LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086966.D
Acq On : 13 May 2016 10:35
Operator : UM/SJ
Sample : H2916-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

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-BF050916.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	12	rVB	714072	1087366	14.63%	2.165%
2	1.747	12	14	53	rVB	2839608	7434312	100.00%	14.804%
3	4.764	276	278	294	rBV	426451	752025	10.12%	1.497%
4	5.221	315	318	320	rBV	4582263	5094755	68.53%	10.145%
5	5.622	351	353	362	rVB	54797	87185	1.17%	0.174%
6	6.296	408	412	414	rBV	4027092	5585303	75.13%	11.122%
7	6.399	418	421	423	rBV	4921665	5104241	68.66%	10.164%
8	6.616	438	440	443	rBV	690611	925894	12.45%	1.844%
9	6.776	452	454	457	rBV	3350659	3430827	46.15%	6.832%
10	7.199	488	491	493	rBV	3266367	3444209	46.33%	6.858%
11	7.336	500	503	508	rVB	74650	130652	1.76%	0.260%
12	7.907	551	553	556	rBV	1256127	1137159	15.30%	2.264%
13	8.993	645	648	650	rBV	4102499	4626462	62.23%	9.213%
14	9.393	680	683	685	rBV	864938	1018702	13.70%	2.029%
15	9.599	699	701	703	rBV	136662	131701	1.77%	0.262%
16	9.656	703	706	708	rBV	1200744	1076130	14.48%	2.143%
17	10.102	743	745	746	rVB	243462	187219	2.52%	0.373%
18	10.319	761	764	767	rBV	78785	122419	1.65%	0.244%
19	10.445	772	775	778	rBV	2385313	2358660	31.73%	4.697%
20	10.571	784	786	793	rVB	248469	309606	4.16%	0.617%
21	11.016	823	825	826	rBV	141038	116864	1.57%	0.233%
22	11.131	833	835	838	rBV	925848	827190	11.13%	1.647%
23	11.394	853	858	861	rBV2	37347	90254	1.21%	0.180%
24	11.679	881	883	887	rBV	63374	80555	1.08%	0.160%
25	12.719	971	974	976	rBV	3500265	3293323	44.30%	6.558%
26	13.634	1049	1054	1061	rBV	73306	240956	3.24%	0.480%
27	13.759	1062	1065	1067	rBV	932633	861428	11.59%	1.715%
28	15.120	1182	1184	1187	rBV	578618	663853	8.93%	1.322%

Sum of corrected areas: 50219250

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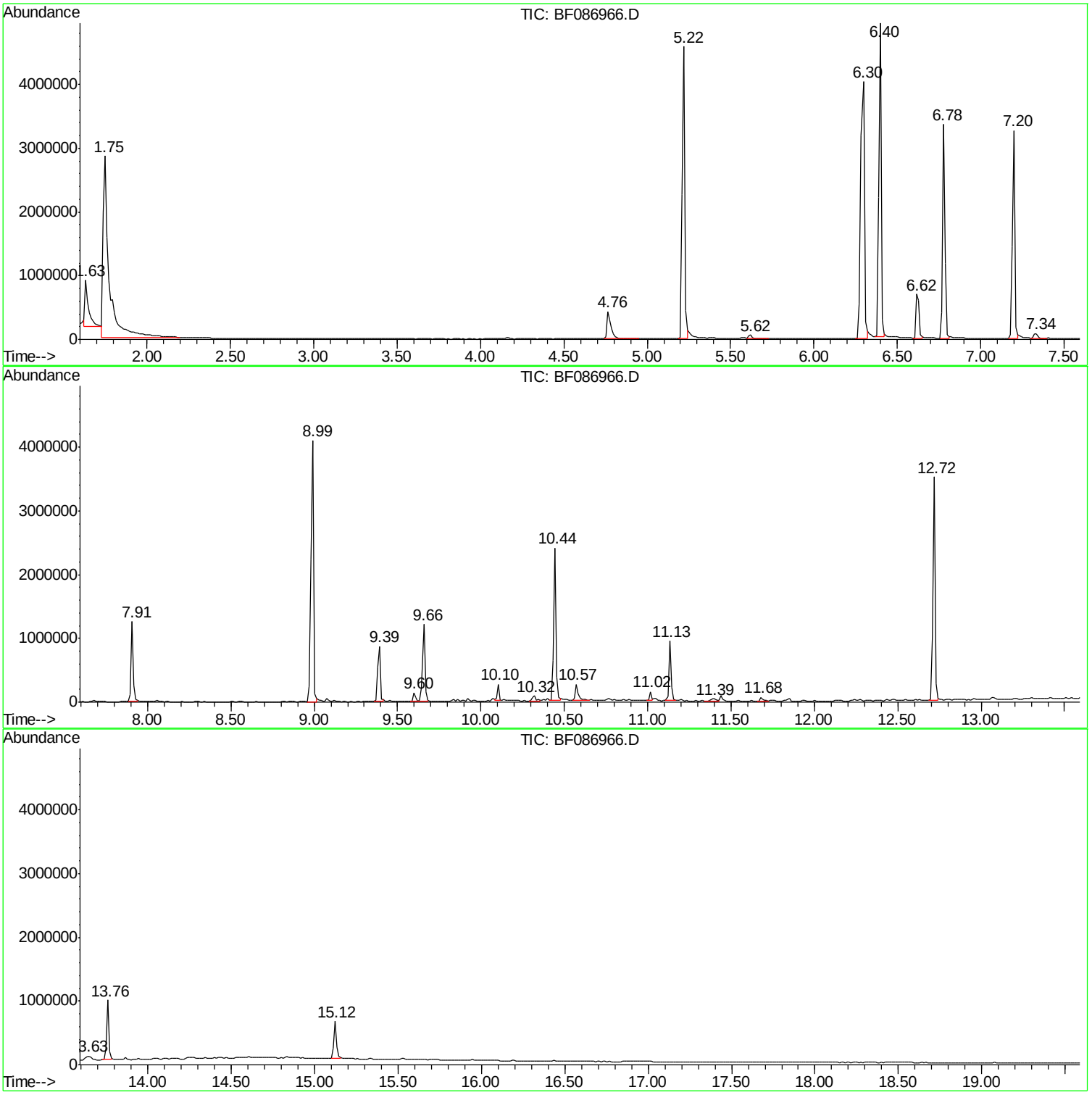
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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\BF051216\
Data File : BF086966.D
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Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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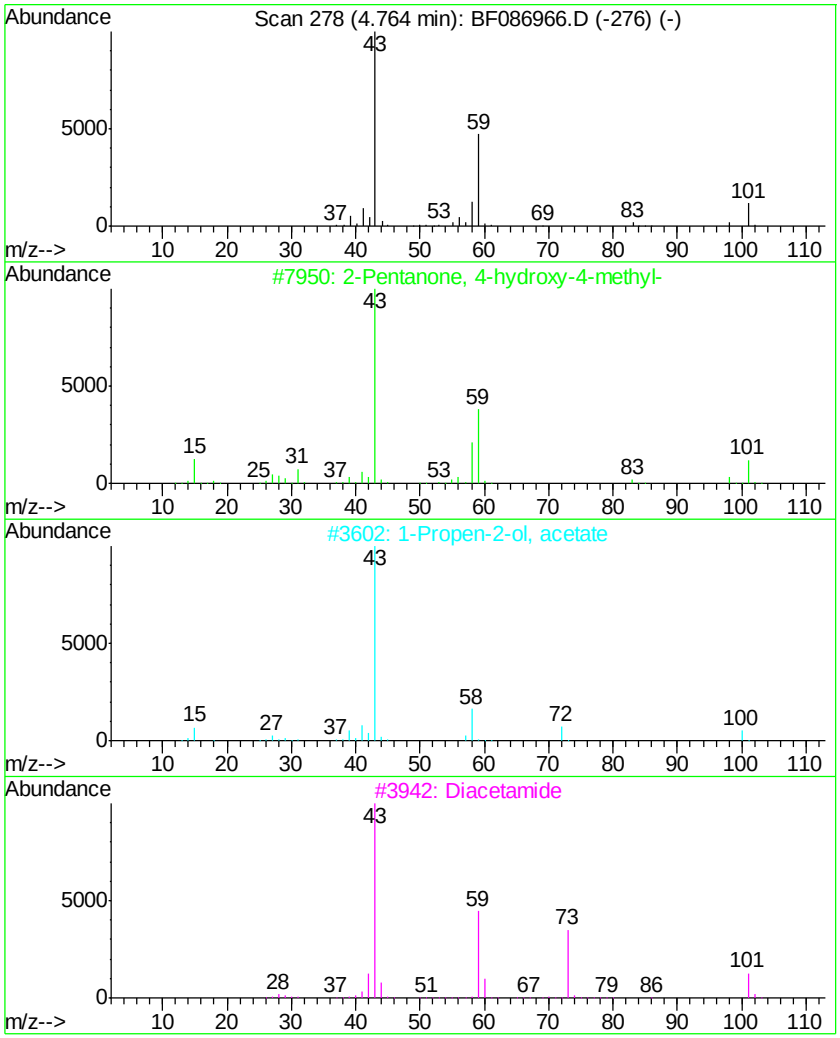
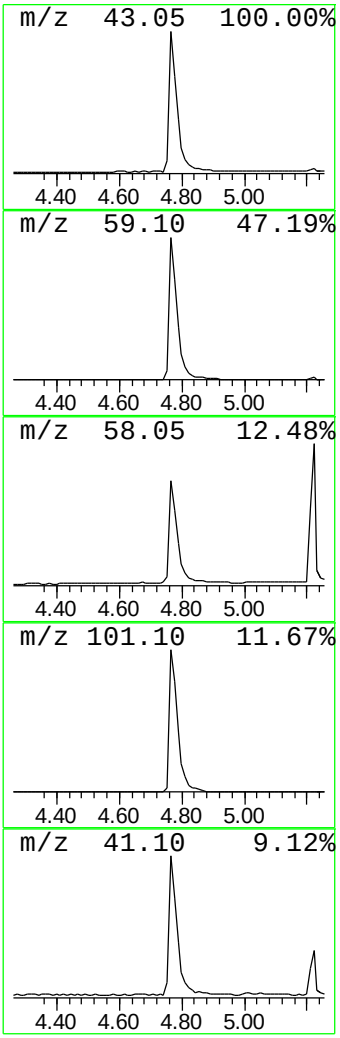
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	16.24 ng	752025	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	Butane	58	C4H10	000106-97-8	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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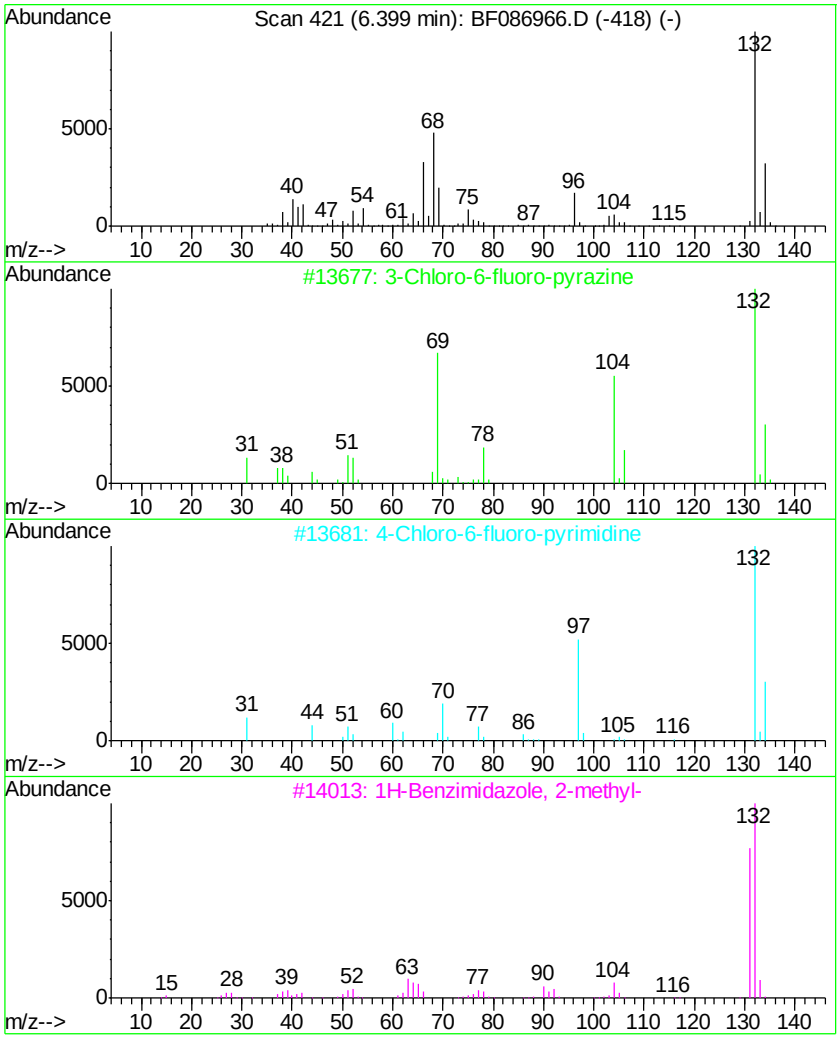
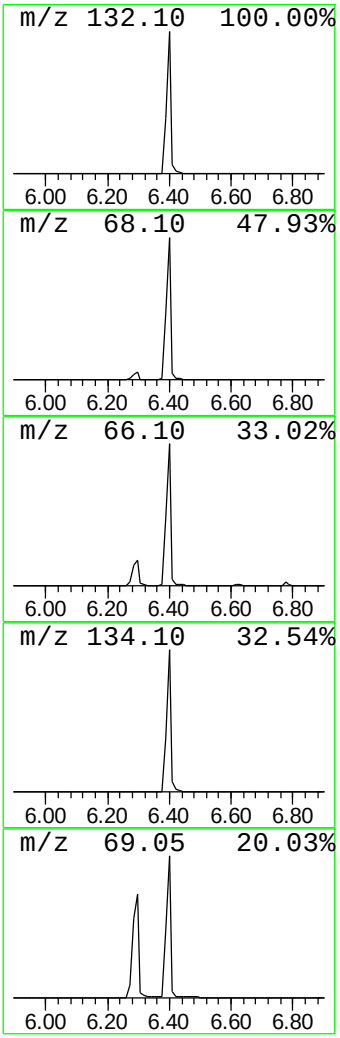
Peak Number 4 unknown6.40 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	110.26 ng	5104240	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





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Operator : UM/SJ
Sample : H2916-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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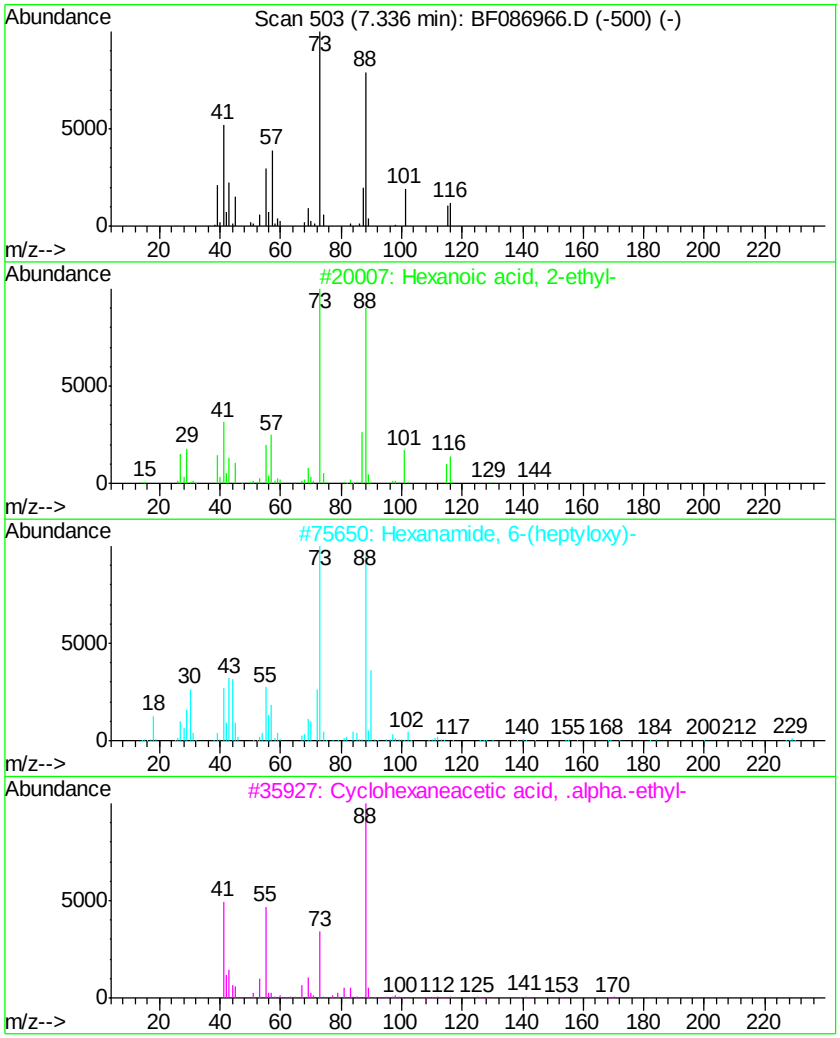
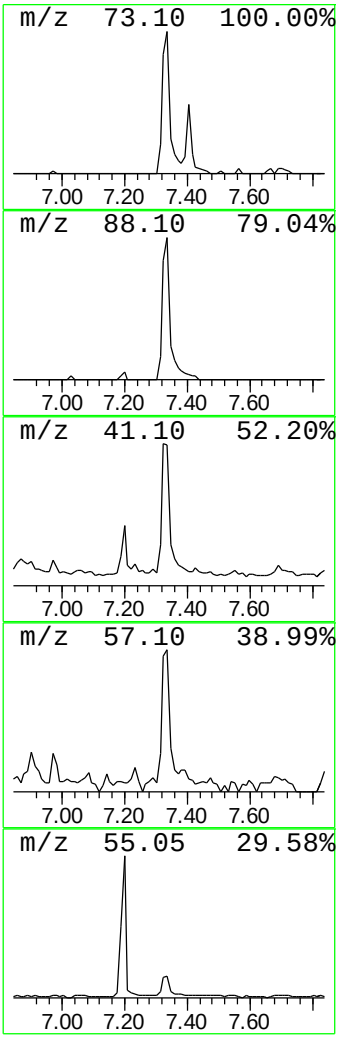
Peak Number 6 Hexanoic acid, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.34	2.30 ng	130652	Naphthalene-d8	7.91

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2	Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	40
3	Cyclohexaneacetic acid, .alpha.-...	170	C10H18O2	006051-00-9	28
4	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	28
5	Methyl (R)-(-)-3-hydroxy-2-methy...	118	C5H10O3	072657-23-9	25





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Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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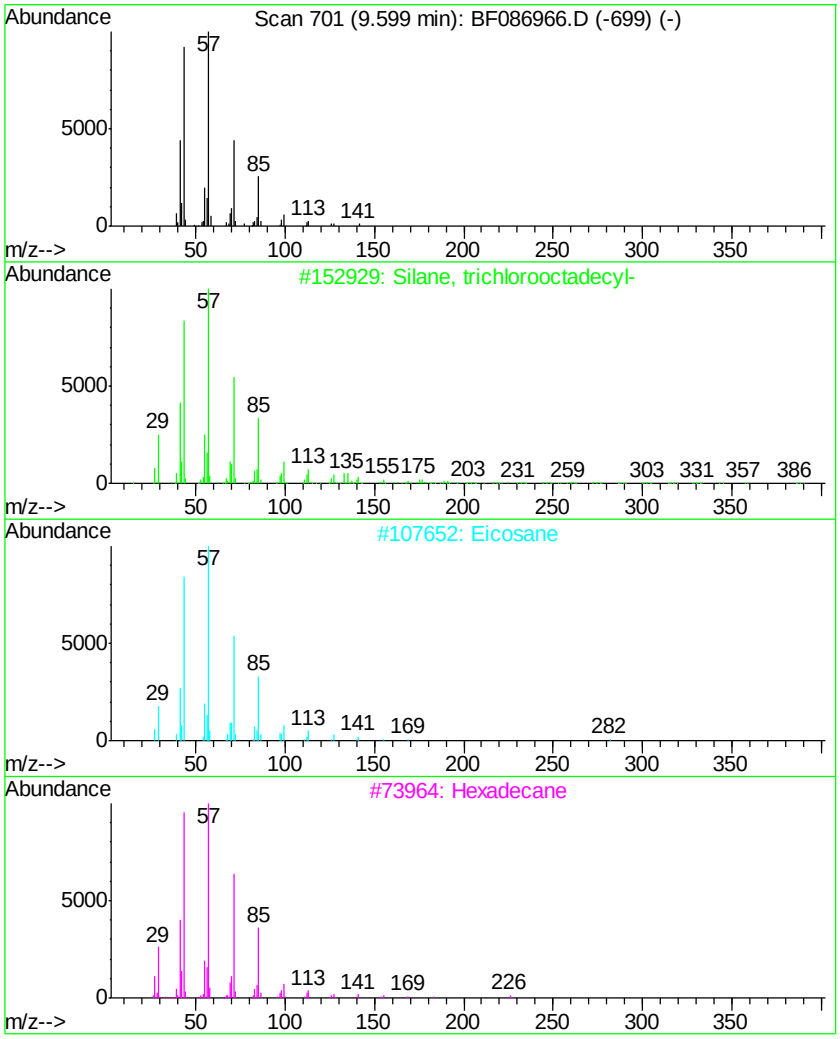
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

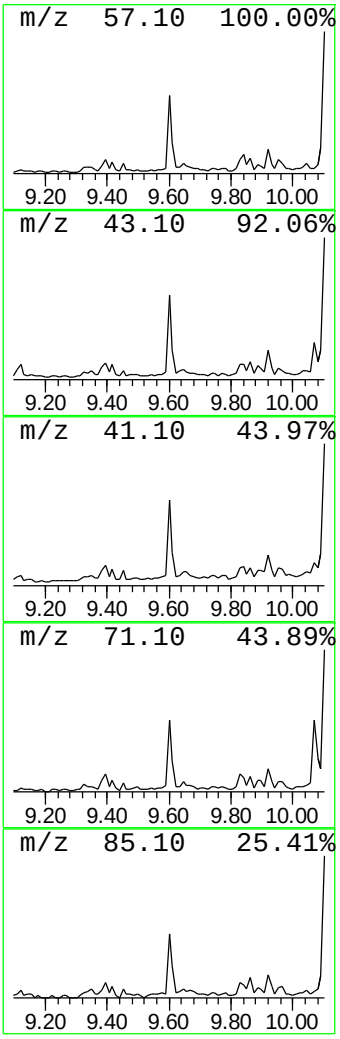
****

Peak Number 7 Silane, trichlorooctadecyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	2.45 ng	131701	Acenaphthene-d10	9.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	90
2	Eicosane	282	C20H42	000112-95-8	83
3	Hexadecane	226	C16H34	000544-76-3	80
4	Octadecane	254	C18H38	000593-45-3	80
5	Undecane	156	C11H24	001120-21-4	78





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Operator : UM/SJ
Sample : H2916-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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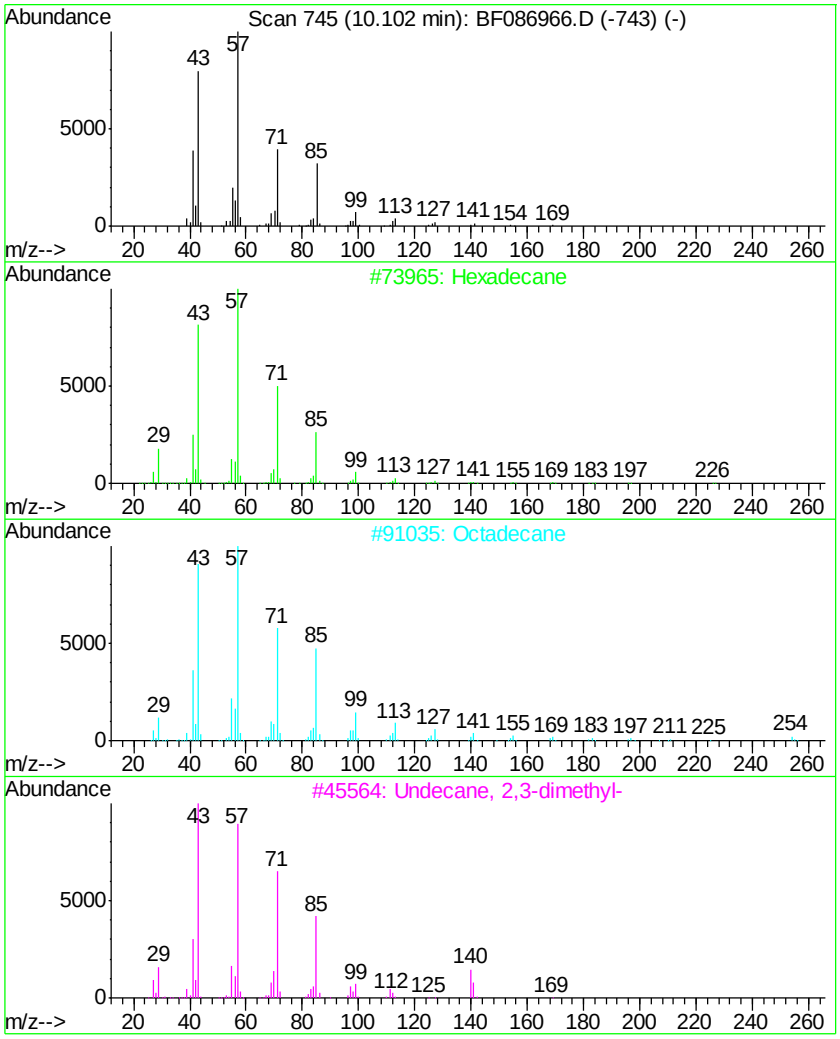
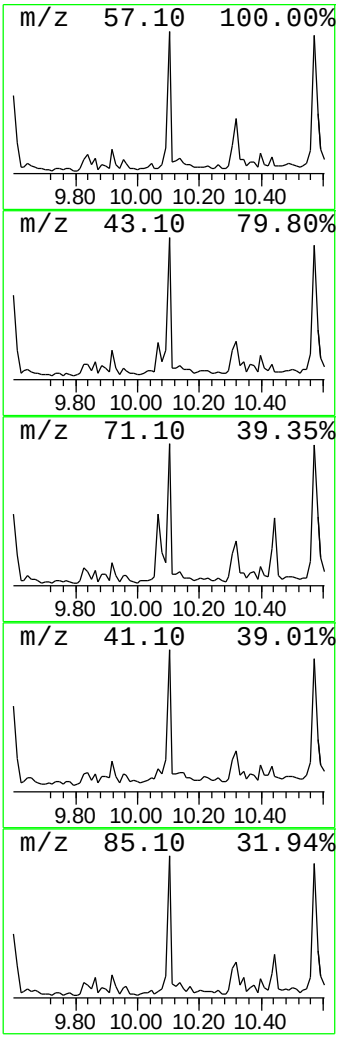
Peak Number 8 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	3.48 ng	187219	Acenaphthene-d10	9.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Octadecane	254	C18H38	000593-45-3	80
3	Undecane, 2,3-dimethyl-	184	C13H28	017312-77-5	72
4	Undecane	156	C11H24	001120-21-4	64
5	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	64





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Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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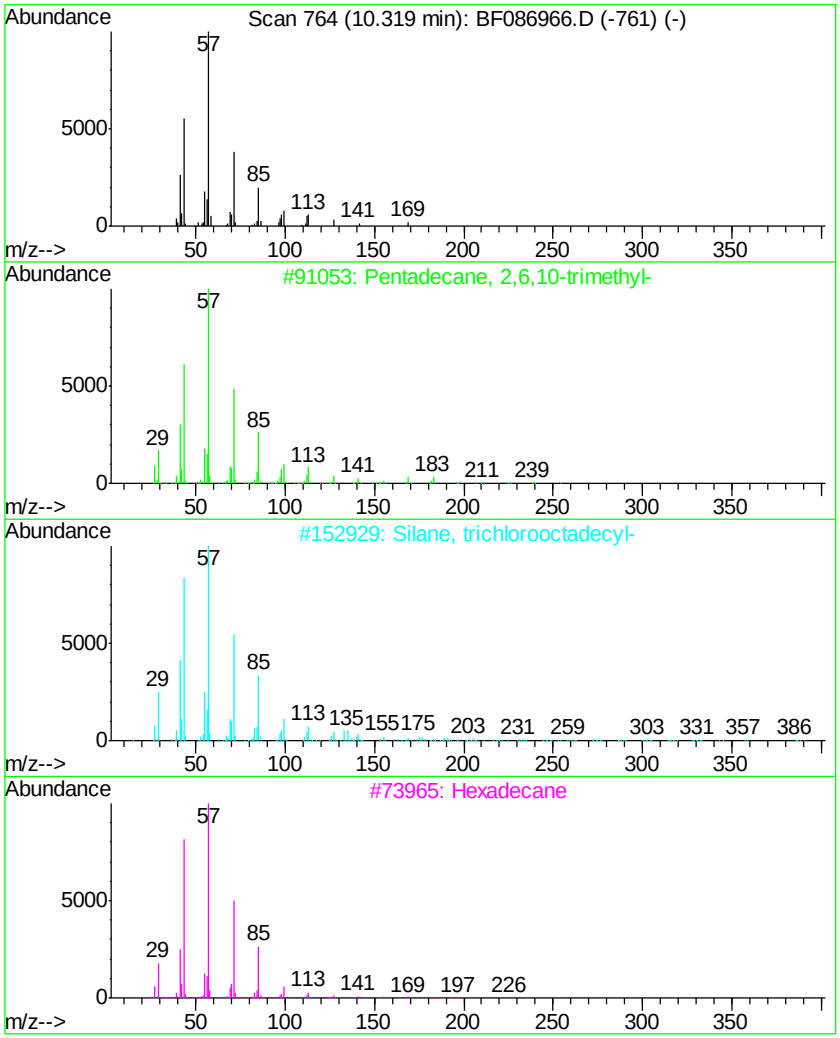
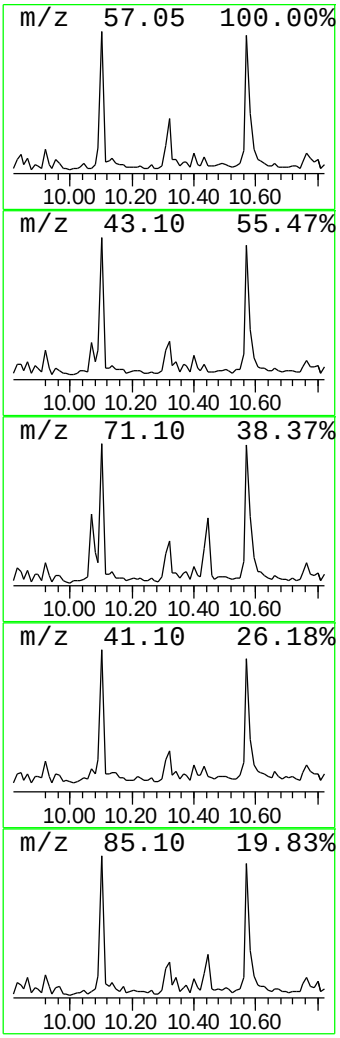
Peak Number 9 Pentadecane, 2,6,10-trimethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.32	2.28 ng	122419	Acenaphthene-d10	9.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	90
2	Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	86
3	Hexadecane	226	C16H34	000544-76-3	80
4	Eicosane	282	C20H42	000112-95-8	72
5	Hentriacontane	437	C31H64	000630-04-6	72





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Sample : H2916-06
Misc :
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Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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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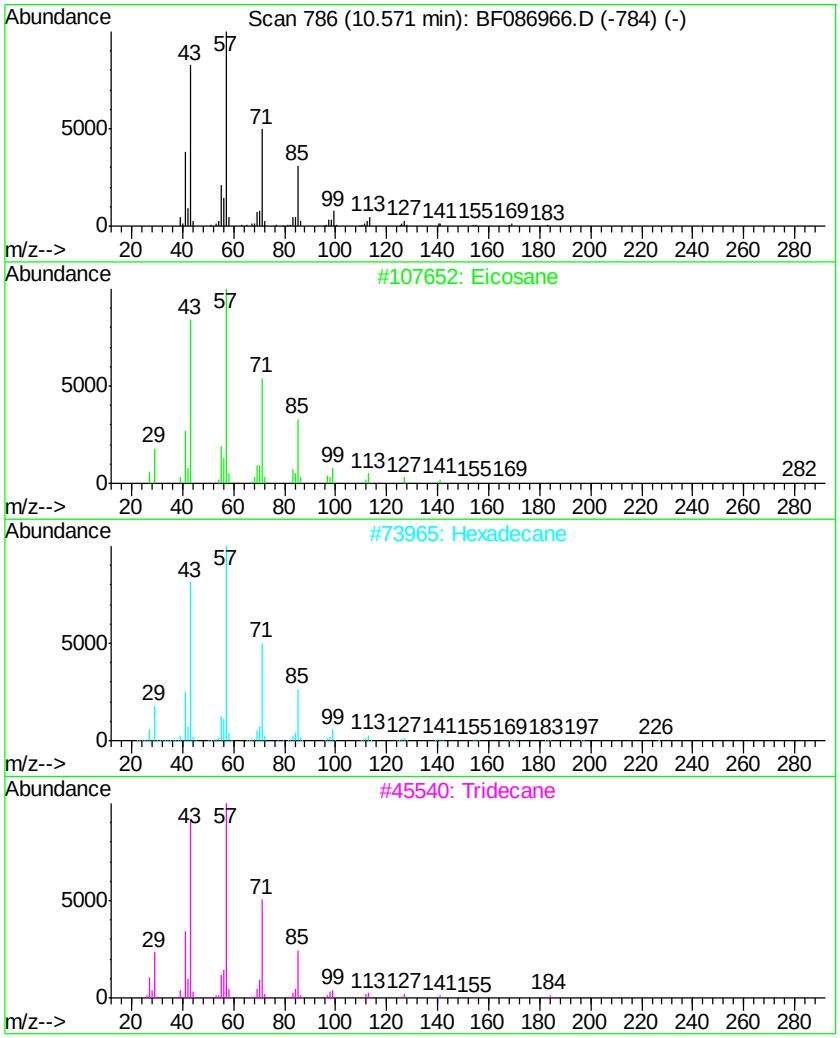
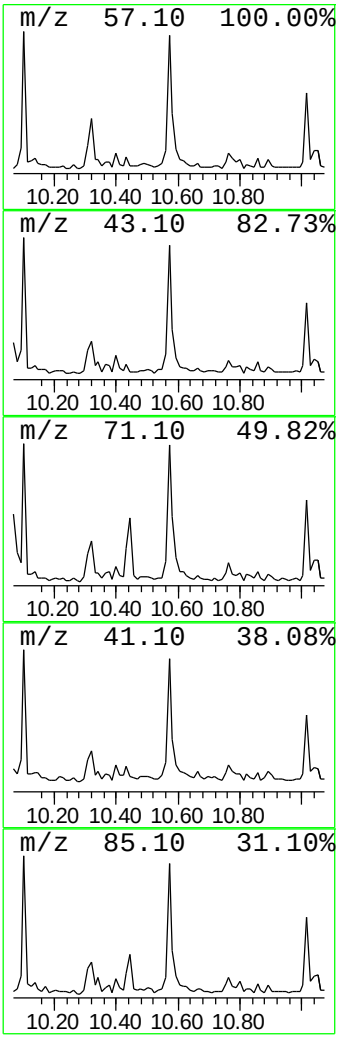
Peak Number 10 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.57	7.49 ng	309606	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	91
3	Tridecane	184	C13H28	000629-50-5	90
4	Octadecane	254	C18H38	000593-45-3	86
5	Tridecane, 7-propyl-	226	C16H34	055045-09-5	80





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Misc :
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Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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TIC Library : C:\DATABASE\NIST02.L
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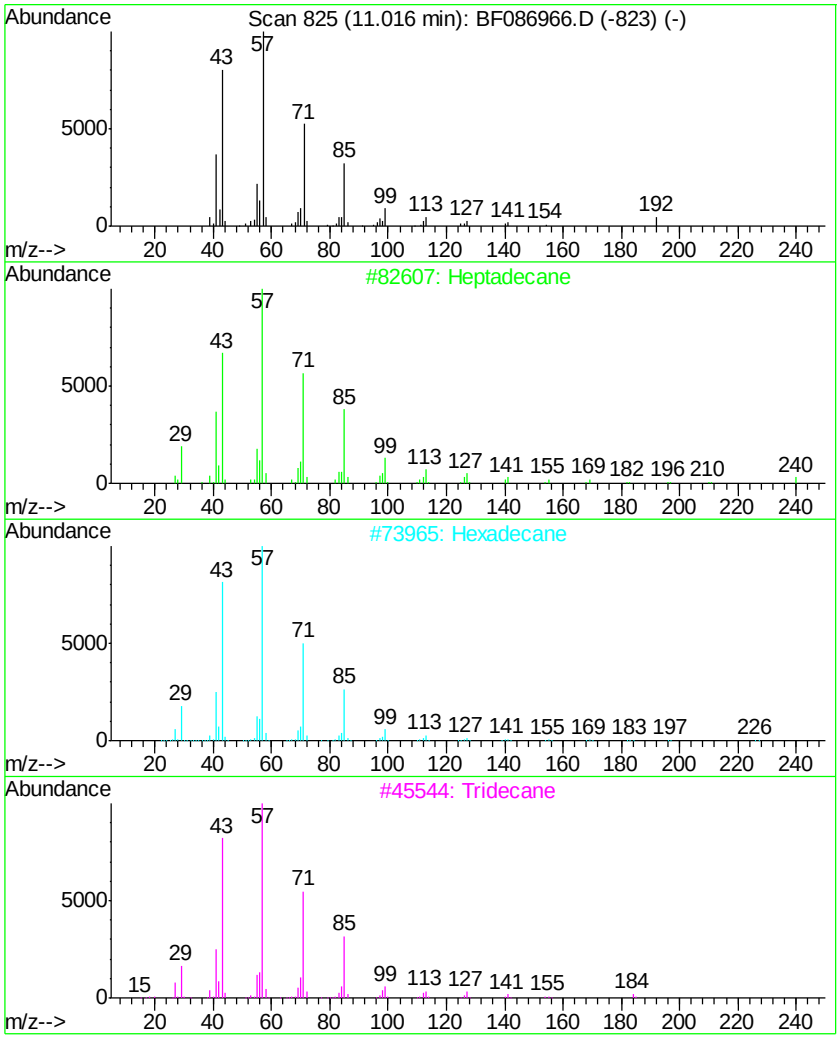
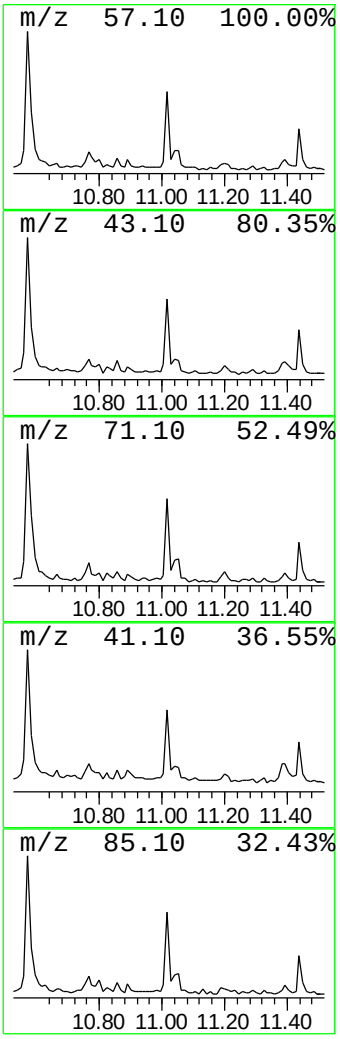
Peak Number 11 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.02	2.83 ng	116864	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Hexadecane	226	C16H34	000544-76-3	87
3	Tridecane	184	C13H28	000629-50-5	86
4	Eicosane	282	C20H42	000112-95-8	83
5	Octadecane	254	C18H38	000593-45-3	80





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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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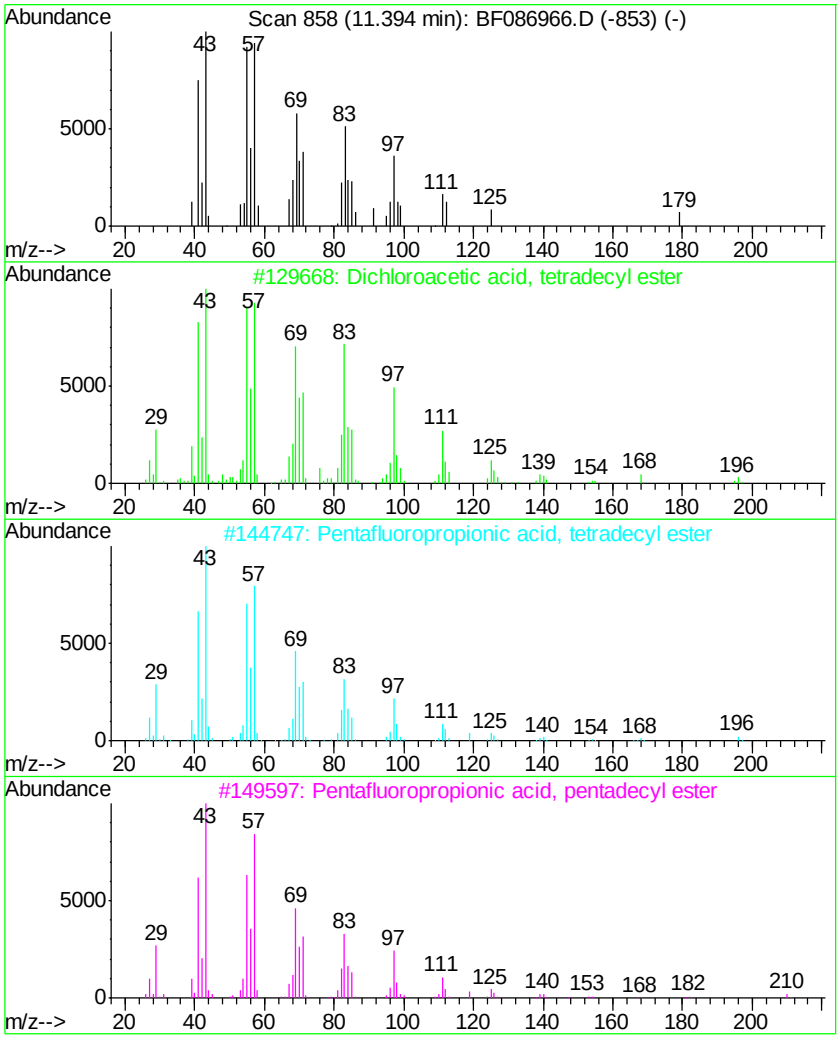
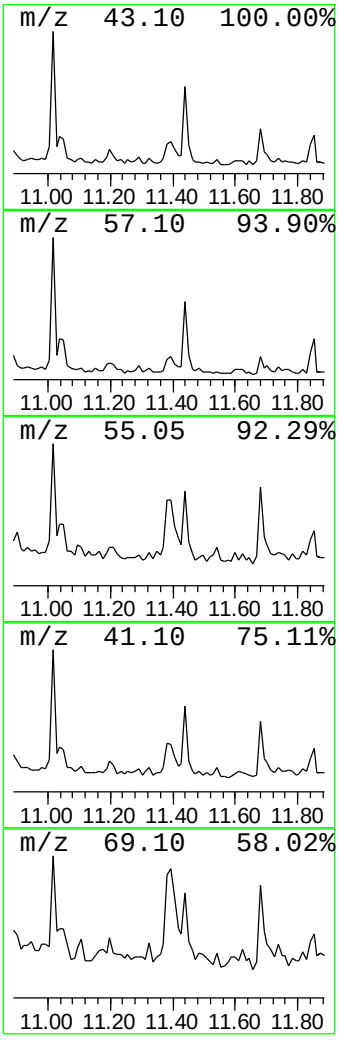
Peak Number 12 Dichloroacetic acid, tetrad... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.39	2.18 ng	90254	Phenanthrene-d10	11.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, tetradecyl ...	324	C16H30Cl2O2	083005-02-1	91
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	1000280-07-5	91
4	11-Tricosene	322	C23H46	052078-56-5	91
5	Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	91





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Sample : H2916-06
Misc :
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Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
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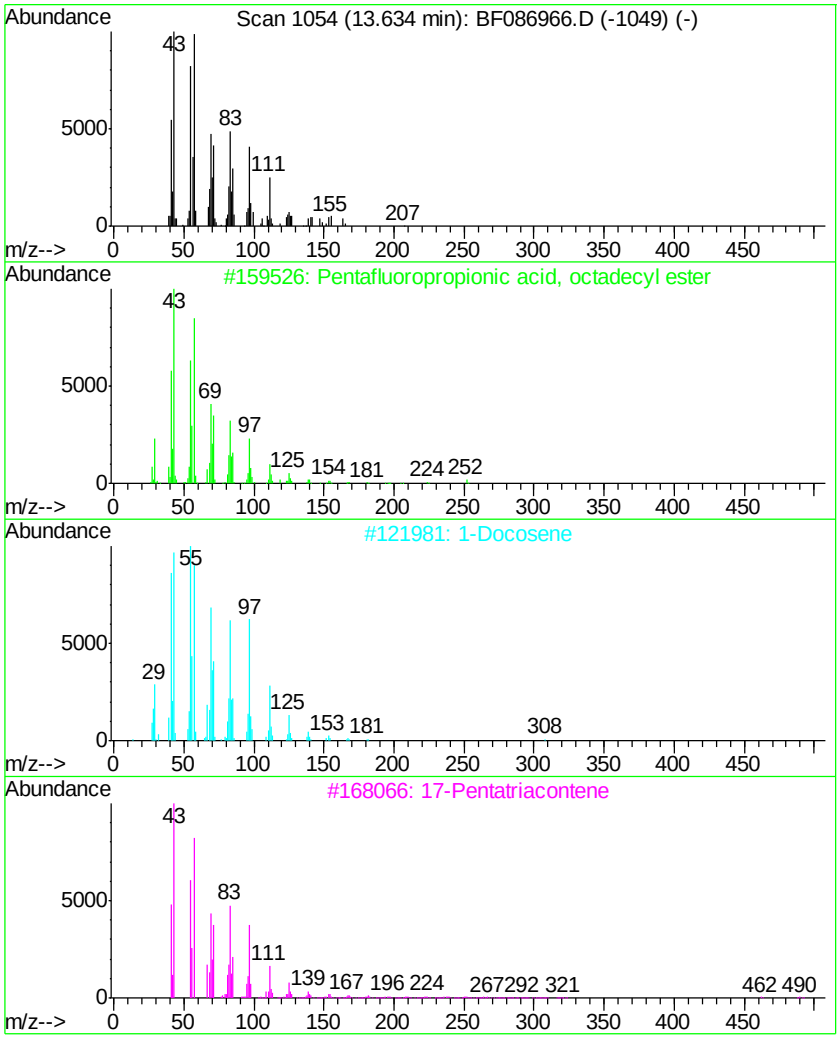
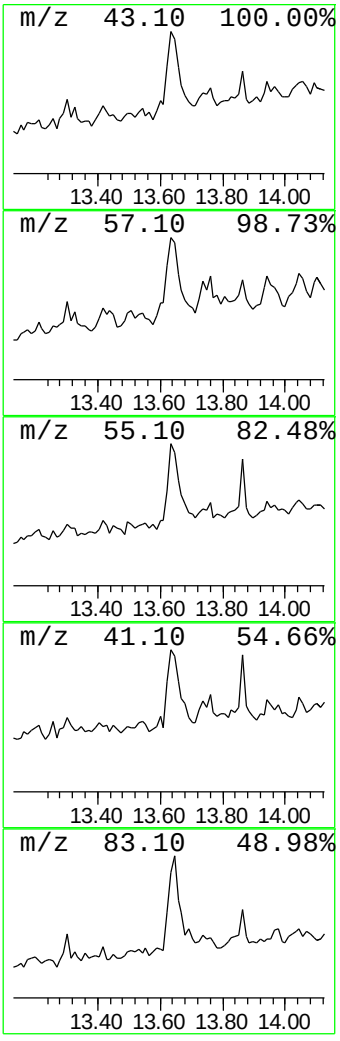
****

Peak Number 13 Pentafluoropropionic acid, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	5.59 ng	240956	Chrysene-d12	13.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
2	1-Docosene	308	C22H44	001599-67-3	90
3	17-Pentatriacontene	491	C35H70	006971-40-0	87
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	87
5	1-Hexacosanol	382	C26H54O	000506-52-5	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051216\
Data File : BF086966.D
Acq On : 13 May 2016 10:35
Operator : UM/SJ
Sample : H2916-06
Misc :
ALS Vial : 40 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : VITALE-FILL-CSPH3-6K

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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...	4.76	16.2	ng	752025	1	6.63	925894	20.0
unknown6.40	6.40	110.3	ng	5104240	1	6.63	925894	20.0
Hexanoic acid, 2-...	7.34	2.3	ng	130652	2	7.91	1137160	20.0
Silane, trichloro...	9.60	2.5	ng	131701	3	9.66	1076130	20.0
Hexadecane	10.10	3.5	ng	187219	3	9.66	1076130	20.0
Pentadecane, 2,6,...	10.32	2.3	ng	122419	3	9.66	1076130	20.0
Eicosane	10.57	7.5	ng	309606	4	11.13	827190	20.0
Heptadecane	11.02	2.8	ng	116864	4	11.13	827190	20.0
Dichloroacetic ac...	11.39	2.2	ng	90254	4	11.13	827190	20.0
Pentafluoropropio...	13.63	5.6	ng	240956	5	13.76	861428	20.0