

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
 Data File : BF136926.D
 Acq On : 04 Jan 2024 01:03
 Operator : CG\JU
 Sample : 05897-18
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 GHL-SS-22

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136926.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	490	500	508	rBV2	21992	29568	2.51%	0.303%
2	5.434	565	569	586	rBV	1341832	1177260	100.00%	12.080%
3	5.639	600	604	608	rBV	18284	17656	1.50%	0.181%
4	6.439	736	740	757	rBV	1173322	1100045	93.44%	11.288%
5	6.610	766	769	772	rBV2	16039	16551	1.41%	0.170%
6	6.781	795	798	804	rBV	373181	300798	25.55%	3.087%
7	7.345	890	894	897	rBV	833965	675567	57.38%	6.932%
8	8.057	1012	1015	1018	rBV	403532	326206	27.71%	3.347%
9	8.775	1133	1137	1140	rBV	19603	17614	1.50%	0.181%
10	8.869	1150	1153	1156	rVB	15229	13190	1.12%	0.135%
11	9.133	1195	1198	1202	rBV	1211304	1072731	91.12%	11.007%
12	9.816	1310	1314	1320	rBV	403762	315909	26.83%	3.242%
13	10.610	1445	1449	1459	rVB	731987	610896	51.89%	6.268%
14	10.733	1465	1470	1474	rBV	19270	22627	1.92%	0.232%
15	11.310	1564	1568	1570	rBV	392774	326299	27.72%	3.348%
16	11.333	1570	1572	1575	rVV	51853	39561	3.36%	0.406%
17	11.386	1578	1581	1583	rVB	17303	13989	1.19%	0.144%
18	11.551	1605	1609	1614	rBV5	13586	18001	1.53%	0.185%
19	11.845	1654	1659	1670	rVB	328479	416745	35.40%	4.276%
20	12.245	1723	1727	1733	rVB8	14557	29210	2.48%	0.300%
21	12.374	1746	1749	1751	rBV3	16555	18613	1.58%	0.191%
22	12.527	1772	1775	1777	rBV	130434	115775	9.83%	1.188%
23	12.633	1788	1793	1804	rVB	237250	335189	28.47%	3.439%
24	12.757	1809	1814	1820	rVB2	94582	107324	9.12%	1.101%
25	12.904	1835	1839	1842	rBV	1298513	1085358	92.19%	11.137%
26	13.092	1869	1871	1873	rVB	22819	17175	1.46%	0.176%
27	13.133	1875	1878	1880	rBV4	20464	26997	2.29%	0.277%
28	13.757	1980	1984	1991	rVV2	182502	312954	26.58%	3.211%
29	13.821	1991	1995	2004	rVB2	144422	222114	18.87%	2.279%
30	13.968	2013	2020	2023	rBV2	389084	458035	38.91%	4.700%
31	13.992	2023	2024	2029	rVB	66720	48402	4.11%	0.497%
32	14.433	2097	2099	2101	rBV	39326	36502	3.10%	0.375%
33	14.462	2101	2104	2108	rVV6	43036	51850	4.40%	0.532%
34	15.133	2215	2218	2224	rBV6	46128	90961	7.73%	0.933%
35	15.451	2268	2272	2281	rVB	208367	277875	23.60%	2.851%

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136926.D
Acq On : 04 Jan 2024 01:03
Operator : CG\JU
Sample : 05897-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-22

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

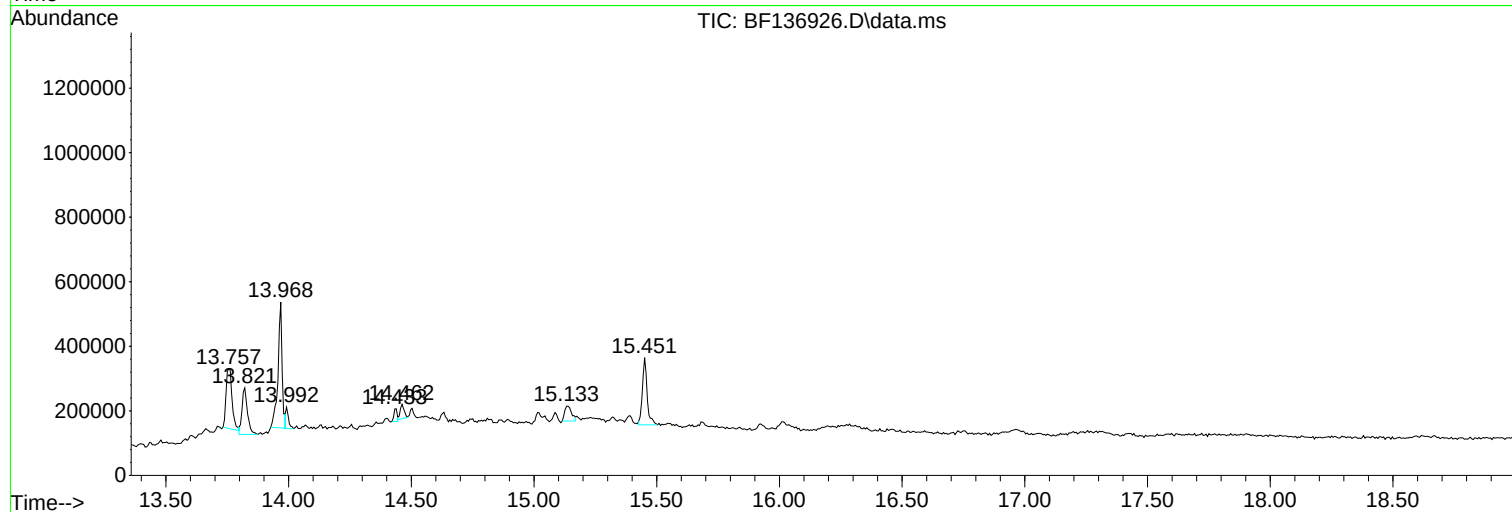
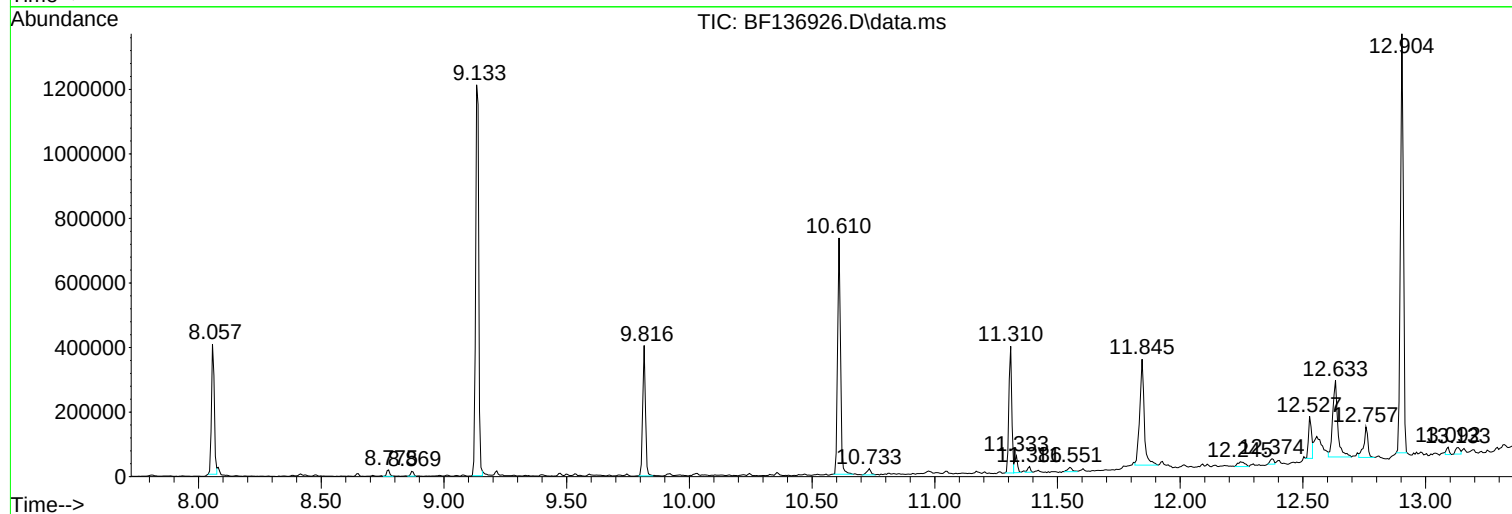
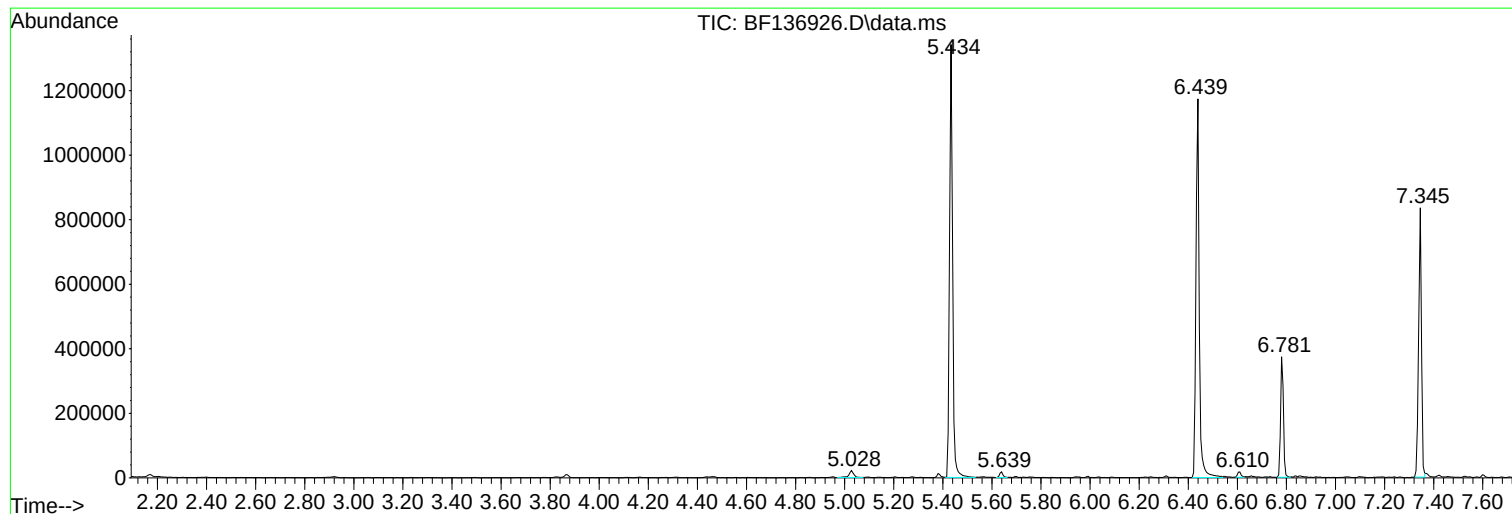
Sum of corrected areas: 9745547

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136926.D
Acq On : 04 Jan 2024 01:03
Operator : CG\JU
Sample : 05897-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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\BF010324\
Data File : BF136926.D
Acq On : 04 Jan 2024 01:03
Operator : CG\JU
Sample : 05897-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-22

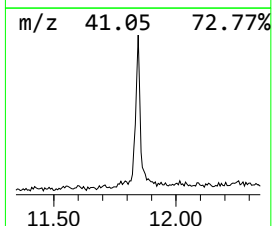
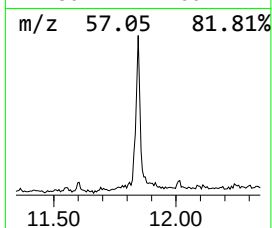
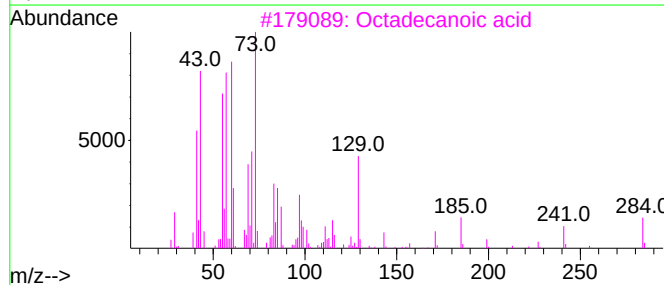
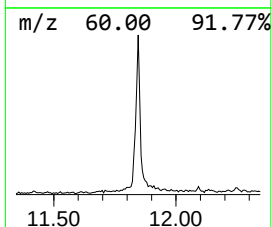
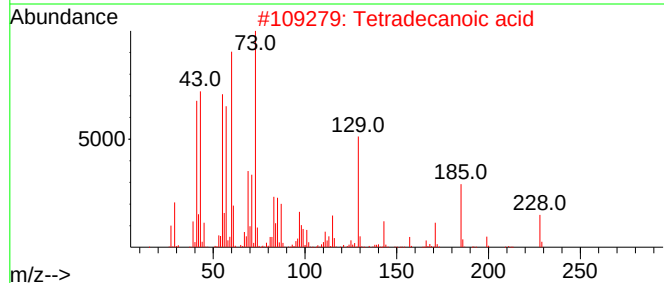
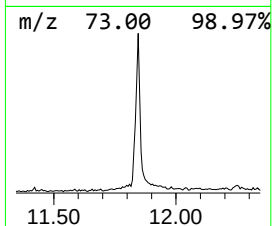
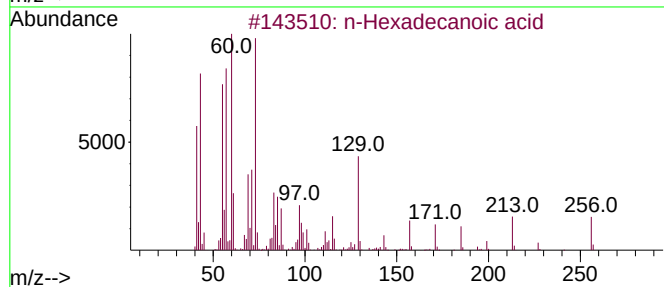
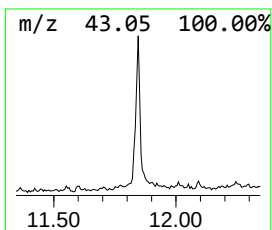
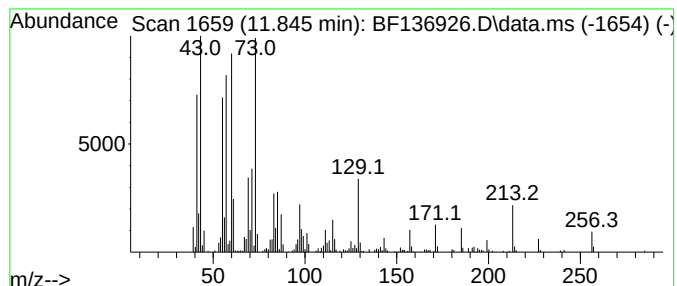
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	25.54 ng	416745	Phenanthrene-d10	11.310

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			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Octanoic acid	144	C8H16O2	000124-07-2	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136926.D
Acq On : 04 Jan 2024 01:03
Operator : CG\JU
Sample : 05897-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-22

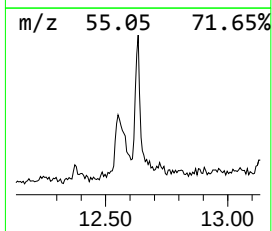
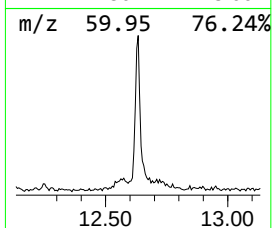
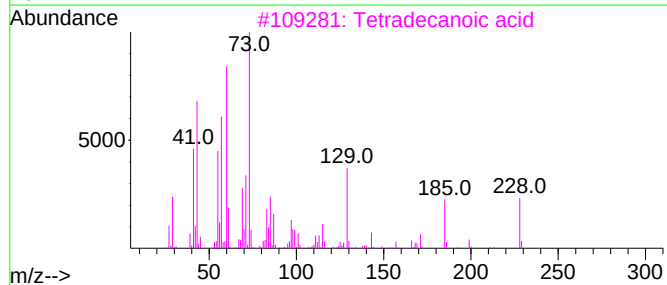
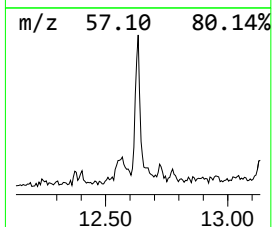
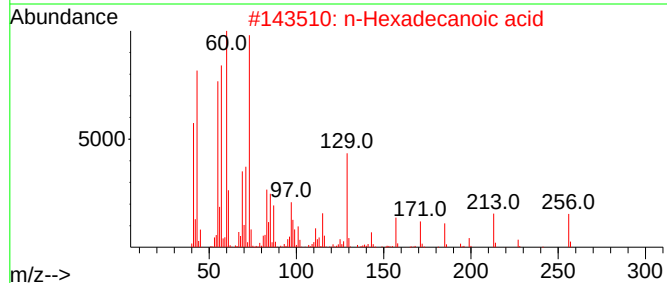
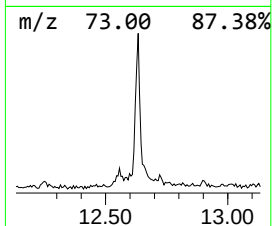
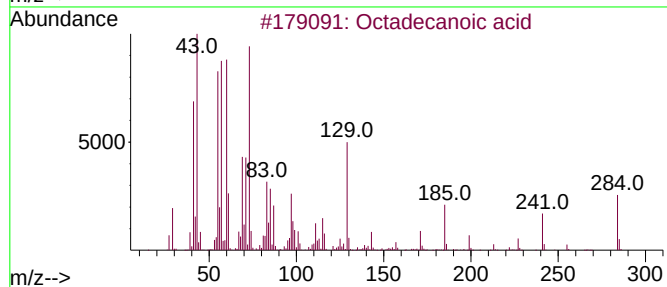
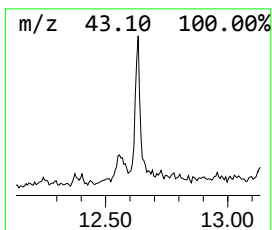
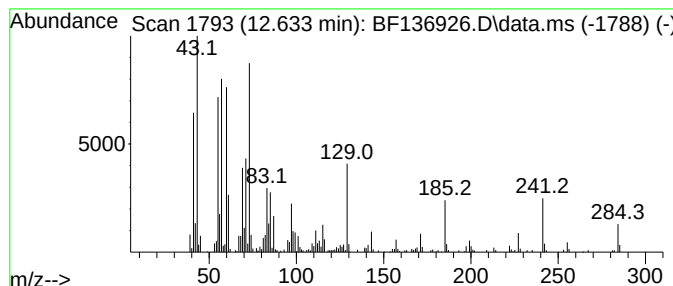
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.633	20.54 ng	335189	Phenanthrene-d10	11.310

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			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	68
5			Tridecanoic acid	214	C13H26O2	000638-53-9	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136926.D
Acq On : 04 Jan 2024 01:03
Operator : CG\JU
Sample : 05897-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-22

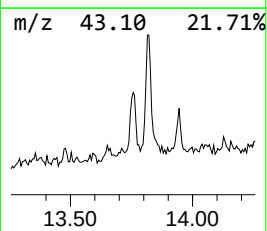
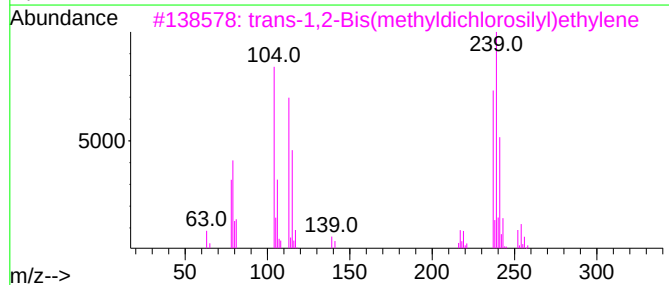
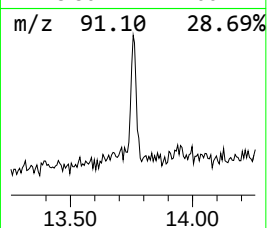
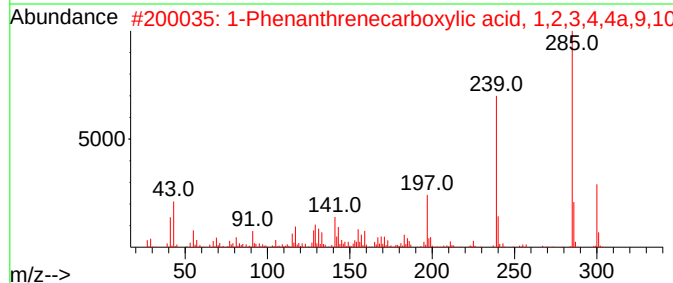
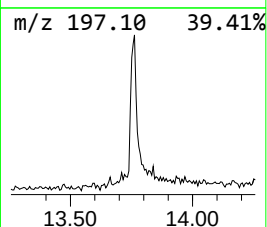
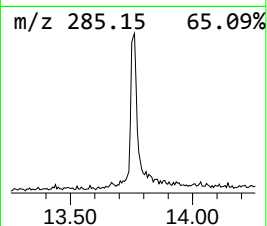
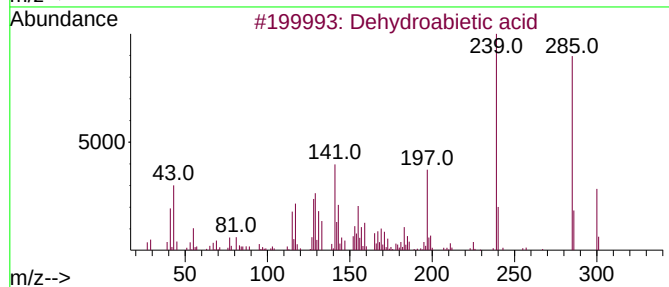
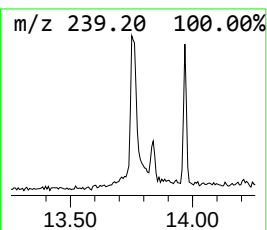
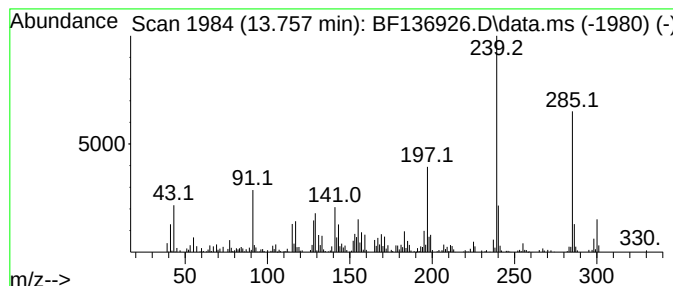
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Dehydroabietic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.757	13.67 ng	312954	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dehydroabietic acid	300	C20H28O2	001740-19-8	99
2			1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	94
3			trans-1,2-Bis(methyldichlorosilyl)...	252	C4H8Cl4Si2	065899-10-7	83
4			3-Quinolinecarboxylic acid, 4-hy...	285	C13H10F3NO3	023851-84-5	47
5			2-Ethylidene-hydrazono-3-methyl-...	239	C10H10ClN3S	1000148-08-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136926.D
Acq On : 04 Jan 2024 01:03
Operator : CG\JU
Sample : 05897-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-22

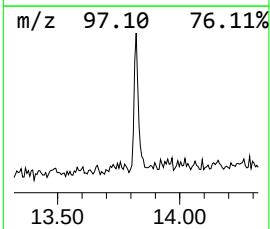
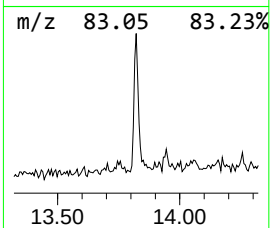
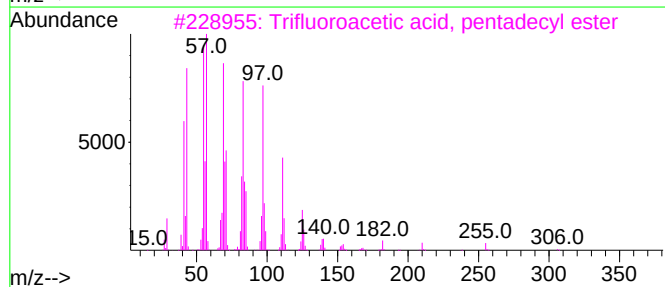
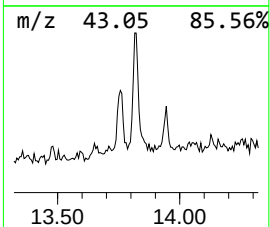
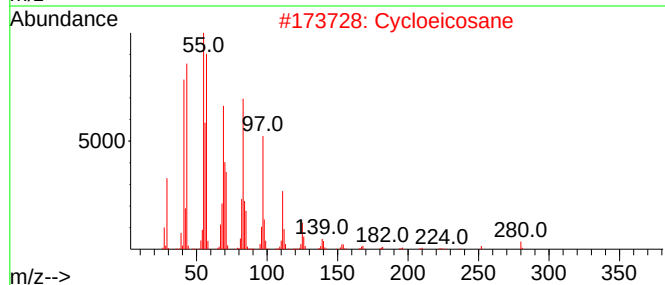
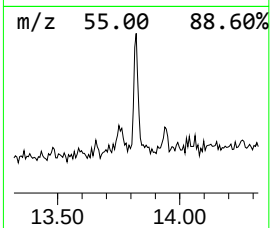
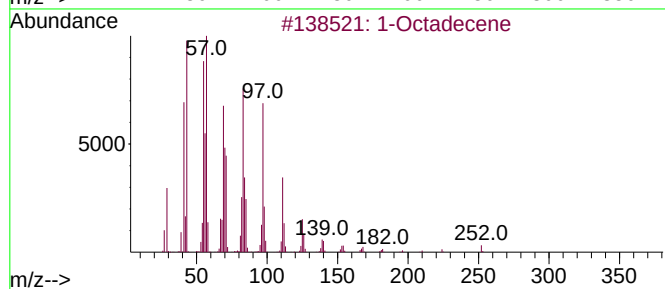
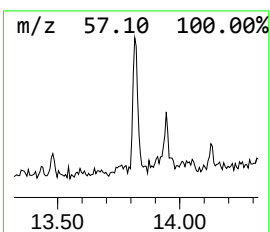
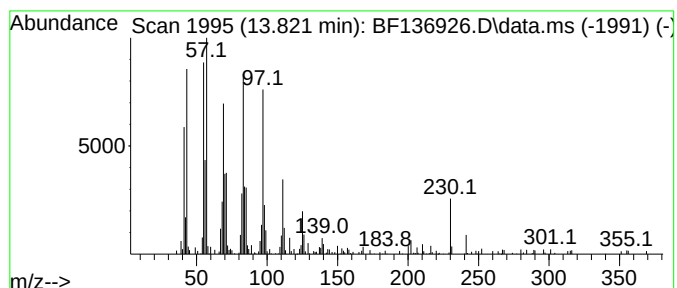
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.821	9.70 ng	222114	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene			252	C18H36	000112-88-9	99
2	Cycloeicosane			280	C20H40	000296-56-0	99
3	Trifluoroacetic acid, pentadecyl...			324	C17H31F3O2	959010-23-2	93
4	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	93
5	Heptafluorobutyric acid, n-tetra...			410	C18H29F7O2	007365-36-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136926.D
Acq On : 04 Jan 2024 01:03
Operator : CG\JU
Sample : 05897-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-22

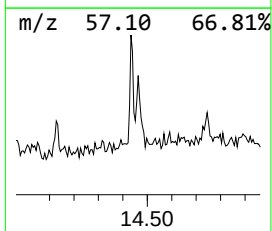
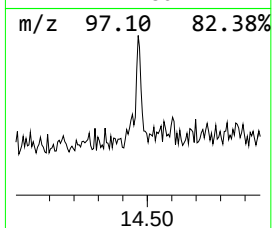
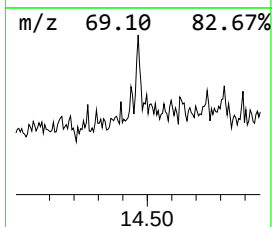
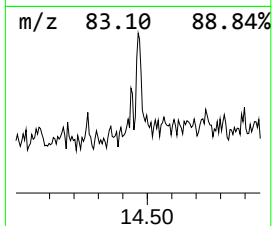
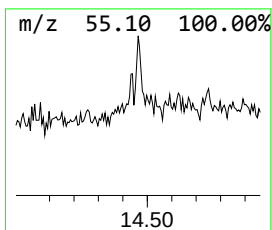
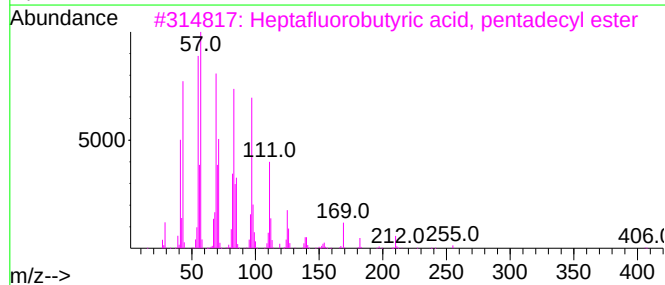
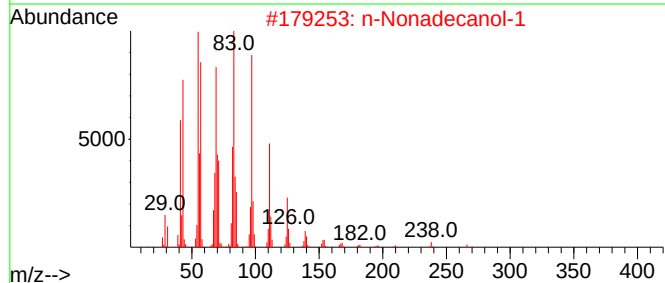
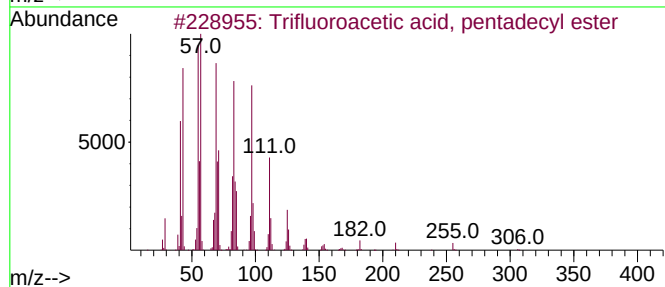
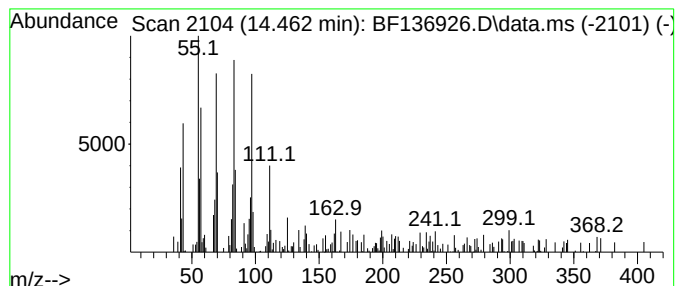
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Trifluoroacetic acid, penta... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.462	2.26 ng	51850	Chrysene-d12	13.968

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	87
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87
4			Cyclopentadecane	210	C15H30	000295-48-7	86
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136926.D
Acq On : 04 Jan 2024 01:03
Operator : CG\JU
Sample : 05897-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-22

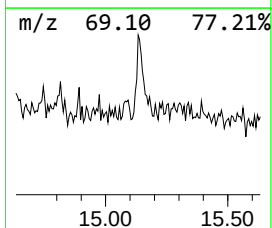
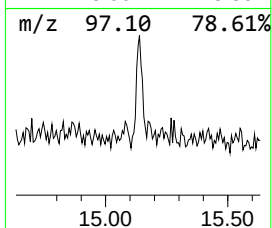
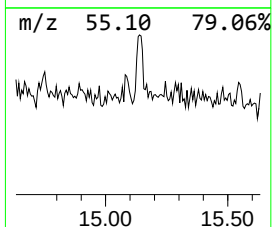
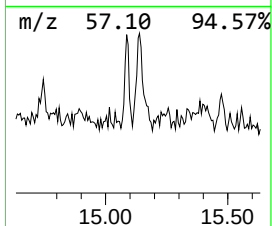
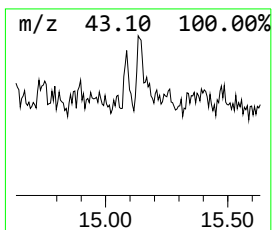
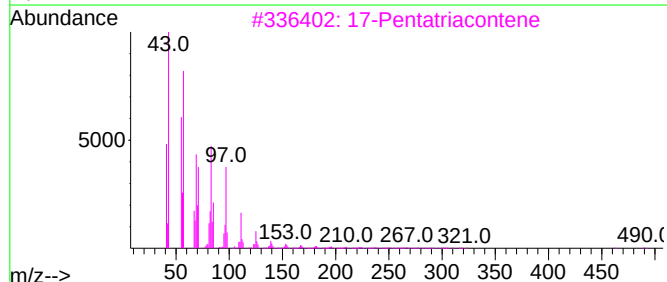
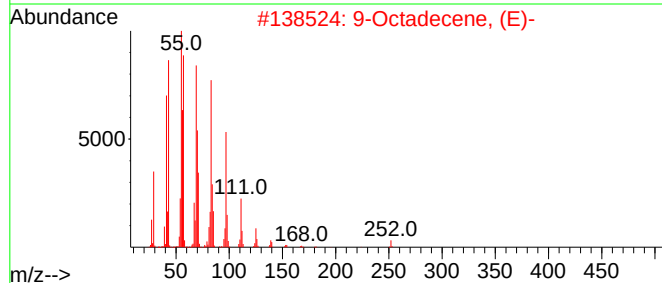
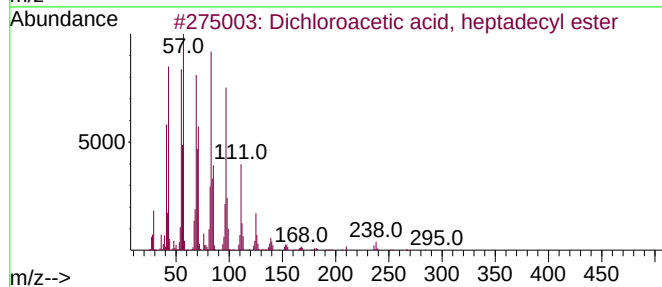
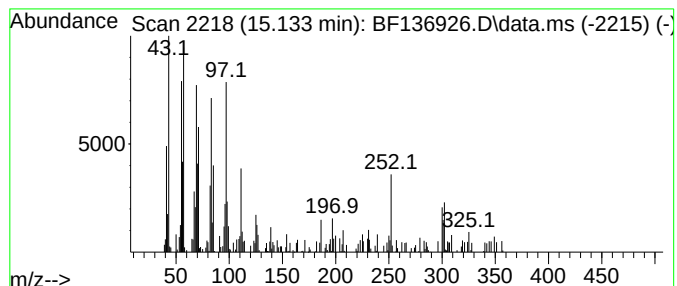
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.133	6.55 ng	90961	Perylene-d12	15.451

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	86
2			9-Octadecene, (E)-	252	C18H36	007206-25-9	70
3			17-Pentatriacontene	491	C35H70	006971-40-0	70
4			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	70
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF010324\
Data File : BF136926.D
Acq On : 04 Jan 2024 01:03
Operator : CG\JU
Sample : 05897-18
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GHL-SS-22

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.845	25.5	ng	416745	4	11.310	326299	20.0
Octadecanoic acid	12.633	20.5	ng	335189	4	11.310	326299	20.0
Dehydroabietic ...	13.757	13.7	ng	312954	5	13.968	458035	20.0
1-Octadecene	13.821	9.7	ng	222114	5	13.968	458035	20.0
Trifluoroacetic...	14.462	2.3	ng	51850	5	13.968	458035	20.0
Dichloroacetic ...	15.133	6.5	ng	90961	6	15.451	277875	20.0