

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016455.D
 Acq On : 16 Apr 2015 11:47
 Operator : TP/IZ
 Sample : G1829-04
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TE-PMW-42

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	2.755	7	11	21	rBV	381104	601563	12.82%	1.873%
2	2.837	21	25	35	rVB	421531	493772	10.52%	1.537%
3	4.776	350	355	362	rVB	66445	95631	2.04%	0.298%
4	5.258	429	437	445	rBV	796783	1127801	24.03%	3.512%
5	6.856	702	709	721	rBV	562262	873988	18.62%	2.721%
6	7.203	761	768	778	rBV	1407579	2144200	45.68%	6.676%
7	7.661	840	846	853	rBV	290908	447169	9.53%	1.392%
8	7.984	893	901	908	rBV	1136062	1735653	36.98%	5.404%
9	8.824	1036	1044	1051	rBV	959121	1530939	32.62%	4.767%
10	10.452	1314	1321	1333	rBV	444588	737699	15.72%	2.297%
11	12.661	1690	1697	1707	rVB	45166	72247	1.54%	0.225%
12	12.925	1733	1742	1753	rBV	2583831	3899073	83.07%	12.140%
13	13.765	1880	1885	1892	rBV	31398	47681	1.02%	0.148%
14	14.306	1969	1977	1985	rBV2	727247	1117015	23.80%	3.478%
15	14.741	2046	2051	2060	rBV	43368	72840	1.55%	0.227%
16	15.546	2182	2188	2195	rBV2	39102	60229	1.28%	0.188%
17	15.669	2199	2209	2214	rBV	60878	83731	1.78%	0.261%
18	15.798	2224	2231	2244	rBV	1882410	2673049	56.95%	8.323%
19	16.080	2274	2279	2284	rVB	112404	149149	3.18%	0.464%
20	16.462	2338	2344	2352	rBV	72044	112338	2.39%	0.350%
21	17.050	2436	2444	2450	rBV2	944886	1319086	28.10%	4.107%
22	17.825	2571	2576	2583	rBV4	32138	63797	1.36%	0.199%
23	17.955	2592	2598	2608	rBV	494150	821125	17.49%	2.557%
24	18.049	2609	2614	2623	rVB	260603	409364	8.72%	1.275%
25	19.112	2787	2795	2811	rBV2	108829	338975	7.22%	1.055%
26	19.236	2811	2816	2833	rVV2	255872	501133	10.68%	1.560%
27	19.682	2886	2892	2903	rVB	3694759	4693580	100.00%	14.614%
28	20.939	3102	3106	3114	rBV	369275	489635	10.43%	1.525%
29	21.145	3137	3141	3145	rBV	209293	233103	4.97%	0.726%
30	21.227	3150	3155	3161	rBV	1042543	1292028	27.53%	4.023%
31	22.226	3310	3325	3347	rVB4	404909	1956118	41.68%	6.091%
32	22.391	3349	3353	3360	rVB	348140	501043	10.68%	1.560%
33	23.460	3529	3535	3546	rVB2	675688	1260073	26.85%	3.923%
34	24.735	3747	3752	3759	rVB5	75716	161479	3.44%	0.503%

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Misc :
ALS Vial : 20 Sample Multiplier: 1

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

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

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

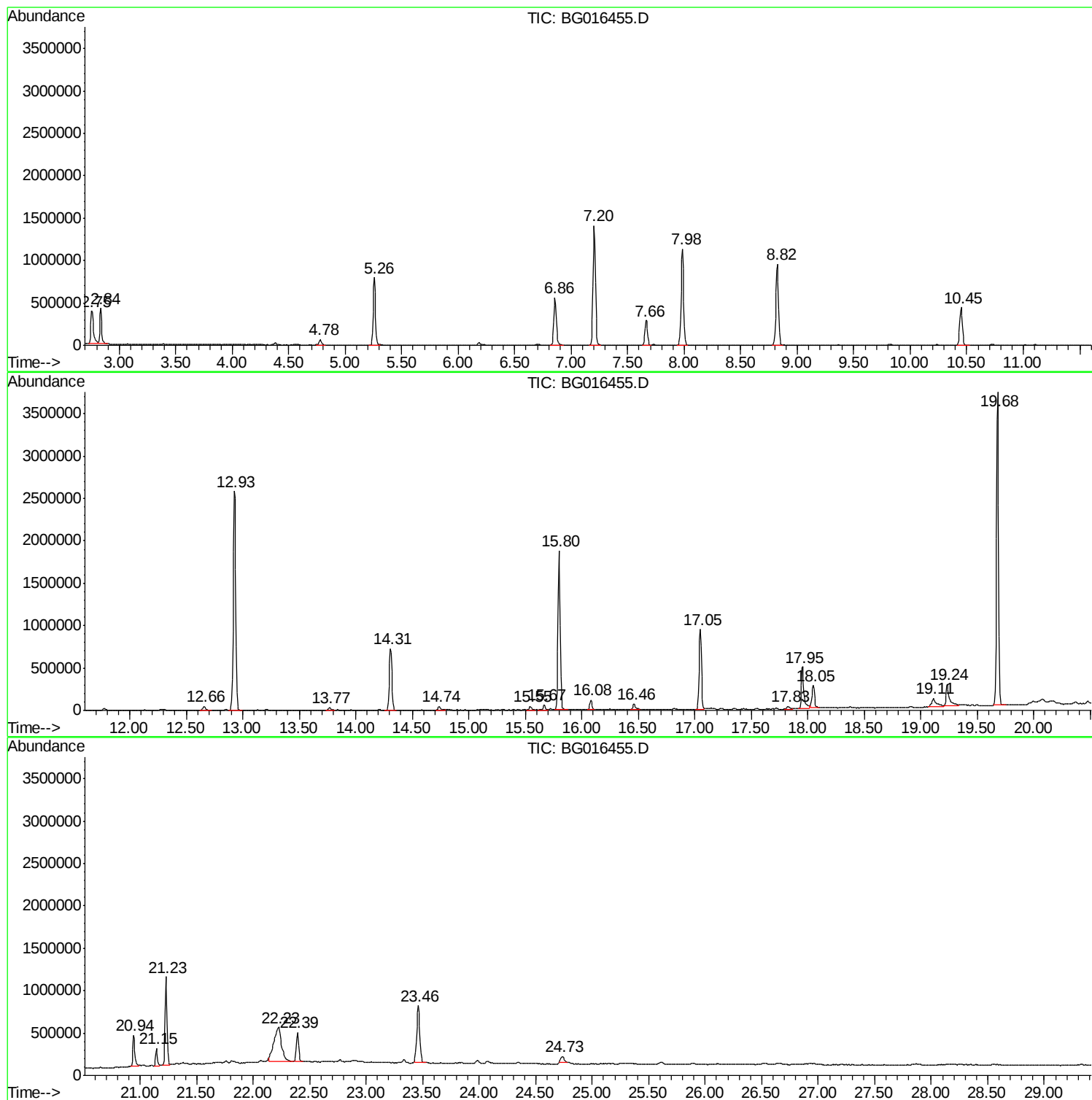
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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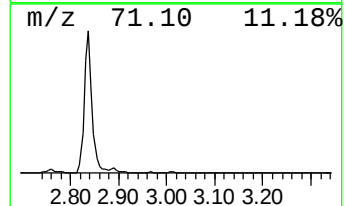
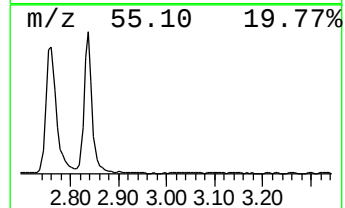
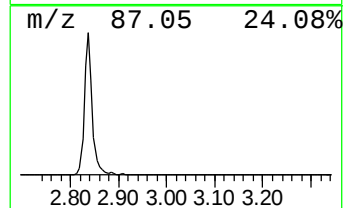
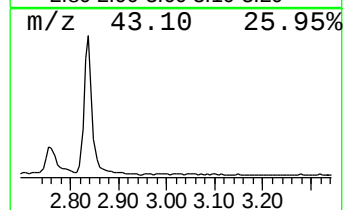
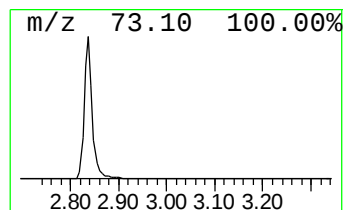
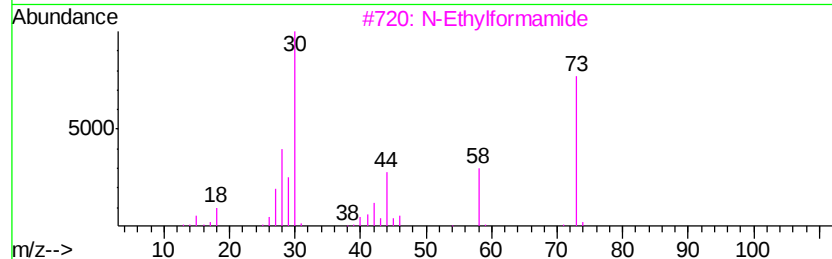
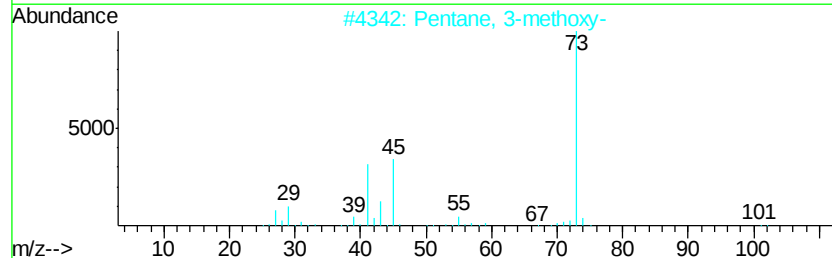
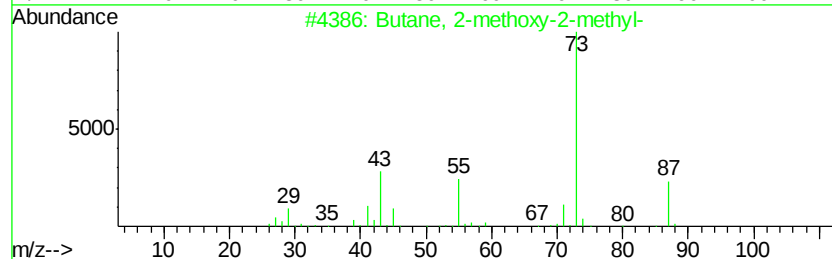
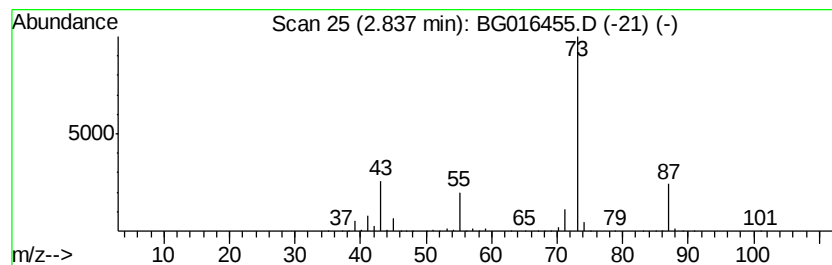
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	22.08 ng	493772	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	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
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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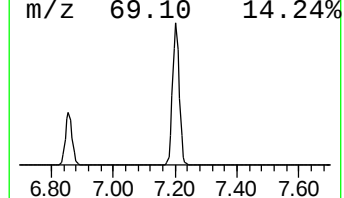
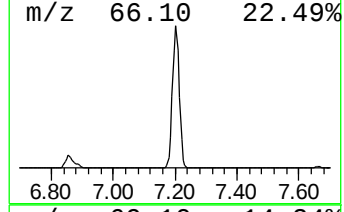
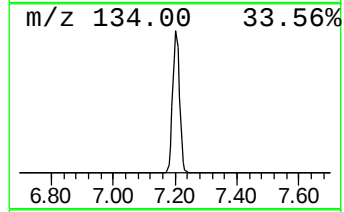
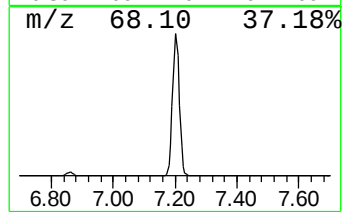
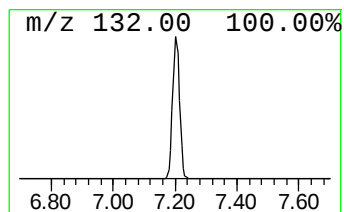
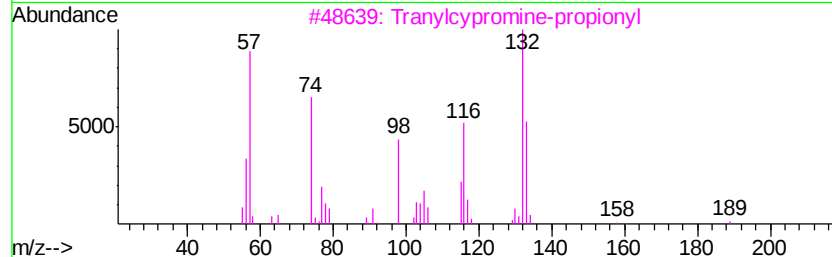
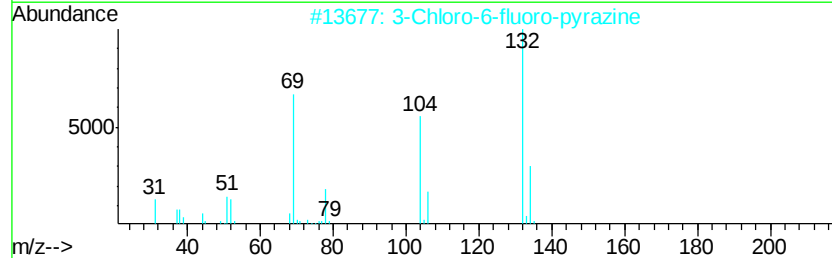
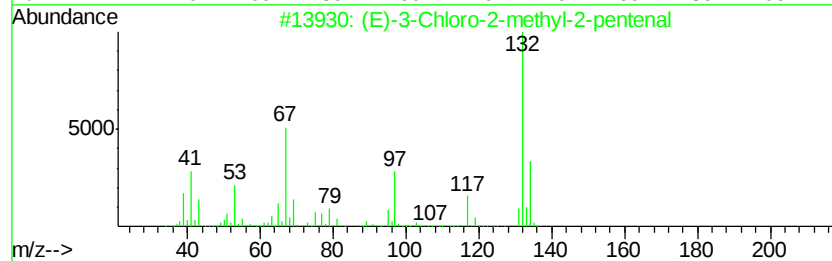
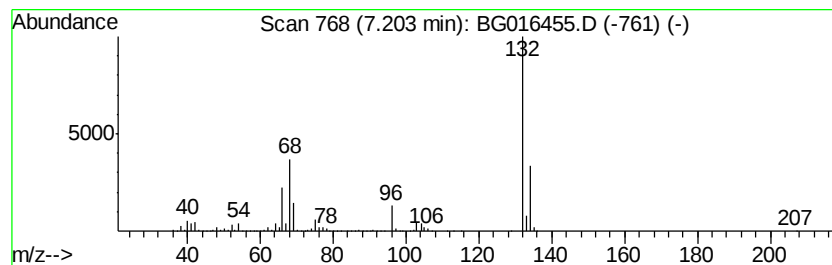
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	95.90 ng	2144200	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	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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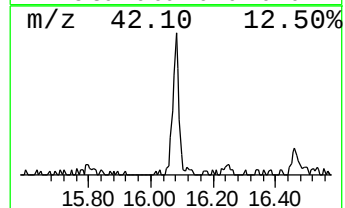
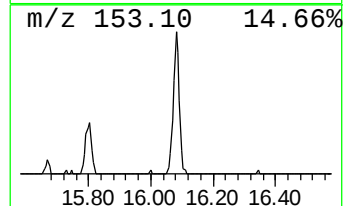
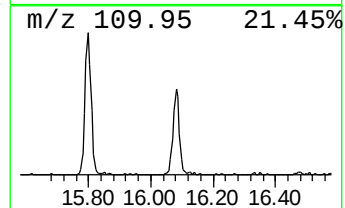
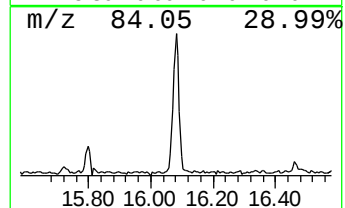
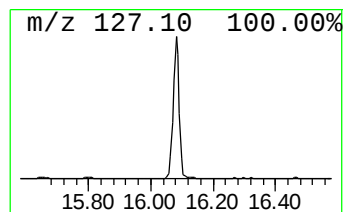
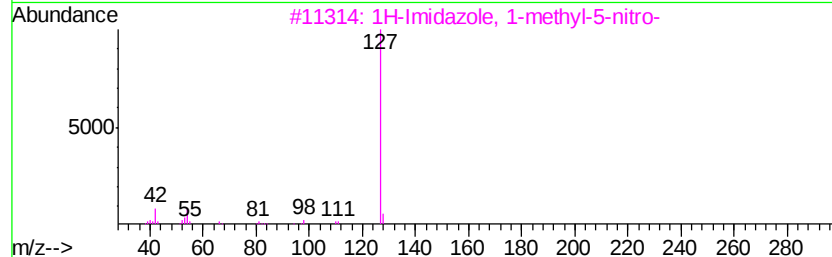
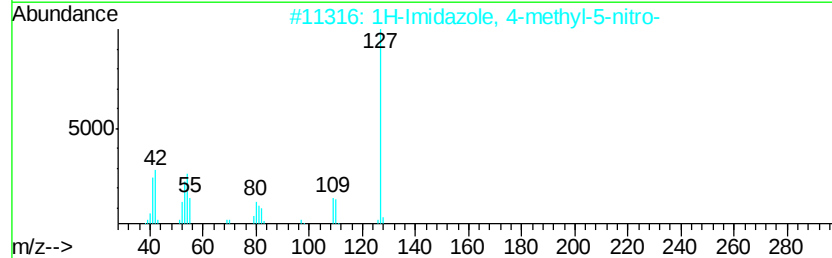
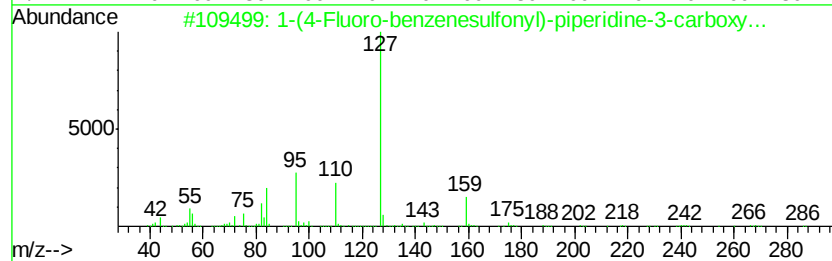
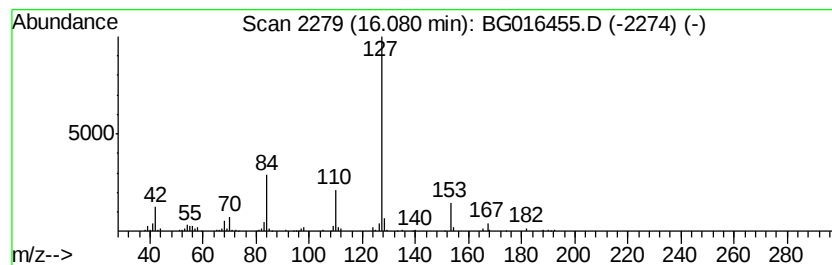
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-(4-Fluoro-benzenesulfonyl... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.		
16.08	2.26 ng	149149	Phenanthrene-d10		17.05		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(4-Fluoro-benzenesulfonyl)-pip...	286	C12H15FN2O3S	1000295-13-0	53
2			1H-Imidazole, 4-methyl-5-nitro-	127	C4H5N3O2	014003-66-8	50
3			1H-Imidazole, 1-methyl-5-nitro-	127	C4H5N3O2	003034-42-2	47
4			1-Ethylhexyl propylphosphonofluo...	238	C11H24F02P	1000298-40-8	47
5			Piperazine, 1-methyl-4-[2-(p-tol...	282	C14H22N2O2S	016191-68-7	40



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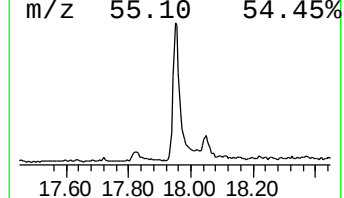
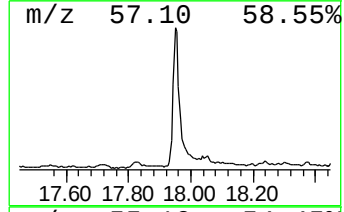
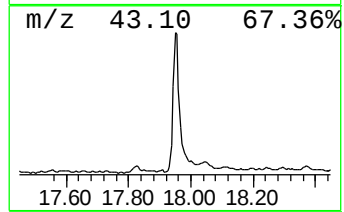
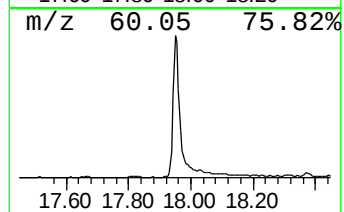
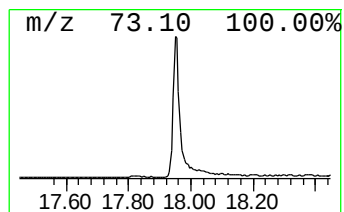
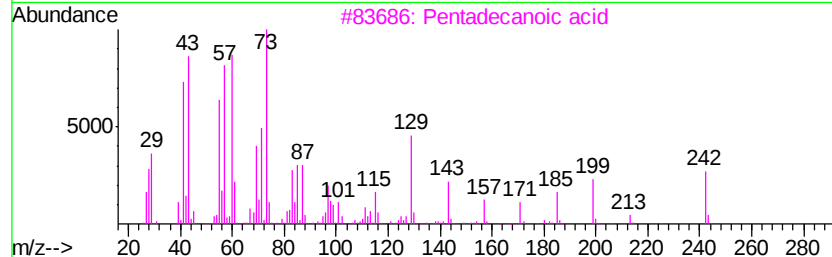
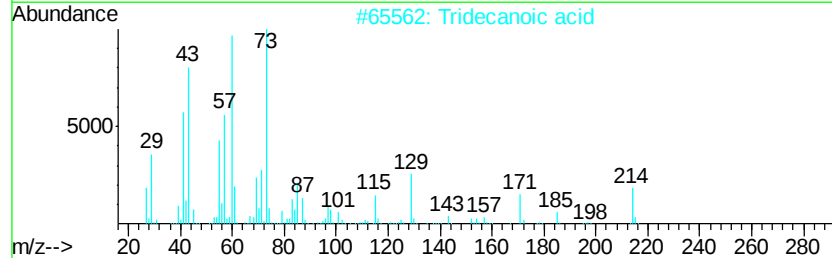
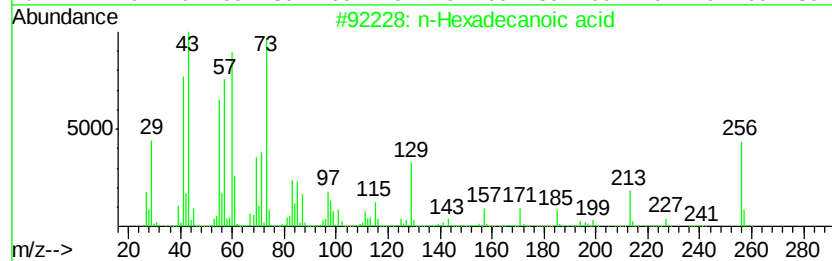
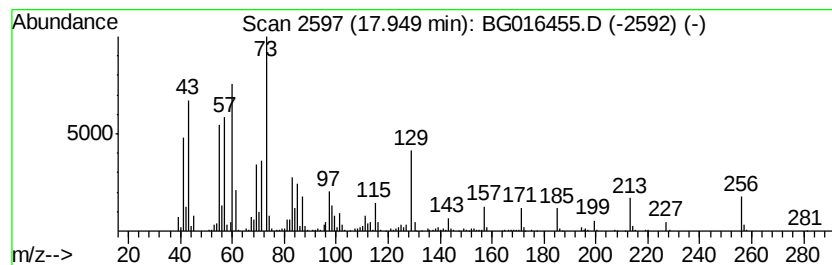
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.95	12.45 ng	821125	Phenanthrene-d10		17.05	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tridecanoic acid		214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	72
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
5	Undecanoic acid		186	C11H22O2	000112-37-8	64



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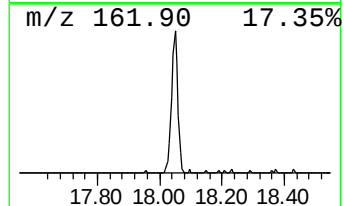
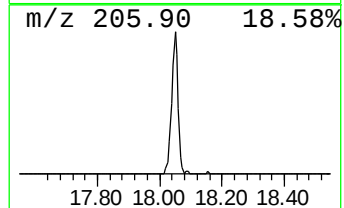
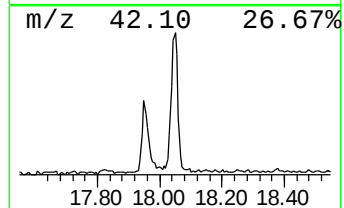
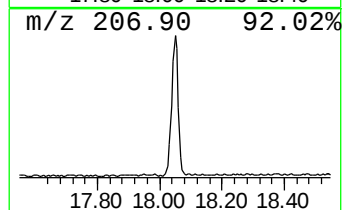
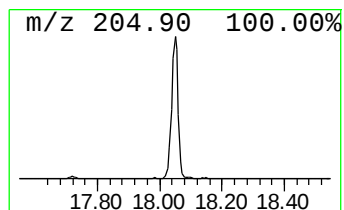
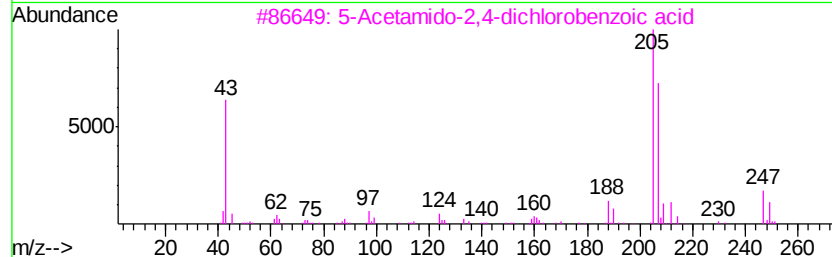
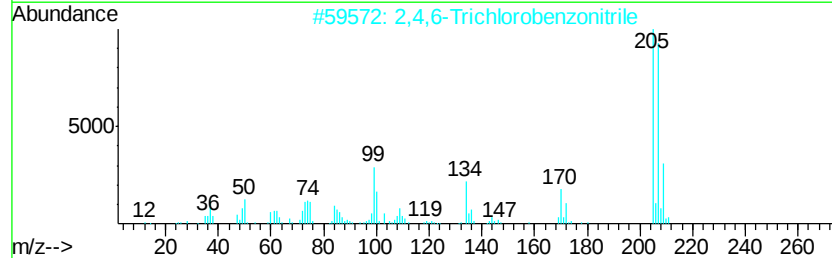
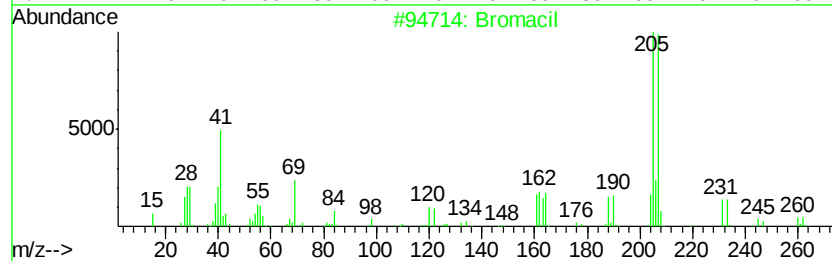
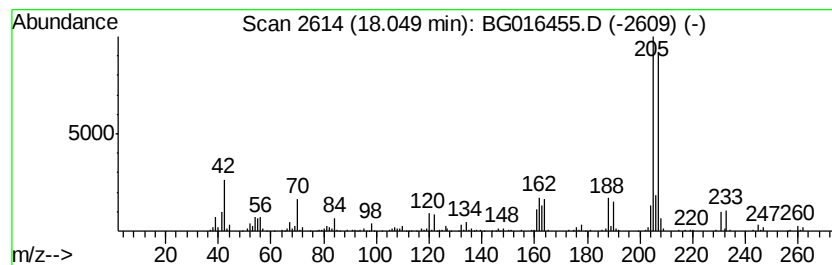
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 8 Bromacil Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.		
18.05	6.21 ng	409364	Phenanthrene-d10	17.05		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromacil	260	C9H13BrN2O2	000314-40-9	98
2		2,4,6-Trichlorobenzonitrile	205	C7H2Cl3N	006575-05-9	53
3		5-Acetamido-2,4-dichlorobenzoic ...	247	C9H7Cl2NO3	050602-49-8	50
4		Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	50
5		5-Chloro-2,3-dihydrofuro(2,3-b)q...	205	C11H8ClNO	064124-92-1	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016455.D
Acq On : 16 Apr 2015 11:47
Operator : TP/IZ
Sample : G1829-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

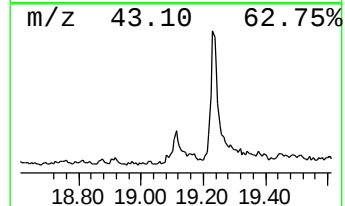
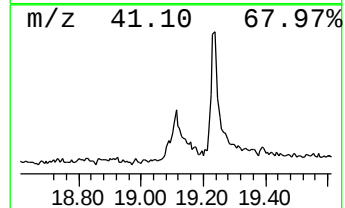
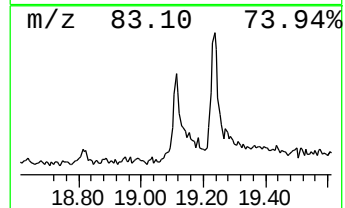
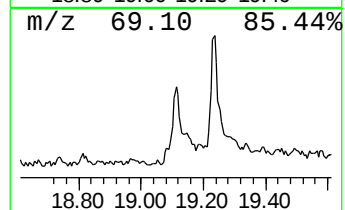
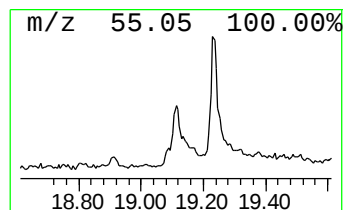
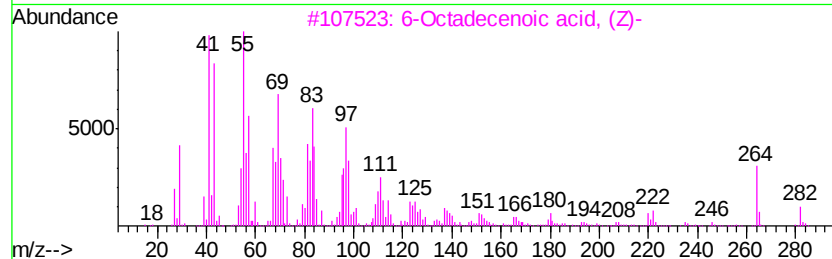
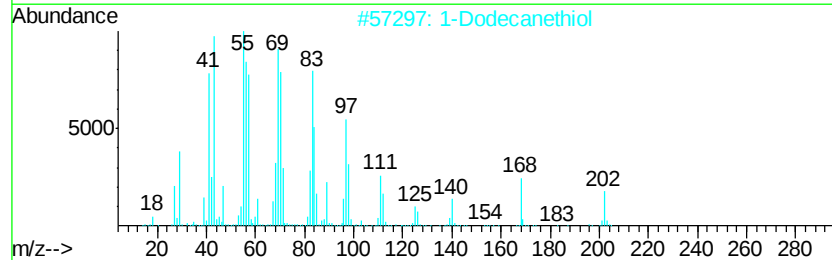
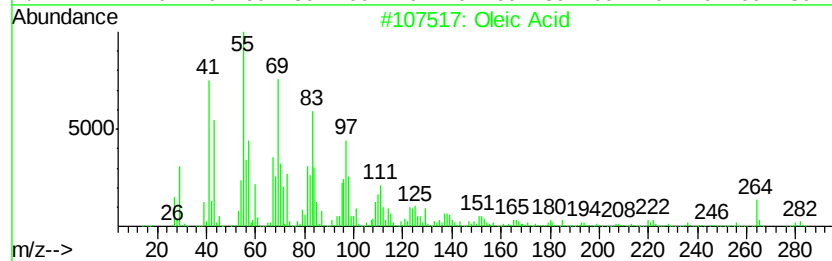
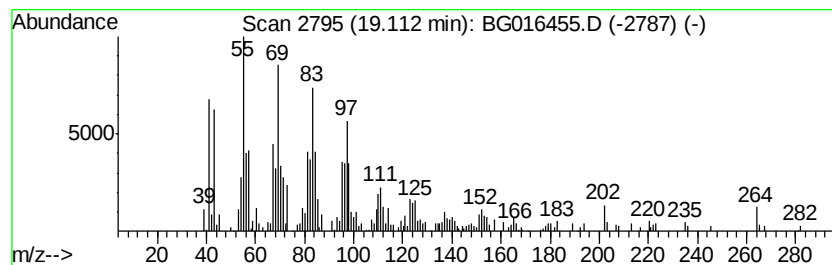
Instrument :
BNA_G
ClientSampleId :
TE-PMW-42

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 9 Oleic Acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.11	5.14 ng	338975	Phenanthrene-d10		17.05
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	94
2	1-Dodecanethiol	202	C12H26S	000112-55-0	83
3	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	83
4	1-Dodecanol	186	C12H26O	000112-53-8	80
5	1-Hexadecanol	242	C16H34O	036653-82-4	76



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016455.D
Acq On : 16 Apr 2015 11:47
Operator : TP/IZ
Sample : G1829-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

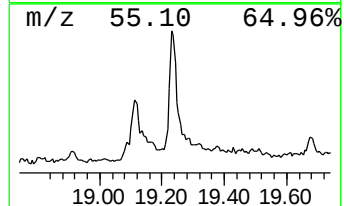
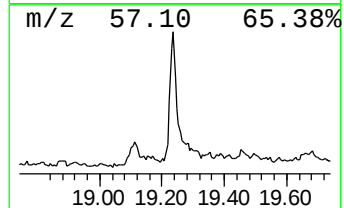
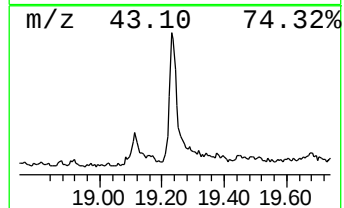
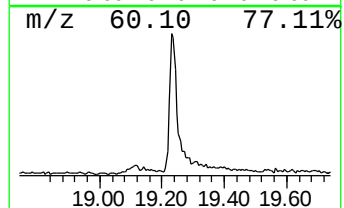
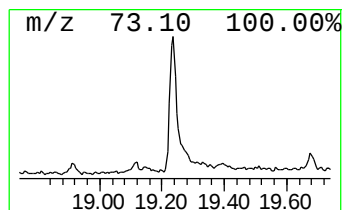
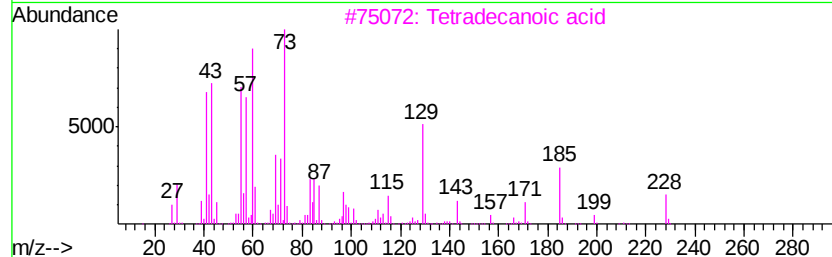
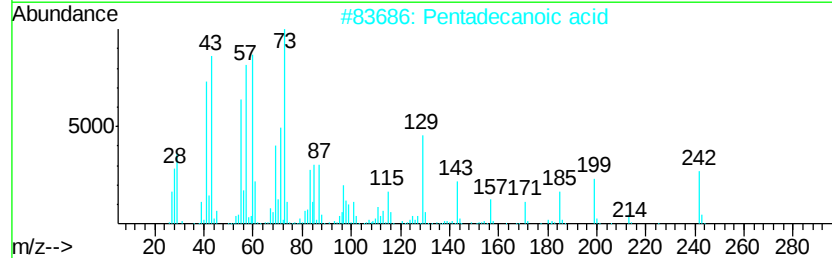
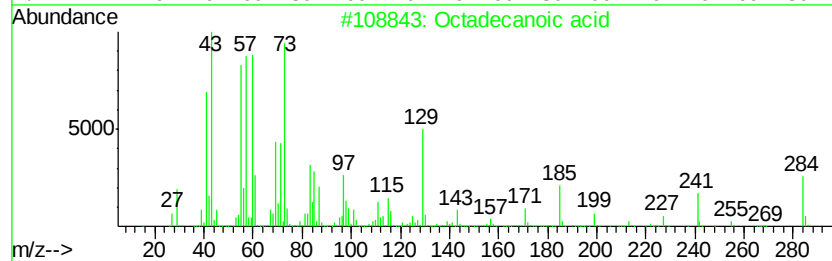
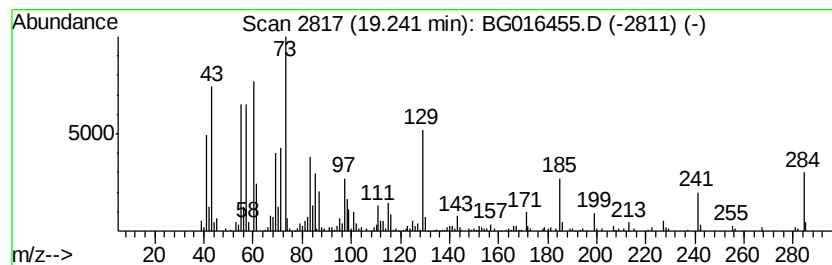
Instrument :
BNA_G
ClientSampleId :
TE-PMW-42

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 10 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.24	7.76 ng	501133	Chrysene-d12	21.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Octadecanoic acid	284 C18H36O2	000057-11-4 99
2		Pentadecanoic acid	242 C15H30O2	001002-84-2 81
3		Tetradecanoic acid	228 C14H28O2	000544-63-8 72
4		Tridecanoic acid	214 C13H26O2	000638-53-9 64
5		n-Decanoic acid	172 C10H20O2	000334-48-5 60



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016455.D
Acq On : 16 Apr 2015 11:47
Operator : TP/IZ
Sample : G1829-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TE-PMW-42

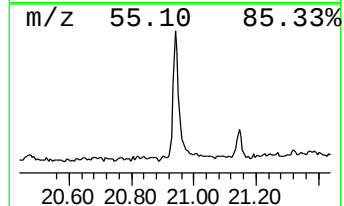
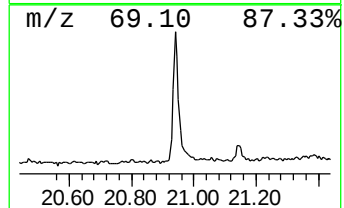
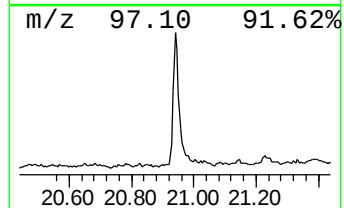
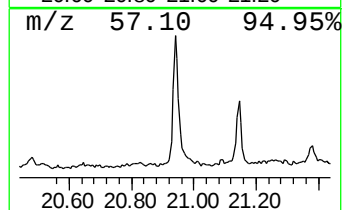
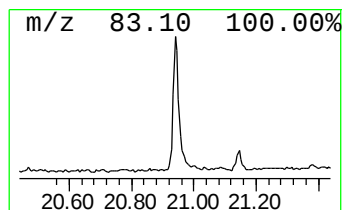
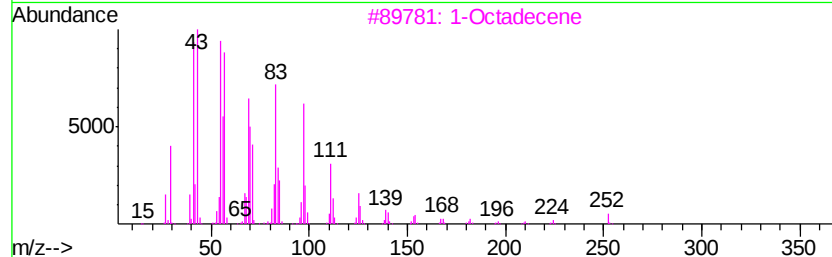
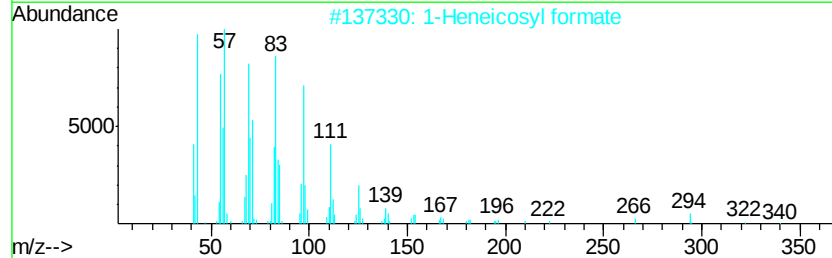
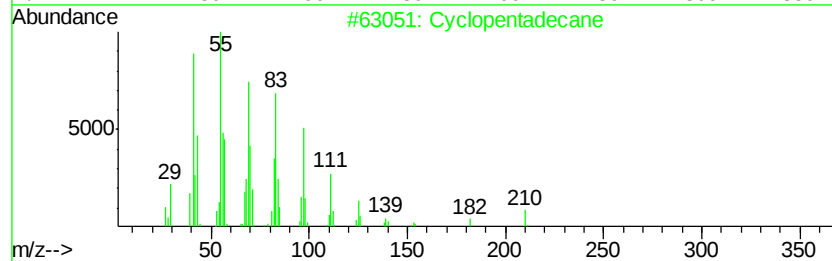
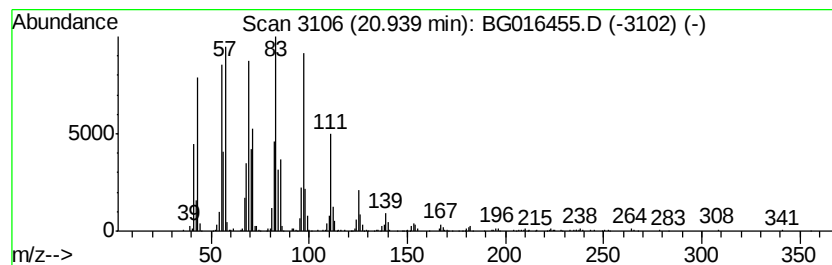
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Cyclopentadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.94	7.58 ng	489635	Chrysene-d12	21.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	95
2		1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3		1-Octadecene	252	C18H36	000112-88-9	92
4		1-Heptadecanol	256	C17H36O	001454-85-9	91
5		1-Hexadecanol	242	C16H34O	036653-82-4	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016455.D
Acq On : 16 Apr 2015 11:47
Operator : TP/IZ
Sample : G1829-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TE-PMW-42

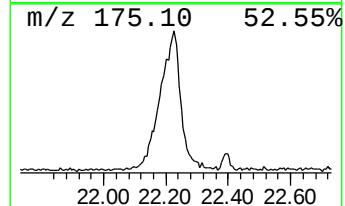
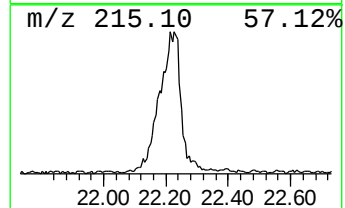
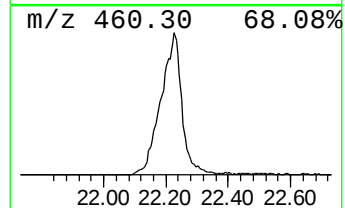
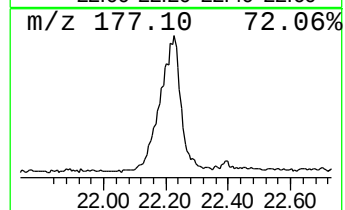
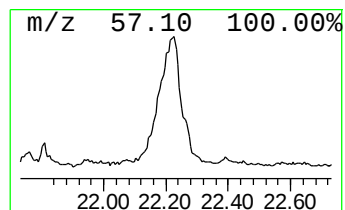
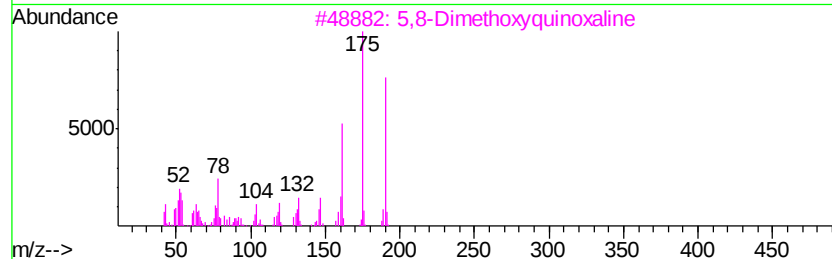
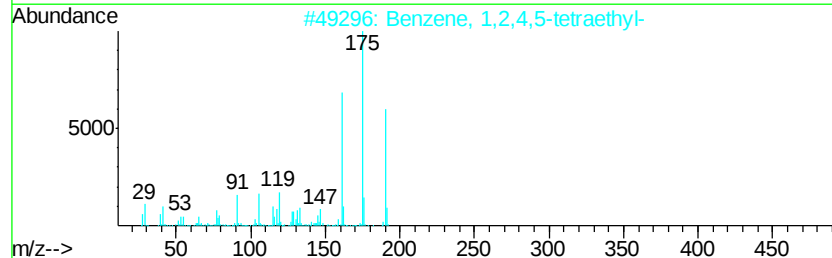
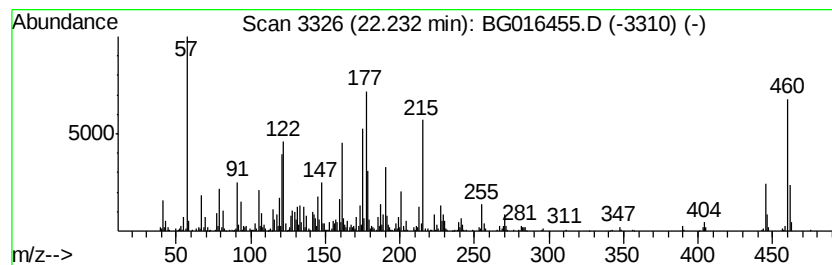
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown22.23 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.23	30.28 ng	1956120	Chrysene-d12	21.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Triazine-2,4,6-triamine, N...	460	C27H24N8	033933-66-3	10
2		Benzene, 1,2,4,5-tetraethyl-	190	C14H22	000635-81-4	10
3		5,8-Dimethoxyquinoxaline	190	C10H10N2O2	019506-19-5	10
4		Benzene, 1,4-bis(3-phenylindol-2...	460	C34H24N2	164936-88-3	10
5		1-Ethyl-2-bromo-1,3,4-triazole	175	C4H6BrN3	064907-56-8	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016455.D
Acq On : 16 Apr 2015 11:47
Operator : TP/IZ
Sample : G1829-04
Misc :
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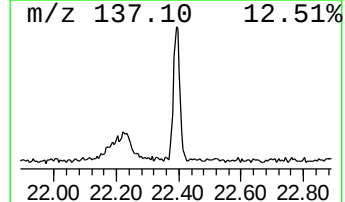
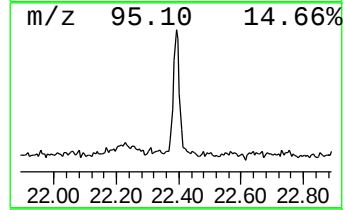
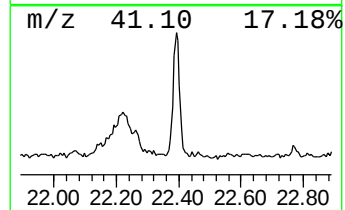
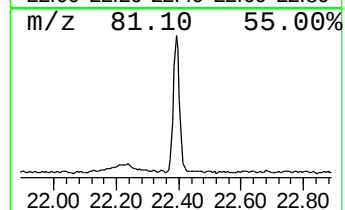
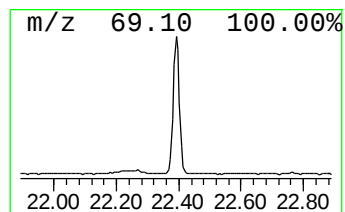
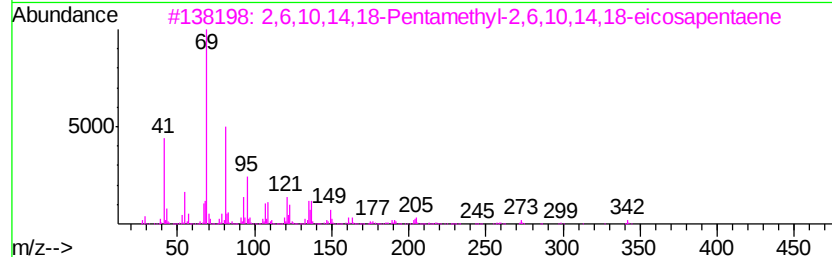
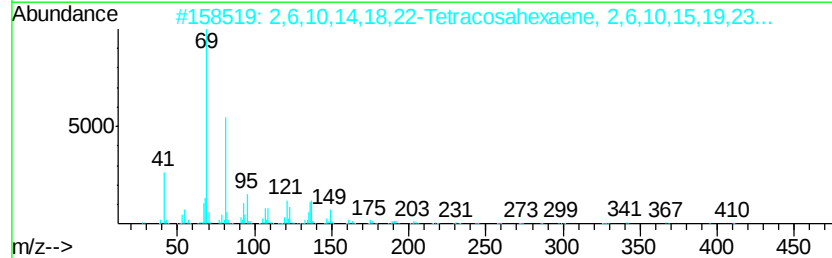
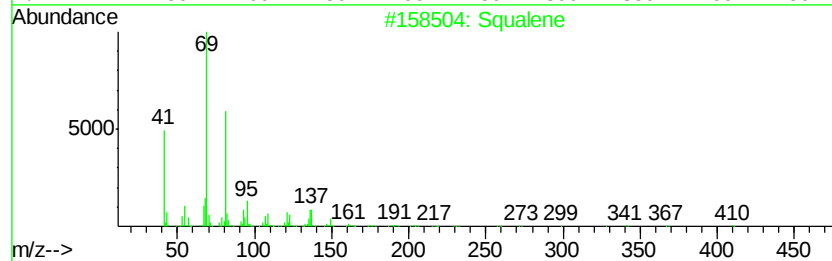
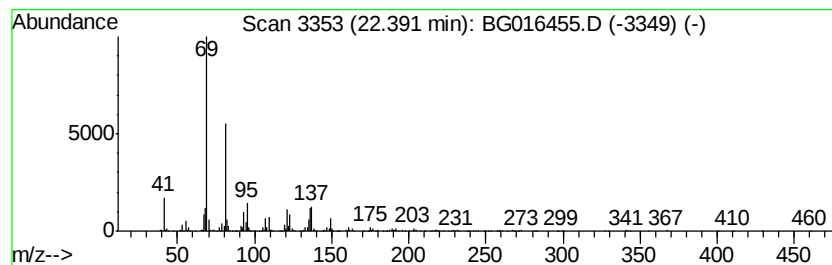
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.39	7.95 ng	501043	Perylene-d12	23.46
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene		410 C30H50	007683-64-9 97
2	2,6,10,14,18,22-Tetracosahexaene...		410 C30H50	000111-02-4 96
3	2,6,10,14,18-Pentamethyl-2,6,10,...		342 C25H42	075581-03-2 93
4	Docosa-2,6,10,14,18-pentaen-22-a...		384 C27H44O	1000163-04-7 83
5	1,5,9-Undecatriene, 2,6,10-trime...		192 C14H24	062951-96-6 74



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
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Acq On : 16 Apr 2015 11:47
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ALS Vial : 20 Sample Multiplier: 1

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ClientSampleId :
TE-PMW-42

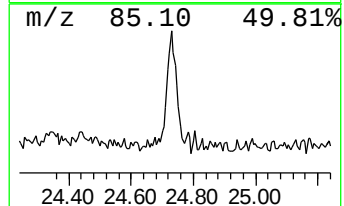
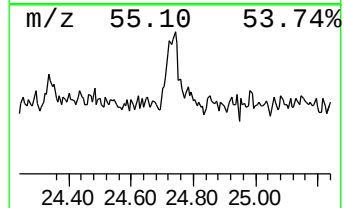
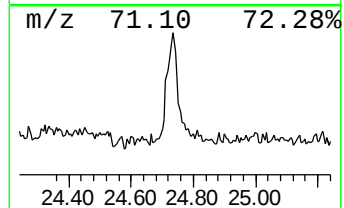
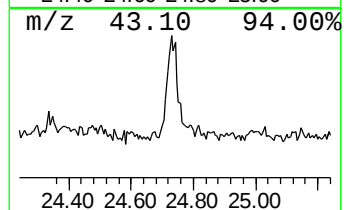
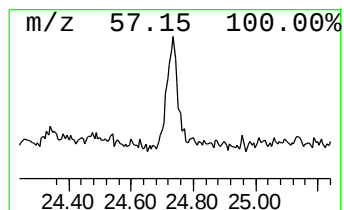
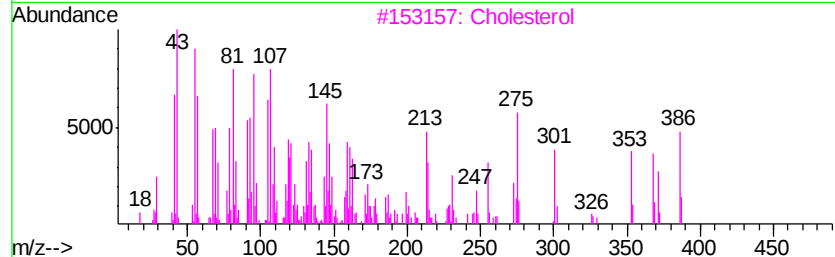
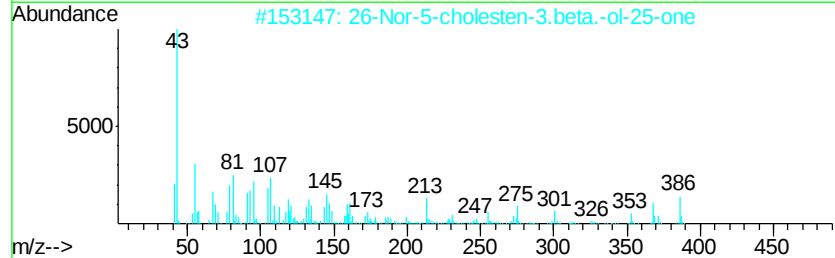
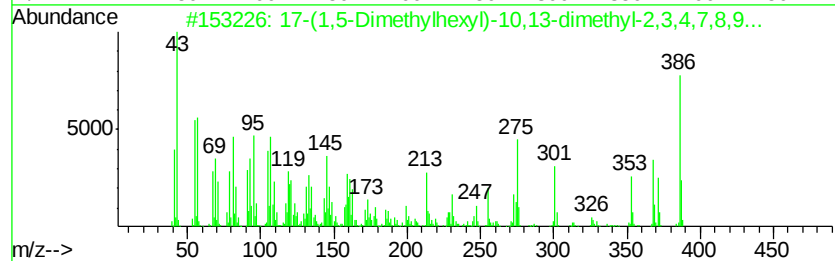
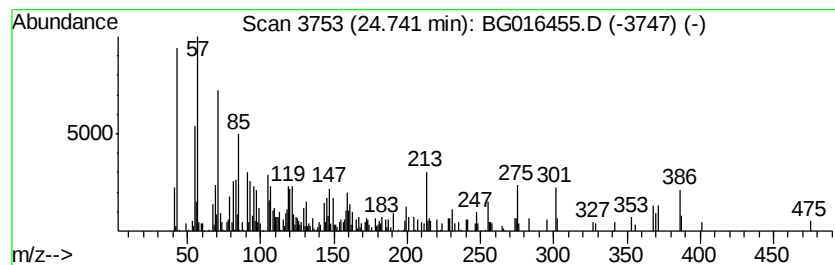
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 17-(1,5-Dimethylhexyl)-10,1... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.74	2.56 ng	161479	Perylene-d12	23.46

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	53
2			26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	53
3			Cholesterol	386	C27H46O	000057-88-5	38
4			Hexadecane	226	C16H34	000544-76-3	35
5			Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	30



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
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Acq On : 16 Apr 2015 11:47
Operator : TP/IZ
Sample : G1829-04
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TE-PMW-42

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...	2.84	22.1	ng	493772	1	7.67	447169	20.0
unknown7.20	7.20	95.9	ng	2144200	1	7.67	447169	20.0
1-(4-Fluoro-benze...	16.08	2.3	ng	149149	4	17.05	1319090	20.0
n-Hexadecanoic acid	17.95	12.4	ng	821125	4	17.05	1319090	20.0
Bromacil	18.05	6.2	ng	409364	4	17.05	1319090	20.0
Oleic Acid	19.11	5.1	ng	338975	4	17.05	1319090	20.0
Octadecanoic acid	19.24	7.8	ng	501133	5	21.23	1292030	20.0
Cyclopentadecane	20.94	7.6	ng	489635	5	21.23	1292030	20.0
unknown22.23	22.23	30.3	ng	1956120	5	21.23	1292030	20.0
Squalene	22.39	8.0	ng	501043	6	23.46	1260070	20.0
17-(1,5-Dimethylh...	24.74	2.6	ng	161479	6	23.46	1260070	20.0