LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024662.D
Acq On : 4 Nov 2016 00:58
Operator : UM/SJ
Sample : H5502-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-79-0.5-1.0

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	3.128	43	49	72	rVB	6161105	10319519	100.00%	21.450%
2	4.720	315	320	331	rVB	128594	211280	2.05%	0.439%
3	5.331	416	424	433	rBV	572642	944630	9.15%	1.963%
4	5.795	496	503	513	rBV	1428064	2419500	23.45%	5.029%
5	7.399	769	776	787	rBV	1625337	2970073	28.78%	6.174%
6	7.793	836	843	851	rBV	1494293	2691299	26.08%	5.594%
7	8.269	917	924	933	rBV	335871	609162	5.90%	1.266%
8	8.592	971	979	987	rVB	1195478	2084222	20.20%	4.332%
9	9.444	1116	1124	1135	rVB	990249	1888149	18.30%	3.925%
10	11.095	1398	1405	1413	rVB	441476	827403	8.02%	1.720%
11	13.504	1807	1815	1826	rBV	2544327	4042258	39.17%	8.402%
12	14.321	1948	1954	1960	rBV	562869	826494	8.01%	1.718%
13	14.885	2043	2050	2057	rVB	773707	1210211	11.73%	2.516%
14	16.365	2295	2302	2314	rBV	1612563	2596016	25.16%	5.396%
15	16.536	2327	2331	2335	rBV3	79122	120044	1.16%	0.250%
16	17.623	2509	2516	2522	rBV	1090936	1688095	16.36%	3.509%
17	17.958	2567	2573	2581	rBV4	54849	111606	1.08%	0.232%
18	20.202	2949	2955	2962	rBV	5341066	7609724	73.74%	15.817%
19	21.495	3171	3175	3184	rBV4	143282	280892	2.72%	0.584%
20	21.918	3240	3247	3256	rVB	1327871	2340459	22.68%	4.865%
21	25.349	3818	3831	3843	rBV2	737450	2318810	22.47%	4.820%

Sum of corrected areas: 48109846

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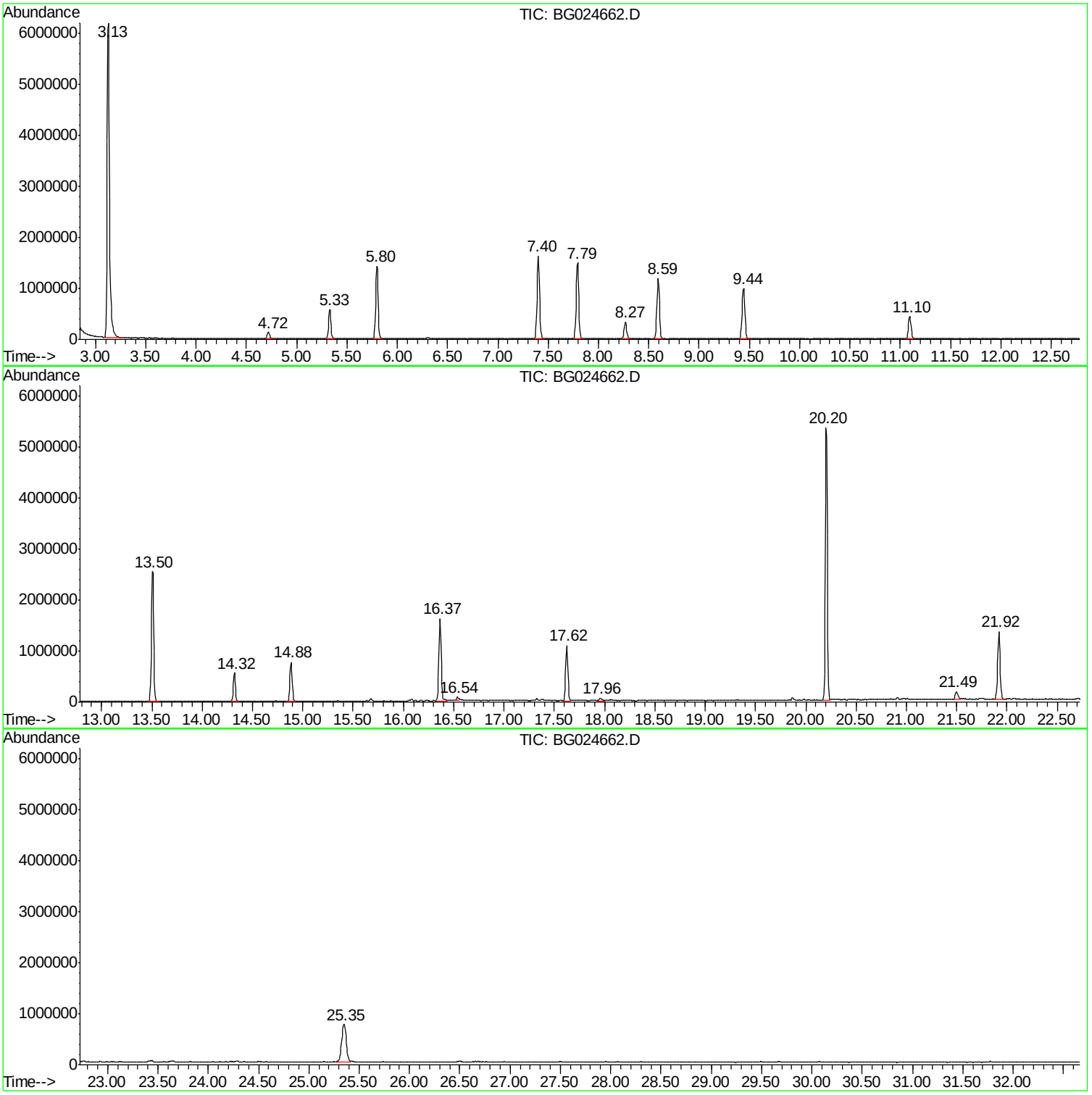
Instrument :
BNA_G
ClientSampleId :
SB-79-0.5-1.0

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024662.D
Acq On : 4 Nov 2016 00:58
Operator : UM/SJ
Sample : H5502-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-79-0.5-1.0

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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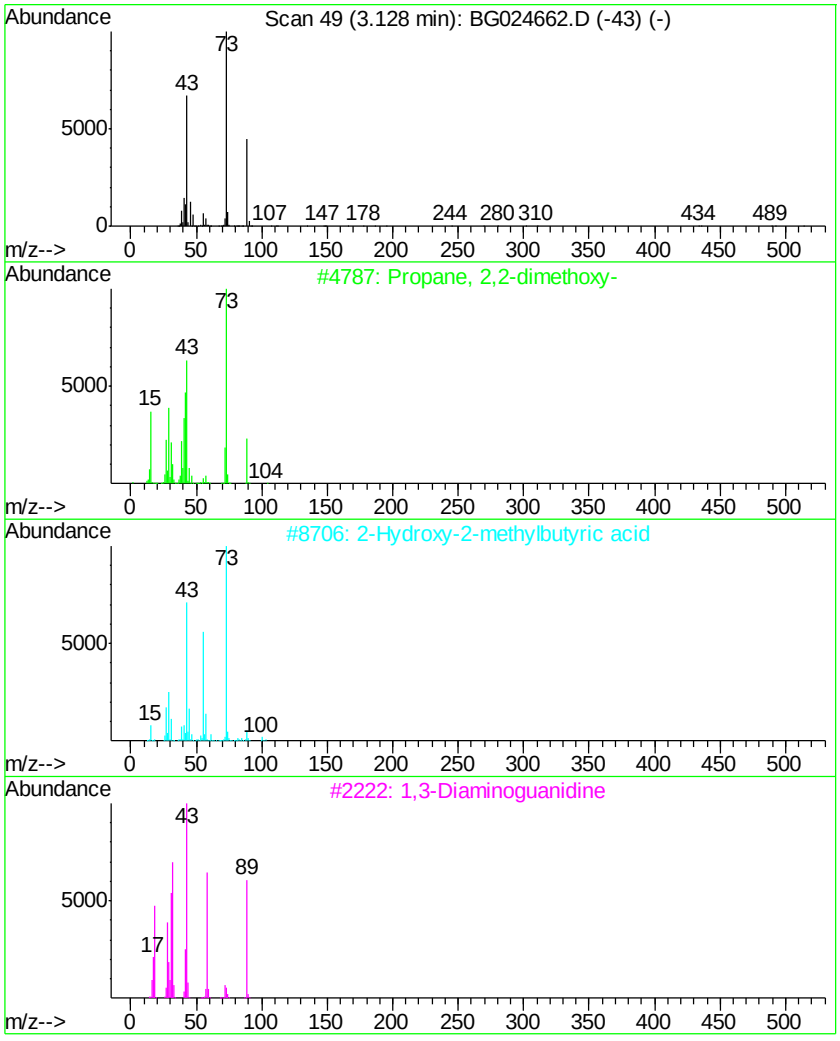
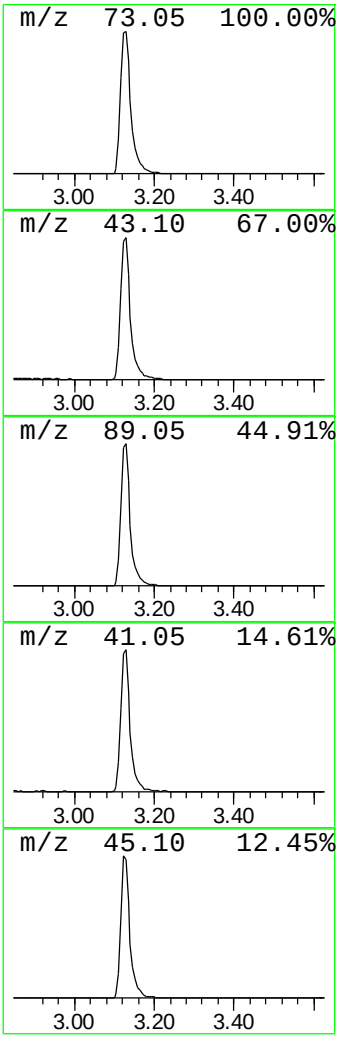
Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	338.81 ng	10319500	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
2	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	17
3	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9





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Misc :
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Instrument : BNA_G
ClientSampleId : SB-79-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
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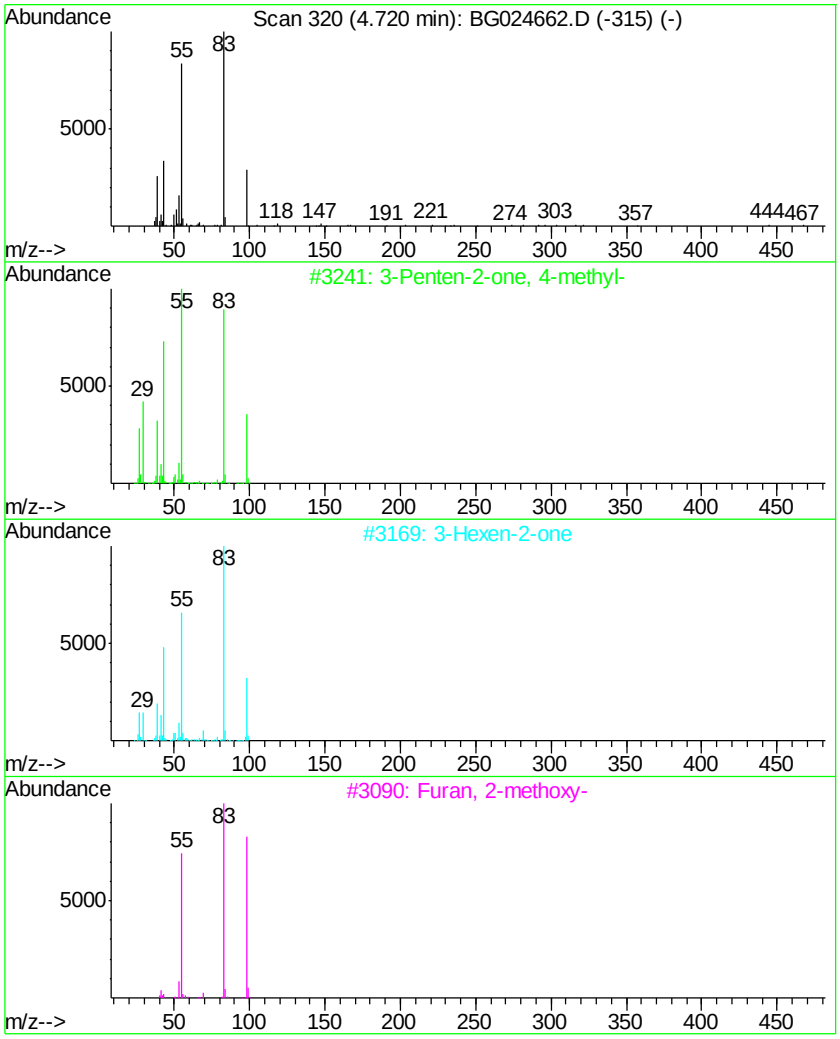
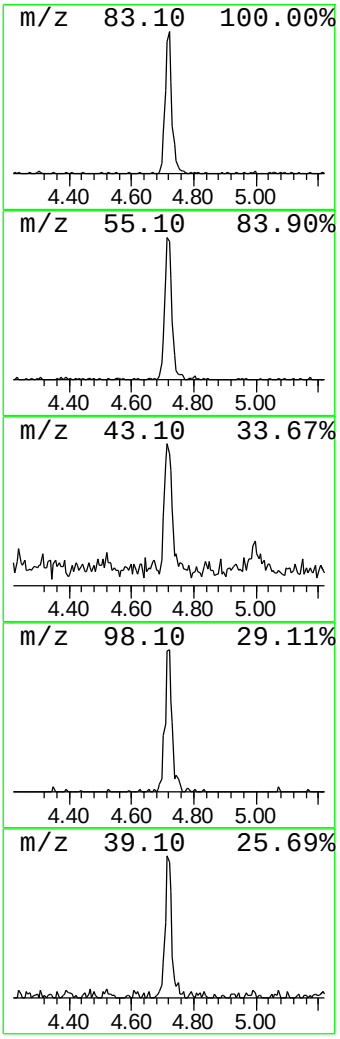
Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	6.94 ng	211280	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2	3-Hexen-2-one	98	C6H10O	000763-93-9	86
3	Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	72





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Sample : H5502-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-79-0.5-1.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
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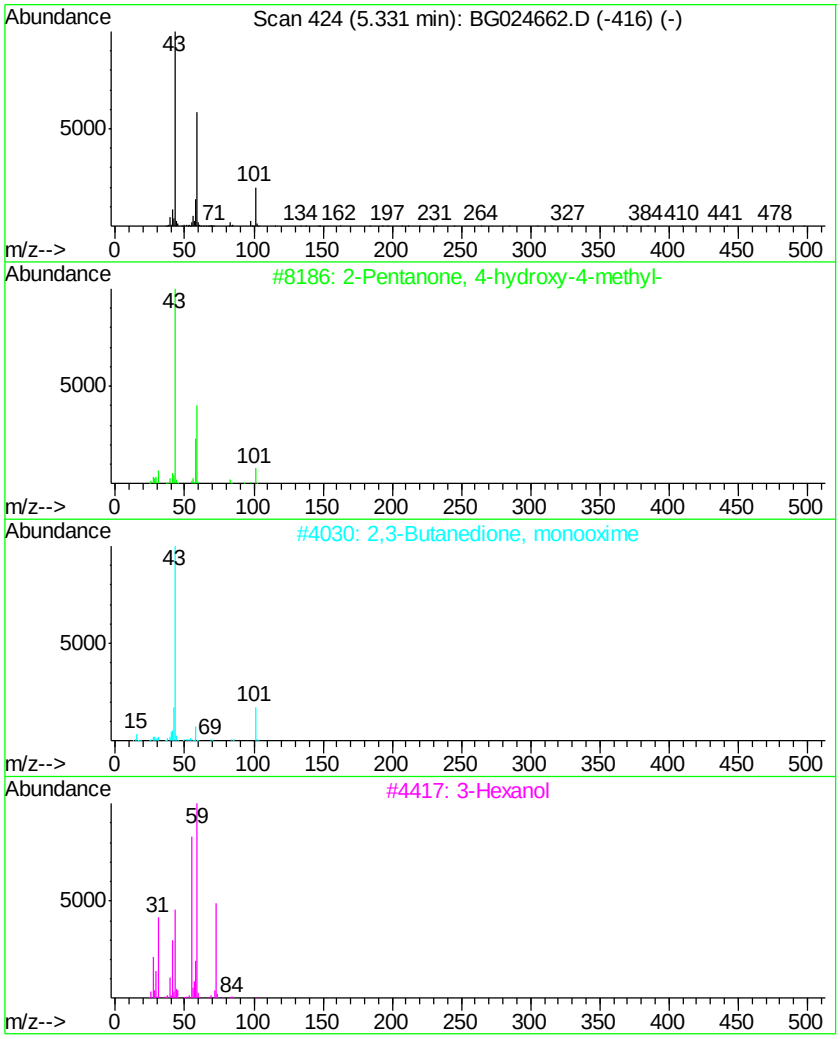
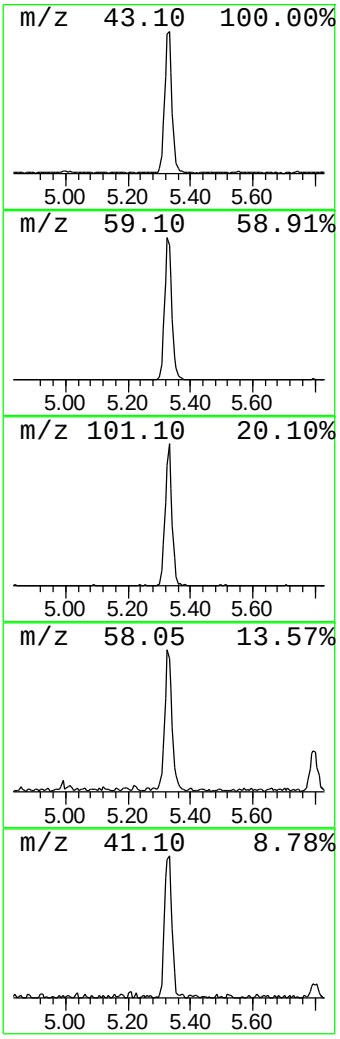
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	31.01 ng	944630	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	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Sample : H5502-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-79-0.5-1.0

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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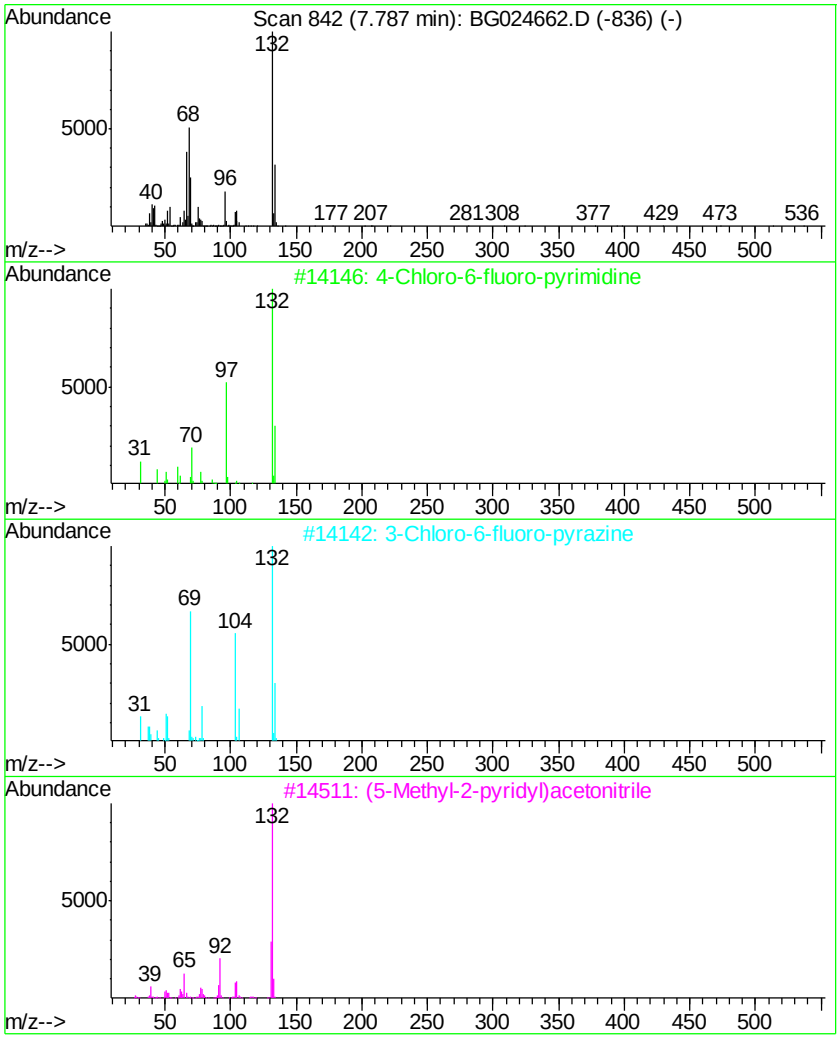
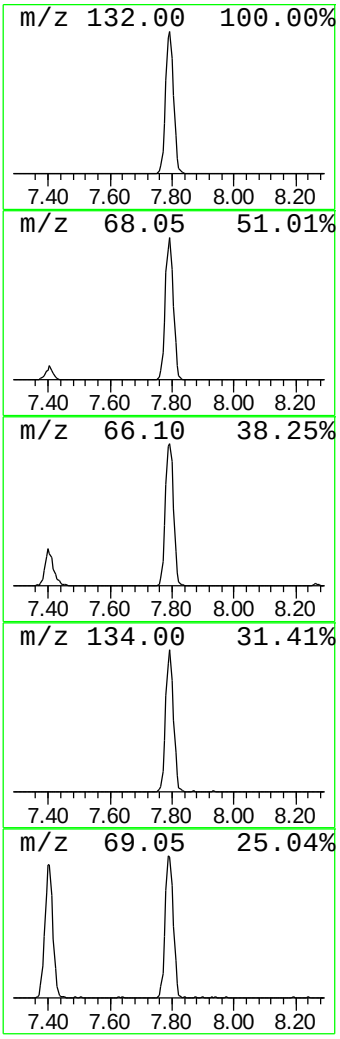
Peak Number 4 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	88.36 ng	2691300	1,4-Dichlorobenzene-d4	8.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	22
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	12
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Sample : H5502-01
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-79-0.5-1.0

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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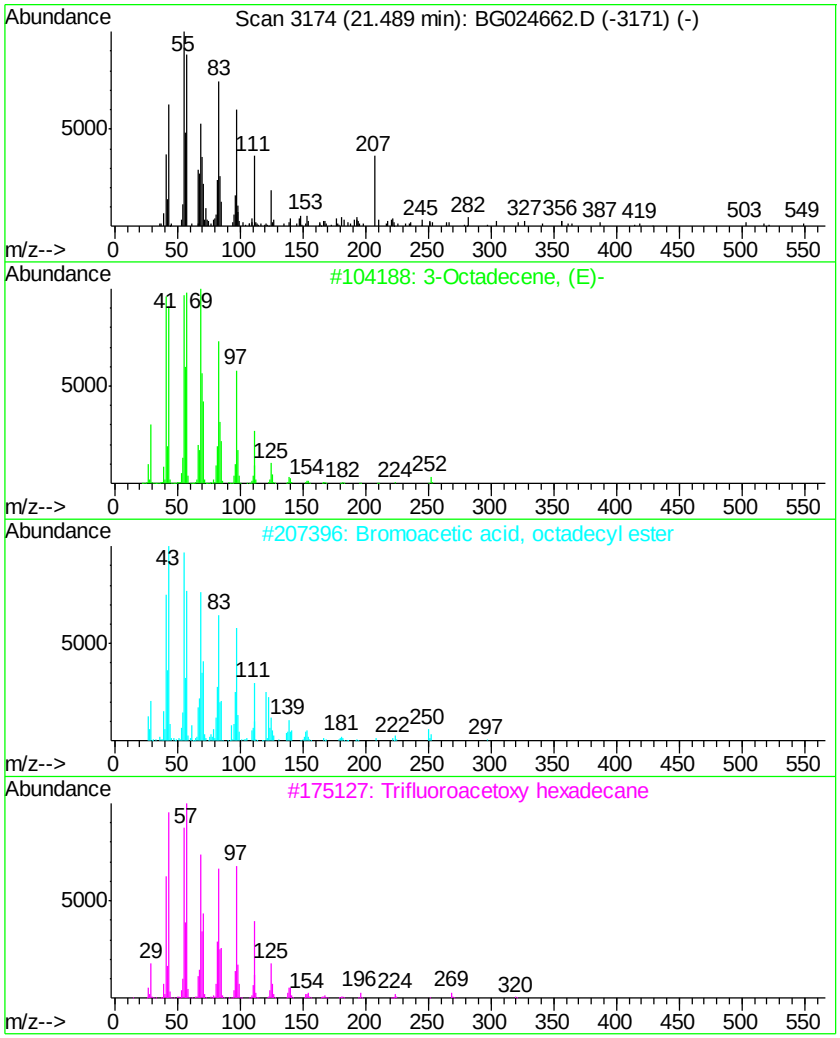
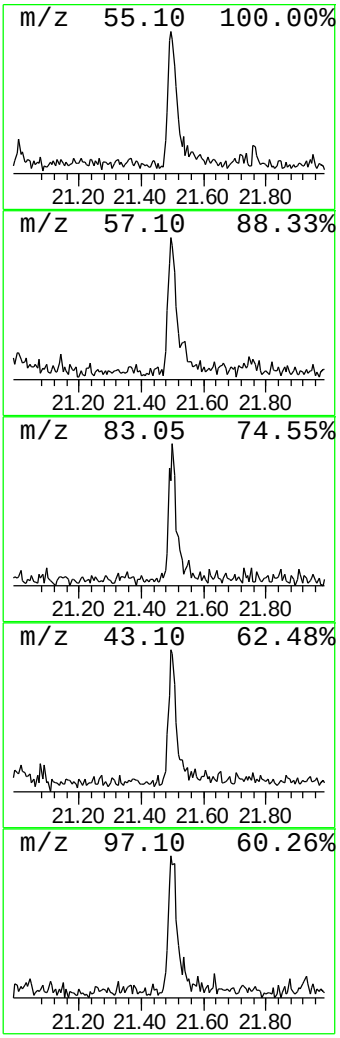
Peak Number 6 3-Octadecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.49	2.40 ng	280892	Chrysene-d12	21.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octadecene, (E)-	252	C18H36	007206-19-1	90
2	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	81
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
4	1-Pentadecene	210	C15H30	013360-61-7	62
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	50





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	338.8	ng	10319500	1	8.27	609162	20.0
3-Penten-2-one, 4...	4.72	6.9	ng	211280	1	8.27	609162	20.0
2-Pentanone, 4-hy...	5.33	31.0	ng	944630	1	8.27	609162	20.0
unknown7.79	7.79	88.4	ng	2691300	1	8.27	609162	20.0
3-Octadecene, (E)-	21.49	2.4	ng	280892	5	21.92	2340460	20.0