

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
 Data File : BF124233.D
 Acq On : 10 Jun 2021 15:01
 Operator : JU/CG
 Sample : M2650-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DELAWANNA-RT10-STOCKPILE-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_F\METHODS\8270-BF060321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124233.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.187	13	17	22	rBB2	15650	17744	1.28%	0.215%
2	5.057	502	505	512	rVB	40229	48171	3.49%	0.584%
3	5.475	572	576	590	rBB	963989	880572	63.72%	10.681%
4	6.492	744	749	752	rBV	949383	881743	63.81%	10.695%
5	6.681	778	781	788	rBV	15462	16625	1.20%	0.202%
6	6.845	806	809	813	rBB	258688	202497	14.65%	2.456%
7	7.410	901	905	908	rBV	684906	596668	43.18%	7.237%
8	8.128	1024	1027	1031	rBV	312703	258733	18.72%	3.138%
9	9.204	1206	1210	1213	rBV	1372921	1190801	86.17%	14.444%
10	9.598	1274	1277	1280	rBV	237949	172533	12.49%	2.093%
11	9.886	1322	1326	1329	rBV	427049	322617	23.35%	3.913%
12	10.675	1456	1460	1464	rBV	980900	871951	63.10%	10.577%
13	11.374	1575	1579	1582	rBV	420647	356858	25.82%	4.329%
14	11.898	1665	1668	1677	rBV2	103699	99300	7.19%	1.204%
15	12.586	1779	1785	1789	rBV	13463	15701	1.14%	0.190%
16	12.680	1798	1801	1807	rBV3	20405	19382	1.40%	0.235%
17	12.963	1844	1849	1852	rBV	1391379	1381848	100.00%	16.761%
18	13.863	1997	2002	2016	rBV4	84262	197650	14.30%	2.397%
19	14.015	2024	2028	2031	rVB	306859	270421	19.57%	3.280%
20	14.474	2104	2106	2109	rBV2	17684	14847	1.07%	0.180%
21	14.786	2156	2159	2164	rVB5	18087	18040	1.31%	0.219%
22	14.862	2168	2172	2176	rVB2	22032	27629	2.00%	0.335%
23	15.121	2214	2216	2221	rBV5	14414	18790	1.36%	0.228%
24	15.492	2275	2279	2284	rBV	201963	260635	18.86%	3.161%
25	15.945	2351	2356	2362	rVB6	20325	33063	2.39%	0.401%
26	16.033	2365	2371	2372	rBV5	13200	19952	1.44%	0.242%
27	17.045	2538	2543	2545	rBV5	10400	17793	1.29%	0.216%
28	17.204	2566	2570	2572	rBV4	9336	15186	1.10%	0.184%
29	18.139	2725	2729	2733	rVB5	9107	16466	1.19%	0.200%

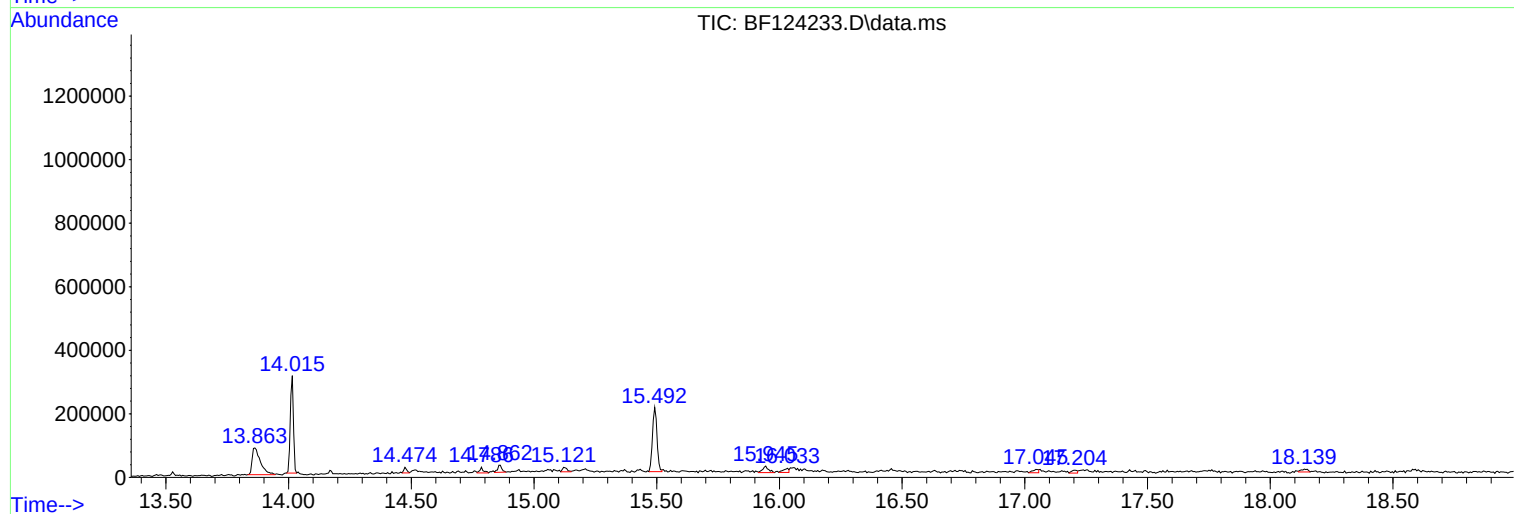
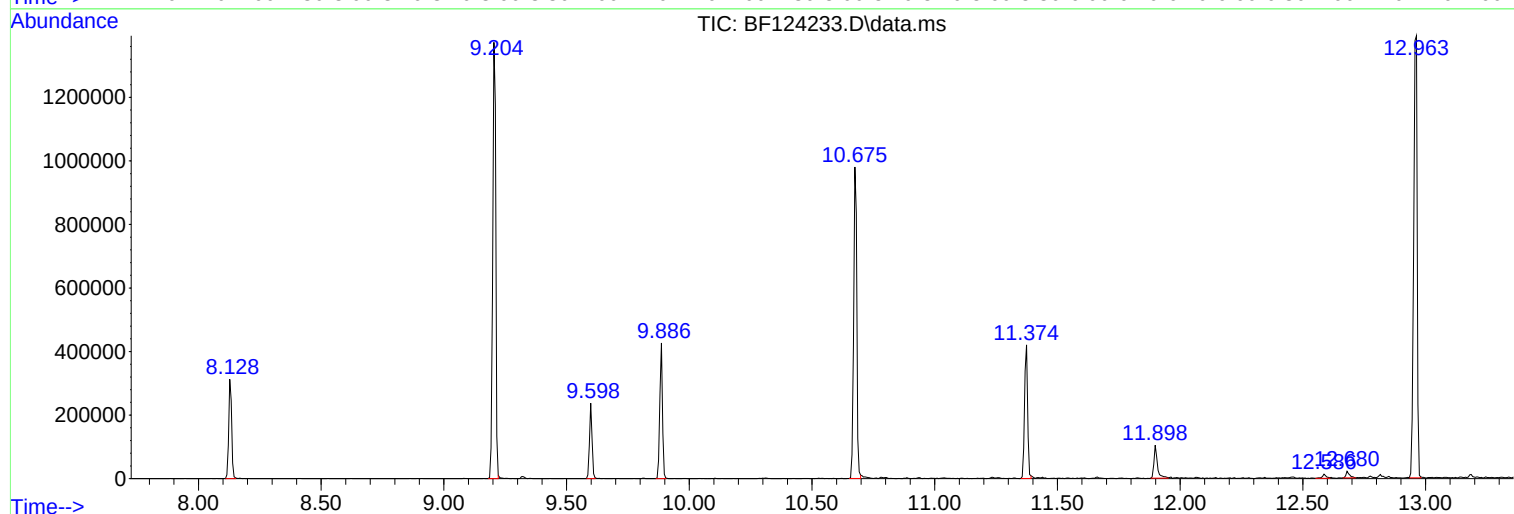
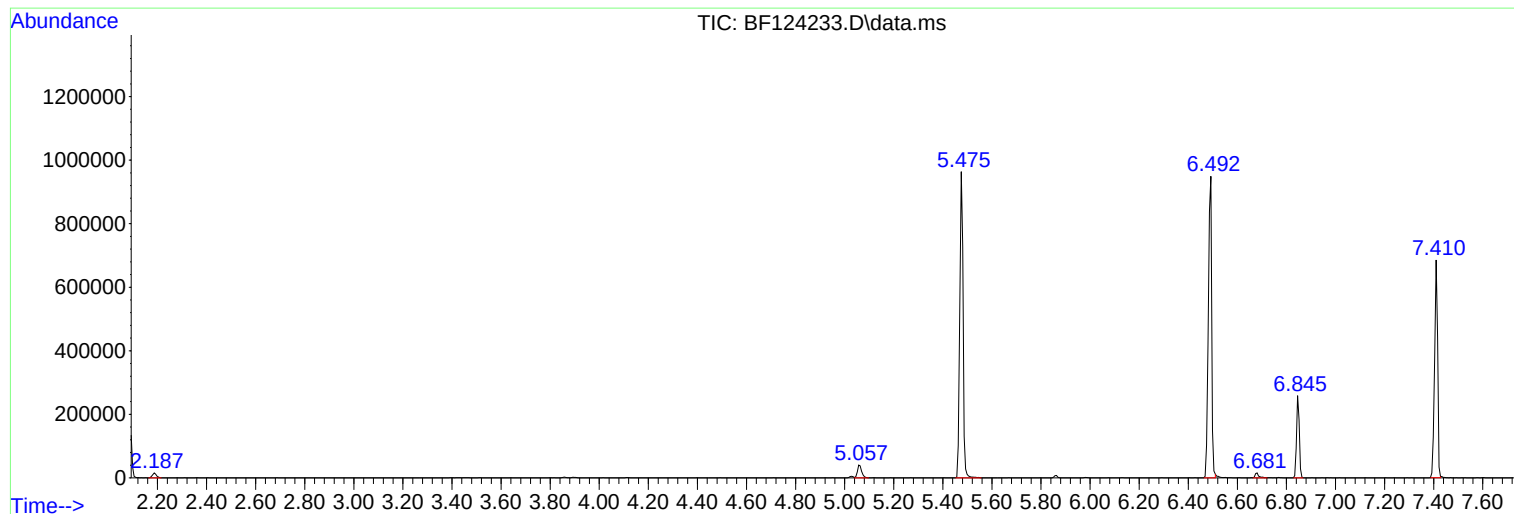
Sum of corrected areas: 8244216

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124233.D
Acq On : 10 Jun 2021 15:01
Operator : JU/CG
Sample : M2650-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DELAWANNA-RT10-STOCKPILE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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\BF061021\
Data File : BF124233.D
Acq On : 10 Jun 2021 15:01
Operator : JU/CG
Sample : M2650-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DELAWANNA-RT10-STOCKPILE-1

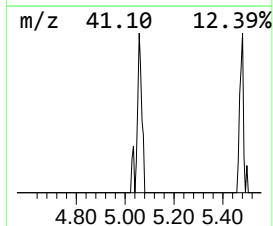
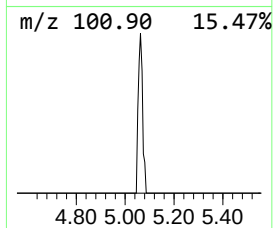
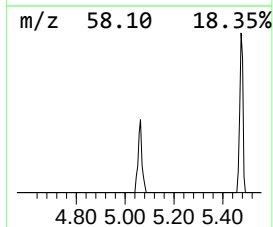
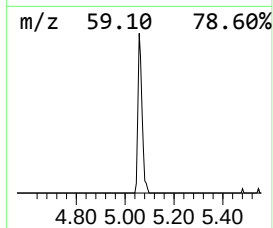
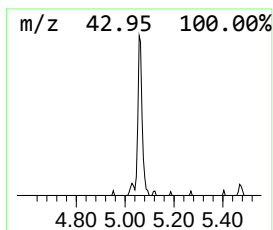
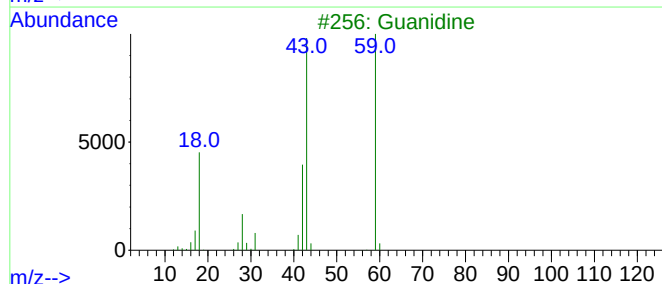
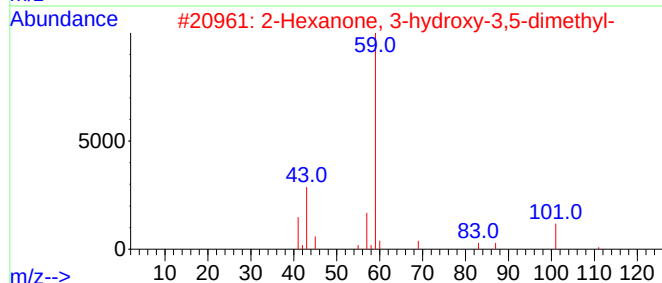
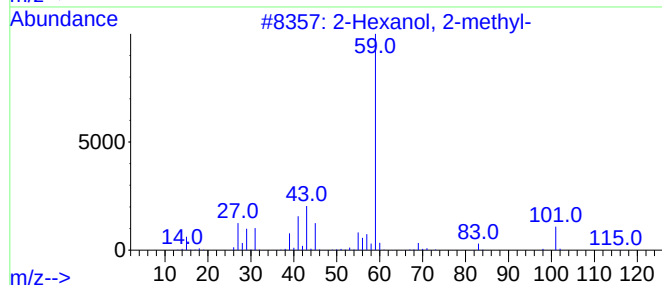
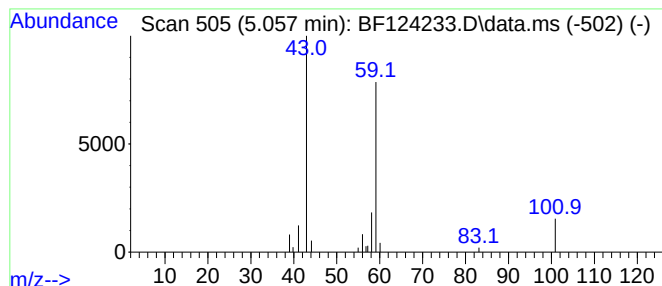
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown5.057 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.057	4.76 ng	48171	1,4-Dichlorobenzene-d4	6.845

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-		116	C7H16O		000625-23-0	38
2	2-Hexanone, 3-hydroxy-3,5-dimethyl-		144	C8H16O2		006321-14-8	36
3	Guanidine		59	CH5N3		000113-00-8	9
4	Oxirane, [(1-methylethoxy)methyl]-		116	C6H12O2		004016-14-2	9
5	3-Hexanol, 4-ethyl-		130	C8H18O		019780-44-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124233.D
Acq On : 10 Jun 2021 15:01
Operator : JU/CG
Sample : M2650-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DELAWANNA-RT10-STOCKPILE-1

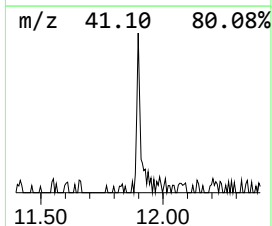
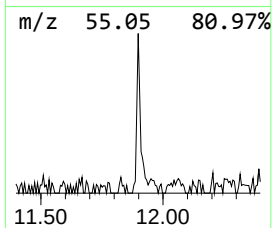
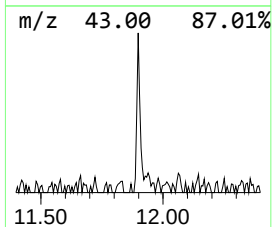
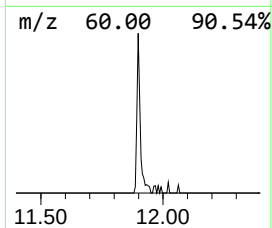
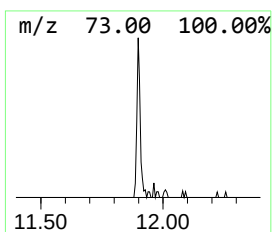
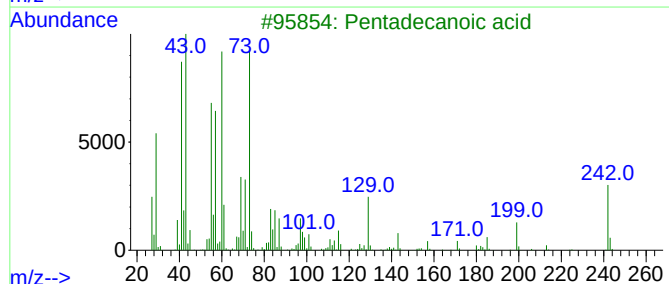
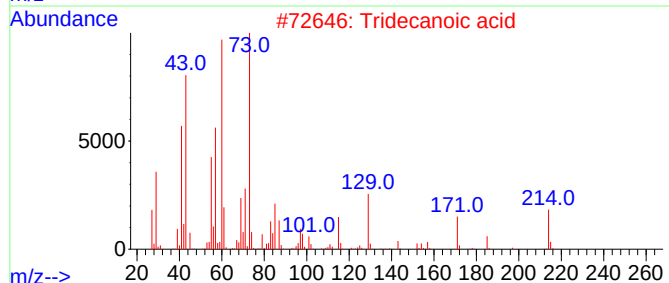
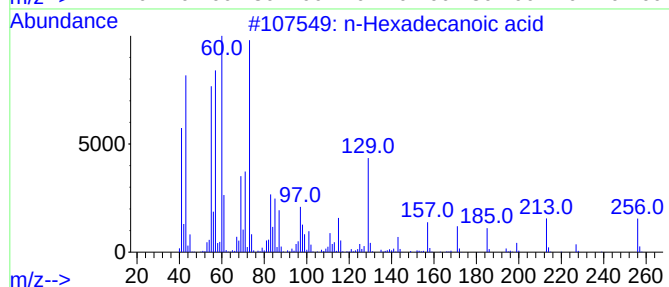
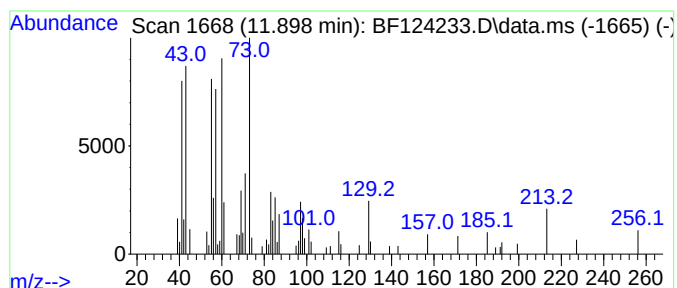
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.898	5.57 ng	99300	Phenanthrene-d10	11.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
2			Tridecanoic acid	214	C13H26O2	000638-53-9	59
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124233.D
Acq On : 10 Jun 2021 15:01
Operator : JU/CG
Sample : M2650-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

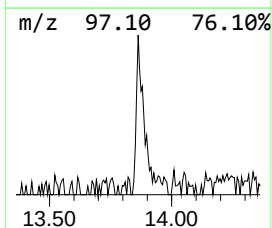
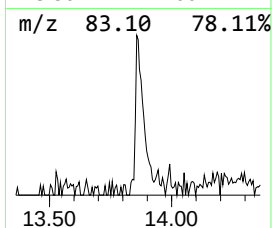
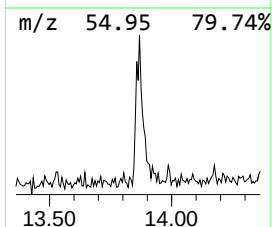
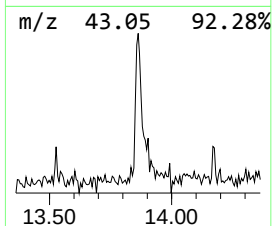
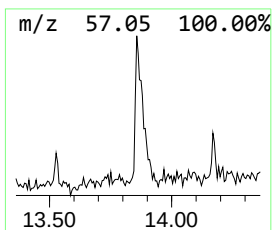
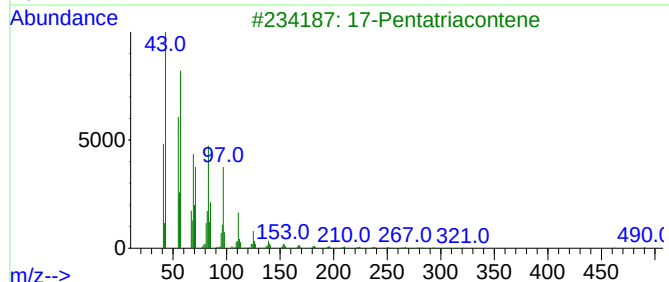
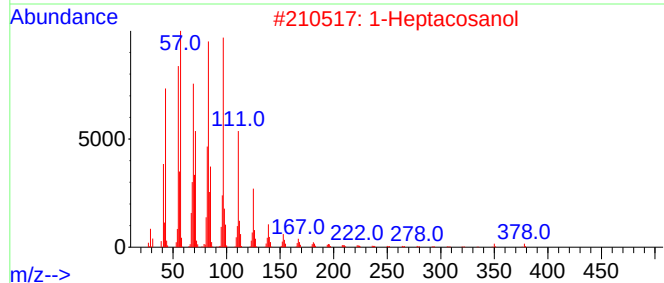
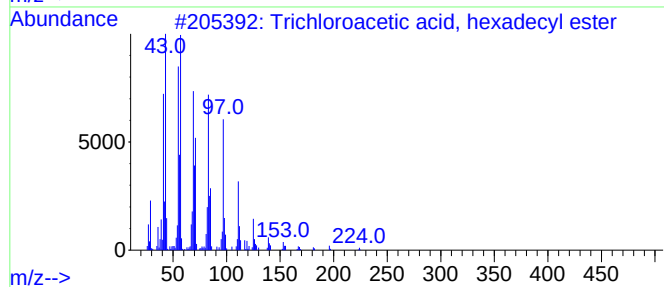
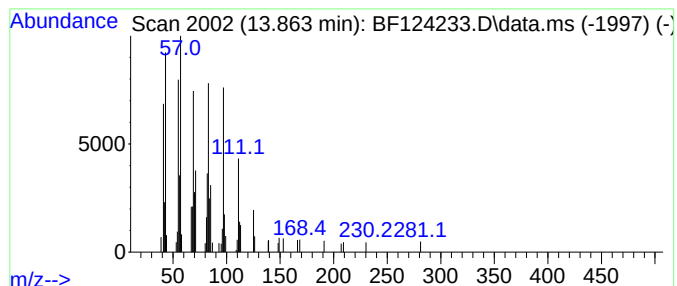
Instrument :
BNA_F
ClientSampleId :
DELAWANNA-RT10-STOCKPILE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Trichloroacetic acid, hexad... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.863	14.62 ng	197650	Chrysene-d12	14.015	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	17-Pentatriacontene	491	C35H70	006971-40-0	91
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
5	Octacosanol	410	C28H58O	000557-61-9	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124233.D
Acq On : 10 Jun 2021 15:01
Operator : JU/CG
Sample : M2650-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DELAWANNA-RT10-STOCKPILE-1

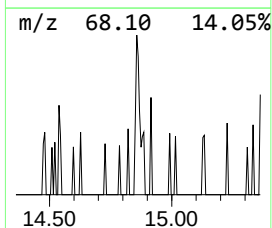
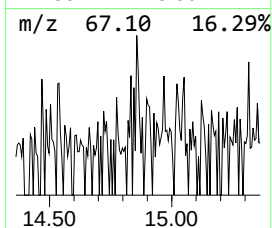
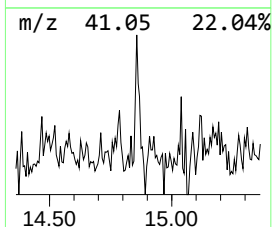
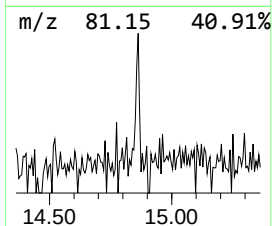
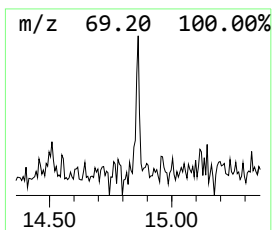
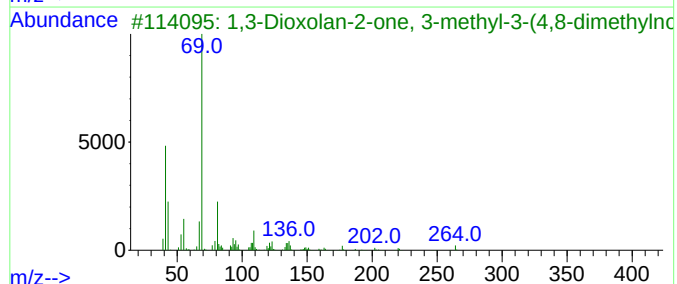
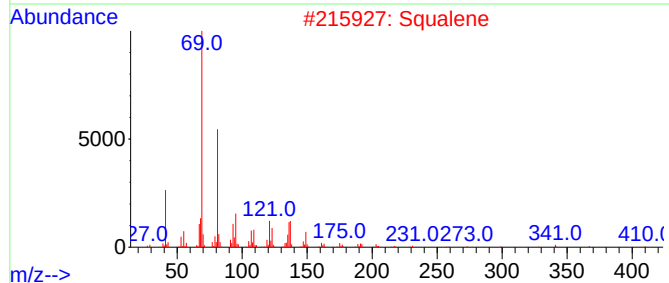
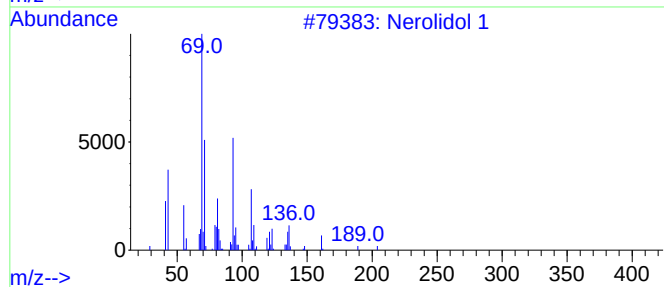
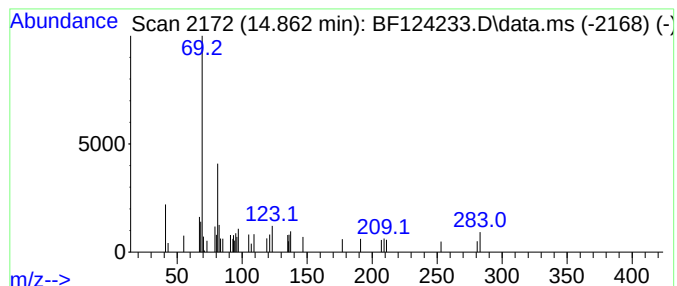
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Nerolidol 1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.863	2.12 ng	27629	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nerolidol 1	222	C15H26O	1000285-43-5	52
2			Squalene	410	C30H50	000111-02-4	50
3			1,3-Dioxolan-2-one, 3-methyl-3-(...	264	C16H24O3	336879-76-6	50
4			Supraene	410	C30H50	007683-64-9	50
5			5-Hexen-1-ol, 2-(2-methyl-1-prop...	154	C10H18O	018675-19-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124233.D
Acq On : 10 Jun 2021 15:01
Operator : JU/CG
Sample : M2650-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DELAWANNA-RT10-STOCKPILE-1

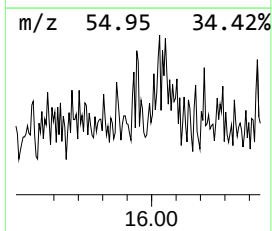
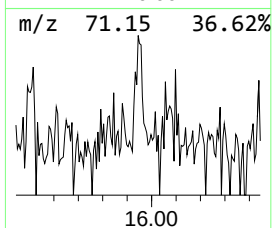
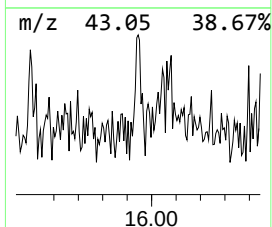
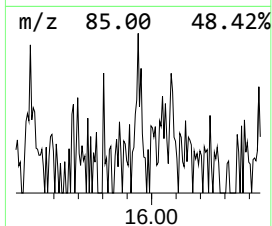
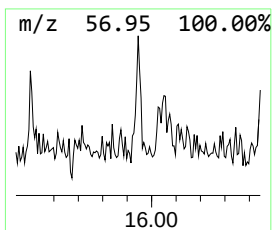
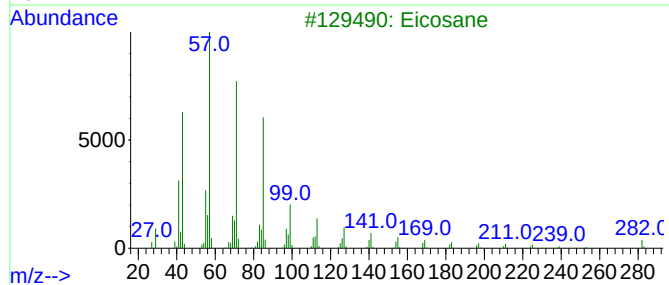
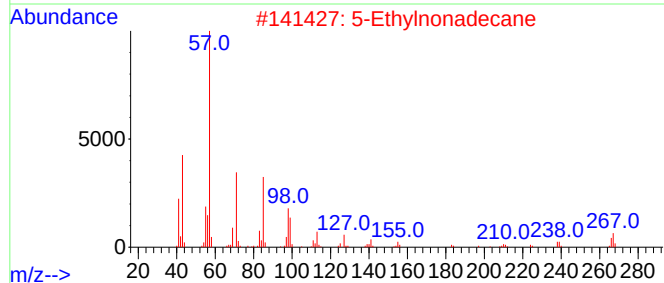
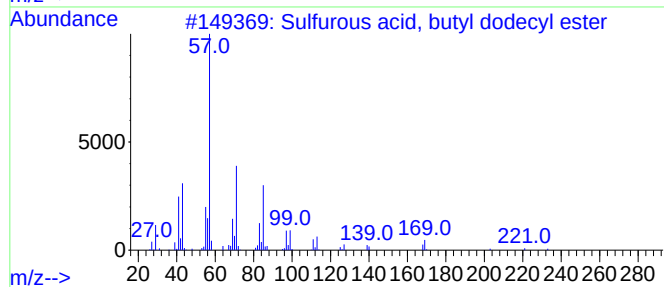
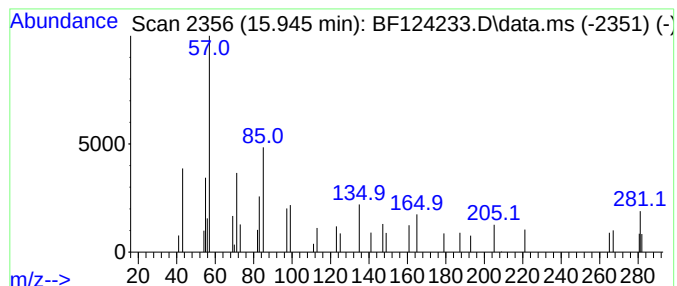
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown15.945 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	2.54 ng	33063	Perylene-d12	15.492

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl dodecyl ester	306	C16H34O3S	1000309-17-9	37
2			5-Ethylnonadecane	296	C21H44	1000360-43-1	32
3			Eicosane	282	C20H42	000112-95-8	25
4			Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	25
5			Heptadecane	240	C17H36	000629-78-7	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF061021\
Data File : BF124233.D
Acq On : 10 Jun 2021 15:01
Operator : JU/CG
Sample : M2650-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DELAWANNA-RT10-STOCKPILE-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF060321.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
unknown5.057	5.057	4.8	ng	48171	1	6.845	202497	20.0
n-Hexadecanoic ...	11.898	5.6	ng	99300	4	11.374	356858	20.0
Trichloroacetic...	13.863	14.6	ng	197650	5	14.015	270421	20.0
Nerolidol 1	14.863	2.1	ng	27629	6	15.492	260635	20.0
unknown15.945	15.945	2.5	ng	33063	6	15.492	260635	20.0