

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100323\
 Data File : BF135546.D
 Acq On : 03 Oct 2023 17:27
 Operator : CG\JU
 Sample : 04666-01 10X
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VNJ-201

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: BF135546.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.375	555	559	575	rBV	229635	308277	6.29%	1.813%
2	6.392	729	732	744	rBV	251400	312567	6.38%	1.839%
3	6.734	787	790	797	rBV	1033614	993015	20.27%	5.841%
4	7.304	884	887	895	rBV	182001	197816	4.04%	1.164%
5	8.016	1001	1008	1014	rBV	1573018	1284729	26.23%	7.557%
6	9.092	1187	1191	1195	rBV	425882	328951	6.72%	1.935%
7	9.175	1200	1205	1207	rBV	56206	56523	1.15%	0.332%
8	9.769	1303	1306	1310	rVB	1321467	1183186	24.16%	6.960%
9	10.569	1439	1442	1446	rBV	112575	114646	2.34%	0.674%
10	10.680	1458	1461	1466	rBV2	79188	124843	2.55%	0.734%
11	10.886	1491	1496	1499	rBV5	32952	50724	1.04%	0.298%
12	11.157	1540	1542	1549	rVB	55892	57642	1.18%	0.339%
13	11.263	1557	1560	1563	rBV	1244207	1033085	21.09%	6.077%
14	11.810	1645	1653	1664	rVB	2283604	3502246	71.50%	20.602%
15	12.457	1759	1763	1765	rBV3	45023	65221	1.33%	0.384%
16	12.492	1765	1769	1771	rBV2	271889	371989	7.59%	2.188%
17	12.598	1780	1787	1797	rVB	2989574	4898142	100.00%	28.813%
18	12.716	1805	1807	1812	rVB2	81506	91045	1.86%	0.536%
19	12.857	1828	1831	1838	rVB	310536	280516	5.73%	1.650%
20	13.921	2008	2012	2015	rBV	873496	784355	16.01%	4.614%
21	15.386	2257	2261	2267	rBV	518525	686652	14.02%	4.039%
22	16.480	2443	2447	2455	rVB3	152807	273591	5.59%	1.609%

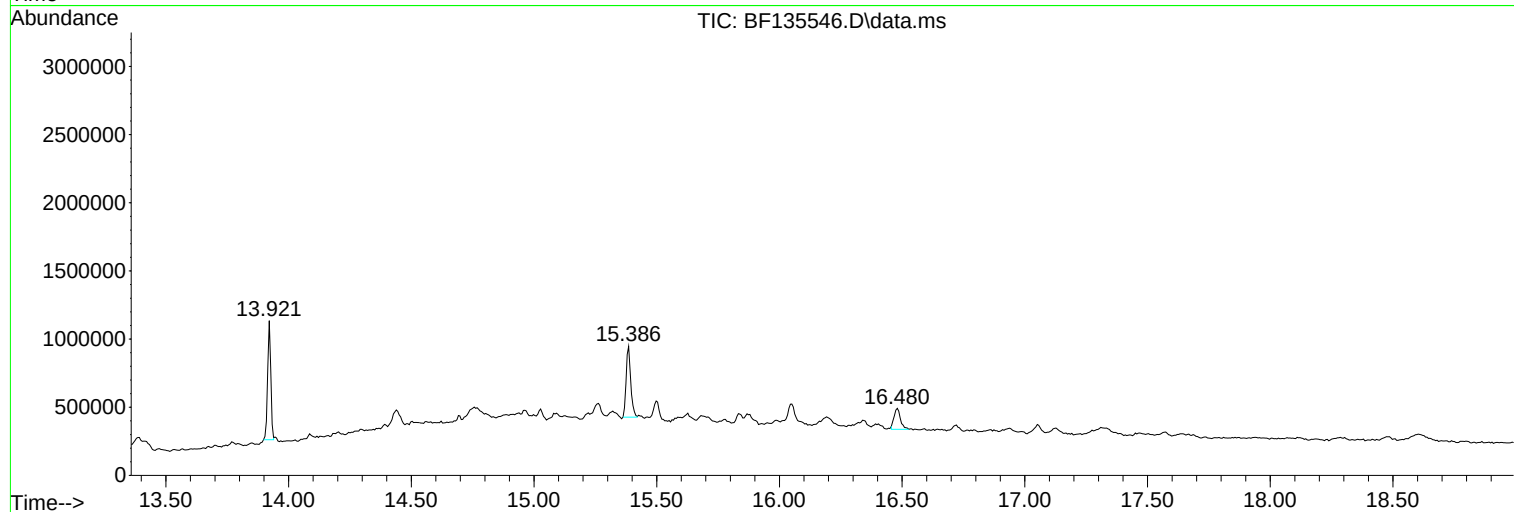
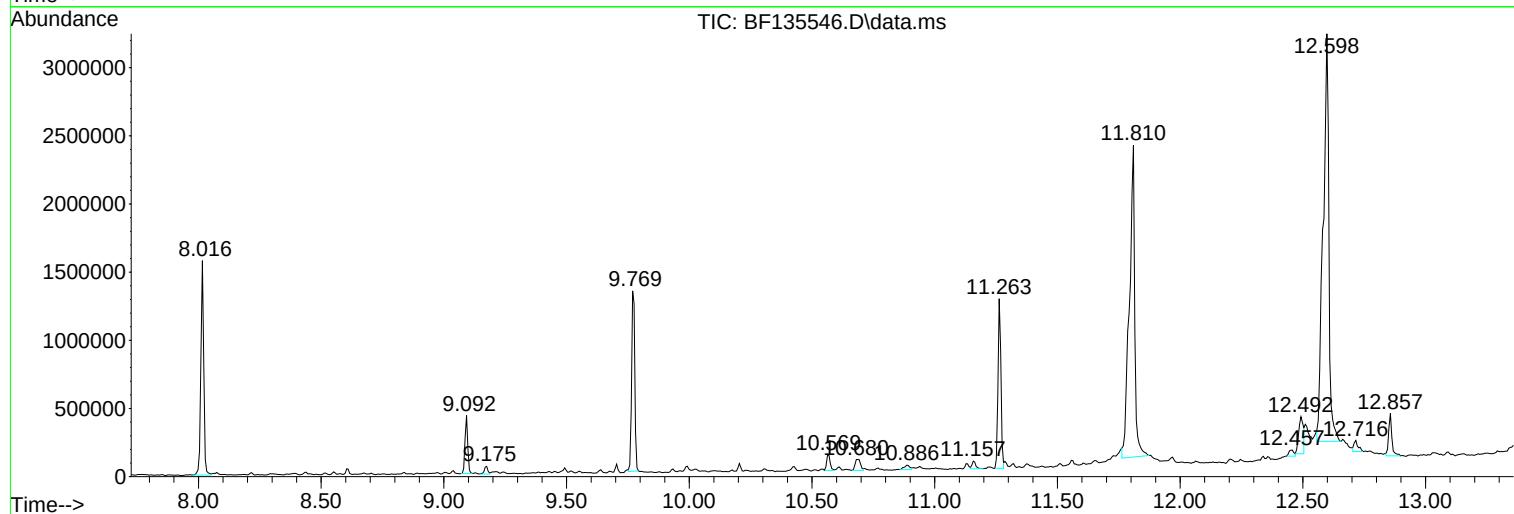
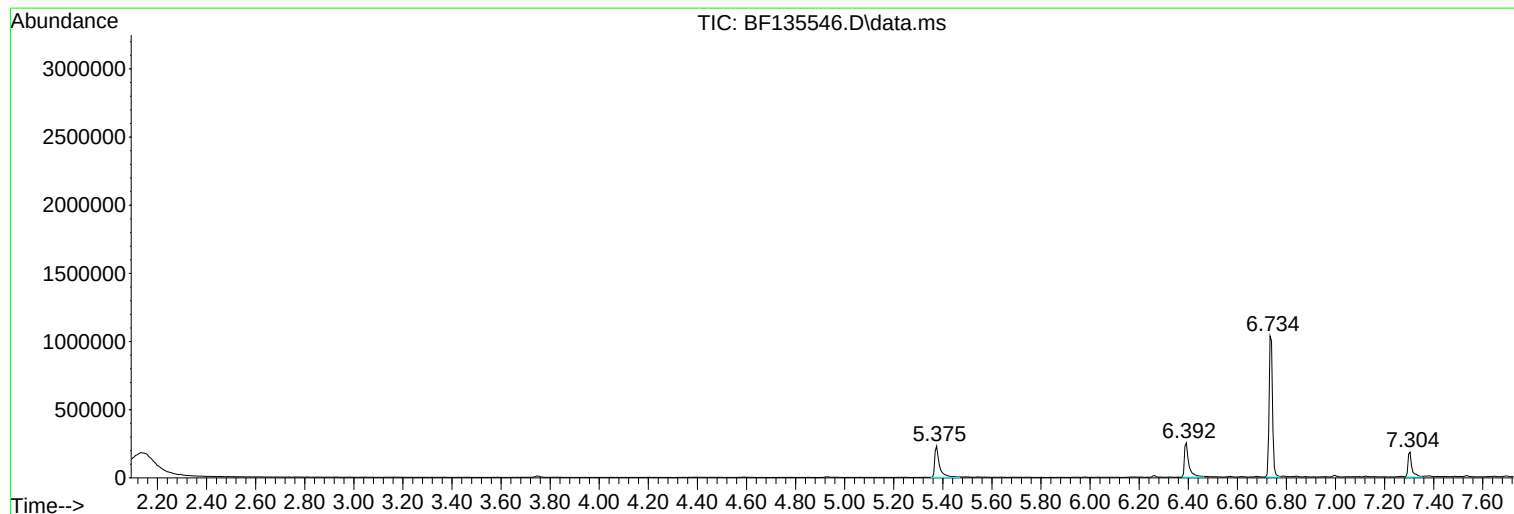
Sum of corrected areas: 16999761

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100323\
Data File : BF135546.D
Acq On : 03 Oct 2023 17:27
Operator : CG\JU
Sample : 04666-01 10X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-201

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\BF100323\
Data File : BF135546.D
Acq On : 03 Oct 2023 17:27
Operator : CG\JU
Sample : 04666-01 10X
Misc :
ALS Vial : 5 Sample Multiplier: 1

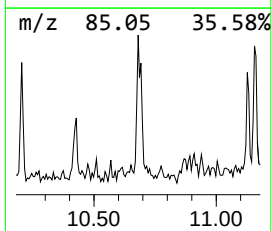
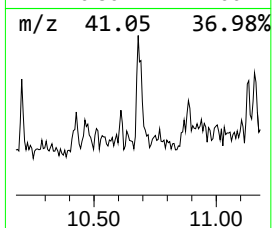
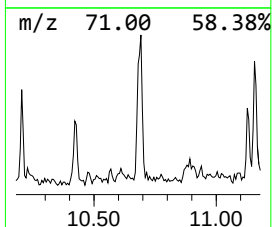
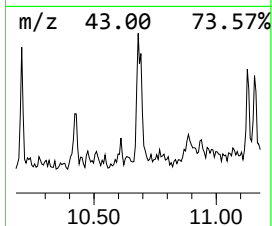
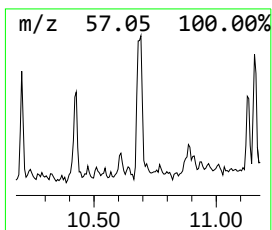
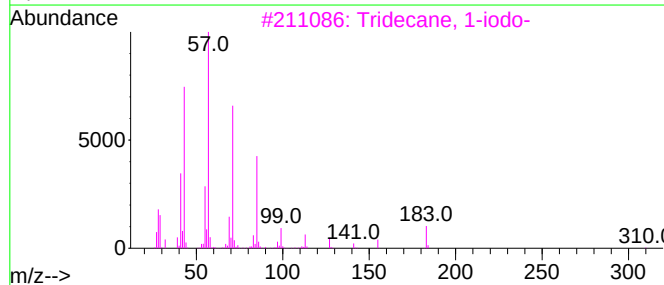
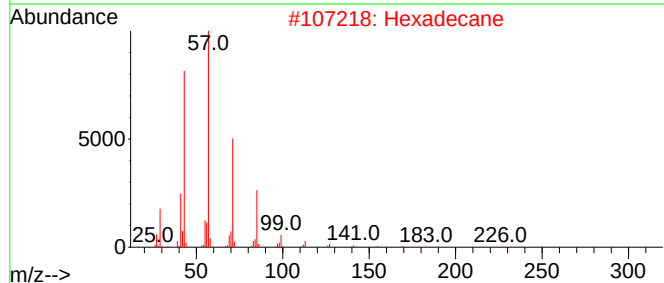
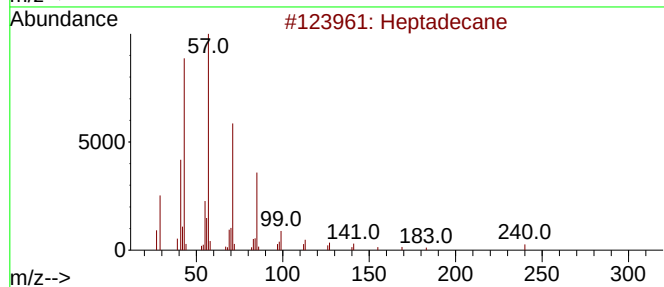
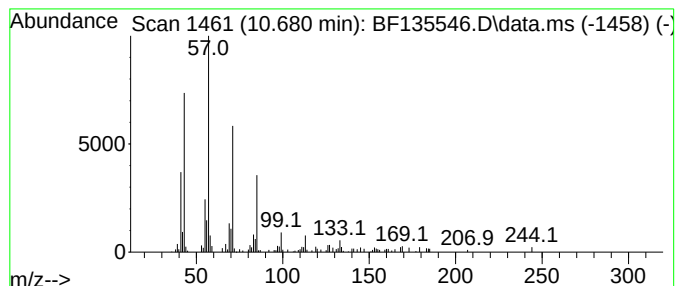
Instrument :
BNA_F
ClientSampleId :
VNJ-201

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 Heptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.680	2.42 ng	124843	Phenanthrene-d10		11.263	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Heptadecane		240	C17H36	000629-78-7	80
2	Hexadecane		226	C16H34	000544-76-3	80
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	80
4	Tetradecane		198	C14H30	000629-59-4	72
5	Dodecane, 1-iodo-		296	C12H25I	004292-19-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100323\
Data File : BF135546.D
Acq On : 03 Oct 2023 17:27
Operator : CG\JU
Sample : 04666-01 10X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-201

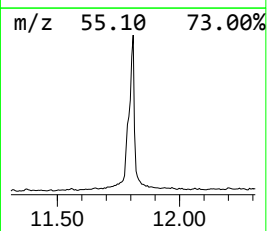
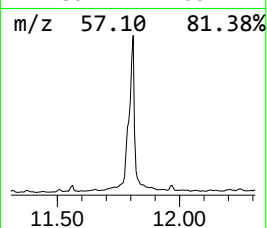
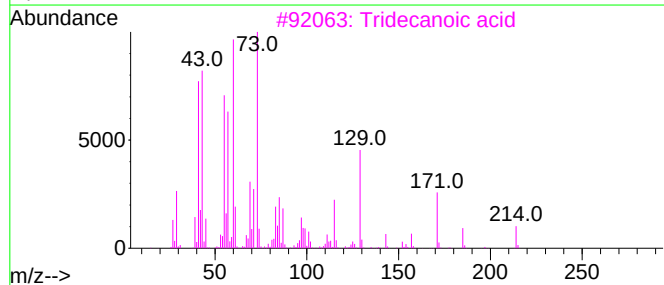
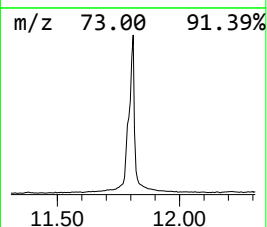
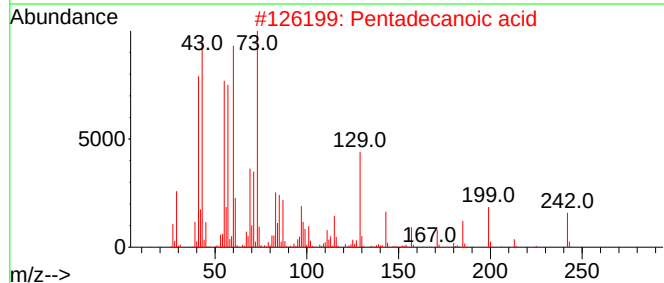
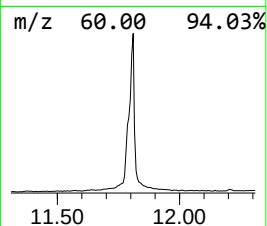
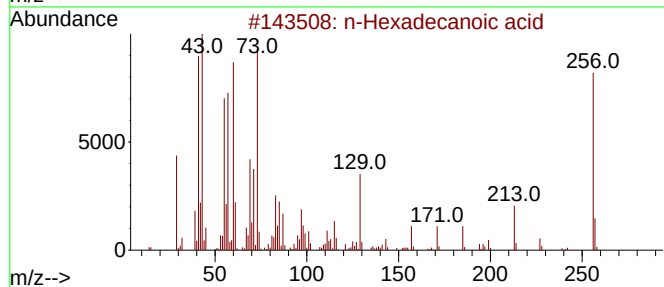
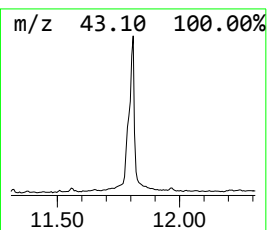
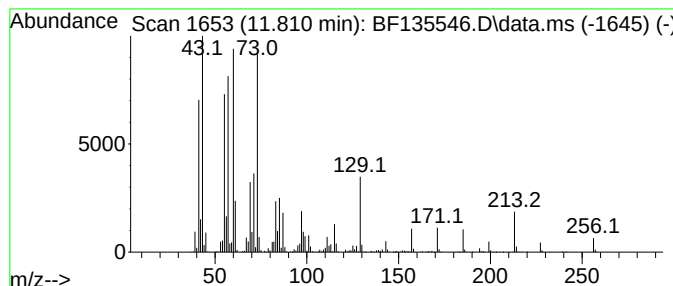
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	67.80 ng	3502250	Phenanthrene-d10	11.263

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100323\
Data File : BF135546.D
Acq On : 03 Oct 2023 17:27
Operator : CG\JU
Sample : 04666-01 10X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-201

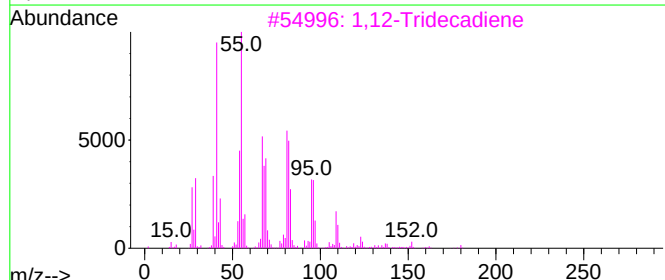
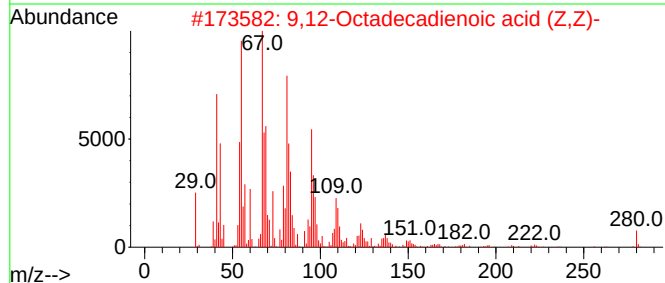
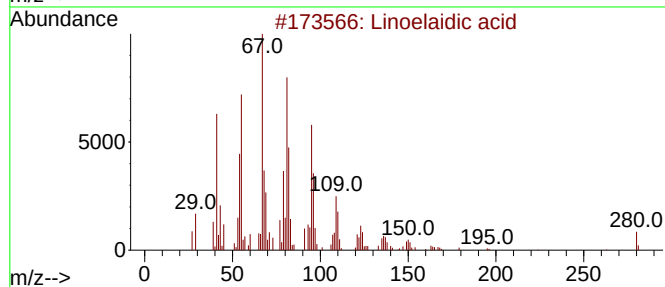
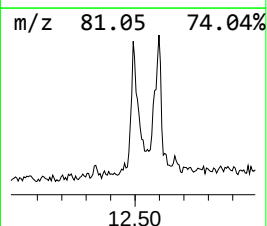
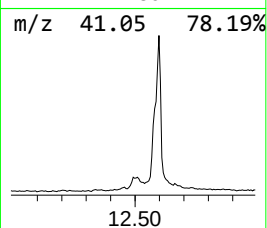
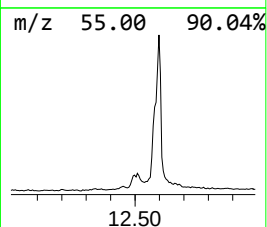
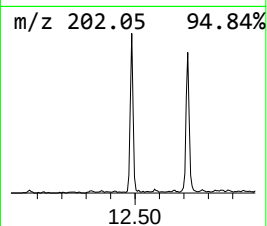
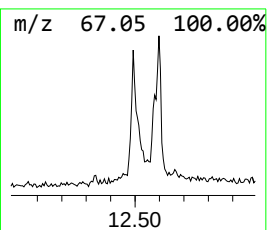
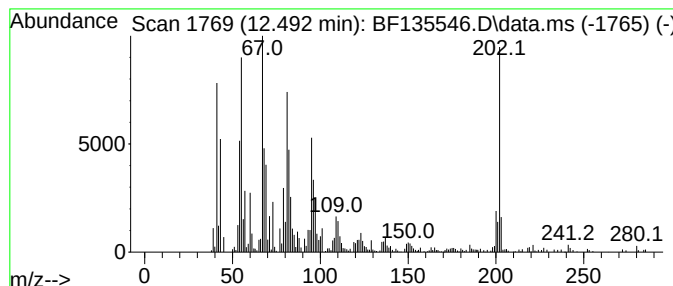
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Linoelaidic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.492	7.20 ng	371989	Phenanthrene-d10	11.263

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Linoelaidic acid	280	C18H32O2	000506-21-8	98
2			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	83
3			1,12-Tridecadiene	180	C13H24	021964-48-7	80
4			1,11-Dodecadiene	166	C12H22	005876-87-9	78
5			Cyclodecene, (Z)-	138	C10H18	000935-31-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100323\
Data File : BF135546.D
Acq On : 03 Oct 2023 17:27
Operator : CG\JU
Sample : 04666-01 10X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-201

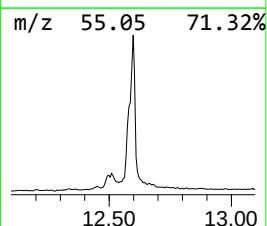
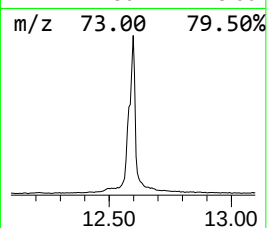
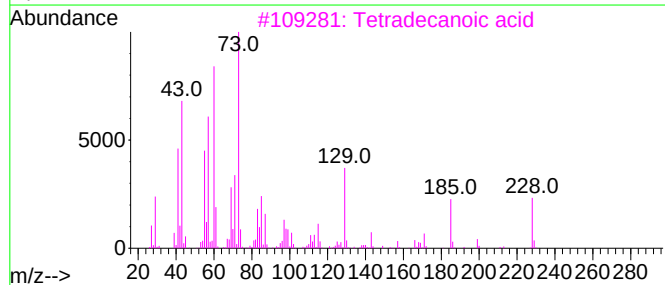
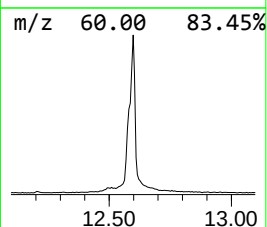
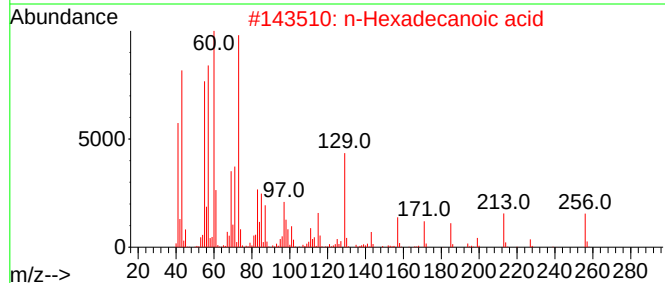
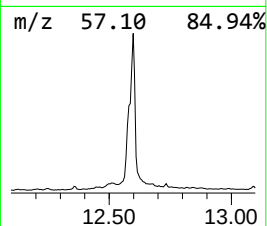
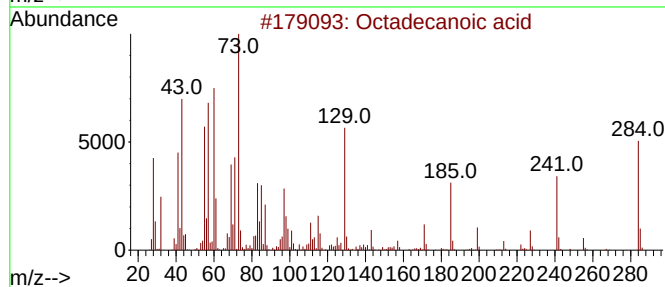
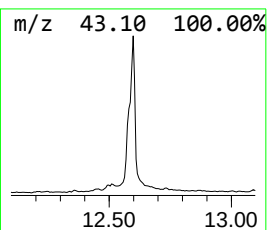
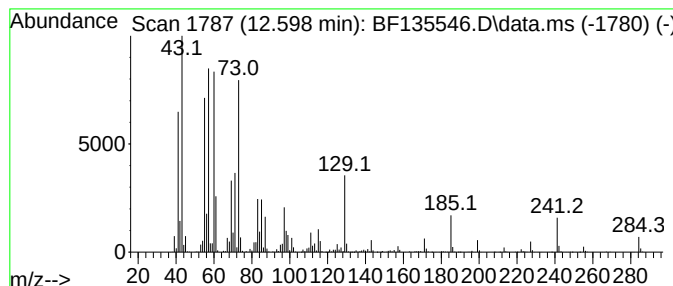
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.598	124.90 ng	4898140	Chrysene-d12	13.921

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	80
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100323\
Data File : BF135546.D
Acq On : 03 Oct 2023 17:27
Operator : CG\JU
Sample : 04666-01 10X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-201

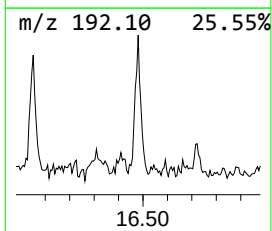
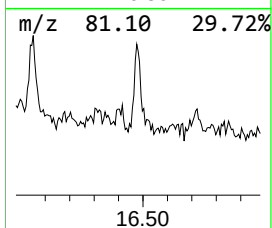
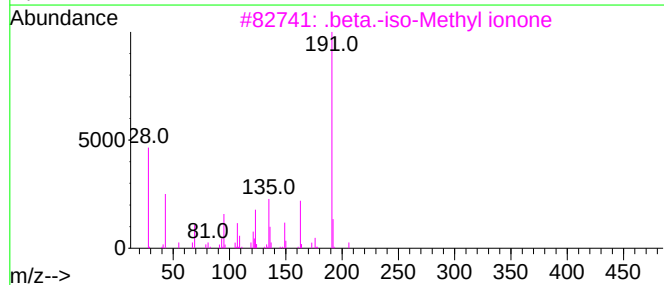
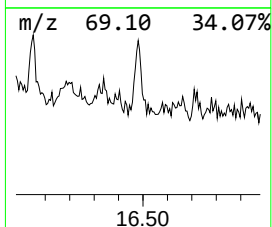
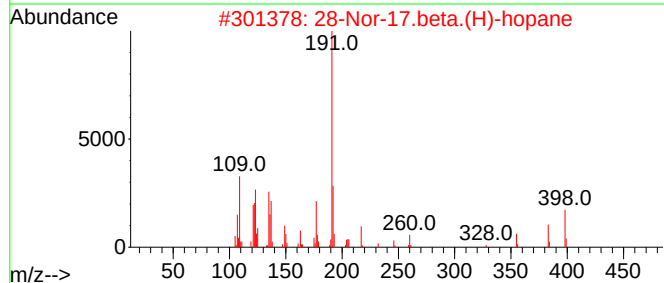
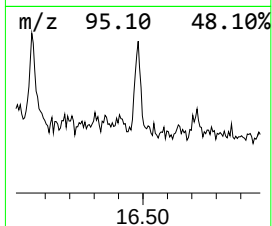
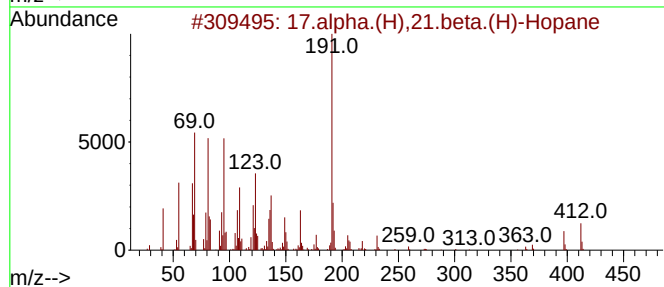
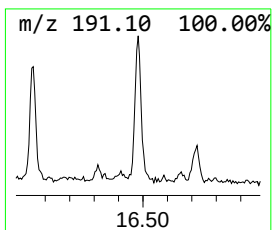
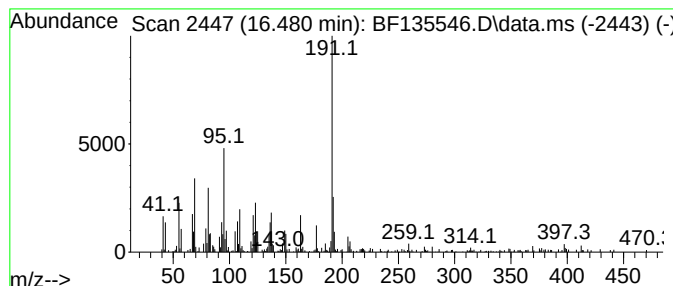
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 17.alpha.(H),21.beta.(H)-Ho... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.480	7.97 ng	273591	Perylene-d12	15.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17.alpha.(H),21.beta.(H)-Hopane	412	C30H52	013849-96-2	90
2			28-Nor-17.beta.(H)-hopane	398	C29H50	036728-72-0	59
3			.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	47
4			1-Penten-3-one, 1-(2,6,6-trimeth...	206	C14H22O	000127-43-5	43
5			2,4,7-Pteridinetriamine, 6-methyl-	191	C7H9N7	017539-50-3	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100323\
Data File : BF135546.D
Acq On : 03 Oct 2023 17:27
Operator : CG\JU
Sample : 04666-01 10X
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VNJ-201

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
Heptadecane	10.680	2.4	ng	124843	4	11.263	1033090	20.0
n-Hexadecanoic ...	11.810	67.8	ng	3502250	4	11.263	1033090	20.0
Linoelaidic acid	12.492	7.2	ng	371989	4	11.263	1033090	20.0
Octadecanoic acid	12.598	124.9	ng	4898140	5	13.921	784355	20.0
17.alpha.(H),21...	16.480	8.0	ng	273591	6	15.386	686652	20.0