LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100517.D
Acq On : 13 Nov 2017 22:15
Operator : SJ/JU
Sample : I6388-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

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-BF110817.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	5.122	511	516	527	rBB	209290	269621	15.98%	1.947%
2	5.516	577	583	586	rBV	1429625	1438104	85.25%	10.387%
3	6.516	748	753	761	rBB	1451337	1500560	88.95%	10.838%
4	6.663	773	778	781	rBV	1624186	1501494	89.01%	10.845%
5	6.892	813	817	820	rVB	574333	446065	26.44%	3.222%
6	7.051	839	844	847	rBB	1302530	1177189	69.78%	8.503%
7	7.451	907	912	915	rBV	936761	883332	52.36%	6.380%
8	8.175	1031	1035	1038	rBV	686431	562470	33.34%	4.063%
9	8.728	1125	1129	1132	rBB	72972	63243	3.75%	0.457%
10	9.245	1212	1217	1220	rBV	1873015	1686913	100.00%	12.184%
11	9.639	1280	1284	1287	rBV	147680	122525	7.26%	0.885%
12	9.928	1329	1333	1337	rBV2	647601	541429	32.10%	3.911%
13	10.639	1450	1454	1457	rBB	197624	151827	9.00%	1.097%
14	10.716	1463	1467	1470	rBV	953523	768828	45.58%	5.553%
15	11.416	1582	1586	1589	rBV	556725	456373	27.05%	3.296%
16	11.927	1670	1673	1676	rBV	27538	22016	1.31%	0.159%
17	12.998	1851	1855	1858	rBV	1435081	1198941	71.07%	8.660%
18	13.880	2002	2005	2013	rBV	138168	137114	8.13%	0.990%
19	14.051	2030	2034	2038	rBV	500527	442459	26.23%	3.196%
20	14.510	2110	2112	2118	rVB6	14045	18170	1.08%	0.131%
21	14.927	2179	2183	2187	rVB	84658	91551	5.43%	0.661%
22	15.533	2281	2286	2292	rVB	271178	338544	20.07%	2.445%
23	15.986	2361	2363	2368	rVB4	19343	26352	1.56%	0.190%

Sum of corrected areas: 13845120

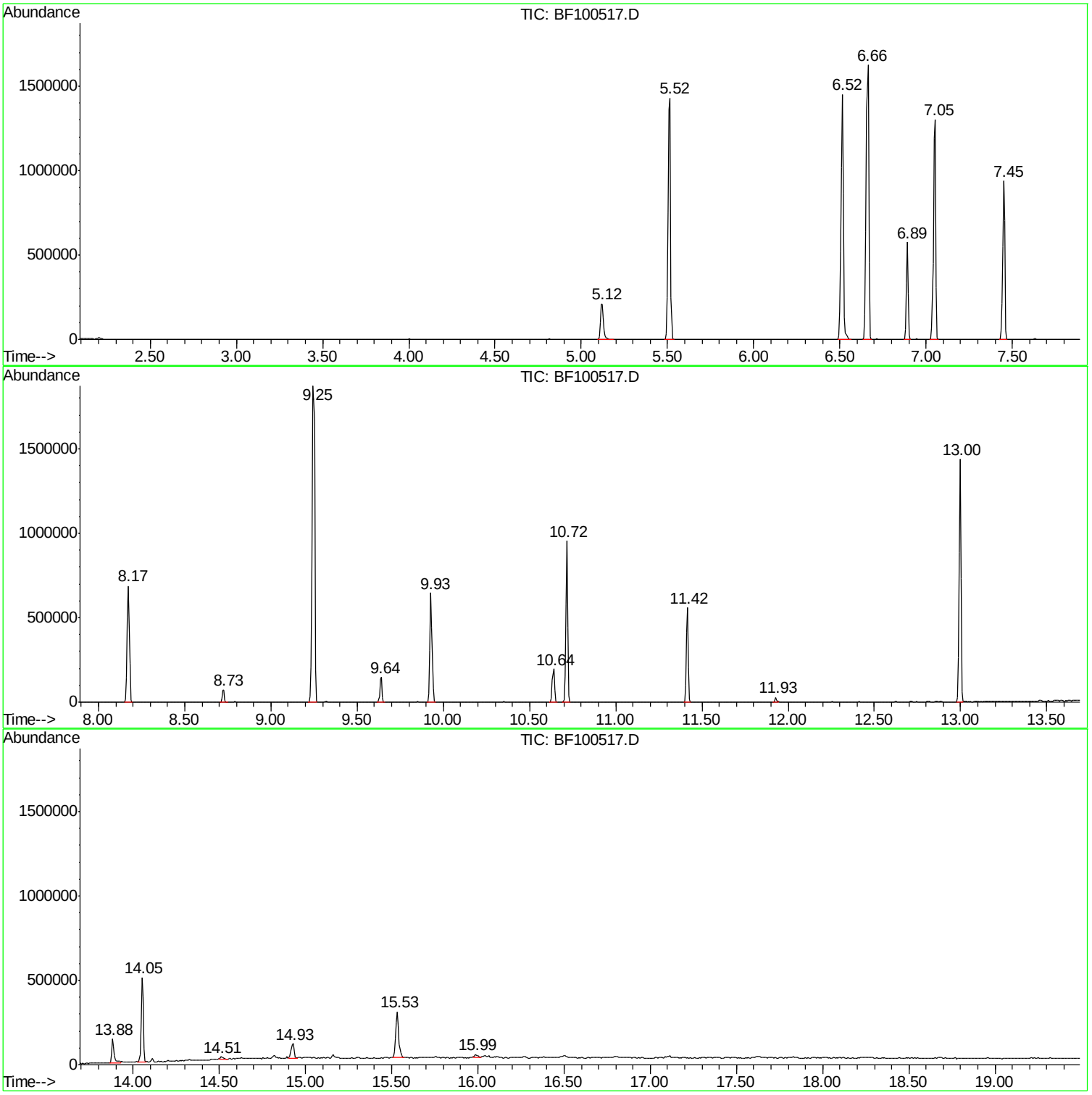
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100517.D
Acq On : 13 Nov 2017 22:15
Operator : SJ/JU
Sample : I6388-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100517.D
Acq On : 13 Nov 2017 22:15
Operator : SJ/JU
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

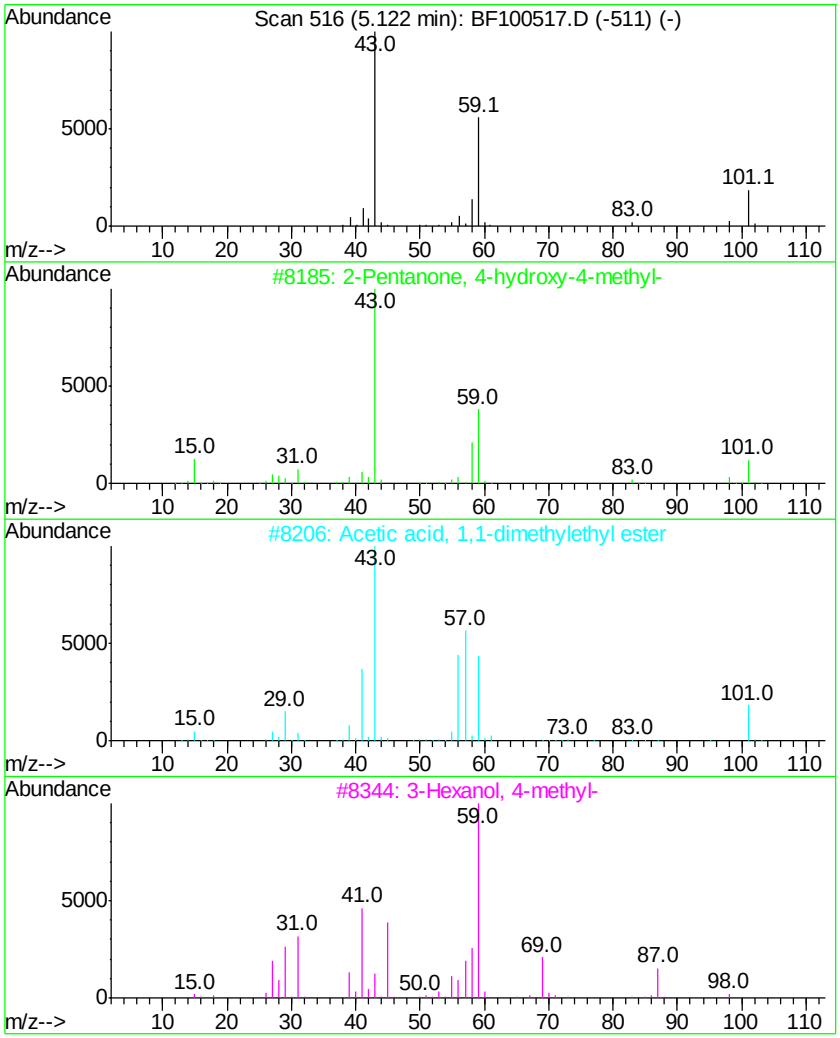
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

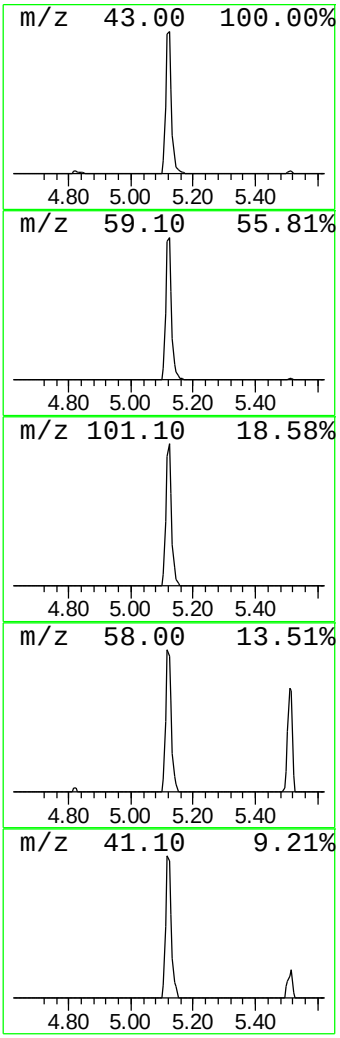
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	12.09 ng	269621	1,4-Dichlorobenzene-d4	6.89

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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
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Acq On : 13 Nov 2017 22:15
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Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

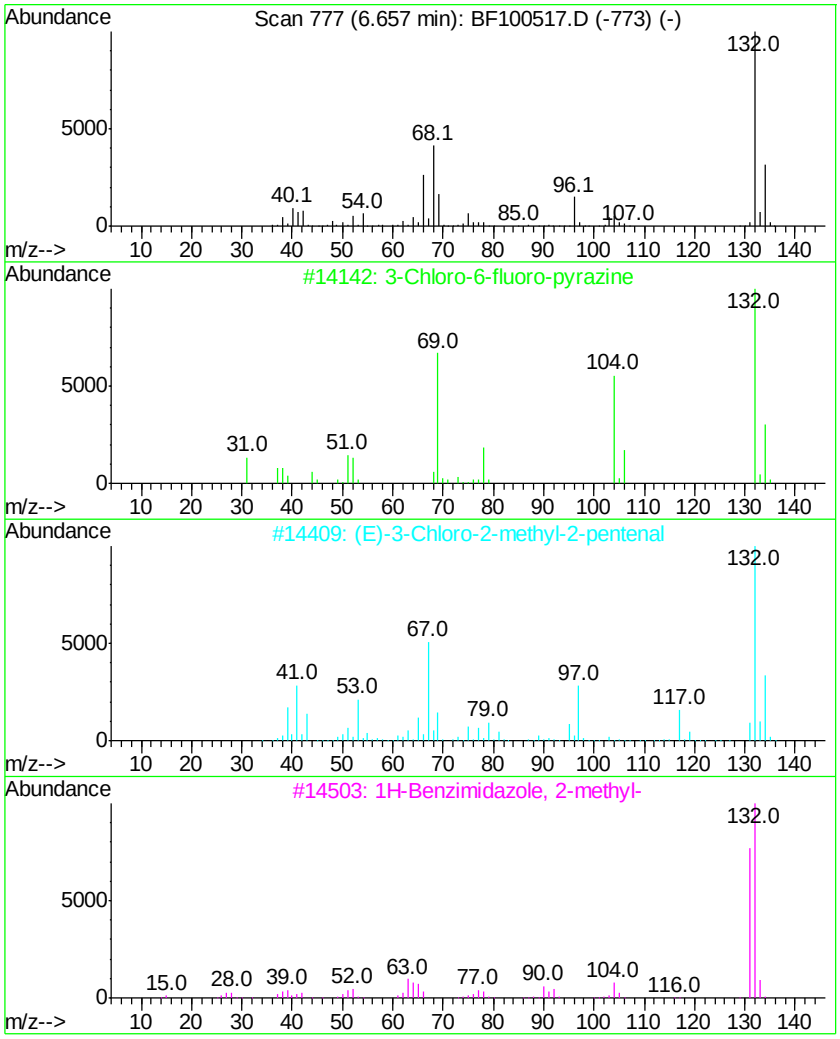
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

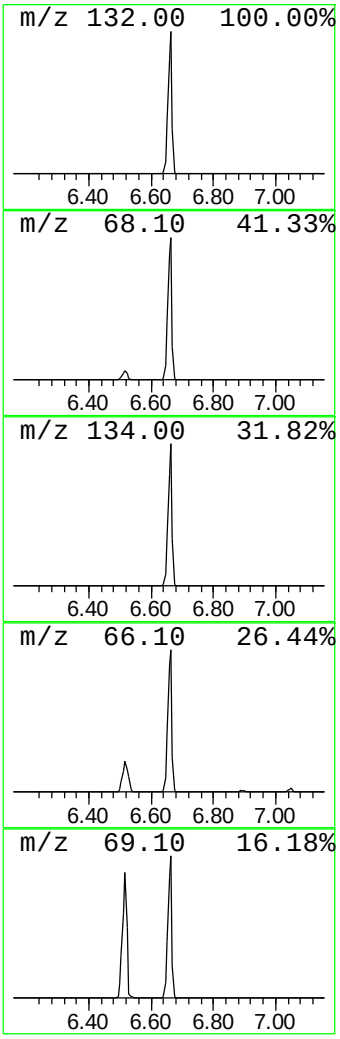
****

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	67.32 ng	1501490	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111317\
Data File : BF100517.D
Acq On : 13 Nov 2017 22:15
Operator : SJ/JU
Sample : I6388-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.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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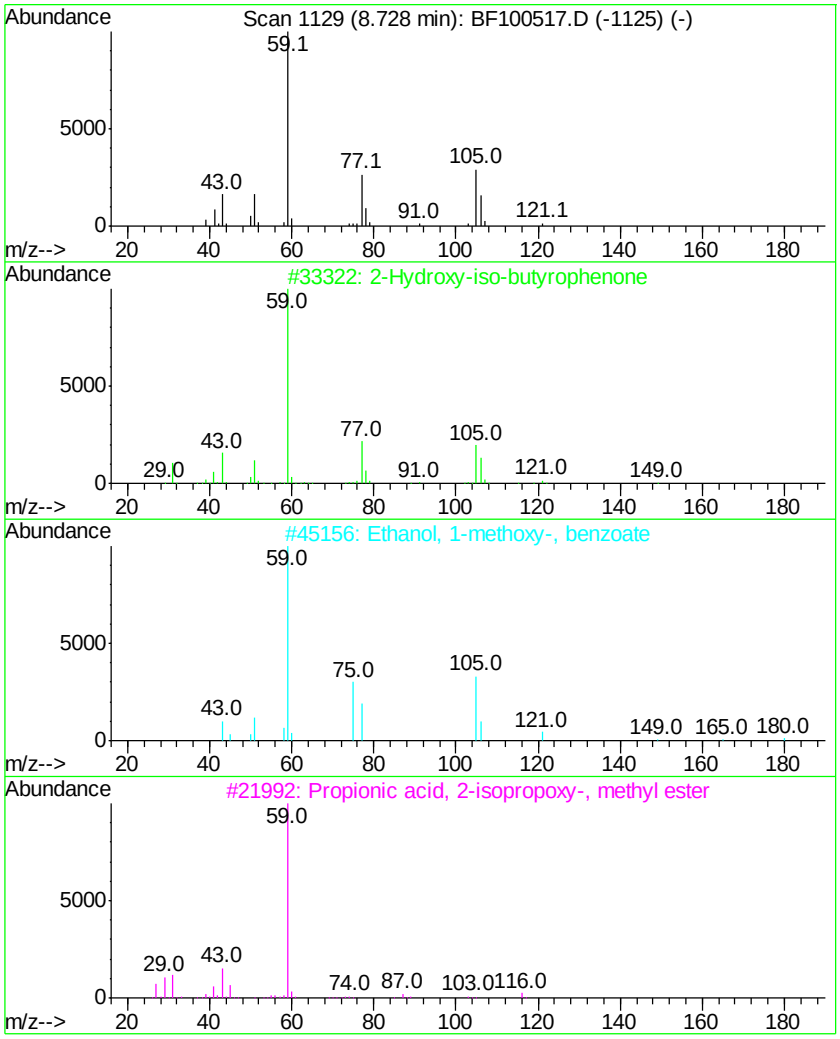
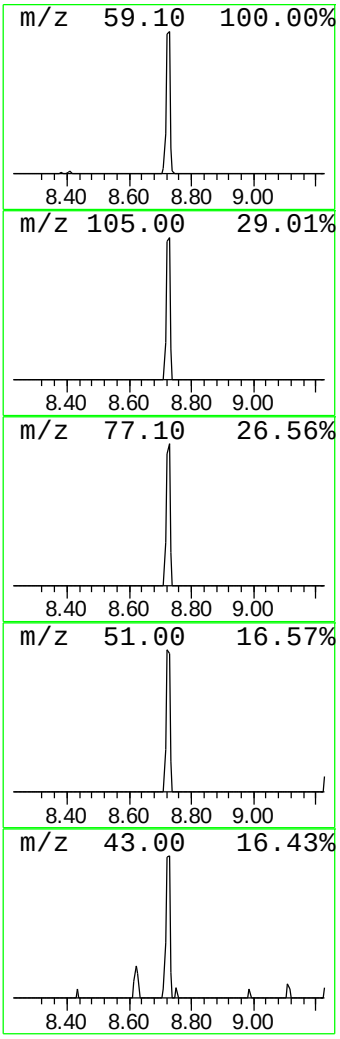
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	2.25 ng	63243	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	86
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3	Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
4	Guanidine	59	CH5N3	000113-00-8	7
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	5





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Acq On : 13 Nov 2017 22:15
Operator : SJ/JU
Sample : I6388-11
Misc :
ALS Vial : 23 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

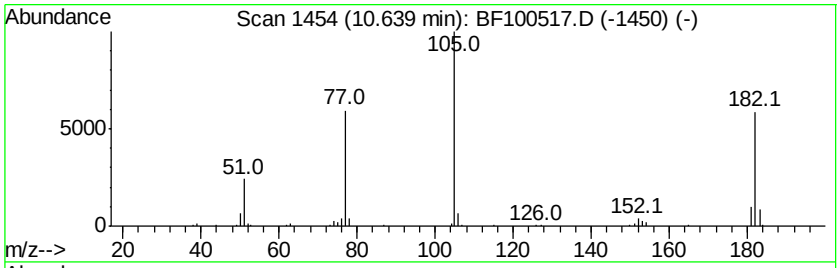
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

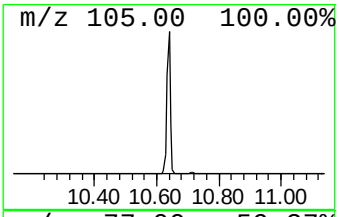
****

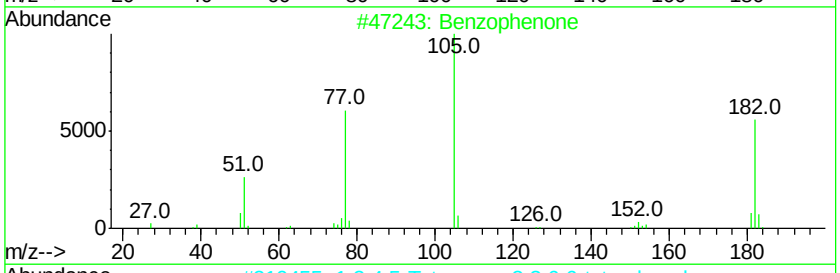
Peak Number 5 Benzophenone Concentration Rank 5

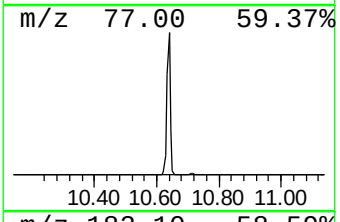
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	5.61 ng	151827	Acenaphthene-d10	9.93

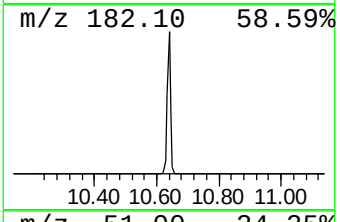
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396	C26H20O4	016204-36-7	78
3	2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9NO2	037791-41-6	47
4	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5	Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47

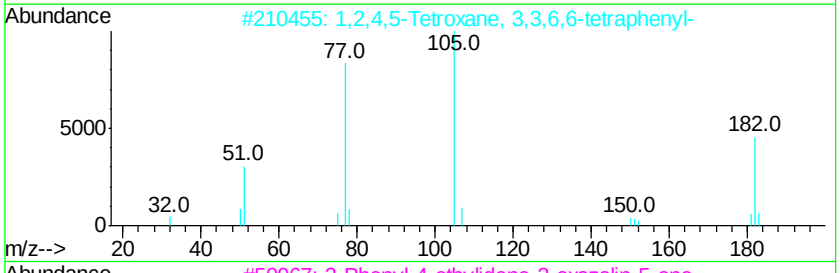


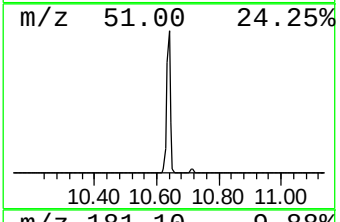


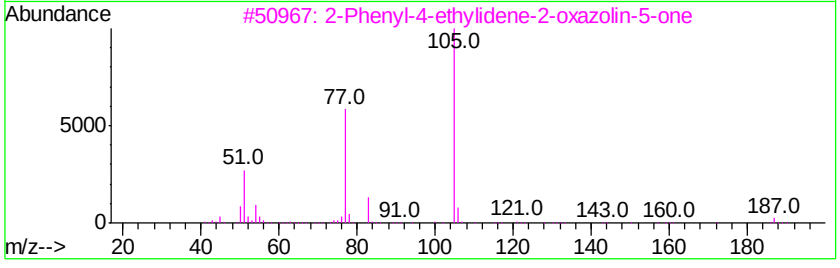


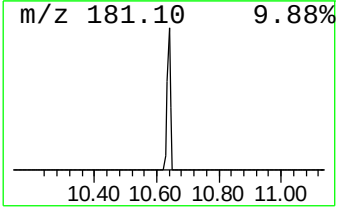












Library Search Compound Report

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Misc :
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Instrument : BNA_F
ClientSampleId : 3N-6

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

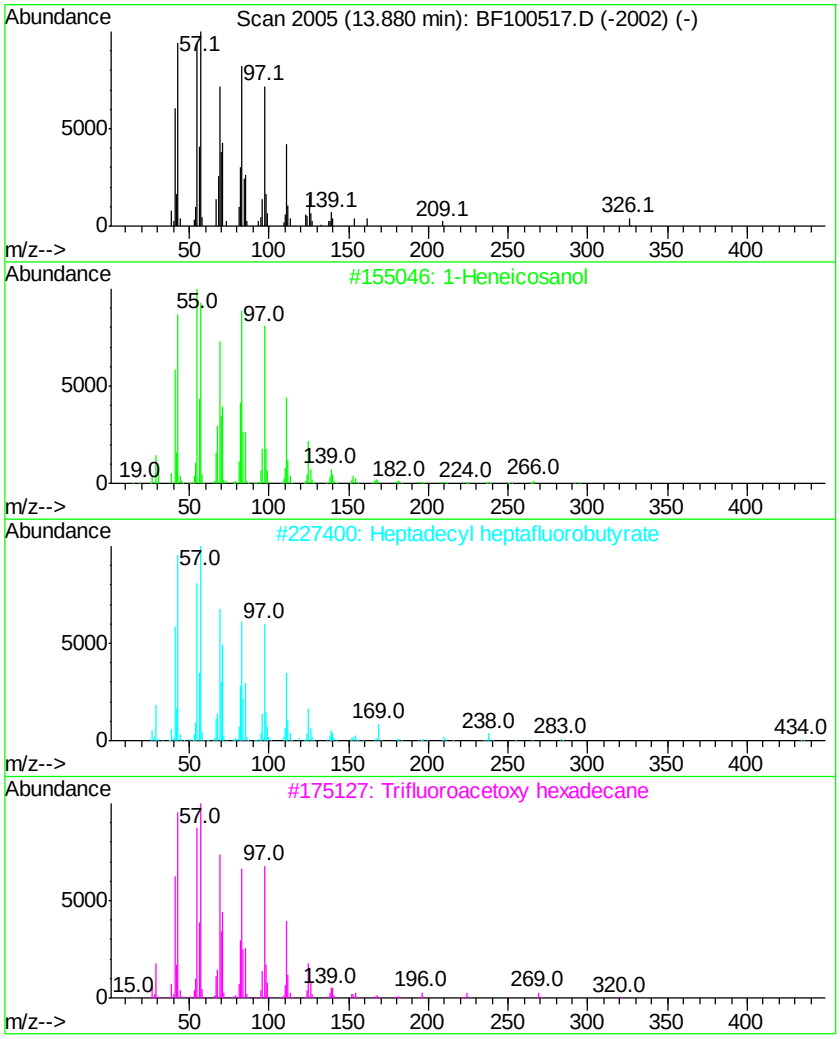
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

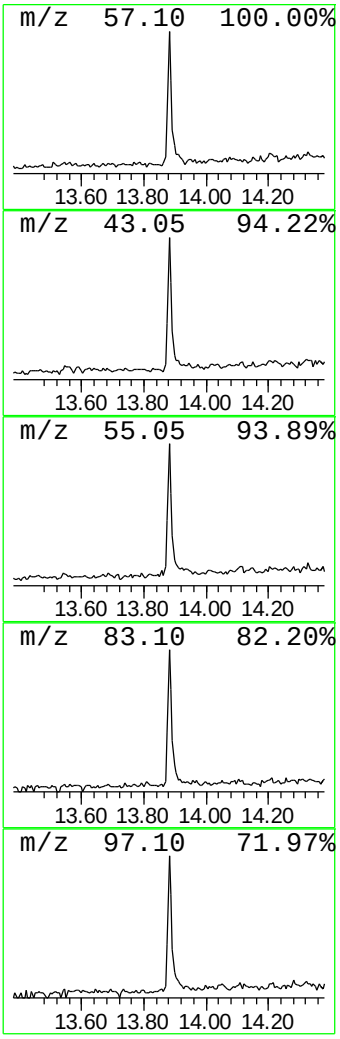
****

Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	6.20 ng	137114	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

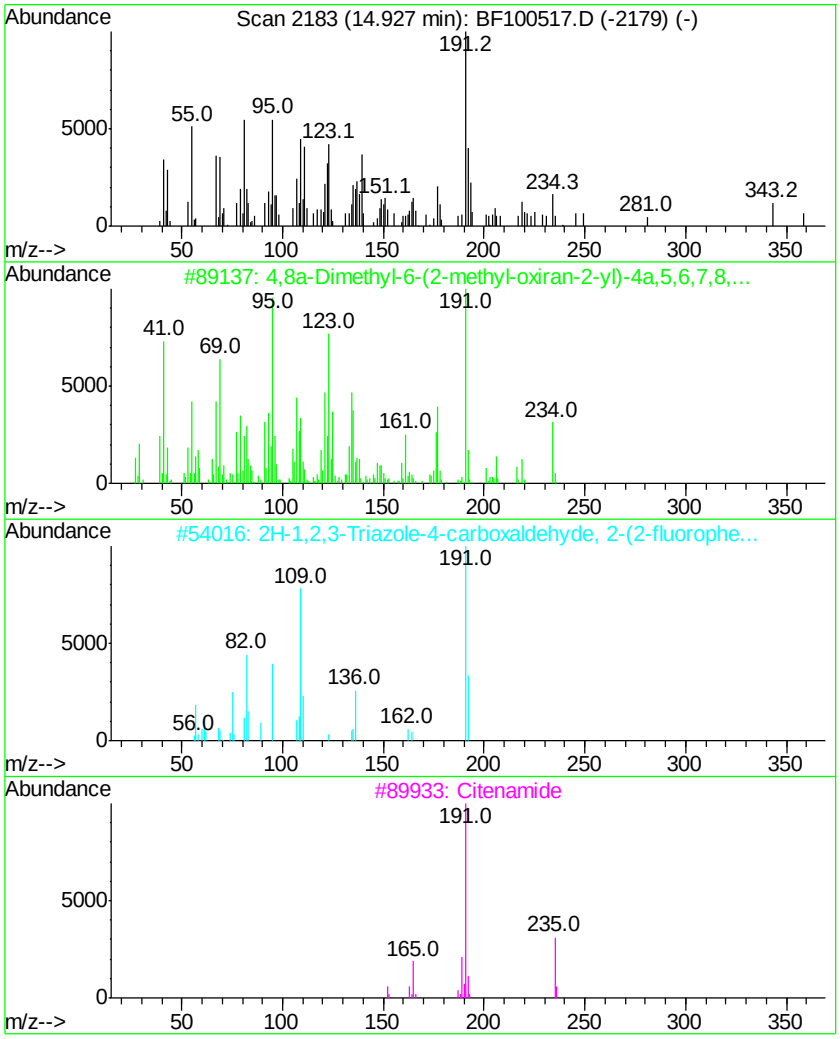
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

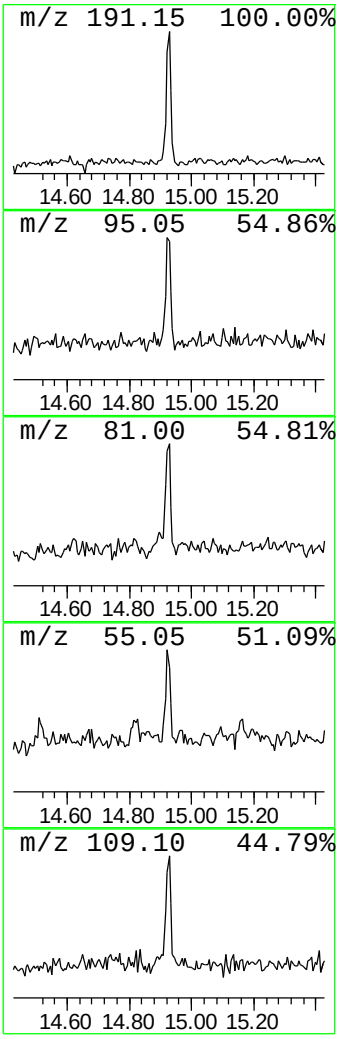
****

Peak Number 7 unknown14.93 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	5.41 ng	91551	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8a-Dimethyl-6-(2-methyl-oxiran...	234	C15H22O2	1000189-11-4	38
2	2H-1,2,3-Triazole-4-carboxaldehy...	191	C9H6FN3O	051306-43-5	38
3	Citenamide	235	C16H13NO	010423-37-7	35
4	Bicyclo[2.2.1]heptane, 2,2,3-tri...	138	C10H18	020536-40-7	25
5	1-(3-Nitro-phenyl)-pyrrolidine	192	C10H12N2O2	1000300-34-7	25





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.12	12.1	ng	269621	1	6.89	446065	20.0
unknown6.66	6.66	67.3	ng	1501490	1	6.89	446065	20.0
2-Hydroxy-iso-but...	8.73	2.3	ng	63243	2	8.17	562470	20.0
Benzophenone	10.64	5.6	ng	151827	3	9.93	541429	20.0
1-Heneicosanol	13.88	6.2	ng	137114	5	14.05	442459	20.0
unknown14.93	14.93	5.4	ng	91551	6	15.53	338544	20.0