.52
242.93	0.2	0.60
245.12	7.9	29.68
246.12	0.7	2.61
250.04	0.4	1.48
250.19	0.4	1.40
268.15	26.5	100.00
269.14	2.2	8.14
287.14	0.6	2.19
292.15	0.2	0.82
296.20	0.2	0.86
315.19	21.5	81.33
316.21	2.6	9.73
324.13	0.5	1.84

327.16	0.1	0.49
366.01	0.2	0.91
366.23	0.2	0.64
367.16	0.1	0.50
368.26	0.2	0.82
380.23	1.3	4.97
381.18	0.1	0.56
385.27	0.2	0.70
398.25	1.5	5.57
399.20	1.1	4.29
408.25	0.1	0.52
430.33	0.6	2.46
440.24	5.4	20.34
441.10	0.2	0.62
441.31	0.7	2.59
442.27	2.7	10.22
443.29	0.2	0.70
472.30	11.7	44.17
473.30	2.3	8.53

HMG 14 Mass spectral peak lists

Mass spectra were acquired in profile mode, then centroided using the valley detection algorithm. The top 50 peaks are shown. Isolation mass and width are adjusted to capture an entire isotopic envelope, where possible.

SPECTRUM - MS

7-1-13_HMG14_837_MS2_01.raw

ITMS + p ESI E Full ms2 838.00@cid35.00 [230.00-2000.00]

Scan #: 1-20

RT: 0.00-3.55

AV: 20

m/z	Intensity	Relative
329.23	318.4	0.79
406.21	452.9	1.12
444.32	1352.6	3.36
445.33	282.2	0.70
454.31	244.1	0.61
464.27	273.0	0.68
472.32	1195.1	2.97
473.33	270.9	0.67
486.34	36727.4	91.16
487.35	8210.4	20.38
488.36	1431.1	3.55
534.41	317.8	0.79
605.42	5111.2	12.69
605.93	3307.6	8.21
606.43	1370.9	3.40
606.95	423.0	1.05
630.40	345.0	0.86
718.46	597.7	1.48
718.97	280.2	0.70
719.46	372.0	0.92
720.51	242.3	0.60
738.52	8428.1	20.92
739.53	3289.5	8.16
740.53	847.0	2.10
760.45	441.8	1.10
787.54	262.3	0.65
809.07	677.1	1.68
821.06	459.4	1.14
821.56	416.3	1.03
822.07	388.3	0.96
822.59	255.5	0.63
837.12	5303.0	13.16
837.59	4751.3	11.79
838.08	2490.5	6.18
838.57	1036.8	2.57
935.59	2068.9	5.14
936.59	972.3	2.41

937.60	290.9	0.72	
983.67	376.8	0.94	
1079.63		1222.4	3.03
1080.64		671.8	1.67
1135.61		241.2	0.60
1167.63		356.6	0.89
1187.77		40287.7	100.00
1188.77		24538.0	60.91
1189.78		9010.4	22.37
1190.79		2097.9	5.21
1593.95		273.3	0.68
1651.08		411.4	1.02
1652.08		384.7	0.95

SPECTRUM - MS

7-1-13_HMG14_837_MS3_935_01.raw

ITMS + p ESI E Full ms3 838.00@cid35.00 936.00@cid35.00 [255.00-1000.00]

Scan #: 1-20

RT: 0.00-1.20

AV: 20

m/z Intensity Relative

268.07	0.9	0.13
315.27	3.6	0.57
329.28	3.1	0.49
398.37	0.8	0.13
430.25	2.7	0.42
440.25	2.3	0.37
440.40	2.8	0.44
444.32	13.4	2.11
445.23	1.6	0.26
445.38	1.0	0.16
454.17	1.2	0.18
454.34	2.7	0.43
472.30	636.7	100.00
473.32	101.9	16.01
474.35	4.2	0.66
486.33	404.4	63.51
487.35	70.6	11.09
488.34	2.0	0.32
625.42	1.1	0.17
690.42	1.8	0.28
690.75	1.1	0.17
691.59	1.1	0.17
699.46	5.3	0.83
700.33	1.5	0.23
708.48	2.2	0.34
717.44	2.7	0.42
718.46	1.1	0.17
737.57	0.9	0.14
738.68	1.0	0.16

739.60	1.9	0.30
764.37	0.8	0.13
778.52	10.8	1.69
779.48	2.1	0.33
780.69	0.8	0.13
861.72	1.1	0.17
864.65	1.3	0.21
893.27	0.8	0.13
893.65	4.3	0.67
894.61	1.5	0.23
903.49	4.2	0.66
903.64	4.2	0.66
904.52	2.0	0.32
905.49	4.0	0.63
905.68	2.5	0.39
906.37	1.8	0.29
906.60	1.8	0.28
935.56	105.8	16.62
936.59	43.2	6.78
937.58	2.3	0.36
937.78	0.9	0.15

SPECTRUM - MS

7-1-13_HMG14_837_MS4_935_486_01.raw

ITMS + p ESI E Full ms4 838.00@cid35.00 936.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-3.15

AV: 50

m/z	Intensity	Relative
138.18	0.1	0.14
180.04	0.2	0.33
211.09	0.1	0.19
213.08	0.1	0.15
220.08	1.4	2.18
221.06	0.1	0.13
222.17	0.1	0.12
227.13	0.3	0.44
236.10	0.1	0.15
241.12	1.9	2.92
242.13	0.2	0.29
250.05	0.1	0.17
257.09	0.1	0.13
259.12	10.3	16.11
260.21	0.3	0.52
268.16	4.8	7.58
269.16	0.6	1.00
296.18	0.1	0.15
297.24	0.2	0.28
301.13	0.8	1.31
315.01	0.1	0.16

315.17	0.1	0.18
321.15	0.1	0.13
329.22	15.7	24.61
330.23	2.3	3.62
339.19	0.1	0.16
382.17	0.1	0.13
382.31	0.1	0.16
394.38	0.1	0.15
395.24	0.2	0.24
396.27	0.1	0.17
396.48	0.1	0.14
410.36	0.1	0.12
412.17	0.5	0.83
412.34	0.8	1.33
413.25	0.2	0.24
415.31	0.6	0.99
416.31	0.1	0.20
431.17	0.1	0.14
440.22	0.1	0.22
440.35	0.1	0.22
444.30	63.8	100.00
445.30	9.9	15.47
454.16	0.3	0.43
454.35	0.5	0.82
455.09	0.1	0.17
456.32	2.3	3.68
457.40	0.2	0.33
486.33	8.0	12.61
487.34	1.3	2.09

SPECTRUM - MS

7-1-13_HMG14_837_MS4_935_472_01.raw

ITMS + p ESI E Full ms4 838.00@cid35.00 936.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-3.06

AV: 50

m/z Intensity Relative

149.04	0.8	2.41
171.04	0.8	2.46
180.04	1.4	4.16
188.06	0.4	1.26
194.07	1.1	3.36
195.06	0.3	0.85
199.06	0.3	0.78
204.04	2.3	7.08
210.02	0.2	0.74
218.08	0.4	1.28
220.10	4.2	12.65
221.06	0.3	0.98
227.10	22.4	68.20

228.04	0.9	2.66
228.20	1.0	3.18
236.12	7.1	21.74
237.05	0.4	1.10
243.10	0.5	1.52
243.26	0.3	0.84
245.10	10.7	32.42
246.09	0.8	2.37
250.12	0.6	1.71
268.15	32.9	100.00
269.15	3.0	9.27
287.19	0.6	1.92
288.17	0.3	0.89
301.27	0.2	0.70
315.20	26.5	80.62
316.20	2.5	7.63
324.16	0.3	0.90
353.24	0.3	1.01
366.25	0.4	1.19
367.07	0.2	0.73
367.21	0.3	0.98
368.29	0.3	0.89
380.24	2.1	6.36
381.24	0.4	1.32
398.25	4.3	13.15
399.22	1.4	4.36
401.18	0.3	0.82
408.26	0.5	1.52
430.33	2.3	6.88
431.20	0.2	0.75
431.35	0.2	0.73
440.27	10.9	33.26
441.23	1.3	3.85
442.28	3.4	10.23
443.20	0.3	0.86
472.30	14.6	44.56
473.30	2.4	7.45

HMG 16 peak lists

SPECTRUM - MS

10-9-13_HMG16_837_MS2_01.raw

ITMS + p ESI E Full ms2 837.80@cid35.00 [230.00-2000.00]

Scan #: 1-20

RT: 0.00-1.75

AV: 20

m/z	Intensity	Relative
420.17	329.2	2.17
444.27	701.5	4.63
464.21	606.1	4.00
486.28	12974.4	85.64
487.28	2894.9	19.11
488.29	571.2	3.77
514.29	275.8	1.82
534.33	194.4	1.28
605.34	5145.3	33.96
605.85	3231.1	21.33
606.35	1363.7	9.00
606.86	442.8	2.92
616.29	206.9	1.37
664.40	622.9	4.11
665.38	230.1	1.52
704.35	876.1	5.78
705.33	304.0	2.01
706.39	2176.8	14.37
707.40	777.1	5.13
708.41	196.3	1.30
718.46	507.0	3.35
720.46	886.9	5.85
722.44	271.4	1.79
724.42	1331.6	8.79
725.40	510.9	3.37
727.91	281.3	1.86
728.40	231.6	1.53
746.32	748.6	4.94
747.32	272.6	1.80
778.42	969.9	6.40
780.38	352.2	2.32
836.38	243.6	1.61
837.00	2550.9	16.84
837.46	2226.0	14.69
837.95	1187.9	7.84
838.43	619.4	4.09
838.94	189.9	1.25
1079.48	1069.9	7.06
1080.49	558.0	3.68
1081.50	198.7	1.31
1167.45	320.1	2.11

1187.61	15149.8	100.00
1188.61	9062.2	59.82
1189.61	3396.0	22.42
1190.62	921.4	6.08
1209.49	501.5	3.31
1210.51	277.4	1.83
1650.85	575.1	3.80
1651.86	497.4	3.28
1652.87	266.3	1.76

SPECTRUM - MS

10-9-13_HMG16_837_MS3_605_01.raw

ITMS + p ESI E Full ms3 837.80@cid35.00 606.00@cid35.00 [165.00-1200.00]

Scan #: 1-50

RT: 0.00-4.82

AV: 50

m/z Intensity Relative

196.09	62.7	5.97
386.18	42.2	4.02
387.18	8.2	0.78
418.17	10.0	0.96
432.14	26.0	2.48
464.21	89.1	8.50
465.21	18.0	1.72
474.31	9.1	0.87
484.29	17.4	1.65
486.28	562.6	53.63
487.28	124.1	11.82
488.30	24.1	2.29
496.28	10.4	0.99
514.29	46.8	4.47
515.29	11.5	1.10
534.34	84.7	8.07
535.34	22.4	2.13
546.32	11.5	1.09
555.84	9.2	0.88
556.28	12.4	1.18
568.29	24.3	2.31
589.35	13.0	1.24
590.35	56.3	5.36
590.86	13.9	1.33
591.34	14.6	1.39
605.36	130.7	12.46
605.84	80.4	7.66
606.34	33.6	3.20
606.86	10.2	0.97
616.30	67.9	6.47
617.31	19.4	1.85
664.41	41.5	3.96
665.39	13.7	1.30

676.35	53.9	5.14	
677.36	15.7	1.50	
704.36	212.5	20.25	
705.34	67.9	6.47	
706.36	16.0	1.52	
714.26	17.6	1.68	
724.43	719.4	68.57	
725.41	250.8	23.90	
726.42	57.0	5.43	
746.33	340.6	32.47	
747.33	112.8	10.76	
748.34	24.3	2.31	
969.53	14.3	1.36	
1187.63		1049.1	100.00
1188.64		608.6	58.02
1189.64		217.3	20.71
1190.65		50.6	4.82

SPECTRUM - MS

10-9-13_HMG16_837_MS4_605_486_01.raw

ITMS + p ESI E Full ms4 837.80@cid35.00 606.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-4.17

AV: 50

m/z Intensity Relative

180.09	0.2	0.22
220.07	1.6	1.47
221.12	0.2	0.15
227.05	0.4	0.33
241.11	2.8	2.56
242.11	0.3	0.26
257.07	0.2	0.19
259.11	11.2	10.11
260.11	1.1	0.95
268.12	5.7	5.14
269.13	0.6	0.59
297.18	0.4	0.33
301.14	0.6	0.53
314.18	0.3	0.27
315.20	0.2	0.19
329.18	19.4	17.54
330.19	2.7	2.42
331.23	0.3	0.23
353.25	0.3	0.27
368.72	0.7	0.65
369.08	0.7	0.62
370.72	0.8	0.69
371.09	1.0	0.92
387.23	0.2	0.16
394.24	0.2	0.20

410.24	0.4	0.34
412.21	1.5	1.39
413.27	0.2	0.20
415.24	1.9	1.69
416.32	0.2	0.15
426.22	0.3	0.26
426.39	0.2	0.18
426.90	0.2	0.17
427.34	0.2	0.15
428.75	0.7	0.59
429.07	0.9	0.77
429.94	0.2	0.15
431.20	0.3	0.25
440.25	0.2	0.16
444.26	110.6	100.00
445.27	21.0	19.01
446.25	3.2	2.92
454.28	1.0	0.90
455.26	0.3	0.24
456.27	4.3	3.90
457.29	0.8	0.75
458.30	0.2	0.15
486.27	10.8	9.74
487.27	2.2	2.03
488.27	0.4	0.34

SPECTRUM - MS

10-9-13_HMG16_837_MS3_486_01.raw

ITMS + p ESI E Full ms3 837.80@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-2.47

AV: 50

m/z Intensity Relative

180.03	6.6	0.20
188.03	3.6	0.11
211.07	3.8	0.12
213.07	4.1	0.13
218.05	3.1	0.09
220.07	36.8	1.13
221.08	4.1	0.13
227.05	6.3	0.19
236.08	3.5	0.11
241.09	65.2	2.00
242.10	5.8	0.18
257.07	4.8	0.15
259.10	249.7	7.67
260.11	22.7	0.70
261.12	3.9	0.12
268.12	113.8	3.49
269.13	12.3	0.38

297.13	10.9	0.33	
301.11	12.8	0.39	
329.18	354.6	10.88	
330.19	54.3	1.67	
331.16	7.2	0.22	
352.18	2.6	0.08	
353.17	16.2	0.50	
354.18	2.8	0.09	
371.11	4.2	0.13	
380.18	6.9	0.21	
382.22	4.0	0.12	
384.20	3.8	0.12	
394.20	4.4	0.13	
410.20	9.4	0.29	
412.20	48.2	1.48	
413.21	10.8	0.33	
414.23	2.4	0.07	
415.24	54.7	1.68	
416.23	10.3	0.32	
426.26	3.9	0.12	
431.25	4.3	0.13	
440.15	3.9	0.12	
440.31	2.7	0.08	
444.26	3257.7		100.00
445.26	638.8	19.61	
446.25	100.6	3.09	
454.24	14.0	0.43	
456.25	52.4	1.61	
457.24	11.8	0.36	
458.22	2.4	0.07	
486.26	275.6	8.46	
487.27	62.8	1.93	
488.28	10.3	0.32	

HMG 18 Mass spectral peak lists

SPECTRUM - MS

10-9-13_HMG18_837_MS2_01.raw

ITMS + p ESI E Full ms2 837.80@cid35.00 [230.00-2000.00]

Scan #: 1-20

RT: 0.00-1.71

AV: 20

m/z	Intensity	Relative	
329.18	353.9	0.76	
406.15	524.2	1.12	
444.26	1537.0		3.29
445.27	331.5	0.71	
454.24	277.0	0.59	
464.20	317.6	0.68	
472.25	1413.1		3.02
473.26	341.8	0.73	
486.27	41367.5		88.43
487.28	9517.1		20.34
488.28	1802.9		3.85
534.32	400.4	0.86	
605.33	5801.3		12.40
605.85	3770.1		8.06
606.34	1584.2		3.39
606.83	553.0	1.18	
630.30	387.0	0.83	
718.37	1143.9		2.45
719.34	318.6	0.68	
720.45	1027.4		2.20
738.42	9968.2		21.31
739.42	3869.5		8.27
740.43	1022.7		2.19
760.34	534.7	1.14	
778.39	753.3	1.61	
780.34	314.7	0.67	
820.93	575.6	1.23	
821.43	519.4	1.11	
821.95	468.6	1.00	
836.37	274.8	0.59	
837.01	6761.6		14.45
837.47	5908.7		12.63
837.96	3188.1		6.81
838.45	1349.3		2.88
838.95	425.3	0.91	
935.45	2422.6		5.18
936.46	1112.7		2.38
937.46	331.4	0.71	
983.53	470.1	1.00	
1079.47		1445.7	3.09
1080.49		757.7	1.62

1135.44	295.1	0.63
1167.46	401.1	0.86
1187.61	46780.9	100.00
1188.61	27865.4	59.57
1189.61	10347.6	22.12
1190.62	2741.2	5.86
1191.61	524.0	1.12
1650.84	516.3	1.10
1651.84	421.3	0.90

SPECTRUM - MS

10-9-13_HMG18_837_MS3_935_01.raw

ITMS + p ESI E Full ms3 837.80@cid35.00 936.00@cid35.00 [255.00-1000.00]

Scan #: 1-20

RT: 0.00-1.14

AV: 20

m/z Intensity Relative

268.11	1.3	0.20
315.19	2.4	0.36
329.19	3.3	0.49
430.23	2.3	0.34
430.38	1.1	0.16
440.28	4.1	0.61
444.33	8.2	1.22
445.15	2.5	0.37
454.21	2.5	0.38
454.36	0.9	0.13
455.29	1.0	0.15
472.23	674.8	100.00
473.24	123.1	18.24
474.01	1.9	0.28
474.22	9.1	1.34
474.37	4.0	0.60
486.26	423.7	62.79
487.27	82.5	12.23
488.32	8.2	1.21
504.21	1.0	0.15
690.32	0.9	0.14
690.49	1.0	0.14
691.06	1.0	0.15
691.27	1.0	0.14
699.56	1.0	0.15
708.29	1.5	0.22
717.29	5.6	0.82
738.38	0.9	0.13
766.42	1.7	0.25
778.47	8.0	1.19
779.44	3.2	0.48
829.33	1.8	0.26
830.50	1.0	0.14

864.47	1.8	0.27
888.29	0.9	0.13
893.59	4.8	0.71
894.51	3.6	0.54
903.49	2.8	0.41
903.61	1.5	0.23
904.42	1.2	0.17
905.42	7.1	1.05
906.36	2.5	0.37
906.58	1.2	0.18
935.03	1.4	0.21
935.45	112.1	16.62
936.06	1.2	0.18
936.46	56.8	8.42
937.22	2.7	0.40
937.37	4.9	0.72
937.52	5.8	0.86

SPECTRUM - MS

10-9-13_HMG18_837_MS4_935_486_01.raw

ITMS + p ESI E Full ms4 837.80@cid35.00 936.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-3.20

AV: 50

m/z	Intensity	Relative
180.06	0.1	0.16
188.01	0.2	0.30
213.05	0.2	0.27
220.07	1.8	2.26
221.06	0.3	0.33
221.21	0.1	0.12
227.12	0.1	0.18
236.15	0.1	0.12
241.10	2.1	2.65
242.11	0.2	0.29
250.06	0.1	0.16
257.14	0.3	0.35
259.09	9.0	11.26
260.08	0.9	1.11
266.02	0.1	0.16
268.12	6.1	7.63
269.12	0.8	1.02
297.13	0.2	0.30
301.17	0.4	0.56
315.10	0.1	0.12
329.17	18.4	23.14
330.17	2.4	3.06
331.20	0.1	0.13
339.06	0.1	0.12
352.16	0.1	0.12

353.16	0.3	0.38
366.29	0.2	0.25
380.16	0.2	0.21
384.13	0.1	0.13
384.29	0.2	0.19
394.20	0.1	0.15
412.18	0.9	1.14
412.38	0.4	0.54
413.12	0.1	0.13
415.25	1.0	1.27
416.32	0.1	0.18
426.20	0.1	0.16
440.08	0.2	0.24
444.24	79.6	100.00
445.25	12.9	16.18
446.30	0.8	0.96
454.21	0.3	0.37
454.33	0.2	0.24
456.23	2.0	2.55
457.24	0.4	0.47
458.26	0.1	0.15
486.23	9.8	12.28
487.04	0.2	0.21
487.29	0.9	1.17
488.29	0.1	0.17

SPECTRUM - MS

10-9-13_HMG18_837_MS4_935_472_02.raw

ITMS + p ESI E Full ms4 837.80@cid35.00 936.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-100

RT: 0.00-7.18

AV: 100

m/z Intensity Relative

148.97	1.1	2.95
171.00	0.9	2.57
180.03	1.3	3.54
188.02	0.7	1.95
194.04	1.2	3.23
203.98	2.4	6.69
210.05	0.2	0.68
218.04	0.5	1.40
220.06	4.4	11.97
221.08	0.4	1.10
227.07	25.7	70.31
228.07	1.8	4.97
232.05	0.4	0.99
236.05	7.6	20.91
237.03	0.6	1.54
243.07	0.5	1.49
245.07	12.5	34.38

246.07	1.0	2.87
250.09	0.6	1.61
268.11	36.5	100.00
269.11	3.6	9.84
287.10	1.4	3.82
301.12	0.2	0.61
315.14	30.6	83.88
316.15	3.2	8.90
317.17	0.4	0.96
324.12	0.7	1.91
325.13	0.3	0.84
327.18	0.2	0.64
339.14	0.3	0.75
353.14	0.2	0.62
366.16	0.5	1.38
367.15	0.8	2.20
368.16	0.7	2.00
380.19	2.4	6.45
381.20	0.3	0.87
385.15	0.5	1.30
396.18	0.2	0.62
398.17	5.0	13.75
399.18	2.0	5.49
401.20	0.6	1.59
408.18	0.8	2.15
430.24	2.4	6.66
431.19	0.3	0.94
440.18	12.6	34.62
441.19	2.1	5.62
442.21	4.3	11.69
443.23	0.8	2.09
472.23	8.7	23.79
473.25	1.6	4.48

HMG 20 MSn peak lists.

SPECTRUM - MS

8-12-13_HMG20_924_MS2_01.raw

ITMS + p ESI E Full ms2 924.60@cid35.00 [250.00-2000.00]

Scan #: 1-20

RT: 0.00-1.71

AV: 20

m/z	Intensity	Relative
444.26	101.9	0.95
464.20	73.1	0.68
486.27	2486.0	23.27
487.28	536.8	5.02
514.28	87.8	0.82
534.33	272.1	2.55
535.33	75.0	0.70
589.35	349.8	3.27
589.85	240.7	2.25
590.36	110.7	1.04
598.32	69.0	0.65
616.29	83.2	0.78
660.36	910.2	8.52
661.37	282.4	2.64
664.40	124.3	1.16
692.39	10683.8	100.00
692.89	8213.2	76.88
693.39	2937.3	27.49
693.91	325.9	3.05
704.34	274.2	2.57
705.32	95.0	0.89
706.38	420.5	3.94
707.40	154.0	1.44
724.41	516.0	4.83
725.40	190.8	1.79
746.32	190.3	1.78
814.95	116.2	1.09
815.45	113.3	1.06
820.94	767.2	7.18
821.44	733.1	6.86
821.95	348.4	3.26
829.96	145.7	1.36
830.45	134.8	1.26
850.42	144.9	1.36
924.04	1400.9	13.11
924.51	1686.8	15.79
924.99	1029.2	9.63
925.49	154.1	1.44
1155.58	255.5	2.39
1156.60	169.3	1.58
1187.60	723.8	6.78

1188.61	436.4	4.08	
1189.61	130.0	1.22	
1253.56	173.7	1.63	
1254.58	104.7	0.98	
1361.70	2983.3		27.92
1362.70	2198.8		20.58
1363.71	753.1	7.05	
1825.02	69.3	0.65	
1826.02	76.9	0.72	

SPECTRUM - MS

8-12-13_HMG20_924_MS3_692_01.raw

ITMS + p ESI E Full ms3 924.60@cid35.00 693.00@cid35.00 [190.00-1400.00]

Scan #: 1-50

RT: 0.00-4.02

AV: 50

m/z Intensity Relative

386.16	49.6	5.15
472.23	68.1	7.08
486.28	56.9	5.92
514.26	83.2	8.65
534.31	717.1	74.55
535.32	181.7	18.89
536.33	28.8	3.00
552.30	36.1	3.76
589.34	961.9	100.00
589.84	561.8	58.41
590.33	289.7	30.12
590.84	57.8	6.01
591.33	35.4	3.68
598.31	194.8	20.25
598.82	112.0	11.65
599.31	43.8	4.55
616.27	103.5	10.76
617.29	28.5	2.96
642.86	95.7	9.95
643.36	58.1	6.04
644.32	59.5	6.19
660.34	382.9	39.81
661.35	104.4	10.85
664.39	36.5	3.80
676.38	34.6	3.60
692.37	205.3	21.35
692.88	150.0	15.59
693.38	59.0	6.13
704.34	80.5	8.37
720.34	84.3	8.77
724.40	567.2	58.97
725.39	194.4	20.21
726.39	38.2	3.97

746.31	98.5	10.24	
747.31	32.0	3.32	
748.38	46.1	4.79	
794.37	79.7	8.29	
850.41	369.0	38.37	
851.41	140.4	14.59	
852.39	35.5	3.69	
1143.59		44.4	4.61
1155.57		228.1	23.72
1156.58		131.1	13.63
1157.59		47.7	4.96
1173.57		100.2	10.42
1174.57		54.7	5.68
1361.69		567.2	58.97
1362.69		377.1	39.20
1363.70		138.9	14.44
1364.71		29.7	3.09

SPECTRUM - MS

8-12-13_HMG20_924_MS4_692_660_01.raw

ITMS + p ESI E Full ms4 924.60@cid35.00 693.00@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-50

RT: 0.00-3.37

AV: 50

m/z	Intensity	Relative
211.05	0.4	1.47
220.11	0.4	1.45
229.10	1.6	6.02
236.09	0.7	2.62
241.16	0.8	3.08
259.10	13.9	52.80
260.10	1.6	6.10
301.09	0.7	2.85
329.17	1.9	7.16
368.16	0.4	1.51
380.18	1.1	4.05
381.15	0.4	1.66
382.21	2.4	8.95
383.19	0.7	2.65
383.33	0.4	1.40
384.17	0.5	1.95
385.25	0.4	1.37
394.21	2.1	7.94
398.22	2.6	9.75
399.20	0.7	2.80
412.23	0.7	2.77
424.20	1.5	5.81
430.24	1.8	7.01
431.22	0.3	1.04
442.24	0.5	2.06

447.16	0.4	1.68
447.34	0.5	1.99
454.22	2.6	9.96
455.36	0.4	1.39
456.24	5.6	21.50
457.15	0.5	1.80
457.35	0.6	2.41
470.28	0.5	1.78
472.24	26.3	100.00
473.33	3.3	12.67
515.30	0.3	1.05
558.31	0.3	1.06
584.23	0.9	3.38
584.42	0.3	1.06
585.34	0.3	1.22
586.30	22.3	84.76
587.30	5.3	20.33
589.33	2.8	10.63
590.46	0.4	1.47
614.37	0.7	2.50
618.33	14.0	53.20
619.35	4.0	15.09
630.28	0.3	1.05
660.36	9.0	34.34
661.37	2.6	9.80

SPECTRUM - MS

8-12-13_HMG20_924_MS3_486_01.raw

ITMS + p ESI E Full ms3 924.60@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-100

RT: 0.00-5.17

AV: 100

m/z Intensity Relative

180.01	2.4	0.37
188.03	1.4	0.21
194.03	0.9	0.13
211.05	1.1	0.17
213.06	0.8	0.13
218.06	0.7	0.11
220.06	13.1	1.99
221.08	1.2	0.18
227.05	2.4	0.36
236.06	0.9	0.14
241.09	17.4	2.65
242.10	1.8	0.27
250.09	0.7	0.11
257.07	1.1	0.17
259.09	70.6	10.72
260.10	6.4	0.97
268.11	40.7	6.18

269.11	3.9	0.59
297.12	3.3	0.50
298.09	0.6	0.10
301.11	3.9	0.60
312.14	0.7	0.11
314.15	1.5	0.22
315.14	0.9	0.13
326.17	0.7	0.10
329.17	129.4	19.66
330.17	15.8	2.41
353.10	1.5	0.23
353.27	1.2	0.18
380.19	1.1	0.16
382.23	1.2	0.18
384.22	1.0	0.16
387.17	1.2	0.18
394.19	1.7	0.25
410.23	2.3	0.35
412.19	10.8	1.64
413.18	2.0	0.31
415.22	11.6	1.76
416.22	2.4	0.36
426.23	2.5	0.38
431.21	1.1	0.17
440.20	1.1	0.17
444.24	658.0	100.00
445.24	120.2	18.27
454.22	5.9	0.89
455.33	0.9	0.13
456.25	27.8	4.23
457.26	6.8	1.04
486.25	47.1	7.15
487.26	9.2	1.40

HMG 21 Mass spectral peak lists

SPECTRUM - MS

7-2-13_HMG21_924_MS2_01.raw

ITMS + p ESI E Full ms2 924.60@cid35.00 [250.00-2000.00]

Scan #: 1-20

RT: 0.00-1.56

AV: 20

m/z	Intensity	Relative
406.18	1924.3	1.76
472.29	7434.4	6.81
534.38	7187.9	6.59
535.38	1943.2	1.78
586.34	2906.1	2.66
605.39	2239.7	2.05
660.41	84872.7	77.76
661.42	25907.4	23.74
662.42	5527.0	5.06
738.48	108195.9	99.13
739.49	40596.7	37.20
740.49	9493.6	8.70
768.98	9886.5	9.06
769.49	7737.9	7.09
769.98	3642.1	3.34
784.51	1679.5	1.54
806.00	38826.5	35.57
806.50	32070.6	29.38
807.00	15813.8	14.49
807.50	5786.5	5.30
821.02	51053.2	46.78
821.52	42881.9	39.29
822.03	20626.2	18.90
822.54	7254.9	6.65
830.02	4451.8	4.08
830.53	3961.3	3.63
831.02	1859.7	1.70
873.49	4348.2	3.98
874.52	5167.2	4.73
875.03	2789.0	2.56
875.53	2016.1	1.85
903.53	2262.0	2.07
908.05	2390.3	2.19
908.55	2413.0	2.21
924.11	29149.4	26.71
924.59	28105.8	25.75
925.07	15030.9	13.77
925.56	6877.8	6.30
1079.55	5456.4	5.00
1080.57	2665.1	2.44
1109.61	40471.2	37.08

1110.61	20946.3	19.19
1111.62	6740.0	6.18
1187.69	109141.9	100.00
1188.69	62386.2	57.16
1189.70	22634.9	20.74
1190.70	5181.6	4.75
1588.90	12621.6	11.56
1589.91	10046.7	9.21
1590.92	4808.1	4.41

SPECTRUM - MS

7-2-13_HMG21_924_MS3_1109_01.raw

ITMS + p ESI E Full ms3 924.60@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-20

RT: 0.00-2.21

AV: 20

m/z Intensity Relative

398.20	2.3	0.17
424.23	13.3	0.99
430.27	3.0	0.22
440.23	2.8	0.21
442.29	4.4	0.33
454.28	8.5	0.64
456.28	2.6	0.19
472.28	697.6	51.98
473.29	113.5	8.46
474.30	13.0	0.97
586.34	21.1	1.57
587.28	2.3	0.17
587.44	2.7	0.20
611.37	3.6	0.27
618.38	7.8	0.58
632.38	2.7	0.20
660.40	1341.9	100.00
661.41	333.8	24.87
662.42	42.4	3.16
667.37	8.7	0.65
716.43	3.6	0.27
799.43	129.8	9.67
800.44	40.8	3.04
801.49	7.5	0.56
829.44	13.6	1.02
830.50	3.8	0.28
831.43	3.4	0.25
831.60	3.0	0.22
864.58	3.3	0.24
873.49	875.1	65.22
874.50	305.3	22.75
875.52	53.6	3.99
882.54	5.2	0.38

883.50	2.3	0.17
891.50	4.6	0.34
903.53	248.9	18.55
904.53	88.1	6.57
905.52	21.5	1.60
921.52	7.5	0.56
952.51	32.3	2.41
953.61	10.9	0.82
954.54	2.5	0.19
1067.52		6.8 0.51
1067.73		5.2 0.39
1068.60		6.3 0.47
1079.56		8.4 0.63
1080.57		2.3 0.17
1109.62		510.0 38.00
1110.61		271.9 20.26
1111.62		83.1 6.20

SPECTRUM - MS

7-2-13_HMG21_924_MS4_1109_660_01.raw

ITMS + p ESI E Full ms4 924.60@cid35.00 1110.00@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-50

RT: 0.00-6.22

AV: 50

m/z	Intensity	Relative
229.11	23.9	6.15
236.09	15.3	3.92
241.13	16.6	4.25
259.13	330.7	84.89
260.13	22.5	5.78
301.15	7.3	1.87
329.21	9.8	2.53
355.22	6.6	1.70
364.23	13.0	3.33
368.22	6.6	1.69
380.22	9.6	2.46
382.24	21.6	5.56
384.23	9.9	2.53
385.23	5.8	1.48
394.26	9.4	2.41
398.23	16.0	4.11
399.23	9.8	2.53
400.25	5.8	1.49
412.25	21.5	5.53
424.23	24.8	6.37
426.26	20.6	5.29
430.29	24.6	6.32
440.26	6.3	1.62
442.28	86.6	22.22
443.28	15.0	3.84

447.29	11.9	3.06
454.25	31.3	8.03
456.27	43.6	11.20
457.29	6.2	1.60
470.26	7.2	1.84
472.27	389.6	100.00
473.29	60.5	15.53
486.29	6.6	1.70
515.32	11.1	2.84
540.30	6.1	1.56
554.31	5.6	1.43
556.35	9.2	2.37
570.32	6.6	1.70
584.31	19.0	4.87
586.34	268.0	68.80
587.35	56.0	14.38
589.36	100.1	25.70
590.37	20.6	5.29
614.35	40.0	10.28
615.37	8.4	2.17
618.38	361.9	92.91
619.39	73.4	18.84
630.38	10.1	2.60
660.40	246.2	63.20
661.42	51.8	13.30

SPECTRUM - MS

7-2-13_HMG21_924_MS4_1109_472_01.raw

ITMS + p ESI E Full ms4 924.60@cid35.00 1110.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-4.33

AV: 50

m/z Intensity Relative

149.02	0.7	1.95
171.10	0.7	2.14
180.04	0.9	2.49
188.07	0.6	1.81
193.97	0.4	1.11
194.11	0.5	1.36
203.77	0.1	0.38
204.04	1.0	2.80
208.16	0.2	0.58
218.10	0.3	0.90
220.09	3.6	10.42
221.12	0.2	0.52
227.09	21.8	63.25
228.06	1.0	2.91
228.21	0.5	1.59
236.08	3.5	10.20
236.97	0.2	0.44

237.14	0.1	0.39
243.10	0.2	0.67
245.09	10.4	30.18
246.14	0.6	1.84
250.12	0.3	0.76
258.80	0.1	0.37
259.20	0.6	1.67
268.14	34.4	100.00
269.14	2.2	6.45
273.03	0.1	0.39
287.16	0.9	2.59
301.16	0.1	0.43
315.17	26.2	75.99
316.19	3.1	8.95
324.28	0.3	0.73
366.20	0.2	0.72
367.29	0.2	0.47
368.21	0.4	1.31
380.21	1.3	3.74
381.26	0.2	0.49
396.24	0.3	0.76
398.21	3.0	8.57
399.25	0.9	2.53
401.30	0.2	0.48
408.19	0.3	0.83
430.27	3.3	9.60
431.27	0.5	1.33
440.23	6.5	18.92
441.24	1.2	3.35
442.39	2.0	5.76
443.22	0.6	1.71
472.28	15.4	44.77
473.28	2.0	5.72

HMG 27 Mass spectral peak lists

SPECTRUM - MS

10-10-13_HMG27_837_MS2_01.raw

ITMS + p ESI E Full ms2 837.80@cid35.00 [230.00-2000.00]

Scan #: 1-20

RT: 0.00-1.77

AV: 20

m/z	Intensity	Relative
259.10	425.9	6.86
412.21	263.9	4.25
472.25	106.3	1.71
486.26	3618.2	58.27
487.26	816.0	13.14
488.27	156.8	2.53
581.31	75.3	1.21
605.33	584.7	9.42
605.84	370.4	5.96
606.34	162.4	2.62
681.87	1094.8	17.63
682.38	812.3	13.08
682.88	384.9	6.20
683.39	135.4	2.18
700.41	93.9	1.51
718.36	230.7	3.72
718.86	1795.4	28.92
719.37	1325.4	21.34
719.87	617.3	9.94
720.40	510.9	8.23
720.88	89.9	1.45
722.42	101.3	1.63
738.41	1003.9	16.17
739.41	386.9	6.23
740.42	106.2	1.71
760.32	64.9	1.04
776.39	56.7	0.91
778.39	260.3	4.19
780.38	109.0	1.76
808.93	89.7	1.45
809.43	67.3	1.08
836.35	67.4	1.08
836.98	748.0	12.05
837.45	676.2	10.89
837.95	346.0	5.57
838.42	179.7	2.89
935.44	252.4	4.06
936.45	115.9	1.87
1079.47	146.5	2.36
1080.48	76.5	1.23
1167.45	59.0	0.95

1187.59	6209.3	100.00
1188.59	3722.6	59.95
1189.59	1416.5	22.81
1190.60	400.9	6.46
1191.60	83.3	1.34
1414.69	1421.2	22.89
1415.69	1022.5	16.47
1416.70	445.5	7.17
1417.72	166.7	2.68

SPECTRUM - MS

10-10-13_HMG27_837_MS3_935_01.raw

ITMS + p ESI E Full ms3 837.80@cid35.00 936.00@cid35.00 [255.00-1000.00]

Scan #: 1-20

RT: 0.00-1.17

AV: 20

m/z Intensity Relative

268.08	0.5	0.27
315.09	0.9	0.47
380.09	0.5	0.27
384.16	0.6	0.29
412.26	2.1	1.04
424.18	0.8	0.39
425.20	0.9	0.43
440.22	0.8	0.39
472.23	198.0	100.00
473.25	32.7	16.50
474.20	2.1	1.05
474.36	2.2	1.10
486.25	62.0	31.33
487.26	11.3	5.69
488.21	0.5	0.26
488.35	0.5	0.23
607.43	0.4	0.21
625.31	20.5	10.38
626.42	1.8	0.90
626.53	1.3	0.67
657.25	0.4	0.21
657.40	0.5	0.25
670.34	0.4	0.22
690.38	0.6	0.32
699.35	132.1	66.71
700.35	41.7	21.06
701.17	1.3	0.65
701.39	4.3	2.19
708.43	0.6	0.31
717.22	0.4	0.20
738.41	2.7	1.34
739.48	1.0	0.51
766.36	1.8	0.92

766.53	0.7	0.38
767.50	0.8	0.41
778.29	0.9	0.44
778.53	0.7	0.36
779.34	0.5	0.24
779.45	0.4	0.20
881.23	0.5	0.23
893.52	0.4	0.22
894.43	0.8	0.40
905.30	1.0	0.49
905.50	0.7	0.33
906.35	0.9	0.45
935.36	22.8	11.50
935.56	15.4	7.76
936.49	13.3	6.70
937.35	2.5	1.25
937.62	1.4	0.72

SPECTRUM - MS

10-10-13_HMG27_837_MS4_935_486_01.raw

ITMS + p ESI E Full ms4 837.80@cid35.00 936.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-3.73

AV: 50

m/z	Intensity	Relative
208.08	0.3	5.02
209.04	0.0	0.41
209.21	0.0	0.59
211.09	0.0	0.40
218.02	0.0	0.47
220.04	0.0	0.63
227.03	0.0	0.68
230.99	0.0	0.29
241.06	0.3	4.98
242.14	0.0	0.41
250.09	0.2	4.86
250.96	0.0	0.27
251.13	0.0	0.67
252.08	0.7	13.33
253.01	0.1	1.03
253.18	0.0	0.38
257.10	0.1	1.86
258.19	0.0	0.28
259.10	4.8	94.87
260.16	0.3	6.13
268.15	0.1	1.64
294.12	0.0	0.29
307.09	0.0	0.86
311.02	0.0	0.29
314.06	0.0	0.62

329.29	0.0	0.37
341.25	0.1	1.19
371.17	0.0	0.42
379.28	0.0	0.36
382.16	0.1	1.11
384.19	0.1	2.68
384.87	0.0	0.32
385.12	0.0	0.46
412.21	5.1	100.00
412.81	0.0	0.31
413.23	0.8	14.93
414.27	0.1	1.14
414.42	0.0	0.45
415.09	0.1	1.50
415.25	0.0	0.67
426.23	0.0	0.90
431.29	0.0	0.31
444.25	2.5	49.73
445.26	0.4	7.43
452.11	0.0	0.29
454.30	0.0	0.31
456.27	0.0	0.30
471.09	0.0	0.34
486.24	0.7	13.59
487.21	0.2	3.75

SPECTRUM - MS

10-10-13_HMG27_837_MS4_935_472_01.raw

ITMS + p ESI E Full ms4 837.80@cid35.00 936.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-100

RT: 0.00-8.56

AV: 100

m/z Intensity Relative

148.96	0.2	2.24
171.00	0.2	2.59
178.11	0.0	0.48
180.02	0.3	3.61
188.06	0.2	2.41
194.02	0.2	2.25
204.00	0.3	3.88
210.07	0.0	0.62
218.00	0.1	1.24
220.06	1.0	13.13
221.09	0.1	1.42
227.07	4.9	65.53
228.10	0.3	4.43
236.07	0.9	12.67
237.06	0.1	0.89
243.13	0.1	1.01
245.08	2.2	29.65

246.08	0.2	2.23
250.08	0.1	0.95
268.12	7.5	100.00
269.12	0.7	9.24
270.16	0.1	0.81
287.10	0.3	3.89
292.05	0.0	0.48
315.15	6.3	84.05
316.17	0.7	9.12
317.24	0.0	0.60
324.13	0.1	1.75
325.12	0.0	0.64
339.21	0.1	0.91
366.11	0.1	0.80
367.18	0.1	1.19
368.17	0.2	2.28
370.22	0.1	0.68
380.18	0.4	5.96
385.07	0.0	0.62
385.24	0.0	0.50
398.27	0.3	4.31
399.20	0.3	3.95
401.10	0.0	0.62
401.24	0.1	0.70
408.18	0.1	1.49
430.24	0.3	3.57
440.19	1.6	20.83
441.20	0.3	3.50
442.22	0.8	10.87
443.31	0.1	1.20
472.23	1.5	19.83
473.20	0.2	3.31
473.37	0.1	1.47

HMG 28 Mass spectral peak lists

SPECTRUM - MS

7-12-13_HMG28_924_MS2_01.raw

ITMS + p ESI E Full ms2 924.40@cid35.00 [250.00-2000.00]

Scan #: 1-20

RT: 0.00-1.66

AV: 20

m/z	Intensity	Relative	
406.15	1973.3	1.60	
472.25	8188.4	6.63	
534.33	8521.7	6.90	
535.34	2245.8	1.82	
586.31	3617.7	2.93	
605.34	2960.3	2.40	
660.36	91296.3	73.88	
661.37	26561.0	21.49	
662.38	5484.2	4.44	
738.43	123570.7	100.00	
739.43	44546.8	36.05	
740.43	9982.7	8.08	
768.93	14842.5	12.01	
769.43	11562.0	9.36	
769.93	5333.1	4.32	
805.94	59131.8	47.85	
806.44	48878.9	39.56	
806.95	23714.1	19.19	
807.46	7731.5	6.26	
820.96	26786.0	21.68	
821.47	21613.0	17.49	
821.97	10335.4	8.36	
822.48	3192.9	2.58	
829.96	5617.9	4.55	
830.47	4966.0	4.02	
830.98	2074.1	1.68	
873.44	6532.7	5.29	
874.47	6557.1	5.31	
874.98	2863.7	2.32	
875.46	2272.2	1.84	
907.98	2844.5	2.30	
908.49	2565.4	2.08	
924.04	41177.5	33.32	
924.52	38420.2	31.09	
925.00	22006.5	17.81	
925.51	9444.6	7.64	
1079.49	6026.0	4.88	
1080.50	2992.7	2.42	
1109.53	45182.3	36.56	
1110.54	22574.5	18.27	
1111.56	7105.2	5.75	

1187.61	117738.4	95.28
1188.62	67856.1	54.91
1189.62	23646.9	19.14
1190.63	4630.9	3.75
1400.70	1978.2	1.60
1588.81	18963.7	15.35
1589.81	15458.8	12.51
1590.82	6913.4	5.59
1591.81	1982.8	1.60

SPECTRUM - MS

7-12-13_HMG28_924_MS3_1109_01.raw

ITMS + p ESI E Full ms3 924.40@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-20

RT: 0.00-2.50

AV: 20

m/z	Intensity	Relative
424.22	83.1	1.26
425.16	13.3	0.20
442.25	29.8	0.45
454.29	16.7	0.25
472.24	3546.0	53.86
473.25	531.8	8.08
474.28	54.0	0.82
500.24	13.0	0.20
586.29	104.8	1.59
587.27	18.6	0.28
611.34	20.2	0.31
618.34	42.4	0.64
625.30	15.5	0.24
660.35	6583.6	100.00
661.37	1519.0	23.07
662.37	197.6	3.00
667.31	47.5	0.72
685.36	17.5	0.27
716.38	18.9	0.29
799.38	837.4	12.72
800.38	260.0	3.95
801.32	23.2	0.35
801.48	25.9	0.39
829.46	45.4	0.69
831.52	25.2	0.38
832.45	20.5	0.31
864.54	22.1	0.34
873.43	6188.6	94.00
874.43	1980.3	30.08
875.46	329.6	5.01
882.46	90.3	1.37
883.35	19.2	0.29
883.53	13.4	0.20

891.46	14.7	0.22	
903.46	695.9	10.57	
904.47	210.6	3.20	
905.52	39.4	0.60	
921.51	39.0	0.59	
952.46	257.1	3.91	
953.40	46.9	0.71	
953.60	33.6	0.51	
954.57	13.2	0.20	
1038.52		13.6	0.21
1067.61		51.3	0.78
1068.51		18.6	0.28
1068.68		17.3	0.26
1079.49		31.8	0.48
1109.53	1638.0		24.88
1110.54	889.4	13.51	
1111.55	253.9	3.86	

SPECTRUM - MS

7-12-13_HMG28_924_MS4_1109_660_01.raw

ITMS + p ESI E Full ms4 924.40@cid35.00 1110.00@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-100

RT: 0.00-12.66

AV: 100

m/z	Intensity	Relative
229.09	25.0	7.72
236.06	11.7	3.62
241.09	13.7	4.24
259.10	323.5	100.00
260.11	25.3	7.81
287.09	5.2	1.62
301.12	6.1	1.89
329.18	4.6	1.43
338.19	5.2	1.60
364.18	14.3	4.41
368.19	5.7	1.76
380.18	5.4	1.66
382.20	13.4	4.13
384.18	5.8	1.78
398.19	11.5	3.56
399.20	5.5	1.69
400.23	7.4	2.28
412.21	19.8	6.11
424.19	23.1	7.14
426.21	24.0	7.43
430.25	11.6	3.57
440.18	5.4	1.66
442.25	98.0	30.29
443.26	15.7	4.85
447.25	7.2	2.24

454.22	21.3	6.59
456.22	22.7	7.02
470.24	5.1	1.58
472.23	196.1	60.60
473.24	30.3	9.37
486.23	7.3	2.26
515.27	11.3	3.51
540.22	5.5	1.71
554.24	5.4	1.66
556.31	8.5	2.62
570.28	8.8	2.72
584.29	14.2	4.40
586.29	233.8	72.26
587.31	49.6	15.33
588.33	5.7	1.77
589.32	81.9	25.30
590.31	20.4	6.31
614.29	37.4	11.55
615.29	8.9	2.74
618.33	258.6	79.93
619.34	56.9	17.59
620.35	7.1	2.20
630.32	9.0	2.79
660.35	77.6	23.98
661.36	15.5	4.80

SPECTRUM - MS

7-12-13_HMG28_924_MS4_1109_472_01.raw

ITMS + p ESI E Full ms4 924.40@cid35.00 1110.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-5.64

AV: 50

m/z Intensity Relative

149.02	1.9	1.15
171.00	3.4	2.04
178.10	0.7	0.45
180.02	5.9	3.55
188.05	3.4	2.04
194.06	3.7	2.23
204.01	6.1	3.65
218.06	1.8	1.10
218.84	0.8	0.46
220.06	21.0	12.66
221.04	1.6	0.98
227.07	105.4	63.39
228.09	8.3	5.00
236.07	17.5	10.50
237.05	1.6	0.95
243.10	1.2	0.75
245.07	51.7	31.10

246.15	2.5	1.52
250.10	1.1	0.69
259.10	7.7	4.65
268.12	166.3	100.00
269.12	14.8	8.89
287.08	6.3	3.77
301.13	0.8	0.51
315.15	135.4	81.43
316.15	15.2	9.11
317.13	1.1	0.65
324.21	0.9	0.56
327.22	0.8	0.46
348.24	0.8	0.48
366.10	1.1	0.67
367.14	1.9	1.17
368.20	3.6	2.18
380.21	7.5	4.48
385.18	0.8	0.51
398.20	14.7	8.84
399.25	3.1	1.88
401.26	0.7	0.44
408.09	0.8	0.48
408.31	0.8	0.49
412.16	1.2	0.72
430.26	13.4	8.07
431.23	1.0	0.59
440.19	33.7	20.25
441.20	4.7	2.81
442.21	18.9	11.38
443.25	2.1	1.28
472.24	67.5	40.60
473.30	11.0	6.61
474.32	2.9	1.77

SPECTRUM - MS

8-12-13_HMG29_924_MS2_01.raw

ITMS + p ESI E Full ms2 924.60@cid35.00 [250.00-2000.00]

Scan #: 1-20

RT: 0.00-1.58

AV: 20

m/z	Intensity	Relative
406.18	229.6	0.44
415.27	742.0	1.42
431.25	299.7	0.57
433.28	25491.8	48.89
434.28	5347.5	10.26
435.30	613.4	1.18
472.29	505.5	0.97
534.37	496.6	0.95
581.37	254.2	0.49
581.87	216.7	0.42
586.36	3923.9	7.53
587.37	1236.0	2.37
605.39	452.3	0.87
605.90	361.5	0.69
660.40	41073.4	78.78
661.41	14784.4	28.36
662.42	2208.9	4.24
681.94	2581.7	4.95
682.45	2699.0	5.18
682.96	973.6	1.87
699.42	524.9	1.01
700.41	223.1	0.43
718.94	2428.0	4.66
719.45	2627.8	5.04
719.95	1036.4	1.99
738.48	11729.6	22.50
739.49	5331.4	10.23
740.49	905.4	1.74
830.03	268.1	0.51
830.53	391.4	0.75
874.54	202.1	0.39
875.03	325.1	0.62
875.55	192.9	0.37
908.56	236.7	0.45
924.12	6436.2	12.35
924.58	11153.4	21.39
925.08	6483.0	12.43
1079.57	624.6	1.20
1080.58	423.7	0.81
1109.62	2921.6	5.60

1110.63	2002.9	3.84
1111.65	525.1	1.01
1187.70	52136.2	100.00
1188.70	42886.8	82.26
1189.71	12060.8	23.13
1340.73	308.2	0.59
1341.76	353.2	0.68
1414.82	18320.8	35.14
1415.82	19489.3	37.38
1416.83	6819.4	13.08

SPECTRUM - MS

8-12-13_HMG29_924_MS3_1109_01.raw

ITMS + p ESI E Full ms3 924.60@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-50

RT: 0.00-3.24

AV: 50

m/z Intensity Relative

415.25	5.0	0.55
415.41	2.3	0.26
424.02	1.7	0.19
424.24	11.9	1.30
425.28	1.6	0.18
430.10	1.5	0.17
430.33	1.8	0.19
431.26	1.7	0.19
433.27	117.5	12.84
434.33	8.1	0.89
454.22	3.0	0.33
472.28	350.5	38.29
473.30	40.5	4.43
542.31	6.6	0.72
543.31	1.3	0.14
558.27	4.0	0.44
586.34	30.9	3.38
587.38	6.8	0.74
618.44	2.4	0.26
625.35	79.6	8.69
626.42	14.3	1.57
628.41	5.2	0.57
629.29	1.2	0.14
653.43	1.9	0.20
657.43	14.2	1.55
658.45	3.5	0.38
660.40	689.9	75.35
661.41	128.6	14.05
669.46	1.5	0.17
699.41	915.5	100.00
700.41	195.7	21.38
701.36	1.3	0.14

717.42	2.7	0.30	
864.53	1.3	0.14	
882.38	1.3	0.14	
882.59	4.4	0.48	
883.52	2.4	0.26	
921.36	1.7	0.18	
921.54	2.7	0.29	
952.51	30.0	3.27	
953.51	10.9	1.19	
1038.53		1.5	0.16
1067.46		1.5	0.17
1067.58		1.4	0.15
1079.59		5.1	0.56
1079.76		1.3	0.14
1080.67		1.7	0.18
1109.69		79.3	8.66
1110.52		26.2	2.86
1110.74		21.8	2.39

SPECTRUM - MS

8-12-13_HMG29_924_MS4_1109_660_02.raw

ITMS + p ESI E Full ms4 924.60@cid35.00 1110.00@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-100

RT: 0.00-6.39

AV: 100

m/z	Intensity	Relative
208.14	0.4	0.23
211.09	0.3	0.22
243.09	0.5	0.29
245.08	5.0	3.17
246.08	0.5	0.30
250.15	0.6	0.36
268.13	0.4	0.23
285.08	0.6	0.38
313.13	0.8	0.52
323.23	0.5	0.30
351.18	0.3	0.18
353.19	3.0	1.89
354.35	0.3	0.16
380.22	0.2	0.13
383.20	2.0	1.24
384.17	0.4	0.24
387.22	1.2	0.76
398.20	5.4	3.42
399.24	0.4	0.26
401.20	0.5	0.28
415.24	19.2	12.12
416.25	2.1	1.32
417.26	0.6	0.37
431.22	4.8	3.05

432.21	0.7	0.46
433.24	158.4	100.00
434.26	21.5	13.55
472.25	21.1	13.34
473.26	3.8	2.40
490.27	0.3	0.17
515.26	1.6	0.99
530.35	0.5	0.29
544.32	0.2	0.12
554.26	0.3	0.16
556.28	0.2	0.12
558.09	2.0	1.27
558.29	1.7	1.10
559.31	0.4	0.24
584.35	0.3	0.21
586.31	72.2	45.58
587.31	14.9	9.42
589.29	0.8	0.50
589.47	0.4	0.26
590.20	0.2	0.14
614.31	0.7	0.42
618.36	16.9	10.65
619.35	2.8	1.79
628.25	0.2	0.14
660.37	10.1	6.40
661.37	1.5	0.97

SPECTRUM - MS

8-12-13_HMG29_924_MS4_1109_472_02.raw

ITMS + p ESI E Full ms4 924.60@cid35.00 1110.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-100

RT: 0.00-6.04

AV: 100

m/z Intensity Relative

149.01	0.1	0.87
171.01	0.4	3.05
180.05	0.5	3.81
188.02	0.2	1.94
189.09	0.1	0.52
194.01	0.1	1.20
204.04	0.6	4.64
208.14	0.1	0.65
218.02	0.2	1.44
220.07	1.5	12.64
222.18	0.1	0.69
227.08	7.3	60.73
228.07	0.3	2.88
228.25	0.1	0.77
232.08	0.1	0.60
236.06	0.9	7.20

245.08	4.1	34.02
246.06	0.1	0.61
246.17	0.1	0.57
250.11	0.2	1.69
268.13	12.0	100.00
269.12	1.1	9.51
287.19	0.2	1.68
315.15	10.3	85.97
316.17	1.1	9.37
324.09	0.2	1.41
324.23	0.2	1.31
366.10	0.1	0.74
367.28	0.1	0.76
368.28	0.2	1.76
370.34	0.1	0.67
380.18	0.3	2.25
385.77	0.1	0.67
396.24	0.1	0.66
398.21	1.3	10.93
399.10	0.1	1.09
399.25	0.3	2.11
401.22	0.3	2.16
408.28	0.1	1.03
412.20	0.1	0.72
430.31	0.3	2.69
440.20	1.7	14.16
441.28	0.2	1.80
442.16	1.1	9.21
442.36	0.7	5.48
443.27	0.1	1.03
443.37	0.1	0.94
472.26	3.8	32.01
473.20	0.3	2.48
473.39	0.1	0.70

HMG 31 Mass spectral peak lists

SPECTRUM - MS

8-16-13_HMG31_924_MS2_01.raw

ITMS + p ESI E Full ms2 924.40@cid35.00 [250.00-2000.00]

Scan #: 1-20

RT: 0.00-1.57

AV: 20

m/z	Intensity	Relative	
486.25	32906.3	19.84	
487.26	7025.2	4.23	
534.31	1303.4	0.79	
589.33	5127.9	3.09	
589.83	3352.1	2.02	
590.33	1486.0	0.90	
630.28	1442.0	0.87	
646.31	3600.5	2.17	
647.33	1156.4	0.70	
660.33	2771.8	1.67	
692.37	165898.6	100.00	
692.87	112047.3	67.54	
693.36	44349.1	26.73	
693.88	11194.2	6.75	
718.30	2443.3	1.47	
738.39	17979.9	10.84	
739.40	6818.6	4.11	
740.40	1494.0	0.90	
760.31	1373.8	0.83	
768.89	1937.5	1.17	
769.40	1567.0	0.94	
805.90	9790.1	5.90	
806.40	7485.5	4.51	
806.90	3636.3	2.19	
820.91	6711.9	4.05	
821.41	5794.9	3.49	
821.92	2962.5	1.79	
829.93	3265.3	1.97	
830.43	2924.2	1.76	
830.93	1411.1	0.85	
924.00	22580.2	13.61	
924.47	21012.3	12.67	
924.95	11746.9	7.08	
925.45	4959.0	2.99	
1109.49	3527.6	2.13	
1110.50	1833.7	1.11	
1155.55	5490.8	3.31	
1156.55	3276.1	1.97	
1157.56	3644.9	2.20	
1158.57	1721.5	1.04	
1187.57	3457.0	2.08	

1188.58	1992.4	1.20
1253.52	1841.3	1.11
1254.53	1157.1	0.70
1361.64	40738.6	24.56
1362.65	26779.4	16.14
1363.65	10380.3	6.26
1364.66	2419.8	1.46
1588.75	2661.0	1.60
1589.76	2013.4	1.21

SPECTRUM - MS

8-16-13_HMG31_924_MS3_1109_01.raw

ITMS + p ESI E Full ms3 924.40@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-50

RT: 0.00-3.21

AV: 50

m/z Intensity Relative

382.19	4.8	0.45
384.22	2.8	0.27
385.14	26.4	2.50
412.13	3.5	0.33
424.17	4.0	0.37
440.36	2.9	0.27
442.26	7.2	0.68
444.19	6.7	0.63
458.16	6.9	0.65
458.34	2.7	0.25
486.25	265.5	25.07
487.23	32.4	3.06
572.32	21.3	2.01
573.17	5.4	0.51
573.31	6.0	0.57
575.37	7.5	0.70
598.27	8.3	0.78
646.30	1059.1	100.00
647.31	199.6	18.85
690.32	9.0	0.85
690.45	6.6	0.62
706.27	10.5	0.99
707.98	4.1	0.38
708.40	61.4	5.79
709.31	18.5	1.74
778.38	7.0	0.66
799.38	15.5	1.47
800.36	4.7	0.44
843.39	3.4	0.32
873.39	143.6	13.56
874.32	35.7	3.38
874.52	20.6	1.95
891.34	8.7	0.82

903.43	11.0	1.04	
904.40	3.5	0.33	
905.25	19.5	1.84	
905.43	31.0	2.92	
906.18	3.2	0.30	
906.42	11.0	1.03	
921.30	2.7	0.26	
921.46	5.4	0.51	
922.52	3.6	0.34	
1003.48		3.3	0.31
1035.40		9.8	0.93
1038.50		5.5	0.52
1067.35		6.4	0.60
1067.63		7.1	0.67
1077.43		5.9	0.55
1109.47		73.6	6.95
1110.58		21.2	2.00

SPECTRUM - MS

8-16-13_HMG31_924_MS4_1109_646_01.raw

ITMS + p ESI E Full ms4 924.40@cid35.00 1110.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-100

RT: 0.00-7.28

AV: 100

m/z	Intensity	Relative
194.07	0.6	1.04
204.01	1.2	2.18
211.06	0.5	0.98
218.03	0.7	1.29
220.10	1.0	1.93
227.06	8.0	14.86
229.09	3.9	7.16
236.05	5.1	9.49
243.08	0.6	1.08
245.08	17.9	33.19
246.08	1.0	1.79
287.08	1.2	2.20
292.10	0.6	1.08
315.13	2.4	4.49
343.15	2.6	4.84
353.14	0.6	1.10
366.14	1.4	2.64
367.17	0.6	1.08
368.18	1.8	3.30
369.19	1.0	1.89
378.17	2.0	3.66
380.20	2.8	5.21
382.19	5.0	9.26
383.20	1.0	1.91
384.17	5.2	9.57

385.16	54.0	100.00
386.17	6.8	12.54
396.23	0.6	1.02
398.18	1.4	2.58
408.18	0.7	1.30
424.19	4.8	8.84
425.18	0.8	1.51
433.28	0.8	1.39
440.18	12.9	23.85
441.21	2.4	4.44
442.22	13.6	25.11
443.24	2.0	3.64
458.21	5.6	10.42
459.30	0.5	0.99
498.25	0.5	1.00
572.28	53.2	98.61
573.29	16.7	30.91
574.22	0.7	1.34
574.40	0.7	1.22
575.30	17.0	31.40
576.31	3.8	6.95
604.33	3.3	6.17
605.33	1.1	2.09
646.32	9.4	17.34
647.29	2.3	4.32

SPECTRUM - MS

8-16-13_HMG31_924_MS4_1109_486_01.raw

ITMS + p ESI E Full ms4 924.40@cid35.00 1110.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-100

RT: 0.00-6.20

AV: 100

m/z Intensity Relative

180.09	0.1	0.49
184.44	0.2	0.83
188.03	0.1	0.48
189.13	0.1	0.28
191.62	0.1	0.47
207.98	0.1	0.38
208.11	0.1	0.53
211.04	0.2	1.02
217.98	0.1	0.34
218.09	0.1	0.37
220.08	0.9	4.41
220.99	0.1	0.35
227.04	0.1	0.58
241.09	1.2	6.07
250.10	0.9	4.29
252.09	0.3	1.26
259.10	8.8	42.57

260.13	0.6	2.82
268.12	3.3	16.09
269.06	0.1	0.33
297.08	0.3	1.32
301.20	0.2	0.99
304.33	0.1	0.43
314.01	0.1	0.33
329.17	9.8	47.63
330.19	0.8	4.10
365.93	0.1	0.33
380.09	0.1	0.60
381.11	0.1	0.33
384.25	0.2	0.89
395.28	0.1	0.52
410.21	0.1	0.49
412.20	3.6	17.48
413.23	0.8	4.07
414.99	0.1	0.38
415.20	0.2	0.97
427.25	0.1	0.50
431.01	0.1	0.64
444.24	20.6	100.00
445.15	3.2	15.45
445.31	2.5	12.22
454.21	0.2	1.01
456.12	0.6	2.68
456.32	1.0	4.64
457.37	0.1	0.41
484.73	0.1	0.51
486.11	2.3	11.04
486.33	1.7	8.28
487.25	0.5	2.66
487.40	0.5	2.33

SPECTRUM - MS

8-16-13_HMG31_924_MS3_605_01.raw

ITMS + p ESI E Full ms3 924.40@cid35.00 605.80@cid35.00 [165.00-1300.00]

Scan #: 1-101

RT: 0.00-15.46

AV: 101

m/z Intensity Relative

196.08	0.8	3.18
284.11	0.3	1.07
285.15	0.3	1.08
386.19	0.5	2.08
415.23	0.9	3.84
432.18	0.3	1.33
445.27	0.2	0.89
464.23	1.1	4.71
470.26	1.0	4.05

471.24	0.9	3.65
472.23	0.4	1.61
484.36	0.2	0.78
486.28	8.5	35.46
487.29	1.6	6.65
496.28	0.3	1.08
514.29	0.6	2.54
534.36	1.8	7.41
535.36	0.4	1.83
568.30	0.3	1.25
590.38	1.6	6.69
590.86	0.5	1.93
591.36	0.4	1.60
605.33	2.7	11.40
605.85	1.6	6.55
606.35	0.5	1.97
616.31	1.0	3.97
664.44	0.4	1.72
676.37	1.0	4.23
677.40	0.2	0.93
704.37	2.7	11.15
705.34	1.0	4.16
724.45	10.5	43.47
725.44	3.4	14.32
726.45	0.6	2.31
738.48	0.9	3.82
739.45	1.9	8.05
740.48	1.2	5.09
746.36	4.8	20.11
747.36	1.5	6.13
748.38	0.2	0.83
760.29	0.2	0.79
761.33	0.2	0.75
761.49	0.2	0.77
762.41	0.2	0.81
970.70	0.2	0.68
980.59	0.3	1.07
1186.69	0.9	3.64
1187.68	24.0	100.00
1188.68	12.6	52.20
1189.68	4.0	16.57

SPECTRUM - MS

8-16-13_HMG31_924_MS3_660_01.raw

ITMS + p ESI E Full ms3 924.40@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-100

RT: 0.00-5.48

AV: 100

m/z	Intensity	Relative
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229.08	6.0	2.50
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241.11	3.1	1.32
245.07	7.5	3.15
259.10	65.9	27.72
260.10	6.9	2.92
353.18	4.9	2.07
364.18	2.2	0.94
380.22	2.5	1.06
382.22	4.4	1.85
383.19	4.4	1.85
387.23	2.4	1.00
394.22	2.2	0.91
398.20	11.4	4.78
399.19	3.3	1.40
412.21	4.5	1.90
415.23	27.7	11.66
416.24	4.2	1.78
424.20	6.1	2.58
426.21	5.3	2.23
430.26	6.0	2.51
431.21	8.6	3.61
433.24	237.8	100.00
434.24	40.0	16.82
435.24	5.1	2.15
442.26	18.6	7.82
443.25	3.6	1.50
447.26	2.6	1.09
454.31	2.8	1.19
456.24	10.1	4.23
470.25	2.6	1.10
472.24	108.9	45.78
473.24	20.7	8.69
486.26	21.5	9.02
487.26	3.9	1.66
515.26	5.2	2.20
558.21	4.0	1.69
584.28	4.5	1.89
586.30	158.6	66.69
587.30	42.2	17.75
588.31	7.3	3.08
589.33	21.1	8.88
590.32	5.5	2.31
614.31	8.0	3.38
615.33	2.9	1.21
618.33	89.1	37.45
619.34	26.0	10.92
620.35	3.9	1.65
630.31	2.6	1.11
660.37	27.7	11.66
661.37	10.1	4.23

SPECTRUM - MS

8-16-13_HMG31_924_MS4_605_486_02.raw

ITMS + p ESI E Full ms4 924.40@cid35.00 605.80@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-291

RT: 0.00-37.83

AV: 291

m/z	Intensity	Relative
188.02	0.0	0.36
211.08	0.0	0.64
216.99	0.0	0.27
218.05	0.0	0.27
220.11	0.0	1.33
236.08	0.0	0.36
241.09	0.1	2.72
242.09	0.0	0.24
249.52	0.0	0.23
250.16	0.0	0.39
252.11	0.0	0.23
256.32	0.0	0.26
257.13	0.0	0.25
259.13	0.2	7.65
260.09	0.0	1.05
268.11	0.1	4.78
269.10	0.0	0.41
301.21	0.0	0.78
315.17	0.0	0.34
329.20	0.3	12.80
330.15	0.0	1.14
330.33	0.0	0.33
335.07	0.0	0.26
352.02	0.0	0.24
369.08	0.0	0.42
371.33	0.0	0.27
384.18	0.0	0.38
384.39	0.0	0.29
387.18	0.0	0.27
392.41	0.0	0.31
399.24	0.0	0.28
410.19	0.0	0.64
411.23	0.0	0.45
412.07	0.0	0.66
412.26	0.0	0.75
413.33	0.0	0.34
415.12	0.0	0.64
415.26	0.0	0.50
415.37	0.0	0.39
426.18	0.0	0.26
431.22	0.0	0.37
444.28	2.6	100.00
445.27	0.4	17.13
454.21	0.0	0.80

456.28	0.1	4.47
457.13	0.0	0.33
457.32	0.0	0.76
457.56	0.0	0.23
486.28	0.0	1.25
487.13	0.0	0.25

HMG 33 Mass spectral peak lists

SPECTRUM - MS

7-22-13_HMG33_1061_MS2_01.raw

ITMS + p ESI E Full ms2 1062.00@cid35.00 [290.00-2000.00]

Scan #: 1-20

RT: 0.00-1.61

AV: 20

m/z	Intensity	Relative
412.21	118.1	2.19
472.24	86.3	1.60
486.25	3072.0	57.07
487.26	566.2	10.52
598.31	98.6	1.83
605.32	80.7	1.50
674.87	158.2	2.94
675.36	106.6	1.98
699.34	84.5	1.57
706.39	138.9	2.58
711.86	226.5	4.21
712.36	138.9	2.58
724.41	262.8	4.88
829.95	5195.1	96.51
830.45	3858.8	71.68
830.95	1636.2	30.40
831.51	218.1	4.05
906.46	841.9	15.64
906.96	701.4	13.03
907.47	338.5	6.29
935.44	297.1	5.52
936.46	111.7	2.08
943.49	4436.1	82.41
943.99	3674.1	68.25
944.50	1767.7	32.84
944.99	253.2	4.70
952.48	93.6	1.74
1032.51	89.2	1.66
1061.56	2566.4	47.68
1062.04	2746.7	51.02
1062.52	1797.0	33.38
1063.06	308.3	5.73
1173.57	1243.8	23.11
1174.58	632.5	11.75
1175.60	175.0	3.25
1187.59	531.0	9.86
1188.59	274.8	5.10
1400.69	764.3	14.20
1401.70	498.6	9.26
1402.79	110.2	2.05
1528.68	170.2	3.16

1529.70	112.9	2.10
1628.81	81.9	1.52
1636.83	5383.0	100.00
1637.84	3773.4	70.10
1638.84	1498.7	27.84
1639.85	142.9	2.66
1864.03	1139.8	21.17
1865.04	942.1	17.50
1866.04	459.4	8.53

SPECTRUM - MS

7-22-13_HMG33_1061_MS3_830_01.raw

ITMS + p ESI E Full ms3 1062.00@cid35.00 830.40@cid35.00 [225.00-2000.00]

Scan #: 1-20

RT: 0.00-5.98

AV: 20

m/z Intensity Relative

259.10	26.9	5.83
412.21	16.8	3.64
472.24	31.0	6.72
473.25	5.5	1.20
486.26	265.8	57.56
487.26	55.0	11.90
488.27	7.7	1.67
534.33	11.1	2.40
598.32	51.0	11.05
598.83	30.7	6.64
599.32	10.6	2.30
605.33	34.8	7.53
605.85	21.3	4.60
606.34	7.4	1.61
664.40	12.5	2.70
674.87	51.6	11.17
675.37	37.5	8.13
675.87	13.5	2.93
704.36	11.5	2.48
706.39	39.7	8.60
707.40	13.2	2.86
711.87	71.9	15.57
712.36	50.7	10.99
712.87	20.3	4.39
713.41	5.8	1.25
724.42	65.6	14.22
725.40	23.7	5.14
746.32	12.9	2.80
829.97	105.1	22.76
830.45	99.2	21.48
830.95	51.9	11.24
831.47	17.6	3.82
935.45	18.0	3.90

936.47	7.1	1.54	
1065.49		20.0	4.34
1066.46		9.0	1.96
1125.54		5.4	1.18
1173.59		461.8	100.00
1174.60		270.0	58.47
1175.60		80.0	17.33
1176.62		11.9	2.58
1187.60		39.1	8.47
1188.61		23.0	4.98
1189.61		6.4	1.38
1195.51		5.4	1.17
1400.71		100.5	21.77
1401.71		70.8	15.33
1402.72		25.2	5.46
1636.84		11.9	2.59
1637.85		10.6	2.30

SPECTRUM - MS

7-22-13_HMG33_1061_MS3_934_01.raw

ITMS + p ESI E Full ms3 1062.00@cid35.00 936.00@cid35.00 [255.00-1000.00]

Scan #: 1-20

RT: 0.00-3.01

AV: 20

m/z	Intensity	Relative
268.11	0.2	0.46
315.21	0.2	0.45
398.25	0.1	0.36
412.21	0.6	1.86
413.15	0.1	0.22
423.95	0.1	0.26
424.21	0.5	1.35
425.11	0.1	0.24
425.25	0.1	0.37
431.32	0.1	0.35
440.17	0.1	0.35
440.30	0.1	0.22
441.27	0.1	0.23
472.23	34.7	100.00
473.24	9.1	26.39
486.25	15.9	45.86
487.24	3.6	10.50
625.27	4.9	14.00
626.30	1.6	4.51
657.35	0.2	0.69
662.47	0.1	0.20
669.39	0.1	0.28
690.45	0.2	0.66
699.34	26.7	77.16
700.34	12.2	35.19

701.40	0.1	0.42
706.35	0.2	0.64
708.18	0.1	0.35
708.35	0.1	0.28
708.50	0.2	0.72
709.38	0.3	0.74
717.22	0.1	0.36
717.40	0.1	0.22
718.42	0.1	0.20
728.38	0.1	0.26
739.46	0.1	0.30
778.29	0.3	0.84
778.47	0.2	0.55
779.38	0.2	0.47
861.47	0.2	0.57
864.76	0.1	0.32
875.59	0.1	0.30
893.48	0.2	0.45
894.38	0.1	0.40
903.46	0.2	0.49
904.33	0.1	0.37
905.52	0.1	0.34
935.43	7.7	22.17
936.52	4.1	11.72
936.97	0.1	0.24

SPECTRUM - MS

7-22-13_HMG33_1061_MS4_934_486_01.raw

ITMS + p ESI E Full ms4 1062.00@cid35.00 936.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-8.70

AV: 50

m/z Intensity Relative

138.90	0.0	0.31
178.00	0.0	0.51
188.13	0.0	0.74
208.05	0.1	4.21
211.16	0.0	0.34
212.99	0.0	0.95
213.16	0.0	0.38
218.11	0.0	0.82
220.17	0.0	0.49
222.12	0.0	0.66
241.14	0.1	4.13
242.12	0.0	0.32
250.09	0.1	6.30
251.05	0.0	0.82
252.13	0.3	14.02
253.25	0.0	0.59
257.12	0.0	1.46

259.09	1.9	99.62
259.94	0.0	2.40
260.13	0.1	6.24
268.08	0.1	3.67
269.20	0.0	0.37
269.85	0.0	0.48
302.04	0.0	0.38
329.13	0.0	1.18
329.27	0.0	1.13
330.20	0.0	0.62
336.06	0.0	0.54
341.28	0.0	2.30
370.15	0.0	0.29
380.08	0.0	0.31
382.09	0.0	0.79
383.87	0.0	0.36
384.23	0.1	2.64
385.24	0.0	0.38
396.21	0.0	0.39
409.08	0.0	0.39
410.32	0.0	0.93
412.19	1.9	100.00
413.28	0.2	9.92
415.09	0.0	1.38
415.33	0.0	1.85
431.19	0.0	0.36
440.17	0.0	0.46
441.25	0.0	0.33
444.23	1.3	69.46
445.25	0.2	12.00
454.34	0.0	0.65
486.29	0.4	20.71
487.28	0.1	6.79

SPECTRUM - MS

7-22-13_HMG33_1061_MS3_486_01.raw

ITMS + p ESI E Full ms3 1062.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-2.69

AV: 50

m/z Intensity Relative

177.09	0.6	0.17
178.04	3.9	1.05
194.03	0.5	0.13
208.07	15.5	4.14
209.07	0.9	0.23
210.95	0.4	0.11
211.07	0.5	0.13
218.03	2.0	0.53
241.08	14.4	3.86

242.10	1.2	0.33
250.09	26.8	7.17
251.08	1.4	0.37
252.09	45.1	12.08
253.09	4.0	1.06
257.07	5.4	1.45
258.07	0.4	0.11
259.09	332.1	88.97
260.11	26.4	7.08
268.13	6.2	1.67
269.19	0.4	0.11
282.13	0.8	0.22
301.05	1.4	0.37
301.23	0.8	0.22
302.09	0.6	0.15
329.21	0.8	0.22
338.13	0.9	0.25
341.18	3.4	0.92
356.21	1.9	0.51
370.19	0.6	0.16
380.27	1.0	0.26
382.20	5.2	1.40
383.23	0.7	0.19
384.13	10.3	2.77
385.13	1.3	0.36
394.21	0.5	0.12
410.24	4.3	1.16
411.19	0.5	0.13
412.20	373.2	100.00
413.21	49.7	13.32
415.22	4.4	1.19
416.21	0.9	0.24
426.40	0.6	0.16
440.26	0.6	0.16
444.24	143.9	38.54
445.25	22.7	6.09
450.30	0.5	0.13
454.27	1.5	0.40
456.36	2.1	0.56
486.24	67.8	18.17
487.26	11.8	3.17

SPECTRUM - MS

7-22-13_HMG33_1061_MS4_934_472_01.raw

ITMS + p ESI E Full ms4 1062.00@cid35.00 936.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-51

RT: 0.00-8.88

AV: 51

m/z Intensity Relative

149.00 0.1 2.09

171.02	0.1	2.15
178.04	0.0	0.58
180.01	0.1	3.32
188.03	0.1	1.92
194.09	0.1	2.57
203.93	0.1	2.40
204.08	0.1	2.75
210.05	0.0	0.61
218.10	0.1	1.61
218.26	0.0	0.57
220.07	0.3	7.94
221.08	0.0	1.50
227.07	1.8	55.57
228.06	0.1	3.96
236.07	0.4	13.01
237.11	0.0	0.58
243.06	0.1	1.86
245.07	0.9	29.07
246.07	0.1	1.93
250.18	0.0	0.68
268.11	2.8	89.34
269.09	0.3	9.99
283.09	0.0	0.67
287.08	0.1	2.21
315.14	2.4	75.21
316.16	0.3	9.17
324.18	0.1	2.47
339.20	0.0	0.61
366.21	0.0	0.62
368.15	0.0	1.51
369.27	0.0	0.57
380.18	0.2	6.60
385.17	0.0	1.35
398.17	0.5	16.38
398.94	0.0	0.87
399.20	0.2	5.55
400.27	0.0	0.56
401.27	0.0	1.17
408.11	0.0	0.93
408.29	0.0	0.84
430.31	0.1	3.60
440.18	0.9	28.78
441.05	0.0	1.36
441.23	0.1	1.82
442.19	0.2	7.15
442.45	0.0	0.57
443.24	0.0	1.10
472.24	3.2	100.00
473.24	0.5	16.90

HMG 34 Mass spectral peak lists

SPECTRUM - MS

12-18-13_HMG34_1011_MS2_01.raw

ITMS + p ESI E Full ms2 1011.60@cid35.00 [275.00-2000.00]

Scan #: 1-21

RT: 0.00-5.11

AV: 21

m/z	Intensity	Relative
433.29	715.3	39.23
434.29	138.3	7.58
534.40	75.4	4.14
738.49	1020.4	55.97
739.49	398.5	21.86
740.50	101.2	5.55
760.44	149.7	8.21
768.99	114.7	6.29
769.47	96.9	5.32
776.48	419.0	22.98
778.47	1340.1	73.50
780.47	752.5	41.27
805.99	273.3	14.99
806.48	242.6	13.31
806.99	121.9	6.68
834.46	1252.3	68.68
835.47	498.3	27.33
836.47	196.6	10.78
873.48	82.0	4.50
874.45	72.6	3.98
892.37	326.1	17.89
894.35	660.9	36.25
896.31	231.2	12.68
917.04	84.5	4.63
917.54	87.4	4.79
950.31	119.3	6.54
952.30	572.1	31.38
953.37	107.0	5.87
954.28	316.5	17.36
979.46	82.8	4.54
982.37	72.2	3.96
1010.33		707.0 38.78
1011.18		1190.3 65.28
1011.58		1097.9 60.22
1012.08		1081.7 59.33
1012.52		355.5 19.50
1187.65		1823.2 100.00
1188.65		1124.5 61.68
1189.62		415.6 22.79
1190.63		101.9 5.59
1283.64		328.0 17.99

1284.64	210.1	11.52
1285.62	79.3	4.35
1588.81	760.3	41.70
1589.81	629.2	34.51
1590.81	302.3	16.58
1591.82	100.8	5.53
1881.62	82.9	4.55
1883.61	105.9	5.81
1885.60	70.8	3.88

SPECTRUM - MS

12-18-13_HMG34_1011_MS3_1283_01.raw

ITMS + p ESI E Full ms3 1011.60@cid35.00 1284.00@cid35.00 [350.00-1300.00]

Scan #: 1-20

RT: 0.00-3.19

AV: 20

m/z Intensity Relative

415.25	0.2	0.39
424.20	0.5	1.01
433.25	3.3	6.81
434.26	0.5	1.09
442.22	0.1	0.16
472.29	5.5	11.23
473.28	1.1	2.28
500.27	0.1	0.18
572.24	0.2	0.33
611.18	0.1	0.19
611.37	0.1	0.21
612.32	0.1	0.16
628.38	0.1	0.28
642.32	0.1	0.16
646.36	0.4	0.78
660.41	0.1	0.26
667.36	0.2	0.36
685.41	0.2	0.49
686.39	0.1	0.19
716.38	0.6	1.15
717.41	0.1	0.30
760.40	2.0	4.18
761.42	0.5	1.11
799.33	2.7	5.52
799.52	1.9	3.86
800.41	1.1	2.20
801.37	0.1	0.18
801.52	0.1	0.21
831.34	0.3	0.70
831.55	0.4	0.90
832.53	0.1	0.27
834.45	36.1	73.61
835.46	9.7	19.86

836.45	1.3	2.63	
873.45	49.0	100.00	
874.46	15.5	31.71	
875.48	2.2	4.40	
1056.46		0.2	0.31
1056.69		0.1	0.17
1095.64		0.2	0.48
1096.59		0.1	0.28
1126.58		1.6	3.32
1127.48		0.4	0.92
1127.69		0.3	0.63
1241.69		0.1	0.22
1253.61		0.2	0.48
1254.55		0.1	0.18
1283.65		9.1	18.62
1284.65		6.2	12.67
1285.62		1.6	3.22

SPECTRUM - MS

12-18-13_HMG34_1011_MS4_1283_472_01.raw

ITMS + p ESI E Full ms4 1011.60@cid35.00 1284.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-14.35

AV: 50

m/z Intensity Relative

141.35	0.0	1.07
148.96	0.0	1.63
171.05	0.0	4.51
187.85	0.0	1.00
188.01	0.0	1.65
188.15	0.0	1.09
189.99	0.0	1.65
194.02	0.0	2.08
204.04	0.0	3.08
218.01	0.0	1.42
220.11	0.0	9.25
227.06	0.1	64.62
228.22	0.0	2.45
236.06	0.0	11.67
243.16	0.0	1.94
245.10	0.1	37.06
246.08	0.0	2.52
249.97	0.0	1.16
268.13	0.2	100.00
269.13	0.0	4.16
270.05	0.0	1.52
283.20	0.0	1.24
287.13	0.0	1.08
315.15	0.2	80.39
316.07	0.0	3.10

316.24	0.0	3.31
317.33	0.0	1.24
324.23	0.0	1.11
357.10	0.0	1.19
365.86	0.0	1.21
368.19	0.0	1.92
369.26	0.0	1.55
374.88	0.0	1.21
380.01	0.0	2.35
380.22	0.0	5.59
397.65	0.0	1.19
398.22	0.0	10.76
399.20	0.0	2.56
401.30	0.0	3.29
430.23	0.0	4.68
440.23	0.0	16.92
441.17	0.0	4.26
442.11	0.0	4.75
442.30	0.0	7.43
472.20	0.1	29.95
472.37	0.1	33.45
472.60	0.0	1.38
473.21	0.0	7.00
473.37	0.0	2.82
474.12	0.0	1.24

SPECTRUM - MS

12-18-13_HMG34_1011_MS4_1283_834_01.raw

ITMS + p ESI E Full ms4 1011.60@cid35.00 1284.00@cid35.00 835.00@cid35.00 [225.00-900.00]

Scan #: 1-50

RT: 0.00-8.74

AV: 50

m/z Intensity Relative

245.09	0.1	1.58
323.22	0.0	0.49
353.16	0.1	1.39
364.16	0.1	1.32
368.17	0.1	1.49
383.21	0.0	0.91
387.26	0.0	0.68
400.27	0.0	0.60
401.23	0.0	0.57
415.23	0.3	8.16
416.25	0.1	1.45
424.27	0.1	1.48
426.29	0.0	0.71
431.25	0.1	1.31
433.24	4.3	100.00
434.32	0.4	8.51
435.31	0.0	0.68

442.25	0.2	4.24
443.28	0.0	0.94
572.31	0.2	3.67
573.37	0.0	1.05
586.39	0.0	0.86
621.32	0.0	0.80
628.41	0.0	0.46
629.36	0.0	0.42
632.31	0.0	0.49
644.38	0.0	0.51
646.34	1.8	43.44
647.34	0.4	9.97
648.38	0.0	1.07
660.35	0.0	0.79
689.31	0.0	1.05
689.47	0.0	1.03
690.32	0.0	0.44
744.38	0.0	0.71
758.51	0.0	0.55
760.39	2.0	46.53
761.42	0.6	13.84
762.27	0.0	1.01
762.49	0.0	0.81
763.40	0.1	3.06
764.34	0.0	0.76
788.41	0.1	2.11
789.49	0.0	0.45
792.42	0.4	9.54
793.50	0.1	2.21
794.52	0.0	0.46
804.41	0.0	0.62
834.44	0.6	13.72
835.44	0.2	3.73

SPECTRUM - MS

12-18-13_HMG34_1011_MS5_1283_834_646_03.raw

ITMS + p ESI E Full ms5 1011.60@cid35.00 1284.00@cid35.00 835.00@cid35.00 647.00@cid35.00
[175.00-700.00]

Scan #: 1-36

RT: 0.00-92.38

AV: 36

m/z	Intensity	Relative
193.56	0.0	2.24
196.96	0.0	3.87
220.04	0.0	3.73
229.07	0.0	5.17
234.07	0.0	2.32
236.04	0.0	3.50
245.10	0.0	34.72
266.16	0.0	2.21

270.77	0.0	1.00
283.99	0.0	3.10
287.18	0.0	2.11
291.99	0.0	2.34
332.16	0.0	3.41
350.13	0.0	3.29
364.22	0.0	4.11
368.21	0.0	8.20
368.39	0.0	3.79
369.26	0.0	2.60
382.13	0.0	5.88
384.10	0.0	3.25
384.29	0.0	2.29
385.04	0.0	1.13
392.22	0.0	3.55
398.23	0.0	6.92
415.16	0.0	1.95
417.32	0.0	1.64
424.19	0.0	18.52
426.02	0.0	1.86
426.17	0.0	2.86
426.35	0.0	9.03
433.34	0.0	58.56
434.26	0.0	23.40
436.21	0.0	7.38
440.38	0.0	3.84
442.24	0.0	2.13
458.17	0.0	2.00
458.34	0.0	4.41
459.27	0.0	3.56
466.14	0.0	1.39
475.17	0.0	0.85
540.40	0.0	4.29
565.68	0.0	5.12
572.35	0.0	100.00
573.27	0.0	30.22
574.23	0.0	0.86
582.30	0.0	1.51
626.05	0.0	2.43
646.25	0.0	95.49
646.45	0.0	86.83
647.28	0.0	23.39

HMG 37 Mass spectral peak lists

SPECTRUM - MS

6-26-13_HMG37_1011_MS2_02.raw

ITMS + p ESI E Full ms2 1011.60@cid35.00 [275.00-2000.00]

Scan #: 1-20

RT: 0.00-1.55

AV: 20

m/z	Intensity	Relative
433.30	28716.4	38.54
434.31	4676.4	6.28
486.32	2698.7	3.62
534.40	1391.7	1.87
586.38	4698.6	6.31
587.38	1209.2	1.62
646.41	1306.8	1.75
660.43	51329.6	68.88
661.44	13649.5	18.32
662.45	1844.4	2.48
692.48	22424.2	30.09
692.98	14223.9	19.09
693.49	4790.4	6.43
738.51	21111.9	28.33
739.51	6866.9	9.22
769.02	3966.7	5.32
769.52	2978.3	4.00
780.54	27979.9	37.55
781.05	4362.2	5.85
806.03	18458.6	24.77
806.53	13597.0	18.25
807.03	5356.9	7.19
857.05	1273.8	1.71
893.09	1730.7	2.32
893.59	1421.6	1.91
894.09	6152.8	8.26
894.58	1222.2	1.64
908.08	1844.9	2.48
908.59	1615.0	2.17
909.10	1863.5	2.50
917.11	1532.7	2.06
917.60	1306.7	1.75
918.11	1548.1	2.08
1011.20	18227.7	24.46
1011.68	20518.6	27.54
1012.16	20340.8	27.30
1012.64	3167.8	4.25
1155.73	1596.9	2.14
1253.72	1206.6	1.62
1283.76	6509.7	8.74
1284.77	3453.6	4.63

1361.84	74515.5	100.00
1362.85	46684.4	62.65
1363.86	15180.1	20.37
1537.98	8534.9	11.45
1538.98	1416.8	1.90
1588.98	26707.5	35.84
1589.99	19521.4	26.20
1590.99	7857.2	10.54
1765.15	1830.7	2.46

SPECTRUM - MS

6-26-13_HMG37_1011_MS3_1283_01.raw

ITMS + p ESI E Full ms3 1011.60@cid35.00 1284.00@cid35.00 [350.00-1300.00]

Scan #: 1-50

RT: 0.00-4.05

AV: 50

m/z Intensity Relative

385.26	1.7	0.45
398.26	1.3	0.33
424.29	1.1	0.28
433.29	25.2	6.56
434.22	2.1	0.55
434.40	1.5	0.39
470.30	2.3	0.59
472.35	1.8	0.48
524.34	2.5	0.65
572.38	4.4	1.14
573.46	1.0	0.27
575.43	1.2	0.31
586.35	8.7	2.27
587.43	1.4	0.37
598.35	11.8	3.08
599.45	3.0	0.78
646.42	144.6	37.72
647.43	32.0	8.34
660.44	154.4	40.26
661.45	41.4	10.79
669.45	1.4	0.37
799.47	33.2	8.65
800.50	11.0	2.87
831.56	2.0	0.53
834.55	1.5	0.40
864.45	1.3	0.35
864.62	2.3	0.60
873.55	383.4	100.00
874.56	145.9	38.05
880.54	2.3	0.59
882.52	25.2	6.56
883.43	5.5	1.44
883.66	4.3	1.13

952.49	1.9	0.50	
952.68	1.5	0.38	
953.66	1.3	0.34	
973.68	2.4	0.62	
974.66	1.3	0.33	
1047.66		35.2	9.18
1048.68		17.3	4.51
1077.62		1.3	0.34
1078.71		1.1	0.28
1079.62		10.9	2.86
1080.58		1.9	0.49
1080.79		1.7	0.45
1209.83		1.2	0.30
1241.68		1.2	0.30
1242.78		1.0	0.25
1283.87		21.2	5.52
1284.78		32.4	8.45

SPECTRUM - MS

6-26-13_HMG37_1011_MS4_1283_660_01.raw

ITMS + p ESI E Full ms4 1011.60@cid35.00 1284.00@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-50

RT: 0.00-5.55

AV: 50

m/z	Intensity	Relative
201.04	0.3	0.47
245.06	0.5	0.72
245.21	0.8	1.10
250.07	0.2	0.34
250.19	0.3	0.44
258.94	0.4	0.60
259.14	1.3	1.93
260.13	0.2	0.36
313.24	0.2	0.33
323.25	0.3	0.39
353.24	0.3	0.43
370.35	0.2	0.26
383.28	1.0	1.41
387.18	0.2	0.33
387.32	0.3	0.44
389.82	0.2	0.26
398.25	1.3	1.97
399.29	0.4	0.60
412.25	0.3	0.38
415.34	5.1	7.47
416.21	0.3	0.50
416.39	0.2	0.35
431.29	2.0	2.86
432.38	0.3	0.44
433.30	68.3	100.00

434.30	7.7	11.30
437.83	0.3	0.49
442.22	0.4	0.52
443.44	0.2	0.36
455.24	0.2	0.32
472.33	8.0	11.77
473.27	0.8	1.12
473.46	0.2	0.32
500.22	0.3	0.50
515.20	0.3	0.46
516.47	0.2	0.36
556.48	0.2	0.31
558.24	1.9	2.76
586.40	37.2	54.48
587.38	6.1	8.98
589.40	0.7	1.09
614.48	0.3	0.49
618.43	7.5	11.03
619.33	0.4	0.58
619.46	0.3	0.48
652.34	0.2	0.26
660.33	2.0	2.99
660.54	1.9	2.77
661.53	0.4	0.61
661.69	0.2	0.25

SPECTRUM - MS

6-26-13_HMG37_1011_MS4_1283_646_01.raw

ITMS + p ESI E Full ms4 1011.60@cid35.00 1284.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-50

RT: 0.00-14.08

AV: 50

m/z Intensity Relative

194.08	0.2	1.03
204.04	0.3	1.61
211.13	0.2	1.44
218.09	0.2	1.16
220.07	0.5	2.85
227.10	1.9	11.58
229.12	0.9	5.66
230.15	0.2	1.16
236.09	1.5	8.87
243.07	0.2	1.20
245.12	5.2	31.06
246.12	0.3	1.70
287.15	0.4	2.53
292.14	0.2	1.07
315.21	0.7	4.06
343.23	0.5	3.27
352.11	0.3	2.02

354.15	0.2	0.90
366.31	0.3	1.55
367.23	0.2	1.47
368.25	0.5	3.05
369.22	0.3	1.67
378.26	0.3	1.80
380.26	0.7	4.23
382.26	1.5	9.27
383.31	0.1	0.73
384.23	1.7	10.05
385.22	12.4	74.58
386.33	0.6	3.32
398.20	0.7	3.99
408.30	0.2	1.23
424.25	1.6	9.75
425.44	0.1	0.76
433.27	0.2	1.27
440.28	3.1	18.40
441.25	0.3	1.84
442.29	4.5	27.08
443.31	0.4	2.56
458.29	2.1	12.73
459.29	0.2	1.15
569.13	0.2	1.09
572.37	16.6	100.00
573.37	4.3	25.85
574.44	0.1	0.73
575.39	3.9	23.36
576.40	0.5	3.00
586.52	0.2	1.15
604.43	0.7	4.34
646.43	1.4	8.52
647.47	0.1	0.76

HMG 41 Mass spectral peak lists

SPECTRUM - MS

6-27-13_HMG41_1149_MS2_01.raw

ITMS + p ESI E Full ms2 1149.00@cid35.00 [315.00-2000.00]

Scan #: 1-20

RT: 0.00-1.90

AV: 20

m/z	Intensity	Relative
486.31	1702.9	14.38
487.32	326.3	2.76
534.38	143.5	1.21
646.40	165.3	1.40
685.45	2022.5	17.08
685.97	1243.7	10.50
686.46	434.9	3.67
706.45	158.5	1.34
724.49	368.9	3.12
761.99	139.7	1.18
799.01	765.5	6.46
799.52	558.5	4.72
800.01	266.5	2.25
814.03	211.8	1.79
814.52	167.2	1.41
917.10	11841.5	100.00
917.60	9828.1	83.00
918.10	4342.0	36.67
918.62	380.8	3.22
954.29	282.9	2.39
993.61	348.3	2.94
994.10	310.5	2.62
994.62	162.9	1.38
1012.28	439.4	3.71
1030.66	3188.4	26.93
1031.16	2961.1	25.01
1031.66	1562.7	13.20
1032.29	282.7	2.39
1045.65	414.2	3.50
1046.13	382.6	3.23
1046.63	219.0	1.85
1054.65	212.9	1.80
1055.15	163.4	1.38
1109.65	255.0	2.15
1120.68	128.1	1.08
1148.71	3559.1	30.06
1149.21	3944.4	33.31
1149.70	2593.5	21.90
1150.21	260.3	2.20
1187.71	340.4	2.87
1188.72	177.7	1.50

1347.82	1490.8	12.59
1348.82	931.5	7.87
1349.83	301.1	2.54
1574.95	471.9	3.99
1575.95	353.8	2.99
1576.97	137.7	1.16
1811.18	2432.2	20.54
1812.19	1998.2	16.87
1813.20	874.0	7.38

SPECTRUM - MS

6-27-13_HMG41_1149_MS3_1109_01.raw

ITMS + p ESI E Full ms3 1149.00@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-20

RT: 0.00-3.63

AV: 20

m/z	Intensity	Relative
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343.20	0.1	0.31
382.36	0.1	0.49
385.22	1.0	3.58
398.27	0.4	1.35
412.30	0.1	0.39
424.25	0.1	0.40
440.26	0.2	0.54
442.37	0.1	0.30
458.22	0.1	0.38
472.28	0.3	1.18
486.30	4.9	17.30
487.34	0.7	2.60
572.33	0.6	2.18
573.32	0.2	0.55
575.34	0.4	1.47
576.45	0.1	0.30
598.26	0.2	0.86
598.43	0.2	0.54
599.35	0.1	0.29
646.39	28.4	100.00
647.41	5.6	19.58
685.33	0.1	0.29
690.37	0.3	1.11
690.57	0.1	0.29
708.51	1.1	3.74
709.42	0.5	1.92
778.45	0.2	0.60
778.57	0.1	0.38
799.44	2.6	9.09
799.74	0.3	1.12
800.43	0.4	1.43
800.62	0.2	0.61
830.47	0.1	0.30

843.53	0.1	0.38
873.52	19.0	66.65
874.52	5.2	18.25
891.65	0.1	0.31
903.62	0.1	0.48
905.49	1.0	3.49
906.43	0.1	0.30
916.07	0.1	0.33
921.42	0.1	0.52
921.67	0.2	0.69
931.07	0.1	0.27
1015.60		0.3 0.90
1035.62		0.3 1.04
1051.83		0.1 0.27
1067.56		0.3 0.96
1109.64		7.7 26.99
1110.63		4.4 15.32

SPECTRUM - MS

6-27-13_HMG41_1149_MS4_1109_486_01.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1110.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-10.18

AV: 50

m/z Intensity Relative

154.99	0.0	2.83
164.27	0.0	0.84
176.04	0.0	0.88
180.10	0.0	0.97
208.07	0.0	3.90
224.41	0.0	1.70
227.25	0.0	1.33
232.32	0.0	0.75
241.14	0.0	6.84
241.78	0.0	1.15
249.95	0.0	1.28
250.17	0.0	2.15
250.79	0.0	1.07
251.15	0.0	1.17
251.84	0.0	0.77
252.16	0.0	10.17
259.13	0.4	85.09
260.12	0.0	10.57
268.09	0.0	2.57
292.43	0.0	1.36
316.28	0.0	1.46
329.16	0.0	8.44
329.36	0.0	4.89
330.25	0.0	1.32
338.55	0.0	0.78

341.16	0.0	1.05
345.49	0.0	0.74
370.21	0.0	2.25
376.12	0.0	1.70
382.13	0.0	2.50
382.32	0.0	1.43
383.74	0.0	1.11
383.99	0.0	0.89
384.17	0.0	3.76
409.41	0.0	1.77
412.25	0.5	100.00
413.16	0.0	8.54
413.37	0.0	5.07
444.35	0.1	28.19
445.35	0.0	8.68
454.29	0.0	1.50
455.96	0.0	0.77
456.33	0.0	0.96
456.50	0.0	1.98
486.07	0.0	1.83
486.40	0.0	10.86
486.96	0.0	2.35
487.26	0.0	3.45
487.51	0.0	0.89
498.45	0.0	1.68

SPECTRUM - MS

6-27-13_HMG41_1149_MS4_1109_646_02.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1110.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-60

RT: 0.00-12.71

AV: 60

m/z Intensity Relative

194.07	0.0	0.64
204.02	0.0	1.23
211.08	0.0	1.14
219.95	0.0	0.57
227.09	0.3	11.59
228.07	0.0	0.54
229.11	0.1	4.25
230.11	0.0	0.57
236.09	0.2	8.39
243.00	0.0	1.06
243.23	0.0	0.59
245.12	0.8	28.50
287.18	0.0	1.36
311.24	0.0	0.74
315.22	0.1	4.11
316.22	0.0	0.67
324.14	0.0	1.29

343.20	0.1	3.11
353.27	0.0	0.91
366.06	0.0	0.83
366.23	0.1	2.37
367.17	0.1	2.17
368.24	0.1	2.80
369.20	0.0	1.25
371.19	0.0	1.05
378.22	0.1	4.79
380.22	0.1	4.75
382.24	0.2	7.90
384.27	0.1	4.59
385.20	2.6	100.00
386.24	0.2	5.84
392.18	0.0	0.55
397.26	0.0	0.59
398.20	0.0	1.81
424.27	0.2	6.43
433.30	0.0	1.61
440.26	0.6	21.90
441.24	0.1	2.62
442.27	0.5	18.79
443.30	0.1	3.12
458.28	0.3	10.05
572.35	2.1	79.72
573.34	0.6	23.23
574.35	0.1	1.95
574.54	0.0	0.58
575.37	0.8	30.67
576.38	0.1	4.94
604.47	0.1	3.70
646.39	0.6	23.40
647.35	0.1	2.79

SPECTRUM - MS

6-27-13_HMG41_1149_MS3_486_01.raw

ITMS + p ESI E Full ms3 1149.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-20

RT: 0.00-2.22

AV: 20

m/z Intensity Relative

168.18	0.3	0.33
178.08	0.8	0.77
208.08	5.3	5.01
211.07	0.3	0.24
218.10	0.4	0.33
220.09	0.3	0.27
241.09	4.6	4.37
242.18	0.4	0.37
250.12	9.4	8.94

251.12	0.9	0.81
252.14	12.0	11.44
253.21	0.6	0.61
257.09	0.8	0.76
257.26	0.5	0.51
259.13	99.6	94.84
260.15	7.5	7.13
268.15	4.3	4.11
281.15	1.2	1.17
282.13	0.6	0.62
301.21	0.6	0.56
312.21	0.4	0.37
314.19	0.9	0.82
329.20	4.2	4.00
330.25	0.6	0.53
341.15	1.2	1.10
356.21	0.3	0.32
356.37	0.5	0.52
370.30	0.5	0.43
380.23	0.4	0.41
382.35	1.3	1.27
384.21	3.8	3.65
385.22	0.3	0.26
394.31	0.3	0.32
408.38	0.3	0.27
410.24	0.9	0.83
412.26	105.0	100.00
413.26	18.6	17.74
414.32	0.6	0.54
415.27	2.0	1.94
426.33	0.9	0.87
427.23	0.7	0.62
440.21	1.7	1.58
444.30	59.8	56.93
445.29	9.0	8.60
454.42	0.4	0.42
455.30	0.3	0.24
456.34	2.9	2.73
457.37	1.2	1.16
486.30	101.2	96.36
487.31	22.2	21.12

HMG 45 Mass spectral peak lists

SPECTRUM - MS

10-23-13_HMG45_1062_MS2_01.raw

ITMS + p ESI E Full ms2 1062.40@cid35.00 [290.00-2000.00]

Scan #: 1-20

RT: 0.00-1.60

AV: 20

m/z	Intensity	Relative
444.27	224.9	1.18
486.27	7201.0	37.91
487.28	1541.0	8.11
488.29	275.1	1.45
534.33	571.5	3.01
598.33	260.7	1.37
738.42	5583.8	29.40
739.43	1993.1	10.49
740.43	513.5	2.70
829.98	18993.3	100.00
830.47	14735.0	77.58
830.97	7018.8	36.95
831.47	2308.0	12.15
831.97	637.4	3.36
906.47	250.8	1.32
906.97	228.5	1.20
921.46	895.4	4.71
922.46	396.3	2.09
943.50	732.3	3.86
944.01	705.1	3.71
944.51	465.2	2.45
952.49	441.1	2.32
952.99	427.3	2.25
953.51	235.2	1.24
983.52	412.6	2.17
984.54	209.1	1.10
1008.52	252.0	1.33
1009.02	251.9	1.33
1012.03	262.9	1.38
1012.52	272.2	1.43
1045.54	367.1	1.93
1046.01	388.6	2.05
1046.53	370.9	1.95
1047.04	233.8	1.23
1061.60	3478.4	18.31
1062.07	3638.7	19.16
1062.56	2320.4	12.22
1063.06	1157.1	6.09
1063.54	523.5	2.76
1173.57	3420.2	18.01
1174.58	2010.7	10.59

1175.59	718.9	3.79	
1187.61	244.3	1.29	
1384.66	2083.6		10.97
1385.67	1322.3		6.96
1386.66	505.8	2.66	
1636.82	5276.9		27.78
1637.83	4135.2		21.77
1638.84	1966.2		10.35
1639.84	624.4	3.29	

SPECTRUM - MS

10-23-13_HMG45_1062_MS3_830_01.raw

ITMS + p ESI E Full ms3 1062.40@cid35.00 830.40@cid35.00 [225.00-1800.00]

Scan #: 1-20

RT: 0.00-2.17

AV: 20

m/z	Intensity	Relative
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444.26	50.8	4.55
458.23	50.3	4.51
464.23	13.4	1.20
472.25	17.7	1.58
486.27	1007.2	90.22
487.28	211.1	18.91
488.29	31.1	2.79
514.28	15.3	1.37
534.33	31.1	2.78
598.33	102.8	9.21
598.85	54.2	4.85
599.34	20.7	1.85
630.33	30.5	2.73
676.35	32.9	2.95
718.35	44.4	3.98
719.36	16.0	1.43
720.92	27.5	2.46
721.41	23.5	2.11
738.43	563.0	50.43
739.43	197.2	17.67
740.43	44.4	3.97
760.37	24.5	2.19
776.95	19.1	1.71
777.45	17.4	1.56
780.44	26.6	2.38
780.94	19.4	1.74
813.95	31.9	2.86
814.45	28.5	2.56
814.96	47.9	4.29
815.48	34.9	3.13
815.98	14.5	1.30
829.99	255.3	22.87
830.48	216.2	19.36

830.98	100.6	9.01	
831.48	34.7	3.11	
921.47	227.2	20.35	
922.48	94.0	8.42	
923.49	34.8	3.11	
983.54	79.0	7.08	
984.55	36.3	3.26	
1065.49		80.0	7.16
1066.47		38.4	3.44
1173.59	1116.3		100.00
1174.60	619.0	55.45	
1175.61	198.2	17.76	
1176.62	34.2	3.06	
1187.64	27.4	2.46	
1188.63	15.8	1.42	
1636.85	34.4	3.08	
1637.85	28.8	2.58	

SPECTRUM - MS

10-23-13_HMG45_1062_MS4_830_1174_01.raw

ITMS + p ESI E Full ms4 1062.40@cid35.00 830.40@cid35.00 1174.00@cid35.00 [320.00-1200.00]

Scan #: 1-20

RT: 0.00-1.81

AV: 20

m/z	Intensity	Relative
384.28	0.9	0.11
435.25	5.2	0.68
444.25	0.5	0.06
447.18	0.7	0.09
447.35	0.5	0.06
456.31	1.2	0.16
458.23	3.5	0.45
470.37	0.5	0.07
472.30	1.0	0.13
474.33	1.4	0.18
486.29	5.8	0.76
487.35	0.9	0.12
492.37	0.5	0.06
502.31	1.5	0.19
516.33	2.1	0.27
517.37	0.5	0.07
534.33	119.3	15.60
535.35	22.7	2.97
536.35	2.6	0.33
562.35	1.2	0.16
590.35	2.4	0.31
591.28	0.5	0.07
620.39	0.6	0.07
639.37	14.3	1.87
640.39	2.8	0.37

665.31	0.5	0.07	
690.39	1.4	0.18	
706.49	1.6	0.20	
707.45	0.6	0.08	
720.44	0.7	0.10	
724.43	14.8	1.93	
725.41	3.7	0.48	
738.43	764.8	100.00	
739.43	192.5	25.17	
740.44	29.4	3.85	
882.48	0.5	0.06	
983.55	43.1	5.64	
984.57	14.8	1.93	
985.53	3.0	0.40	
1067.60		1.3	0.17
1074.53		4.8	0.63
1075.56		2.1	0.27
1141.58		4.4	0.58
1142.44		0.9	0.12
1142.64		1.4	0.18
1143.53		0.9	0.11
1143.72		0.7	0.10
1173.60		59.1	7.72
1174.60		30.9	4.04
1175.62		10.9	1.43

SPECTRUM - MS

10-23-13_HMG45_1062_MS3_1384_01.raw

ITMS + p ESI E Full ms3 1062.40@cid35.00 1385.40@cid35.00 [380.00-1400.00]

Scan #: 1-50

RT: 0.00-8.25

AV: 50

m/z Intensity Relative

458.23	68.3	10.63
459.24	10.0	1.56
486.26	96.5	15.01
487.28	14.5	2.26
488.25	1.8	0.28
546.23	2.0	0.31
546.43	2.6	0.40
574.34	8.8	1.37
620.33	3.3	0.52
676.36	11.8	1.84
677.27	1.6	0.24
677.46	1.5	0.24
694.33	7.2	1.12
695.26	1.5	0.23
703.44	1.7	0.26
764.40	21.5	3.34
765.37	5.8	0.90

815.35	1.6	0.25	
847.44	2.7	0.42	
850.41	3.5	0.55	
879.50	3.3	0.51	
889.46	5.1	0.79	
890.45	2.4	0.38	
921.46	642.6	100.00	
922.47	191.3	29.77	
923.48	31.1	4.84	
935.53	3.1	0.48	
1139.40		2.3	0.36
1140.59		1.5	0.23
1157.56		11.4	1.77
1158.66		3.5	0.55
1166.62		4.3	0.67
1167.52		2.8	0.43
1227.57		48.7	7.57
1228.59		21.2	3.30
1229.71		2.1	0.33
1278.59		7.1	1.10
1279.62		4.3	0.68
1313.61		2.8	0.44
1342.62		4.6	0.72
1342.82		1.6	0.25
1343.67		3.1	0.48
1352.66		8.0	1.24
1353.75		1.5	0.24
1354.65		8.6	1.34
1355.70		2.6	0.41
1384.65		44.7	6.96
1385.56		16.8	2.62
1385.78		15.2	2.36
1386.68		10.2	1.59

SPECTRUM - MS

10-23-13_HMG45_1062_MS4_1384_486_01.raw

ITMS + p ESI E Full ms4 1062.40@cid35.00 1385.40@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-8.09

AV: 50

m/z	Intensity	Relative
180.05	0.0	0.42
180.17	0.0	0.26
188.13	0.0	0.33
204.07	0.0	0.21
220.08	0.3	3.12
227.09	0.1	0.60
236.04	0.0	0.28
241.08	0.5	5.15
242.11	0.0	0.42

250.07	0.0	0.18
257.05	0.0	0.35
259.11	1.8	17.50
260.15	0.1	0.94
268.11	1.2	11.66
269.14	0.1	0.91
297.16	0.1	0.56
301.17	0.1	0.76
315.18	0.0	0.28
329.18	3.8	37.73
330.16	0.4	4.46
331.26	0.0	0.19
337.33	0.0	0.19
343.76	0.0	0.24
353.20	0.1	0.75
380.19	0.0	0.33
382.21	0.0	0.41
384.27	0.0	0.18
394.25	0.0	0.42
410.20	0.0	0.38
411.83	0.0	0.31
412.19	0.2	1.91
413.14	0.0	0.25
415.24	0.2	1.68
416.23	0.0	0.43
426.19	0.0	0.20
440.14	0.0	0.30
440.32	0.0	0.21
443.87	0.1	0.97
444.26	10.0	100.00
445.26	1.7	16.73
446.25	0.2	1.93
454.24	0.1	0.67
455.19	0.0	0.18
456.24	0.5	4.76
457.26	0.0	0.48
470.02	0.1	0.85
478.37	0.1	0.57
486.27	1.4	13.53
487.17	0.2	1.55
488.35	0.1	0.50

SPECTRUM - MS

10-23-13_HMG45_1062_MS4_1384_921_01.raw

ITMS + p ESI E Full ms4 1062.40@cid35.00 1385.40@cid35.00 922.00@cid35.00 [250.00-1000.00]

Scan #: 1-50

RT: 0.00-4.86

AV: 50

m/z	Intensity	Relative
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268.14	0.6	0.79
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426.19	0.6	0.74
444.26	1.6	1.99
454.24	0.4	0.51
458.23	81.1	100.00
459.24	10.9	13.42
460.24	0.8	0.99
472.25	0.4	0.48
486.27	57.6	71.01
487.27	8.6	10.56
488.26	0.6	0.73
504.27	0.4	0.51
546.28	2.3	2.83
547.31	0.4	0.44
574.32	5.3	6.57
575.33	1.0	1.25
620.31	2.3	2.84
621.33	0.4	0.52
646.34	1.3	1.59
676.35	11.4	14.03
677.35	2.4	2.97
678.33	0.4	0.50
692.26	0.9	1.16
692.43	0.7	0.82
694.35	7.0	8.66
695.36	1.5	1.89
703.38	2.0	2.43
704.45	0.4	0.46
764.41	17.9	22.04
765.39	4.7	5.86
766.40	0.5	0.65
815.40	2.4	2.92
816.34	0.7	0.84
816.51	0.4	0.55
817.41	0.4	0.44
829.33	0.8	1.00
829.53	0.7	0.82
847.40	3.6	4.41
848.41	2.3	2.86
850.42	3.2	3.94
851.43	1.1	1.38
879.44	3.5	4.34
880.47	1.1	1.35
889.42	7.9	9.73
890.43	2.2	2.76
891.44	3.9	4.79
892.43	1.0	1.20
921.46	9.9	12.24
922.48	3.7	4.53
923.46	0.4	0.50

SPECTRUM - MS

10-23-13_HMG45_1062_MS5_1384_921_486_01.raw

ITMS + p ESI E Full ms5 1062.40@cid35.00 1385.40@cid35.00 922.00@cid35.00 487.00@cid35.00

[130.00-500.00]

Scan #: 1-50

RT: 0.00-15.53

AV: 50

m/z	Intensity	Relative
178.03	0.0	0.13
179.96	0.0	0.40
180.10	0.0	0.25
181.12	0.0	0.11
188.02	0.0	0.31
211.13	0.0	0.13
213.13	0.0	0.22
218.06	0.0	0.12
220.05	0.1	2.11
227.12	0.0	0.32
235.95	0.0	0.11
236.06	0.0	0.16
241.11	0.1	3.60
242.09	0.0	0.39
243.13	0.0	0.12
250.10	0.0	0.12
259.10	0.5	13.57
260.12	0.0	0.76
268.13	0.3	7.62
269.24	0.0	0.27
281.96	0.0	0.24
293.91	0.0	0.15
297.17	0.0	0.44
301.09	0.0	1.00
329.18	1.0	25.56
330.20	0.1	2.71
339.23	0.0	0.15
353.14	0.0	0.41
380.08	0.0	0.29
382.24	0.0	0.23
394.18	0.0	0.25
410.22	0.0	0.32
412.26	0.1	1.45
413.13	0.0	0.12
413.31	0.0	0.15
415.23	0.1	1.54
415.46	0.0	0.14
416.26	0.0	0.42
431.23	0.0	0.31
440.33	0.0	0.21
444.25	3.9	100.00
445.26	0.5	13.01
446.30	0.0	0.68

454.27	0.0	0.20
454.43	0.0	0.15
456.31	0.1	2.02
457.33	0.0	0.38
486.27	0.5	12.65
487.26	0.1	1.89
488.33	0.0	0.13

SPECTRUM - MS

10-23-13_HMG45_1062_MS5_1384_921_458_01.raw

ITMS + p ESI E Full ms5 1062.40@cid35.00 1385.40@cid35.00 922.00@cid35.00 459.00@cid35.00
[125.00-500.00]

Scan #: 1-51

RT: 0.00-13.95

AV: 51

m/z	Intensity	Relative
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149.05	0.0	0.51
157.00	0.0	0.41
162.01	0.0	0.21
180.06	0.0	0.96
181.10	0.0	0.24
188.04	0.0	0.80
194.04	0.1	1.56
203.99	0.1	1.78
213.05	0.4	10.19
214.07	0.0	0.80
217.99	0.0	0.27
218.15	0.0	0.19
220.07	0.2	4.99
222.08	0.0	0.23
229.10	0.0	0.42
231.05	0.5	12.25
232.07	0.0	0.69
236.08	0.2	5.89
237.08	0.0	0.26
238.12	0.0	0.31
250.03	0.0	0.51
268.12	3.8	100.00
269.11	0.3	6.78
273.05	0.1	1.37
301.13	0.9	24.72
302.15	0.1	1.57
303.09	0.0	0.32
324.11	0.0	0.58
352.18	0.0	0.53
353.21	0.0	0.31
354.27	0.0	0.38
366.15	0.0	0.95
366.33	0.0	0.32
384.15	0.1	3.60

385.05	0.0	0.65
385.24	0.1	1.34
386.27	0.0	0.20
394.17	0.0	0.21
398.30	0.0	0.19
416.31	0.0	0.93
417.24	0.0	0.20
426.11	0.1	3.52
426.28	0.1	3.35
427.21	0.1	1.40
428.19	0.2	4.64
429.25	0.0	0.56
430.19	0.0	0.20
458.22	3.6	93.61
459.25	0.4	10.86
460.28	0.0	0.65

HMG 47 Mass spectral peak lists

SPECTRUM - MS

8-22-13_HMG47_1148_MS2_01.raw

ITMS + p ESI E Full ms2 1149.00@cid35.00 [315.00-2000.00]

Scan #: 1-20

RT: 0.00-1.57

AV: 20

m/z	Intensity	Relative
486.30	2668.1	12.20
487.30	491.9	2.25
534.36	148.7	0.68
646.36	823.9	3.77
647.37	202.5	0.93
685.42	2235.5	10.22
685.93	1454.8	6.65
686.43	490.8	2.24
706.43	348.6	1.59
724.46	686.0	3.14
725.44	243.4	1.11
813.98	762.2	3.49
814.48	684.3	3.13
814.98	333.7	1.53
917.06	21865.3	100.00
917.55	18318.6	83.78
918.05	8353.6	38.20
918.55	1152.7	5.27
1039.57	198.5	0.91
1040.09	181.2	0.83
1045.60	1039.6	4.75
1046.07	1018.3	4.66
1046.57	585.4	2.68
1054.59	307.2	1.40
1055.10	308.1	1.41
1055.61	159.1	0.73
1079.53	157.9	0.72
1109.58	523.9	2.40
1110.58	245.0	1.12
1132.62	149.6	0.68
1133.10	161.8	0.74
1133.62	141.4	0.65
1148.66	4029.8	18.43
1149.15	4438.1	20.30
1149.62	3032.2	13.87
1150.13	656.1	3.00
1187.66	1736.8	7.94
1188.67	953.1	4.36
1189.68	273.2	1.25
1347.73	775.3	3.55
1348.73	526.1	2.41

1349.73	162.9	0.74	
1604.89	386.2	1.77	
1605.89	324.9	1.49	
1606.90	264.8	1.21	
1607.88	125.6	0.57	
1811.06	2580.9		11.80
1812.07	2211.0		10.11
1813.08	1001.6		4.58
1814.07	153.1	0.70	

SPECTRUM - MS

8-22-13_HMG47_1148_MS3_1109_01.raw

ITMS + p ESI E Full ms3 1149.00@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-20

RT: 0.00-1.41

AV: 20

m/z Intensity Relative

368.31	0.4	0.22
385.17	5.4	2.99
440.15	1.1	0.59
440.37	0.6	0.35
442.34	0.7	0.40
444.30	1.2	0.65
454.25	0.7	0.40
458.16	0.6	0.31
486.30	47.2	26.21
487.32	6.4	3.57
572.06	0.8	0.46
572.27	1.9	1.04
572.46	1.7	0.93
573.42	1.1	0.58
575.29	0.7	0.39
575.45	1.0	0.55
576.34	0.4	0.21
604.40	0.7	0.40
646.36	180.3	100.00
647.37	33.4	18.55
660.42	0.4	0.22
690.20	0.7	0.38
690.41	1.9	1.05
706.23	0.6	0.34
706.40	0.6	0.36
708.39	12.4	6.91
709.31	1.2	0.69
709.47	1.0	0.54
778.38	1.1	0.62
873.49	0.7	0.37
879.50	0.4	0.21
903.38	1.1	0.58
903.59	0.4	0.20

904.48	0.4	0.23
905.44	5.7	3.14
906.51	1.5	0.81
921.54	0.4	0.25
1003.59		0.6 0.31
1007.64		0.4 0.22
1035.41		1.0 0.58
1035.59		0.6 0.34
1038.55		0.6 0.35
1067.63		0.9 0.50
1068.41		0.5 0.26
1068.57		0.4 0.21
1077.64		1.7 0.94
1079.65		1.3 0.71
1080.56		0.4 0.20
1109.58		25.2 14.00
1110.58		14.0 7.77

SPECTRUM - MS

8-22-13_HMG47_1148_MS4_1109_486_02.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1110.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-8.47

AV: 50

m/z	Intensity	Relative
179.97	0.0	0.47
180.11	0.0	0.46
188.07	0.0	0.14
211.12	0.0	0.45
213.16	0.0	0.13
218.08	0.0	0.20
220.09	0.3	4.49
221.06	0.0	0.55
227.09	0.0	0.61
236.11	0.0	0.40
241.07	0.3	4.70
242.18	0.0	0.14
250.11	0.0	0.54
257.09	0.0	0.36
259.11	1.3	19.42
260.07	0.1	0.92
260.22	0.0	0.58
268.13	0.9	14.07
269.09	0.1	0.96
282.12	0.0	0.16
297.20	0.1	0.92
298.21	0.0	0.18
301.14	0.1	1.76
315.21	0.0	0.17
329.18	3.0	45.36

330.17	0.4	5.62
353.08	0.0	0.19
353.28	0.0	0.35
367.24	0.0	0.20
380.17	0.0	0.53
385.24	0.0	0.17
394.18	0.0	0.42
399.26	0.0	0.22
410.30	0.0	0.31
411.93	0.0	0.14
412.22	0.2	2.31
415.21	0.1	1.35
415.37	0.0	0.59
416.17	0.0	0.14
427.19	0.0	0.27
440.07	0.0	0.15
443.02	0.0	0.14
444.27	6.5	100.00
445.27	1.0	15.19
454.24	0.1	0.78
455.24	0.0	0.14
456.25	0.4	5.80
457.32	0.0	0.71
486.28	1.4	21.92
487.31	0.2	2.78

SPECTRUM - MS

8-22-13_HMG47_1148_MS4_1109_646_02.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1110.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-50

RT: 0.00-9.13

AV: 50

m/z Intensity Relative

204.02	0.3	1.80
211.06	0.2	0.99
218.07	0.2	1.11
220.07	0.3	2.03
227.07	1.9	11.92
228.07	0.1	0.72
229.10	0.9	5.64
236.07	1.4	8.65
237.09	0.1	0.67
243.08	0.1	0.83
245.09	4.8	30.29
246.11	0.3	2.03
287.11	0.3	2.06
292.08	0.1	0.93
311.09	0.1	0.71
315.16	0.6	3.76
343.17	0.7	4.26

353.15	0.2	1.00
366.16	0.4	2.61
367.19	0.4	2.39
368.19	0.6	3.69
369.18	0.3	1.66
378.18	0.6	3.64
380.20	0.7	4.51
381.20	0.1	0.62
382.22	1.4	8.83
383.22	0.2	1.57
384.19	1.4	8.63
385.17	15.8	100.00
386.19	1.7	11.04
398.26	0.2	1.51
408.18	0.2	1.00
424.21	1.3	8.32
425.25	0.1	0.88
433.25	0.2	1.11
440.21	3.5	22.14
441.23	0.5	3.45
442.25	3.4	21.34
443.23	0.5	2.94
458.23	1.5	9.55
459.25	0.3	1.77
572.30	13.9	87.74
573.31	4.6	28.99
574.43	0.1	0.85
575.32	4.6	29.32
576.33	1.0	6.24
604.34	0.9	5.93
605.41	0.1	0.87
646.34	4.3	27.42
647.36	1.0	6.22

SPECTRUM - MS

8-22-13_HMG47_1148_MS3_486_02.raw

ITMS + p ESI E Full ms3 1149.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-13.30

AV: 50

m/z Intensity Relative

178.04	0.9	0.14
180.03	4.6	0.71
188.04	2.6	0.41
194.04	0.8	0.13
204.02	1.1	0.17
211.07	1.8	0.28
213.09	1.5	0.24
218.05	1.4	0.21
220.08	24.5	3.84

221.08	2.3	0.36
227.07	3.5	0.54
236.08	1.7	0.26
241.10	29.3	4.58
242.11	2.7	0.42
250.11	1.5	0.24
257.10	1.7	0.27
259.11	121.8	19.03
260.12	11.2	1.75
268.13	81.2	12.69
269.13	8.2	1.29
297.15	5.3	0.84
298.14	0.7	0.11
301.14	8.0	1.26
302.14	0.9	0.15
314.17	0.7	0.12
315.16	1.4	0.22
329.19	262.2	40.97
330.20	35.3	5.52
352.20	0.7	0.11
353.19	3.1	0.48
380.20	1.5	0.23
382.22	1.9	0.30
384.22	1.2	0.19
394.23	2.7	0.42
410.22	2.6	0.41
412.22	12.6	1.97
413.23	2.6	0.40
415.25	10.6	1.66
416.26	2.0	0.31
426.25	1.7	0.27
431.22	1.5	0.23
440.23	1.2	0.19
444.27	640.1	100.00
445.27	129.0	20.16
454.25	7.0	1.10
455.26	1.5	0.24
456.27	38.6	6.03
457.28	8.3	1.29
486.28	105.5	16.48
487.29	22.2	3.47

HMG 49 Mass spectral peak lists

SPECTRUM - MS

4-26-13_HMO-49_1148_MS2_01.raw

ITMS + p ESI E Full ms2 1149.40@cid35.00 [315.00-2000.00]

Scan #: 1-20

RT: 0.00-1.74

AV: 20

m/z	Intensity	Relative
486.08	15870.9	12.61
487.09	3241.3	2.57
646.13	1389.2	1.10
685.17	15342.0	12.19
685.68	11013.6	8.75
686.17	4660.2	3.70
686.70	1215.9	0.97
706.15	1402.6	1.11
724.17	2917.7	2.32
761.65	1282.3	1.02
798.68	6167.4	4.90
799.16	5069.1	4.03
799.64	2696.5	2.14
813.65	1654.5	1.31
814.15	1527.9	1.21
916.69	125901.3	100.00
917.16	113571.0	90.21
917.67	57558.1	45.72
918.19	18512.8	14.70
993.17	2866.6	2.28
993.67	3279.2	2.60
994.17	1954.0	1.55
1030.19	33644.4	26.72
1030.68	33787.5	26.84
1031.18	19999.7	15.89
1031.70	7734.8	6.14
1045.18	4526.6	3.60
1045.68	4368.6	3.47
1046.18	2885.9	2.29
1046.69	1215.2	0.97
1054.17	1967.2	1.56
1054.66	2011.5	1.60
1109.14	2528.7	2.01
1110.15	1368.9	1.09
1148.24	19809.7	15.73
1148.71	22164.2	17.60
1149.18	14879.7	11.82
1149.68	7898.4	6.27
1187.19	3470.7	2.76
1188.19	2235.8	1.78
1347.24	12815.3	10.18

1348.24	8906.8	7.07
1349.22	3468.9	2.76
1574.27	4090.5	3.25
1575.26	3419.6	2.72
1576.28	1602.7	1.27
1810.32	26018.9	20.67
1811.33	22990.9	18.26
1812.33	11291.3	8.97
1813.32	3410.6	2.71

SPECTRUM - MS

4-26-13_HMO-49_1148_MS3_1109_01.raw

ITMS + p ESI E Full ms3 1149.40@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-50

RT: 0.00-6.52

AV: 50

m/z Intensity Relative

384.05	1.1	0.37
385.05	9.8	3.26
386.08	1.3	0.42
398.12	1.4	0.48
412.07	2.0	0.68
440.01	2.4	0.81
442.06	2.1	0.71
454.03	1.0	0.32
458.09	2.3	0.75
470.07	1.0	0.32
472.03	2.4	0.81
486.07	51.5	17.12
487.08	7.8	2.59
572.09	7.0	2.34
573.10	2.6	0.86
575.12	4.1	1.35
598.06	5.4	1.80
599.08	1.4	0.47
646.11	301.1	100.00
647.12	76.8	25.52
660.09	1.0	0.34
690.06	2.9	0.95
691.09	0.8	0.27
708.08	23.7	7.88
709.10	6.2	2.07
778.12	2.1	0.70
779.13	1.0	0.32
799.10	26.7	8.87
800.11	9.9	3.28
873.14	197.2	65.50
874.15	74.7	24.82
875.22	1.0	0.35
879.14	0.9	0.31

891.11	2.1	0.71
903.04	2.7	0.91
904.11	1.4	0.45
905.09	11.3	3.77
906.11	4.3	1.42
916.65	1.2	0.40
917.16	1.1	0.38
921.18	2.1	0.70
922.19	1.1	0.36
1015.17		8.7 2.88
1015.67		4.8 1.60
1035.14		2.8 0.95
1036.02		0.8 0.28
1067.17		3.5 1.17
1068.18		2.3 0.75
1109.15		24.6 8.18
1110.14		16.0 5.32

SPECTRUM - MS

4-26-13_HMO-49_1148_MS4_1109_486_01.raw

ITMS + p ESI E Full ms4 1149.40@cid35.00 1110.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-100

RT: 0.00-12.02

AV: 100

m/z	Intensity	Relative
177.92	0.0	1.33
179.97	0.0	0.62
196.06	0.0	0.43
208.09	0.1	2.20
208.92	0.0	0.68
210.93	0.0	0.44
220.06	0.0	1.23
241.01	0.2	5.80
242.01	0.0	0.55
250.04	0.2	5.93
250.93	0.0	0.87
252.01	0.3	10.39
257.01	0.0	0.57
259.01	3.1	97.77
259.77	0.0	0.60
260.00	0.1	4.24
263.84	0.0	0.39
267.99	0.2	7.24
268.17	0.1	1.58
297.05	0.0	0.40
300.98	0.1	2.19
320.99	0.0	0.46
329.05	0.4	11.89
330.04	0.1	1.74
351.95	0.0	0.39

352.85	0.0	1.27
356.99	0.0	0.62
379.83	0.0	0.63
380.05	0.0	0.66
380.95	0.0	1.26
381.18	0.0	0.75
382.07	0.0	1.04
382.24	0.0	0.45
384.02	0.0	0.83
385.11	0.0	0.45
393.93	0.0	1.44
412.08	3.2	100.00
413.07	0.5	15.68
414.99	0.0	0.55
424.13	0.0	0.47
444.09	2.1	64.52
445.12	0.4	11.34
454.00	0.0	0.51
455.16	0.0	0.81
456.02	0.0	1.02
456.16	0.0	0.94
486.12	0.4	11.74
486.92	0.0	1.13
487.08	0.0	0.92
487.23	0.0	0.86

SPECTRUM - MS

4-26-13_HMO-49_1148_MS4_1109_646_02.raw

ITMS + p ESI E Full ms4 1149.40@cid35.00 1110.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-100

RT: 0.00-14.42

AV: 100

m/z Intensity Relative

193.94	0.1	1.10
203.94	0.2	1.60
217.98	0.1	1.01
219.99	0.2	1.67
226.98	1.4	12.32
229.00	0.7	6.20
235.97	1.0	8.87
244.99	3.2	28.17
246.04	0.2	1.98
287.00	0.2	2.01
291.98	0.1	0.72
315.02	0.4	3.81
343.04	0.6	4.97
366.01	0.3	2.66
366.97	0.1	1.22
367.14	0.2	1.65
368.01	0.3	2.47

369.13	0.1	0.81
371.08	0.1	0.92
378.05	0.5	4.39
380.07	0.4	3.94
382.06	0.8	7.03
383.09	0.1	1.13
384.05	0.9	7.92
385.05	11.4	100.00
386.05	1.5	13.44
398.06	0.4	3.28
408.03	0.2	1.76
424.05	0.7	5.96
425.06	0.1	1.00
433.05	0.2	1.54
440.04	2.6	22.93
441.08	0.2	2.10
442.05	2.2	18.98
443.16	0.2	1.33
458.09	1.1	9.22
459.08	0.1	1.00
530.06	0.1	0.71
572.08	9.1	79.55
573.10	3.1	27.12
574.10	0.3	2.79
575.10	3.5	30.84
576.05	0.5	4.31
576.22	0.3	2.38
604.04	0.4	3.11
604.20	0.3	3.01
605.10	0.1	1.31
605.26	0.1	0.71
646.13	1.9	16.79
647.16	0.3	2.38

SPECTRUM - MS

4-26-13_HMO-49_1148_MS3_486_01.raw

ITMS + p ESI E Full ms3 1149.40@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-2.23

AV: 50

m/z Intensity Relative

177.93	14.5	1.08
207.99	73.5	5.47
208.92	4.5	0.33
209.07	4.7	0.35
217.90	8.3	0.62
218.07	5.7	0.42
220.02	6.6	0.49
241.00	66.5	4.95
242.06	5.2	0.39

249.96	102.5	7.63	
250.99	12.3	0.92	
252.00	171.8	12.79	
253.00	17.8	1.33	
256.95	18.0	1.34	
259.00	1338.4		99.65
260.01	108.9	8.11	
268.01	40.4	3.00	
300.84	3.5	0.26	
301.06	7.1	0.53	
312.05	3.7	0.27	
314.08	3.5	0.26	
329.04	74.8	5.57	
330.05	12.5	0.93	
338.03	4.0	0.30	
338.95	3.7	0.28	
341.02	7.9	0.59	
356.06	6.2	0.46	
370.14	5.0	0.37	
380.07	3.7	0.27	
382.06	14.6	1.09	
384.01	37.9	2.82	
384.97	3.4	0.25	
385.17	3.8	0.29	
394.02	4.0	0.29	
410.03	11.5	0.86	
411.06	3.5	0.26	
412.07	1343.2		100.00
413.04	252.5	18.80	
414.99	17.9	1.33	
415.14	11.0	0.82	
416.07	4.1	0.31	
426.12	4.3	0.32	
440.06	4.6	0.34	
444.10	739.6	55.07	
445.09	129.6	9.65	
454.08	8.9	0.67	
456.13	38.9	2.90	
457.16	7.5	0.56	
486.07	334.2	24.88	
487.09	60.6	4.51	

HMG 51 Mass spectral peak lists

SPECTRUM - MS

12-17-13_HMG51_1149_MS2_01.raw

ITMS + p ESI E Full ms2 1149.00@cid35.00 [315.00-2000.00]

Scan #: 1-20

RT: 0.00-2.05

AV: 20

m/z	Intensity	Relative
433.24	88.2	7.34
486.29	92.6	7.71
534.35	72.9	6.07
660.34	434.3	36.14
661.35	115.8	9.64
738.43	549.5	45.73
739.44	189.8	15.80
778.42	65.1	5.42
780.42	94.5	7.87
829.97	265.9	22.13
830.47	215.6	17.94
830.97	95.2	7.92
916.99	538.5	44.81
917.49	468.6	39.00
917.99	219.7	18.28
918.49	65.4	5.45
952.20	62.7	5.22
954.20	310.5	25.84
993.50	331.4	27.58
994.01	305.2	25.40
994.51	159.5	13.27
1012.13	460.9	38.35
1030.53	1201.8	100.00
1031.02	1083.3	90.15
1031.52	595.3	49.53
1032.11	343.0	28.54
1045.49	64.2	5.34
1046.01	61.8	5.14
1079.19	118.0	9.82
1080.19	61.4	5.11
1089.21	59.4	4.94
1090.18	89.7	7.47
1118.19	53.4	4.45
1148.08	181.8	15.13
1148.60	491.5	40.90
1149.08	581.0	48.35
1149.55	376.1	31.29
1150.06	185.1	15.40
1173.59	88.0	7.33
1174.58	50.5	4.20
1187.59	68.7	5.72

1558.72	264.9	22.04
1559.72	182.7	15.20
1560.70	71.0	5.91
1636.77	628.6	52.30
1637.78	468.5	38.99
1638.79	193.7	16.12
1639.80	53.1	4.42
1863.89	113.7	9.46
1864.91	97.9	8.14

SPECTRUM - MS

12-18-13_HMG51_1149_MS3_917_01.raw

ITMS + p ESI E Full ms3 1149.00@cid35.00 917.40@cid35.00 [250.00-2000.00]

Scan #: 1-20

RT: 0.00-1.93

AV: 20

m/z Intensity Relative

385.18	4.0	2.36
433.24	24.6	14.62
440.18	4.2	2.47
458.26	4.1	2.44
472.28	8.1	4.79
534.36	11.5	6.82
586.32	5.6	3.35
605.33	9.3	5.53
605.85	6.1	3.63
646.33	96.4	57.27
647.33	23.2	13.78
660.33	73.9	43.88
661.36	18.4	10.93
711.90	12.6	7.51
712.40	7.3	4.32
724.40	15.0	8.92
725.45	4.3	2.55
738.43	129.2	76.76
739.44	38.9	23.09
740.45	7.9	4.71
761.88	4.5	2.65
776.88	6.8	4.06
777.41	6.5	3.88
798.92	15.1	8.98
799.45	9.6	5.68
799.92	3.8	2.23
813.93	124.2	73.76
814.42	96.2	57.14
814.93	38.2	22.69
815.43	11.4	6.77
822.95	4.2	2.52
867.47	5.0	2.98
917.01	51.3	30.47

917.50	42.5	25.25	
917.99	21.4	12.71	
918.50	5.4	3.21	
1065.48		5.1	3.05
1079.41		6.1	3.61
1095.52		51.8	30.77
1096.51		22.3	13.28
1097.53		6.1	3.61
1109.53		6.7	4.01
1173.61		104.5	62.07
1174.62		49.8	29.61
1175.59		14.3	8.48
1187.61		168.3	100.00
1188.61		88.2	52.40
1189.56		17.8	10.56
1400.84		12.7	7.56
1401.69		15.2	9.05

SPECTRUM - MS

12-18-13_HMG51_1149_MS4_917_1173_01.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 917.40@cid35.00 1174.00@cid35.00 [320.00-1200.00]

Scan #: 1-20

RT: 0.00-2.74

AV: 20

m/z	Intensity	Relative
435.24	0.6	1.74
458.29	0.1	0.38
470.22	0.2	0.46
472.22	0.5	1.37
472.41	0.2	0.52
474.36	0.2	0.58
486.33	0.7	1.94
487.32	0.1	0.27
502.24	0.2	0.60
502.39	0.2	0.53
516.38	0.1	0.35
534.34	13.6	38.02
535.34	3.2	8.83
536.32	0.4	0.99
590.34	0.3	0.74
625.36	0.3	0.82
626.35	0.1	0.28
639.40	0.3	0.82
662.12	0.1	0.28
662.37	0.3	0.72
690.40	0.1	0.29
692.37	0.1	0.25
692.51	0.1	0.28
706.46	0.1	0.32
724.41	35.7	100.00

725.41	9.6	27.02	
726.43	1.2	3.31	
738.44	23.5	65.89	
739.45	6.2	17.47	
740.48	0.6	1.82	
969.55	0.8	2.33	
970.56	0.2	0.66	
970.70	0.2	0.46	
983.43	0.7	1.90	
983.62	0.8	2.31	
984.55	0.4	1.23	
1067.56		0.3	0.76
1068.45		0.1	0.39
1074.25		0.1	0.24
1074.54		0.5	1.43
1075.51		0.1	0.32
1075.69		0.1	0.24
1141.52		1.0	2.83
1142.53		0.3	0.83
1143.48		0.2	0.58
1143.67		0.1	0.33
1173.62		5.7	15.83
1174.64		2.6	7.22
1175.54		0.6	1.61
1175.70		0.4	0.99

SPECTRUM - MS

12-18-13_HMG51_1149_MS4_917_1187_01.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 917.40@cid35.00 1188.00@cid35.00 [325.00-1200.00]

Scan #: 1-21

RT: 0.00-2.77

AV: 21

m/z Intensity Relative

435.24	0.7	0.68
456.37	0.2	0.18
457.32	0.1	0.09
470.29	0.1	0.10
472.30	0.7	0.68
473.26	0.1	0.13
474.34	0.1	0.14
486.33	0.8	0.80
487.30	0.1	0.10
492.43	0.1	0.09
502.27	0.2	0.20
516.25	0.2	0.23
516.44	0.1	0.12
517.34	0.1	0.09
534.35	14.8	14.89
535.35	3.0	3.01
536.31	0.3	0.30

562.29	0.1	0.15	
590.39	0.2	0.21	
620.41	0.1	0.07	
621.44	0.1	0.08	
639.26	1.1	1.12	
639.44	0.9	0.87	
640.38	0.4	0.44	
665.39	0.1	0.09	
676.45	0.1	0.07	
688.35	0.1	0.07	
690.32	0.1	0.09	
690.50	0.1	0.08	
706.37	0.5	0.52	
707.56	0.1	0.08	
720.36	0.1	0.07	
738.43	99.1	100.00	
739.43	27.6	27.85	
740.44	3.2	3.28	
896.50	0.1	0.08	
965.49	0.3	0.26	
983.51	1.4	1.37	
984.55	0.4	0.40	
1081.61		0.1	0.10
1082.41		0.1	0.08
1088.54		0.6	0.60
1089.49		0.3	0.29
1089.73		0.1	0.08
1155.61		0.6	0.57
1156.53		0.4	0.37
1157.64		0.1	0.09
1187.61		16.1	16.29
1188.60		9.1	9.23
1189.60		2.6	2.63

SPECTRUM - MS

12-17-13_HMG51_1149_MS3_1558_01.raw

ITMS + p ESI E Full ms3 1149.00@cid35.00 1559.40@cid35.00 [425.00-1600.00]

Scan #: 1-20

RT: 0.00-1.89

AV: 20

m/z Intensity Relative

458.17	0.7	1.73
458.33	0.8	2.05
472.34	0.3	0.71
486.27	1.9	4.87
574.38	0.2	0.61
620.29	0.3	0.85
646.29	1.8	4.78
660.43	1.9	5.02
661.39	0.7	1.96

676.37	0.5	1.20
694.31	0.3	0.77
764.27	0.4	1.11
764.43	0.4	0.99
785.35	0.2	0.65
859.38	1.0	2.54
873.46	1.0	2.53
874.39	0.3	0.77
889.42	0.4	1.16
920.97	0.2	0.64
921.44	24.9	65.22
922.44	7.1	18.57
923.43	1.0	2.74
1095.49		8.8 22.94
1096.51		2.9 7.70
1097.53		0.4 1.03
1109.50		3.0 7.73
1110.50		0.7 1.91
1110.67		0.4 1.14
1116.59		0.2 0.59
1165.56		0.6 1.54
1248.66		4.5 11.89
1249.58		3.8 9.96
1250.67		0.4 0.93
1322.60		38.2 100.00
1323.61		18.7 48.86
1324.73		3.1 8.03
1331.62		0.7 1.72
1332.57		0.3 0.81
1340.52		0.6 1.47
1352.67		2.1 5.62
1353.63		1.1 2.98
1354.69		0.3 0.67
1401.59		2.4 6.35
1401.79		1.4 3.65
1402.66		1.6 4.26
1403.67		0.5 1.21
1528.77		0.7 1.77
1558.72		14.4 37.76
1559.73		9.5 24.86
1560.72		3.4 8.83

SPECTRUM - MS

12-17-13_HMG51_1149_MS4_1558_660_01.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1559.40@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-50

RT: 0.00-21.03

AV: 50

m/z	Intensity	Relative
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229.07	0.0	7.98
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236.06	0.0	2.93
241.06	0.0	1.58
259.12	0.2	79.02
260.05	0.0	6.64
260.22	0.0	2.62
302.12	0.0	1.82
325.14	0.0	1.60
364.16	0.0	2.79
367.98	0.0	1.70
382.19	0.0	2.51
384.19	0.0	1.82
398.23	0.0	2.62
400.28	0.0	2.14
412.43	0.0	1.70
413.16	0.0	2.08
424.18	0.0	5.39
424.33	0.0	2.41
425.25	0.0	1.92
426.20	0.0	9.95
442.22	0.0	20.62
443.32	0.0	1.73
454.27	0.0	5.52
456.23	0.0	1.73
457.28	0.0	1.63
472.31	0.0	17.42
473.23	0.0	1.57
473.42	0.0	4.06
486.33	0.0	2.56
515.35	0.0	2.19
516.35	0.0	1.63
523.86	0.0	21.55
554.20	0.0	1.64
556.24	0.0	1.79
586.28	0.2	100.00
587.29	0.0	19.18
588.25	0.0	2.14
588.99	0.0	1.54
589.33	0.0	18.07
590.35	0.0	5.64
614.22	0.0	3.38
614.37	0.0	5.31
615.25	0.0	1.71
616.42	0.0	2.99
618.31	0.1	35.52
619.37	0.0	12.31
660.09	0.0	13.27
660.22	0.0	8.26
660.42	0.2	77.16
661.24	0.0	13.68

SPECTRUM - MS

12-18-13_HMG51_1149_MS4_1558_1109_01.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1559.40@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-51

RT: 0.00-30.52

AV: 51

m/z	Intensity	Relative
385.17	0.0	5.22
398.23	0.0	1.09
412.24	0.0	1.08
440.06	0.0	0.47
440.18	0.0	0.43
442.20	0.0	0.78
454.17	0.0	0.36
458.27	0.0	0.40
458.37	0.0	0.36
472.23	0.0	0.71
486.26	0.1	15.12
487.24	0.0	1.63
572.24	0.0	1.11
572.42	0.0	0.41
573.10	0.0	0.35
573.40	0.0	0.46
575.34	0.0	1.30
598.23	0.0	1.25
598.49	0.0	0.41
611.33	0.0	0.37
646.31	0.7	100.00
647.32	0.1	17.13
648.24	0.0	1.36
648.37	0.0	0.75
660.41	0.0	0.41
690.31	0.0	1.00
690.52	0.0	0.38
706.25	0.0	0.49
706.39	0.0	0.44
708.42	0.0	4.82
709.33	0.0	0.79
709.52	0.0	0.48
778.42	0.0	0.41
799.37	0.1	10.93
800.41	0.0	1.56
831.40	0.0	0.38
873.41	0.6	81.53
874.40	0.1	18.96
875.46	0.0	2.25
891.46	0.0	0.49
903.48	0.0	0.86
905.41	0.0	2.79
906.51	0.0	0.76
921.50	0.0	0.37

1067.37	0.0	0.65
1068.47	0.0	0.33
1109.51	0.3	41.88
1110.50	0.1	18.08
1111.50	0.0	2.78
1111.68	0.0	0.66

SPECTRUM - MS

12-18-13_HMG51_1149_MS3_1109_01.raw

ITMS + p ESI E Full ms3 1149.00@cid35.00 1109.40@cid35.00 [305.00-1200.00]

Scan #: 1-20

RT: 0.00-5.55

AV: 20

m/z Intensity Relative

385.24	0.1	1.43
398.27	0.0	1.11
433.24	0.2	5.12
472.27	0.7	17.91
473.27	0.0	0.87
486.28	0.5	13.45
487.25	0.0	1.10
572.31	0.1	2.61
575.32	0.0	1.27
586.26	0.1	1.77
598.21	0.1	1.74
598.38	0.0	0.60
625.29	0.2	5.13
646.33	3.9	100.00
647.35	0.5	12.66
660.33	1.2	31.40
661.37	0.1	2.12
699.36	1.3	33.56
700.31	0.1	2.46
700.51	0.1	1.39
706.41	0.0	0.80
708.32	0.4	9.56
709.26	0.0	0.76
709.48	0.0	0.97
738.45	0.1	3.03
778.40	0.0	0.74
799.40	0.3	7.98
800.35	0.1	1.33
873.43	2.2	56.66
874.45	0.4	11.50
882.50	0.0	0.76
903.42	0.0	1.09
903.55	0.0	1.00
905.45	0.2	4.79
906.44	0.0	0.69
921.41	0.0	1.06

927.47	0.0	0.60	
928.00	0.0	0.72	
928.41	0.0	0.69	
952.46	0.1	1.40	
992.47	0.0	1.21	
993.24	0.0	0.64	
1011.49		0.3	6.89
1012.55		0.1	1.33
1038.47		0.0	0.61
1067.50		0.0	1.22
1109.01		0.0	1.04
1109.53		2.2	55.72
1109.95		0.1	1.49
1110.51		0.9	22.15

SPECTRUM - MS

12-18-13_HMG51_1149_MS4_1109_660_01.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1109.40@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-50

RT: 0.00-45.44

AV: 50

m/z Intensity Relative

180.83	0.0	0.59
201.39	0.0	0.56
211.03	0.0	0.89
211.27	0.0	0.68
229.11	0.0	1.02
244.82	0.0	0.76
245.25	0.0	0.77
250.12	0.0	0.89
259.06	0.0	1.30
259.17	0.0	1.08
260.20	0.0	0.64
297.17	0.0	0.61
313.21	0.0	0.62
323.26	0.0	1.12
350.18	0.0	0.59
352.30	0.0	0.93
353.28	0.0	2.18
368.23	0.0	0.62
380.14	0.0	0.76
383.21	0.0	1.54
398.18	0.0	7.23
399.30	0.0	0.65
415.29	0.0	7.49
424.25	0.0	1.60
431.32	0.0	1.93
433.24	0.1	100.00
434.19	0.0	6.18
472.34	0.0	15.17

473.26	0.0	1.52
486.19	0.0	0.57
512.33	0.0	1.40
515.08	0.0	1.42
515.29	0.0	1.12
554.07	0.0	0.64
557.97	0.0	0.66
586.31	0.1	45.76
587.23	0.0	1.55
589.26	0.0	2.07
614.27	0.0	0.82
614.46	0.0	1.19
615.25	0.0	0.81
618.32	0.0	10.07
618.45	0.0	6.54
619.31	0.0	1.54
619.46	0.0	0.65
660.39	0.0	20.73
661.24	0.0	1.39
661.43	0.0	0.60
698.51	0.0	0.90
699.06	0.0	1.23

SPECTRUM - MS

12-18-13_HMG51_1149_MS4_1109_646_01.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1109.40@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-43

RT: 0.00-21.39

AV: 43

m/z	Intensity	Relative
193.93	0.0	1.00
204.00	0.0	4.96
211.05	0.0	1.04
218.09	0.0	1.24
220.14	0.0	1.29
227.06	0.0	9.56
229.11	0.0	6.03
232.00	0.0	0.82
236.13	0.0	3.98
243.05	0.0	0.94
245.08	0.1	37.41
246.16	0.0	1.36
287.10	0.0	3.25
308.18	0.0	0.96
315.18	0.0	4.00
324.05	0.0	1.14
343.14	0.0	1.74
353.14	0.0	1.15
366.21	0.0	1.74
368.24	0.0	2.35

369.13	0.0	1.01
378.20	0.0	1.66
380.20	0.0	4.35
382.06	0.0	1.50
382.26	0.0	3.55
383.21	0.0	1.01
384.12	0.0	3.14
384.26	0.0	2.92
385.17	0.1	62.09
386.12	0.0	3.23
386.29	0.0	3.37
399.14	0.0	1.03
424.23	0.0	7.26
433.20	0.0	1.97
440.22	0.0	16.70
441.19	0.0	2.88
442.22	0.0	21.34
443.19	0.0	1.88
443.34	0.0	1.27
458.06	0.0	1.02
458.26	0.0	7.27
542.33	0.0	0.91
572.27	0.2	100.00
573.29	0.0	19.59
575.33	0.0	21.30
576.41	0.0	1.98
604.37	0.0	3.39
646.38	0.0	21.63
647.33	0.0	1.32
666.89	0.0	0.82

SPECTRUM - MS

12-18-13_HMG51_1149_MS4_1109_486_01.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1109.40@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-42.49

AV: 50

m/z	Intensity	Relative
133.46	0.0	1.80
168.07	0.0	2.06
176.16	0.0	1.50
180.28	0.0	0.32
207.98	0.0	6.16
218.11	0.0	2.91
219.96	0.0	0.90
229.72	0.0	1.02
241.02	0.0	0.54
242.05	0.0	0.96
245.52	0.0	0.26
249.99	0.0	2.23

250.13	0.0	1.02
252.11	0.0	14.68
252.99	0.0	3.55
257.05	0.0	1.41
257.26	0.0	2.73
259.10	0.0	100.00
259.51	0.0	0.00
259.64	0.0	0.00
260.10	0.0	4.66
268.03	0.0	2.43
268.15	0.0	6.97
284.81	0.0	1.30
341.23	0.0	0.38
357.20	0.0	1.55
382.24	0.0	1.70
385.30	0.0	0.87
390.30	0.0	0.23
393.97	0.0	2.20
412.14	0.0	83.38
412.29	0.0	39.04
412.67	0.0	0.00
413.17	0.0	4.51
413.38	0.0	1.15
421.38	0.0	2.30
438.94	0.0	0.45
444.23	0.0	49.15
444.64	0.0	0.00
445.27	0.0	1.33
454.27	0.0	4.15
454.93	0.0	0.49
455.33	0.0	3.49
456.01	0.0	1.04
456.42	0.0	0.85
476.08	0.0	0.38
486.03	0.0	6.38
486.29	0.0	22.15
486.70	0.0	0.00
487.26	0.0	2.38

SPECTRUM - MS

12-18-13_HMG51_1149_MS4_1109_472_03.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1109.40@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-100

RT: 0.00-87.25

AV: 100

m/z	Intensity	Relative
133.18	0.0	5.90
137.57	0.0	3.06
165.18	0.0	4.04
171.02	0.0	2.85

179.97	0.0	7.91
181.76	0.0	4.16
187.98	0.0	2.61
198.00	0.0	3.08
203.99	0.0	2.78
208.11	0.0	2.89
220.11	0.0	7.46
224.08	0.0	1.41
226.34	0.0	5.20
227.02	0.0	82.46
228.09	0.0	11.24
230.92	0.0	3.11
236.09	0.0	6.44
236.20	0.0	3.76
236.98	0.0	5.61
240.50	0.0	4.28
245.03	0.0	25.52
245.21	0.0	6.52
252.76	0.0	1.43
268.11	0.0	100.00
269.23	0.0	9.84
309.02	0.0	3.00
314.85	0.0	4.02
315.23	0.0	40.56
316.14	0.0	2.31
324.12	0.0	4.21
325.26	0.0	1.61
327.22	0.0	2.67
380.10	0.0	2.19
381.18	0.0	4.13
381.33	0.0	2.62
396.36	0.0	1.75
398.17	0.0	97.25
399.10	0.0	8.81
399.29	0.0	6.54
412.27	0.0	1.68
430.30	0.0	10.31
440.14	0.0	9.87
440.31	0.0	6.22
442.25	0.0	9.11
442.64	0.0	2.58
443.25	0.0	4.33
472.27	0.0	16.20
476.51	0.0	6.84
485.85	0.0	3.56
496.94	0.0	3.50

SPECTRUM - MS

12-17-13_HMG51_1149_MS3_830_01.raw

ITMS + p ESI E Full ms3 1149.00@cid35.00 830.40@cid35.00 [225.00-2000.00]

Scan #: 1-20

RT: 0.00-4.90

AV: 20

m/z	Intensity	Relative
386.16	0.8	1.30
444.25	2.2	3.70
458.25	2.3	3.86
486.28	45.7	77.63
487.27	9.8	16.70
488.27	1.4	2.35
514.27	0.8	1.43
534.34	1.4	2.45
598.30	4.2	7.13
598.82	2.9	4.94
599.34	1.0	1.71
630.30	1.7	2.91
676.32	2.0	3.34
677.31	0.7	1.15
718.34	2.4	4.09
719.35	0.9	1.55
720.90	1.4	2.44
721.39	1.3	2.14
738.43	29.9	50.83
739.43	11.0	18.65
740.45	2.0	3.36
760.33	1.4	2.39
776.87	1.0	1.67
777.38	0.9	1.56
780.43	1.3	2.19
780.94	1.1	1.92
813.91	1.9	3.24
814.41	1.5	2.51
814.93	2.5	4.20
815.43	2.2	3.72
815.96	1.0	1.70
829.96	11.7	19.94
830.46	10.1	17.19
830.96	5.2	8.82
831.45	1.1	1.86
921.43	12.4	21.07
922.45	5.4	9.18
923.45	1.8	3.13
983.50	4.6	7.80
984.50	2.3	3.94
1065.46	4.2	7.14
1066.47	2.2	3.81
1153.48	1.1	1.92
1173.59	58.9	100.00
1174.59	34.8	59.01
1175.57	10.3	17.55
1176.58	1.2	2.10

1636.78	1.9	3.17
1637.79	1.7	2.85
1638.81	0.9	1.49

SPECTRUM - MS

12-17-13_HMG51_1149_MS4_830_921_01.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 830.40@cid35.00 922.00@cid35.00 [250.00-1000.00]

Scan #: 1-50

RT: 0.00-25.24

AV: 50

m/z	Intensity	Relative
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268.10	0.0	1.27
301.16	0.0	0.54
329.17	0.0	0.63
444.25	0.1	1.95
454.22	0.0	0.61
458.24	3.5	100.00
459.24	0.6	17.42
460.21	0.1	2.01
486.28	2.1	60.03
487.26	0.4	12.20
488.28	0.1	1.50
546.25	0.1	3.11
547.27	0.0	0.54
574.31	0.3	7.26
575.33	0.1	1.96
620.29	0.1	2.93
621.31	0.0	0.67
646.29	0.1	1.43
676.31	0.5	14.28
677.32	0.2	4.30
678.34	0.0	1.01
692.31	0.0	1.28
694.33	0.4	10.31
695.32	0.1	2.44
696.39	0.2	6.74
703.34	0.1	2.85
704.31	0.0	0.77
724.40	0.3	7.47
764.37	1.0	27.60
765.37	0.3	8.65
766.38	0.1	1.54
793.43	0.0	0.66
815.31	0.1	1.67
815.48	0.0	1.36
816.41	0.1	2.00
829.32	0.0	0.85
829.49	0.0	0.87
847.37	0.1	4.00
848.37	0.1	3.20

850.43	0.2	4.55
851.51	0.0	0.67
879.56	0.1	2.25
880.43	0.1	1.82
889.39	0.3	9.86
890.39	0.1	3.65
891.40	0.2	5.34
892.52	0.0	1.10
921.42	0.2	4.68
922.46	0.1	2.13
923.36	0.0	0.64

SPECTRUM - MS

12-17-13_HMG51_1149_MS5_830_921_486_01.raw

ITMS + p ESI E Full ms5 1149.00@cid35.00 830.40@cid35.00 922.00@cid35.00 487.00@cid35.00
[130.00-500.00]

Scan #: 1-18

RT: 0.00-8.23

AV: 18

m/z Intensity Relative

146.82	0.0	0.91
161.91	0.0	0.23
178.11	0.0	0.92
179.05	0.0	0.31
194.21	0.0	0.27
198.98	0.0	0.30
220.09	0.0	5.21
226.99	0.0	0.46
241.12	0.0	4.12
242.09	0.0	1.38
243.27	0.0	0.67
256.92	0.0	1.34
257.11	0.0	1.73
259.08	0.1	18.07
260.00	0.0	1.14
268.09	0.0	3.94
269.09	0.0	0.53
281.94	0.0	0.39
283.40	0.0	1.54
297.21	0.0	2.19
300.89	0.0	0.31
301.05	0.0	0.63
303.88	0.0	1.41
326.47	0.0	0.37
329.14	0.1	30.74
329.40	0.0	1.38
330.05	0.0	0.75
330.21	0.0	0.85
330.33	0.0	0.49
331.14	0.0	0.55

353.12	0.0	0.27
373.10	0.0	1.48
382.15	0.0	0.62
398.03	0.0	1.71
411.97	0.0	1.04
415.25	0.0	2.66
415.43	0.0	0.52
424.12	0.0	0.61
431.17	0.0	1.56
444.27	0.3	100.00
445.24	0.0	12.00
445.45	0.0	2.00
446.18	0.0	1.36
446.29	0.0	0.93
455.19	0.0	0.65
456.25	0.0	6.88
479.54	0.0	0.31
486.29	0.2	54.24
487.27	0.0	14.52
488.34	0.0	2.20

SPECTRUM - MS

12-17-13_HMG51_1149_MS5_830_921_458_01.raw

ITMS + p ESI E Full ms5 1149.00@cid35.00 830.40@cid35.00 922.00@cid35.00 459.00@cid35.00

[125.00-500.00]

Scan #: 1-50

RT: 0.00-20.32

AV: 50

m/z	Intensity	Relative
149.02	0.0	1.36
178.07	0.0	0.41
179.76	0.0	0.48
180.01	0.0	3.48
181.11	0.0	0.40
188.01	0.0	1.09
190.09	0.0	0.47
193.91	0.0	0.34
194.11	0.0	0.51
196.09	0.0	0.35
204.04	0.0	1.93
213.04	0.0	12.13
214.03	0.0	0.54
217.97	0.0	0.46
218.14	0.0	0.82
220.04	0.0	8.50
220.89	0.0	0.66
231.06	0.1	12.71
232.01	0.0	0.50
236.15	0.0	4.65
236.99	0.0	0.37

240.55	0.0	0.38
262.80	0.0	0.34
268.11	0.4	100.00
269.09	0.0	7.90
270.13	0.0	0.67
273.24	0.0	0.54
287.14	0.0	0.43
301.14	0.1	28.13
302.02	0.0	1.92
302.27	0.0	1.29
303.07	0.0	0.50
313.10	0.0	0.36
352.17	0.0	0.47
353.14	0.0	0.33
366.16	0.0	2.23
371.06	0.0	0.31
371.26	0.0	0.36
384.22	0.0	2.06
385.10	0.0	1.09
385.21	0.0	0.73
416.08	0.0	0.77
422.52	0.0	0.45
426.12	0.0	4.59
427.27	0.0	1.23
428.18	0.0	4.36
429.27	0.0	1.10
458.23	0.1	21.53
459.32	0.0	1.84
460.22	0.0	0.60

SPECTRUM - MS

12-20-13_HMG51_MS4_1149_1558_1095_01.raw

ITMS + p ESI E Full ms4 1149.00@cid35.00 1559.40@cid35.00 1096.00@cid35.00 [300.00-1100.00]

Scan #: 1-21

RT: 0.00-9.38

AV: 21

m/z Intensity Relative

385.21	0.0	2.27
410.08	0.0	1.36
422.00	0.0	0.71
440.15	0.0	1.24
458.25	0.2	24.03
459.12	0.0	0.97
459.37	0.0	1.07
472.26	0.2	36.20
473.17	0.0	1.63
473.31	0.0	1.76
572.28	0.0	1.91
575.30	0.0	0.97
612.25	0.0	2.26

646.39	0.2	37.52
647.29	0.1	9.21
660.32	0.3	51.65
661.36	0.1	9.85
678.10	0.0	0.83
785.30	0.0	4.29
785.50	0.0	0.98
794.50	0.0	0.85
795.29	0.0	0.75
815.41	0.0	4.08
836.37	0.0	1.71
859.40	0.1	20.32
860.35	0.0	3.95
861.49	0.0	0.91
864.26	0.0	0.75
866.16	0.0	0.88
866.38	0.0	2.70
866.57	0.0	2.51
867.57	0.0	1.46
868.45	0.0	1.19
889.33	0.1	20.28
889.52	0.1	16.53
890.41	0.0	6.63
891.41	0.0	5.07
927.38	0.0	0.71
938.53	0.0	3.19
939.46	0.0	0.87
1017.40	0.0	0.94
1022.49	0.0	0.86
1023.36	0.0	1.54
1024.41	0.0	5.31
1063.57	0.0	1.42
1095.47	0.7	100.00
1096.45	0.2	27.15
1096.64	0.1	20.61
1097.33	0.0	2.23
1097.66	0.0	2.01

SPECTRUM - MS

12-20-13_HMG51_MS5_1149_1558_1095_472_02.raw

ITMS + p ESI E Full ms5 1149.00@cid35.00 1559.40@cid35.00 1096.00@cid35.00 473.00@cid35.00
[130.00-500.00]

Scan #: 1-76

RT: 0.00-173.92

AV: 76

m/z	Intensity	Relative
148.91	0.0	3.16
161.97	0.0	2.07
165.16	0.0	2.14
170.98	0.0	3.46

178.07	0.0	2.29
194.05	0.0	5.17
204.12	0.0	5.86
220.05	0.0	8.65
227.08	0.0	49.60
228.13	0.0	7.41
236.12	0.0	8.17
240.04	0.0	3.08
245.06	0.0	34.73
250.13	0.0	5.10
268.09	0.0	100.00
269.15	0.0	5.02
276.83	0.0	2.89
283.16	0.0	4.98
286.00	0.0	1.96
287.14	0.0	4.24
315.08	0.0	44.35
315.22	0.0	35.37
322.35	0.0	2.25
323.69	0.0	3.45
327.09	0.0	2.28
330.16	0.0	4.05
357.24	0.0	2.76
367.23	0.0	2.66
368.82	0.0	3.15
374.65	0.0	2.90
379.90	0.0	1.99
380.20	0.0	4.02
396.10	0.0	3.30
398.18	0.0	11.05
398.30	0.0	10.97
399.17	0.0	6.10
401.10	0.0	3.82
408.24	0.0	4.24
430.25	0.0	5.78
437.55	0.0	1.93
440.02	0.0	12.13
440.28	0.0	22.13
441.12	0.0	9.46
441.39	0.0	9.89
441.97	0.0	2.28
442.21	0.0	2.10
454.99	0.0	3.29
456.28	0.0	2.05
467.20	0.0	2.50
472.33	0.0	2.90

HMG 54 Mass spectral peak lists

SPECTRUM - MS

12-18-13_HMG54_1235_MS2_01.raw

ITMS + p ESI E Full ms2 1236.00@cid35.00 [340.00-2000.00]

Scan #: 1-20

RT: 0.00-1.50

AV: 20

m/z	Intensity	Relative
486.27	6743.1	7.35
646.30	5244.1	5.72
660.34	5121.1	5.58
685.38	3999.4	4.36
685.89	2799.4	3.05
692.39	5575.2	6.08
692.89	3952.5	4.31
693.39	1712.6	1.87
724.38	2590.2	2.82
738.41	4093.4	4.46
900.94	6998.8	7.63
901.45	6366.0	6.94
901.94	4034.6	4.40
902.45	1684.8	1.84
916.96	7600.2	8.29
917.45	6455.0	7.04
917.96	3066.1	3.34
1003.99	91701.4	100.00
1004.50	84882.0	92.56
1004.98	44477.3	48.50
1005.50	15524.1	16.93
1006.01	2791.7	3.04
1109.48	4689.8	5.11
1110.49	2274.7	2.48
1117.53	1719.0	1.87
1118.05	2210.1	2.41
1132.54	9841.1	10.73
1133.04	9972.8	10.88
1133.54	6640.8	7.24
1134.02	2988.6	3.26
1141.51	2349.9	2.56
1142.03	2115.4	2.31
1235.64	17456.2	19.04
1236.11	21173.9	23.09
1236.58	15104.1	16.47
1237.07	7590.8	8.28
1237.56	1977.0	2.16
1347.59	3108.0	3.39
1348.61	2128.1	2.32
1361.62	13506.7	14.73
1362.63	8789.4	9.58

1363.64	3331.8	3.63
1732.74	1881.3	2.05
1778.83	1948.3	2.12
1779.84	1662.2	1.81
1810.83	3484.0	3.80
1811.84	2764.8	3.02
1984.99	9089.0	9.91
1986.00	8202.8	8.95
1986.98	4295.8	4.68

SPECTRUM - MS

12-18-13_HMG54_1235_MS3_1004_01.raw

ITMS + p ESI E Full ms3 1236.00@cid35.00 1004.60@cid35.00 [275.00-2000.00]

Scan #: 1-20

RT: 0.00-1.73

AV: 20

m/z Intensity Relative

385.15	360.1	2.50
534.33	839.6	5.82
589.33	428.7	2.97
646.30	8102.7	56.16
647.31	1873.9	12.99
660.33	4156.3	28.81
661.34	1000.8	6.94
664.38	418.6	2.90
685.37	3316.4	22.99
685.88	1981.3	13.73
686.37	571.1	3.96
692.38	11591.5	80.35
692.88	6533.6	45.29
693.37	2110.2	14.63
693.87	421.3	2.92
704.30	580.6	4.02
706.38	1358.4	9.42
724.38	2154.8	14.94
725.39	649.2	4.50
738.41	2279.1	15.80
739.40	651.8	4.52
746.29	451.5	3.13
798.91	584.7	4.05
799.39	423.9	2.94
863.91	559.6	3.88
864.42	432.4	3.00
900.93	13568.4	94.05
901.44	10195.2	70.67
901.93	5397.8	37.42
902.44	2061.9	14.29
902.96	542.8	3.76
909.95	1137.6	7.89
910.45	766.3	5.31

1003.99	5054.6	35.04
1004.49	4773.6	33.09
1004.97	2592.3	17.97
1005.49	927.6	6.43
1141.50	391.7	2.72
1155.52	803.0	5.57
1156.53	356.7	2.47
1253.52	747.9	5.18
1254.54	373.6	2.59
1269.55	975.7	6.76
1270.56	456.4	3.16
1347.60	4216.2	29.23
1348.62	2170.9	15.05
1349.61	603.1	4.18
1361.62	14426.6	100.00
1362.63	7847.4	54.39
1363.64	2260.5	15.67

SPECTRUM - MS

12-18-13_HMG54_1235_MS4_1004_1347_01.raw

ITMS + p ESI E Full ms4 1236.00@cid35.00 1004.60@cid35.00 1348.00@cid35.00 [370.00-1400.00]

Scan #: 1-20

RT: 0.00-4.56

AV: 20

m/z Intensity Relative

435.26	7.2	0.84
436.25	1.3	0.15
456.31	1.3	0.16
470.28	1.3	0.15
472.30	0.9	0.11
474.29	3.1	0.36
486.33	4.7	0.55
487.33	0.9	0.10
492.34	1.5	0.18
502.30	2.3	0.26
516.32	2.1	0.24
534.35	193.1	22.45
535.35	36.5	4.24
536.32	3.0	0.35
562.32	1.0	0.12
572.30	0.7	0.08
590.33	1.8	0.21
625.34	8.5	0.99
626.35	1.9	0.22
646.33	19.4	2.25
647.34	3.8	0.44
676.34	1.7	0.20
692.48	1.2	0.14
706.41	0.9	0.11
722.40	0.9	0.11

724.41	860.2	100.00
725.42	209.1	24.30
726.43	25.1	2.92
752.43	0.8	0.09
836.43	4.8	0.56
837.41	1.2	0.14
877.48	0.7	0.08
898.51	0.6	0.07
919.46	1.7	0.19
921.49	0.9	0.10
1067.53	7.8	0.90
1068.51	3.1	0.36
1141.55	45.8	5.33
1142.56	18.4	2.14
1143.58	20.7	2.40
1144.59	6.6	0.77
1145.59	1.4	0.17
1159.58	2.8	0.33
1160.59	1.4	0.16
1248.60	4.5	0.52
1249.71	1.1	0.13
1315.64	1.9	0.22
1347.66	124.5	14.47
1348.66	76.8	8.93
1349.67	21.4	2.49

SPECTRUM - MS

12-18-13_HMG54_1235_MS4_1004_1361_01.raw

ITMS + p ESI E Full ms4 1236.00@cid35.00 1004.60@cid35.00 1362.00@cid35.00 [370.00-2000.00]

Scan #: 1-20

RT: 0.00-5.34

AV: 20

m/z	Intensity	Relative
435.26	19.8	1.16
474.30	8.2	0.48
486.33	20.0	1.18
502.30	7.4	0.44
516.31	9.1	0.53
534.35	534.2	31.41
535.35	110.9	6.52
536.34	10.4	0.61
562.33	15.0	0.88
590.34	9.8	0.57
625.34	22.9	1.35
639.35	10.8	0.64
644.33	7.9	0.46
646.33	15.7	0.92
660.35	81.5	4.80
661.36	17.6	1.04
662.36	11.4	0.67

706.41	12.0	0.71	
720.38	8.3	0.49	
724.41	1700.4		100.00
725.42	441.2	25.95	
726.43	55.9	3.28	
738.44	585.2	34.42	
739.44	152.1	8.94	
740.45	19.4	1.14	
748.41	10.7	0.63	
850.43	39.4	2.32	
851.42	11.5	0.68	
863.46	11.2	0.66	
877.48	11.4	0.67	
919.48	18.6	1.09	
921.47	9.4	0.55	
1081.52		114.1	6.71
1082.53		48.1	2.83
1083.54		10.8	0.63
1143.58		43.0	2.53
1144.59		19.4	1.14
1155.57		306.3	18.01
1156.57		129.2	7.60
1157.58		83.8	4.93
1158.60		25.2	1.48
1173.59		32.2	1.90
1174.59		14.4	0.85
1262.62		29.1	1.71
1263.62		14.2	0.84
1329.66		18.2	1.07
1330.68		8.4	0.49
1361.70		430.0	25.29
1362.68		258.7	15.22
1363.68		76.0	4.47

SPECTRUM - MS

12-18-13_HMG54_1235_MS3_1732_01.raw

ITMS + p ESI E Full ms3 1236.00@cid35.00 1733.40@cid35.00 [475.00-1800.00]

Scan #: 1-20

RT: 0.00-3.43

AV: 20

m/z Intensity Relative

486.38	0.6	0.56
646.31	41.4	40.13
647.31	9.6	9.28
648.30	1.5	1.47
708.36	0.6	0.59
868.47	1.2	1.19
873.49	1.9	1.85
874.31	0.6	0.57
903.44	0.6	0.59

989.45	0.8	0.79
1063.49		15.8 15.30
1064.51		7.3 7.08
1065.49		2.8 2.67
1109.50		40.1 38.83
1110.50		16.7 16.15
1111.57		2.4 2.33
1269.56		103.2 100.00
1270.57		49.5 48.02
1271.55		11.9 11.54
1283.53		0.6 0.58
1290.57		1.8 1.79
1291.62		0.5 0.50
1313.47		1.3 1.22
1313.68		0.8 0.81
1314.61		0.9 0.88
1329.47		0.9 0.85
1329.69		0.9 0.88
1331.57		12.9 12.55
1332.59		6.5 6.30
1333.70		1.0 1.00
1401.73		2.7 2.66
1402.48		0.8 0.74
1402.68		1.2 1.17
1496.67		8.3 8.05
1497.81		2.2 2.15
1498.80		0.9 0.89
1526.63		38.2 37.01
1527.64		22.8 22.08
1528.65		13.4 12.95
1529.73		1.7 1.61
1530.50		0.6 0.54
1530.74		0.7 0.64
1544.65		1.8 1.70
1545.68		1.1 1.02
1658.61		1.0 0.93
1658.81		0.7 0.68
1659.73		0.6 0.62
1732.77		43.5 42.19
1733.77		37.8 36.64
1734.78		18.9 18.32

SPECTRUM - MS

12-18-13_HMG54_1235_MS4_1732_1109_01.raw

ITMS + p ESI E Full ms4 1236.00@cid35.00 1733.40@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-20

RT: 0.00-3.29

AV: 20

m/z Intensity Relative

384.18 0.1 0.83

385.15	0.4	3.81	
440.12	0.1	0.65	
442.31	0.1	0.71	
454.14	0.1	0.57	
458.32	0.1	0.95	
472.36	0.1	0.53	
486.32	1.8	17.53	
487.35	0.1	1.18	
504.39	0.1	0.56	
572.22	0.1	1.16	
573.32	0.1	1.05	
575.31	0.2	1.44	
598.13	0.1	0.64	
598.36	0.1	0.66	
634.28	0.1	0.55	
646.32	10.5	100.00	
647.34	1.4	13.20	
648.36	0.1	1.03	
660.37	0.1	0.67	
690.22	0.1	0.74	
690.34	0.1	0.80	
690.47	0.1	0.91	
708.25	0.3	2.84	
708.41	0.4	3.41	
709.24	0.1	0.71	
709.48	0.1	0.72	
778.26	0.1	1.15	
799.17	0.1	1.11	
799.45	0.3	2.60	
800.15	0.1	0.79	
873.29	1.6	15.49	
873.50	1.6	15.25	
874.01	0.0	0.47	
874.47	0.5	4.92	
875.38	0.1	0.73	
875.50	0.0	0.47	
891.54	0.1	0.59	
904.52	0.1	0.53	
905.30	0.2	1.75	
905.46	0.1	0.91	
905.57	0.1	0.74	
906.35	0.1	0.53	
921.45	0.1	0.64	
1038.56		0.1	0.51
1068.65		0.1	0.63
1080.44		0.0	0.47
1109.49		1.9	17.78
1110.39		0.5	4.49
1110.57		0.4	3.84

SPECTRUM - MS

12-18-13_HMG54_1235_MS5_1732_1109_486_02.raw

ITMS + p ESI E Full ms5 1236.00@cid35.00 1733.40@cid35.00 1110.00@cid35.00 487.00@cid35.00
[130.00-500.00]

Scan #: 1-100

RT: 0.00-46.04

AV: 100

m/z	Intensity	Relative
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179.96	0.0	0.34
187.10	0.0	0.48
197.14	0.0	0.66
208.08	0.0	1.50
208.24	0.0	0.33
220.03	0.0	3.73
221.16	0.0	0.76
227.15	0.0	0.44
235.53	0.0	0.68
235.98	0.0	0.77
241.08	0.0	7.57
242.05	0.0	0.84
245.03	0.0	0.42
250.10	0.0	1.89
251.58	0.0	0.73
252.10	0.0	2.63
257.06	0.0	0.78
259.11	0.2	46.06
259.47	0.0	0.50
259.97	0.0	1.05
260.20	0.0	1.77
268.11	0.1	16.17
269.15	0.0	2.00
286.45	0.0	0.91
297.15	0.0	0.64
301.04	0.0	0.98
329.16	0.1	43.28
330.04	0.0	0.62
330.25	0.0	1.42
366.21	0.0	1.76
371.17	0.0	0.59
377.76	0.0	0.59
384.19	0.0	0.70
394.03	0.0	0.51
412.18	0.1	31.77
413.13	0.0	1.74
413.28	0.0	2.28
415.10	0.0	0.54
415.35	0.0	0.72
418.35	0.0	0.96
431.23	0.0	1.00
440.10	0.0	0.44
444.25	0.3	100.00

445.26	0.0	11.41
454.08	0.0	0.35
454.32	0.0	1.30
456.31	0.0	3.87
468.60	0.0	0.73
486.26	0.1	17.38
487.30	0.0	1.49

SPECTRUM - MS

12-18-13_HMG54_1235_MS5_1732_1109_646_01.raw

ITMS + p ESI E Full ms5 1236.00@cid35.00 1733.40@cid35.00 1110.00@cid35.00 647.00@cid35.00
[175.00-700.00]

Scan #: 1-50

RT: 0.00-11.33

AV: 50

m/z	Intensity	Relative
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194.01	0.0	0.96
204.00	0.0	3.13
218.07	0.0	0.90
220.08	0.0	1.24
227.04	0.1	8.70
229.08	0.1	4.66
236.06	0.1	7.71
245.10	0.3	25.35
246.04	0.0	0.78
287.08	0.0	2.09
287.27	0.0	0.91
315.05	0.0	1.77
315.24	0.0	1.69
324.22	0.0	0.93
343.15	0.1	5.17
353.15	0.0	1.01
366.20	0.0	1.66
366.98	0.0	0.99
367.11	0.0	1.00
368.18	0.0	0.79
369.18	0.0	2.54
371.30	0.0	0.77
378.21	0.0	1.78
380.17	0.0	2.95
382.22	0.1	7.92
384.19	0.1	8.05
385.17	1.3	100.00
386.17	0.1	9.82
397.04	0.0	0.78
397.26	0.0	0.87
398.23	0.0	2.46
424.27	0.1	4.43
433.12	0.0	1.06
440.18	0.3	21.62

441.22	0.0	1.66
442.21	0.2	17.71
443.30	0.0	1.39
458.22	0.2	11.77
530.21	0.0	0.84
542.43	0.0	1.05
545.47	0.0	0.75
572.29	0.8	65.75
572.83	0.0	0.74
573.31	0.3	23.60
574.29	0.0	0.78
575.32	0.3	26.07
576.28	0.0	2.59
604.31	0.1	6.64
646.31	0.3	25.58
647.40	0.0	2.86

SPECTRUM - MS

1-16-14_HMG54_1235_MS4_1732_646_02.raw

ITMS + p ESI E Full ms4 1236.00@cid35.00 1733.40@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-100

RT: 0.00-15.06

AV: 100

m/z Intensity Relative

204.10	0.1	1.40
211.15	0.1	0.95
218.09	0.1	1.19
220.04	0.1	2.06
227.07	0.7	13.42
229.09	0.3	5.32
236.17	0.3	5.73
245.11	1.7	30.32
246.14	0.1	1.31
287.18	0.1	2.21
315.30	0.1	1.44
324.15	0.1	1.41
336.31	0.1	0.96
343.15	0.2	4.08
366.18	0.2	3.99
367.21	0.2	2.91
368.20	0.2	3.16
368.37	0.1	0.92
369.16	0.1	1.05
369.33	0.1	1.06
371.24	0.1	0.98
378.24	0.1	1.69
380.08	0.1	1.57
380.28	0.2	3.18
382.18	0.2	4.53
382.34	0.2	3.01

383.26	0.1	2.31
384.21	0.6	10.40
385.21	5.5	100.00
386.21	0.7	12.99
398.29	0.1	1.76
424.24	0.3	6.36
440.25	1.1	20.86
441.22	0.1	1.88
442.25	1.2	21.82
443.27	0.2	4.05
458.22	0.3	5.80
458.39	0.2	3.70
459.29	0.1	1.54
498.19	0.1	1.11
542.35	0.1	0.98
572.33	4.2	77.12
573.33	1.5	26.86
574.29	0.3	5.18
574.49	0.1	1.30
575.37	1.7	31.30
576.41	0.3	5.63
604.37	0.2	4.31
646.38	0.6	11.57
647.42	0.1	1.26

SPECTRUM - MS

12-18-13_HMG54_1235_MS3_660_01.raw

ITMS + p ESI E Full ms3 1236.00@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-50

RT: 0.00-6.22

AV: 50

m/z Intensity Relative

211.07	2.3	0.95
229.07	10.0	4.16
236.03	4.6	1.89
241.07	6.3	2.60
257.06	2.5	1.02
259.11	72.4	29.98
260.10	7.3	3.02
301.11	3.7	1.53
329.16	7.5	3.12
355.17	3.2	1.31
380.16	5.9	2.44
382.20	11.5	4.75
383.19	4.5	1.88
384.21	5.9	2.44
385.19	3.6	1.48
394.20	6.9	2.87
398.18	10.3	4.28
399.18	6.2	2.57

412.17	5.2	2.17
424.20	6.6	2.72
430.23	16.3	6.75
431.24	3.0	1.23
442.22	6.6	2.74
447.24	7.1	2.94
454.19	13.9	5.75
455.21	2.5	1.03
456.21	28.8	11.94
457.22	5.3	2.19
470.21	4.4	1.83
472.25	241.4	100.00
473.25	50.5	20.94
474.23	7.4	3.06
486.27	8.9	3.69
515.26	2.7	1.12
556.28	2.3	0.94
562.30	5.7	2.34
584.23	9.9	4.09
586.28	86.9	35.99
587.27	24.3	10.08
588.29	5.0	2.07
589.30	29.7	12.32
590.31	10.0	4.15
614.27	8.3	3.42
618.32	138.7	57.46
619.33	39.7	16.44
620.34	7.1	2.94
630.30	5.2	2.15
660.33	51.5	21.34
661.34	15.1	6.24
662.34	3.4	1.39

SPECTRUM - MS

1-16-14_HMG54_1235_MS3_917_01.raw

ITMS + p ESI E Full ms3 1236.00@cid35.00 918.00@cid35.00 [250.00-2000.00]

Scan #: 1-20

RT: 0.00-1.76

AV: 20

m/z Intensity Relative

444.30	13.7	0.63
486.30	447.5	20.78
487.28	95.9	4.45
488.32	10.6	0.49
514.33	20.2	0.94
534.39	44.3	2.06
535.33	12.5	0.58
582.34	57.3	2.66
582.90	22.7	1.05
583.33	13.8	0.64

616.32	28.1	1.31	
646.33	49.0	2.28	
685.41	2153.5		100.00
685.92	1407.9		65.38
686.41	497.0	23.08	
686.90	80.8	3.75	
687.30	10.7	0.50	
704.36	62.8	2.92	
705.28	10.0	0.47	
706.34	16.4	0.76	
706.51	12.6	0.59	
724.43	406.0	18.85	
725.43	139.0	6.46	
726.44	20.8	0.97	
746.36	48.1	2.23	
794.53	11.6	0.54	
807.97	14.8	0.69	
813.95	83.0	3.85	
814.47	66.4	3.08	
814.95	36.6	1.70	
822.94	50.9	2.36	
823.46	51.9	2.41	
901.87	11.6	0.54	
902.03	11.0	0.51	
902.48	9.9	0.46	
917.01	304.3	14.13	
917.49	270.3	12.55	
918.01	132.7	6.16	
918.53	37.2	1.73	
1109.54		121.9	5.66
1110.56		58.7	2.72
1141.62		59.7	2.77
1142.58		30.6	1.42
1143.60		19.0	0.88
1143.77		17.8	0.83
1144.65		10.1	0.47
1347.68		571.0	26.51
1348.70		347.3	16.13
1349.72		112.6	5.23
1350.67		13.8	0.64

SPECTRUM - MS

1-16-14_HMG54_1235_MS4_917_1109_01.raw

ITMS + p ESI E Full ms4 1236.00@cid35.00 918.00@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-20

RT: 0.00-1.50

AV: 20

m/z Intensity Relative

364.16	0.2	0.48
384.29	0.2	0.41

385.19	1.7	3.68	
412.19	0.2	0.53	
424.19	0.3	0.56	
442.23	0.2	0.46	
458.11	0.2	0.52	
458.35	0.5	1.05	
486.30	11.1	23.74	
487.06	0.2	0.51	
487.29	0.7	1.41	
487.44	0.6	1.38	
488.10	0.3	0.54	
572.30	1.0	2.04	
573.23	0.6	1.34	
575.37	0.4	0.82	
604.33	0.2	0.46	
614.23	0.3	0.56	
646.35	46.7	100.00	
647.38	9.1	19.46	
648.44	0.3	0.63	
675.07	0.2	0.41	
690.13	0.4	0.83	
708.44	1.4	3.06	
709.23	0.3	0.57	
709.42	0.2	0.50	
799.40	0.2	0.42	
802.59	0.2	0.43	
848.33	0.3	0.59	
891.62	0.6	1.19	
892.46	0.4	0.89	
905.43	0.6	1.18	
906.51	0.2	0.48	
922.35	0.2	0.49	
926.79	0.2	0.38	
989.13	0.3	0.73	
990.44	0.3	0.54	
1003.40		0.3	0.59
1036.59		0.3	0.65
1067.73		0.2	0.44
1068.57		0.3	0.66
1077.50		0.2	0.53
1078.43		0.3	0.71
1079.59		1.2	2.51
1080.57		0.6	1.30
1109.59		7.4	15.93
1110.56		4.3	9.24
1110.85		0.3	0.61
1111.42		0.3	0.68
1111.68		0.3	0.69

SPECTRUM - MS

1-16-14_HMG54_1235_MS5_917_1109_486_03.raw

ITMS + p ESI E Full ms5 1236.00@cid35.00 918.00@cid35.00 1110.00@cid35.00 487.00@cid35.00
[130.00-500.00]

Scan #: 1-106

RT: 0.00-17.45

AV: 106

m/z	Intensity	Relative
151.58	0.0	0.81
179.90	0.0	1.00
187.15	0.0	0.71
204.05	0.0	0.61
211.19	0.0	1.21
219.98	0.0	2.26
220.13	0.0	3.79
229.21	0.0	0.56
229.81	0.0	0.58
241.04	0.0	4.89
251.35	0.0	1.48
254.42	0.0	0.64
258.69	0.0	0.52
259.13	0.2	24.02
260.06	0.0	0.85
268.14	0.1	16.80
269.09	0.0	1.85
278.14	0.0	0.86
293.24	0.0	0.63
301.03	0.0	0.95
315.29	0.0	0.81
329.18	0.3	50.21
329.55	0.0	1.38
330.12	0.0	4.02
330.28	0.0	5.24
331.34	0.0	1.12
338.90	0.0	1.07
353.08	0.0	0.53
362.08	0.0	1.19
390.28	0.0	1.79
394.16	0.0	0.57
410.31	0.0	0.77
412.24	0.0	0.87
415.23	0.0	5.40
424.39	0.0	1.09
426.57	0.0	0.58
431.21	0.0	1.05
434.95	0.0	0.65
444.30	0.7	100.00
445.34	0.1	14.91
446.29	0.0	0.73
448.03	0.0	0.65
454.31	0.0	1.32
455.15	0.0	0.67

456.22	0.0	7.22
456.37	0.0	2.37
486.24	0.0	6.01
486.38	0.0	4.34
488.38	0.0	1.02
489.50	0.0	0.71

SPECTRUM - MS

1-16-14_HMG54_1235_MS5_917_1109_646_03.raw

ITMS + p ESI E Full ms5 1236.00@cid35.00 918.00@cid35.00 1110.00@cid35.00 647.00@cid35.00
[175.00-700.00]

Scan #: 1-286

RT: 0.00-48.81

AV: 286

m/z	Intensity	Relative
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194.06	0.0	0.76
204.05	0.0	2.07
211.07	0.0	0.75
220.09	0.0	1.33
227.06	0.2	10.43
229.05	0.1	3.72
236.05	0.2	8.16
243.02	0.0	1.00
245.11	0.4	17.36
246.15	0.0	1.53
287.24	0.0	1.96
315.15	0.1	2.39
343.17	0.1	4.95
353.19	0.0	0.73
366.15	0.1	2.62
367.20	0.0	1.13
368.21	0.1	2.26
369.20	0.0	1.42
371.19	0.0	1.07
378.22	0.1	3.99
379.21	0.0	0.96
380.21	0.1	3.40
382.23	0.1	3.94
384.19	0.1	5.34
385.19	2.4	100.00
386.19	0.3	12.41
387.18	0.0	1.46
398.15	0.1	2.43
424.28	0.1	3.12
433.15	0.0	0.90
433.32	0.0	0.91
440.19	0.4	15.44
441.22	0.1	3.60
442.23	0.3	10.86
458.28	0.2	7.86

459.29	0.0	0.77
498.26	0.0	0.77
530.39	0.0	0.76
572.30	1.2	50.97
573.31	0.6	23.76
574.26	0.1	2.82
574.44	0.0	2.07
575.34	0.8	32.43
576.31	0.2	7.57
577.22	0.0	0.73
604.34	0.2	6.57
605.31	0.0	1.57
646.38	0.2	7.86
647.24	0.0	1.56
647.50	0.0	1.08

HMG 55 Mass spectral peak lists

SPECTRUM - MS

7-22-13_HMG55_1236_MS2_01.raw

ITMS + p ESI E Full ms2 1236.10@cid35.00 [340.00-2000.00]

Scan #: 1-20

RT: 0.00-3.69

AV: 20

m/z	Intensity	Relative
486.28	149.1	8.94
646.36	58.2	3.49
660.38	387.0	23.20
661.39	108.9	6.53
685.40	160.0	9.59
685.91	107.2	6.43
692.41	88.7	5.32
692.92	58.7	3.52
724.45	86.9	5.21
885.99	79.6	4.77
886.51	69.0	4.13
901.02	62.0	3.72
901.51	56.2	3.37
917.03	437.3	26.22
917.53	378.2	22.68
918.03	159.9	9.59
918.54	46.0	2.76
1004.09	1667.8	100.00
1004.58	1549.3	92.89
1005.09	778.8	46.70
1005.57	227.1	13.61
1080.59	67.9	4.07
1081.08	64.5	3.87
1109.56	106.7	6.40
1110.57	51.4	3.08
1117.63	679.0	40.71
1118.13	713.2	42.76
1118.63	405.5	24.31
1119.14	147.6	8.85
1132.61	123.8	7.42
1133.10	125.5	7.52
1133.61	76.5	4.59
1141.62	67.9	4.07
1142.11	62.1	3.72
1142.62	42.5	2.55
1235.69	598.3	35.87
1236.18	754.8	45.25
1236.66	524.8	31.46
1237.16	230.3	13.81
1347.73	209.4	12.55
1348.74	132.2	7.92

1349.74	43.3	2.60
1361.72	176.2	10.57
1362.73	105.2	6.31
1811.06	336.8	20.19
1812.06	276.9	16.60
1813.07	130.6	7.83
1985.27	208.8	12.52
1986.28	199.4	11.96
1987.28	94.0	5.64

SPECTRUM - MS

7-22-13_HMG55_1236_MS3_1109_01.raw

ITMS + p ESI E Full ms3 1236.10@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-20

RT: 0.00-3.44

AV: 20

m/z Intensity Relative

385.19	2.5	3.44
386.17	0.3	0.45
398.19	0.5	0.69
412.25	0.7	0.97
440.21	0.5	0.72
442.20	0.4	0.55
454.26	0.3	0.42
458.27	0.3	0.44
472.27	0.4	0.52
486.26	13.7	18.67
487.28	2.3	3.09
572.30	1.4	1.89
573.22	0.5	0.62
573.41	0.4	0.57
575.32	1.1	1.49
598.29	1.2	1.68
599.32	0.5	0.66
646.34	73.3	100.00
647.36	17.2	23.41
648.35	2.4	3.31
660.38	0.3	0.43
690.40	0.8	1.03
708.36	4.7	6.34
709.38	0.8	1.05
778.37	0.4	0.50
780.48	0.6	0.81
782.54	1.1	1.56
784.45	2.5	3.35
786.44	0.5	0.73
799.41	5.4	7.41
800.41	1.9	2.56
872.39	0.4	0.57
873.46	39.2	53.48

874.46	16.2	22.15	
875.47	2.5	3.41	
876.37	1.0	1.33	
891.43	0.4	0.52	
903.41	0.6	0.76	
905.43	1.6	2.14	
921.47	0.7	0.94	
958.23	1.6	2.17	
960.25	0.5	0.67	
1035.51		0.7	0.92
1050.27		0.4	0.54
1067.53		1.1	1.56
1079.58		0.3	0.44
1108.26		1.9	2.60
1109.56		15.4	20.99
1110.54		9.1	12.41
1111.60		2.3	3.17

SPECTRUM - MS

7-22-13_HMG55_1236_MS4_1109_486_02.raw

ITMS + p ESI E Full ms4 1236.10@cid35.00 1110.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-9.67

AV: 50

m/z	Intensity	Relative
149.01	0.0	0.74
154.01	0.0	0.88
178.01	0.0	1.37
208.08	0.0	4.22
211.10	0.0	0.84
218.00	0.0	0.60
220.03	0.0	2.08
221.05	0.0	0.90
241.04	0.0	2.58
241.19	0.0	1.75
248.06	0.0	0.60
250.15	0.1	6.36
252.03	0.1	8.15
252.18	0.1	5.21
252.97	0.0	0.67
257.12	0.0	1.29
257.26	0.0	0.76
259.10	1.1	97.07
260.08	0.1	5.59
260.22	0.0	4.09
268.15	0.1	10.41
268.99	0.0	1.70
273.99	0.0	0.64
297.15	0.0	0.60
301.16	0.0	1.85

325.79	0.0	1.06
326.12	0.0	0.71
329.18	0.3	29.27
330.19	0.0	3.44
336.13	0.0	0.69
352.24	0.0	1.08
382.30	0.0	0.61
383.86	0.0	0.77
384.13	0.0	2.01
384.46	0.0	0.62
412.22	1.2	100.00
413.23	0.1	11.19
414.20	0.0	0.66
415.13	0.0	1.49
415.29	0.0	2.57
416.12	0.0	0.69
430.92	0.0	0.65
444.26	1.0	82.59
445.12	0.1	7.19
445.31	0.1	11.19
454.32	0.0	0.94
456.29	0.0	1.15
484.16	0.0	0.66
486.30	0.4	32.36
487.46	0.0	2.46

SPECTRUM - MS

7-22-13_HMG55_1236_MS4_1109_646_01.raw

ITMS + p ESI E Full ms4 1236.10@cid35.00 1110.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-50

RT: 0.00-9.68

AV: 50

m/z Intensity Relative

194.02	0.1	1.09
203.99	0.2	1.74
211.06	0.1	0.96
220.08	0.1	1.05
227.08	1.0	11.25
228.12	0.1	0.63
229.10	0.4	4.38
236.07	0.6	7.00
245.08	1.8	19.20
246.08	0.1	1.26
287.12	0.1	1.60
292.05	0.1	0.63
315.14	0.2	2.52
343.16	0.4	4.67
366.17	0.3	2.81
367.19	0.2	1.73
368.19	0.2	2.36

369.27	0.1	0.71
371.18	0.1	1.35
378.19	0.4	3.91
379.17	0.1	0.60
380.19	0.3	3.71
381.17	0.1	0.75
382.21	0.5	5.45
383.21	0.1	1.16
384.17	0.5	5.50
385.17	9.2	100.00
386.19	1.0	10.42
396.30	0.1	0.81
398.23	0.1	1.15
408.26	0.1	0.78
424.19	0.5	5.54
433.34	0.1	0.77
440.21	1.7	18.37
441.23	0.3	3.33
442.23	1.3	13.76
443.28	0.1	1.15
458.22	0.8	8.28
459.18	0.1	1.14
498.19	0.1	0.76
530.24	0.1	0.68
572.29	5.4	58.66
573.30	2.1	22.38
574.31	0.2	2.60
575.32	2.8	30.80
576.34	0.6	6.10
604.34	0.6	6.83
605.37	0.1	0.96
646.32	1.5	16.12
647.34	0.4	3.99

SPECTRUM - MS

7-22-13_HMG55_1236_MS3_660_01.raw

ITMS + p ESI E Full ms3 1236.10@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-50

RT: 0.00-11.58

AV: 50

m/z Intensity Relative

229.11	1.7	6.93
236.07	1.0	3.89
241.10	0.9	3.77
259.11	24.6	100.00
260.12	2.1	8.35
287.12	0.4	1.69
301.14	0.4	1.47
325.17	0.3	1.42
338.20	0.4	1.68

350.19	0.3	1.39
364.19	1.0	4.18
368.19	0.4	1.44
369.21	0.4	1.45
382.22	0.8	3.06
398.21	0.6	2.34
400.23	0.7	2.71
412.23	1.3	5.45
424.20	2.1	8.55
426.22	2.0	8.05
430.25	0.6	2.38
440.20	0.4	1.78
442.26	8.3	33.63
443.26	1.4	5.78
447.26	0.5	1.99
454.23	1.2	4.79
456.25	1.2	4.95
472.24	11.4	46.07
473.24	2.1	8.57
486.26	1.1	4.39
515.29	0.9	3.70
540.25	0.5	1.96
554.31	0.4	1.65
556.33	0.7	2.76
562.33	0.8	3.19
570.30	0.6	2.45
584.29	1.0	3.87
586.31	15.2	61.72
587.32	3.9	15.97
589.33	6.7	27.26
590.35	1.6	6.62
597.36	0.9	3.45
597.84	0.3	1.41
614.32	3.0	12.00
615.32	0.8	3.05
618.35	19.2	77.76
619.36	4.8	19.37
624.36	0.5	1.85
630.34	0.7	2.79
660.38	9.6	38.81
661.40	1.9	7.91

HMG 56 Mass spectral peak lists

SPECTRUM - MS

6-27-13_HMG56_1235_MS2_01.raw

ITMS + p ESI E Full ms2 1236.00@cid35.00 [340.00-2000.00]

Scan #: 1-20

RT: 0.00-1.68

AV: 20

m/z	Intensity	Relative
433.28	426.4	11.58
486.31	391.3	10.63
646.41	145.0	3.94
660.42	1624.8	44.15
661.43	442.8	12.03
685.45	465.5	12.65
685.96	296.2	8.05
692.46	133.2	3.62
724.49	279.1	7.58
799.01	344.4	9.36
799.52	246.5	6.70
901.07	137.7	3.74
917.10	1314.4	35.71
917.59	1070.6	29.09
918.09	459.5	12.48
1004.15	3680.6	100.00
1004.65	3443.7	93.56
1005.15	1688.1	45.87
1005.66	287.2	7.80
1030.66	1100.6	29.90
1031.15	1021.1	27.74
1031.65	518.0	14.07
1109.64	317.6	8.63
1110.64	142.1	3.86
1117.70	1031.0	28.01
1118.20	1082.2	29.40
1118.70	633.2	17.20
1132.69	357.8	9.72
1133.18	399.4	10.85
1133.68	238.4	6.48
1141.69	167.1	4.54
1142.19	160.9	4.37
1235.24	139.8	3.80
1235.78	2186.0	59.39
1236.26	2741.5	74.49
1236.74	1798.0	48.85
1237.25	362.9	9.86
1347.82	865.9	23.53
1348.82	529.5	14.39
1349.82	156.0	4.24
1361.82	442.9	12.03

1362.82	252.7	6.87
1574.96	462.3	12.56
1575.95	357.1	9.70
1811.18	1566.9	42.57
1812.19	1333.2	36.22
1813.19	575.5	15.64
1985.39	602.5	16.37
1986.41	541.1	14.70
1987.41	263.5	7.16

SPECTRUM - MS

6-27-13_HMG56_1235_MS3_1109_01.raw

ITMS + p ESI E Full ms3 1236.00@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-50

RT: 0.00-4.82

AV: 50

m/z Intensity Relative

343.27	0.1	0.26
384.19	0.2	0.38
385.20	1.8	3.38
386.21	0.2	0.40
398.24	0.4	0.78
412.22	0.3	0.66
412.40	0.2	0.37
440.24	0.3	0.61
442.27	0.3	0.62
454.25	0.3	0.50
458.31	0.3	0.65
470.34	0.1	0.23
472.27	0.4	0.73
486.30	8.5	16.20
487.31	1.3	2.39
524.24	0.1	0.28
572.36	0.8	1.53
573.30	0.3	0.66
575.37	0.6	1.22
598.42	0.7	1.34
599.25	0.1	0.28
599.40	0.2	0.29
604.47	0.1	0.23
646.39	52.8	100.00
647.40	9.3	17.58
660.48	0.2	0.31
669.48	0.1	0.24
690.42	0.3	0.63
691.40	0.1	0.23
706.40	0.2	0.28
708.42	3.2	5.97
709.40	0.6	1.10
778.40	0.1	0.25

778.56	0.1	0.20	
799.45	6.1	11.61	
800.47	1.8	3.35	
873.52	42.6	80.63	
874.53	11.7	22.12	
891.55	0.4	0.75	
903.43	0.3	0.51	
903.61	0.3	0.54	
905.61	0.7	1.25	
906.59	0.2	0.37	
1035.50		0.2	0.37
1035.70		0.3	0.52
1038.57		0.2	0.30
1067.62		0.6	1.21
1068.63		0.3	0.60
1109.63		5.2	9.76
1110.63		2.1	3.93

SPECTRUM - MS

1-16-14_HMG56_1235_MS4_1109_486_02.raw

ITMS + p ESI E Full ms4 1236.00@cid35.00 1110.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-100

RT: 0.00-30.87

AV: 100

m/z	Intensity	Relative
178.04	0.0	1.46
208.11	0.0	2.71
209.06	0.0	0.51
210.04	0.0	0.62
211.12	0.0	0.86
217.37	0.0	1.39
227.24	0.0	0.35
241.06	0.0	7.15
250.08	0.0	5.66
251.06	0.0	0.56
252.11	0.0	13.04
253.11	0.0	2.87
254.02	0.0	0.50
257.04	0.0	0.29
257.20	0.0	0.61
259.10	0.3	94.19
260.02	0.0	3.15
260.16	0.0	3.86
268.13	0.0	1.82
289.89	0.0	0.53
301.23	0.0	0.59
314.09	0.0	0.44
324.04	0.0	0.53
329.14	0.0	0.46
329.26	0.0	0.40

330.02	0.0	0.43
338.13	0.0	0.26
339.06	0.0	0.45
341.04	0.0	0.48
362.03	0.0	0.34
366.92	0.0	0.36
367.23	0.0	0.79
368.29	0.0	0.35
370.26	0.0	0.40
383.97	0.0	0.79
384.25	0.0	2.10
391.38	0.0	1.09
395.08	0.0	0.48
408.37	0.0	0.50
412.18	0.3	100.00
413.21	0.0	12.82
415.21	0.0	1.95
432.15	0.0	0.54
444.26	0.1	29.95
445.12	0.0	2.81
445.28	0.0	2.96
454.24	0.0	0.38
456.37	0.0	0.36
486.22	0.0	7.39
487.24	0.0	2.13

SPECTRUM - MS

6-27-13_HMG56_1235_MS4_1109_646_01.raw

ITMS + p ESI E Full ms4 1236.00@cid35.00 1110.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-100

RT: 0.00-9.83

AV: 100

m/z Intensity Relative

194.14	0.0	0.63
204.01	0.0	1.02
218.06	0.0	0.83
220.16	0.0	0.65
227.09	0.6	12.41
229.11	0.2	5.38
236.09	0.4	8.89
245.10	0.9	20.35
287.18	0.0	0.94
315.26	0.0	1.00
324.22	0.0	0.81
343.29	0.1	2.32
344.14	0.0	0.59
353.25	0.0	0.91
366.13	0.1	1.39
366.30	0.0	0.76
367.12	0.1	1.21

368.30	0.1	1.35
369.23	0.1	1.41
369.38	0.0	0.76
371.20	0.0	0.97
378.25	0.2	3.53
380.21	0.2	3.91
382.27	0.2	4.56
384.24	0.3	5.54
385.21	4.6	100.00
386.21	0.5	9.72
398.27	0.1	2.15
408.27	0.1	1.08
424.25	0.3	6.05
440.26	0.8	16.60
441.19	0.1	2.48
442.29	0.7	15.46
443.24	0.1	1.57
443.38	0.0	0.97
458.26	0.4	9.70
498.27	0.0	0.66
501.38	0.0	0.83
517.30	0.0	0.98
530.37	0.0	0.64
542.24	0.0	0.66
572.34	2.9	61.94
573.36	0.9	19.35
574.40	0.1	1.19
575.36	1.5	32.18
576.45	0.1	3.23
604.40	0.3	6.59
605.47	0.0	0.93
646.46	0.3	6.40
647.51	0.1	1.30

SPECTRUM - MS

6-27-13_HMG56_1235_MS3_660_01.raw

ITMS + p ESI E Full ms3 1236.00@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-50

RT: 0.00-3.68

AV: 50

m/z Intensity Relative

208.09	1.3	0.43
211.09	1.0	0.35
227.09	0.8	0.29
229.12	1.1	0.39
245.10	10.6	3.59
250.11	1.8	0.59
259.13	4.2	1.40
285.14	1.5	0.50
313.16	2.0	0.68

323.20	1.4	0.46
353.21	6.6	2.24
354.22	0.8	0.27
382.23	1.0	0.33
383.24	5.4	1.83
384.21	1.0	0.33
387.27	4.0	1.34
398.24	12.4	4.17
399.23	2.0	0.68
415.27	40.2	13.58
416.28	6.4	2.15
417.26	1.3	0.44
424.24	1.5	0.51
430.29	2.3	0.79
431.24	10.6	3.58
432.27	1.2	0.40
433.28	296.0	100.00
434.28	44.9	15.16
454.21	0.8	0.27
456.33	1.6	0.55
472.28	70.4	23.77
473.30	11.8	3.99
486.29	1.1	0.37
515.32	4.3	1.44
516.35	1.1	0.36
554.36	0.9	0.31
558.24	5.1	1.73
559.36	0.9	0.30
562.45	1.9	0.63
586.36	138.6	46.83
587.37	33.7	11.37
589.38	4.3	1.45
590.41	1.1	0.39
597.40	2.3	0.77
597.89	1.2	0.41
614.36	2.3	0.76
618.39	46.4	15.67
619.39	11.3	3.81
624.39	1.3	0.42
660.42	41.6	14.06
661.43	8.9	3.01

SPECTRUM - MS

6-27-13_HMG56_1235_MS3_486_01.raw

ITMS + p ESI E Full ms3 1236.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-3.67

AV: 50

m/z	Intensity	Relative
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177.04	0.1	0.19
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178.05	0.4	1.10
208.09	2.1	5.56
209.12	0.2	0.52
211.12	0.1	0.21
218.10	0.2	0.61
227.08	0.1	0.19
241.12	1.3	3.54
242.11	0.1	0.31
250.11	3.4	8.99
251.10	0.5	1.23
252.13	5.3	14.07
253.15	0.6	1.61
257.11	0.7	1.83
259.13	36.9	98.12
260.14	2.8	7.40
268.17	0.6	1.50
301.29	0.1	0.33
312.16	0.1	0.38
314.20	0.4	0.95
326.18	0.1	0.32
329.22	0.1	0.38
338.15	0.1	0.26
339.21	0.1	0.32
341.19	0.3	0.68
352.22	0.1	0.23
356.23	0.1	0.40
357.25	0.1	0.35
370.28	0.2	0.57
380.21	0.1	0.19
382.27	0.3	0.72
384.17	1.5	3.87
385.23	0.2	0.50
387.19	0.1	0.28
410.20	0.2	0.60
410.33	0.1	0.40
412.25	37.6	100.00
413.26	6.2	16.51
415.28	0.5	1.27
426.13	0.1	0.22
426.33	0.3	0.73
427.35	0.1	0.23
444.29	12.4	33.13
445.29	2.1	5.61
454.31	0.6	1.64
455.35	0.1	0.33
456.35	3.1	8.34
457.35	0.7	1.78
486.29	8.1	21.63
487.33	1.5	3.97

HMG 60 Mass spectral peak lists

SPECTRUM - MS

12-17-13_HMG60_1236_MS2_01.raw

ITMS + p ESI E Full ms2 1236.10@cid35.00 [340.00-2000.00]

Scan #: 1-20

RT: 0.00-1.98

AV: 20

m/z	Intensity	Relative
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433.22	139.6	33.88
434.23	24.5	5.94
486.25	19.0	4.60
586.28	23.1	5.61
660.31	280.9	68.16
661.32	79.8	19.36
724.38	28.0	6.80
779.42	20.7	5.03
834.39	73.8	17.89
835.39	29.9	7.25
916.97	153.3	37.19
917.46	143.0	34.69
917.96	75.0	18.19
918.47	22.6	5.48
935.40	20.0	4.86
993.46	27.2	6.60
993.98	29.0	7.04
1003.98	96.1	23.31
1004.49	92.4	22.42
1004.98	51.2	12.41
1030.51	297.1	72.09
1030.99	297.2	72.12
1031.48	176.1	42.74
1031.99	61.9	15.02
1062.16	33.7	8.17
1117.53	72.3	17.54
1118.04	99.2	24.07
1118.54	57.1	13.85
1119.07	22.3	5.41
1120.09	32.2	7.82
1173.56	66.1	16.05
1174.57	38.0	9.23
1235.62	296.0	71.83
1236.10	397.7	96.48
1236.58	283.2	68.70
1237.08	150.9	36.62
1361.60	23.1	5.61
1400.65	69.0	16.73
1401.66	45.9	11.13
1402.64	21.0	5.10
1535.69	29.3	7.11

1536.70	22.0	5.33
1636.74	84.0	20.38
1637.75	68.2	16.55
1638.76	31.2	7.58
1810.85	412.1	100.00
1811.86	351.6	85.32
1812.86	178.6	43.33
1813.88	51.4	12.47
1984.98	36.3	8.82

SPECTRUM - MS

12-17-13_HMG60_1236_MS3_917_01.raw

ITMS + p ESI E Full ms3 1236.10@cid35.00 917.50@cid35.00 [250.00-2000.00]

Scan #: 1-21

RT: 0.00-4.30

AV: 21

m/z Intensity Relative

415.21	0.7	1.08
433.22	21.2	35.07
434.23	3.9	6.47
435.23	0.6	0.94
472.26	1.5	2.43
534.34	1.6	2.73
586.28	3.7	6.10
587.27	1.0	1.58
660.31	40.7	67.42
661.32	12.4	20.62
662.32	2.3	3.79
664.40	0.8	1.36
674.85	1.2	1.96
675.33	0.9	1.56
692.38	6.5	10.78
692.89	4.3	7.21
693.38	1.8	3.03
699.34	0.6	0.92
704.33	0.6	1.04
706.40	2.4	3.97
707.39	0.9	1.44
711.84	1.2	1.95
712.35	0.8	1.34
724.38	11.5	19.04
725.40	4.3	7.08
726.41	0.8	1.32
814.92	0.6	1.07
822.92	0.6	0.97
823.45	0.6	0.94
916.97	18.0	29.90
917.47	18.9	31.29
917.97	11.0	18.28
918.47	3.3	5.47

1065.45	1.3	2.15
1066.44	0.8	1.31
1109.50	3.7	6.08
1110.49	1.8	2.99
1173.58	60.3	100.00
1174.58	35.3	58.52
1175.56	11.1	18.36
1176.55	1.5	2.44
1326.61	0.5	0.75
1361.62	1.6	2.71
1362.63	1.2	2.00
1363.63	0.5	0.77
1400.67	20.3	33.66
1401.68	14.4	23.88
1402.65	5.2	8.59
1403.66	0.9	1.56
1418.65	0.5	0.79

SPECTRUM - MS

12-17-13_HMG60_1236_MS4_917_1173_01.raw

ITMS + p ESI E Full ms4 1236.10@cid35.00 917.50@cid35.00 1174.00@cid35.00 [320.00-1200.00]

Scan #: 1-20

RT: 0.00-3.77

AV: 20

m/z Intensity Relative

384.15	0.0	0.11
384.34	0.0	0.13
435.30	0.3	0.80
436.27	0.1	0.20
456.31	0.1	0.14
470.39	0.0	0.11
472.20	0.3	0.76
472.40	0.2	0.44
473.27	0.0	0.12
474.26	0.2	0.44
486.32	0.3	0.93
487.30	0.1	0.23
492.27	0.1	0.18
502.30	0.1	0.22
516.26	0.1	0.23
534.33	10.5	29.30
535.33	2.1	5.80
536.06	0.0	0.11
536.34	0.1	0.40
562.34	0.1	0.37
590.31	0.2	0.55
625.35	0.4	0.98
626.31	0.1	0.31
651.33	0.0	0.12
662.29	0.3	0.94

663.36	0.1	0.39
692.35	0.1	0.27
724.39	36.0	100.00
725.39	9.7	26.87
726.41	1.2	3.39
752.46	0.0	0.12
877.42	0.1	0.17
921.45	0.1	0.21
969.48	1.4	3.75
970.47	0.5	1.44
971.57	0.1	0.20
1067.52		0.3 0.96
1068.50		0.1 0.38
1074.49		0.4 1.10
1075.58		0.1 0.30
1100.56		0.0 0.11
1131.63		0.1 0.16
1141.55		0.4 1.05
1142.46		0.2 0.58
1142.69		0.1 0.32
1143.53		0.2 0.65
1144.51		0.1 0.16
1173.59		3.7 10.27
1174.57		2.0 5.62
1175.53		0.7 1.85

SPECTRUM - MS

12-17-13_HMG60_1236_MS3_1109_01.raw

ITMS + p ESI E Full ms3 1236.10@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-50

RT: 0.00-35.61

AV: 50

m/z Intensity Relative

424.25	0.0	1.25
433.21	0.2	11.16
434.32	0.0	0.96
472.25	0.6	33.48
473.24	0.1	6.10
586.28	0.1	4.32
625.26	0.2	10.53
626.29	0.0	1.50
657.44	0.0	1.14
660.31	1.3	72.96
661.31	0.3	18.18
662.34	0.0	1.05
699.34	1.8	100.00
700.34	0.5	25.57
701.40	0.0	0.94
948.47	0.0	0.72
952.41	0.1	2.88

980.44	0.2	12.84	
981.35	0.0	2.41	
1021.38		0.0	0.66
1028.32		0.0	0.72
1034.53		0.0	1.52
1036.38		0.0	1.17
1036.61		0.0	0.68
1040.47		0.0	0.76
1048.33		0.0	0.73
1048.61		0.0	0.86
1049.17		0.0	0.72
1050.51		0.0	0.67
1051.44		0.0	0.67
1058.47		0.0	0.78
1064.44		0.0	1.32
1070.64		0.0	2.08
1072.51	0.2	13.17	
1073.38	0.0	0.78	
1073.58	0.0	0.68	
1076.43	0.2	12.51	
1077.35	0.0	1.11	
1077.56	0.0	0.71	
1078.59	0.0	1.84	
1079.27	0.0	1.01	
1079.44	0.0	0.87	
1079.63	0.0	1.02	
1080.05	0.0	0.66	
1080.31	0.0	1.34	
1090.56	0.1	5.47	
1108.45	0.1	4.53	
1109.47	0.3	14.65	
1110.46	0.1	7.48	
1111.44	0.0	0.71	

SPECTRUM - MS

12-17-13_HMG60_1236_MS4_1109_472_01.raw

ITMS + p ESI E Full ms4 1236.10@cid35.00 1110.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-81.63

AV: 50

m/z	Intensity	Relative
148.96	0.0	1.70
154.81	0.0	0.78
170.99	0.0	4.14
179.96	0.0	4.03
180.13	0.0	1.12
193.97	0.0	5.22
203.87	0.0	1.05
204.09	0.0	2.30
218.06	0.0	2.52

220.07	0.0	15.12
221.13	0.0	0.80
227.06	0.0	63.90
228.13	0.0	1.27
236.03	0.0	11.65
237.05	0.0	1.05
237.98	0.0	1.42
243.12	0.0	2.89
245.08	0.0	23.51
245.99	0.0	1.42
250.07	0.0	1.12
252.11	0.0	0.87
268.10	0.0	100.00
269.19	0.0	11.13
286.93	0.0	0.83
287.11	0.0	2.27
315.15	0.0	97.43
316.17	0.0	7.92
324.14	0.0	2.59
325.31	0.0	1.21
327.20	0.0	1.08
353.14	0.0	1.02
366.20	0.0	1.26
368.12	0.0	1.11
369.88	0.0	1.14
380.21	0.0	4.00
396.33	0.0	1.68
398.26	0.0	9.28
399.16	0.0	2.44
408.26	0.0	1.17
430.12	0.0	1.56
430.33	0.0	1.17
439.87	0.0	1.13
440.20	0.0	13.78
442.12	0.0	4.21
442.28	0.0	4.46
442.54	0.0	0.82
455.28	0.0	0.90
472.30	0.0	10.48
473.31	0.0	1.41
480.96	0.0	1.19

SPECTRUM - MS

12-17-13_HMG60_1236_MS4_1109_660_01.raw

ITMS + p ESI E Full ms4 1236.10@cid35.00 1110.00@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-51

RT: 0.00-28.05

AV: 51

m/z	Intensity	Relative
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210.97	0.0	0.50
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211.93	0.0	0.26
245.08	0.0	3.21
246.01	0.0	0.27
246.19	0.0	0.46
313.13	0.0	0.48
323.16	0.0	0.51
353.02	0.0	0.57
353.19	0.0	1.39
366.25	0.0	0.51
368.17	0.0	0.33
383.23	0.0	1.38
387.22	0.0	0.63
398.20	0.0	2.10
415.21	0.0	9.64
416.25	0.0	0.77
431.27	0.0	1.38
432.27	0.0	0.41
433.22	0.5	100.00
434.20	0.0	9.29
435.23	0.0	0.33
472.24	0.1	12.27
473.21	0.0	1.07
473.37	0.0	0.40
475.49	0.0	0.34
513.24	0.0	0.34
515.28	0.0	1.07
530.27	0.0	0.30
544.27	0.0	0.37
556.27	0.0	0.49
557.32	0.0	0.25
558.22	0.0	1.36
559.18	0.0	0.51
584.27	0.0	0.32
586.27	0.2	45.49
586.98	0.0	0.39
587.29	0.0	8.68
587.61	0.0	0.42
588.29	0.0	0.71
589.43	0.0	0.54
614.30	0.0	0.25
617.96	0.0	0.25
618.34	0.0	9.20
619.22	0.0	0.70
619.39	0.0	1.28
628.30	0.0	0.41
659.98	0.0	0.89
660.32	0.1	18.95
661.07	0.0	0.56
661.44	0.0	1.67

SPECTRUM - MS

12-17-13_HMG60_1236_MS3_1004_01.raw

ITMS + p ESI E Full ms3 1236.10@cid35.00 1004.60@cid35.00 [275.00-2000.00]

Scan #: 1-20

RT: 0.00-4.21

AV: 20

m/z Intensity Relative

433.22	6.7	34.37
434.22	1.1	5.54
472.27	1.6	8.23
514.28	0.6	3.18
534.33	0.7	3.32
664.38	1.5	7.42
685.37	0.6	3.23
704.31	1.0	5.26
706.39	3.8	19.39
707.39	1.3	6.78
724.39	3.4	17.42
725.40	1.2	6.19
760.45	0.6	3.28
768.49	0.6	3.03
770.41	0.8	4.10
779.42	19.6	100.00
779.92	14.4	73.40
780.43	5.7	29.05
780.93	1.3	6.43
798.88	0.9	4.84
799.40	0.7	3.73
834.40	11.3	57.58
835.42	4.1	20.96
836.41	0.8	4.04
886.35	1.1	5.36
888.27	1.6	8.10
901.95	1.1	5.55
902.46	1.1	5.83
902.95	0.5	2.58
909.96	1.6	8.30
910.46	1.7	8.50
910.97	0.8	4.12
946.22	1.2	5.99
1004.00	6.9	34.99
1004.51	7.4	37.52
1004.99	4.5	22.98
1005.53	1.8	9.30
1065.45	2.1	10.78
1066.45	0.9	4.71
1125.56	1.6	8.03
1126.57	0.9	4.38
1173.59	16.3	83.01
1174.58	9.3	47.25
1175.56	2.7	13.63

1535.70	2.4	12.42
1536.72	1.7	8.60
1574.73	9.4	47.76
1575.76	7.9	40.20
1576.76	2.6	13.21
1577.70	0.5	2.73

SPECTRUM - MS

12-17-13_HMG60_1236_MS4_1004_1174_01.raw

ITMS + p ESI E Full ms4 1236.10@cid35.00 1004.60@cid35.00 1174.00@cid35.00 [320.00-1200.00]

Scan #: 1-20

RT: 0.00-4.22

AV: 20

m/z Intensity Relative

435.24	0.1	1.43
470.32	0.0	0.35
472.30	0.1	1.57
474.27	0.0	0.37
486.17	0.0	0.24
486.37	0.0	0.32
487.22	0.0	0.41
492.38	0.0	0.23
502.15	0.0	0.28
516.30	0.0	0.37
534.33	2.0	28.24
535.33	0.4	5.30
536.32	0.0	0.27
562.28	0.0	0.31
590.49	0.0	0.22
591.35	0.0	0.19
625.37	0.1	1.93
626.30	0.0	0.21
637.43	0.0	0.28
662.25	0.0	0.62
692.30	0.0	0.27
706.38	0.0	0.25
724.38	7.1	100.00
725.40	1.8	25.40
726.39	0.1	1.81
726.58	0.1	0.76
863.22	0.0	0.19
951.43	0.0	0.46
952.52	0.0	0.22
969.47	0.1	1.77
969.61	0.1	0.95
970.48	0.1	1.05
971.58	0.0	0.22
1014.09	0.0	0.22
1067.43	0.0	0.48
1067.62	0.0	0.51

1074.53	0.0	0.48
1075.34	0.0	0.24
1075.54	0.0	0.31
1141.42	0.1	0.89
1141.67	0.0	0.37
1142.42	0.0	0.44
1142.68	0.0	0.56
1143.55	0.0	0.70
1144.58	0.0	0.22
1173.59	0.8	10.73
1174.50	0.3	4.06
1174.68	0.2	3.13
1174.94	0.0	0.19
1175.68	0.0	0.65

SPECTRUM - MS

12-17-13_HMG60_1236_MS3_834_01.raw

ITMS + p ESI E Full ms3 1236.10@cid35.00 835.00@cid35.00 [225.00-900.00]

Scan #: 1-50

RT: 0.00-12.82

AV: 50

m/z Intensity Relative

245.15	0.1	0.69
299.12	0.0	0.41
353.14	0.1	1.09
364.16	0.1	0.91
368.16	0.1	1.04
383.16	0.1	1.35
384.15	0.0	0.45
387.20	0.0	0.38
401.16	0.0	0.45
415.21	0.9	8.07
416.23	0.1	1.18
424.19	0.2	2.18
426.21	0.1	1.02
431.23	0.2	1.44
433.21	10.6	100.00
434.22	1.8	17.51
435.23	0.2	2.08
442.22	0.5	4.90
443.21	0.1	0.91
558.21	0.1	0.67
572.25	0.4	3.45
573.24	0.1	1.11
586.28	0.2	1.84
604.28	0.1	0.57
621.32	0.1	0.87
628.29	0.1	1.19
632.29	0.0	0.40
646.28	4.5	42.15

647.30	1.2	11.81
648.29	0.2	2.08
660.28	0.2	1.83
689.32	0.1	1.40
690.32	0.1	0.49
730.34	0.1	0.50
758.32	0.1	0.78
759.39	0.0	0.38
760.34	5.3	50.55
761.35	1.9	17.82
762.36	0.3	2.92
763.31	0.4	3.41
764.40	0.1	0.79
788.32	0.2	1.99
789.25	0.0	0.37
792.38	1.0	9.89
793.40	0.4	3.43
794.41	0.1	0.88
804.27	0.0	0.46
834.38	1.6	15.29
835.41	0.6	5.21
836.46	0.1	0.87

SPECTRUM - MS

12-17-13_HMG60_1236_MS4_834_646_01.raw

ITMS + p ESI E Full ms4 1236.10@cid35.00 835.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-50

RT: 0.00-12.18

AV: 50

m/z	Intensity	Relative
204.95	0.0	1.01
218.11	0.0	1.64
220.13	0.0	1.37
227.10	0.0	1.32
229.05	0.0	8.00
230.03	0.0	1.12
236.09	0.0	5.22
237.09	0.0	0.94
245.10	0.1	13.11
246.08	0.0	1.15
335.93	0.0	1.21
350.05	0.0	1.44
364.11	0.0	3.55
364.31	0.0	2.11
365.10	0.0	1.09
365.28	0.0	1.21
366.22	0.0	1.20
368.15	0.0	6.29
369.12	0.0	3.66
382.15	0.0	1.21

384.12	0.0	2.49
385.23	0.0	1.32
396.14	0.0	0.85
398.16	0.0	3.26
398.34	0.0	0.98
408.12	0.0	1.13
415.17	0.0	2.85
417.21	0.0	3.12
424.20	0.1	11.62
425.31	0.0	1.51
426.23	0.0	3.86
433.22	0.5	100.00
434.22	0.1	18.13
435.24	0.0	2.14
440.16	0.0	2.20
442.18	0.0	4.62
442.42	0.0	1.13
458.24	0.0	7.80
459.26	0.0	0.97
475.08	0.0	2.69
540.19	0.0	2.54
554.26	0.0	1.37
572.25	0.5	89.54
573.17	0.1	17.80
573.38	0.0	8.13
574.34	0.0	3.17
576.18	0.0	1.06
604.30	0.0	3.30
646.38	0.1	10.04
647.28	0.0	4.75

SPECTRUM - MS

12-17-13_HMG60_1236_MS3_935_01.raw

ITMS + p ESI E Full ms3 1236.10@cid35.00 936.00@cid35.00 [255.00-1000.00]

Scan #: 1-20

RT: 0.00-3.96

AV: 20

m/z Intensity Relative

398.16	0.0	0.76
412.15	0.1	2.21
413.22	0.0	0.51
424.21	0.1	1.48
430.15	0.0	0.46
440.23	0.0	0.51
472.25	4.5	98.60
473.35	0.5	10.10
474.25	0.1	1.81
486.26	2.3	50.25
487.24	0.5	11.06
488.19	0.0	0.81

625.28	0.8	17.30
626.39	0.1	3.09
627.31	0.0	0.89
657.24	0.0	0.98
699.34	4.6	100.00
700.33	1.3	28.35
701.29	0.3	6.33
708.21	0.0	0.33
712.41	0.0	0.37
724.19	0.0	0.35
724.31	0.0	0.50
724.52	0.0	1.04
778.40	0.0	0.63
780.48	0.0	0.48
788.39	0.0	0.44
818.25	0.0	0.39
825.76	0.0	0.39
830.00	0.0	0.41
859.46	0.0	0.44
864.32	0.0	0.97
864.55	0.0	0.49
875.43	0.0	0.52
889.40	0.0	0.42
893.41	0.1	1.22
899.32	0.0	1.03
899.50	0.1	1.80
899.98	0.1	1.27
900.35	0.0	0.65
903.34	0.0	0.48
904.30	0.0	0.89
905.30	0.0	0.48
917.30	0.0	0.35
919.34	0.0	0.40
935.40	1.2	25.26
936.42	0.6	13.91
936.99	0.0	0.37
937.40	0.1	2.50
937.60	0.0	0.98

SPECTRUM - MS

12-17-13_HMG60_1236_MS4_935_486_01.raw

ITMS + p ESI E Full ms4 1236.10@cid35.00 936.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-36.36

AV: 50

m/z	Intensity	Relative
177.90	0.0	0.57
190.01	0.0	0.40
208.05	0.0	5.42
208.76	0.0	0.27

209.06	0.0	0.59
210.11	0.0	0.31
211.16	0.0	0.33
213.05	0.0	0.80
218.08	0.0	0.53
227.00	0.0	0.38
241.08	0.0	6.35
242.14	0.0	0.40
243.09	0.0	0.42
250.09	0.0	8.52
251.07	0.0	1.35
252.18	0.0	9.08
253.04	0.0	0.69
257.08	0.0	1.97
259.10	0.1	91.64
260.14	0.0	8.67
268.11	0.0	3.40
273.12	0.0	0.59
286.92	0.0	0.32
298.22	0.0	0.36
301.07	0.0	0.58
337.99	0.0	0.29
341.30	0.0	0.27
342.29	0.0	0.29
365.74	0.0	0.29
370.25	0.0	0.66
378.99	0.0	0.53
382.20	0.0	2.48
384.05	0.0	3.71
384.23	0.0	1.64
385.21	0.0	1.03
393.98	0.0	0.66
410.25	0.0	1.35
412.20	0.1	100.00
413.21	0.0	18.70
414.25	0.0	2.20
415.18	0.0	3.24
431.15	0.0	0.41
444.24	0.1	62.51
445.26	0.0	10.52
446.29	0.0	1.63
453.98	0.0	0.30
462.50	0.0	0.43
486.26	0.1	40.55
487.25	0.0	3.90
487.52	0.0	0.39

SPECTRUM - MS

12-17-13_HMG60_1236_MS4_935_472_01.raw

ITMS + p ESI E Full ms4 1236.10@cid35.00 936.00@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-54.93

AV: 50

m/z	Intensity	Relative
148.95	0.0	3.07
170.99	0.0	1.61
178.06	0.0	1.02
187.97	0.0	1.96
193.99	0.0	6.49
203.93	0.0	5.06
204.09	0.0	7.35
218.07	0.0	1.42
220.05	0.0	12.34
220.98	0.0	0.89
227.05	0.1	67.65
228.07	0.0	5.08
232.08	0.0	1.81
236.09	0.0	16.23
237.01	0.0	1.24
243.06	0.0	1.02
245.10	0.0	38.21
246.11	0.0	1.09
250.10	0.0	2.16
268.10	0.1	100.00
269.13	0.0	6.70
287.09	0.0	2.85
315.14	0.1	80.98
316.18	0.0	6.50
317.11	0.0	0.91
317.24	0.0	1.04
324.17	0.0	1.36
339.18	0.0	1.35
365.95	0.0	1.30
367.23	0.0	1.48
380.01	0.0	1.03
380.23	0.0	6.27
381.11	0.0	1.03
385.10	0.0	0.95
396.20	0.0	1.97
398.16	0.0	15.64
399.14	0.0	5.36
408.21	0.0	1.17
430.27	0.0	5.19
431.23	0.0	0.94
440.15	0.0	34.71
441.12	0.0	3.86
441.33	0.0	1.09
442.23	0.0	7.85
443.26	0.0	1.36
471.94	0.0	1.36
472.25	0.1	54.67

473.01	0.0	1.36
473.27	0.0	7.23
474.36	0.0	1.67

HMG 62 Mass spectral peak lists

Mass spectra were acquired in profile mode, then centroided using the valley detection algorithm. The top 50 peaks are shown. Isolation mass and width are adjusted to capture an entire isotopic envelope, where possible.

SPECTRUM - MS

6-28-13_HMG62_1235_MS2_01.raw

ITMS + p ESI E Full ms2 1236.50@cid35.00 [340.00-2000.00]

Scan #: 1-20

RT: 0.00-1.65

AV: 20

m/z	Intensity	Relative
433.28	588.7	40.62
434.28	98.8	6.82
486.31	84.4	5.82
660.40	557.6	38.47
661.42	152.7	10.53
724.49	151.4	10.45
760.46	83.4	5.76
799.00	91.1	6.28
834.50	778.9	53.74
835.51	270.4	18.65
917.09	337.3	23.27
917.58	295.2	20.37
918.08	162.4	11.20
993.58	103.9	7.17
994.10	103.2	7.12
1004.15	1449.5	100.00
1004.65	1347.3	92.95
1005.14	746.2	51.48
1005.63	282.8	19.51
1030.64	655.6	45.23
1031.14	633.9	43.73
1031.64	354.4	24.45
1032.13	132.2	9.12
1117.69	390.1	26.91
1118.19	441.0	30.43
1118.70	294.5	20.32
1119.20	157.5	10.86
1173.68	161.1	11.11
1174.71	95.1	6.56
1187.70	168.4	11.62
1188.69	93.4	6.44
1207.72	110.1	7.60
1235.76	1057.8	72.98
1236.26	1288.9	88.92
1236.75	966.8	66.70
1237.24	533.6	36.81
1237.75	87.6	6.05

1283.72	92.7	6.40	
1347.81	162.8	11.23	
1348.81	109.1	7.53	
1574.94	213.2	14.71	
1575.93	164.1	11.32	
1636.98	1135.6		78.35
1637.99	837.5	57.78	
1639.00	391.7	27.02	
1639.99	108.1	7.46	
1811.15	812.5	56.06	
1812.16	675.3	46.59	
1813.16	365.9	25.25	
1814.15	118.2	8.15	

SPECTRUM - MS

6-28-13_HMG62_1235_MS3_486_01.raw

ITMS + p ESI E Full ms3 1236.50@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-7.93

AV: 50

m/z Intensity Relative

178.06	0.1	0.99
208.09	0.3	6.43
209.15	0.0	0.66
218.14	0.0	0.45
241.17	0.2	4.86
250.04	0.2	4.52
250.19	0.2	4.19
251.17	0.0	0.85
252.13	0.7	13.71
253.12	0.1	1.70
257.11	0.1	1.58
259.13	5.1	99.29
260.14	0.5	9.88
268.26	0.1	1.51
282.21	0.1	1.07
298.06	0.0	0.40
301.16	0.0	0.97
312.18	0.1	1.77
314.22	0.1	2.45
315.25	0.0	0.39
326.15	0.1	1.20
329.21	0.1	2.33
341.12	0.0	0.85
356.33	0.0	0.38
370.18	0.0	0.45
380.24	0.0	0.47
382.09	0.0	0.43
382.29	0.1	1.18

384.17	0.2	4.54
385.29	0.0	0.43
387.16	0.0	0.42
387.31	0.0	0.39
410.25	0.1	1.45
411.15	0.0	0.38
412.24	5.1	100.00
413.26	0.9	17.78
415.23	0.1	2.00
416.19	0.0	0.58
426.33	0.1	1.14
427.26	0.1	1.10
429.19	0.0	0.38
444.29	3.1	60.18
445.27	0.7	13.25
454.34	0.2	3.50
455.32	0.0	0.61
456.35	1.0	19.95
457.37	0.2	4.77
471.21	0.0	0.76
486.30	1.5	30.28
487.33	0.4	7.08

SPECTRUM - MS

6-28-13_HMG62_1235_MS3_1283_01.raw

ITMS + p ESI E Full ms3 1236.50@cid35.00 1284.40@cid35.00 [350.00-1300.00]

Scan #: 1-20

RT: 0.00-4.82

AV: 20

m/z	Intensity	Relative
415.28	0.0	0.25
424.29	0.1	0.63
433.26	1.3	6.96
434.30	0.1	0.73
472.27	1.6	9.04
473.30	0.3	1.79
572.39	0.1	0.45
586.36	0.2	0.94
598.34	0.2	0.94
628.42	0.1	0.45
646.39	1.7	9.54
647.45	0.3	1.56
648.45	0.1	0.51
660.42	1.9	10.78
661.41	0.4	2.14
667.55	0.0	0.27
685.41	0.0	0.26
716.49	0.0	0.24
760.47	0.4	2.47
761.36	0.1	0.51

761.54	0.0	0.26
799.45	1.4	7.64
800.30	0.2	1.00
800.52	0.3	1.58
801.51	0.1	0.41
802.33	0.1	0.42
821.49	0.0	0.26
831.57	0.1	0.53
834.51	8.5	46.98
835.51	2.9	16.06
836.37	0.2	0.97
836.58	0.5	2.51
873.51	18.0	100.00
874.51	5.4	30.02
875.52	1.2	6.76
880.47	0.0	0.27
882.45	0.2	1.22
882.68	0.1	0.54
883.50	0.1	0.48
952.63	0.1	0.31
1077.54	0.0	0.27
1079.41	0.1	0.28
1079.55	0.1	0.31
1095.66	0.2	1.01
1126.74	0.2	1.17
1127.64	0.1	0.62
1253.67	0.1	0.32
1283.71	3.1	17.20
1284.73	2.0	11.17
1285.77	0.8	4.18

SPECTRUM - MS

6-28-13_HMG62_1235_MS5_1284_472_01.raw

ITMS + p ESI E Full ms4 1236.50@cid35.00 1284.40@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-33.10

AV: 50

m/z	Intensity	Relative
134.10	0.0	1.62
136.83	0.0	1.46
184.10	0.0	1.73
187.97	0.0	3.02
188.10	0.0	1.54
192.79	0.0	1.49
196.30	0.0	2.41
204.13	0.0	2.95
215.36	0.0	1.58
220.08	0.0	24.09
227.10	0.1	61.21
228.12	0.0	3.12

234.91	0.0	3.22
236.06	0.0	4.12
236.21	0.0	2.20
245.10	0.0	28.82
246.14	0.0	1.43
251.84	0.0	2.82
260.86	0.0	2.16
262.82	0.0	2.62
268.15	0.1	100.00
269.08	0.0	1.84
269.24	0.0	2.57
271.48	0.0	1.43
287.18	0.0	4.08
287.33	0.0	1.41
300.67	0.0	2.03
315.22	0.1	67.70
315.59	0.0	1.92
316.19	0.0	6.48
327.35	0.0	3.21
343.02	0.0	1.84
354.61	0.0	1.76
355.06	0.0	2.90
368.24	0.0	2.31
380.27	0.0	2.18
398.26	0.0	20.71
399.10	0.0	2.46
399.25	0.0	3.54
422.12	0.0	1.83
440.14	0.0	8.50
440.33	0.0	5.56
441.33	0.0	1.98
441.89	0.0	3.30
442.18	0.0	1.53
442.31	0.0	1.80
472.27	0.0	31.25
473.25	0.0	4.93
476.20	0.0	2.13
485.80	0.0	1.37

SPECTRUM - MS

6-28-13_HMG62_1235_MS4_1284_834_01.raw

ITMS + p ESI E Full ms4 1236.50@cid35.00 1284.40@cid35.00 835.00@cid35.00 [225.00-900.00]

Scan #: 1-40

RT: 0.00-8.93

AV: 40

m/z	Intensity	Relative
245.12	0.0	1.29
271.09	0.0	0.57
353.33	0.0	0.84
354.34	0.0	0.72

368.31	0.0	1.33
383.30	0.0	1.24
402.30	0.0	0.86
415.27	0.2	10.30
416.31	0.0	1.32
424.04	0.0	0.91
424.25	0.0	1.02
424.41	0.0	0.78
426.35	0.0	0.75
431.33	0.0	1.30
433.28	1.9	100.00
434.30	0.3	17.54
435.30	0.0	0.62
442.27	0.1	5.31
442.50	0.0	1.23
443.33	0.0	1.01
572.14	0.0	0.91
572.40	0.0	2.35
573.25	0.0	0.99
573.49	0.0	0.94
586.39	0.0	0.60
587.43	0.0	1.05
621.50	0.0	0.80
628.21	0.0	0.86
628.35	0.0	0.88
646.40	0.9	46.79
647.44	0.2	9.40
648.26	0.0	1.24
648.40	0.0	1.60
689.46	0.0	1.10
690.45	0.0	0.93
760.46	0.9	46.46
761.48	0.2	11.82
762.47	0.0	1.10
763.55	0.1	3.82
788.49	0.0	1.46
789.43	0.0	0.88
792.21	0.0	1.24
792.41	0.1	5.30
792.58	0.1	6.02
793.45	0.1	3.69
805.45	0.0	0.71
834.45	0.2	9.82
834.64	0.1	7.65
835.60	0.1	2.69
835.79	0.0	0.95

SPECTRUM - MS

6-28-13_HMG62_1235_MS4_1283_660_01.raw

ITMS + p ESI E Full ms4 1236.50@cid35.00 1284.40@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-40

RT: 0.00-9.88

AV: 40

m/z	Intensity	Relative
208.05	0.0	0.96
217.20	0.0	0.95
239.43	0.0	0.94
245.12	0.0	1.51
250.42	0.0	0.49
259.03	0.0	0.94
313.89	0.0	0.93
353.39	0.0	0.79
369.74	0.0	0.91
380.29	0.0	0.63
395.02	0.0	1.10
398.06	0.0	1.25
398.28	0.0	1.88
401.40	0.0	0.60
415.14	0.0	1.91
415.34	0.0	10.34
416.30	0.0	0.85
417.34	0.0	0.86
431.27	0.0	5.93
432.22	0.0	1.86
433.29	0.5	100.00
434.21	0.1	11.21
434.39	0.0	9.42
442.98	0.0	0.56
472.17	0.0	3.44
472.33	0.0	5.00
473.06	0.0	0.59
473.33	0.0	1.84
490.53	0.0	0.61
497.31	0.0	0.59
514.02	0.0	0.68
514.58	0.0	0.50
524.09	0.0	0.56
558.28	0.0	1.61
558.54	0.0	0.78
562.49	0.0	0.87
568.21	0.0	1.58
571.50	0.0	0.61
586.35	0.2	38.10
587.37	0.1	15.26
589.44	0.0	1.33
600.40	0.0	0.72
614.20	0.0	1.65
614.43	0.0	0.75
615.48	0.0	1.80
618.28	0.0	4.79
618.48	0.0	1.81

619.48	0.0	2.31
660.38	0.0	10.82
661.46	0.0	3.40

SPECTRUM - MS

6-28-13_HMG62_1235_MS5_1284_834_646_01.raw

ITMS + p ESI E Full ms5 1236.50@cid35.00 1284.40@cid35.00 835.00@cid35.00 647.00@cid35.00
[175.00-700.00]

Scan #: 1-50

RT: 0.00-26.86

AV: 50

m/z	Intensity	Relative
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211.09	0.0	1.51
218.03	0.0	1.43
220.02	0.0	1.68
229.14	0.0	5.20
236.10	0.0	2.82
245.14	0.0	12.15
265.63	0.0	1.69
269.31	0.0	1.52
271.14	0.0	1.39
274.24	0.0	1.53
276.82	0.0	1.74
332.34	0.0	1.76
364.19	0.0	3.37
368.22	0.0	4.37
369.26	0.0	1.34
382.19	0.0	1.38
384.18	0.0	2.79
384.85	0.0	1.72
398.21	0.0	3.12
398.41	0.0	2.35
417.24	0.0	1.60
424.31	0.0	2.93
426.17	0.0	3.03
426.31	0.0	1.97
433.28	0.1	100.00
434.27	0.0	13.07
435.36	0.0	4.31
439.09	0.0	3.28
439.98	0.0	1.94
442.22	0.0	2.34
456.13	0.0	3.83
458.07	0.0	1.59
458.29	0.0	4.54
461.46	0.0	2.70
482.70	0.0	1.47
504.06	0.0	1.39
521.18	0.0	1.92
544.52	0.0	1.36

571.99	0.0	2.53
572.36	0.1	65.90
573.19	0.0	8.66
573.35	0.0	18.08
582.23	0.0	1.78
623.90	0.0	1.66
625.09	0.0	3.45
632.13	0.0	1.98
646.34	0.0	9.93
646.44	0.0	7.09
646.62	0.0	2.00
697.05	0.0	3.07

SPECTRUM - MS

6-28-13_HMG62_1235_MS4_1283_646_02.raw

ITMS + p ESI E Full ms4 1236.50@cid35.00 1284.40@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-100

RT: 0.00-28.20

AV: 100

m/z Intensity Relative

196.38	0.0	1.50
213.36	0.0	1.39
227.13	0.0	11.19
229.10	0.0	3.79
236.12	0.0	5.51
245.11	0.1	29.27
245.99	0.0	1.95
283.14	0.0	1.42
315.11	0.0	4.15
343.23	0.0	3.40
356.67	0.0	1.42
363.46	0.0	1.88
366.30	0.0	1.80
368.47	0.0	1.81
371.18	0.0	1.40
378.15	0.0	2.14
380.26	0.0	2.73
382.24	0.0	8.71
383.31	0.0	2.26
384.23	0.0	13.37
384.41	0.0	2.94
385.20	0.1	58.65
386.06	0.0	1.53
386.25	0.0	6.57
398.23	0.0	1.49
398.41	0.0	2.28
424.29	0.0	4.36
425.28	0.0	1.41
430.65	0.0	2.25
433.35	0.0	15.50

434.23	0.0	2.31
440.27	0.0	19.92
442.30	0.1	23.89
442.90	0.0	1.63
443.36	0.0	2.27
458.28	0.0	8.74
459.26	0.0	1.86
486.60	0.0	1.37
530.26	0.0	2.27
558.25	0.0	1.67
571.95	0.0	1.71
572.35	0.2	100.00
573.34	0.1	32.71
574.29	0.0	4.65
574.56	0.0	1.44
575.04	0.0	1.53
575.37	0.0	11.36
576.35	0.0	5.84
604.42	0.0	2.47
646.48	0.0	4.72

SPECTRUM - MS

6-28-13_HMG62_1235_MS4_834_646_01.raw

ITMS + p ESI E Full ms4 1236.50@cid35.00 835.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-50

RT: 0.00-9.22

AV: 50

m/z	Intensity	Relative
204.04	0.0	0.66
218.01	0.1	1.67
219.94	0.0	0.57
220.14	0.1	1.92
227.14	0.1	1.20
229.10	0.4	9.09
236.07	0.2	5.12
245.11	0.6	11.65
246.07	0.0	0.71
311.09	0.0	0.50
332.17	0.0	0.84
350.15	0.1	1.12
351.25	0.0	0.51
364.22	0.3	5.25
365.18	0.0	0.63
366.15	0.0	0.62
366.39	0.0	0.58
368.20	0.4	7.90
369.23	0.1	2.23
382.16	0.1	1.77
382.34	0.0	0.86
384.16	0.1	1.84

384.34	0.0	0.56
385.11	0.0	0.87
385.28	0.0	0.63
398.24	0.2	3.36
415.25	0.1	2.47
417.27	0.1	2.59
424.24	0.5	10.00
425.21	0.1	1.51
426.21	0.1	3.07
426.39	0.1	1.56
427.25	0.1	1.15
433.27	4.9	100.00
434.29	0.7	14.14
440.34	0.1	2.48
442.35	0.2	3.81
457.99	0.0	0.71
458.27	0.3	7.03
459.37	0.0	0.52
475.24	0.0	0.53
540.13	0.0	0.53
540.34	0.1	1.22
572.32	3.8	78.15
573.34	0.9	17.44
575.29	0.0	1.02
575.43	0.0	0.95
604.41	0.0	0.67
646.36	0.6	12.03
647.41	0.2	3.91

SPECTRUM - MS

6-28-13_HMG62_1235_MS3_1109_01.raw

ITMS + p ESI E Full ms3 1236.50@cid35.00 1110.40@cid35.00 [305.00-1200.00]

Scan #: 1-20

RT: 0.00-9.90

AV: 20

m/z Intensity Relative

433.21	0.0	3.66
472.29	0.6	52.84
473.35	0.1	7.58
646.25	0.0	2.79
646.49	0.0	3.16
660.42	1.1	100.00
661.43	0.3	29.58
830.54	0.0	2.84
873.63	0.0	2.81
874.53	0.0	2.41
903.55	0.6	56.08
904.49	0.2	16.32
904.70	0.2	14.06
914.47	0.0	2.53

952.63	0.0	4.45	
964.11	0.1	5.86	
965.04	0.0	4.33	
987.06	0.0	4.20	
987.63	0.0	3.33	
988.25	0.0	3.31	
1042.27		0.0	2.58
1051.77		0.1	11.75
1052.37		0.1	6.36
1067.36		0.0	3.28
1067.58		0.0	2.92
1072.63		0.1	6.18
1073.10		0.1	7.45
1073.67		0.1	12.79
1074.16		0.0	2.38
1077.46		0.1	4.68
1077.74		0.1	12.72
1078.44		0.0	2.71
1078.62		0.0	3.35
1079.70		0.1	9.44
1080.13		0.0	2.42
1080.43		0.0	3.37
1080.89		0.0	3.90
1081.11		0.0	4.10
1081.35		0.1	7.54
1081.63		0.0	3.52
1089.21		0.0	3.26
1090.72		0.0	4.29
1091.73		0.0	3.33
1109.57		0.1	11.59
1109.79		0.2	14.91
1109.97		0.1	4.74
1110.32		0.2	21.64
1110.81		0.2	14.13
1111.25		0.1	5.15
1111.78		0.0	2.61

SPECTRUM - MS

6-28-13_HMG62_1235_MS4_1109_660_01.raw

ITMS + p ESI E Full ms4 1236.50@cid35.00 1110.40@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-112

RT: 0.00-89.52

AV: 112

m/z	Intensity	Relative
211.07	0.0	1.87
217.54	0.0	1.23
227.07	0.0	1.18
229.14	0.0	3.27
236.16	0.0	1.96
241.06	0.0	1.77

259.13	0.0	27.36
260.17	0.0	3.26
309.07	0.0	1.21
329.10	0.0	1.85
329.25	0.0	2.88
338.26	0.0	1.89
359.21	0.0	1.19
380.29	0.0	3.00
382.22	0.0	11.27
384.27	0.0	3.02
394.17	0.0	3.07
394.37	0.0	1.91
398.22	0.0	4.60
424.31	0.0	2.02
430.31	0.0	6.62
431.20	0.0	1.28
433.29	0.0	6.00
434.27	0.0	1.28
442.37	0.0	1.40
454.26	0.0	7.80
456.28	0.0	11.78
457.31	0.0	2.56
470.32	0.0	1.19
472.29	0.1	100.00
473.33	0.0	12.03
504.53	0.0	1.51
542.39	0.0	1.63
556.28	0.0	1.19
558.22	0.0	1.18
572.27	0.0	1.25
584.06	0.0	1.46
584.43	0.0	2.72
586.36	0.0	35.28
587.36	0.0	5.38
589.38	0.0	16.09
590.46	0.0	3.01
614.51	0.0	2.55
618.38	0.1	63.00
619.36	0.0	12.01
630.46	0.0	1.37
644.68	0.0	1.11
660.42	0.0	10.85
661.40	0.0	1.19
661.58	0.0	1.20

SPECTRUM - MS

6-28-13_HMG62_1235_MS4_1109_472_01.raw

ITMS + p ESI E Full ms4 1236.50@cid35.00 1110.40@cid35.00 473.00@cid35.00 [130.00-500.00]

Scan #: 1-88

RT: 0.00-56.29

AV: 88

m/z	Intensity	Relative
130.78	0.0	2.82
148.95	0.0	3.20
151.34	0.0	2.56
163.07	0.0	2.68
169.85	0.0	4.68
172.07	0.0	3.25
175.86	0.0	2.91
180.10	0.0	4.39
203.93	0.0	2.91
212.77	0.0	3.30
216.31	0.0	3.48
218.03	0.0	2.79
220.09	0.0	7.51
220.25	0.0	2.61
227.08	0.0	61.46
228.14	0.0	3.65
236.02	0.0	5.67
245.11	0.0	40.80
250.44	0.0	9.49
255.87	0.0	2.60
267.77	0.0	3.10
268.14	0.0	97.24
268.99	0.0	4.03
269.29	0.0	2.95
287.14	0.0	5.07
312.64	0.0	3.09
315.20	0.0	100.00
316.18	0.0	2.94
321.48	0.0	3.30
324.12	0.0	3.56
334.16	0.0	3.38
346.89	0.0	3.69
380.29	0.0	6.33
381.97	0.0	3.12
391.46	0.0	4.00
396.38	0.0	3.22
397.05	0.0	4.69
398.23	0.0	5.54
399.20	0.0	8.61
428.55	0.0	2.57
430.27	0.0	28.86
440.08	0.0	5.93
440.24	0.0	9.00
441.46	0.0	3.68
442.07	0.0	4.99
442.30	0.0	4.39
472.18	0.0	8.86
472.30	0.0	11.01
472.44	0.0	15.26

483.40 0.0 2.92

HMG 65 Mass spectral peak lists

SPECTRUM - MS

10-23-13_HMG65_1286_MS2_01.raw

ITMS + p ESI E Full ms2 1287.00@cid35.00 [350.00-2000.00]

Scan #: 1-20

RT: 0.00-1.79

AV: 20

m/z	Intensity	Relative
486.27	333.8	16.13
487.28	73.6	3.56
724.43	86.8	4.19
725.41	30.7	1.48
822.97	360.0	17.40
823.48	300.2	14.50
823.98	145.4	7.03
824.47	52.8	2.55
921.46	40.2	1.94
936.52	114.9	5.55
937.02	99.8	4.82
937.53	57.3	2.77
1054.57	2069.8	100.00
1055.06	2002.1	96.73
1055.57	1163.2	56.20
1056.07	495.8	23.96
1056.58	161.3	7.79
1092.15	31.9	1.54
1131.11	66.2	3.20
1131.59	79.1	3.82
1132.10	45.3	2.19
1150.14	45.5	2.20
1159.58	67.8	3.28
1160.57	39.2	1.90
1168.11	420.9	20.34
1168.61	445.9	21.54
1169.12	293.4	14.18
1169.62	131.2	6.34
1170.13	86.1	4.16
1177.11	32.7	1.58
1177.62	31.8	1.54
1187.58	88.3	4.27
1188.63	47.3	2.29
1217.16	41.1	1.99
1218.13	54.0	2.61
1219.13	48.7	2.35
1228.06	61.1	2.95
1285.08	67.6	3.27
1285.78	378.3	18.28
1286.22	695.0	33.58
1286.69	883.7	42.70

1287.15	675.3	32.63
1287.67	378.8	18.30
1288.14	195.6	9.45
1288.69	41.2	1.99
1384.68	78.1	3.77
1385.69	49.5	2.39
1622.85	215.3	10.40
1623.85	174.6	8.43
1624.86	86.7	4.19

SPECTRUM - MS

10-23-13_HMG65_1286_MS3_1054_01.raw

ITMS + p ESI E Full ms3 1287.00@cid35.00 1055.20@cid35.00 [290.00-2000.00]

Scan #: 1-20

RT: 0.00-2.22

AV: 20

m/z Intensity Relative

486.27	167.5	34.05	
487.27	29.0	5.88	
534.32	27.1	5.50	
535.35	5.8	1.19	
706.38	8.6	1.75	
724.42	83.8	17.04	
725.40	23.4	4.76	
822.97	492.0	100.00	
823.47	302.3	61.45	
823.97	116.9	23.76	
824.47	31.6	6.42	
824.96	6.1	1.24	
855.36	7.4	1.51	
899.48	18.5	3.77	
899.98	14.3	2.91	
900.48	6.1	1.23	
921.47	33.0	6.71	
922.49	12.6	2.57	
936.51	83.0	16.87	
937.03	61.4	12.48	
937.53	22.5	4.57	
938.04	9.7	1.96	
945.51	12.1	2.47	
945.99	8.5	1.72	
969.53	7.2	1.45	
1001.52	6.3	1.28	
1038.55	8.0	1.62	
1039.05	6.2	1.27	
1039.53	9.1	1.85	
1040.04	6.6	1.34	
1054.58	107.0	21.76	
1055.07	97.3	19.79	
1055.57	59.6	12.11	

1056.07	24.6	5.00
1056.57	7.8	1.58
1159.59	67.4	13.70
1160.60	30.6	6.21
1161.60	9.2	1.87
1187.63	19.4	3.95
1188.61	8.7	1.77
1384.70	35.4	7.19
1385.69	17.3	3.52
1386.70	10.3	2.09
1514.72	6.8	1.39
1574.74	8.6	1.74
1622.85	175.5	35.67
1623.86	109.3	22.21
1624.97	21.3	4.32
1625.88	9.5	1.93
1850.04	7.3	1.48

SPECTRUM - MS

10-23-13_HMG65_1286_MS4_1054_823_01.raw

ITMS + p ESI E Full ms4 1287.00@cid35.00 1055.20@cid35.00 823.40@cid35.00 [225.00-2000.00]

Scan #: 1-21

RT: 0.00-4.36

AV: 21

m/z Intensity Relative

444.27	3.2	3.72
458.23	2.9	3.45
486.27	68.4	80.63
487.28	12.4	14.56
488.28	1.4	1.68
514.29	1.7	2.00
534.33	12.1	14.27
535.32	2.5	2.98
591.33	7.4	8.68
591.80	3.0	3.51
592.32	1.1	1.31
616.30	1.6	1.84
664.41	2.9	3.36
676.36	2.9	3.41
704.35	3.2	3.80
705.35	1.8	2.06
706.40	7.6	8.90
707.41	2.6	3.05
713.90	1.9	2.28
714.39	1.8	2.16
724.42	32.1	37.85
725.40	9.5	11.17
726.41	1.6	1.85
746.33	2.6	3.05
769.92	1.6	1.88

773.42	1.6	1.87
806.94	2.7	3.23
807.45	1.7	1.95
807.95	3.9	4.64
808.45	2.7	3.18
822.97	37.0	43.60
823.47	28.0	32.98
823.97	10.7	12.56
824.48	2.9	3.43
921.46	14.7	17.35
922.48	5.3	6.26
923.50	1.4	1.64
969.53	6.5	7.67
970.53	2.6	3.06
981.49	1.3	1.50
1051.48		5.5 6.52
1052.46		2.3 2.76
1111.54		6.1 7.13
1112.54		2.7 3.21
1159.59		84.9 100.00
1160.60		40.5 47.67
1161.61		10.0 11.81
1187.61		1.8 2.13
1622.85		5.9 6.96
1623.86		4.3 5.08

SPECTRUM - MS

11-5-13_HMG65_1286_MS3_486_02.raw

ITMS + p ESI E Full ms3 1287.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-100

RT: 0.00-29.37

AV: 100

m/z Intensity Relative

178.04	0.1	0.33
180.02	0.2	0.71
188.03	0.1	0.42
208.07	0.3	1.14
211.07	0.1	0.34
218.05	0.1	0.36
220.07	1.0	3.57
221.08	0.1	0.43
227.06	0.2	0.55
236.06	0.1	0.29
241.09	1.4	5.01
242.11	0.2	0.61
250.08	0.4	1.60
252.10	0.7	2.48
257.09	0.2	0.57
259.10	9.8	35.82
260.11	1.1	3.84

261.12	0.2	0.61
268.12	3.2	11.56
269.12	0.4	1.54
297.12	0.2	0.83
301.11	0.3	1.24
314.16	0.1	0.35
315.17	0.1	0.29
329.18	10.1	36.83
330.18	1.6	5.86
331.17	0.2	0.89
353.17	0.1	0.48
382.20	0.2	0.57
384.16	0.2	0.80
394.22	0.1	0.40
410.20	0.1	0.53
412.20	5.7	20.75
413.21	1.2	4.41
414.23	0.2	0.77
415.24	0.5	1.84
416.24	0.1	0.45
426.25	0.1	0.51
440.20	0.1	0.29
444.25	27.4	100.00
445.25	6.2	22.65
446.25	1.0	3.78
454.25	0.4	1.31
455.23	0.1	0.38
456.26	1.9	6.91
457.26	0.5	1.78
458.26	0.1	0.39
486.26	1.8	6.48
487.27	0.4	1.52
488.27	0.1	0.31

SPECTRUM - MS

10-23-13_HMG65_1286_MS3_1384_01.raw

ITMS + p ESI E Full ms3 1287.00@cid35.00 1385.40@cid35.00 [380.00-1400.00]

Scan #: 1-20

RT: 0.00-5.15

AV: 20

m/z Intensity Relative

458.22	1.6	10.01
459.24	0.3	1.92
486.27	2.6	15.90
487.27	0.4	2.45
534.35	0.2	1.04
546.26	0.1	0.66
574.32	0.2	1.47
620.34	0.1	0.52
676.34	0.3	2.10

677.35	0.1	0.43	
694.24	0.1	0.49	
694.43	0.1	0.57	
703.44	0.1	0.48	
724.42	0.3	2.17	
764.40	0.5	2.94	
765.38	0.2	1.03	
850.42	0.1	0.46	
877.48	0.1	0.42	
879.49	0.1	0.69	
889.40	0.2	1.07	
921.46	16.1	100.00	
922.47	5.4	33.50	
923.49	1.1	6.98	
951.51	0.5	3.23	
1074.49		0.4	2.18
1075.57		0.1	0.48
1111.57		0.1	0.49
1139.65		0.1	0.60
1140.61		0.1	0.52
1148.57		1.5	9.40
1149.65		0.5	3.14
1150.43		0.1	0.45
1157.58		0.3	1.64
1166.35		0.1	0.44
1166.61		0.2	1.09
1196.63		0.2	0.96
1227.62		1.0	6.25
1228.68		0.3	1.84
1229.60		0.1	0.42
1278.64		0.2	0.97
1312.63		0.5	3.26
1342.54		0.1	0.84
1343.64		0.1	0.50
1352.61		0.2	1.02
1354.61		0.1	0.58
1354.76		0.1	0.57
1355.80		0.1	0.53
1384.69		2.5	15.45
1385.69		1.7	10.79
1386.70		1.0	6.11

SPECTRUM - MS

10-23-13_HMG65_1286_MS4_1384_921_01.raw

ITMS + p ESI E Full ms4 1287.00@cid35.00 1385.40@cid35.00 922.00@cid35.00 [250.00-1000.00]

Scan #: 1-50

RT: 0.00-29.17

AV: 50

m/z	Intensity	Relative
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268.10	0.0	1.23
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426.13	0.0	0.58
444.24	0.1	2.88
445.27	0.0	0.51
454.24	0.0	0.67
458.23	1.9	100.00
459.23	0.2	11.45
460.31	0.0	0.74
486.26	1.6	82.70
487.28	0.2	10.61
546.31	0.1	2.66
547.21	0.0	0.54
574.33	0.2	8.02
575.38	0.0	1.15
620.30	0.1	3.72
621.20	0.0	0.48
621.37	0.0	0.53
646.32	0.0	2.07
655.32	0.0	0.64
676.34	0.3	15.48
677.34	0.1	2.96
692.32	0.0	1.83
694.36	0.2	9.75
695.41	0.0	0.91
703.42	0.0	1.84
724.55	0.0	0.49
734.39	0.0	0.51
752.39	0.0	0.75
764.41	0.4	23.06
765.39	0.1	4.61
815.41	0.1	3.30
816.27	0.0	0.78
816.41	0.0	0.49
816.56	0.0	0.49
829.37	0.0	1.32
829.55	0.0	0.83
847.41	0.1	6.49
848.41	0.0	2.61
850.45	0.1	6.33
851.55	0.0	1.06
857.36	0.0	0.53
879.42	0.1	5.07
880.43	0.0	1.22
889.42	0.2	12.26
890.42	0.1	2.67
891.46	0.1	3.71
892.40	0.0	0.93
921.47	0.3	15.89
922.46	0.1	5.04
923.45	0.0	0.49

SPECTRUM - MS

10-23-13_HMG65_1286_MS5_1384_921_486_01.raw

ITMS + p ESI E Full ms5 1287.00@cid35.00 1385.40@cid35.00 922.00@cid35.00 487.00@cid35.00

[130.00-500.00]

Scan #: 1-51

RT: 0.00-55.35

AV: 51

m/z Intensity Relative

155.09	0.0	0.19
179.97	0.0	0.59
180.18	0.0	0.19
192.18	0.0	0.37
199.15	0.0	0.17
200.08	0.0	0.26
220.10	0.0	2.14
227.09	0.0	0.41
235.94	0.0	0.17
241.09	0.0	3.44
242.08	0.0	0.26
250.13	0.0	0.26
257.09	0.0	0.18
259.10	0.0	13.43
260.11	0.0	1.15
268.11	0.0	8.41
269.01	0.0	0.16
269.18	0.0	0.18
297.22	0.0	0.23
301.13	0.0	1.19
312.33	0.0	0.28
325.07	0.0	0.17
329.18	0.1	25.21
330.18	0.0	1.84
331.14	0.0	0.32
353.18	0.0	1.61
384.16	0.0	0.38
394.18	0.0	0.54
410.23	0.0	0.17
412.13	0.0	1.19
412.31	0.0	0.72
413.24	0.0	0.27
414.98	0.0	0.27
415.18	0.0	1.75
415.33	0.0	0.77
416.31	0.0	0.17
424.35	0.0	0.27
431.13	0.0	0.20
441.26	0.0	0.20
444.25	0.2	100.00
445.26	0.0	15.92
446.16	0.0	0.79
446.39	0.0	0.34

453.97	0.0	0.20
454.26	0.0	0.26
456.21	0.0	2.95
457.25	0.0	0.19
486.25	0.1	29.37
487.29	0.0	4.54
488.24	0.0	0.55

SPECTRUM - MS

10-23-13_HMG65_1286_MS5_1384_921_458_01.raw

ITMS + p ESI E Full ms5 1287.00@cid35.00 1385.40@cid35.00 922.00@cid35.00 459.00@cid35.00
[125.00-500.00]

Scan #: 1-50

RT: 0.00-50.04

AV: 50

m/z	Intensity	Relative
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149.08	0.0	1.15
156.95	0.0	0.43
177.96	0.0	0.33
180.08	0.0	0.80
188.04	0.0	0.81
189.14	0.0	0.47
194.04	0.0	0.82
194.16	0.0	0.32
204.00	0.0	3.21
204.16	0.0	0.59
209.59	0.0	0.44
213.06	0.0	13.29
214.06	0.0	0.41
218.10	0.0	0.95
220.08	0.0	7.70
221.15	0.0	0.40
228.10	0.0	0.35
231.06	0.0	15.53
232.17	0.0	0.37
236.06	0.0	6.84
237.06	0.0	0.63
243.69	0.0	0.60
250.12	0.0	0.90
268.11	0.2	100.00
269.11	0.0	7.26
273.05	0.0	1.06
301.13	0.1	24.53
302.03	0.0	1.14
302.19	0.0	0.63
310.14	0.0	0.35
324.17	0.0	0.47
329.24	0.0	0.64
336.17	0.0	0.37
352.26	0.0	0.37

354.31	0.0	0.53
362.15	0.0	0.33
366.09	0.0	0.58
366.24	0.0	0.53
371.25	0.0	0.34
384.13	0.0	5.16
385.19	0.0	1.86
416.24	0.0	1.44
426.11	0.0	4.67
426.28	0.0	3.41
427.18	0.0	1.29
427.35	0.0	0.74
428.23	0.0	4.42
458.22	0.0	12.83
459.09	0.0	0.39
459.22	0.0	0.33

HMG 66 Mass spectral peak lists

SPECTRUM - MS

11-5-13_HMG66_1286_MS2_01.raw

ITMS + p ESI E Full ms2 1287.00@cid35.00 [350.00-2000.00]

Scan #: 1-20

RT: 0.00-4.60

AV: 20

m/z	Intensity	Relative
486.28	228.6	17.07
487.29	51.1	3.82
534.35	15.7	1.17
724.43	78.0	5.82
725.40	31.0	2.32
822.96	167.3	12.49
823.45	150.4	11.23
823.96	78.4	5.85
824.46	32.1	2.40
921.45	57.3	4.28
922.47	26.6	1.99
1040.54		15.2 1.14
1041.06		13.6 1.02
1053.53		13.0 0.97
1054.01		19.0 1.42
1054.56	1233.9	92.12
1055.02	1339.4	100.00
1055.52	769.0	57.41
1056.03	328.4	24.52
1056.53	105.1	7.85
1057.03	20.7	1.55
1159.54	29.2	2.18
1160.53	18.1	1.35
1170.14	14.4	1.07
1177.08	26.9	2.01
1177.57	33.9	2.53
1178.09	24.5	1.83
1187.58	155.0	11.57
1188.58	91.7	6.85
1189.57	38.4	2.87
1228.03	14.4	1.07
1233.07	14.1	1.05
1233.56	16.2	1.21
1270.10	21.8	1.62
1270.60	26.6	1.99
1271.10	25.5	1.90
1271.62	17.5	1.31
1286.18	153.2	11.44
1286.64	235.9	17.61
1287.08	155.1	11.58
1287.60	85.3	6.37

1288.09	40.5	3.02
1384.62	90.2	6.73
1385.63	59.2	4.42
1386.62	25.6	1.91
1432.69	15.8	1.18
1622.77	160.3	11.97
1623.77	132.9	9.92
1624.77	65.7	4.90
1625.78	23.3	1.74

SPECTRUM - MS

11-5-13_HMG66_1286_MS3_1055_01.raw

ITMS + p ESI E Full ms3 1287.00@cid35.00 1055.00@cid35.00 [290.00-2000.00]

Scan #: 1-20

RT: 0.00-3.97

AV: 20

m/z	Intensity	Relative
444.26	25.1	2.24
458.22	60.7	5.43
486.27	638.6	57.12
487.28	142.8	12.77
488.28	24.6	2.20
534.33	72.1	6.45
605.33	21.9	1.96
676.34	24.9	2.22
704.34	34.6	3.10
706.38	43.9	3.93
724.41	390.4	34.92
725.40	143.9	12.87
726.40	35.0	3.13
822.96	1118.0	100.00
823.45	957.6	85.65
823.96	453.2	40.54
824.46	135.5	12.12
824.96	26.5	2.37
921.45	305.8	27.35
922.46	133.0	11.90
923.47	35.8	3.20
945.50	41.8	3.73
945.98	41.2	3.69
946.49	25.3	2.26
1002.02	22.5	2.02
1038.53	34.1	3.05
1039.02	38.6	3.46
1039.52	46.8	4.18
1040.02	37.4	3.35
1054.59	325.1	29.08
1055.06	378.0	33.81
1055.54	253.8	22.70
1056.04	118.9	10.63

1056.55	38.1	3.40
1159.55	155.5	13.91
1160.56	94.4	8.45
1161.57	34.4	3.08
1187.60	346.1	30.95
1188.60	206.3	18.45
1189.61	79.5	7.11
1384.66	128.5	11.50
1385.65	89.8	8.03
1386.65	34.1	3.05
1432.73	33.5	3.00
1433.71	24.4	2.18
1514.67	29.5	2.64
1622.80	628.1	56.18
1623.81	518.2	46.35
1624.82	248.0	22.18
1625.82	72.4	6.48

SPECTRUM - MS

11-5-13_HMG66_1286_MS4_1055_823_01.raw

ITMS + p ESI E Full ms4 1287.00@cid35.00 1055.00@cid35.00 823.40@cid35.00 [225.00-1800.00]

Scan #: 1-20

RT: 0.00-2.85

AV: 20

m/z Intensity Relative

386.16	3.1	2.41
444.26	6.7	5.21
458.22	24.1	18.61
459.23	4.4	3.43
486.26	122.1	94.46
487.27	25.0	19.37
488.27	3.6	2.77
514.26	6.2	4.80
534.32	9.8	7.62
591.32	11.0	8.54
591.80	6.4	4.97
605.31	14.1	10.92
605.82	8.3	6.41
606.32	3.1	2.42
616.28	7.6	5.85
664.40	4.5	3.48
676.34	5.0	3.84
704.34	17.7	13.68
705.30	6.1	4.72
706.37	7.0	5.44
713.89	4.2	3.22
714.37	3.6	2.76
724.41	119.3	92.33
725.39	39.1	30.28
726.41	8.8	6.78

746.31	12.3	9.50
747.30	3.7	2.89
806.90	5.1	3.91
807.42	4.2	3.25
807.93	8.3	6.45
808.43	5.4	4.15
822.96	40.6	31.37
823.45	32.8	25.35
823.95	15.7	12.15
824.44	5.3	4.13
921.44	50.2	38.85
922.46	21.1	16.35
923.47	4.9	3.82
969.49	8.3	6.42
970.49	4.4	3.38
1051.45		5.6 4.30
1159.55		129.3 100.00
1160.55		69.8 54.03
1161.56		21.3 16.48
1162.56		3.2 2.47
1187.60		32.3 24.98
1188.60		17.8 13.75
1189.61		4.9 3.79
1622.81		7.5 5.81
1623.80		5.1 3.98

SPECTRUM - MS

11-5-13_HMG66_1286_MS5_1055_823_1160_01.raw

ITMS + p ESI E Full ms5 1287.00@cid35.00 1055.00@cid35.00 823.40@cid35.00 1160.20@cid35.00 [315.00-1200.00]

Scan #: 1-20

RT: 0.00-2.63

AV: 20

m/z Intensity Relative

370.11	0.0	0.06
384.11	0.1	0.07
433.20	0.1	0.16
435.25	0.6	0.83
436.29	0.1	0.07
444.22	0.1	0.08
456.37	0.1	0.11
458.23	0.2	0.30
470.31	0.1	0.08
472.27	0.1	0.14
474.22	0.1	0.12
474.38	0.2	0.26
475.34	0.1	0.11
486.32	0.5	0.63
502.21	0.1	0.15
502.35	0.1	0.15

516.34	0.1	0.19
534.32	16.3	21.63
535.33	3.7	4.86
536.35	0.3	0.36
562.30	0.0	0.06
563.37	0.1	0.07
590.30	0.1	0.19
590.46	0.1	0.11
616.28	0.0	0.07
620.44	0.0	0.06
625.33	0.8	1.03
626.43	0.1	0.07
676.32	0.1	0.11
692.15	0.1	0.07
692.40	0.1	0.10
723.45	0.1	0.09
724.40	75.4	100.00
725.39	18.9	25.05
726.40	2.5	3.30
969.48	2.0	2.71
970.43	0.5	0.62
970.63	0.5	0.68
971.53	0.1	0.08
1054.41		0.1 0.07
1060.48		0.2 0.24
1060.67		0.1 0.14
1061.54		0.1 0.10
1127.48		0.2 0.25
1127.67		0.1 0.09
1129.40		0.1 0.07
1129.67		0.1 0.08
1159.54		5.7 7.56
1160.55		3.0 3.97
1161.57		0.7 0.97

SPECTRUM - MS

11-5-13_HMG66_1286_MS3_1384_01.raw

ITMS + p ESI E Full ms3 1287.00@cid35.00 1385.40@cid35.00 [380.00-1400.00]

Scan #: 1-20

RT: 0.00-5.83

AV: 20

m/z Intensity Relative

444.20	0.1	0.53
458.21	2.1	11.45
459.25	0.3	1.74
486.25	2.4	13.40
487.32	0.3	1.72
546.17	0.1	0.62
546.30	0.1	0.36
574.33	0.2	1.08

676.39	0.3	1.55
677.28	0.1	0.37
694.29	0.2	0.89
694.47	0.1	0.34
695.44	0.1	0.50
764.44	0.4	2.20
765.37	0.1	0.72
815.36	0.1	0.42
850.38	0.2	1.18
873.43	0.1	0.32
879.50	0.1	0.44
880.43	0.1	0.31
889.48	0.1	0.47
891.33	0.1	0.32
921.42	18.2	100.00
922.44	5.6	30.95
923.49	0.6	3.16
1074.51	0.1	0.55
1139.56	0.1	0.44
1157.46	0.4	2.00
1158.48	0.1	0.32
1166.37	0.1	0.65
1166.60	0.1	0.76
1187.62	0.1	0.38
1227.53	1.3	7.26
1228.47	0.4	2.35
1228.62	0.3	1.86
1228.76	0.1	0.60
1229.47	0.1	0.47
1278.46	0.1	0.73
1278.60	0.1	0.71
1279.52	0.1	0.79
1313.69	0.1	0.34
1342.68	0.1	0.40
1343.61	0.1	0.64
1352.35	0.1	0.43
1352.61	0.3	1.51
1354.60	0.3	1.66
1355.57	0.1	0.62
1384.62	1.3	7.04
1385.64	1.1	5.89
1386.66	0.4	2.12

SPECTRUM - MS

11-5-13_HMG66_1286_MS4_1384_921_01.raw

ITMS + p ESI E Full ms4 1287.00@cid35.00 1385.40@cid35.00 922.00@cid35.00 [250.00-1000.00]

Scan #: 1-20

RT: 0.00-5.37

AV: 20

m/z Intensity Relative

268.19	0.0	0.48
301.12	0.0	0.56
329.24	0.0	0.46
444.26	0.2	2.30
456.23	0.0	0.45
458.21	7.6	100.00
459.22	1.0	13.41
460.23	0.1	1.41
486.26	4.9	64.52
487.26	0.8	10.88
488.28	0.1	1.15
546.29	0.1	1.64
547.25	0.0	0.52
574.31	0.5	6.28
575.34	0.1	1.27
620.27	0.2	2.59
646.25	0.1	0.83
646.45	0.0	0.58
655.26	0.0	0.59
676.32	1.1	14.65
677.39	0.1	1.94
678.36	0.1	0.83
692.32	0.1	1.47
694.34	0.6	8.27
695.35	0.1	1.82
703.36	0.1	1.65
704.41	0.1	0.71
764.37	1.6	21.53
765.35	0.5	6.28
766.41	0.1	0.75
815.38	0.2	2.67
816.38	0.1	1.35
829.32	0.1	0.72
829.48	0.1	0.82
847.43	0.2	3.07
848.42	0.1	1.56
849.38	0.0	0.59
850.39	0.4	4.90
851.46	0.1	1.07
879.34	0.2	2.03
879.54	0.1	1.81
880.43	0.1	1.54
889.38	0.8	10.15
890.33	0.1	1.19
890.49	0.1	1.41
891.42	0.3	4.26
892.43	0.1	1.36
921.42	2.0	26.07
922.42	0.6	8.04
923.49	0.1	1.49

SPECTRUM - MS

11-5-13_HMG66_1286_MS5_1384_921_486_01.raw

ITMS + p ESI E Full ms5 1287.00@cid35.00 1385.40@cid35.00 922.00@cid35.00 487.00@cid35.00
[130.00-500.00]

Scan #: 1-50

RT: 0.00-17.47

AV: 50

m/z	Intensity	Relative
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167.98	0.0	0.18
168.11	0.0	0.18
184.95	0.0	0.28
213.03	0.0	0.24
220.09	0.0	2.89
221.06	0.0	0.17
226.91	0.0	0.36
227.13	0.0	0.22
236.19	0.0	0.44
241.05	0.0	2.59
242.25	0.0	0.17
243.17	0.0	0.20
244.96	0.0	0.23
259.11	0.1	12.24
260.05	0.0	0.61
260.31	0.0	0.30
268.10	0.1	6.80
269.06	0.0	0.80
297.10	0.0	0.30
297.23	0.0	0.29
301.20	0.0	0.64
329.15	0.2	27.56
330.05	0.0	1.33
330.20	0.0	1.78
353.09	0.0	0.30
371.25	0.0	0.19
382.26	0.0	0.21
383.09	0.0	0.17
385.29	0.0	0.21
394.09	0.0	0.37
410.24	0.0	0.19
412.21	0.0	1.09
415.03	0.0	0.86
415.26	0.0	1.09
416.25	0.0	0.94
426.23	0.0	0.30
440.23	0.0	0.40
444.24	0.8	100.00
445.25	0.1	15.62
446.24	0.0	0.55
446.37	0.0	0.28
454.34	0.0	0.23

455.20	0.0	0.40
456.31	0.0	3.29
458.09	0.0	0.35
458.35	0.0	0.23
486.26	0.2	24.34
487.35	0.0	1.66
488.30	0.0	0.47
488.40	0.0	0.24

SPECTRUM - MS

11-5-13_HMG66_1286_MS5_1384_921_458_01.raw

ITMS + p ESI E Full ms5 1287.00@cid35.00 1385.40@cid35.00 922.00@cid35.00 459.00@cid35.00

[125.00-500.00]

Scan #: 1-50

RT: 0.00-38.75

AV: 50

m/z	Intensity	Relative
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148.99	0.0	2.07
180.13	0.0	0.61
181.05	0.0	0.22
188.07	0.0	0.37
194.04	0.0	2.30
195.14	0.0	0.36
203.86	0.0	0.47
204.05	0.0	1.43
206.15	0.0	0.30
213.05	0.0	12.83
214.06	0.0	0.69
219.97	0.0	3.41
220.13	0.0	3.64
221.03	0.0	0.33
231.05	0.0	11.46
232.10	0.0	0.61
236.06	0.0	4.31
237.06	0.0	0.49
250.14	0.0	1.07
268.11	0.4	100.00
269.13	0.0	8.03
270.17	0.0	0.91
273.04	0.0	0.56
284.05	0.0	0.34
301.13	0.1	29.44
302.13	0.0	1.97
313.19	0.0	0.47
324.05	0.0	0.41
326.13	0.0	0.33
353.97	0.0	0.43
354.15	0.0	0.57
366.21	0.0	0.35
371.12	0.0	0.34

384.01	0.0	1.07
384.20	0.0	2.52
385.22	0.0	1.08
386.08	0.0	0.27
387.27	0.0	0.42
396.30	0.0	0.31
416.22	0.0	1.09
426.18	0.0	6.67
427.05	0.0	0.63
427.28	0.0	0.29
427.90	0.0	0.23
428.16	0.0	2.64
428.34	0.0	1.00
429.15	0.0	0.49
458.20	0.0	9.47
459.21	0.0	2.09
460.18	0.0	0.27

SPECTRUM - MS

11-5-13_HMG66_1286_MS3_486_03.raw

ITMS + p ESI E Full ms3 1287.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-4.38

AV: 50

m/z Intensity Relative

178.02	0.2	0.19
180.01	0.7	0.79
188.06	0.5	0.51
211.10	0.2	0.20
213.08	0.2	0.26
218.04	0.2	0.21
220.07	3.5	3.84
221.07	0.4	0.41
227.05	0.5	0.56
236.07	0.2	0.27
241.09	4.0	4.39
242.10	0.4	0.45
250.12	0.2	0.24
257.09	0.2	0.22
259.10	18.5	20.27
260.11	2.0	2.18
261.12	0.3	0.33
268.12	11.9	13.04
269.12	1.5	1.68
297.14	0.7	0.81
301.11	1.3	1.39
302.14	0.2	0.21
315.18	0.3	0.29
329.17	37.8	41.36
330.18	5.9	6.48

331.17	0.9	1.01
353.17	0.5	0.55
380.19	0.2	0.27
382.26	0.3	0.30
384.22	0.2	0.19
394.22	0.5	0.56
410.20	0.3	0.38
411.21	0.2	0.17
412.19	1.7	1.89
413.26	0.3	0.31
415.24	1.5	1.63
416.24	0.5	0.54
426.14	0.2	0.25
431.19	0.2	0.26
444.25	91.3	100.00
445.25	20.6	22.51
446.25	3.7	4.06
454.23	1.1	1.15
455.25	0.2	0.27
456.25	5.5	6.02
457.26	1.5	1.63
458.15	0.2	0.17
486.26	15.9	17.41
487.26	4.0	4.43
488.27	0.7	0.79

HMG 67 Mass spectral peak lists

SPECTRUM - MS

12-16-13_HMG67_1286_MS2_01.raw

ITMS + p ESI E Full ms2 1287.00@cid35.00 [350.00-2000.00]

Scan #: 1-20

RT: 0.00-1.62

AV: 20

m/z	Intensity	Relative
486.33	564.8	14.72
487.32	115.0	3.00
724.47	224.8	5.86
823.02	422.2	11.00
823.53	335.5	8.74
824.03	159.7	4.16
899.55	129.6	3.38
900.04	117.1	3.05
921.51	156.4	4.08
936.56	357.6	9.32
937.06	319.3	8.32
937.57	185.0	4.82
938.10	78.3	2.04
1054.63	3838.3	100.00
1055.13	3655.0	95.23
1055.62	1997.9	52.05
1056.13	841.4	21.92
1056.62	257.3	6.70
1131.15	804.5	20.96
1131.66	817.7	21.30
1132.16	501.9	13.08
1132.66	224.4	5.85
1133.15	83.3	2.17
1148.60	109.3	2.85
1150.29	118.1	3.08
1167.20	82.5	2.15
1168.17	2915.7	75.96
1168.66	3063.9	79.82
1169.16	1871.4	48.76
1169.67	841.1	21.91
1170.17	415.1	10.81
1177.16	89.7	2.34
1177.67	101.3	2.64
1187.70	537.9	14.01
1188.69	323.4	8.43
1189.65	121.2	3.16
1228.18	139.6	3.64
1286.25	1355.4	35.31
1286.73	1649.2	42.97
1287.21	1288.2	33.56
1287.72	719.3	18.74

1288.22	319.2	8.32
1384.73	312.5	8.14
1385.74	181.4	4.73
1386.75	86.4	2.25
1622.88	456.1	11.88
1623.89	352.7	9.19
1624.89	170.2	4.43
1850.01	121.9	3.18
1851.04	96.0	2.50

SPECTRUM - MS

12-16-13_HMG67_1286_MS3_486_01.raw

ITMS + p ESI E Full ms3 1287.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-50

RT: 0.00-4.69

AV: 50

m/z Intensity Relative

178.02	0.2	0.67
180.02	0.3	0.82
208.09	1.1	3.11
211.07	0.2	0.54
218.09	0.2	0.51
220.06	1.4	4.06
221.09	0.2	0.61
227.01	0.1	0.40
241.10	2.0	5.74
242.12	0.2	0.60
250.06	1.0	2.69
250.21	0.5	1.32
252.13	1.8	5.13
253.14	0.1	0.39
257.12	0.4	1.19
259.14	22.4	62.88
260.13	2.3	6.43
261.11	0.3	0.85
268.12	4.2	11.72
269.09	0.4	1.10
269.25	0.2	0.52
297.24	0.3	0.75
301.14	0.6	1.81
329.20	13.3	37.45
330.18	1.7	4.77
331.22	0.2	0.53
338.19	0.1	0.36
352.13	0.1	0.38
353.21	0.2	0.67
380.24	0.2	0.65
382.22	0.2	0.68
382.43	0.1	0.35
384.19	0.6	1.67

385.20	0.1	0.40
410.27	0.2	0.52
412.24	16.4	46.15
413.24	3.2	8.87
414.26	0.3	0.94
415.27	0.6	1.73
416.29	0.2	0.48
426.38	0.1	0.36
444.30	35.6	100.00
445.32	7.6	21.43
446.27	1.1	3.01
454.26	0.4	1.06
456.28	2.2	6.24
457.31	0.5	1.45
486.31	11.4	32.04
487.33	2.7	7.52
488.28	0.4	0.99

SPECTRUM - MS

12-16-13_HMG67_1286_MS3_1385_01.raw

ITMS + p ESI E Full ms3 1287.00@cid35.00 1385.40@cid35.00 [380.00-1400.00]

Scan #: 1-20

RT: 0.00-3.13

AV: 20

m/z	Intensity	Relative
458.29	3.0	11.90
459.27	0.5	1.97
486.32	2.7	10.63
487.31	0.6	2.39
534.44	0.2	0.62
546.31	0.2	0.86
574.39	0.3	1.11
611.30	0.1	0.50
676.39	0.6	2.30
677.42	0.2	0.75
685.44	0.4	1.42
694.39	0.3	1.27
724.47	1.2	4.57
764.45	1.1	4.41
765.50	0.1	0.57
850.45	0.2	0.65
873.23	0.1	0.52
873.48	0.4	1.53
889.49	0.2	0.79
921.50	25.5	100.00
922.51	9.6	37.54
923.51	2.1	8.20
991.55	0.5	1.88
992.58	0.2	0.73
1074.55		3.7 14.52

1075.58	1.4	5.33
1076.63	0.3	1.18
1139.59	0.3	1.34
1148.60	15.2	59.49
1149.62	7.0	27.50
1150.63	2.3	8.81
1157.75	0.3	1.04
1158.64	0.2	0.69
1166.68	0.3	1.27
1167.76	0.1	0.57
1187.76	0.2	0.92
1188.68	0.1	0.53
1215.69	0.7	2.82
1216.65	0.5	1.96
1217.68	0.2	0.69
1227.74	1.5	5.98
1228.68	1.1	4.31
1229.53	0.2	0.71
1229.76	0.2	0.88
1352.71	0.1	0.53
1354.73	0.4	1.49
1355.66	0.1	0.58
1384.73	7.6	29.95
1385.74	6.0	23.46
1386.75	2.8	11.15

SPECTRUM - MS

12-16-13_HMG67_1286_MS4_1385_921_01.raw

ITMS + p ESI E Full ms4 1287.00@cid35.00 1385.40@cid35.00 922.00@cid35.00 [250.00-1000.00]

Scan #: 1-50

RT: 0.00-13.20

AV: 50

m/z Intensity Relative

268.11	0.1	0.85
301.18	0.1	0.62
329.19	0.1	0.52
426.22	0.1	0.44
444.30	0.2	1.40
454.24	0.1	0.51
458.28	13.6	100.00
459.27	1.8	13.06
460.24	0.1	1.08
486.31	7.1	51.99
487.30	1.1	7.91
546.29	0.3	2.25
574.35	0.7	5.47
575.38	0.1	1.02
620.33	0.4	2.78
621.32	0.1	0.44
646.43	0.1	0.97

655.35	0.1	0.52
676.36	1.6	12.07
677.36	0.3	2.01
685.38	0.5	3.52
686.38	0.1	0.54
692.44	0.2	1.20
694.38	1.2	8.56
695.38	0.2	1.73
703.34	0.2	1.59
703.51	0.1	1.03
704.42	0.1	0.57
724.44	0.3	1.92
725.46	0.1	0.52
752.49	0.1	0.46
764.41	3.1	23.02
765.43	0.8	5.56
766.39	0.1	0.46
815.42	0.3	2.17
816.43	0.2	1.31
829.45	0.2	1.34
847.43	0.5	3.72
848.43	0.3	1.94
850.45	0.5	3.54
851.58	0.1	0.46
879.47	0.4	2.95
880.62	0.1	0.58
889.43	1.1	7.82
890.43	0.3	1.91
891.46	0.5	3.71
892.46	0.1	0.73
921.49	2.3	17.05
922.49	0.8	5.91
923.52	0.1	0.90

SPECTRUM - MS

12-16-13_HMG67_1286_MS5_1385_921_486_01.raw

ITMS + p ESI E Full ms5 1287.00@cid35.00 1385.40@cid35.00 922.00@cid35.00 487.00@cid35.00

[130.00-500.00]

Scan #: 1-50

RT: 0.00-27.54

AV: 50

m/z Intensity Relative

175.23	0.0	0.26
178.04	0.0	0.45
180.07	0.0	0.71
207.97	0.0	0.48
218.14	0.0	0.61
220.17	0.0	2.04
241.10	0.0	3.71
242.11	0.0	0.74

250.02	0.0	0.28
252.15	0.0	0.54
257.15	0.0	0.66
259.13	0.1	18.16
260.13	0.0	0.92
268.12	0.0	11.86
269.11	0.0	0.99
293.11	0.0	0.23
297.13	0.0	0.57
297.25	0.0	0.23
301.08	0.0	0.33
301.23	0.0	0.33
315.15	0.0	0.24
329.20	0.1	32.09
330.24	0.0	1.99
353.23	0.0	0.39
367.90	0.0	0.48
381.15	0.0	0.53
382.29	0.0	0.96
394.24	0.0	0.91
395.17	0.0	0.49
410.24	0.0	0.45
412.18	0.0	4.50
412.37	0.0	0.95
412.86	0.0	0.22
413.14	0.0	0.49
415.26	0.0	1.45
416.20	0.0	0.37
416.37	0.0	0.47
431.27	0.0	0.80
440.22	0.0	0.28
444.28	0.4	100.00
445.32	0.0	9.76
446.15	0.0	0.32
446.39	0.0	0.83
456.35	0.0	2.54
456.98	0.0	0.25
457.38	0.0	0.47
479.94	0.0	0.34
486.30	0.1	28.58
487.10	0.0	0.37
487.34	0.0	4.05

SPECTRUM - MS

12-16-13_HMG67_1286_MS5_1385_921_458_01.raw

ITMS + p ESI E Full ms5 1287.00@cid35.00 1385.40@cid35.00 922.00@cid35.00 459.00@cid35.00

[125.00-500.00]

Scan #: 1-50

RT: 0.00-17.47

AV: 50

m/z Intensity Relative

143.21	0.0	1.02
145.10	0.0	0.32
148.93	0.0	0.62
156.94	0.0	0.69
178.02	0.0	0.37
179.99	0.0	1.63
194.01	0.0	0.55
194.21	0.0	0.85
194.98	0.0	0.34
203.89	0.0	0.55
204.11	0.0	0.53
213.04	0.1	11.30
214.03	0.0	0.45
218.00	0.0	0.51
218.14	0.0	0.35
220.09	0.0	4.28
231.09	0.1	12.52
232.15	0.0	0.58
236.02	0.0	3.68
236.96	0.0	0.30
250.03	0.0	0.44
258.25	0.0	0.36
258.53	0.0	0.23
268.12	0.9	100.00
269.09	0.1	8.79
270.06	0.0	0.62
273.07	0.0	1.30
273.24	0.0	1.09
299.79	0.0	0.23
301.16	0.2	23.65
302.20	0.0	1.85
324.16	0.0	0.28
354.19	0.0	0.52
366.18	0.0	0.38
382.16	0.0	0.36
384.08	0.0	0.95
384.27	0.0	1.57
385.17	0.0	0.90
416.28	0.0	0.56
426.14	0.0	1.04
426.29	0.0	1.92
426.45	0.0	0.92
427.24	0.0	0.23
428.36	0.0	2.35
429.14	0.0	0.26
429.26	0.0	0.41
458.27	0.5	60.54
459.30	0.1	10.77
459.61	0.0	0.25
460.19	0.0	1.36

SPECTRUM - MS

12-16-13_HMG67_1286_MS3_1054_01.raw

ITMS + p ESI E Full ms3 1287.00@cid35.00 1055.20@cid35.00 [290.00-2000.00]

Scan #: 1-20

RT: 0.00-3.84

AV: 20

m/z Intensity Relative

458.27	14.8	5.67
486.31	141.8	54.12
487.30	31.8	12.12
534.37	12.7	4.83
676.36	7.1	2.71
704.36	8.2	3.13
706.43	12.0	4.59
724.43	80.2	30.60
725.44	29.7	11.33
822.99	262.1	100.00
823.49	220.3	84.07
823.99	103.0	39.31
824.47	31.0	11.85
899.52	35.0	13.36
900.00	35.0	13.36
900.48	18.2	6.96
921.46	79.3	30.28
922.48	34.7	13.26
923.48	9.2	3.51
936.52	95.1	36.30
937.03	91.5	34.91
937.54	47.3	18.04
938.04	18.2	6.93
945.53	10.7	4.09
946.03	10.6	4.05
1038.53	8.5	3.24
1039.05	9.3	3.55
1039.54	9.4	3.58
1040.06	7.4	2.83
1054.61	62.1	23.70
1055.09	75.9	28.95
1055.58	48.5	18.49
1056.07	22.4	8.54
1159.61	34.7	13.23
1160.61	21.4	8.16
1161.60	6.9	2.63
1187.65	100.0	38.14
1188.65	60.8	23.21
1189.63	20.9	7.96
1384.69	24.3	9.28
1385.69	16.7	6.39
1386.70	8.5	3.26

1432.75	8.9	3.41
1514.72	7.7	2.93
1622.83	177.5	67.73
1623.84	141.3	53.93
1624.85	64.3	24.55
1625.85	17.6	6.72
1849.95	7.9	3.02
1850.96	7.0	2.67

SPECTRUM - MS

12-16-13_HMG67_1286_MS4_1054_823_01.raw

ITMS + p ESI E Full ms4 1287.00@cid35.00 1055.20@cid35.00 823.40@cid35.00 [225.00-2000.00]

Scan #: 1-20

RT: 0.00-3.65

AV: 20

m/z Intensity Relative

444.28	2.1	3.96
458.26	10.8	20.30
459.27	1.9	3.58
486.30	45.5	85.32
487.30	9.1	17.16
514.30	2.5	4.63
534.36	4.0	7.45
591.32	3.9	7.31
591.81	2.8	5.18
605.35	6.2	11.71
605.85	3.7	7.02
606.36	1.4	2.55
616.31	3.2	5.98
664.41	1.8	3.30
676.35	2.2	4.06
704.36	7.4	13.98
705.36	2.9	5.40
706.42	3.3	6.19
713.95	1.6	2.96
714.42	1.4	2.53
724.43	47.6	89.34
725.44	16.6	31.07
726.44	2.8	5.21
727.94	1.6	3.03
728.40	1.3	2.49
746.35	4.8	9.06
747.35	1.4	2.62
773.46	1.3	2.47
806.95	2.0	3.75
807.45	1.7	3.27
807.97	2.9	5.53
808.46	2.0	3.68
822.99	15.3	28.78
823.49	13.6	25.56

823.98	6.1	11.36	
824.47	1.9	3.59	
921.47	19.6	36.74	
922.48	8.7	16.31	
923.46	1.7	3.25	
969.61	2.0	3.66	
970.52	1.9	3.54	
1051.47		2.3	4.40
1159.60		53.3	100.00
1160.61		28.3	53.08
1161.60		8.0	14.94
1187.66		16.2	30.44
1188.66		8.9	16.61
1189.63		2.7	5.15
1622.82		3.1	5.74
1623.82		2.3	4.27

SPECTRUM - MS

12-16-13_HMG67_1286_MS5_1054_823_1160_01.raw

ITMS + p ESI E Full ms5 1287.00@cid35.00 1055.20@cid35.00 823.40@cid35.00 1160.40@cid35.00
[315.00-1200.00]

Scan #: 1-20

RT: 0.00-4.65

AV: 20

m/z	Intensity	Relative
384.30	0.0	0.07
426.32	0.0	0.06
435.23	0.4	0.51
435.42	0.1	0.20
436.30	0.1	0.08
438.24	0.0	0.05
444.37	0.0	0.07
454.25	0.0	0.06
456.37	0.1	0.10
458.28	0.3	0.48
472.30	0.1	0.08
474.31	0.1	0.20
475.35	0.1	0.09
486.48	0.2	0.27
487.39	0.0	0.05
502.31	0.1	0.14
516.34	0.1	0.18
534.36	13.4	19.43
535.36	2.7	3.83
536.33	0.3	0.47
562.31	0.1	0.14
578.34	0.0	0.05
590.30	0.1	0.13
590.47	0.1	0.08
591.47	0.1	0.08

625.40	0.4	0.60	
626.34	0.1	0.14	
676.41	0.2	0.28	
682.53	0.0	0.05	
692.50	0.1	0.18	
696.43	0.1	0.11	
706.29	0.0	0.05	
724.42	69.2	100.00	
725.44	18.0	25.99	
726.45	2.5	3.64	
969.52	1.6	2.38	
970.53	0.7	1.04	
971.51	0.1	0.13	
971.66	0.1	0.08	
1053.53		0.1	0.09
1060.73		0.1	0.10
1061.57		0.1	0.07
1127.40		0.1	0.11
1127.63		0.2	0.29
1128.65		0.1	0.11
1129.57		0.1	0.12
1130.56		0.0	0.07
1159.59		6.4	9.22
1160.61		3.2	4.66
1161.70		0.6	0.87

SPECTRUM - MS

7-22-13_HMG69_1323_MS2_01.raw

ITMS + p ESI E Full ms2 1323.00@cid35.00 [360.00-2000.00]

Scan #: 1-20

RT: 0.00-3.02

AV: 20

m/z	Intensity	Relative
433.28	702.0	10.37
486.31	479.1	7.08
646.39	310.2	4.58
660.41	434.8	6.42
685.44	323.9	4.78
724.49	513.5	7.58
779.50	439.8	6.50
780.01	314.4	4.64
834.51	3241.7	47.88
835.51	1126.5	16.64
886.04	496.4	7.33
886.56	504.6	7.45
917.08	871.3	12.87
917.58	683.3	10.09
1004.14	1167.5	17.25
1004.64	1033.8	15.27
1005.14	506.1	7.48
1091.18	5729.7	84.64
1091.68	5882.9	86.90
1092.18	3120.1	46.09
1092.68	538.8	7.96
1109.63	683.5	10.10
1110.64	344.9	5.09
1117.68	2598.9	38.39
1118.18	2705.0	39.96
1118.69	1522.7	22.49
1204.75	938.4	13.86
1205.25	1135.6	16.77
1205.75	719.5	10.63
1219.72	1035.7	15.30
1220.21	1196.8	17.68
1220.73	802.0	11.85
1228.72	376.9	5.57
1229.23	461.6	6.82
1229.73	320.4	4.73
1322.81	5194.0	76.72
1323.28	6769.7	100.00
1323.77	5221.7	77.13
1324.27	1394.6	20.60
1347.79	765.0	11.30
1348.80	490.1	7.24

1535.90	865.1	12.78
1536.90	599.1	8.85
1749.08	587.9	8.68
1750.09	542.7	8.02
1811.15	3351.9	49.51
1812.16	2736.3	40.42
1813.17	1184.5	17.50
1985.38	424.7	6.27
1986.38	390.1	5.76

SPECTRUM - MS

7-23-13_HMG69_1323_MS3_660_01.raw

ITMS + p ESI E Full ms3 1323.00@cid35.00 661.00@cid35.00 [180.00-700.00]

Scan #: 1-50

RT: 0.00-5.92

AV: 50

m/z Intensity Relative

229.09	3.4	4.68
236.07	1.9	2.62
241.08	2.1	2.91
257.10	0.9	1.26
259.10	27.5	37.59
260.10	2.0	2.76
301.15	1.4	1.91
329.18	3.4	4.63
350.19	1.7	2.35
355.22	0.8	1.16
380.17	2.0	2.75
381.19	0.9	1.28
382.22	5.2	7.17
383.21	1.5	2.12
384.11	0.8	1.06
384.29	0.8	1.14
385.23	0.9	1.27
394.22	3.6	4.93
398.20	4.8	6.52
399.22	2.2	2.99
412.19	2.2	3.04
424.22	7.3	10.01
425.18	1.0	1.34
430.25	4.7	6.38
431.22	0.9	1.18
442.24	2.2	2.95
447.28	2.2	3.07
454.22	5.7	7.76
456.24	11.6	15.85
457.26	1.8	2.44
470.25	1.7	2.31
472.24	73.1	100.00
473.26	13.6	18.58

486.27	6.7	9.22
562.31	7.9	10.83
563.31	1.2	1.67
584.27	2.5	3.44
586.30	39.7	54.27
587.30	9.4	12.92
589.32	9.2	12.55
590.33	2.0	2.71
597.31	2.0	2.78
614.30	2.6	3.58
616.34	1.2	1.64
618.34	41.2	56.38
619.34	10.0	13.65
624.32	1.2	1.64
630.37	1.1	1.56
660.36	24.7	33.75
661.37	6.9	9.45

SPECTRUM - MS

7-22-13_HMG69_1323_MS3_834_01.raw

ITMS + p ESI E Full ms3 1323.00@cid35.00 835.00@cid35.00 [225.00-900.00]

Scan #: 1-50

RT: 0.00-8.13

AV: 50

m/z	Intensity	Relative
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245.11	5.4	1.13
353.22	6.0	1.26
364.23	4.8	1.02
368.23	4.1	0.86
369.23	2.1	0.43
383.24	6.7	1.41
384.23	2.0	0.43
387.27	3.0	0.64
401.25	2.0	0.42
415.28	39.5	8.33
416.29	5.7	1.20
417.31	2.2	0.46
424.24	7.6	1.61
426.27	4.1	0.86
431.25	6.7	1.40
433.29	474.2	100.00
434.30	68.8	14.50
435.31	5.1	1.07
442.31	26.5	5.59
443.32	4.1	0.86
458.28	1.9	0.41
558.28	2.2	0.47
572.36	17.2	3.63
573.36	4.6	0.97
586.39	7.6	1.61

604.41	2.7	0.57
621.43	4.8	1.02
628.39	5.4	1.13
630.39	2.2	0.47
644.42	2.2	0.46
646.41	209.7	44.21
647.42	49.5	10.44
648.43	4.8	1.02
660.40	6.1	1.29
689.45	8.6	1.80
730.49	2.7	0.57
758.47	3.8	0.80
760.48	196.7	41.48
761.48	56.6	11.92
762.48	4.6	0.98
763.48	14.6	3.09
764.49	4.6	0.96
788.48	10.1	2.14
789.48	2.9	0.60
792.51	52.6	11.08
793.52	16.3	3.43
804.50	3.3	0.69
834.54	57.9	12.21
835.54	20.0	4.22
836.56	3.2	0.68

SPECTRUM - MS

7-22-13_HMG69_1323_MS4_834_646_01.raw

ITMS + p ESI E Full ms4 1323.00@cid35.00 835.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-50

RT: 0.00-8.55

AV: 50

m/z Intensity Relative

197.14	0.1	0.40
204.04	0.2	0.70
218.10	0.3	1.06
220.11	0.5	1.93
227.11	0.2	0.91
229.13	2.3	8.31
236.12	1.0	3.80
243.15	0.1	0.42
245.12	3.1	11.52
246.14	0.2	0.77
287.14	0.1	0.48
295.15	0.2	0.60
350.23	0.4	1.42
353.20	0.1	0.52
364.25	1.1	4.19
365.24	0.2	0.57
366.17	0.2	0.62

368.24	1.4	5.24
369.23	0.5	1.87
382.22	0.6	2.28
382.41	0.2	0.63
383.30	0.1	0.48
384.30	0.3	1.25
385.23	0.3	0.99
392.25	0.1	0.52
398.36	0.6	2.17
415.29	0.7	2.54
417.31	0.9	3.20
424.27	2.5	9.04
425.26	0.3	1.09
426.29	1.3	4.59
427.28	0.1	0.41
433.30	27.3	100.00
434.32	3.3	12.22
440.28	0.8	2.94
442.30	1.4	5.28
443.32	0.1	0.44
458.29	2.0	7.36
459.29	0.3	1.24
475.37	0.1	0.51
499.25	0.1	0.44
540.42	0.5	1.96
541.35	0.2	0.63
572.37	23.2	85.02
573.37	4.8	17.66
575.39	0.4	1.57
604.45	0.4	1.61
614.33	0.2	0.58
646.41	4.0	14.71
647.43	1.2	4.39

SPECTRUM - MS

7-22-13_HMG69_1323_MS3_1109_01.raw

ITMS + p ESI E Full ms3 1323.00@cid35.00 1110.00@cid35.00 [305.00-1200.00]

Scan #: 1-20

RT: 0.00-2.91

AV: 20

m/z Intensity Relative

378.27	0.3	0.24
382.29	0.3	0.25
385.21	6.2	4.37
386.30	0.3	0.25
398.26	0.7	0.51
412.27	1.0	0.68
440.25	1.6	1.11
442.39	0.5	0.38
444.35	0.3	0.22

454.30	0.4	0.27
458.29	1.0	0.73
470.33	0.4	0.29
472.28	0.4	0.29
486.31	27.4	19.39
487.33	4.5	3.19
572.34	3.1	2.16
573.36	1.0	0.74
575.38	2.5	1.73
598.32	2.5	1.74
599.35	0.5	0.33
604.47	0.4	0.28
646.39	141.5	100.00
647.40	24.5	17.34
660.28	0.3	0.22
690.20	0.4	0.27
690.42	0.9	0.65
708.43	7.7	5.41
709.44	1.7	1.17
778.53	1.0	0.68
799.46	10.5	7.39
800.53	2.1	1.49
873.52	72.1	50.94
874.53	19.9	14.04
891.56	0.5	0.33
903.62	0.7	0.48
905.34	0.9	0.63
905.57	1.8	1.30
906.42	0.4	0.30
906.56	0.5	0.32
921.62	0.6	0.42
922.60	0.4	0.25
1035.48		0.5 0.38
1035.69		0.4 0.31
1067.66		1.7 1.18
1068.53		0.6 0.42
1073.64		1.1 0.77
1074.10		0.9 0.63
1077.52		0.3 0.24
1109.63	42.8	30.23
1110.64	23.1	16.35

SPECTRUM - MS

7-22-13_HMG69_1323_MS4_1109_646_01.raw

ITMS + p ESI E Full ms4 1323.00@cid35.00 1110.00@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-50

RT: 0.00-8.60

AV: 50

m/z Intensity Relative

194.03 0.1 0.76

204.03	0.3	1.70
211.07	0.1	0.66
220.12	0.2	1.02
227.10	1.6	9.78
228.13	0.1	0.66
229.13	0.6	3.39
236.11	1.1	6.41
243.13	0.1	0.57
245.11	2.9	17.49
287.07	0.1	0.80
315.19	0.4	2.14
324.20	0.1	0.78
339.19	0.1	0.59
343.21	0.8	5.05
353.16	0.2	0.95
366.23	0.3	2.02
367.20	0.3	1.89
368.22	0.3	1.58
369.26	0.2	1.21
371.26	0.1	0.65
378.23	0.7	4.40
380.25	0.6	3.69
382.27	0.8	4.76
384.23	0.7	4.02
385.22	16.6	100.00
386.23	1.3	7.92
396.24	0.1	0.63
398.25	0.2	1.44
408.25	0.1	0.80
424.31	0.6	3.64
425.22	0.1	0.68
433.32	0.3	1.54
440.26	2.6	15.49
441.26	0.4	2.13
442.29	2.0	12.08
443.30	0.3	1.70
458.28	1.3	7.91
459.31	0.2	1.15
498.21	0.1	0.59
530.38	0.2	1.16
572.36	8.5	51.36
573.36	3.5	21.23
574.30	0.1	0.70
574.45	0.1	0.86
575.38	5.0	30.01
576.41	0.9	5.19
604.39	1.1	6.71
646.41	5.3	32.08
647.42	0.9	5.29

SPECTRUM - MS

7-22-13_HMG69_1323_MS4_1109_486_02.raw

ITMS + p ESI E Full ms4 1323.00@cid35.00 1110.00@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-100

RT: 0.00-13.80

AV: 100

m/z Intensity Relative

161.40	0.0	0.44
178.15	0.0	0.60
188.04	0.0	0.49
190.42	0.0	0.43
198.14	0.0	0.61
208.15	0.0	2.06
211.01	0.0	0.79
218.29	0.0	0.51
220.07	0.0	2.23
237.32	0.0	0.49
238.03	0.0	0.74
241.13	0.2	8.17
250.12	0.1	6.04
250.99	0.0	0.44
251.98	0.1	2.67
252.16	0.1	6.46
253.15	0.0	1.40
257.16	0.0	2.05
259.13	1.4	71.58
260.12	0.1	5.53
267.89	0.0	0.71
268.25	0.1	4.89
269.20	0.0	0.48
286.99	0.0	0.43
297.19	0.0	0.95
301.19	0.0	2.27
329.21	0.8	39.72
330.17	0.0	2.35
330.42	0.0	0.56
338.33	0.0	0.47
369.98	0.0	0.50
382.24	0.0	0.96
384.03	0.0	0.68
384.19	0.1	2.82
389.26	0.0	0.53
394.28	0.0	0.61
412.26	1.4	69.15
413.30	0.1	5.07
415.26	0.0	1.75
436.78	0.0	0.48
440.40	0.0	0.50
442.00	0.0	0.46
444.30	2.0	100.00
445.30	0.3	14.71

454.36	0.0	0.43
456.33	0.0	1.62
456.47	0.0	1.34
457.26	0.0	0.67
486.29	0.2	12.55
487.27	0.0	1.14

SPECTRUM - MS

7-23-13_HMG69_1323_MS3_1004_01.raw

ITMS + p ESI E Full ms3 1323.00@cid35.00 1004.50@cid35.00 [275.00-2000.00]

Scan #: 1-50

RT: 0.00-10.71

AV: 50

m/z	Intensity	Relative
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472.24	6.1	2.58
534.33	30.1	12.80
535.34	6.7	2.86
646.34	26.9	11.44
647.35	6.8	2.91
660.37	148.9	63.31
661.38	37.7	16.03
662.39	5.7	2.41
664.42	5.1	2.19
685.39	74.8	31.82
685.90	46.7	19.85
686.39	13.7	5.84
692.39	44.4	18.90
692.90	27.7	11.78
693.41	7.9	3.37
704.36	6.3	2.67
706.40	17.5	7.46
707.40	5.1	2.15
724.43	131.7	56.03
725.41	38.0	16.16
726.41	6.1	2.59
797.96	5.2	2.19
863.98	9.4	4.00
864.48	8.0	3.42
901.00	235.1	100.00
901.50	208.9	88.85
902.00	92.0	39.12
902.50	23.8	10.11
902.99	5.2	2.21
910.02	15.5	6.59
910.51	13.5	5.75
911.00	4.9	2.07
954.52	4.3	1.84
1004.07		21.6 9.19
1004.57		20.7 8.80
1005.06		12.0 5.10

1077.55	7.4	3.16
1141.58	5.7	2.44
1143.62	5.0	2.14
1239.58	9.1	3.86
1240.59	4.9	2.09
1283.64	55.0	23.38
1284.65	29.1	12.37
1285.66	7.2	3.05
1347.71	184.1	78.29
1348.72	110.9	47.16
1349.72	29.7	12.65
1361.70	26.4	11.24
1362.71	13.9	5.93
1363.72	4.5	1.92

SPECTRUM - MS

7-23-13_HMG69_1323_MS4_1004_1283_01.raw

ITMS + p ESI E Full ms4 1323.00@cid35.00 1004.50@cid35.00 1284.00@cid35.00 [350.00-1300.00]

Scan #: 1-50

RT: 0.00-8.44

AV: 50

m/z Intensity Relative

384.08	0.1	0.71
385.12	0.0	0.56
385.32	0.0	0.68
454.37	0.1	1.03
472.25	0.2	3.06
572.34	0.1	1.68
573.40	0.1	0.77
575.34	0.2	2.16
586.31	0.1	1.30
589.40	0.0	0.61
598.26	0.0	0.65
602.23	0.1	0.85
604.32	0.1	1.30
618.37	0.1	1.08
632.47	0.0	0.61
646.33	6.2	84.25
647.34	1.1	14.99
660.36	7.3	100.00
661.44	0.7	8.87
841.49	0.0	0.59
842.54	0.1	0.77
864.41	0.1	0.90
880.61	0.1	0.75
882.46	0.7	9.77
883.63	0.1	1.29
952.48	0.1	1.44
952.61	0.1	1.01
1003.48	0.4	6.00

1004.50	0.1	1.44
1008.79	0.1	0.72
1017.50	0.1	1.16
1036.46	0.1	0.68
1077.54	5.4	73.45
1078.55	1.8	24.50
1079.56	0.3	4.75
1080.29	0.1	0.82
1080.59	0.1	1.88
1095.67	0.1	1.96
1209.67	0.0	0.62
1212.62	0.1	0.89
1212.77	0.1	0.81
1241.45	0.1	0.76
1241.58	0.0	0.60
1241.75	0.1	1.31
1242.69	0.1	1.04
1251.49	0.0	0.57
1283.60	1.1	14.32
1283.81	0.4	5.28
1284.68	0.3	4.76
1284.82	0.2	3.36

SPECTRUM - MS

7-23-13_HMG69_1323_MS5_1004_1283_646_02.raw

ITMS + p ESI E Full ms5 1323.00@cid35.00 1004.50@cid35.00 1284.00@cid35.00 647.00@cid35.00
[175.00-700.00]

Scan #: 1-116

RT: 0.00-24.60

AV: 116

m/z	Intensity	Relative
193.97	0.0	0.98
203.98	0.0	2.02
227.10	0.1	11.51
229.03	0.0	3.31
236.04	0.0	3.66
236.18	0.0	3.02
245.09	0.1	20.40
292.24	0.0	1.02
315.21	0.0	1.94
343.18	0.0	3.07
343.95	0.0	1.14
344.11	0.0	0.85
366.09	0.0	0.90
367.18	0.0	1.72
368.04	0.0	0.88
368.25	0.0	1.23
371.20	0.0	1.14
378.16	0.0	3.69
378.42	0.0	1.13

380.21	0.0	1.95
380.33	0.0	1.29
382.25	0.0	1.46
384.21	0.0	4.81
385.19	0.5	100.00
386.20	0.0	8.06
398.11	0.0	1.29
408.19	0.0	1.61
412.32	0.0	2.52
424.23	0.0	5.56
440.03	0.0	2.69
440.28	0.0	6.84
440.98	0.0	1.76
441.31	0.0	1.10
442.09	0.0	2.43
442.29	0.0	8.43
458.27	0.0	4.44
492.54	0.0	1.35
499.16	0.0	1.02
572.32	0.2	41.30
573.31	0.1	20.00
574.31	0.0	1.44
574.47	0.0	1.20
575.40	0.1	21.05
576.32	0.0	2.22
576.51	0.0	0.92
604.34	0.0	6.76
604.57	0.0	1.23
646.14	0.0	1.40
646.37	0.0	7.06
647.40	0.0	3.14

SPECTRUM - MS

7-23-13_HMG69_1323_MS5_1004_1283_660_02.raw

ITMS + p ESI E Full ms5 1323.00@cid35.00 1004.50@cid35.00 1284.00@cid35.00 661.00@cid35.00
[180.00-700.00]

Scan #: 1-100

RT: 0.00-19.59

AV: 100

m/z Intensity Relative

218.12	0.0	1.29
229.17	0.0	3.14
241.09	0.0	3.49
241.29	0.0	1.17
259.12	0.2	29.81
301.16	0.0	1.55
329.14	0.0	1.36
329.32	0.0	1.20
330.26	0.0	1.25
332.11	0.0	1.34

368.36	0.0	1.31
371.10	0.0	1.26
371.29	0.0	1.20
380.23	0.0	3.60
382.22	0.0	6.41
382.37	0.0	2.88
383.31	0.0	1.83
384.18	0.0	5.03
394.10	0.0	1.23
394.29	0.0	4.20
398.12	0.0	4.89
424.19	0.0	2.78
430.24	0.0	8.59
430.45	0.0	1.38
431.25	0.0	1.51
442.31	0.0	1.33
447.26	0.0	1.71
454.20	0.0	3.67
456.16	0.0	7.56
456.35	0.0	4.31
457.34	0.0	1.74
470.26	0.0	2.49
472.25	0.6	100.00
473.26	0.1	10.87
540.28	0.0	1.21
584.41	0.0	2.30
586.23	0.2	28.30
586.45	0.1	21.31
587.28	0.1	9.64
588.36	0.0	2.43
589.27	0.1	15.25
614.14	0.0	1.91
614.30	0.0	3.68
618.36	0.3	58.54
619.38	0.0	6.31
619.56	0.0	3.39
628.36	0.0	2.06
628.50	0.0	1.68
660.42	0.0	5.58
661.38	0.0	3.31

HMG 76 Mass spectral peak lists

SPECTRUM - MS

7-23-13_HMG76_981_MS2_01.raw

ITMS + p ESI E Full ms2 981.80@cid35.00 [270.00-2000.00]

Scan #: 1-20

RT: 0.00-1.73

AV: 20

m/z	Intensity	Relative
486.28	2145.7	31.12
487.29	446.1	6.47
646.36	169.7	2.46
685.41	245.5	3.56
826.82	2743.6	39.79
827.15	3682.8	53.42
827.48	2291.5	33.24
827.83	1119.7	16.24
828.23	389.9	5.66
902.52	504.7	7.32
902.86	746.7	10.83
903.19	452.0	6.56
903.52	312.6	4.53
912.52	178.6	2.59
912.85	262.9	3.81
913.20	177.9	2.58
917.05	980.9	14.23
917.54	836.0	12.13
918.05	418.1	6.06
918.54	249.8	3.62
918.88	190.5	2.76
981.26	1326.4	19.24
981.58	2349.2	34.07
981.90	1544.6	22.40
982.22	986.4	14.31
982.58	523.6	7.60
997.08	438.7	6.36
997.59	451.7	6.55
998.09	249.4	3.62
1109.58	630.1	9.14
1110.60	633.3	9.18
1111.14	361.6	5.24
1111.63	295.7	4.29
1174.60	398.0	5.77
1175.11	459.8	6.67
1175.61	307.9	4.47
1228.69	5624.0	81.57
1229.18	6894.6	100.00
1229.68	4062.3	58.92
1230.19	1977.5	28.68
1230.69	528.1	7.66

1342.24	1421.7	20.62
1342.74	1974.2	28.63
1343.24	1236.9	17.94
1343.75	631.1	9.15
1344.26	191.1	2.77
1460.30	607.4	8.81
1460.80	957.2	13.88
1461.31	644.4	9.35
1461.80	387.7	5.62

SPECTRUM - MS

7-23-13_HMG76_981_MS3_1229_01.raw

ITMS + p ESI E Full ms3 981.80@cid35.00 1229.00@cid35.00 [335.00-2000.00]

Scan #: 1-50

RT: 0.00-4.77

AV: 50

m/z Intensity Relative

486.29	78.4	7.23
646.36	148.5	13.69
647.37	34.8	3.21
685.41	150.5	13.88
685.92	88.0	8.11
686.43	27.1	2.50
706.43	19.1	1.76
724.45	45.2	4.17
798.96	16.5	1.52
894.02	73.6	6.79
894.52	64.4	5.94
895.02	45.8	4.22
895.53	20.6	1.90
917.05	205.6	18.96
917.56	157.6	14.54
918.05	62.3	5.75
997.10	1084.3	100.00
997.60	889.3	82.02
998.10	407.1	37.54
998.59	101.6	9.37
1073.60	31.2	2.88
1074.08	25.5	2.35
1074.57	14.4	1.33
1109.59	51.2	4.72
1110.63	242.7	22.39
1111.14	205.0	18.91
1111.65	118.3	10.91
1112.15	30.1	2.77
1125.64	142.0	13.10
1126.13	123.6	11.39
1126.62	98.1	9.04
1127.13	36.1	3.32
1134.64	28.4	2.62

1135.13	27.7	2.55
1228.68	150.7	13.89
1229.17	182.1	16.80
1229.69	119.4	11.01
1230.21	42.4	3.91
1347.75	212.8	19.63
1348.75	126.3	11.65
1349.78	38.9	3.59
1574.87	15.9	1.47
1765.02	21.2	1.96
1766.05	14.5	1.34
1811.08	105.3	9.71
1812.09	75.1	6.93
1813.11	29.7	2.73
1971.27	138.8	12.80
1972.29	109.1	10.06
1973.30	47.6	4.39

SPECTRUM - MS

7-23-13_HMG76_981_MS4_1229_997_01.raw

ITMS + p ESI E Full ms4 981.80@cid35.00 1229.00@cid35.00 997.50@cid35.00 [270.00-2000.00]

Scan #: 1-51

RT: 0.00-5.33

AV: 51

m/z Intensity Relative

385.19	3.2	2.15
440.23	2.4	1.64
458.26	2.6	1.76
514.28	2.5	1.66
534.39	5.9	3.95
572.32	1.9	1.30
582.36	4.8	3.21
582.91	1.9	1.30
591.35	1.5	1.02
616.30	2.4	1.64
646.38	90.9	61.02
647.48	9.5	6.37
648.43	1.9	1.29
664.44	4.3	2.91
685.43	121.1	81.35
685.94	48.4	32.49
686.22	1.9	1.29
686.44	12.2	8.18
704.40	5.5	3.69
706.43	12.7	8.54
707.47	2.8	1.87
724.46	18.9	12.72
725.45	5.1	3.45
746.38	4.5	3.00
791.03	1.7	1.15

791.95	6.1	4.11
792.47	3.0	2.01
857.02	6.2	4.13
886.03	3.5	2.36
894.04	95.6	64.18
894.54	53.8	36.16
895.05	36.0	24.20
895.54	16.0	10.73
896.07	3.6	2.40
903.03	10.9	7.32
903.52	4.1	2.78
904.06	1.9	1.30
947.55	2.1	1.44
997.12	40.2	27.02
997.60	34.2	22.95
998.10	16.0	10.72
1141.64		6.8 4.59
1143.68		2.2 1.47
1239.62		8.0 5.35
1240.63		2.5 1.69
1347.78		148.9 100.00
1348.79		58.5 39.29
1349.78		11.2 7.50
1766.13		2.1 1.38
1971.41		1.7 1.16

SPECTRUM - MS

7-23-13_HMG76_981_MS5_1229_997_646_02.raw

ITMS + p ESI E Full ms5 981.80@cid35.00 1229.00@cid35.00 997.50@cid35.00 647.00@cid35.00
[175.00-700.00]

Scan #: 1-50

RT: 0.00-8.84

AV: 50

m/z Intensity Relative

204.01	0.2	1.67
220.06	0.2	1.28
227.09	1.2	10.25
229.13	0.4	3.71
236.09	0.8	7.17
243.09	0.1	1.04
245.09	2.4	20.57
246.19	0.1	0.84
287.13	0.2	1.55
315.07	0.2	1.84
315.25	0.2	1.90
343.27	0.3	2.18
350.21	0.1	0.71
353.18	0.1	1.05
366.24	0.3	2.29
367.24	0.2	1.79

368.21	0.3	2.76
369.18	0.2	1.39
371.18	0.1	0.76
378.23	0.6	4.79
380.34	0.2	1.80
382.23	0.7	5.76
383.28	0.1	0.98
384.21	0.8	6.56
385.19	11.8	100.00
386.21	1.4	11.91
398.25	0.2	1.27
408.16	0.1	1.06
424.20	0.6	5.33
425.21	0.1	1.23
433.29	0.2	1.77
440.23	1.9	16.40
441.31	0.2	2.00
442.27	1.8	15.22
443.22	0.1	1.17
443.35	0.2	1.34
458.25	0.9	7.62
459.21	0.1	0.76
459.35	0.1	0.88
503.32	0.1	0.74
530.31	0.1	0.89
531.28	0.1	0.75
572.34	6.3	53.01
573.33	2.8	23.89
574.36	0.3	2.39
575.34	3.5	29.26
576.35	0.9	8.00
604.41	0.8	6.53
646.34	1.9	16.02
647.41	0.4	3.75

SPECTRUM - MS

7-23-13_HMG76_981_MS3_1109_02.raw

ITMS + p ESI E Full ms3 981.80@cid35.00 1109.60@cid35.00 [305.00-1200.00]

Scan #: 1-50

RT: 0.00-9.71

AV: 50

m/z Intensity Relative

380.21	0.0	0.18
385.19	1.0	3.76
398.20	0.2	0.65
412.22	0.3	0.98
424.25	0.0	0.19
440.24	0.2	0.81
442.20	0.1	0.41
442.35	0.1	0.30

444.25	0.1	0.27
454.27	0.1	0.32
458.29	0.1	0.51
470.28	0.1	0.38
472.04	0.0	0.15
472.28	0.1	0.50
486.29	4.9	18.68
524.40	0.0	0.18
572.31	0.5	1.84
573.32	0.1	0.30
575.34	0.4	1.58
598.30	0.4	1.47
604.44	0.1	0.27
646.37	26.1	100.00
660.33	0.1	0.21
685.38	0.1	0.26
690.40	0.2	0.93
706.40	0.1	0.30
708.39	1.3	5.01
778.55	0.1	0.21
799.43	2.6	9.98
831.40	0.0	0.14
831.56	0.0	0.15
873.49	18.1	69.50
875.52	0.1	0.36
891.46	0.1	0.35
903.43	0.2	0.61
905.47	0.6	2.35
908.05	0.0	0.16
908.52	0.2	0.79
921.32	0.1	0.20
921.55	0.1	0.48
922.15	0.0	0.15
922.55	0.2	0.67
922.74	0.0	0.15
1003.55	0.0	0.17
1006.05	0.1	0.40
1035.59	0.2	0.64
1038.51	0.1	0.24
1067.59	0.3	1.30
1109.13	0.1	0.36
1109.62	3.7	14.24

SPECTRUM - MS

7-23-13_HMG76_981_MS4_1109_646_01.raw

ITMS + p ESI E Full ms4 981.80@cid35.00 1109.60@cid35.00 647.00@cid35.00 [175.00-700.00]

Scan #: 1-89

RT: 0.00-45.25

AV: 89

m/z Intensity Relative

194.01	0.0	0.78
204.05	0.0	1.47
211.12	0.0	0.62
218.06	0.0	0.75
220.11	0.0	0.76
227.08	0.1	11.24
229.12	0.0	4.43
236.15	0.0	3.98
245.10	0.2	21.20
284.14	0.0	0.44
287.18	0.0	0.76
292.11	0.0	0.74
311.16	0.0	0.69
315.17	0.0	3.21
324.22	0.0	0.71
343.22	0.0	4.06
353.19	0.0	1.26
364.17	0.0	0.40
366.13	0.0	2.41
367.20	0.0	1.53
368.24	0.0	1.66
369.22	0.0	1.55
371.11	0.0	0.40
371.35	0.0	0.46
378.04	0.0	1.88
378.24	0.0	3.45
380.21	0.0	4.57
382.22	0.0	5.53
384.16	0.0	5.86
385.18	0.8	100.00
396.31	0.0	0.38
398.23	0.0	2.00
408.26	0.0	0.62
422.21	0.0	0.41
424.20	0.0	5.61
433.23	0.0	1.24
440.23	0.1	16.59
442.24	0.1	15.41
456.20	0.0	0.58
457.80	0.0	0.56
458.22	0.1	10.84
498.27	0.0	0.70
530.29	0.0	1.27
572.32	0.6	69.04
573.32	0.1	14.60
575.33	0.3	34.54
600.39	0.0	0.44
604.19	0.0	2.48
604.43	0.0	5.98
646.37	0.4	50.98

SPECTRUM - MS

10-4-13_HMG76_981_MS4_1109_486_01.raw

ITMS + p ESI Full ms4 981.80@cid35.00 1109.60@cid35.00 487.00@cid35.00 [130.00-500.00]

Scan #: 1-101

RT: 0.00-25.64

AV: 101

m/z	Intensity	Relative
149.18	0.0	0.37
162.00	0.0	0.31
176.04	0.0	0.23
176.97	0.0	0.28
178.08	0.0	1.41
180.06	0.0	0.36
188.07	0.0	0.49
192.06	0.0	0.17
194.04	0.0	0.39
199.20	0.0	0.24
204.16	0.0	0.16
208.15	0.0	7.07
211.07	0.0	0.53
218.18	0.0	0.62
218.45	0.0	0.23
220.19	0.0	1.53
222.11	0.0	0.22
227.22	0.0	0.25
241.11	0.0	7.33
250.13	0.0	6.30
252.12	0.0	14.01
257.13	0.0	2.51
259.13	0.2	97.19
268.10	0.0	7.22
301.24	0.0	1.19
308.91	0.0	0.19
315.42	0.0	0.17
324.38	0.0	0.35
329.20	0.0	21.16
329.83	0.0	0.21
341.27	0.0	1.17
342.31	0.0	0.38
356.58	0.0	0.44
368.14	0.0	0.52
380.10	0.0	0.17
382.30	0.0	0.78
384.27	0.0	3.26
387.33	0.0	0.18
394.14	0.0	0.21
396.62	0.0	0.34
410.15	0.0	1.75
410.55	0.0	0.35
412.24	0.2	100.00

413.25	0.0	0.31
415.29	0.0	0.79
444.25	0.2	67.27
454.29	0.0	0.60
456.18	0.0	3.02
458.28	0.0	0.30
486.17	0.0	1.35

SPECTRUM - MS

10-4-13_HMG76_981_MS6_827_997_894_1348_01.raw

ITMS + p ESI E Full ms6 981.80@cid35.00 827.40@cid35.00 997.60@cid35.00 895.00@cid35.00
1348.20@cid35.00 [370.00-1400.00]

Scan #: 1-101

RT: 0.00-41.54

AV: 101

m/z	Intensity	Relative
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435.33	0.0	0.66
486.09	0.0	0.47
486.36	0.0	1.26
502.33	0.0	0.70
520.41	0.0	0.42
534.35	0.1	26.23
535.39	0.0	4.61
536.41	0.0	0.50
625.39	0.0	1.66
646.29	0.0	2.17
646.49	0.0	1.13
647.45	0.0	0.39
706.47	0.0	0.64
708.21	0.0	0.44
722.42	0.0	0.65
724.44	0.4	100.00
725.43	0.1	27.87
726.37	0.0	1.17
726.50	0.0	1.02
836.51	0.0	0.68
837.49	0.0	0.48
863.37	0.0	0.34
863.57	0.0	0.41
877.46	0.0	0.95
919.60	0.0	1.05
921.50	0.0	0.34
937.55	0.0	0.53
1045.76	0.0	0.37
1067.53	0.0	3.39
1067.74	0.0	0.98
1068.69	0.0	0.57
1141.17	0.0	0.60
1141.61	0.0	11.06
1142.58	0.0	4.05

1142.73	0.0	1.86
1142.92	0.0	0.47
1143.52	0.0	2.50
1143.70	0.0	3.33
1144.69	0.0	2.91
1159.61	0.0	1.79
1160.55	0.0	0.65
1160.79	0.0	0.41
1230.49	0.0	0.38
1248.75	0.0	1.88
1315.51	0.0	0.70
1315.75	0.0	0.77
1347.59	0.0	1.03
1347.79	0.0	2.83
1348.76	0.0	2.54
1349.77	0.0	0.87