

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
 Data File : BG016389.D
 Acq On : 14 Apr 2015 9:30
 Operator : TP/IZ
 Sample : G1744-07
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TD-3

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-BG040615.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	2.776	9	15	24	rBV	141529	326738	13.71%	1.528%
2	2.858	24	29	34	rVV	96660	152400	6.40%	0.713%
3	2.899	34	36	45	rVB2	23326	32919	1.38%	0.154%
4	4.791	352	358	367	rVB	132831	191127	8.02%	0.894%
5	5.267	432	439	447	rBV	1005666	1456699	61.14%	6.812%
6	6.859	703	710	722	rBV	1045029	1604521	67.34%	7.503%
7	7.212	763	770	780	rBV	1062462	1615689	67.81%	7.555%
8	7.676	843	849	856	rVB	298574	456041	19.14%	2.133%
9	7.993	895	903	910	rVB	756631	1167933	49.02%	5.462%
10	8.833	1038	1046	1055	rBV	578772	954717	40.07%	4.465%
11	10.461	1316	1323	1330	rBV	425111	696455	29.23%	3.257%
12	12.935	1737	1744	1751	rBV	1388882	1963536	82.41%	9.182%
13	13.775	1882	1887	1895	rBV	75109	104190	4.37%	0.487%
14	14.315	1973	1979	1991	rVB2	627085	910965	38.23%	4.260%
15	15.167	2120	2124	2130	rVB2	25250	33156	1.39%	0.155%
16	15.802	2225	2232	2243	rBV	861104	1246585	52.32%	5.829%
17	16.031	2267	2271	2280	rBV	29219	48436	2.03%	0.227%
18	16.818	2401	2405	2412	rBV2	17923	30091	1.26%	0.141%
19	17.053	2439	2445	2454	rBV2	718033	1036838	43.52%	4.849%
20	17.952	2593	2598	2607	rBV2	101876	164032	6.88%	0.767%
21	19.239	2812	2817	2826	rBV5	38885	80079	3.36%	0.374%
22	19.386	2837	2842	2852	rVB	542855	622404	26.12%	2.911%
23	19.462	2852	2855	2858	rVV	22900	24490	1.03%	0.115%
24	19.497	2858	2861	2868	rVB	71488	83678	3.51%	0.391%
25	19.685	2887	2893	2903	rBV	1873322	2382619	100.00%	11.142%
26	20.373	3004	3010	3015	rBV2	27674	41341	1.74%	0.193%
27	20.426	3015	3019	3024	rVV	421816	450125	18.89%	2.105%
28	20.490	3026	3030	3033	rVV2	56138	72383	3.04%	0.338%
29	20.526	3033	3036	3040	rVB	42784	43878	1.84%	0.205%
30	20.949	3103	3108	3117	rBV	247564	368026	15.45%	1.721%
31	21.231	3151	3156	3167	rBV	855771	1104080	46.34%	5.163%
32	21.383	3179	3182	3186	rVB	96085	97479	4.09%	0.456%
33	21.812	3251	3255	3261	rBV	87972	122686	5.15%	0.574%
34	22.271	3329	3333	3338	rBV	95674	117707	4.94%	0.550%

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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

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Peak separation: 5

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35	22.400	3351	3355	3359	rVB	41974	54980	2.31%	0.257%
36	22.776	3414	3419	3425	rBV	71327	110331	4.63%	0.516%
37	23.346	3511	3516	3521	rBV	55460	94569	3.97%	0.442%
38	23.463	3529	3536	3547	rBV	582070	1055824	44.31%	4.937%
39	23.992	3621	3626	3635	rVB2	45333	88557	3.72%	0.414%
40	24.744	3750	3754	3760	rVB4	35194	64703	2.72%	0.303%
41	26.525	4052	4057	4069	rVB4	34227	111486	4.68%	0.521%

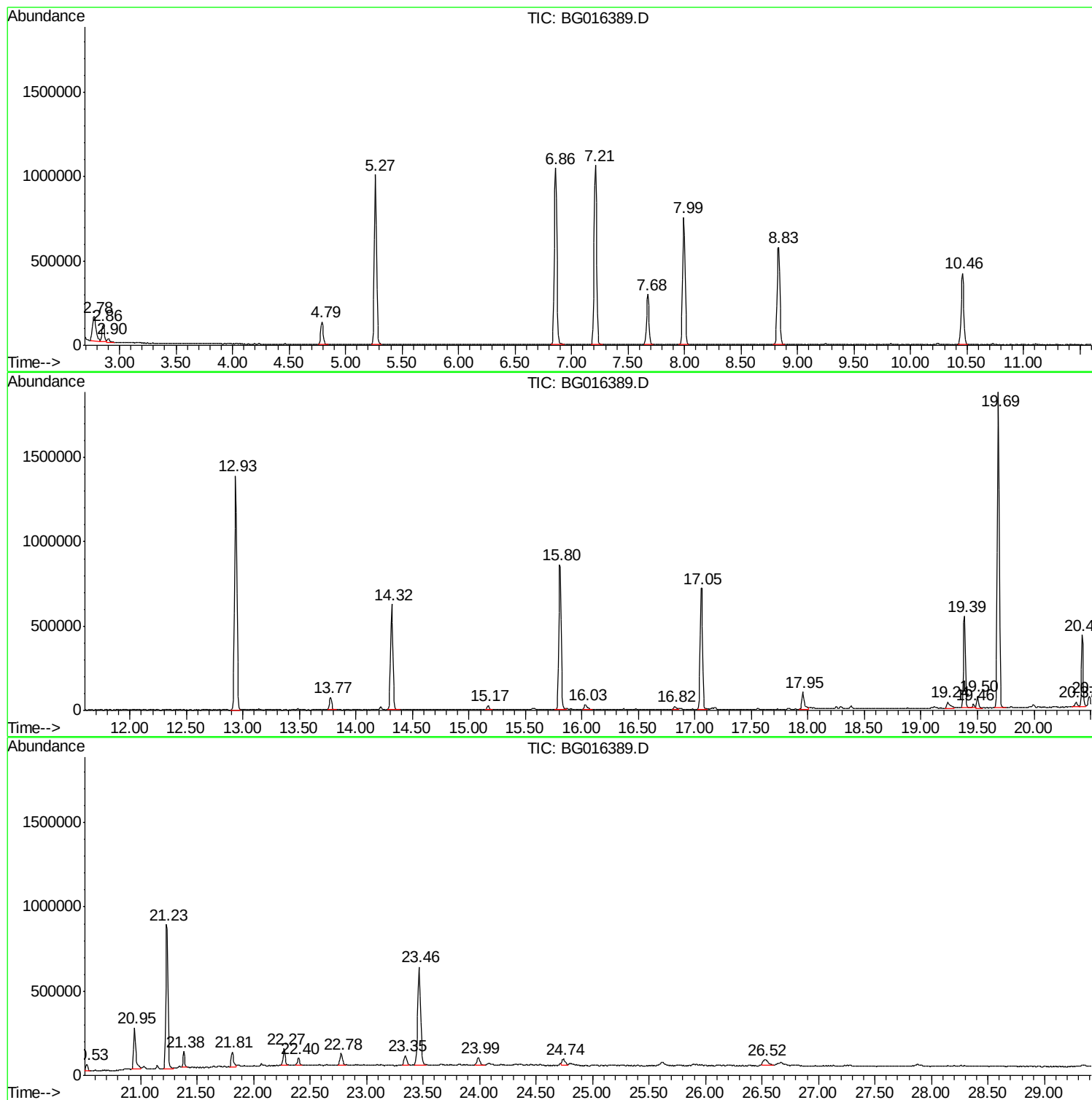
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Instrument :
BNA_G
ClientSampled :
TD-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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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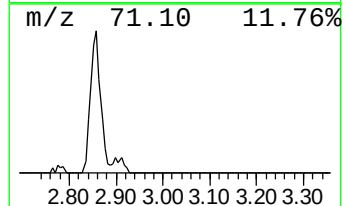
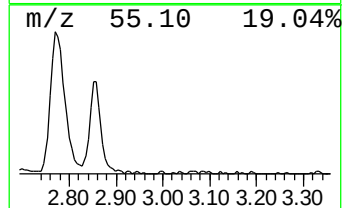
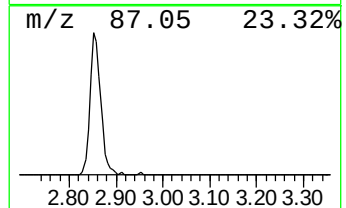
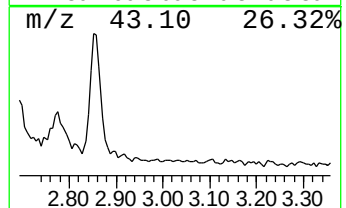
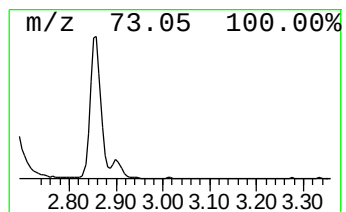
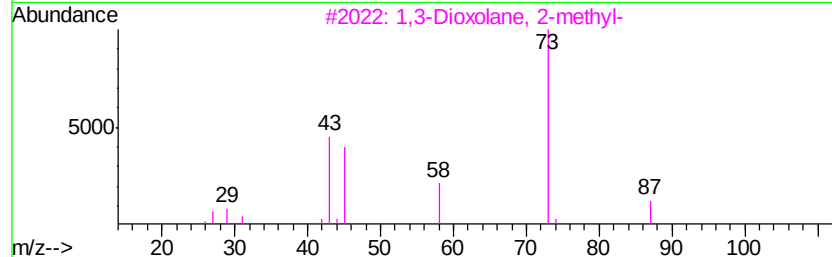
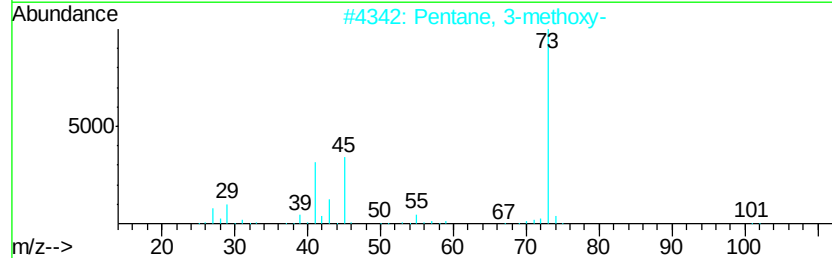
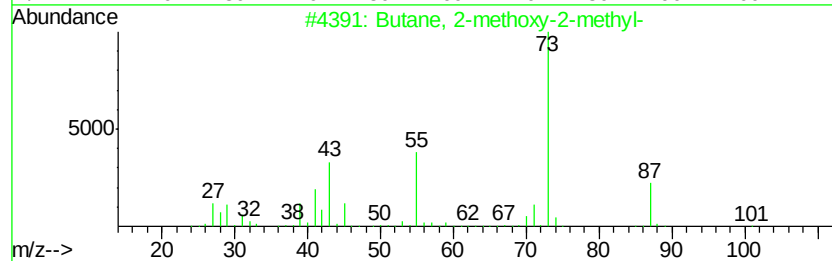
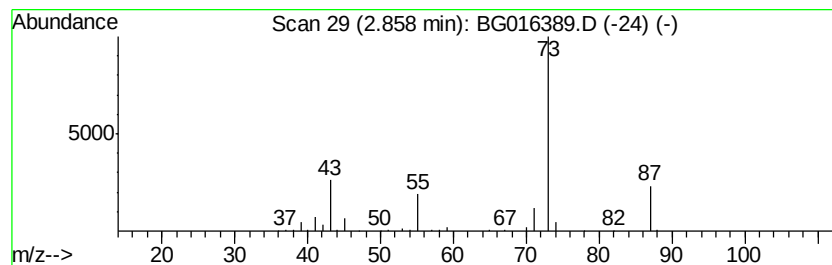
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	6.68 ng	152400	1,4-Dichlorobenzene-d4	7.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	9



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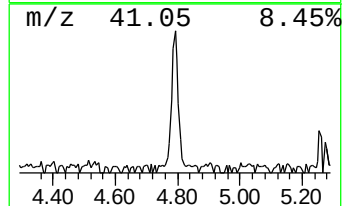
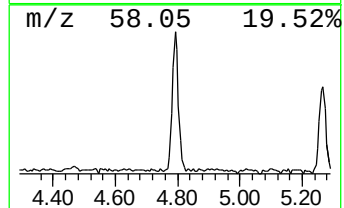
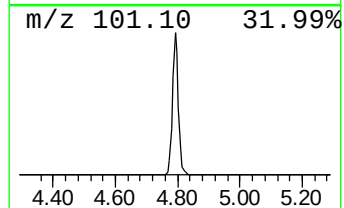
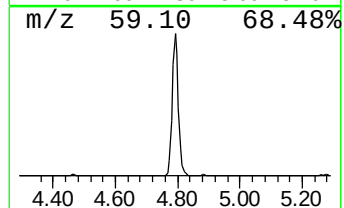
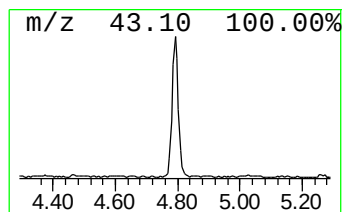
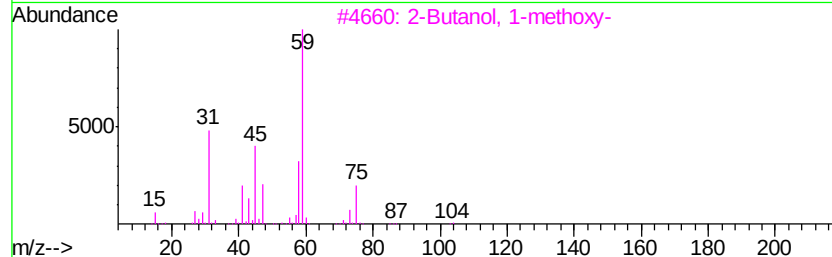
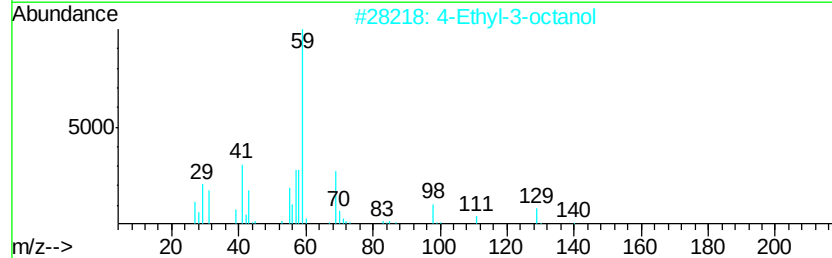
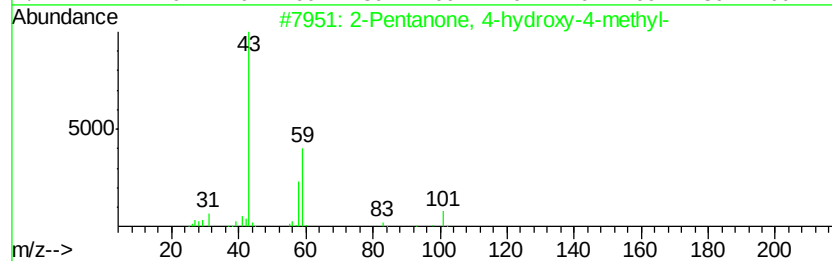
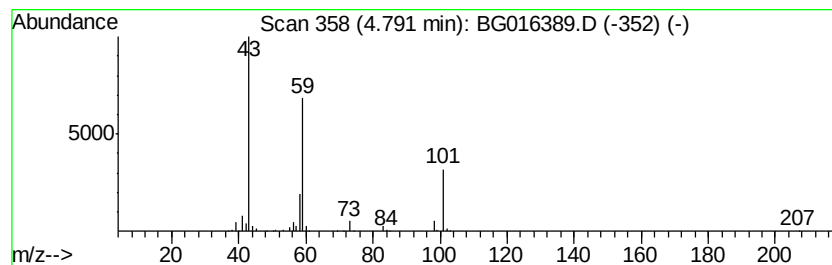
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	8.38 ng	191127	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		4-Ethyl-3-octanol	158	C10H22O	019781-26-1	47
3		2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	37
4		2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25



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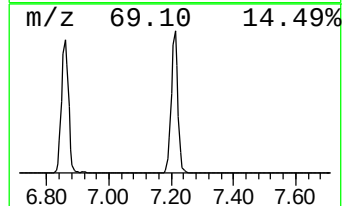
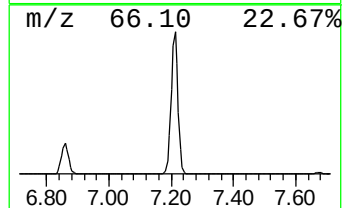
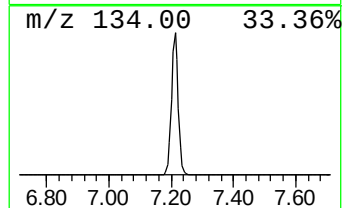
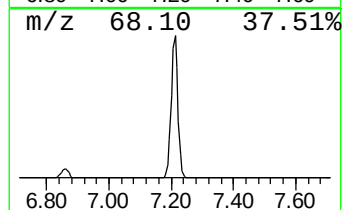
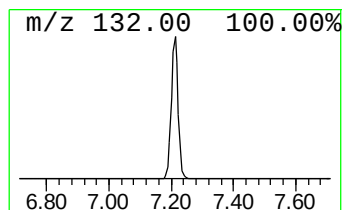
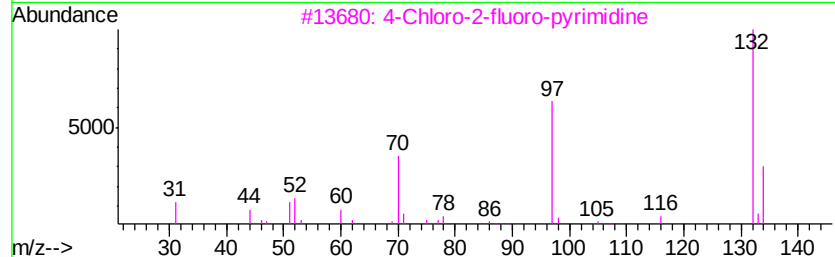
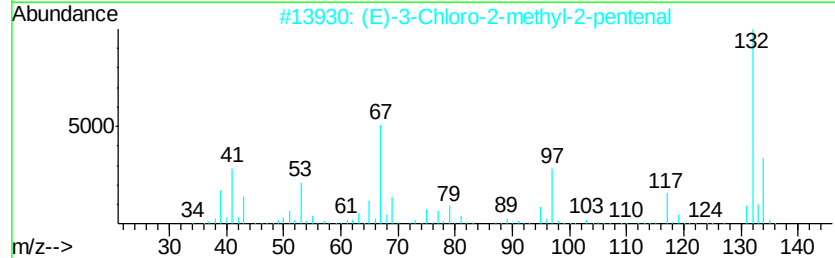
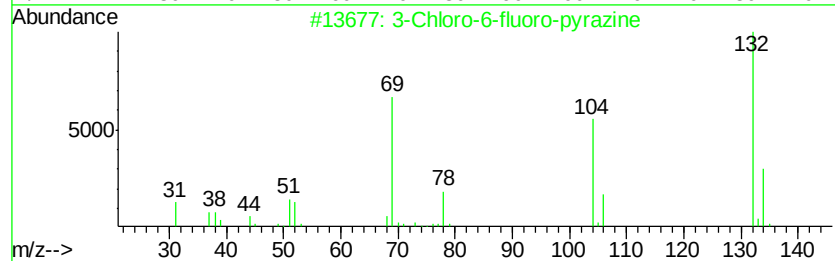
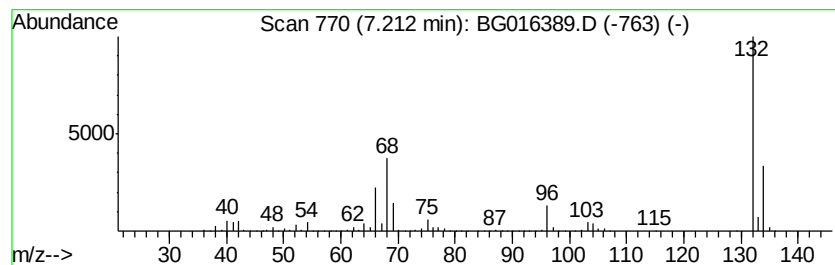
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	70.86 ng	1615690	1,4-Dichlorobenzene-d4	7.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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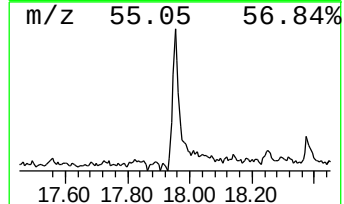
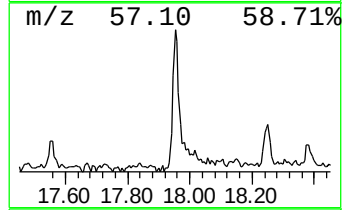
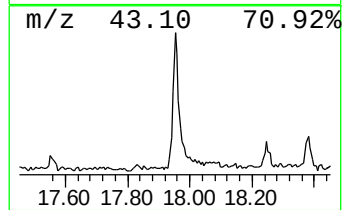
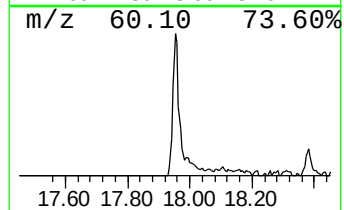
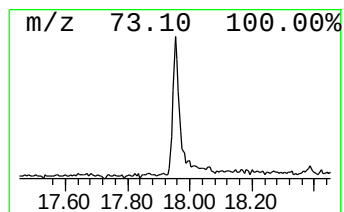
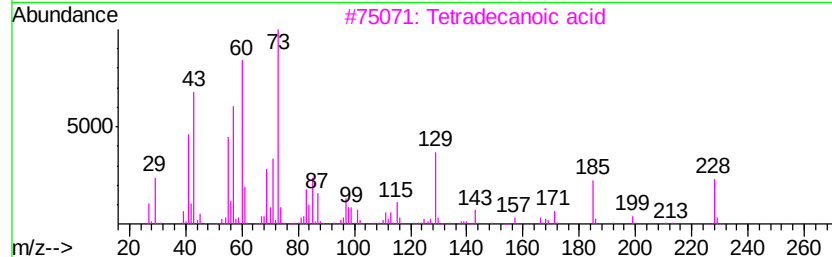
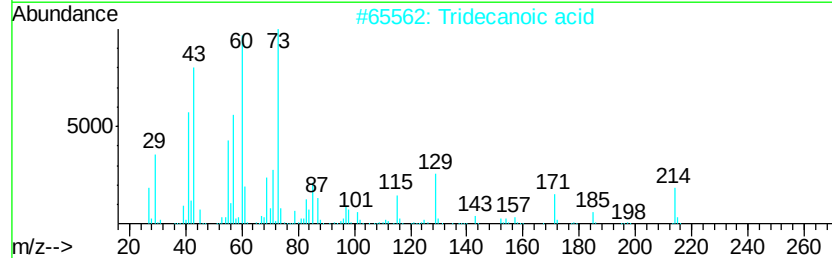
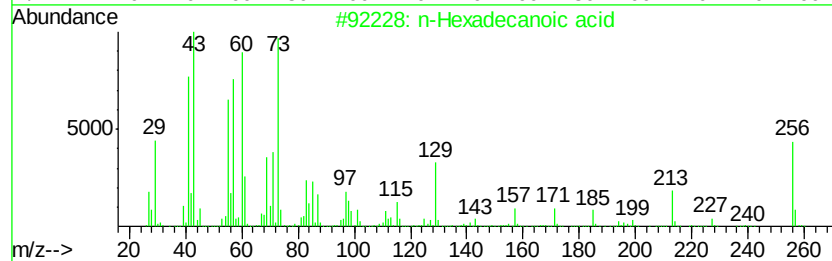
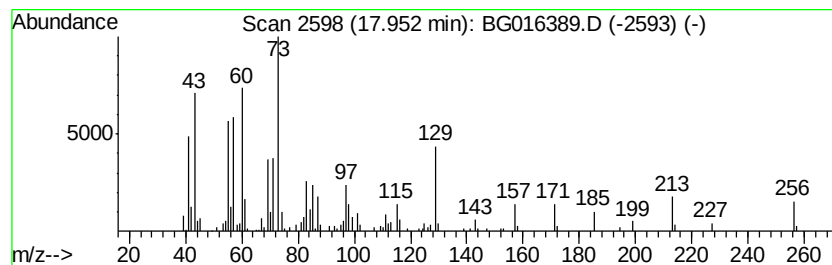
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	3.16 ng	164032	Phenanthrene-d10	17.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tridecanoic acid	214	C13H26O2	000638-53-9	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		n-Decanoic acid	172	C10H20O2	000334-48-5	64
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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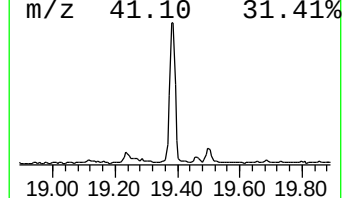
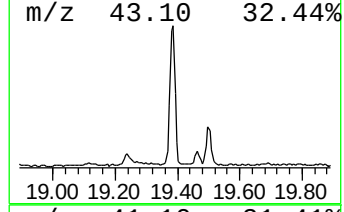
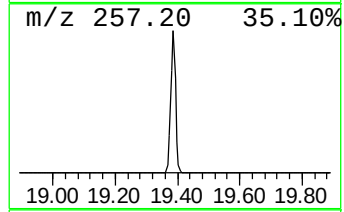
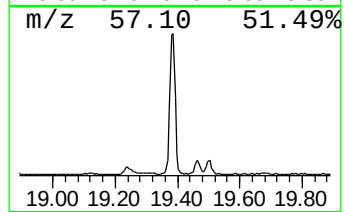
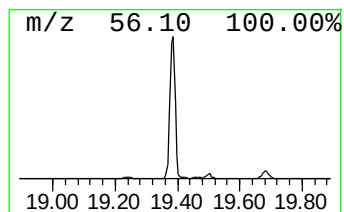
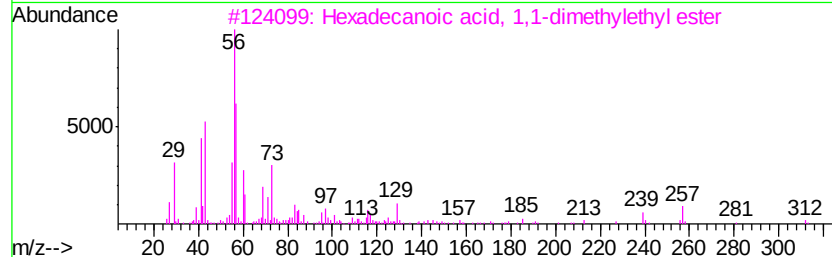
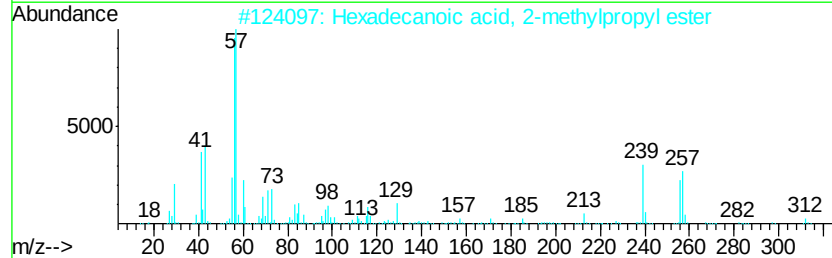
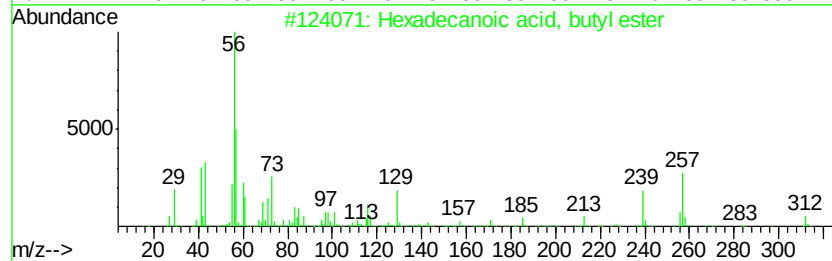
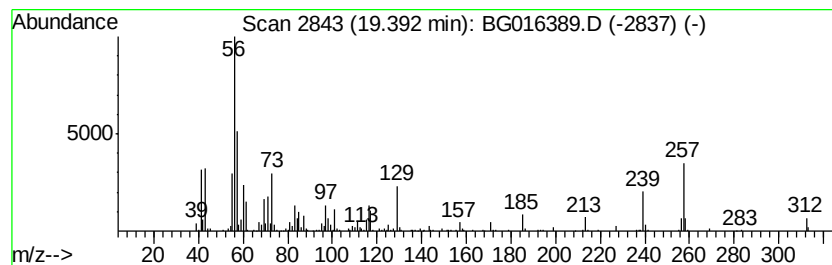
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	11.27 ng	622404	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	99
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	81
3		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	49
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	30



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016389.D
Acq On : 14 Apr 2015 9:30
Operator : TP/IZ
Sample : G1744-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-3

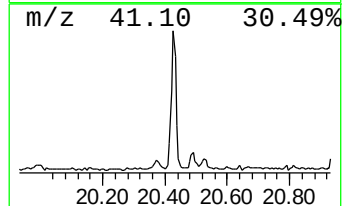
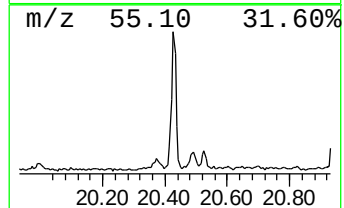
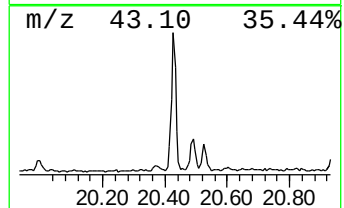
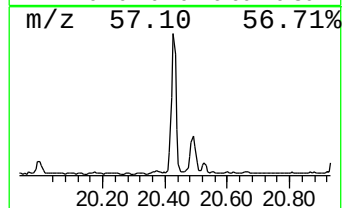
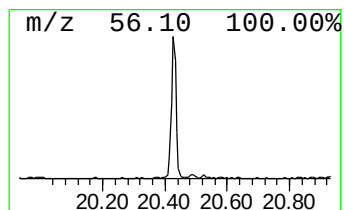
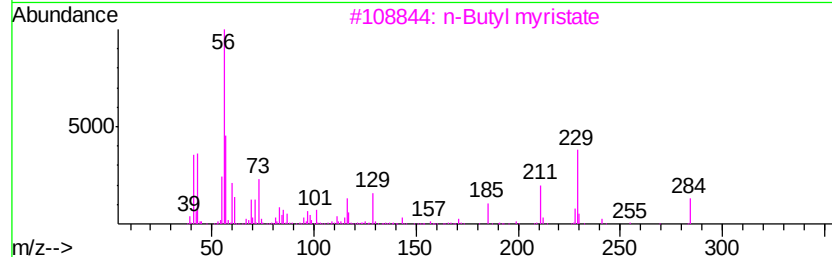
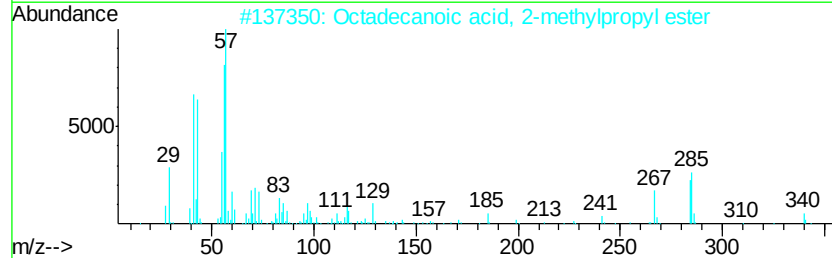
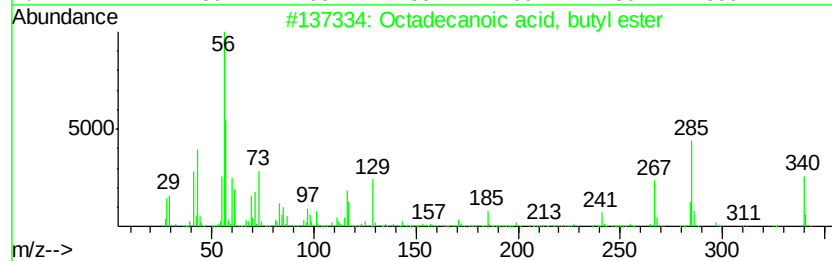
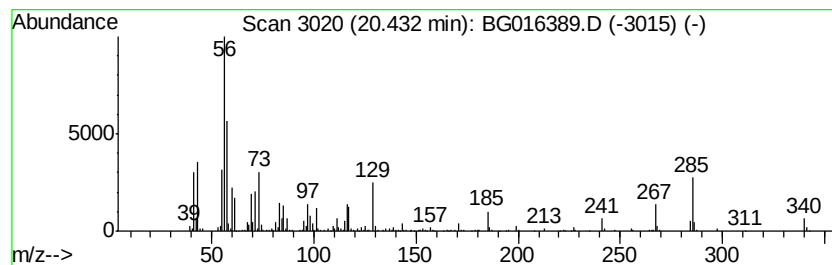
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	8.15 ng	450125	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	97
2		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	70
3		n-Butyl myristate	284	C18H36O2	000110-36-1	53
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		1,4-Dioxaspiro[2.4]heptan-5-one, ...	142	C7H10O3	126091-79-0	27



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016389.D
Acq On : 14 Apr 2015 9:30
Operator : TP/IZ
Sample : G1744-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

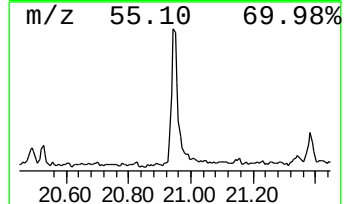
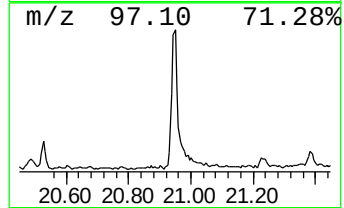
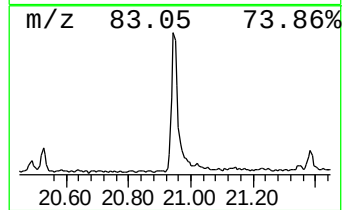
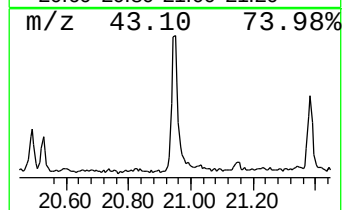
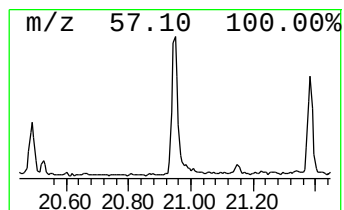
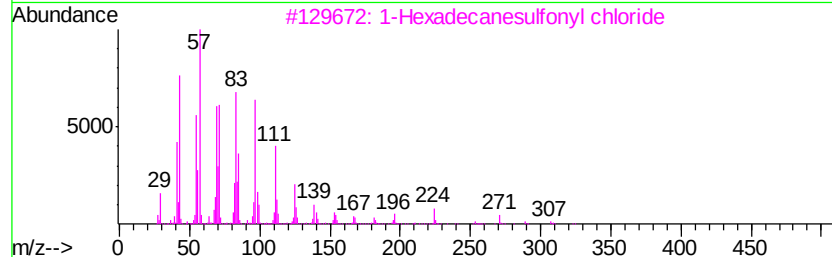
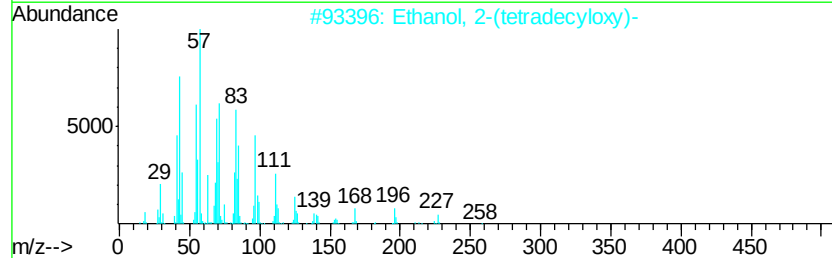
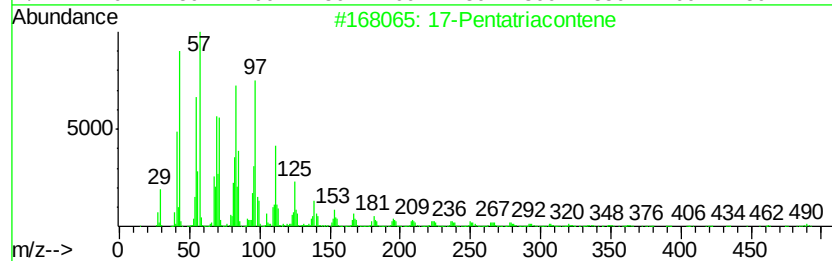
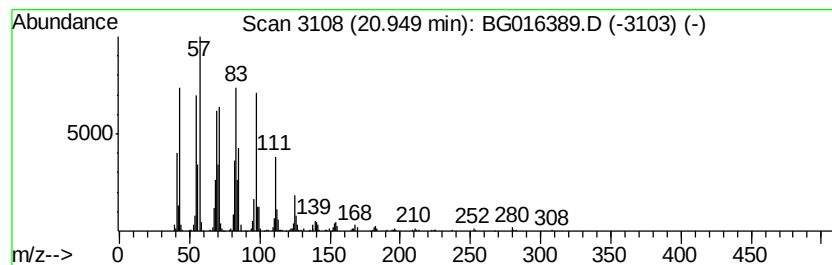
Instrument :
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ClientSampleId :
TD-3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 17-Pentatriacontene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.95	6.67 ng	368026	Chrysene-d12	21.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		17-Pentatriacontene	491 C35H70	006971-40-0 91
2		Ethanol, 2-(tetradecyloxy)-	258 C16H34O2	002136-70-1 91
3		1-Hexadecanesulfonyl chloride	324 C16H33ClO2S	038775-38-1 91
4		Heptafluorobutanoic acid, hepta...	452 C21H35F7O2	1000282-97-3 90
5		Pentafluoropropionic acid, hepta...	402 C20H35F5O2	1000283-04-2 90



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016389.D
Acq On : 14 Apr 2015 9:30
Operator : TP/IZ
Sample : G1744-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-3

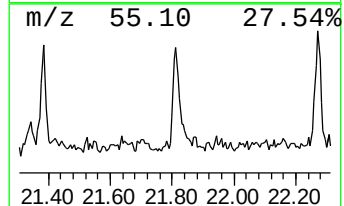
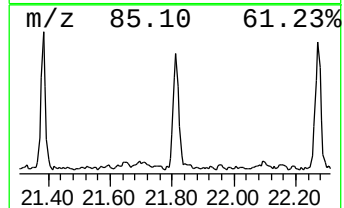
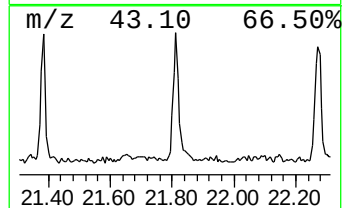
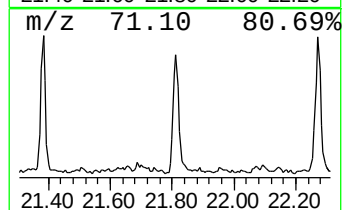
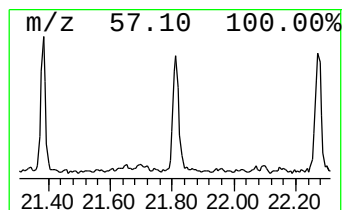
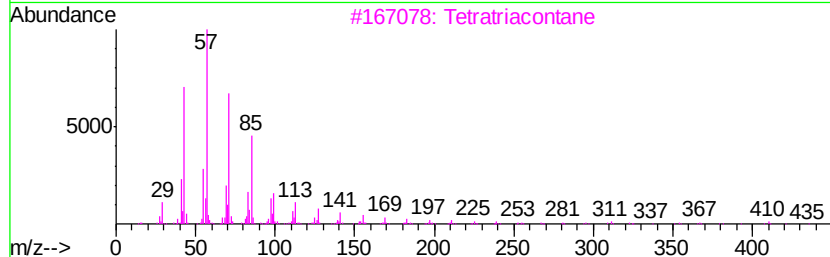
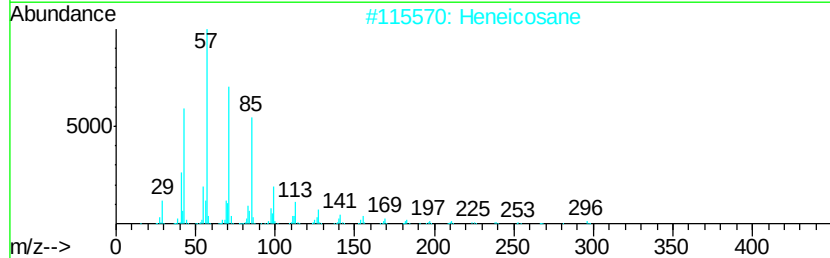
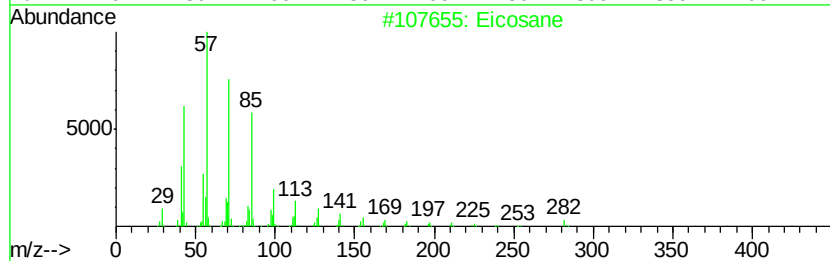
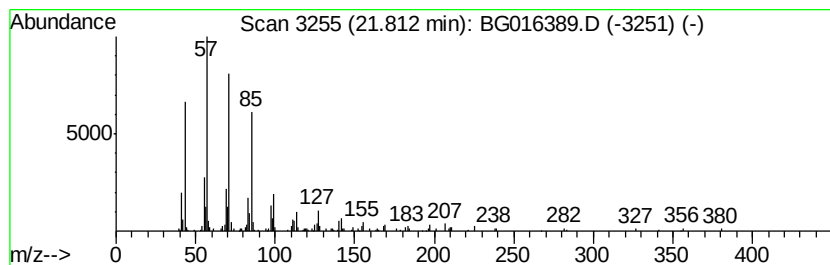
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Eicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.81	2.22 ng	122686	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	98
2		Heneicosane	296	C21H44	000629-94-7	91
3		Tetratriacontane	479	C34H70	014167-59-0	91
4		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5		Triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016389.D
Acq On : 14 Apr 2015 9:30
Operator : TP/IZ
Sample : G1744-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-3

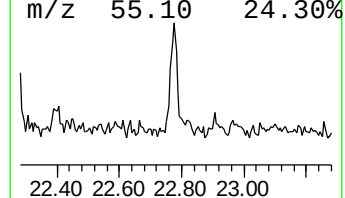
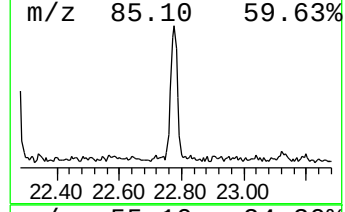
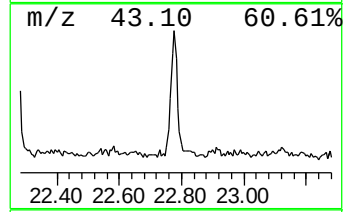
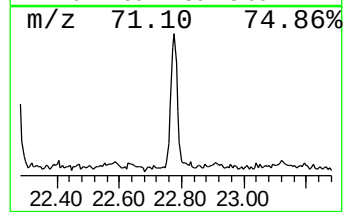
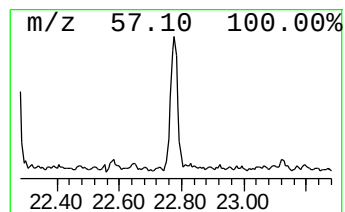
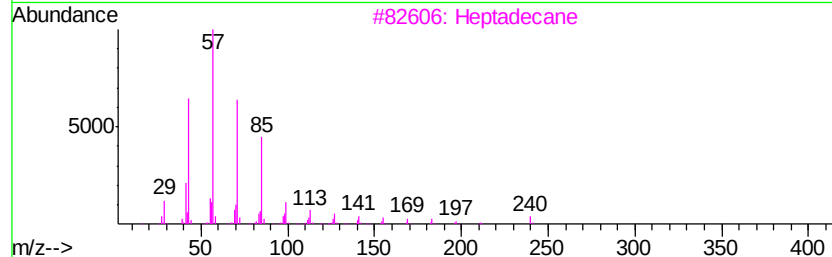
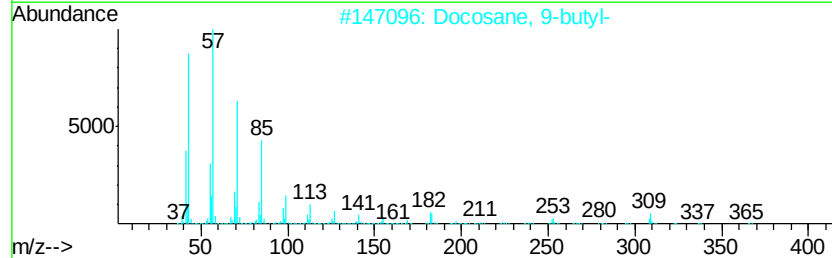
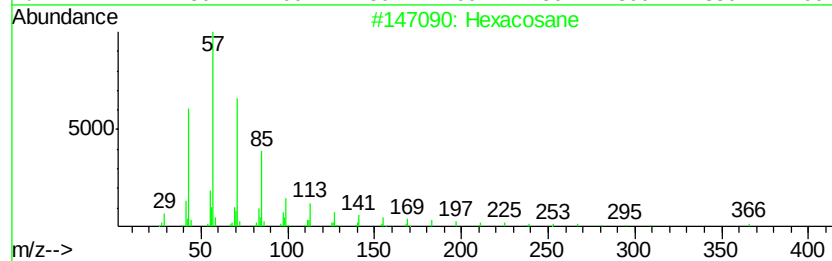
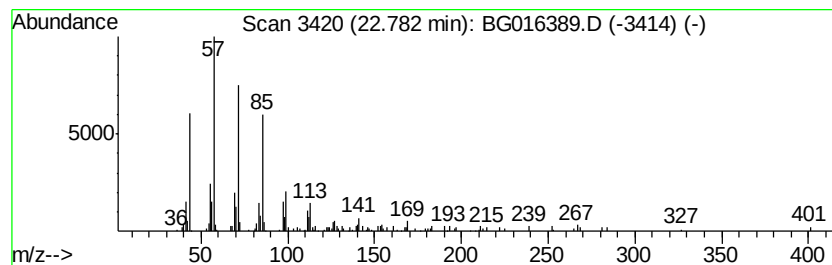
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Hexacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.78	2.09 ng	110331	Perylene-d12	23.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexacosane	366	C26H54	000630-01-3	90
2		Docosane, 9-butyl-	366	C26H54	055282-14-9	87
3		Heptadecane	240	C17H36	000629-78-7	87
4		Triacontane	422	C30H62	000638-68-6	87
5		Docosane	310	C22H46	000629-97-0	87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
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Acq On : 14 Apr 2015 9:30
Operator : TP/IZ
Sample : G1744-07
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
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ClientSampleID :
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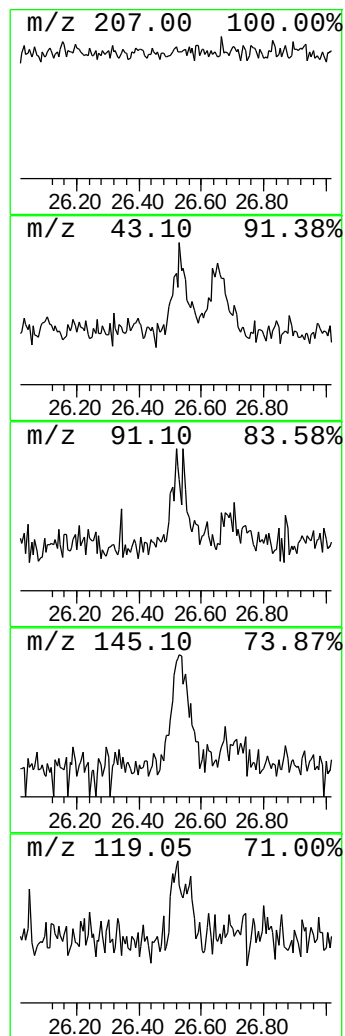
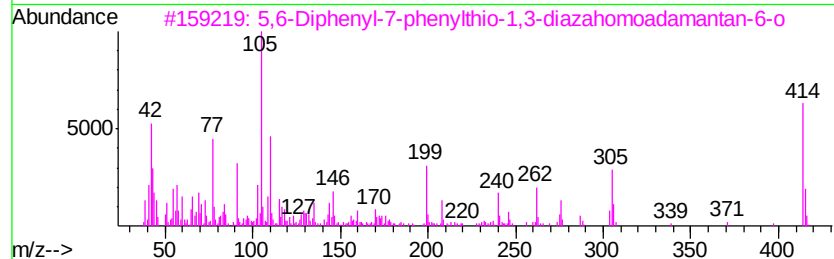
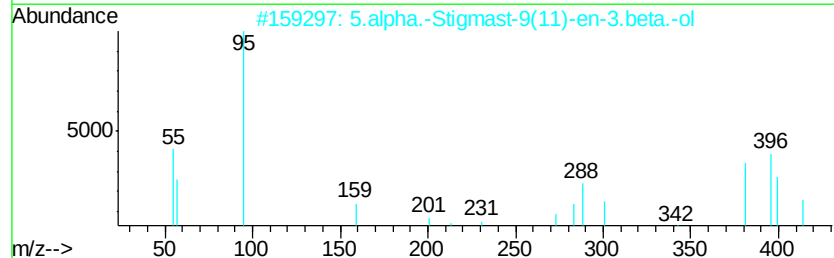
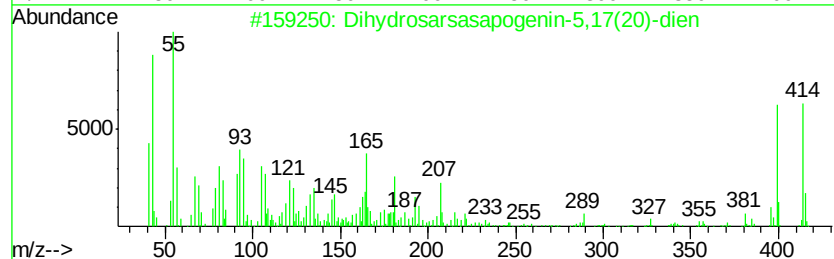
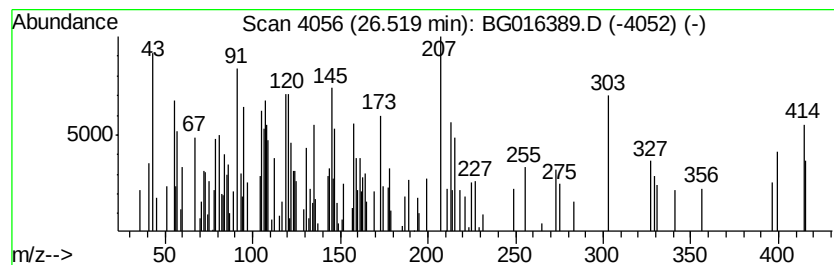
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown26.52 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.52	2.11 ng	111486	Perylene-d12	23.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dihydrosarsasapogenin-5,17(20)-dien	414	C27H42O3	096974-10-6	10
2		5.alpha.-Stigmast-9(11)-en-3.beta...	414	C29H50O	077794-81-1	10
3		5,6-Diphenyl-7-phenylthio-1,3-di...	414	C26H26N2OS	1000216-35-1	9
4		Glucosamine, 1,3,4,6-O-tetraacet...	451	C21H25NO10	1000127-16-7	9
5		Benzene, 1,3,5-tris(2,2-dimethyl...	414	C21H35I	025347-04-0	7



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016389.D
Acq On : 14 Apr 2015 9:30
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ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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...	2.86	6.7	ng	152400	1	7.68	456041	20.0
2-Pentanone, 4-hy...	4.79	8.4	ng	191127	1	7.68	456041	20.0
unknown7.21	7.21	70.9	ng	1615690	1	7.68	456041	20.0
n-Hexadecanoic acid	17.95	3.2	ng	164032	4	17.05	1036840	20.0
Hexadecanoic acid...	19.39	11.3	ng	622404	5	21.24	1104080	20.0
Octadecanoic acid...	20.43	8.2	ng	450125	5	21.24	1104080	20.0
17-Pentatriacontene	20.95	6.7	ng	368026	5	21.24	1104080	20.0
Eicosane	21.81	2.2	ng	122686	5	21.24	1104080	20.0
Hexacosane	22.78	2.1	ng	110331	6	23.47	1055820	20.0
unknown26.52	26.52	2.1	ng	111486	6	23.47	1055820	20.0