

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
 Data File : BF132742.D
 Acq On : 10 Mar 2023 15:31
 Operator : CG\JU
 Sample : 01853-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20230167-COMPOSITE-1-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_F\Methods\8270-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132742.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.199	440	444	453	rVB	707530	683111	13.13%	2.288%
2	5.604	509	513	523	rBV	1212858	1066410	20.50%	3.572%
3	5.987	574	578	584	rBV	80280	76415	1.47%	0.256%
4	6.604	680	683	693	rVB	758673	695671	13.38%	2.330%
5	6.975	743	746	750	rBV	1391990	1205069	23.17%	4.037%
6	7.545	838	843	846	rVB	3200194	2896850	55.70%	9.704%
7	7.616	852	855	868	rVB3	52383	88206	1.70%	0.295%
8	7.710	868	871	874	rVB	105358	82640	1.59%	0.277%
9	8.263	961	965	968	rBV	2001826	1554248	29.88%	5.207%
10	9.339	1144	1148	1151	rBV	6096669	5200827	100.00%	17.423%
11	9.404	1157	1159	1163	rBV	132716	100529	1.93%	0.337%
12	9.939	1243	1250	1253	rBV	75609	71881	1.38%	0.241%
13	10.022	1261	1264	1268	rVB	2029244	1831006	35.21%	6.134%
14	10.116	1277	1280	1283	rBV	75854	58737	1.13%	0.197%
15	10.739	1382	1386	1389	rBV	859559	740692	14.24%	2.481%
16	10.816	1395	1399	1403	rBV	2174785	1974906	37.97%	6.616%
17	11.045	1435	1438	1443	rVB	124384	106844	2.05%	0.358%
18	11.522	1515	1519	1522	rBV	2304828	1909359	36.71%	6.396%
19	11.616	1532	1535	1538	rBV	146516	113896	2.19%	0.382%
20	11.669	1541	1544	1551	rBV	115998	102796	1.98%	0.344%
21	12.033	1602	1606	1610	rBV	601508	595505	11.45%	1.995%
22	12.280	1645	1648	1652	rVB	226340	180736	3.48%	0.605%
23	12.822	1736	1740	1746	rBV4	90876	138711	2.67%	0.465%
24	13.110	1785	1789	1793	rBV	4959370	4714733	90.65%	15.794%
25	13.322	1821	1825	1830	rVB	109907	117090	2.25%	0.392%
26	13.669	1880	1884	1887	rBV2	92124	95425	1.83%	0.320%
27	13.998	1936	1940	1955	rBV	569822	941899	18.11%	3.155%
28	14.180	1967	1971	1977	rBV	1264071	1113200	21.40%	3.729%
29	14.316	1991	1994	1997	rBV2	59515	72574	1.40%	0.243%
30	15.027	2112	2115	2119	rVB	146389	159490	3.07%	0.534%
31	15.721	2228	2233	2244	rVB2	872722	1161566	22.33%	3.891%

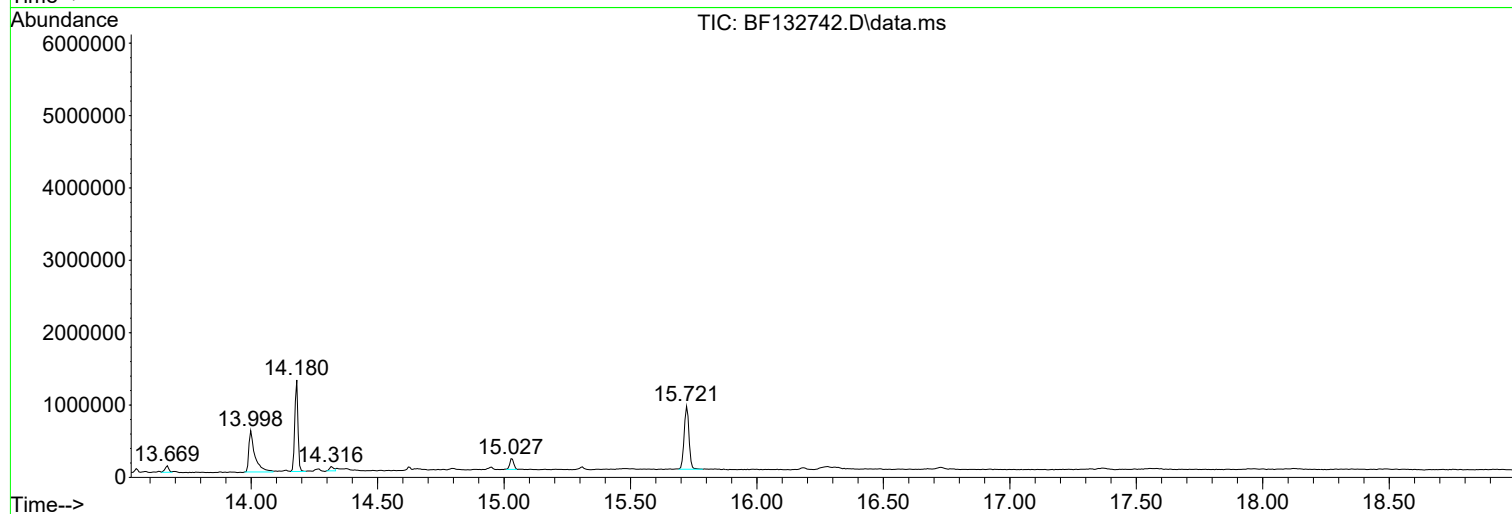
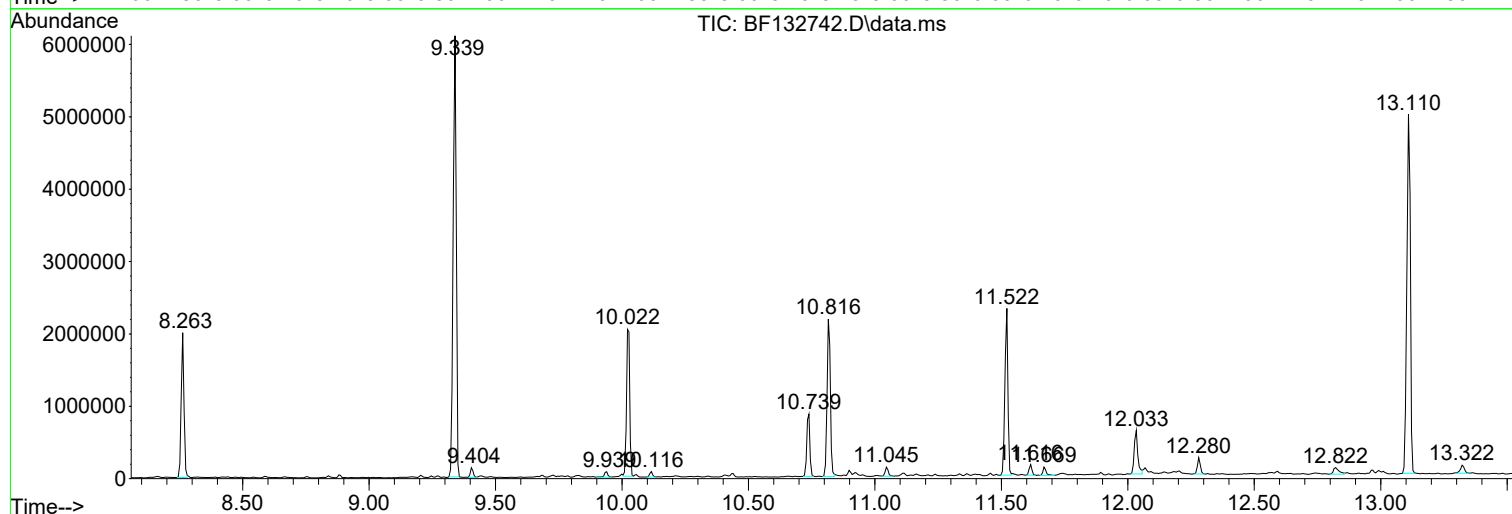
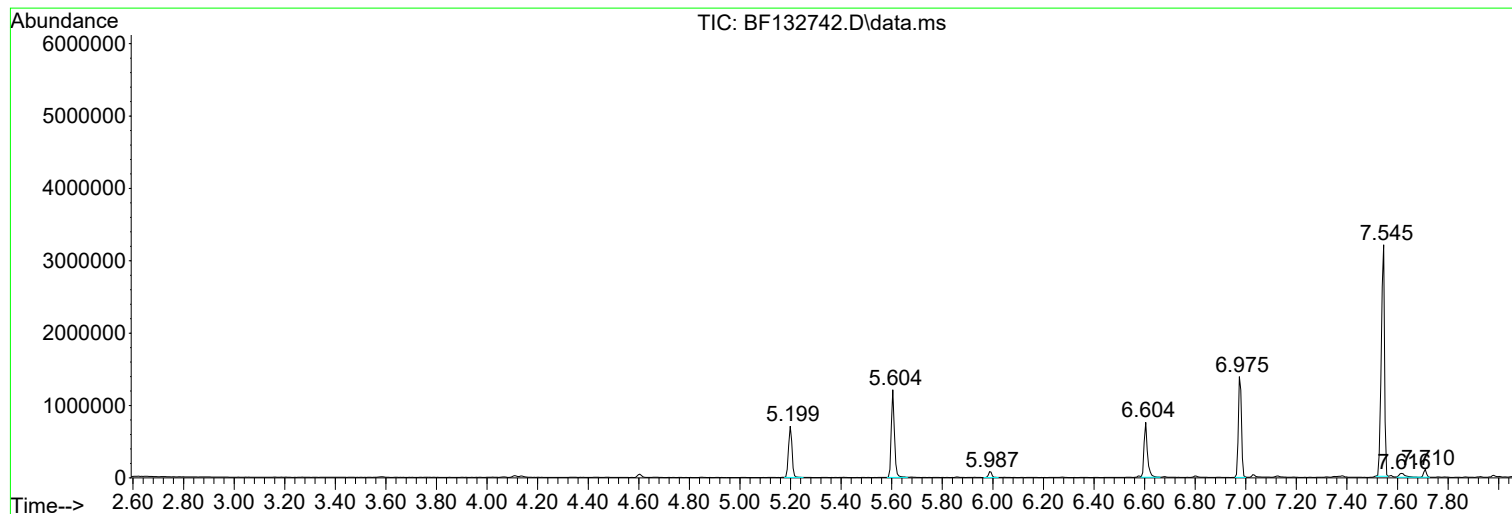
Sum of corrected areas: 29851022

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132742.D
Acq On : 10 Mar 2023 15:31
Operator : CG\JU
Sample : 01853-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230167-COMPOSITE-1-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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\BF031023\
Data File : BF132742.D
Acq On : 10 Mar 2023 15:31
Operator : CG\JU
Sample : 01853-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

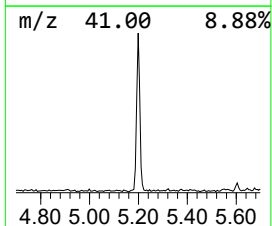
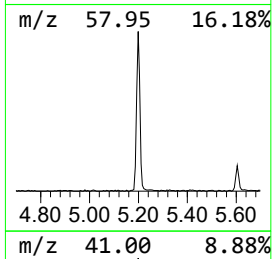
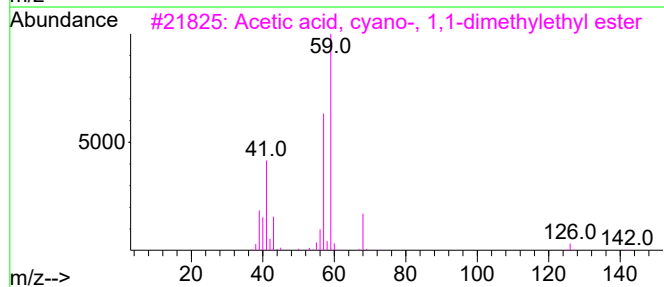
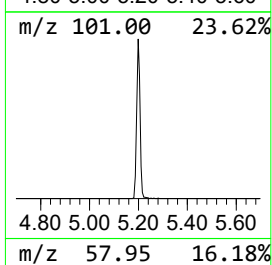
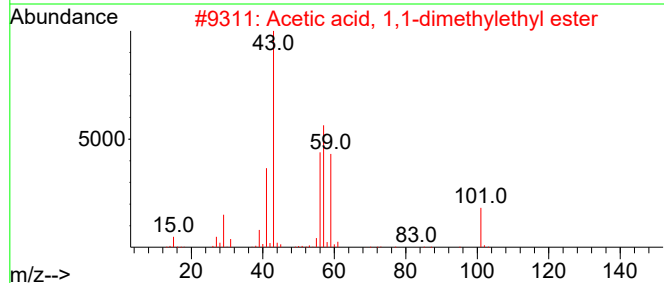
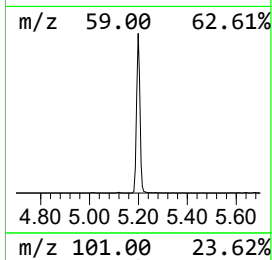
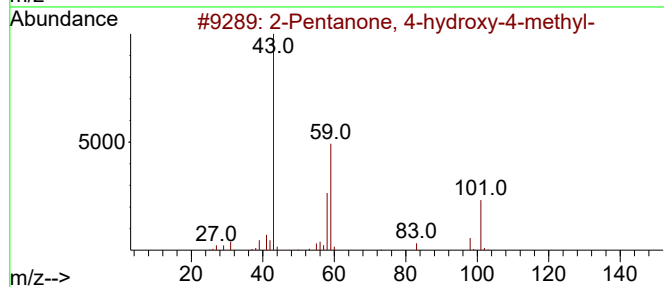
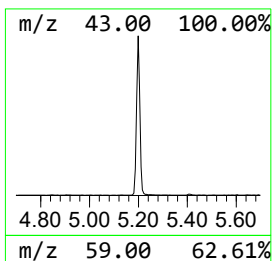
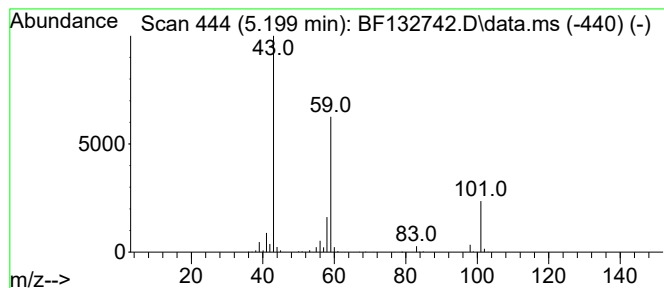
Instrument :
BNA_F
ClientSampleId :
20230167-COMPOSITE-1-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.199	11.34 ng	683111	1,4-Dichlorobenzene-d4	6.975	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132742.D
Acq On : 10 Mar 2023 15:31
Operator : CG\JU
Sample : 01853-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230167-COMPOSITE-1-ELUTRIATE

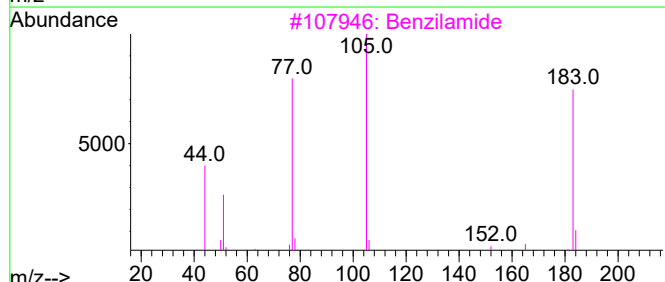
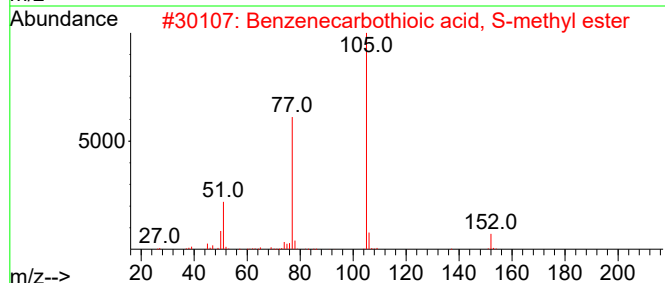
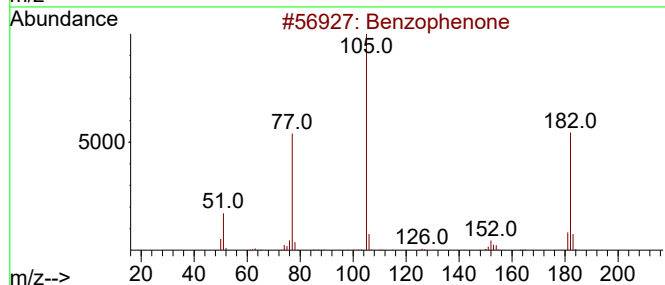
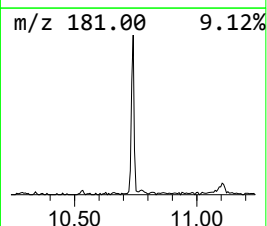
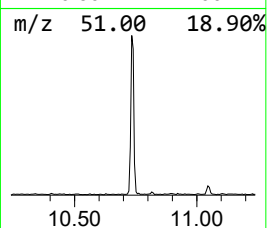
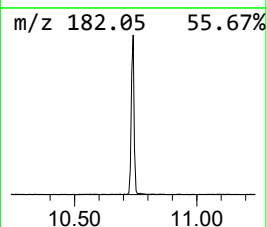
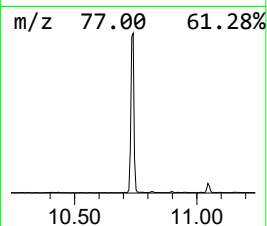
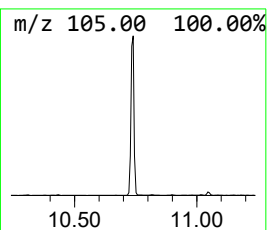
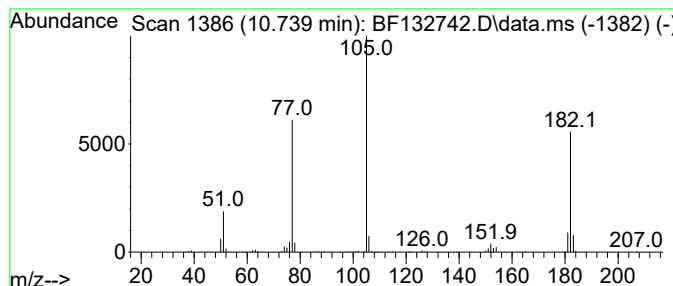
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.739	8.09 ng	740692	Acenaphthene-d10	10.022

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	47
3			Benzilamide	227	C14H13NO2	004746-87-6	47
4			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	43
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132742.D
Acq On : 10 Mar 2023 15:31
Operator : CG\JU
Sample : 01853-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230167-COMPOSITE-1-ELUTRIATE

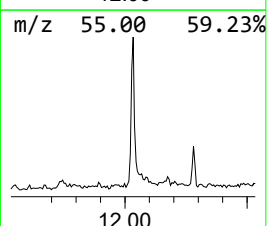
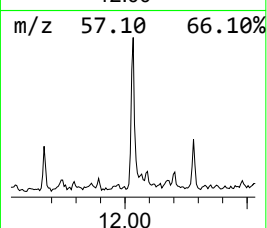
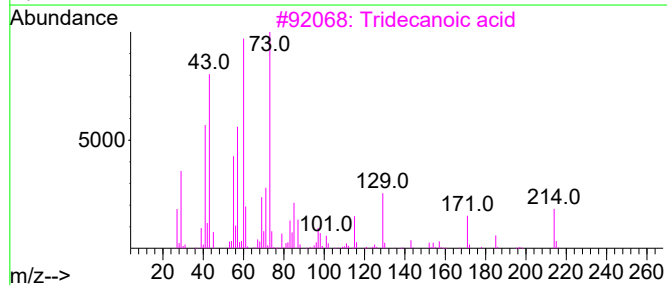
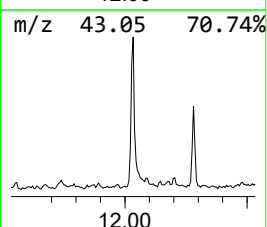
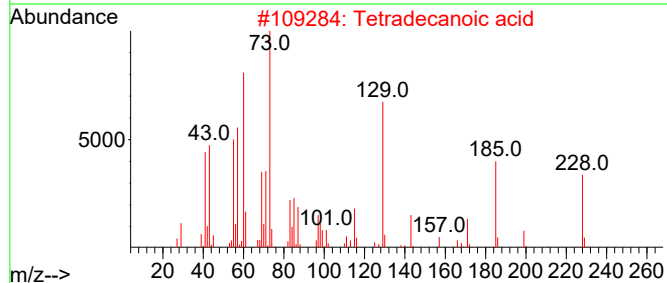
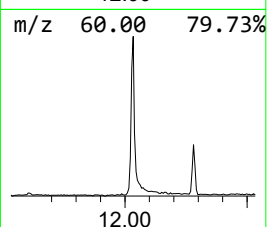
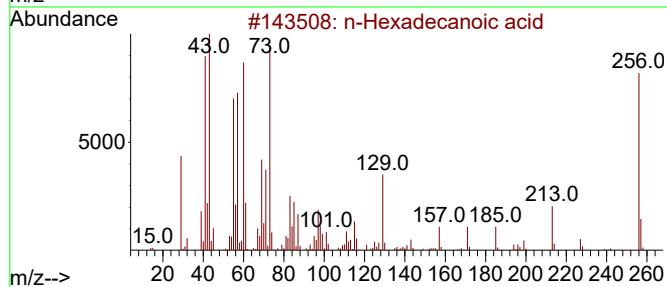
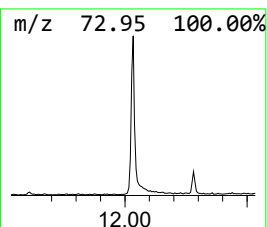
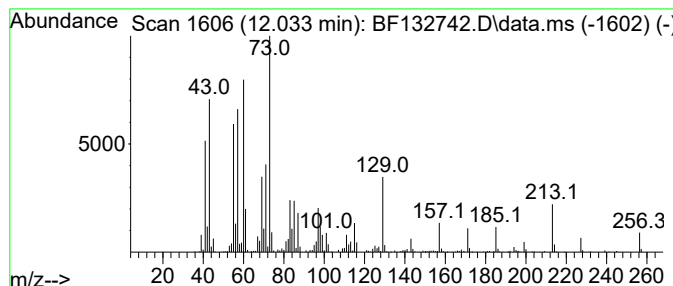
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.033	6.24 ng	595505	Phenanthrene-d10	11.522

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			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132742.D
Acq On : 10 Mar 2023 15:31
Operator : CG\JU
Sample : 01853-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230167-COMPOSITE-1-ELUTRIATE

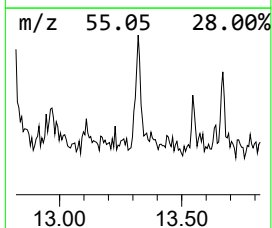
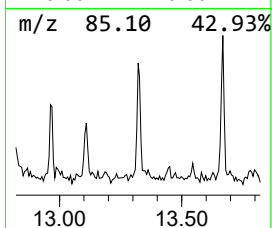
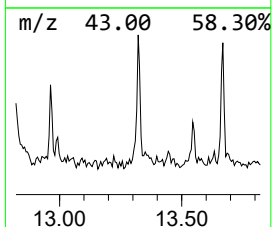
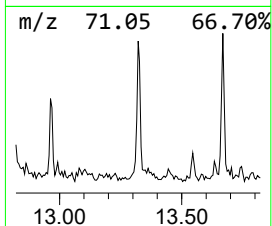
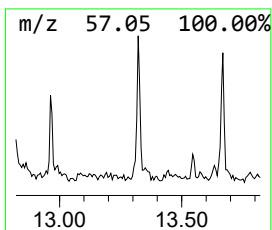
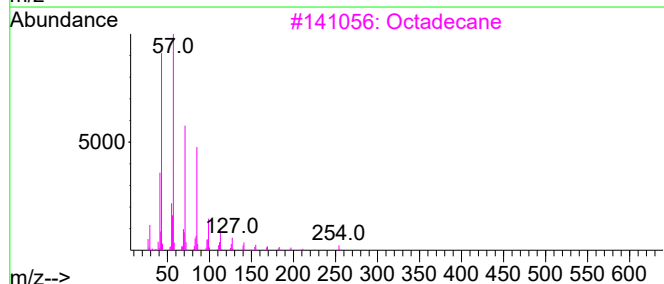
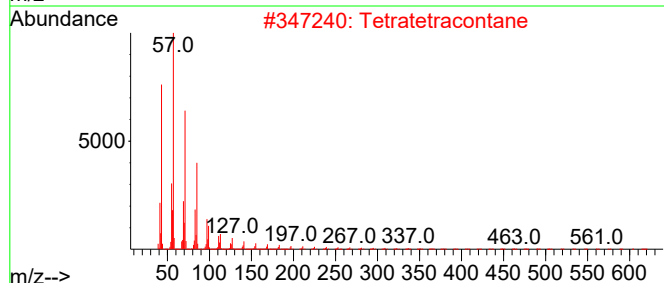
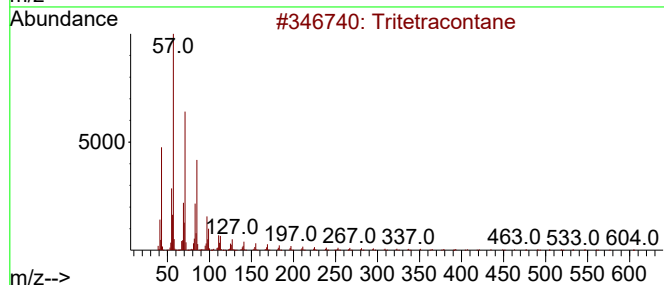
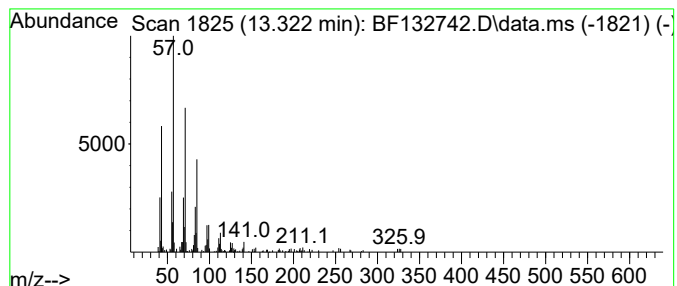
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tritetracontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.322	2.10 ng	117090	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tritetracontane	605	C43H88	007098-21-7	90
2			Tetratetracontane	619	C44H90	007098-22-8	90
3			Octadecane	254	C18H38	000593-45-3	90
4			Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	87
5			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132742.D
Acq On : 10 Mar 2023 15:31
Operator : CG\JU
Sample : 01853-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230167-COMPOSITE-1-ELUTRIATE

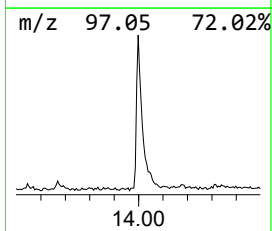
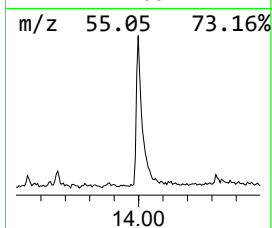
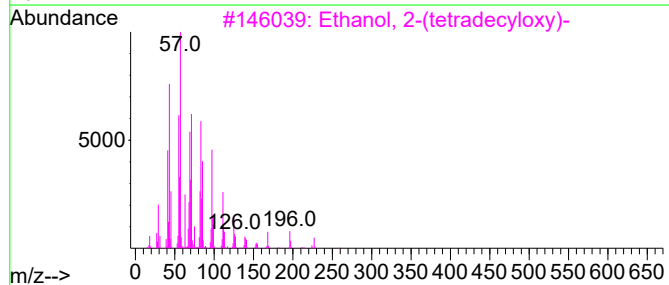
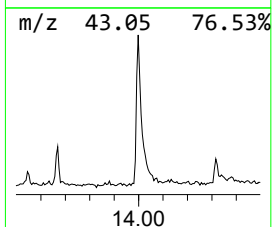
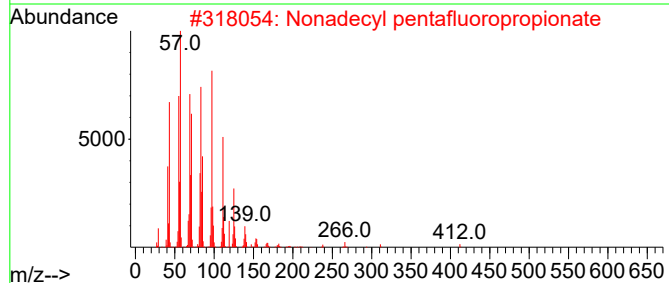
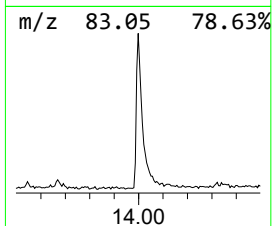
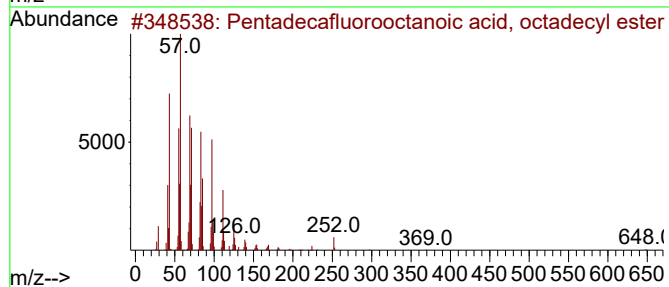
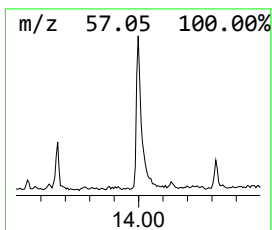
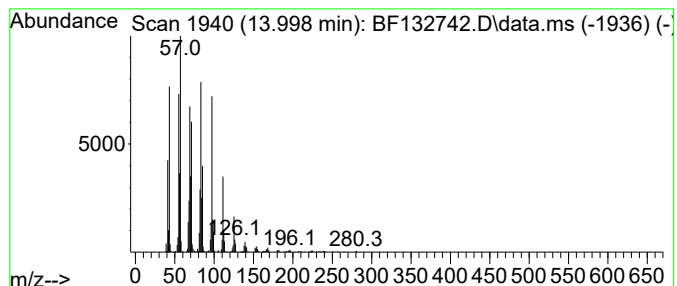
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.998	16.92 ng	941899	Chrysene-d12	14.180

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132742.D
Acq On : 10 Mar 2023 15:31
Operator : CG\JU
Sample : 01853-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230167-COMPOSITE-1-ELUTRIATE

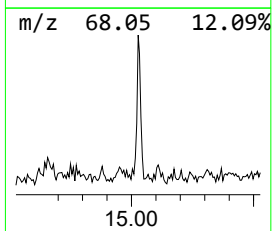
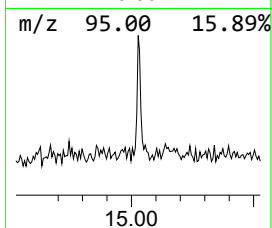
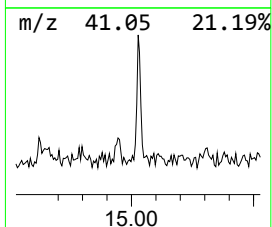
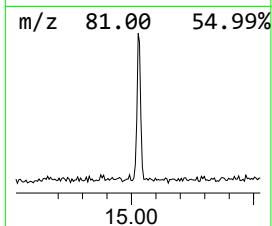
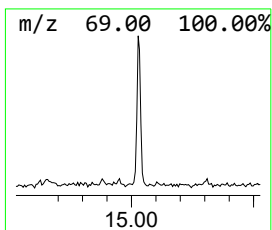
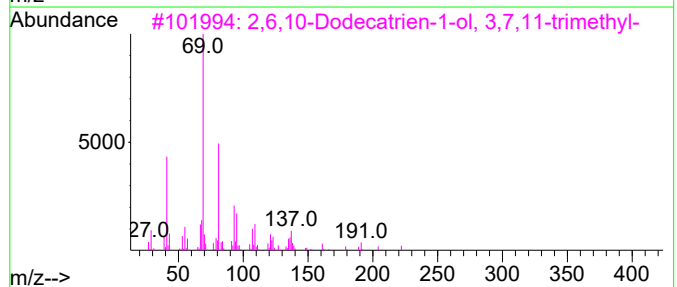
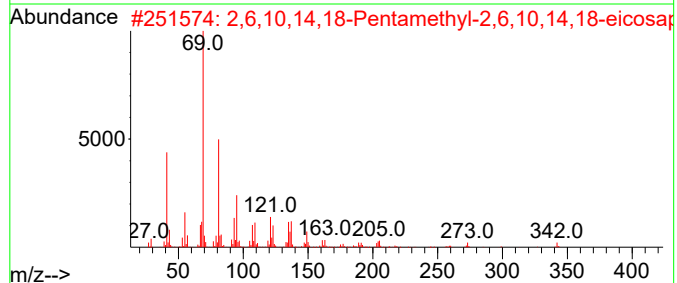
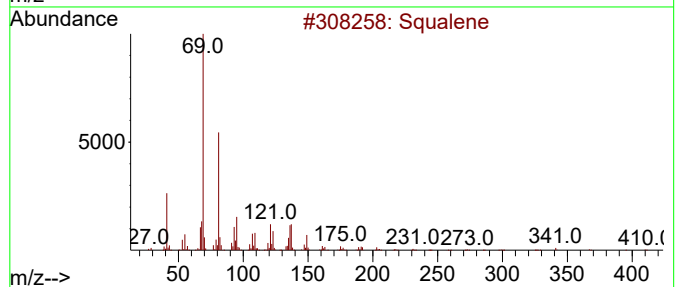
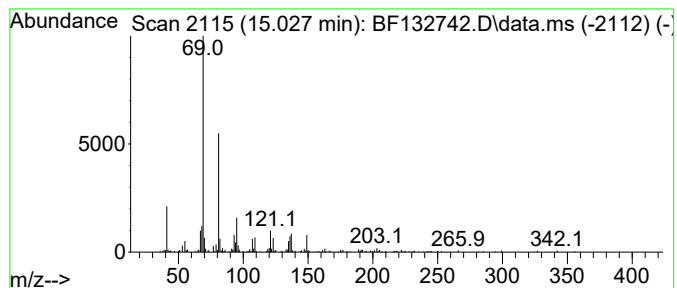
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.027	2.75 ng	159490	Perylene-d12	15.721

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	90
3			2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	90
4			Supraene	410	C30H50	007683-64-9	87
5			Farnesol isomer a	222	C15H26O	1000108-92-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031023\
Data File : BF132742.D
Acq On : 10 Mar 2023 15:31
Operator : CG\JU
Sample : 01853-03
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20230167-COMPOSITE-1-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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
2-Pentanone, 4-...	5.199	11.3	ng	683111	1	6.975	1205070	20.0
Benzophenone	10.739	8.1	ng	740692	3	10.022	1831010	20.0
n-Hexadecanoic ...	12.033	6.2	ng	595505	4	11.522	1909360	20.0
Tritetracontane	13.322	2.1	ng	117090	5	14.180	1113200	20.0
Pentadecafluoro...	13.998	16.9	ng	941899	5	14.180	1113200	20.0
Squalene	15.027	2.8	ng	159490	6	15.721	1161570	20.0