

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
 Data File : BG016360.D
 Acq On : 13 Apr 2015 14:57
 Operator : TP/IZ
 Sample : G1822-02
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 F5-025

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	2.765	8	13	23	rBV2	134325	271089	7.54%	0.996%
2	2.847	23	27	33	rVB	177666	232418	6.46%	0.854%
3	4.780	350	356	366	rVB2	157307	238755	6.64%	0.877%
4	5.256	431	437	448	rBV	1231179	1773283	49.32%	6.514%
5	6.855	699	709	727	rBV	1250401	1961481	54.55%	7.205%
6	7.207	762	769	778	rBV	1251927	1928671	53.64%	7.085%
7	7.454	804	811	821	rVB2	39385	66981	1.86%	0.246%
8	7.671	842	848	856	rBV	343401	531190	14.77%	1.951%
9	7.988	895	902	910	rBV	819749	1296038	36.05%	4.761%
10	8.829	1037	1045	1052	rBV	707088	1119993	31.15%	4.114%
11	10.462	1314	1323	1329	rBV	450465	764893	21.27%	2.810%
12	11.784	1539	1548	1556	rBV	70189	113661	3.16%	0.418%
13	12.936	1737	1744	1758	rVB	1661773	2376646	66.10%	8.730%
14	13.776	1881	1887	1895	rBV	159325	210486	5.85%	0.773%
15	14.316	1972	1979	1987	rBV2	680916	1023463	28.47%	3.760%
16	15.092	2104	2111	2114	rBV	46618	60989	1.70%	0.224%
17	15.679	2201	2211	2217	rBV	421783	559052	15.55%	2.054%
18	15.809	2226	2233	2242	rBV	1168250	1638774	45.58%	6.020%
19	17.060	2440	2446	2451	rBV	906944	1239357	34.47%	4.553%
20	17.953	2592	2598	2608	rBV3	58997	126418	3.52%	0.464%
21	18.294	2652	2656	2668	rBV3	22218	45519	1.27%	0.167%
22	19.117	2790	2796	2801	rBV	30625	48638	1.35%	0.179%
23	19.387	2837	2842	2847	rBV	624335	688153	19.14%	2.528%
24	19.469	2852	2856	2858	rVV3	39918	58597	1.63%	0.215%
25	19.499	2858	2861	2867	rVB	103560	128406	3.57%	0.472%
26	19.687	2887	2893	2900	rBV	2978147	3595451	100.00%	13.208%
27	20.374	3006	3010	3015	rVB2	30382	38543	1.07%	0.142%
28	20.427	3015	3019	3026	rBV	623452	665478	18.51%	2.445%
29	20.491	3026	3030	3033	rVV	69387	84171	2.34%	0.309%
30	20.527	3033	3036	3040	rVB	55271	60030	1.67%	0.221%
31	20.950	3103	3108	3117	rBV	260301	365002	10.15%	1.341%
32	21.238	3150	3157	3161	rBV	1149333	1481970	41.22%	5.444%
33	21.385	3178	3182	3188	rBV	126263	140906	3.92%	0.518%
34	21.813	3251	3255	3262	rBV	113742	141866	3.95%	0.521%

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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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Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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35	22.272	3329	3333	3341	rBV	127355	164281	4.57%	0.603%
36	22.777	3414	3419	3425	rBV2	101429	174866	4.86%	0.642%
37	23.347	3511	3516	3526	rVB2	81597	154219	4.29%	0.567%
38	23.470	3529	3537	3546	rBV2	718806	1413651	39.32%	5.193%
39	23.993	3621	3626	3636	rVB2	66103	123866	3.45%	0.455%
40	24.745	3749	3754	3759	rBV3	50915	115357	3.21%	0.424%

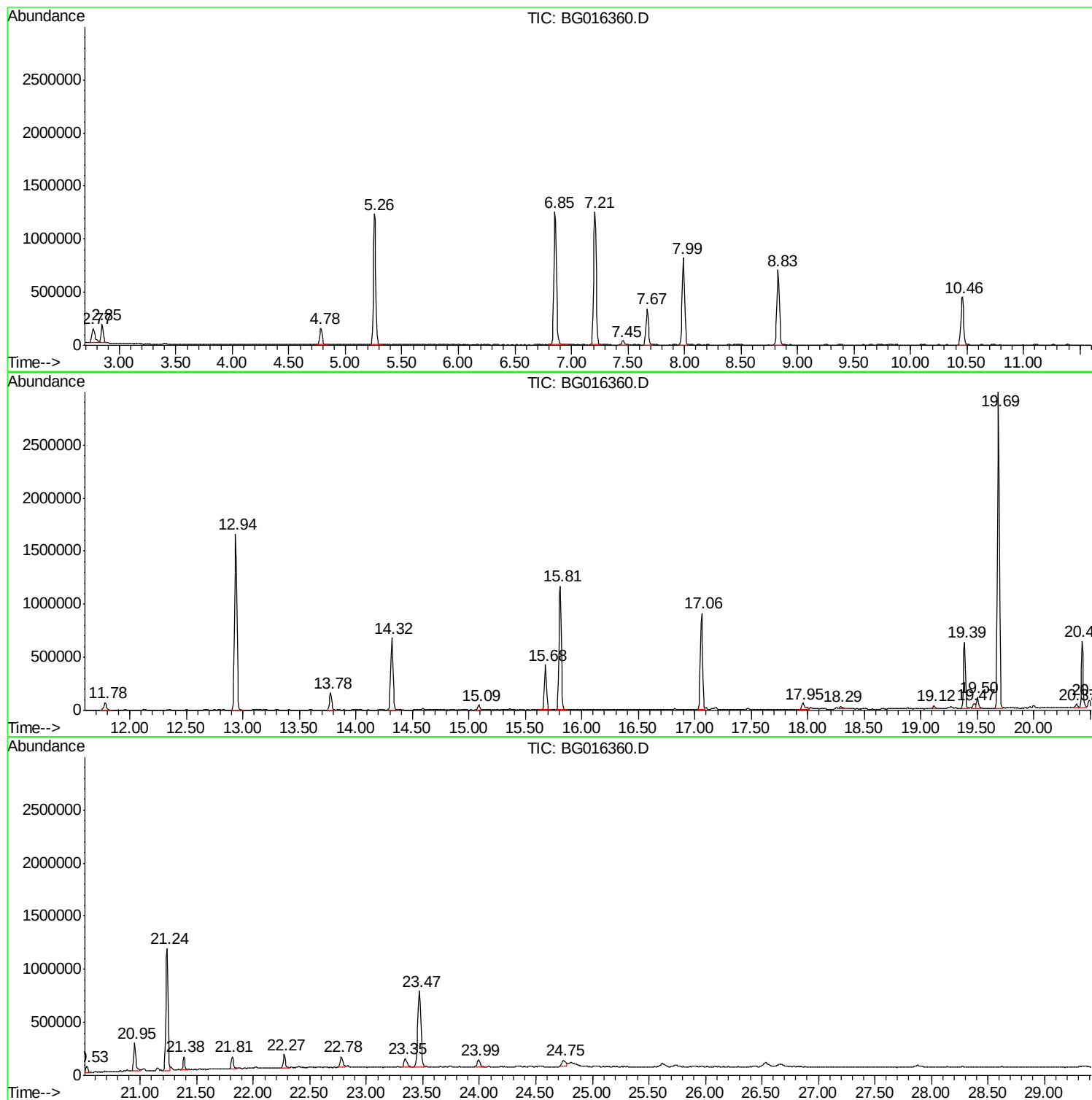
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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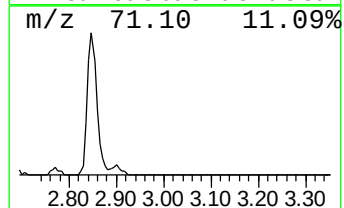
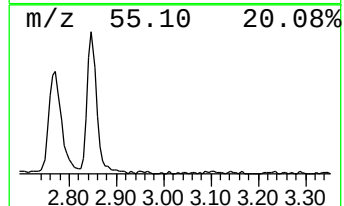
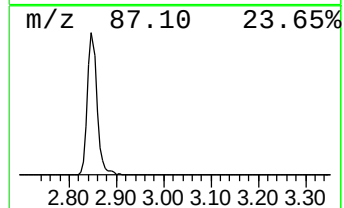
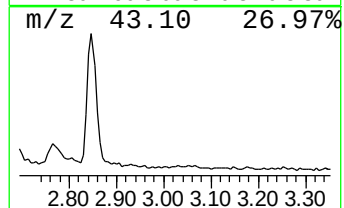
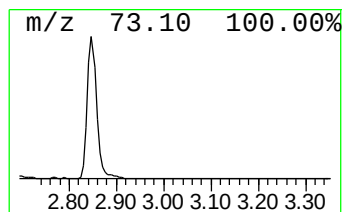
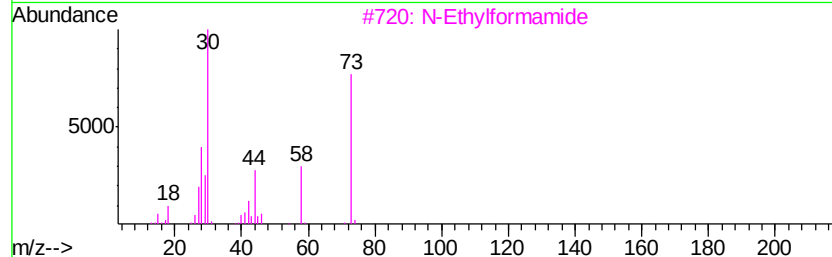
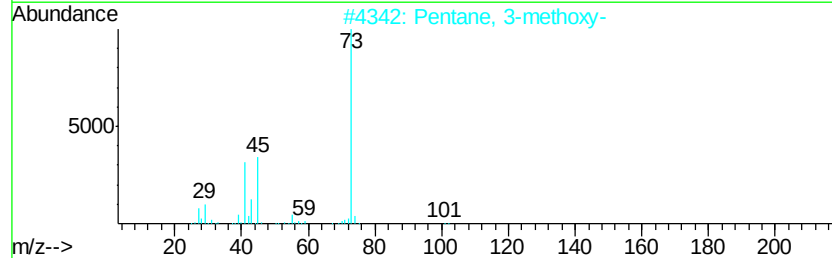
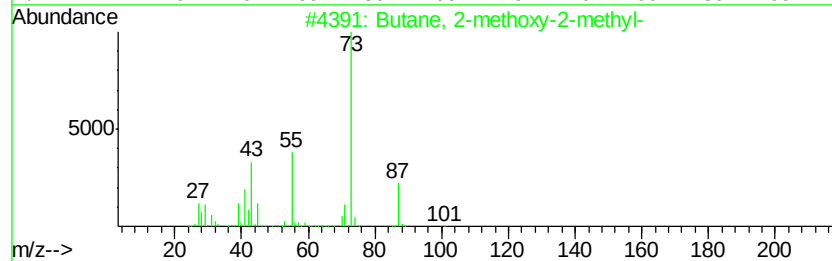
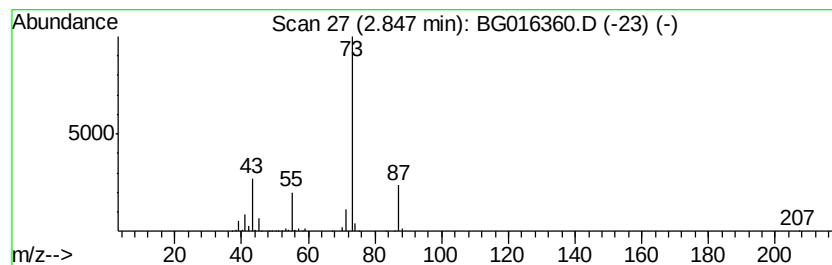
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	8.75 ng	232418	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7



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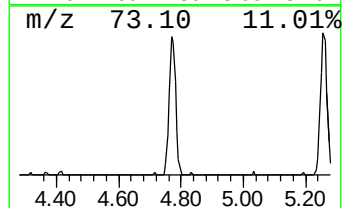
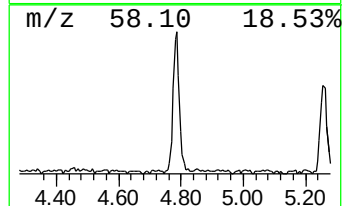
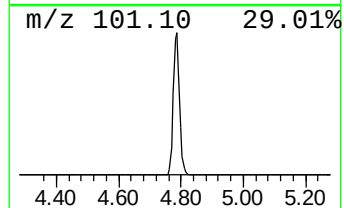
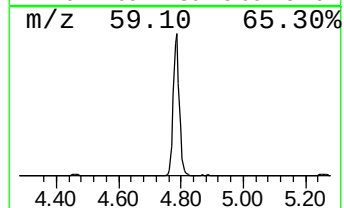
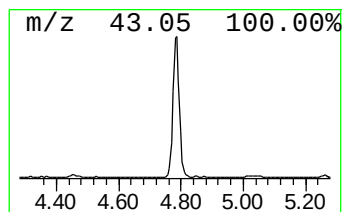
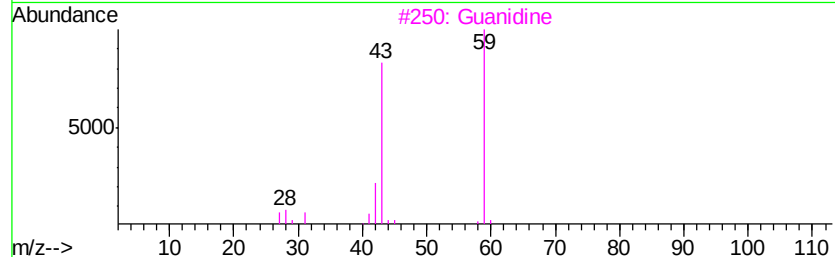
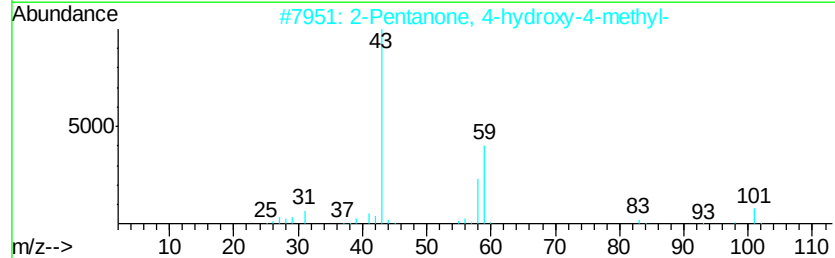
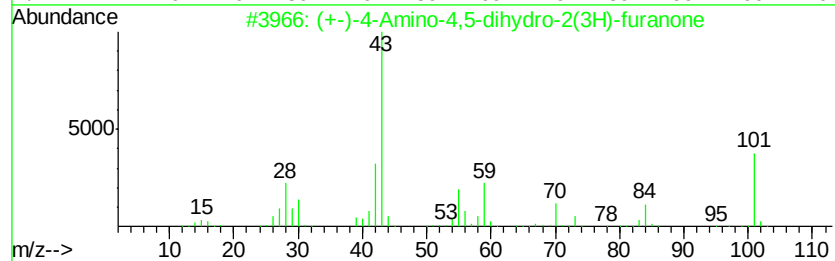
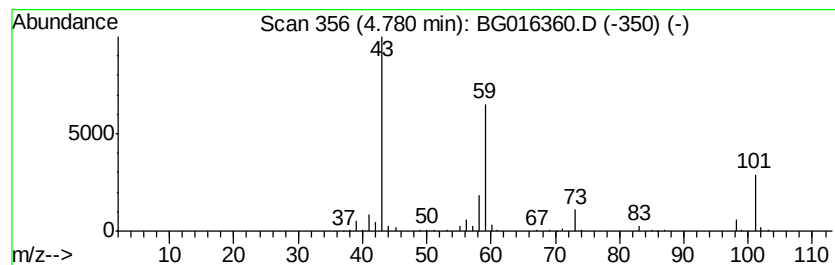
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown4.78 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	8.99 ng	238755	1,4-Dichlorobenzene-d4	7.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-	4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47	
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
3	Guanidine	59	CH5N3	000113-00-8	37		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	25		
5	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	17		



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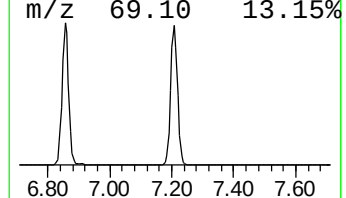
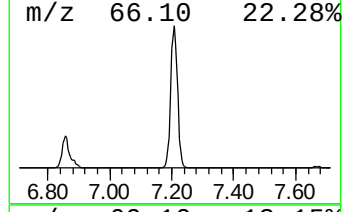
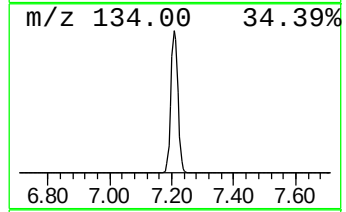
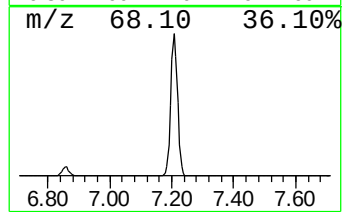
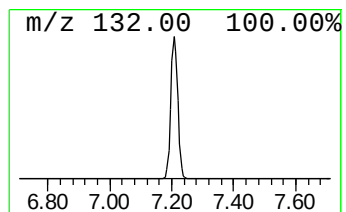
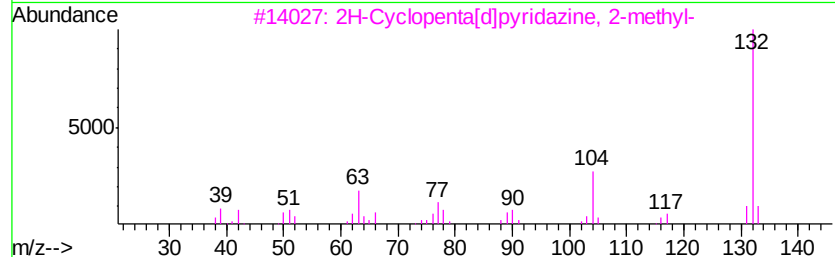
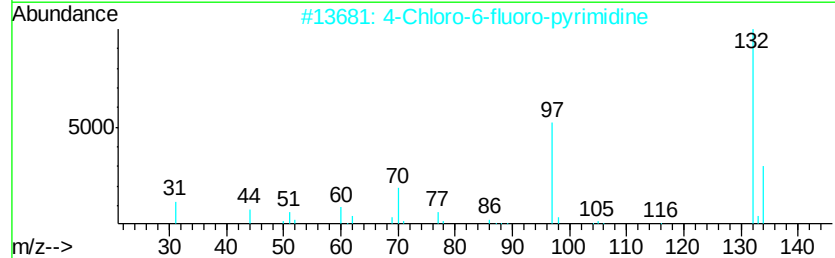
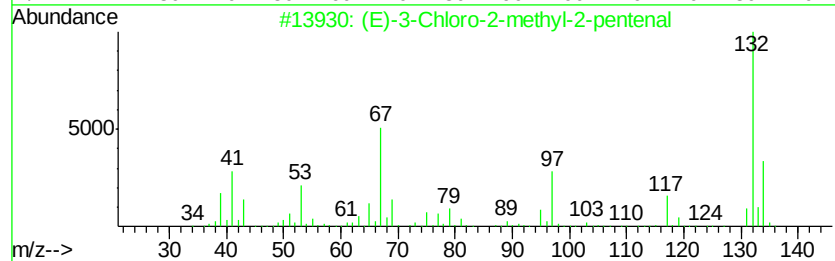
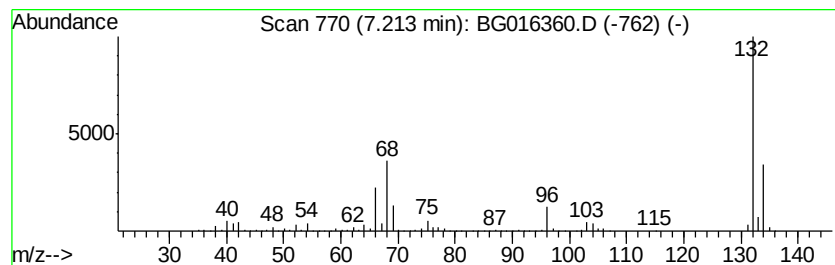
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	72.62 ng	1928670	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
3		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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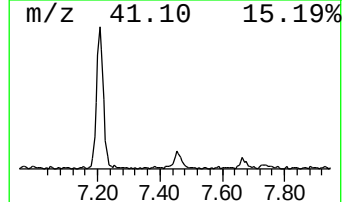
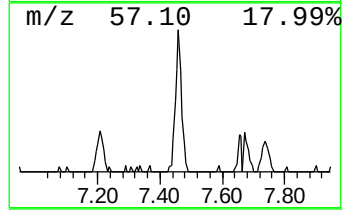
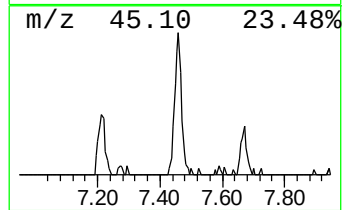
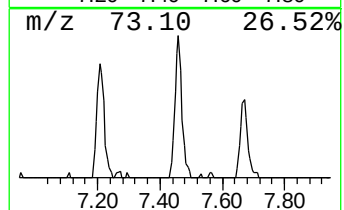
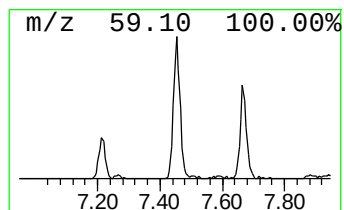
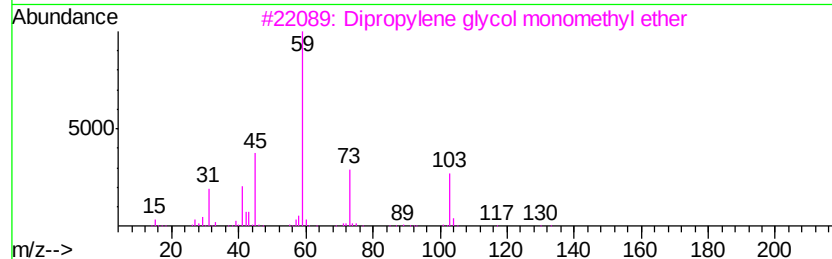
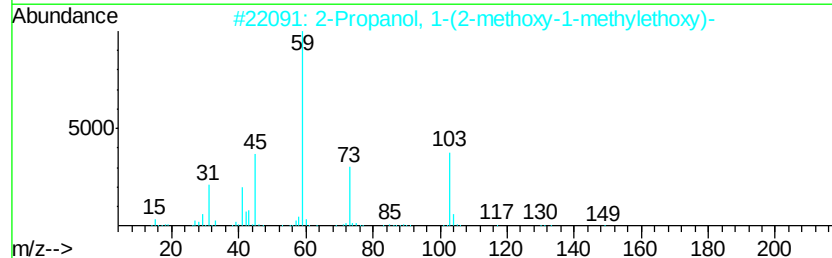
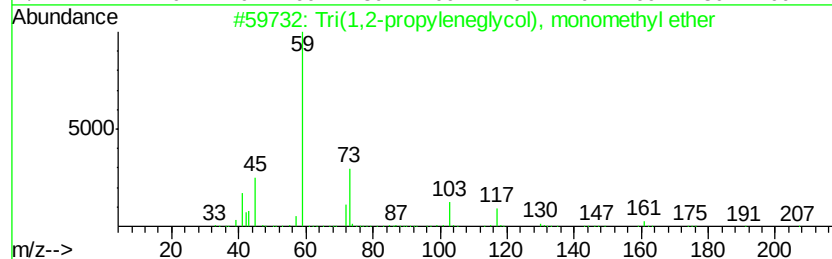
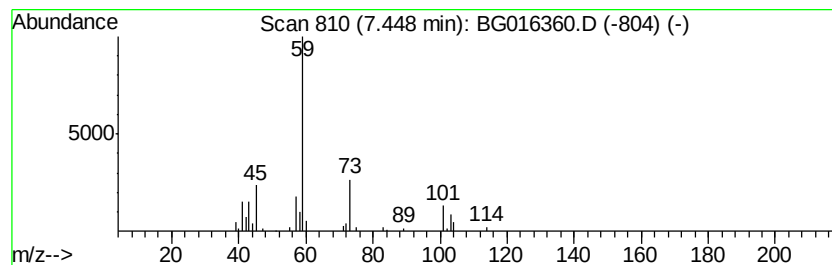
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown7.45 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.45	2.52 ng	66981	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tri(1,2-propyleneglycol), monome...	206	C10H22O4	1000262-26-6	45
2		2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	38
3		Dipropylene glycol monomethyl ether	148	C7H16O3	034590-94-8	38
4		1,2-Dideoxy-L-erythro-pentitol	120	C5H12O3	1000112-47-4	33
5		Propane, 1,2-dimethoxy-	104	C5H12O2	007778-85-0	33



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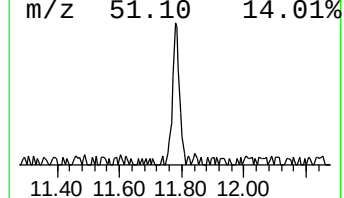
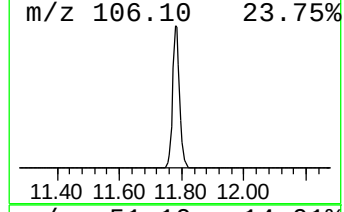
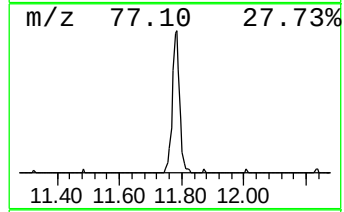
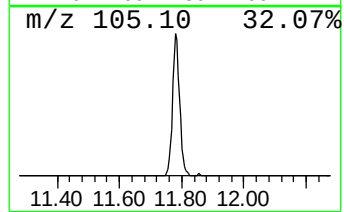
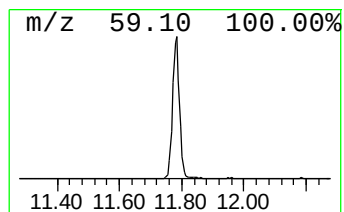
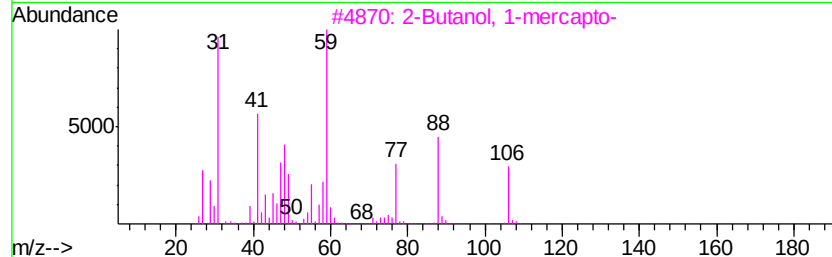
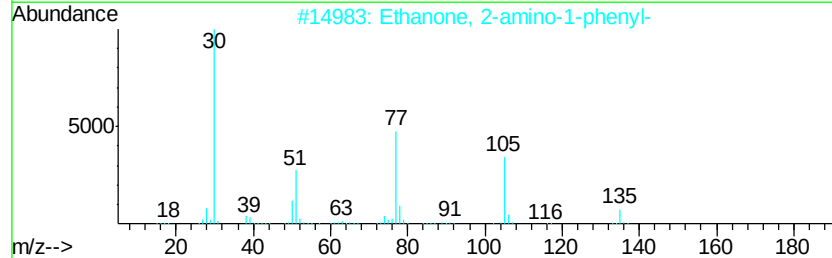
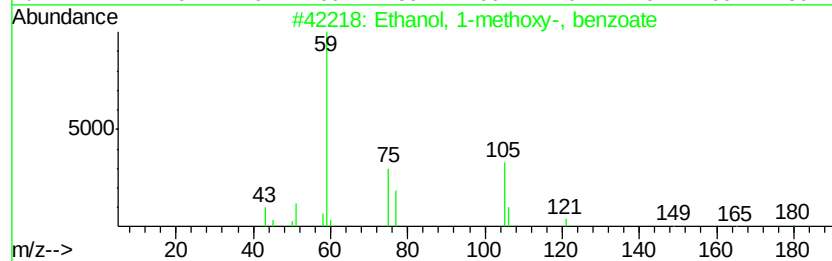
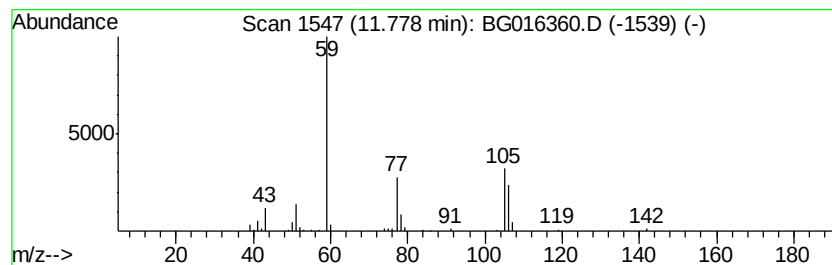
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Peak Number 7 unknown11.78 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.97 ng	113661	Napthalene-d8	10.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	45
2		Ethanone, 2-amino-1-phenyl-	135	C8H9NO	000613-89-8	10
3		2-Butanol, 1-mercapto-	106	C4H10OS	025807-94-7	9
4		Propanedioic acid, (benzoylhydra...	282	C12H14N2O6	1000142-99-9	9
5		Acetic acid, chloro-, methyl ester	108	C3H5ClO2	000096-34-4	9



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Data File : BG016360.D
Acq On : 13 Apr 2015 14:57
Operator : TP/IZ
Sample : G1822-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

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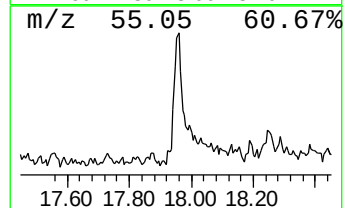
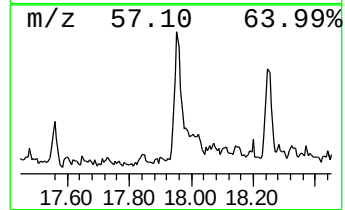
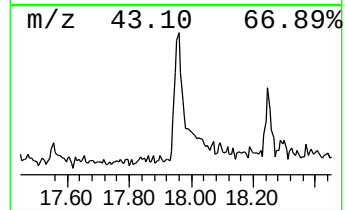
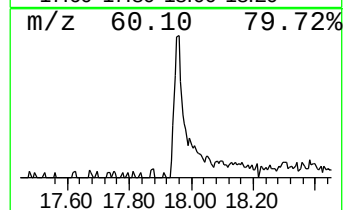
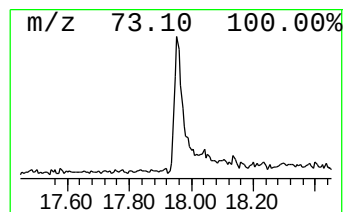
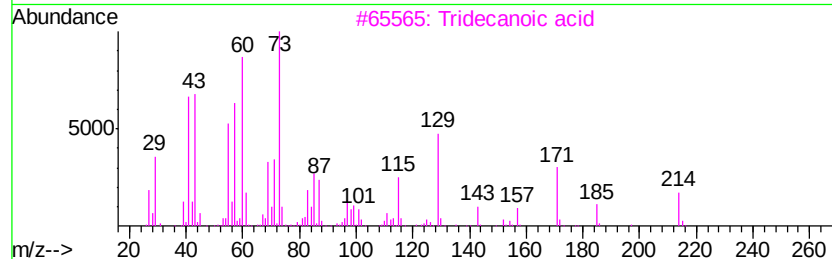
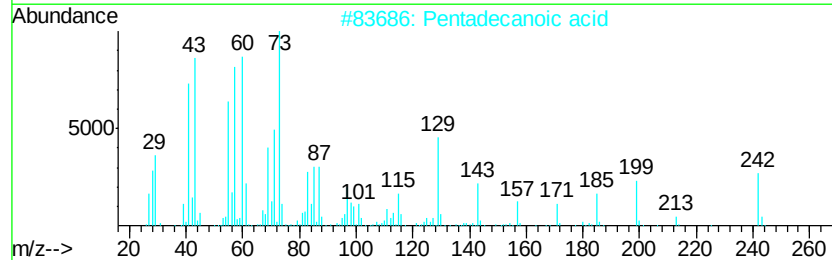
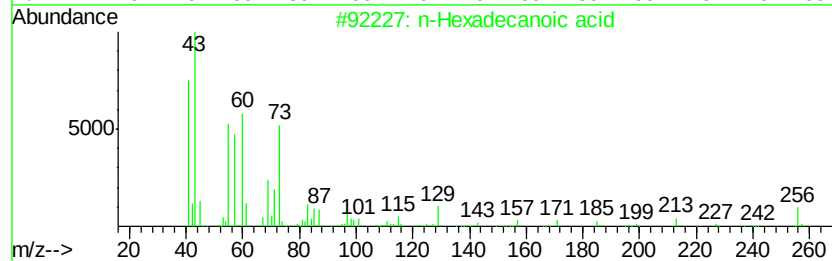
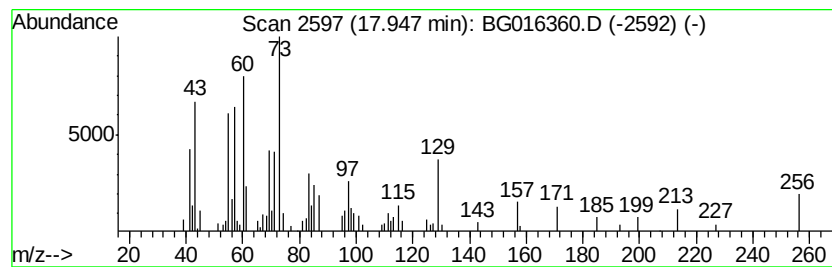
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	2.04 ng	126418	Phenanthrene-d10	17.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3		Tridecanoic acid	214	C13H26O2	000638-53-9	72
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	43



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016360.D
Acq On : 13 Apr 2015 14:57
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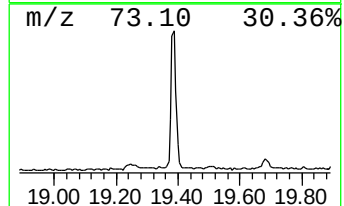
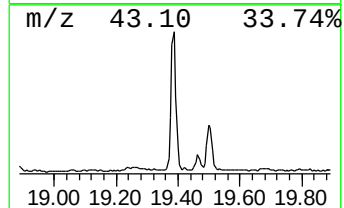
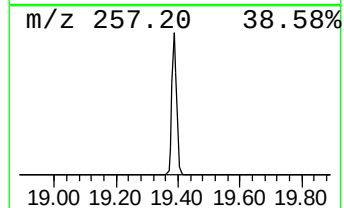
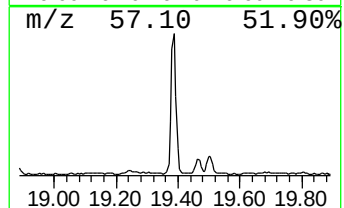
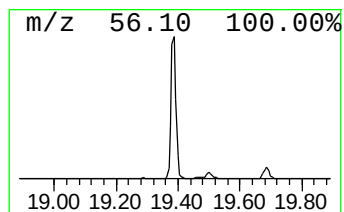
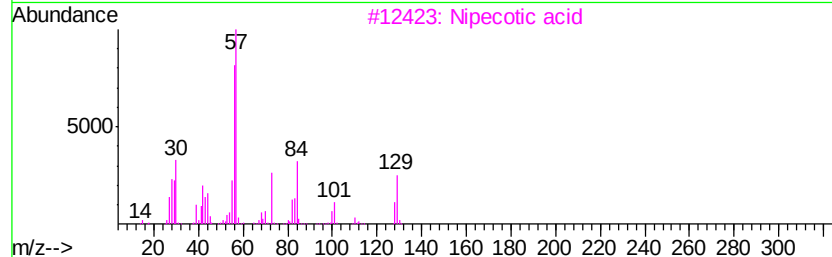
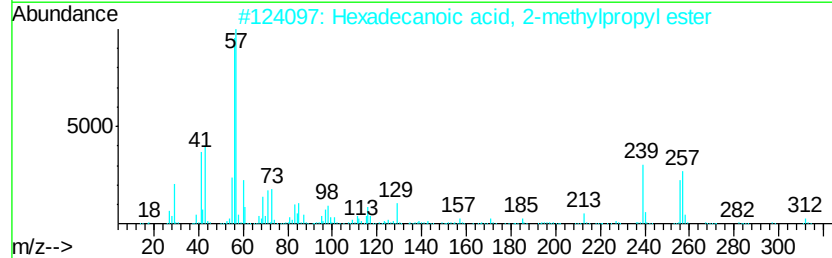
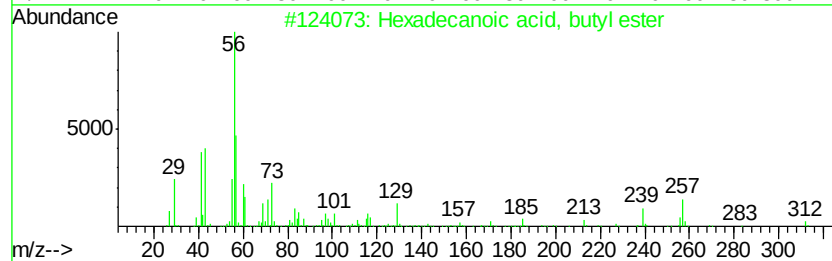
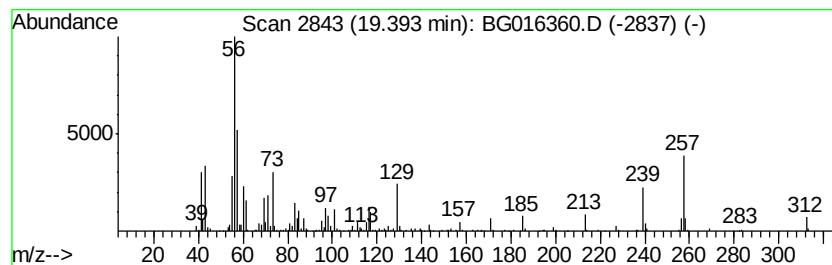
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	9.29 ng	688153	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	98
2		Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	81
3		Nipecotic acid	129	C6H11NO2	000498-95-3	47
4		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	27
5		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	27



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016360.D
Acq On : 13 Apr 2015 14:57
Operator : TP/IZ
Sample : G1822-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

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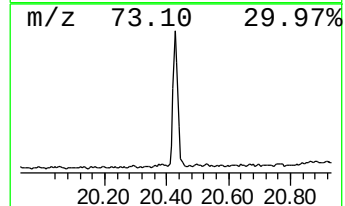
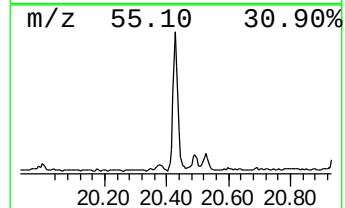
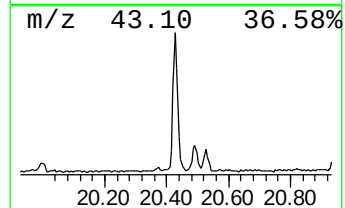
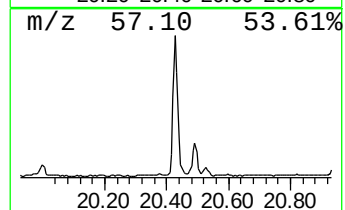
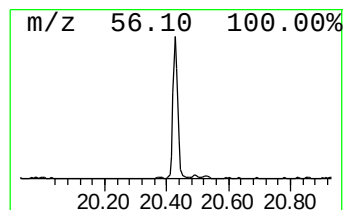
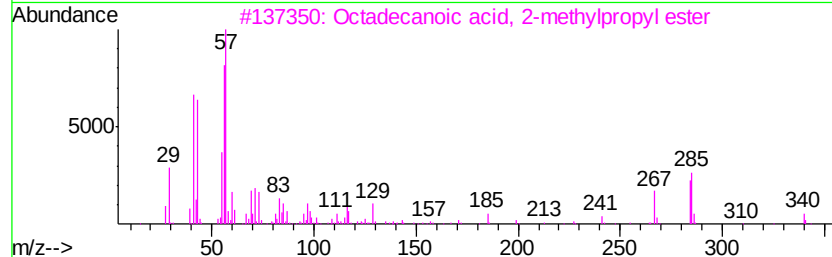
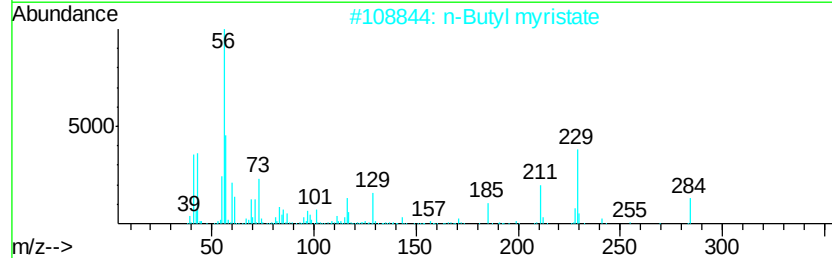
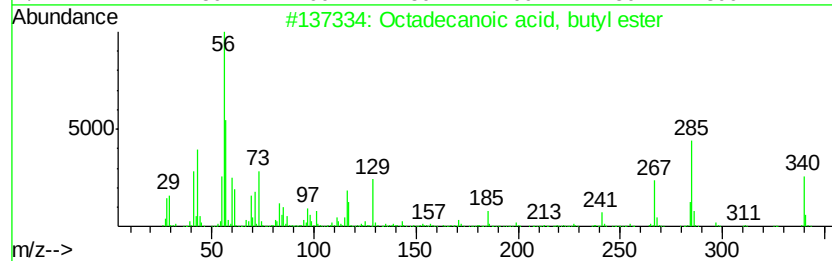
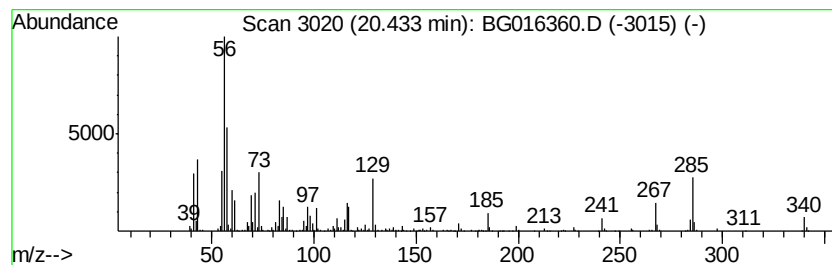
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	8.98 ng	665478	Chrysene-d12	21.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	98
2		n-Butyl myristate	284	C18H36O2	000110-36-1	64
3		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	64
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	27



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016360.D
Acq On : 13 Apr 2015 14:57
Operator : TP/IZ
Sample : G1822-02
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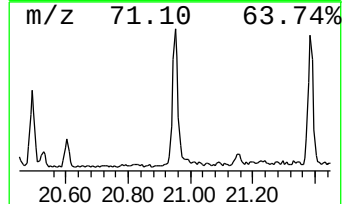
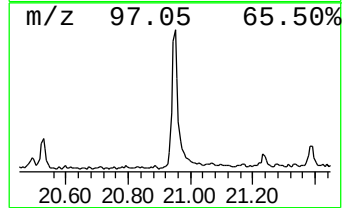
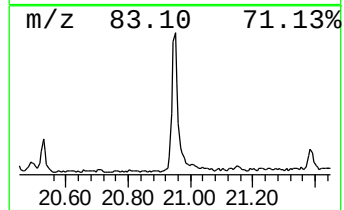
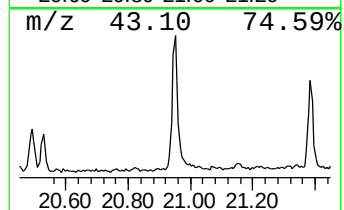
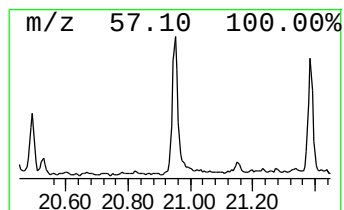
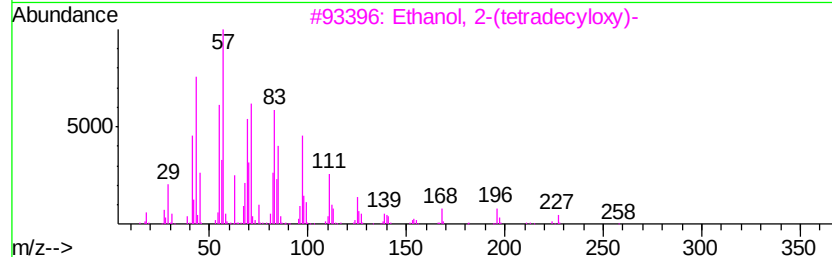
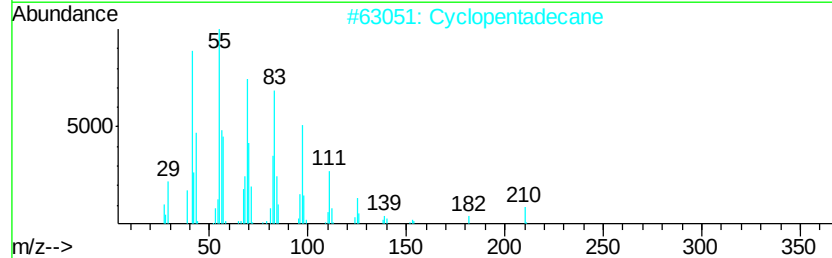
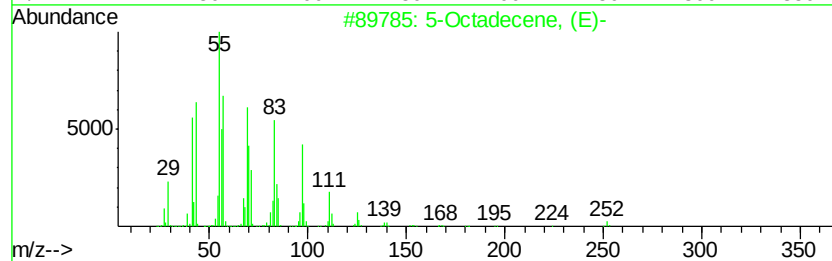
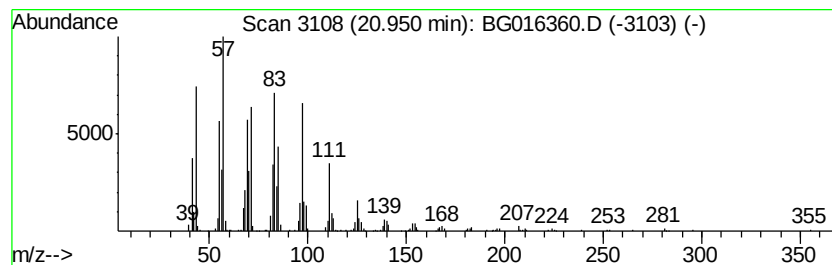
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 5-Octadecene, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.95	4.93 ng	365002	Chrysene-d12	21.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	Cyclopentadecane	210	C15H30	000295-48-7	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	17-Pentatriacontene	491	C35H70	006971-40-0	91
5	1-Docosene	308	C22H44	001599-67-3	90



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
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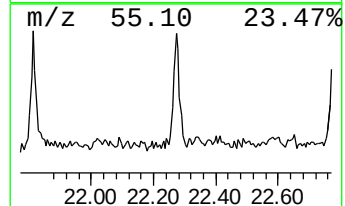
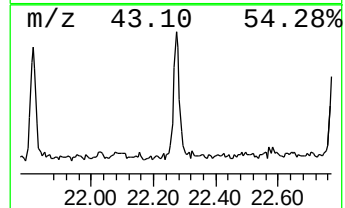
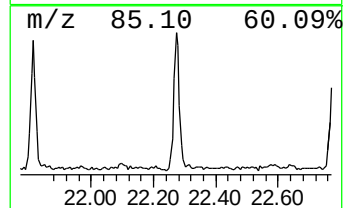
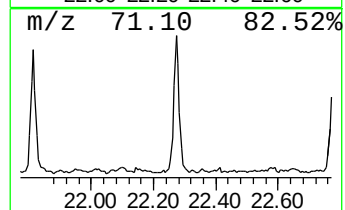
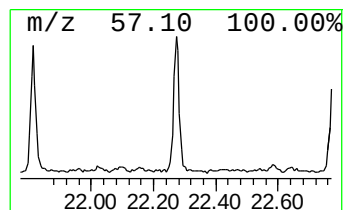
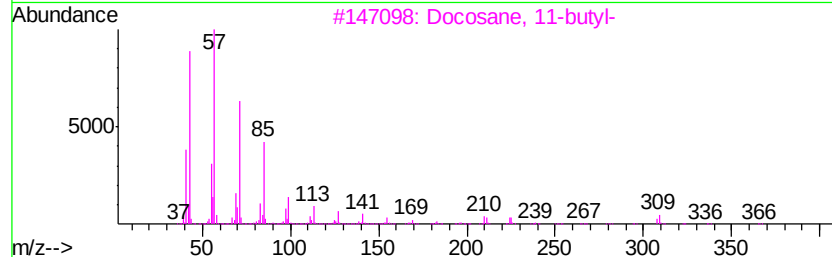
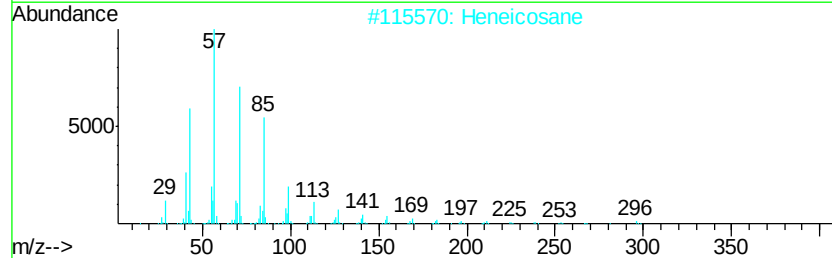
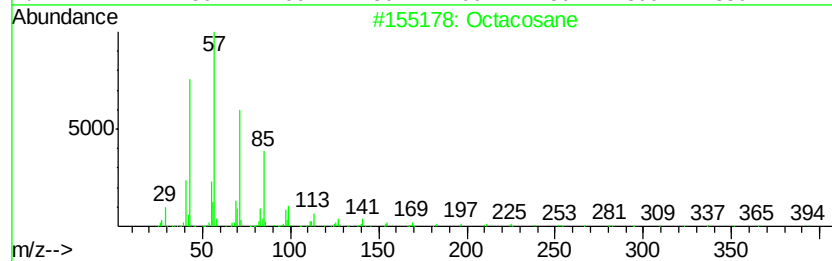
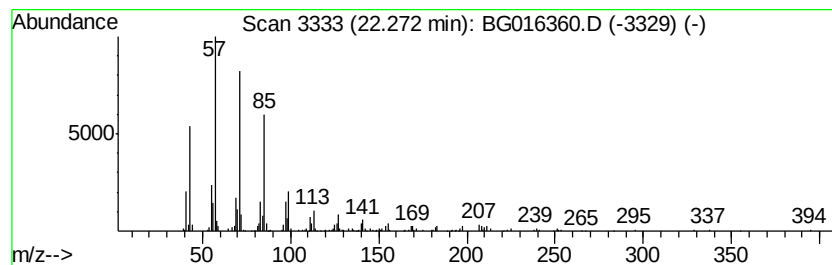
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octacosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.27	2.22 ng	164281	Chrysene-d12	21.24
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octacosane	394	C28H58	000630-02-4 94
2	Heneicosane	296	C21H44	000629-94-7 91
3	Docosane, 11-butyl-	366	C26H54	013475-76-8 91
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9 91
5	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6 91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
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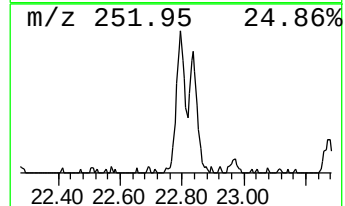
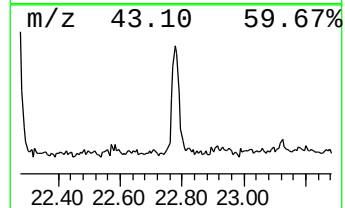
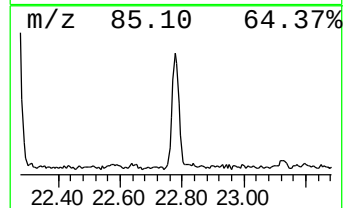
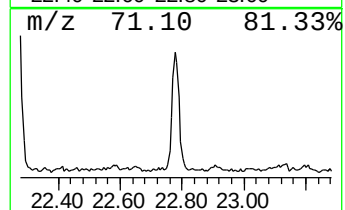
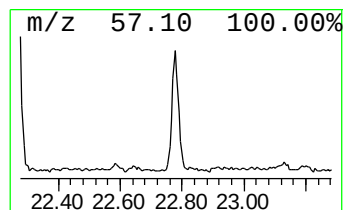
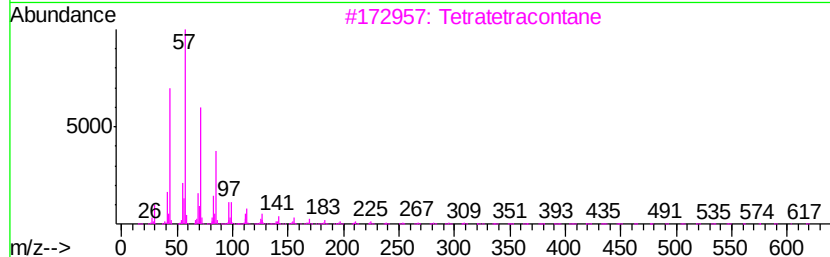
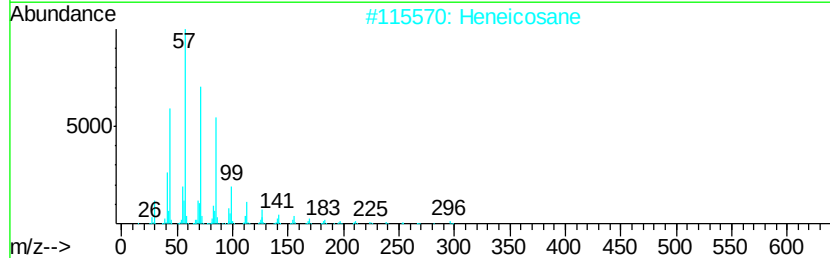
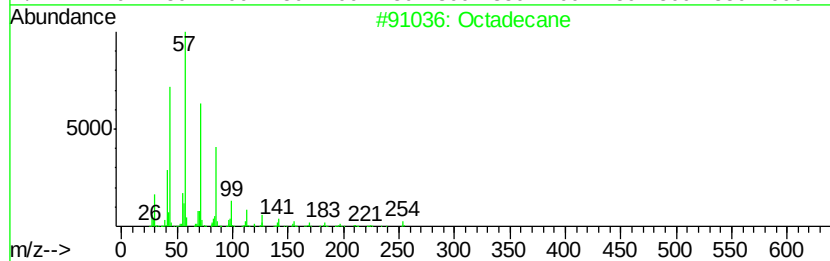
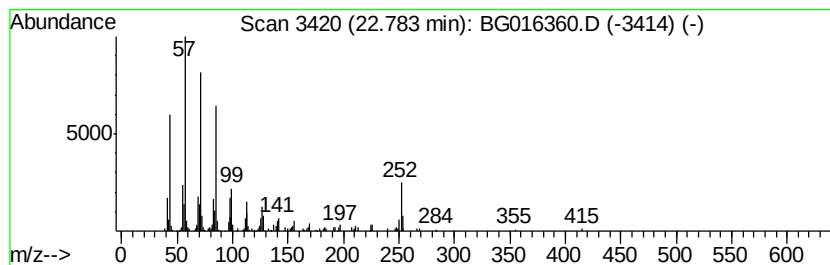
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.78	2.47 ng	174866	Perylene-d12	23.47
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecane	254	C18H38	000593-45-3 95
2	Heneicosane	296	C21H44	000629-94-7 87
3	Tetratetracontane	619	C44H90	007098-22-8 87
4	Heptacosane	380	C27H56	000593-49-7 87
5	Eicosane	282	C20H42	000112-95-8 87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016360.D
Acq On : 13 Apr 2015 14:57
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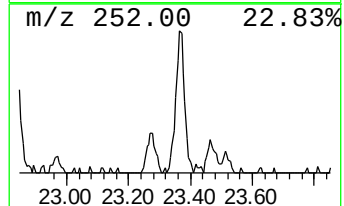
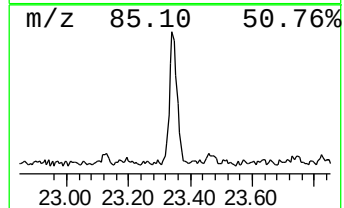
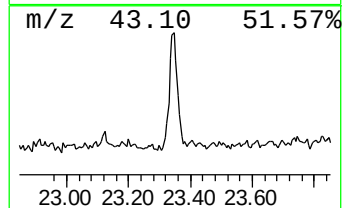
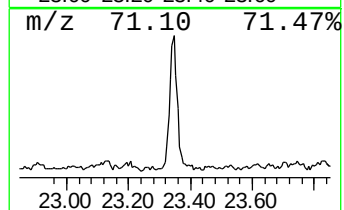
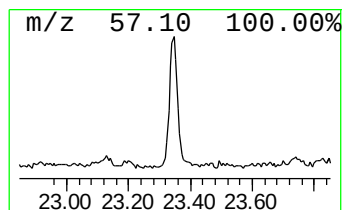
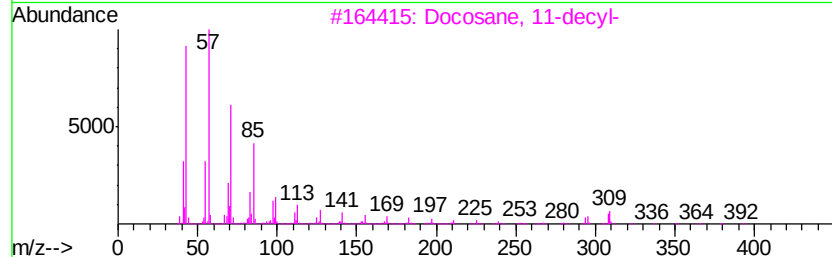
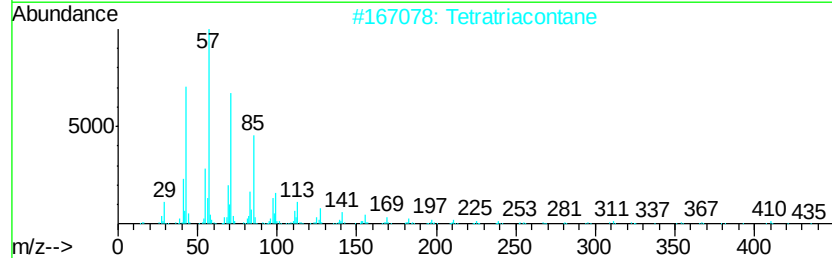
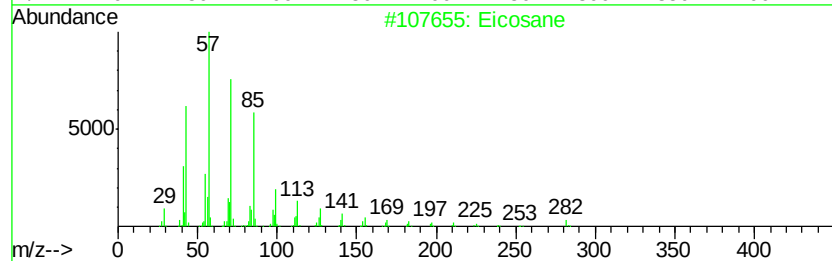
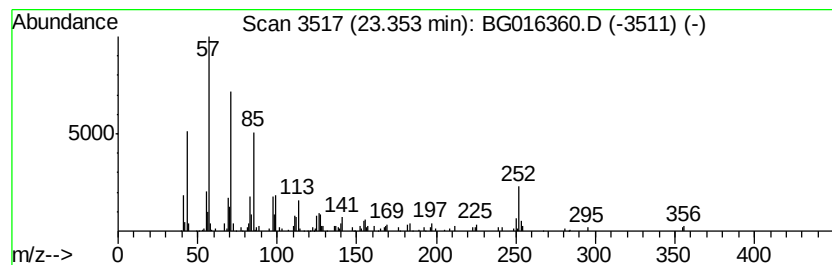
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Eicosane Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.35	2.18 ng	154219	Perylene-d12	23.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Eicosane	282	C20H42	000112-95-8	87
2		Tetratriacontane	479	C34H70	014167-59-0	87
3		Docosane, 11-decyl-	451	C32H66	055401-55-3	87
4		Tetracosane	338	C24H50	000646-31-1	87
5		Hexacosane	366	C26H54	000630-01-3	83



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016360.D
Acq On : 13 Apr 2015 14:57
Operator : TP/IZ
Sample : G1822-02
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F5-025

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	8.8	ng	232418	1	7.67	531190	20.0
unknown4.78	4.78	9.0	ng	238755	1	7.67	531190	20.0
unknown7.21	7.21	72.6	ng	1928670	1	7.67	531190	20.0
unknown7.45	7.45	2.5	ng	66981	1	7.67	531190	20.0
unknown11.78	11.78	3.0	ng	113661	2	10.46	764893	20.0
n-Hexadecanoic acid	17.95	2.0	ng	126418	4	17.06	1239360	20.0
Hexadecanoic acid...	19.39	9.3	ng	688153	5	21.24	1481970	20.0
Octadecanoic acid...	20.43	9.0	ng	665478	5	21.24	1481970	20.0
5-Octadecene, (E)-	20.95	4.9	ng	365002	5	21.24	1481970	20.0
Octacosane	22.27	2.2	ng	164281	5	21.24	1481970	20.0
Octadecane	22.78	2.5	ng	174866	6	23.47	1413650	20.0
Eicosane	23.35	2.2	ng	154219	6	23.47	1413650	20.0