LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040915\
Data File : BF078386.D
Acq On : 10 Apr 2015 6:22
Operator : TP/IZ
Sample : G1782-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB04(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-BF040115.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	1.070	14	16	18	rVB	274375	384468	21.91%	3.448%
2	1.173	21	25	28	rVB	104768	183663	10.46%	1.647%
3	1.321	36	38	41	rVB	73482	93028	5.30%	0.834%
4	1.538	55	57	64	rVV	89316	158910	9.05%	1.425%
5	1.630	64	65	100	rVB	791341	1755072	100.00%	15.739%
6	4.567	320	322	329	rBV	60799	84648	4.82%	0.759%
7	5.150	371	373	383	rBB	640904	781745	44.54%	7.011%
8	6.487	488	490	498	rVB	827635	810448	46.18%	7.268%
9	6.602	498	500	503	rBV	873375	854278	48.67%	7.661%
10	6.887	523	525	527	rBV	186020	203787	11.61%	1.828%
11	7.070	539	541	543	rBV	689611	627452	35.75%	5.627%
12	7.585	583	586	588	rBV	563521	490098	27.92%	4.395%
13	8.465	661	663	665	rBV	291078	284488	16.21%	2.551%
14	9.813	778	781	783	rBV	851300	854153	48.67%	7.660%
15	10.328	824	826	828	rBB	33724	43175	2.46%	0.387%
16	10.625	849	852	854	rBV	312226	340825	19.42%	3.056%
17	11.528	929	931	933	rBV	30472	28535	1.63%	0.256%
18	11.596	935	937	940	rBV	564135	552931	31.50%	4.959%
19	11.848	957	959	963	rVV2	13098	22291	1.27%	0.200%
20	12.442	1009	1011	1013	rBV	264220	331616	18.89%	2.974%
21	13.197	1075	1077	1080	rBV	46706	64575	3.68%	0.579%
22	13.939	1140	1142	1146	rVB	24110	25648	1.46%	0.230%
23	14.100	1152	1156	1162	rBV3	29127	104511	5.95%	0.937%
24	14.214	1164	1166	1170	rVB	22620	31245	1.78%	0.280%
25	14.442	1183	1186	1188	rBV	877502	868108	49.46%	7.785%
26	14.774	1212	1215	1219	rBV4	10254	25106	1.43%	0.225%
27	15.631	1287	1290	1294	rBV	119276	208226	11.86%	1.867%
28	15.711	1294	1297	1299	rBV	338339	392690	22.37%	3.522%
29	15.883	1310	1312	1314	rBV	60787	64117	3.65%	0.575%
30	16.431	1358	1360	1362	rBV2	15943	26777	1.53%	0.240%
31	16.660	1378	1380	1383	rVB3	17582	19728	1.12%	0.177%
32	17.380	1441	1443	1446	rBV	247460	379118	21.60%	3.400%
33	17.963	1492	1494	1498	rBV3	30173	55450	3.16%	0.497%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040915\
Data File : BF078386.D
Acq On : 10 Apr 2015 6:22
Operator : TP/IZ
Sample : G1782-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB04(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-BF040115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

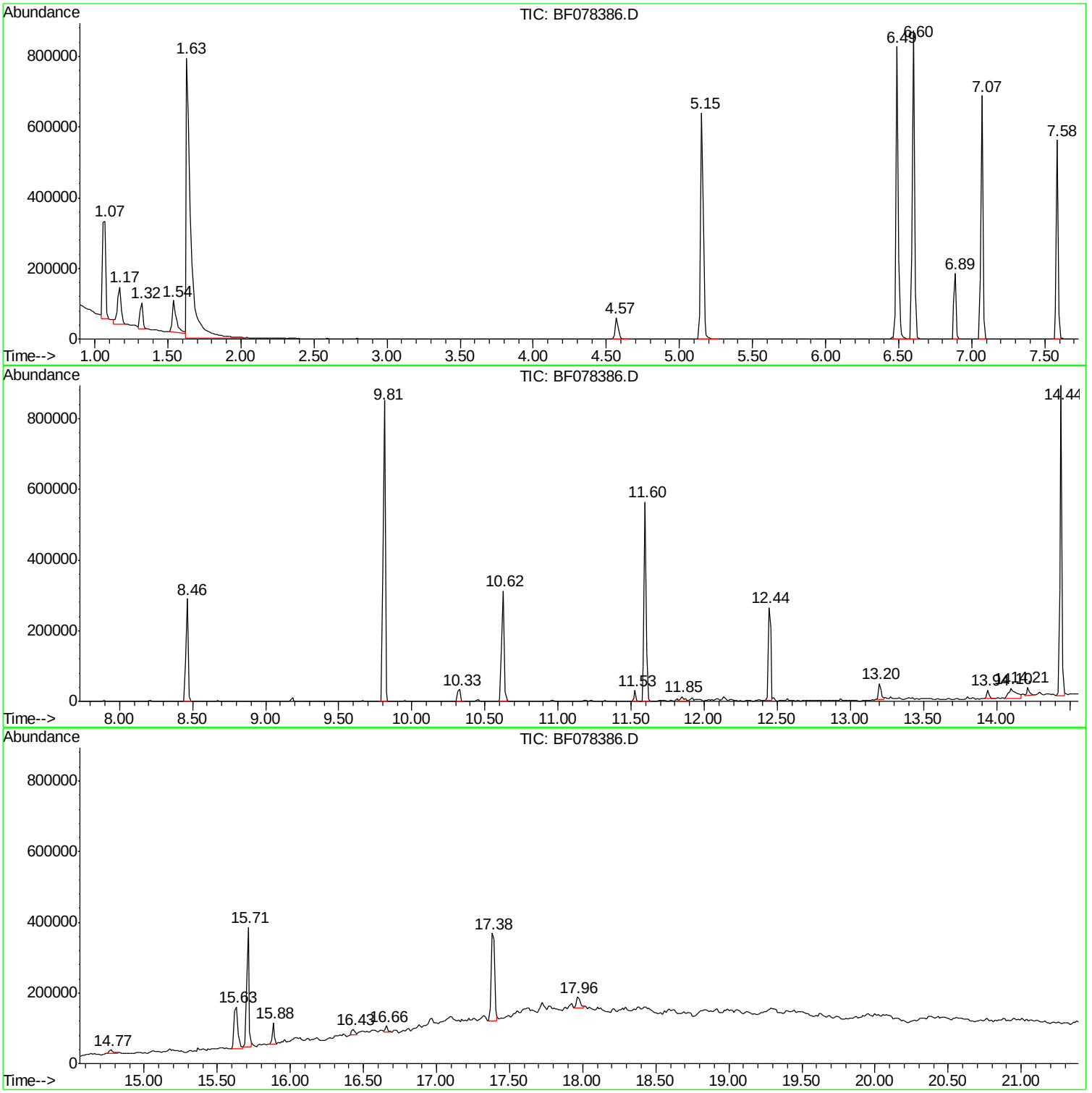
Sum of corrected areas: 11150910

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040915\
Data File : BF078386.D
Acq On : 10 Apr 2015 6:22
Operator : TP/IZ
Sample : G1782-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB04(1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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Acq On : 10 Apr 2015 6:22
Operator : TP/IZ
Sample : G1782-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

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ClientSampleId : SB04(1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
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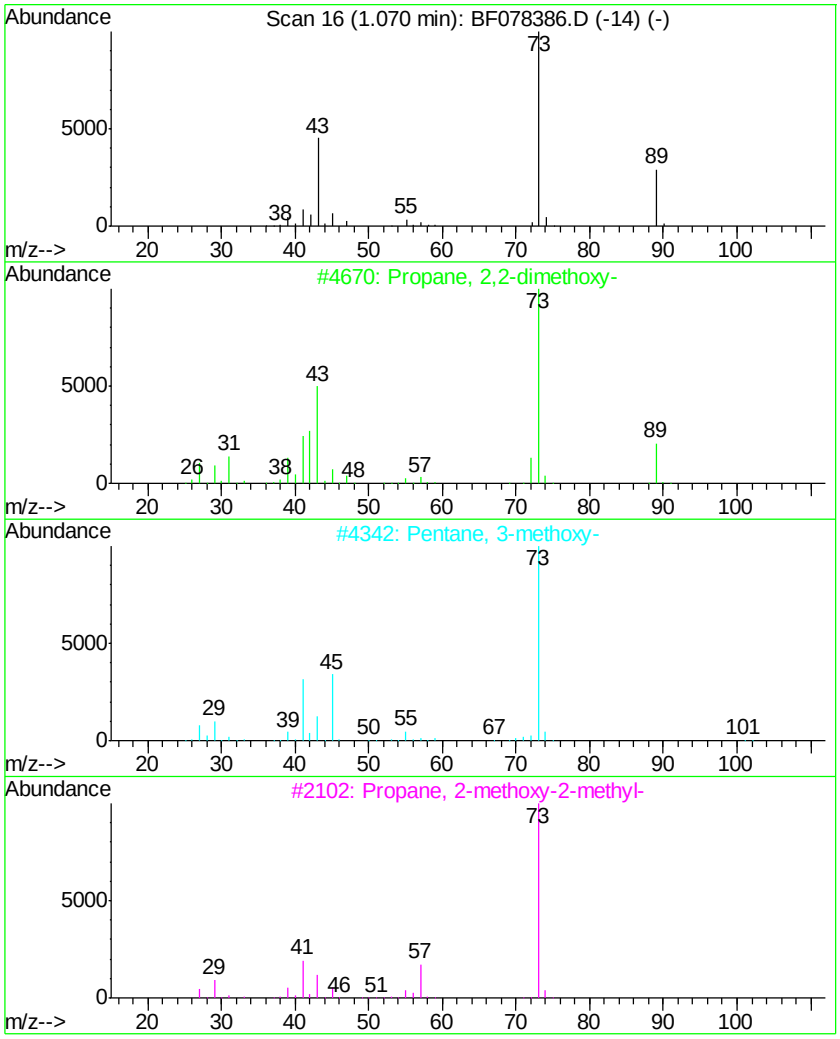
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

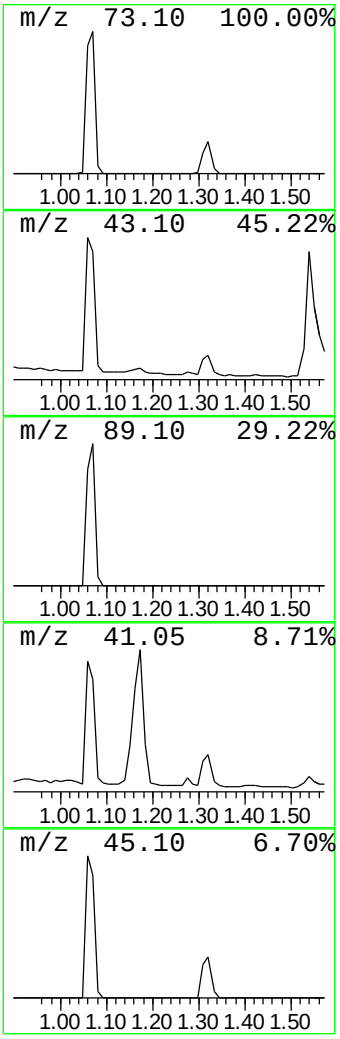
****

Peak Number 1 unknown1.07 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.07	37.73 ng	384468	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	36
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040915\
Data File : BF078386.D
Acq On : 10 Apr 2015 6:22
Operator : TP/IZ
Sample : G1782-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB04(1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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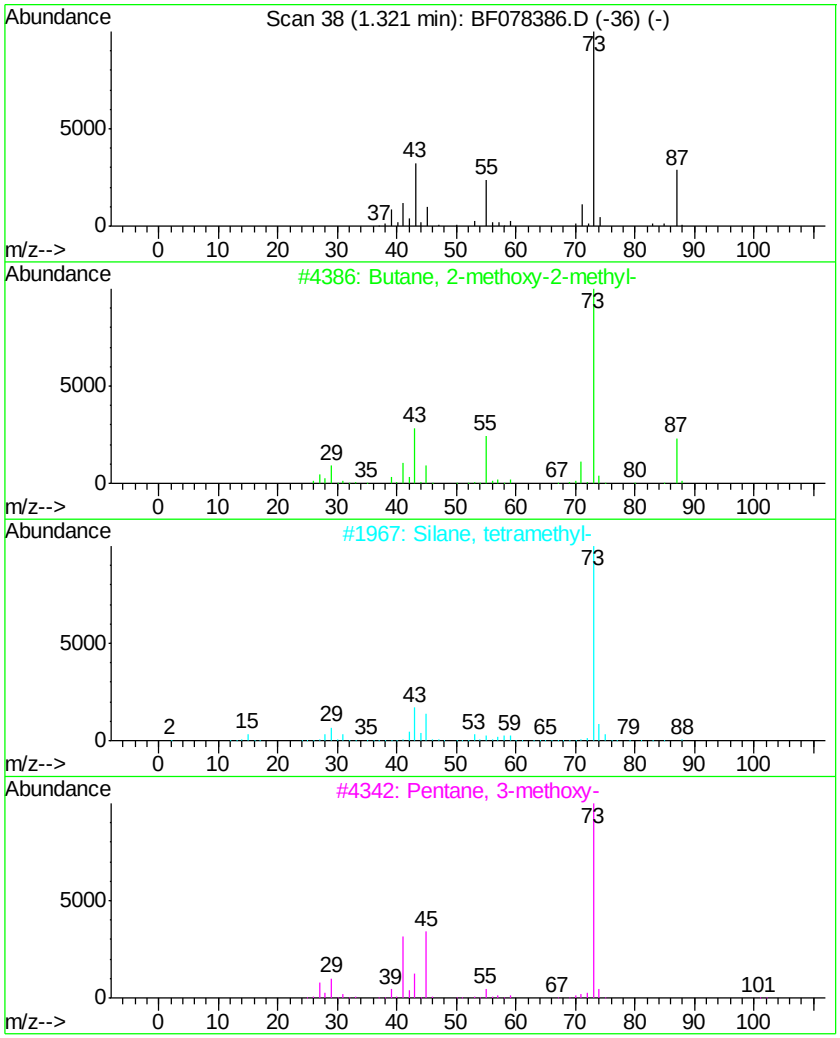
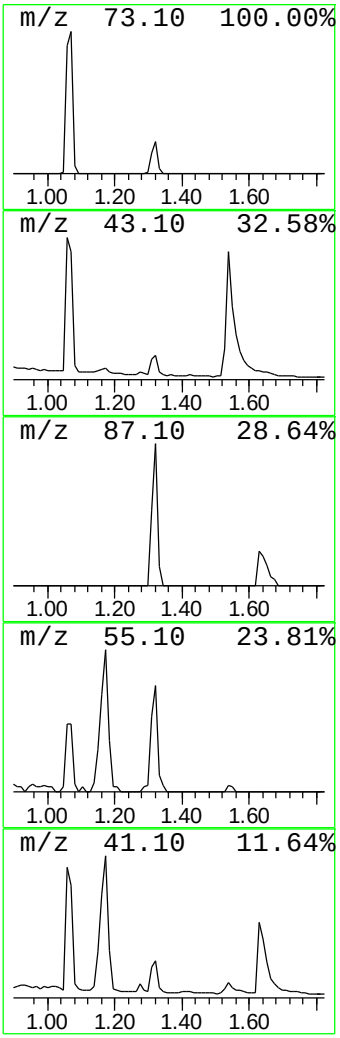
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	9.13 ng	93028	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040915\
Data File : BF078386.D
Acq On : 10 Apr 2015 6:22
Operator : TP/IZ
Sample : G1782-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB04(1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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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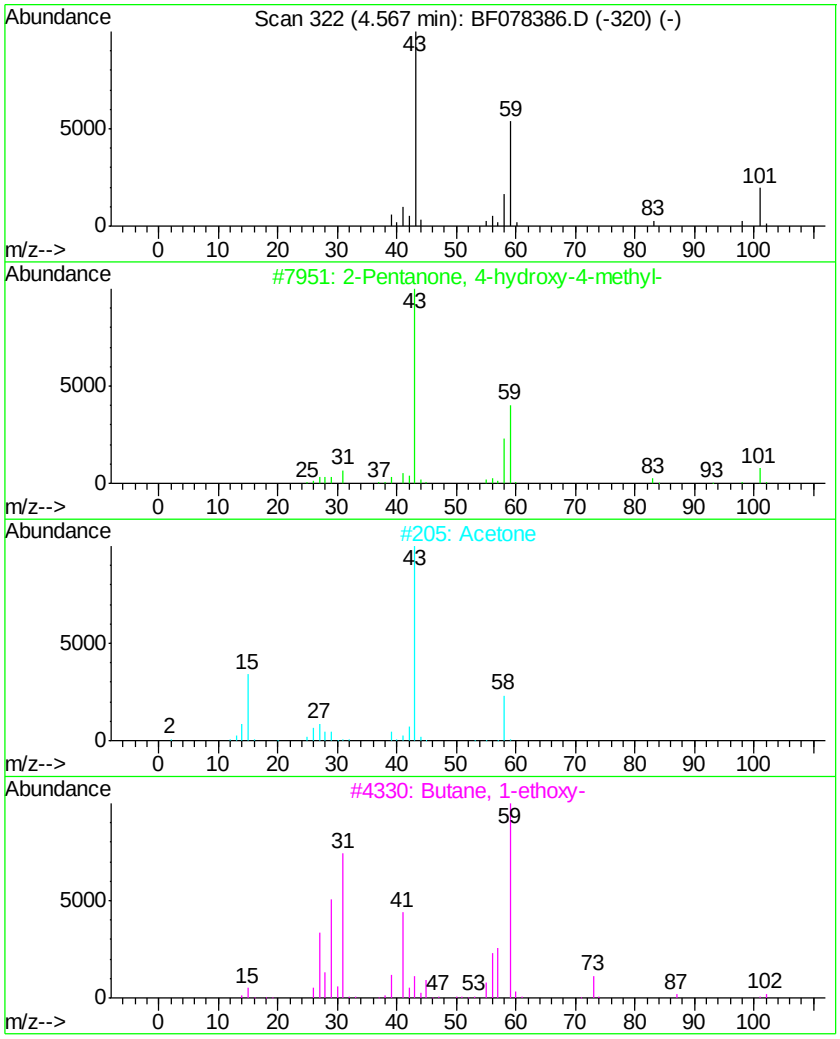
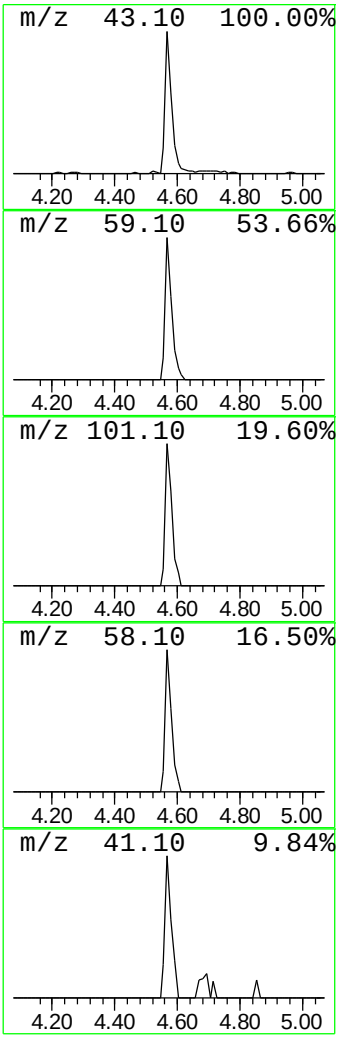
Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	8.31 ng	84648	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	Acetone	58	C3H6O	000067-64-1	9
3	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
5	Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040915\
Data File : BF078386.D
Acq On : 10 Apr 2015 6:22
Operator : TP/IZ
Sample : G1782-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB04(1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

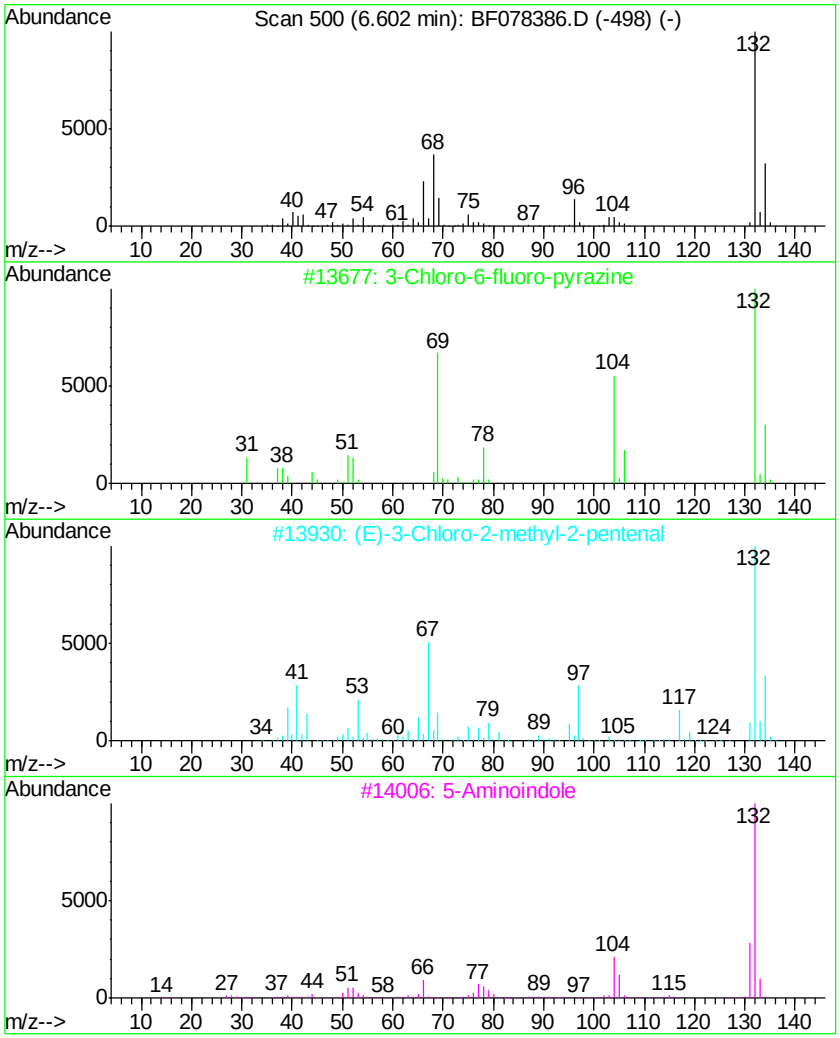
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

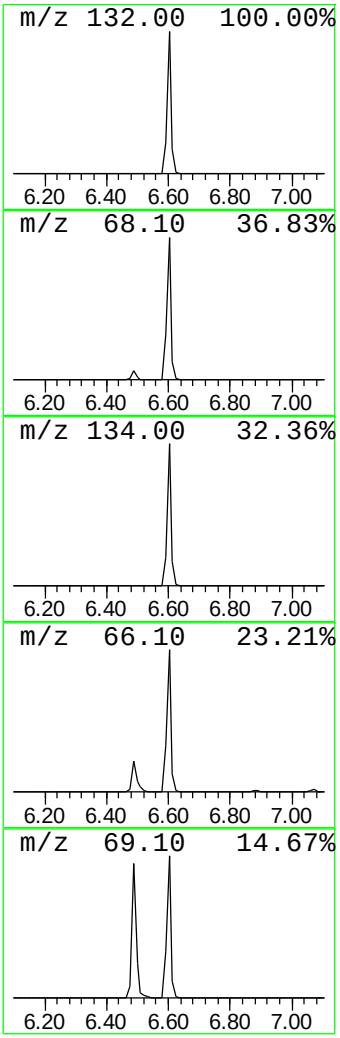
****

Peak Number 7 unknown6.60 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	83.84 ng	854278	1,4-Dichlorobenzene-d4	6.89

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	25
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB04(1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

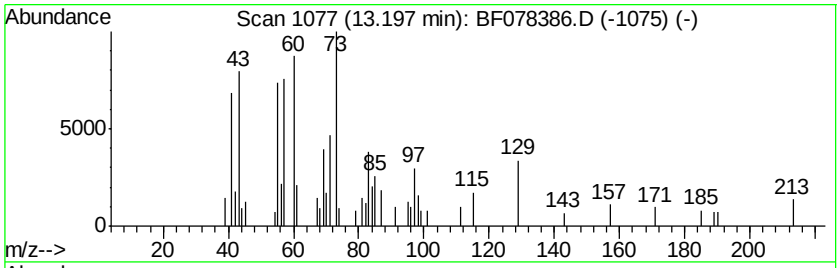
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

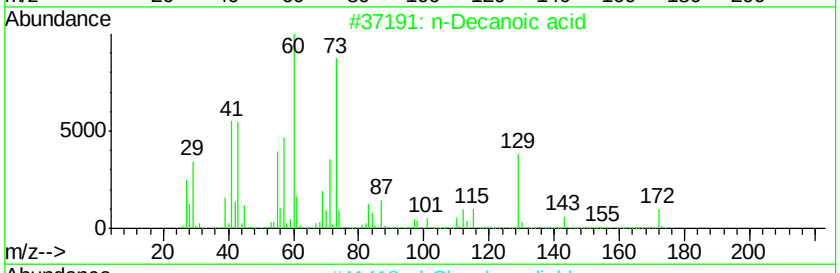
****

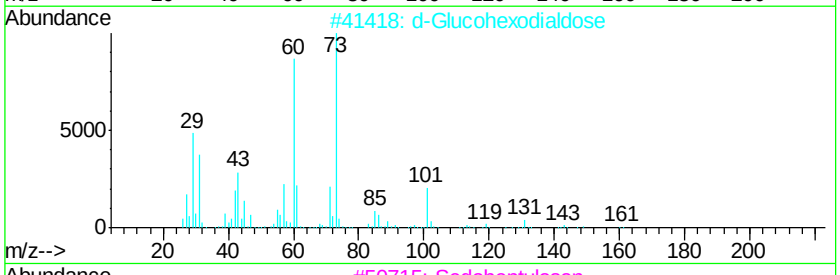
Peak Number 9 unknown13.20 Concentration Rank 11

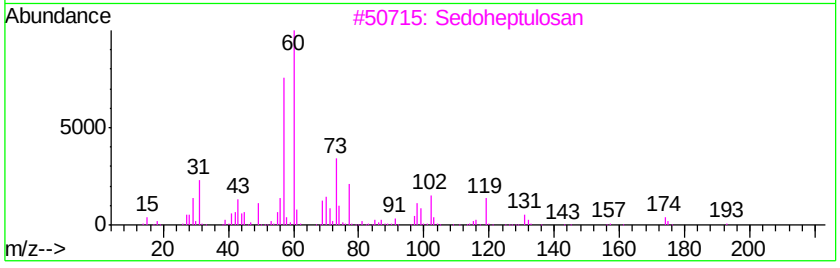
R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	3.89 ng	64575	Phenanthrene-d10	12.44

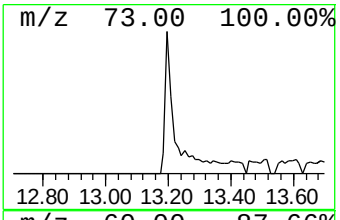
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	47
2	d-Glucohexodialdose	178	C6H10O6	1000149-19-1	35
3	Sedoheptulosan	192	C7H12O6	000469-90-9	22
4	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	22
5	17-Pentatriacontene	491	C35H70	006971-40-0	18

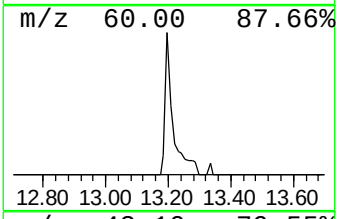


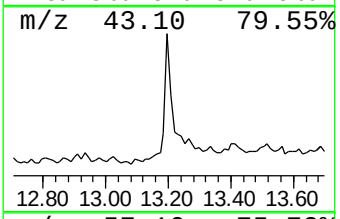


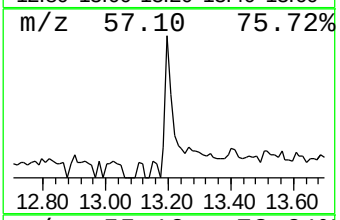


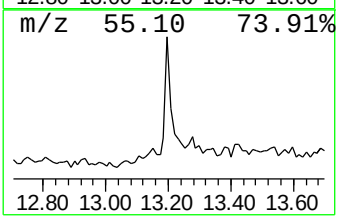












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Instrument : BNA_F
ClientSampleId : SB04(1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

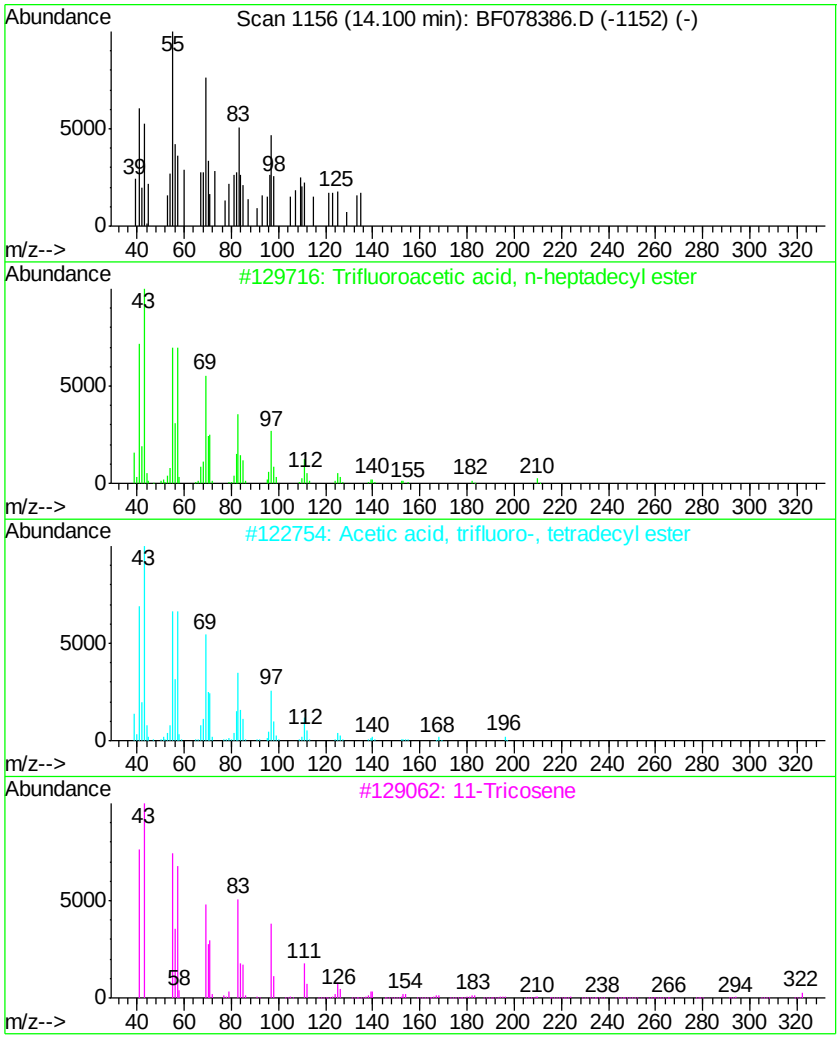
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

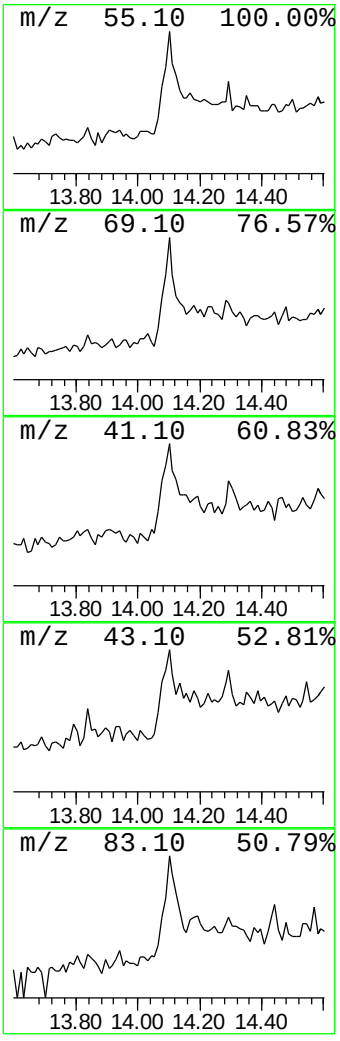
****

Peak Number 10 Trifluoroacetic acid, n-hep... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.10	5.32 ng	104511	Chrysene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	59
2	Acetic acid, trifluoro-, tetrade...	310	C16H29F3O2	006222-02-2	59
3	11-Tricosene	322	C23H46	052078-56-5	47
4	Acetic acid, trifluoro-, decyl e...	254	C12H21F3O2	000333-88-0	43
5	1-Hexadecanol	242	C16H34O	036653-82-4	38





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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

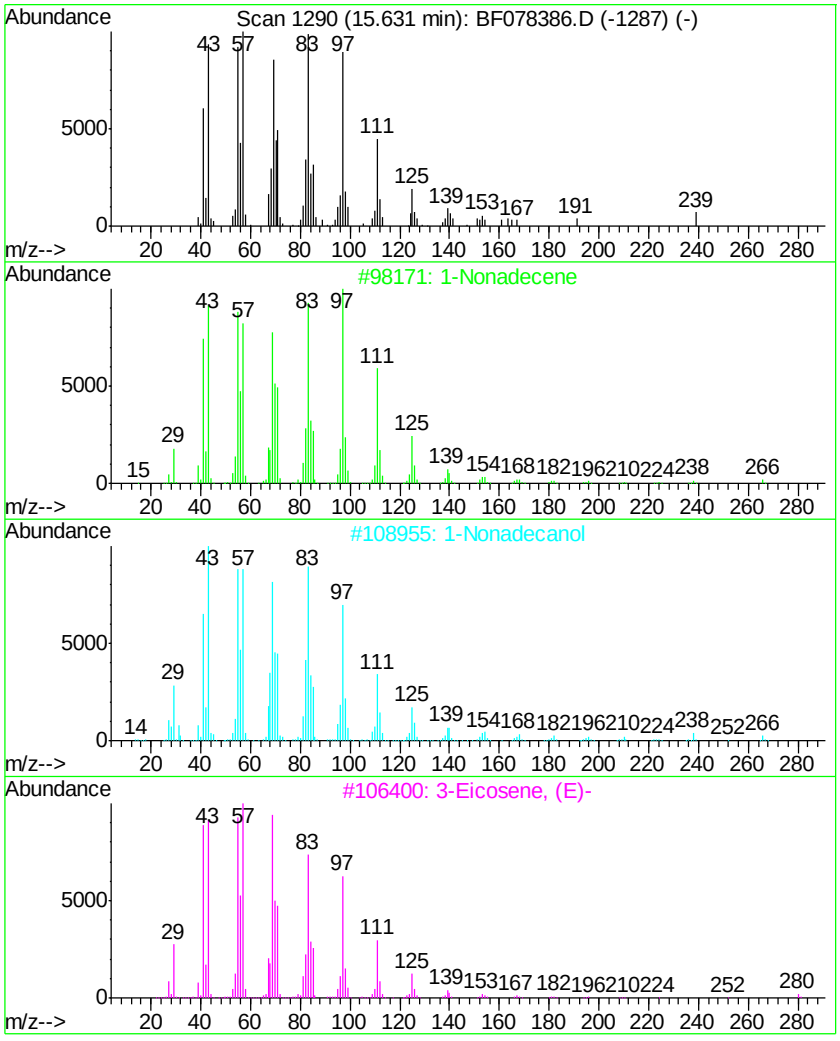
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

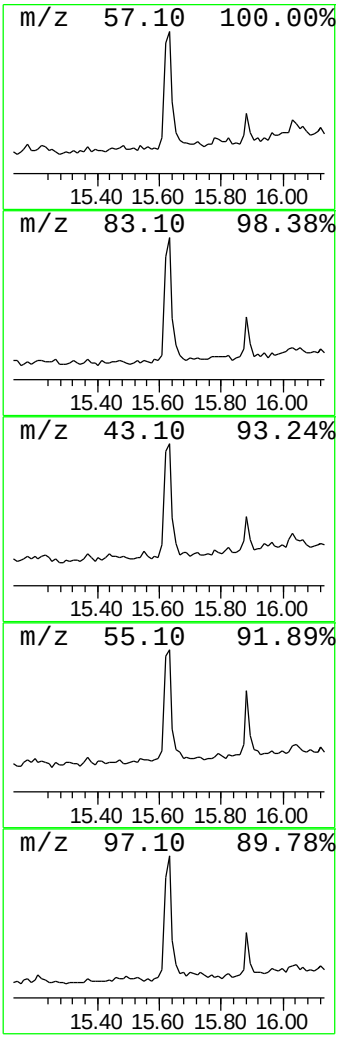
****

Peak Number 11 1-Nonadecene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.63	10.61 ng	208226	Chrysene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	94
2	1-Nonadecanol	284	C19H40O	001454-84-8	93
3	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	91
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040915\
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Misc :
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Instrument : BNA_F
ClientSampleId : SB04(1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
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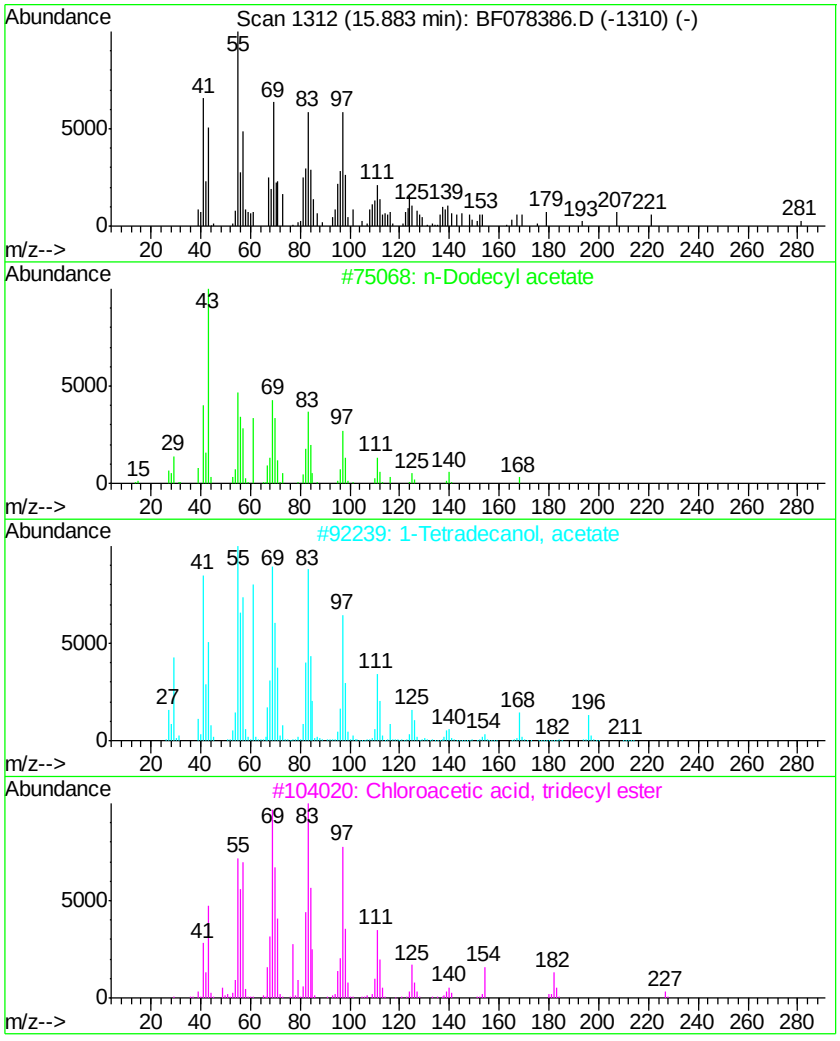
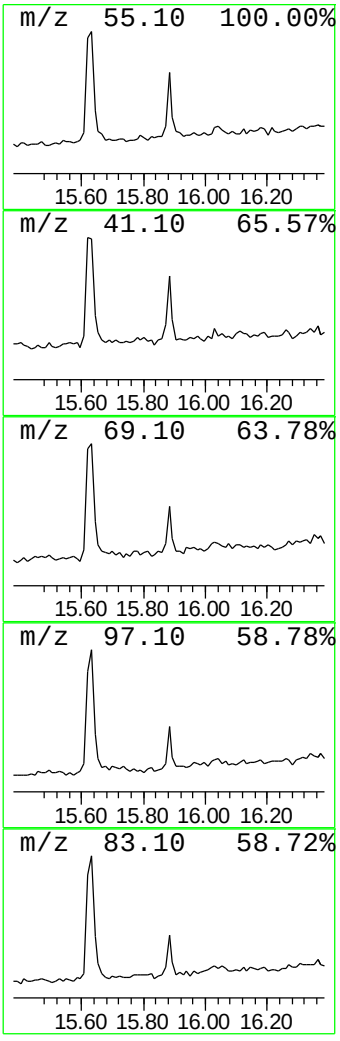
Peak Number 12 n-Dodecyl acetate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.88	3.27 ng	64117	Chrysene-d12	15.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl acetate	228	C14H28O2	000112-66-3	64
2	1-Tetradecanol, acetate	256	C16H32O2	000638-59-5	64
3	Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	64
4	Cyclohexane, 1-(1,5-dimethylhexy...	280	C20H40	056009-20-2	60
5	Isoheptadecanol	256	C17H36O	057289-07-3	58





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040915\
Data File : BF078386.D
Acq On : 10 Apr 2015 6:22
Operator : TP/IZ
Sample : G1782-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB04(1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

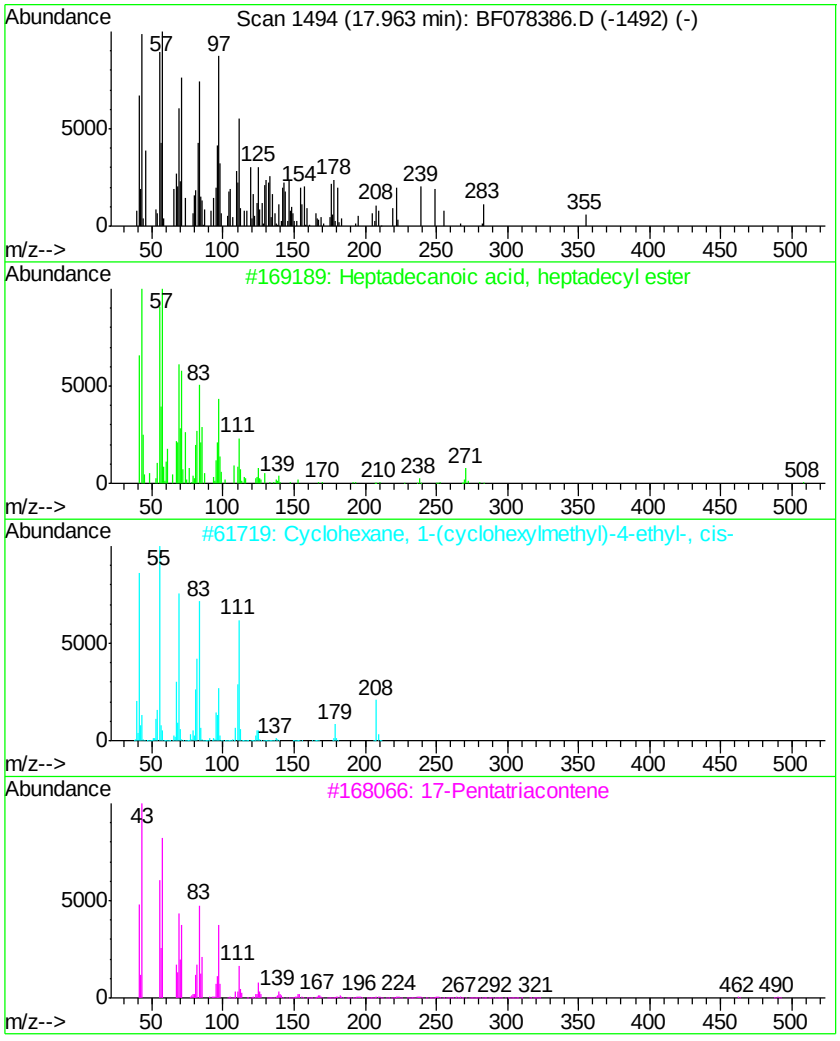
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

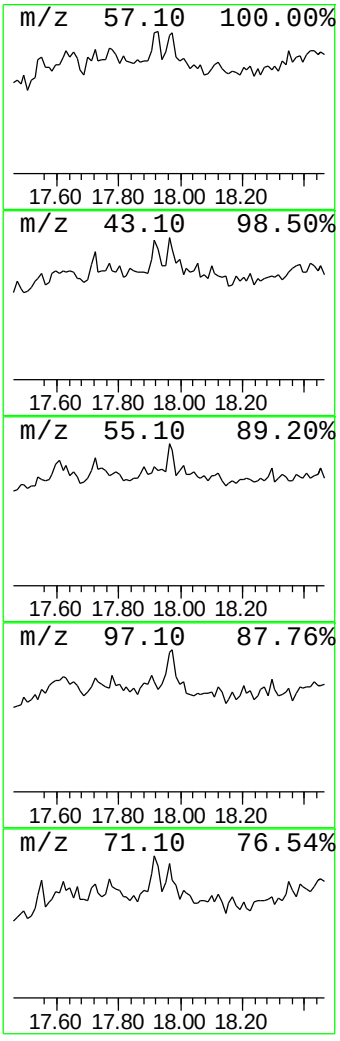
****

Peak Number 13 Heptadecanoic acid, heptade... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	2.93 ng	55450	Perylene-d12	17.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid, heptadecyl e...	509	C34H68O2	036617-50-2	64
2	Cyclohexane, 1-(cyclohexylmethyl...	208	C15H28	054934-95-1	38
3	17-Pentatriacontene	491	C35H70	006971-40-0	30
4	6,10,13-Trimethyltetradecanol	256	C17H36O	1000131-71-0	27
5	Cyclododecanemethanol	198	C13H26O	001892-12-2	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040915\
Data File : BF078386.D
Acq On : 10 Apr 2015 6:22
Operator : TP/IZ
Sample : G1782-14
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB04(1)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040115.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
unknown1.07	1.07	37.7	ng	384468	1	6.89	203787	20.0
Butane, 2-methoxy...	1.32	9.1	ng	93028	1	6.89	203787	20.0
2-Pentanone, 4-hy...	4.57	8.3	ng	84648	1	6.89	203787	20.0
unknown6.60	6.60	83.8	ng	854278	1	6.89	203787	20.0
unknown13.20	13.20	3.9	ng	64575	4	12.44	331616	20.0
Trifluoroacetic a...	14.10	5.3	ng	104511	5	15.71	392690	20.0
1-Nonadecene	15.63	10.6	ng	208226	5	15.71	392690	20.0
n-Dodecyl acetate	15.88	3.3	ng	64117	5	15.71	392690	20.0
Heptadecanoic aci...	17.96	2.9	ng	55450	6	17.39	379118	20.0