

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080216\
 Data File : BG023417.D
 Acq On : 3 Aug 2016 5:02
 Operator : UM/SJ
 Sample : H4288-15
 Misc :
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-66-14.0-15.0

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-BG080116.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	2.991	21	26	54	rVB	4363329	7749766	68.23%	11.897%
2	5.182	393	399	412	rBV	559543	937070	8.25%	1.439%
3	5.664	474	481	493	rBV	2092501	3559376	31.34%	5.464%
4	7.279	748	756	768	rBV	2377420	4338600	38.20%	6.660%
5	7.649	810	819	830	rBV	2257132	3928537	34.58%	6.031%
6	8.119	892	899	910	rVB2	349687	605462	5.33%	0.929%
7	8.448	947	955	963	rBV	1409804	2515302	22.14%	3.861%
8	9.294	1091	1099	1108	rBV	1404269	2533771	22.31%	3.890%
9	10.951	1373	1381	1390	rBV	560829	1030543	9.07%	1.582%
10	13.400	1790	1798	1805	rBV	3919441	6384326	56.20%	9.801%
11	14.223	1932	1938	1945	rBV	699991	986537	8.69%	1.514%
12	14.781	2027	2033	2043	rVB3	1075362	1803294	15.88%	2.768%
13	16.279	2281	2288	2302	rBV	4817400	7490233	65.94%	11.499%
14	16.472	2317	2321	2329	rVB	91024	148236	1.31%	0.228%
15	17.542	2494	2503	2511	rBV2	1837989	2781376	24.49%	4.270%
16	18.411	2646	2651	2659	rBV	330698	486998	4.29%	0.748%
17	19.680	2863	2867	2874	rBV4	79865	132326	1.16%	0.203%
18	19.827	2886	2892	2899	rVB	533586	606790	5.34%	0.932%
19	20.150	2941	2947	2955	rBV	8255216	11359078	100.00%	17.438%
20	20.866	3065	3069	3076	rVB	309583	365251	3.22%	0.561%
21	21.460	3166	3170	3178	rBV3	107243	237798	2.09%	0.365%
22	21.853	3231	3237	3244	rBV	1624038	2583004	22.74%	3.965%
23	25.237	3801	3813	3825	rBV2	866821	2577253	22.69%	3.956%

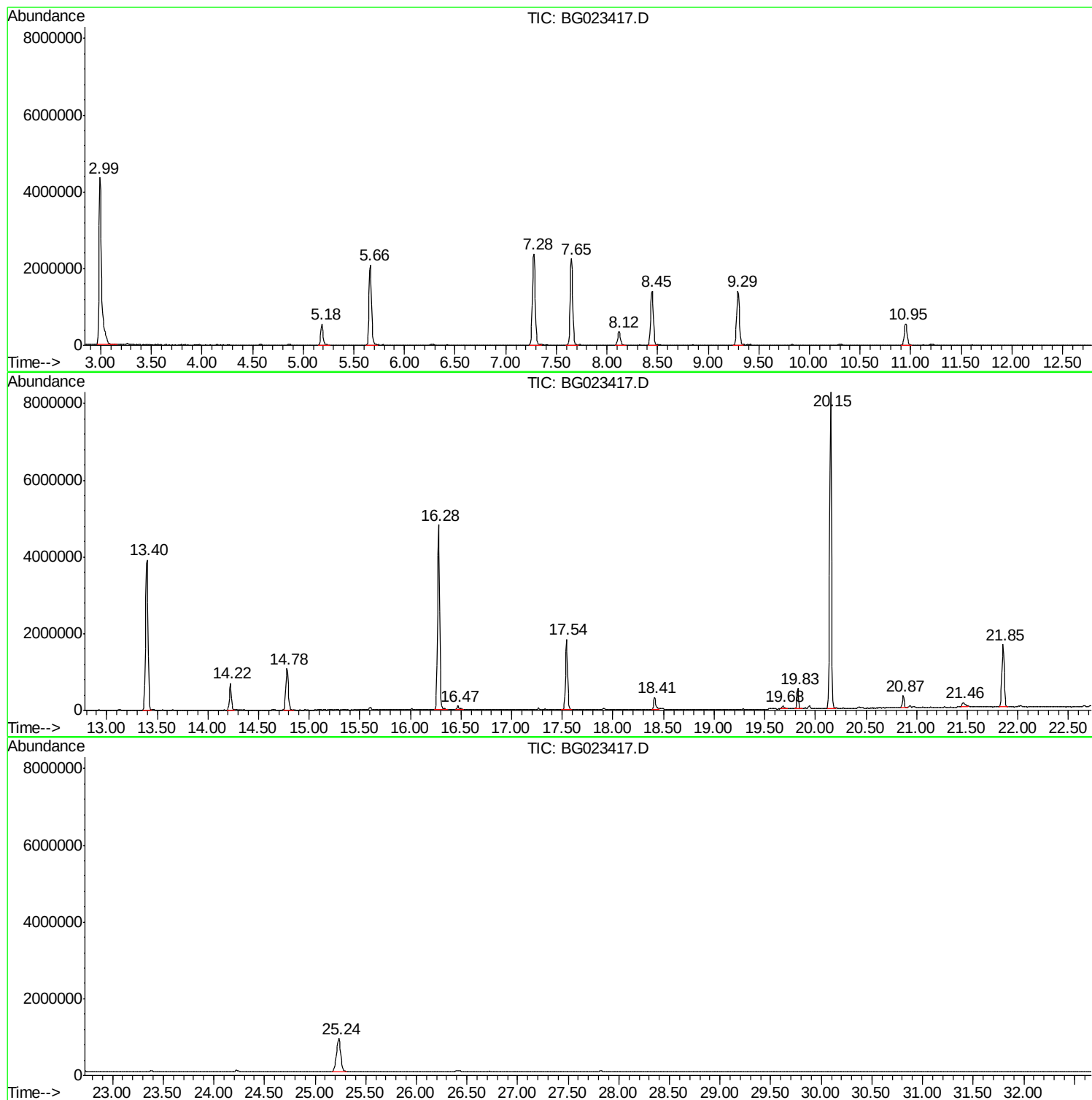
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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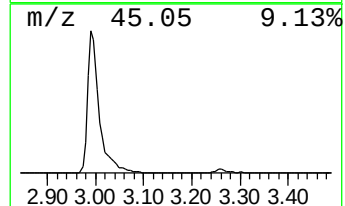
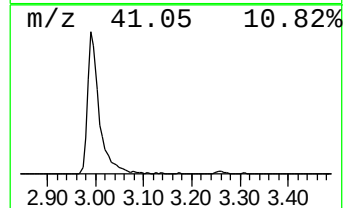
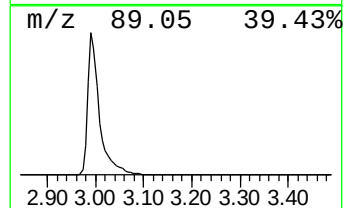
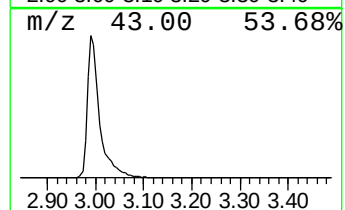
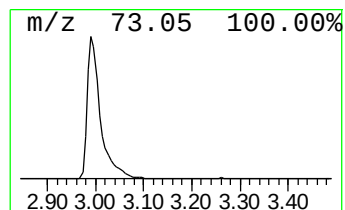
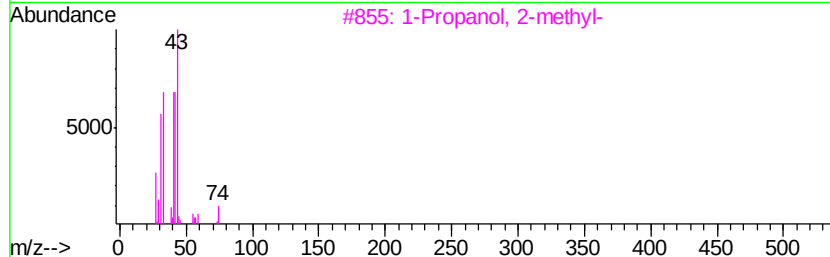
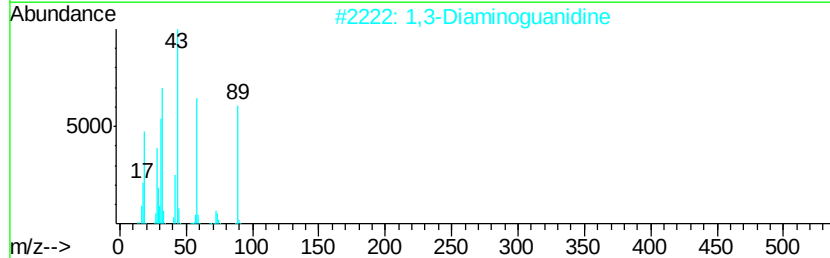
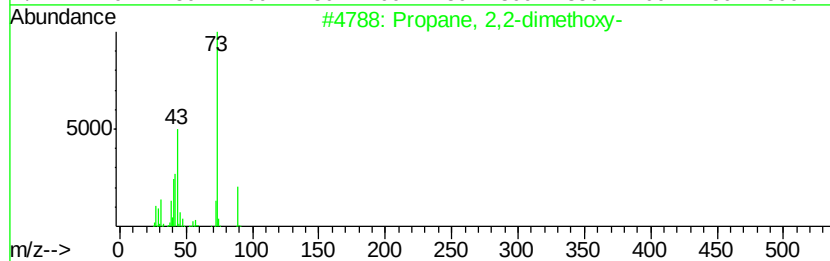
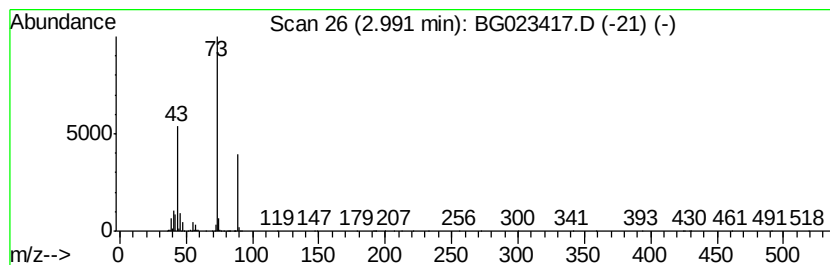
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	256.00 ng	7749770	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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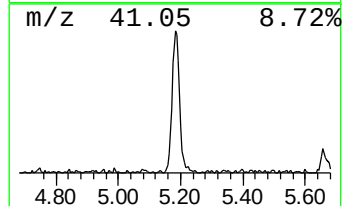
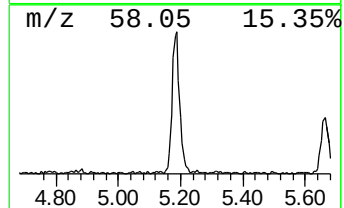
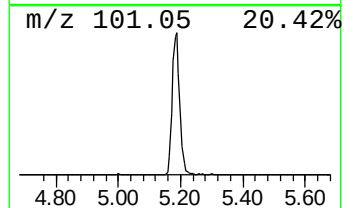
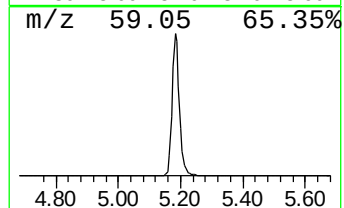
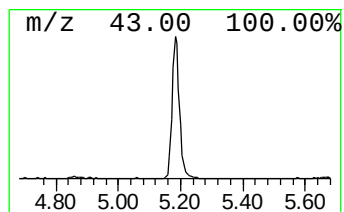
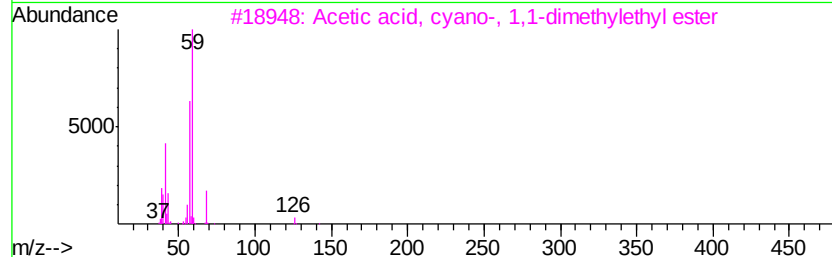
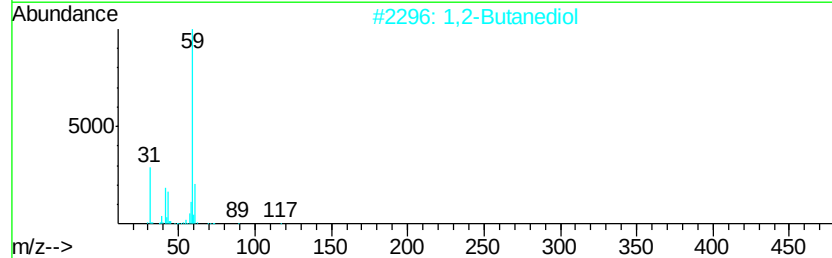
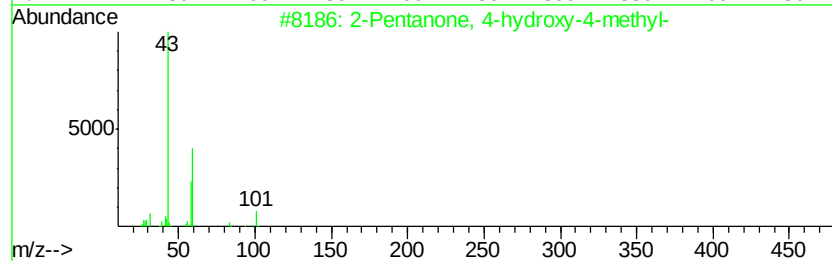
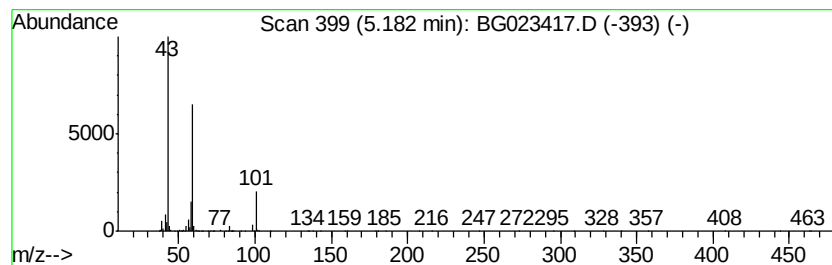
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	30.95 ng	937070	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,2-Butanediol	90	C4H10O2	000584-03-2	23
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Guanidine	59	CH5N3	000113-00-8	9



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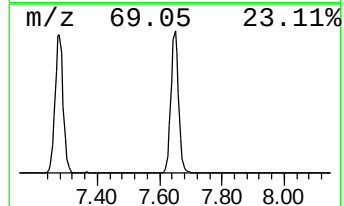
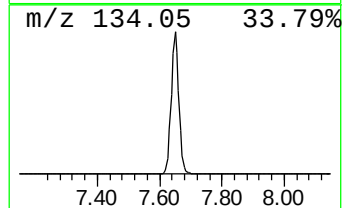
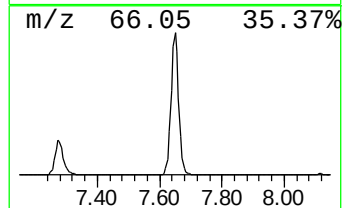
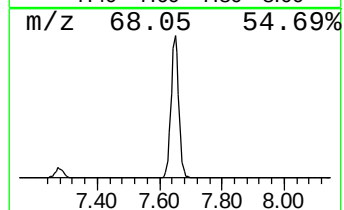
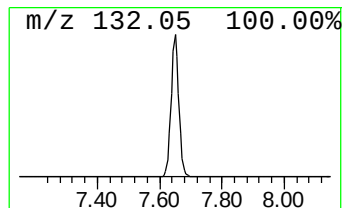
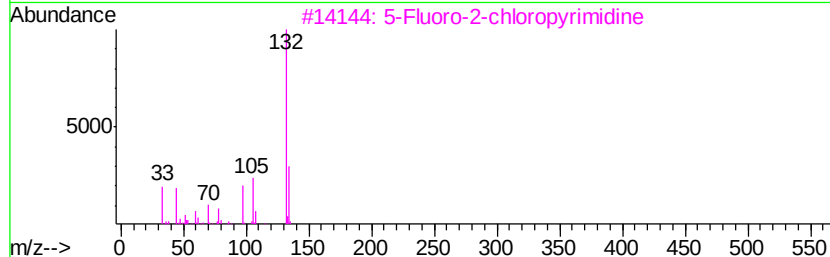
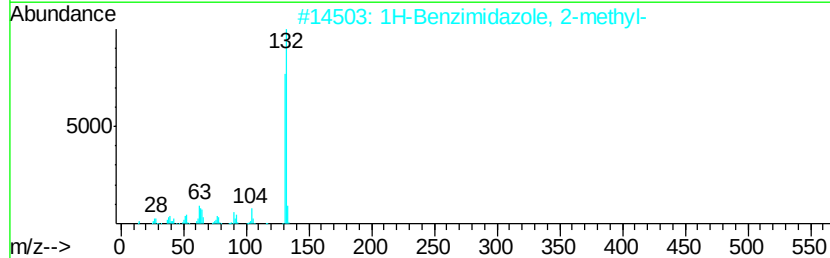
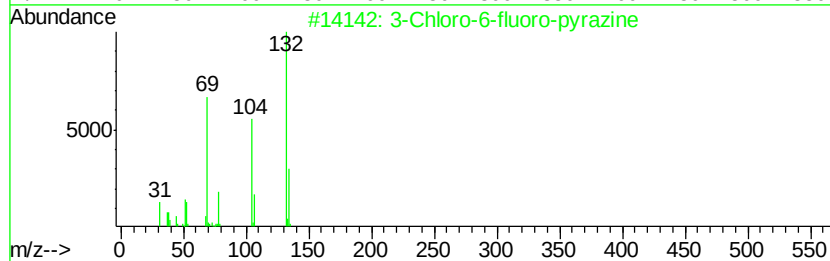
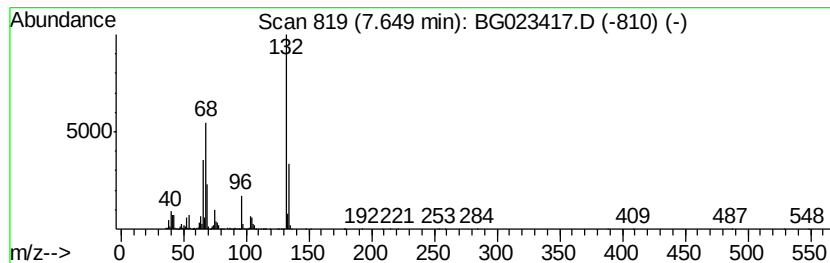
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Peak Number 3 unknown7.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.65	129.77 ng	3928540	1,4-Dichlorobenzene-d4	8.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		N-(-3,4-Methylenedioxyphenyl)isop...	267	C17H17NO2	1000378-96-6	10



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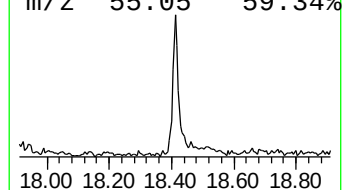
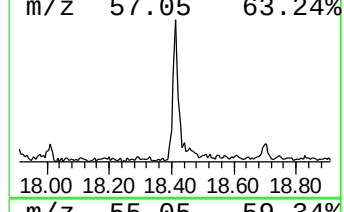
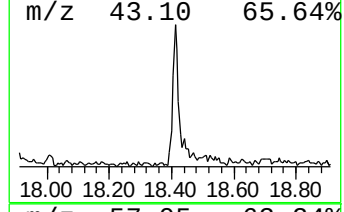
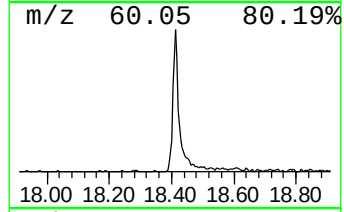
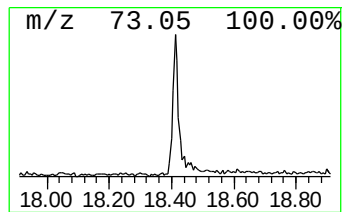
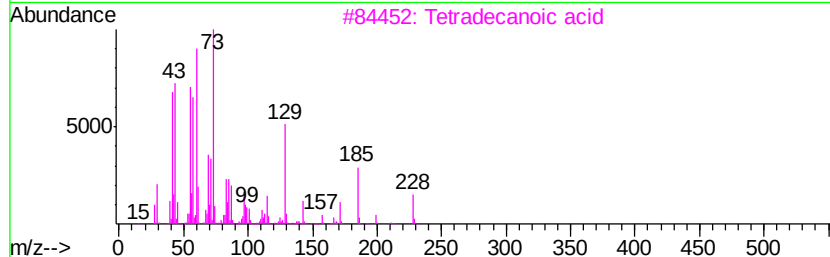
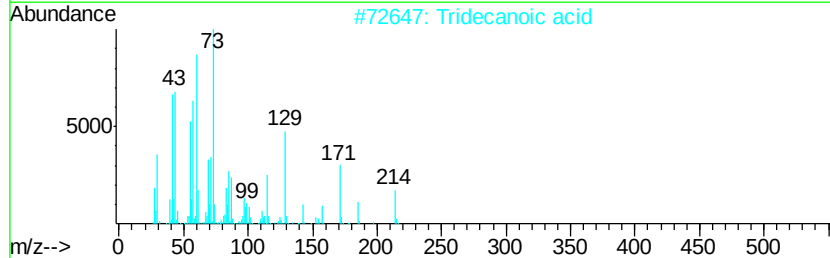
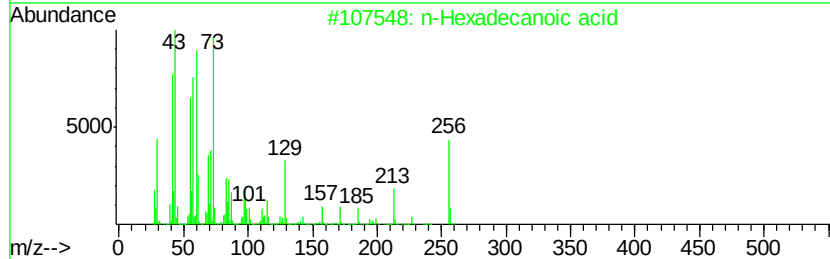
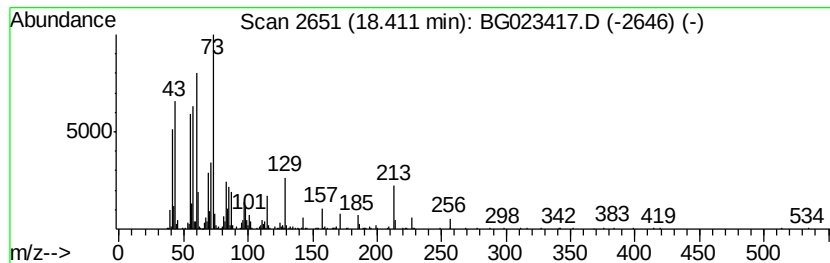
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	3.50 ng	486998	Phenanthrene-d10	17.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5	Dodecanoic acid	200	C12H24O2	000143-07-7	76



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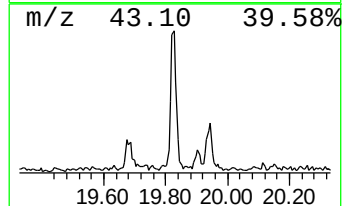
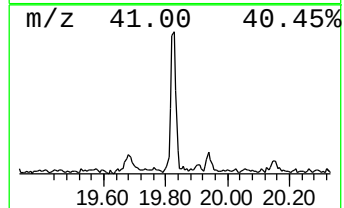
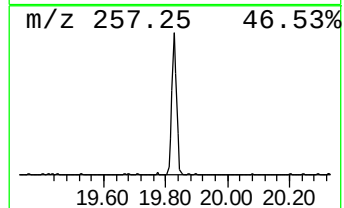
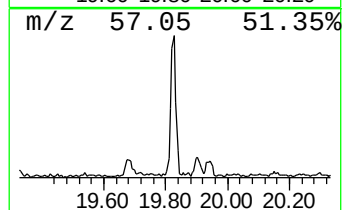
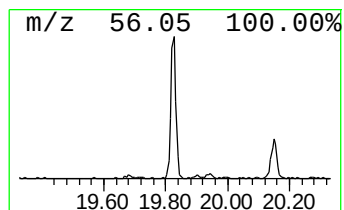
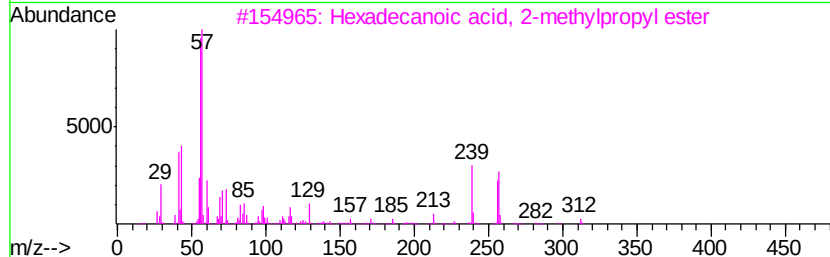
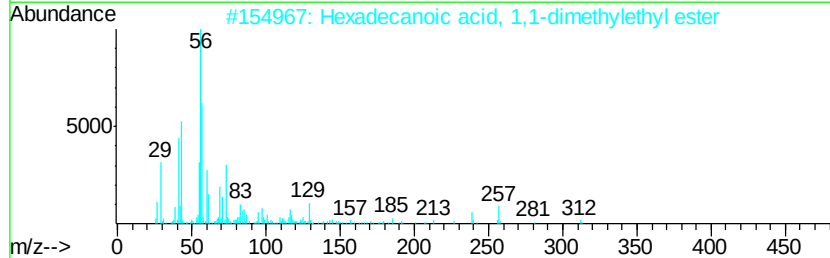
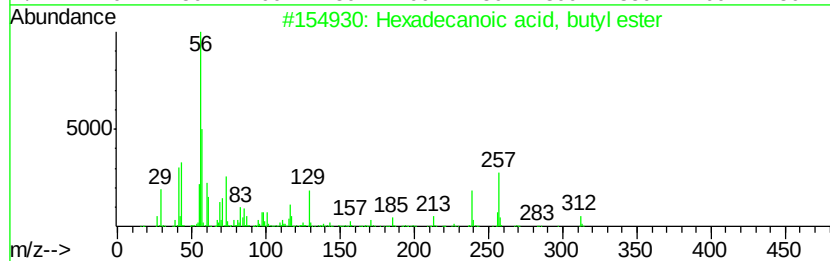
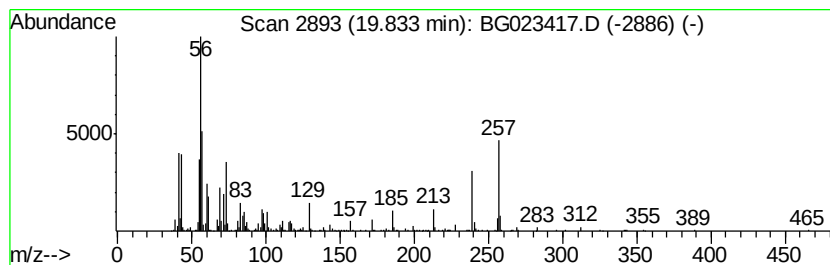
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Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.83	4.70 ng	606790	Chrysene-d12	21.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	89
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	45
4		2-Methyl-1-octadecene	266	C19H38	061868-20-0	27
5		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	27



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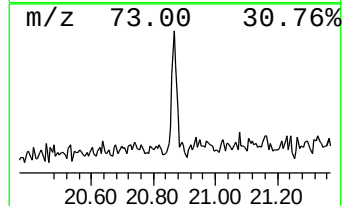
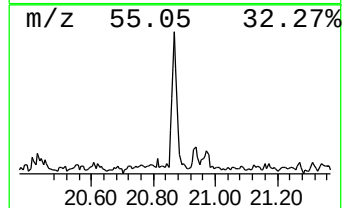
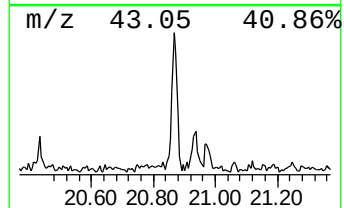
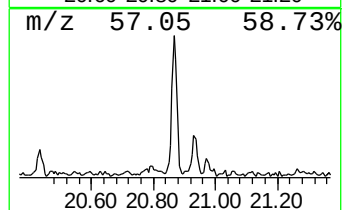
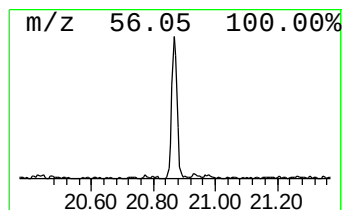
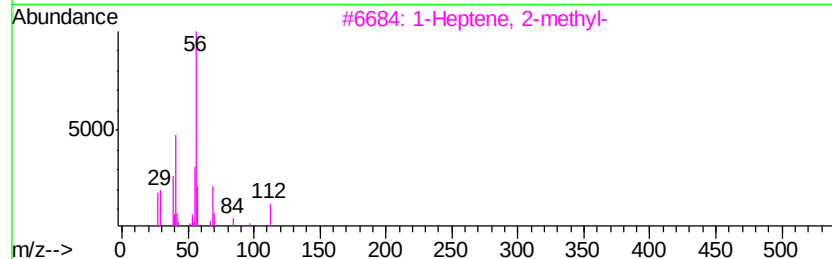
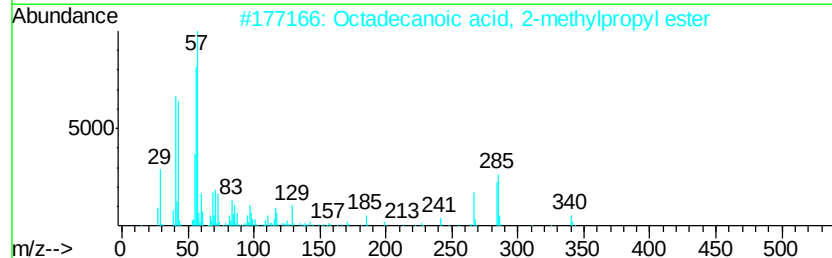
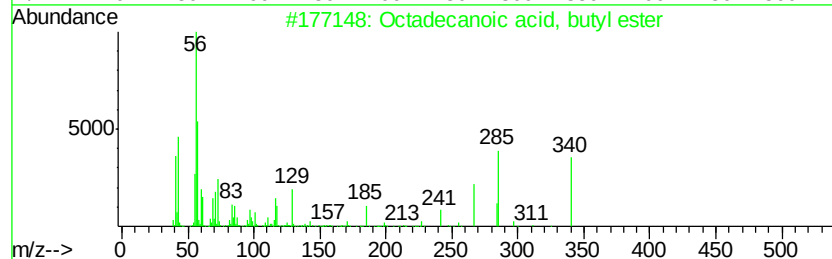
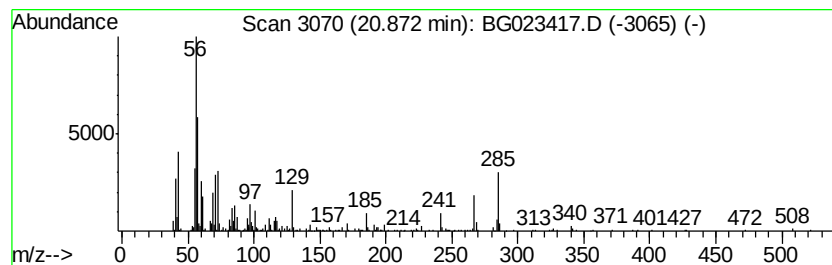
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	2.83 ng	365251	Chrysene-d12	21.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	50
2		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	46
3		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	38
4		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
5		Oxirane, (1-methylbutyl)-	114	C7H14O	053229-39-3	35



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG080216\
Data File : BG023417.D
Acq On : 3 Aug 2016 5:02
Operator : UM/SJ
Sample : H4288-15
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-66-14.0-15.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	2.99	256.0	ng	7749770	1	8.12	605462	20.0
2-Pentanone, 4-hy...	5.18	30.9	ng	937070	1	8.12	605462	20.0
unknown7.65	7.65	129.8	ng	3928540	1	8.12	605462	20.0
n-Hexadecanoic acid	18.41	3.5	ng	486998	4	17.54	2781380	20.0
Hexadecanoic acid...	19.83	4.7	ng	606790	5	21.85	2583000	20.0
Octadecanoic acid...	20.87	2.8	ng	365251	5	21.85	2583000	20.0