

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
 Data File : BG057855.D
 Acq On : 24 Jun 2023 00:08
 Operator : CG/JU
 Sample : 03336-04
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-5

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: BG057855.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	341	rBV	29560	50472	2.63%	0.453%
2	5.496	403	410	418	rBV	612790	947877	49.46%	8.501%
3	7.083	671	680	693	rBV	608064	1002736	52.32%	8.993%
4	7.923	815	823	830	rBV	171802	282167	14.72%	2.531%
5	9.080	1012	1020	1029	rBV	341884	599058	31.26%	5.372%
6	10.725	1291	1300	1307	rBV	231863	404945	21.13%	3.632%
7	13.181	1711	1718	1725	rBV	803344	1261728	65.83%	11.315%
8	14.556	1946	1952	1961	rVB	367376	551208	28.76%	4.943%
9	15.908	2175	2182	2188	rBV	99949	136999	7.15%	1.229%
10	16.043	2198	2205	2217	rBV	731240	1108589	57.84%	9.942%
11	17.300	2412	2419	2430	rVB	463583	680353	35.50%	6.102%
12	18.187	2564	2570	2580	rBV	146975	220869	11.52%	1.981%
13	19.462	2783	2787	2792	rBV2	42151	62618	3.27%	0.562%
14	19.915	2858	2864	2871	rBV	1444111	1916638	100.00%	17.189%
15	21.201	3078	3083	3091	rBV	101530	171968	8.97%	1.542%
16	21.554	3136	3143	3149	rBV	448172	735477	38.37%	6.596%
17	22.993	3383	3388	3396	rBV3	97315	202345	10.56%	1.815%
18	24.703	3670	3679	3691	rVB2	282174	814406	42.49%	7.304%

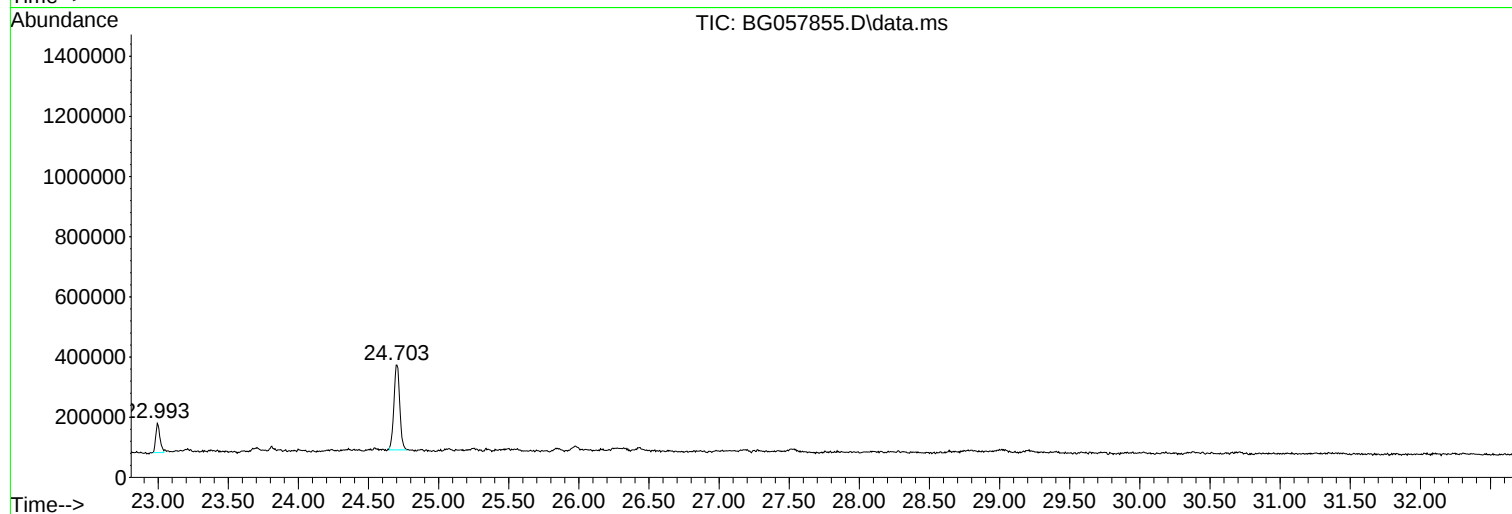
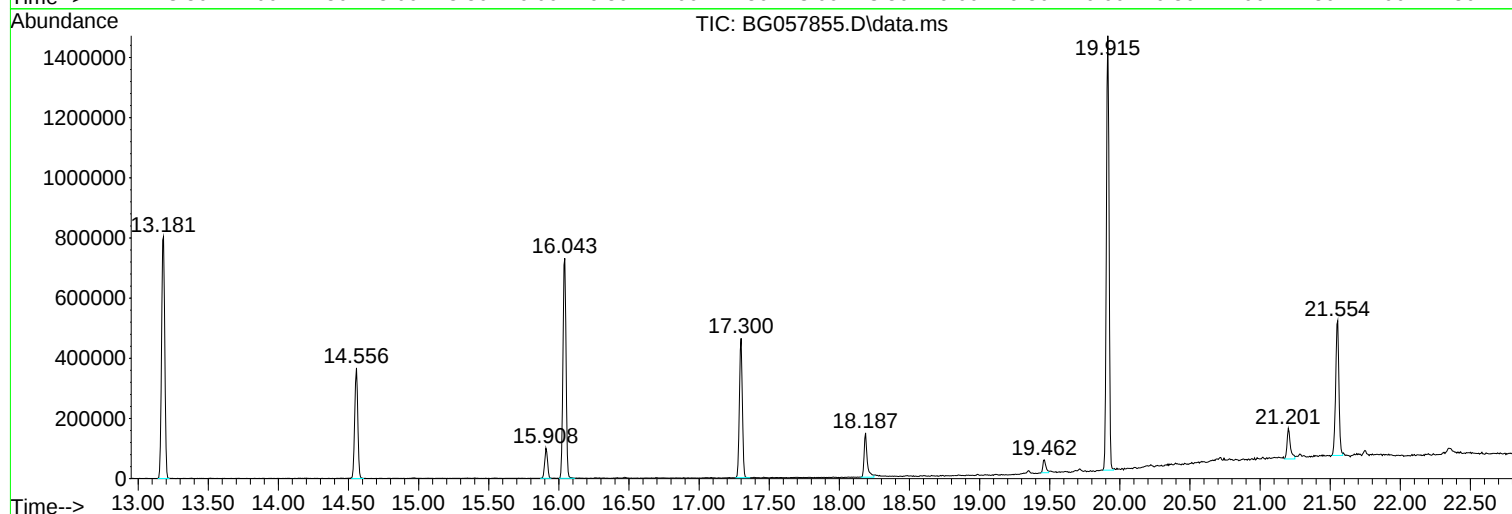
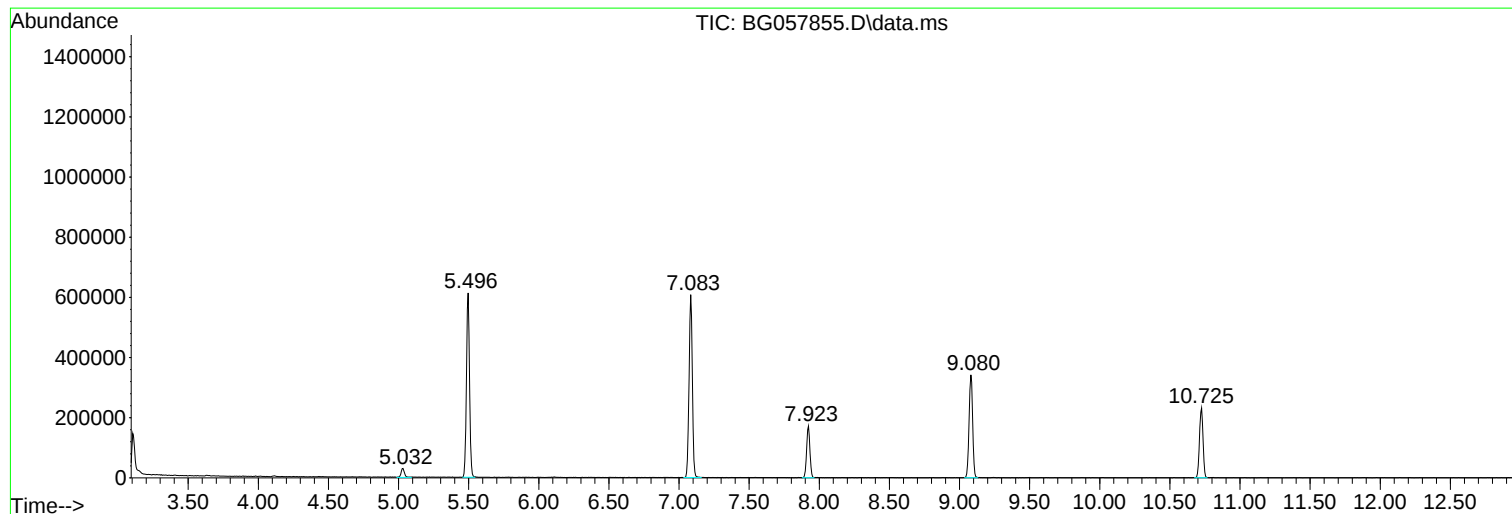
Sum of corrected areas: 11150453

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057855.D
Acq On : 24 Jun 2023 00:08
Operator : CG/JU
Sample : 03336-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-5

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 : BG057855.D
Acq On : 24 Jun 2023 00:08
Operator : CG/JU
Sample : 03336-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-5

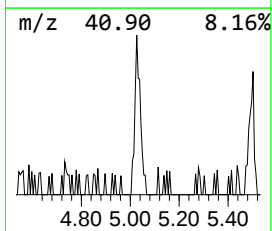
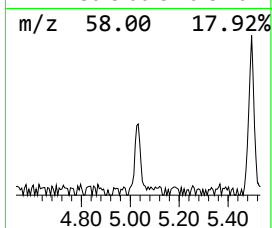
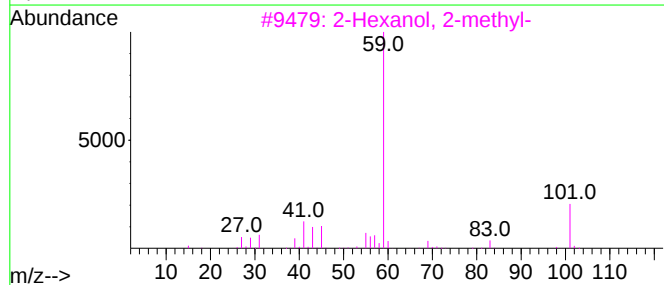
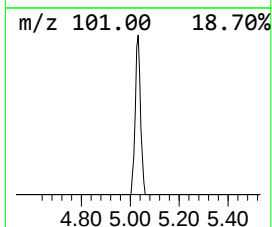
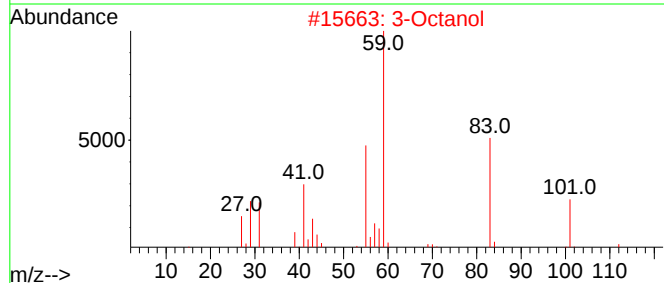
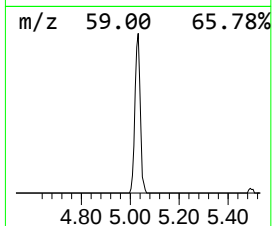
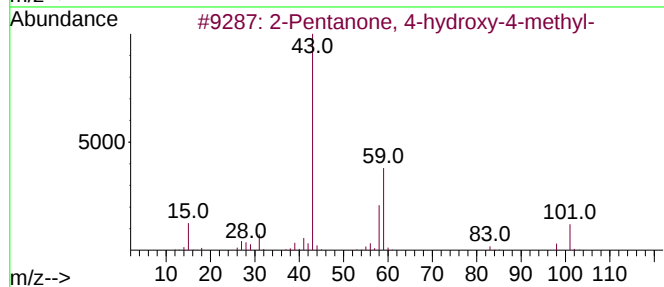
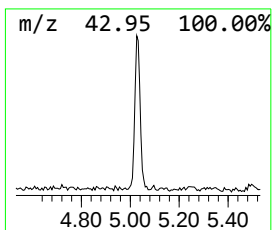
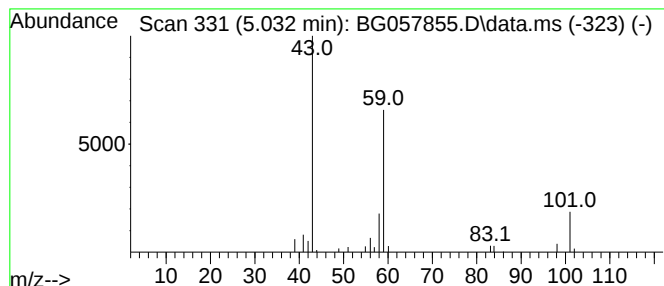
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.032	3.58 ng	50472	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	64
2		3-Octanol	130	C8H18O	000589-98-0	40
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057855.D
Acq On : 24 Jun 2023 00:08
Operator : CG/JU
Sample : 03336-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-5

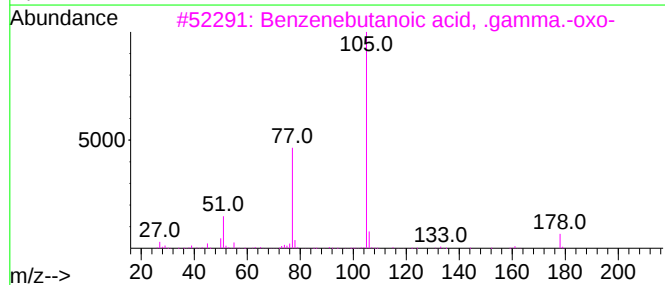
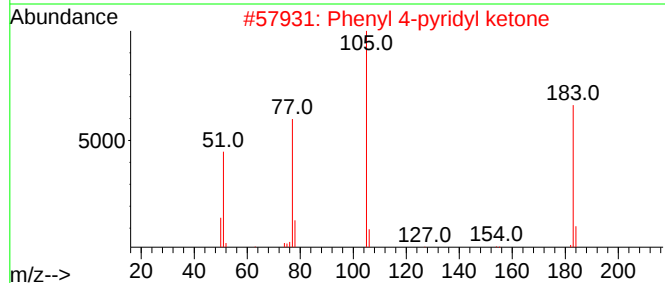
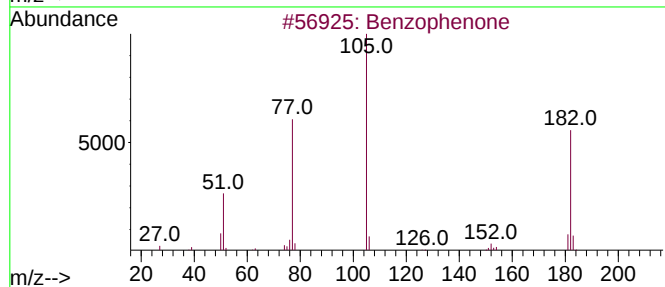
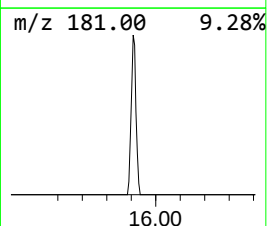
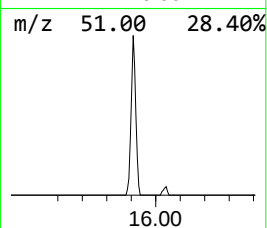
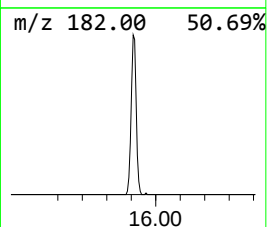
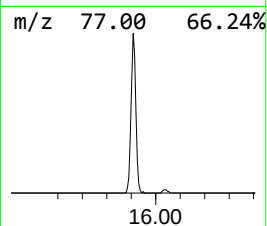
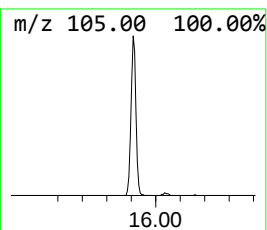
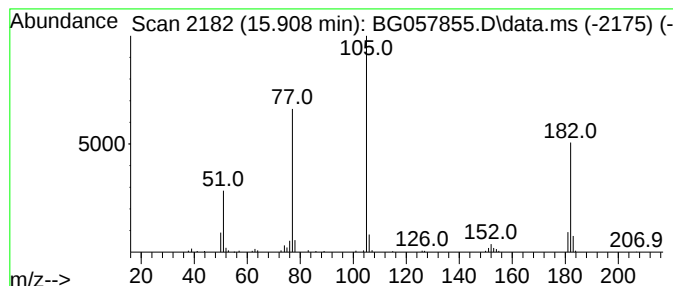
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
15.908	4.97 ng	136999	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	53
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057855.D
Acq On : 24 Jun 2023 00:08
Operator : CG/JU
Sample : 03336-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

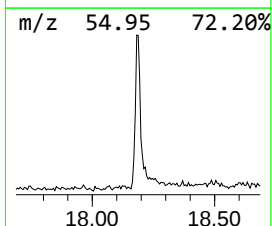
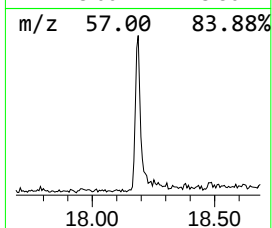
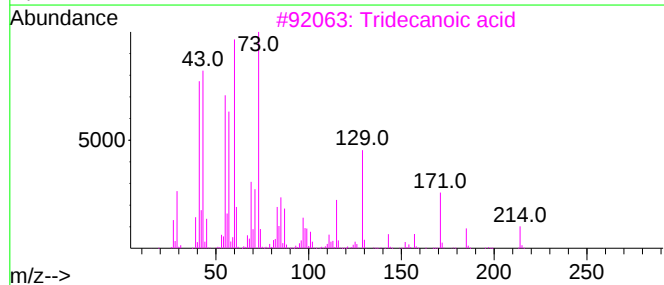
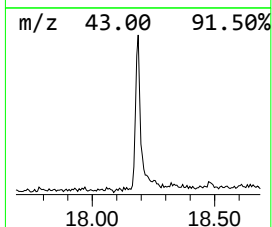
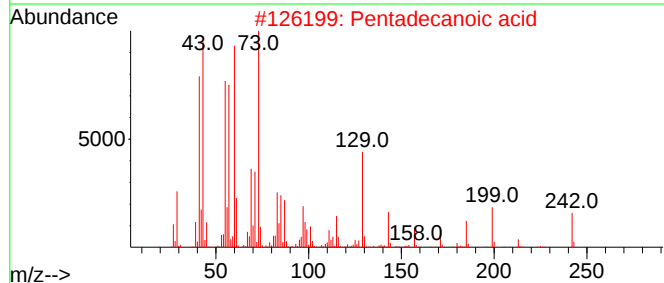
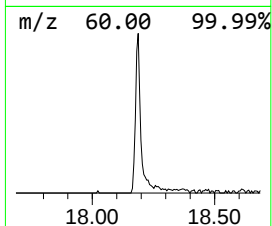
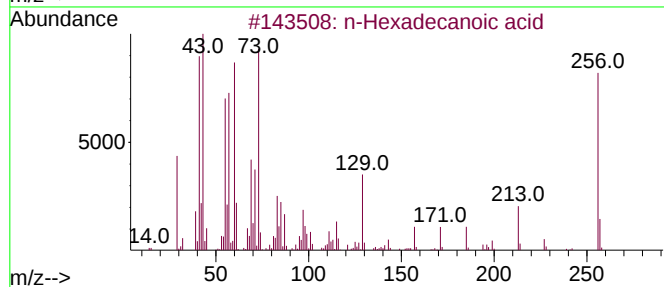
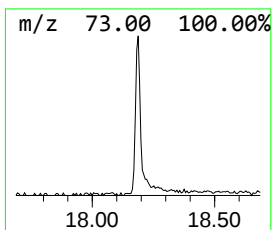
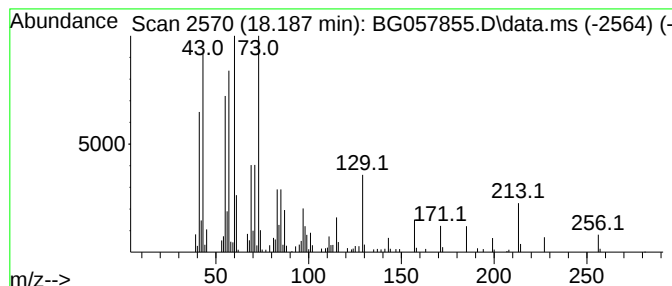
Instrument :
BNA_G
ClientSampleId :
WC-5

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	6.49 ng	220869	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	90
3	Tridecanoic acid		214	C13H26O2	000638-53-9	90
4	Dodecanoic acid		200	C12H24O2	000143-07-7	76
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057855.D
Acq On : 24 Jun 2023 00:08
Operator : CG/JU
Sample : 03336-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-5

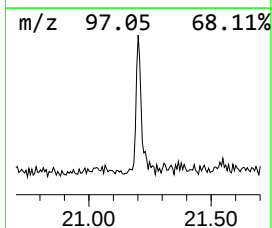
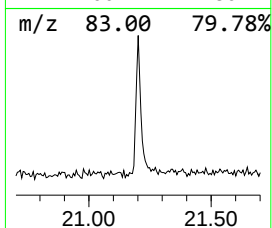
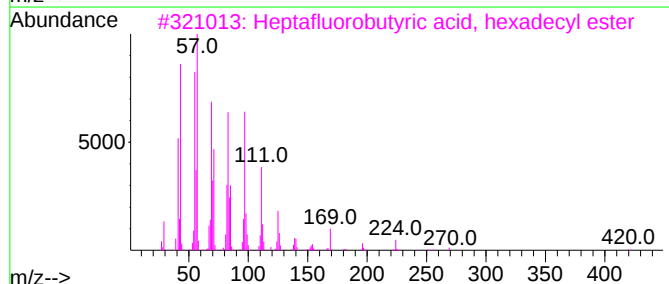
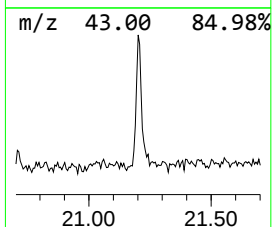
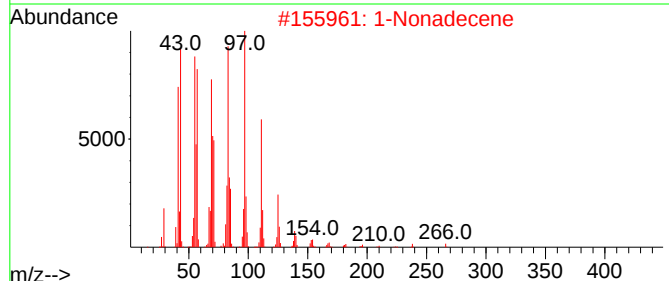
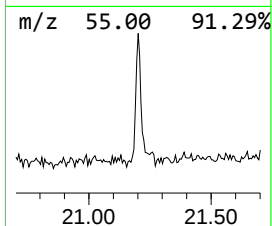
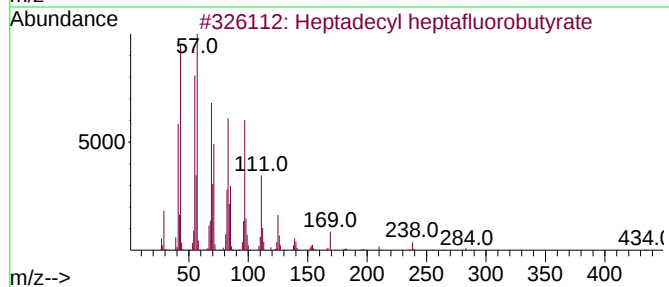
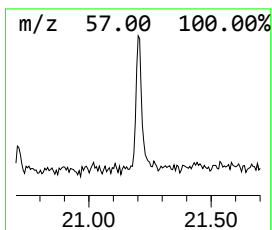
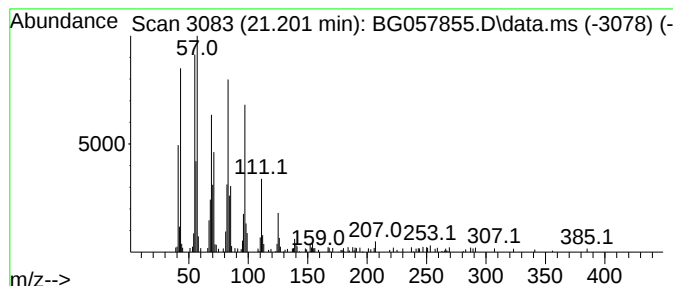
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.201	4.68 ng	171968	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			1-Nonadecene	266	C19H38	018435-45-5	93
3			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
5			Octacosanol	410	C28H58O	000557-61-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057855.D
Acq On : 24 Jun 2023 00:08
Operator : CG/JU
Sample : 03336-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-5

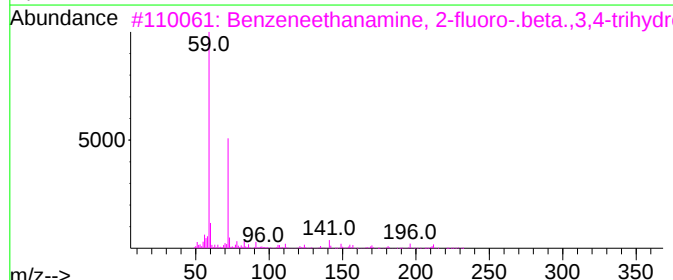
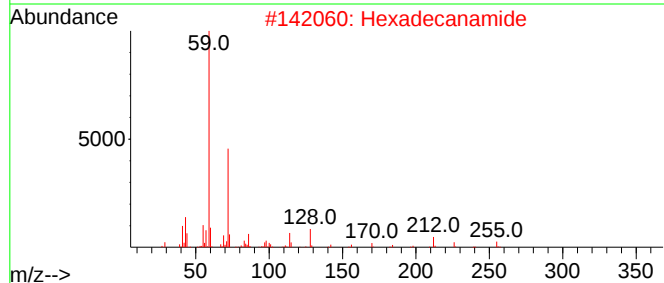
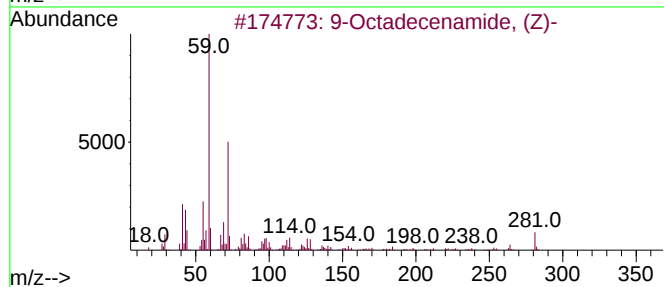
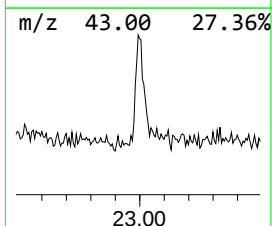
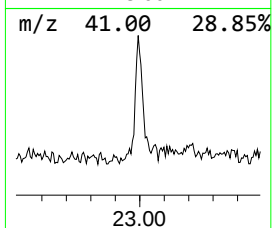
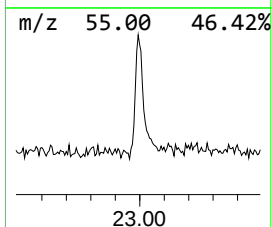
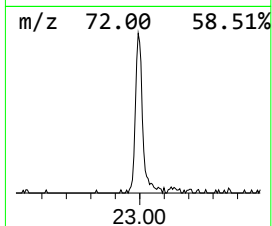
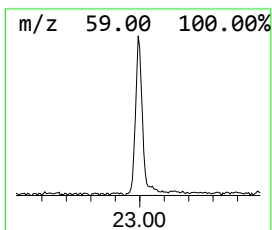
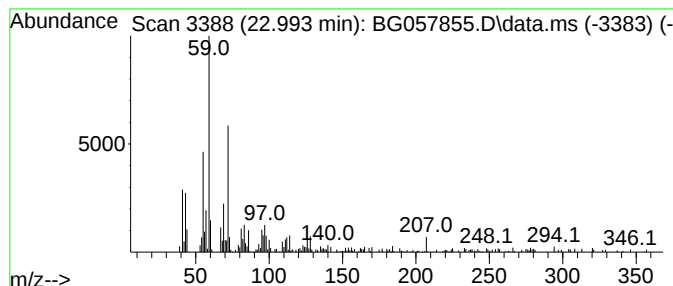
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.993	5.50 ng	202345	Chrysene-d12	21.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2			Hexadecanamide	255	C16H33NO	000629-54-9	72
3			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	64
4			Decanamide-	171	C10H21NO	002319-29-1	53
5			Tetradecanamide	227	C14H29NO	000638-58-4	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057855.D
Acq On : 24 Jun 2023 00:08
Operator : CG/JU
Sample : 03336-04
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-5

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	3.6	ng	50472	1	7.923	282167	20.0
Benzophenone	15.908	5.0	ng	136999	3	14.556	551208	20.0
n-Hexadecanoic ...	18.187	6.5	ng	220869	4	17.300	680353	20.0
Heptadecyl hept...	21.201	4.7	ng	171968	5	21.554	735477	20.0
9-Octadecenamid...	22.993	5.5	ng	202345	5	21.554	735477	20.0