

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
 Data File : BF135191.D
 Acq On : 12 Sep 2023 20:27
 Operator : CG\JU
 Sample : 04336-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TRENCH-B

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	495	499	509	rVB	55812	82524	2.36%	0.347%
2	5.404	559	564	567	rBV	2959757	3091757	88.53%	12.992%
3	6.404	728	734	737	rBV	2800322	3152039	90.25%	13.245%
4	6.763	791	795	798	rBV	770872	640067	18.33%	2.690%
5	7.328	885	891	894	rBV	2016331	2065860	59.15%	8.681%
6	7.763	962	965	973	rBV2	26645	43622	1.25%	0.183%
7	8.039	1007	1012	1015	rBV	1006652	850735	24.36%	3.575%
8	9.122	1190	1196	1199	rBV	3623879	3384933	96.92%	14.224%
9	9.798	1305	1311	1314	rBV	1132836	967672	27.71%	4.066%
10	10.592	1441	1446	1449	rBV	2395023	2247603	64.36%	9.445%
11	11.286	1560	1564	1567	rBV	1236852	1081905	30.98%	4.546%
12	11.310	1567	1568	1572	rVB	116522	73345	2.10%	0.308%
13	11.827	1652	1656	1666	rBV2	394414	399988	11.45%	1.681%
14	12.504	1765	1771	1776	rBV	153026	141119	4.04%	0.593%
15	12.616	1786	1790	1801	rBV2	91016	123109	3.53%	0.517%
16	12.733	1804	1810	1813	rVV	120511	129292	3.70%	0.543%
17	12.892	1831	1837	1840	rBV	3247666	3492428	100.00%	14.676%
18	13.827	1988	1996	2009	rBV4	82371	260755	7.47%	1.096%
19	13.939	2010	2015	2018	rVV	853660	867216	24.83%	3.644%
20	13.963	2018	2019	2027	rVB	54288	52490	1.50%	0.221%
21	14.980	2188	2192	2195	rBV2	32284	47824	1.37%	0.201%
22	15.404	2259	2264	2270	rBV	479912	600838	17.20%	2.525%

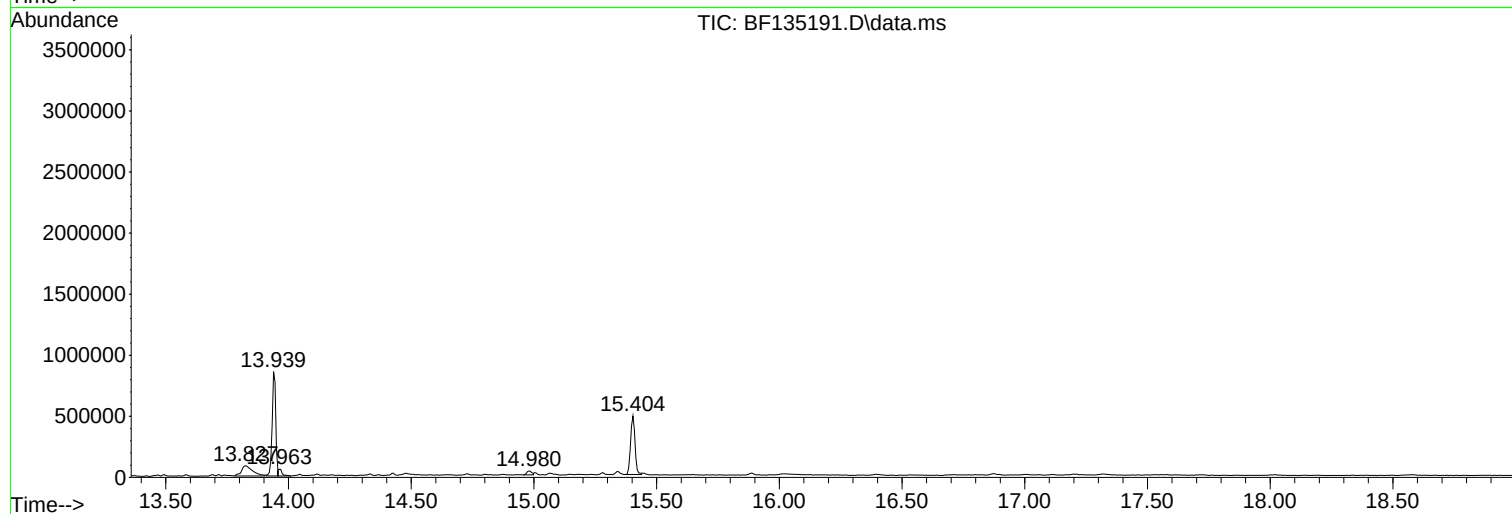
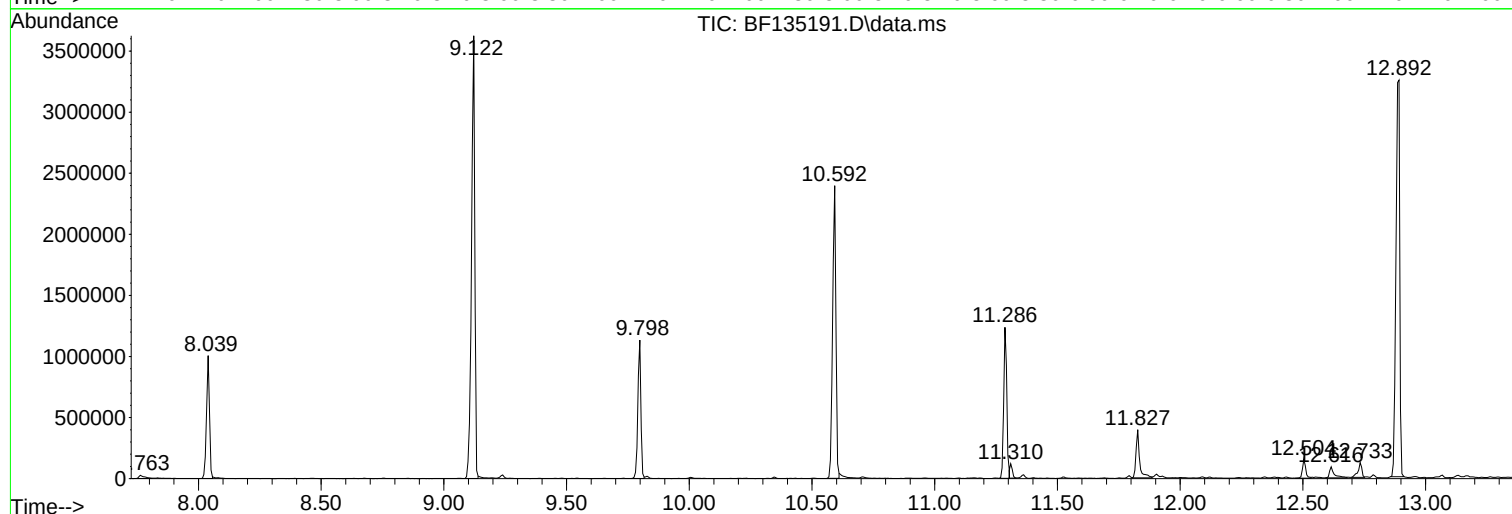
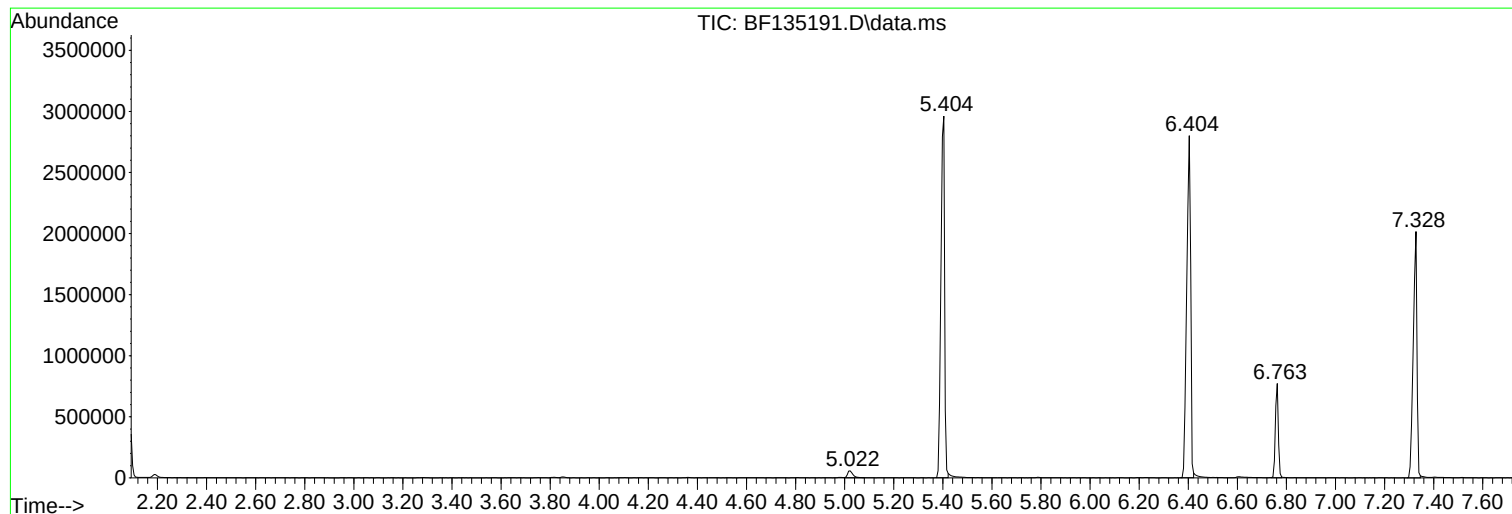
Sum of corrected areas: 23797121

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135191.D
Acq On : 12 Sep 2023 20:27
Operator : CG\JU
Sample : 04336-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRENCH-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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\BF091223\
Data File : BF135191.D
Acq On : 12 Sep 2023 20:27
Operator : CG\JU
Sample : 04336-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRENCH-B

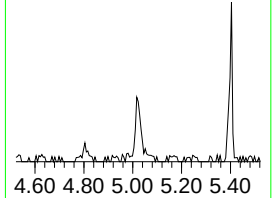
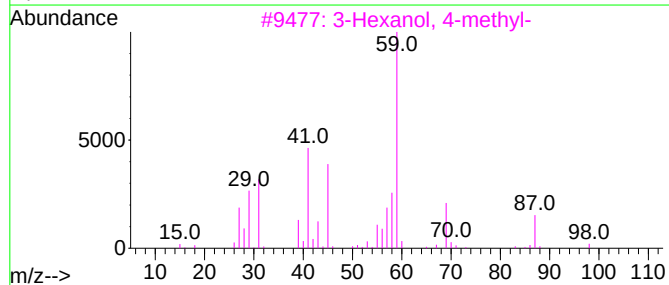
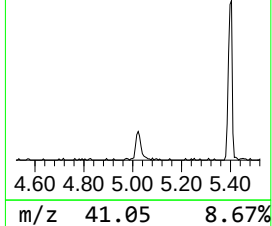
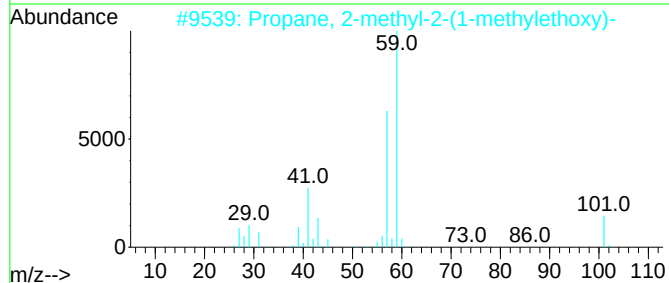
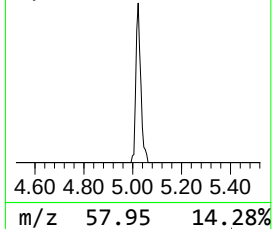
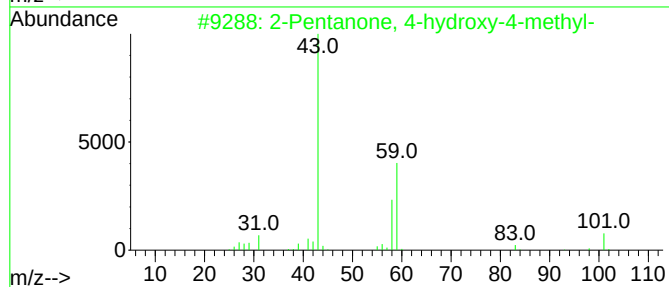
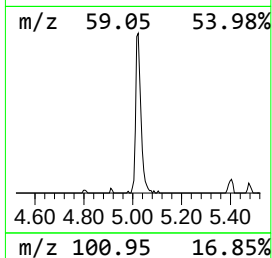
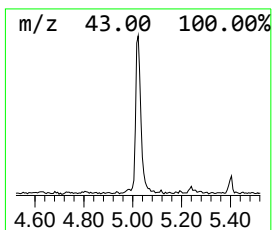
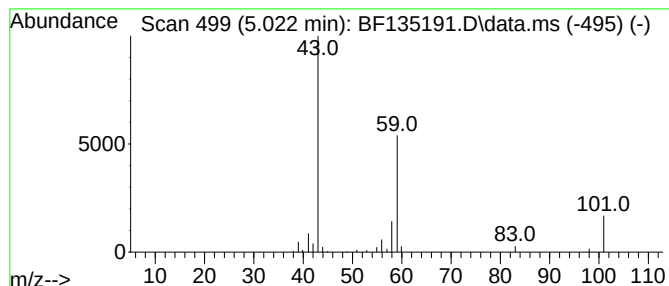
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	2.58 ng	82524	1,4-Dichlorobenzene-d4	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	28		



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135191.D
Acq On : 12 Sep 2023 20:27
Operator : CG\JU
Sample : 04336-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRENCH-B

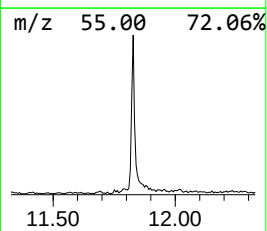
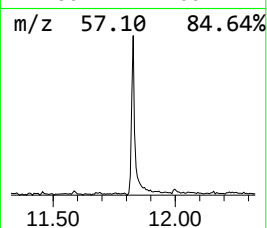
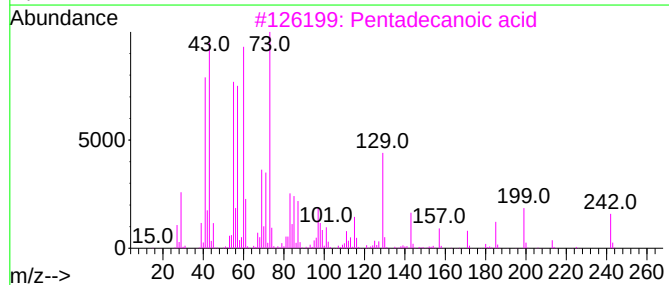
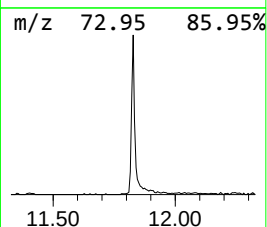
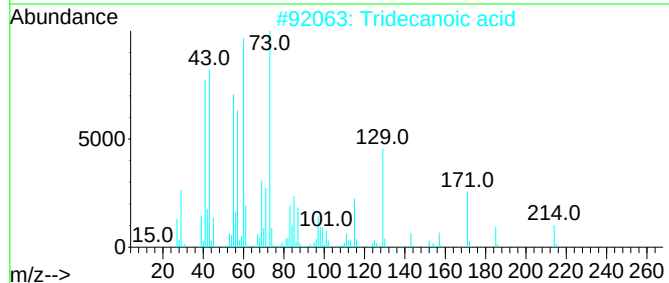
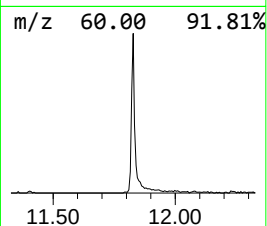
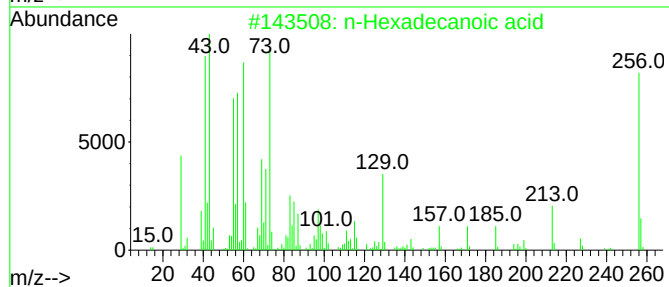
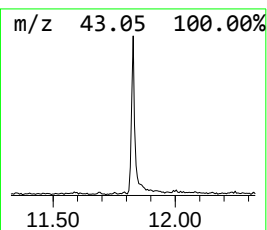
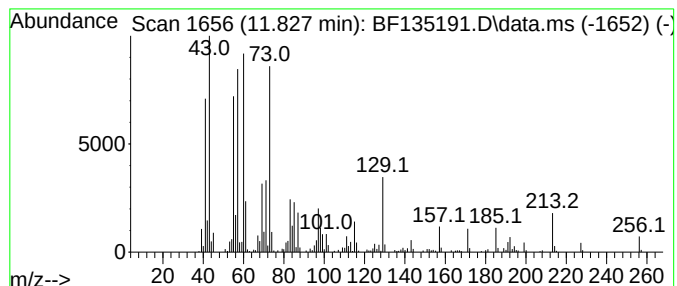
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.827	7.39 ng	399988	Phenanthrene-d10	11.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135191.D
Acq On : 12 Sep 2023 20:27
Operator : CG\JU
Sample : 04336-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRENCH-B

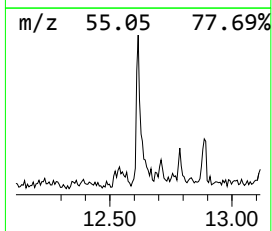
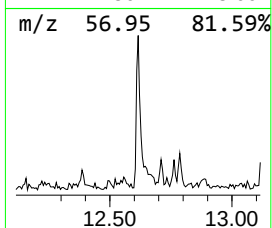
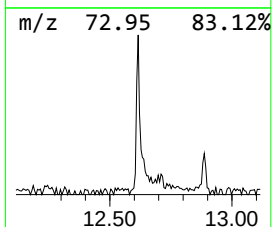
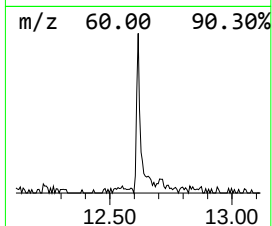
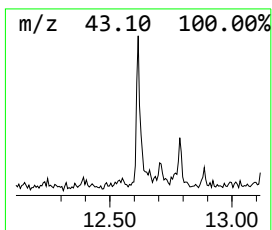
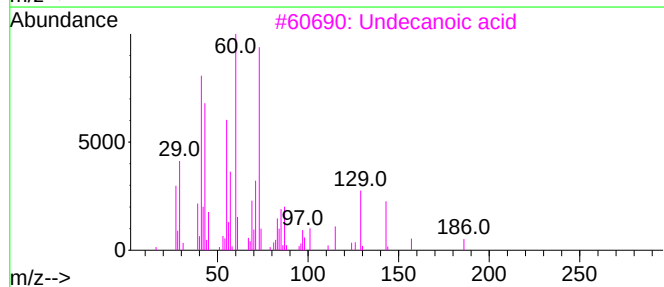
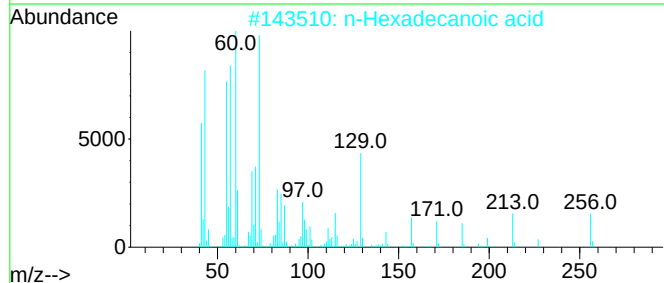
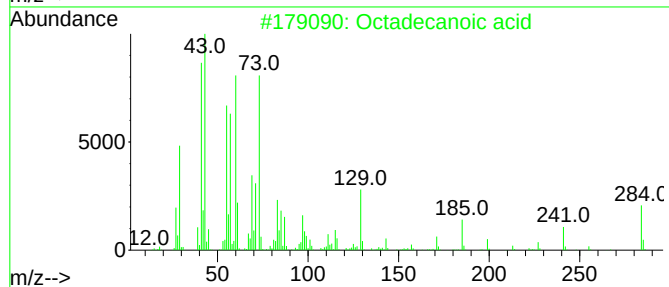
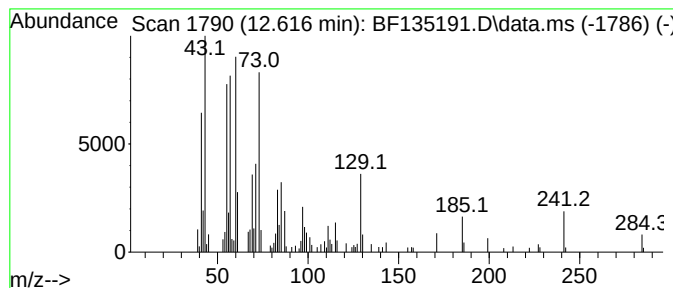
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	2.84 ng	123109	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74
3			Undecanoic acid	186	C11H22O2	000112-37-8	64
4			Nonanoic acid	158	C9H18O2	000112-05-0	46
5			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135191.D
Acq On : 12 Sep 2023 20:27
Operator : CG\JU
Sample : 04336-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRENCH-B

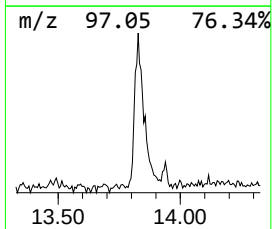
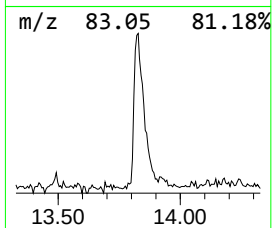
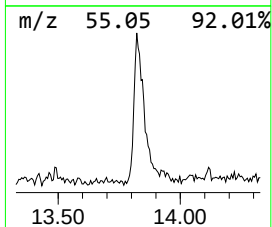
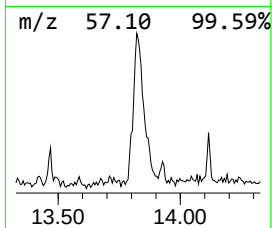
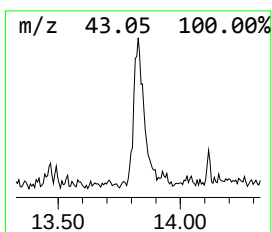
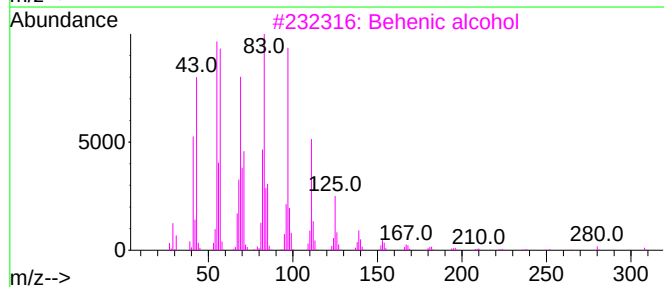
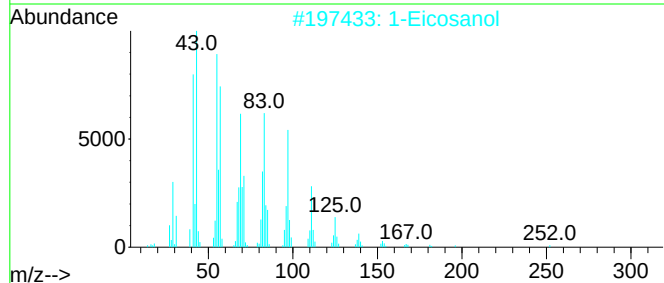
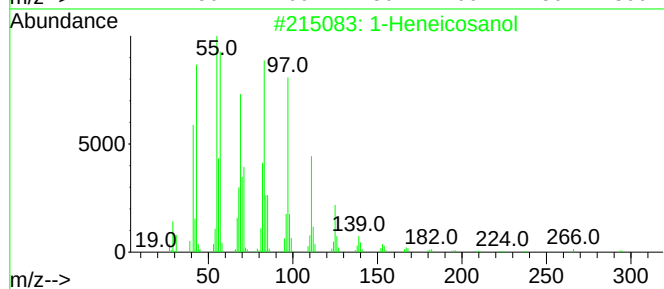
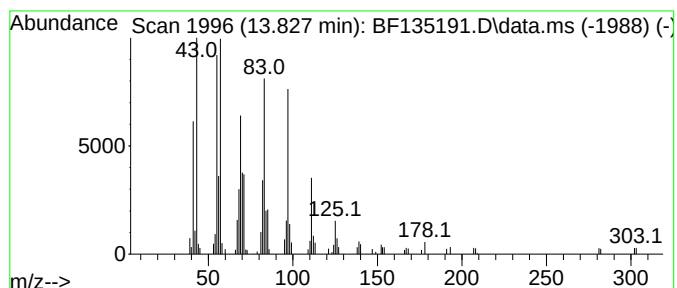
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	6.01 ng	260755	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			1-Eicosanol	298	C20H42O	000629-96-9	91
3			Behenic alcohol	326	C22H46O	000661-19-8	91
4			Eicosyl methyl ether	312	C21H44O	1000406-29-4	91
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091223\
Data File : BF135191.D
Acq On : 12 Sep 2023 20:27
Operator : CG\JU
Sample : 04336-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TRENCH-B

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	2.6	ng	82524	1	6.763	640067	20.0
n-Hexadecanoic ...	11.827	7.4	ng	399988	4	11.286	1081910	20.0
Octadecanoic acid	12.616	2.8	ng	123109	5	13.939	867216	20.0
1-Heneicosanol	13.827	6.0	ng	260755	5	13.939	867216	20.0