LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080322\
Data File : BM036084.D
Acq On : 03 Aug 2022 18:54
Operator : CG/JU
Sample : N3998-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ST-1

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-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036084.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.428	391	398	416	rBV	2578747	3944835	22.02%	4.723%
2	7.034	660	671	689	rBV	2849643	4458874	24.89%	5.338%
3	7.863	805	812	820	rBV	557518	861922	4.81%	1.032%
4	9.034	1002	1011	1026	rBV	1590567	2667614	14.89%	3.194%
5	10.669	1282	1289	1299	rBV	833775	1406053	7.85%	1.683%
6	13.133	1699	1708	1721	rBV	4312010	6307642	35.21%	7.552%
7	14.316	1902	1909	1914	rBV2	104759	190606	1.06%	0.228%
8	14.504	1931	1941	1948	rBV	1487900	2145884	11.98%	2.569%
9	15.986	2184	2193	2202	rBV	4354243	6160773	34.39%	7.376%
10	17.245	2402	2407	2412	rVB	1951217	2619038	14.62%	3.136%
11	18.151	2555	2561	2587	rBV	3465060	5469364	30.53%	6.548%
12	19.303	2753	2757	2760	rBV	266667	329345	1.84%	0.394%
13	19.339	2760	2763	2773	rVB2	172851	303973	1.70%	0.364%
14	19.427	2773	2778	2793	rBV	1492835	2000516	11.17%	2.395%
15	19.868	2848	2853	2859	rBV	8545595	10071950	56.22%	12.059%
16	21.145	3066	3070	3078	rBV	495244	701219	3.91%	0.840%
17	21.345	3101	3104	3108	rVB	201665	216403	1.21%	0.259%
18	21.421	3113	3117	3123	rBV	2891028	3665497	20.46%	4.389%
19	23.791	3513	3520	3531	rVB2	2185528	4300463	24.00%	5.149%
20	24.915	3702	3711	3734	rVB	6142707	17915995	100.00%	21.450%
21	25.209	3753	3761	3763	rBV2	1774518	4108708	22.93%	4.919%
22	26.774	4020	4027	4046	rVB3	1004892	3676988	20.52%	4.402%

Sum of corrected areas: 83523662

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080322\
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Instrument :
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ClientSampleId :
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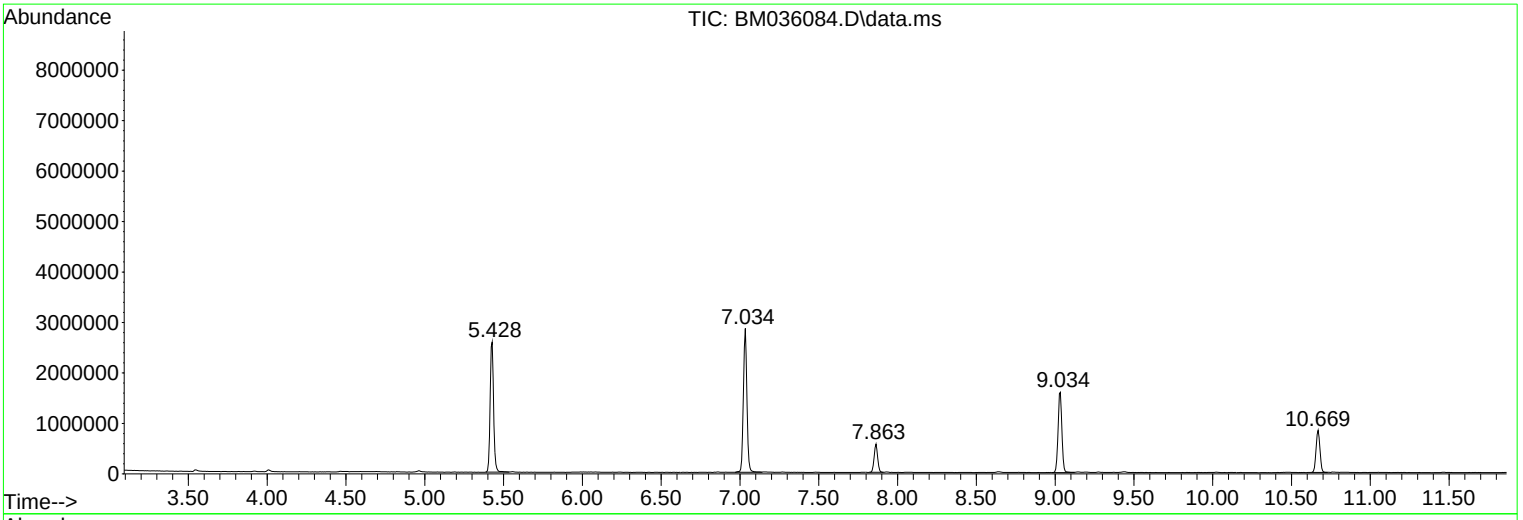
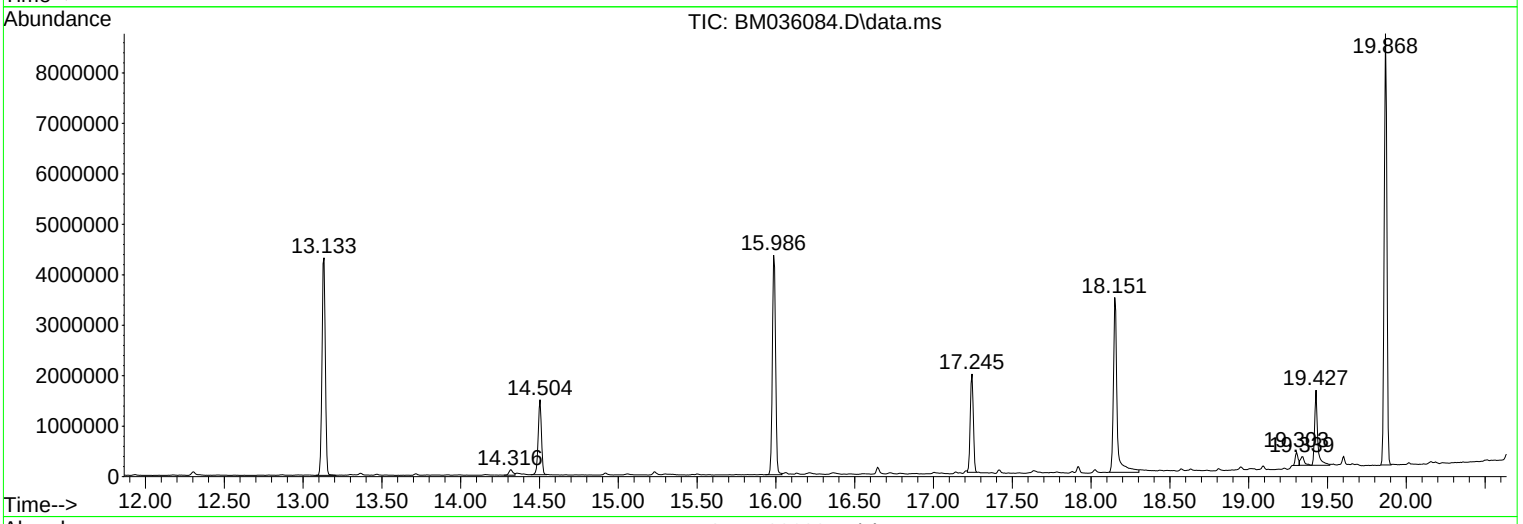
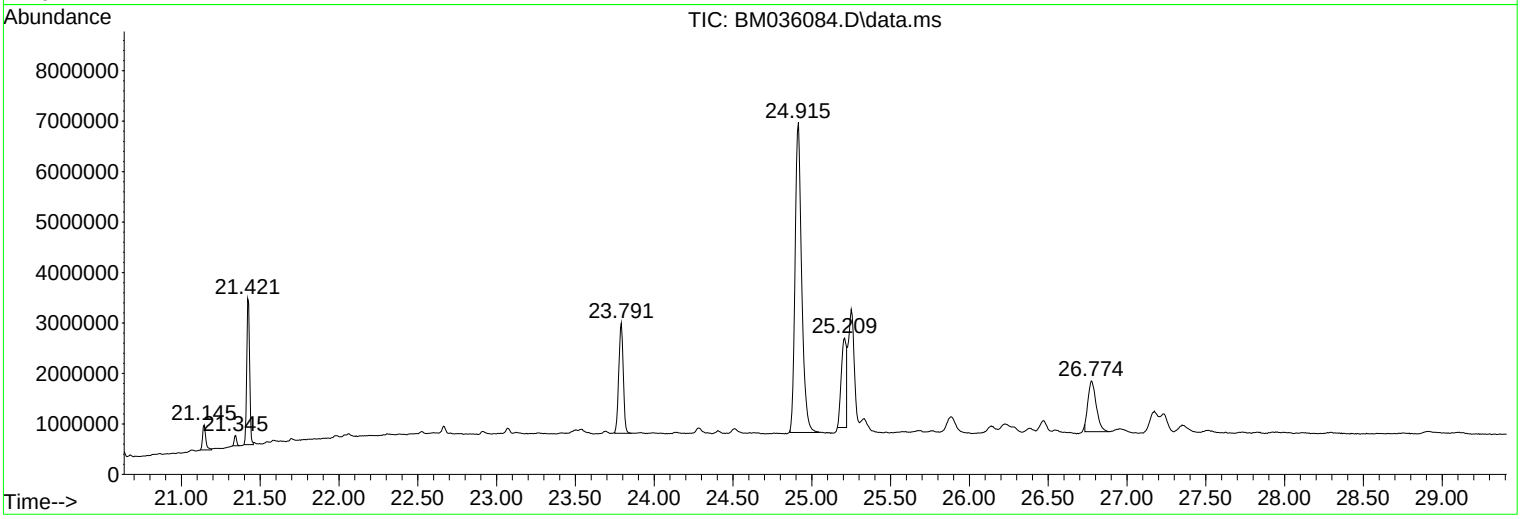
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BM036084.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

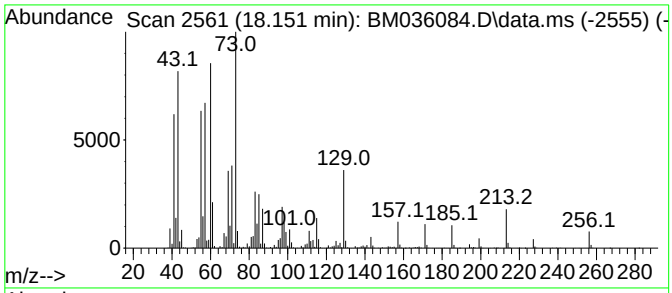
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

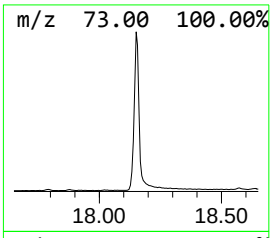
****

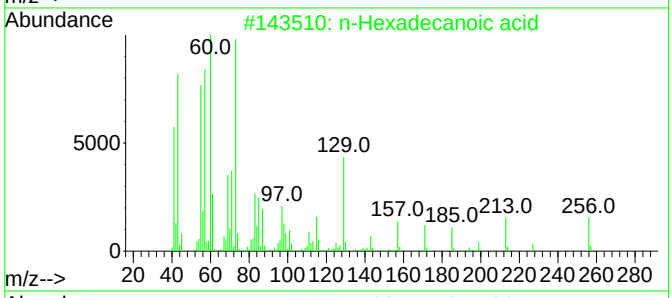
Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

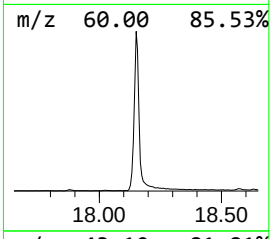
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.151	41.77 ng	5469360	Phenanthrene-d10	17.245

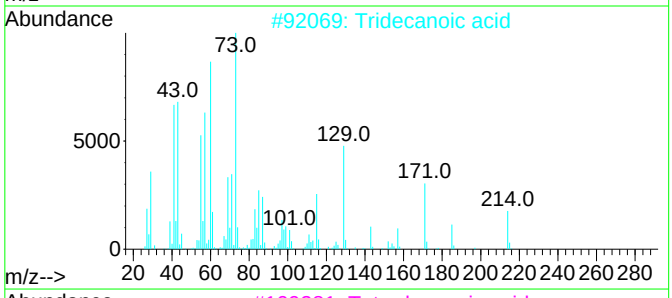
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64

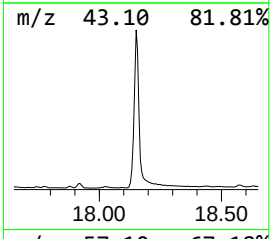


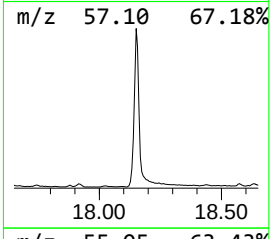


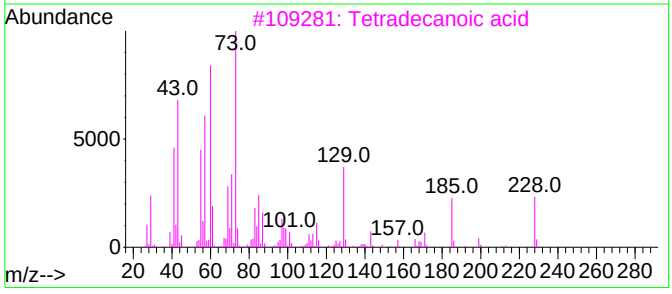


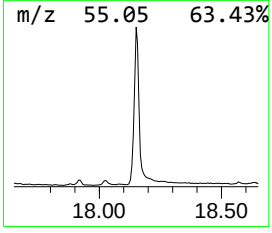












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Data File : BM036084.D
Acq On : 03 Aug 2022 18:54
Operator : CG/JU
Sample : N3998-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
ST-1

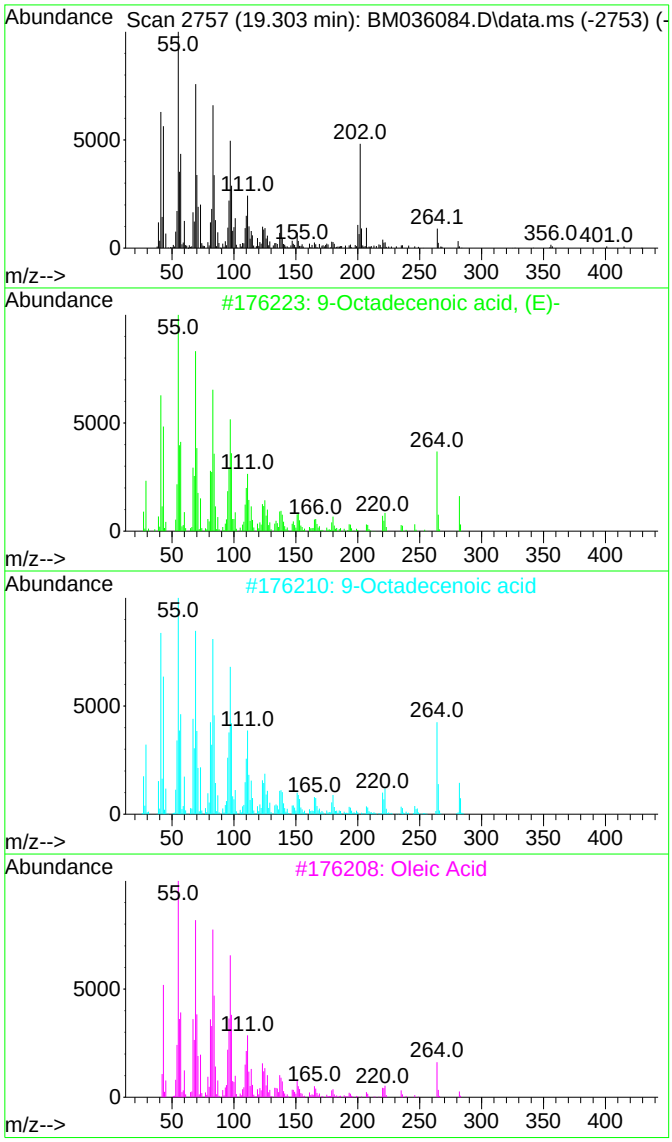
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

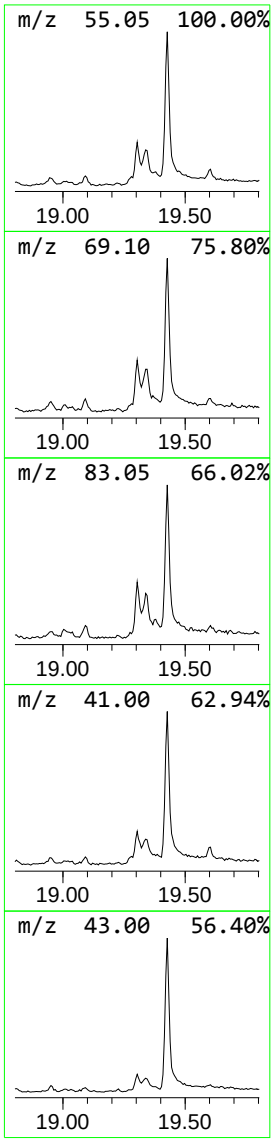
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 9-Octadecenoic acid, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.304	2.52 ng	329345	Phenanthrene-d10	17.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	97
2	9-Octadecenoic acid	282	C18H34O2	002027-47-6	87
3	Oleic Acid	282	C18H34O2	000112-80-1	74
4	1-Hexadecanol	242	C16H34O	036653-82-4	58
5	6-Octadecenoic acid	282	C18H34O2	1000336-66-8	52





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TIC Library : C:\Database\NIST20.L
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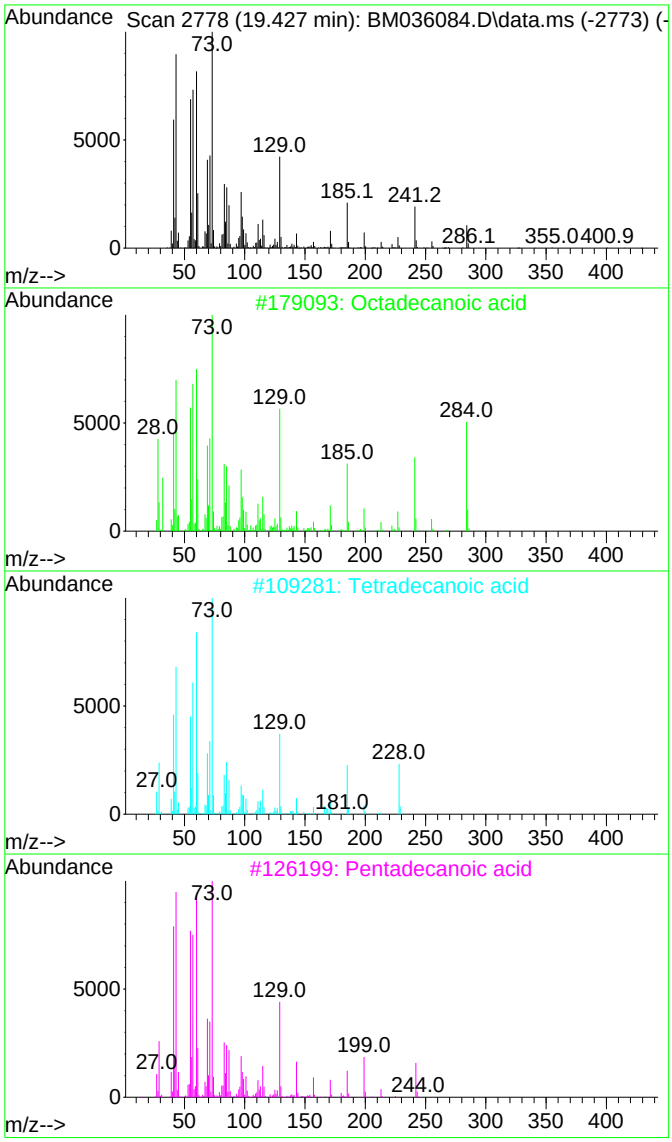
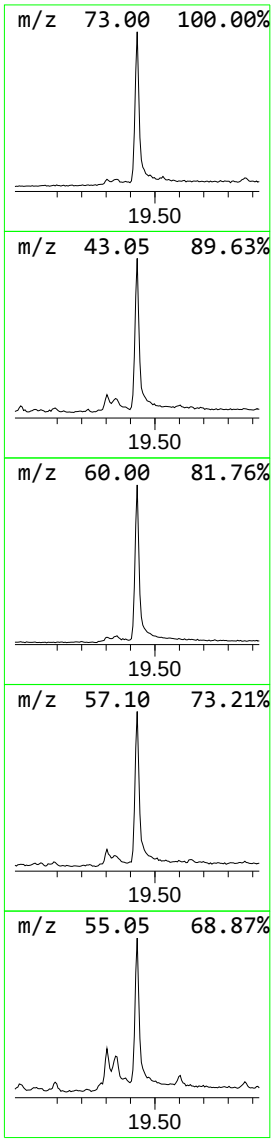
****

Peak Number 3 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.427	10.92 ng	2000520	Chrysene-d12	21.421

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	81
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	Tridecanoic acid	214	C13H26O2	000638-53-9	74





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Data File : BM036084.D
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Operator : CG/JU
Sample : N3998-10
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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TIC Library : C:\Database\NIST20.L
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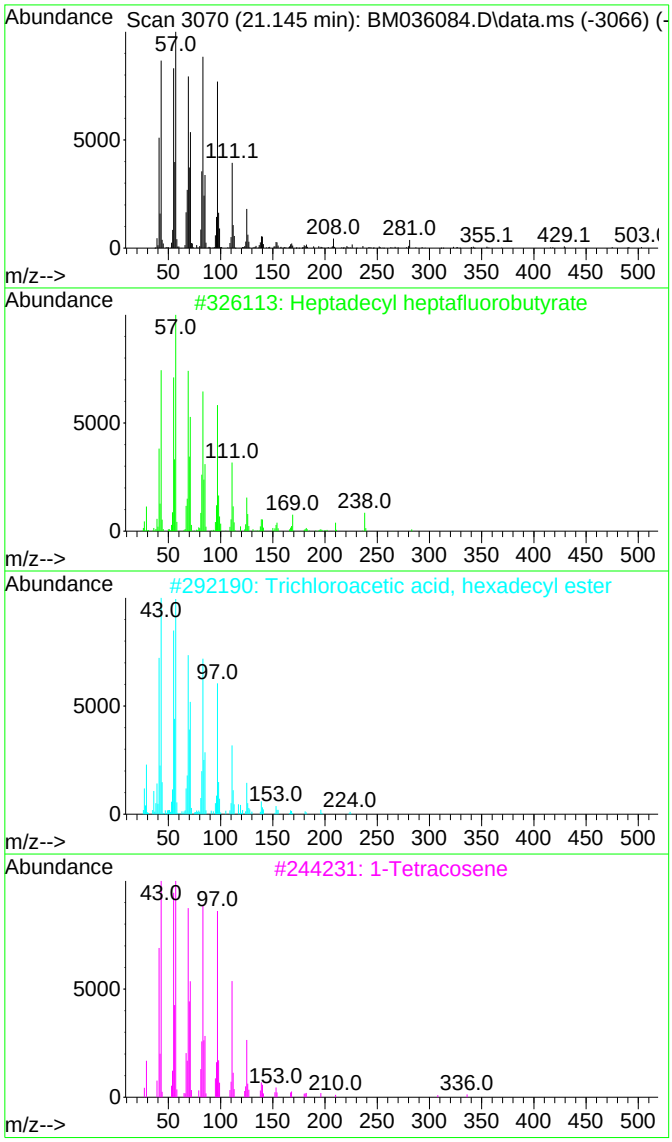
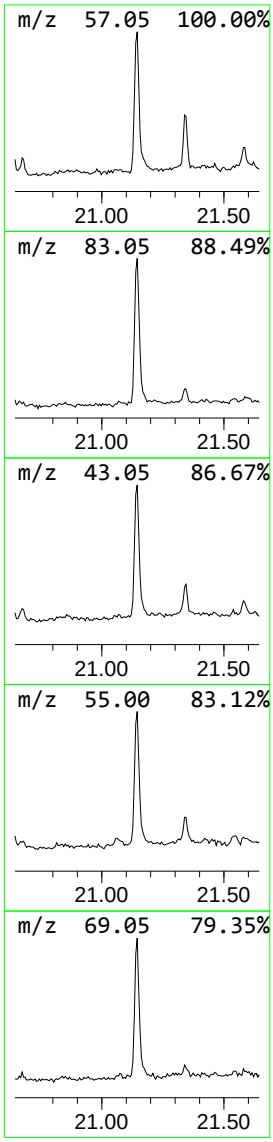
****

Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.145	3.83 ng	701219	Chrysene-d12	21.421

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Tetracosene	336	C24H48	010192-32-2	94
4	Pentacos-1-ene	350	C25H50	016980-85-1	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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BNA_M
ClientSampleId :
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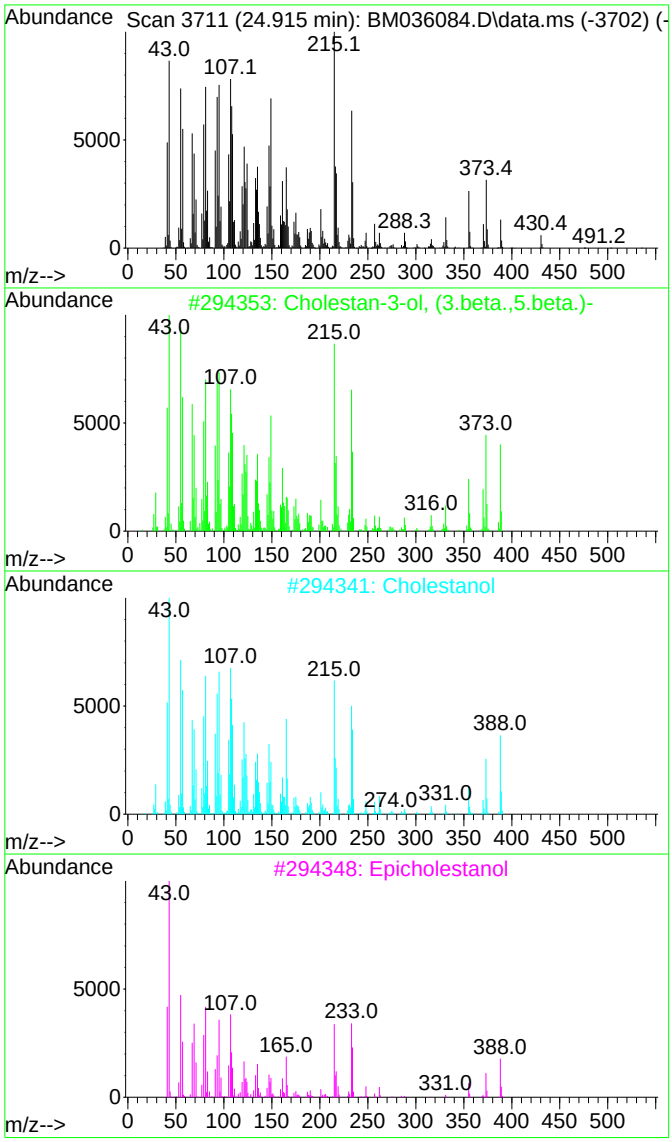
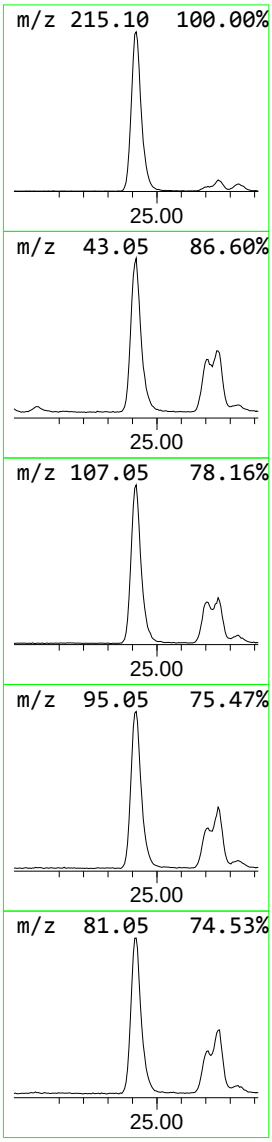
****
Peak Number 5 Cholestan-3-ol, (3.beta.,5.... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.915	83.32 ng	17916000	Perylene-d12	23.791

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	97
2	Cholestanol	388	C27H48O	000080-97-7	83
3	Epicholestanol	388	C27H48O	000516-95-0	83
4	Cholestan-3-ol	388	C27H48O	027409-41-2	53
5	Cholestan-3-ol, (3.alpha.,5.beta.)-	388	C27H48O	000516-92-7	53





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BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

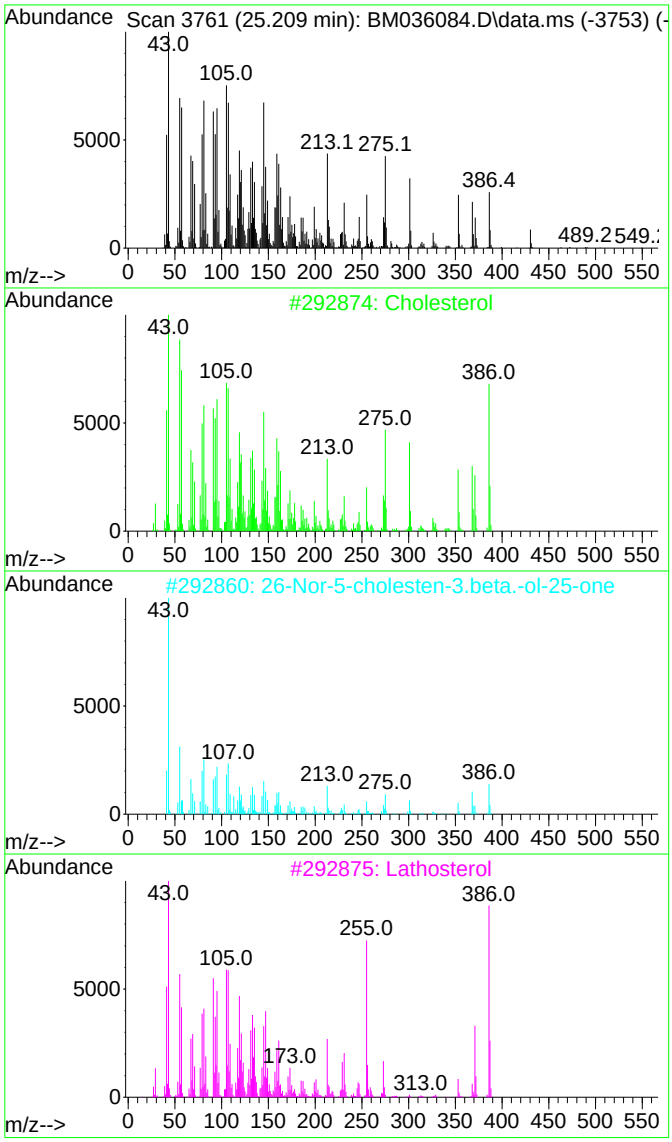
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

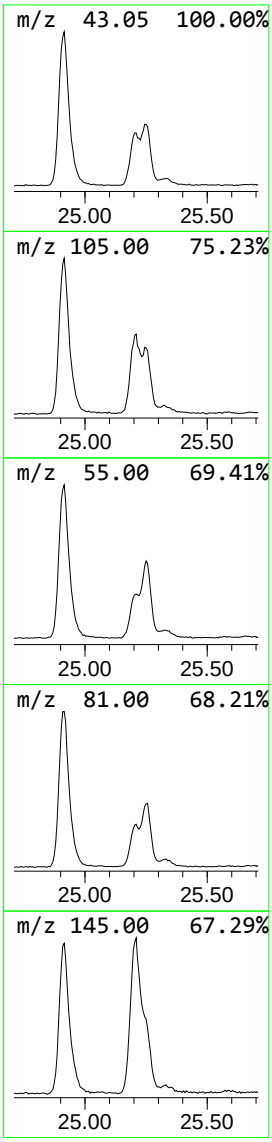
****

Peak Number 6 Cholesterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.209	19.11 ng	4108710	Perylene-d12	23.791

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	98
3	Lathosterol	386	C27H46O	000080-99-9	87
4	Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	70
5	Methyl (25RS)-3.beta.-hydroxy-5-...	430	C28H46O3	056845-86-4	53





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

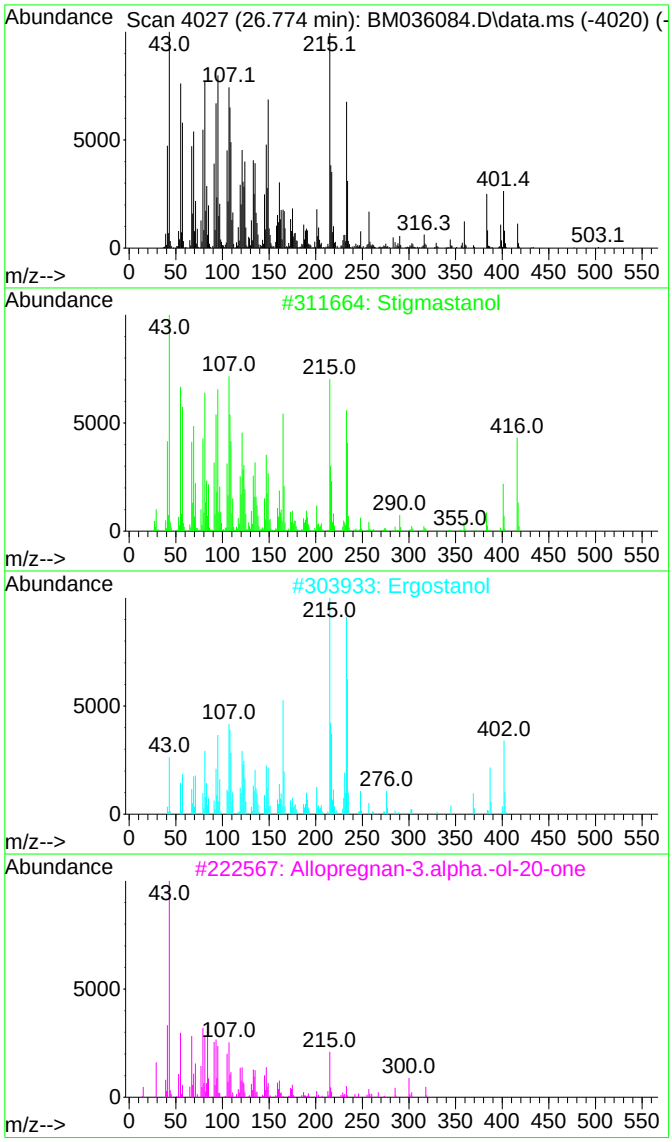
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

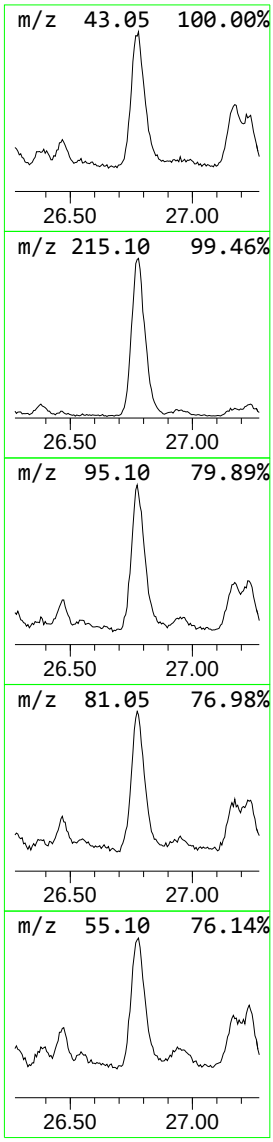
****

Peak Number 7 Stigmastanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.774	17.10 ng	3676990	Perylene-d12	23.791

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmastanol	416	C29H52O	019466-47-8	64
2	Ergostanol	402	C28H50O	006538-02-9	43
3	Allopregnan-3.alpha.-ol-20-one	318	C21H34O2	000516-54-1	27
4	5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332	C22H36O2	070434-92-3	27
5	A-Norcholestan-3-one, 5-ethenyl-...	398	C28H46O	019594-90-2	20





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080322\
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BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	18.151	41.8	ng	5469360	4	17.245	2619040	20.0
9-Octadecenoic ...	19.304	2.5	ng	329345	4	17.245	2619040	20.0
Octadecanoic acid	19.427	10.9	ng	2000520	5	21.421	3665500	20.0
Heptadecyl hept...	21.145	3.8	ng	701219	5	21.421	3665500	20.0
Cholestan-3-ol,...	24.915	83.3	ng	17916000	6	23.791	4300460	20.0
Cholesterol	25.209	19.1	ng	4108710	6	23.791	4300460	20.0
Stigmastanol	26.774	17.1	ng	3676990	6	23.791	4300460	20.0