LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040317\
Data File : BF094133.D
Acq On : 3 Apr 2017 20:55
Operator : SJ/MA
Sample : I2493-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP06-COMP

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-BF032217.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	2.263	61	64	69	rBV	76989	91657	3.97%	0.407%
2	3.340	237	247	249	rBV2	17947	43727	1.90%	0.194%
3	4.010	358	361	367	rBV	74743	81012	3.51%	0.360%
4	4.381	420	424	426	rBV	44404	49496	2.15%	0.220%
5	4.416	426	430	434	rVB	993578	934129	40.49%	4.153%
6	4.640	460	468	471	rBV2	41306	49869	2.16%	0.222%
7	5.363	588	591	594	rBV	44551	45824	1.99%	0.204%
8	5.445	601	605	608	rBV	37170	33403	1.45%	0.148%
9	5.487	608	612	618	rBV	1071657	997603	43.24%	4.435%
10	5.628	632	636	640	rBV	1111898	1018249	44.14%	4.527%
11	5.692	644	647	650	rBV	112589	100737	4.37%	0.448%
12	5.887	676	680	684	rBV	1052449	950006	41.18%	4.223%
13	5.957	688	692	694	rBV	38007	39259	1.70%	0.175%
14	6.063	701	710	713	rBV	890776	795195	34.47%	3.535%
15	6.263	740	744	747	rBV	55290	52152	2.26%	0.232%
16	6.351	755	759	763	rBV2	31100	36133	1.57%	0.161%
17	6.528	783	789	796	rBV	601926	591318	25.63%	2.629%
18	6.792	828	834	837	rBV	33026	31783	1.38%	0.141%
19	6.822	837	839	844	rVB	40329	38346	1.66%	0.170%
20	7.081	879	883	890	rBV4	43272	69273	3.00%	0.308%
21	7.292	915	919	924	rBV2	37131	43532	1.89%	0.194%
22	7.392	931	936	938	rBV	1267997	1251270	54.24%	5.563%
23	7.416	938	940	945	rVB	76716	78097	3.39%	0.347%
24	7.616	969	974	979	rVB	57720	67905	2.94%	0.302%
25	7.822	1003	1009	1011	rBV3	36107	42596	1.85%	0.189%
26	8.257	1079	1083	1087	rBV	103138	92236	4.00%	0.410%
27	8.322	1090	1094	1100	rVV	222423	245307	10.63%	1.091%
28	8.375	1100	1103	1106	rVB	54206	48401	2.10%	0.215%
29	8.569	1129	1136	1141	rBV3	51590	82009	3.55%	0.365%
30	8.710	1155	1160	1164	rBV	1298471	1164421	50.47%	5.177%
31	9.210	1237	1245	1249	rBV	1204565	1165288	50.51%	5.180%
32	9.263	1249	1254	1260	rVB8	16960	40909	1.77%	0.182%
33	9.351	1261	1269	1274	rBV3	90475	152826	6.62%	0.679%
34	9.533	1292	1300	1304	rBV	1235038	1278106	55.40%	5.682%

LSC Area Percent Report

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Operator : SJ/MA
Sample : I2493-04 5X
Misc :
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Instrument : BNA_F
ClientSampleId : LSS-SP06-COMP

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-BF032217.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.786	1340	1343	1348	rVB5	24119	37615	1.63%	0.167%
36	10.075	1388	1392	1396	rBV	717818	717250	31.09%	3.189%
37	10.122	1398	1400	1403	rVB2	43305	38466	1.67%	0.171%
38	10.204	1411	1414	1417	rBV	36474	42878	1.86%	0.191%
39	10.498	1460	1464	1471	rBV	444187	479510	20.79%	2.132%
40	10.586	1477	1479	1485	rVB6	33961	41452	1.80%	0.184%
41	10.710	1497	1500	1501	rBV2	44852	44830	1.94%	0.199%
42	11.104	1564	1567	1572	rVB2	101004	101964	4.42%	0.453%
43	11.304	1598	1601	1605	rBV3	52420	67562	2.93%	0.300%
44	11.357	1606	1610	1612	rVV	1023616	967701	41.95%	4.302%
45	11.380	1612	1614	1617	rVB	181252	159000	6.89%	0.707%
46	11.445	1623	1625	1630	rVB	69354	60606	2.63%	0.269%
47	11.869	1694	1697	1700	rVB	205644	184962	8.02%	0.822%
48	12.851	1861	1864	1867	rVB	294519	294607	12.77%	1.310%
49	13.127	1908	1911	1914	rVB	306146	339762	14.73%	1.510%
50	13.333	1943	1946	1951	rVB	632290	612468	26.55%	2.723%
51	13.951	2048	2051	2056	rVB	597556	626552	27.16%	2.785%
52	14.615	2161	2164	2167	rVB	667957	671027	29.09%	2.983%
53	14.668	2170	2173	2177	rVB	687944	685487	29.71%	3.047%
54	14.904	2209	2213	2222	rVB	1944665	2306931	100.00%	10.256%
55	15.098	2243	2246	2249	rVB	504501	509896	22.10%	2.267%
56	18.568	2829	2836	2850	rVB	689201	1701531	73.76%	7.564%

Sum of corrected areas: 22494131

LSC Report - Integrated Chromatogram

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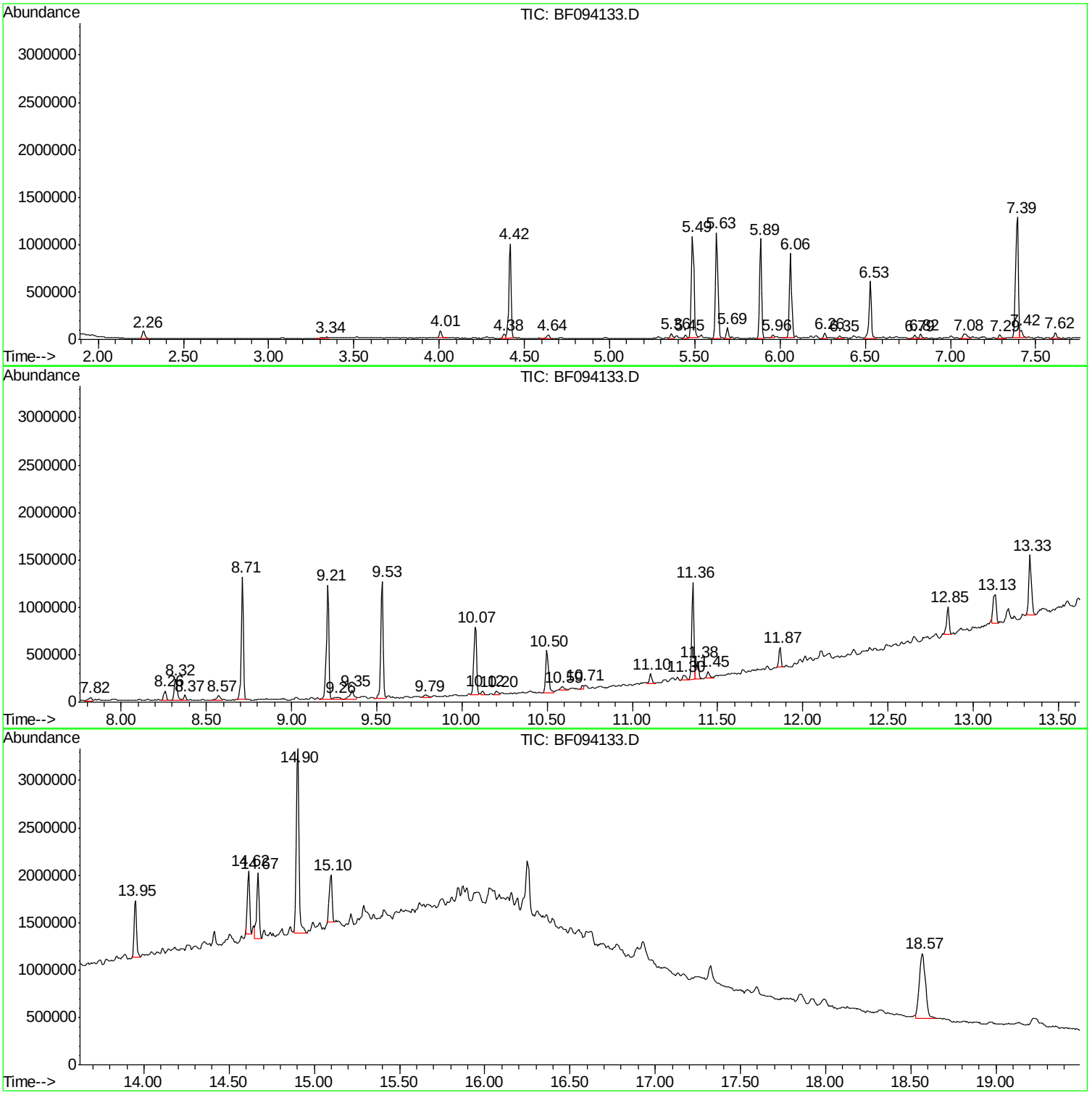
Sample : I2493-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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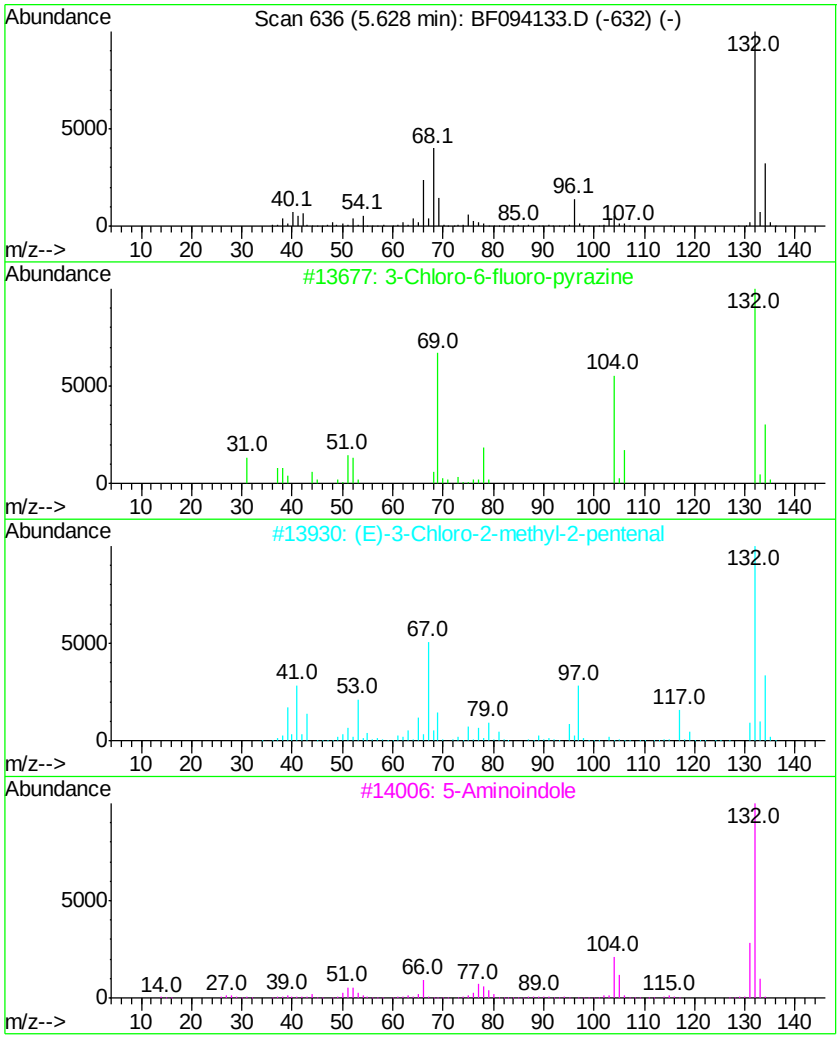
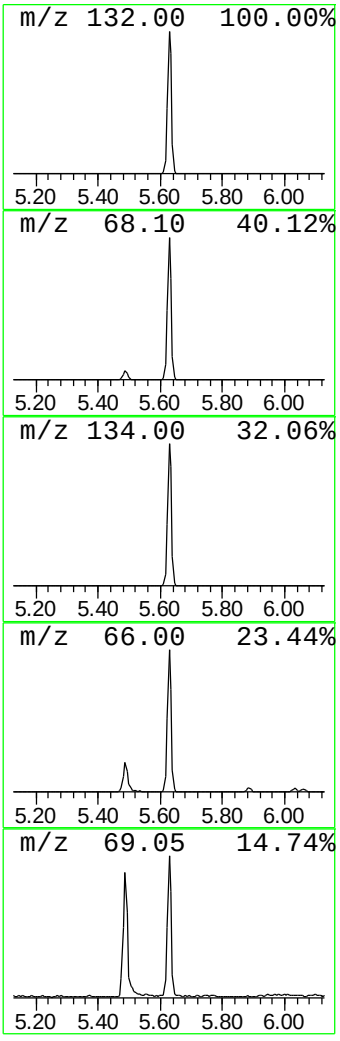
****

Peak Number 1 unknown5.63 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.63	21.44 ng	1018250	1,4-Dichlorobenzene-d4	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9





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Operator : SJ/MA
Sample : I2493-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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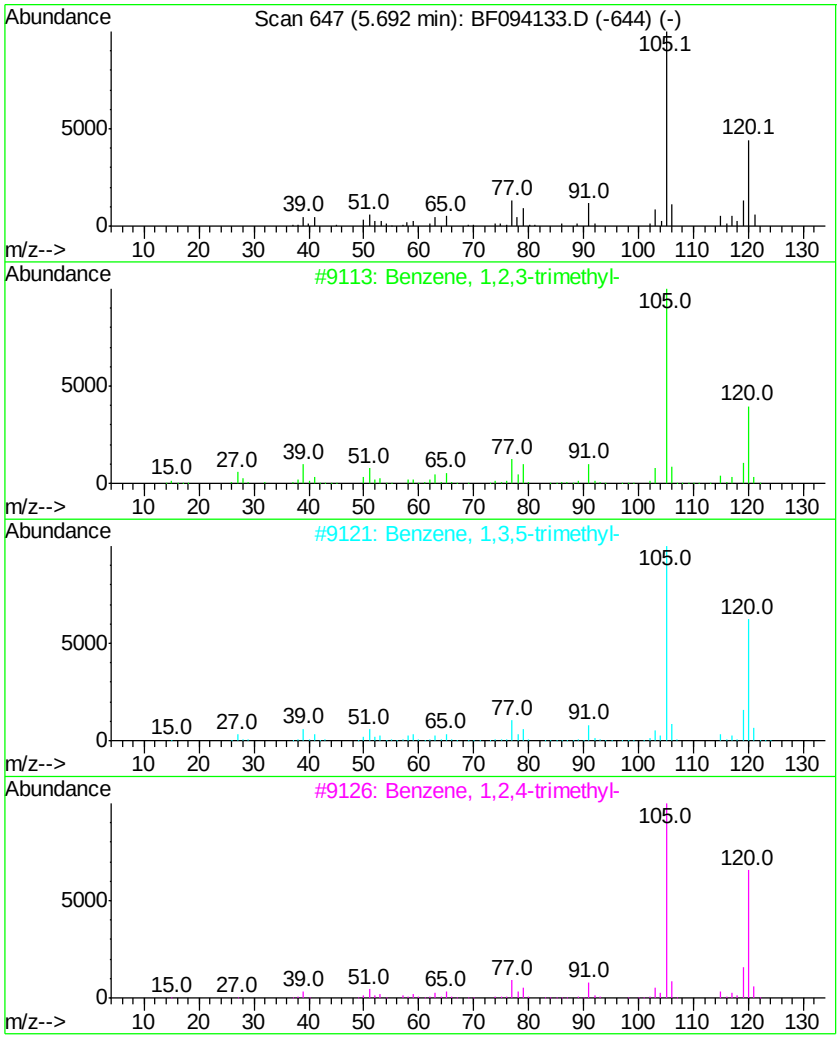
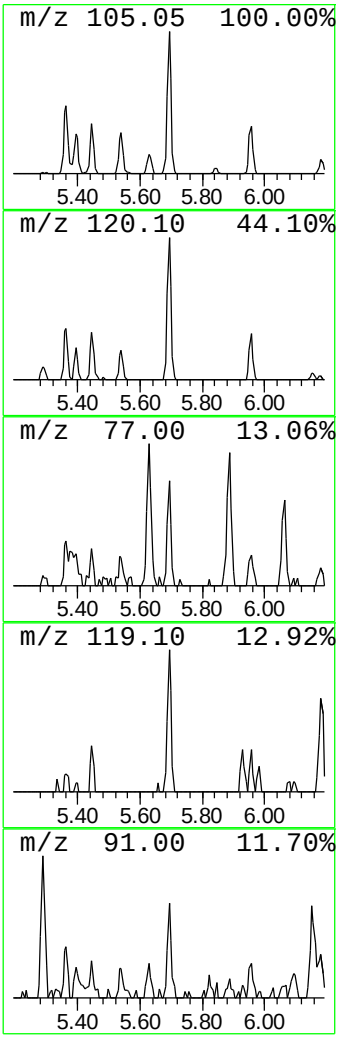
Peak Number 2 Benzene, 1,2,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.69	2.12 ng	100737	1,4-Dichlorobenzene-d4	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	94
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





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Operator : SJ/MA
Sample : I2493-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

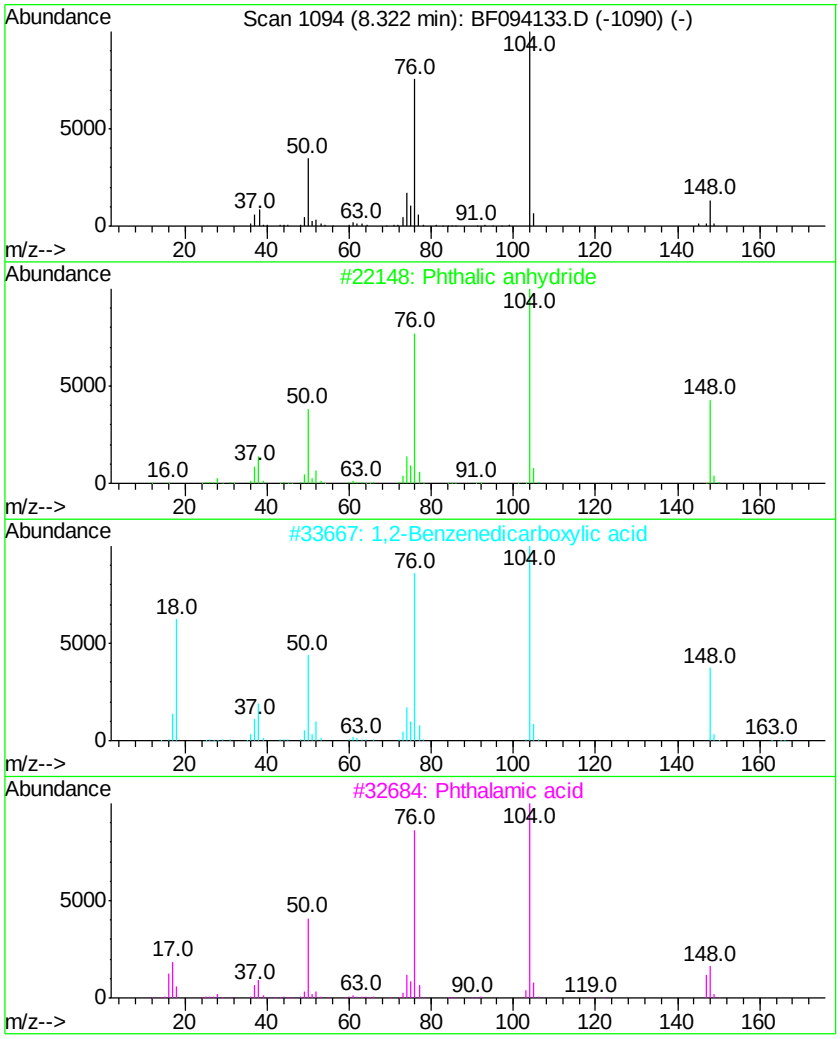
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

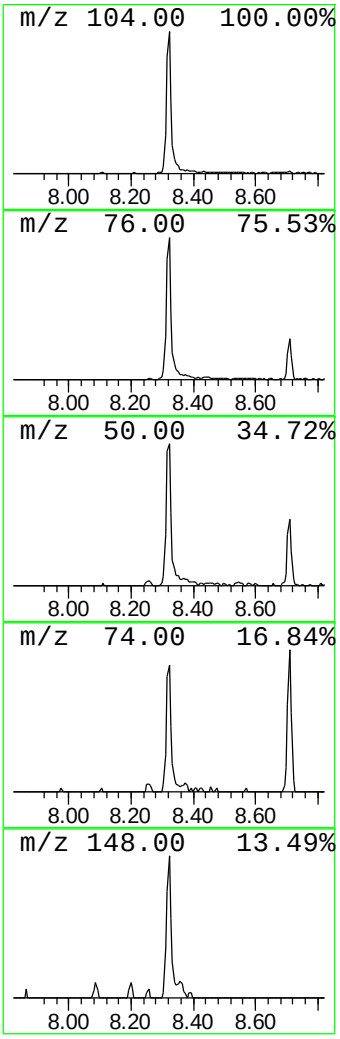
****

Peak Number 4 Phthalic anhydride Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.32	3.92 ng	245307	Naphthalene-d8	7.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic anhydride	148	C8H4O3	000085-44-9	95
2	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	83
3	Phthalamic acid	165	C8H7NO3	000088-97-1	83
4	Bicyclo[4.2.0]octa-1,3,5-triene-...	132	C8H4O2	006383-11-5	80
5	Phthalic acid, monoethyl ester	194	C10H10O4	002306-33-4	74





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Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
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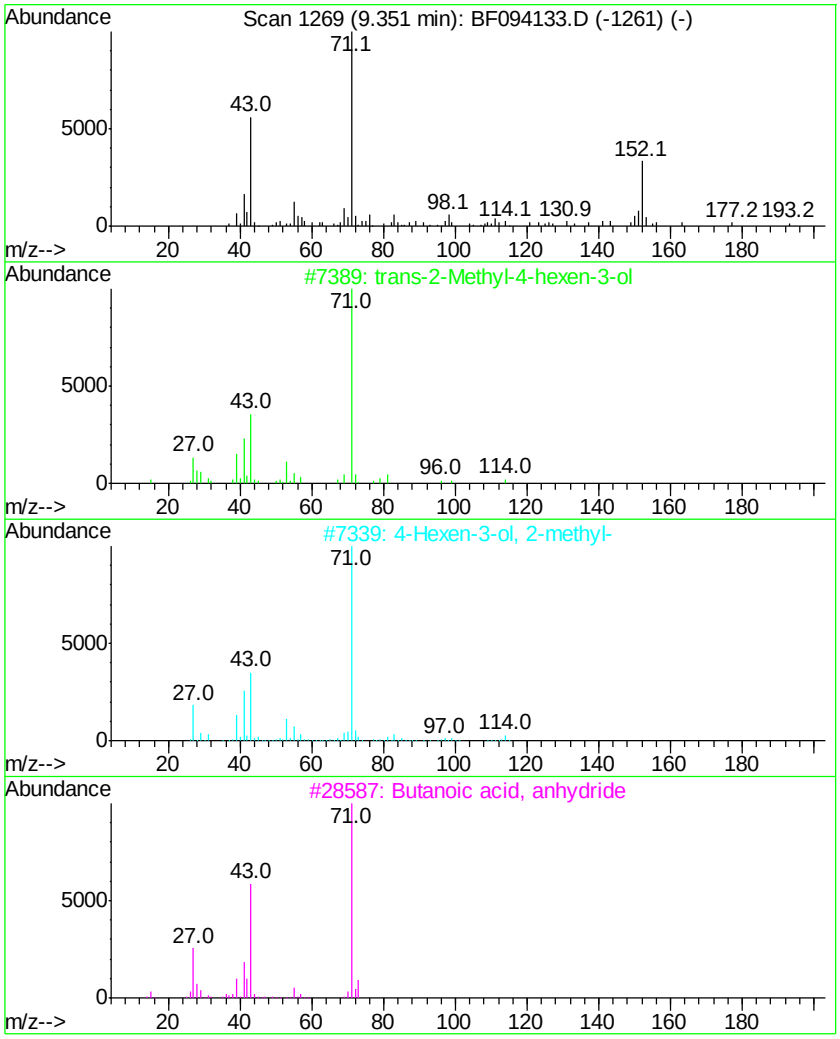
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

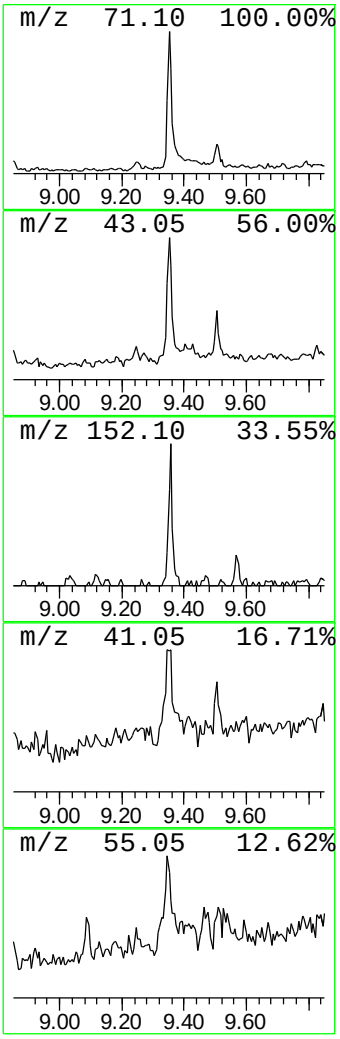
****

Peak Number 5 unknown9.35 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.35	2.39 ng	152826	Acenaphthene-d10	9.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-2-Methyl-4-hexen-3-ol	114	C7H14O	096346-76-8	49
2	4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	47
3	Butanoic acid, anhydride	158	C8H14O3	000106-31-0	47
4	Pentane, 3-bromo-	150	C5H11Br	001809-10-5	47
5	Propanamide, 2-methyl-2-(1-oxobu...	362	C15H17F3N2O5	110990-15-3	47





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Instrument : BNA_F
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TIC Library : C:\DATABASE\NIST02.L
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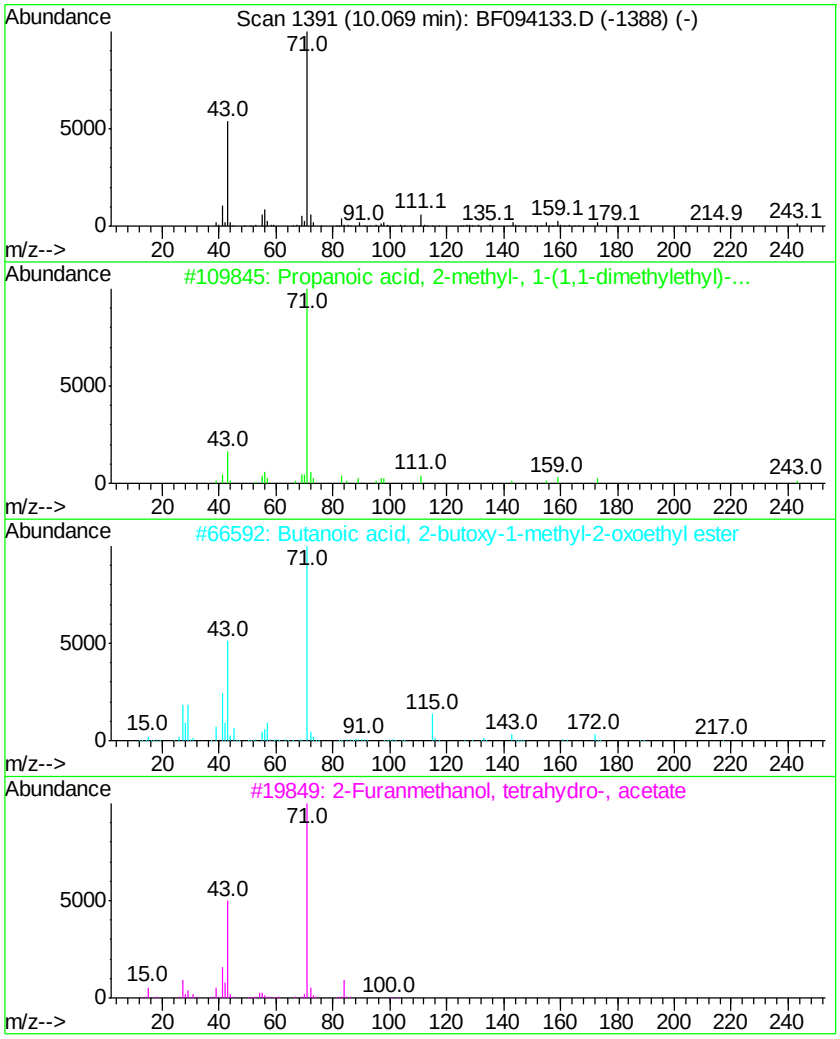
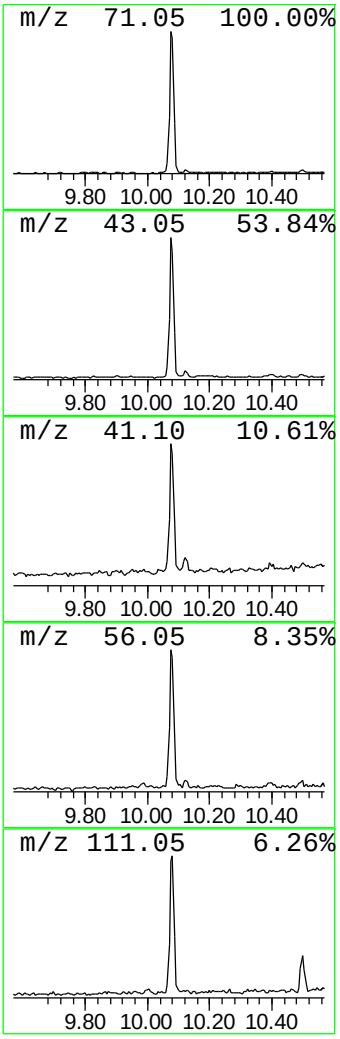
****

Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.07	11.22 ng	717250	Acenaphthene-d10	9.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	78
2	Butanoic acid, 2-butoxy-1-methyl...	216	C11H20O4	007492-70-8	50
3	2-Furanmethanol, tetrahydro-, ac...	144	C7H12O3	000637-64-9	50
4	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	40
5	Octanoic acid, 2-tetrahydrofuryl...	228	C13H24O3	033601-75-1	39





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TIC Library : C:\DATABASE\NIST02.L
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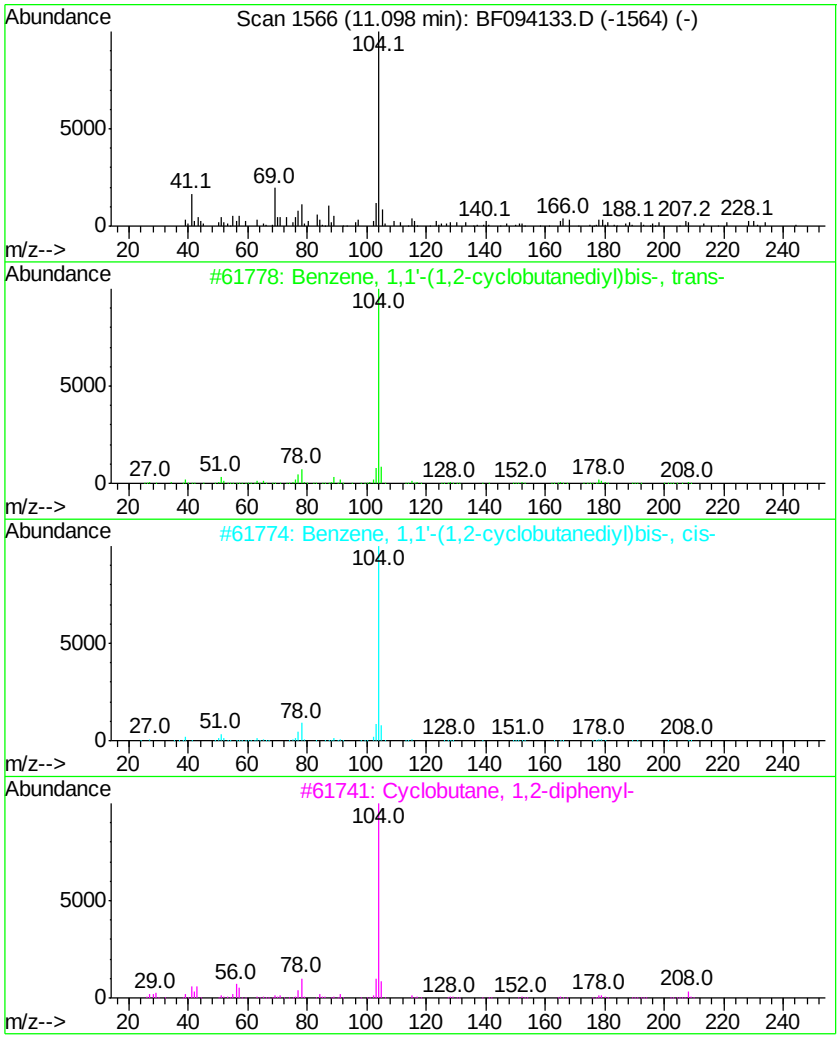
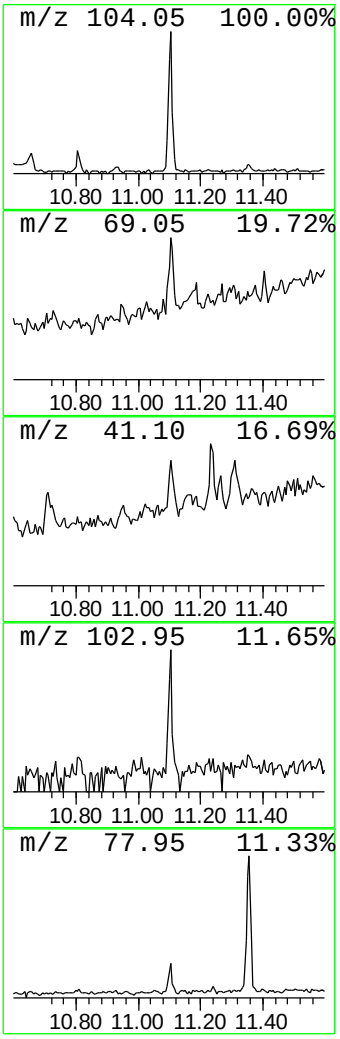
****

Peak Number 7 Benzene, 1,1'-(1,2-cyclobut... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.10	2.11 ng	101964	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	020071-09-4	68
2	Benzene, 1,1'-(1,2-cyclobutanedi...	208	C16H16	007694-30-6	64
3	Cyclobutane, 1,2-diphenyl-	208	C16H16	003018-21-1	59
4	Naphthalene, 1,2,3,4-tetrahydro-...	208	C16H16	029422-13-7	59
5	Cyclobutane, 1,3-diphenyl-, trans-	208	C16H16	025558-23-0	59





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Misc :
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Instrument : BNA_F
ClientSampleId : LSS-SP06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

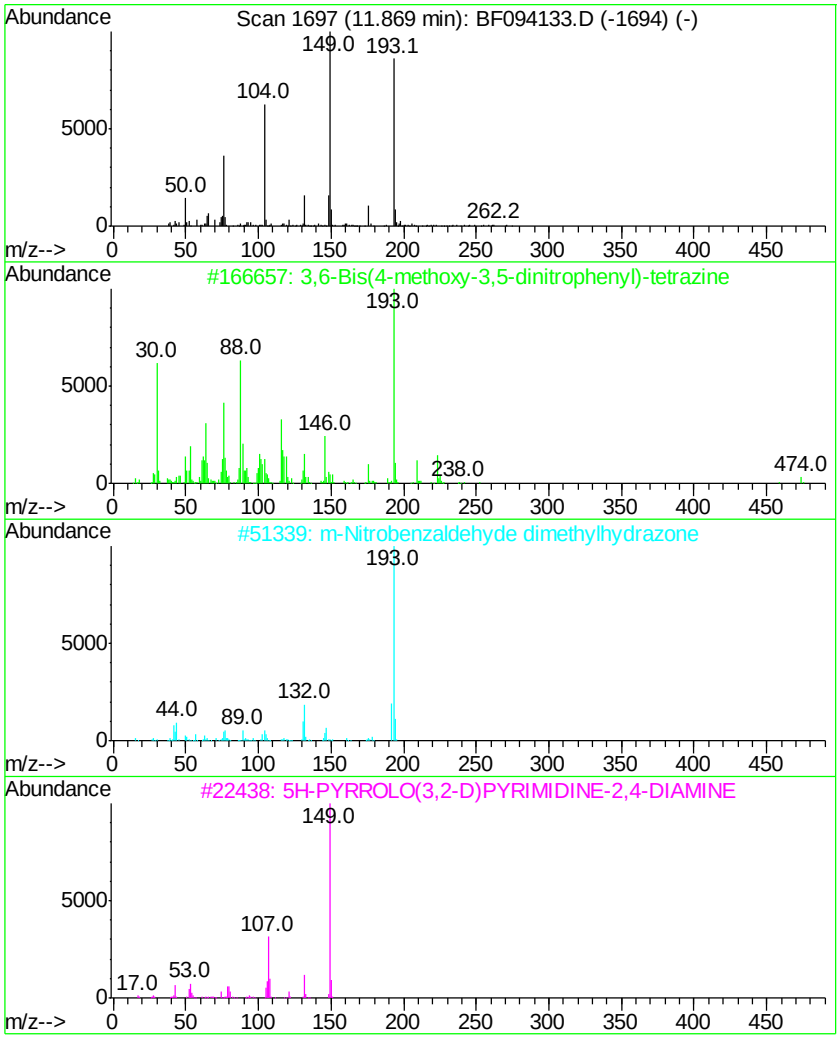
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

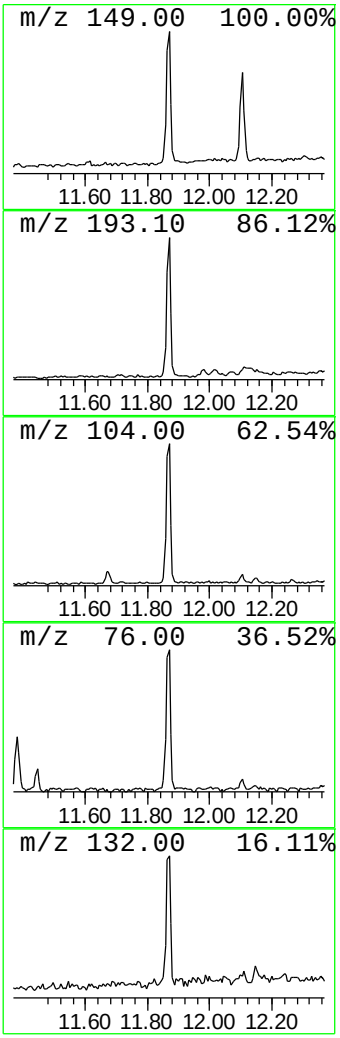
****

Peak Number 8 unknown11.87 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	3.82 ng	184962	Phenanthrene-d10	11.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6-Bis(4-methoxy-3,5-dinitrophe...	474	C16H10N8O10	1000075-22-6	32
2	m-Nitrobenzaldehyde dimethylhydr...	193	C9H11N3O2	032787-76-1	27
3	5H-PYRROLO(3,2-D)PYRIMIDINE-2,4-...	149	C6H7N5	1000244-21-4	22
4	3H-3,10a-Methano-1,2-benzodioxoc...	226	C13H22O3	095906-83-5	14
5	1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000084-78-6	12





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Misc :
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TIC Library : C:\DATABASE\NIST02.L
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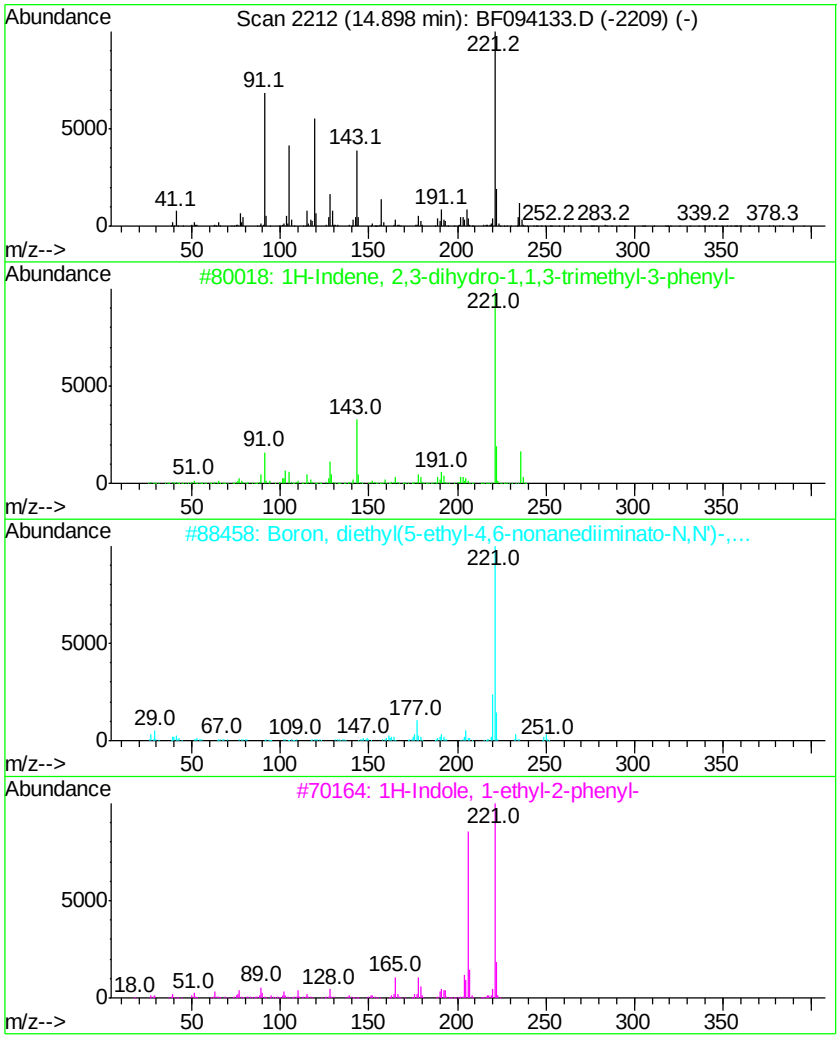
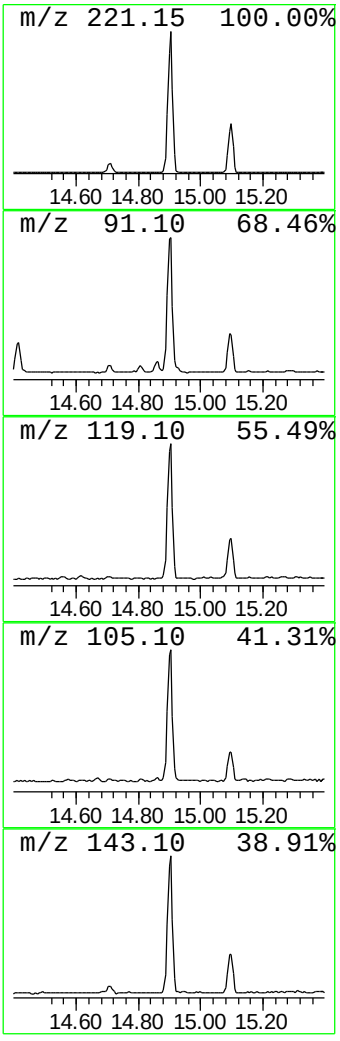
Peak Number 9 unknown14.90 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	68.76 ng	2306930	Chrysene-d12	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	47
2	Boron, diethyl(5-ethyl-4,6-nonan...	250	C15H31BN2	136705-03-8	35
3	1H-Indole, 1-ethyl-2-phenyl-	221	C16H15N	013228-39-2	35
4	Benzene, 1,1'-(1,3,3-trimethyl-1...	236	C18H20	006258-73-7	32
5	3-Methoxy-5-nitrobenzotrifluoride	221	C8H6F3NO3	000328-79-0	27





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Data File : BF094133.D
Acq On : 3 Apr 2017 20:55
Operator : SJ/MA
Sample : I2493-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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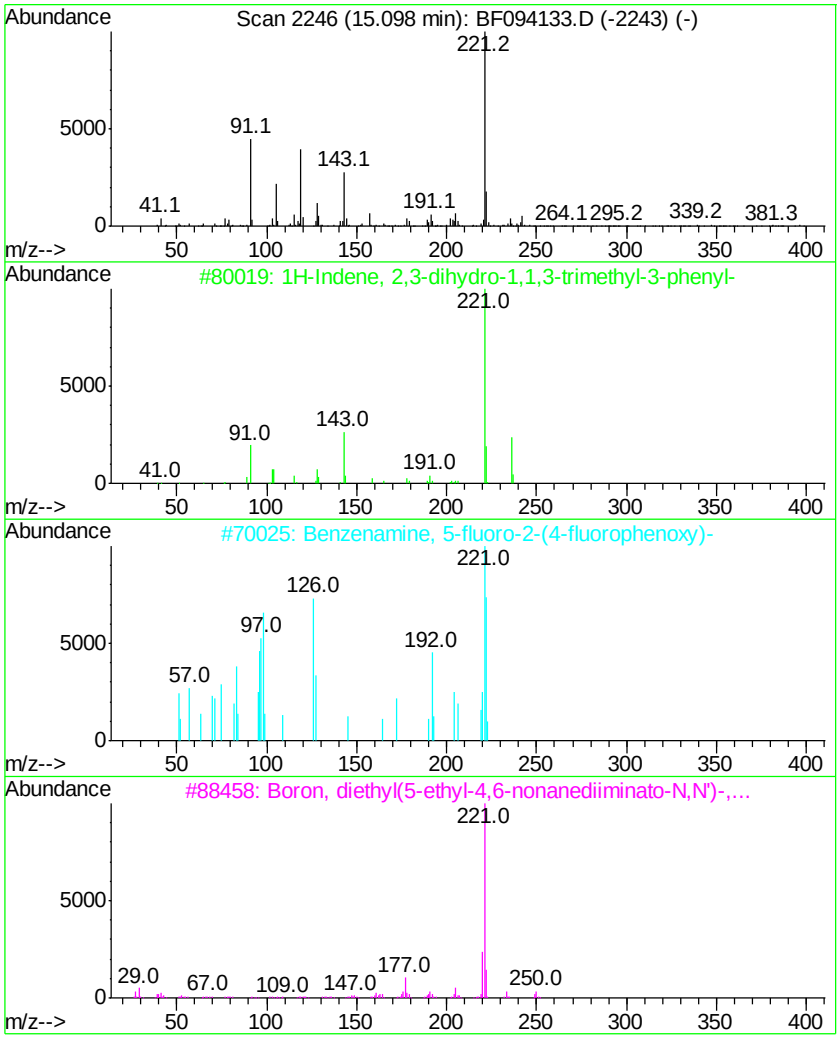
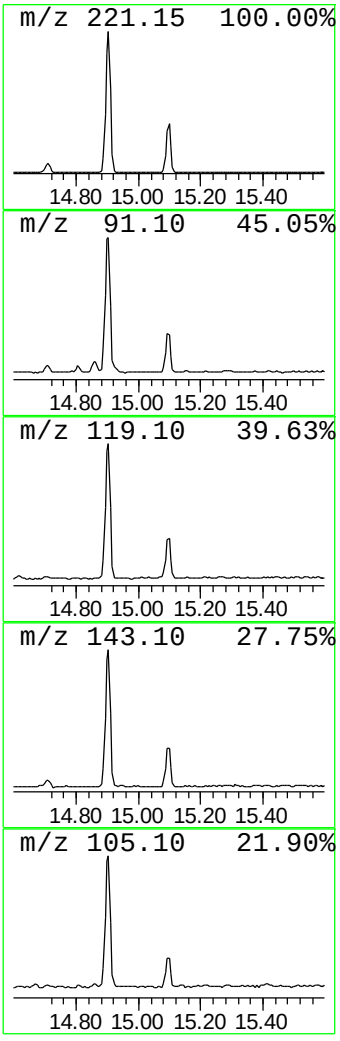
Peak Number 10 unknown15.10 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.10	15.20 ng	509896	Chrysene-d12	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-1,1,3-tri...	236	C18H20	003910-35-8	49
2	Benzenamine, 5-fluoro-2-(4-fluor...	221	C12H9F2NO	020653-64-9	46
3	Boron, diethyl(5-ethyl-4,6-nonan...	250	C15H31BN2	136705-03-8	35
4	1H-Naphtho[2,1-b]pyran-2-carboni...	388	C23H20N2O4	299198-80-4	25
5	1H-1,2,4-Triazole, 3,5-diphenyl-	221	C14H11N3	002039-06-7	25





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040317\
Data File : BF094133.D
Acq On : 3 Apr 2017 20:55
Operator : SJ/MA
Sample : I2493-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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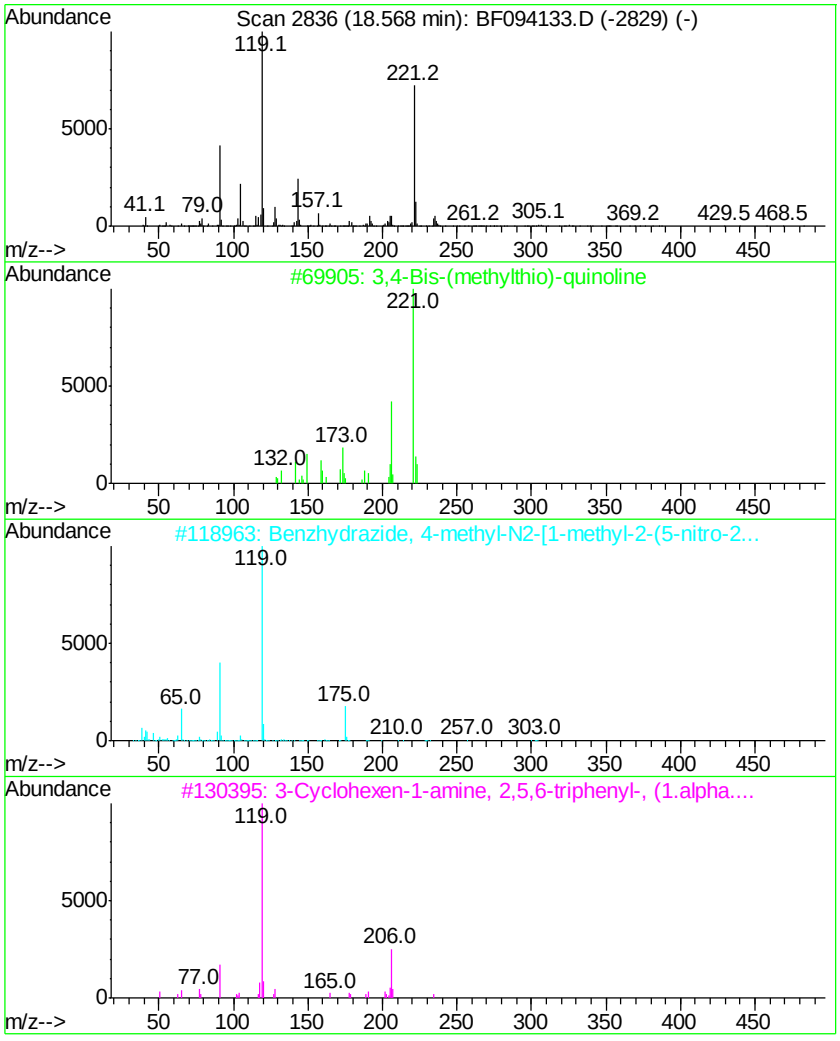
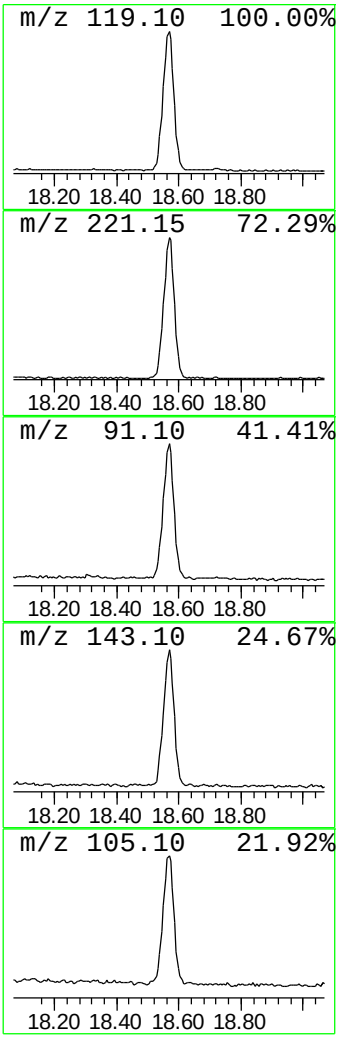
Peak Number 11 unknown18.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.57	66.74 ng	1701530	Perylene-d12	16.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Bis-(methylthio)-quinoline	221	C11H11NS2	074579-34-3	43
2	Benzhydrazide, 4-methyl-N2-[1-me...	303	C12H13N7O3	324021-25-2	38
3	3-Cyclohexen-1-amine, 2,5,6-trip...	325	C24H23N	033512-00-4	38
4	Benzene, (1,1-dimethylnonyl)-	232	C17H28	055191-25-8	35
5	2,4,4,6-Tetramethyl-6-phenyl-1-h...	230	C17H26	1000293-27-9	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040317\
Data File : BF094133.D
Acq On : 3 Apr 2017 20:55
Operator : SJ/MA
Sample : I2493-04 5X
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP06-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.63	5.63	21.4	ng	1018250	1	5.89	950006	20.0
Benzene, 1,2,3-tr...	5.69	2.1	ng	100737	1	5.89	950006	20.0
Phthalic anhydride	8.32	3.9	ng	245307	2	7.39	1251270	20.0
unknown9.35	9.35	2.4	ng	152826	3	9.53	1278110	20.0
Propanoic acid, 2...	10.07	11.2	ng	717250	3	9.53	1278110	20.0
Benzene, 1,1'-(1,...	11.10	2.1	ng	101964	4	11.36	967701	20.0
unknown11.87	11.87	3.8	ng	184962	4	11.36	967701	20.0
unknown14.90	14.90	68.8	ng	2306930	5	14.62	671027	20.0
unknown15.10	15.10	15.2	ng	509896	5	14.62	671027	20.0
unknown18.57	18.57	66.7	ng	1701530	6	16.25	509896	20.0