

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041423\
 Data File : BM039431.D
 Acq On : 14 Apr 2023 13:11
 Operator : CG/JU
 Sample : PB152106BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB152106BL

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-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039431.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.946	292	299	313	rBV	2152964	3119231	26.04%	4.739%
2	5.428	374	381	403	rBV	4935108	7418208	61.92%	11.269%
3	7.051	650	657	680	rBV	4377091	7353956	61.38%	11.172%
4	7.851	786	793	803	rBV	868474	1418413	11.84%	2.155%
5	9.028	984	993	1023	rBV	2618057	4749542	39.65%	7.215%
6	10.663	1262	1271	1288	rBV	1060068	1928062	16.09%	2.929%
7	13.133	1683	1691	1709	rBV	6739850	10243607	85.51%	15.562%
8	14.510	1918	1925	1944	rBV	1624022	2446258	20.42%	3.716%
9	16.004	2173	2179	2203	rBV	4346693	7077816	59.08%	10.752%
10	17.262	2386	2393	2407	rBV	1685729	2628052	21.94%	3.992%
11	18.162	2541	2546	2564	rBV	169423	442393	3.69%	0.672%
12	19.439	2759	2763	2772	rBV	145533	321574	2.68%	0.489%
13	19.580	2783	2787	2792	rBV	170311	194177	1.62%	0.295%
14	19.892	2834	2840	2854	rBV	9110898	11980125	100.00%	18.200%
15	20.627	2962	2965	2970	rBV	157542	178647	1.49%	0.271%
16	21.450	3101	3105	3116	rBV	1553738	2279318	19.03%	3.463%
17	23.838	3505	3511	3523	rVB2	983045	2046434	17.08%	3.109%

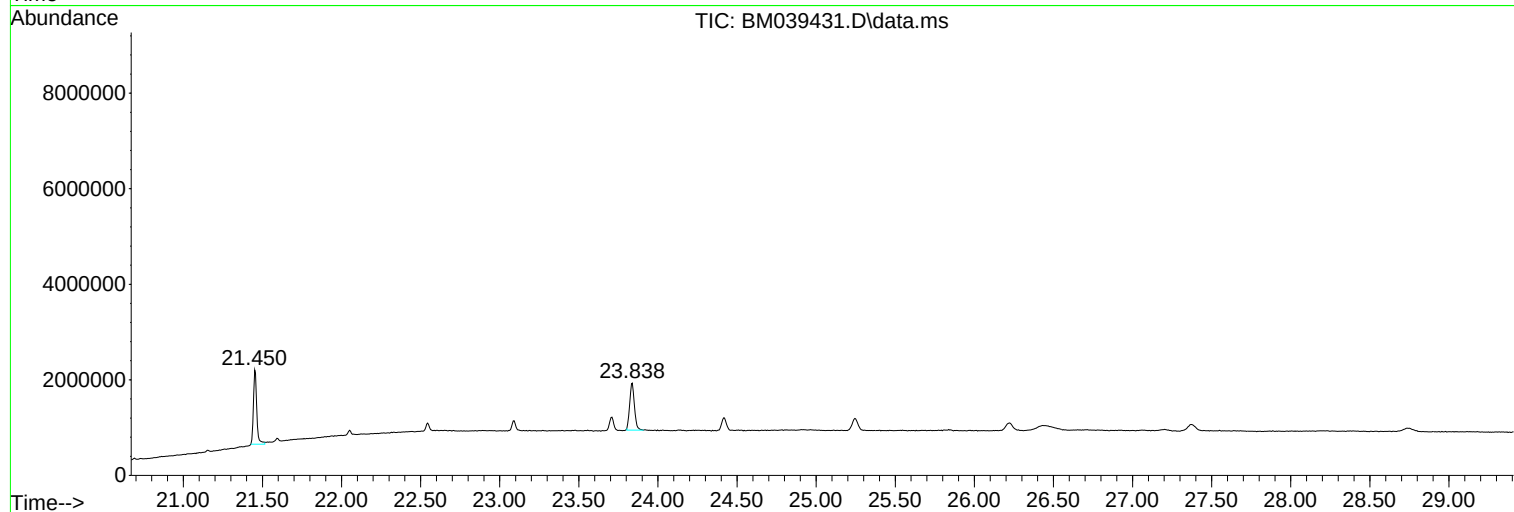
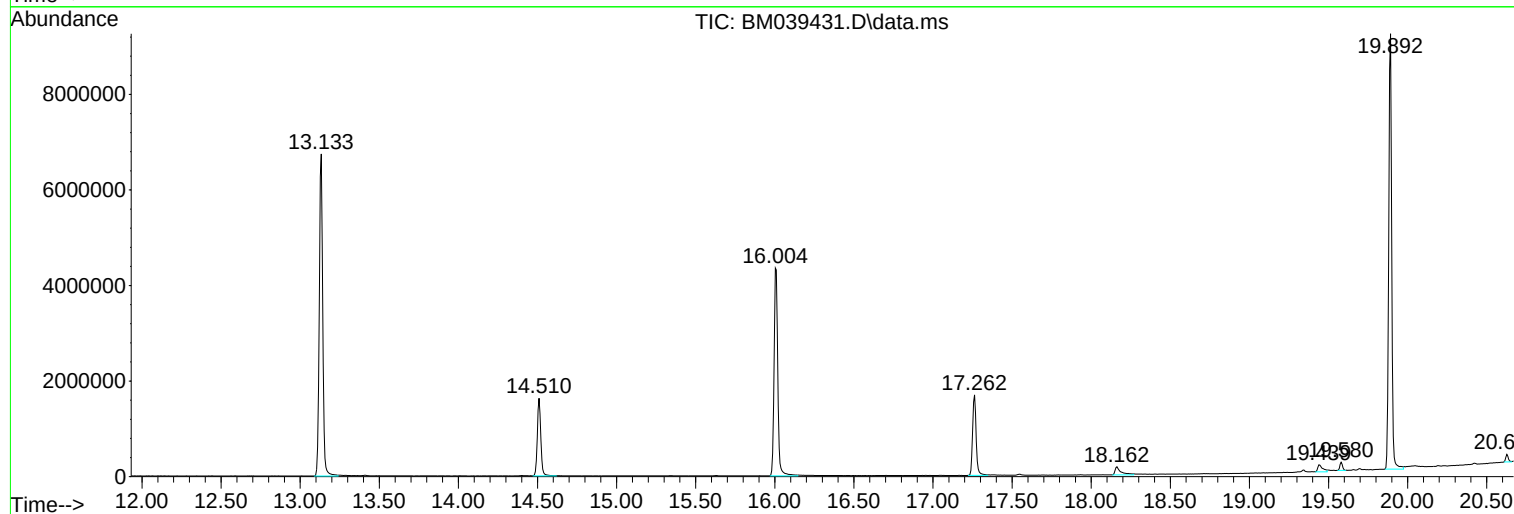
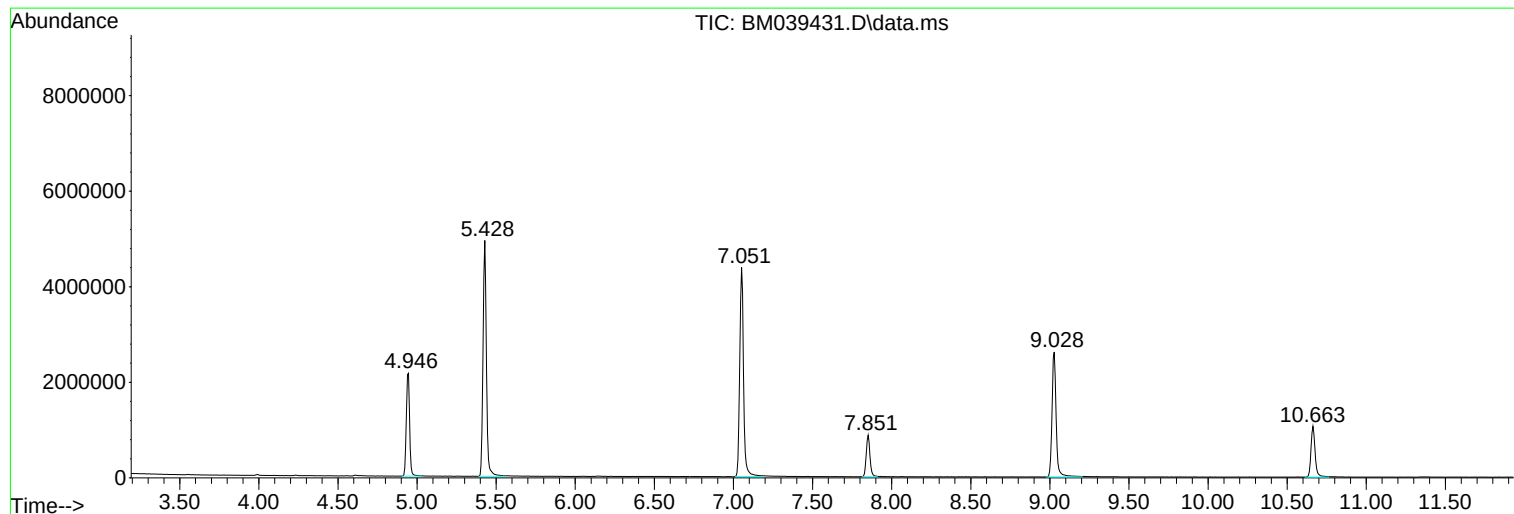
Sum of corrected areas: 65825813

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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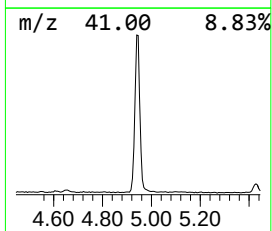
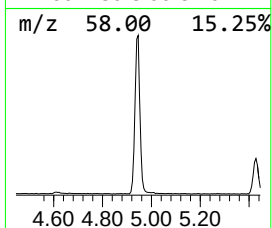
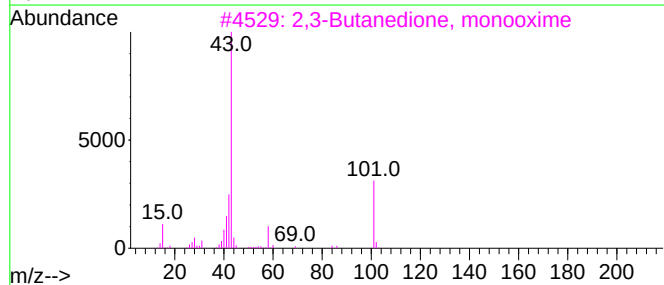
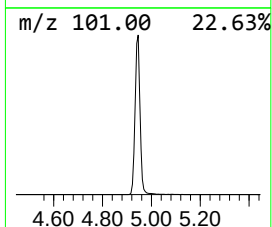
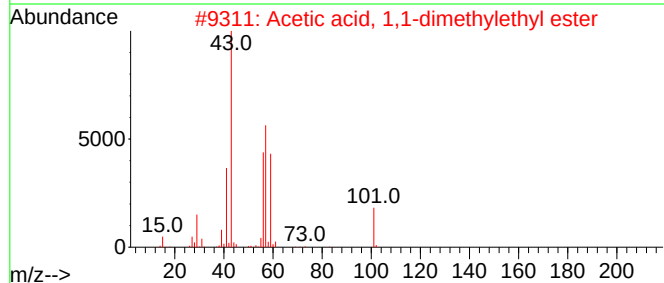
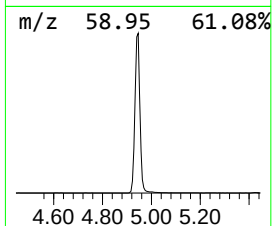
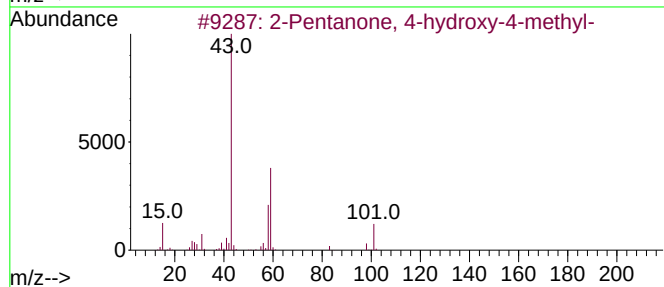
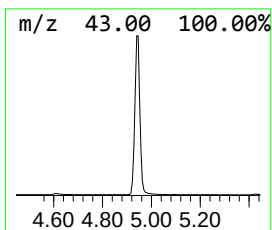
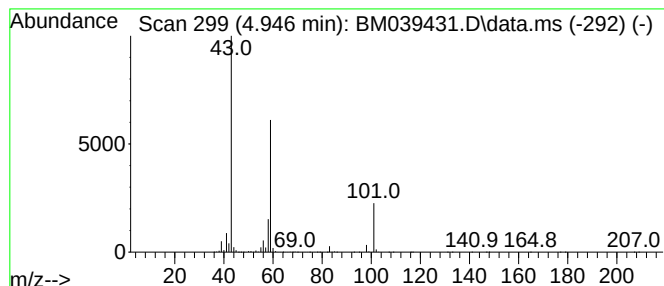
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.946	43.98 ng	3119230	1,4-Dichlorobenzene-d4	7.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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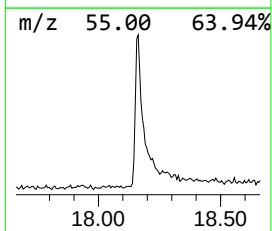
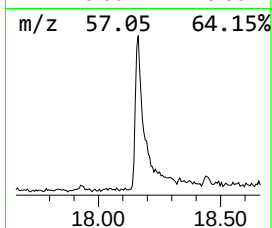
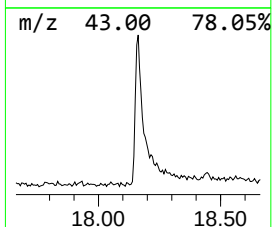
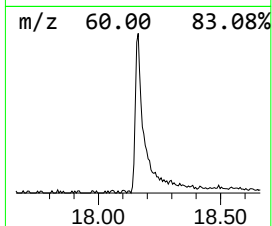
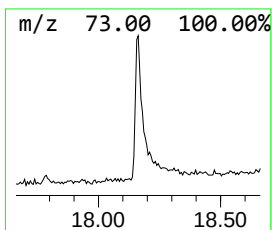
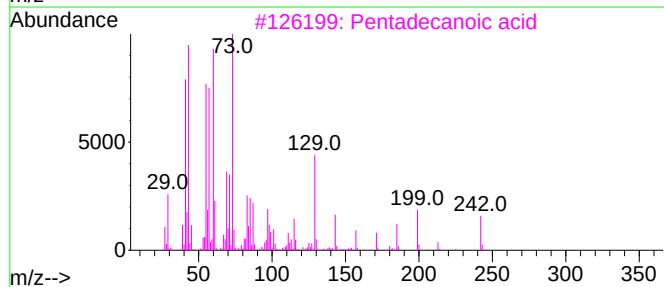
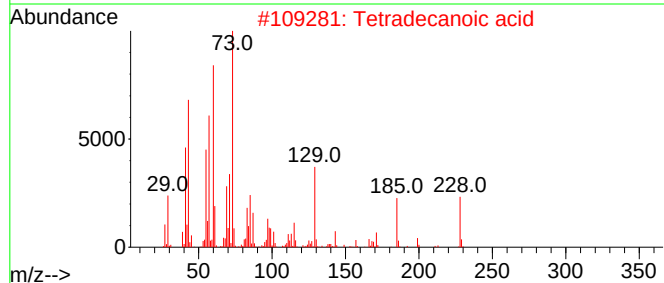
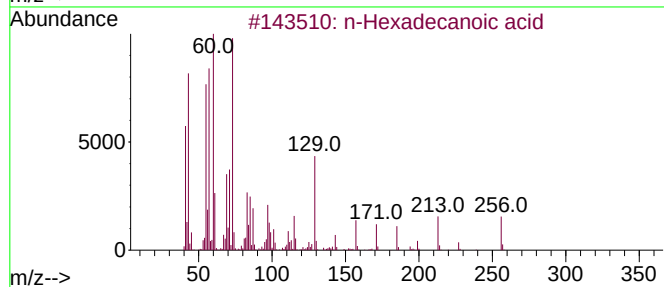
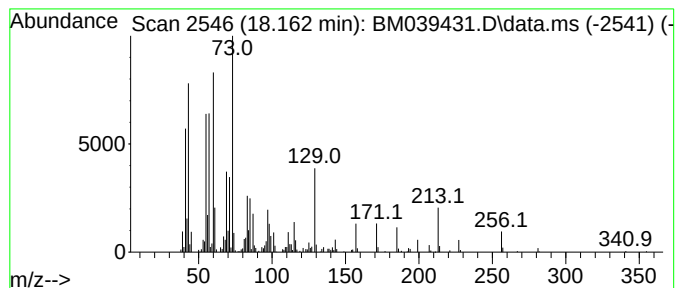
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.162	3.37 ng	442393	Phenanthrene-d10	17.262	
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	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Octadecanoic acid	284	C18H36O2	000057-11-4	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76



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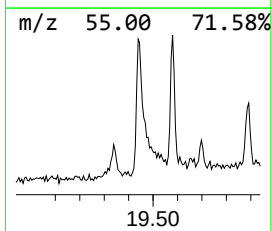
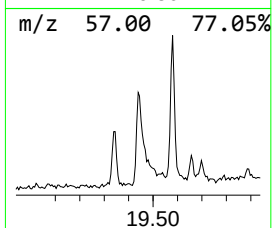
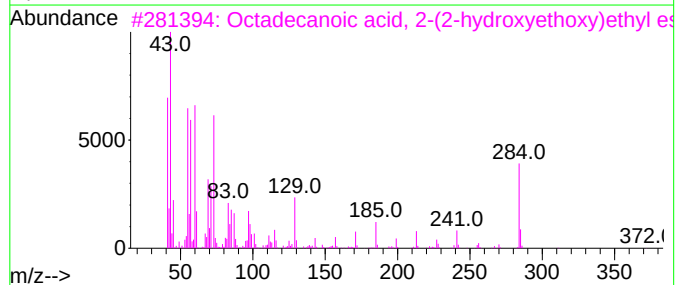
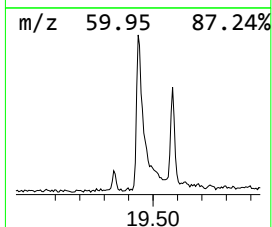
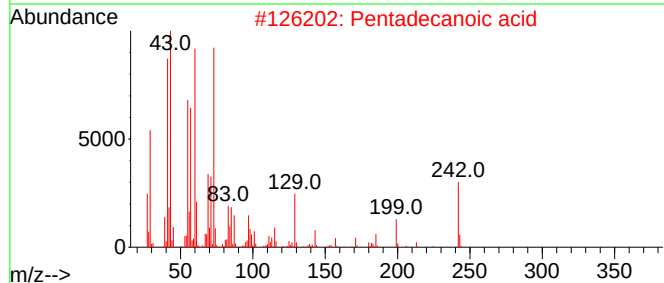
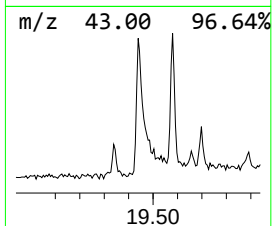
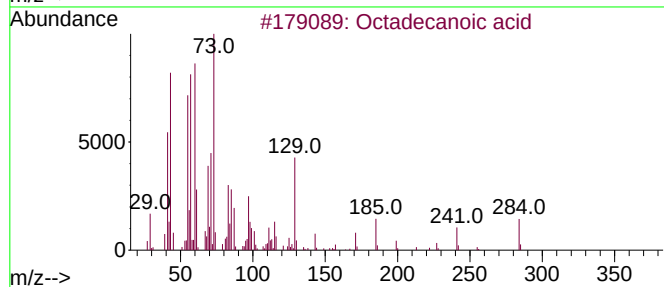
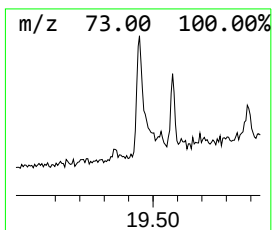
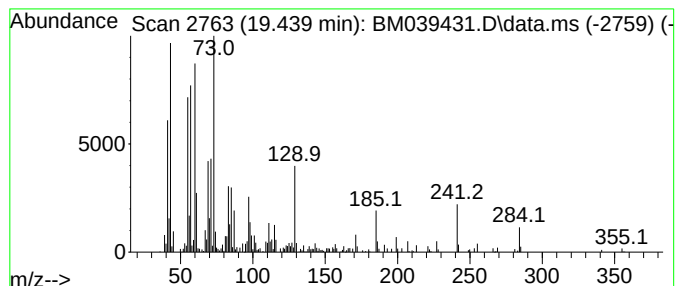
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	2.82 ng	321574	Chrysene-d12	21.450

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.946	44.0	ng	3119230	1	7.851	1418410	20.0
n-Hexadecanoic ...	18.162	3.4	ng	442393	4	17.262	2628050	20.0
Octadecanoic acid	19.439	2.8	ng	321574	5	21.450	2279320	20.0