LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 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-BF121417.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	5.028	496	500	523	rBV	546852	769932	24.75%	2.568%
2	5.434	565	569	592	rBV	2739651	3025318	97.23%	10.092%
3	6.451	738	742	760	rBV	2637054	3111414	100.00%	10.379%
4	6.581	760	764	768	rBV	2913282	2831864	91.02%	9.447%
5	6.810	799	803	811	rBV	966908	870201	27.97%	2.903%
6	6.963	825	829	846	rBV	2440817	2346663	75.42%	7.828%
7	7.375	895	899	911	rBV	1602317	1801307	57.89%	6.009%
8	8.092	1017	1021	1039	rVB	1080724	1101931	35.42%	3.676%
9	9.163	1199	1203	1212	rBV	3041098	2951714	94.87%	9.847%
10	9.563	1265	1271	1277	rBV	135508	141753	4.56%	0.473%
11	9.763	1300	1305	1309	rBV	59952	54968	1.77%	0.183%
12	9.845	1316	1319	1331	rVB	1046147	1043762	33.55%	3.482%
13	10.263	1388	1390	1394	rVB	79408	56355	1.81%	0.188%
14	10.645	1451	1455	1464	rBV	1253548	1379463	44.34%	4.602%
15	10.739	1468	1471	1475	rVB	53294	59349	1.91%	0.198%
16	11.339	1569	1573	1582	rBV	925174	911943	29.31%	3.042%
17	11.857	1657	1661	1669	rBV3	67164	100986	3.25%	0.337%
18	12.557	1777	1780	1784	rBV	104445	99236	3.19%	0.331%
19	12.639	1792	1794	1802	rBV5	28182	48966	1.57%	0.163%
20	12.786	1814	1819	1825	rVB	83159	111589	3.59%	0.372%
21	12.921	1838	1842	1846	rBV	2152074	1915895	61.58%	6.391%
22	13.121	1873	1876	1881	rVB4	41872	69376	2.23%	0.231%
23	13.474	1933	1936	1938	rBV2	42174	43590	1.40%	0.145%
24	13.804	1989	1992	2006	rBV	380034	471626	15.16%	1.573%
25	13.992	2019	2024	2027	rBV	789256	864131	27.77%	2.883%
26	14.439	2095	2100	2106	rBV2	220177	403268	12.96%	1.345%
27	14.874	2171	2174	2182	rVB	176970	178133	5.73%	0.594%
28	15.062	2202	2206	2209	rVV	647870	721842	23.20%	2.408%
29	15.092	2209	2211	2217	rVB	116525	155875	5.01%	0.520%
30	15.462	2270	2274	2282	rVB	563727	745133	23.95%	2.486%
31	15.633	2299	2303	2310	rVB	252580	343220	11.03%	1.145%
32	15.856	2336	2341	2346	rVB	465386	653777	21.01%	2.181%
33	15.915	2348	2351	2357	rVB2	77917	140570	4.52%	0.469%
34	16.639	2469	2474	2484	rVB	241785	451771	14.52%	1.507%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 29976921

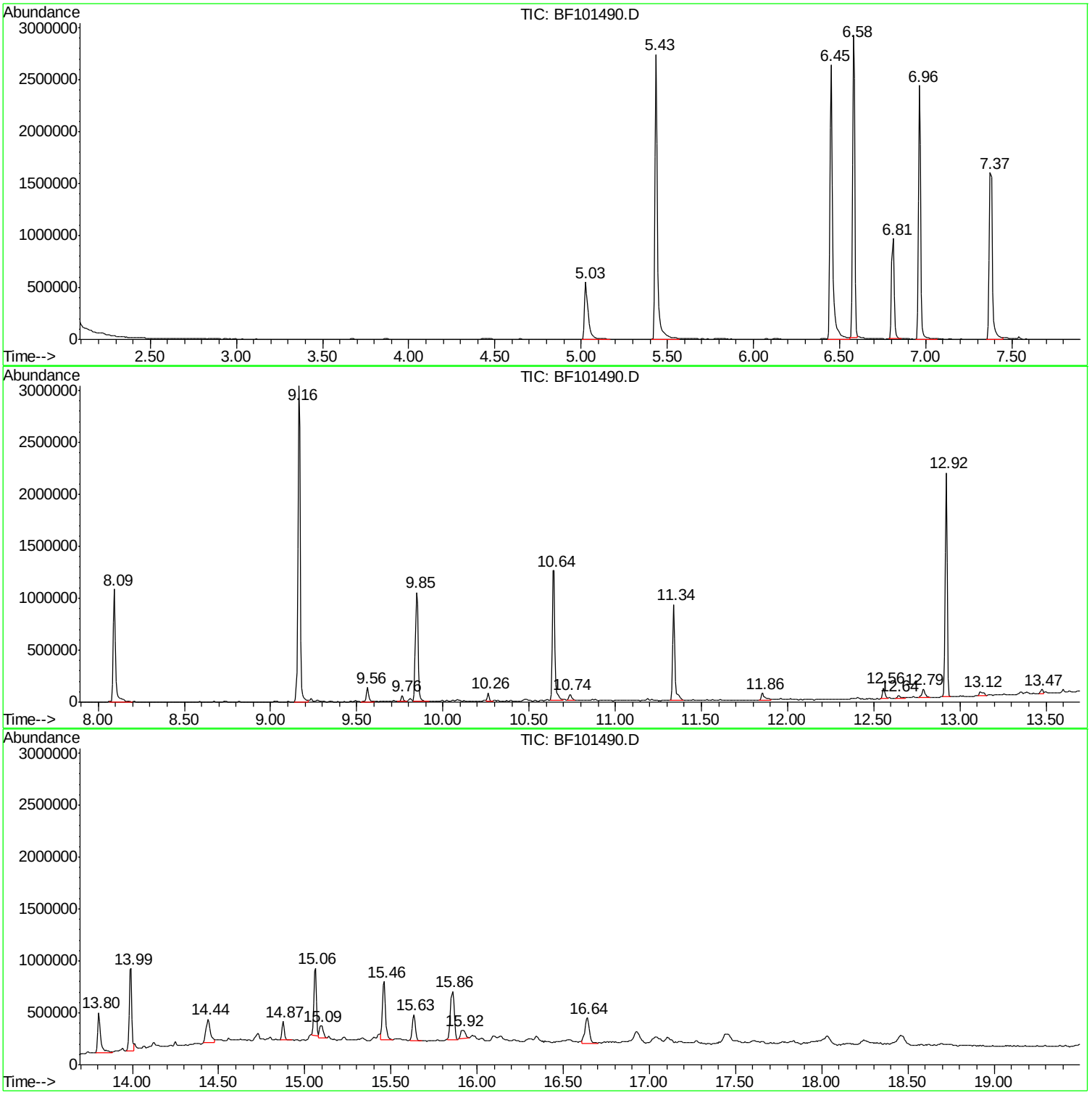
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

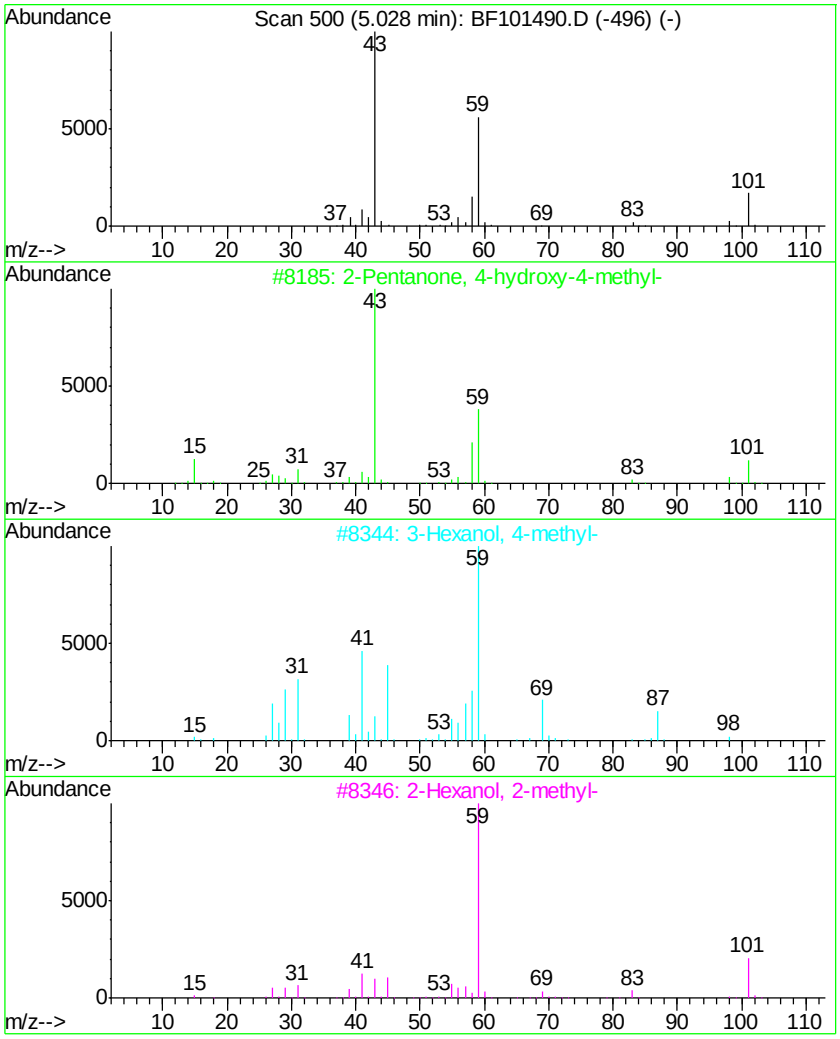
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

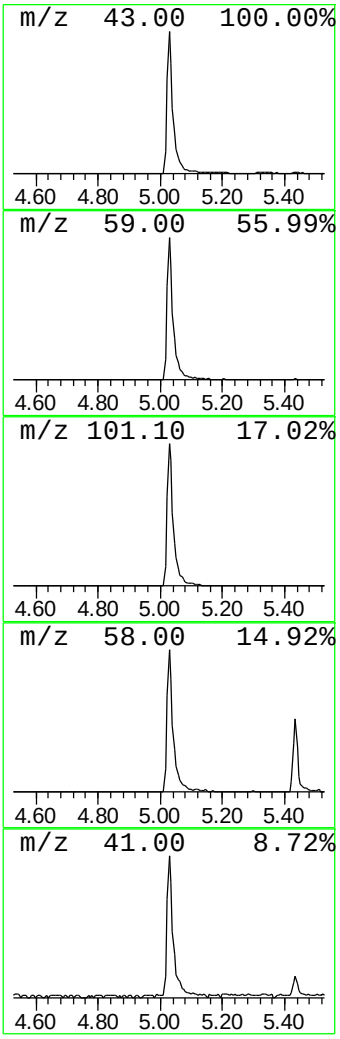
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	17.70 ng	769932	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

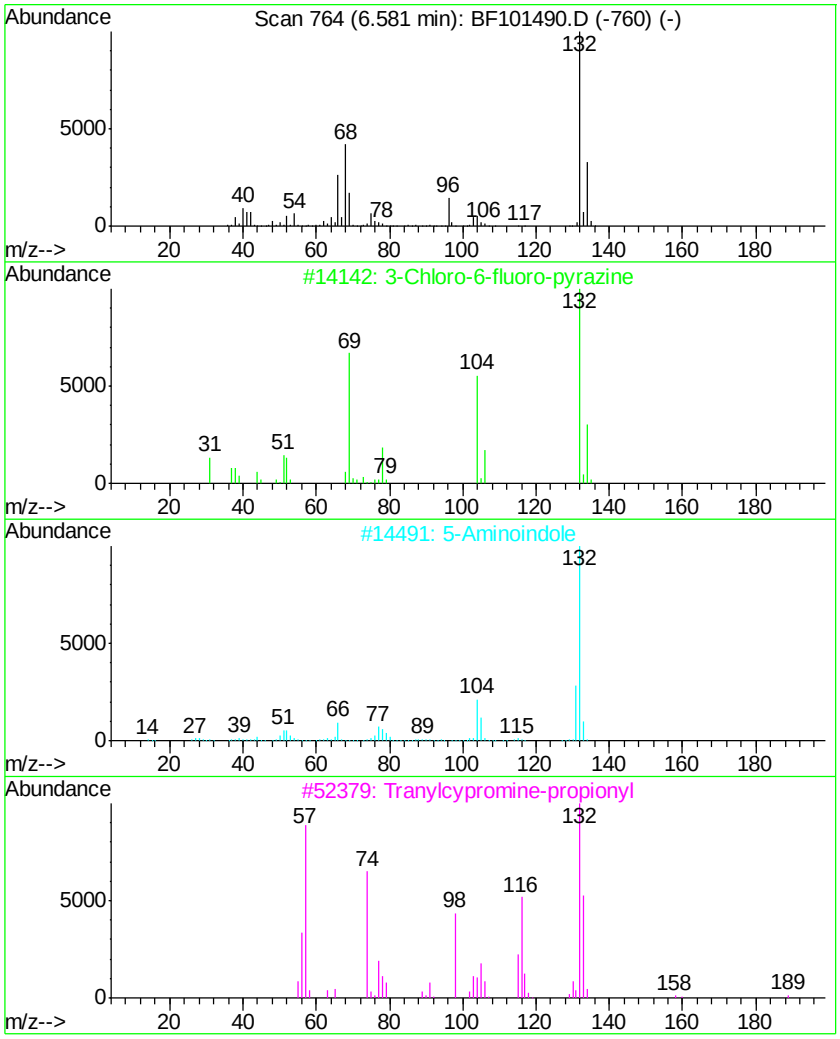
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

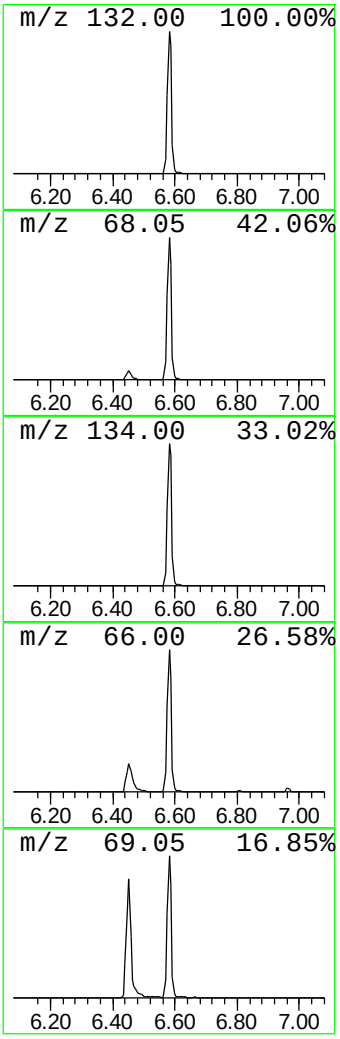
****

Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	65.09 ng	2831860	1,4-Dichlorobenzene-d4	6.81

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

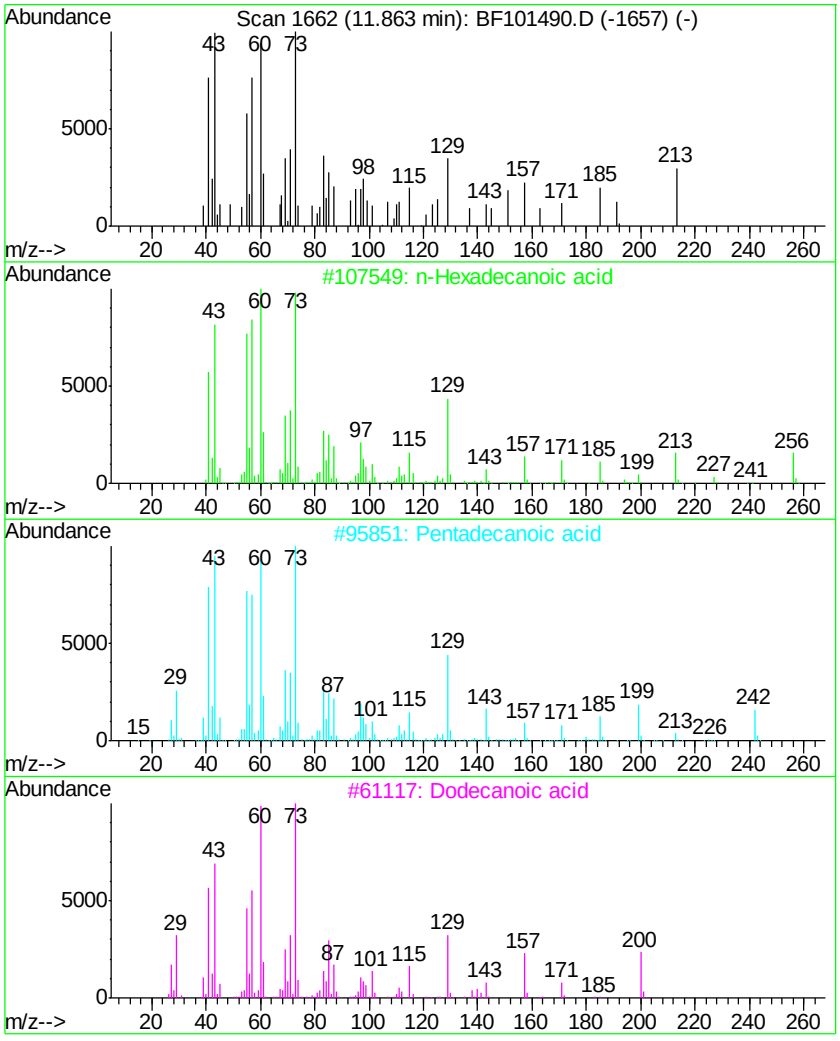
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

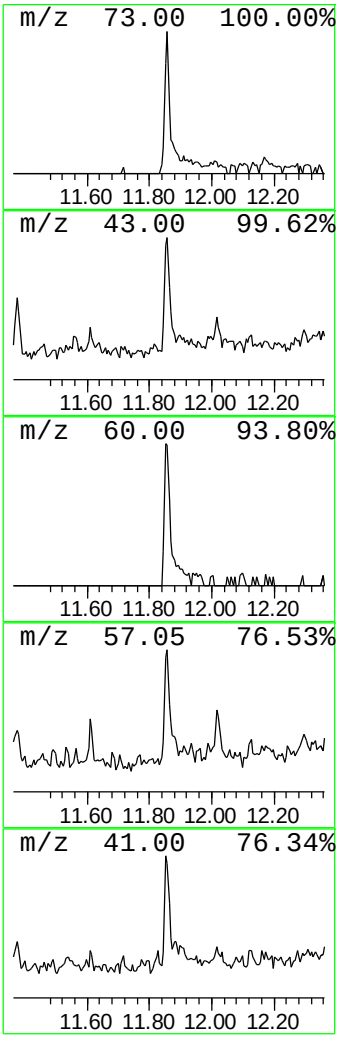
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	2.21 ng	100986	Phenanthrene-d10	11.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3	Dodecanoic acid	200	C12H24O2	000143-07-7	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5	Tridecanoic acid	214	C13H26O2	000638-53-9	53





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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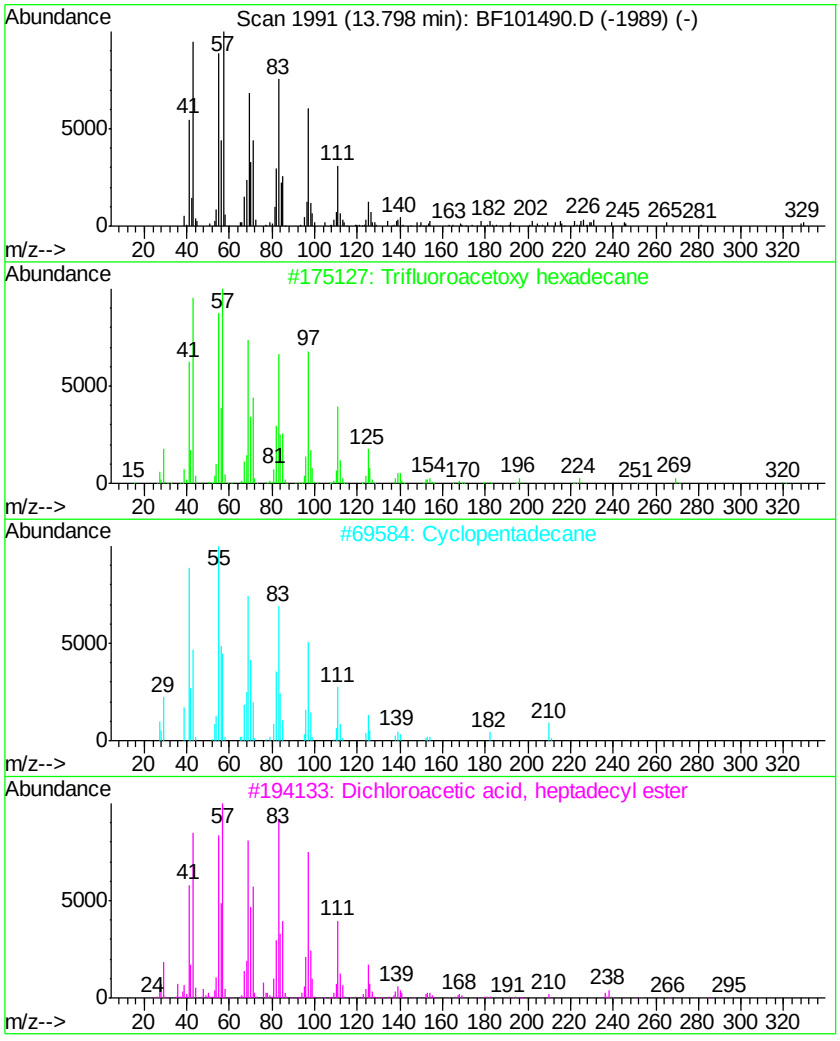
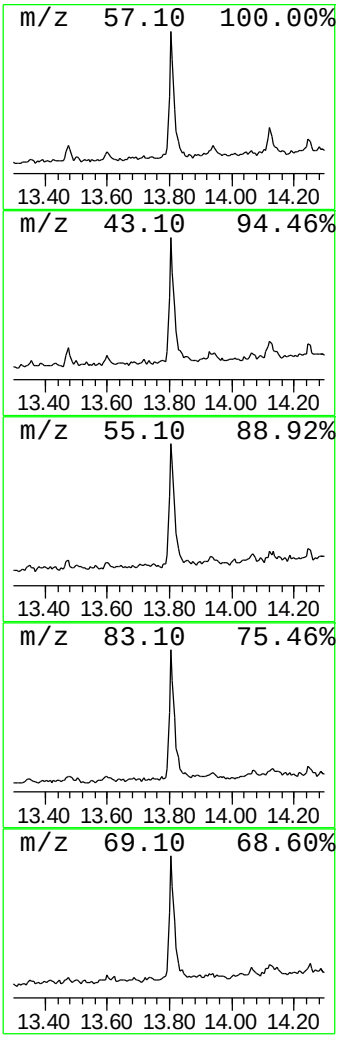
Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	10.92 ng	471626	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4	1-Tricosene	322	C23H46	018835-32-0	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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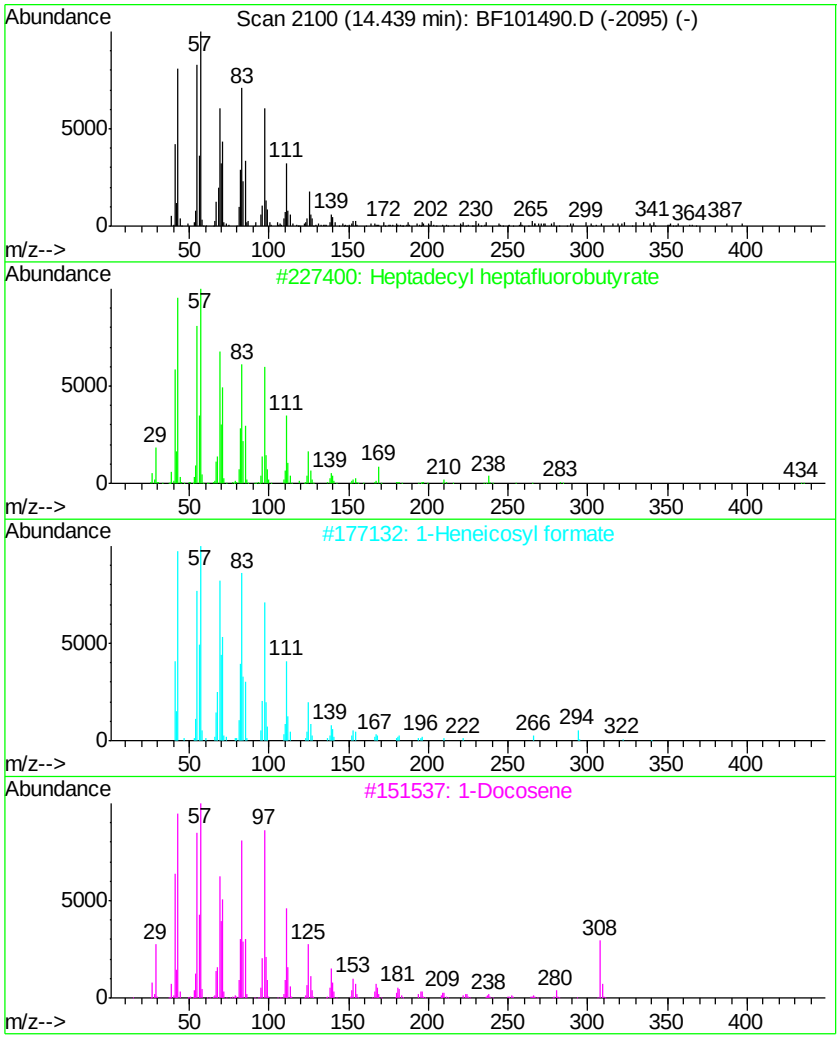
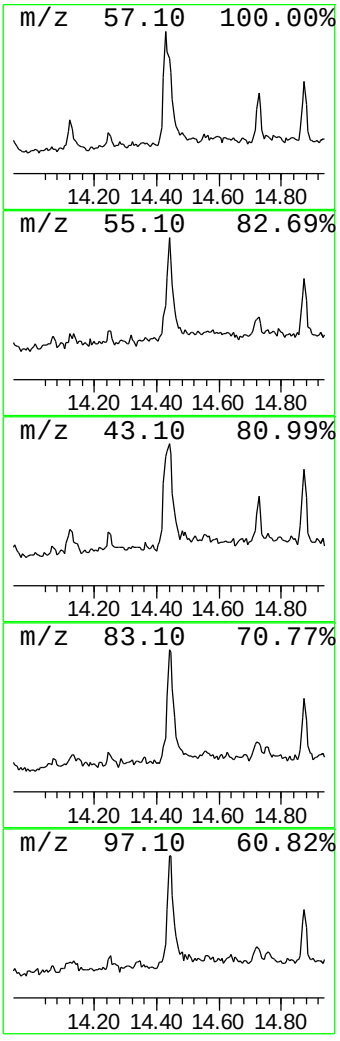
Peak Number 8 Heptadecyl heptafluorobutyrate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.44	9.33 ng	403268	Chrysene-d12	13.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
3	1-Docosene	308	C22H44	001599-67-3	93
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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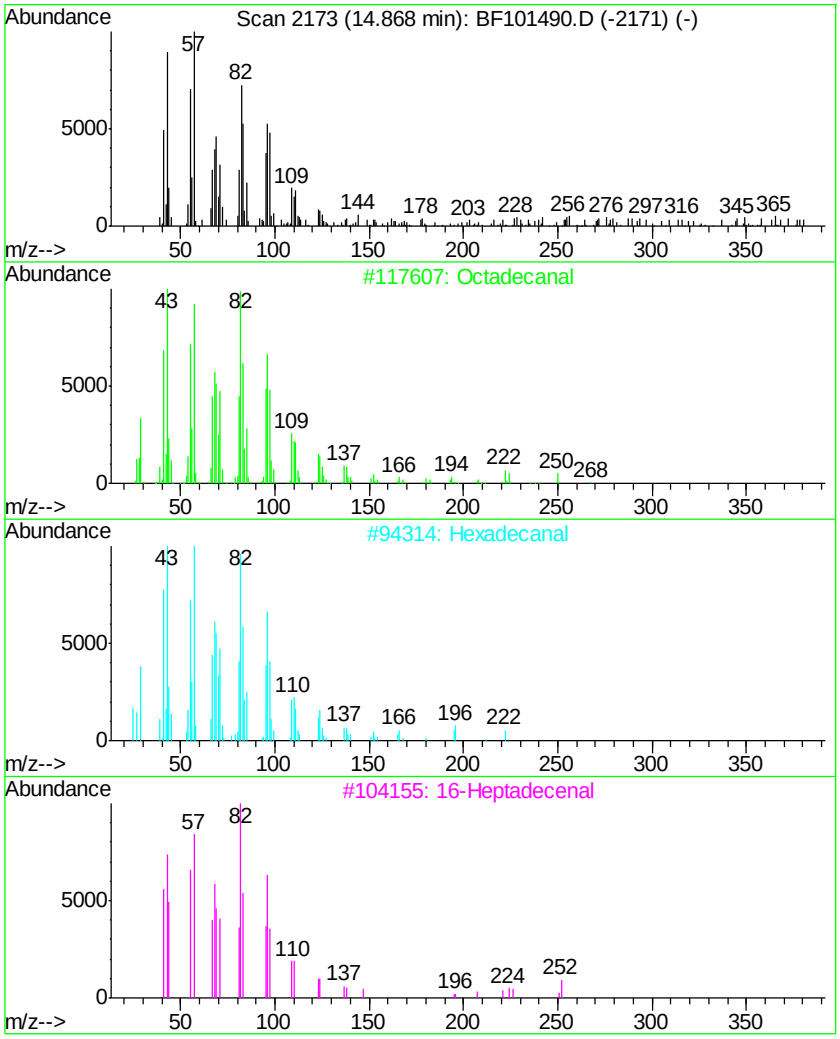
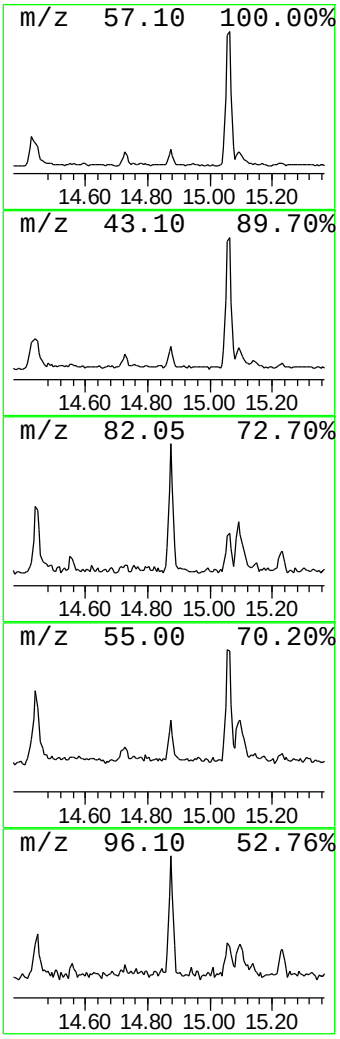
Peak Number 9 Octadecanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.87	4.78 ng	178133	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Hexadecanal	240	C16H32O	000629-80-1	91
3	16-Heptadecenal	252	C17H32O	1000144-57-9	89
4	Heptadecanal	254	C17H34O	1000376-70-0	87
5	1,19-Eicosadiene	278	C20H38	014811-95-1	87





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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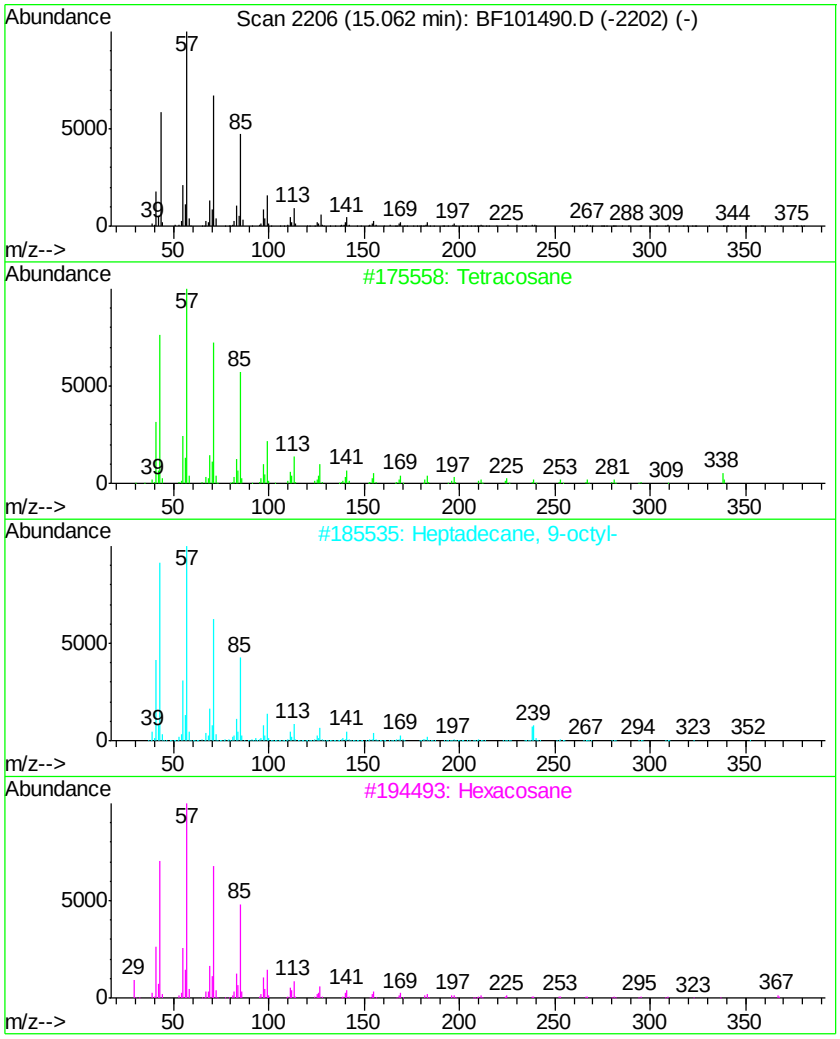
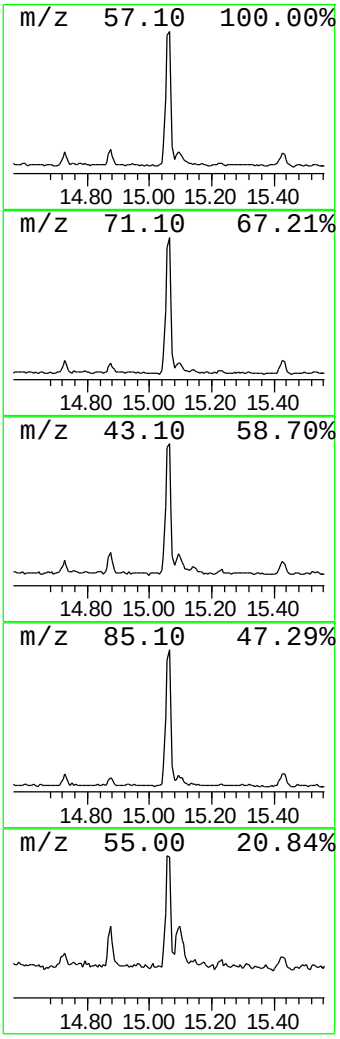
Peak Number 10 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	19.37 ng	721842	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	94
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	92
3	Hexacosane	366	C26H54	000630-01-3	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Docosane	310	C22H46	000629-97-0	91





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Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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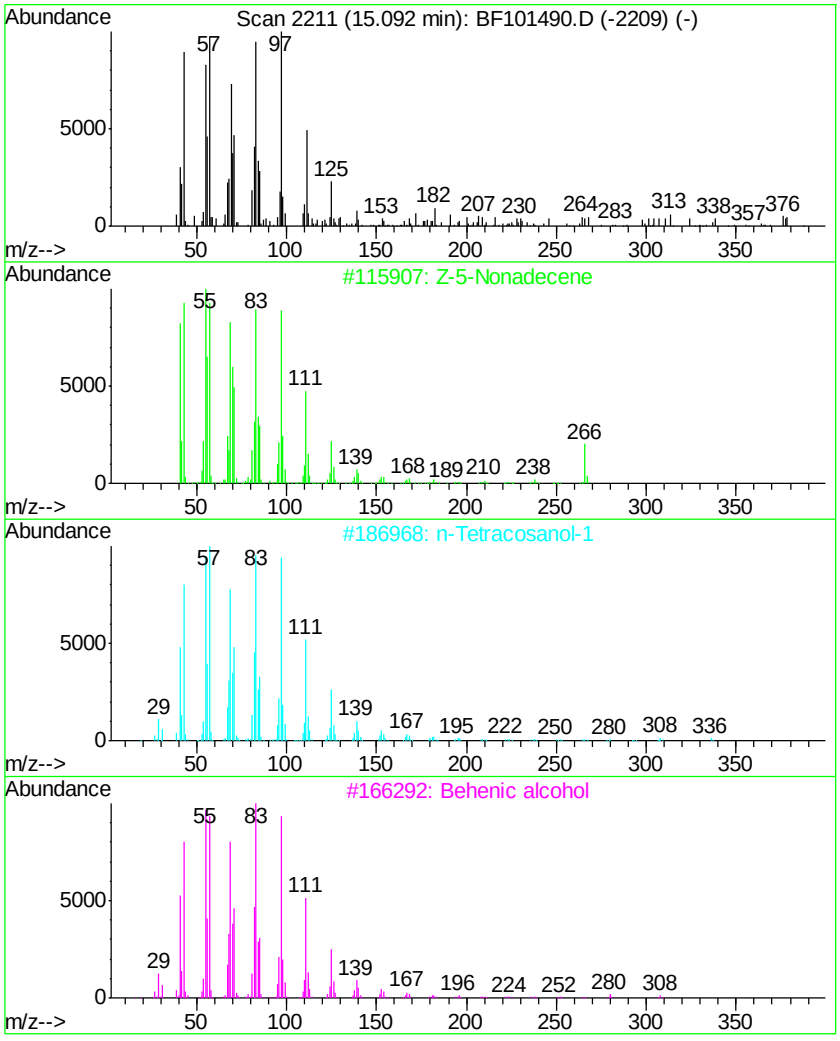
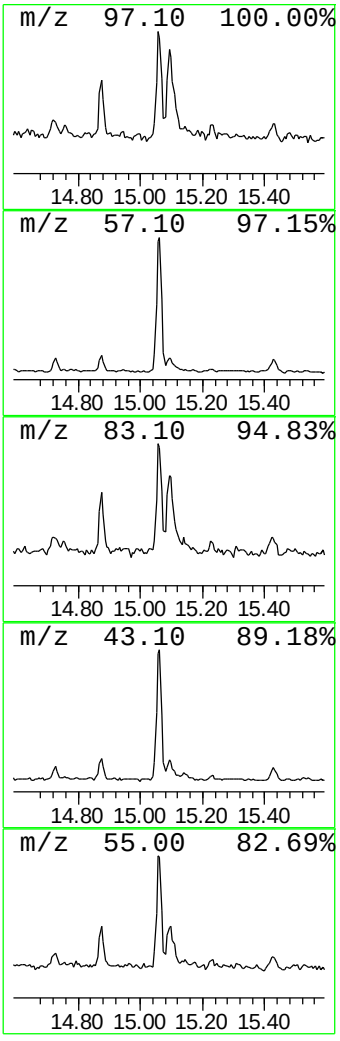
Peak Number 11 Z-5-Nonadecene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	4.18 ng	155875	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-5-Nonadecene	266	C19H38	1000131-11-8	94
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
3	Behenic alcohol	326	C22H46O	000661-19-8	94
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5	1-Heneicosanol	312	C21H44O	015594-90-8	90





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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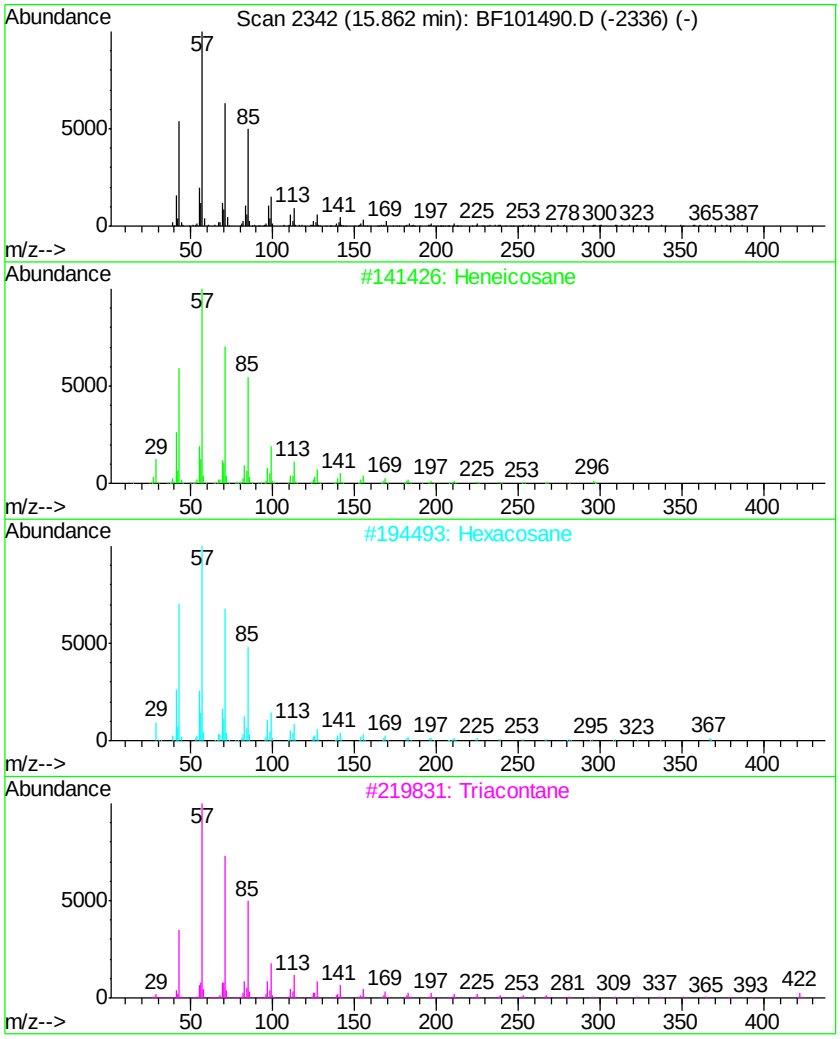
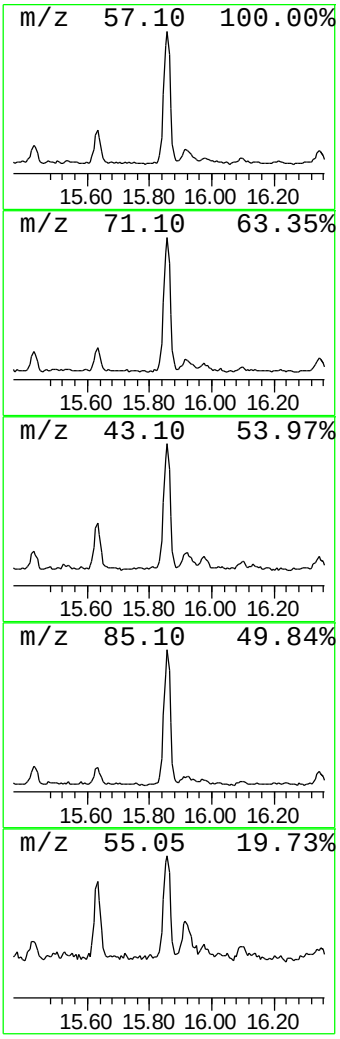
Peak Number 13 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	17.55 ng	653777	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Triacontane	422	C30H62	000638-68-6	90
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
5	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	74





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Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

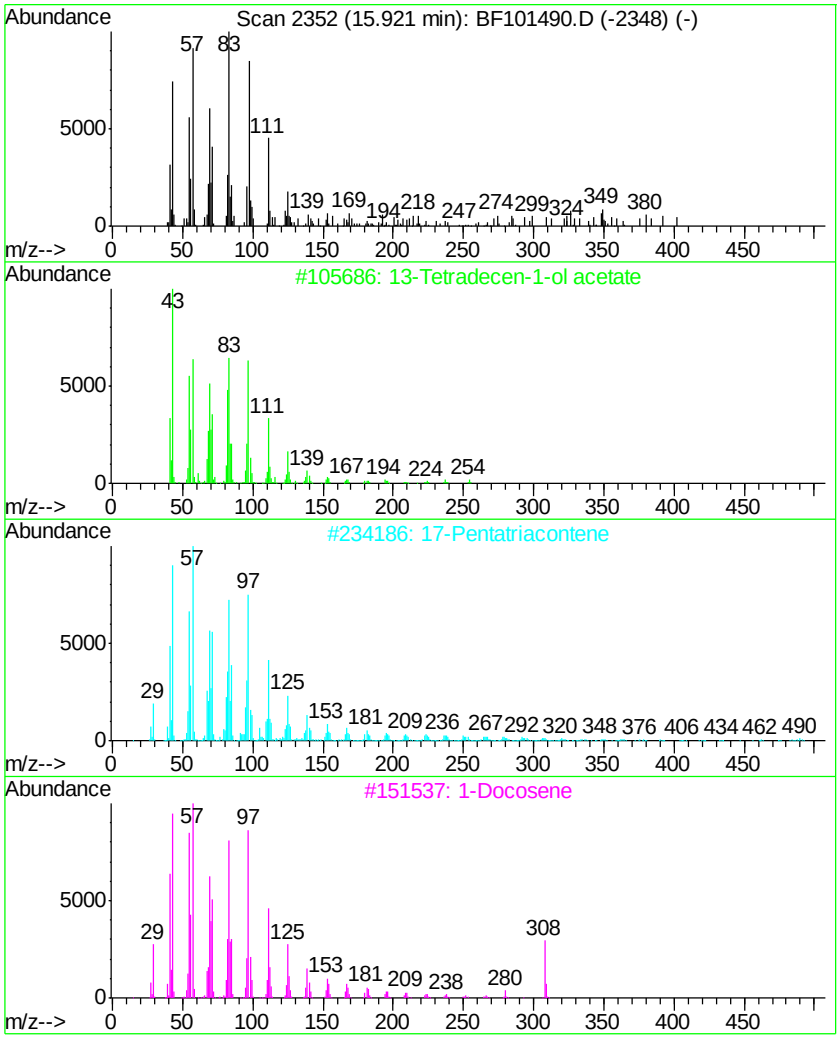
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

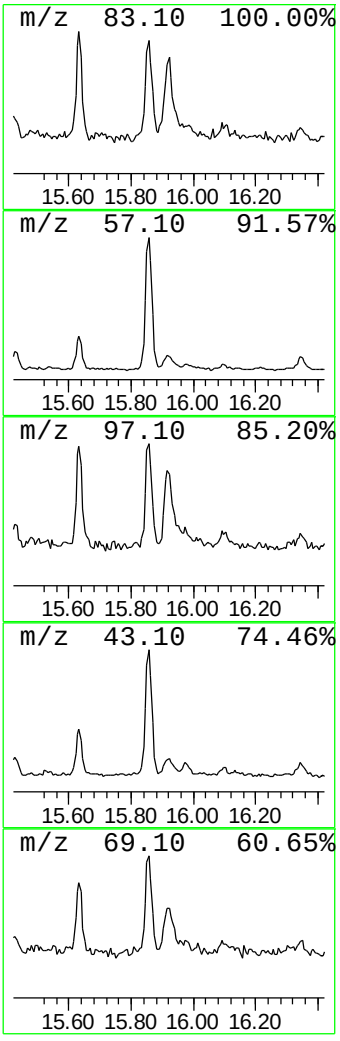
****

Peak Number 14 13-Tetradecen-1-ol acetate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	3.77 ng	140570	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	87
2	17-Pentatriacontene	491	C35H70	006971-40-0	86
3	1-Docosene	308	C22H44	001599-67-3	83
4	9-Tricosene, (Z)-	322	C23H46	027519-02-4	64
5	Cetene	224	C16H32	000629-73-2	56





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

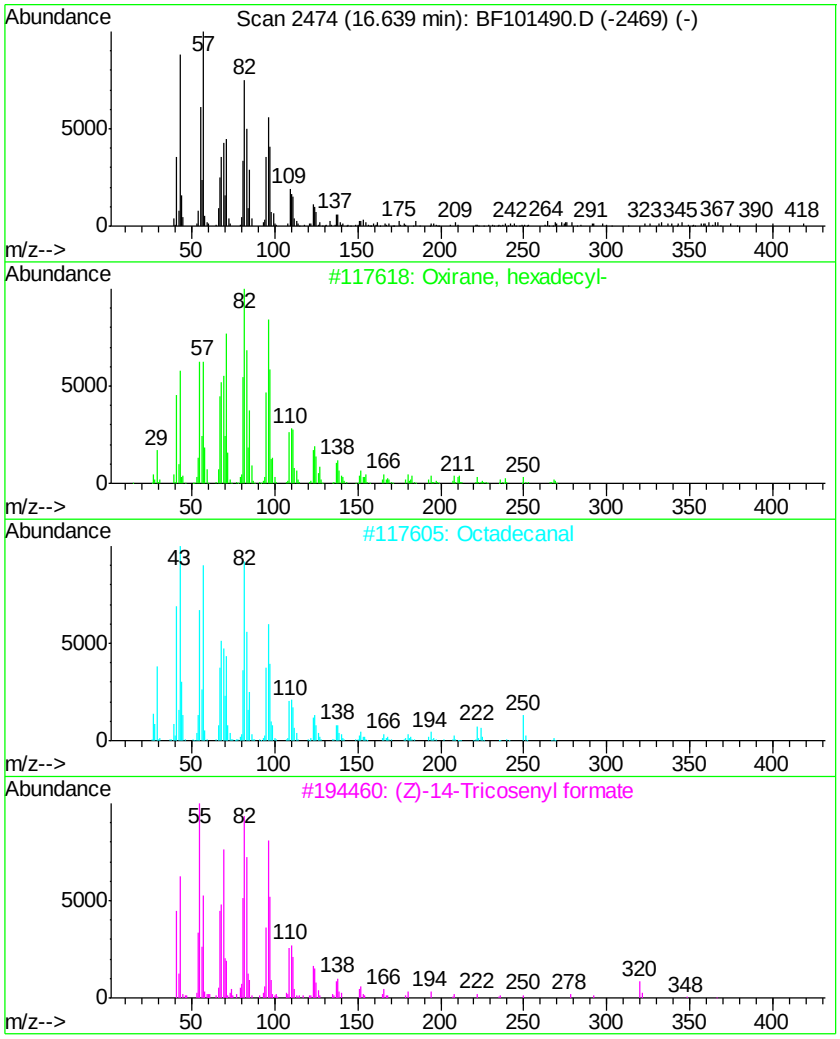
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

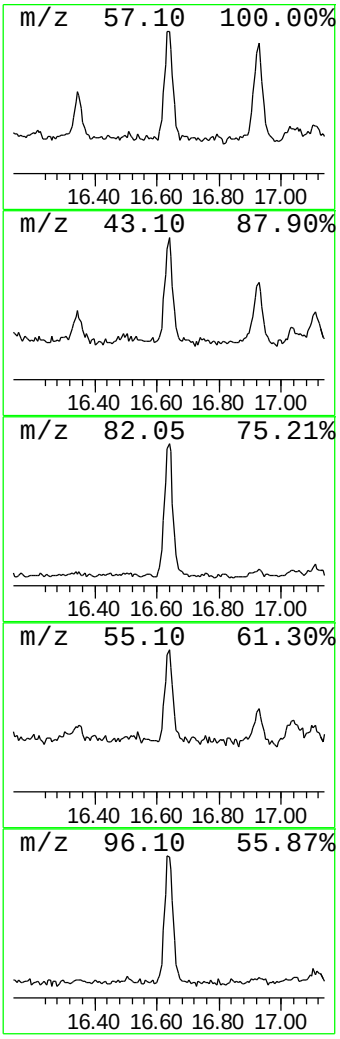
****

Peak Number 15 Oxirane, hexadecyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.64	12.13 ng	451771	Perylene-d12	15.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2	Octadecanal	268	C18H36O	000638-66-4	91
3	(Z)-14-Tricosenyl formate	366	C24H46O2	077899-10-6	90
4	Hexadecanal	240	C16H32O	000629-80-1	86
5	1,15-Pentadecanediol	244	C15H32O2	014722-40-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121817\
Data File : BF101490.D
Acq On : 18 Dec 2017 19:36
Operator : SJ/JU
Sample : I6908-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 1

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	5.03	17.7	ng	769932	1	6.81	870201	20.0
unknown6.58	6.58	65.1	ng	2831860	1	6.81	870201	20.0
n-Hexadecanoic acid	11.86	2.2	ng	100986	4	11.34	911943	20.0
Trifluoroacetoxy ...	13.80	10.9	ng	471626	5	13.99	864131	20.0
Heptadecyl heptaf...	14.44	9.3	ng	403268	5	13.99	864131	20.0
Octadecanal	14.87	4.8	ng	178133	6	15.46	745133	20.0
Tetracosane	15.06	19.4	ng	721842	6	15.46	745133	20.0
Z-5-Nonadecene	15.09	4.2	ng	155875	6	15.46	745133	20.0
Heneicosane	15.86	17.6	ng	653777	6	15.46	745133	20.0
13-Tetradecen-1-o...	15.92	3.8	ng	140570	6	15.46	745133	20.0
Oxirane, hexadecyl-	16.64	12.1	ng	451771	6	15.46	745133	20.0