

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
 Data File : BG017969.D
 Acq On : 19 Jul 2015 22:20
 Operator : TP/UM
 Sample : G2975-11
 Misc :
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 AB-SLOPE-FAIL-6(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	2.864	26	30	45	rVB	385706	513963	10.13%	1.397%
2	3.270	96	99	106	rVB	47667	62567	1.23%	0.170%
3	4.151	244	249	255	rVB	64003	84656	1.67%	0.230%
4	4.739	342	349	358	rBV	1123010	1551925	30.58%	4.219%
5	5.197	420	427	438	rBV	1628345	2417153	47.62%	6.571%
6	5.796	524	529	534	rBV	111283	153679	3.03%	0.418%
7	6.772	687	695	709	rVB	1705736	2723214	53.65%	7.403%
8	7.124	746	755	763	rBV	1766102	2833169	55.82%	7.702%
9	7.582	826	833	843	rBV	358516	576643	11.36%	1.568%
10	7.900	878	887	896	rVB	1257288	2066199	40.71%	5.617%
11	8.740	1020	1030	1039	rBV	1036852	1719366	33.87%	4.674%
12	10.362	1297	1306	1313	rBV	527434	892203	17.58%	2.425%
13	12.859	1721	1731	1739	rBV	2687091	4060356	80.00%	11.038%
14	13.705	1869	1875	1884	rVB	606689	825414	16.26%	2.244%
15	14.239	1960	1966	1973	rBV2	812014	1285758	25.33%	3.495%
16	14.803	2054	2062	2072	rBV	70910	276502	5.45%	0.752%
17	15.080	2102	2109	2112	rBV2	53030	110499	2.18%	0.300%
18	15.738	2214	2221	2231	rBV	2289565	3229444	63.63%	8.779%
19	15.979	2257	2262	2265	rBV	57941	84269	1.66%	0.229%
20	16.772	2390	2397	2401	rBV2	80450	106529	2.10%	0.290%
21	16.995	2429	2435	2443	rBV2	1014060	1508772	29.73%	4.101%
22	17.395	2496	2503	2515	rBV3	149474	247320	4.87%	0.672%
23	17.512	2519	2523	2527	rVB	79279	90213	1.78%	0.245%
24	17.912	2587	2591	2598	rBV3	162903	256601	5.06%	0.698%
25	18.205	2637	2641	2646	rBV2	52474	82376	1.62%	0.224%
26	18.346	2661	2665	2670	rVB2	66111	81788	1.61%	0.222%
27	18.775	2735	2738	2745	rBV3	71609	116771	2.30%	0.317%
28	19.204	2808	2811	2820	rVB10	35472	57197	1.13%	0.155%
29	19.351	2833	2836	2841	rVB4	50033	68710	1.35%	0.187%
30	19.645	2880	2886	2893	rBV	4033534	5075644	100.00%	13.798%
31	20.920	3099	3103	3109	rBV	109370	159949	3.15%	0.435%
32	21.196	3144	3150	3160	rBV	1330913	1626205	32.04%	4.421%
33	22.377	3347	3351	3358	rVB	108891	157272	3.10%	0.428%
34	22.753	3411	3415	3423	rVB4	42455	75505	1.49%	0.205%

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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-BG071715.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.411	3520	3527	3535	rBV2	863594	1608435	31.69%	4.372%
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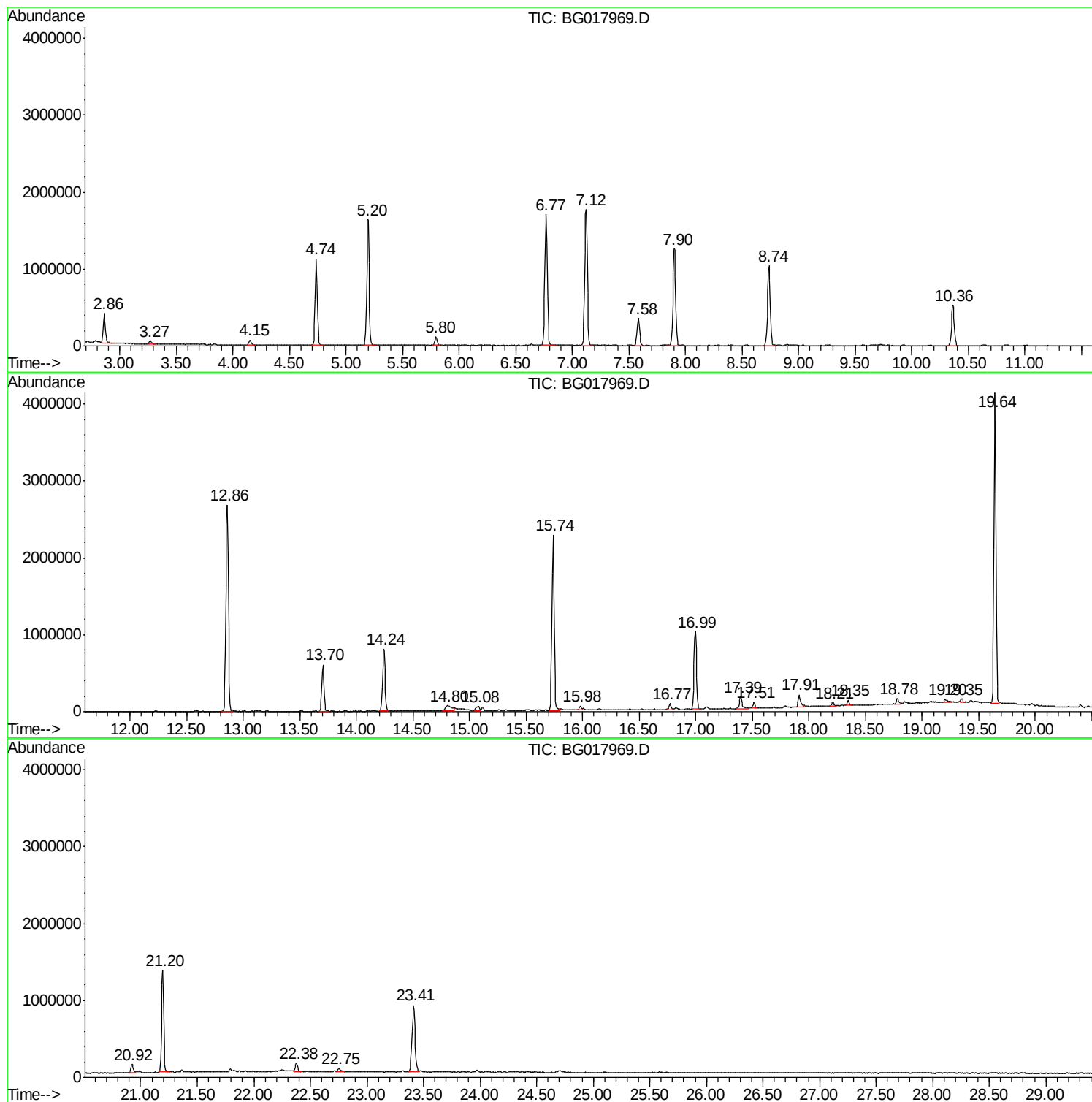
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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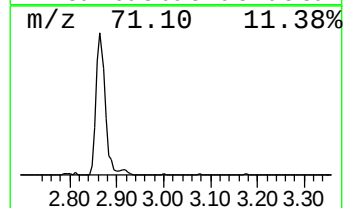
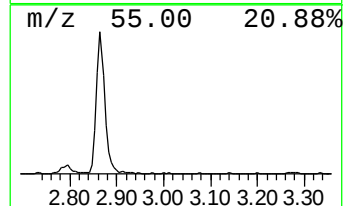
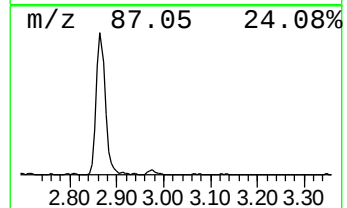
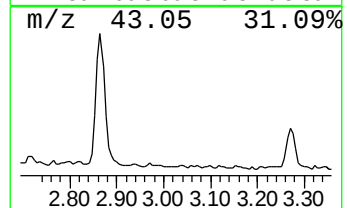
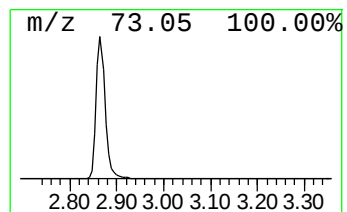
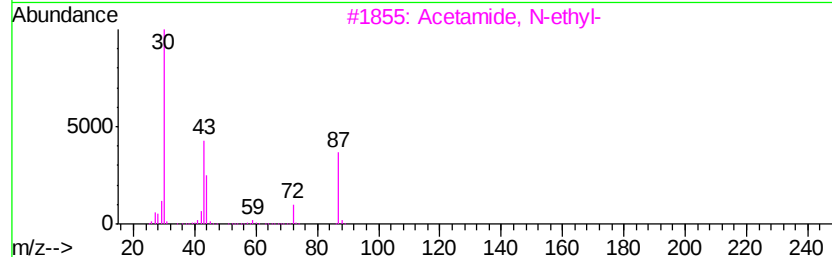
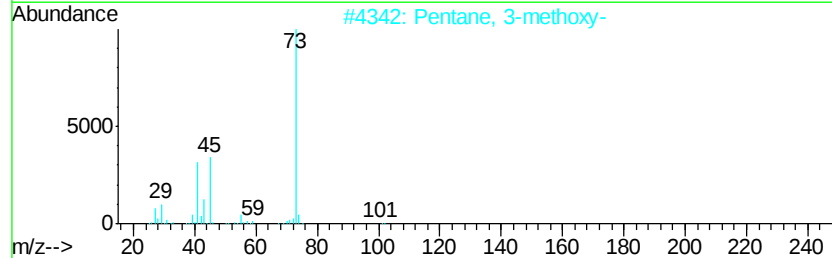
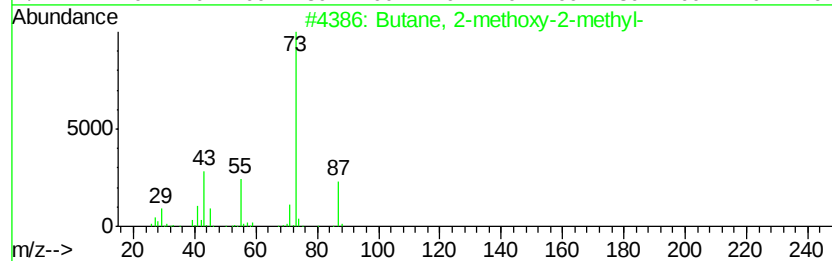
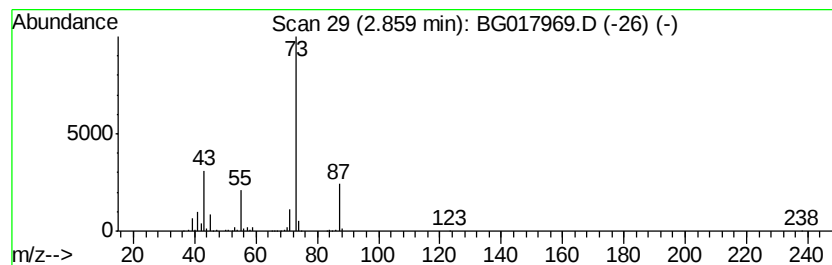
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	17.83 ng	513963	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	86
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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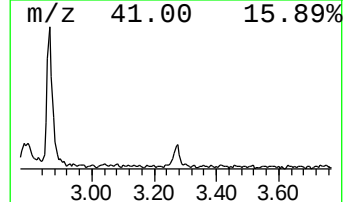
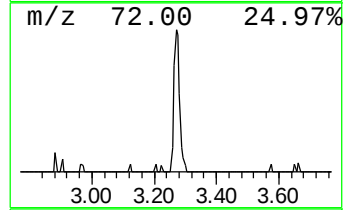
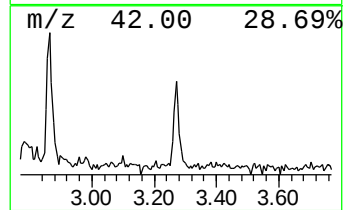
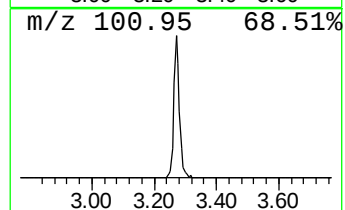
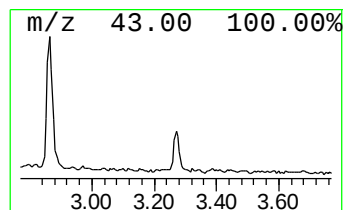
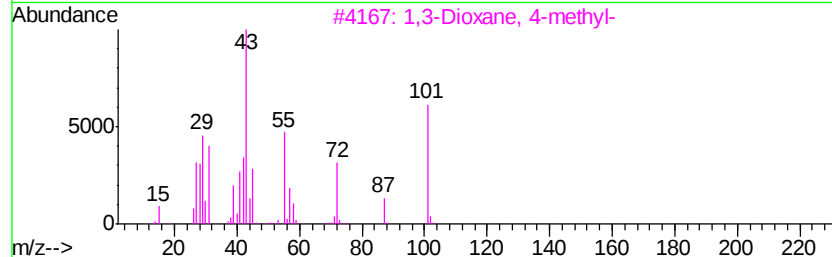
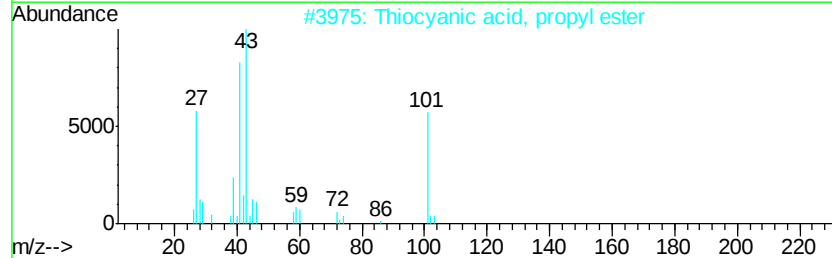
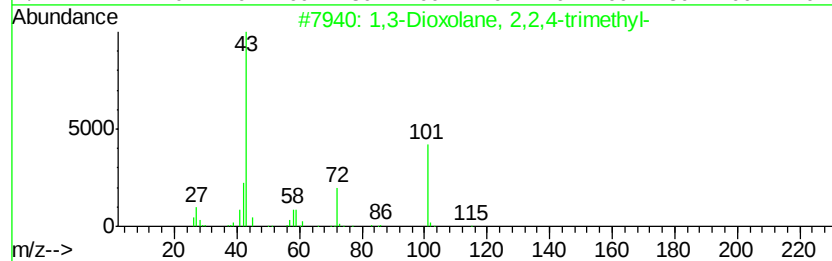
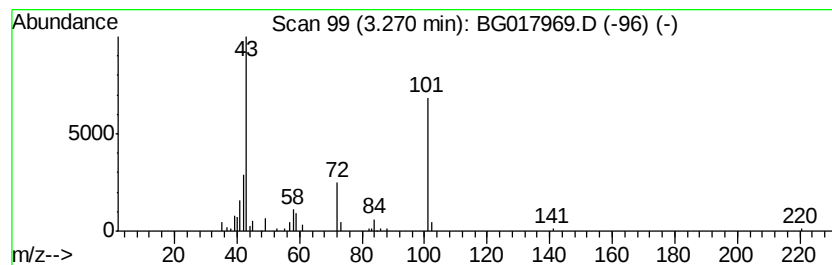
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.27	2.17 ng	62567	1,4-Dichlorobenzene-d4	7.58

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	64
2			Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	47
3			1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	45
4			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	40
5			Propanamide, N,N-dimethyl-	101	C5H11NO	000758-96-3	38



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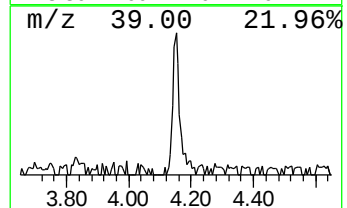
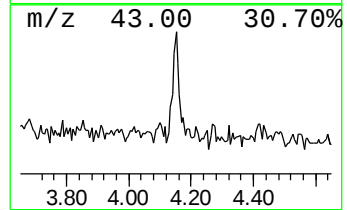
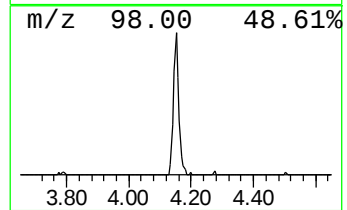
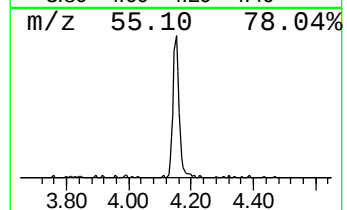
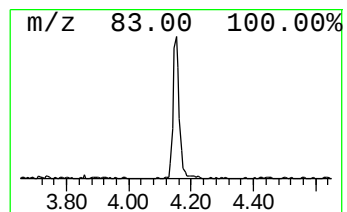
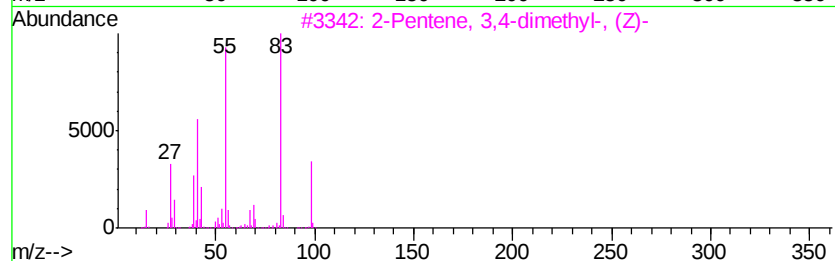
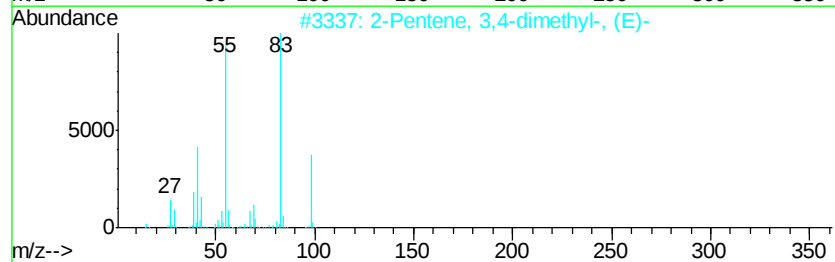
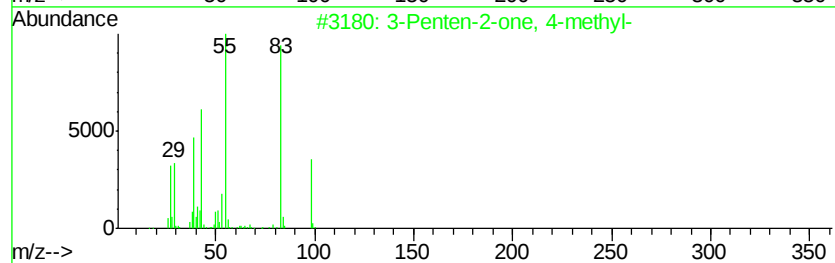
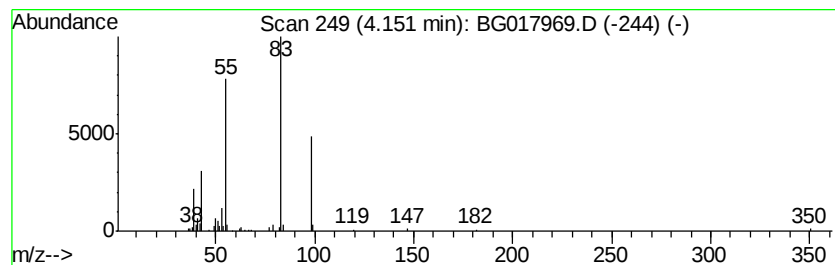
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.15	2.94 ng	84656	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	86
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
3		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	64
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	64
5		Cyclohexane, methyl-	98	C7H14	000108-87-2	56



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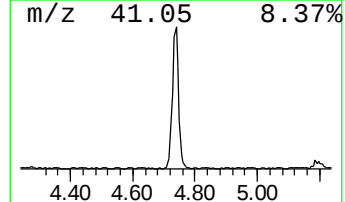
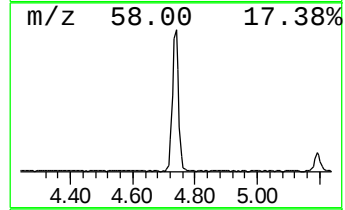
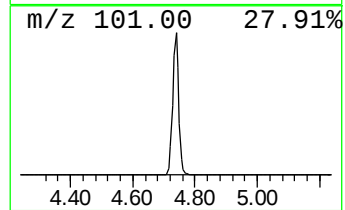
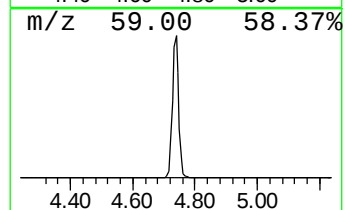
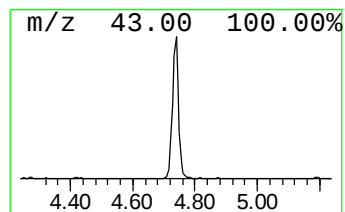
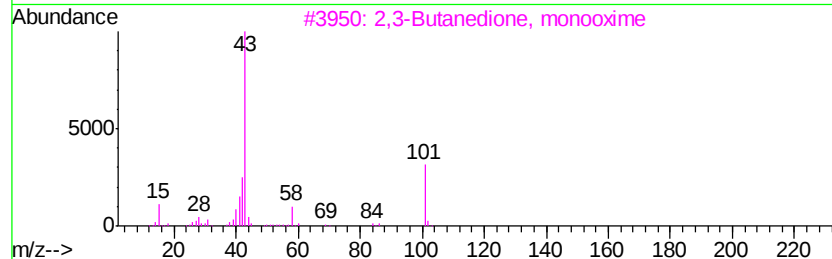
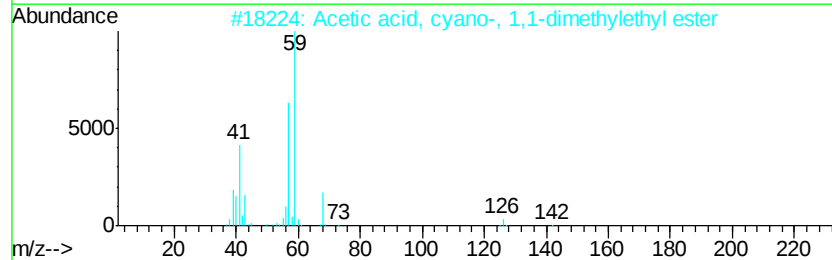
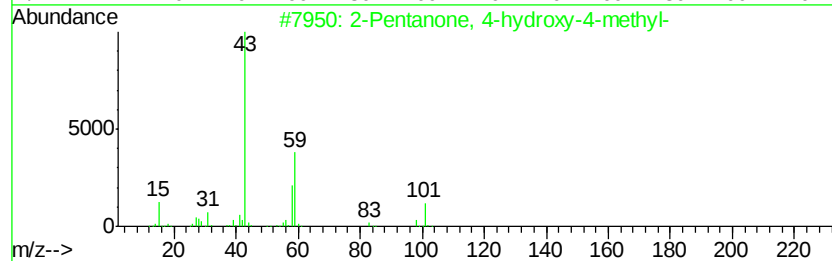
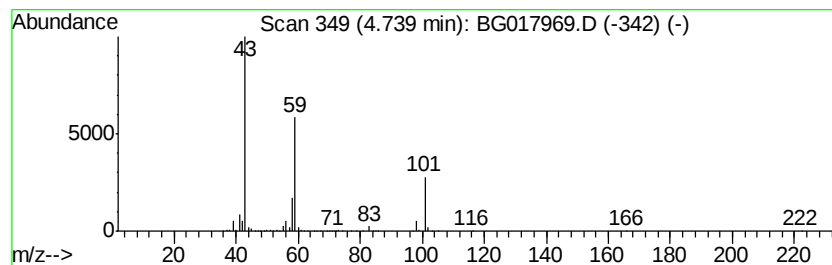
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.74	53.83 ng	1551930	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4		Acetone	58	C3H6O	000067-64-1	10
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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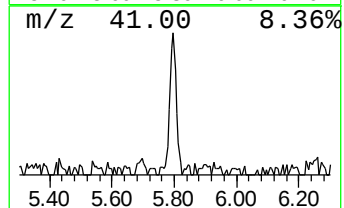
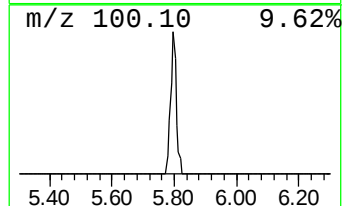
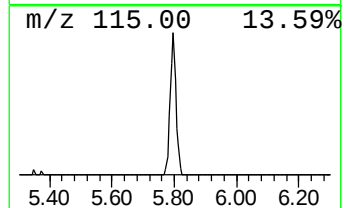
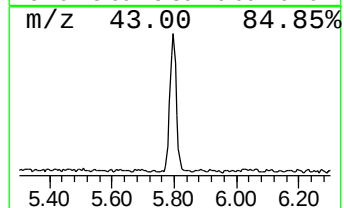
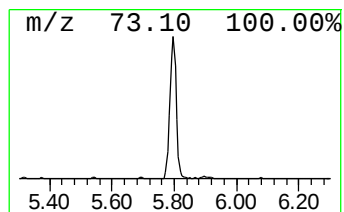
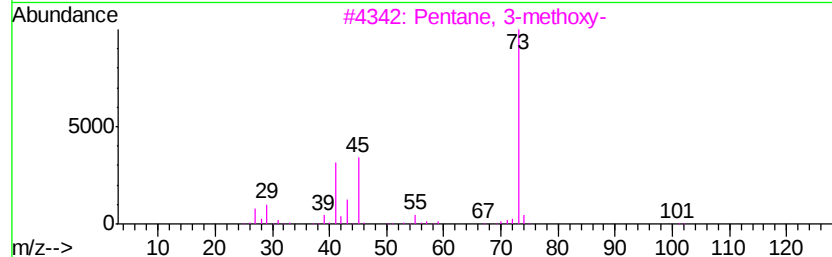
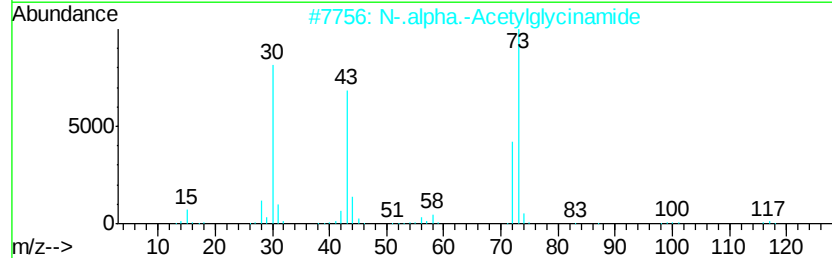
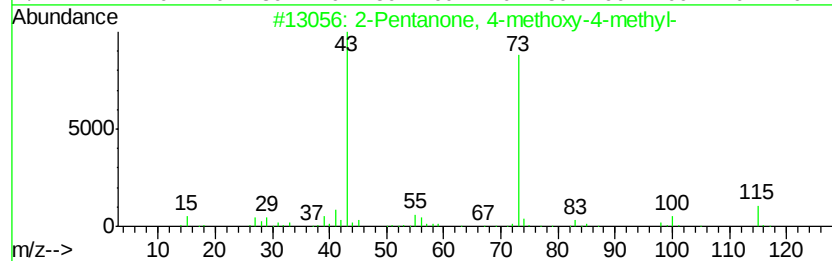
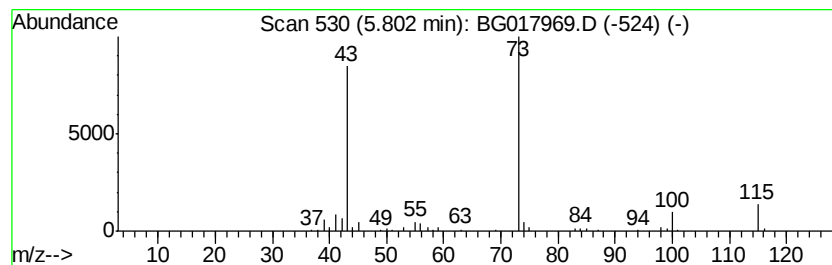
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.80	5.33 ng	153679	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	78
2		N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	38
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4		2,3-Pentanedione	100	C5H8O2	000600-14-6	12
5		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017969.D
Acq On : 19 Jul 2015 22:20
Operator : TP/UM
Sample : G2975-11
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AB-SLOPE-FAIL-6(0-2)

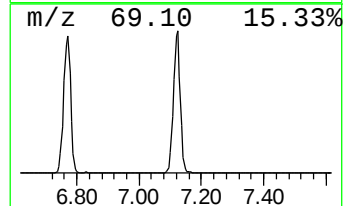
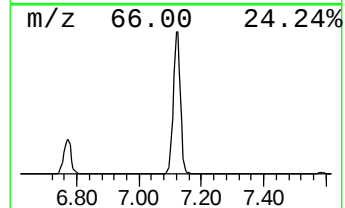
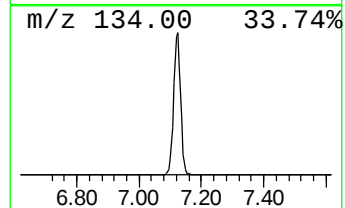
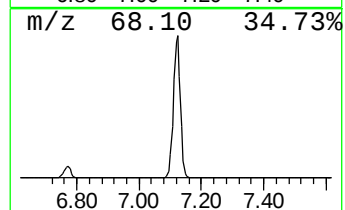
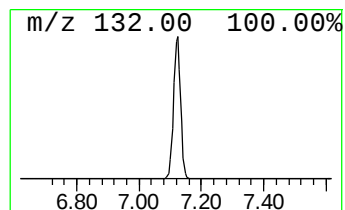
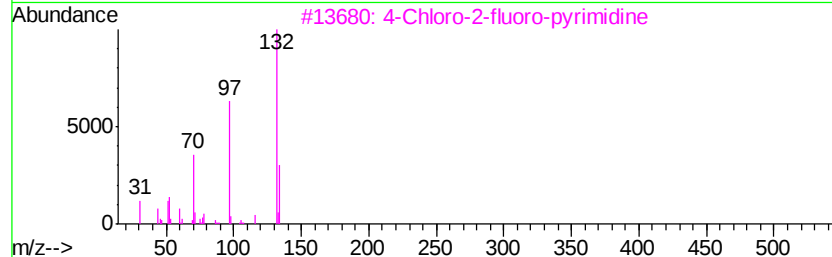
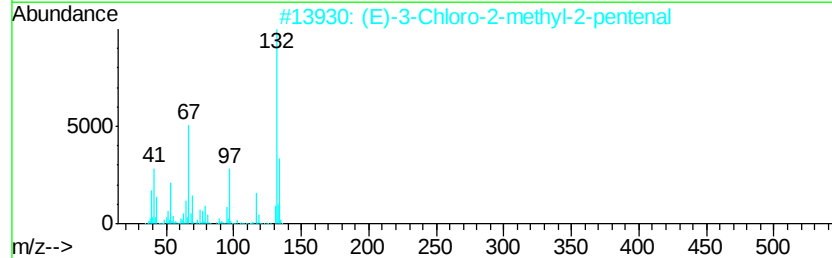
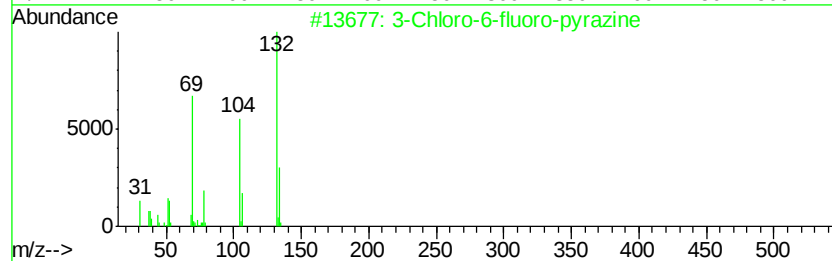
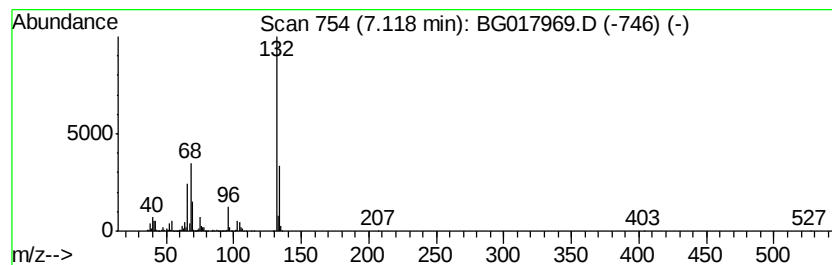
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown7.12 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.12	98.26 ng	2833170	1,4-Dichlorobenzene-d4	7.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017969.D
Acq On : 19 Jul 2015 22:20
Operator : TP/UM
Sample : G2975-11
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AB-SLOPE-FAIL-6(0-2)

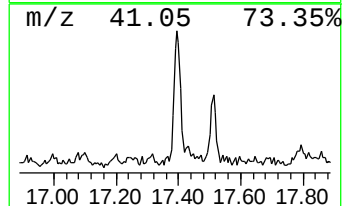
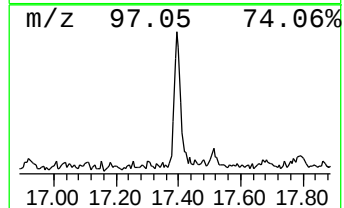
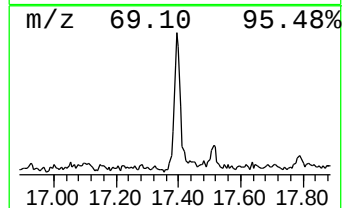
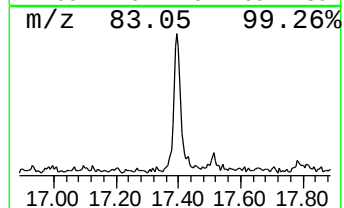
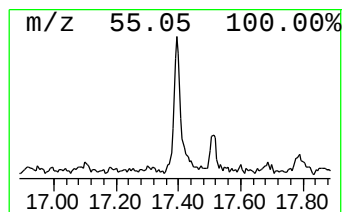
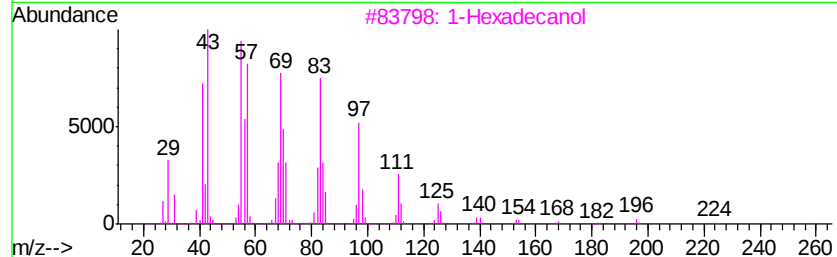
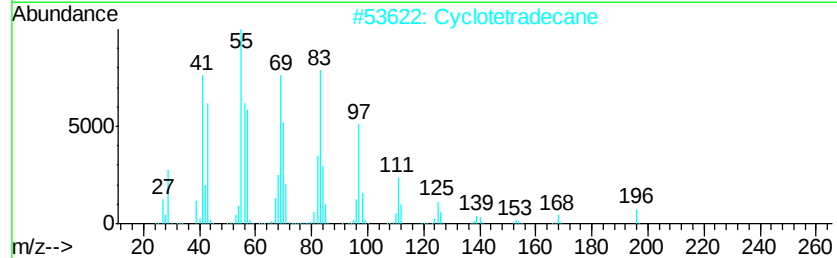
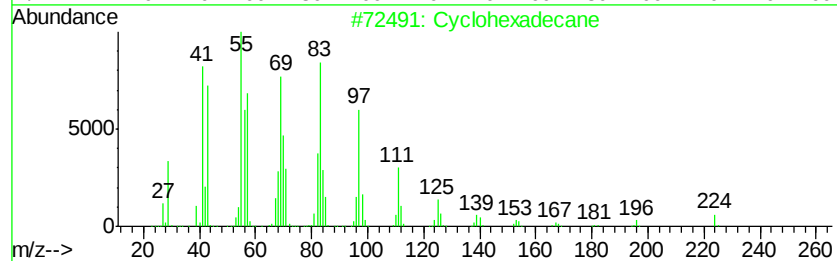
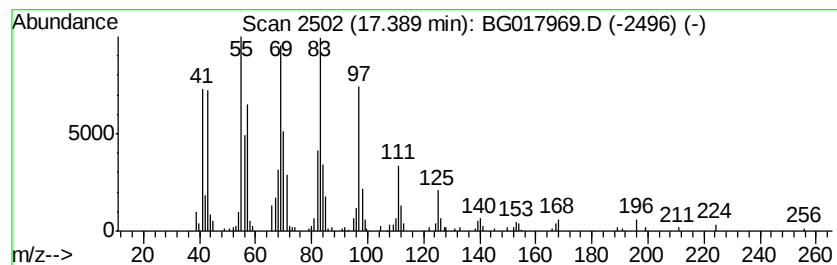
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Cyclohexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.39	3.28 ng	247320	Phenanthrene-d10	17.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexadecane	224	C16H32	000295-65-8	97
2		Cyclotetradecane	196	C14H28	000295-17-0	95
3		1-Hexadecanol	242	C16H34O	036653-82-4	91
4		1-Pentadecanol	228	C15H32O	000629-76-5	90
5		3-Heptafluorobutyroxytetradecane	410	C18H29F7O2	1000245-49-8	83



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017969.D
Acq On : 19 Jul 2015 22:20
Operator : TP/UM
Sample : G2975-11
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AB-SLOPE-FAIL-6(0-2)

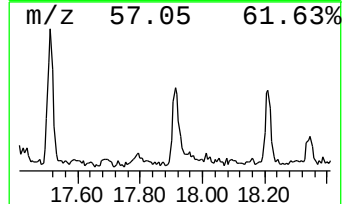
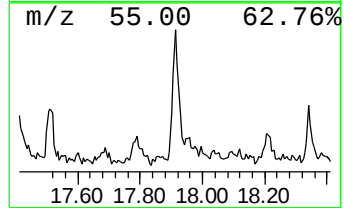
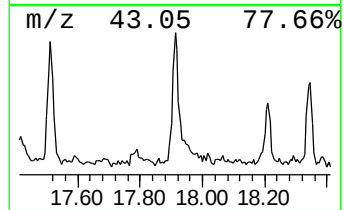
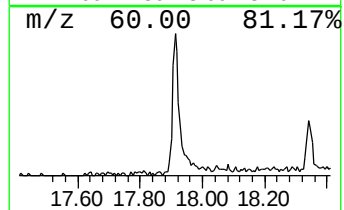
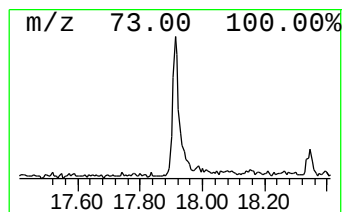
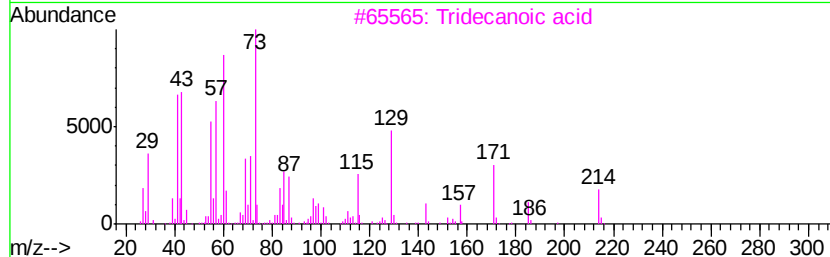
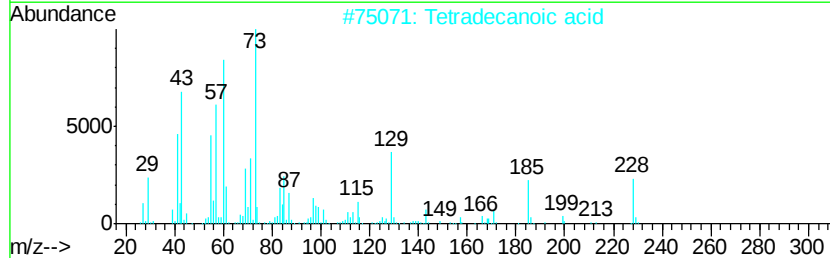
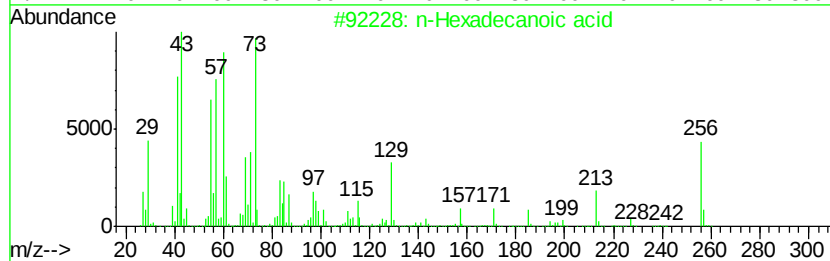
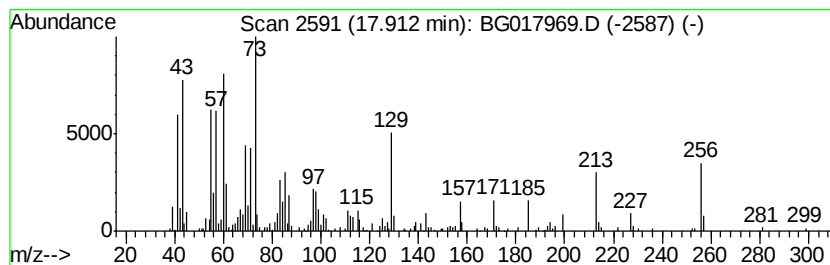
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.91	3.40 ng	256601	Phenanthrene-d10	17.00

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			Octane, 2,3,3-trimethyl-	156	C11H24	062016-30-2	11
5			Docosane, 2,21-dimethyl-	338	C24H50	077536-31-3	11



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071915\
Data File : BG017969.D
Acq On : 19 Jul 2015 22:20
Operator : TP/UM
Sample : G2975-11
Misc :
ALS Vial : 45 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AB-SLOPE-FAIL-6(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	17.8	ng	513963	1	7.58	576643	20.0
1,3-Dioxolane, 2,...	3.27	2.2	ng	62567	1	7.58	576643	20.0
3-Penten-2-one, 4...	4.15	2.9	ng	84656	1	7.58	576643	20.0
2-Pentanone, 4-hy...	4.74	53.8	ng	1551930	1	7.58	576643	20.0
2-Pentanone, 4-me...	5.80	5.3	ng	153679	1	7.58	576643	20.0
unknown7.12	7.12	98.3	ng	2833170	1	7.58	576643	20.0
Cyclohexadecane	17.39	3.3	ng	247320	4	17.00	1508770	20.0
n-Hexadecanoic acid	17.91	3.4	ng	256601	4	17.00	1508770	20.0