LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
Data File : BF088664.D
Acq On : 3 Jul 2016 23:19
Operator : UM/SJ
Sample : H3817-08
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BS-2C-8.5-9FT

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-BF063016.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	1.850	21	23	35	rVB	43692	61426	2.01%	0.233%
2	2.010	35	37	40	rBV	51928	73905	2.42%	0.281%
3	3.015	122	125	141	rBV	94355	209823	6.88%	0.797%
4	4.958	292	295	299	rVB	142938	209096	6.85%	0.794%
5	5.381	329	332	334	rBV	2625357	2774926	90.94%	10.536%
6	6.421	420	423	425	rBV	2674380	3051318	100.00%	11.586%
7	6.547	431	434	437	rBV	2399503	2665843	87.37%	10.122%
8	6.787	452	455	456	rBV	549224	660456	21.64%	2.508%
9	6.936	466	468	471	rVB	1923073	1971373	64.61%	7.485%
10	7.347	501	504	506	rBV	1747656	1753635	57.47%	6.658%
11	8.067	564	567	569	rBV	1071386	909579	29.81%	3.454%
12	9.142	658	661	664	rBB	2599077	2668095	87.44%	10.130%
13	9.542	693	696	698	rVB	309817	369638	12.11%	1.403%
14	9.816	717	720	722	rBV	1253132	1097079	35.95%	4.165%
15	10.605	786	789	791	rBV	1622580	1822214	59.72%	6.919%
16	11.176	837	839	840	rBV	94005	77389	2.54%	0.294%
17	11.291	847	849	851	rVB	1131335	992349	32.52%	3.768%
18	11.359	851	855	859	rVB2	24613	61204	2.01%	0.232%
19	11.599	875	876	879	rVB	49296	48223	1.58%	0.183%
20	12.708	971	973	976	rBV	183423	169116	5.54%	0.642%
21	12.788	976	980	982	rVB2	45261	46956	1.54%	0.178%
22	12.879	985	988	990	rBV	2470610	2408176	78.92%	9.144%
23	13.416	1033	1035	1037	rBV	133775	123667	4.05%	0.470%
24	13.805	1066	1069	1076	rBV	133093	324456	10.63%	1.232%
25	13.919	1076	1079	1081	rVV	879720	951716	31.19%	3.614%
26	14.445	1123	1125	1131	rBV2	26815	62298	2.04%	0.237%
27	15.302	1197	1200	1203	rBV	490145	676382	22.17%	2.568%
28	15.862	1243	1249	1258	rBV2	21880	96974	3.18%	0.368%

Sum of corrected areas: 26337312

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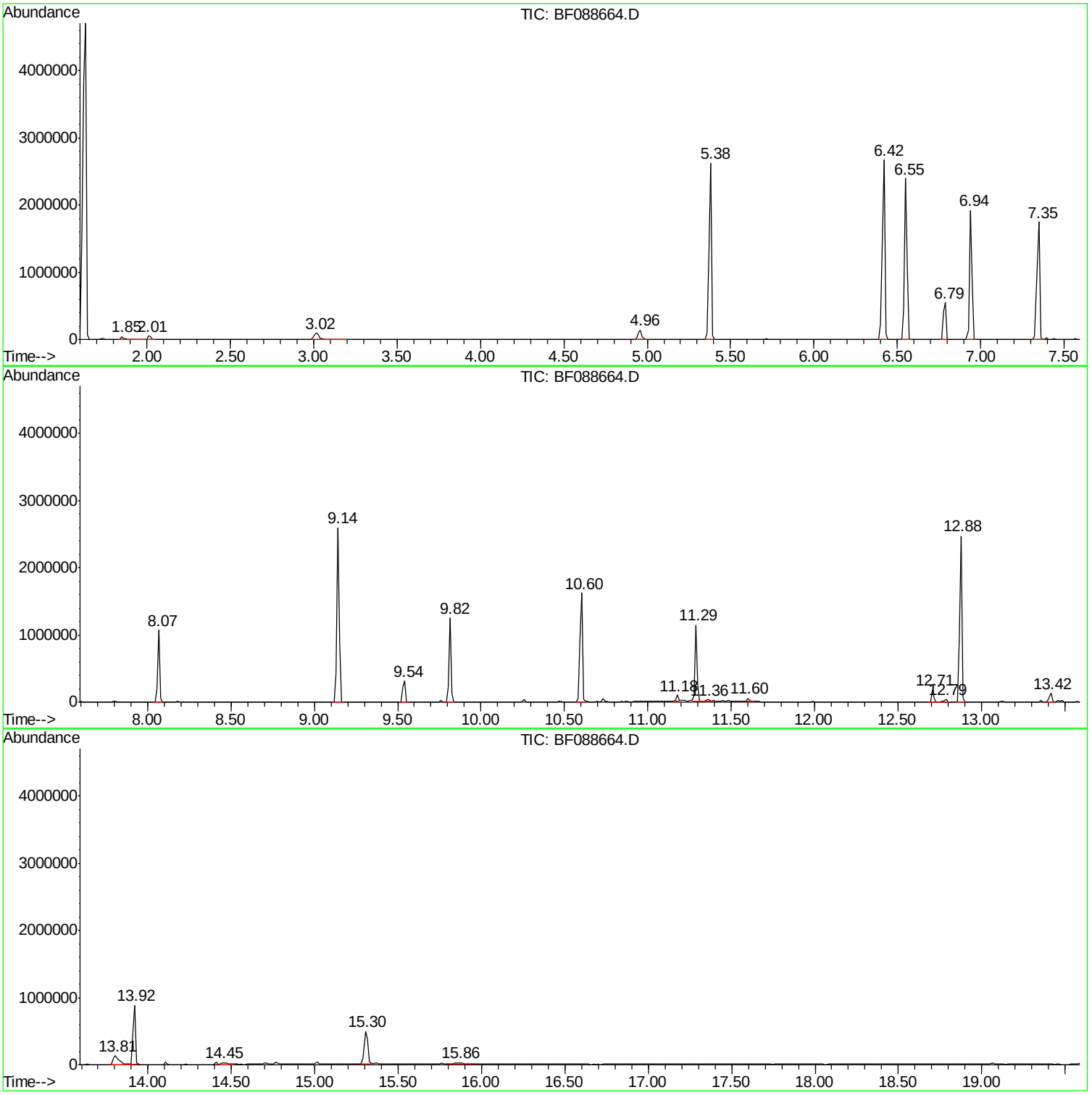
Instrument :
BNA_F
ClientSampleId :
BS-2C-8.5-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
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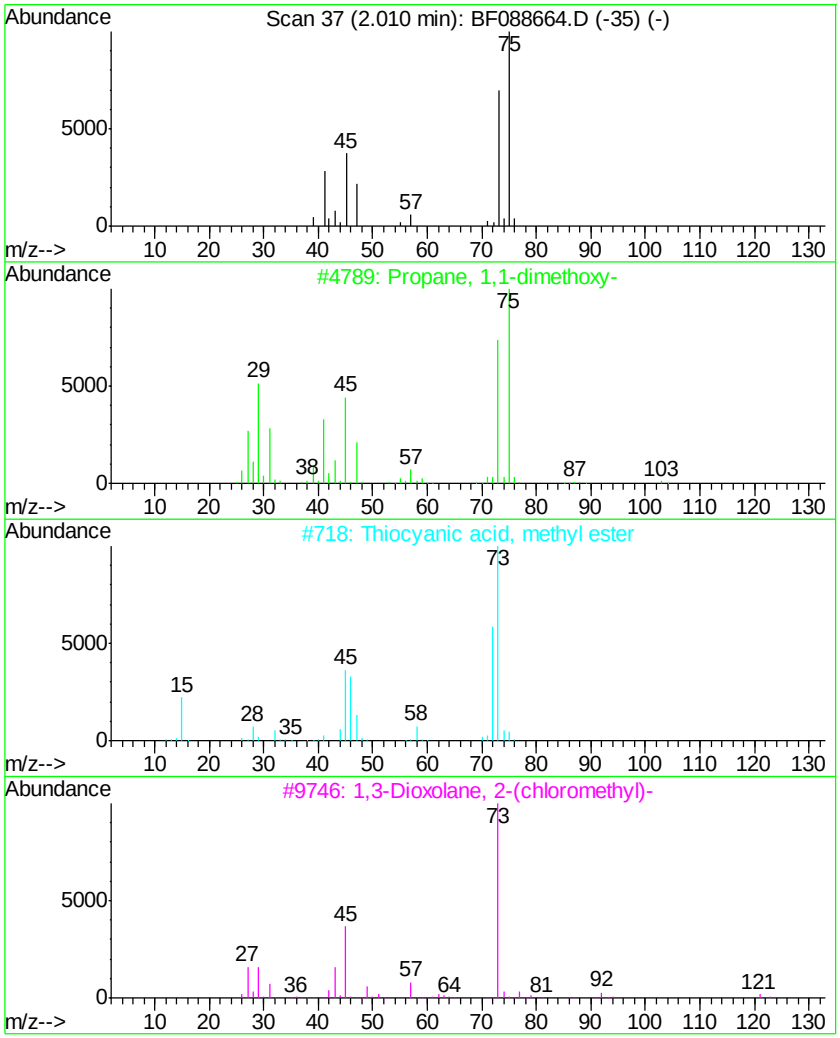
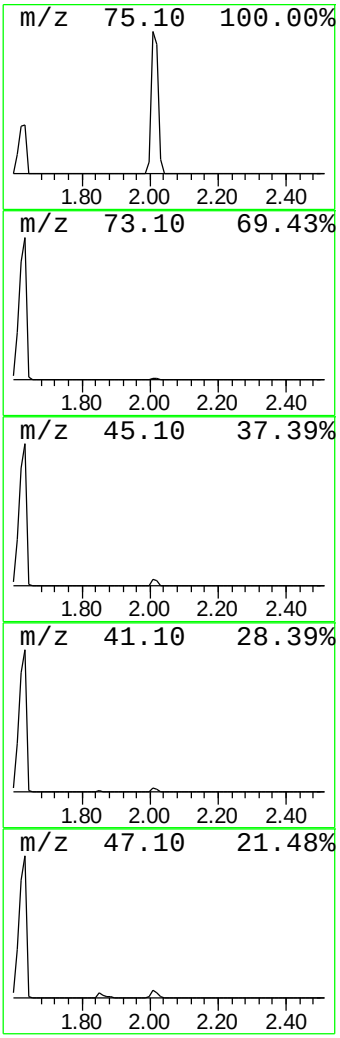
****

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	2.24 ng	73905	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2	Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
3	1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
4	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





Library Search Compound Report

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Operator : UM/SJ
Sample : H3817-08
Misc :
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Instrument : BNA_F
ClientSampleId : BS-2C-8.5-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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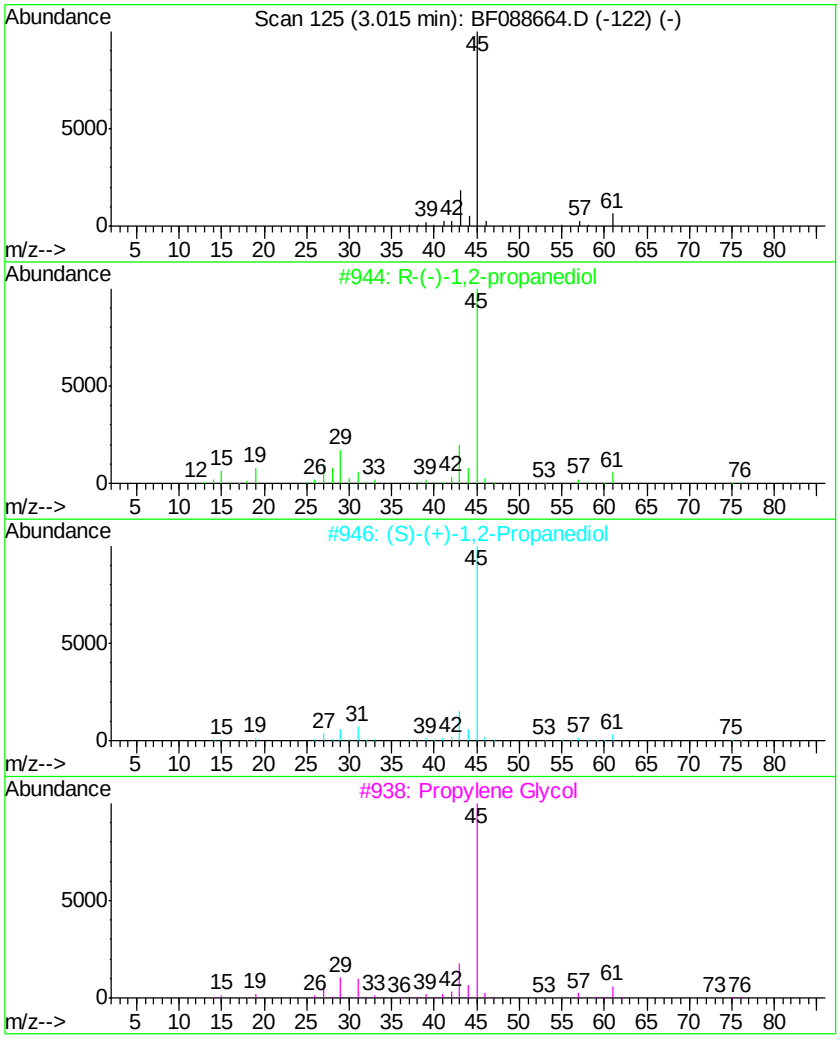
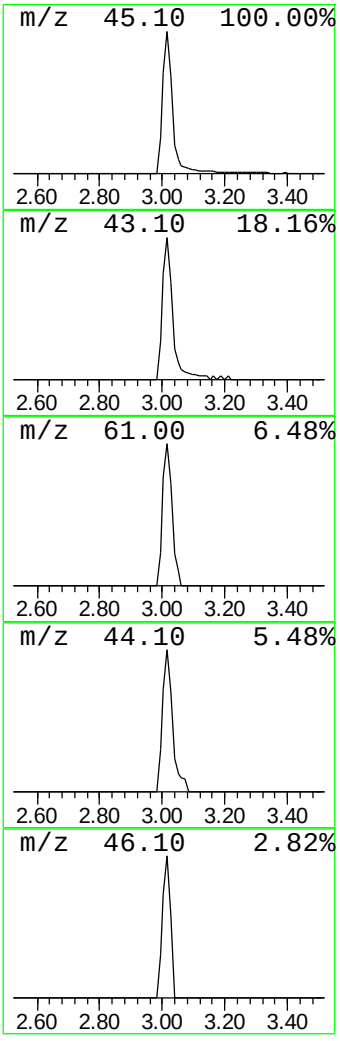
Peak Number 2 unknown3.02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.02	6.35 ng	209823	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	002155-30-8	9
5	Formamide	45	CH3NO	000075-12-7	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF070316\
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Operator : UM/SJ
Sample : H3817-08
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BS-2C-8.5-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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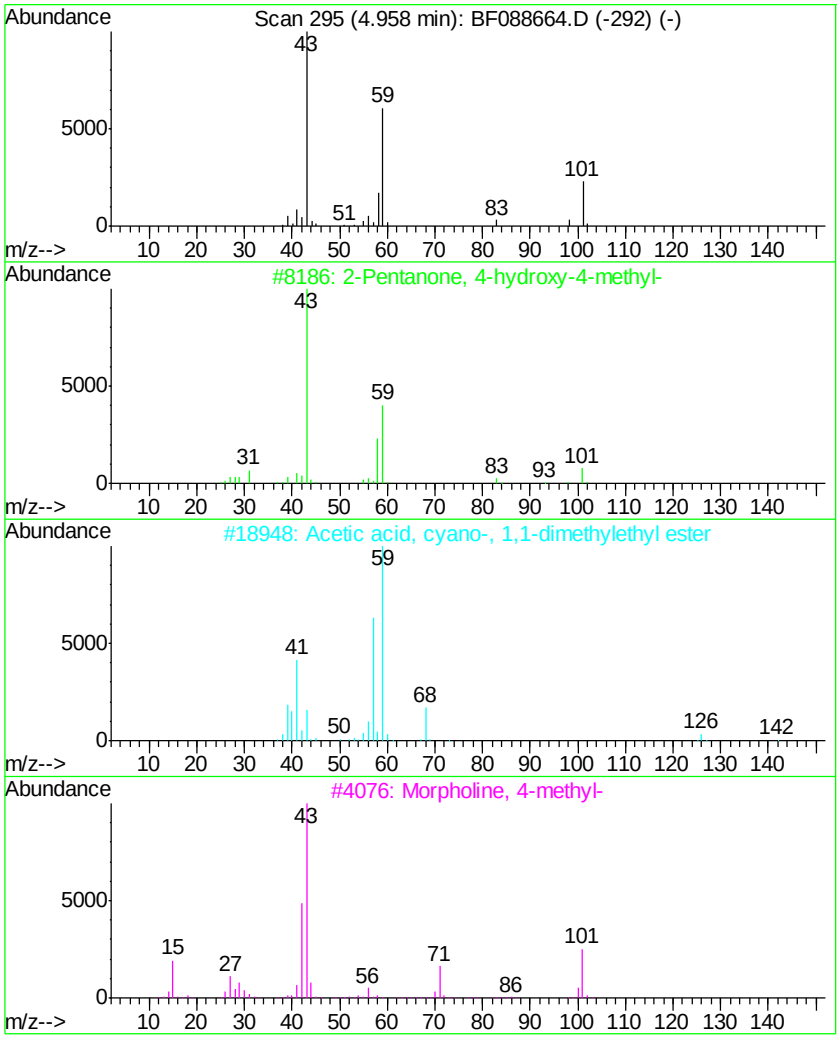
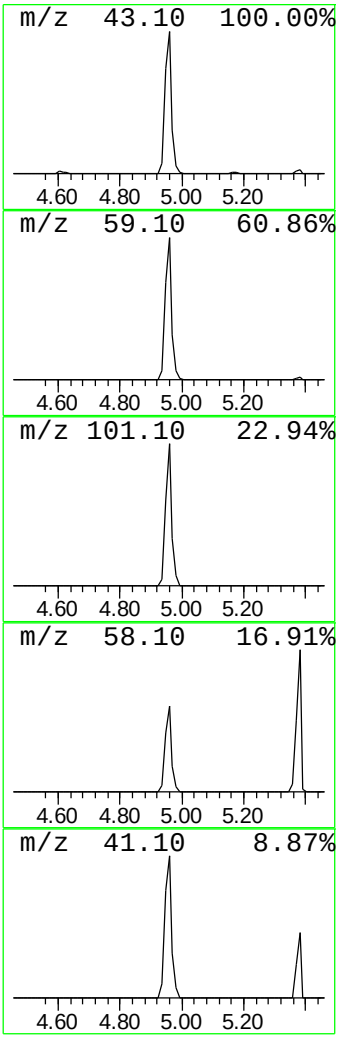
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	6.33 ng	209096	1,4-Dichlorobenzene-d4	6.79

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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BS-2C-8.5-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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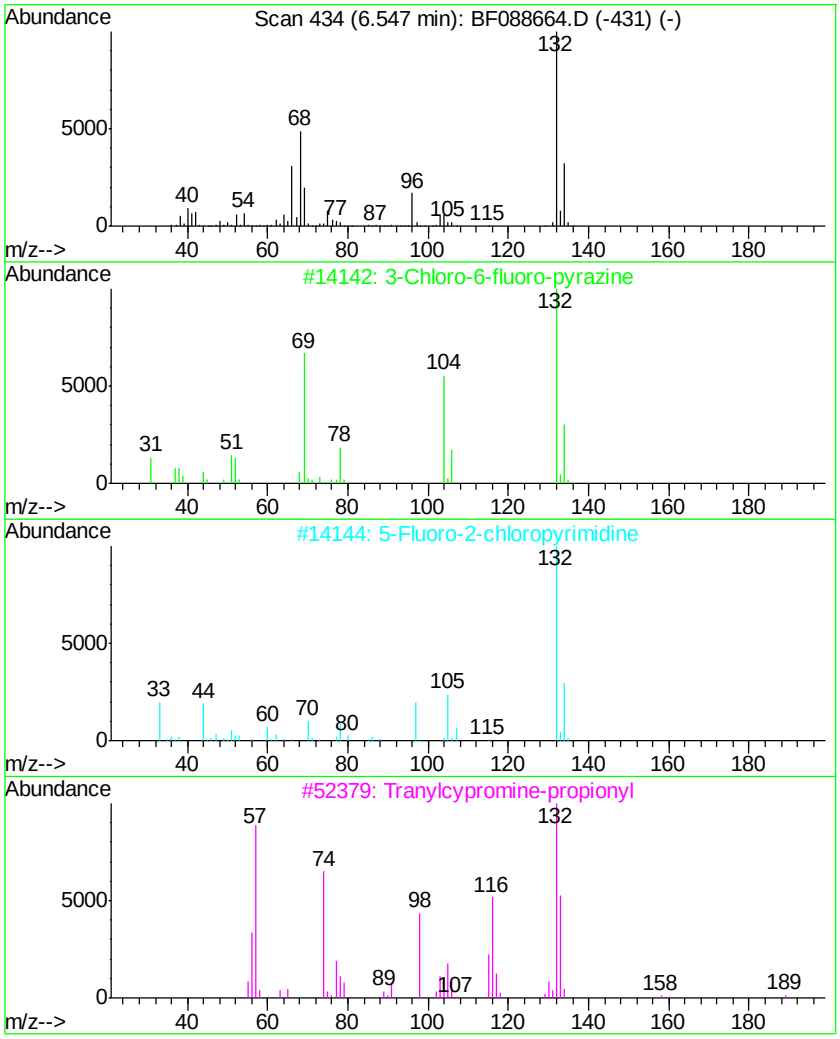
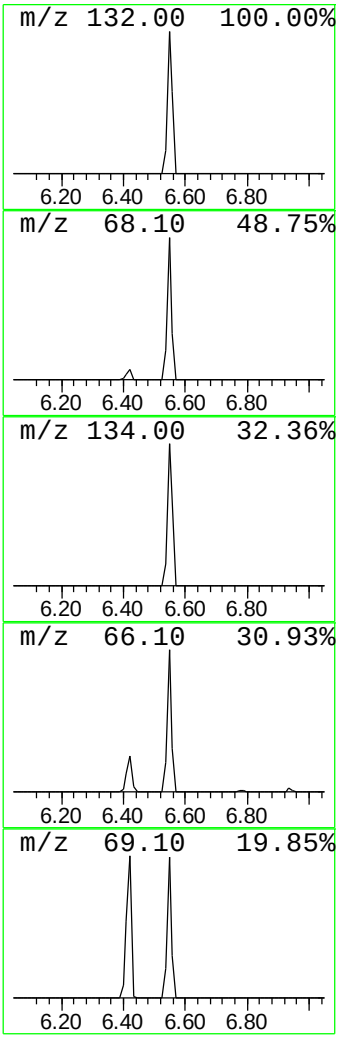
****

Peak Number 4 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	80.73 ng	2665840	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Misc :
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Instrument : BNA_F
ClientSampleId : BS-2C-8.5-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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TIC Library : C:\Database\NIST11.L
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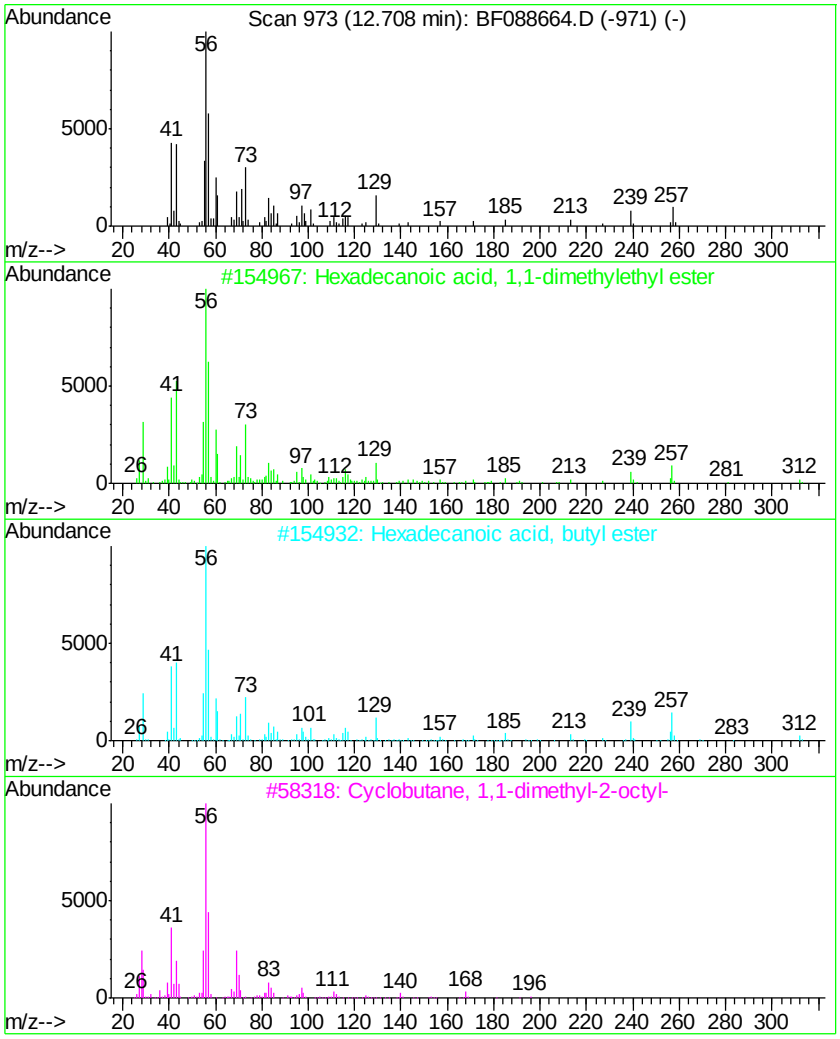
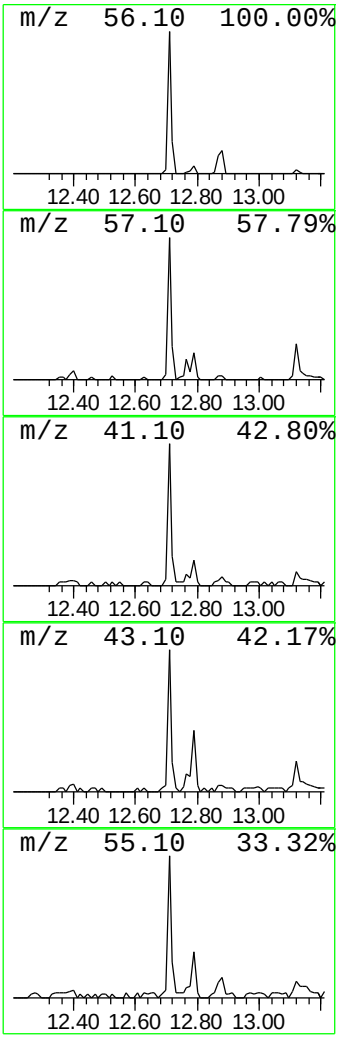
****

Peak Number 6 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	3.55 ng	169116	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	72
3	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	38
5	Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37





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Instrument : BNA_F
ClientSampleId : BS-2C-8.5-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
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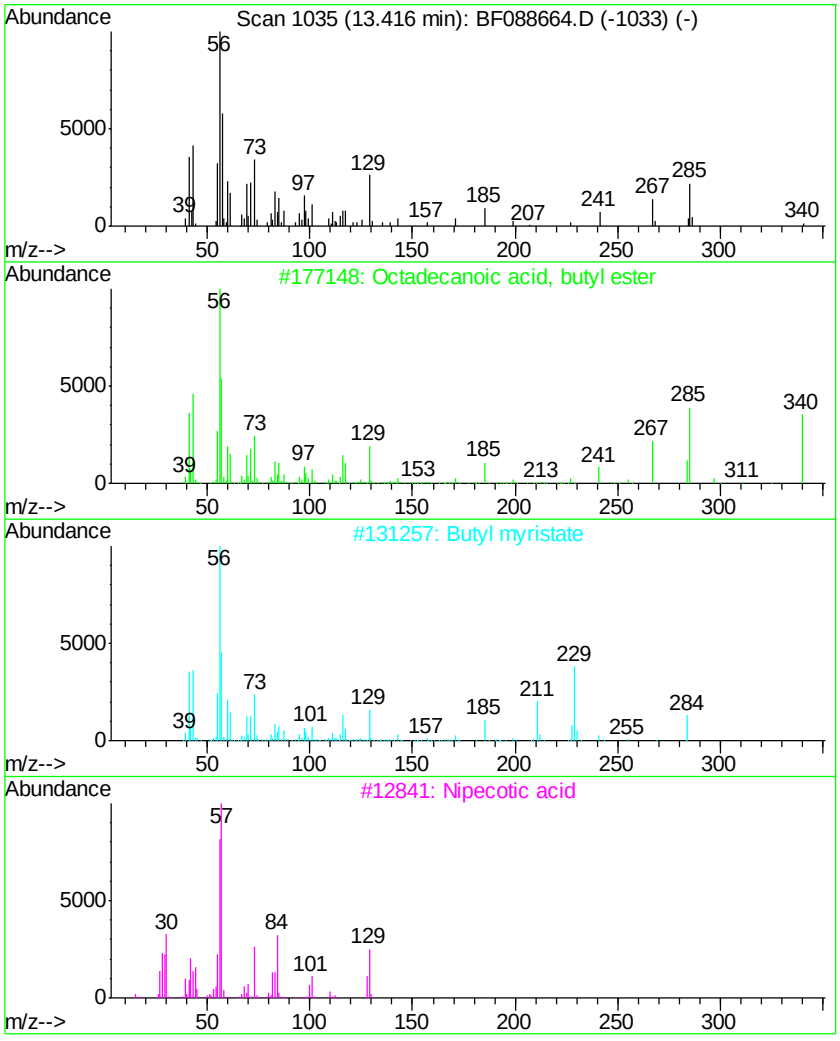
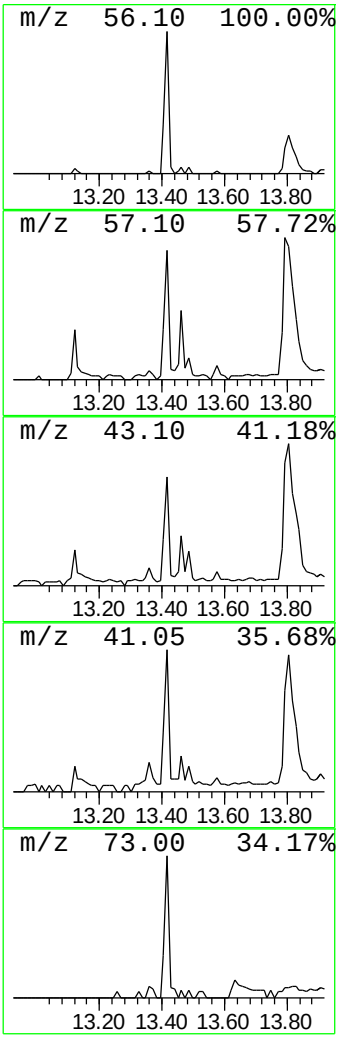
Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.42	2.60 ng	123667	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	93
2	Butyl myristate	284	C18H36O2	000110-36-1	59
3	Nipecotic acid	129	C6H11NO2	000498-95-3	50
4	Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	38
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32





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Instrument : BNA_F
ClientSampleId : BS-2C-8.5-9FT

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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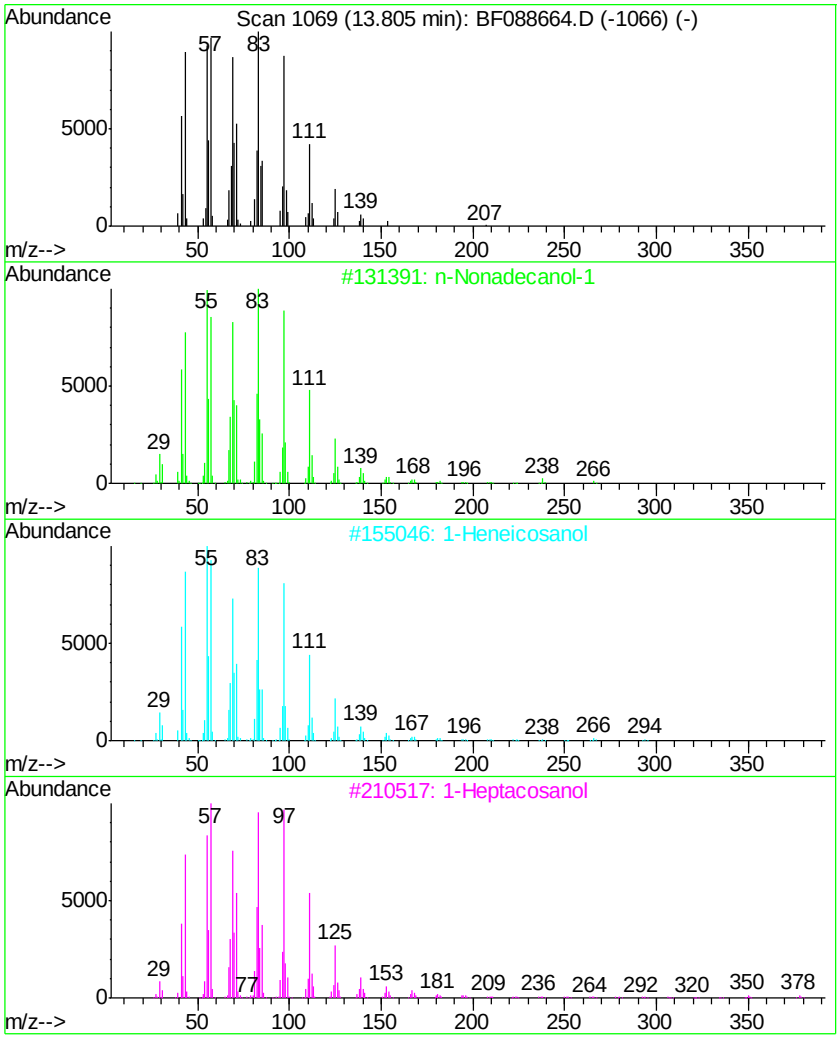
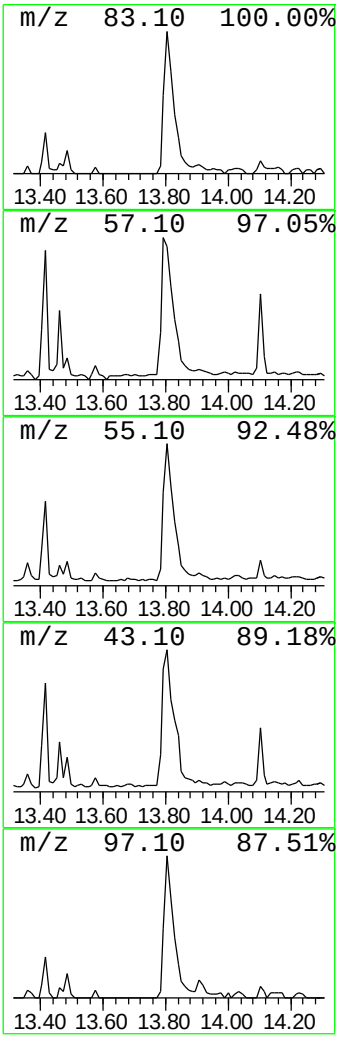
Peak Number 8 n-Nonadecanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	6.82 ng	324456	Chrysene-d12	13.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	94
3	1-Heptacosanol	396	C27H56O	002004-39-9	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	Behenic alcohol	326	C22H46O	000661-19-8	91





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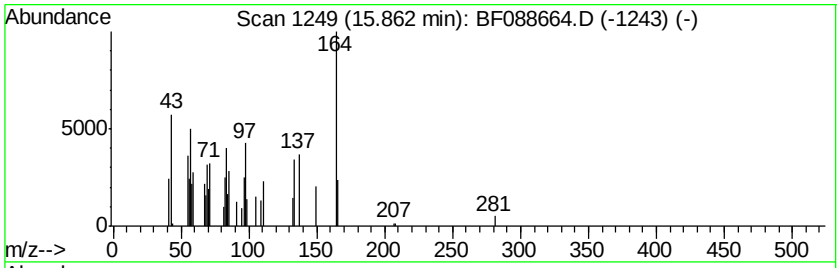
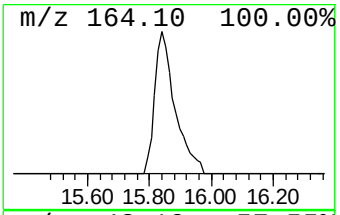
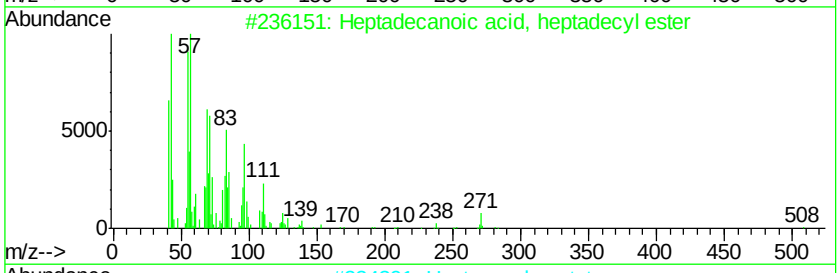
Peak Number 9 unknown15.86 Concentration Rank 7

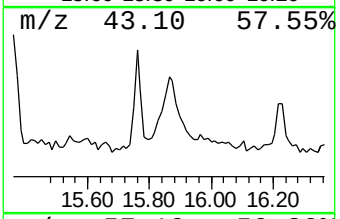
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.86	2.87 ng	96974	Perylene-d12	15.30

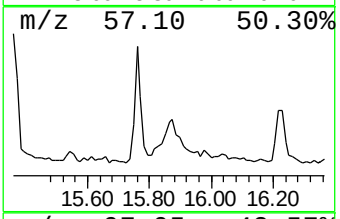
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, heptadecyl e...	509	C34H68O2	036617-50-2	38
2	Heptacosyl acetate	438	C29H58O2	1000351-78-2	30
3	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	30
4	1-Heptacosanol	396	C27H56O	002004-39-9	30
5	17-Pentatriacontene	491	C35H70	006971-40-0	30

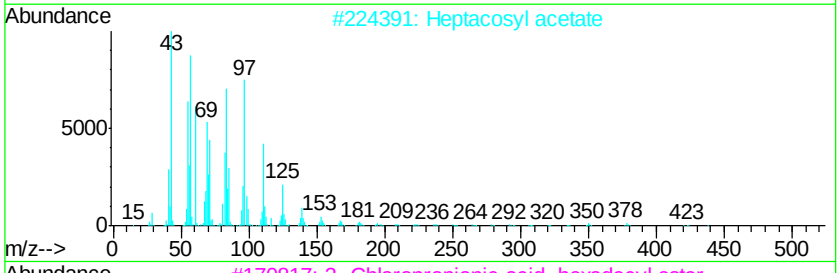


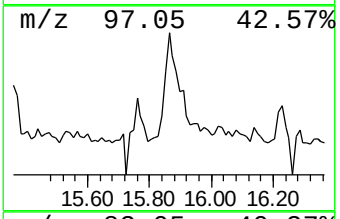


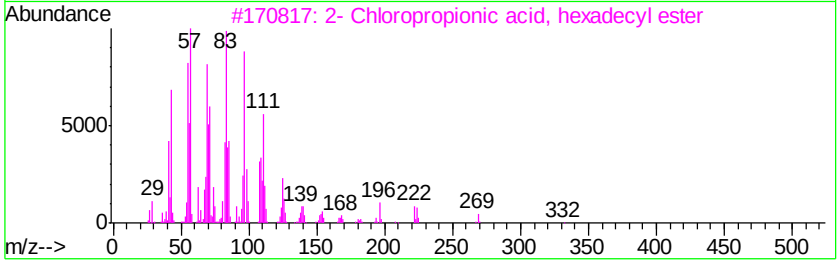


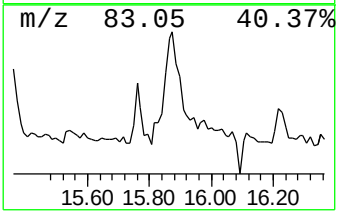












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070316\
Data File : BF088664.D
Acq On : 3 Jul 2016 23:19
Operator : UM/SJ
Sample : H3817-08
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : BS-2C-8.5-9FT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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
Propane, 1,1-dime...	2.01	2.2	ng	73905	1	6.79	660456	20.0
unknown3.02	3.02	6.3	ng	209823	1	6.79	660456	20.0
2-Pentanone, 4-hy...	4.96	6.3	ng	209096	1	6.79	660456	20.0
unknown6.55	6.55	80.7	ng	2665840	1	6.79	660456	20.0
Hexadecanoic acid...	12.71	3.5	ng	169116	5	13.92	951716	20.0
Octadecanoic acid...	13.42	2.6	ng	123667	5	13.92	951716	20.0
n-Nonadecanol-1	13.81	6.8	ng	324456	5	13.92	951716	20.0
unknown15.86	15.86	2.9	ng	96974	6	15.30	676382	20.0