

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
 Data File : BG029303.D
 Acq On : 17 Oct 2017 16:14
 Operator : SJ/JU
 Sample : I5794-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ENV-106-5(10-15)

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-BG101617.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	5.245	326	333	343	rBV	243665	369529	8.67%	1.324%
2	5.721	407	414	428	rBV	1212291	1940203	45.52%	6.954%
3	7.325	678	687	701	rBV	1267033	2344613	55.01%	8.403%
4	7.701	743	751	766	rBV	1250573	2138682	50.18%	7.665%
5	8.171	823	831	838	rBV	222046	382113	8.97%	1.369%
6	8.494	878	886	898	rVB	841108	1472887	34.56%	5.279%
7	9.334	1020	1029	1042	rBV	758235	1342873	31.51%	4.813%
8	10.985	1300	1310	1318	rBV	347636	629750	14.78%	2.257%
9	13.412	1715	1723	1733	rBV	1985646	3125591	73.33%	11.202%
10	14.229	1855	1862	1869	rBV	609954	873811	20.50%	3.132%
11	14.787	1949	1957	1965	rBV2	589620	950305	22.30%	3.406%
12	16.132	2179	2186	2191	rBV	91895	129987	3.05%	0.466%
13	16.267	2202	2209	2224	rBV	1911498	2947114	69.15%	10.562%
14	17.525	2416	2423	2431	rBV	780240	1179783	27.68%	4.228%
15	18.394	2566	2571	2581	rBV2	275660	396877	9.31%	1.422%
16	19.652	2780	2785	2795	rBV	107948	158208	3.71%	0.567%
17	20.116	2858	2864	2873	rVB	3192171	4262120	100.00%	15.275%
18	21.414	3080	3085	3097	rBV	140705	250885	5.89%	0.899%
19	21.796	3142	3150	3163	rVB2	817400	1375844	32.28%	4.931%
20	23.518	3436	3443	3452	rVB	156930	315363	7.40%	1.130%
21	25.104	3703	3713	3725	rBV3	425230	1315750	30.87%	4.716%

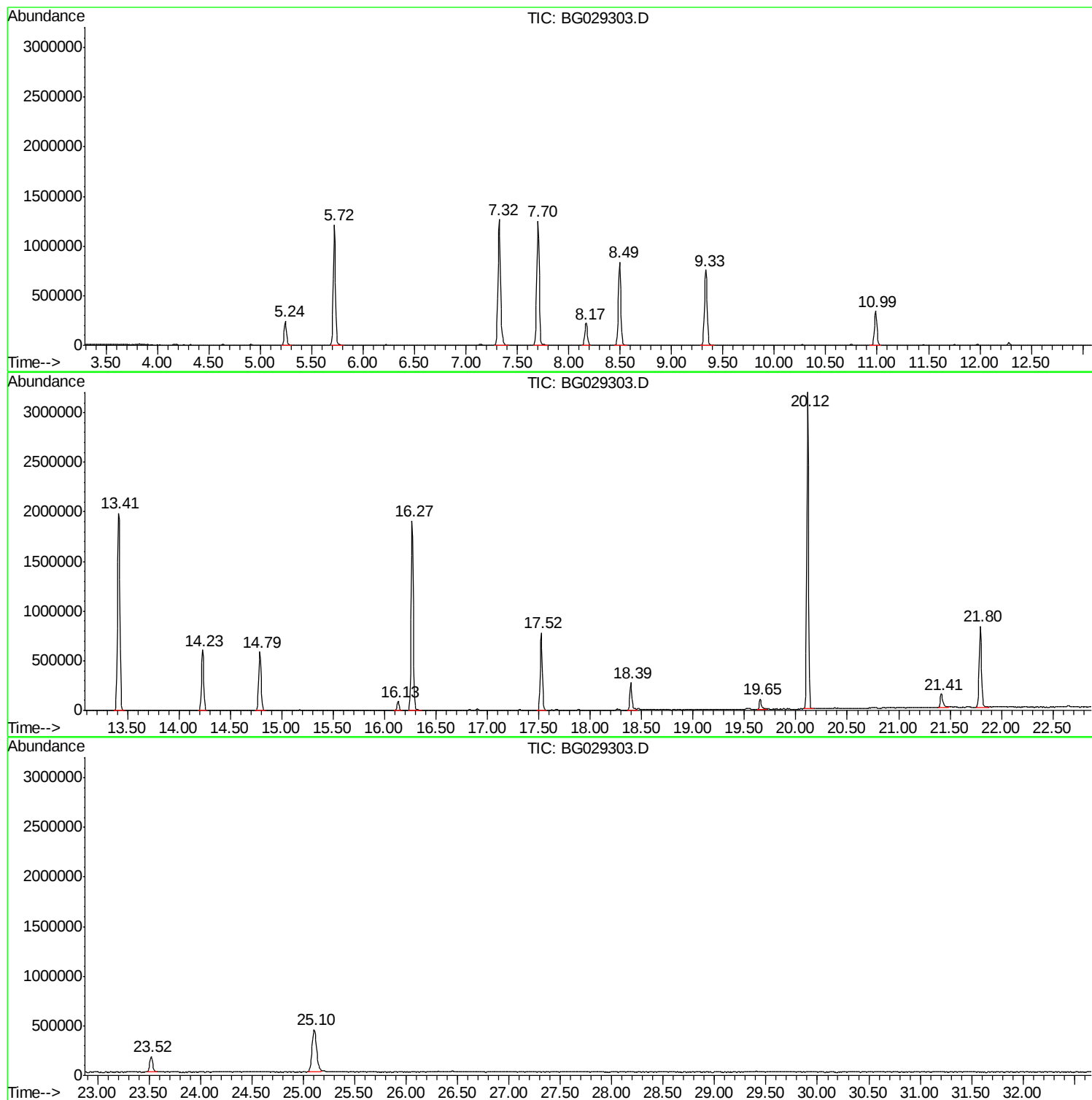
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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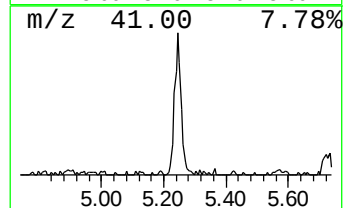
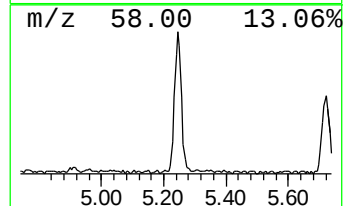
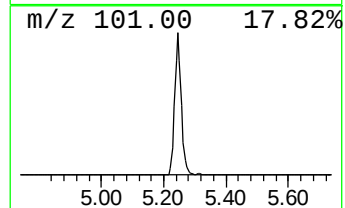
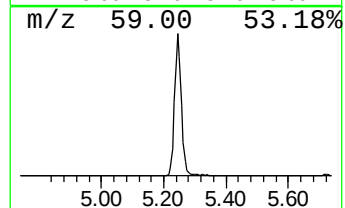
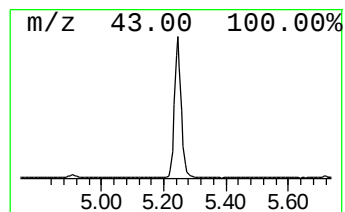
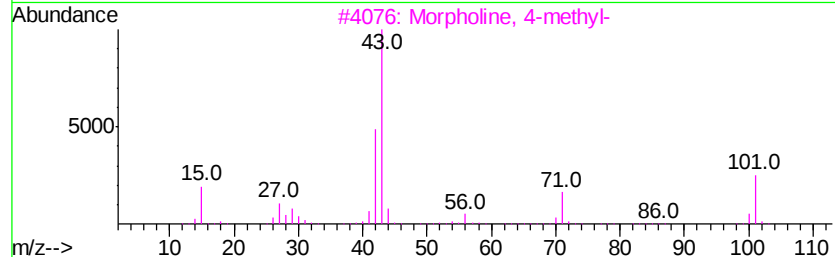
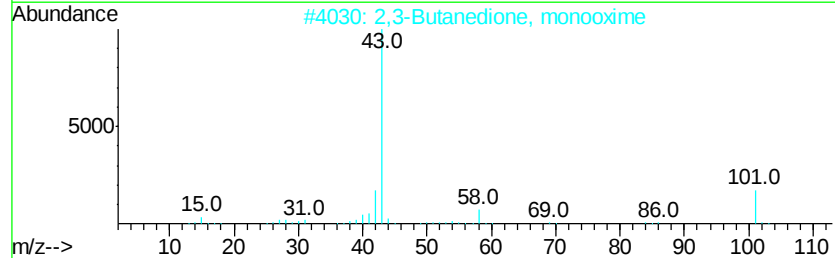
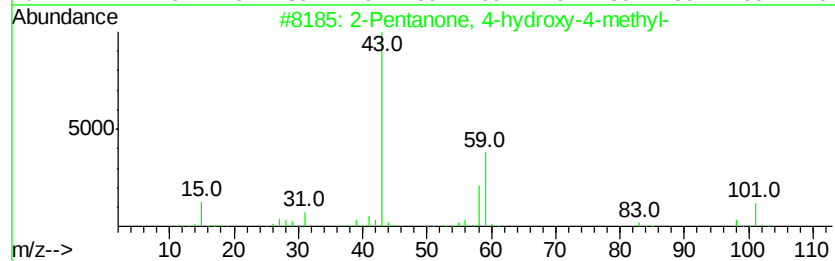
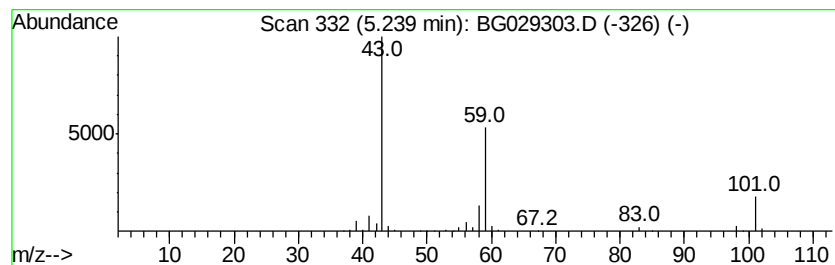
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.24	19.34 ng	369529	1,4-Dichlorobenzene-d4	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9



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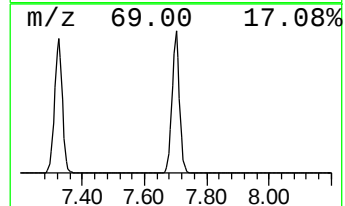
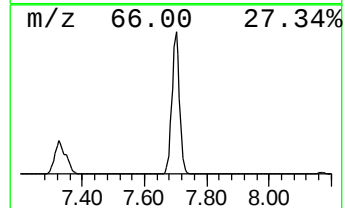
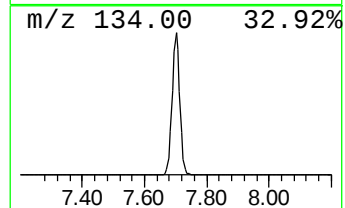
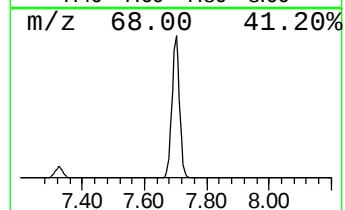
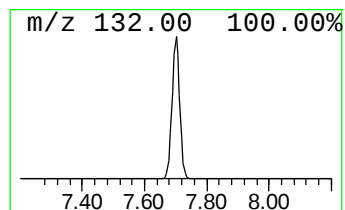
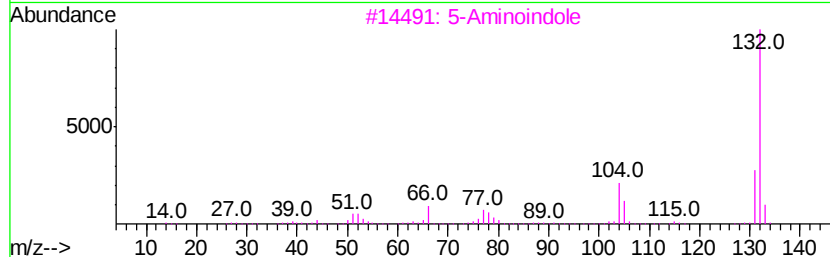
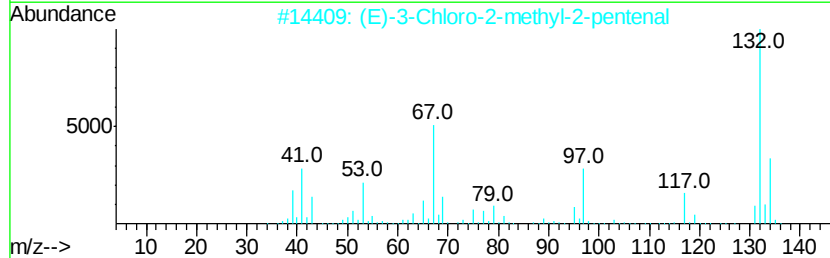
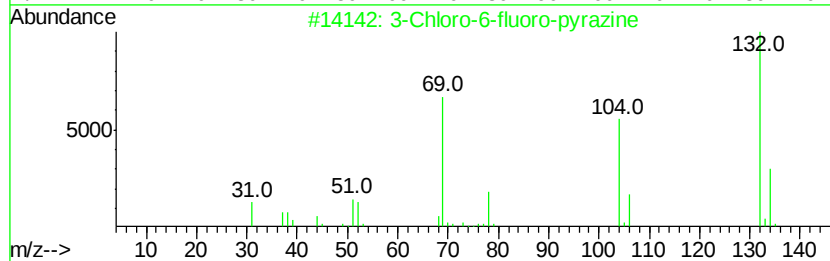
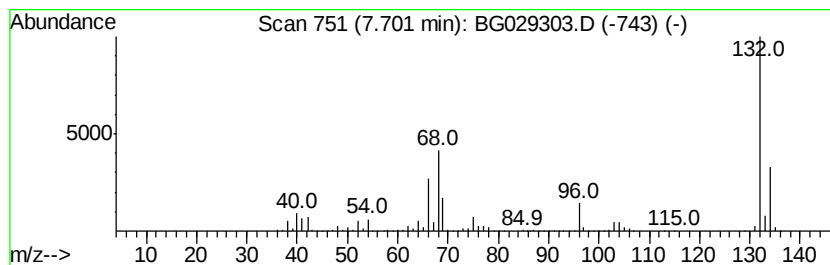
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Peak Number 2 unknown7.70 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	111.94 ng	2138680	1,4-Dichlorobenzene-d4	8.17

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	27
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Amphetaminil	250	C17H18N2	017590-01-1	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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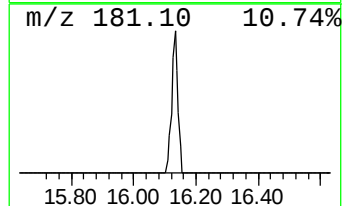
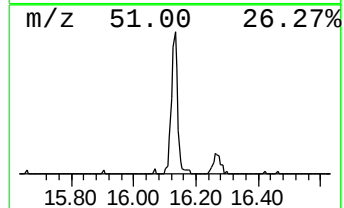
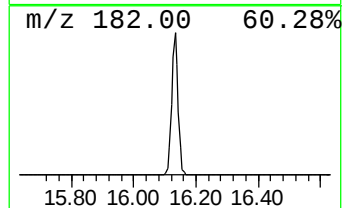
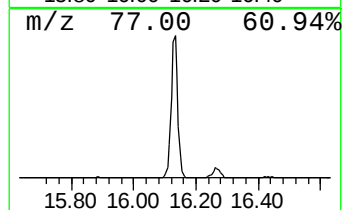
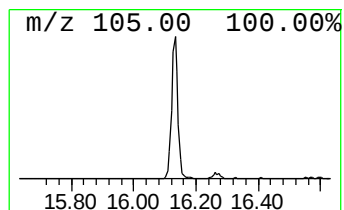
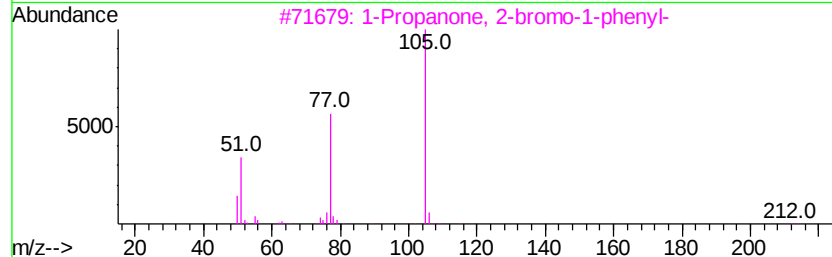
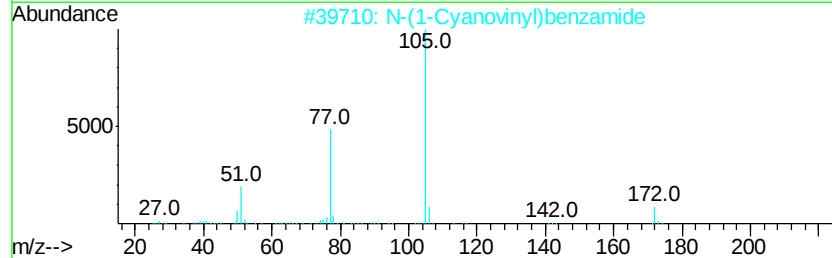
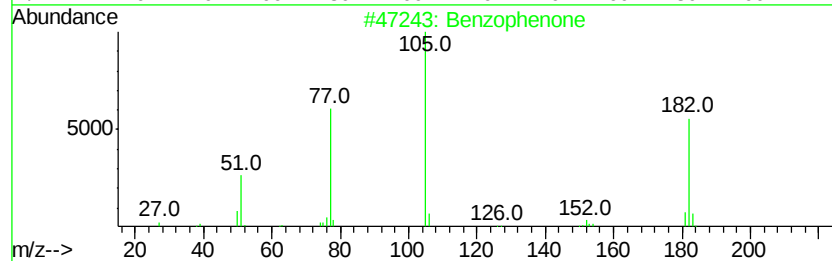
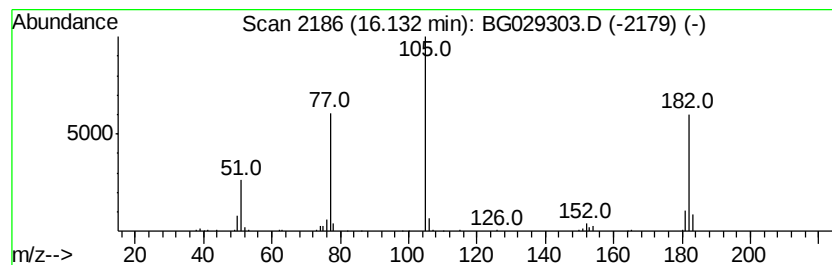
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Peak Number 4 Benzophenone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.13	2.74 ng	129987	Acenaphthene-d10	14.79	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
5	1,2,4-Triazine-3,5(2H,4H)-dione, ...	249	C10H7N3O3S	024168-34-1	47



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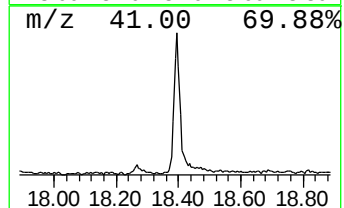
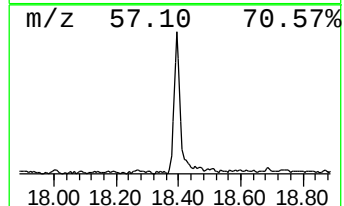
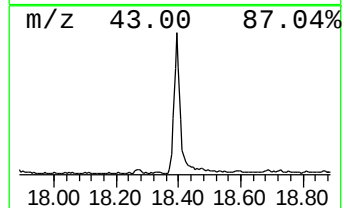
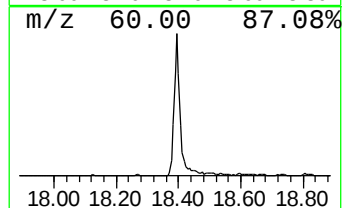
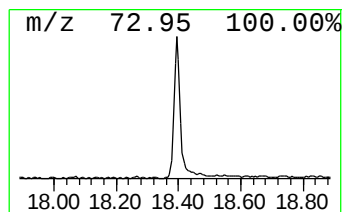
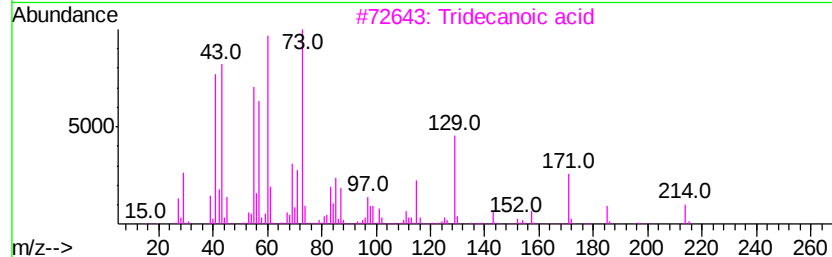
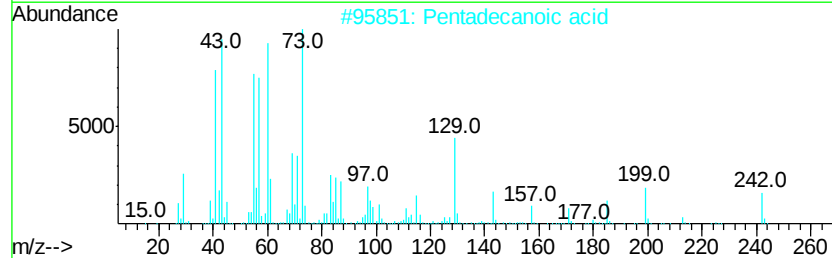
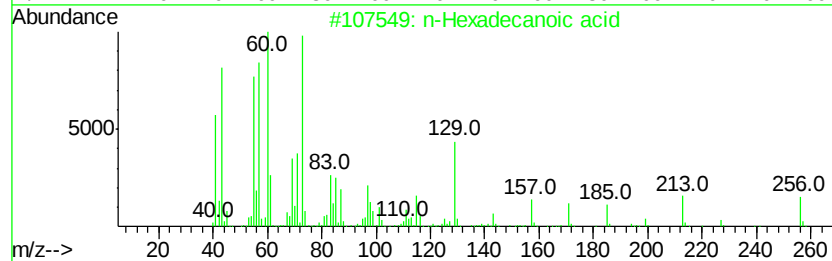
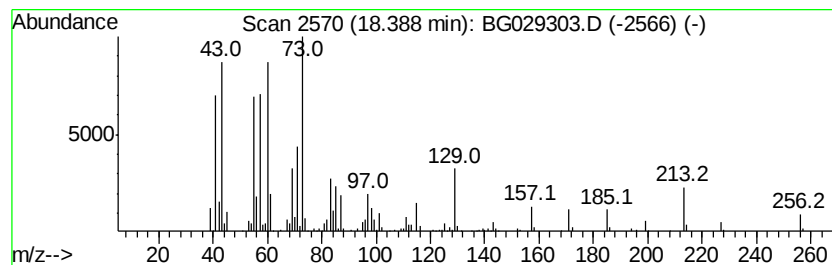
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.39	6.73 ng	396877	Phenanthrene-d10	17.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58



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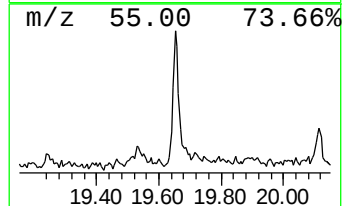
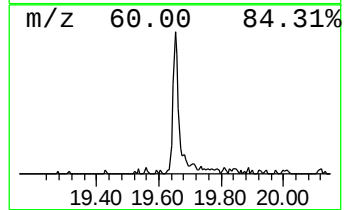
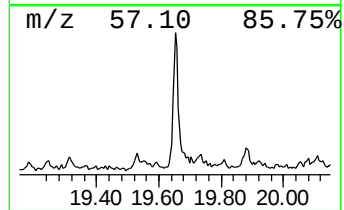
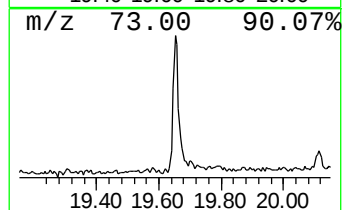
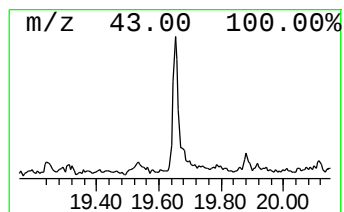
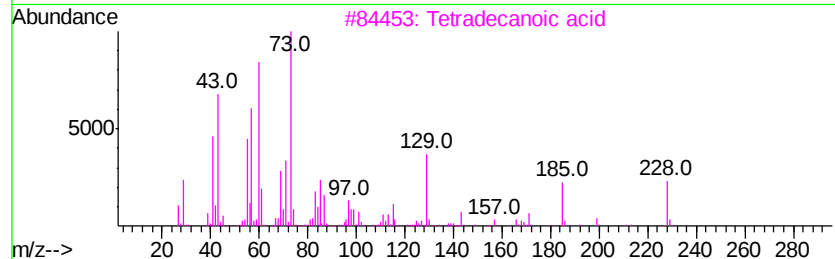
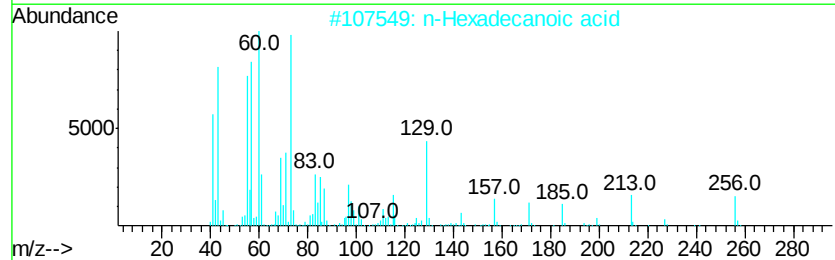
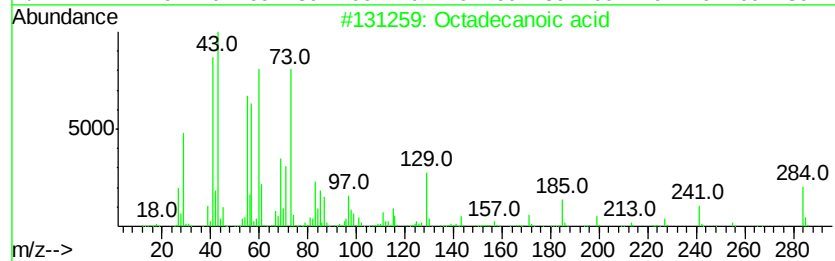
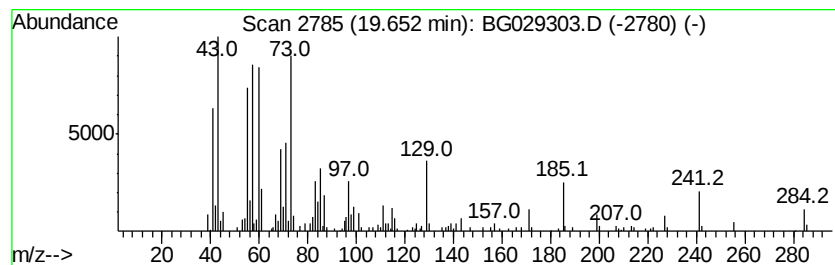
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Peak Number 6 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.65	2.68 ng	158208	Phenanthrene-d10		17.52
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	68
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64



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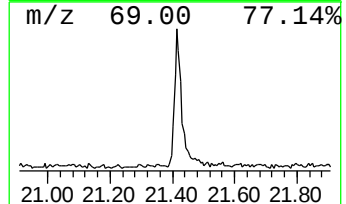
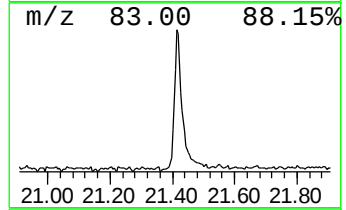
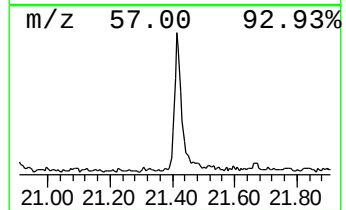
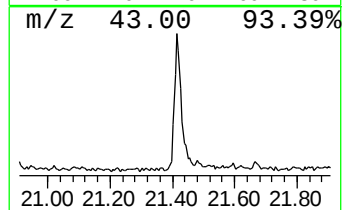
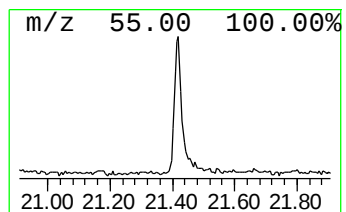
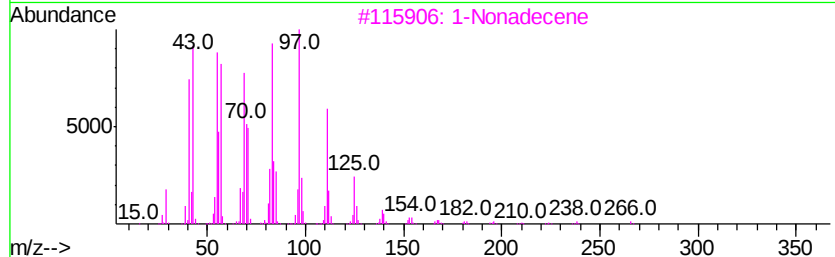
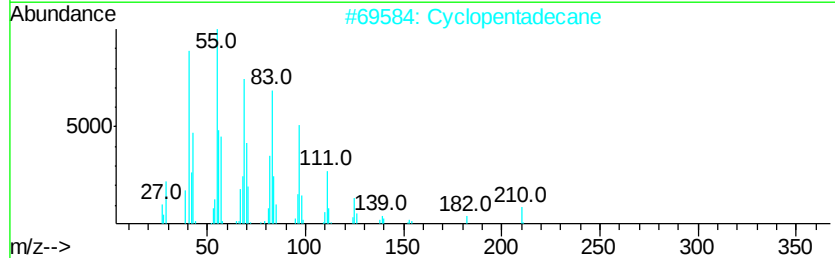
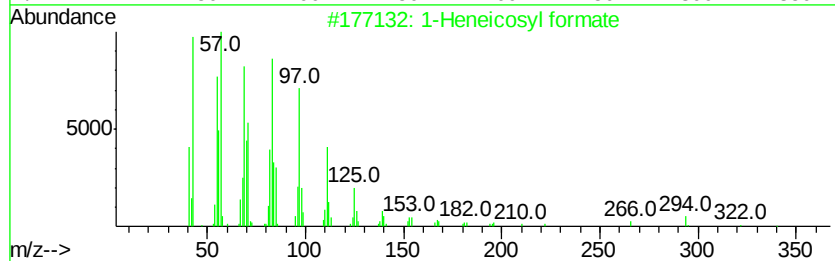
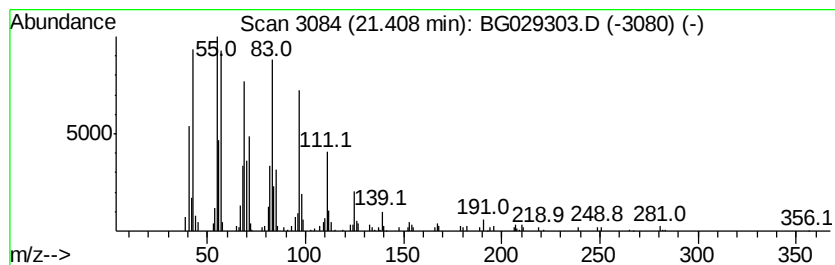
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ClientSampleId :
ENV-106-5(10-15)

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Heneicosyl formate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.41	3.65 ng	250885	Chrysene-d12	21.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
2	Cyclopentadecane	210	C15H30	000295-48-7	93
3	1-Nonadecene	266	C19H38	018435-45-5	91
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5	Behenic alcohol	326	C22H46O	000661-19-8	91



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101717\
Data File : BG029303.D
Acq On : 17 Oct 2017 16:14
Operator : SJ/JU
Sample : I5794-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ENV-106-5(10-15)

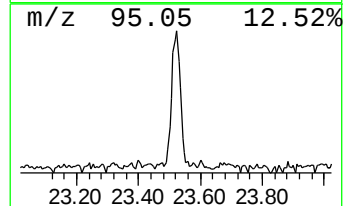
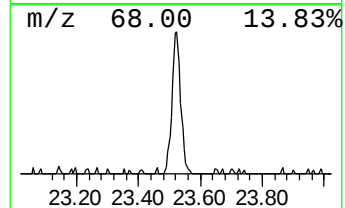
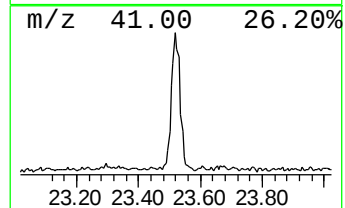
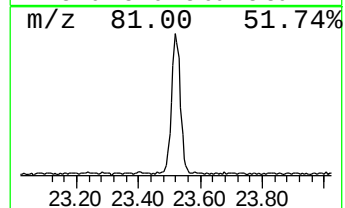
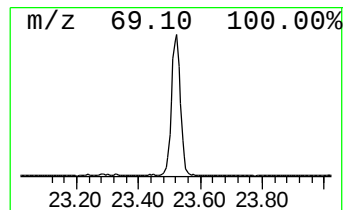
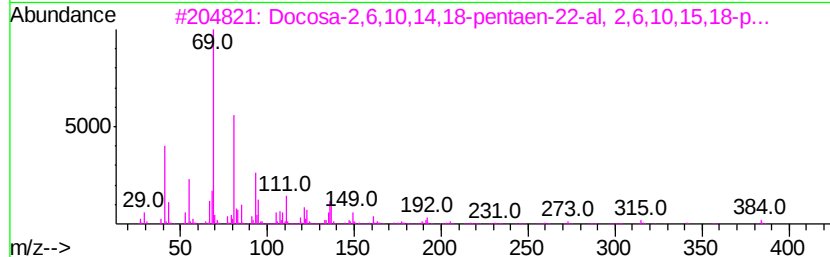
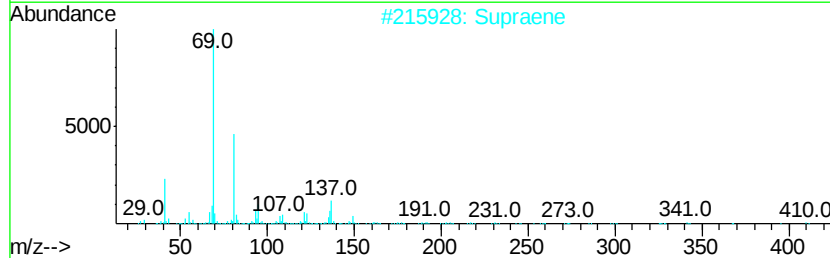
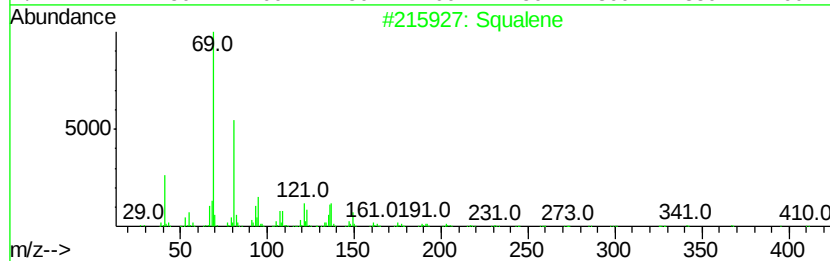
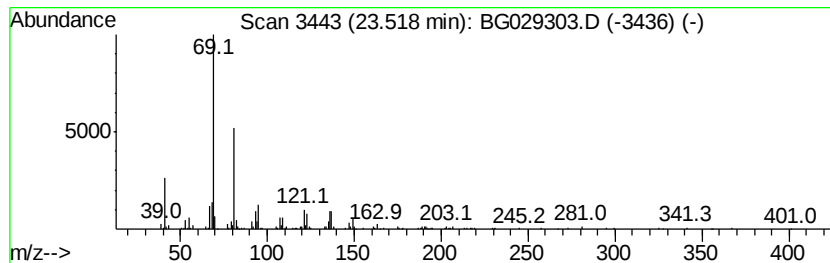
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.52	4.79 ng	315363	Perylene-d12	25.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	87
3		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83
4		2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	78
5		trans-Farnesol	222	C15H26O	000106-28-5	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101717\
Data File : BG029303.D
Acq On : 17 Oct 2017 16:14
Operator : SJ/JU
Sample : I5794-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
ENV-106-5(10-15)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101617.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
2-Pentanone, 4-hy...	5.24	19.3	ng	369529	1	8.17	382113	20.0
unknown7.70	7.70	111.9	ng	2138680	1	8.17	382113	20.0
Benzophenone	16.13	2.7	ng	129987	3	14.79	950305	20.0
n-Hexadecanoic acid	18.39	6.7	ng	396877	4	17.52	1179780	20.0
Octadecanoic acid	19.65	2.7	ng	158208	4	17.52	1179780	20.0
1-Heneicosyl formate	21.41	3.6	ng	250885	5	21.80	1375840	20.0
Squalene	23.52	4.8	ng	315363	6	25.10	1315750	20.0