

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
 Data File : BG017966.D
 Acq On : 19 Jul 2015 20:34
 Operator : TP/UM
 Sample : G2975-01
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 AB-SLOPE-FAIL-1(0-2)

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-BG071715.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	2.782	13	16	21	rBV3	38782	66172	1.34%	0.176%
2	2.864	25	30	35	rBV	630999	776079	15.71%	2.063%
3	2.905	35	37	43	rVB2	44134	53385	1.08%	0.142%
4	4.151	244	249	256	rBV	65580	91627	1.85%	0.244%
5	4.738	342	349	358	rVB	1180392	1658375	33.57%	4.409%
6	5.196	420	427	438	rBV	1844140	2660556	53.85%	7.073%
7	5.796	523	529	536	rBV	118534	169443	3.43%	0.450%
8	6.771	687	695	712	rVB	1880895	2903875	58.78%	7.720%
9	7.123	747	755	765	rBV	1894797	3061801	61.97%	8.140%
10	7.582	827	833	843	rVB	326486	525411	10.63%	1.397%
11	7.905	880	888	896	rBV	1343710	2166383	43.85%	5.760%
12	8.739	1022	1030	1038	rBV	1109464	1800587	36.45%	4.787%
13	10.361	1299	1306	1314	rVB	463320	787288	15.94%	2.093%
14	12.858	1724	1731	1738	rBV	2648422	3982881	80.62%	10.589%
15	13.704	1868	1875	1885	rVB	576438	809835	16.39%	2.153%
16	14.245	1960	1967	1975	rBV2	720354	1104701	22.36%	2.937%
17	15.079	2101	2109	2112	rBV2	37987	84115	1.70%	0.224%
18	15.737	2215	2221	2230	rBV	2059582	2964488	60.00%	7.881%
19	15.978	2258	2262	2274	rBV	51591	93756	1.90%	0.249%
20	16.771	2392	2397	2402	rBV2	67721	90871	1.84%	0.242%
21	16.994	2429	2435	2445	rBV2	916320	1296302	26.24%	3.446%
22	17.394	2496	2503	2514	rBV	216320	338710	6.86%	0.900%
23	17.511	2519	2523	2528	rVB	76954	89424	1.81%	0.238%
24	17.911	2587	2591	2597	rBV2	123148	187286	3.79%	0.498%
25	18.205	2636	2641	2646	rBV	56406	72562	1.47%	0.193%
26	18.340	2660	2664	2669	rBV2	115173	136291	2.76%	0.362%
27	18.775	2733	2738	2747	rBV	648189	845806	17.12%	2.249%
28	19.068	2782	2788	2797	rBV8	17501	50546	1.02%	0.134%
29	19.203	2807	2811	2817	rBV6	34033	56432	1.14%	0.150%
30	19.644	2879	2886	2897	rBV	3938034	4940439	100.00%	13.135%
31	20.296	2993	2997	3003	rBV	63660	80157	1.62%	0.213%
32	20.919	3099	3103	3112	rBV	133364	207201	4.19%	0.551%
33	21.195	3144	3150	3158	rBV	1160959	1452545	29.40%	3.862%
34	22.376	3346	3351	3361	rVB	387309	529410	10.72%	1.407%

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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

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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.410	3520	3527	3540	rVB	749171	1420895	28.76%	3.778%
36	24.697	3741	3746	3747	rBV5	39742	57952	1.17%	0.154%

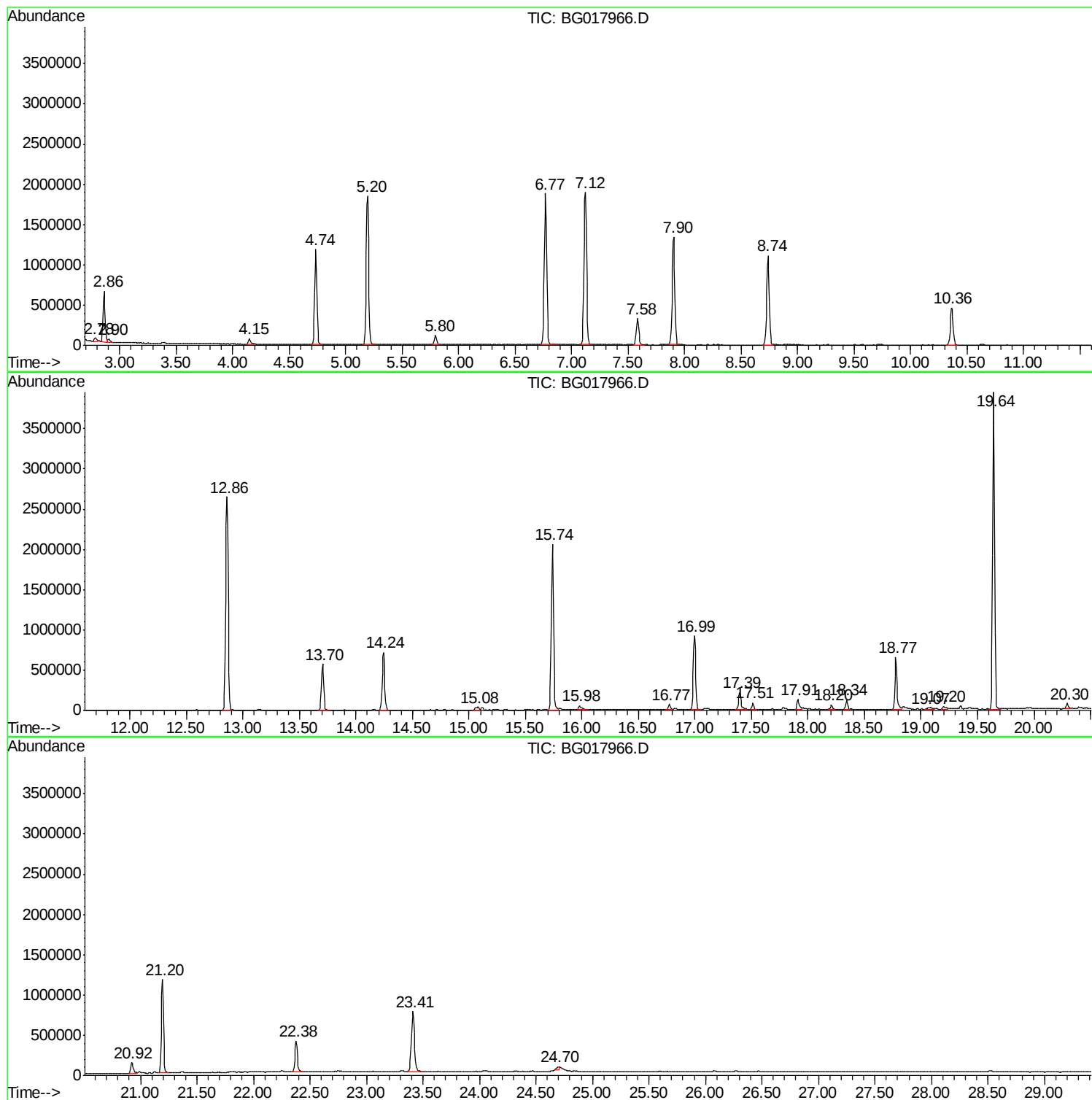
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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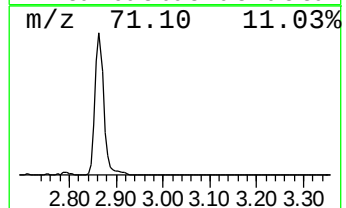
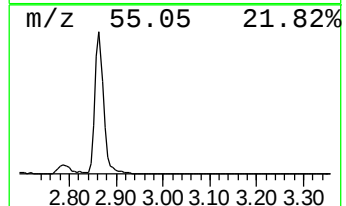
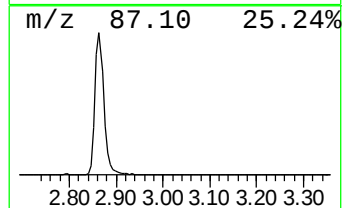
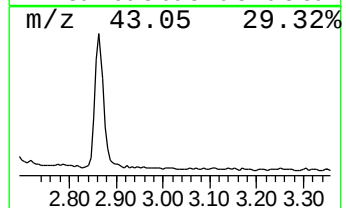
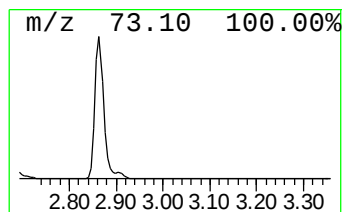
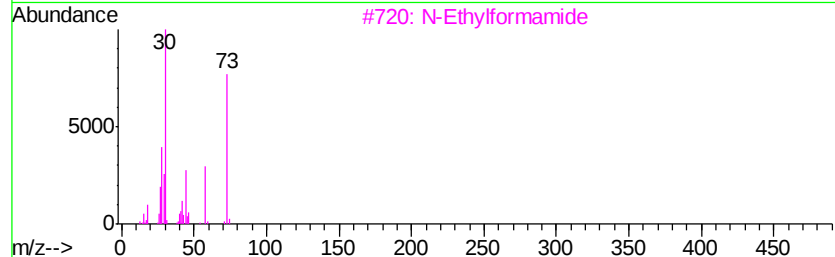
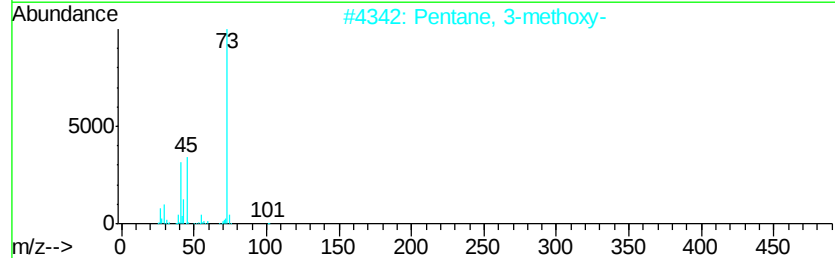
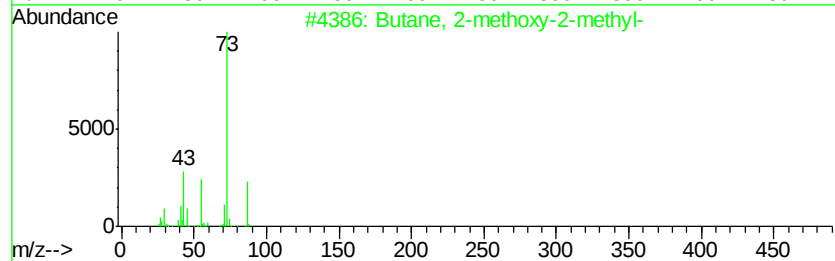
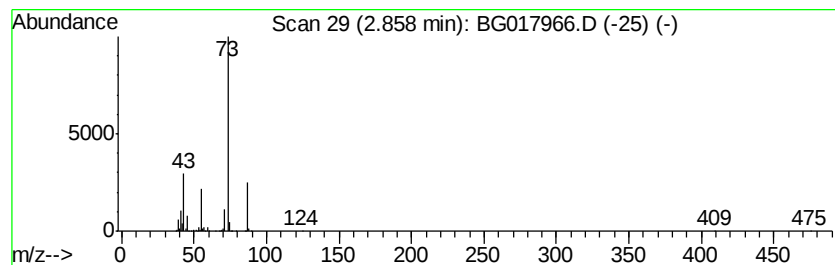
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	29.54 ng	776079	1,4-Dichlorobenzene-d4	7.59

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86	
2	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23	
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9	
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9	
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9	



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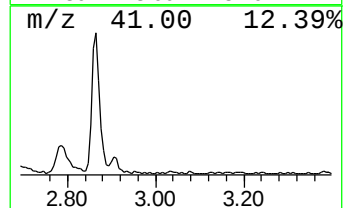
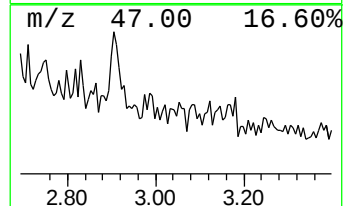
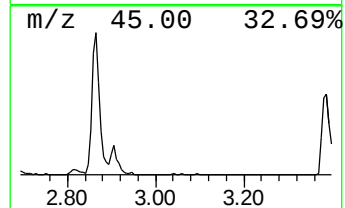
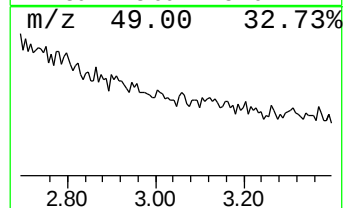
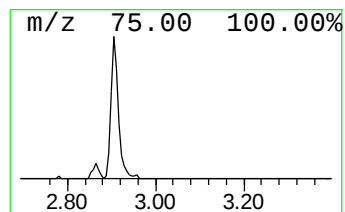
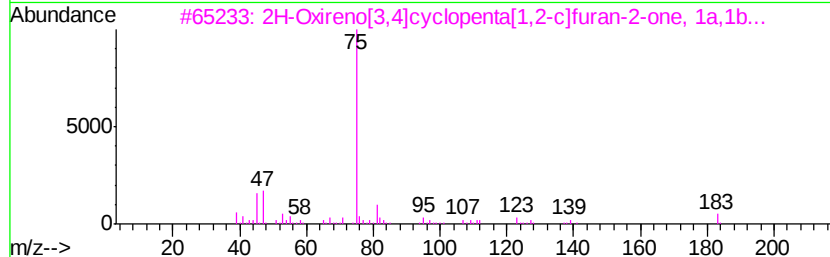
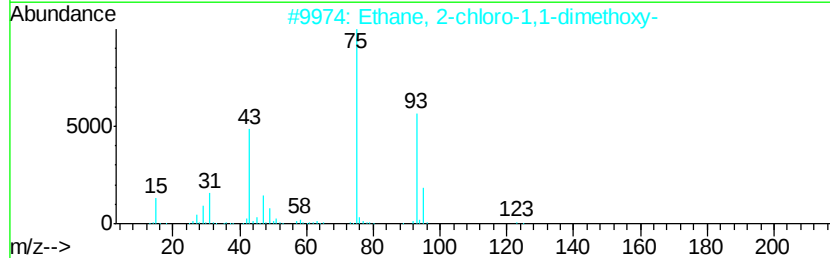
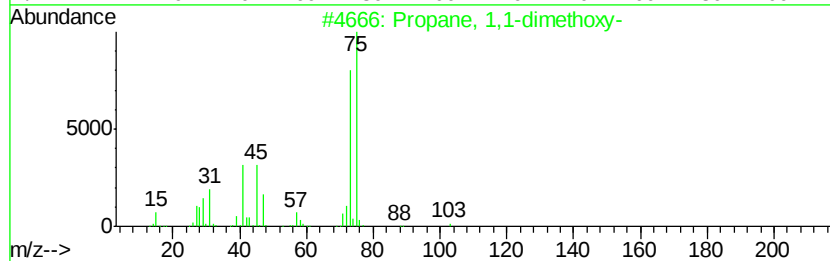
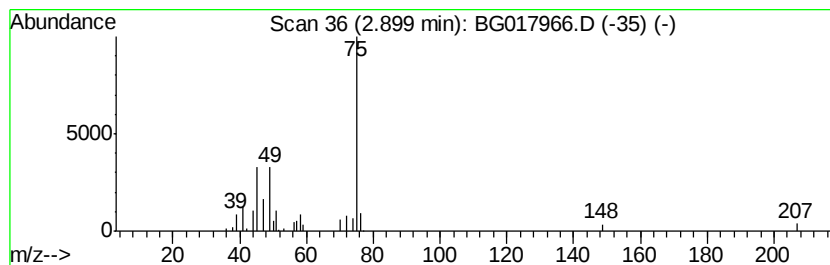
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.90	2.03 ng	53385	1,4-Dichlorobenzene-d4	7.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	56
2		Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	38
3		2H-Oxireno[3,4]cyclopenta[1,2-c]...	214	C10H14O5	1000141-74-6	9
4		Propane, 3-chloro-1,1-dimethoxy-	138	C5H11ClO2	035502-06-8	9
5		Silanol, trimethyl-	90	C3H10OSi	001066-40-6	9



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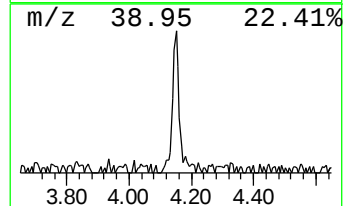
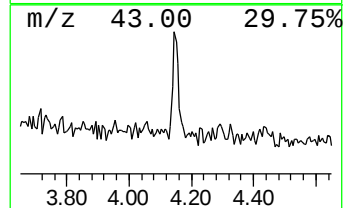
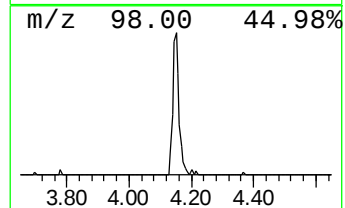
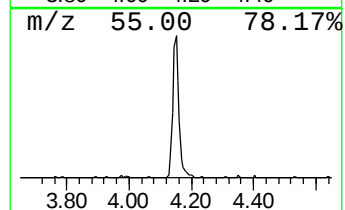
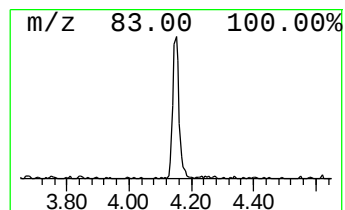
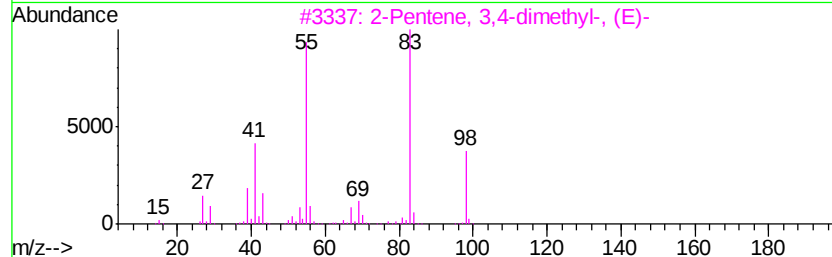
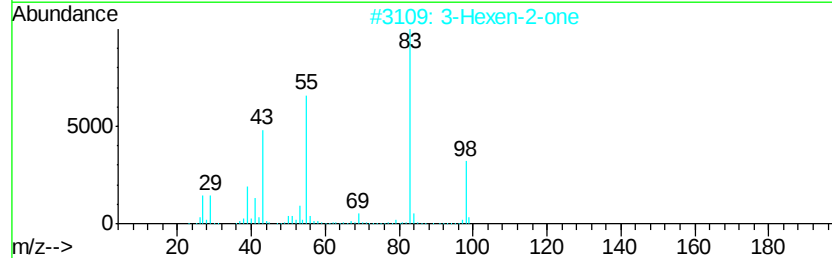
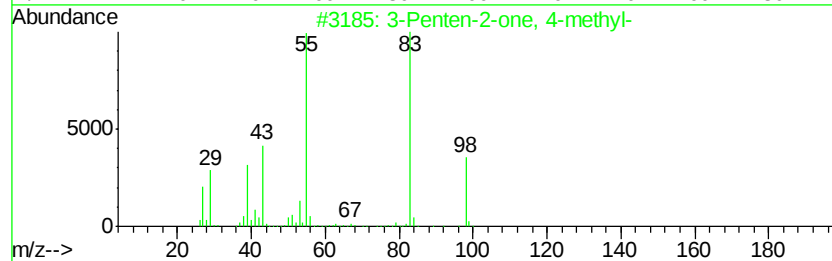
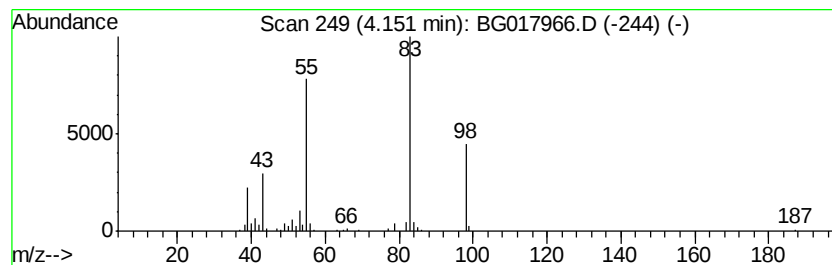
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.15	3.49 ng	91627	1,4-Dichlorobenzene-d4	7.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2			3-Hexen-2-one	98	C6H10O	000763-93-9	86
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	78
5			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	78



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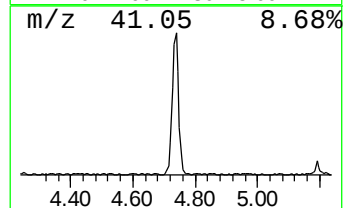
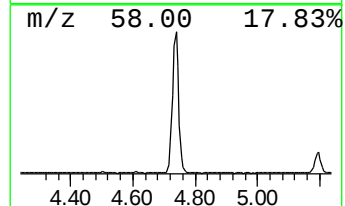
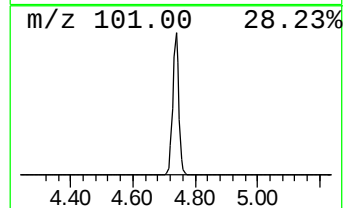
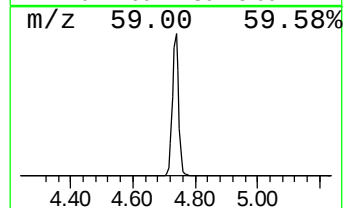
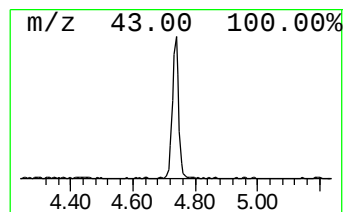
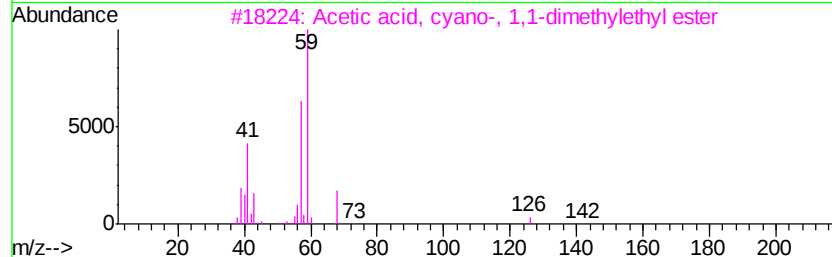
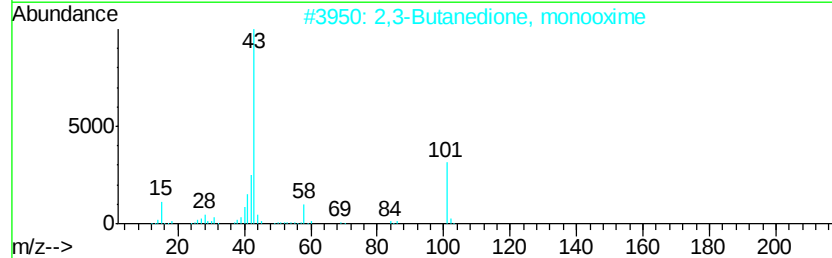
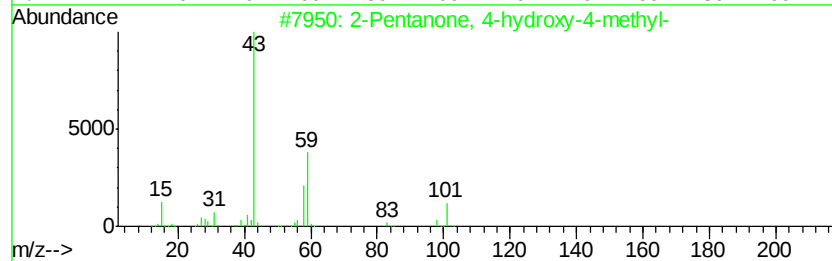
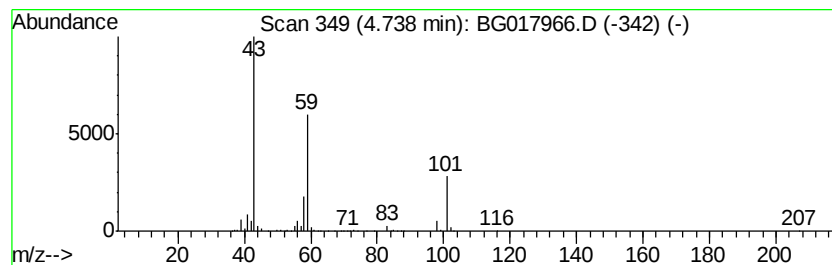
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	63.13 ng	1658380	1,4-Dichlorobenzene-d4	7.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		Acetone	58	C3H6O	000067-64-1	10
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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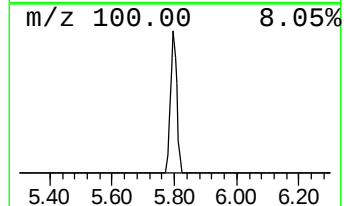
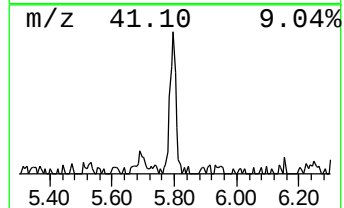
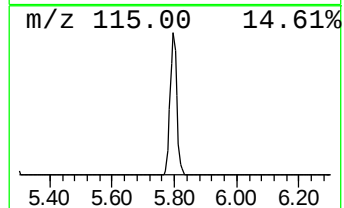
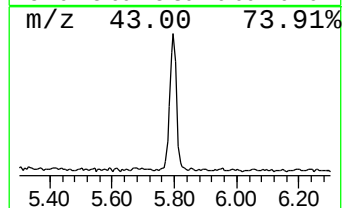
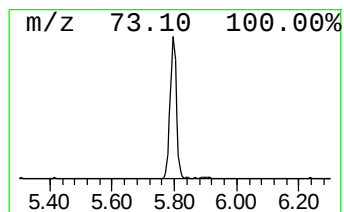
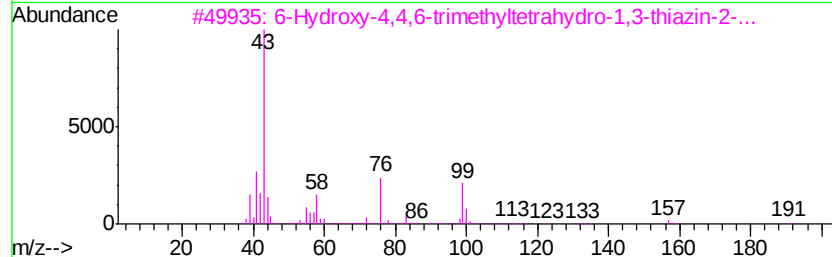
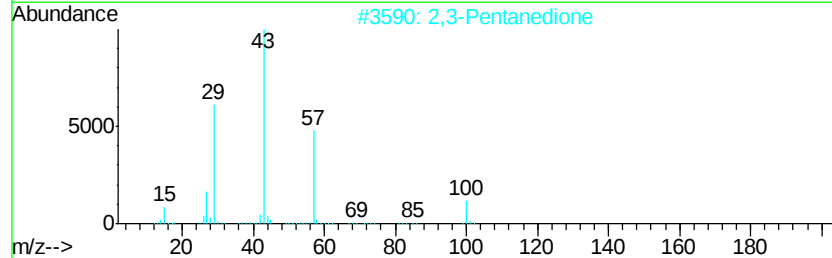
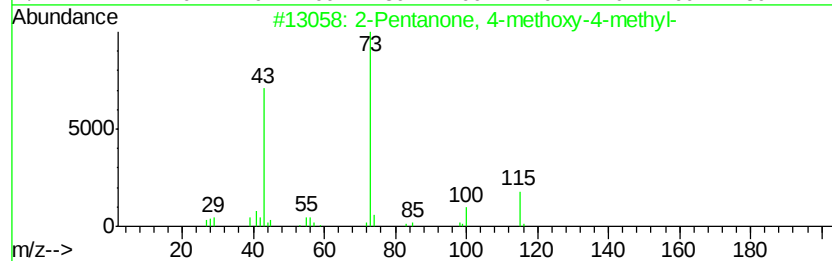
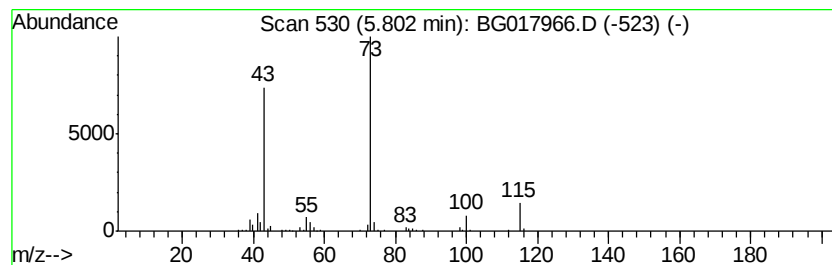
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-methoxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.80	6.45 ng	169443	1,4-Dichlorobenzene-d4	7.59

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		2,3-Pentanedione	100	C5H8O2	000600-14-6	22
3		6-Hydroxy-4,4,6-trimethyltetrahy...	191	C7H13NO2	016504-29-3	12
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		Methyl Isobutyl Ketone	100	C6H12O	000108-10-1	12



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017966.D
Acq On : 19 Jul 2015 20:34
Operator : TP/UM
Sample : G2975-01
Misc :
ALS Vial : 42 Sample Multiplier: 1

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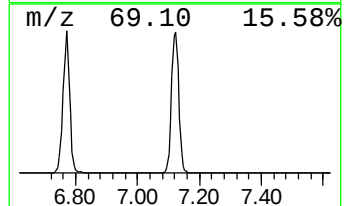
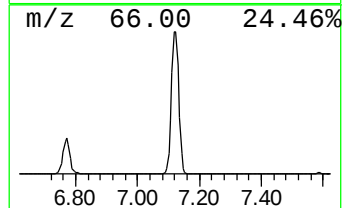
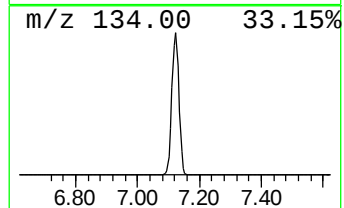
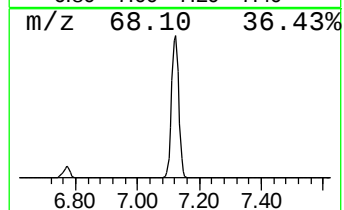
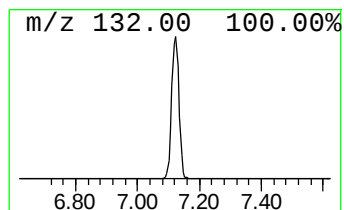
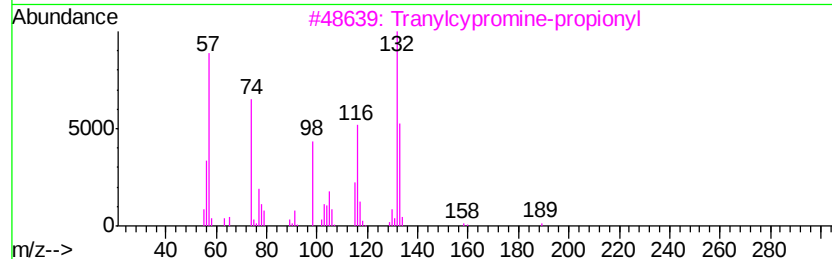
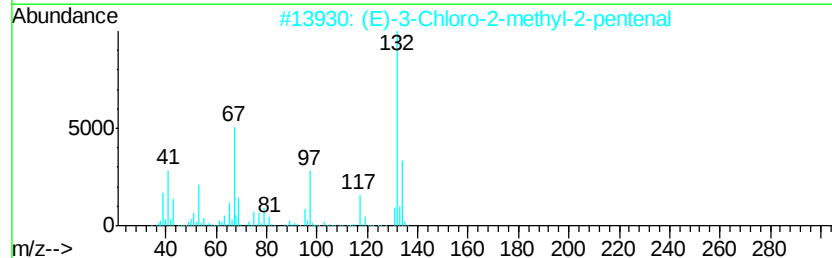
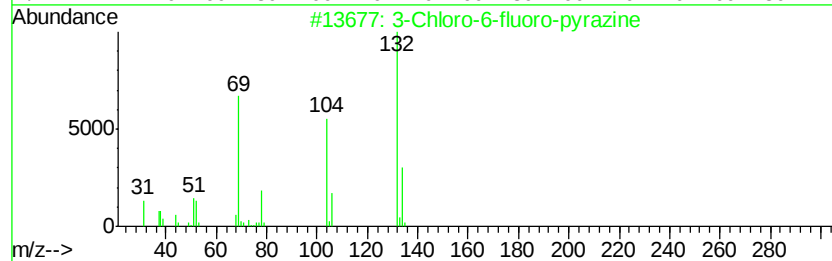
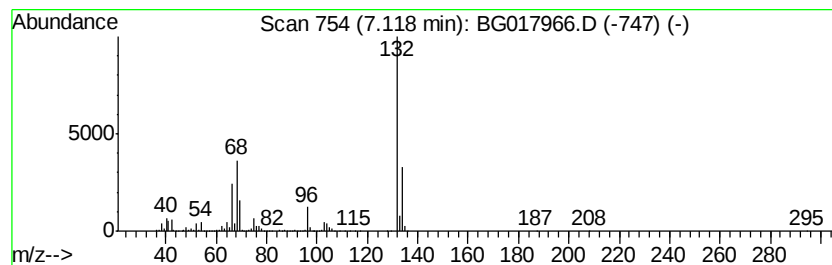
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown7.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	116.55 ng	3061800	1,4-Dichlorobenzene-d4	7.59

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017966.D
Acq On : 19 Jul 2015 20:34
Operator : TP/UM
Sample : G2975-01
Misc :
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Instrument :
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ClientSampleId :
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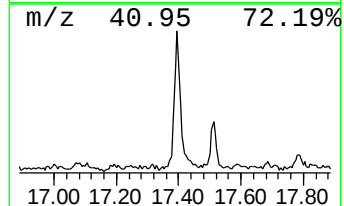
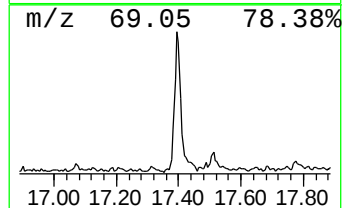
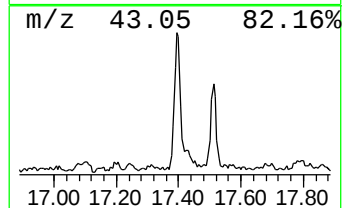
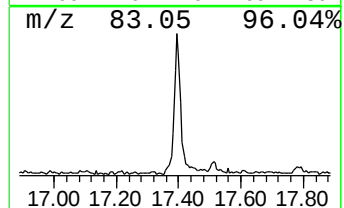
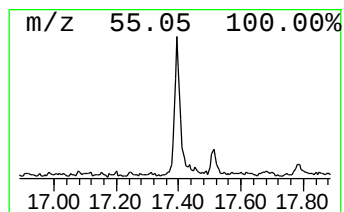
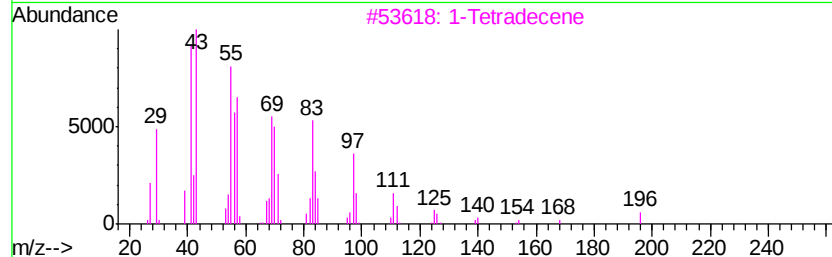
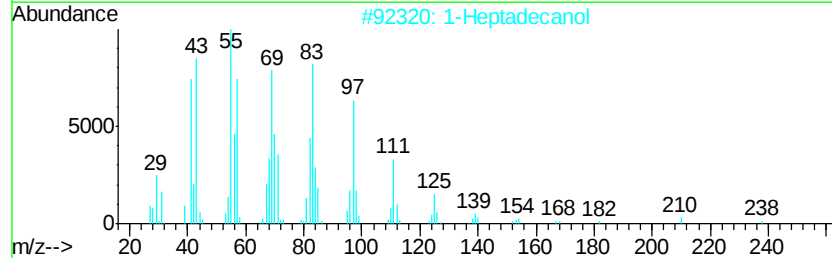
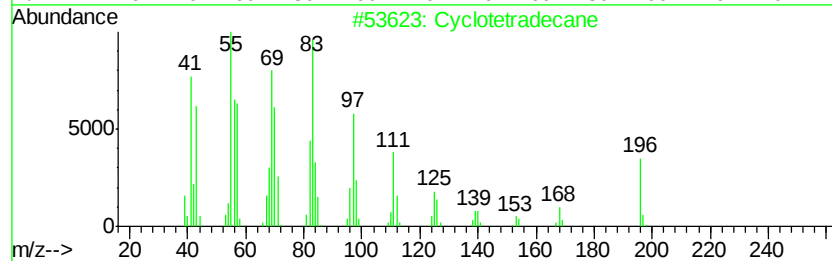
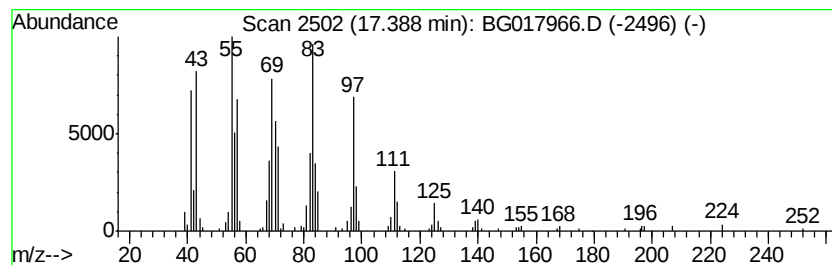
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclotetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	5.23 ng	338710	Phenanthrene-d10	16.99

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclotetradecane	196	C14H28	000295-17-0	96
2		1-Heptadecanol	256	C17H36O	001454-85-9	95
3		1-Tetradecene	196	C14H28	001120-36-1	94
4		Cyclohexadecane	224	C16H32	000295-65-8	94
5		1-Pentadecanol	228	C15H32O	000629-76-5	94



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017966.D
Acq On : 19 Jul 2015 20:34
Operator : TP/UM
Sample : G2975-01
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
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ClientSampleId :
AB-SLOPE-FAIL-1(0-2)

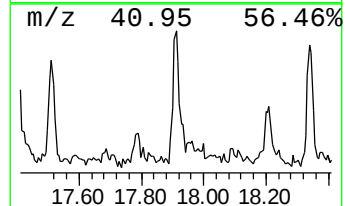
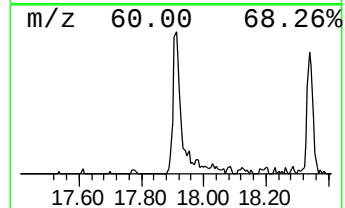
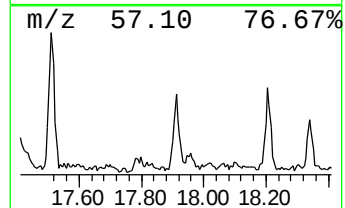
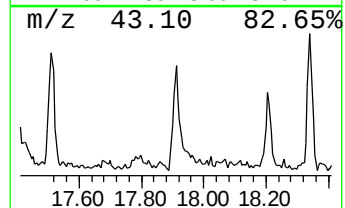
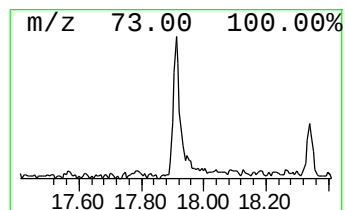
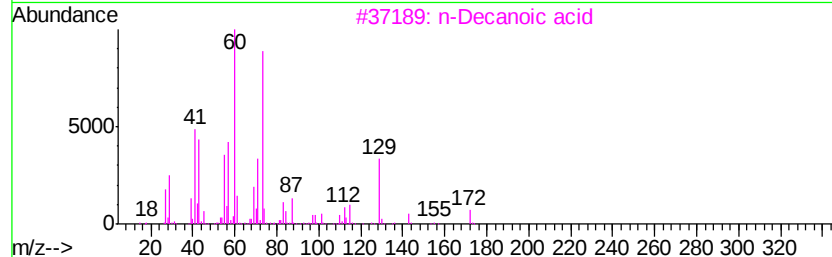
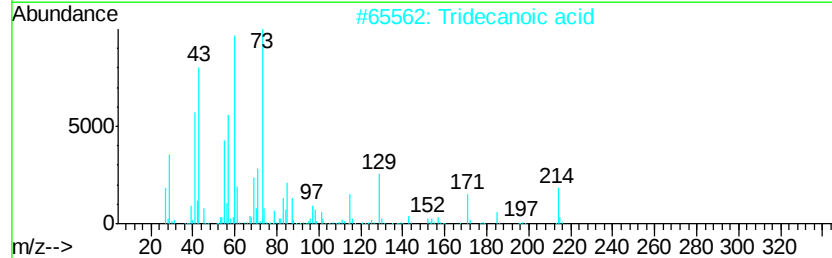
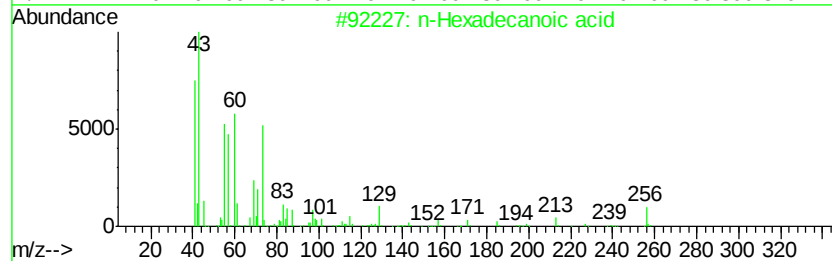
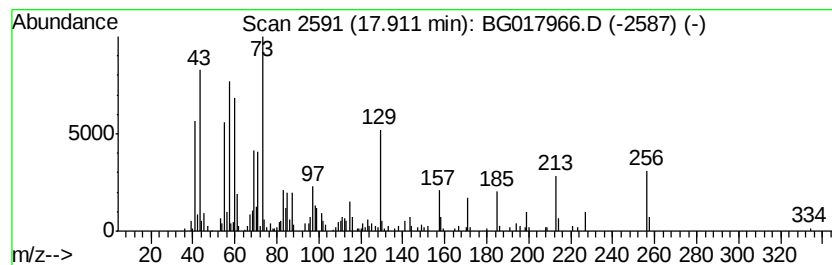
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	2.89 ng	187286	Phenanthrene-d10	16.99

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	70
3			n-Decanoic acid	172	C10H20O2	000334-48-5	50
4			Dodecanoic acid	200	C12H24O2	000143-07-7	49
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	49



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017966.D
Acq On : 19 Jul 2015 20:34
Operator : TP/UM
Sample : G2975-01
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
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ClientSampleId :
AB-SLOPE-FAIL-1(0-2)

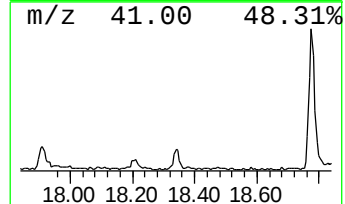
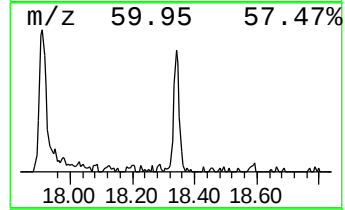
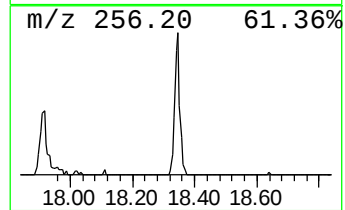
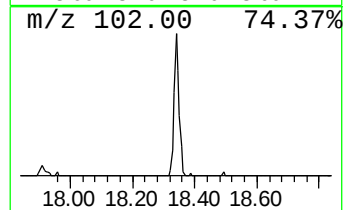
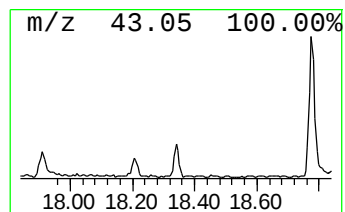
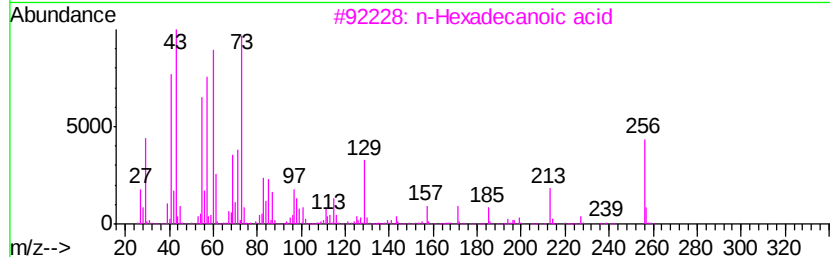
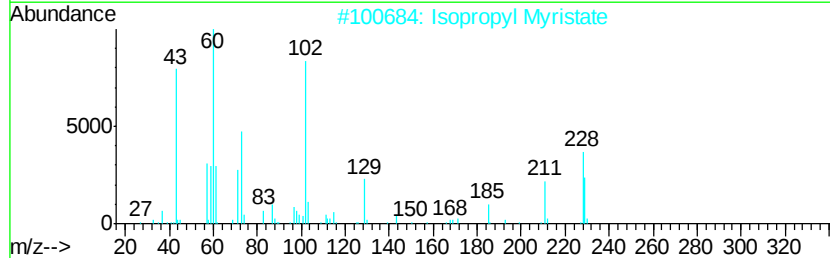
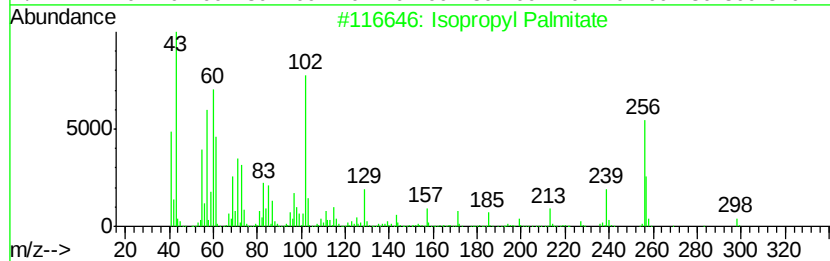
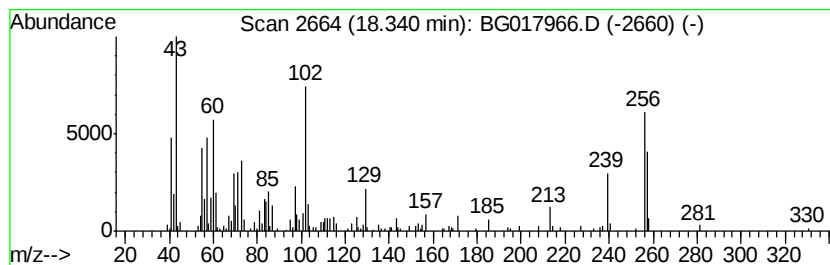
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Isopropyl Palmitate Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	2.10 ng	136291	Phenanthrene-d10	16.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Palmitate	298	C19H38O2	000142-91-6	74
2		Isopropyl Myristate	270	C17H34O2	000110-27-0	43
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	42
4		Urea, (2-thiazolin-2-yl)-	145	C4H7N3OS	015823-99-1	27
5		Silanamine, 1,1,1-trimethyl-N-[2...	281	C14H27NOSi2	054965-31-0	14



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017966.D
Acq On : 19 Jul 2015 20:34
Operator : TP/UM
Sample : G2975-01
Misc :
ALS Vial : 42 Sample Multiplier: 1

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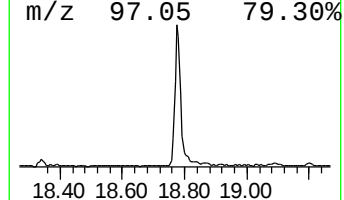
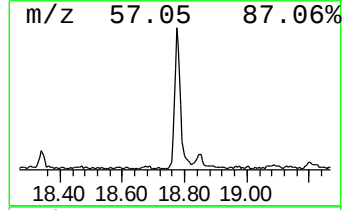
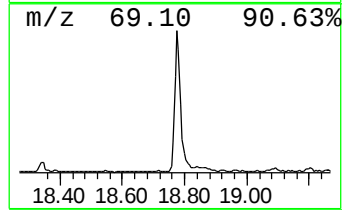
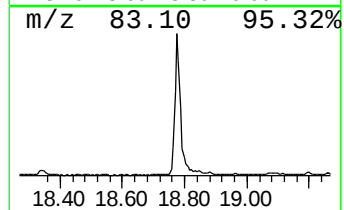
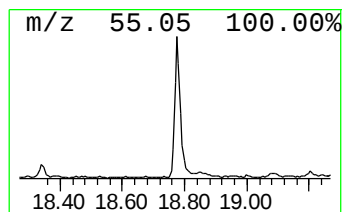
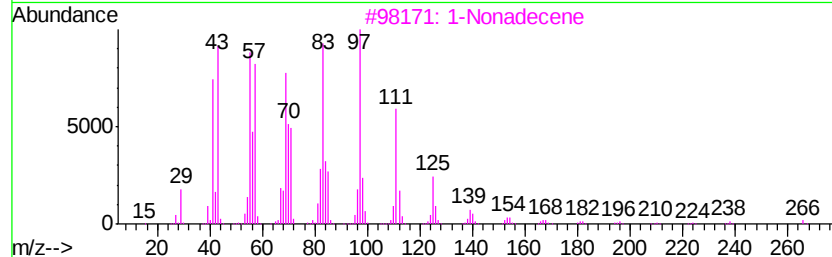
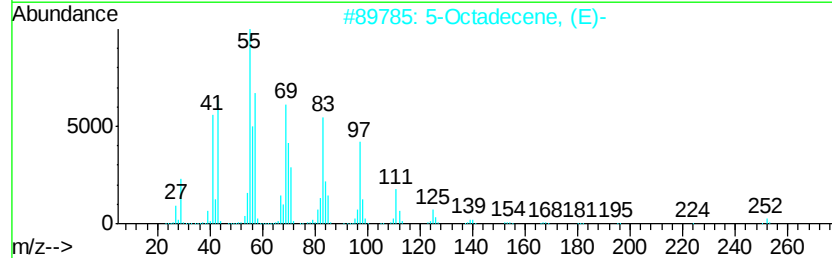
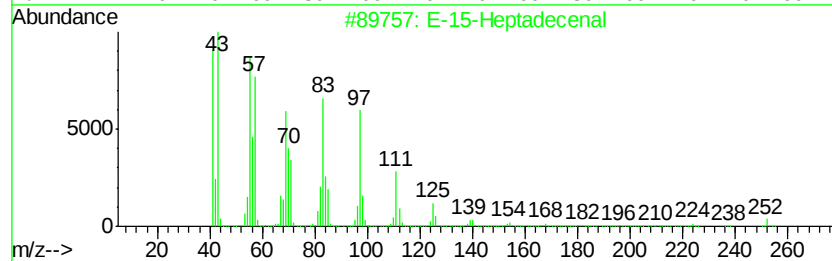
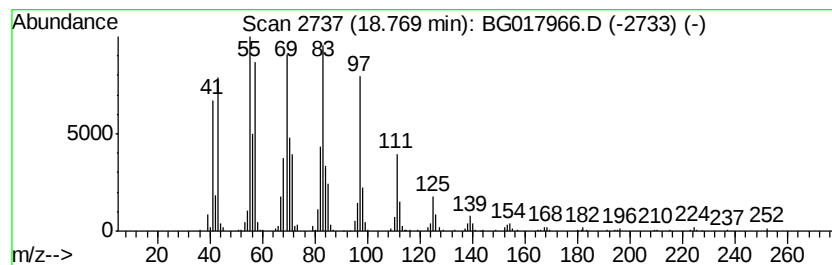
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.77	13.05 ng	845806	Phenanthrene-d10	16.99

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	E-15-Heptadecenal	252	C17H32O	1000130-97-9	99
2		5-Octadecene, (E)-	252	C18H36	007206-21-5	98
3		1-Nonadecene	266	C19H38	018435-45-5	95
4		1-Octadecene	252	C18H36	000112-88-9	94
5		Cyclohexadecane	224	C16H32	000295-65-8	94



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
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Acq On : 19 Jul 2015 20:34
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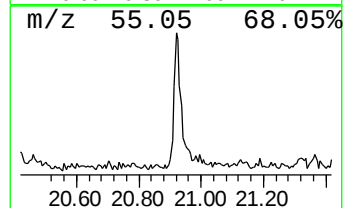
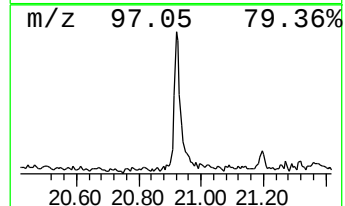
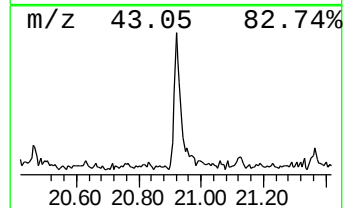
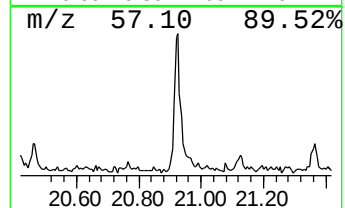
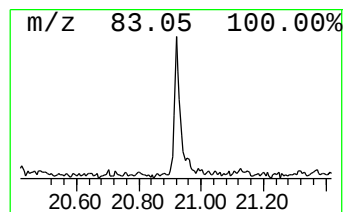
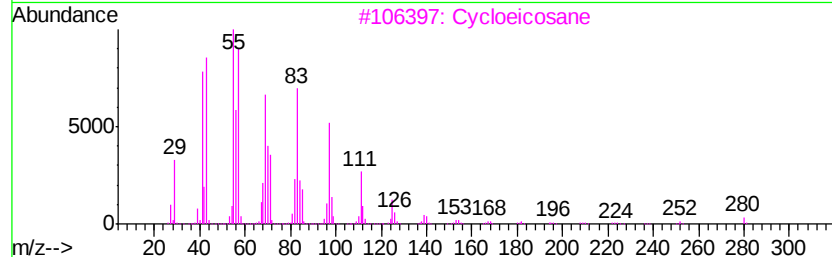
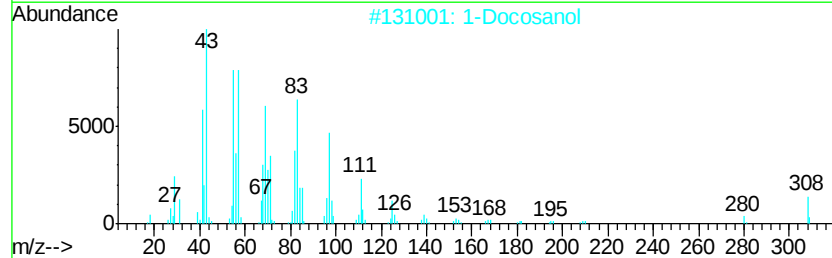
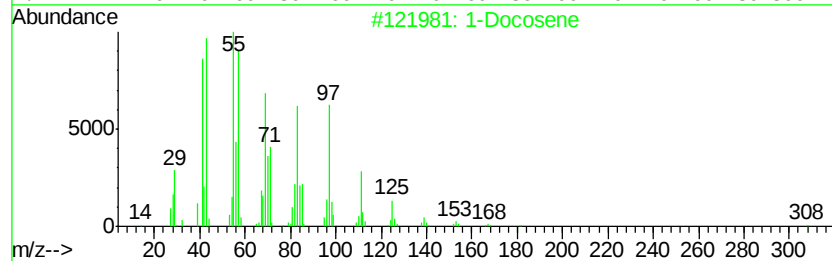
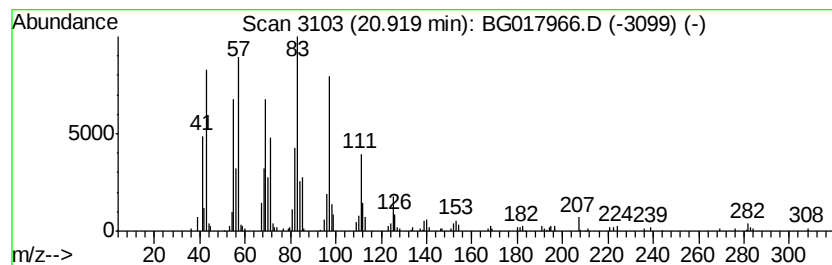
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Docosene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.92	2.85 ng	207201	Chrysene-d12	21.20	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	94
2	1-Docosanol	326	C22H46O	000661-19-8	87
3	Cycloeicosane	280	C20H40	000296-56-0	86
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	58
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	53



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017966.D
Acq On : 19 Jul 2015 20:34
Operator : TP/UM
Sample : G2975-01
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ALS Vial : 42 Sample Multiplier: 1

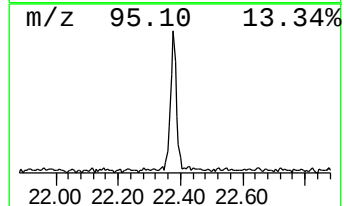
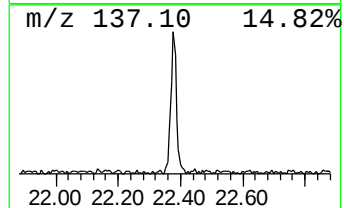
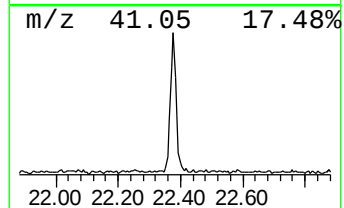
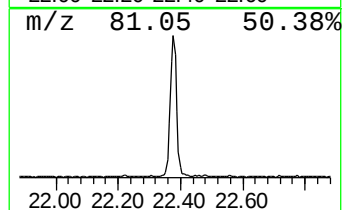
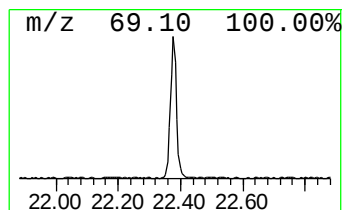
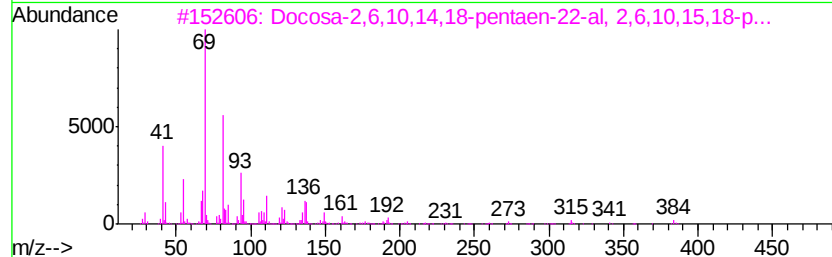
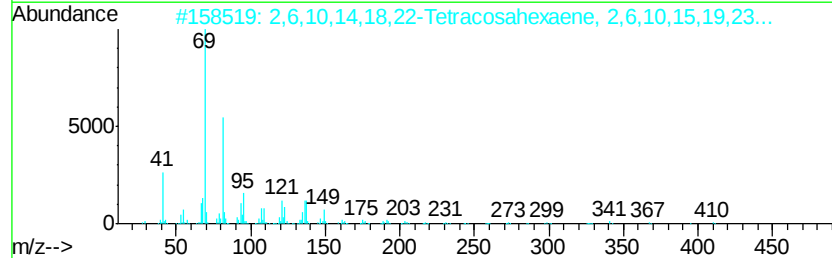
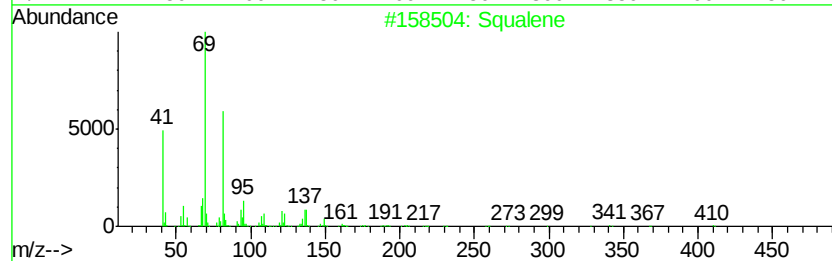
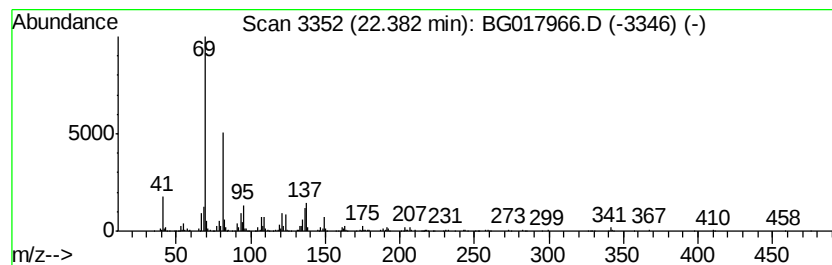
Instrument :
BNA_G
ClientSampleId :
AB-SLOPE-FAIL-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.38	7.45 ng	529410	Perylene-d12	23.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	99
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	91
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
5	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017966.D
Acq On : 19 Jul 2015 20:34
Operator : TP/UM
Sample : G2975-01
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AB-SLOPE-FAIL-1(0-2)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.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	29.5	ng	776079	1	7.59	525411	20.0
Propane, 1,1-dime...	2.90	2.0	ng	53385	1	7.59	525411	20.0
3-Penten-2-one, 4...	4.15	3.5	ng	91627	1	7.59	525411	20.0
2-Pentanone, 4-hy...	4.74	63.1	ng	1658380	1	7.59	525411	20.0
2-Pentanone, 4-me...	5.80	6.5	ng	169443	1	7.59	525411	20.0
unknown7.12	7.12	116.6	ng	3061800	1	7.59	525411	20.0
Cyclotetradecane	17.39	5.2	ng	338710	4	16.99	1296300	20.0
n-Hexadecanoic acid	17.91	2.9	ng	187286	4	16.99	1296300	20.0
Isopropyl Palmitate	18.34	2.1	ng	136291	4	16.99	1296300	20.0
E-15-Heptadecenal	18.77	13.1	ng	845806	4	16.99	1296300	20.0
1-Docosene	20.92	2.9	ng	207201	5	21.20	1452550	20.0
Squalene	22.38	7.5	ng	529410	6	23.41	1420900	20.0