LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093622.D
Acq On : 13 Mar 2017 22:01
Operator : SJ/MA
Sample : I2230-08
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-4-CHAR

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	2.481	50	52	63	rVB	74775	181123	1.12%	0.254%
2	3.144	108	110	130	rBV	1149596	2367779	14.58%	3.323%
3	4.218	198	204	206	rBV	6307517	16243539	100.00%	22.799%
4	4.470	223	226	229	rBV	2782843	3806412	23.43%	5.343%
5	4.893	261	263	276	rVB2	105354	358770	2.21%	0.504%
6	5.316	298	300	315	rBV	3786611	5721420	35.22%	8.030%
7	6.333	386	389	391	rBV	2477389	2529713	15.57%	3.551%
8	6.379	391	393	400	rVV	1794452	3747811	23.07%	5.260%
9	6.482	400	402	416	rVB	4654318	5434423	33.46%	7.628%
10	6.710	420	422	430	rVB	998806	1165485	7.18%	1.636%
11	6.859	433	435	438	rBV	3897471	3980228	24.50%	5.587%
12	6.939	440	442	447	rVV	202511	264338	1.63%	0.371%
13	7.019	447	449	462	rVB	649827	782409	4.82%	1.098%
14	7.282	470	472	484	rBV	3108789	3827060	23.56%	5.372%
15	7.476	487	489	495	rBV	691269	952633	5.86%	1.337%
16	7.853	519	522	533	rBV	661005	921488	5.67%	1.293%
17	8.002	533	535	545	rVB	1466740	1747821	10.76%	2.453%
18	8.527	578	581	591	rBV2	240552	570996	3.52%	0.801%
19	8.825	604	607	609	rBV	1443186	1282386	7.89%	1.800%
20	9.076	626	629	632	rBV	4306468	5917157	36.43%	8.305%
21	9.762	686	689	696	rVB	571289	806138	4.96%	1.131%
22	10.551	756	758	761	rBV2	2315932	3007553	18.52%	4.221%
23	11.248	817	819	826	rBV	1207101	1320521	8.13%	1.853%
24	12.836	955	958	961	rBV	3608793	3972509	24.46%	5.576%
25	13.899	1049	1051	1060	rBV	190985	337056	2.08%	0.473%

Sum of corrected areas: 71246768

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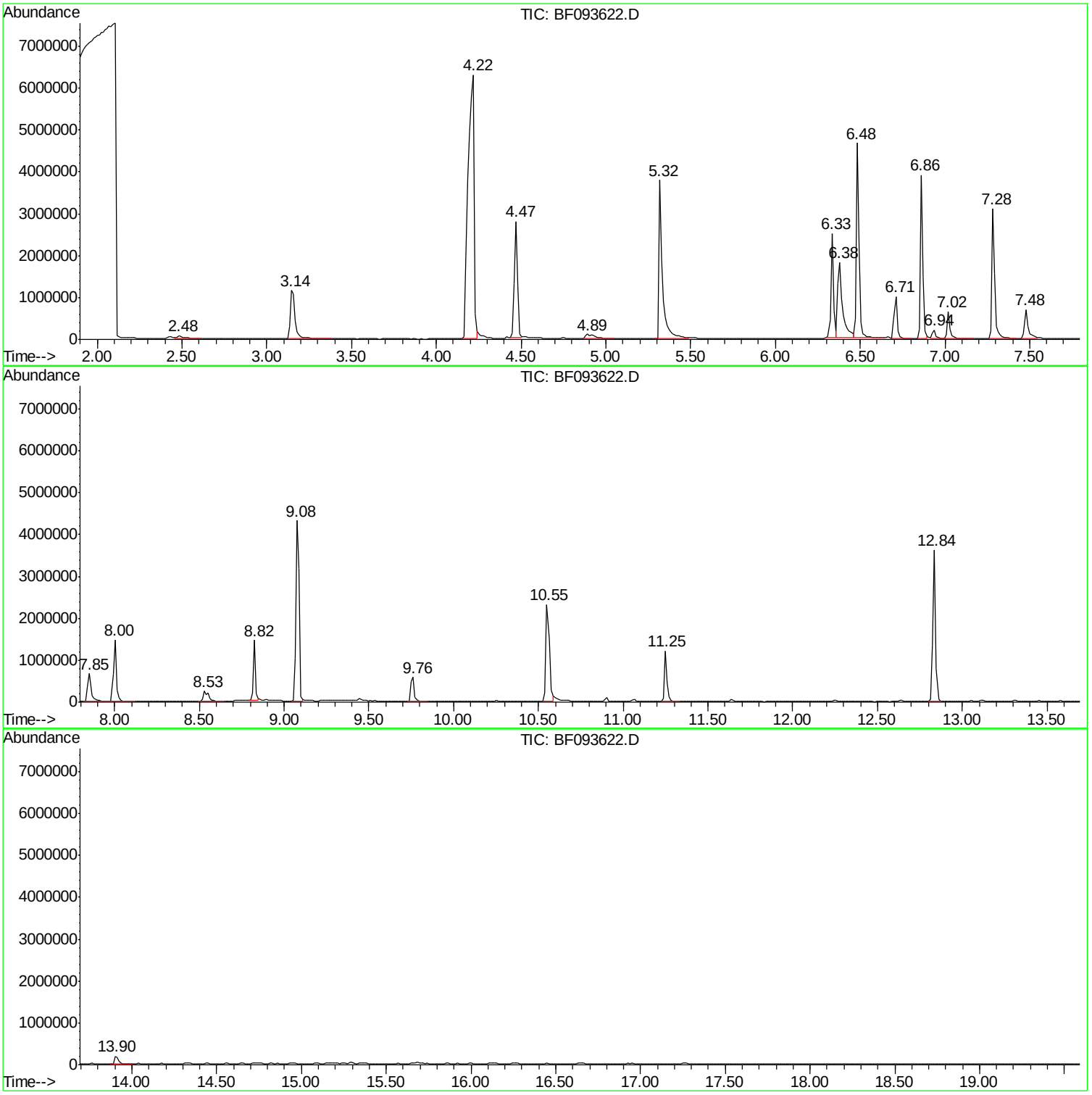
Instrument :
BNA_F
ClientSampleId :
COMPOSITE-4-CHAR

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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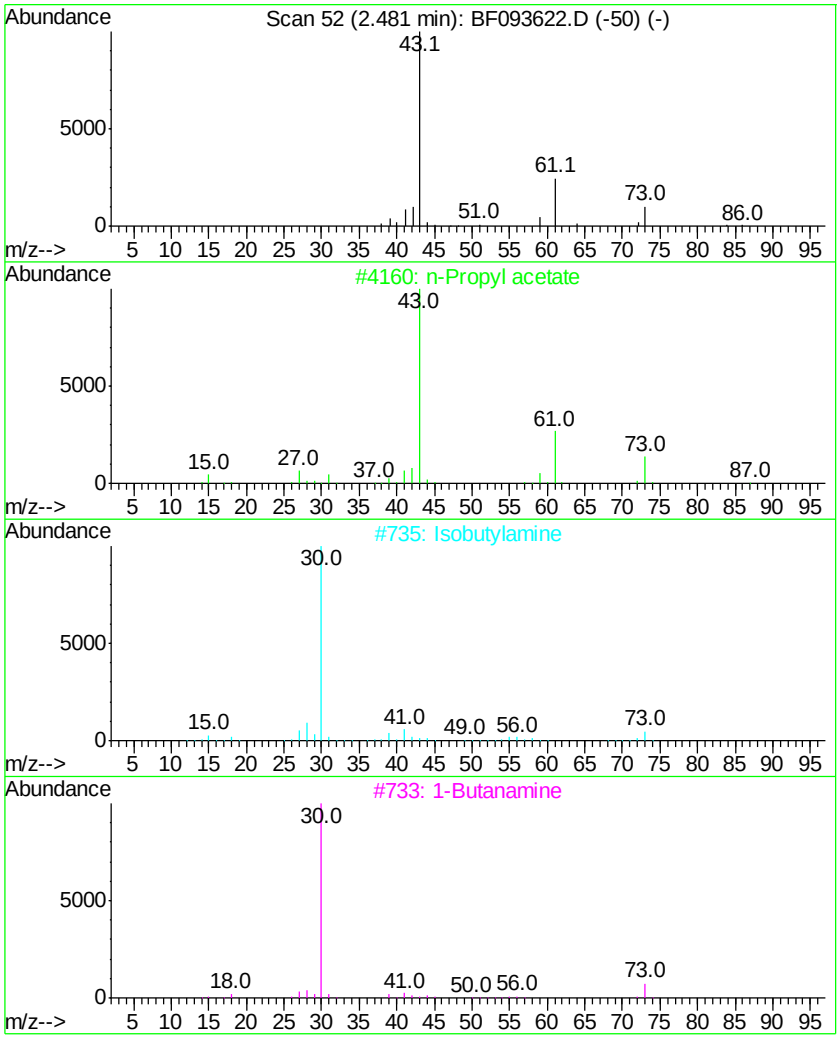
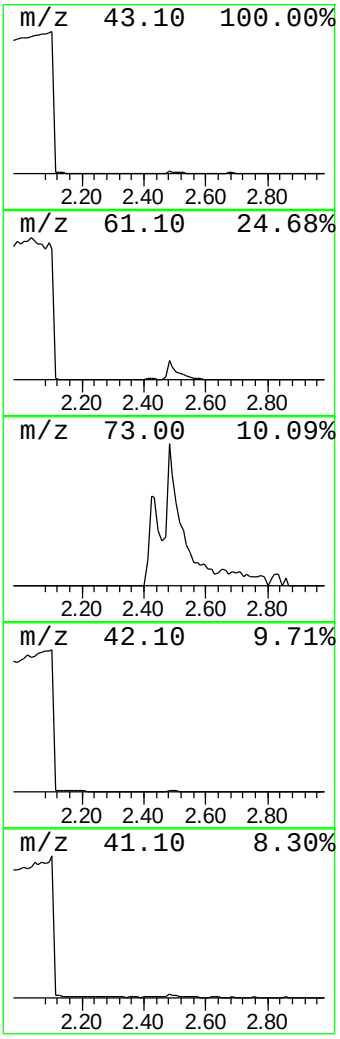
Peak Number 1 n-Propyl acetate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.48	3.11 ng	181123	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	Isobutylamine	73	C4H11N	000078-81-9	7
3	1-Butanamine	73	C4H11N	000109-73-9	5
4	Pentane	72	C5H12	000109-66-0	4
5	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4





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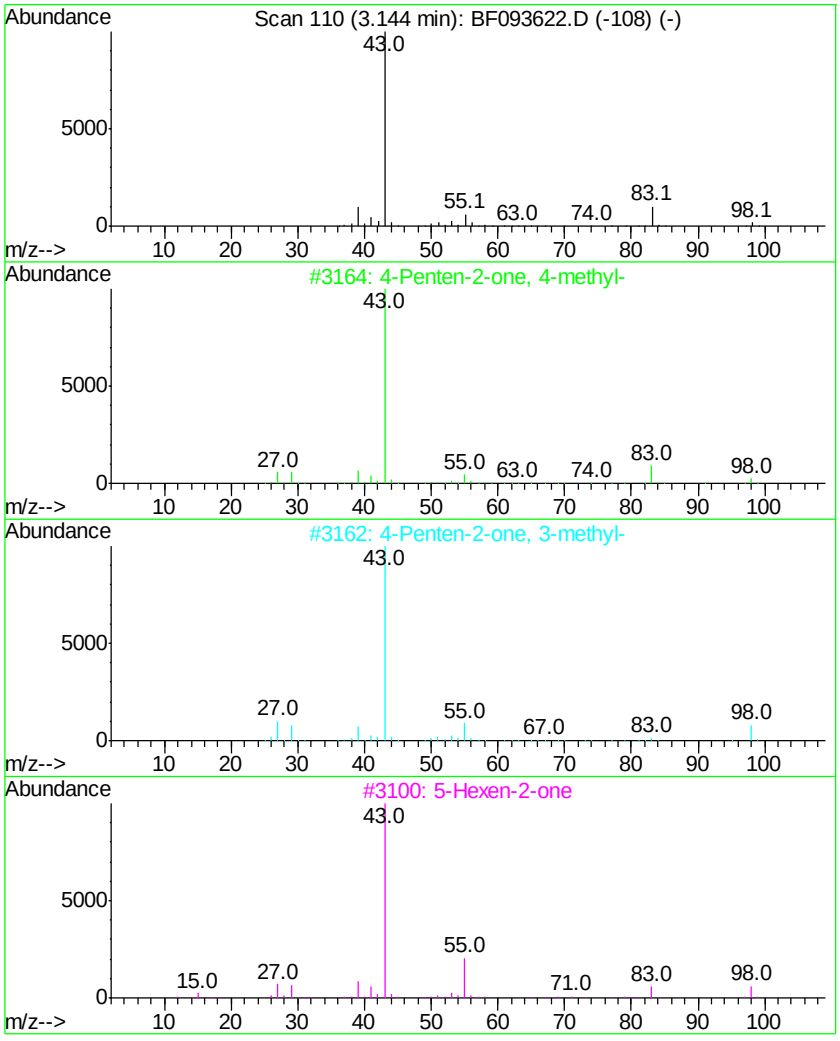
TIC Integration Parameters: LSCINT.P

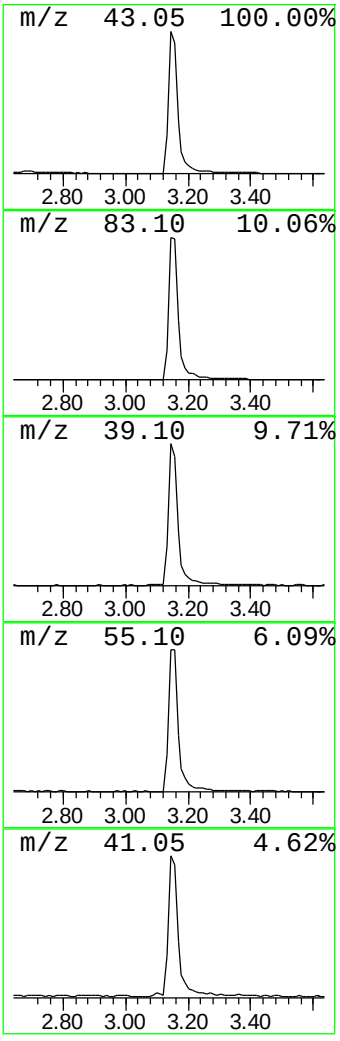
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.14	40.63 ng	2367780	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	72
2	4-Penten-2-one, 3-methyl-	98	C6H10O	000758-87-2	47
3	5-Hexen-2-one	98	C6H10O	000109-49-9	36
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	30
5	4-Hexen-2-one	98	C6H10O	025659-22-7	9





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Operator : SJ/MA
Sample : I2230-08
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Instrument : BNA_F
ClientSampleId : COMPOSITE-4-CHAR

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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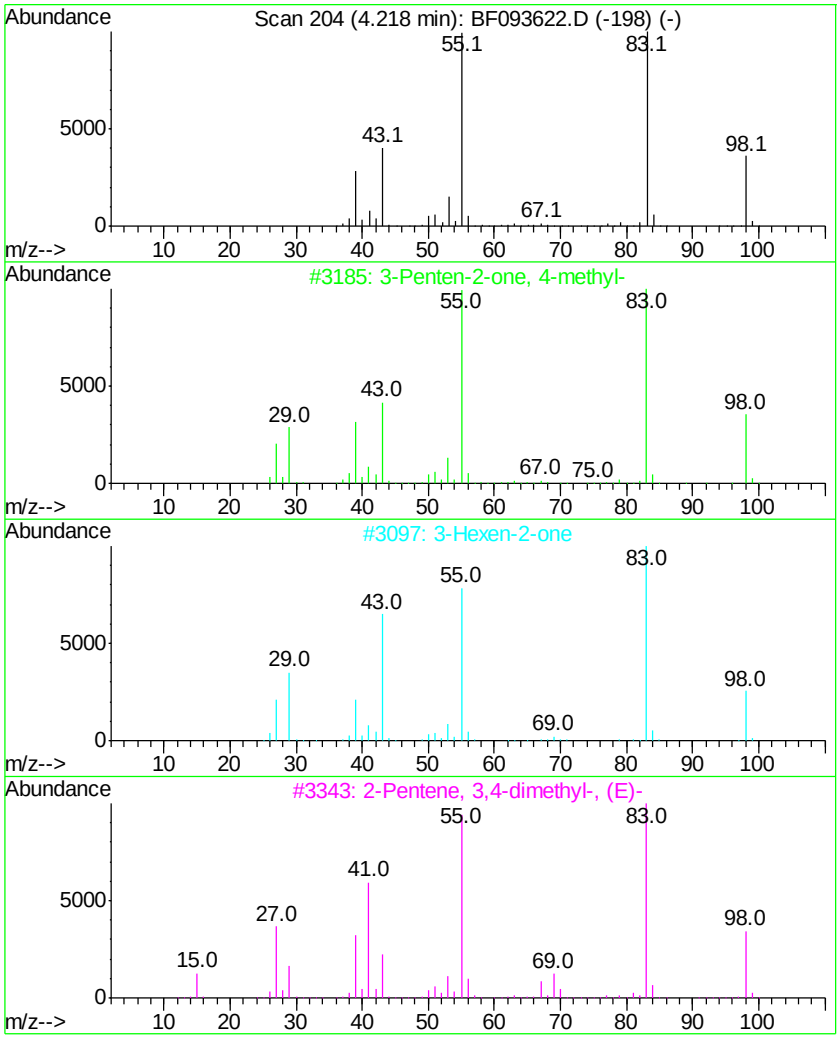
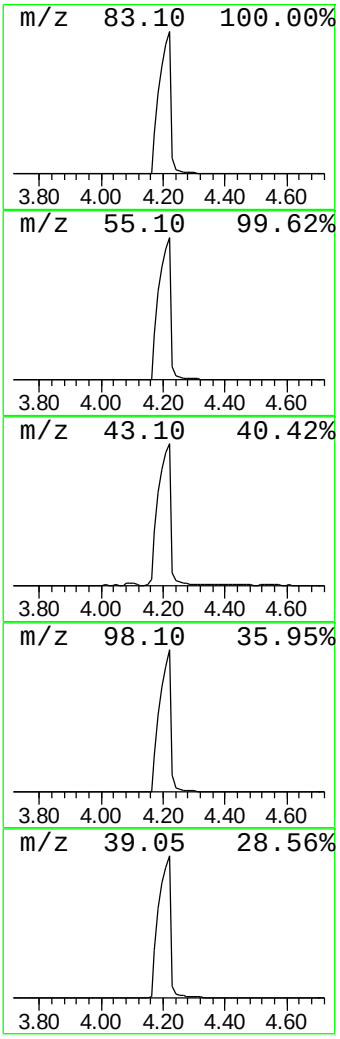
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.22	278.74 ng	16243500	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	95
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, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86





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Sample : I2230-08
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-4-CHAR

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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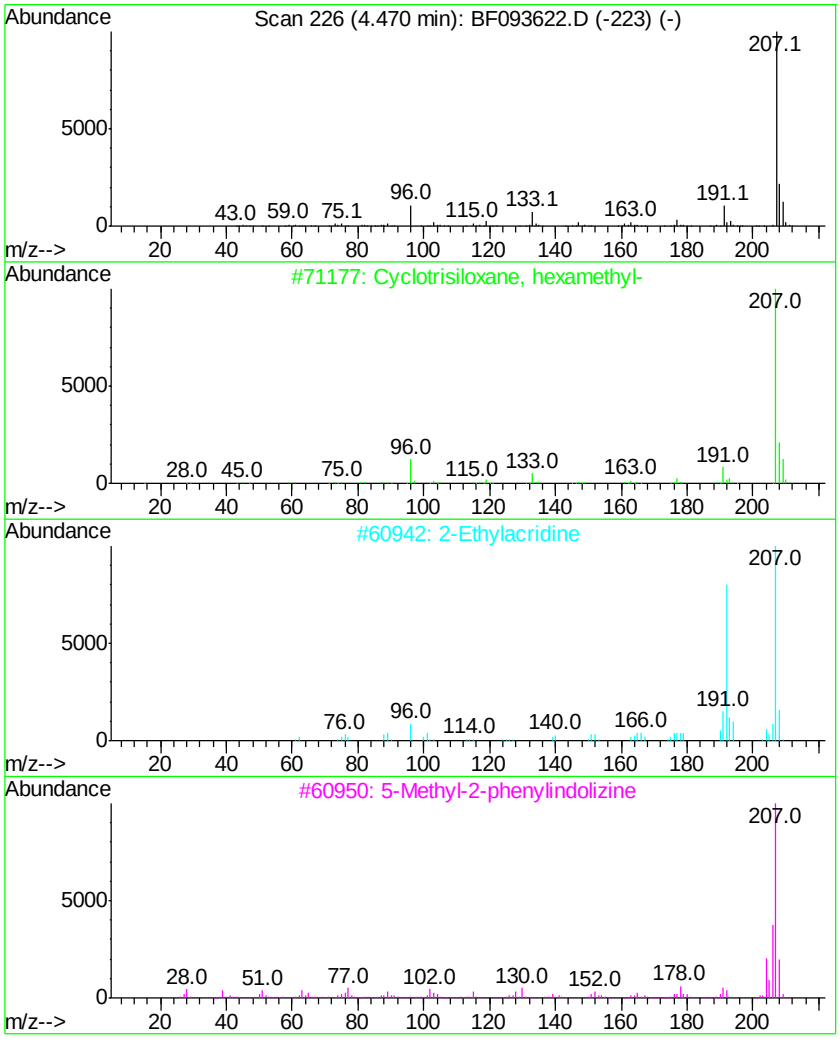
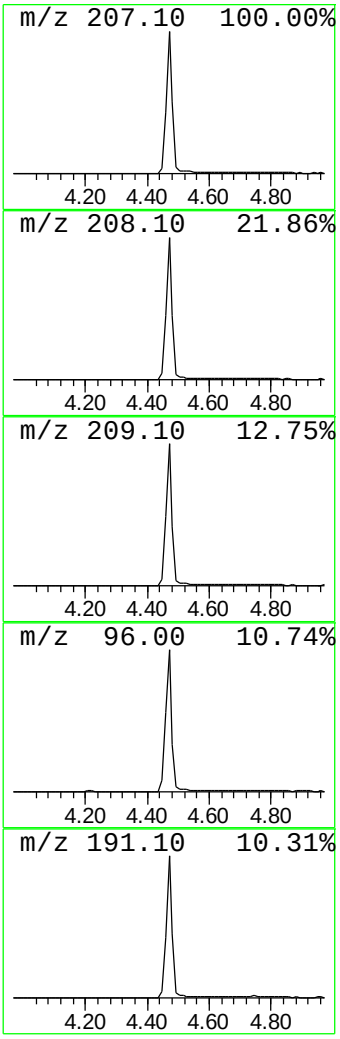
Peak Number 4 Cyclotrisiloxane, hexamethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.47	65.32 ng	3806410	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	2-Ethylacridine	207	C15H13N	055751-83-2	45
3	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	39
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	38
5	1,3,5-Triazine, 2-chloro-4,6-bis...	207	C5H6ClN3S2	004407-40-3	9





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Data File : BF093622.D
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Operator : SJ/MA
Sample : I2230-08
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-4-CHAR

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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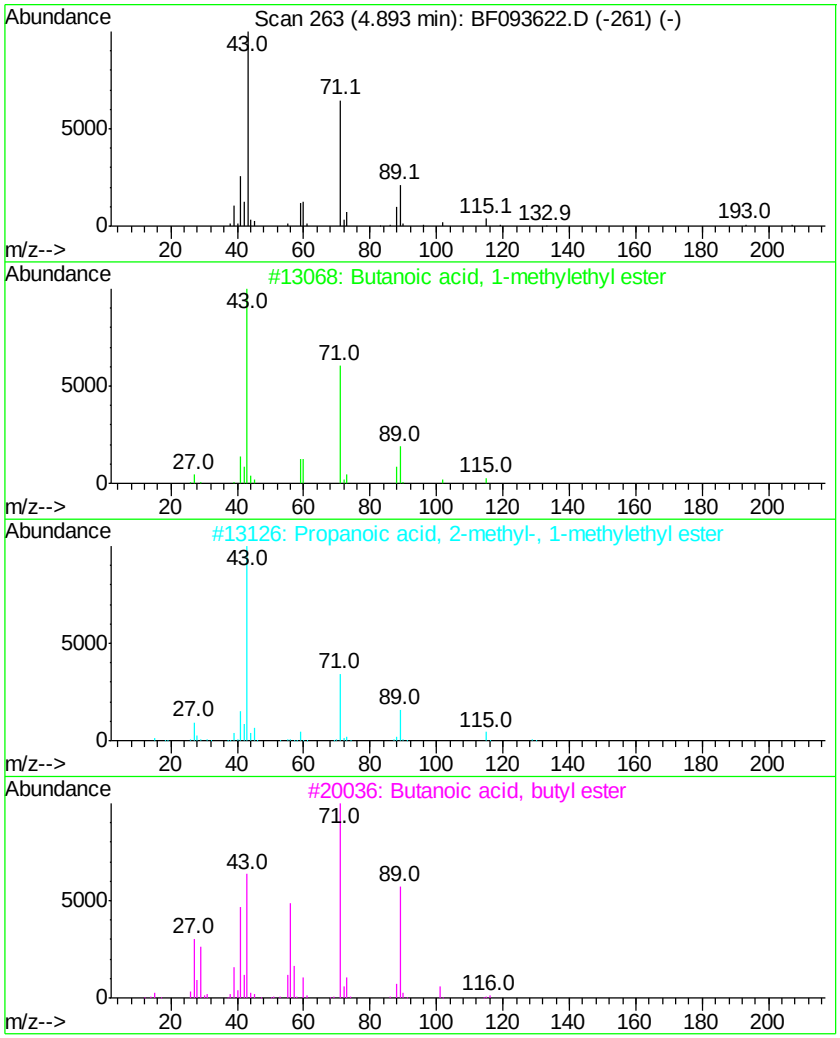
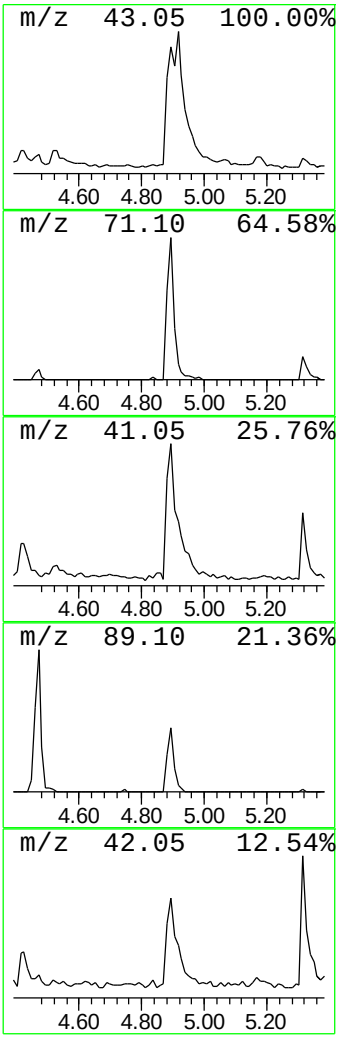
****

Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	6.16 ng	358770	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	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	64
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	53
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	45





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Instrument : BNA_F
ClientSampleId : COMPOSITE-4-CHAR

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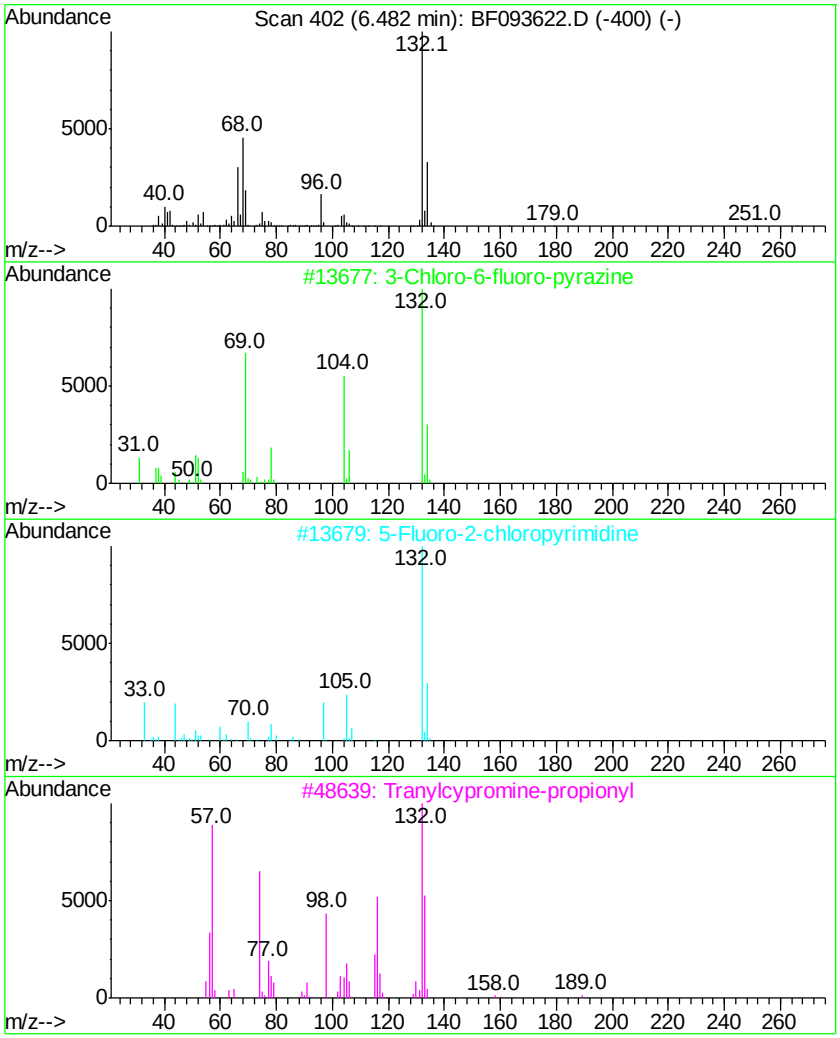
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

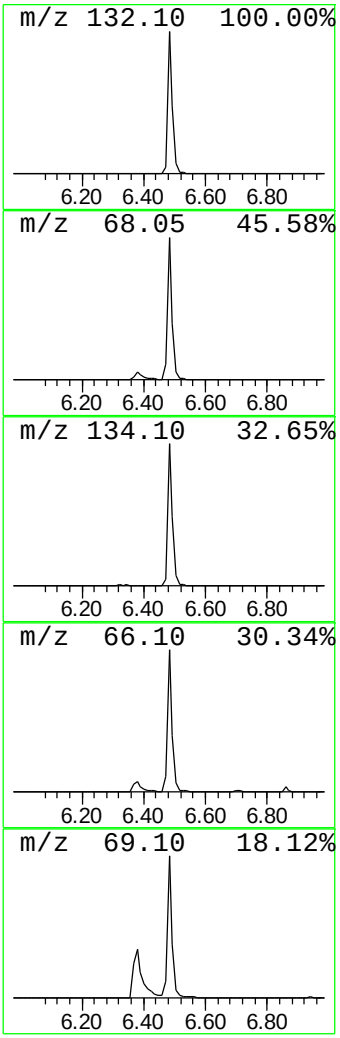
****

Peak Number 6 unknown6.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	93.26 ng	5434420	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	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
5	Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9





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Instrument : BNA_F
ClientSampleId : COMPOSITE-4-CHAR

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

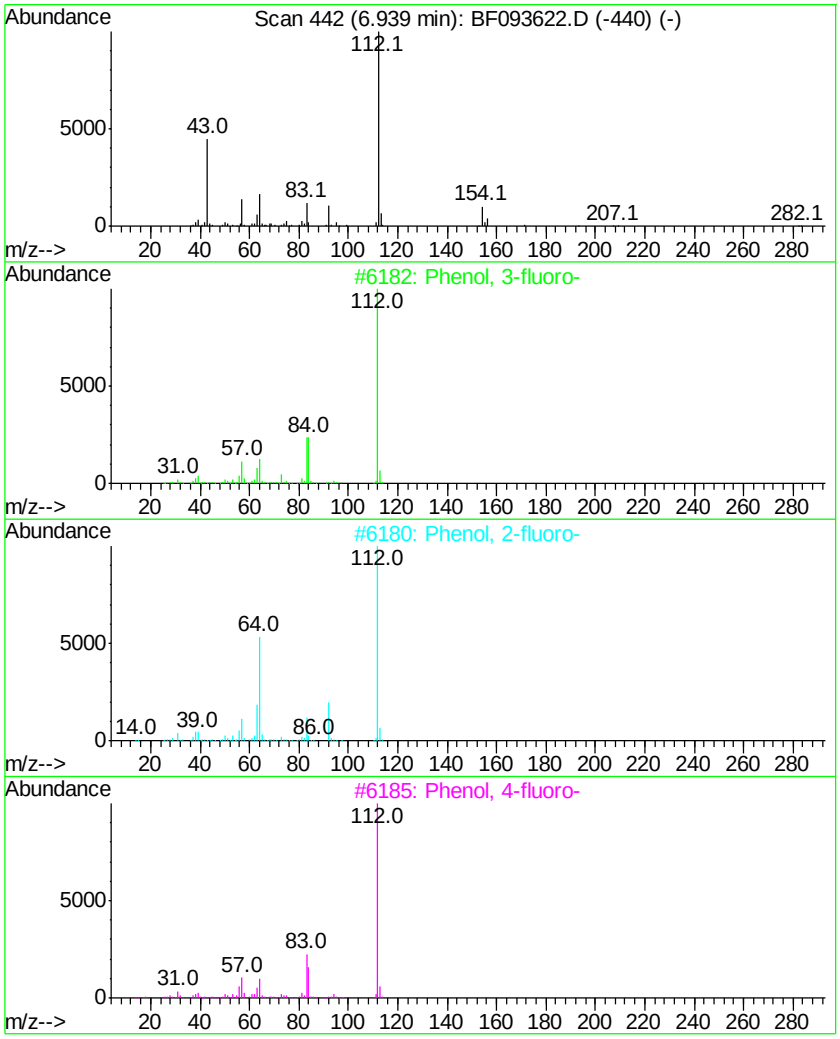
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

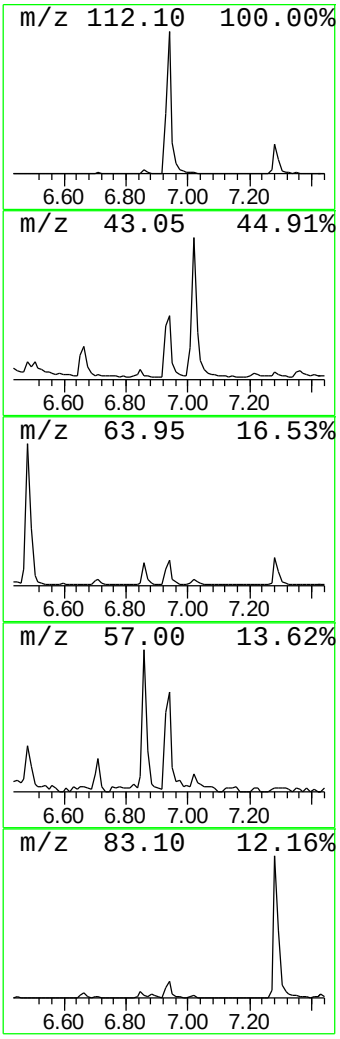
****

Peak Number 8 Phenol, 3-fluoro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	4.54 ng	264338	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-fluoro-	112	C6H5FO	000372-20-3	72
2	Phenol, 2-fluoro-	112	C6H5FO	000367-12-4	64
3	Phenol, 4-fluoro-	112	C6H5FO	000371-41-5	64
4	1,4-Cyclohexanedione	112	C6H8O2	000637-88-7	50
5	Benzene, 1-ethoxy-4-fluoro-	140	C8H9FO	000459-26-7	45





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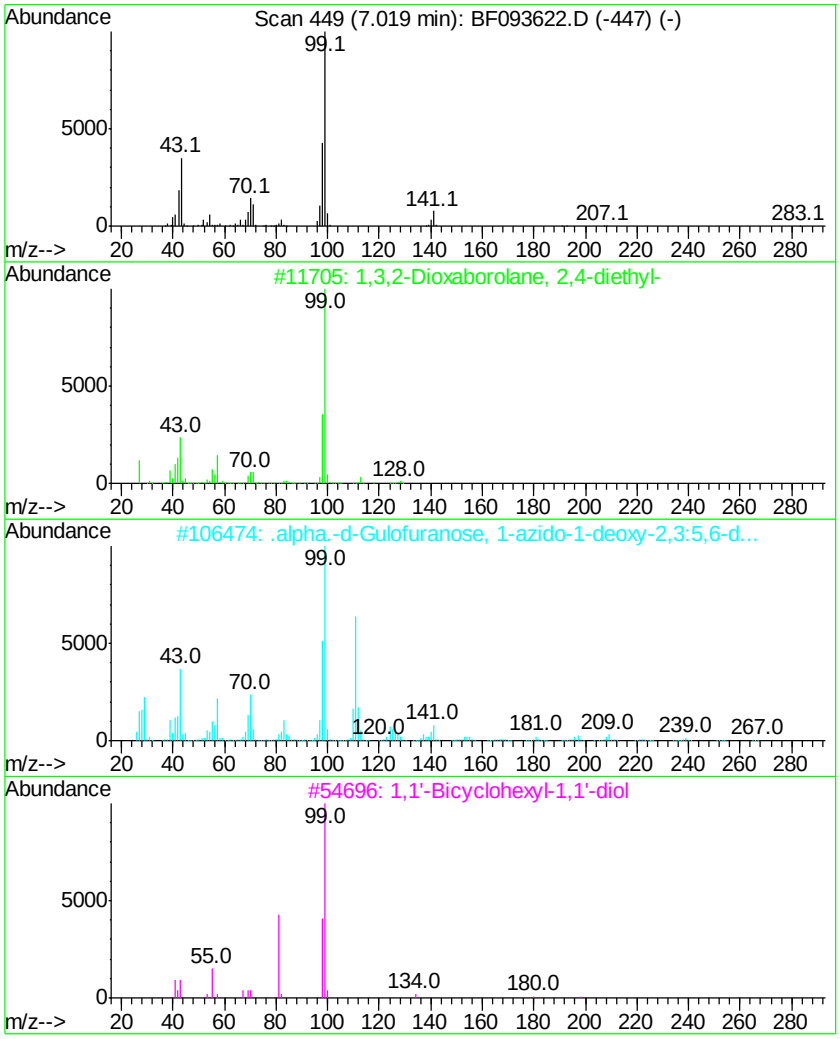
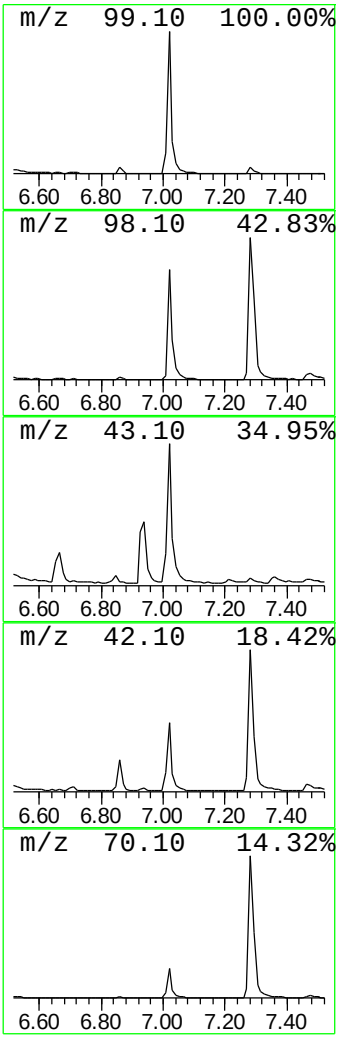
****

Peak Number 9 1,3,2-Dioxaborolane, 2,4-di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	13.43 ng	782409	1,4-Dichlorobenzene-d4	6.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,2-Dioxaborolane, 2,4-diethyl-	128	C6H13BO2	057633-63-3	56
2	.alpha.-d-Gulofuranose, 1-azido-...	281	C10H17B2N3O5	1000149-82-2	50
3	1,1'-Bicyclohexyl-1,1'-diol	198	C12H22O2	002888-11-1	38
4	2,2'-Bioxepane	198	C12H22O2	074793-02-5	38
5	Bis(2-ethylhexyl)hydrogen phosphate	322	C16H35O4P	000298-07-7	37





Library Search Compound Report

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

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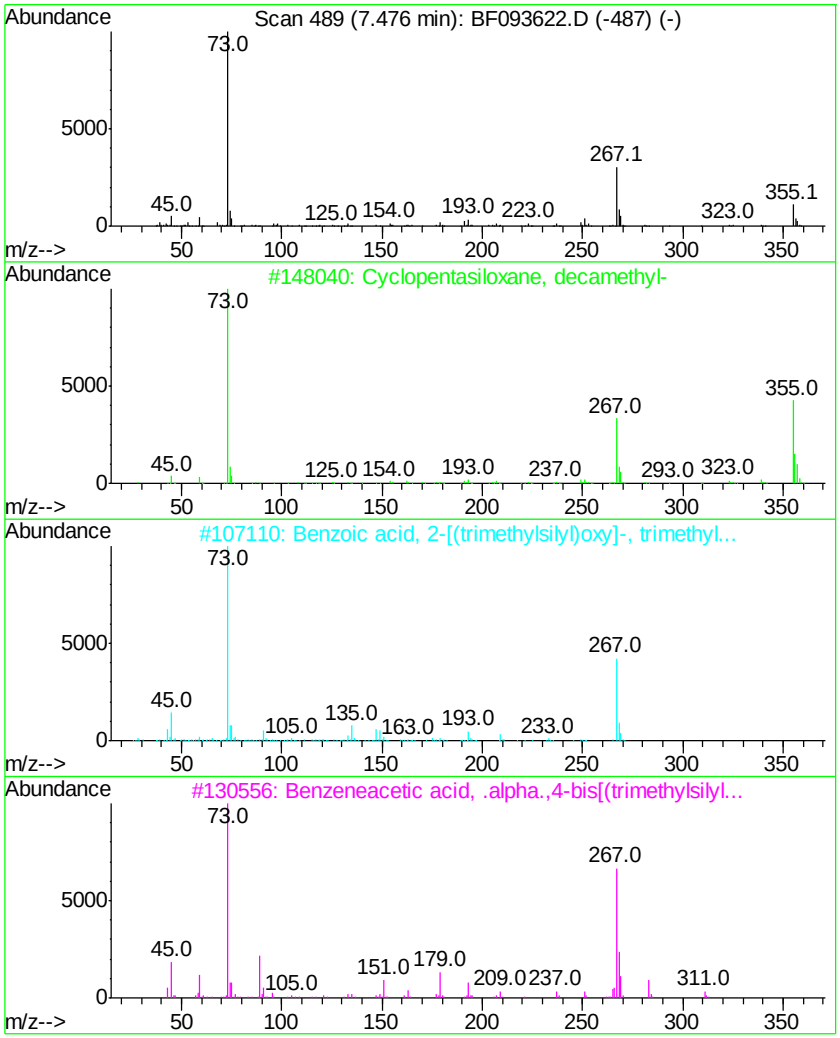
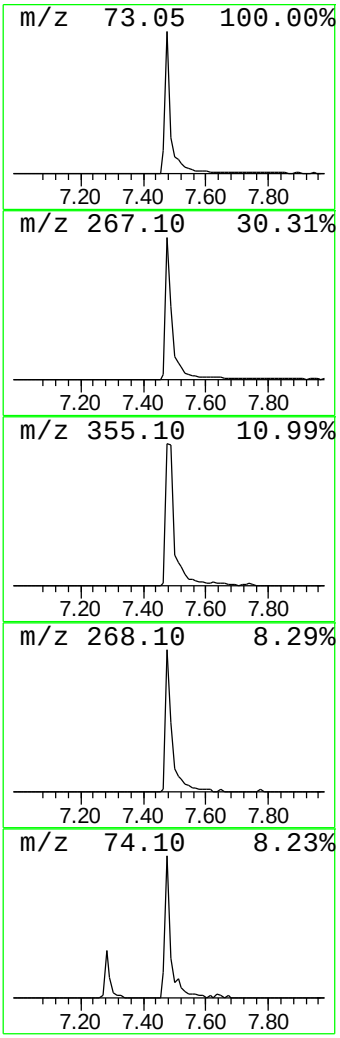
Peak Number 10 Cyclopentasiloxane, decamet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	10.90 ng	952633	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	91
2	Benzoic acid, 2-[(trimethylsilyl...	282	C13H22O3Si2	003789-85-3	33
3	Benzeneacetic acid, .alpha.,4-bi...	326	C15H26O4Si2	055334-40-2	30
4	Benzoic acid, 2,5-bis(trimethyls...	370	C16H30O4Si3	003618-20-0	22
5	Benzoic acid, 2,6-bis[(trimethyl...	370	C16H30O4Si3	003782-85-2	16





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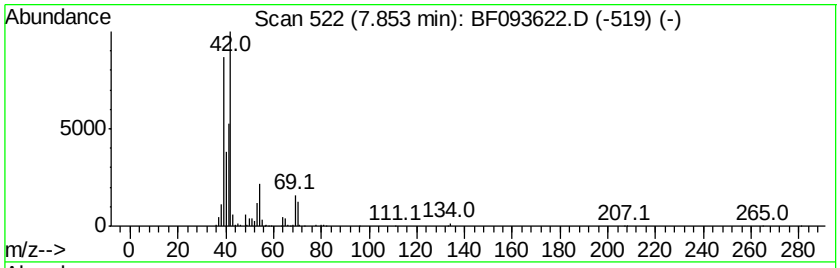
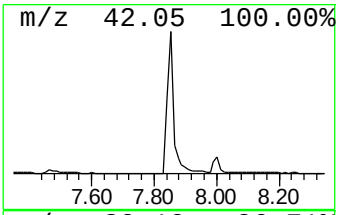
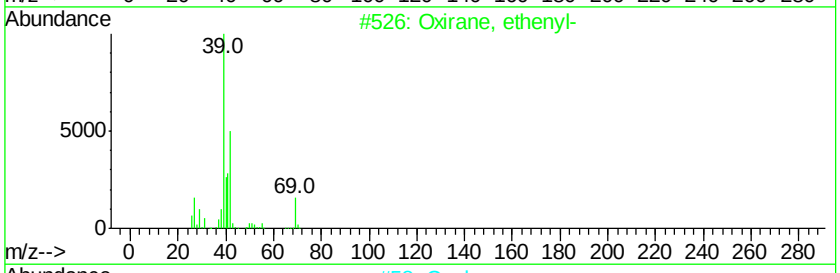
Peak Number 11 Oxirane, ethenyl- Concentration Rank 9

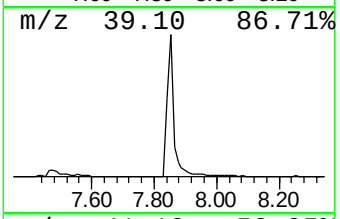
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.85	10.54 ng	921488	Naphthalene-d8	8.00

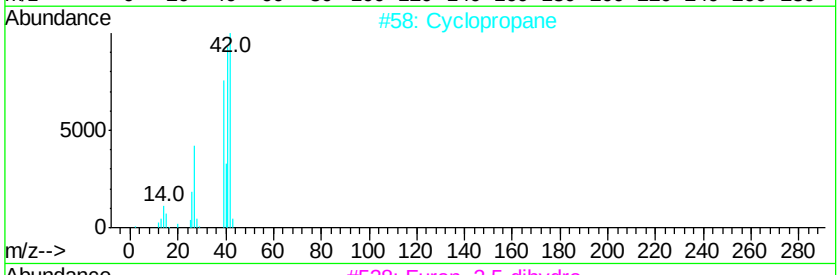
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, ethenyl-	70	C4H6O	000930-22-3	64
2	Cyclopropane	42	C3H6	000075-19-4	56
3	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	50
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	10
5	3-Aminopropionitrile	70	C3H6N2	000151-18-8	10

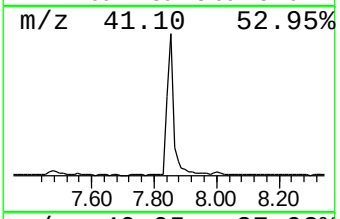


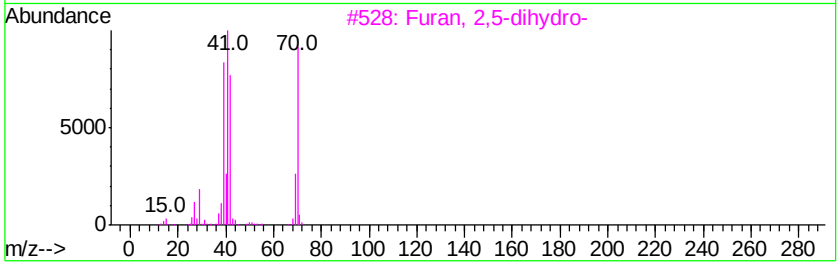


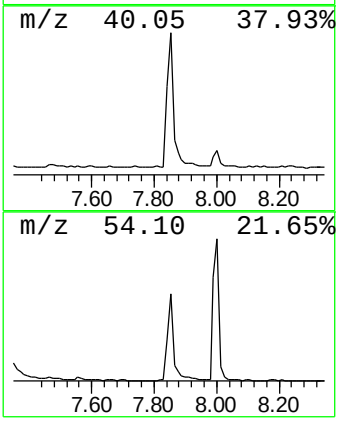












Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093622.D
Acq On : 13 Mar 2017 22:01
Operator : SJ/MA
Sample : I2230-08
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-4-CHAR

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

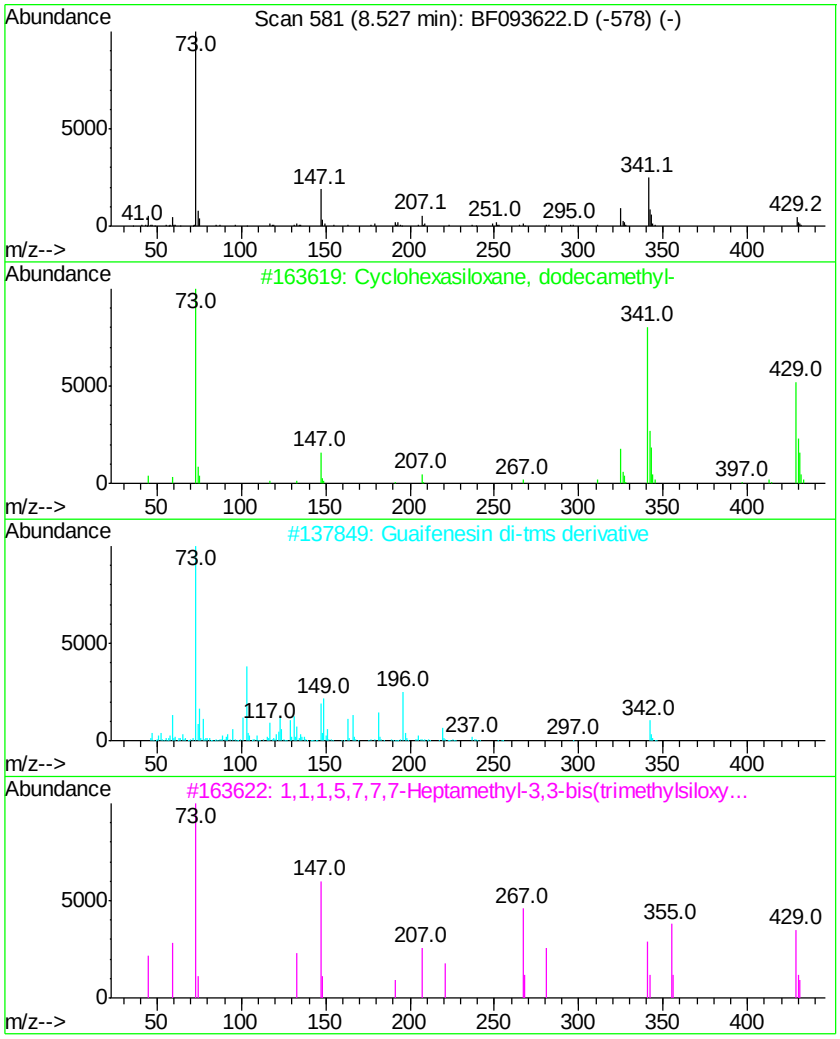
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

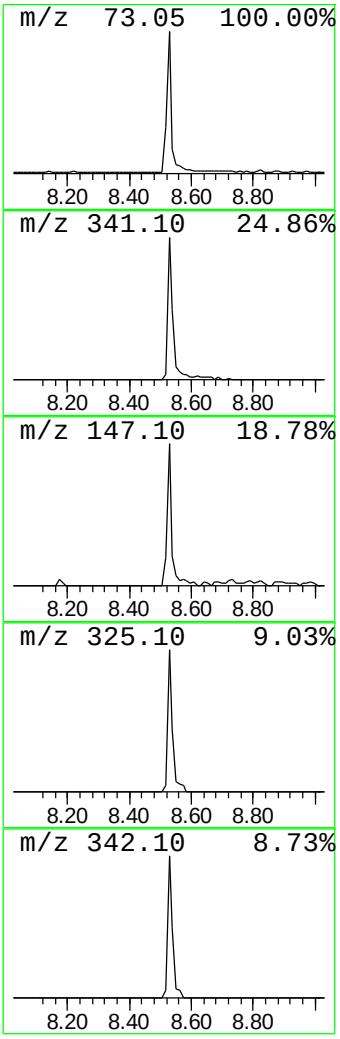
****

Peak Number 12 Cyclohexasiloxane, dodecame... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.53	6.53 ng	570996	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexasiloxane, dodecamethyl-	444	C12H36O6Si6	000540-97-6	91
2	Guaifenesin di-tms derivative	342	C16H30O4Si2	107966-19-8	17
3	1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	16
4	2,2'-Bis(trimethylsilyloxy)diphe...	344	C19H28O2Si2	097993-26-5	14
5	Octasiloxane, 1,1,3,3,5,5,7,7,9,...	578	C16H50O7Si8	019095-24-0	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF031317\
Data File : BF093622.D
Acq On : 13 Mar 2017 22:01
Operator : SJ/MA
Sample : I2230-08
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-4-CHAR

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

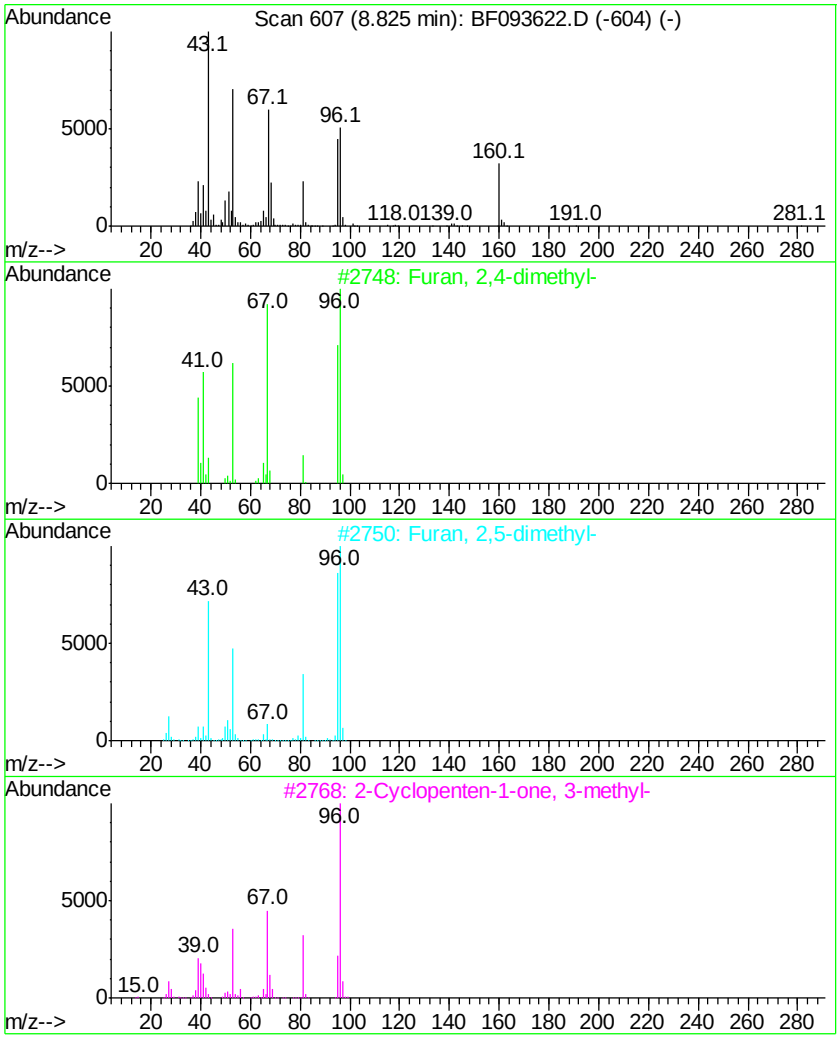
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

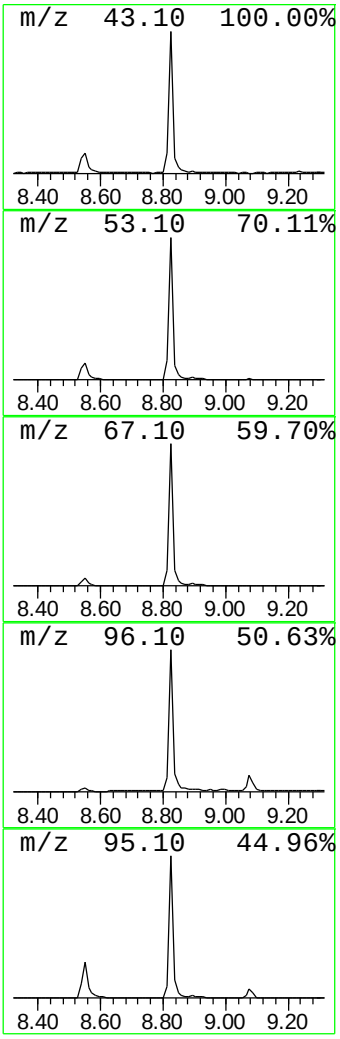
****

Peak Number 13 Furan, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.82	14.67 ng	1282390	Naphthalene-d8	8.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,4-dimethyl-	96	C6H8O	003710-43-8	80
2	Furan, 2,5-dimethyl-	96	C6H8O	000625-86-5	68
3	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	002758-18-1	53
4	1-Pentyn-3-one, 4-methyl-	96	C6H8O	013531-82-3	53
5	1-Butyne, 3-methyl-	68	C5H8	000598-23-2	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031317\
Data File : BF093622.D
Acq On : 13 Mar 2017 22:01
Operator : SJ/MA
Sample : I2230-08
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : COMPOSITE-4-CHAR

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	2.48	3.1	ng	181123	1	6.71	1165490	20.0
4-Penten-2-one, 4...	3.14	40.6	ng	2367780	1	6.71	1165490	20.0
3-Penten-2-one, 4...	4.22	278.7	ng	16243500	1	6.71	1165490	20.0
Cyclotrisiloxane,...	4.47	65.3	ng	3806410	1	6.71	1165490	20.0
Butanoic acid, 1-...	4.89	6.2	ng	358770	1	6.71	1165490	20.0
unknown6.48	6.48	93.3	ng	5434420	1	6.71	1165490	20.0
Phenol, 3-fluoro-	6.94	4.5	ng	264338	1	6.71	1165490	20.0
1,3,2-Dioxaborola...	7.02	13.4	ng	782409	1	6.71	1165490	20.0
Cyclopentasiloxan...	7.48	10.9	ng	952633	2	8.00	1747820	20.0
Oxirane, ethenyl-	7.85	10.5	ng	921488	2	8.00	1747820	20.0
Cyclohexasiloxane...	8.53	6.5	ng	570996	2	8.00	1747820	20.0
Furan, 2,4-dimethyl-	8.82	14.7	ng	1282390	2	8.00	1747820	20.0