LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084357.D
Acq On : 10 Jan 2016 11:38
Operator : SJ/UM
Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

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-BF123115.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	5.047	257	259	267	rVB	1469318	2409073	27.05%	2.873%
2	5.481	294	297	299	rBV	7016587	8878245	99.67%	10.589%
3	6.510	383	387	389	rBV	7335716	8442315	94.78%	10.069%
4	6.636	395	398	400	rBV	7007712	8907321	100.00%	10.623%
5	6.853	415	417	419	rBV	2302579	1858631	20.87%	2.217%
6	7.013	428	431	433	rBV	6970162	6301602	70.75%	7.516%
7	7.424	463	467	469	rBV	5130748	5547608	62.28%	6.616%
8	8.145	527	530	532	rBV	2410347	2494713	28.01%	2.975%
9	9.219	621	624	627	rBV	7815563	7917416	88.89%	9.443%
10	9.619	656	659	660	rBV	1176651	1348586	15.14%	1.608%
11	9.825	674	677	681	rBV2	127487	228185	2.56%	0.272%
12	9.893	681	683	686	rVB	2933613	2662282	29.89%	3.175%
13	10.328	720	721	723	rVB	364537	293153	3.29%	0.350%
14	10.545	737	740	744	rBV	110647	213996	2.40%	0.255%
15	10.682	749	752	755	rVV2	4341777	5851587	65.69%	6.979%
16	10.796	759	762	767	rVB	356514	638159	7.16%	0.761%
17	10.991	778	779	784	rBV2	43203	93220	1.05%	0.111%
18	11.253	799	802	803	rBV	257285	251911	2.83%	0.300%
19	11.379	811	813	815	rVV	3142914	2731627	30.67%	3.258%
20	11.436	815	818	822	rVB2	50932	109828	1.23%	0.131%
21	11.676	837	839	841	rBV	181345	141784	1.59%	0.169%
22	11.928	858	861	864	rBV4	73533	170652	1.92%	0.204%
23	12.088	872	875	877	rBV	191084	200025	2.25%	0.239%
24	12.476	907	909	913	rVB	64163	93674	1.05%	0.112%
25	12.796	934	937	938	rBV	260227	333572	3.74%	0.398%
26	12.854	940	942	949	rVB	594978	815774	9.16%	0.973%
27	12.968	949	952	955	rBV	7144402	7645758	85.84%	9.119%
28	13.276	977	979	983	rBV	132997	191637	2.15%	0.229%
29	13.494	992	998	1000	rBV2	310661	440355	4.94%	0.525%
30	13.871	1028	1031	1039	rBV	721239	997815	11.20%	1.190%
31	14.008	1041	1043	1046	rBV	1690761	2386952	26.80%	2.847%
32	14.191	1056	1059	1061	rBV	92864	109870	1.23%	0.131%
33	14.488	1084	1085	1090	rBV2	74553	126685	1.42%	0.151%
34	14.797	1109	1112	1114	rVB	60644	90401	1.01%	0.108%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084357.D
Acq On : 10 Jan 2016 11:38
Operator : SJ/UM
Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.865	1116	1118	1120	rBV	170882	160837	1.81%	0.192%
36	15.117	1137	1140	1142	rBV	93988	114068	1.28%	0.136%
37	15.437	1165	1168	1171	rBV	1072867	1542565	17.32%	1.840%
38	15.482	1171	1172	1176	rVB	91879	98892	1.11%	0.118%
39	15.894	1206	1208	1211	rBV	78849	123881	1.39%	0.148%
40	15.962	1211	1214	1223	rVB6	36947	136202	1.53%	0.162%
41	16.374	1247	1250	1255	rBV2	72605	159720	1.79%	0.190%
42	16.945	1296	1300	1304	rBV	59833	131075	1.47%	0.156%
43	17.403	1337	1340	1345	rBV6	30730	97294	1.09%	0.116%
44	17.608	1355	1358	1365	rVB	57282	144596	1.62%	0.172%
45	18.397	1424	1427	1433	rVB	37730	102937	1.16%	0.123%
46	19.346	1505	1510	1515	rBV2	35091	109371	1.23%	0.130%

Sum of corrected areas: 83845850

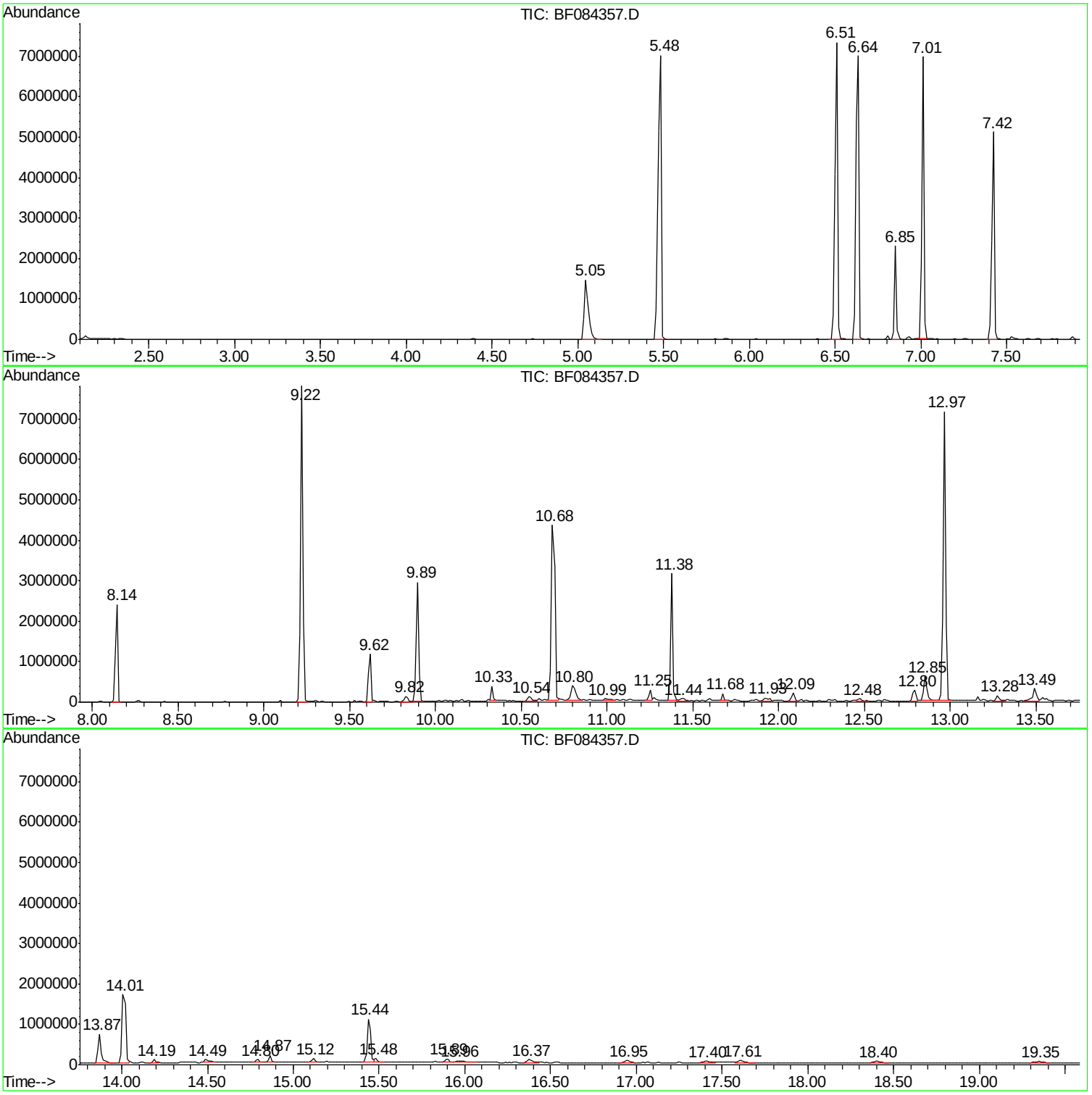
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084357.D
Acq On : 10 Jan 2016 11:38
Operator : SJ/UM
Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084357.D
Acq On : 10 Jan 2016 11:38
Operator : SJ/UM
Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

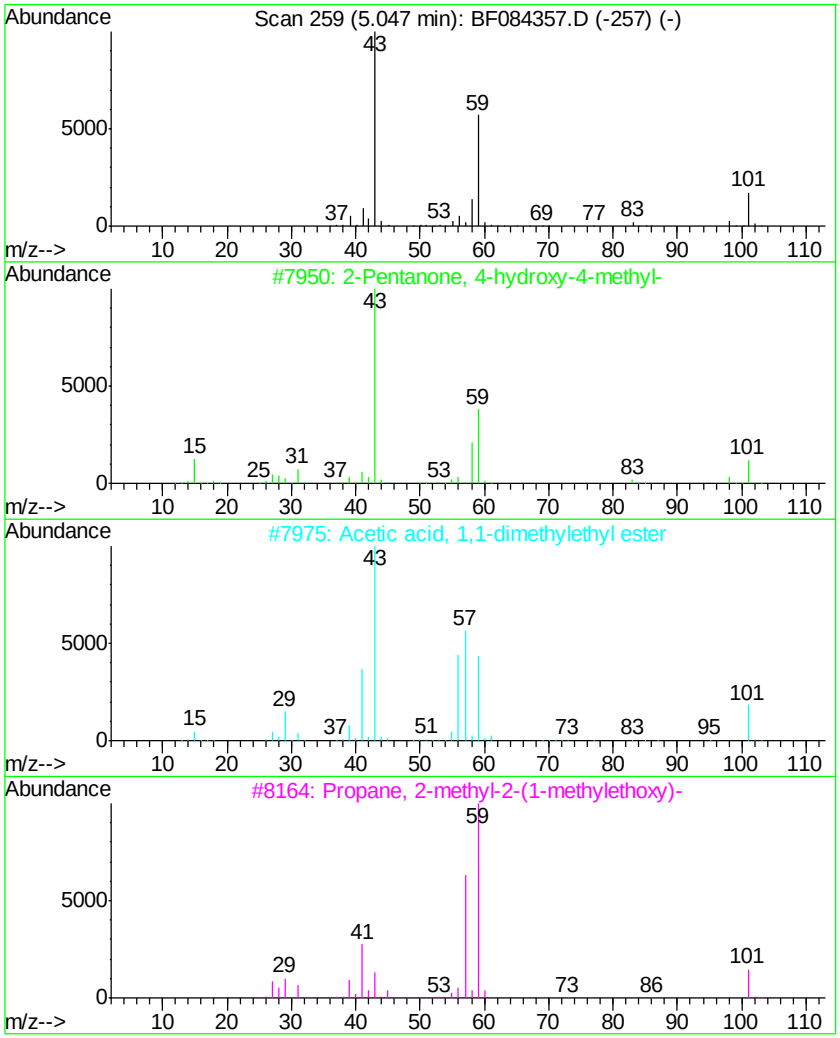
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

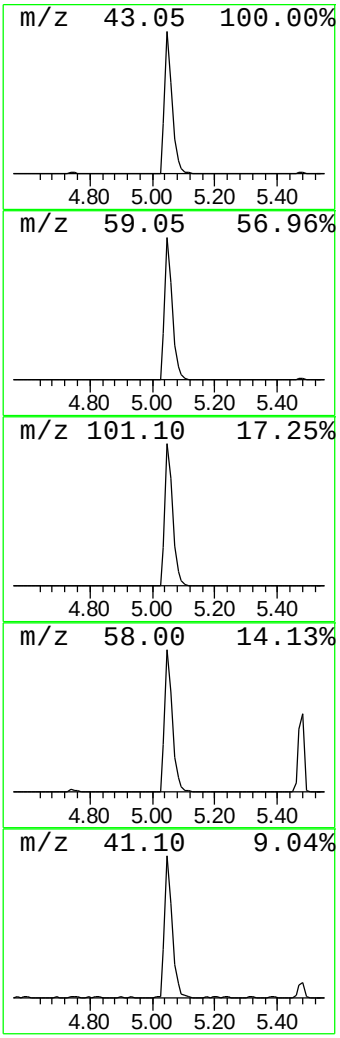
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	25.92 ng	2409070	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084357.D
Acq On : 10 Jan 2016 11:38
Operator : SJ/UM
Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

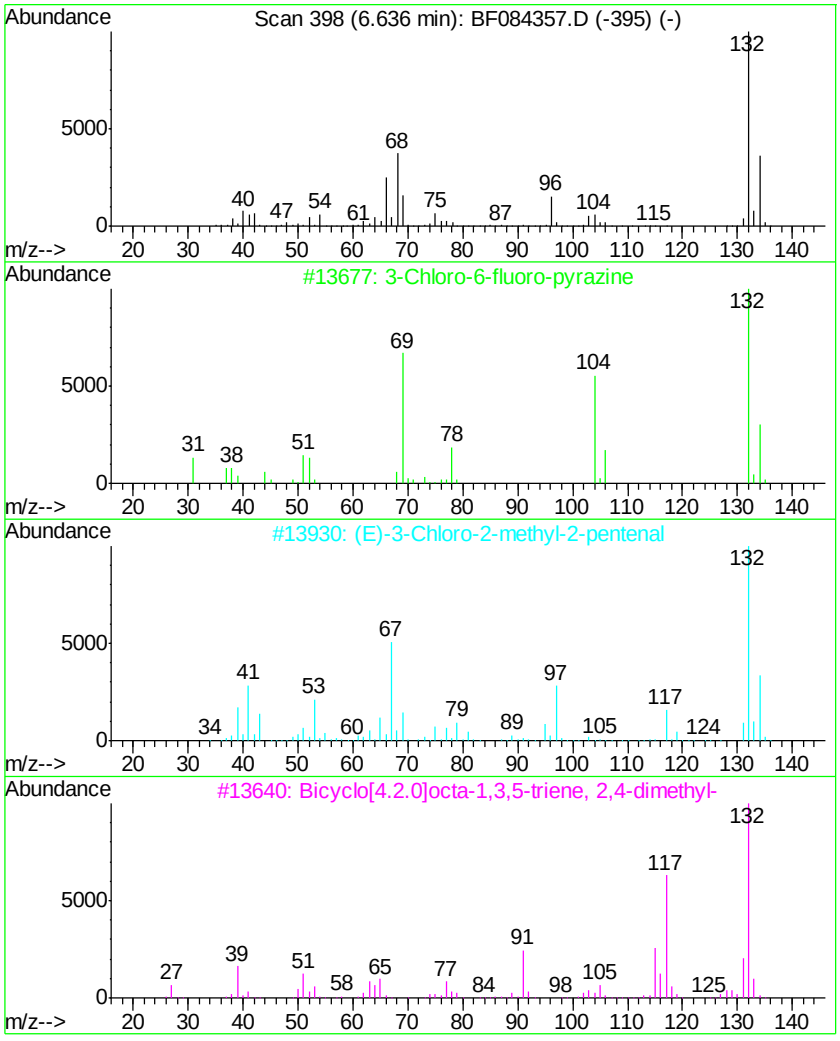
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

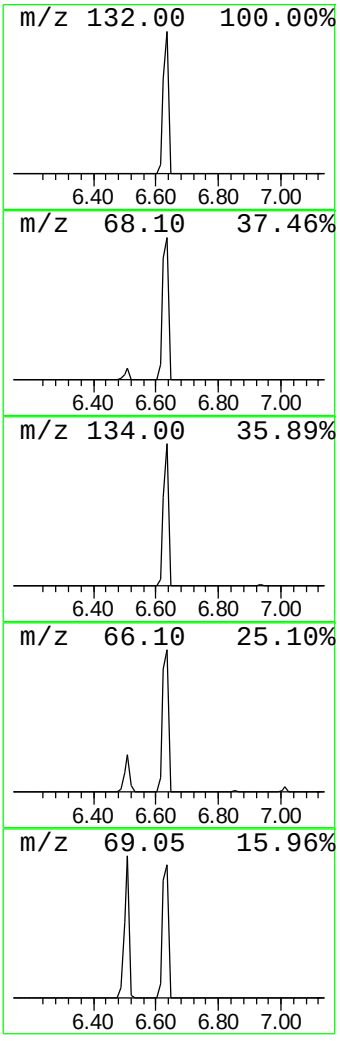
****

Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	95.85 ng	8907320	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	5-Aminoindole	132	C8H8N2	005192-03-0	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084357.D
Acq On : 10 Jan 2016 11:38
Operator : SJ/UM
Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

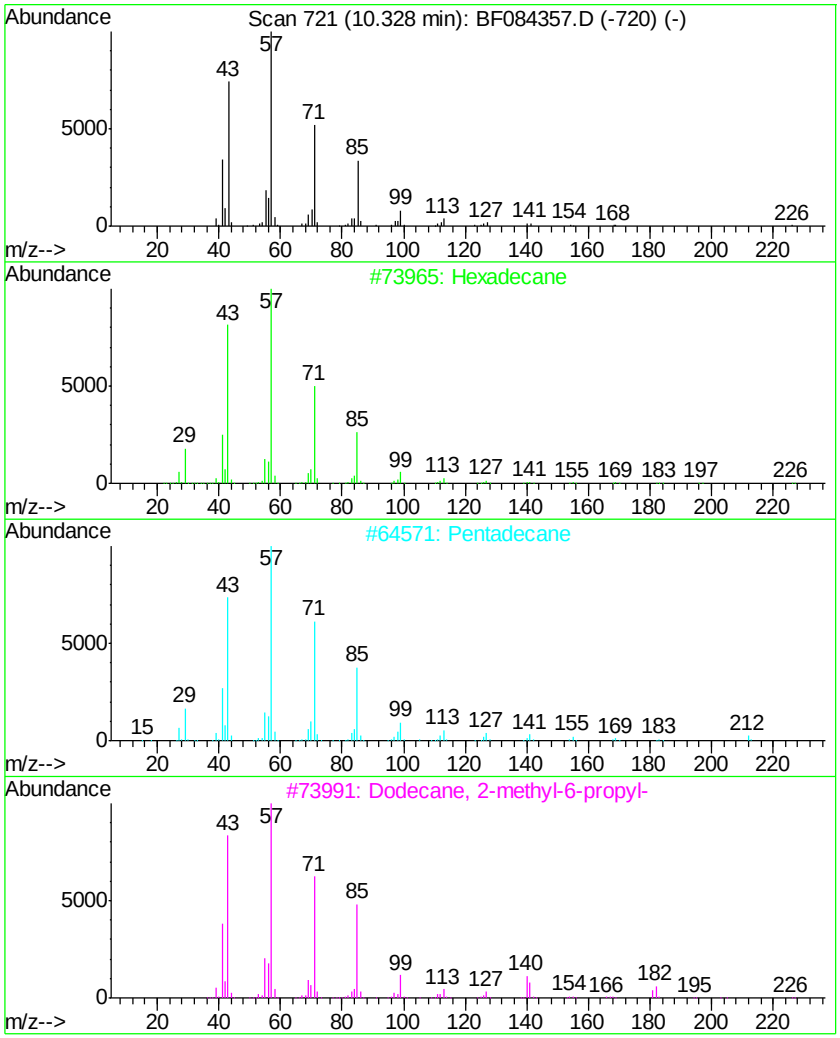
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

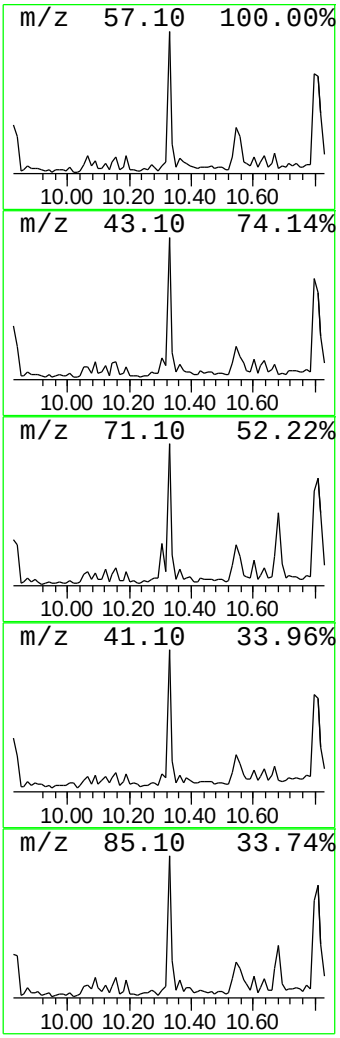
****

Peak Number 4 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.33	2.20 ng	293153	Acenaphthene-d10	9.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	91
2	Pentadecane	212	C15H32	000629-62-9	86
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	78
4	Bacchotricuneatin c	342	C20H22O5	066563-30-2	72
5	1-Iodoundecane	282	C11H23I	004282-44-4	64





Data Path : Z:\HPCHEM1\BNA F\DATA\BF011016\
Data File : BF084357.D
Acq On : 10 Jan 2016 11:38
Operator : SJ/UM
Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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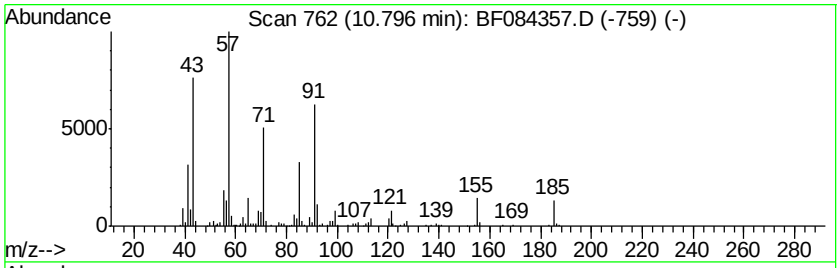
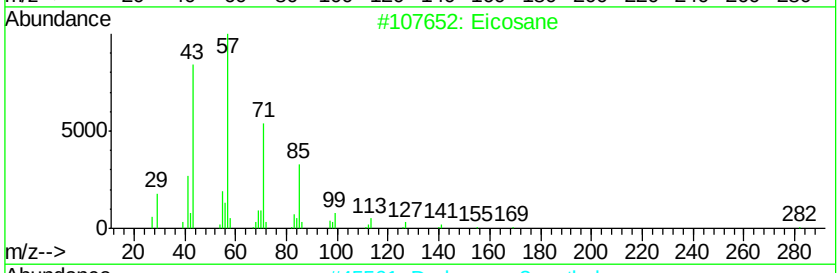
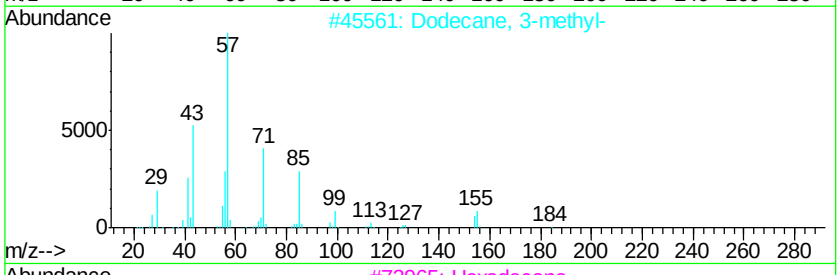
Peak Number 5 Eicosane Concentration Rank 6

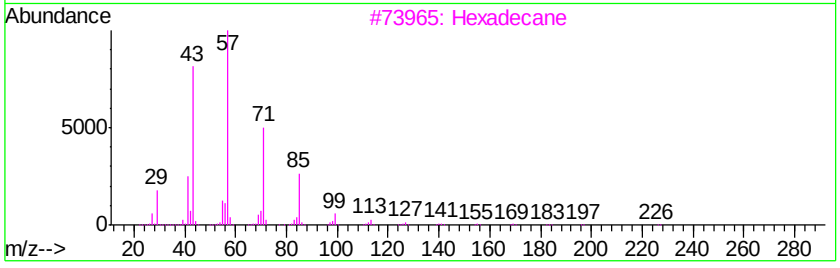
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	4.67 ng	638159	Phenanthrene-d10	11.38

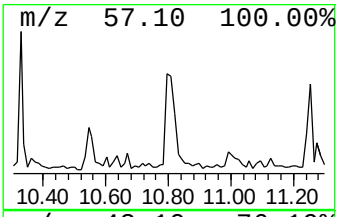
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	60
2	Dodecane, 3-methyl-	184	C13H28	017312-57-1	53
3	Hexadecane	226	C16H34	000544-76-3	53
4	Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	47
5	Pentadecane, 7-methyl-	226	C16H34	006165-40-8	47

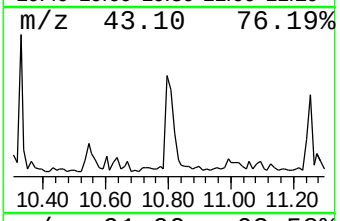


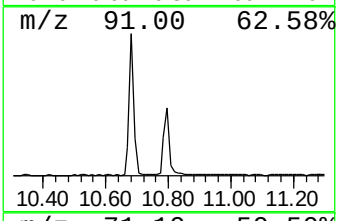


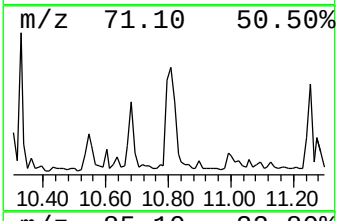


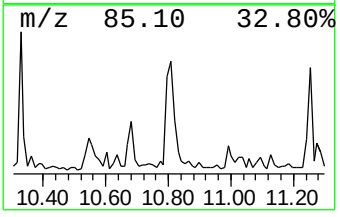












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Acq On : 10 Jan 2016 11:38
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Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

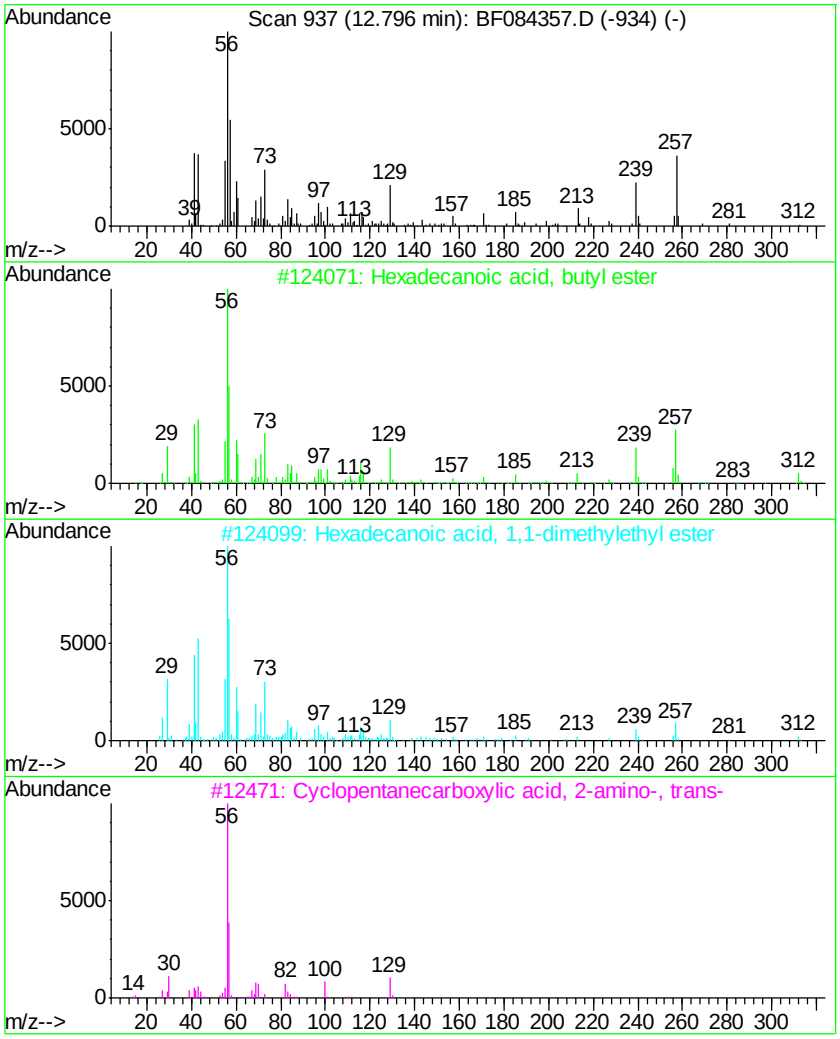
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

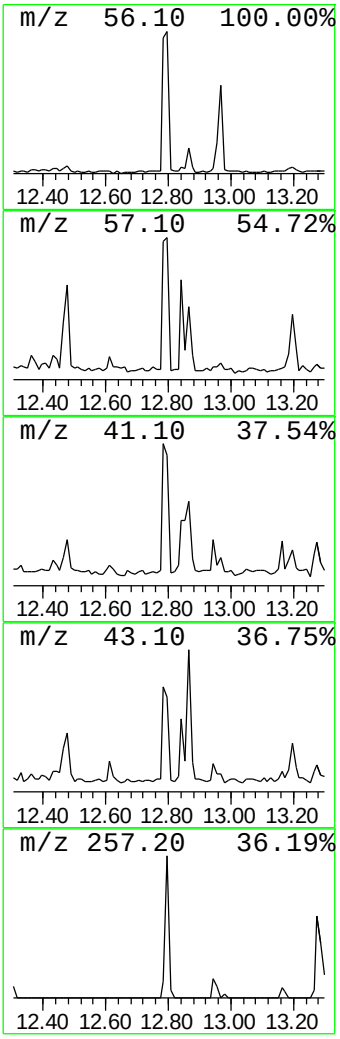
****

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	2.79 ng	333572	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	35
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	32
5	2,2-Dimethyl-1,3-butanediol	118	C6H14O2	000076-35-7	27





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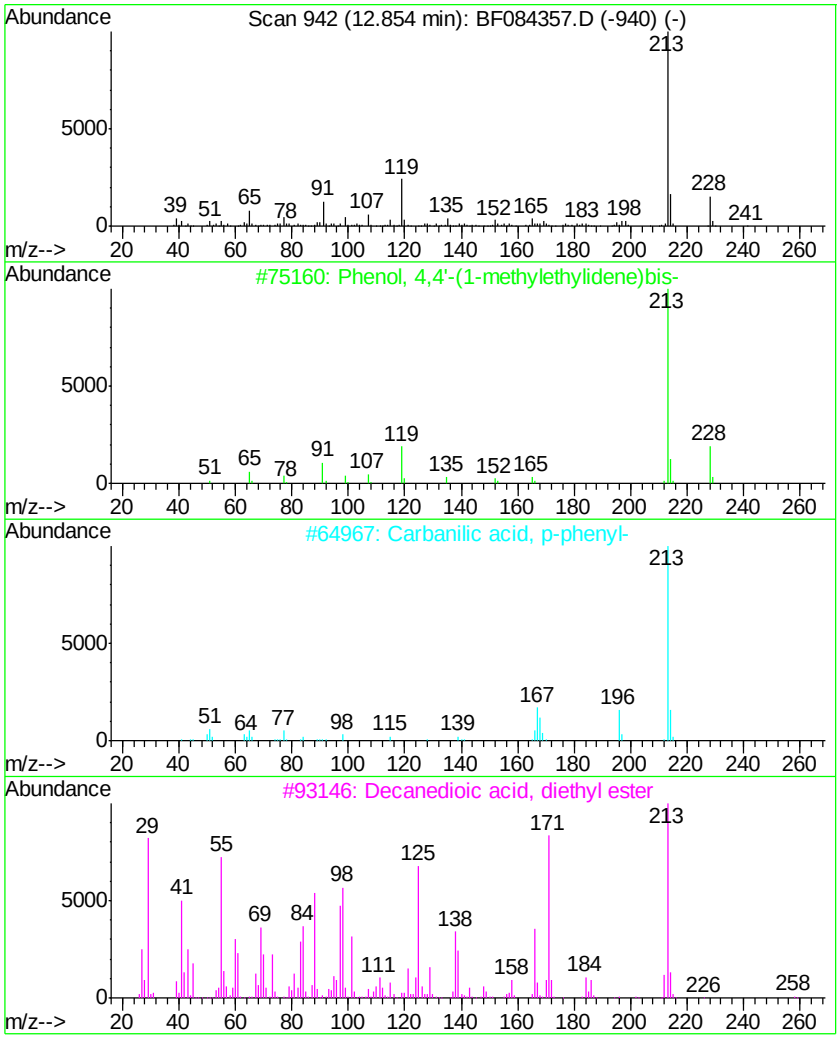
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

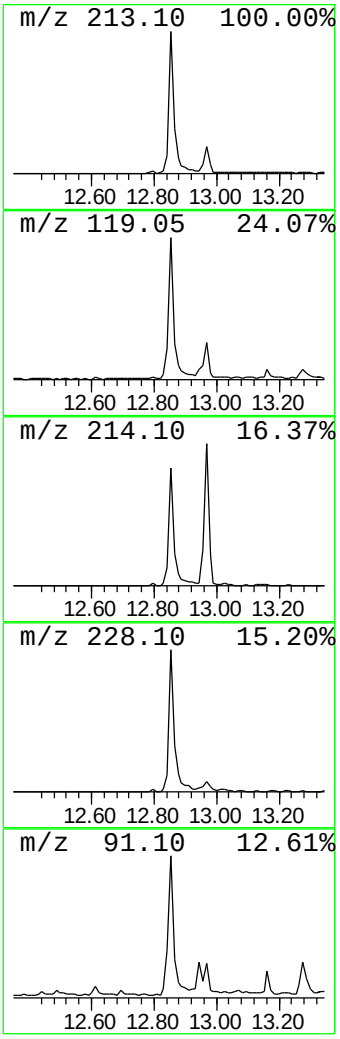
****

Peak Number 7 Phenol, 4,4'-(1-methylethyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	6.84 ng	815774	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	96
2	Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	50
3	Decanedioic acid, diethyl ester	258	C14H26O4	000110-40-7	50
4	Pyridine, 2-(5-trifluoromethyl-3...	213	C9H6F3N3	003974-71-8	42
5	N-Benzyl-p-anisidine	213	C14H15NO	017377-95-6	40





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Data File : BF084357.D
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Sample : H1043-04
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

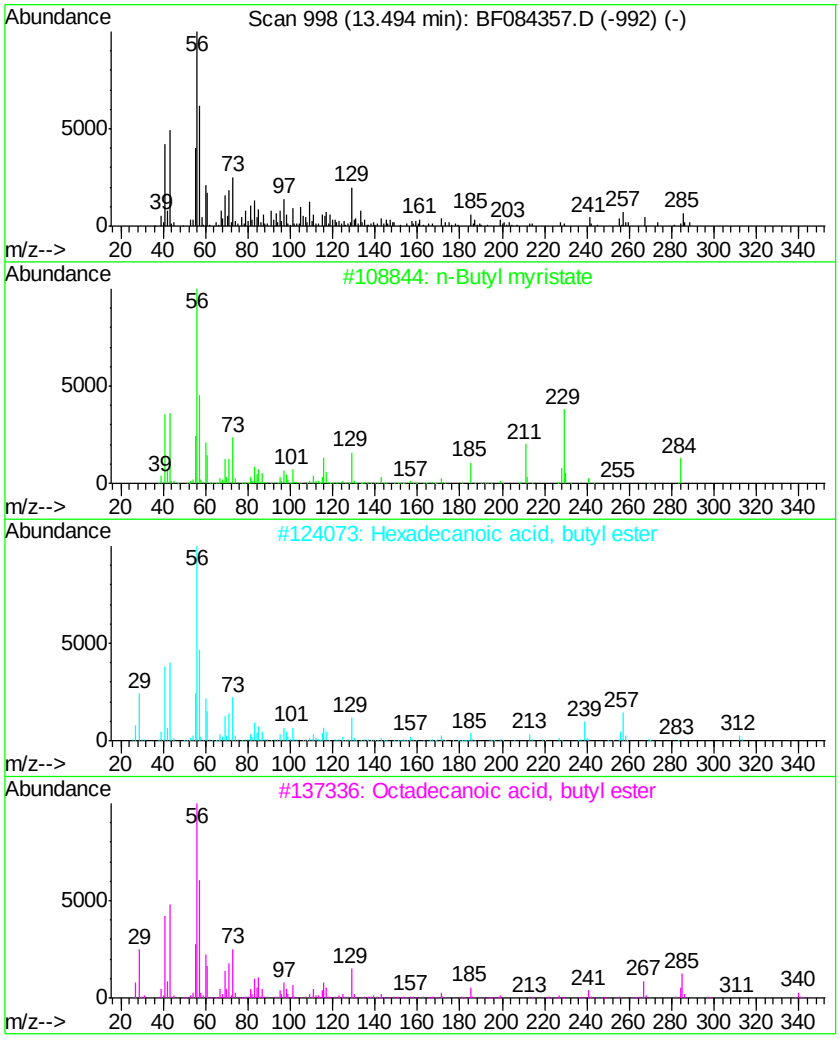
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

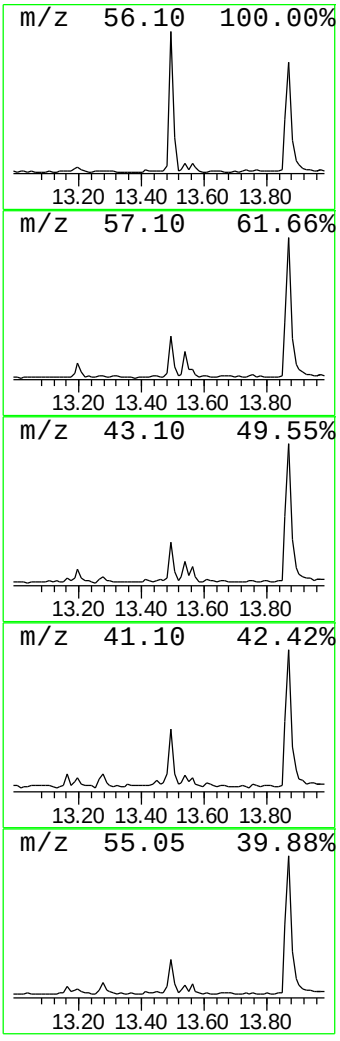
****

Peak Number 8 n-Butyl myristate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	3.69 ng	440355	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl myristate	284	C18H36O2	000110-36-1	86
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	83
3	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	72
4	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	64
5	Isobutyl laurate	256	C16H32O2	037811-72-6	58





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Data File : BF084357.D
Acq On : 10 Jan 2016 11:38
Operator : SJ/UM
Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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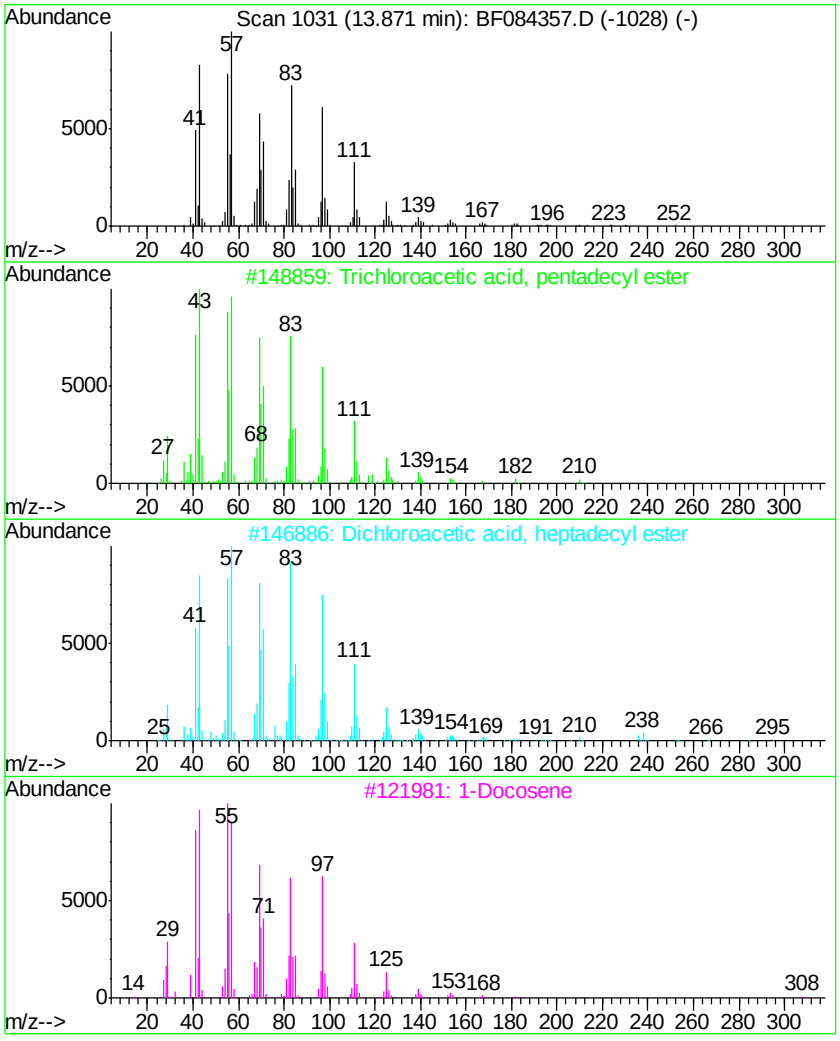
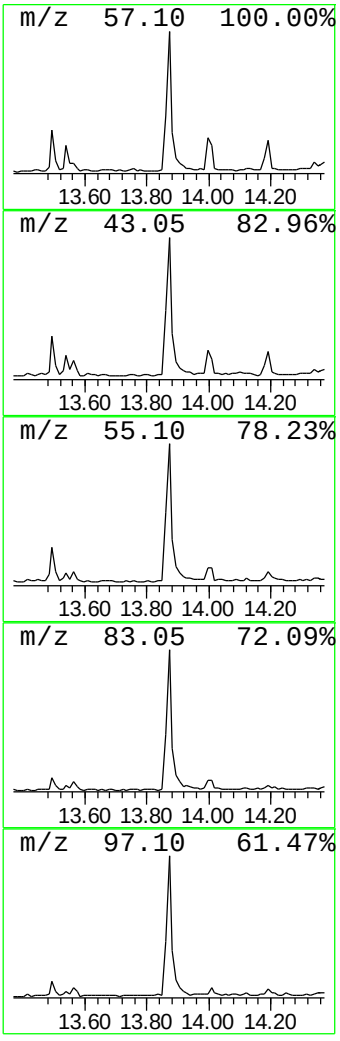
Peak Number 9 Trichloroacetic acid, penta... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	8.36 ng	997815	Chrysene-d12	14.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3	1-Docosene	308	C22H44	001599-67-3	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	91





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Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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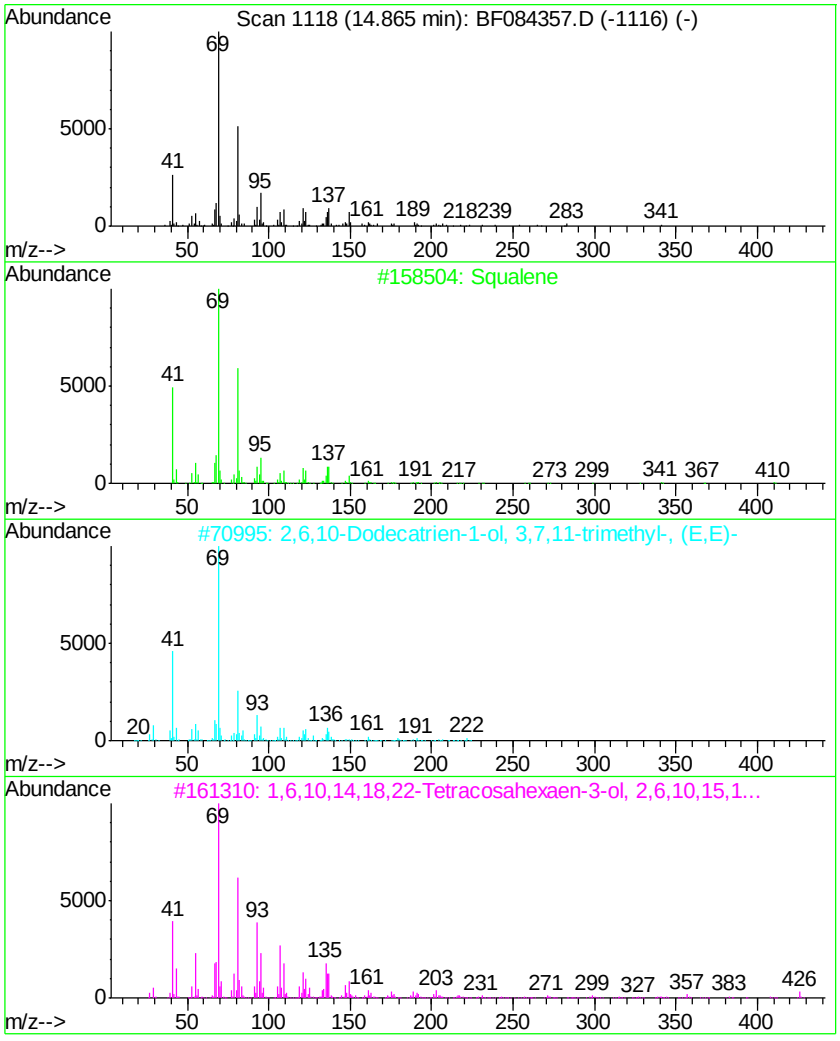
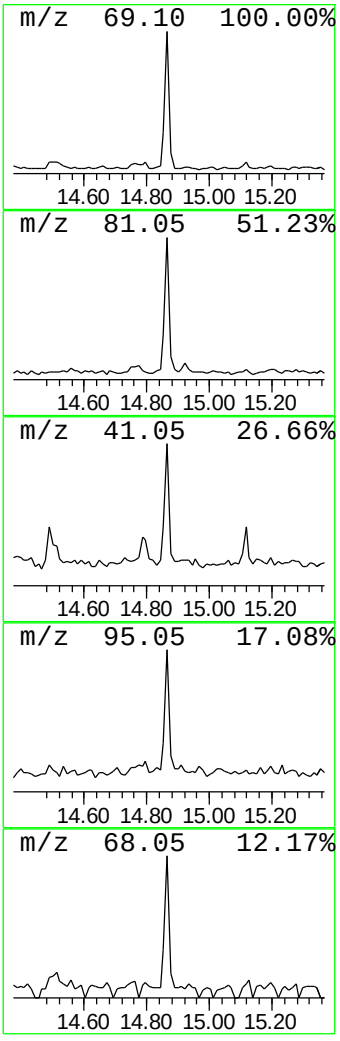
Peak Number 10 Squalene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	2.09 ng	160837	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	000106-28-5	80
3	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H50O	054159-46-5	72
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72
5	5,9,13-Pentadecatrien-2-one, 6,1...	262	C18H30O	001117-52-8	64





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Data File : BF084357.D
Acq On : 10 Jan 2016 11:38
Operator : SJ/UM
Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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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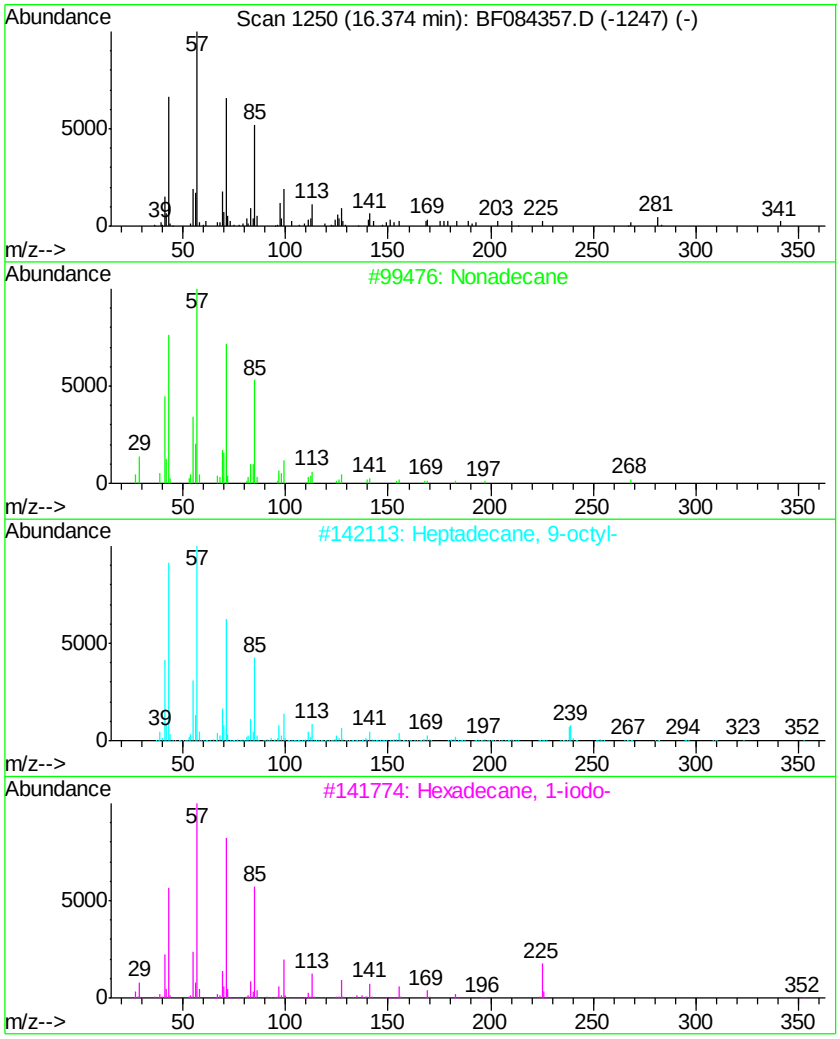
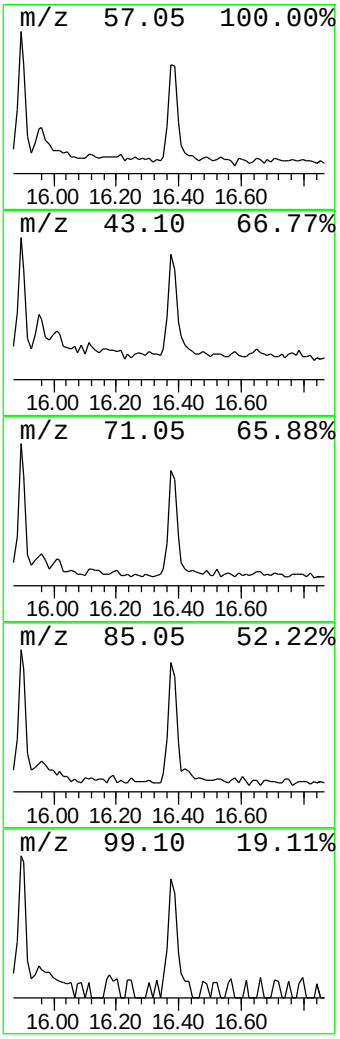
Peak Number 11 Nonadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.37	2.07 ng	159720	Perylene-d12	15.44

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	86
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
4	Docosane	310	C22H46	000629-97-0	86
5	2-Bromo dodecane	248	C12H25Br	013187-99-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011016\
Data File : BF084357.D
Acq On : 10 Jan 2016 11:38
Operator : SJ/UM
Sample : H1043-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2N(0-10)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	25.9	ng	2409070	1	6.85	1858630	20.0
unknown6.64	6.64	95.8	ng	8907320	1	6.85	1858630	20.0
Hexadecane	10.33	2.2	ng	293153	3	9.89	2662280	20.0
Eicosane	10.80	4.7	ng	638159	4	11.38	2731630	20.0
Hexadecanoic acid...	12.80	2.8	ng	333572	5	14.02	2386950	20.0
Phenol, 4,4'-(1-m...	12.85	6.8	ng	815774	5	14.02	2386950	20.0
n-Butyl myristate	13.49	3.7	ng	440355	5	14.02	2386950	20.0
Trichloroacetic a...	13.87	8.4	ng	997815	5	14.02	2386950	20.0
Squalene	14.87	2.1	ng	160837	6	15.44	1542570	20.0
Nonadecane	16.37	2.1	ng	159720	6	15.44	1542570	20.0