LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100716\
Data File : BF090441.D
Acq On : 7 Oct 2016 13:07
Operator : UM/SJ
Sample : H5121-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-T1

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_F\METHODS\8270-BF100516.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	4.554	192	194	197	rBV	155684	165479	1.73%	0.284%
2	5.183	246	249	251	rBV	571864	762087	7.97%	1.309%
3	5.583	282	284	287	rBV	2778137	3287128	34.38%	5.645%
4	6.600	370	373	375	rBV	2669543	2299120	24.05%	3.948%
5	6.749	383	386	389	rBV	5424033	5393583	56.41%	9.262%
6	6.989	404	407	409	rBV	1118283	1460506	15.27%	2.508%
7	7.046	409	412	414	rVV	204773	192951	2.02%	0.331%
8	7.137	418	420	423	rVB	3857560	5042183	52.73%	8.659%
9	7.549	453	456	458	rBV	4271179	4544851	47.53%	7.805%
10	8.269	517	519	522	rBV	1898911	2001798	20.94%	3.438%
11	9.355	611	614	616	rBV	8195660	7935038	82.99%	13.626%
12	9.743	646	648	650	rBV	346071	278432	2.91%	0.478%
13	10.029	671	673	676	rVB	1647488	2285273	23.90%	3.924%
14	10.829	739	743	745	rBV	5058443	5444726	56.94%	9.350%
15	10.943	749	753	758	rVB2	84425	122968	1.29%	0.211%
16	11.526	801	804	806	rBV	2903269	2564154	26.82%	4.403%
17	12.052	847	850	852	rBV	243202	322028	3.37%	0.553%
18	12.841	916	919	926	rBV	261030	342901	3.59%	0.589%
19	13.126	940	944	946	rBV	7099888	9561673	100.00%	16.420%
20	14.018	1019	1022	1030	rBV2	76240	157373	1.65%	0.270%
21	14.167	1033	1035	1038	rVV	1694741	2315650	24.22%	3.976%
22	15.675	1163	1167	1169	rBV	1231634	1753543	18.34%	3.011%

Sum of corrected areas: 58233445

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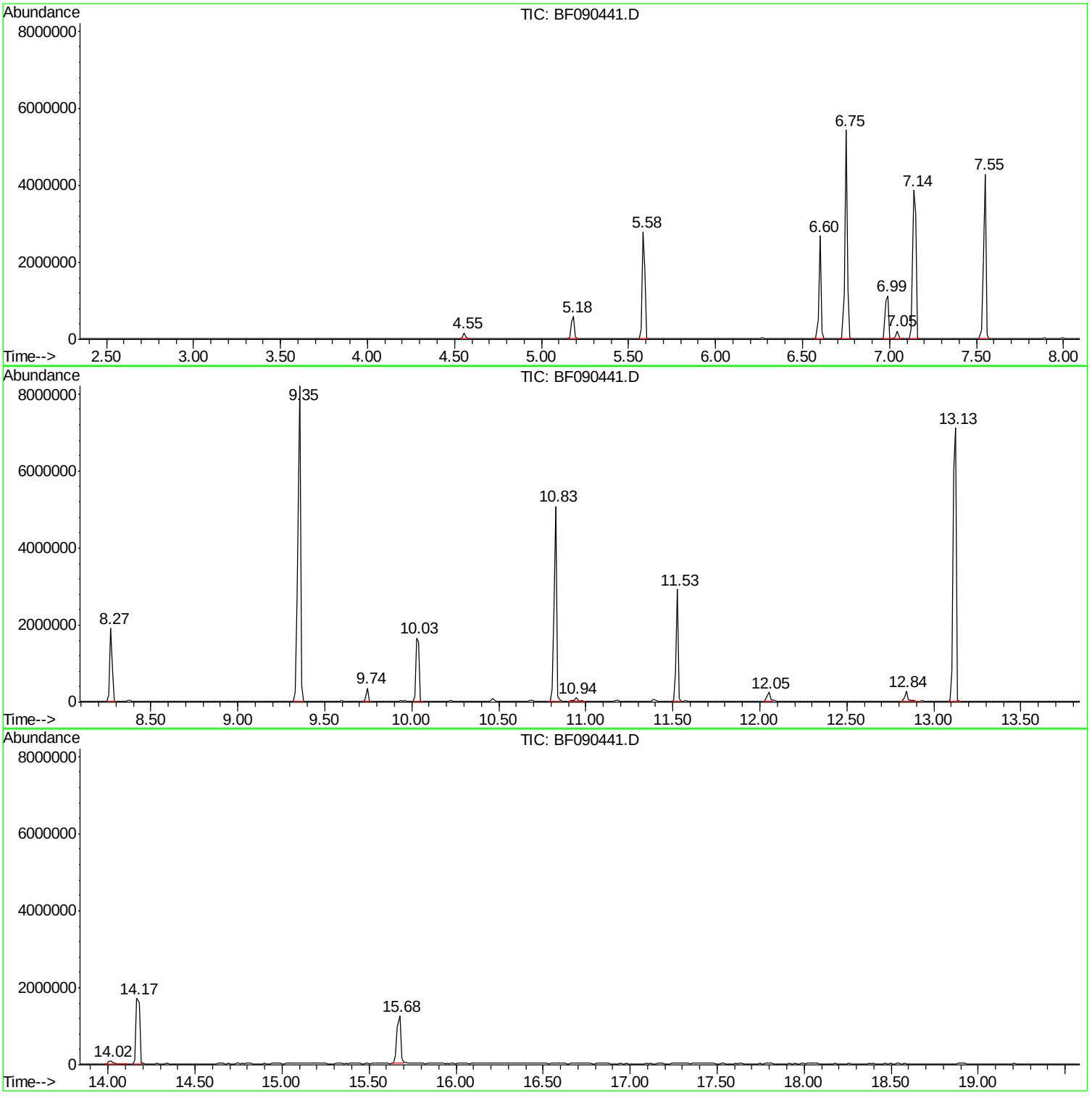
Instrument :
BNA_F
ClientSampleId :
WS-T1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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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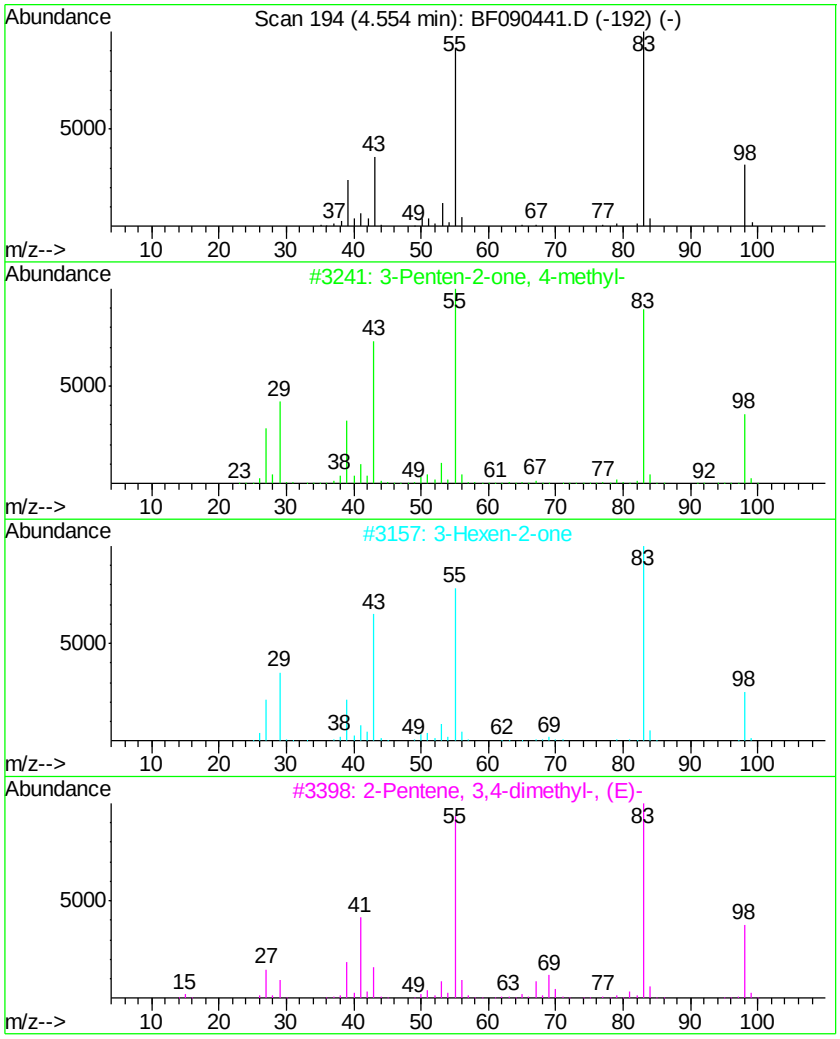
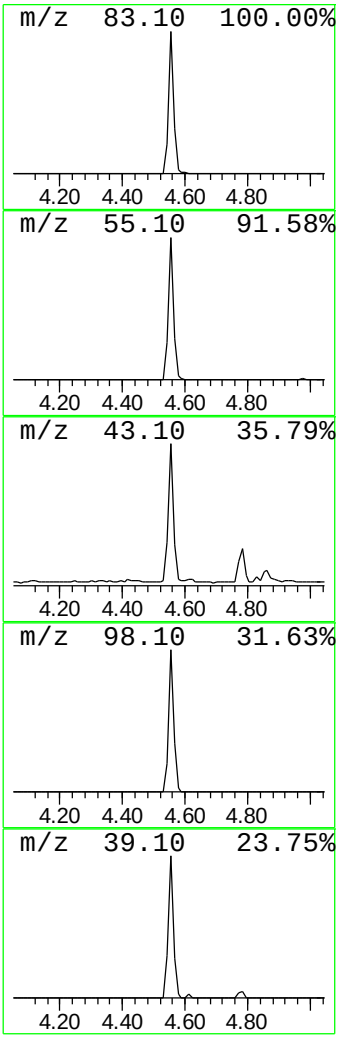
Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.55	2.27 ng	165479	1,4-Dichlorobenzene-d4	6.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5	2,4-Azetidinedione, 3,3-diethyl-	141	C7H11NO2	042282-85-9	78





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Operator : UM/SJ
Sample : H5121-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-T1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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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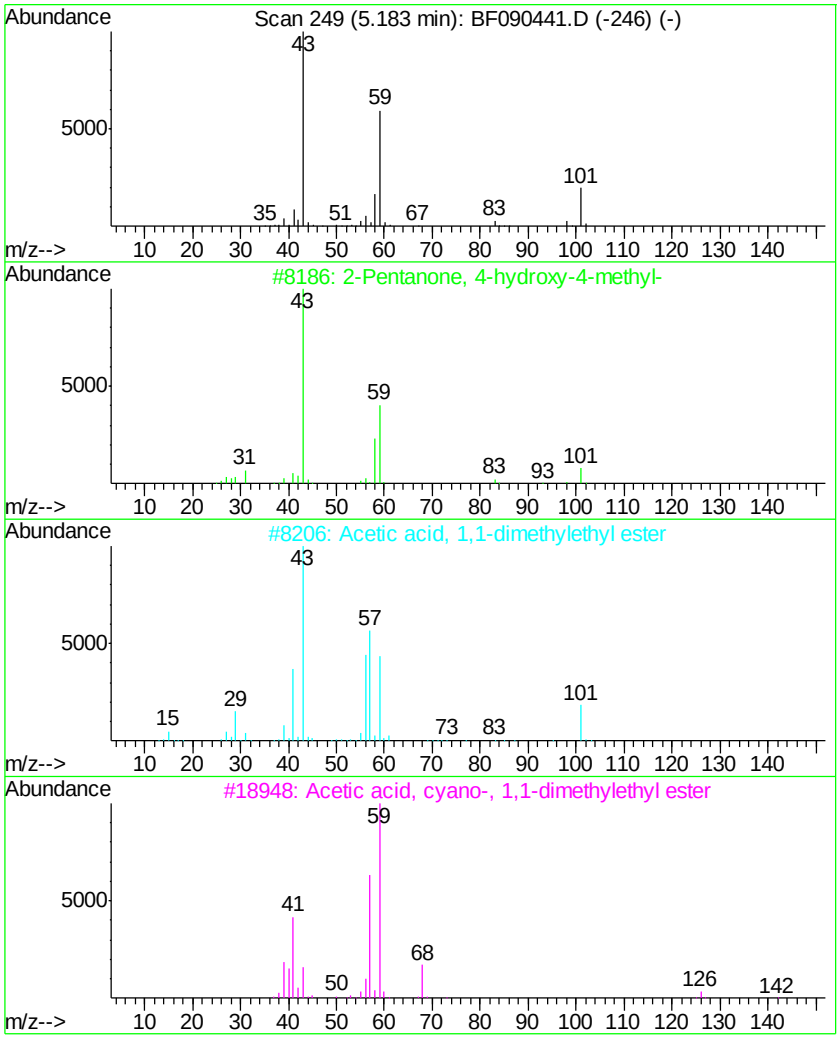
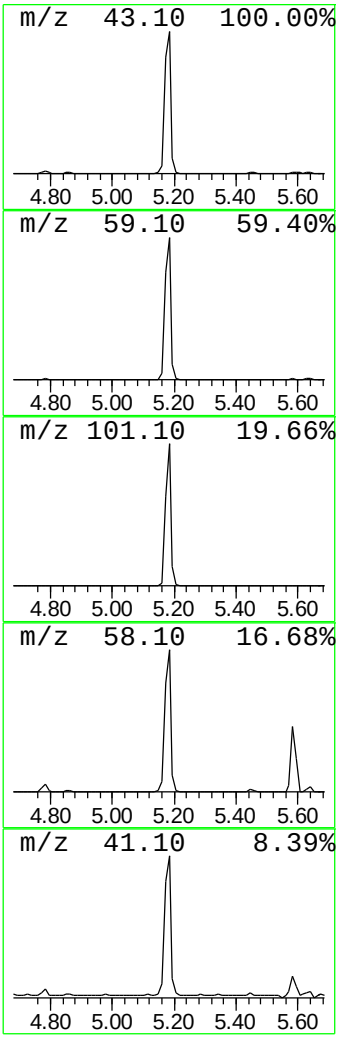
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	10.44 ng	762087	1,4-Dichlorobenzene-d4	6.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Acetone	58	C3H6O	000067-64-1	9





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Operator : UM/SJ
Sample : H5121-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-T1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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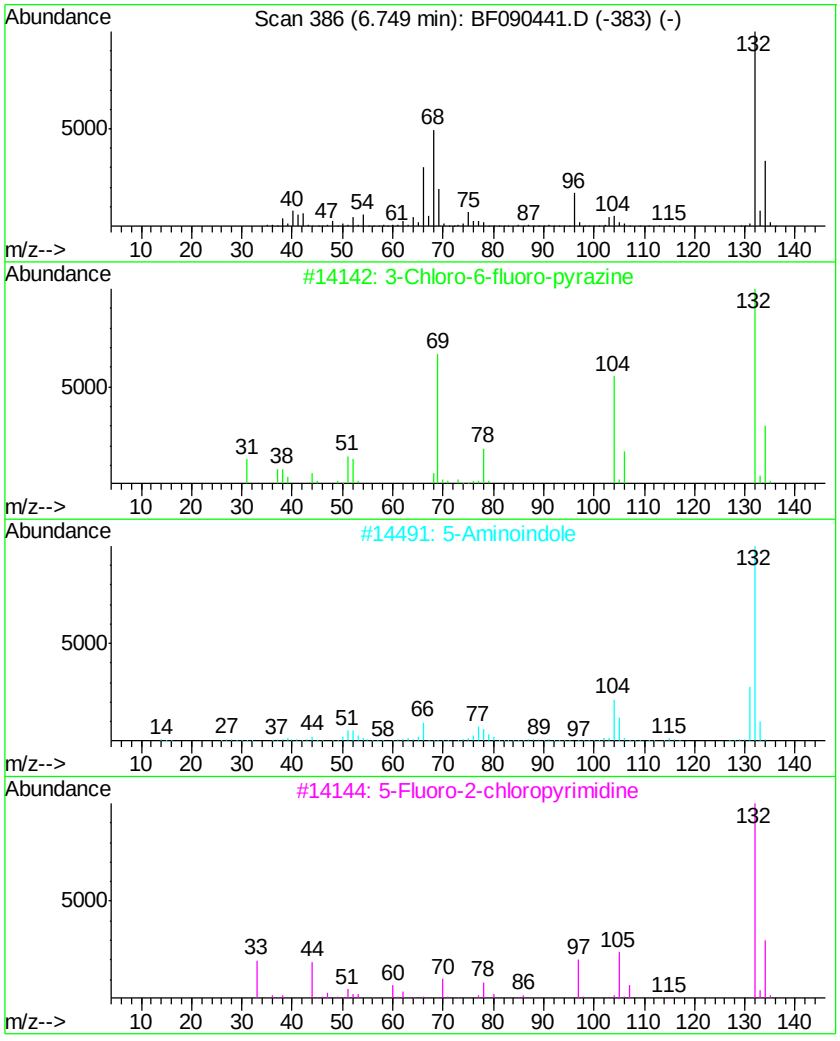
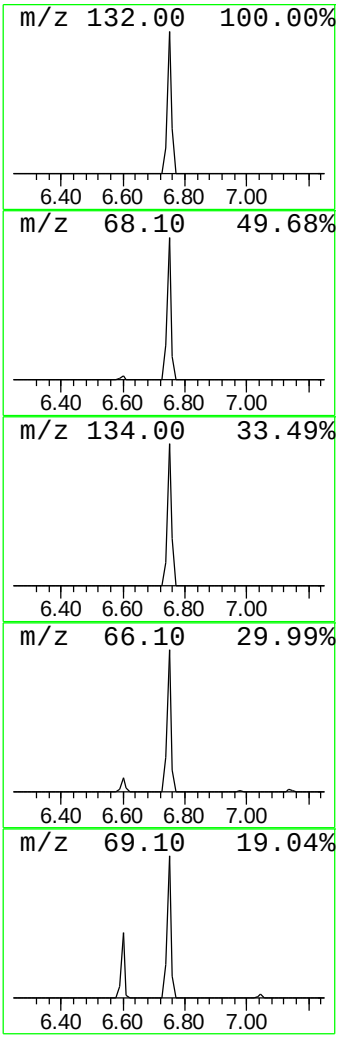
Peak Number 3 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	73.86 ng	5393580	1,4-Dichlorobenzene-d4	6.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9





Library Search Compound Report

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Operator : UM/SJ
Sample : H5121-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-T1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.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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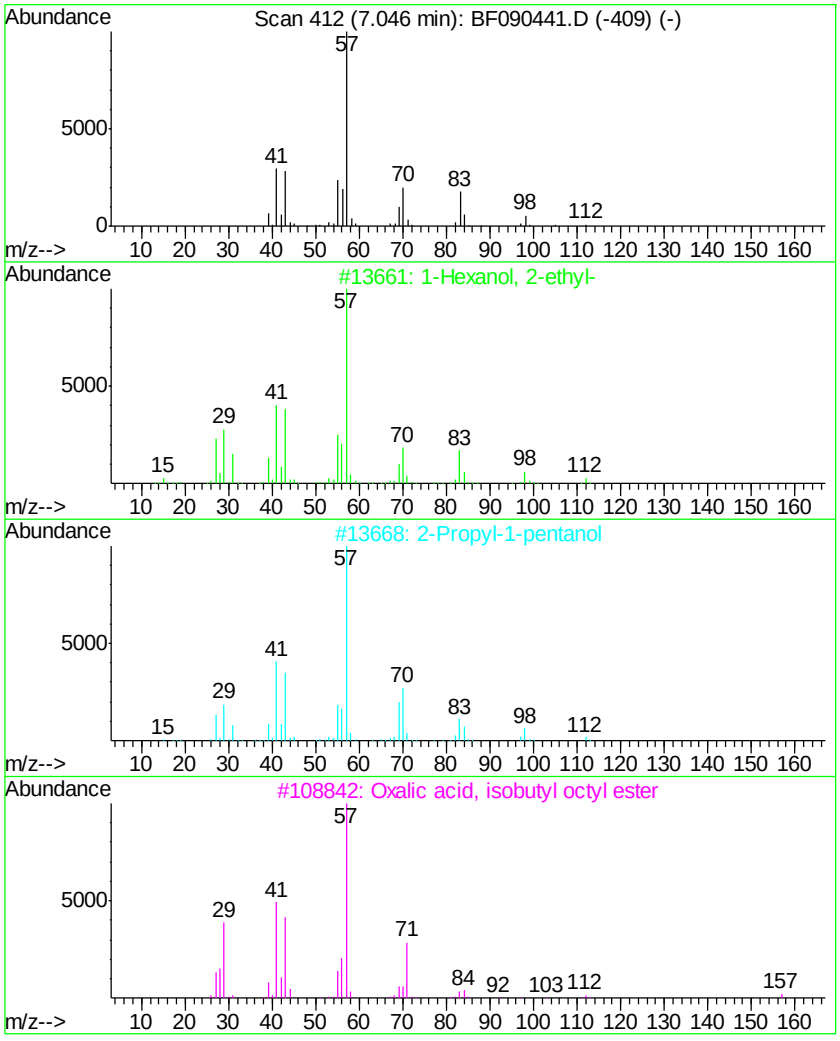
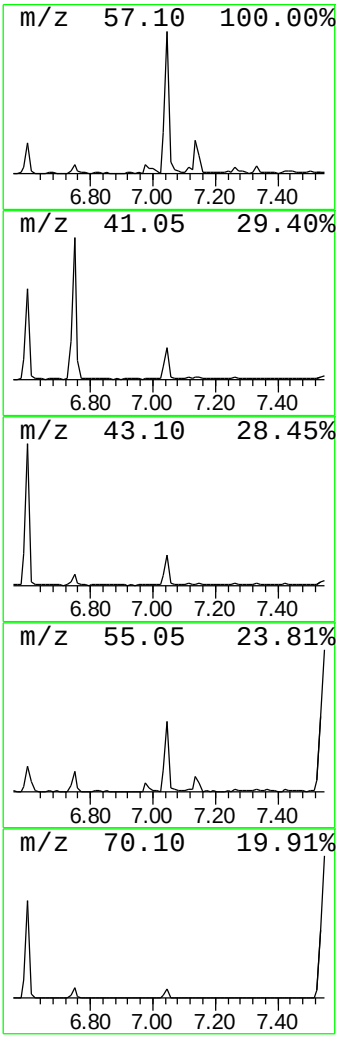
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	2.64 ng	192951	1,4-Dichlorobenzene-d4	6.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47
4	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	45





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Instrument : BNA_F
ClientSampleId : WS-T1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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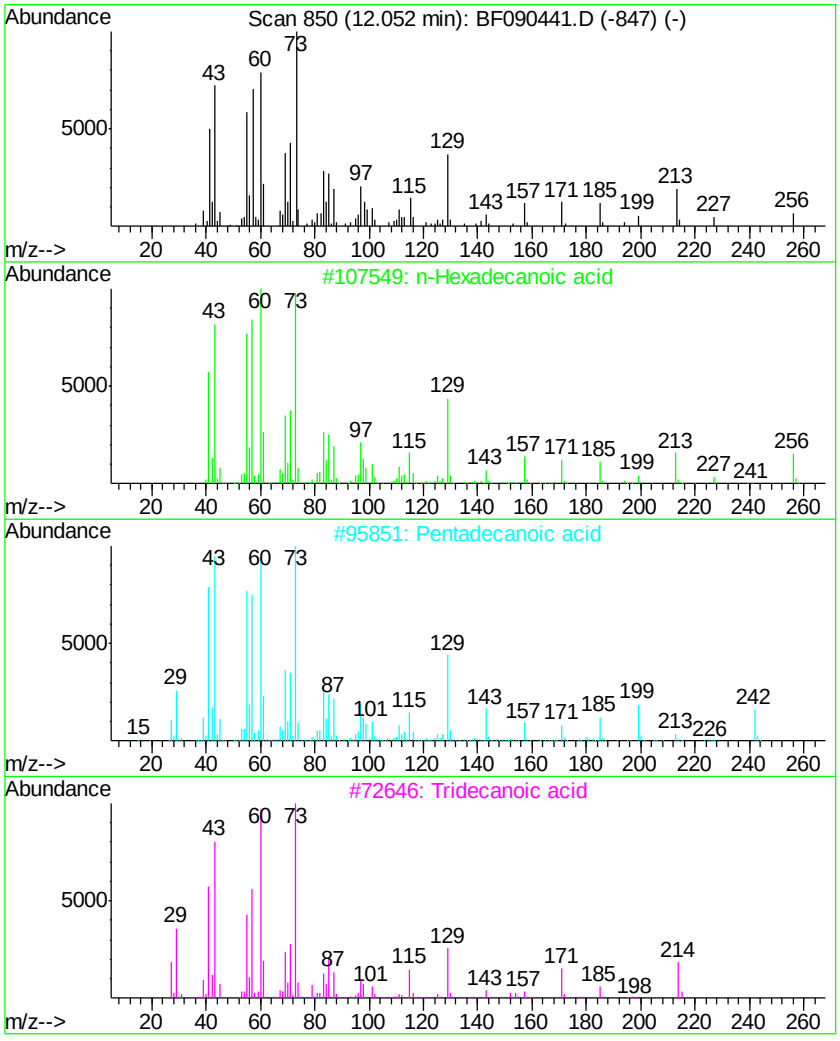
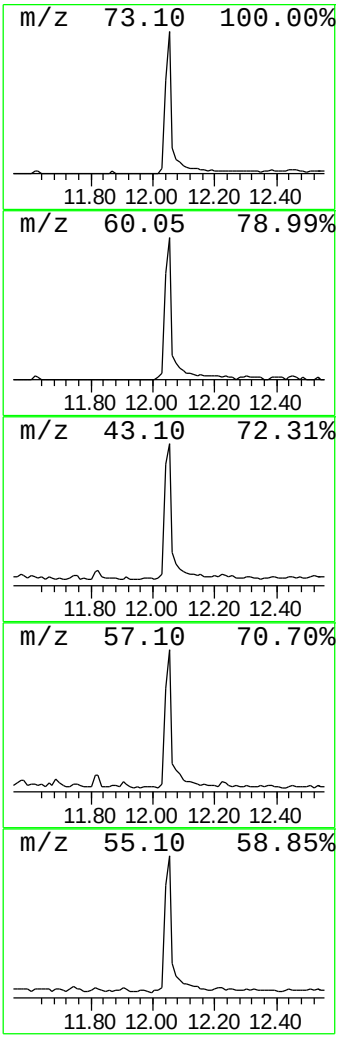
Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	2.51 ng	322028	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25





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Operator : UM/SJ
Sample : H5121-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : WS-T1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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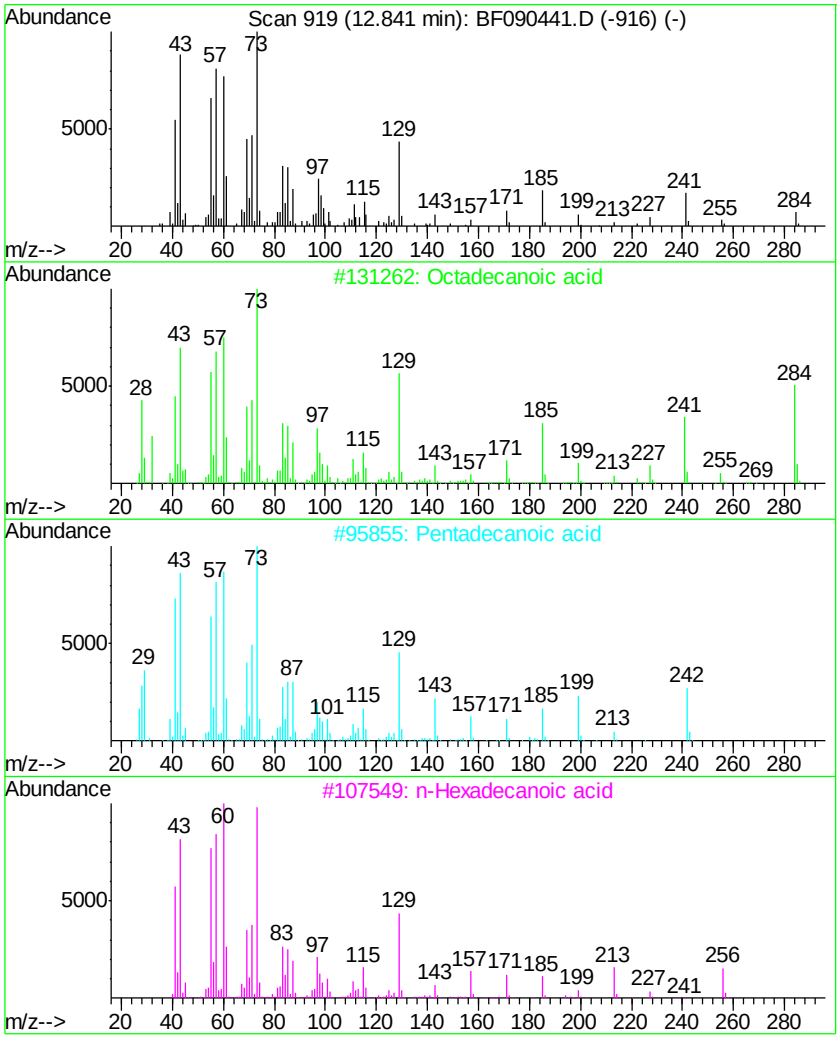
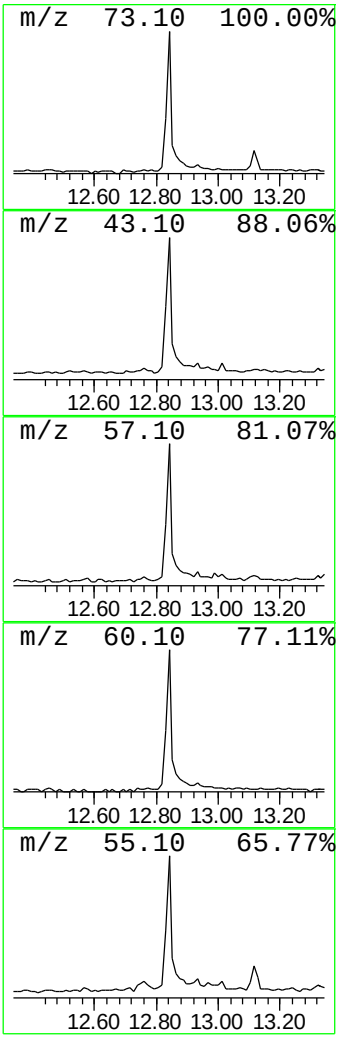
Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	2.67 ng	342901	Phenanthrene-d10	11.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4	n-PROPYL NONYL ETHER	186	C12H26O	1000130-69-3	25
5	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1000309-70-5	20





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.55	2.3	ng	165479	1	6.99	1460510	20.0
2-Pentanone, 4-hy...	5.18	10.4	ng	762087	1	6.99	1460510	20.0
unknown6.75	6.75	73.9	ng	5393580	1	6.99	1460510	20.0
1-Hexanol, 2-ethyl-	7.05	2.6	ng	192951	1	6.99	1460510	20.0
n-Hexadecanoic acid	12.05	2.5	ng	322028	4	11.53	2564150	20.0
Octadecanoic acid	12.84	2.7	ng	342901	4	11.53	2564150	20.0