

Data Path : Z:\HPCHEM1\BNA G\DATA\BG041916\
 Data File : BG021748.D
 Acq On : 19 Apr 2016 00:17
 Operator : UM/SJ
 Sample : H2537-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B6(15-17)

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-BG041316.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	3.093	38	43	62	rVB	1641096	2484917	100.00%	16.095%
2	3.363	84	89	100	rVB	24161	39515	1.59%	0.256%
3	5.290	411	417	423	rBV	52914	83953	3.38%	0.544%
4	5.760	489	497	508	rBV	541731	888756	35.77%	5.757%
5	7.364	760	770	783	rBV	554454	1002732	40.35%	6.495%
6	7.746	825	835	842	rBV	536157	956062	38.47%	6.193%
7	8.210	907	914	927	rVB	110536	192479	7.75%	1.247%
8	8.539	961	970	979	rBV	388336	702951	28.29%	4.553%
9	9.380	1101	1113	1121	rBV	348651	628407	25.29%	4.070%
10	11.031	1386	1394	1402	rBV	156460	289425	11.65%	1.875%
11	13.451	1798	1806	1812	rBV	933322	1502157	60.45%	9.730%
12	14.262	1938	1944	1950	rBV	96739	142804	5.75%	0.925%
13	14.691	2012	2017	2021	rBV	22966	28288	1.14%	0.183%
14	14.820	2033	2039	2047	rVB2	260875	418351	16.84%	2.710%
15	15.637	2173	2178	2182	rVB	42993	55367	2.23%	0.359%
16	16.042	2238	2247	2250	rBV4	12810	29686	1.19%	0.192%
17	16.301	2285	2291	2299	rVB	696005	1094828	44.06%	7.091%
18	16.495	2319	2324	2334	rBV	44775	82552	3.32%	0.535%
19	17.282	2452	2458	2462	rBV	26420	34648	1.39%	0.224%
20	17.558	2498	2505	2510	rBV2	306707	502331	20.22%	3.254%
21	19.591	2846	2851	2855	rBV	21949	29581	1.19%	0.192%
22	19.820	2885	2890	2897	rVB	194991	220994	8.89%	1.431%
23	19.897	2899	2903	2906	rVV3	21657	29607	1.19%	0.192%
24	19.932	2906	2909	2920	rVB2	40816	70936	2.85%	0.459%
25	20.143	2938	2945	2951	rBV	1549223	2142291	86.21%	13.876%
26	20.425	2989	2993	2998	rVB	36362	41959	1.69%	0.272%
27	20.854	3062	3066	3073	rVV	157341	171311	6.89%	1.110%
28	20.919	3073	3077	3081	rVV	40145	52162	2.10%	0.338%
29	20.960	3081	3084	3089	rVB3	20701	25823	1.04%	0.167%
30	21.436	3162	3165	3172	rVB	38825	51584	2.08%	0.334%
31	21.824	3224	3231	3239	rBV	364273	620686	24.98%	4.020%
32	22.000	3257	3261	3266	rBV	30745	42321	1.70%	0.274%
33	22.623	3364	3367	3373	rVB2	21779	36213	1.46%	0.235%
34	23.328	3481	3487	3494	rBV5	33100	84991	3.42%	0.551%

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ClientSampleId :
B6(15-17)

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-BG041316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.539	3519	3523	3529	rVB	32060	60738	2.44%	0.393%
36	25.161	3789	3799	3809	rBV2	203983	597313	24.04%	3.869%

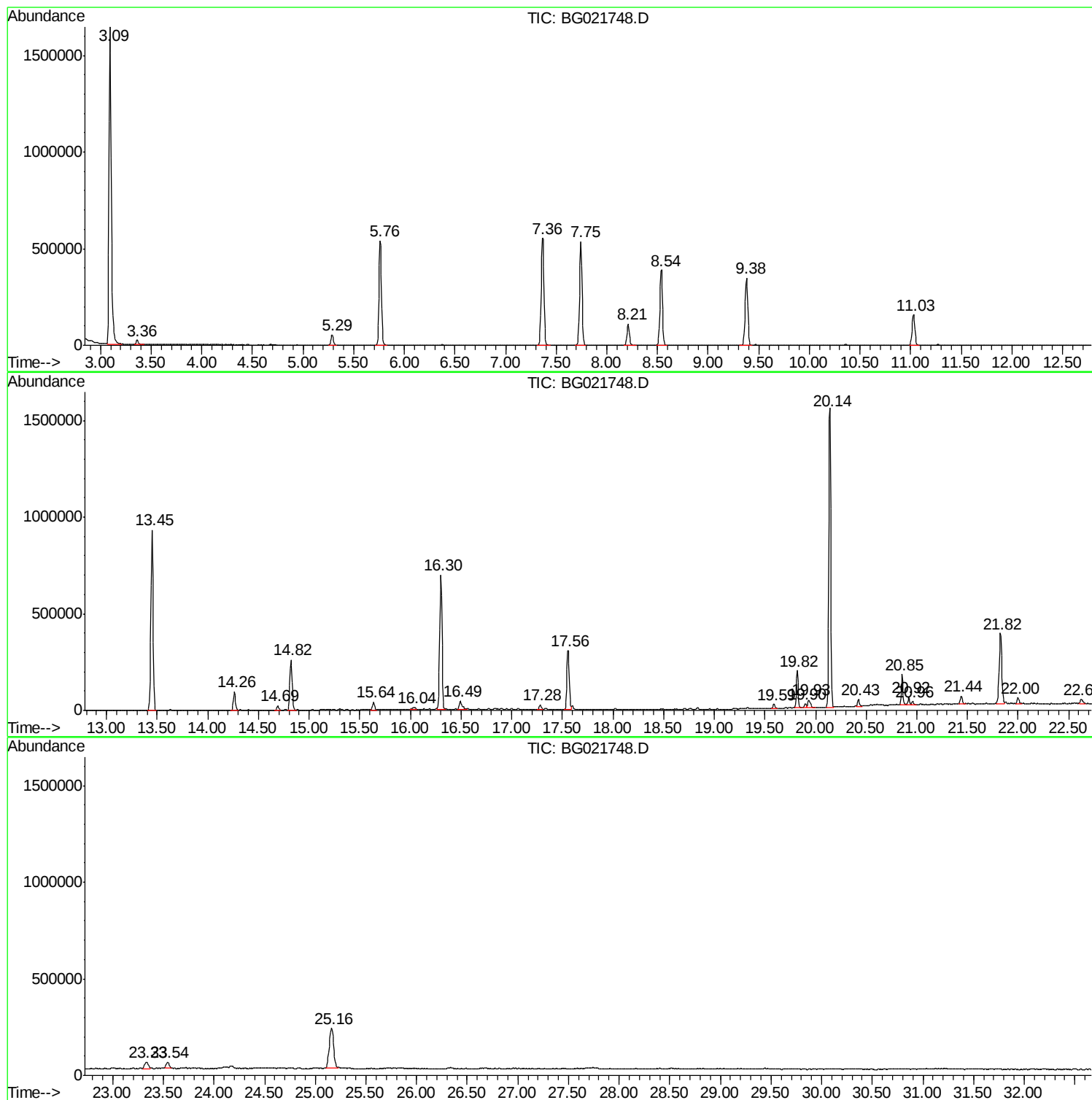
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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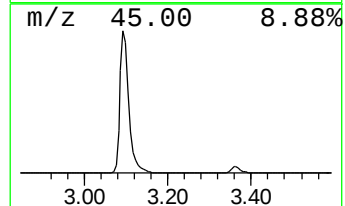
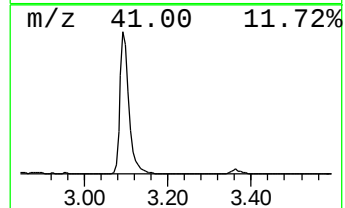
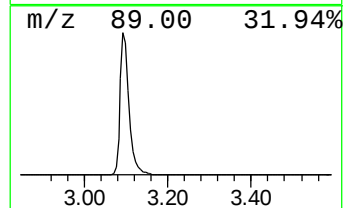
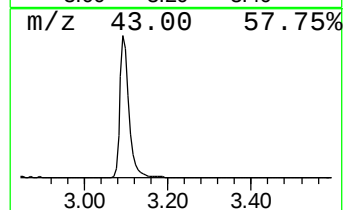
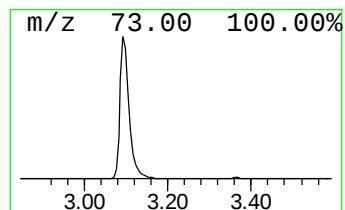
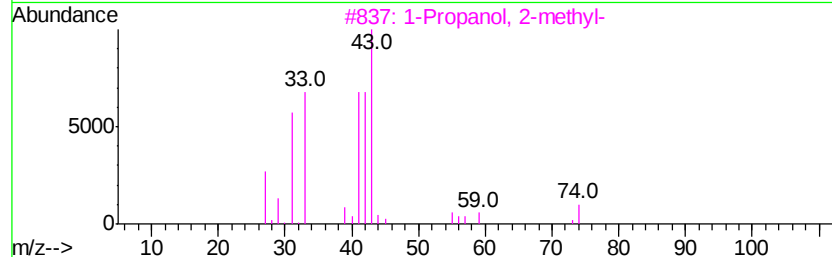
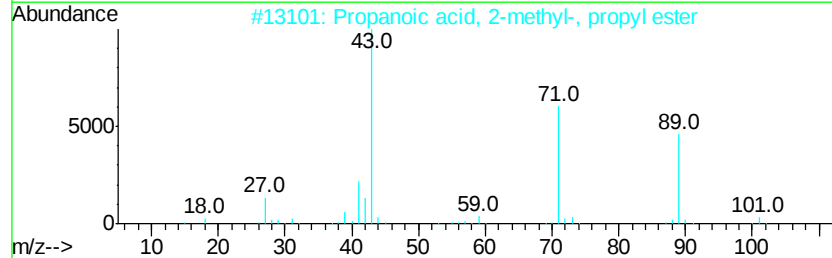
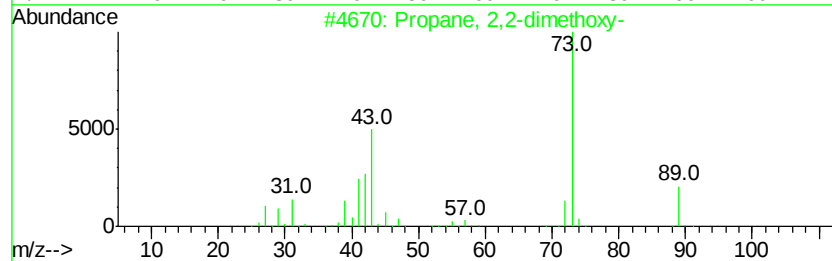
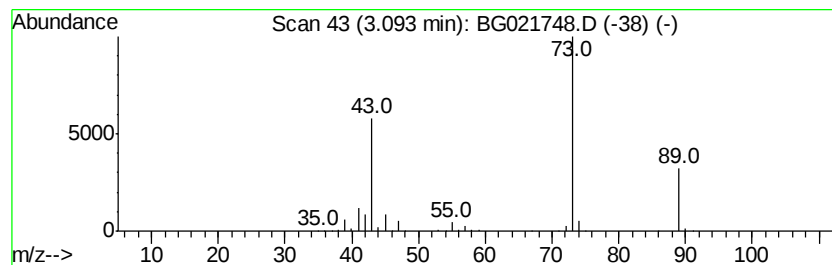
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown3.09 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.09	258.20 ng	2484920	1,4-Dichlorobenzene-d4	8.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2	Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	23
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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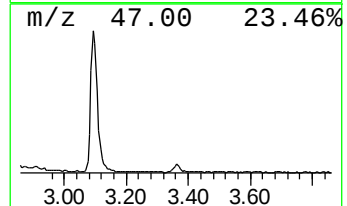
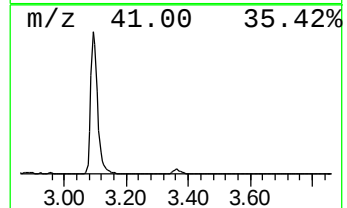
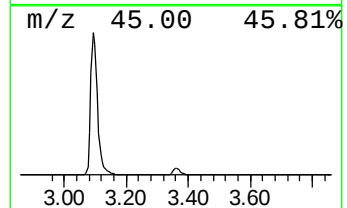
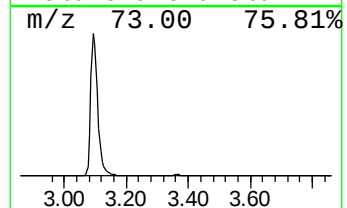
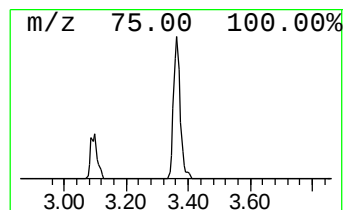
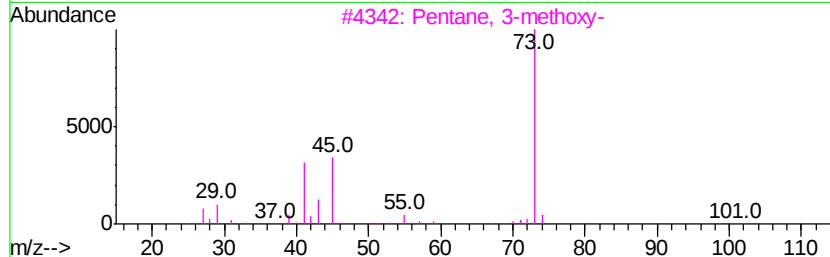
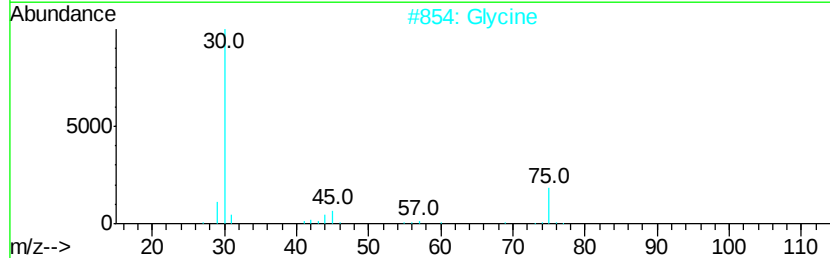
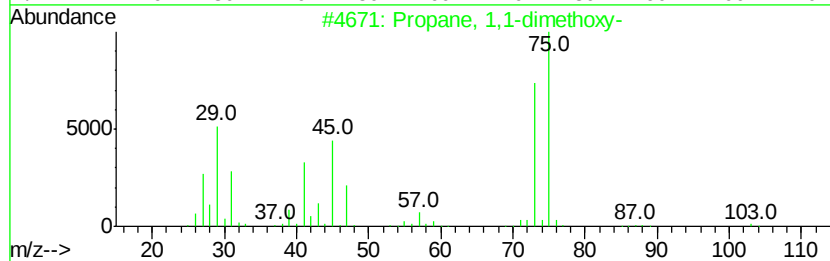
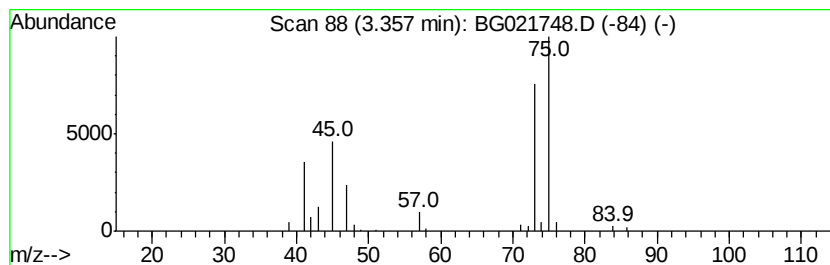
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.36	4.11 ng	39515	1,4-Dichlorobenzene-d4	8.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2			Glycine	75	C2H5NO2	000056-40-6	9
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4			1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9
5			1,3-Dioxolane, 2-(1-bromoethyl)-	180	C5H9BrO2	005267-73-2	9



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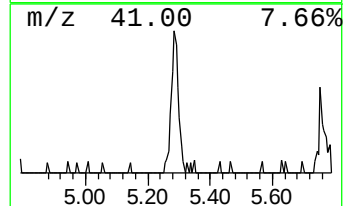
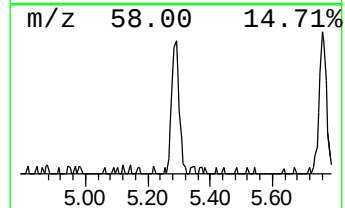
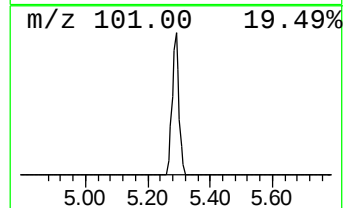
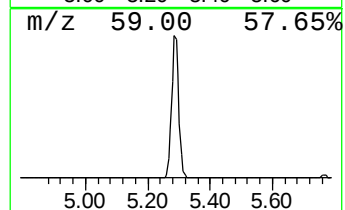
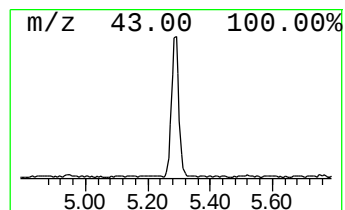
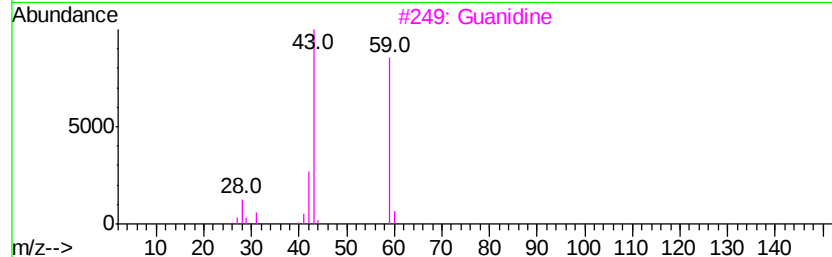
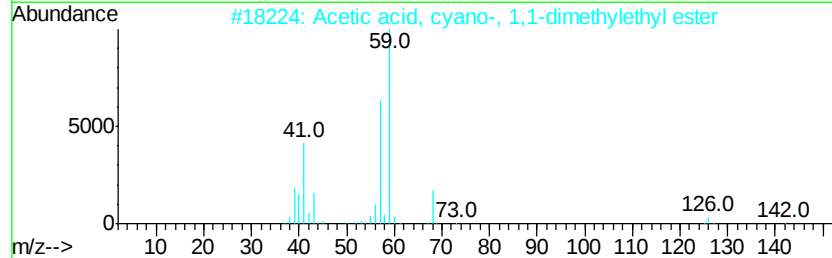
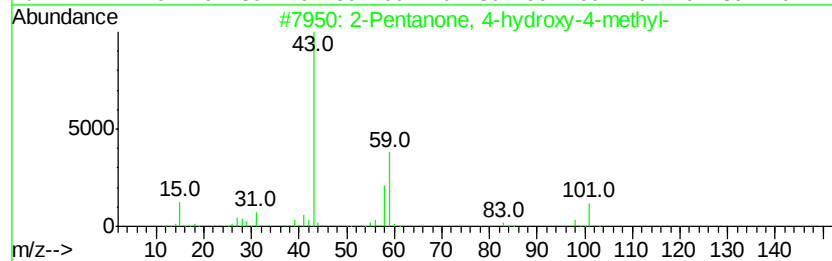
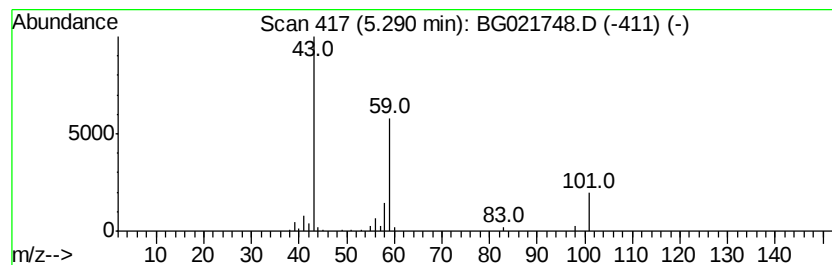
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.29	8.72 ng	83953	1,4-Dichlorobenzene-d4	8.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3			Guanidine	59	CH5N3	000113-00-8	9
4			4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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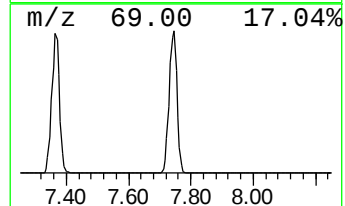
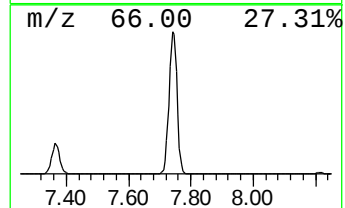
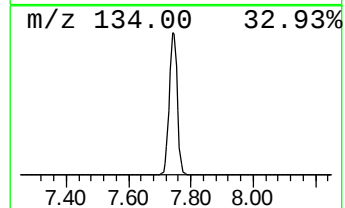
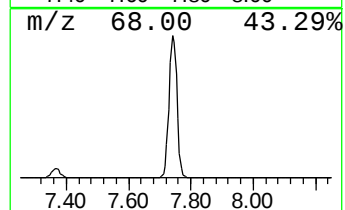
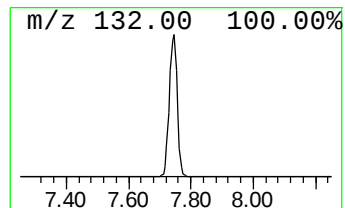
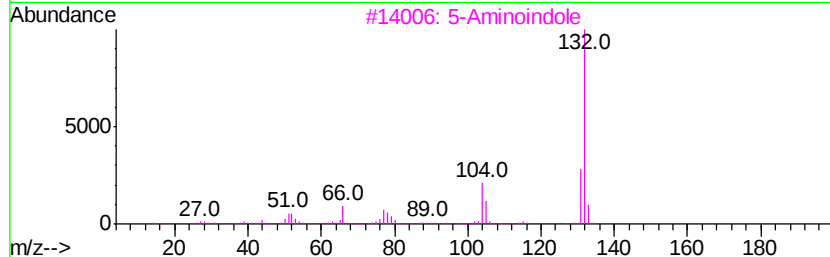
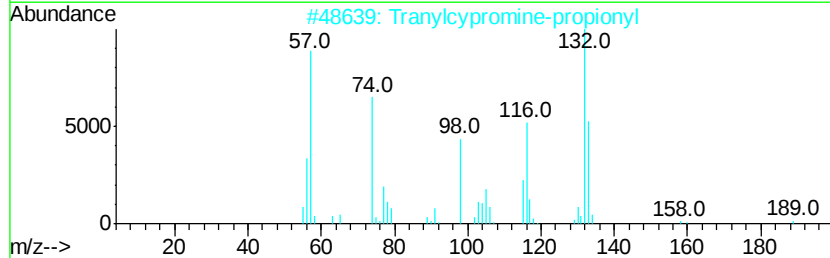
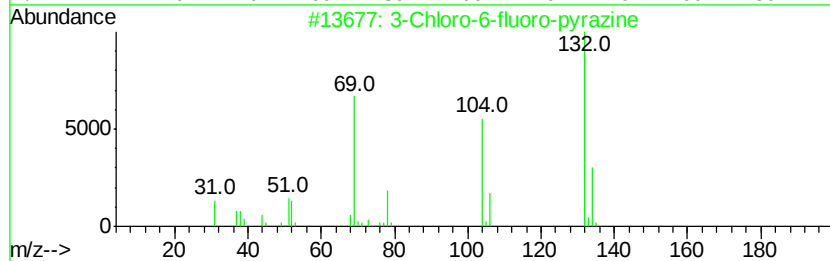
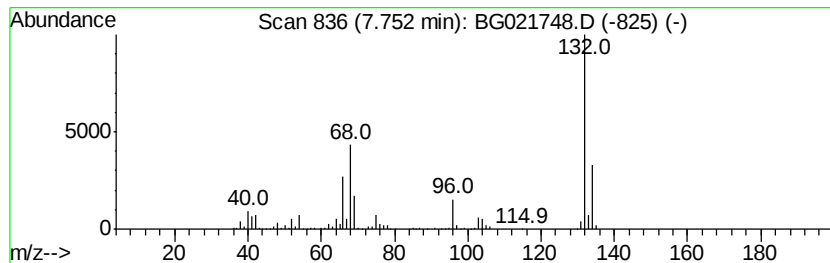
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.75 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	99.34 ng	956062	1,4-Dichlorobenzene-d4	8.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		Xenon	132	Xe	007440-63-3	9
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



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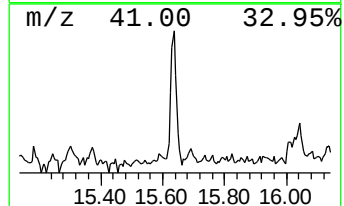
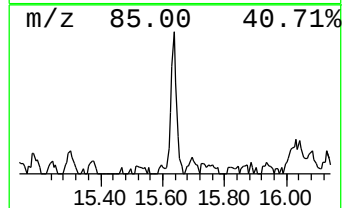
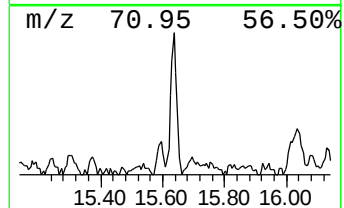
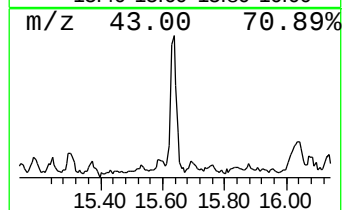
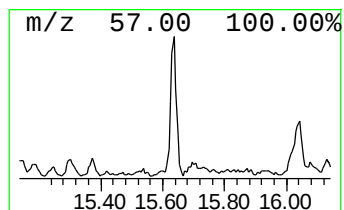
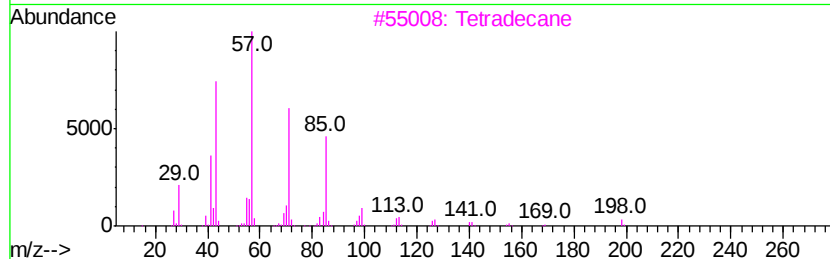
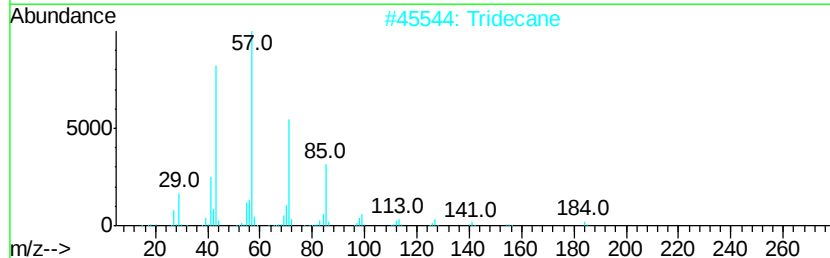
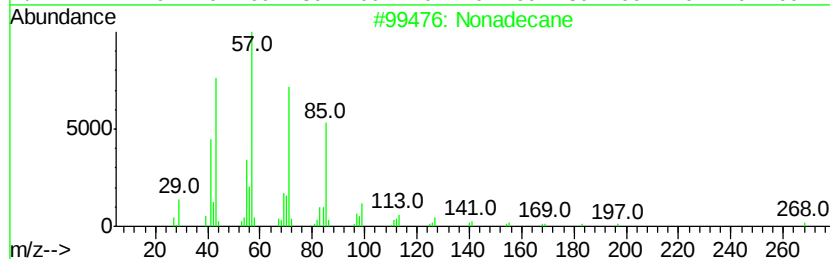
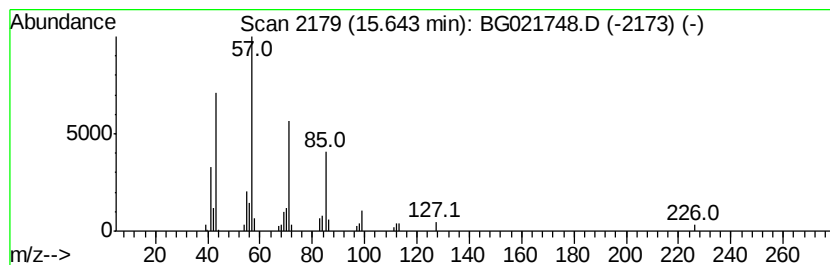
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Nonadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.64	2.65 ng	55367	Acenaphthene-d10	14.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane		268	C19H40	000629-92-5	87
2	Tridecane		184	C13H28	000629-50-5	86
3	Tetradecane		198	C14H30	000629-59-4	86
4	Eicosane		282	C20H42	000112-95-8	83
5	Hexadecane		226	C16H34	000544-76-3	83



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ClientSampleId :
B6(15-17)

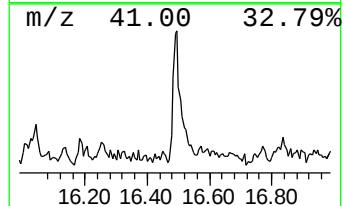
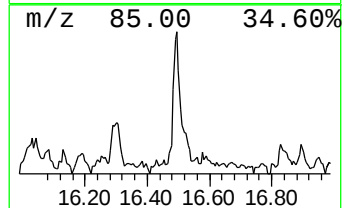
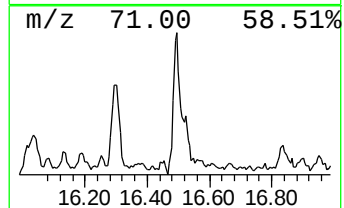
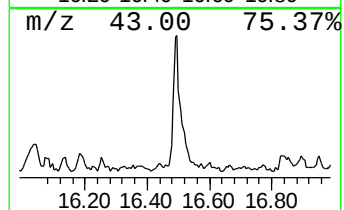
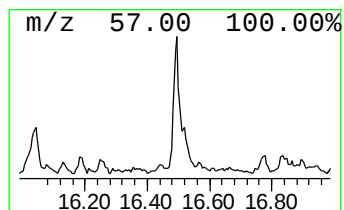
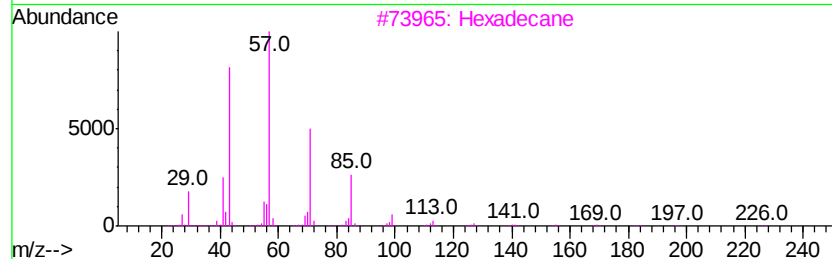
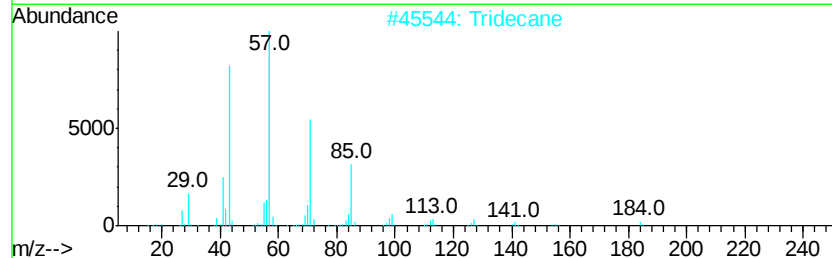
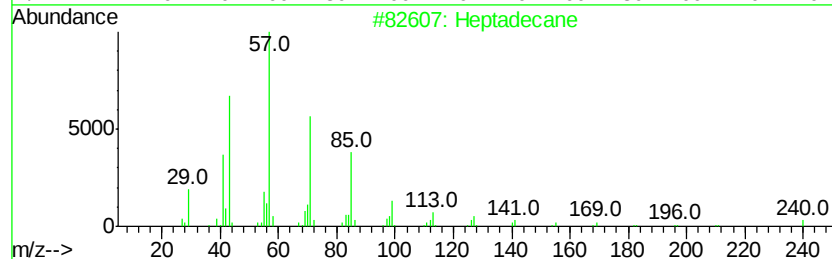
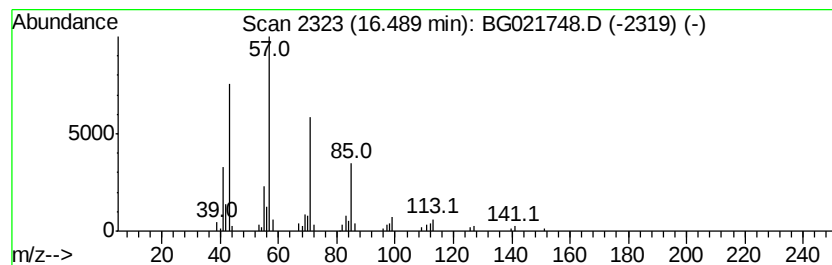
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	3.29 ng	82552	Phenanthrene-d10	17.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	90
2	Tridecane		184	C13H28	000629-50-5	90
3	Hexadecane		226	C16H34	000544-76-3	86
4	Pentadecane		212	C15H32	000629-62-9	83
5	Pentane, 2,2,3,3-tetramethyl-		128	C9H20	007154-79-2	53



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041916\
Data File : BG021748.D
Acq On : 19 Apr 2016 00:17
Operator : UM/SJ
Sample : H2537-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
B6(15-17)

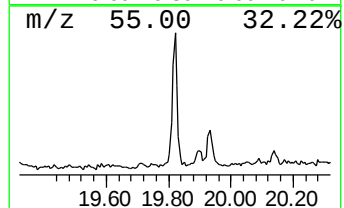
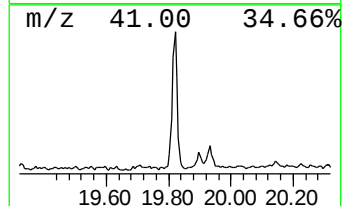
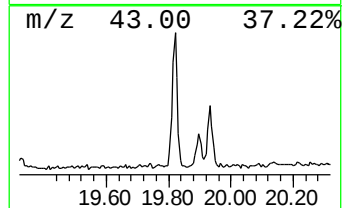
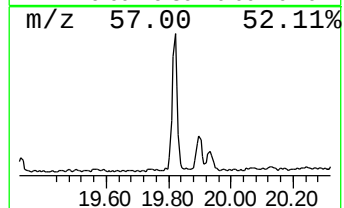
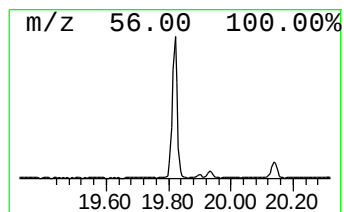
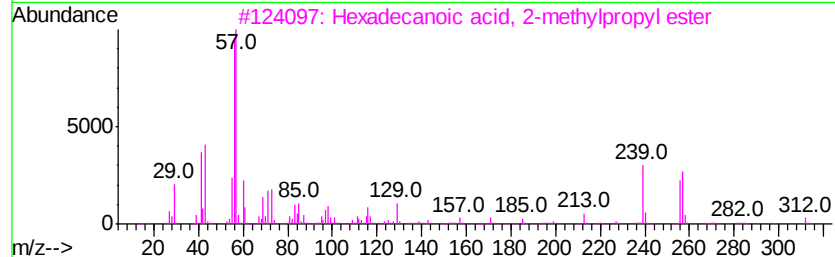
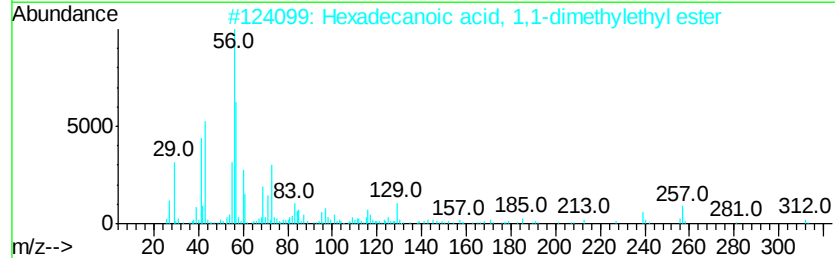
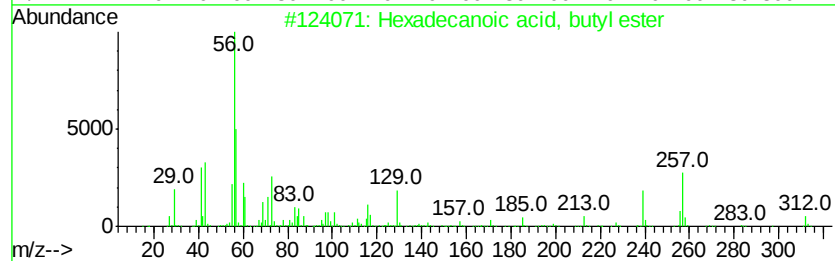
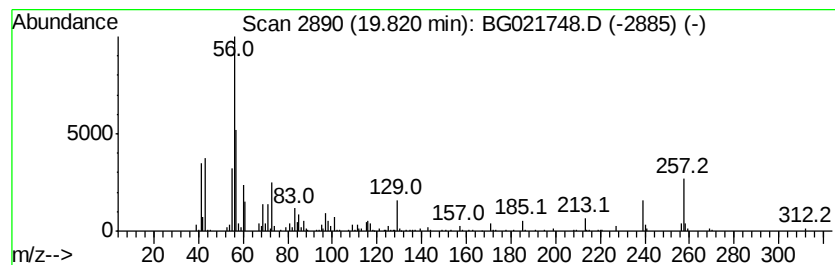
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.82	7.12 ng	220994	Chrysene-d12	21.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	90
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	64
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	040482-05-1	38
5		Cyclohexanol, 4-amino-, trans-	115	C6H13NO	027489-62-9	30



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041916\
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Acq On : 19 Apr 2016 00:17
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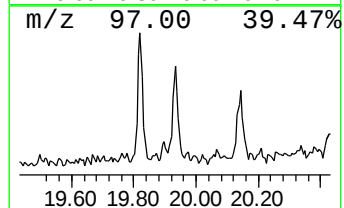
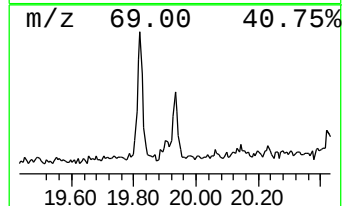
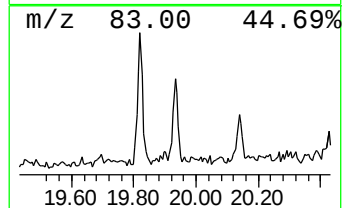
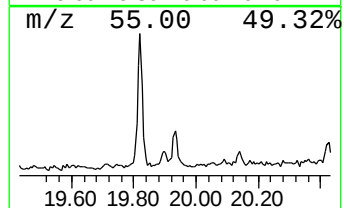
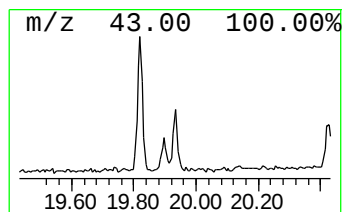
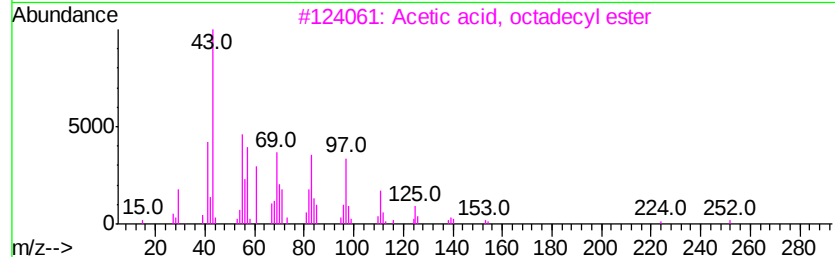
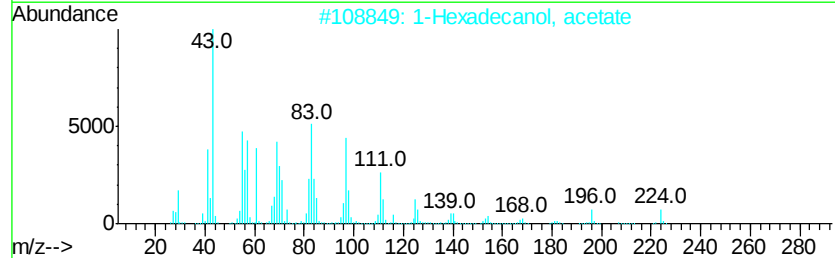
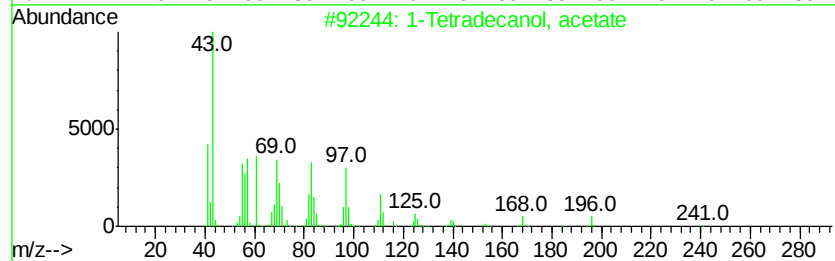
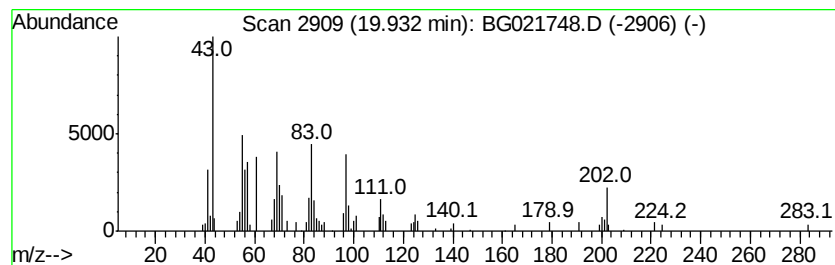
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Tetradecanol, acetate Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.93	2.29 ng	70936	Chrysene-d12		21.82
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetradecanol, acetate	256	C16H32O2	000638-59-5	87
2	1-Hexadecanol, acetate	284	C18H36O2	000629-70-9	87
3	Acetic acid, octadecyl ester	312	C20H40O2	000822-23-1	87
4	1-Heptadecanol, acetate	298	C19H38O2	000822-20-8	83
5	1-Pentadecanol acetate	270	C17H34O2	000629-58-3	72



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041916\
Data File : BG021748.D
Acq On : 19 Apr 2016 00:17
Operator : UM/SJ
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Misc :
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Instrument :
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ClientSampleId :
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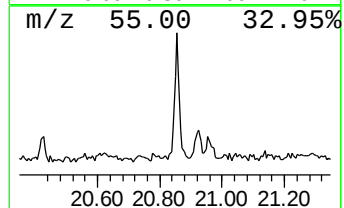
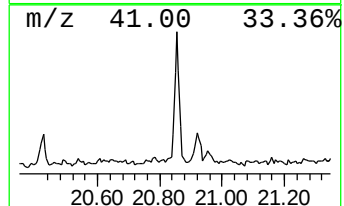
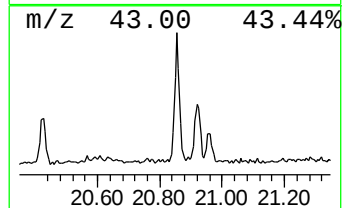
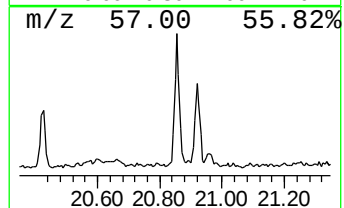
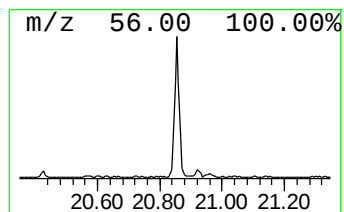
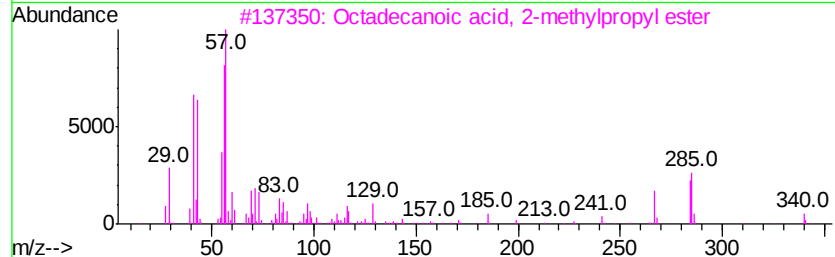
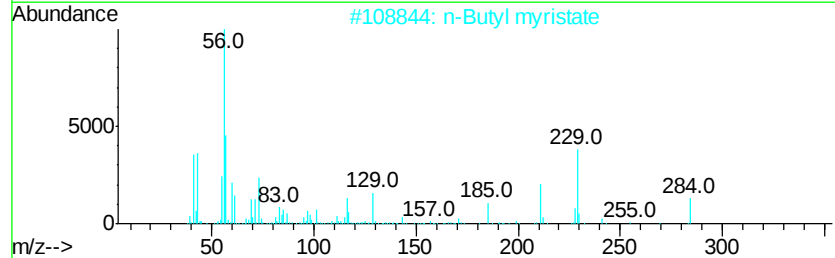
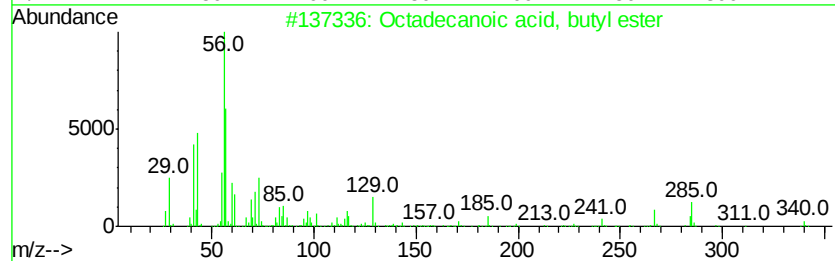
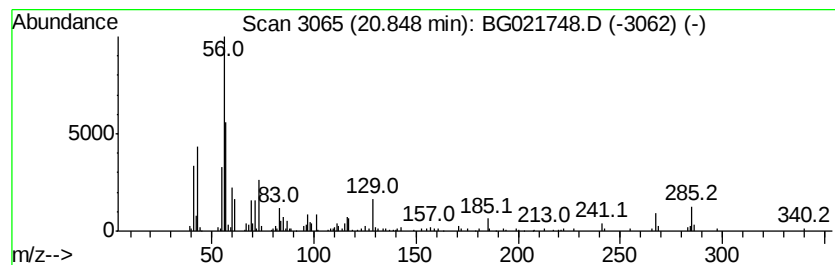
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	5.52 ng	171311	Chrysene-d12	21.82

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	97
2			n-Butyl myristate	284	C18H36O2	000110-36-1	64
3			Octadecanoic acid, 2-methylpropyl ester	340	C22H44O2	000646-13-9	43
4			Cyclopropane, 1-(1-methylethyl)-	210	C15H30	041977-39-3	38
5			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	35



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041916\
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ClientSampleId :
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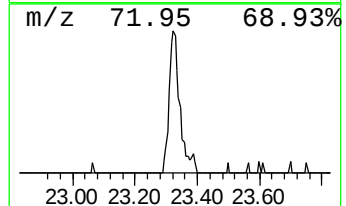
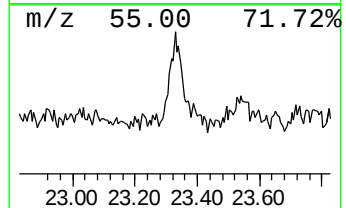
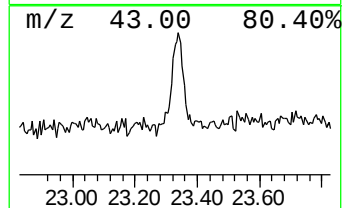
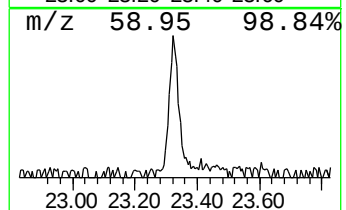
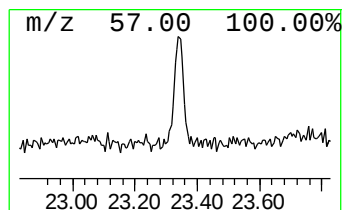
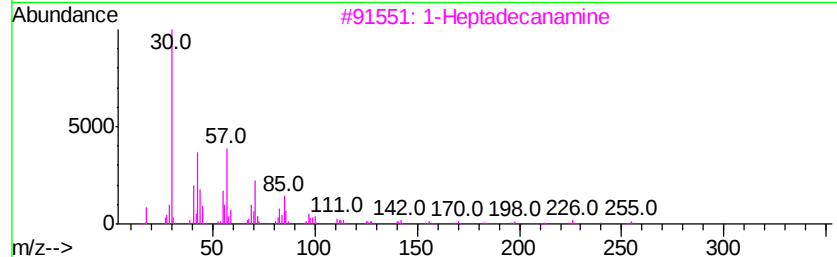
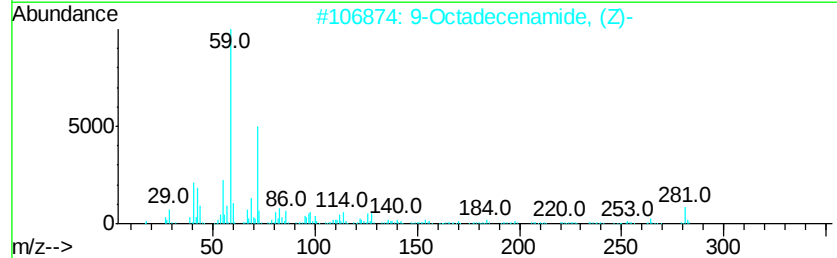
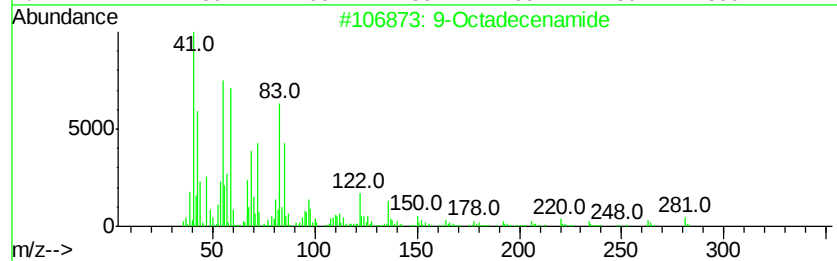
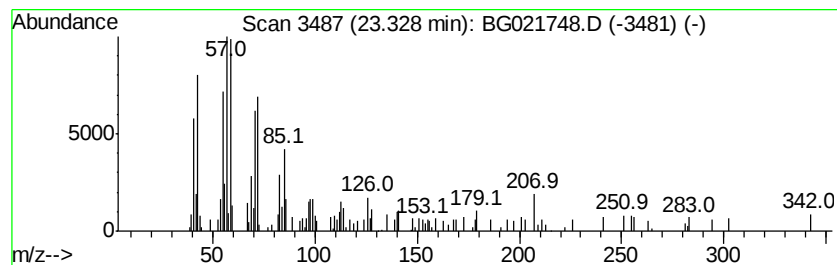
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 9-Octadecenamide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.33	2.74 ng	84991	Chrysene-d12	21.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide	281	C18H35NO	003322-62-1	52
2		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	50
3		1-Heptadecanamine	255	C17H37N	004200-95-7	42
4		Hexadecanamide	255	C16H33NO	000629-54-9	38
5		Hexadecane	226	C16H34	000544-76-3	35



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041916\
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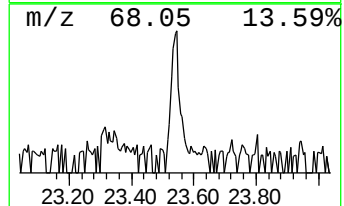
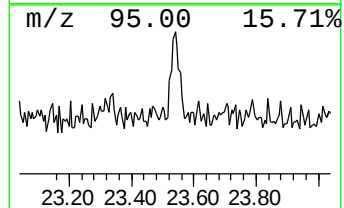
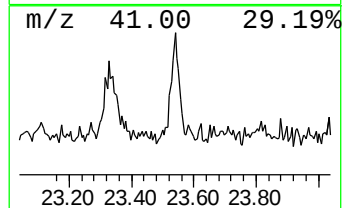
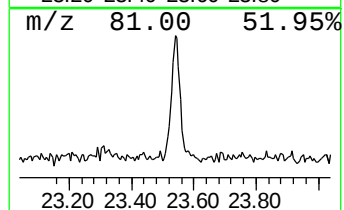
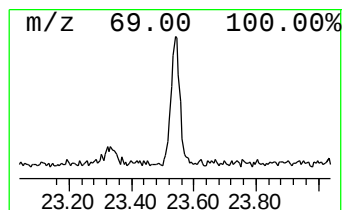
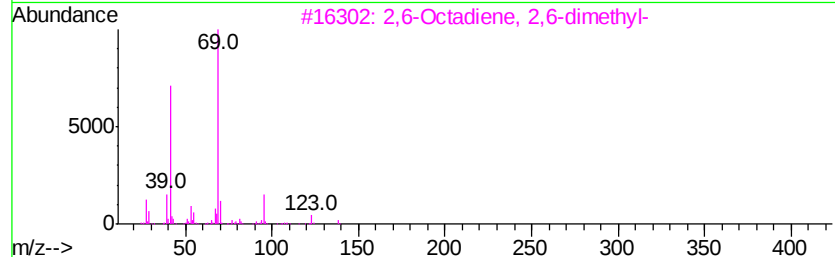
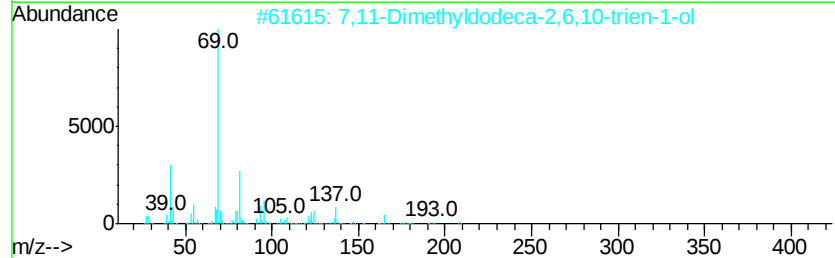
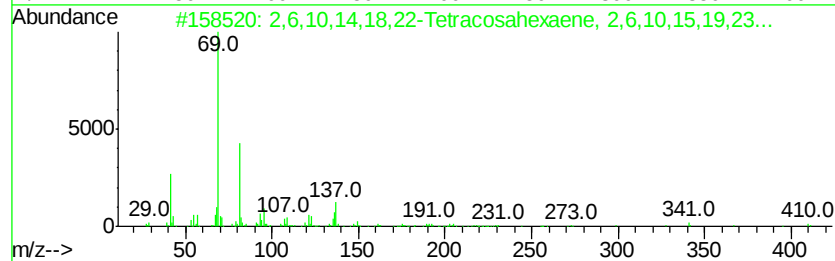
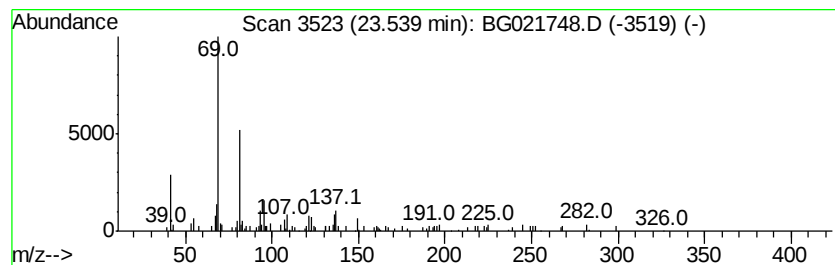
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 2,6,10,14,18,22-Tetracosae... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.54	2.03 ng	60738	Perylene-d12	25.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	80		
2	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80		
3	2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	64		
4	Squalene	410	C30H50	007683-64-9	64		
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59		



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041916\
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Acq On : 19 Apr 2016 00:17
Operator : UM/SJ
Sample : H2537-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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					#	RT	Resp	Conc
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Propane, 1,1-dime...	3.36	4.1	ng	39515	1	8.21	192479	20.0
2-Pentanone, 4-hy...	5.29	8.7	ng	83953	1	8.21	192479	20.0
unknown7.75	7.75	99.3	ng	956062	1	8.21	192479	20.0
Nonadecane	15.64	2.6	ng	55367	3	14.82	418351	20.0
Heptadecane	16.49	3.3	ng	82552	4	17.55	502331	20.0
Hexadecanoic acid...	19.82	7.1	ng	220994	5	21.82	620686	20.0
1-Tetradecanol, a...	19.93	2.3	ng	70936	5	21.82	620686	20.0
Octadecanoic acid...	20.85	5.5	ng	171311	5	21.82	620686	20.0
9-Octadecenamide	23.33	2.7	ng	84991	5	21.82	620686	20.0
2,6,10,14,18,22-T...	23.54	2.0	ng	60738	6	25.16	597313	20.0