

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
 Data File : BM035155.D
 Acq On : 19 May 2022 16:24
 Operator : CG/JU
 Sample : N2864-05
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P011-SS003-0612-01

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_M\Methods\8270-BM042722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM035155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	322	328	333	rBV2	45845	69017	1.36%	0.210%
2	5.481	400	407	419	rBV	1850568	2644075	52.10%	8.060%
3	7.075	670	678	688	rBV	1770303	2797430	55.12%	8.527%
4	7.904	811	819	827	rBV	553622	855415	16.86%	2.607%
5	9.063	1008	1016	1026	rBV	1109863	1811123	35.69%	5.521%
6	10.704	1288	1295	1305	rVB	685428	1152380	22.71%	3.513%
7	13.169	1707	1714	1724	rBV	2587867	3749646	73.88%	11.430%
8	14.545	1941	1948	1964	rVB	972538	1483637	29.23%	4.522%
9	14.963	2010	2019	2031	rBV2	57789	113995	2.25%	0.347%
10	16.027	2194	2200	2207	rBV	2126590	2947110	58.07%	8.983%
11	16.539	2282	2287	2300	rVB	77888	130066	2.56%	0.396%
12	17.286	2408	2414	2421	rVB	1216395	1667217	32.85%	5.082%
13	18.080	2542	2549	2555	rBV6	23227	52090	1.03%	0.159%
14	18.192	2562	2568	2578	rBV	645446	986175	19.43%	3.006%
15	19.321	2755	2760	2762	rBV2	174592	265284	5.23%	0.809%
16	19.351	2762	2765	2780	rVV2	344618	724182	14.27%	2.207%
17	19.468	2780	2785	2795	rVV	452458	643862	12.69%	1.963%
18	19.598	2803	2807	2822	rVB2	147431	339073	6.68%	1.034%
19	19.827	2842	2846	2854	rBV2	160382	251858	4.96%	0.768%
20	19.909	2855	2860	2866	rVB	4230964	5075071	100.00%	15.470%
21	20.409	2941	2945	2956	rBV	227685	395387	7.79%	1.205%
22	21.186	3073	3077	3087	rBV	678625	817548	16.11%	2.492%
23	21.468	3121	3125	3132	rVB	1470756	1811057	35.69%	5.520%
24	23.856	3525	3531	3541	rVB2	1011914	2023578	39.87%	6.168%

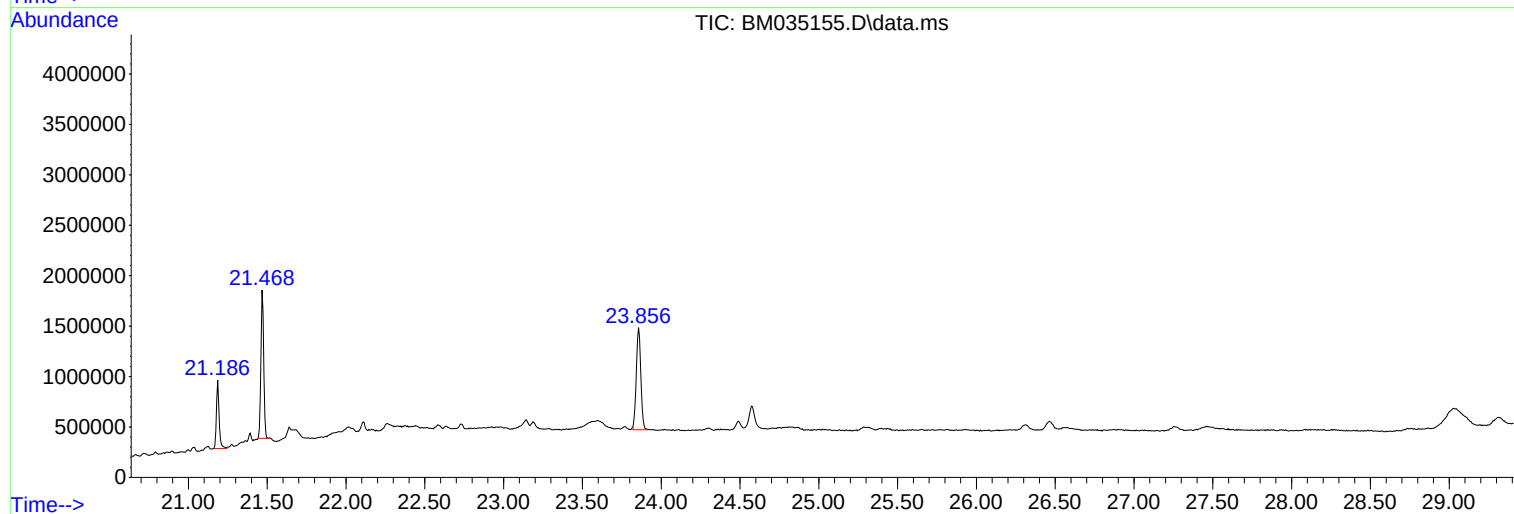
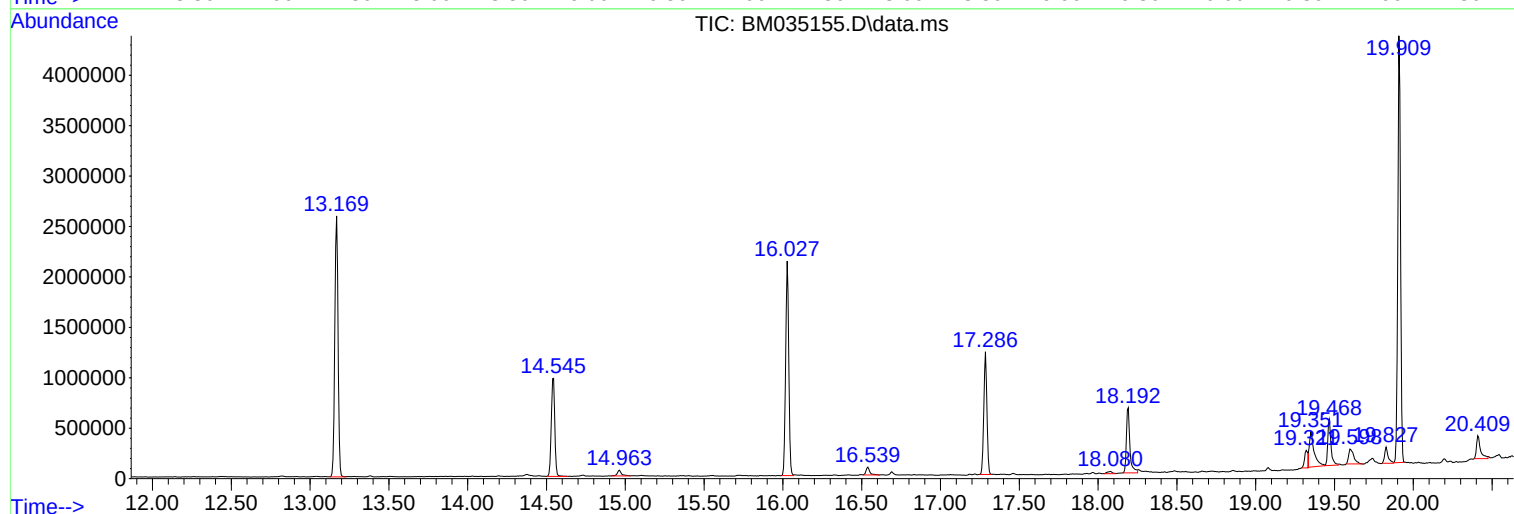
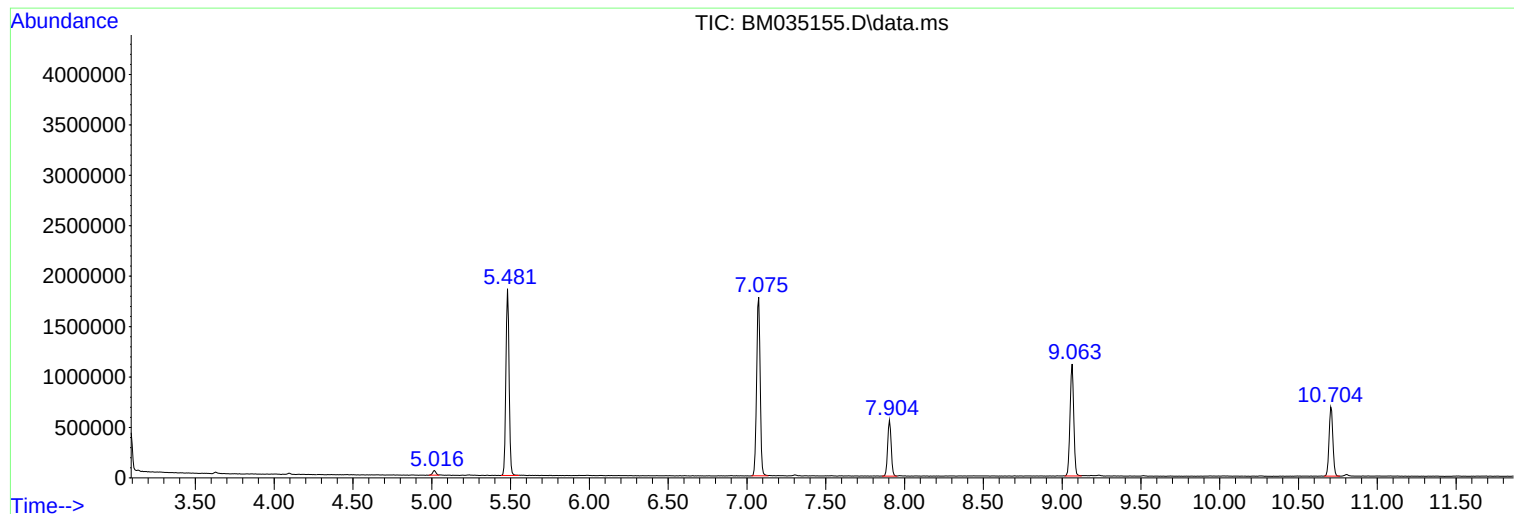
Sum of corrected areas: 32806276

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035155.D
Acq On : 19 May 2022 16:24
Operator : CG/JU
Sample : N2864-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P011-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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_M\Data\BM051922\
Data File : BM035155.D
Acq On : 19 May 2022 16:24
Operator : CG/JU
Sample : N2864-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P011-SS003-0612-01

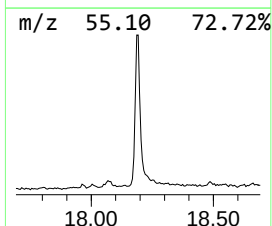
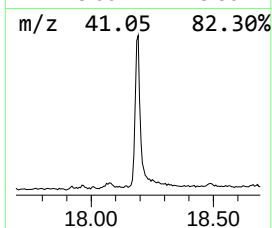
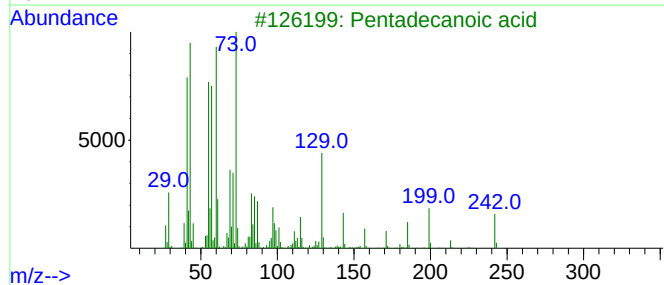
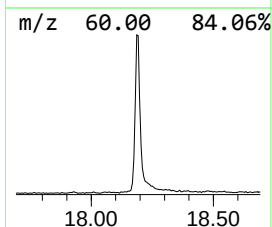
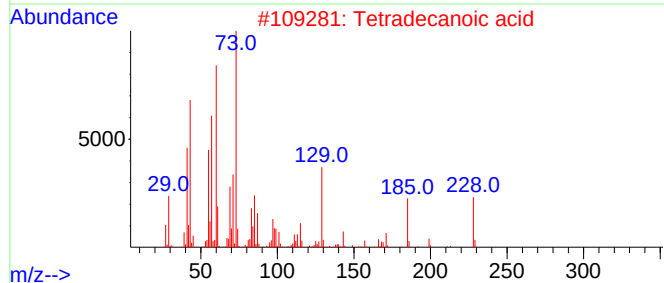
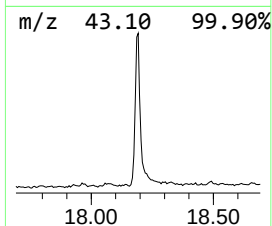
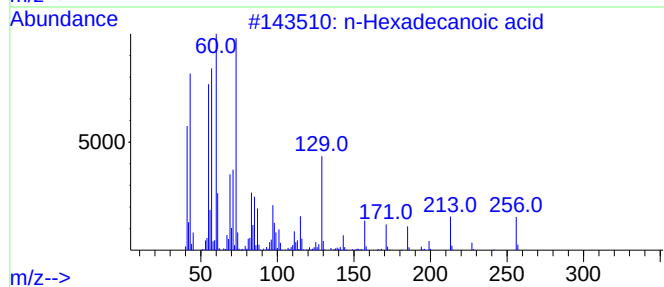
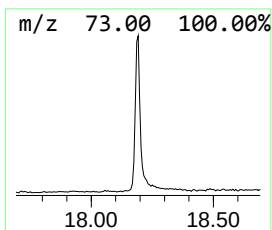
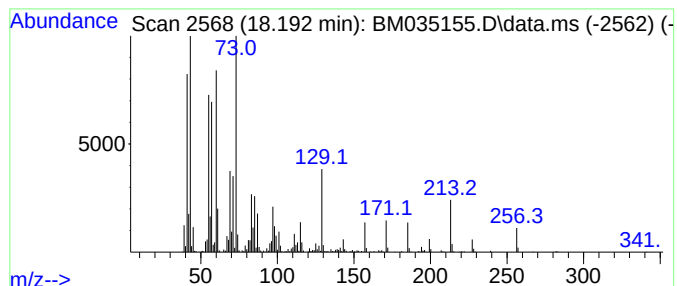
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	11.83 ng	986175	Phenanthrene-d10	17.286

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			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035155.D
Acq On : 19 May 2022 16:24
Operator : CG/JU
Sample : N2864-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P011-SS003-0612-01

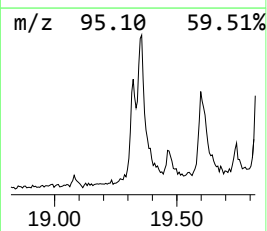
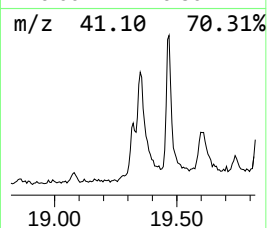
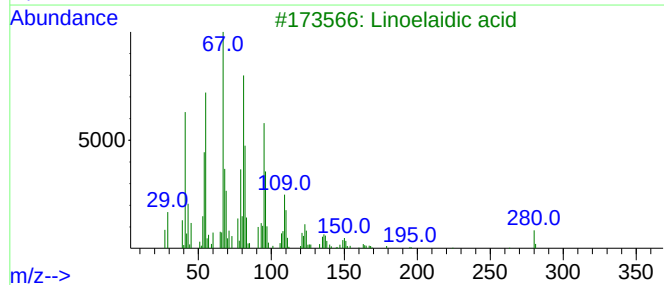
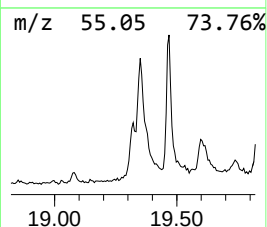
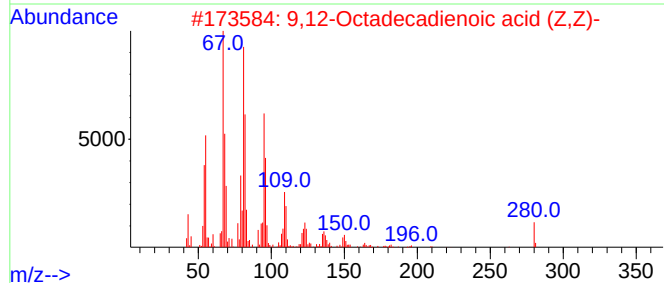
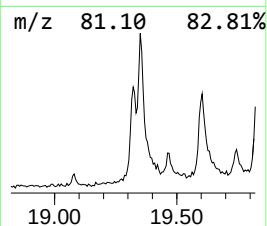
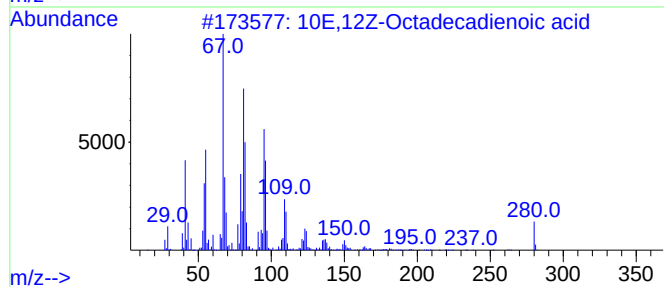
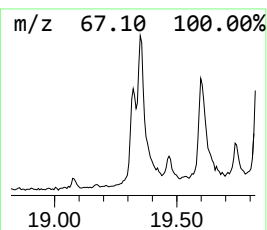
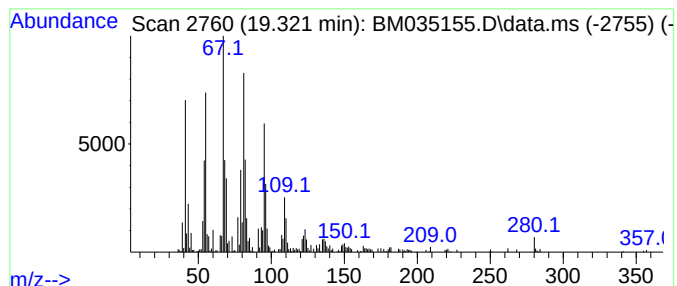
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 10E,12Z-Octadecadienoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.321	3.18 ng	265284	Phenanthrene-d10	17.286

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	10E,12Z-Octadecadienoic acid			280	C18H32O2	002420-56-6	99
2	9,12-Octadecadienoic acid (Z,Z)-			280	C18H32O2	000060-33-3	98
3	Linoelaidic acid			280	C18H32O2	000506-21-8	96
4	7-Hexadecyne			222	C16H30	074685-28-2	93
5	6-Tetradecyne			194	C14H26	003730-08-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035155.D
Acq On : 19 May 2022 16:24
Operator : CG/JU
Sample : N2864-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

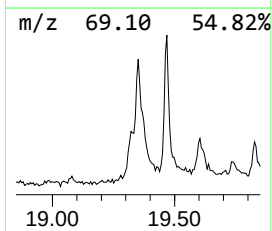
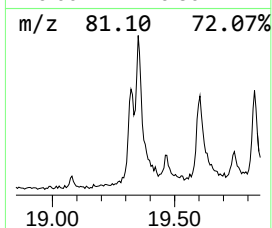
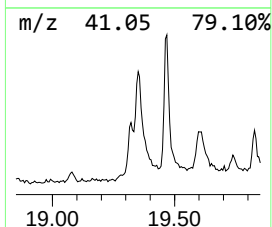
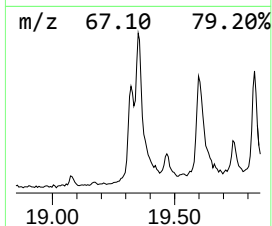
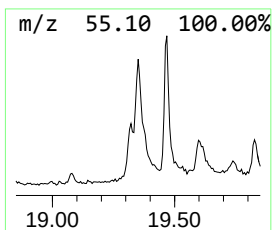
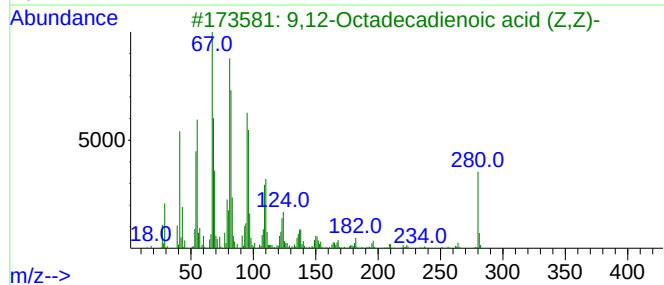
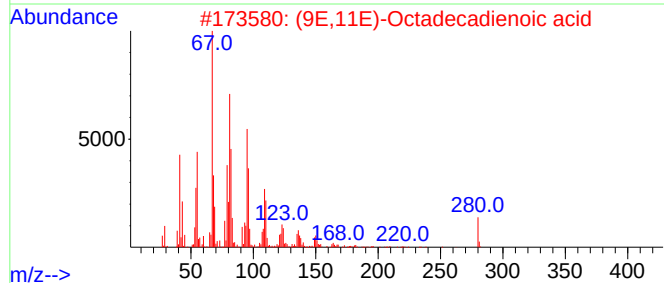
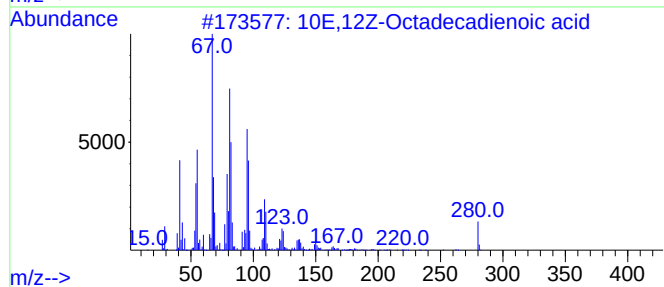
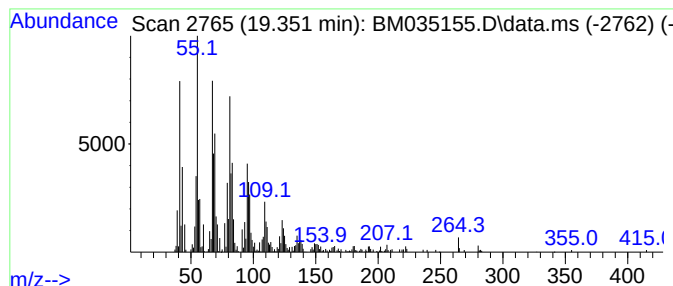
Instrument :
BNA_M
ClientSampleId :
P011-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 (9E,11E)-Octadecadienoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
19.351	8.69 ng	724182	Phenanthrene-d10			17.286
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	10E,12Z-Octadecadienoic acid		280	C18H32O2	002420-56-6	97
2	(9E,11E)-Octadecadienoic acid		280	C18H32O2	000544-71-8	97
3	9,12-Octadecadienoic acid (Z,Z)-		280	C18H32O2	000060-33-3	95
4	9,17-Octadecadienal, (Z)-		264	C18H32O	056554-35-9	94
5	12-Methyl-E,E-2,13-octadecadien-...		280	C19H36O	1010130-90-4	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035155.D
Acq On : 19 May 2022 16:24
Operator : CG/JU
Sample : N2864-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P011-SS003-0612-01

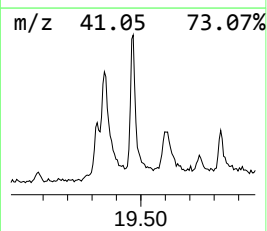
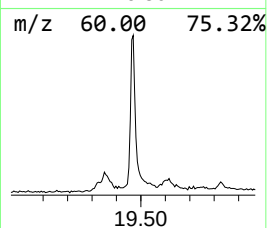
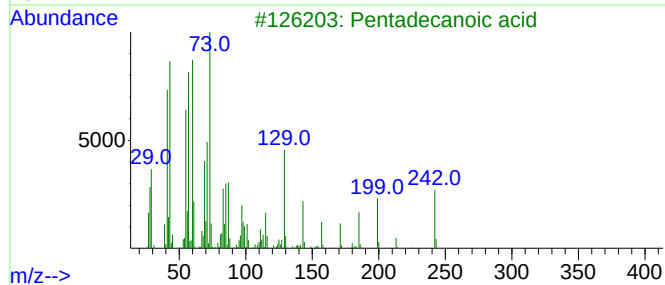
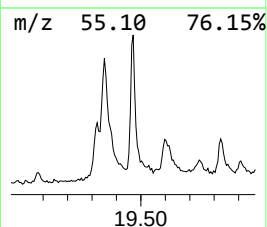
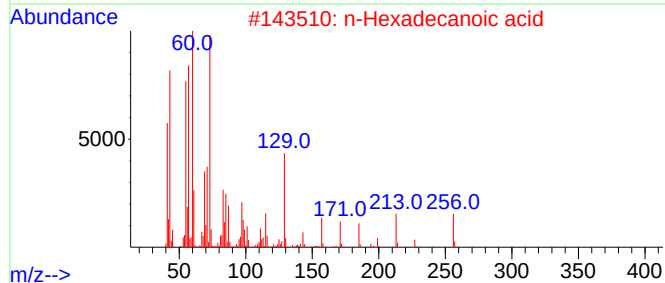
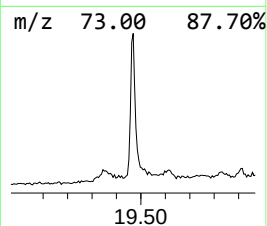
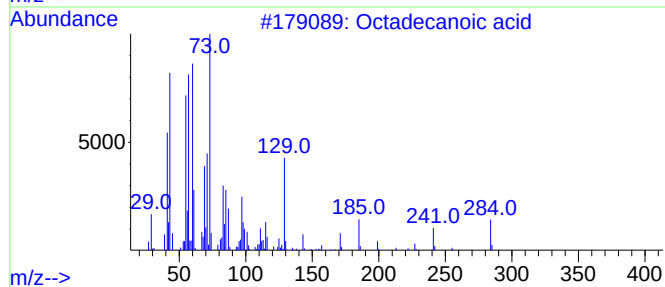
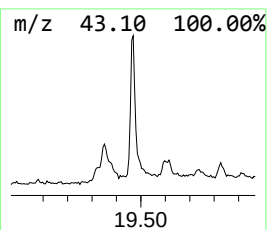
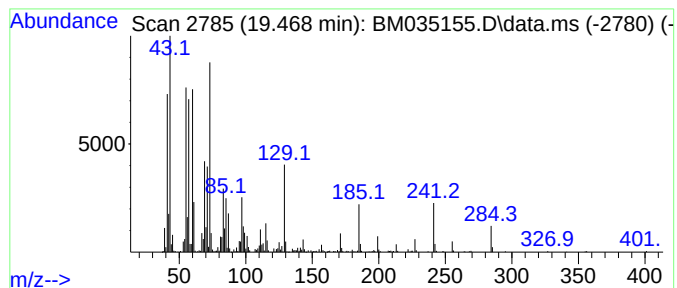
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.468	7.11 ng	643862	Chrysene-d12	21.468

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	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	70



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035155.D
Acq On : 19 May 2022 16:24
Operator : CG/JU
Sample : N2864-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P011-SS003-0612-01

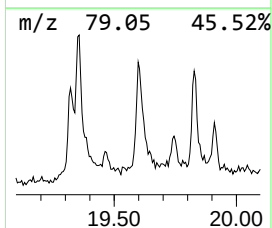
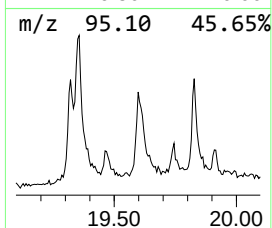
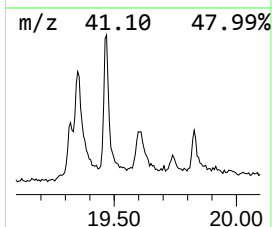
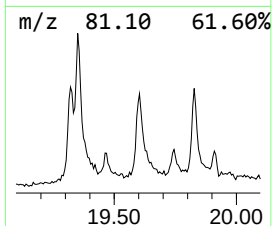
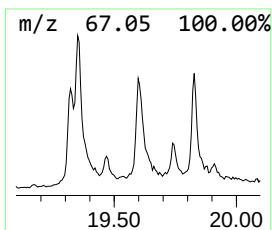
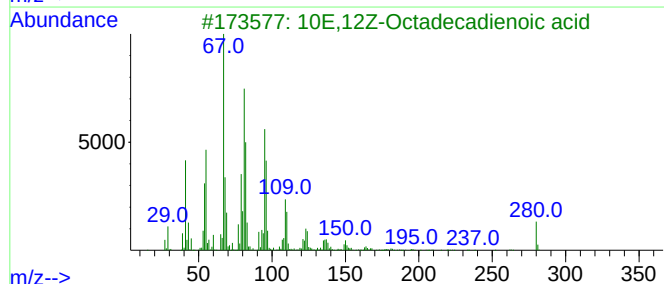
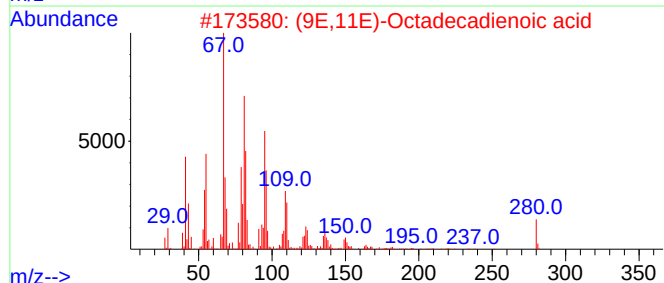
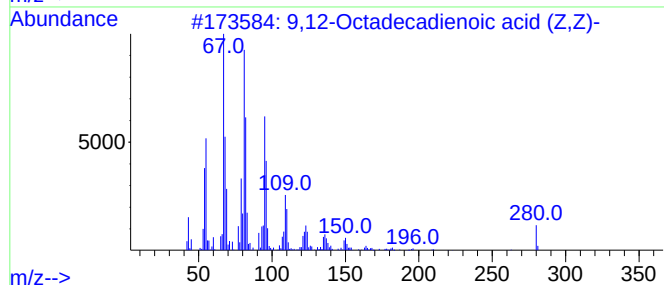
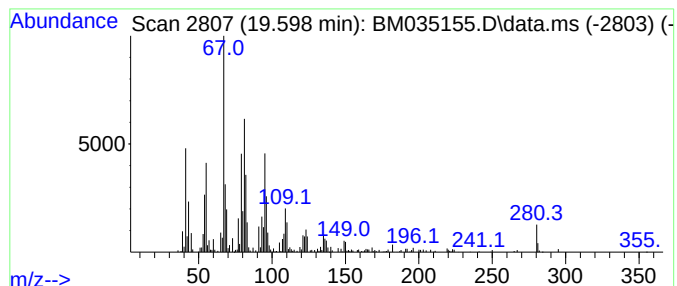
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.598	3.74 ng	339073	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2			(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	97
3			10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	97
4			Methyl 9,12-heptadecadienoate	280	C18H32O2	1000336-36-2	97
5			Linoelaidic acid	280	C18H32O2	000506-21-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035155.D
Acq On : 19 May 2022 16:24
Operator : CG/JU
Sample : N2864-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P011-SS003-0612-01

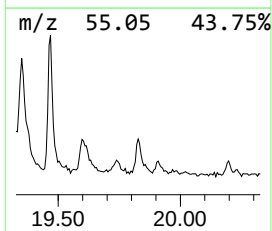
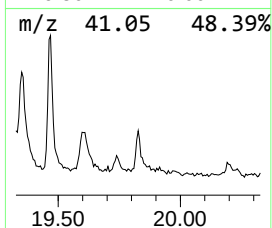
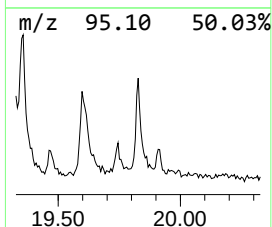
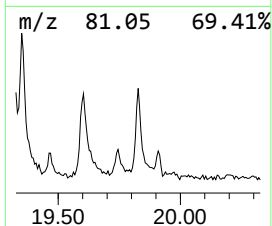
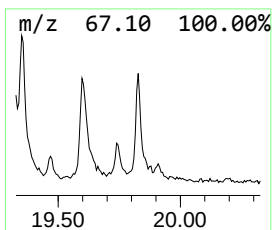
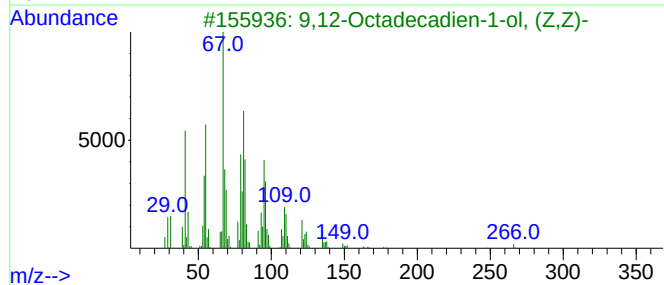
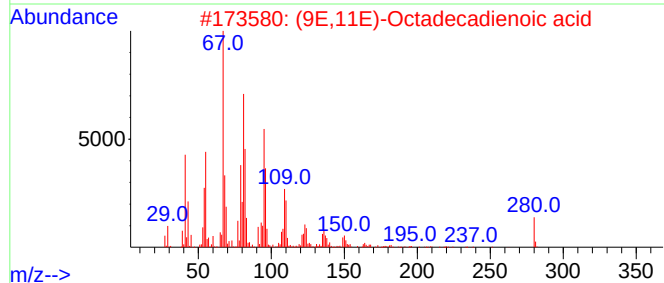
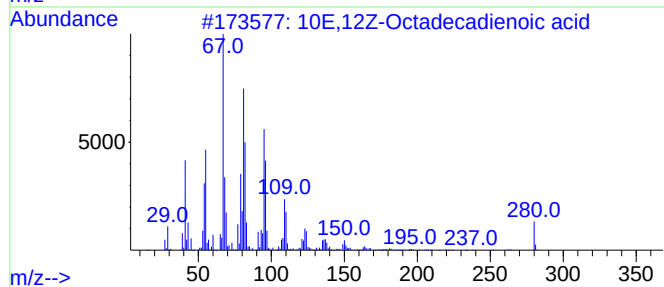
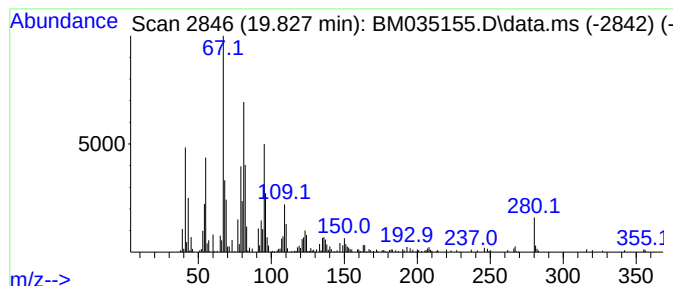
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,E-11,Z-13-Octadecatriene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.827	2.78 ng	251858	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	10E,12Z-Octadecadienoic acid			280	C18H32O2	002420-56-6	98
2	(9E,11E)-Octadecadienoic acid			280	C18H32O2	000544-71-8	98
3	9,12-Octadecadien-1-ol, (Z,Z)-			266	C18H34O	000506-43-4	95
4	9,12-Octadecadienoic acid (Z,Z)-			280	C18H32O2	000060-33-3	91
5	1,E-11,Z-13-Octadecatriene			248	C18H32	080625-36-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035155.D
Acq On : 19 May 2022 16:24
Operator : CG/JU
Sample : N2864-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

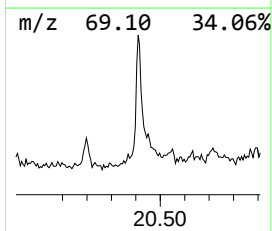
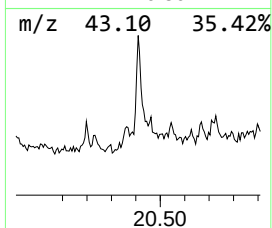
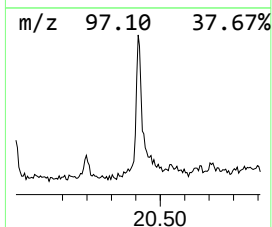
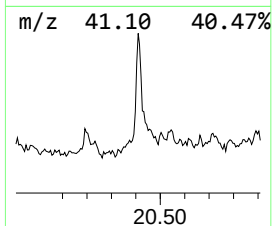
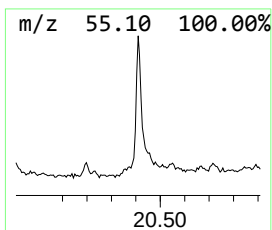
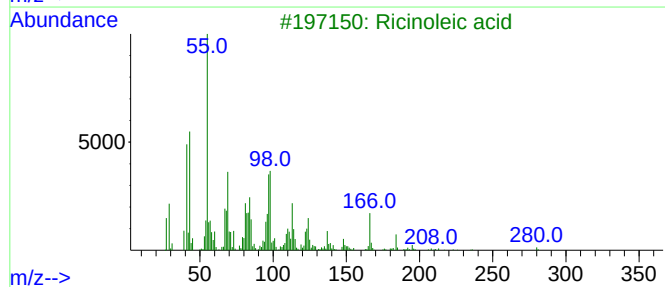
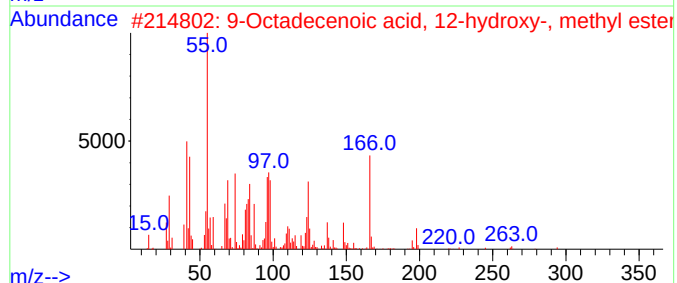
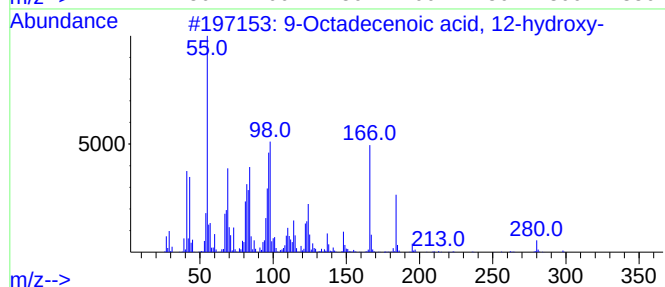
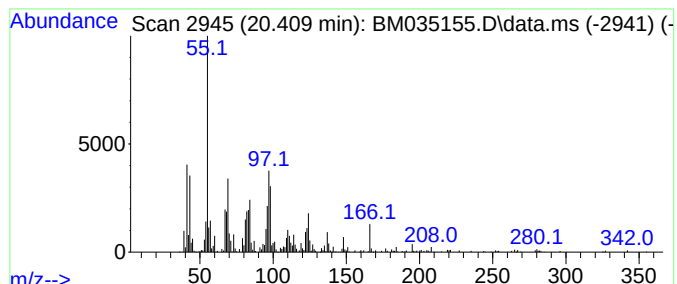
Instrument :
BNA_M
ClientSampleId :
P011-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenoic acid, 12-hyd... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.409	4.37 ng	395387	Chrysene-d12	21.468	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, 12-hydroxy-	298	C18H34O3	007431-95-0	87
2	9-Octadecenoic acid, 12-hydroxy-...	312	C19H36O3	000141-24-2	86
3	Ricinoleic acid	298	C18H34O3	000141-22-0	83
4	Chloromethyl 5-chloroundecanoate	268	C12H22Cl2O2	080418-91-3	52
5	Oxacycloheptadecan-2-one	254	C16H30O2	000109-29-5	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035155.D
Acq On : 19 May 2022 16:24
Operator : CG/JU
Sample : N2864-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P011-SS003-0612-01

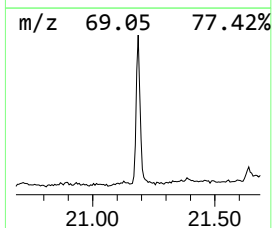
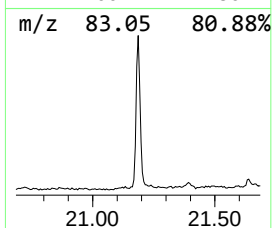
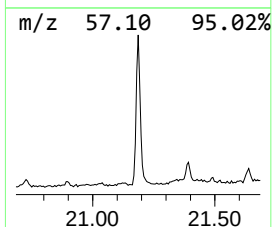
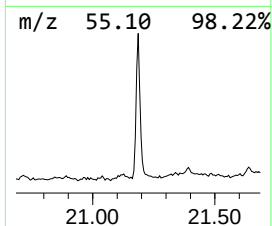
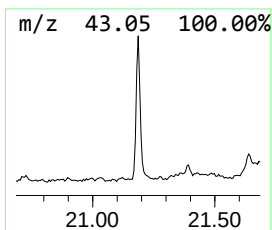
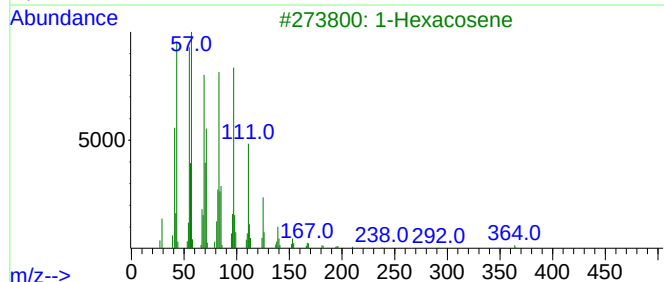
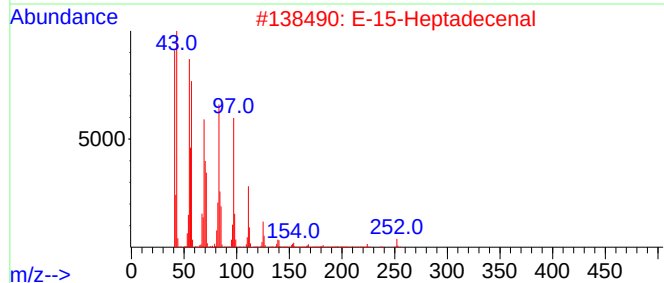
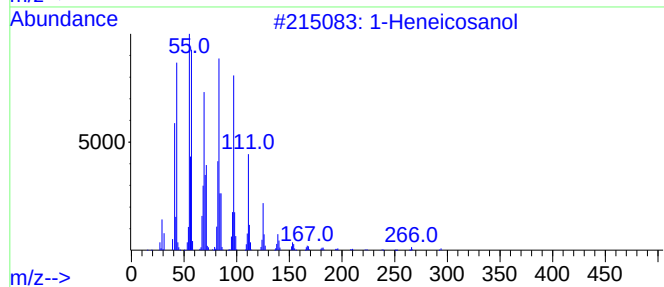
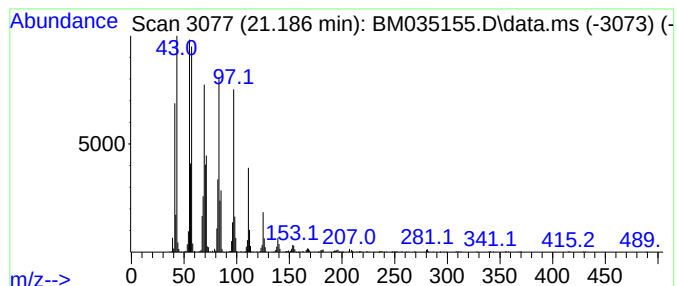
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1-Heneicosanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.186	9.03 ng	817548	Chrysene-d12	21.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	95
2			E-15-Heptadecenal	252	C17H32O	1000130-97-9	95
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			1-Tetracosene	336	C24H48	010192-32-2	94
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM051922\
Data File : BM035155.D
Acq On : 19 May 2022 16:24
Operator : CG/JU
Sample : N2864-05
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P011-SS003-0612-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.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
n-Hexadecanoic ...	18.192	11.8	ng	986175	4	17.286	1667220	20.0
10E,12Z-Octadec...	19.321	3.2	ng	265284	4	17.286	1667220	20.0
(9E,11E)-Octade...	19.351	8.7	ng	724182	4	17.286	1667220	20.0
Octadecanoic acid	19.468	7.1	ng	643862	5	21.468	1811060	20.0
9,12-Octadecadi...	19.598	3.7	ng	339073	5	21.468	1811060	20.0
1,E-11,Z-13-Oct...	19.827	2.8	ng	251858	5	21.468	1811060	20.0
9-Octadecenoic ...	20.409	4.4	ng	395387	5	21.468	1811060	20.0
1-Heneicosanol	21.186	9.0	ng	817548	5	21.468	1811060	20.0