

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052322\
 Data File : BM035197.D
 Acq On : 23 May 2022 16:57
 Operator : CG/JU
 Sample : N2894-18
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 P008-SS002-2430-01

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: BM035197.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.481	400	407	419	rBV	1923165	2731623	4.71%	1.872%
2	7.075	669	678	688	rBV	1770946	2793922	4.81%	1.915%
3	7.898	812	818	828	rVB	487493	791594	1.36%	0.543%
4	9.063	1008	1016	1024	rBV	1094785	1842007	3.17%	1.263%
5	10.704	1287	1295	1303	rBV	617853	1045151	1.80%	0.716%
6	13.163	1707	1713	1720	rBV	2767396	4139137	7.13%	2.837%
7	14.539	1941	1947	1953	rBV	947825	1398008	2.41%	0.958%
8	16.027	2194	2200	2206	rBV	2330901	3269913	5.63%	2.241%
9	17.280	2408	2413	2425	rVB	1091146	1686904	2.91%	1.156%
10	18.227	2552	2574	2598	rVB	15886893	47110271	81.18%	32.290%
11	19.268	2747	2751	2755	rBV	758616	1072714	1.85%	0.735%
12	19.327	2756	2761	2763	rVV	1649681	2439403	4.20%	1.672%
13	19.351	2763	2765	2771	rVV	1365264	2421886	4.17%	1.660%
14	19.504	2772	2791	2808	rVB	23210284	58031634	100.00%	39.776%
15	19.909	2855	2860	2865	rBV	4927697	5798697	9.99%	3.975%
16	19.968	2865	2870	2878	rVB	427257	757909	1.31%	0.519%
17	20.774	3002	3007	3018	rVB	490423	917219	1.58%	0.629%
18	20.945	3031	3036	3047	rVB	359290	608219	1.05%	0.417%
19	21.468	3120	3125	3139	rBV	2085783	3030708	5.22%	2.077%
20	22.162	3238	3243	3250	rBV	742691	1175265	2.03%	0.806%
21	23.844	3522	3529	3539	rVB3	1243648	2834409	4.88%	1.943%

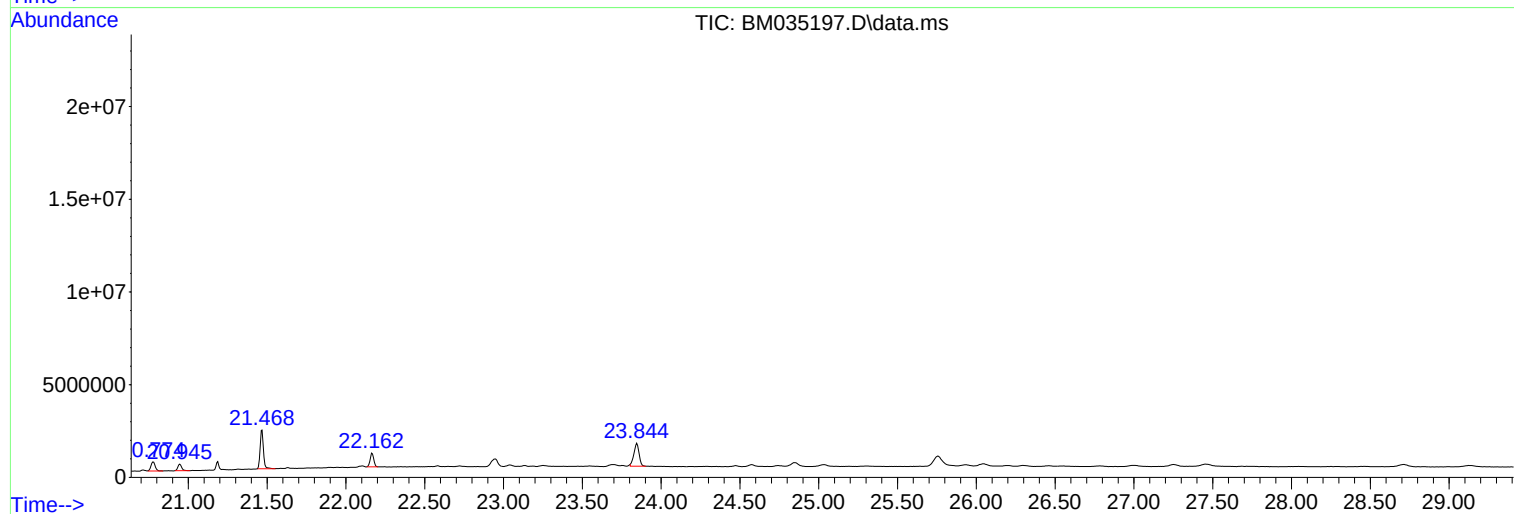
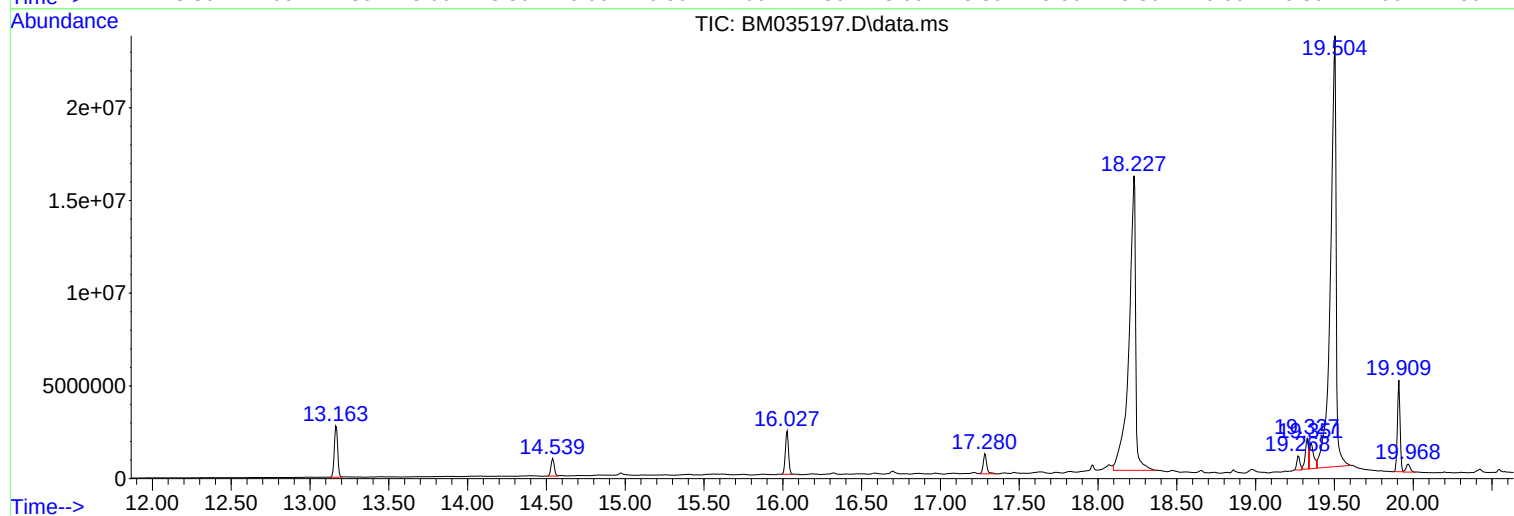
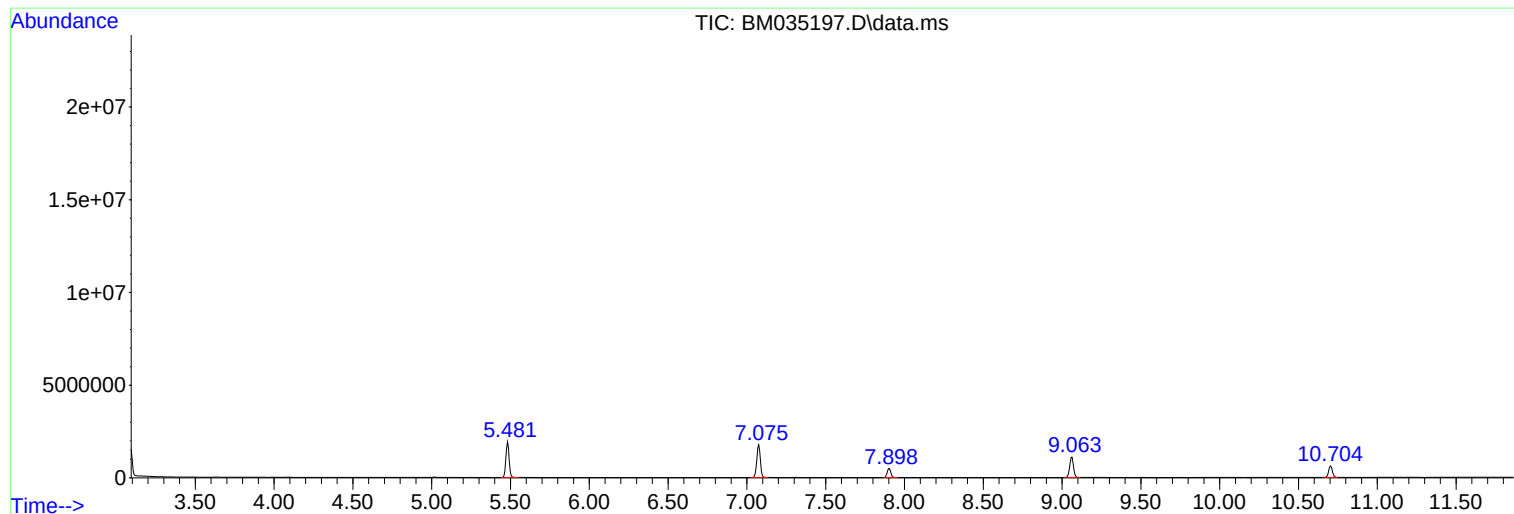
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM042722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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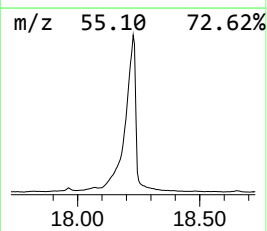
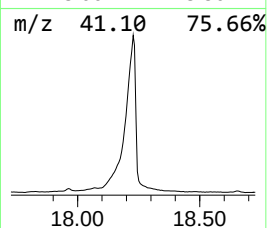
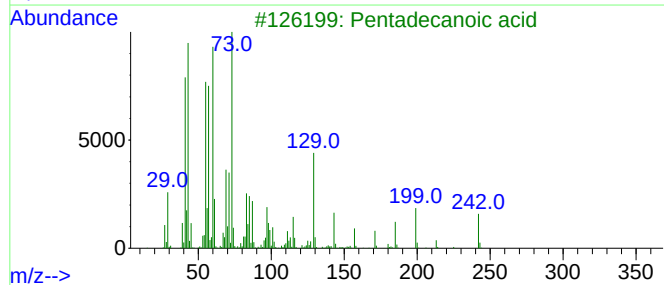
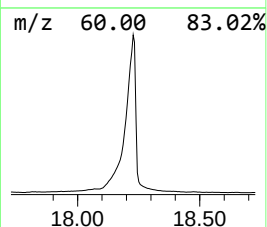
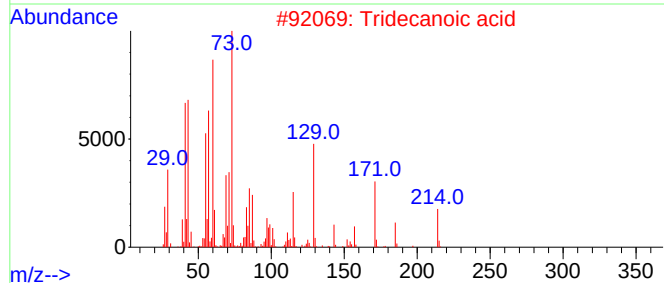
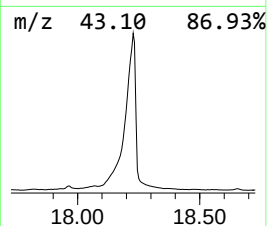
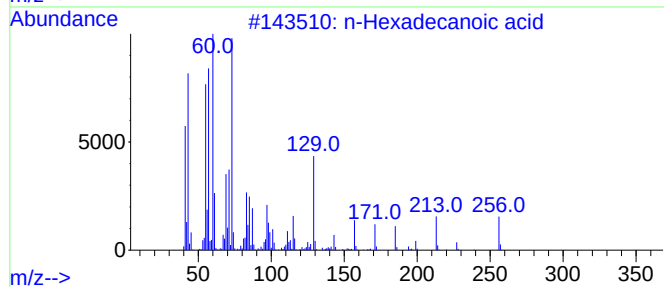
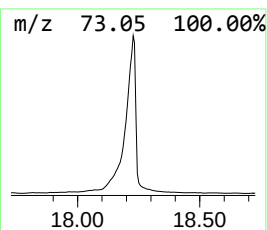
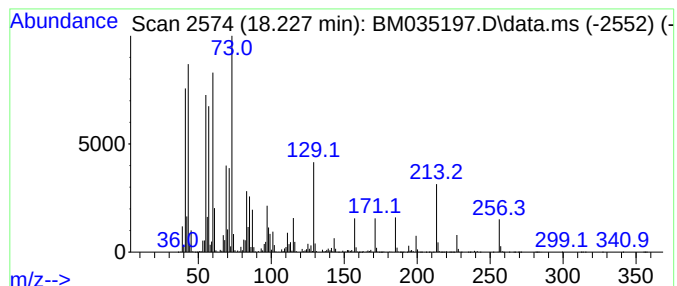
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.227	558.54 ng	47110300	Phenanthrene-d10	17.280

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Undecanoic acid	186	C11H22O2	000112-37-8	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	68



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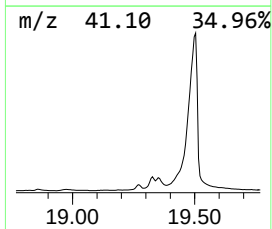
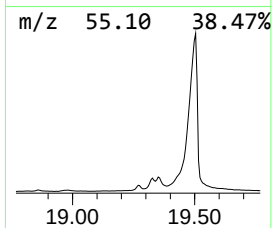
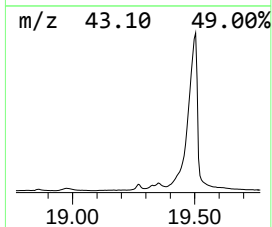
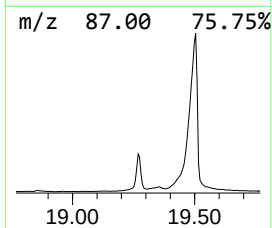
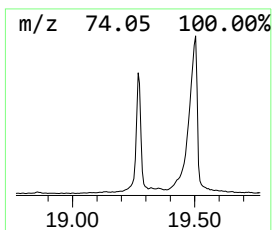
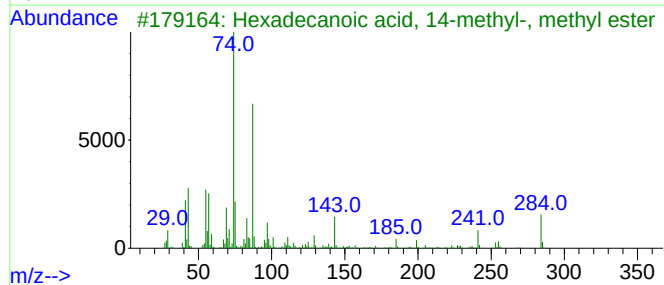
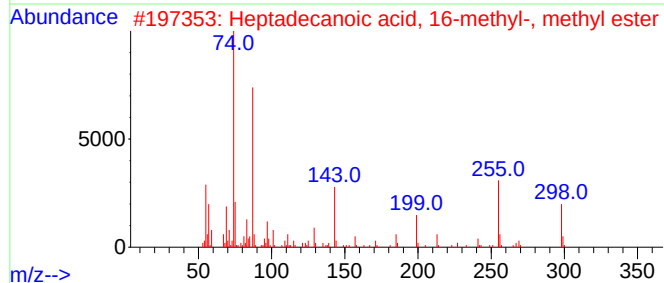
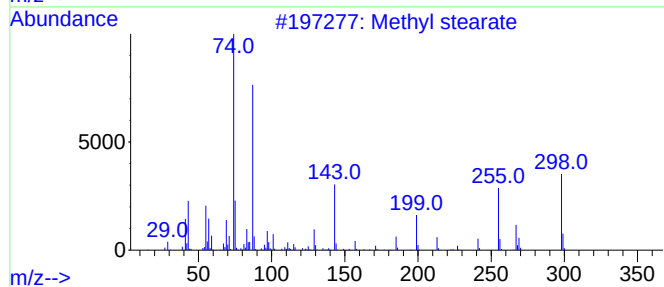
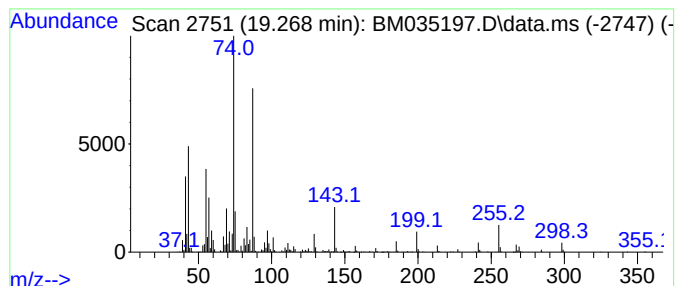
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Methyl stearate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.268	12.72 ng	1072710	Phenanthrene-d10	17.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	94
3			Hexadecanoic acid, 14-methyl-, m...	284	C18H36O2	002490-49-5	90
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
5			Methyl 9-methyltetradecanoate	256	C16H32O2	213617-69-7	87



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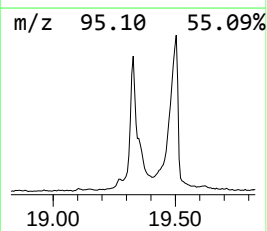
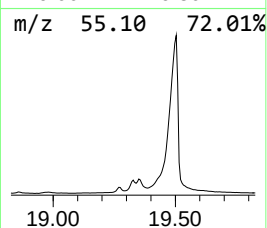
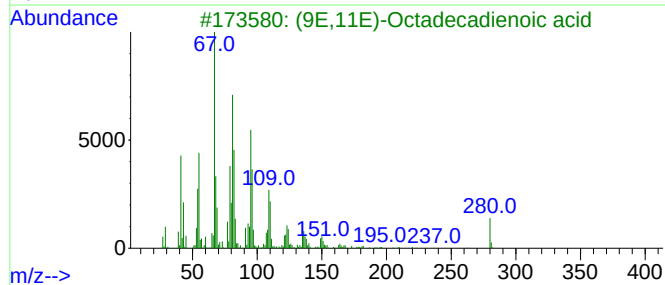
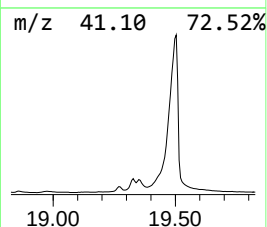
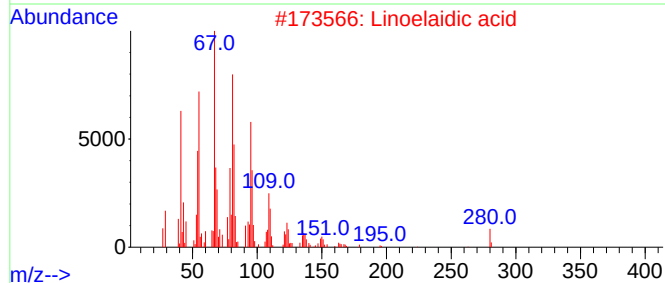
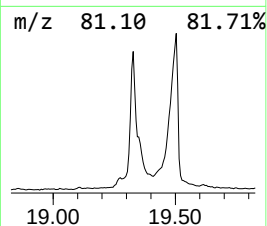
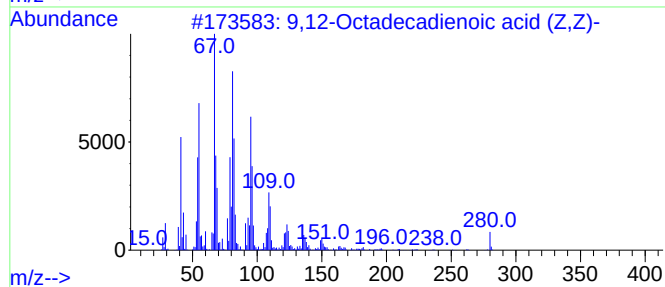
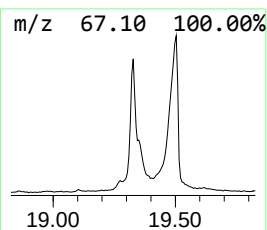
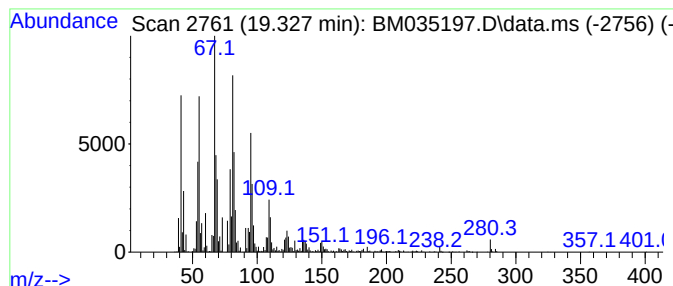
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 9,12-Octadecadienoic acid (... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.327	28.92 ng	2439400	Phenanthrene-d10	17.280

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2			Linoelaidic acid	280	C18H32O2	000506-21-8	99
3			(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	99
4			10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	99
5			2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	90



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Misc :
ALS Vial : 4 Sample Multiplier: 1

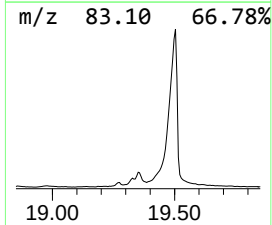
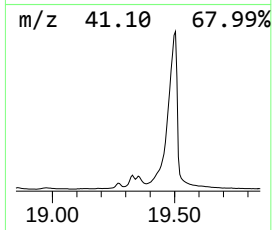
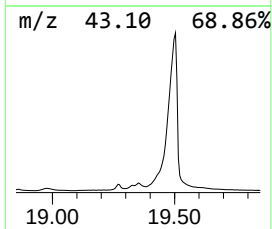
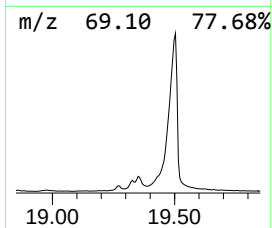
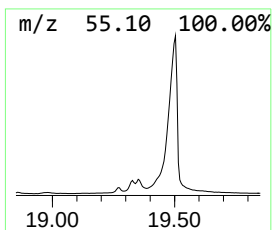
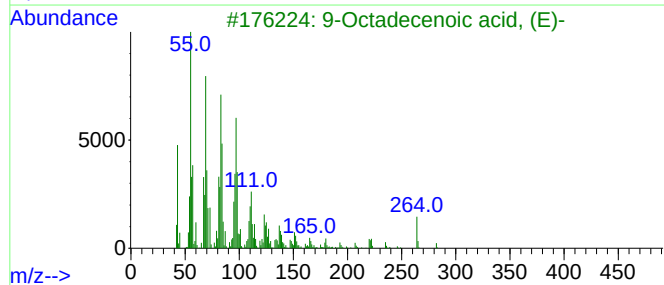
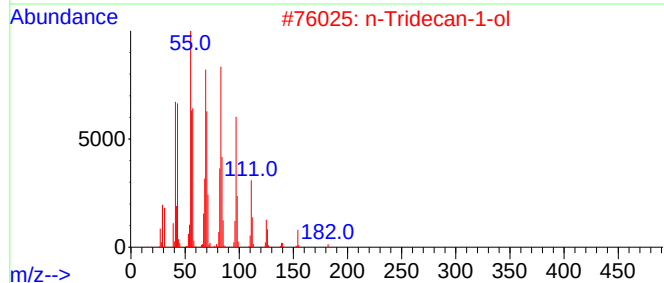
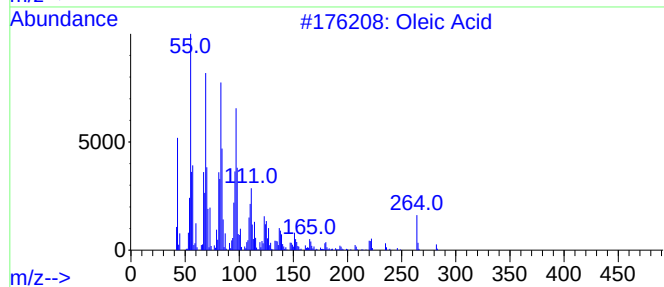
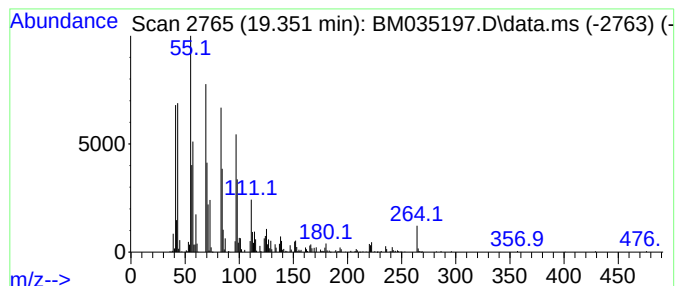
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Peak Number 4 Oleic Acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.351	28.71 ng	2421890	Phenanthrene-d10		17.280	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Oleic Acid		282	C18H34O2	000112-80-1	90
2	n-Tridecan-1-ol		200	C13H28O	000112-70-9	83
3	9-Octadecenoic acid, (E)-		282	C18H34O2	000112-79-8	81
4	1-Hexadecanol		242	C16H34O	036653-82-4	68
5	Cyclohexadecane		224	C16H32	000295-65-8	68



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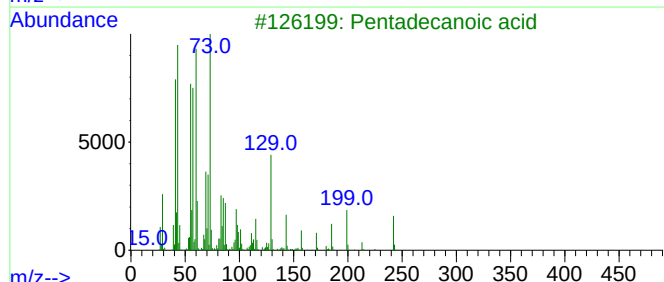
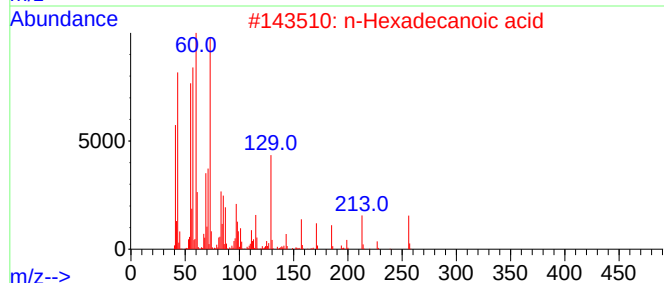
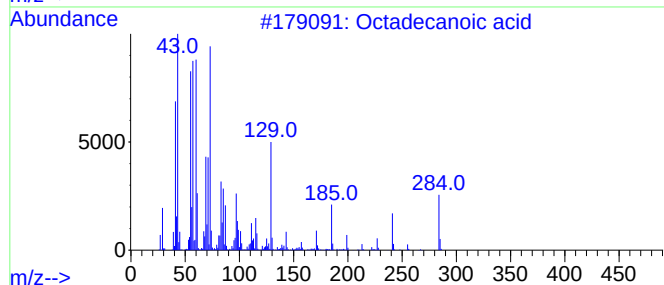
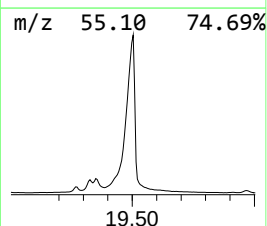
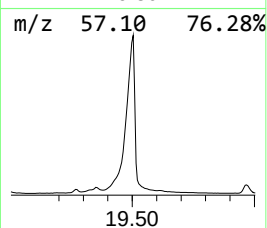
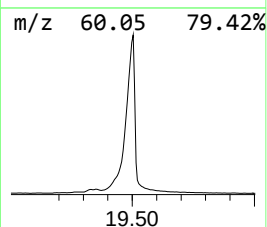
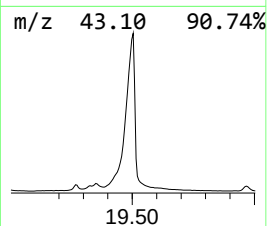
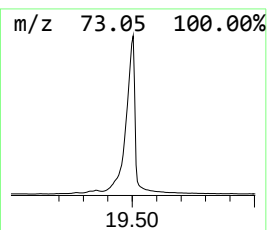
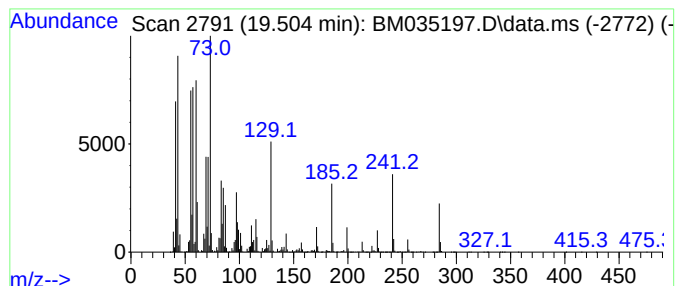
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.504	382.96 ng	58031600	Chrysene-d12	21.462

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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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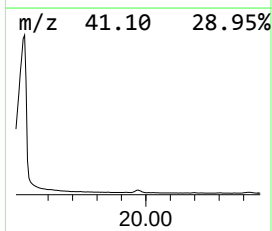
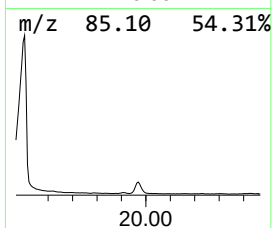
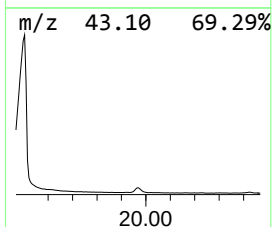
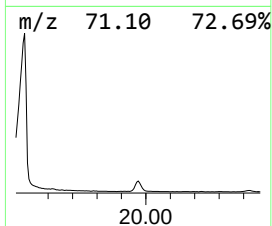
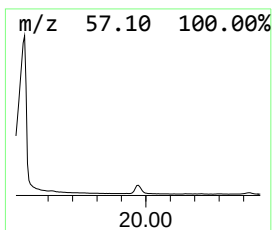
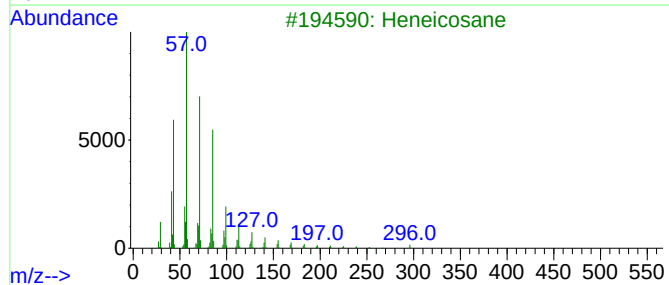
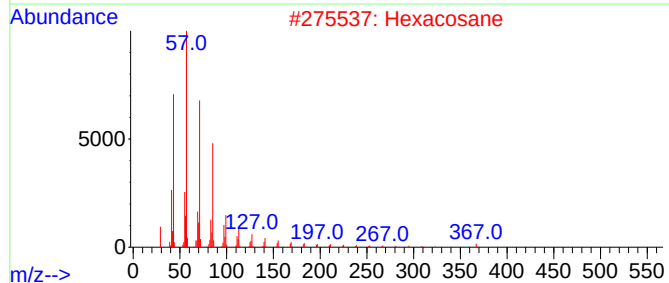
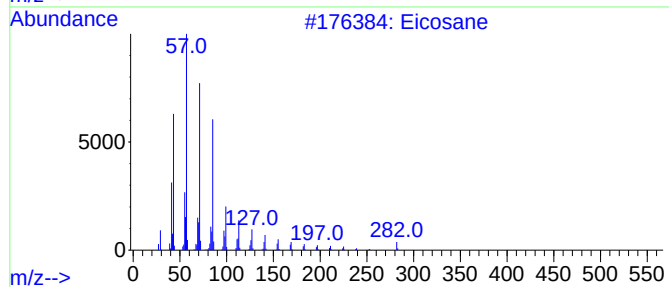
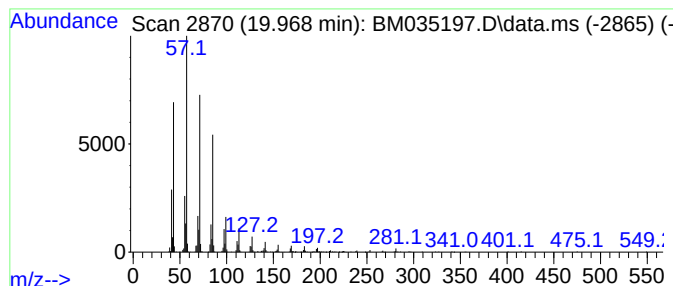
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.968	5.00 ng	757909	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Hexacosane	366	C26H54	000630-01-3	90
3			Heneicosane	296	C21H44	000629-94-7	90
4			Octacosane	394	C28H58	000630-02-4	90
5			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052322\
Data File : BM035197.D
Acq On : 23 May 2022 16:57
Operator : CG/JU
Sample : N2894-18
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
P008-SS002-2430-01

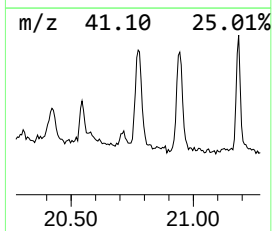
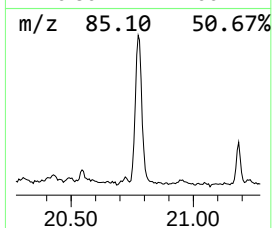
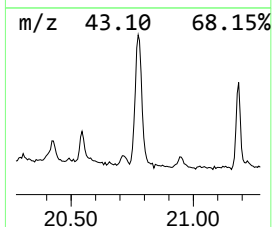
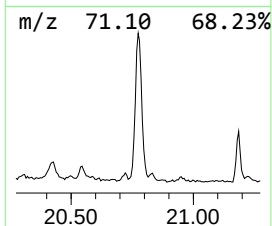
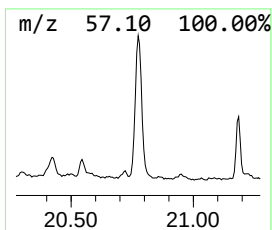
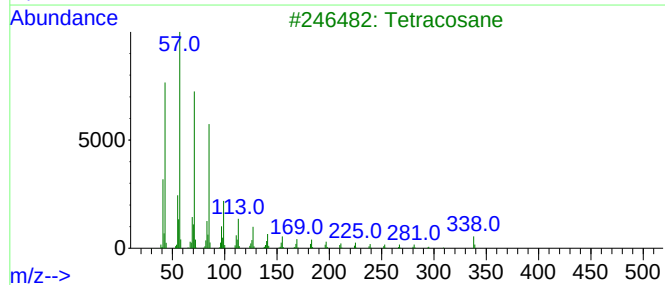
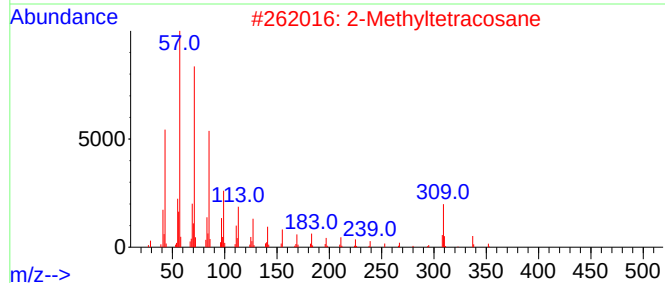
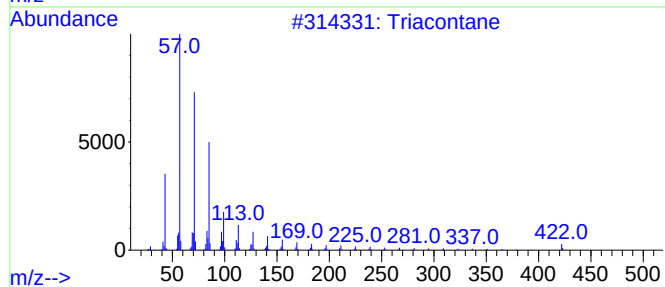
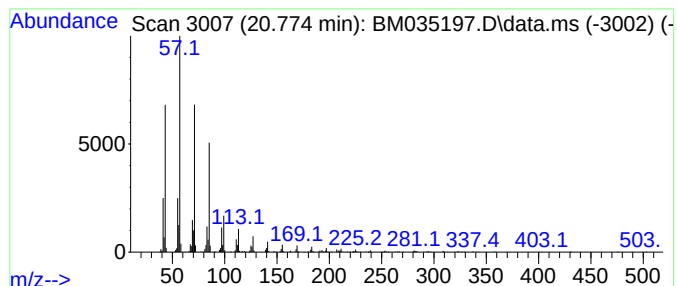
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.774	6.05 ng	917219	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triacontane	422	C30H62	000638-68-6	91
2			2-Methyltetracosane	352	C25H52	001560-78-7	91
3			Tetracosane	338	C24H50	000646-31-1	91
4			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052322\
Data File : BM035197.D
Acq On : 23 May 2022 16:57
Operator : CG/JU
Sample : N2894-18
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P008-SS002-2430-01

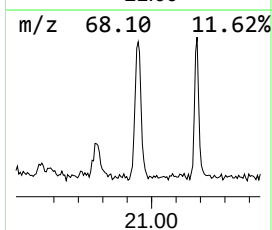
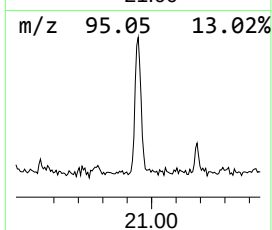
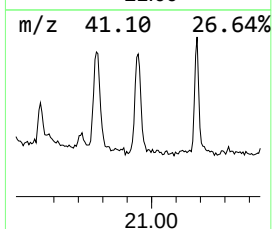
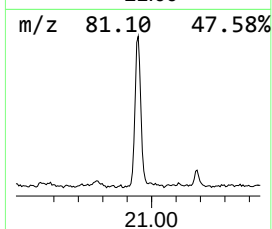
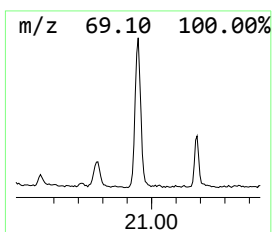
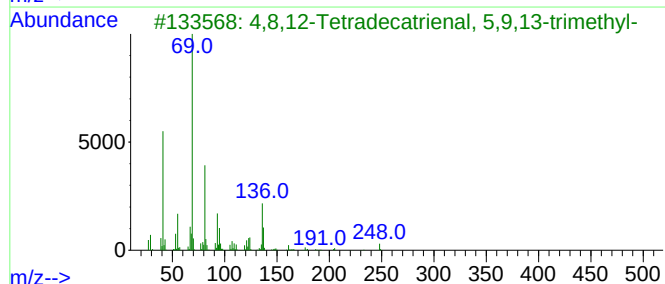
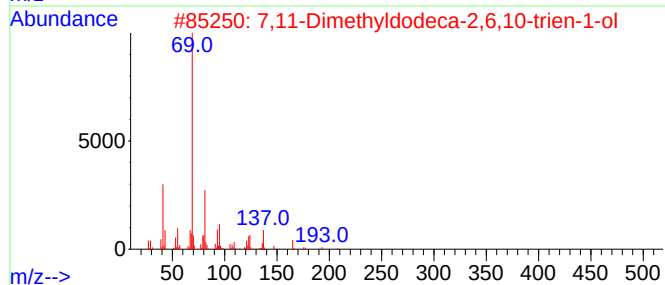
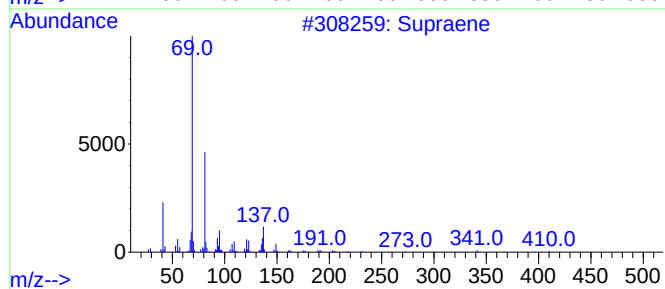
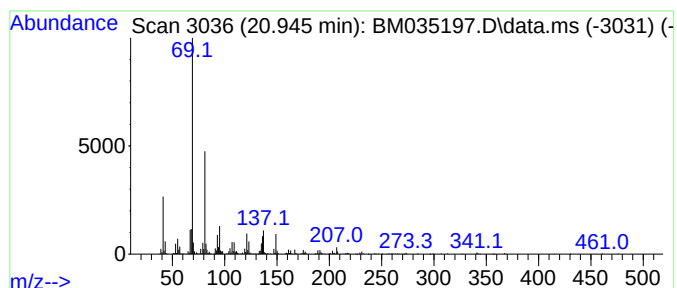
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Supraene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.945	4.01 ng	608219	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	90
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
4			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50
5			1,5-Heptadiene, 3,4-dimethyl-	124	C9H16	1000061-77-9	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052322\
Data File : BM035197.D
Acq On : 23 May 2022 16:57
Operator : CG/JU
Sample : N2894-18
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P008-SS002-2430-01

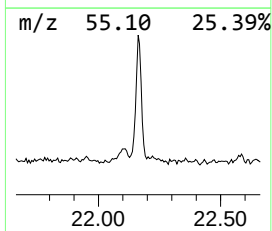
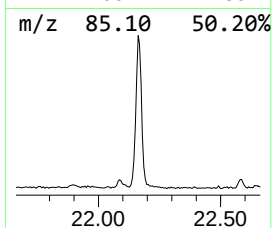
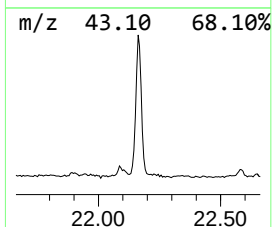
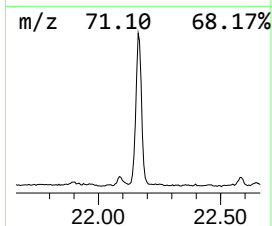
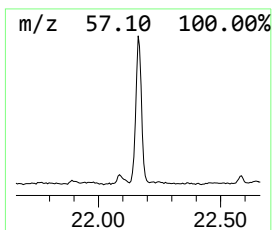
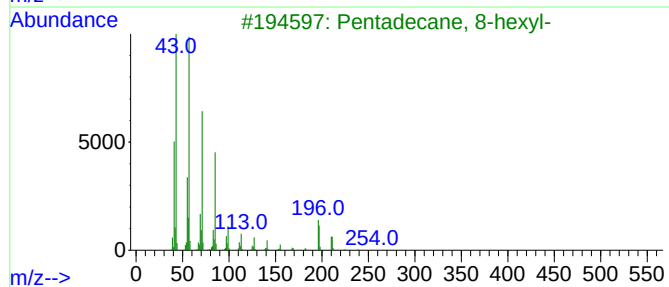
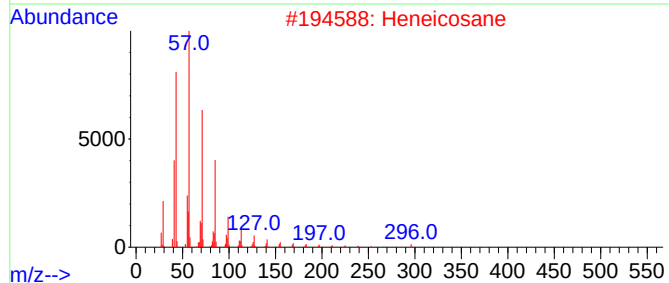
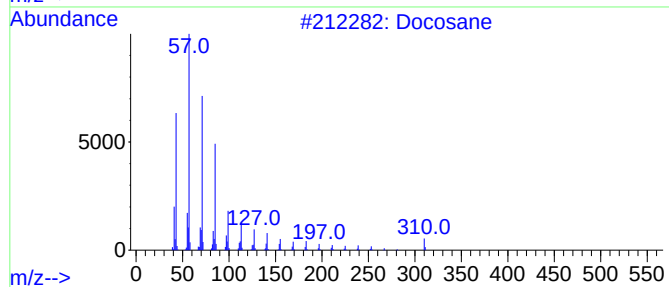
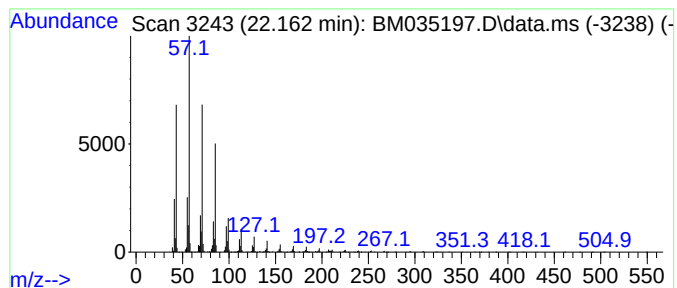
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Docosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.162	7.76 ng	1175270	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	97
2			Heneicosane	296	C21H44	000629-94-7	97
3			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
4			Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	94
5			triacontane	422	C30H62	000638-68-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM052322\
Data File : BM035197.D
Acq On : 23 May 2022 16:57
Operator : CG/JU
Sample : N2894-18
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
P008-SS002-2430-01

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Methyl stearate	19.268	12.7	ng	1072710	4	17.280	1686900	20.0
9,12-Octadecadi...	19.327	28.9	ng	2439400	4	17.280	1686900	20.0
Oleic Acid	19.351	28.7	ng	2421890	4	17.280	1686900	20.0
Octadecanoic acid	19.504	383.0	ng	58031600	5	21.462	3030710	20.0
Eicosane	19.968	5.0	ng	757909	5	21.462	3030710	20.0
Triacontane	20.774	6.0	ng	917219	5	21.462	3030710	20.0
Supraene	20.945	4.0	ng	608219	5	21.462	3030710	20.0
Docosane	22.162	7.8	ng	1175270	5	21.462	3030710	20.0