LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093632.D
Acq On : 14 Mar 2017 2:58
Operator : SJ/MA
Sample : I2199-24
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-97

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	2.356	38	41	45	rBV	51132	89543	1.52%	0.178%
2	2.424	45	47	57	rVB	57078	162229	2.76%	0.322%
3	3.110	104	107	129	rBV	280498	743294	12.62%	1.477%
4	4.161	196	199	218	rBV	2572886	4322674	73.42%	8.588%
5	4.401	218	220	222	rBV	48691	79088	1.34%	0.157%
6	4.459	222	225	228	rVB	619912	895632	15.21%	1.779%
7	4.881	259	262	274	rBV2	161271	411695	6.99%	0.818%
8	5.316	297	300	319	rBV	2841748	5406071	91.82%	10.740%
9	6.333	386	389	391	rBV	748917	690683	11.73%	1.372%
10	6.367	391	392	400	rVV	2919278	4354463	73.96%	8.651%
11	6.482	400	402	405	rVB	4708164	4778303	81.16%	9.493%
12	6.710	420	422	433	rVB	987675	1107087	18.80%	2.199%
13	6.859	433	435	438	rBV	3832989	3859168	65.54%	7.667%
14	7.019	447	449	457	rVB	321264	433690	7.37%	0.862%
15	7.282	470	472	487	rBV	2888958	3591578	61.00%	7.135%
16	7.476	487	489	500	rVB	158415	218210	3.71%	0.434%
17	8.002	533	535	544	rBV	1310658	1495994	25.41%	2.972%
18	8.528	576	581	585	rBV	73250	84434	1.43%	0.168%
19	9.088	627	630	632	rBV	4326920	5887837	100.00%	11.697%
20	9.762	686	689	698	rVB	881072	1094013	18.58%	2.173%
21	10.551	756	758	761	rBV2	2183387	2997670	50.91%	5.956%
22	11.248	817	819	826	rBV	1508040	1537615	26.12%	3.055%
23	12.654	940	942	944	rVB	114546	105304	1.79%	0.209%
24	12.837	955	958	961	rBV	4457734	5041177	85.62%	10.015%
25	13.362	1001	1004	1006	rVB	78696	71248	1.21%	0.142%
26	13.900	1049	1051	1061	rBV	627966	770379	13.08%	1.531%
27	15.340	1175	1177	1185	rVB5	41224	105387	1.79%	0.209%

Sum of corrected areas: 50334466

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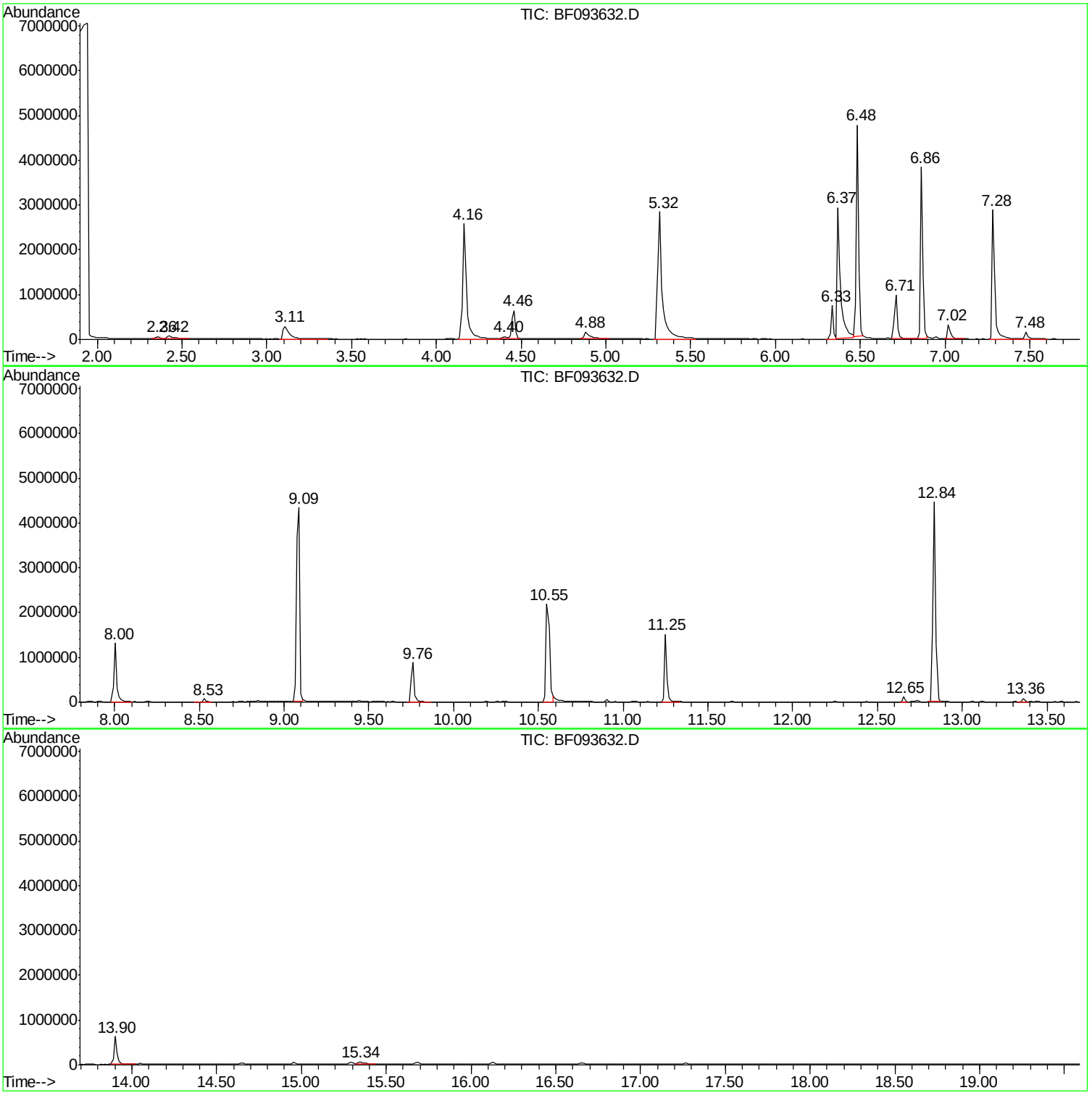
Instrument :
BNA_F
ClientSampleId :
D-97

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 Integration Parameters: LSCINT.P

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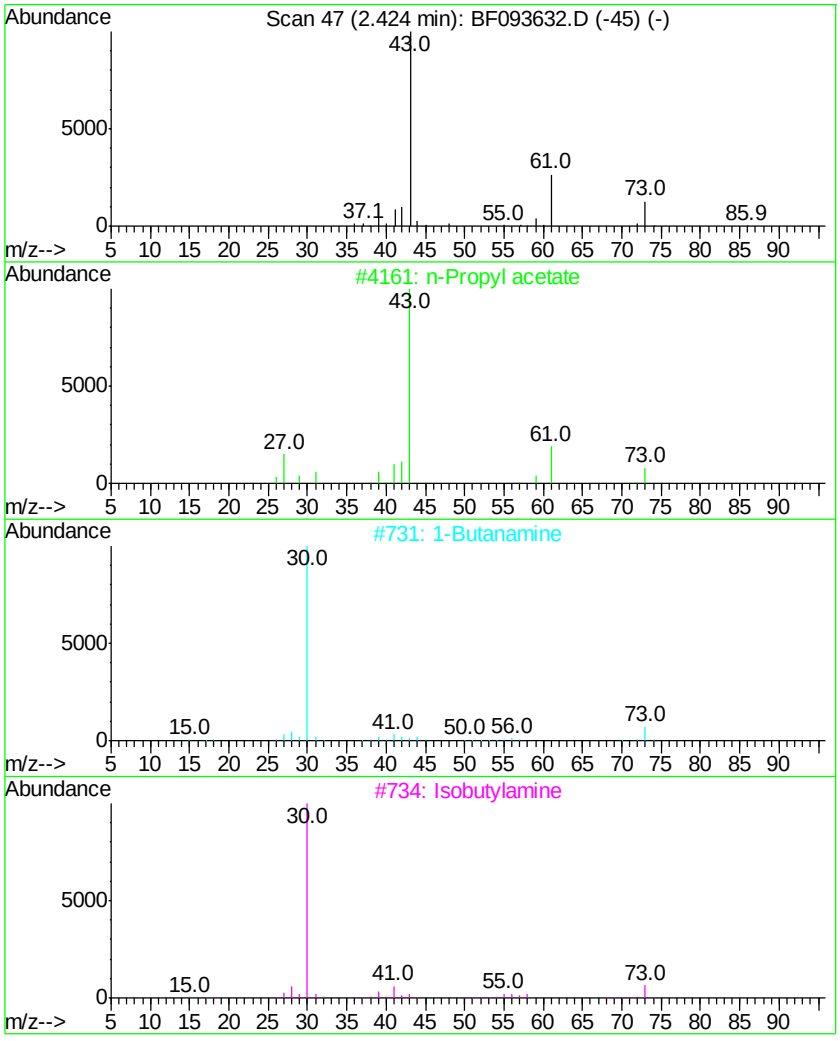
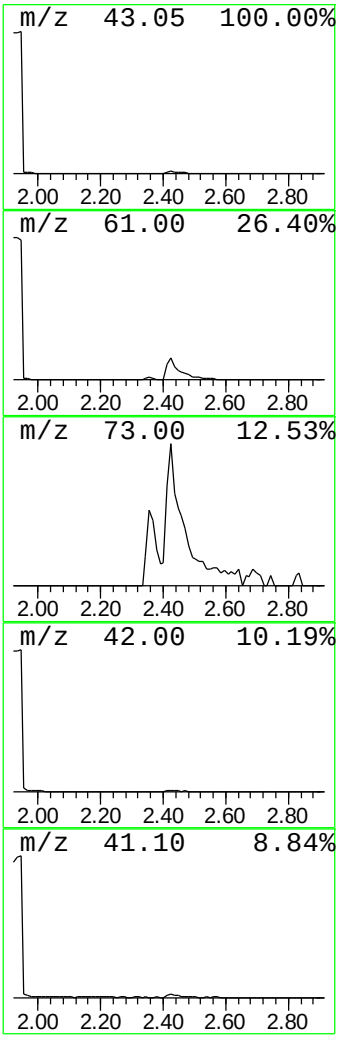
Peak Number 1 n-Propyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.42	2.93 ng	162229	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	1-Butanamine	73	C4H11N	000109-73-9	7
3	Isobutylamine	73	C4H11N	000078-81-9	5
4	Pentane	72	C5H12	000109-66-0	4
5	Hydrogen azide	43	HN3	007782-79-8	4





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093632.D
Acq On : 14 Mar 2017 2:58
Operator : SJ/MA
Sample : I2199-24
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-97

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

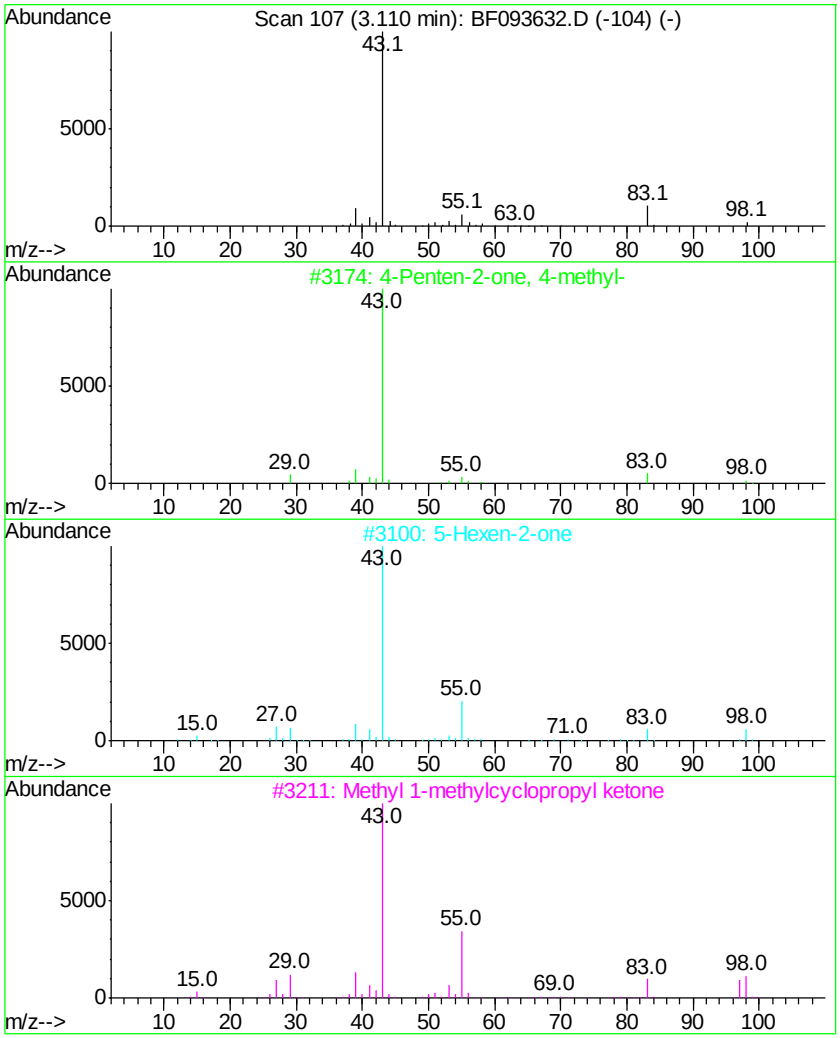
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

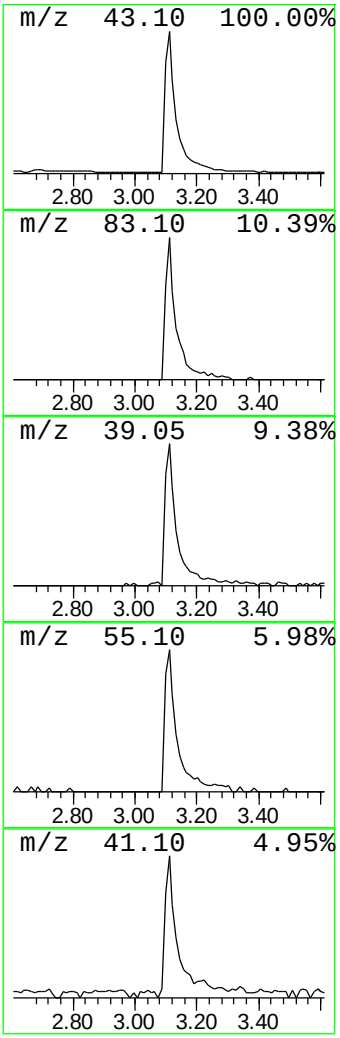
****

Peak Number 2 4-Penten-2-one, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.11	13.43 ng	743294	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	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	37
4	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	37
5	Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9





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Data File : BF093632.D
Acq On : 14 Mar 2017 2:58
Operator : SJ/MA
Sample : I2199-24
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-97

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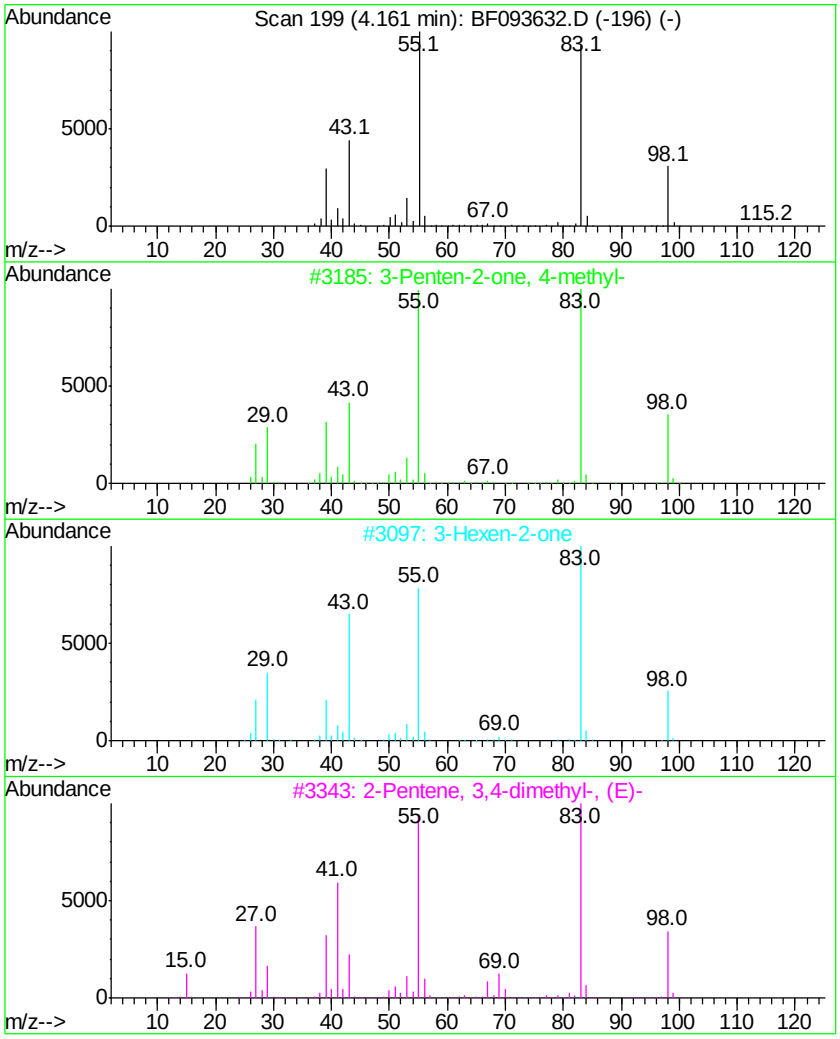
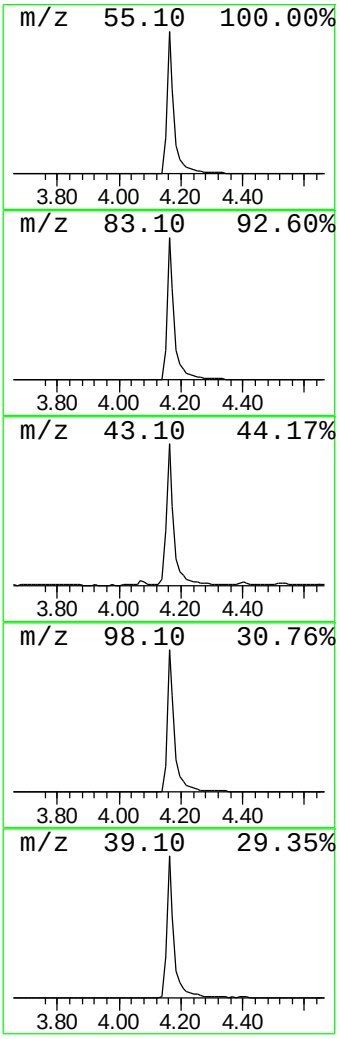
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	78.09 ng	4322670	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, 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, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86





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Instrument : BNA_F
ClientSampleId : D-97

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

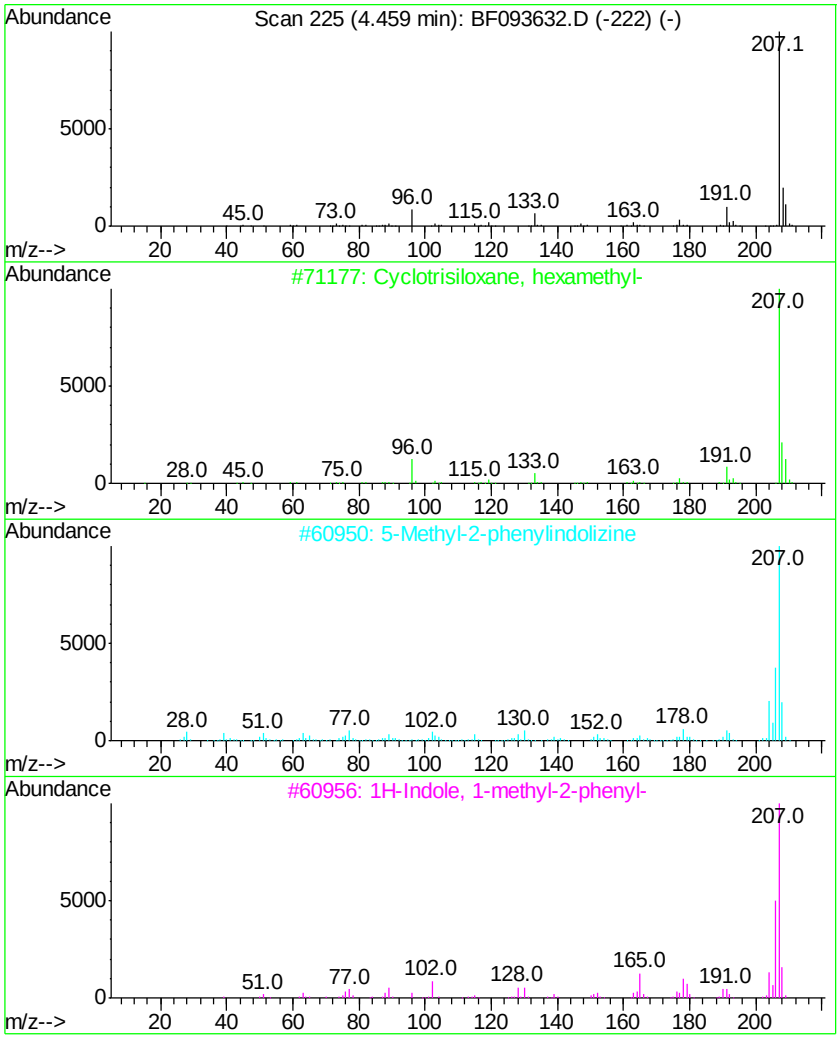
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

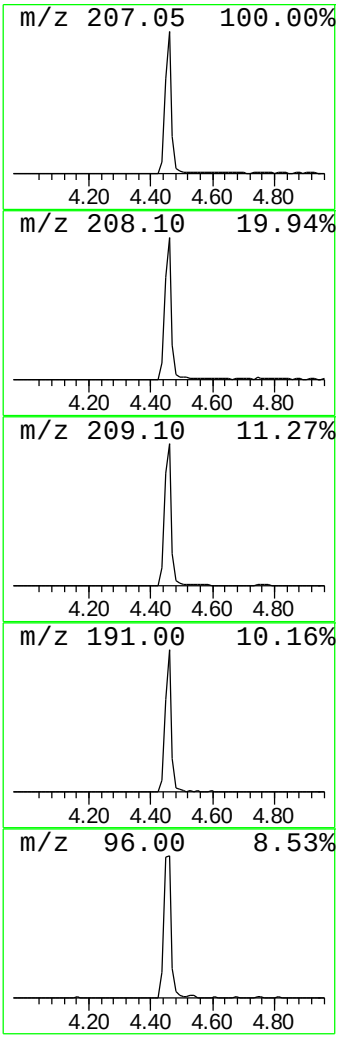
****

Peak Number 4 Cyclotrisiloxane, hexamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	16.18 ng	895632	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	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	39
3	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	39
4	Benzo[h]quinoline, 2,4-dimethyl-	207	C15H13N	000605-67-4	39
5	2-Ethylacridine	207	C15H13N	055751-83-2	36





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093632.D
Acq On : 14 Mar 2017 2:58
Operator : SJ/MA
Sample : I2199-24
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D-97

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
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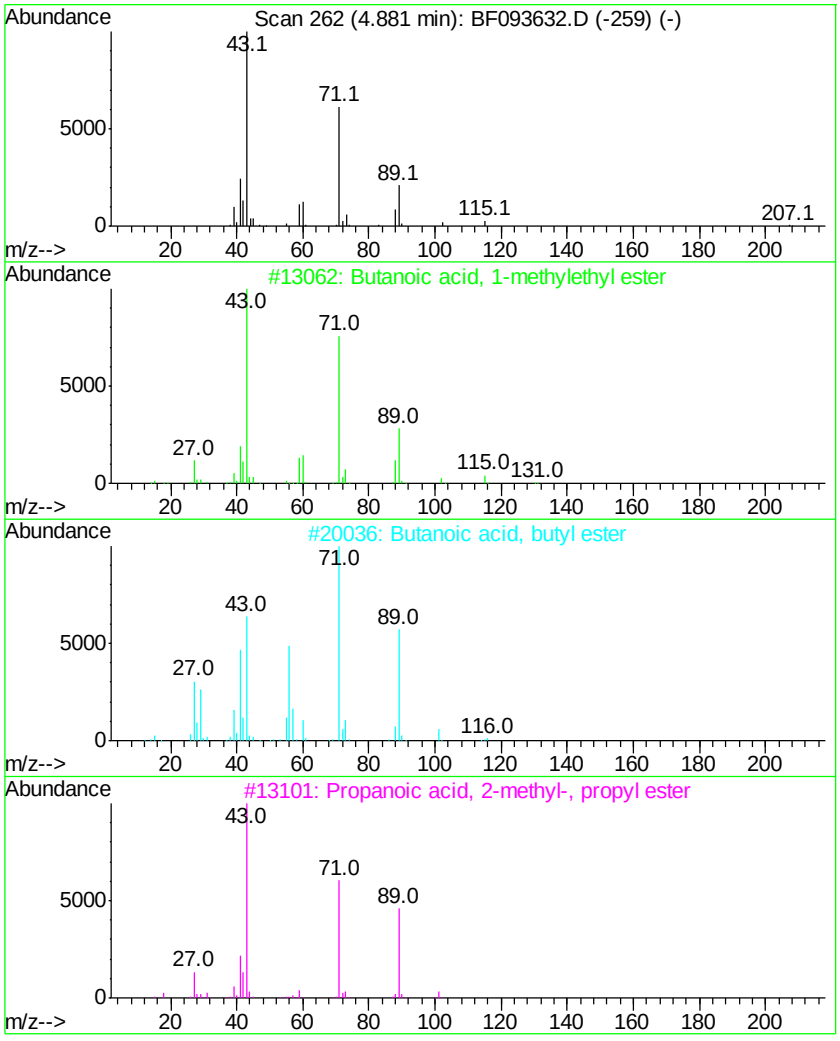
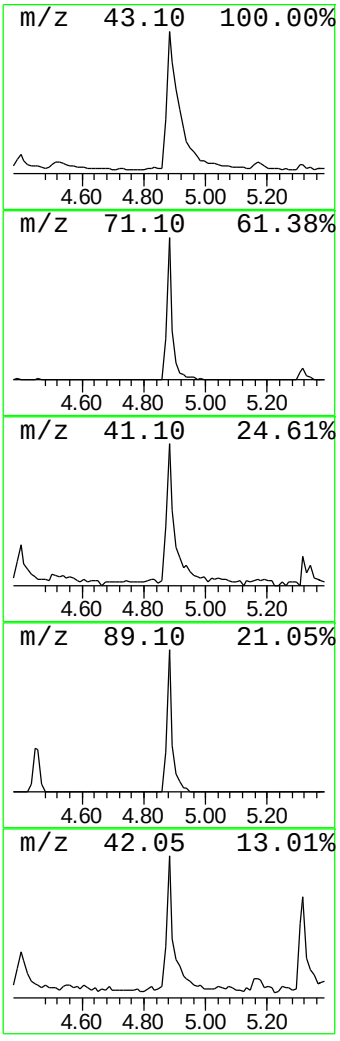
****

Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.88	7.44 ng	411695	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50





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Sample : I2199-24
Misc :
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Instrument : BNA_F
ClientSampleId : D-97

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

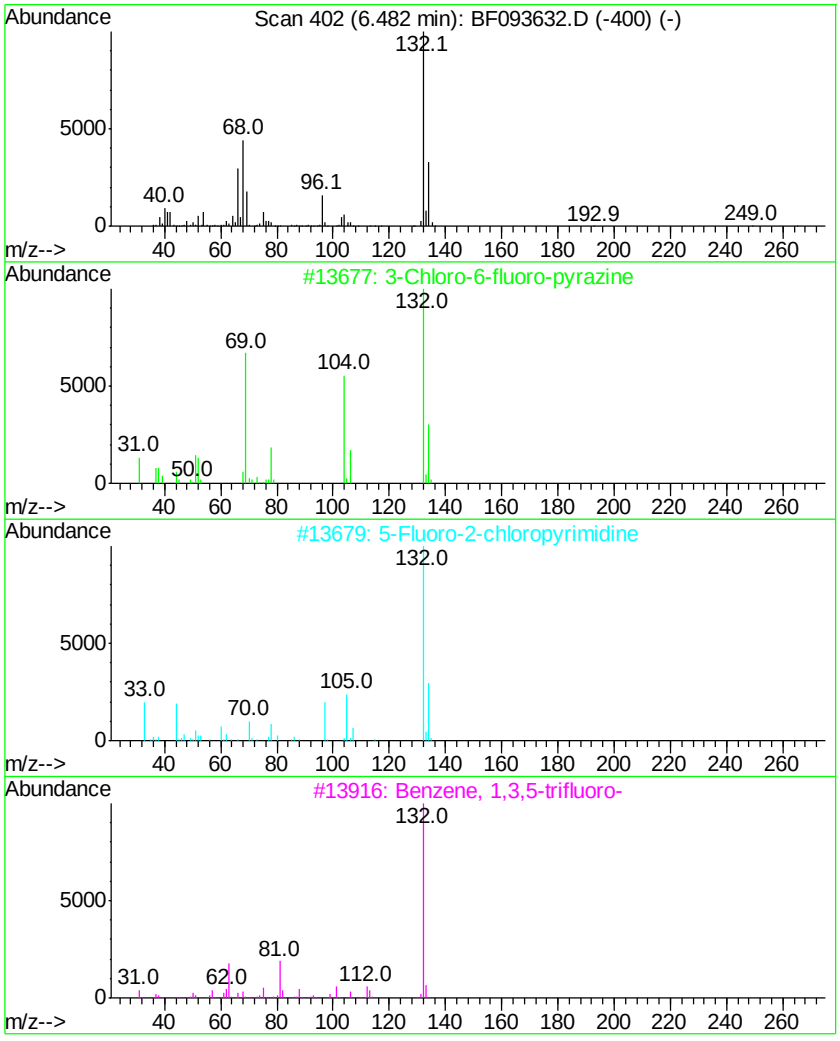
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

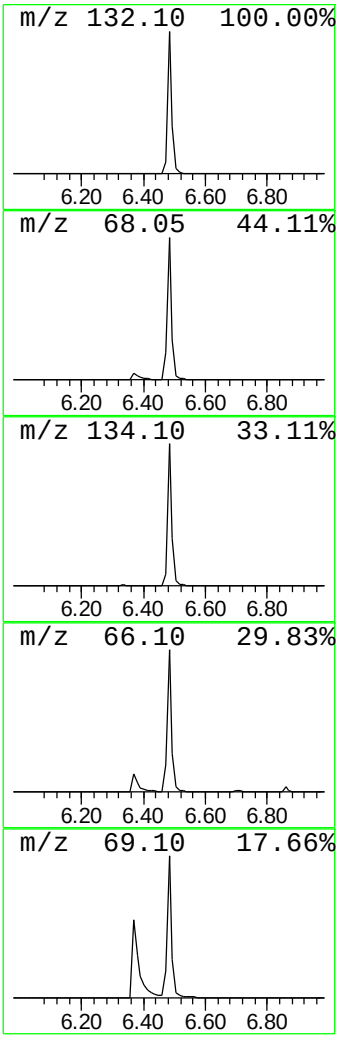
****

Peak Number 6 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	86.32 ng	4778300	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	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





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Instrument : BNA_F
ClientSampleId : D-97

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

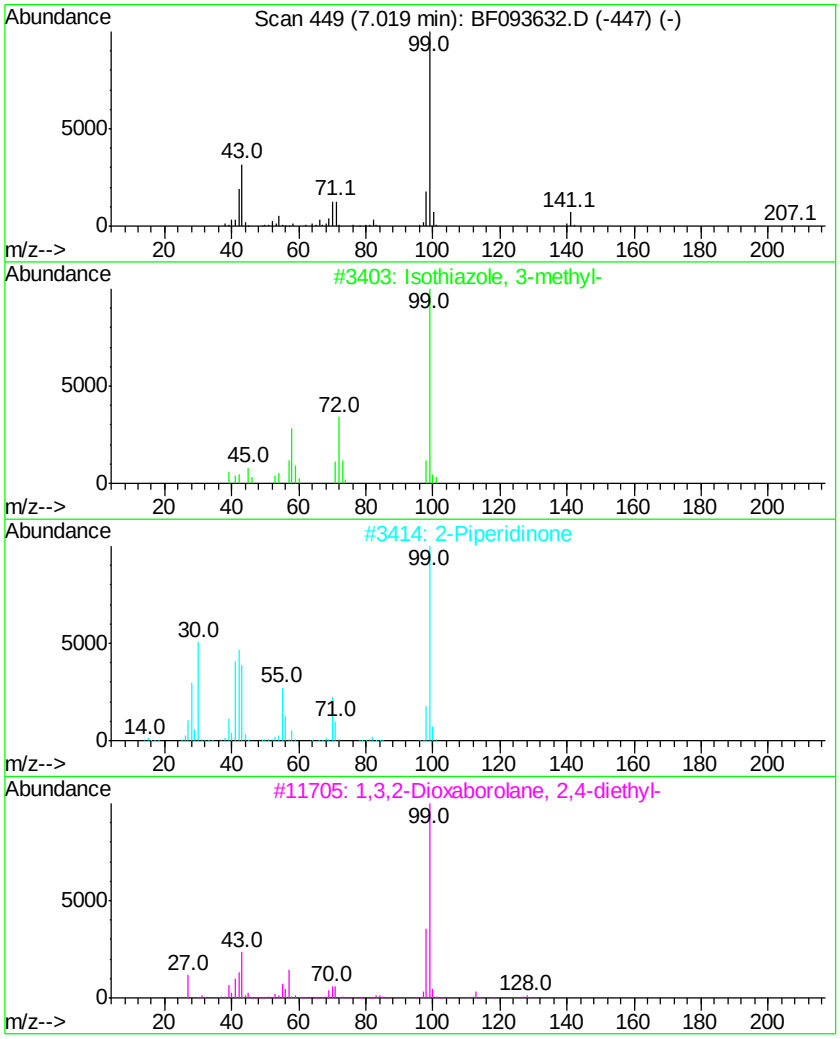
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

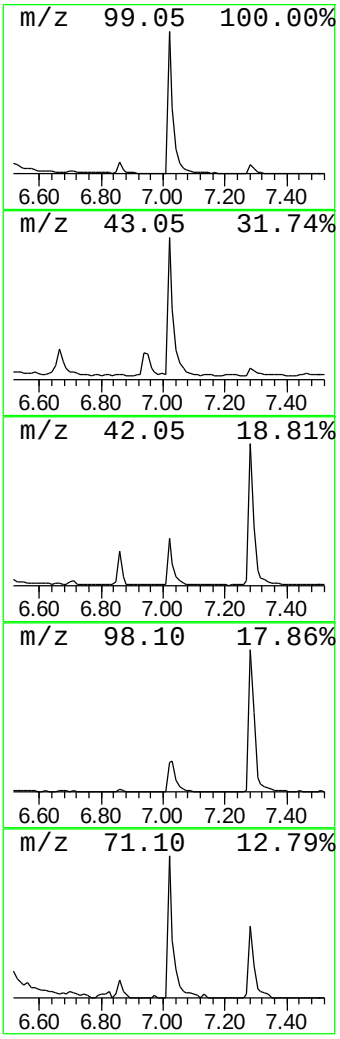
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	7.83 ng	433690	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isothiazole, 3-methyl-	99	C4H5NS	000693-92-5	59
2	2-Piperidinone	99	C5H9NO	000675-20-7	45
3	1,3,2-Dioxaborolane, 2,4-diethyl-	128	C6H13BO2	057633-63-3	40
4	Hexanoic acid, anhydride	214	C12H22O3	002051-49-2	38
5	Cyclohexanol, 1-(2-nitropropyl)-	187	C9H17NO3	103077-77-6	38





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Misc :
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Instrument : BNA_F
ClientSampleId : D-97

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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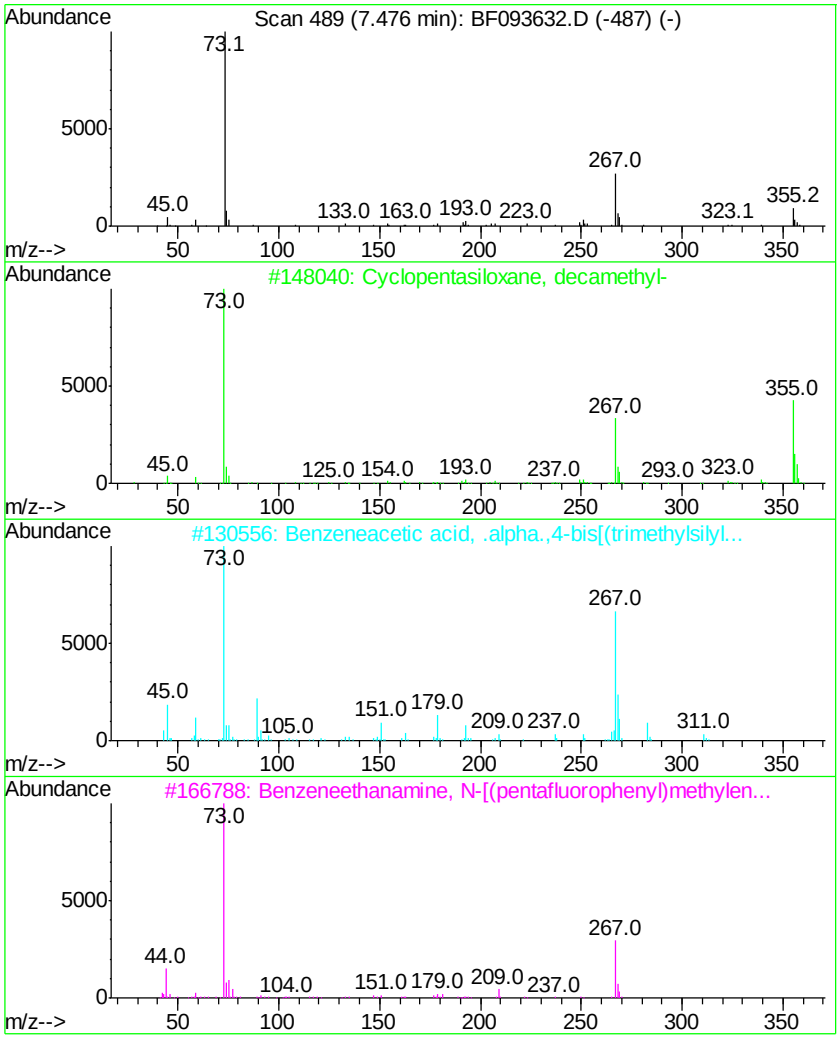
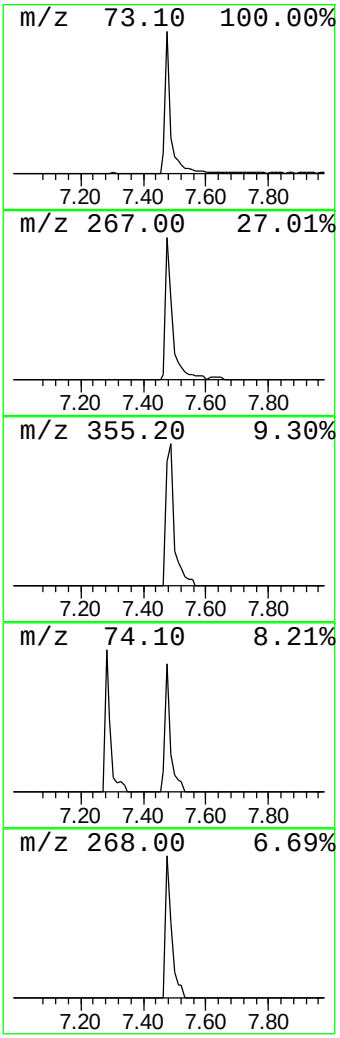
Peak Number 9 Cyclopentasiloxane, decamet... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	2.92 ng	218210	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	90
2	Benzeneacetic acid, .alpha.,4-bi...	326	C15H26O4Si2	055334-40-2	40
3	Benzeneethanamine, N-[(pentafluo...	475	C21H26F5NO2Si2	055429-85-1	40
4	Pentasiloxane, 1,1,3,3,5,5,7,7,9...	356	C10H32O4Si5	000995-83-5	38
5	Benzoic acid, 4-[(trimethylsilyl...	282	C13H22O3Si2	002078-13-9	33





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Misc :
ALS Vial : 32 Sample Multiplier: 1

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

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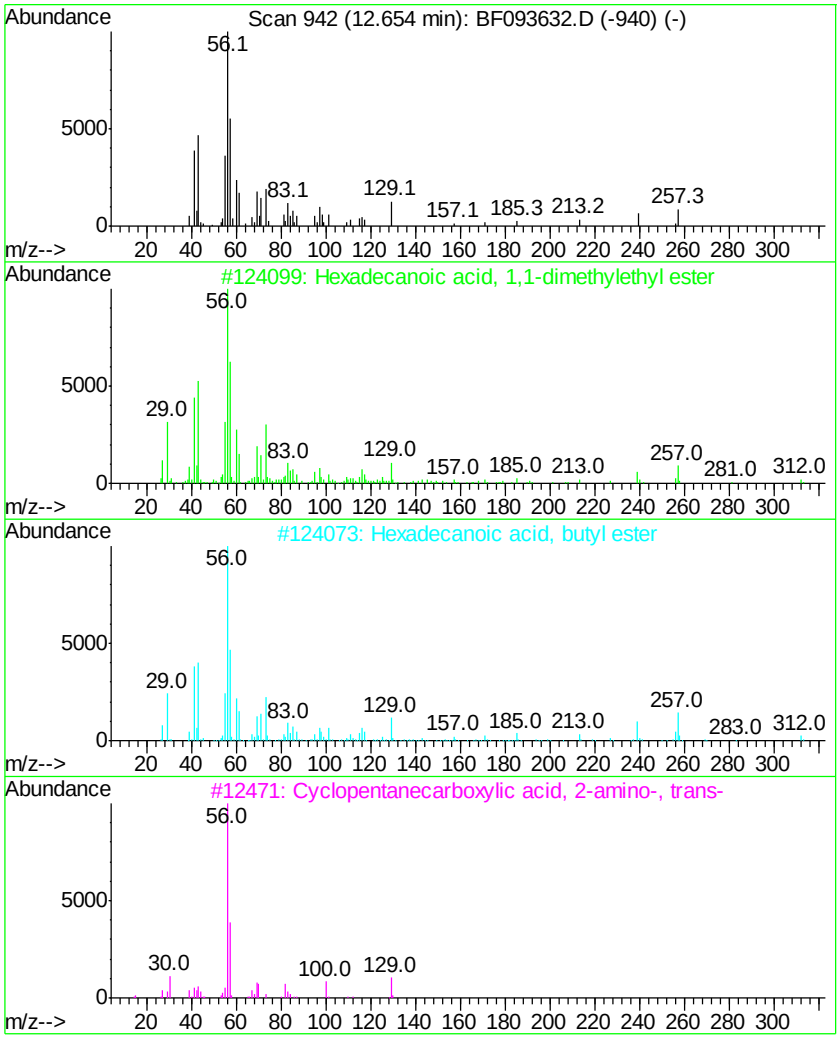
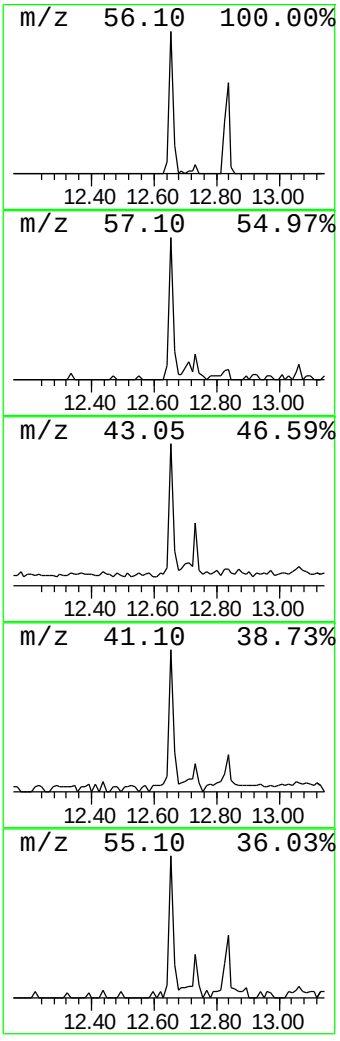
Peak Number 10 Hexadecanoic acid, 1,1-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.73 ng	105304	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, butyl ester	312	C20H40O2	000111-06-8	52
3	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	37
4	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	37
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093632.D
Acq On : 14 Mar 2017 2:58
Operator : SJ/MA
Sample : I2199-24
Misc :
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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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	2.42	2.9	ng	162229	1	6.71	1107090	20.0
4-Penten-2-one, 4...	3.11	13.4	ng	743294	1	6.71	1107090	20.0
3-Penten-2-one, 4...	4.16	78.1	ng	4322670	1	6.71	1107090	20.0
Cyclotrisiloxane,...	4.46	16.2	ng	895632	1	6.71	1107090	20.0
Butanoic acid, 1-...	4.88	7.4	ng	411695	1	6.71	1107090	20.0
unknown6.48	6.48	86.3	ng	4778300	1	6.71	1107090	20.0
Isothiazole, 3-me...	7.02	7.8	ng	433690	1	6.71	1107090	20.0
Cyclopentasiloxan...	7.48	2.9	ng	218210	2	8.00	1495990	20.0
Hexadecanoic acid...	12.65	2.7	ng	105304	5	13.90	770379	20.0