

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
 Data File : BG059764.D
 Acq On : 18 Nov 2023 14:32
 Operator : MA/JU
 Sample : 05385-01 5X
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 HR-02-11102023

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-BG111623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059764.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.833	410	416	424	rVB	122031	192344	4.71%	1.525%
2	7.460	686	693	702	rBV	137950	248294	6.08%	1.968%
3	8.347	835	844	850	rBV	138236	255221	6.25%	2.023%
4	9.540	1041	1047	1054	rVB2	98815	178047	4.36%	1.412%
5	11.191	1321	1328	1335	rVB	191756	359465	8.81%	2.850%
6	13.048	1638	1644	1648	rBV8	23094	42076	1.03%	0.334%
7	13.594	1731	1737	1745	rVB2	414870	647469	15.87%	5.133%
8	13.712	1753	1757	1764	rVB9	25360	49906	1.22%	0.396%
9	13.794	1766	1771	1777	rVB7	37127	64704	1.59%	0.513%
10	14.781	1933	1939	1944	rBV10	35188	56490	1.38%	0.448%
11	14.969	1963	1971	1978	rBV	394680	623107	15.27%	4.940%
12	15.727	2094	2100	2105	rBV7	44645	75165	1.84%	0.596%
13	16.121	2161	2167	2175	rBV7	29975	69929	1.71%	0.554%
14	16.456	2215	2224	2229	rBV2	281138	477256	11.70%	3.784%
15	16.591	2241	2247	2252	rBV6	53657	101382	2.48%	0.804%
16	17.378	2378	2381	2386	rVB6	37507	56800	1.39%	0.450%
17	17.725	2435	2440	2450	rVB	451929	701482	17.19%	5.561%
18	18.118	2505	2507	2512	rVB6	36450	43732	1.07%	0.347%
19	18.312	2535	2540	2546	rBV	460518	571261	14.00%	4.529%
20	18.536	2574	2578	2584	rVB7	72802	97971	2.40%	0.777%
21	19.446	2728	2733	2736	rBV	3332288	4080620	100.00%	32.351%
22	19.476	2736	2738	2747	rVB3	1476754	1931431	47.33%	15.312%
23	19.599	2755	2759	2763	rVB2	237621	274572	6.73%	2.177%
24	19.658	2766	2769	2772	rBV4	100490	146272	3.58%	1.160%
25	20.298	2873	2878	2883	rVB	545279	750939	18.40%	5.953%
26	22.055	3172	3177	3182	rVB2	304417	517701	12.69%	4.104%

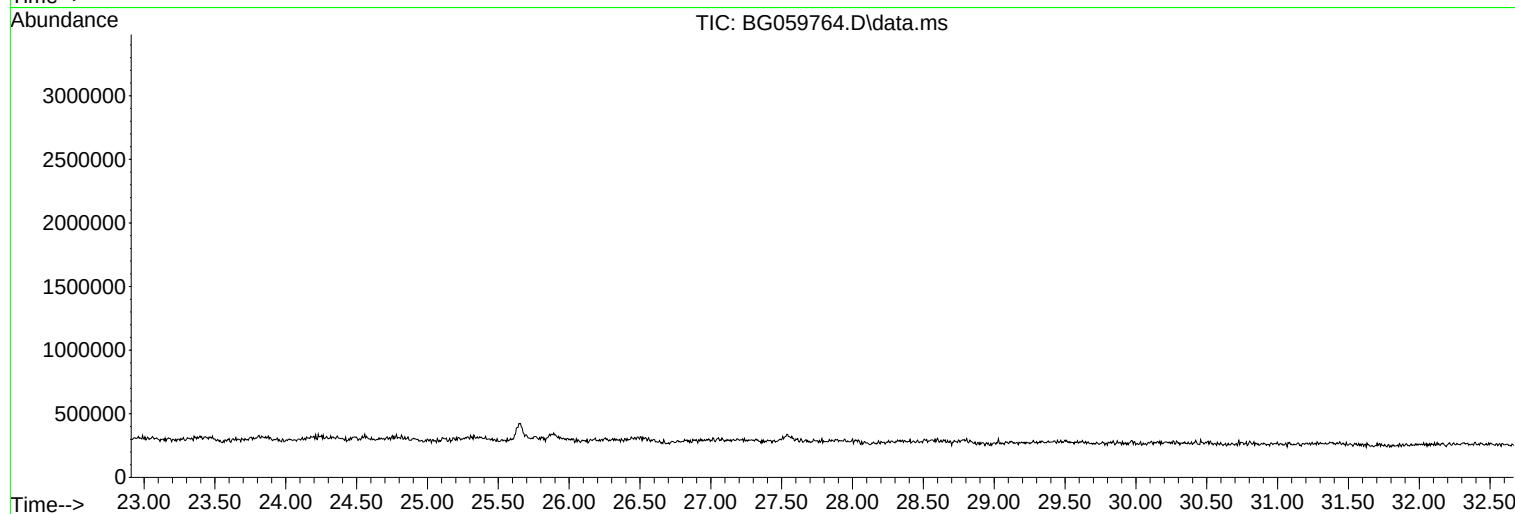
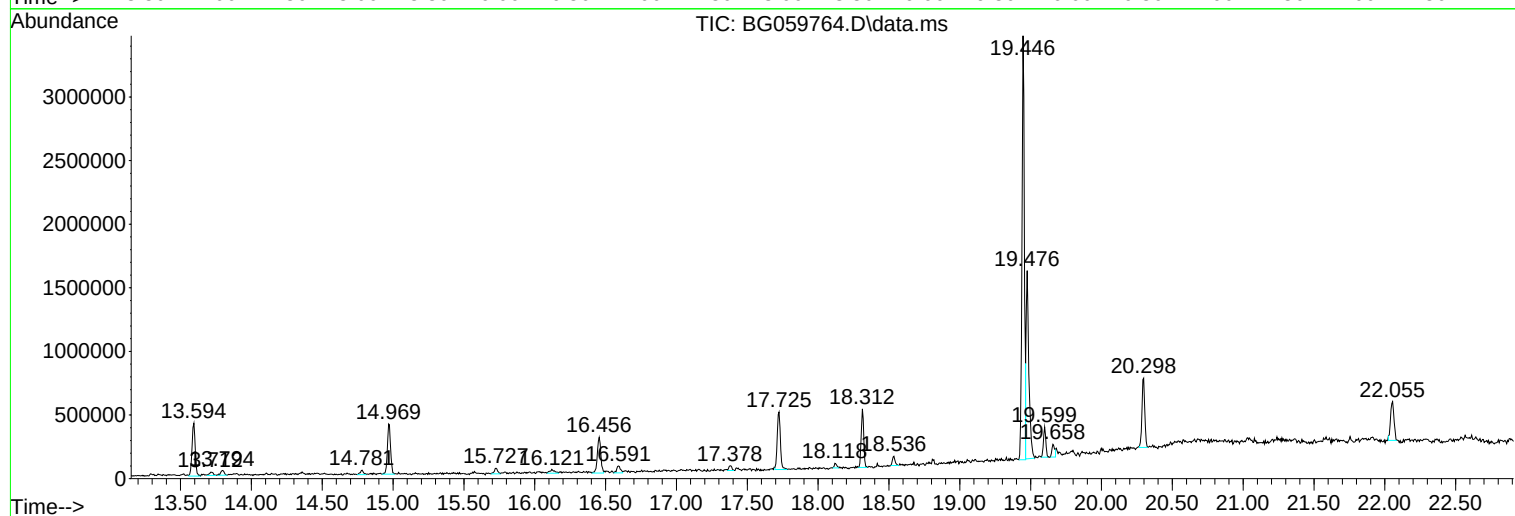
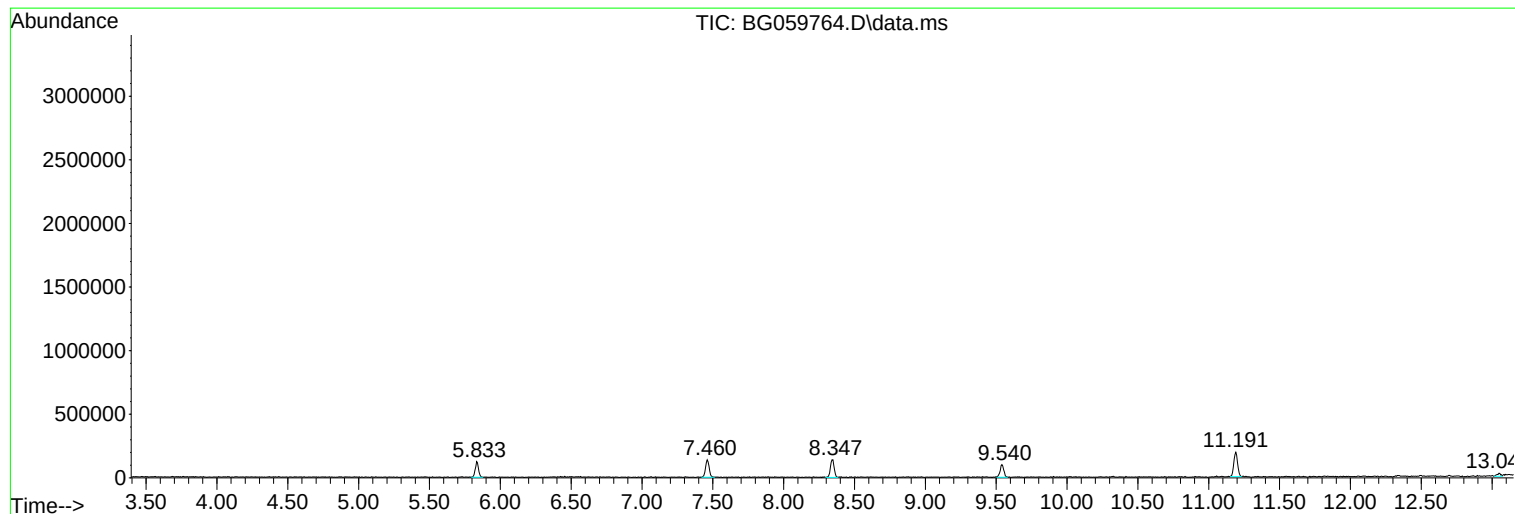
Sum of corrected areas: 12613636

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

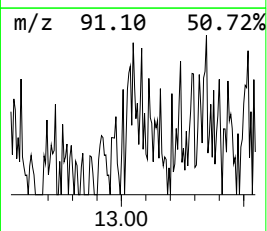
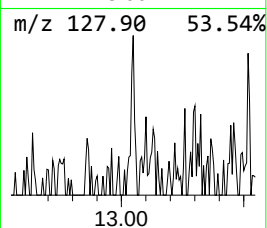
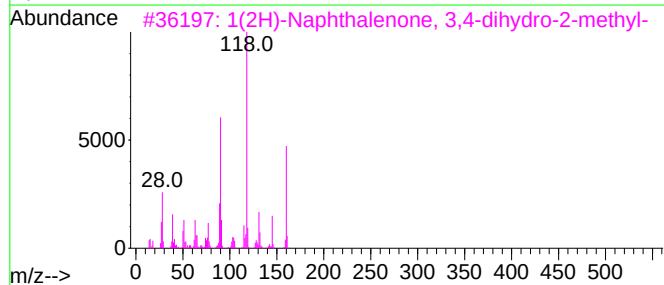
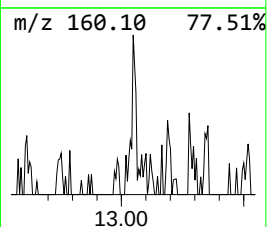
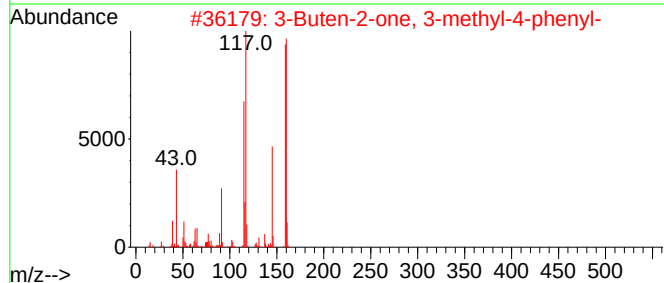
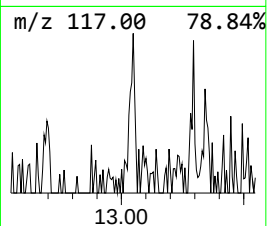
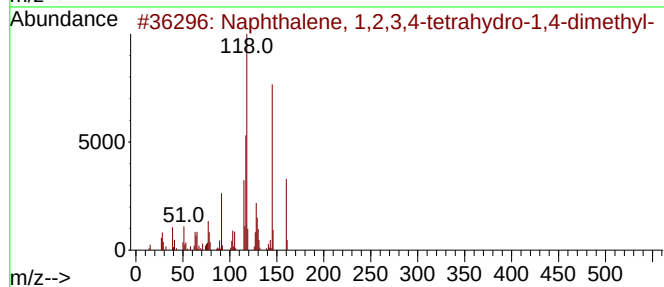
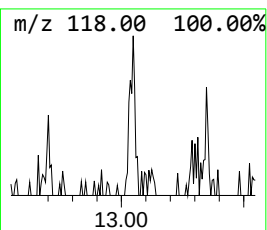
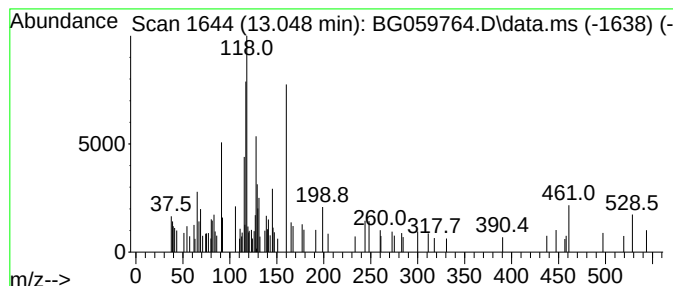
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Naphthalene, 1,2,3,4-tetra... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.048	2.34 ng	42076	Naphthalene-d8	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,2,3,4-tetrahydro-...	160	C12H16	004175-54-6	52
2			3-Buten-2-one, 3-methyl-4-phenyl-	160	C11H12O	001901-26-4	38
3			1(2H)-Naphthalenone, 3,4-dihydro...	160	C11H12O	001590-08-5	38
4			1-Methyl-2-tetralone	160	C11H12O	004024-14-0	30
5			Propanoic acid, 2-methyl-, 3-phe...	206	C13H18O2	000103-58-2	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

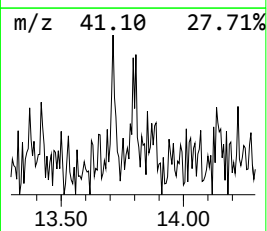
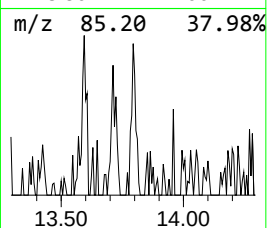
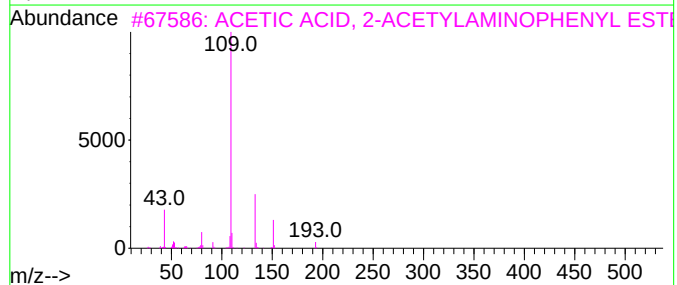
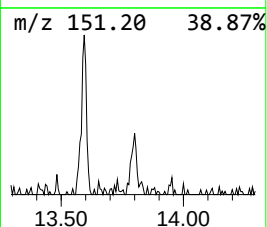
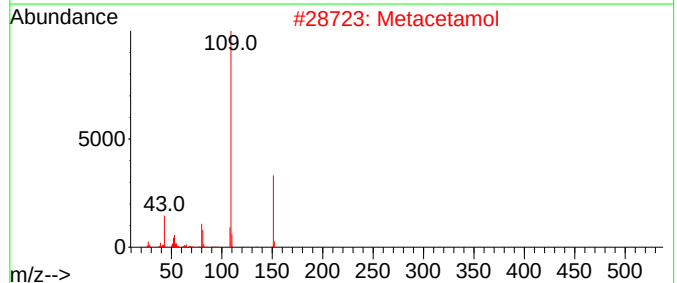
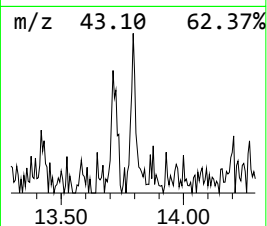
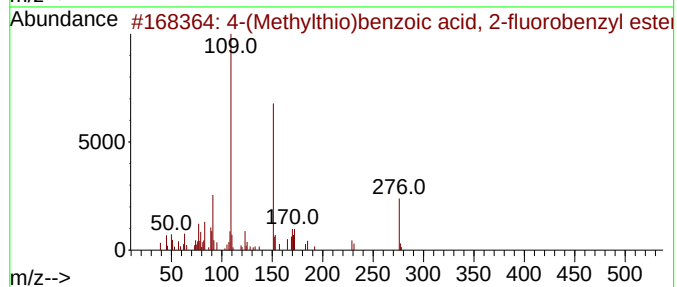
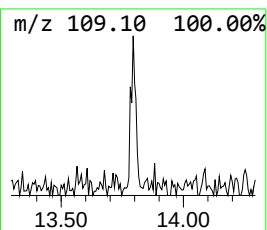
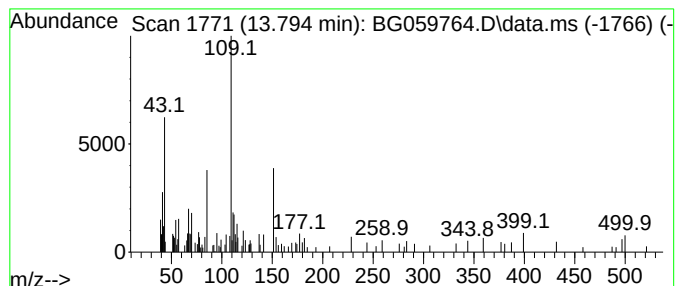
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 4-(Methylthio)benzoic acid,... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.794	2.08 ng	64704	Acenaphthene-d10	14.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(Methylthio)benzoic acid, 2-fl...	276	C15H13FO2S	1000375-06-4	53
2			Metacetamol	151	C8H9NO2	000621-42-1	42
3			ACETIC ACID, 2-ACETYLAMINOPHENYL...	193	C10H11NO3	005467-64-1	38
4			2,3-Pyridinediamine	109	C5H7N3	000452-58-4	38
5			2-Amino-4-methylpyrimidine	109	C5H7N3	000108-52-1	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

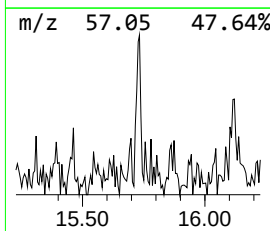
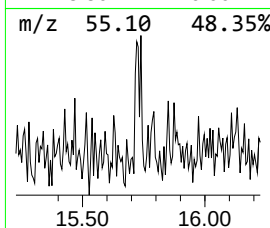
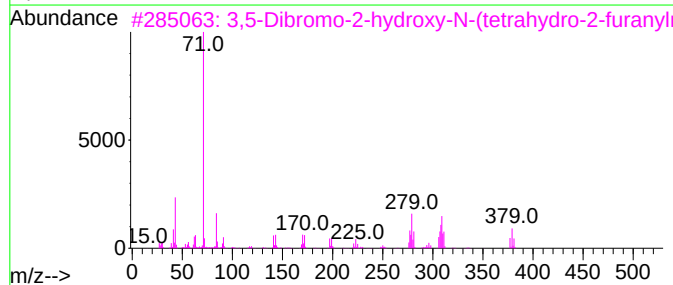
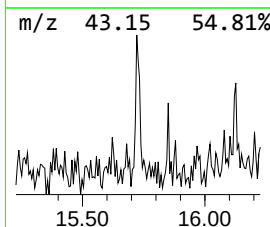
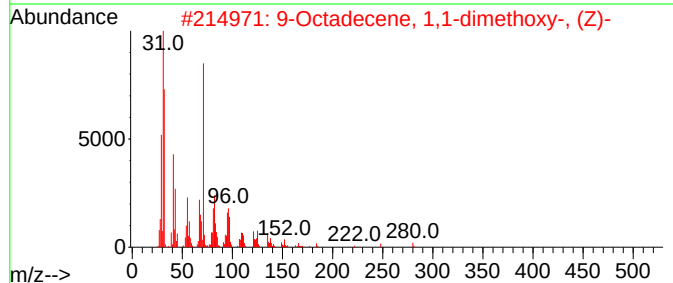
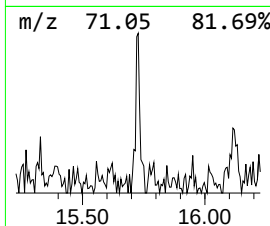
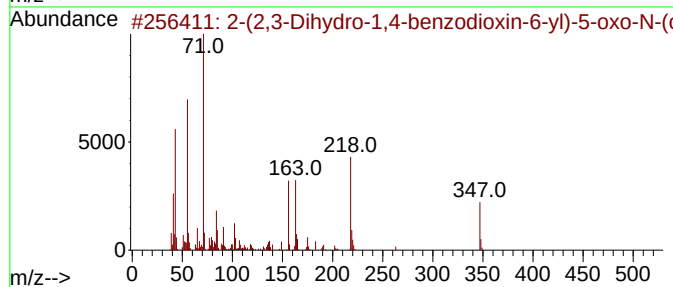
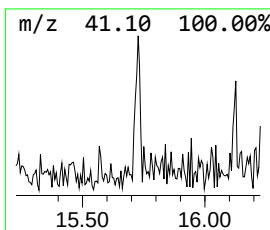
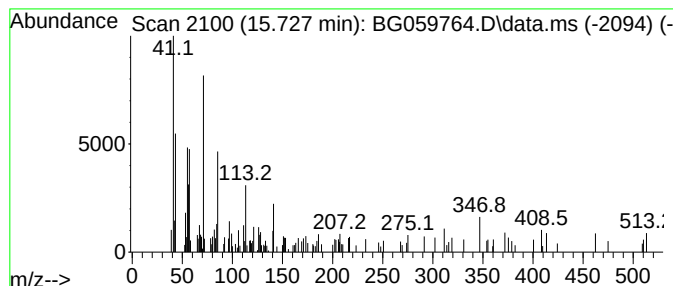
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown15.727 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.727	2.41 ng	75165	Acenaphthene-d10	14.975

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2,3-Dihydro-1,4-benzodioxin-6-yl)-5-oxo-N-(4-aminophenyl)-2H-benzofuran-3-carboxamide	347	C18H21NO6	1000387-38-3	43		
2	9-Octadecene, 1,1-dimethoxy-, (Z)-	312	C20H40O2	015677-71-1	17		
3	3,5-Dibromo-2-hydroxy-N-(tetrahydro-2-furanyl)acetamide	377	C12H13Br2NO3	015686-77-8	9		
4	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	9		
5	2-Furanmethanamine, tetrahydro-	101	C5H11NO	004795-29-3	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

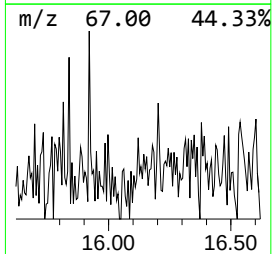
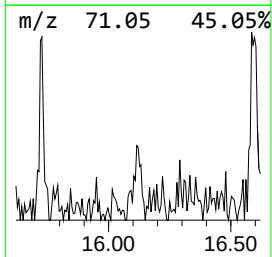
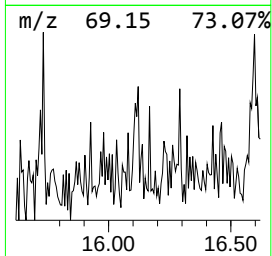
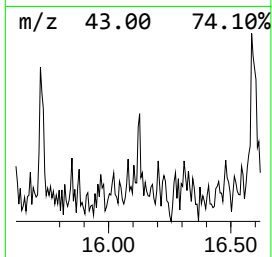
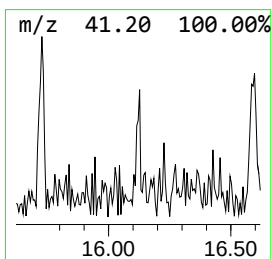
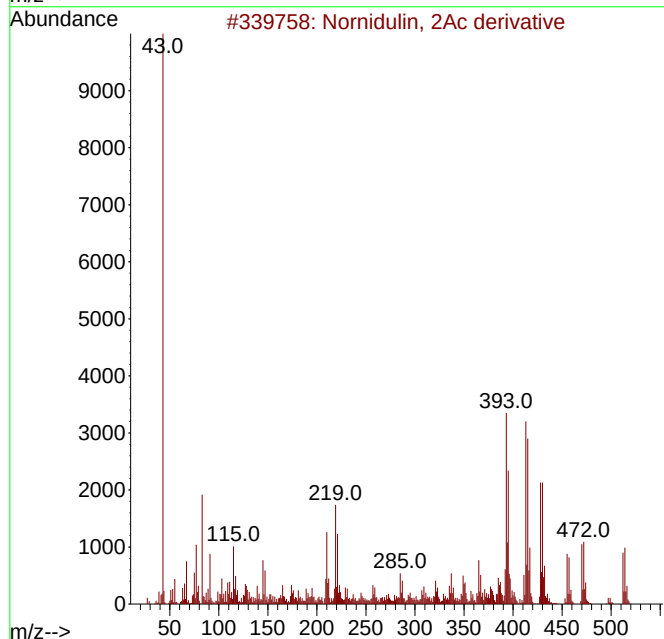
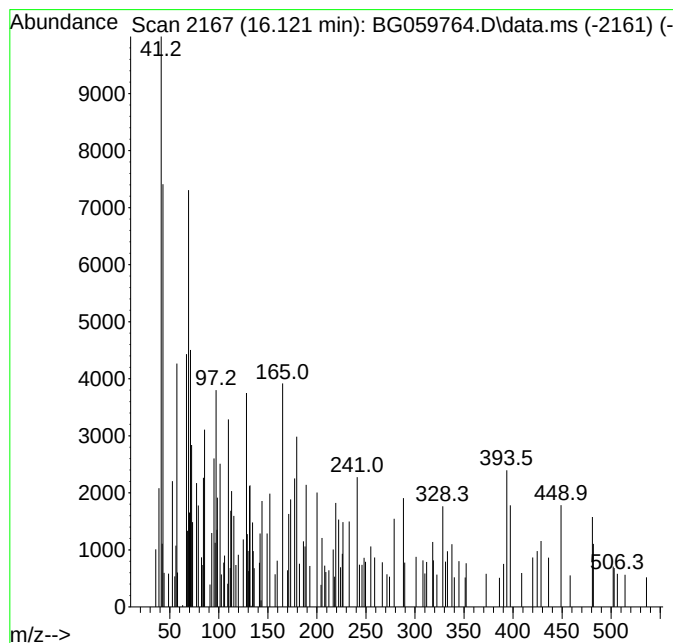
Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown16.121 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.121	2.24 ng	69929	Acenaphthene-d10	14.975
Hit# of	1	Tentative ID	MW MolForm	CAS# Qual
1	Norridulin, 2Ac derivative	512	C23H19Cl3O7	1000480-54-4 10



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

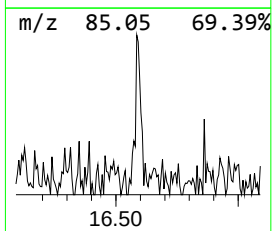
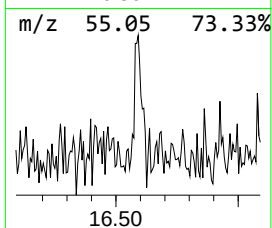
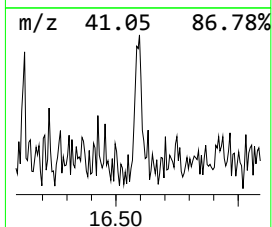
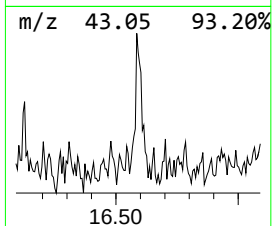
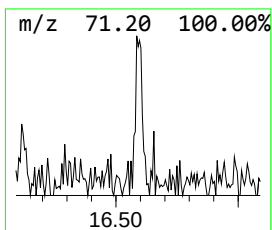
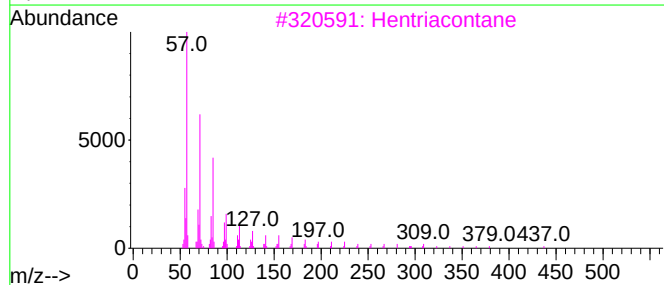
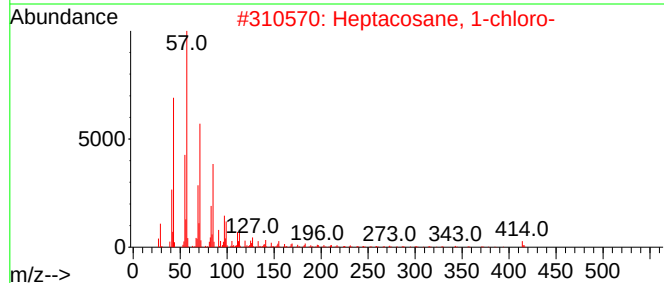
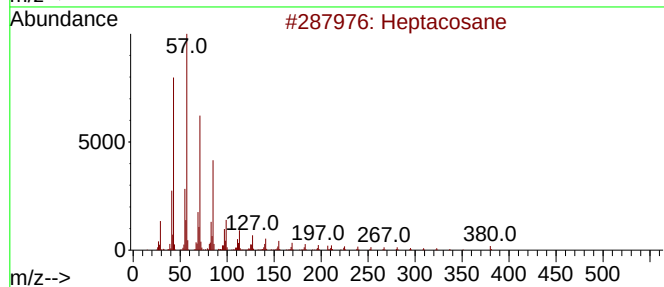
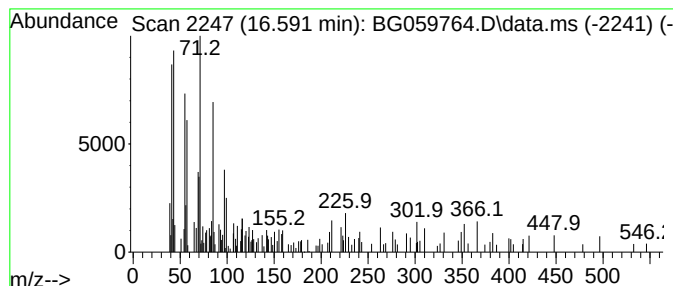
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.591	2.89 ng	101382	Phenanthrene-d10	17.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	64
2			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	62
3			Hentriacontane	437	C31H64	000630-04-6	50
4			Hexacosane	366	C26H54	000630-01-3	49
5			Heptadecane	240	C17H36	000629-78-7	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

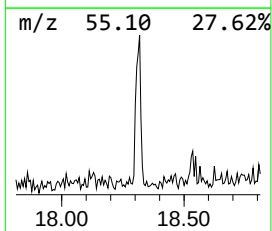
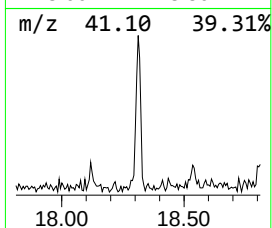
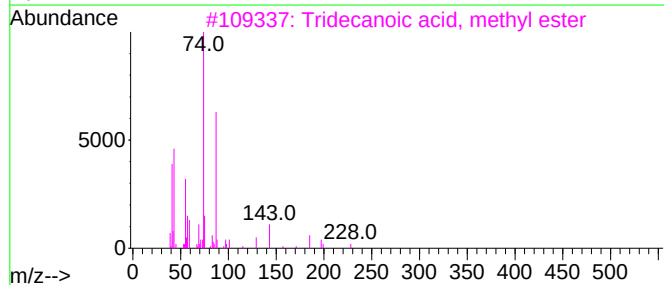
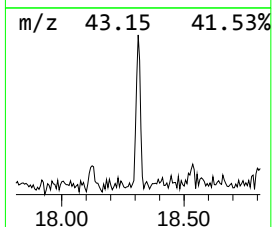
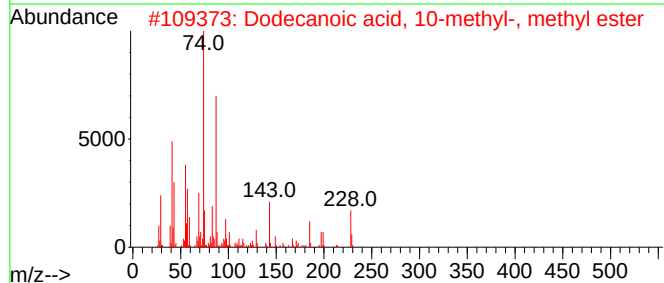
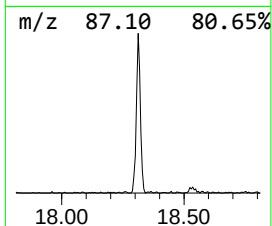
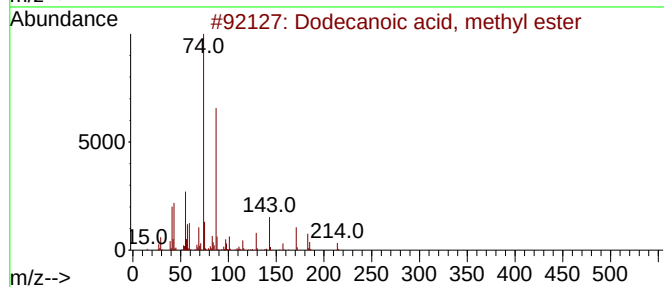
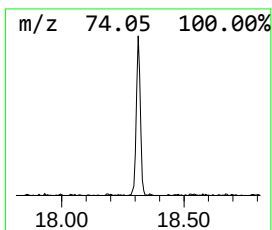
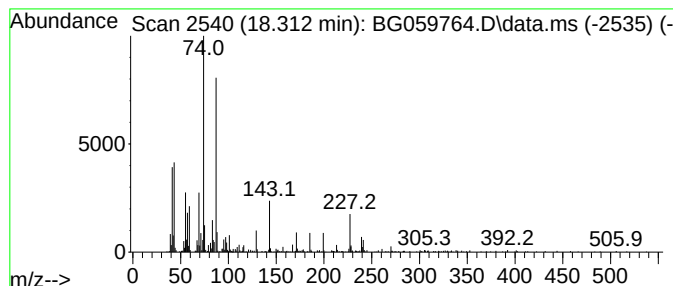
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dodecanoic acid, methyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.312	16.29 ng	571261	Phenanthrene-d10	17.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	93
2			Dodecanoic acid, 10-methyl-, met...	228	C14H28O2	005129-65-7	91
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	83
4			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	81
5			Methyl tetradecanoate	242	C15H30O2	000124-10-7	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

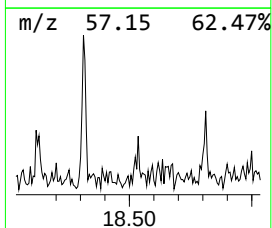
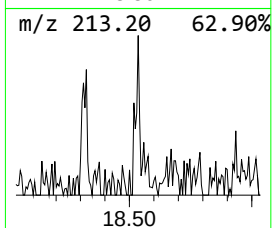
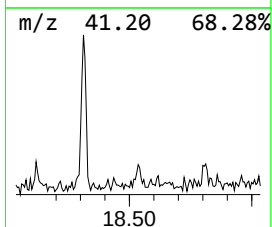
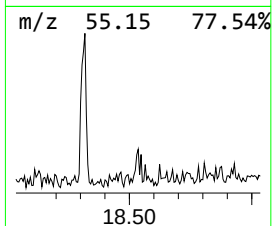
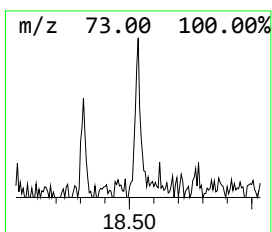
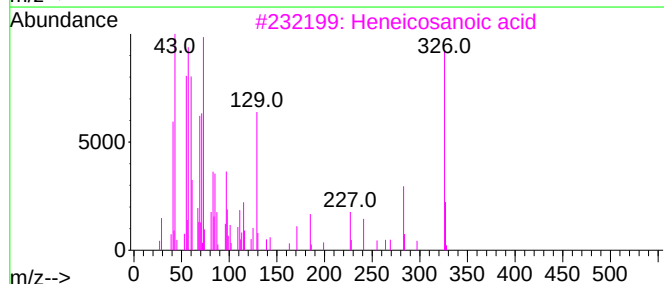
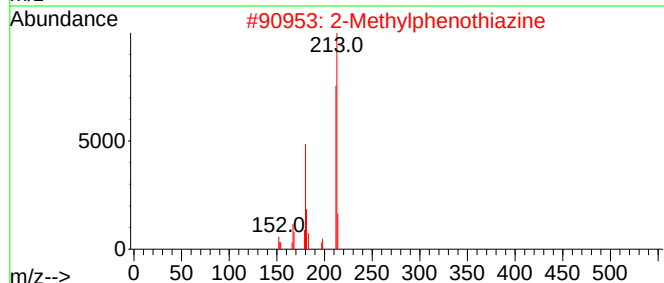
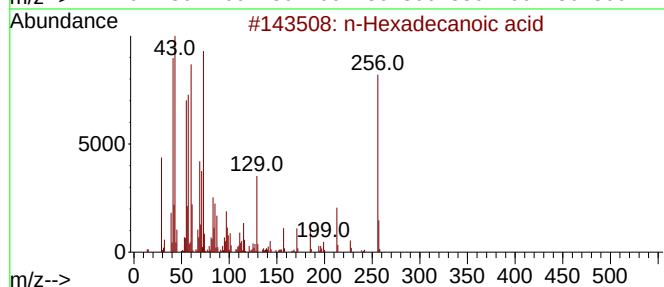
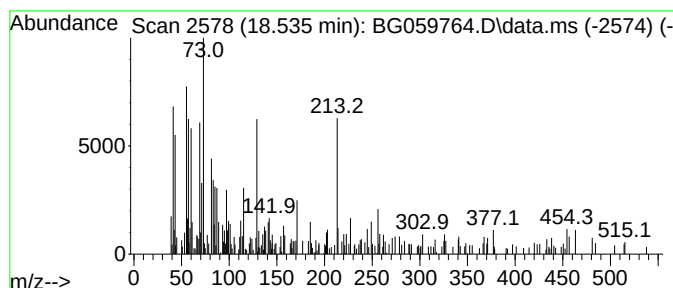
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.535	2.79 ng	97971	Phenanthrene-d10	17.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
2			2-Methylphenothiazine	213	C13H11NS	005828-51-3	38
3			Heneicosanoic acid	326	C21H42O2	002363-71-5	38
4			Pyrido[3,4-c]coumarine, 3,4-dihy...	213	C12H7NO3	040547-98-6	11
5			1-Methyl-3-(pyrazol-1-yl)-3H-ind...	213	C12H11N3O	1000388-50-6	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

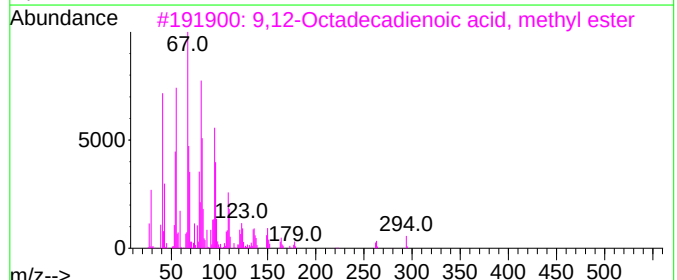
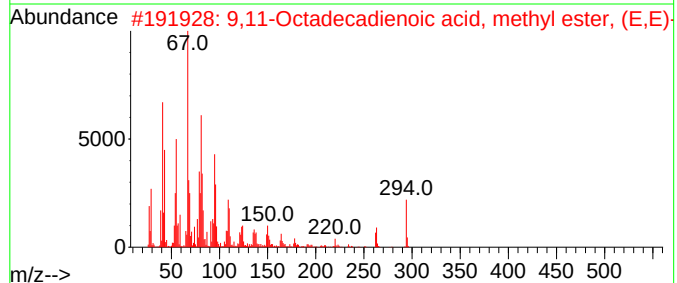
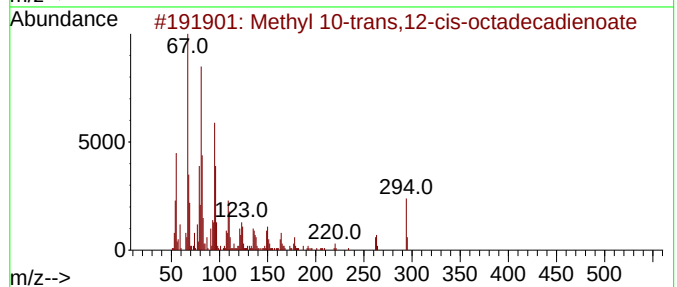
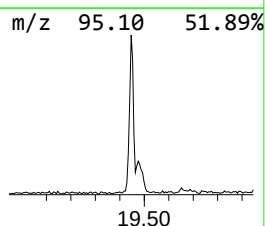
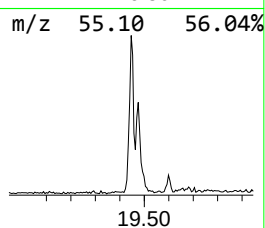
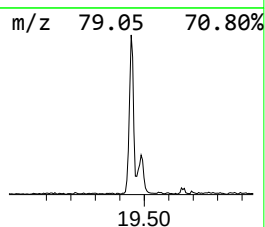
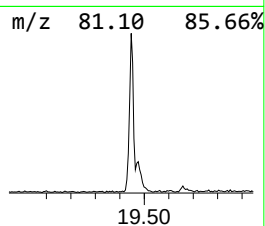
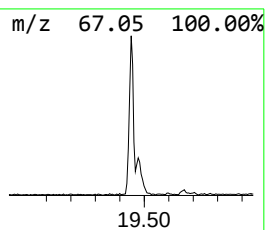
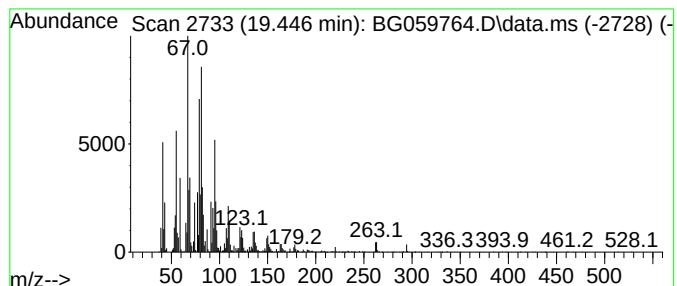
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Methyl 10-trans,12-cis-octa... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.446	116.34 ng	4080620	Phenanthrene-d10	17.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 10-trans,12-cis-octadecad...	294	C19H34O2	1000336-44-2	89
2			9,11-Octadecadienoic acid, methy...	294	C19H34O2	013038-47-6	86
3			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	84
4			Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	013058-52-1	80
5			9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

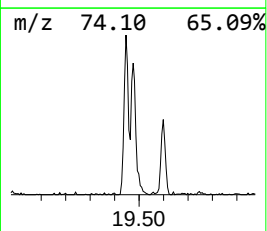
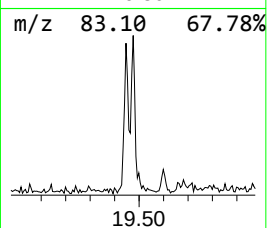
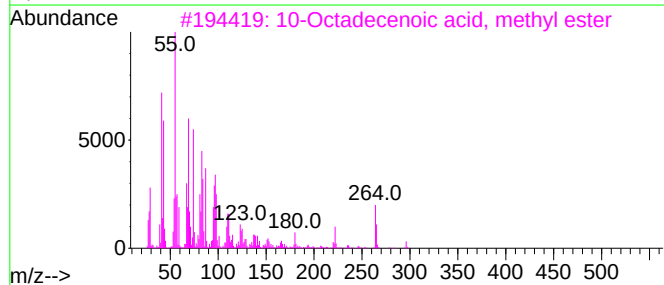
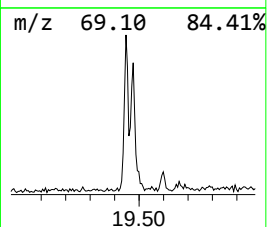
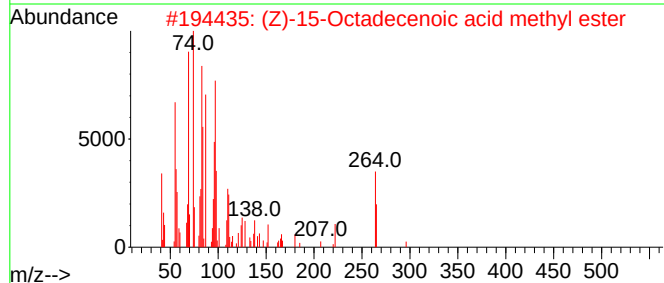
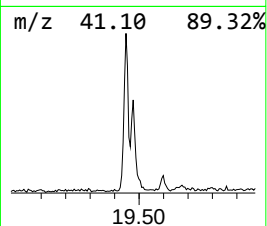
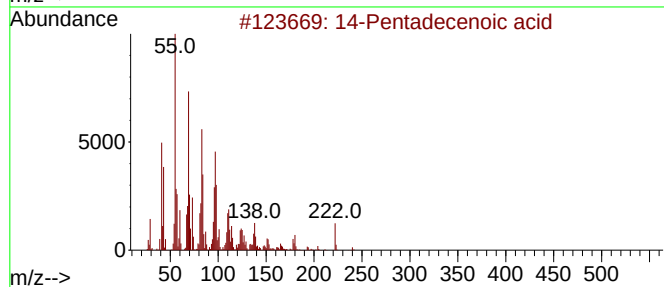
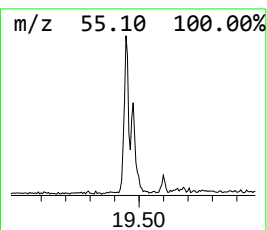
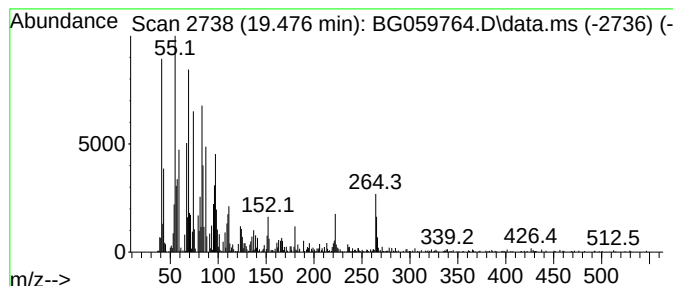
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 14-Pentadecenoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.476	55.07 ng	1931430	Phenanthrene-d10	17.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			14-Pentadecenoic acid	240	C15H28O2	017351-34-7	78
2			(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	72
3			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	60
4			cis-9-Octadecenoic acid, propyl ...	324	C21H40O2	1000405-15-0	58
5			1-cis-Vaccenoylglycerol	356	C21H40O4	020379-67-3	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

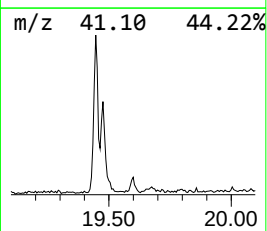
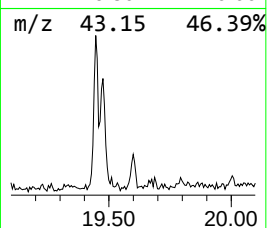
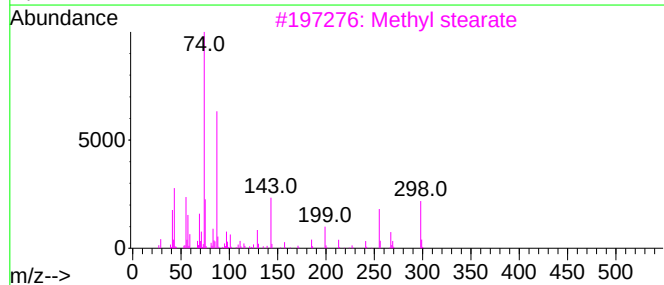
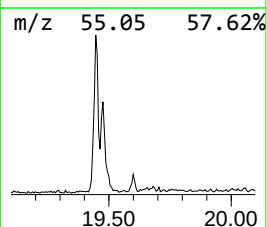
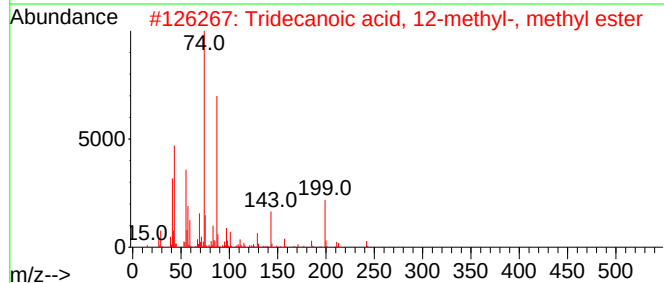
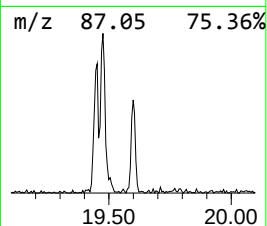
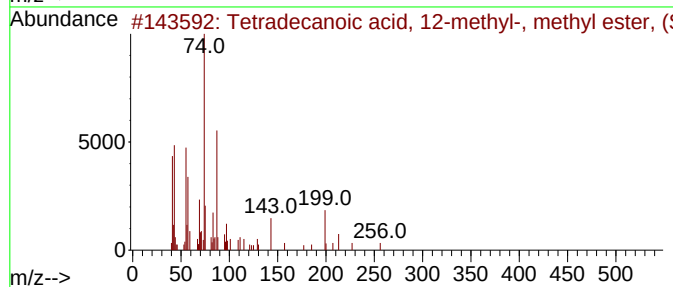
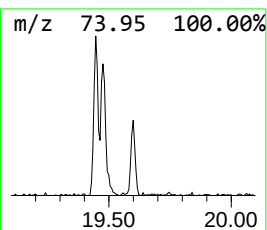
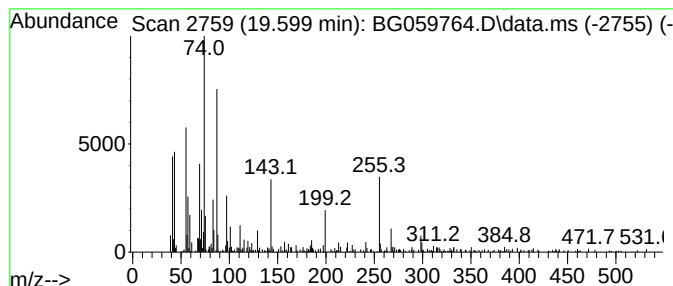
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Tetradecanoic acid, 12-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.599	7.83 ng	274572	Phenanthrene-d10	17.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid, 12-methyl-, ...	256	C16H32O2	062691-05-8	74
2			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	74
3			Methyl stearate	298	C19H38O2	000112-61-8	72
4			Methyl 8,10-dimethyl-hexadecanoa...	298	C19H38O2	1000336-39-7	70
5			Octacosanoic acid, methyl ester	438	C29H58O2	055682-92-3	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

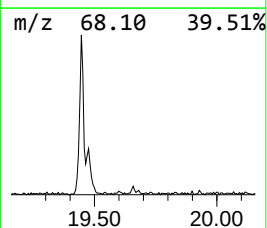
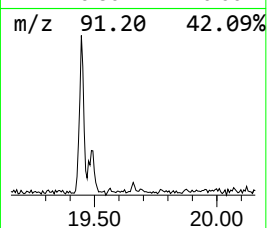
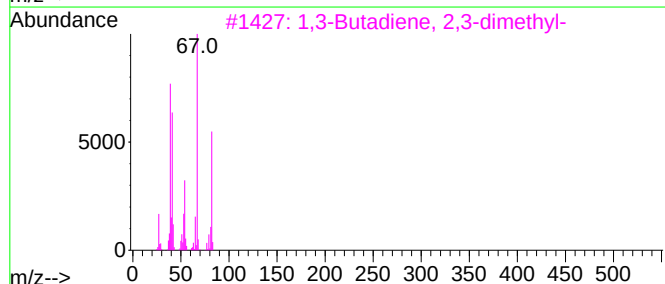
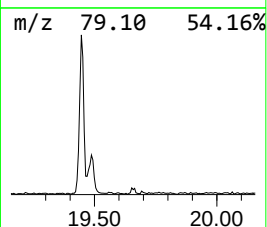
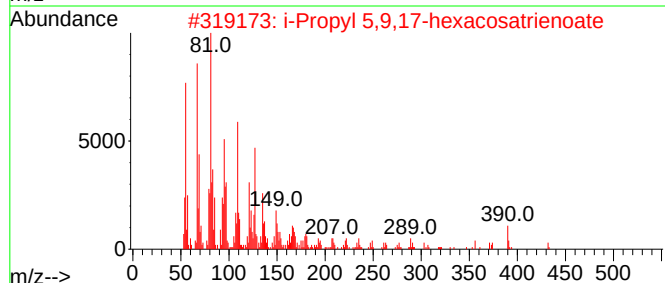
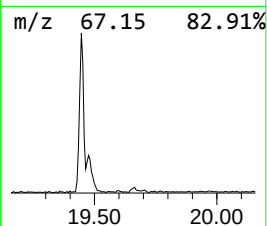
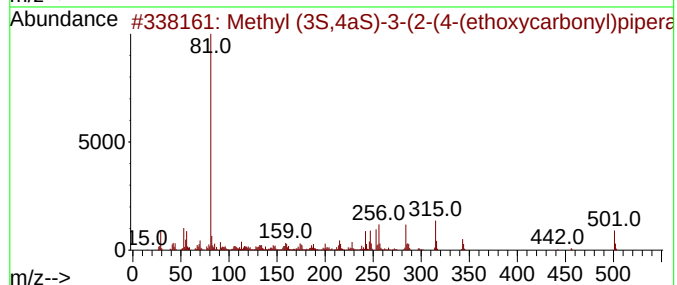
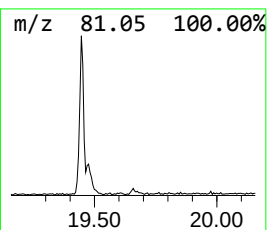
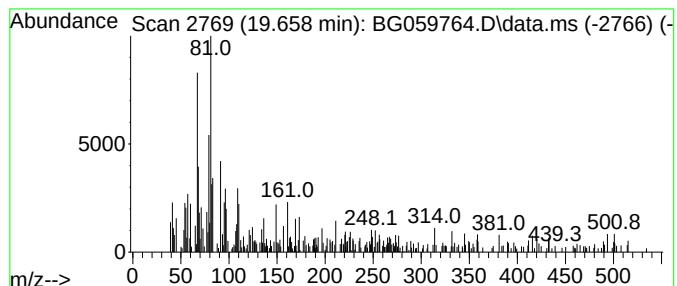
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown19.658 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.658	4.17 ng	146272	Phenanthrene-d10	17.725

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl (3S,4aS)-3-(2-(4-(ethoxyc...	501	C26H35N3O7	1010483-63-5	35
2			i-Propyl 5,9,17-hexacosatrienoate	432	C29H52O2	1000336-59-4	30
3			1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	27
4			Ethyl (3S,4aS)-1-(furan-2-ylmeth...	432	C22H28N2O5S	1000483-65-9	12
5			N-[Imino(2-nitrocyclohexyl)oxoim...	316	C12H20N4O6	104486-72-8	12



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111723\
Data File : BG059764.D
Acq On : 18 Nov 2023 14:32
Operator : MA/JU
Sample : 05385-01 5X
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
HR-02-11102023

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Naphthalene, 1,...	13.048	2.3	ng	42076	2	11.191	359465	20.0
4-(Methylthio)b...	13.794	2.1	ng	64704	3	14.975	623107	20.0
unknown15.727	15.727	2.4	ng	75165	3	14.975	623107	20.0
unknown16.121	16.121	2.2	ng	69929	3	14.975	623107	20.0
Heptacosane	16.591	2.9	ng	101382	4	17.725	701482	20.0
Dodecanoic acid...	18.312	16.3	ng	571261	4	17.725	701482	20.0
n-Hexadecanoic ...	18.535	2.8	ng	97971	4	17.725	701482	20.0
Methyl 10-trans...	19.446	116.3	ng	4080620	4	17.725	701482	20.0
14-Pentadecenoic...	19.476	55.1	ng	1931430	4	17.725	701482	20.0
Tetradecanoic a...	19.599	7.8	ng	274572	4	17.725	701482	20.0
unknown19.658	19.658	4.2	ng	146272	4	17.725	701482	20.0