LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075535.D
Acq On : 15 Nov 2014 12:04
Operator : TP / JJ
Sample : F4706-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(5-7)-111114

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-BF111214.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	1.612	43	46	49	rBV	4134468	4801632	100.00%	27.261%
2	1.761	56	59	64	rVB	147846	241458	5.03%	1.371%
3	1.955	73	76	84	rBV2	166051	323643	6.74%	1.837%
4	5.339	370	372	377	rVB	359069	388620	8.09%	2.206%
5	5.841	413	416	418	rBV	907298	1124017	23.41%	6.382%
6	7.087	523	525	528	rBV	1080465	1100821	22.93%	6.250%
7	7.259	537	540	542	rBV	1184863	1141483	23.77%	6.481%
8	7.544	563	565	568	rBV	253084	310202	6.46%	1.761%
9	7.739	580	582	584	rVB	854342	794968	16.56%	4.513%
10	8.242	623	626	628	rBV	635560	671101	13.98%	3.810%
11	9.133	701	704	706	rBV	405728	433502	9.03%	2.461%
12	10.470	819	821	824	rBV	1038030	1047558	21.82%	5.947%
13	10.973	863	865	867	rVB	170501	141586	2.95%	0.804%
14	11.305	892	894	897	rVB	444775	466281	9.71%	2.647%
15	12.208	971	973	975	rBV	134697	119837	2.50%	0.680%
16	12.288	977	980	983	rBV	769432	738988	15.39%	4.196%
17	13.156	1053	1056	1059	rBV	529335	503410	10.48%	2.858%
18	13.854	1115	1117	1120	rBV	72862	84974	1.77%	0.482%
19	14.962	1211	1214	1217	rBV	57530	70081	1.46%	0.398%
20	15.145	1228	1230	1233	rVB	863684	1075705	22.40%	6.107%
21	16.345	1330	1335	1341	rBV4	44443	185342	3.86%	1.052%
22	16.448	1341	1344	1346	rVV	525791	577392	12.02%	3.278%
23	16.871	1376	1381	1390	rVB10	26527	154722	3.22%	0.878%
24	18.151	1490	1493	1496	rBV	494242	678297	14.13%	3.851%
25	18.506	1518	1524	1525	rBV6	19783	57122	1.19%	0.324%
26	19.031	1566	1570	1579	rVB7	58402	253763	5.28%	1.441%
27	19.203	1581	1585	1586	rBV3	18034	49291	1.03%	0.280%
28	19.649	1617	1624	1626	rBV7	17606	77710	1.62%	0.441%

Sum of corrected areas: 17613506

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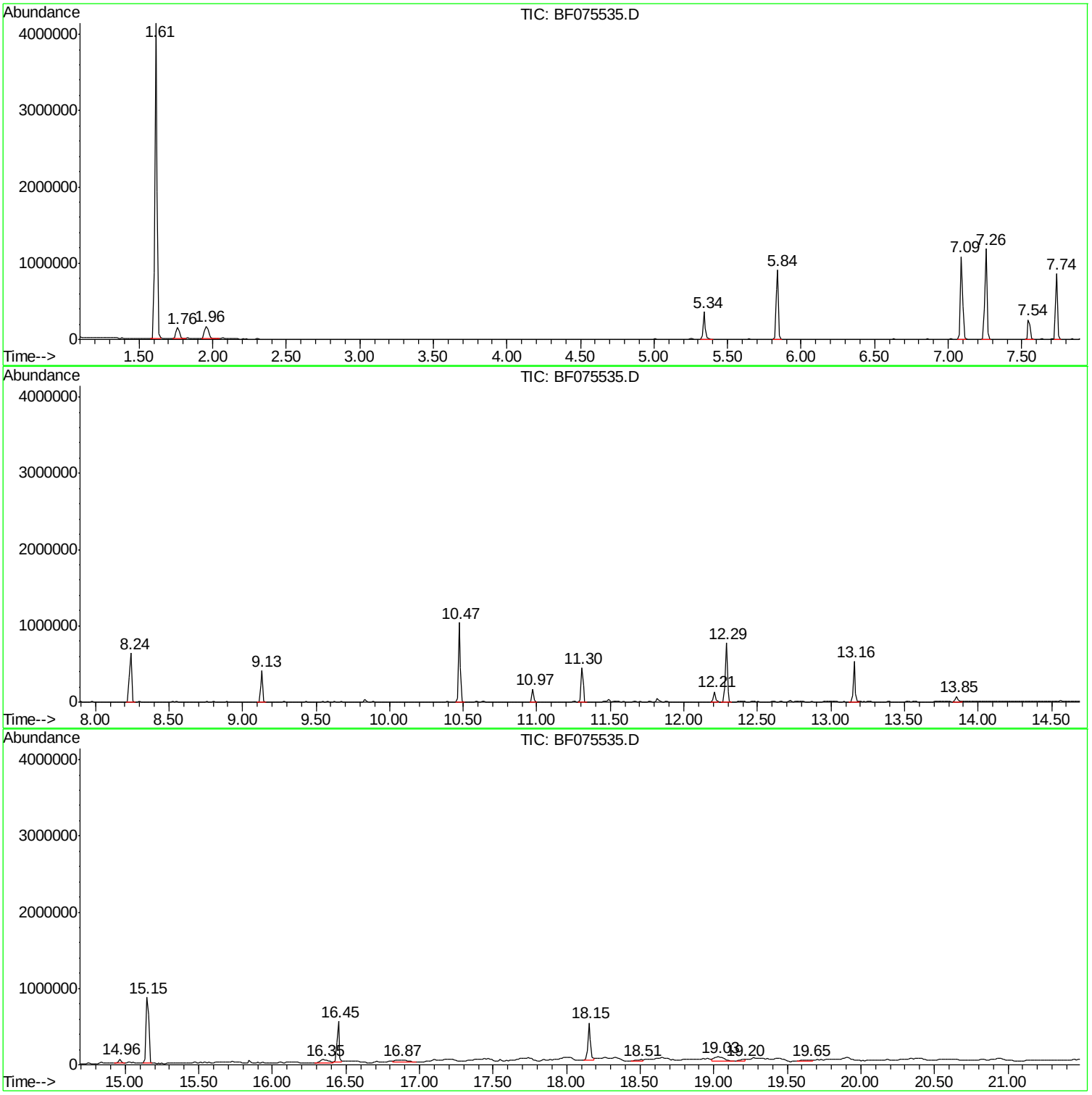
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-10(5-7)-111114

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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TIC Library : C:\DATABASE\NIST02.L
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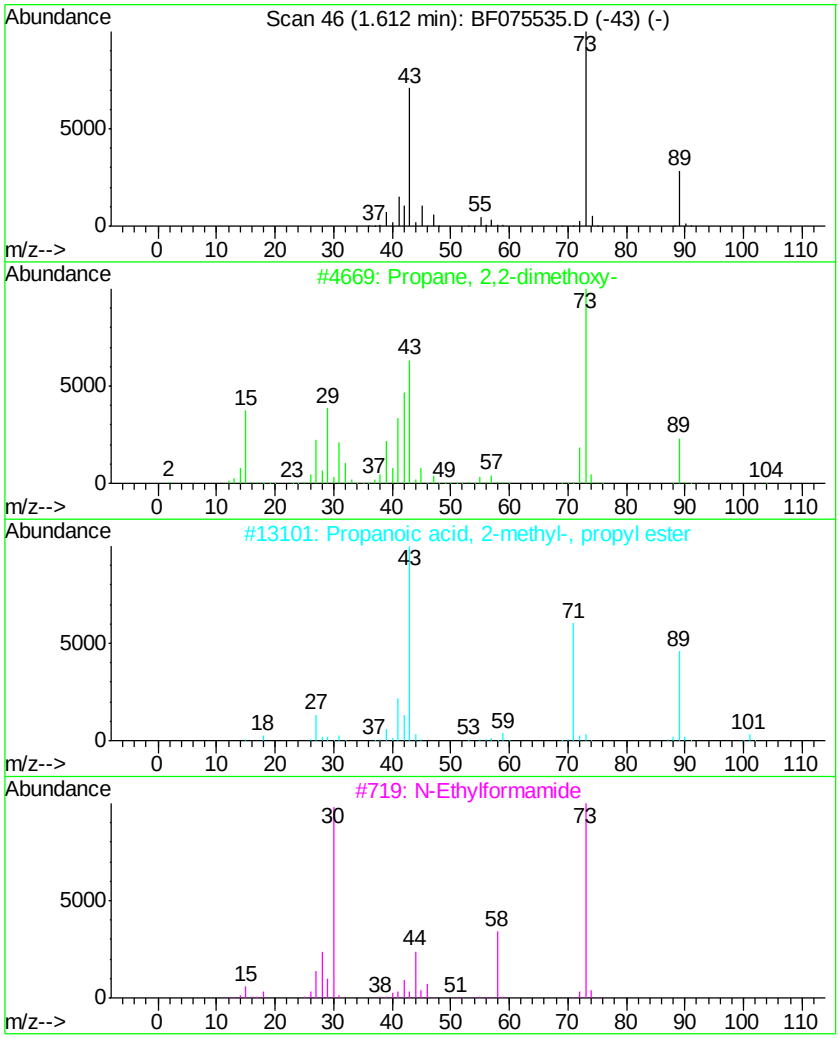
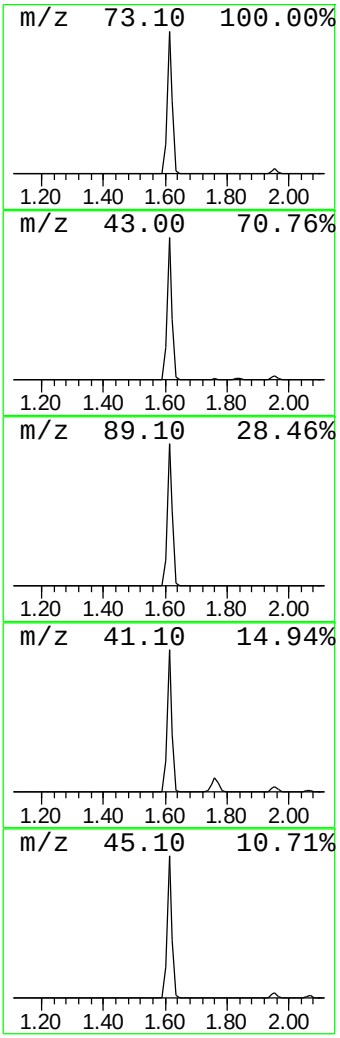
****

Peak Number 1 unknown1.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.61	309.58 ng	4801630	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	45
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	23
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9





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Operator : TP / JJ
Sample : F4706-09
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ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(5-7)-111114

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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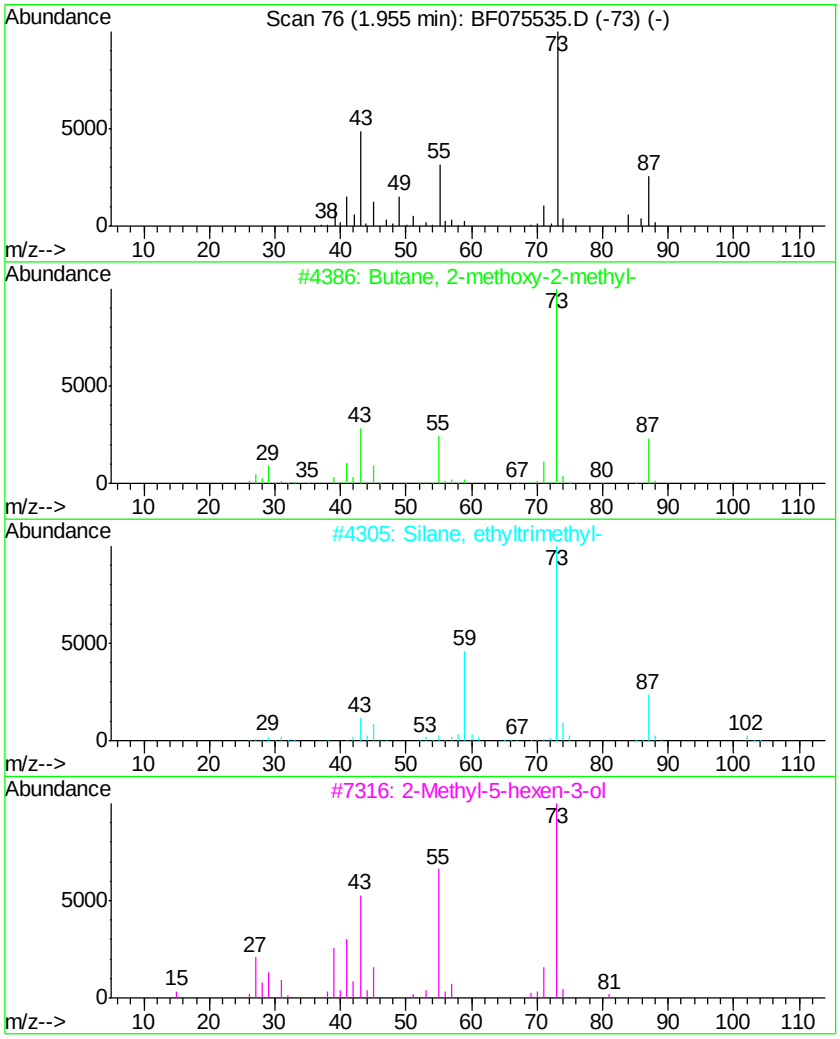
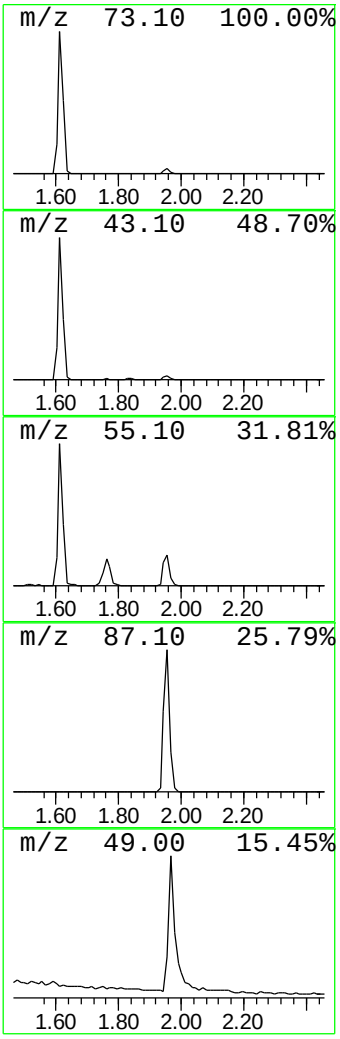
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.96	20.87 ng	323643	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	53
2	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	28
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5	1-Pentanamine	87	C5H13N	000110-58-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075535.D
Acq On : 15 Nov 2014 12:04
Operator : TP / JJ
Sample : F4706-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(5-7)-111114

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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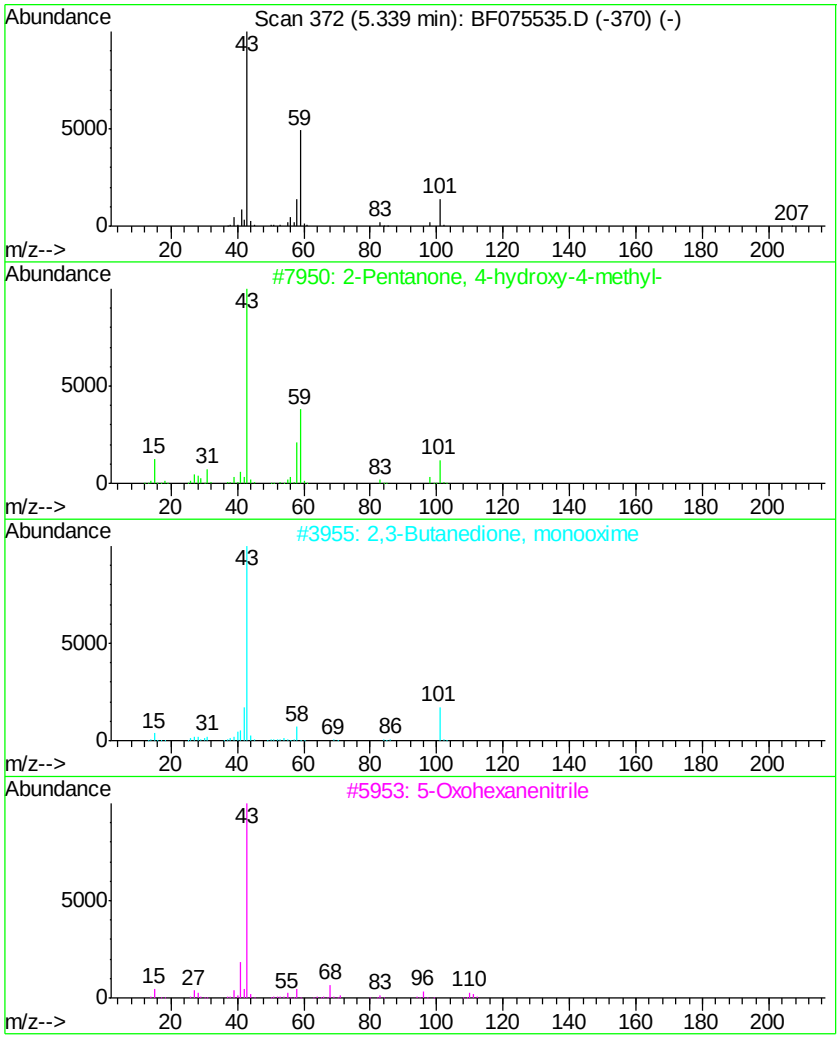
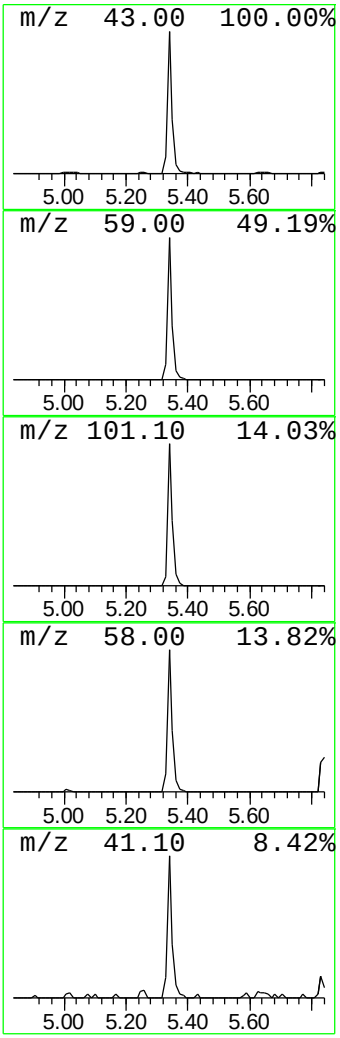
Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.34	25.06 ng	388620	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
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Acq On : 15 Nov 2014 12:04
Operator : TP / JJ
Sample : F4706-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(5-7)-111114

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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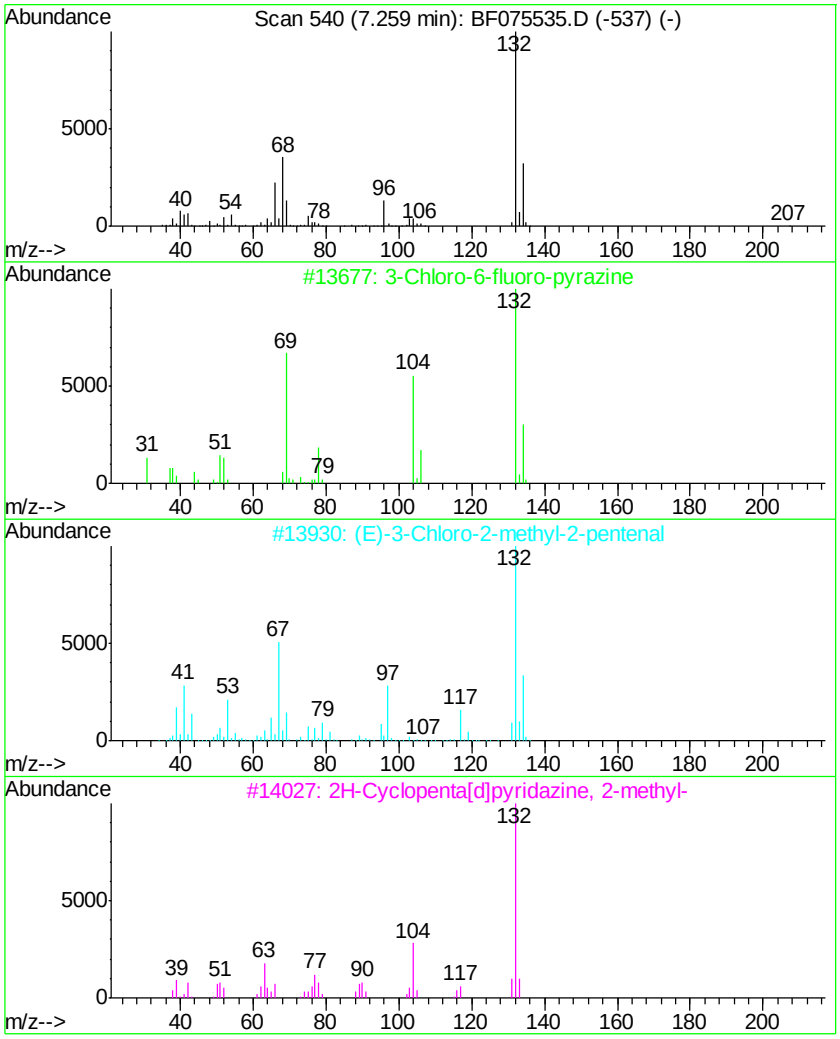
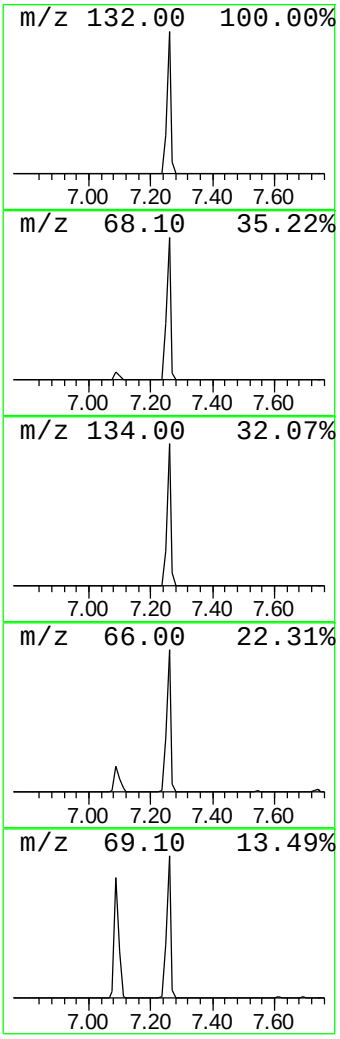
Peak Number 5 unknown7.26 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.26	73.60 ng	1141480	1,4-Dichlorobenzene-d4	7.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
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Sample : F4706-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(5-7)-111114

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
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TIC Library : C:\DATABASE\NIST02.L
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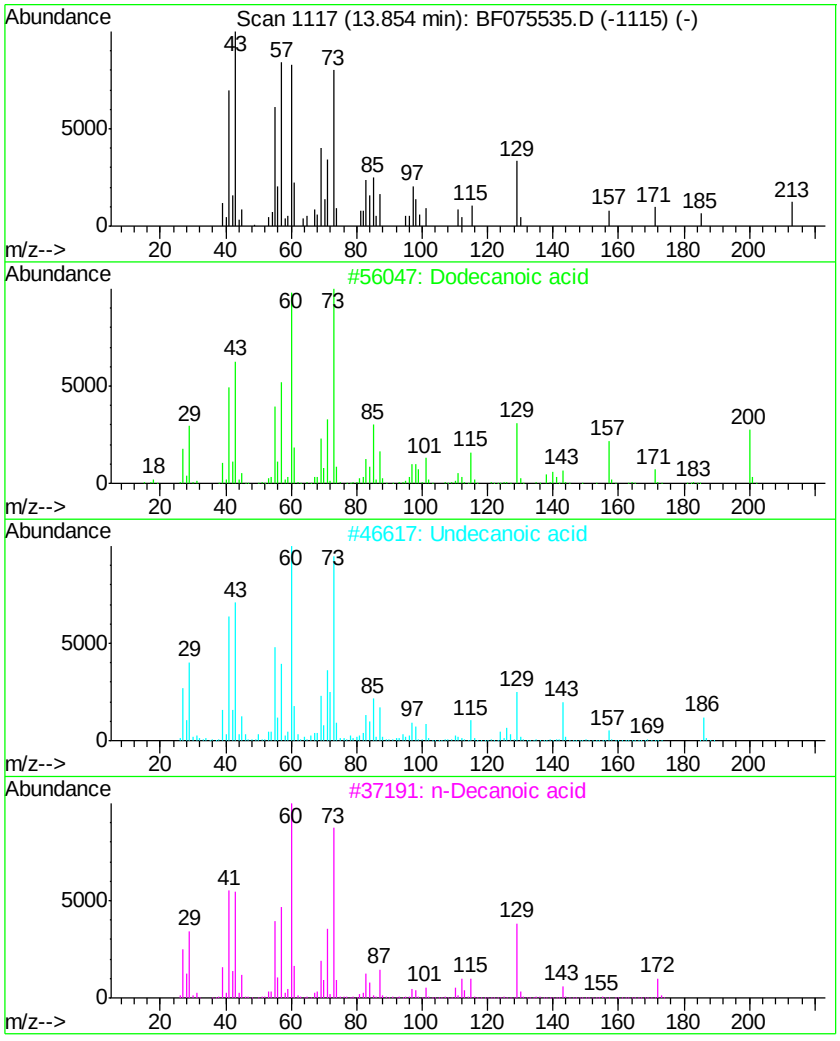
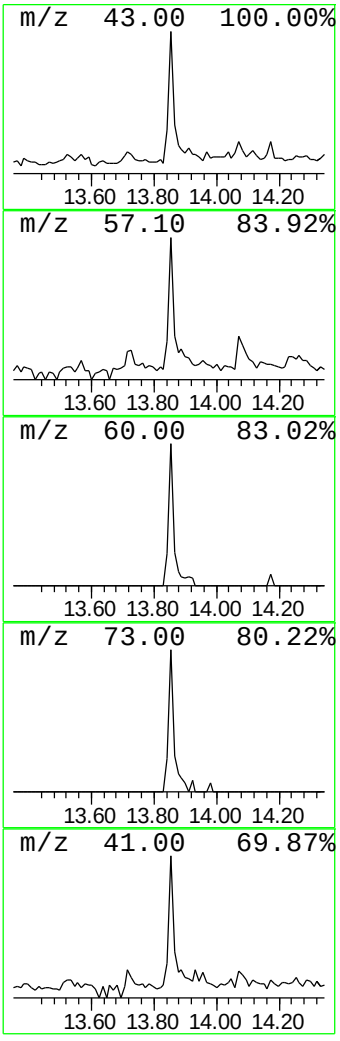
Peak Number 8 Dodecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.85	3.38 ng	84974	Phenanthrene-d10	13.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	72
2	Undecanoic acid	186	C11H22O2	000112-37-8	59
3	n-Decanoic acid	172	C10H20O2	000334-48-5	50
4	Nonanoic acid	158	C9H18O2	000112-05-0	47
5	Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
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TIC Library : C:\DATABASE\NIST02.L
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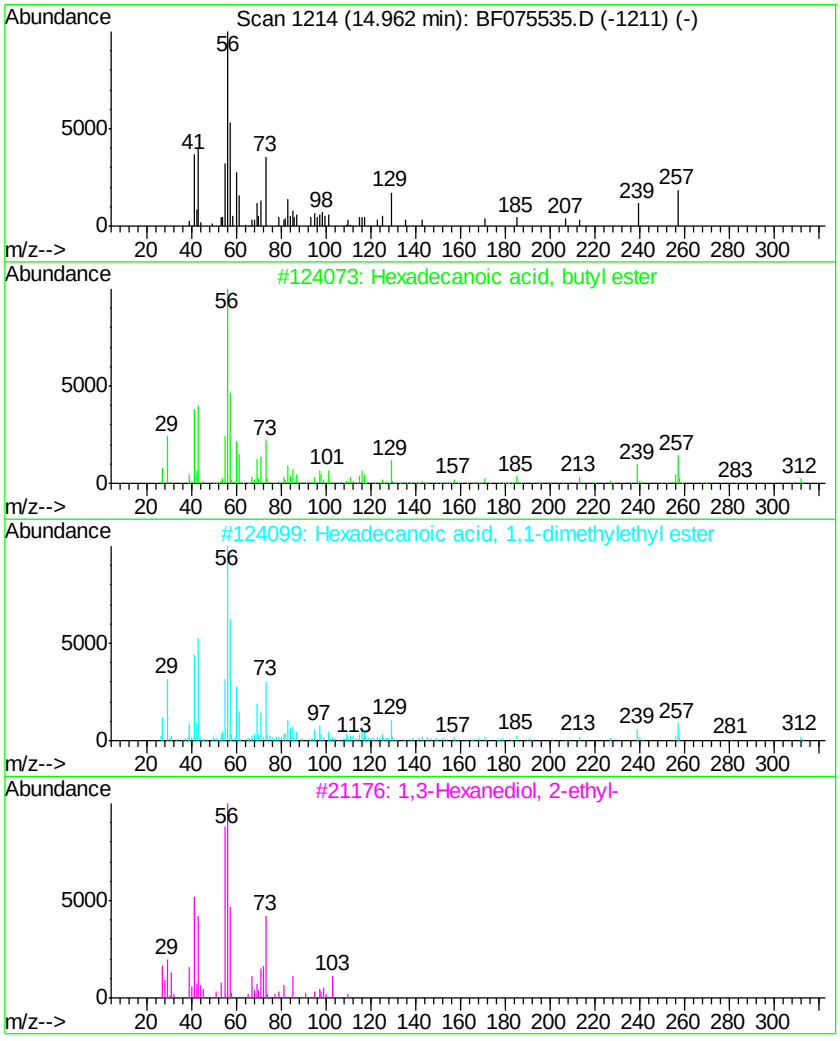
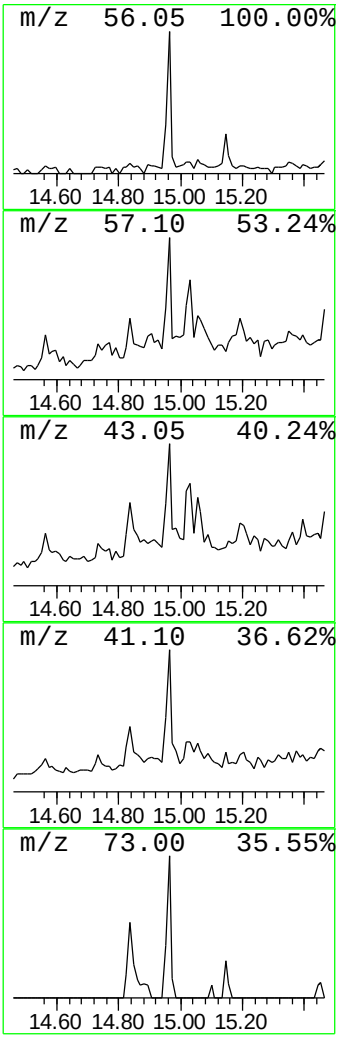
Peak Number 9 Hexadecanoic acid, butyl ester Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	2.43 ng	70081	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	90
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	80
3	1,3-Hexanediol, 2-ethyl-	146	C8H18O2	000094-96-2	37
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35





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Instrument : BNA_F
ClientSampleId : SB-10(5-7)-111114

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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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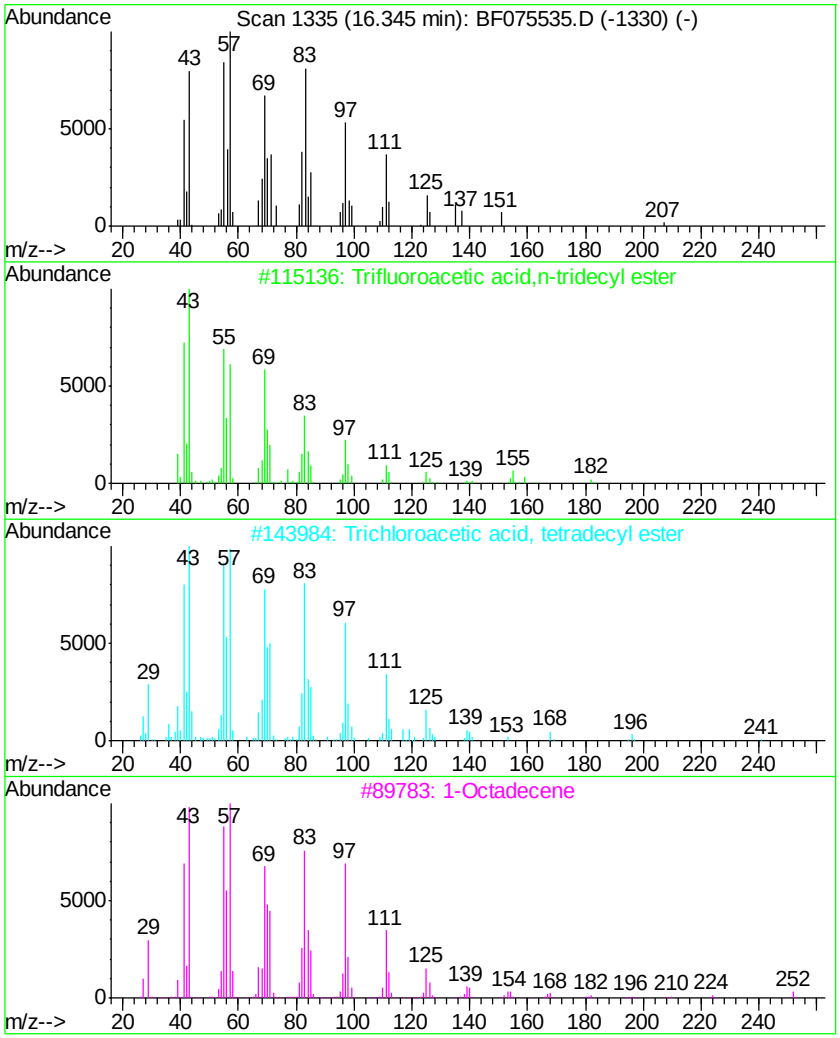
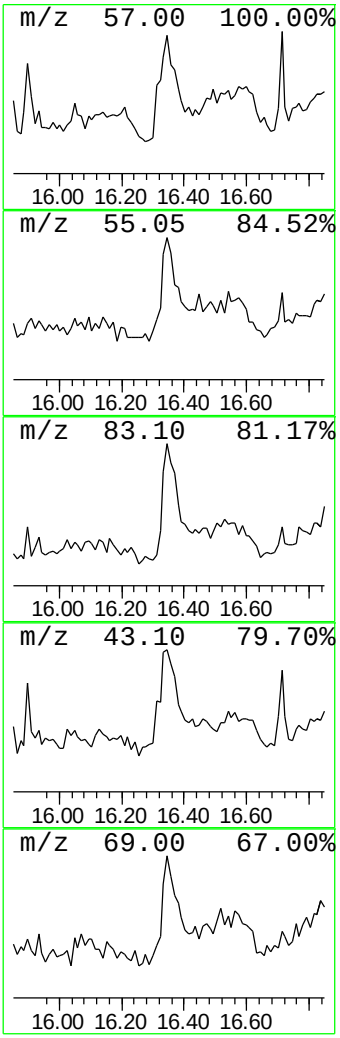
Peak Number 10 Trifluoroacetic acid,n-trid... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.35	6.42 ng	185342	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	80
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	74
3	1-Octadecene	252	C18H36	000112-88-9	64
4	17-Pentatriacontene	491	C35H70	006971-40-0	52
5	1-Hexadecanol	242	C16H34O	036653-82-4	52





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TIC Library : C:\DATABASE\NIST02.L
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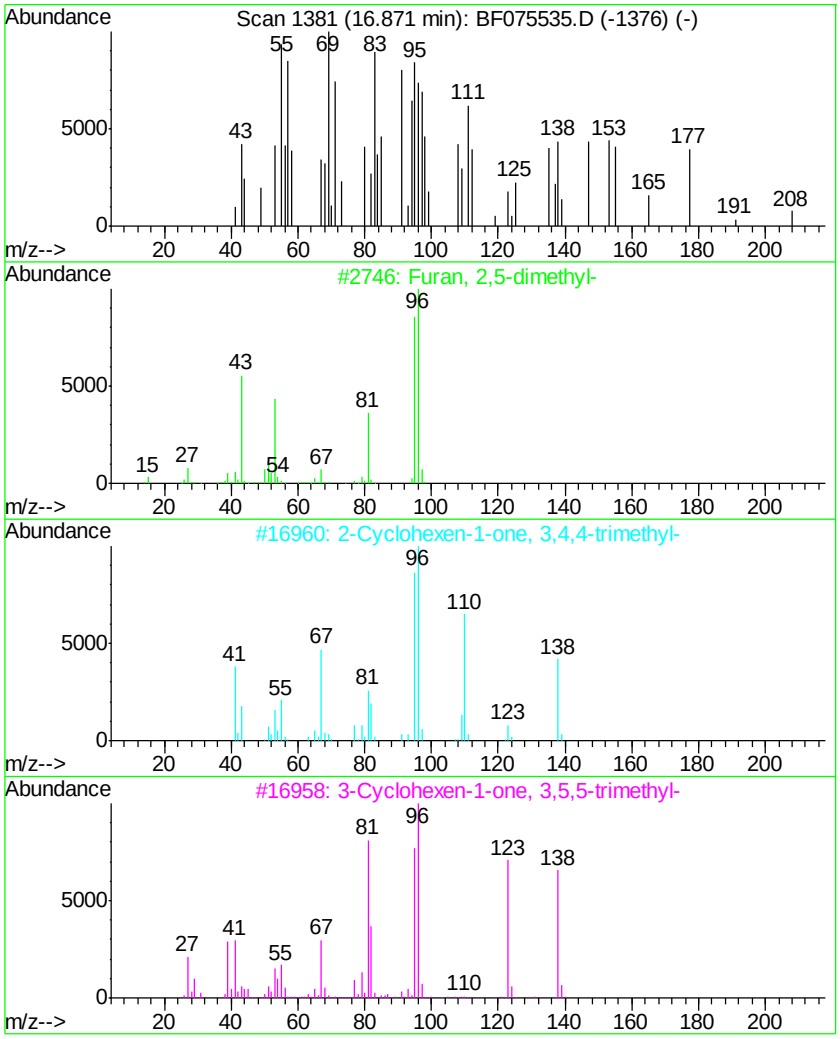
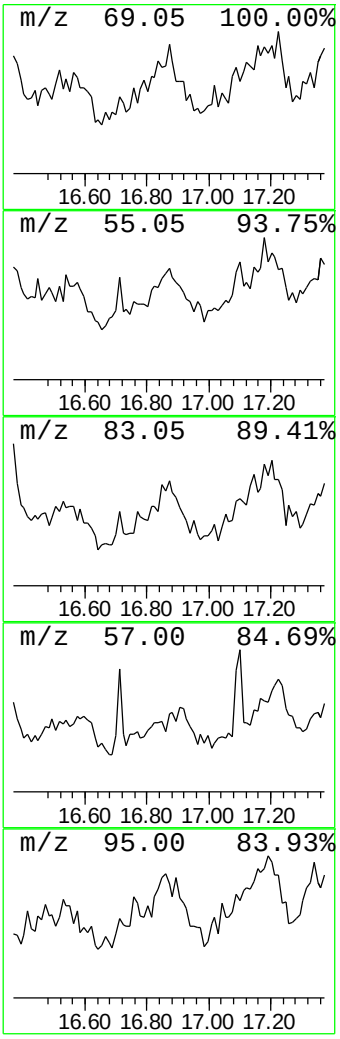
Peak Number 11 unknown16.87 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.87	5.36 ng	154722	Chrysene-d12	16.45

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	38
2	2-Cyclohexen-1-one, 3,4,4-trimet...	138	C9H14O	017299-41-1	14
3	3-Cyclohexen-1-one, 3,5,5-trimet...	138	C9H14O	000471-01-2	10
4	2R-Acetoxymethyl-1,3,5-trimethyl...	282	C17H30O3	1000144-12-6	10
5	Chloromethyl 6-chlorododecanoate	282	C13H24Cl2O2	080419-02-9	10





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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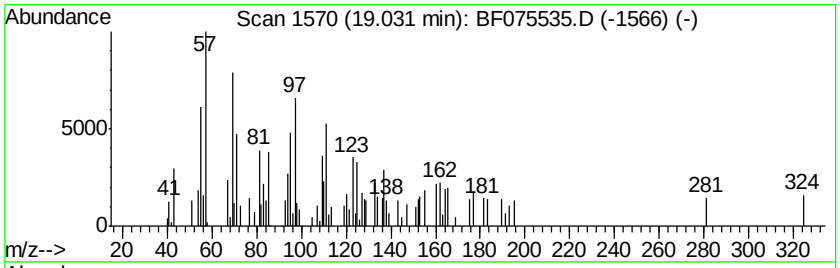
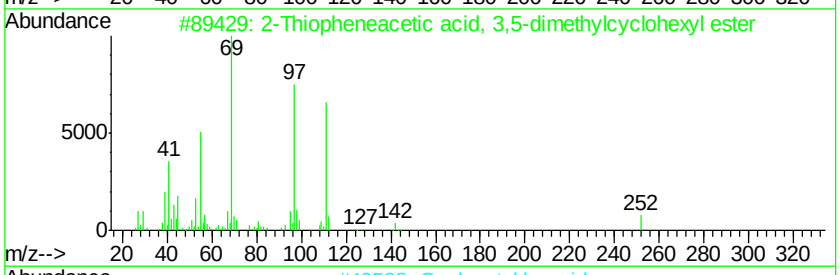
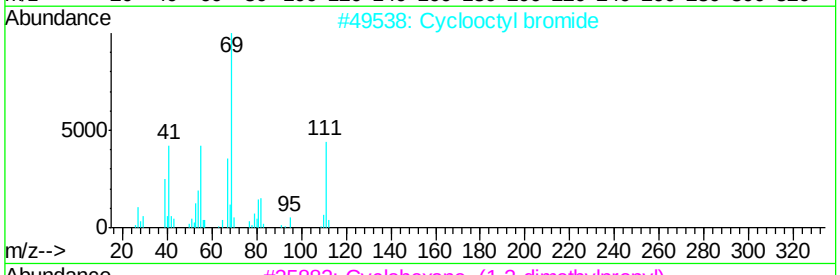
Peak Number 12 unknown19.03 Concentration Rank 7

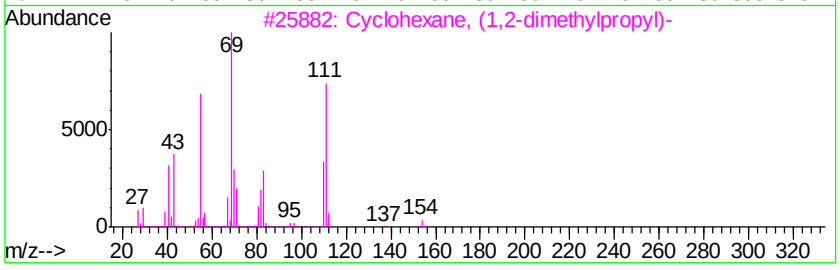
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.03	7.48 ng	253763	Perylene-d12	18.15

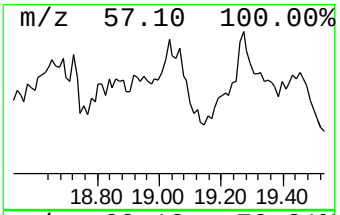
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Thiopheneacetic acid, 3,5-dime...	252	C14H20O2S	1000278-92-2	38
2	Cyclooctyl bromide	190	C8H15Br	001556-09-8	27
3	Cyclohexane, (1,2-dimethylpropyl)-	154	C11H22	051284-29-8	27
4	Cyclopentanecarboxylic acid, 3-t...	296	C19H36O2	1000280-58-5	27
5	Cyclohexane, 1-ethyl-2,4-dimethyl-	140	C10H20	061142-69-6	27

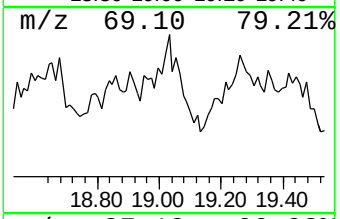


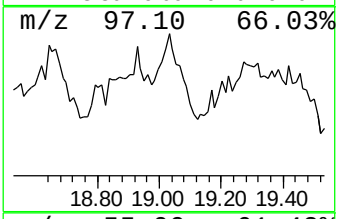


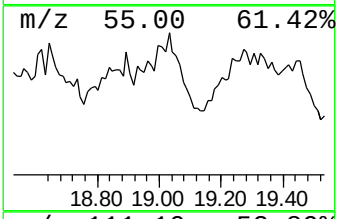


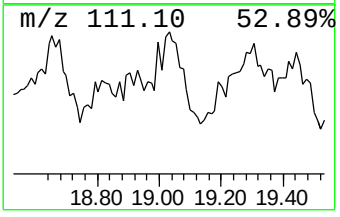












Data Path : Z:\HPCHEM1\BNA F\DATA\BF111414\
Data File : BF075535.D
Acq On : 15 Nov 2014 12:04
Operator : TP / JJ
Sample : F4706-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(5-7)-111114

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

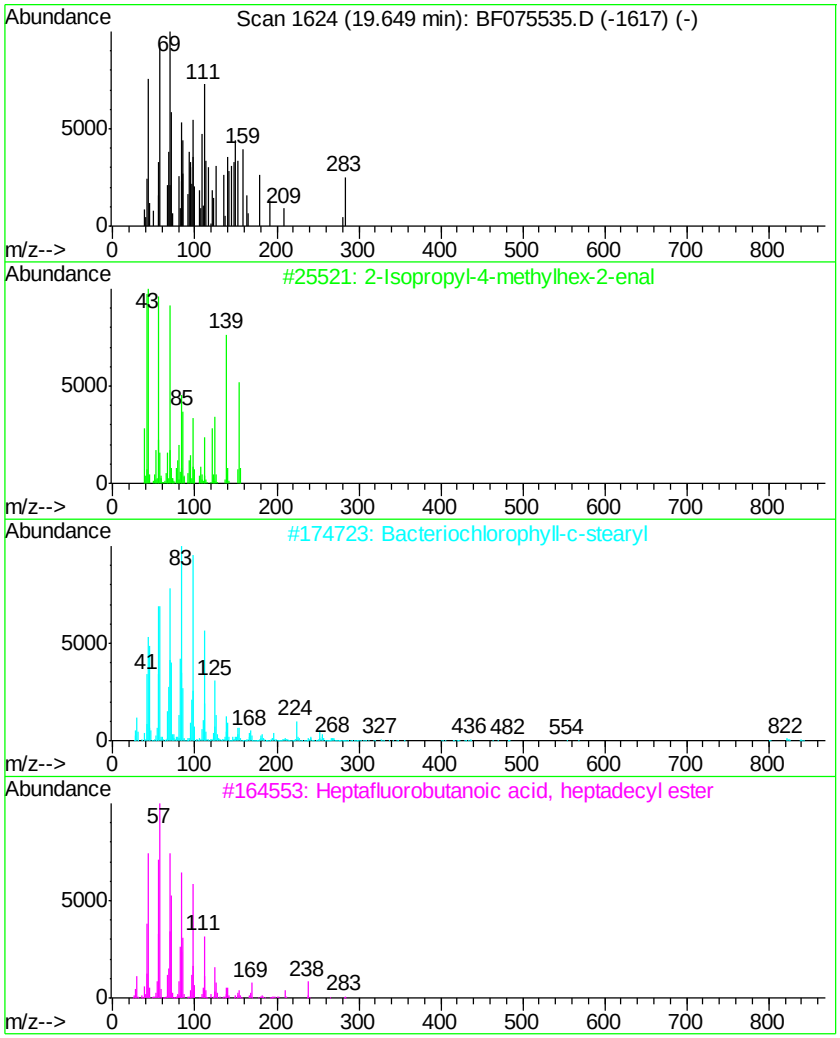
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

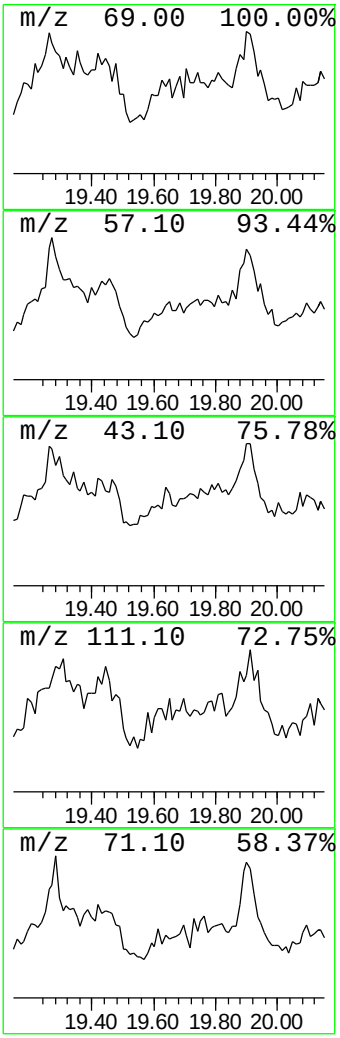
****

Peak Number 13 unknown19.65 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.65	2.29 ng	77710	Perylene-d12	18.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropyl-4-methylhex-2-enal	154	C10H18O	072668-37-2	27
2	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1000164-49-7	16
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	16
4	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	16
5	2-Thiophenecarboxylic acid, 4-te...	324	C19H32O2S	1000280-66-3	16





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111414\
Data File : BF075535.D
Acq On : 15 Nov 2014 12:04
Operator : TP / JJ
Sample : F4706-09
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-10(5-7)-111114

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF111214.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
unknown1.61	1.61	309.6	ng	4801630	1	7.54	310202	20.0
Butane, 2-methoxy...	1.96	20.9	ng	323643	1	7.54	310202	20.0
2-Pentanone, 4-hy...	5.34	25.1	ng	388620	1	7.54	310202	20.0
unknown7.26	7.26	73.6	ng	1141480	1	7.54	310202	20.0
Dodecanoic acid	13.85	3.4	ng	84974	4	13.16	503410	20.0
Hexadecanoic acid...	14.96	2.4	ng	70081	5	16.45	577392	20.0
Trifluoroacetic a...	16.35	6.4	ng	185342	5	16.45	577392	20.0
unknown16.87	16.87	5.4	ng	154722	5	16.45	577392	20.0
unknown19.03	19.03	7.5	ng	253763	6	18.15	678297	20.0
unknown19.65	19.65	2.3	ng	77710	6	18.15	678297	20.0