LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023396.D
Acq On : 2 Aug 2016 11:21
Operator : UM/SJ
Sample : H4145-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9536

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_G\METHODS\8270-BG080116.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	3.848	166	172	189	rBV	1166446	1933067	8.73%	0.576%
2	5.188	392	400	409	rBV	794260	1251306	5.65%	0.373%
3	5.663	474	481	496	rBV	2649433	4304910	19.43%	1.283%
4	7.279	748	756	769	rBV	2834196	4985855	22.51%	1.485%
5	7.649	810	819	829	rBV	2669287	4680504	21.13%	1.394%
6	8.007	872	880	890	rVV	3447953	5849324	26.40%	1.743%
7	8.119	892	899	902	rVV	443686	769216	3.47%	0.229%
8	8.154	902	905	914	rVB	684284	1117773	5.05%	0.333%
9	8.448	948	955	958	rBV	1891862	3589726	16.20%	1.069%
10	8.477	958	960	968	rVB	1496798	2127997	9.61%	0.634%
11	9.212	1077	1085	1092	rBV	1159020	2049823	9.25%	0.611%
12	9.300	1092	1100	1104	rVV	1696507	3315116	14.96%	0.988%
13	9.341	1104	1107	1114	rVB	1222708	1895329	8.56%	0.565%
14	9.864	1186	1196	1203	rBV	4156948	7576177	34.20%	2.257%
15	10.345	1271	1278	1286	rVB	1469969	2379913	10.74%	0.709%
16	10.956	1369	1382	1385	rBV	643895	1264764	5.71%	0.377%
17	11.003	1385	1390	1399	rVB	3066731	5782260	26.10%	1.723%
18	11.279	1430	1437	1449	rVB	1824026	3132829	14.14%	0.933%
19	12.607	1654	1663	1674	rBV	2399227	4048613	18.27%	1.206%
20	12.954	1713	1722	1730	rBV	3839108	6669777	30.11%	1.987%
21	13.400	1789	1798	1805	rBV	4718988	7647172	34.52%	2.278%
22	13.664	1835	1843	1854	rBV	7404247	12573163	56.75%	3.746%
23	14.234	1932	1940	1946	rBV	4522574	7463929	33.69%	2.224%
24	14.363	1955	1962	1969	rVB	2929735	4428548	19.99%	1.319%
25	14.786	2026	2034	2045	rVB2	1117316	1857542	8.38%	0.553%
26	15.151	2090	2096	2098	rBV	2665902	3902548	17.62%	1.163%
27	15.186	2098	2102	2112	rVB	4509347	7267131	32.80%	2.165%
28	15.597	2165	2172	2178	rBV	6840046	10304246	46.51%	3.070%
29	15.826	2204	2211	2220	rVB	7938265	11732146	52.96%	3.495%
30	16.044	2241	2248	2263	rBV	6832890	10349148	46.71%	3.083%
31	16.284	2281	2289	2299	rBV	3594089	5752687	25.97%	1.714%
32	16.725	2357	2364	2371	rVB	6545249	9346586	42.19%	2.785%
33	16.848	2378	2385	2391	rVB	3216427	4868463	21.98%	1.450%
34	17.547	2497	2504	2506	rBV	1386380	2078481	9.38%	0.619%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023396.D
Acq On : 2 Aug 2016 11:21
Operator : UM/SJ
Sample : H4145-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9536

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_G\METHODS\8270-BG080116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	17.594	2506	2512	2519	rVB	8067176	14132966	63.79%	4.211%
36	18.499	2659	2666	2671	rBV	5221021	7709524	34.80%	2.297%
37	19.844	2890	2895	2901	rBV	154172	223395	1.01%	0.067%
38	19.968	2908	2916	2927	rBV	9469581	15659306	70.68%	4.665%
39	20.156	2941	2948	2954	rBV	7414948	10442231	47.13%	3.111%
40	20.843	3058	3065	3070	rBV	10619913	13679809	61.75%	4.076%
41	21.718	3208	3214	3222	rBV	4277350	6075072	27.42%	1.810%
42	21.847	3227	3236	3243	rBV2	9680404	22154166	100.00%	6.600%
43	21.924	3243	3249	3261	rVB	10311167	18889112	85.26%	5.627%
44	24.168	3619	3631	3637	rBV	3710126	10169049	45.90%	3.030%
45	24.232	3637	3642	3652	rVB	1583875	3616385	16.32%	1.077%
46	25.108	3774	3791	3804	rBV	6174757	21138787	95.42%	6.298%
47	25.243	3804	3814	3826	rVB2	831791	2408275	10.87%	0.717%
48	27.011	4106	4115	4126	rVB4	138005	512757	2.31%	0.153%
49	29.132	4454	4476	4477	rBV3	1996218	7554963	34.10%	2.251%
50	30.348	4659	4683	4704	rVB3	2439567	12996804	58.67%	3.872%

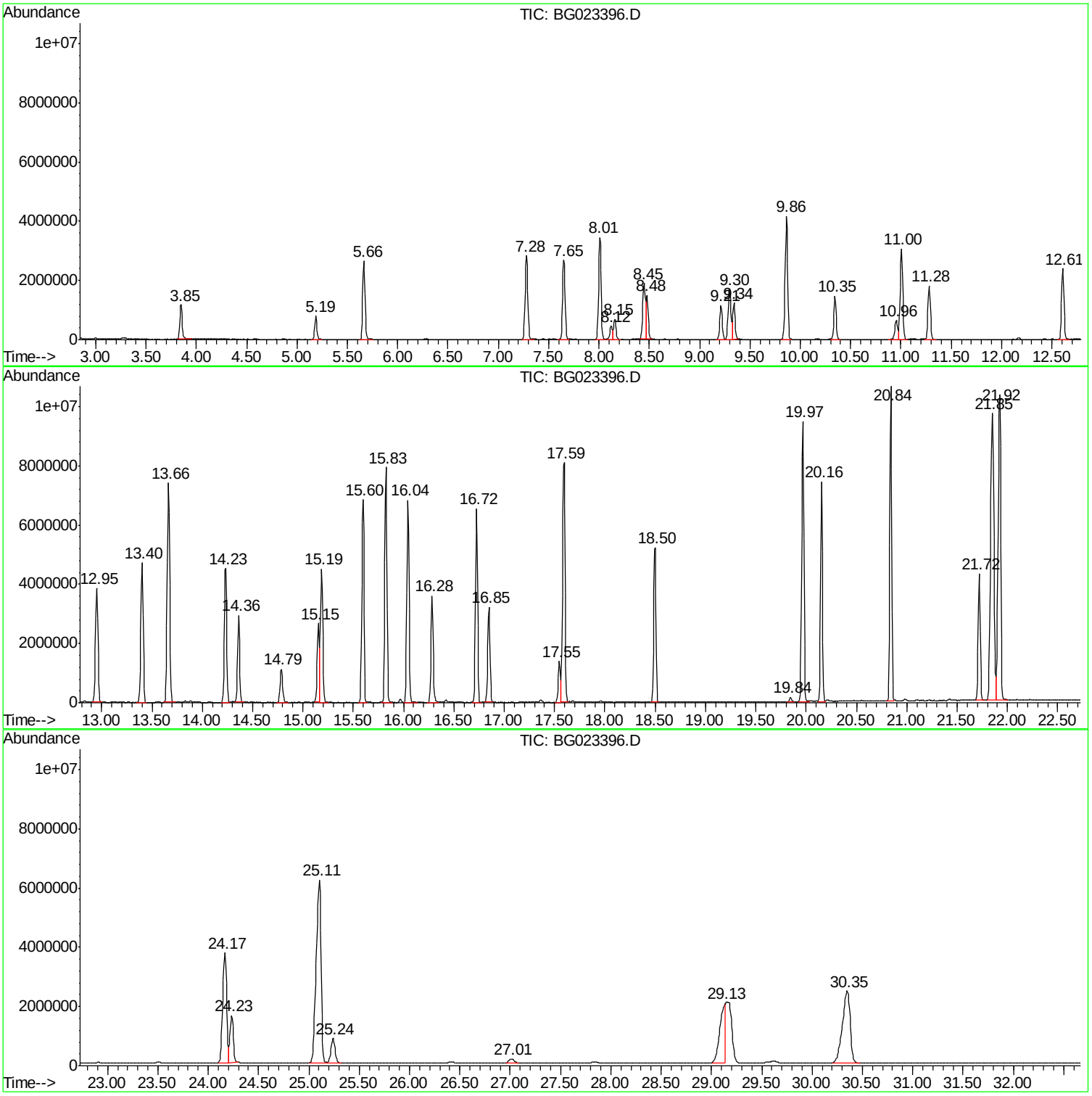
Sum of corrected areas: 335658670

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023396.D
Acq On : 2 Aug 2016 11:21
Operator : UM/SJ
Sample : H4145-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
9536

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023396.D
Acq On : 2 Aug 2016 11:21
Operator : UM/SJ
Sample : H4145-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9536

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

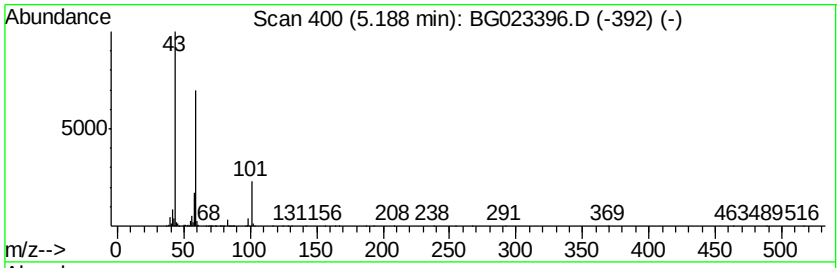
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

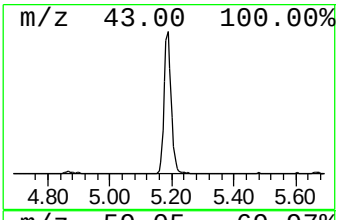
****

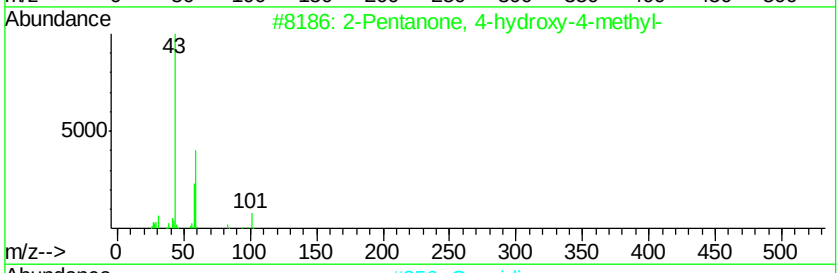
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

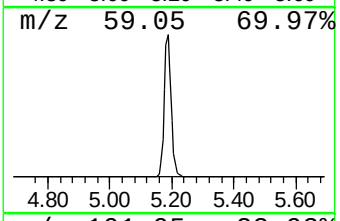
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	32.53 ng	1251310	1,4-Dichlorobenzene-d4	8.12

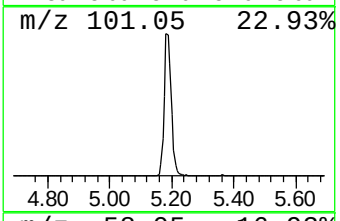
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Guanidine	59	CH5N3	000113-00-8	43
3	1,2-Butanediol	90	C4H10O2	000584-03-2	23
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	Acetone	58	C3H6O	000067-64-1	9

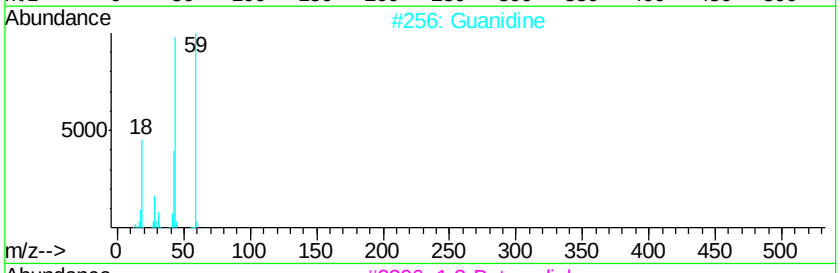


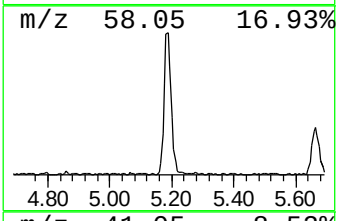


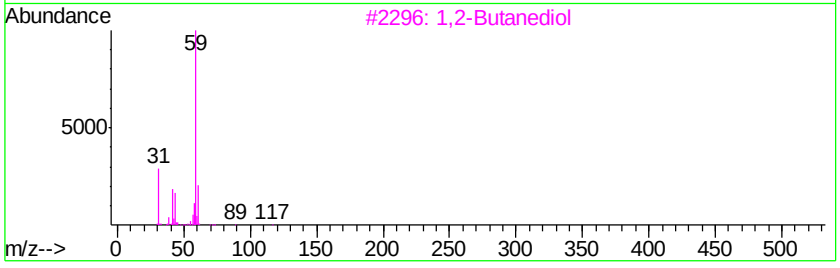


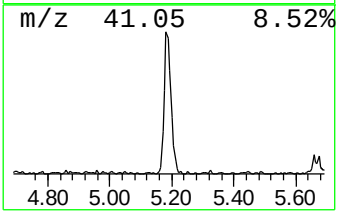












Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023396.D
Acq On : 2 Aug 2016 11:21
Operator : UM/SJ
Sample : H4145-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9536

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

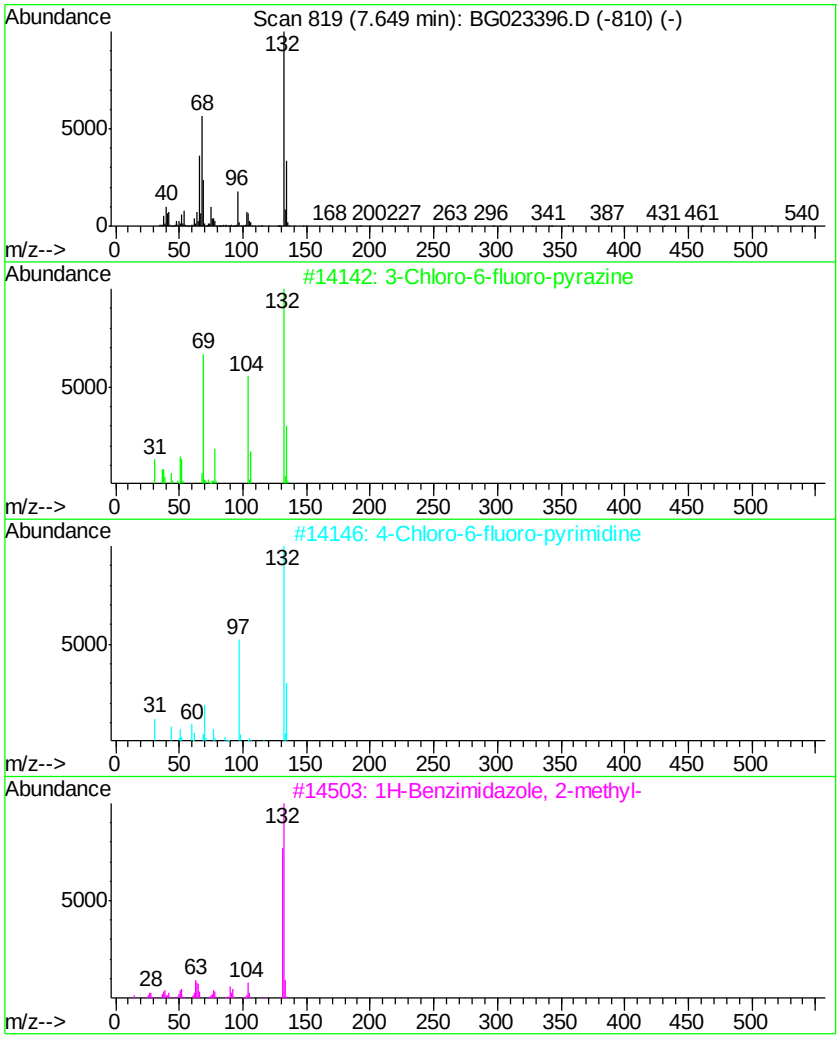
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

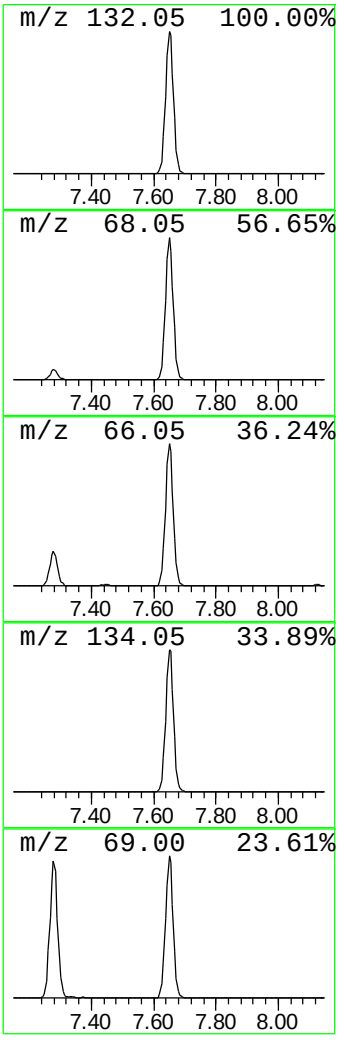
****

Peak Number 2 unknown7.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	121.70 ng	4680500	1,4-Dichlorobenzene-d4	8.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
Data File : BG023396.D
Acq On : 2 Aug 2016 11:21
Operator : UM/SJ
Sample : H4145-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9536

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

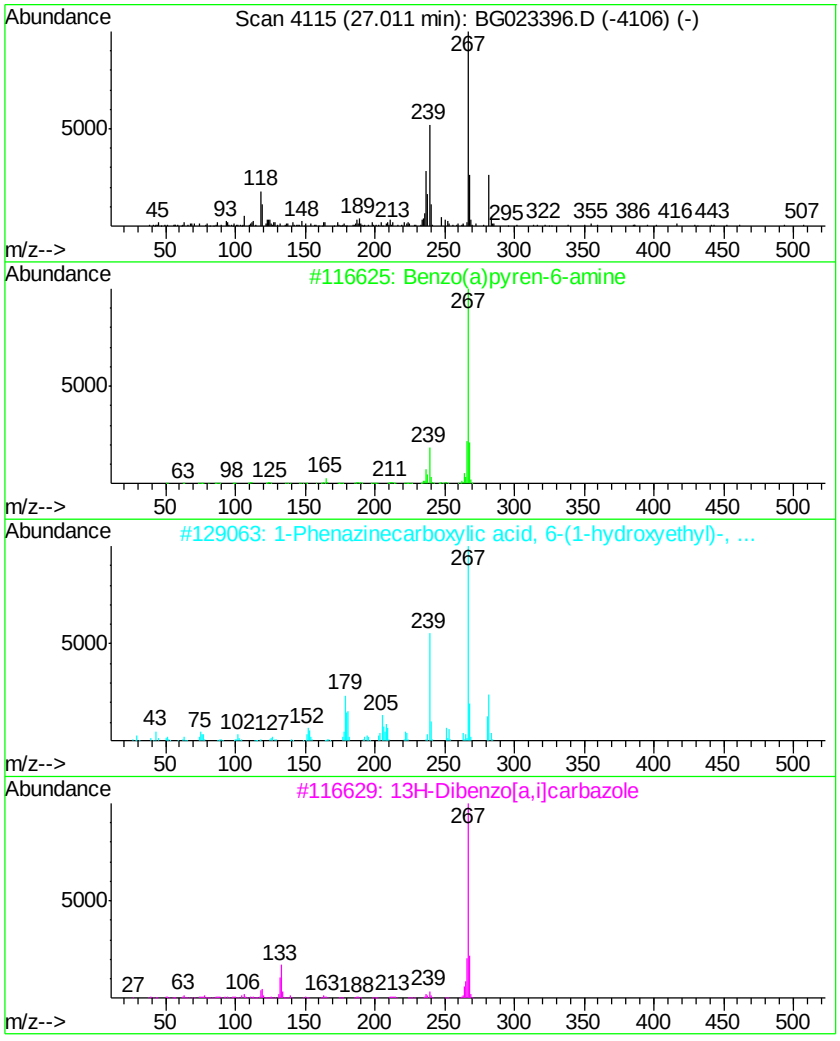
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

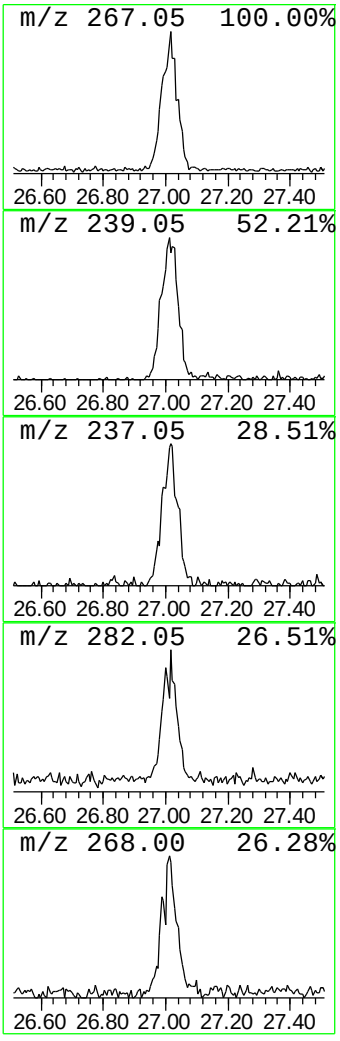
****

Peak Number 3 Benzo(a)pyren-6-amine Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.01	4.26 ng	512757	Perylene-d12	25.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo(a)pyren-6-amine	267	C20H13N	007428-83-3	91
2	1-Phenazinecarboxylic acid, 6-(1...	282	C16H14N2O3	073634-72-7	81
3	13H-Dibenzo[a,i]carbazole	267	C20H13N	000239-64-5	50
4	3,12b-Dimethyl-1,2,3,5,6,7,12,12...	282	C18H22N2O	1000297-42-3	47
5	Ether, bis(p-tert-butylphenyl)	282	C20H26O	024085-65-2	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG080216\
Data File : BG023396.D
Acq On : 2 Aug 2016 11:21
Operator : UM/SJ
Sample : H4145-14
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 9536

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
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...	5.19	32.5	ng	1251310	1	8.12	769216	20.0
unknown7.65	7.65	121.7	ng	4680500	1	8.12	769216	20.0
Benzo(a)pyren-6-a...	27.01	4.3	ng	512757	6	25.24	2408280	20.0