

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
 Data File : BF135023.D
 Acq On : 31 Aug 2023 01:21
 Operator : CG\JU
 Sample : 04196-22
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 OR-345-COMP-04

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-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135023.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	11	15	21	rBV	45184	61069	1.63%	0.226%
2	5.022	495	499	507	rVB	99293	136559	3.65%	0.505%
3	5.410	560	565	568	rBV	3575727	3554772	95.01%	13.146%
4	6.416	730	736	739	rBV	3121566	3493162	93.36%	12.918%
5	6.604	765	768	773	rBV	172447	136079	3.64%	0.503%
6	6.769	793	796	800	rBV	947364	786648	21.03%	2.909%
7	7.333	887	892	895	rBV	2141487	2319167	61.99%	8.576%
8	8.051	1009	1014	1017	rBV	1226777	1024947	27.39%	3.790%
9	9.133	1192	1198	1201	rBV	4210950	3741474	100.00%	13.836%
10	9.257	1213	1219	1222	rBV	2446018	2410290	64.42%	8.913%
11	9.810	1308	1313	1316	rBV	1205343	1032821	27.60%	3.819%
12	10.598	1443	1447	1451	rBV	2002617	1959836	52.38%	7.248%
13	10.769	1472	1476	1481	rBV	80866	78342	2.09%	0.290%
14	10.886	1492	1496	1502	rBV	64414	62337	1.67%	0.231%
15	10.945	1502	1506	1508	rBV	49352	43921	1.17%	0.162%
16	11.298	1562	1566	1570	rBV	989966	826249	22.08%	3.056%
17	11.839	1653	1658	1670	rBV	494790	484651	12.95%	1.792%
18	12.415	1754	1756	1760	rVB	137107	110200	2.95%	0.408%
19	12.563	1774	1781	1784	rVB	109192	103918	2.78%	0.384%
20	12.627	1789	1792	1804	rBV	111038	131099	3.50%	0.485%
21	12.898	1834	1838	1842	rBV	2624262	2494038	66.66%	9.223%
22	13.327	1895	1911	1912	rBV6	88559	301428	8.06%	1.115%
23	13.809	1988	1993	2000	rBV3	152649	240607	6.43%	0.890%
24	13.957	2014	2018	2021	rBV	734742	646616	17.28%	2.391%
25	14.821	2161	2165	2169	rVB	158026	157138	4.20%	0.581%
26	15.427	2262	2268	2273	rBV	548432	703669	18.81%	2.602%

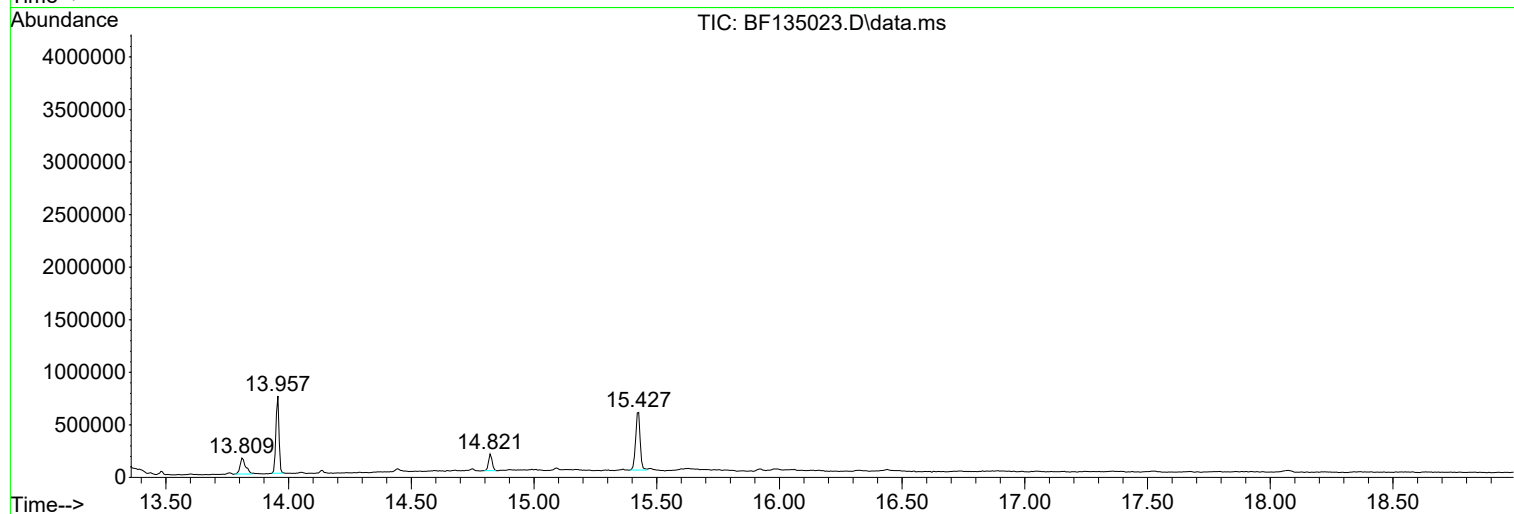
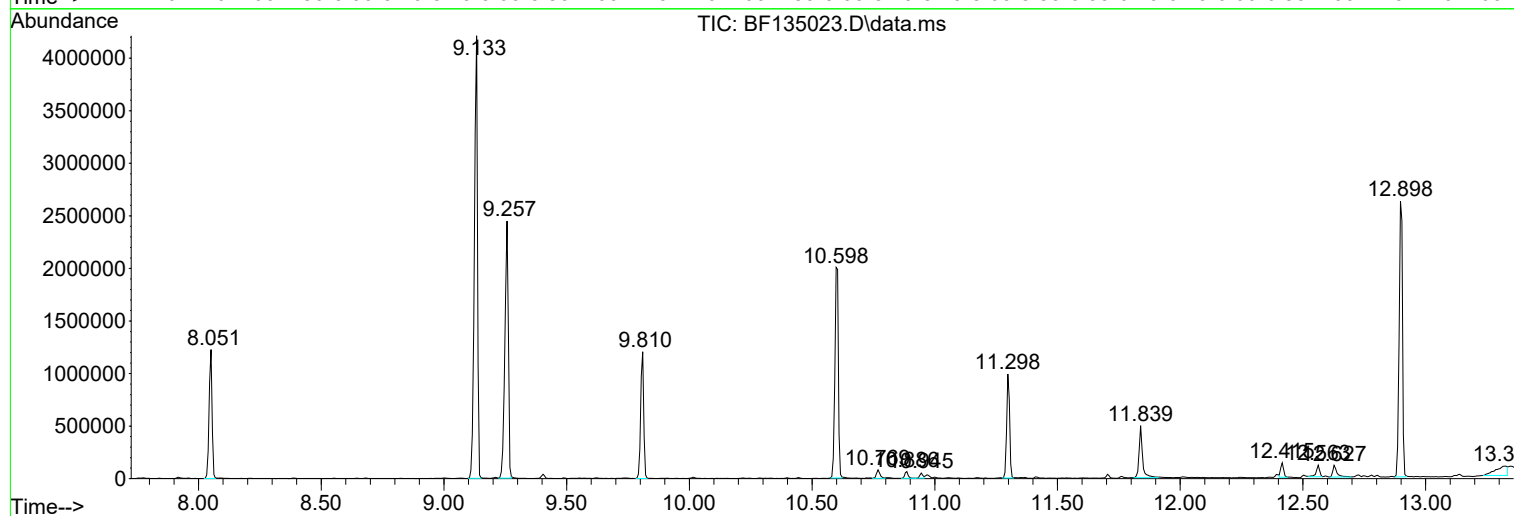
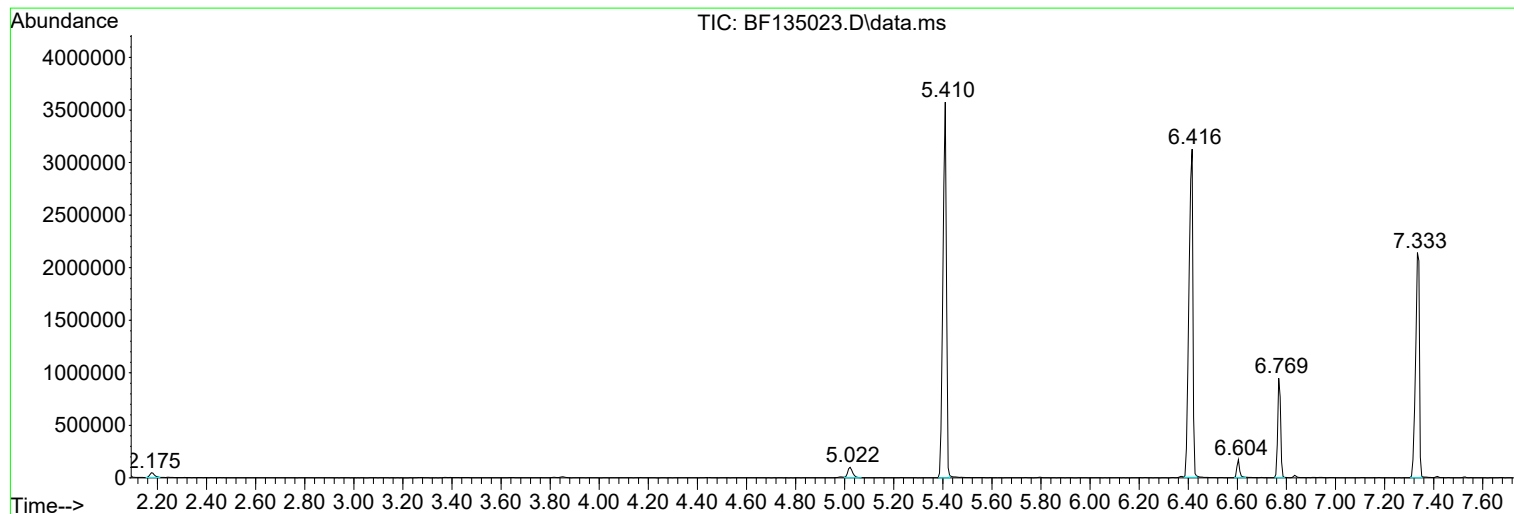
Sum of corrected areas: 27041037

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

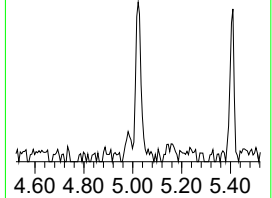
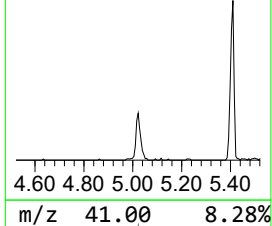
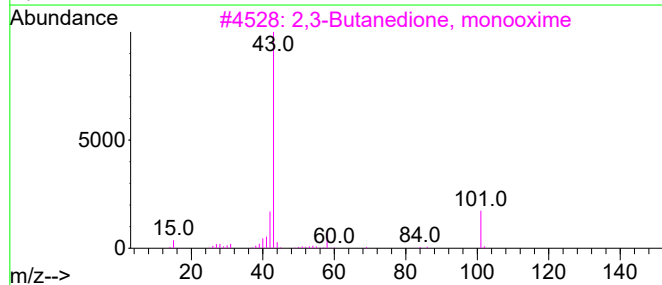
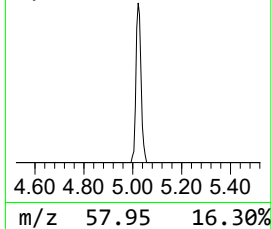
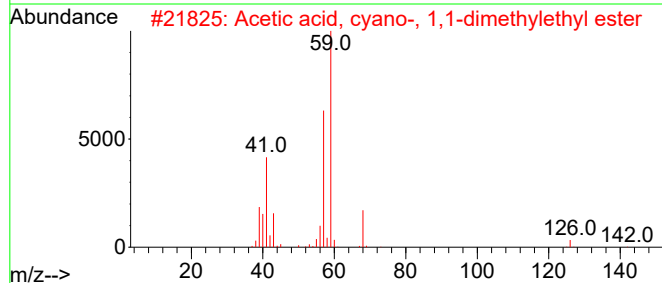
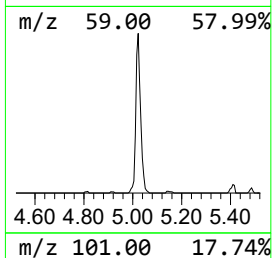
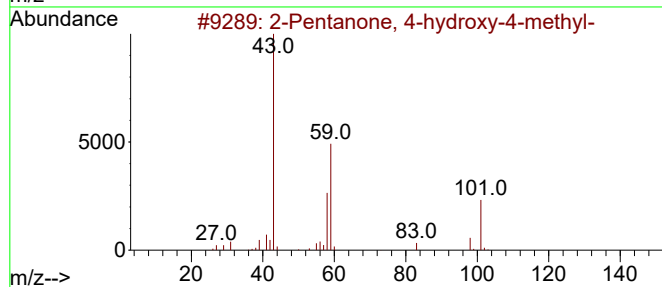
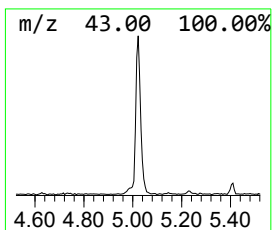
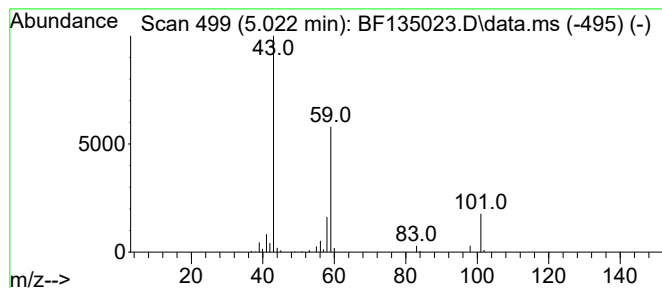
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	3.47 ng	136559	1,4-Dichlorobenzene-d4	6.769

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			5-Hexen-2-one	98	C6H10O	000109-49-9	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

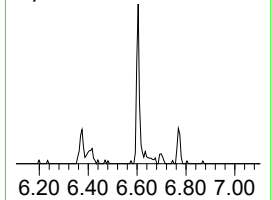
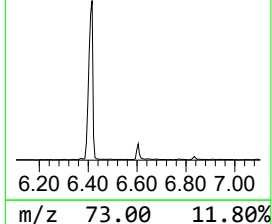
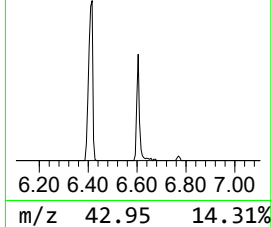
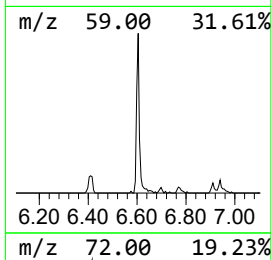
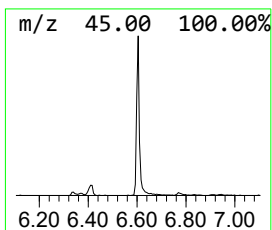
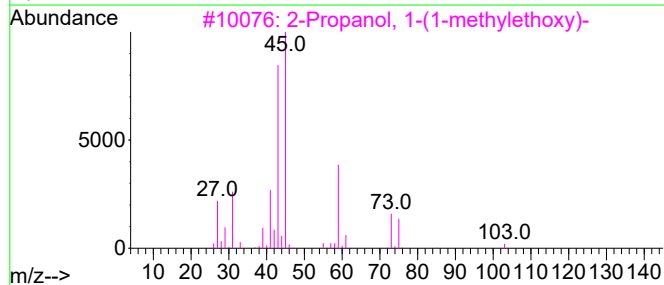
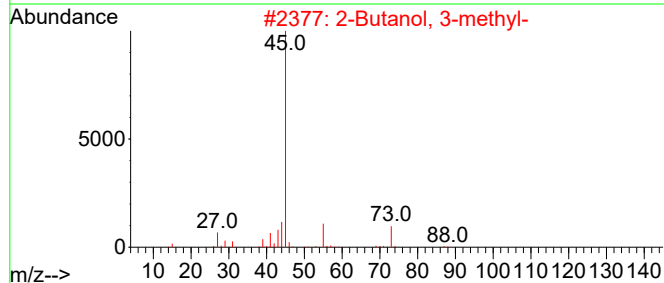
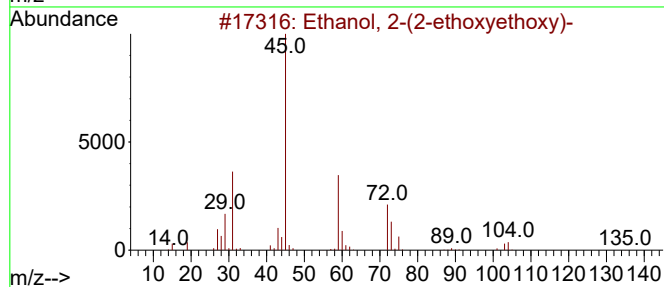
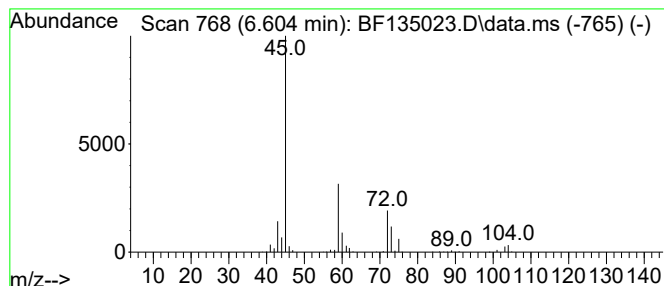
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.604	3.46 ng	136079	1,4-Dichlorobenzene-d4	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	47
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
4			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	36
5			Ethanol, 2-[2-(2-propenyloxy)eth...]	146	C7H14O3	015075-50-0	33



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

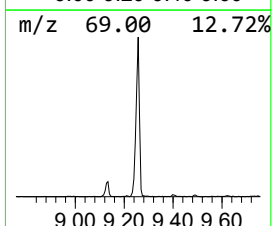
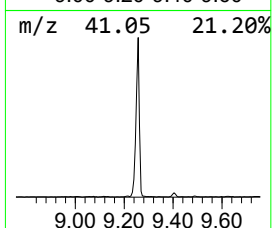
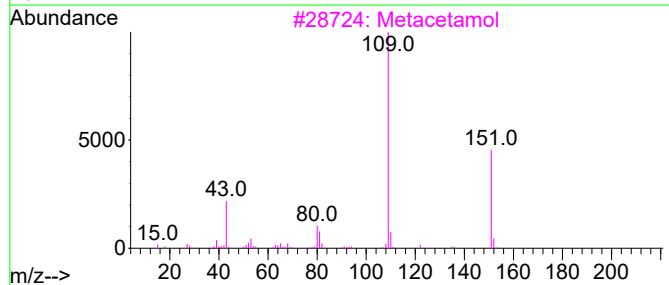
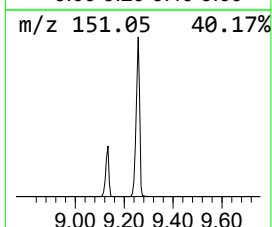
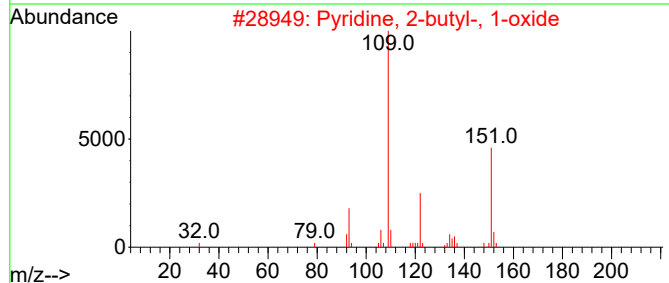
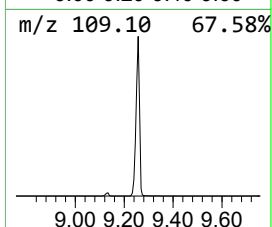
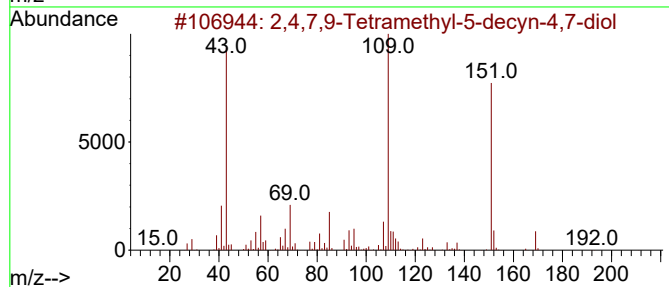
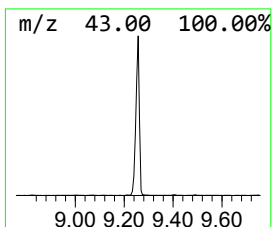
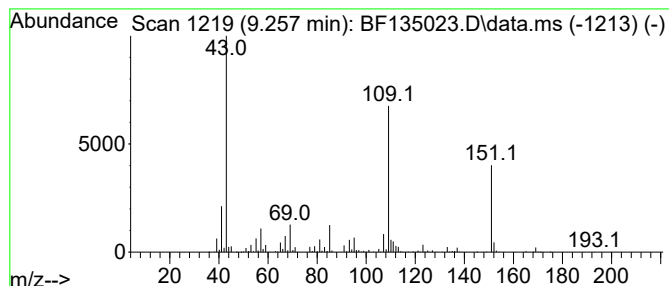
Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
9.257	46.67 ng	2410290	Acenaphthene-d10		9.810	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...		226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide		151	C9H13NO	031396-32-4	59
3	Metacetamol		151	C8H9NO2	000621-42-1	53
4	4-Amino-2-methylpyrimidine		109	C5H7N3	000074-69-1	27
5	Cyclohexanol, 3,3,5-trimethyl-		142	C9H18O	000116-02-9	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

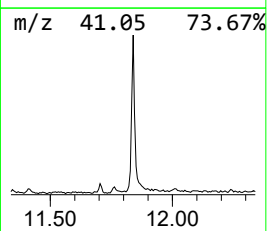
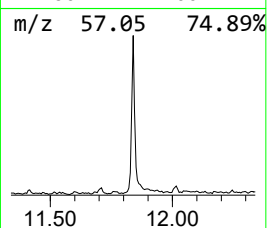
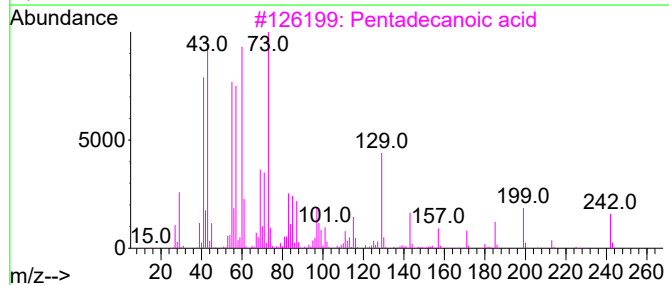
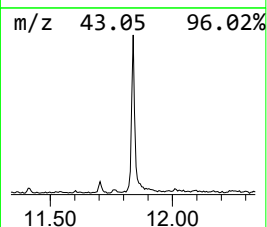
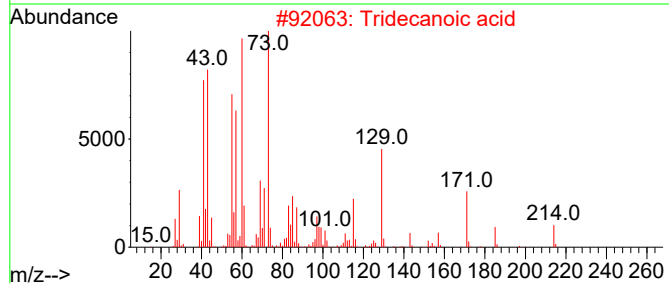
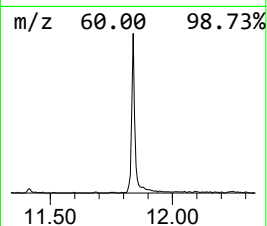
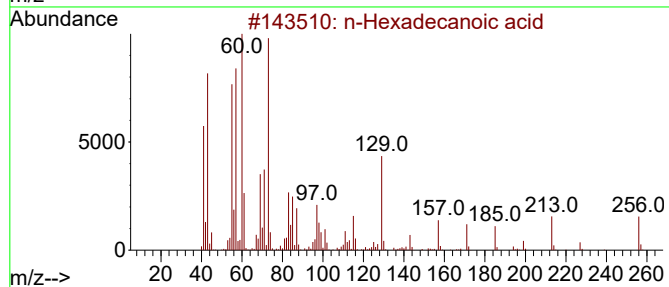
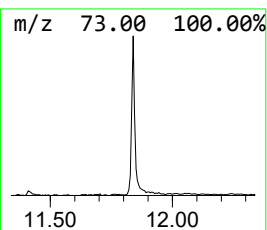
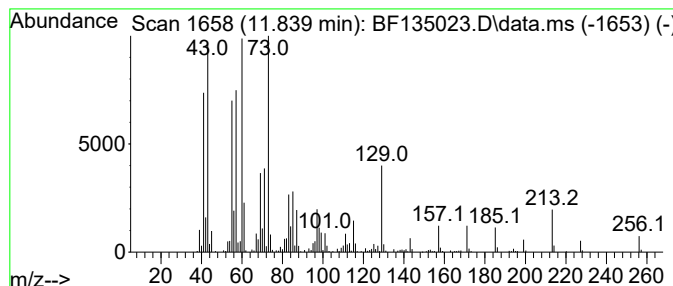
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	11.73 ng	484651	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

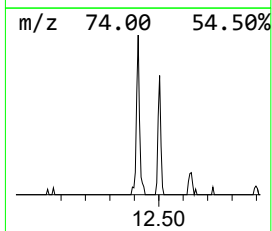
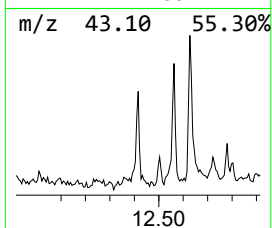
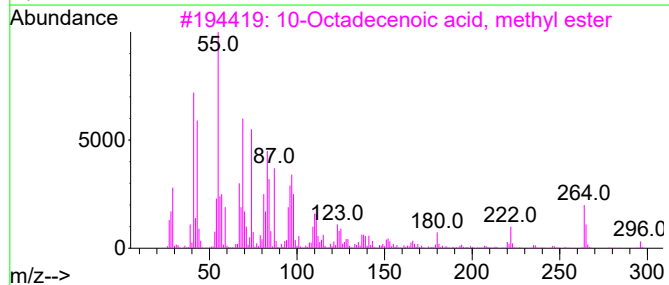
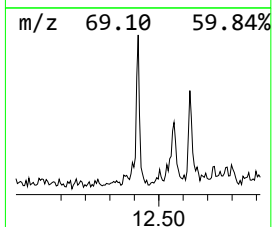
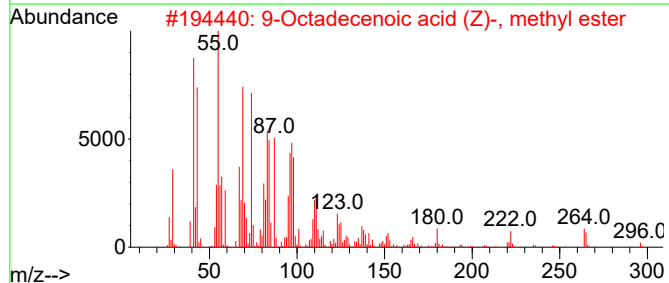
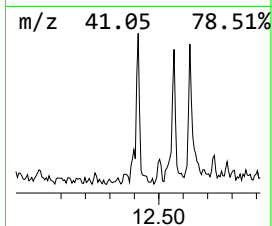
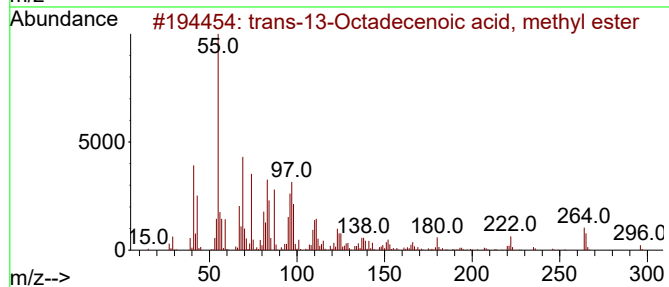
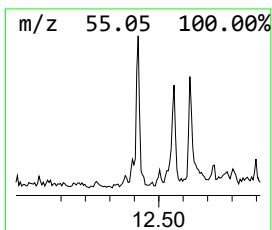
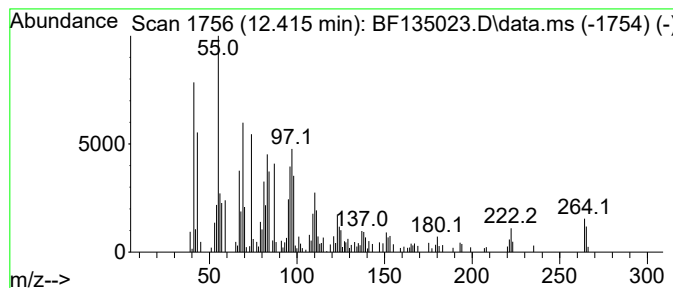
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 trans-13-Octadecenoic acid,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.416	2.67 ng	110200	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	94
2			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	93
3			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
4			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	86
5			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

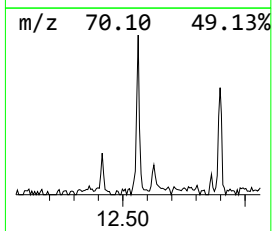
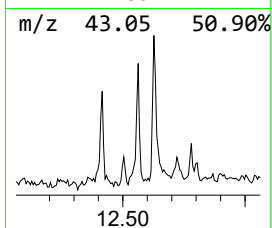
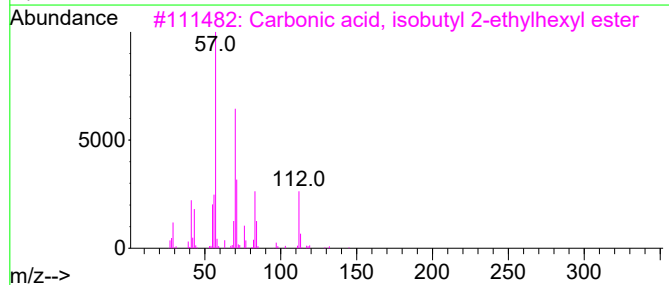
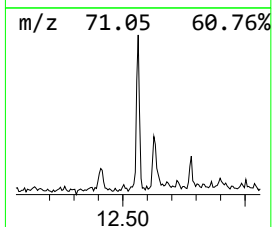
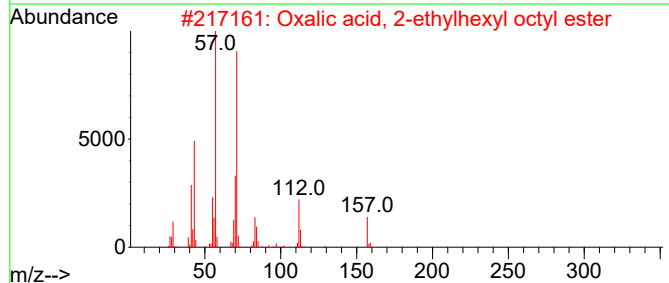
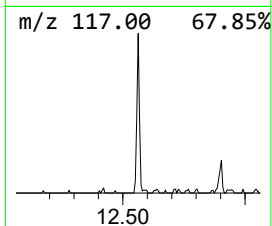
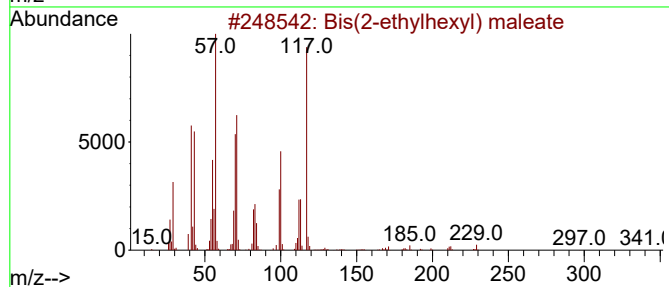
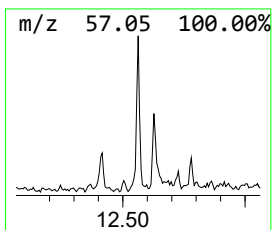
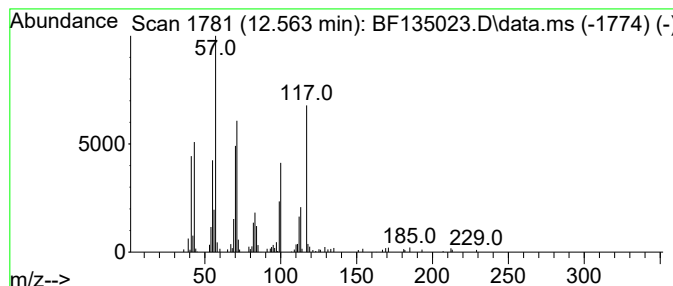
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Bis(2-ethylhexyl) maleate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.563	2.52 ng	103918	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	90
2			Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	35
3			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000383-13-3	35
4			1-Decene, 4-methyl-	154	C11H22	013151-29-6	35
5			3-Hexanone	100	C6H12O	000589-38-8	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

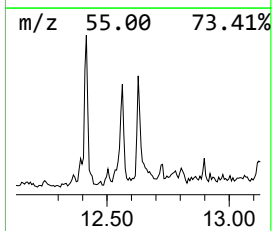
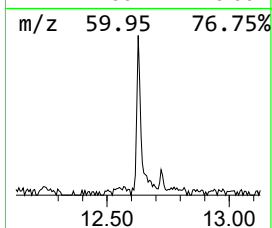
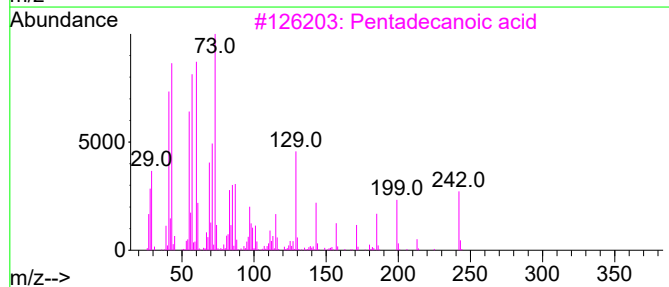
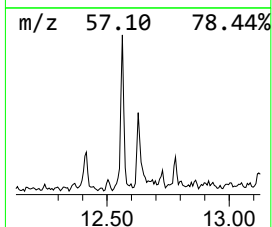
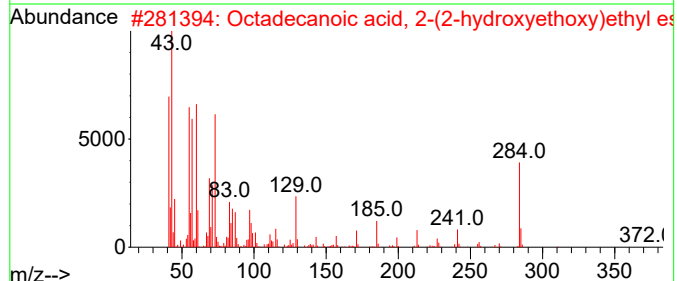
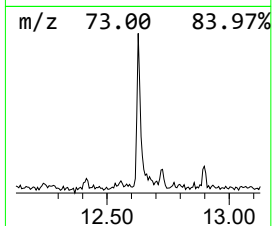
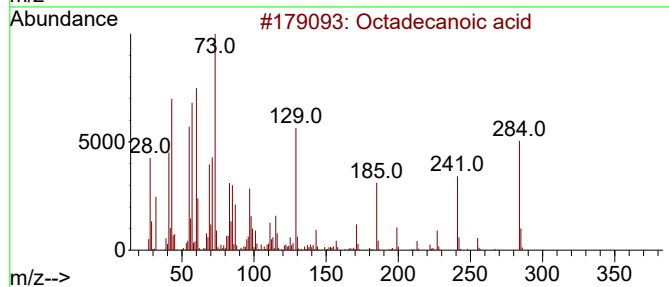
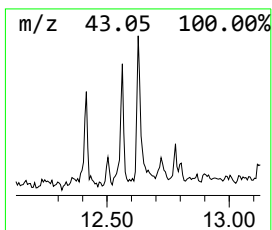
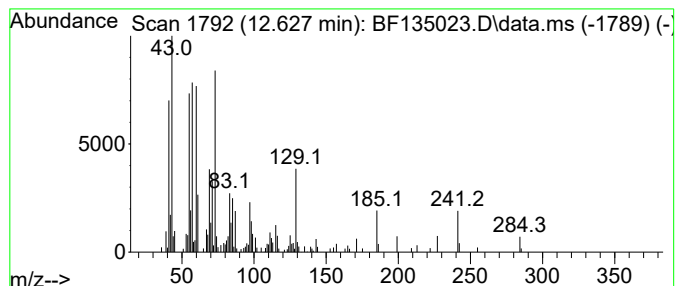
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.627	3.17 ng	131099	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	94
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Undecanoic acid	186	C11H22O2	000112-37-8	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

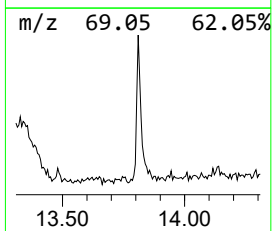
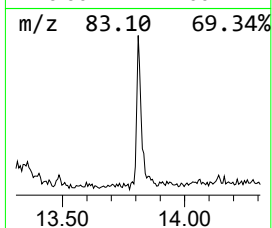
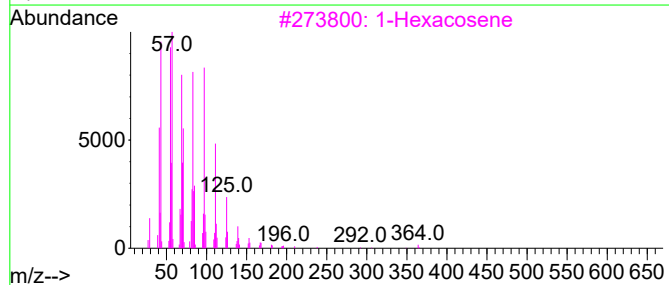
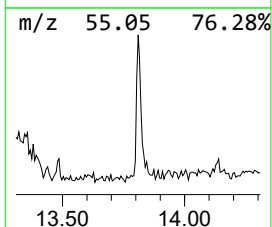
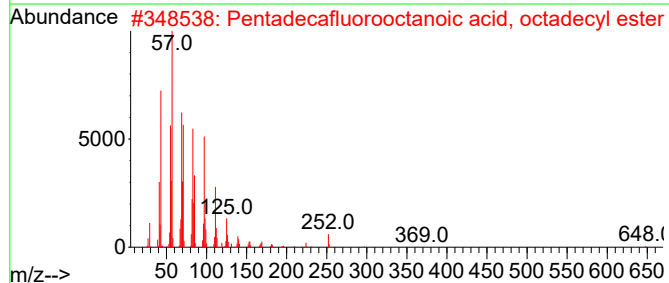
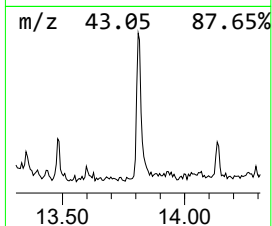
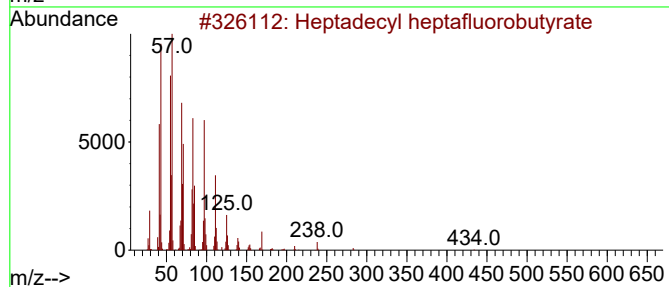
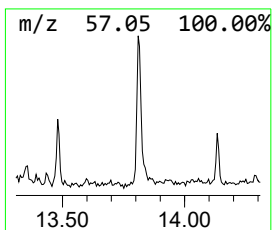
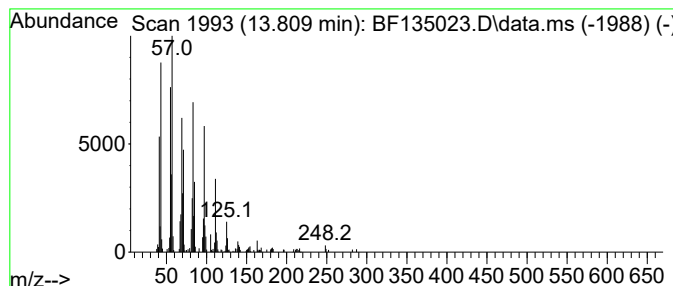
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	7.44 ng	240607	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

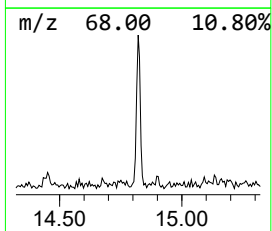
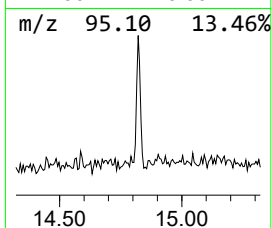
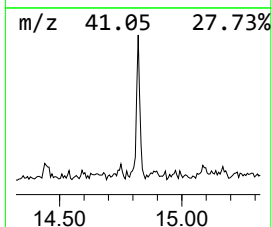
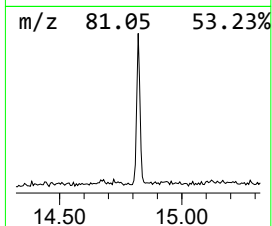
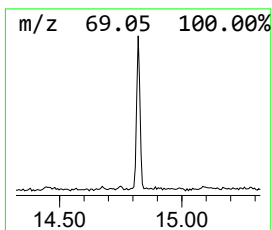
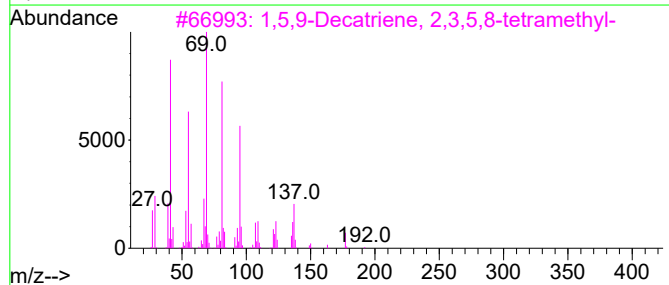
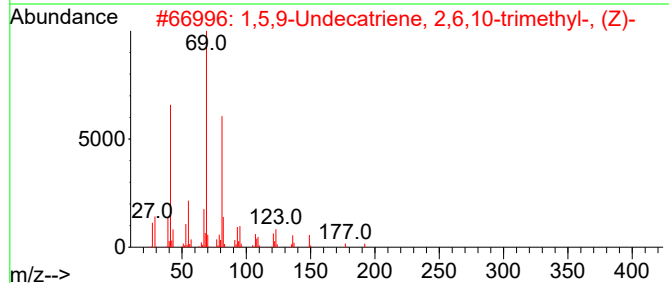
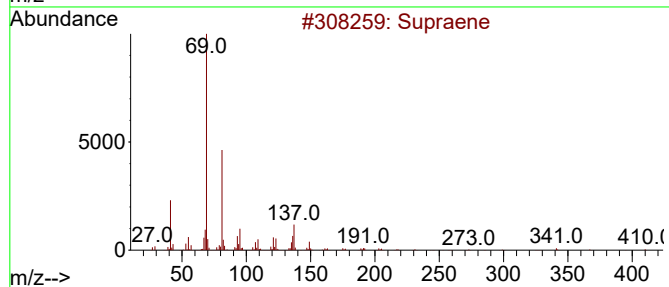
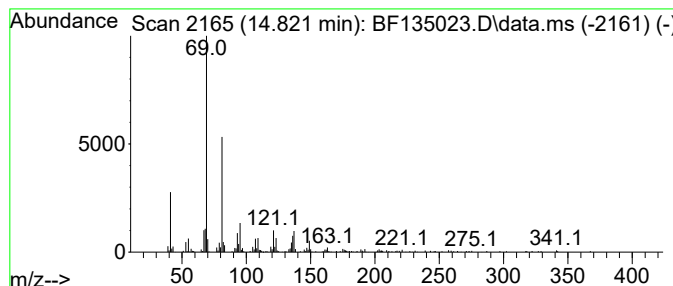
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.821	4.47 ng	157138	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	90
3			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
4			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5			2,6,10,14-Hexadecatetraenoic aci...	318	C21H34O2	042207-88-5	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF083023\
Data File : BF135023.D
Acq On : 31 Aug 2023 01:21
Operator : CG\JU
Sample : 04196-22
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
OR-345-COMP-04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.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-...	5.022	3.5	ng	136559	1	6.769	786648	20.0
Ethanol, 2-(2-e...	6.604	3.5	ng	136079	1	6.769	786648	20.0
2,4,7,9-Tetrame...	9.257	46.7	ng	2410290	3	9.810	1032820	20.0
n-Hexadecanoic ...	11.839	11.7	ng	484651	4	11.298	826249	20.0
trans-13-Octade...	12.416	2.7	ng	110200	4	11.298	826249	20.0
Bis(2-ethylhexy...	12.563	2.5	ng	103918	4	11.298	826249	20.0
Octadecanoic acid	12.627	3.2	ng	131099	4	11.298	826249	20.0
Cyclohexane, 3,...	13.327	9.3	ng	301428	5	13.957	646616	20.0
Heptadecyl hept...	13.810	7.4	ng	240607	5	13.957	646616	20.0
Supraene	14.821	4.5	ng	157138	6	15.427	703669	20.0