

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
 Data File : BG017021.D
 Acq On : 10 May 2015 12:00
 Operator : TP/IZ
 Sample : G2151-12
 Misc :
 ALS Vial : 63 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TU012-SB-20-7.5

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-BG050515.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	2.775	11	15	28	rVB	4345040	5006162	100.00%	17.380%
2	2.916	34	39	43	rBV2	147953	261740	5.23%	0.909%
3	2.992	48	52	56	rBV	179023	265015	5.29%	0.920%
4	3.897	199	206	211	rBV2	44220	71158	1.42%	0.247%
5	3.991	218	222	230	rVB	77238	109451	2.19%	0.380%
6	4.790	353	358	360	rBV2	37084	51378	1.03%	0.178%
7	4.908	373	378	384	rVB	79446	118773	2.37%	0.412%
8	5.319	432	448	452	rBV2	112026	347625	6.94%	1.207%
9	5.384	452	459	466	rVB	1041975	1544096	30.84%	5.361%
10	6.206	589	599	606	rBV	53443	108351	2.16%	0.376%
11	6.970	721	729	738	rBV	1195209	1890185	37.76%	6.562%
12	7.328	779	790	798	rBV	1113203	1762578	35.21%	6.119%
13	7.787	862	868	876	rVB	226408	361955	7.23%	1.257%
14	8.110	916	923	930	rBV	747518	1172246	23.42%	4.070%
15	8.944	1057	1065	1072	rBV	679936	1144517	22.86%	3.973%
16	9.843	1211	1218	1226	rBV	39413	98363	1.96%	0.341%
17	10.578	1336	1343	1351	rBV	323362	548091	10.95%	1.903%
18	13.051	1755	1764	1770	rBV	1598331	2408379	48.11%	8.361%
19	13.880	1901	1905	1915	rBV	74685	103737	2.07%	0.360%
20	14.426	1988	1998	2005	rBV2	531647	815543	16.29%	2.831%
21	15.912	2245	2251	2259	rBV	1542585	2229854	44.54%	7.742%
22	16.136	2286	2289	2297	rVB2	35248	53959	1.08%	0.187%
23	17.170	2459	2465	2470	rBV2	705538	984653	19.67%	3.418%
24	18.069	2610	2618	2628	rBV	272637	423286	8.46%	1.470%
25	19.226	2812	2815	2821	rVB2	60201	82631	1.65%	0.287%
26	19.344	2831	2835	2839	rBV2	121171	155524	3.11%	0.540%
27	19.591	2873	2877	2883	rVB3	42557	87957	1.76%	0.305%
28	19.796	2906	2912	2919	rBV	2850203	3398512	67.89%	11.799%
29	21.054	3122	3126	3135	rBV	443743	547165	10.93%	1.900%
30	21.200	3147	3151	3156	rBV4	41517	51519	1.03%	0.179%
31	21.347	3170	3176	3180	rBV	795390	1053198	21.04%	3.656%
32	21.494	3198	3201	3210	rVB7	46333	69655	1.39%	0.242%
33	21.952	3273	3279	3283	rBV2	170954	290299	5.80%	1.008%
34	22.123	3303	3308	3314	rVB3	47266	81900	1.64%	0.284%

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Instrument :
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ClientSampleId :
TU012-SB-20-7.5

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	22.934	3442	3446	3449	rBV3	61209	94496	1.89%	0.328%
36	23.645	3560	3567	3574	rBV2	481061	943989	18.86%	3.277%
37	24.285	3673	3676	3681	rBV6	39990	65885	1.32%	0.229%

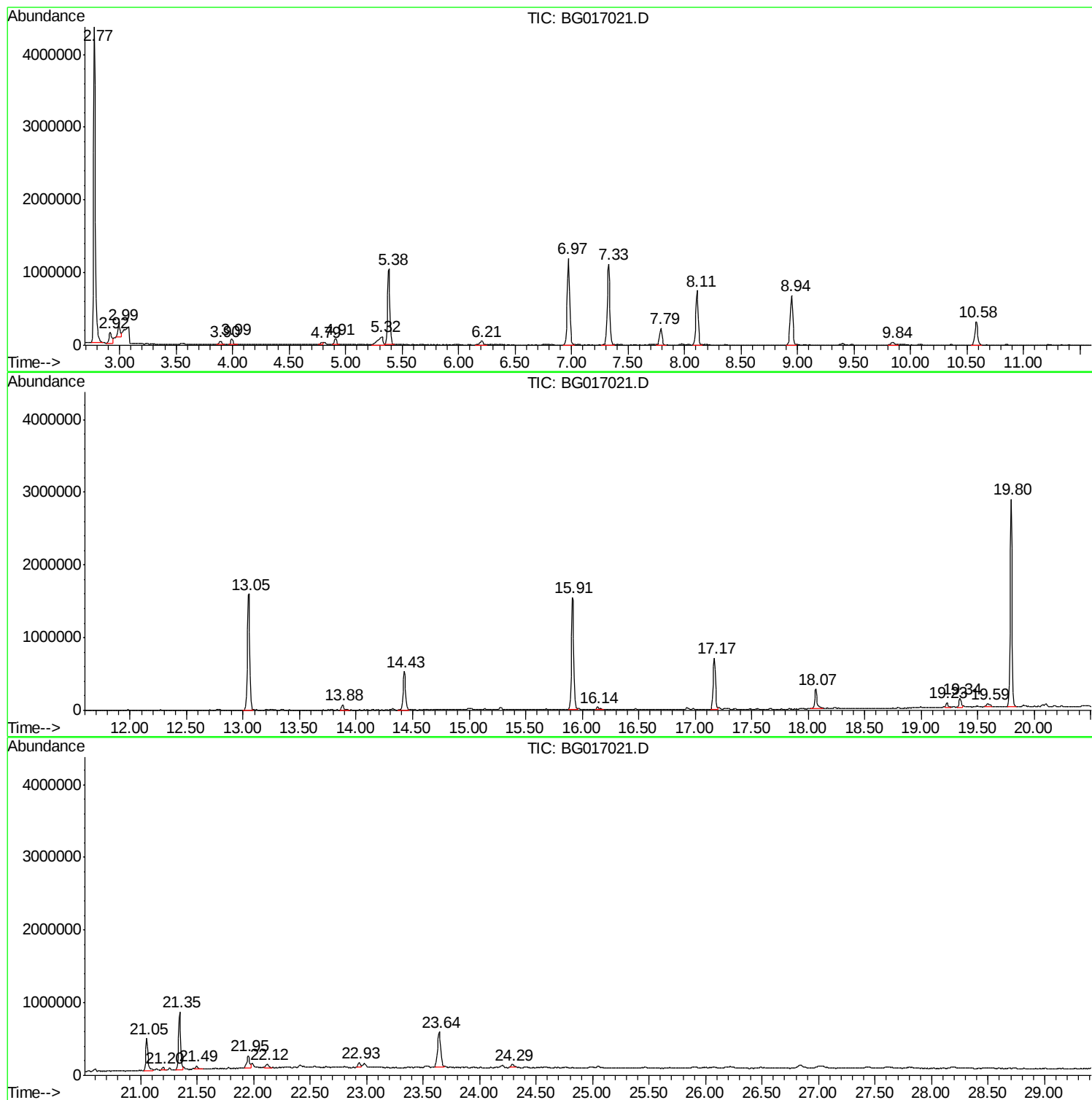
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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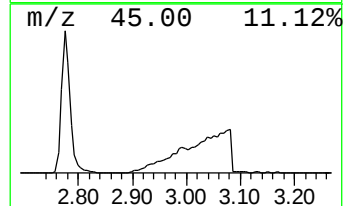
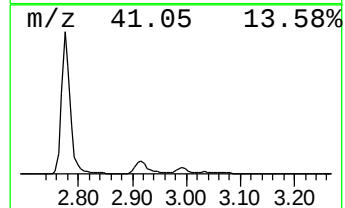
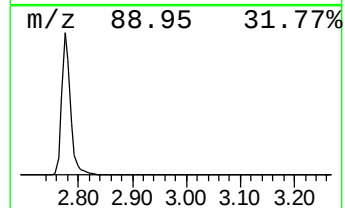
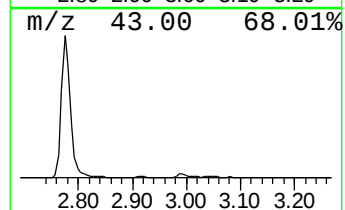
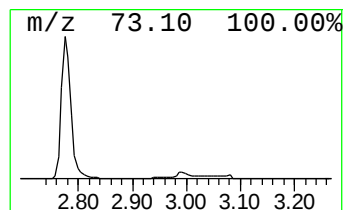
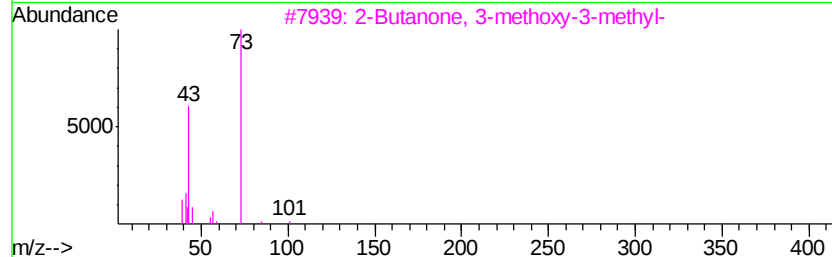
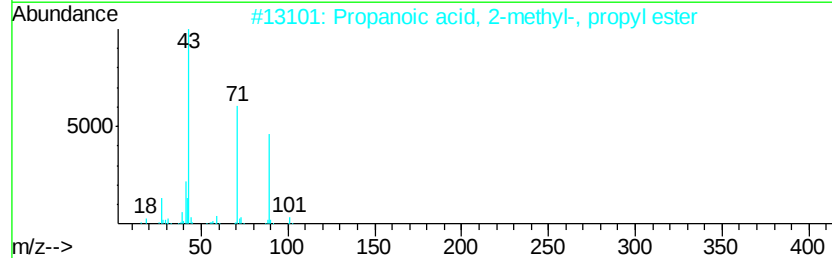
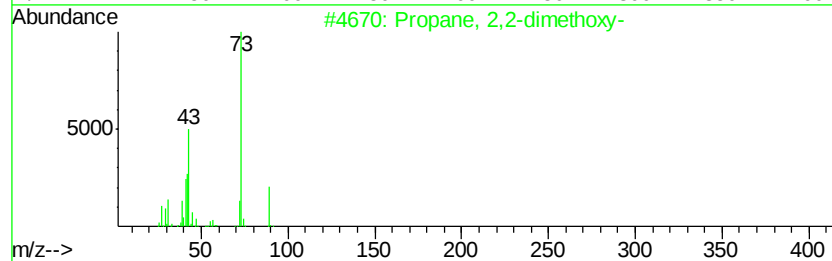
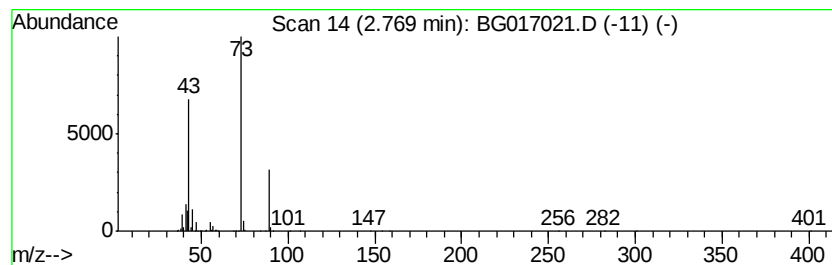
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.77	276.62 ng	5006160	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	39
2		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	35
3		2-Butanone, 3-methoxy-3-methyl-	116	C6H12O2	036687-98-6	28
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9



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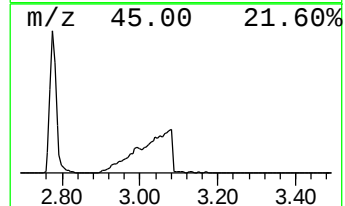
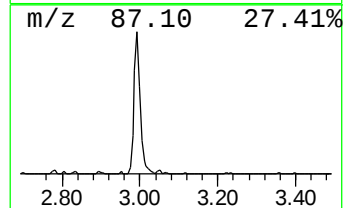
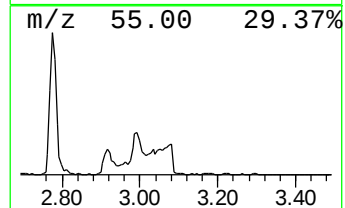
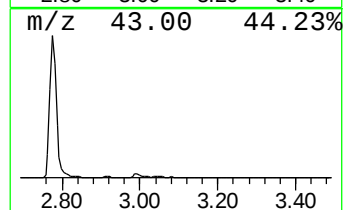
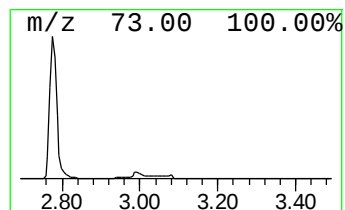
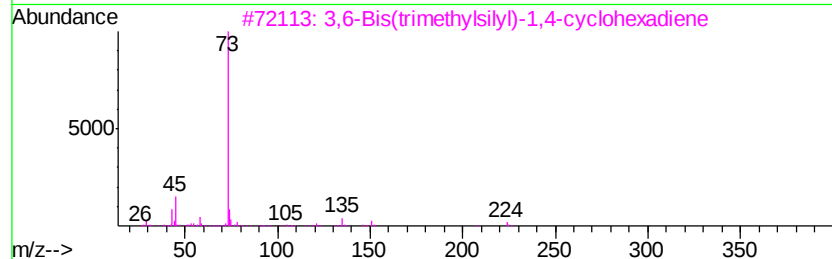
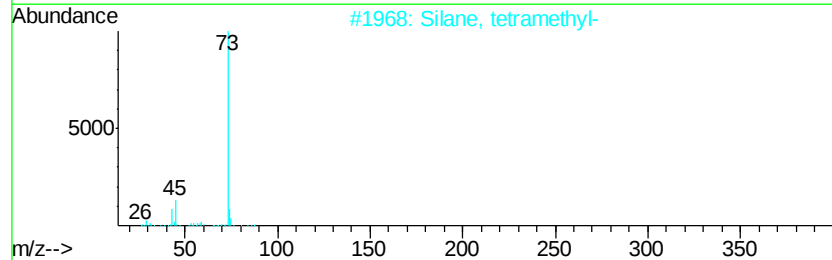
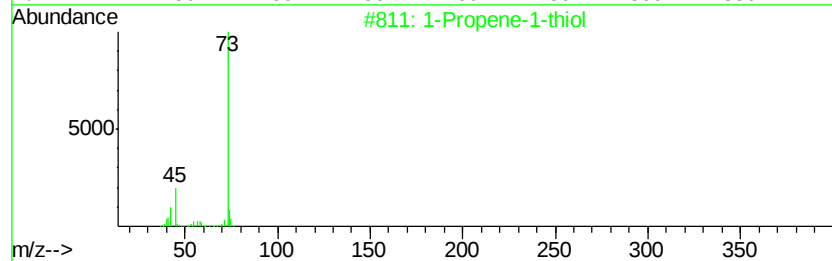
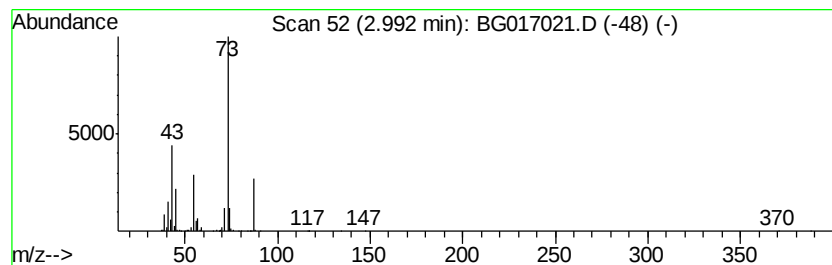
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown2.99 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	14.64 ng	265015	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propene-1-thiol	74	C3H6S	000925-89-3	47
2		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
3		3,6-Bis(trimethylsilyl)-1,4-cycl...	224	C12H24Si2	018090-43-2	37
4		1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	33
5		Myo-Inositol, 4-C-methyl-	194	C7H14O6	000472-95-7	28



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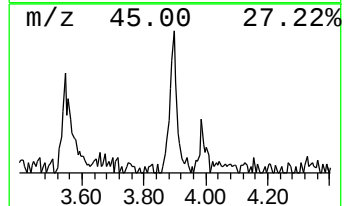
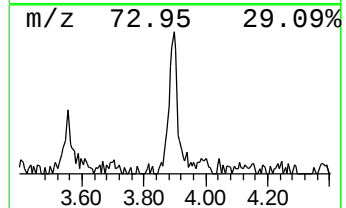
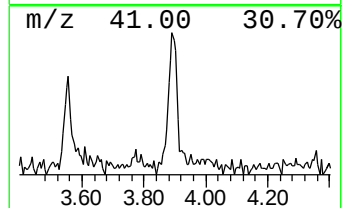
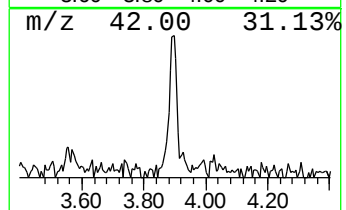
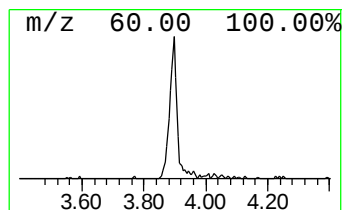
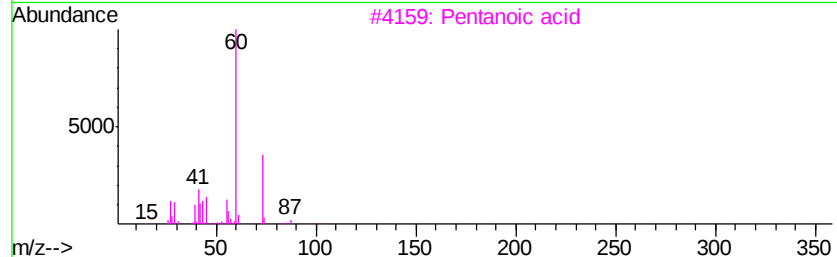
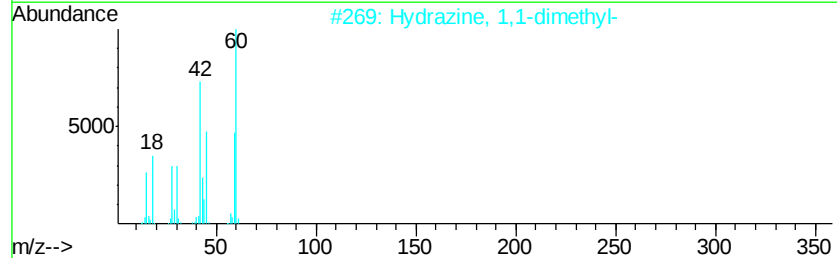
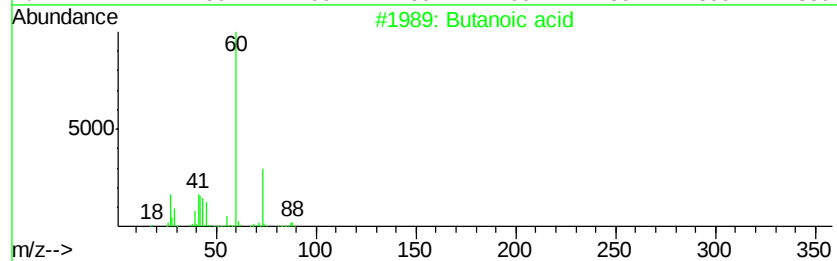
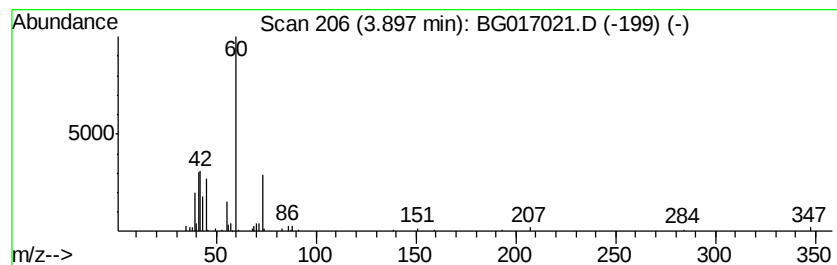
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown3.90 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.90	3.93 ng	71158	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid	88	C4H8O2	000107-92-6	38
2		Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
3		Pentanoic acid	102	C5H10O2	000109-52-4	9
4		5-Hexenoic acid	114	C6H10O2	001577-22-6	9
5		1,3,5-Trithiane, 2,4,6-trimethyl-	180	C6H12S3	002765-04-0	9



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ALS Vial : 63 Sample Multiplier: 1

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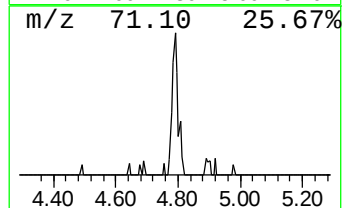
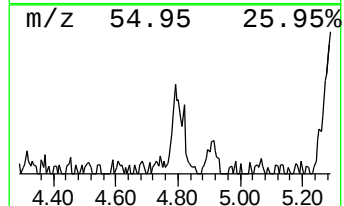
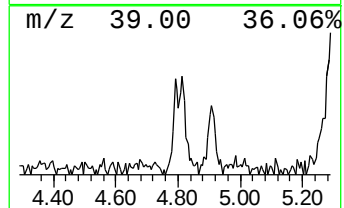
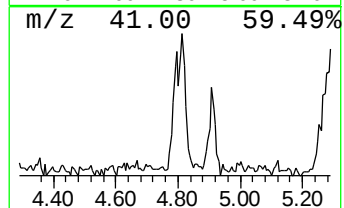
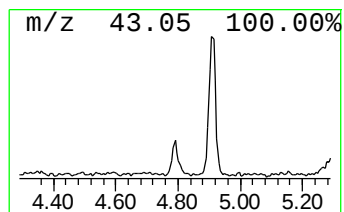
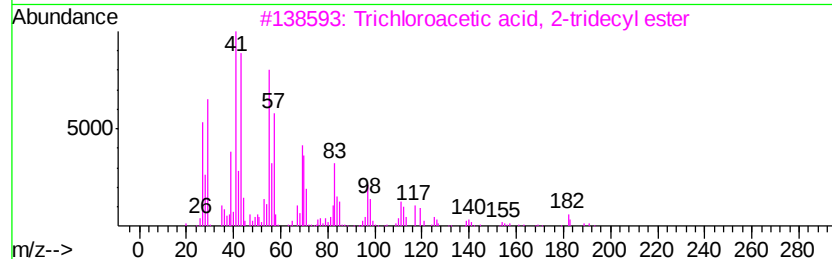
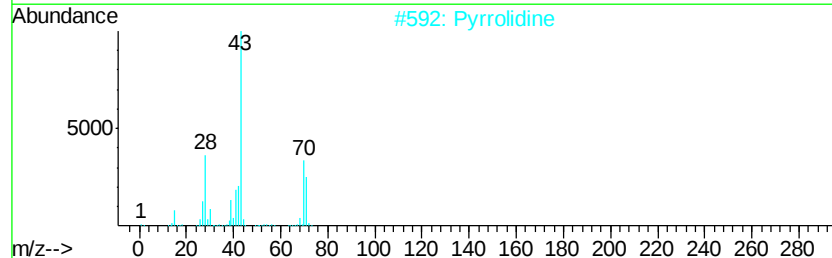
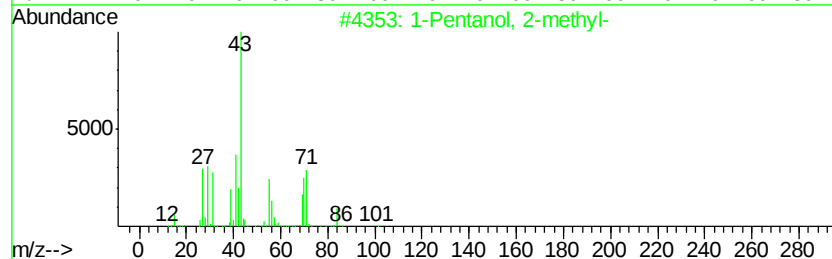
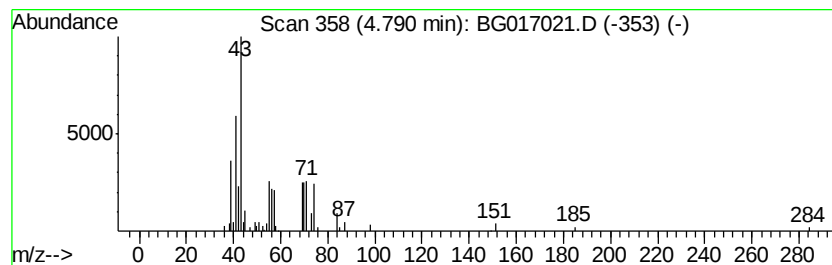
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown4.79 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	2.84 ng	51378	1,4-Dichlorobenzene-d4	7.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	47	
2	Pyrrolidine	71	C4H9N	000123-75-1	38	
3	Trichloroacetic acid, 2-tridecyl...	344	C15H27Cl3O2	1000282-06-3	37	
4	3-Tridecene, (E)-	182	C13H26	041446-57-5	32	
5	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	32	



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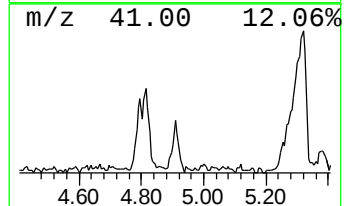
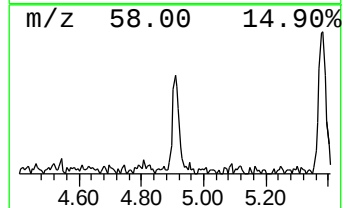
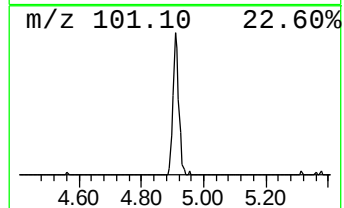
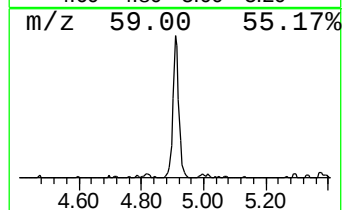
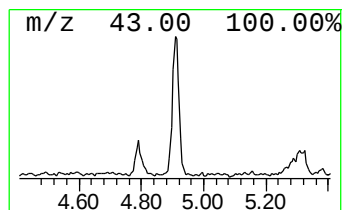
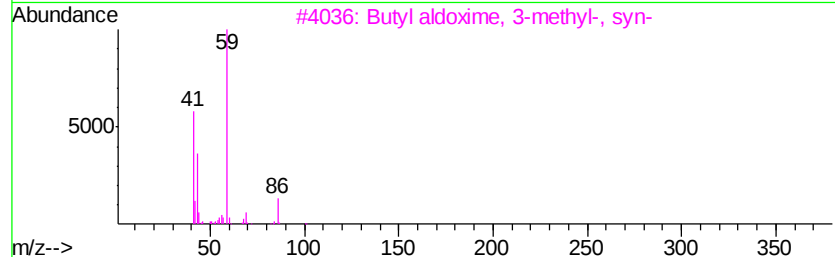
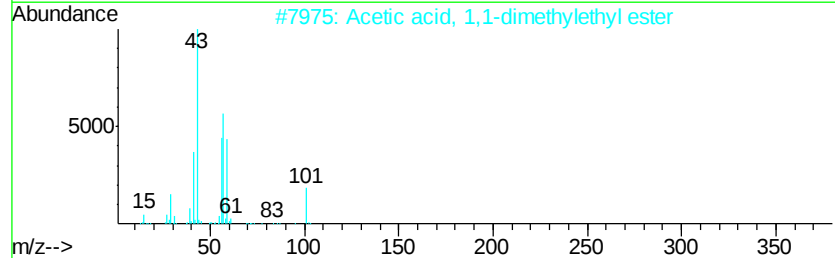
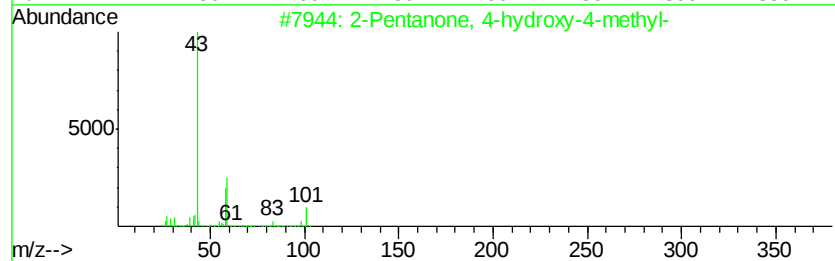
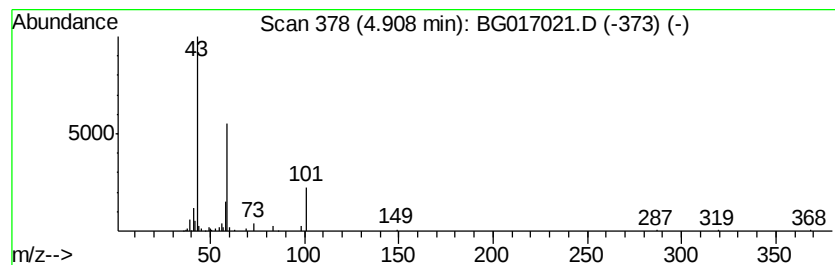
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	6.56 ng	118773	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	22
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	17
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017021.D
Acq On : 10 May 2015 12:00
Operator : TP/IZ
Sample : G2151-12
Misc :
ALS Vial : 63 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TU012-SB-20-7.5

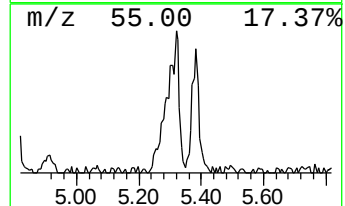
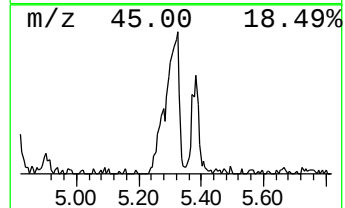
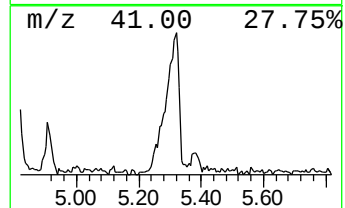
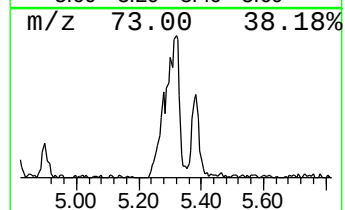
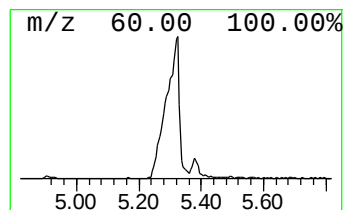
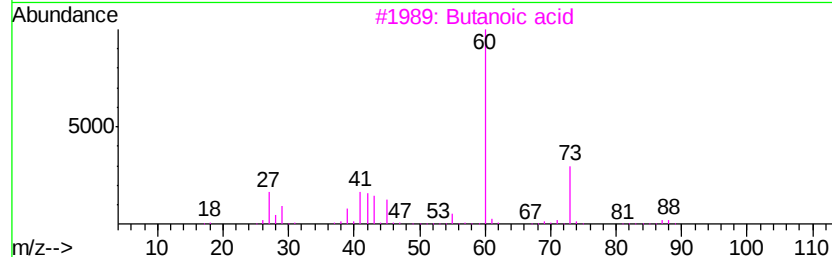
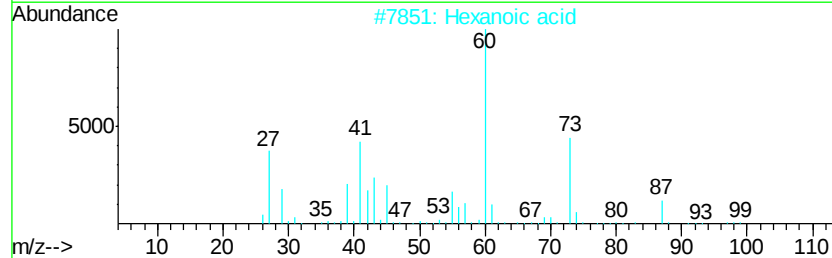
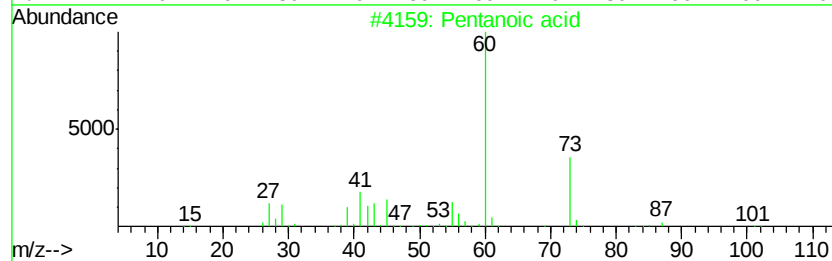
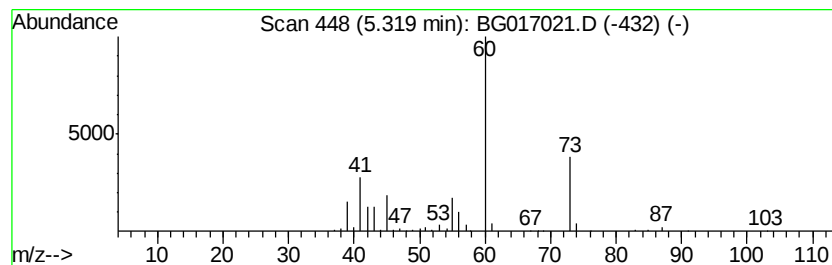
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	19.21 ng	347625	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid	102	C5H10O2	000109-52-4	83
2		Hexanoic acid	116	C6H12O2	000142-62-1	72
3		Butanoic acid	88	C4H8O2	000107-92-6	50
4		Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	40
5		Hexanoic acid, 6-bromo-	194	C6H11BrO2	004224-70-8	39



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017021.D
Acq On : 10 May 2015 12:00
Operator : TP/IZ
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Misc :
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ClientSampleId :
TU012-SB-20-7.5

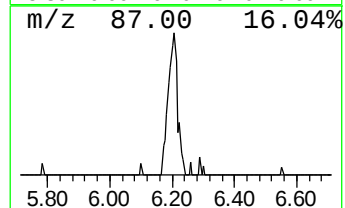
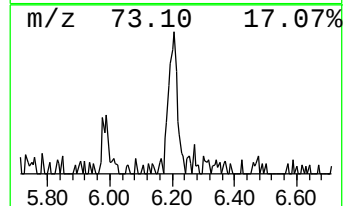
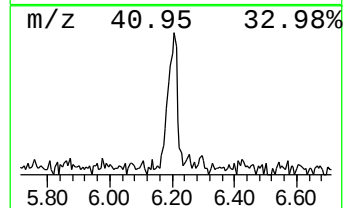
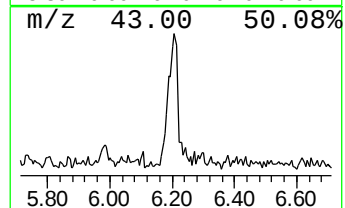
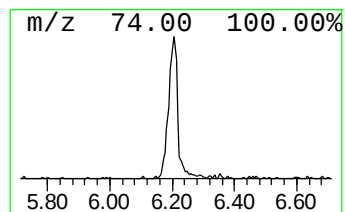
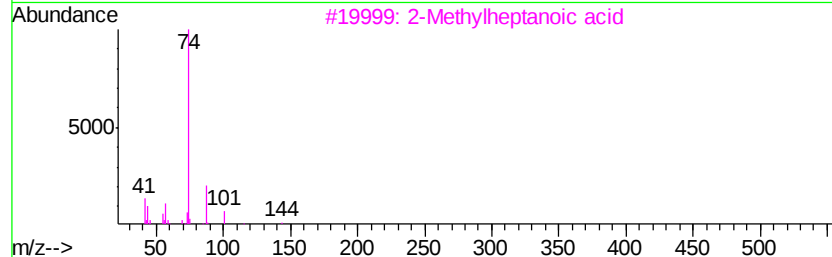
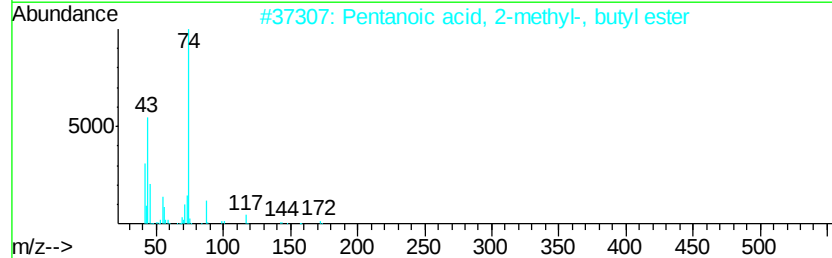
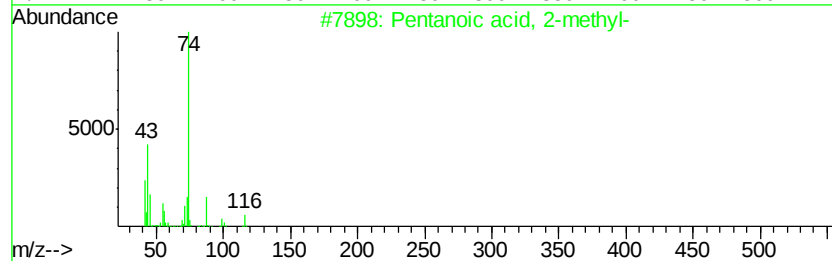
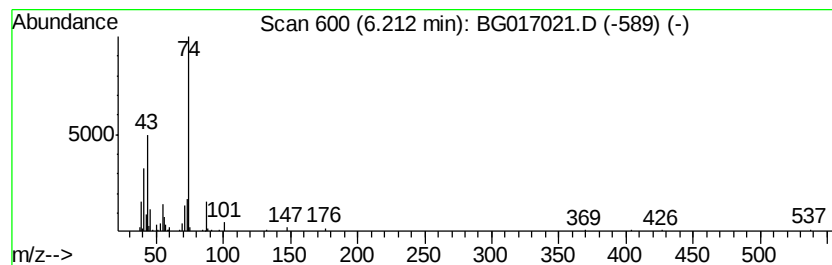
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentanoic acid, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.21	5.99 ng	108351	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	74
2		Pentanoic acid, 2-methyl-, butyl...	172	C10H20O2	006297-41-2	64
3		2-Methylheptanoic acid	144	C8H16O2	001188-02-9	53
4		Diethanolamine	105	C4H11NO2	000111-42-2	40
5		Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017021.D
Acq On : 10 May 2015 12:00
Operator : TP/IZ
Sample : G2151-12
Misc :
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ClientSampleId :
TU012-SB-20-7.5

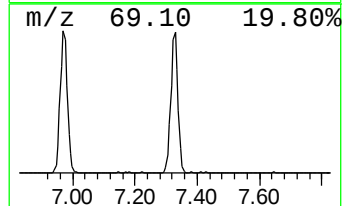
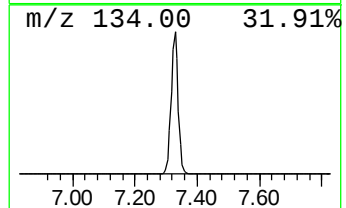
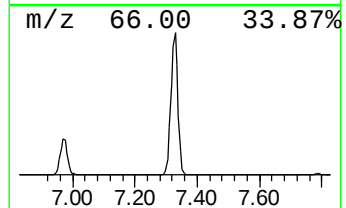
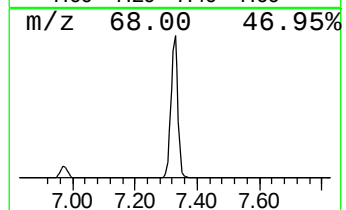
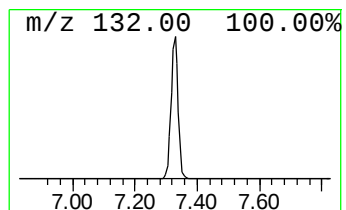
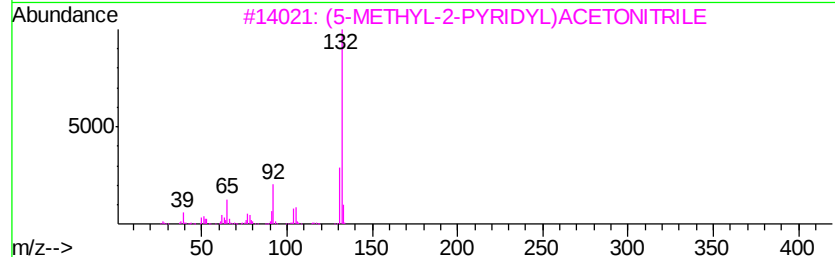
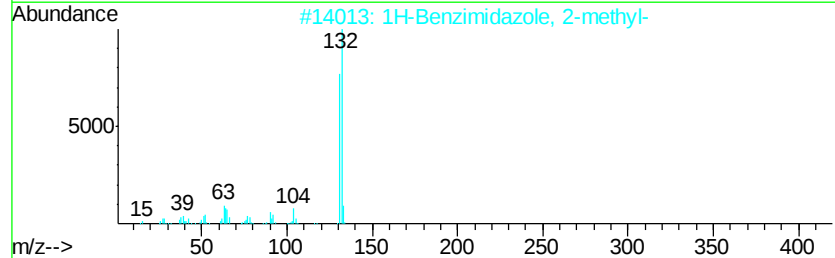
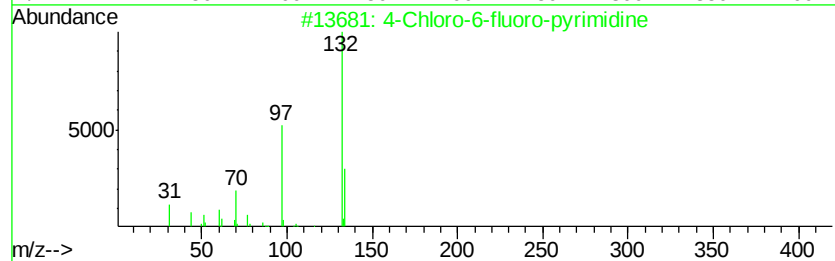
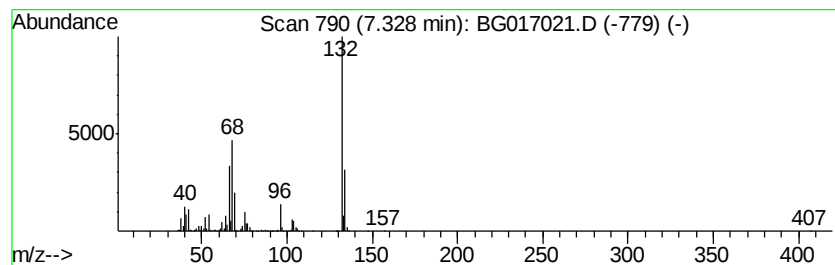
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown7.33 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.33	97.39 ng	1762580	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	22
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	13
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017021.D
Acq On : 10 May 2015 12:00
Operator : TP/IZ
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Misc :
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Instrument :
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ClientSampleId :
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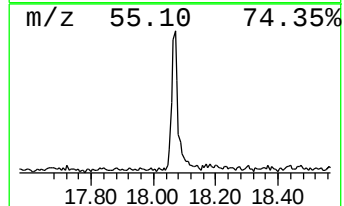
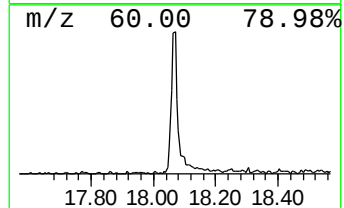
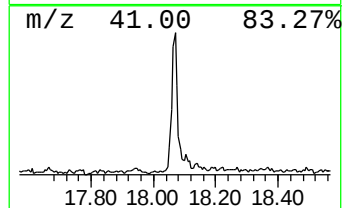
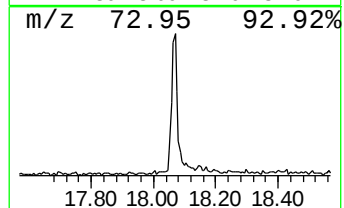
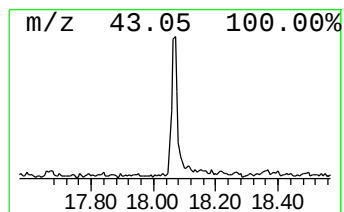
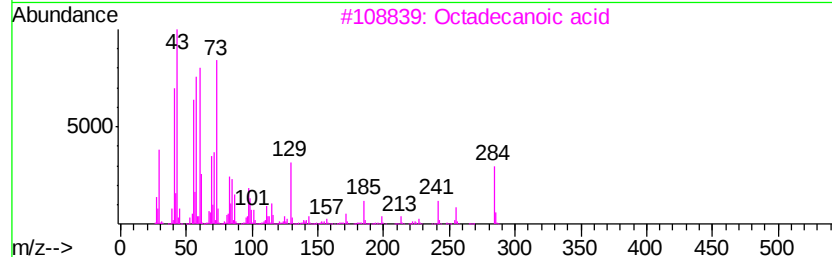
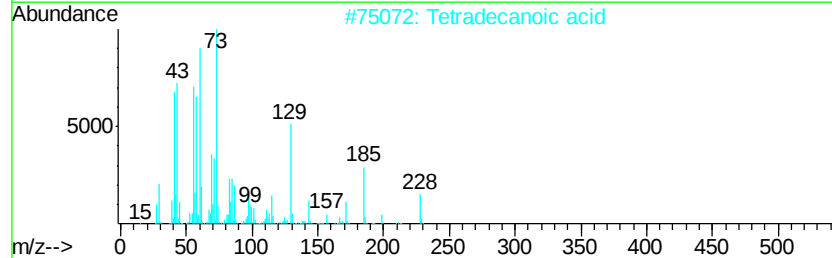
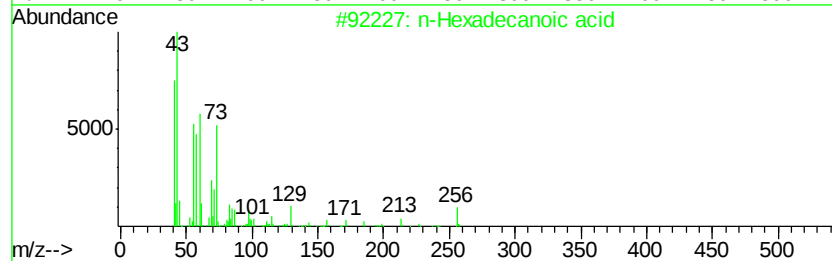
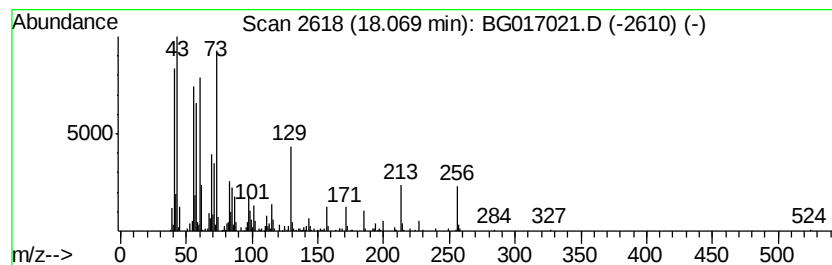
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.07	8.60 ng	423286	Phenanthrene-d10	17.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	76
3		Octadecanoic acid	284	C18H36O2	000057-11-4	64
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\BG050815\
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Operator : TP/IZ
Sample : G2151-12
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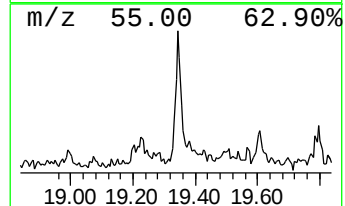
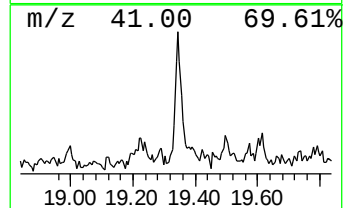
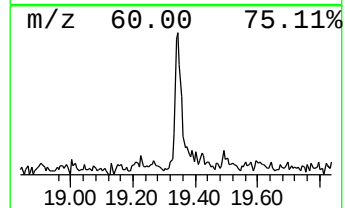
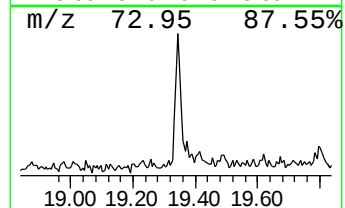
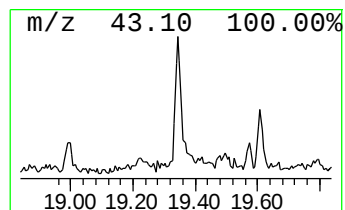
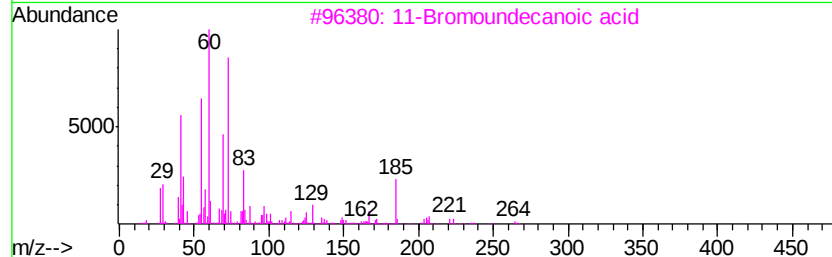
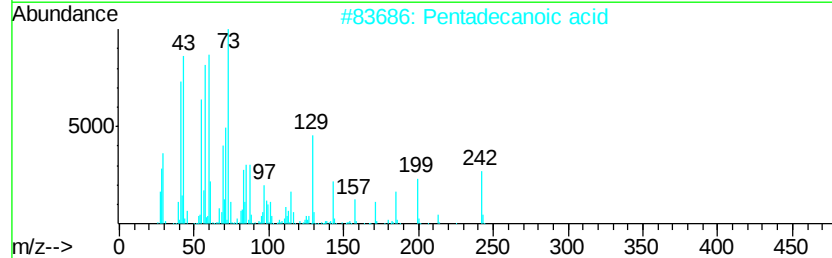
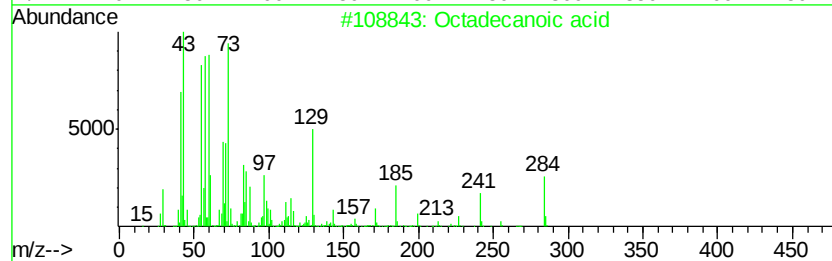
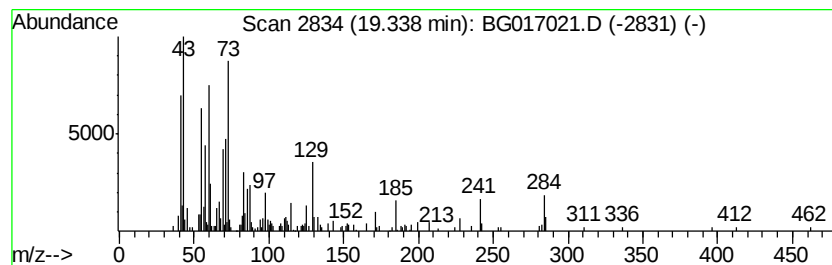
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Octadecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.34	2.95 ng	155524	Chrysene-d12		21.35	
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	46
3		11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35
4		Nonanoic acid	158	C9H18O2	000112-05-0	25
5		Hexadecane, 1-chloro-	260	C16H33Cl	004860-03-1	18



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017021.D
Acq On : 10 May 2015 12:00
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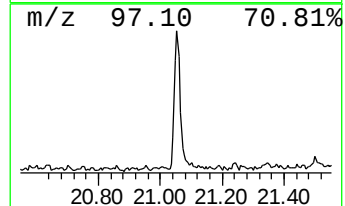
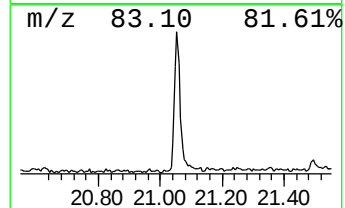
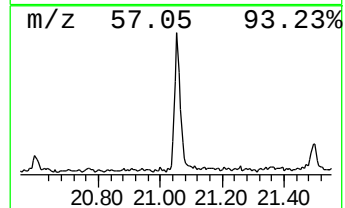
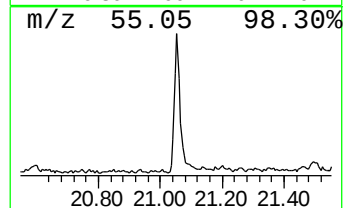
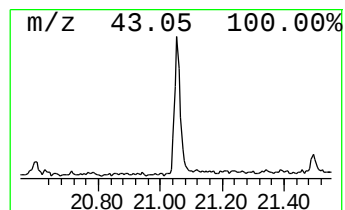
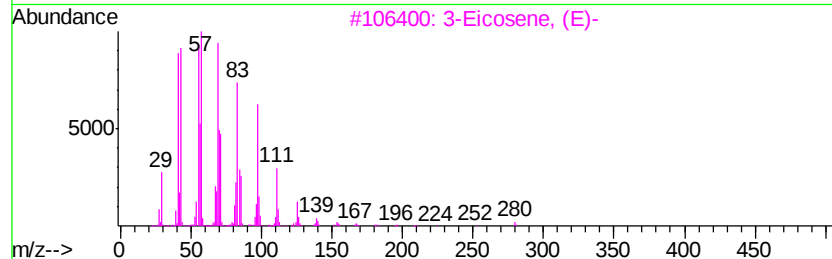
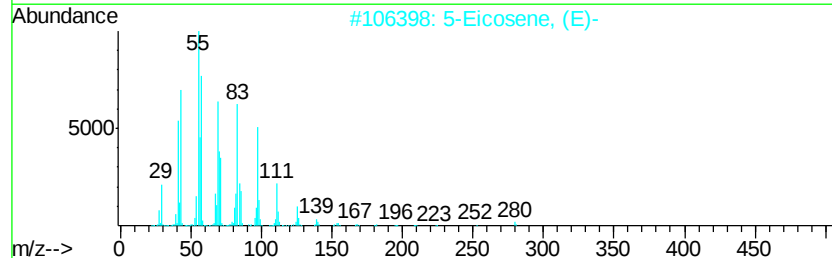
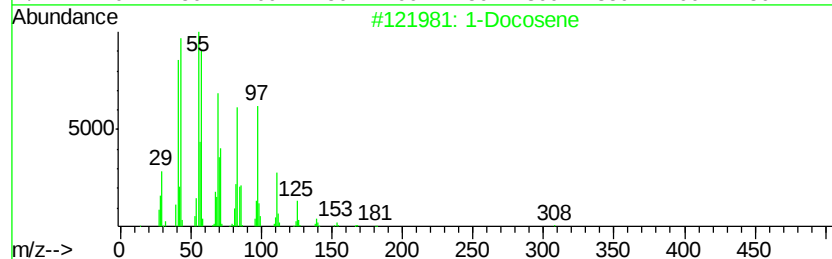
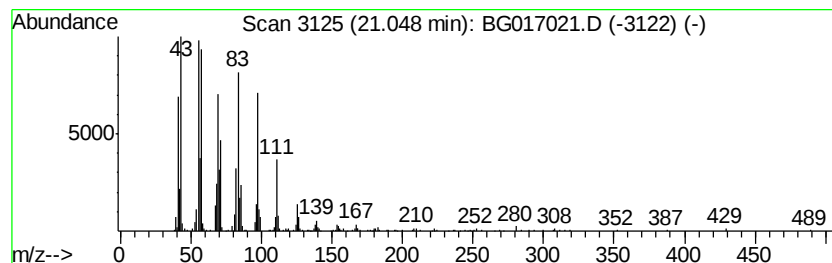
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 1-Docosene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.05	10.39 ng	547165	Chrysene-d12	21.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	99
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	96
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	96
4		Z-5-Nonadecene	266	C19H38	1000131-11-8	94
5		1-Heneicosyl formate	340	C22H44O2	077899-03-7	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
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Acq On : 10 May 2015 12:00
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ClientSampleId :
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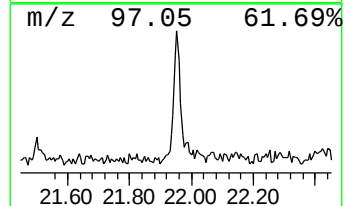
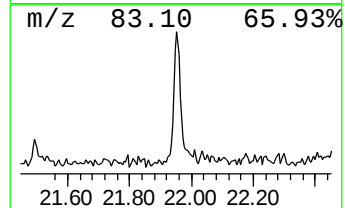
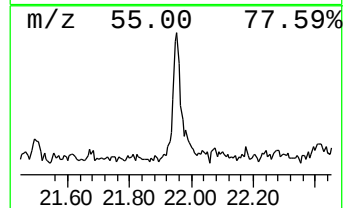
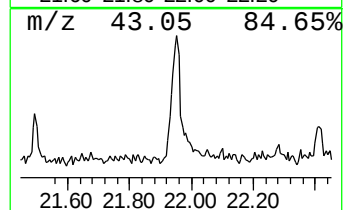
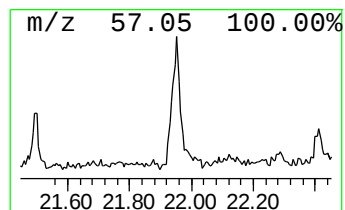
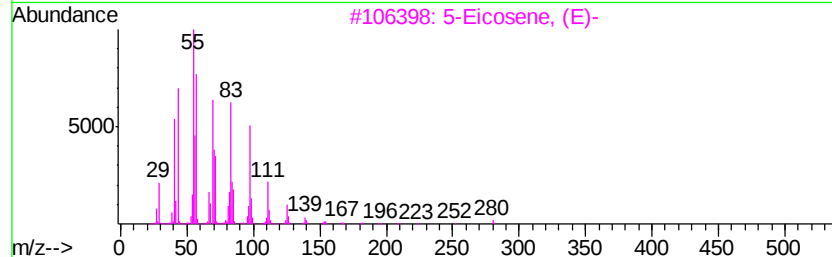
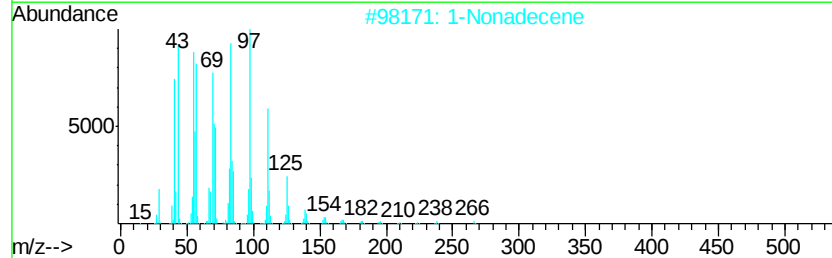
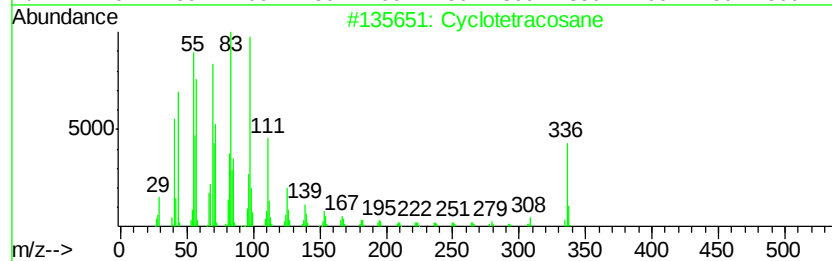
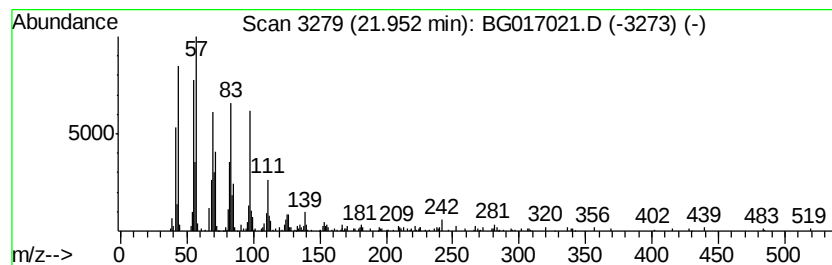
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Cyclotetracosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.95	5.51 ng	290299	Chrysene-d12	21.35

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetracosane	336	C24H48	000297-03-0	97
2			1-Nonadecene	266	C19H38	018435-45-5	96
3			5-Eicosene, (E)-	280	C20H40	074685-30-6	94
4			Cyclohexadecane	224	C16H32	000295-65-8	94
5			1-Docosene	308	C22H44	001599-67-3	94



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG017021.D
Acq On : 10 May 2015 12:00
Operator : TP/IZ
Sample : G2151-12
Misc :
ALS Vial : 63 Sample Multiplier: 1

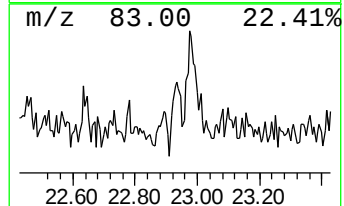
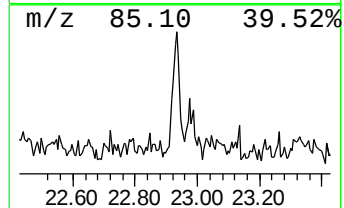
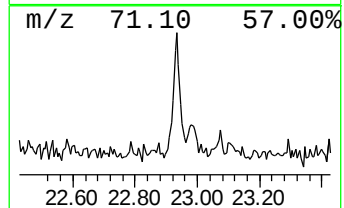
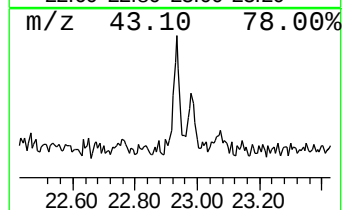
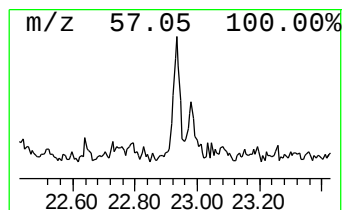
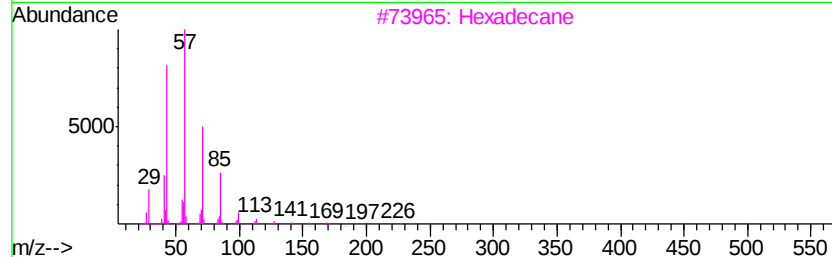
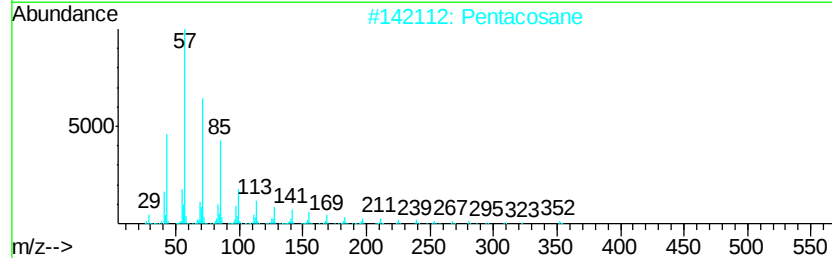
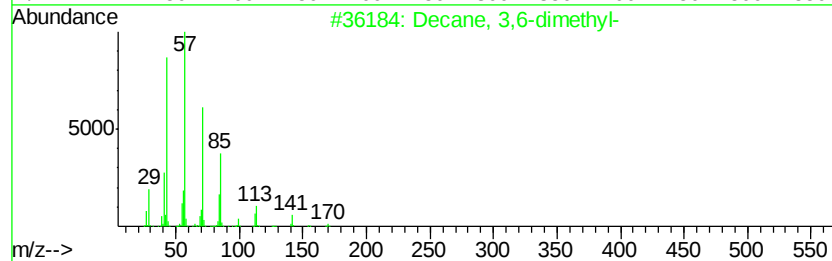
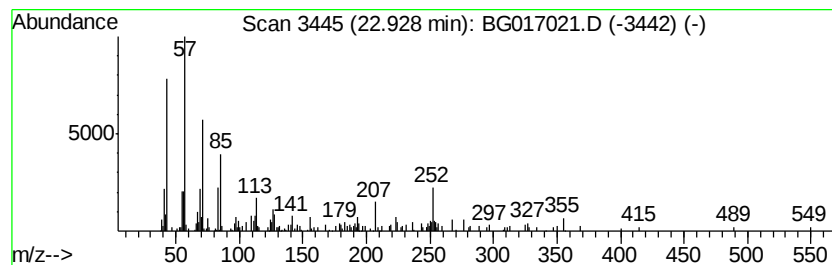
Instrument :
BNA_G
ClientSampleId :
TU012-SB-20-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Decane, 3,6-dimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.93	2.00 ng	94496	Perylene-d12	23.64	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	55
2	Pentacosane	352	C25H52	000629-99-2	55
3	Hexadecane	226	C16H34	000544-76-3	55
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	49
5	2,6-Dimethyldecane	170	C12H26	013150-81-7	49



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
 Data File : BG017021.D
 Acq On : 10 May 2015 12:00
 Operator : TP/IZ
 Sample : G2151-12
 Misc :
 ALS Vial : 63 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TU012-SB-20-7.5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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
unknown2.77	2.77	276.6	ng	5006160	1	7.79	361955	20.0
unknown2.99	2.99	14.6	ng	265015	1	7.79	361955	20.0
unknown3.90	3.90	3.9	ng	71158	1	7.79	361955	20.0
unknown4.79	4.79	2.8	ng	51378	1	7.79	361955	20.0
2-Pentanone, 4-hy...	4.91	6.6	ng	118773	1	7.79	361955	20.0
Pentanoic acid	5.32	19.2	ng	347625	1	7.79	361955	20.0
Pentanoic acid, 2...	6.21	6.0	ng	108351	1	7.79	361955	20.0
unknown7.33	7.33	97.4	ng	1762580	1	7.79	361955	20.0
n-Hexadecanoic acid	18.07	8.6	ng	423286	4	17.17	984653	20.0
Octadecanoic acid	19.34	3.0	ng	155524	5	21.35	1053200	20.0
1-Docosene	21.05	10.4	ng	547165	5	21.35	1053200	20.0
Cyclotetracosane	21.95	5.5	ng	290299	5	21.35	1053200	20.0
Decane, 3,6-dimet...	22.93	2.0	ng	94496	6	23.64	943989	20.0