LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093636.D
Acq On : 14 Mar 2017 4:48
Operator : SJ/MA
Sample : I2199-28
Misc :
ALS Vial : 36 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-107

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	47	49	68	rVB	99331	281542	4.48%	0.533%
2	4.161	197	199	203	rBV	75363	124808	1.98%	0.236%
3	4.230	203	205	216	rVB	36642	119021	1.89%	0.225%
4	4.413	218	221	224	rBV	63434	134445	2.14%	0.255%
5	4.870	259	261	286	rBV	1291918	2614517	41.56%	4.953%
6	5.316	298	300	326	rBV	4105818	6286212	99.93%	11.908%
7	5.716	333	335	344	rVB	68524	119316	1.90%	0.226%
8	6.367	391	392	400	rBV	2931781	5690599	90.46%	10.780%
9	6.481	400	402	405	rVB	4891644	5281184	83.96%	10.004%
10	6.710	420	422	431	rVB	989893	1145980	18.22%	2.171%
11	6.859	433	435	438	rBV	4077298	4203368	66.82%	7.962%
12	7.282	470	472	475	rBV	3043343	3779091	60.08%	7.159%
13	8.002	533	535	545	rBV	1341302	1560009	24.80%	2.955%
14	9.087	626	630	632	rBV	4139768	6290471	100.00%	11.916%
15	9.762	686	689	691	rBV	1250485	1668492	26.52%	3.161%
16	10.550	756	758	761	rBV2	2343745	3335278	53.02%	6.318%
17	11.248	817	819	825	rBV	1834276	1739207	27.65%	3.295%
18	12.654	940	942	945	rBV	316272	272155	4.33%	0.516%
19	12.836	955	958	961	rBV	4466625	5465823	86.89%	10.354%
20	13.362	1002	1004	1006	rBV	177602	178296	2.83%	0.338%
21	13.899	1049	1051	1060	rBV	1045058	1405193	22.34%	2.662%
22	15.305	1171	1174	1188	rVB	643729	1025272	16.30%	1.942%
23	15.682	1202	1207	1212	rBV	41187	69559	1.11%	0.132%

Sum of corrected areas: 52789838

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Misc :
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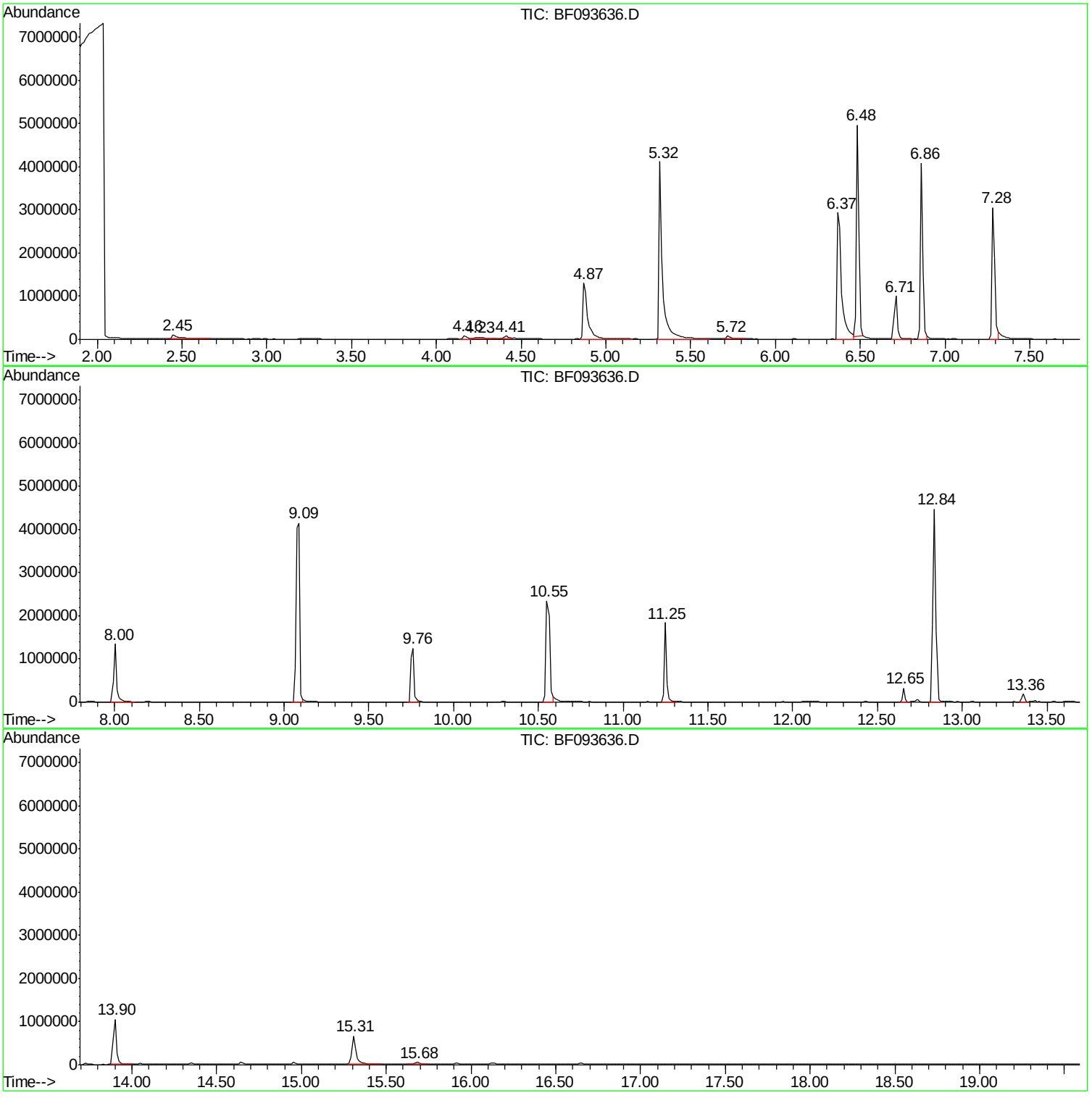
Instrument : BNA_F
ClientSampleId : D-107

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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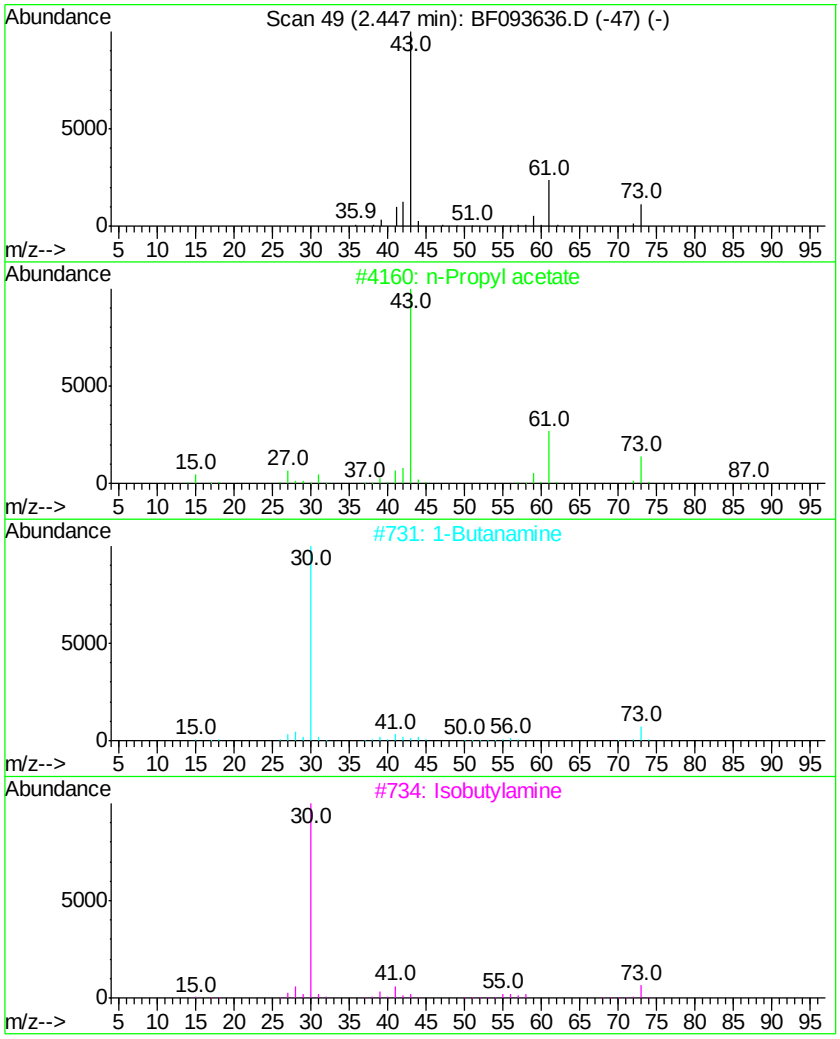
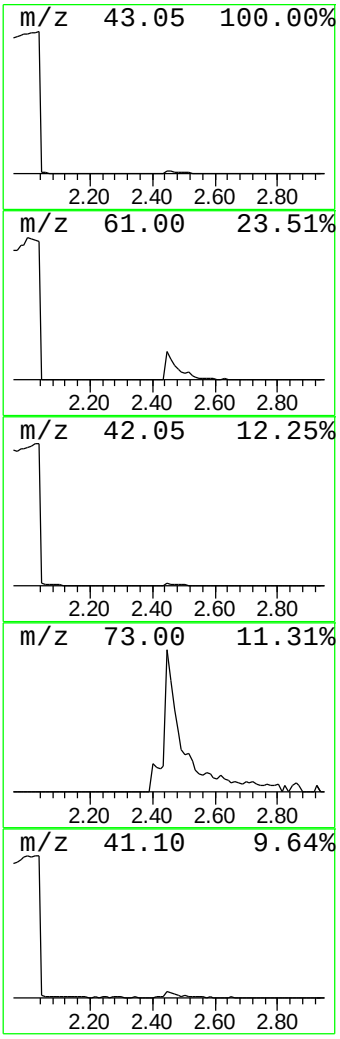
****

Peak Number 1 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	4.91 ng	281542	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	5
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	Butane, 2-methyl-	72	C5H12	000078-78-4	5
5	Pentane	72	C5H12	000109-66-0	4





Library Search Compound Report

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

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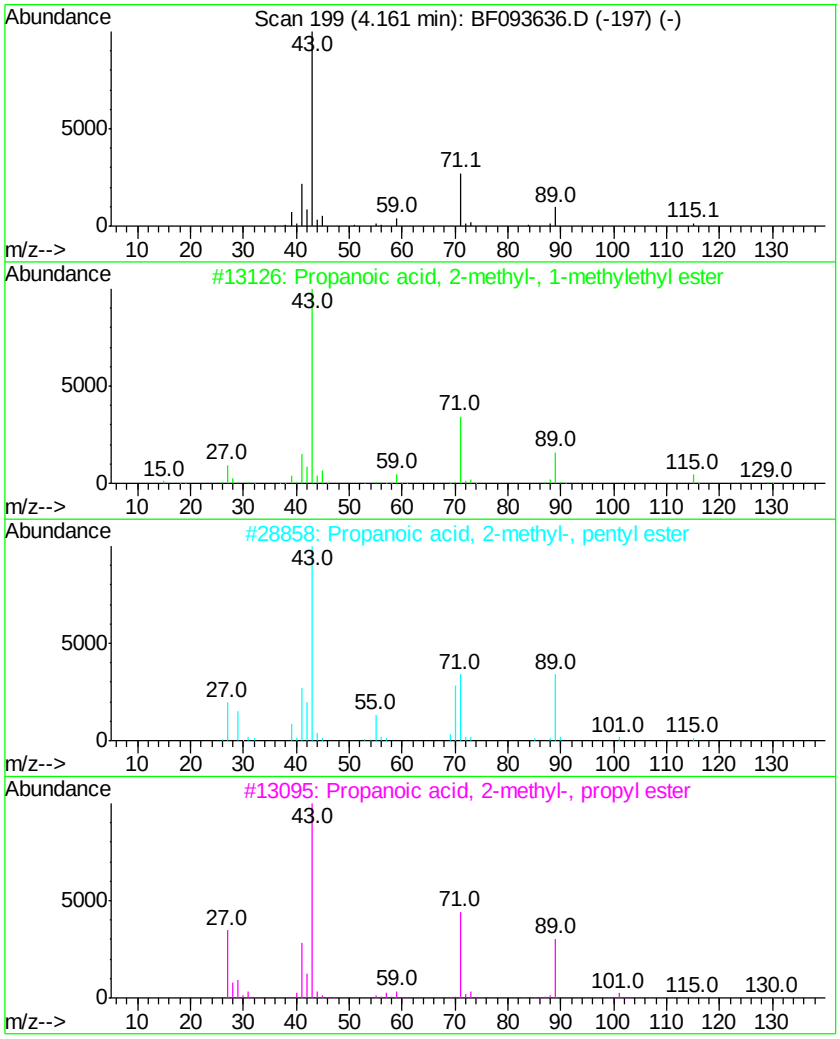
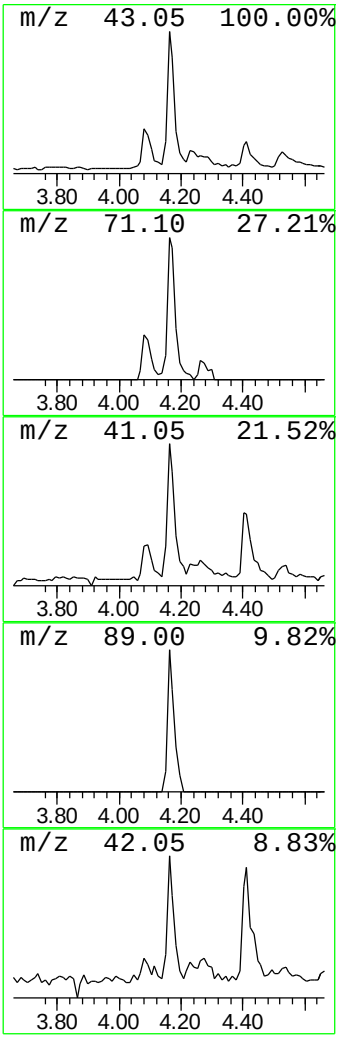
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	2.18 ng	124808	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	33
3	Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	28
4	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	28
5	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	9





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Operator : SJ/MA
Sample : I2199-28
Misc :
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Instrument : BNA_F
ClientSampleId : D-107

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

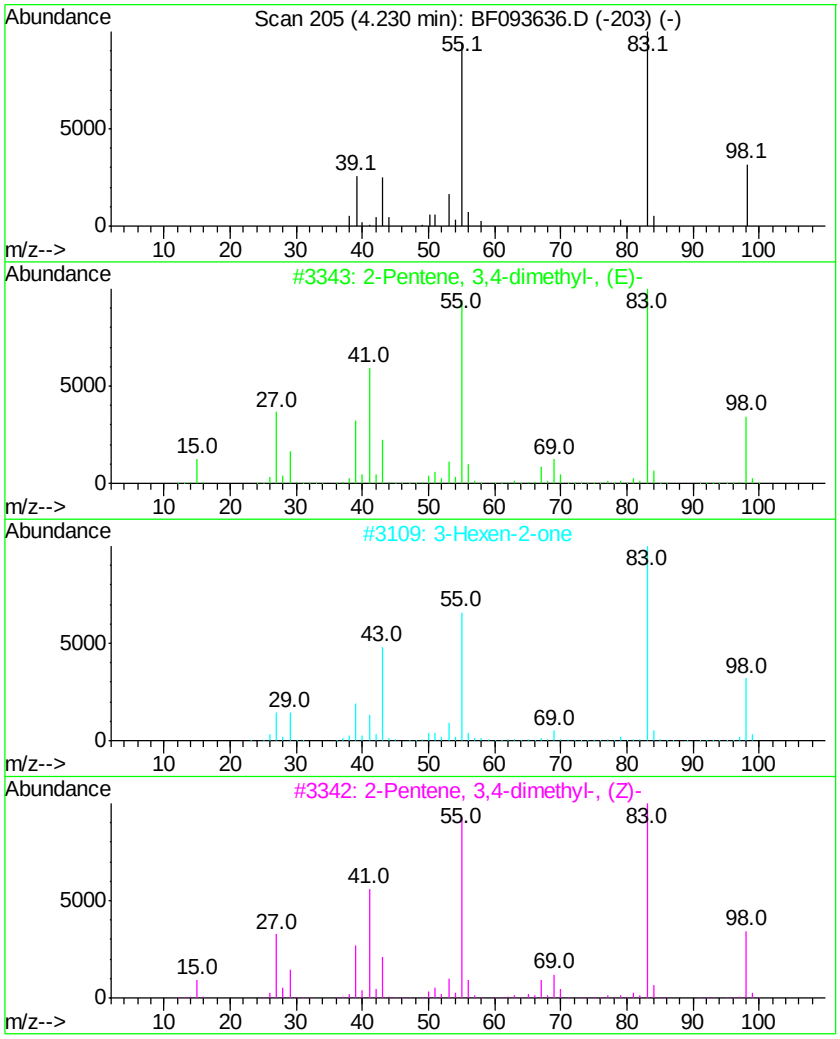
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

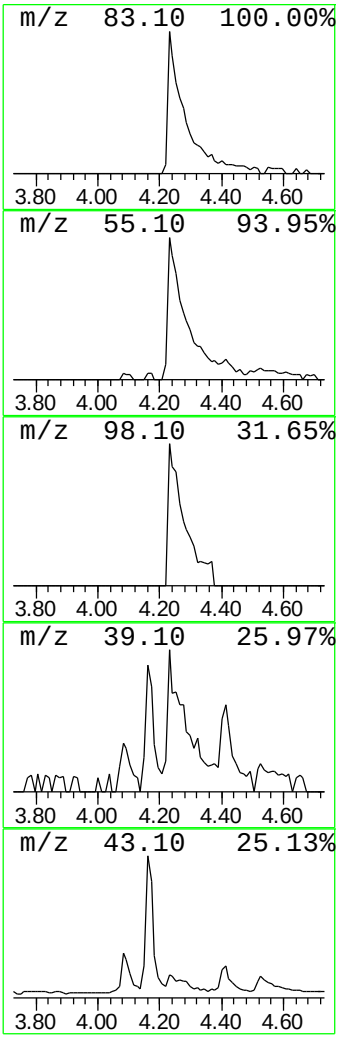
****

Peak Number 3 2-Pentene, 3,4-dimethyl-, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.23	2.08 ng	119021	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
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, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86





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Instrument : BNA_F
ClientSampleId : D-107

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
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TIC Library : C:\DATABASE\NIST02.L
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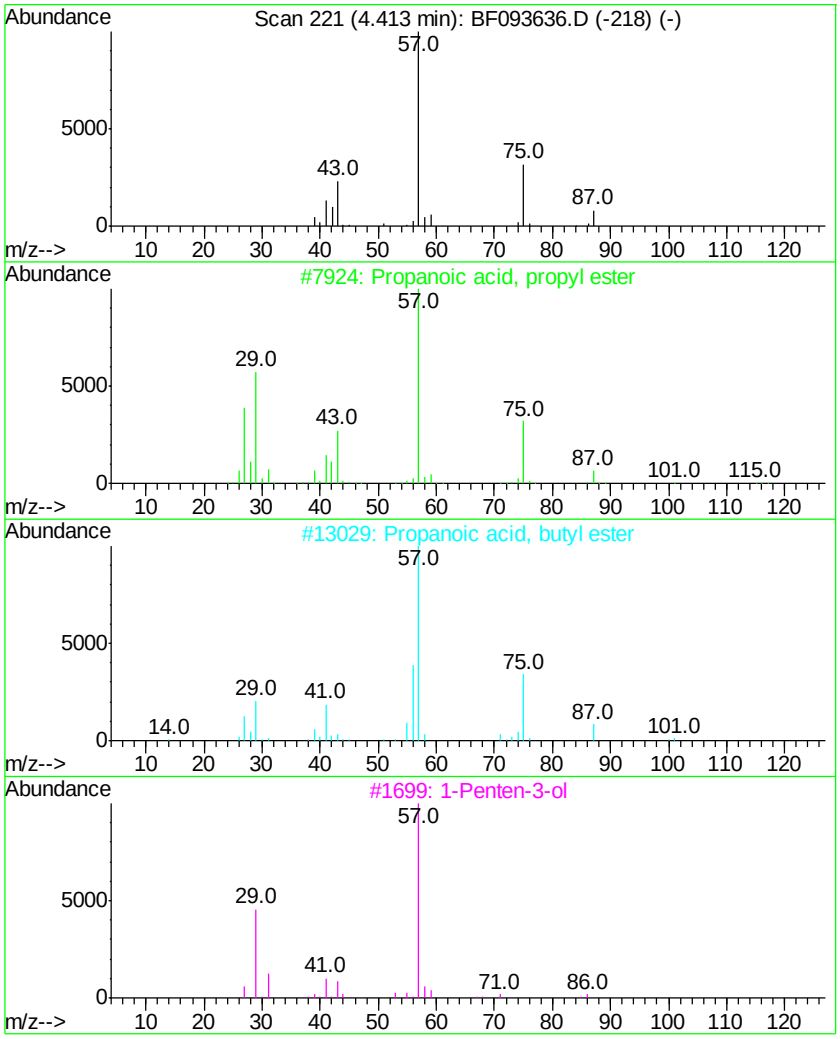
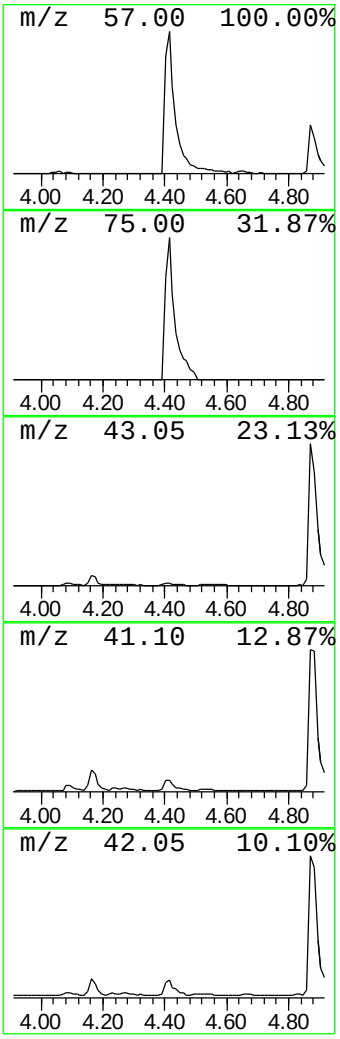
****

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	2.35 ng	134445	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	78
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	36
3	1-Penten-3-ol	86	C5H10O	000616-25-1	9
4	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	9
5	1-Pentanamine	87	C5H13N	000110-58-7	7





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
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Sample : I2199-28
Misc :
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Instrument : BNA_F
ClientSampleId : D-107

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

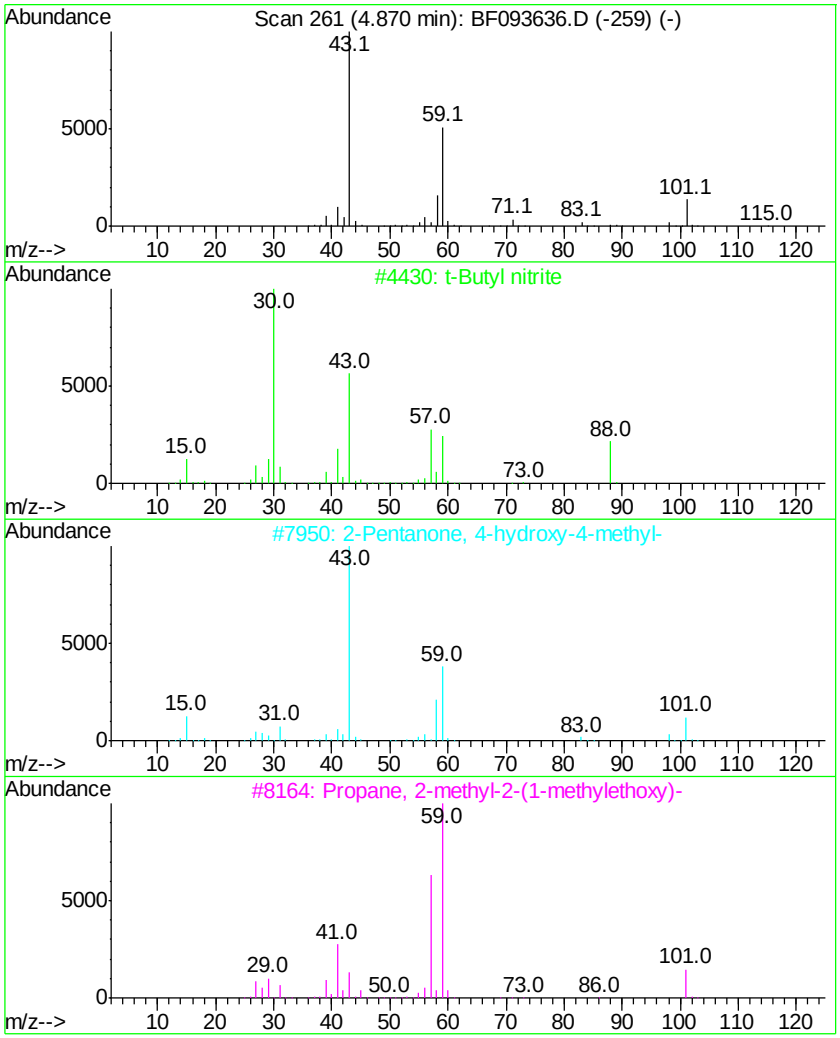
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

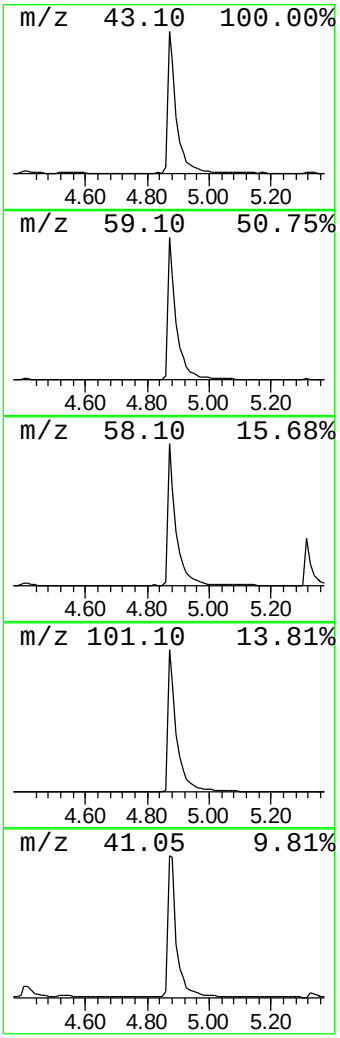
****

Peak Number 5 unknown4.87 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	45.63 ng	2614520	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	t-Butyl nitrite	103	C4H9NO2	000540-80-7	39
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Library Search Compound Report

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Sample : I2199-28
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Instrument : BNA_F
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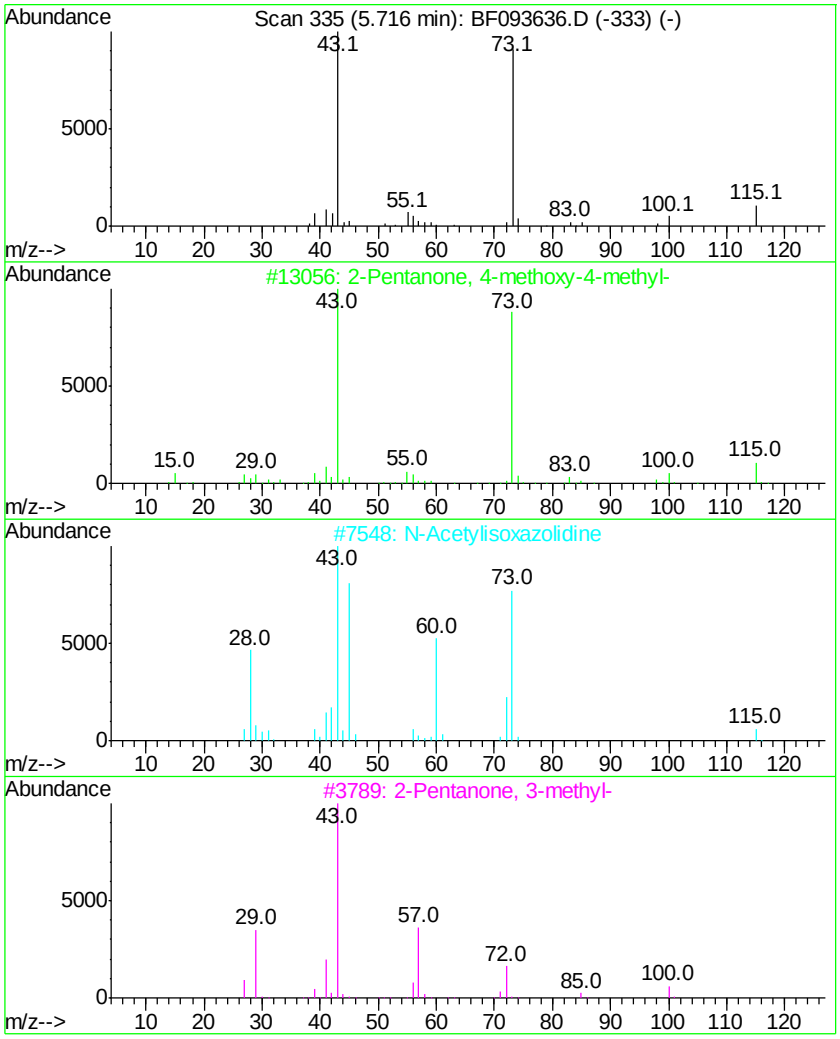
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

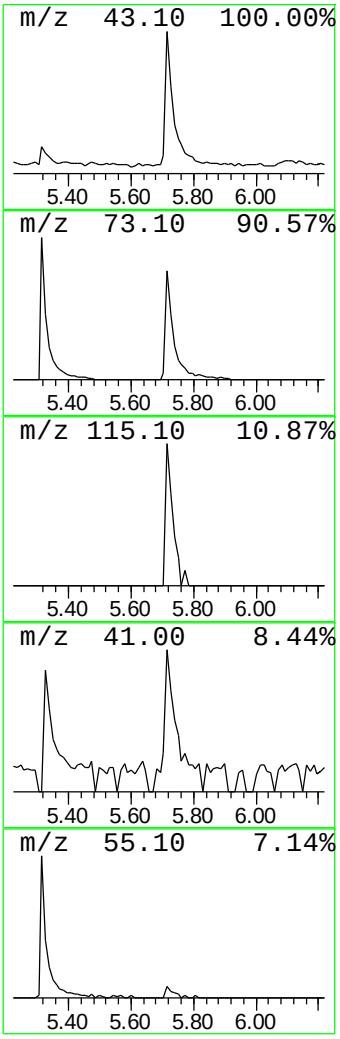
****

Peak Number 6 2-Pentanone, 4-methoxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	2.08 ng	119316	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	83
2	N-Acetylisoxazolidine	115	C5H9NO2	115615-36-6	38
3	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	16
4	2-Hexanone	100	C6H12O	000591-78-6	10
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10





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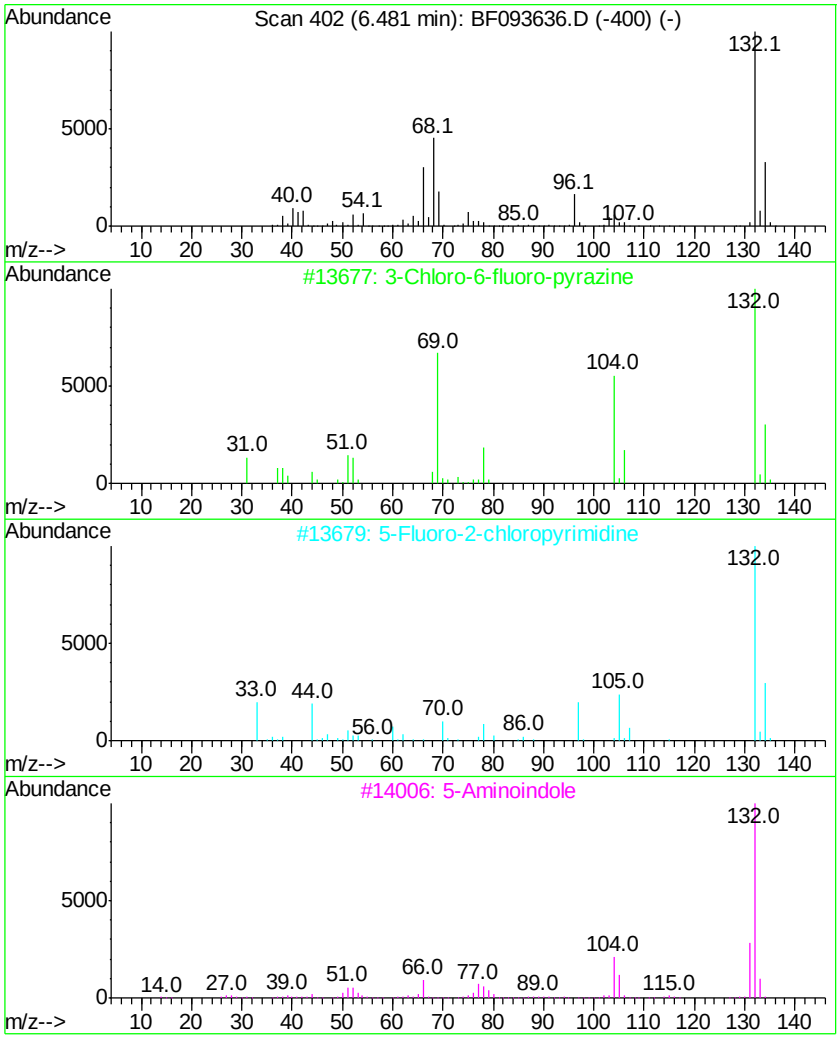
TIC Integration Parameters: LSCINT.P

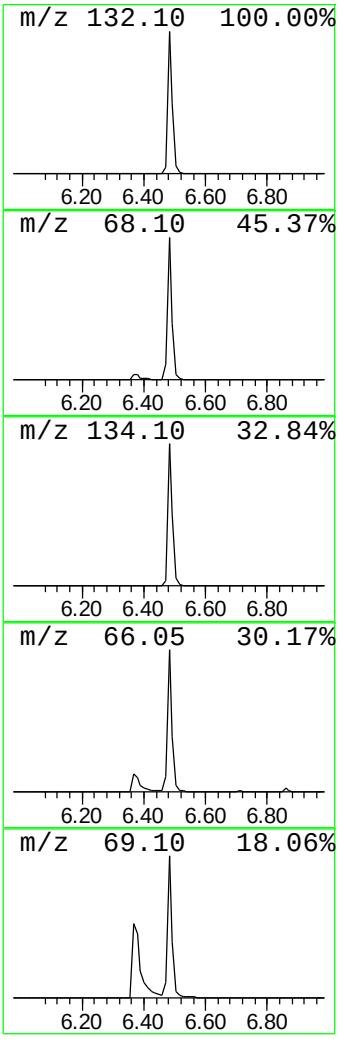
****

Peak Number 7 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	92.17 ng	5281180	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	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

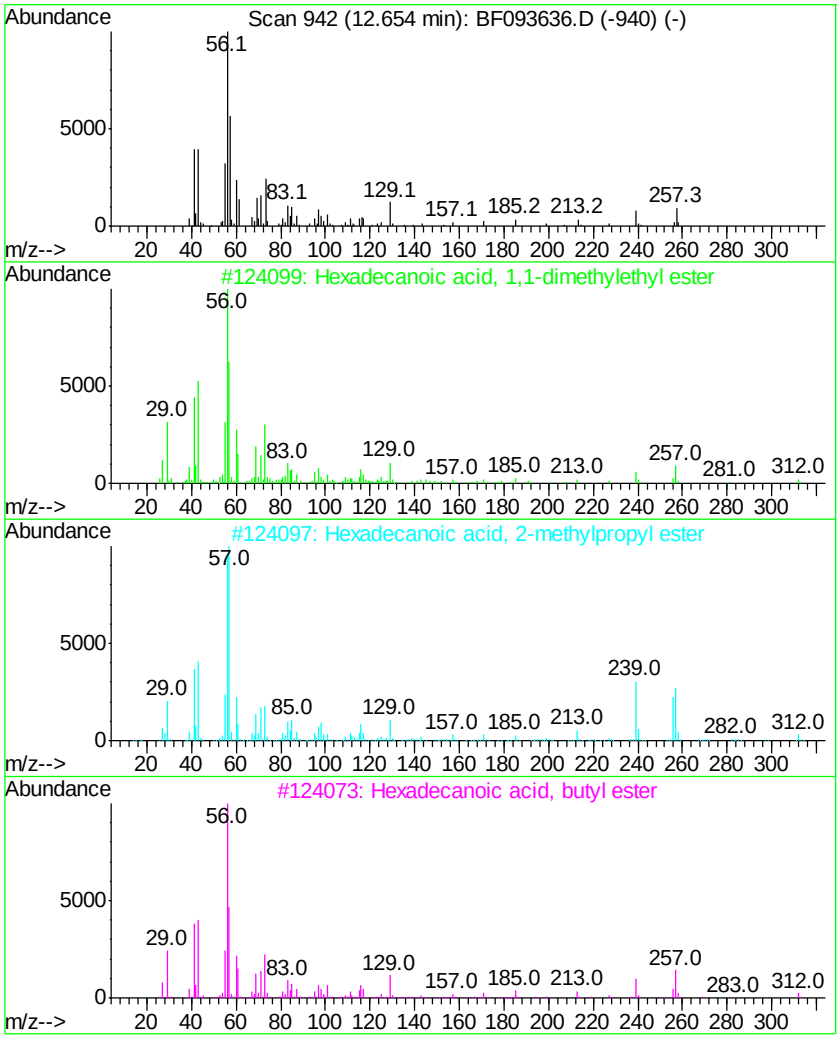
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

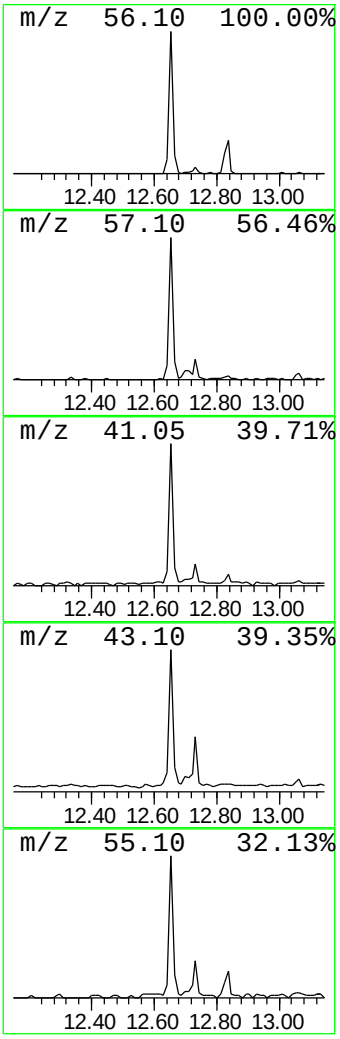
****

Peak Number 9 Hexadecanoic acid, 1,1-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	3.87 ng	272155	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	62
2	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	59
3	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	58
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
5	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	43





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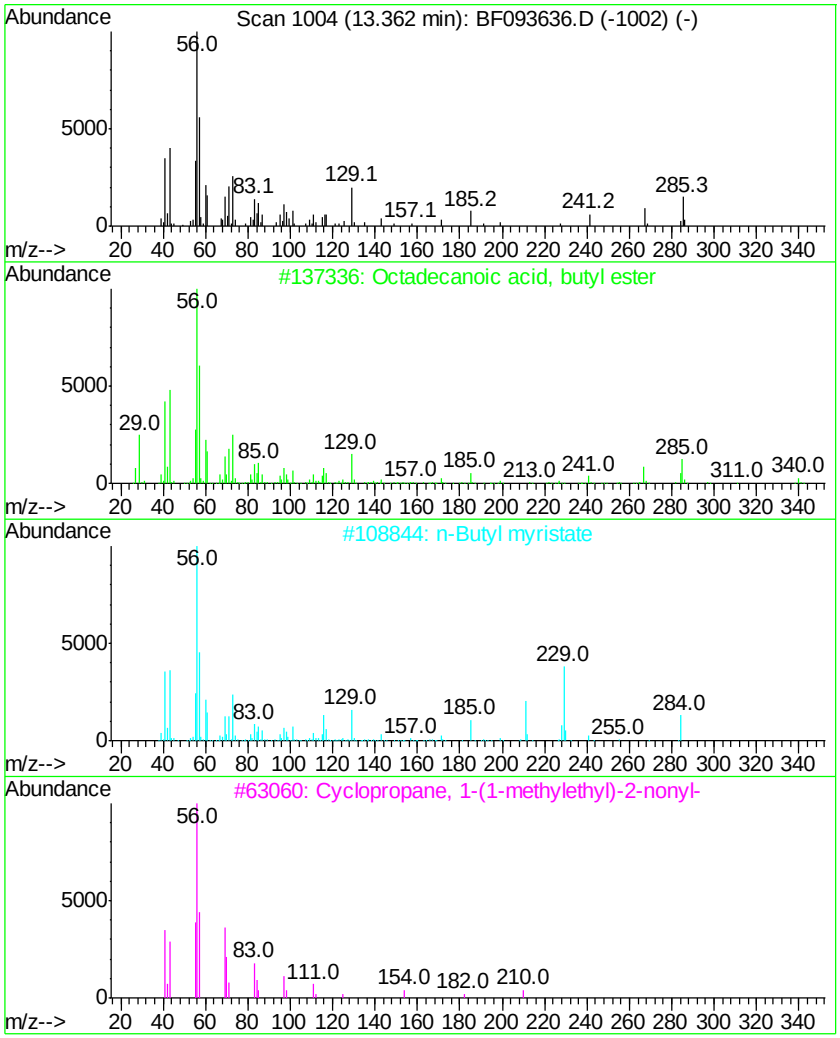
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

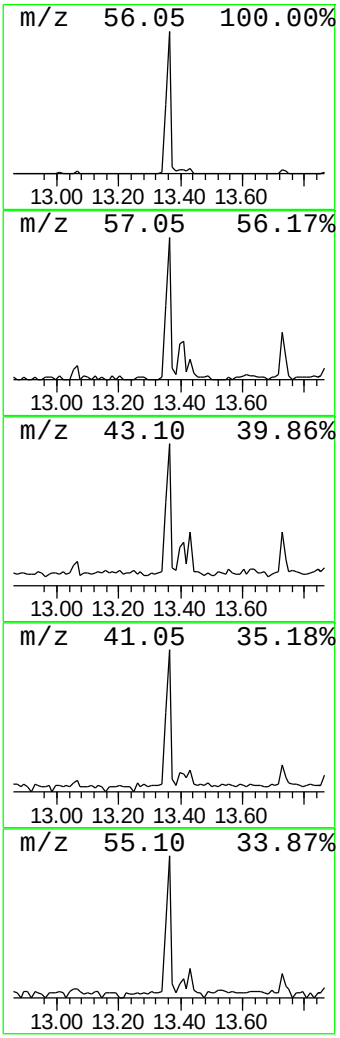
****

Peak Number 10 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.36	2.54 ng	178296	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2	n-Butyl myristate	284	C18H36O2	000110-36-1	53
3	Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	35
4	2-Methyl-1-octadecene	266	C19H38	061868-20-0	35
5	2-Methyl-n-1-tridecene	196	C14H28	018094-01-4	27





Tentatively Identified Compound (LSC) summary

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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.45	4.9	ng	281542	1	6.71	1145980	20.0
Propanoic acid, 2...	4.16	2.2	ng	124808	1	6.71	1145980	20.0
2-Pentene, 3,4-di...	4.23	2.1	ng	119021	1	6.71	1145980	20.0
Propanoic acid, p...	4.41	2.4	ng	134445	1	6.71	1145980	20.0
unknown4.87	4.87	45.6	ng	2614520	1	6.71	1145980	20.0
2-Pentanone, 4-me...	5.72	2.1	ng	119316	1	6.71	1145980	20.0
unknown6.48	6.48	92.2	ng	5281180	1	6.71	1145980	20.0
Hexadecanoic acid...	12.65	3.9	ng	272155	5	13.90	1405190	20.0
Octadecanoic acid...	13.36	2.5	ng	178296	5	13.90	1405190	20.0