

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111221\
 Data File : BF126155.D
 Acq On : 12 Nov 2021 14:16
 Operator : JU/CG
 Sample : M4572-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3

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_F\METHODS\8270-BF110321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.039	498	502	507	rBV	478286	506395	7.43%	1.731%
2	5.451	568	572	576	rBV	1866643	1743815	25.60%	5.959%
3	6.463	740	744	755	rVB	1408370	1187769	17.43%	4.059%
4	6.839	805	808	812	rBV	953798	757211	11.11%	2.588%
5	6.904	816	819	829	rBV	100884	162592	2.39%	0.556%
6	7.404	899	904	907	rBV	3160637	2996937	43.99%	10.242%
7	8.122	1023	1026	1030	rBV	1077186	964455	14.16%	3.296%
8	9.204	1205	1210	1213	rBV	7238658	5734381	84.17%	19.597%
9	9.880	1321	1325	1328	rBV	1413386	1194482	17.53%	4.082%
10	10.668	1454	1459	1462	rBV	4045268	3400346	49.91%	11.621%
11	11.363	1574	1577	1581	rVB	1587874	1285793	18.87%	4.394%
12	11.904	1664	1669	1676	rBV	617885	650571	9.55%	2.223%
13	12.957	1843	1848	1851	rBV	7916890	6812862	100.00%	23.283%
14	14.004	2021	2026	2030	rBV	1290863	1153374	16.93%	3.942%
15	15.468	2270	2275	2280	rBV	586740	710160	10.42%	2.427%

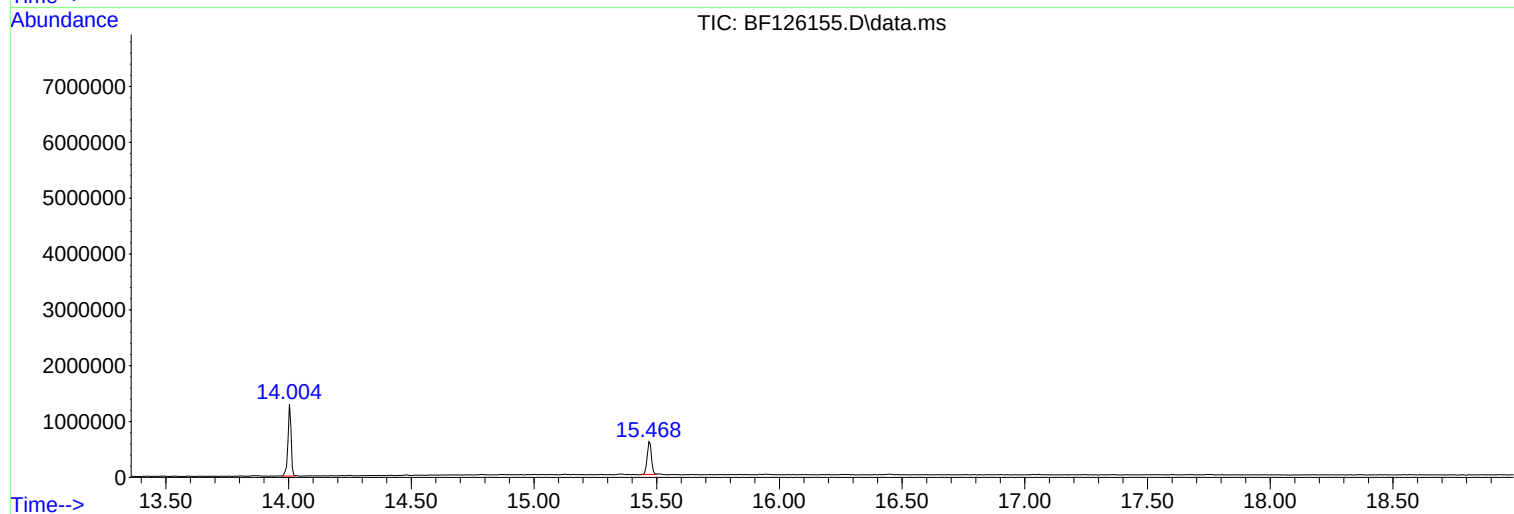
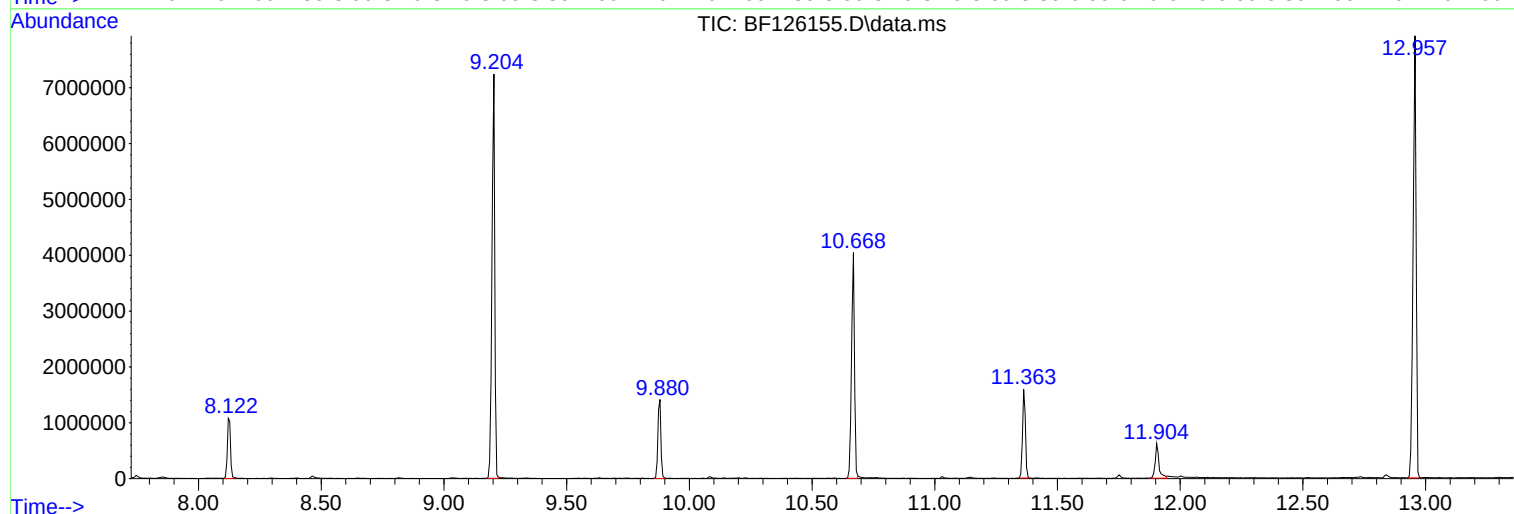
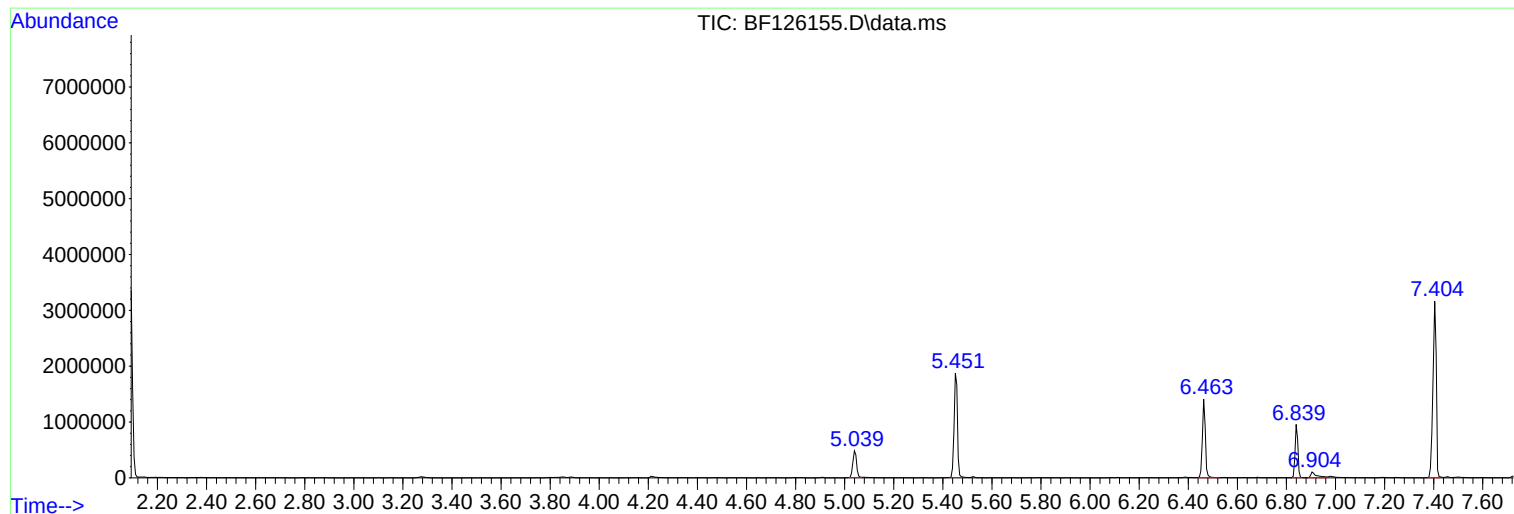
Sum of corrected areas: 29261143

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF110321.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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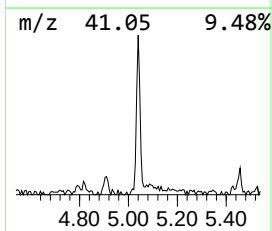
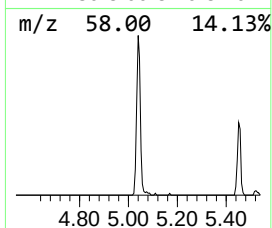
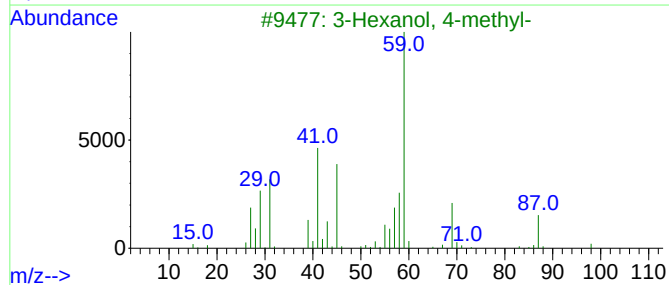
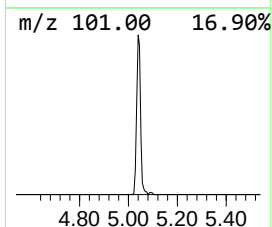
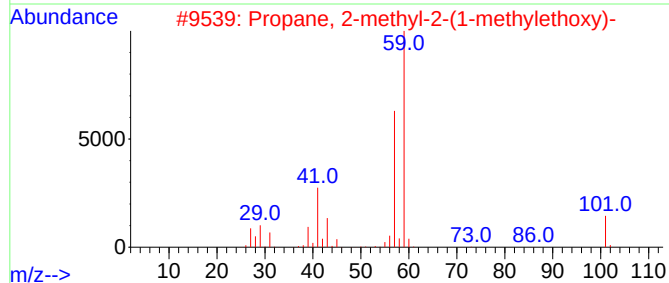
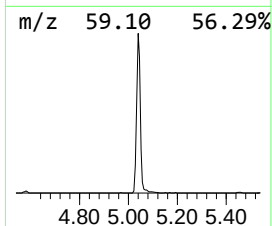
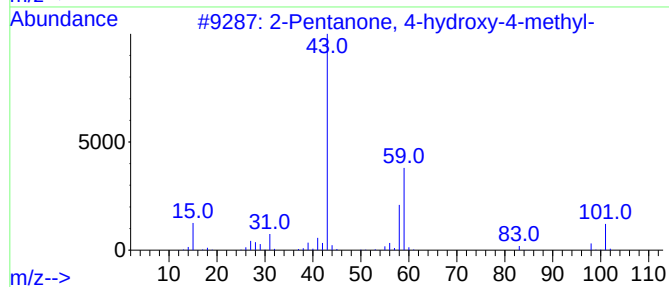
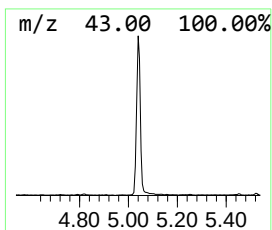
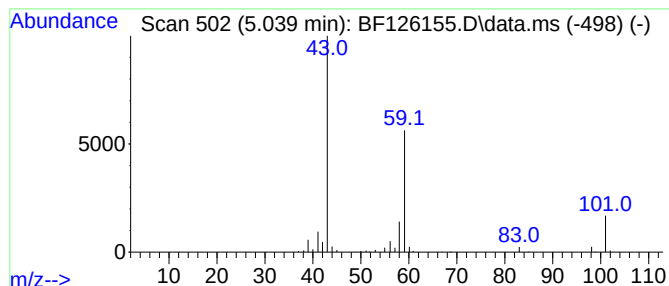
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TIC Library : C:\Database\NIST20.L
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.039	13.38 ng	506395	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



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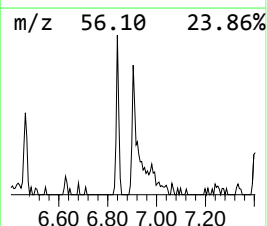
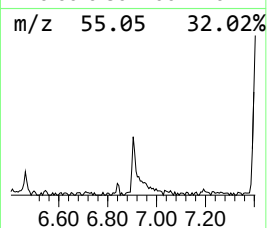
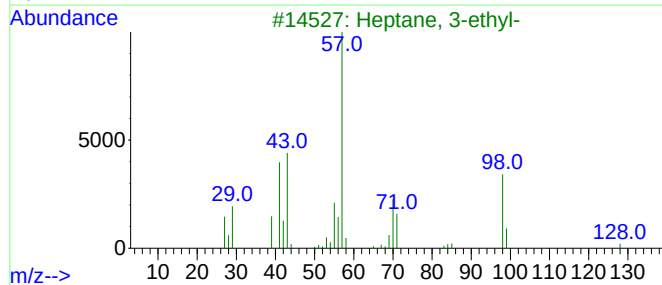
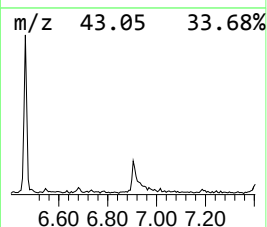
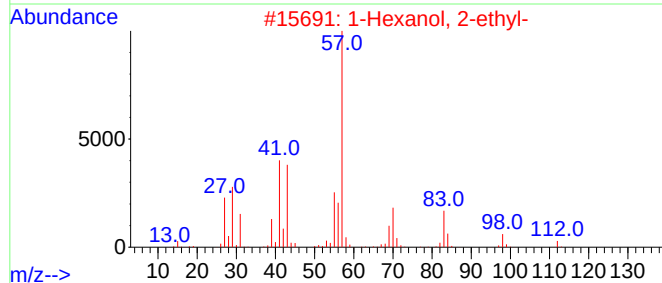
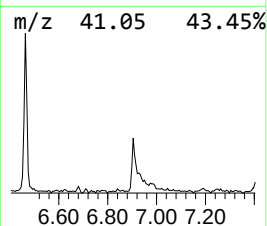
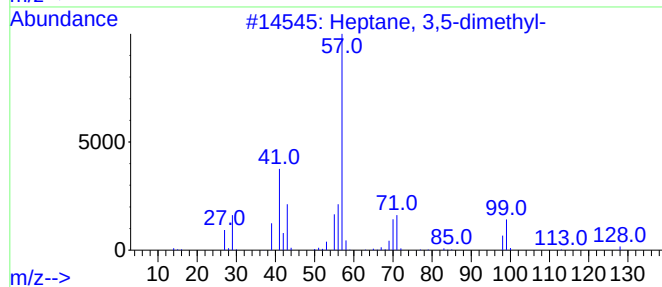
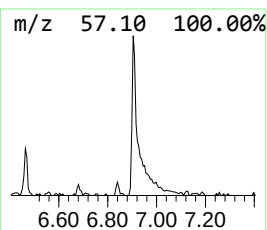
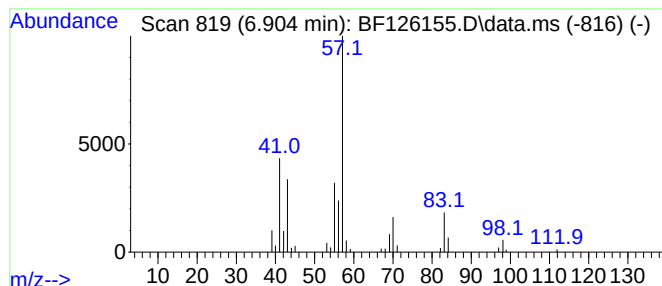
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Peak Number 2 Heptane, 3,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.904	4.29 ng	162592	1,4-Dichlorobenzene-d4	6.839

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	53
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
3			Heptane, 3-ethyl-	128	C9H20	015869-80-4	50
4			2-Propyl-1-Pentanol, trifluoroac...	226	C10H17F3O2	1000365-19-7	50
5			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50



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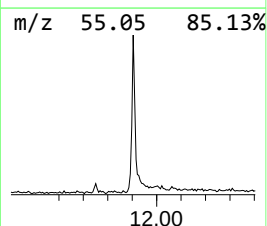
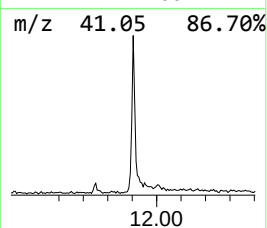
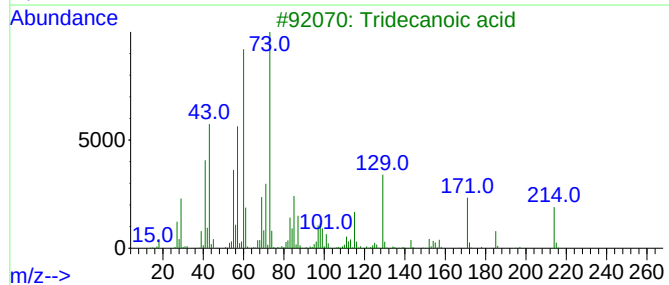
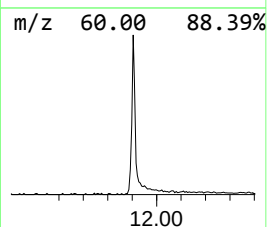
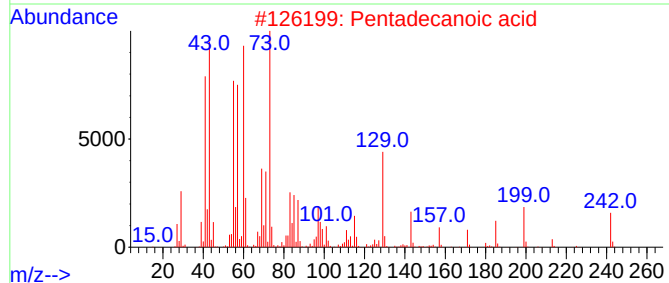
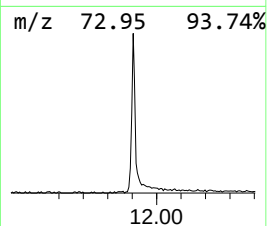
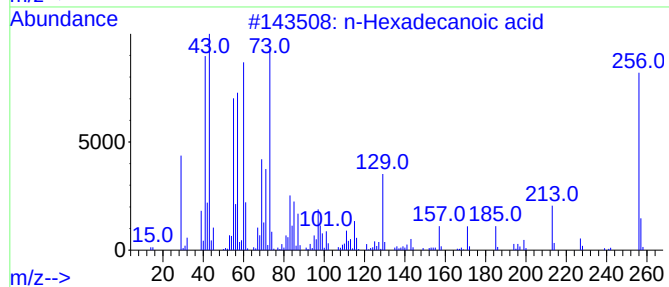
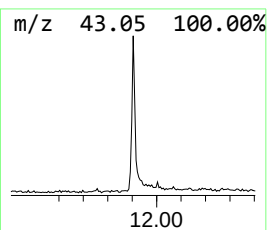
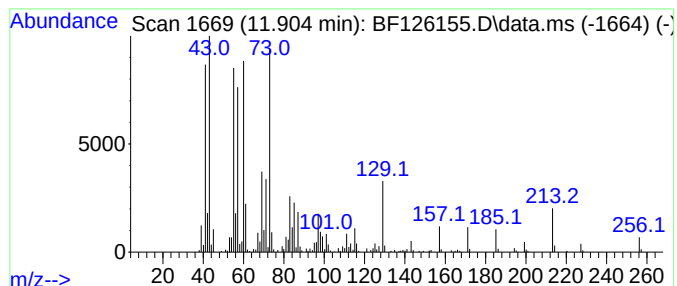
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.904	10.12 ng	650571	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.039	13.4	ng	506395	1	6.839	757211	20.0
Heptane, 3,5-di...	6.904	4.3	ng	162592	1	6.839	757211	20.0
n-Hexadecanoic ...	11.904	10.1	ng	650571	4	11.363	1285790	20.0