LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF111417\
Data File : BF100546.D
Acq On : 14 Nov 2017 16:54
Operator : SJ/JU
Sample : I6389-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-11

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	4.499	407	410	416	rBV	24471	27694	1.05%	0.122%
2	5.110	510	514	526	rVB	399800	503544	19.11%	2.216%
3	5.504	576	581	585	rBV	2403915	2494555	94.68%	10.978%
4	6.510	747	752	762	rVB	2373644	2634795	100.00%	11.595%
5	6.657	772	777	780	rBV	2434825	2499205	94.85%	10.999%
6	6.887	812	816	819	rVB	947040	791117	30.03%	3.482%
7	7.040	838	842	846	rVB	2106796	1898461	72.05%	8.355%
8	7.445	906	911	914	rBV	1727114	1561497	59.26%	6.872%
9	8.169	1029	1034	1037	rVB	1063583	994641	37.75%	4.377%
10	8.716	1123	1127	1131	rBV	232610	184603	7.01%	0.812%
11	8.910	1156	1160	1162	rBV	24694	26740	1.01%	0.118%
12	9.239	1211	1216	1219	rBV	2744069	2292255	87.00%	10.088%
13	9.628	1279	1282	1286	rVB	366861	288658	10.96%	1.270%
14	9.922	1328	1332	1336	rBV	1127271	944802	35.86%	4.158%
15	10.633	1449	1453	1456	rBV	557439	464909	17.64%	2.046%
16	10.710	1462	1466	1469	rBV	1304362	1148405	43.59%	5.054%
17	11.404	1581	1584	1587	rBV	858208	789424	29.96%	3.474%
18	11.922	1667	1672	1675	rBV4	23267	29728	1.13%	0.131%
19	12.986	1849	1853	1857	rBV	1734893	1650384	62.64%	7.263%
20	13.874	2001	2004	2013	rBV	78460	85665	3.25%	0.377%
21	14.045	2029	2033	2036	rBV	854941	769395	29.20%	3.386%
22	14.498	2108	2110	2115	rBV4	21675	33620	1.28%	0.148%
23	14.886	2174	2176	2179	rVB2	33914	28842	1.09%	0.127%
24	15.521	2279	2284	2294	rVB	438013	579998	22.01%	2.552%

Sum of corrected areas: 22722937

LSC Report - Integrated Chromatogram

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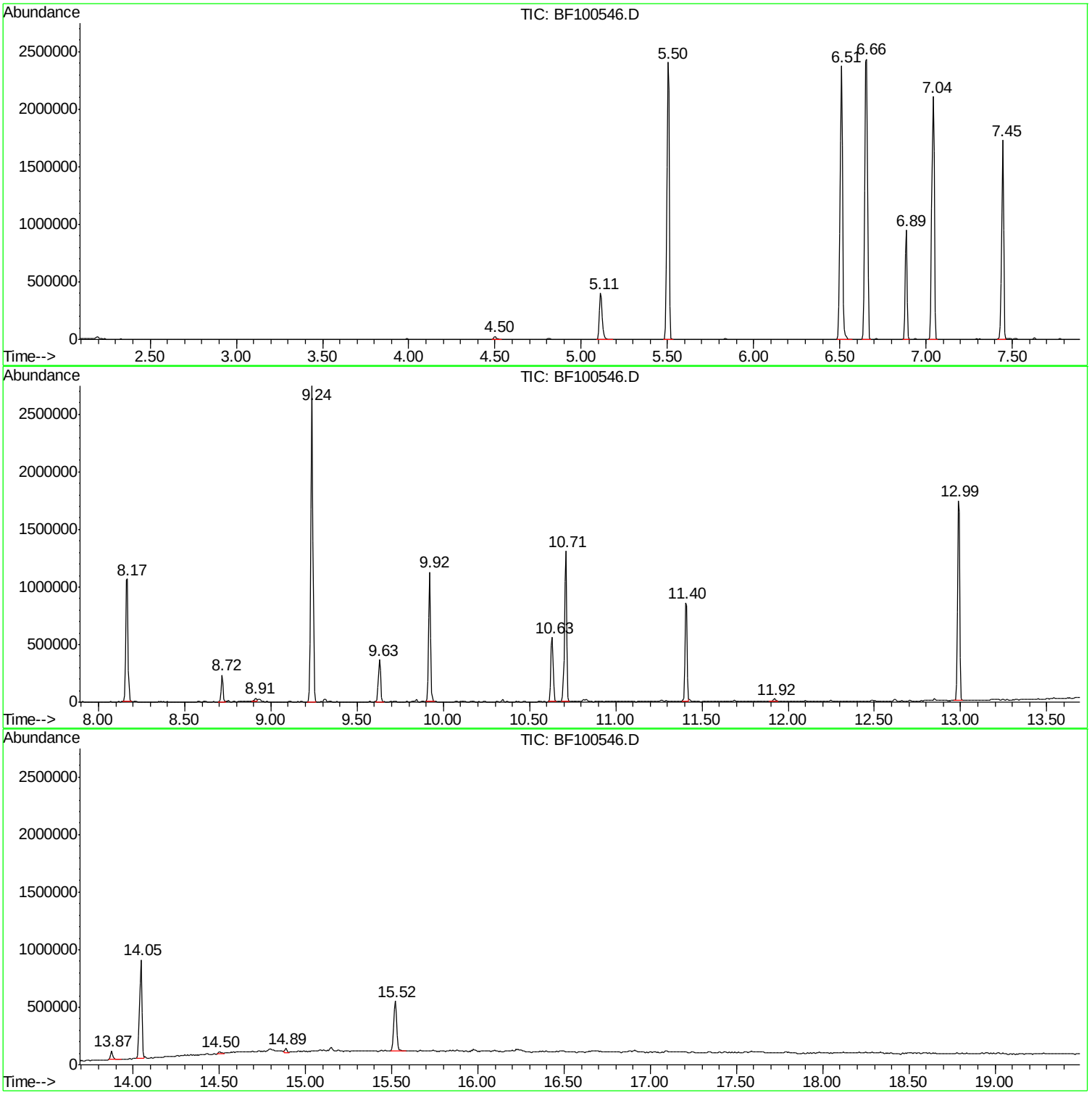
Operator : SJ/JU
Sample : I6389-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-11

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

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Data File : BF100546.D
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ClientSampleId : 3N-11

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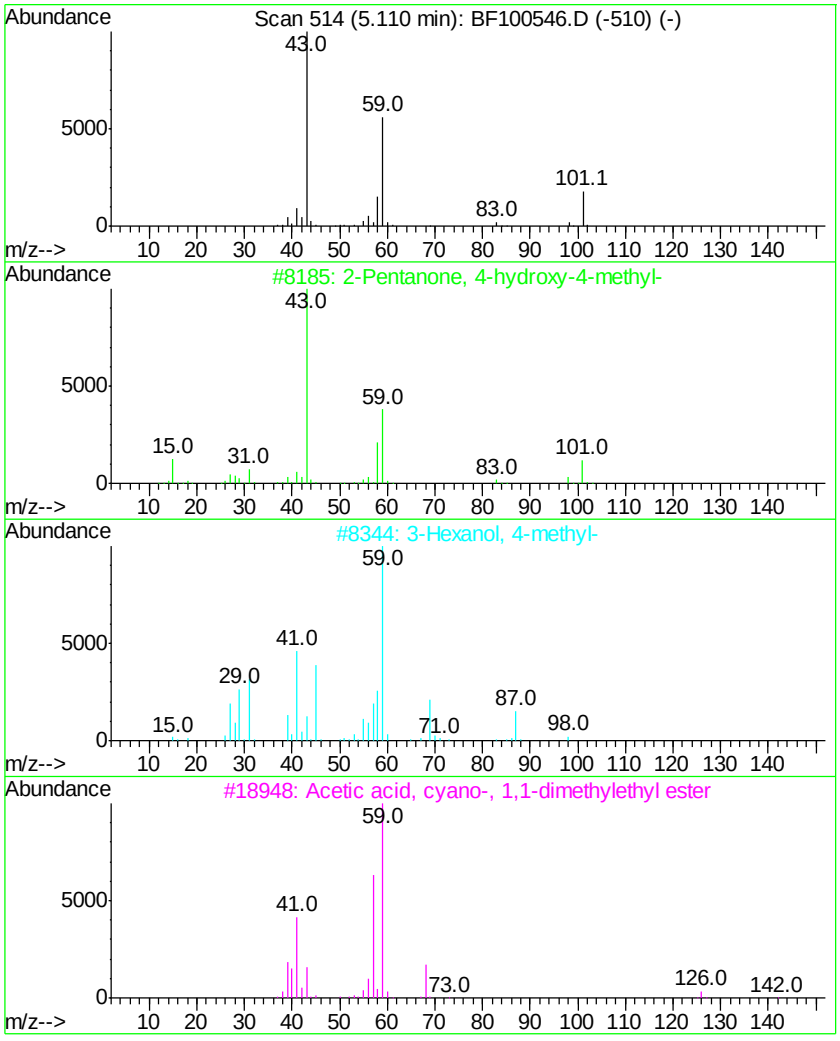
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

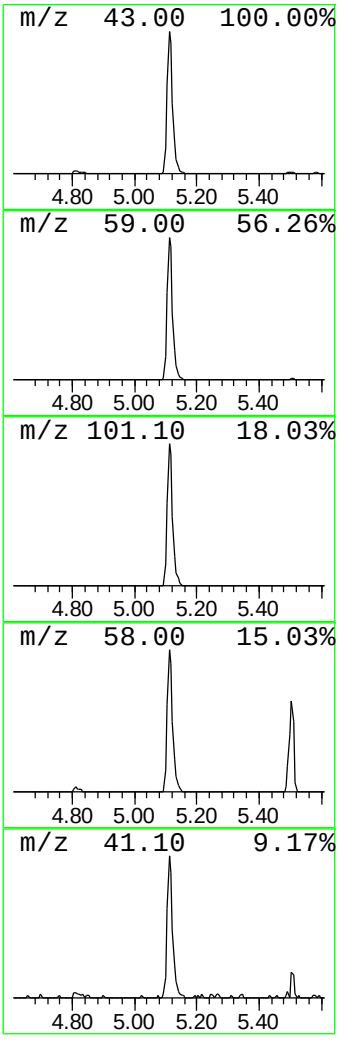
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	12.73 ng	503544	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	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

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Data File : BF100546.D
Acq On : 14 Nov 2017 16:54
Operator : SJ/JU
Sample : I6389-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-11

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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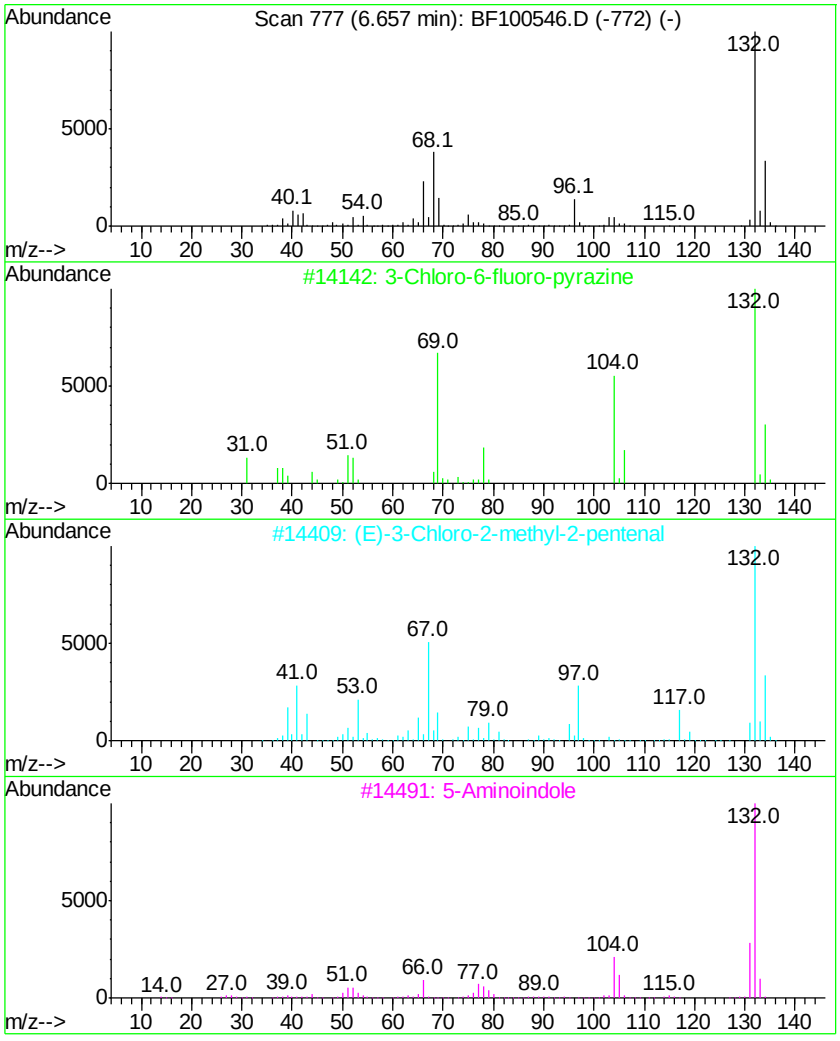
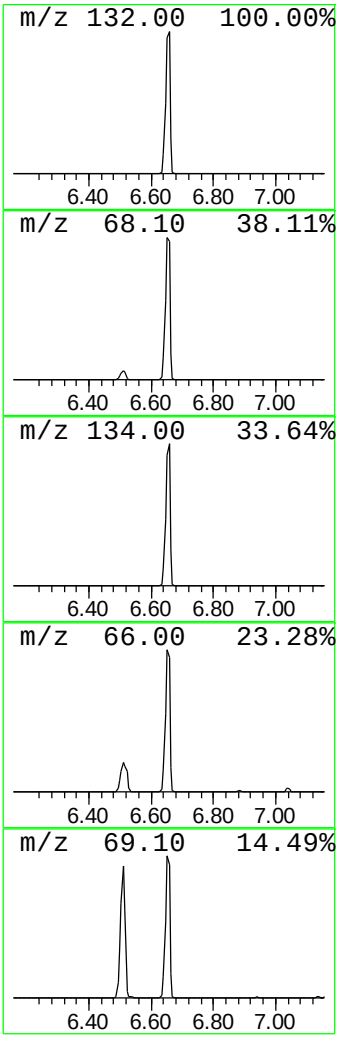
Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	63.18 ng	2499210	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	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

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Data File : BF100546.D
Acq On : 14 Nov 2017 16:54
Operator : SJ/JU
Sample : I6389-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-11

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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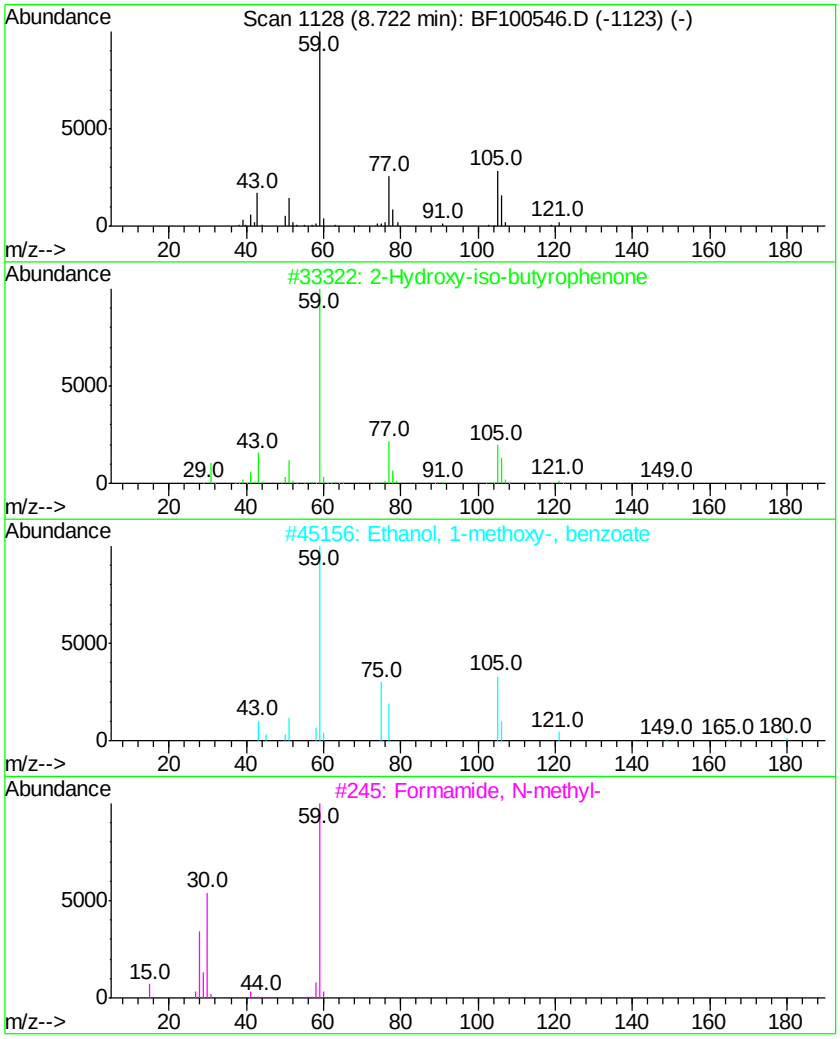
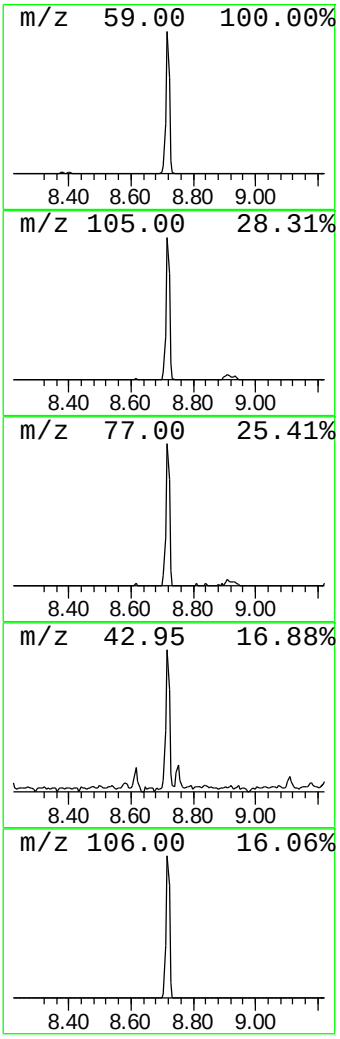
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	3.71 ng	184603	Naphthalene-d8	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	64
3	Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
4	Guanidine	59	CH5N3	000113-00-8	7
5	Acetamide	59	C2H5NO	000060-35-5	5





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Acq On : 14 Nov 2017 16:54
Operator : SJ/JU
Sample : I6389-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 3N-11

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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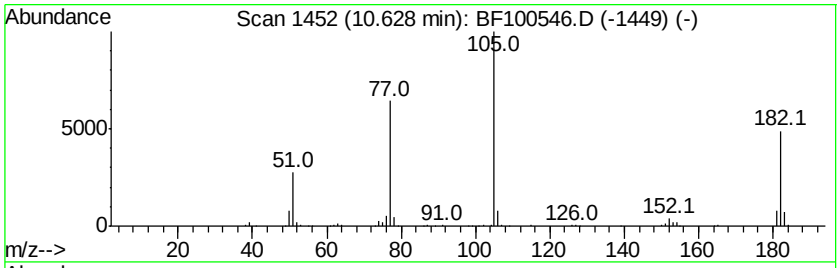
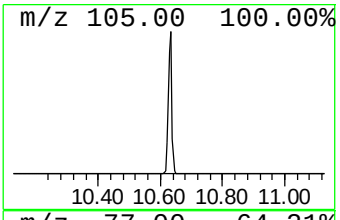
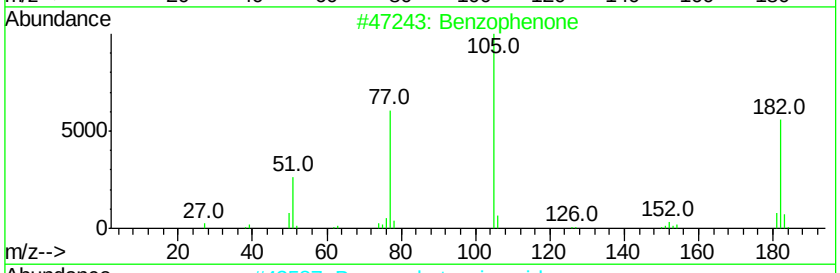
Peak Number 5 Benzophenone Concentration Rank 4

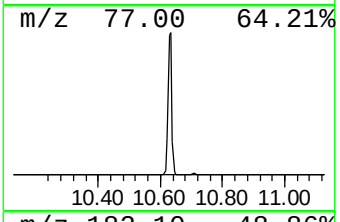
R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	9.84 ng	464909	Acenaphthene-d10	9.92

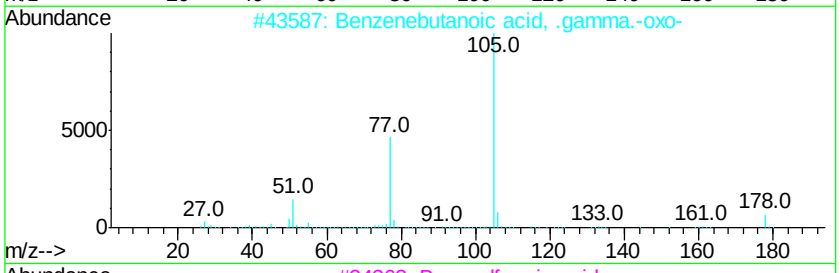
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
3	Benzoylformic acid	150	C8H6O3	000611-73-4	47
4	Vinyl benzoate	148	C9H8O2	000769-78-8	47
5	Benzopinacol	366	C26H22O2	000464-72-2	47

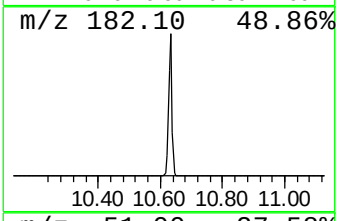


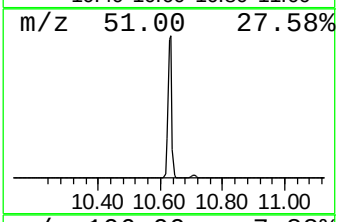


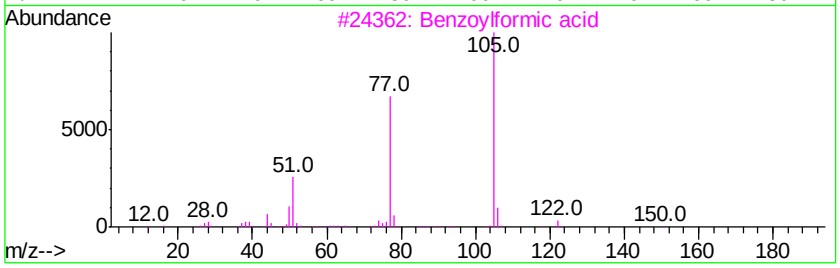


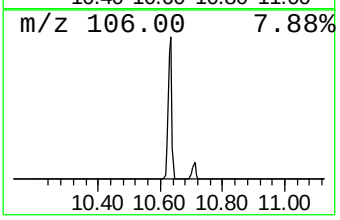












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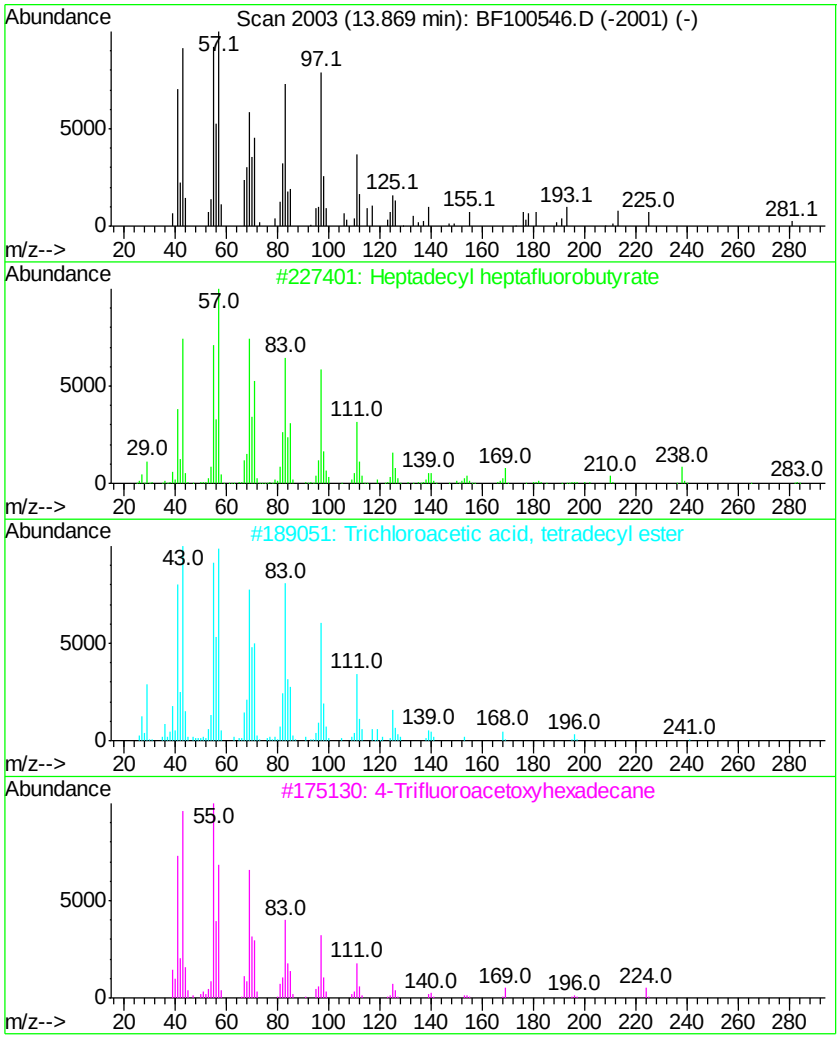
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

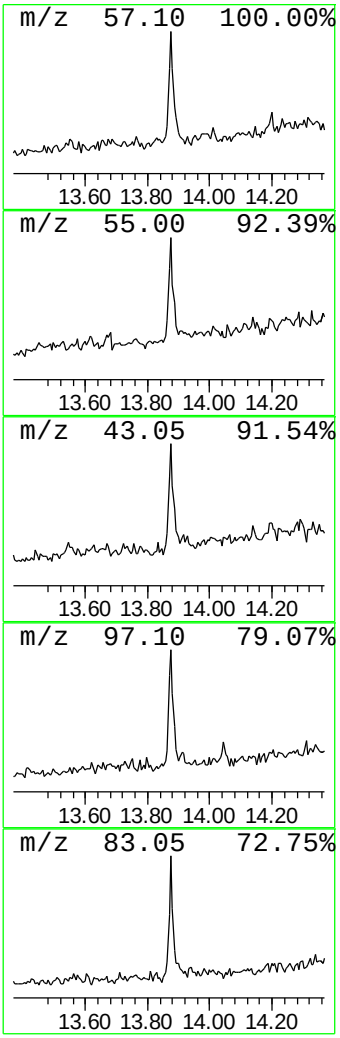
****

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.23 ng	85665	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
3	4-Trifluoroacetoxyhexadecane	338	C18H33F3O2	1000215-97-5	91
4	11-Tricosene	322	C23H46	052078-56-5	91
5	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91





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
2-Pentanone, 4-hy...	5.11	12.7	ng	503544	1	6.89	791117	20.0
unknown6.66	6.66	63.2	ng	2499210	1	6.89	791117	20.0
2-Hydroxy-iso-but...	8.72	3.7	ng	184603	2	8.17	994641	20.0
Benzophenone	10.63	9.8	ng	464909	3	9.92	944802	20.0
Heptadecyl heptaf...	13.87	2.2	ng	85665	5	14.05	769395	20.0