LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040715\
Data File : BF078324.D
Acq On : 8 Apr 2015 6:04
Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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	1.093	16	18	20	rBV	1038756	1021089	94.57%	10.636%
2	1.196	24	27	31	rVB	87308	147296	13.64%	1.534%
3	1.356	38	41	43	rVB	49131	67623	6.26%	0.704%
4	1.664	66	68	76	rBV	33677	59113	5.47%	0.616%
5	4.624	325	327	336	rVB	58930	80352	7.44%	0.837%
6	5.207	375	378	386	rBV	486376	663557	61.46%	6.912%
7	6.533	491	494	496	rBV	565470	702432	65.06%	7.317%
8	6.648	502	504	507	rBV	773687	732603	67.85%	7.631%
9	6.933	527	529	531	rBV	177472	171862	15.92%	1.790%
10	7.116	543	545	548	rBV	618446	561159	51.97%	5.845%
11	7.630	588	590	592	rBV	494368	430698	39.89%	4.486%
12	8.511	664	667	669	rBV	269191	242825	22.49%	2.529%
13	9.231	728	730	732	rBV	33610	30719	2.85%	0.320%
14	9.859	783	785	787	rBV	1057162	899284	83.29%	9.367%
15	10.374	828	830	832	rBV	56012	52136	4.83%	0.543%
16	10.671	854	856	861	rVB2	291270	298445	27.64%	3.109%
17	11.219	902	904	908	rBV	11396	21350	1.98%	0.222%
18	11.574	933	935	938	rVB	130537	135185	12.52%	1.408%
19	11.654	939	942	944	rBV	431316	544762	50.45%	5.674%
20	11.894	961	963	964	rBV	18470	14198	1.31%	0.148%
21	12.500	1014	1016	1018	rBV	309303	296073	27.42%	3.084%
22	12.751	1033	1038	1041	rBV	14897	18780	1.74%	0.196%
23	13.254	1080	1082	1083	rBV	21696	30317	2.81%	0.316%
24	13.460	1097	1100	1103	rBV4	7000	20534	1.90%	0.214%
25	13.780	1124	1128	1129	rBV4	6913	15605	1.45%	0.163%
26	13.974	1144	1145	1148	rBV	8137	10980	1.02%	0.114%
27	14.054	1150	1152	1155	rVV2	14364	19608	1.82%	0.204%
28	14.500	1188	1191	1193	rVB	776524	1079733	100.00%	11.247%
29	14.820	1217	1219	1221	rBV2	8645	15618	1.45%	0.163%
30	15.677	1292	1294	1299	rBV	176928	268694	24.89%	2.799%
31	15.768	1299	1302	1304	rVV	316784	400064	37.05%	4.167%
32	15.940	1315	1317	1320	rBV	34000	47603	4.41%	0.496%
33	16.054	1325	1327	1328	rVV	18488	24367	2.26%	0.254%
34	16.088	1328	1330	1332	rVB2	23000	31073	2.88%	0.324%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040715\
Data File : BF078324.D
Acq On : 8 Apr 2015 6:04
Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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

35	16.534	1367	1369	1374	rVB2	51150	84653	7.84%	0.882%
36	17.426	1445	1447	1452	rBV	245109	359789	33.32%	3.748%

Sum of corrected areas: 9600179

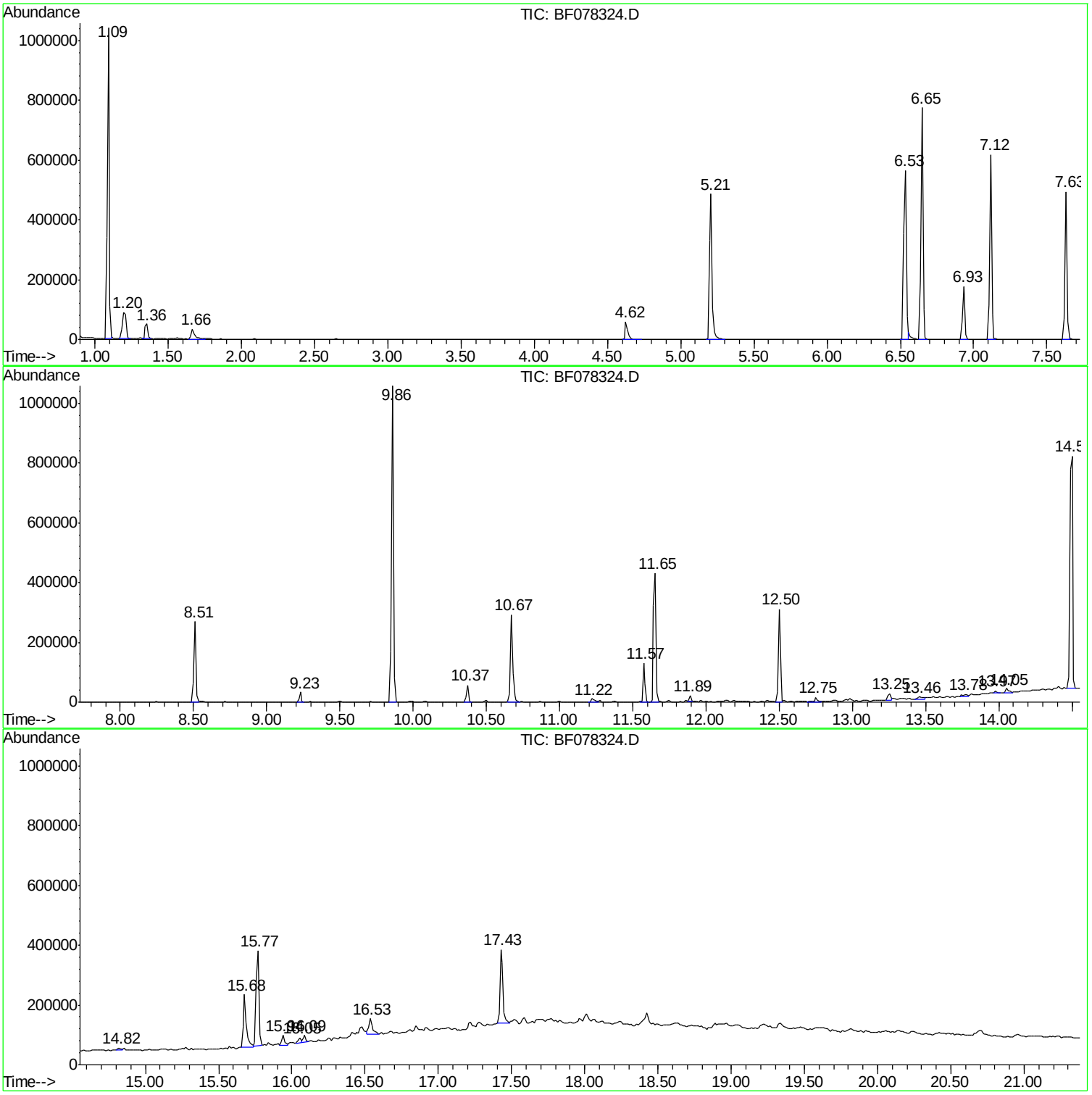
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040715\
Data File : BF078324.D
Acq On : 8 Apr 2015 6:04
Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040715\
Data File : BF078324.D
Acq On : 8 Apr 2015 6:04
Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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

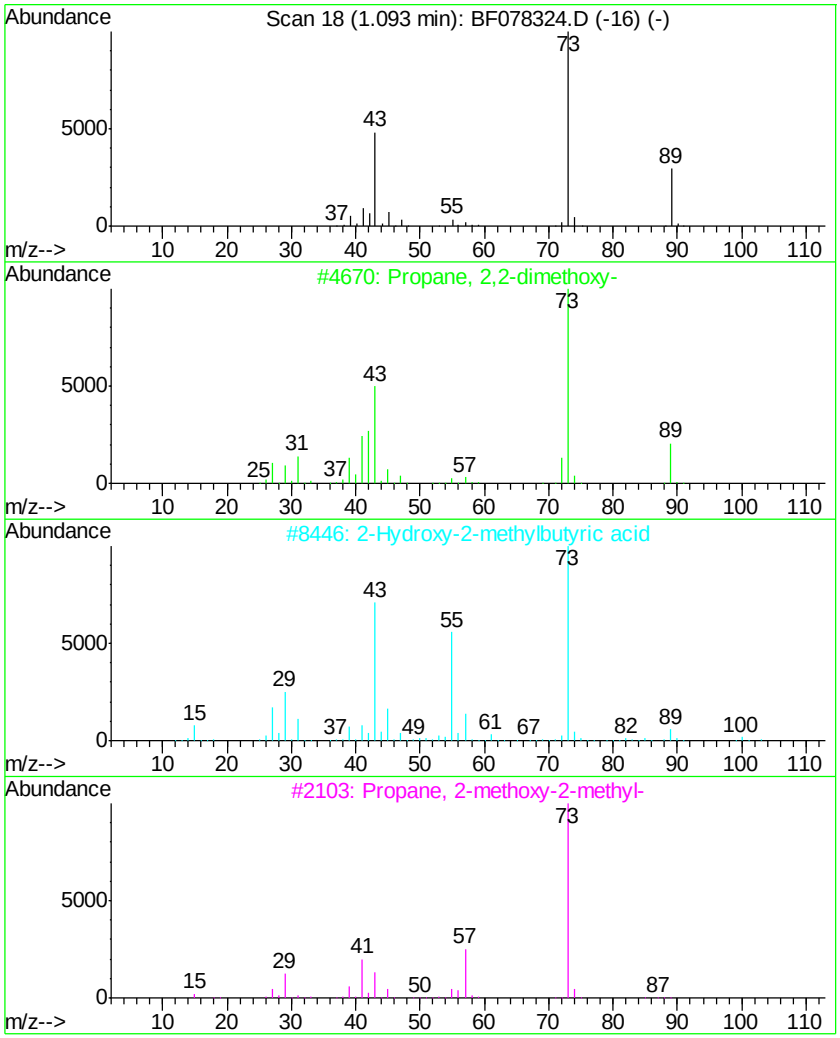
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

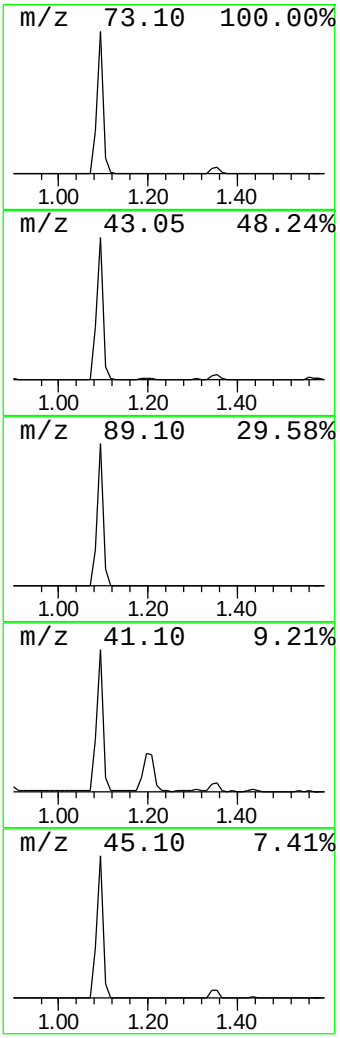
****

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.09	118.83 ng	1021090	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
3	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	5
5	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	4





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040715\
Data File : BF078324.D
Acq On : 8 Apr 2015 6:04
Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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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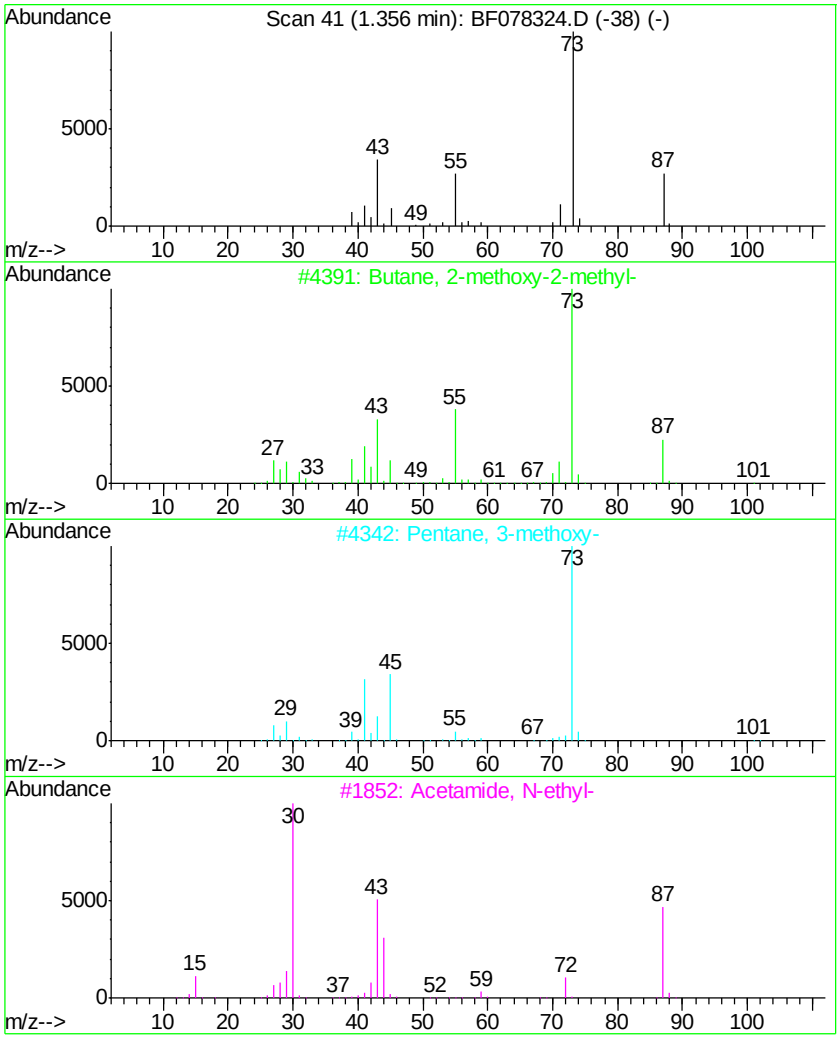
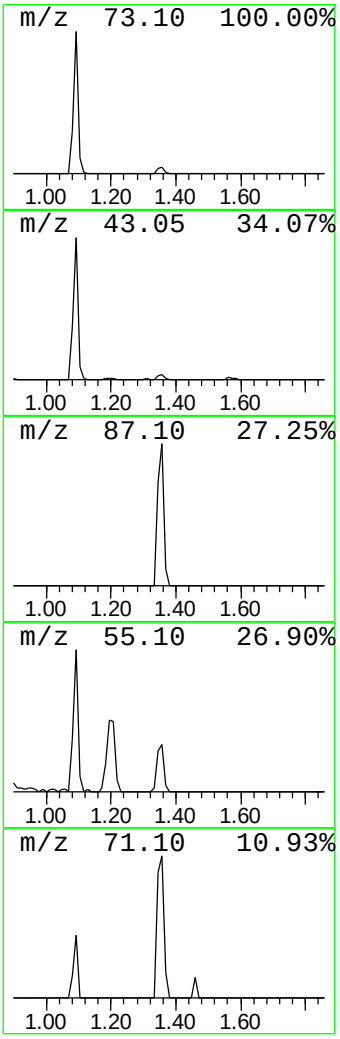
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.36	7.87 ng	67623	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	16
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\BF040715\
Data File : BF078324.D
Acq On : 8 Apr 2015 6:04
Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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

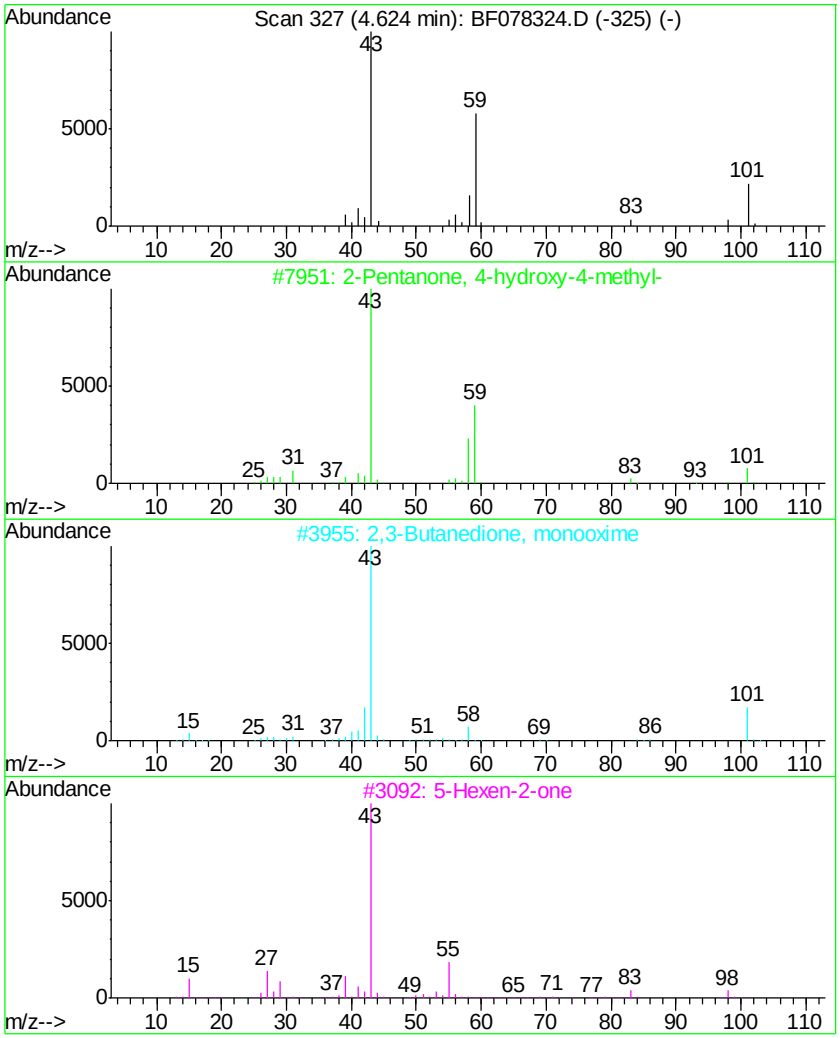
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

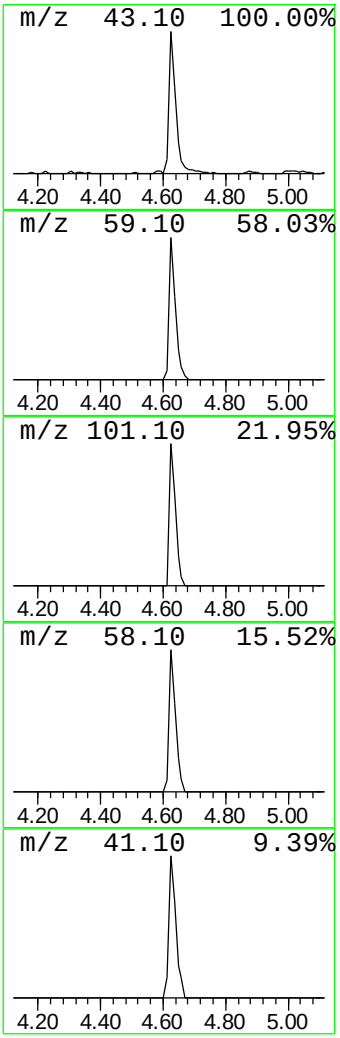
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.62	9.35 ng	80352	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040715\
Data File : BF078324.D
Acq On : 8 Apr 2015 6:04
Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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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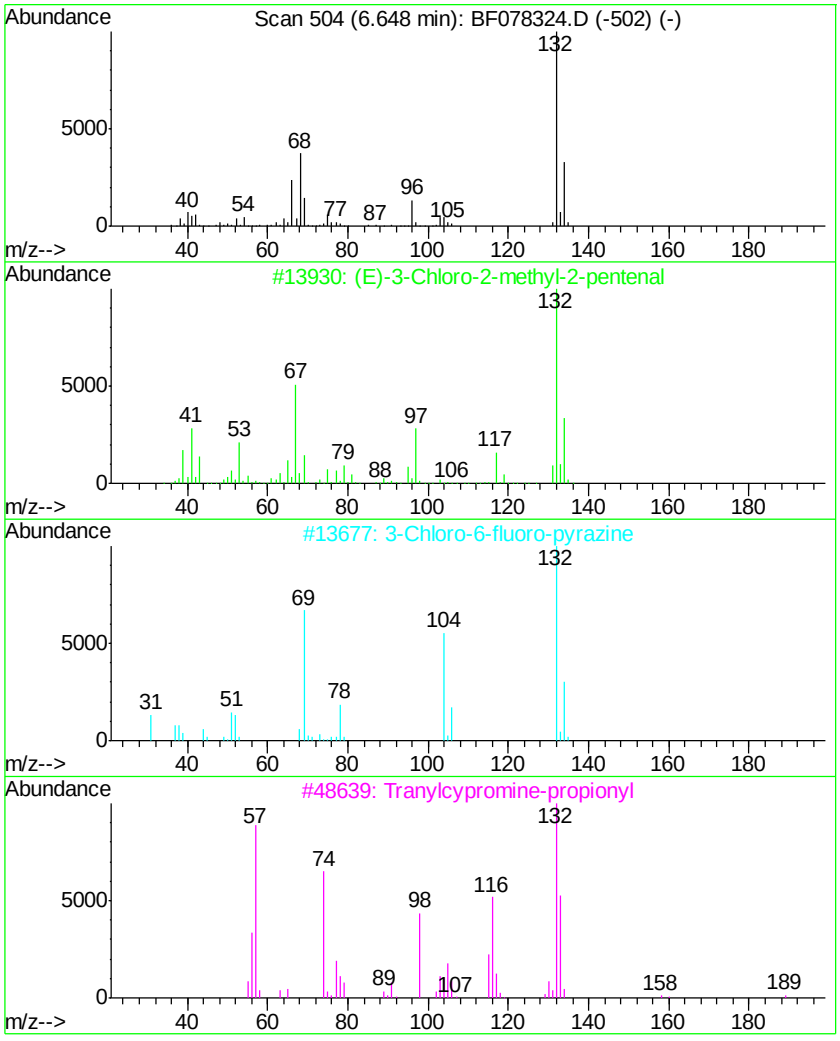
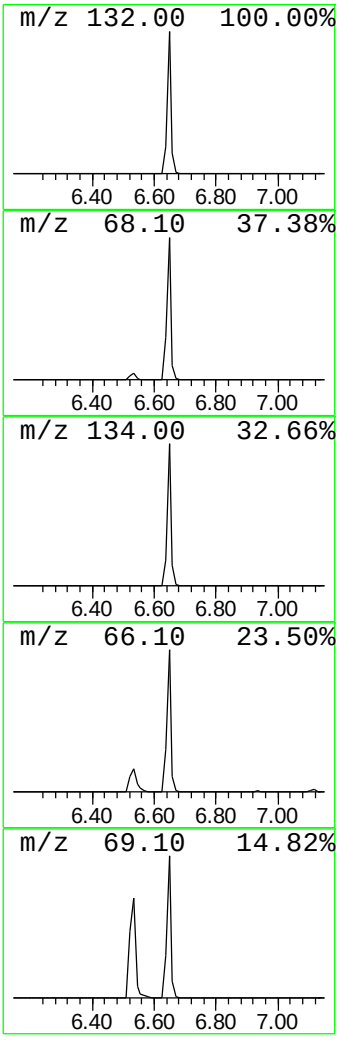
Peak Number 6 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	85.25 ng	732603	1,4-Dichlorobenzene-d4	6.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Acq On : 8 Apr 2015 6:04
Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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

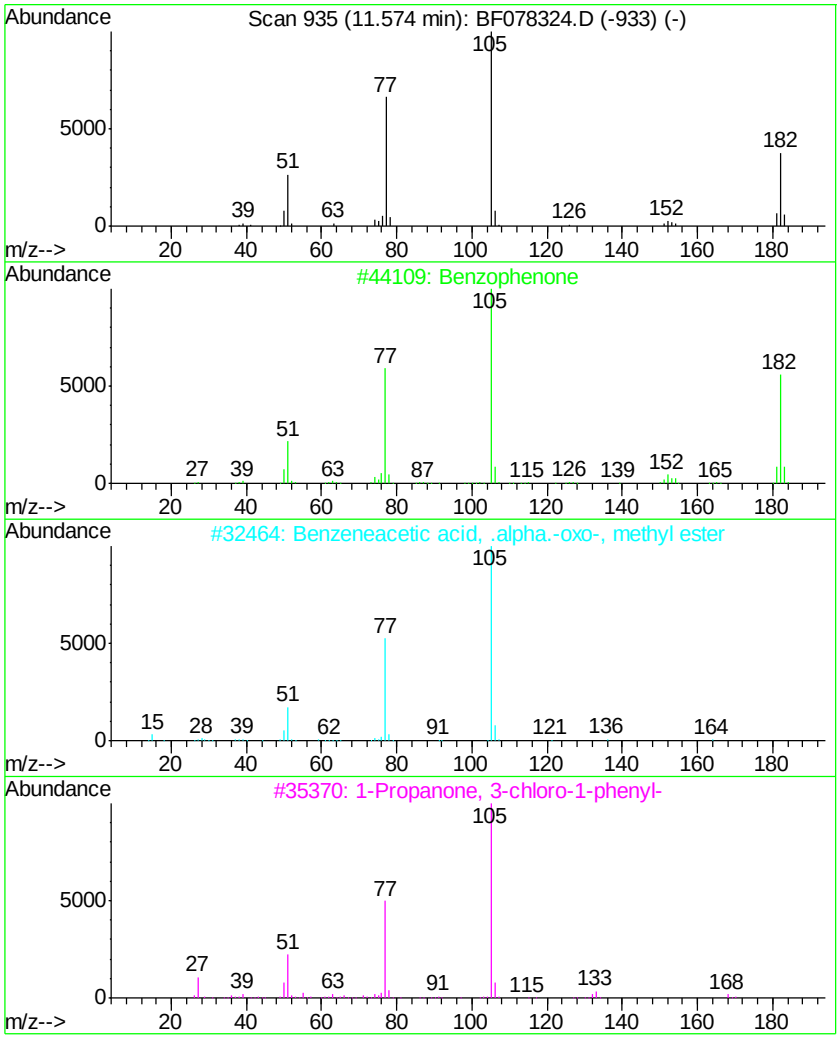
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

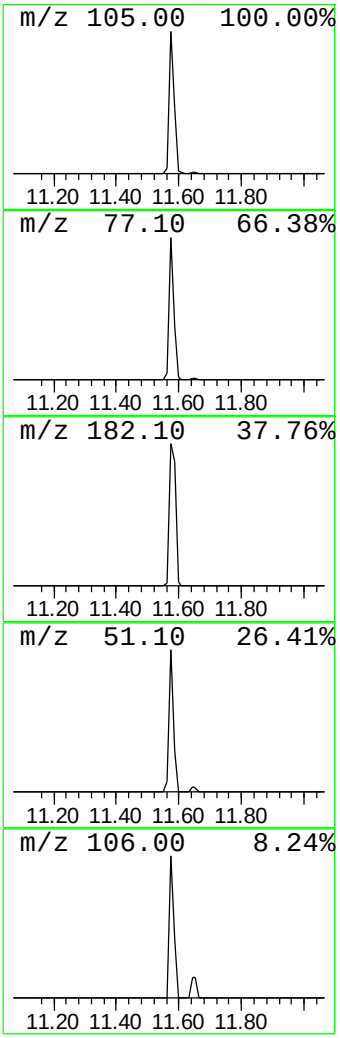
****

Peak Number 9 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	9.06 ng	135185	Acenaphthene-d10	10.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	53
3	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	53
4	1-Butanone, 1-phenyl-	148	C10H12O	000495-40-9	53
5	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	53





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040715\
Data File : BF078324.D
Acq On : 8 Apr 2015 6:04
Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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

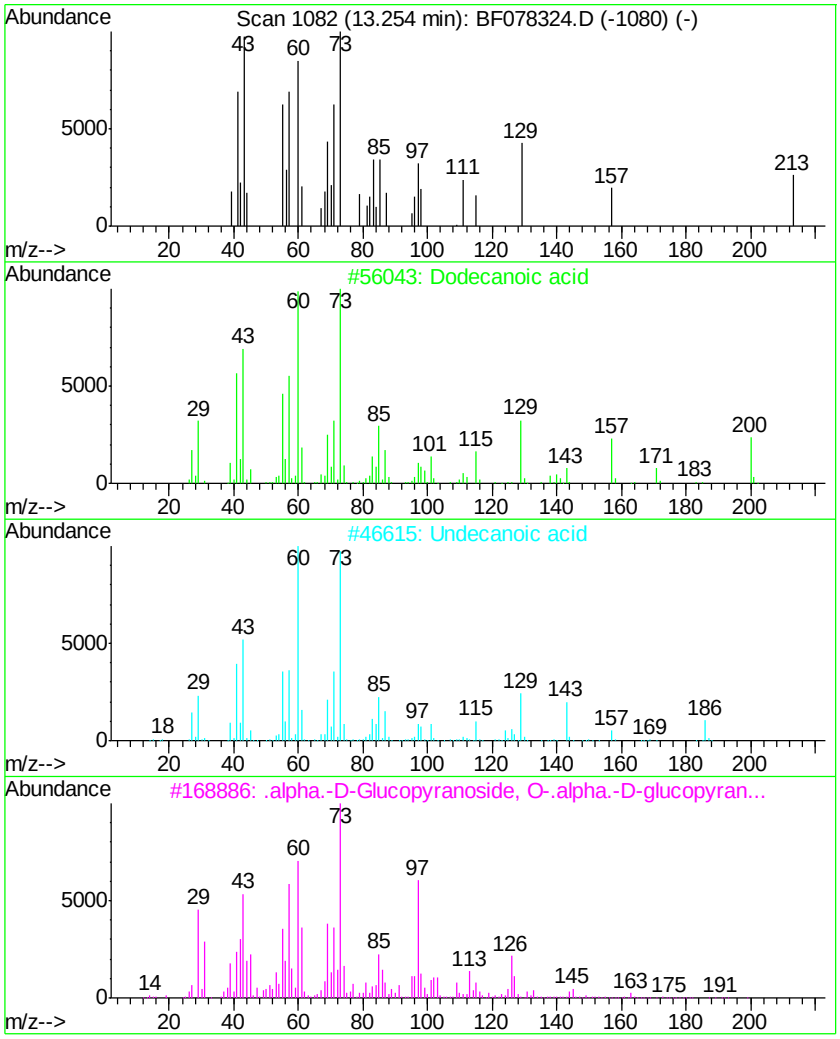
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

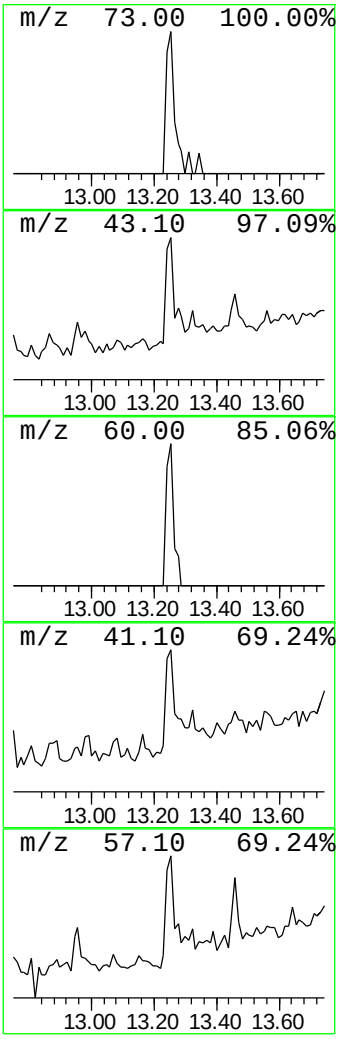
****

Peak Number 10 Dodecanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.25	2.05 ng	30317	Phenanthrene-d10	12.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	50
2	Undecanoic acid	186	C11H22O2	000112-37-8	43
3	.alpha.-D-Glucopyranoside, O-.al...	504	C18H32O16	000597-12-6	38
4	.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	38
5	1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	25





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Sample : G1783-05
Misc :
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Instrument : BNA_F
ClientSampleId : FD-5

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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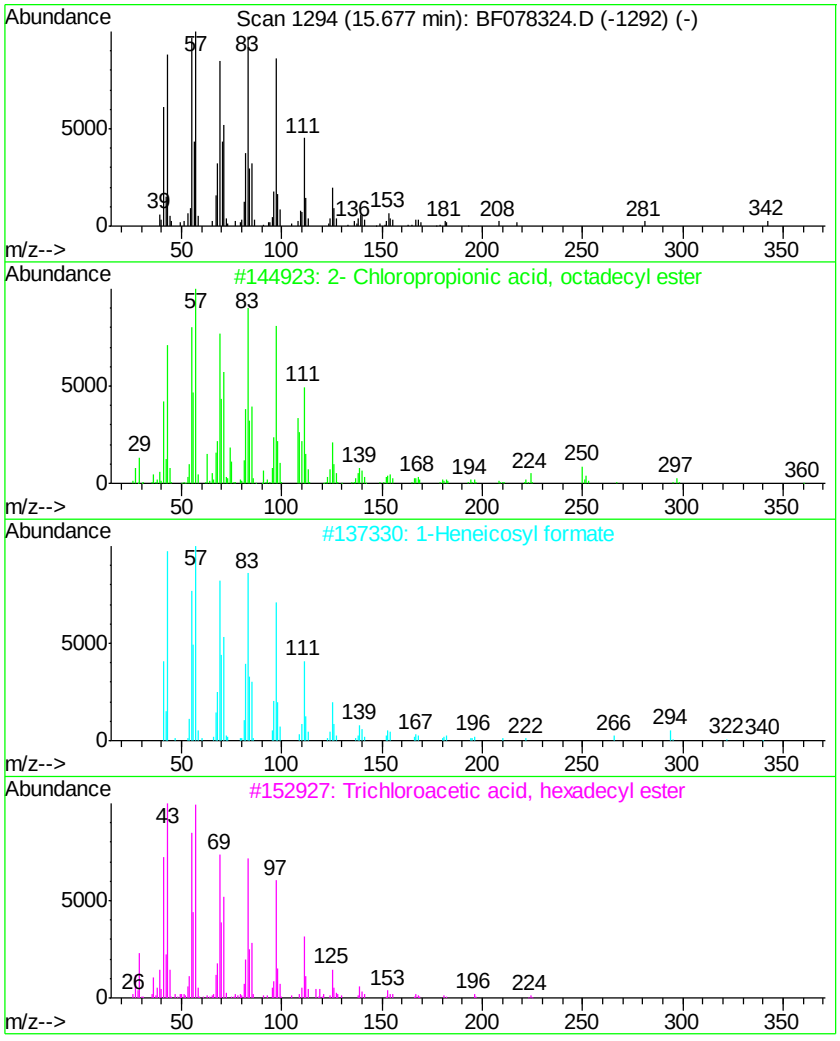
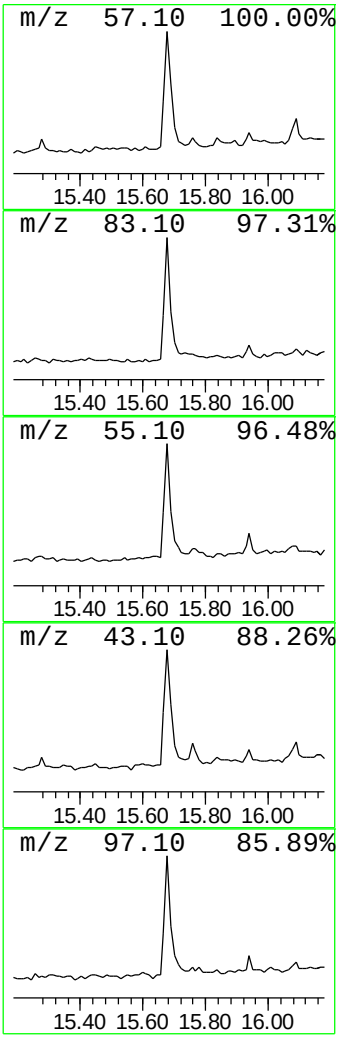
Peak Number 11 2- Chloropropionic acid, oc... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	13.43 ng	268694	Chrysene-d12	15.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
3	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
4	1-Nonadecene	266	C19H38	018435-45-5	91
5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91





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ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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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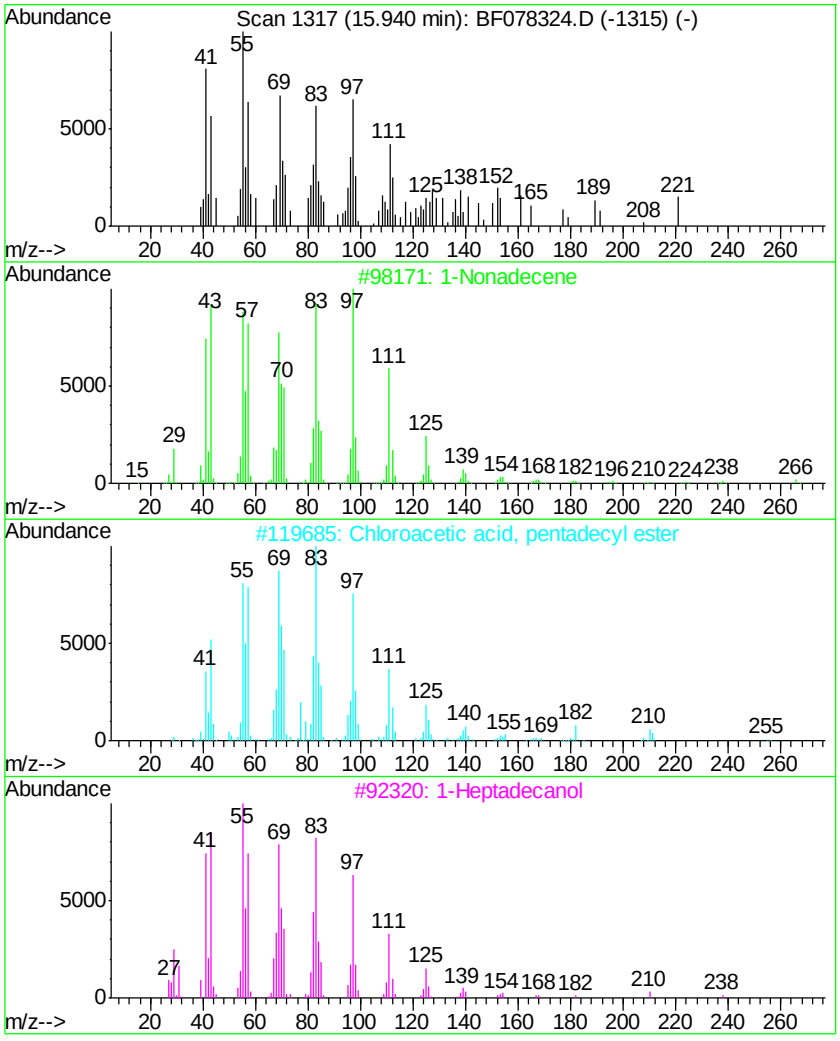
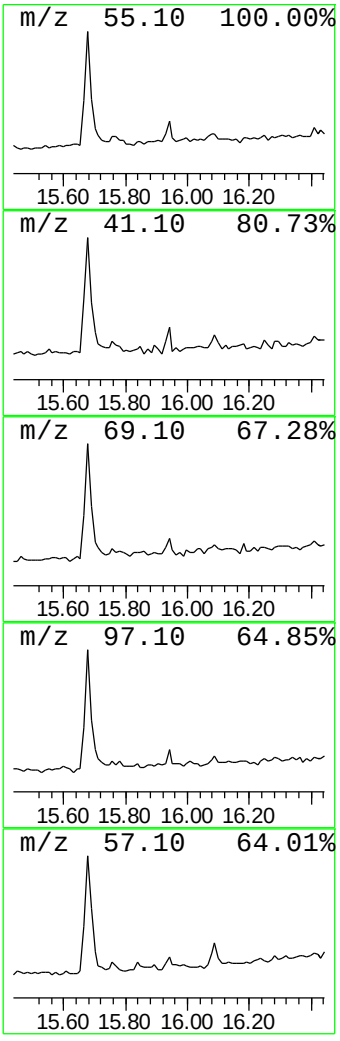
Peak Number 12 1-Nonadecene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	2.38 ng	47603	Chrysene-d12	15.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	58
2	Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	53
3	1-Heptadecanol	256	C17H36O	001454-85-9	49
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	46
5	Isotridecanol-	200	C13H28O	027458-92-0	46





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040715\
Data File : BF078324.D
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Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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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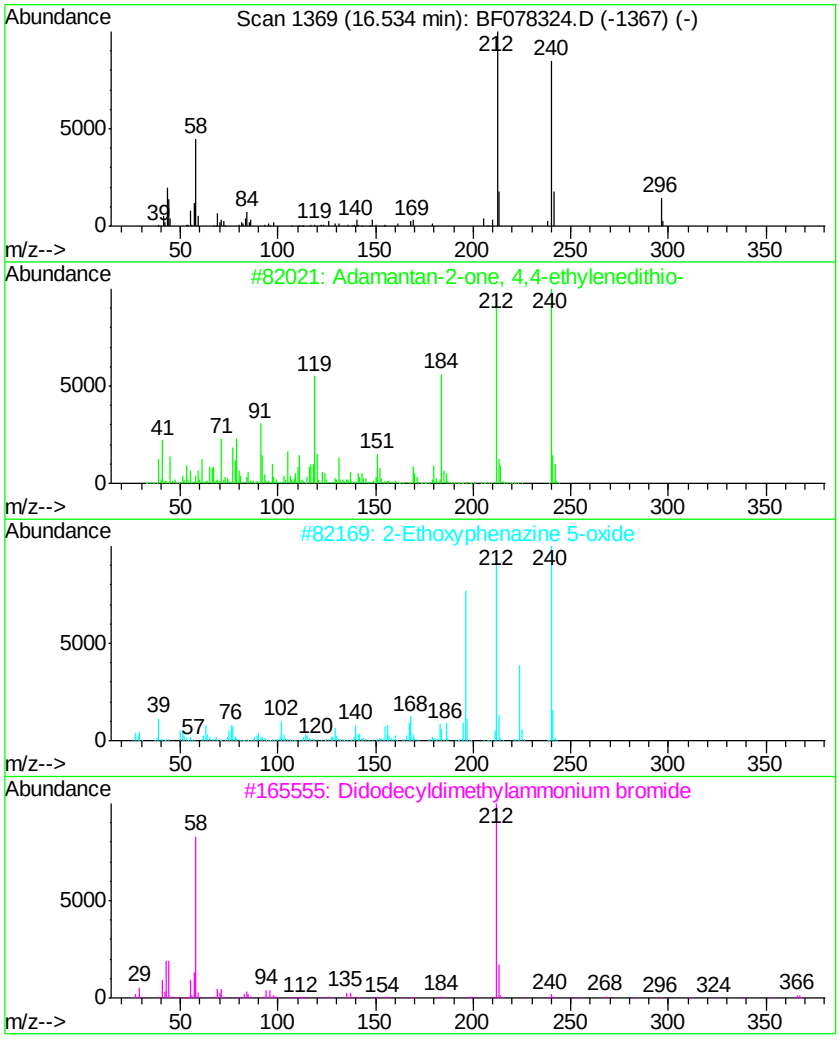
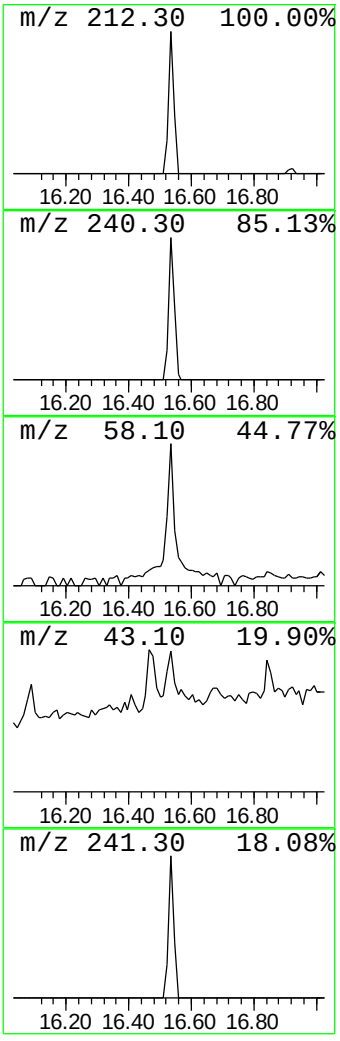
Peak Number 13 unknown16.53 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	4.23 ng	84653	Chrysene-d12	15.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantan-2-one, 4,4-ethylenedit...	240	C12H16OS2	1000210-52-6	45
2	2-Ethoxyphenazine 5-oxide	240	C14H12N2O2	018274-46-9	38
3	Didodecyldimethylammonium bromide	461	C26H56BrN	003282-73-3	37
4	Quinoxaline, 6-chloro-2-phenyl-	240	C14H9ClN2	025187-19-3	27
5	2,7-Phenazinediyl diacetate	296	C16H12N2O4	029606-39-1	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040715\
Data File : BF078324.D
Acq On : 8 Apr 2015 6:04
Operator : TP/IZ
Sample : G1783-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : FD-5

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
Propane, 2,2-dime...	1.09	118.8	ng	1021090	1	6.93	171862	20.0
Butane, 2-methoxy...	1.36	7.9	ng	67623	1	6.93	171862	20.0
2-Pentanone, 4-hy...	4.62	9.3	ng	80352	1	6.93	171862	20.0
unknown6.65	6.65	85.3	ng	732603	1	6.93	171862	20.0
Benzophenone	11.57	9.1	ng	135185	3	10.67	298445	20.0
Dodecanoic acid	13.25	2.0	ng	30317	4	12.50	296073	20.0
2- Chloropropioni...	15.68	13.4	ng	268694	5	15.77	400064	20.0
1-Nonadecene	15.94	2.4	ng	47603	5	15.77	400064	20.0
unknown16.53	16.53	4.2	ng	84653	5	15.77	400064	20.0