

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080823\
 Data File : BG058646.D
 Acq On : 8 Aug 2023 17:10
 Operator : MA/JU
 Sample : 03903-14
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-04W

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-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058646.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.382	384	390	400	rBV	367067	580055	17.55%	4.158%
2	6.981	656	662	676	rBV	215108	389483	11.78%	2.792%
3	7.815	797	804	809	rBV	132264	227971	6.90%	1.634%
4	7.868	809	813	823	rVB2	30124	50398	1.52%	0.361%
5	8.978	994	1002	1018	rBV	450836	833658	25.22%	5.976%
6	9.119	1021	1026	1036	rVV4	19156	50398	1.52%	0.361%
7	9.954	1162	1168	1177	rBV3	21659	51714	1.56%	0.371%
8	10.612	1273	1280	1292	rBV	197792	367845	11.13%	2.637%
9	11.434	1413	1420	1432	rBV	81641	178958	5.41%	1.283%
10	13.079	1692	1700	1714	rBV	1281159	1997703	60.44%	14.321%
11	14.460	1928	1935	1944	rVB	383274	595328	18.01%	4.268%
12	14.883	2002	2007	2023	rBV4	30342	62709	1.90%	0.450%
13	15.277	2065	2074	2081	rVB2	24170	41155	1.25%	0.295%
14	15.817	2160	2166	2175	rBV2	56518	82479	2.50%	0.591%
15	15.952	2181	2189	2211	rBV	1192371	1887710	57.12%	13.532%
16	17.204	2396	2402	2414	rBV	544187	822856	24.90%	5.899%
17	17.862	2510	2514	2520	rBV5	22817	33810	1.02%	0.242%
18	18.091	2547	2553	2562	rBV	118481	198697	6.01%	1.424%
19	19.372	2766	2771	2785	rBV2	46786	85442	2.59%	0.613%
20	19.501	2789	2793	2803	rVB	31418	47111	1.43%	0.338%
21	19.824	2842	2848	2855	rBV	2538960	3304993	100.00%	23.693%
22	21.129	3062	3070	3086	rBV5	36348	160260	4.85%	1.149%
23	21.446	3117	3124	3132	rBV2	530918	858472	25.98%	6.154%
24	24.519	3632	3647	3664	rBV2	329108	1040325	31.48%	7.458%

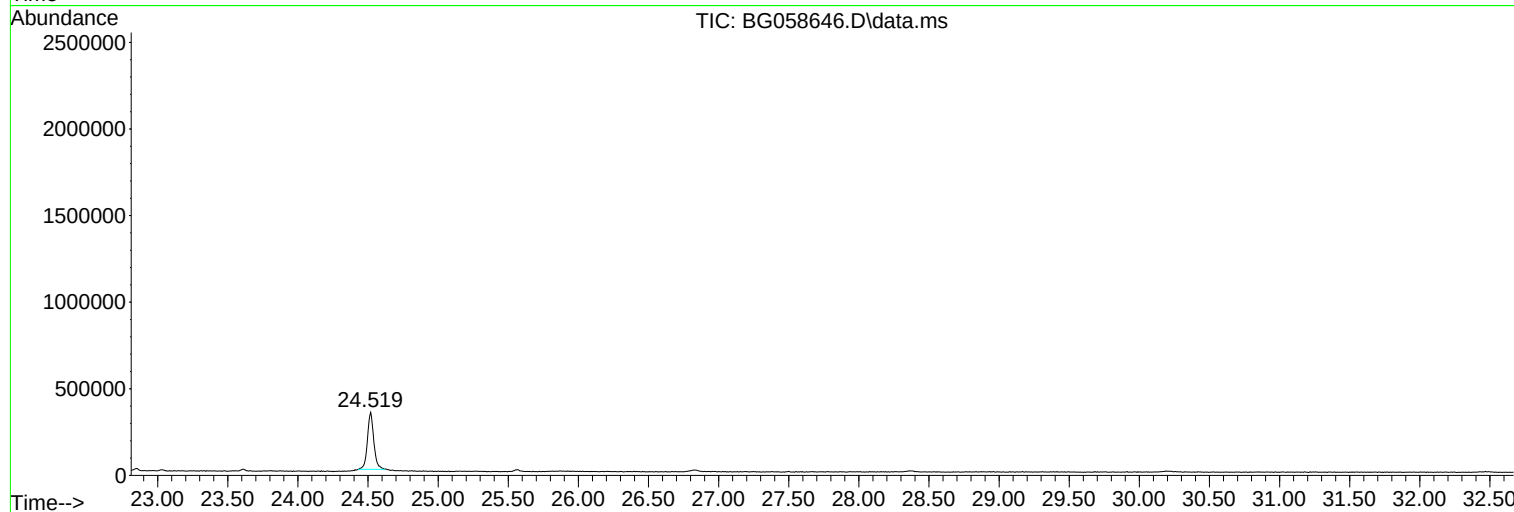
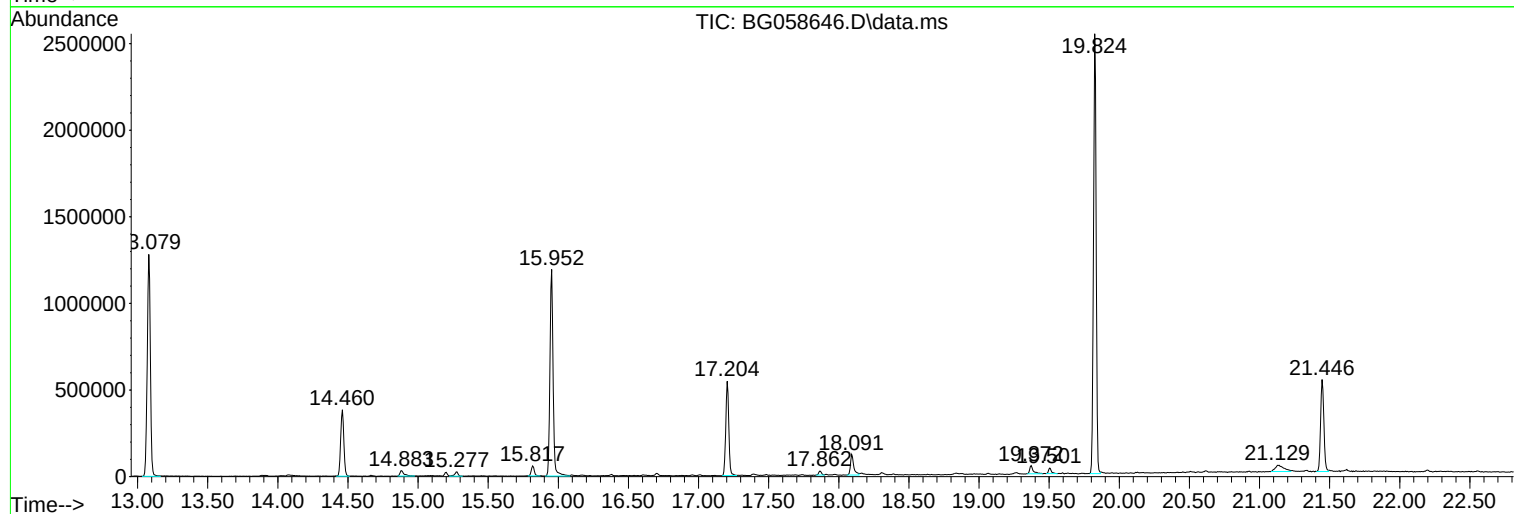
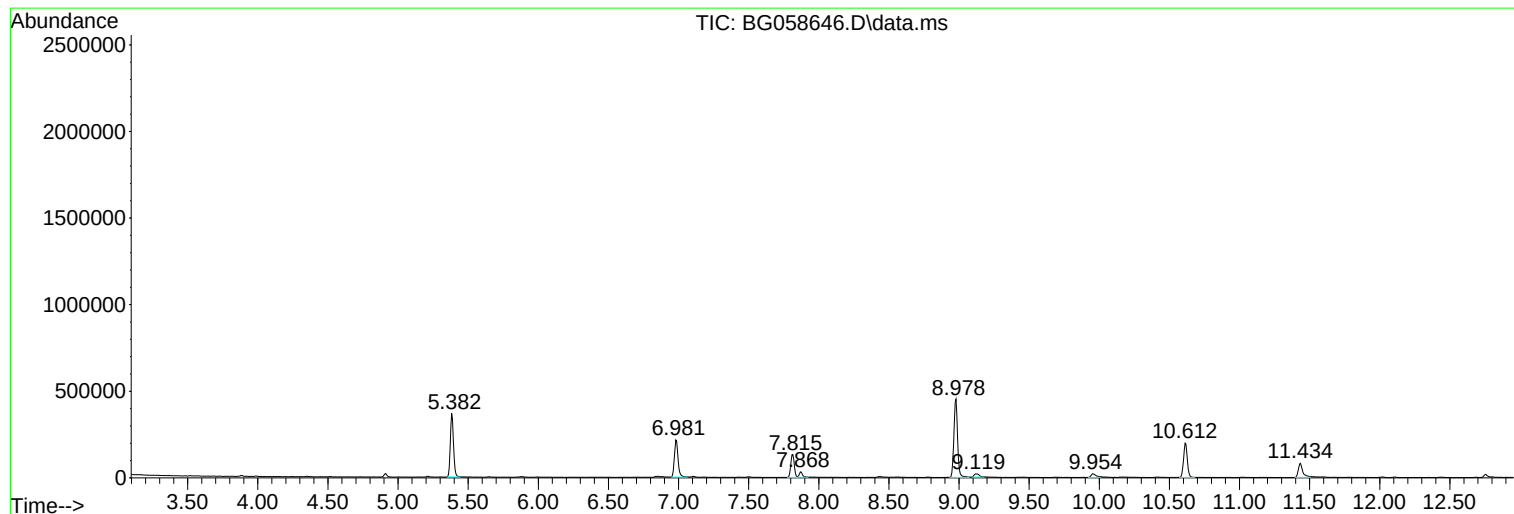
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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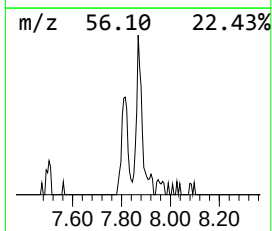
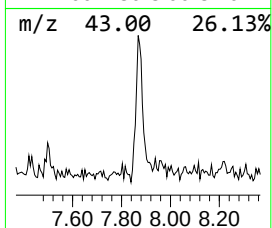
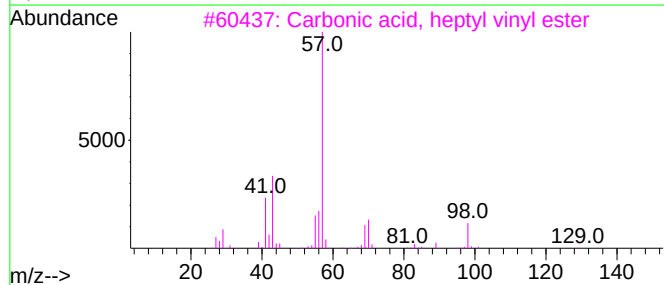
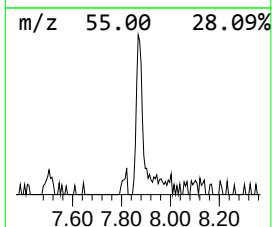
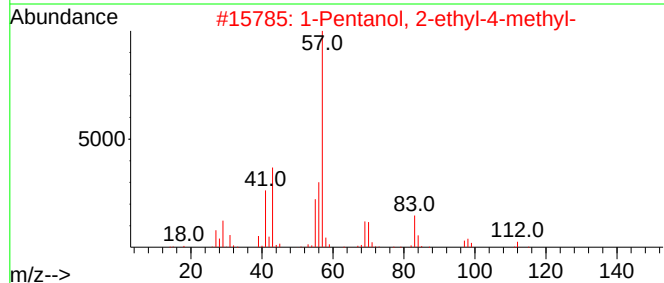
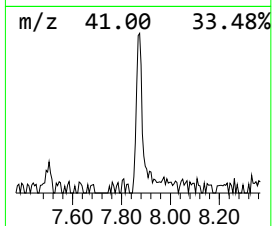
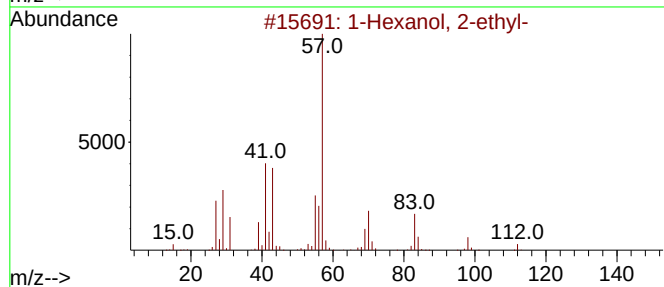
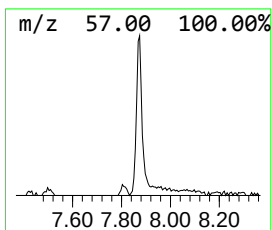
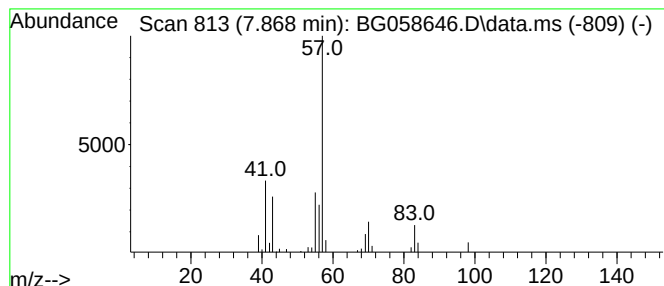
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.868	4.42 ng	50398	1,4-Dichlorobenzene-d4	7.809

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	78
3		Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	50
4		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	43
5		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	38



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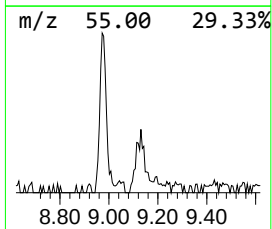
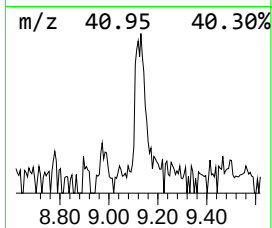
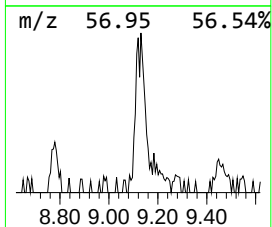
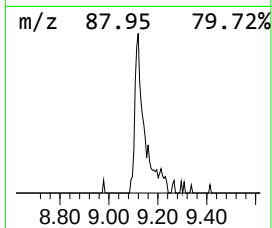
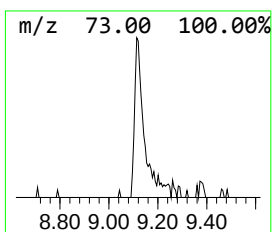
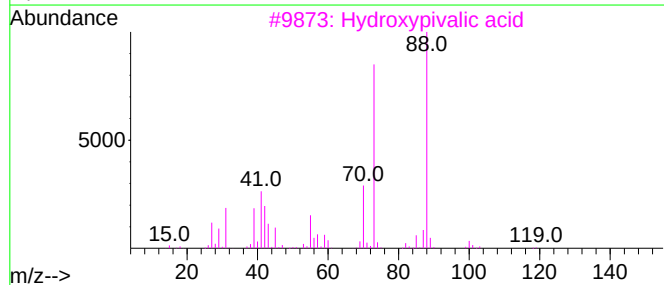
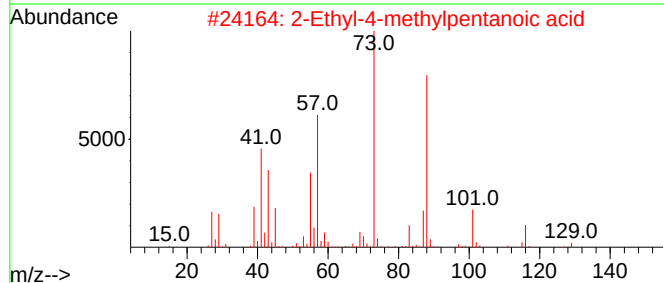
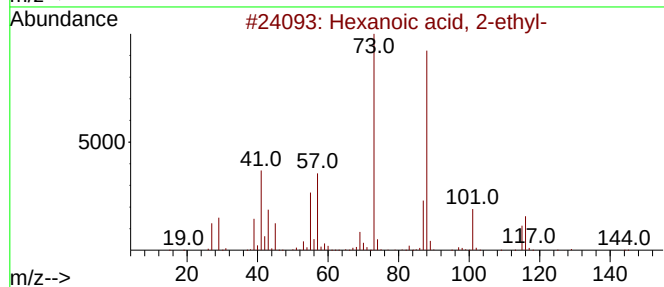
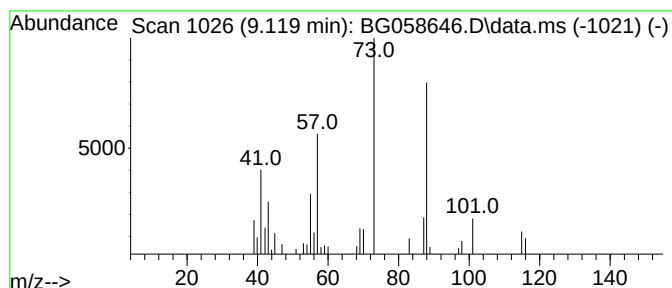
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.119	4.42 ng	50398	1,4-Dichlorobenzene-d4	7.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	78
2			2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	72
3			Hydroxypivalic acid	118	C5H10O3	004835-90-9	53
4			Urea, ethyl-	88	C3H8N2O	000625-52-5	50
5			3-Furanol, tetrahydro-	88	C4H8O2	000453-20-3	43



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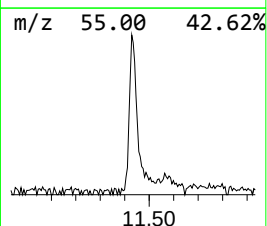
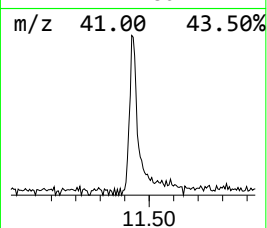
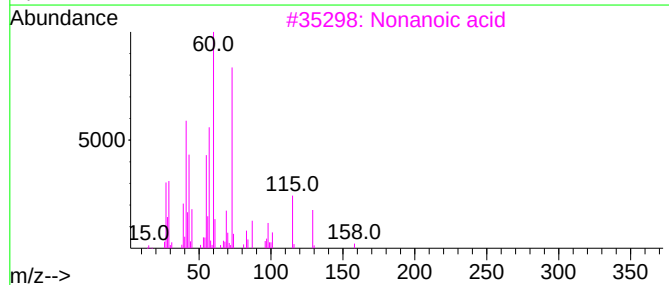
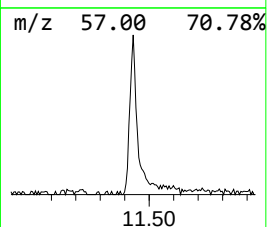
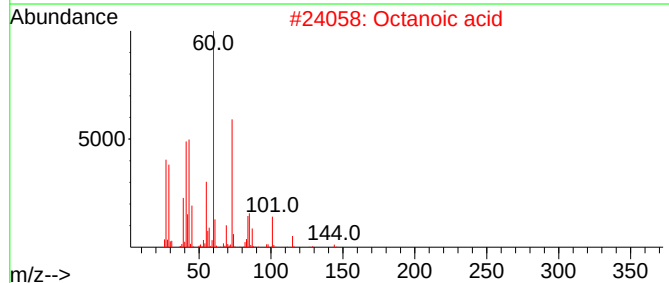
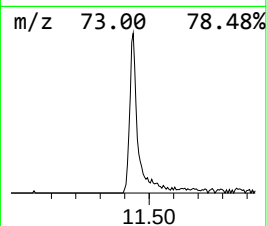
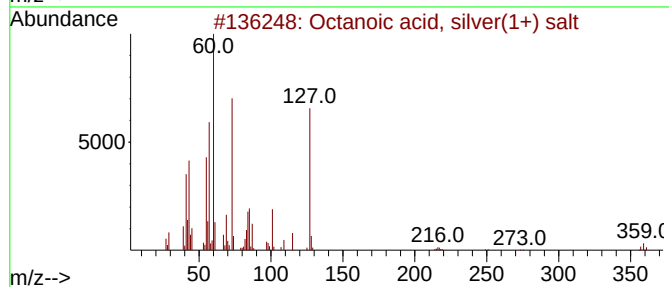
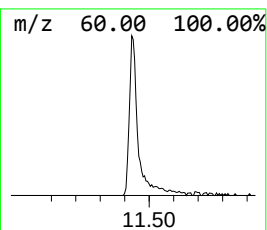
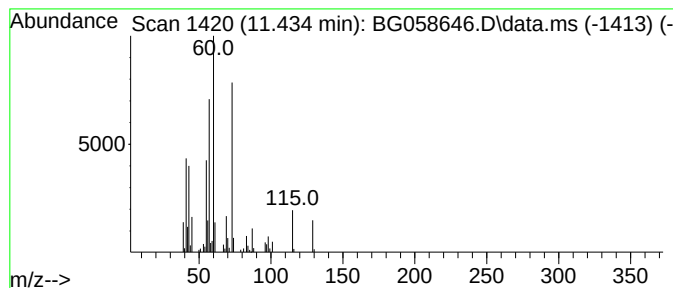
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Peak Number 3 Octanoic acid, silver(1+) salt Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.434	9.73 ng	178958	Naphthalene-d8	10.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	58
2			Octanoic acid	144	C8H16O2	000124-07-2	53
3			Nonanoic acid	158	C9H18O2	000112-05-0	53
4			Hexanoic acid	116	C6H12O2	000142-62-1	53
5			Heptanoic acid	130	C7H14O2	000111-14-8	50



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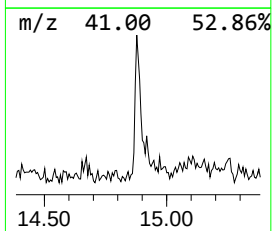
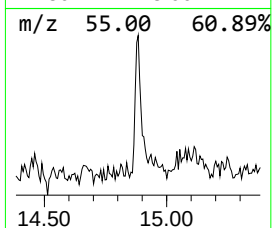
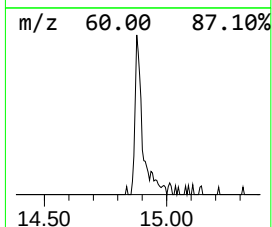
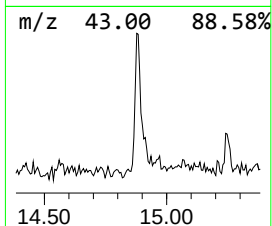
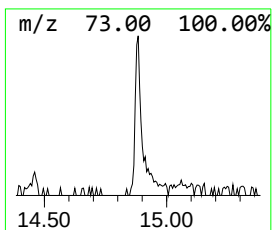
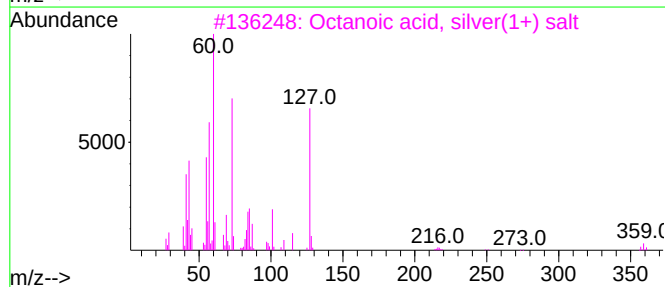
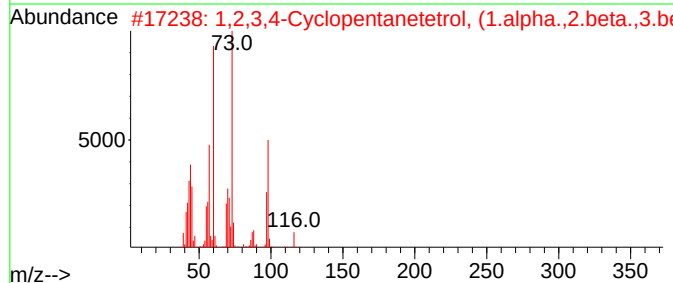
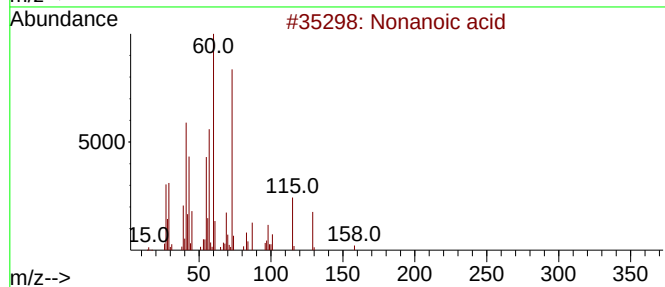
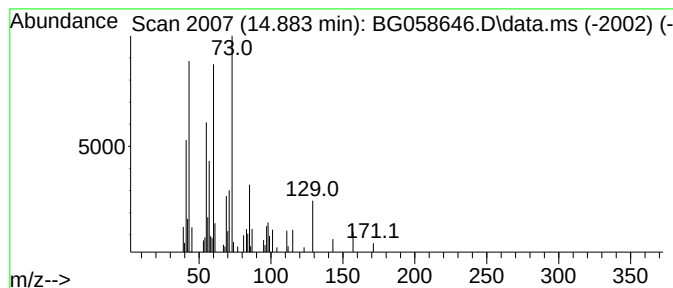
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Peak Number 4 Nonanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.883	2.11 ng	62709	Acenaphthene-d10	14.460

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	50
2			1,2,3,4-Cyclopentanetetrol, (1.a...	134	C5H10O4	014003-71-5	47
3			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	43
4			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	43
5			Octanoic acid	144	C8H16O2	000124-07-2	43



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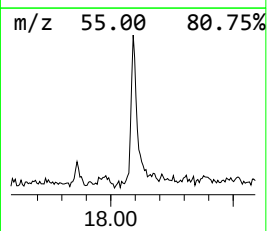
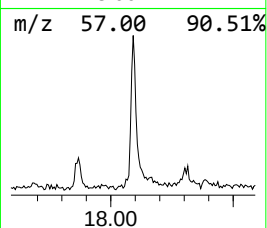
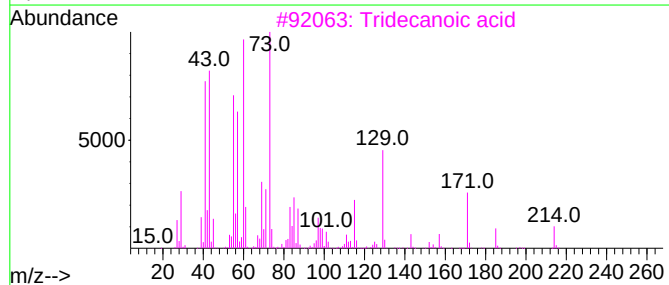
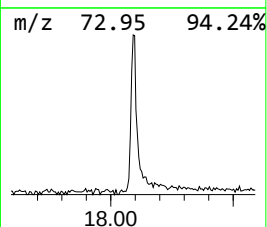
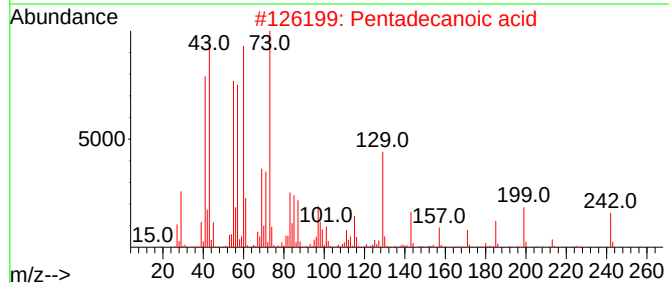
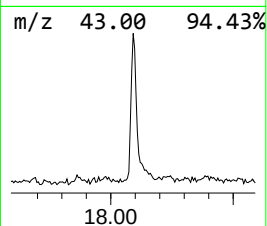
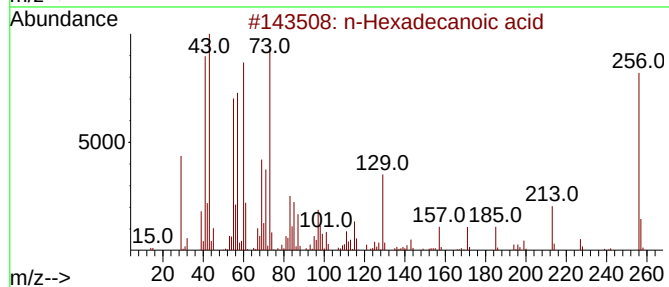
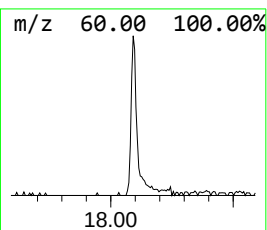
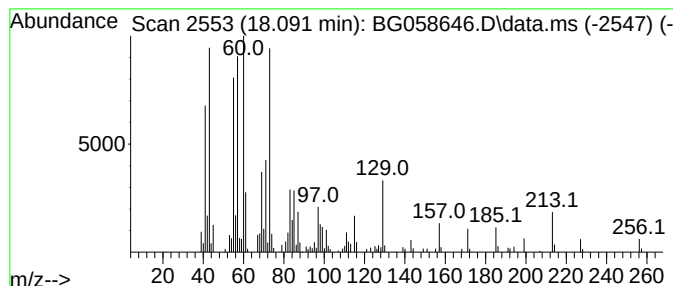
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.091	4.83 ng	198697	Phenanthrene-d10	17.204

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			n-Decanoic acid	172	C10H20O2	000334-48-5	58
5			Octanoic acid	144	C8H16O2	000124-07-2	46



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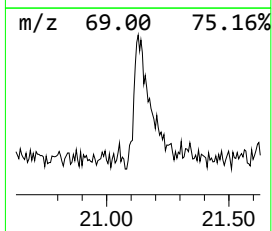
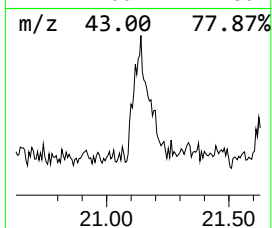
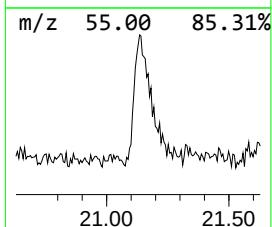
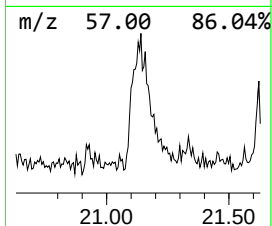
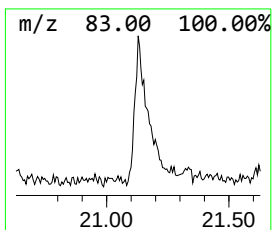
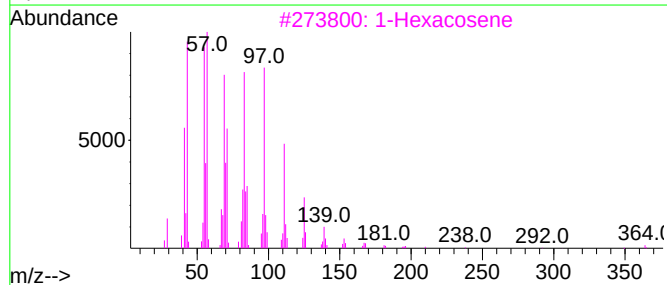
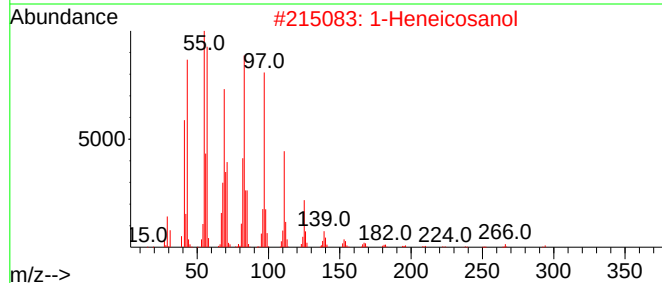
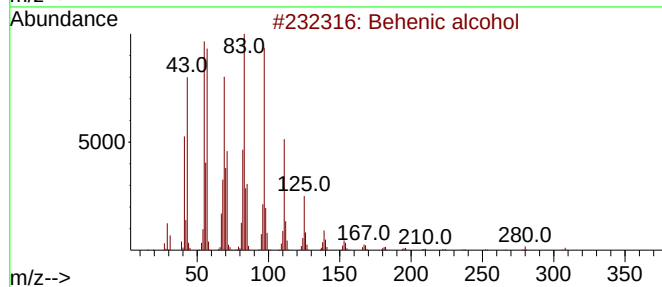
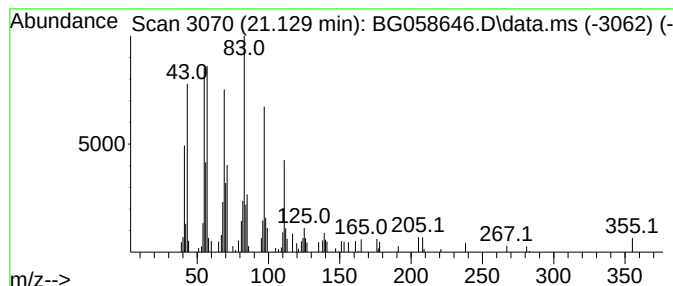
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.129	3.73 ng	160260	Chrysene-d12	21.446

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	91
3			1-Hexacosene	364	C26H52	018835-33-1	91
4			1-Tetracosene	336	C24H48	010192-32-2	83
5			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080823\
Data File : BG058646.D
Acq On : 8 Aug 2023 17:10
Operator : MA/JU
Sample : 03903-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-04W

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	7.868	4.4	ng	50398	1	7.809	227971	20.0
Hexanoic acid, ...	9.119	4.4	ng	50398	1	7.809	227971	20.0
Octanoic acid, ...	11.434	9.7	ng	178958	2	10.612	367845	20.0
Nonanoic acid	14.883	2.1	ng	62709	3	14.460	595328	20.0
n-Hexadecanoic ...	18.091	4.8	ng	198697	4	17.204	822856	20.0
Behenic alcohol	21.129	3.7	ng	160260	5	21.446	858472	20.0