

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102323\
 Data File : BM042409.D
 Acq On : 23 Oct 2023 19:22
 Operator : MA/JU
 Sample : PB156324BL
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB156324BL

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: BM042409.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.446	209	214	220	rBV	143271	184882	2.66%	0.476%
2	5.075	315	321	332	rVB	1289824	1714226	24.69%	4.410%
3	5.522	390	397	410	rBV	3588869	5099848	73.46%	13.120%
4	7.145	666	673	688	rBV	3373001	5220990	75.20%	13.432%
5	7.992	811	817	827	rVB	529405	847453	12.21%	2.180%
6	9.192	1012	1021	1036	rBV	1955245	3172926	45.70%	8.163%
7	10.816	1289	1297	1305	rBV	667878	1094318	15.76%	2.815%
8	13.263	1705	1713	1724	rBV	3923747	5598385	80.64%	14.403%
9	14.639	1941	1947	1956	rBV	817792	1176708	16.95%	3.027%
10	16.133	2194	2201	2213	rVB	2619865	3521117	50.72%	9.059%
11	17.392	2408	2415	2425	rBV	891049	1249706	18.00%	3.215%
12	18.233	2552	2558	2572	rBV	94528	183532	2.64%	0.472%
13	19.515	2771	2776	2786	rBV2	63822	113031	1.63%	0.291%
14	20.003	2854	2859	2868	rBV	6097046	6942440	100.00%	17.861%
15	21.574	3121	3126	3133	rBV	1002738	1274375	18.36%	3.279%
16	24.044	3539	3546	3559	rVB	717045	1476050	21.26%	3.797%

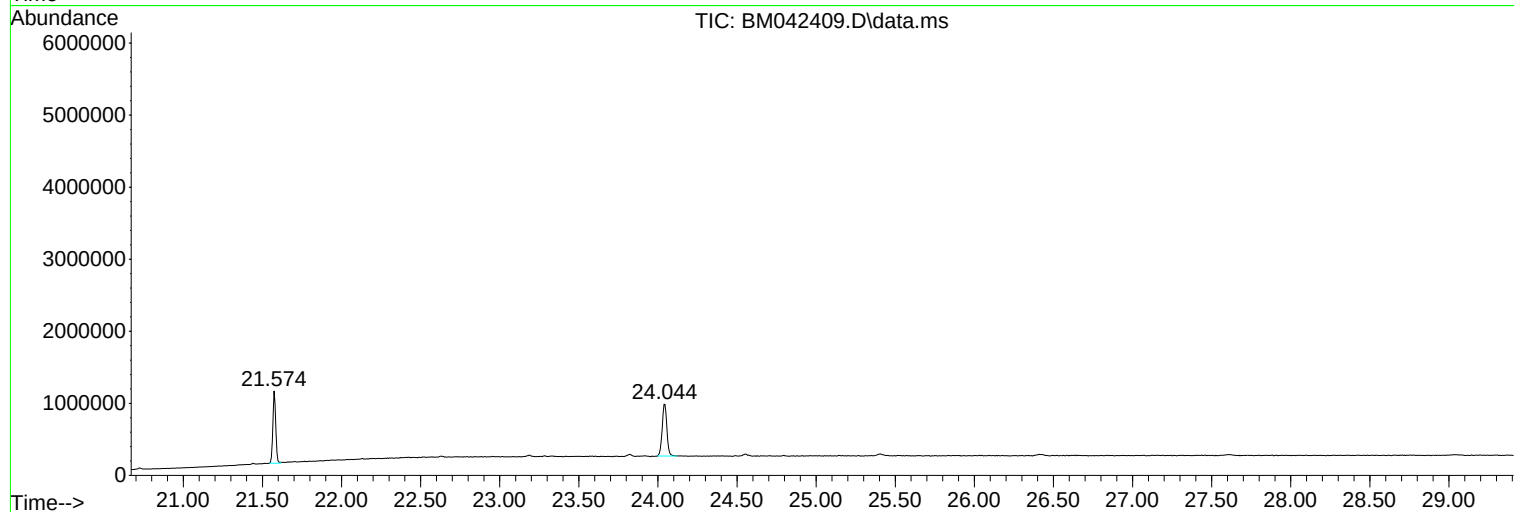
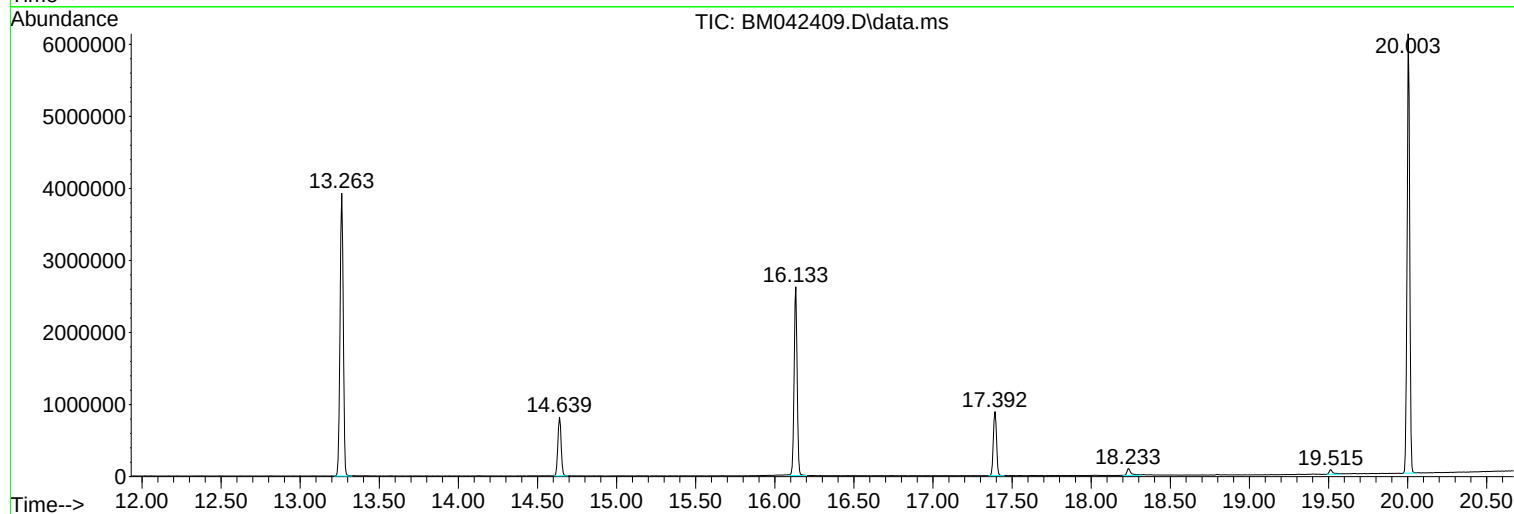
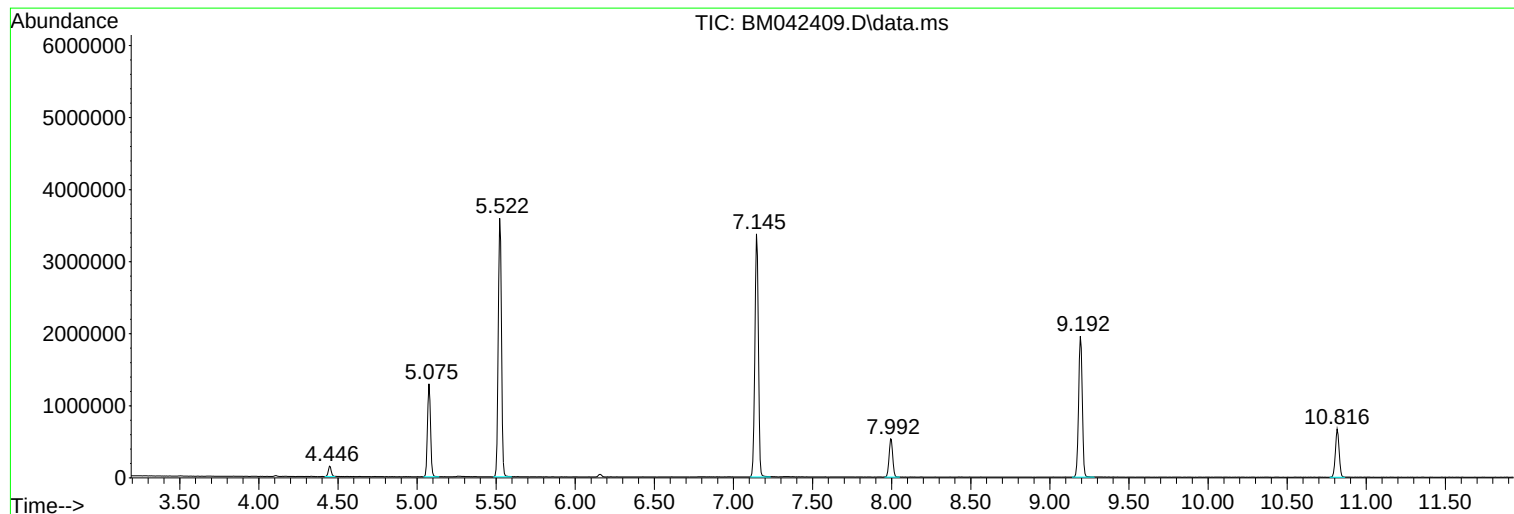
Sum of corrected areas: 38869987

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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



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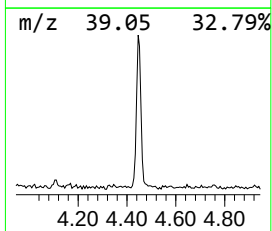
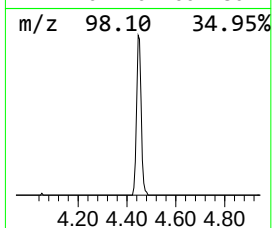
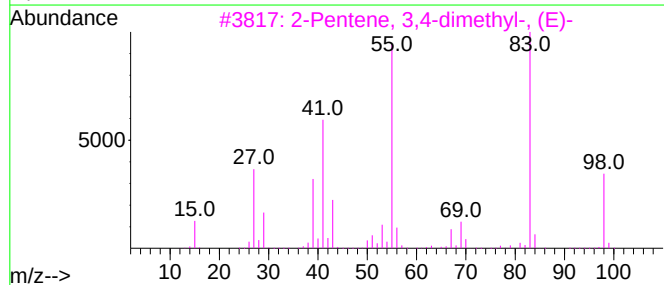
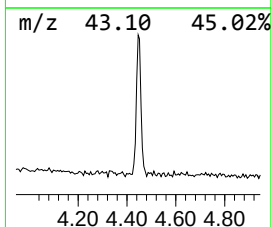
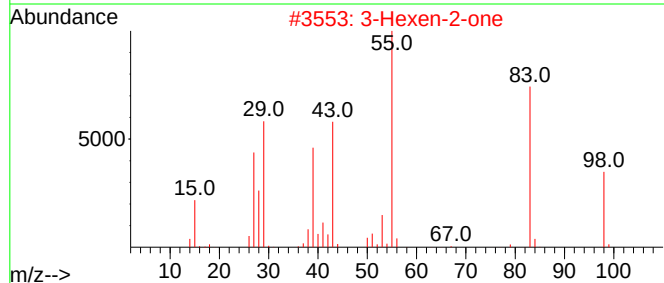
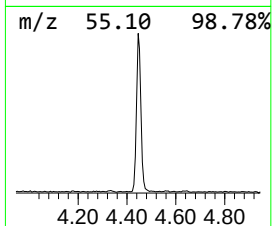
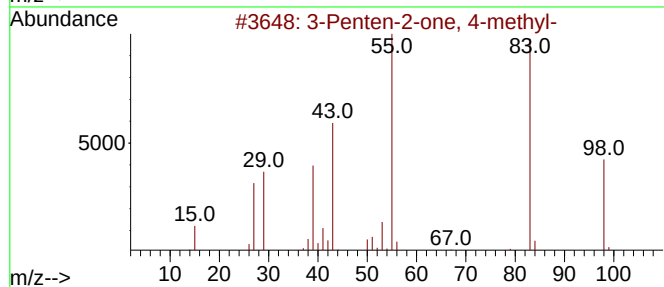
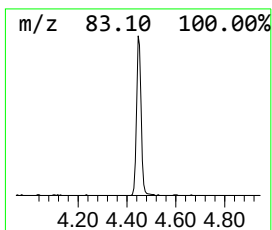
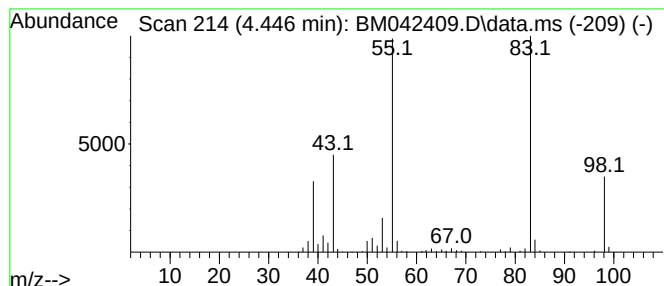
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.446	4.36 ng	184882	1,4-Dichlorobenzene-d4	7.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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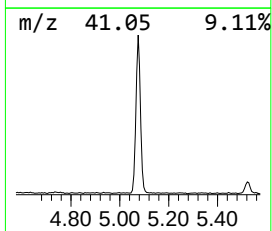
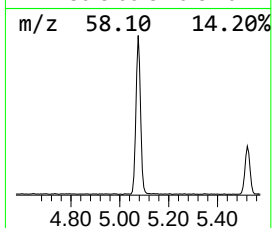
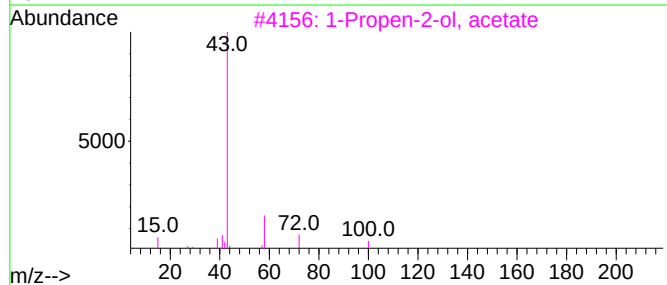
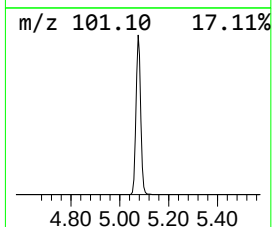
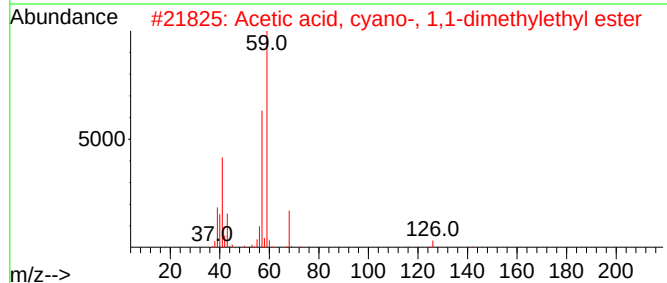
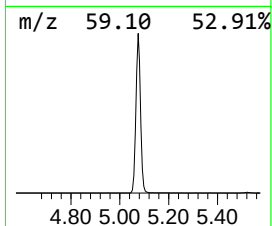
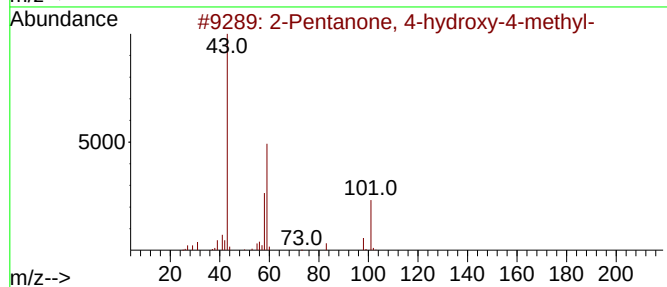
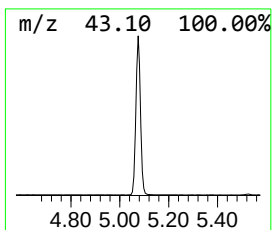
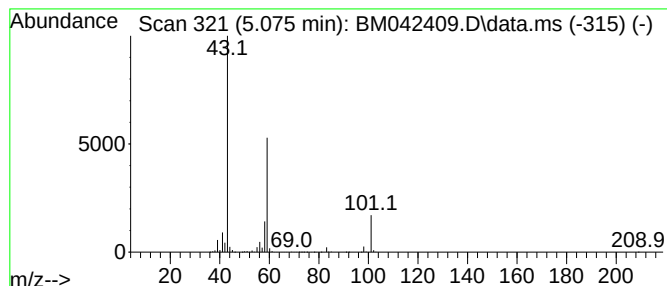
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	40.46 ng	1714230	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	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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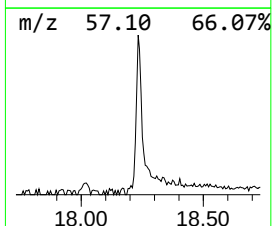
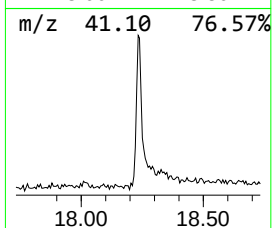
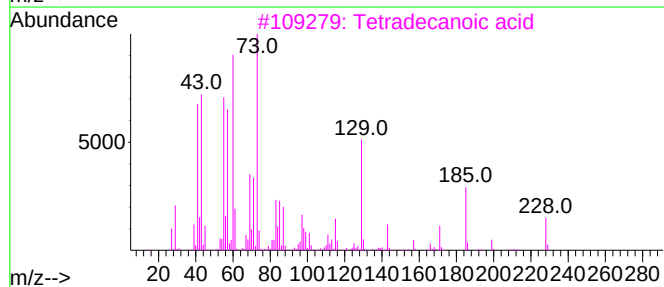
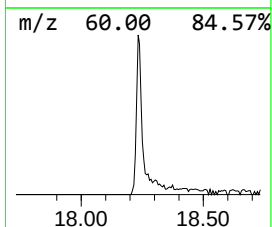
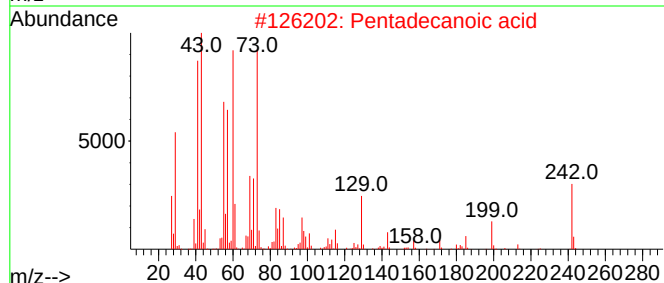
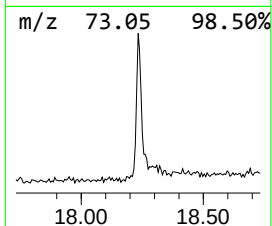
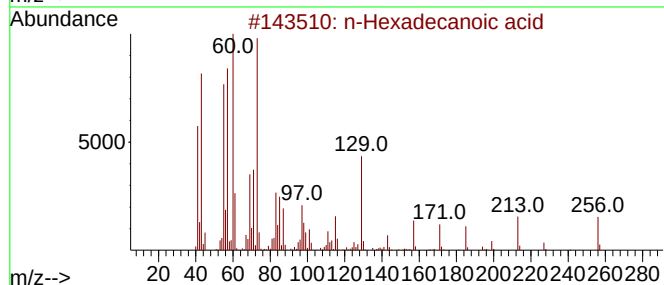
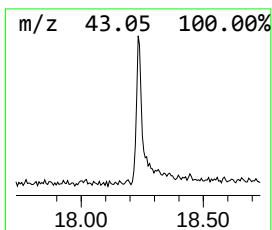
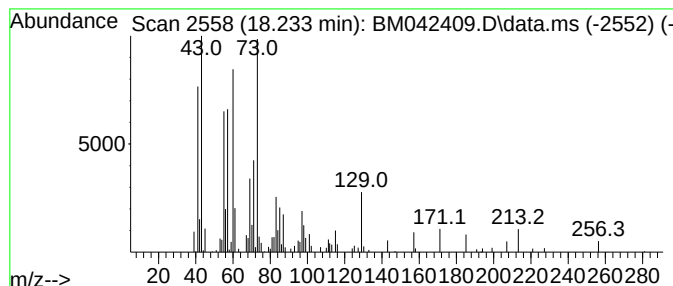
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.233	2.94 ng	183532	Phenanthrene-d10	17.392

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20
5			Oxalic acid, allyl pentadecyl ester	340	C20H36O4	1000309-24-3	18



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.446	4.4	ng	184882	1	7.998	847453	20.0
2-Pentanone, 4-...	5.075	40.5	ng	1714230	1	7.998	847453	20.0
n-Hexadecanoic ...	18.233	2.9	ng	183532	4	17.392	1249710	20.0