LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093637.D
Acq On : 14 Mar 2017 5:16
Operator : SJ/MA
Sample : I2199-29
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-110

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	48	50	63	rVB	70126	214723	3.47%	0.413%
2	3.133	106	109	124	rBV	396563	895736	14.46%	1.721%
3	4.173	197	200	218	rBV	1733998	3019808	48.76%	5.803%
4	4.401	218	220	223	rVV	59175	114078	1.84%	0.219%
5	4.459	223	225	228	rVB	239794	331082	5.35%	0.636%
6	4.893	260	263	281	rBV2	339135	877192	14.16%	1.686%
7	5.316	298	300	330	rBV	4336767	6192701	100.00%	11.899%
8	6.333	386	389	391	rBV	235749	207307	3.35%	0.398%
9	6.367	391	392	400	rBV2	3211847	5398013	87.17%	10.372%
10	6.482	400	402	405	rVB	5068456	5151343	83.18%	9.898%
11	6.710	420	422	431	rVB	984892	1136672	18.36%	2.184%
12	6.859	433	435	438	rBV	4008283	4168595	67.31%	8.010%
13	7.030	448	450	459	rVB	108568	162043	2.62%	0.311%
14	7.282	470	472	475	rBV	3121443	3704659	59.82%	7.119%
15	8.002	533	535	550	rVB	1284634	1474455	23.81%	2.833%
16	9.076	626	629	632	rBV	3996787	6025649	97.30%	11.578%
17	9.762	686	689	691	rBV	1121967	1441317	23.27%	2.770%
18	10.551	756	758	761	rBV2	2193419	3172518	51.23%	6.096%
19	11.248	817	819	831	rVB	1614365	1598180	25.81%	3.071%
20	12.654	940	942	944	rBV	166657	141809	2.29%	0.272%
21	12.837	955	958	961	rBV	4507875	5145815	83.09%	9.888%
22	13.362	1001	1004	1006	rBV	102430	103075	1.66%	0.198%
23	13.900	1049	1051	1059	rBV	915031	1148349	18.54%	2.207%
24	15.328	1174	1176	1188	rVB2	91937	217066	3.51%	0.417%

Sum of corrected areas: 52042185

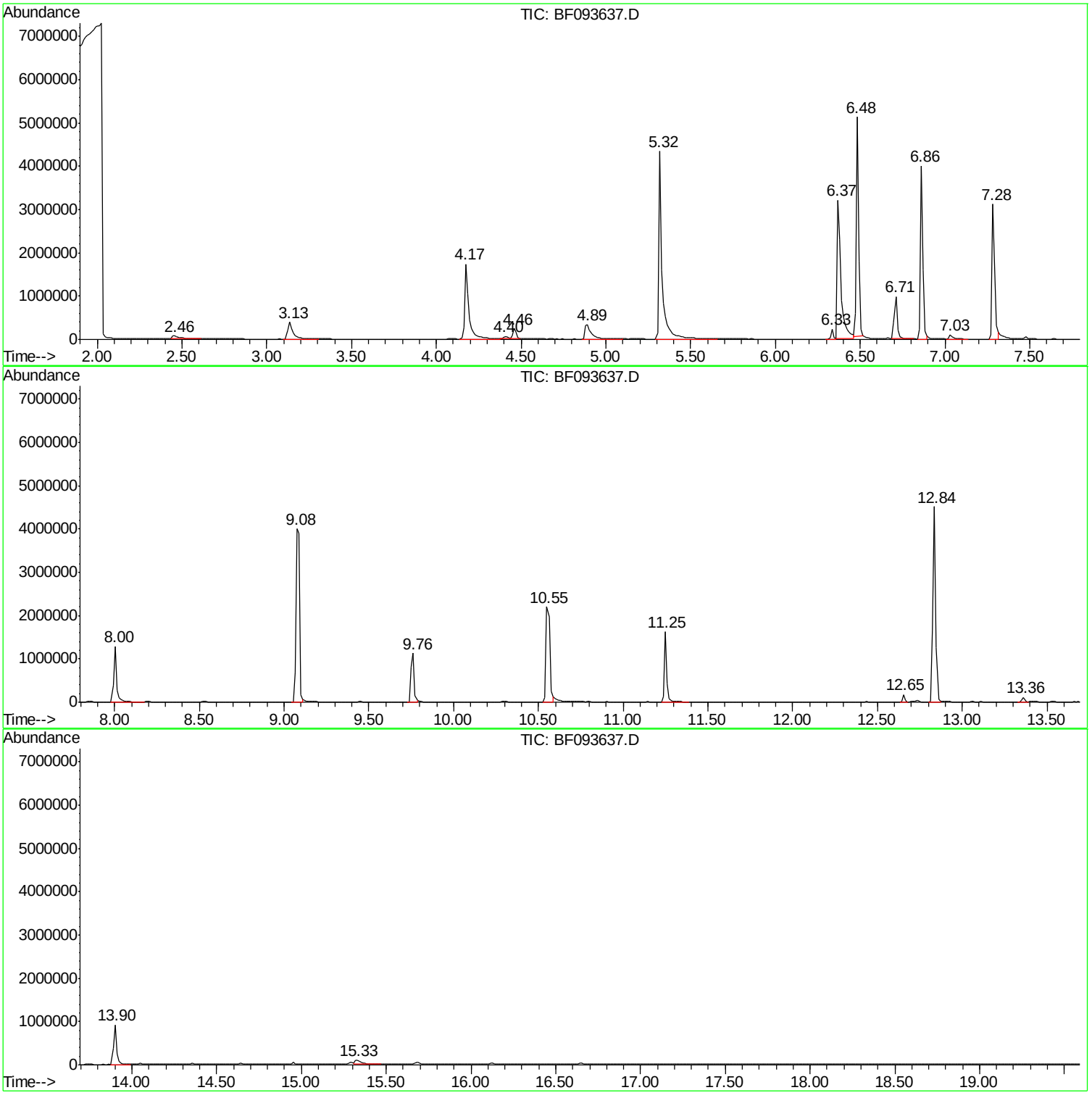
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093637.D
Acq On : 14 Mar 2017 5:16
Operator : SJ/MA
Sample : I2199-29
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-110

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

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093637.D
Acq On : 14 Mar 2017 5:16
Operator : SJ/MA
Sample : I2199-29
Misc :
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Instrument : BNA_F
ClientSampleId : D-110

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

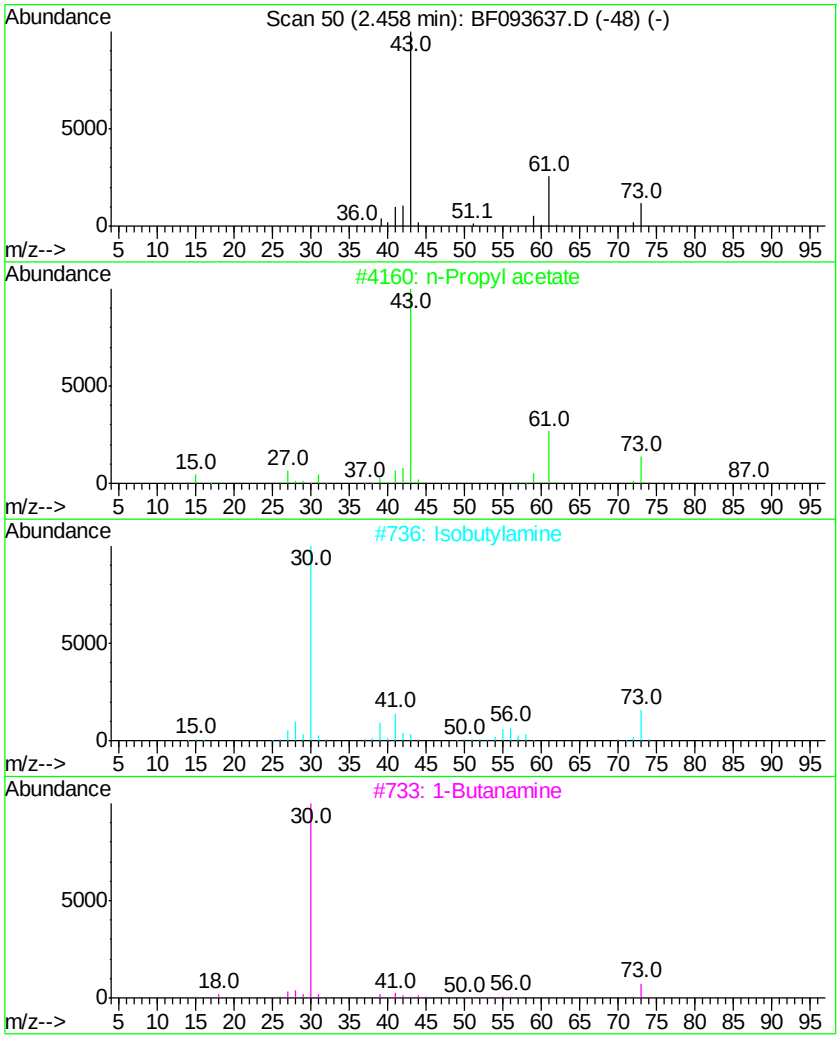
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

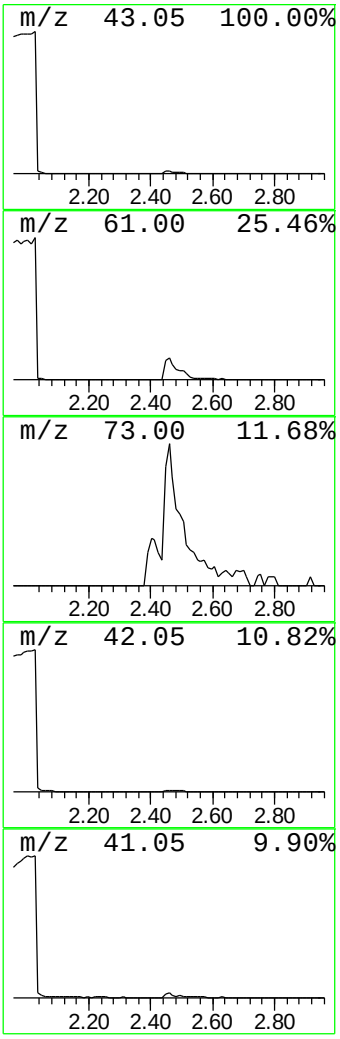
****

Peak Number 1 n-Propyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.46	3.78 ng	214723	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	Isobutylamine	73	C4H11N	000078-81-9	5
3	1-Butanamine	73	C4H11N	000109-73-9	4
4	Pentane	72	C5H12	000109-66-0	4
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093637.D
Acq On : 14 Mar 2017 5:16
Operator : SJ/MA
Sample : I2199-29
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-110

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

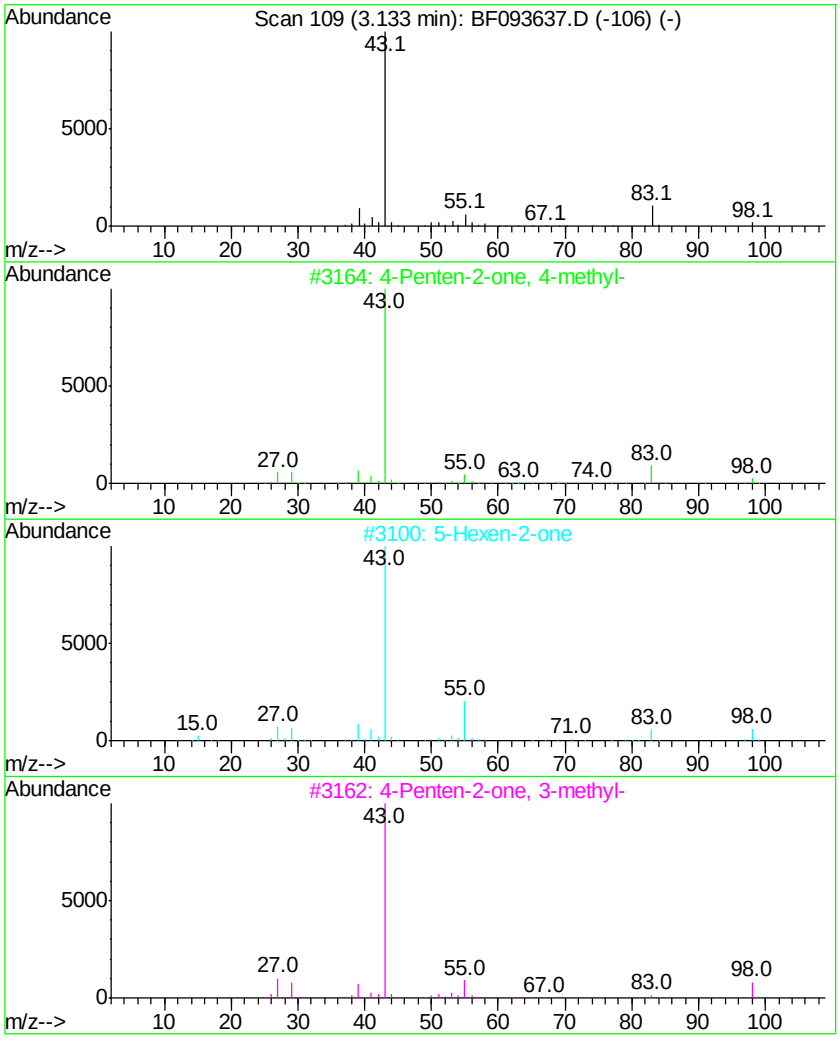
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

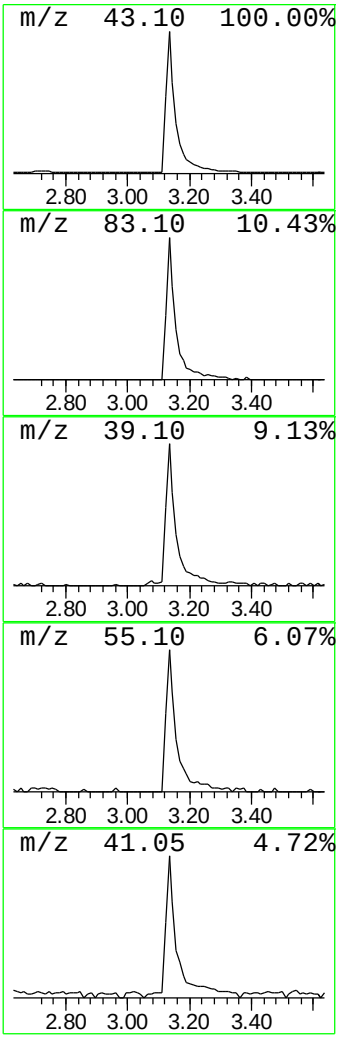
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	15.76 ng	895736	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-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	38
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	9
5	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093637.D
Acq On : 14 Mar 2017 5:16
Operator : SJ/MA
Sample : I2199-29
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-110

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

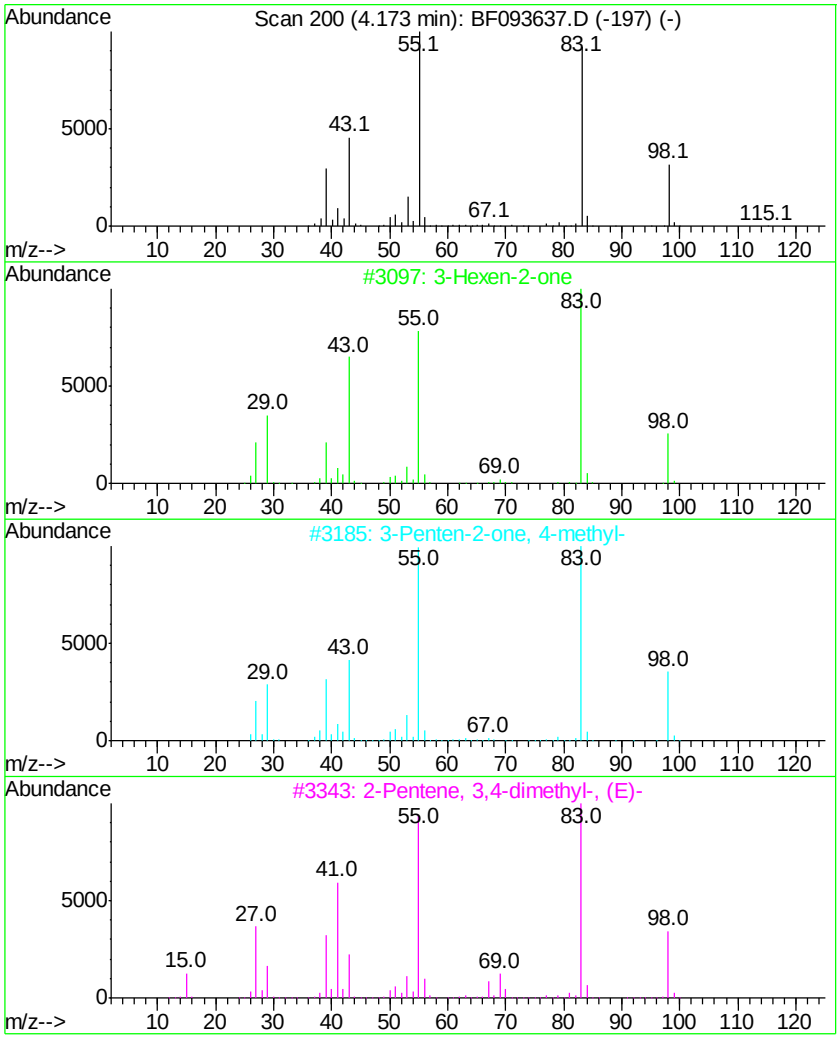
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

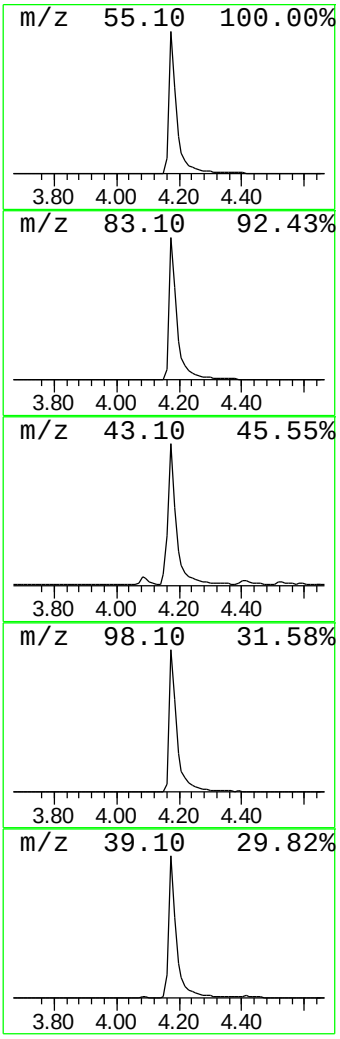
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.17	53.13 ng	3019810	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, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093637.D
Acq On : 14 Mar 2017 5:16
Operator : SJ/MA
Sample : I2199-29
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-110

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

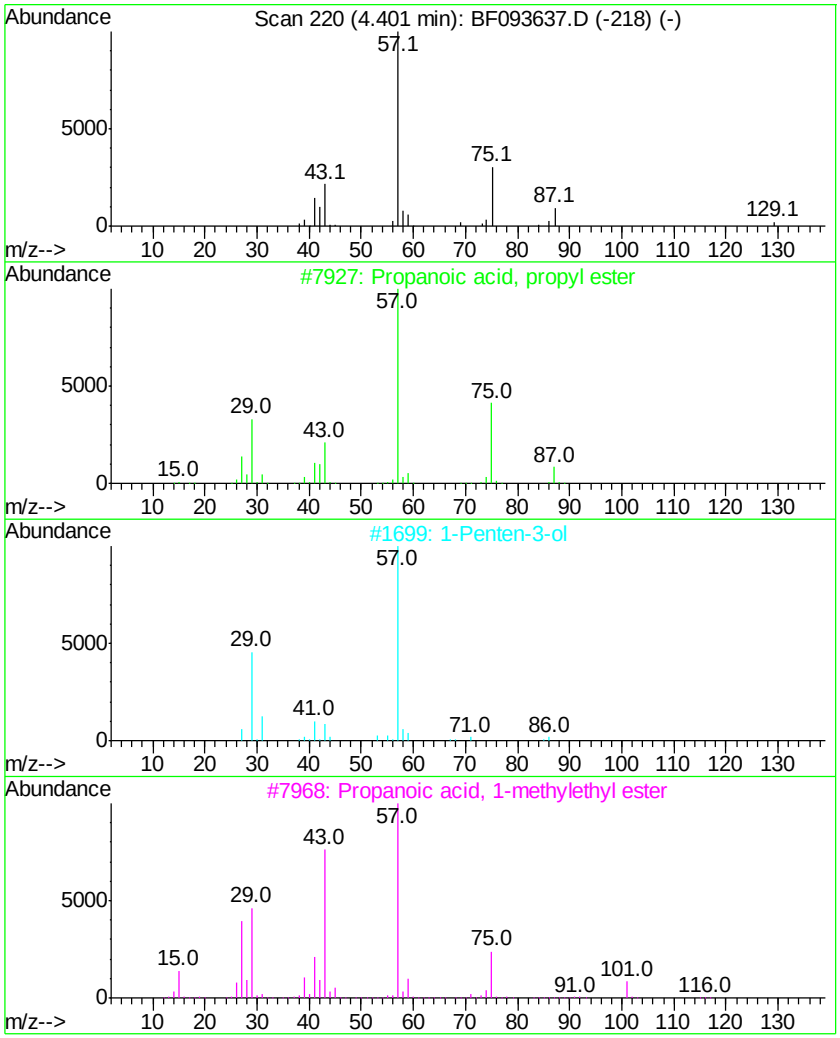
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

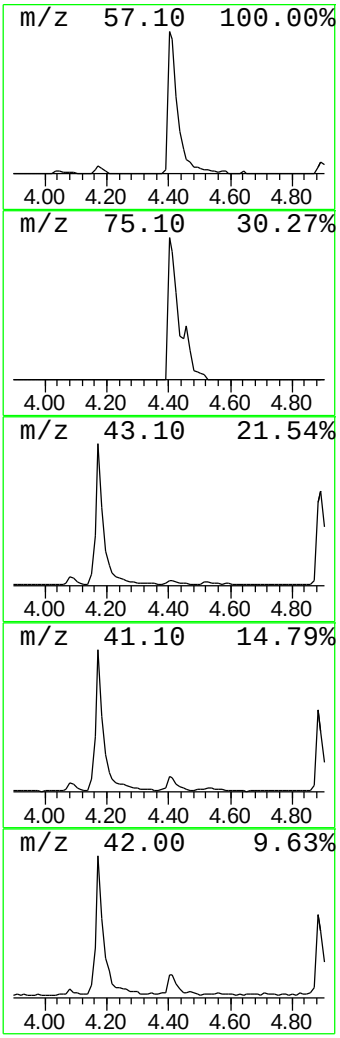
****

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	2.01 ng	114078	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	72
2	1-Penten-3-ol	86	C5H10O	000616-25-1	9
3	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	9
4	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	9
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093637.D
Acq On : 14 Mar 2017 5:16
Operator : SJ/MA
Sample : I2199-29
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-110

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

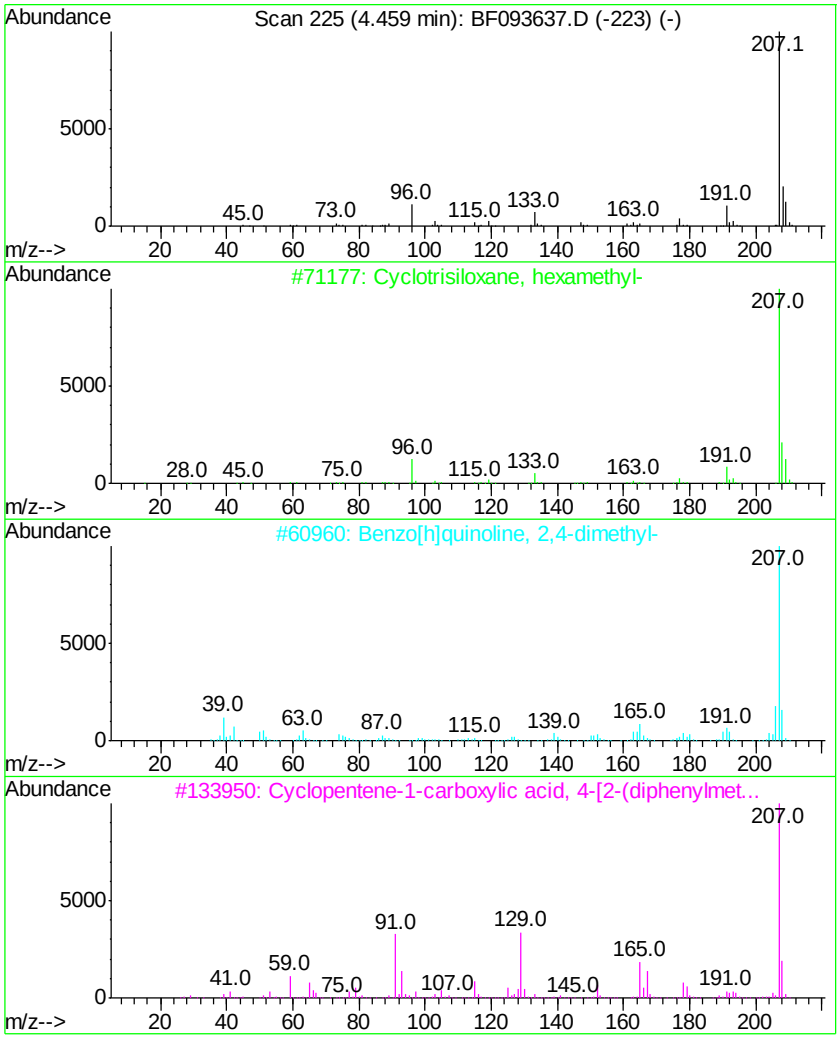
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

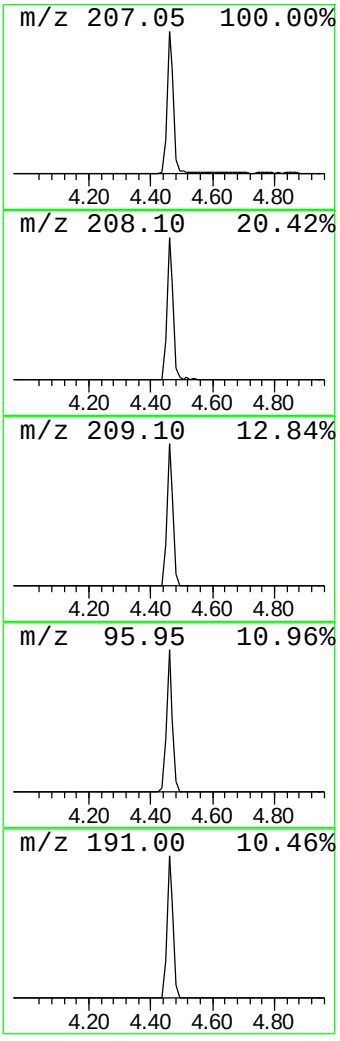
****

Peak Number 5 Cyclotrisiloxane, hexamethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	5.83 ng	331082	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	Cyclopentene-1-carboxylic acid, ...	332	C23H24O2	1000159-40-6	38
4	N-(2-Acetylcyclopentylidene)cycl...	207	C13H21NO	1000100-48-5	9
5	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
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Operator : SJ/MA
Sample : I2199-29
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-110

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

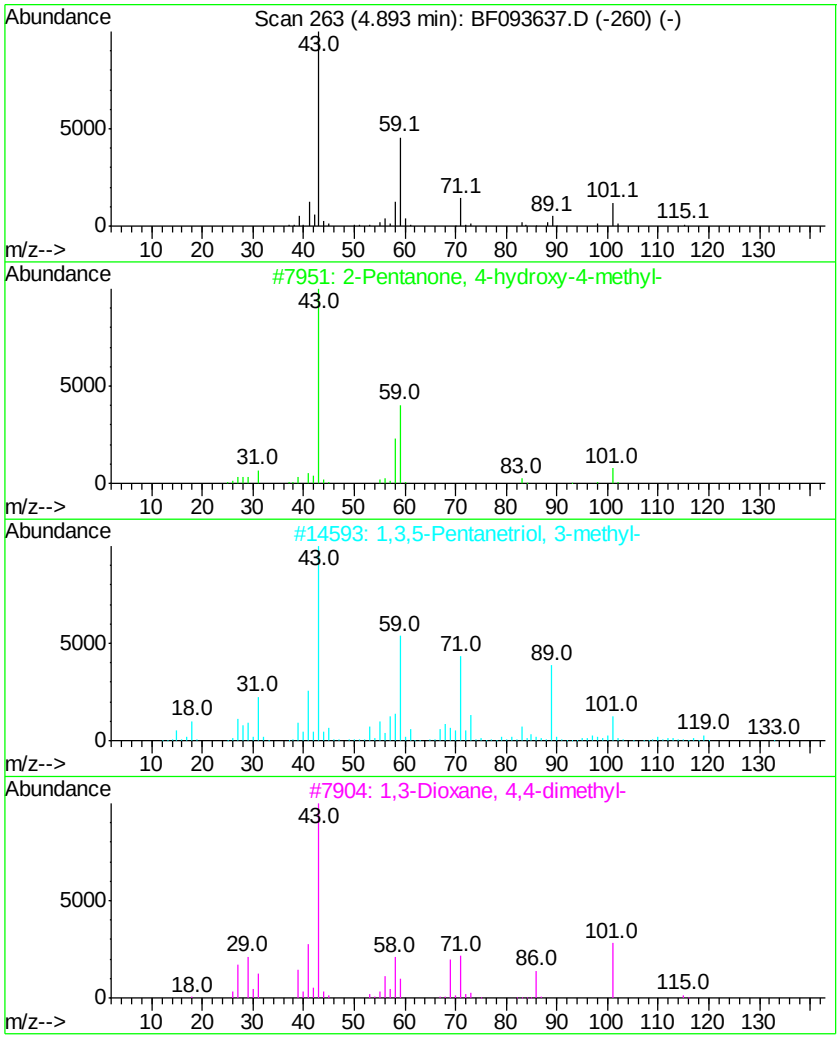
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

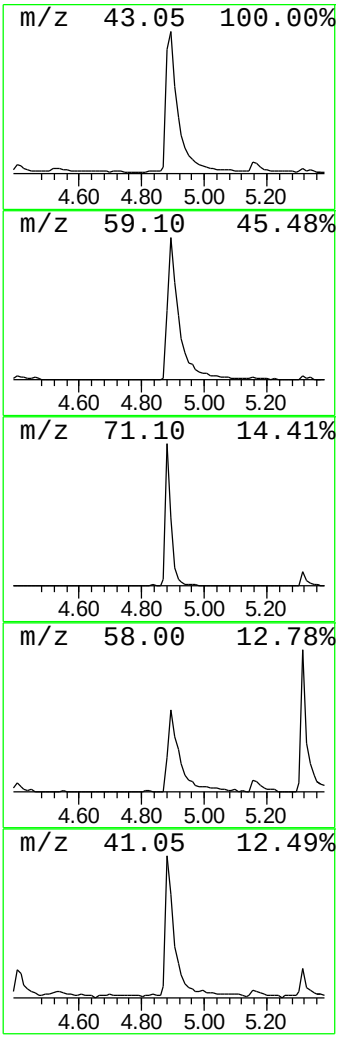
****

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	15.43 ng	877192	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	1,3-Dioxane, 4,4-dimethyl-	116	C6H12O2	000766-15-4	10
4	Diacetamide	101	C4H7NO2	000625-77-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : I2199-29
Misc :
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Instrument : BNA_F
ClientSampleId : D-110

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

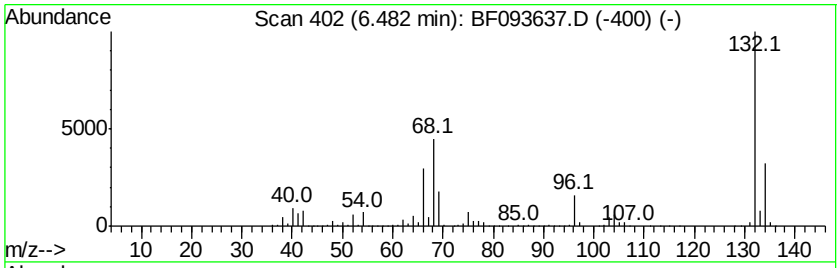
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

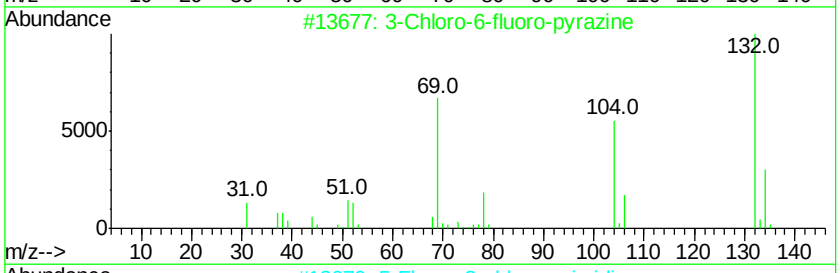
****

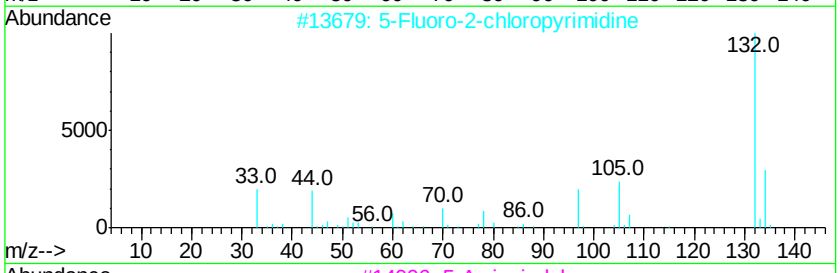
Peak Number 7 unknown6.48 Concentration Rank 1

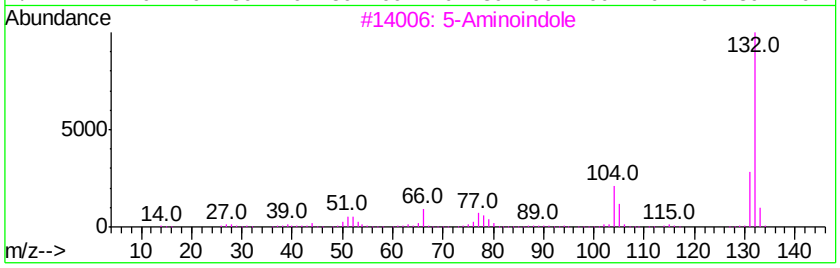
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	90.64 ng	5151340	1,4-Dichlorobenzene-d4	6.71

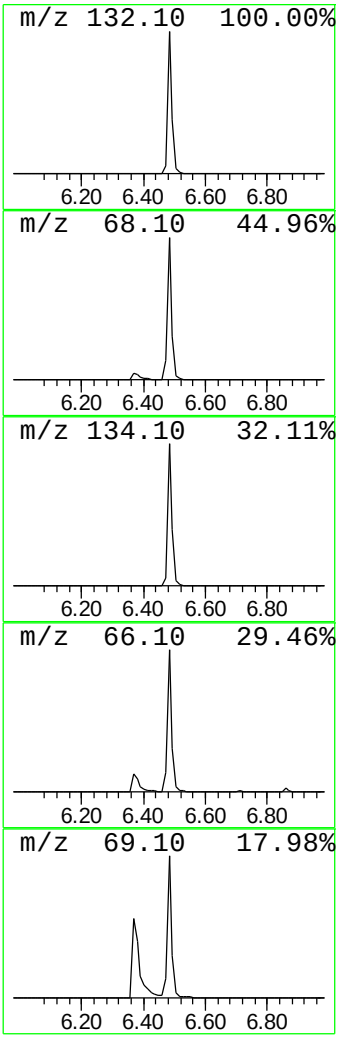
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9











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

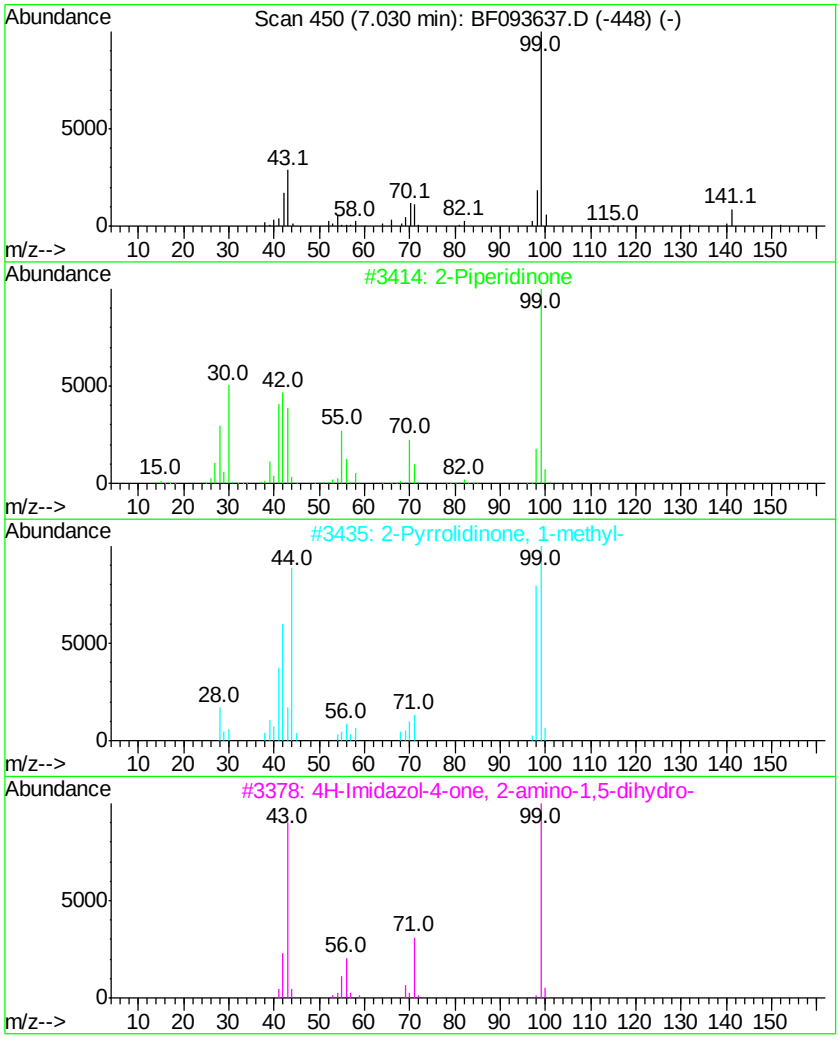
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

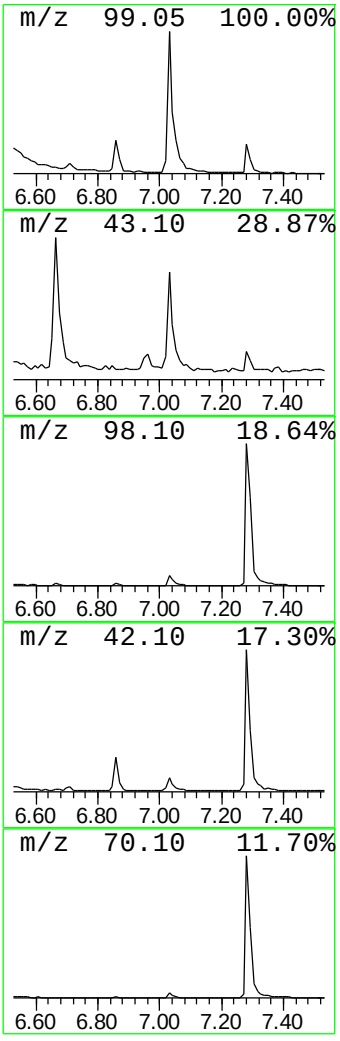
****

Peak Number 9 2-Piperidinone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	2.85 ng	162043	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Piperidinone	99	C5H9NO	000675-20-7	78
2	2-Pyrrolidinone, 1-methyl-	99	C5H9NO	000872-50-4	50
3	4H-Imidazol-4-one, 2-amino-1,5-d...	99	C3H5N3O	000503-86-6	42
4	3,5-Diamino-1,2,4-triazole	99	C2H5N5	001455-77-2	42
5	1,3,2-Dioxaborolane, 2,4-diethyl-	128	C6H13BO2	057633-63-3	40





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093637.D
Acq On : 14 Mar 2017 5:16
Operator : SJ/MA
Sample : I2199-29
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-110

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

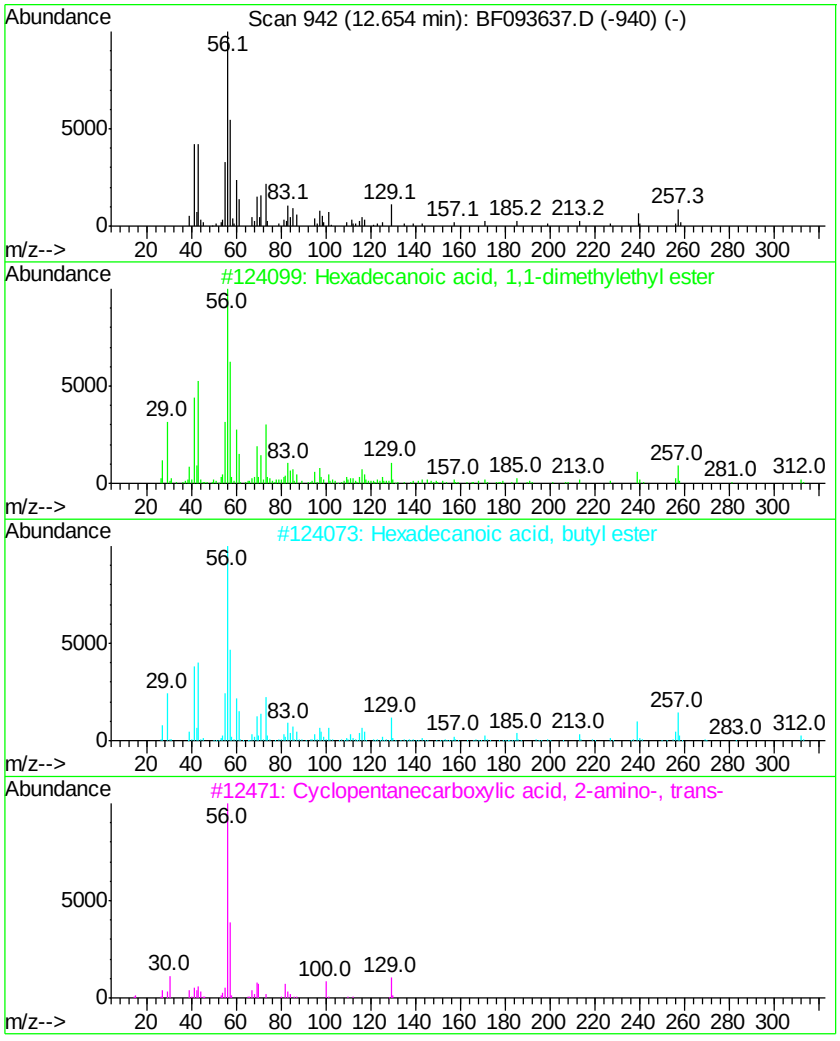
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

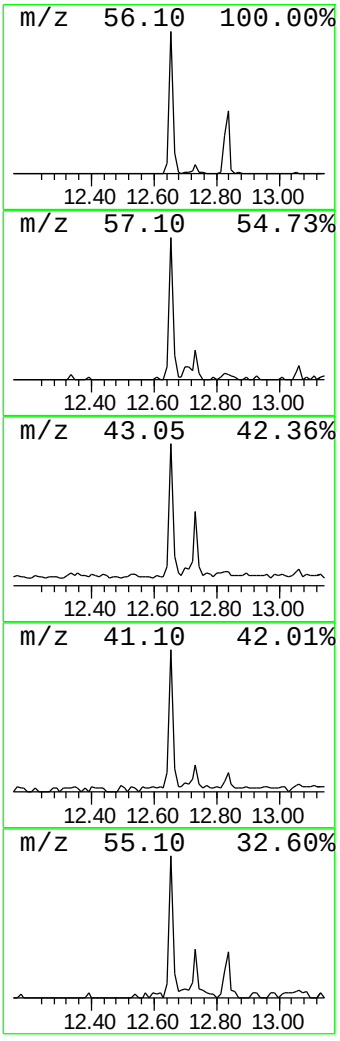
****

Peak Number 10 Hexadecanoic acid, 1,1-dime... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.47 ng	141809	Chrysene-d12	13.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	76
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	53
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	43
4	Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	43
5	Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093637.D
Acq On : 14 Mar 2017 5:16
Operator : SJ/MA
Sample : I2199-29
Misc :
ALS Vial : 37 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-110

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
n-Propyl acetate	2.46	3.8	ng	214723	1	6.71	1136670	20.0
4-Penten-2-one, 4...	3.13	15.8	ng	895736	1	6.71	1136670	20.0
3-Hexen-2-one	4.17	53.1	ng	3019810	1	6.71	1136670	20.0
Propanoic acid, p...	4.40	2.0	ng	114078	1	6.71	1136670	20.0
Cyclotrisiloxane,...	4.46	5.8	ng	331082	1	6.71	1136670	20.0
2-Pentanone, 4-hy...	4.89	15.4	ng	877192	1	6.71	1136670	20.0
unknown6.48	6.48	90.6	ng	5151340	1	6.71	1136670	20.0
2-Piperidinone	7.03	2.9	ng	162043	1	6.71	1136670	20.0
Hexadecanoic acid...	12.65	2.5	ng	141809	5	13.90	1148350	20.0