

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
 Data File : BG048618.D
 Acq On : 7 Apr 2021 15:39
 Operator : CG/JU
 Sample : M1951-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SW-1

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-BG033021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048618.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.640	384	392	399	rBV	321060	496981	20.54%	4.583%
2	7.244	657	665	676	rVB	230891	407752	16.85%	3.760%
3	8.091	801	809	815	rBV	103303	179633	7.42%	1.657%
4	9.260	1001	1008	1017	rVB	366801	656612	27.14%	6.055%
5	10.917	1283	1290	1296	rBV	132610	238269	9.85%	2.197%
6	13.367	1699	1707	1714	rBV	922778	1458771	60.29%	13.452%
7	13.625	1745	1751	1758	rBV	201039	317659	13.13%	2.929%
8	14.183	1841	1846	1851	rBV	35334	49281	2.04%	0.454%
9	14.742	1933	1941	1949	rBV	196176	312863	12.93%	2.885%
10	15.141	2004	2009	2014	rBV5	18903	32140	1.33%	0.296%
11	15.852	2124	2130	2142	rVB3	75995	129255	5.34%	1.192%
12	16.234	2189	2195	2206	rBV	803058	1258173	52.00%	11.603%
13	17.497	2404	2410	2417	rBV	256474	412161	17.03%	3.801%
14	17.791	2453	2460	2468	rBV	18007	40753	1.68%	0.376%
15	18.384	2555	2561	2568	rBV	340182	520341	21.50%	4.798%
16	18.890	2641	2647	2653	rBV8	26671	75079	3.10%	0.692%
17	19.142	2684	2690	2695	rBV4	22930	36929	1.53%	0.341%
18	19.230	2701	2705	2713	rBV7	27176	47311	1.96%	0.436%
19	19.548	2756	2759	2763	rVB4	30747	42063	1.74%	0.388%
20	19.648	2772	2776	2784	rBV	183645	235306	9.72%	2.170%
21	20.112	2848	2855	2864	rVB	1848309	2419746	100.00%	22.314%
22	20.899	2985	2989	2992	rVB6	18747	25537	1.06%	0.235%
23	21.416	3072	3077	3090	rBV2	145497	245617	10.15%	2.265%
24	21.563	3098	3102	3103	rBV4	22381	26297	1.09%	0.243%
25	21.581	3103	3105	3114	rVB8	28833	62910	2.60%	0.580%
26	21.798	3135	3142	3151	rVB	266230	476280	19.68%	4.392%
27	21.986	3170	3174	3180	rVB7	22717	32786	1.35%	0.302%
28	22.615	3277	3281	3288	rBV9	22979	43632	1.80%	0.402%
29	24.013	3509	3519	3526	rBV9	29135	108850	4.50%	1.004%
30	25.135	3701	3710	3724	rVB2	146016	454922	18.80%	4.195%

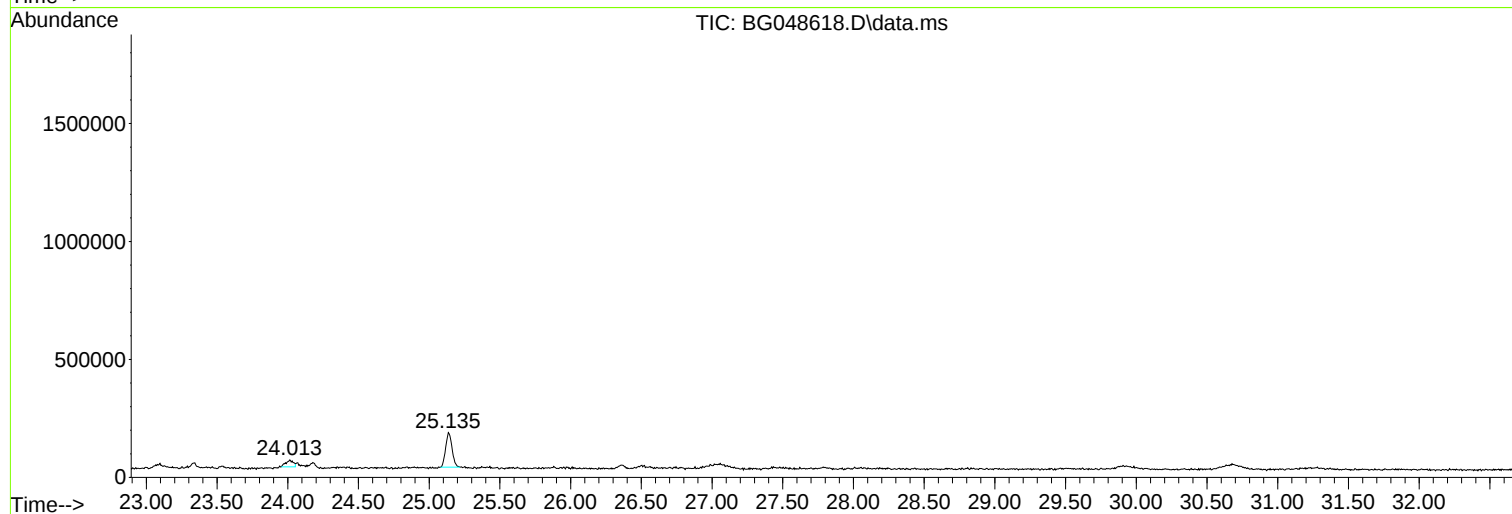
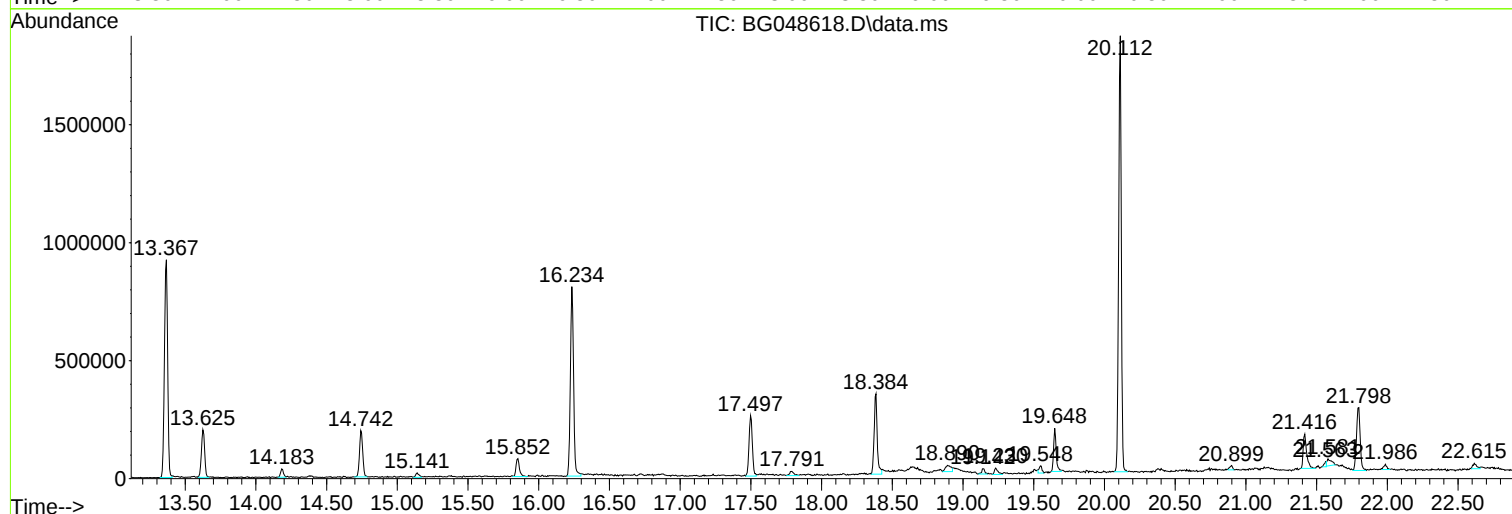
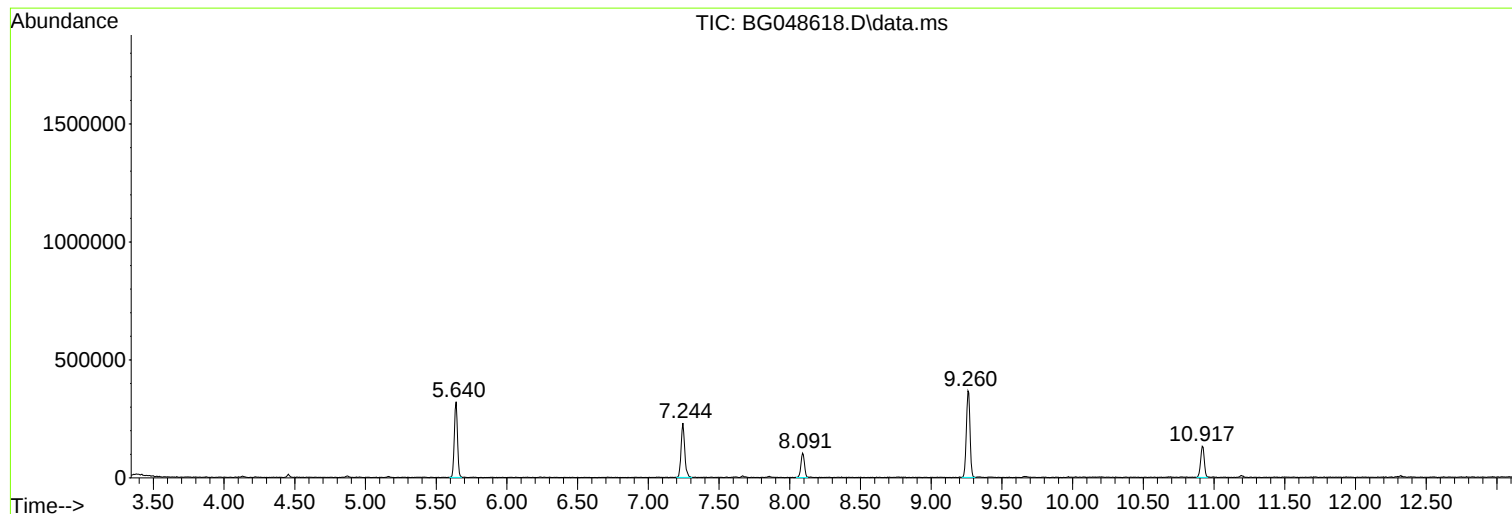
Sum of corrected areas: 10843909

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

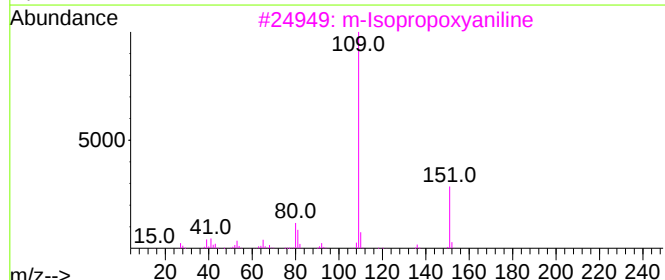
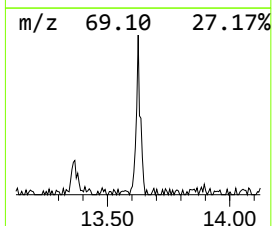
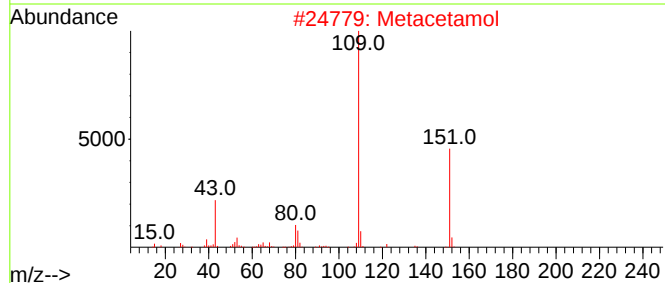
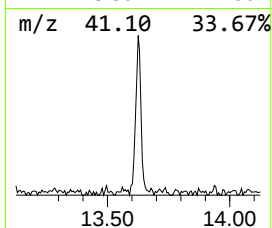
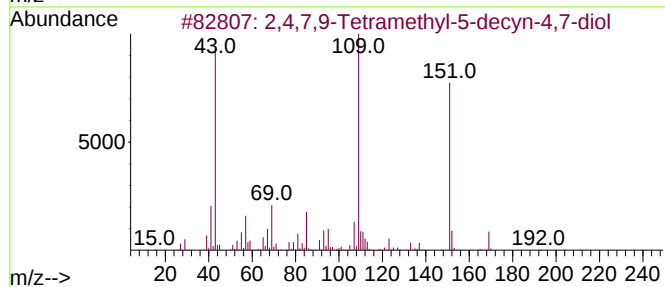
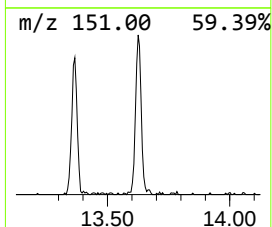
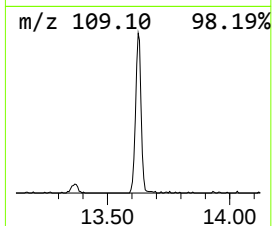
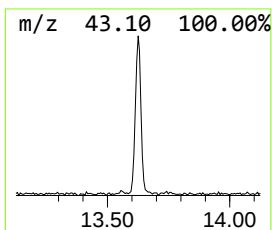
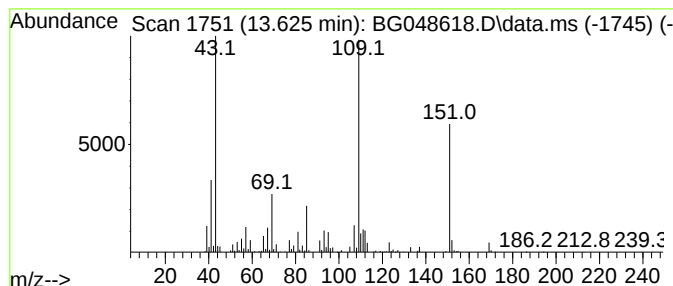
Instrument :
BNA_G
ClientSampleId :
SW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.625	20.31 ng	317659	Acenaphthene-d10	14.742	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	52
2	Metacetamol	151	C8H9NO2	000621-42-1	52
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50
4	Tiocarlide	400	C23H32N2O2S	000910-86-1	50
5	Acetaminophen	151	C8H9NO2	000103-90-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-1

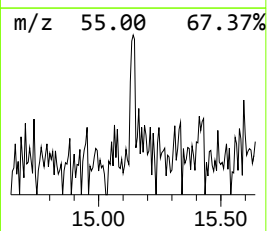
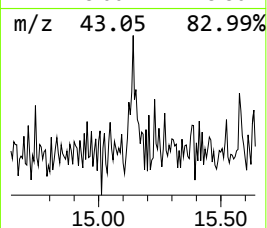
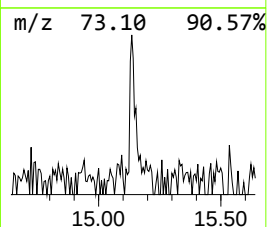
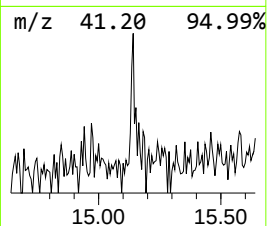
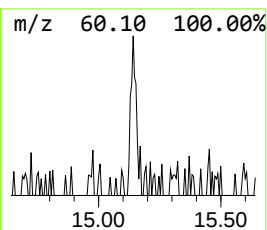
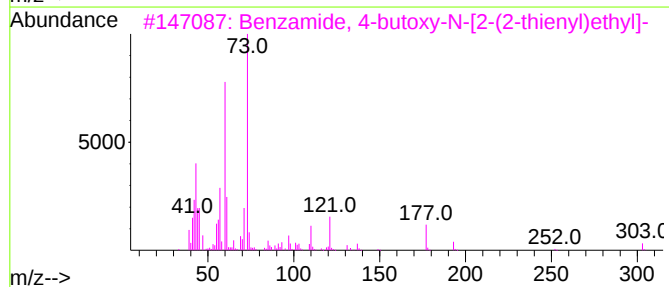
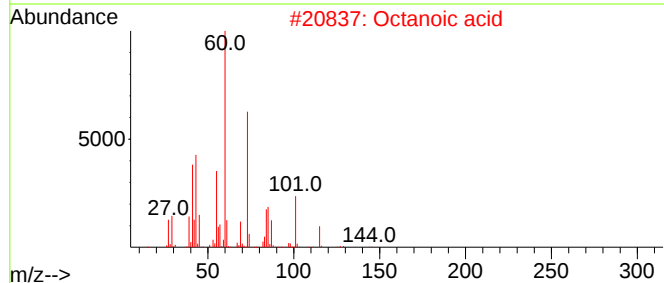
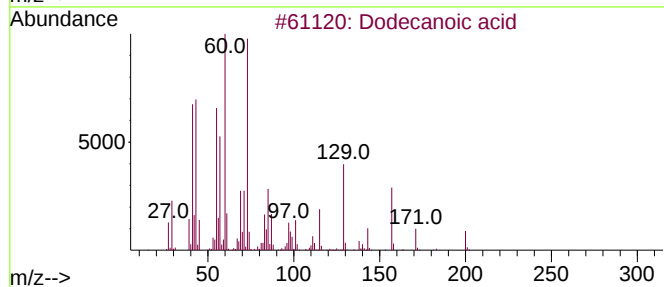
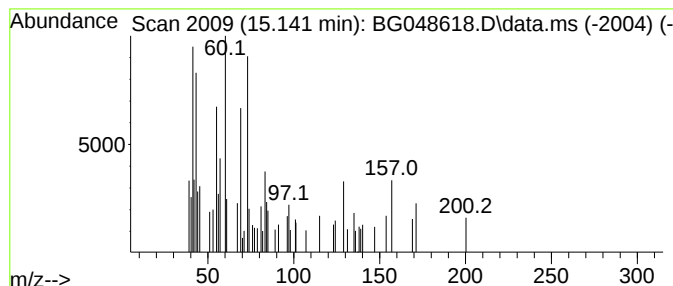
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.141	2.05 ng	32140	Acenaphthene-d10	14.742

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	59
2			Octanoic acid	144	C8H16O2	000124-07-2	50
3			Benzamide, 4-butoxy-N-[2-(2-thie...	303	C17H21NO2S	1000319-87-5	38
4			Maltose	342	C12H22O11	000069-79-4	35
5			Lactose	342	C12H22O11	000063-42-3	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-1

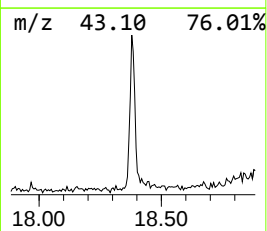
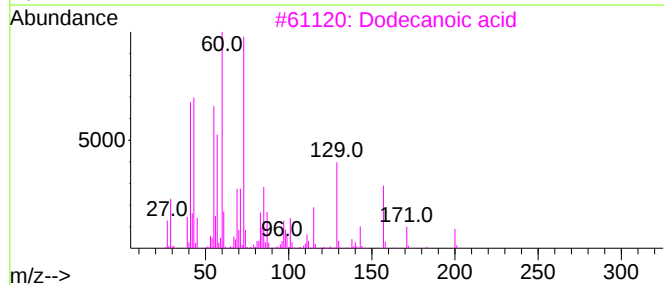
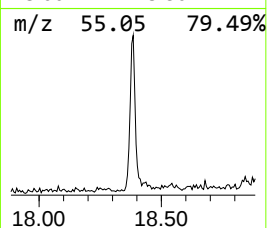
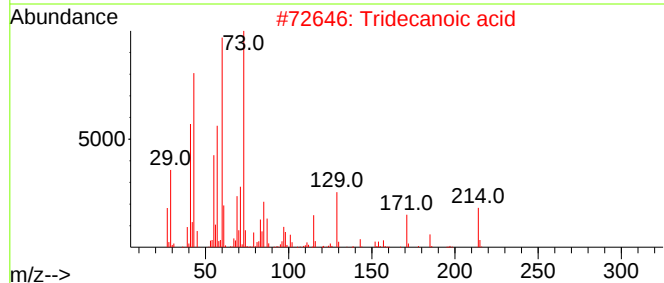
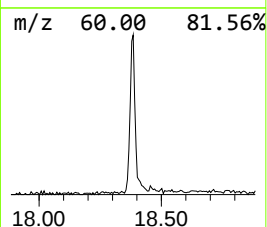
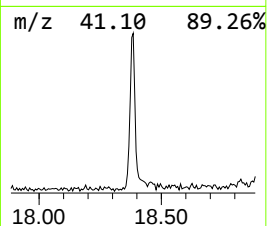
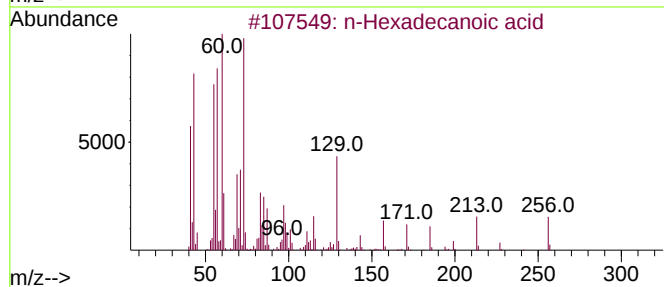
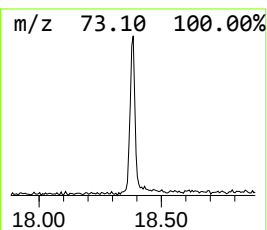
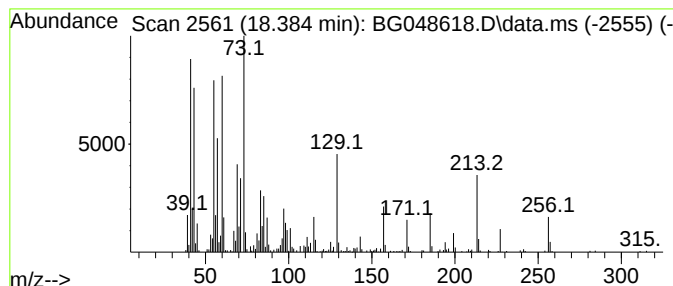
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.384	25.25 ng	520341	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Dodecanoic acid	200	C12H24O2	000143-07-7	62
4			Undecanoic acid	186	C11H22O2	000112-37-8	60
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-1

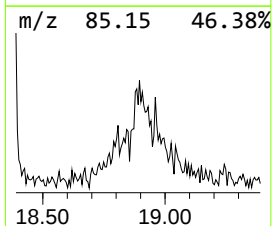
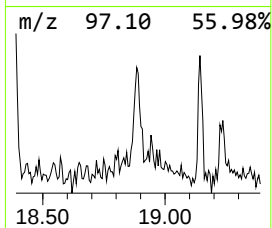
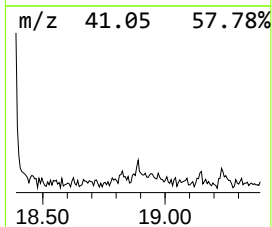
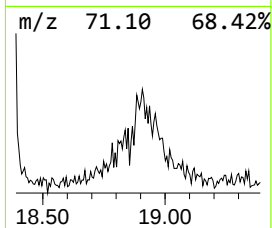
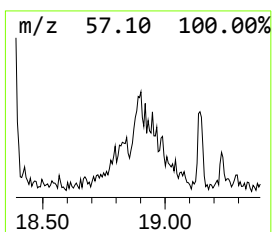
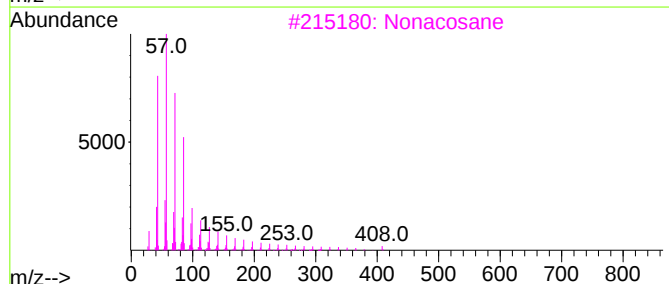
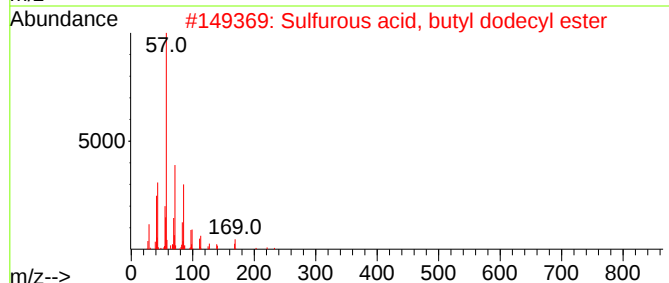
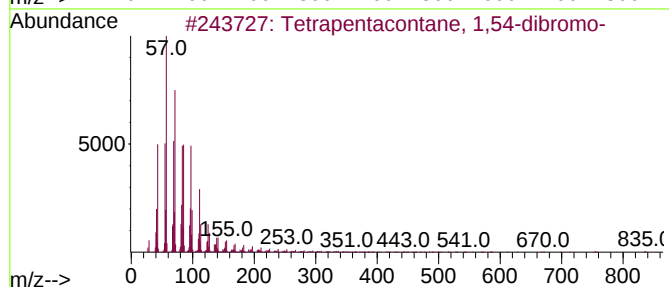
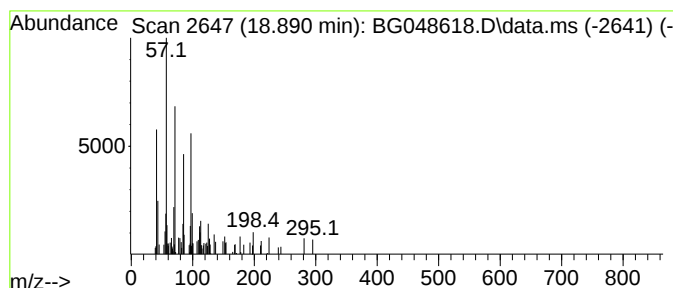
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetrapentacontane, 1,54-dib... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.890	3.64 ng	75079	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	74
2			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	49
3			Nonacosane	408	C29H60	000630-03-5	47
4			Hexadecane, 3-methyl-	240	C17H36	006418-43-5	47
5			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

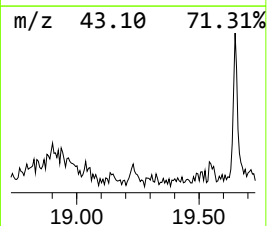
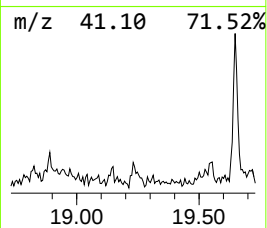
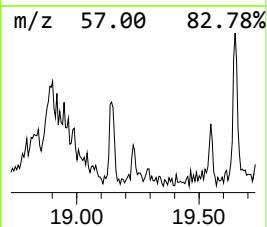
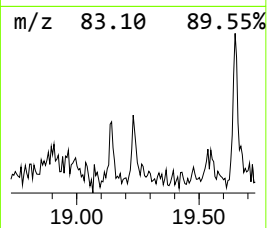
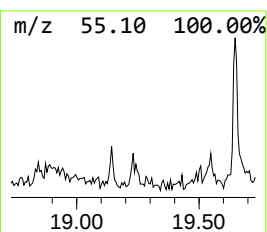
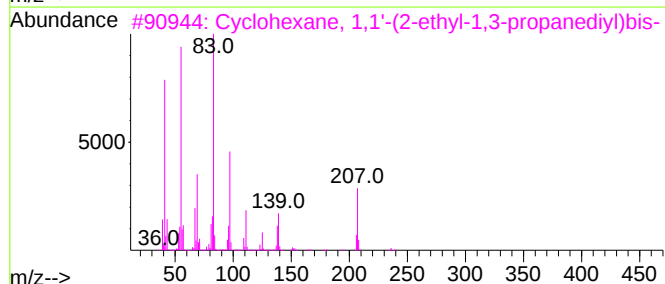
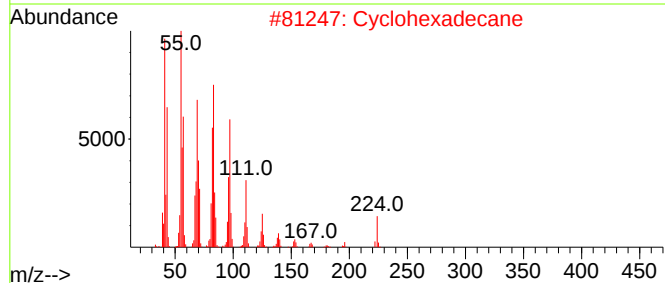
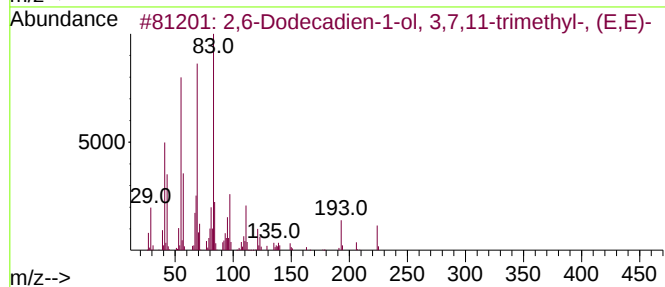
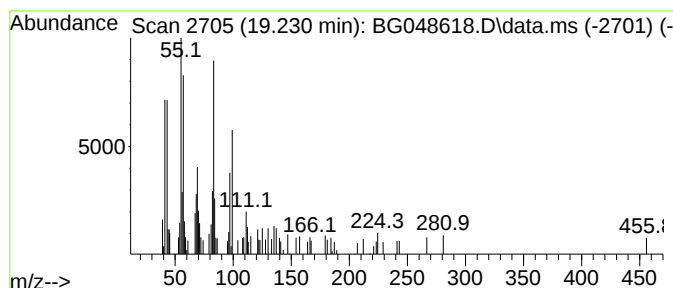
Instrument :
BNA_G
ClientSampleId :
SW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2,6-Dodecadien-1-ol, 3,7,11... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.230	2.30 ng	47311	Phenanthrene-d10		17.497	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,6-Dodecadien-1-ol, 3,7,11-trim...		224	C15H28O	020576-56-1	58
2	Cyclohexadecane		224	C16H32	000295-65-8	53
3	Cyclohexane, 1,1'-(2-ethyl-1,3-p...		236	C17H32	054833-34-0	46
4	Cyclohexane, 1,1'-(2-methyl-1,3-...		222	C16H30	002883-08-1	46
5	3-Hexene, 2,2-dimethyl-, (E)-		112	C8H16	000690-93-7	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-1

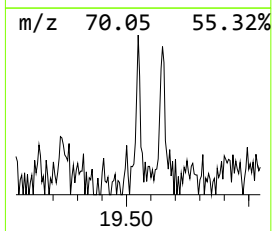
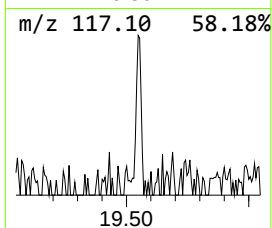
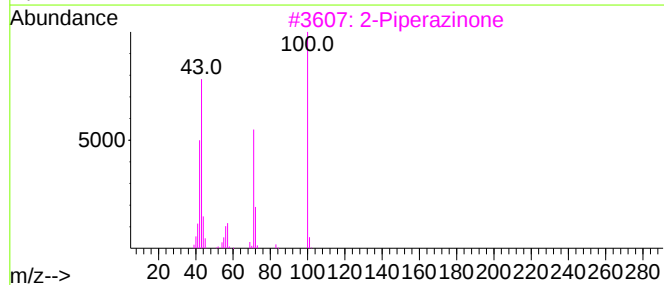
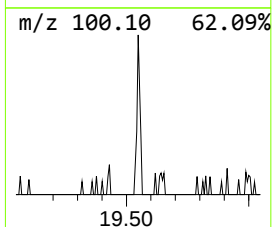
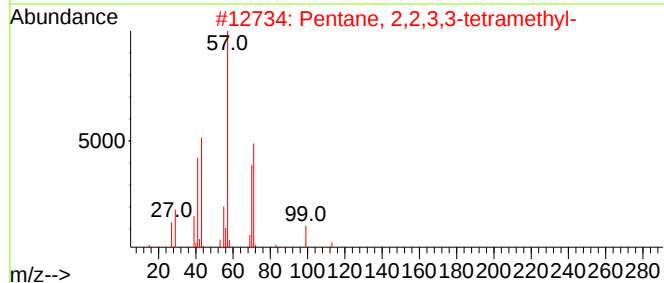
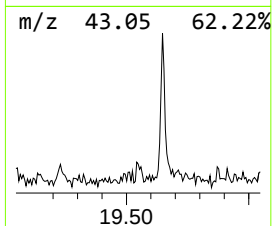
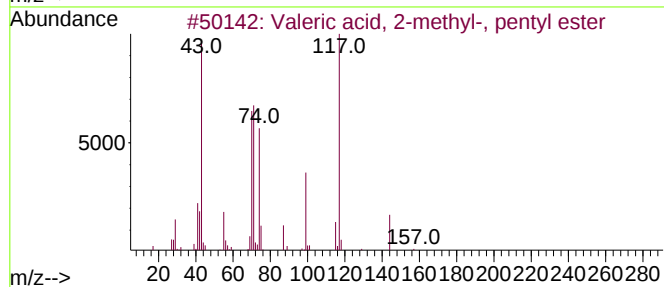
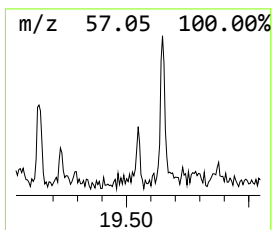
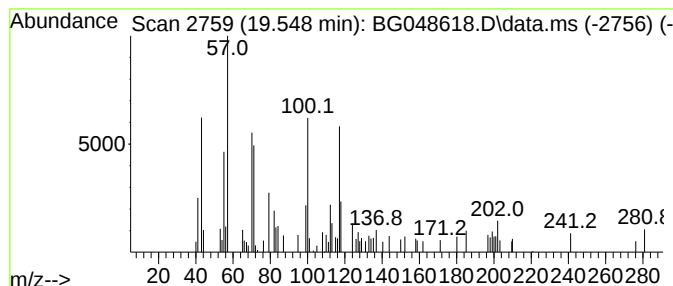
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown19.54 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.548	2.04 ng	42063	Phenanthrene-d10	17.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Valeric acid, 2-methyl-, pentyl ...	186	C11H22O2	006297-48-9	27
2			Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	22
3			2-Piperazinone	100	C4H8N2O	005625-67-2	18
4			Heptadecane, 7-methyl-	254	C18H38	020959-33-5	14
5			3-Trifluoromethylcinnamic acid, ...	328	C18H23F3O2	1000293-54-5	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-1

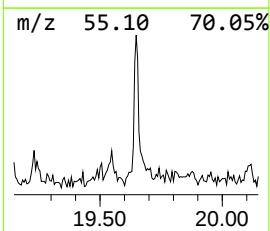
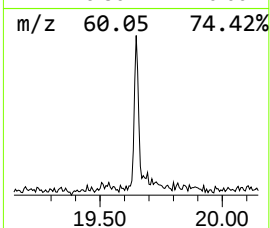
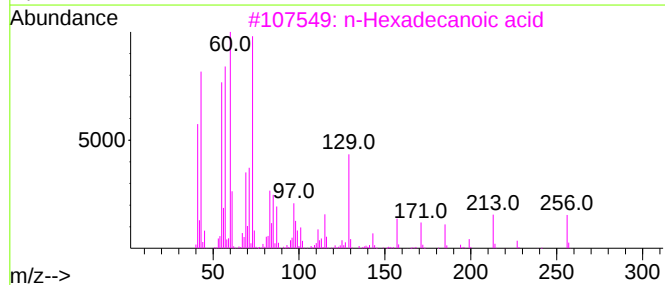
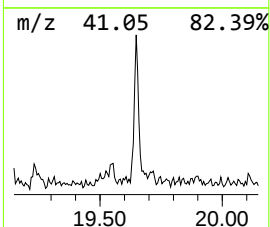
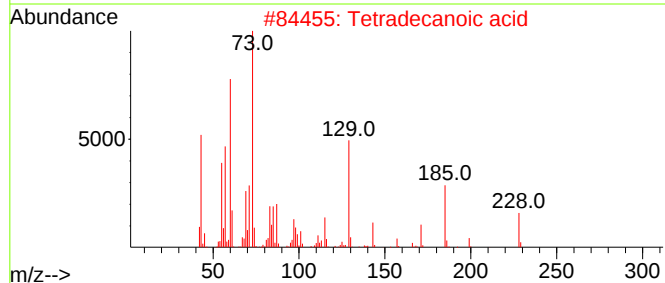
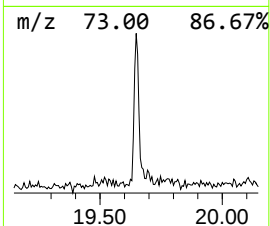
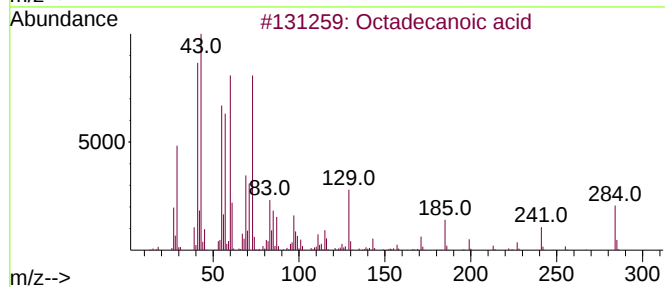
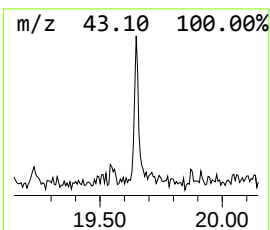
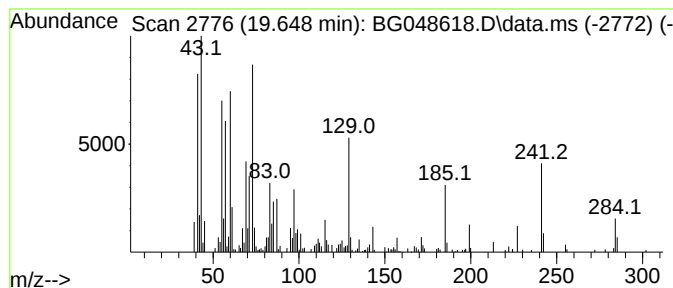
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.648	9.88 ng	235306	Chrysene-d12	21.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	83
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58
4			n-Decanoic acid	172	C10H20O2	000334-48-5	55
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-1

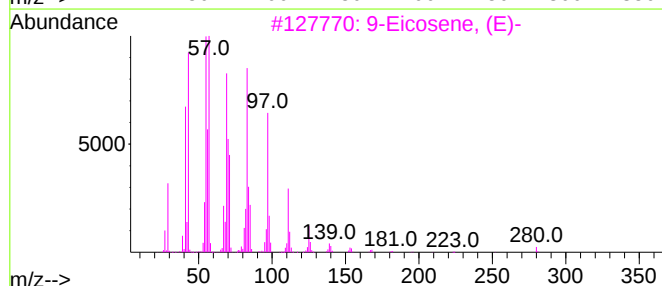
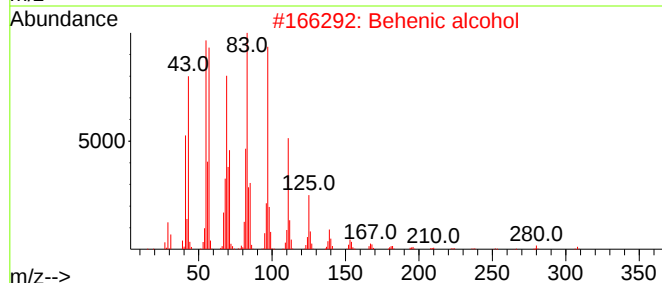
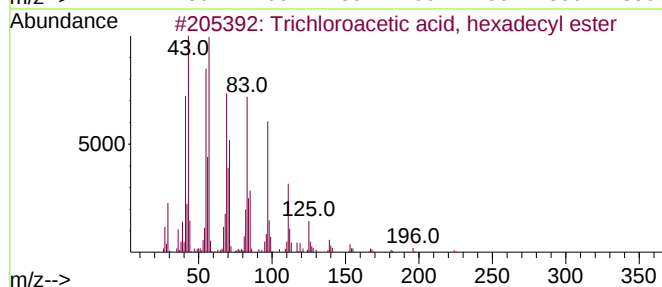
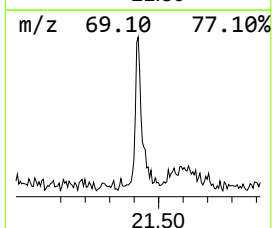
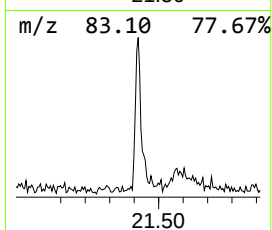
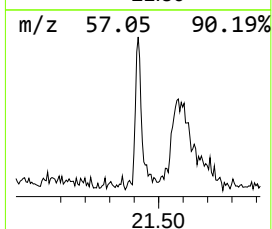
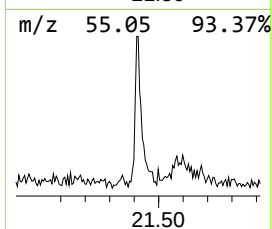
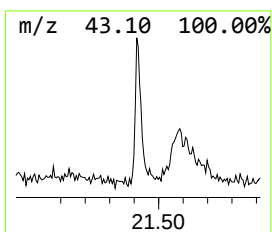
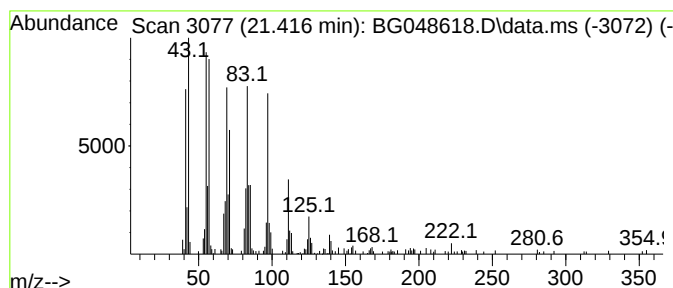
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Trichloroacetic acid, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	10.31 ng	245617	Chrysene-d12	21.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			Behenic alcohol	326	C22H46O	000661-19-8	93
3			9-Eicosene, (E)-	280	C20H40	074685-29-3	91
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-1

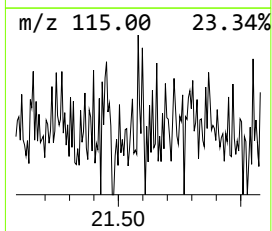
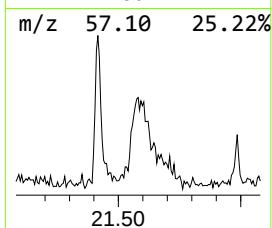
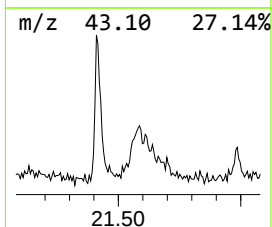
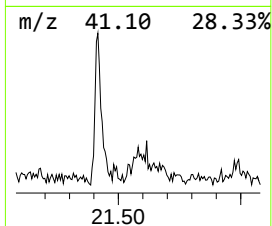
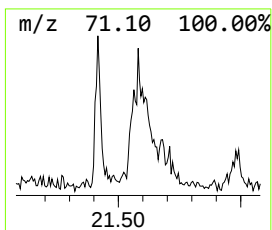
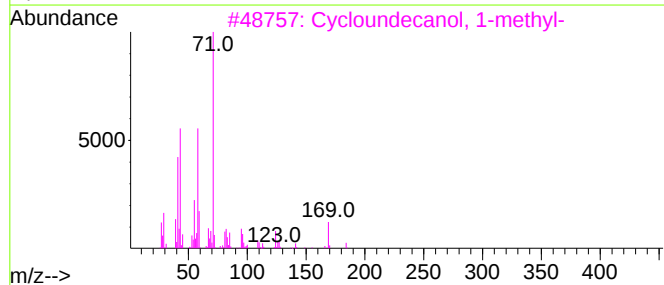
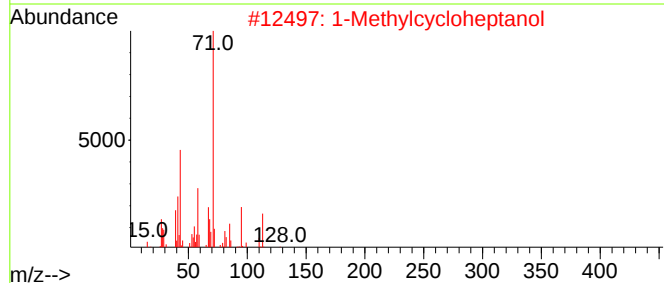
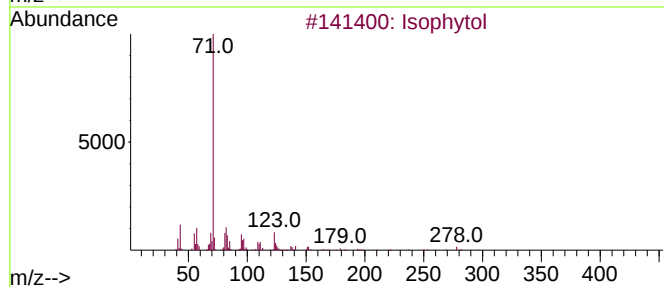
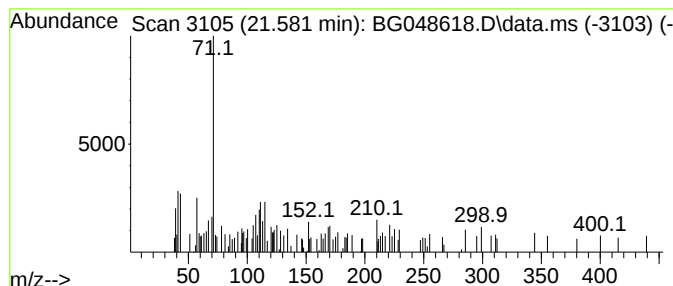
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 unknown21.58 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.581	2.64 ng	62910	Chrysene-d12	21.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isophytol	296	C20H40O	000505-32-8	38
2			1-Methylcycloheptanol	128	C8H16O	003761-94-2	38
3			Cycloundecanol, 1-methyl-	184	C12H24O	076154-15-9	35
4			Z-1-Methoxy-2-pentene	100	C6H12O	1000279-59-4	35
5			Ether, 1-dodecenyl methyl	198	C13H26O	026537-04-2	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

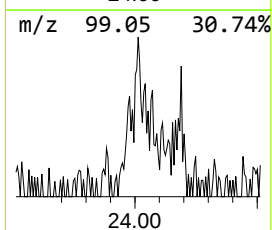
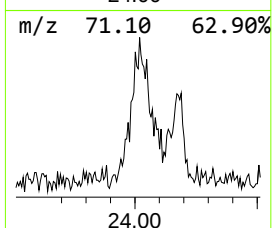
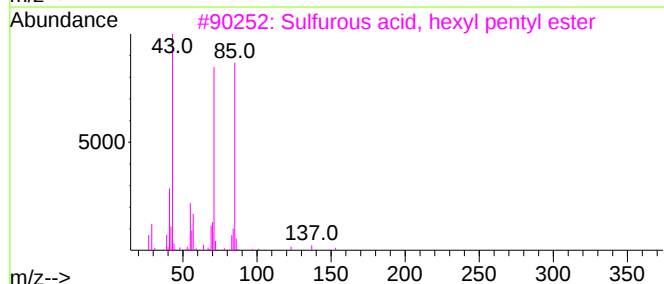
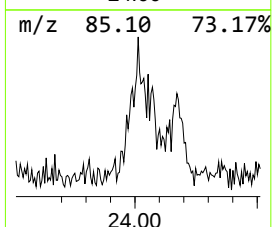
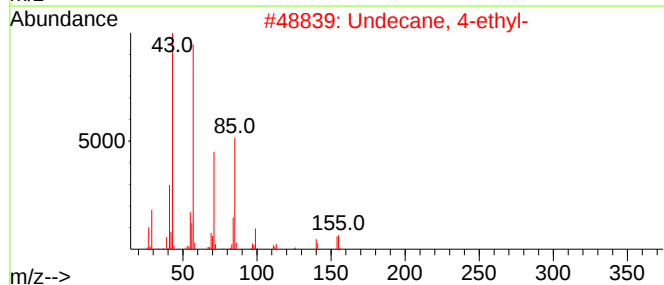
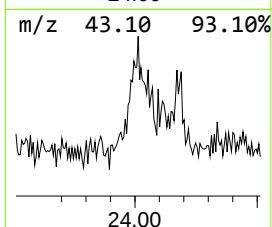
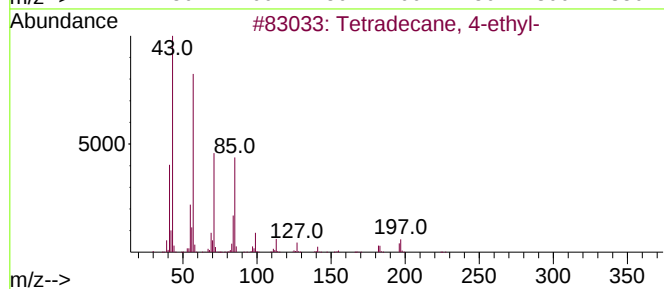
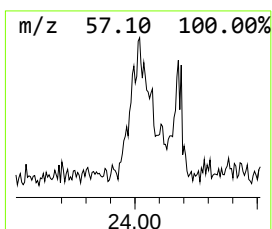
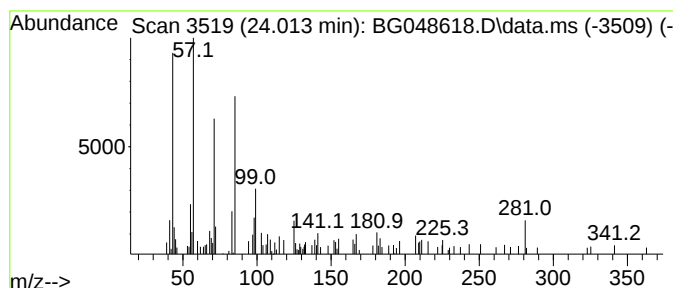
Instrument :
BNA_G
ClientSampleId :
SW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Tetradecane, 4-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.013	4.79 ng	108850	Perylene-d12	25.135	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	53
2	Undecane, 4-ethyl-	184	C13H28	017312-59-3	53
3	Sulfurous acid, hexyl pentyl ester	236	C11H24O3S	1000309-14-1	50
4	Eicosane	282	C20H42	000112-95-8	45
5	4-Octanone, 2,3-epoxy-2-methyl-	156	C9H16O2	017257-83-9	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040721\
Data File : BG048618.D
Acq On : 7 Apr 2021 15:39
Operator : CG/JU
Sample : M1951-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SW-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,4,7,9-Tetrame...	13.625	20.3	ng	317659	3	14.742	312863	20.0
Dodecanoic acid	15.141	2.0	ng	32140	3	14.742	312863	20.0
n-Hexadecanoic ...	18.384	25.3	ng	520341	4	17.497	412161	20.0
Tetrapentaconta...	18.890	3.6	ng	75079	4	17.497	412161	20.0
2,6-Dodecadien-...	19.230	2.3	ng	47311	4	17.497	412161	20.0
unknown19.54	19.548	2.0	ng	42063	4	17.497	412161	20.0
Octadecanoic acid	19.648	9.9	ng	235306	5	21.792	476280	20.0
Trichloroacetic...	21.416	10.3	ng	245617	5	21.792	476280	20.0
unknown21.58	21.581	2.6	ng	62910	5	21.792	476280	20.0
Tetradecane, 4-...	24.013	4.8	ng	108850	6	25.135	454922	20.0