

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
 Data File : BF122417.D
 Acq On : 20 Nov 2020 22:25
 Operator : JU/CG
 Sample : L4829-04
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-4

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_F\METHODS\8270-BF110920.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF122417.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.475	572	576	580	rBV	2591296	2481705	31.21%	5.714%
2	6.487	744	748	761	rBV	1742337	1761043	22.14%	4.055%
3	6.863	808	812	815	rBV	1568348	1283007	16.13%	2.954%
4	7.428	902	908	911	rBV	3946451	3805088	47.85%	8.761%
5	7.634	939	943	946	rVB	114232	107247	1.35%	0.247%
6	8.151	1027	1031	1034	rBV	1922668	1702155	21.40%	3.919%
7	9.228	1209	1214	1217	rBV	7123394	6977350	87.74%	16.066%
8	9.622	1277	1281	1284	rBV	238130	202837	2.55%	0.467%
9	9.910	1325	1330	1333	rBV	2264544	2075390	26.10%	4.779%
10	10.698	1459	1464	1467	rBV	5273514	5025340	63.19%	11.571%
11	11.392	1578	1582	1586	rBV	2367884	2209435	27.78%	5.087%
12	11.927	1669	1673	1686	rBV2	452111	618555	7.78%	1.424%
13	12.380	1746	1750	1753	rBV	290669	242803	3.05%	0.559%
14	12.633	1790	1793	1798	rBV	76384	83972	1.06%	0.193%
15	12.716	1804	1807	1817	rBV	280201	406784	5.12%	0.937%
16	12.992	1848	1854	1857	rBV	7638732	7952644	100.00%	18.311%
17	13.604	1955	1958	1962	rVB	175850	153971	1.94%	0.355%
18	13.892	2003	2007	2023	rBV	570307	974814	12.26%	2.245%
19	14.039	2028	2032	2036	rBV	2672060	2413963	30.35%	5.558%
20	14.516	2108	2113	2115	rBV2	81591	92485	1.16%	0.213%
21	15.174	2221	2225	2229	rVB	83677	97601	1.23%	0.225%
22	15.521	2278	2284	2288	rBV	1972219	2432040	30.58%	5.600%
23	15.563	2288	2291	2296	rVB	79453	102627	1.29%	0.236%
24	16.004	2362	2366	2371	rVB2	60125	90027	1.13%	0.207%
25	16.074	2373	2378	2386	rBV5	46155	137211	1.73%	0.316%

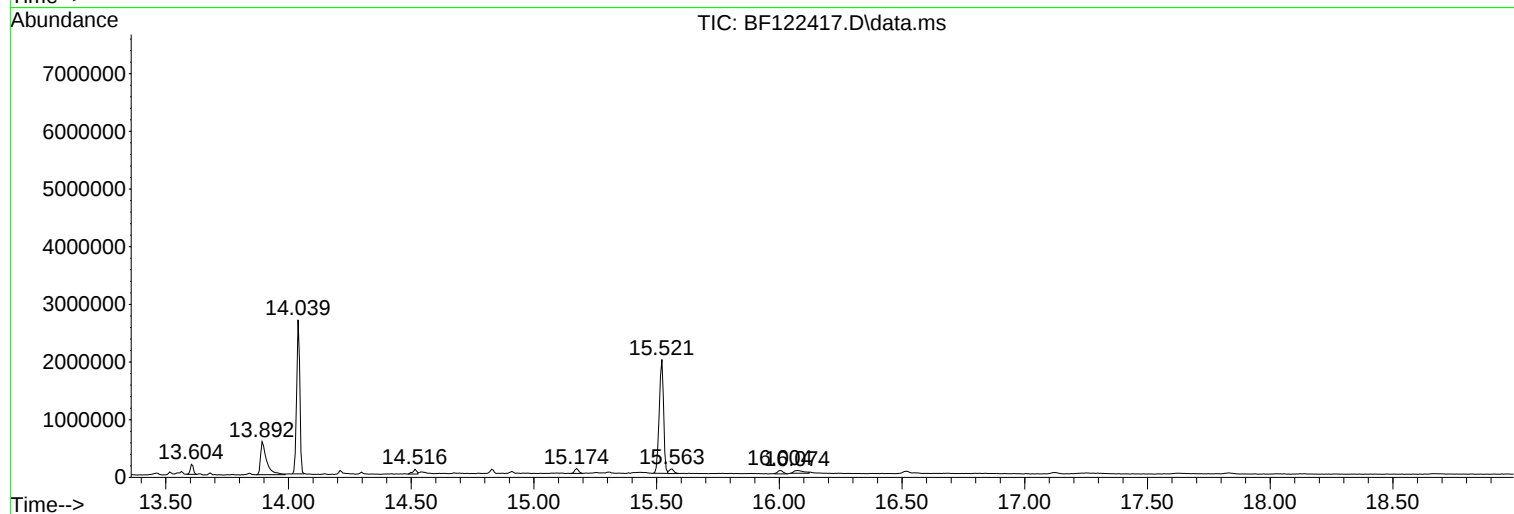
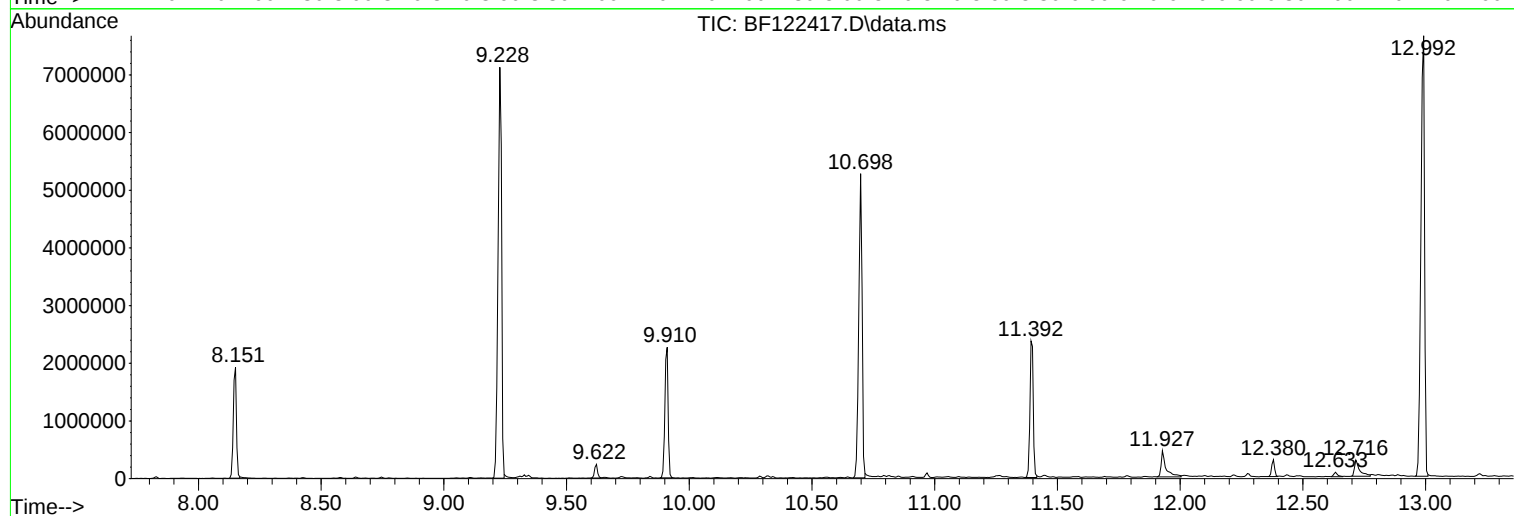
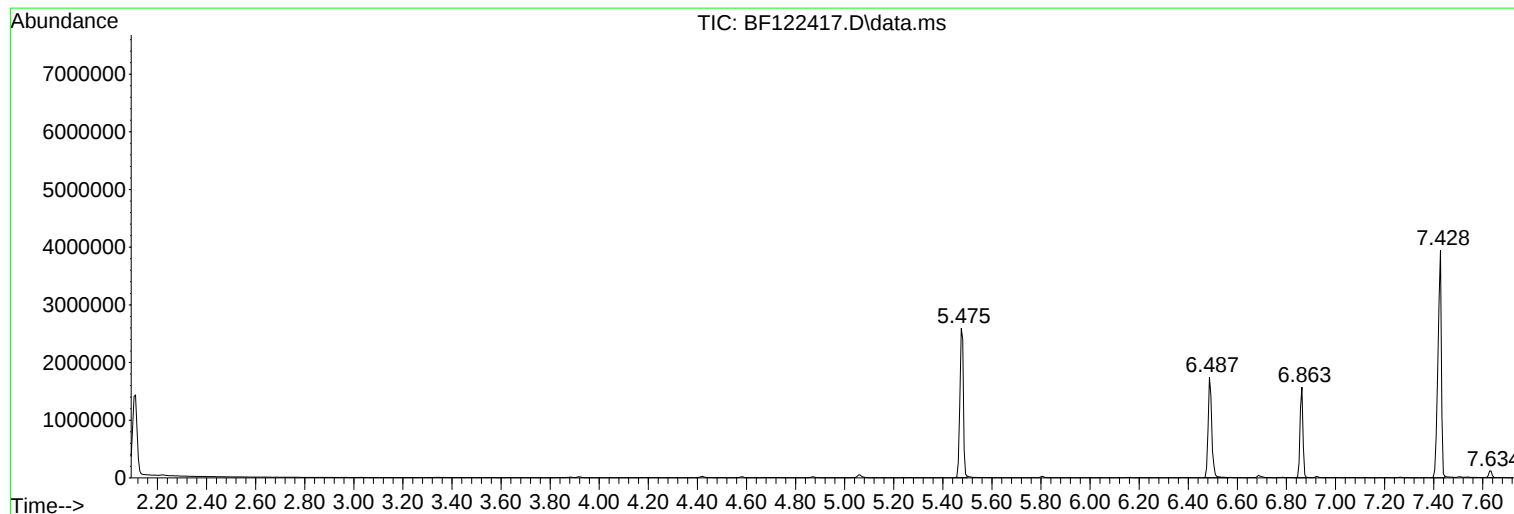
Sum of corrected areas: 43430094

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122417.D
Acq On : 20 Nov 2020 22:25
Operator : JU/CG
Sample : L4829-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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_F\Data\BF112020\
Data File : BF122417.D
Acq On : 20 Nov 2020 22:25
Operator : JU/CG
Sample : L4829-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

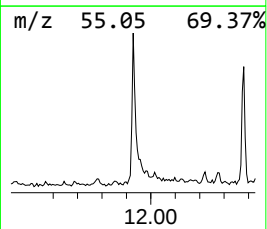
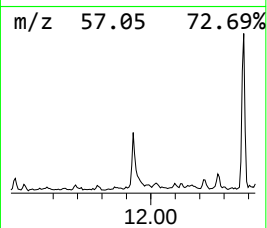
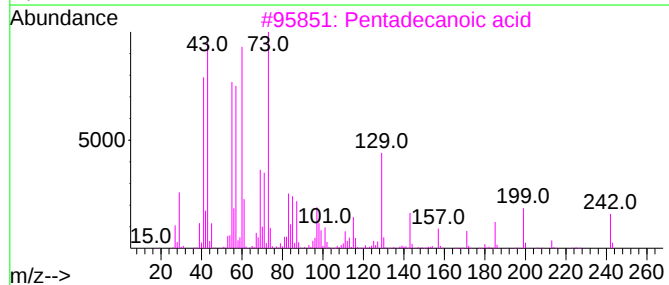
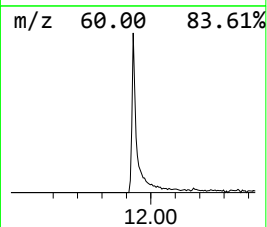
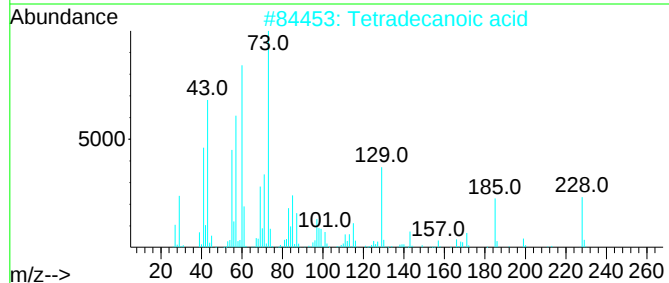
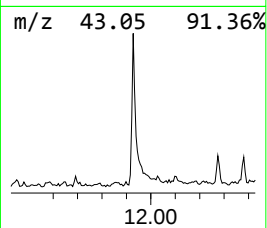
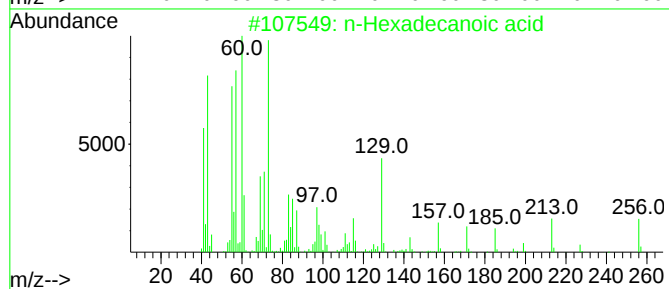
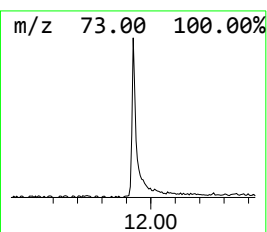
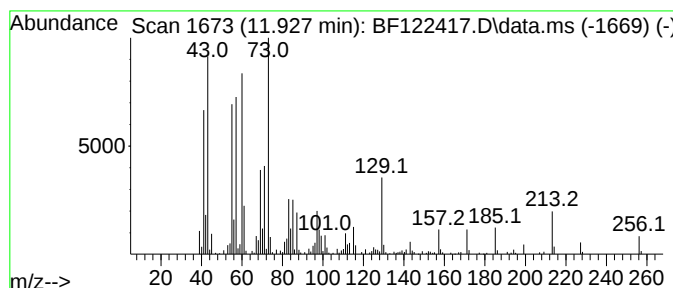
Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.927	5.60 ng	618555	Phenanthrene-d10	11.392	
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	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122417.D
Acq On : 20 Nov 2020 22:25
Operator : JU/CG
Sample : L4829-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

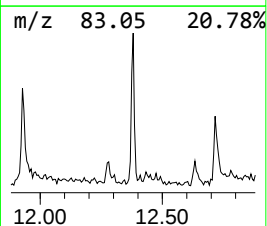
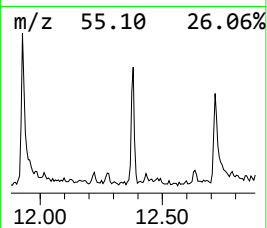
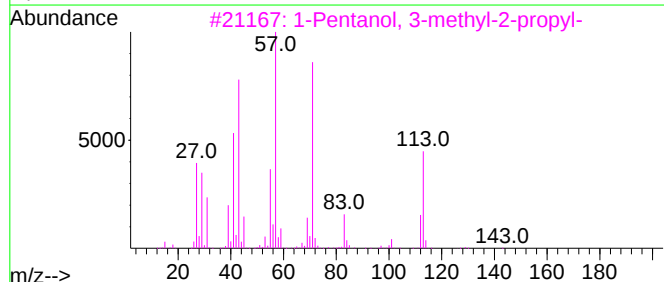
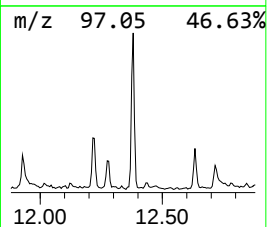
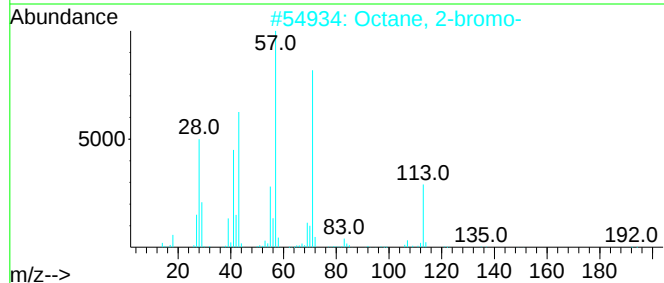
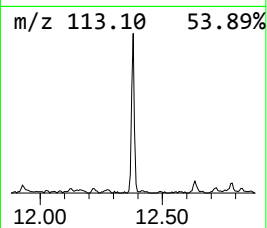
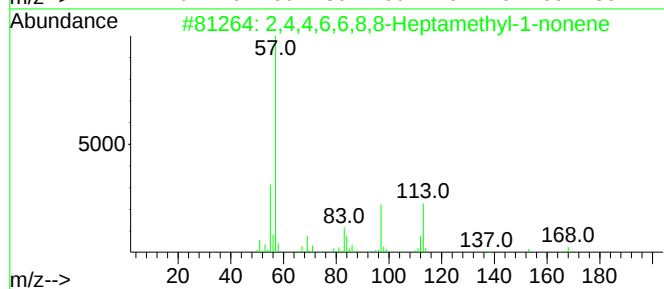
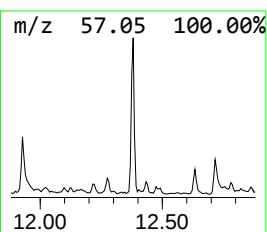
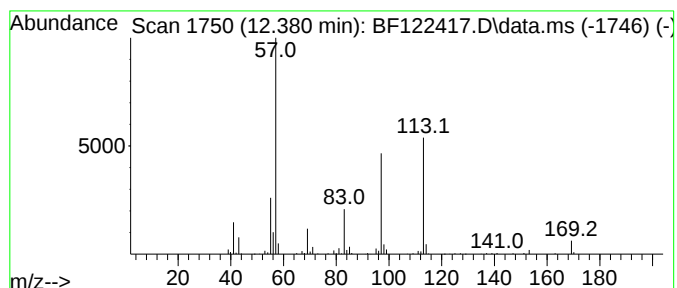
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown12.380 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.380	2.20 ng	242803	Phenanthrene-d10	11.392

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	43
2			Octane, 2-bromo-	192	C8H17Br	000557-35-7	43
3			1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40
4			Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	32
5			Vardenafil	488	C23H32N6O4S	224785-90-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122417.D
Acq On : 20 Nov 2020 22:25
Operator : JU/CG
Sample : L4829-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

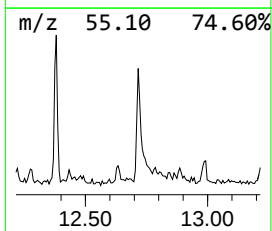
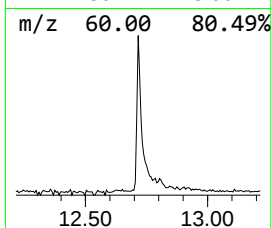
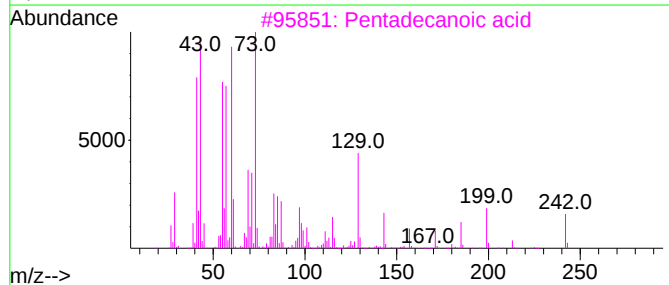
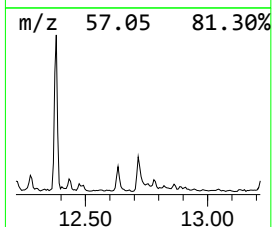
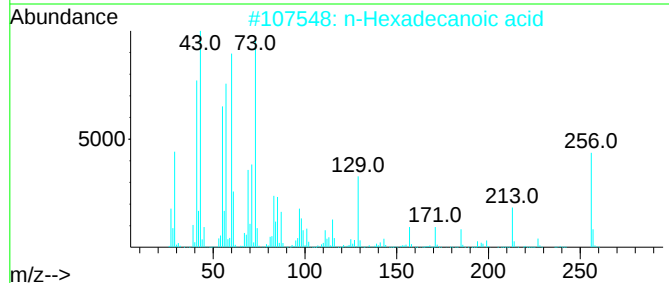
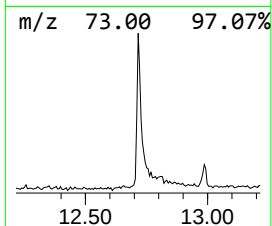
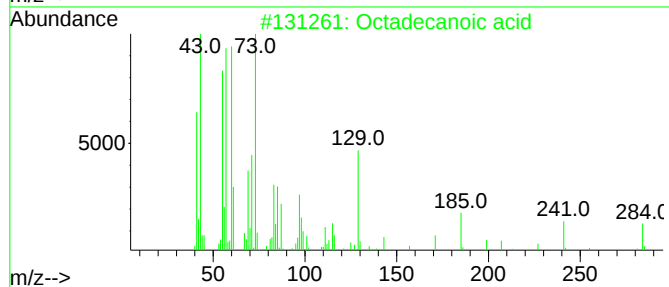
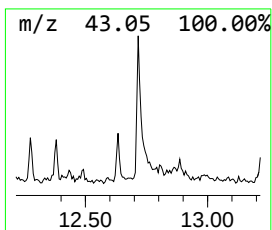
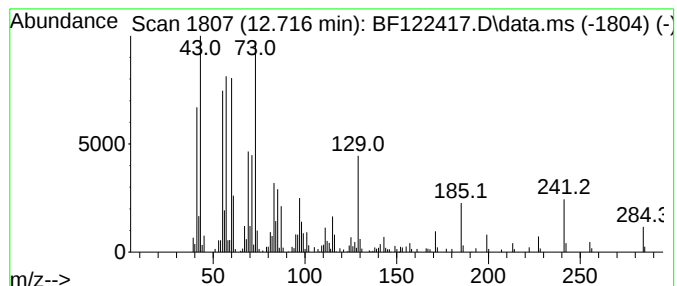
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
12.716	3.68 ng	406784	Phenanthrene-d10	11.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122417.D
Acq On : 20 Nov 2020 22:25
Operator : JU/CG
Sample : L4829-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

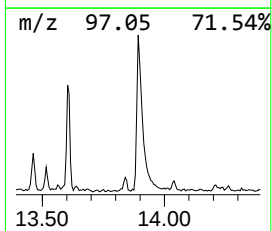
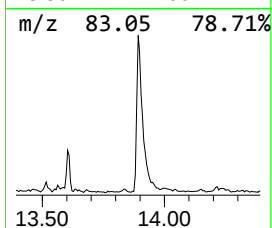
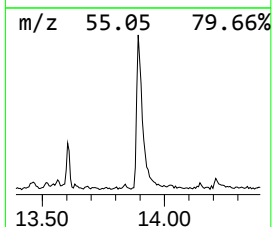
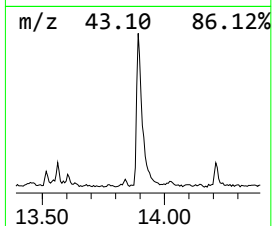
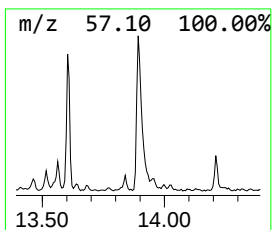
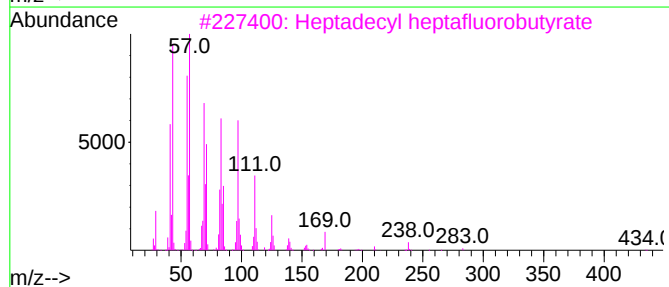
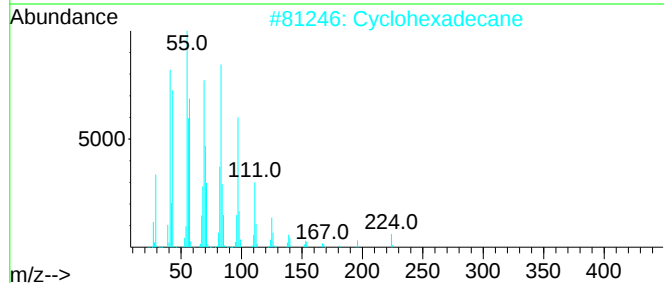
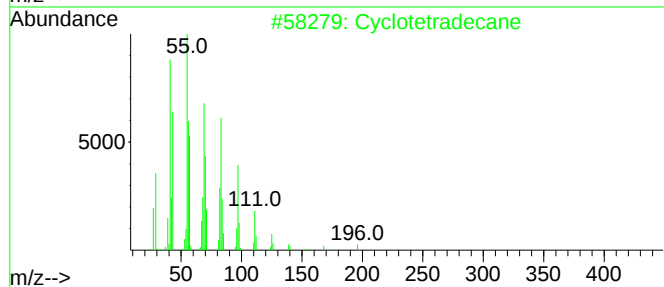
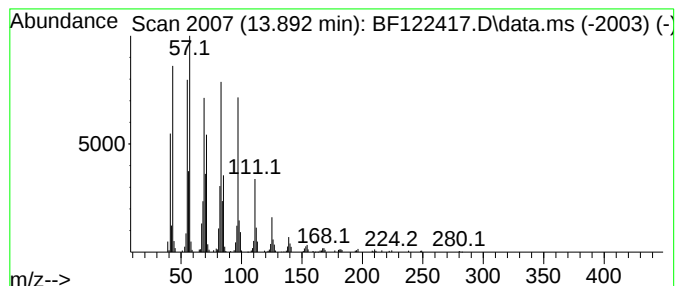
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Cyclotetradecane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.892	8.08 ng	974814	Chrysene-d12	14.039

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclotetradecane	196	C14H28	000295-17-0	96
2			Cyclohexadecane	224	C16H32	000295-65-8	95
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
5			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112020\
Data File : BF122417.D
Acq On : 20 Nov 2020 22:25
Operator : JU/CG
Sample : L4829-04
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MW-4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110920.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 ...	11.927	5.6	ng	618555	4	11.392	2209440	20.0
unknown12.380	12.380	2.2	ng	242803	4	11.392	2209440	20.0
Octadecanoic acid	12.716	3.7	ng	406784	4	11.392	2209440	20.0
Cyclotetradecane	13.892	8.1	ng	974814	5	14.039	2413960	20.0