LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG072816\
Data File : BG023316.D
Acq On : 28 Jul 2016 21:06
Operator : UM/SJ
Sample : H4205-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-39-12.0-13.0

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.002	23	28	49	rBV	8276339	13687415	100.00%	15.215%
2	3.654	135	139	144	rBV	109017	137615	1.01%	0.153%
3	5.193	395	401	411	rBV	641937	973371	7.11%	1.082%
4	5.669	475	482	495	rBV	3208953	5373587	39.26%	5.973%
5	7.290	750	758	771	rBV	3455981	6155504	44.97%	6.843%
6	7.661	812	821	831	rBV	3269834	5833131	42.62%	6.484%
7	8.136	893	902	907	rBV	620609	1075718	7.86%	1.196%
8	8.459	948	957	966	rBV	2364376	4140744	30.25%	4.603%
9	9.311	1094	1102	1111	rBV	2110783	3868096	28.26%	4.300%
10	10.974	1377	1385	1396	rVB	958134	1725405	12.61%	1.918%
11	13.423	1794	1802	1809	rBV	5494948	8808524	64.35%	9.792%
12	14.246	1936	1942	1948	rBV	1333741	1943325	14.20%	2.160%
13	14.810	2031	2038	2045	rVB2	1560701	2644165	19.32%	2.939%
14	15.626	2165	2177	2183	rVB4	74603	153503	1.12%	0.171%
15	16.302	2286	2292	2306	rBV	4963986	8018609	58.58%	8.914%
16	16.496	2321	2325	2329	rBV2	102800	142802	1.04%	0.159%
17	17.571	2499	2508	2521	rBV2	2209252	3475092	25.39%	3.863%
18	18.440	2651	2656	2667	rBV3	147617	298981	2.18%	0.332%
19	19.715	2868	2873	2879	rBV8	70583	143470	1.05%	0.159%
20	19.856	2892	2897	2901	rBV	496664	598151	4.37%	0.665%
21	20.179	2946	2952	2959	rBV	8914788	12398059	90.58%	13.782%
22	20.901	3070	3075	3079	rBV	381750	436871	3.19%	0.486%
23	21.894	3234	3244	3255	rBV	2176635	3920603	28.64%	4.358%
24	22.423	3329	3334	3341	rBV2	121846	202891	1.48%	0.226%
25	25.295	3812	3823	3838	rBV2	1254226	3803765	27.79%	4.228%

Sum of corrected areas: 89959397

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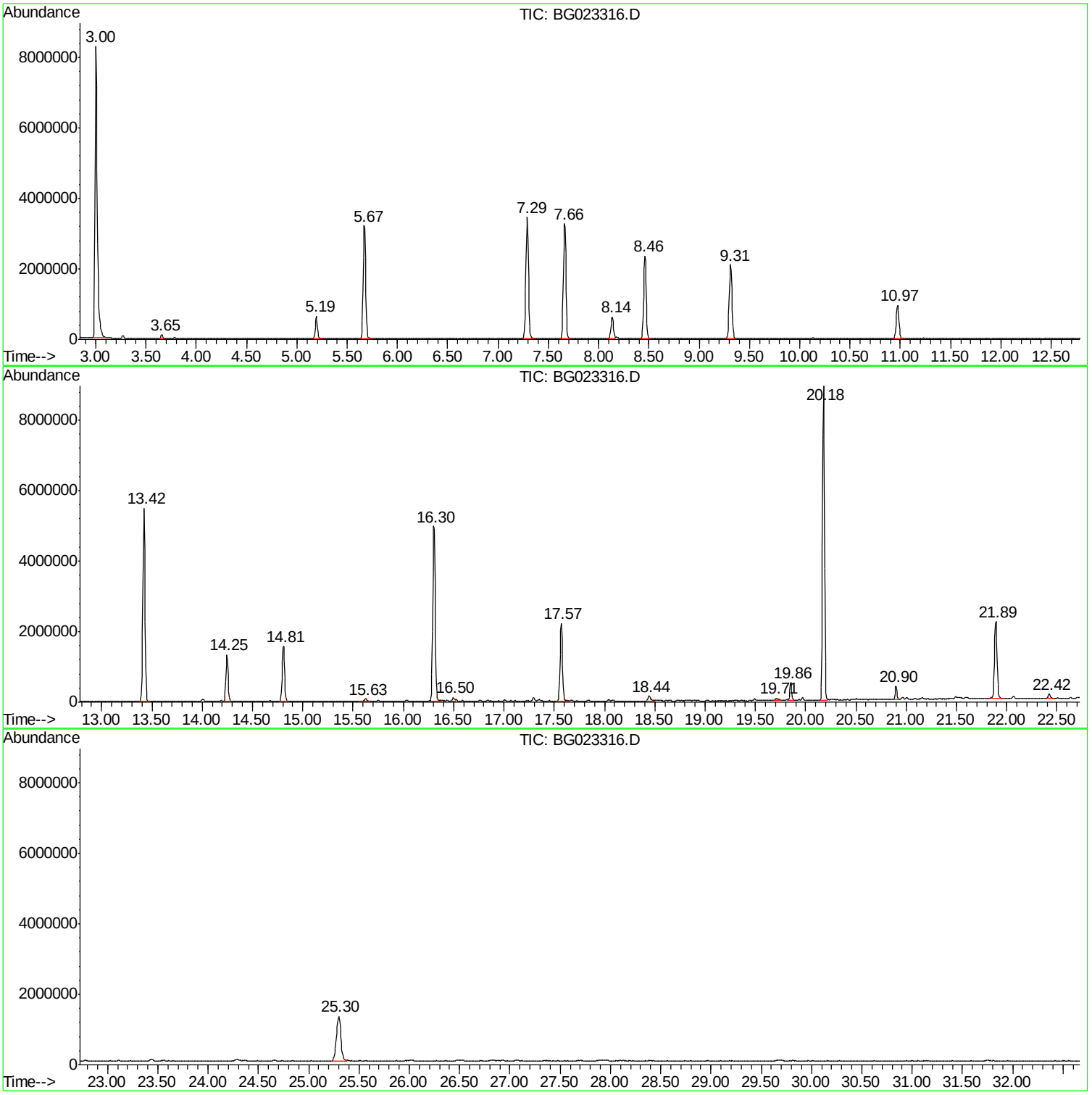
ClientSampleId : SB-39-12.0-13.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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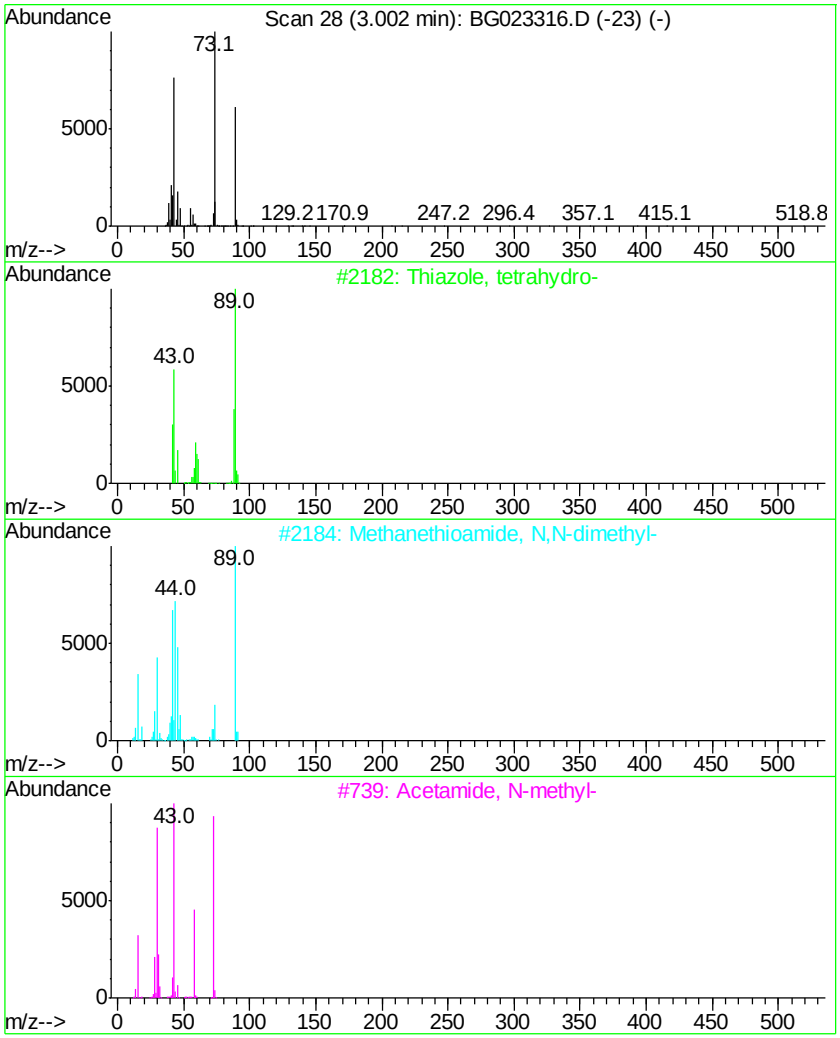
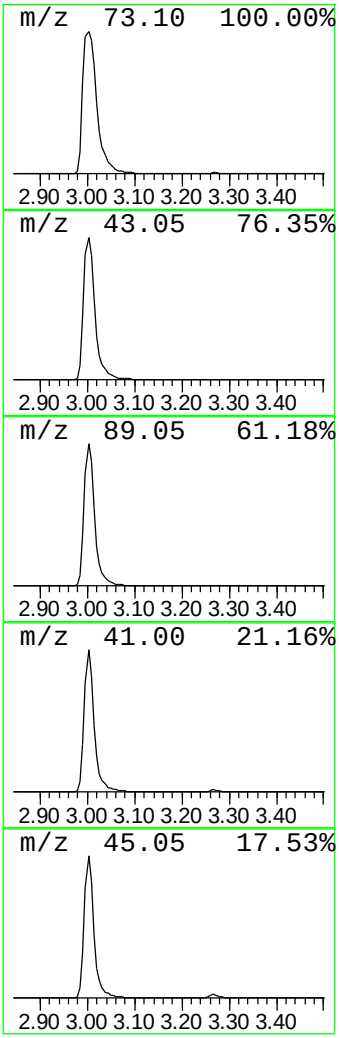
Peak Number 1 unknown3.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	254.48 ng	13687400	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	37
2	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	37
3	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4	2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	12
5	1-Propene-1-thiol	74	C3H6S	000925-89-3	9





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ClientSampleId : SB-39-12.0-13.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
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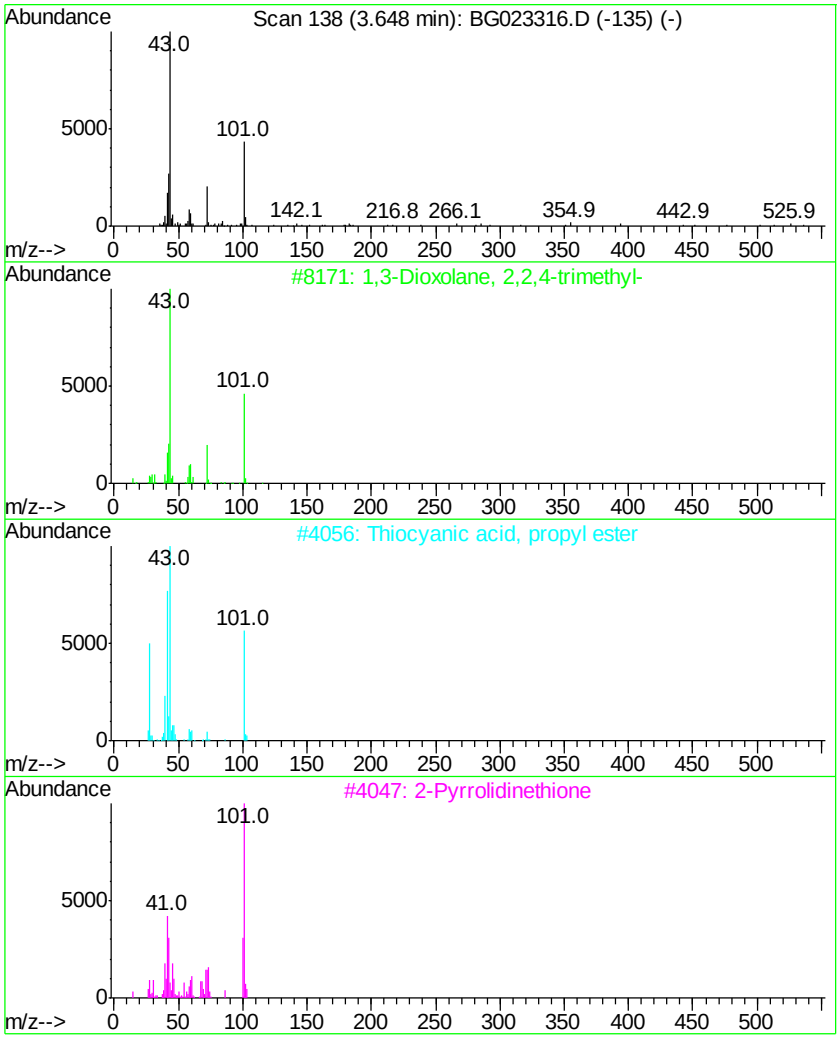
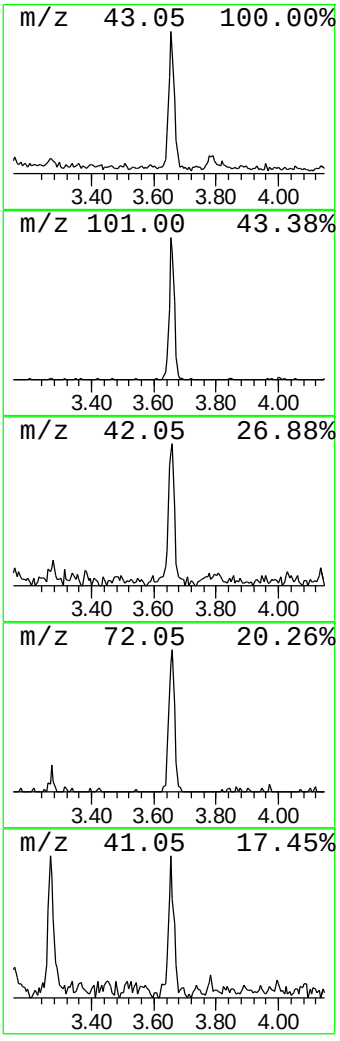
Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.65	2.56 ng	137615	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	56
2	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	50
3	2-Pyrrolidinethione	101	C4H7NS	002295-35-4	45
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	9





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Instrument : BNA_G
ClientSampleId : SB-39-12.0-13.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
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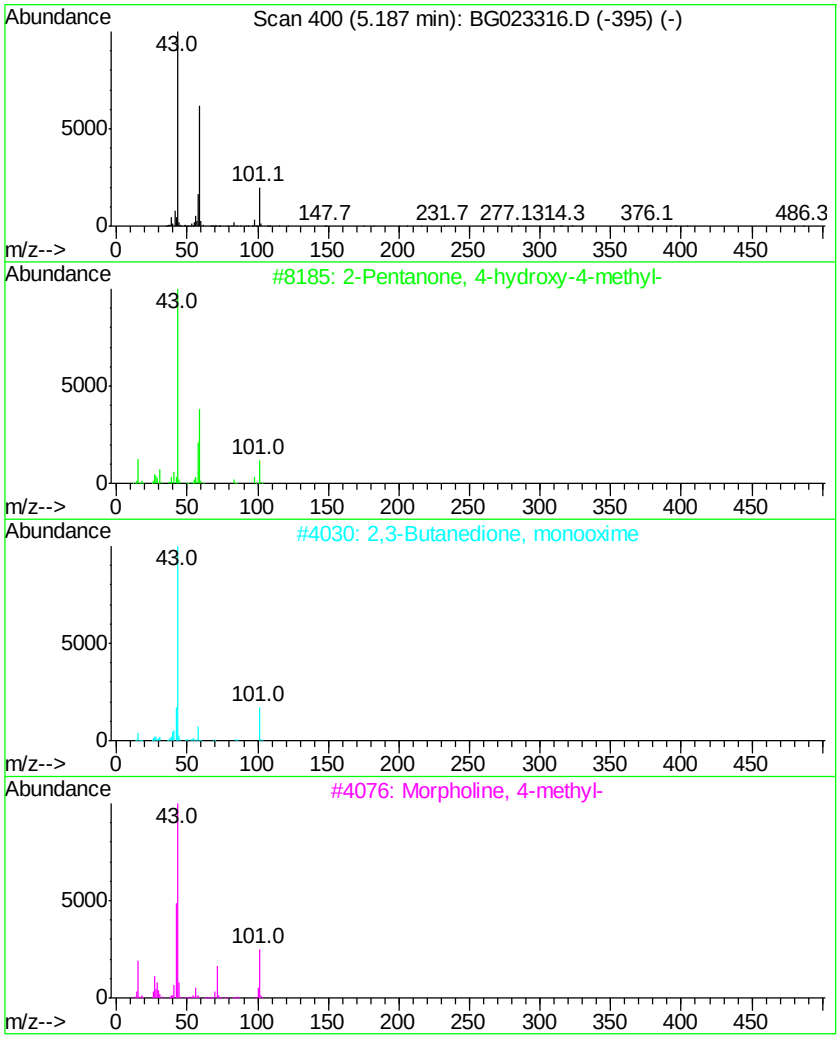
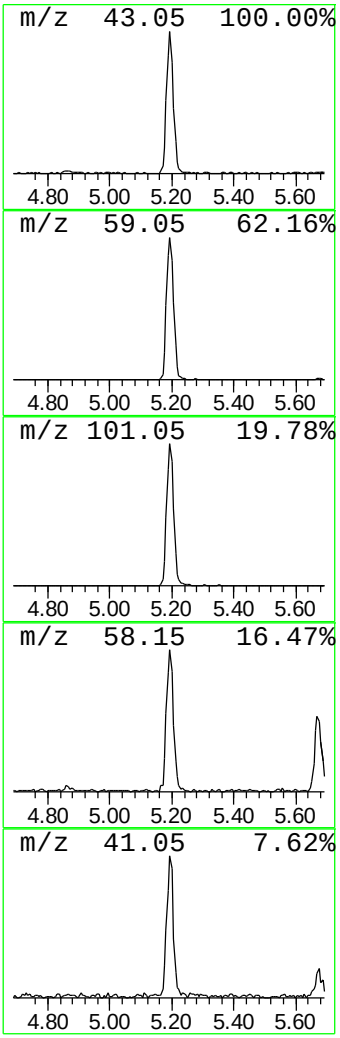
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	18.10 ng	973371	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Acetone	58	C3H6O	000067-64-1	9
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9





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ClientSampleId : SB-39-12.0-13.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG072616.M
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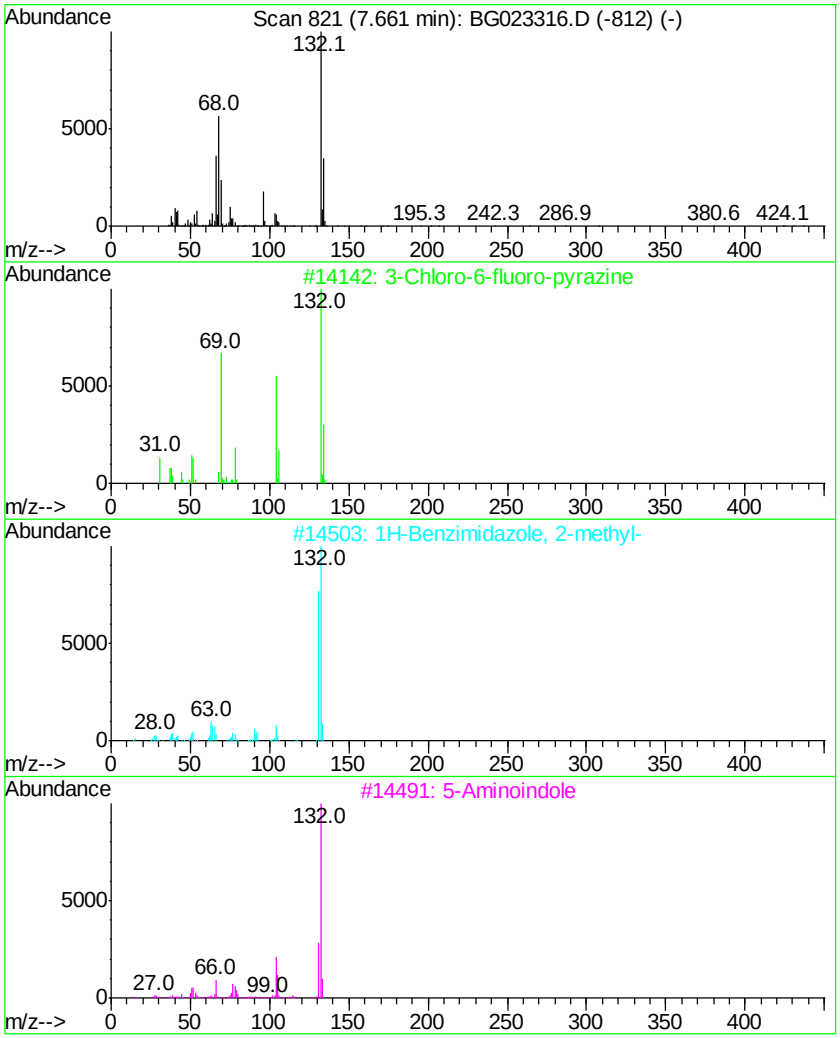
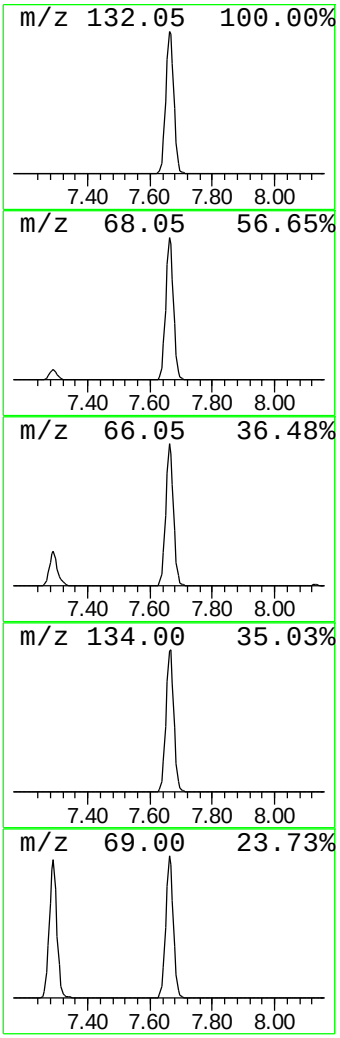
Peak Number 4 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	108.45 ng	5833130	1,4-Dichlorobenzene-d4	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Aminoindole	132	C8H8N2	005192-03-0	22
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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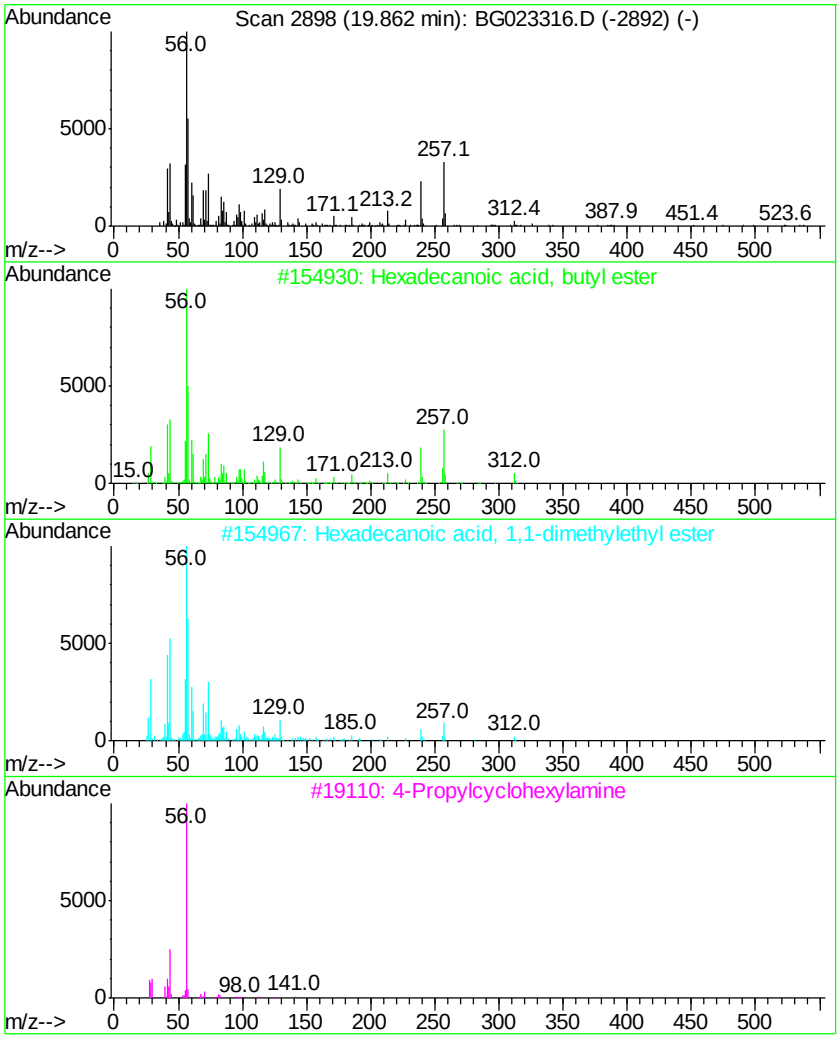
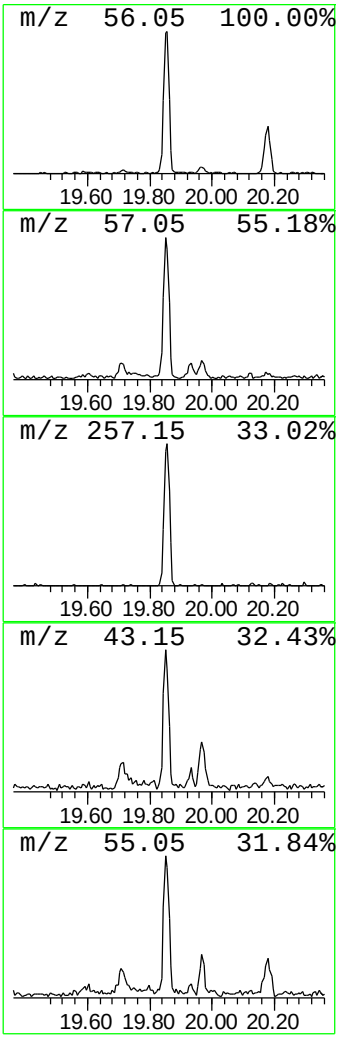
Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.86	3.05 ng	598151	Chrysene-d12	21.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	86
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	83
3	4-Propylcyclohexylamine	141	C9H19N	102653-37-2	27
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	27





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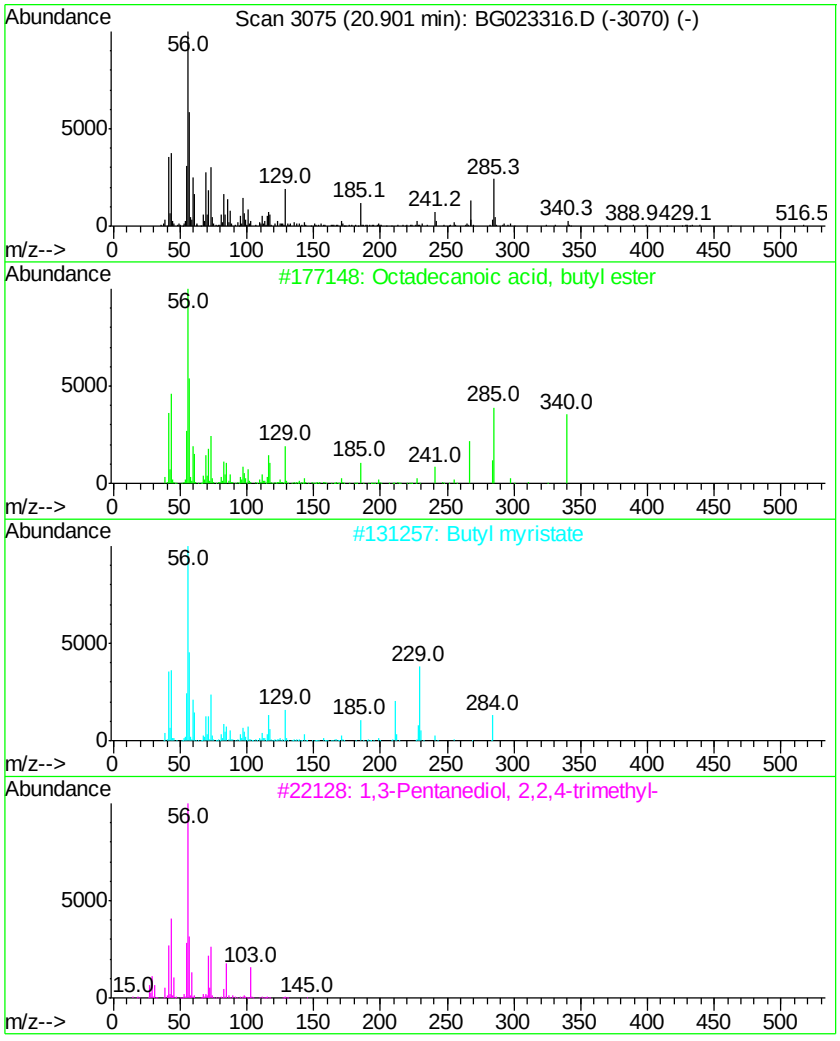
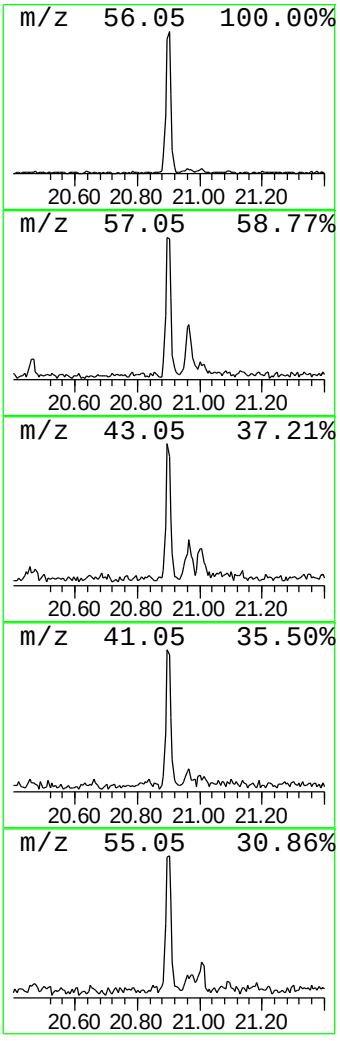
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.90	2.23 ng	436871	Chrysene-d12	21.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	76
2	Butyl myristate	284	C18H36O2	000110-36-1	68
3	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	38
4	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	37
5	3-Amino-2,2-dimethyl-1-propanol	103	C5H13NO	026734-09-8	35





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.00	3.00	254.5	ng	13687400	1	8.14	1075720	20.0
1,3-Dioxolane, 2,...	3.65	2.6	ng	137615	1	8.14	1075720	20.0
2-Pentanone, 4-hy...	5.19	18.1	ng	973371	1	8.14	1075720	20.0
unknown7.66	7.66	108.5	ng	5833130	1	8.14	1075720	20.0
Hexadecanoic acid...	19.86	3.0	ng	598151	5	21.89	3920600	20.0
Octadecanoic acid...	20.90	2.2	ng	436871	5	21.89	3920600	20.0