

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
 Data File : BF127985.D
 Acq On : 28 Apr 2022 17:13
 Operator : CG\JU
 Sample : N2588-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MH-2

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-BF042222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127985.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.551	550	555	558	rBV	2372928	2172114	83.90%	12.104%
2	6.551	720	725	728	rBV	2305127	2247429	86.80%	12.523%
3	6.928	786	789	793	rVB	657424	514340	19.87%	2.866%
4	7.492	880	885	888	rBV	1690014	1522838	58.82%	8.486%
5	8.210	1003	1007	1011	rBV	718374	645654	24.94%	3.598%
6	9.286	1185	1190	1193	rBV	2920058	2589073	100.00%	14.427%
7	9.969	1302	1306	1313	rVB	888691	726953	28.08%	4.051%
8	10.763	1436	1441	1444	rBV	1693489	1588267	61.35%	8.850%
9	11.463	1556	1560	1564	rBV	873197	725982	28.04%	4.045%
10	11.804	1603	1618	1623	rBV8	40805	162189	6.26%	0.904%
11	11.975	1644	1647	1655	rBV	132341	123363	4.76%	0.687%
12	12.227	1687	1690	1694	rVB	1669492	1382575	53.40%	7.704%
13	12.639	1748	1760	1765	rBV6	40296	152866	5.90%	0.852%
14	13.051	1825	1830	1833	rBV	2312515	2154735	83.22%	12.007%
15	14.074	1991	2004	2006	rBV3	50638	111373	4.30%	0.621%
16	14.104	2006	2009	2022	rVB	484153	520390	20.10%	2.900%
17	14.957	2150	2154	2159	rVB	126794	124714	4.82%	0.695%
18	15.615	2261	2266	2272	rBV	374571	481025	18.58%	2.680%

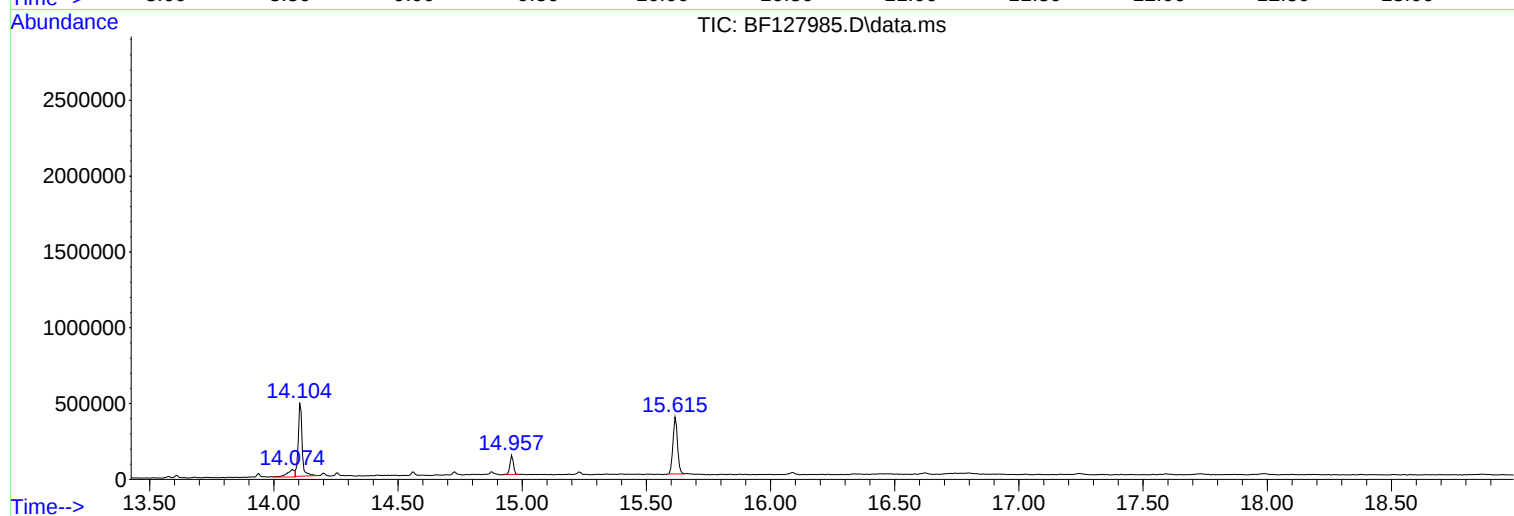
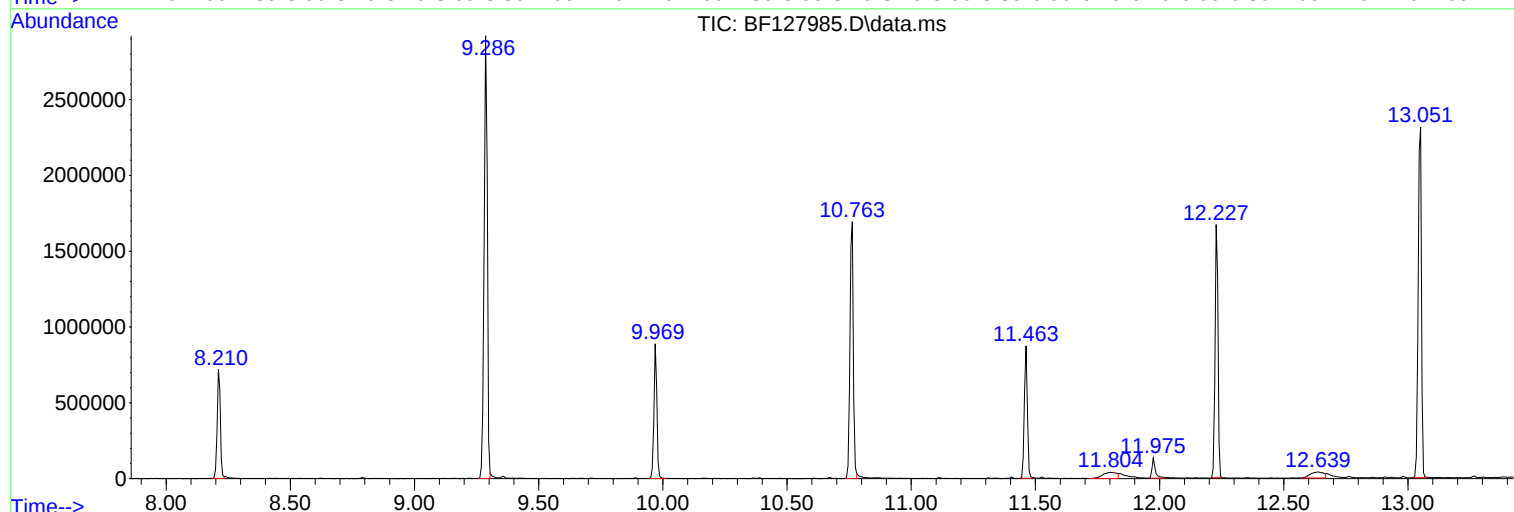
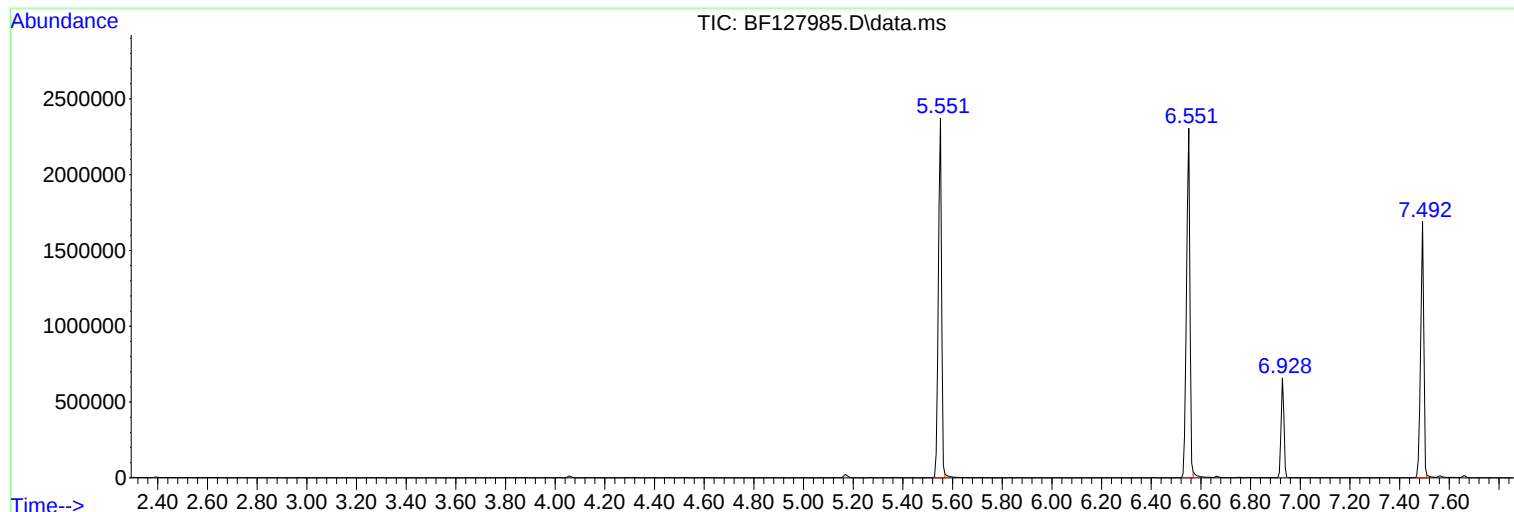
Sum of corrected areas: 17945880

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
Data File : BF127985.D
Acq On : 28 Apr 2022 17:13
Operator : CG\JU
Sample : N2588-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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_F\Data\BF042822\
Data File : BF127985.D
Acq On : 28 Apr 2022 17:13
Operator : CG\JU
Sample : N2588-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

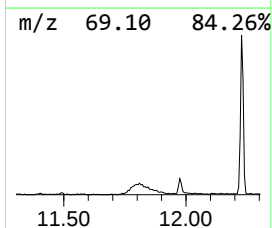
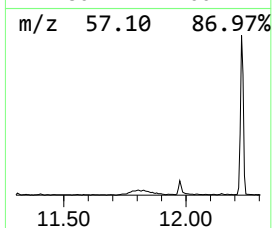
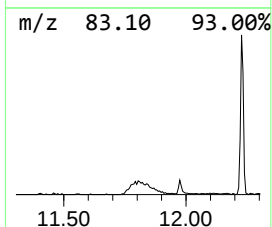
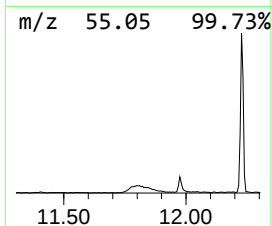
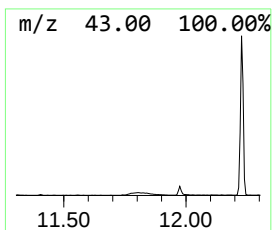
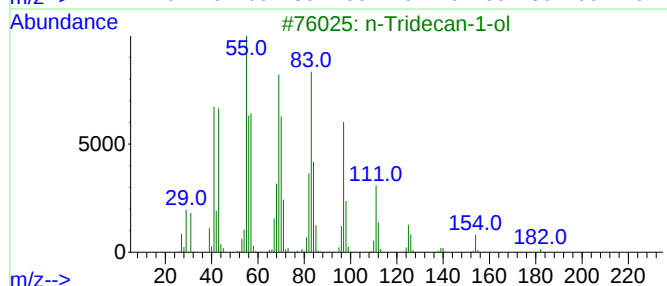
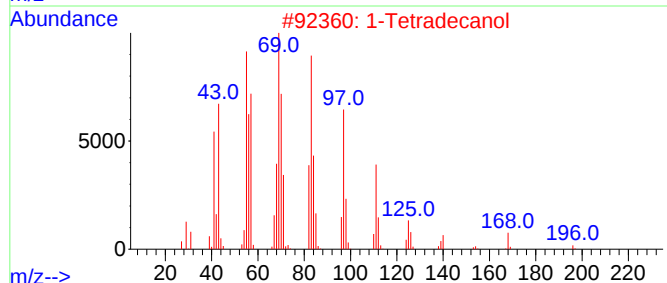
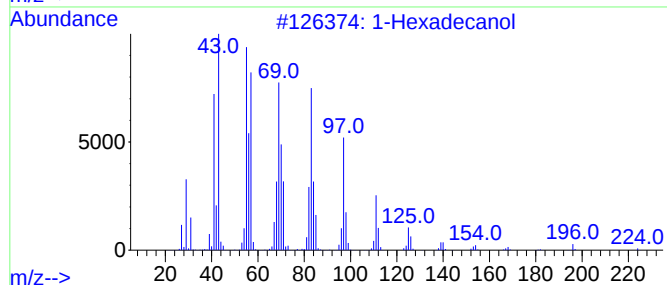
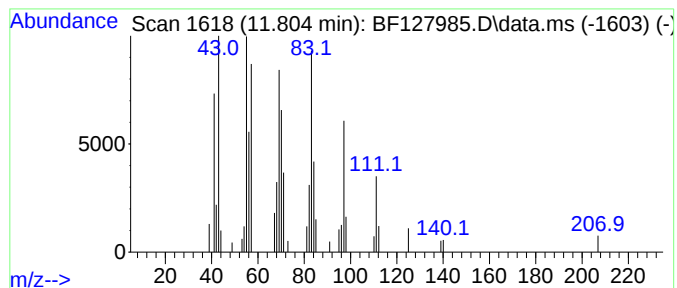
Instrument :
BNA_F
ClientSampleId :
MH-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Hexadecanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.804	4.47 ng	162189	Phenanthrene-d10	11.463	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	95
2	1-Tetradecanol	214	C14H30O	000112-72-1	91
3	n-Tridecan-1-ol	200	C13H28O	000112-70-9	91
4	9-Octadecene, (E)-	252	C18H36	007206-25-9	91
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
Data File : BF127985.D
Acq On : 28 Apr 2022 17:13
Operator : CG\JU
Sample : N2588-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-2

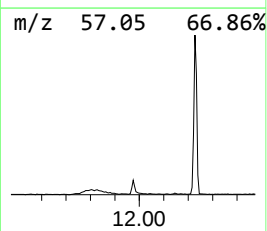
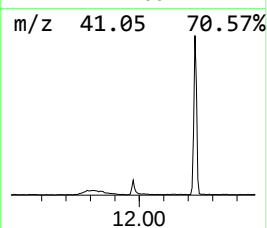
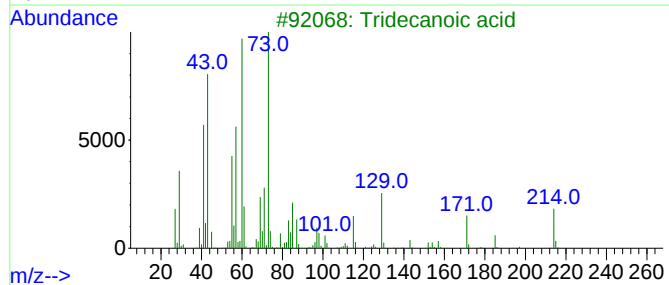
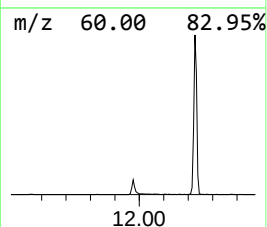
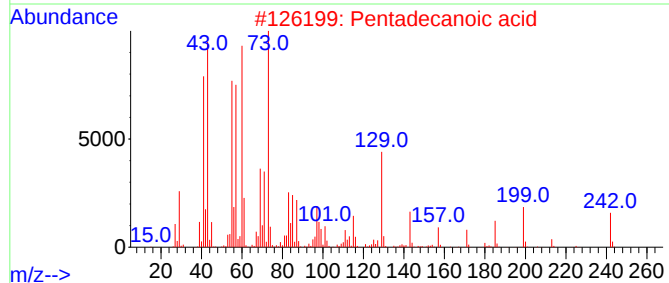
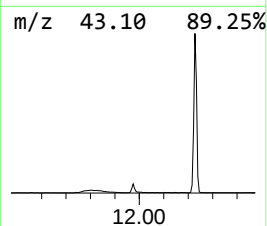
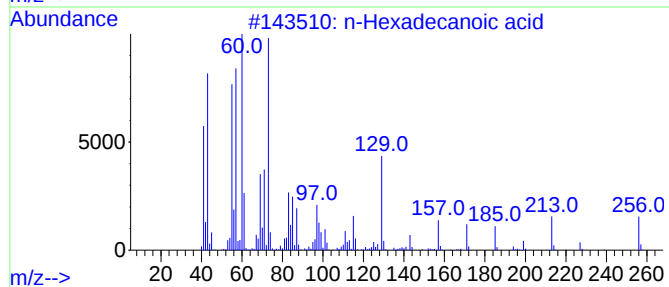
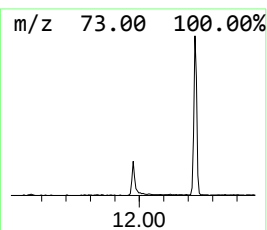
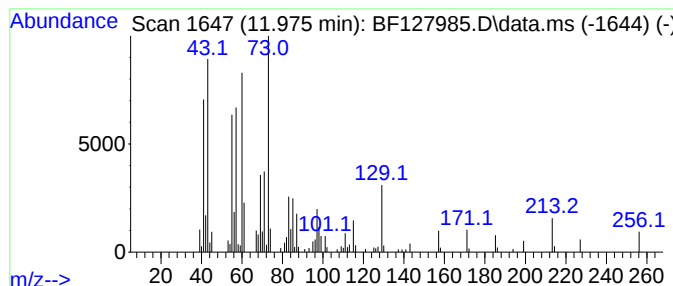
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.975	3.40 ng	123363	Phenanthrene-d10	11.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	76
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
Data File : BF127985.D
Acq On : 28 Apr 2022 17:13
Operator : CG\JU
Sample : N2588-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-2

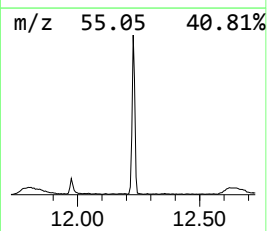
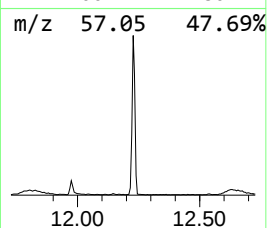
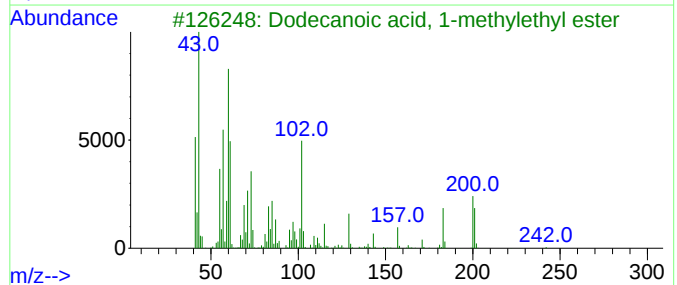
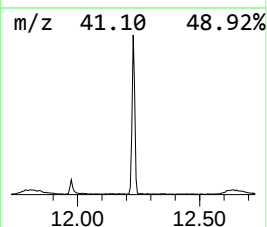
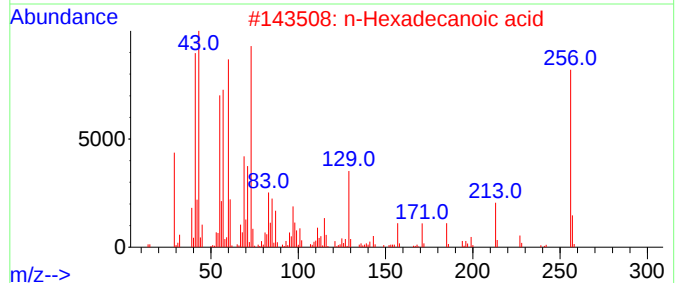
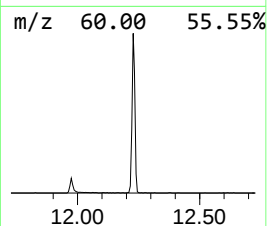
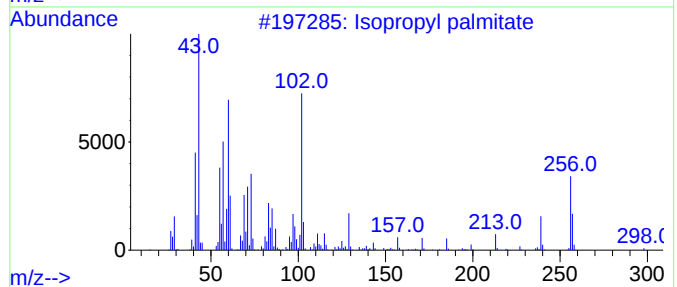
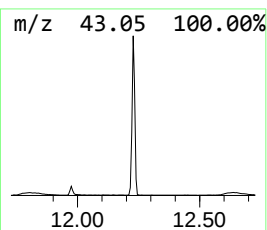
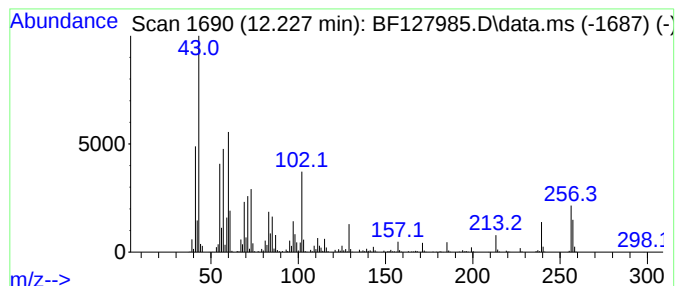
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Isopropyl palmitate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.227	38.09 ng	1382580	Phenanthrene-d10	11.463

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl palmitate	298	C19H38O2	000142-91-6	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	43
4			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	38
5			Methyl-.beta.-D-thiogalactoside	194	C7H14O6	001824-94-8	32



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
Data File : BF127985.D
Acq On : 28 Apr 2022 17:13
Operator : CG\JU
Sample : N2588-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

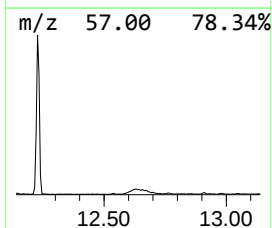
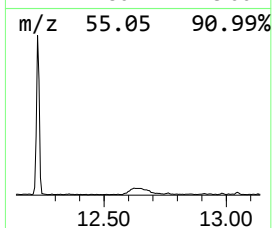
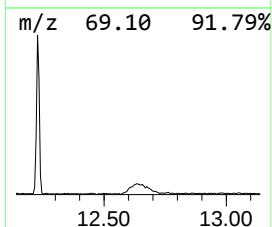
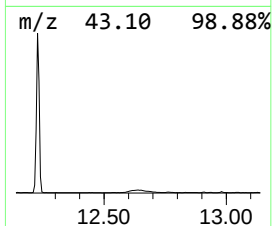
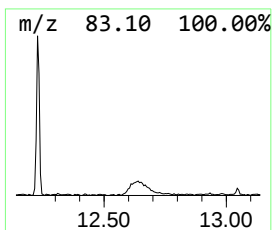
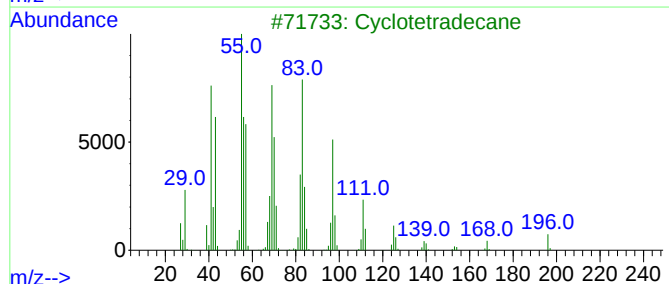
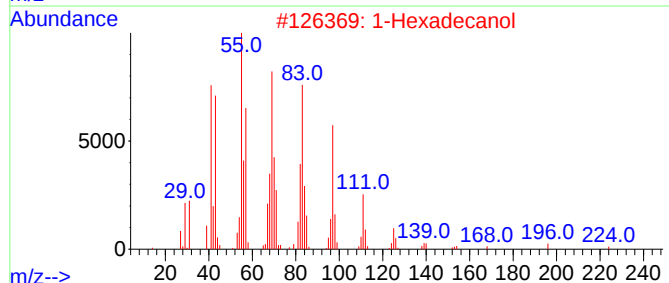
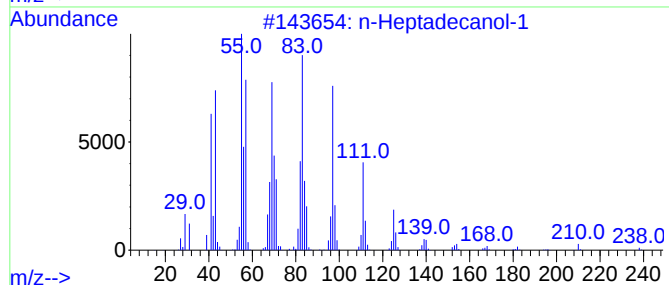
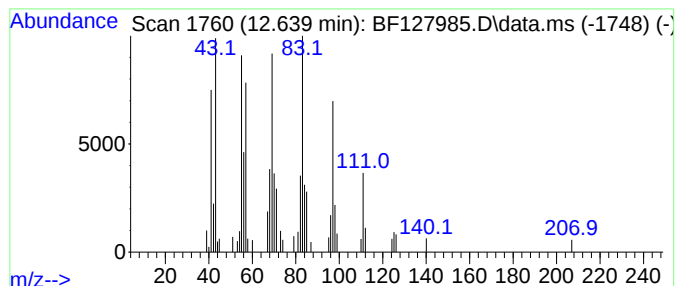
Instrument :
BNA_F
ClientSampleId :
MH-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Heptadecanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.639	4.21 ng	152866	Phenanthrene-d10		11.463	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Heptadecanol-1		256	C17H36O	001454-85-9	91
2	1-Hexadecanol		242	C16H34O	036653-82-4	81
3	Cyclotetradecane		196	C14H28	000295-17-0	72
4	n-Nonadecanol-1		284	C19H40O	001454-84-8	70
5	Trifluoroacetoxy hexadecane		338	C18H33F3O2	006222-03-3	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
Data File : BF127985.D
Acq On : 28 Apr 2022 17:13
Operator : CG\JU
Sample : N2588-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-2

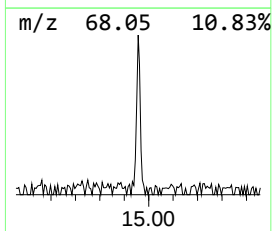
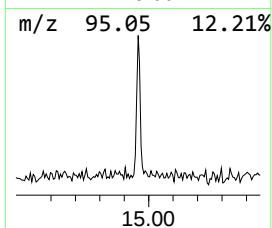
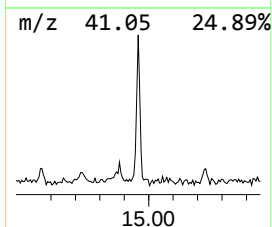
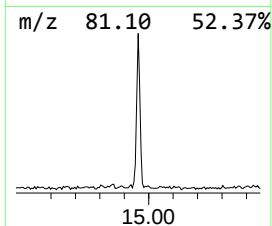
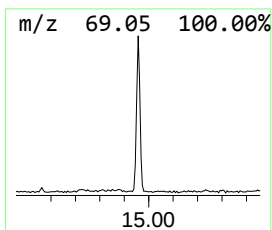
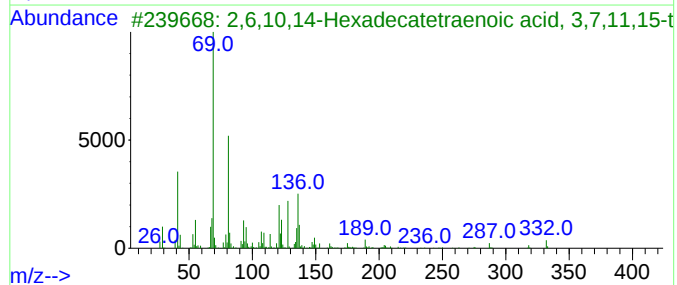
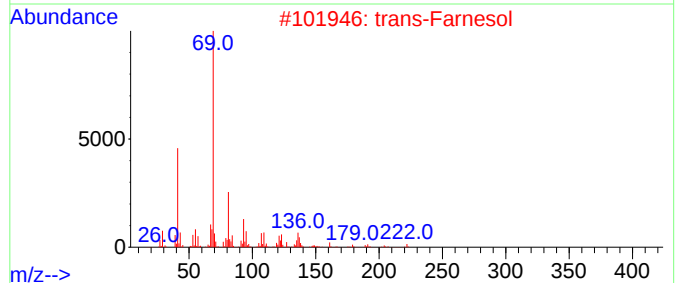
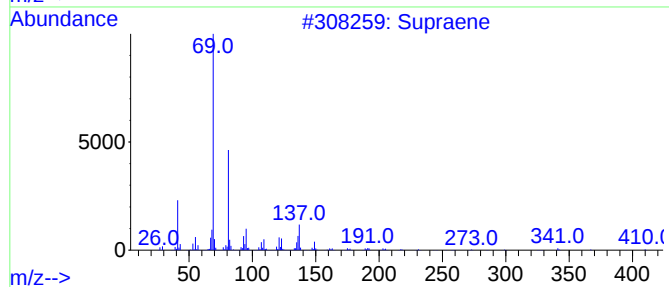
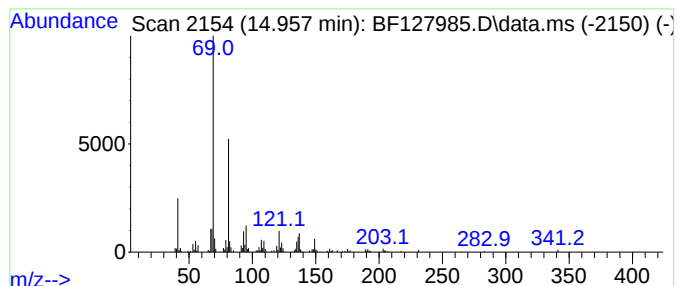
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Supraene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.957	5.19 ng	124714	Perylene-d12	15.615

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	87
2			trans-Farnesol	222	C15H26O	000106-28-5	72
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	58
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042822\
Data File : BF127985.D
Acq On : 28 Apr 2022 17:13
Operator : CG\JU
Sample : N2588-03
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexadecanol	11.804	4.5	ng	162189	4	11.463	725982	20.0
n-Hexadecanoic ...	11.975	3.4	ng	123363	4	11.463	725982	20.0
Isopropyl palmi...	12.227	38.1	ng	1382580	4	11.463	725982	20.0
n-Heptadecanol-1	12.639	4.2	ng	152866	4	11.463	725982	20.0
Supraene	14.957	5.2	ng	124714	6	15.615	481025	20.0