LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024675.D
Acq On : 4 Nov 2016 10:10
Operator : UM/SJ
Sample : H5509-08
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-94-19.5-20.0

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-BG102516.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	3.126	44	49	70	rVB	7491482	13334050	100.00%	21.500%
2	5.329	419	424	433	rVB	444169	726653	5.45%	1.172%
3	5.799	496	504	512	rBV	2121655	3569189	26.77%	5.755%
4	7.403	769	777	787	rBV	2220196	4018419	30.14%	6.479%
5	7.791	835	843	856	rBV	2077429	3756447	28.17%	6.057%
6	8.267	917	924	937	rVB2	370212	670023	5.02%	1.080%
7	8.590	970	979	989	rVB	1528605	2788609	20.91%	4.496%
8	9.442	1116	1124	1134	rBV	1333094	2521915	18.91%	4.066%
9	11.093	1396	1405	1413	rBV	495919	906576	6.80%	1.462%
10	13.508	1806	1816	1828	rBV	3235004	5127479	38.45%	8.268%
11	14.319	1948	1954	1967	rBV	1139261	1653336	12.40%	2.666%
12	14.883	2041	2050	2056	rBV	783866	1272246	9.54%	2.051%
13	16.363	2295	2302	2313	rBV	3278052	5154310	38.66%	8.311%
14	16.534	2327	2331	2335	rBV3	92503	136732	1.03%	0.220%
15	17.621	2510	2516	2529	rBV	1060778	1736149	13.02%	2.799%
16	17.956	2568	2573	2582	rBV2	156262	255215	1.91%	0.412%
17	18.467	2656	2660	2666	rBV2	128525	200624	1.50%	0.323%
18	19.865	2893	2898	2903	rBV	281663	338578	2.54%	0.546%
19	20.206	2949	2956	2963	rBV	6193985	8575990	64.32%	13.828%
20	20.905	3070	3075	3078	rBV2	214422	271274	2.03%	0.437%
21	21.493	3171	3175	3182	rBV2	203531	327143	2.45%	0.528%
22	21.916	3240	3247	3254	rBV	1324584	2301635	17.26%	3.711%
23	25.347	3817	3831	3843	rVB3	759572	2374953	17.81%	3.829%

Sum of corrected areas: 62017545

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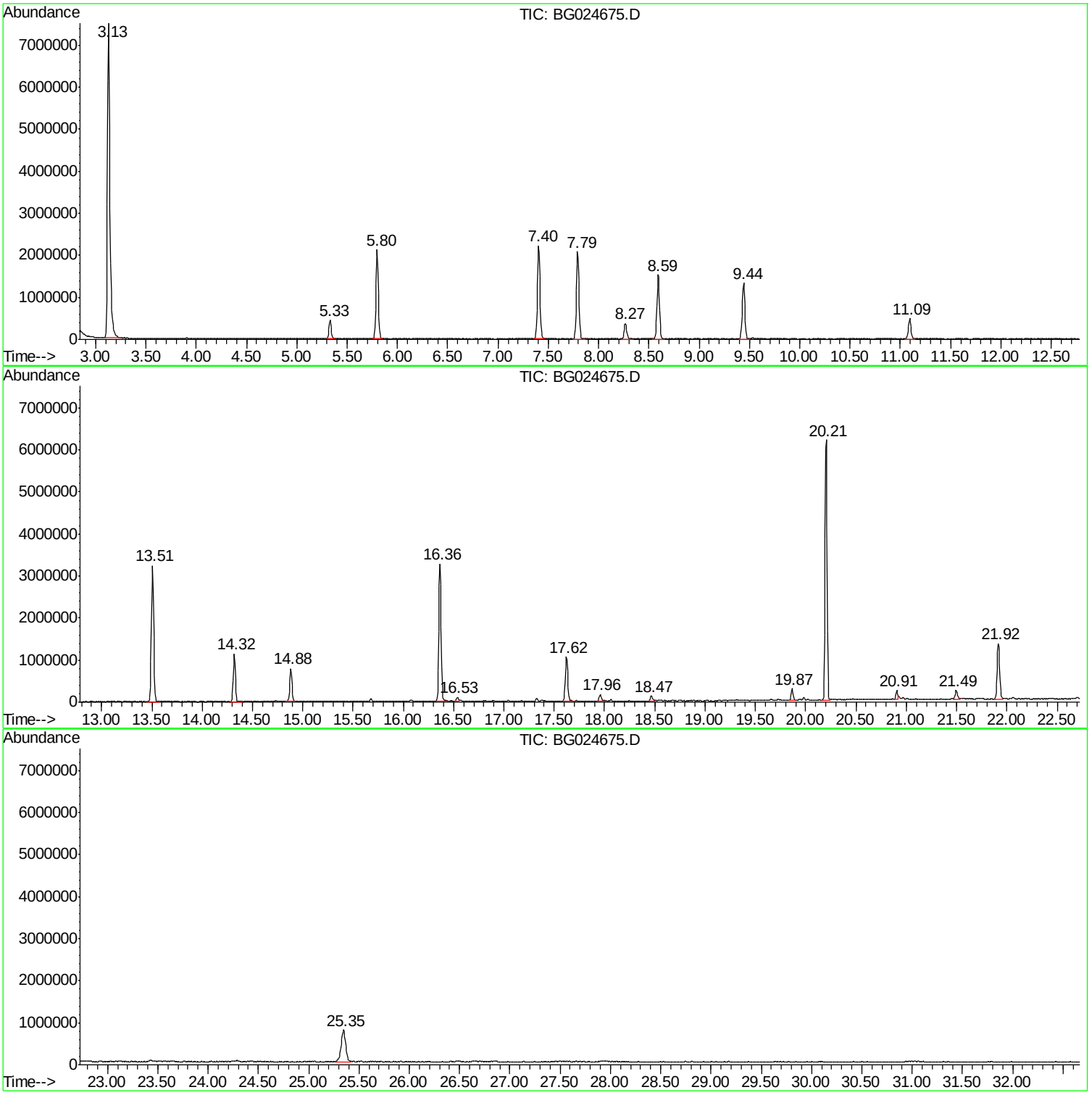
Instrument :
BNA_G
ClientSampleId :
SB-94-19.5-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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Instrument : BNA_G
ClientSampleId : SB-94-19.5-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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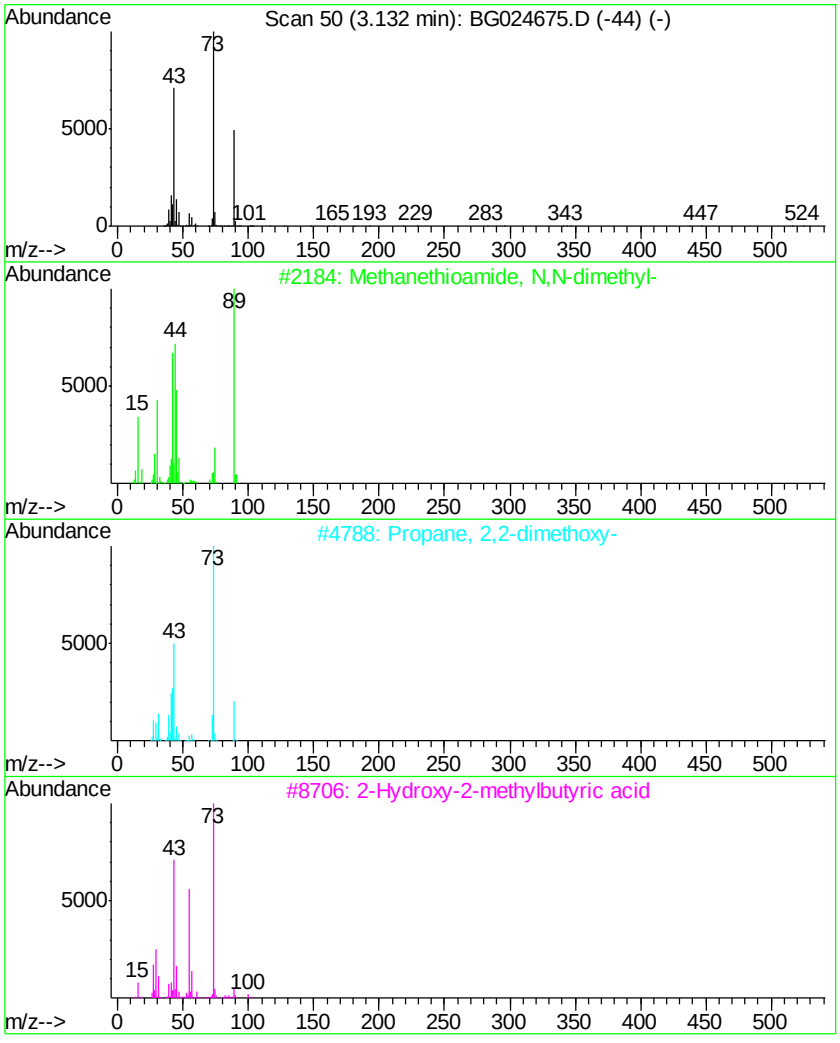
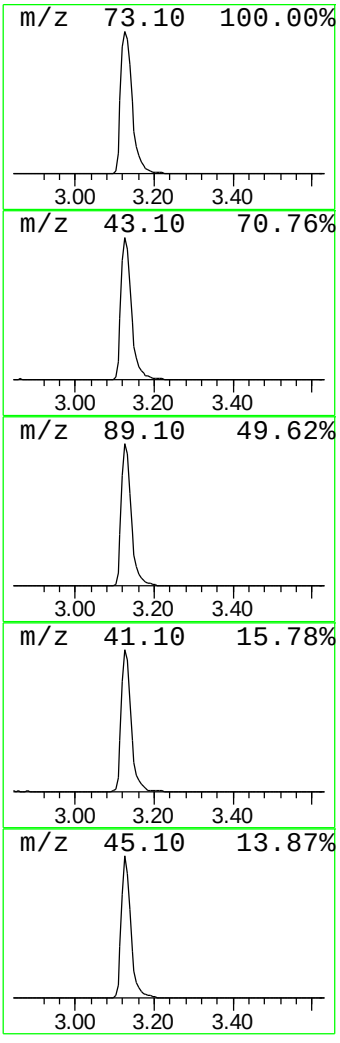
Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	398.02 ng	13334100	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	42
2	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	23
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	12
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10





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Sample : H5509-08
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Instrument : BNA_G
ClientSampleId : SB-94-19.5-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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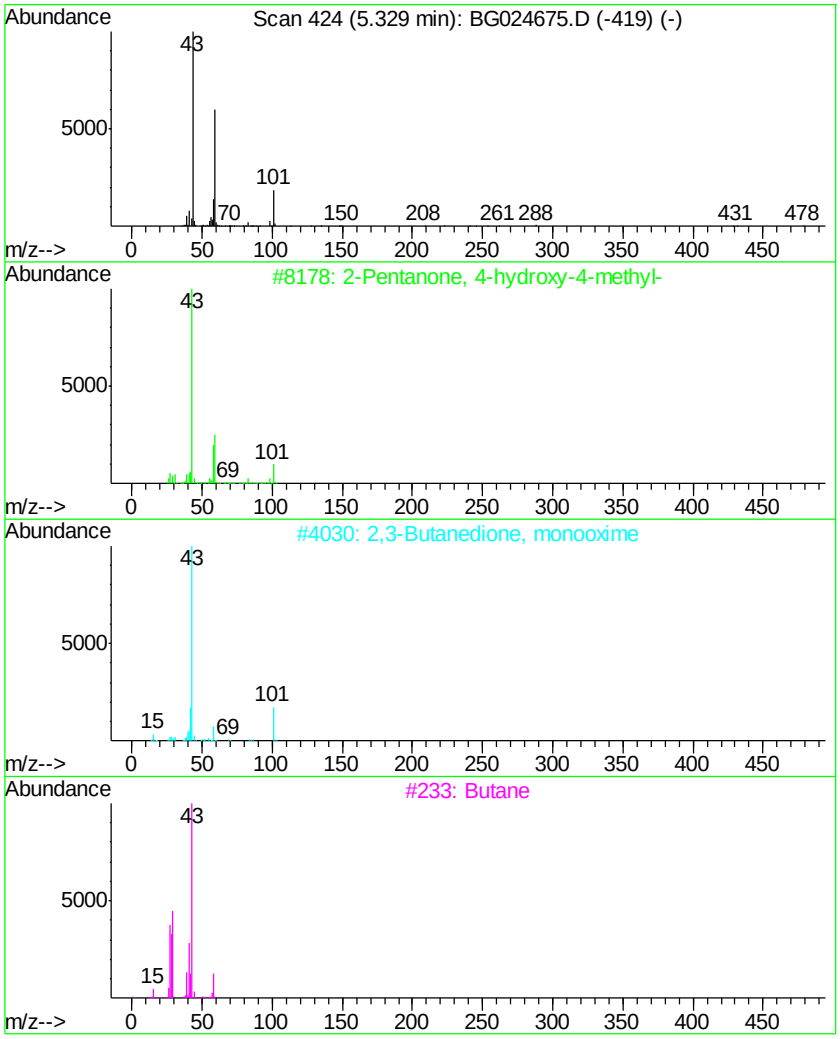
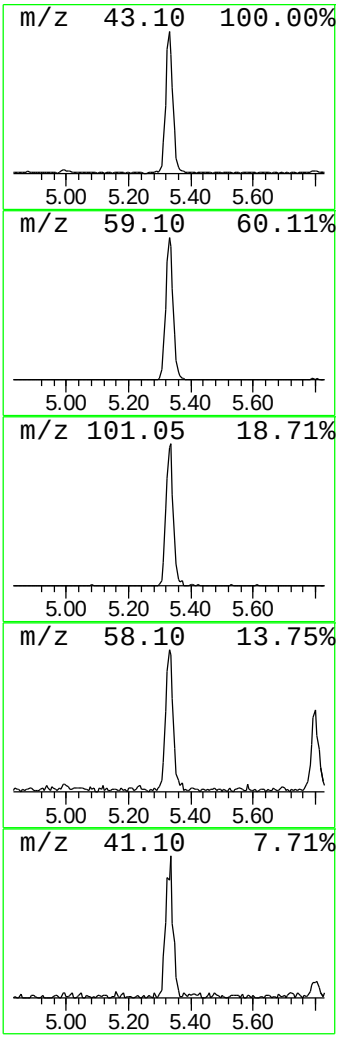
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	21.69 ng	726653	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3	Butane	58	C4H10	000106-97-8	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : UM/SJ
Sample : H5509-08
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-94-19.5-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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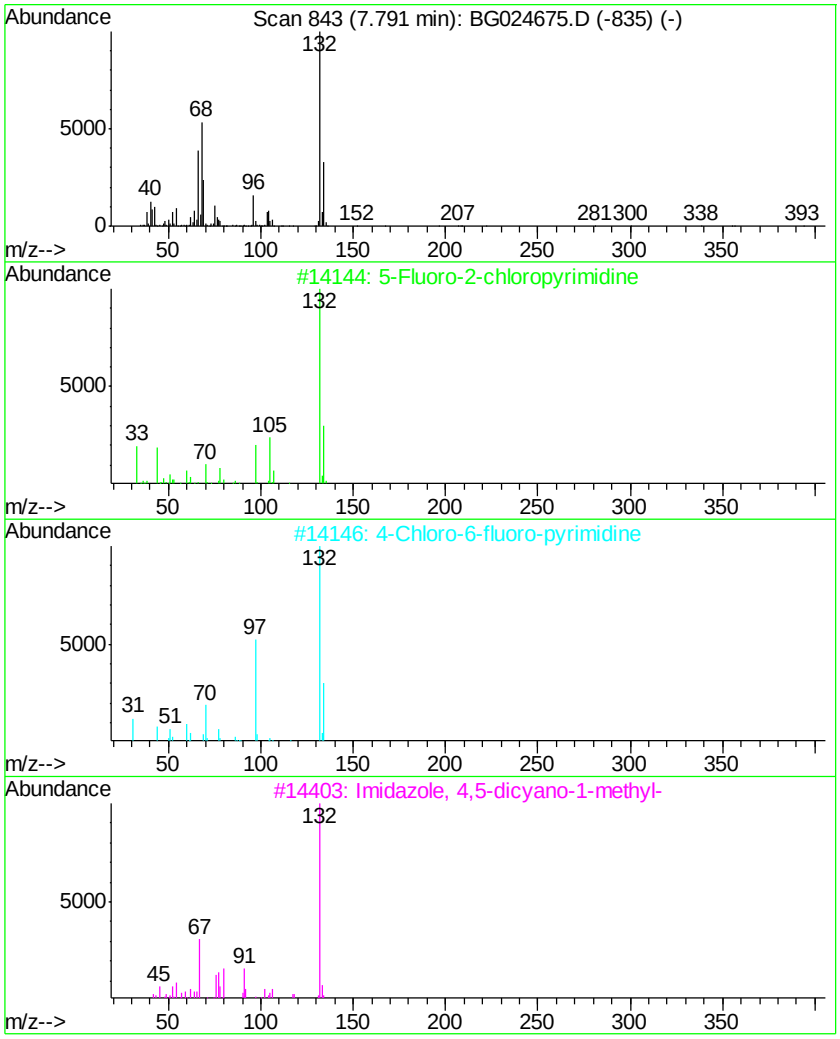
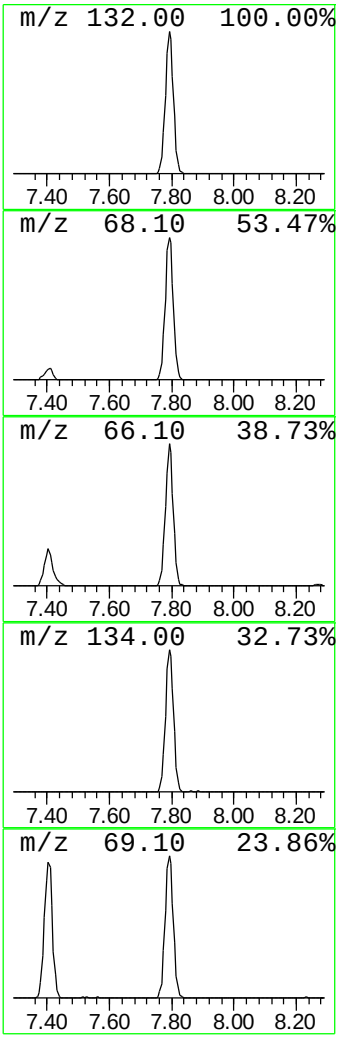
Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	112.13 ng	3756450	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	10
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
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Operator : UM/SJ
Sample : H5509-08
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-94-19.5-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

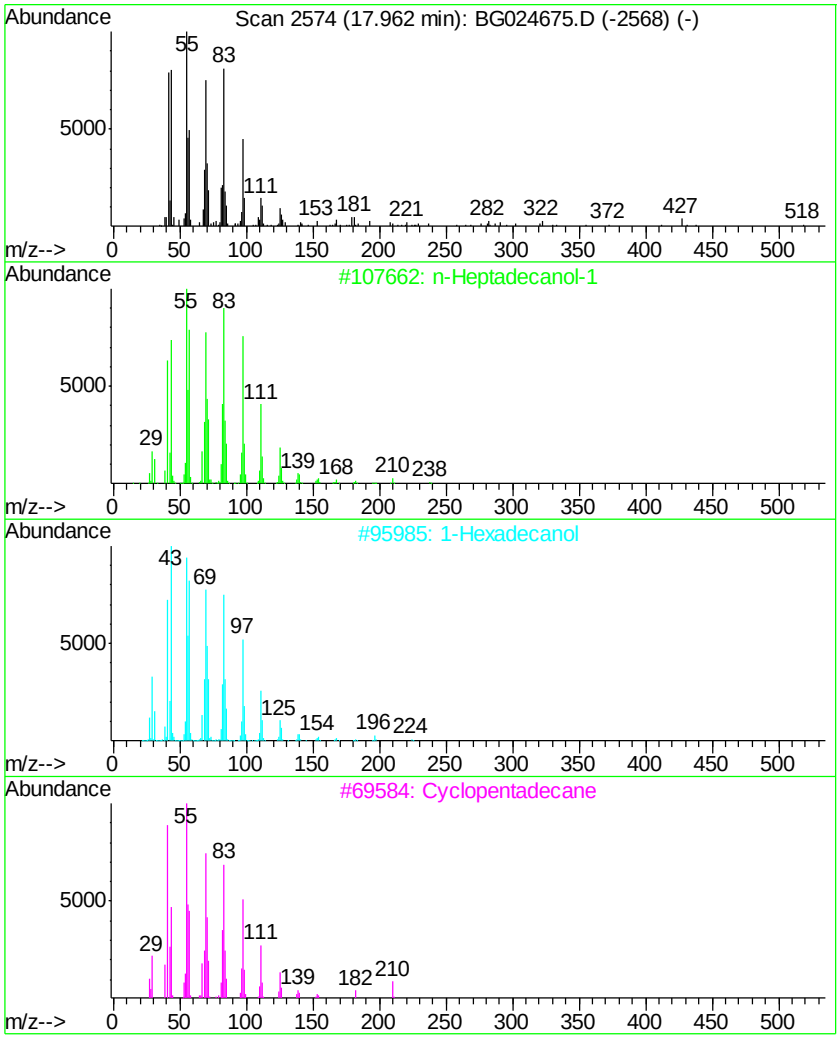
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

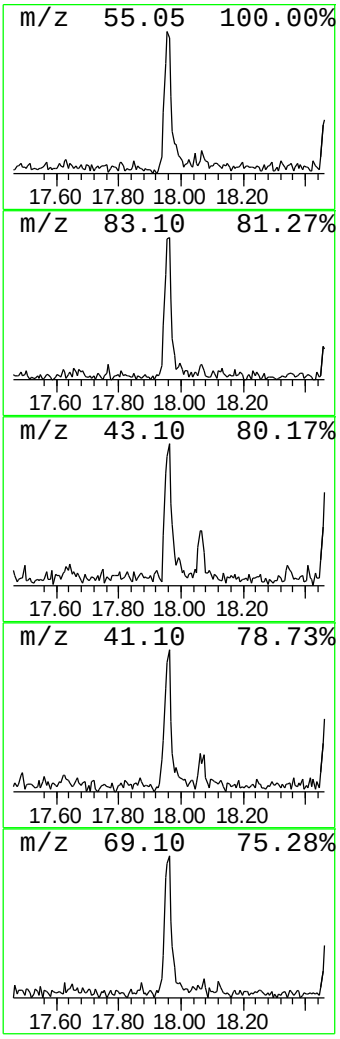
****

Peak Number 5 n-Heptadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	2.94 ng	255215	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1	256	C17H36O	001454-85-9	87
2	1-Hexadecanol	242	C16H34O	036653-82-4	87
3	Cyclopentadecane	210	C15H30	000295-48-7	83
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	83
5	1-Octadecene	252	C18H36	000112-88-9	70





Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024675.D
Acq On : 4 Nov 2016 10:10
Operator : UM/SJ
Sample : H5509-08
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-94-19.5-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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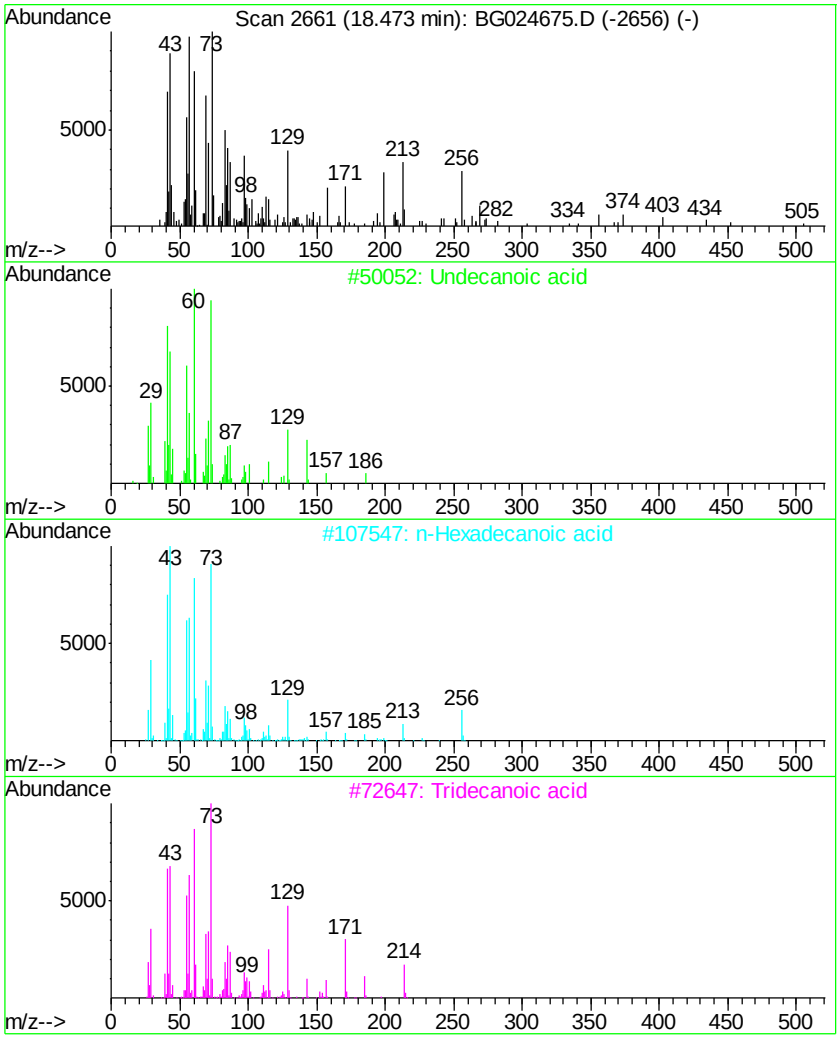
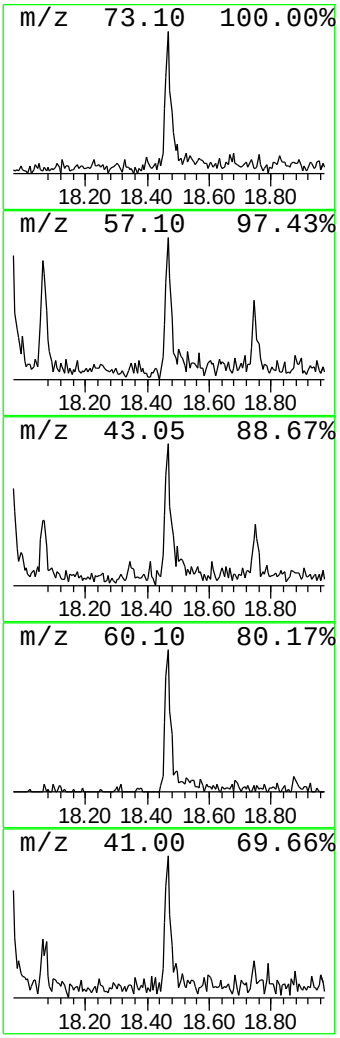
Peak Number 6 Undecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.31 ng	200624	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	89
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3	Tridecanoic acid	214	C13H26O2	000638-53-9	70
4	Methyl 2,6-anhydro-.alpha.-d-alt...	176	C7H12O5	1000130-02-0	50
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





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Sample : H5509-08
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-94-19.5-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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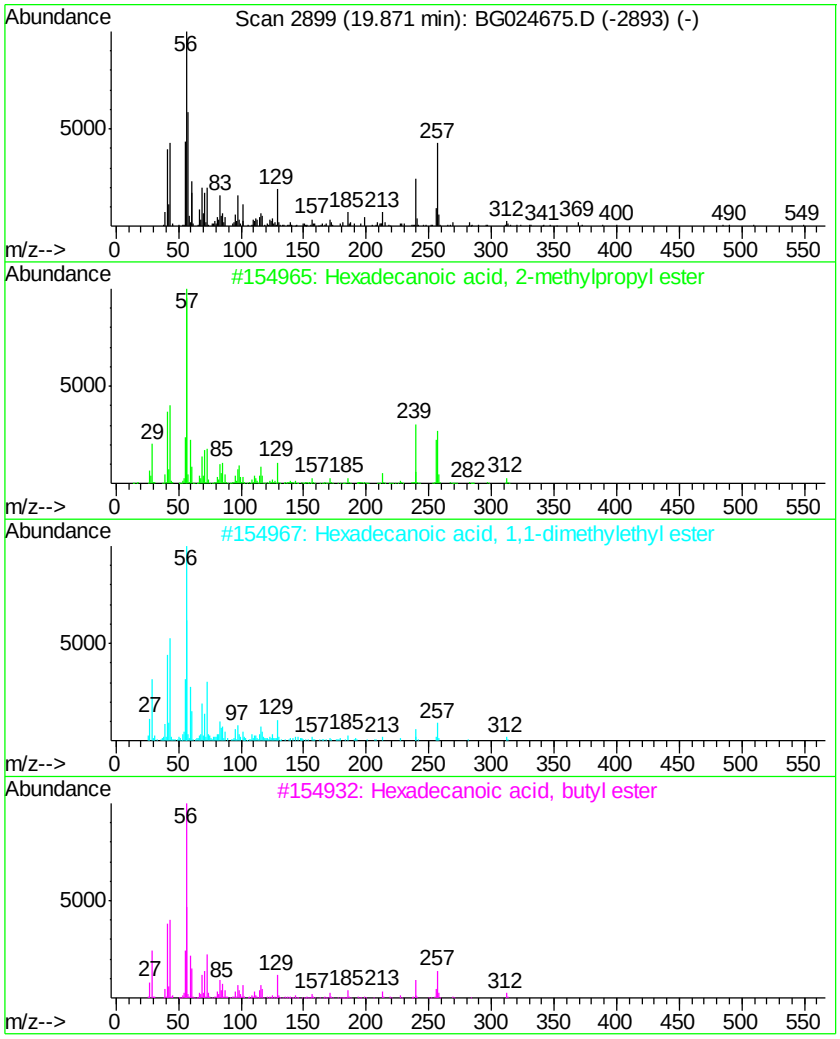
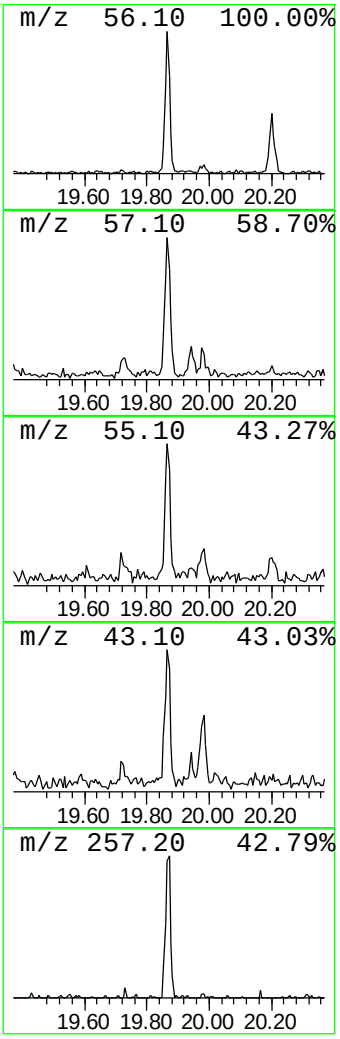
Peak Number 7 Hexadecanoic acid, 2-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.87	2.94 ng	338578	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	86
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	78
3	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	78
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
5	Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	43





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Instrument : BNA_G
ClientSampleId : SB-94-19.5-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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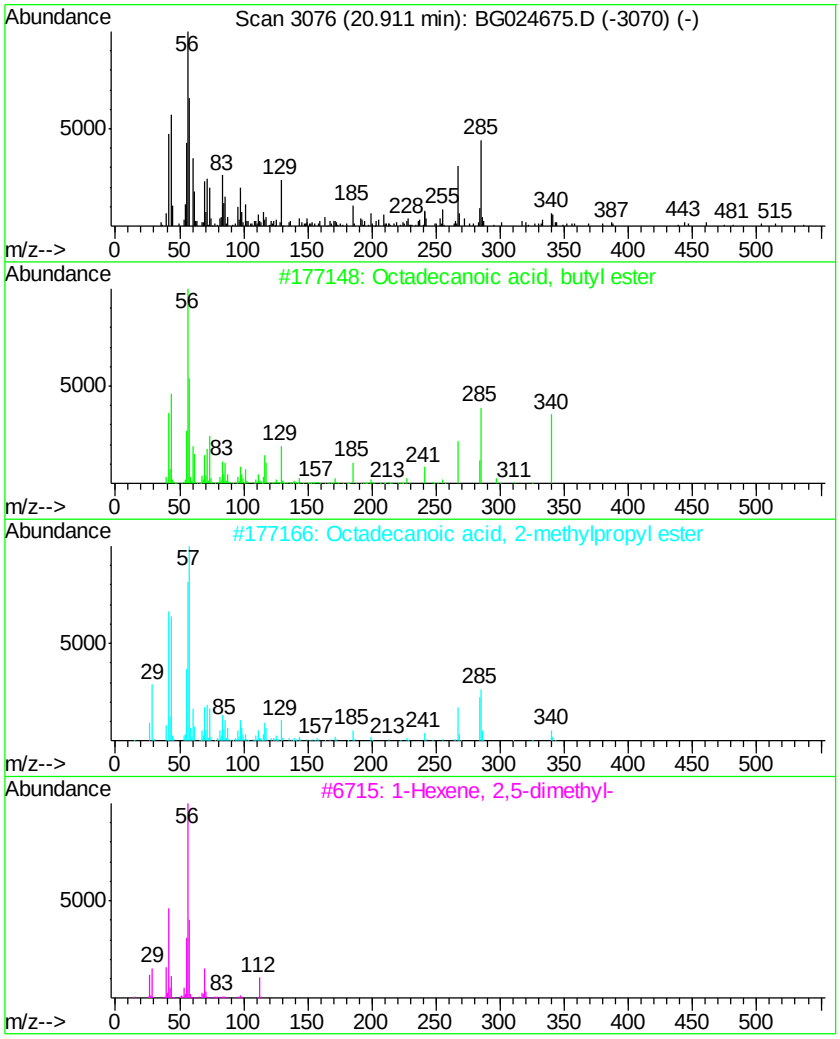
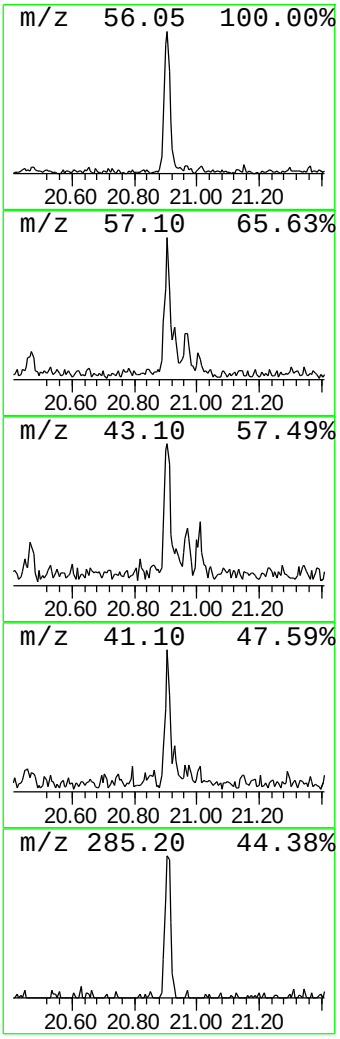
Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.91	2.36 ng	271274	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	72
3	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30
4	Cyclododecylamine	183	C12H25N	001502-03-0	27
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27





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ALS Vial : 43 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-94-19.5-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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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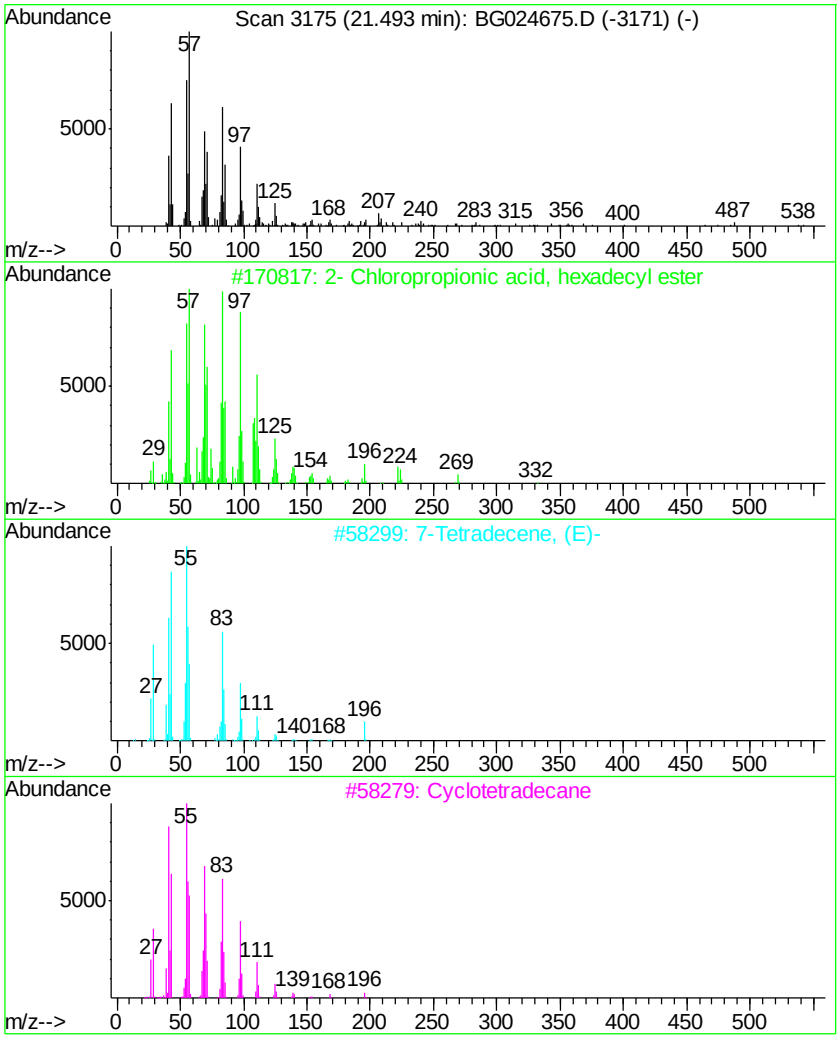
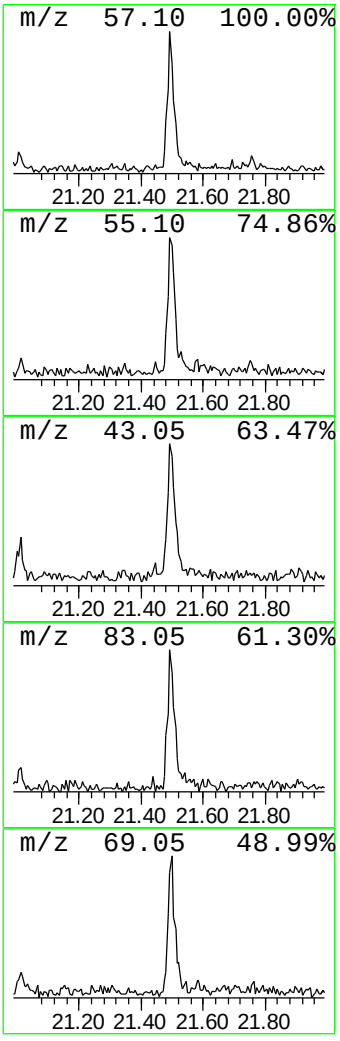
Peak Number 9 2- Chloropropionic acid, he... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.49	2.84 ng	327143	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	87
2	7-Tetradecene, (E)-	196	C14H28	041446-63-3	81
3	Cyclotetradecane	196	C14H28	000295-17-0	74
4	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	74
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	74





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown3.13	3.13	398.0	ng	13334100	1	8.27	670023	20.0
2-Pentanone, 4-hy...	5.33	21.7	ng	726653	1	8.27	670023	20.0
unknown7.79	7.79	112.1	ng	3756450	1	8.27	670023	20.0
n-Heptadecanol-1	17.96	2.9	ng	255215	4	17.62	1736150	20.0
Undecanoic acid	18.47	2.3	ng	200624	4	17.62	1736150	20.0
Hexadecanoic acid...	19.87	2.9	ng	338578	5	21.92	2301640	20.0
Octadecanoic acid...	20.91	2.4	ng	271274	5	21.92	2301640	20.0
2- Chloropropioni...	21.49	2.8	ng	327143	5	21.92	2301640	20.0