

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
 Data File : BM041229.D
 Acq On : 01 Aug 2023 17:46
 Operator : MA/JU
 Sample : 03715-07
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 T842-FH-04-CT

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-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041229.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	365	372	386	rBV	1982679	2830800	30.83%	5.516%
2	6.987	638	646	661	rBV	1870427	2930907	31.92%	5.711%
3	7.798	778	784	792	rBV	580639	893667	9.73%	1.741%
4	8.975	976	984	999	rBV	1119434	1865150	20.31%	3.634%
5	10.610	1254	1262	1275	rBV	719378	1200950	13.08%	2.340%
6	13.086	1675	1683	1693	rBV	2855550	4245028	46.22%	8.272%
7	13.927	1819	1826	1833	rBV	114268	171489	1.87%	0.334%
8	14.468	1911	1918	1928	rVV	1026072	1529755	16.66%	2.981%
9	15.968	2166	2173	2191	rBV	2551412	3462267	37.70%	6.746%
10	17.227	2380	2387	2393	rBV	1312016	1833910	19.97%	3.573%
11	18.133	2535	2541	2558	rBV	2856019	4128930	44.96%	8.045%
12	18.798	2650	2654	2667	rBV	243465	416143	4.53%	0.811%
13	18.992	2683	2687	2693	rBV	75724	110517	1.20%	0.215%
14	19.262	2730	2733	2735	rBV	104439	130613	1.42%	0.255%
15	19.292	2735	2738	2748	rVB2	207942	398068	4.33%	0.776%
16	19.409	2754	2758	2773	rBV	1619560	2306140	25.11%	4.494%
17	19.862	2830	2835	2846	rBV	5778348	7103769	77.35%	13.842%
18	20.903	3009	3012	3018	rBV	242175	305938	3.33%	0.596%
19	21.133	3048	3051	3059	rVB	316833	412689	4.49%	0.804%
20	21.427	3097	3101	3112	rBV	1586679	2185860	23.80%	4.259%
21	23.803	3499	3505	3512	rVB	1033383	1981469	21.58%	3.861%
22	24.491	3616	3622	3635	rVB	622454	1692842	18.43%	3.299%
23	27.132	4061	4071	4093	rVB2	2492310	9183425	100.00%	17.894%

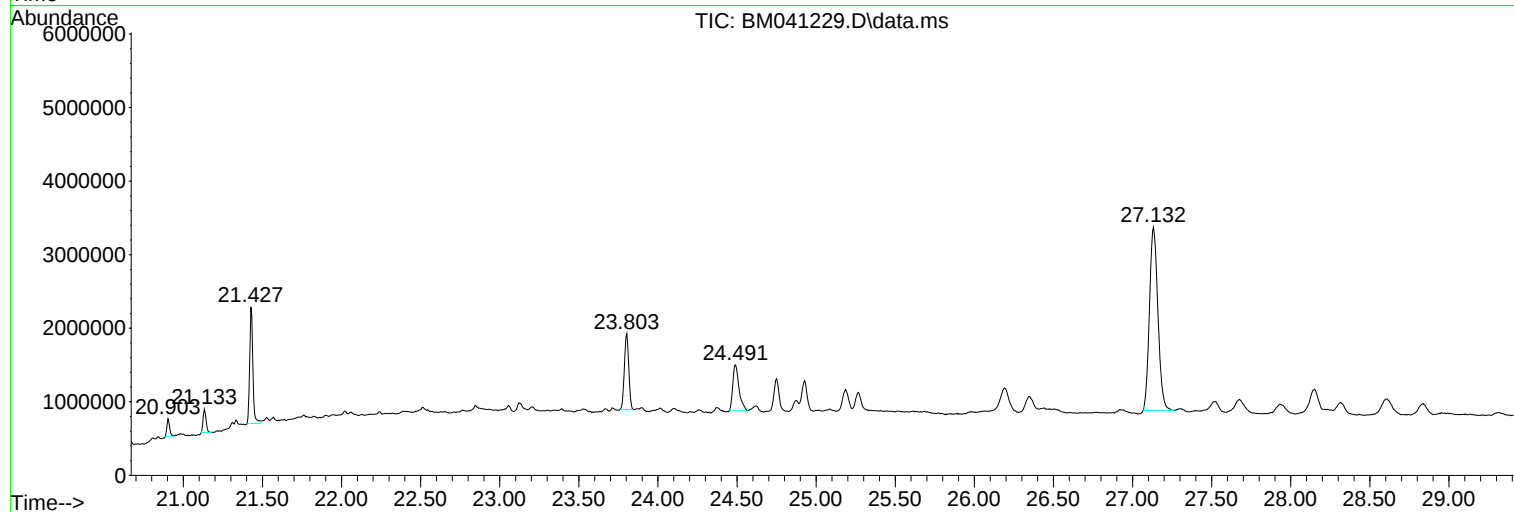
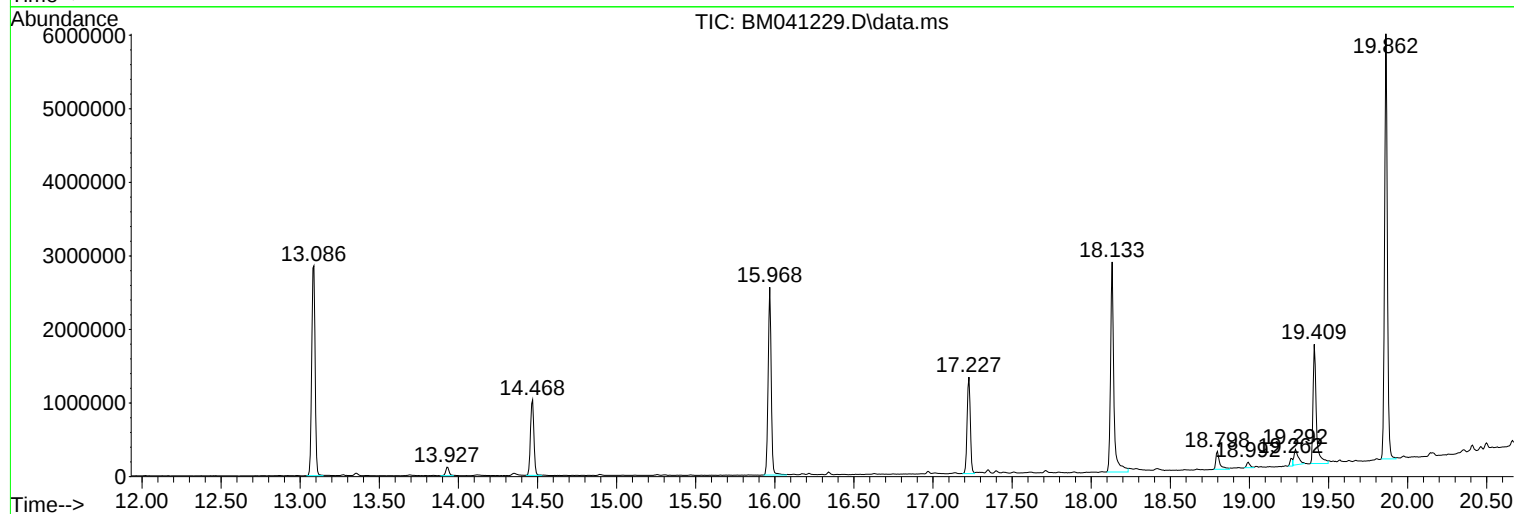
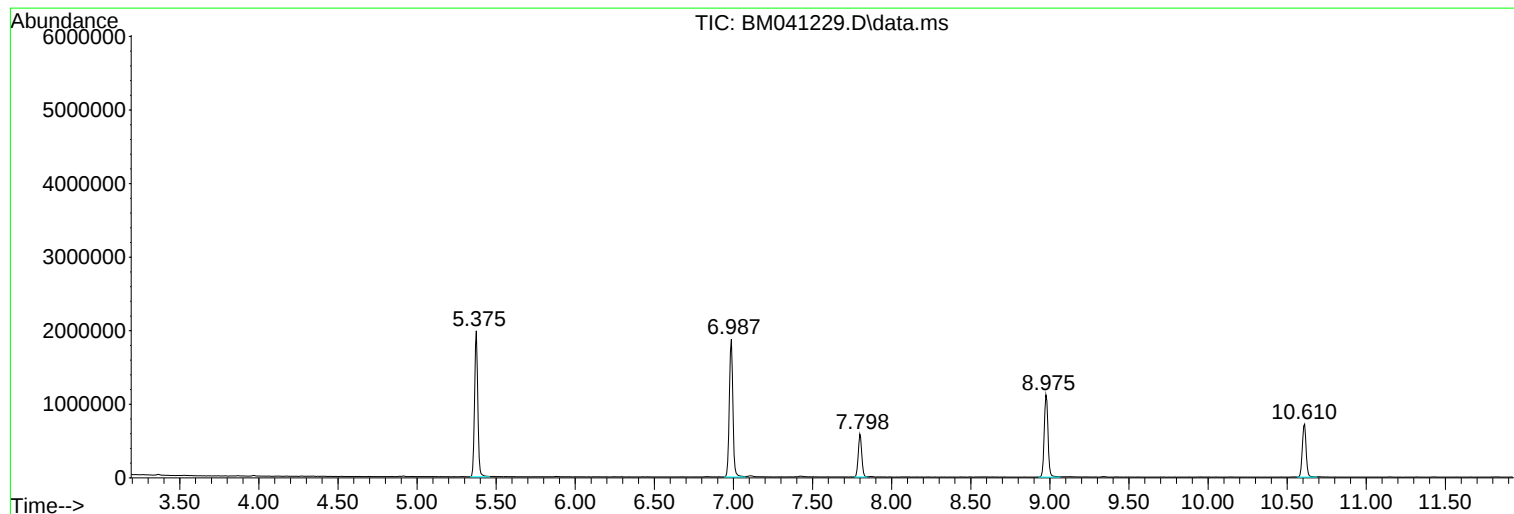
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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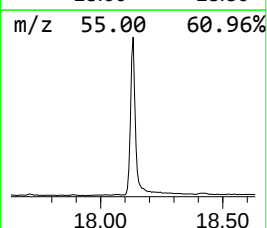
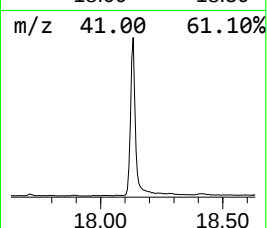
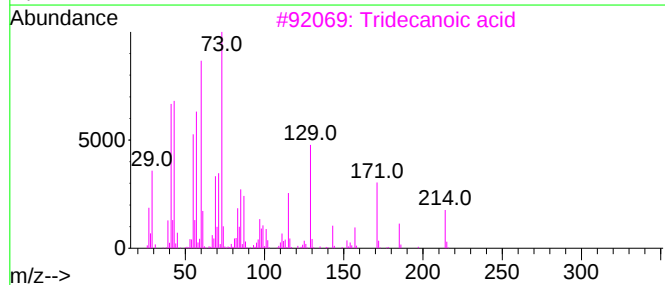
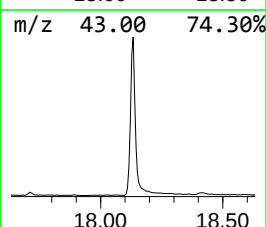
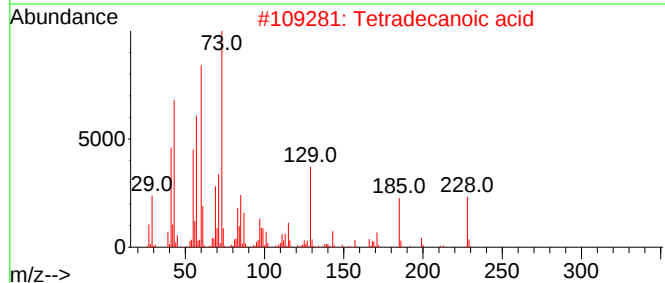
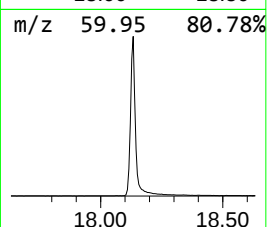
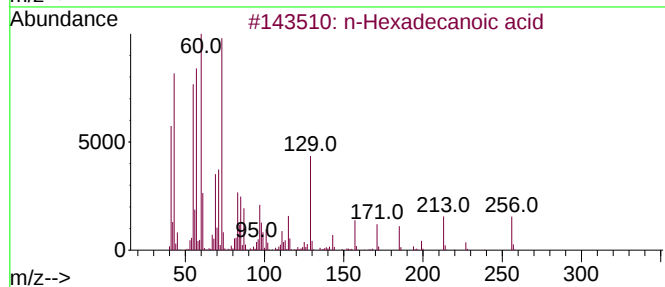
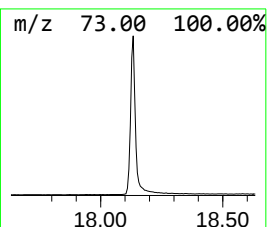
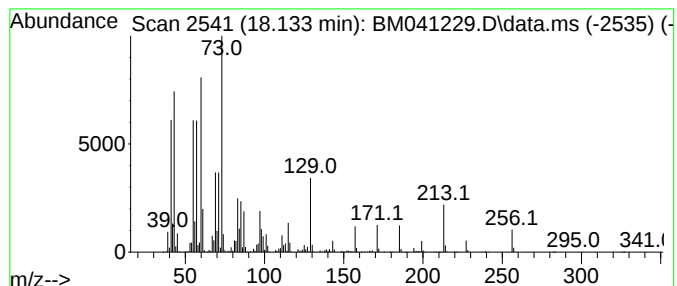
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.133	45.03 ng	4128930	Phenanthrene-d10	17.227

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	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	47



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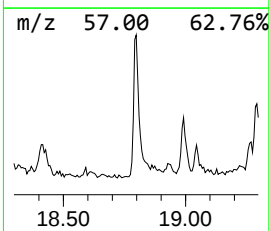
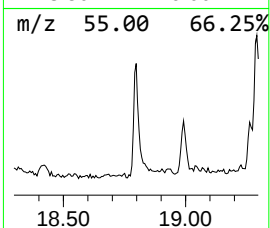
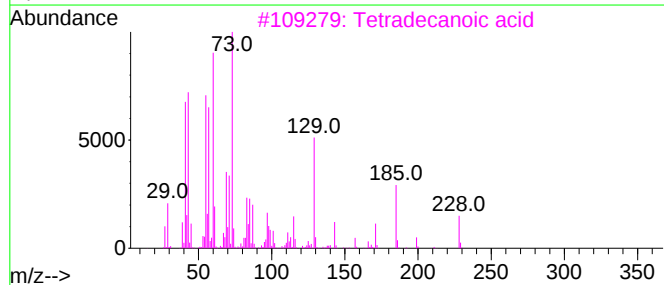
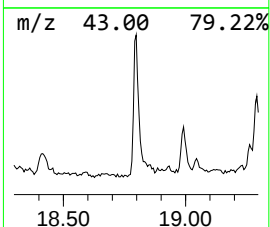
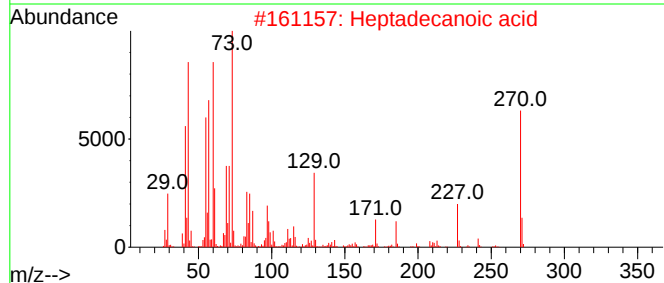
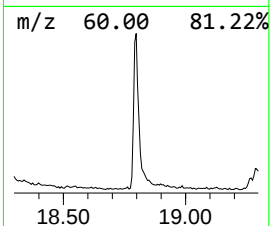
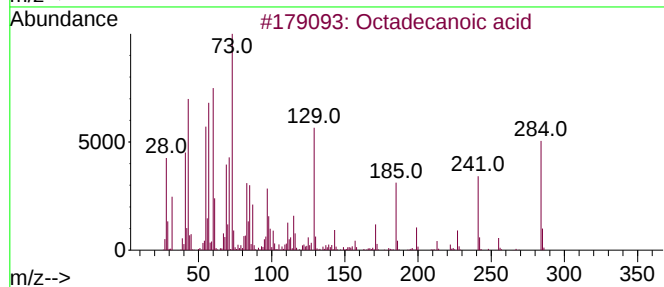
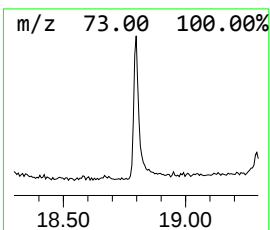
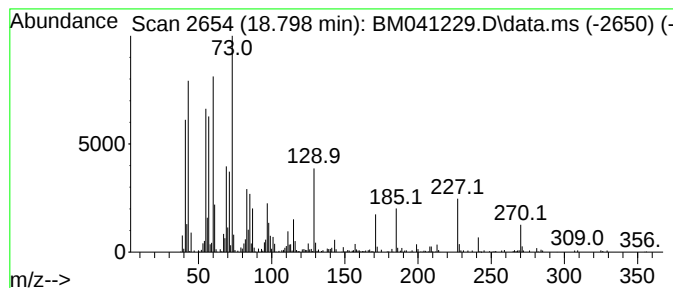
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.798	4.54 ng	416143	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Heptadecanoic acid	270	C17H34O2	000506-12-7	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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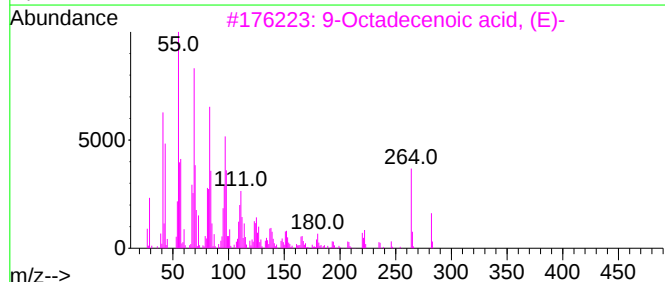
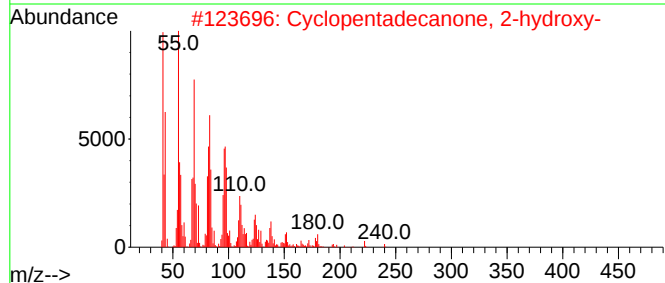
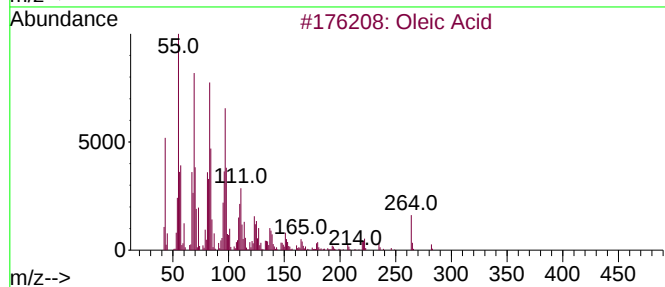
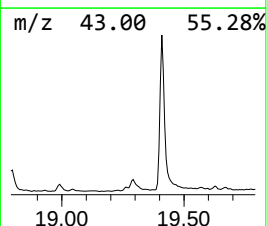
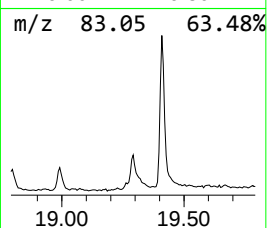
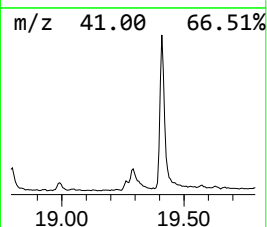
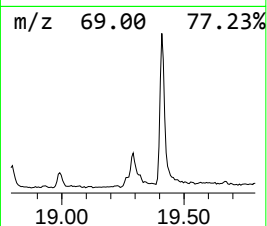
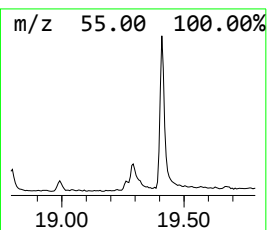
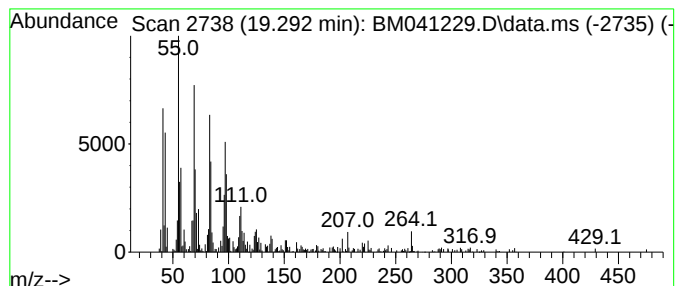
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Oleic Acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.292	4.34 ng	398068	Phenanthrene-d10	17.227

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oleic Acid	282	C18H34O2	000112-80-1	91
2			Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	89
3			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	87
4			Oleyl alcohol, trifluoroacetate	364	C20H35F3O2	1000352-68-4	81
5			14-Pentadecenoic acid	240	C15H28O2	017351-34-7	68



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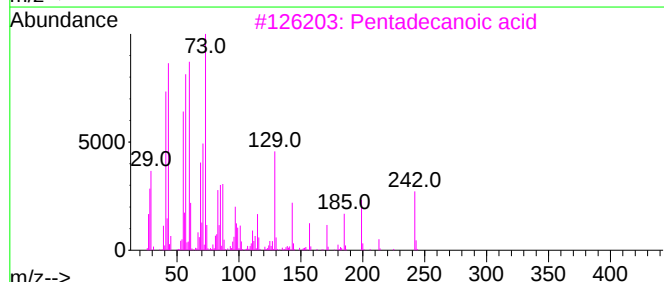
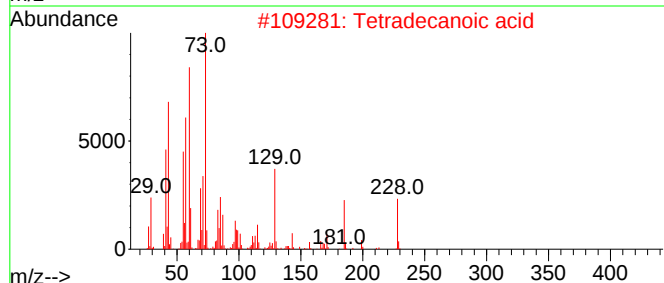
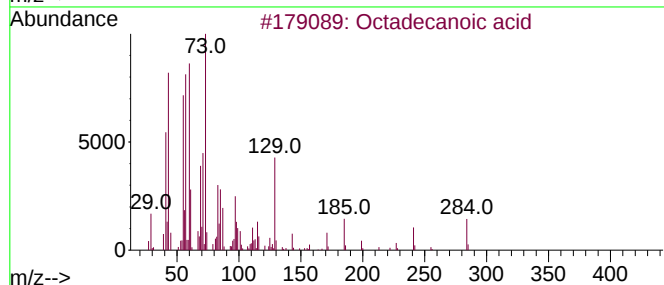
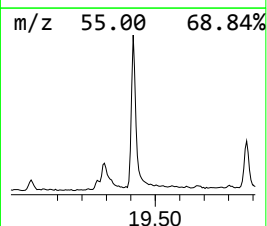
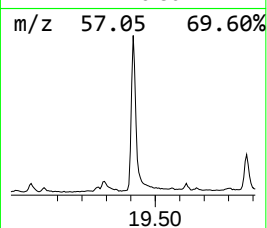
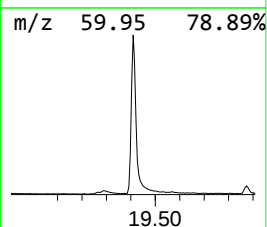
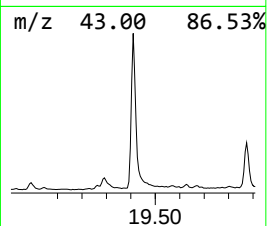
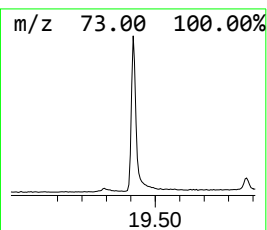
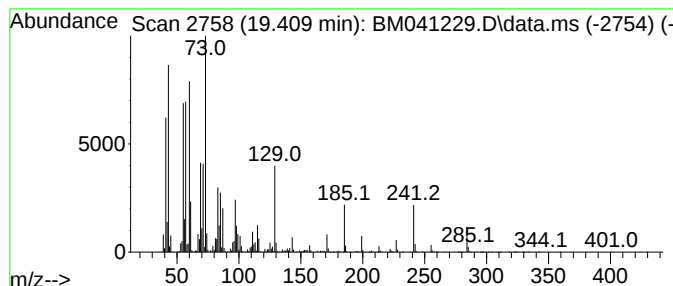
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.409	21.10 ng	2306140	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	74
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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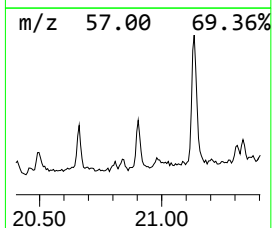
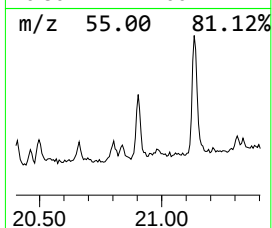
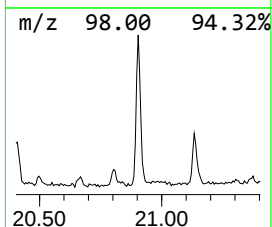
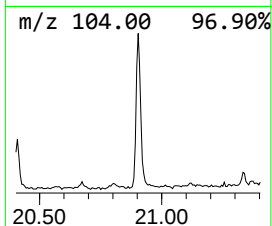
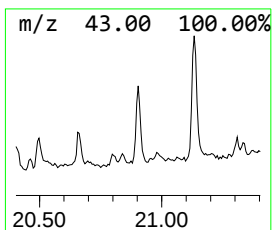
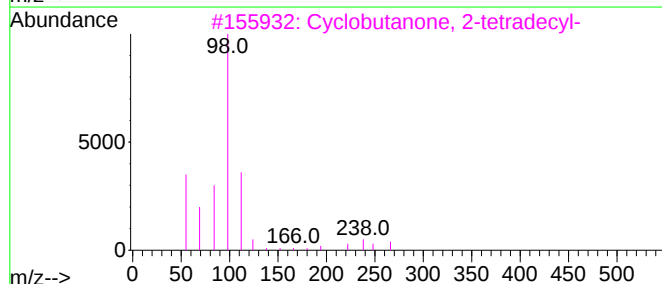
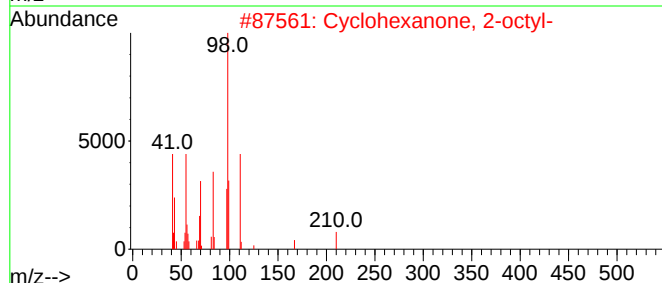
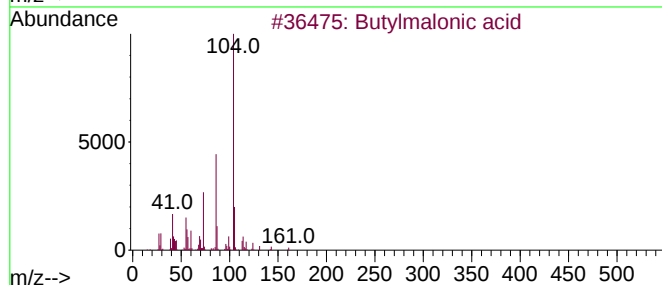
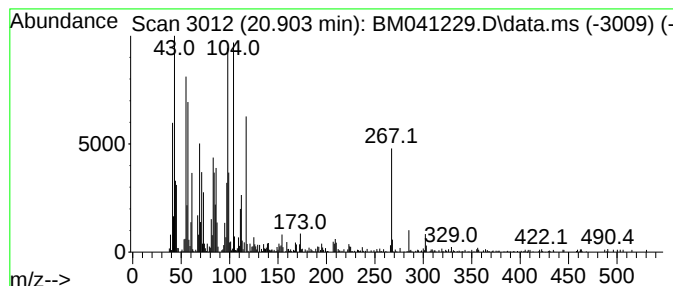
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown20.903 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.903	2.80 ng	305938	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylmalonic acid	160	C7H12O4	000534-59-8	30
2			Cyclohexanone, 2-octyl-	210	C14H26O	006814-21-7	15
3			Cyclobutanone, 2-tetradecyl-	266	C18H34O	035493-47-1	14
4			n-Hexylamine, N-acetyl-1-cyano-	168	C9H16N2O	1000227-04-0	14
5			AB-005	352	C23H32N2O	895155-25-6	11



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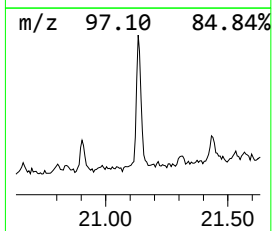
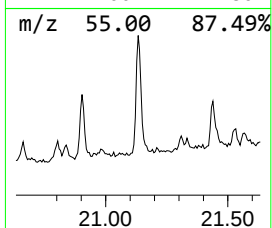
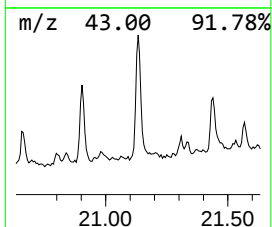
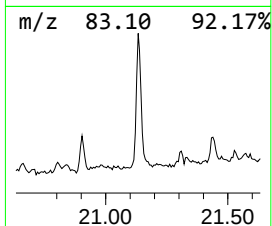
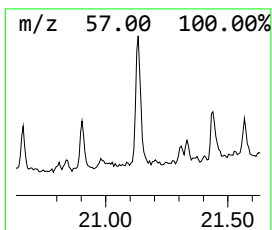
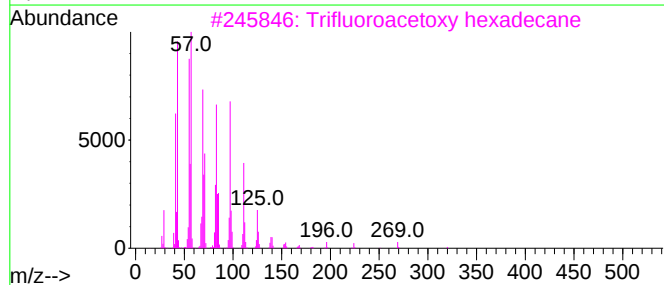
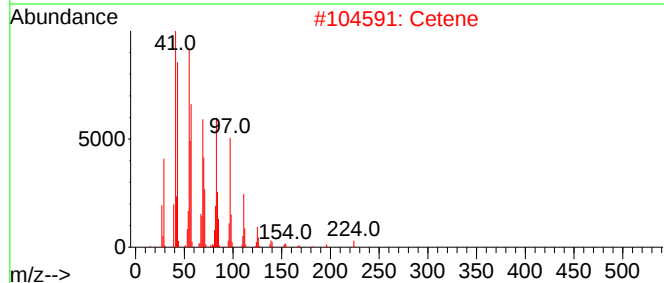
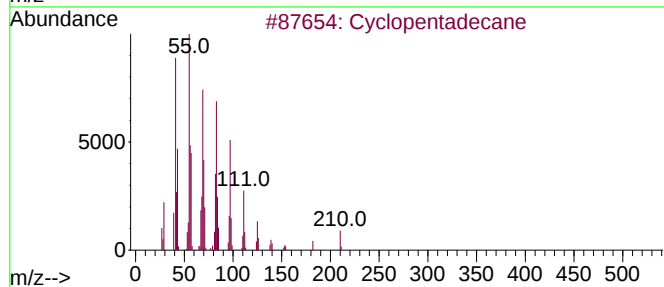
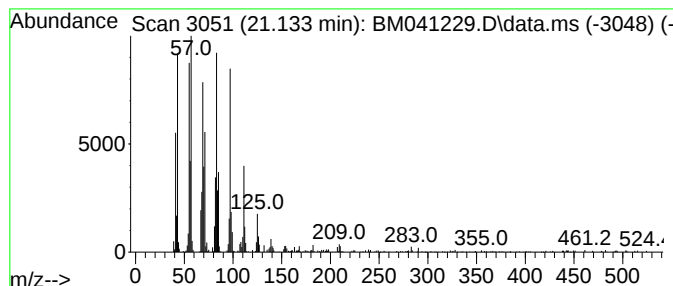
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclopentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.133	3.78 ng	412689	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	97
2			Cetene	224	C16H32	000629-73-2	95
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
5			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041229.D
Acq On : 01 Aug 2023 17:46
Operator : MA/JU
Sample : 03715-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
T842-FH-04-CT

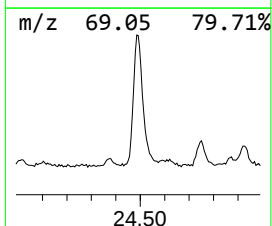
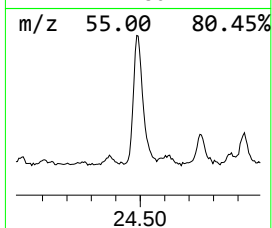
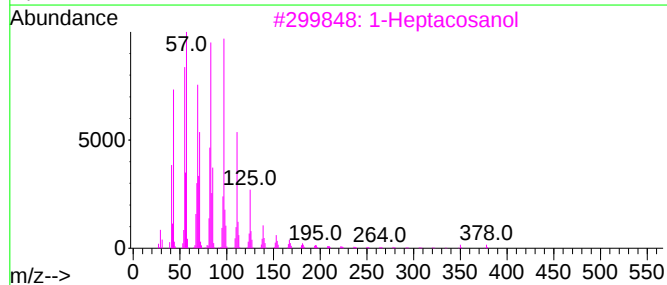
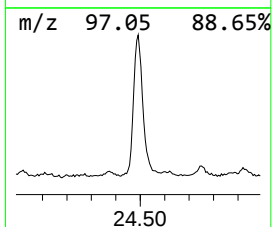
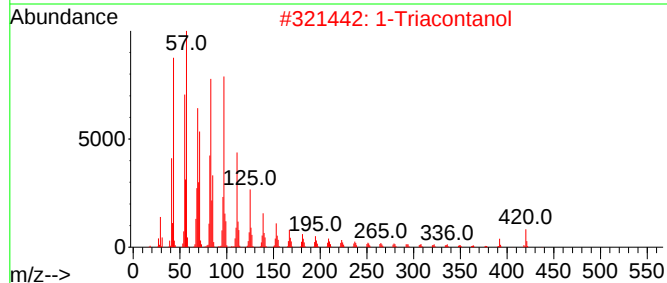
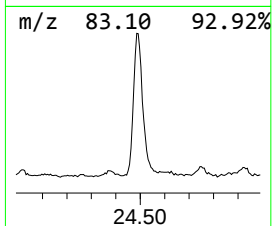
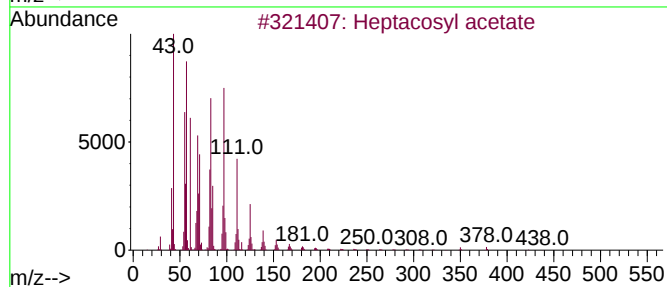
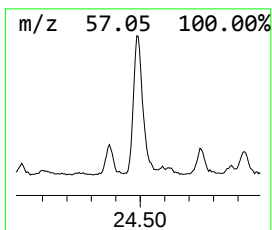
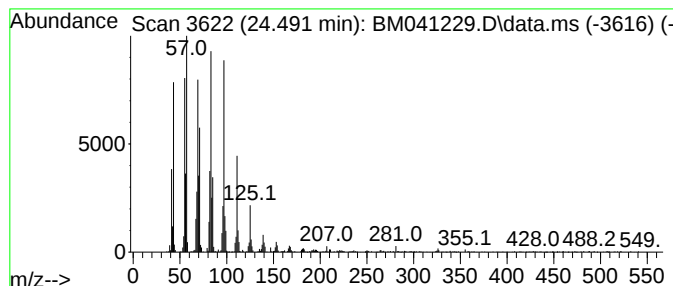
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.491	17.09 ng	1692840	Perylene-d12	23.803

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosyl acetate	438	C29H58O2	1000351-78-2	95
2			1-Triacontanol	438	C30H62O	000593-50-0	95
3			1-Heptacosanol	396	C27H56O	002004-39-9	95
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041229.D
Acq On : 01 Aug 2023 17:46
Operator : MA/JU
Sample : 03715-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
T842-FH-04-CT

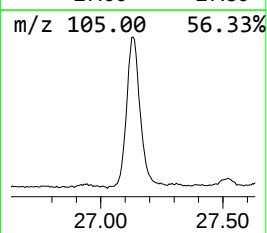
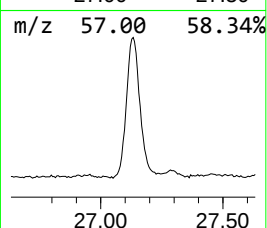
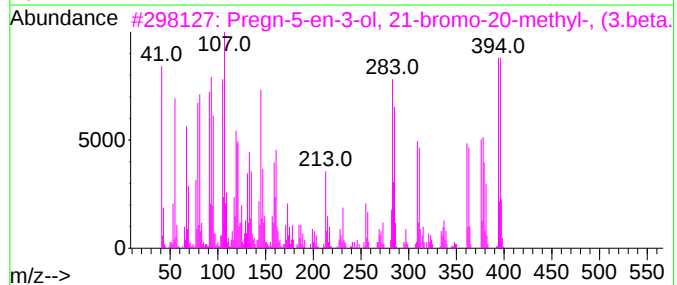
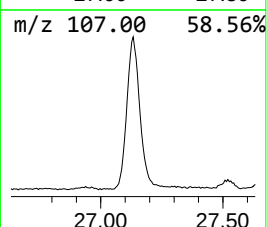
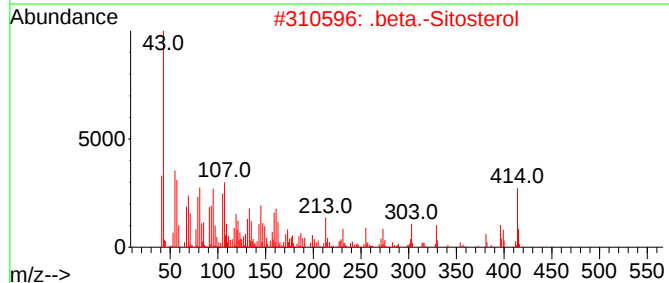
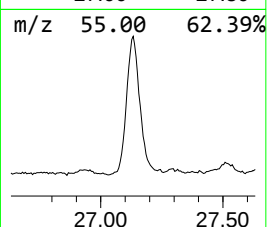
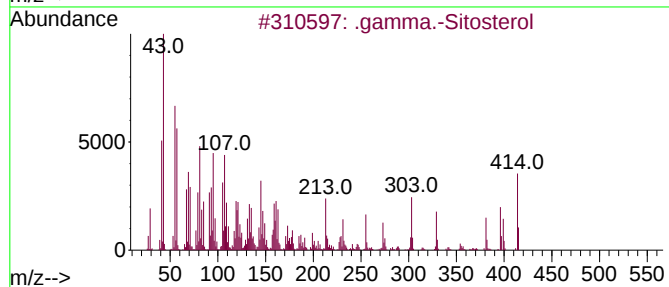
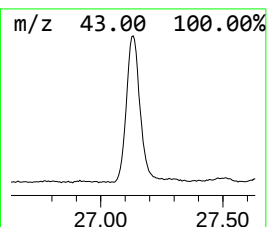
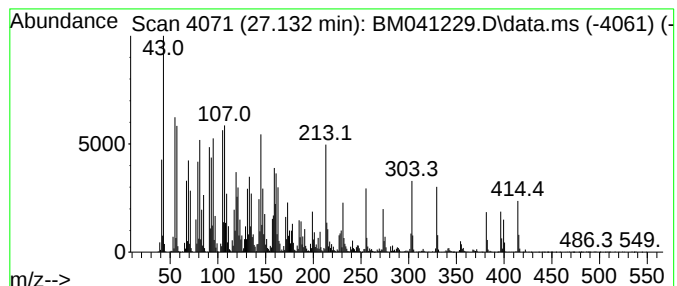
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.132	92.69 ng	9183430	Perylene-d12	23.803

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	gamma.-Sitosterol	414	C29H50O	000083-47-6	99	
2	.	beta.-Sitosterol	414	C29H50O	000083-46-5	99	
3	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	94		
4	Campesterol	400	C28H48O	000474-62-4	62		
5	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	49		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080123\
Data File : BM041229.D
Acq On : 01 Aug 2023 17:46
Operator : MA/JU
Sample : 03715-07
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
T842-FH-04-CT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM072823.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
n-Hexadecanoic ...	18.133	45.0	ng	4128930	4	17.227	1833910	20.0
Octadecanoic acid	18.798	4.5	ng	416143	4	17.227	1833910	20.0
Oleic Acid	19.292	4.3	ng	398068	4	17.227	1833910	20.0
Tetradecanoic acid	19.409	21.1	ng	2306140	5	21.427	2185860	20.0
unknown20.903	20.903	2.8	ng	305938	5	21.427	2185860	20.0
Cyclopentadecane	21.133	3.8	ng	412689	5	21.427	2185860	20.0
Heptacosyl acetate	24.491	17.1	ng	1692840	6	23.803	1981470	20.0
.gamma.-Sitosterol	27.132	92.7	ng	9183430	6	23.803	1981470	20.0