

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
 Data File : BG016966.D
 Acq On : 8 May 2015 20:38
 Operator : TP/IZ
 Sample : G2058-13
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MPE-15

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-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	2.919	34	39	47	rBV	320520	524178	9.73%	1.709%
2	2.990	47	51	63	rVB	646647	864969	16.06%	2.821%
3	4.911	373	378	384	rBV	62791	88753	1.65%	0.289%
4	5.375	451	457	466	rBV	642206	891029	16.55%	2.906%
5	6.956	718	726	738	rBV	446525	693628	12.88%	2.262%
6	7.326	781	789	796	rBV	1210157	1914478	35.55%	6.243%
7	7.790	862	868	875	rBV	360296	562070	10.44%	1.833%
8	8.113	915	923	929	rBV	981931	1563376	29.03%	5.098%
9	8.947	1056	1065	1074	rBV	987228	1639264	30.44%	5.346%
10	10.587	1335	1344	1351	rBV	530071	887462	16.48%	2.894%
11	12.784	1713	1718	1726	rVB2	104048	152189	2.83%	0.496%
12	13.054	1756	1764	1771	rBV	2536926	3792689	70.43%	12.369%
13	14.429	1990	1998	2006	rBV2	839436	1328666	24.67%	4.333%
14	14.864	2065	2072	2083	rBV	511596	799952	14.86%	2.609%
15	15.786	2226	2229	2236	rVB	58855	84360	1.57%	0.275%
16	15.916	2245	2251	2268	rVB	2218627	3303928	61.35%	10.775%
17	17.173	2459	2465	2472	rBV2	1130456	1613809	29.97%	5.263%
18	18.072	2613	2618	2628	rBV	327563	477352	8.86%	1.557%
19	19.353	2832	2836	2846	rVB2	233450	321994	5.98%	1.050%
20	19.799	2906	2912	2918	rBV	4446957	5384998	100.00%	17.561%
21	21.057	3122	3126	3133	rBV	173365	243255	4.52%	0.793%
22	21.350	3170	3176	3190	rBV	1378694	1773978	32.94%	5.785%
23	22.502	3368	3372	3377	rBV2	68398	102166	1.90%	0.333%
24	23.648	3560	3567	3574	rVB2	878543	1655146	30.74%	5.398%

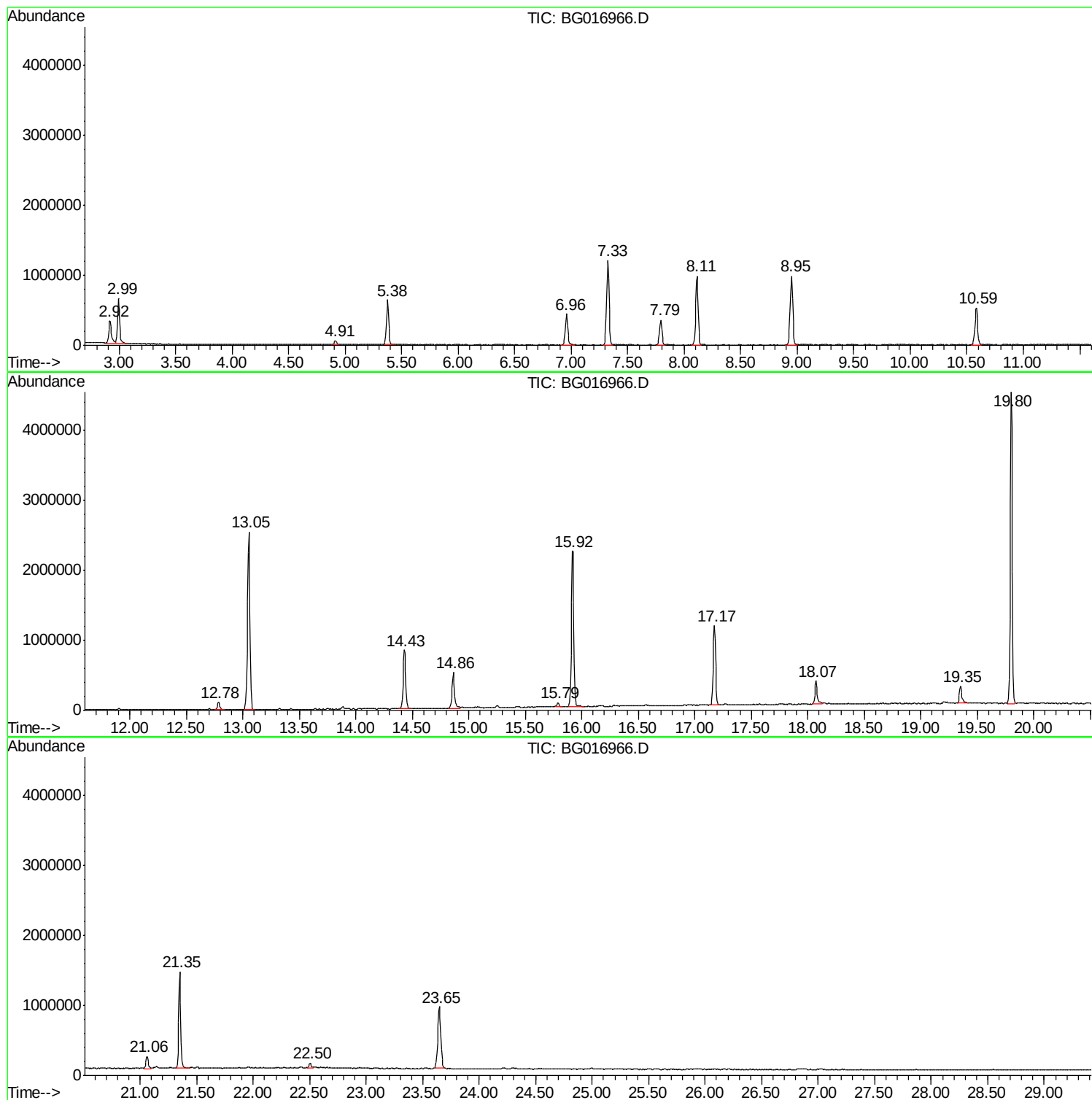
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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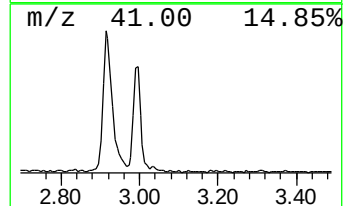
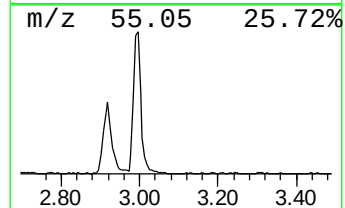
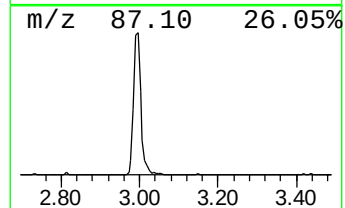
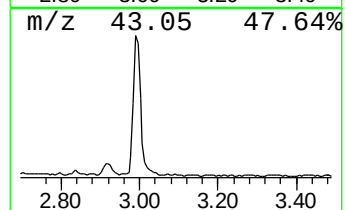
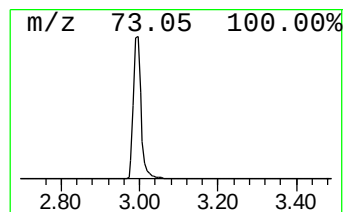
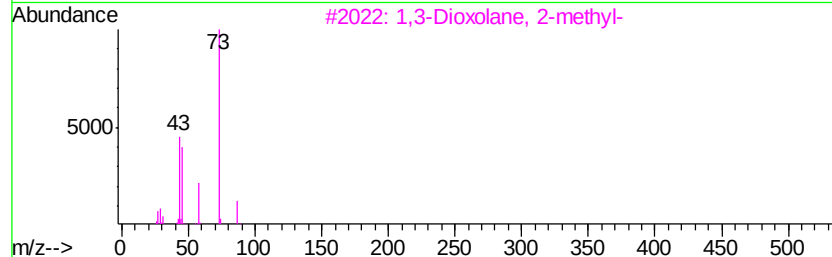
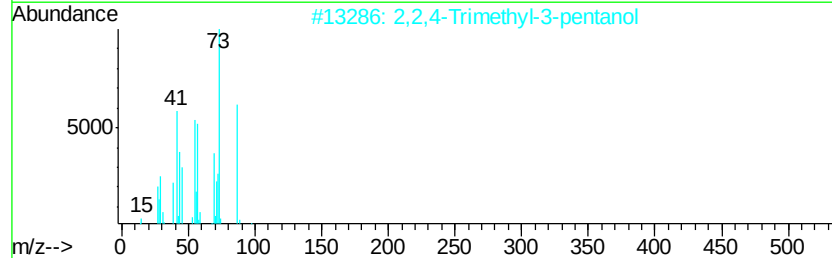
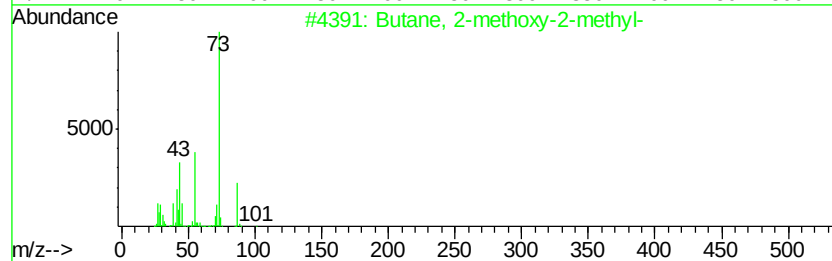
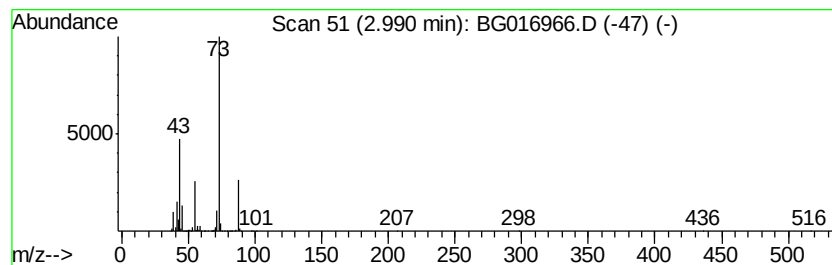
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	30.78 ng	864969	1,4-Dichlorobenzene-d4	7.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78	
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64	
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23	
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9	
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9	



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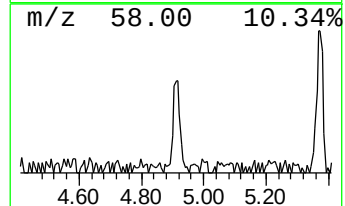
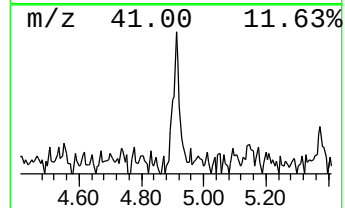
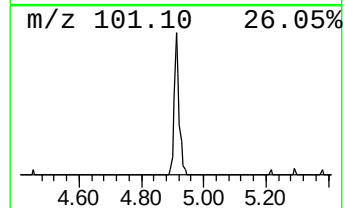
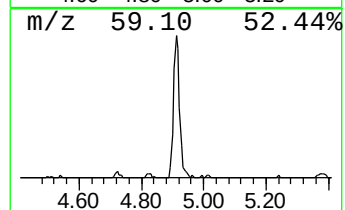
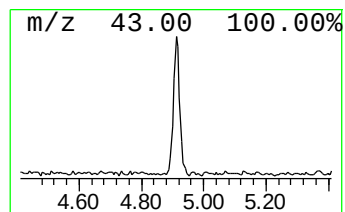
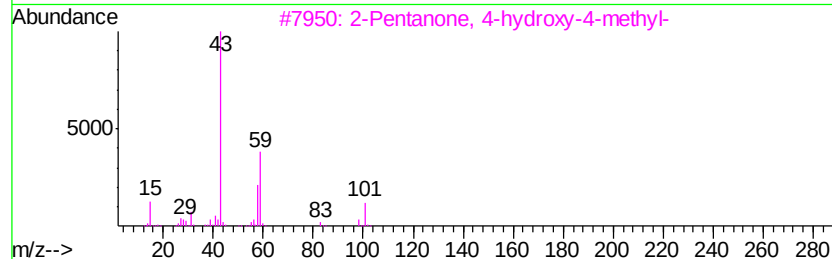
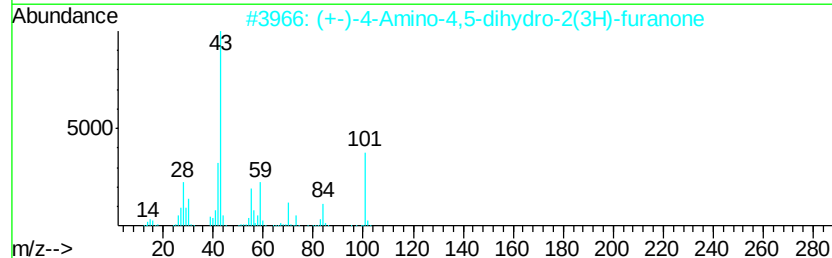
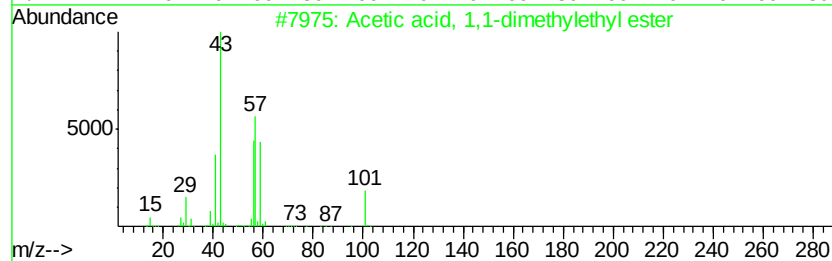
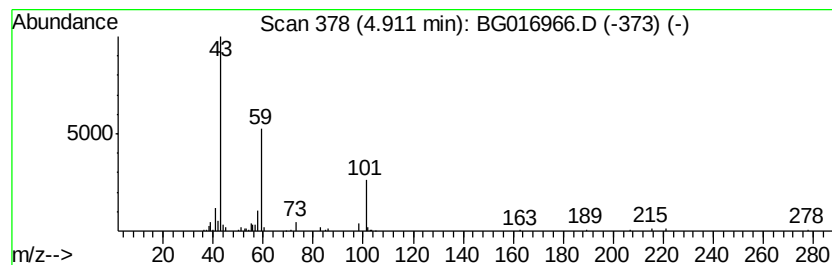
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Peak Number 3 unknown4.91 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	3.16 ng	88753	1,4-Dichlorobenzene-d4	7.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	45
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
5			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25



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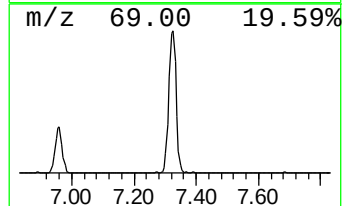
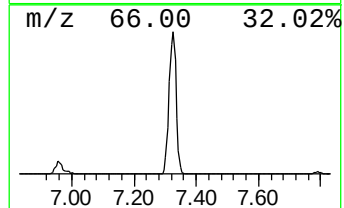
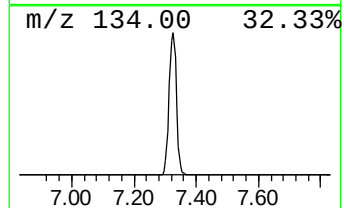
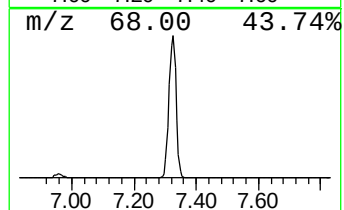
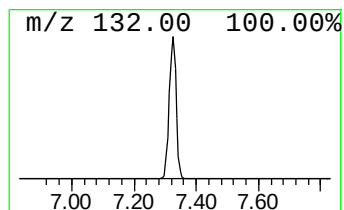
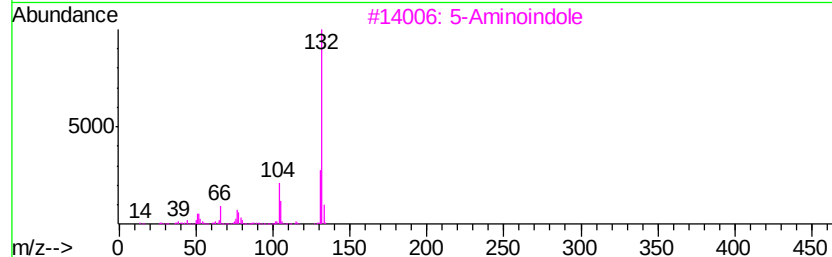
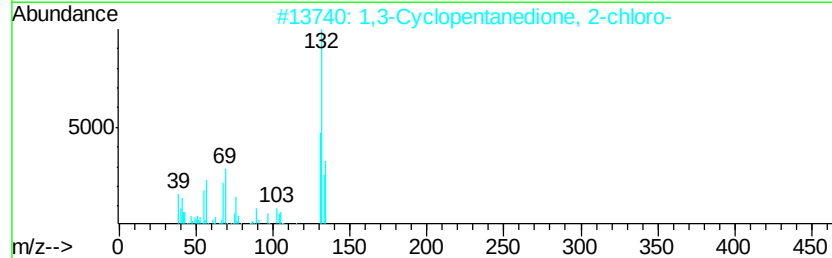
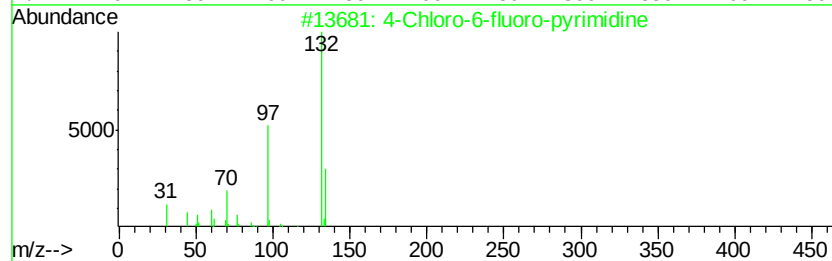
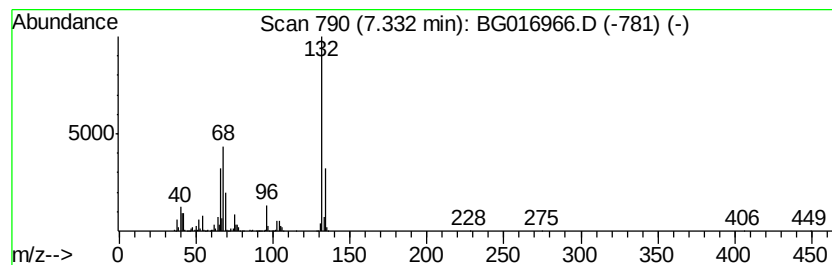
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Peak Number 4 unknown7.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.33	68.12 ng	1914480	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		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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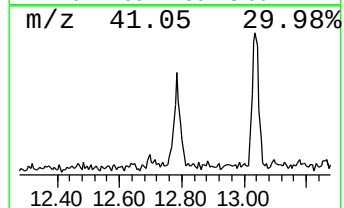
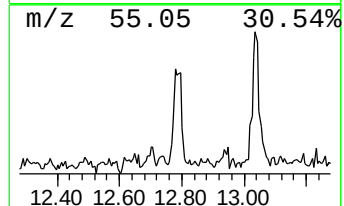
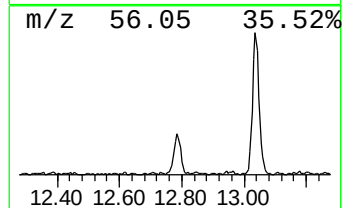
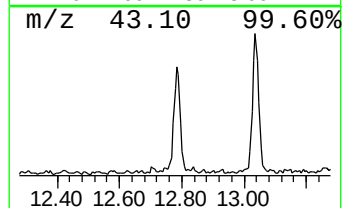
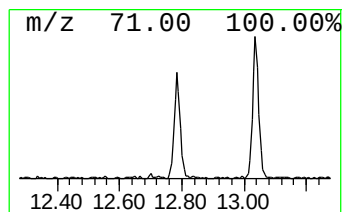
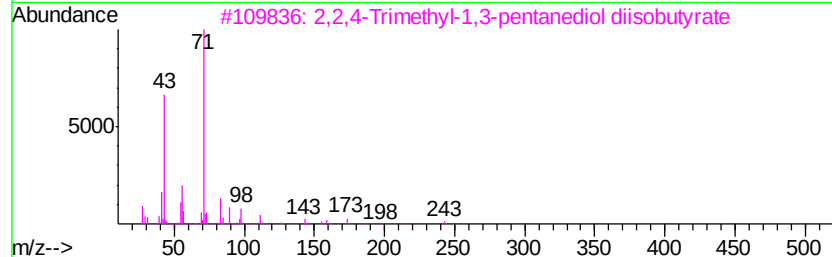
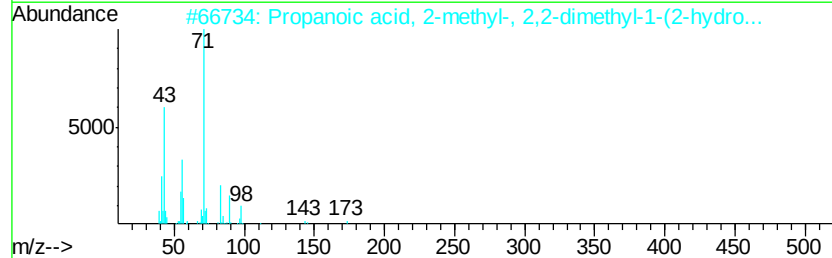
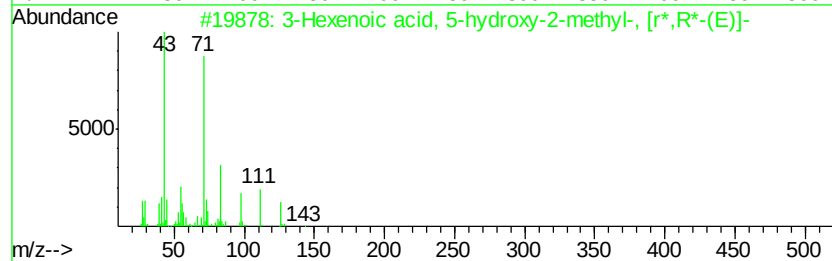
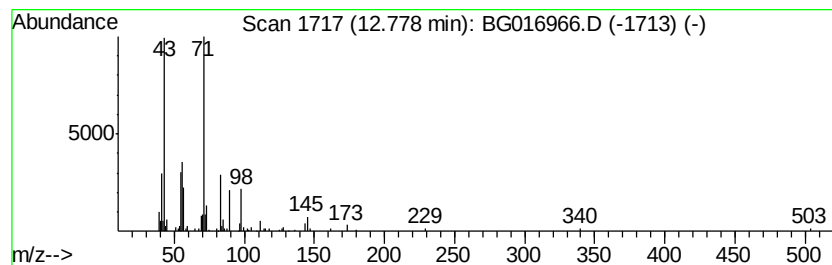
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 6 3-Hexenoic acid, 5-hydroxy-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.78	2.29 ng	152189	Acenaphthene-d10	14.43
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	3-Hexenoic acid, 5-hydroxy-2-met...	144 C7H12O3	110678-36-9	59
2	Propanoic acid, 2-methyl-, 2,2-d...	216 C12H24O3	074367-33-2	50
3	2,2,4-Trimethyl-1,3-pentanediol ...	286 C16H30O4	006846-50-0	47
4	Butanoic acid, 1-methylethyl ester	130 C7H14O2	000638-11-9	38
5	Propanoic acid, 2-methyl-, 2-met...	144 C8H16O2	000097-85-8	38



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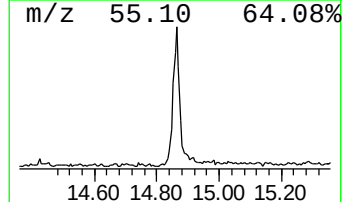
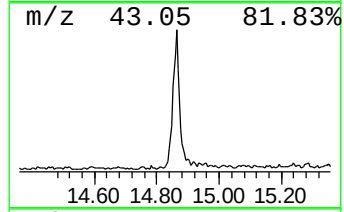
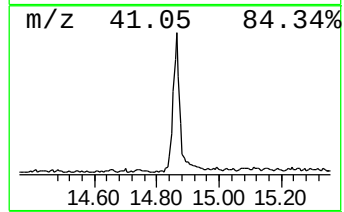
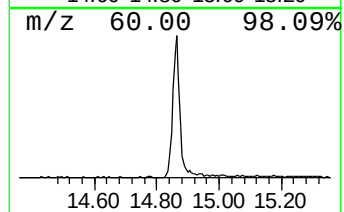
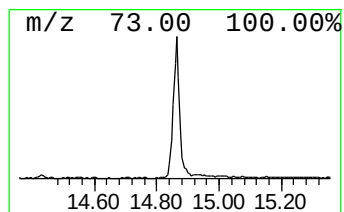
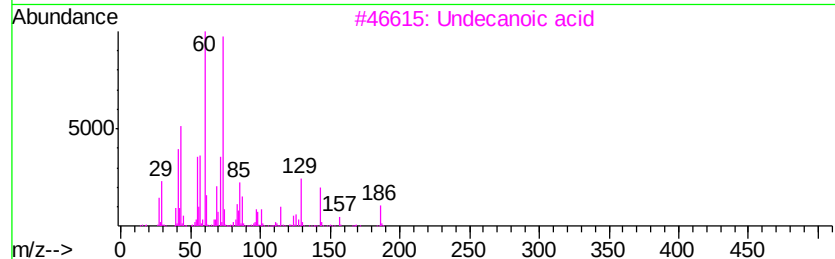
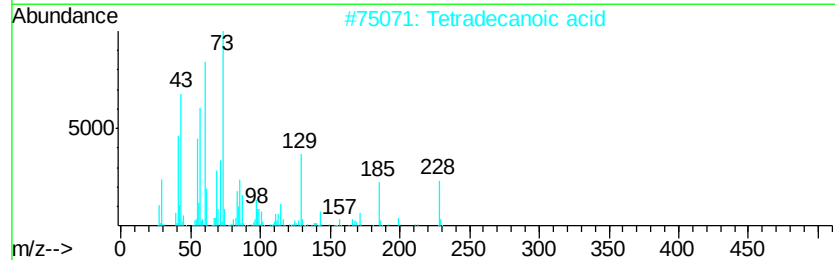
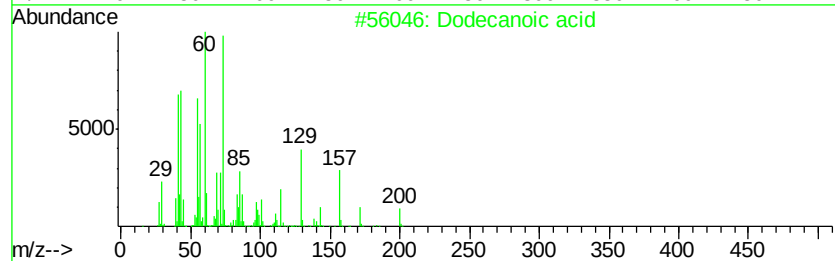
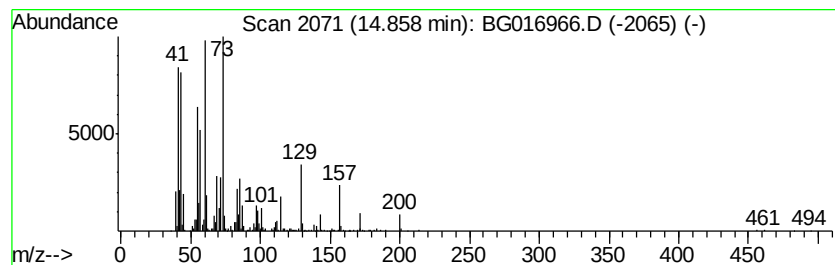
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Peak Number 7 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.86	12.04 ng	799952	Acenaphthene-d10	14.43
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Dodecanoic acid	200 C12H24O2	000143-07-7	99
2	Tetradecanoic acid	228 C14H28O2	000544-63-8	72
3	Undecanoic acid	186 C11H22O2	000112-37-8	72
4	Tridecanoic acid	214 C13H26O2	000638-53-9	64
5	Pentadecanoic acid	242 C15H30O2	001002-84-2	58



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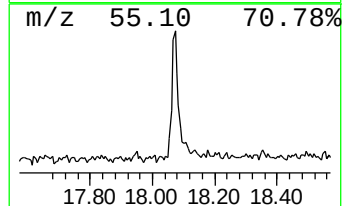
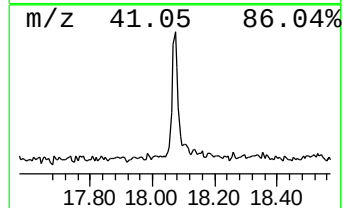
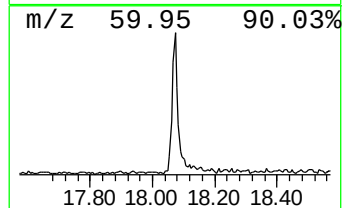
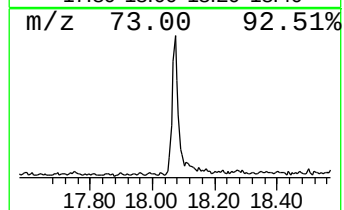
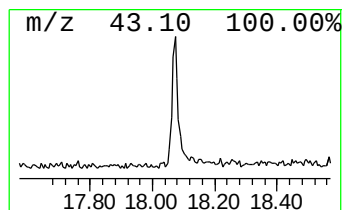
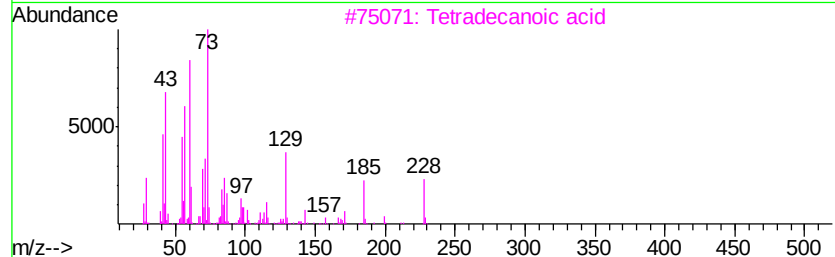
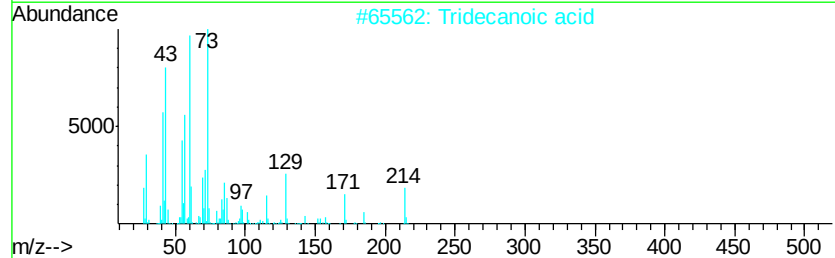
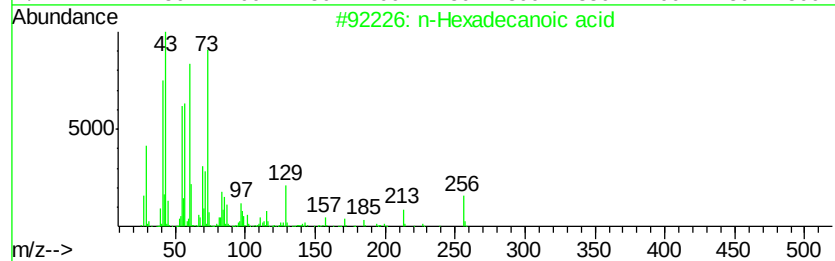
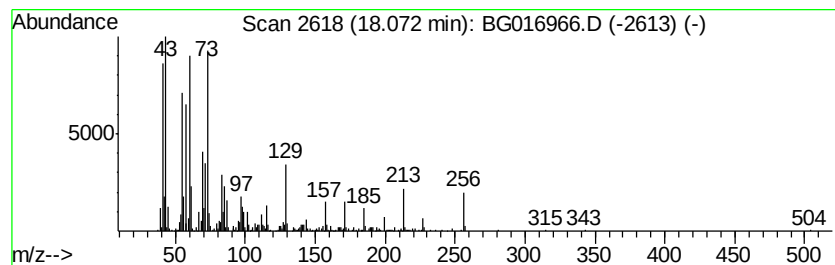
Instrument :
BNA_G
ClientSampleId :
MPE-15

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 8 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.07	5.92 ng	477352	Phenanthrene-d10	17.17	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016966.D
Acq On : 8 May 2015 20:38
Operator : TP/IZ
Sample : G2058-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MPE-15

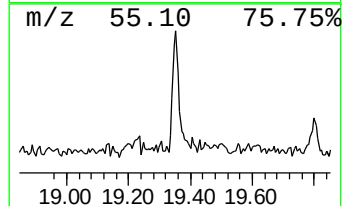
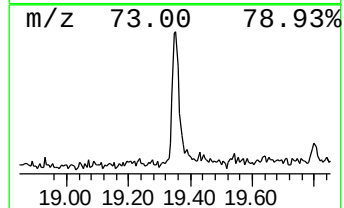
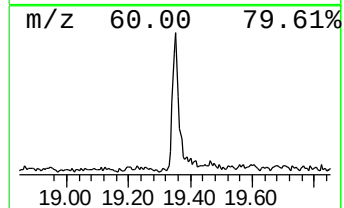
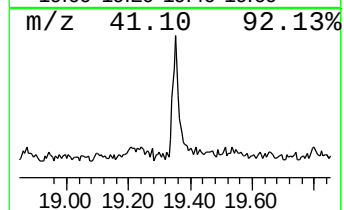
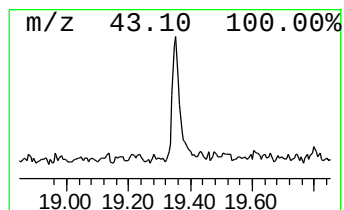
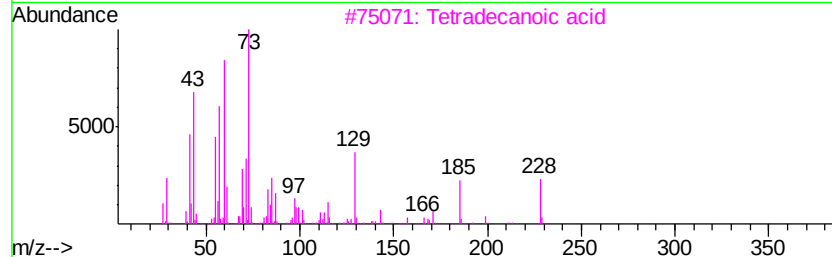
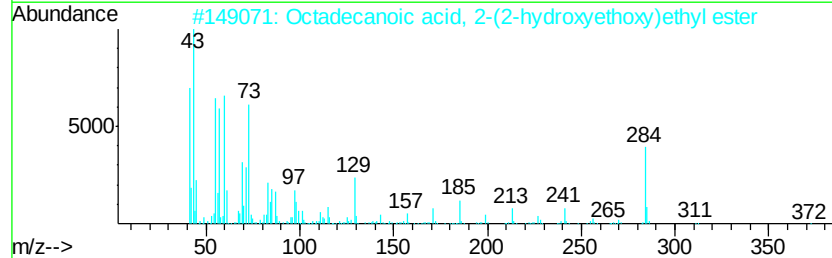
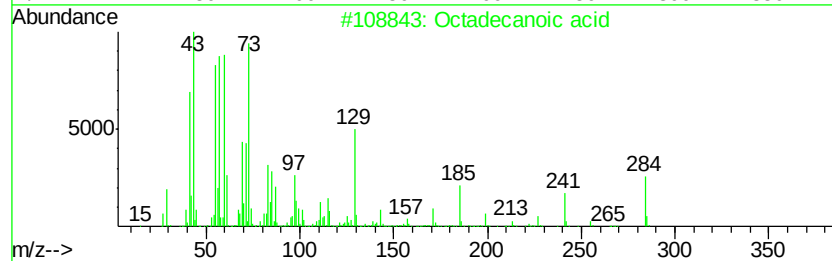
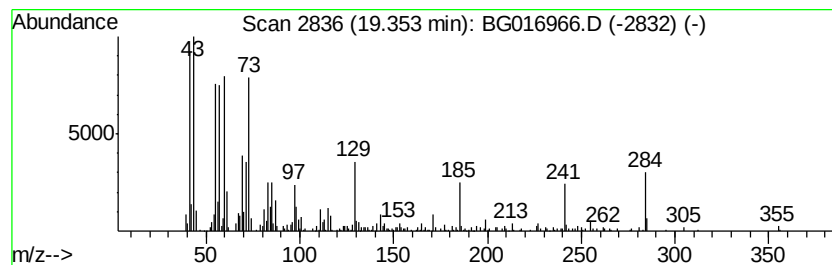
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.35	3.63 ng	321994	Chrysene-d12	21.35

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid		284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...		372	C22H44O4	000106-11-6	80
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	76
4	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	58
5	Dodecanoic acid		200	C12H24O2	000143-07-7	52



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016966.D
Acq On : 8 May 2015 20:38
Operator : TP/IZ
Sample : G2058-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MPE-15

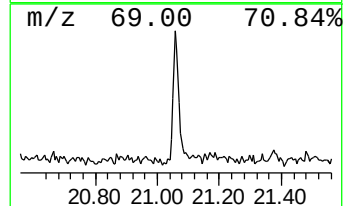
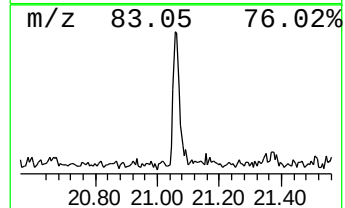
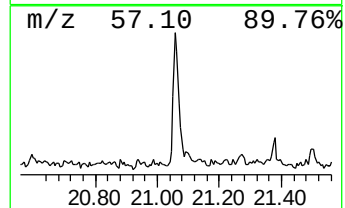
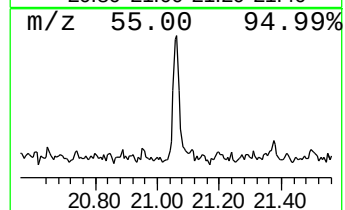
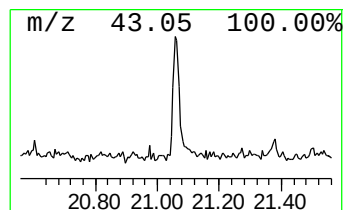
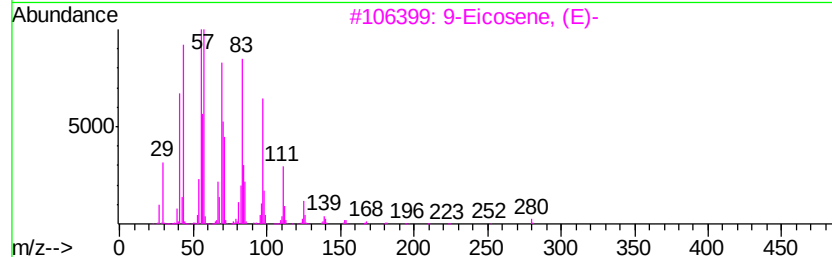
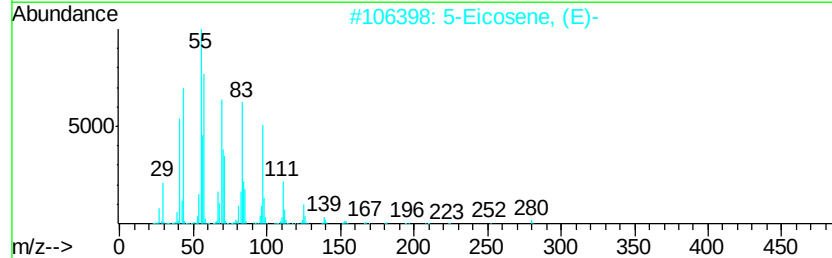
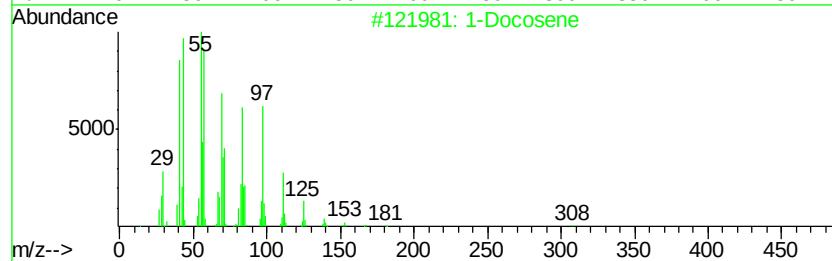
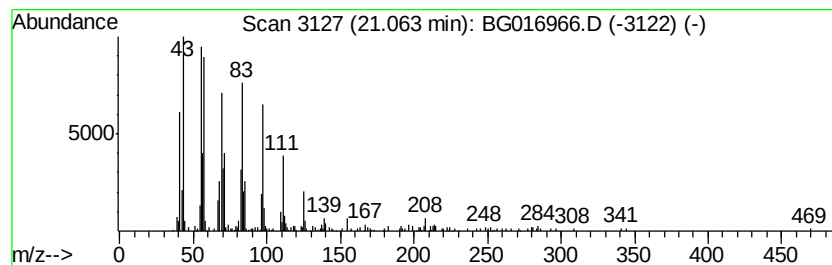
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Docosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.06	2.74 ng	243255	Chrysene-d12	21.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	95
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	94
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	93
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
5		cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	87



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Sample : G2058-13
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MPE-15

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
Butane, 2-methoxy...	2.99	30.8	ng	864969	1	7.79	562070	20.0
unknown4.91	4.91	3.2	ng	88753	1	7.79	562070	20.0
unknown7.33	7.33	68.1	ng	1914480	1	7.79	562070	20.0
3-Hexenoic acid, ...	12.78	2.3	ng	152189	3	14.43	1328670	20.0
Dodecanoic acid	14.86	12.0	ng	799952	3	14.43	1328670	20.0
n-Hexadecanoic acid	18.07	5.9	ng	477352	4	17.17	1613810	20.0
Octadecanoic acid	19.35	3.6	ng	321994	5	21.35	1773980	20.0
1-Docosene	21.06	2.7	ng	243255	5	21.35	1773980	20.0