

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
 Data File : BG057862.D
 Acq On : 24 Jun 2023 5:04
 Operator : CG/JU
 Sample : 03336-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-6

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: BG057862.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	323	331	338	rBV	54246	84404	3.17%	0.578%
2	5.496	403	410	422	rBV	940562	1491579	55.94%	10.211%
3	7.089	672	681	693	rBV	921627	1564570	58.67%	10.710%
4	7.923	817	823	830	rBV	188242	313196	11.75%	2.144%
5	9.086	1013	1021	1030	rBV	547526	964390	36.17%	6.602%
6	10.726	1292	1300	1309	rBV	267260	464894	17.43%	3.182%
7	13.181	1710	1718	1725	rBV	1310295	2047997	76.80%	14.020%
8	14.556	1946	1952	1962	rVB2	387881	596346	22.36%	4.082%
9	15.914	2177	2183	2190	rBV	107468	153087	5.74%	1.048%
10	16.043	2199	2205	2218	rBV	1041122	1570205	58.88%	10.749%
11	17.300	2412	2419	2425	rBV	473995	701135	26.29%	4.800%
12	18.187	2565	2570	2580	rBV	133255	208835	7.83%	1.430%
13	19.351	2763	2768	2776	rBV2	20396	41572	1.56%	0.285%
14	19.462	2783	2787	2796	rBV5	36970	74264	2.78%	0.508%
15	19.921	2859	2865	2872	rVB	1936119	2666622	100.00%	18.254%
16	21.207	3080	3084	3091	rVB	76830	111307	4.17%	0.762%
17	21.554	3138	3143	3149	rVB	425489	689202	25.85%	4.718%
18	22.999	3385	3389	3398	rVB3	80656	156149	5.86%	1.069%
19	24.709	3673	3680	3695	rVB2	248976	708299	26.56%	4.849%

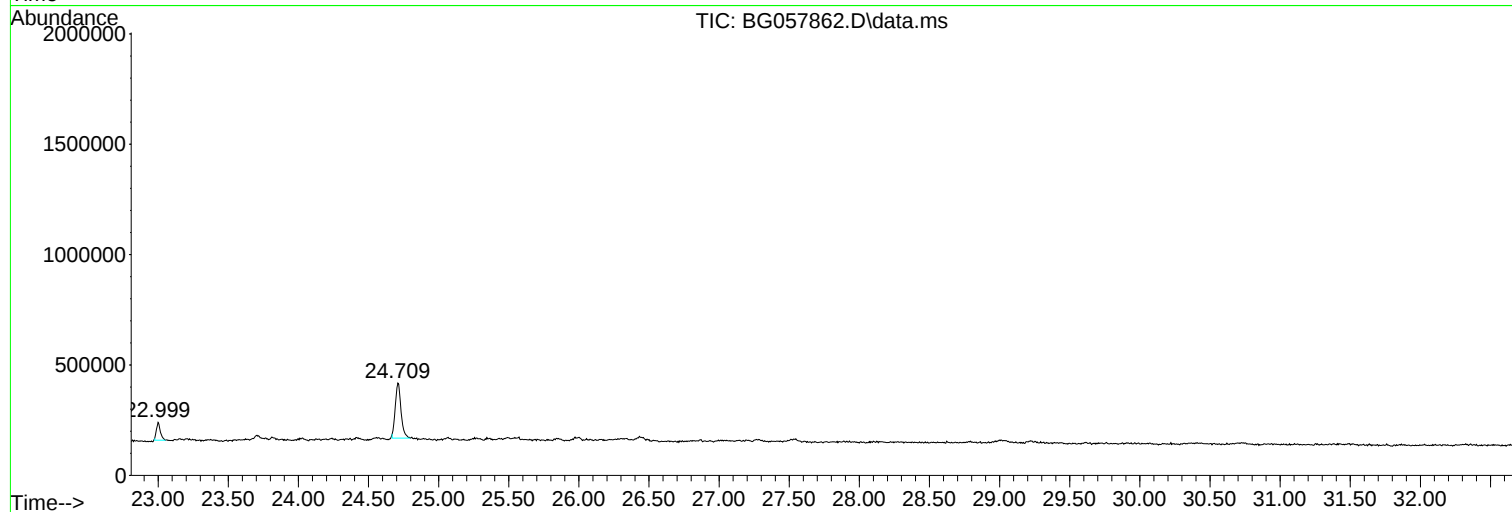
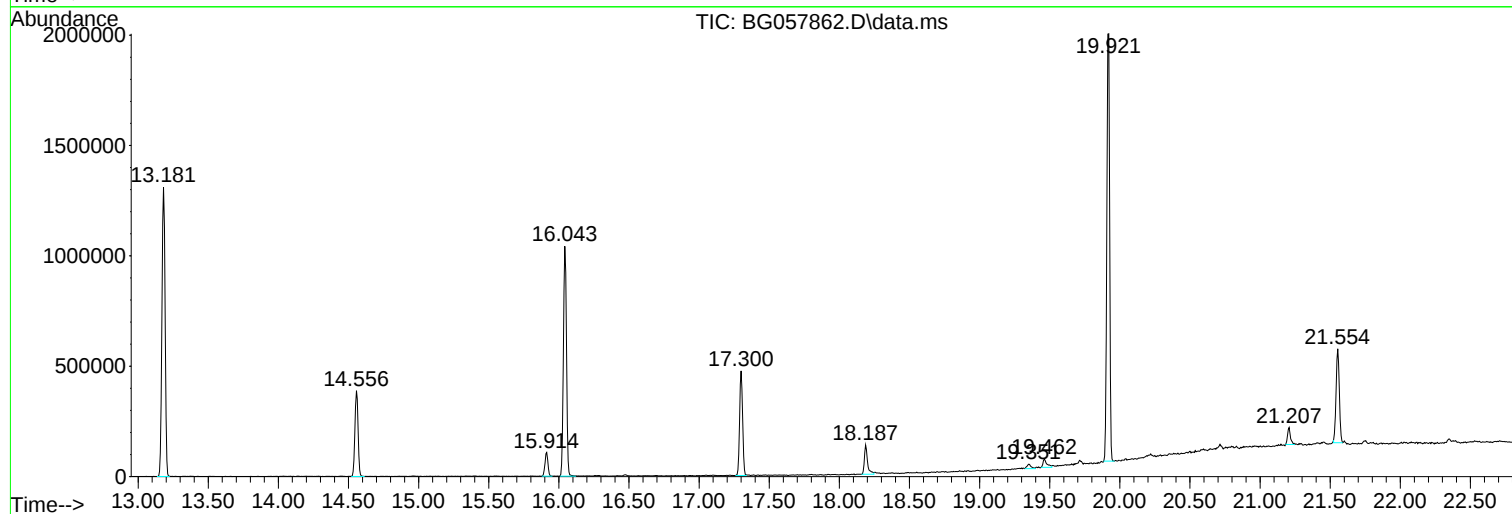
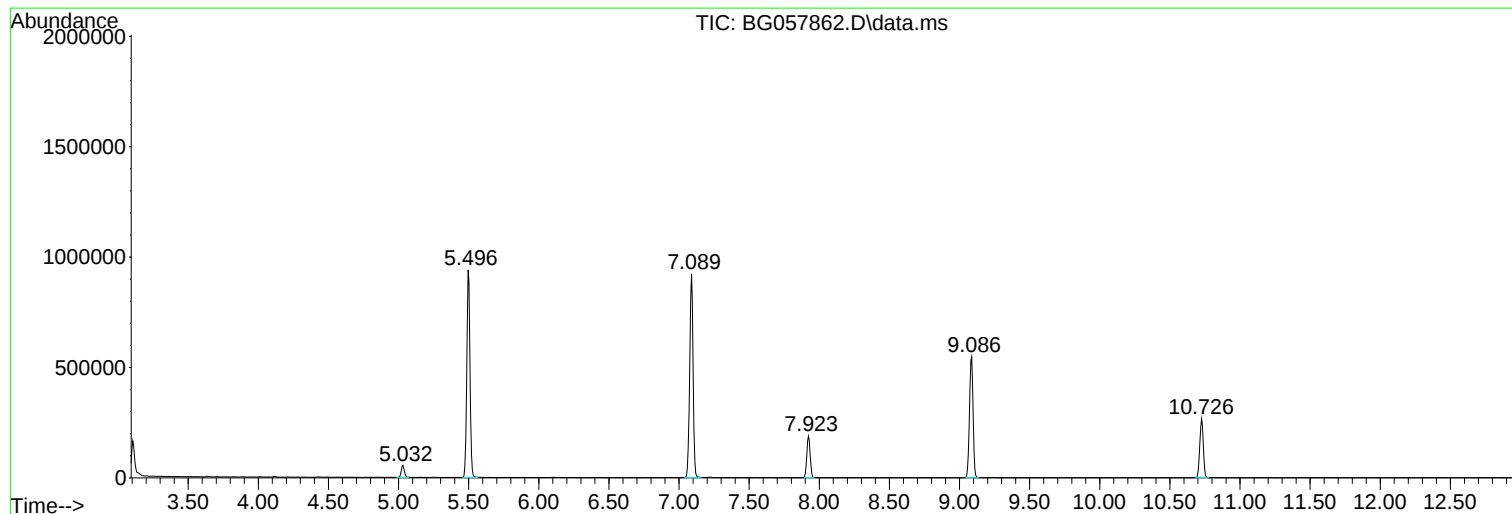
Sum of corrected areas: 14608053

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057862.D
Acq On : 24 Jun 2023 5:04
Operator : CG/JU
Sample : 03336-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-6

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057862.D
Acq On : 24 Jun 2023 5:04
Operator : CG/JU
Sample : 03336-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-6

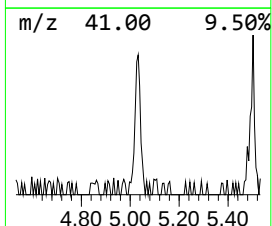
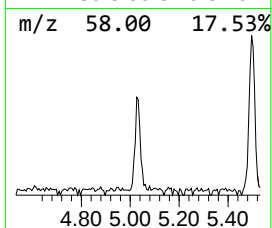
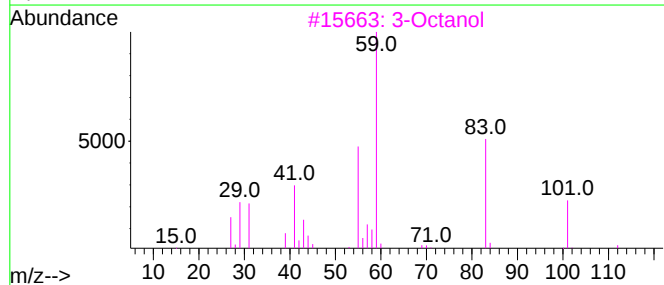
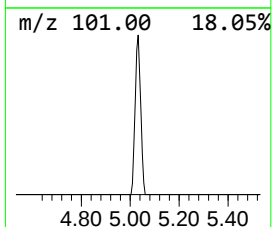
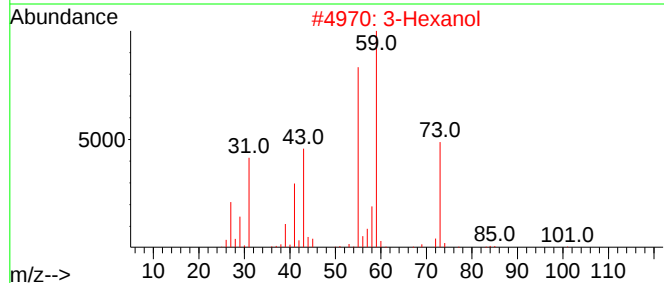
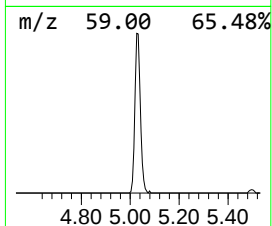
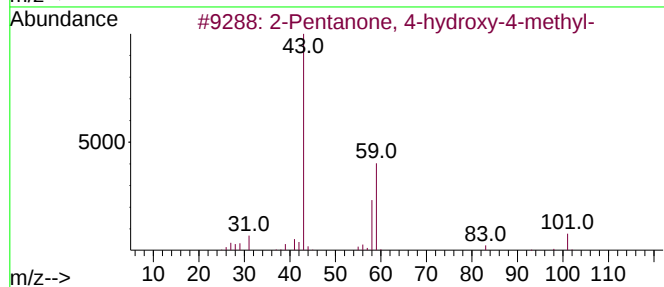
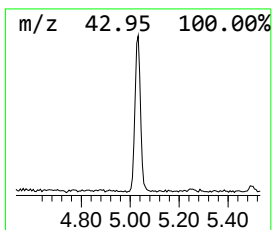
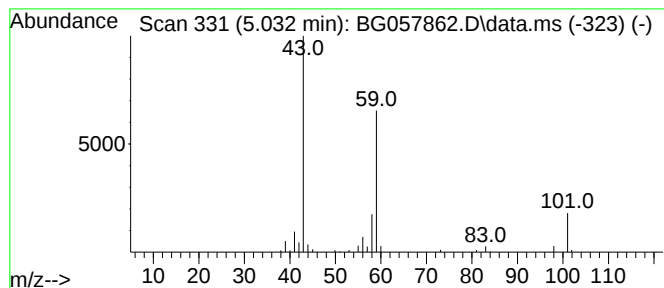
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.032	5.39 ng	84404	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	50		
2	3-Hexanol	102	C6H14O	000623-37-0	33		
3	3-Octanol	130	C8H18O	000589-98-0	33		
4	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	28		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057862.D
Acq On : 24 Jun 2023 5:04
Operator : CG/JU
Sample : 03336-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-6

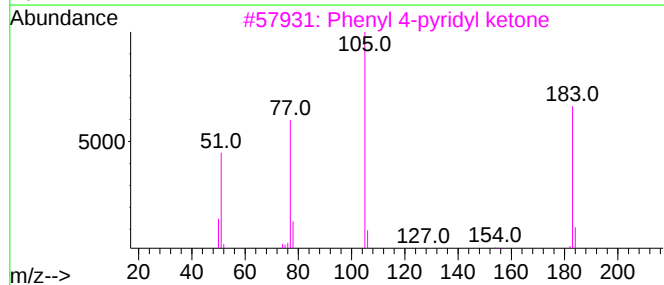
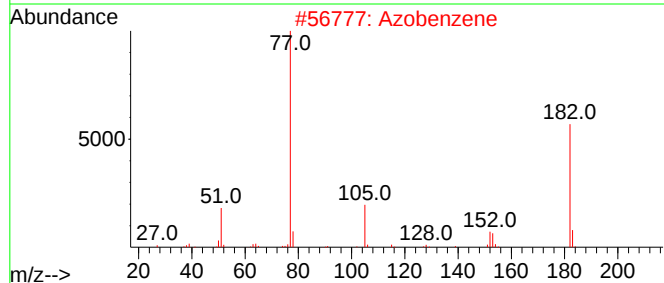
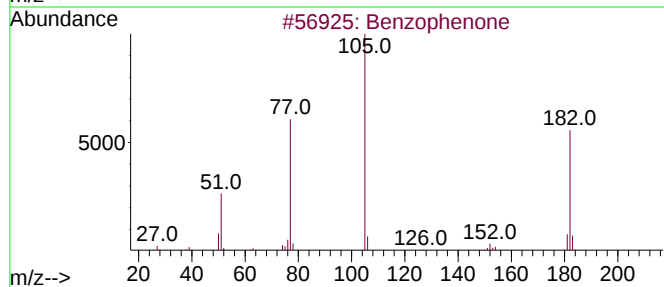
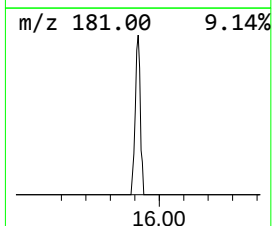
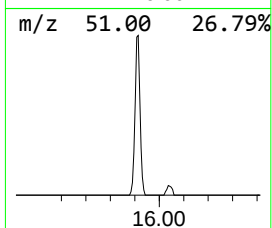
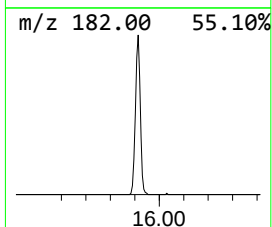
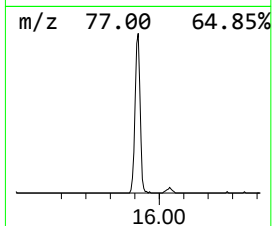
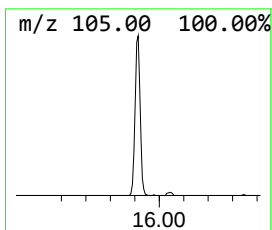
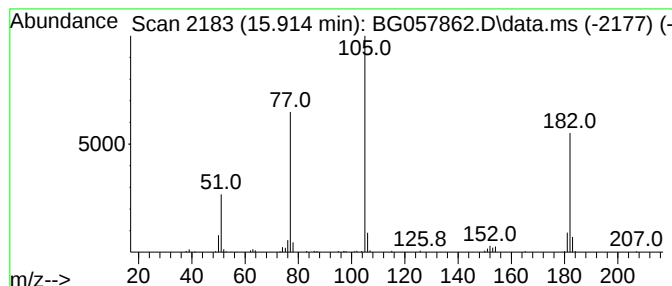
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	5.13 ng	153087	Acenaphthene-d10	14.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	53
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057862.D
Acq On : 24 Jun 2023 5:04
Operator : CG/JU
Sample : 03336-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-6

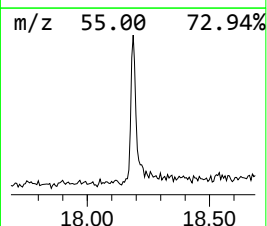
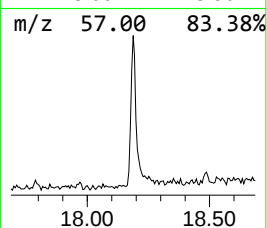
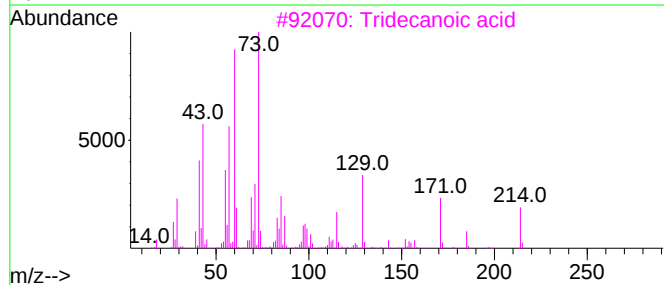
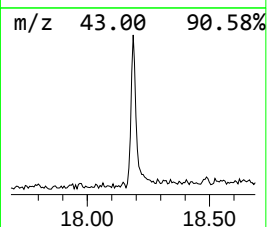
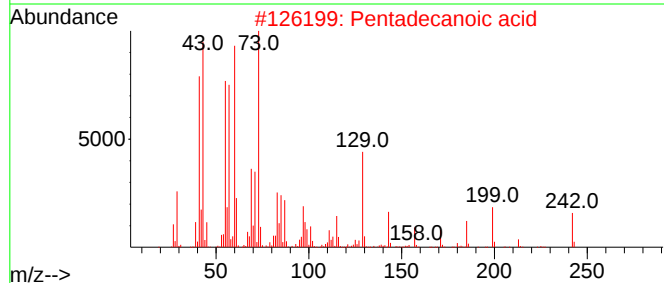
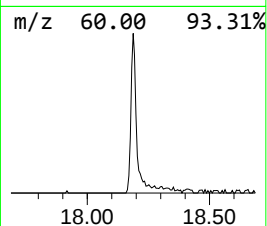
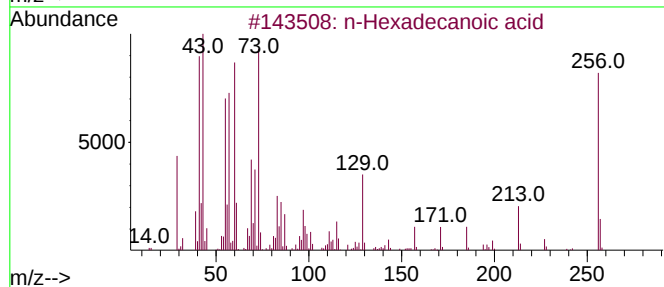
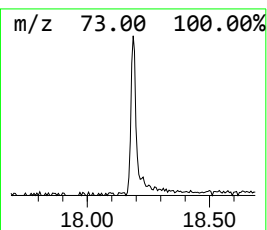
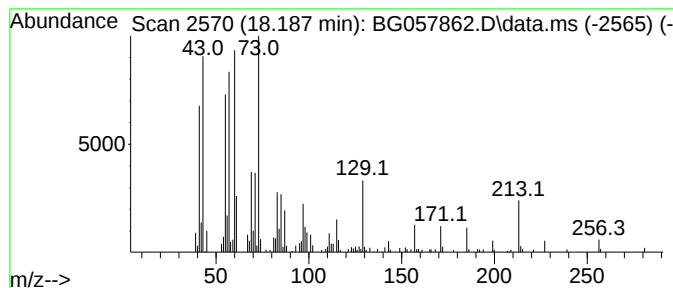
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.187	5.96 ng	208835	Phenanthrene-d10	17.300

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	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057862.D
Acq On : 24 Jun 2023 5:04
Operator : CG/JU
Sample : 03336-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-6

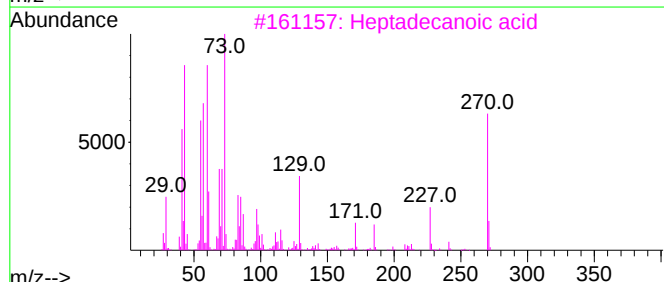
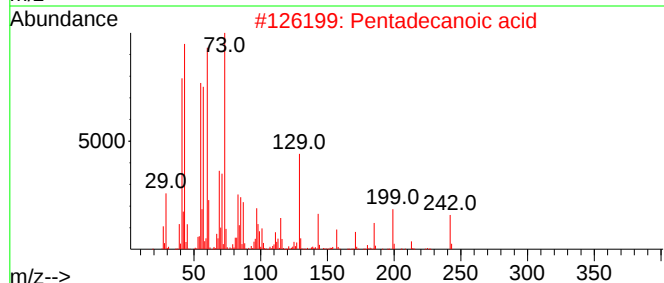
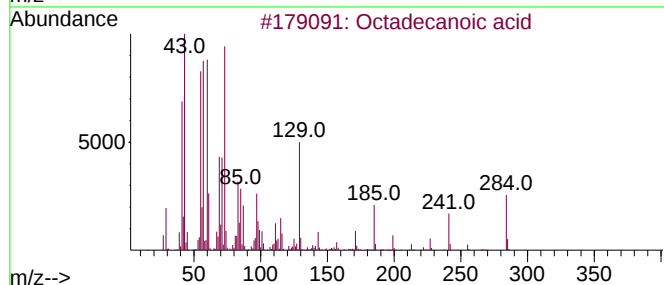
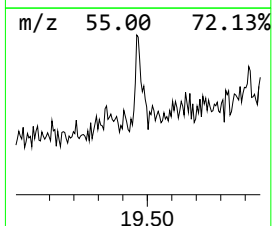
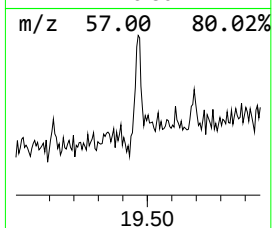
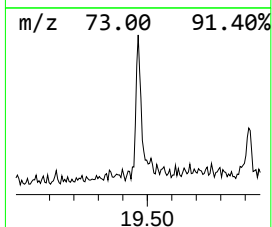
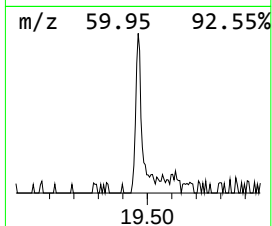
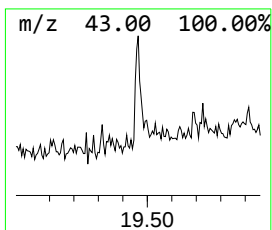
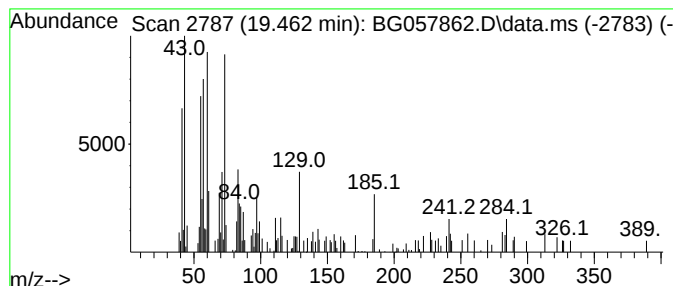
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.462	2.16 ng	74264	Chrysene-d12	21.554

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	83
3			Heptadecanoic acid	270	C17H34O2	000506-12-7	62
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057862.D
Acq On : 24 Jun 2023 5:04
Operator : CG/JU
Sample : 03336-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-6

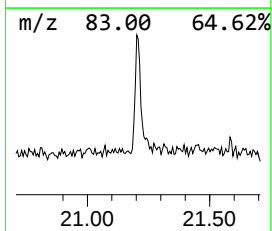
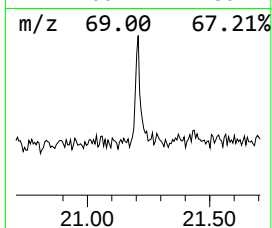
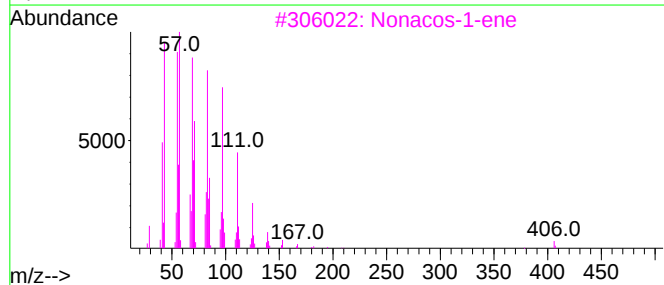
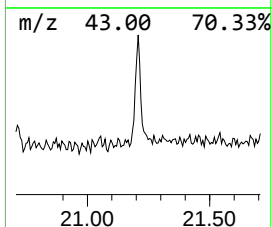
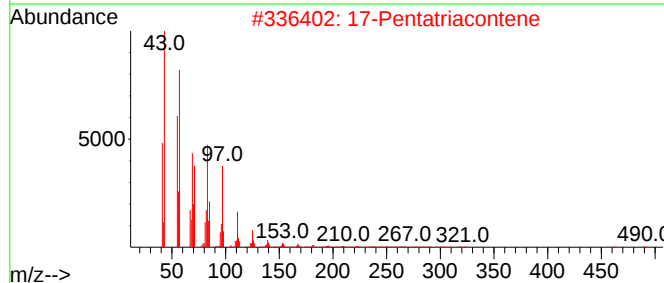
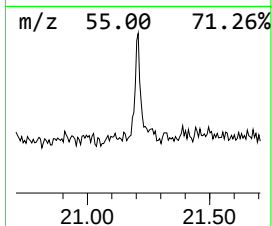
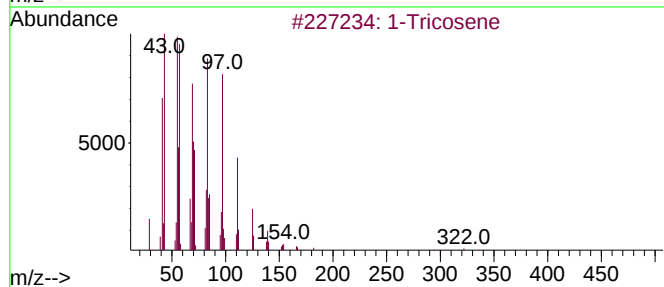
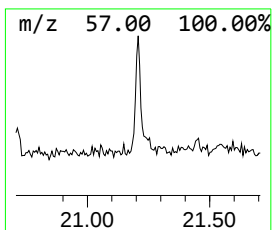
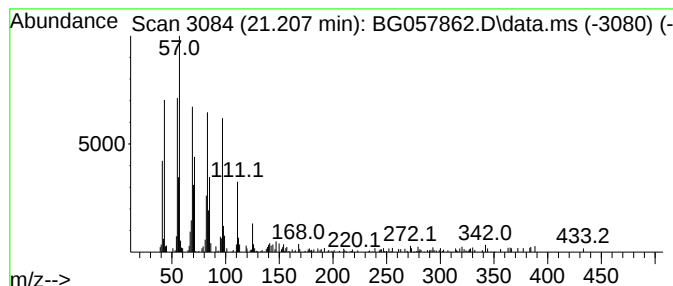
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Tricosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.207	3.23 ng	111307	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Tricosene	322	C23H46	018835-32-0	95
2			17-Pentatriacontene	491	C35H70	006971-40-0	91
3			Nonacos-1-ene	406	C29H58	018835-35-3	91
4			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5			9-Tricosanol, acetate	382	C25H50O2	039754-92-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057862.D
Acq On : 24 Jun 2023 5:04
Operator : CG/JU
Sample : 03336-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-6

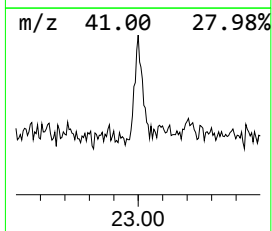
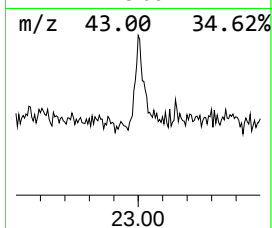
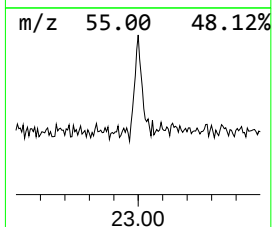
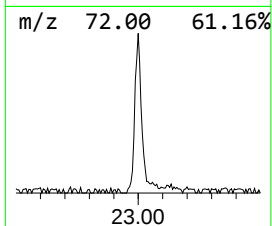
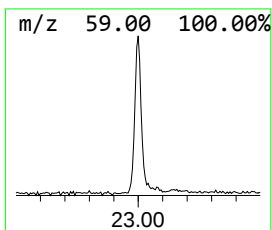
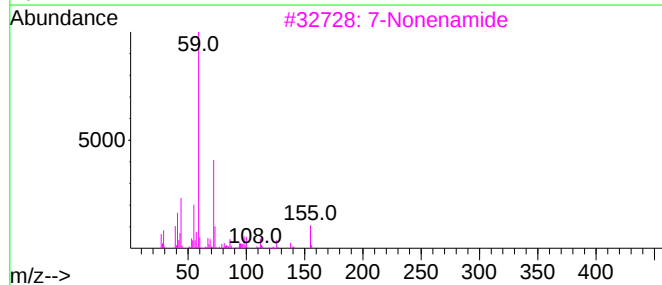
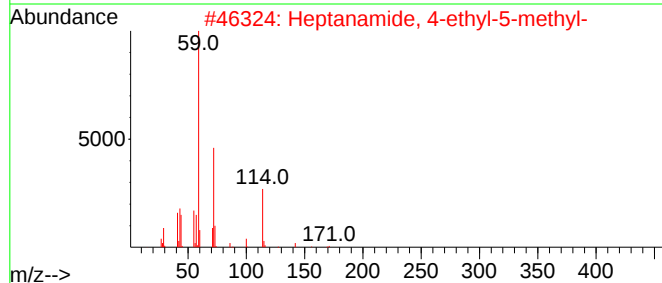
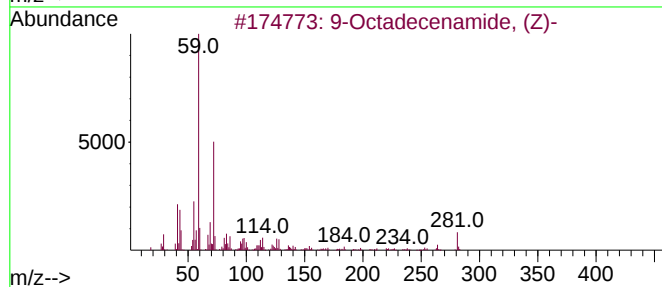
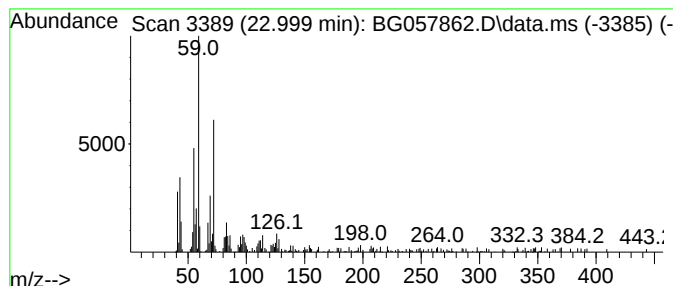
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.999	4.53 ng	156149	Chrysene-d12	21.554

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	86
2		Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
3		7-Nonenamide	155	C9H17NO	090949-53-4	64
4		Dodecanamide	199	C12H25NO	001120-16-7	59
5		N-ethyl-N-(1-methyl-2-[4-(methyl...	251	C14H21NOS	1000365-85-2	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057862.D
Acq On : 24 Jun 2023 5:04
Operator : CG/JU
Sample : 03336-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-6

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-...	5.032	5.4	ng	84404	1	7.923	313196	20.0
Benzophenone	15.914	5.1	ng	153087	3	14.556	596346	20.0
n-Hexadecanoic ...	18.187	6.0	ng	208835	4	17.300	701135	20.0
Octadecanoic acid	19.462	2.2	ng	74264	5	21.554	689202	20.0
1-Tricosene	21.207	3.2	ng	111307	5	21.554	689202	20.0
9-Octadecenamid...	22.999	4.5	ng	156149	5	21.554	689202	20.0