LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
Data File : BF100603.D
Acq On : 15 Nov 2017 22:56
Operator : SJ/JU
Sample : I6426-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110917-TIDO-E-D-B

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	2.181	13	16	27	rVB3	51172	98654	2.81%	0.478%
2	5.098	509	512	521	rVB	199782	228995	6.53%	1.109%
3	5.498	575	580	583	rBV	1396171	1236794	35.26%	5.988%
4	6.498	746	750	761	rVB	999073	809798	23.09%	3.921%
5	6.651	771	776	779	rBV	2147269	2026933	57.79%	9.813%
6	6.881	812	815	819	rBV	807506	659968	18.82%	3.195%
7	7.039	838	842	845	rBV	2773859	2609781	74.41%	12.635%
8	7.445	905	911	914	rBV	1993564	2170039	61.87%	10.506%
9	8.163	1029	1033	1036	rBV	1028170	824818	23.52%	3.993%
10	8.716	1123	1127	1130	rBV	117202	91743	2.62%	0.444%
11	9.239	1211	1216	1219	rBV	3612422	3507478	100.00%	16.982%
12	9.627	1279	1282	1285	rBV	56039	43143	1.23%	0.209%
13	9.916	1328	1331	1335	rVB	891230	765651	21.83%	3.707%
14	10.627	1448	1452	1455	rBV	226338	173228	4.94%	0.839%
15	10.704	1461	1465	1468	rBV	1301741	1124565	32.06%	5.445%
16	11.404	1580	1584	1587	rBV	661682	602077	17.17%	2.915%
17	12.798	1818	1821	1824	rBV	80040	58015	1.65%	0.281%
18	12.986	1848	1853	1856	rBV	2458292	2225568	63.45%	10.775%
19	13.504	1938	1941	1944	rBV	57573	45588	1.30%	0.221%
20	13.874	1998	2004	2012	rBV	23753	35671	1.02%	0.173%
21	14.039	2028	2032	2035	rBV	680998	595121	16.97%	2.881%
22	14.721	2144	2148	2155	rBV	91158	100341	2.86%	0.486%
23	15.509	2277	2282	2289	rBV	498280	620664	17.70%	3.005%

Sum of corrected areas: 20654633

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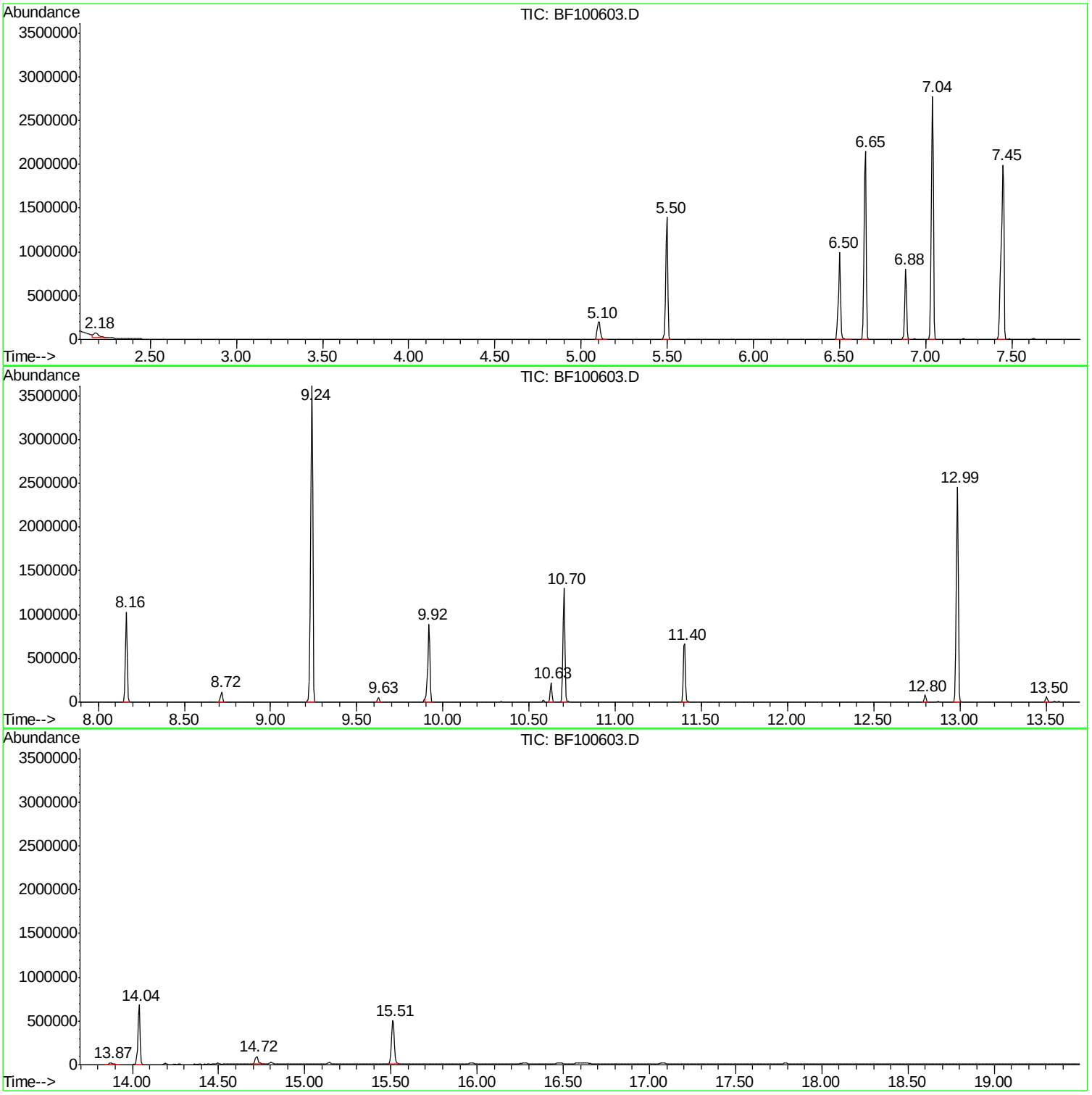
ClientSampleId :
110917-TIDO-E-D-B

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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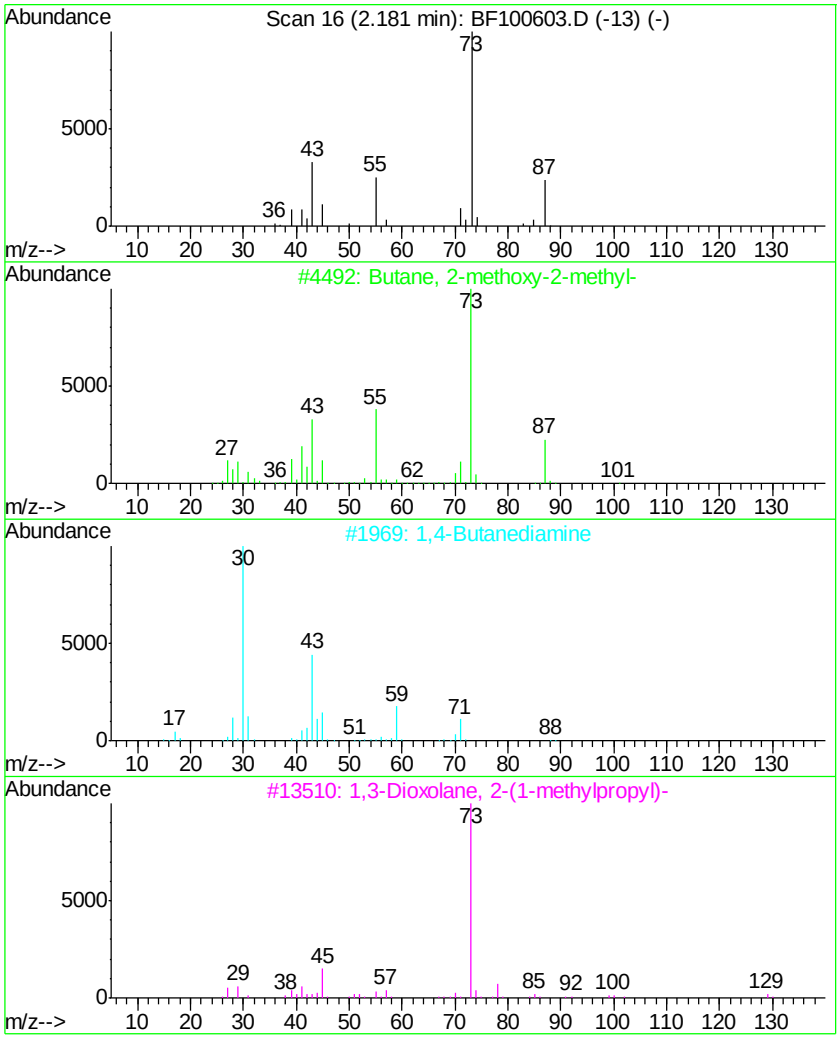
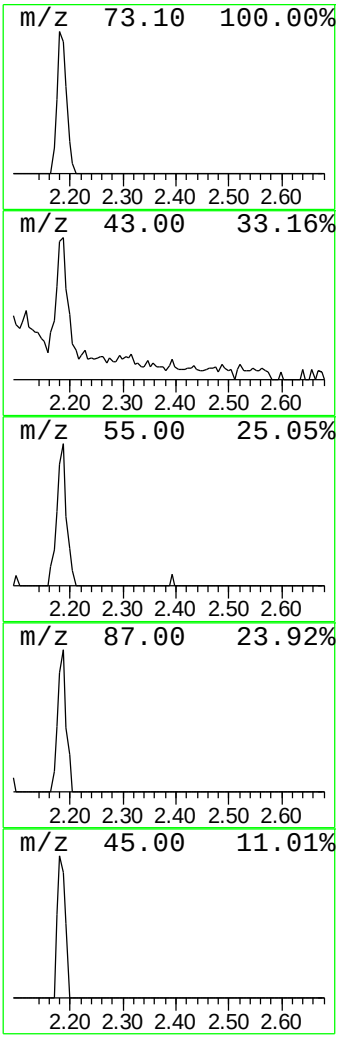
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	2.99 ng	98654	1,4-Dichlorobenzene-d4	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	1,4-Butanediamine	88	C4H12N2	000110-60-1	9
3	1,3-Dioxolane, 2-(1-methylpropyl)-	130	C7H14O2	014447-25-7	9
4	1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	5





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
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Sample : I6426-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : 110917-TIDO-E-D-B

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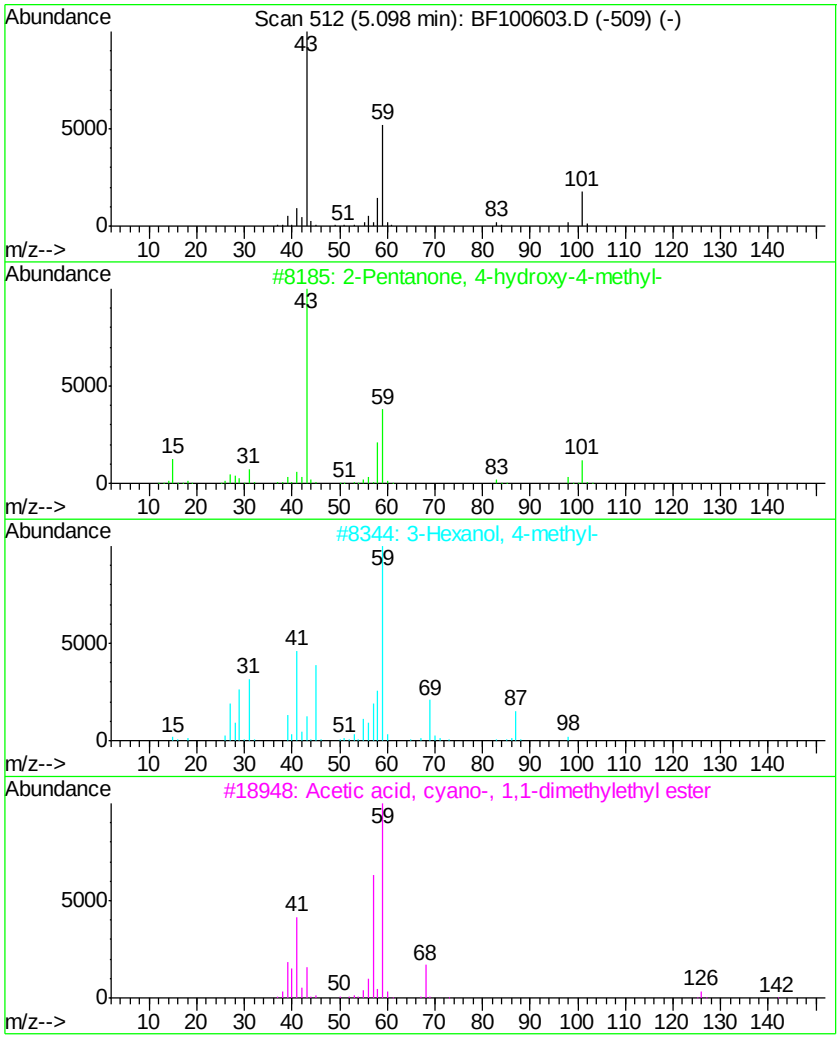
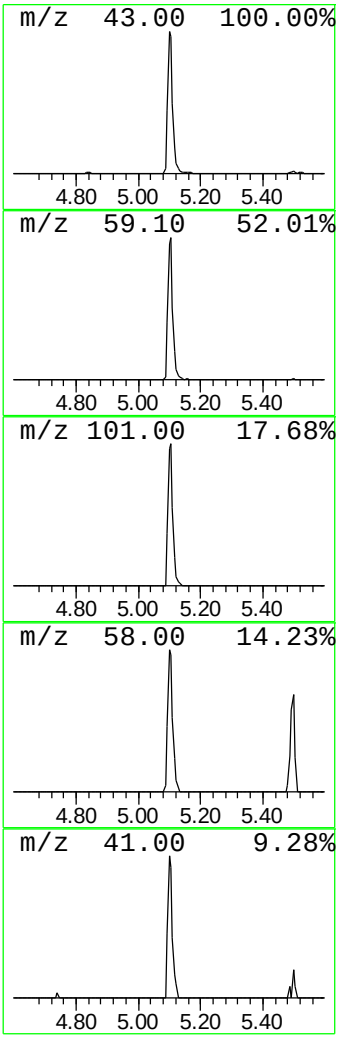
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.94 ng	228995	1,4-Dichlorobenzene-d4	6.88

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	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





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Operator : SJ/JU
Sample : I6426-01
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
110917-TIDO-E-D-B

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

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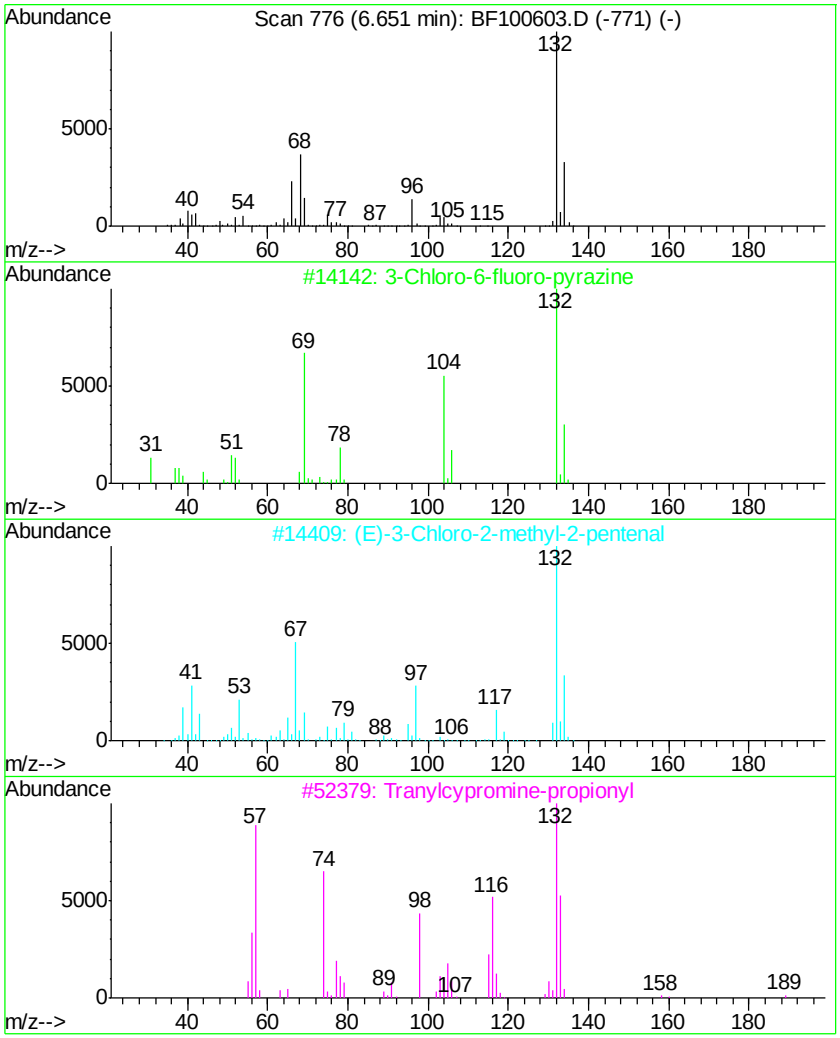
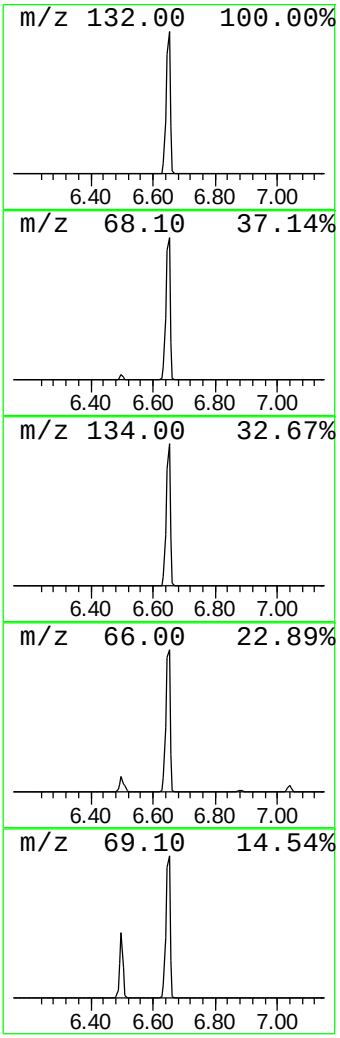
Peak Number 3 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	61.43 ng	2026930	1,4-Dichlorobenzene-d4	6.88

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	35
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





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ClientSampleId : 110917-TIDO-E-D-B

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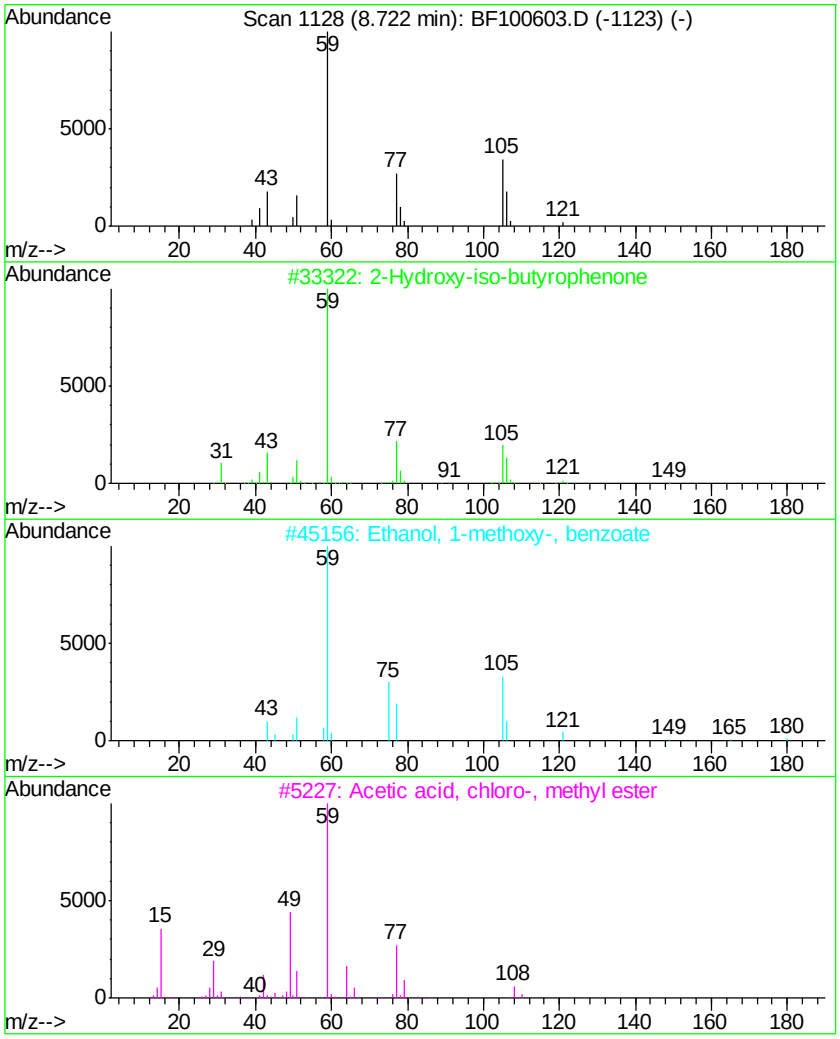
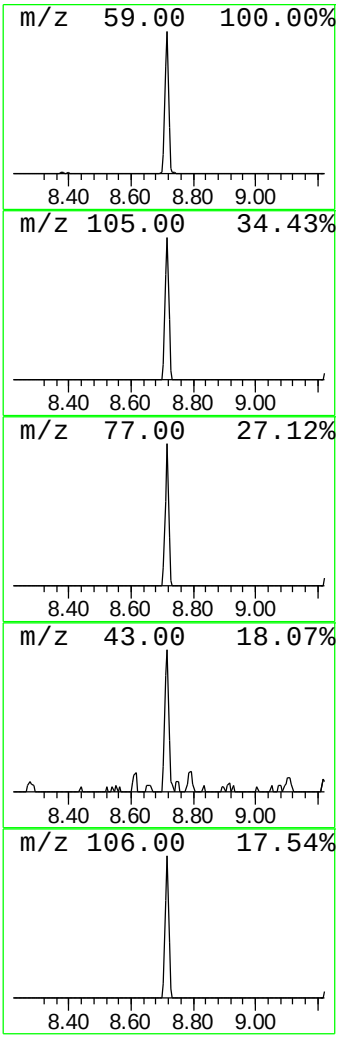
Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.22 ng	91743	Naphthalene-d8	8.16

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	56
3	Acetic acid, chloro-, methyl ester	108	C3H5ClO2	000096-34-4	9
4	Guanidine	59	CH5N3	000113-00-8	7
5	Acetamide	59	C2H5NO	000060-35-5	5





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

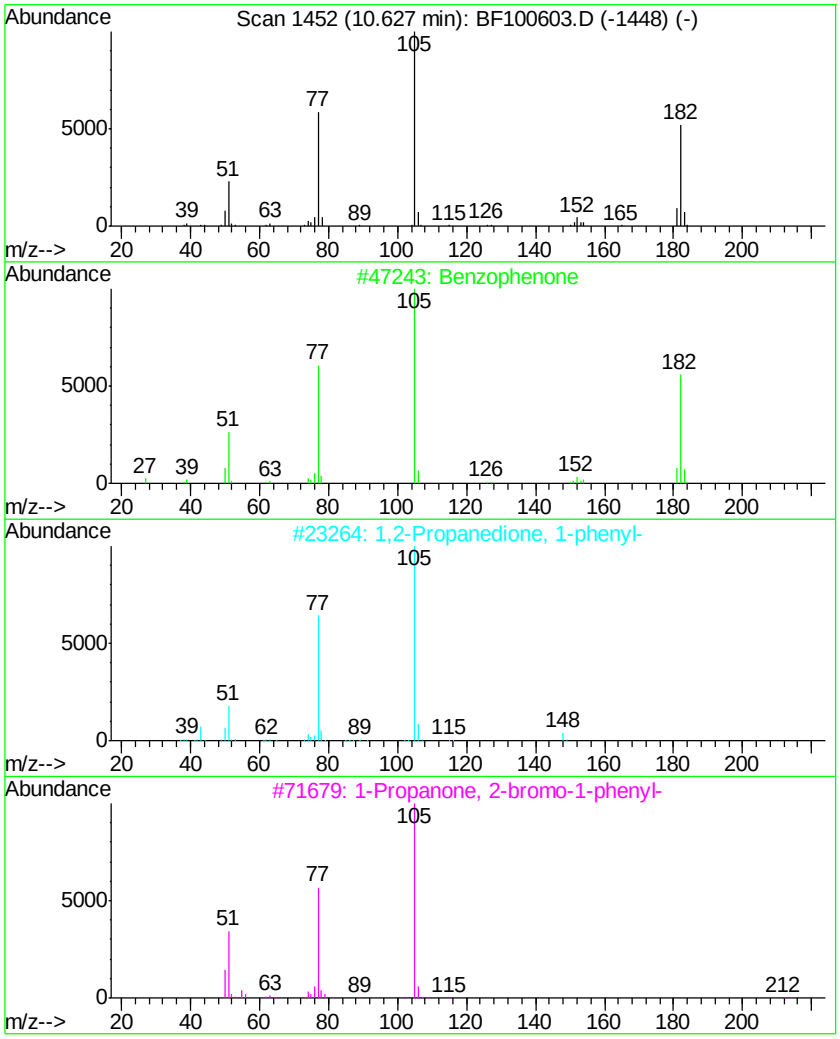
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

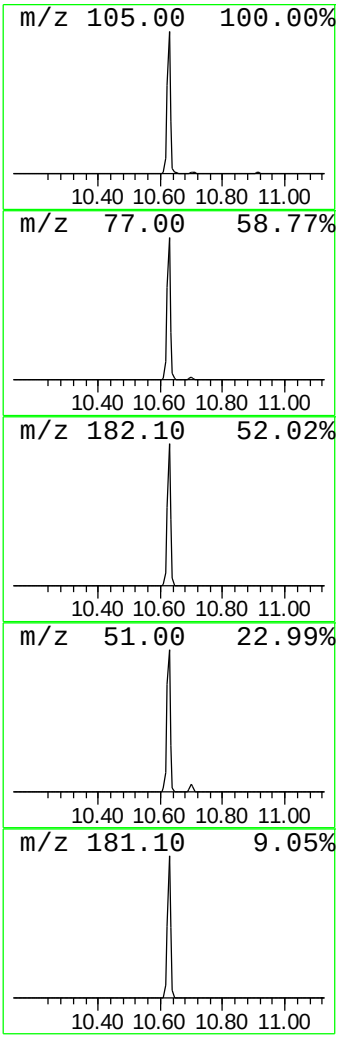
****

Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	4.52 ng	173228	Acenaphthene-d10	9.92

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5	2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47





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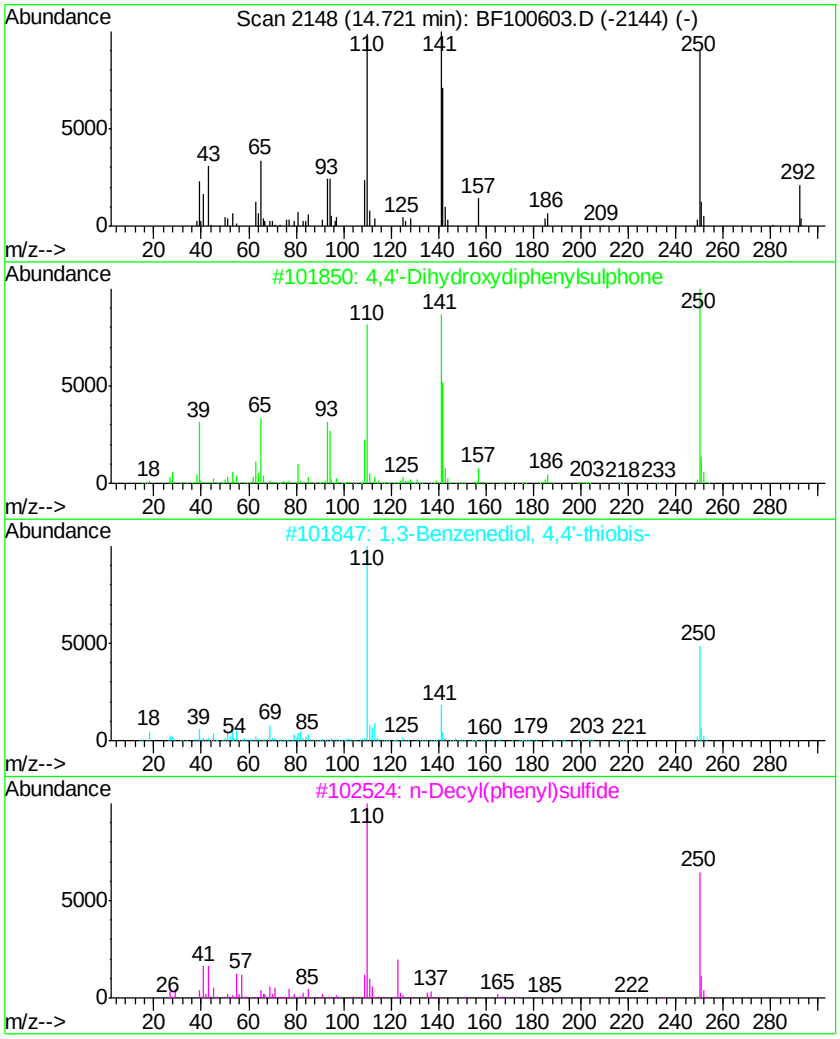
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

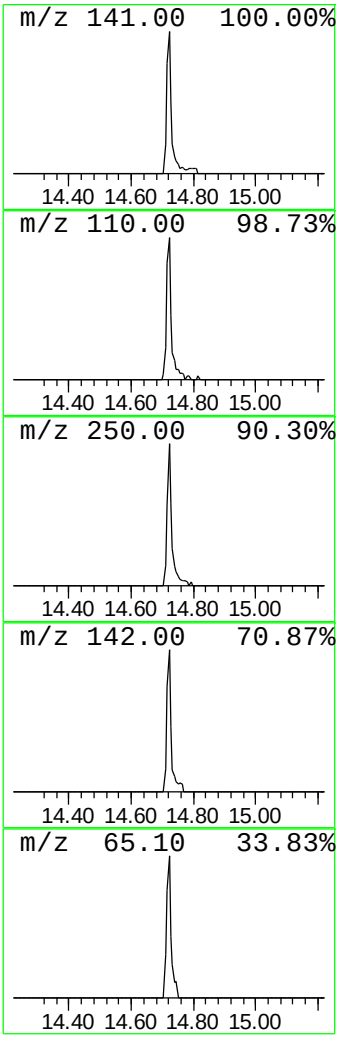
****

Peak Number 7 4,4'-Dihydroxydiphenylsulphone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.72	3.37 ng	100341	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	97
2	1,3-Benzenediol, 4,4'-thiobis-	250	C12H10O4S	000097-29-0	64
3	n-Decyl(phenyl)sulfide	250	C16H26S	013910-18-4	38
4	1H-Pyrazole-5-carboxylic acid, 4...	141	C4H7N5O	1000327-48-2	25
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	18





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
Butane, 2-methoxy...	2.18	3.0	ng	98654	1	6.88	659968	20.0
2-Pentanone, 4-hy...	5.10	6.9	ng	228995	1	6.88	659968	20.0
unknown6.65	6.65	61.4	ng	2026930	1	6.88	659968	20.0
2-Hydroxy-iso-but...	8.72	2.2	ng	91743	2	8.16	824818	20.0
Benzophenone	10.63	4.5	ng	173228	3	9.92	765651	20.0
4,4'-Dihydroxydip...	14.72	3.4	ng	100341	5	14.04	595121	20.0