

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
 Data File : BG048043.D
 Acq On : 28 Jan 2021 1:00
 Operator : CG/JU
 Sample : M1226-04
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 0055-052-COMP-I-ELUTRIATE

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-BG012521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048043.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.680	390	398	408	rBV	548059	864306	20.85%	5.039%
2	7.266	661	668	682	rVB	394158	726328	17.52%	4.235%
3	8.124	807	814	820	rBV	176575	288595	6.96%	1.683%
4	9.287	1003	1012	1020	rBV	598118	1023972	24.70%	5.970%
5	10.938	1284	1293	1300	rBV	223527	390910	9.43%	2.279%
6	13.370	1700	1707	1714	rBV	1508309	2320958	56.00%	13.531%
7	14.187	1841	1846	1851	rBV2	32471	47211	1.14%	0.275%
8	14.745	1933	1941	1950	rVB	376950	570809	13.77%	3.328%
9	16.226	2186	2193	2204	rBV	1305208	2062067	49.75%	12.022%
10	17.489	2401	2408	2414	rVB	490241	736826	17.78%	4.296%
11	18.371	2552	2558	2565	rBV	407039	569859	13.75%	3.322%
12	18.441	2566	2570	2575	rVB	109007	146844	3.54%	0.856%
13	19.134	2684	2688	2693	rBV	93597	117473	2.83%	0.685%
14	19.634	2768	2773	2784	rBV	287923	399269	9.63%	2.328%
15	19.769	2792	2796	2803	rVB	31206	43751	1.06%	0.255%
16	20.092	2845	2851	2856	rBV	3301834	4144911	100.00%	24.165%
17	20.774	2964	2967	2972	rVB2	38062	44547	1.07%	0.260%
18	20.991	3000	3004	3009	rBV	127737	173523	4.19%	1.012%
19	21.396	3068	3073	3083	rBV2	340986	511860	12.35%	2.984%
20	21.649	3112	3116	3121	rVB	44983	63140	1.52%	0.368%
21	21.761	3129	3135	3142	rVB2	557515	916539	22.11%	5.343%
22	25.045	3684	3694	3703	rBV2	303049	880750	21.25%	5.135%
23	26.385	3918	3922	3933	rVB9	42247	108073	2.61%	0.630%

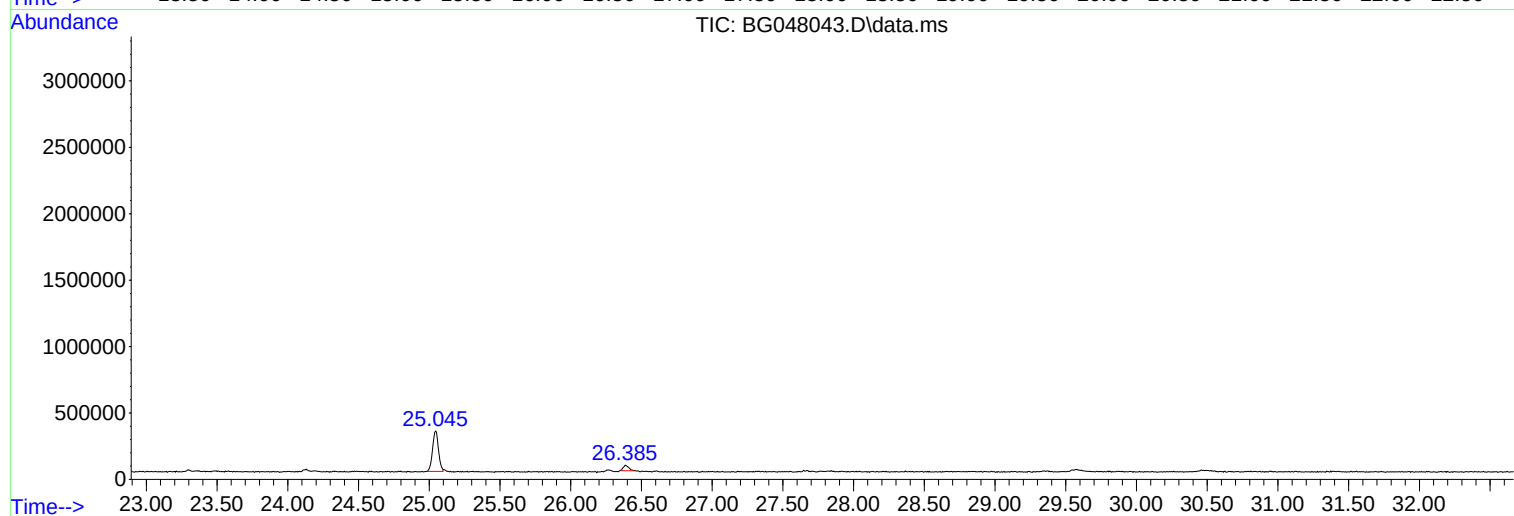
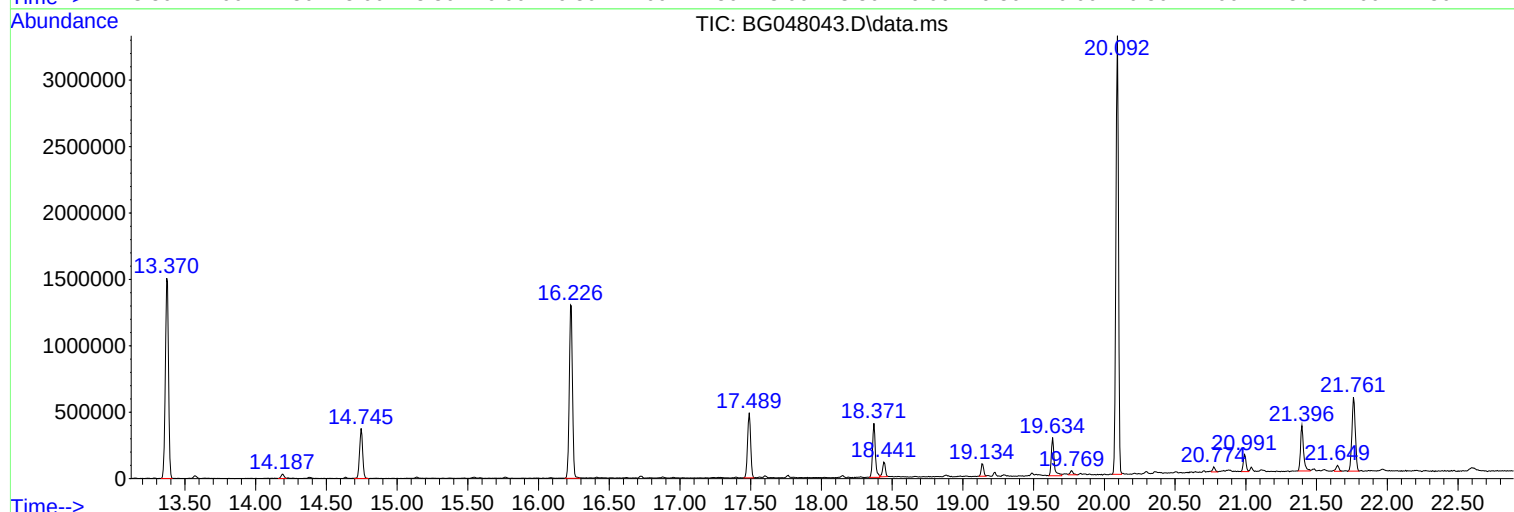
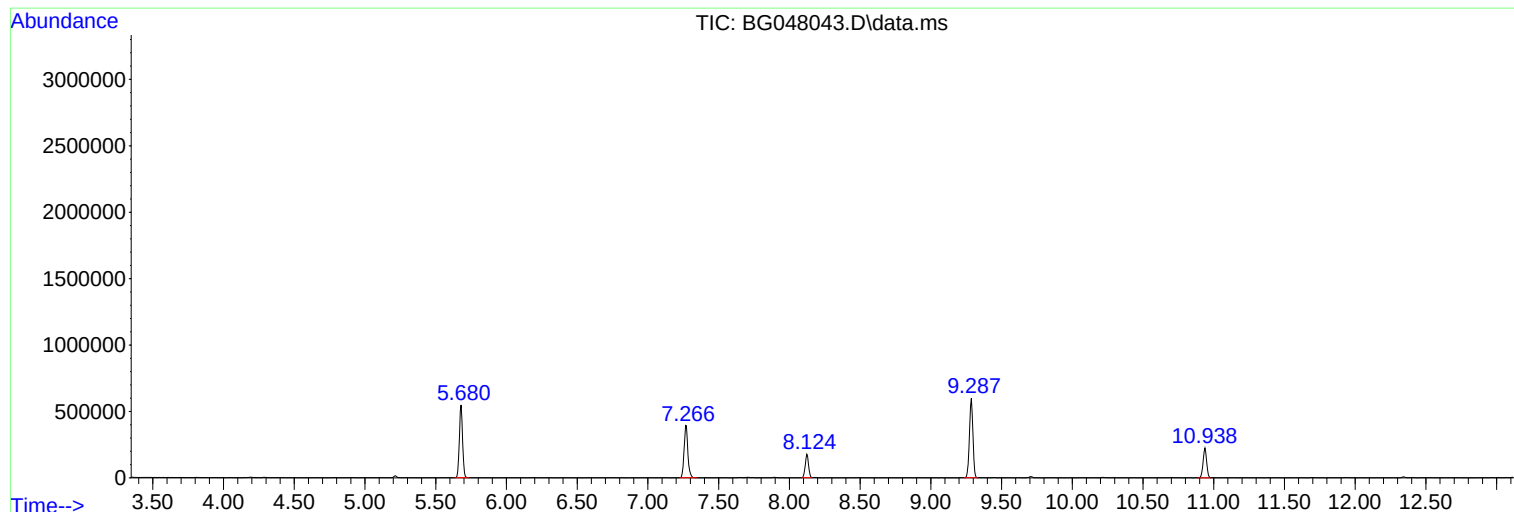
Sum of corrected areas: 17152521

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048043.D
Acq On : 28 Jan 2021 1:00
Operator : CG/JU
Sample : M1226-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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\BG012721\
Data File : BG048043.D
Acq On : 28 Jan 2021 1:00
Operator : CG/JU
Sample : M1226-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

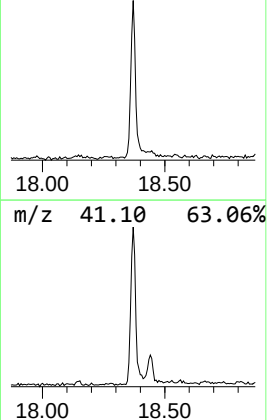
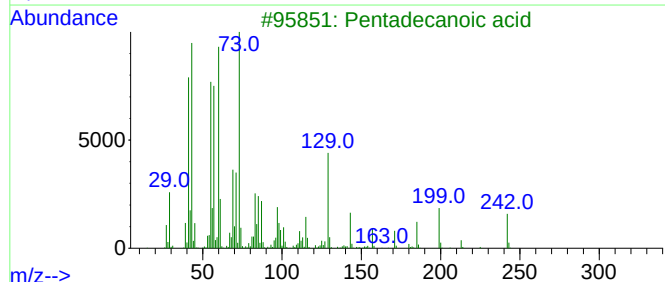
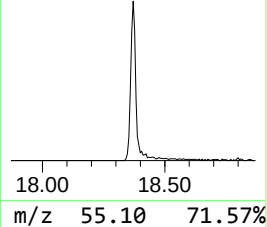
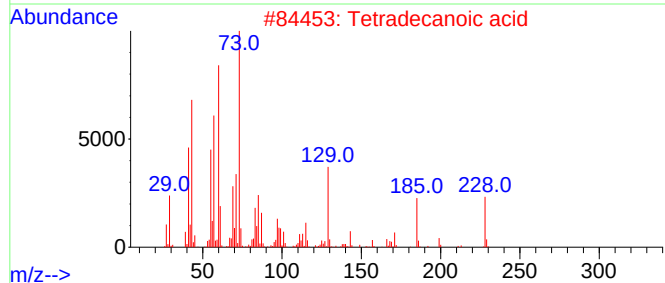
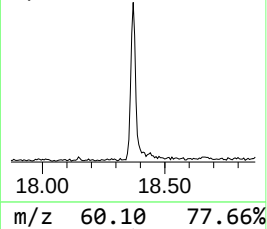
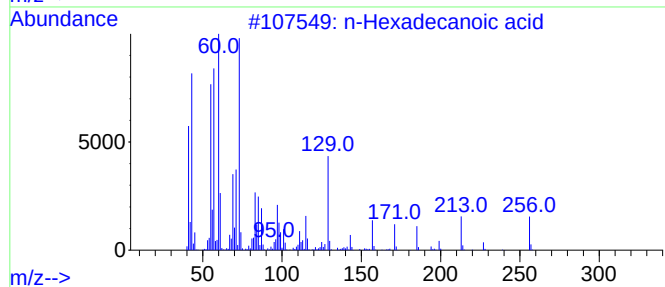
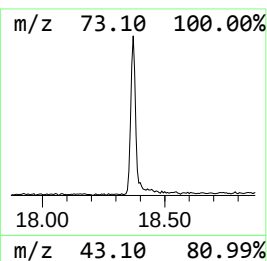
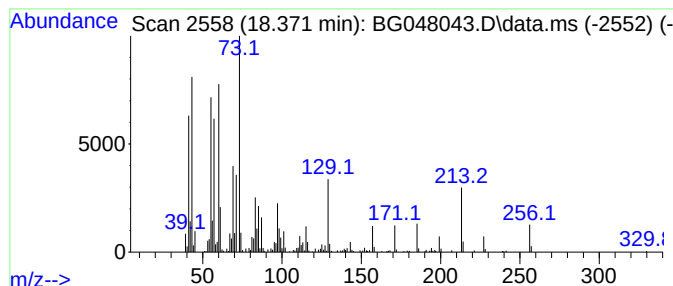
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.371	15.47 ng	569859	Phenanthrene-d10	17.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Octadecanoic acid	284	C18H36O2	000057-11-4	81
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048043.D
Acq On : 28 Jan 2021 1:00
Operator : CG/JU
Sample : M1226-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

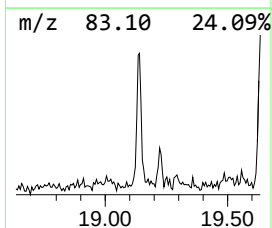
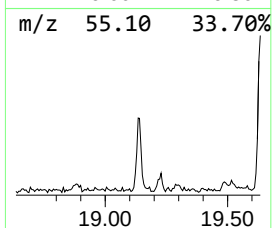
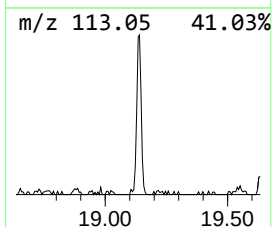
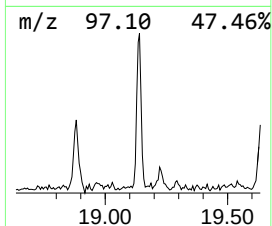
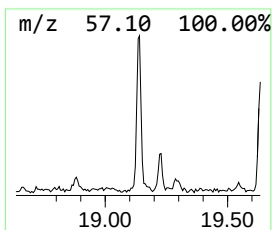
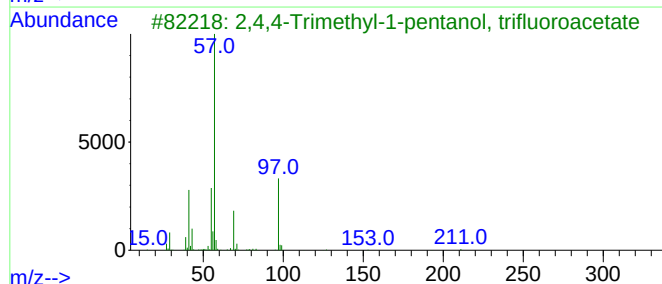
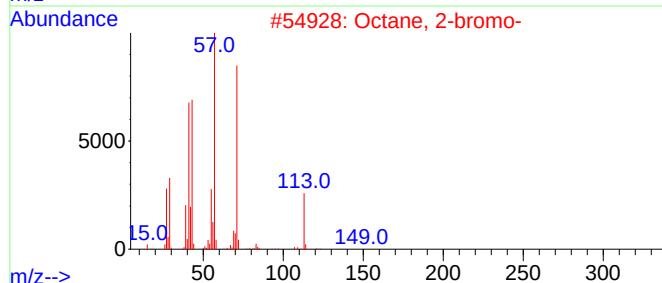
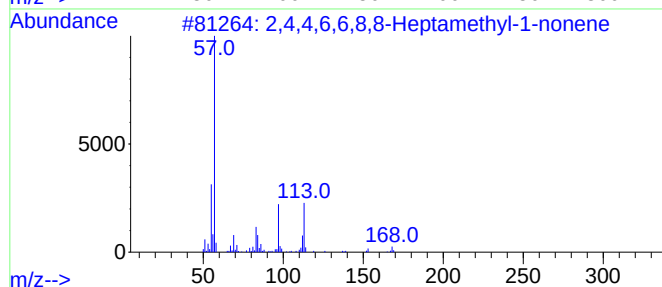
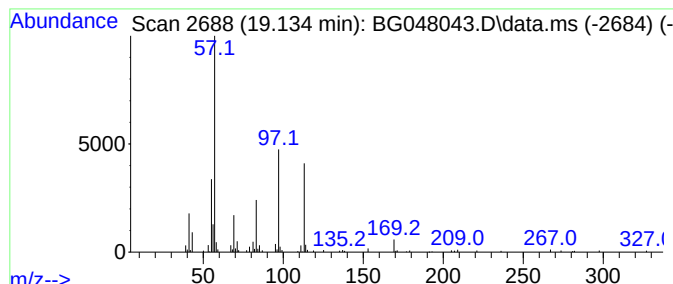
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.134	3.19 ng	117473	Phenanthrene-d10	17.489

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	72	
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	43	
3	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	35	
4	4-Methylnonanoic acid	172	C10H20O2	045019-28-1	28	
5	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	28	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048043.D
Acq On : 28 Jan 2021 1:00
Operator : CG/JU
Sample : M1226-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

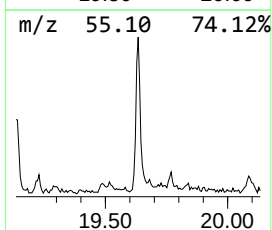
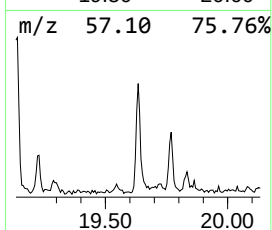
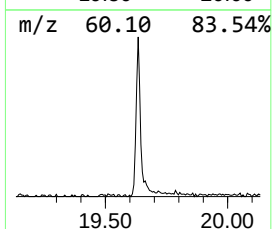
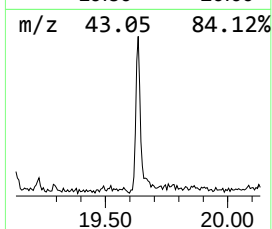
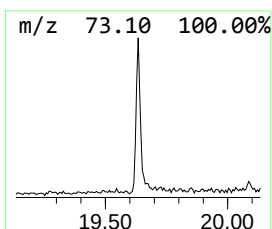
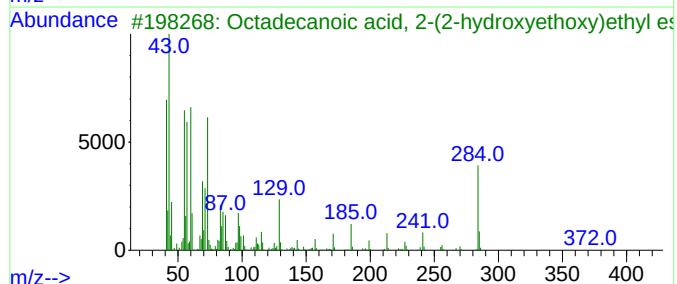
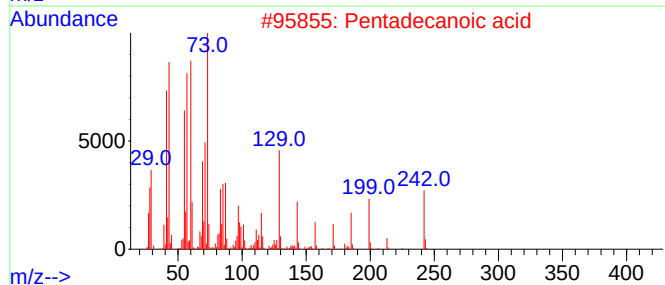
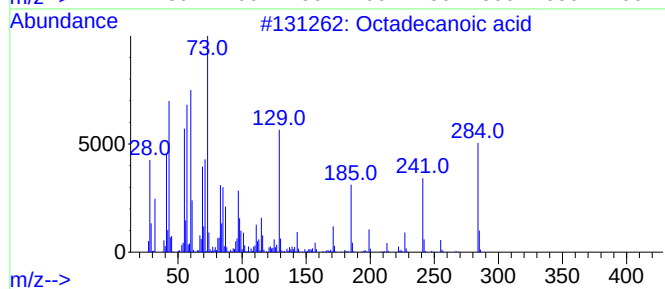
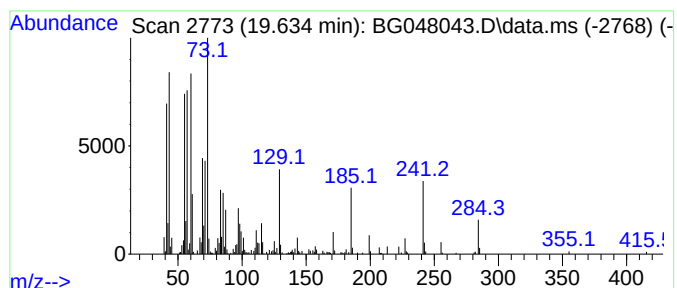
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.634	8.71 ng	399269	Chrysene-d12	21.761

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048043.D
Acq On : 28 Jan 2021 1:00
Operator : CG/JU
Sample : M1226-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

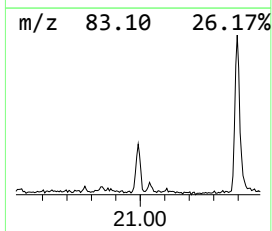
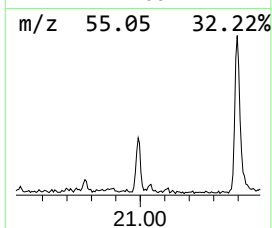
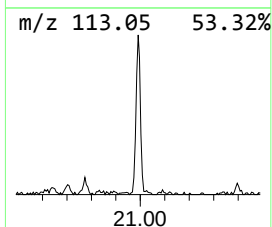
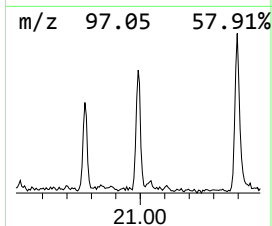
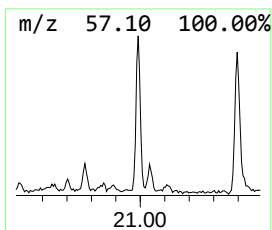
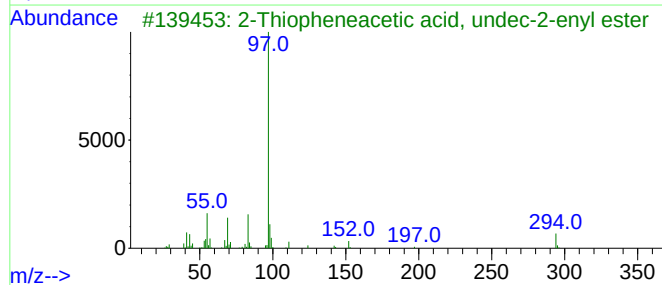
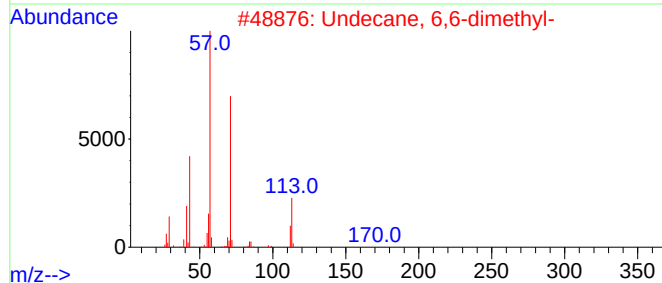
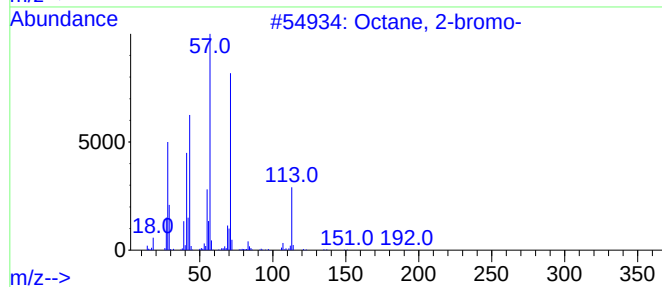
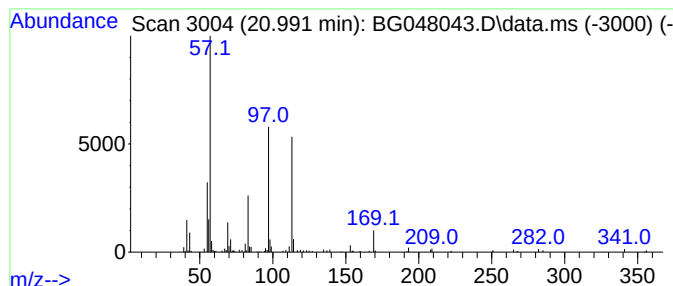
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown20.991 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.991	3.79 ng	173523	Chrysene-d12	21.761

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-		192	C8H17Br		000557-35-7	35
2	Undecane, 6,6-dimethyl-		184	C13H28		017312-76-4	25
3	2-Thiopheneacetic acid, undec-2-...		294	C17H26O2S		1000299-39-0	25
4	2,4,4-Trimethyl-1-pentanol, hept...		326	C12H17F7O2		1000365-01-4	25
5	2,4,4,6,6,8,8-Heptamethyl-1-nonene		224	C16H32		015796-04-0	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048043.D
Acq On : 28 Jan 2021 1:00
Operator : CG/JU
Sample : M1226-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

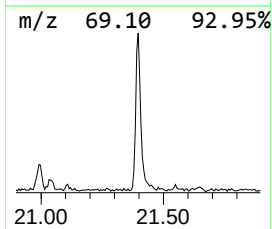
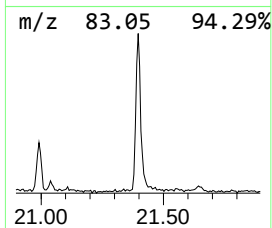
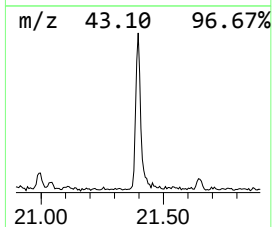
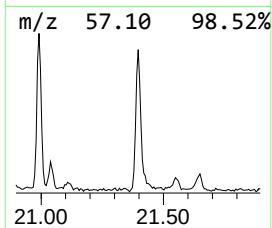
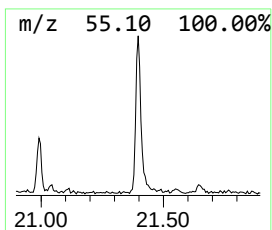
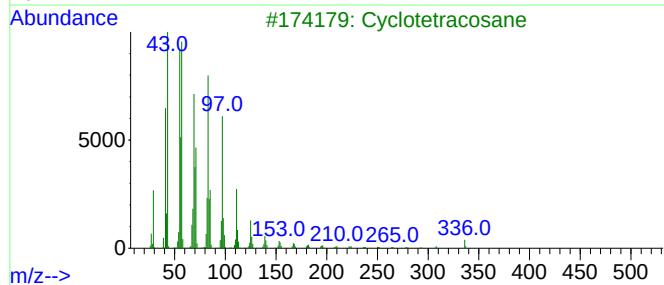
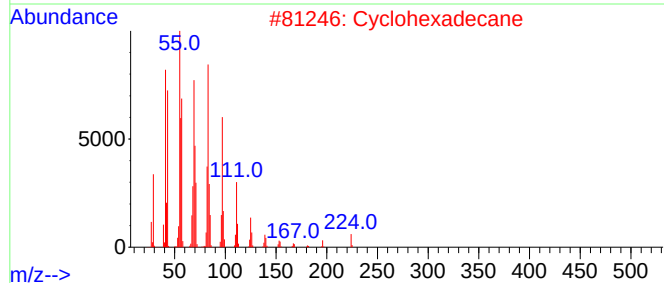
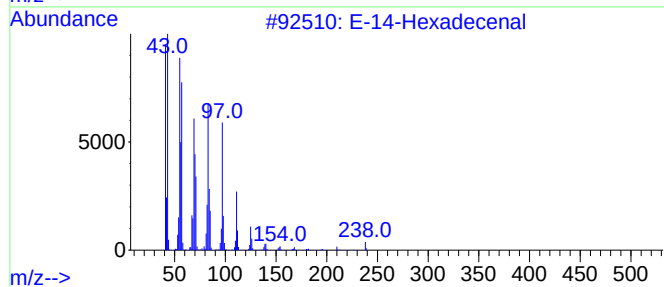
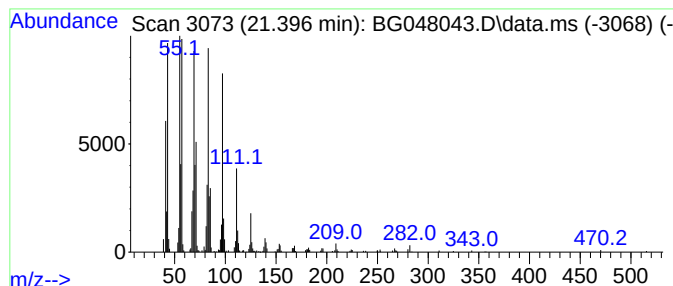
Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 E-14-Hexadecenal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.396	11.17 ng	511860	Chrysene-d12	21.761	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-14-Hexadecenal	238	C16H30O	330207-53-9	92
2	Cyclohexadecane	224	C16H32	000295-65-8	91
3	Cyclotetracosane	336	C24H48	000297-03-0	86
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	81
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048043.D
Acq On : 28 Jan 2021 1:00
Operator : CG/JU
Sample : M1226-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

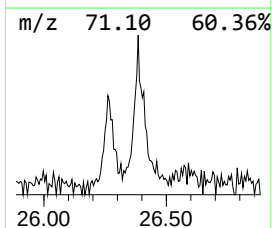
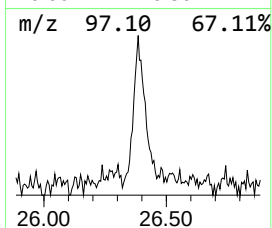
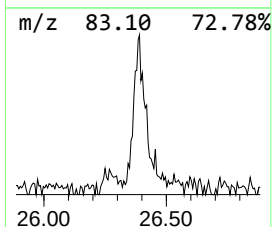
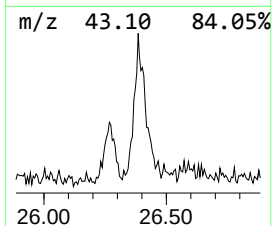
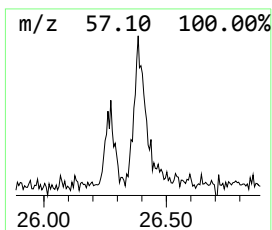
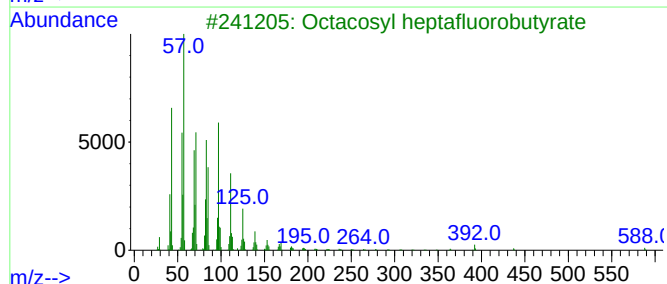
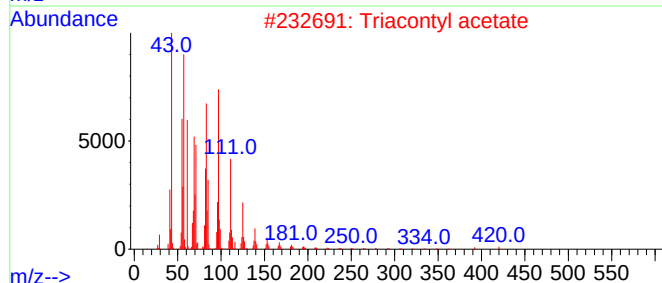
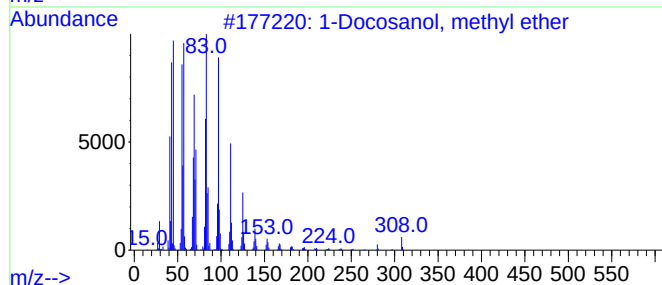
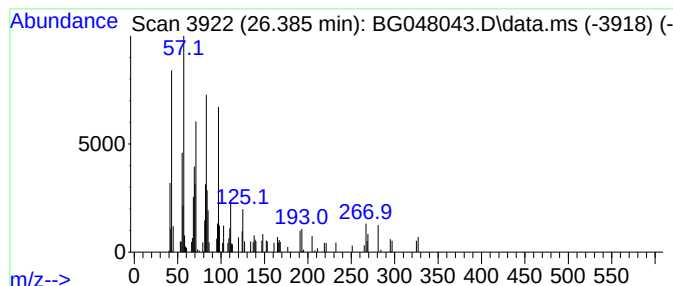
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Docosanol, methyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.385	2.45 ng	108073	Perylene-d12	25.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosanol, methyl ether			340	C23H48O	1000333-91-9	53
2	Triacontyl acetate			480	C32H64O2	041755-58-2	53
3	Octacosyl heptafluorobutyrate			606	C32H57F7O2	1000351-83-6	52
4	1-Heptacosanol			396	C27H56O	002004-39-9	52
5	Hexacosyl pentafluoropropionate			528	C29H53F5O2	1000351-81-2	52



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048043.D
Acq On : 28 Jan 2021 1:00
Operator : CG/JU
Sample : M1226-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0055-052-COMP-I-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.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
n-Hexadecanoic ...	18.371	15.5	ng	569859	4	17.489	736826	20.0
2,4,4,6,6,8,8-H...	19.134	3.2	ng	117473	4	17.489	736826	20.0
Octadecanoic acid	19.634	8.7	ng	399269	5	21.761	916539	20.0
unknown20.991	20.991	3.8	ng	173523	5	21.761	916539	20.0
E-14-Hexadecenal	21.396	11.2	ng	511860	5	21.761	916539	20.0
1-Docosanol, me...	26.385	2.5	ng	108073	6	25.045	880750	20.0