

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051315\
 Data File : BG017111.D
 Acq On : 13 May 2015 17:28
 Operator : TP/IZ
 Sample : G2194-14
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TU021-TW-02

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-BG051315.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.800	12	19	28	rBV	235816	401143	8.59%	1.856%
2	2.876	28	32	41	rVB	595615	713260	15.28%	3.301%
3	4.815	357	362	367	rBV2	33808	49591	1.06%	0.229%
4	5.303	438	445	455	rBV	555172	795180	17.03%	3.680%
5	6.907	711	718	725	rBV	382540	568782	12.18%	2.632%
6	7.247	770	776	784	rBV	1005395	1571111	33.66%	7.271%
7	7.711	848	855	862	rVB	198262	322162	6.90%	1.491%
8	8.029	901	909	916	rBV	803353	1281822	27.46%	5.932%
9	8.869	1045	1052	1060	rBV	789979	1272488	27.26%	5.889%
10	10.502	1324	1330	1336	rBV	270637	456117	9.77%	2.111%
11	12.712	1701	1706	1713	rBV	55513	87580	1.88%	0.405%
12	12.982	1743	1752	1760	rBV	1948581	2922199	62.60%	13.523%
13	14.363	1979	1987	1993	rBV3	439917	659027	14.12%	3.050%
14	15.861	2235	2242	2254	rBV	1791692	2609977	55.91%	12.078%
15	17.112	2448	2455	2461	rBV	583006	820561	17.58%	3.797%
16	18.011	2604	2608	2614	rBV	175158	244482	5.24%	1.131%
17	19.298	2823	2827	2834	rBV2	92630	122317	2.62%	0.566%
18	19.744	2897	2903	2910	rBV	3796096	4668166	100.00%	21.603%
19	21.008	3115	3118	3124	rBV4	102432	128426	2.75%	0.594%
20	21.213	3145	3153	3156	rBV	50648	71710	1.54%	0.332%
21	21.296	3161	3167	3172	rBV	727045	885648	18.97%	4.099%
22	22.482	3365	3369	3374	rVB	93006	128229	2.75%	0.593%
23	23.564	3545	3553	3560	rBV2	427700	829009	17.76%	3.836%

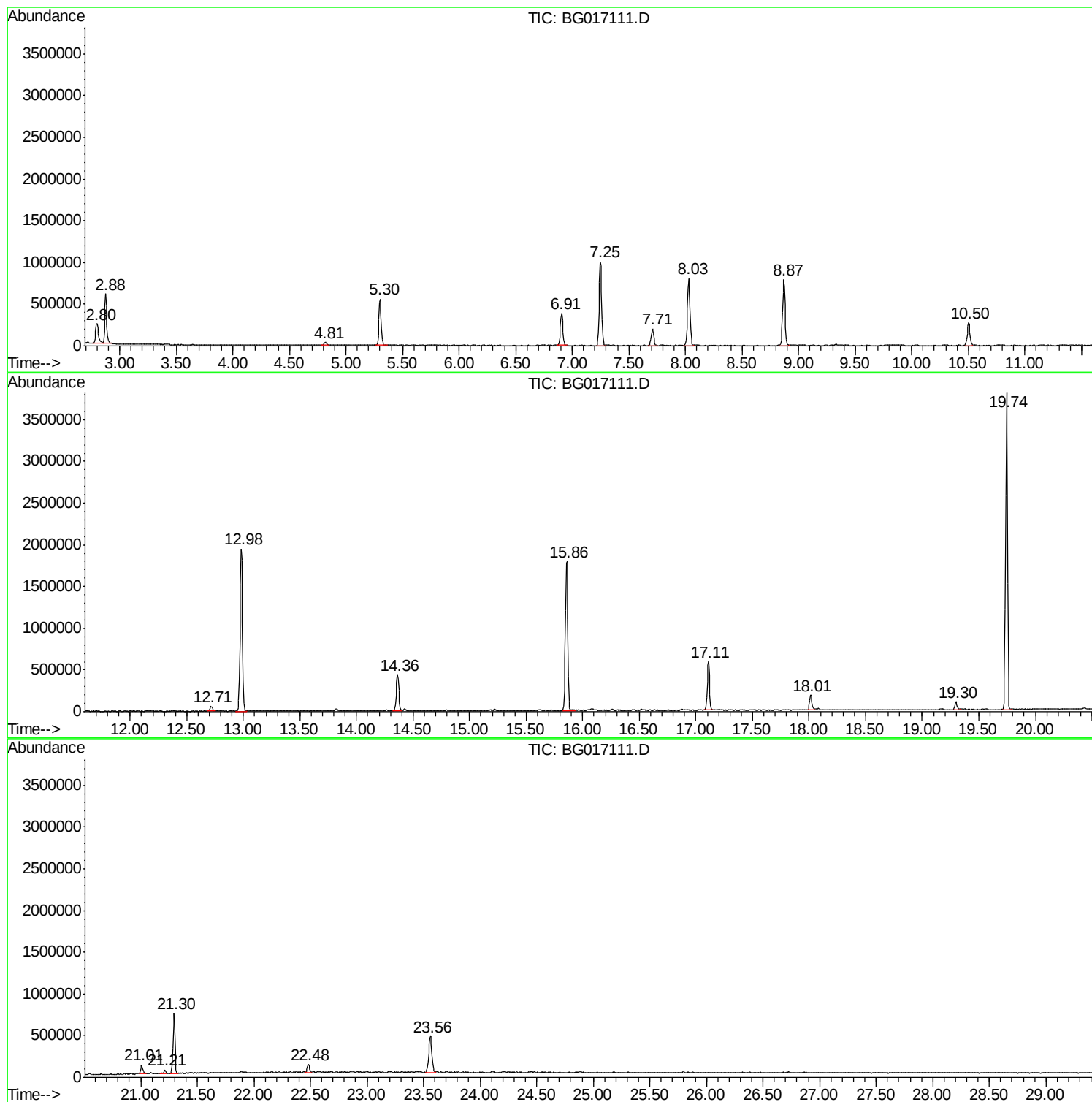
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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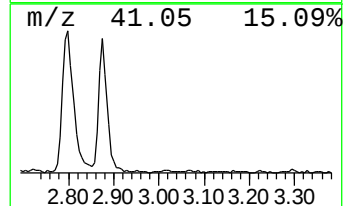
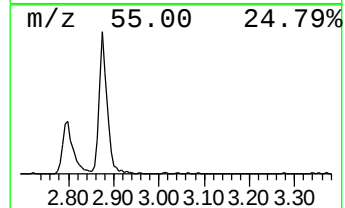
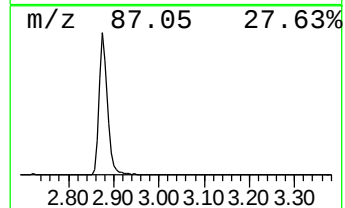
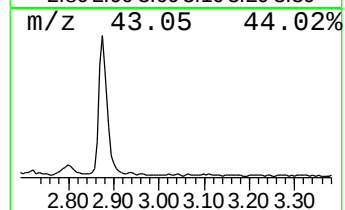
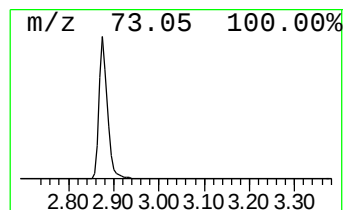
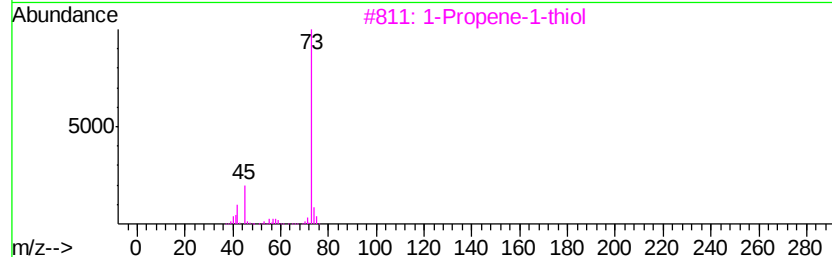
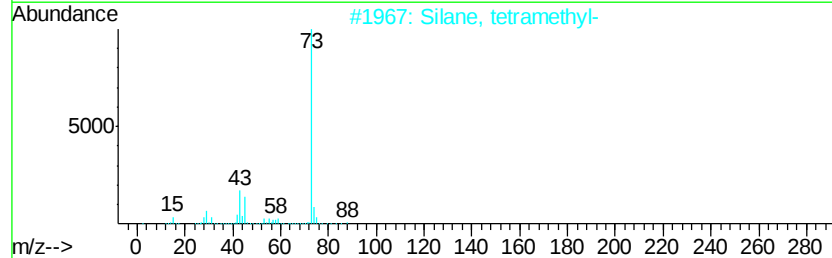
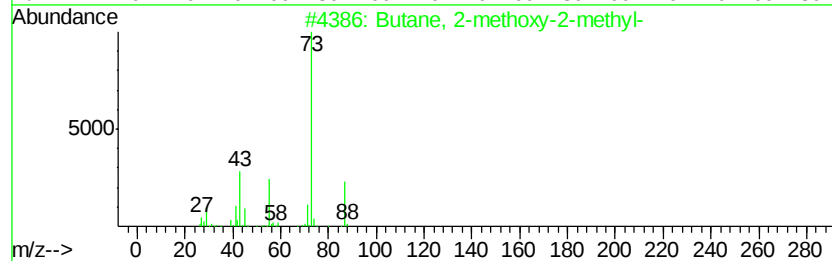
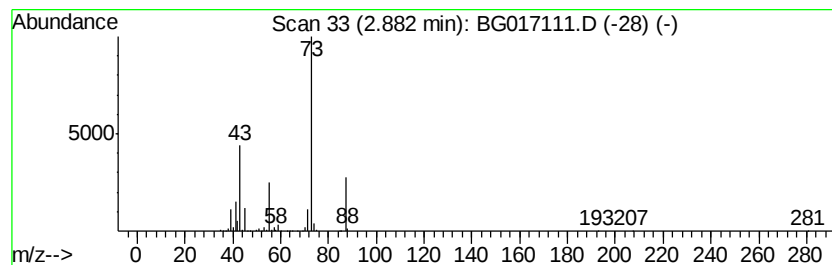
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	44.28 ng	713260	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
3		1-Propene-1-thiol	74	C3H6S	000925-89-3	12
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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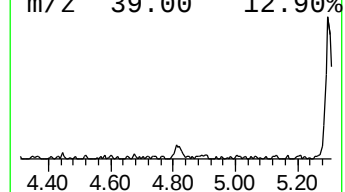
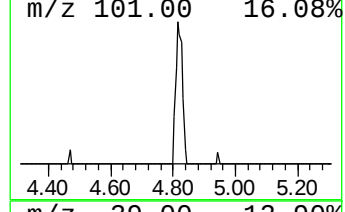
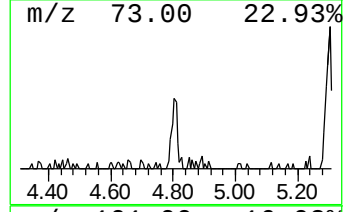
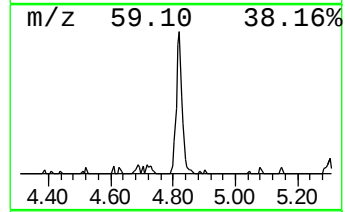
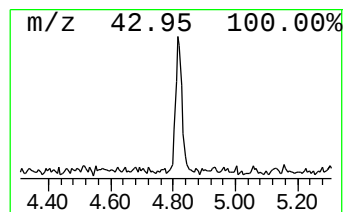
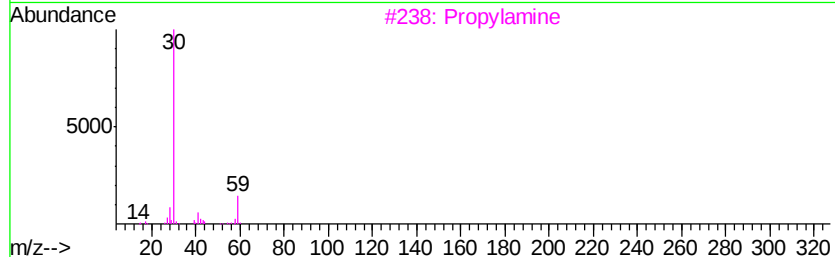
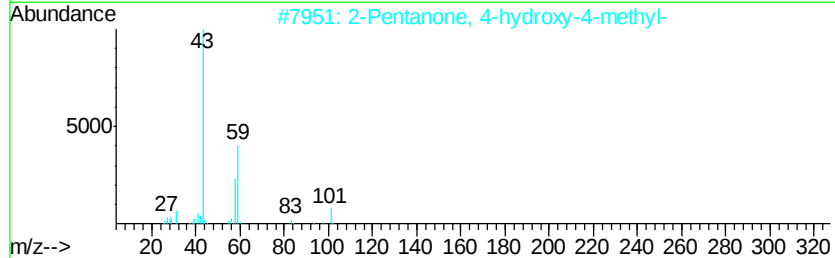
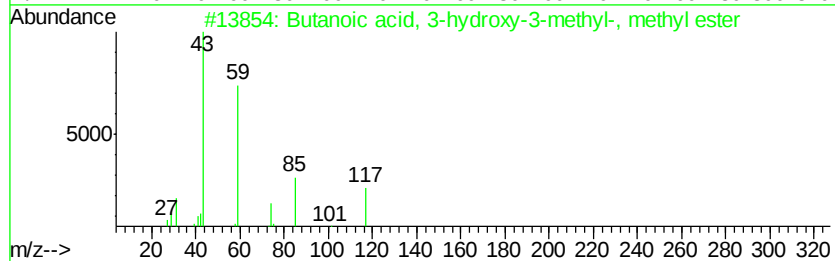
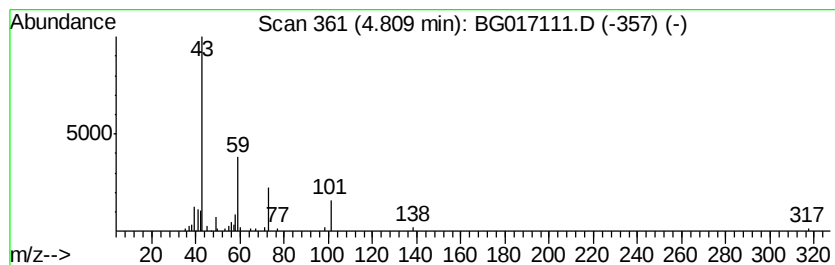
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown4.81 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.81	3.08 ng	49591	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 3-hydroxy-3-methyl...	132	C6H12O3	006149-45-7	38
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	36
3		Propylamine	59	C3H9N	000107-10-8	9
4		Diacetamide	101	C4H7NO2	000625-77-4	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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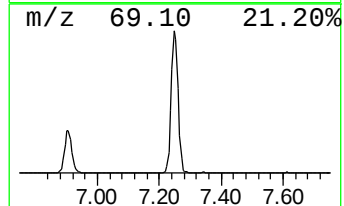
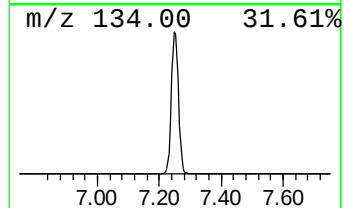
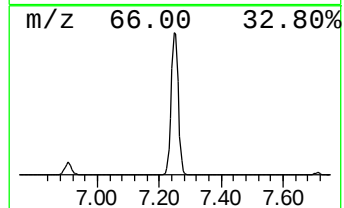
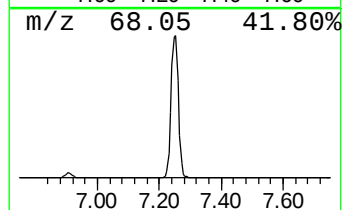
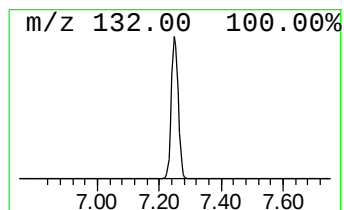
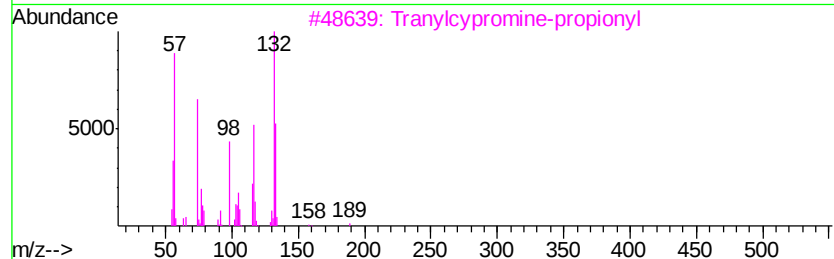
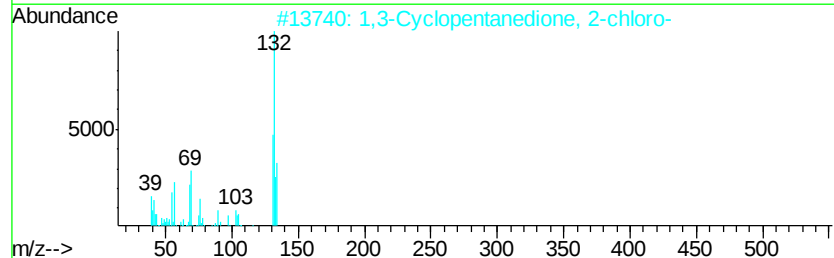
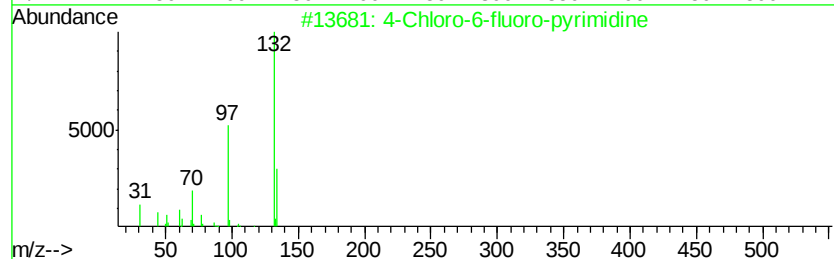
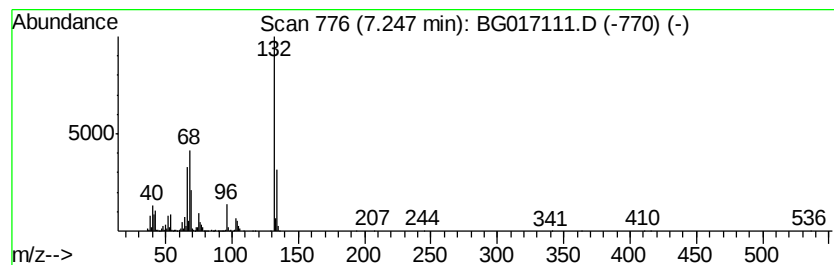
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 4 unknown7.25 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.25	97.54 ng	1571110	1,4-Dichlorobenzene-d4	7.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	12



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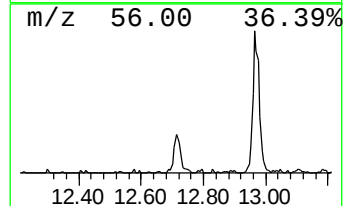
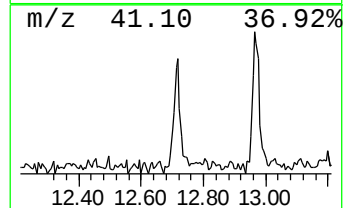
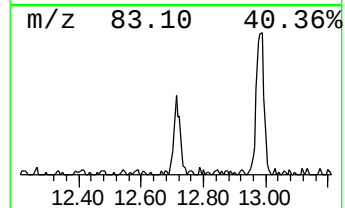
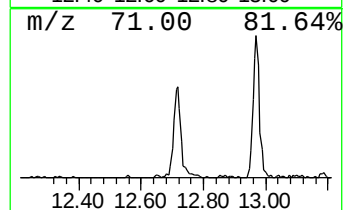
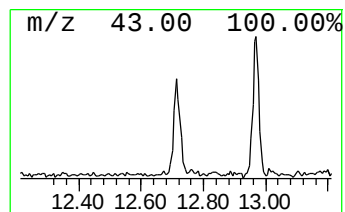
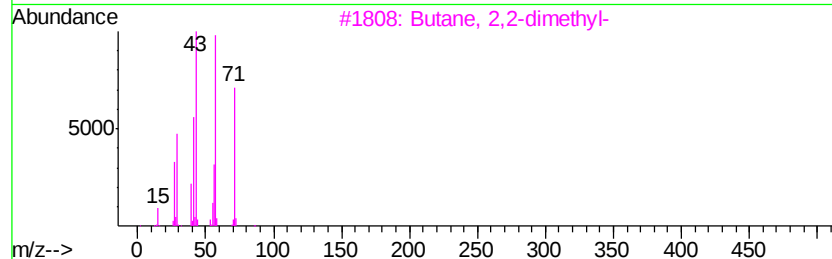
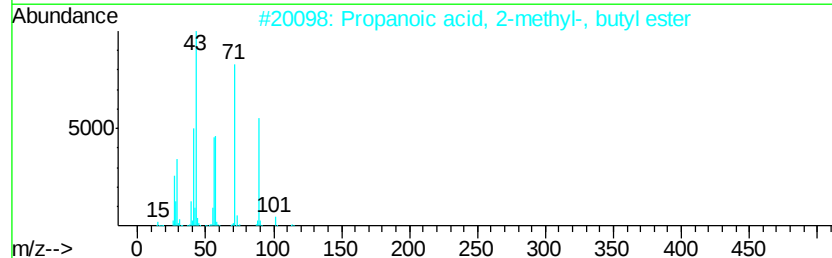
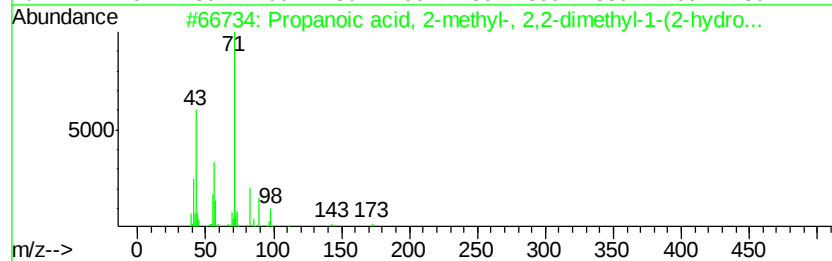
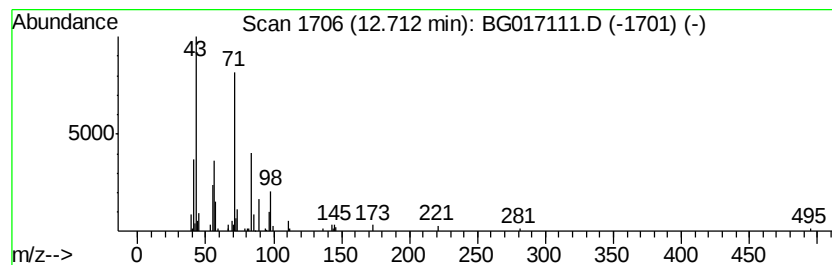
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	2.66 ng	87580	Acenaphthene-d10	14.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	53
2		Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	43
3		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
4		Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	38
5		1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	37



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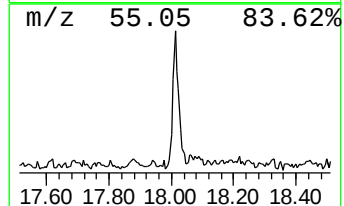
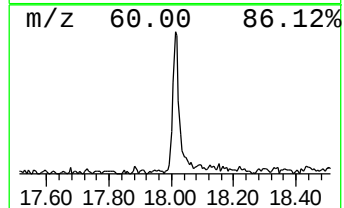
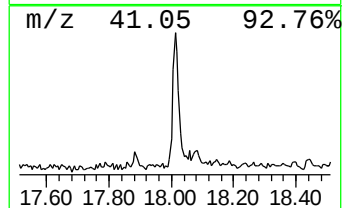
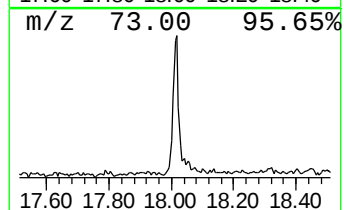
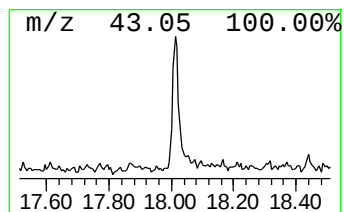
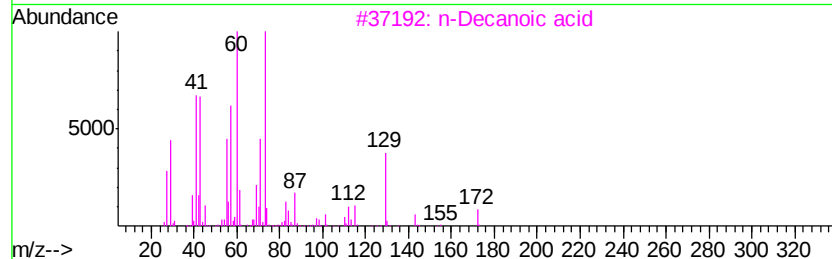
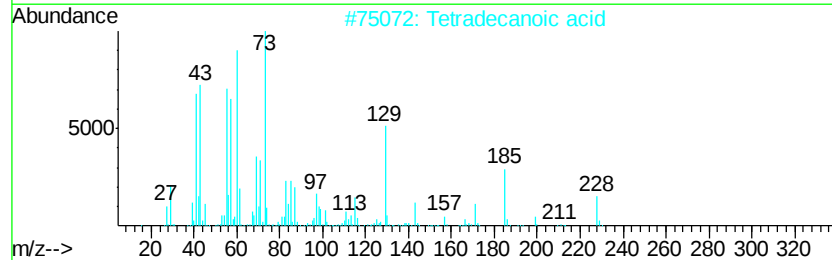
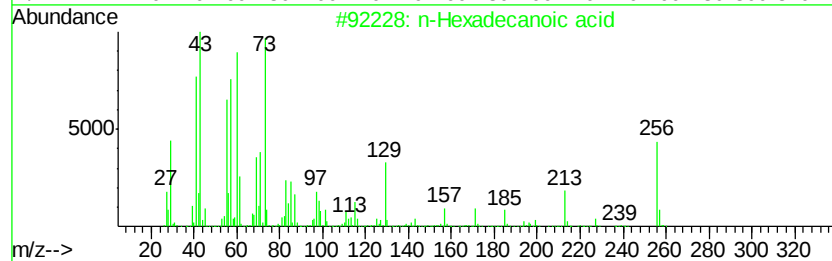
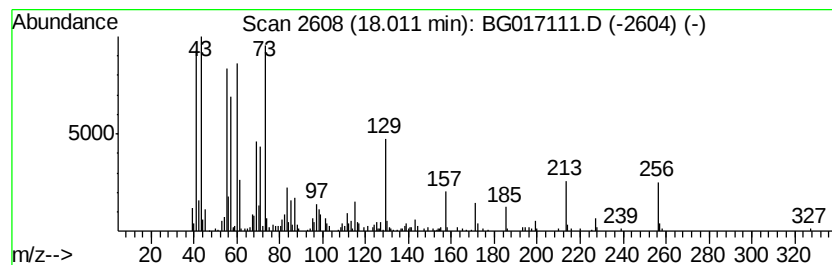
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.01	5.96 ng	244482	Phenanthrene-d10	17.11	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	n-Decanoic acid	172	C10H20O2	000334-48-5	62
4	4-Oxazolidinone, 2-hydroxy-3-met...	201	C10H19NO3	056440-43-8	35
5	Heptanoic acid	130	C7H14O2	000111-14-8	27



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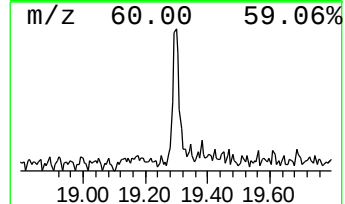
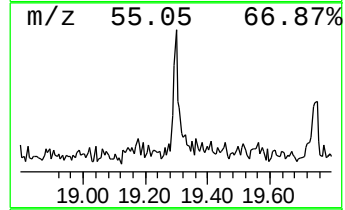
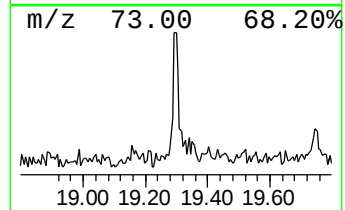
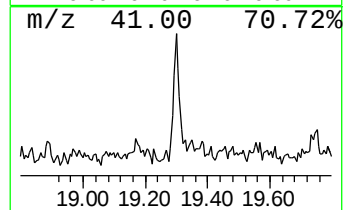
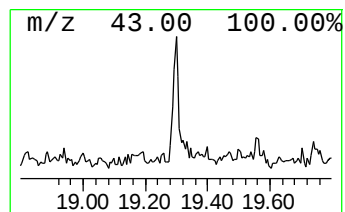
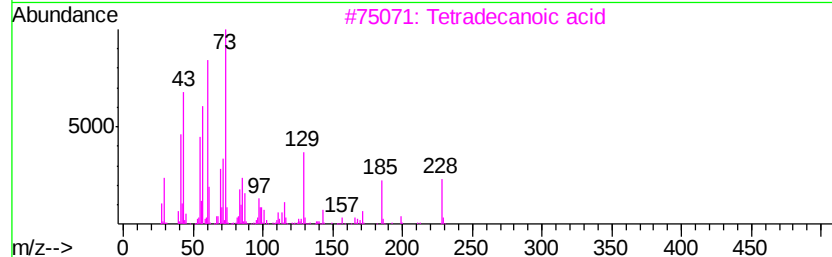
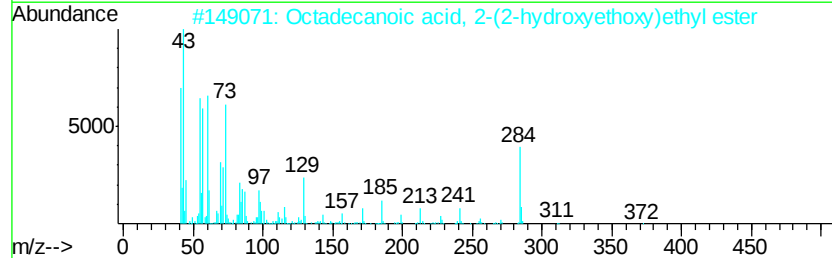
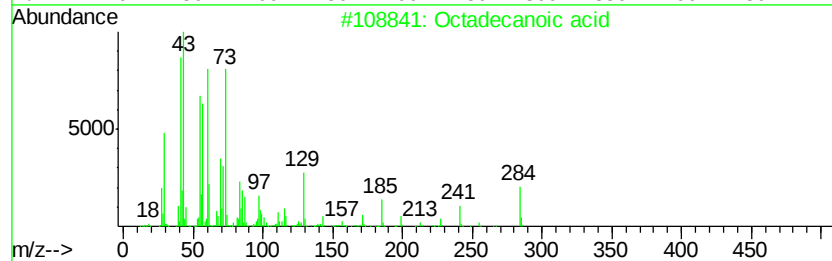
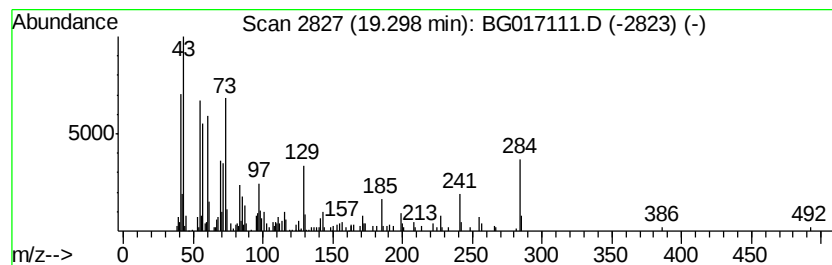
Instrument :
BNA_G
ClientSampleId :
TU021-TW-02

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

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

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.30	2.76 ng	122317	Chrysene-d12	21.30
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Octadecanoic acid	284 C18H36O2	000057-11-4	93
2	Octadecanoic acid, 2-(2-hydroxye...	372 C22H44O4	000106-11-6	50
3	Tetradecanoic acid	228 C14H28O2	000544-63-8	43
4	n-Decanoic acid	172 C10H20O2	000334-48-5	42
5	Pentadecanoic acid	242 C15H30O2	001002-84-2	42



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051315\
Data File : BG017111.D
Acq On : 13 May 2015 17:28
Operator : TP/IZ
Sample : G2194-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TU021-TW-02

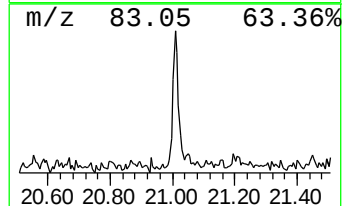
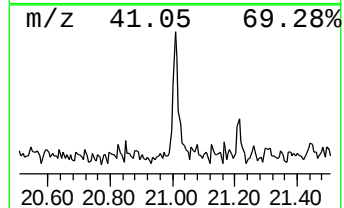
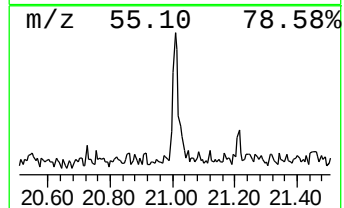
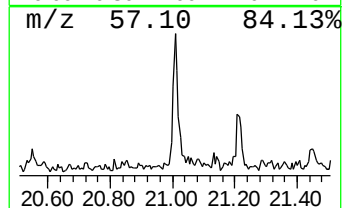
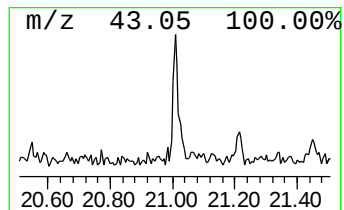
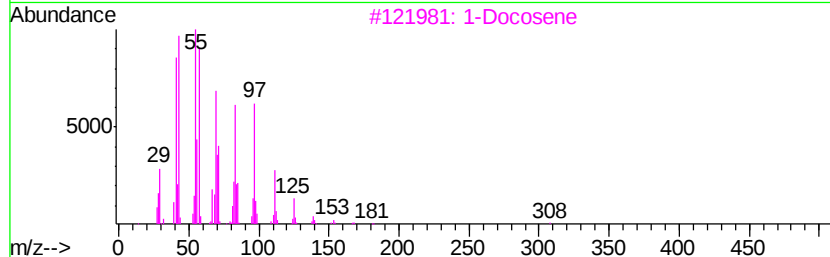
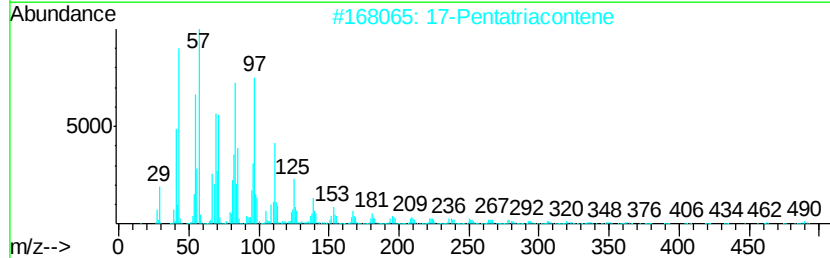
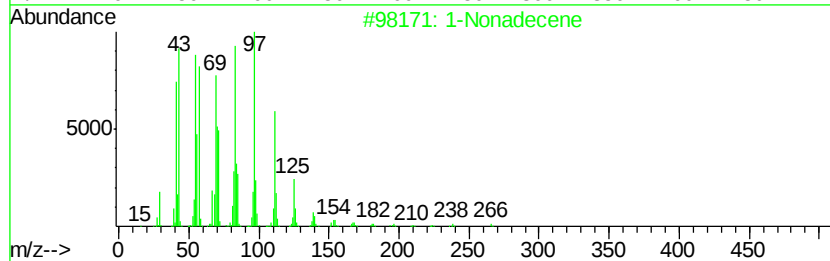
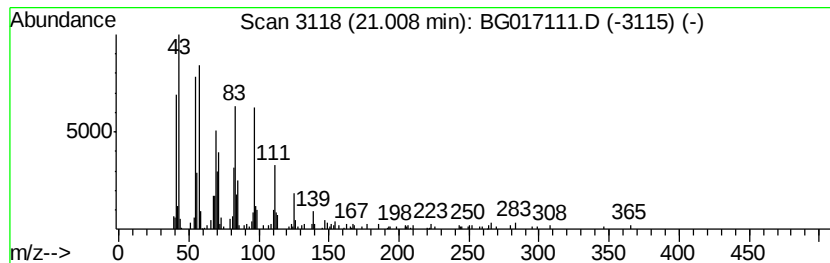
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Nonadecene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.01	2.90 ng	128426	Chrysene-d12	21.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Nonadecene	266	C19H38	018435-45-5	97
2		17-Pentatriacontene	491	C35H70	006971-40-0	91
3		1-Docosene	308	C22H44	001599-67-3	91
4		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	91
5		Acetic acid, trifluoro-, hexadec...	338	C18H33F3O2	006222-03-3	87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG051315\
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Acq On : 13 May 2015 17:28
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Sample : G2194-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TU021-TW-02

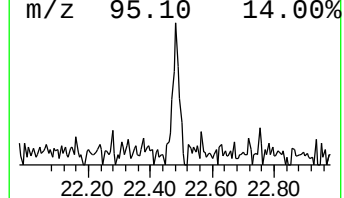
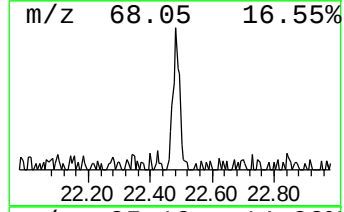
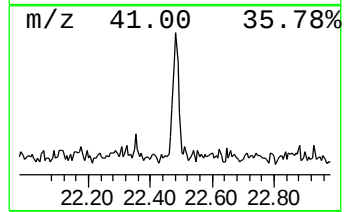
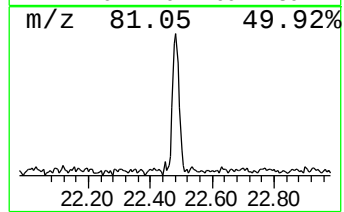
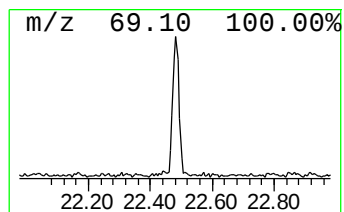
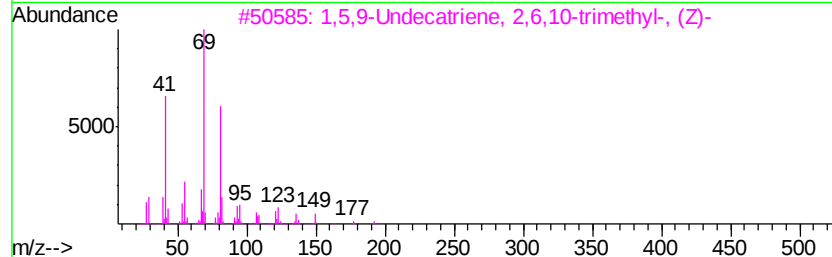
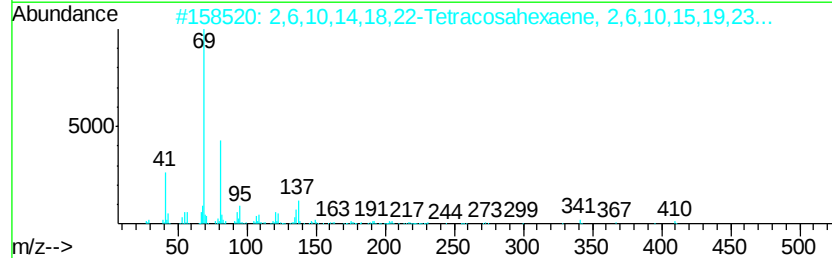
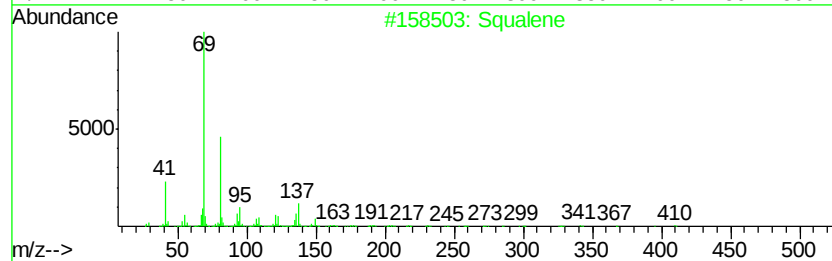
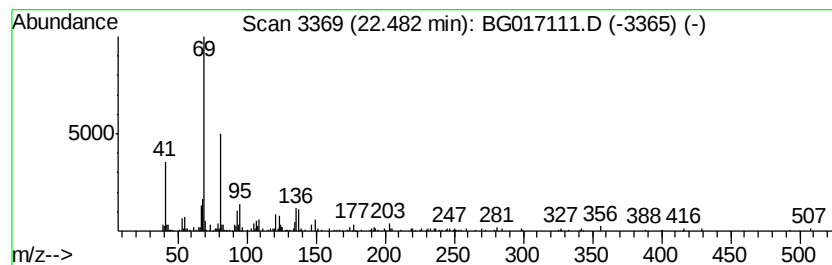
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG051315.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.48	3.09 ng	128229	Perylene-d12	23.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	83
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	80
3		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	76
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64



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Acq On : 13 May 2015 17:28
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Sample : G2194-14
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TU021-TW-02

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

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.88	44.3	ng	713260	1	7.71	322162	20.0
unknown4.81	4.81	3.1	ng	49591	1	7.71	322162	20.0
unknown7.25	7.25	97.5	ng	1571110	1	7.71	322162	20.0
Propanoic acid, 2...	12.71	2.7	ng	87580	3	14.36	659027	20.0
n-Hexadecanoic acid	18.01	6.0	ng	244482	4	17.11	820561	20.0
Octadecanoic acid	19.30	2.8	ng	122317	5	21.30	885648	20.0
1-Nonadecene	21.01	2.9	ng	128426	5	21.30	885648	20.0
Squalene	22.48	3.1	ng	128229	6	23.56	829009	20.0