LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093610.D
Acq On : 13 Mar 2017 16:35
Operator : SJ/MA
Sample : I2174-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-67

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	2.344	37	40	44	rBV	41672	71021	1.55%	0.168%
2	2.401	44	45	55	rVB	50567	129522	2.82%	0.307%
3	3.087	103	105	122	rBV	320485	750507	16.36%	1.778%
4	4.161	196	199	217	rBV	1065516	2090153	45.57%	4.951%
5	4.447	222	224	228	rVB	154322	231003	5.04%	0.547%
6	4.870	259	261	277	rBV	272527	547317	11.93%	1.296%
7	5.316	298	300	316	rBV	2489836	4586474	100.00%	10.863%
8	6.333	387	389	391	rBV	199166	194725	4.25%	0.461%
9	6.367	391	392	400	rVV	3098383	3879257	84.58%	9.188%
10	6.482	400	402	405	rVB	4317434	4198097	91.53%	9.943%
11	6.710	420	422	429	rVB	902662	962426	20.98%	2.280%
12	6.859	433	435	441	rBV	3172762	3325162	72.50%	7.876%
13	7.019	448	449	456	rVB2	153292	235067	5.13%	0.557%
14	7.282	470	472	484	rBV	2697974	3020796	65.86%	7.155%
15	7.476	487	489	499	rVB2	52785	123027	2.68%	0.291%
16	8.002	532	535	540	rBV2	1280814	2340822	51.04%	5.544%
17	8.722	597	598	601	rBV	147825	146119	3.19%	0.346%
18	8.825	605	607	615	rVB	79516	116116	2.53%	0.275%
19	9.076	627	629	632	rBV	3486103	4533174	98.84%	10.737%
20	9.373	653	655	659	rBV	53985	100793	2.20%	0.239%
21	9.762	686	689	691	rBV	977687	1191709	25.98%	2.823%
22	10.048	711	714	721	rBV	109352	256323	5.59%	0.607%
23	10.151	721	723	731	rVB2	76084	181838	3.96%	0.431%
24	10.551	756	758	766	rBV	2076135	2582034	56.30%	6.116%
25	11.248	817	819	824	rBV	1499386	1417085	30.90%	3.356%
26	12.837	955	958	960	rBV	4026931	3947522	86.07%	9.350%
27	13.900	1049	1051	1062	rBV	695186	817927	17.83%	1.937%
28	15.328	1171	1176	1182	rBV3	105699	243846	5.32%	0.578%

Sum of corrected areas: 42219862

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Operator : SJ/MA
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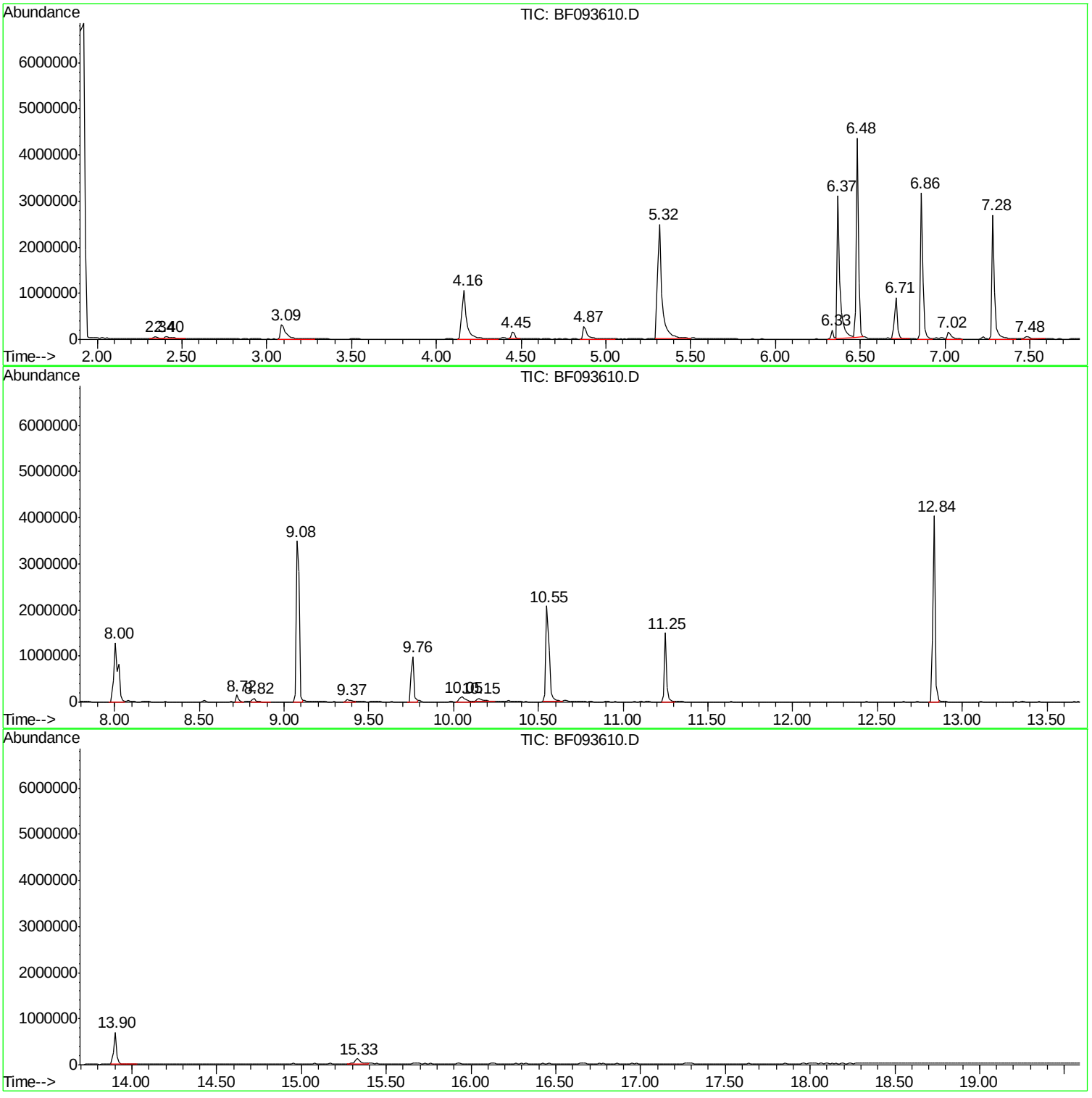
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-67

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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Operator : SJ/MA
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

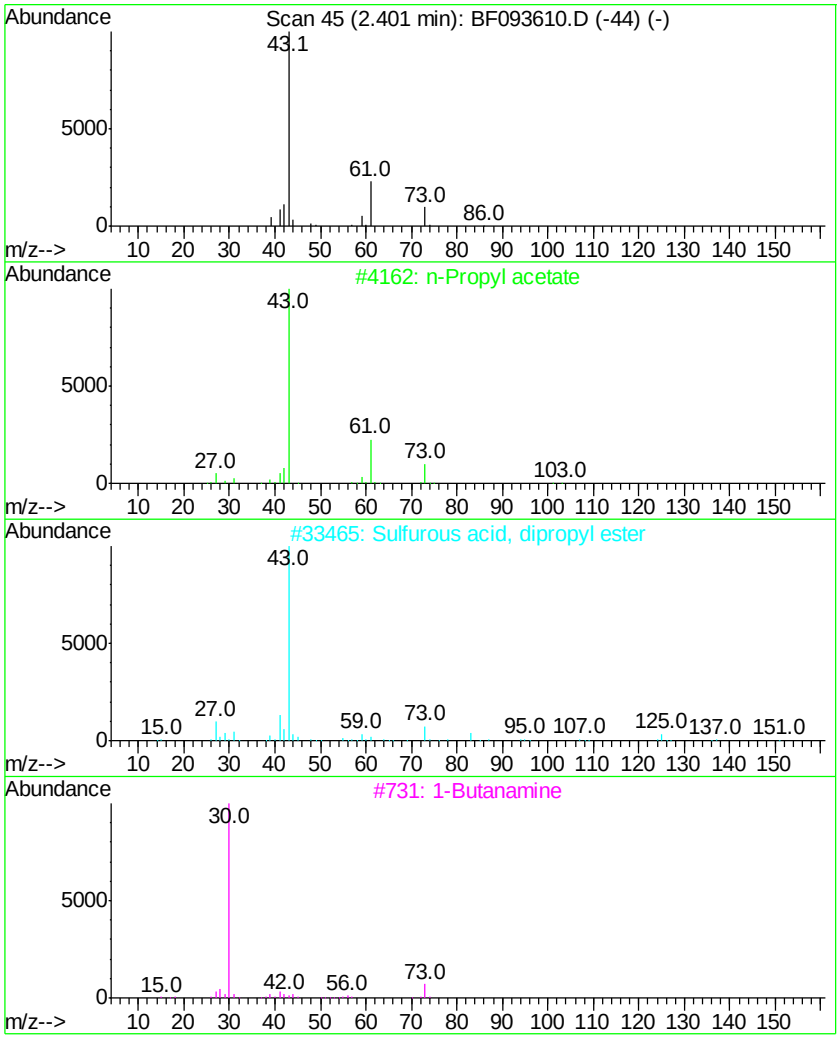
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

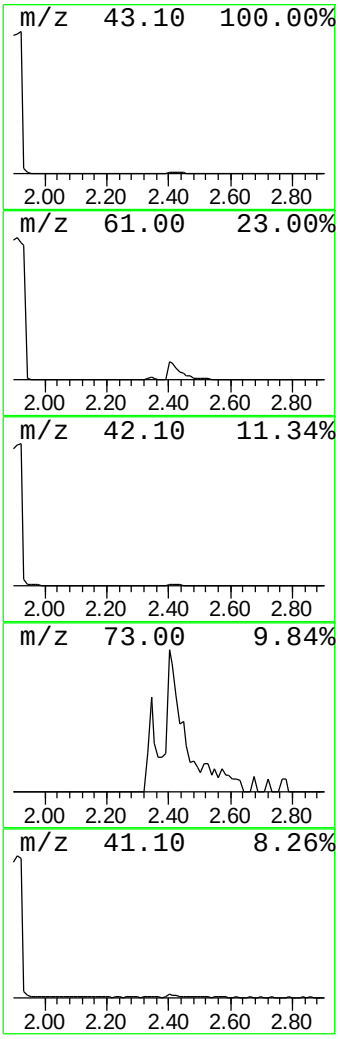
****

Peak Number 1 n-Propyl acetate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.40	2.69 ng	129522	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	Sulfurous acid, dipropyl ester	166	C6H14O3S	000623-98-3	9
3	1-Butanamine	73	C4H11N	000109-73-9	5
4	Isobutylamine	73	C4H11N	000078-81-9	4
5	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	4





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Data File : BF093610.D
Acq On : 13 Mar 2017 16:35
Operator : SJ/MA
Sample : I2174-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-67

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

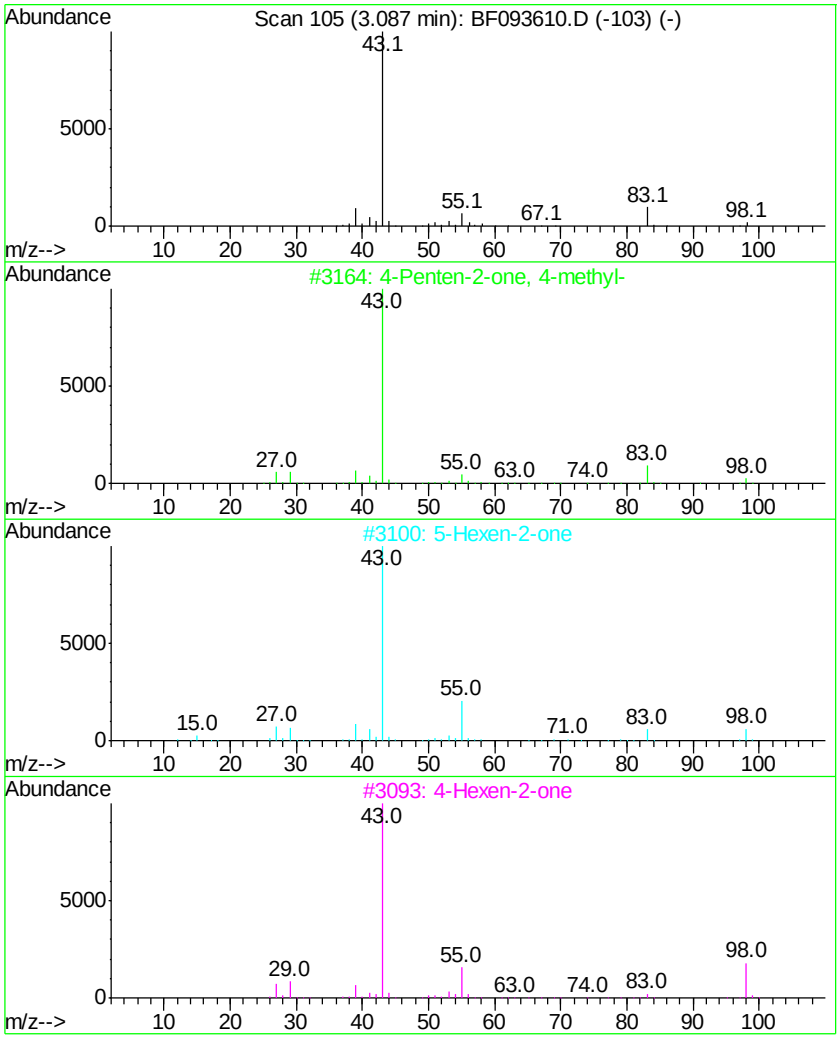
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

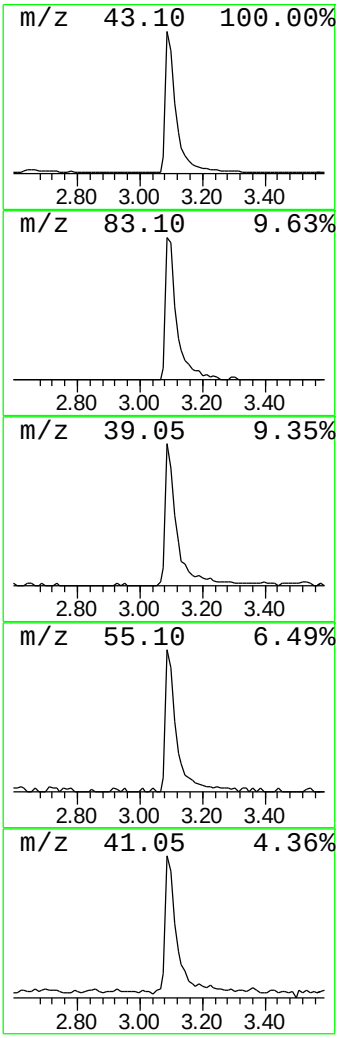
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.09	15.60 ng	750507	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	80
2	5-Hexen-2-one	98	C6H10O	000109-49-9	38
3	4-Hexen-2-one	98	C6H10O	025659-22-7	9
4	2-Vinylethyl acetate	114	C6H10O2	001576-84-7	9
5	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9





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Data File : BF093610.D
Acq On : 13 Mar 2017 16:35
Operator : SJ/MA
Sample : I2174-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-67

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

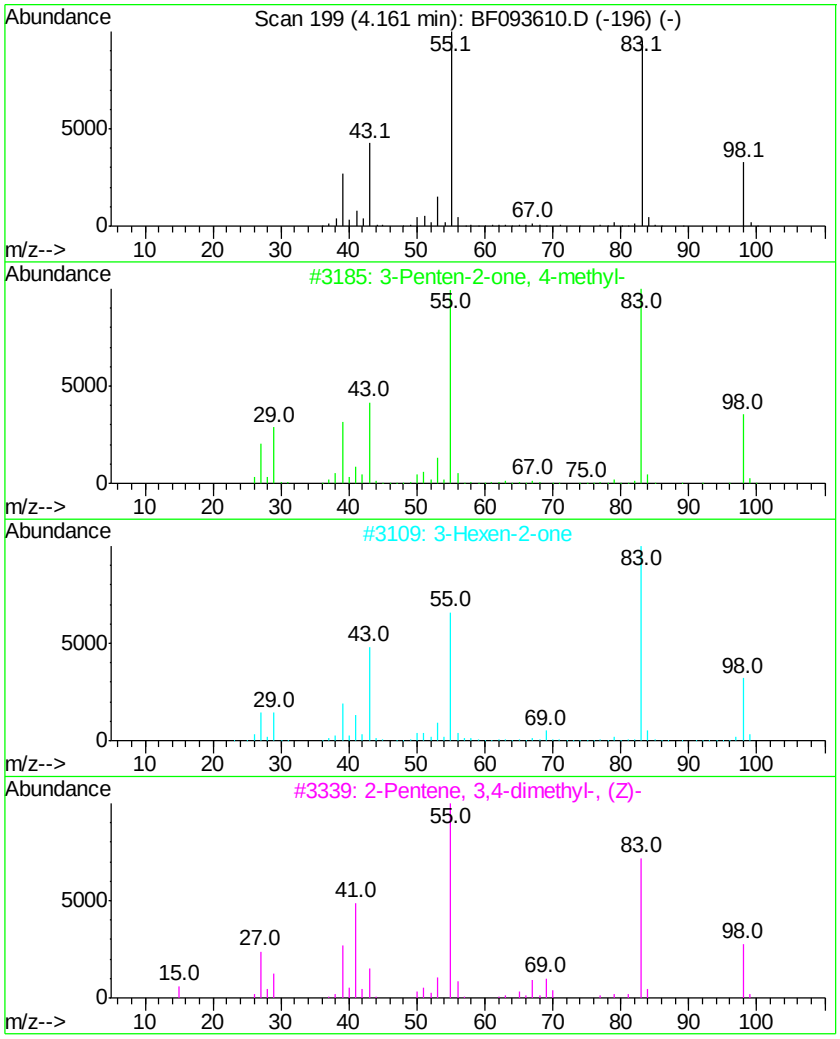
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

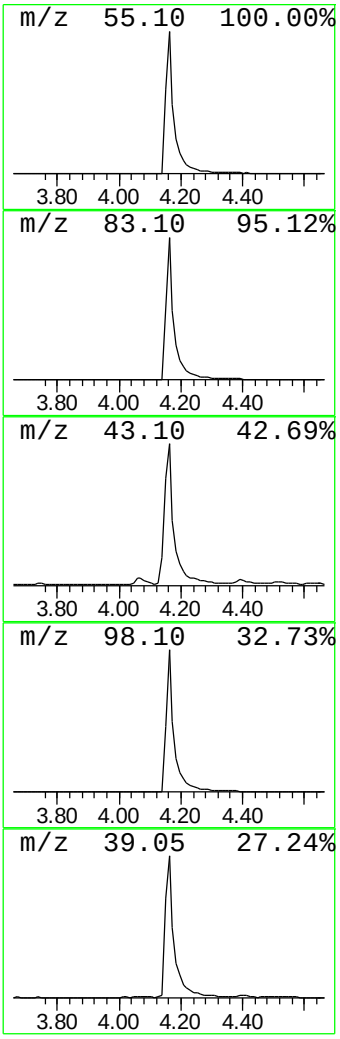
****

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	43.44 ng	2090150	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78





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Sample : I2174-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-67

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

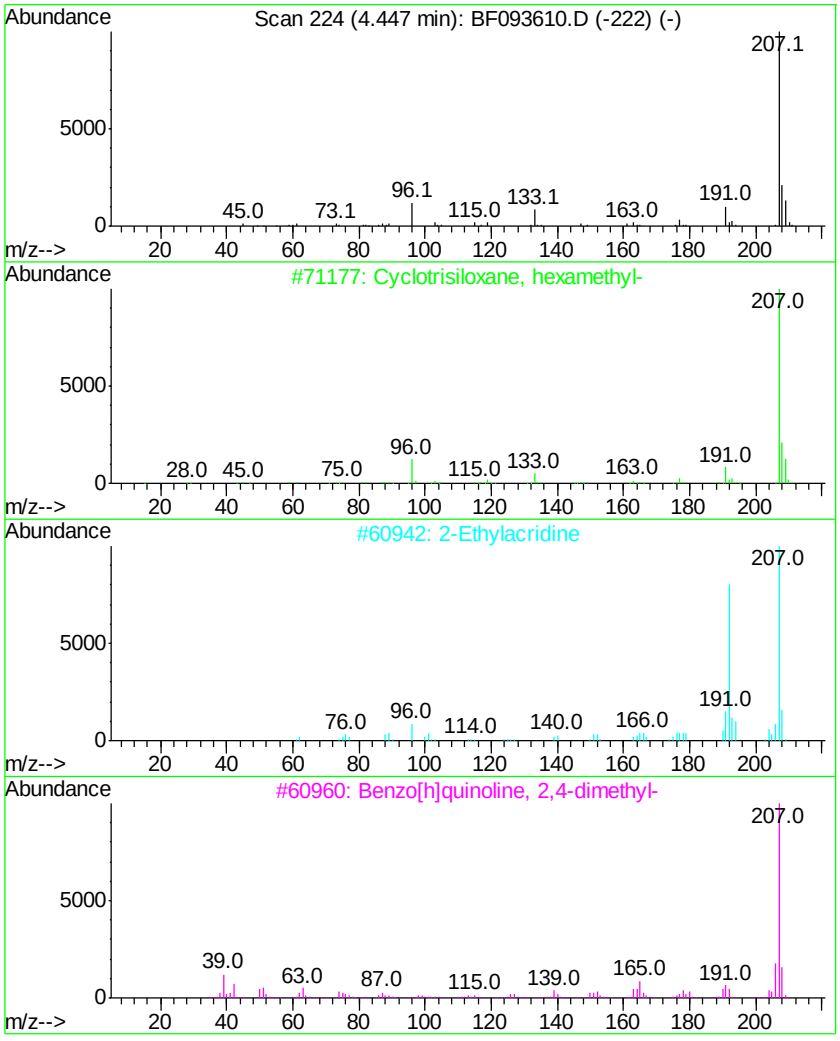
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

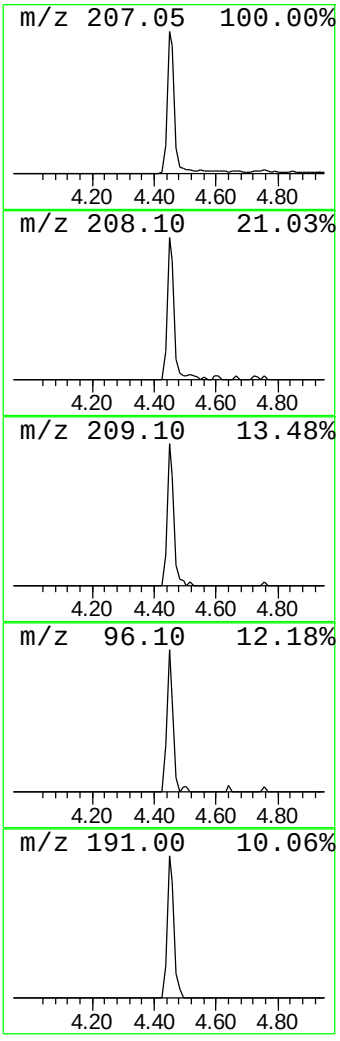
****

Peak Number 4 Cyclotrisiloxane, hexamethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.45	4.80 ng	231003	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	2-Ethylacridine	207	C15H13N	055751-83-2	45
3	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	39
4	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	39
5	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093610.D
Acq On : 13 Mar 2017 16:35
Operator : SJ/MA
Sample : I2174-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-67

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

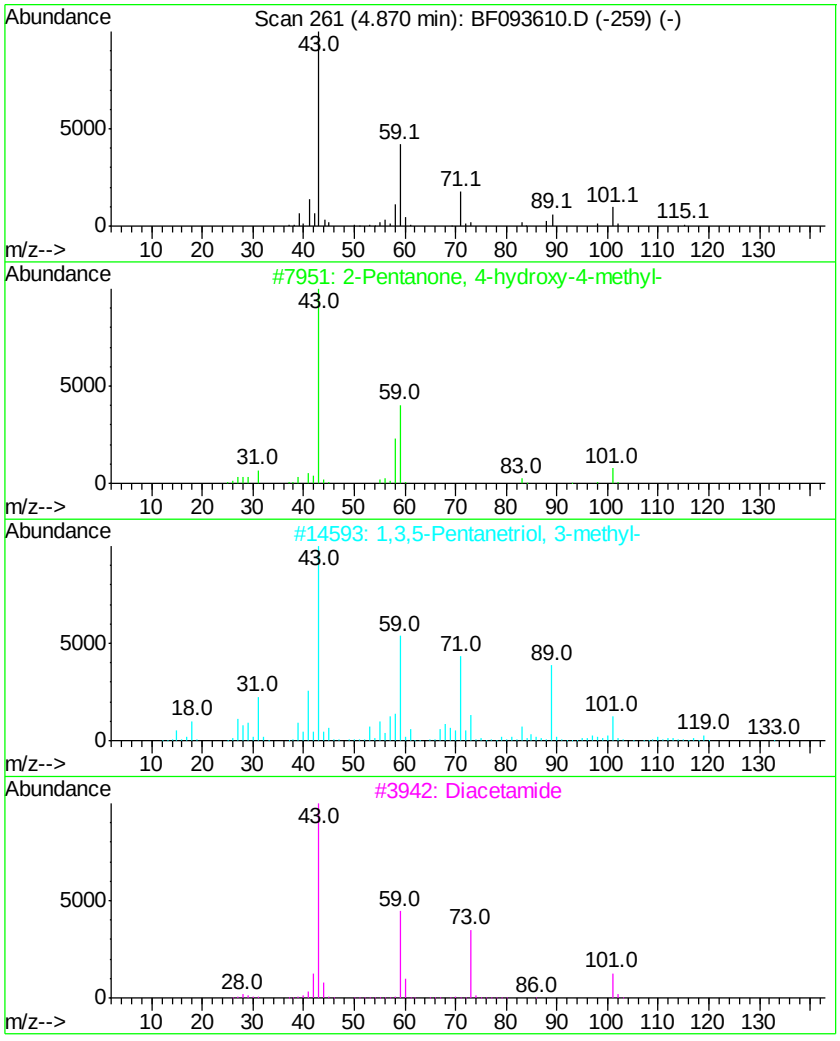
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

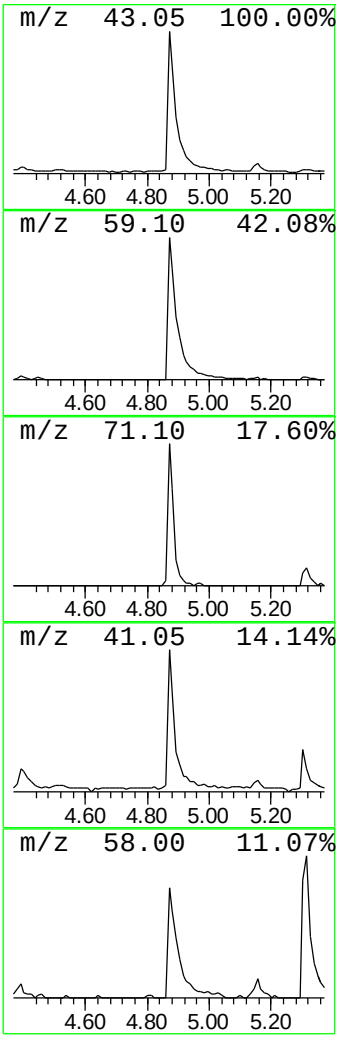
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	11.37 ng	547317	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	40
2	1,3,5-Pentanetriol, 3-methyl-	134	C6H14O3	007564-64-9	38
3	Diacetamide	101	C4H7NO2	000625-77-4	33
4	2-Pentene, 2-methoxy-	100	C6H12O	061142-47-0	33
5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	12





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Sample : I2174-20
Misc :
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Instrument : BNA_F
ClientSampleId : D-67

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

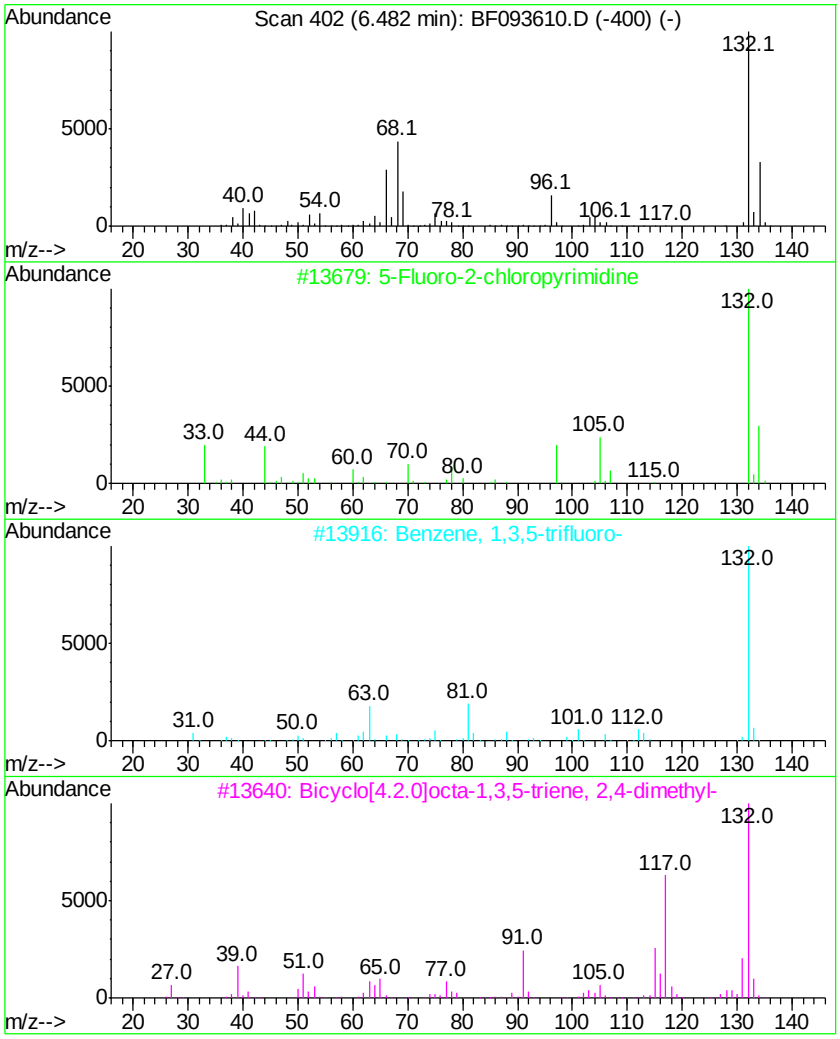
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

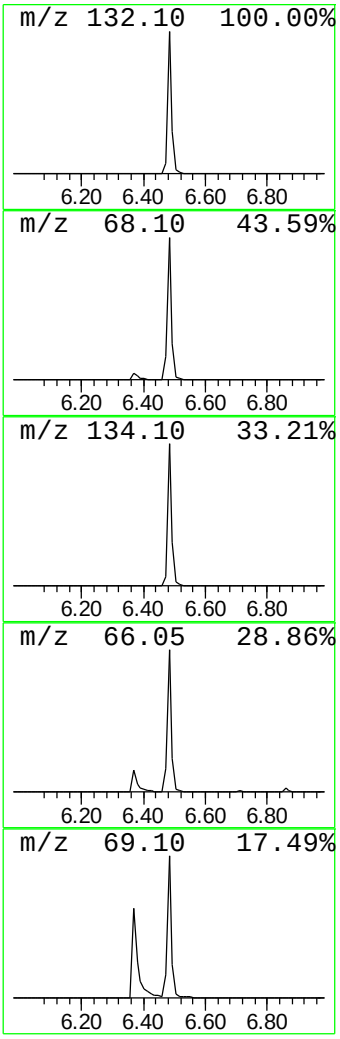
****

Peak Number 6 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	87.24 ng	4198100	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093610.D
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Operator : SJ/MA
Sample : I2174-20
Misc :
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Instrument : BNA_F
ClientSampleId : D-67

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

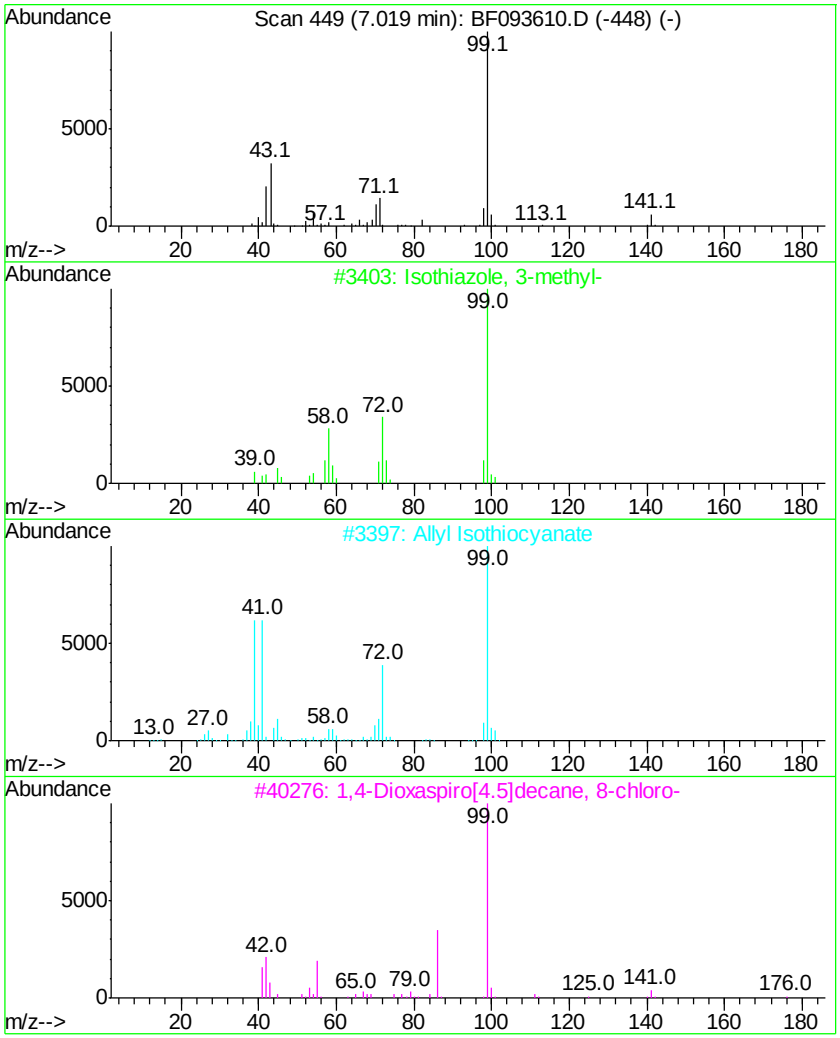
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

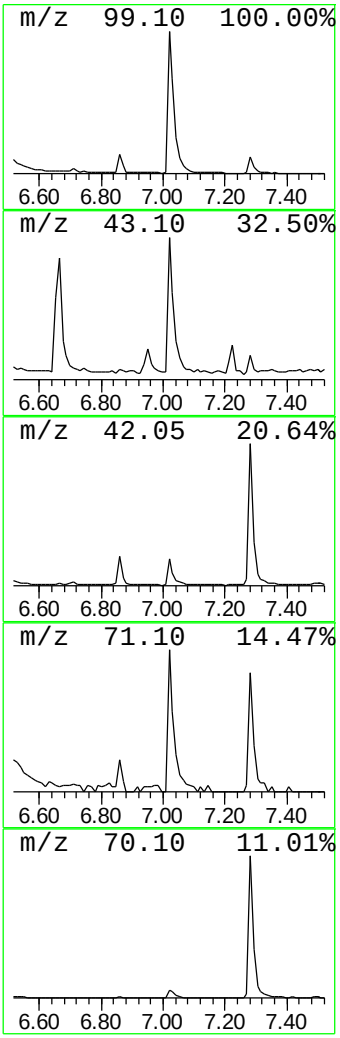
****

Peak Number 8 Isothiazole, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	4.88 ng	235067	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isothiazole, 3-methyl-	99	C4H5NS	000693-92-5	50
2	Allyl Isothiocyanate	99	C4H5NS	000057-06-7	45
3	1,4-Dioxaspiro[4.5]decane, 8-chl...	176	C8H13ClO2	055724-03-3	42
4	Hexanoic acid, 1-cyclopentylethy...	212	C13H24O2	1000279-28-7	39
5	3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	38





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Instrument : BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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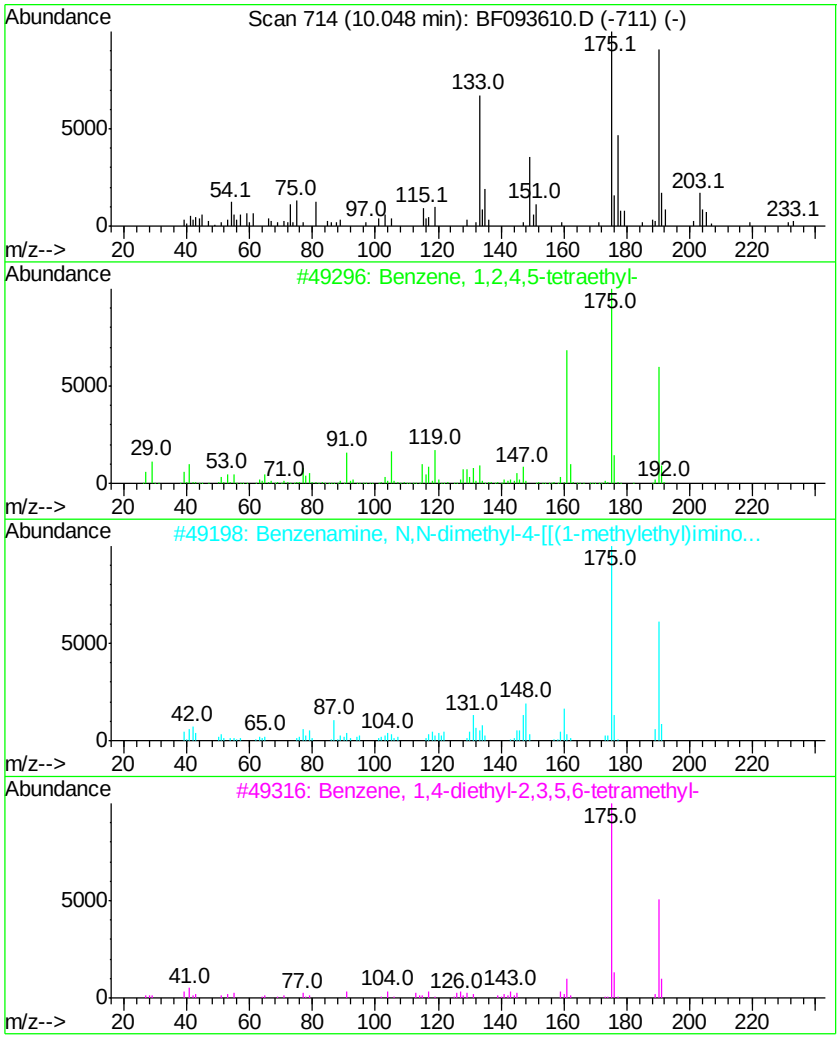
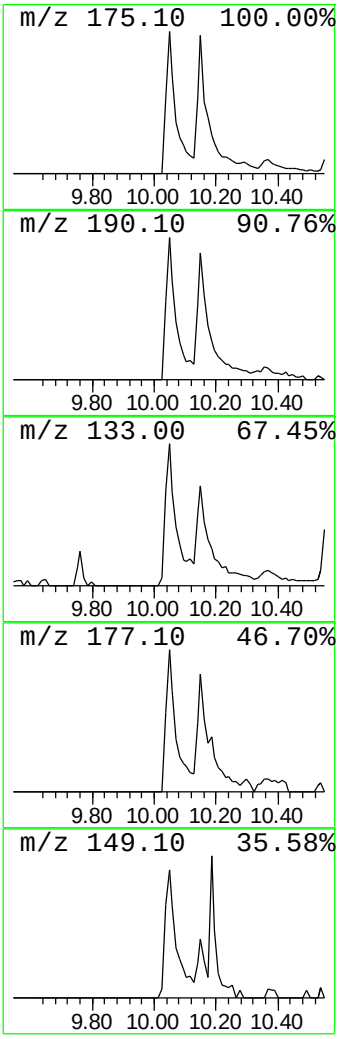
Peak Number 9 unknown10.05 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.05	4.30 ng	256323	Acenaphthene-d10	9.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,4,5-tetraethyl-	190	C14H22	000635-81-4	49
2	Benzenamine, N,N-dimethyl-4-[[(1...	190	C12H18N2	027976-83-6	47
3	Benzene, 1,4-diethyl-2,3,5,6-tet...	190	C14H22	033962-13-9	47
4	4,7-Dimethoxy-2-methyl-1H-indene	190	C12H14O2	1000188-03-2	47
5	5,8-Dimethoxyquinoxaline	190	C10H10N2O2	019506-19-5	43





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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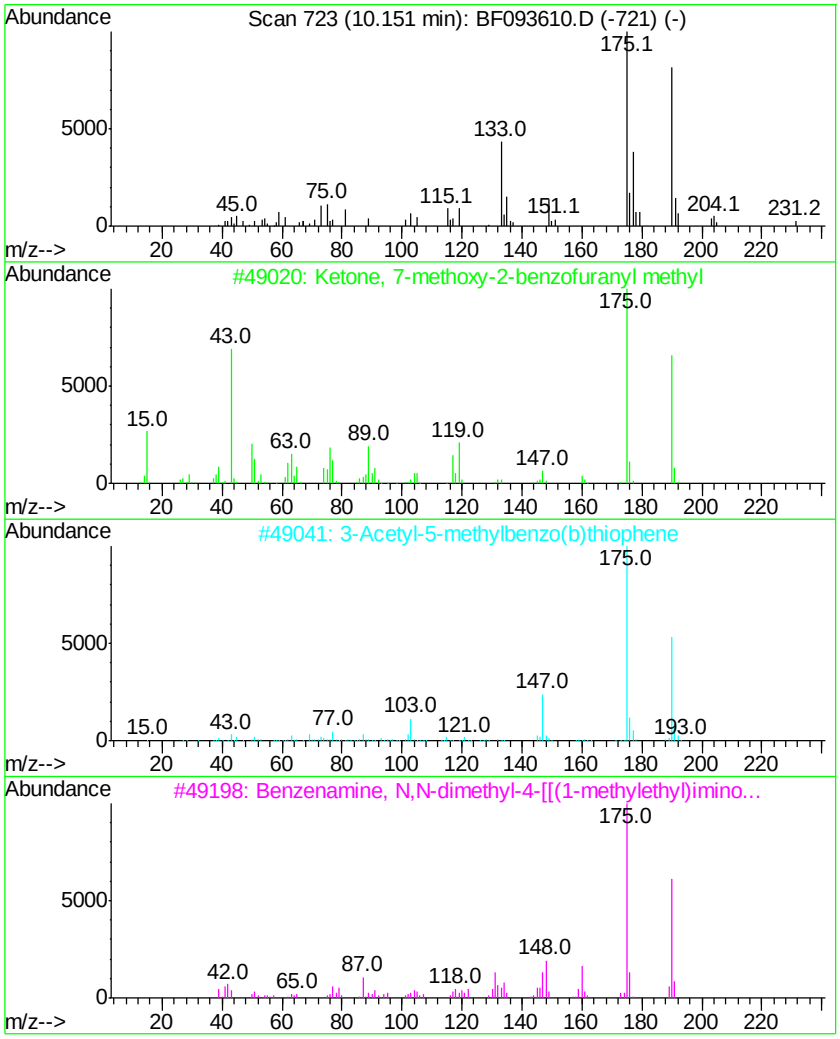
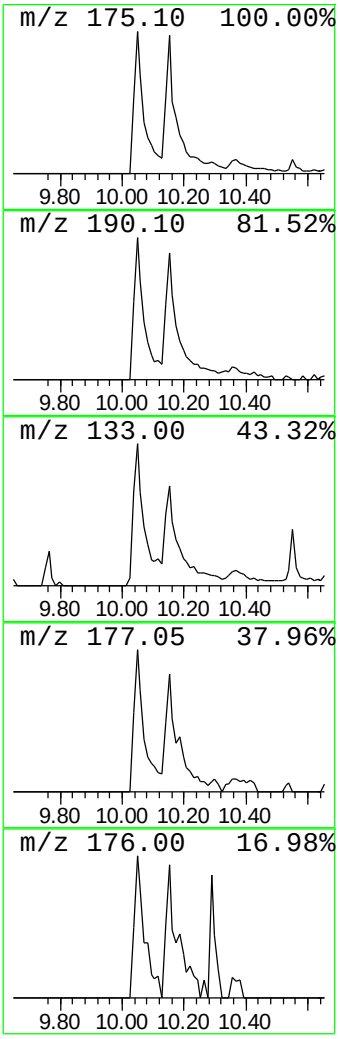
Peak Number 10 Ketone, 7-methoxy-2-benzofu... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.15	3.05 ng	181838	Acenaphthene-d10	9.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ketone, 7-methoxy-2-benzofuranyl...	190	C11H10O3	043071-52-9	53
2	3-Acetyl-5-methylbenzo(b)thiophene	190	C11H10OS	002046-76-6	52
3	Benzenamine, N,N-dimethyl-4-[[(1...	190	C12H18N2	027976-83-6	52
4	Benzene, 1,3-diethyl-2,4,5,6-tet...	190	C14H22	033781-72-5	52
5	2-Acetyl-6-methylbenzo(b)thiophene	190	C11H10OS	001467-89-6	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.40	2.7	ng	129522	1	6.71	962426	20.0
4-Penten-2-one, 4...	3.09	15.6	ng	750507	1	6.71	962426	20.0
3-Penten-2-one, 4...	4.16	43.4	ng	2090150	1	6.71	962426	20.0
Cyclotrisiloxane,...	4.45	4.8	ng	231003	1	6.71	962426	20.0
2-Pentanone, 4-hy...	4.87	11.4	ng	547317	1	6.71	962426	20.0
unknown6.48	6.48	87.2	ng	4198100	1	6.71	962426	20.0
Isothiazole, 3-me...	7.02	4.9	ng	235067	1	6.71	962426	20.0
unknown10.05	10.05	4.3	ng	256323	3	9.76	1191710	20.0
Ketone, 7-methoxy...	10.15	3.0	ng	181838	3	9.76	1191710	20.0