

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
 Data File : BG015930.D
 Acq On : 27 Jan 2015 2:05
 Operator : TP/IZ
 Sample : G1139-08
 Misc : S
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 121B2A

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.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	2.828	19	24	32	rBV	403879	677819	7.30%	1.513%
2	2.904	32	37	43	rVB	655474	823921	8.87%	1.840%
3	3.133	72	76	82	rBV2	169140	220970	2.38%	0.493%
4	4.814	359	362	368	rBV2	81494	113727	1.22%	0.254%
5	5.278	436	441	448	rBV	688708	1052380	11.33%	2.350%
6	6.870	706	712	718	rBV	442666	694448	7.48%	1.550%
7	7.223	762	772	779	rBV	1429767	2195304	23.64%	4.901%
8	7.687	844	851	857	rBV2	441510	703948	7.58%	1.572%
9	8.004	898	905	912	rBV	1568645	2456305	26.45%	5.484%
10	8.844	1041	1048	1055	rBV	1415373	2321082	25.00%	5.182%
11	10.472	1318	1325	1330	rBV2	585321	973217	10.48%	2.173%
12	10.519	1330	1333	1341	rVB2	66631	121926	1.31%	0.272%
13	11.312	1460	1468	1476	rBV4	67517	164386	1.77%	0.367%
14	11.565	1505	1511	1519	rVB7	44296	101728	1.10%	0.227%
15	11.829	1549	1556	1560	rBV3	96736	152195	1.64%	0.340%
16	12.364	1640	1647	1651	rBV3	63766	113680	1.22%	0.254%
17	12.581	1677	1684	1687	rBV6	55665	98553	1.06%	0.220%
18	12.945	1736	1746	1753	rBV	3623534	5410497	58.27%	12.080%
19	13.333	1806	1812	1817	rBV4	210704	312946	3.37%	0.699%
20	13.915	1908	1911	1917	rVB4	75659	108820	1.17%	0.243%
21	14.332	1973	1982	1986	rBV3	979725	1532581	16.51%	3.422%
22	14.373	1986	1989	1995	rVB	132464	195126	2.10%	0.436%
23	14.450	1998	2002	2006	rBV2	79782	109143	1.18%	0.244%
24	15.419	2163	2167	2172	rVB3	143177	193219	2.08%	0.431%
25	15.537	2175	2187	2193	rBV2	842223	1361802	14.67%	3.040%
26	15.824	2224	2236	2246	rBV	3158888	4407761	47.47%	9.841%
27	16.277	2310	2313	2318	rVB3	81974	106951	1.15%	0.239%
28	17.076	2441	2449	2455	rBV	1557076	2194590	23.64%	4.900%
29	17.752	2554	2564	2569	rBV	86048	115751	1.25%	0.258%
30	17.940	2592	2596	2600	rBV3	87572	126437	1.36%	0.282%
31	18.045	2609	2614	2624	rVB	249750	339673	3.66%	0.758%
32	18.404	2670	2675	2680	rVB3	67454	99501	1.07%	0.222%
33	18.504	2687	2692	2696	rBV4	126340	170478	1.84%	0.381%
34	19.714	2891	2898	2903	rBV	6910711	9285294	100.00%	20.731%

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Misc : S
ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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

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35	21.265	3157	3162	3171	rBV	2374502	2985343	32.15%	6.665%
36	23.521	3538	3546	3556	rBV	1389101	2748365	29.60%	6.136%

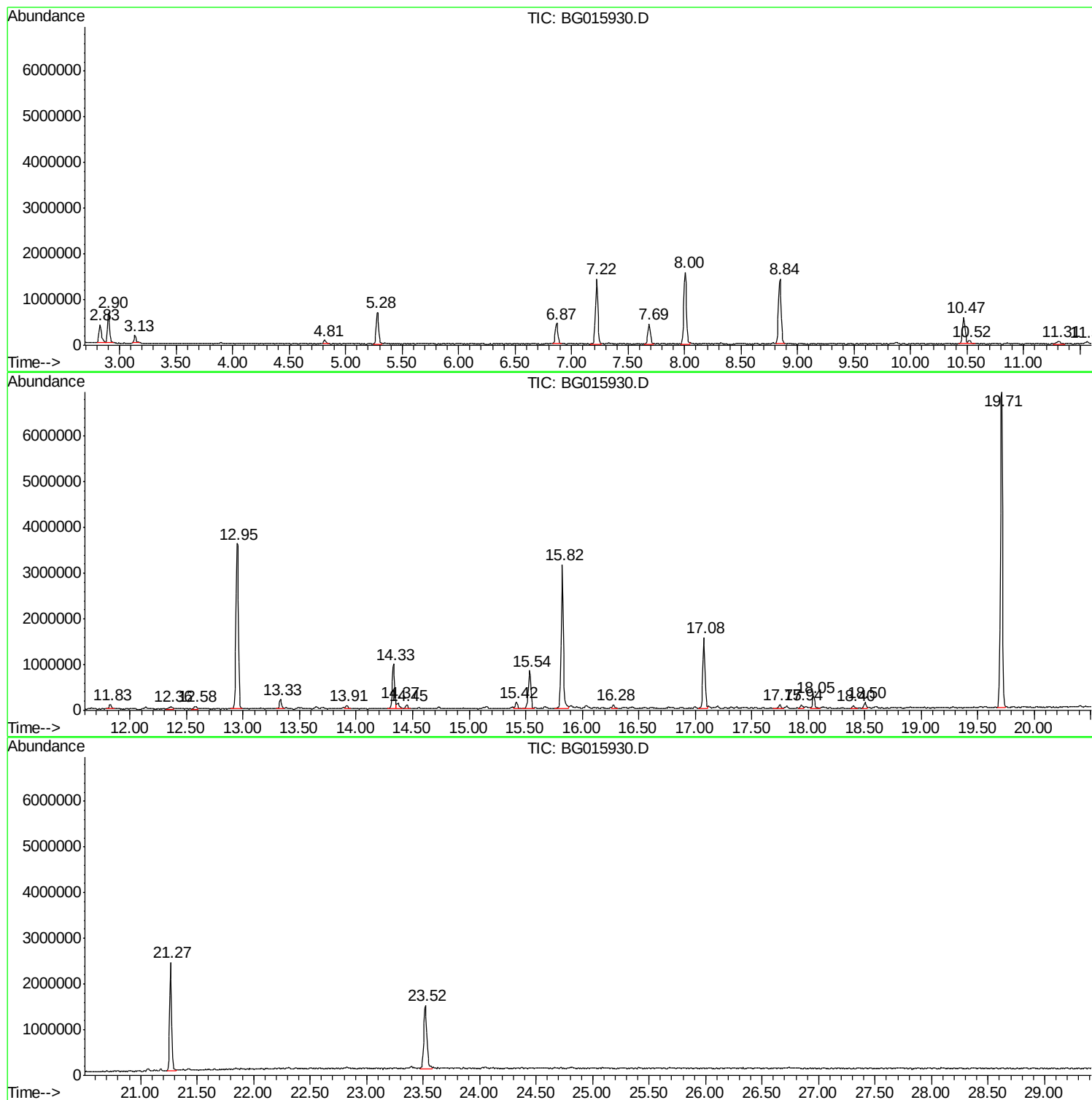
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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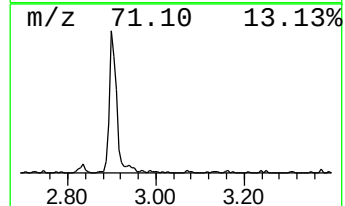
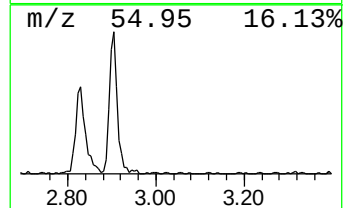
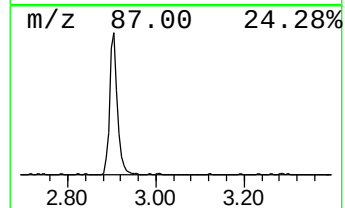
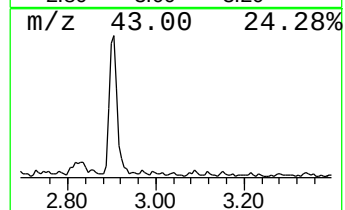
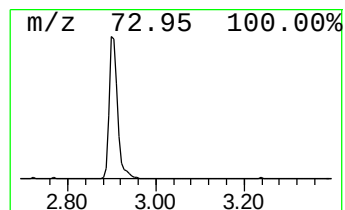
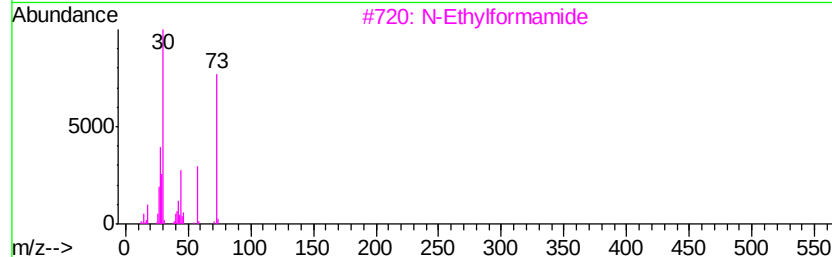
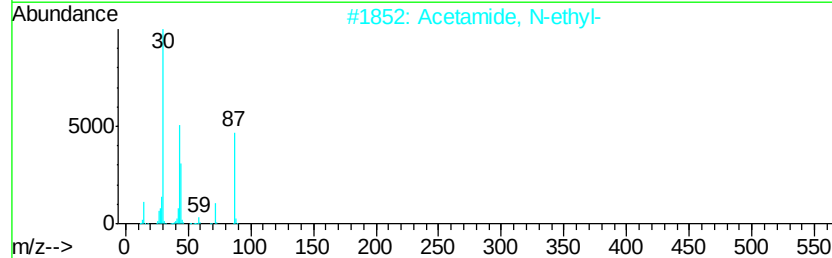
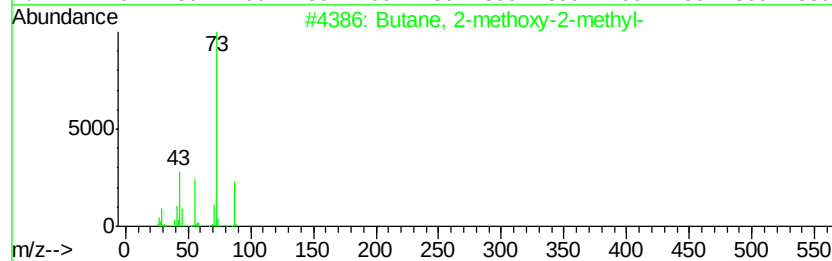
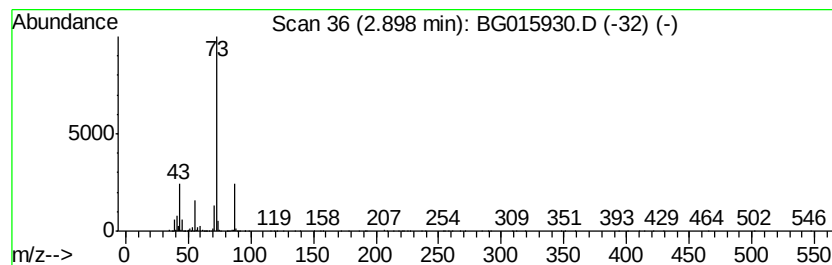
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	23.41 ng	823921	1,4-Dichlorobenzene-d4	7.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
5		Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	9



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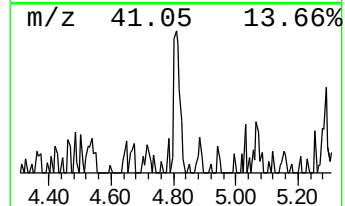
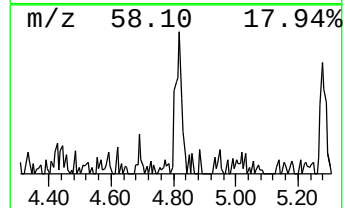
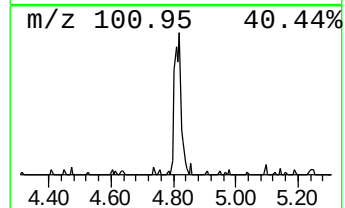
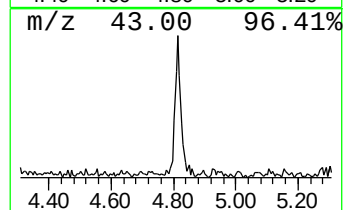
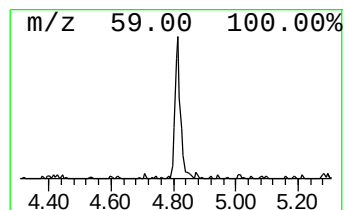
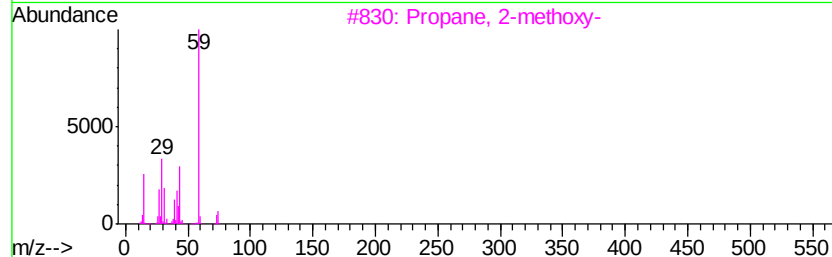
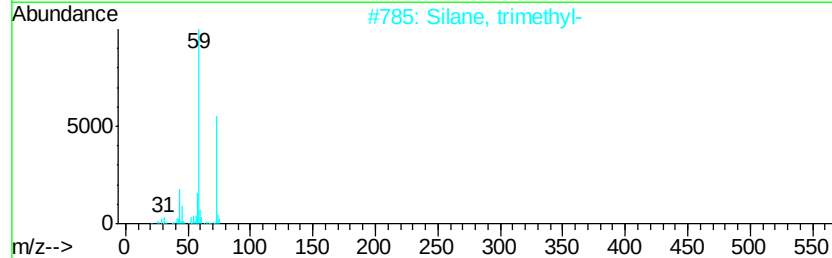
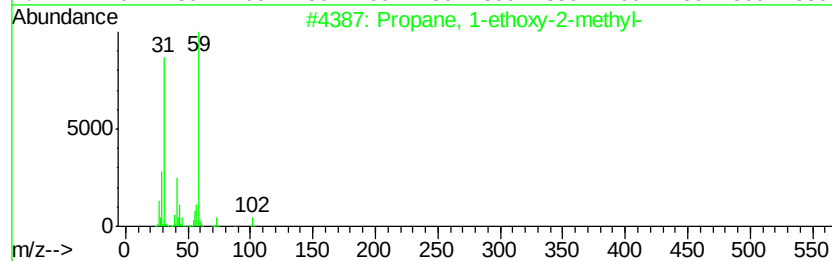
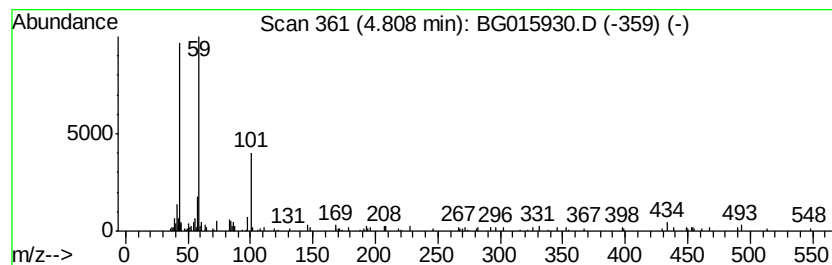
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Propane, 1-ethoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	3.23 ng	113727	1,4-Dichlorobenzene-d4	7.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	50	
2	Silane, trimethyl-	74	C3H10Si	000993-07-7	50	
3	Propane, 2-methoxy-	74	C4H10O	000598-53-8	40	
4	1-Propanol, 3,3'-oxybis-	134	C6H14O3	002396-61-4	40	
5	Butanoic acid, 4-(2,4,5-trichlor...	296	C11H11Cl3O2	025333-21-5	39	



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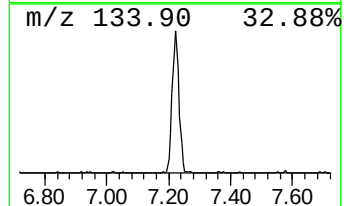
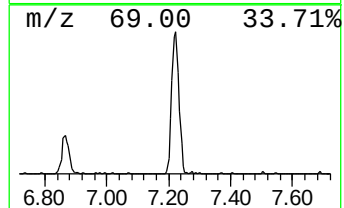
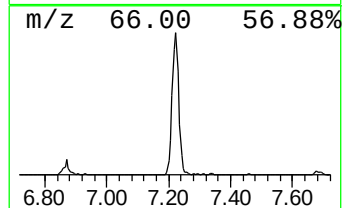
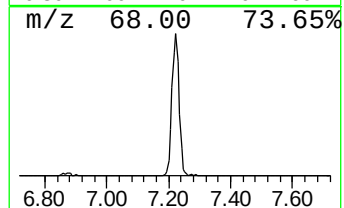
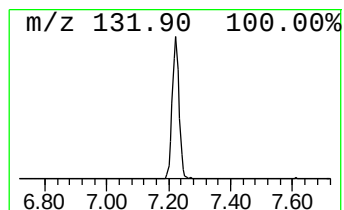
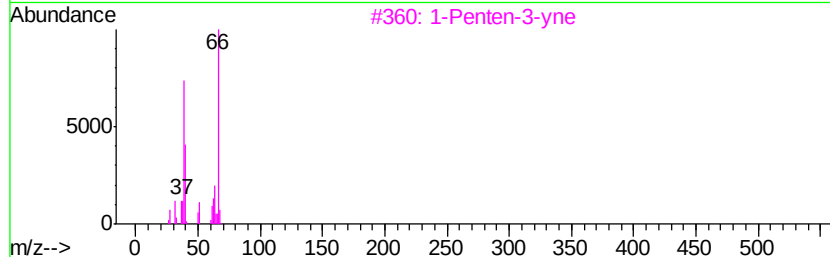
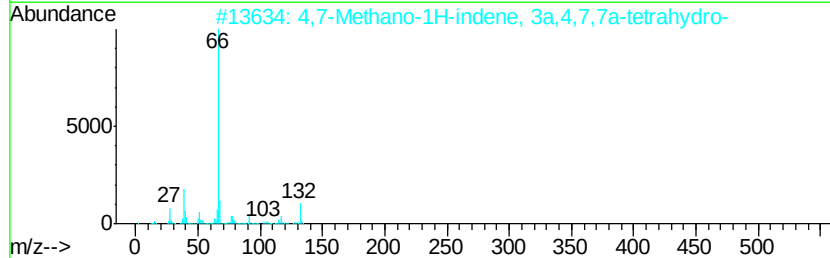
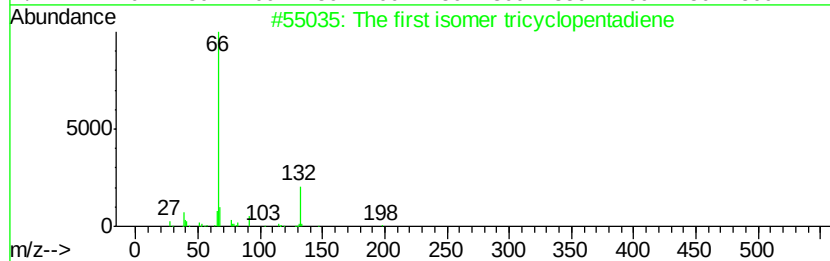
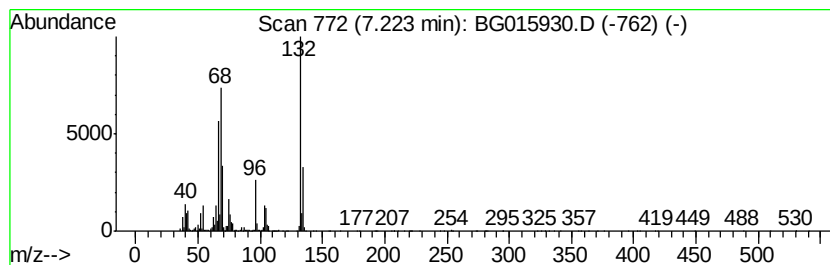
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.22 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	62.37 ng	2195300	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	The first isomer tricyclopentadiene	198	C15H18	1000222-21-0	47
2		4,7-Methano-1H-indene, 3a,4,7,7a...	132	C10H12	000077-73-6	38
3		1-Penten-3-yne	66	C5H6	000646-05-9	30
4		Silane, bicyclo[2.2.1]hept-5-en-...	226	C7H9Cl3Si	014319-64-3	27
5		Bicyclo[2.2.1]hept-5-ene-2-aceti...	180	C11H16O2	074876-17-8	16



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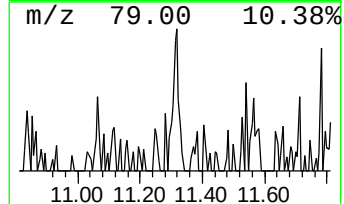
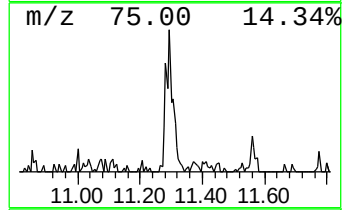
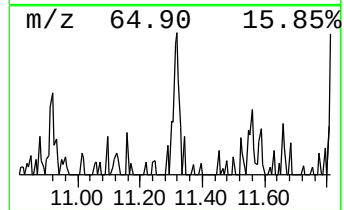
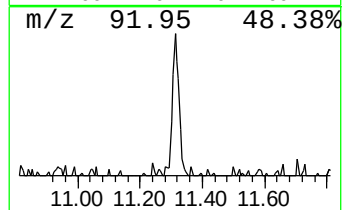
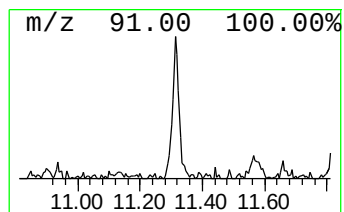
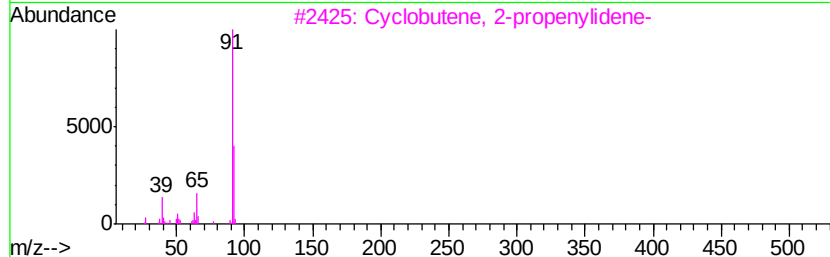
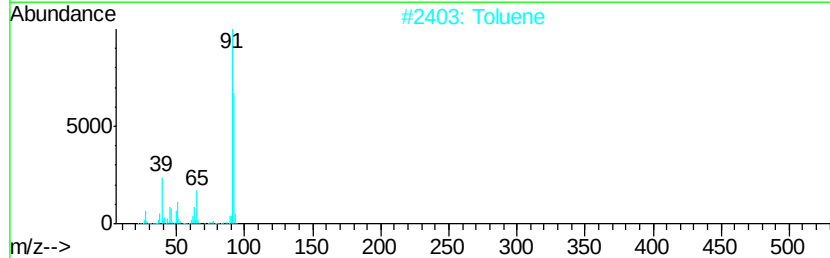
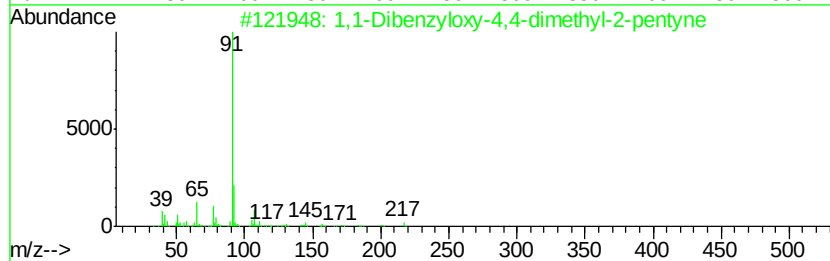
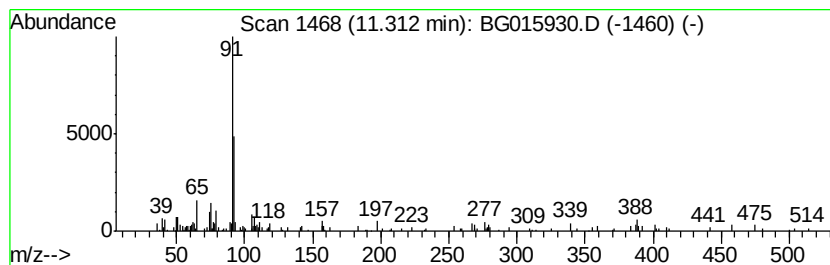
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1,1-Dibenzoyloxy-4,4-dimethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.31	3.38 ng	164386	Naphthalene-d8	10.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1-Dibenzoyloxy-4,4-dimethyl-2-p...	308	C21H24O2	212687-75-7	50
2		Toluene	92	C7H8	000108-88-3	49
3		Cyclobutene, 2-propenylidene-	92	C7H8	052097-85-5	49
4		Spiro[2.4]hepta-4,6-diene	92	C7H8	000765-46-8	49
5		1,6-Heptadien-3-yne	92	C7H8	005150-80-1	47



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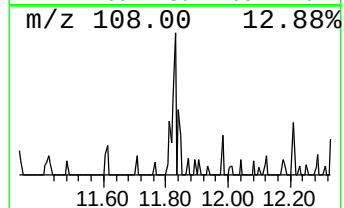
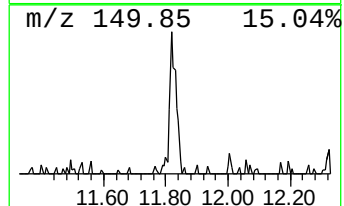
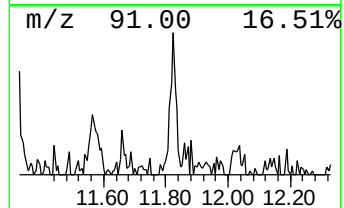
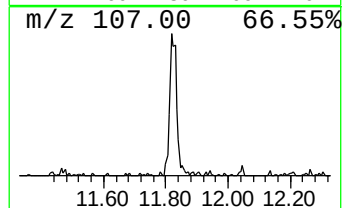
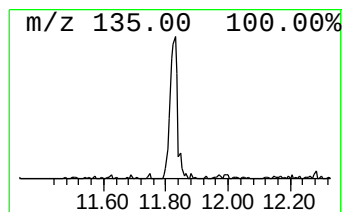
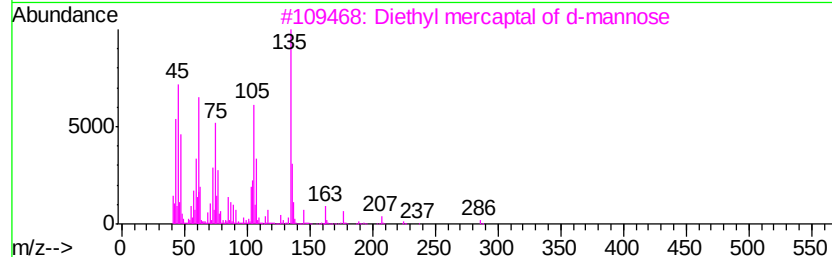
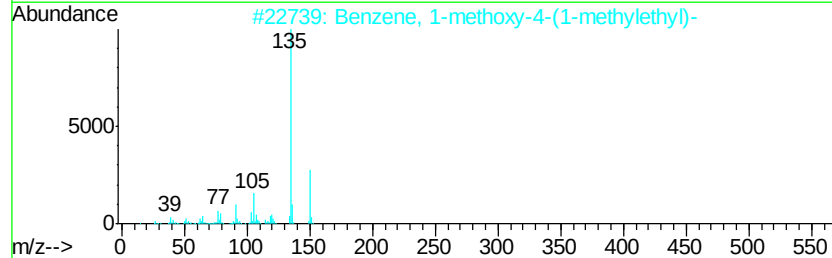
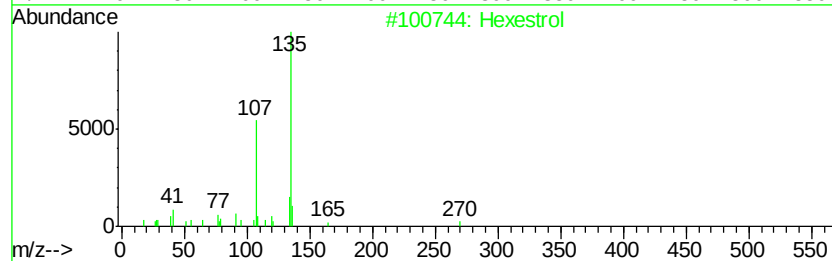
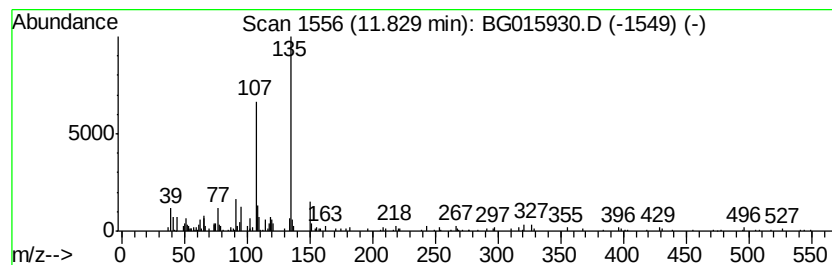
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Peak Number 8 Hexestrol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.83	3.13 ng	152195	Naphthalene-d8	10.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexestrol	270	C18H22O2	005635-50-7	72
2		Benzene, 1-methoxy-4-(1-methylet...	150	C10H14O	004132-48-3	47
3		Diethyl mercaptal of d-mannose	286	C10H22O5S2	006748-69-2	46
4		5-[3,4-Methylenedioxybenzyl]-2-t...	250	C11H10N2O3S	028824-68-2	43
5		[1,3]-Oxazino[5,6-c]quinoline,3-...	418	C21H17F3N2O4	041958-08-1	43



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Sample : G1139-08
Misc : S
ALS Vial : 16 Sample Multiplier: 1

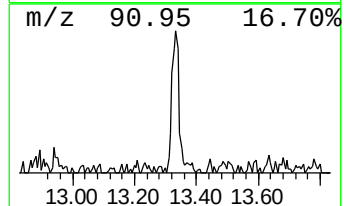
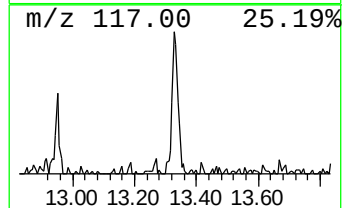
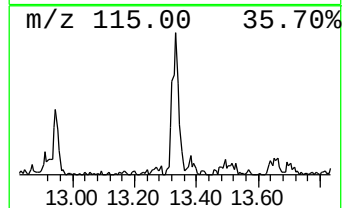
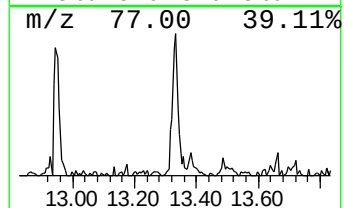
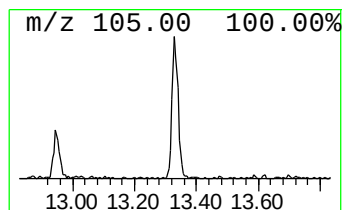
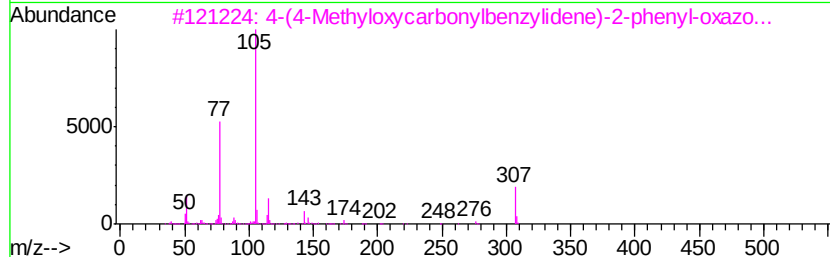
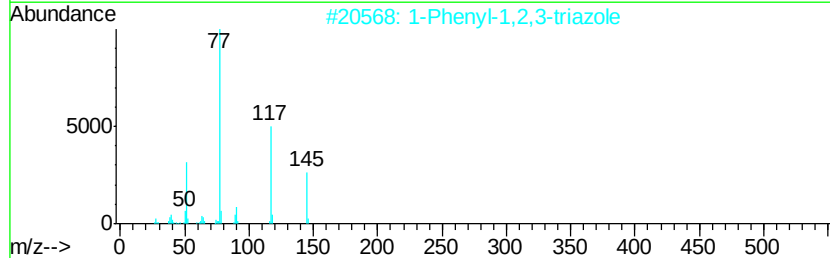
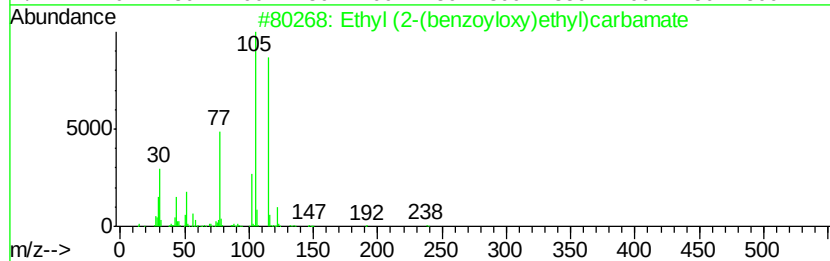
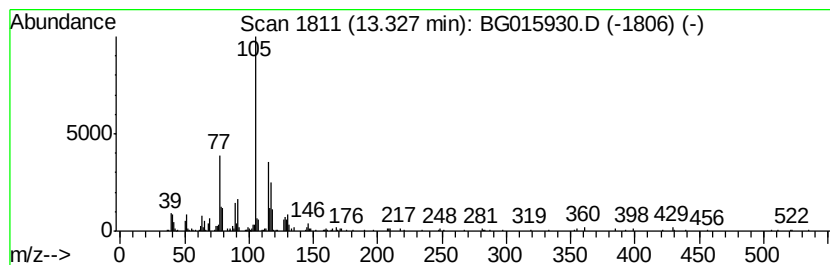
Instrument :
BNA_G
ClientSampleId :
121B2A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown13.33 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	4.08 ng	312946	Acenaphthene-d10	14.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Ethyl (2-(benzoyloxy)ethyl)carba...	237 C12H15N04	091642-01-2 47
2		1-Phenyl-1,2,3-triazole	145 C8H7N3	001453-81-2 35
3		4-(4-Methyloxycarbonylbenzyliden...	307 C18H13N04	329023-63-4 22
4		1H-Pyrazole-3-carboxaldehyde, 5-...	172 C10H8N2O	057204-65-6 16
5		Benzene, 1-butynyl-	130 C10H10	000622-76-4 14



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015930.D
Acq On : 27 Jan 2015 2:05
Operator : TP/IZ
Sample : G1139-08
Misc : S
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
121B2A

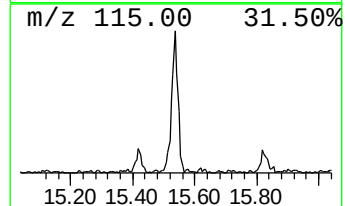
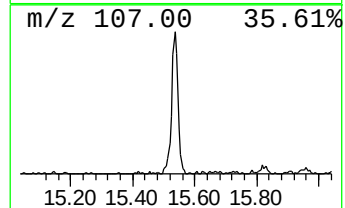
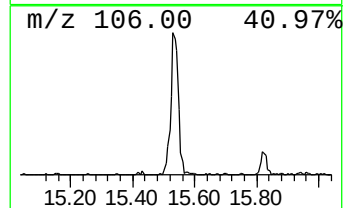
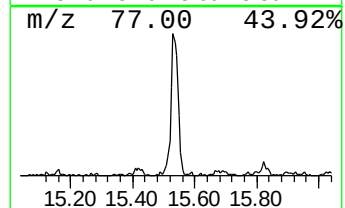
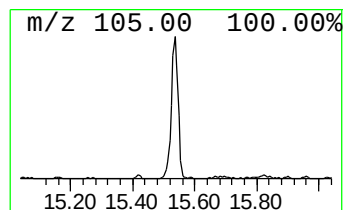
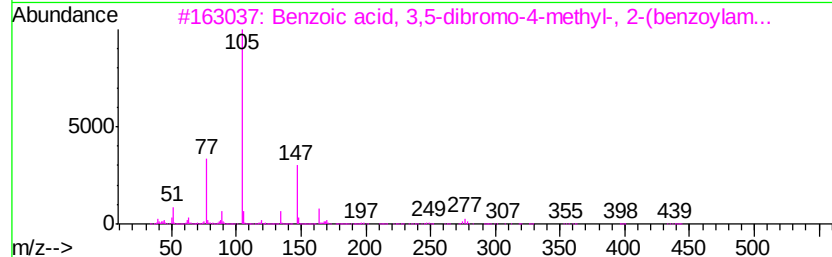
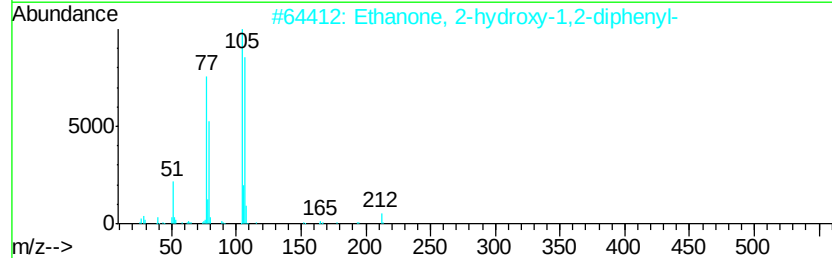
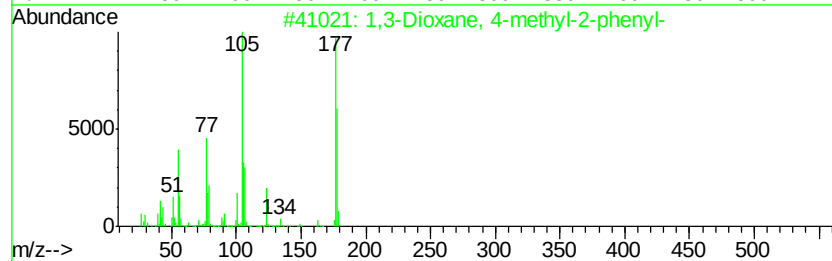
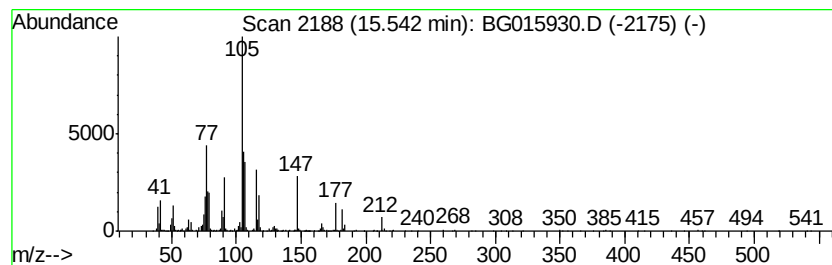
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1,3-Dioxane, 4-methyl-2-phe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	17.77 ng	1361800	Acenaphthene-d10	14.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dioxane, 4-methyl-2-phenyl-	178	C11H14O2	000774-44-7	53
2		Ethanone, 2-hydroxy-1,2-diphenyl-	212	C14H12O2	000119-53-9	43
3		Benzoic acid, 3,5-dibromo-4-meth...	439	C17H15Br2NO3	1000258-73-5	41
4		Benzoin	212	C14H12O2	000579-44-2	38
5		Benzamide, N-(1,1-dimethylethyl)-	177	C11H15NO	005894-65-5	27



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015930.D
Acq On : 27 Jan 2015 2:05
Operator : TP/IZ
Sample : G1139-08
Misc : S
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
121B2A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.90	23.4	ng	823921	1	7.69	703948	20.0
Propane, 1-ethoxy...	4.81	3.2	ng	113727	1	7.69	703948	20.0
unknown7.22	7.22	62.4	ng	2195300	1	7.69	703948	20.0
1,1-Dibenzylloxy-4...	11.31	3.4	ng	164386	2	10.47	973217	20.0
Hexestrol	11.83	3.1	ng	152195	2	10.47	973217	20.0
unknown13.33	13.33	4.1	ng	312946	3	14.33	1532580	20.0
1,3-Dioxane, 4-me...	15.54	17.8	ng	1361800	3	14.33	1532580	20.0