

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
 Data File : BG057891.D
 Acq On : 28 Jun 2023 13:51
 Operator : CG/JU
 Sample : 03366-03 2X
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB38

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-BG062723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057891.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.026	325	330	339	rVB	35417	52851	4.85%	0.574%
2	5.496	403	410	422	rVB	401364	657848	60.34%	7.141%
3	7.083	672	680	689	rBV	417168	703584	64.54%	7.637%
4	7.917	815	822	831	rBV	230735	386416	35.45%	4.194%
5	9.080	1011	1020	1028	rBV	244674	430224	39.46%	4.670%
6	10.720	1292	1299	1307	rVB	316285	569514	52.24%	6.182%
7	13.176	1710	1717	1724	rBV	614172	928694	85.19%	10.080%
8	14.556	1945	1952	1960	rBV	479464	736703	67.58%	7.997%
9	15.908	2176	2182	2190	rVB	58677	84738	7.77%	0.920%
10	16.037	2198	2204	2212	rBV	454065	699448	64.16%	7.592%
11	17.300	2412	2419	2424	rBV	561368	847800	77.77%	9.202%
12	17.341	2424	2426	2431	rVB3	22506	26099	2.39%	0.283%
13	18.187	2565	2570	2575	rBV	73863	137528	12.62%	1.493%
14	19.351	2764	2768	2775	rBV	76387	110981	10.18%	1.205%
15	19.715	2827	2830	2834	rVB	61124	81766	7.50%	0.888%
16	19.915	2859	2864	2868	rVB	869561	1090159	100.00%	11.833%
17	21.554	3137	3143	3148	rBV2	474807	788660	72.34%	8.560%
18	24.709	3673	3680	3701	rVB	278271	879797	80.70%	9.550%

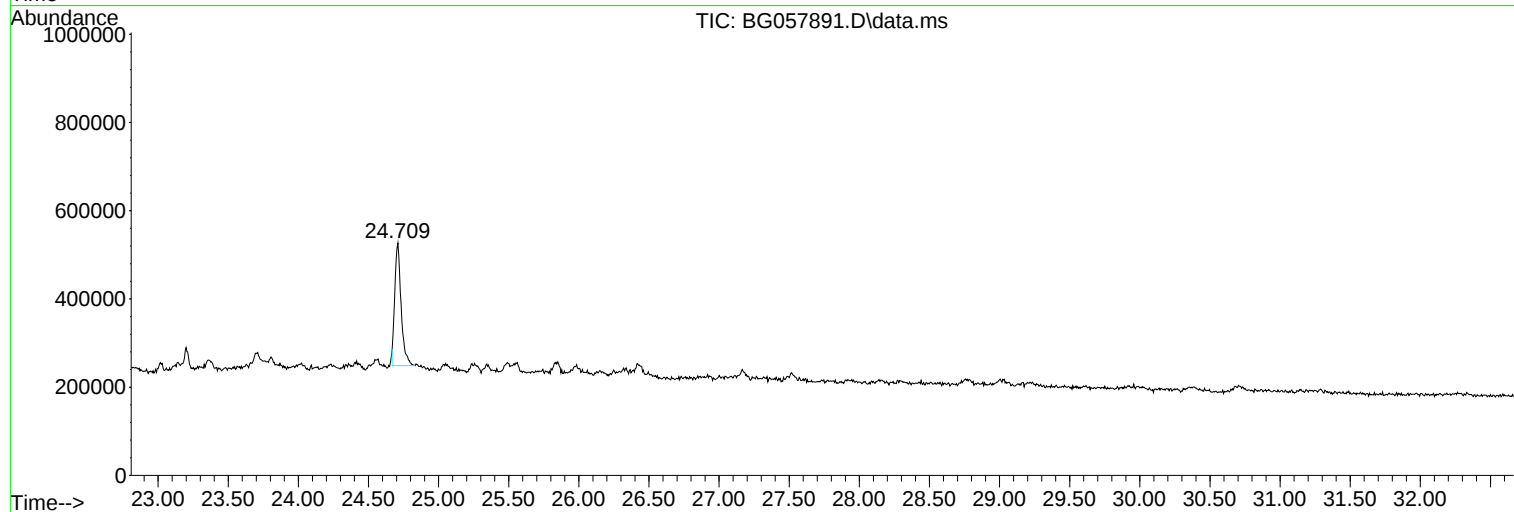
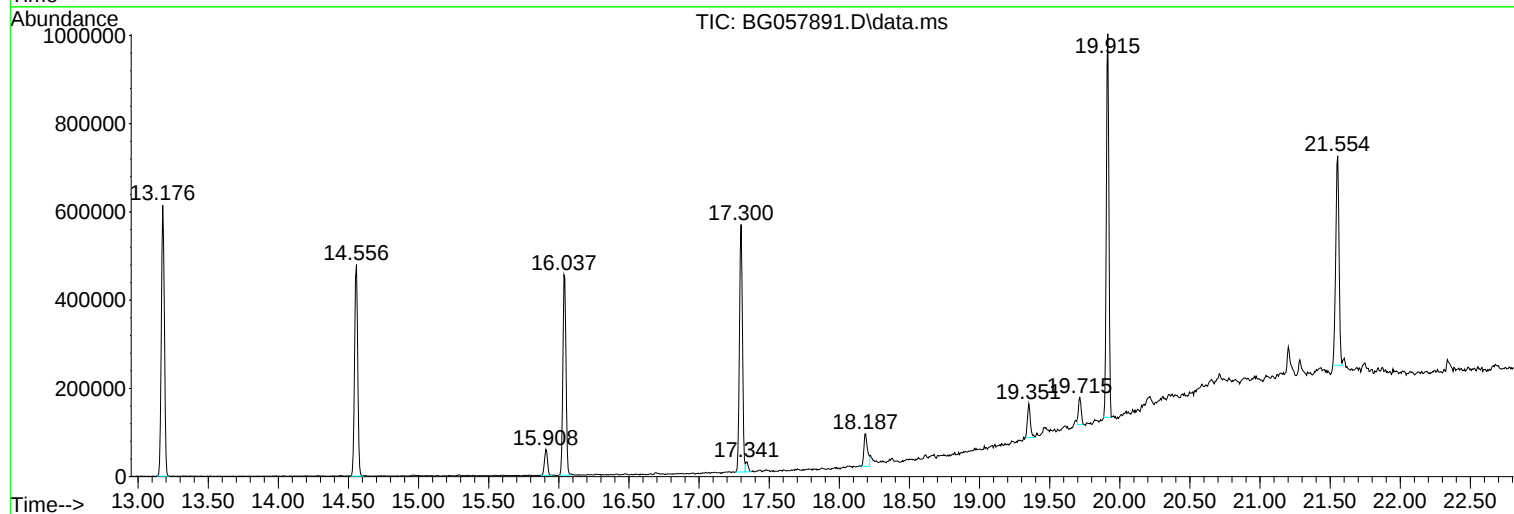
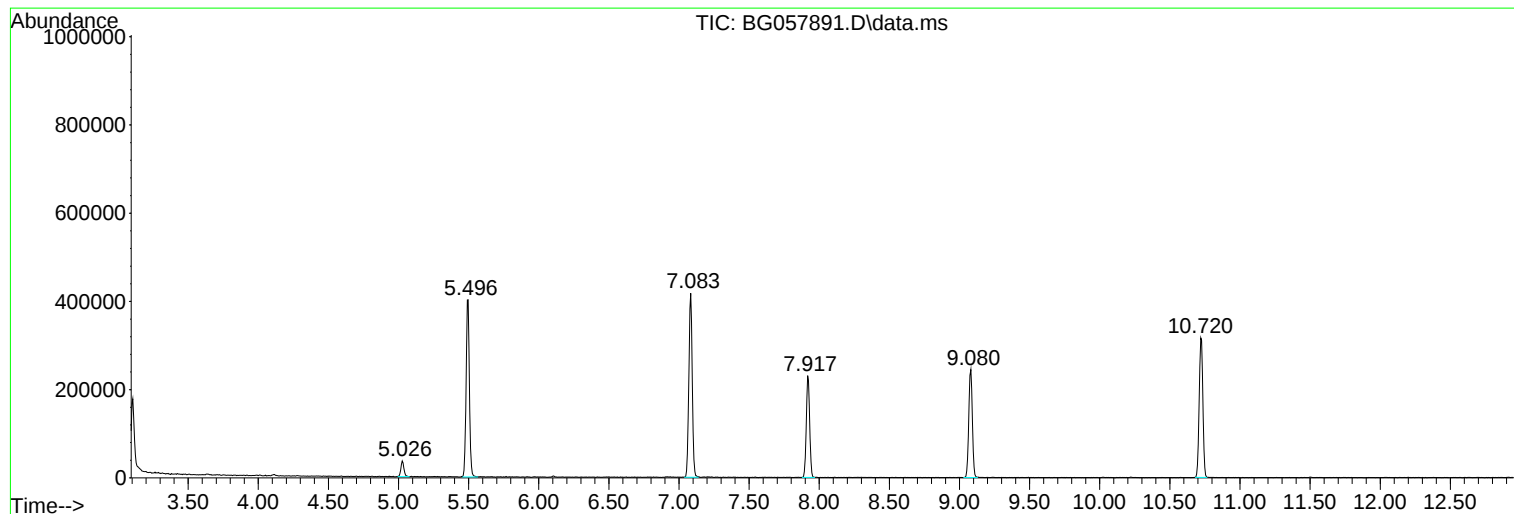
Sum of corrected areas: 9212810

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
Data File : BG057891.D
Acq On : 28 Jun 2023 13:51
Operator : CG/JU
Sample : 03366-03 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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\BG062823\
Data File : BG057891.D
Acq On : 28 Jun 2023 13:51
Operator : CG/JU
Sample : 03366-03 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB38

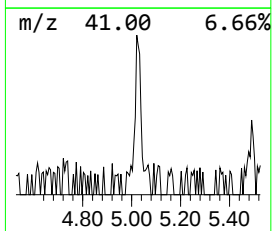
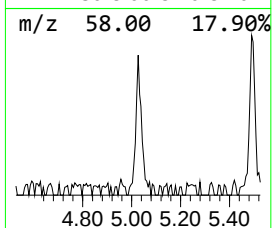
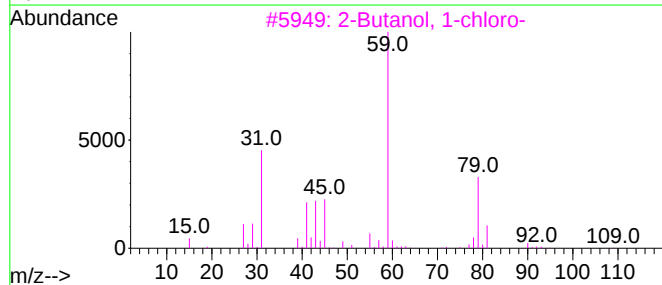
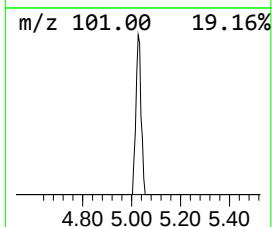
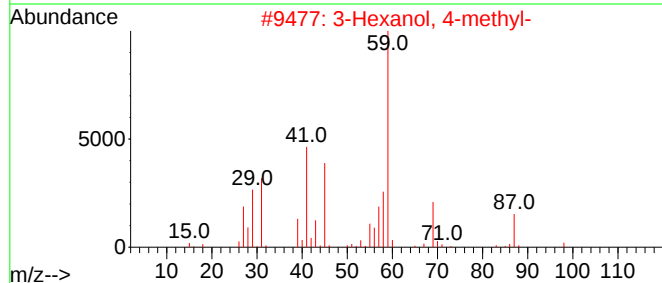
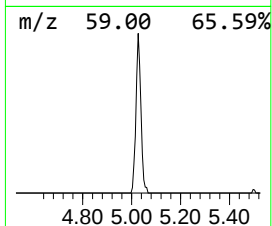
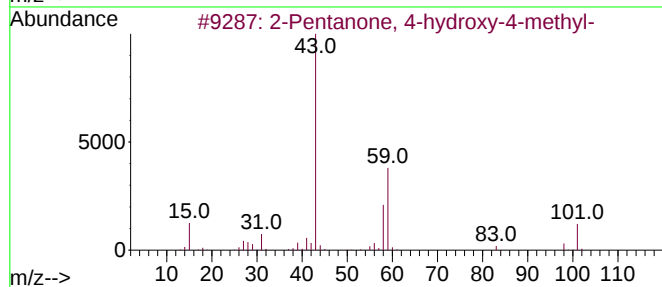
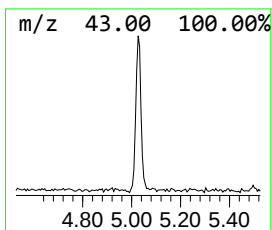
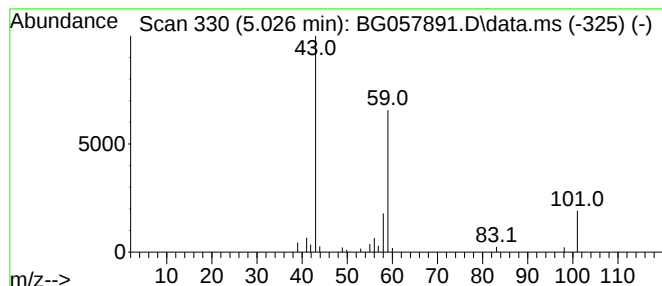
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.026	2.74 ng	52851	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	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25		
3	2-Butanol, 1-chloro-	108	C4H9ClO	001873-25-2	17		
4	Guanidine	59	CH5N3	000113-00-8	9		
5	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
Data File : BG057891.D
Acq On : 28 Jun 2023 13:51
Operator : CG/JU
Sample : 03366-03 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB38

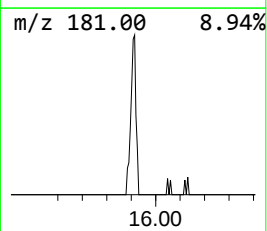
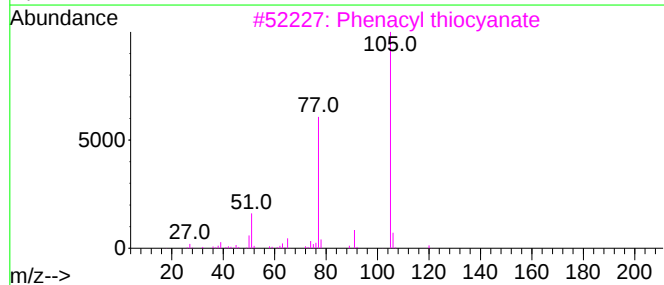
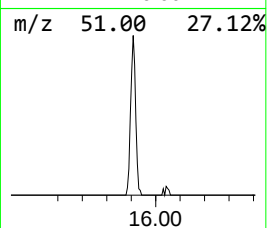
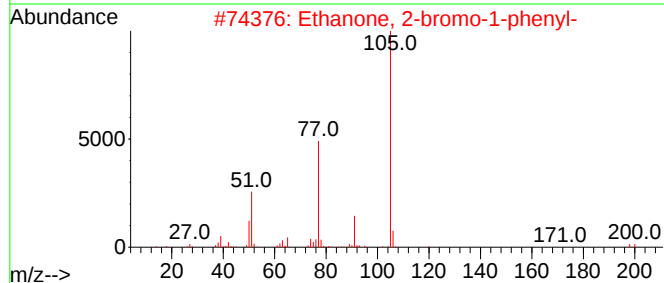
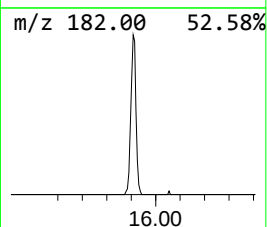
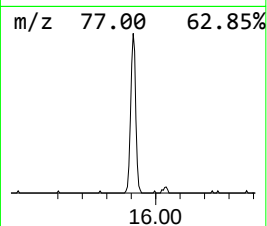
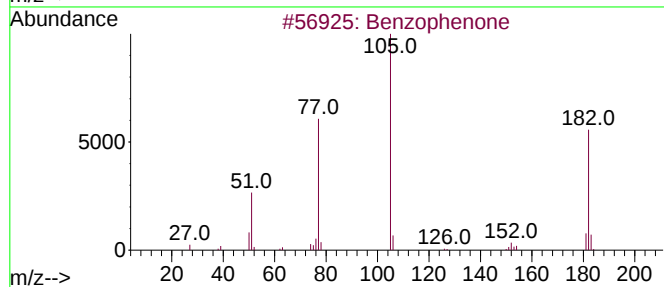
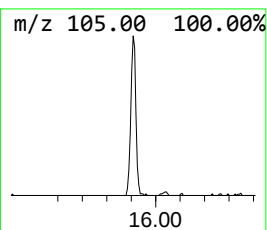
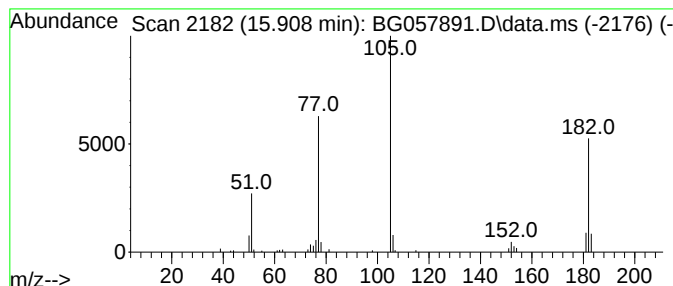
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
15.908	2.30 ng	84738	Acenaphthene-d10	14.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	47
3		Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	47
4		N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	47
5		N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
Data File : BG057891.D
Acq On : 28 Jun 2023 13:51
Operator : CG/JU
Sample : 03366-03 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB38

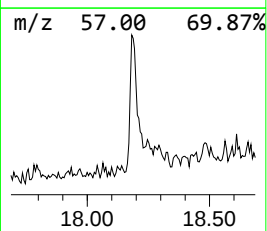
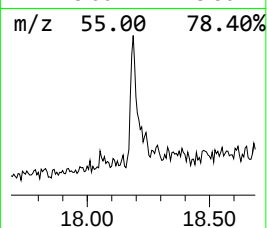
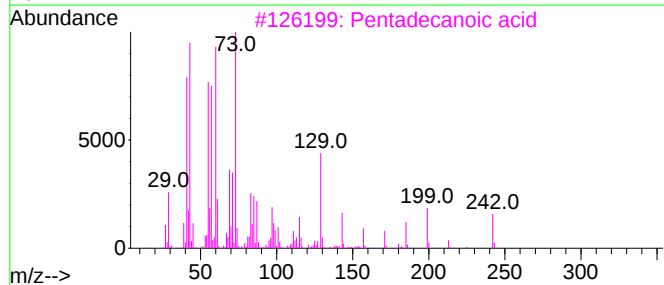
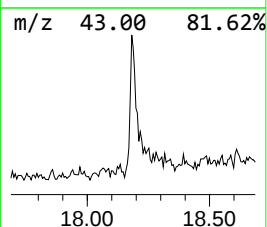
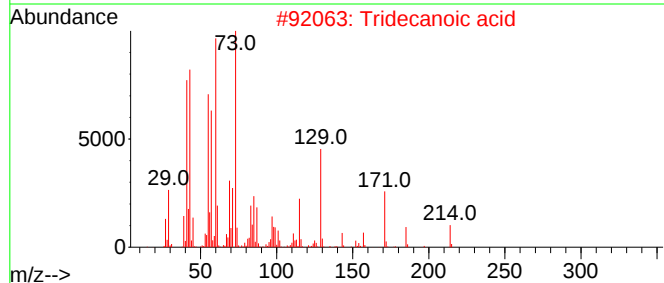
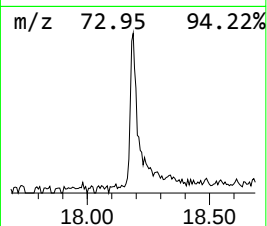
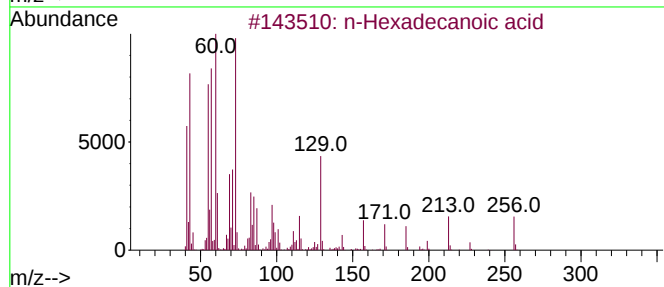
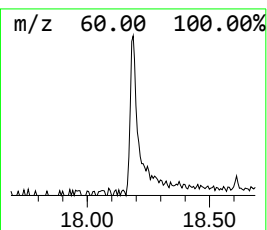
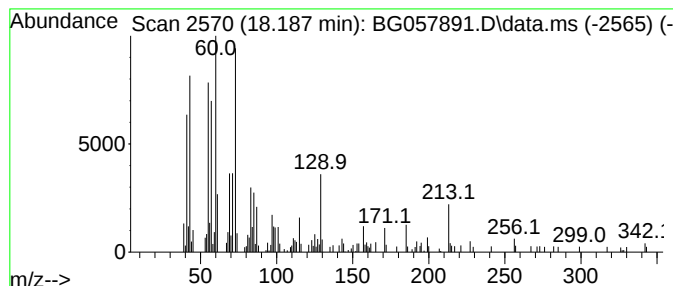
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	3.24 ng	137528	Phenanthrene-d10	17.300

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
Data File : BG057891.D
Acq On : 28 Jun 2023 13:51
Operator : CG/JU
Sample : 03366-03 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB38

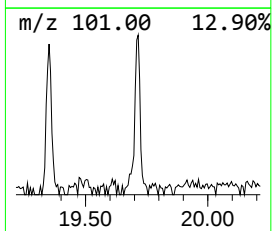
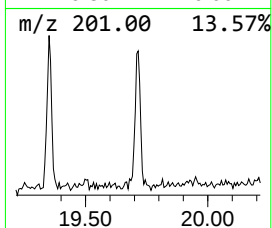
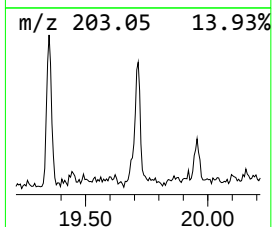
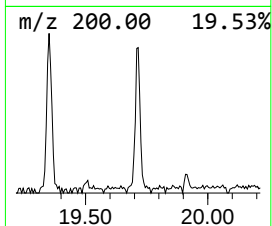
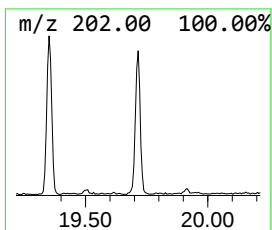
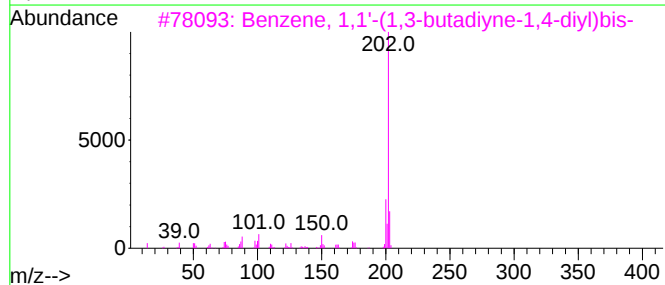
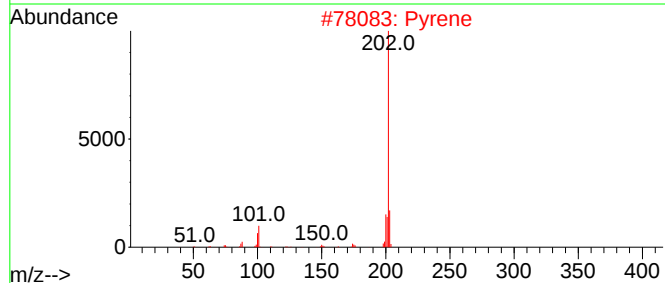
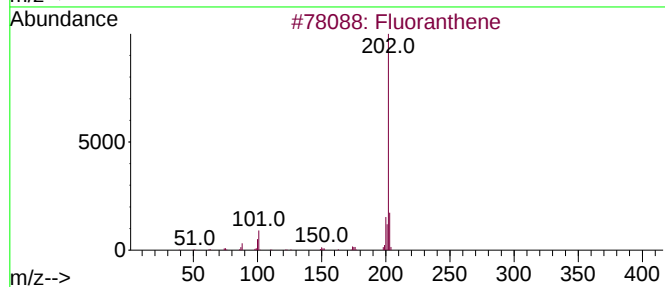
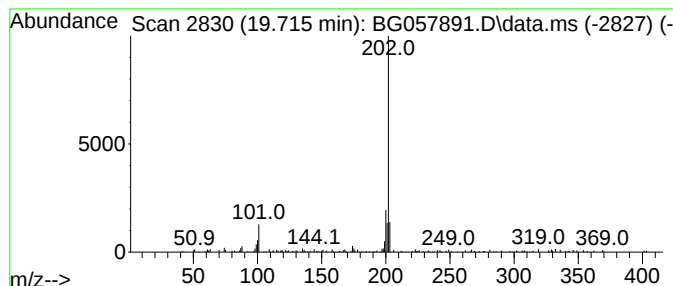
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.715	2.07 ng	81766	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluoranthene	202	C16H10	000206-44-0	76
2			Pyrene	202	C16H10	000129-00-0	68
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	50
4			1-Leucyl-1-leucine, N,N'-dimethy...	514	C28H54N2O6	1000328-59-6	47
5			1-Methyl-7,11-dithiaspiro[5,5] u...	202	C10H18S2	107678-22-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062823\
Data File : BG057891.D
Acq On : 28 Jun 2023 13:51
Operator : CG/JU
Sample : 03366-03 2X
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB38

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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-...	5.026	2.7	ng	52851	1	7.923	386416	20.0
Benzophenone	15.908	2.3	ng	84738	3	14.556	736703	20.0
n-Hexadecanoic ...	18.187	3.2	ng	137528	4	17.300	847800	20.0
Benzene, 1,1'-(...	19.715	2.1	ng	81766	5	21.554	788660	20.0