

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
 Data File : BM042416.D
 Acq On : 24 Oct 2023 13:01
 Operator : MA/JU
 Sample : 04920-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 LSS-B3-COMP-101623

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-BM102123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042416.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	317	321	327	rVB	159425	212040	4.17%	0.599%
2	5.522	391	397	410	rBV	1834026	2594045	50.99%	7.333%
3	7.145	666	673	683	rBV	1784001	2732008	53.70%	7.723%
4	7.586	743	748	757	rBV2	32690	53732	1.06%	0.152%
5	7.992	811	817	828	rBV	470923	756835	14.88%	2.139%
6	9.192	1011	1021	1031	rBV	1051034	1696601	33.35%	4.796%
7	10.816	1289	1297	1305	rBV	608423	994872	19.56%	2.812%
8	13.263	1706	1713	1724	rBV	2173860	3178098	62.47%	8.984%
9	14.639	1941	1947	1960	rVB	832667	1217796	23.94%	3.442%
10	15.010	2003	2010	2018	rBV	90355	158526	3.12%	0.448%
11	16.133	2192	2201	2213	rBV	1823733	2666172	52.41%	7.537%
12	17.392	2408	2415	2422	rBV	1082157	1500659	29.50%	4.242%
13	18.245	2551	2560	2580	rBV	3049968	5087355	100.00%	14.381%
14	19.374	2748	2752	2753	rBV2	85781	95737	1.88%	0.271%
15	19.397	2753	2756	2767	rVV2	132789	289987	5.70%	0.820%
16	19.515	2771	2776	2797	rVV	2454227	3696738	72.67%	10.450%
17	20.003	2854	2859	2867	rVB	3828772	4433316	87.14%	12.532%
18	21.233	3064	3068	3076	rBV	301331	425013	8.35%	1.201%
19	21.574	3121	3126	3131	rVB	1302341	1732413	34.05%	4.897%
20	24.038	3538	3545	3556	rVB	900671	1854042	36.44%	5.241%

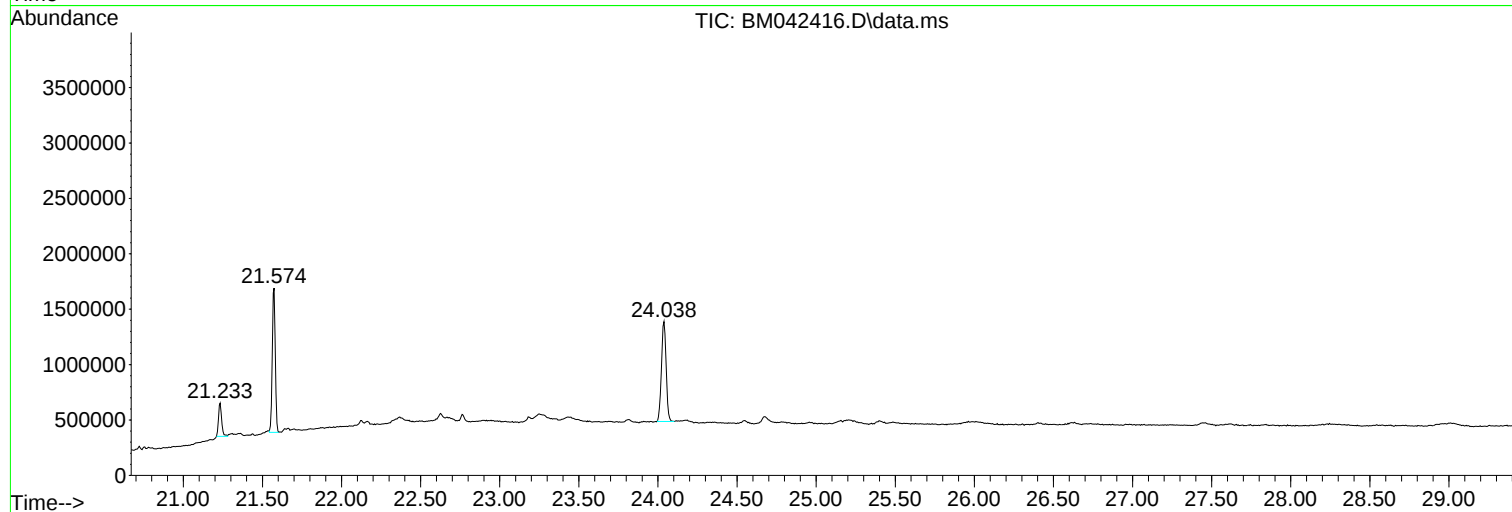
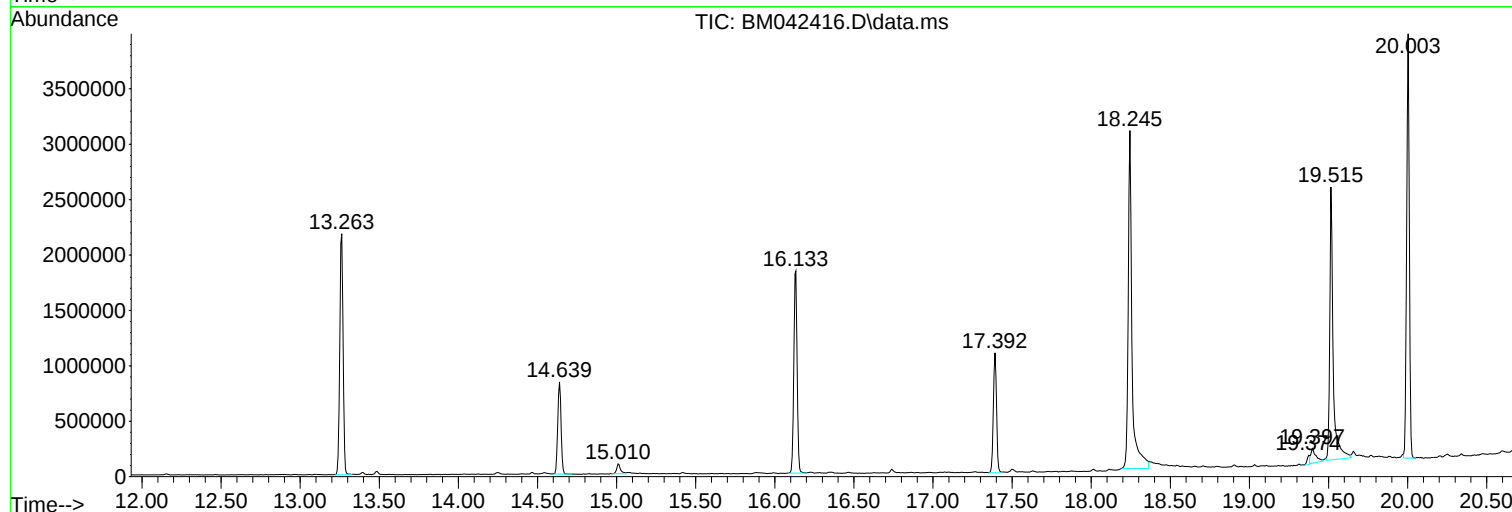
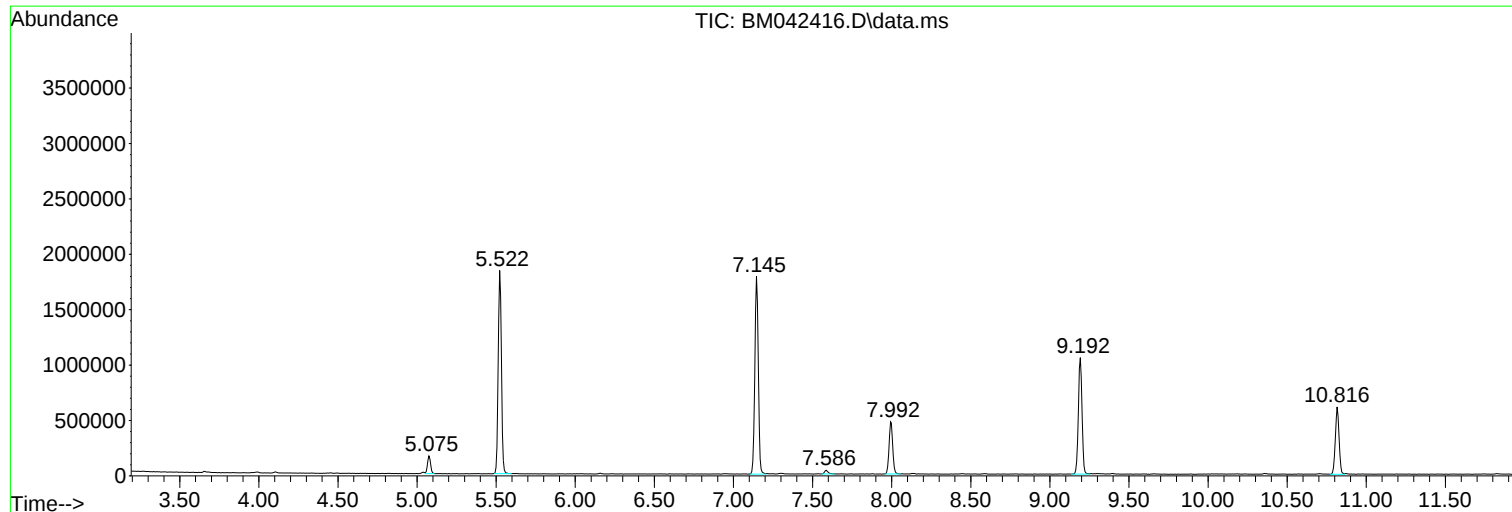
Sum of corrected areas: 35375985

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042416.D
Acq On : 24 Oct 2023 13:01
Operator : MA/JU
Sample : 04920-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B3-COMP-101623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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\BM102423\
Data File : BM042416.D
Acq On : 24 Oct 2023 13:01
Operator : MA/JU
Sample : 04920-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B3-COMP-101623

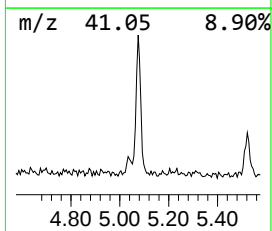
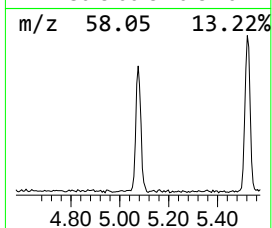
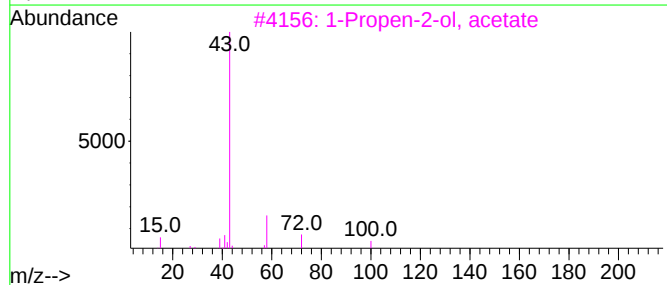
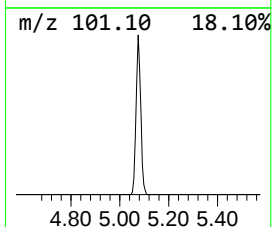
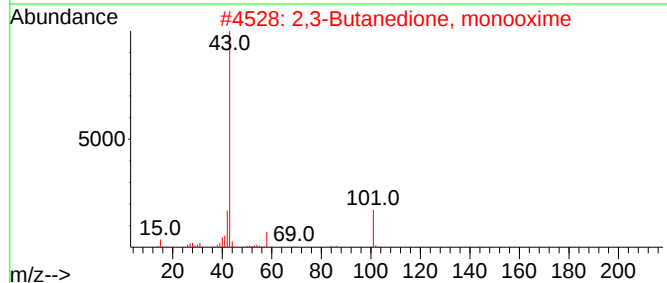
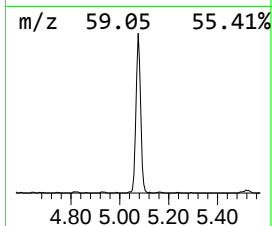
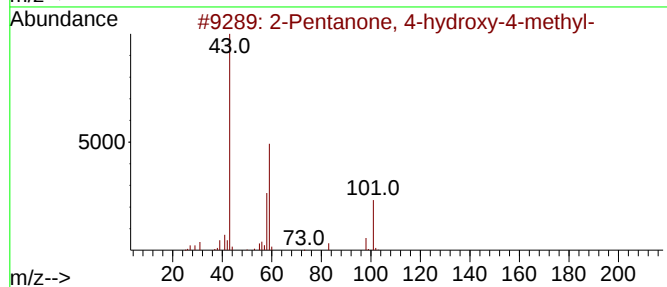
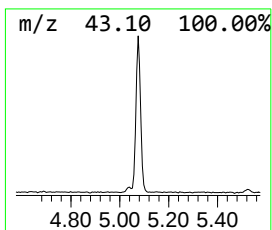
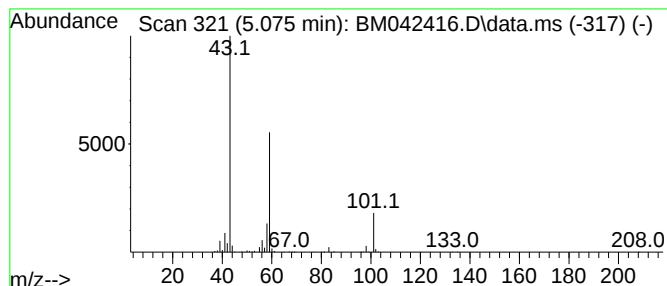
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	5.60 ng	212040	1,4-Dichlorobenzene-d4	7.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042416.D
Acq On : 24 Oct 2023 13:01
Operator : MA/JU
Sample : 04920-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B3-COMP-101623

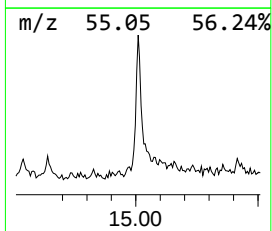
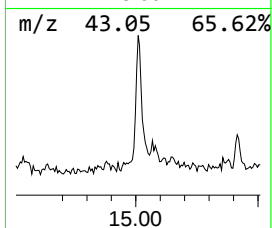
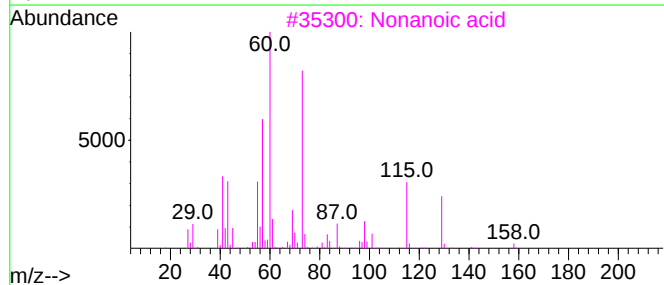
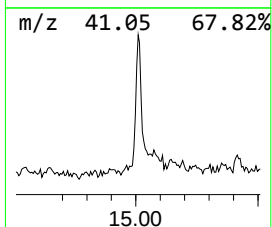
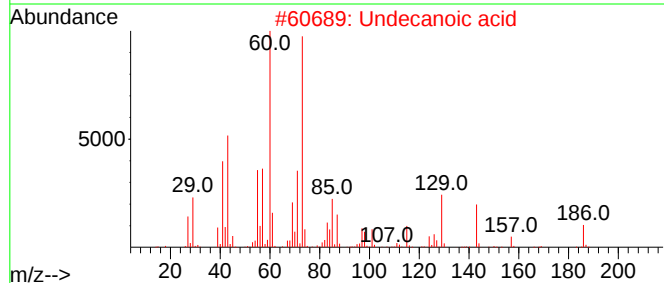
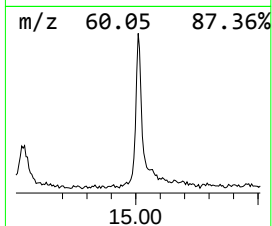
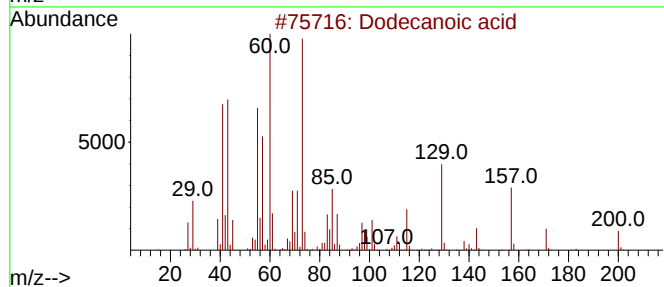
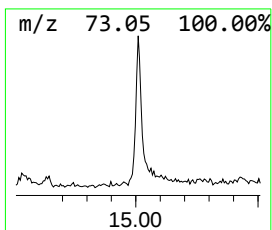
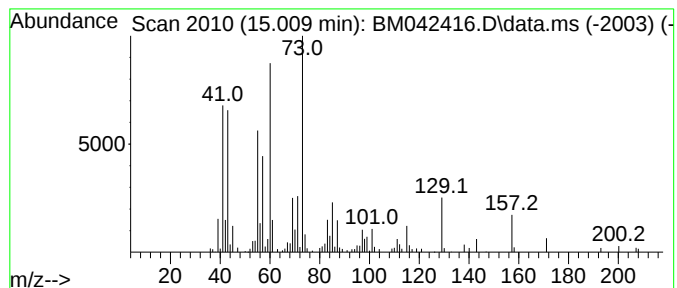
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Dodecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.009	2.60 ng	158526	Acenaphthene-d10	14.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	97
2			Undecanoic acid	186	C11H22O2	000112-37-8	90
3			Nonanoic acid	158	C9H18O2	000112-05-0	64
4			Butanoic acid	88	C4H8O2	000107-92-6	35
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042416.D
Acq On : 24 Oct 2023 13:01
Operator : MA/JU
Sample : 04920-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

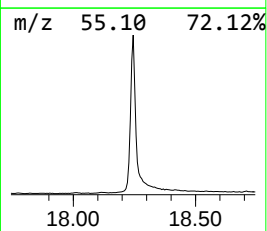
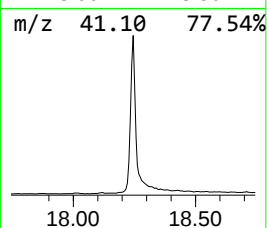
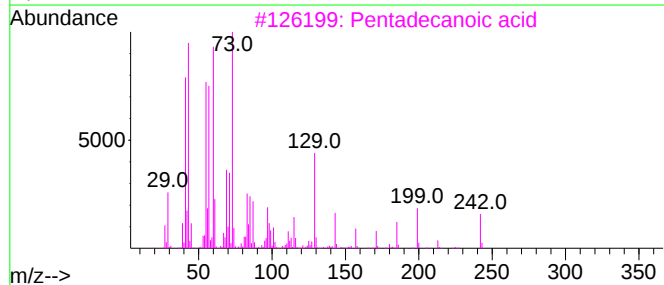
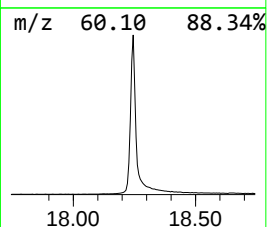
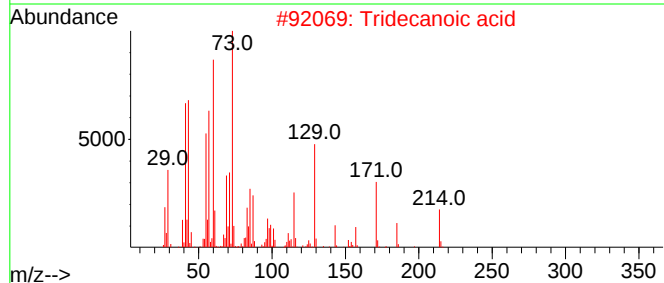
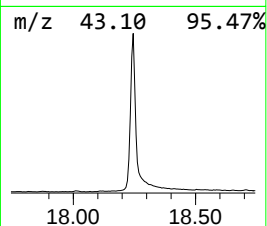
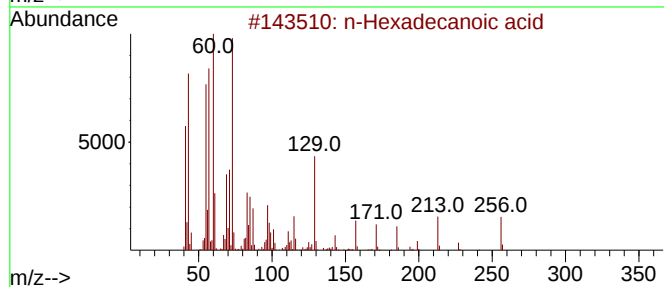
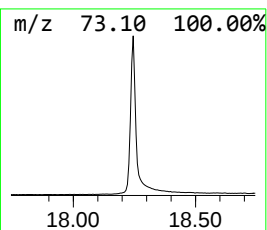
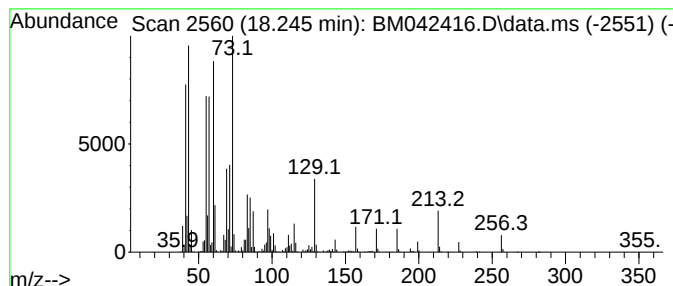
Instrument :
BNA_M
ClientSampleId :
LSS-B3-COMP-101623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.245	67.80 ng	5087360	Phenanthrene-d10		17.392	
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	87
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	74
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042416.D
Acq On : 24 Oct 2023 13:01
Operator : MA/JU
Sample : 04920-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B3-COMP-101623

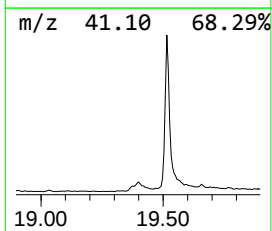
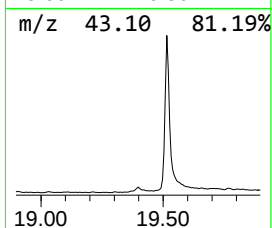
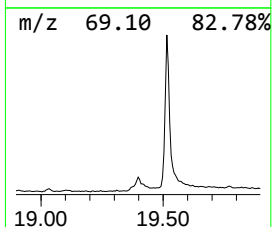
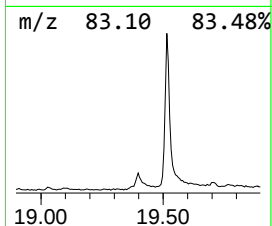
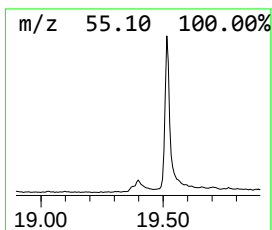
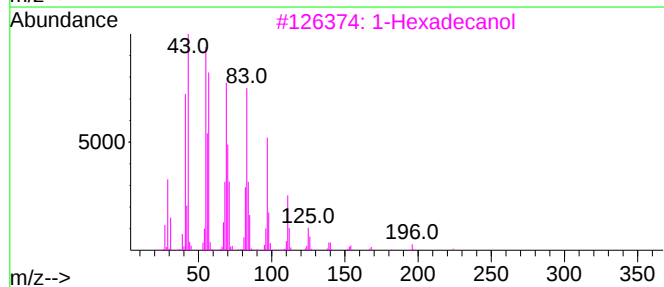
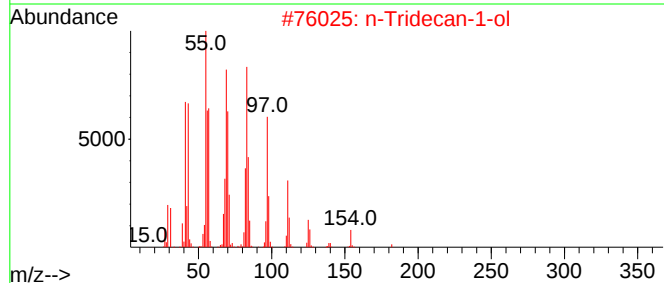
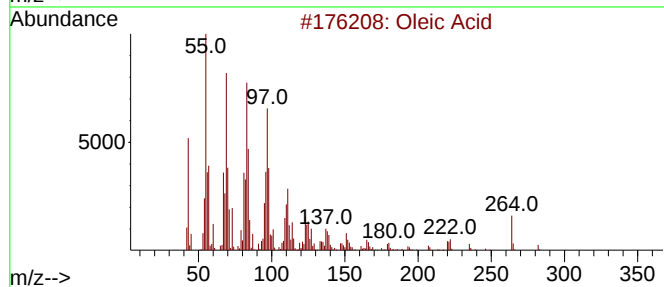
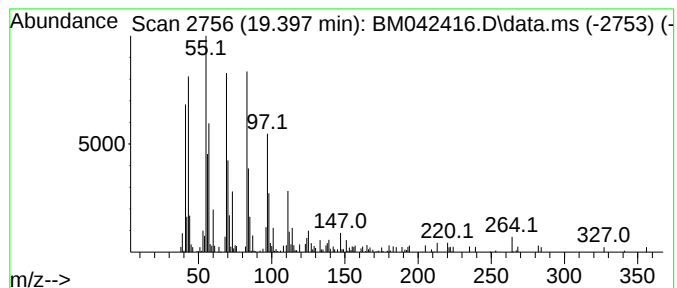
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Oleic Acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.397	3.86 ng	289987	Phenanthrene-d10	17.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oleic Acid	282	C18H34O2	000112-80-1	87
2			n-Tridecan-1-ol	200	C13H28O	000112-70-9	81
3			1-Hexadecanol	242	C16H34O	036653-82-4	68
4			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	64
5			1-Octadecanol	270	C18H38O	000112-92-5	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042416.D
Acq On : 24 Oct 2023 13:01
Operator : MA/JU
Sample : 04920-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B3-COMP-101623

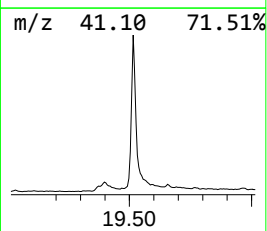
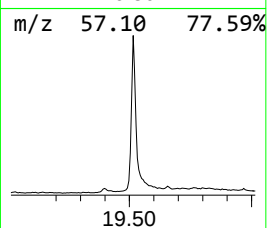
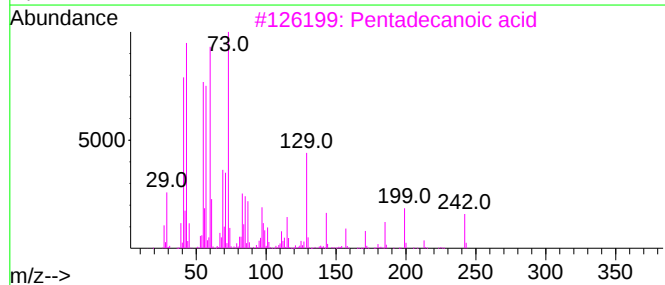
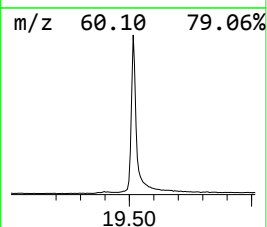
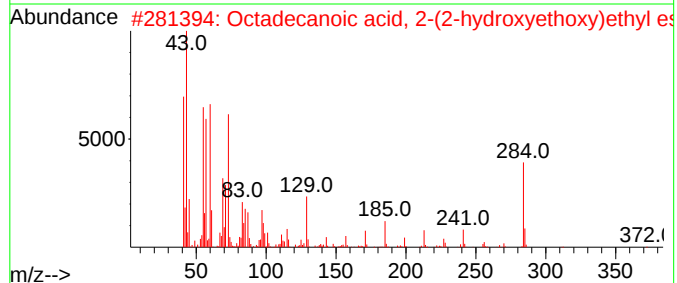
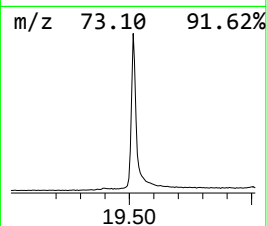
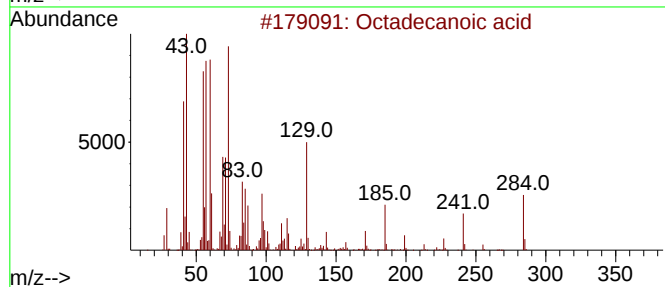
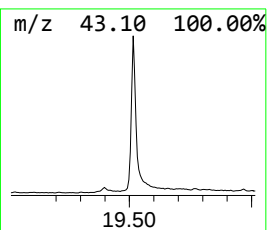
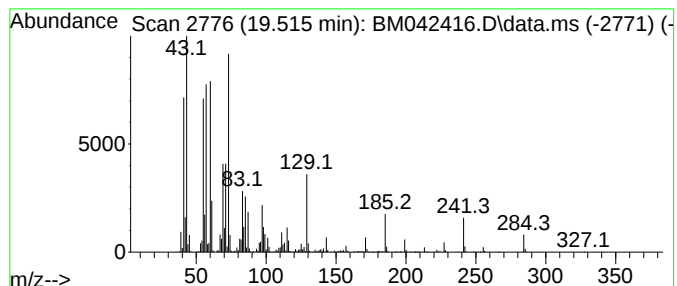
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	42.68 ng	3696740	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	78
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042416.D
Acq On : 24 Oct 2023 13:01
Operator : MA/JU
Sample : 04920-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B3-COMP-101623

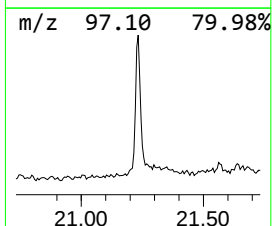
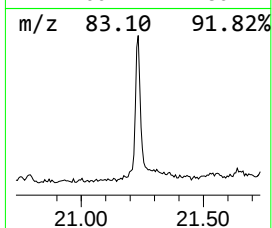
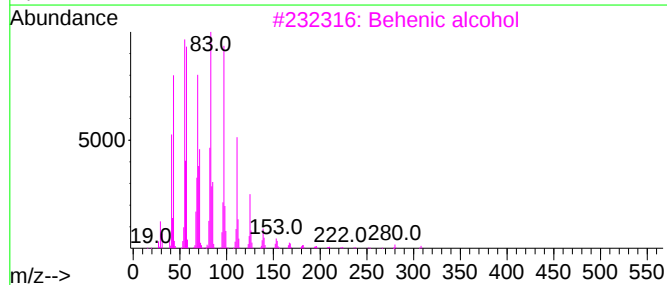
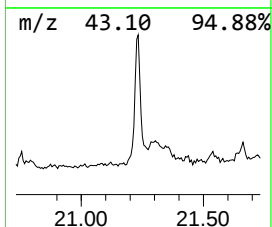
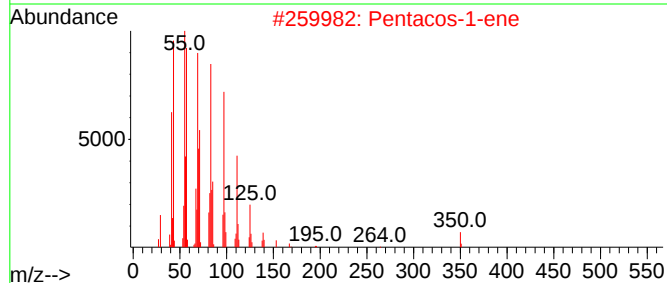
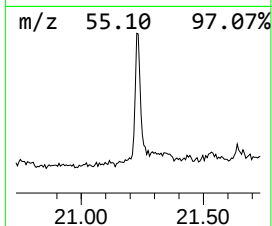
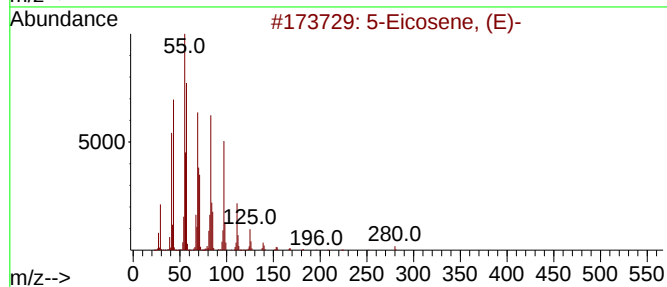
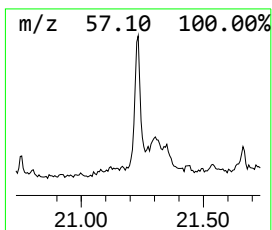
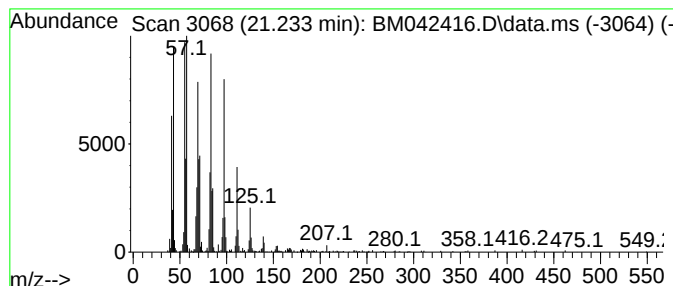
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	4.91 ng	425013	Chrysene-d12	21.574

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		Pentacos-1-ene	350	C25H50	016980-85-1	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		1-Tetracosene	336	C24H48	010192-32-2	94
5		Heptacos-1-ene	378	C27H54	015306-27-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102423\
Data File : BM042416.D
Acq On : 24 Oct 2023 13:01
Operator : MA/JU
Sample : 04920-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
LSS-B3-COMP-101623

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.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-...	5.075	5.6	ng	212040	1	7.998	756835	20.0
Dodecanoic acid	15.009	2.6	ng	158526	3	14.639	1217800	20.0
n-Hexadecanoic ...	18.245	67.8	ng	5087360	4	17.392	1500660	20.0
Oleic Acid	19.397	3.9	ng	289987	4	17.392	1500660	20.0
Octadecanoic acid	19.515	42.7	ng	3696740	5	21.574	1732410	20.0
5-Eicosene, (E)-	21.233	4.9	ng	425013	5	21.574	1732410	20.0