LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092519\
Data File : BG042930.D
Acq On : 25 Sep 2019 16:33
Operator : JU
Sample : K4839-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-BN-WP

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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	3.178	9	15	24	rBV	139431	321755	5.13%	0.273%
2	3.261	24	29	48	rVB	574645	1012951	16.16%	0.860%
3	3.866	127	132	147	rBV	349642	593734	9.47%	0.504%
4	5.658	428	437	452	rBV	1150448	1921767	30.66%	1.631%
5	7.244	698	707	722	rBV	1275900	2233495	35.63%	1.896%
6	7.614	759	770	780	rBV	1193426	2126620	33.92%	1.805%
7	7.967	821	830	837	rBV	918101	1648867	26.30%	1.400%
8	8.108	840	854	865	rVV2	1138182	2313885	36.91%	1.964%
9	8.402	896	904	907	rBV	936489	1880040	29.99%	1.596%
10	8.607	930	939	946	rBV	368689	769186	12.27%	0.653%
11	8.878	977	985	995	rBV	771855	1263737	20.16%	1.073%
12	9.160	1025	1033	1040	rBV	1333068	2394281	38.19%	2.032%
13	9.236	1040	1046	1050	rVV	725465	1406778	22.44%	1.194%
14	9.277	1050	1053	1069	rVB	847473	1437872	22.94%	1.221%
15	9.800	1134	1142	1153	rBV	210543	374190	5.97%	0.318%
16	10.282	1217	1224	1234	rBV	275656	469556	7.49%	0.399%
17	10.740	1294	1302	1312	rBV	784783	1406312	22.43%	1.194%
18	10.881	1316	1326	1340	rVB	245925	482572	7.70%	0.410%
19	11.222	1376	1384	1398	rBV	1837341	3198566	51.03%	2.715%
20	12.532	1599	1607	1620	rBV	1512280	2591910	41.35%	2.200%
21	12.879	1658	1666	1674	rBV	1341757	2113075	33.71%	1.794%
22	13.319	1734	1741	1752	rBV	2073585	3282774	52.37%	2.787%
23	13.572	1772	1784	1797	rBV	790254	1290784	20.59%	1.096%
24	14.154	1875	1883	1891	rBV	2445850	3652976	58.27%	3.101%
25	14.265	1895	1902	1914	rVB	608319	877805	14.00%	0.745%
26	14.424	1918	1929	1937	rBV	2442237	4112423	65.60%	3.491%
27	14.694	1967	1975	1980	rBV	394693	646224	10.31%	0.549%
28	14.765	1980	1987	1998	rVB	3700722	5926776	94.55%	5.031%
29	15.053	2028	2036	2039	rBV	1117376	1777892	28.36%	1.509%
30	15.094	2039	2043	2054	rVB	2040598	3121473	49.80%	2.650%
31	15.511	2107	2114	2126	rVB	3105115	4229610	67.47%	3.590%
32	15.734	2145	2152	2162	rBV	2115845	3033389	48.39%	2.575%
33	15.946	2181	2188	2200	rBV	1018077	1487120	23.72%	1.262%
34	16.181	2221	2228	2243	rBV	1704812	2568250	40.97%	2.180%

LSC Area Percent Report

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Misc :
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Instrument : BNA_G
ClientSampleId : PT-BN-WP

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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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.751	2317	2325	2333	rBV	1854205	2901909	46.29%	2.463%
36	17.438	2435	2442	2454	rBV2	521123	849818	13.56%	0.721%
37	19.489	2784	2791	2802	rBV	2771985	4039653	64.44%	3.429%
38	19.730	2827	2832	2841	rVB	44570	77023	1.23%	0.065%
39	19.853	2844	2853	2861	rBV	2949496	4352406	69.43%	3.695%
40	20.047	2880	2886	2895	rBV	4614082	6268614	100.00%	5.321%
41	20.740	2998	3004	3009	rBV	4351334	5300094	84.55%	4.499%
42	21.433	3118	3122	3133	rVB	74428	121638	1.94%	0.103%
43	21.604	3145	3151	3157	rVB	1947920	2622684	41.84%	2.226%
44	21.710	3163	3169	3173	rBV	612216	1089207	17.38%	0.925%
45	21.757	3173	3177	3185	rVB	1266468	2039493	32.53%	1.731%
46	22.744	3343	3345	3351	rVB	45417	70606	1.13%	0.060%
47	22.826	3351	3359	3368	rVB	3115685	5634335	89.88%	4.783%
48	23.225	3423	3427	3435	rVB2	53340	99298	1.58%	0.084%
49	23.995	3547	3558	3573	rVB	2399709	6205653	99.00%	5.268%
50	24.941	3711	3719	3737	rVB	361607	1155449	18.43%	0.981%
51	28.631	4333	4347	4365	rVB2	681796	2976430	47.48%	2.527%
52	29.794	4527	4545	4564	rVB2	792186	4031207	64.31%	3.422%

Sum of corrected areas: 117804162

LSC Report - Integrated Chromatogram

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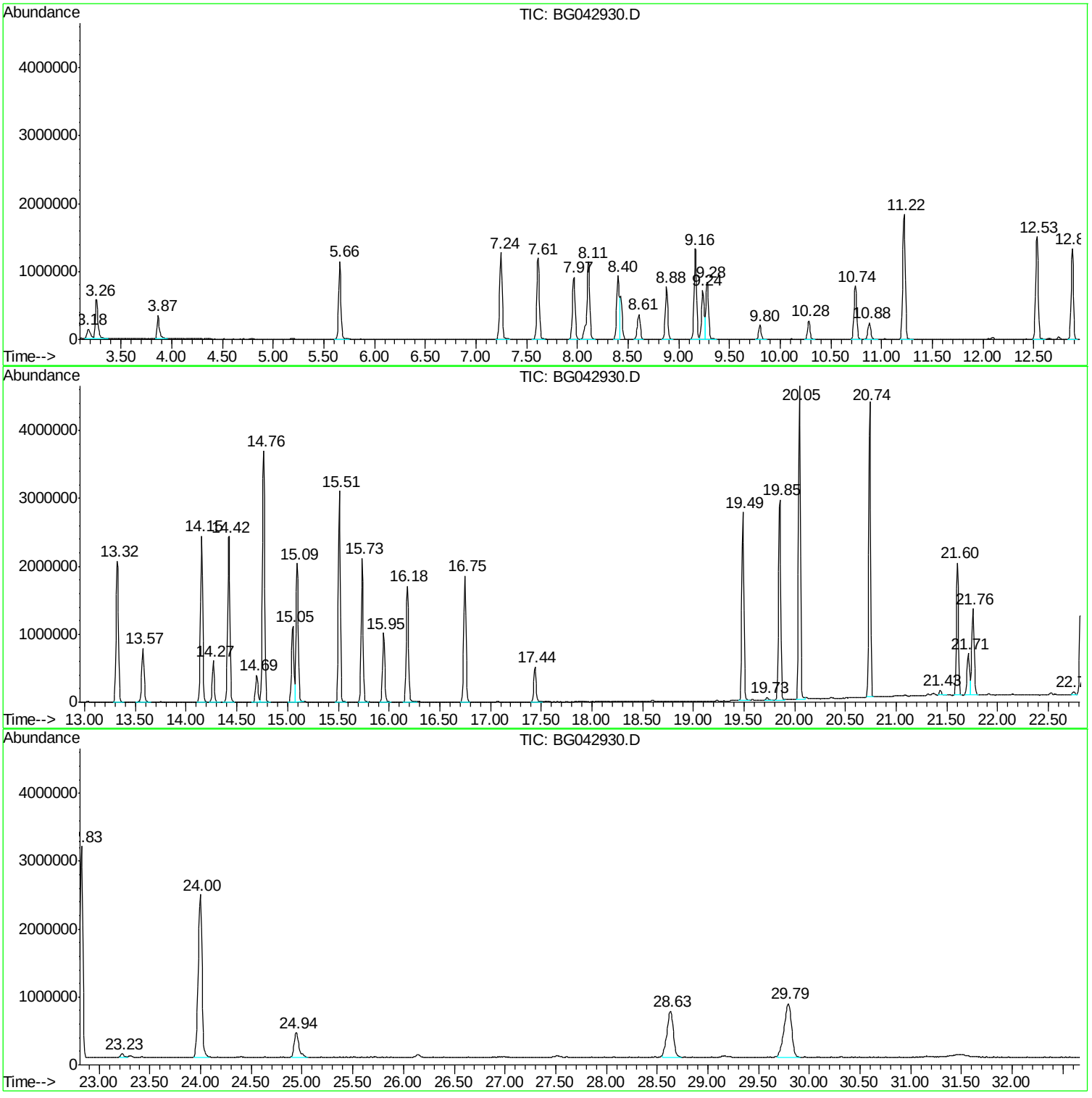
Operator : JU
Sample : K4839-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-BN-WP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.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:\SVOASRV\HPCHEM1\BNA G\DATA\BG092519\
Data File : BG042930.D
Acq On : 25 Sep 2019 16:33
Operator : JU
Sample : K4839-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-BN-WP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

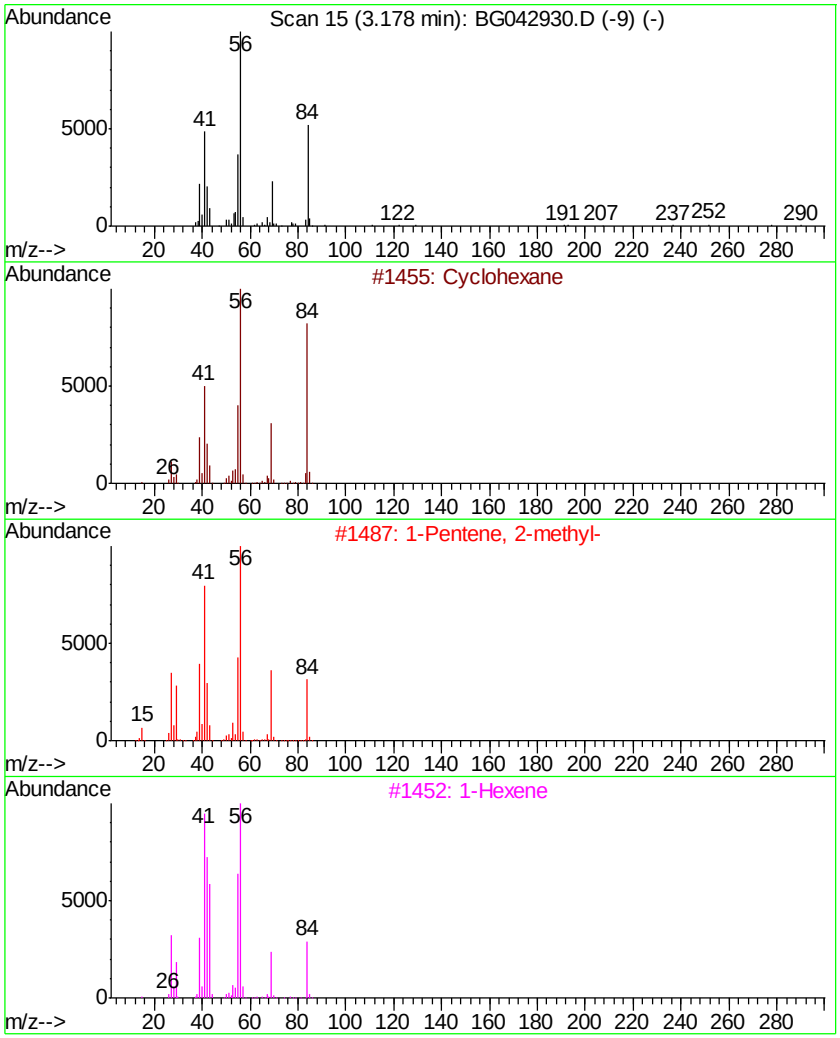
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

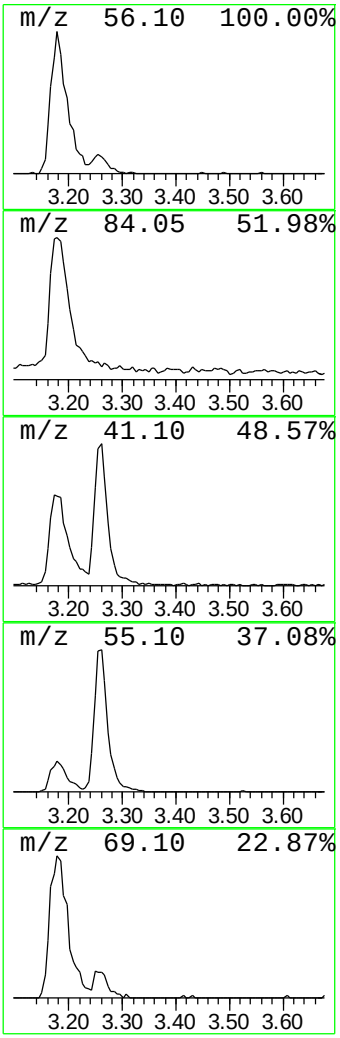
****

Peak Number 1 Cyclohexane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	2.78 ng	321755	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane	84	C6H12	000110-82-7	90
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	80
3	1-Hexene	84	C6H12	000592-41-6	50
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	50
5	Vigabatrin	129	C6H11NO2	060643-86-9	47





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Sample : K4839-03
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-BN-WP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

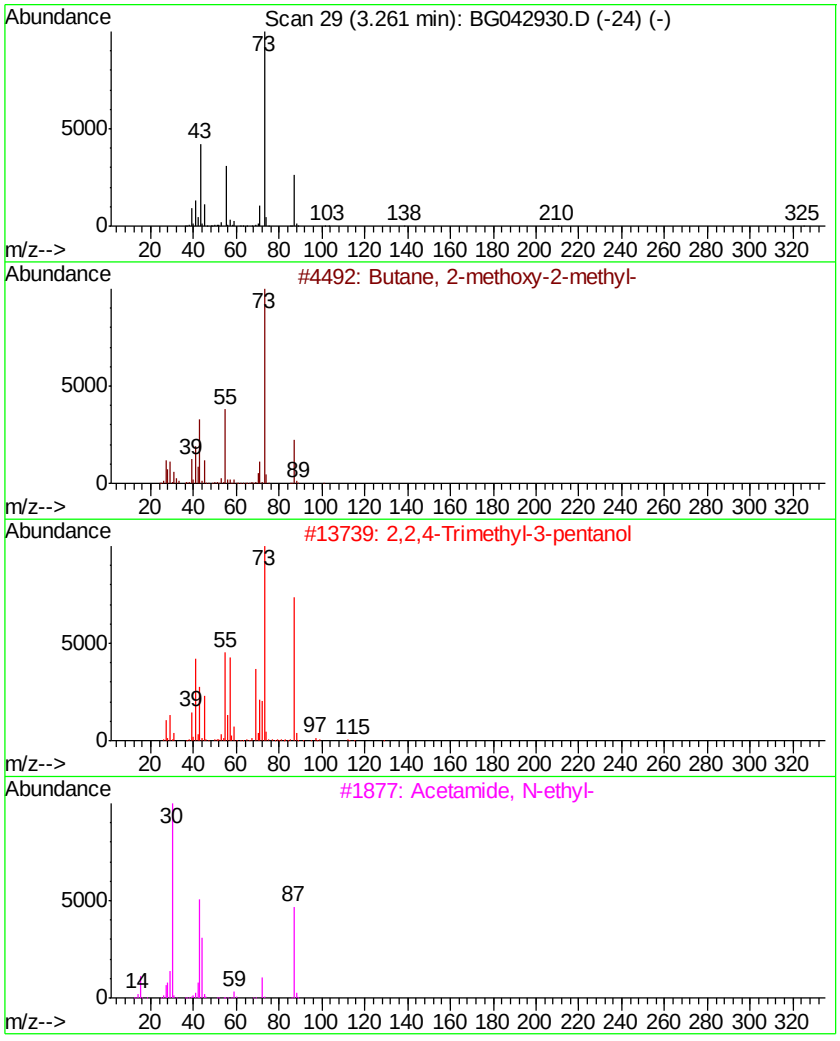
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

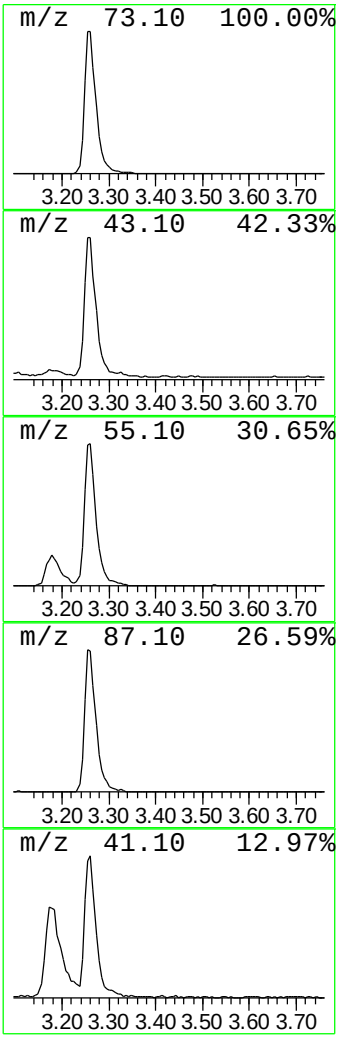
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.26	8.76 ng	1012950	1,4-Dichlorobenzene-d4	8.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	35
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG092519\
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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : PT-BN-WP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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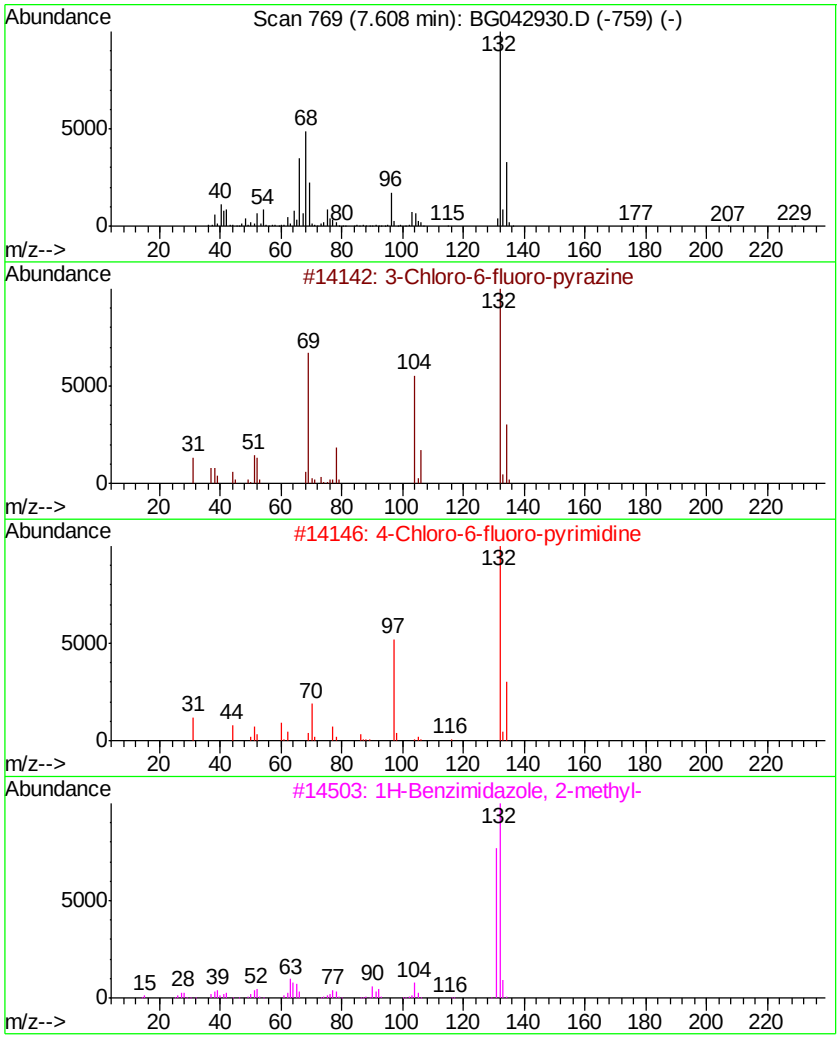
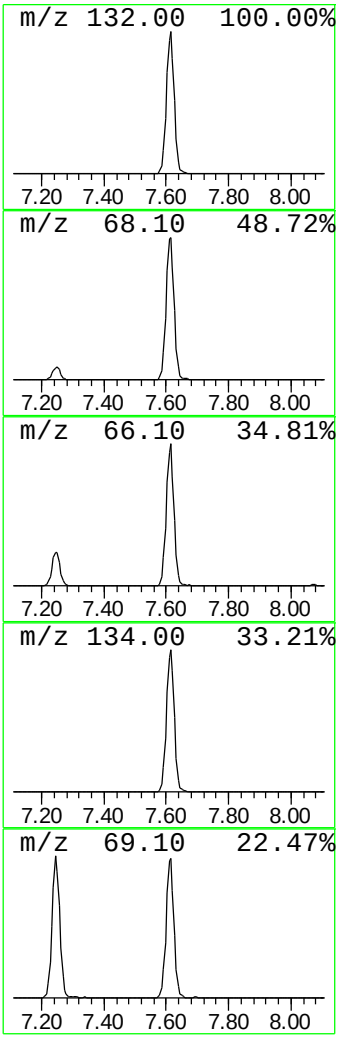
****

Peak Number 3 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	18.38 ng	2126620	1,4-Dichlorobenzene-d4	8.07

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	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	Pyrazolo(2,3-a)pyridine, 7-methyl-	132	C8H8N2	034760-58-2	22





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Instrument : BNA_G
ClientSampleId : PT-BN-WP

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

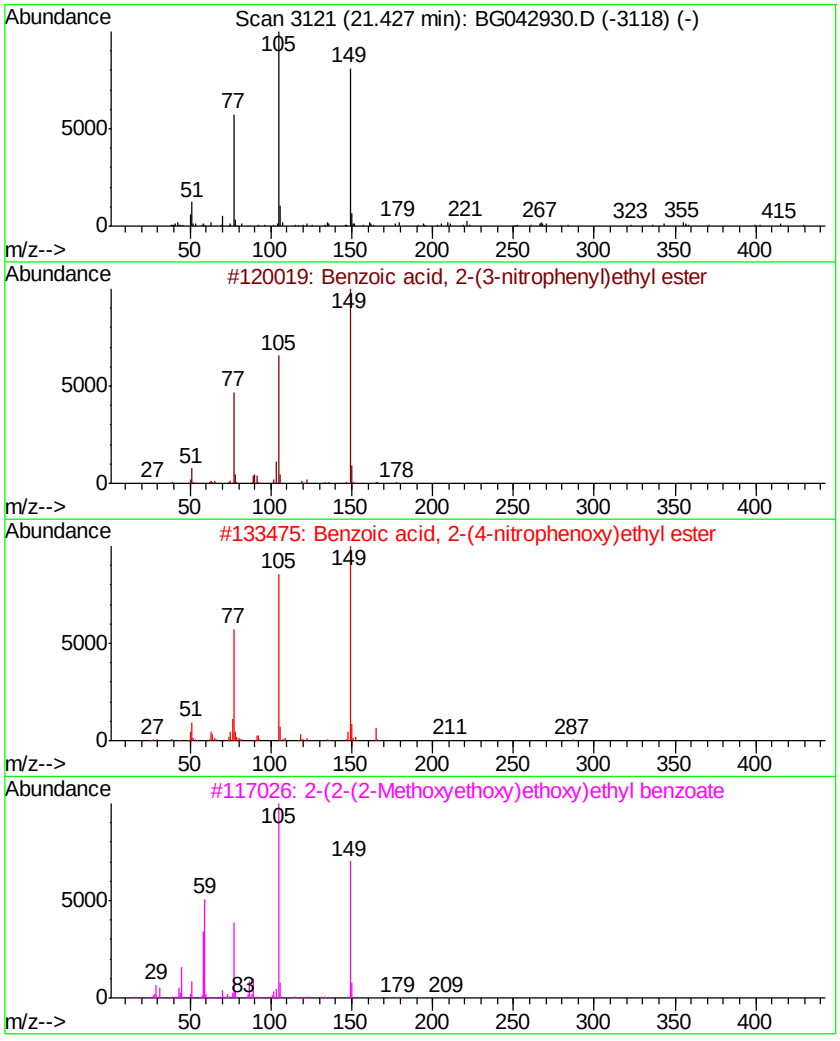
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

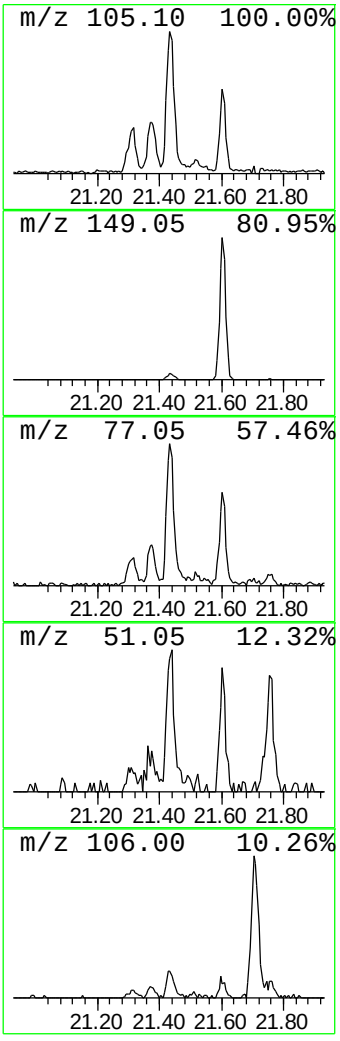
****

Peak Number 4 Benzoic acid, 2-(3-nitrophe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.43	2.23 ng	121638	Chrysene-d12	21.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	72
2	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	64
3	2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	59
4	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59
5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	59





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
Cyclohexane	3.18	2.8	ng	321755	1	8.07	2313890	20.0
Butane, 2-methoxy...	3.26	8.8	ng	1012950	1	8.07	2313890	20.0
unknown7.61	7.61	18.4	ng	2126620	1	8.07	2313890	20.0
Benzoic acid, 2-(...	21.43	2.2	ng	121638	5	21.71	1089210	20.0