

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012023\
 Data File : BG056375.D
 Acq On : 20 Jan 2023 20:09
 Operator : CG/JU
 Sample : 01232-10
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DUP01

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:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056375.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.341	343	349	360	rBV	120079	186235	7.41%	1.615%
2	5.829	425	432	440	rBV	486676	824049	32.77%	7.148%
3	7.444	699	707	716	rBV	499074	885949	35.23%	7.685%
4	8.302	847	853	864	rBB	141438	236440	9.40%	2.051%
5	9.477	1046	1053	1064	rVB	299977	534839	21.27%	4.639%
6	11.134	1327	1335	1343	rBV	188075	337371	13.42%	2.926%
7	13.543	1738	1745	1753	rBV	1182507	1803591	71.72%	15.645%
8	14.918	1969	1979	1990	rBV	348738	525006	20.88%	4.554%
9	16.258	2197	2207	2211	rBV	45485	70581	2.81%	0.612%
10	16.399	2223	2231	2239	rBV	789836	1215605	48.34%	10.544%
11	17.656	2438	2445	2457	rBV	417331	652855	25.96%	5.663%
12	18.496	2584	2588	2597	rBV	99856	144287	5.74%	1.252%
13	19.401	2738	2742	2745	rBV4	22049	33362	1.33%	0.289%
14	19.648	2780	2784	2787	rBV	41989	48860	1.94%	0.424%
15	19.753	2799	2802	2805	rBV4	23794	30209	1.20%	0.262%
16	19.889	2821	2825	2831	rBV	154676	180912	7.19%	1.569%
17	20.194	2874	2877	2878	rBV	61676	61275	2.44%	0.532%
18	20.229	2878	2883	2888	rVB	2014566	2514690	100.00%	21.813%
19	21.528	3101	3104	3114	rVB2	64240	114017	4.53%	0.989%
20	21.945	3170	3175	3181	rVB2	374999	641047	25.49%	5.561%
21	25.388	3755	3761	3772	rVB3	155530	487318	19.38%	4.227%

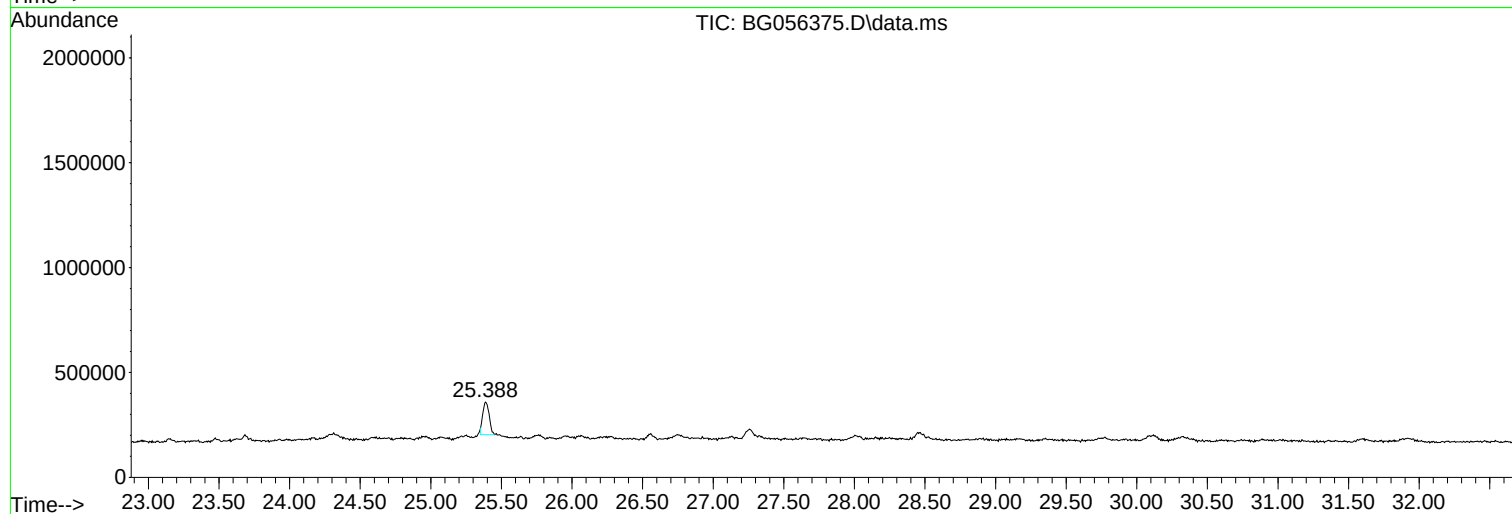
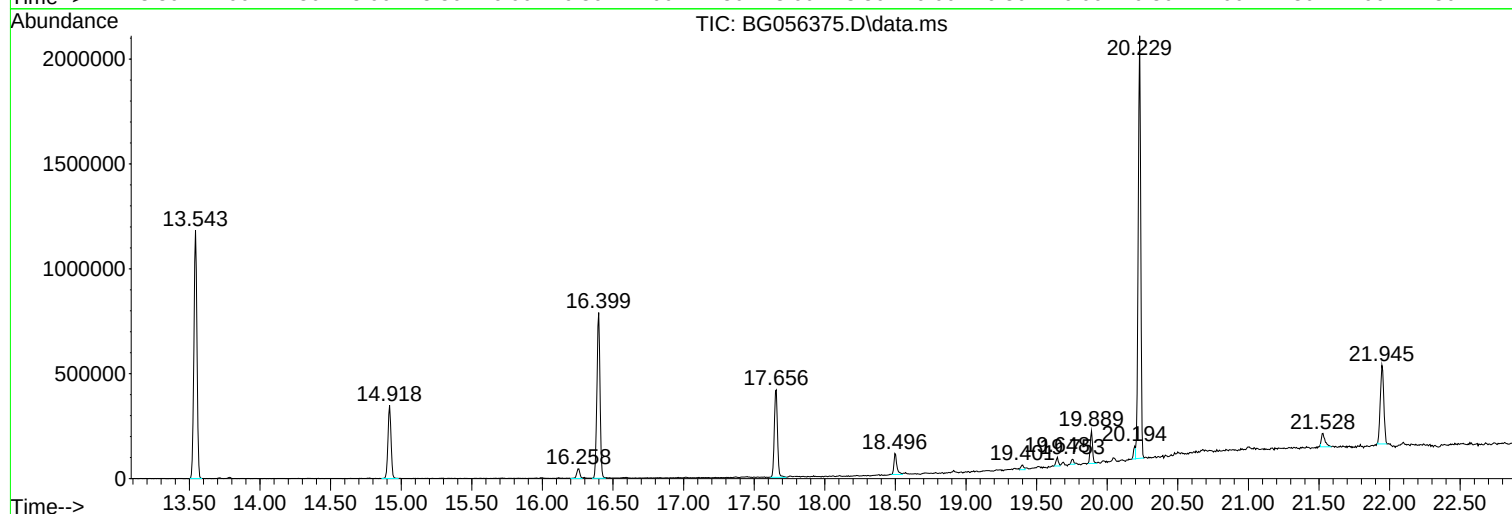
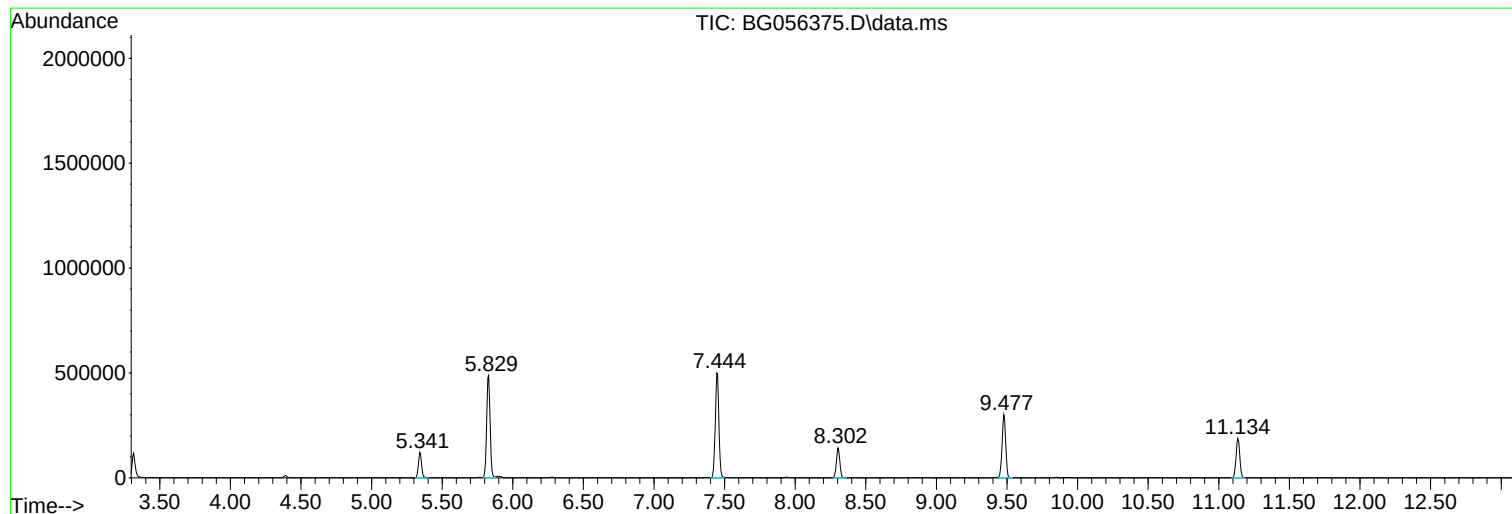
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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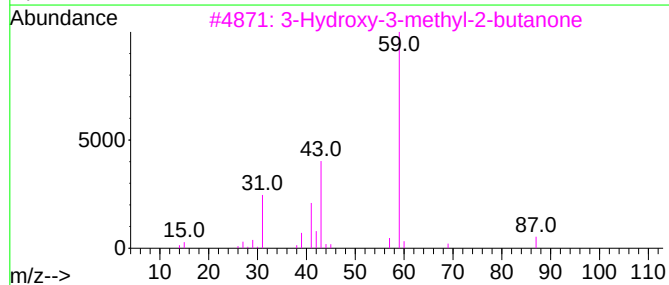
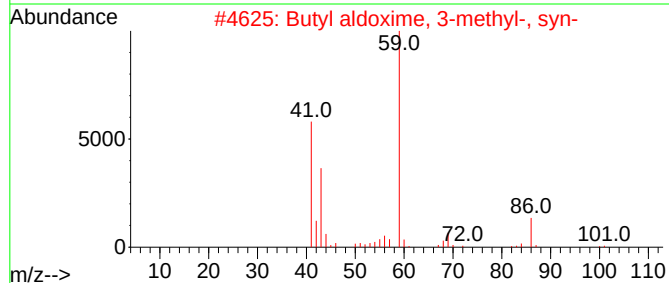
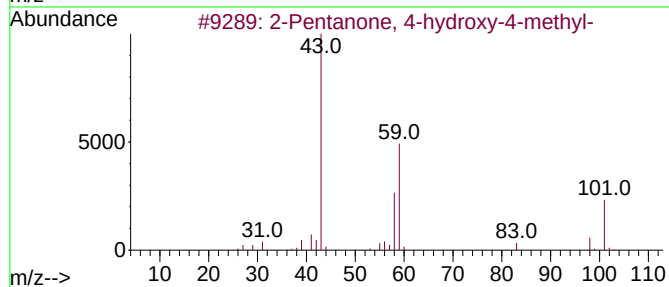
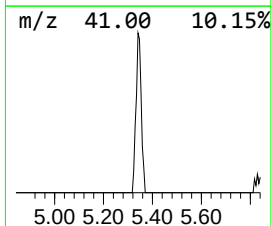
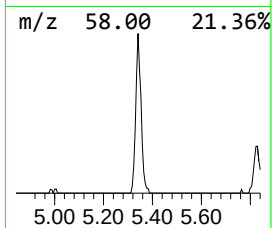
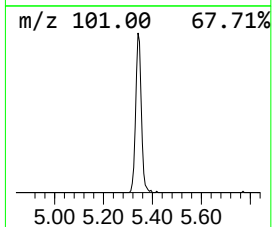
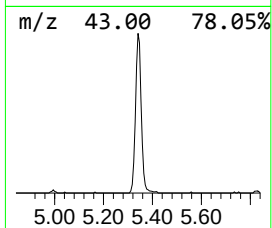
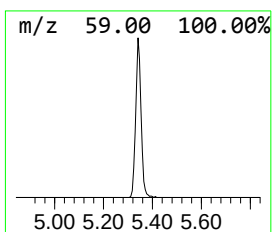
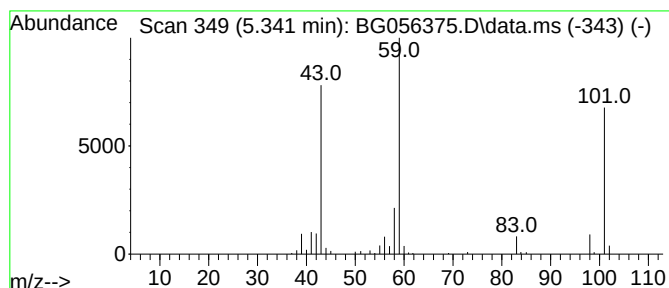
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.341	15.75 ng	186235	1,4-Dichlorobenzene-d4	8.302

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	35	
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32	
4	Guanidine	59	CH5N3	000113-00-8	32	
5	Oxirane, tetramethyl-	100	C6H12O	005076-20-0	23	



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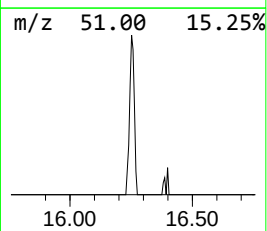
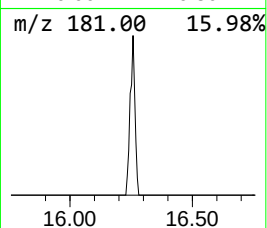
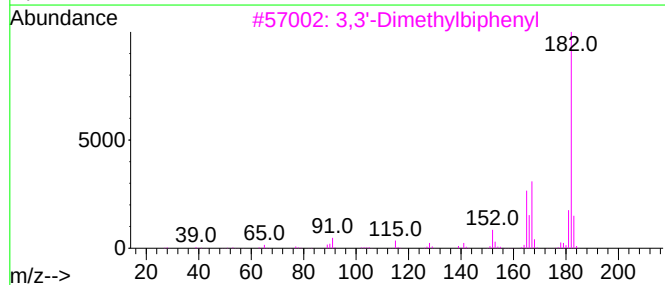
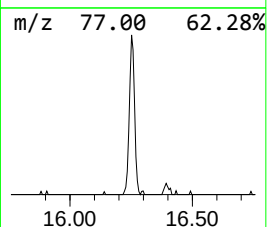
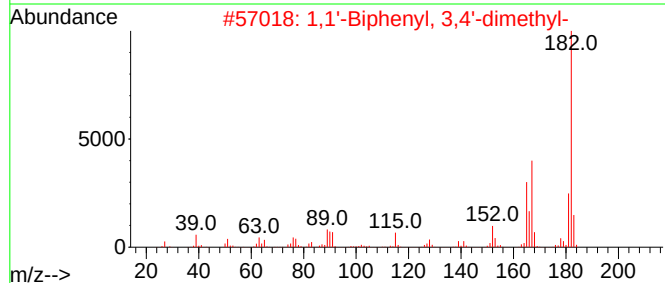
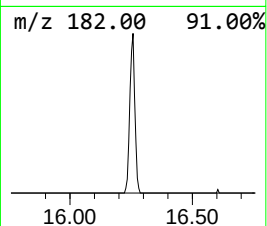
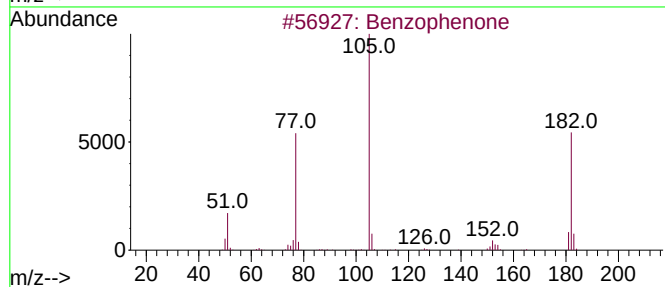
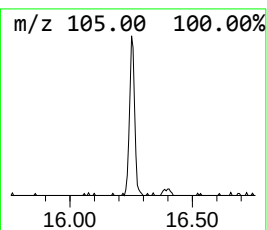
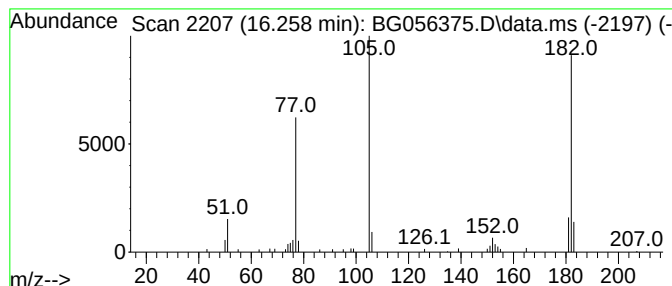
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.258	2.69 ng	70581	Acenaphthene-d10	14.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	91
2			1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	46
3			3,3'-Dimethylbiphenyl	182	C14H14	000612-75-9	43
4			2,4,6-Trimethoxytoluene	182	C10H14O3	014107-97-2	43
5			Methyl benzilate	242	C15H14O3	000076-89-1	38



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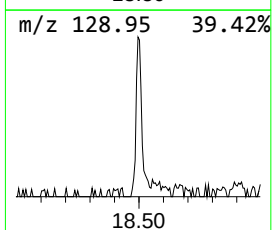
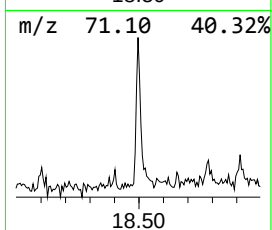
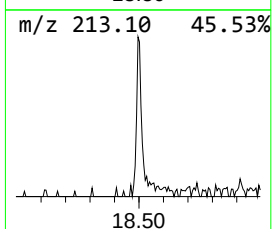
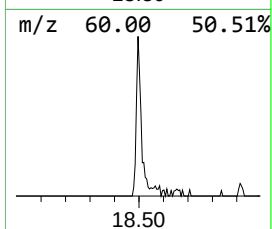
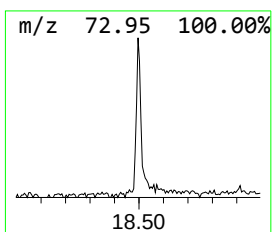
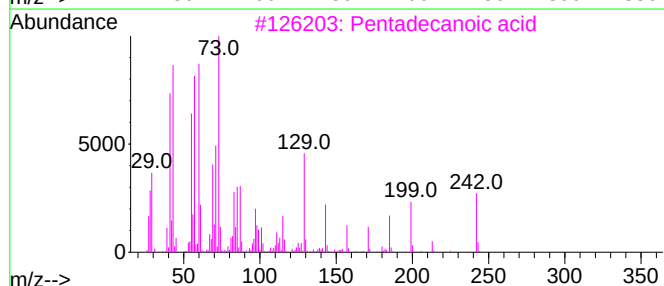
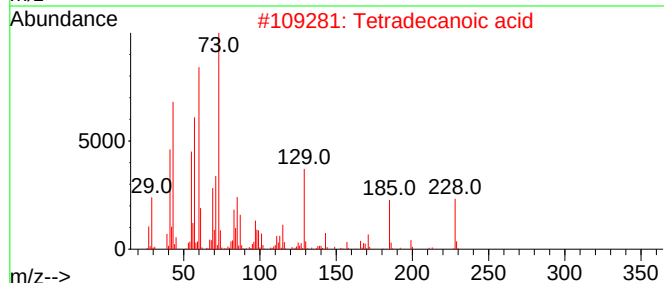
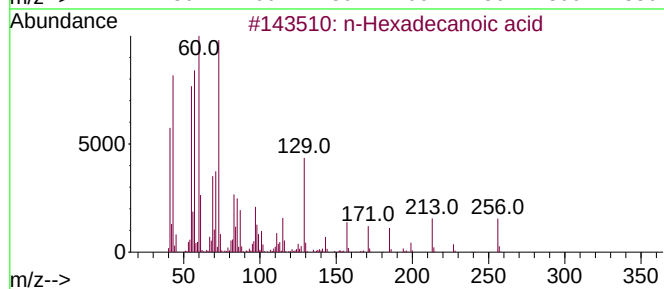
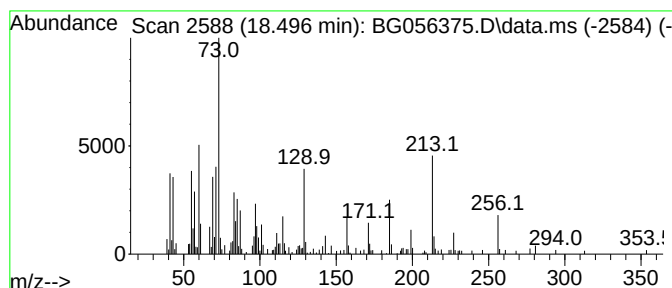
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.496	4.42 ng	144287	Phenanthrene-d10	17.656	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4	Undecanoic acid	186	C11H22O2	000112-37-8	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



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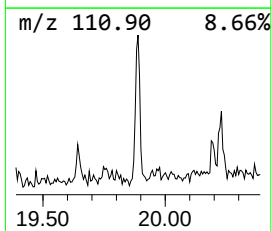
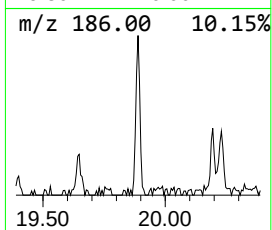
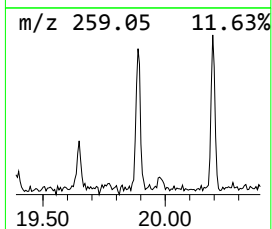
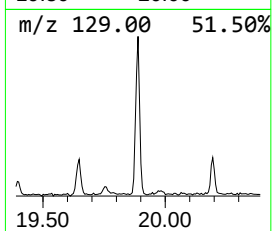
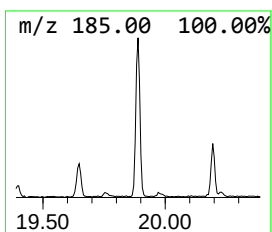
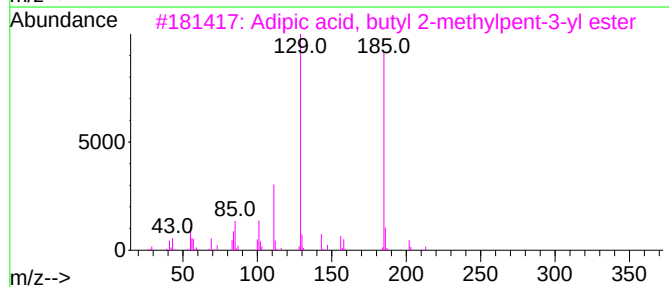
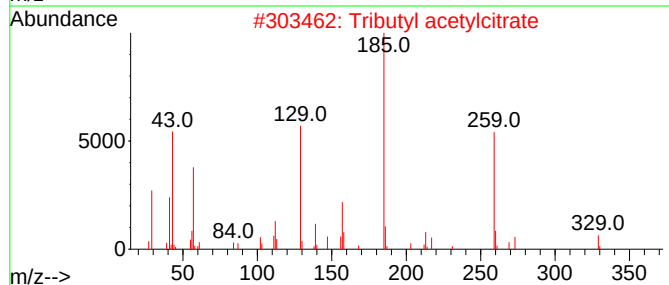
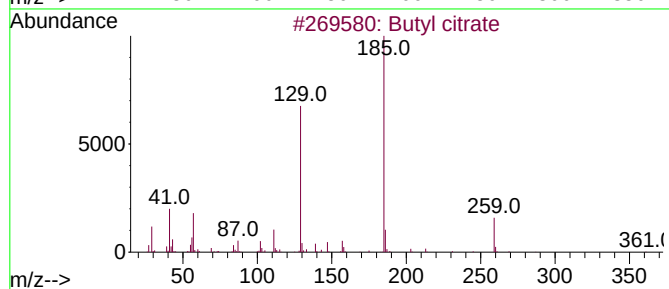
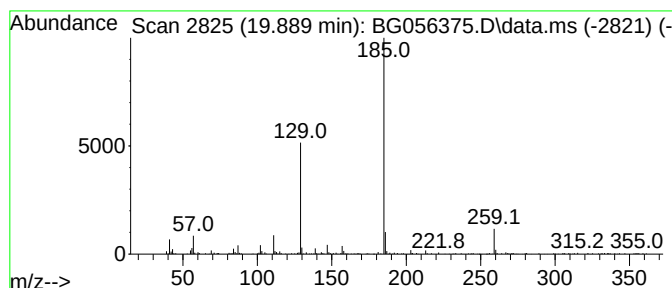
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Butyl citrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.889	5.64 ng	180912	Chrysene-d12	21.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butyl citrate	360	C18H32O7	000077-94-1	91
2			Tributyl acetylcitrate	402	C20H34O8	000077-90-7	78
3			Adipic acid, butyl 2-methylpent-...	286	C16H30O4	1010353-55-8	64
4			Adipic acid, butyl 2-decyl ester	342	C20H38O4	1000353-59-7	64
5			Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	50



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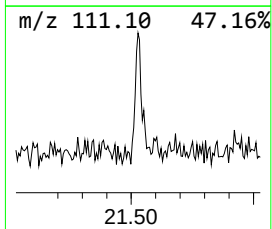
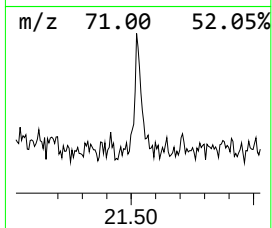
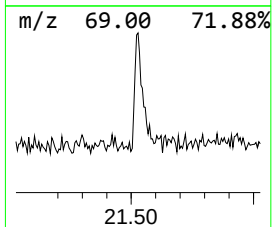
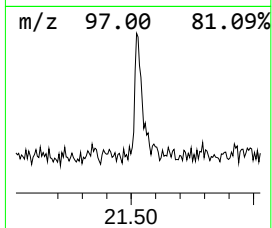
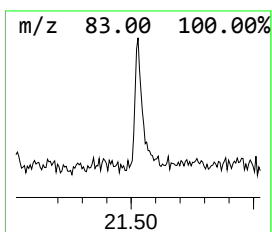
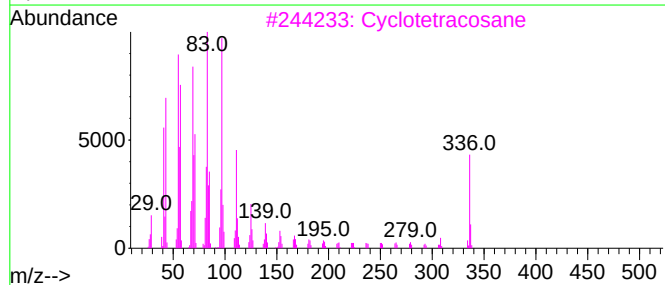
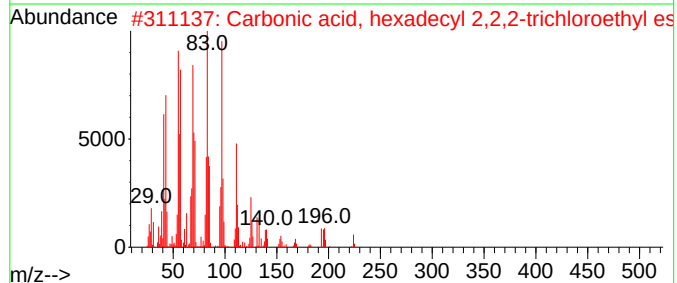
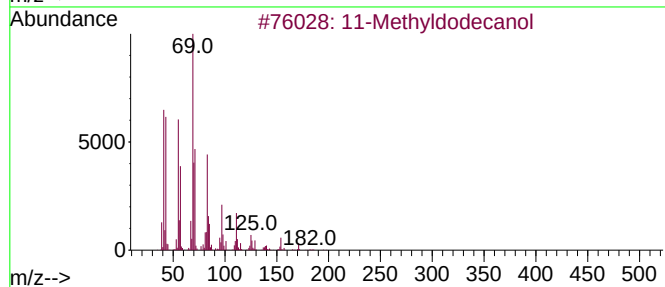
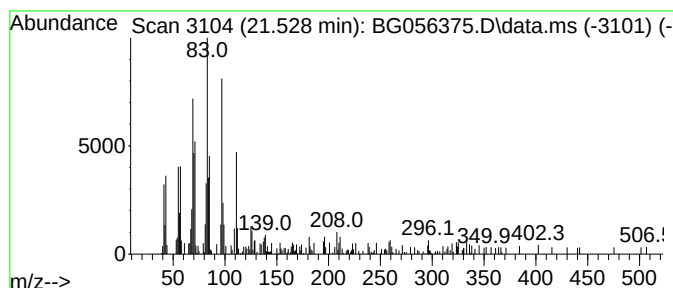
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 11-Methyldodecanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.528	3.56 ng	114017	Chrysene-d12	21.945

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11-Methyldodecanol	200	C13H28O	085763-57-1	74
2			Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	72
3			Cyclotetracosane	336	C24H48	000297-03-0	64
4			Cyclopentadecane	210	C15H30	000295-48-7	59
5			n-Pentadecanol	228	C15H32O	000629-76-5	58



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.341	15.8	ng	186235	1	8.302	236440	20.0
Benzophenone	16.258	2.7	ng	70581	3	14.918	525006	20.0
n-Hexadecanoic ...	18.496	4.4	ng	144287	4	17.656	652855	20.0
Butyl citrate	19.889	5.6	ng	180912	5	21.945	641047	20.0
11-Methyldodecanol	21.528	3.6	ng	114017	5	21.945	641047	20.0