LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099392.D
Acq On : 12 Oct 2017 13:37
Operator : SJ/JU
Sample : I5758-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB8

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-BF092317.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	2.175	12	15	46	rVB4	95547	307386	9.00%	1.149%
2	2.381	47	50	58	rVB	45419	69541	2.04%	0.260%
3	3.487	236	238	254	rBV	16082	53838	1.58%	0.201%
4	5.092	507	511	526	rBV	370971	563404	16.49%	2.105%
5	5.487	573	578	581	rBV	2734563	2953395	86.46%	11.036%
6	6.492	743	749	752	rBV	2585214	3034681	88.84%	11.340%
7	6.628	767	772	775	rBV	3034919	3060892	89.61%	11.438%
8	6.851	807	810	814	rBV	785688	620266	18.16%	2.318%
9	7.010	832	837	840	rBV	2588420	2426333	71.03%	9.067%
10	7.422	901	907	910	rBV	1830122	1952833	57.17%	7.297%
11	8.133	1023	1028	1031	rBV	991638	852226	24.95%	3.185%
12	9.210	1205	1211	1214	rBV	3518221	3415975	100.00%	12.765%
13	9.598	1273	1277	1282	rBV	511620	416272	12.19%	1.555%
14	9.886	1322	1326	1330	rBV2	1073989	901718	26.40%	3.369%
15	10.680	1456	1461	1464	rBV	1781325	1714378	50.19%	6.406%
16	10.774	1475	1477	1484	rVB	40438	42331	1.24%	0.158%
17	11.374	1575	1579	1582	rBV	943327	793176	23.22%	2.964%
18	12.957	1843	1848	1851	rBV	2425047	2293966	67.15%	8.572%
19	13.833	1994	1997	2010	rBV2	92525	118927	3.48%	0.444%
20	14.010	2024	2027	2031	rBV	571220	490347	14.35%	1.832%
21	14.621	2127	2131	2136	rVB	168563	150639	4.41%	0.563%
22	15.480	2272	2277	2287	rBV	439888	528957	15.48%	1.977%

Sum of corrected areas: 26761481

LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
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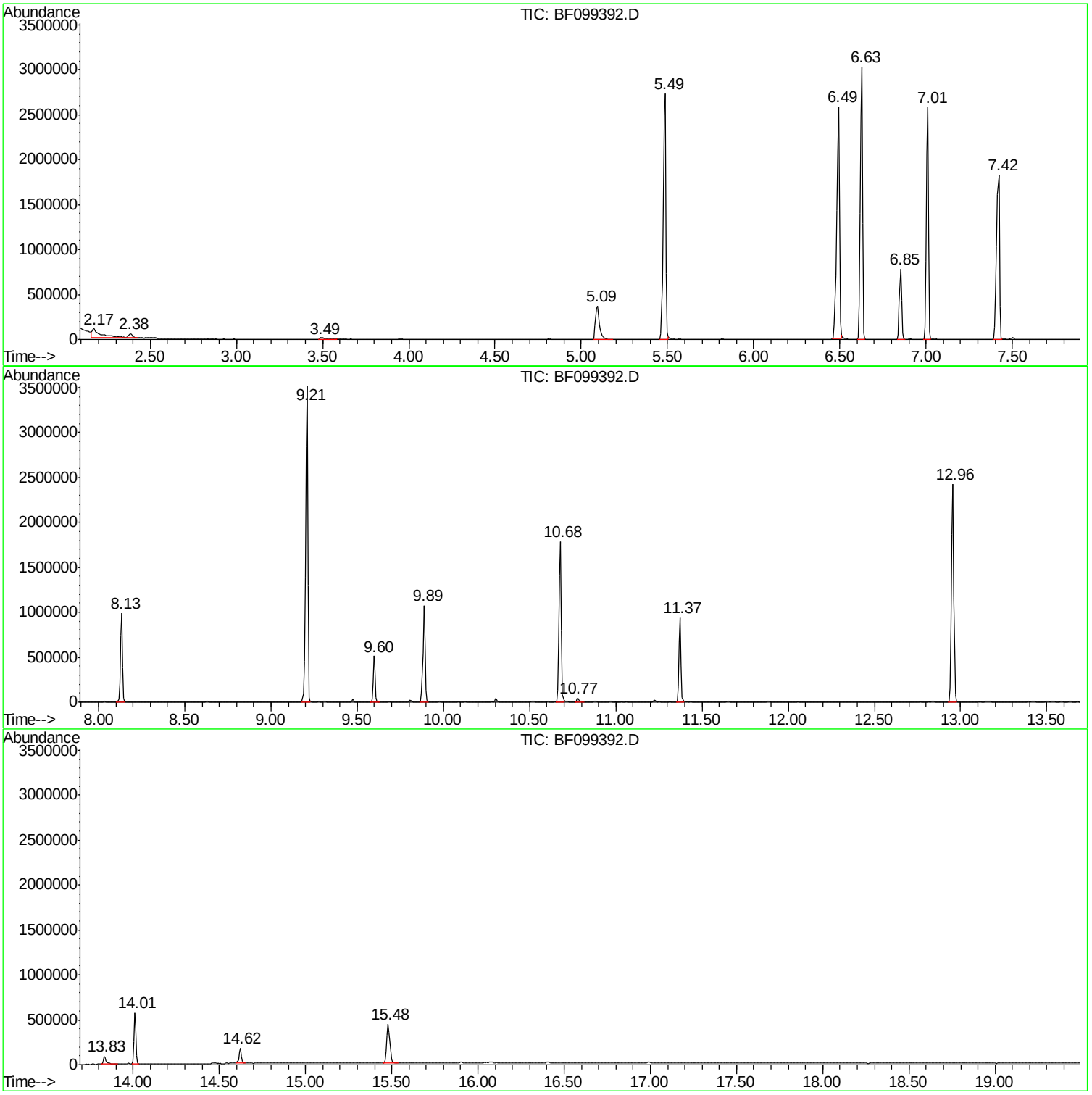
Operator : SJ/JU
Sample : I5758-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099392.D
Acq On : 12 Oct 2017 13:37
Operator : SJ/JU
Sample : I5758-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

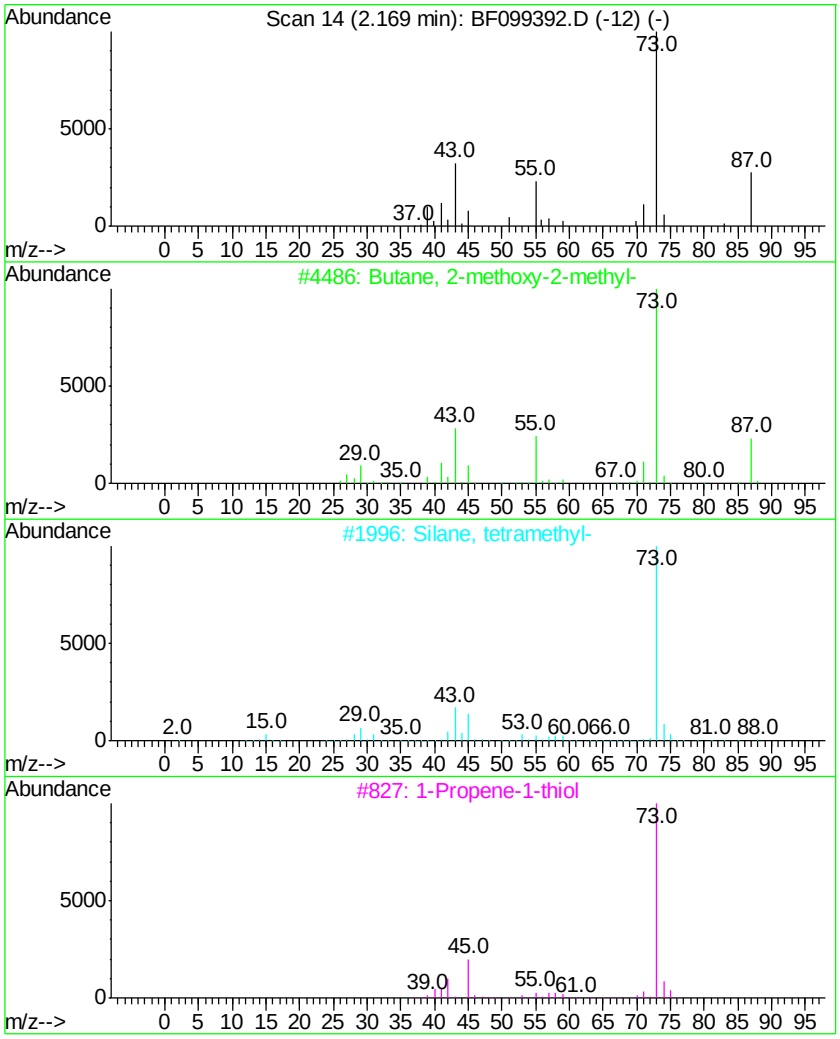
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

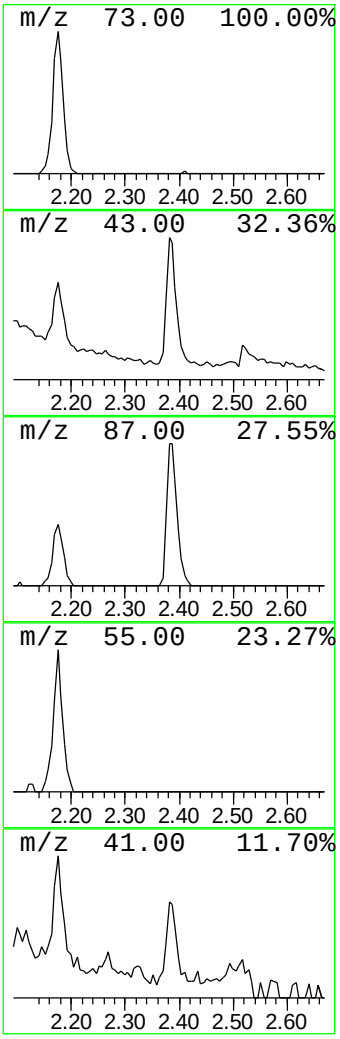
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	9.91 ng	307386	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3	1-Propene-1-thiol	74	C3H6S	000925-89-3	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	1,4-Butanediamine	88	C4H12N2	000110-60-1	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099392.D
Acq On : 12 Oct 2017 13:37
Operator : SJ/JU
Sample : I5758-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

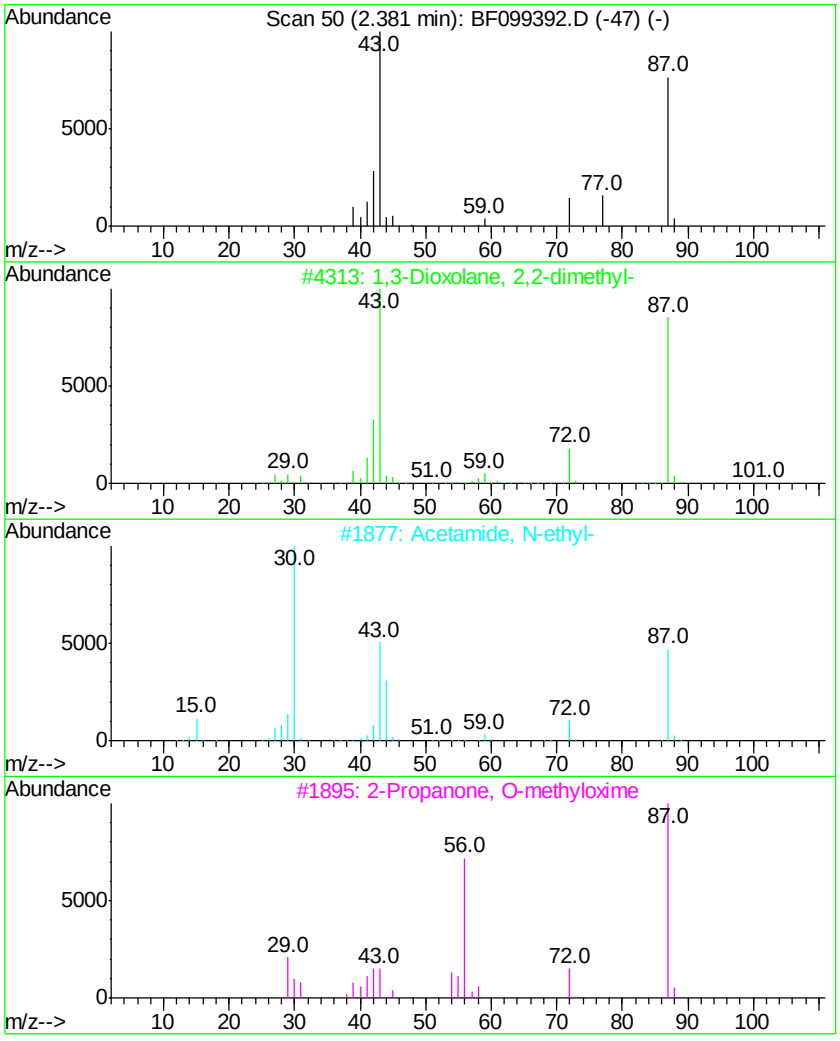
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

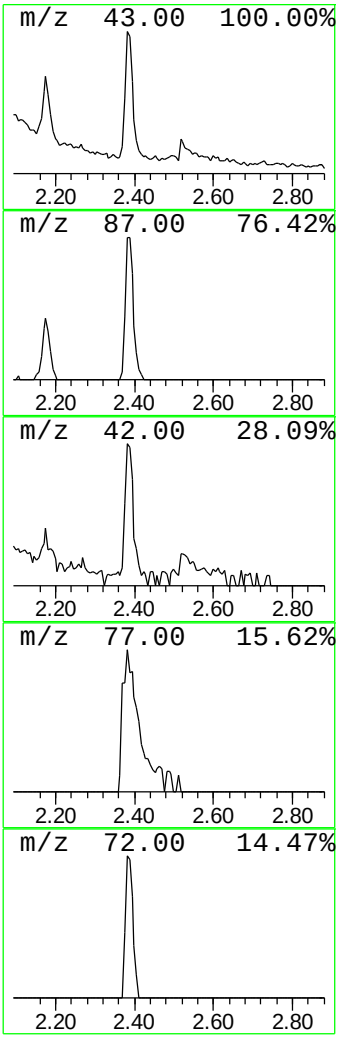
****

Peak Number 2 1,3-Dioxolane, 2,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.38	2.24 ng	69541	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2-dimethyl-	102	C5H10O2	002916-31-6	78
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50
3	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	42
4	Ethanol, 2,2'-oxybis-, diacetate	190	C8H14O5	000628-68-2	38
5	Morpholine	87	C4H9NO	000110-91-8	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099392.D
Acq On : 12 Oct 2017 13:37
Operator : SJ/JU
Sample : I5758-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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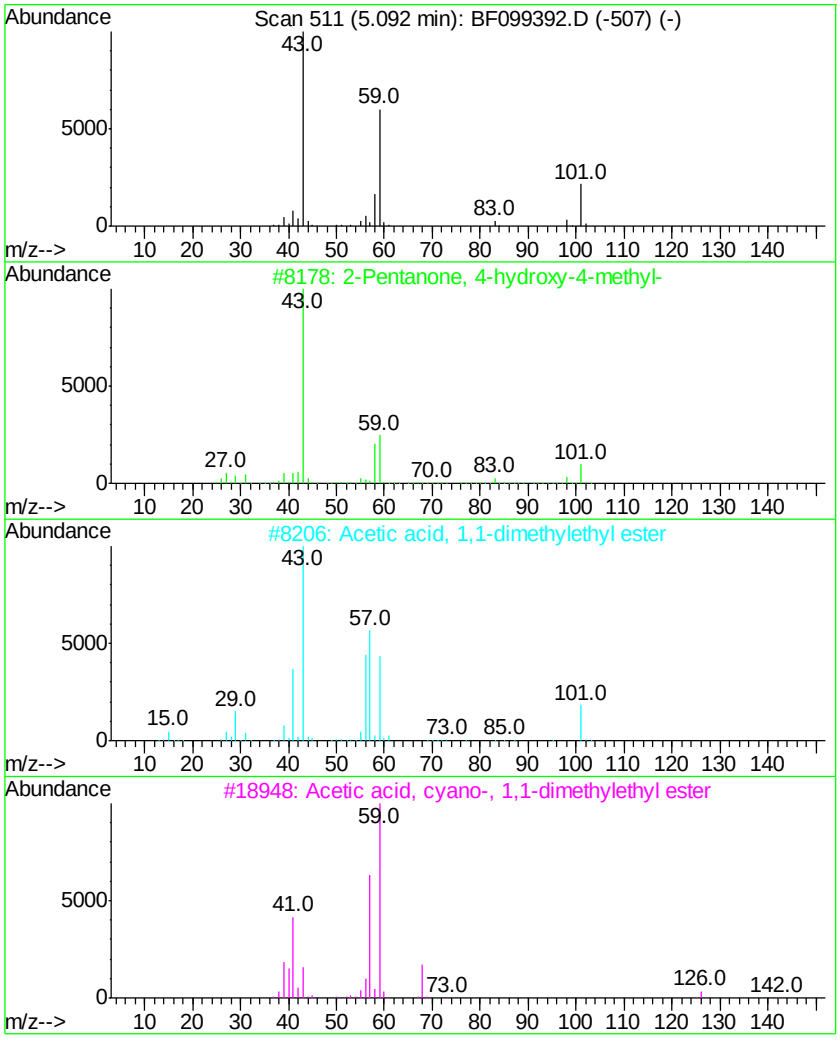
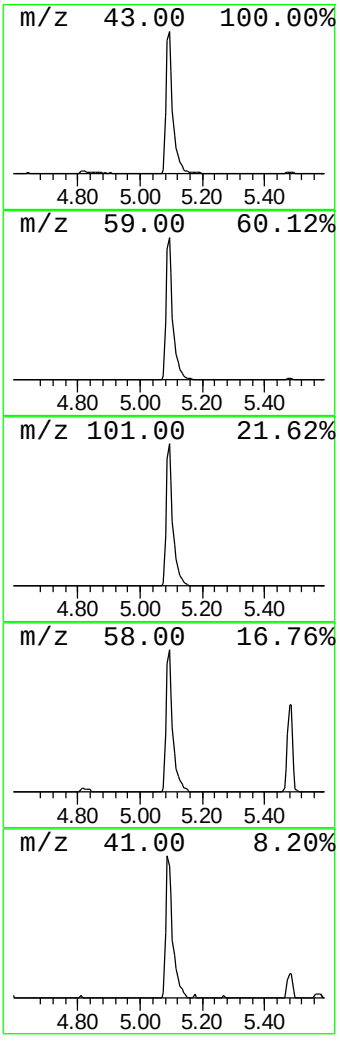
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	18.17 ng	563404	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
Data File : BF099392.D
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Operator : SJ/JU
Sample : I5758-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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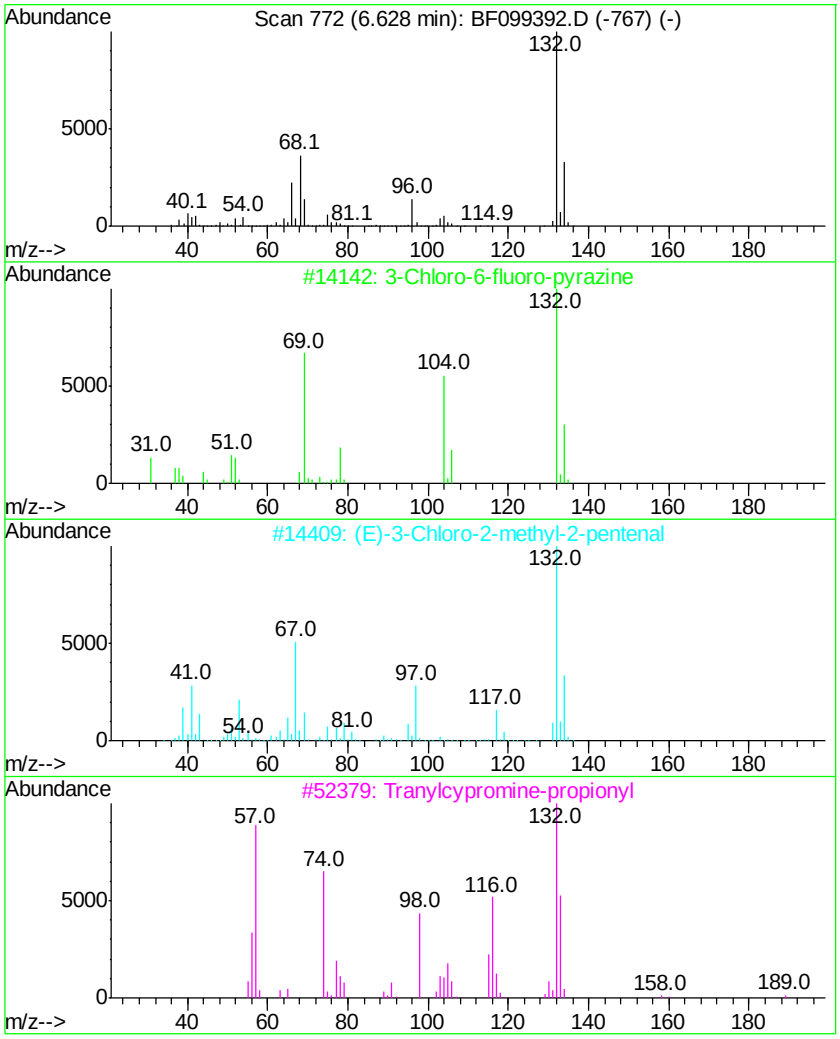
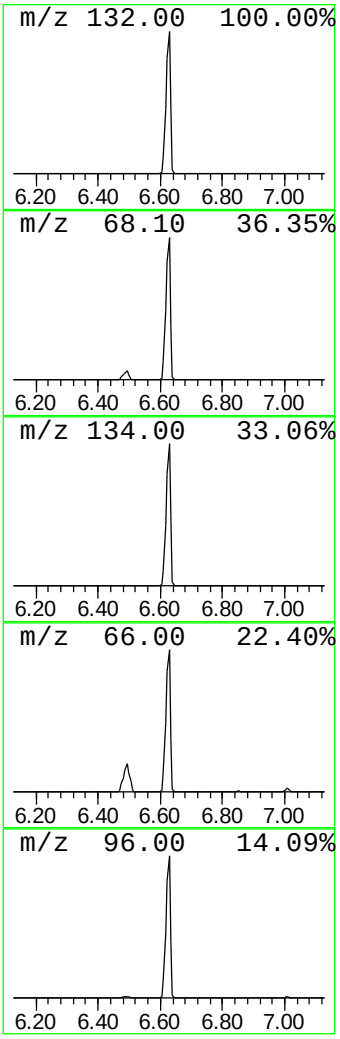
Peak Number 4 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	98.70 ng	3060890	1,4-Dichlorobenzene-d4	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF101217\
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Operator : SJ/JU
Sample : I5758-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

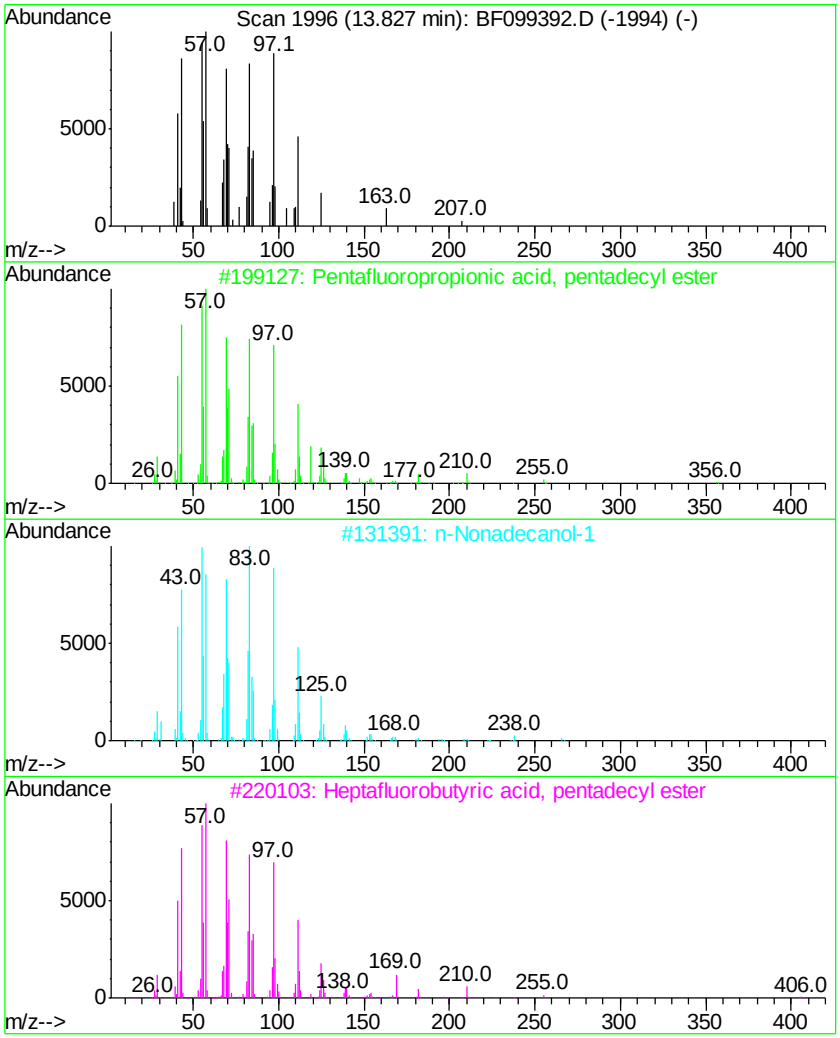
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

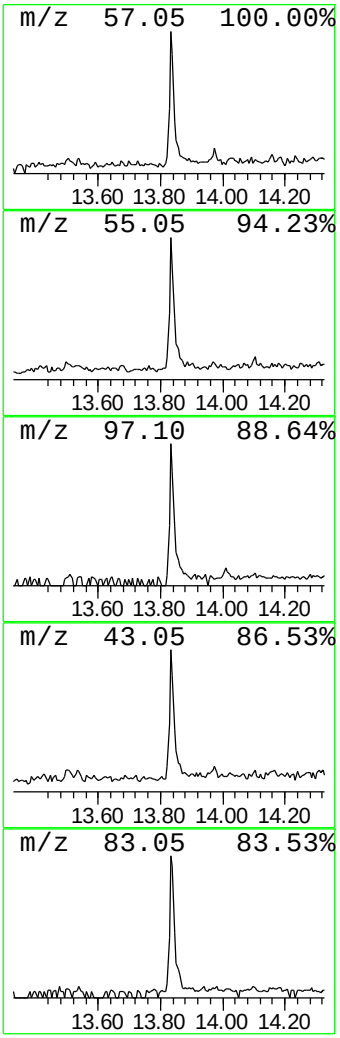
****

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.83	4.85 ng	118927	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
4	Behenic alcohol	326	C22H46O	000661-19-8	95
5	1-Heneicosanol	312	C21H44O	015594-90-8	95





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Operator : SJ/JU
Sample : I5758-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB8

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

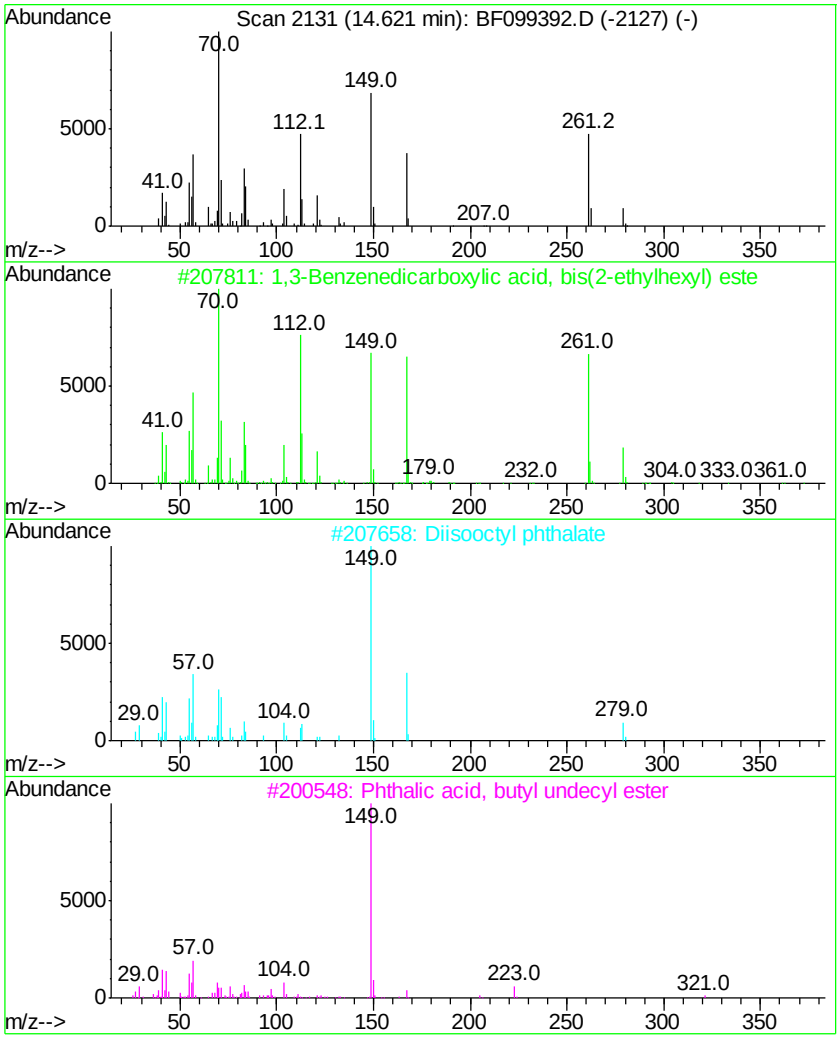
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

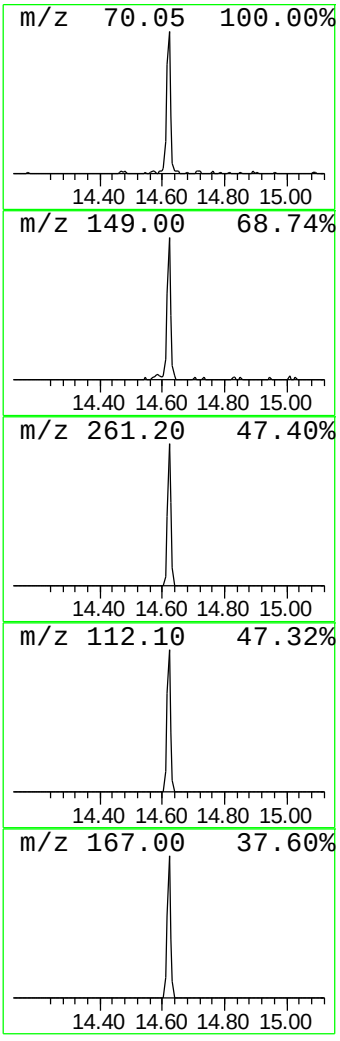
****

Peak Number 7 unknown14.62 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	6.14 ng	150639	Chrysene-d12	14.01

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	49
2	Diisooctyl phthalate	390	C24H38O4	000131-20-4	22
3	Phthalic acid, butyl undecyl ester	376	C23H36O4	1000308-91-2	22
4	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	14
5	Cyclohexanamine, N-methyl-	113	C7H15N	000100-60-7	14





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.17	9.9	ng	307386	1	6.85	620266	20.0
1,3-Dioxolane, 2,...	2.38	2.2	ng	69541	1	6.85	620266	20.0
2-Pentanone, 4-hy...	5.09	18.2	ng	563404	1	6.85	620266	20.0
unknown6.63	6.63	98.7	ng	3060890	1	6.85	620266	20.0
Pentafluoropropio...	13.83	4.8	ng	118927	5	14.01	490347	20.0
unknown14.62	14.62	6.1	ng	150639	5	14.01	490347	20.0