

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
 Data File : BG017243.D
 Acq On : 22 May 2015 13:12
 Operator : TP/IZ
 Sample : G2255-11
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DUP-0274-150512

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-BG051315.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	2.769	9	14	23	rBV2	67581	152270	28.02%	3.395%
2	2.851	23	28	42	rVB	235414	380651	70.04%	8.488%
3	3.151	75	79	86	rVB4	8653	13115	2.41%	0.292%
4	4.309	270	276	286	rVB	33394	52357	9.63%	1.167%
5	4.990	387	392	402	rBV6	9337	18412	3.39%	0.411%
6	5.272	436	440	447	rVB2	14318	21764	4.00%	0.485%
7	6.882	710	714	720	rBV3	8528	13569	2.50%	0.303%
8	7.217	767	771	779	rVB	27902	44257	8.14%	0.987%
9	7.681	843	850	858	rVB	141728	216116	39.77%	4.819%
10	7.998	899	904	909	rBV	30581	48476	8.92%	1.081%
11	8.839	1042	1047	1055	rVB	28993	48631	8.95%	1.084%
12	10.472	1318	1325	1332	rBV	188089	303340	55.82%	6.764%
13	11.124	1430	1436	1442	rVB5	3824	5767	1.06%	0.129%
14	12.681	1697	1701	1710	rBV3	15192	24580	4.52%	0.548%
15	12.951	1738	1747	1754	rBV2	84907	142693	26.26%	3.182%
16	13.233	1790	1795	1801	rBV3	50483	78438	14.43%	1.749%
17	13.792	1886	1890	1894	rBV	22113	27724	5.10%	0.618%
18	13.868	1900	1903	1909	rVB4	7342	10493	1.93%	0.234%
19	14.332	1975	1982	1990	rBV2	258870	401238	73.83%	8.947%
20	14.873	2065	2074	2079	rBV6	2924	7252	1.33%	0.162%
21	15.084	2105	2110	2112	rVB2	4737	6048	1.11%	0.135%
22	15.349	2152	2155	2160	rVB6	3797	5456	1.00%	0.122%
23	15.460	2171	2174	2179	rBV2	15823	21236	3.91%	0.474%
24	15.542	2183	2188	2191	rBV7	5543	8577	1.58%	0.191%
25	15.824	2229	2236	2246	rBV3	56301	100766	18.54%	2.247%
26	16.054	2272	2275	2278	rBV	6606	7948	1.46%	0.177%
27	16.359	2320	2327	2331	rBV2	13353	18915	3.48%	0.422%
28	16.847	2405	2410	2413	rBV5	9146	13657	2.51%	0.305%
29	17.082	2444	2450	2456	rVB	333878	467046	85.94%	10.414%
30	17.317	2486	2490	2493	rBV4	4943	6450	1.19%	0.144%
31	17.464	2512	2515	2521	rBV4	6679	10660	1.96%	0.238%
32	17.587	2532	2536	2538	rBV3	5719	6826	1.26%	0.152%
33	17.752	2561	2564	2570	rBV6	6349	7384	1.36%	0.165%
34	17.981	2599	2603	2609	rBV2	63633	83061	15.28%	1.852%

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35	18.045	2612	2614	2618	rVB3	7239	9895	1.82%	0.221%
36	18.280	2650	2654	2658	rBV4	4916	8100	1.49%	0.181%
37	18.327	2658	2662	2665	rVV6	3978	7163	1.32%	0.160%
38	18.844	2747	2750	2755	rBV6	4724	6170	1.14%	0.138%
39	19.267	2818	2822	2832	rBV3	41052	59133	10.88%	1.319%
40	19.414	2843	2847	2851	rVB2	50368	58680	10.80%	1.308%
41	19.491	2857	2860	2864	rBV3	6959	9644	1.77%	0.215%
42	19.532	2864	2867	2870	rVB3	9847	10939	2.01%	0.244%
43	19.714	2893	2898	2905	rVB	176597	224859	41.37%	5.014%
44	20.025	2948	2951	2955	rVB5	9032	11320	2.08%	0.252%
45	20.172	2973	2976	2981	rBV6	6690	9052	1.67%	0.202%
46	20.460	3021	3025	3028	rBV	57558	58740	10.81%	1.310%
47	20.519	3032	3035	3038	rVB3	11444	12055	2.22%	0.269%
48	20.983	3109	3114	3118	rBV2	47480	68365	12.58%	1.524%
49	21.059	3126	3127	3131	rVB4	9415	6478	1.19%	0.144%
50	21.165	3142	3145	3146	rBV3	8571	9446	1.74%	0.211%
51	21.183	3146	3148	3151	rVB3	17135	17644	3.25%	0.393%
52	21.265	3157	3162	3167	rBV	465241	543472	100.00%	12.118%
53	21.412	3185	3187	3193	rBV6	9570	10071	1.85%	0.225%
54	21.853	3259	3262	3264	rBV4	11558	16078	2.96%	0.359%
55	21.900	3268	3270	3274	rVB5	8795	8456	1.56%	0.189%
56	22.446	3359	3363	3367	rVB4	15792	22063	4.06%	0.492%
57	23.515	3538	3545	3554	rVB2	271106	515233	94.80%	11.489%
58	27.287	4185	4187	4191	rBV4	5268	6456	1.19%	0.144%

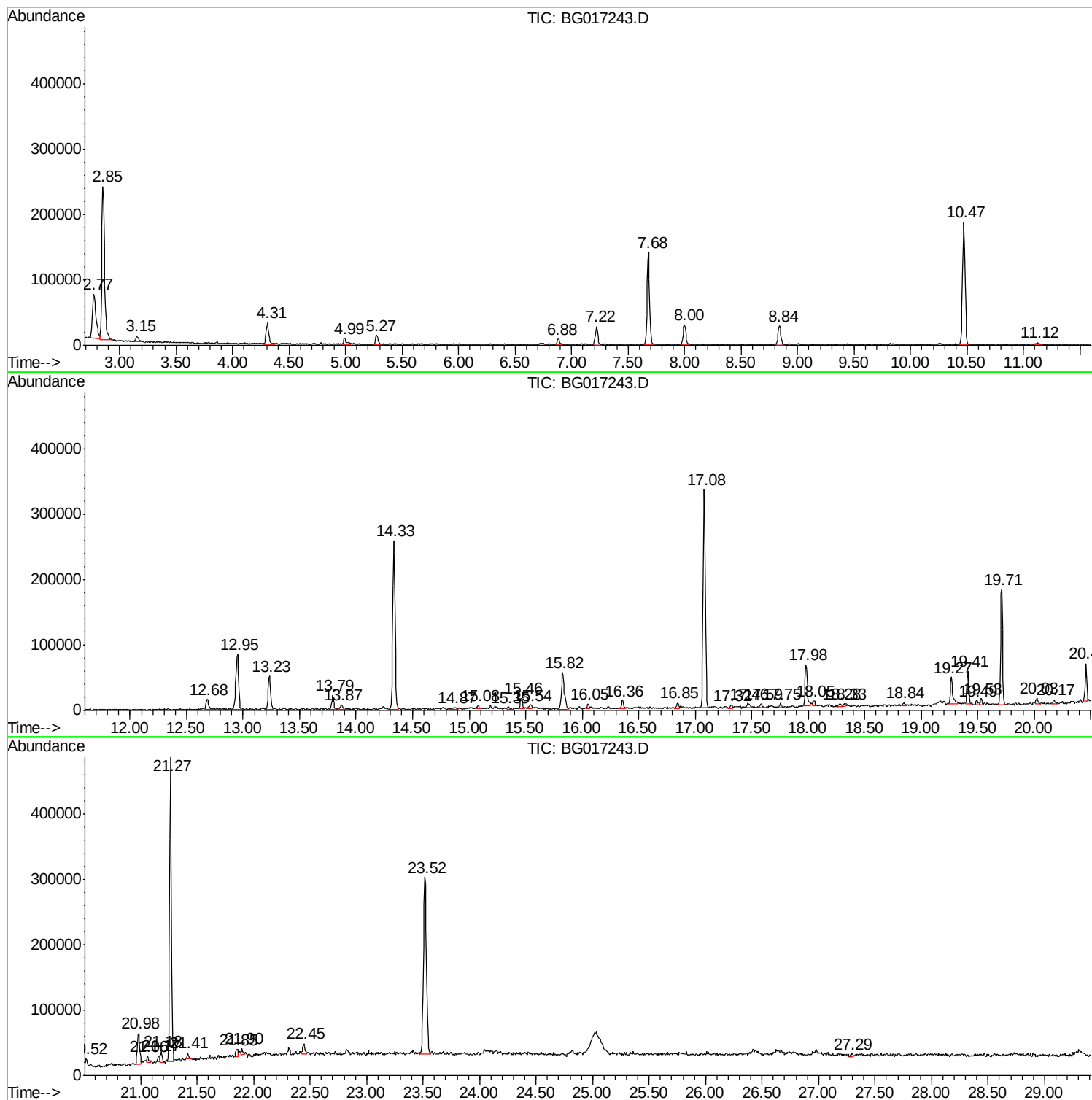
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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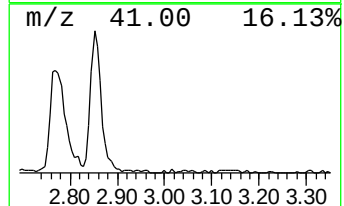
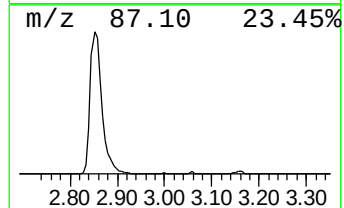
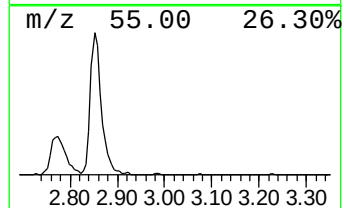
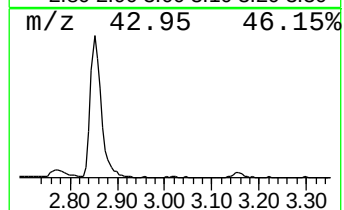
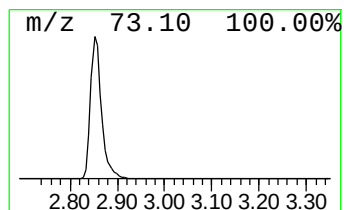
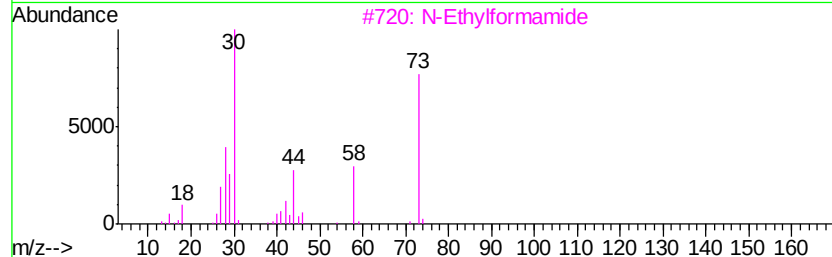
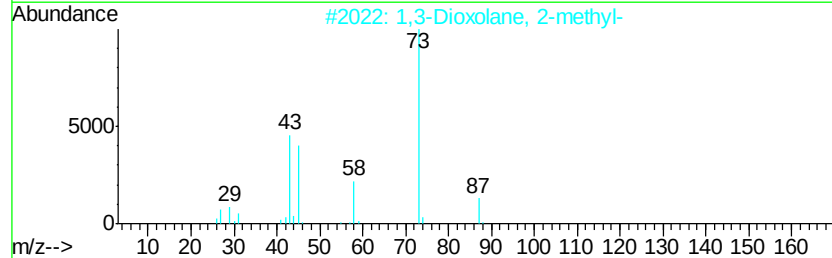
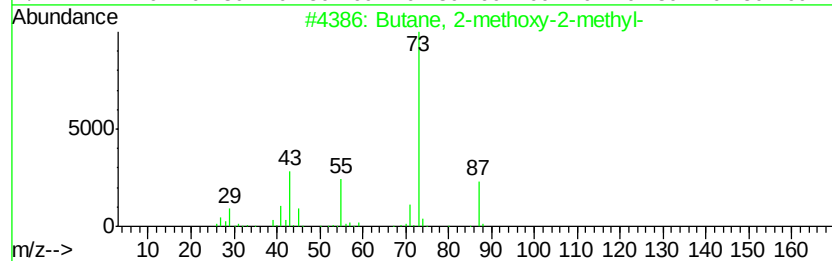
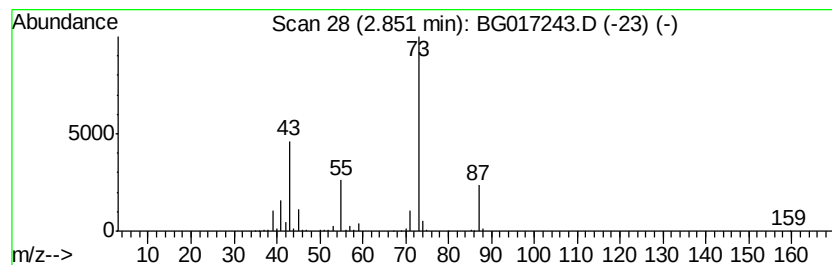
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	35.23 ng	380651	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	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, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	9



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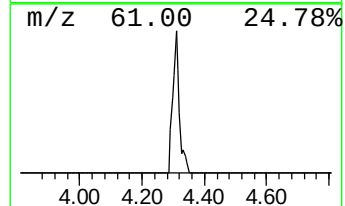
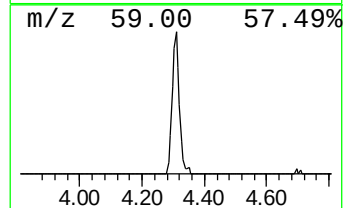
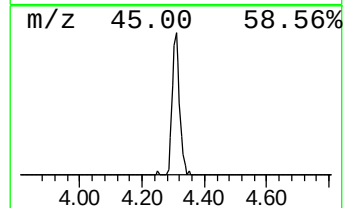
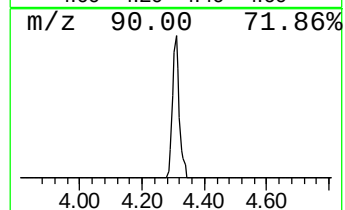
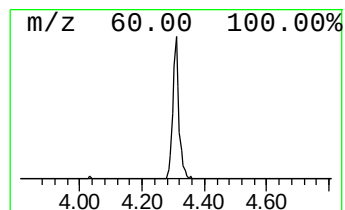
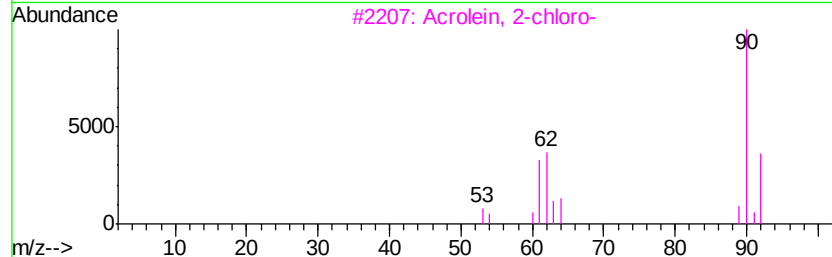
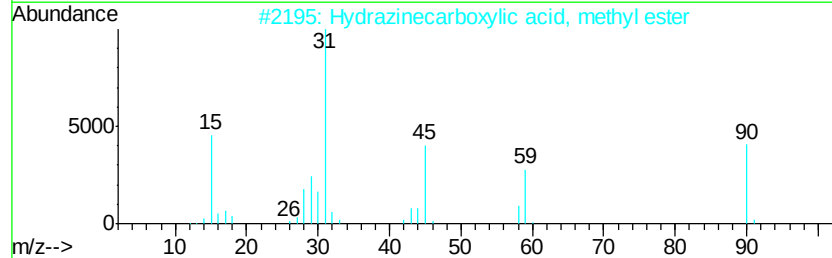
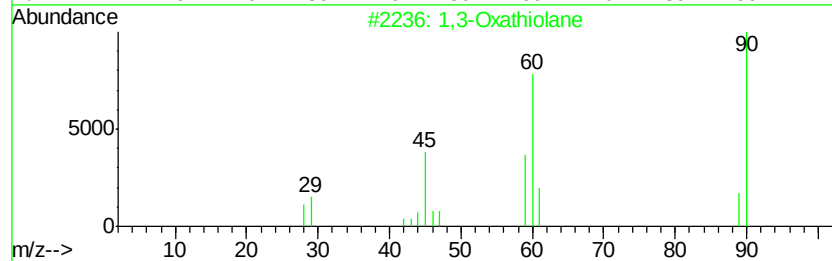
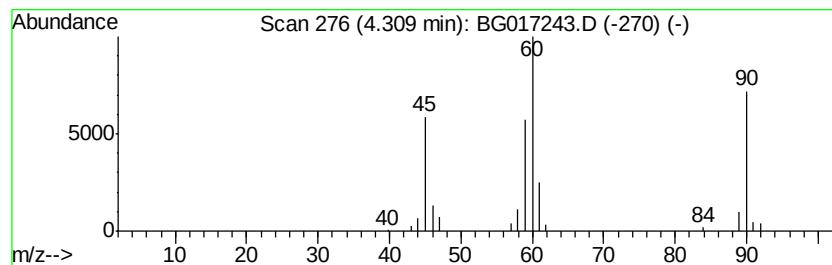
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown4.31 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.31	4.85 ng	52357	1,4-Dichlorobenzene-d4	7.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Oxathiolane	90	C3H6OS	002094-97-5	43
2			Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	17
3			Acrolein, 2-chloro-	90	C3H3ClO	000683-51-2	10
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5			Thiirane	60	C2H4S	000420-12-2	9



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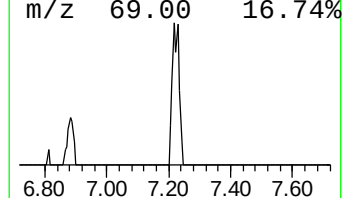
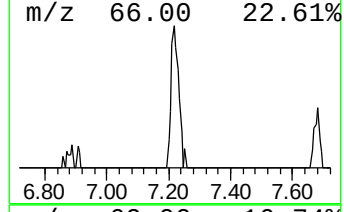
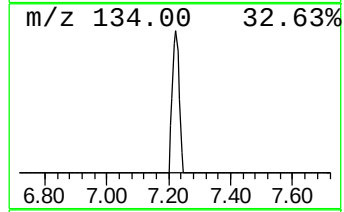
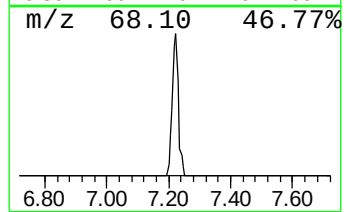
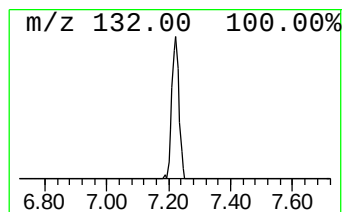
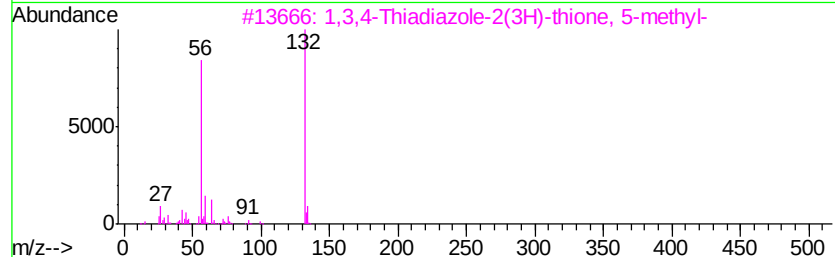
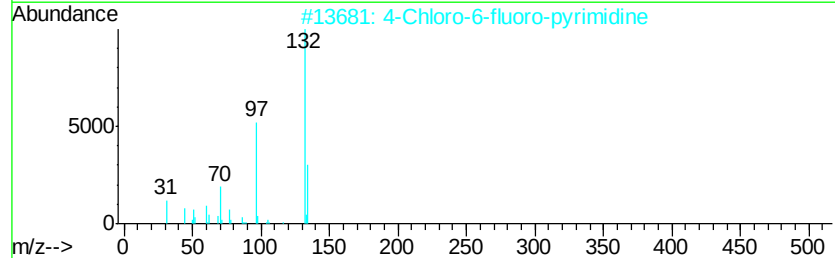
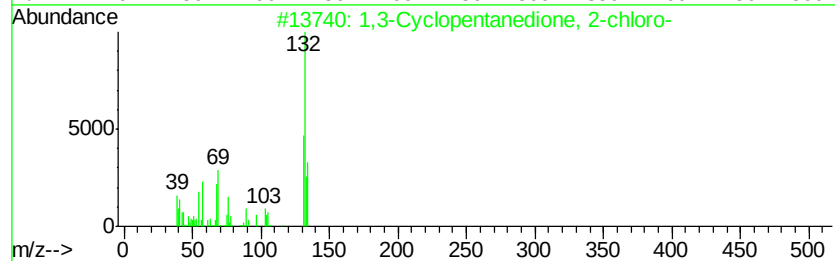
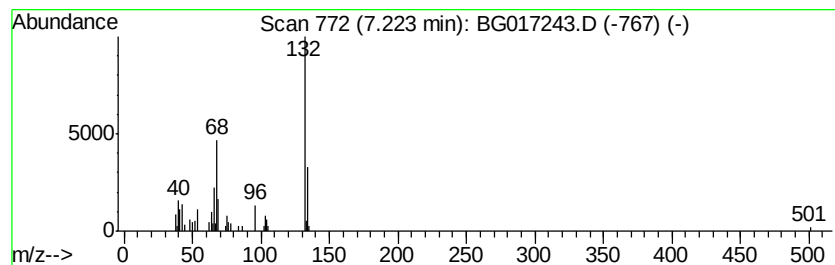
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.22 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	4.10 ng	44257	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	37
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27
4		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



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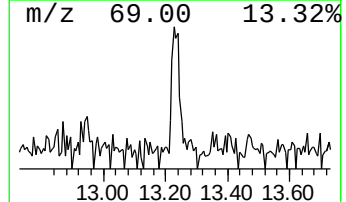
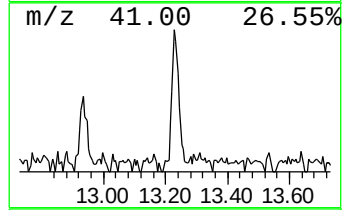
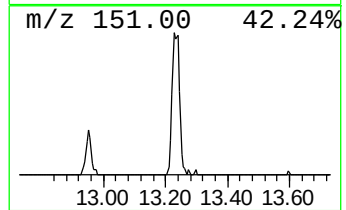
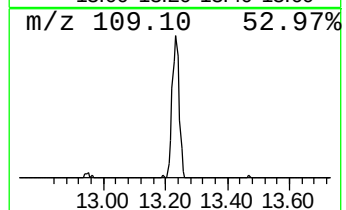
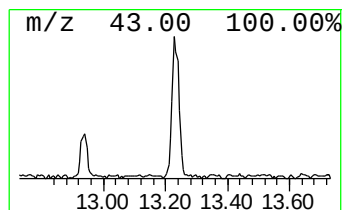
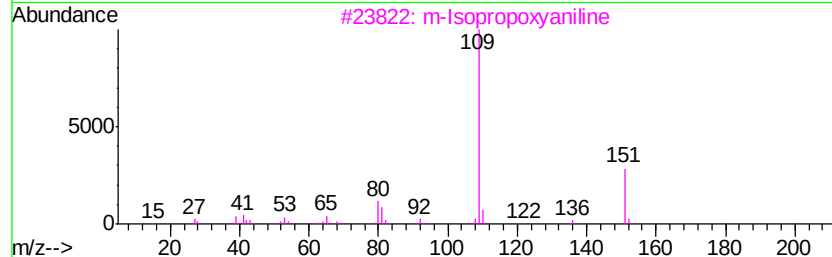
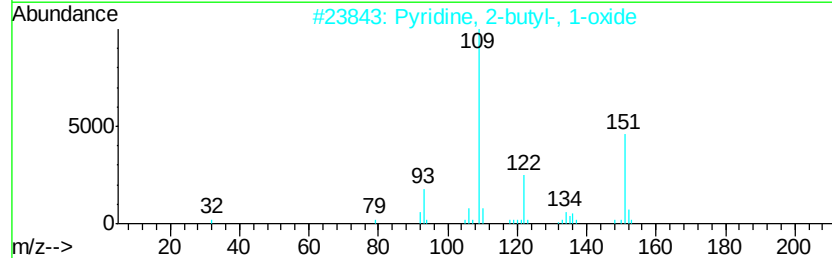
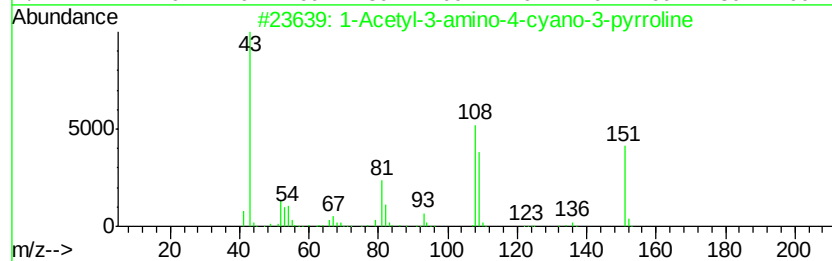
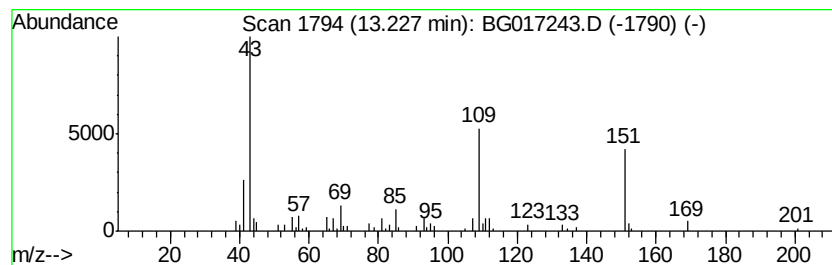
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Acetyl-3-amino-4-cyano-3-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.23	3.91 ng	78438	Acenaphthene-d10		14.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Acetyl-3-amino-4-cyano-3-pyrro...	151	C7H9N3O	002125-74-8	50
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	50
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50
4	Metacetamol	151	C8H9NO2	000621-42-1	50
5	Acetaminophen	151	C8H9NO2	000103-90-2	50



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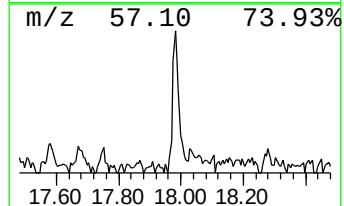
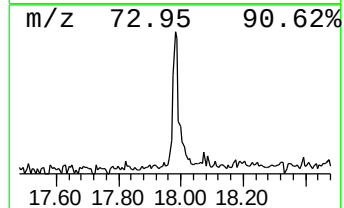
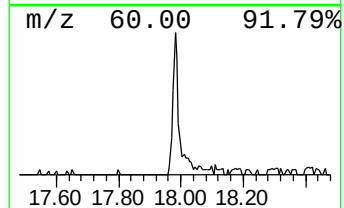
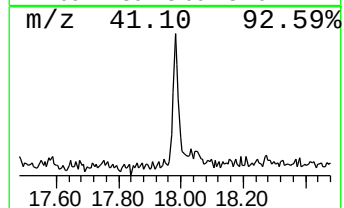
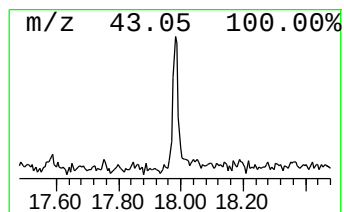
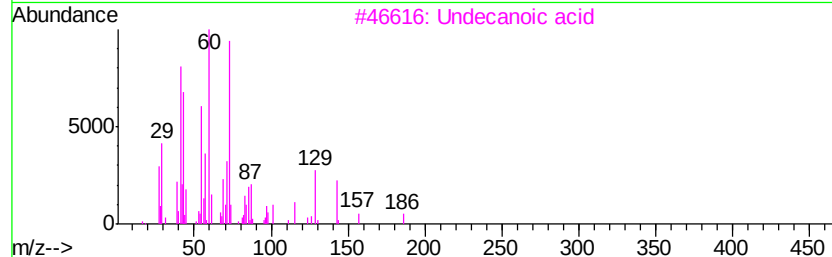
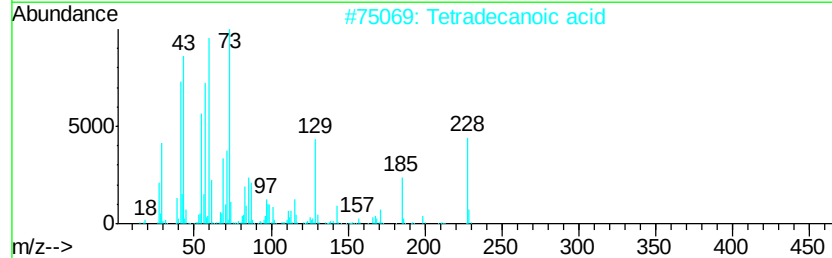
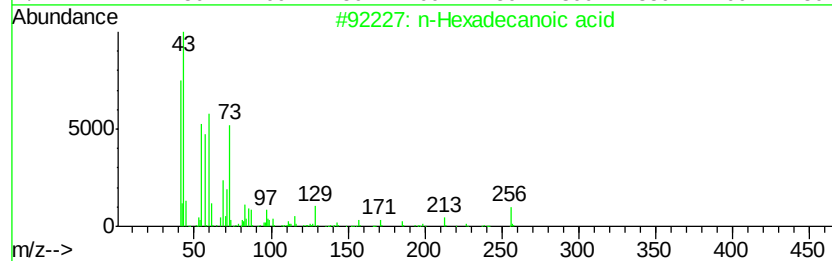
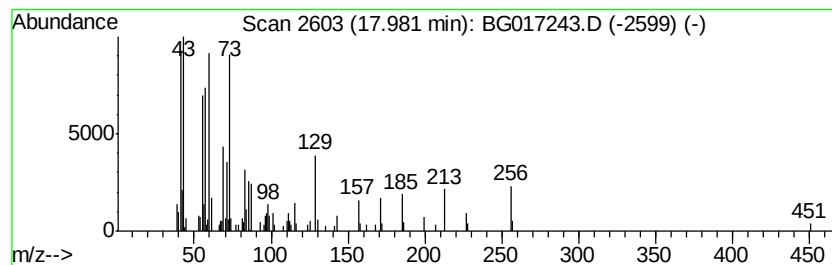
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.98	3.56 ng	83061	Phenanthrene-d10	17.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	Undecanoic acid	186	C11H22O2	000112-37-8	70
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017243.D
Acq On : 22 May 2015 13:12
Operator : TP/IZ
Sample : G2255-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0274-150512

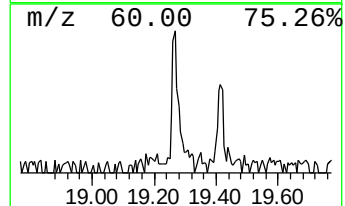
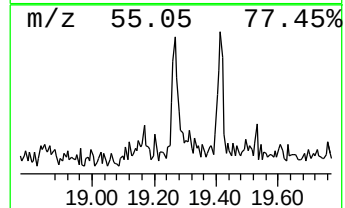
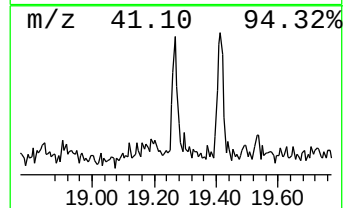
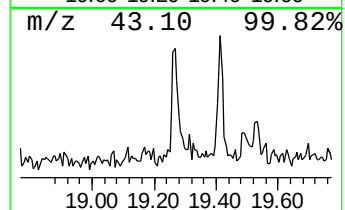
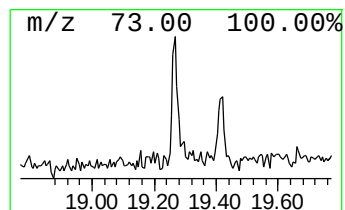
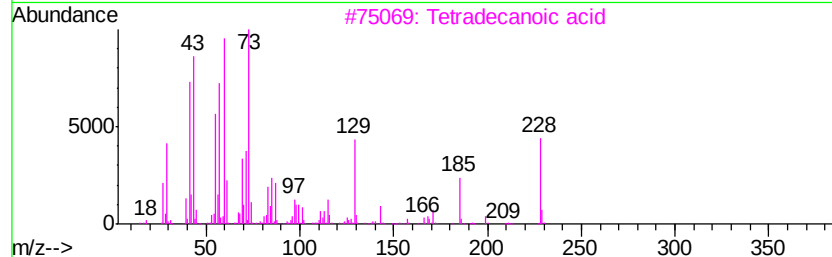
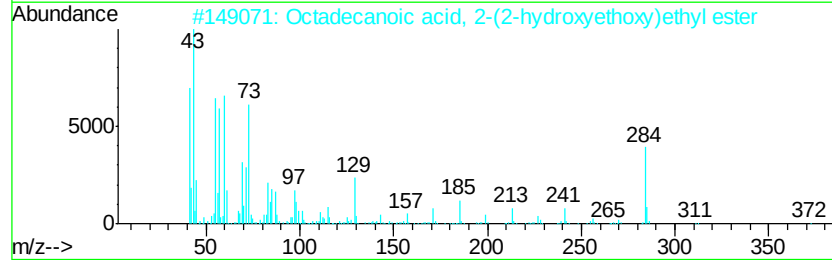
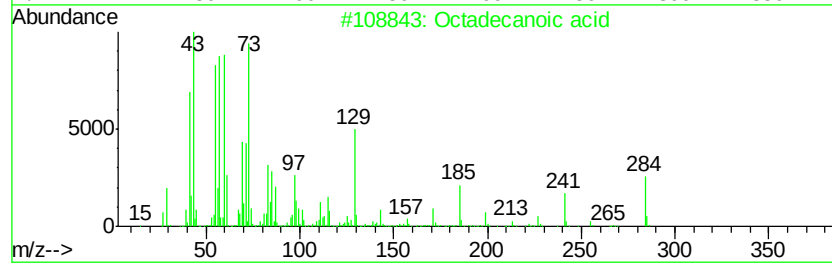
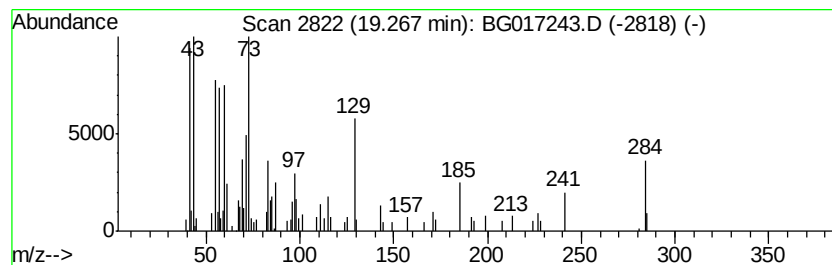
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.27	2.18 ng	59133	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	94
2		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4		n-Decanoic acid	172	C10H20O2	000334-48-5	70
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017243.D
Acq On : 22 May 2015 13:12
Operator : TP/IZ
Sample : G2255-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0274-150512

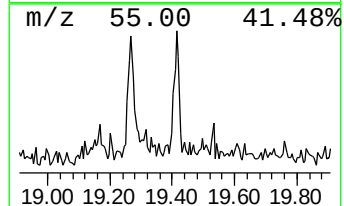
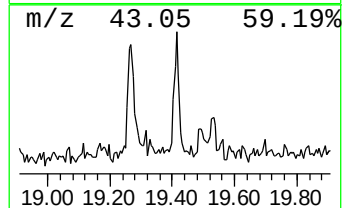
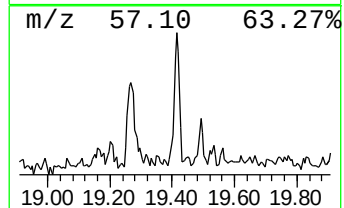
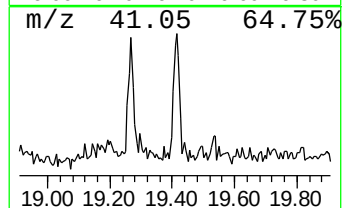
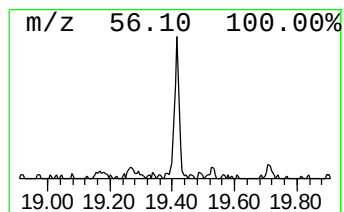
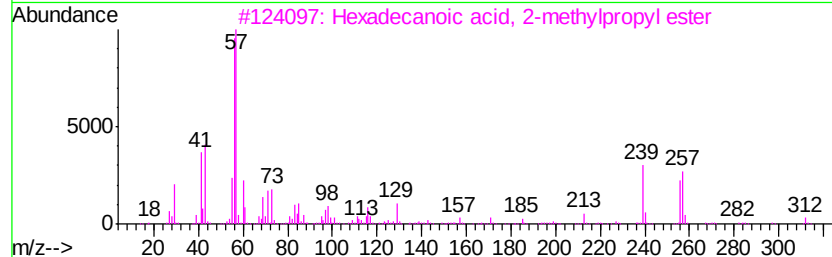
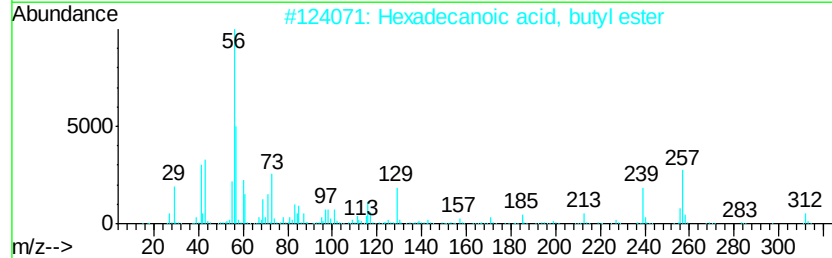
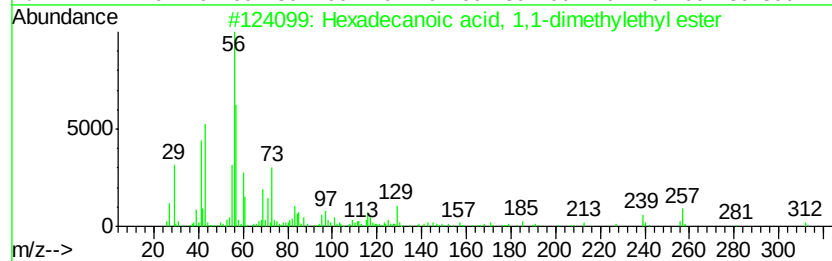
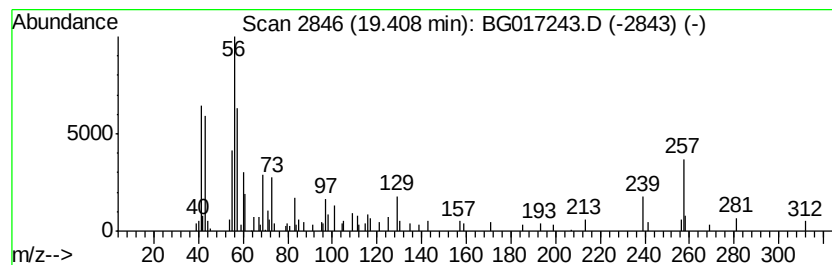
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexadecanoic acid, 1,1-dime... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.41	2.16 ng	58680	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	98
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
3		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	51
4		Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	38
5		Cyclohexanol,2-amino-,trans-	115	C6H13NO	006982-39-4	27



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017243.D
Acq On : 22 May 2015 13:12
Operator : TP/IZ
Sample : G2255-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0274-150512

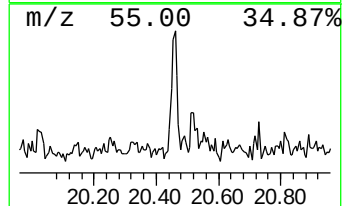
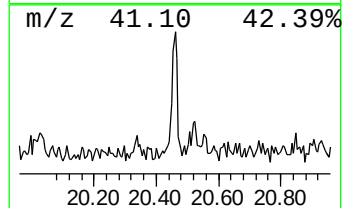
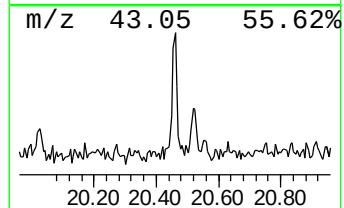
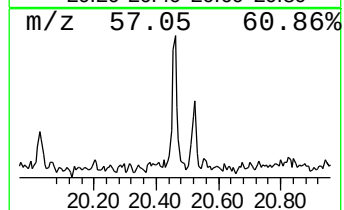
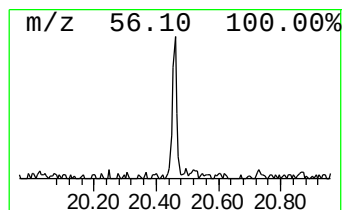
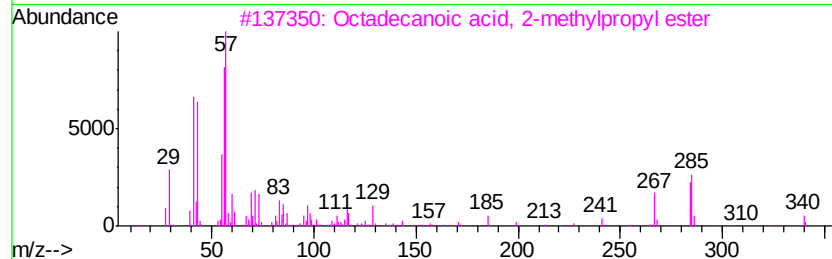
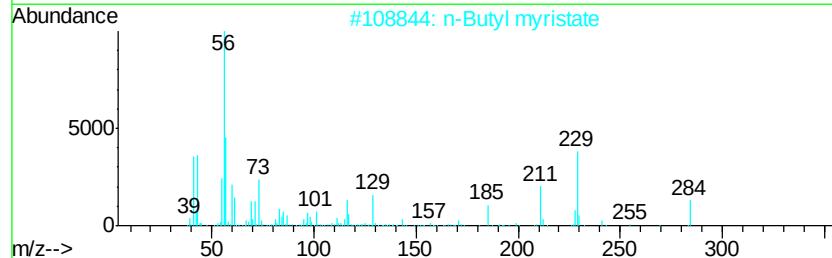
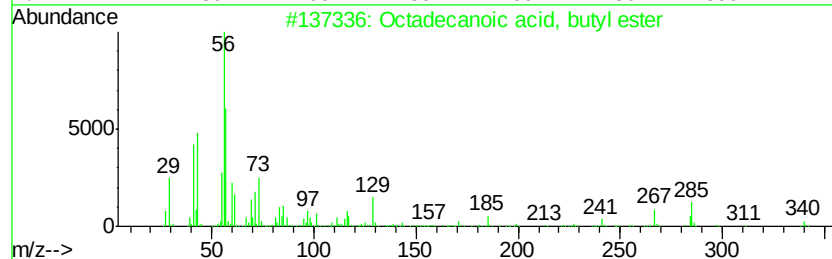
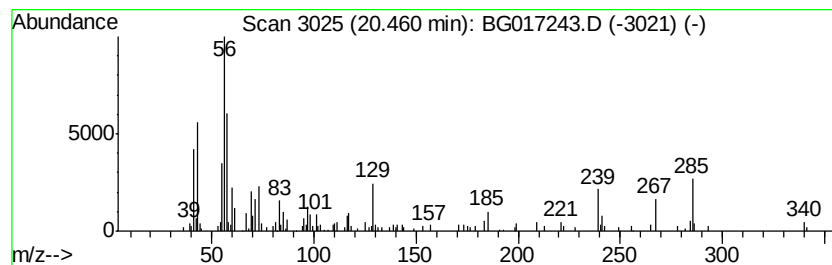
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.46	2.16 ng	58740	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	94
2		n-Butyl myristate	284	C18H36O2	000110-36-1	47
3		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	41
4		Cyclohexane, (1,1-dimethylethyl)-	140	C10H20	003178-22-1	38
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017243.D
Acq On : 22 May 2015 13:12
Operator : TP/IZ
Sample : G2255-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0274-150512

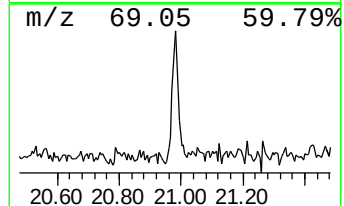
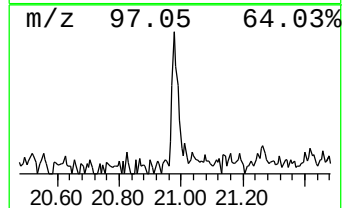
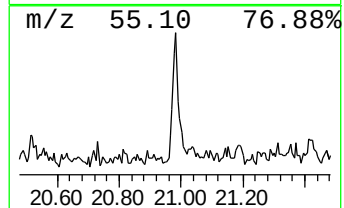
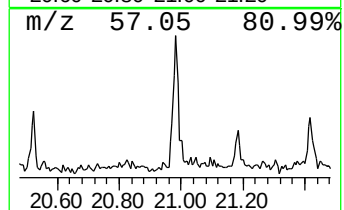
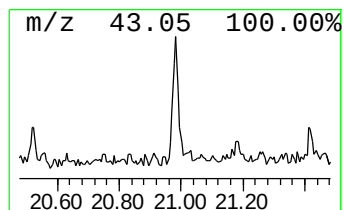
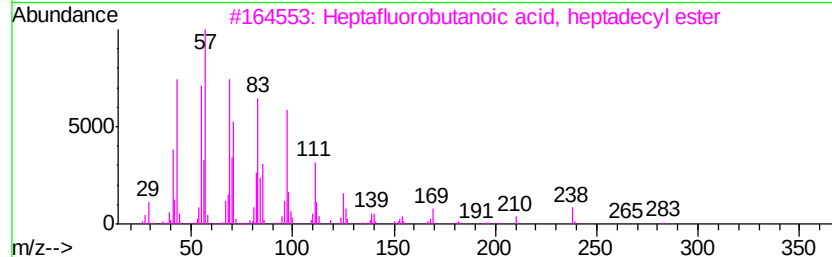
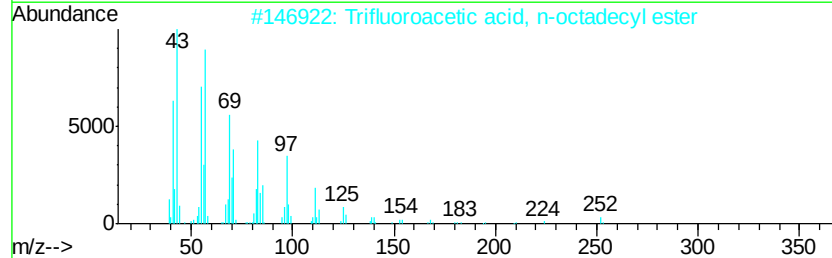
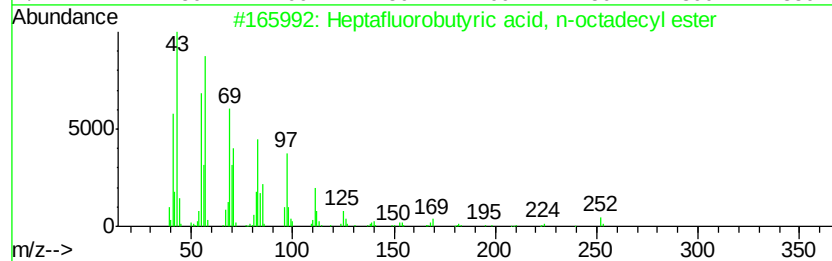
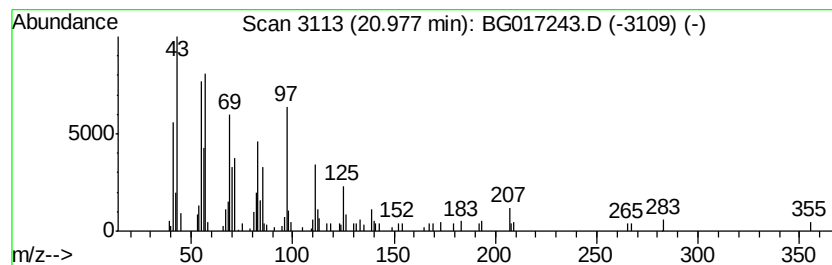
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Heptafluorobutyric acid, n-... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.98	2.52 ng	68365	Chrysene-d12	21.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-octadecyl...	466	C22H37F7O2	000400-57-7	87
2			Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	83
3			Heptafluorobutanoic acid, heptadecyl...	452	C21H35F7O2	1000282-97-3	83
4			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	83
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	81



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG052215\
Data File : BG017243.D
Acq On : 22 May 2015 13:12
Operator : TP/IZ
Sample : G2255-11
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
DUP-0274-150512

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.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
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unknown4.31	4.31	4.8	ng	52357	1	7.68	216116	20.0
unknown7.22	7.22	4.1	ng	44257	1	7.68	216116	20.0
1-Acetyl-3-amino-...	13.23	3.9	ng	78438	3	14.33	401238	20.0
n-Hexadecanoic acid	17.98	3.6	ng	83061	4	17.08	467046	20.0
Octadecanoic acid	19.27	2.2	ng	59133	5	21.27	543472	20.0
Hexadecanoic acid...	19.41	2.2	ng	58680	5	21.27	543472	20.0
Octadecanoic acid...	20.46	2.2	ng	58740	5	21.27	543472	20.0
Heptafluorobutyri...	20.98	2.5	ng	68365	5	21.27	543472	20.0