

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
 Data File : BG057838.D
 Acq On : 23 Jun 2023 12:00
 Operator : CG/JU
 Sample : 03291-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-1

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: BG057838.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.027	325	330	335	rBV	44609	66120	2.31%	0.529%
2	5.491	402	409	419	rBV	373561	565522	19.76%	4.526%
3	7.078	672	679	690	rVB	233008	388338	13.57%	3.108%
4	7.918	816	822	830	rBV	136082	223417	7.81%	1.788%
5	9.081	1011	1020	1030	rBV	494831	854240	29.85%	6.836%
6	10.720	1292	1299	1308	rBV	204070	359917	12.58%	2.880%
7	13.176	1710	1717	1728	rBV	1241961	1966299	68.72%	15.735%
8	14.551	1944	1951	1958	rBV	360890	554859	19.39%	4.440%
9	15.908	2176	2182	2188	rBV	136388	190567	6.66%	1.525%
10	16.038	2197	2204	2215	rBV	1176159	1769185	61.83%	14.158%
11	16.472	2273	2278	2283	rVB	45485	67418	2.36%	0.540%
12	17.295	2412	2418	2426	rBV	481677	725729	25.36%	5.808%
13	18.182	2565	2569	2576	rBV	68736	106827	3.73%	0.855%
14	19.457	2783	2786	2791	rBV2	50418	72398	2.53%	0.579%
15	19.915	2858	2864	2869	rBV	2151615	2861351	100.00%	22.898%
16	21.202	3080	3083	3092	rVB3	47916	82705	2.89%	0.662%
17	21.549	3136	3142	3148	rVB2	439789	720866	25.19%	5.769%
18	22.706	3335	3339	3347	rVB2	49275	85381	2.98%	0.683%
19	24.698	3669	3678	3691	rVB	294822	835003	29.18%	6.682%

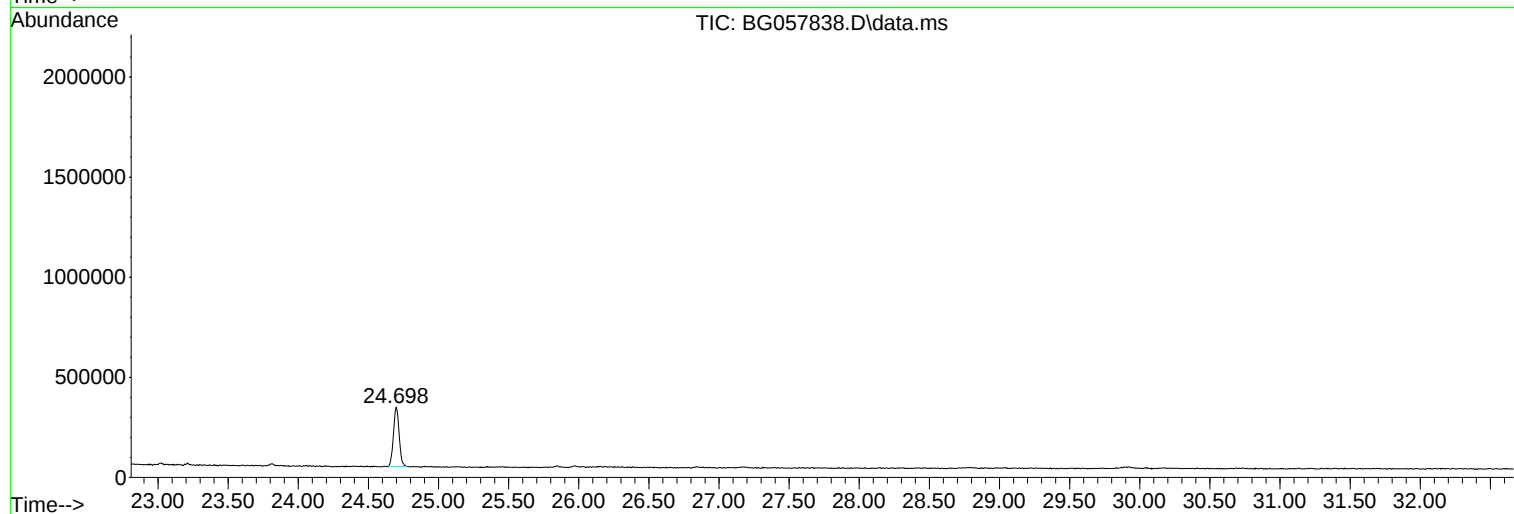
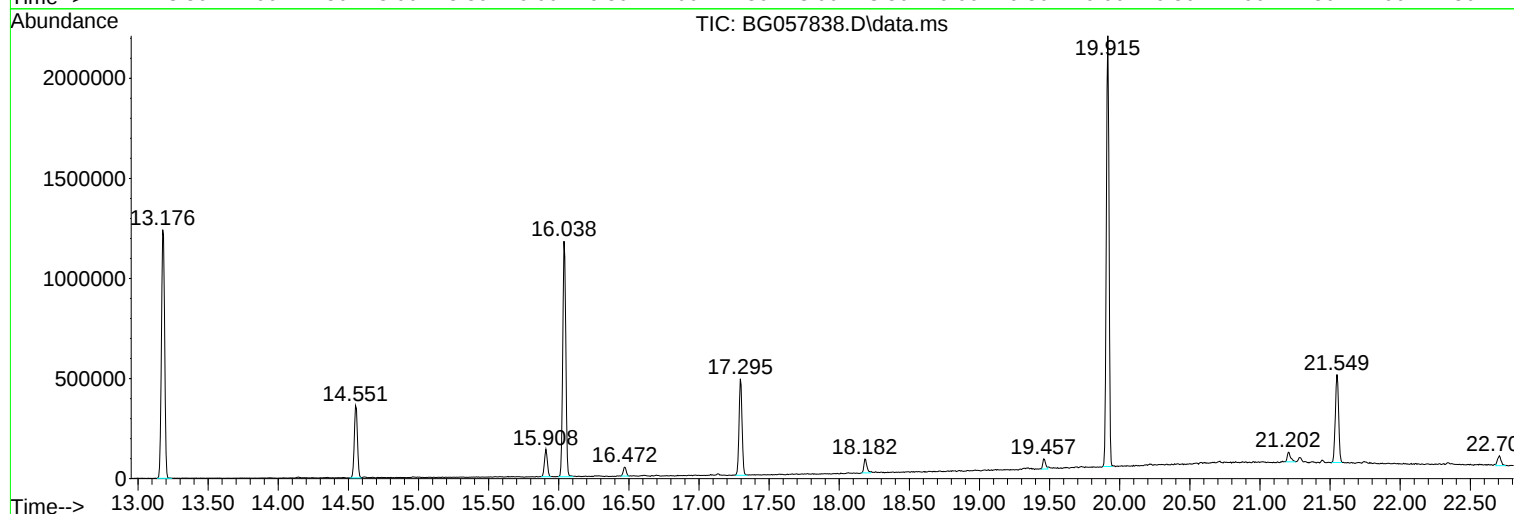
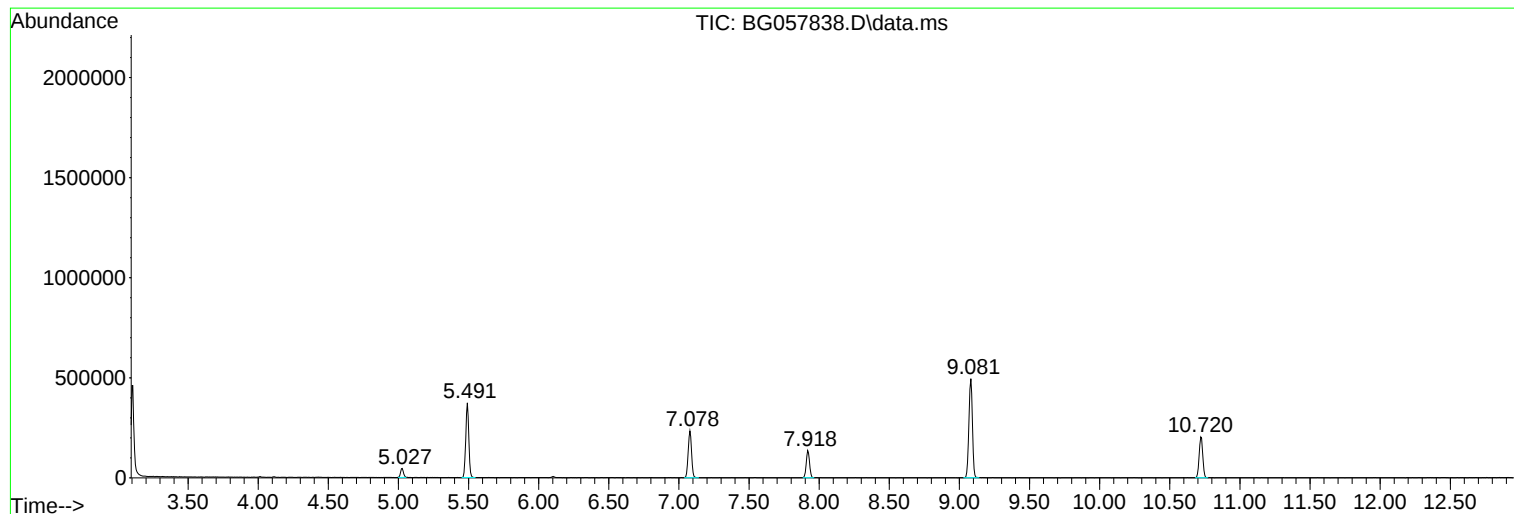
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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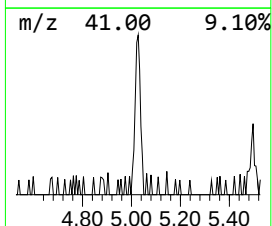
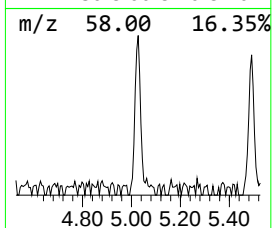
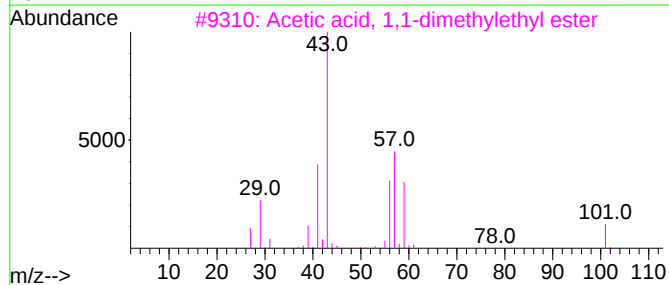
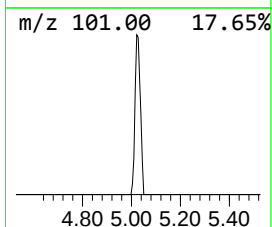
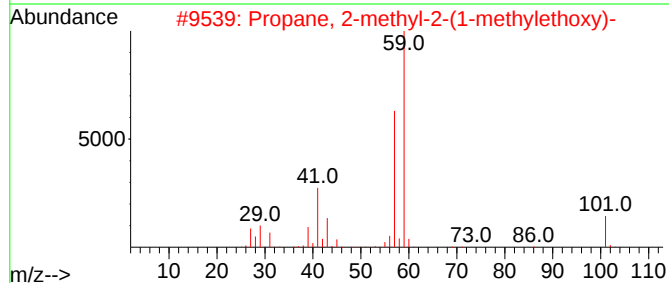
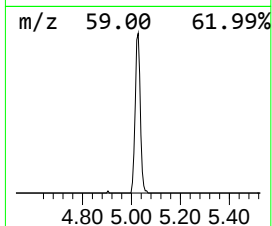
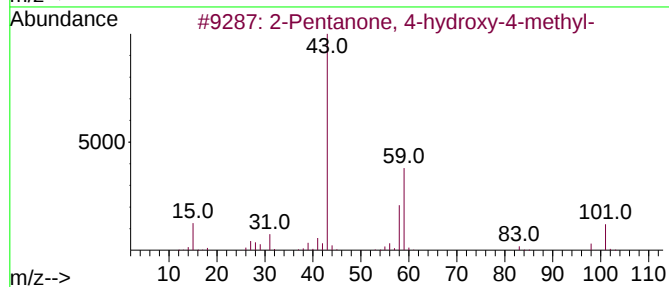
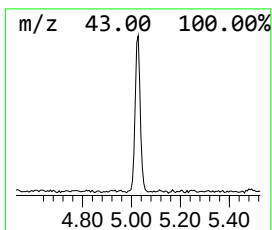
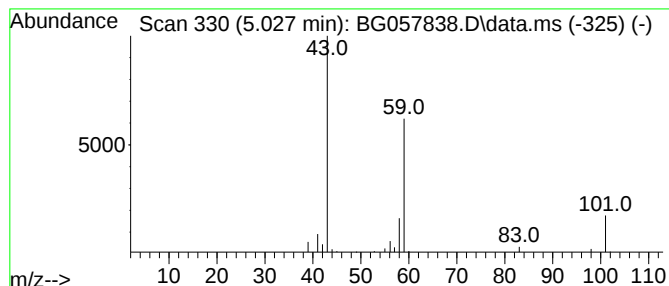
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.027	5.92 ng	66120	1,4-Dichlorobenzene-d4	7.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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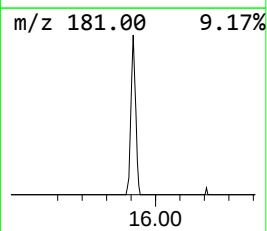
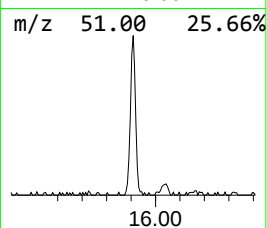
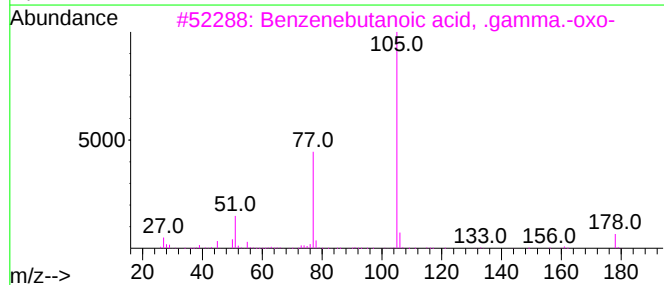
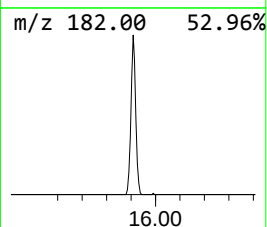
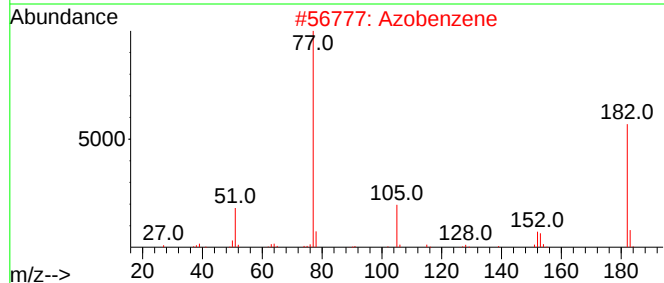
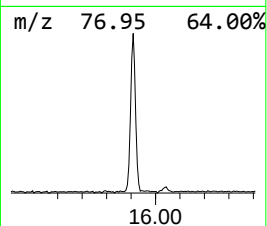
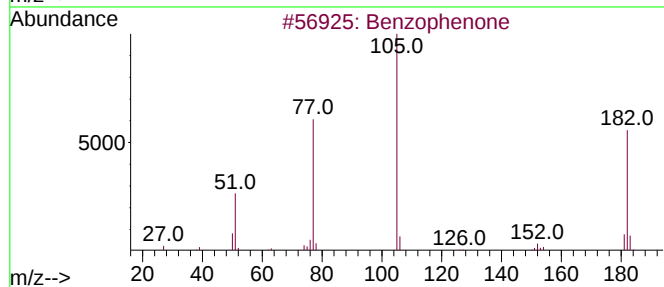
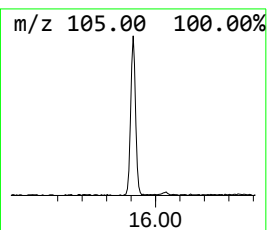
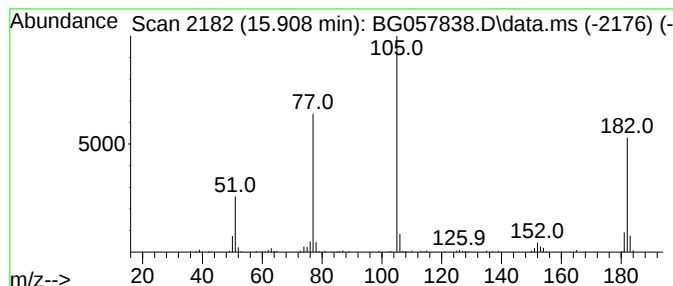
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.908	6.87 ng	190567	Acenaphthene-d10	14.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	59
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			Benzoyl bromide	184	C7H5BrO	000618-32-6	47
5			Methyl benzilate	242	C15H14O3	000076-89-1	47



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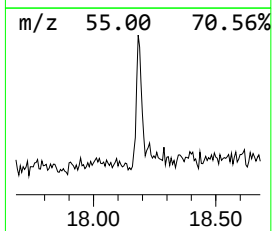
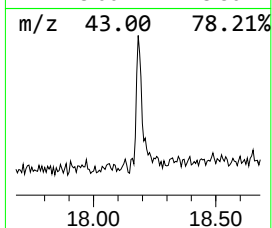
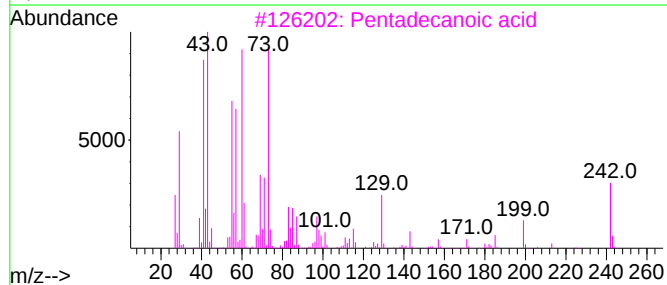
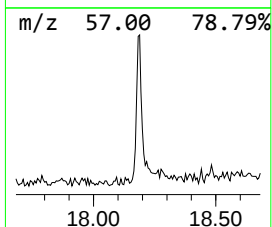
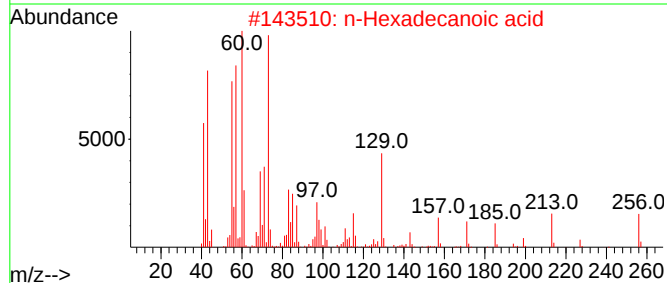
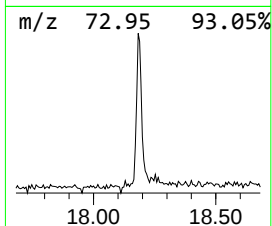
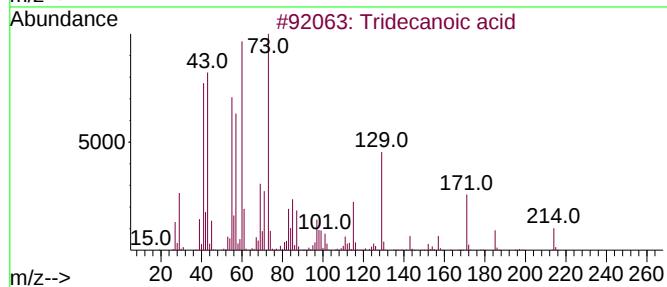
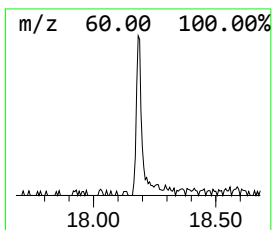
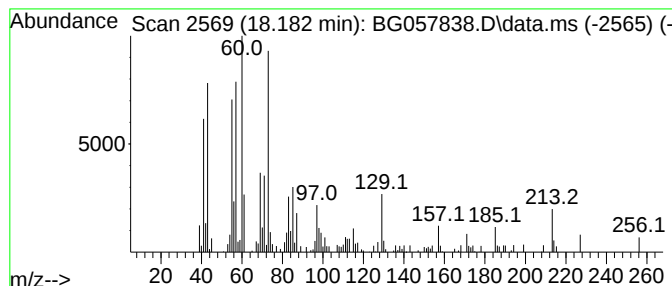
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Peak Number 3 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.182	2.94 ng	106827	Phenanthrene-d10	17.295

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	74
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4			Nonanoic acid	158	C9H18O2	000112-05-0	55
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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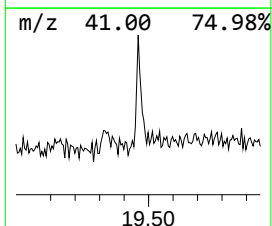
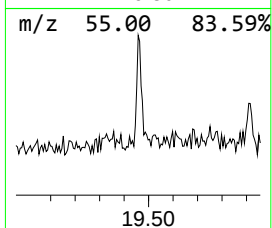
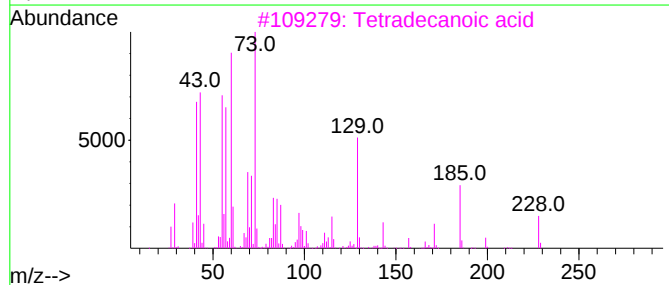
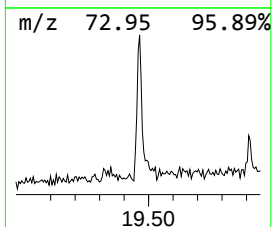
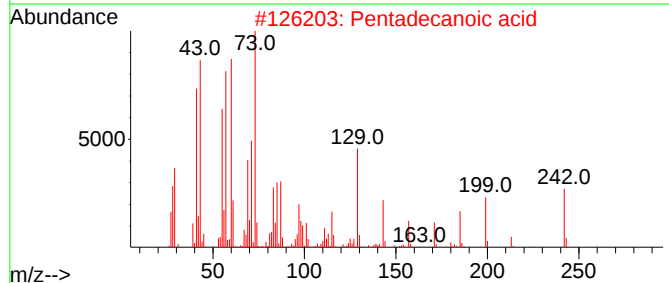
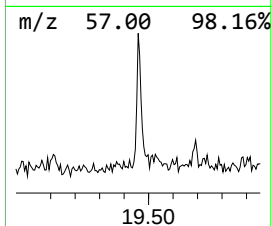
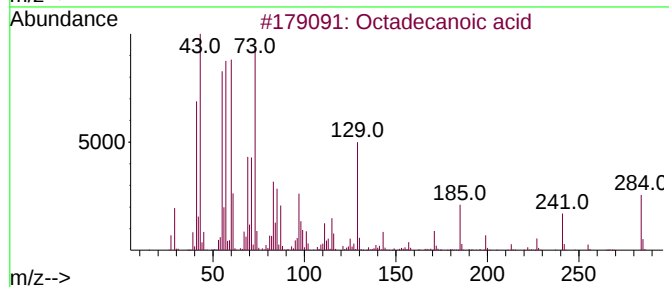
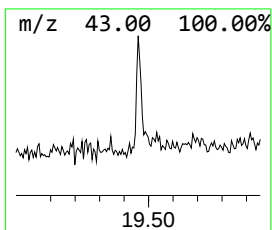
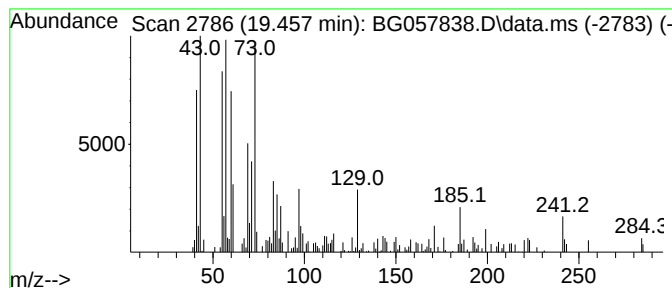
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.457	2.01 ng	72398	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	95
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4			Pentadecane	212	C15H32	000629-62-9	25
5			Tridecane	184	C13H28	000629-50-5	25



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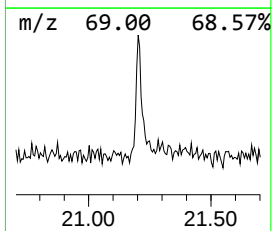
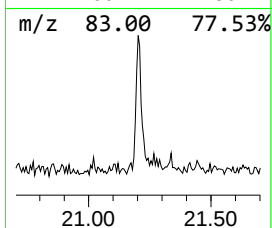
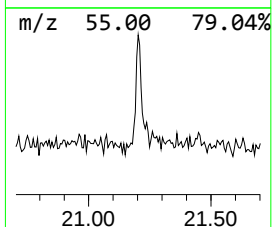
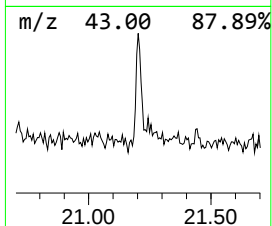
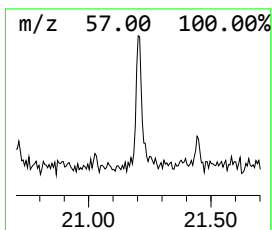
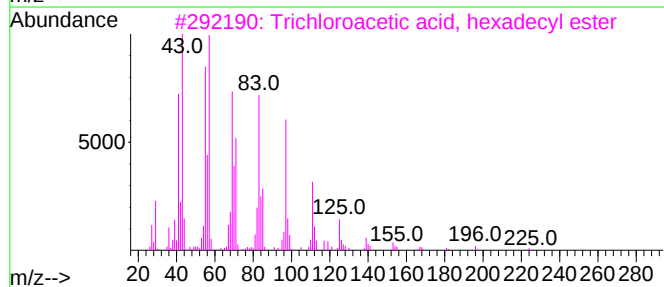
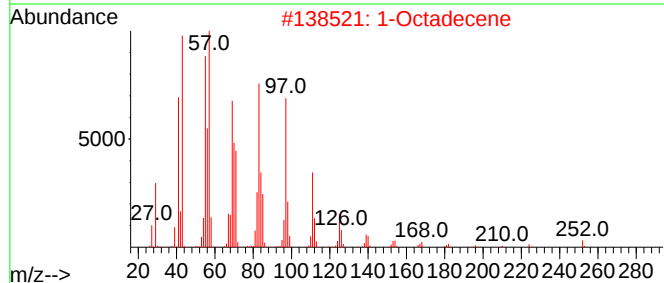
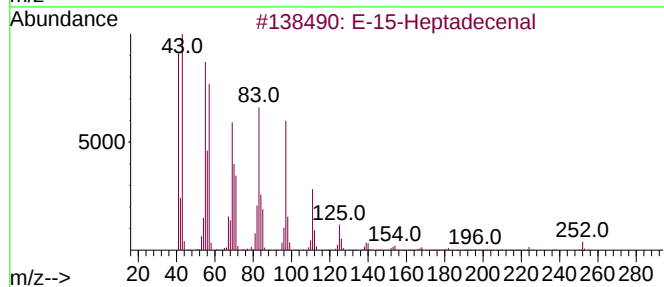
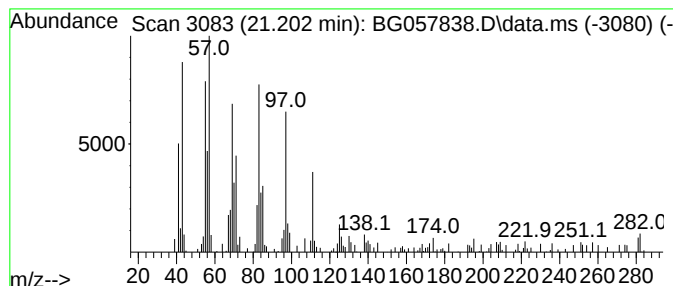
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Peak Number 5 E-15-Heptadecenal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.202	2.29 ng	82705	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal			252	C17H32O	1000130-97-9	93
2	1-Octadecene			252	C18H36	000112-88-9	93
3	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	91
4	Trichloroacetic acid, pentadecyl...			372	C17H31Cl3O2	074339-53-0	91
5	2-Heptadecenal			252	C17H32O	1000143-48-6	90



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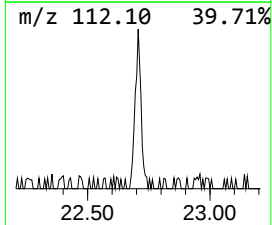
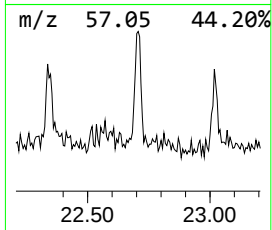
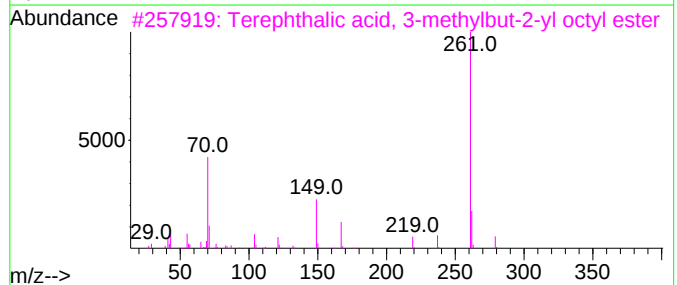
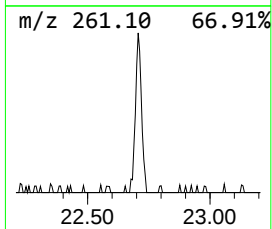
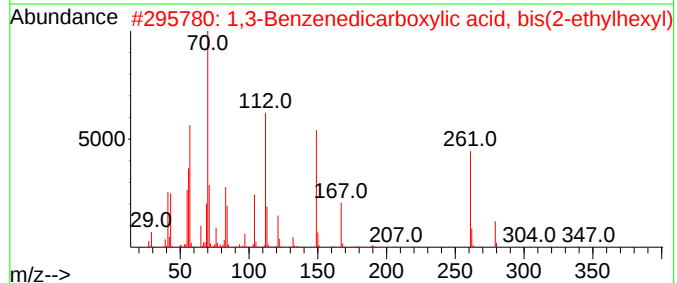
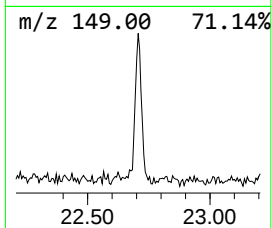
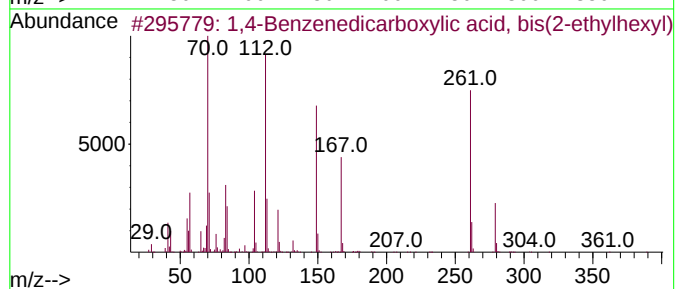
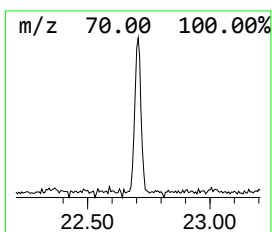
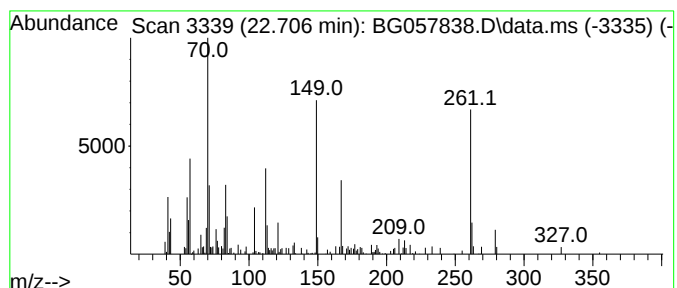
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.706	2.37 ng	85381	Chrysene-d12	21.549

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64	
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	64	
3	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	59	
4	Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	38	
5	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	35	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057838.D
Acq On : 23 Jun 2023 12:00
Operator : CG/JU
Sample : 03291-01
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.027	5.9	ng	66120	1	7.918	223417	20.0
Benzophenone	15.908	6.9	ng	190567	3	14.551	554859	20.0
Tridecanoic acid	18.182	2.9	ng	106827	4	17.295	725729	20.0
Octadecanoic acid	19.457	2.0	ng	72398	5	21.549	720866	20.0
E-15-Heptadecenal	21.202	2.3	ng	82705	5	21.549	720866	20.0
1,4-Benzenedica...	22.706	2.4	ng	85381	5	21.549	720866	20.0