

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
 Data File : BG016387.D
 Acq On : 14 Apr 2015 8:21
 Operator : TP/IZ
 Sample : G1831-05
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PE-11

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	2.770	9	14	23	rBV	161806	329339	11.48%	1.230%
2	2.853	23	28	34	rVB	123333	173789	6.06%	0.649%
3	4.786	352	357	368	rVB	169420	244779	8.54%	0.914%
4	5.261	432	438	447	rBV	1322568	1842356	64.24%	6.882%
5	6.860	703	710	722	rBV	1361182	2098014	73.16%	7.837%
6	7.212	762	770	778	rBV	1330219	2052767	71.58%	7.668%
7	7.676	841	849	857	rBV	341467	534479	18.64%	1.996%
8	7.994	895	903	910	rBV	940066	1459610	50.90%	5.452%
9	8.828	1038	1045	1056	rBV	739344	1225963	42.75%	4.579%
10	10.461	1315	1323	1330	rBV	503307	828222	28.88%	3.094%
11	11.783	1542	1548	1558	rVB	31574	51821	1.81%	0.194%
12	12.935	1737	1744	1751	rBV	1484124	2214083	77.21%	8.270%
13	13.775	1881	1887	1892	rBV	82620	111722	3.90%	0.417%
14	14.316	1973	1979	1988	rBV2	723331	1081641	37.72%	4.040%
15	15.679	2203	2211	2217	rBV	128861	172776	6.02%	0.645%
16	15.808	2226	2233	2243	rBV	1042424	1506048	52.52%	5.625%
17	17.059	2439	2446	2451	rBV2	907007	1282780	44.73%	4.792%
18	17.101	2451	2453	2458	rVB	27891	28877	1.01%	0.108%
19	17.958	2592	2599	2606	rBV	104724	171620	5.98%	0.641%
20	19.116	2789	2796	2803	rBV	65266	97059	3.38%	0.363%
21	19.239	2813	2817	2824	rBV6	28684	56403	1.97%	0.211%
22	19.386	2834	2842	2847	rBV	489681	567622	19.79%	2.120%
23	19.474	2850	2857	2859	rVV2	57082	103351	3.60%	0.386%
24	19.504	2859	2862	2867	rVB	90831	105187	3.67%	0.393%
25	19.686	2887	2893	2902	rBV	2443385	2867743	100.00%	10.712%
26	19.997	2943	2946	2950	rVB	25595	29041	1.01%	0.108%
27	20.373	3005	3010	3014	rBV5	23917	33623	1.17%	0.126%
28	20.426	3015	3019	3025	rVV	373094	431637	15.05%	1.612%
29	20.491	3026	3030	3033	rVV	74339	86604	3.02%	0.323%
30	20.526	3033	3036	3040	rVB	53155	55860	1.95%	0.209%
31	20.949	3103	3108	3120	rBV	517549	733374	25.57%	2.739%
32	21.237	3151	3157	3162	rBV	1122218	1485184	51.79%	5.548%
33	21.384	3179	3182	3186	rBV	131328	134802	4.70%	0.504%
34	21.813	3251	3255	3265	rBV	113592	177194	6.18%	0.662%

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

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

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

35	22.277	3329	3334	3340	rVB	113617	156037	5.44%	0.583%
36	22.400	3352	3355	3363	rVB2	31359	48618	1.70%	0.182%
37	22.776	3415	3419	3434	rVB3	98546	221015	7.71%	0.826%
38	23.340	3511	3515	3525	rBV3	73510	151700	5.29%	0.567%
39	23.464	3529	3536	3550	rVB2	721323	1422177	49.59%	5.312%
40	23.992	3621	3626	3634	rVB3	60134	119912	4.18%	0.448%
41	24.081	3637	3641	3648	rVV7	25165	48659	1.70%	0.182%
42	24.744	3749	3754	3760	rBV2	40281	80065	2.79%	0.299%
43	26.531	4052	4058	4069	rBV2	50904	148258	5.17%	0.554%

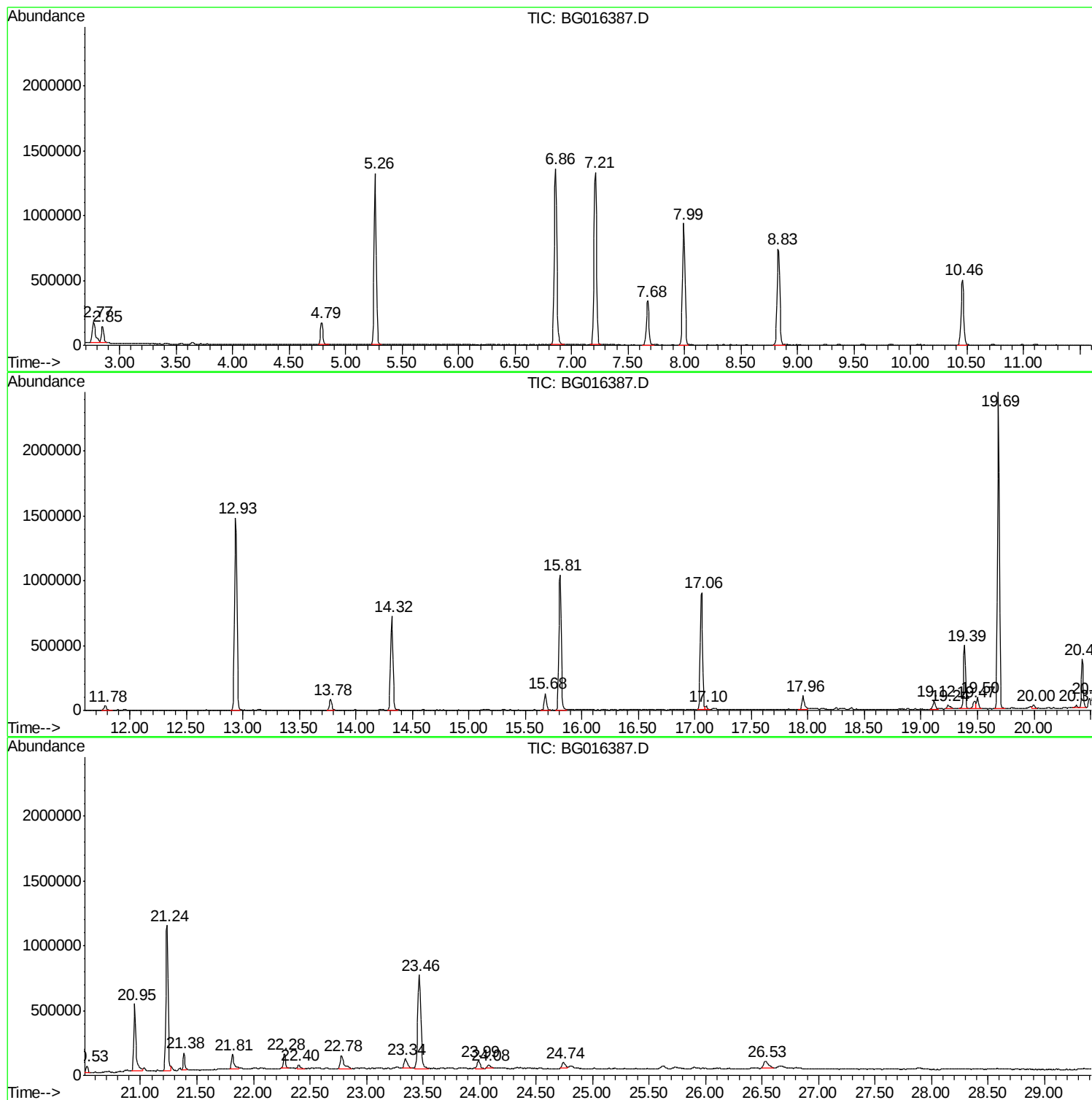
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BNA_G
ClientSampled :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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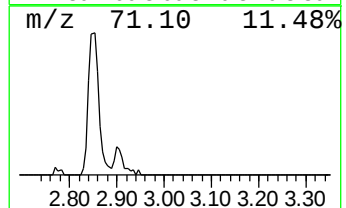
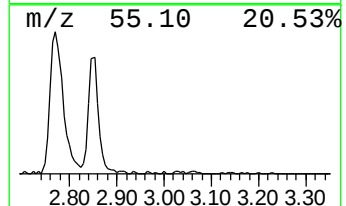
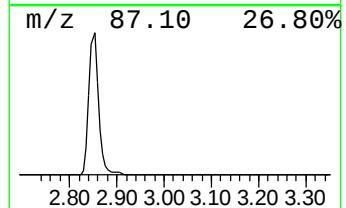
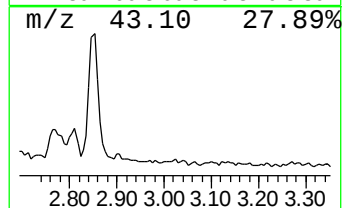
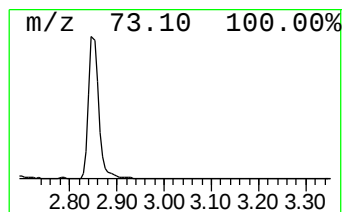
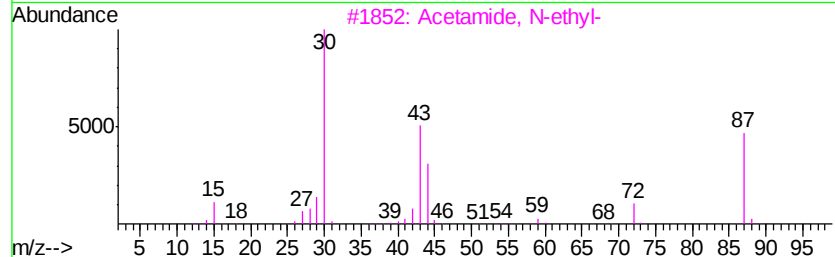
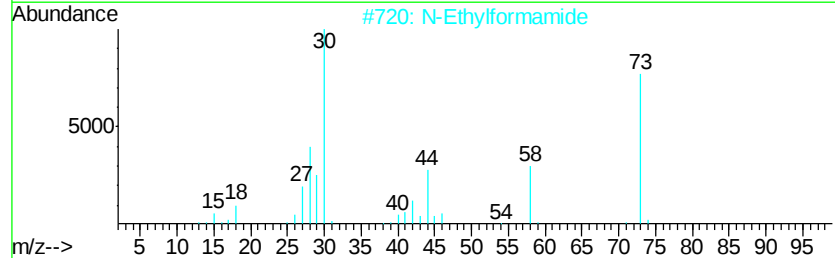
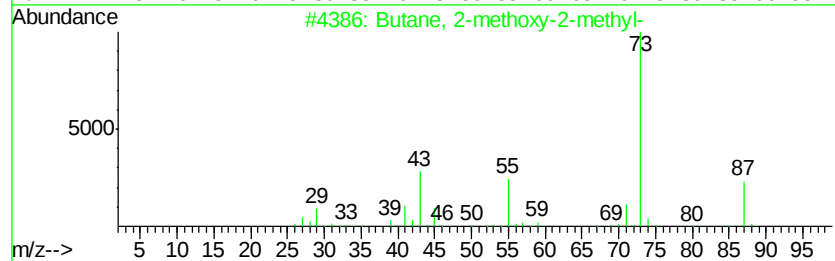
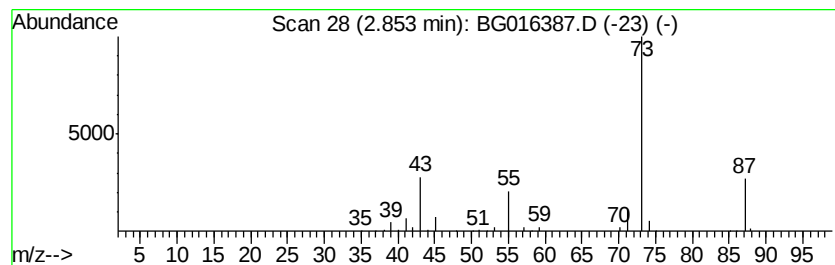
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.85	6.50 ng	173789	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	78
2			N-Ethylformamide	73	C3H7NO	000627-45-2	9
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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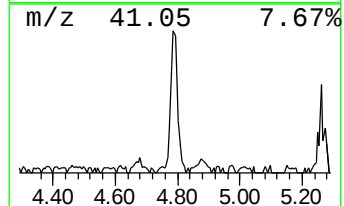
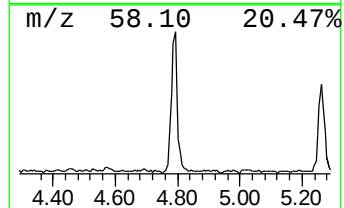
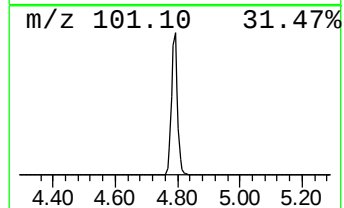
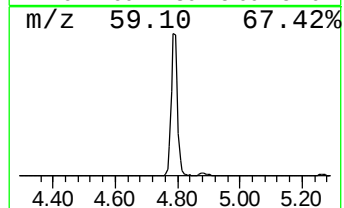
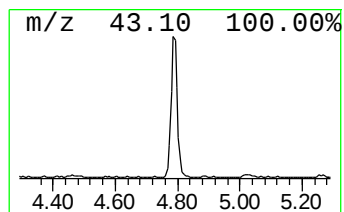
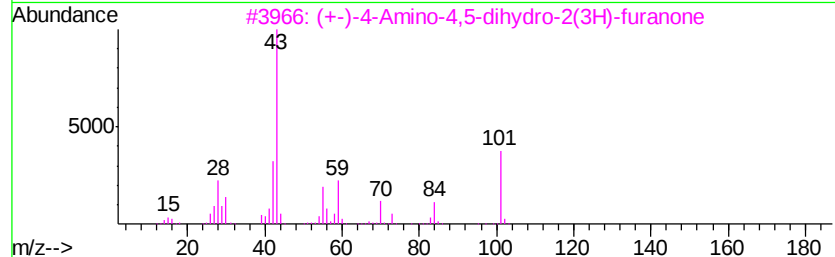
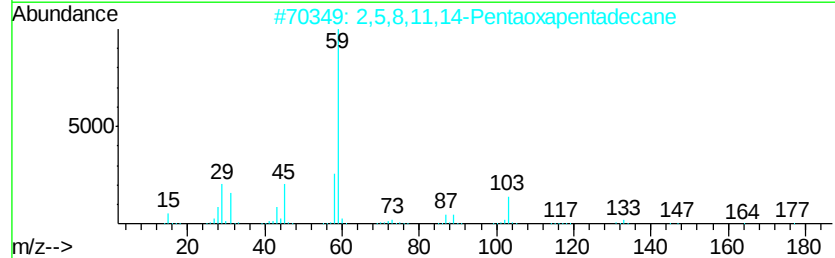
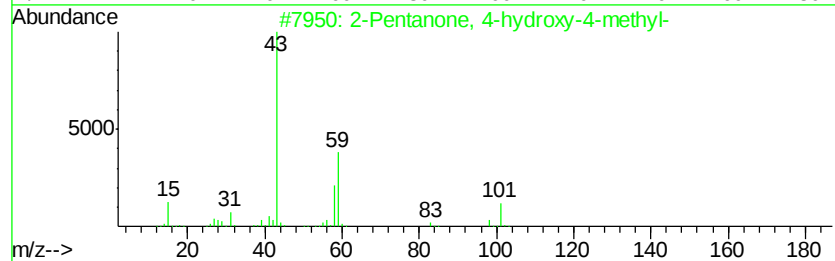
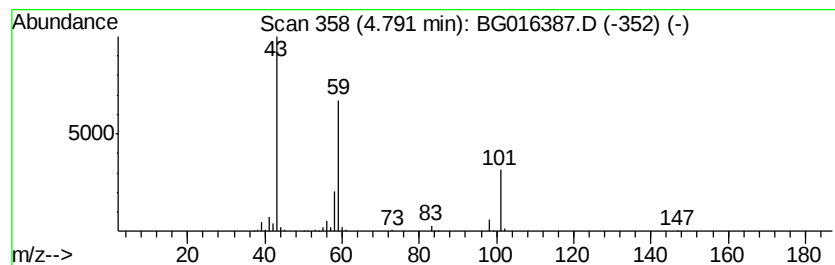
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	9.16 ng	244779	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	50
2		2,5,8,11,14-Pentaoxapentadecane	222	C10H22O5	000143-24-8	25
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	25
4		2,5,8,11,14,17-Hexaoxaoctadecane	266	C12H26O6	001191-87-3	23
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23



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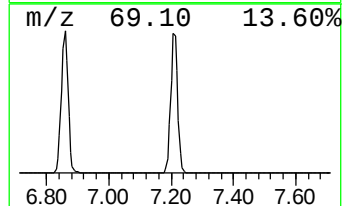
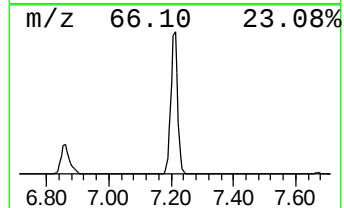
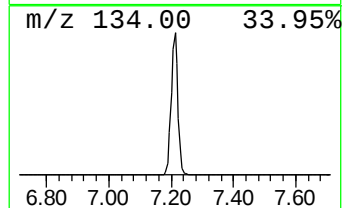
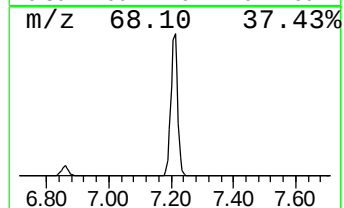
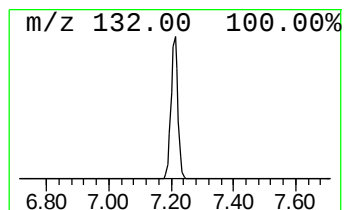
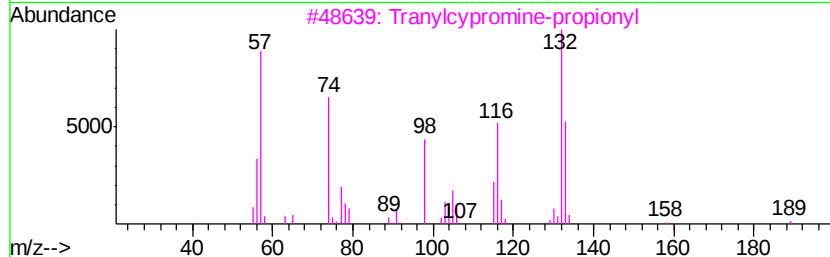
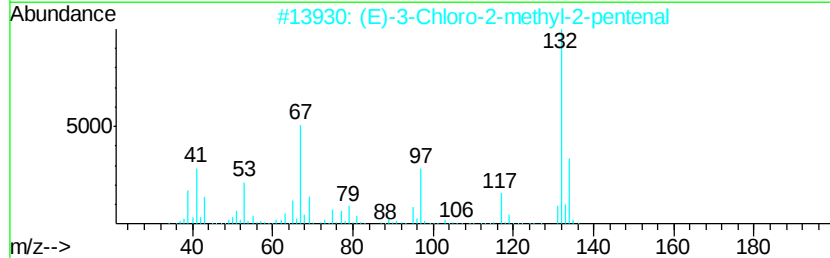
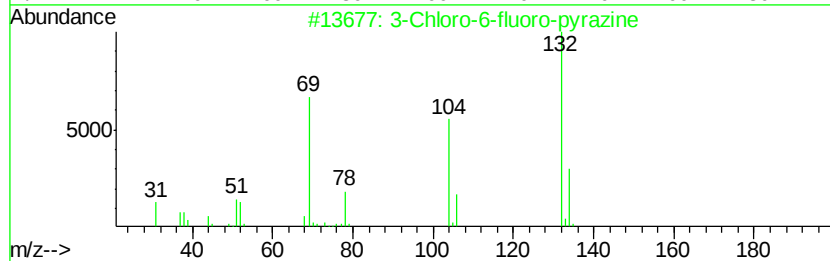
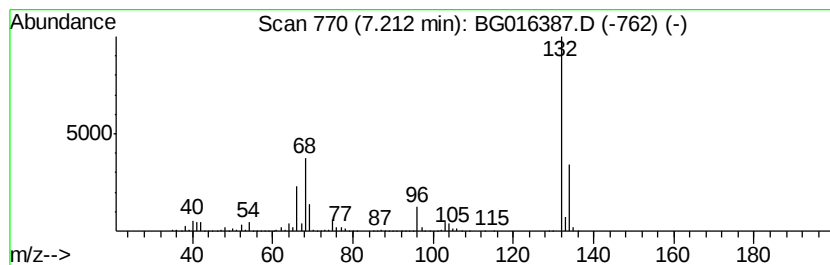
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	76.81 ng	2052770	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	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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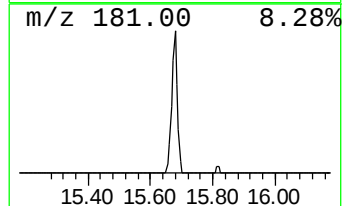
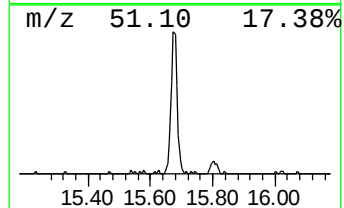
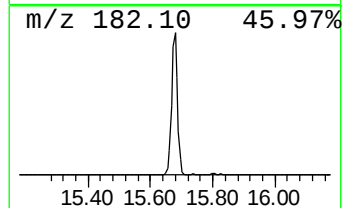
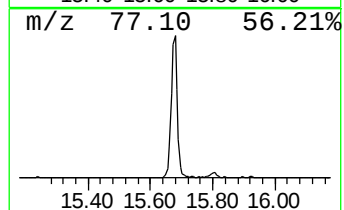
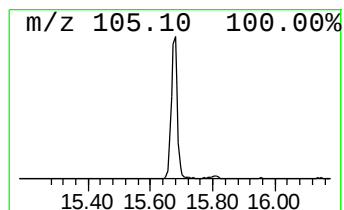
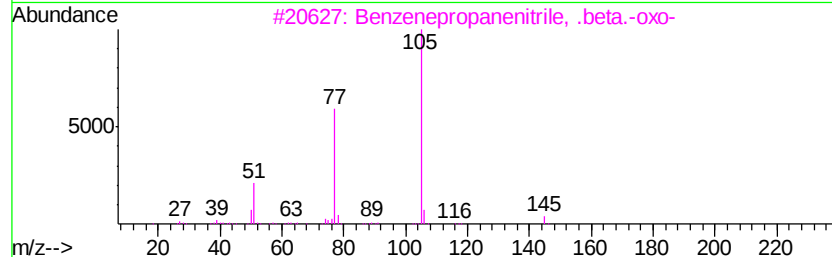
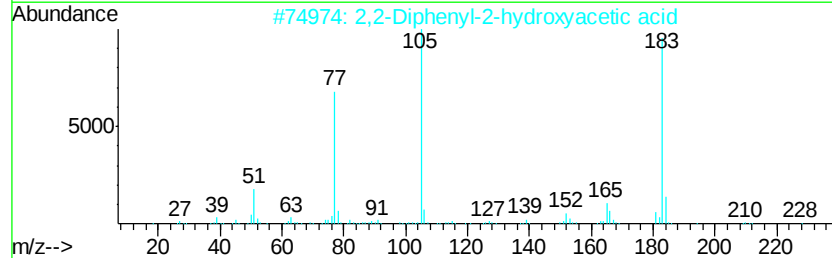
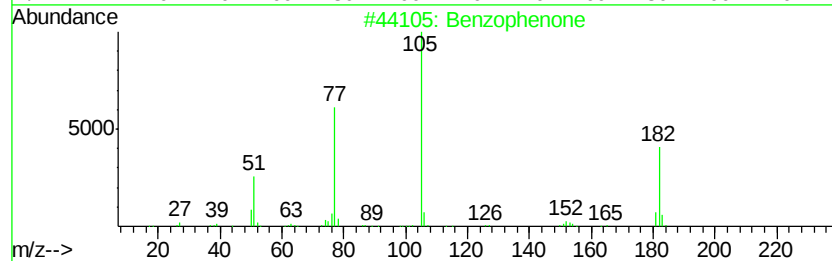
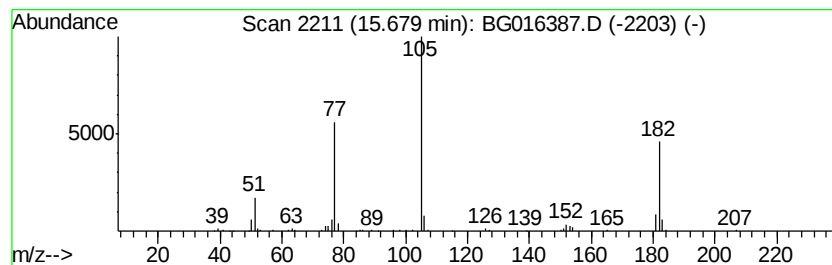
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzophenone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.68	3.19 ng	172776	Acenaphthene-d10	14.32

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	95
2		2,2-Diphenyl-2-hydroxyacetic acid	228	C14H12O3	000076-93-7	47
3		Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43
4		Benzofurazan-5-carbohydrazide, N...	282	C14H10N4O3	1000272-94-4	43
5		Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	43



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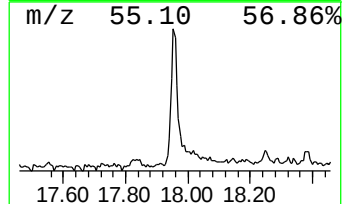
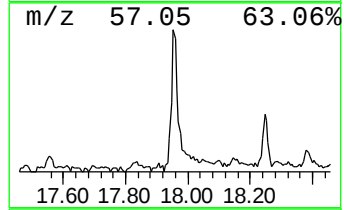
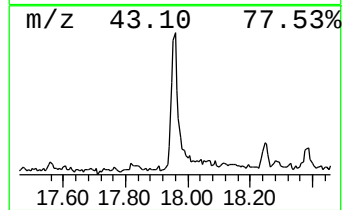
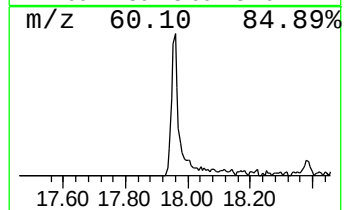
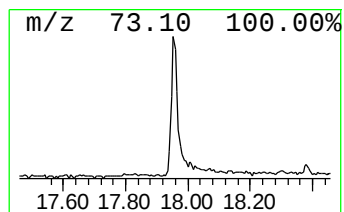
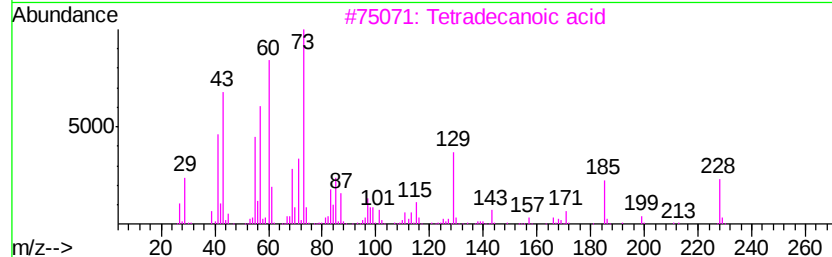
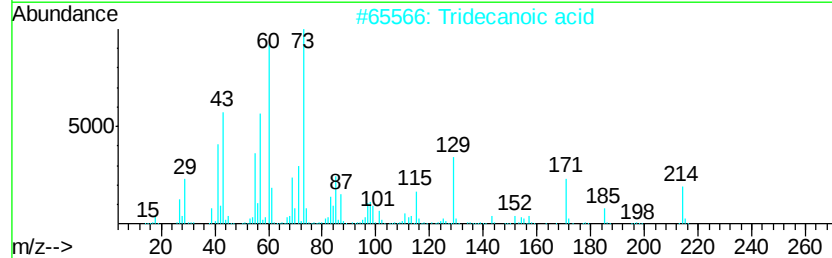
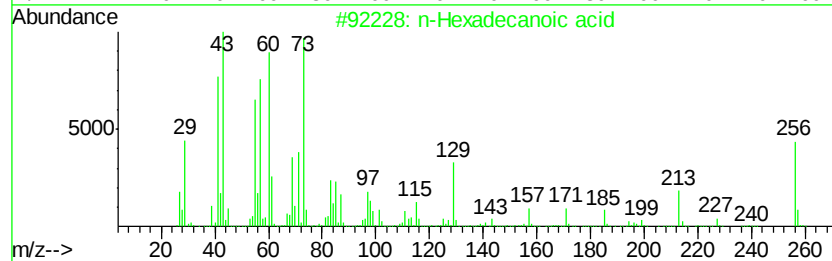
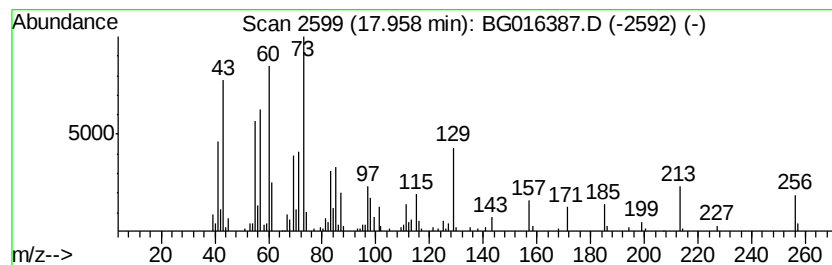
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.96	2.68 ng	171620	Phenanthrene-d10	17.06

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	74
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Undecanoic acid	186	C11H22O2	000112-37-8	72
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	72



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016387.D
Acq On : 14 Apr 2015 8:21
Operator : TP/IZ
Sample : G1831-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PE-11

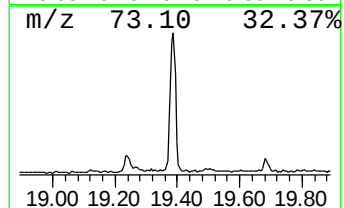
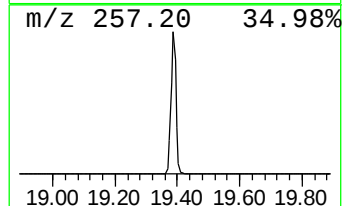
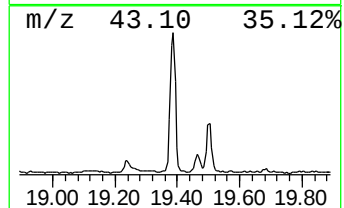
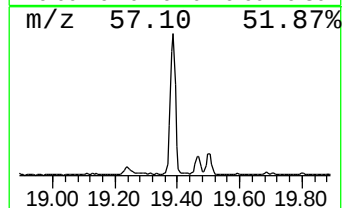
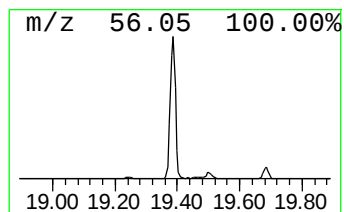
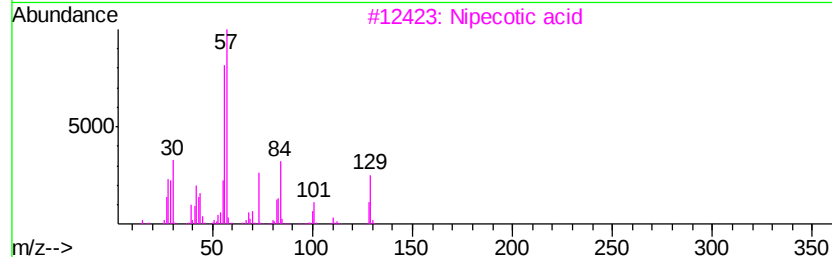
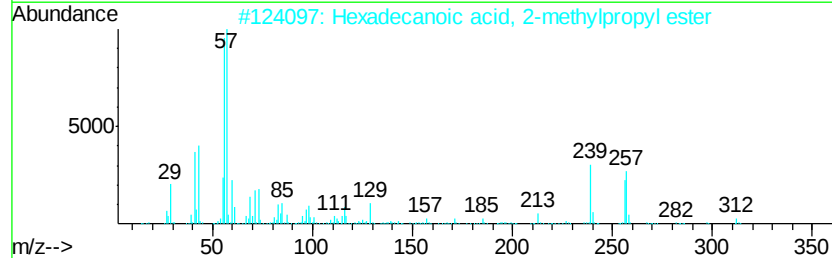
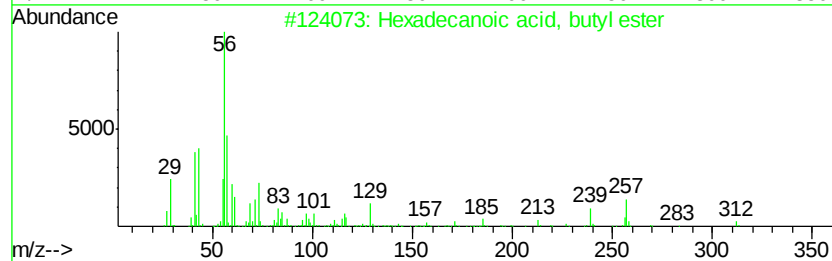
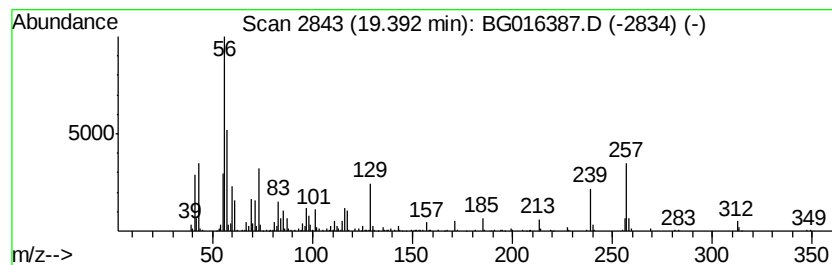
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	7.64 ng	567622	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		Nipecotic acid	129	C6H11NO2	000498-95-3	47
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27
5		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
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Acq On : 14 Apr 2015 8:21
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ClientSampleId :
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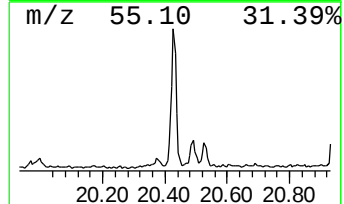
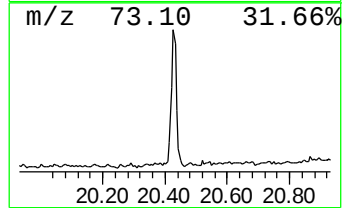
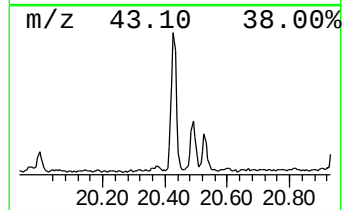
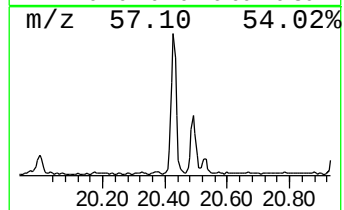
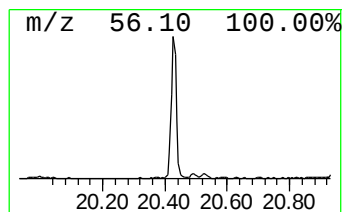
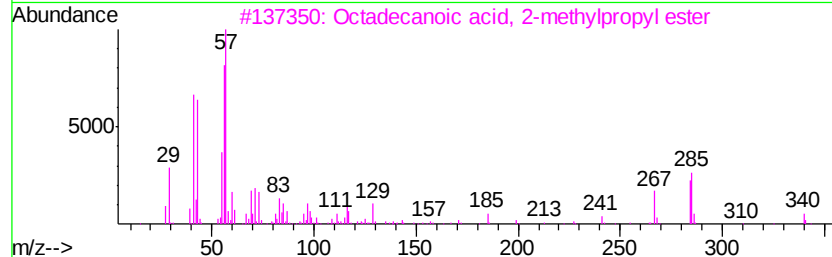
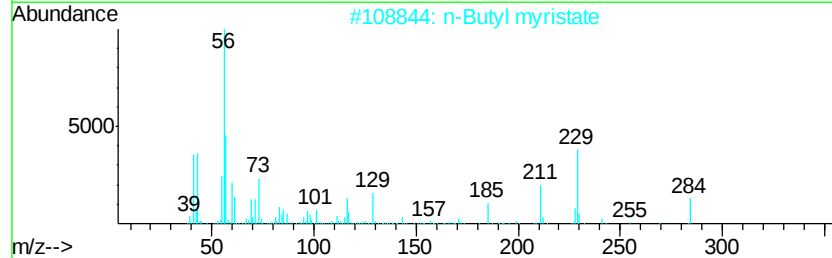
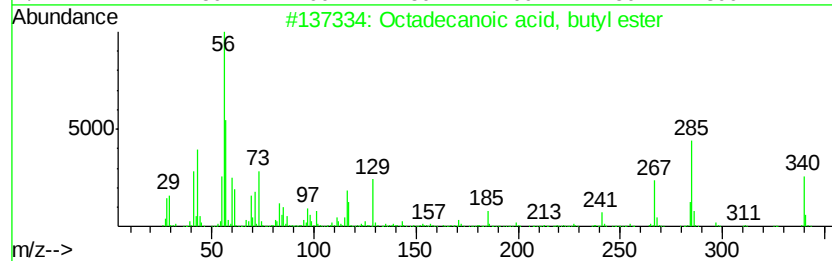
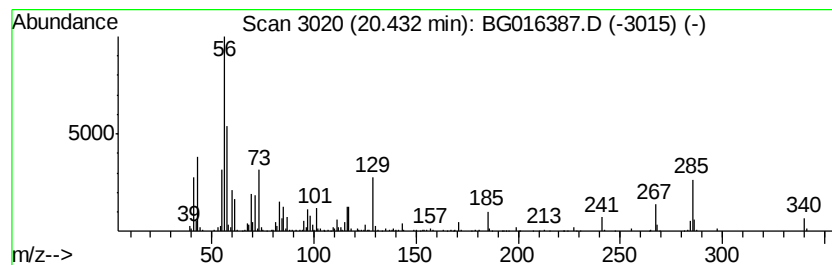
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	5.81 ng	431637	Chrysene-d12	21.24

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	99
2			n-Butyl myristate	284	C18H36O2	000110-36-1	58
3			Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	55
4			Nipecotic acid	129	C6H11NO2	000498-95-3	47
5			1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016387.D
Acq On : 14 Apr 2015 8:21
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Sample : G1831-05
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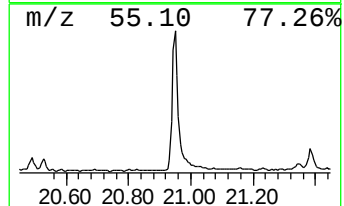
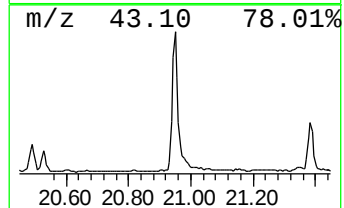
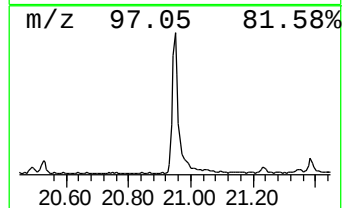
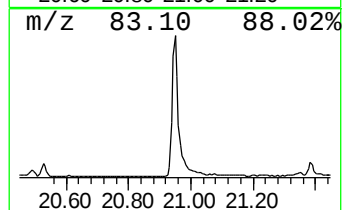
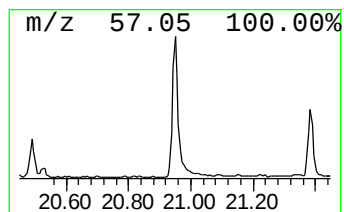
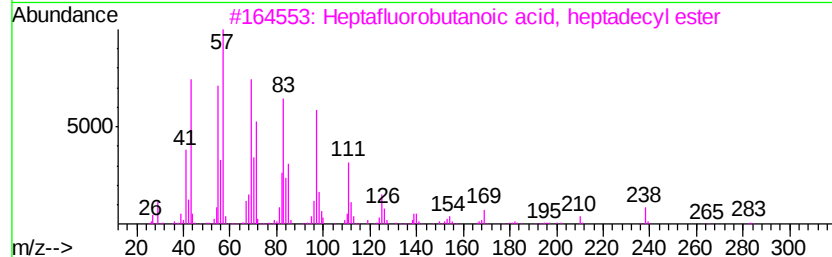
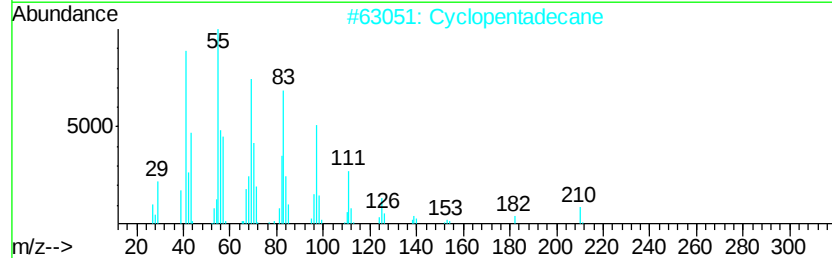
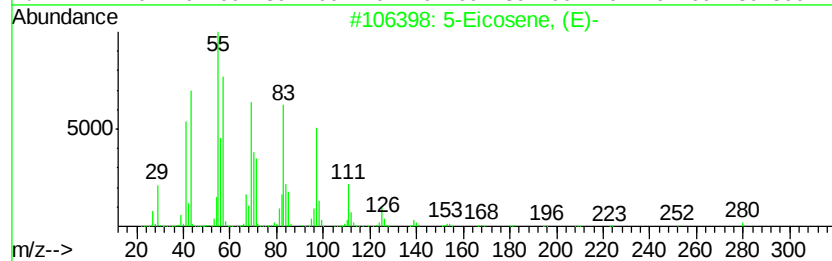
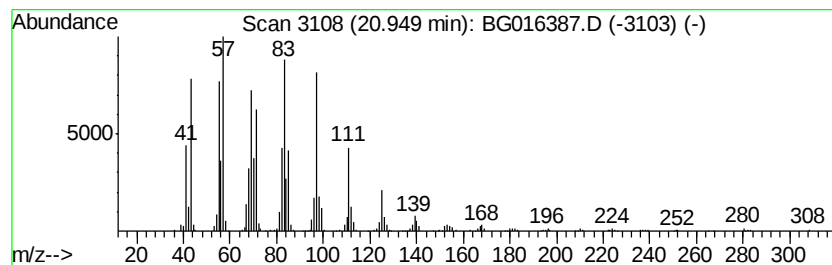
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.95	9.88 ng	733374	Chrysene-d12	21.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	93
4	E-14-Hexadecenal	238	C16H30O	330207-53-9	91
5	1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91



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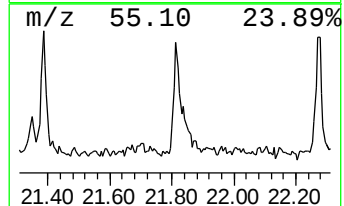
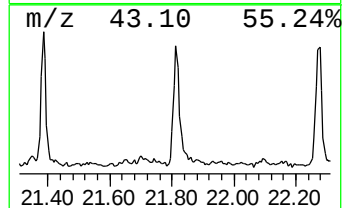
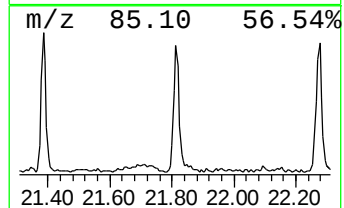
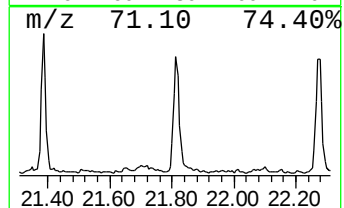
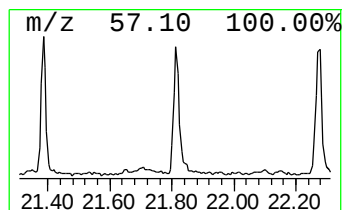
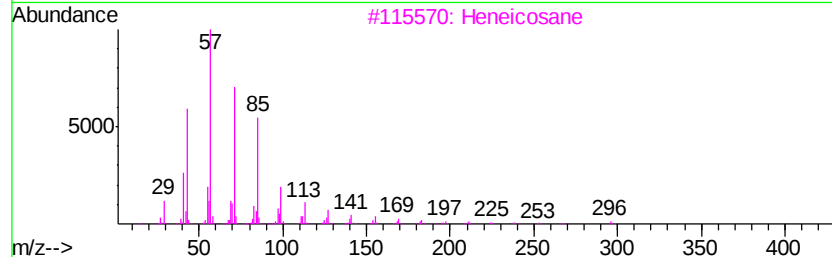
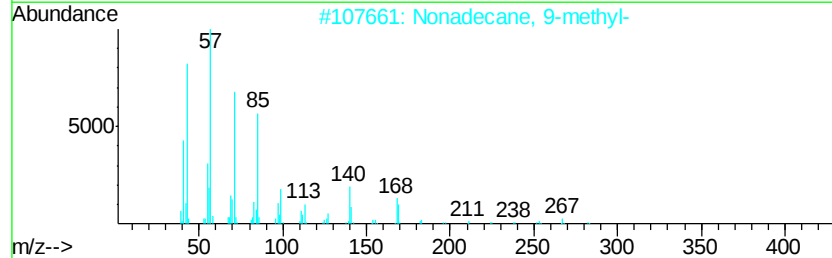
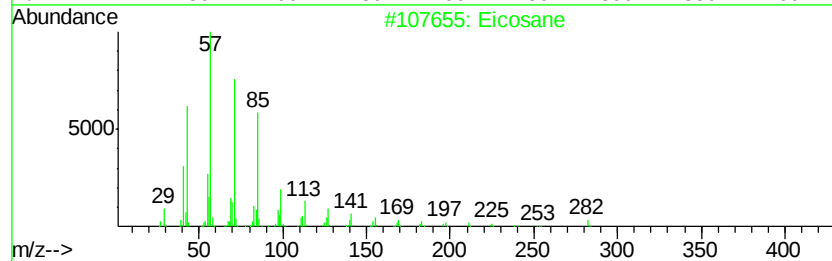
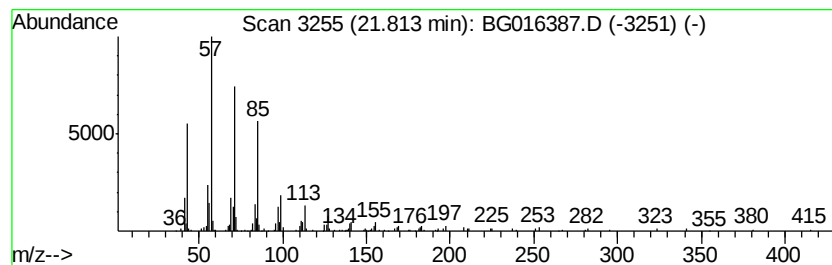
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Eicosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.81	2.39 ng	177194	Chrysene-d12	21.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Eicosane		282 C20H42	000112-95-8 98
2	Nonadecane, 9-methyl-		282 C20H42	013287-24-6 94
3	Heneicosane		296 C21H44	000629-94-7 91
4	Tetracosane		338 C24H50	000646-31-1 91
5	Octacosane		394 C28H58	000630-02-4 91



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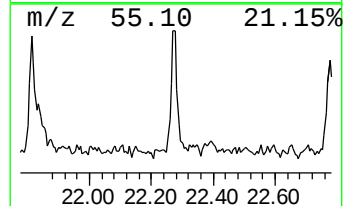
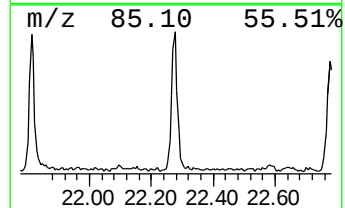
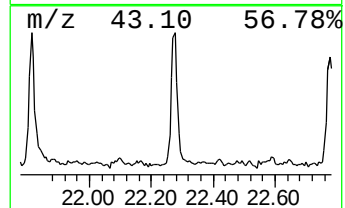
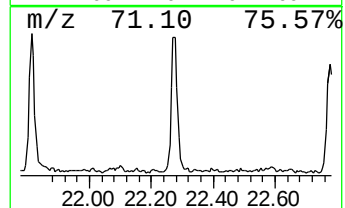
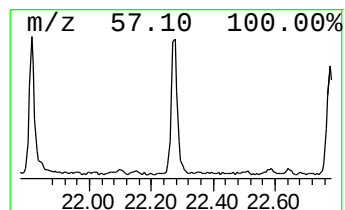
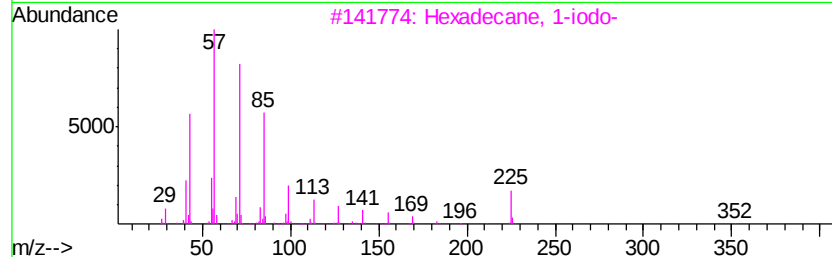
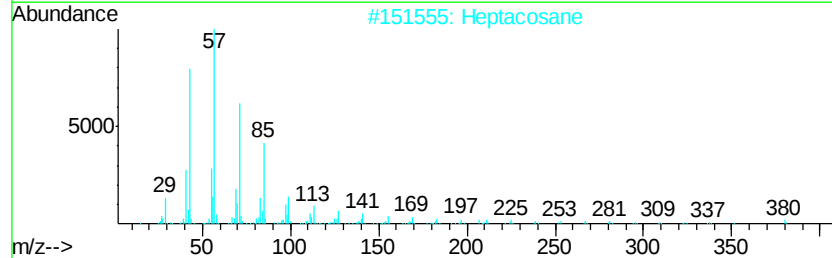
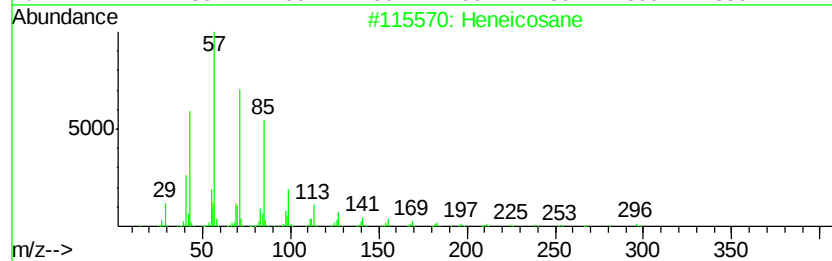
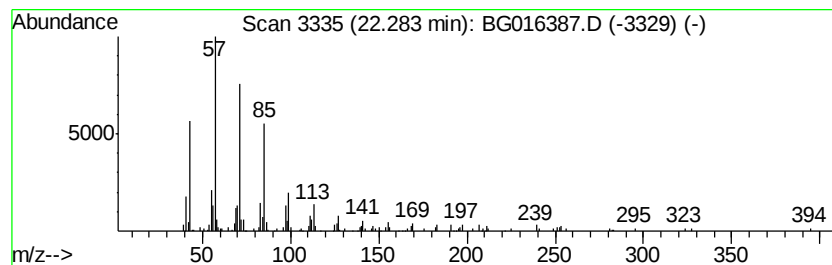
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heneicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	2.10 ng	156037	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heneicosane	296	C21H44	000629-94-7	90
2		Heptacosane	380	C27H56	000593-49-7	90
3		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
4		Heptadecane	240	C17H36	000629-78-7	87
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87



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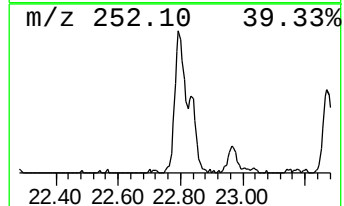
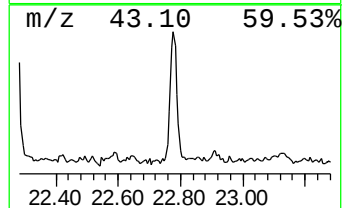
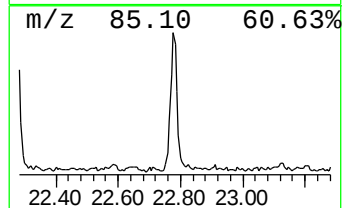
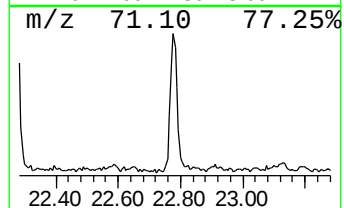
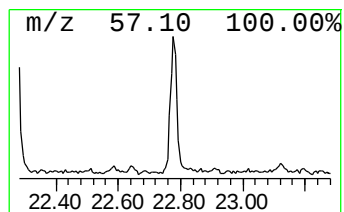
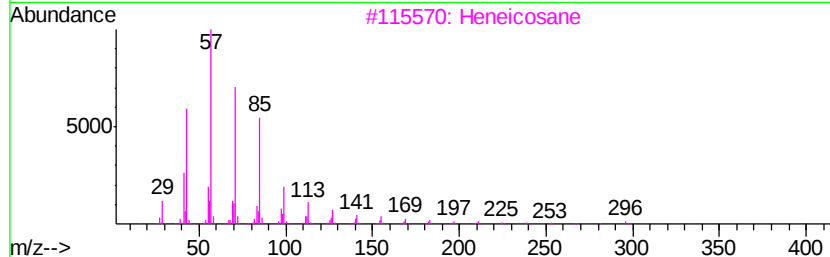
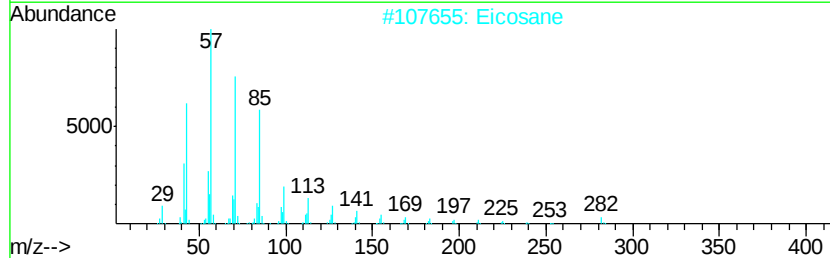
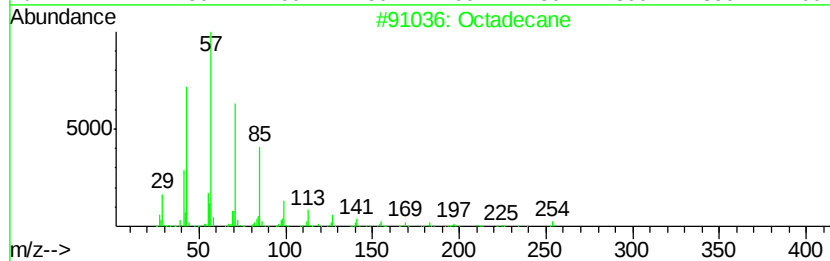
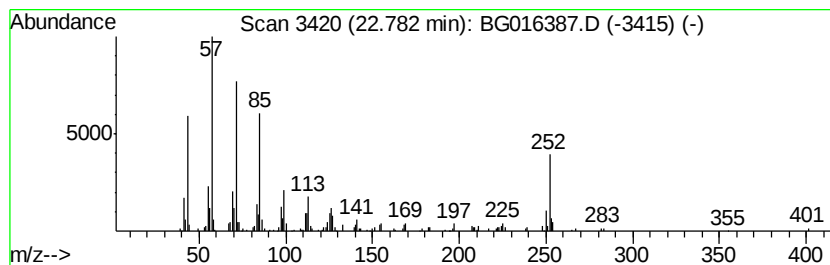
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Octadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.78	3.11 ng	221015	Perylene-d12	23.47

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	95
2			Eicosane	282	C20H42	000112-95-8	94
3			Heneicosane	296	C21H44	000629-94-7	90
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5			Heptadecane	240	C17H36	000629-78-7	83



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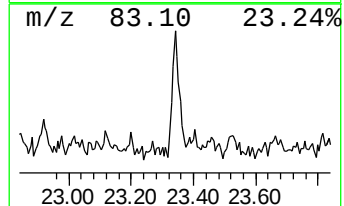
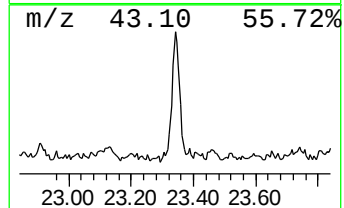
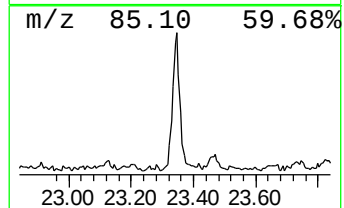
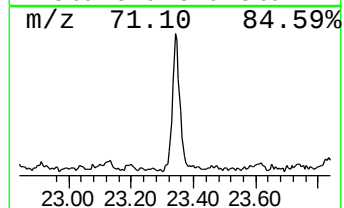
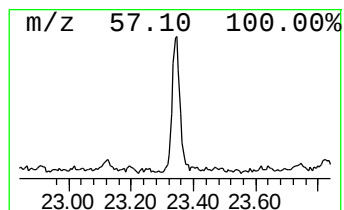
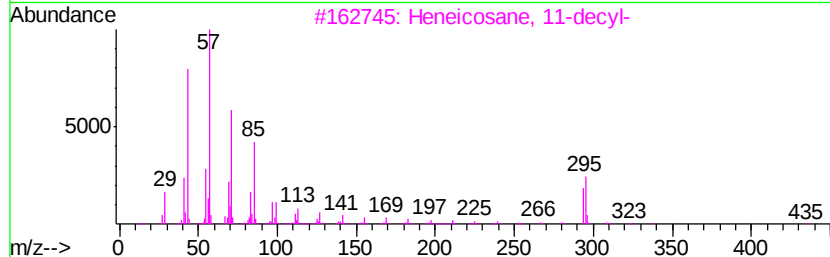
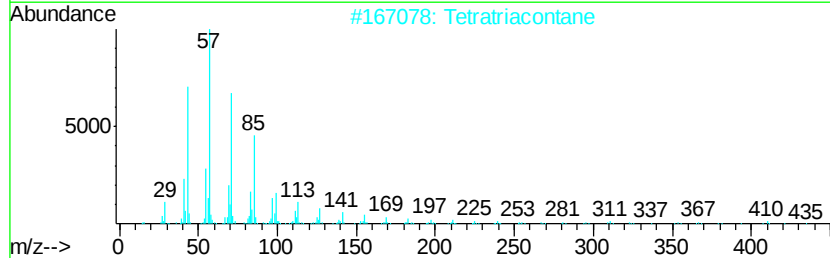
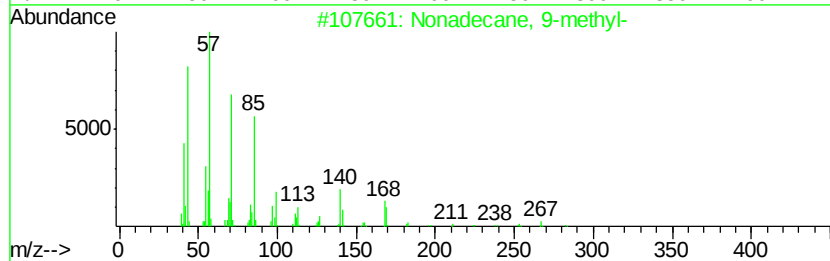
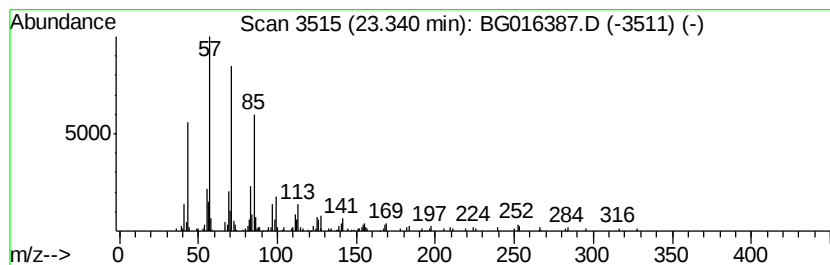
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Nonadecane, 9-methyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.34	2.13 ng	151700	Perylene-d12	23.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2		Tetratriacontane	479	C34H70	014167-59-0	91
3		Heneicosane, 11-decyl-	437	C31H64	055320-06-4	91
4		Heneicosane	296	C21H44	000629-94-7	87
5		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016387.D
Acq On : 14 Apr 2015 8:21
Operator : TP/IZ
Sample : G1831-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

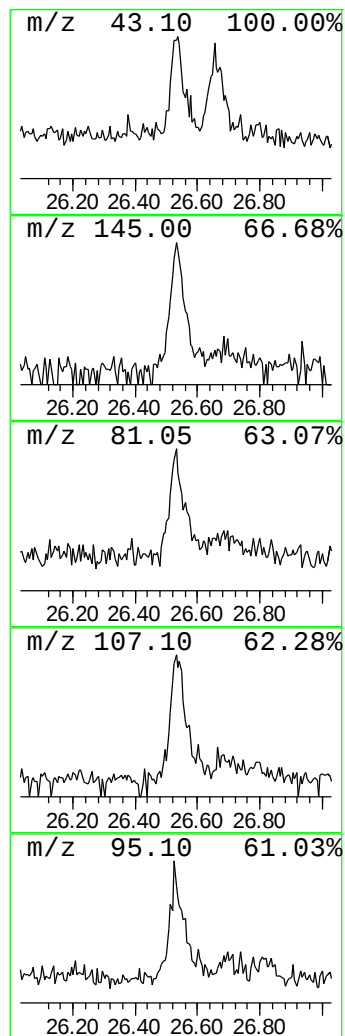
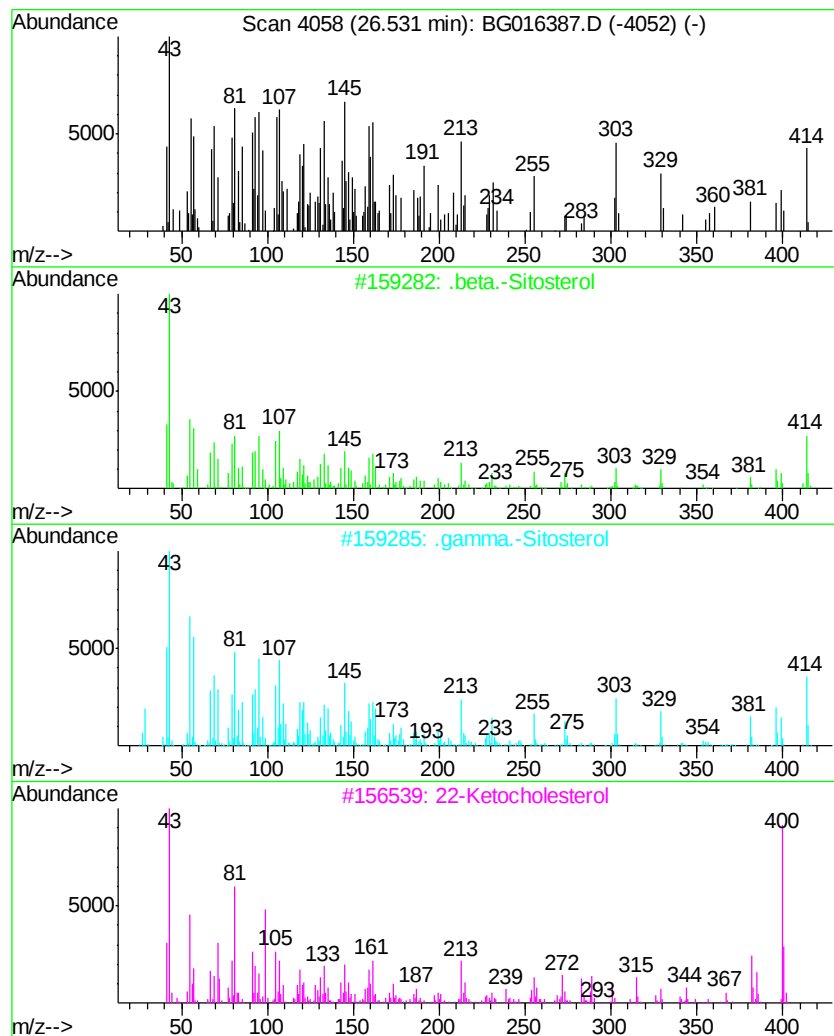
Instrument :
BNA_G
ClientSampleId :
PE-11

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 15 .beta.-Sitosterol Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.53	2.08 ng	148258	Perylene-d12	23.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Sitosterol	414 C29H50O	000083-46-5 93
2		.gamma.-Sitosterol	414 C29H50O	000083-47-6 83
3		22-Ketocholesterol	400 C27H44O2	1000127-06-3 32
4		Ergost-5-en-3-ol, (3.beta.)-	400 C28H48O	004651-51-8 22
5		5-Cholestene-3-ol, 24-methyl-	400 C28H48O	1000214-17-4 16



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016387.D
Acq On : 14 Apr 2015 8:21
Operator : TP/IZ
Sample : G1831-05
Misc :
ALS Vial : 27 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PE-11

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...	2.85	6.5	ng	173789	1	7.68	534479	20.0
2-Pentanone, 4-hy...	4.79	9.2	ng	244779	1	7.68	534479	20.0
unknown7.21	7.21	76.8	ng	2052770	1	7.68	534479	20.0
Benzophenone	15.68	3.2	ng	172776	3	14.32	1081640	20.0
n-Hexadecanoic acid	17.96	2.7	ng	171620	4	17.06	1282780	20.0
Hexadecanoic acid...	19.39	7.6	ng	567622	5	21.24	1485180	20.0
Octadecanoic acid...	20.43	5.8	ng	431637	5	21.24	1485180	20.0
5-Eicosene, (E)-	20.95	9.9	ng	733374	5	21.24	1485180	20.0
Eicosane	21.81	2.4	ng	177194	5	21.24	1485180	20.0
Heneicosane	22.28	2.1	ng	156037	5	21.24	1485180	20.0
Octadecane	22.78	3.1	ng	221015	6	23.47	1422180	20.0
Nonadecane, 9-met...	23.34	2.1	ng	151700	6	23.47	1422180	20.0
.beta.-Sitosterol	26.53	2.1	ng	148258	6	23.47	1422180	20.0