LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093639.D
Acq On : 14 Mar 2017 6:11
Operator : SJ/MA
Sample : I2201-17
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-112

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	2.458	47	50	62	rVB	75712	211896	3.28%	0.396%
2	4.161	197	199	204	rBV	78435	132520	2.05%	0.247%
3	4.241	204	206	218	rVV	29880	122080	1.89%	0.228%
4	4.413	218	221	229	rVB2	57322	136666	2.11%	0.255%
5	4.870	259	261	278	rBV	1314690	2740909	42.40%	5.119%
6	5.316	298	300	322	rBV	4380970	6263798	96.89%	11.697%
7	5.716	333	335	348	rVB	89414	163949	2.54%	0.306%
8	6.367	390	392	400	rBV	3353998	5561530	86.03%	10.386%
9	6.481	400	402	405	rVB	5084919	5308891	82.12%	9.914%
10	6.710	419	422	433	rVB	1037203	1207823	18.68%	2.256%
11	6.859	433	435	438	rBV	4118121	4388335	67.88%	8.195%
12	7.282	470	472	475	rBV	3176729	3993882	61.78%	7.458%
13	8.002	533	535	547	rVB	1398698	1592581	24.63%	2.974%
14	9.076	626	629	632	rBV	4371811	6464799	100.00%	12.073%
15	9.762	686	689	691	rBV	1258515	1745727	27.00%	3.260%
16	10.276	733	734	740	rBV	129690	167842	2.60%	0.313%
17	10.550	756	758	761	rBV2	2501275	3390420	52.44%	6.331%
18	11.248	816	819	825	rBV	1860486	1783739	27.59%	3.331%
19	11.625	850	852	855	rVB	128719	168448	2.61%	0.315%
20	12.836	955	958	961	rBV	4706432	5545859	85.79%	10.357%
21	13.899	1049	1051	1061	rVB	981480	1517620	23.48%	2.834%
22	15.305	1171	1174	1185	rBV	578389	939327	14.53%	1.754%

Sum of corrected areas: 53548641

LSC Report - Integrated Chromatogram

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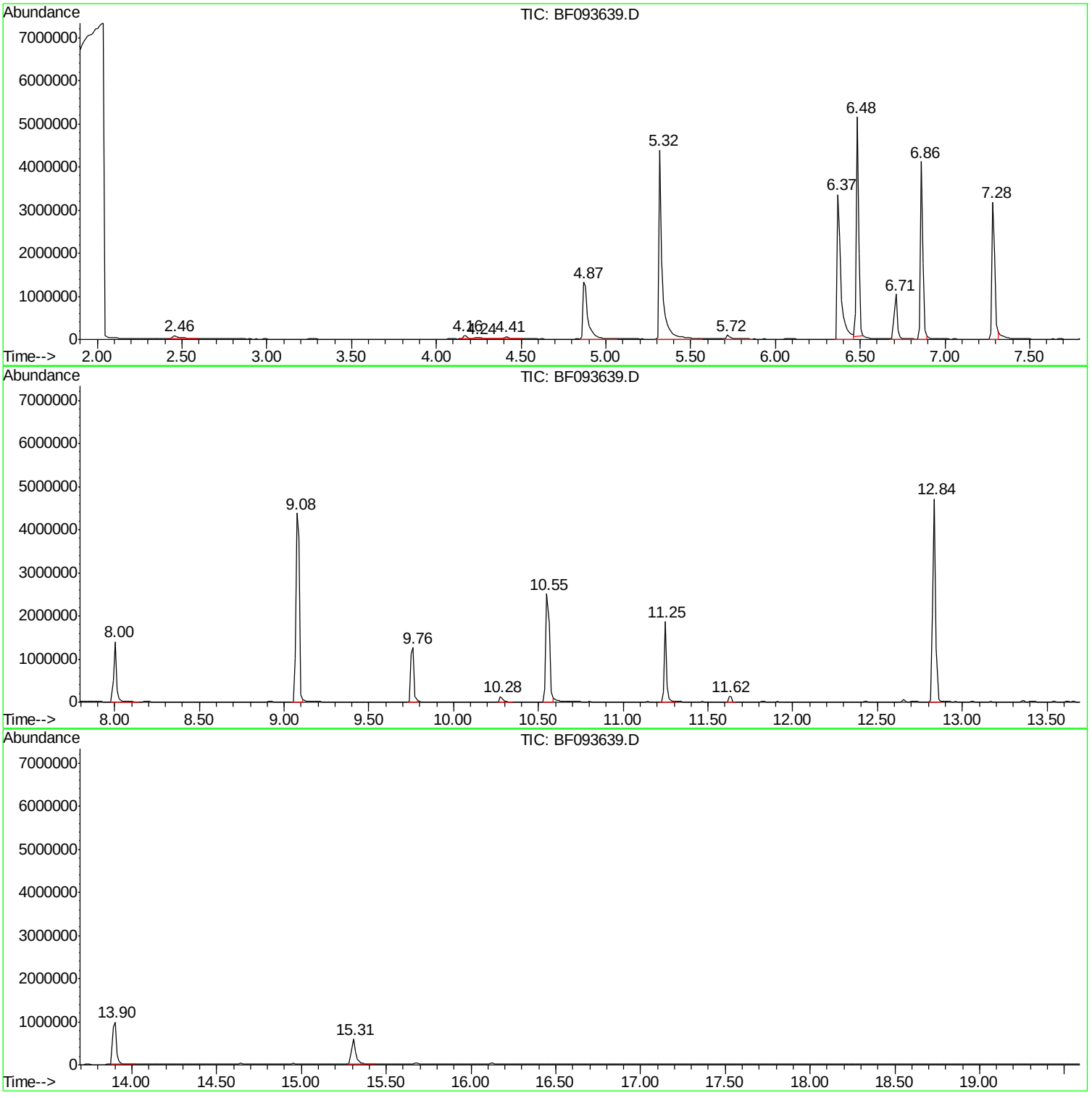
Operator : SJ/MA
Sample : I2201-17
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-112

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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Data File : BF093639.D
Acq On : 14 Mar 2017 6:11
Operator : SJ/MA
Sample : I2201-17
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ClientSampleId : D-112

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

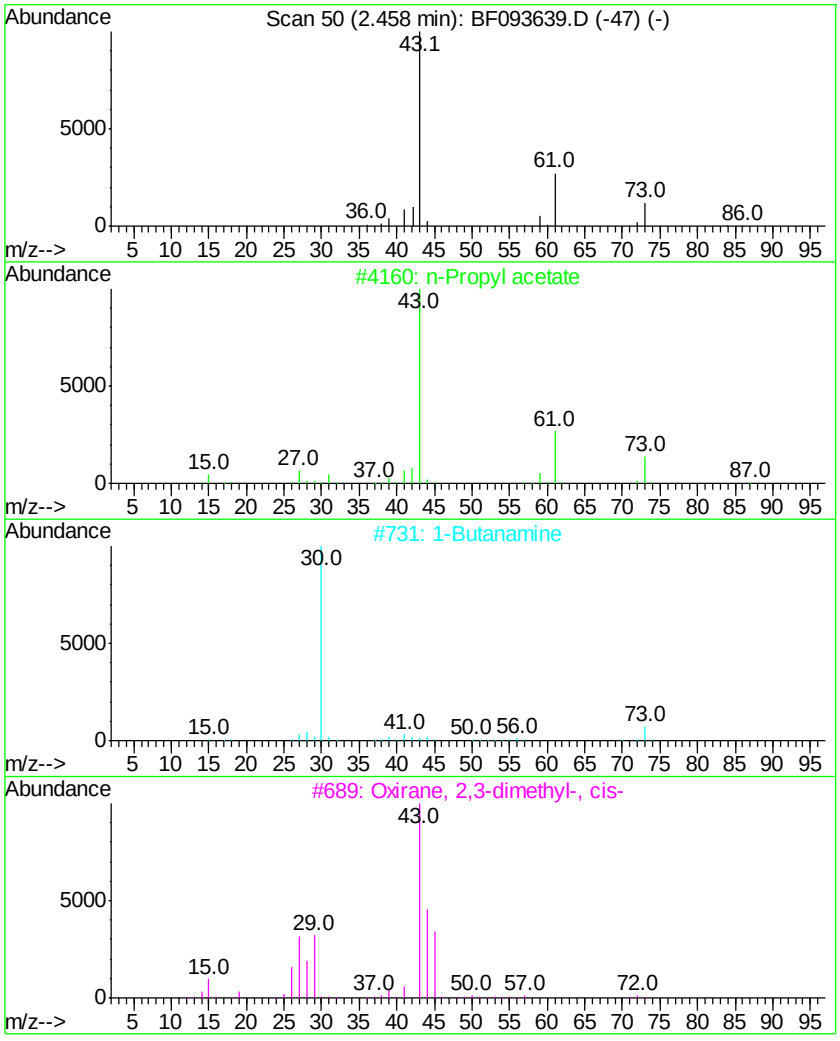
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

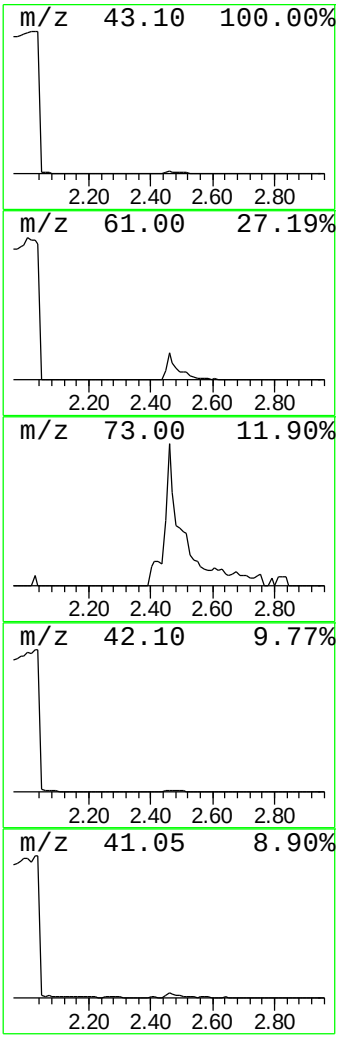
****

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.46	3.51 ng	211896	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	1-Butanamine	73	C4H11N	000109-73-9	7
3	Oxirane, 2,3-dimethyl-, cis-	72	C4H8O	001758-33-4	5
4	Isobutylamine	73	C4H11N	000078-81-9	5
5	Pentane	72	C5H12	000109-66-0	4





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093639.D
Acq On : 14 Mar 2017 6:11
Operator : SJ/MA
Sample : I2201-17
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-112

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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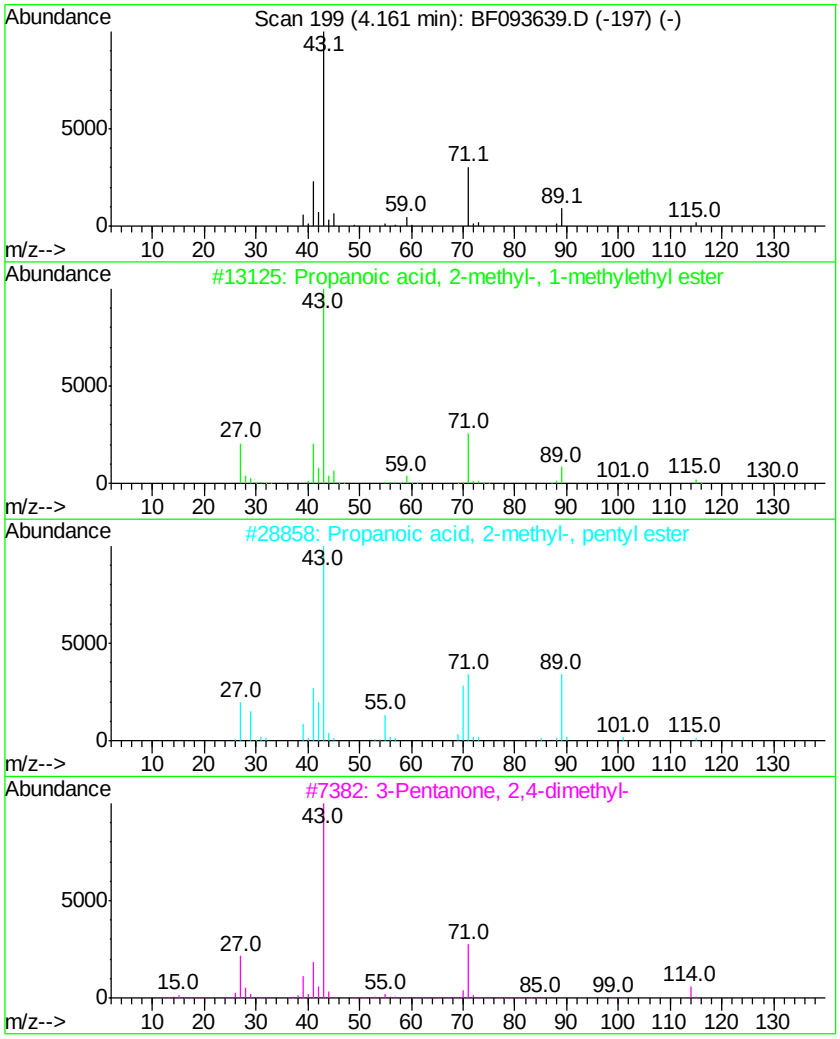
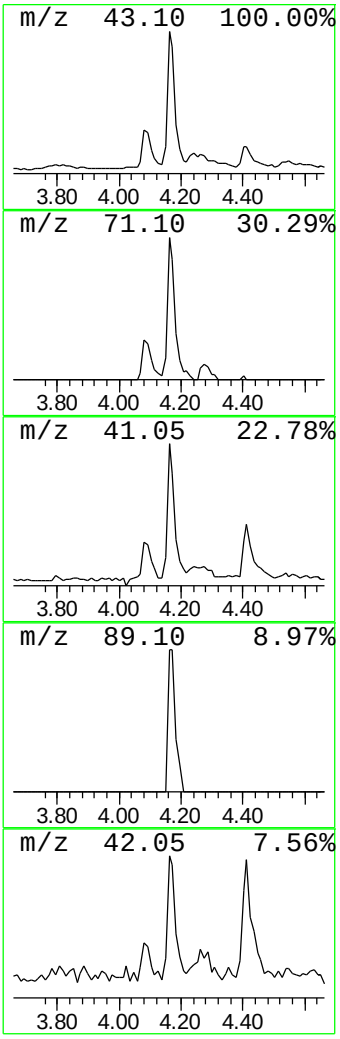
Peak Number 2 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	2.19 ng	132520	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	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	33
4	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	27
5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	9





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Data File : BF093639.D
Acq On : 14 Mar 2017 6:11
Operator : SJ/MA
Sample : I2201-17
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-112

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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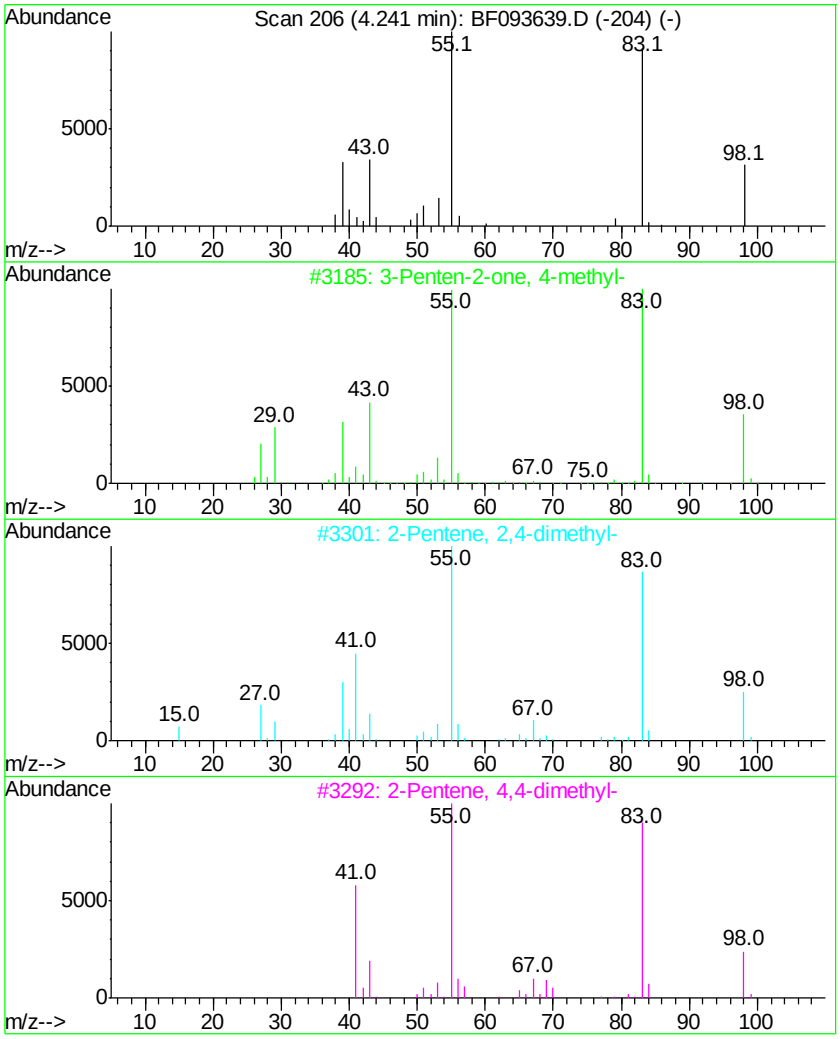
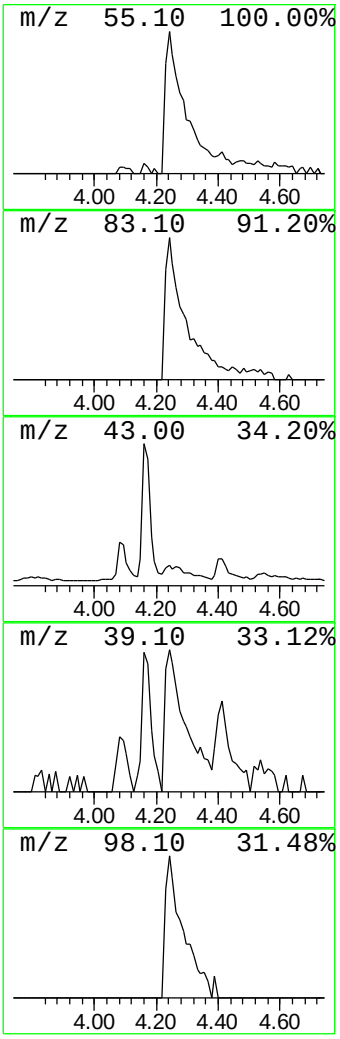
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.24	2.02 ng	122080	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	86
2	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
3	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	72
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	72
5	3-Hexen-2-one	98	C6H10O	000763-93-9	72





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Acq On : 14 Mar 2017 6:11
Operator : SJ/MA
Sample : I2201-17
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-112

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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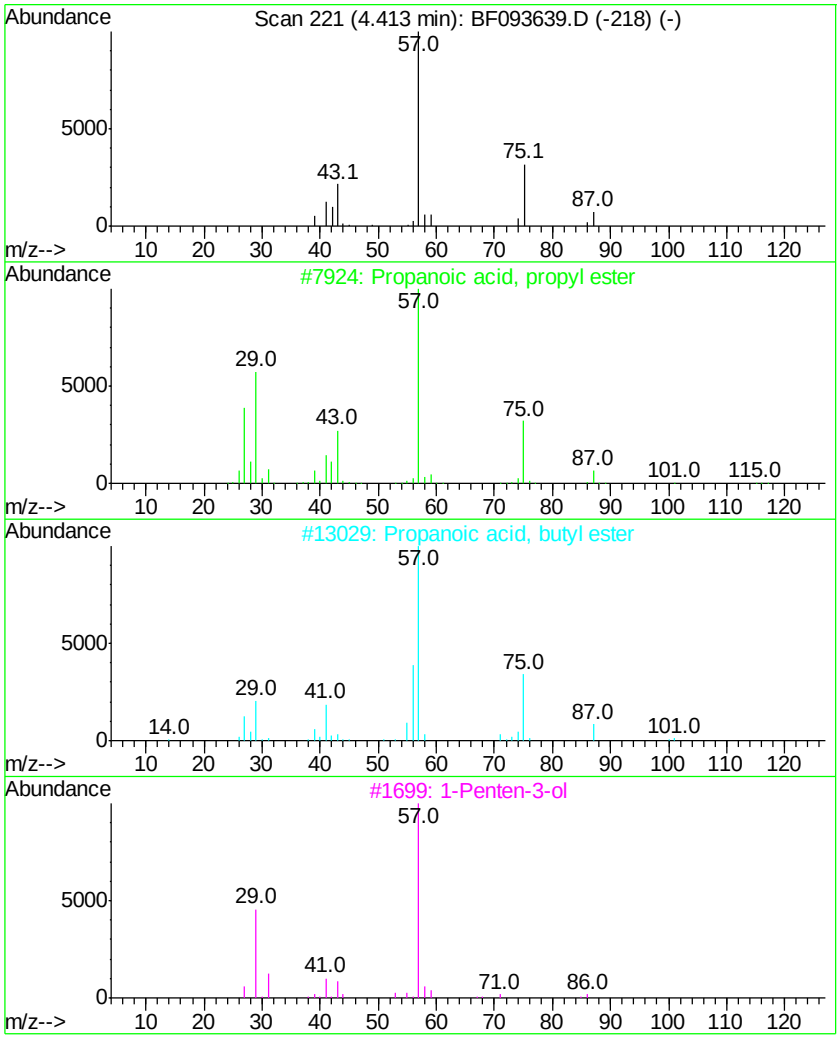
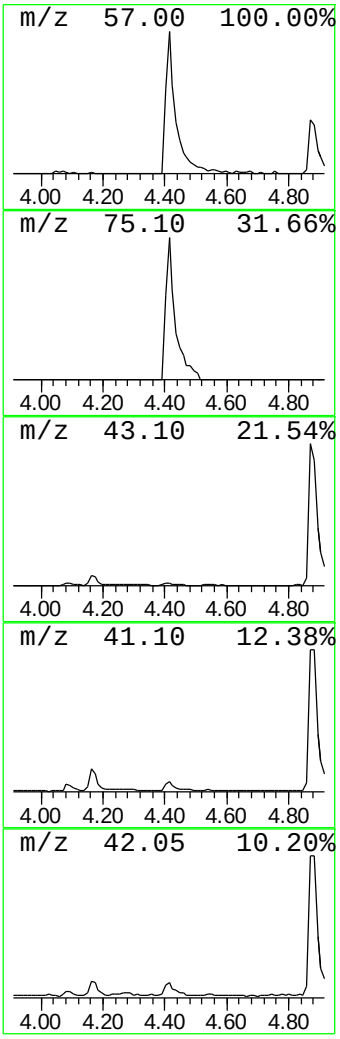
Peak Number 4 Propanoic acid, propyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	2.26 ng	136666	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	64
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38
3	1-Penten-3-ol	86	C5H10O	000616-25-1	16
4	1-Pentanamine	87	C5H13N	000110-58-7	7
5	Azetidine	57	C3H7N	000503-29-7	7





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Operator : SJ/MA
Sample : I2201-17
Misc :
ALS Vial : 39 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-112

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

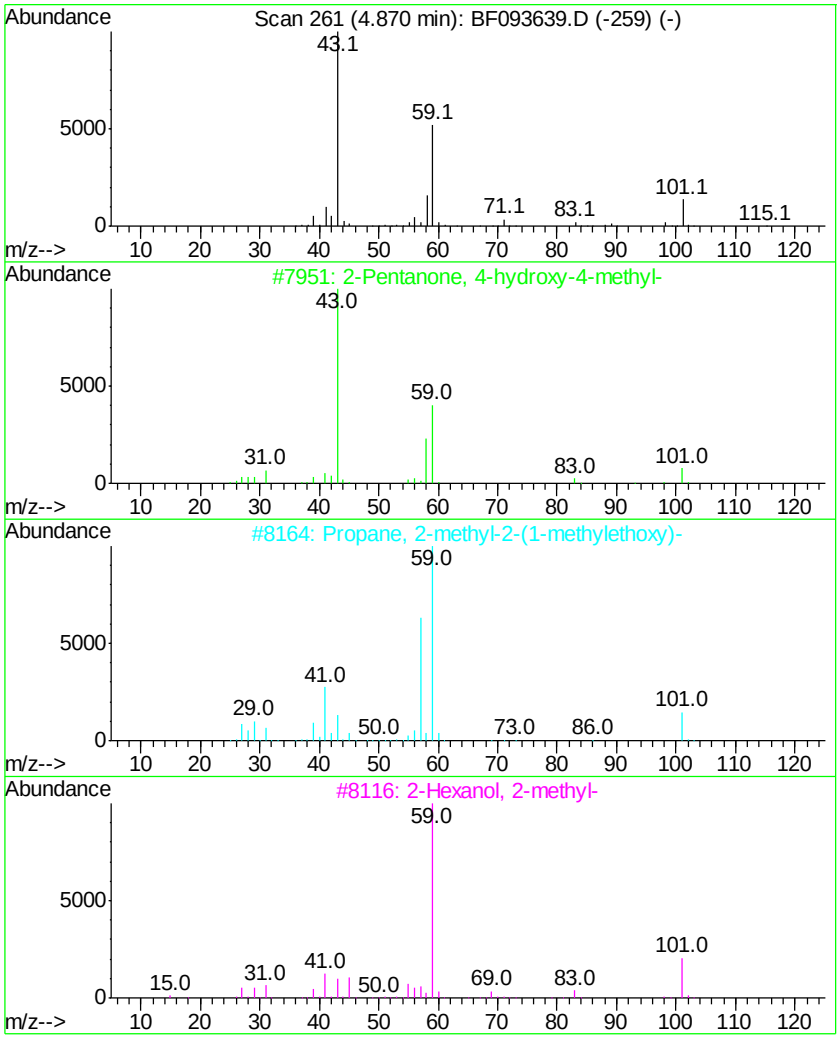
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

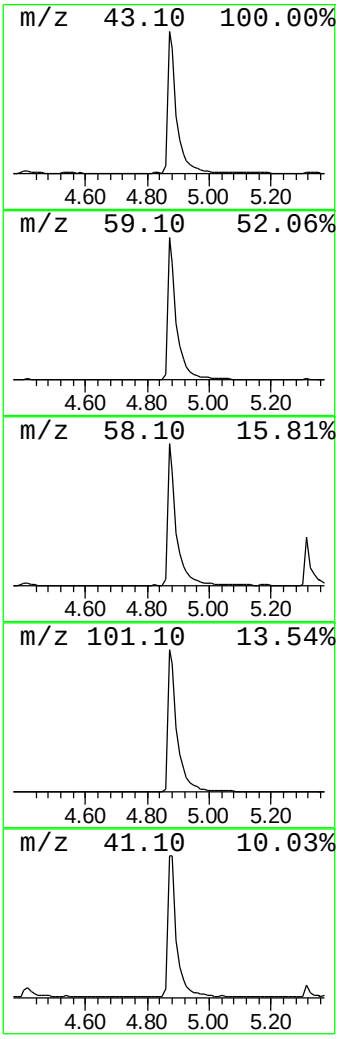
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	45.39 ng	2740910	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	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23





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Misc :
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Instrument : BNA_F
ClientSampleId : D-112

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

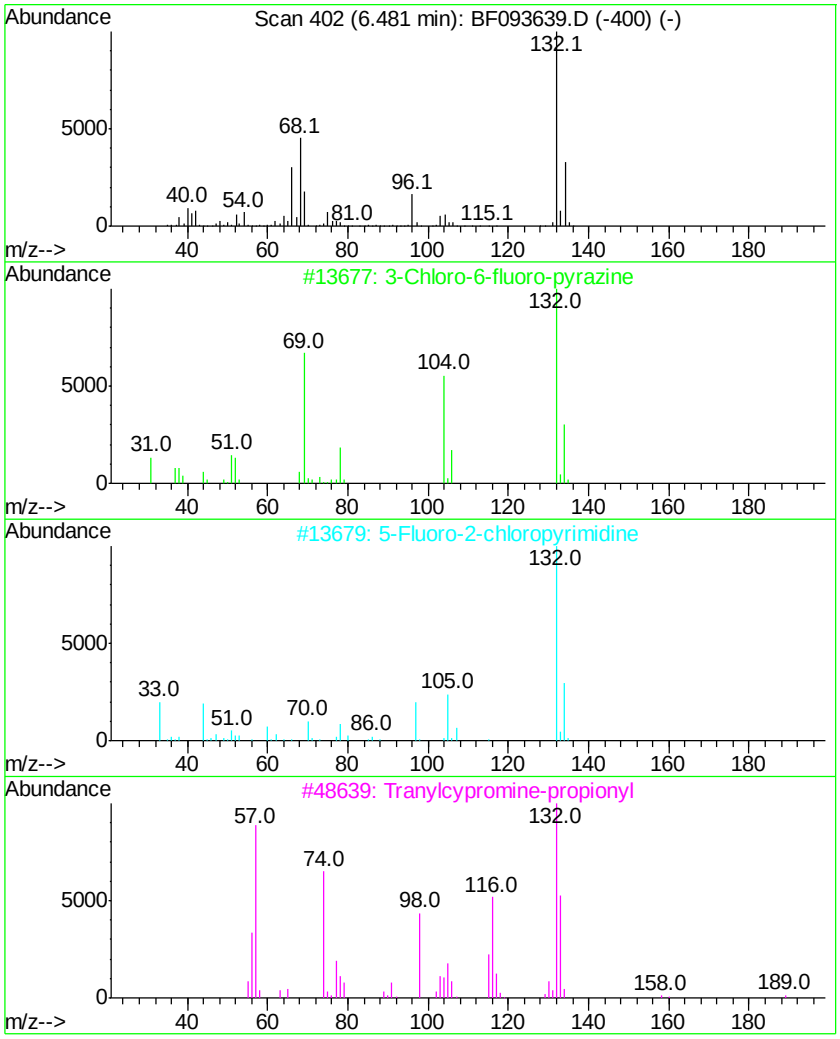
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

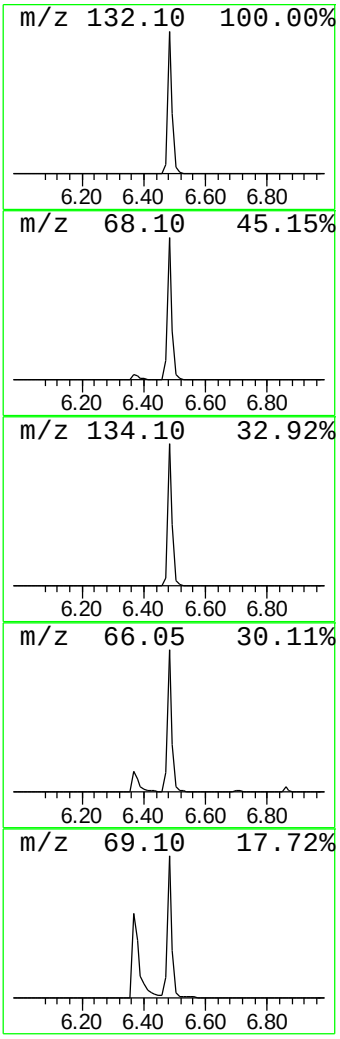
****

Peak Number 7 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	87.91 ng	5308890	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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
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	2.46	3.5	ng	211896	1	6.71	1207820	20.0
Propanoic acid, 2...	4.16	2.2	ng	132520	1	6.71	1207820	20.0
3-Penten-2-one, 4...	4.24	2.0	ng	122080	1	6.71	1207820	20.0
Propanoic acid, p...	4.41	2.3	ng	136666	1	6.71	1207820	20.0
2-Pentanone, 4-hy...	4.87	45.4	ng	2740910	1	6.71	1207820	20.0
unknown6.48	6.48	87.9	ng	5308890	1	6.71	1207820	20.0