

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016450.D
 Acq On : 16 Apr 2015 8:54
 Operator : TP/IZ
 Sample : G1829-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TE-PMW-43

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	2.761	7	12	21	rBV	381522	605464	13.33%	2.170%
2	2.837	21	25	32	rVB	426475	478878	10.55%	1.716%
3	4.782	350	356	363	rBV	57087	85273	1.88%	0.306%
4	5.258	431	437	445	rBV	696073	971240	21.39%	3.480%
5	6.856	703	709	725	rVB	461759	719654	15.85%	2.579%
6	7.203	761	768	777	rBV	1320308	1994462	43.92%	7.147%
7	7.667	840	847	856	rBV	281640	444077	9.78%	1.591%
8	7.984	894	901	911	rVB	1062754	1666636	36.70%	5.972%
9	8.824	1037	1044	1055	rVB	912179	1462472	32.21%	5.240%
10	10.452	1313	1321	1327	rBV	427232	719927	15.85%	2.580%
11	12.925	1735	1742	1753	rVB	2440906	3731259	82.17%	13.370%
12	13.766	1880	1885	1893	rVB	36218	52156	1.15%	0.187%
13	14.306	1970	1977	1985	rBV2	716650	1066124	23.48%	3.820%
14	15.669	2200	2209	2215	rBV	56804	88893	1.96%	0.319%
15	15.798	2225	2231	2245	rBV	1842709	2642962	58.20%	9.470%
16	16.462	2338	2344	2350	rBV2	43022	64821	1.43%	0.232%
17	17.050	2435	2444	2449	rBV2	933929	1301049	28.65%	4.662%
18	17.826	2569	2576	2584	rBV10	29119	64992	1.43%	0.233%
19	17.949	2592	2597	2606	rBV	267593	412021	9.07%	1.476%
20	18.378	2666	2670	2674	rVB2	38385	46406	1.02%	0.166%
21	19.112	2788	2795	2810	rBV2	93669	276657	6.09%	0.991%
22	19.236	2812	2816	2831	rVB	121875	217578	4.79%	0.780%
23	19.682	2886	2892	2897	rBV	3587336	4541124	100.00%	16.272%
24	20.223	2980	2984	2989	rVB	113051	142341	3.13%	0.510%
25	20.910	3098	3101	3103	rBV	51288	51598	1.14%	0.185%
26	20.945	3103	3107	3116	rVB	285695	401382	8.84%	1.438%
27	21.145	3137	3141	3146	rBV	250367	272063	5.99%	0.975%
28	21.227	3150	3155	3161	rBV	984051	1282488	28.24%	4.595%
29	22.397	3349	3354	3361	rVB	688963	908817	20.01%	3.257%
30	23.460	3529	3535	3544	rVB2	666098	1194787	26.31%	4.281%

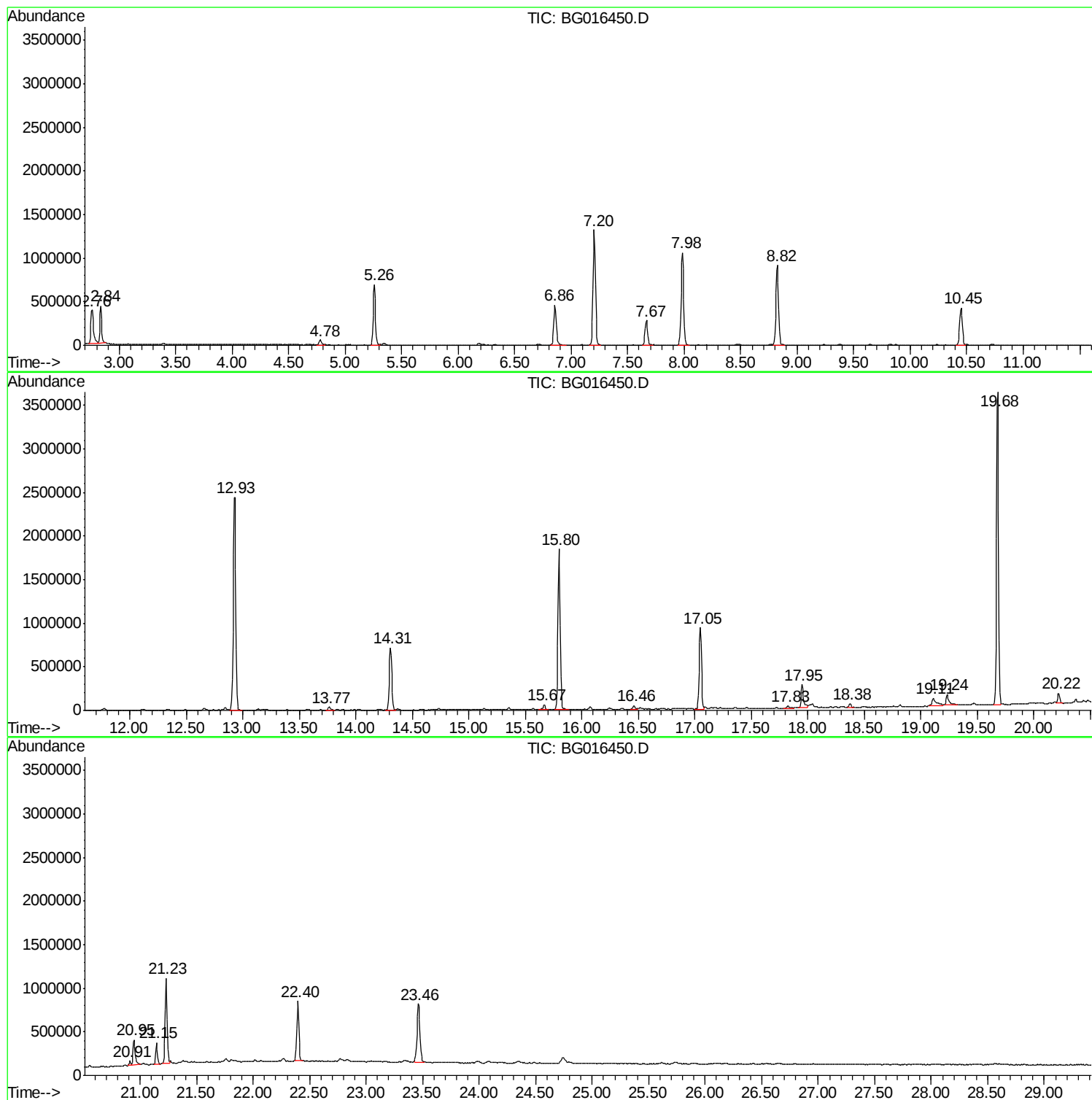
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
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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



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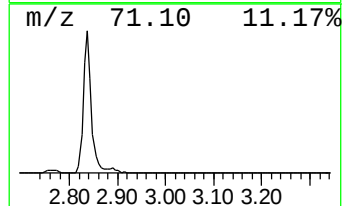
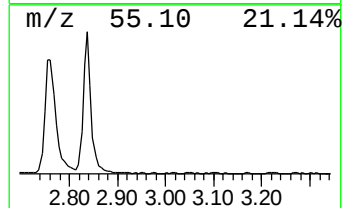
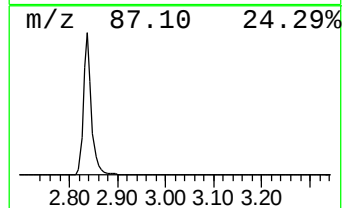
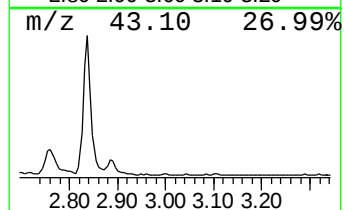
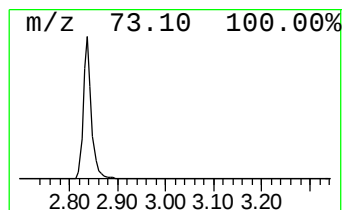
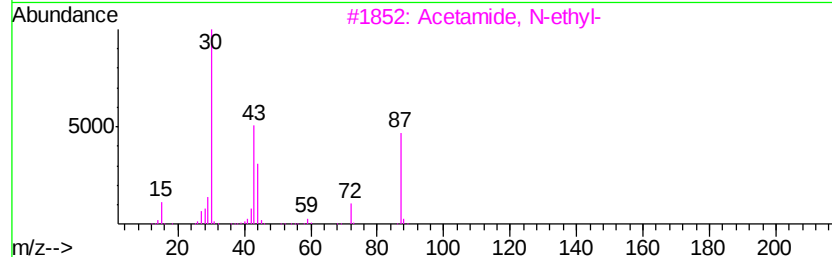
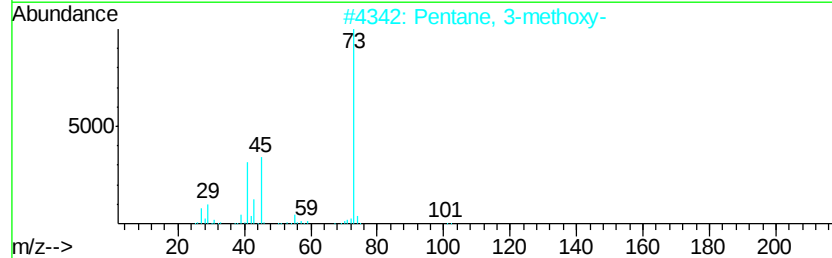
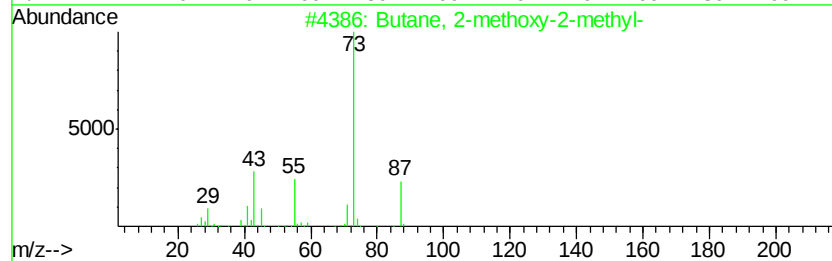
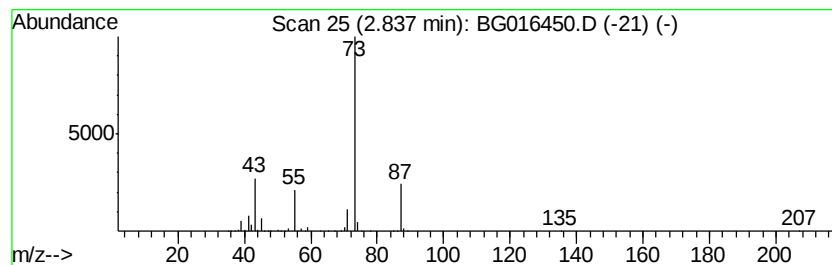
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	21.57 ng	478878	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	23
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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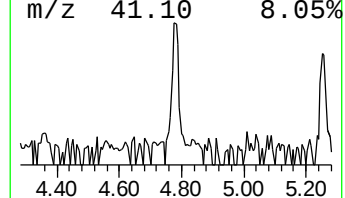
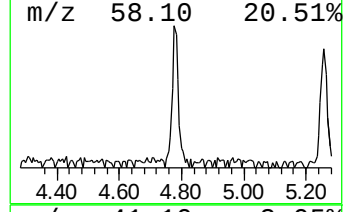
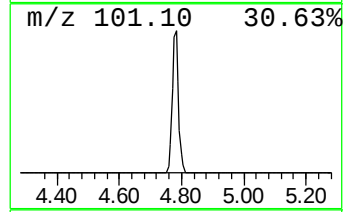
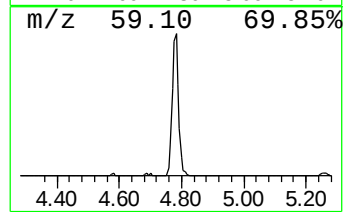
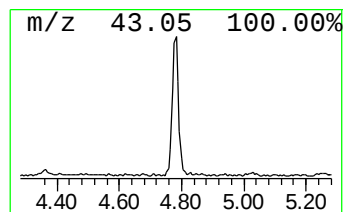
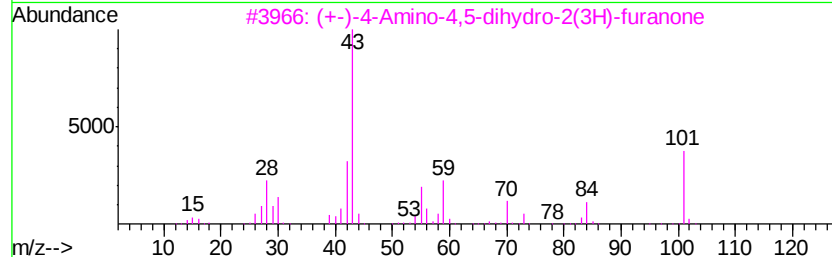
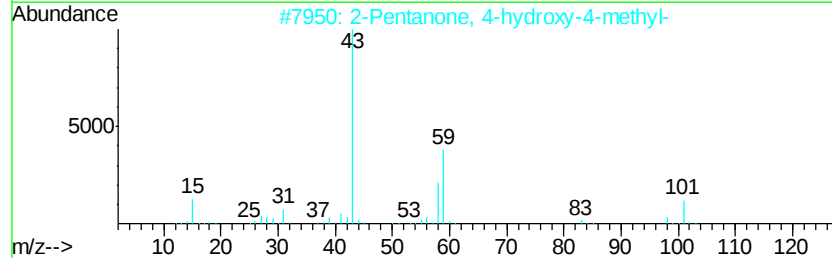
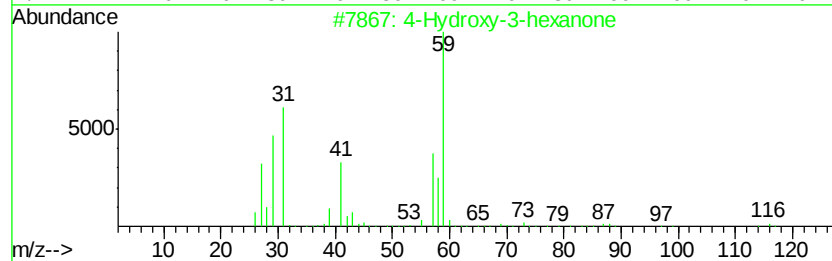
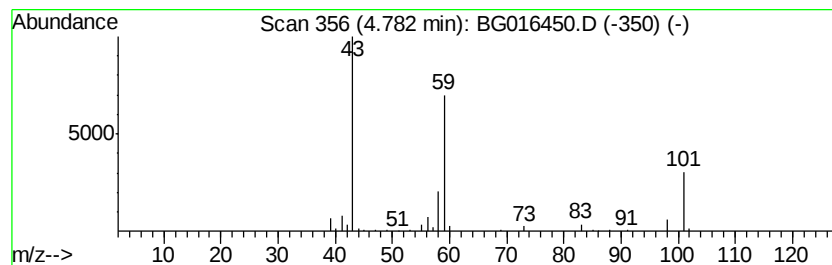
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown4.78 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	3.84 ng	85273	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	43
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
3		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	23
4		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	12
5		Hexanamide	115	C6H13NO	000628-02-4	12



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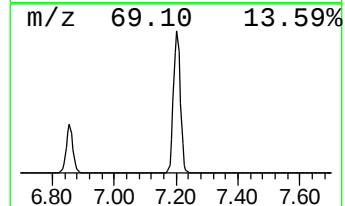
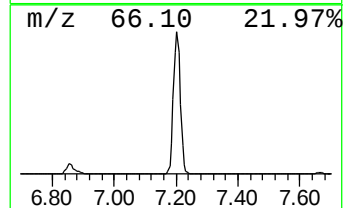
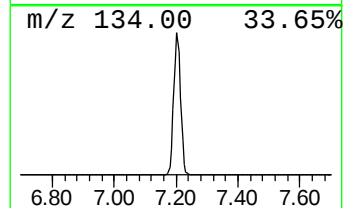
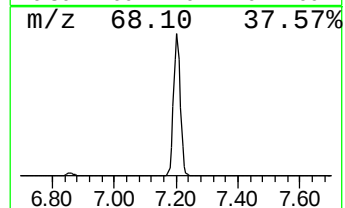
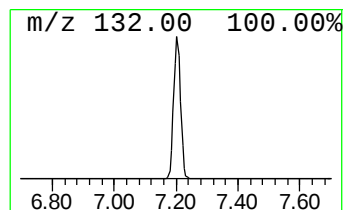
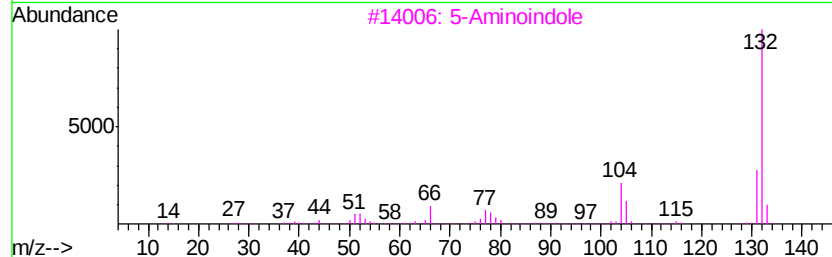
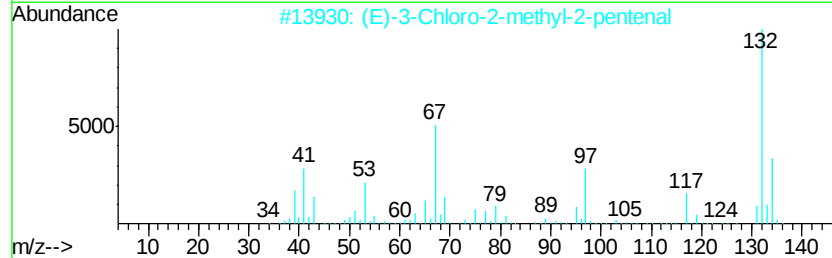
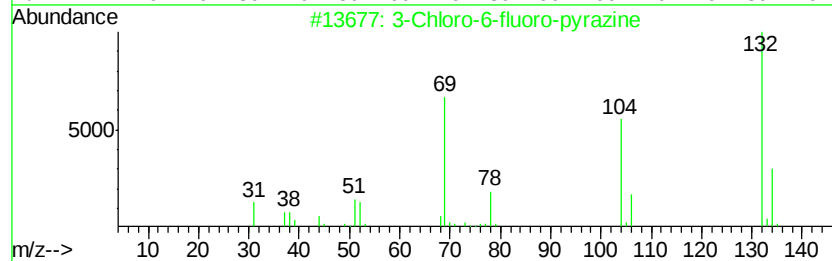
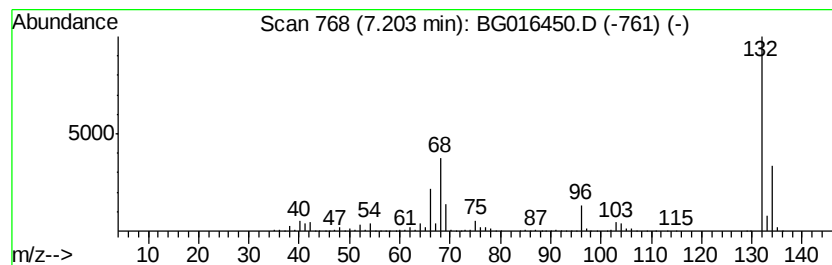
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	89.83 ng	1994460	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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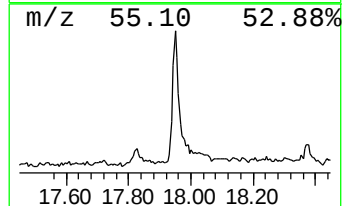
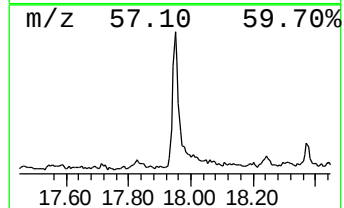
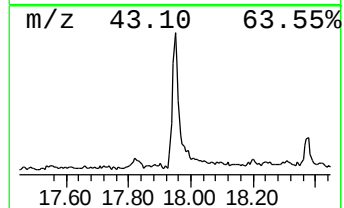
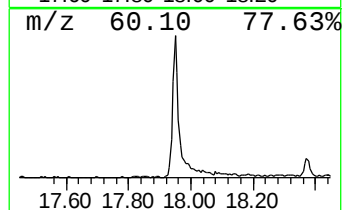
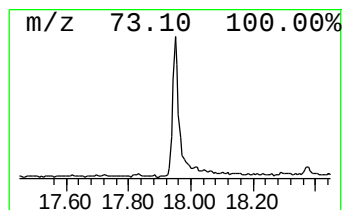
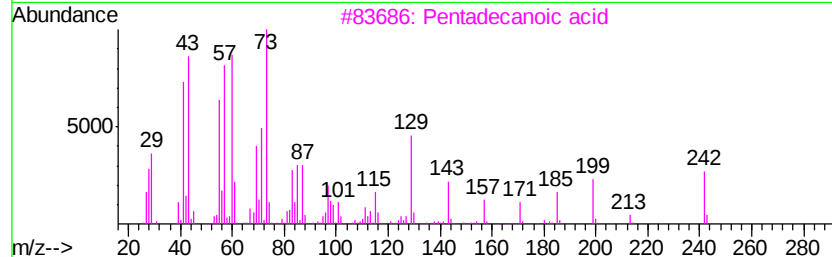
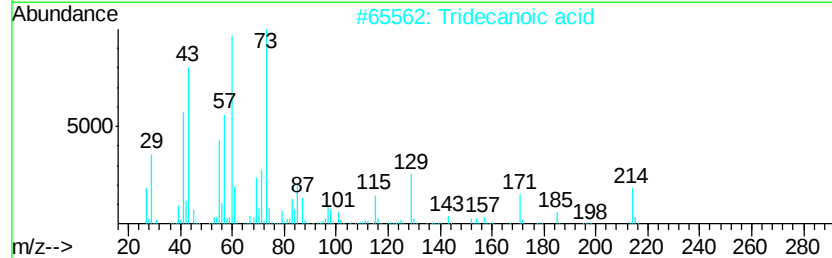
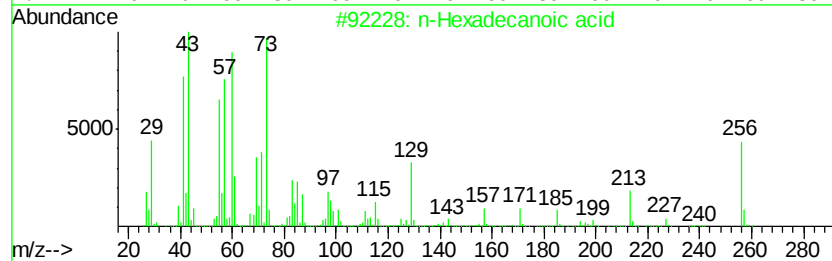
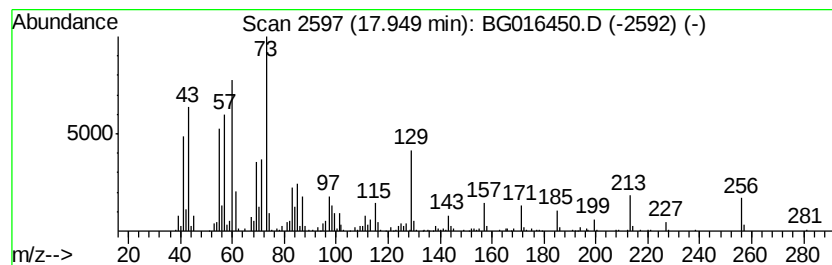
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.95	6.33 ng	412021	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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



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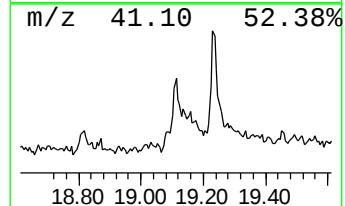
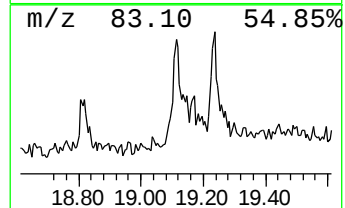
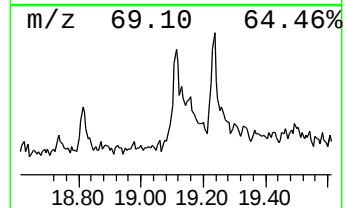
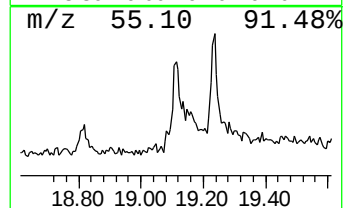
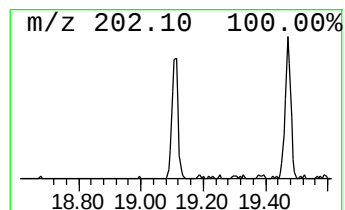
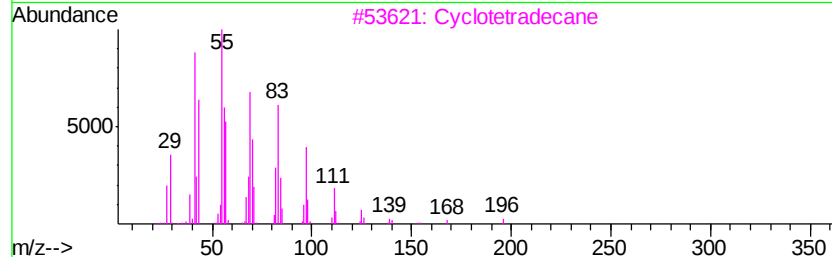
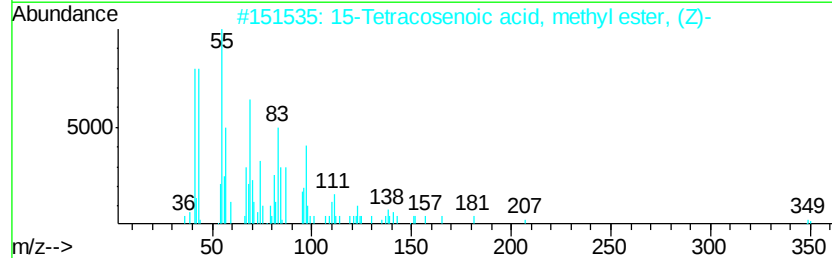
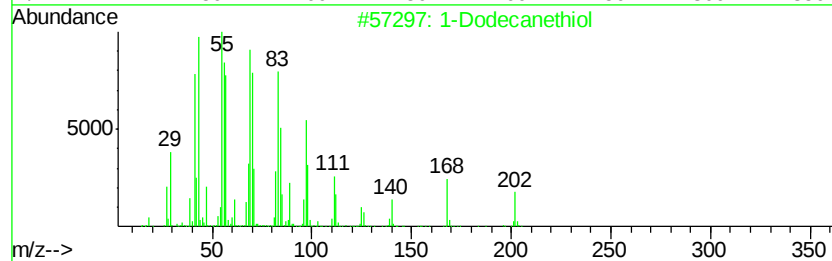
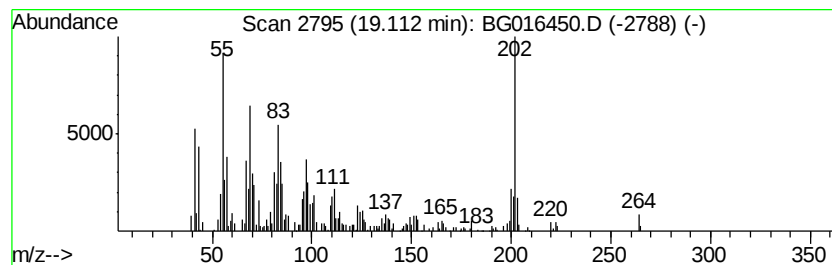
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 7 1-Dodecanethiol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.11	4.25 ng	276657	Phenanthrene-d10	17.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanethiol		202	C12H26S	000112-55-0	64
2	15-Tetracosenoic acid, methyl es...		380	C25H48O2	002733-88-2	50
3	Cyclotetradecane		196	C14H28	000295-17-0	42
4	5-Tetradecene, (Z)-		196	C14H28	041446-62-2	38
5	Oxacyclotetradecan-2-one, 13-met...		226	C14H26O2	057092-32-7	38



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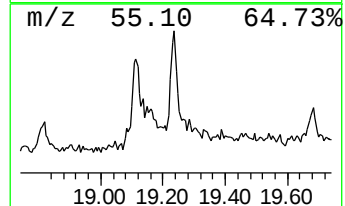
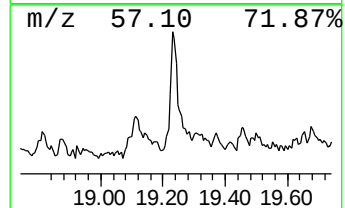
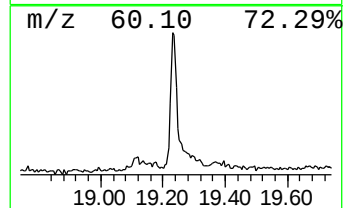
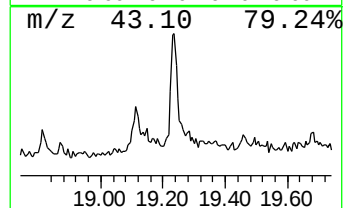
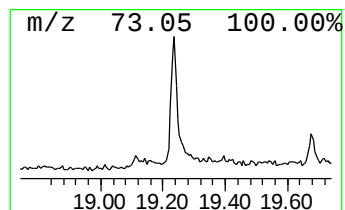
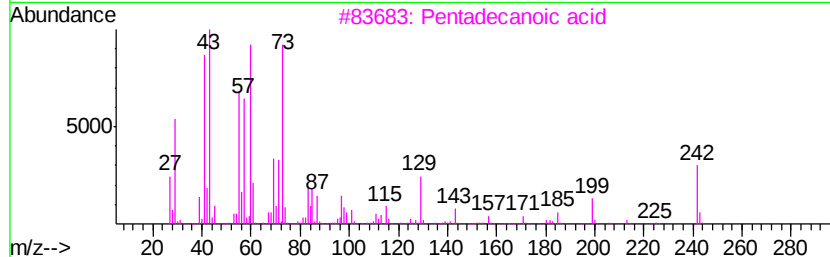
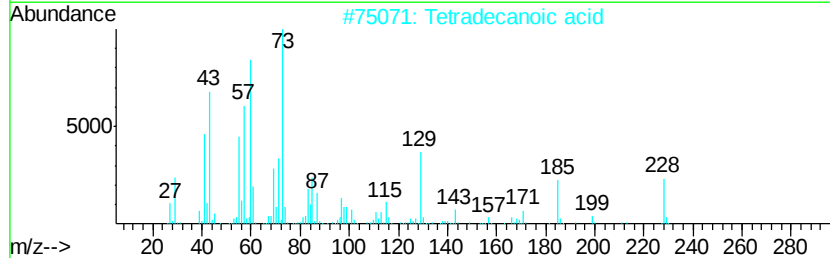
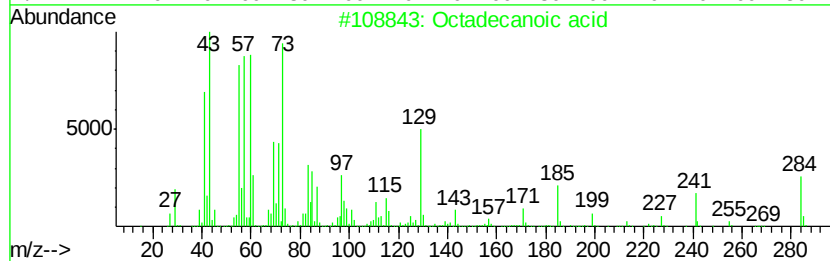
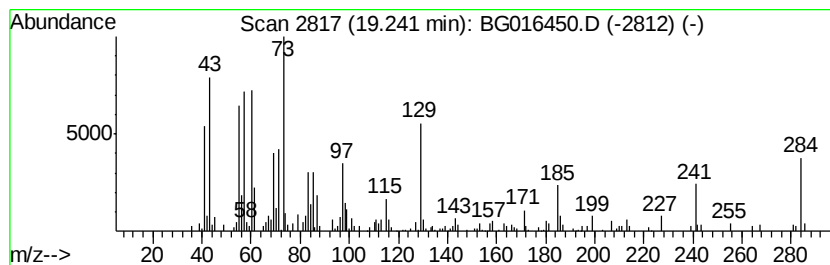
Instrument :
BNA_G
ClientSampleId :
TE-PMW-43

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 8 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.24	3.39 ng	217578	Chrysene-d12	21.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	55
5	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	25



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016450.D
Acq On : 16 Apr 2015 8:54
Operator : TP/IZ
Sample : G1829-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

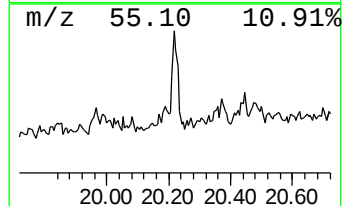
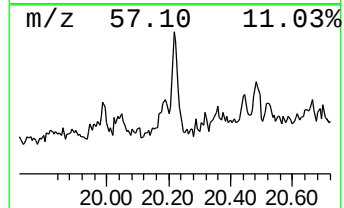
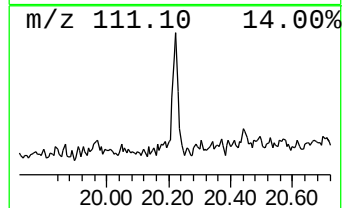
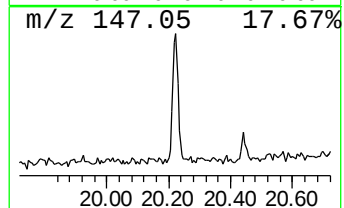
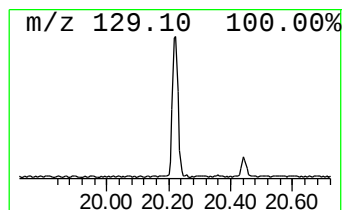
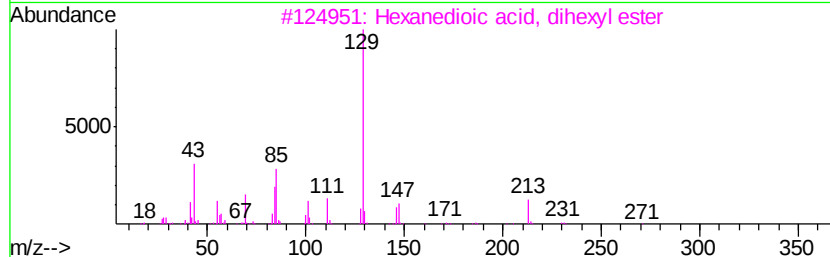
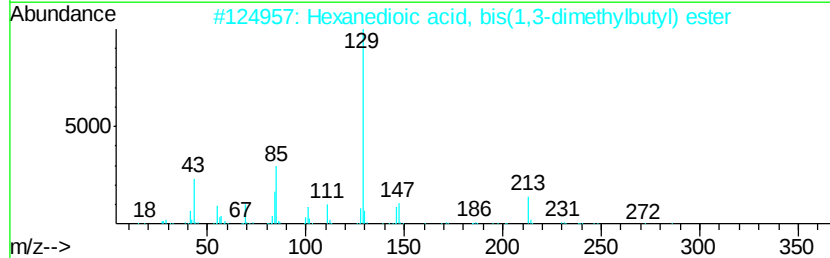
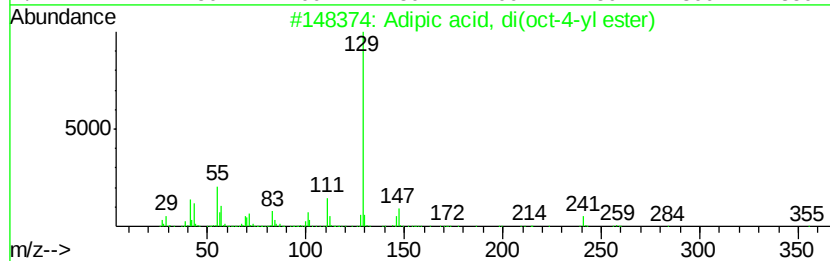
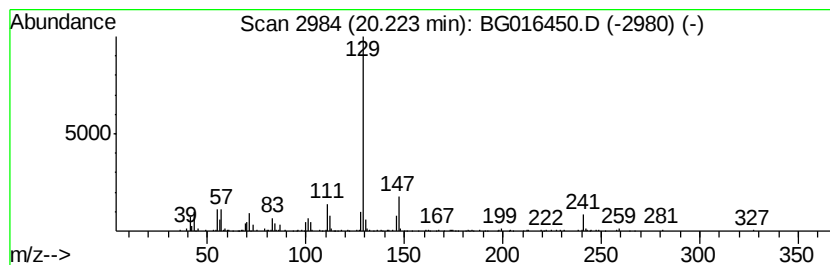
Instrument :
BNA_G
ClientSampleId :
TE-PMW-43

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 Adipic acid, di(oct-4-yl es... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.22	2.22 ng	142341	Chrysene-d12	21.23
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Adipic acid, di(oct-4-yl ester)	370 C22H42O4	1000160-80-1	91
2	Hexanedioic acid, bis(1,3-dimeth...	314 C18H34O4	055125-22-9	78
3	Hexanedioic acid, dihexyl ester	314 C18H34O4	000110-33-8	64
4	Hexanedioic acid, mono(2-ethylhe...	258 C14H26O4	004337-65-9	59
5	Hexanedioic acid, bis(2-ethylhex...	370 C22H42O4	000103-23-1	56



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016450.D
Acq On : 16 Apr 2015 8:54
Operator : TP/IZ
Sample : G1829-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

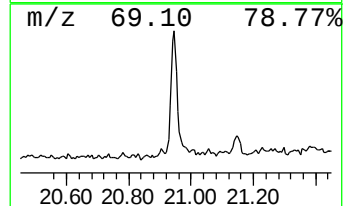
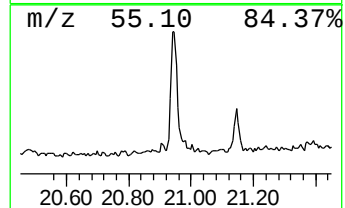
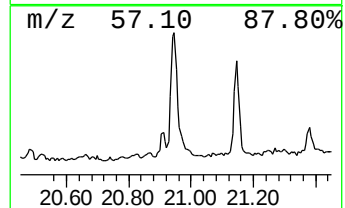
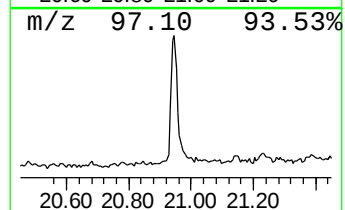
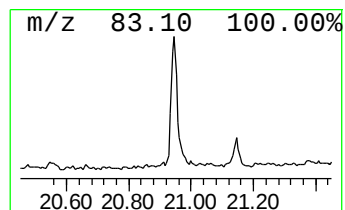
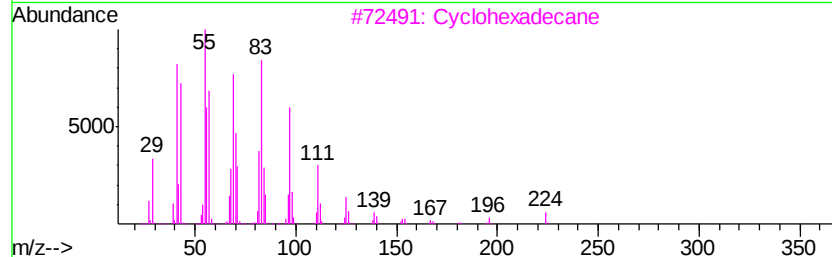
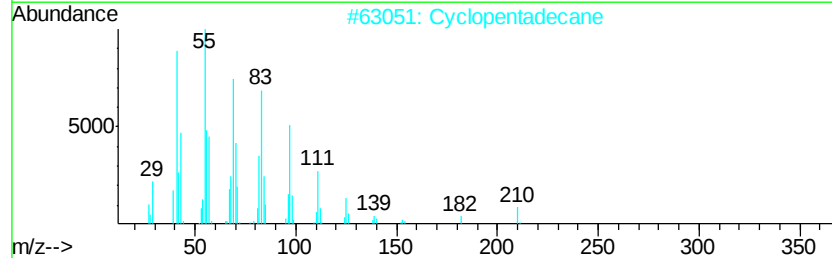
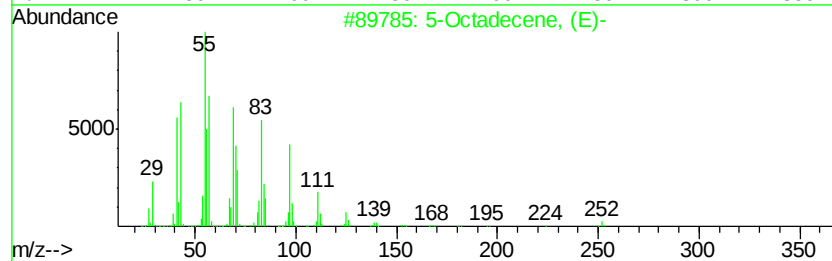
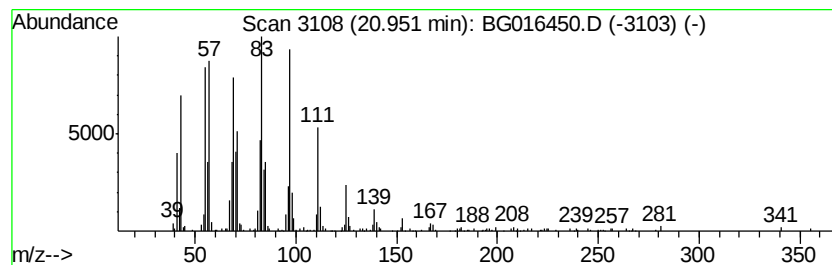
Instrument :
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ClientSampleId :
TE-PMW-43

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 5-Octadecene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.95	6.26 ng	401382	Chrysene-d12	21.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	95
2	Cyclopentadecane	210	C15H30	000295-48-7	95
3	Cyclohexadecane	224	C16H32	000295-65-8	93
4	Cyclotetradecane	196	C14H28	000295-17-0	93
5	1-Heptadecanol	256	C17H36O	001454-85-9	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016450.D
Acq On : 16 Apr 2015 8:54
Operator : TP/IZ
Sample : G1829-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

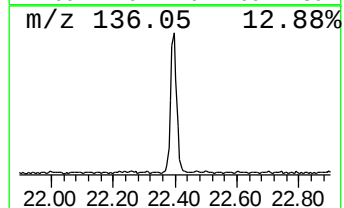
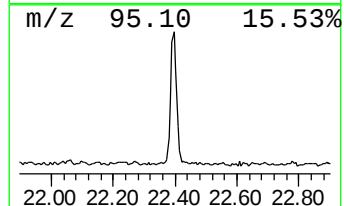
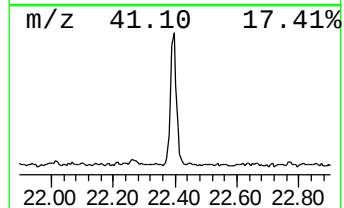
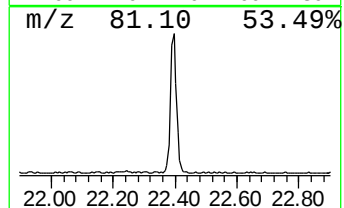
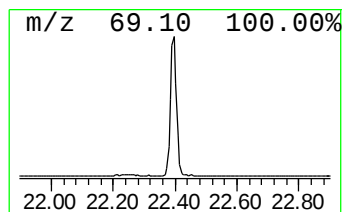
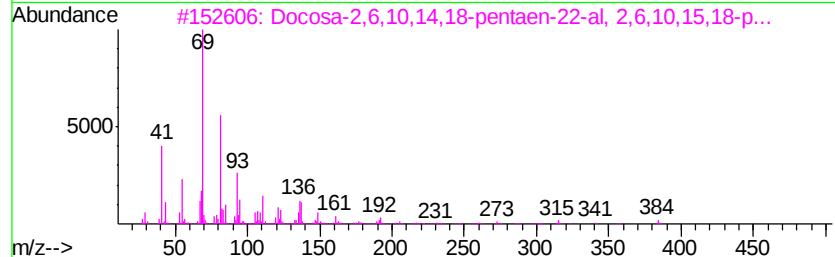
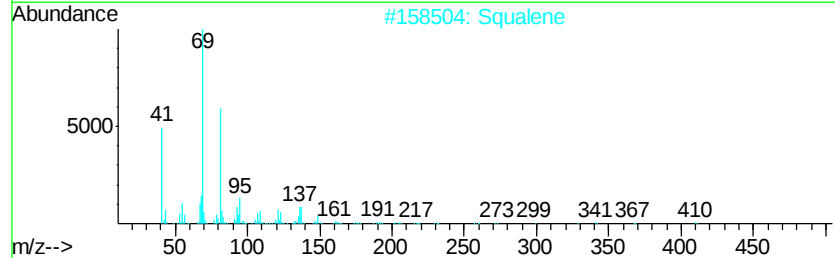
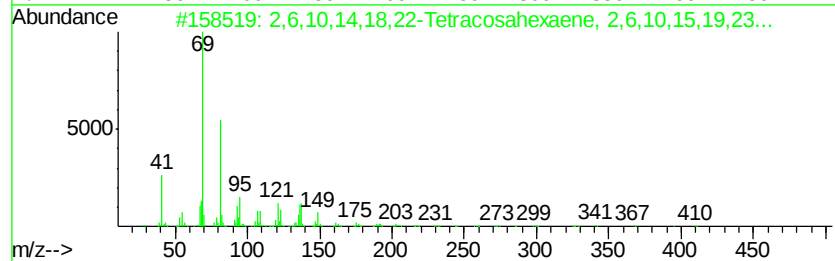
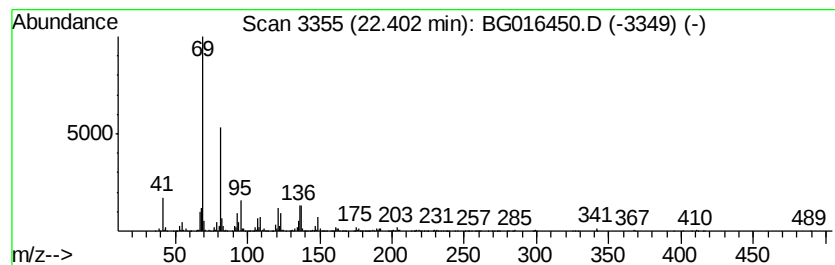
Instrument :
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ClientSampleId :
TE-PMW-43

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 11 2,6,10,14,18,22-Tetracosae... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.40	15.21 ng	908817	Perylene-d12	23.46	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	99
2	Squalene	410	C30H50	007683-64-9	98
3	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	74
5	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016450.D
Acq On : 16 Apr 2015 8:54
Operator : TP/IZ
Sample : G1829-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TE-PMW-43

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	21.6	ng	478878	1	7.67	444077	20.0
unknown4.78	4.78	3.8	ng	85273	1	7.67	444077	20.0
unknown7.20	7.20	89.8	ng	1994460	1	7.67	444077	20.0
n-Hexadecanoic acid	17.95	6.3	ng	412021	4	17.05	1301050	20.0
1-Dodecanethiol	19.11	4.3	ng	276657	4	17.05	1301050	20.0
Octadecanoic acid	19.24	3.4	ng	217578	5	21.23	1282490	20.0
Adipic acid, di(o...	20.22	2.2	ng	142341	5	21.23	1282490	20.0
5-Octadecene, (E)-	20.95	6.3	ng	401382	5	21.23	1282490	20.0
2,6,10,14,18,22-T...	22.40	15.2	ng	908817	6	23.46	1194790	20.0