

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
 Data File : BG057829.D
 Acq On : 23 Jun 2023 5:18
 Operator : CG/JU
 Sample : 03320-19
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-14A

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057829.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.032	324	331	340	rBV	492944	737098	27.40%	4.684%
2	5.496	403	410	423	rVB	952286	1454061	54.05%	9.240%
3	6.107	508	514	521	rBV	21305	29785	1.11%	0.189%
4	7.089	670	681	691	rBV	927994	1573481	58.49%	9.999%
5	7.923	816	823	831	rBV	194526	314060	11.67%	1.996%
6	9.086	1012	1021	1032	rBV	546800	964399	35.85%	6.129%
7	10.726	1293	1300	1309	rVB	277099	472298	17.56%	3.001%
8	13.182	1711	1718	1725	rBV	1292300	1956606	72.73%	12.434%
9	14.556	1945	1952	1961	rVB	417363	633133	23.53%	4.024%
10	15.914	2177	2183	2189	rBV	156938	224021	8.33%	1.424%
11	16.043	2198	2205	2216	rBV	1092232	1662922	61.81%	10.568%
12	17.300	2411	2419	2426	rBV	510878	743030	27.62%	4.722%
13	18.187	2565	2570	2581	rBV	182961	280258	10.42%	1.781%
14	19.462	2783	2787	2792	rBV	50502	70908	2.64%	0.451%
15	19.915	2858	2864	2870	rBV	1938858	2690358	100.00%	17.097%
16	21.207	3080	3084	3093	rVV3	96316	160495	5.97%	1.020%
17	21.284	3094	3097	3106	rVB	44936	73141	2.72%	0.465%
18	21.554	3137	3143	3151	rVB	457240	750916	27.91%	4.772%
19	22.347	3274	3278	3280	rBV5	21015	31362	1.17%	0.199%
20	23.211	3421	3425	3433	rVB	69859	122127	4.54%	0.776%
21	24.703	3671	3679	3692	rVB	265693	791348	29.41%	5.029%

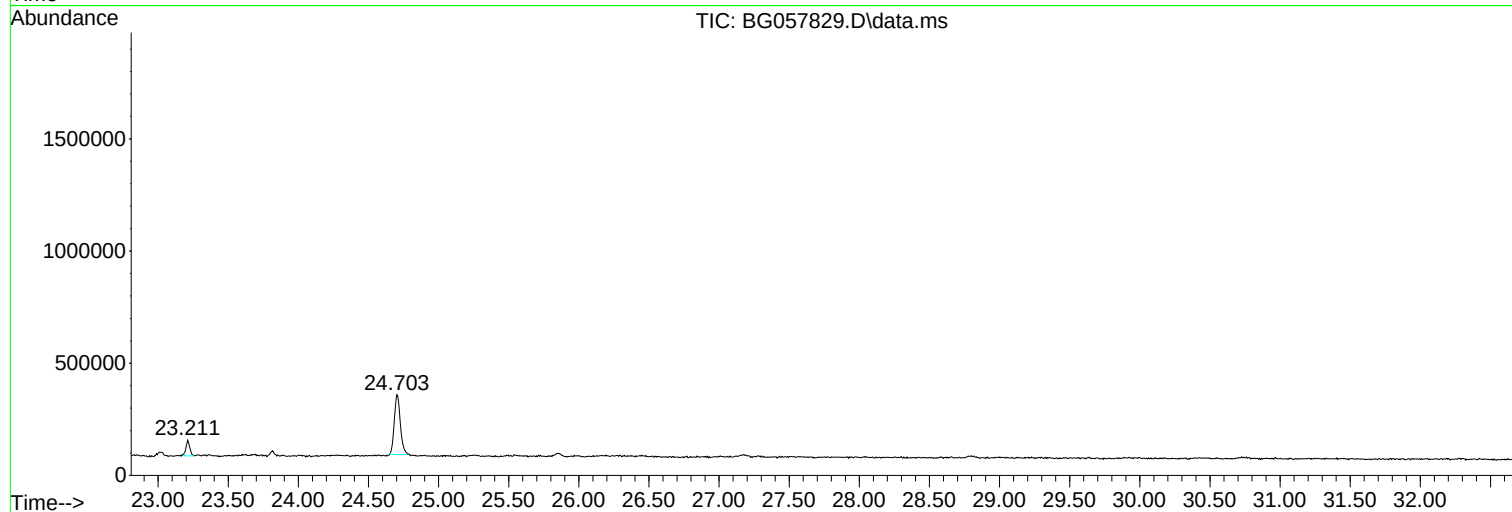
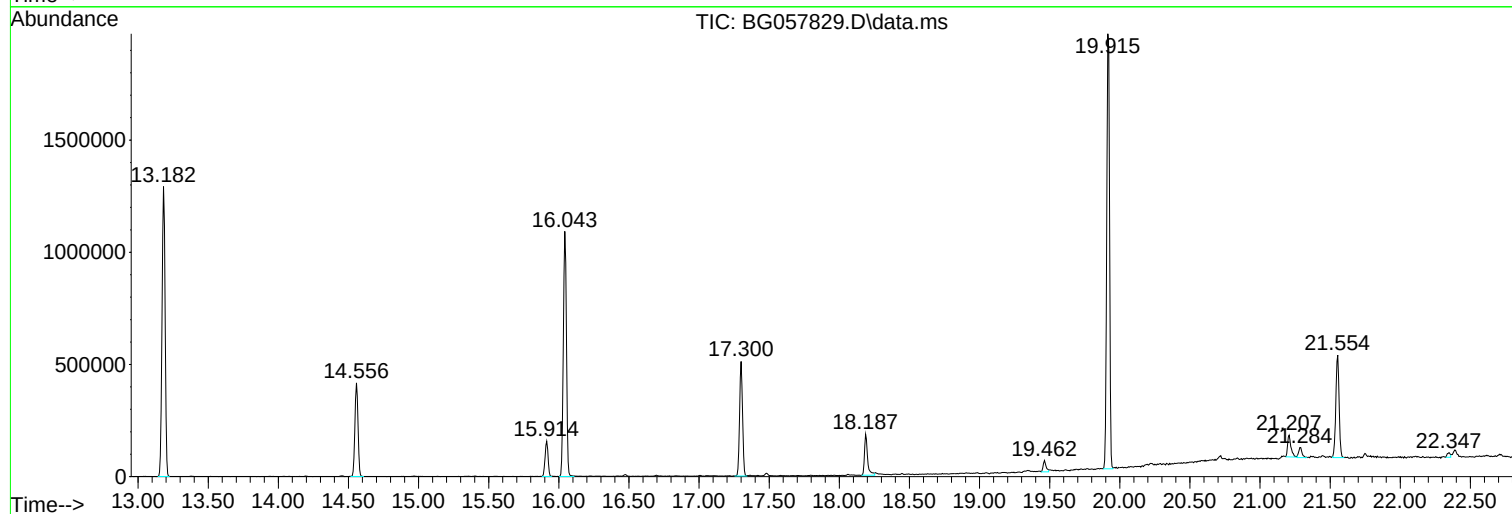
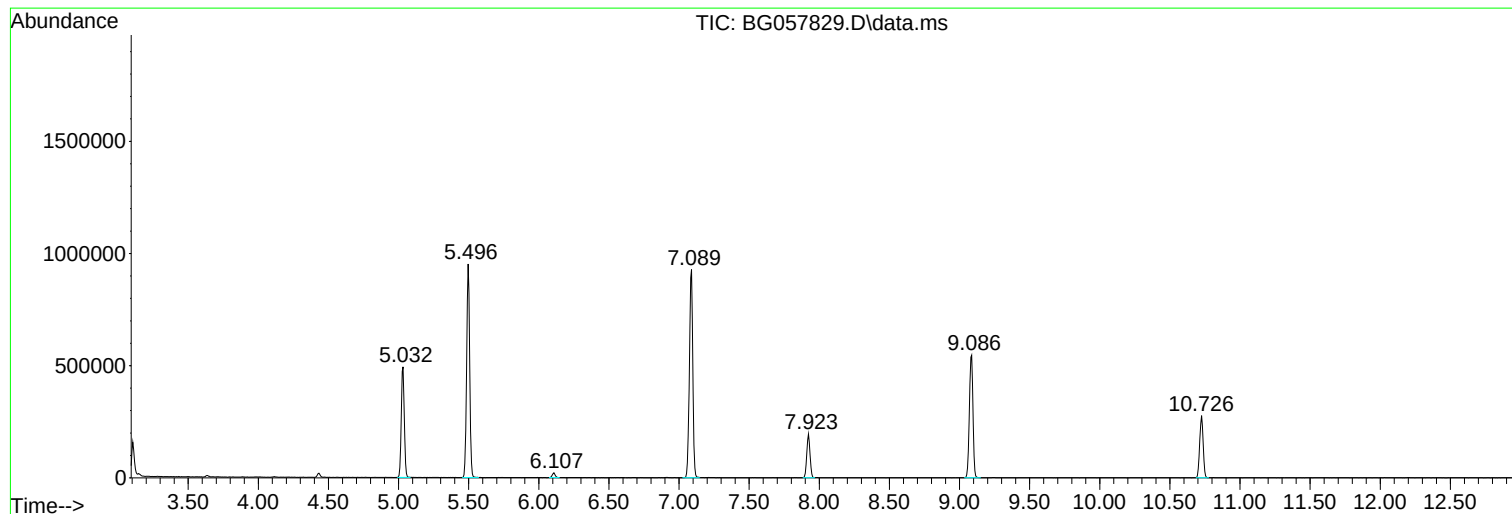
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG057829.D
Acq On : 23 Jun 2023 5:18
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ALS Vial : 16 Sample Multiplier: 1

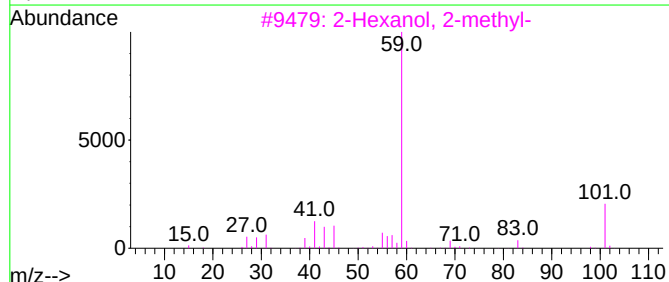
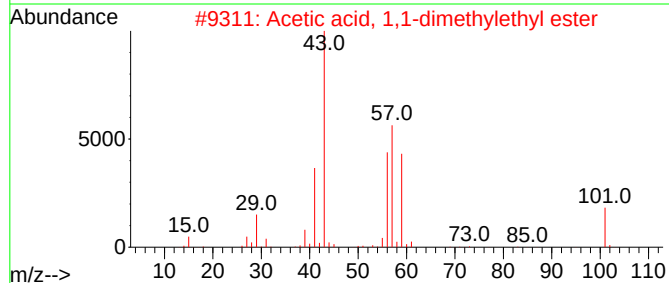
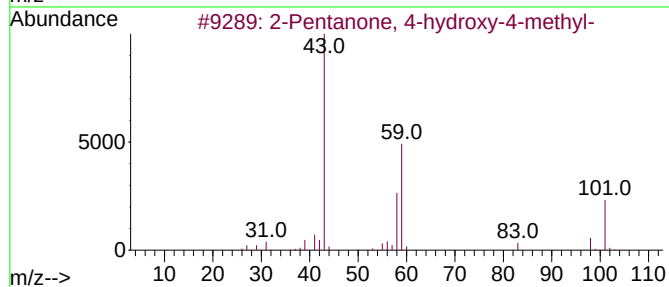
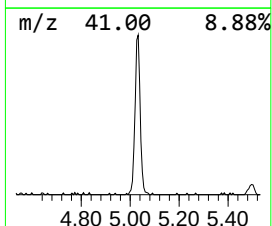
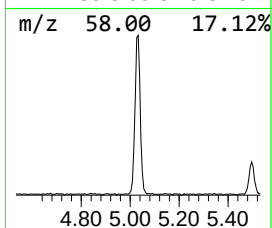
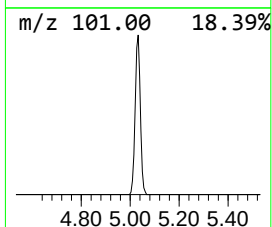
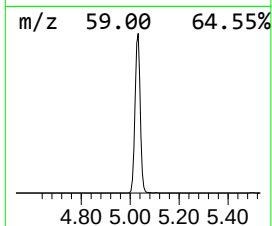
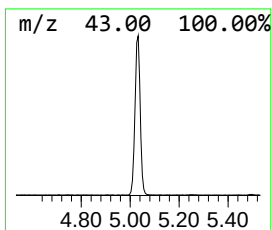
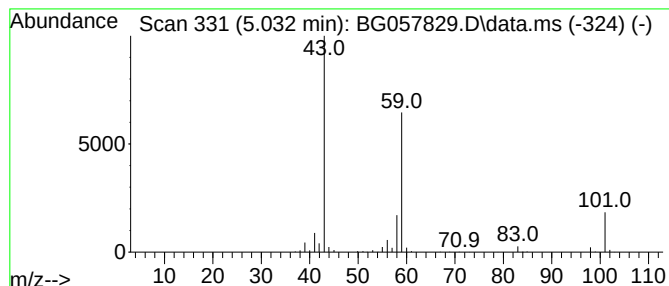
Instrument :
BNA_G
ClientSampleId :
WC-14A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
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.
5.032	46.94 ng	737098	1,4-Dichlorobenzene-d4			7.923
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	38
4	Propane, 2-methyl-2-(1-methyleth...		116	C7H16O	017348-59-3	33
5	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	33



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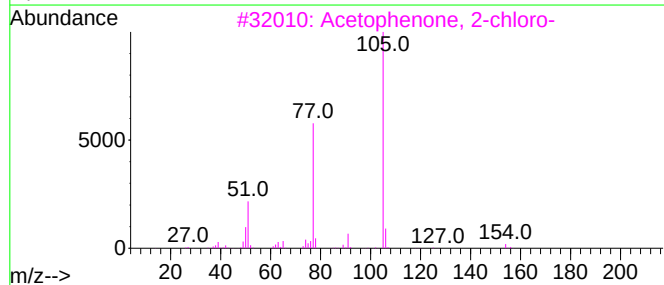
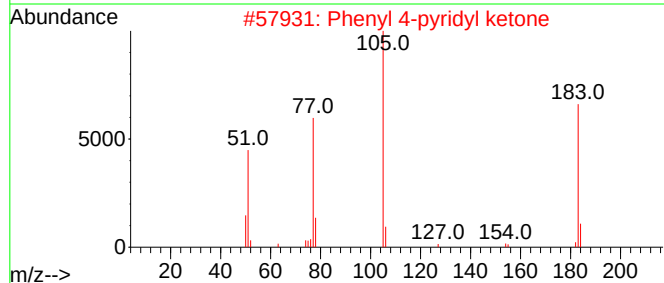
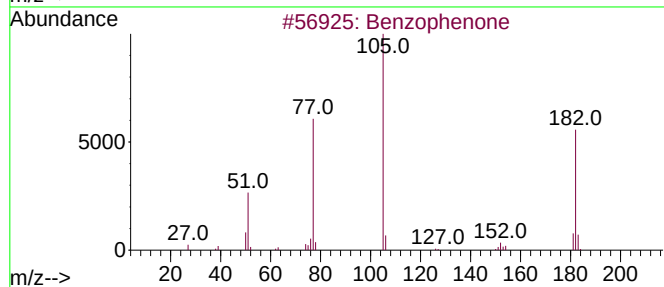
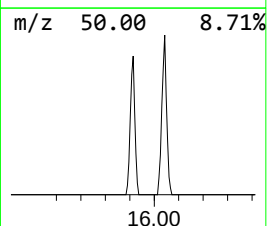
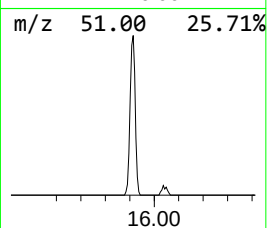
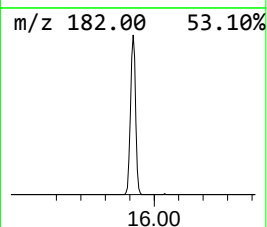
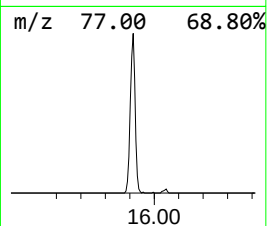
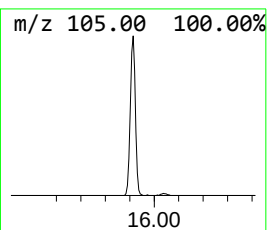
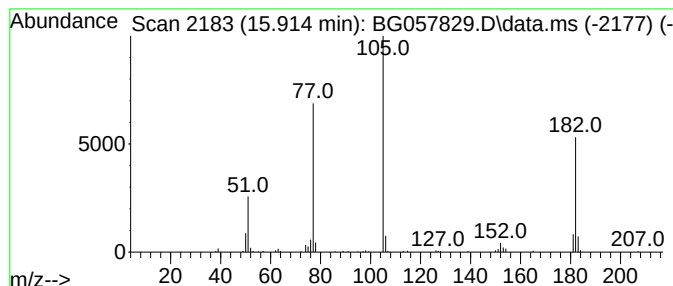
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.914	7.08 ng	224021	Acenaphthene-d10	14.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
5			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47



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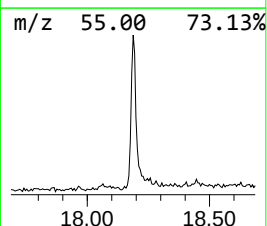
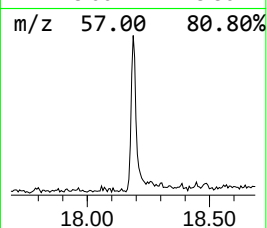
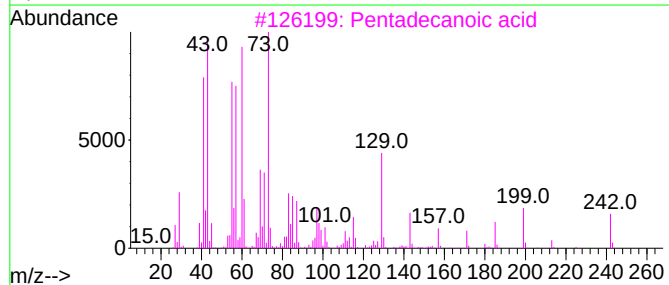
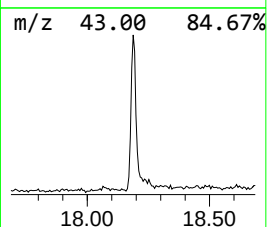
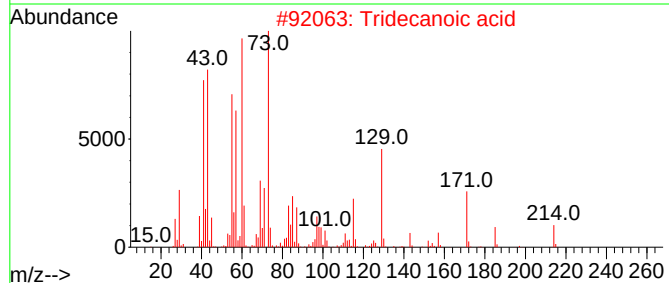
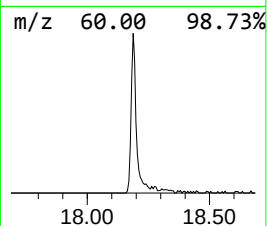
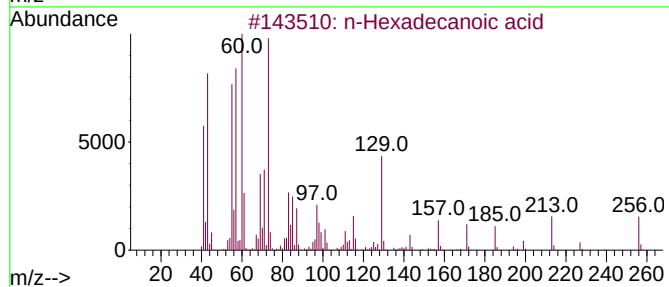
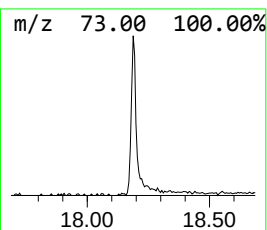
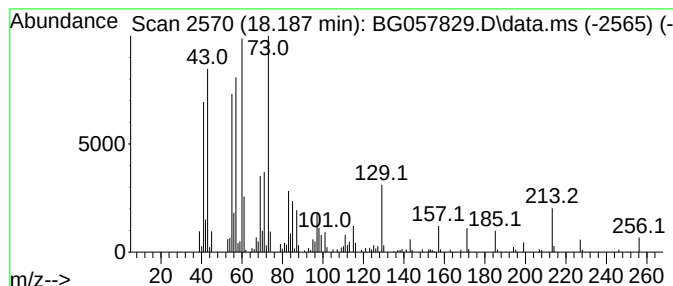
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.187	7.54 ng	280258	Phenanthrene-d10		17.300	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	94
2	Tridecanoic acid		214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
5	Undecanoic acid		186	C11H22O2	000112-37-8	64



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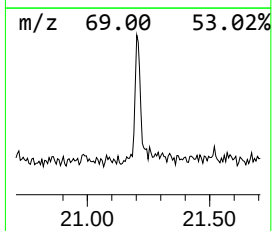
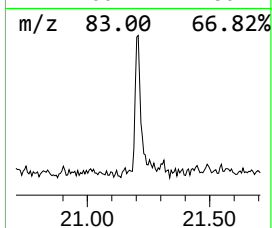
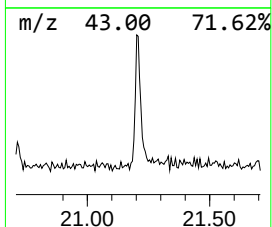
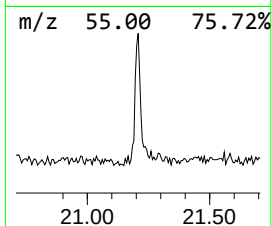
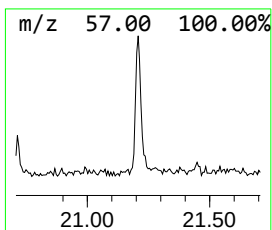
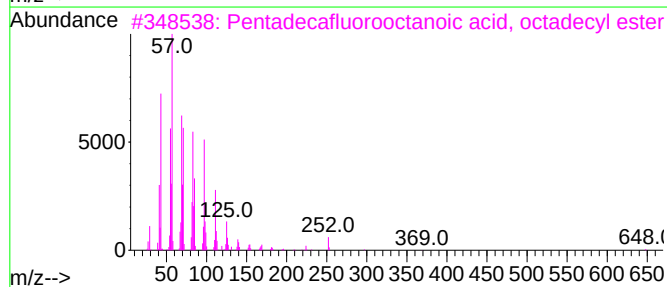
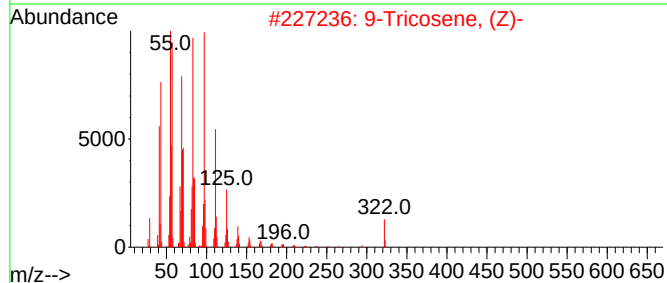
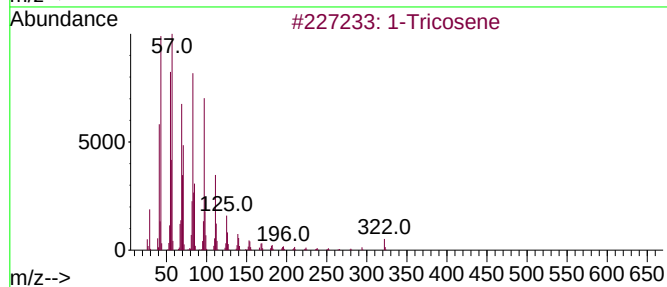
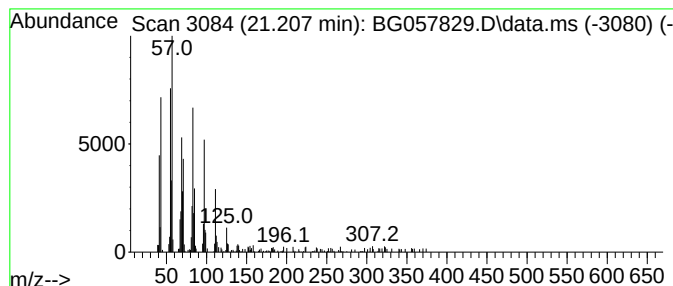
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.207	4.27 ng	160495	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene			322	C23H46	018835-32-0	95
2	9-Tricosene, (Z)-			322	C23H46	027519-02-4	93
3	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	93
4	Nonadecyl trifluoroacetate			380	C21H39F3O2	1000351-76-3	91
5	Cyclodocosane, ethyl-			336	C24H48	1000151-22-6	91



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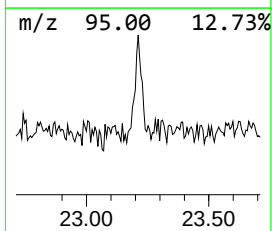
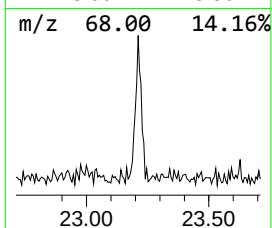
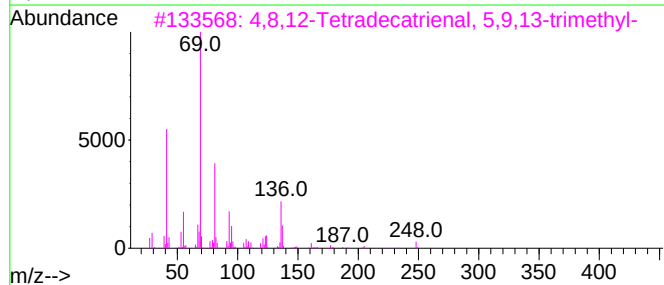
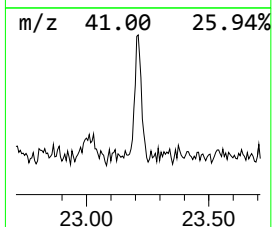
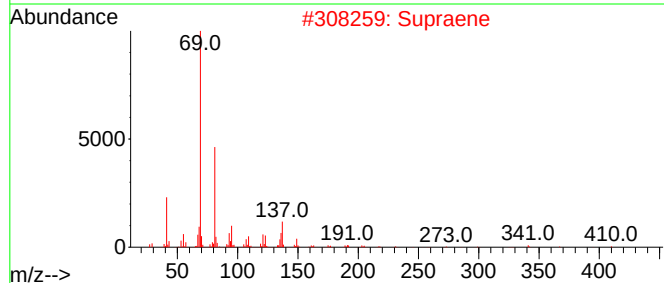
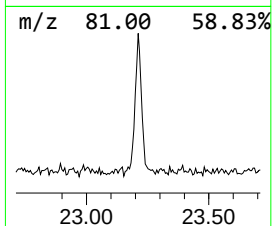
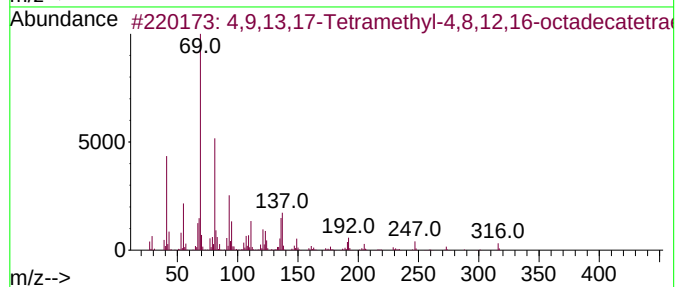
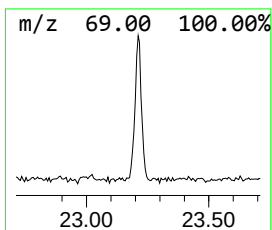
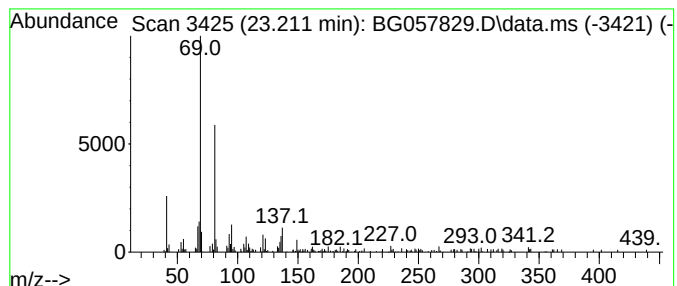
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 4,9,13,17-Tetramethyl-4,8,11... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.211	3.09 ng	122127	Perylene-d12	24.703

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	87		
2	Supraene	410	C30H50	007683-64-9	83		
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72		
4	Squalene	410	C30H50	000111-02-4	72		
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.032	46.9	ng	737098	1	7.923	314060	20.0
Benzophenone	15.914	7.1	ng	224021	3	14.556	633133	20.0
n-Hexadecanoic ...	18.187	7.5	ng	280258	4	17.300	743030	20.0
1-Tricosene	21.207	4.3	ng	160495	5	21.554	750916	20.0
4,9,13,17-Tetra...	23.211	3.1	ng	122127	6	24.703	791348	20.0