LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093644.D
Acq On : 14 Mar 2017 8:29
Operator : SJ/MA
Sample : I2201-20
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-120

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	2.447	44	49	60	rBV	87037	244223	3.85%	0.458%
2	4.161	196	199	201	rBV	90183	121826	1.92%	0.228%
3	4.195	201	202	218	rVV	152707	440790	6.95%	0.826%
4	4.401	218	220	229	rVB	62331	142010	2.24%	0.266%
5	4.870	259	261	284	rBV	1263539	2554231	40.28%	4.789%
6	5.316	298	300	327	rBV	4439689	6170816	97.31%	11.569%
7	5.716	333	335	342	rVB	76313	122957	1.94%	0.231%
8	6.367	390	392	400	rBV	3597633	5574610	87.90%	10.452%
9	6.481	400	402	405	rVB	5060669	5318236	83.86%	9.971%
10	6.710	419	422	430	rVB	1035119	1216633	19.18%	2.281%
11	6.859	433	435	438	rBV	4009901	4215087	66.47%	7.903%
12	7.281	470	472	475	rBV	3070101	3854806	60.79%	7.227%
13	8.002	532	535	549	rBV	1424634	1673009	26.38%	3.137%
14	9.076	626	629	632	rBV	4231483	6341650	100.00%	11.890%
15	9.750	686	688	691	rBV	1193336	1745250	27.52%	3.272%
16	10.550	756	758	761	rBV2	2415687	3361337	53.00%	6.302%
17	11.248	816	819	825	rBV	1803022	1795927	28.32%	3.367%
18	12.653	940	942	944	rBV	178865	146193	2.31%	0.274%
19	12.836	955	958	961	rBV	4726407	5550637	87.53%	10.407%
20	13.362	1001	1004	1006	rBV	90517	101554	1.60%	0.190%
21	13.888	1048	1050	1062	rVB	1023413	1548168	24.41%	2.903%
22	15.305	1171	1174	1185	rVB	684110	1097880	17.31%	2.058%

Sum of corrected areas: 53337830

LSC Report - Integrated Chromatogram

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Misc :
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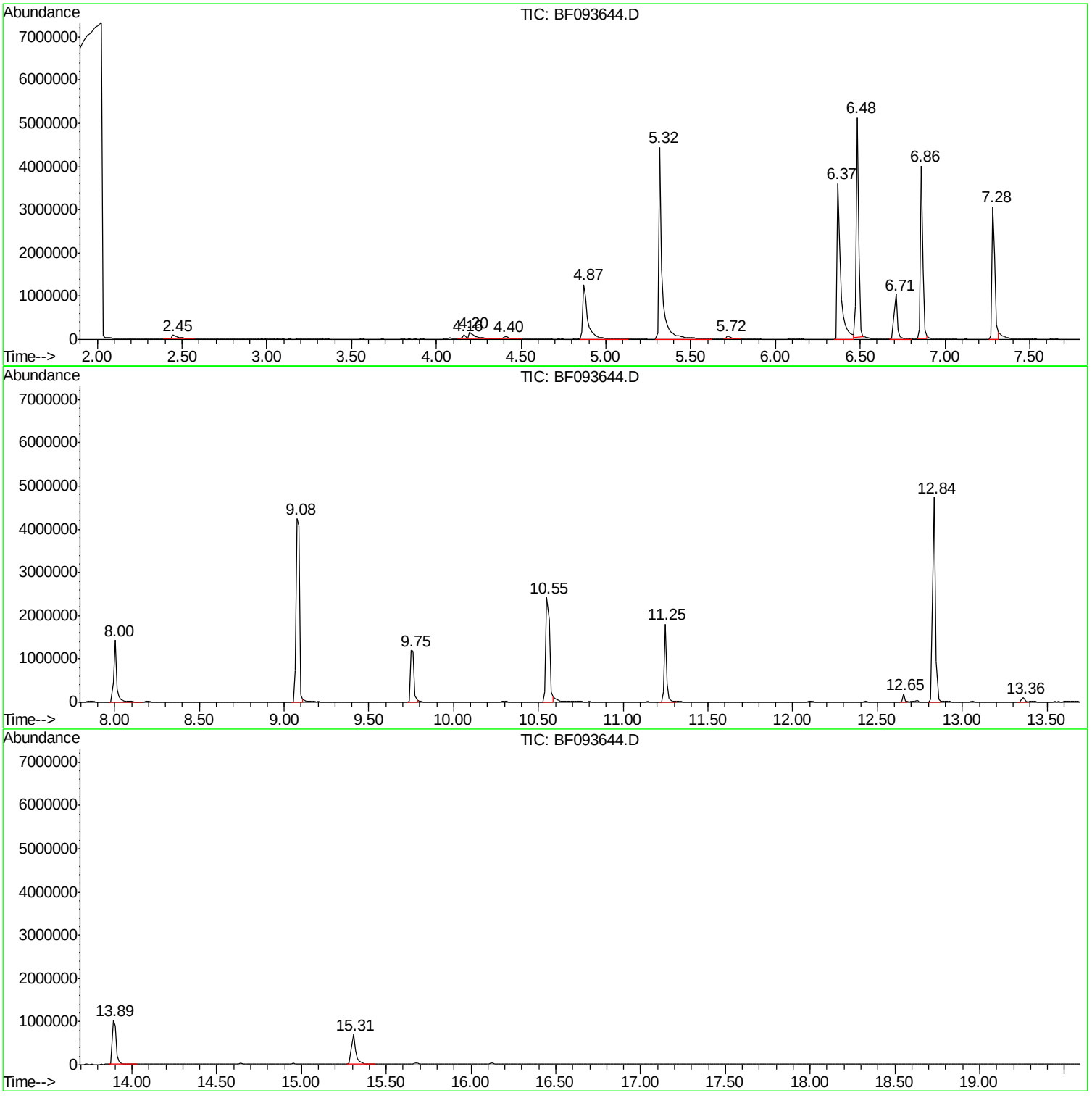
Instrument : BNA_F
ClientSampleId : D-120

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

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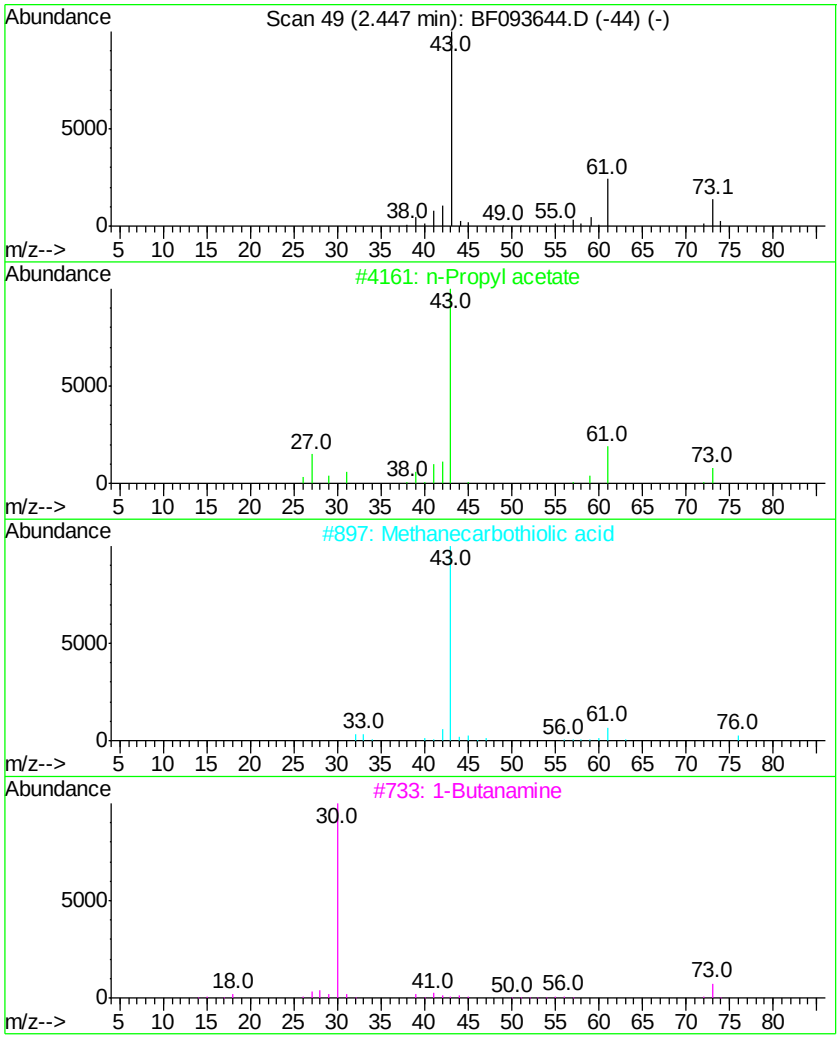
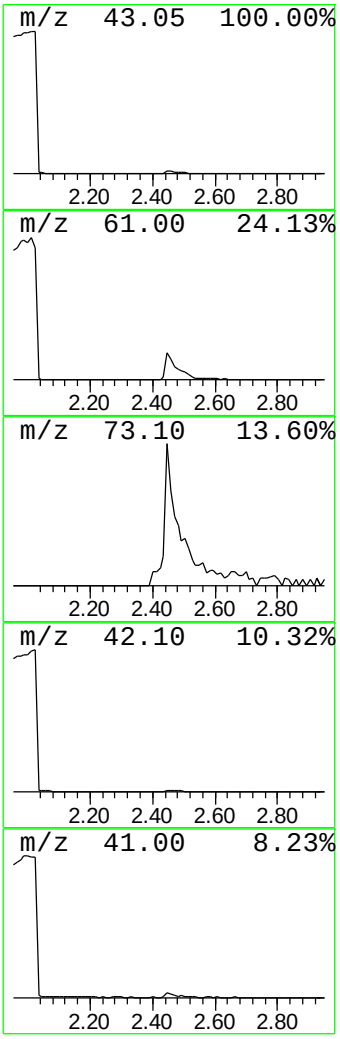
Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	4.01 ng	244223	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	72
2	Methanecarbothiolic acid	76	C2H4OS	000507-09-5	9
3	1-Butanamine	73	C4H11N	000109-73-9	7
4	Pentane	72	C5H12	000109-66-0	7
5	Isobutylamine	73	C4H11N	000078-81-9	5





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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
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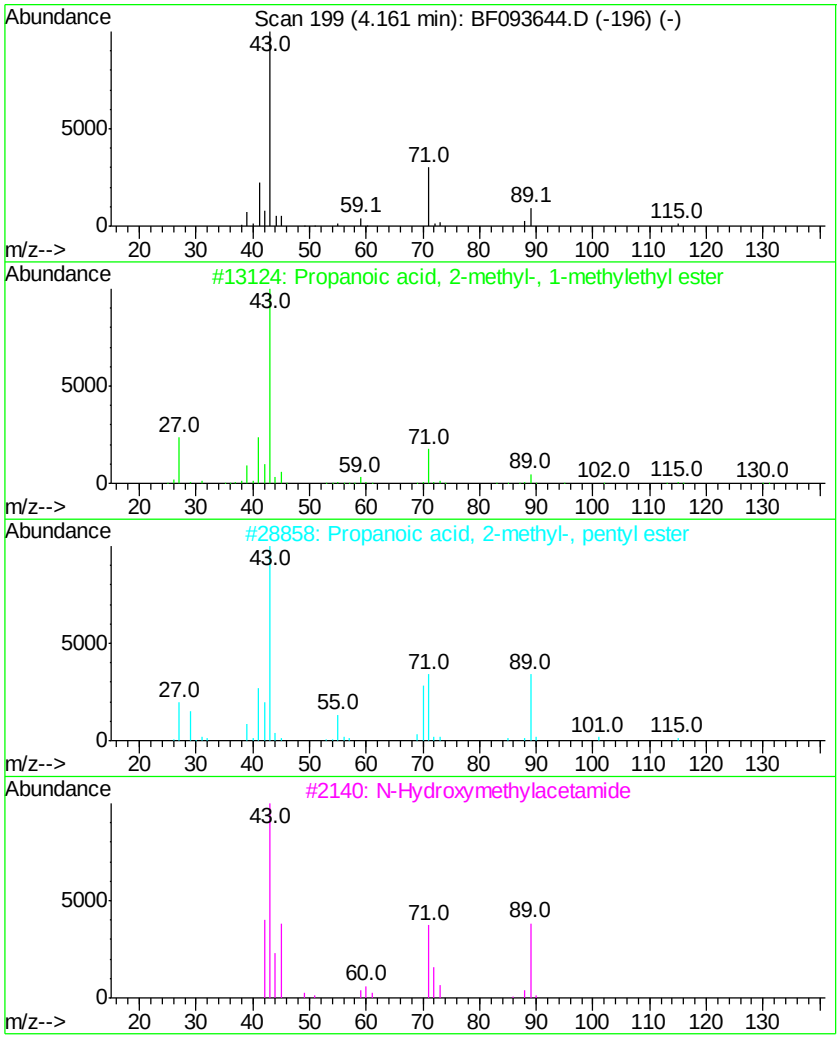
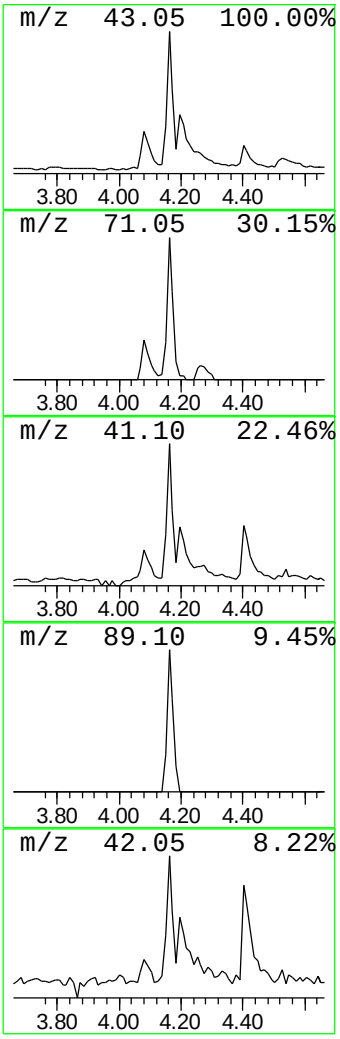
Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	2.00 ng	121826	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	38
3	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	9
4	.beta.-Alanine	89	C3H7NO2	000107-95-9	9
5	Propanoic acid, 2-methyl-, hexyl...	172	C10H20O2	002349-07-7	9





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Operator : SJ/MA
Sample : I2201-20
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-120

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

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TIC Integration Parameters: LSCINT.P

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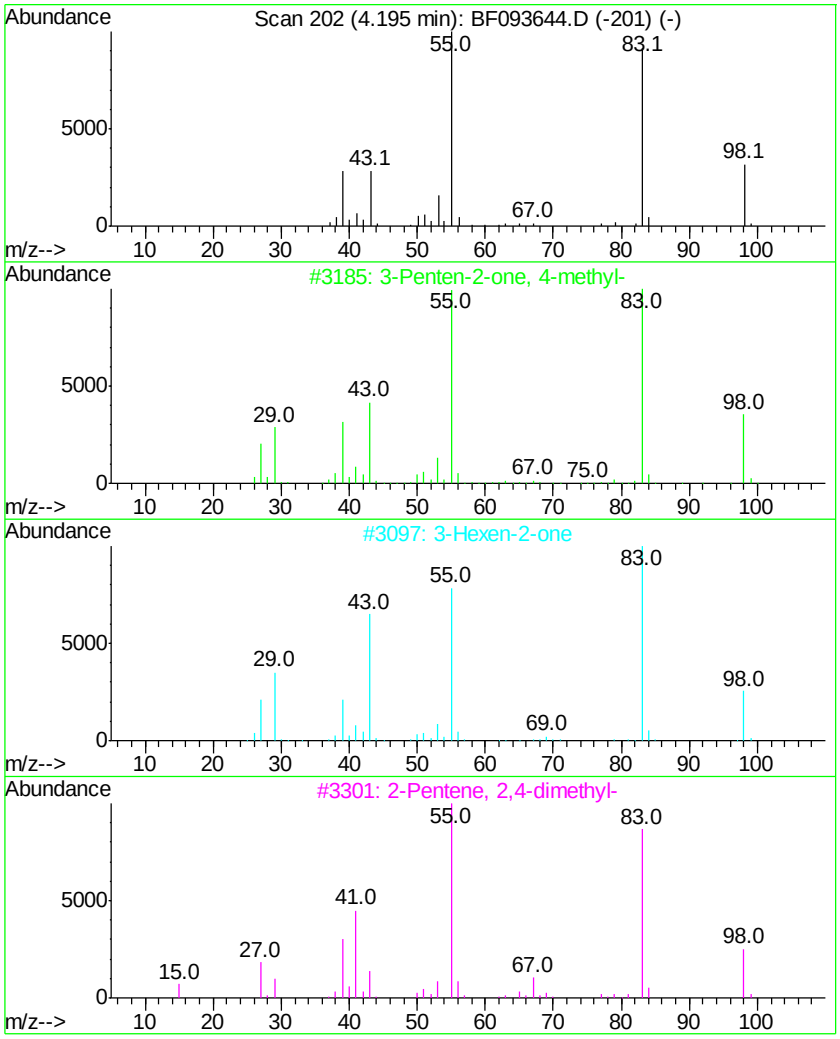
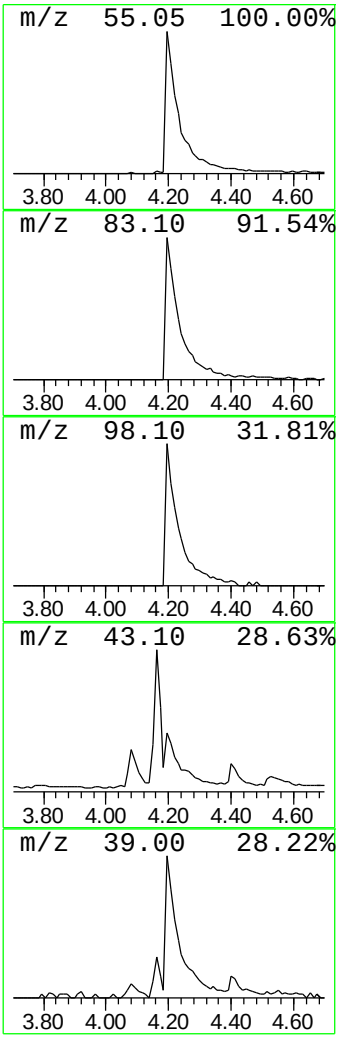
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.20	7.25 ng	440790	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	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78
5	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78





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Operator : SJ/MA
Sample : I2201-20
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-120

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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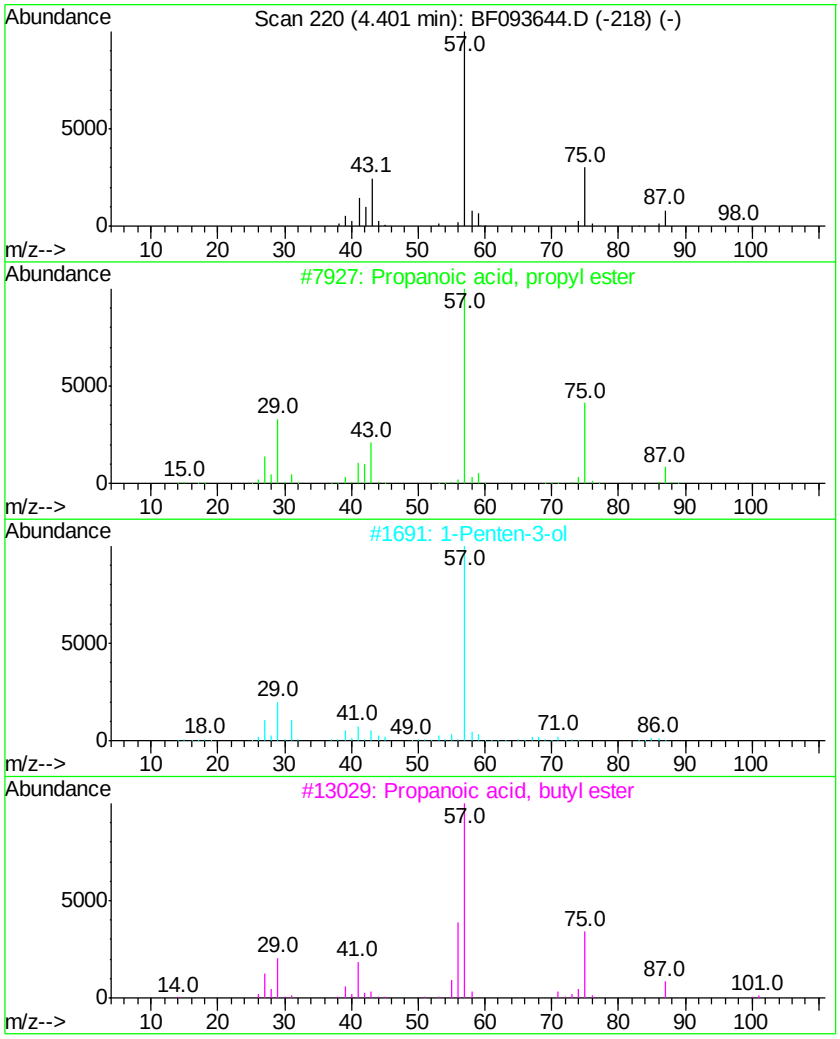
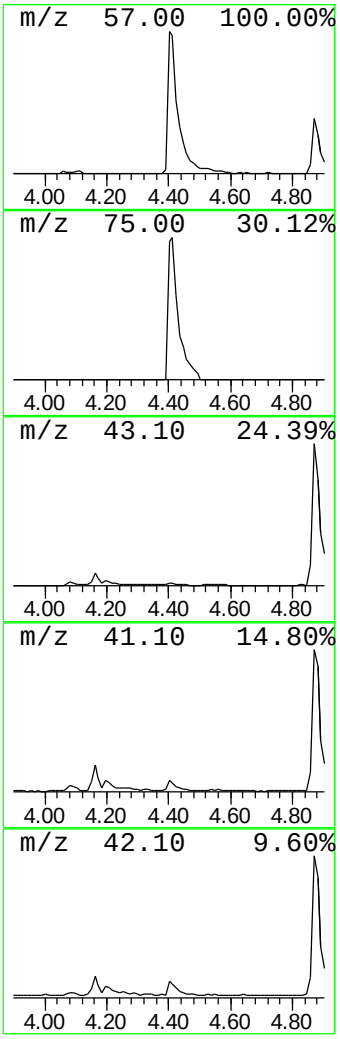
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	2.33 ng	142010	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	74
2	1-Penten-3-ol	86	C5H10O	000616-25-1	9
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9
4	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9
5	1-Pentanamine	87	C5H13N	000110-58-7	7





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Operator : SJ/MA
Sample : I2201-20
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-120

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

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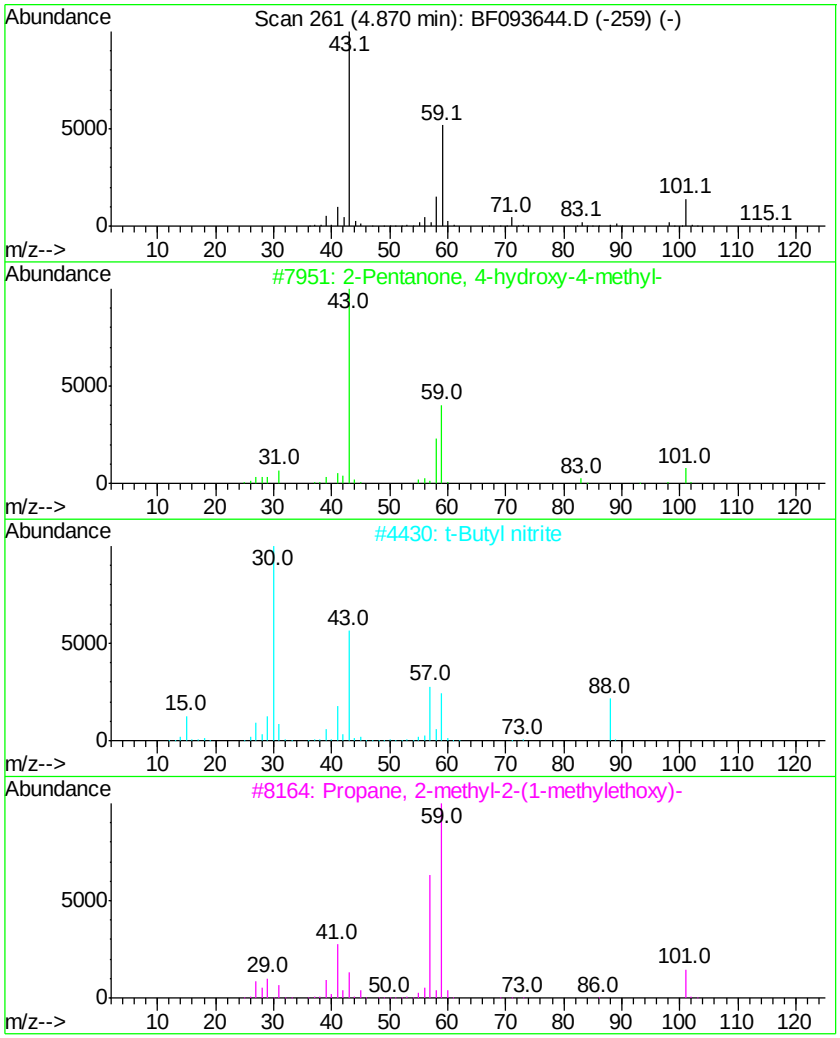
TIC Integration Parameters: LSCINT.P

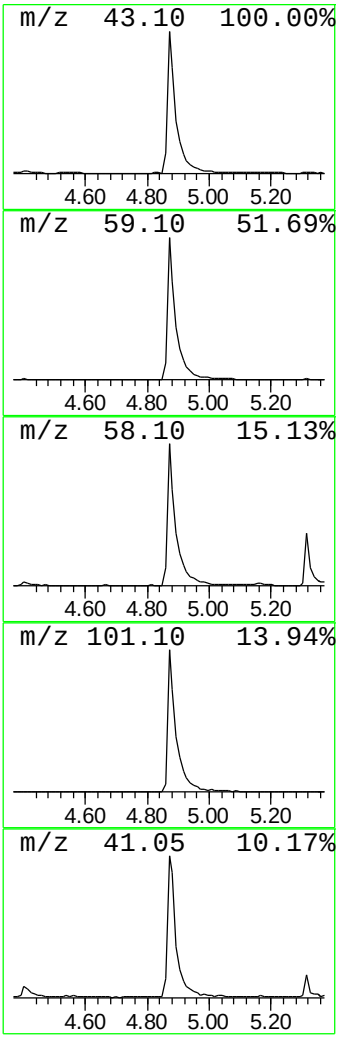
****

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	41.99 ng	2554230	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	45
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25





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Instrument : BNA_F
ClientSampleId : D-120

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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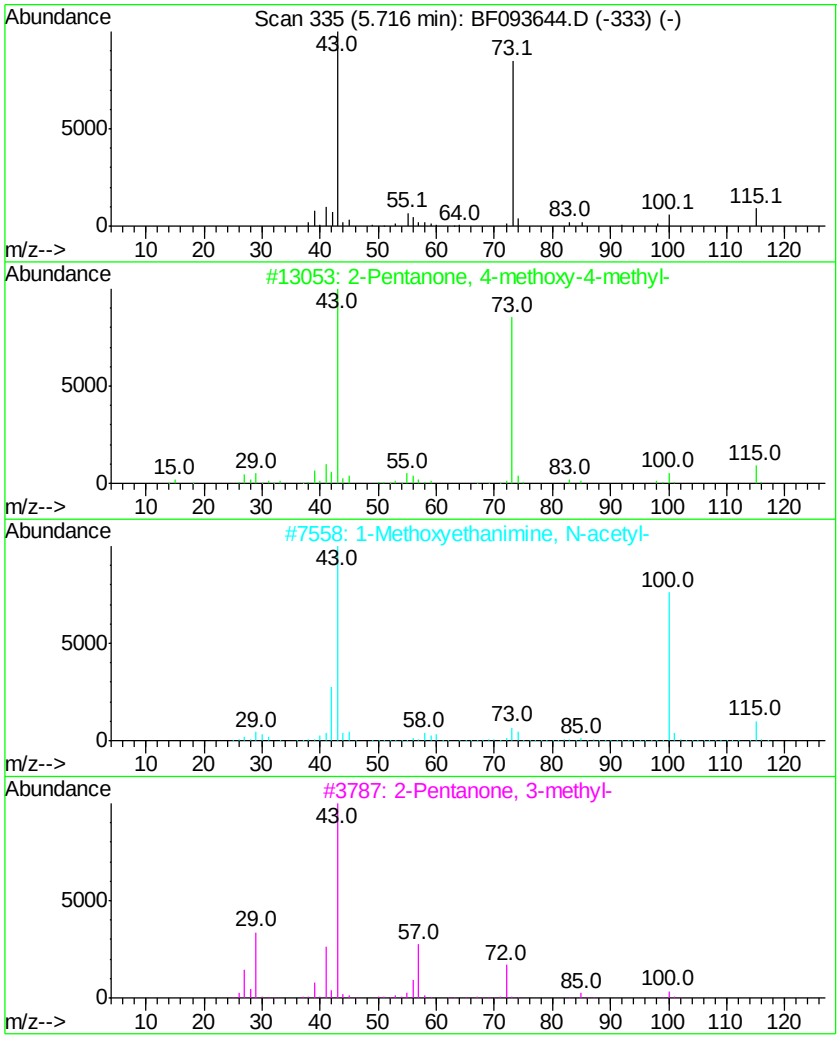
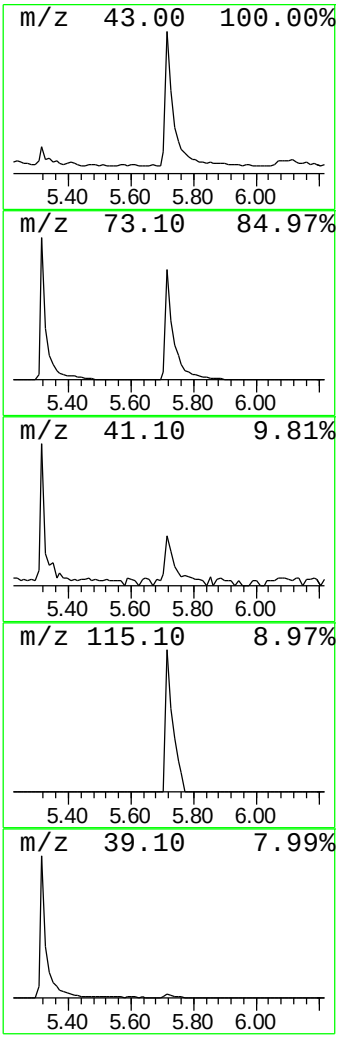
Peak Number 6 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.02 ng	122957	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	90
2	1-Methoxyethanimine, N-acetyl-	115	C5H9NO2	099028-43-0	25
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	12
4	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	12
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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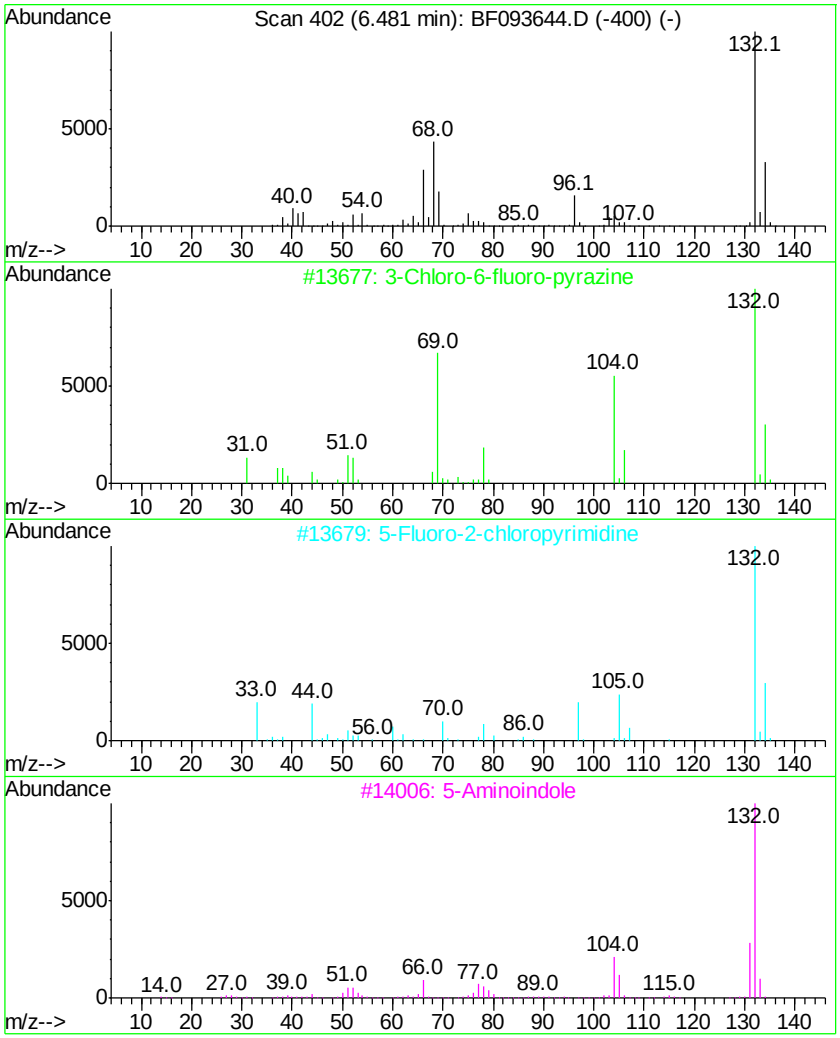
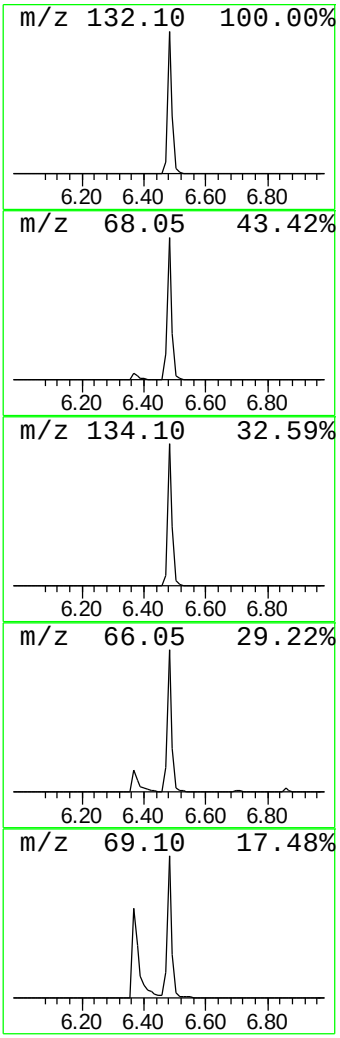
Peak Number 7 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	87.43 ng	5318240	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





Tentatively Identified Compound (LSC) summary

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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
n-Propyl acetate	2.45	4.0	ng	244223	1	6.71	1216630	20.0
Propanoic acid, 2...	4.16	2.0	ng	121826	1	6.71	1216630	20.0
3-Penten-2-one, 4...	4.20	7.3	ng	440790	1	6.71	1216630	20.0
Propanoic acid, p...	4.40	2.3	ng	142010	1	6.71	1216630	20.0
2-Pentanone, 4-hy...	4.87	42.0	ng	2554230	1	6.71	1216630	20.0
2-Pentanone, 4-me...	5.72	2.0	ng	122957	1	6.71	1216630	20.0
unknown6.48	6.48	87.4	ng	5318240	1	6.71	1216630	20.0