LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093613.D
Acq On : 13 Mar 2017 17:56
Operator : SJ/MA
Sample : I2174-23
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-74

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-BF030717.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	2.355	39	41	45	rBV	74549	118862	2.37%	0.259%
2	2.424	45	47	55	rVB	44105	130977	2.61%	0.285%
3	3.098	103	106	128	rBV	339530	803388	15.99%	1.750%
4	4.161	196	199	217	rBV	1784193	3016141	60.04%	6.572%
5	4.458	222	225	228	rVB	785451	1237400	24.63%	2.696%
6	4.881	259	262	277	rBV	252032	501252	9.98%	1.092%
7	5.316	297	300	325	rBV	3055537	4990036	99.33%	10.872%
8	6.333	387	389	391	rBV	1199598	1112635	22.15%	2.424%
9	6.367	391	392	400	rVV	3011533	4140021	82.41%	9.020%
10	6.482	400	402	405	rVB	4568201	4511963	89.82%	9.831%
11	6.710	420	422	433	rVB	953856	1013348	20.17%	2.208%
12	6.859	433	435	438	rBV	3351748	3527359	70.22%	7.685%
13	7.019	447	449	459	rVB2	145556	255695	5.09%	0.557%
14	7.282	470	472	487	rBV	2829449	3265320	65.00%	7.114%
15	7.476	487	489	502	rVV	255991	431921	8.60%	0.941%
16	8.002	532	535	548	rVB	1221615	1349076	26.85%	2.939%
17	8.527	578	581	584	rBV	113685	121734	2.42%	0.265%
18	9.076	627	629	632	rBV	3561948	5023583	100.00%	10.945%
19	9.385	654	656	660	rBV	33556	85964	1.71%	0.187%
20	9.762	686	689	691	rBV	863716	1064977	21.20%	2.320%
21	10.048	712	714	721	rBV	65686	200906	4.00%	0.438%
22	10.150	721	723	731	rVB	44896	122856	2.45%	0.268%
23	10.550	756	758	761	rBV	2149316	2658478	52.92%	5.792%
24	11.248	817	819	825	rBV	1388058	1364308	27.16%	2.973%
25	12.836	955	958	960	rBV	4027862	4176494	83.14%	9.100%
26	13.899	1048	1051	1058	rBV	404246	513664	10.23%	1.119%
27	15.340	1174	1177	1183	rVB3	65272	158790	3.16%	0.346%

Sum of corrected areas: 45897148

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Misc :
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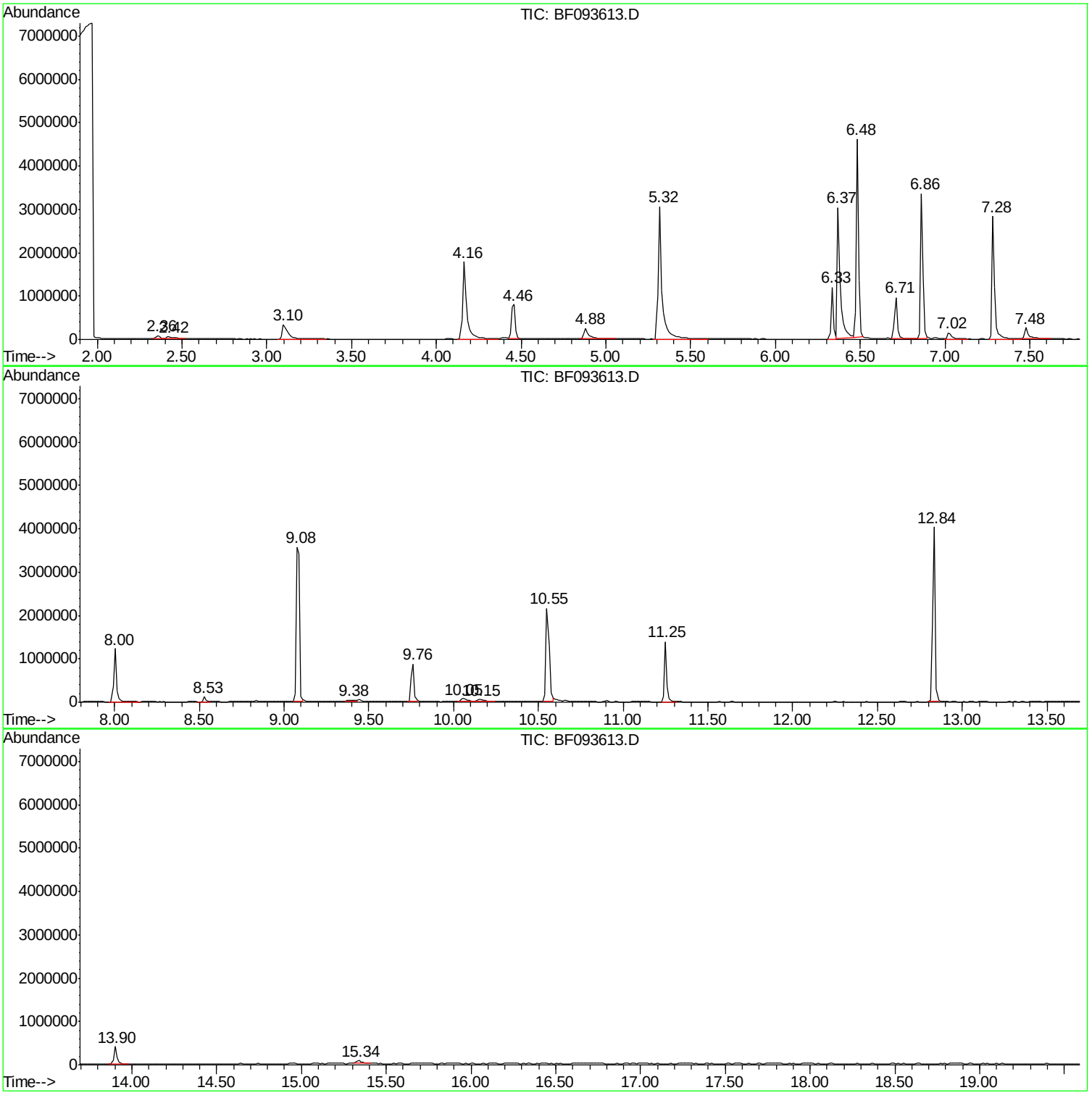
Instrument : BNA_F
ClientSampleId : D-74

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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

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Misc :
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Instrument : BNA_F
ClientSampleId : D-74

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

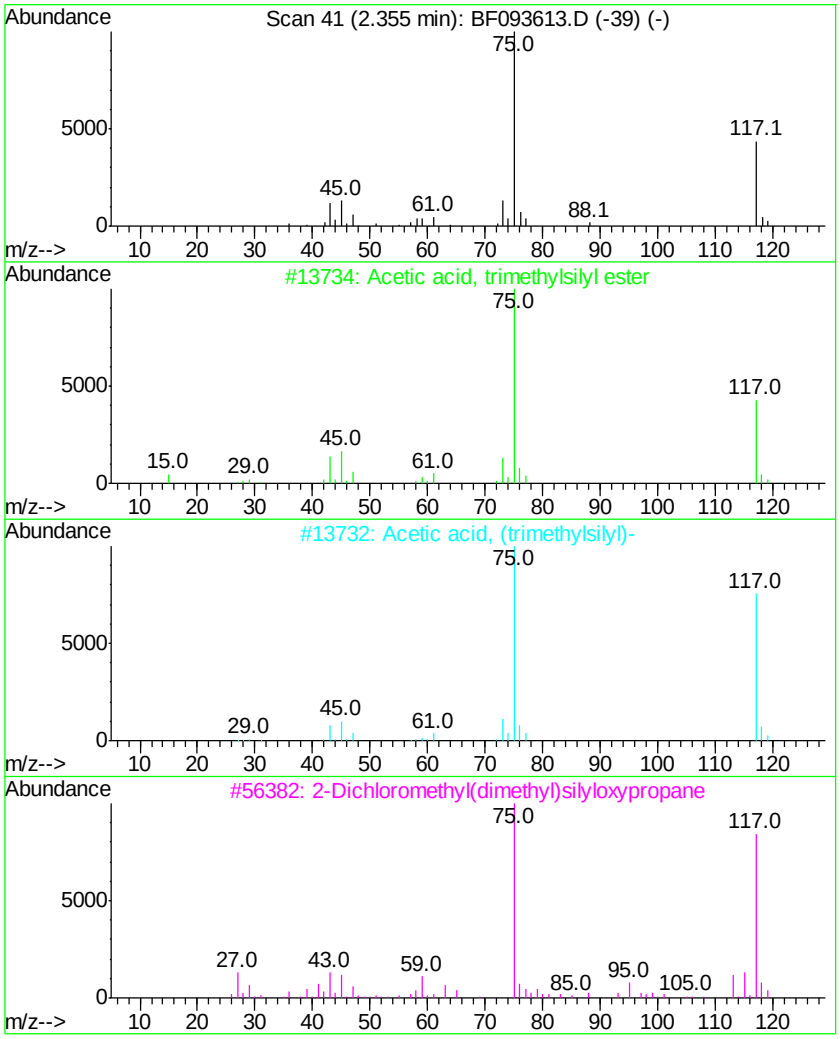
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

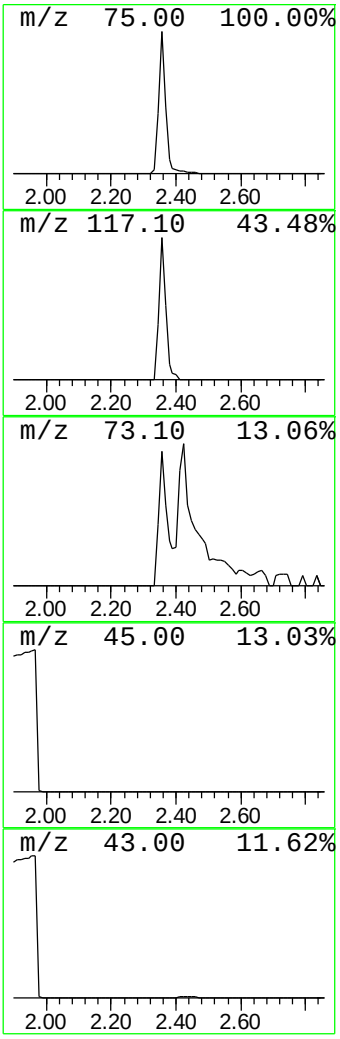
****

Peak Number 1 Acetic acid, trimethylsilyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.36	2.35 ng	118862	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, trimethylsilyl ester	132	C5H12O2Si	018147-36-9	90
2	Acetic acid, (trimethylsilyl)-	132	C5H12O2Si	002345-38-2	83
3	2-Dichloromethyl(dimethyl)silylo...	200	C6H14Cl2OSi	018209-57-9	56
4	Silane, trimethylpropoxy-	132	C6H16OSi	001825-63-4	56
5	Silane, trimethyl(1-methylethoxy)-	132	C6H16OSi	001825-64-5	56





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Data File : BF093613.D
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Operator : SJ/MA
Sample : I2174-23
Misc :
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Instrument : BNA_F
ClientSampleId : D-74

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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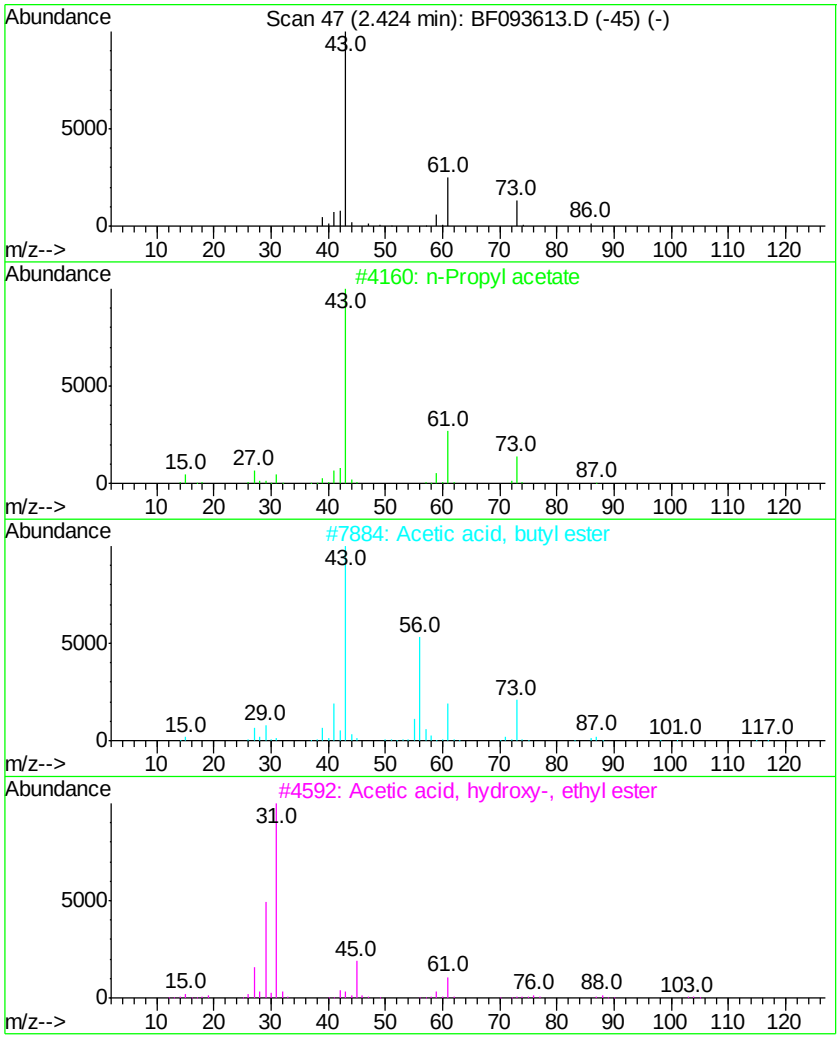
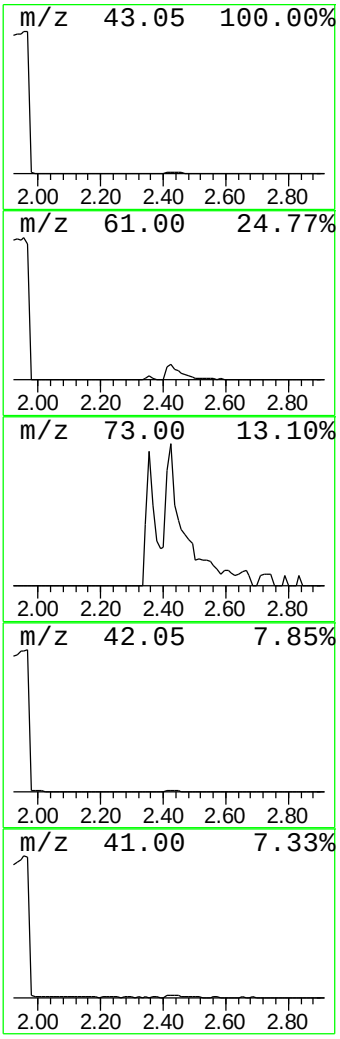
Peak Number 2 n-Propyl acetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.42	2.59 ng	130977	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	4
3	Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	4
4	1-Butanamine	73	C4H11N	000109-73-9	4
5	Isobutylamine	73	C4H11N	000078-81-9	3





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Operator : SJ/MA
Sample : I2174-23
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-74

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
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TIC Library : C:\DATABASE\NIST02.L
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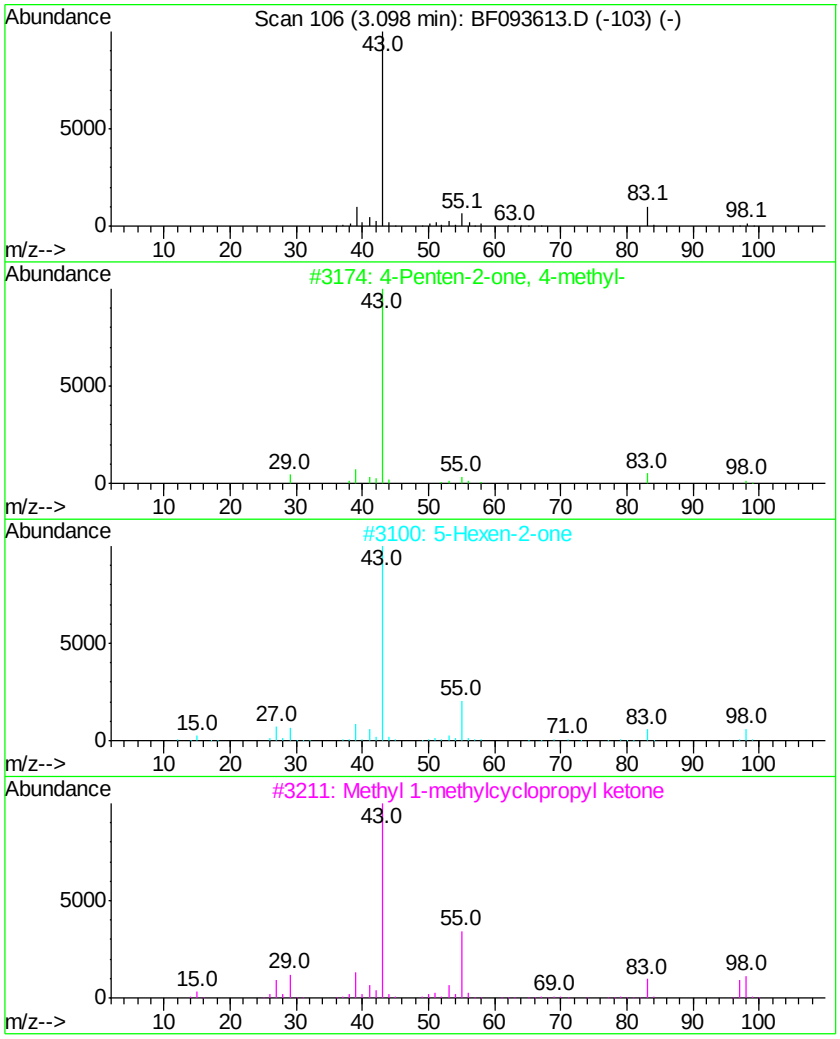
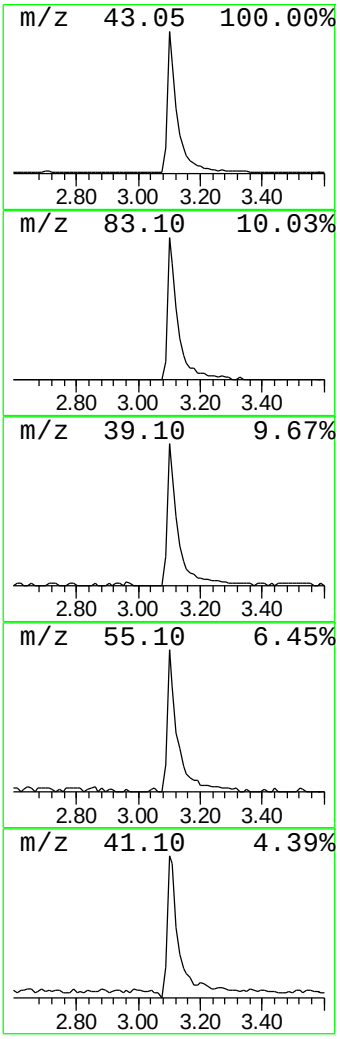
Peak Number 3 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.10	15.86 ng	803388	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	72
2	5-Hexen-2-one	98	C6H10O	000109-49-9	36
3	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	25
4	Pent-3-enylamine	85	C5H11N	087156-70-5	9
5	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	9





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ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-74

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

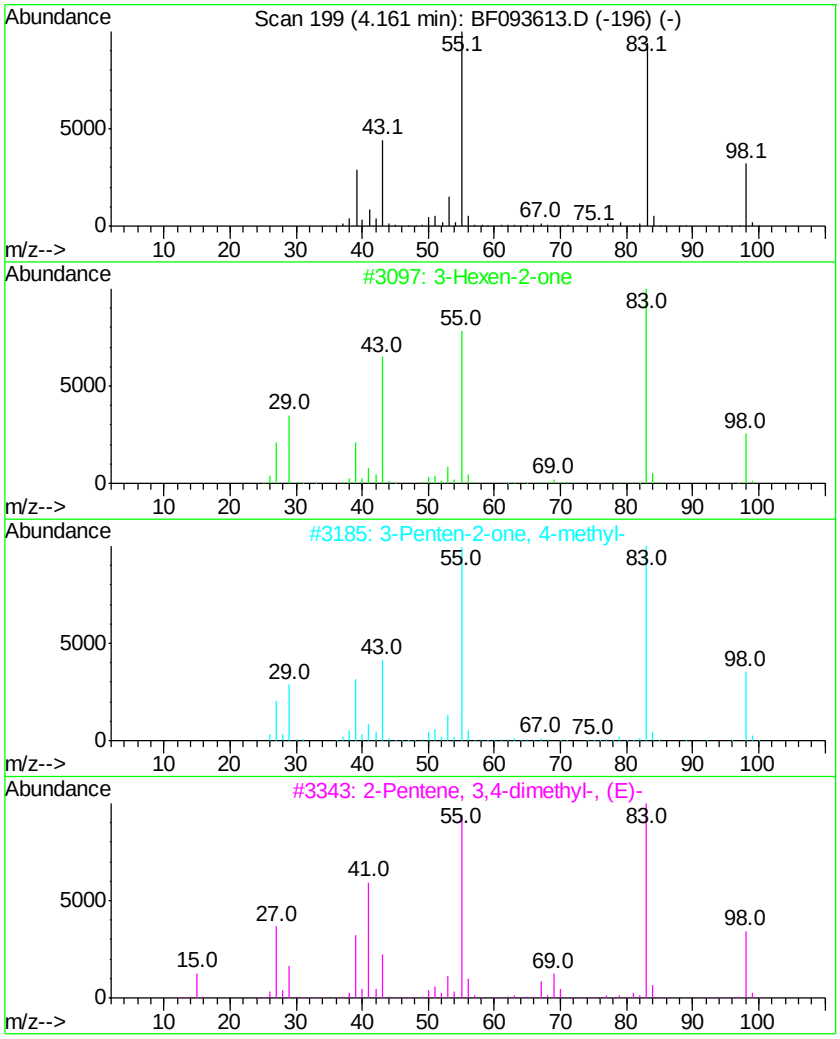
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

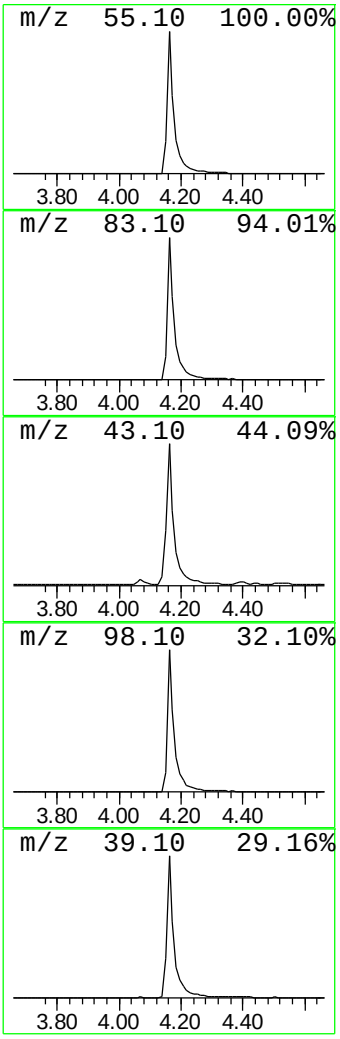
****

Peak Number 4 3-Hexen-2-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	59.53 ng	3016140	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





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Sample : I2174-23
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-74

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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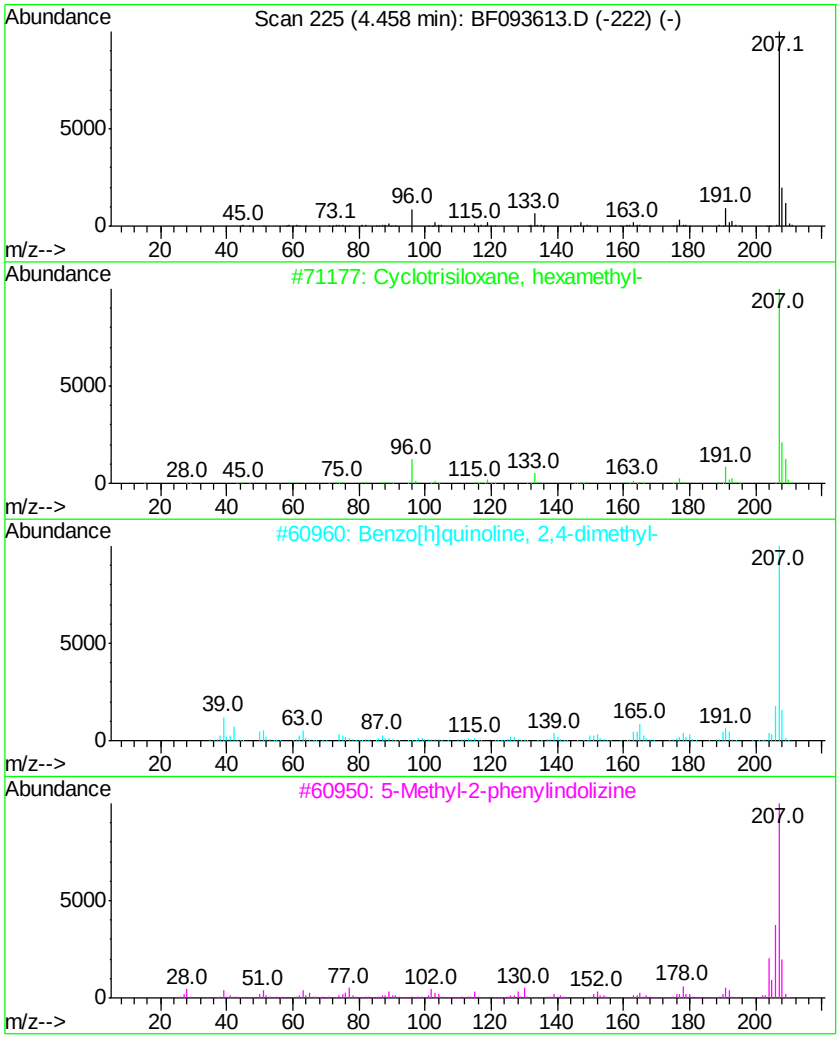
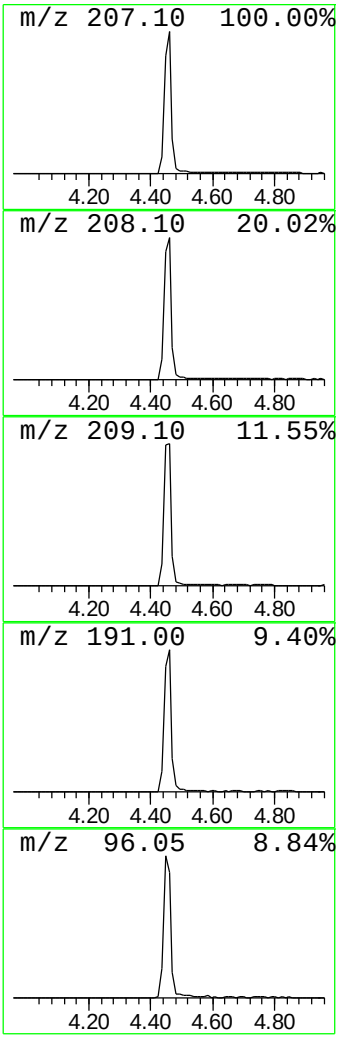
****

Peak Number 5 Cyclotrisiloxane, hexamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	24.42 ng	1237400	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	91
2	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	39
3	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	39
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	39
5	Benz[b]-1,4-oxazepine-4(5H)-thio...	207	C11H13NOS	1000258-63-4	9





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Misc :
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Instrument : BNA_F
ClientSampleId : D-74

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

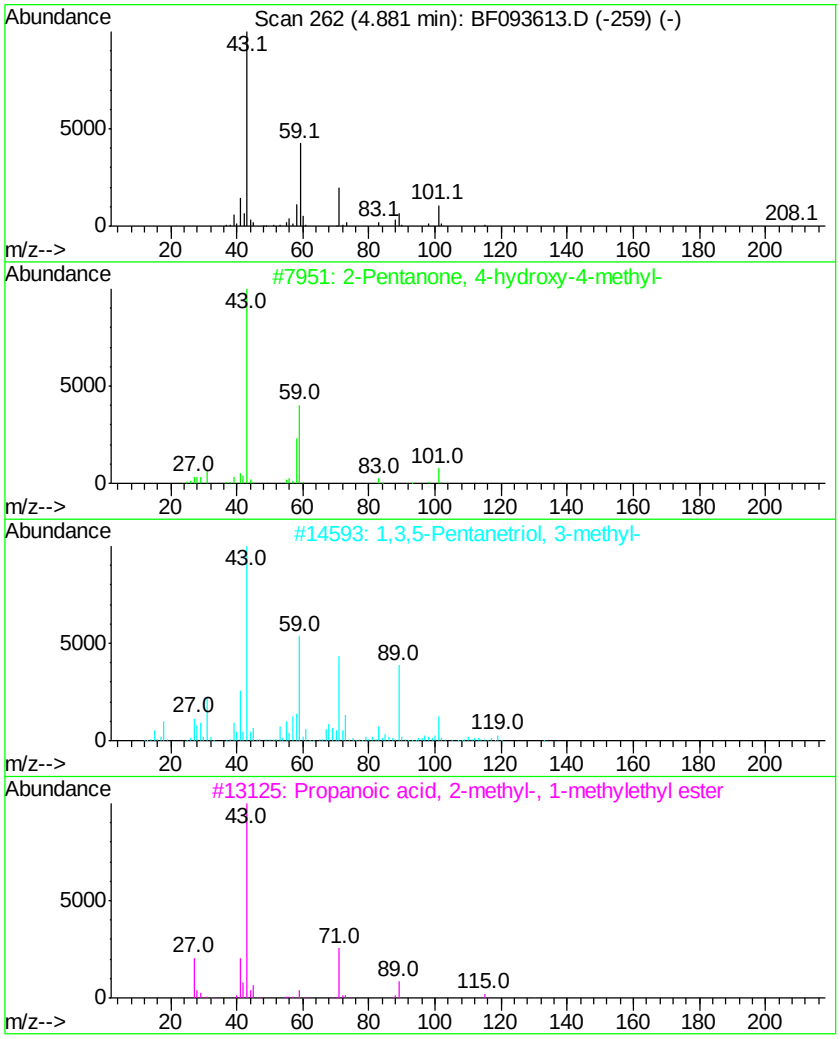
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

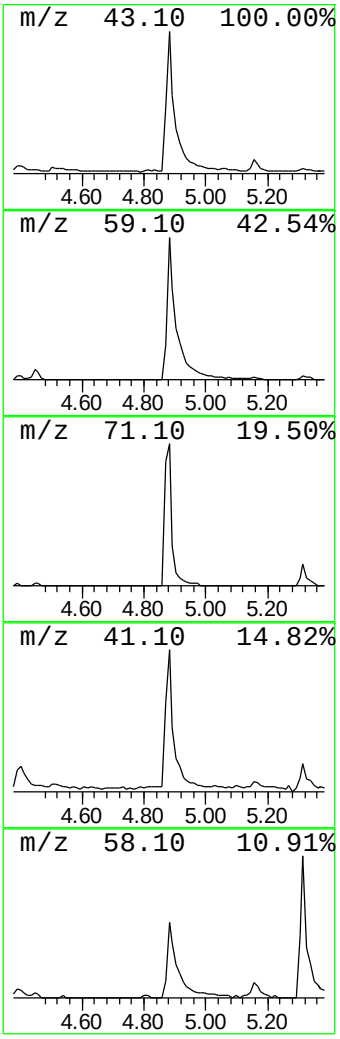
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	9.89 ng	501252	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2	1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	36
3	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	22
4	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	12
5	Formamide, N-butyl-	101	C5H11NO	000871-71-6	9





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Instrument : BNA_F
ClientSampleId : D-74

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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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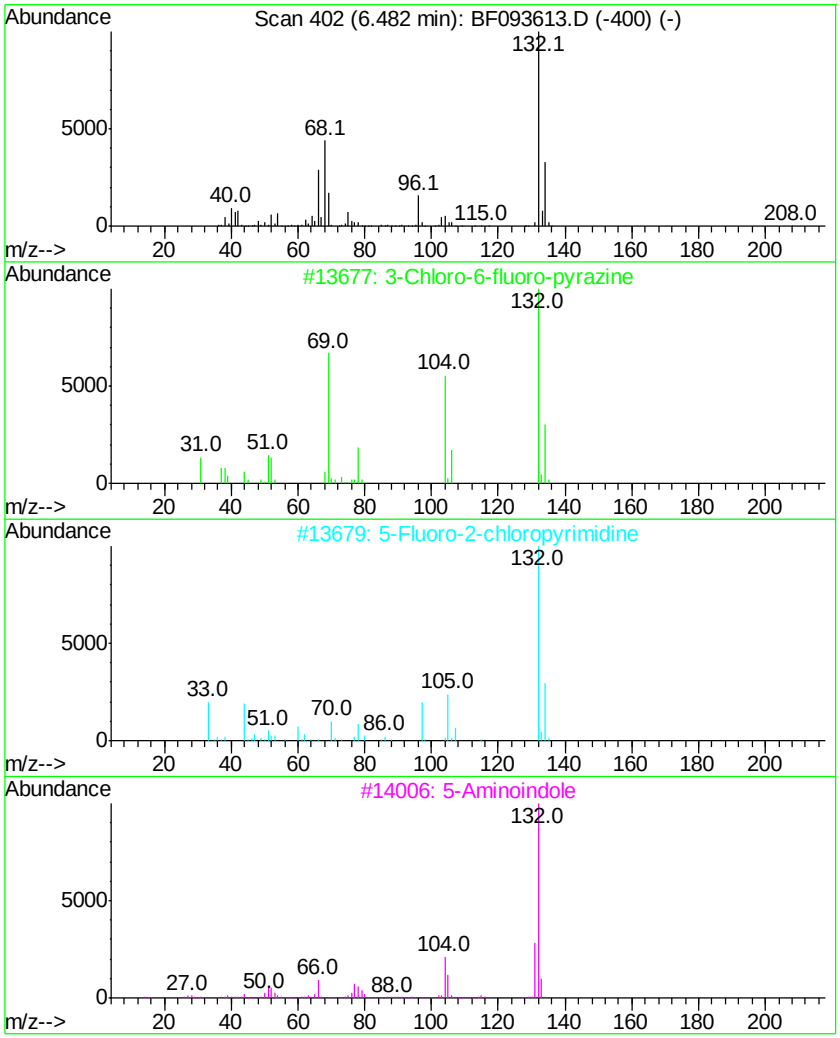
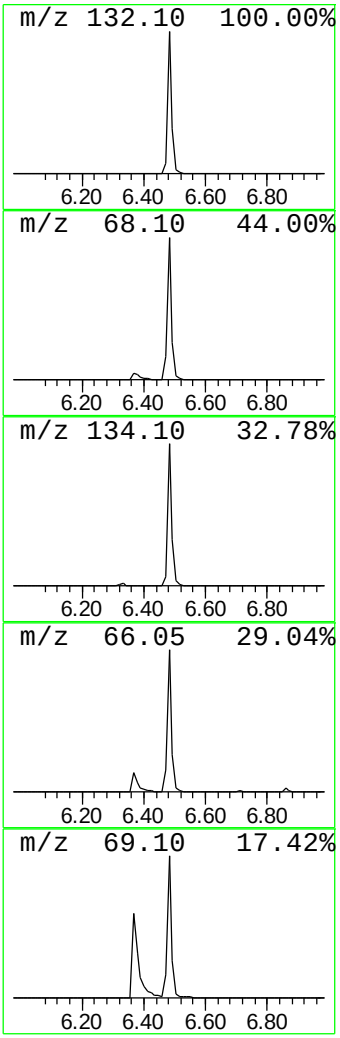
Peak Number 7 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	89.05 ng	4511960	1,4-Dichlorobenzene-d4	6.71

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	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9





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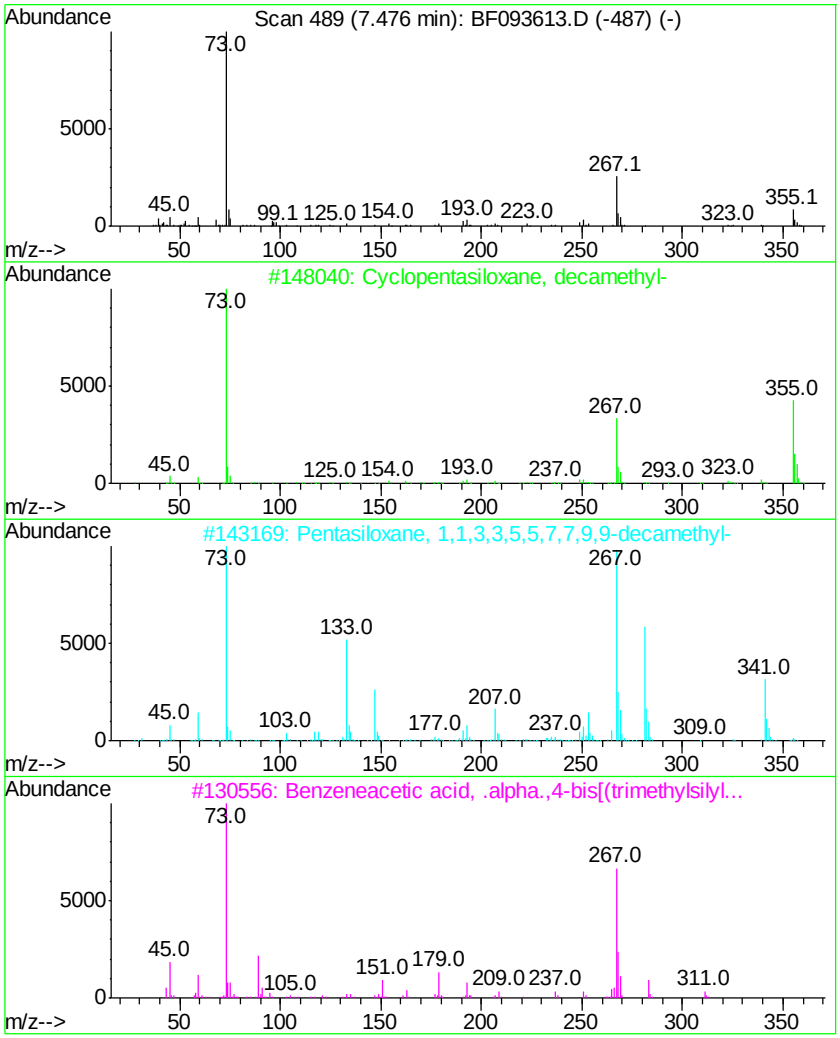
TIC Integration Parameters: LSCINT.P

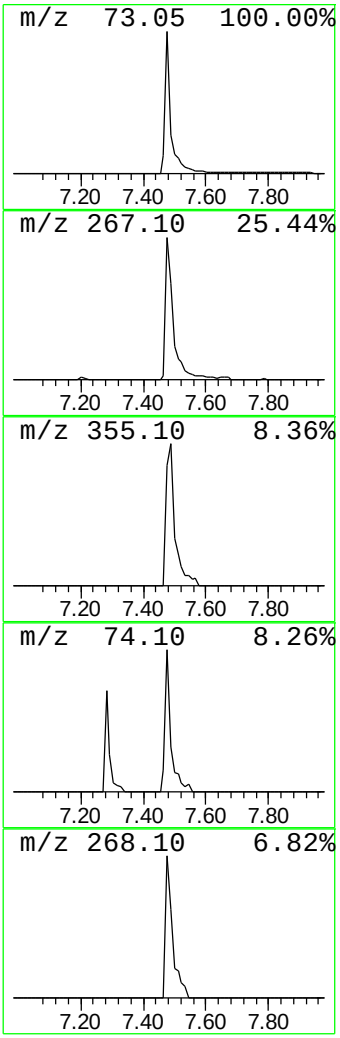
****

Peak Number 10 Cyclopentasiloxane, decamet... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	6.40 ng	431921	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	90
2	Pentasiloxane, 1,1,3,3,5,5,7,7,9...	356	C10H32O4Si5	000995-83-5	56
3	Benzeneacetic acid, .alpha.,4-bi...	326	C15H26O4Si2	055334-40-2	38
4	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	37
5	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	36





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

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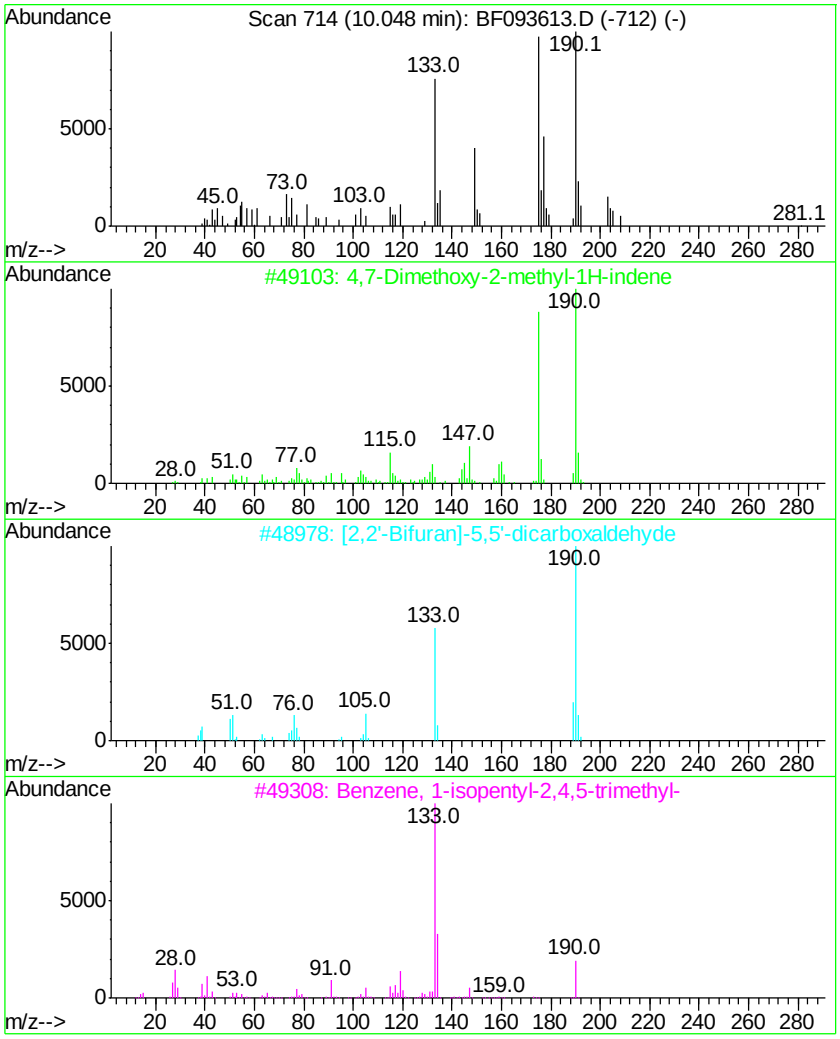
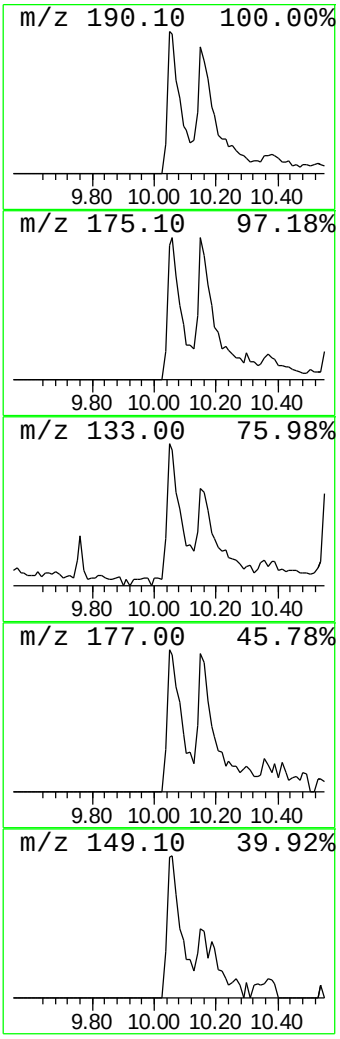
Peak Number 11 unknown10.05 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.05	3.77 ng	200906	Acenaphthene-d10	9.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,7-Dimethoxy-2-methyl-1H-indene	190	C12H14O2	1000188-03-2	35
2	[2,2'-Bifuran]-5,5'-dicarboxalde...	190	C10H6O4	005905-01-1	35
3	Benzene, 1-isopentyl-2,4,5-trime...	190	C14H22	010425-90-8	27
4	Thiophene, 3-methyl-2,5-bis(meth...	190	C7H10S3	050878-68-7	25
5	3(E)-Hydroxyimino-1,2,2,5,6,7-he...	207	C13H21NO	1000140-10-5	16





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Instrument : BNA_F
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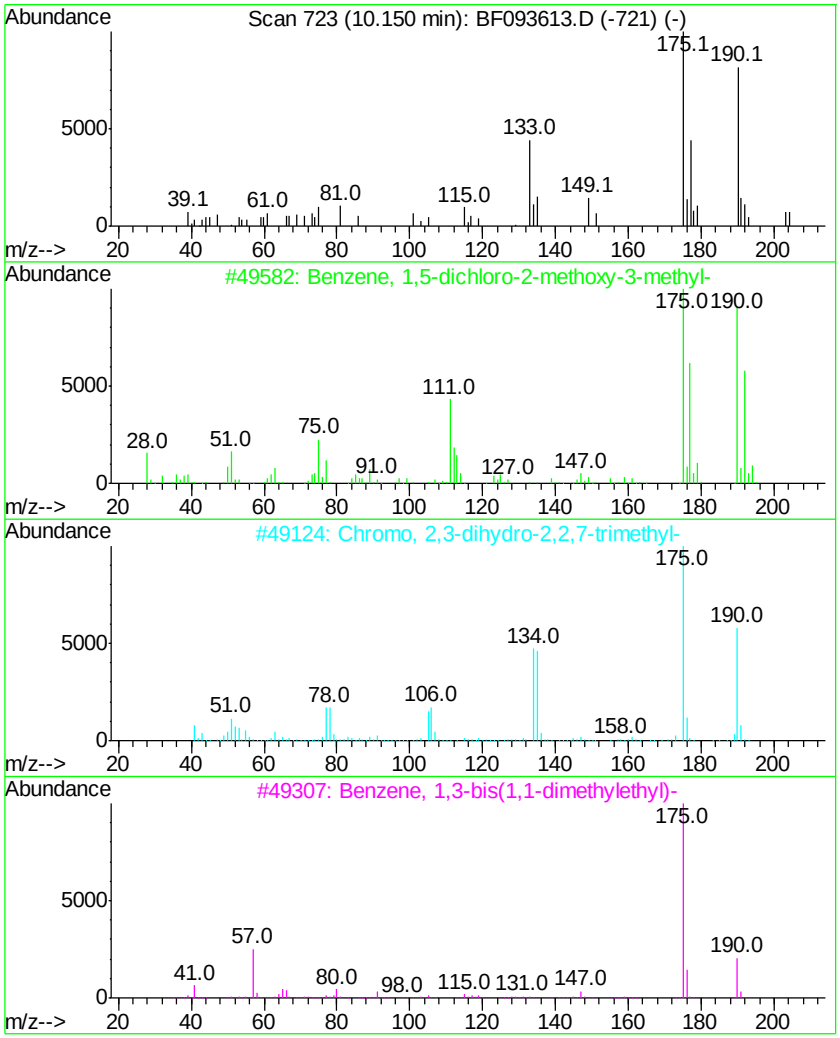
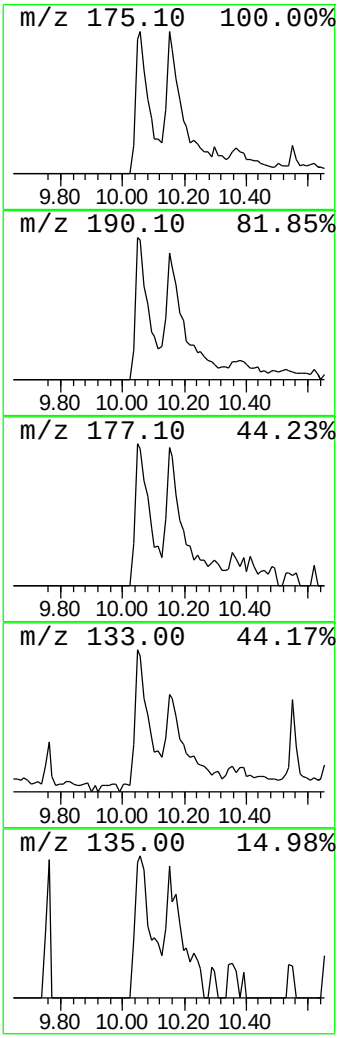
Peak Number 12 Benzene, 1,5-dichloro-2-met... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.15	2.31 ng	122856	Acenaphthene-d10	9.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,5-dichloro-2-methoxy-...	190	C8H8Cl2O	013334-73-1	58
2	Chromo, 2,3-dihydro-2,2,7-trimet...	190	C12H14O2	110411-30-8	50
3	Benzene, 1,3-bis(1,1-dimethyleth...	190	C14H22	001014-60-4	49
4	4,7-Dimethoxy-2-methyl-1H-indene	190	C12H14O2	1000188-03-2	49
5	Benzenamine, N,N-dimethyl-4-[[(1...	190	C12H18N2	027976-83-6	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093613.D
Acq On : 13 Mar 2017 17:56
Operator : SJ/MA
Sample : I2174-23
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-74

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.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
Acetic acid, trim...	2.36	2.4	ng	118862	1	6.71	1013350	20.0
n-Propyl acetate	2.42	2.6	ng	130977	1	6.71	1013350	20.0
4-Penten-2-one, 4...	3.10	15.9	ng	803388	1	6.71	1013350	20.0
3-Hexen-2-one	4.16	59.5	ng	3016140	1	6.71	1013350	20.0
Cyclotrisiloxane,...	4.46	24.4	ng	1237400	1	6.71	1013350	20.0
2-Pentanone, 4-hy...	4.88	9.9	ng	501252	1	6.71	1013350	20.0
unknown6.48	6.48	89.0	ng	4511960	1	6.71	1013350	20.0
Cyclopentasiloxan...	7.48	6.4	ng	431921	2	8.00	1349080	20.0
unknown10.05	10.05	3.8	ng	200906	3	9.76	1064980	20.0
Benzene, 1,5-dich...	10.15	2.3	ng	122856	3	9.76	1064980	20.0