LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG022716\
Data File : BG021108.D
Acq On : 27 Feb 2016 10:32
Operator : UM/SJ
Sample : H1558-18
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-20

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-BG022616.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	3.090	38	43	50	rBV	54632	74932	9.78%	2.251%
2	3.231	62	67	75	rVB3	7432	14987	1.96%	0.450%
3	5.258	405	412	422	rBB	32040	48006	6.26%	1.442%
4	5.722	485	491	498	rBB	155377	237850	31.04%	7.146%
5	7.315	755	762	769	rBV	157783	267930	34.96%	8.049%
6	7.697	820	827	834	rBB	160136	261405	34.11%	7.853%
7	8.167	902	907	913	rBB2	20465	33147	4.33%	0.996%
8	8.490	956	962	969	rBB	104729	177771	23.20%	5.341%
9	9.330	1098	1105	1112	rBB	97129	166025	21.67%	4.988%
10	10.981	1379	1386	1393	rBB	28659	49217	6.42%	1.479%
11	13.402	1792	1798	1805	rBB	250460	377130	49.21%	11.330%
12	14.218	1932	1937	1943	rBB	40461	55472	7.24%	1.667%
13	14.777	2026	2032	2038	rBB2	46453	71605	9.34%	2.151%
14	15.599	2169	2172	2177	rBB	8025	9603	1.25%	0.288%
15	16.251	2275	2283	2290	rBB2	229307	335792	43.82%	10.088%
16	16.457	2314	2318	2321	rBV	8216	10596	1.38%	0.318%
17	17.509	2491	2497	2503	rBV	67552	97435	12.72%	2.927%
18	18.378	2641	2645	2651	rVB2	8752	10844	1.42%	0.326%
19	20.100	2932	2938	2944	rVB	629452	766297	100.00%	23.021%
20	21.398	3155	3159	3167	rVB3	12661	17851	2.33%	0.536%
21	21.774	3216	3223	3231	rVB	81924	133489	17.42%	4.010%
22	25.059	3772	3782	3792	rBV2	40329	111257	14.52%	3.342%

Sum of corrected areas: 3328641

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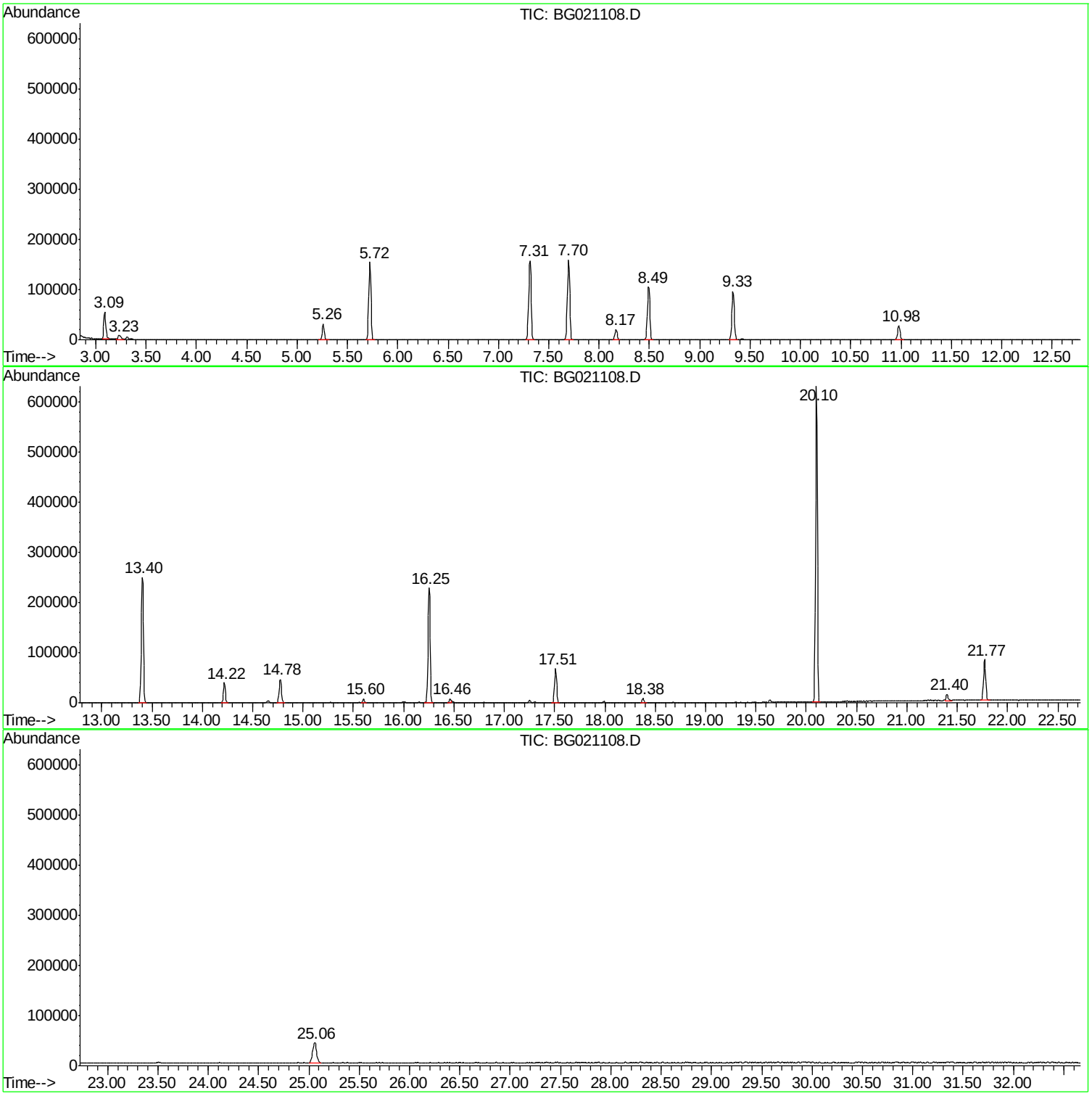
Instrument :
BNA_G
ClientSampleId :
S-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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Sample : H1558-18
Misc :
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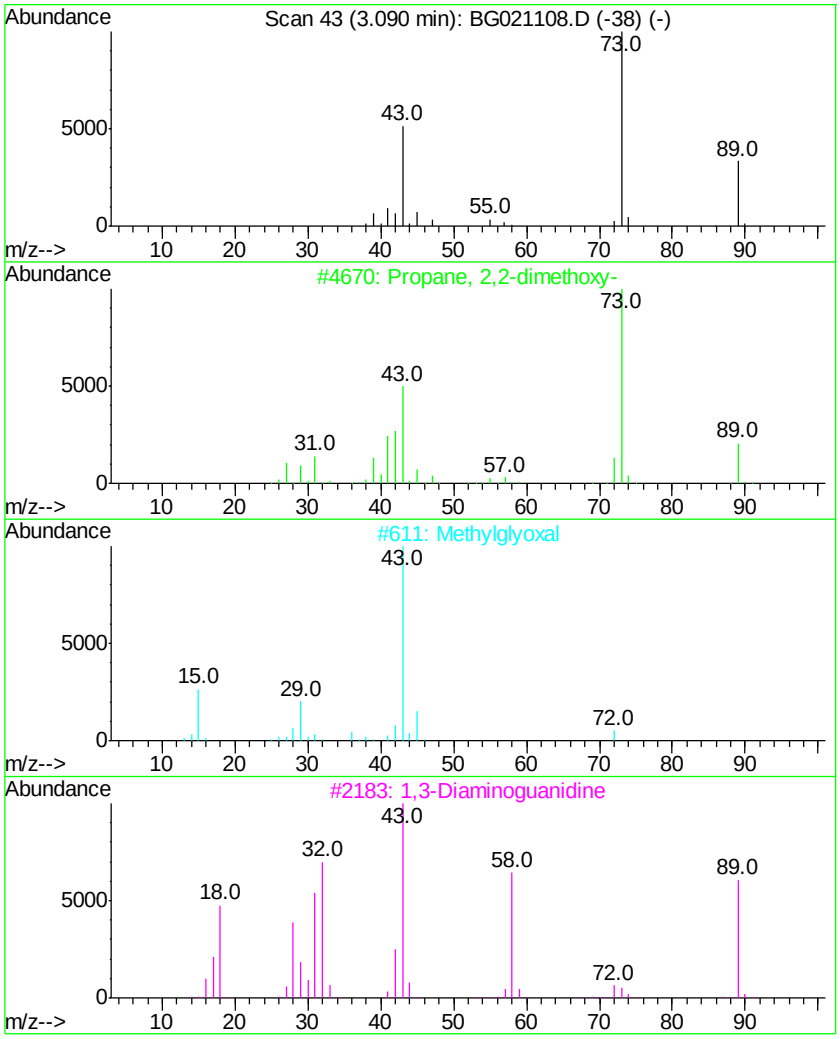
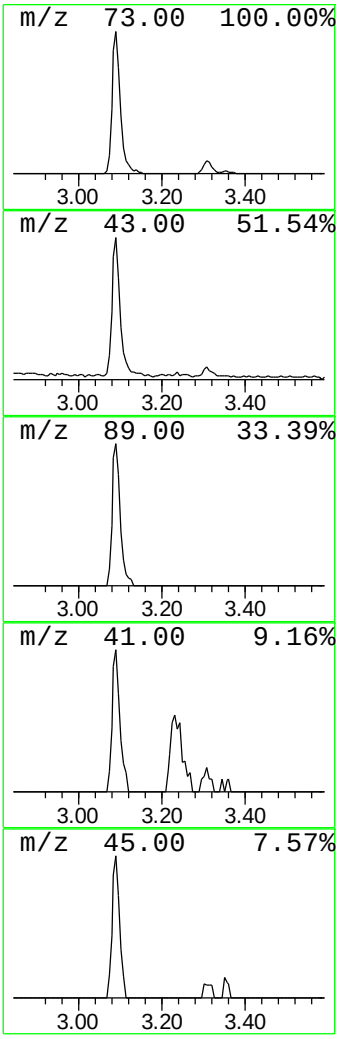
****

Peak Number 1 unknown3.09 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.09	45.21 ng	74932	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	Methylglyoxal	72	C3H4O2	000078-98-8	9
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9





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Operator : UM/SJ
Sample : H1558-18
Misc :
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Instrument : BNA_G
ClientSampleId : S-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
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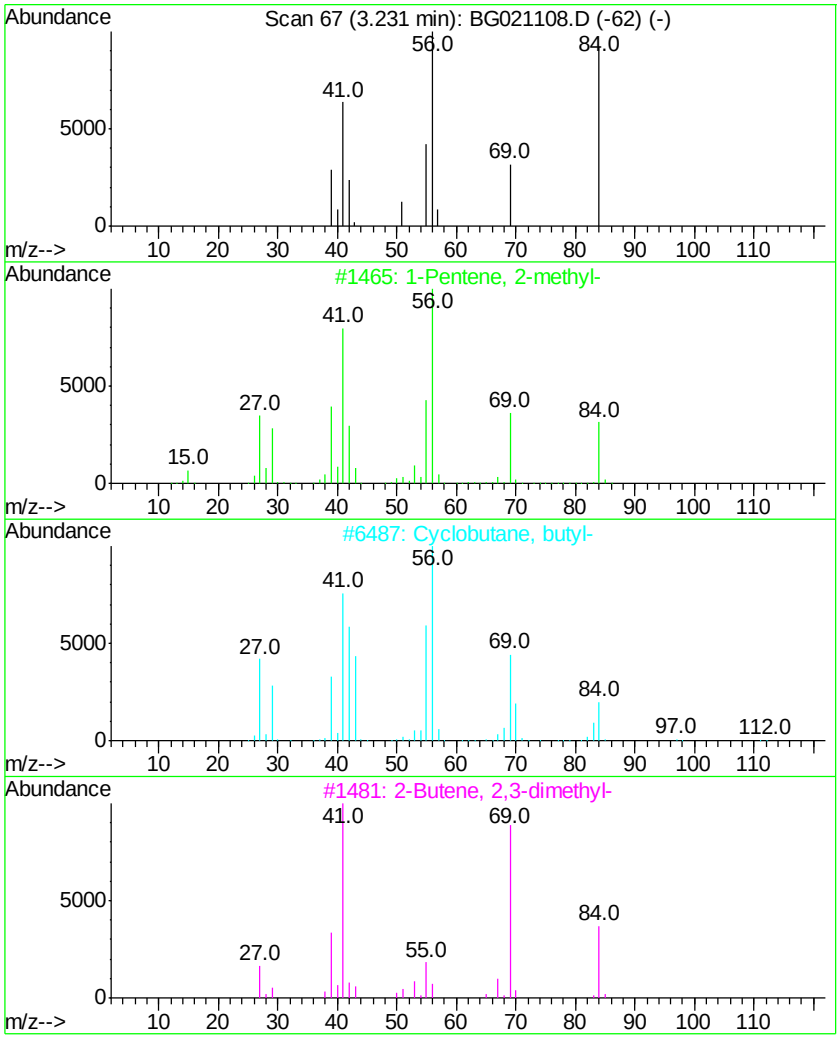
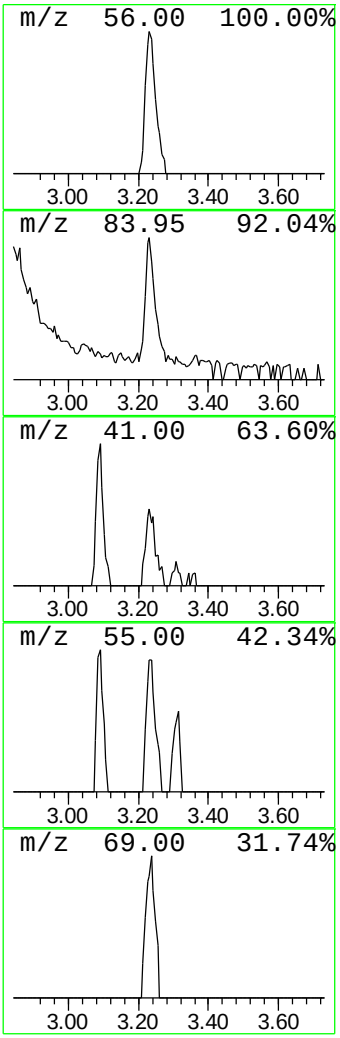
****

Peak Number 2 1-Pentene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	9.04 ng	14987	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	83
2	Cyclobutane, butyl-	112	C8H16	013152-44-8	23
3	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	9
4	2,3,4,5-Tetrahydropyridazine	84	C4H8N2	000694-06-4	9
5	Cyclopentane, methyl-	84	C6H12	000096-37-7	9





Library Search Compound Report

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Operator : UM/SJ
Sample : H1558-18
Misc :
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Instrument : BNA_G
ClientSampleId : S-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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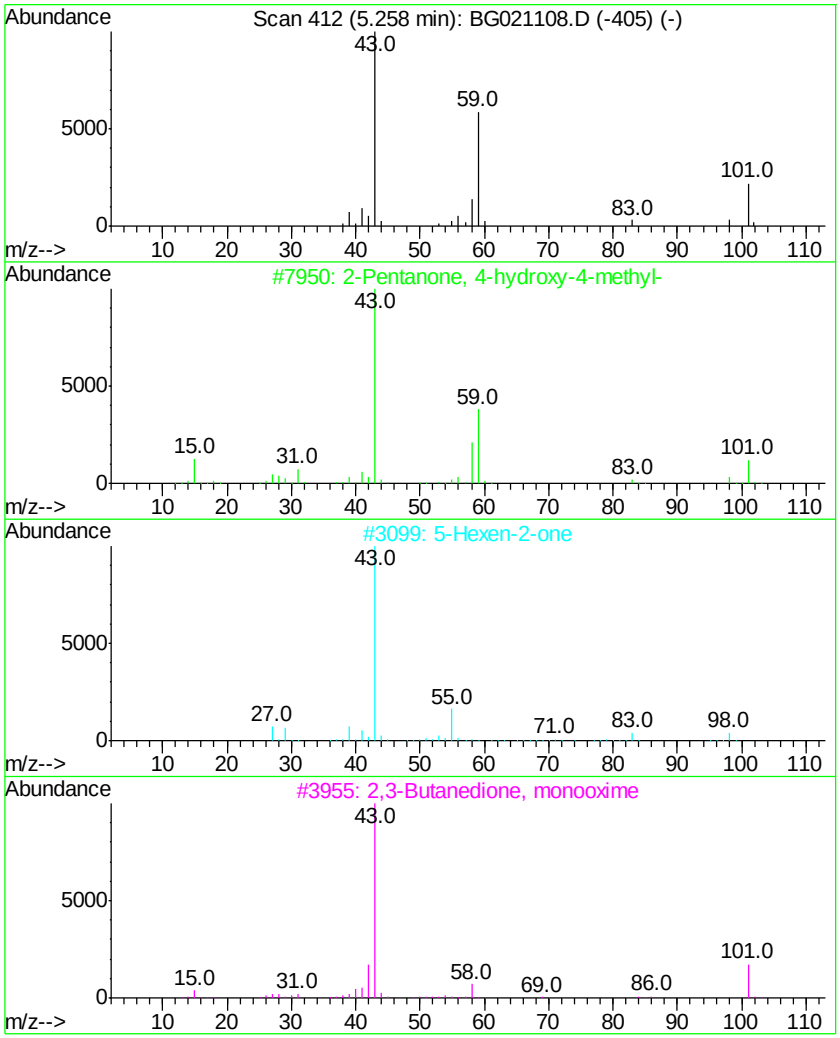
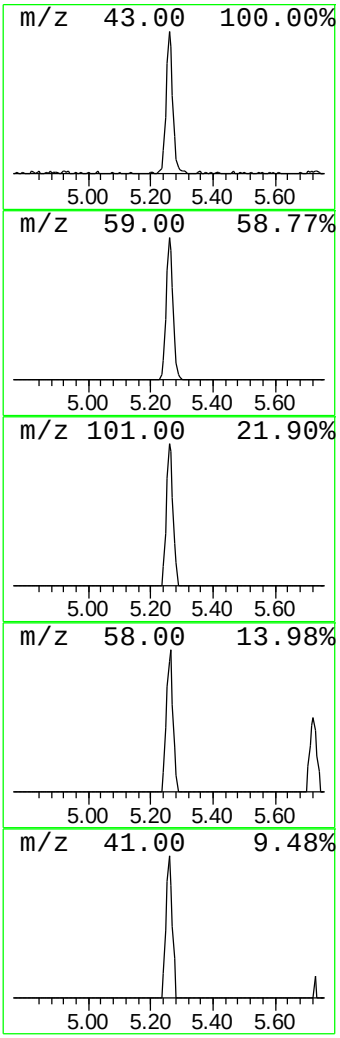
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	28.97 ng	48006	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Sample : H1558-18
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : S-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
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TIC Library : C:\DATABASE\NIST02.L
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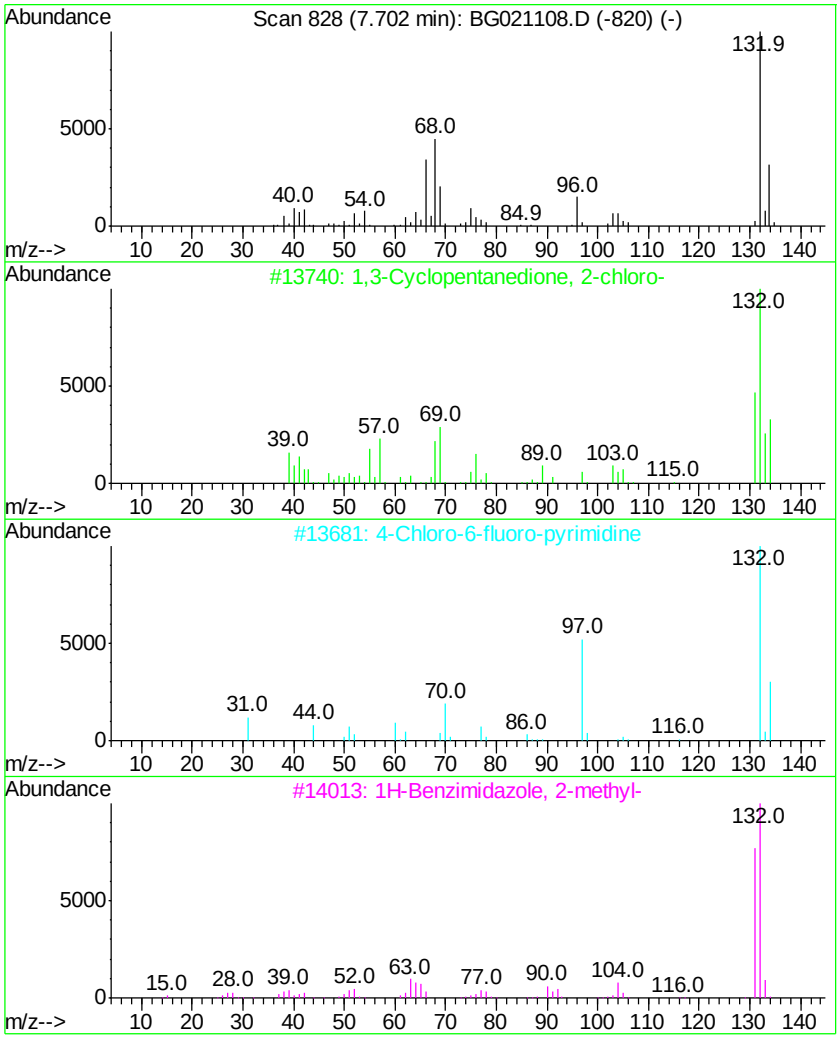
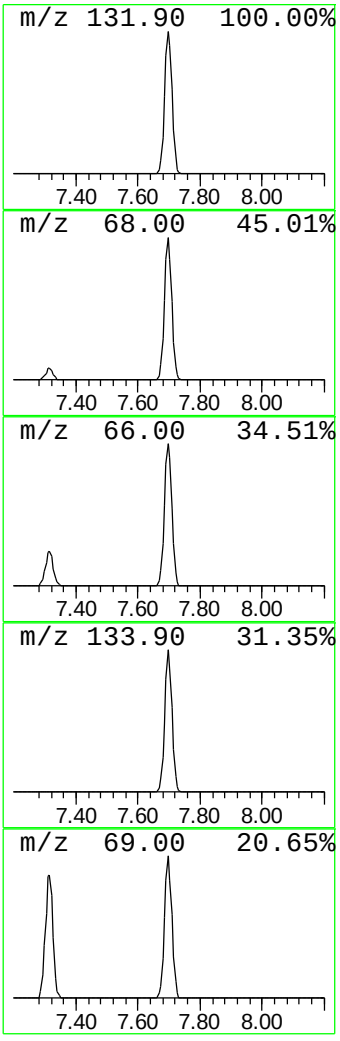
****

Peak Number 4 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	157.73 ng	261405	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	38
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	12





Data Path : Z:\HPCHEM1\BNA G\DATA\BG022716\
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Operator : UM/SJ
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Misc :
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Instrument : BNA_G
ClientSampleId : S-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG022616.M
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TIC Library : C:\DATABASE\NIST02.L
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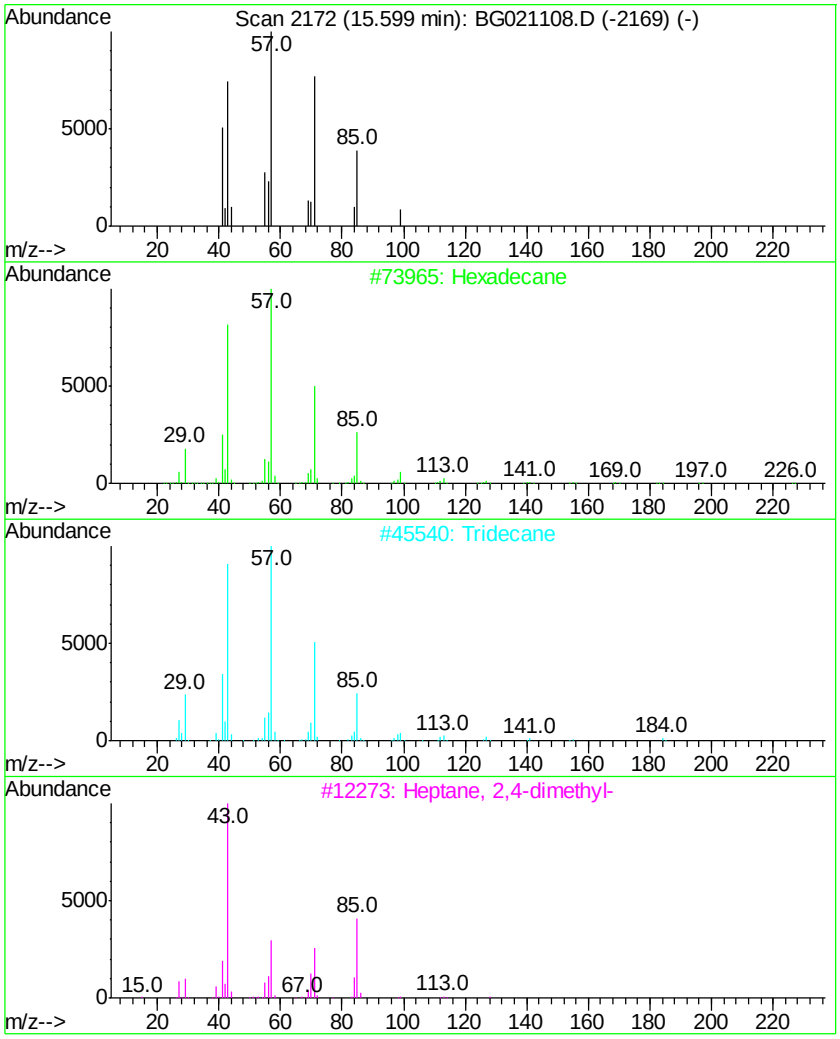
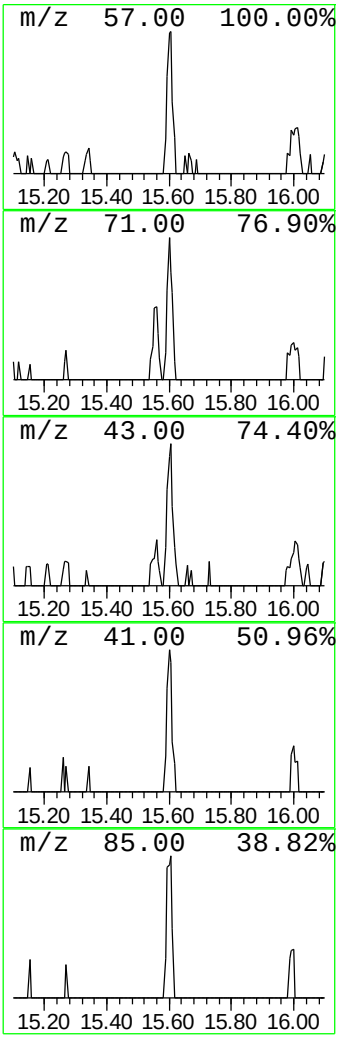
****

Peak Number 6 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.60	2.68 ng	9603	Acenaphthene-d10	14.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	78
2	Tridecane	184	C13H28	000629-50-5	72
3	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	56
4	Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	50
5	Undecane	156	C11H24	001120-21-4	42





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Instrument : BNA_G
ClientSampleId : S-20

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TIC Library : C:\DATABASE\NIST02.L
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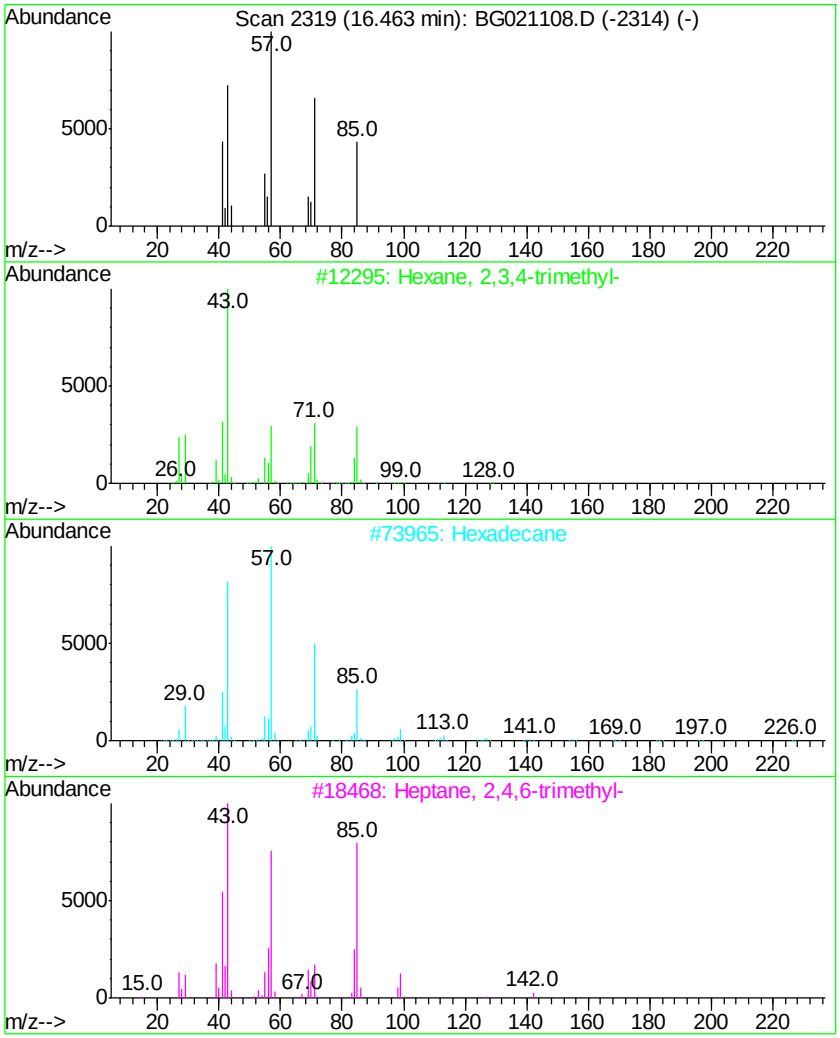
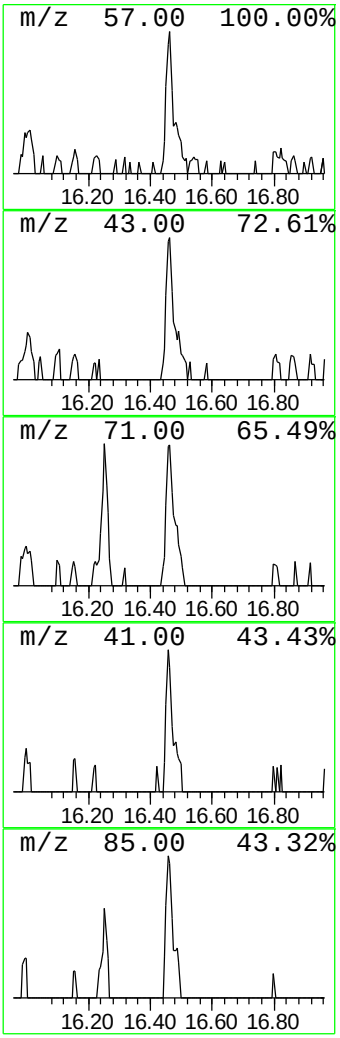
****

Peak Number 7 Hexane, 2,3,4-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.46	2.17 ng	10596	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53
2	Hexadecane	226	C16H34	000544-76-3	45
3	Heptane, 2,4,6-trimethyl-	142	C10H22	002613-61-8	43
4	Hexane, 2,2,3,3-tetramethyl-	142	C10H22	013475-81-5	40
5	Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	38





Library Search Compound Report

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TIC Library : C:\DATABASE\NIST02.L
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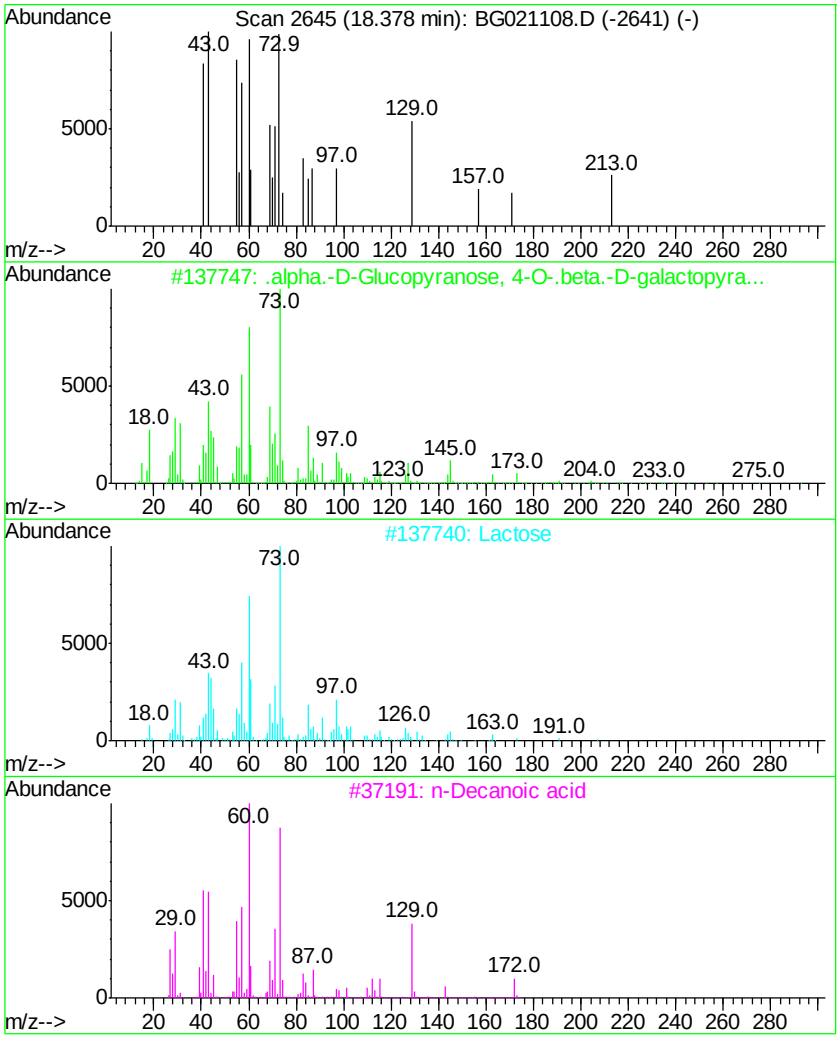
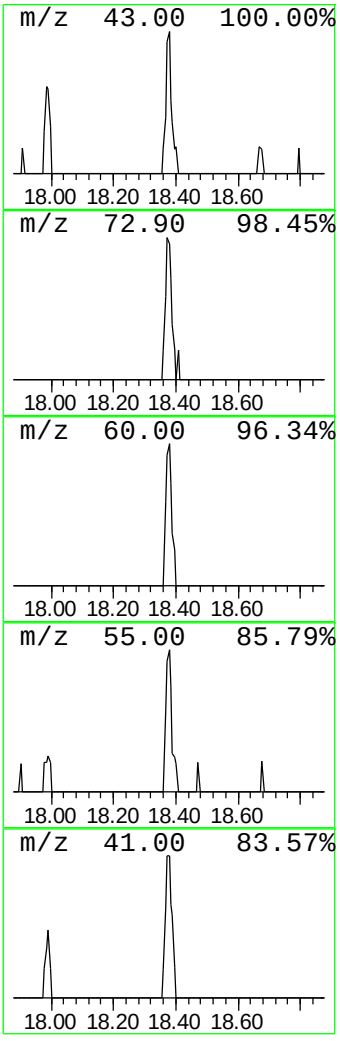
Peak Number 8 unknown18.38 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	2.23 ng	10844	Phenanthrene-d10	17.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	38
2	Lactose	342	C12H22O11	000063-42-3	37
3	n-Decanoic acid	172	C10H20O2	000334-48-5	33
4	1-.beta.-d-Ribofuranosyl-3-[5-te...	269	C8H11N7O4	1000211-51-6	28
5	1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	25





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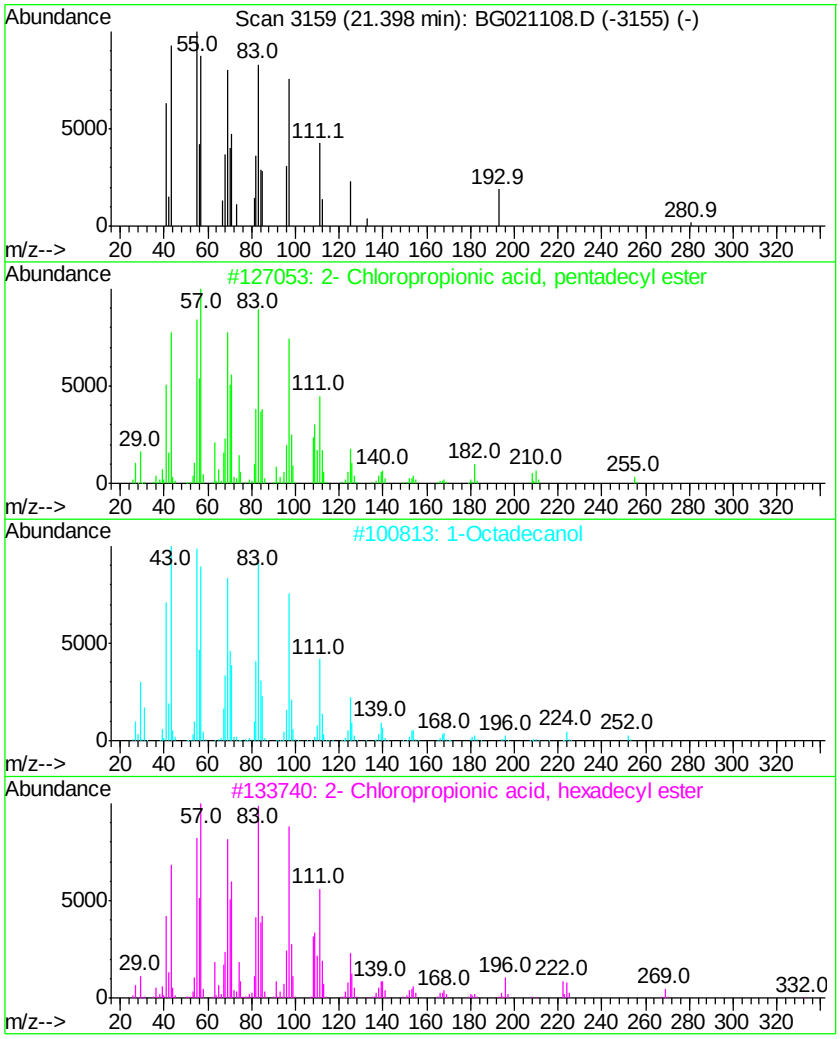
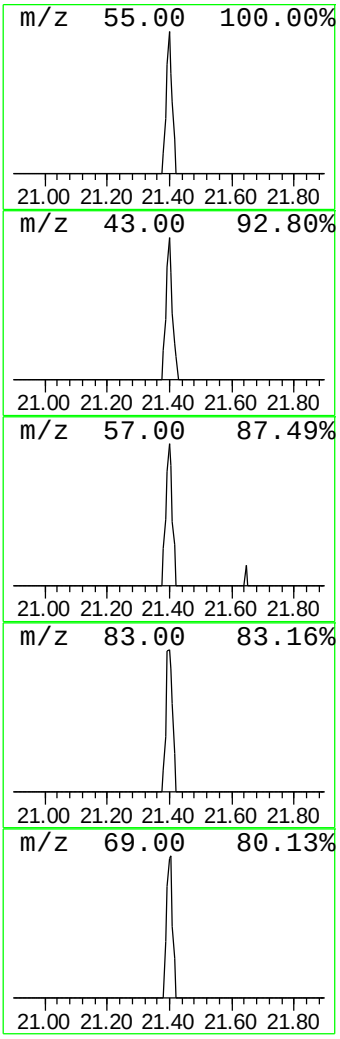
****

Peak Number 9 2- Chloropropionic acid, pe... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	2.67 ng	17851	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	91
2	1-Octadecanol	270	C18H38O	000112-92-5	91
3	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
4	1-Nonadecanol	284	C19H40O	001454-84-8	91
5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91





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
unknown3.09	3.09	45.2	ng	74932	1	8.17	33147	20.0
1-Pentene, 2-methyl-	3.23	9.0	ng	14987	1	8.17	33147	20.0
2-Pentanone, 4-hy...	5.26	29.0	ng	48006	1	8.17	33147	20.0
unknown7.70	7.70	157.7	ng	261405	1	8.17	33147	20.0
Hexadecane	15.60	2.7	ng	9603	3	14.78	71605	20.0
Hexane, 2,3,4-tri...	16.46	2.2	ng	10596	4	17.51	97435	20.0
unknown18.38	18.38	2.2	ng	10844	4	17.51	97435	20.0
2- Chloropropioni...	21.40	2.7	ng	17851	5	21.77	133489	20.0