

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
 Data File : BF133426.D
 Acq On : 17 May 2023 21:55
 Operator : CG\JU
 Sample : 02813-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133426.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.892	472	477	489	rVB	713368	866375	21.98%	3.048%
2	5.328	547	551	561	rBV	3106654	3116346	79.06%	10.965%
3	5.716	614	617	622	rBV	72630	60398	1.53%	0.213%
4	6.363	722	727	735	rBV	3204563	3134526	79.52%	11.029%
5	6.710	783	786	790	rBV	1693763	1353226	34.33%	4.761%
6	7.275	878	882	886	rBV	2217500	2033317	51.58%	7.154%
7	7.998	1001	1005	1008	rBV	2076303	1629165	41.33%	5.732%
8	9.075	1184	1188	1191	rBV	5067035	3941761	100.00%	13.869%
9	9.657	1285	1287	1291	rVB3	55277	51916	1.32%	0.183%
10	9.751	1299	1303	1306	rVB	1750429	1395039	35.39%	4.908%
11	10.157	1369	1372	1374	rBV2	74036	68019	1.73%	0.239%
12	10.463	1421	1424	1427	rBV	136924	118064	3.00%	0.415%
13	10.539	1433	1437	1440	rBV	1603563	1345029	34.12%	4.732%
14	11.233	1552	1555	1558	rBV	1430242	1160170	29.43%	4.082%
15	11.257	1558	1559	1563	rVB	108259	78616	1.99%	0.277%
16	11.733	1638	1640	1643	rBV2	128564	125450	3.18%	0.441%
17	11.774	1644	1647	1651	rVV2	533325	486688	12.35%	1.712%
18	12.445	1758	1761	1765	rBV	251654	210849	5.35%	0.742%
19	12.557	1778	1780	1786	rVB3	91295	84446	2.14%	0.297%
20	12.674	1797	1800	1803	rVB	202452	190367	4.83%	0.670%
21	12.821	1821	1825	1828	rBV	2674364	2296972	58.27%	8.082%
22	13.727	1975	1979	1986	rBV	243967	307838	7.81%	1.083%
23	13.868	1999	2003	2006	rBV2	1052750	1154735	29.29%	4.063%
24	13.898	2006	2008	2010	rVB	132614	104591	2.65%	0.368%
25	14.351	2082	2085	2092	rBV5	171056	345836	8.77%	1.217%
26	14.715	2145	2147	2154	rBV	109700	128910	3.27%	0.454%
27	14.892	2174	2177	2184	rVB	150580	272879	6.92%	0.960%
28	14.968	2187	2190	2193	rBV	291318	311139	7.89%	1.095%
29	15.298	2242	2246	2260	rVB	893323	1577403	40.02%	5.550%
30	15.739	2317	2321	2326	rBV	350559	471065	11.95%	1.657%

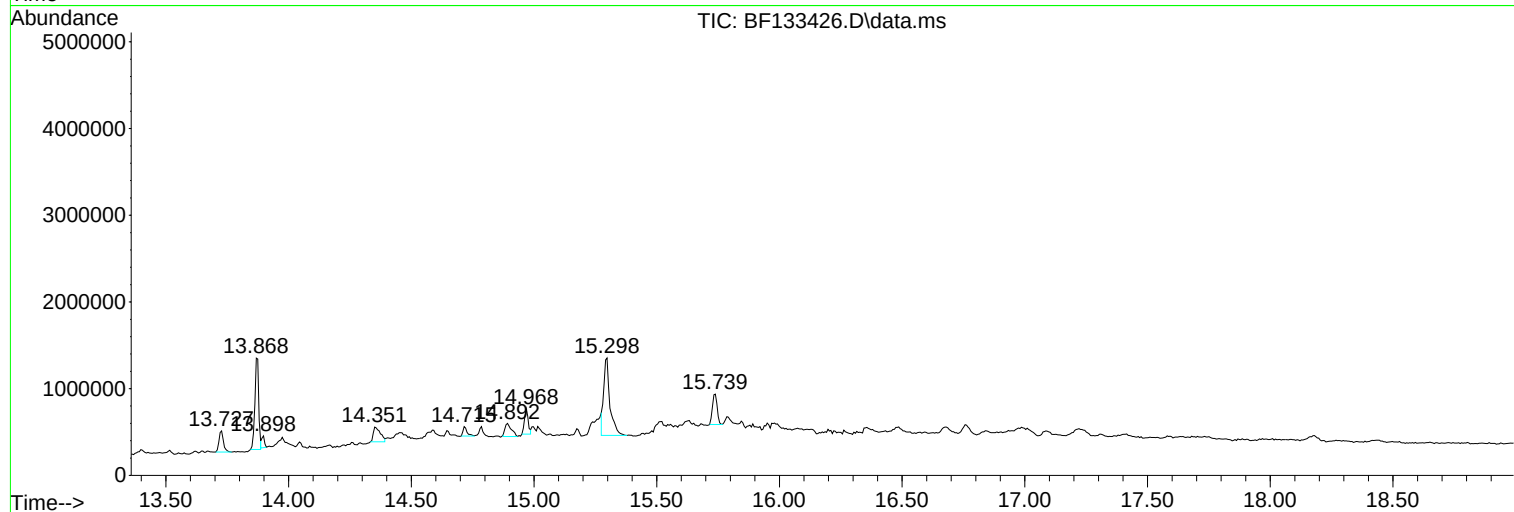
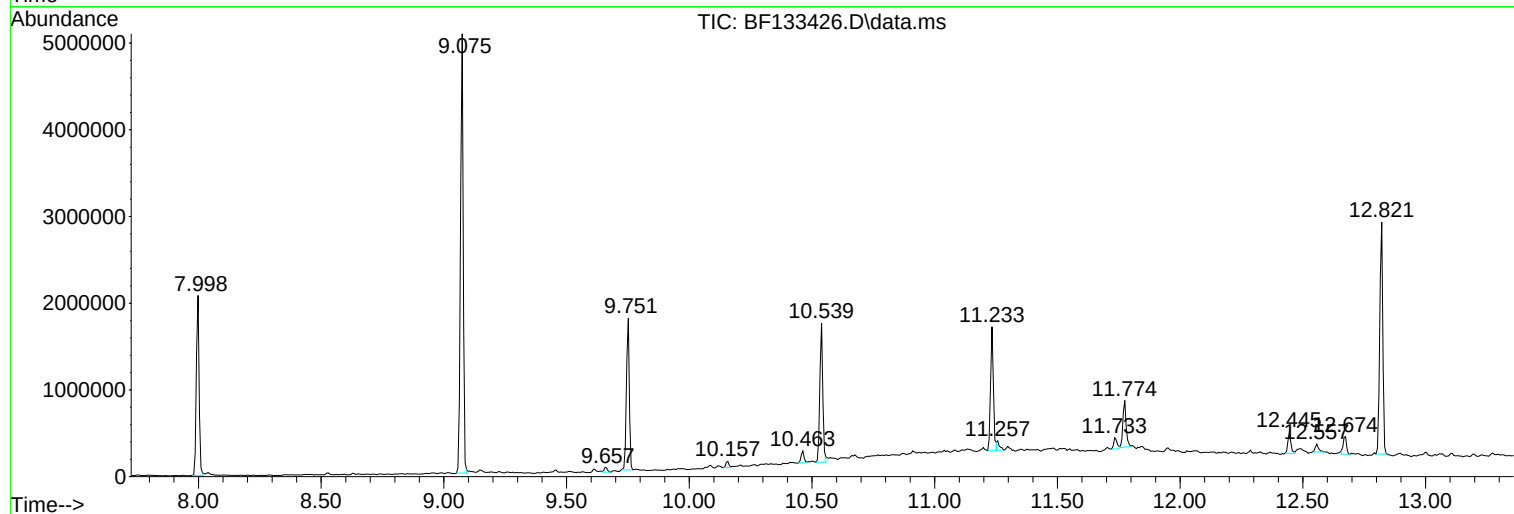
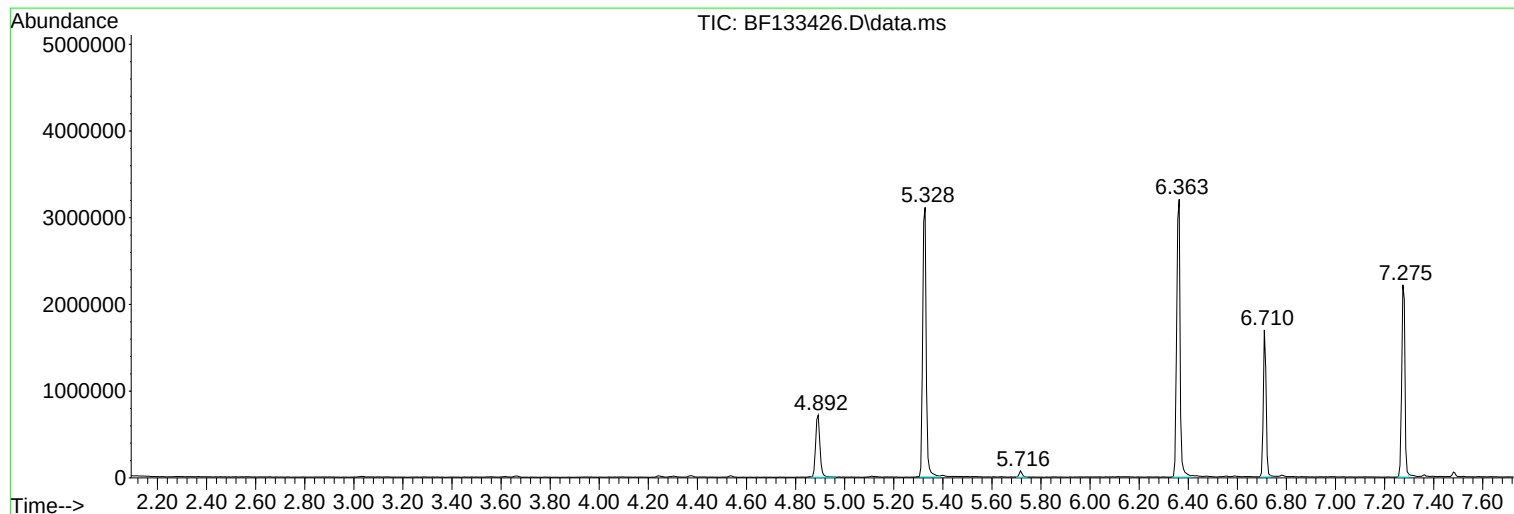
Sum of corrected areas: 28421135

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133426.D
Acq On : 17 May 2023 21:55
Operator : CG\JU
Sample : 02813-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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\BF051723\
Data File : BF133426.D
Acq On : 17 May 2023 21:55
Operator : CG\JU
Sample : 02813-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

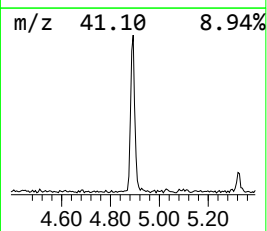
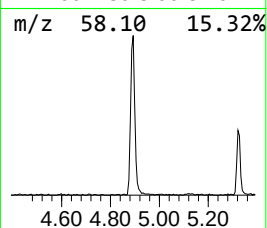
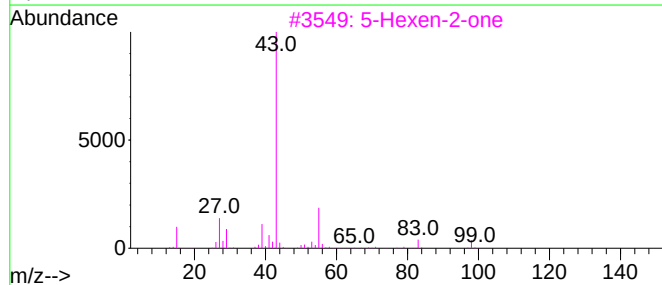
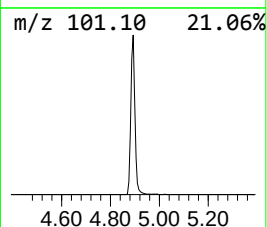
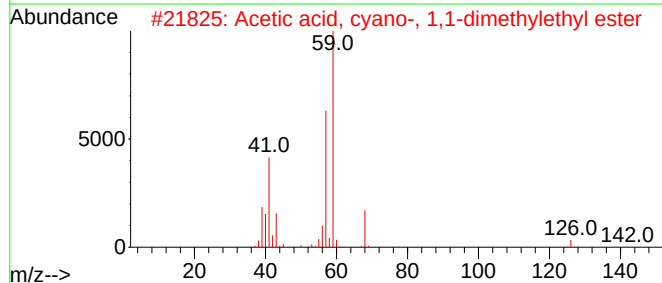
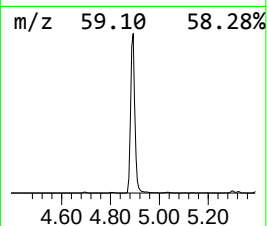
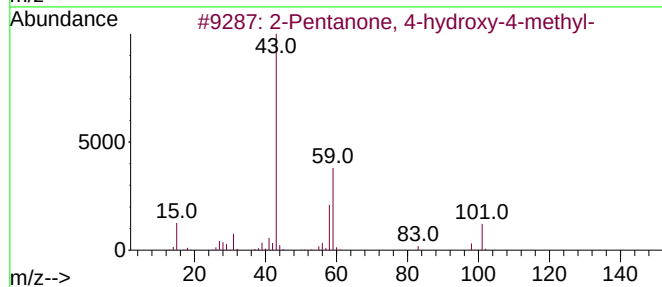
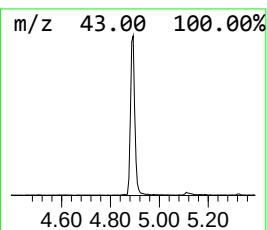
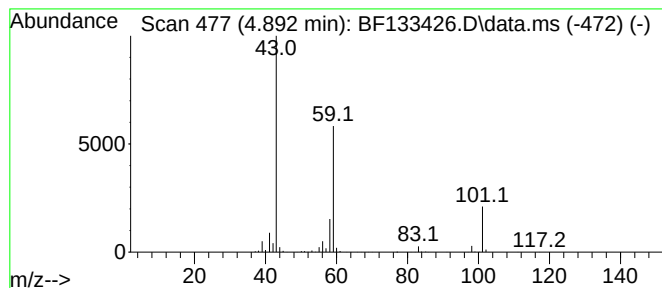
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.892	12.80 ng	866375	1,4-Dichlorobenzene-d4	6.710

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133426.D
Acq On : 17 May 2023 21:55
Operator : CG\JU
Sample : 02813-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

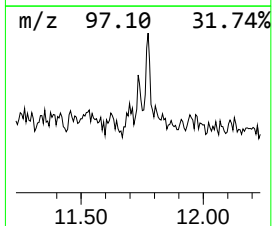
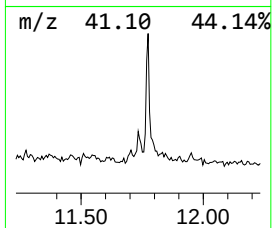
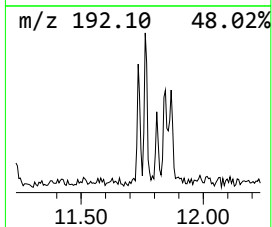
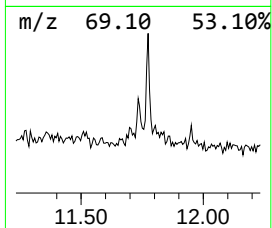
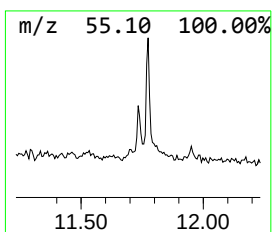
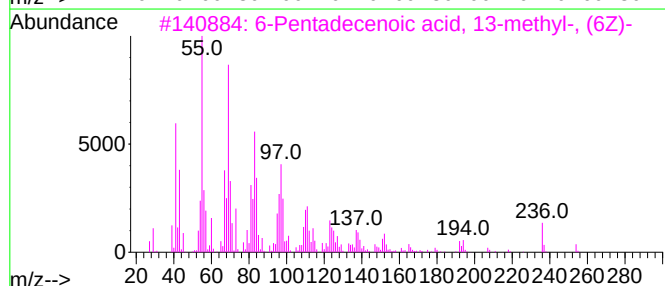
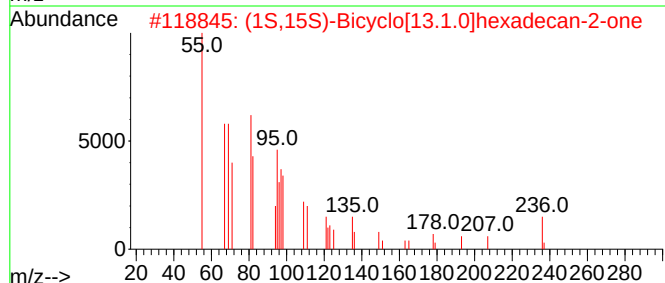
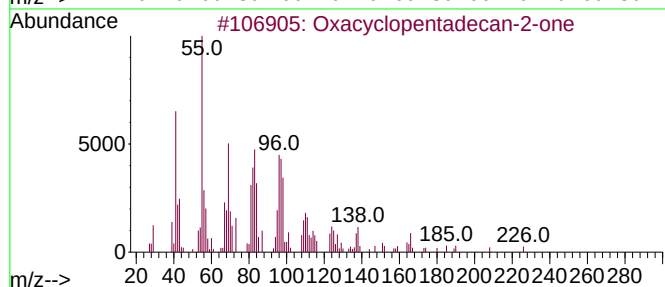
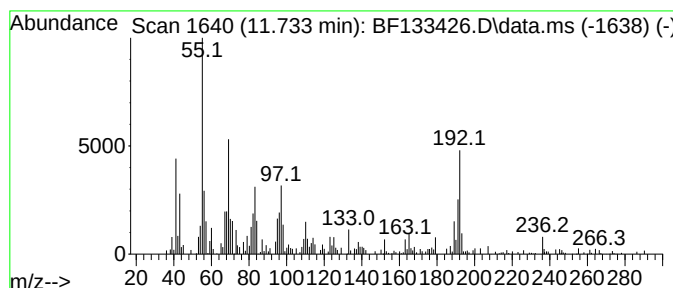
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown11.733 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.733	2.16 ng	125450	Phenanthrene-d10	11.233

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxacyclopentadecan-2-one	226	C14H26O2	003537-83-5	25
2		(1S,15S)-Bicyclo[13.1.0]hexadeca...	236	C16H28O	102572-89-4	25
3		6-Pentadecenoic acid, 13-methyl-...	254	C16H30O2	682751-34-4	22
4		trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	20
5		cis-Vaccenic acid	282	C18H34O2	000506-17-2	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133426.D
Acq On : 17 May 2023 21:55
Operator : CG\JU
Sample : 02813-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

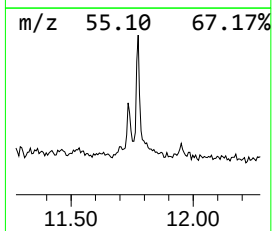
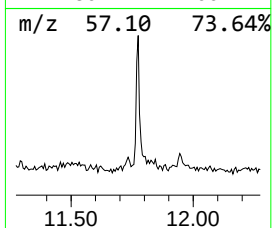
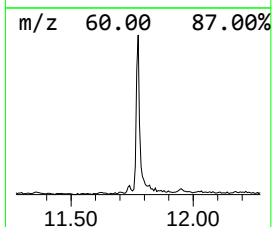
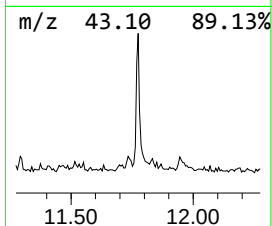
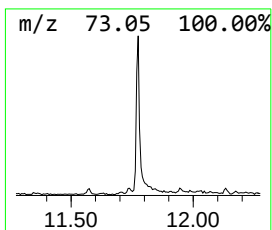
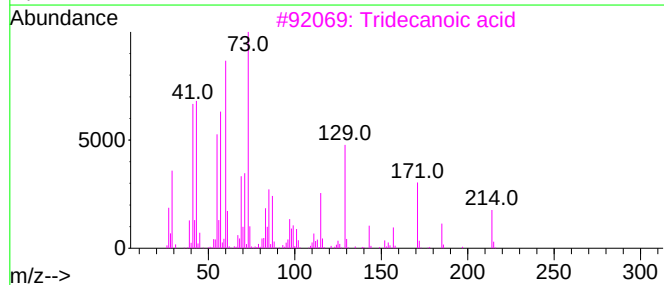
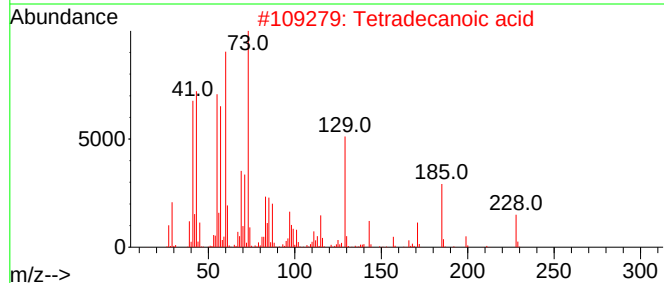
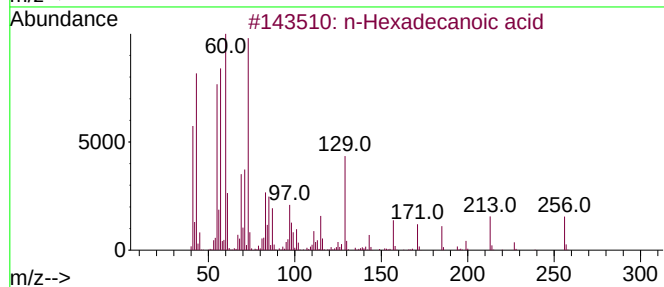
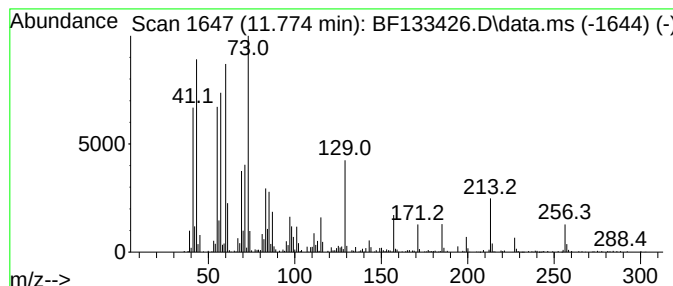
Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.774	8.39 ng	486688	Phenanthrene-d10	11.233	
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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	92
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Octadecanoic acid	284	C18H36O2	000057-11-4	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133426.D
Acq On : 17 May 2023 21:55
Operator : CG\JU
Sample : 02813-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

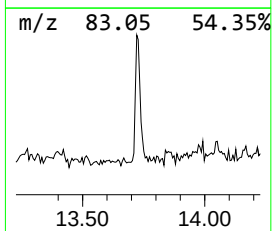
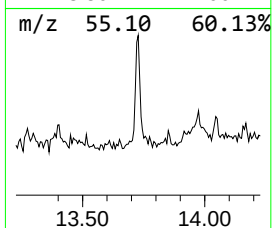
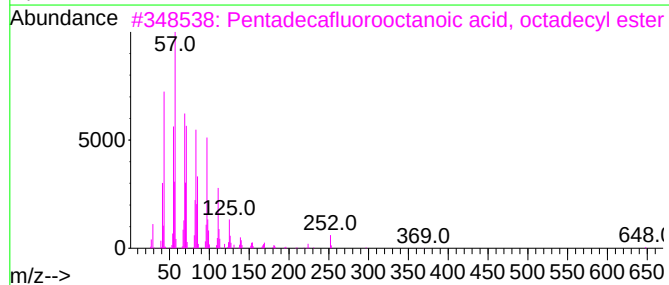
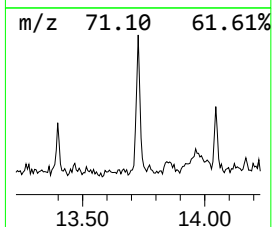
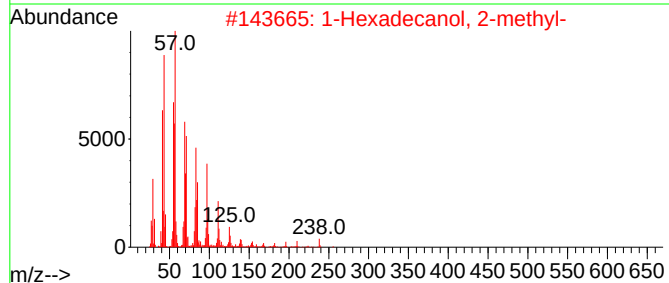
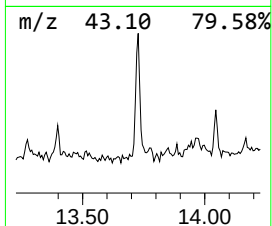
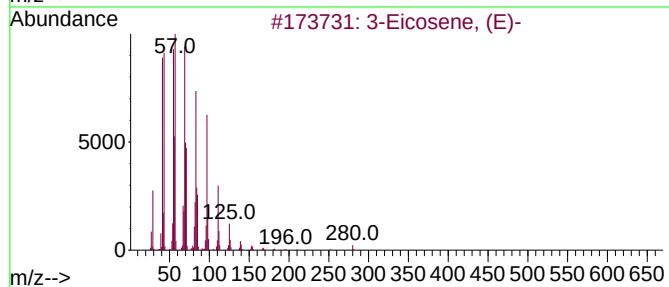
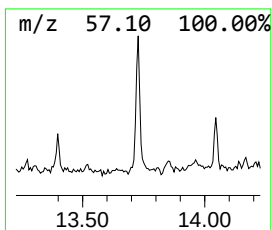
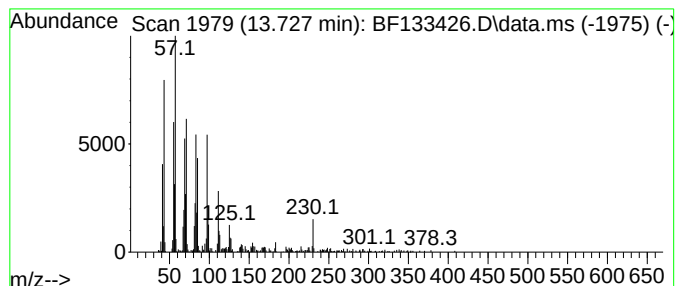
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.727	5.33 ng	307838	Chrysene-d12	13.874

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2		1-Hexadecanol, 2-methyl-	256	C17H36O	002490-48-4	94
3		Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	89
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133426.D
Acq On : 17 May 2023 21:55
Operator : CG\JU
Sample : 02813-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

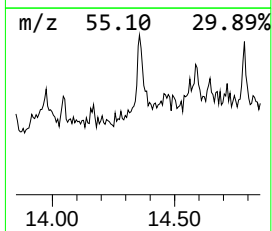
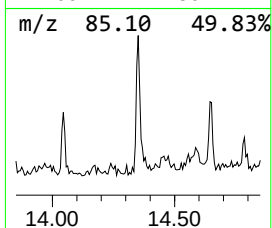
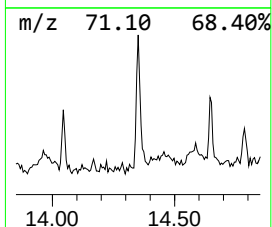
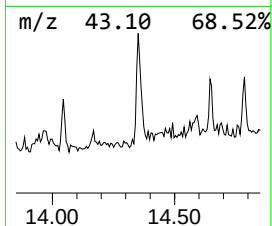
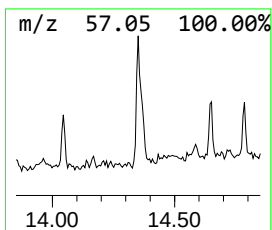
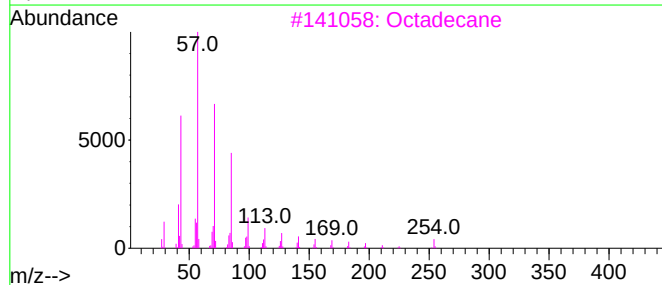
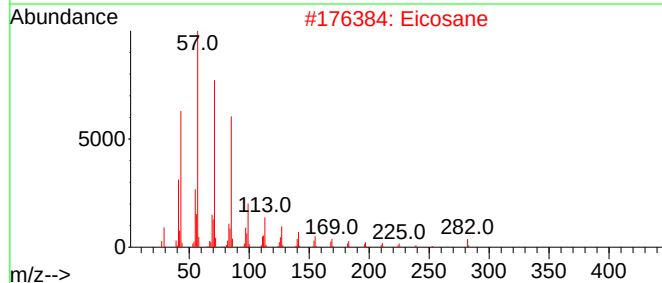
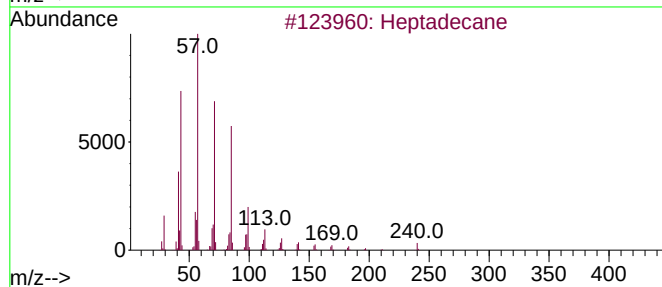
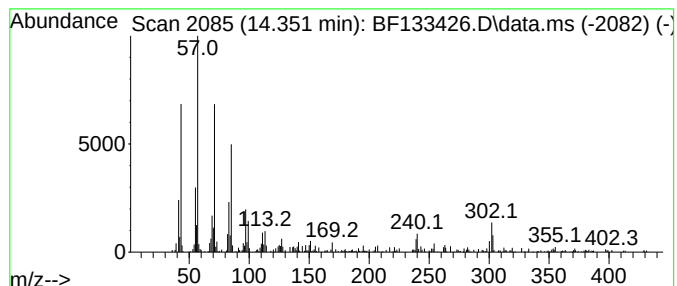
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.351	5.99 ng	345836	Chrysene-d12	13.874

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	93
2			Eicosane	282	C20H42	000112-95-8	91
3			Octadecane	254	C18H38	000593-45-3	91
4			E-14-Hexadecenal	238	C16H30O	330207-53-9	90
5			Heptacosane	380	C27H56	000593-49-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133426.D
Acq On : 17 May 2023 21:55
Operator : CG\JU
Sample : 02813-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

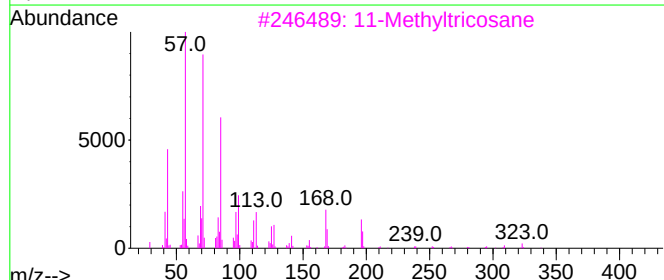
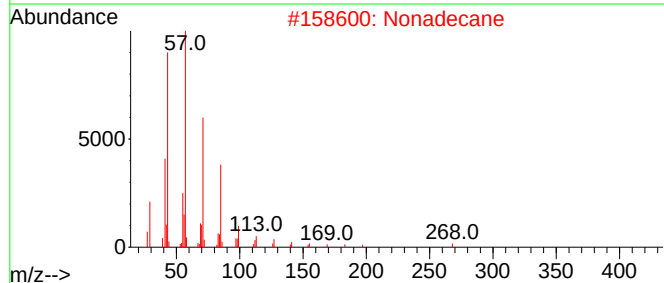
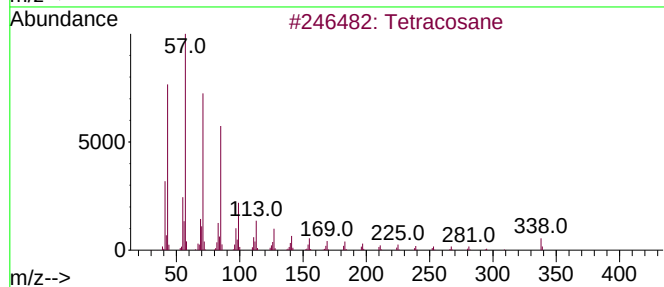
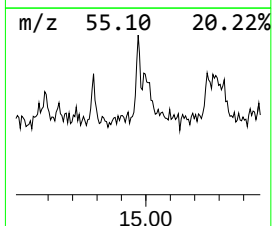
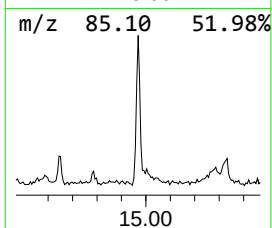
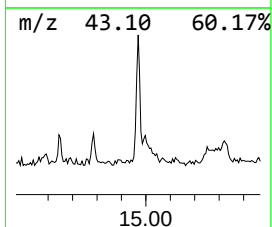
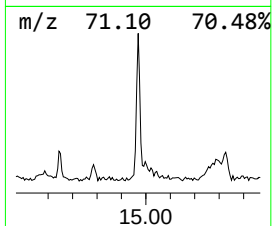
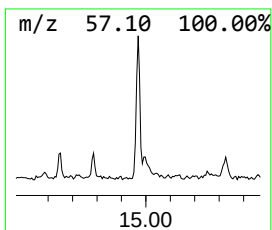
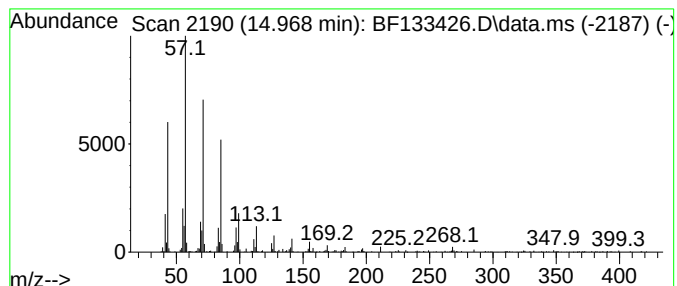
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.968	3.94 ng	311139	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	93
2			Nonadecane	268	C19H40	000629-92-5	93
3			11-Methyltricosane	338	C24H50	027538-41-6	93
4			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
5			Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133426.D
Acq On : 17 May 2023 21:55
Operator : CG\JU
Sample : 02813-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

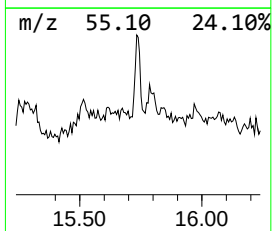
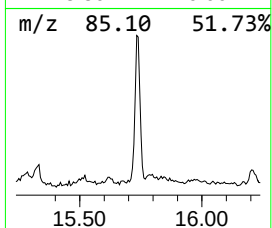
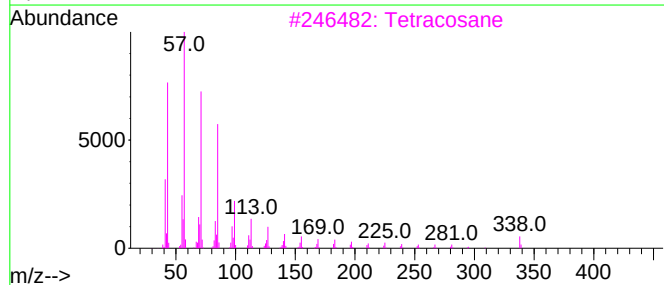
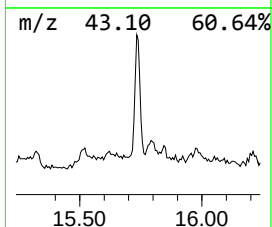
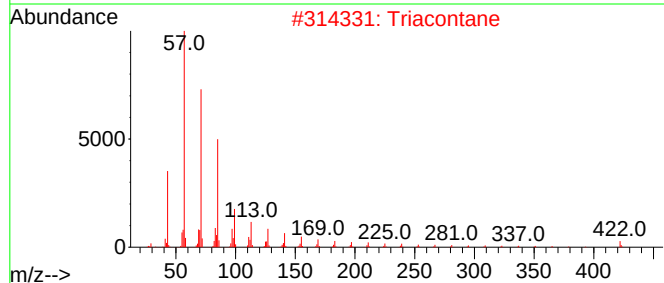
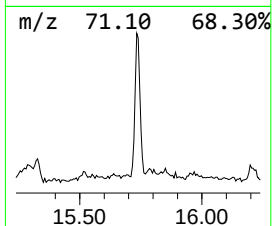
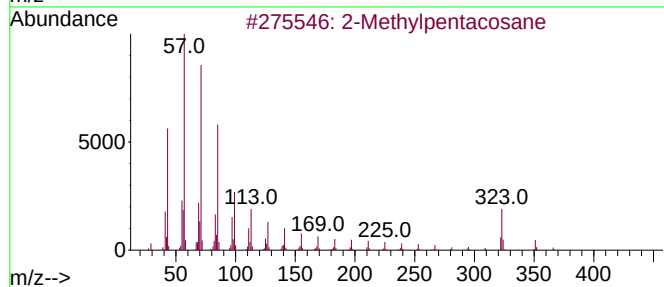
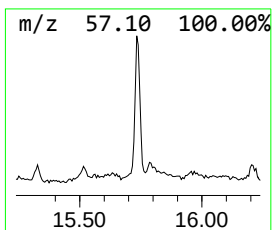
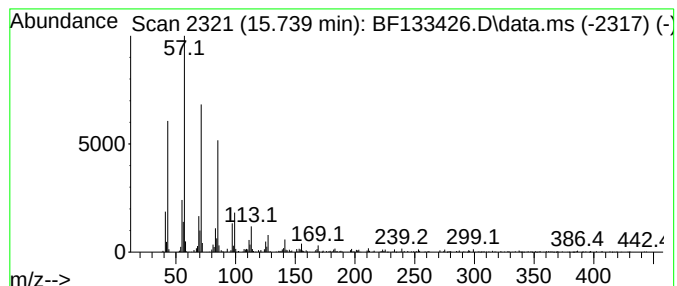
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 2-Methylpentacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.739	5.97 ng	471065	Perylene-d12	15.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methylpentacosane	366	C26H54	000629-87-8	94
2			Triacontane	422	C30H62	000638-68-6	93
3			Tetracosane	338	C24H50	000646-31-1	93
4			11-Methylpentacosane	366	C26H54	015689-71-1	93
5			Octadecane	254	C18H38	000593-45-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051723\
Data File : BF133426.D
Acq On : 17 May 2023 21:55
Operator : CG\JU
Sample : 02813-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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-...	4.892	12.8	ng	866375	1	6.710	1353230	20.0
unknown11.733	11.733	2.2	ng	125450	4	11.233	1160170	20.0
n-Hexadecanoic ...	11.774	8.4	ng	486688	4	11.233	1160170	20.0
3-Eicosene, (E)-	13.727	5.3	ng	307838	5	13.874	1154740	20.0
Heptadecane	14.351	6.0	ng	345836	5	13.874	1154740	20.0
Tetracosane	14.968	3.9	ng	311139	6	15.298	1577400	20.0
2-Methylpentaco...	15.739	6.0	ng	471065	6	15.298	1577400	20.0