LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF093016\
Data File : BF090331.D
Acq On : 1 Oct 2016 00:00
Operator : UM/SJ
Sample : H4998-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B057-6-9

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-BF092016.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	1.633	3	4	55	rVB	2789713	7488258	100.00%	19.622%
2	4.536	256	258	267	rBV	292712	579525	7.74%	1.519%
3	5.039	299	302	304	rBV	2561401	3194914	42.67%	8.372%
4	6.102	393	395	396	rBV	121726	127289	1.70%	0.334%
5	6.136	396	398	401	rVV	2105026	3353697	44.79%	8.788%
6	6.239	404	407	409	rVB	2319005	3184214	42.52%	8.344%
7	6.456	424	426	429	rBV	829527	719873	9.61%	1.886%
8	6.616	437	440	442	rBV	2348128	2302504	30.75%	6.034%
9	7.027	473	476	479	rBV	1262870	1888349	25.22%	4.948%
10	7.748	536	539	541	rBV	1120175	955784	12.76%	2.505%
11	8.833	631	634	636	rBV	2781917	3169205	42.32%	8.305%
12	9.233	666	669	671	rBV	1610862	1441838	19.25%	3.778%
13	9.485	689	691	693	rBV	750808	988762	13.20%	2.591%
14	10.274	758	760	763	rBV2	1264987	1793332	23.95%	4.699%
15	10.422	771	773	777	rBV	77535	108529	1.45%	0.284%
16	10.959	817	820	822	rBV	1047561	907032	12.11%	2.377%
17	12.079	916	918	920	rVB	134450	107915	1.44%	0.283%
18	12.548	956	959	961	rBV	2052403	2205043	29.45%	5.778%
19	12.799	980	981	983	rVB	266148	254352	3.40%	0.667%
20	13.462	1036	1039	1042	rBV2	319547	511112	6.83%	1.339%
21	13.577	1046	1049	1051	rBV	708735	785327	10.49%	2.058%
22	13.782	1064	1067	1072	rBV	44374	87767	1.17%	0.230%
23	14.091	1091	1094	1097	rBV2	327134	398589	5.32%	1.044%
24	14.297	1110	1112	1115	rBV	52424	75842	1.01%	0.199%
25	14.674	1142	1145	1148	rBV	157690	266275	3.56%	0.698%
26	14.903	1162	1165	1168	rBV	400463	663083	8.85%	1.738%
27	15.337	1201	1203	1206	rVB	124682	173243	2.31%	0.454%
28	18.046	1436	1440	1447	rVB2	154958	430236	5.75%	1.127%

Sum of corrected areas: 38161889

LSC Report - Integrated Chromatogram

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Misc :
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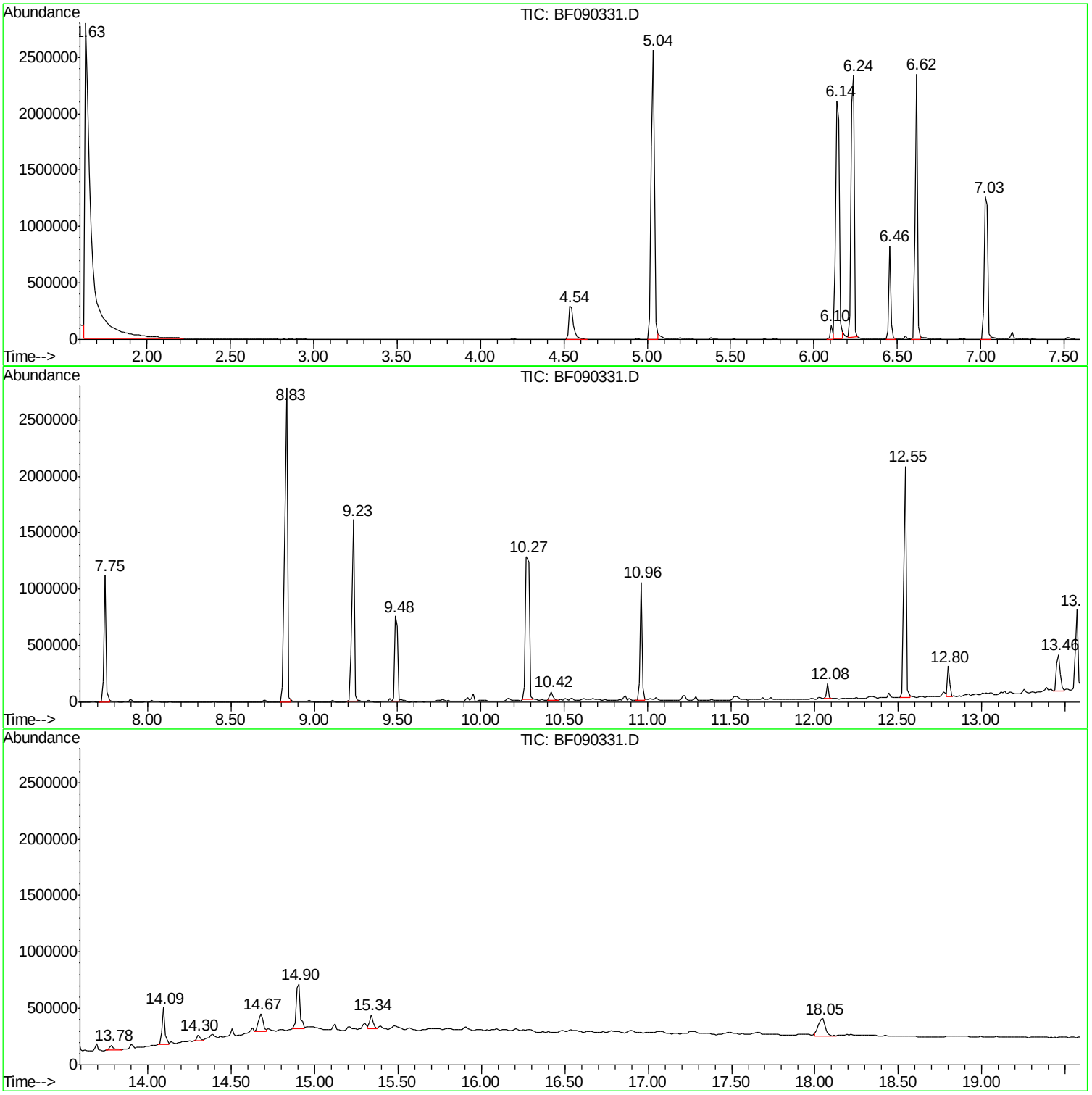
Instrument :
BNA_F
ClientSampleId :
SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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_F
ClientSampleId : SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
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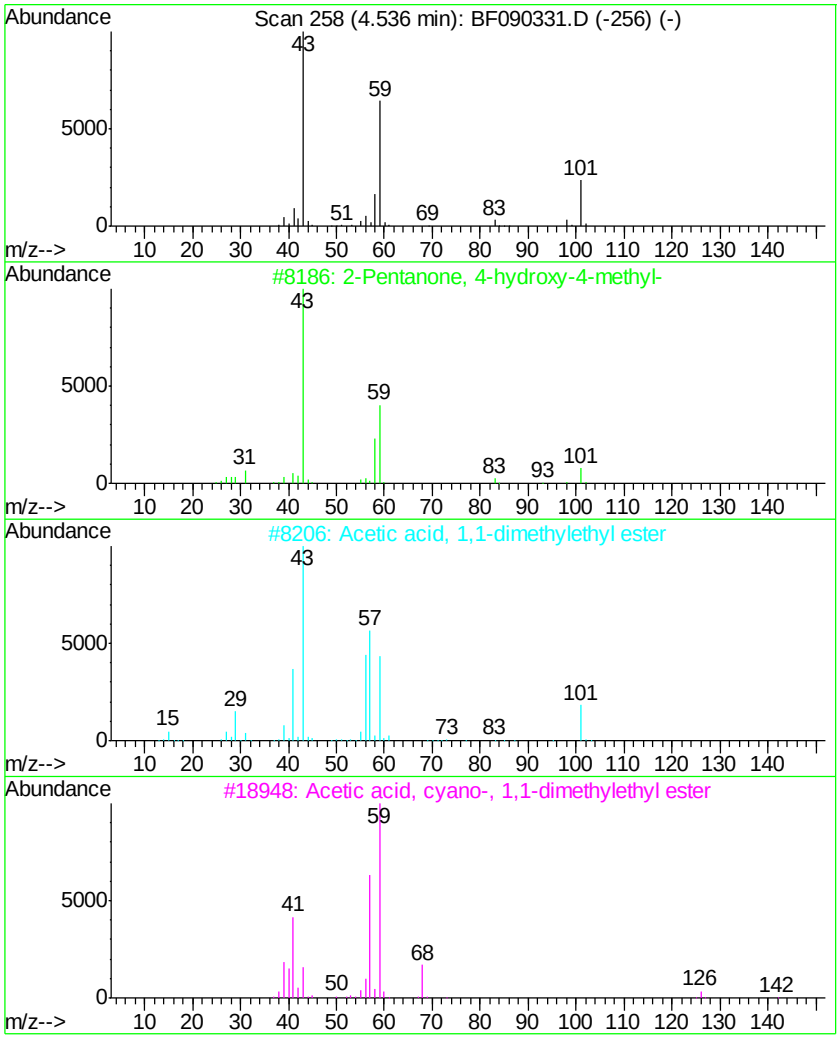
TIC Integration Parameters: LSCINT.P

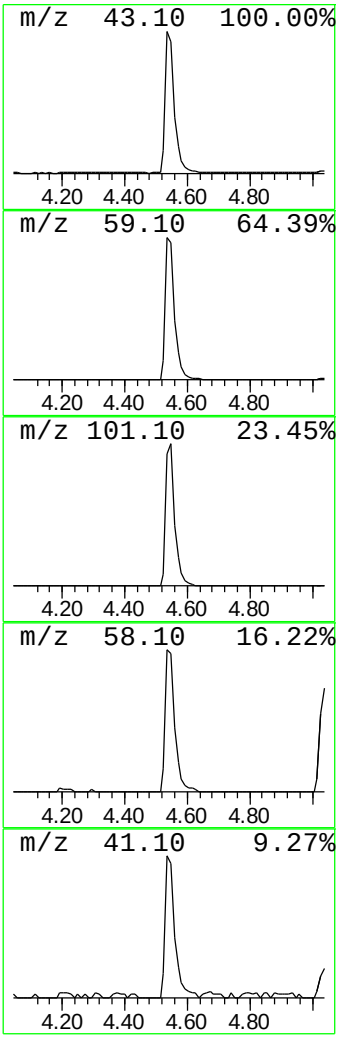
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	16.10 ng	579525	1,4-Dichlorobenzene-d4	6.46

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	25
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Instrument : BNA_F
ClientSampleId : SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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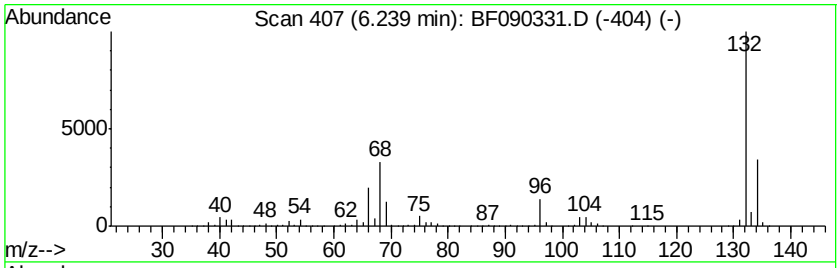
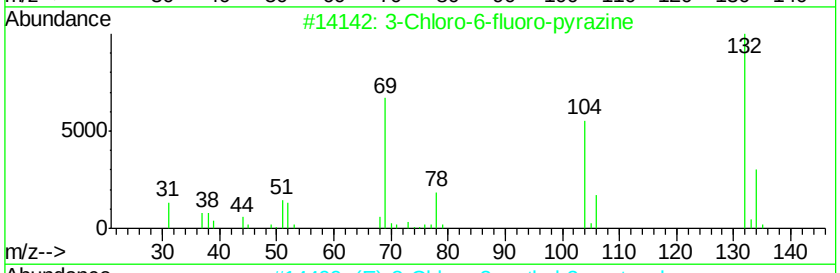
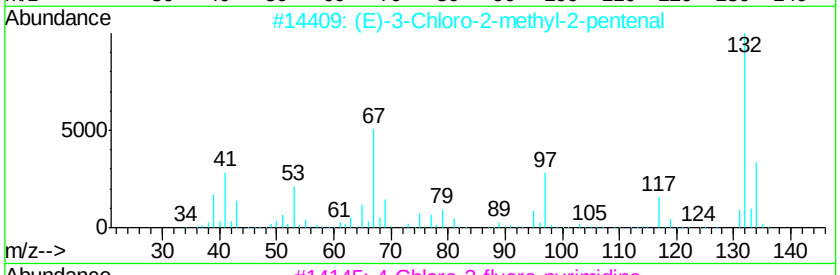
Peak Number 3 unknown6.24 Concentration Rank 2

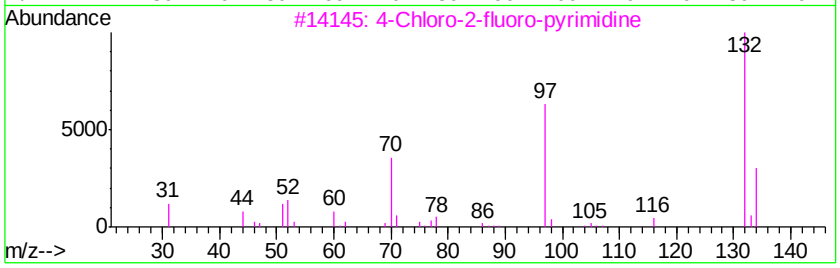
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.24	88.47 ng	3184210	1,4-Dichlorobenzene-d4	6.46

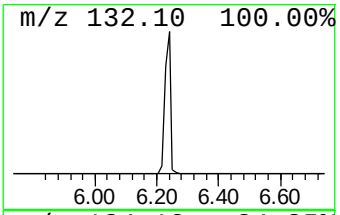
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	Xenon	132	Xe	007440-63-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9

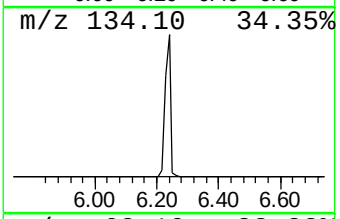


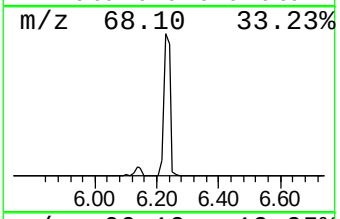


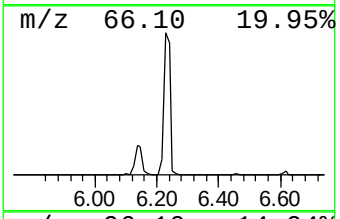


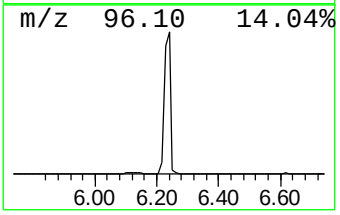












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Data File : BF090331.D
Acq On : 1 Oct 2016 00:00
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ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

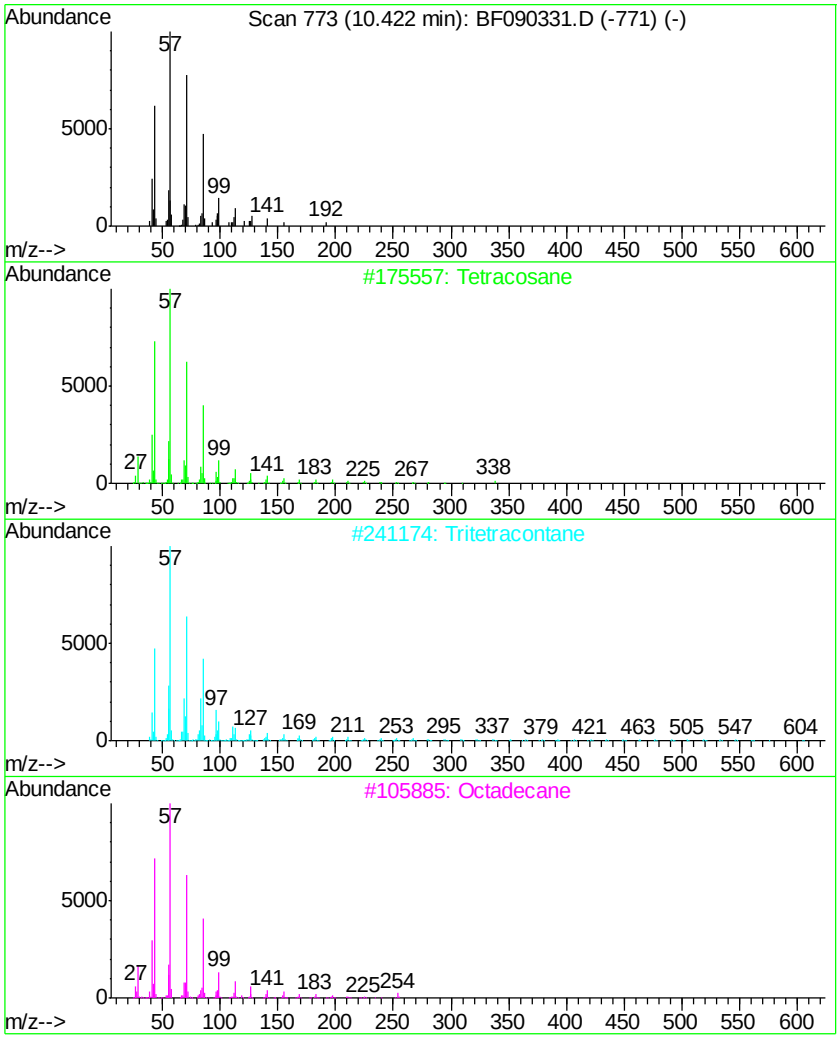
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

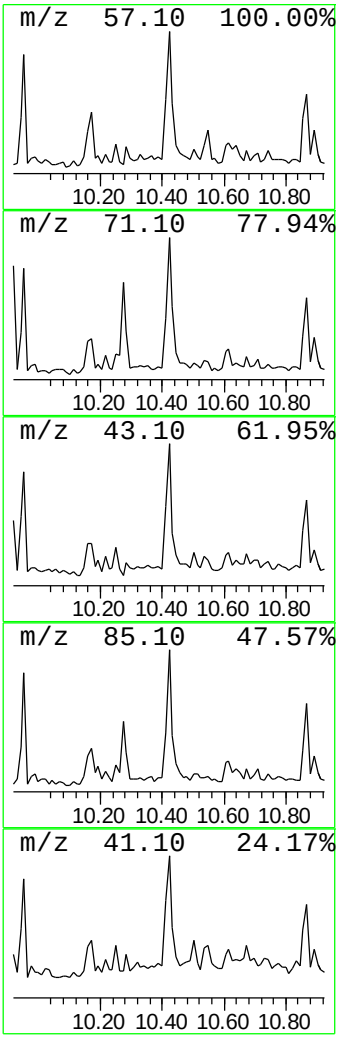
****

Peak Number 5 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.42	2.39 ng	108529	Phenanthrene-d10	10.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Tritetracontane	605	C43H88	007098-21-7	90
3	Octadecane	254	C18H38	000593-45-3	90
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
5	Hexadecane	226	C16H34	000544-76-3	90





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Instrument : BNA_F
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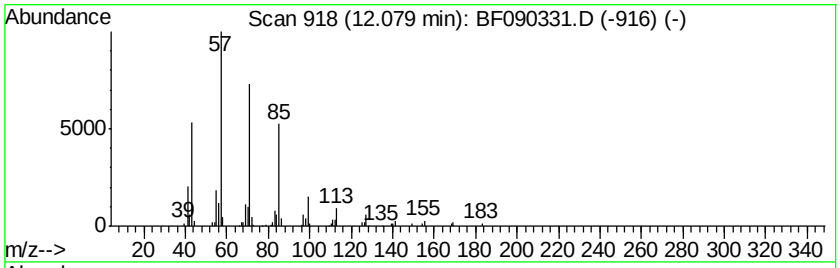
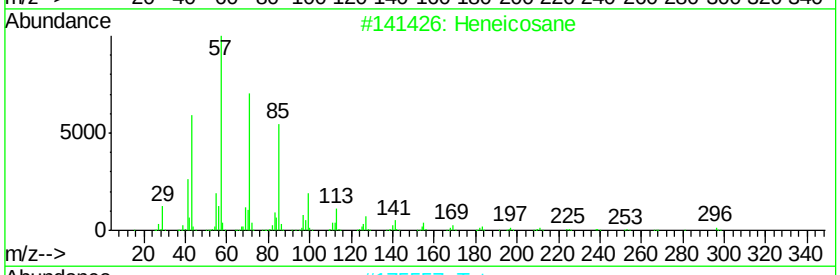
****

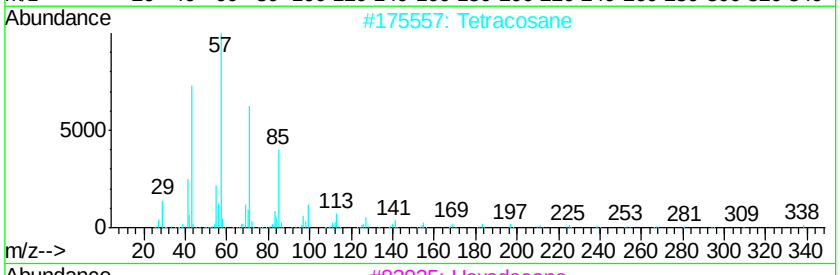
Peak Number 6 Heneicosane Concentration Rank 12

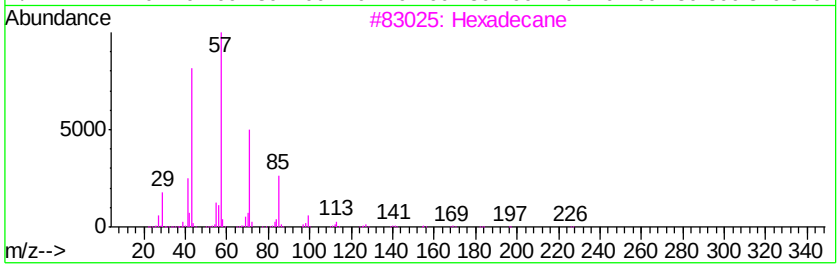
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	2.38 ng	107915	Phenanthrene-d10	10.96

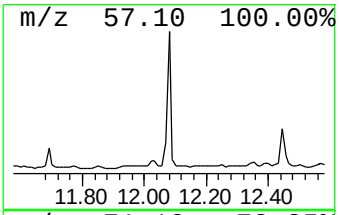
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Tetracosane	338	C24H50	000646-31-1	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	86
5	Pentadecane	212	C15H32	000629-62-9	86

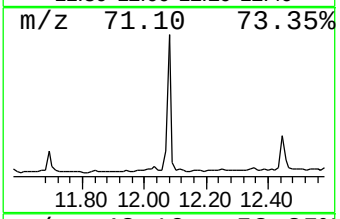


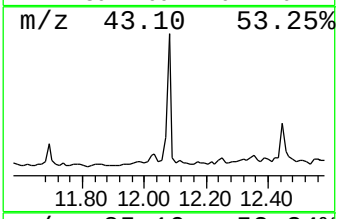


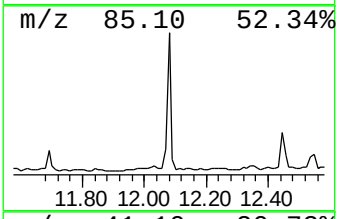


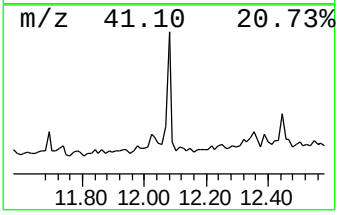












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TIC Library : C:\DATABASE\NIST11.L
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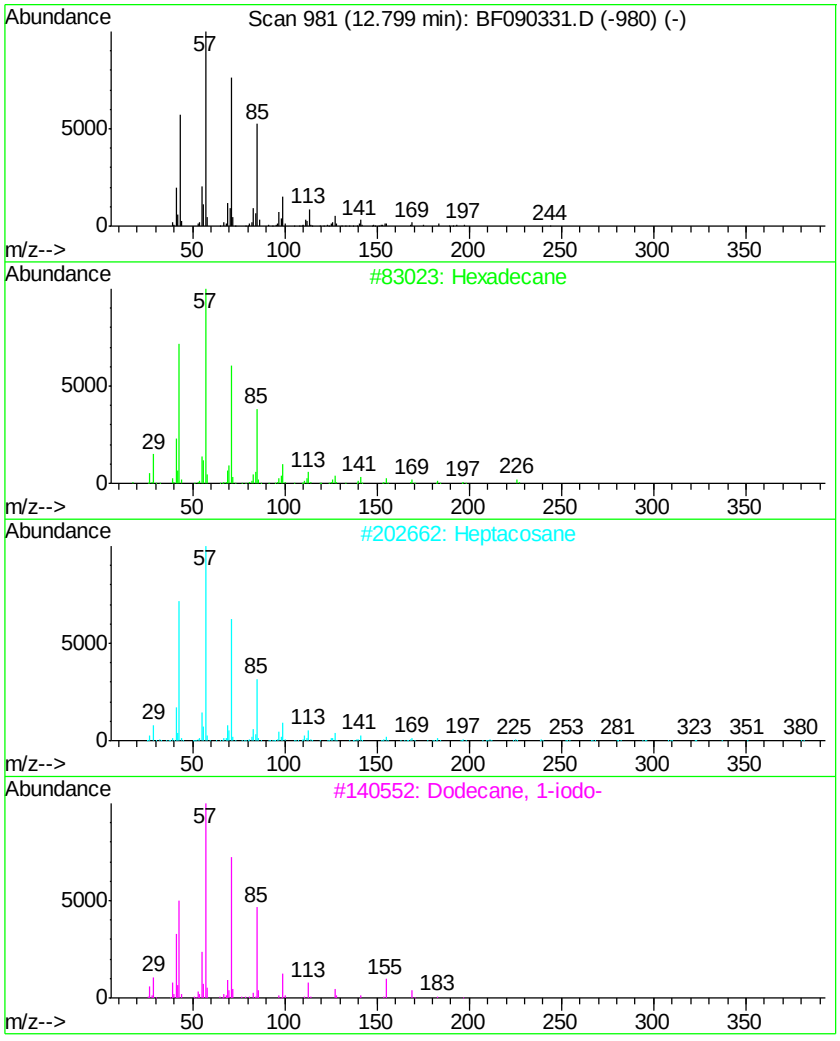
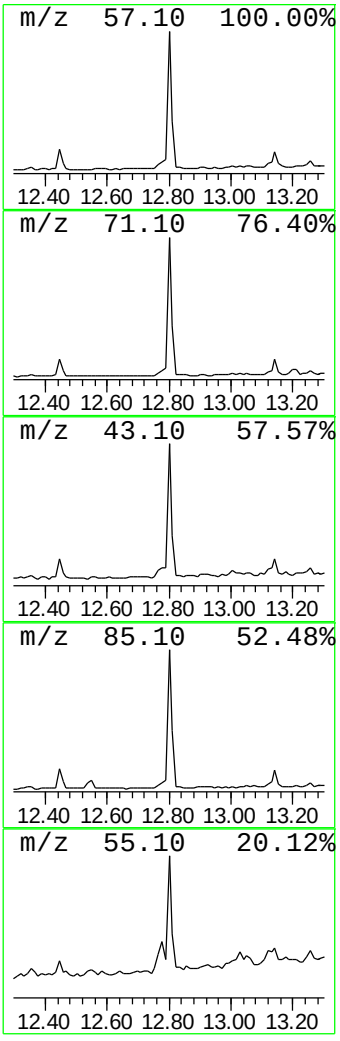
****

Peak Number 7 Hexadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	6.48 ng	254352	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Heptacosane	380	C27H56	000593-49-7	87
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	87
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	80
5	Undecane, 2,7-dimethyl-	184	C13H28	017301-24-5	72





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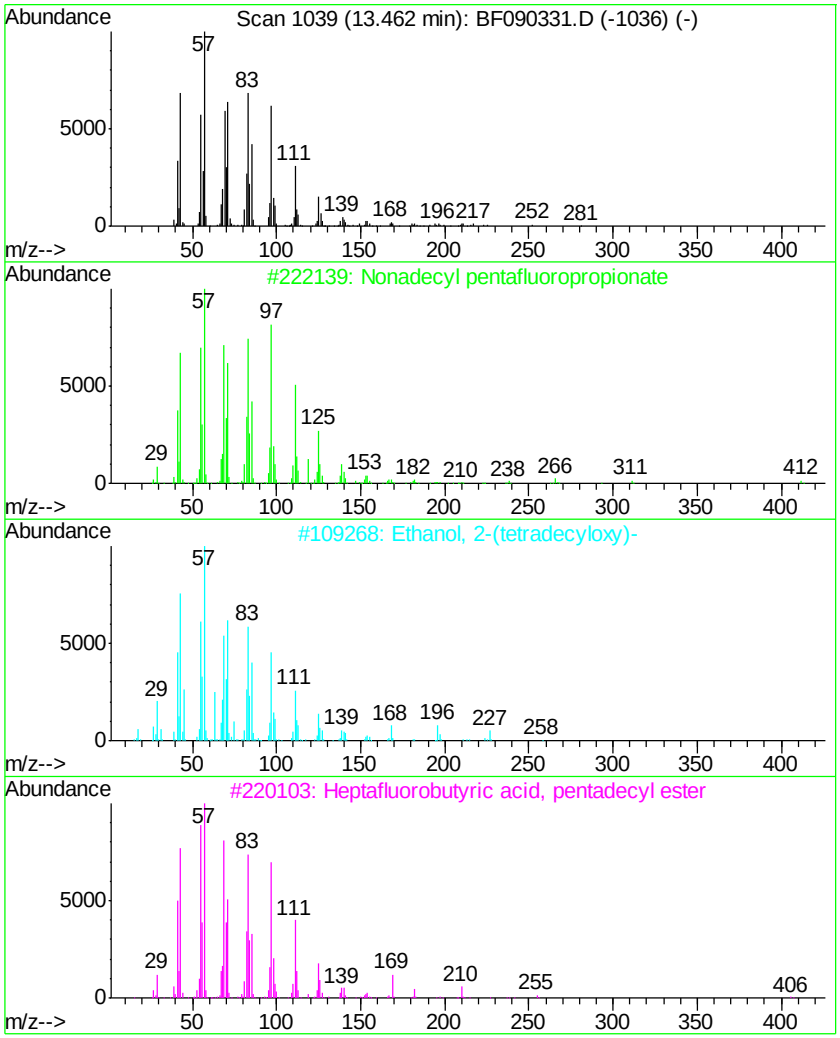
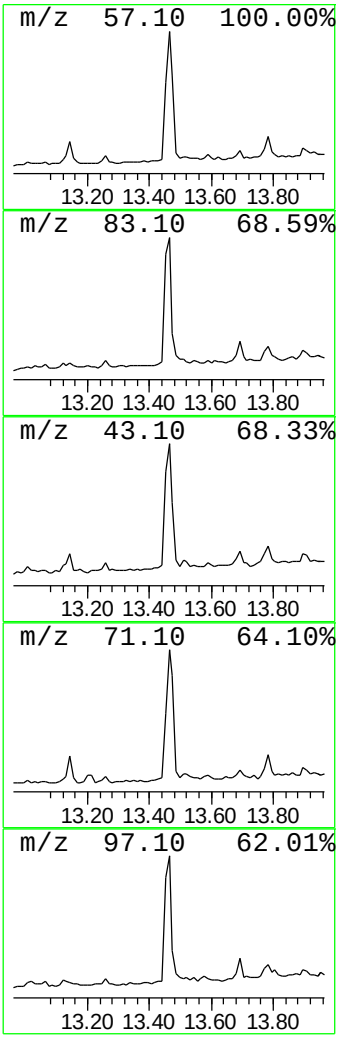
****

Peak Number 8 Nonadecyl pentafluoropropio... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	13.02 ng	511112	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	81
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	81
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81





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Acq On : 1 Oct 2016 00:00
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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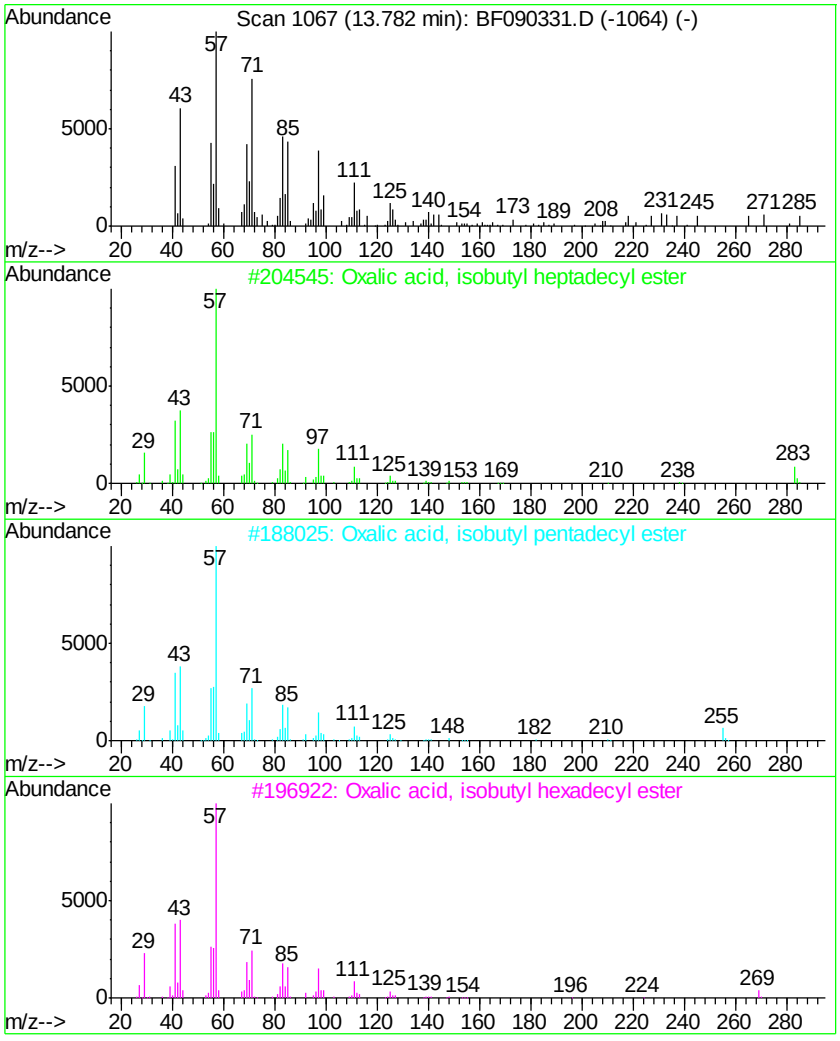
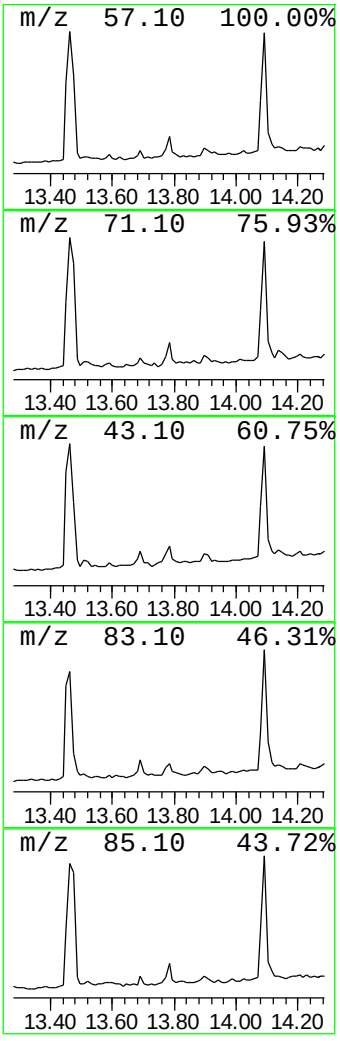
Peak Number 9 Oxalic acid, isobutyl hepta... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	2.24 ng	87767	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	87
2	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	87
3	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87
4	1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	87
5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	76





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Data File : BF090331.D
Acq On : 1 Oct 2016 00:00
Operator : UM/SJ
Sample : H4998-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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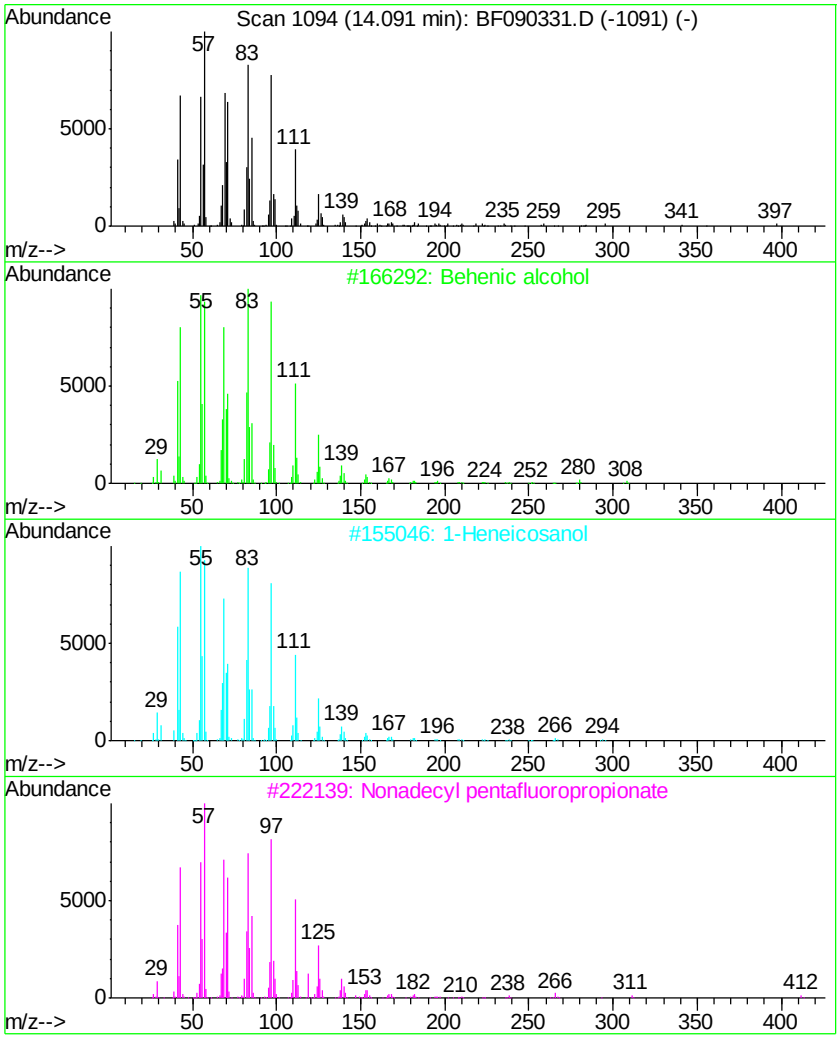
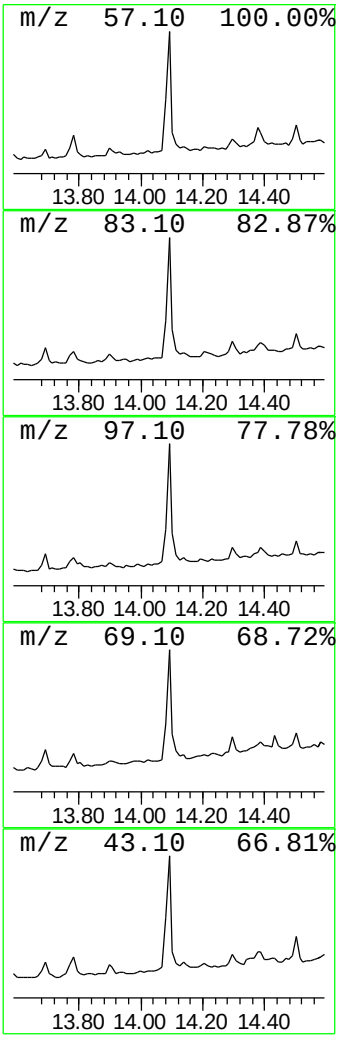
Peak Number 10 Behenic alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.09	10.15 ng	398589	Chrysene-d12	13.58

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	93
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87





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Acq On : 1 Oct 2016 00:00
Operator : UM/SJ
Sample : H4998-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
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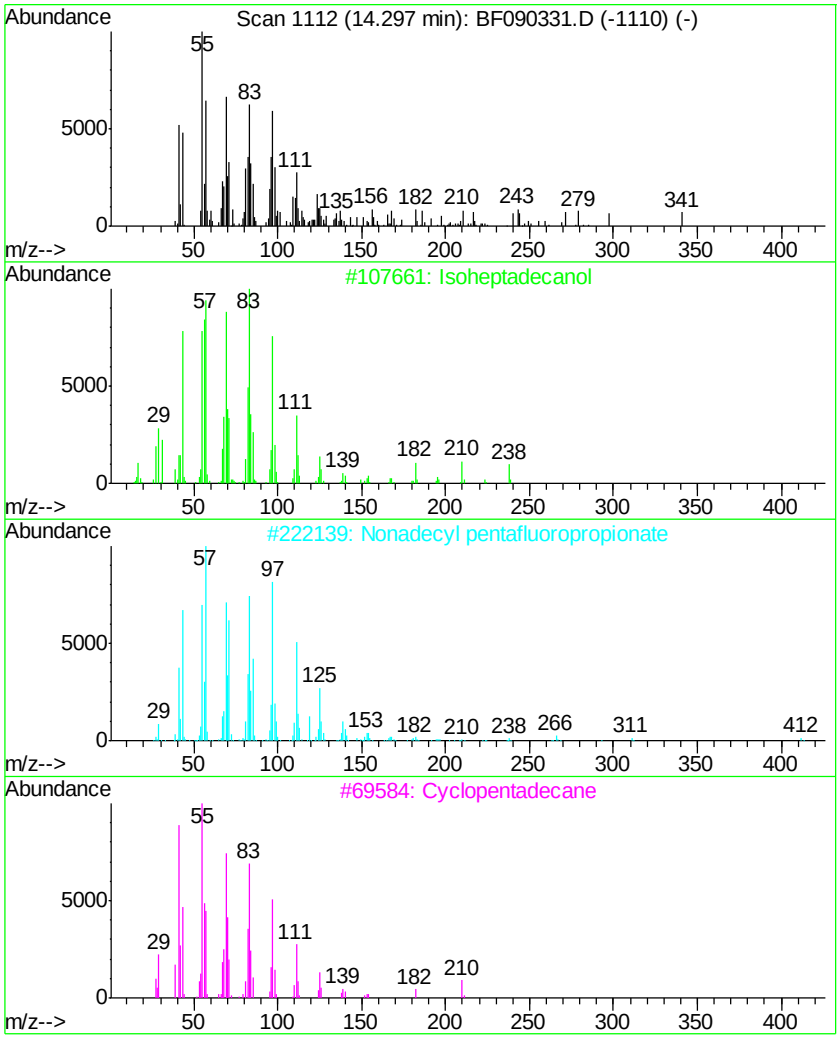
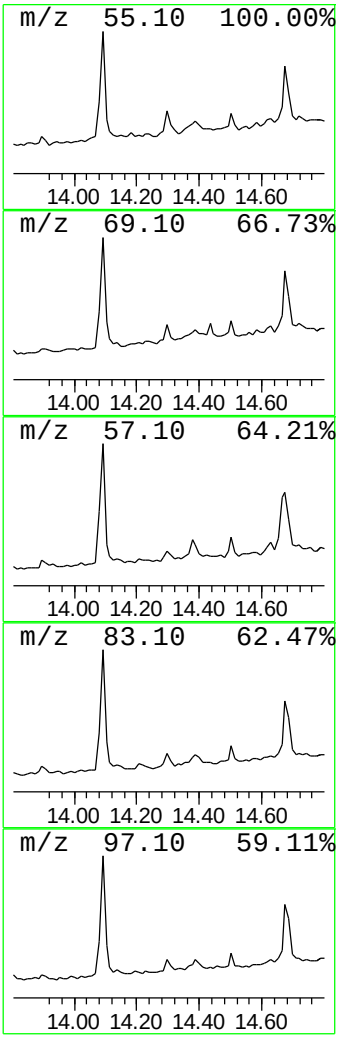
Peak Number 11 Isoheptadecanol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	2.29 ng	75842	Perylene-d12	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isoheptadecanol	256	C17H36O	057289-07-3	68
2	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	62
3	Cyclopentadecane	210	C15H30	000295-48-7	62
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	58
5	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	58





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Data File : BF090331.D
Acq On : 1 Oct 2016 00:00
Operator : UM/SJ
Sample : H4998-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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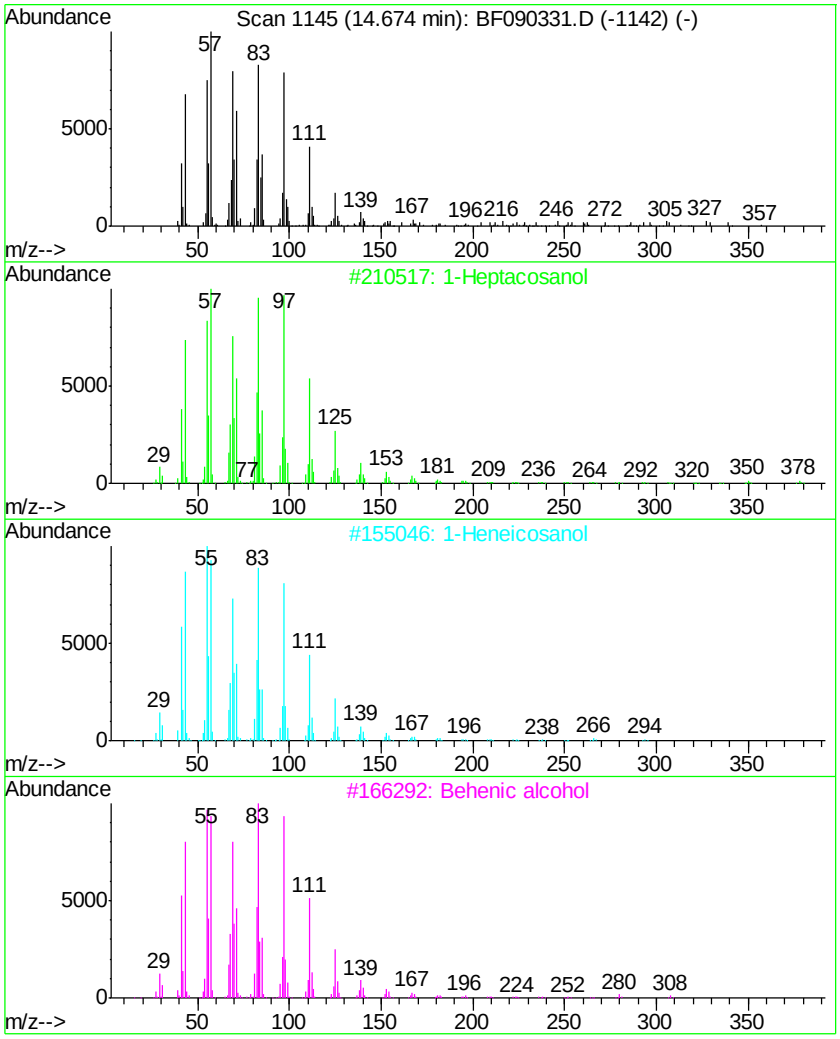
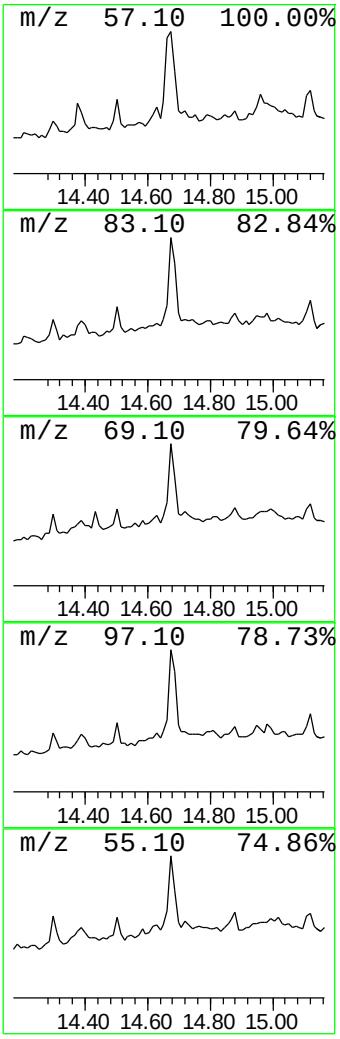
Peak Number 12 1-Heptacosanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.67	8.03 ng	266275	Perylene-d12	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91
5	1-Hexacosanol	382	C26H54O	000506-52-5	91





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Data File : BF090331.D
Acq On : 1 Oct 2016 00:00
Operator : UM/SJ
Sample : H4998-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.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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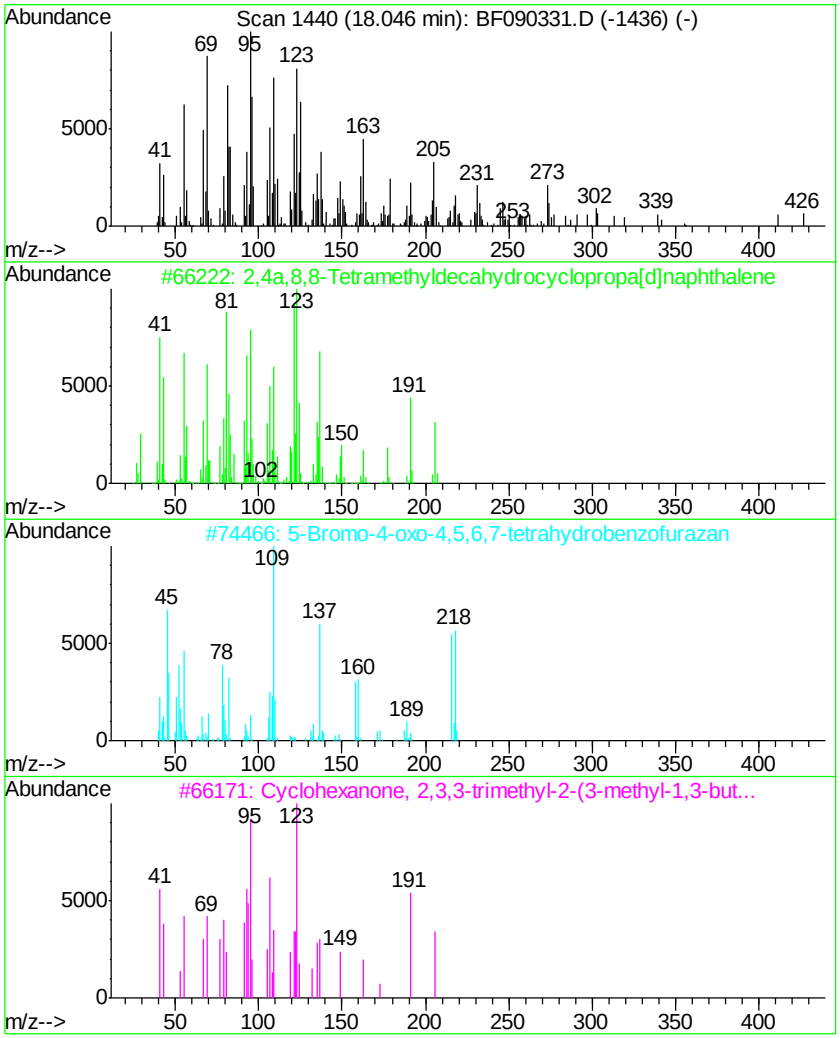
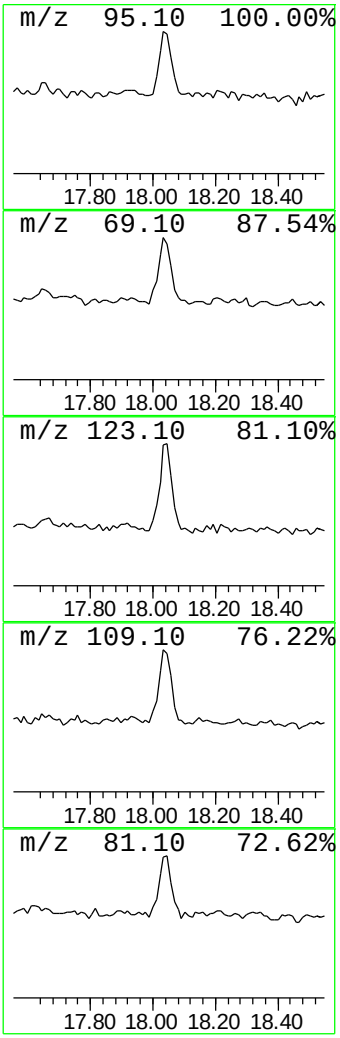
Peak Number 14 2,4a,8,8-Tetramethyldecahyd... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	12.98 ng	430236	Perylene-d12	14.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4a,8,8-Tetramethyldecahydrocyc...	206	C15H26	074022-04-1	64
2	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
3	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	42
4	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-41-8	38
5	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF093016\
Data File : BF090331.D
Acq On : 1 Oct 2016 00:00
Operator : UM/SJ
Sample : H4998-19
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SUP-B057-6-9

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092016.M
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
2-Pentanone, 4-hy...	4.54	16.1	ng	579525	1	6.46	719873	20.0
unknown6.24	6.24	88.5	ng	3184210	1	6.46	719873	20.0
Tetracosane	10.42	2.4	ng	108529	4	10.96	907032	20.0
Heneicosane	12.08	2.4	ng	107915	4	10.96	907032	20.0
Hexadecane	12.80	6.5	ng	254352	5	13.58	785327	20.0
Nonadecyl pentafl...	13.46	13.0	ng	511112	5	13.58	785327	20.0
Oxalic acid, isob...	13.78	2.2	ng	87767	5	13.58	785327	20.0
Behenic alcohol	14.09	10.2	ng	398589	5	13.58	785327	20.0
Isoheptadecanol	14.30	2.3	ng	75842	6	14.90	663083	20.0
1-Heptacosanol	14.67	8.0	ng	266275	6	14.90	663083	20.0
2,4a,8,8-Tetramet...	18.05	13.0	ng	430236	6	14.90	663083	20.0