

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
 Data File : BG057853.D
 Acq On : 23 Jun 2023 22:42
 Operator : CG/JU
 Sample : 03337-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-17

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: BG057853.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	324	330	339	rBV	53382	77474	3.32%	0.599%
2	5.491	402	409	418	rBV	690182	1091541	46.73%	8.444%
3	7.083	672	680	689	rBV	720676	1209455	51.78%	9.356%
4	7.917	816	822	831	rVB	154176	263314	11.27%	2.037%
5	9.081	1011	1020	1028	rBV	398387	685954	29.37%	5.306%
6	10.720	1292	1299	1307	rBV	226162	392356	16.80%	3.035%
7	13.176	1710	1717	1724	rBV	993279	1554096	66.54%	12.022%
8	14.551	1943	1951	1961	rVB	348391	558593	23.92%	4.321%
9	15.908	2176	2182	2189	rBV	91257	126424	5.41%	0.978%
10	16.037	2197	2204	2211	rBV	926258	1408518	60.31%	10.896%
11	17.295	2411	2418	2427	rBV	474969	709319	30.37%	5.487%
12	18.188	2564	2570	2579	rBV	205385	308900	13.23%	2.389%
13	19.457	2783	2786	2794	rBV2	57267	89819	3.85%	0.695%
14	19.915	2858	2864	2870	rVB	1777460	2335625	100.00%	18.067%
15	20.221	2913	2916	2921	rVB	26702	27391	1.17%	0.212%
16	20.714	2996	3000	3004	rBV2	33697	40490	1.73%	0.313%
17	21.202	3078	3083	3093	rBV	205536	318846	13.65%	2.466%
18	21.548	3136	3142	3153	rVB2	451562	733155	31.39%	5.671%
19	21.742	3173	3175	3180	rVB2	42467	48661	2.08%	0.376%
20	22.342	3273	3277	3283	rBV4	38290	72700	3.11%	0.562%
21	24.698	3670	3678	3693	rVB	292735	874824	37.46%	6.767%

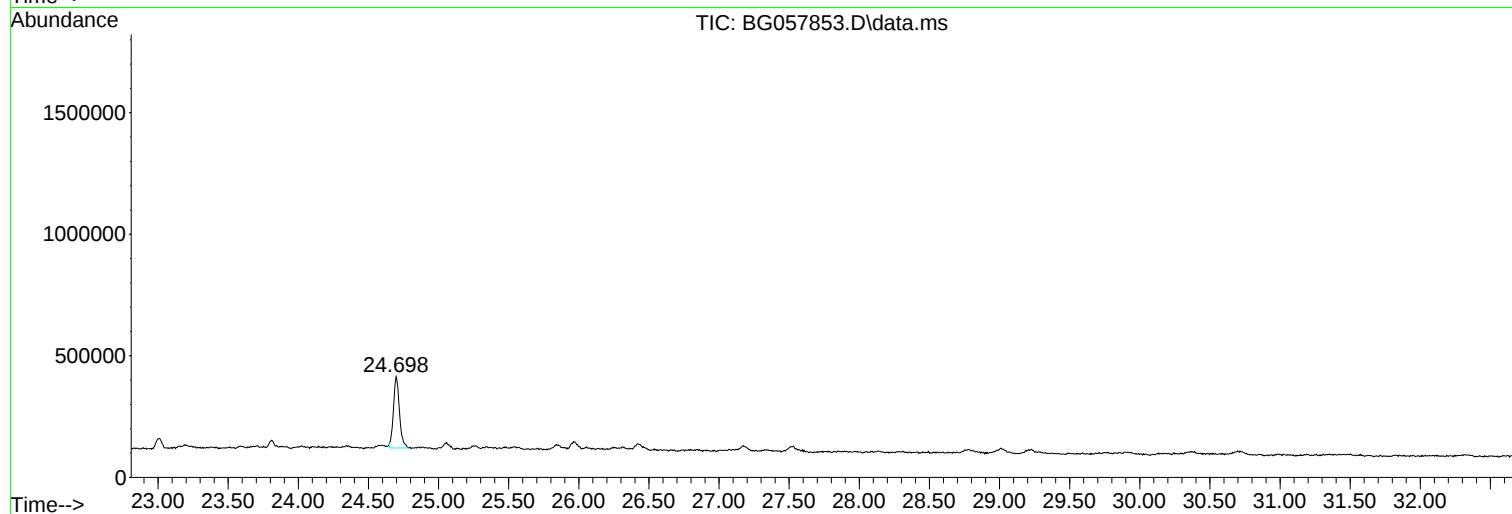
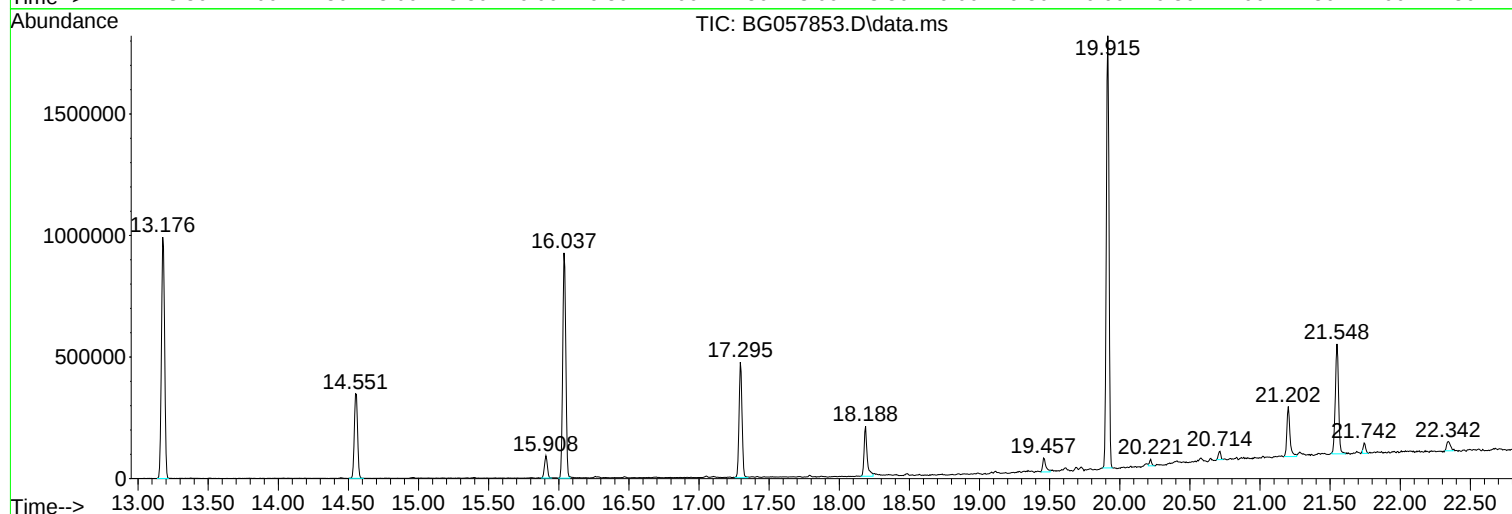
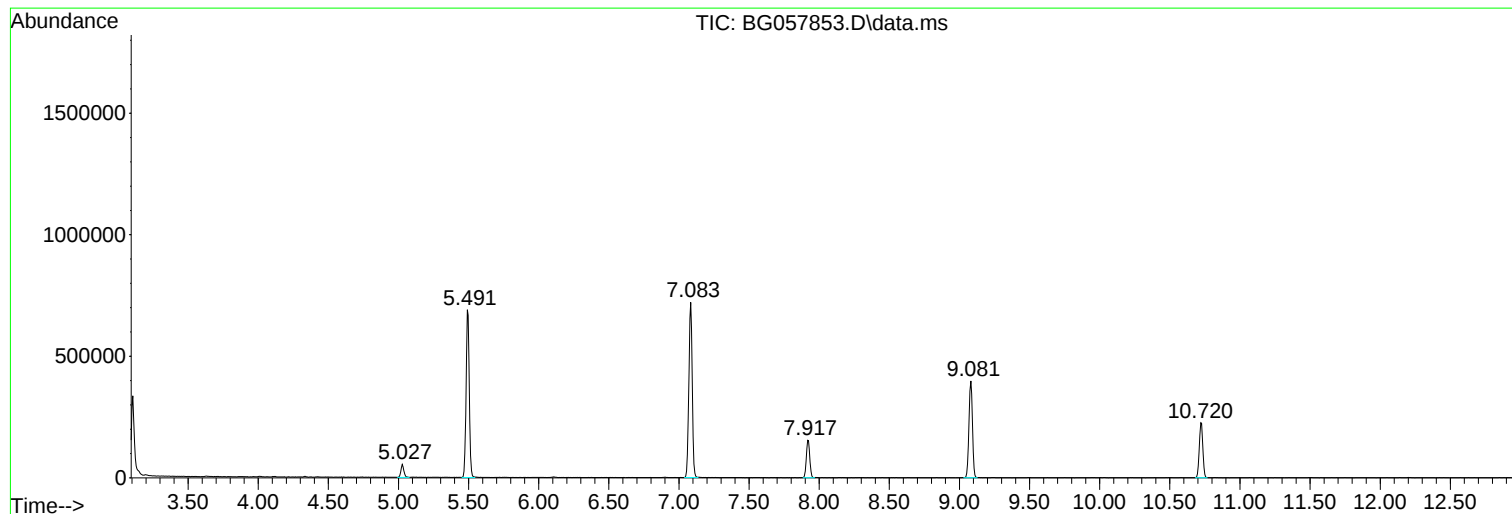
Sum of corrected areas: 12927455

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057853.D
Acq On : 23 Jun 2023 22:42
Operator : CG/JU
Sample : 03337-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-17

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 : BG057853.D
Acq On : 23 Jun 2023 22:42
Operator : CG/JU
Sample : 03337-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-17

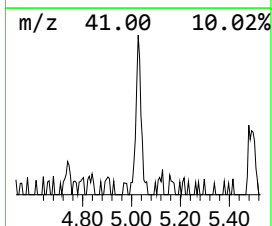
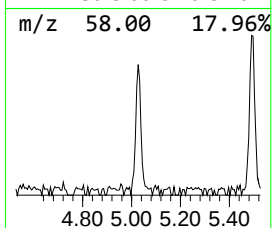
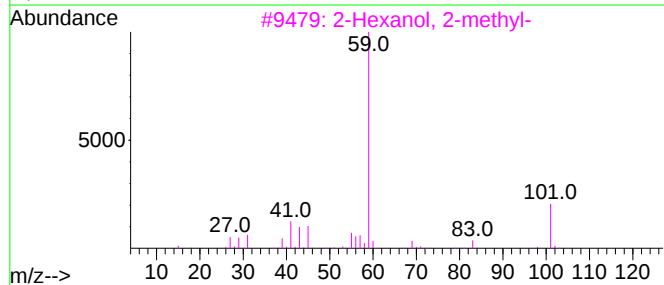
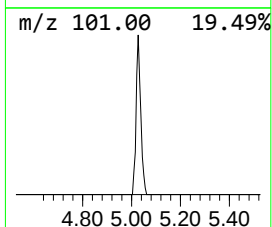
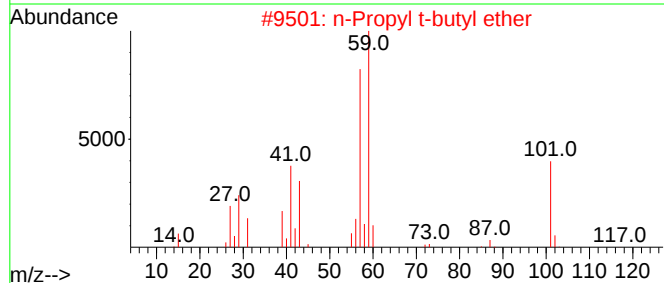
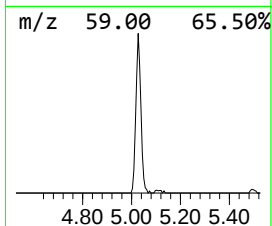
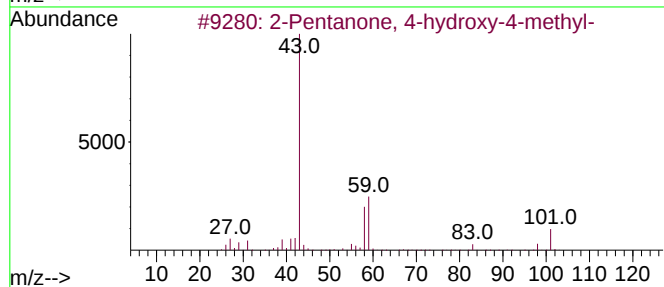
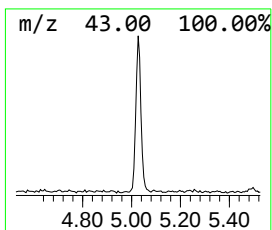
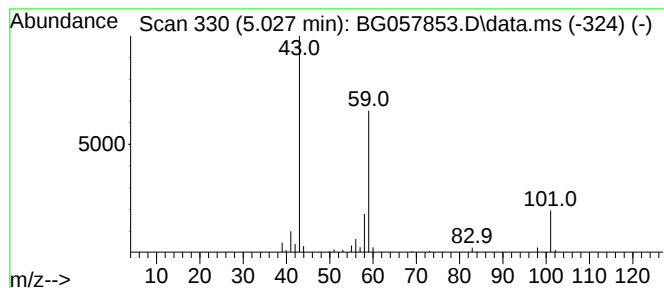
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.027	5.88 ng	77474	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	45	
2	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	36	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
4	3-Hexanol	102	C6H14O	000623-37-0	28	
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057853.D
Acq On : 23 Jun 2023 22:42
Operator : CG/JU
Sample : 03337-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-17

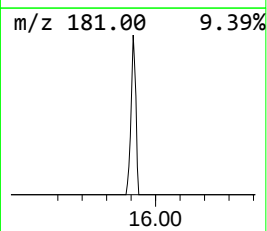
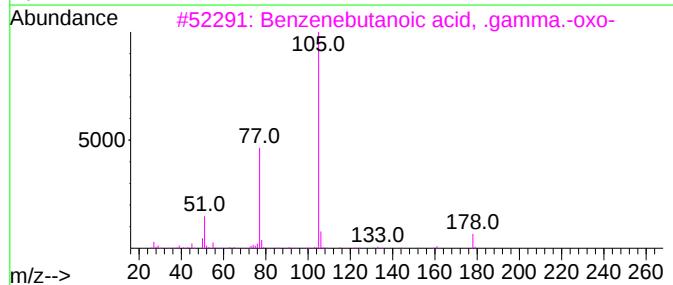
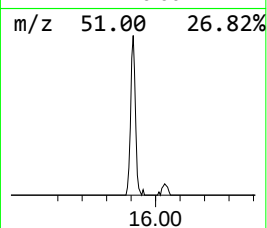
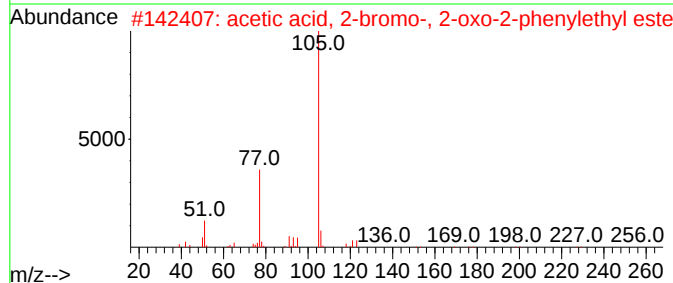
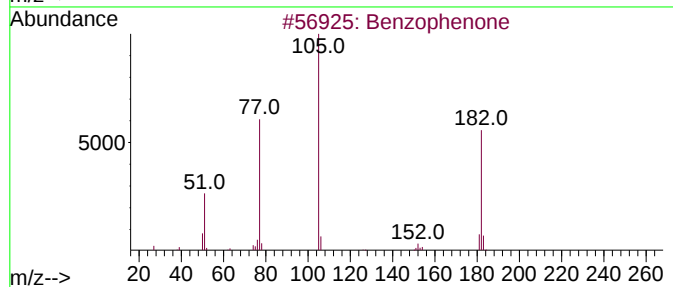
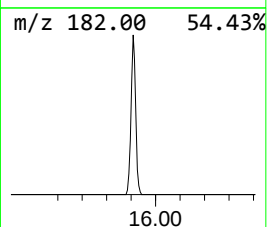
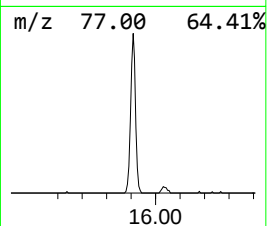
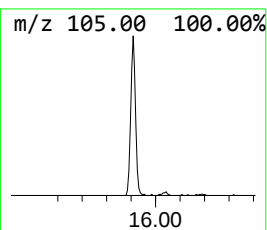
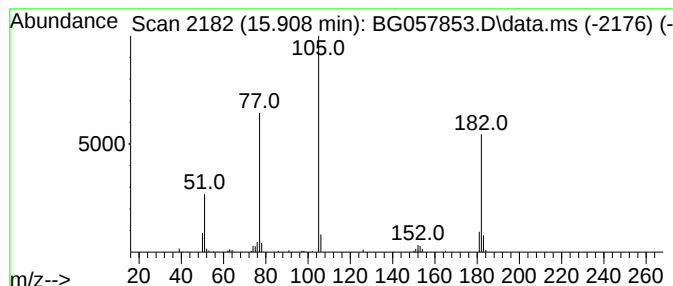
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.908	4.53 ng	126424	Acenaphthene-d10	14.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47
3			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057853.D
Acq On : 23 Jun 2023 22:42
Operator : CG/JU
Sample : 03337-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-17

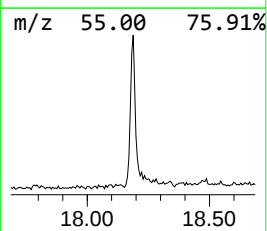
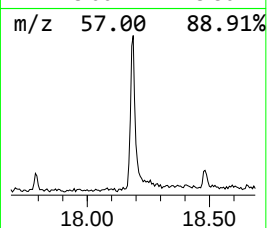
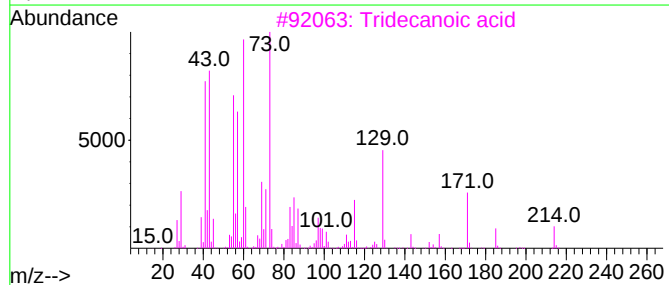
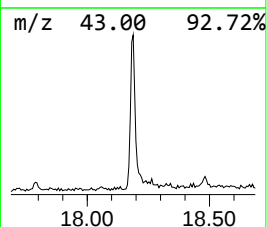
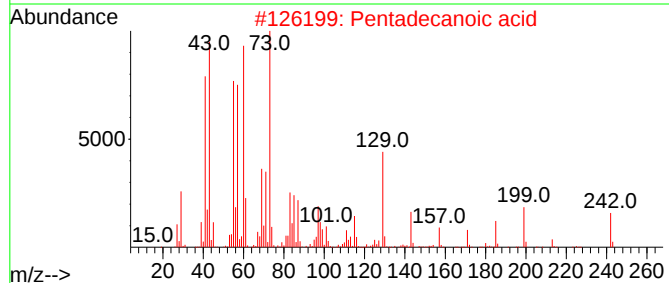
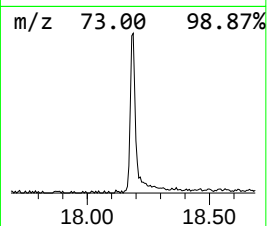
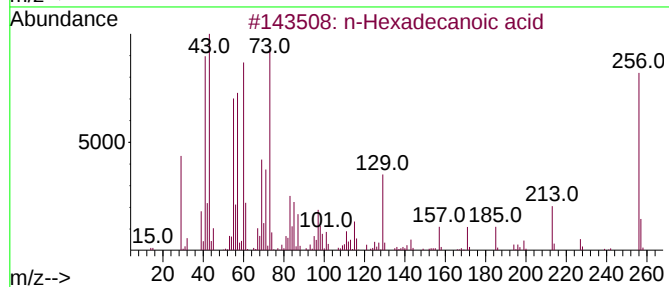
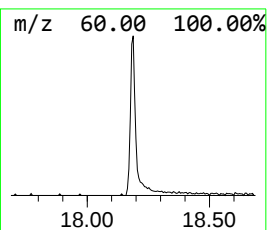
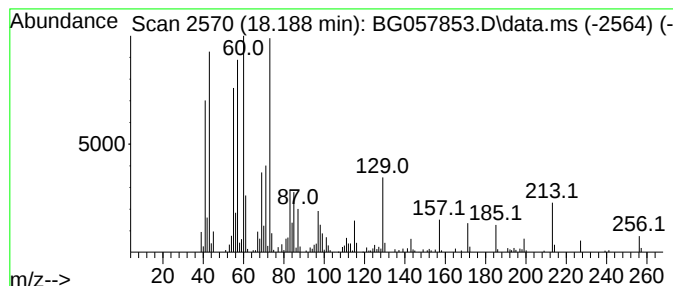
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.188	8.71 ng	308900	Phenanthrene-d10	17.295

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057853.D
Acq On : 23 Jun 2023 22:42
Operator : CG/JU
Sample : 03337-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-17

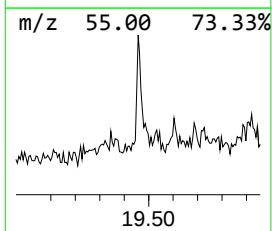
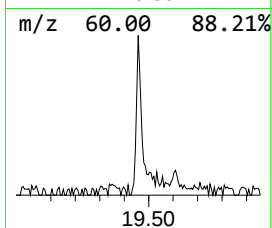
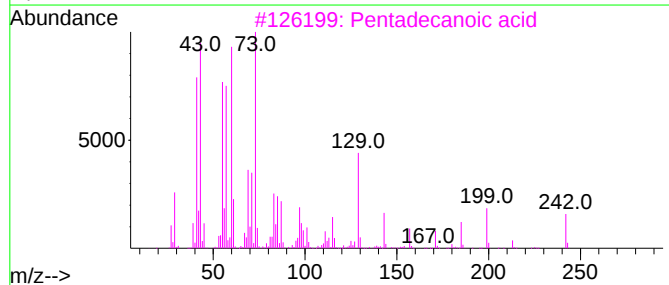
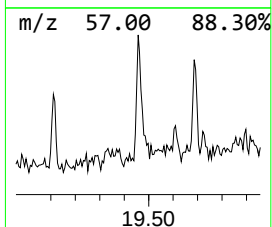
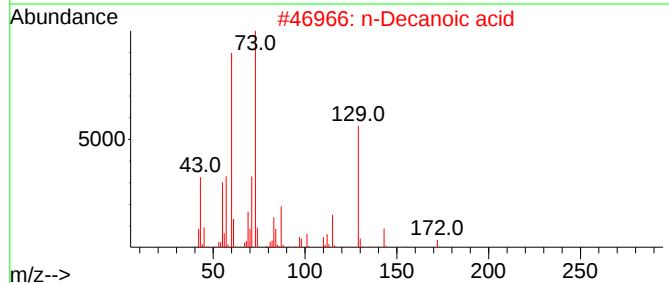
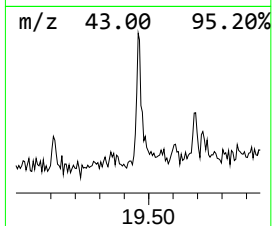
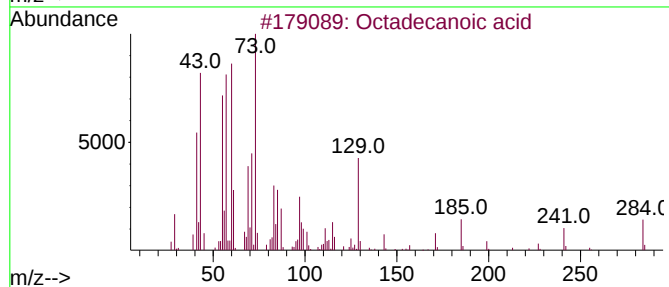
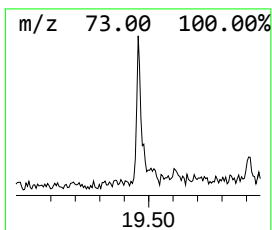
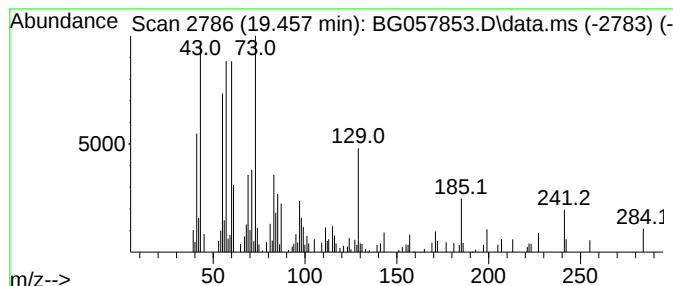
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.457	2.45 ng	89819	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	96
2			n-Decanoic acid	172	C10H20O2	000334-48-5	92
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057853.D
Acq On : 23 Jun 2023 22:42
Operator : CG/JU
Sample : 03337-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-17

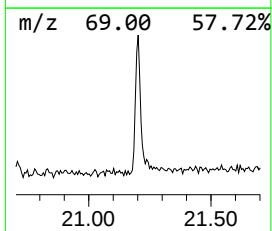
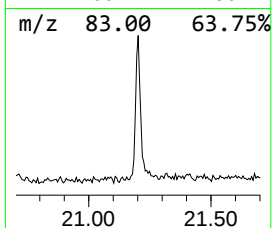
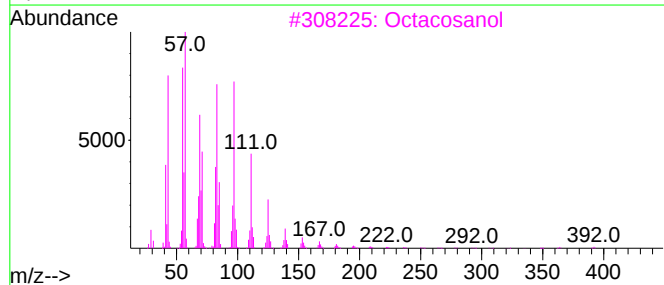
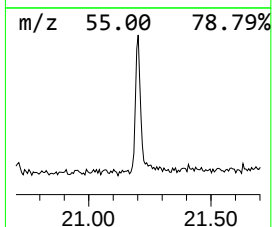
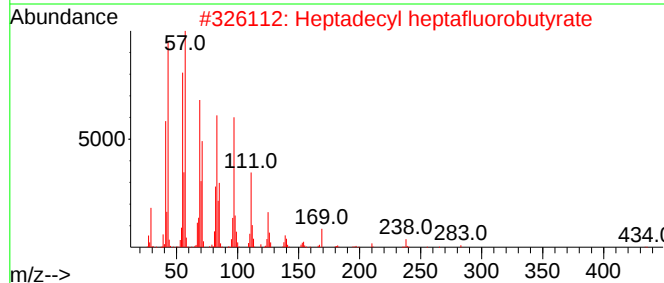
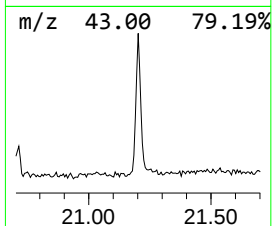
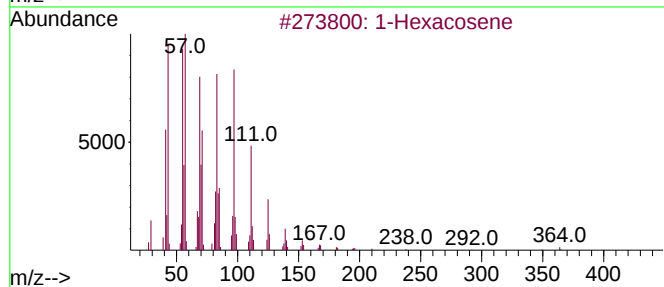
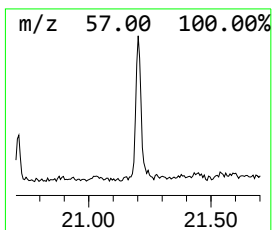
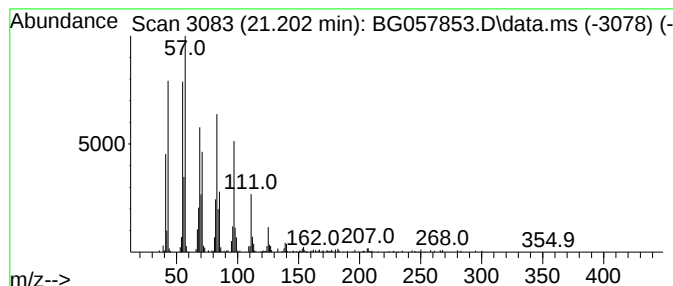
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.202	8.70 ng	318846	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	94
2	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	94
3	Octacosanol			410	C28H58O	000557-61-9	91
4	1-Hexadecanesulfonyl chloride			324	C16H33ClO2S	038775-38-1	91
5	Pentafluoropropionic acid, hepta...			402	C20H35F5O2	959218-78-1	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
Data File : BG057853.D
Acq On : 23 Jun 2023 22:42
Operator : CG/JU
Sample : 03337-04
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-17

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	77474	1	7.923	263314	20.0
Benzophenone	15.908	4.5	ng	126424	3	14.557	558593	20.0
n-Hexadecanoic ...	18.188	8.7	ng	308900	4	17.295	709319	20.0
Octadecanoic acid	19.457	2.5	ng	89819	5	21.549	733155	20.0
1-Hexacosene	21.202	8.7	ng	318846	5	21.549	733155	20.0