LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061216\
Data File : BF087959.D
Acq On : 12 Jun 2016 20:31
Operator : UM/SJ
Sample : H3467-04
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HF-20-WC-1

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-BF060716.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	1.735	11	13	14	rBV	212063	313064	10.06%	1.151%
2	1.861	22	24	26	rBV	525586	866264	27.84%	3.186%
3	2.353	60	67	70	rVB2	11321	46721	1.50%	0.172%
4	2.604	87	89	94	rVB	60884	80253	2.58%	0.295%
5	4.330	237	240	243	rBV	562606	786775	25.29%	2.893%
6	4.993	295	298	305	rBV	312448	560386	18.01%	2.061%
7	5.404	331	334	337	rBV	1941025	2196091	70.58%	8.076%
8	6.444	422	425	427	rBV	2082801	2482576	79.79%	9.130%
9	6.570	433	436	438	rBV	2478148	2463405	79.17%	9.060%
10	6.799	454	456	458	rBV	751601	611393	19.65%	2.249%
11	6.959	467	470	472	rBV	2313798	2128308	68.40%	7.827%
12	7.370	502	506	508	rBV	1673318	1895348	60.92%	6.970%
13	8.090	566	569	572	rBV	785563	947379	30.45%	3.484%
14	9.165	660	663	666	rBV	2622582	3017571	96.98%	11.098%
15	9.839	719	722	737	rBV	978967	959854	30.85%	3.530%
16	10.628	788	791	801	rBV	1633061	1915386	61.56%	7.044%
17	11.325	849	852	854	rBV	731639	949312	30.51%	3.491%
18	12.034	912	914	920	rBV	75053	100579	3.23%	0.370%
19	12.742	973	976	978	rBV	162269	205505	6.60%	0.756%
20	12.811	981	982	985	rVB	44304	35762	1.15%	0.132%
21	12.914	988	991	993	rBV	2758616	3111438	100.00%	11.443%
22	13.439	1035	1037	1039	rBV	144506	134736	4.33%	0.496%
23	13.954	1079	1082	1084	rBV	782055	781464	25.12%	2.874%
24	15.360	1202	1205	1208	rBV	366094	524149	16.85%	1.928%
25	15.405	1208	1209	1220	rVB2	30090	77416	2.49%	0.285%

Sum of corrected areas: 27191135

LSC Report - Integrated Chromatogram

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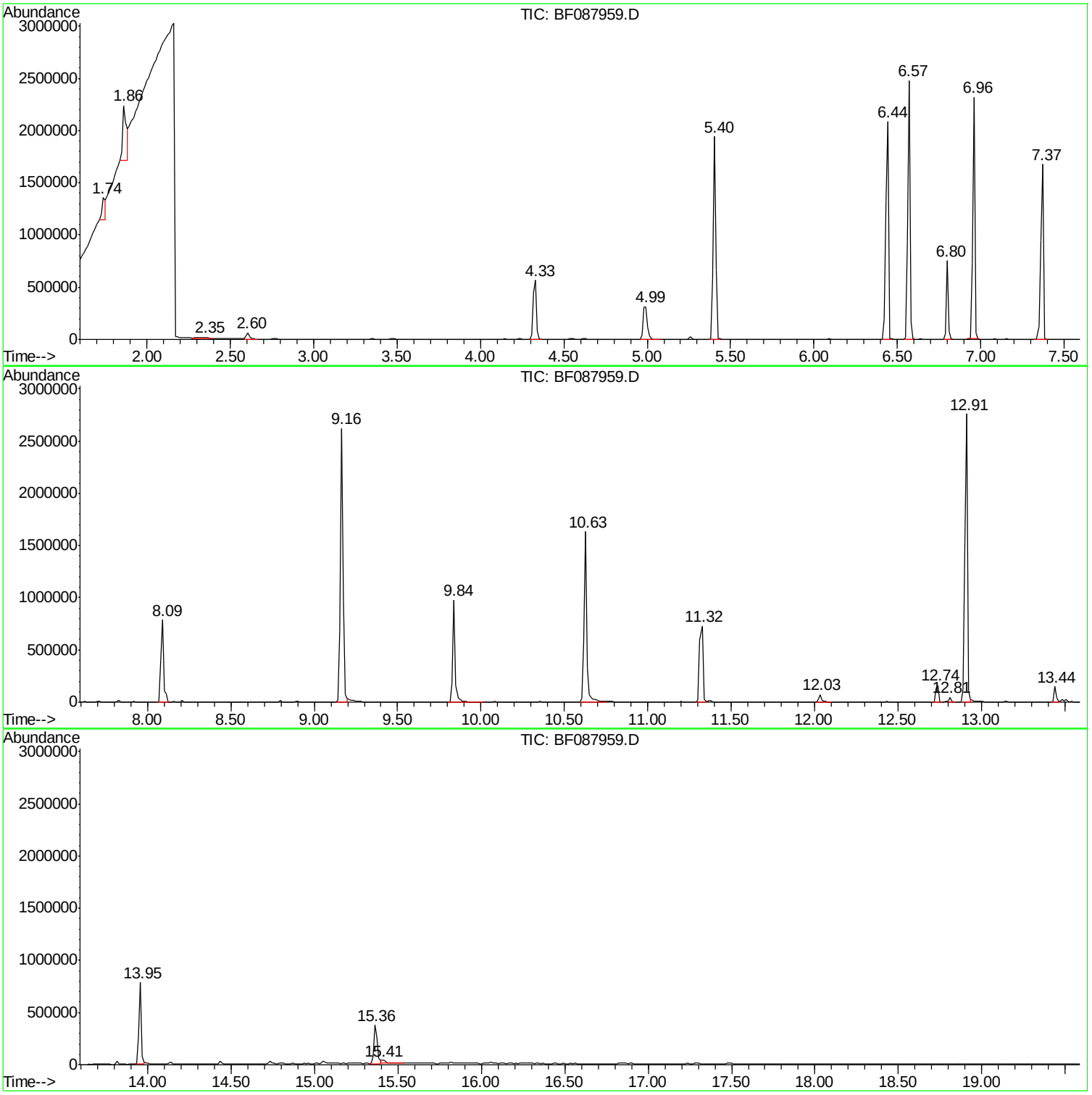
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HF-20-WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061216\
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Operator : UM/SJ
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ClientSampleId : HF-20-WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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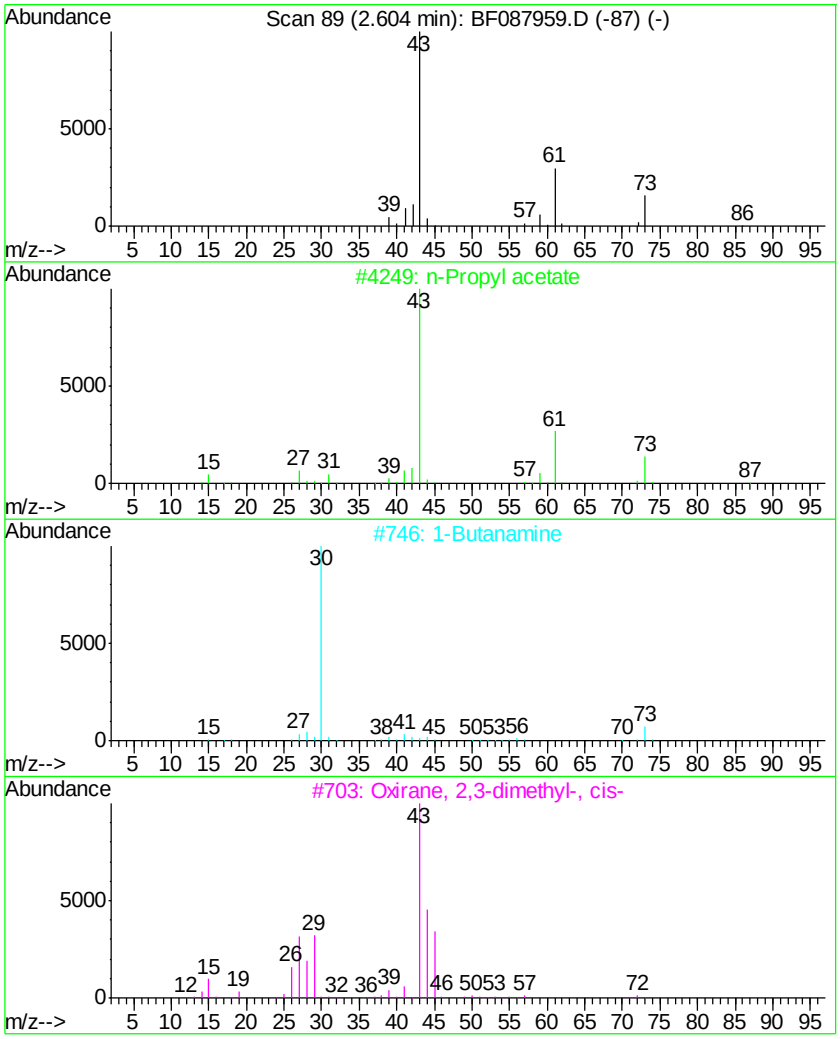
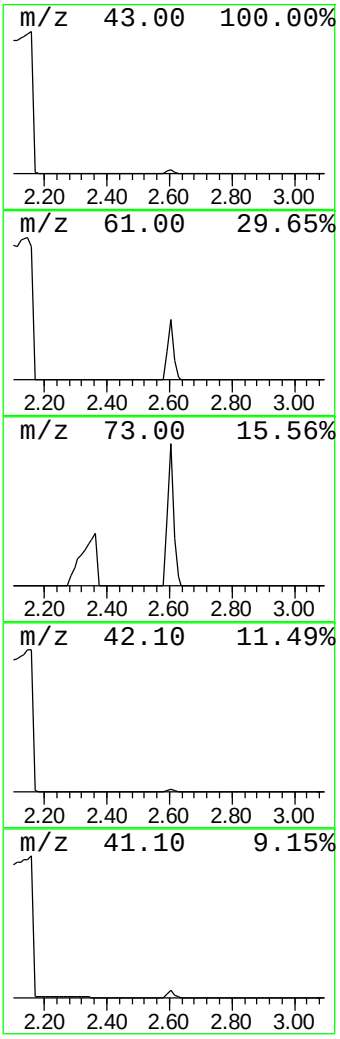
Peak Number 3 n-Propyl acetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.60	2.63 ng	80253	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	7
3	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	7
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	Pentane	72	C5H12	000109-66-0	4





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Acq On : 12 Jun 2016 20:31
Operator : UM/SJ
Sample : H3467-04
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HF-20-WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

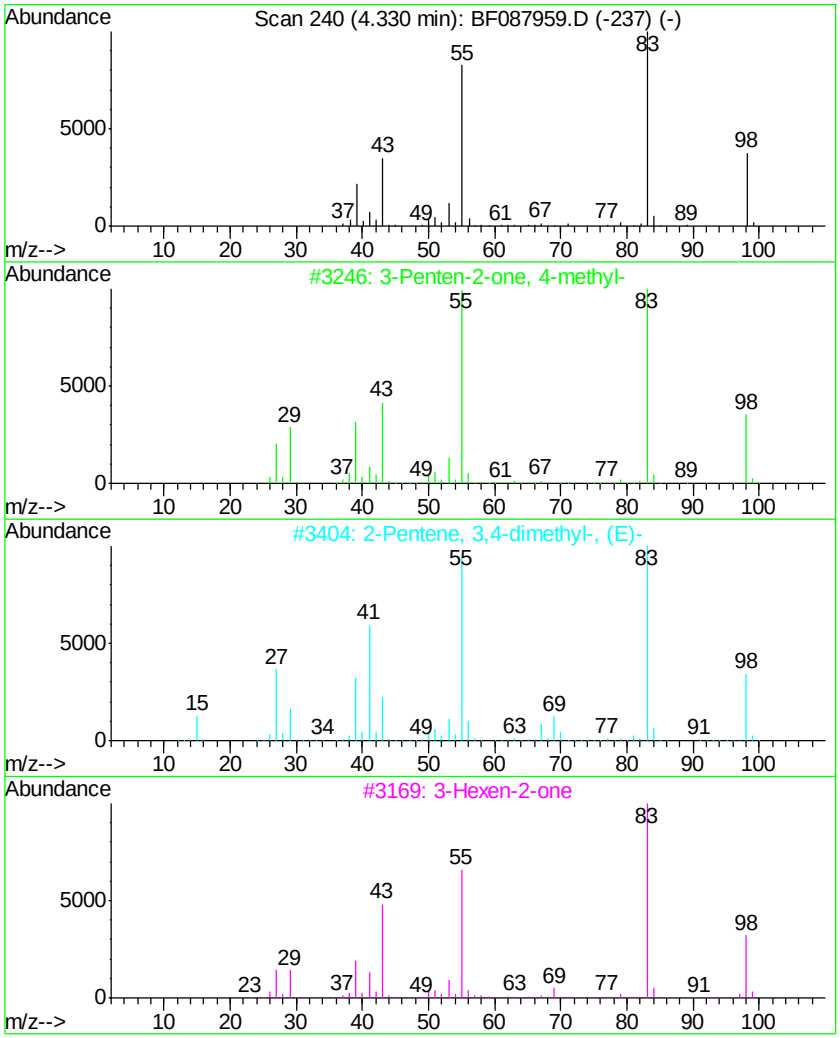
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

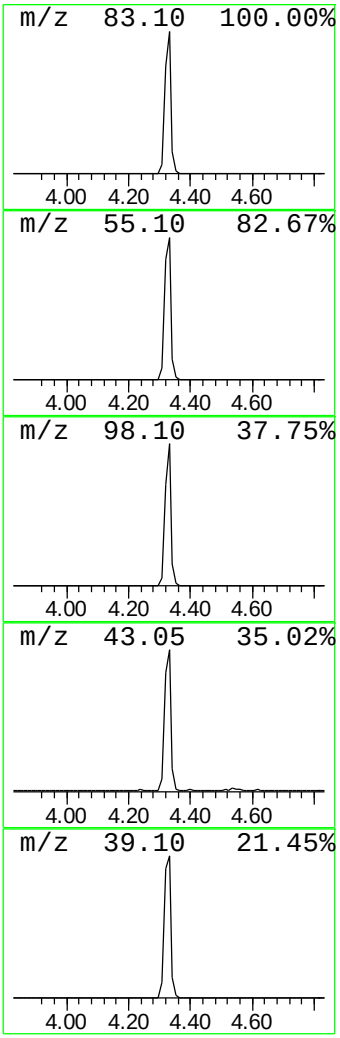
****

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	25.74 ng	786775	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	3-Hexen-2-one	98	C6H10O	000763-93-9	90
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





Data Path : Z:\HPCHEM1\BNA F\DATA\BF061216\
Data File : BF087959.D
Acq On : 12 Jun 2016 20:31
Operator : UM/SJ
Sample : H3467-04
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HF-20-WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

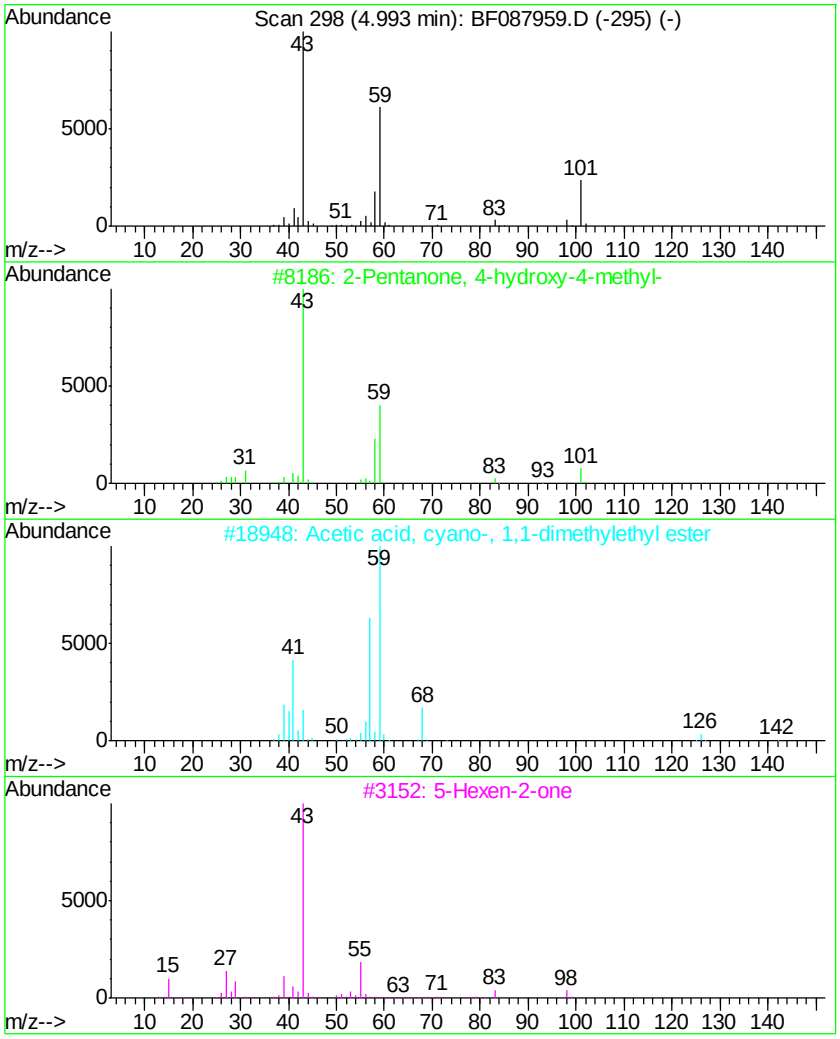
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

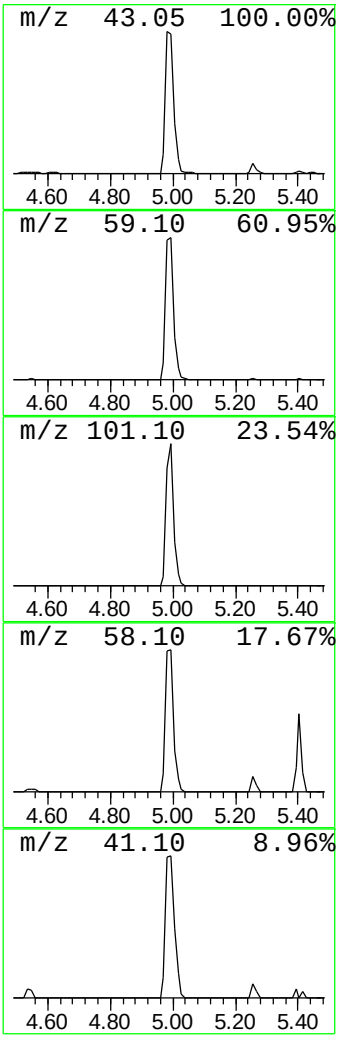
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	18.33 ng	560386	1,4-Dichlorobenzene-d4	6.80

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Acetone	58	C3H6O	000067-64-1	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061216\
Data File : BF087959.D
Acq On : 12 Jun 2016 20:31
Operator : UM/SJ
Sample : H3467-04
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HF-20-WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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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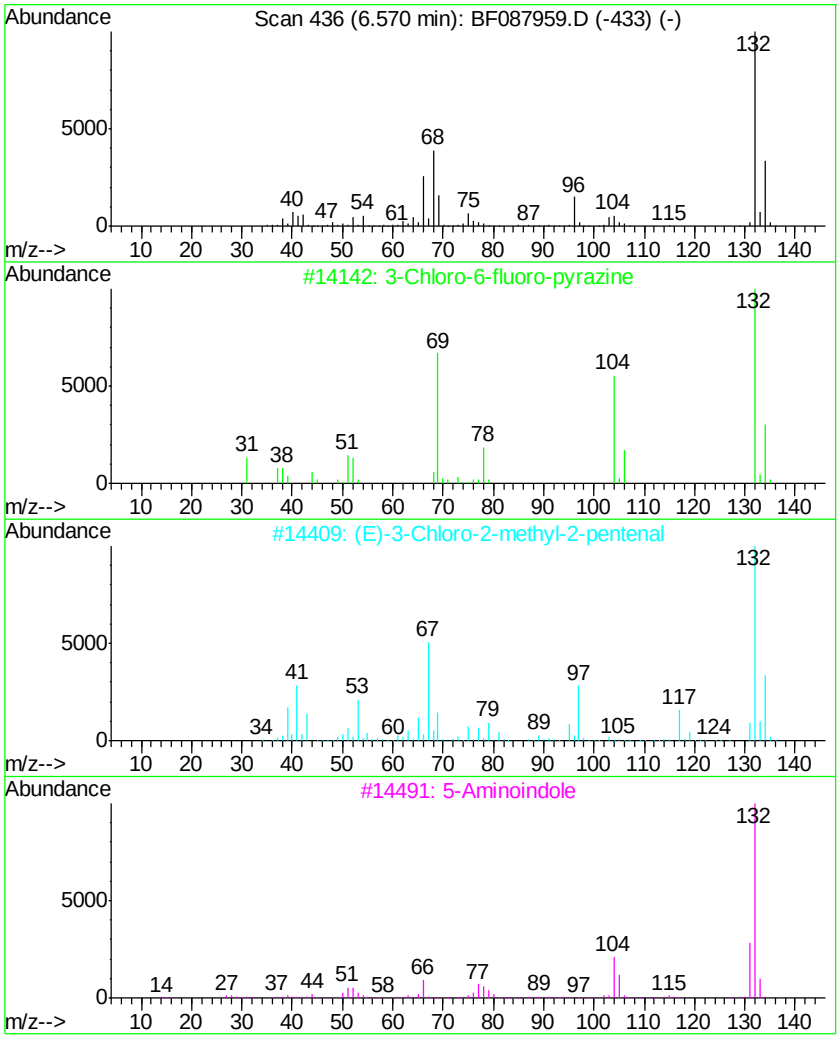
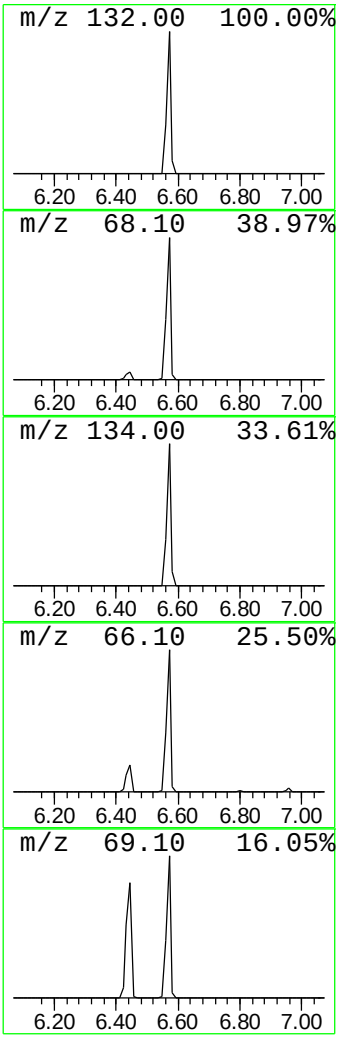
Peak Number 6 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	80.58 ng	2463410	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





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Data File : BF087959.D
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Operator : UM/SJ
Sample : H3467-04
Misc :
ALS Vial : 55 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HF-20-WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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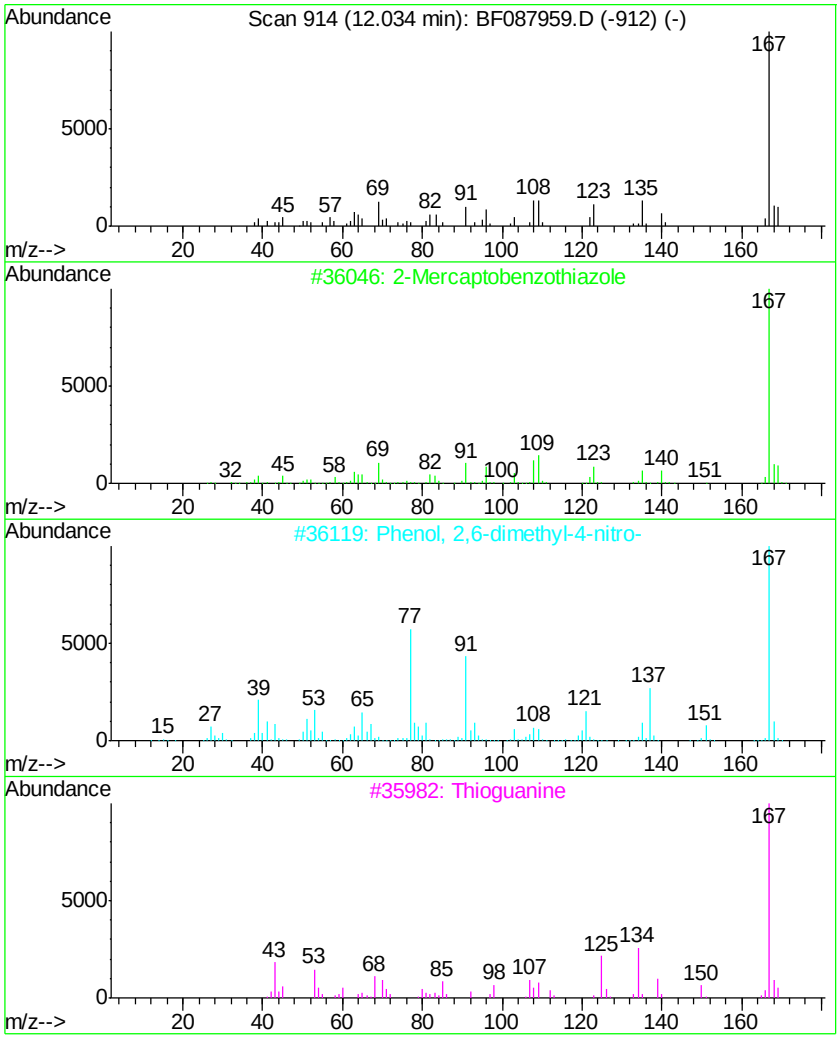
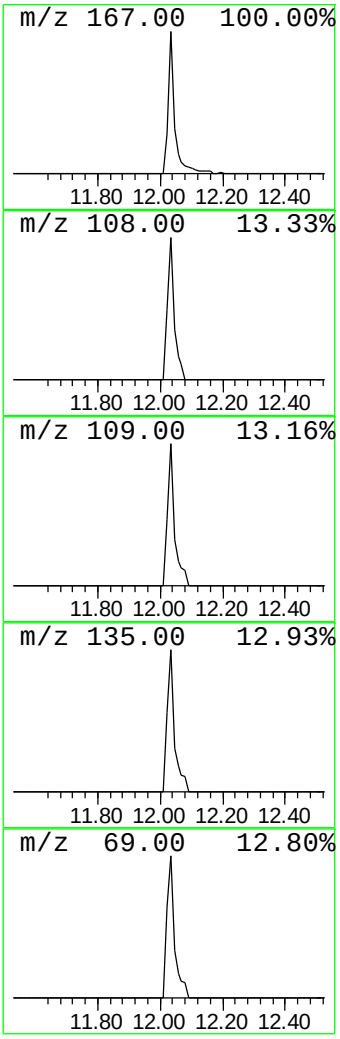
Peak Number 8 2-Mercaptobenzothiazole Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.03	2.12 ng	100579	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Mercaptobenzothiazole	167	C7H5NS2	000149-30-4	96
2	Phenol, 2,6-dimethyl-4-nitro-	167	C8H9NO3	002423-71-4	59
3	Thioguanine	167	C5H5N5S	000154-42-7	59
4	5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	59
5	3-Methoxythiobenzamide	167	C8H9NOS	064559-06-4	45





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Instrument : BNA_F
ClientSampleId : HF-20-WC-1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

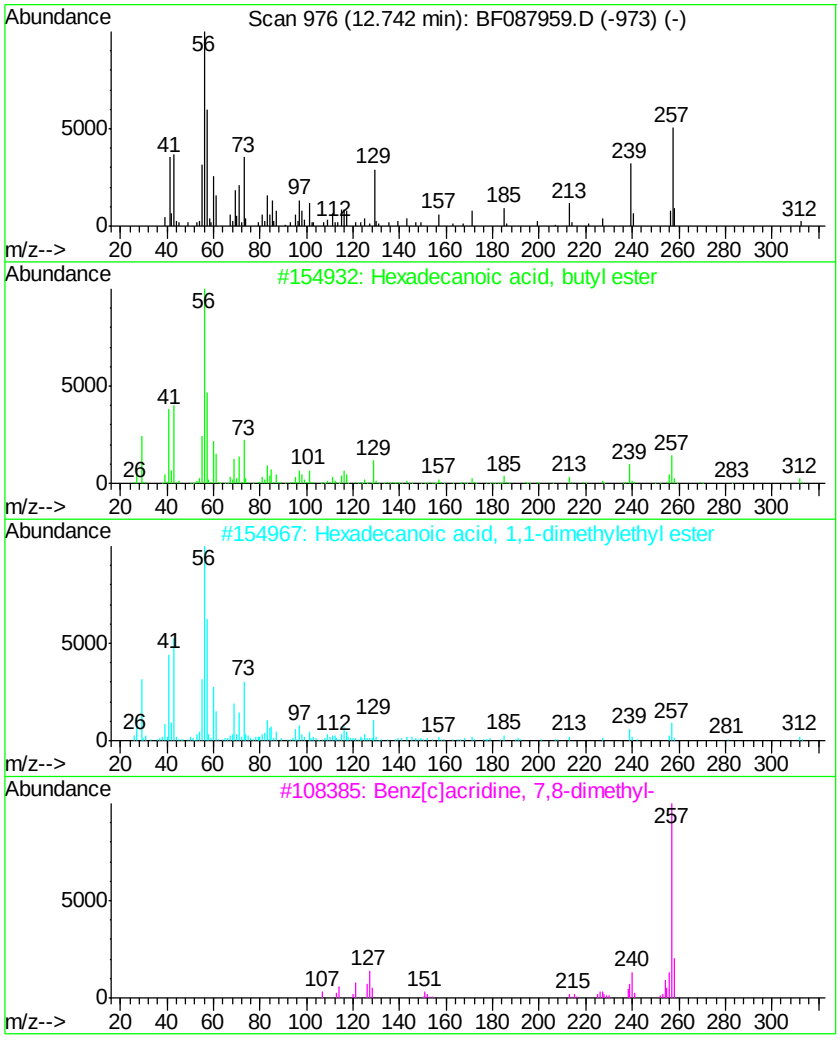
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

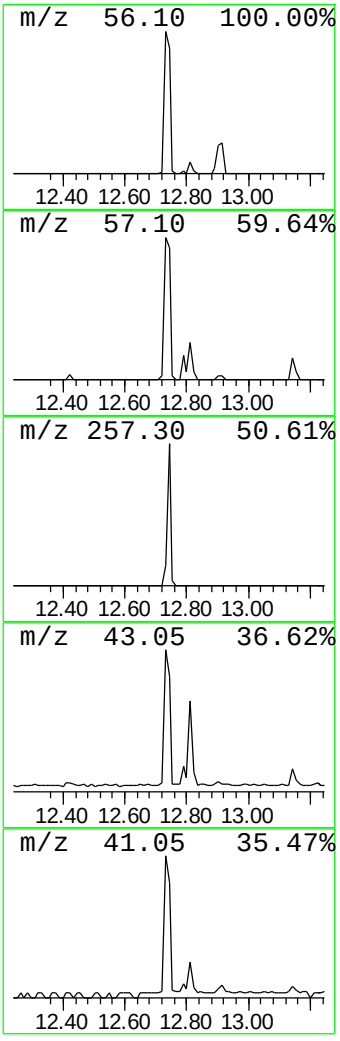
****

Peak Number 9 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	5.26 ng	205505	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	92
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	92
3	Benz[c]acridine, 7,8-dimethyl-	257	C19H15N	003518-01-2	38
4	Nipecotic acid	129	C6H11NO2	000498-95-3	38
5	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	27





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

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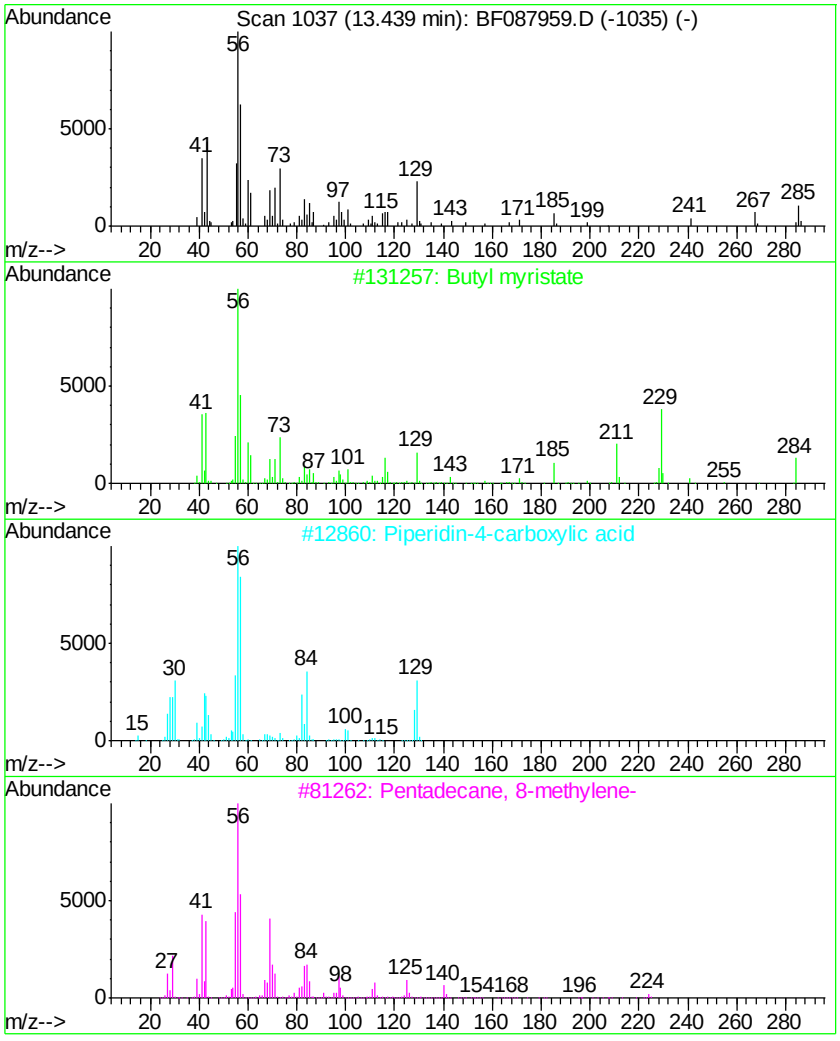
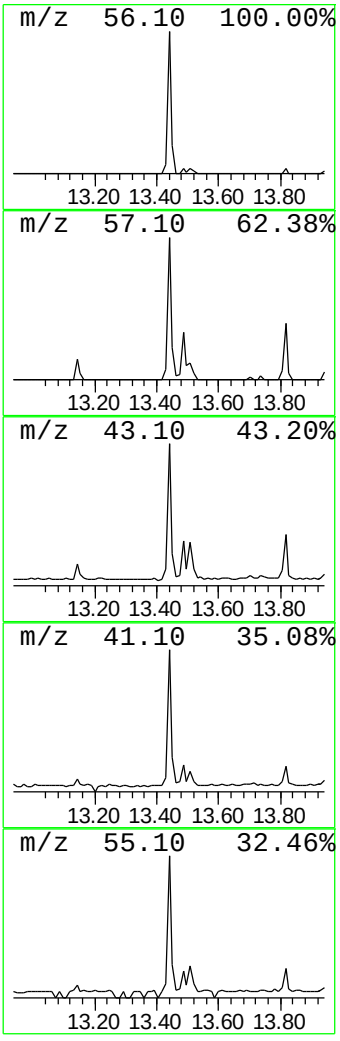
Peak Number 10 Butyl myristate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.44	3.45 ng	134736	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl myristate	284	C18H36O2	000110-36-1	72
2	Piperidin-4-carboxylic acid	129	C6H11NO2	000498-94-2	38
3	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
4	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	35
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	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
n-Propyl acetate	2.60	2.6	ng	80253	1	6.80	611393	20.0
3-Penten-2-one, 4...	4.33	25.7	ng	786775	1	6.80	611393	20.0
2-Pentanone, 4-hy...	4.99	18.3	ng	560386	1	6.80	611393	20.0
unknown6.57	6.57	80.6	ng	2463410	1	6.80	611393	20.0
2-Mercaptobenzoth...	12.03	2.1	ng	100579	4	11.32	949312	20.0
Hexadecanoic acid...	12.74	5.3	ng	205505	5	13.95	781464	20.0
Butyl myristate	13.44	3.5	ng	134736	5	13.95	781464	20.0