LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100958.D
Acq On : 29 Nov 2017 3:03
Operator : SJ/JU
Sample : I6579-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-2-E(7-8)

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	5.098	508	512	523	rBB	85981	116042	6.79%	0.804%
2	5.487	573	578	581	rBV	1722172	1659178	97.11%	11.494%
3	6.492	744	749	752	rBV	1498191	1708470	100.00%	11.836%
4	6.634	768	773	776	rBV	1840059	1699822	99.49%	11.776%
5	6.857	808	811	815	rBV	443809	373821	21.88%	2.590%
6	7.016	834	838	841	rBV	1358415	1142607	66.88%	7.916%
7	7.422	902	907	910	rBV	931934	982506	57.51%	6.806%
8	8.139	1025	1029	1032	rBV	565315	469714	27.49%	3.254%
9	8.692	1120	1123	1131	rBV	105098	87297	5.11%	0.605%
10	9.216	1207	1212	1215	rBV	1741450	1418692	83.04%	9.828%
11	9.604	1275	1278	1282	rBV	83461	67967	3.98%	0.471%
12	9.898	1324	1328	1331	rBV	473853	440159	25.76%	3.049%
13	9.927	1331	1333	1338	rVB	23878	17721	1.04%	0.123%
14	10.610	1444	1449	1452	rBV	439586	363685	21.29%	2.519%
15	10.686	1458	1462	1465	rBV	975651	868103	50.81%	6.014%
16	11.380	1577	1580	1583	rBV	446512	403600	23.62%	2.796%
17	11.404	1583	1584	1588	rVB	108831	71702	4.20%	0.497%
18	11.898	1661	1668	1676	rBV6	21218	40312	2.36%	0.279%
19	11.998	1681	1685	1687	rBV2	16014	17953	1.05%	0.124%
20	12.592	1783	1786	1790	rBV	130881	112456	6.58%	0.779%
21	12.821	1820	1825	1828	rBV	102215	115710	6.77%	0.802%
22	12.968	1845	1850	1853	rBV	1130995	1054646	61.73%	7.306%
23	13.151	1878	1881	1884	rVB	23113	23504	1.38%	0.163%
24	13.216	1890	1892	1896	rBV	26059	24014	1.41%	0.166%
25	13.857	1999	2001	2009	rVB7	21636	31819	1.86%	0.220%
26	14.021	2024	2029	2032	rBV2	478494	489258	28.64%	3.389%
27	14.045	2032	2033	2037	rVB	59057	46565	2.73%	0.323%
28	14.127	2040	2047	2049	rBV6	22720	36114	2.11%	0.250%
29	14.474	2103	2106	2109	rBV5	16721	22057	1.29%	0.153%
30	15.062	2202	2206	2209	rBV	50346	72935	4.27%	0.505%
31	15.368	2254	2258	2263	rVB	30601	47579	2.78%	0.330%
32	15.427	2264	2268	2274	rBV	40364	56898	3.33%	0.394%
33	15.498	2275	2280	2284	rBV	263288	329880	19.31%	2.285%
34	15.927	2351	2353	2360	rVB7	14662	22183	1.30%	0.154%

LSC Area Percent Report

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Operator : SJ/JU
Sample : I6579-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-2-E(7-8)

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

Sum of corrected areas: 14434969

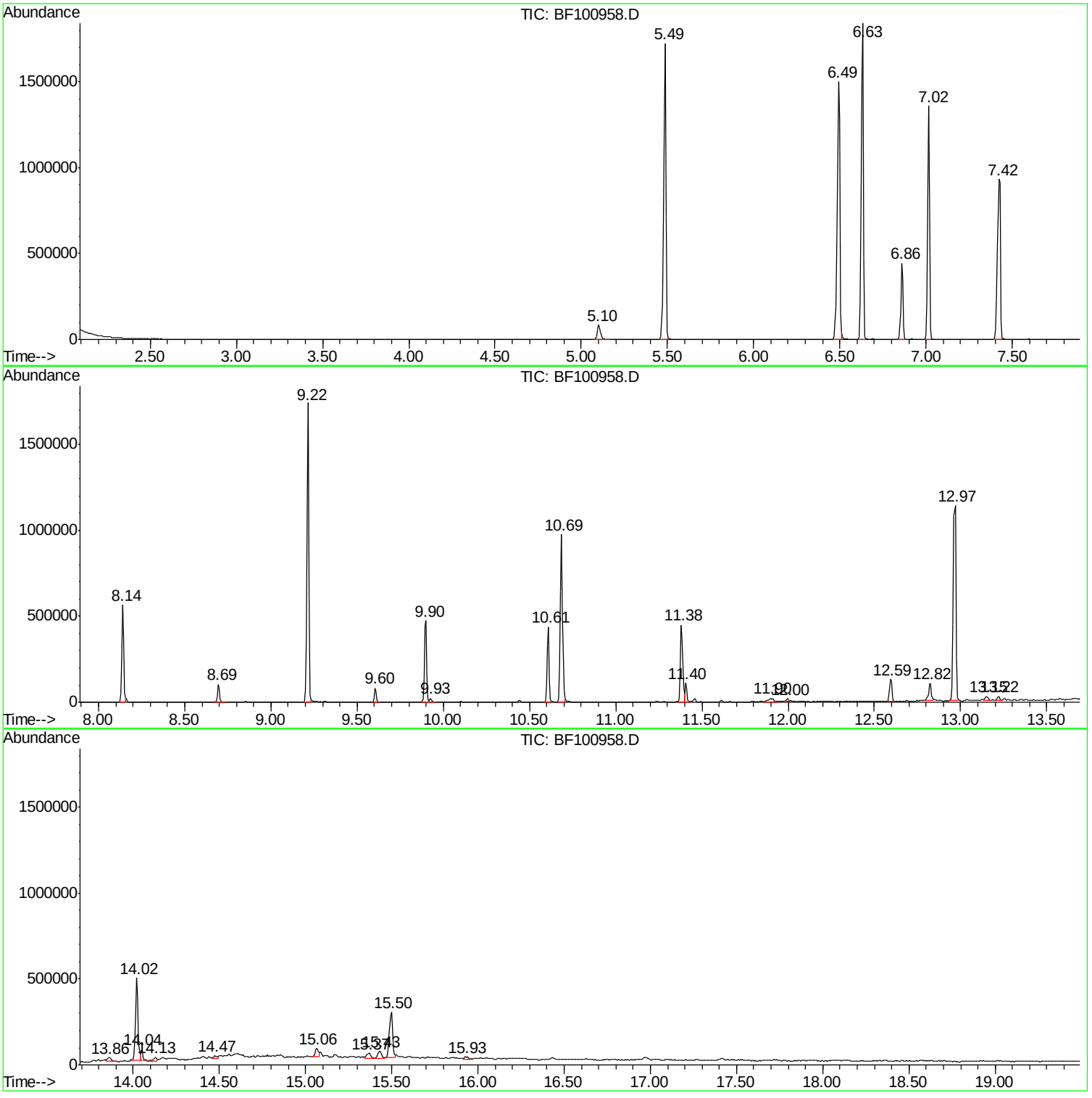
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100958.D
Acq On : 29 Nov 2017 3:03
Operator : SJ/JU
Sample : I6579-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HAR-2-E(7-8)

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 : Z:\HPCHEM1\BNA F\DATA\BF112817\
Data File : BF100958.D
Acq On : 29 Nov 2017 3:03
Operator : SJ/JU
Sample : I6579-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-2-E(7-8)

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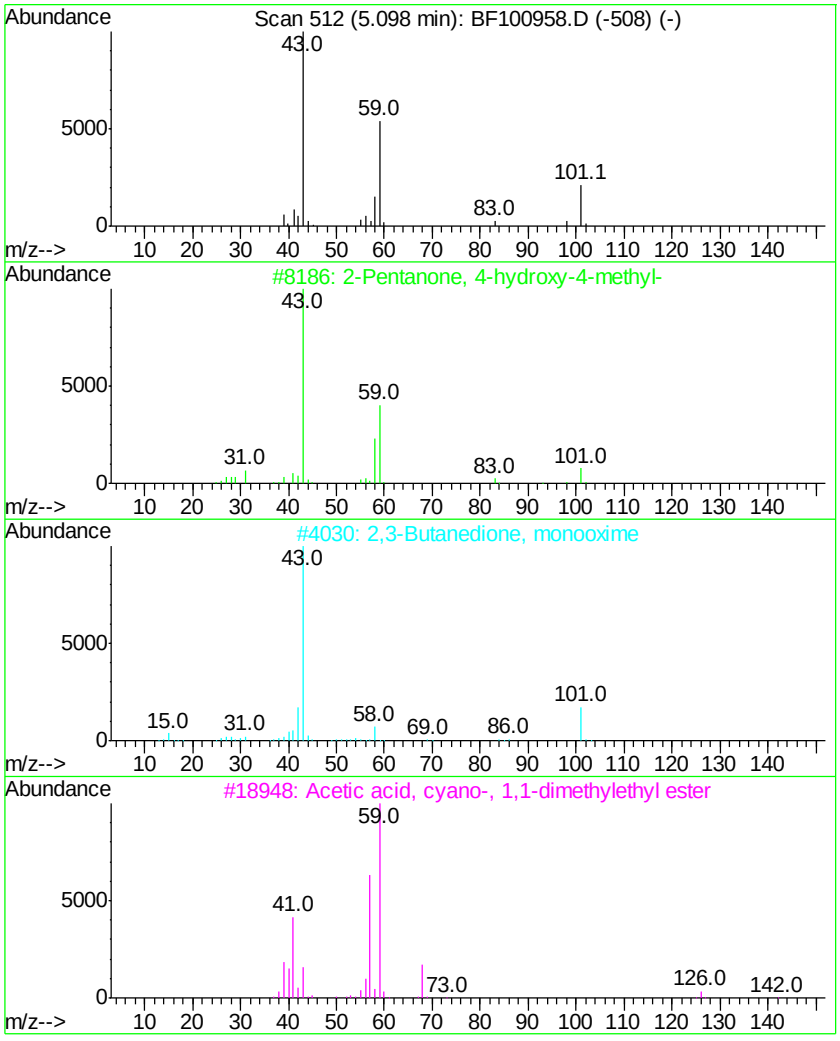
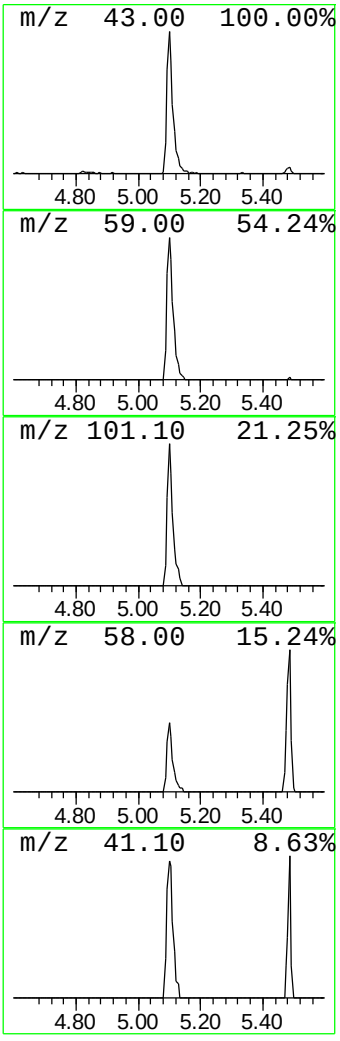
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.21 ng	116042	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9





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Sample : I6579-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-2-E(7-8)

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

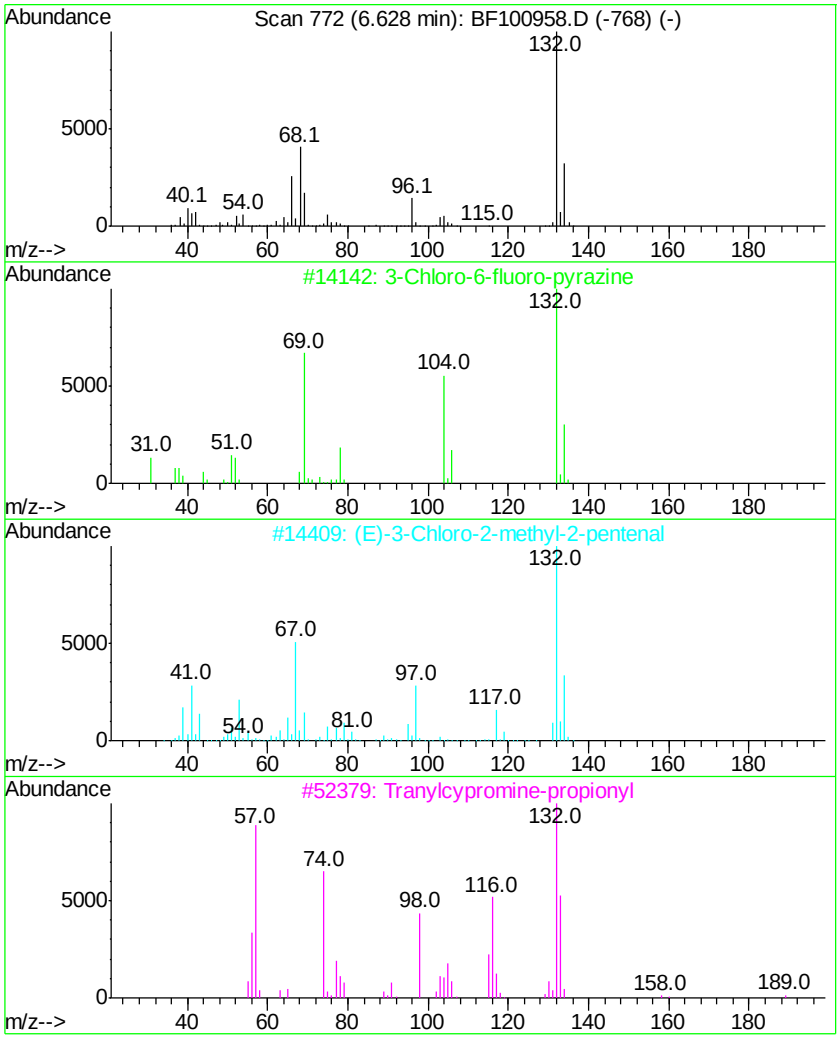
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

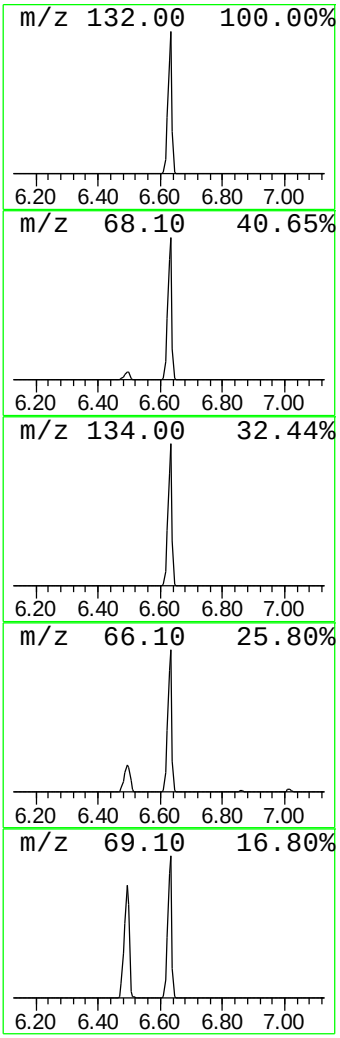
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	90.94 ng	1699820	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
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	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





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Acq On : 29 Nov 2017 3:03
Operator : SJ/JU
Sample : I6579-11
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : HAR-2-E(7-8)

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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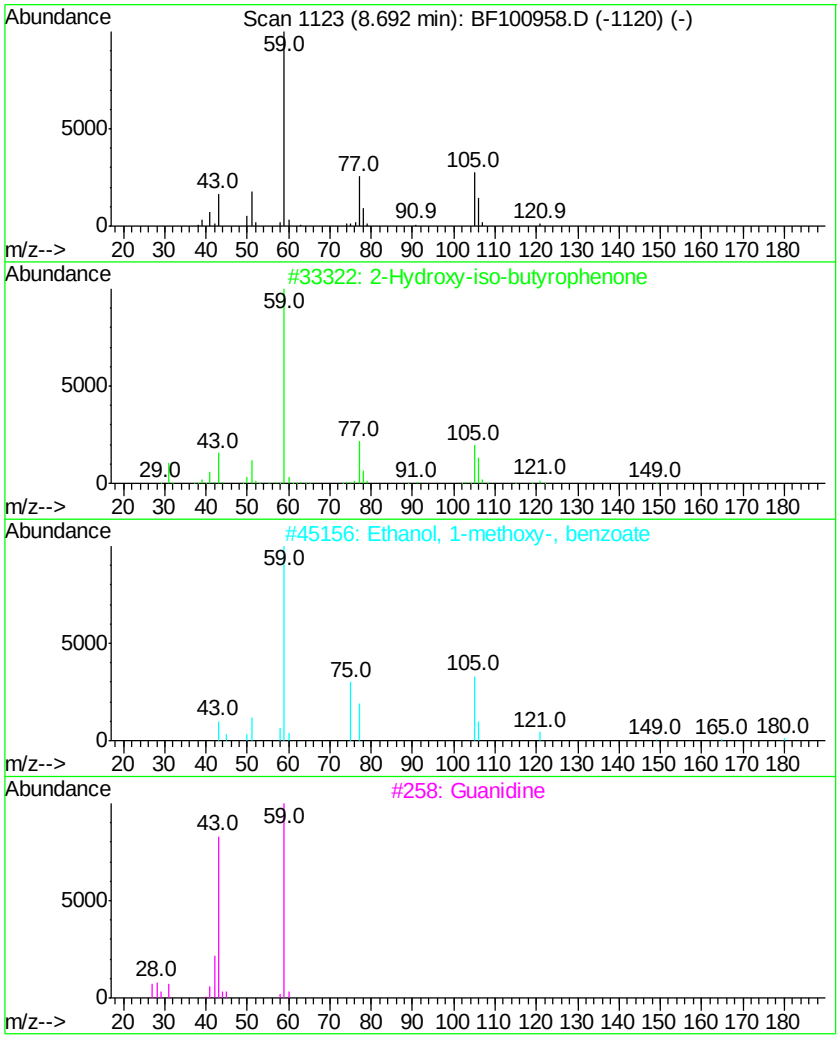
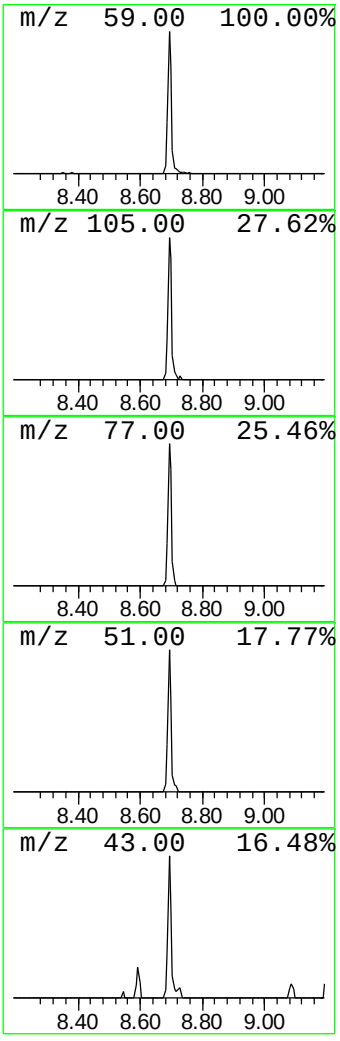
Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	3.72 ng	87297	Naphthalene-d8	8.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	83
2	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	50
3	Guanidine	59	CH5N3	000113-00-8	7
4	Acetamide	59	C2H5NO	000060-35-5	5
5	Formamide, N-methyl-	59	C2H5NO	000123-39-7	4





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Misc :
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Instrument : BNA_F
ClientSampleId : HAR-2-E(7-8)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
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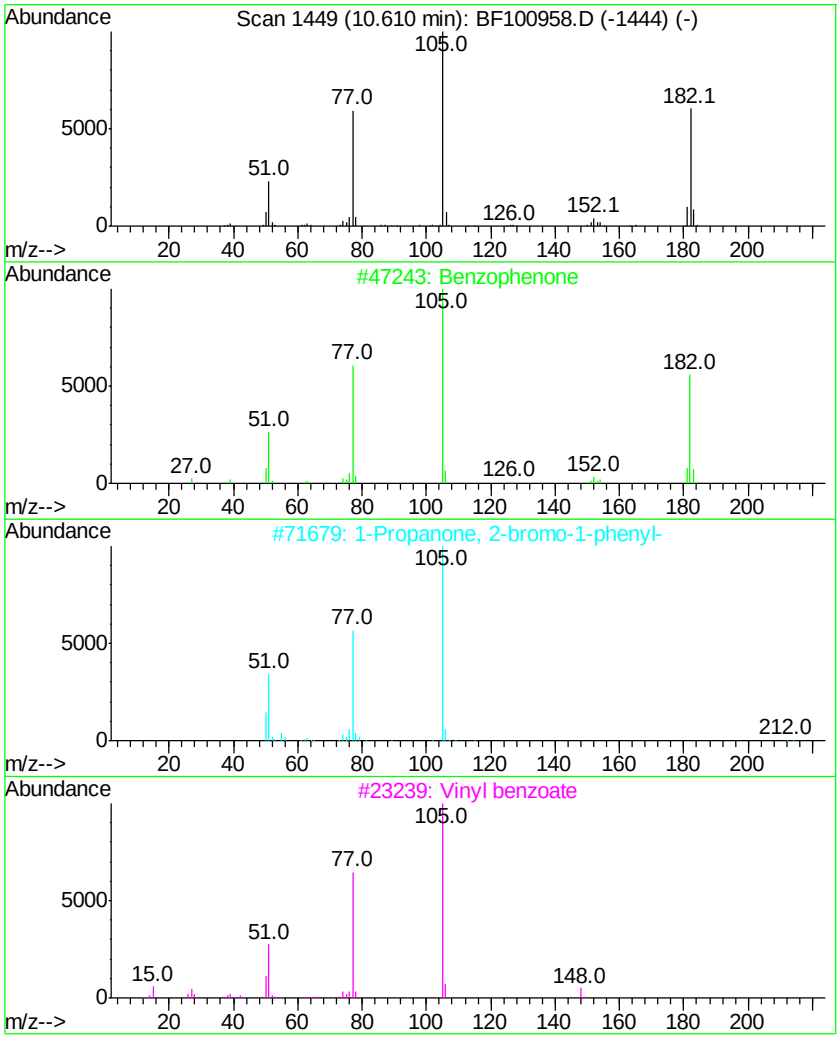
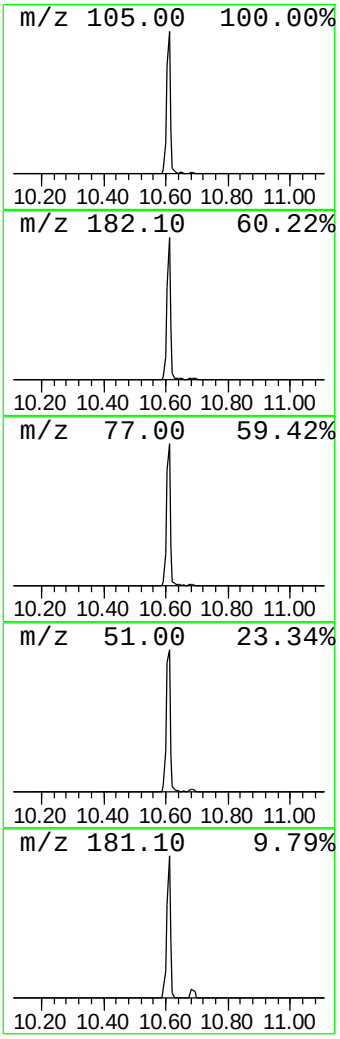
****

Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.61	16.53 ng	363685	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
3	Vinyl benzoate	148	C9H8O2	000769-78-8	47
4	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47





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...	5.10	6.2	ng	116042	1	6.86	373821	20.0
unknown6.63	6.63	90.9	ng	1699820	1	6.86	373821	20.0
2-Hydroxy-iso-but...	8.69	3.7	ng	87297	2	8.14	469714	20.0
Benzophenone	10.61	16.5	ng	363685	3	9.90	440159	20.0