LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040317\
Data File : BF094134.D
Acq On : 3 Apr 2017 21:22
Operator : SJ/MA
Sample : I2493-06 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP07-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	60	64	69	rVB	108674	127989	5.17%	0.813%
2	3.322	232	244	247	rBV6	13479	31673	1.28%	0.201%
3	4.010	358	361	367	rVB	79219	81371	3.29%	0.517%
4	4.381	421	424	426	rBV	36646	40887	1.65%	0.260%
5	4.416	426	430	434	rVB	899604	803408	32.47%	5.105%
6	4.640	464	468	476	rVB2	26021	28400	1.15%	0.180%
7	5.363	588	591	594	rBV	34191	33216	1.34%	0.211%
8	5.445	601	605	608	rBV	31407	30177	1.22%	0.192%
9	5.487	608	612	618	rVV	942849	899430	36.35%	5.715%
10	5.540	618	621	629	rVV2	42952	78312	3.17%	0.498%
11	5.628	632	636	640	rBV	926996	869506	35.14%	5.525%
12	5.692	644	647	650	rBV	77594	71489	2.89%	0.454%
13	5.887	676	680	684	rBV	881932	785305	31.74%	4.990%
14	5.951	684	691	699	rVV4	38989	80848	3.27%	0.514%
15	6.063	706	710	713	rBV	780114	685656	27.71%	4.357%
16	6.263	741	744	748	rBV	44395	42201	1.71%	0.268%
17	6.528	782	789	794	rBV	497111	495189	20.01%	3.146%
18	6.792	829	834	837	rBV	28928	27104	1.10%	0.172%
19	6.822	837	839	844	rVV	40612	37336	1.51%	0.237%
20	7.086	879	884	890	rBV4	36494	64222	2.60%	0.408%
21	7.292	915	919	923	rBV2	36491	40894	1.65%	0.260%
22	7.392	931	936	939	rBV	1040993	1057905	42.76%	6.722%
23	7.416	939	940	946	rVB2	100023	89520	3.62%	0.569%
24	7.822	1003	1009	1012	rBV2	37376	46034	1.86%	0.292%
25	8.257	1079	1083	1087	rBV	82310	79091	3.20%	0.503%
26	8.322	1087	1094	1098	rVV	65313	90815	3.67%	0.577%
27	8.375	1100	1103	1107	rVB	49774	45872	1.85%	0.291%
28	8.710	1156	1160	1164	rVB	1097229	1003723	40.57%	6.378%
29	9.022	1208	1213	1218	rBV3	20724	34116	1.38%	0.217%
30	9.210	1240	1245	1249	rVB	69334	71689	2.90%	0.456%
31	9.351	1263	1269	1275	rBV3	52658	98488	3.98%	0.626%
32	9.533	1292	1300	1304	rBV2	937739	1039009	41.99%	6.602%
33	9.786	1339	1343	1348	rVB5	22444	40006	1.62%	0.254%
34	9.839	1348	1352	1355	rBV4	21529	30230	1.22%	0.192%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040317\
Data File : BF094134.D
Acq On : 3 Apr 2017 21:22
Operator : SJ/MA
Sample : I2493-06 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP07-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	10.080	1390	1393	1397	rVB2	24699	28919	1.17%	0.184%
36	10.122	1397	1400	1403	rVB	37006	31569	1.28%	0.201%
37	10.204	1411	1414	1418	rBV	35371	45952	1.86%	0.292%
38	10.498	1460	1464	1471	rBV	374314	404627	16.35%	2.571%
39	10.586	1477	1479	1483	rBV5	22067	27934	1.13%	0.177%
40	10.710	1497	1500	1502	rBV2	41375	51133	2.07%	0.325%
41	10.763	1506	1509	1513	rVV5	24490	31418	1.27%	0.200%
42	11.104	1565	1567	1572	rVB3	60223	59677	2.41%	0.379%
43	11.263	1592	1594	1597	rVB	40435	32854	1.33%	0.209%
44	11.304	1599	1601	1606	rVB4	38328	43636	1.76%	0.277%
45	11.357	1606	1610	1613	rBV	820509	827356	33.44%	5.257%
46	11.380	1613	1614	1618	rVB	185828	158486	6.41%	1.007%
47	11.445	1623	1625	1629	rVB	67630	65995	2.67%	0.419%
48	12.851	1861	1864	1868	rVB	305538	302599	12.23%	1.923%
49	13.127	1908	1911	1915	rVB	340525	344352	13.92%	2.188%
50	13.215	1921	1926	1935	rBV	1990399	2474170	100.00%	15.721%
51	13.333	1943	1946	1952	rVB	548923	564347	22.81%	3.586%
52	14.615	2160	2164	2167	rBV2	543480	641326	25.92%	4.075%
53	16.251	2440	2442	2449	rVB3	484250	520848	21.05%	3.309%

Sum of corrected areas: 15738309

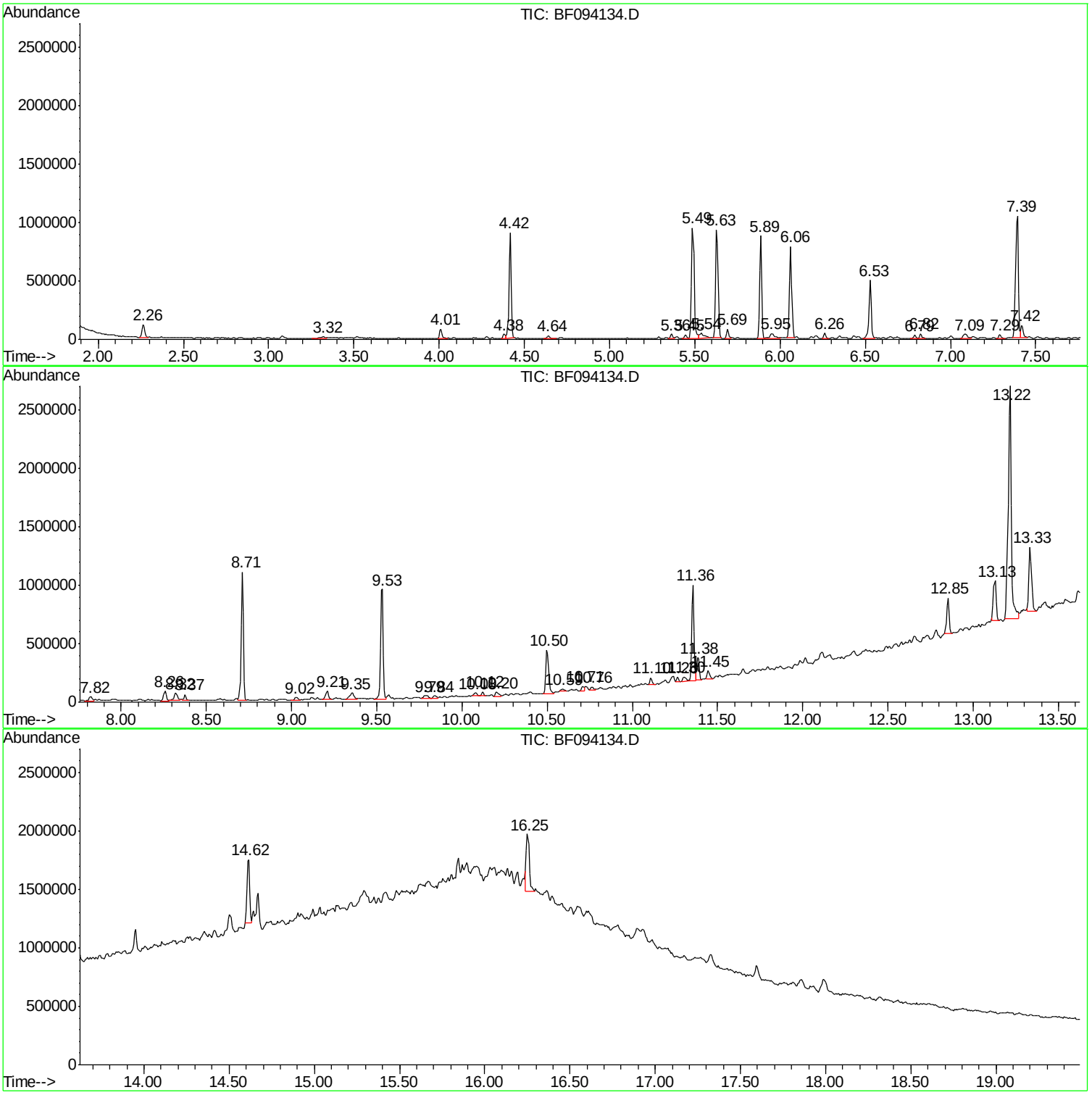
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040317\
Data File : BF094134.D
Acq On : 3 Apr 2017 21:22
Operator : SJ/MA
Sample : I2493-06 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP07-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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF040317\
Data File : BF094134.D
Acq On : 3 Apr 2017 21:22
Operator : SJ/MA
Sample : I2493-06 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP07-COMP

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

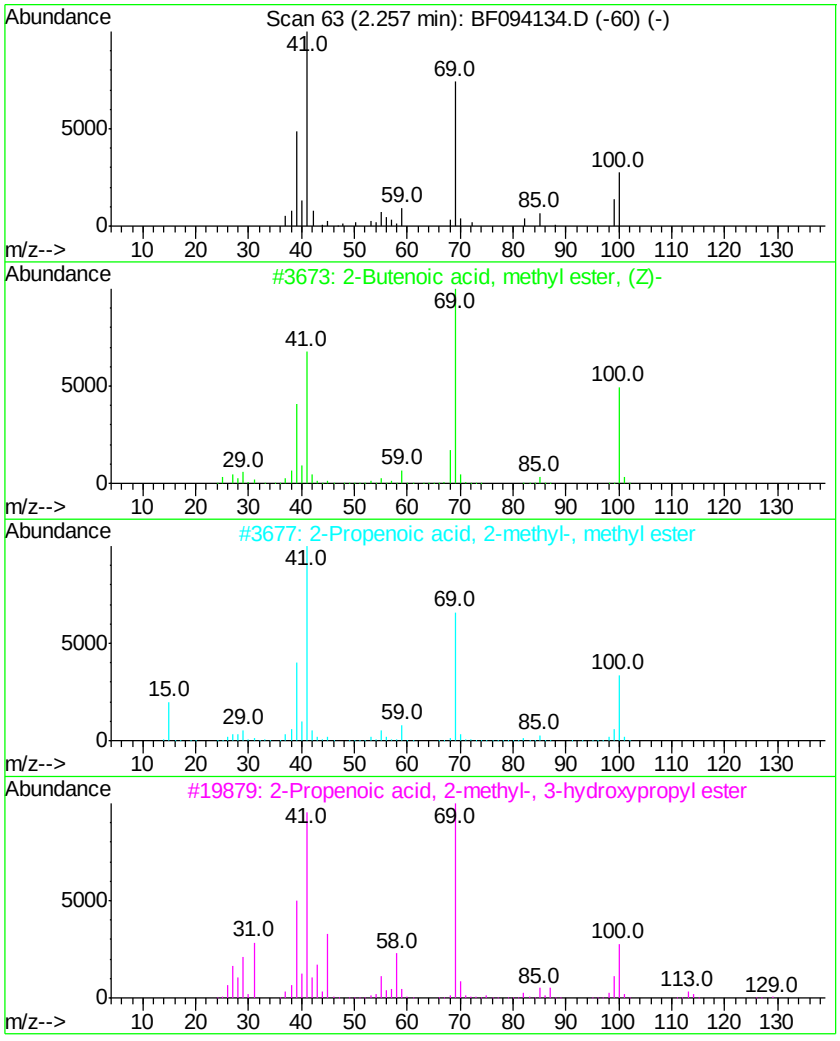
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

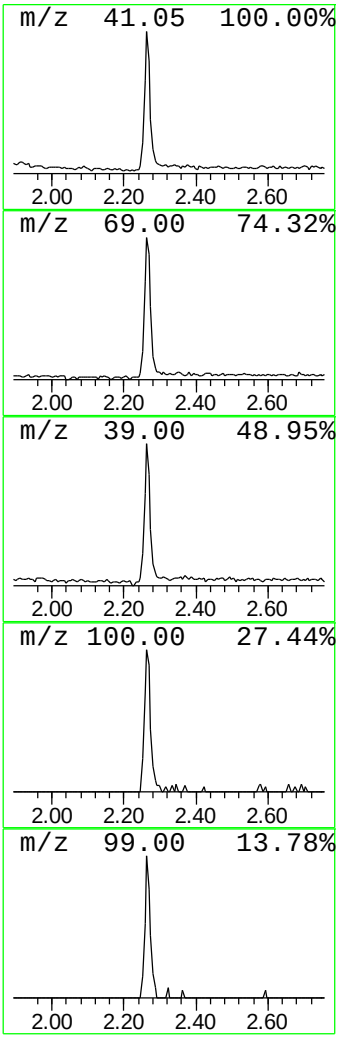
****

Peak Number 1 2-Butenoic acid, methyl est... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	3.26 ng	127989	1,4-Dichlorobenzene-d4	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, methyl ester, (Z)-	100	C5H8O2	004358-59-2	83
2	2-Propenoic acid, 2-methyl-, met...	100	C5H8O2	000080-62-6	80
3	2-Propenoic acid, 2-methyl-, 3-h...	144	C7H12O3	002761-09-3	72
4	2-Propenoic acid, 2-methyl-, 2-h...	144	C7H12O3	000923-26-2	64
5	2-Butenoic acid, methyl ester, (E)-	100	C5H8O2	000623-43-8	45





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040317\
Data File : BF094134.D
Acq On : 3 Apr 2017 21:22
Operator : SJ/MA
Sample : I2493-06 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP07-COMP

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

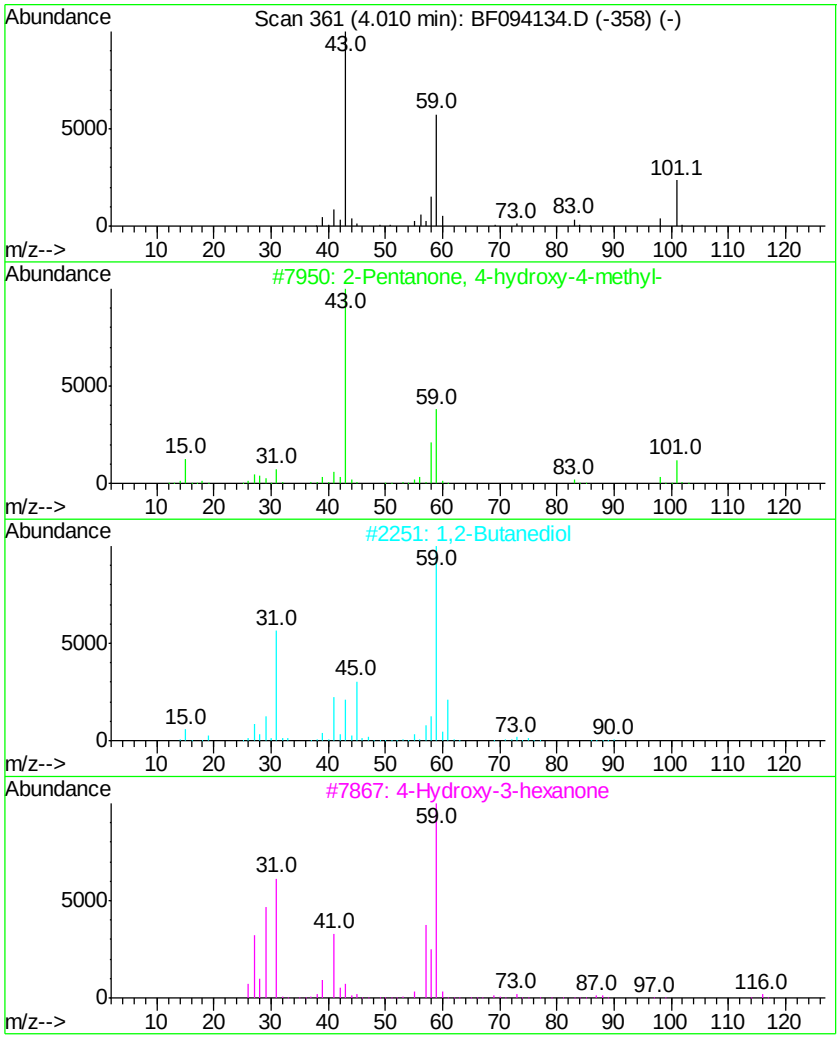
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

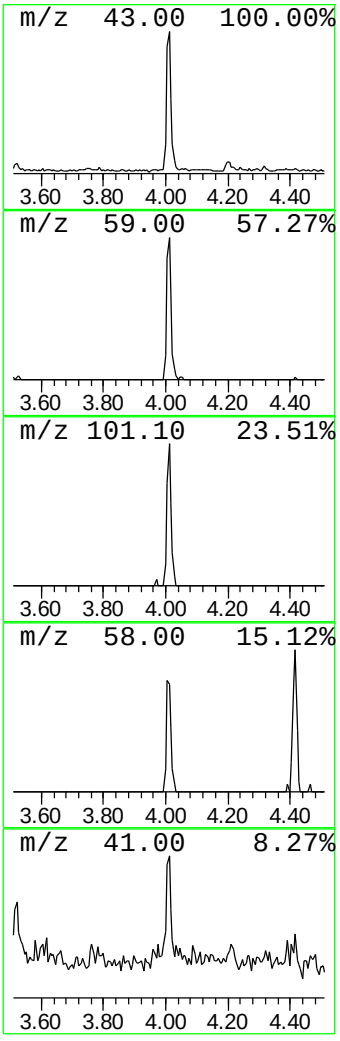
****

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.01	2.07 ng	81371	1,4-Dichlorobenzene-d4	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39
2	1,2-Butanediol	90	C4H10O2	000584-03-2	23
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Guanidine	59	CH5N3	000113-00-8	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040317\
Data File : BF094134.D
Acq On : 3 Apr 2017 21:22
Operator : SJ/MA
Sample : I2493-06 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP07-COMP

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

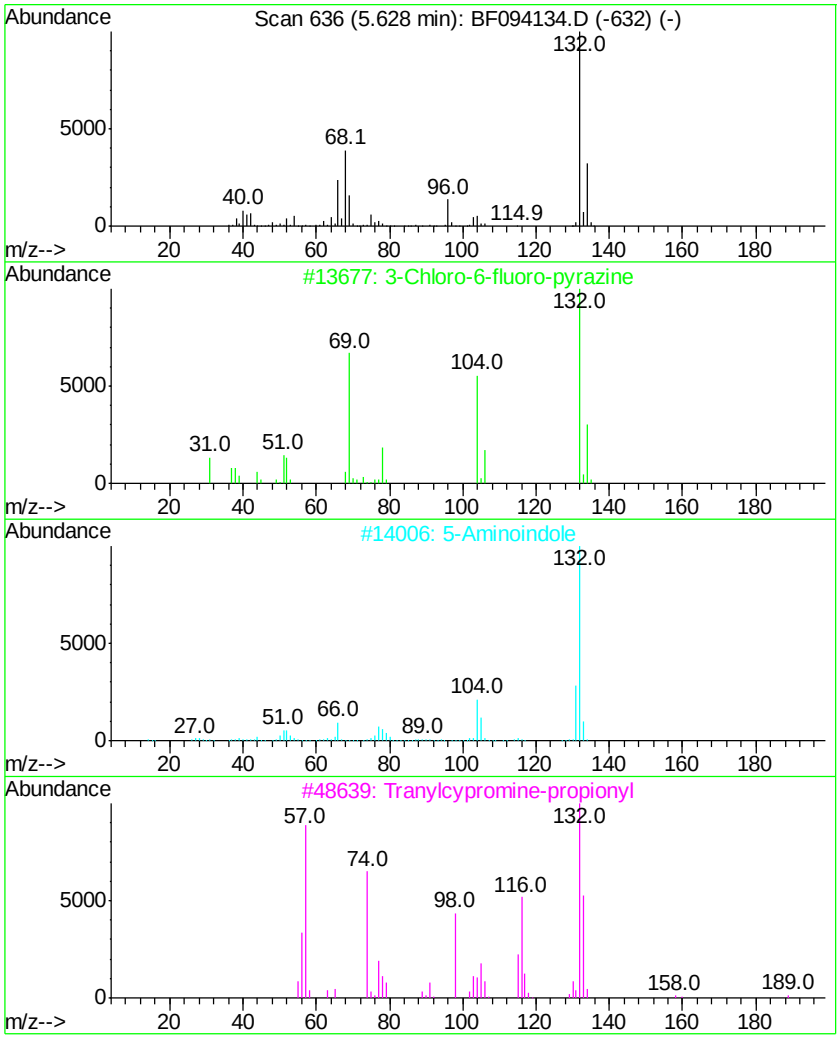
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

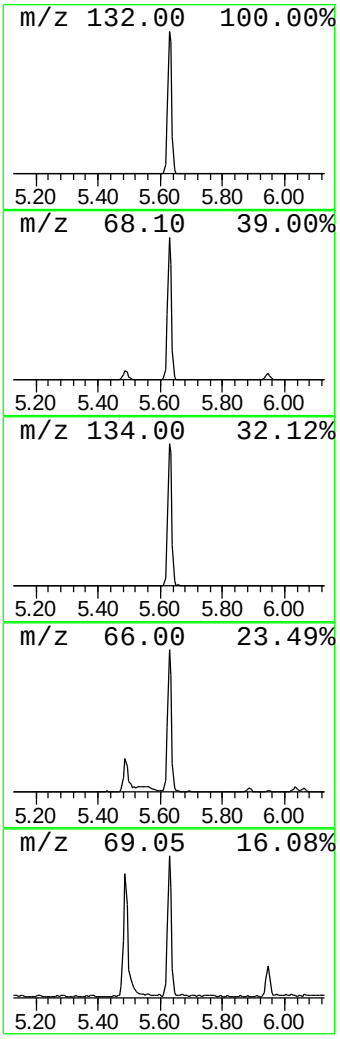
****

Peak Number 3 unknown5.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.63	22.14 ng	869506	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	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF040317\
Data File : BF094134.D
Acq On : 3 Apr 2017 21:22
Operator : SJ/MA
Sample : I2493-06 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP07-COMP

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

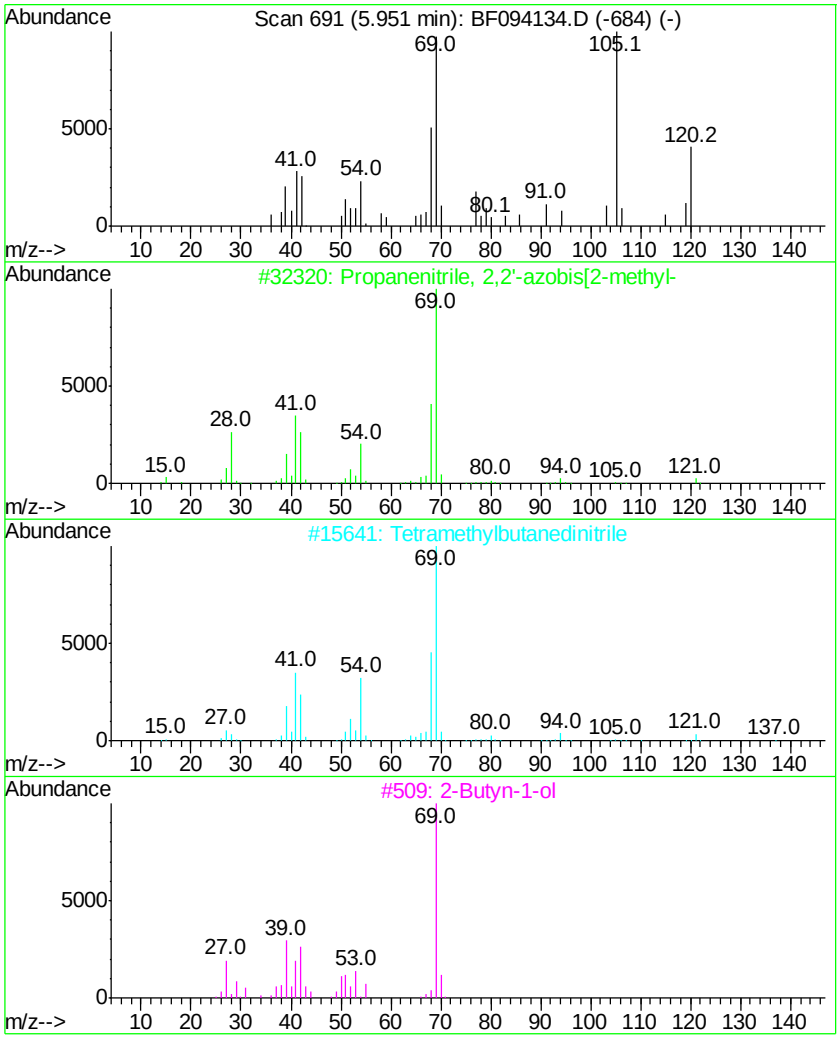
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

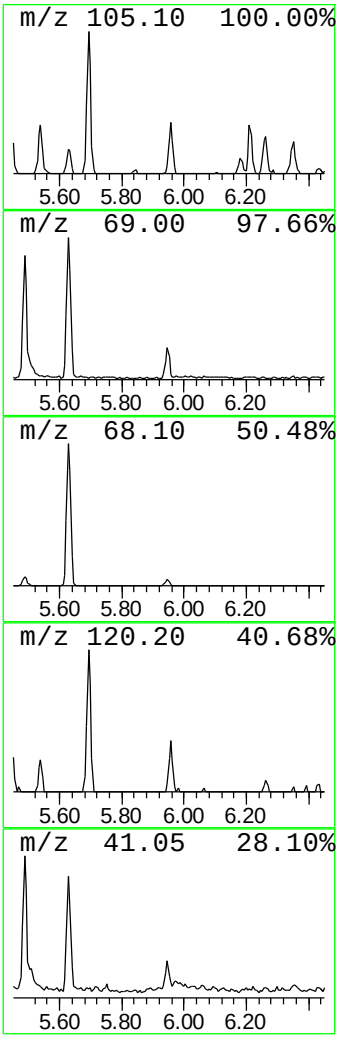
****

Peak Number 4 Propanenitrile, 2,2'-azobis... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.95	2.06 ng	80848	1,4-Dichlorobenzene-d4	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanenitrile, 2,2'-azobis[2-me...	164	C8H12N4	000078-67-1	50
2	Tetramethylbutanedinitrile	136	C8H12N2	003333-52-6	38
3	2-Butyn-1-ol	70	C4H6O	000764-01-2	27
4	Butane, 1,3-dichloro-2-methyl-	140	C5H10Cl2	023010-07-3	27
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	18





Data Path : Z:\HPCHEM1\BNA F\DATA\BF040317\
Data File : BF094134.D
Acq On : 3 Apr 2017 21:22
Operator : SJ/MA
Sample : I2493-06 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP07-COMP

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

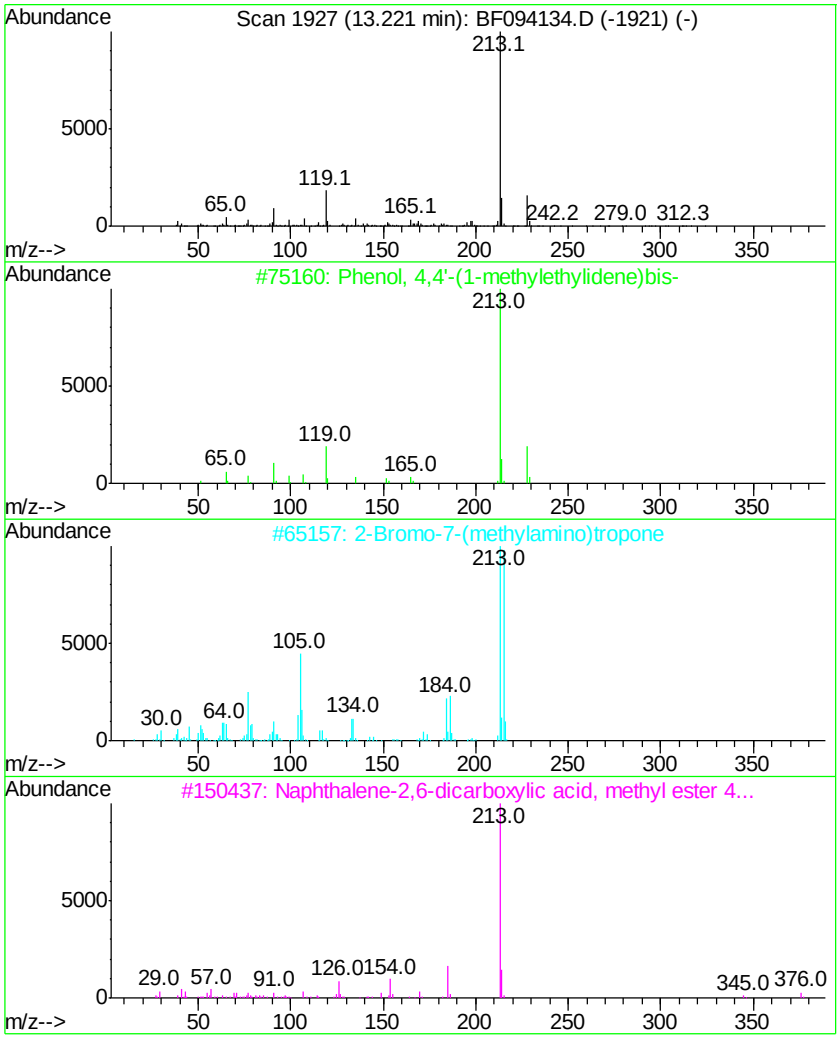
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

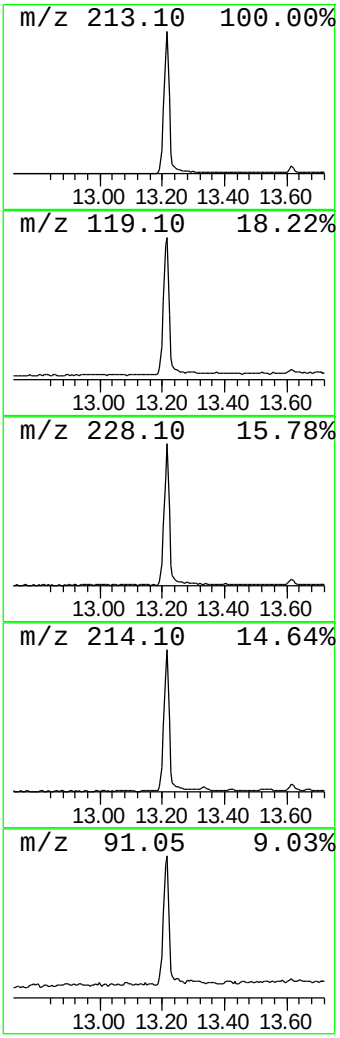
****

Peak Number 6 Phenol, 4,4'-(1-methylethyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.22	77.16 ng	2474170	Chrysene-d12	14.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	97
2	2-Bromo-7-(methylamino)tropone	213	C8H8BrNO	103539-25-9	50
3	Naphthalene-2,6-dicarboxylic aci...	376	C24H24O4	1000189-60-8	50
4	2-Trifluoromethyl-5-hydroxyquino...	213	C10H6F3NO	041958-06-9	45
5	1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	40





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040317\
Data File : BF094134.D
Acq On : 3 Apr 2017 21:22
Operator : SJ/MA
Sample : I2493-06 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : LSS-SP07-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
2-Butenoic acid, ...	2.26	3.3	ng	127989	1	5.89	785305	20.0
2-Pentanone, 4-hy...	4.01	2.1	ng	81371	1	5.89	785305	20.0
unknown5.63	5.63	22.1	ng	869506	1	5.89	785305	20.0
Propanenitrile, 2...	5.95	2.1	ng	80848	1	5.89	785305	20.0
Phenol, 4,4'-(1-m...	13.22	77.2	ng	2474170	5	14.62	641326	20.0