

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
 Data File : BG015965.D
 Acq On : 28 Jan 2015 3:10
 Operator : TP/IZ
 Sample : G1138-09
 Misc :
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 275B2

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	17	24	32	rBV	333916	599210	5.96%	1.130%
2	2.904	32	37	44	rVB	671224	832656	8.28%	1.571%
3	4.420	291	295	301	rVB2	85055	118087	1.17%	0.223%
4	4.814	357	362	369	rVB	182357	237901	2.37%	0.449%
5	5.278	435	441	450	rBV	1122121	1711537	17.01%	3.229%
6	6.870	705	712	720	rBV	780999	1303742	12.96%	2.459%
7	7.223	763	772	781	rBV	2029361	3201860	31.83%	6.040%
8	7.687	843	851	859	rBV	511427	842701	8.38%	1.590%
9	8.004	898	905	914	rBV	1753706	2859737	28.43%	5.394%
10	8.844	1040	1048	1056	rBV	1613838	2652075	26.37%	5.003%
11	10.466	1314	1324	1330	rBV	655006	1150731	11.44%	2.171%
12	10.530	1330	1335	1341	rVB7	58748	114374	1.14%	0.216%
13	11.794	1544	1550	1553	rBV	132014	230013	2.29%	0.434%
14	11.823	1553	1555	1561	rVB4	85573	119106	1.18%	0.225%
15	12.945	1739	1746	1753	rBV	4347885	6468148	64.30%	12.201%
16	13.327	1806	1811	1816	rVB3	125331	187672	1.87%	0.354%
17	13.785	1883	1889	1899	rVB	203216	314962	3.13%	0.594%
18	14.332	1974	1982	1987	rBV2	1154421	1831968	18.21%	3.456%
19	14.367	1987	1988	1994	rVB	104000	106866	1.06%	0.202%
20	15.419	2162	2167	2172	rVB4	95345	126366	1.26%	0.238%
21	15.536	2177	2187	2192	rBV	588537	931430	9.26%	1.757%
22	15.695	2207	2214	2219	rBV	498101	675530	6.72%	1.274%
23	15.824	2230	2236	2247	rBV	4641451	6287808	62.51%	11.861%
24	17.076	2442	2449	2458	rBV2	1722158	2494615	24.80%	4.706%
25	17.981	2600	2603	2608	rBV6	108329	143602	1.43%	0.271%
26	19.714	2892	2898	2905	rBV	8330262	10059064	100.00%	18.975%
27	20.977	3109	3113	3118	rBV2	638285	832978	8.28%	1.571%
28	21.271	3157	3163	3169	rBV	2438947	3210888	31.92%	6.057%
29	23.521	3538	3546	3554	rBV2	1501455	3090331	30.72%	5.829%
30	25.202	3824	3832	3838	rBV2	96024	277204	2.76%	0.523%

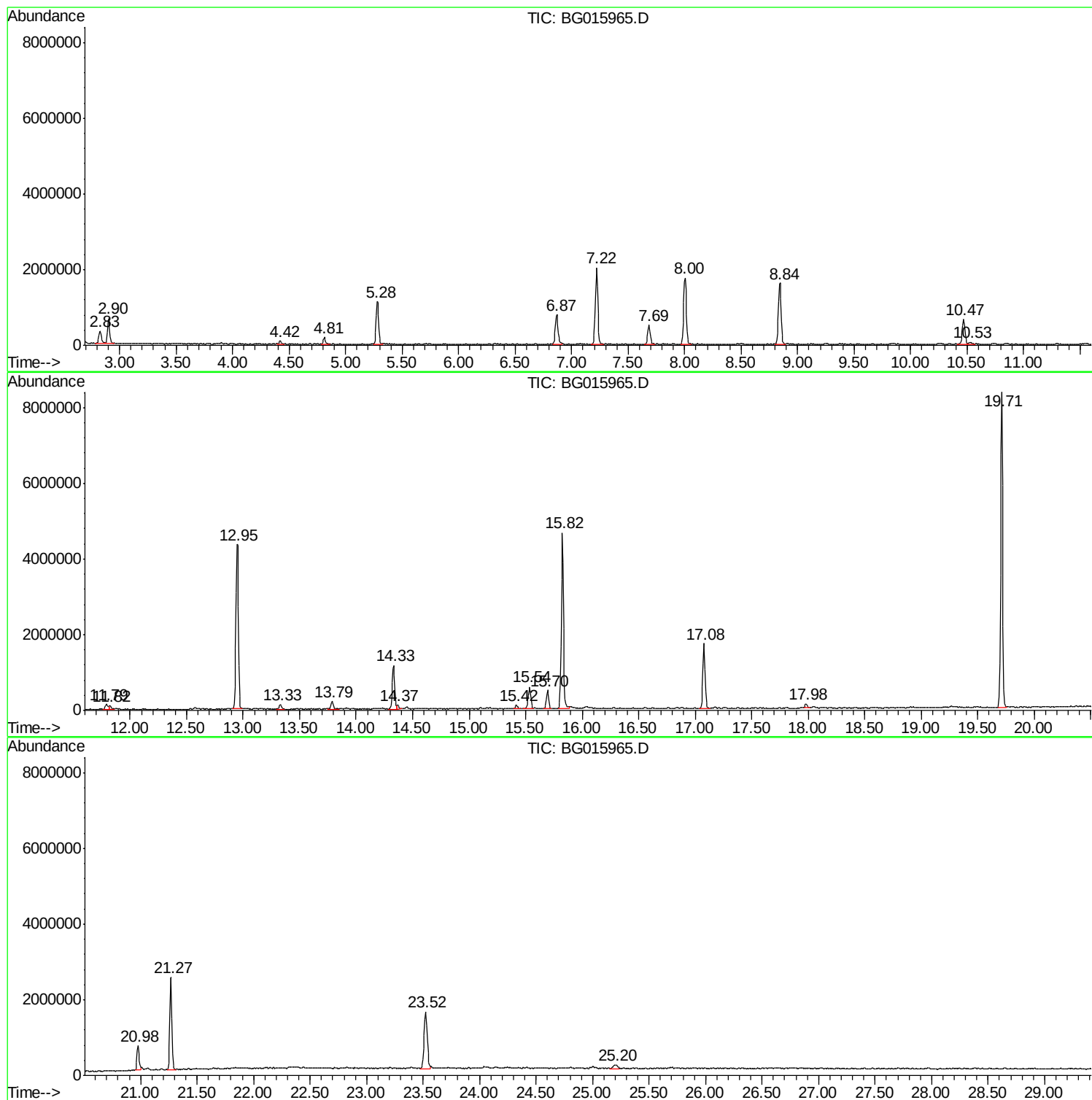
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Instrument :
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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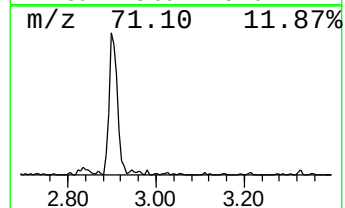
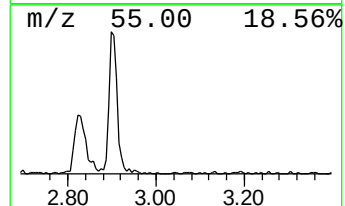
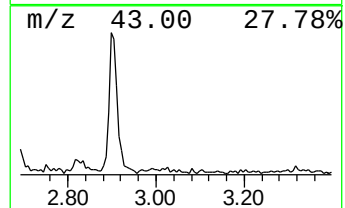
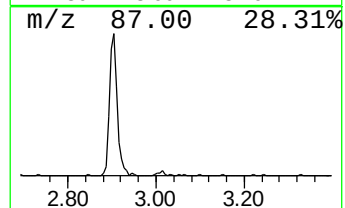
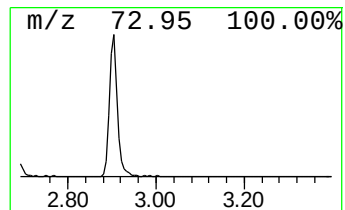
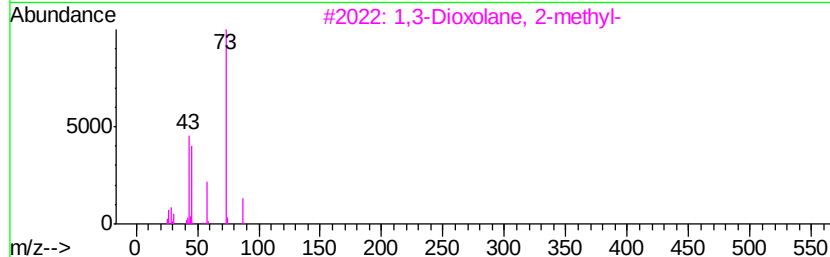
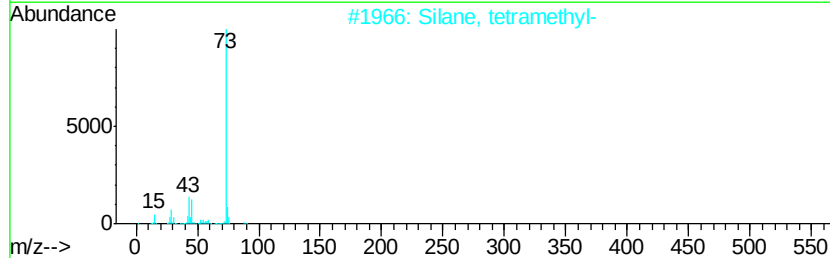
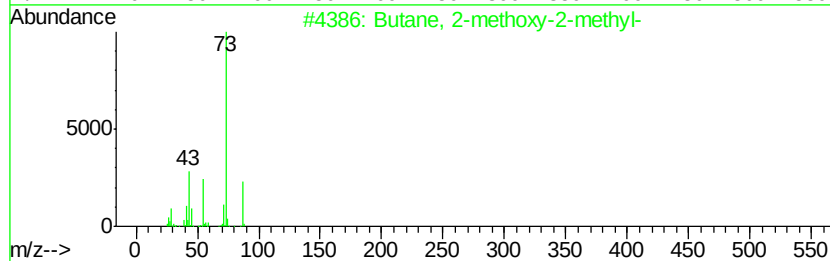
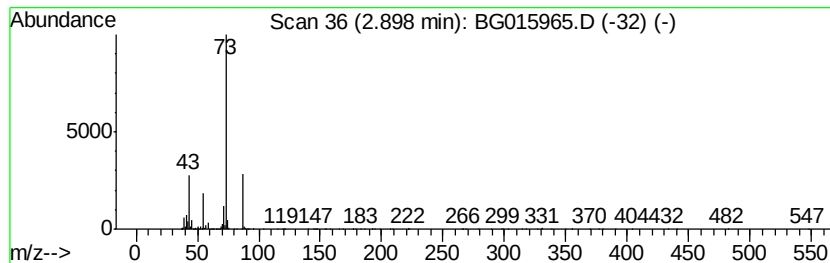
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown2.90 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	19.76 ng	832656	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	40
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		1-Propene-1-thiol	74	C3H6S	000925-89-3	9



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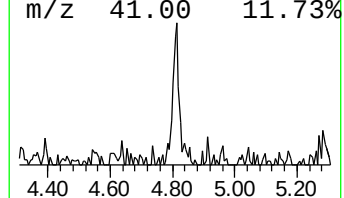
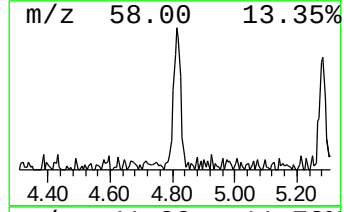
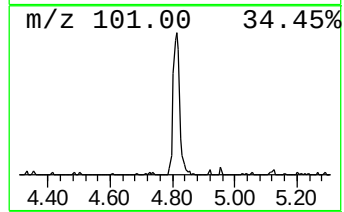
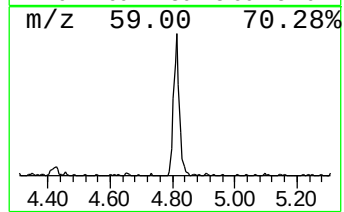
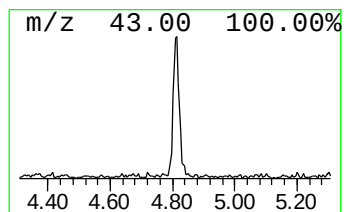
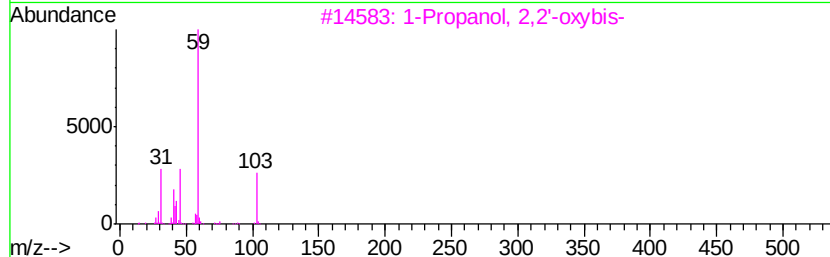
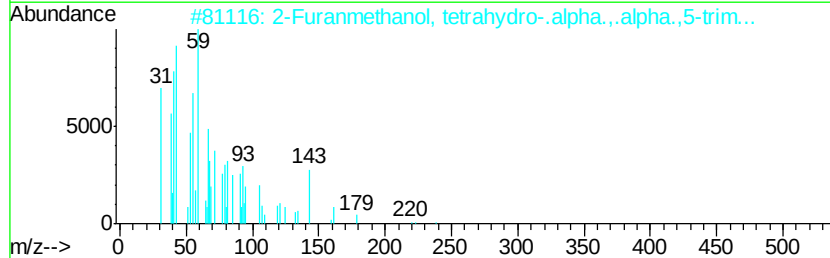
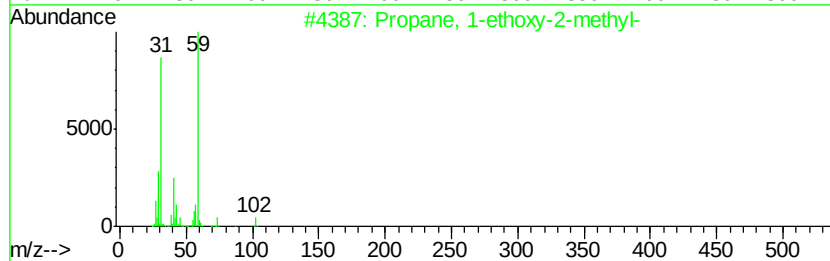
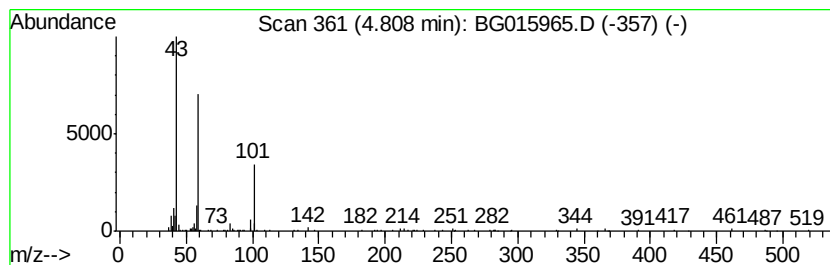
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown4.81 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	5.65 ng	237901	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	40
2			2-Furanmethanol, tetrahydro-.alp...	238	C15H26O2	026184-88-3	40
3			1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	40
4			Pentanedioic acid, dimethyl ester	160	C7H12O4	001119-40-0	39
5			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39



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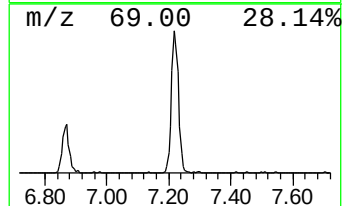
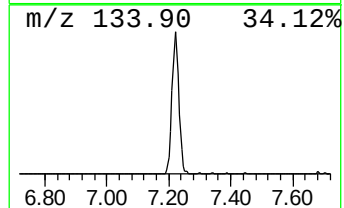
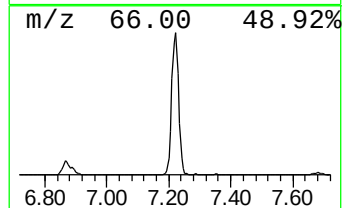
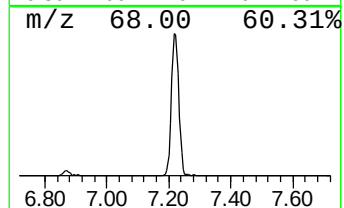
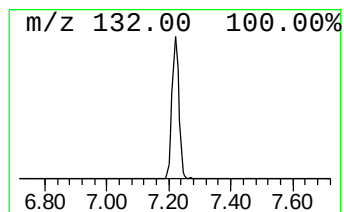
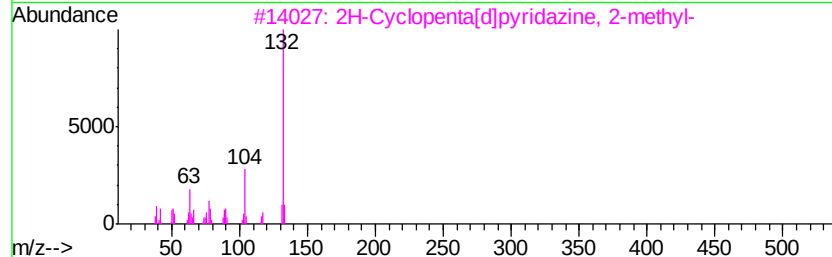
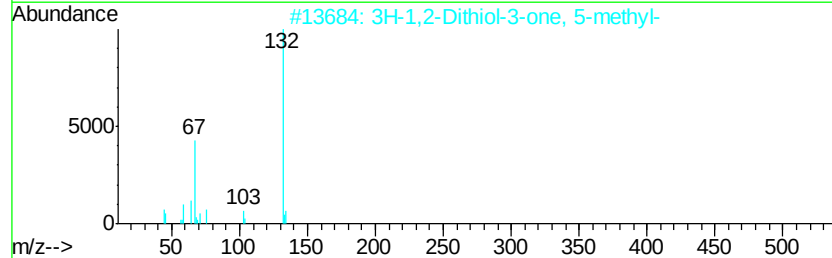
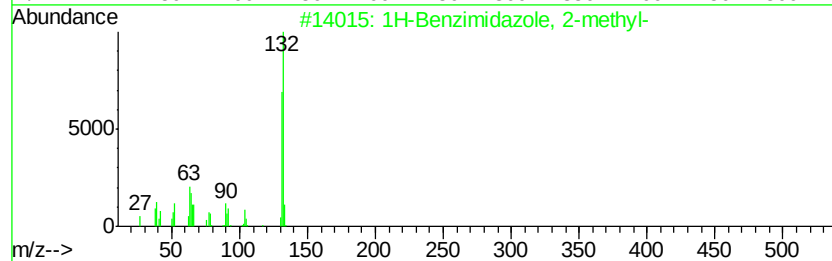
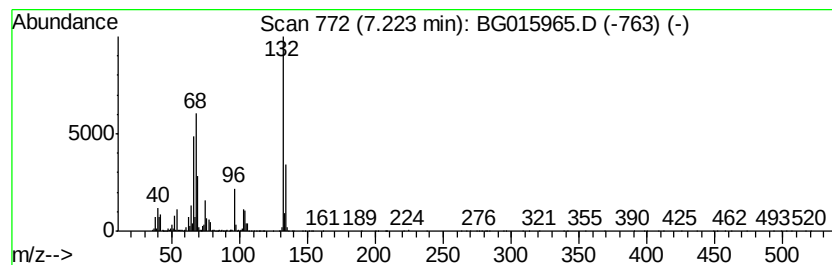
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.22 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	75.99 ng	3201860	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	18
2		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	14
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
5		1H-Indenol	132	C9H8O	056631-57-3	10



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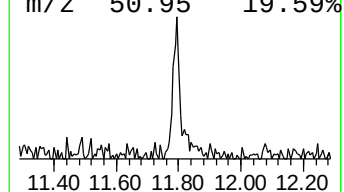
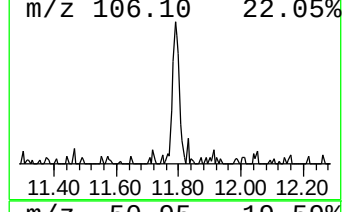
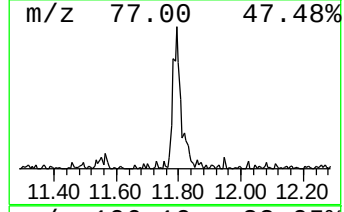
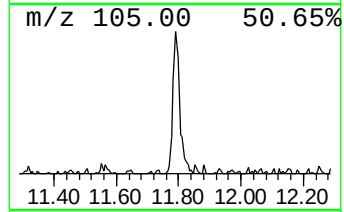
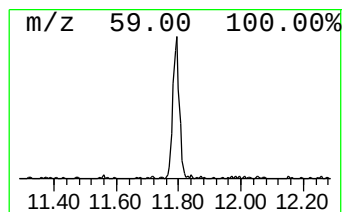
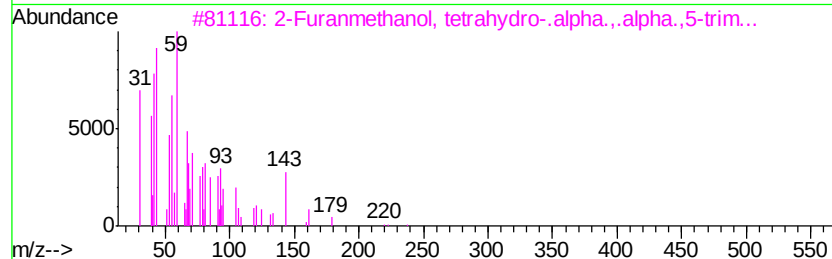
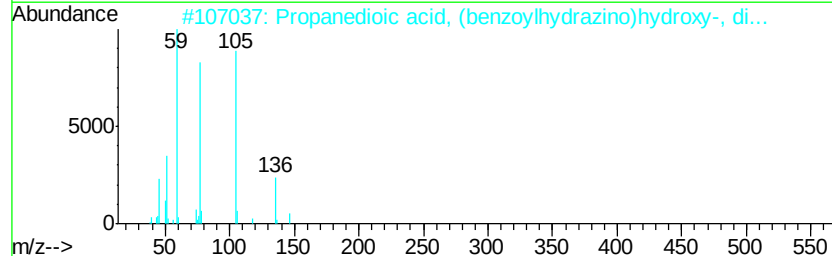
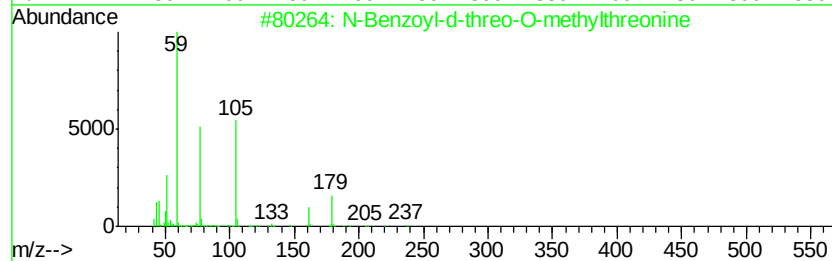
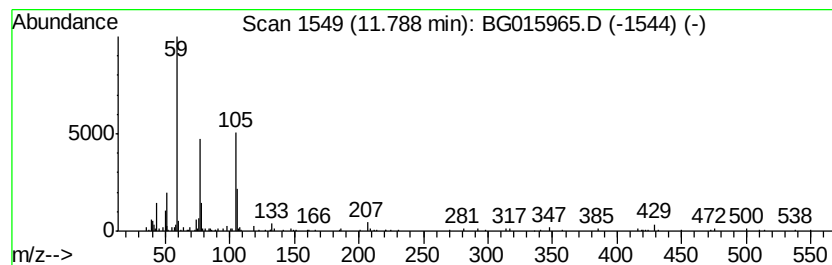
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 N-Benzoyl-d-threo-O-methylt... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.79	4.00 ng	230013	Napthalene-d8	10.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-Benzoyl-d-threo-O-methylthreonine	237	C12H15N04	131644-54-7	72
2		Propanedioic acid, (benzoylhydra...	282	C12H14N2O6	1000142-99-9	42
3		2-Furanmethanol, tetrahydro-.alp...	238	C15H26O2	026184-88-3	38
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
5		Propanoic acid, 2-methoxy-, meth...	118	C5H10O3	017639-76-8	17



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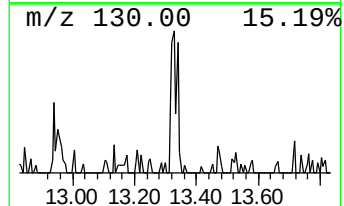
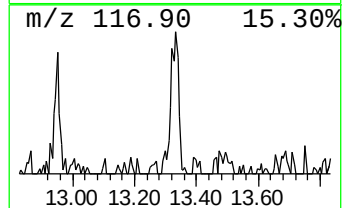
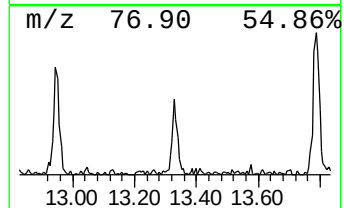
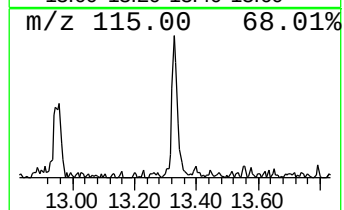
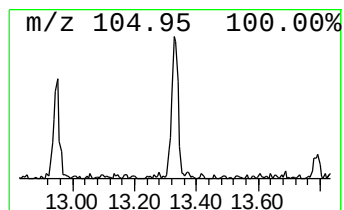
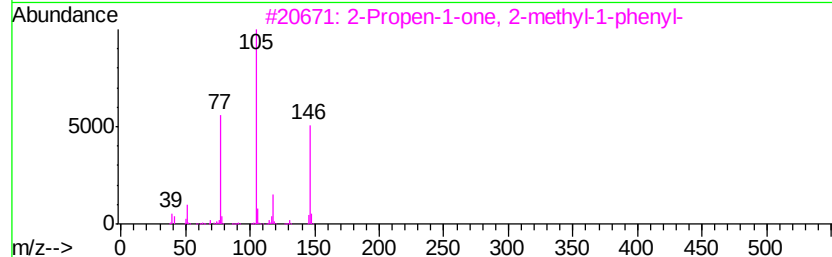
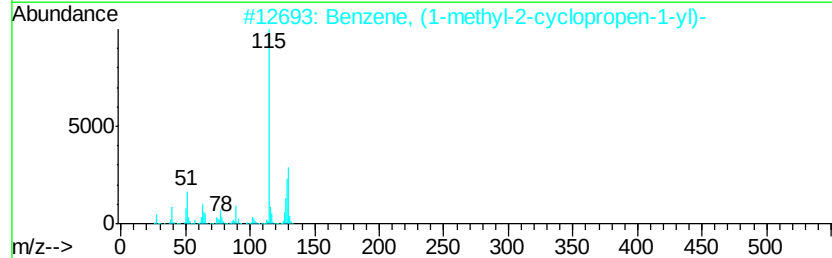
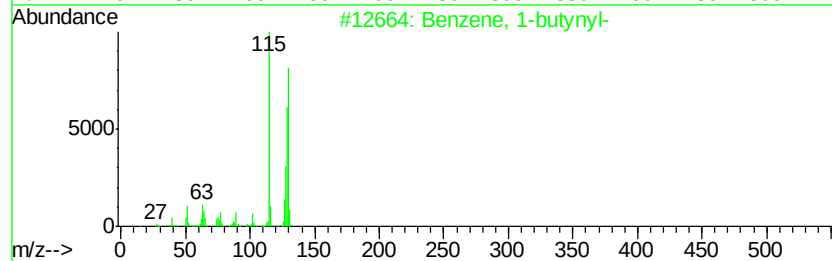
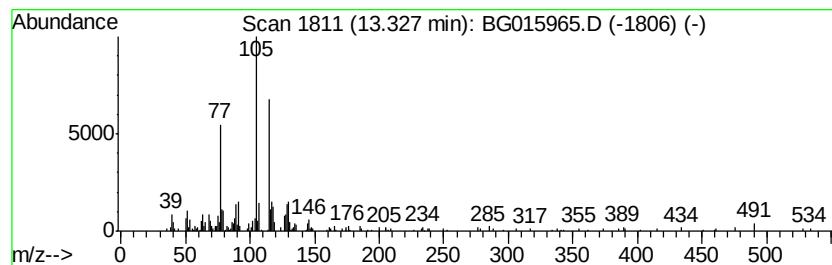
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 9 unknown13.33 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.33	2.05 ng	187672	Acenaphthene-d10	14.33

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-butynyl-	130	C10H10	000622-76-4	41
2		Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	35
3		2-Propen-1-one, 2-methyl-1-phenyl-	146	C10H10O	000769-60-8	25
4		Benzoic acid, methyl ester	136	C8H8O2	000093-58-3	25
5		Tetracyclo[2.2.1.0(2,6).0(3,5)]h...	116	C9H8	081787-74-8	25



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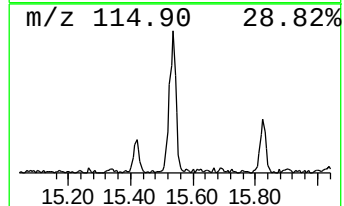
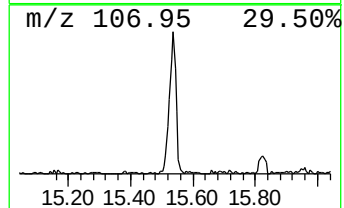
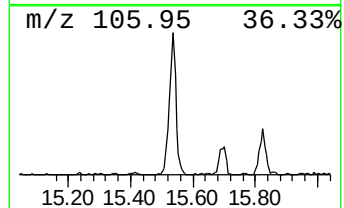
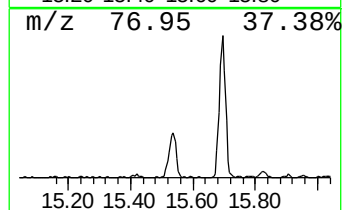
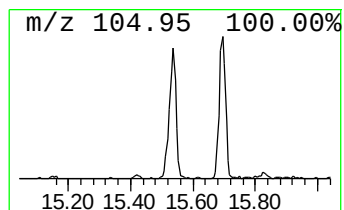
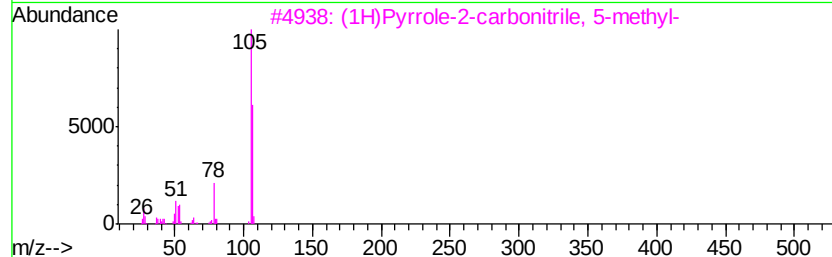
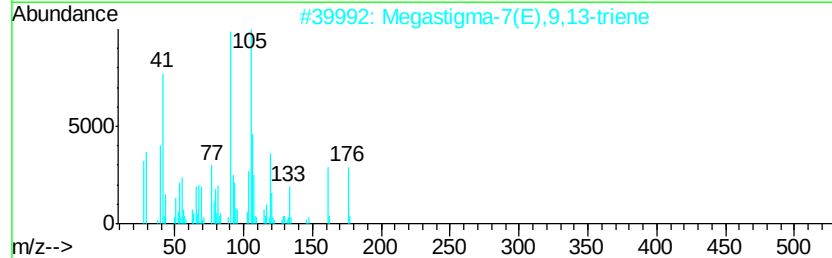
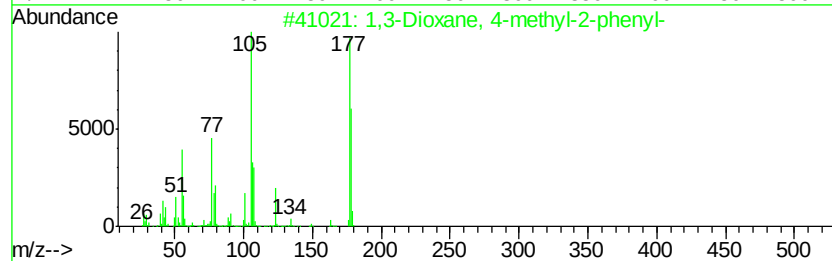
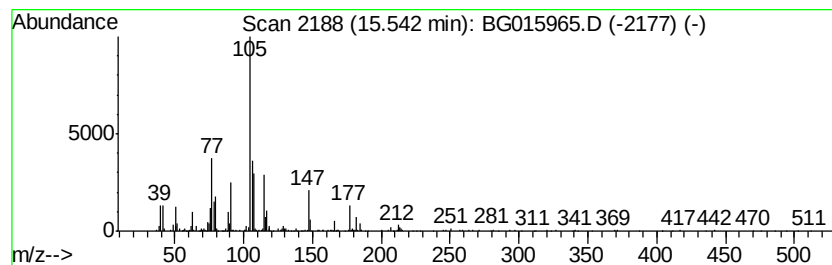
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown15.54 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	10.17 ng	931430	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	38
2		Megastigma-7(E),9,13-triene	176	C13H20	081983-67-7	23
3		(1H)Pyrrole-2-carbonitrile, 5-me...	106	C6H6N2	026173-92-2	18
4		D-Arabinose, cyclic 1,2-ethanedi...	226	C7H14O4S2	003650-67-7	17
5		Benzoin	212	C14H12O2	000579-44-2	10



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015965.D
Acq On : 28 Jan 2015 3:10
Operator : TP/IZ
Sample : G1138-09
Misc :
ALS Vial : 47 Sample Multiplier: 1

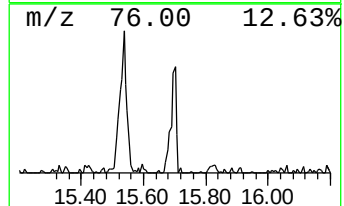
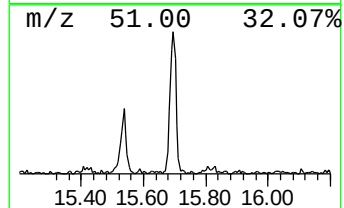
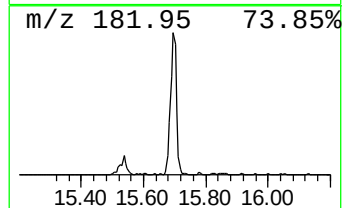
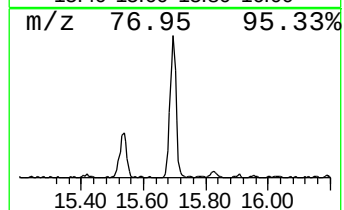
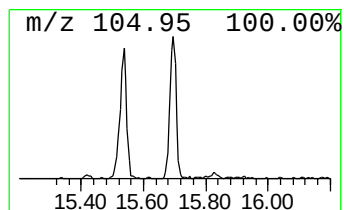
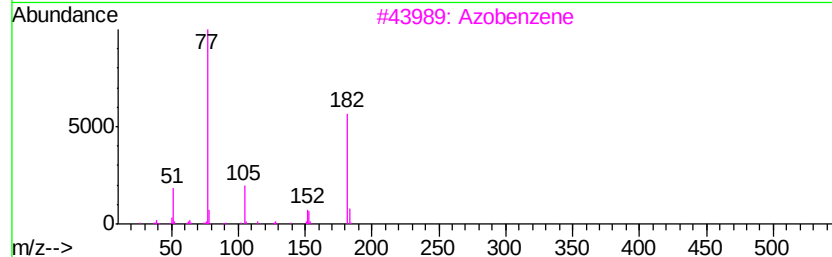
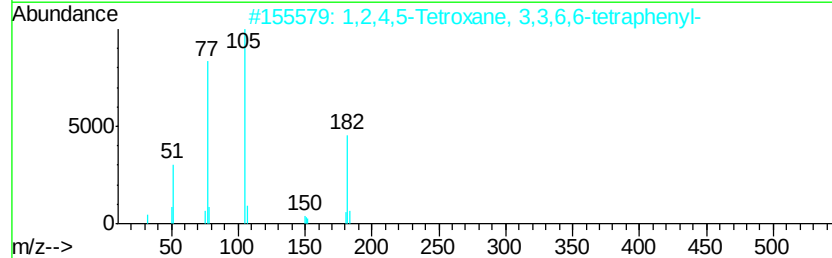
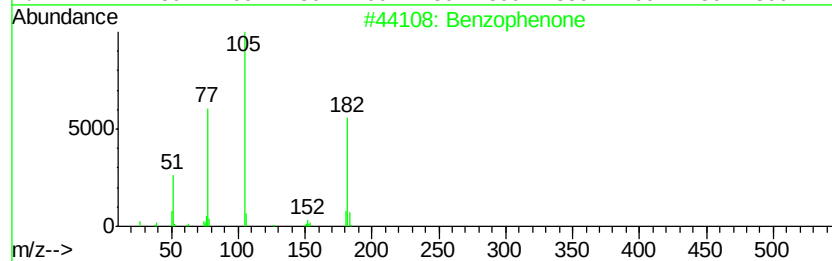
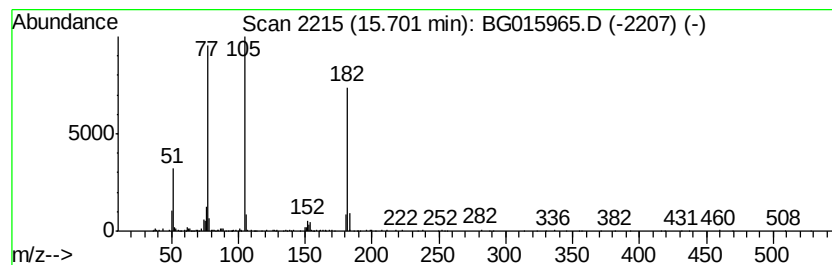
Instrument :
BNA_G
ClientSampleId :
275B2

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 11 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.70	7.37 ng	675530	Acenaphthene-d10	14.33
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 93
2		1,2,4,5-Tetroxane, 3,3,6,6-tetra...	396 C26H20O4	016204-36-7 78
3		Azobenzene	182 C12H10N2	000103-33-3 72
4		(Z)-Butenoic acid, 2-diphenylmet...	279 C18H17NO2	120238-59-7 64
5		Pyrimido[4,5-b]benzothiazole, 1,...	338 C20H22N2OS	339587-49-4 50



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015965.D
Acq On : 28 Jan 2015 3:10
Operator : TP/IZ
Sample : G1138-09
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
275B2

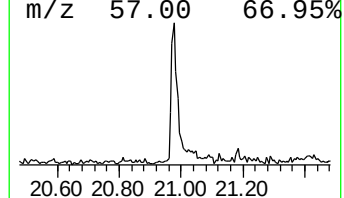
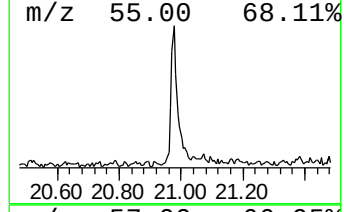
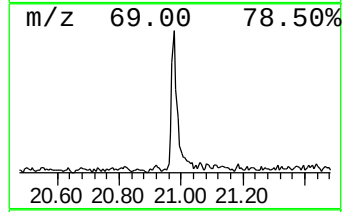
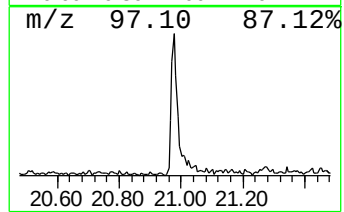
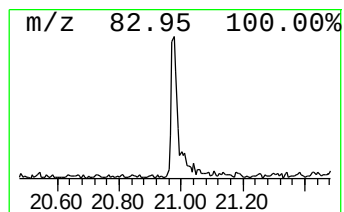
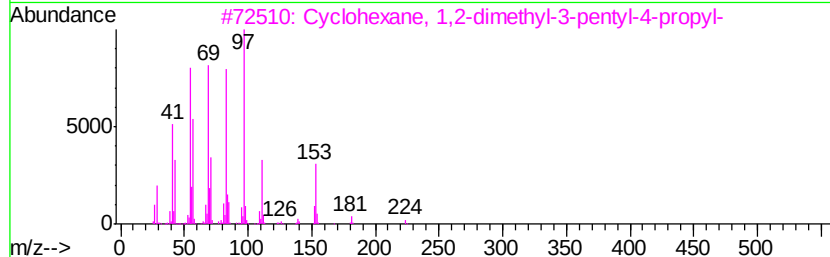
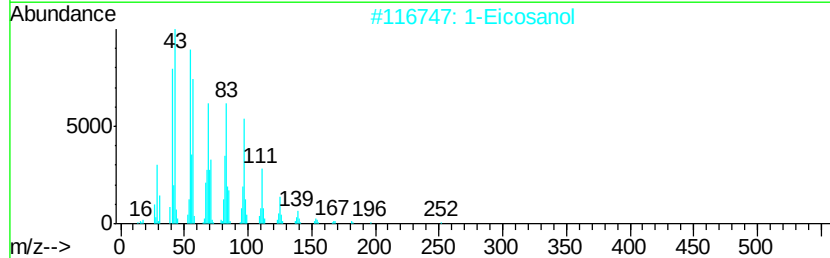
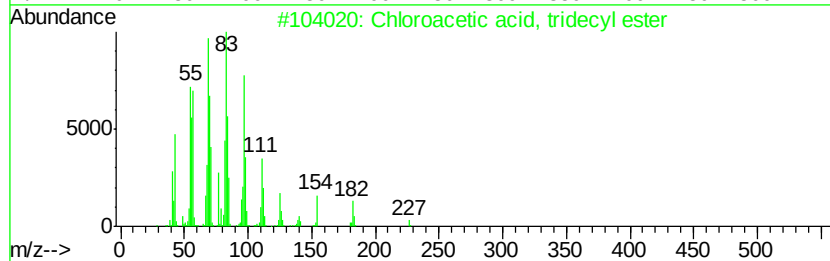
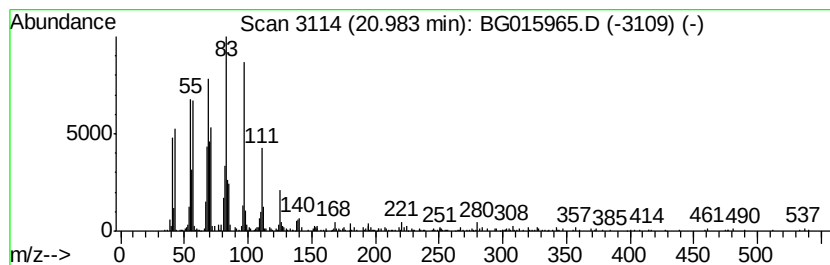
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG012015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Chloroacetic acid, tridecyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.98	5.19 ng	832978	Chrysene-d12	21.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Chloroacetic acid, tridecyl ester	276	C15H29ClO2	018277-85-5	91
2		1-Eicosanol	298	C20H42O	000629-96-9	81
3		Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	81
4		1-Docosene	308	C22H44	001599-67-3	78
5		Cyclotetradecane	196	C14H28	000295-17-0	74



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG012615\
Data File : BG015965.D
Acq On : 28 Jan 2015 3:10
Operator : TP/IZ
Sample : G1138-09
Misc :
ALS Vial : 47 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
275B2

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
unknown2.90	2.90	19.8	ng	832656	1	7.69	842701	20.0
unknown4.81	4.81	5.7	ng	237901	1	7.69	842701	20.0
unknown7.22	7.22	76.0	ng	3201860	1	7.69	842701	20.0
N-Benzoyl-d-threo...	11.79	4.0	ng	230013	2	10.47	1150730	20.0
unknown13.33	13.33	2.0	ng	187672	3	14.33	1831970	20.0
unknown15.54	15.54	10.2	ng	931430	3	14.33	1831970	20.0
Benzophenone	15.70	7.4	ng	675530	3	14.33	1831970	20.0
Chloroacetic acid...	20.98	5.2	ng	832978	5	21.26	3210890	20.0