

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM092023\
 Data File : BM041942.D
 Acq On : 20 Sep 2023 17:25
 Operator : MA/JU
 Sample : 04436-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 B103-05

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-BM091823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041942.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.058	313	318	326	rVB	157949	216907	1.74%	0.334%
2	5.499	385	393	403	rBV	4046698	5772384	46.37%	8.887%
3	7.105	658	666	679	rBV	4081787	6523797	52.41%	10.044%
4	7.958	803	811	821	rBV	1087172	1739370	13.97%	2.678%
5	9.152	1002	1014	1026	rBV	2493080	4066894	32.67%	6.262%
6	10.775	1281	1290	1298	rBV	1506305	2479336	19.92%	3.817%
7	13.222	1699	1706	1713	rBV	5916388	8707398	69.95%	13.406%
8	14.604	1932	1941	1950	rBV	2295070	3374280	27.11%	5.195%
9	16.098	2188	2195	2209	rBV	5280173	7466746	59.98%	11.496%
10	17.357	2403	2409	2422	rBV	2858854	3997169	32.11%	6.154%
11	18.198	2547	2552	2562	rBV	270313	415159	3.33%	0.639%
12	19.968	2847	2853	2862	rBV	10203959	12448598	100.00%	19.166%
13	20.633	2962	2966	2973	rBV	130897	186558	1.50%	0.287%
14	21.192	3057	3061	3071	rBV	419930	649274	5.22%	1.000%
15	21.527	3113	3118	3124	rBV	2903984	3750768	30.13%	5.775%
16	23.945	3522	3529	3542	rVB	1570606	3155719	25.35%	4.859%

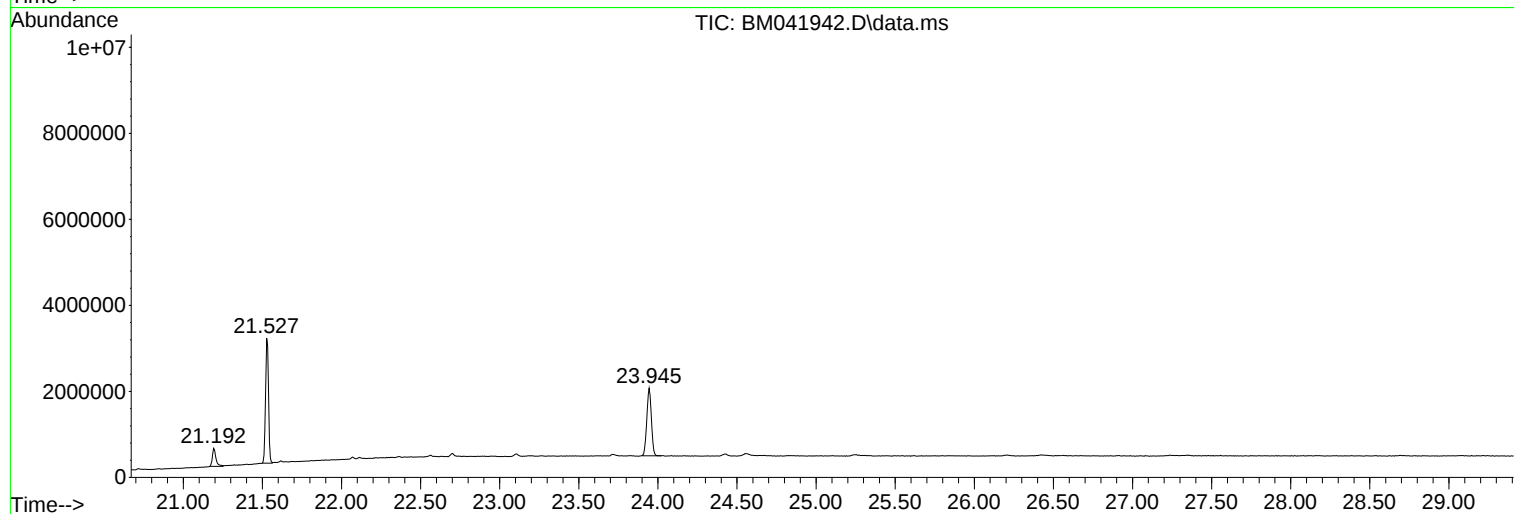
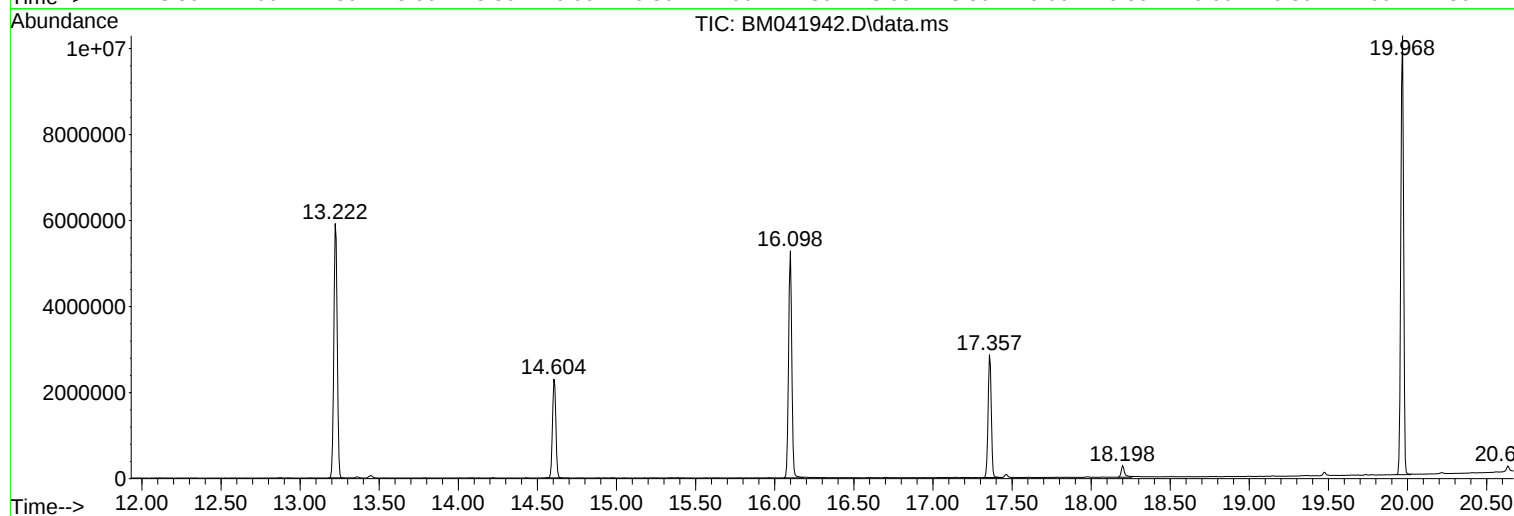
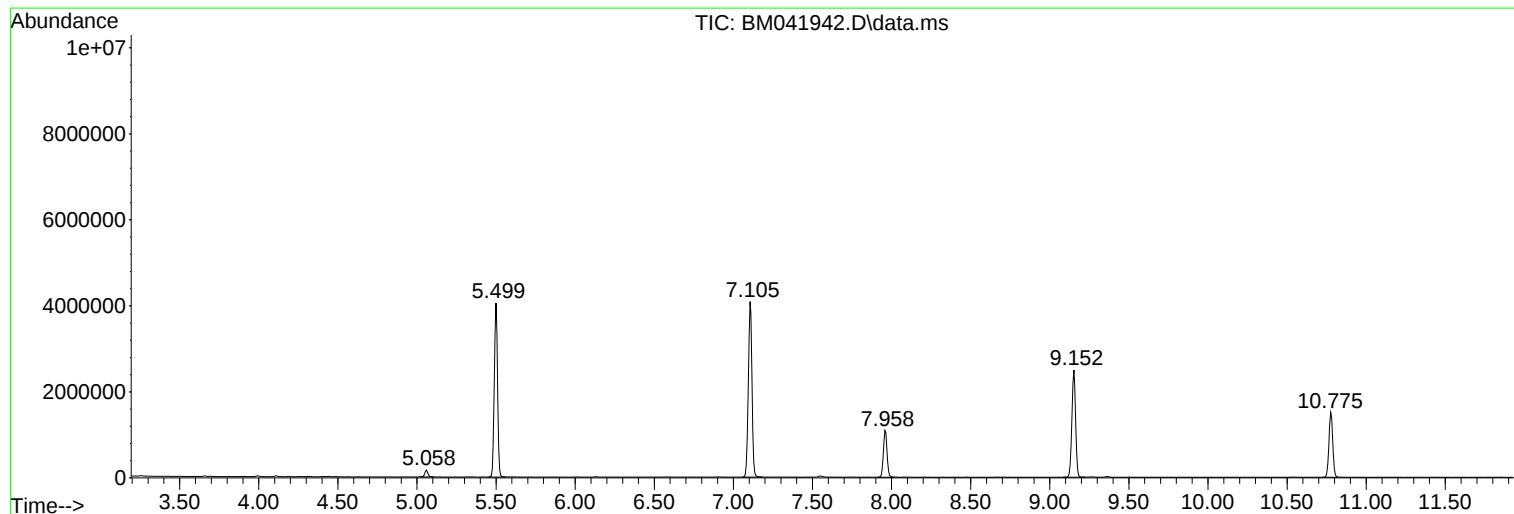
Sum of corrected areas: 64950357

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091823.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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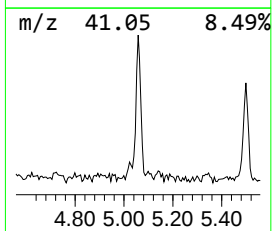
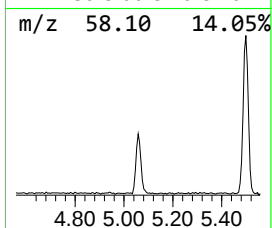
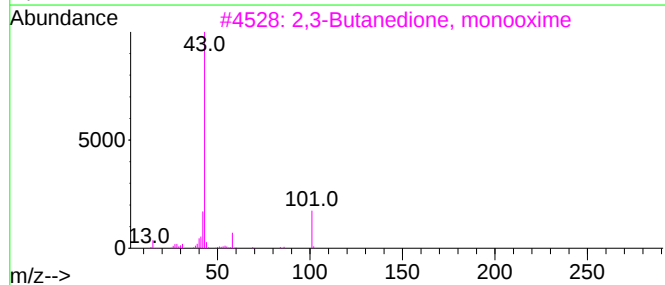
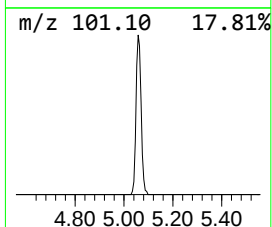
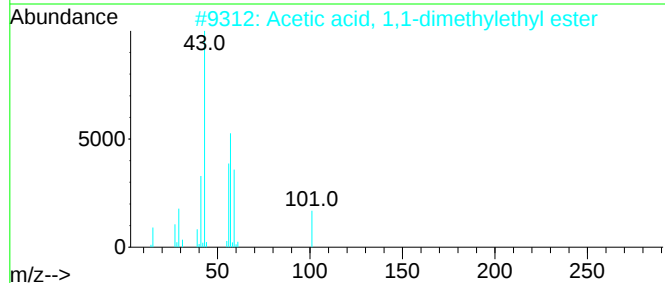
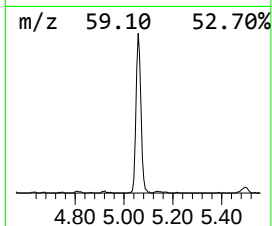
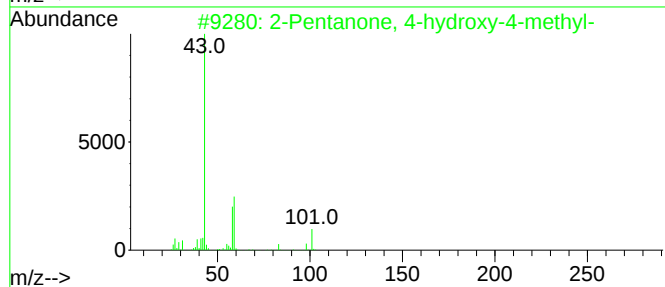
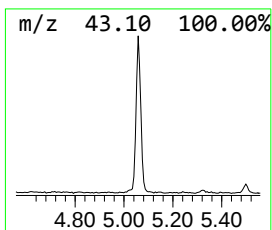
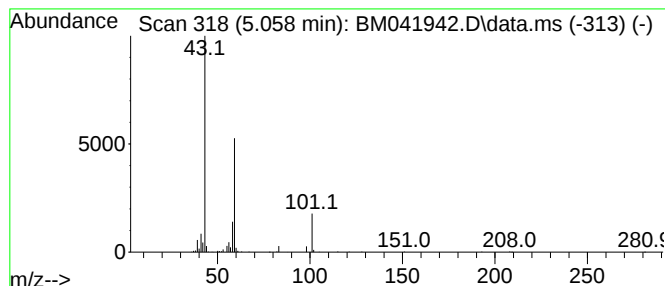
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM091823.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.058	2.49 ng	216907	1,4-Dichlorobenzene-d4	7.957

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	25
5		Hexanamide	115	C6H13NO	000628-02-4	25



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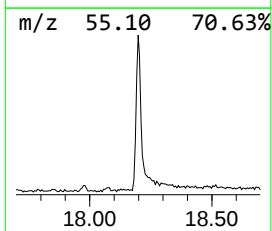
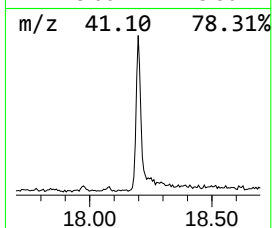
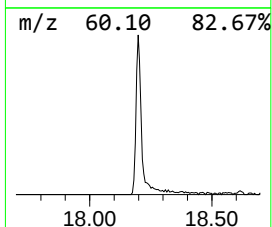
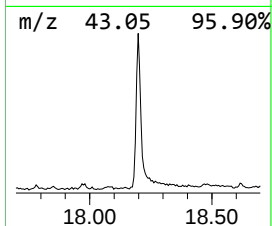
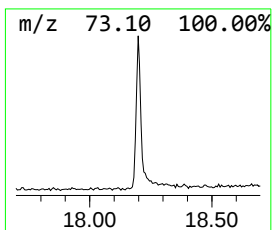
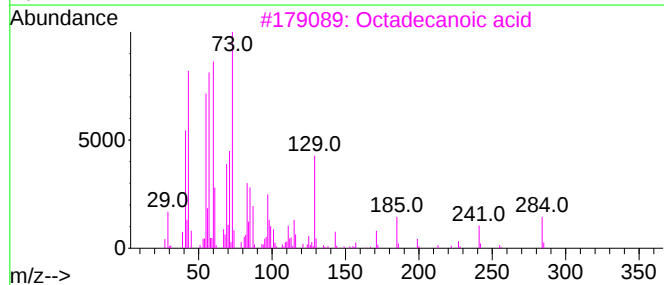
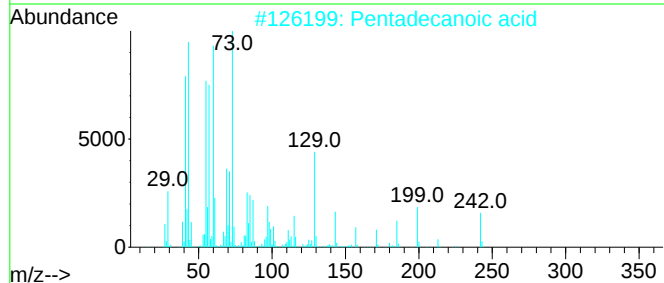
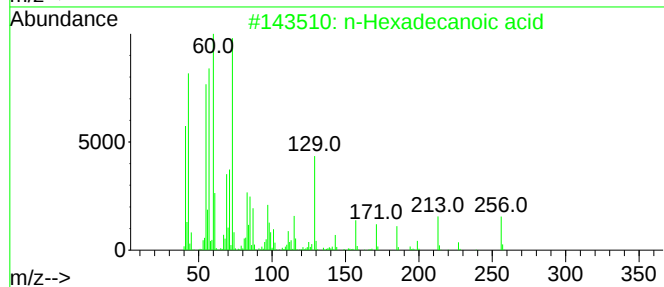
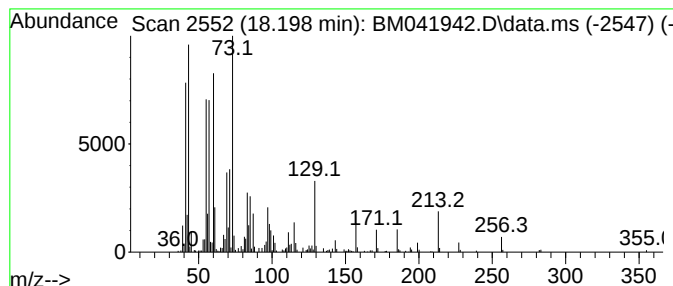
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.198	2.08 ng	415159	Phenanthrene-d10	17.357

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	90
3		Octadecanoic acid	284	C18H36O2	000057-11-4	90
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5		Tridecanoic acid	214	C13H26O2	000638-53-9	87



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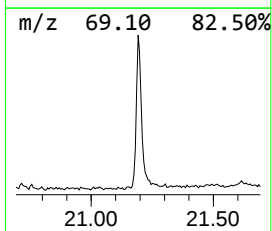
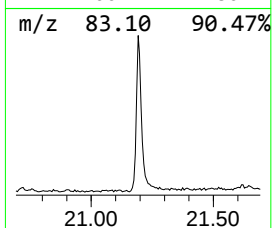
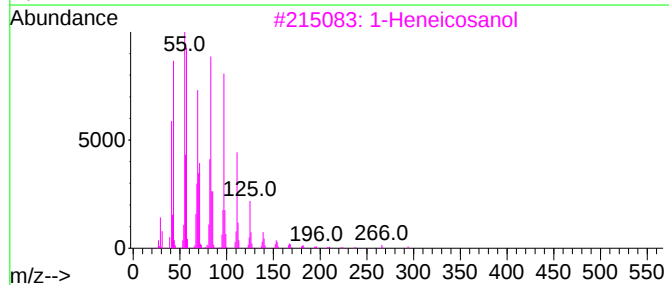
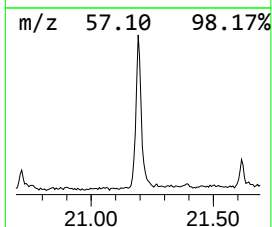
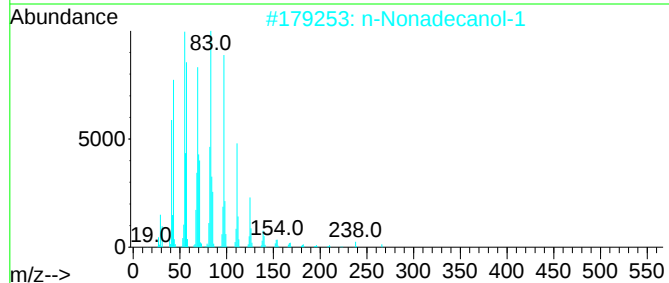
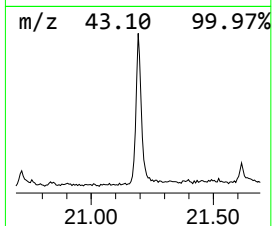
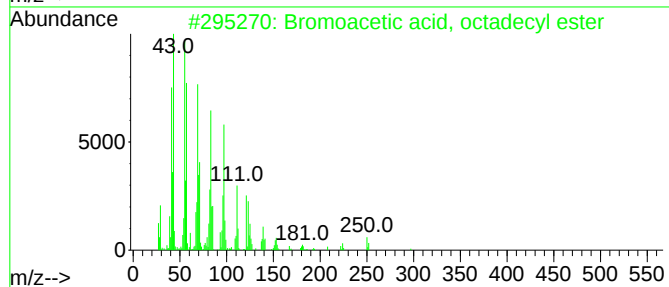
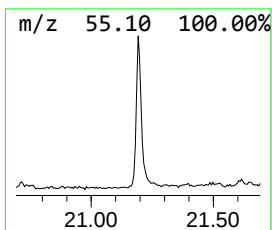
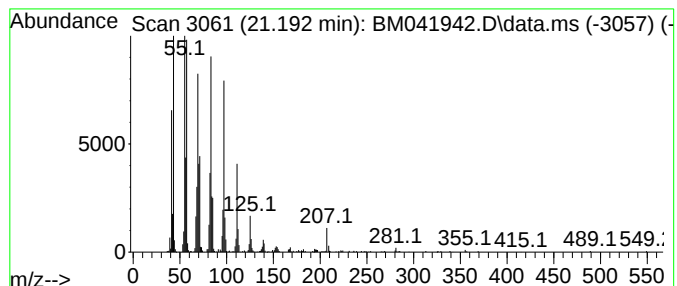
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Peak Number 3 Bromoacetic acid, octadecyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.192	3.46 ng	649274	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	94
4			n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5			3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.058	2.5	ng	216907	1	7.957	1739370	20.0
n-Hexadecanoic ...	18.198	2.1	ng	415159	4	17.357	3997170	20.0
Bromoacetic aci...	21.192	3.5	ng	649274	5	21.527	3750770	20.0