

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
 Data File : BG057631.D
 Acq On : 31 May 2023 21:29
 Operator : CG/JU
 Sample : 02981-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-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_G\Methods\8270-BG052723.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057631.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.370	306	312	318	rBV	11828	18879	1.28%	0.262%
2	5.857	388	395	409	rBV	360374	634032	42.87%	8.804%
3	7.484	665	672	684	rBV	374598	689889	46.65%	9.580%
4	8.336	810	817	825	rBV	104565	173333	11.72%	2.407%
5	9.517	1011	1018	1028	rBV	239566	425298	28.76%	5.906%
6	11.173	1290	1300	1308	rBV	134551	237675	16.07%	3.300%
7	13.576	1702	1709	1722	rVB	662373	1000558	67.66%	13.894%
8	14.951	1937	1943	1951	rVB	212811	333554	22.56%	4.632%
9	16.284	2165	2170	2180	rVB	21149	33039	2.23%	0.459%
10	16.437	2189	2196	2211	rBV	495390	764326	51.69%	10.613%
11	17.688	2404	2409	2421	rVB	273934	426230	28.82%	5.919%
12	18.528	2548	2552	2562	rBV3	22246	51338	3.47%	0.713%
13	20.261	2841	2847	2852	rBV	1116355	1478811	100.00%	20.535%
14	21.548	3063	3066	3079	rVB4	34773	85830	5.80%	1.192%
15	21.994	3135	3142	3150	rVB2	245857	433903	29.34%	6.025%
16	25.478	3727	3735	3749	rVB	135927	414809	28.05%	5.760%

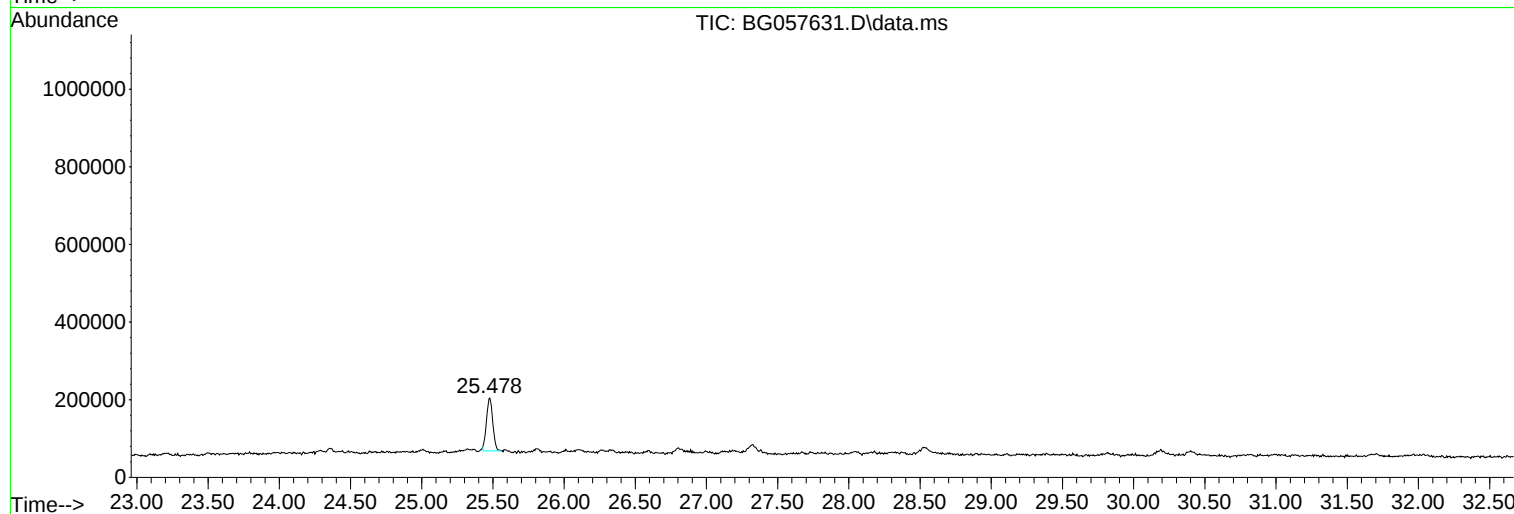
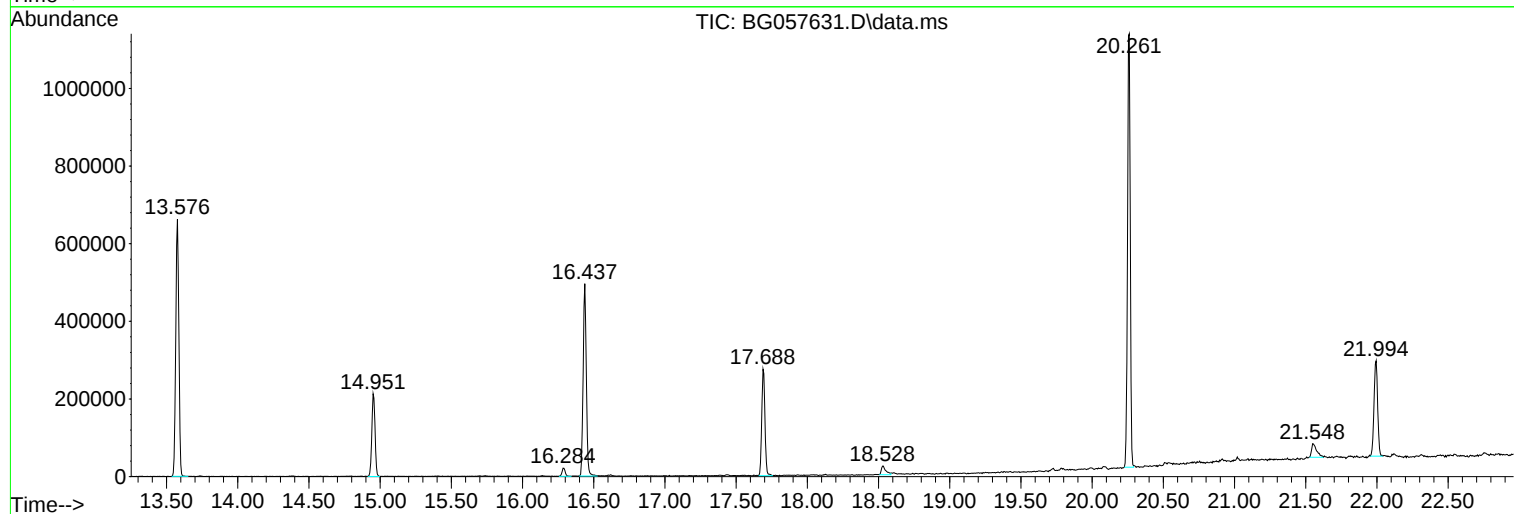
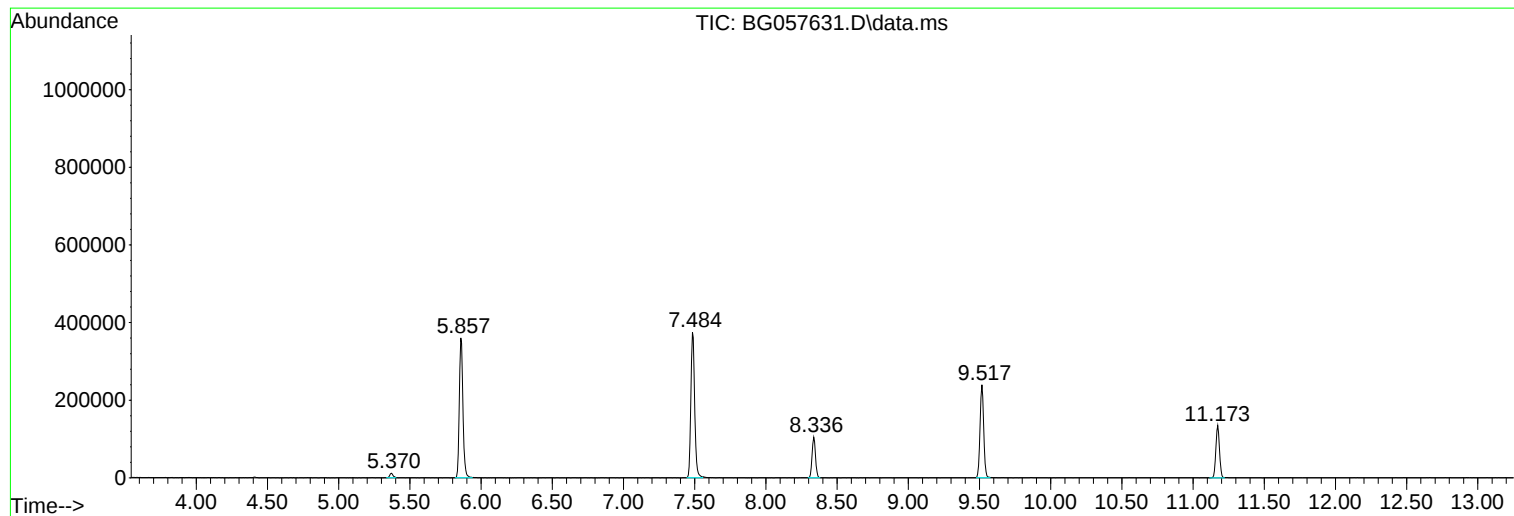
Sum of corrected areas: 7201504

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.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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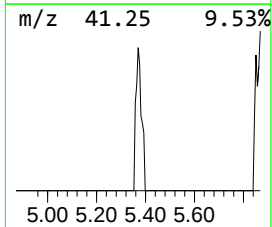
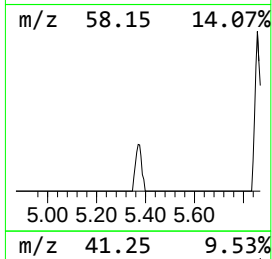
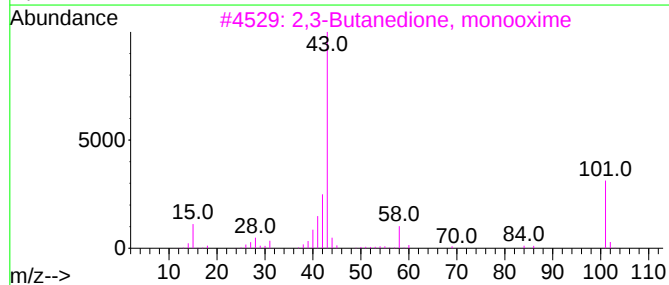
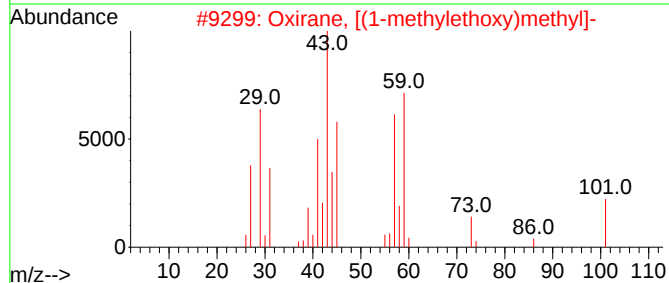
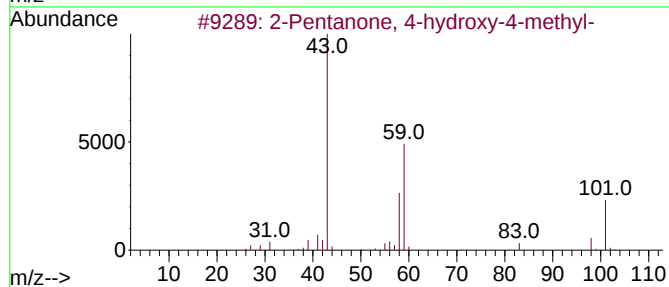
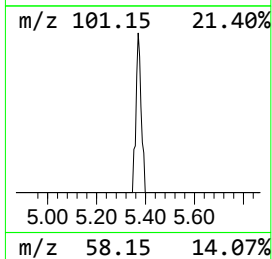
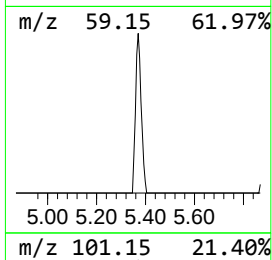
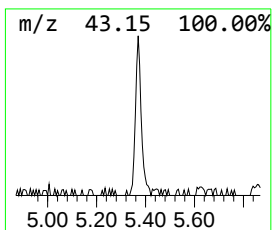
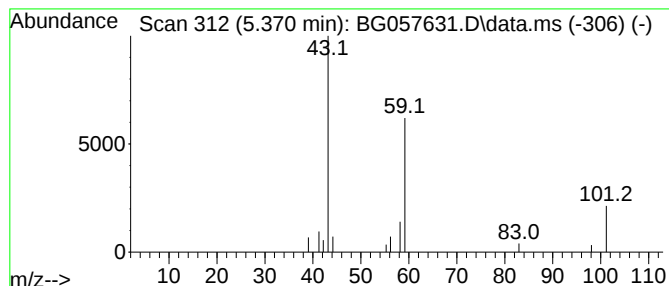
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.370	2.18 ng	18879	1,4-Dichlorobenzene-d4	8.336

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	40	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9	



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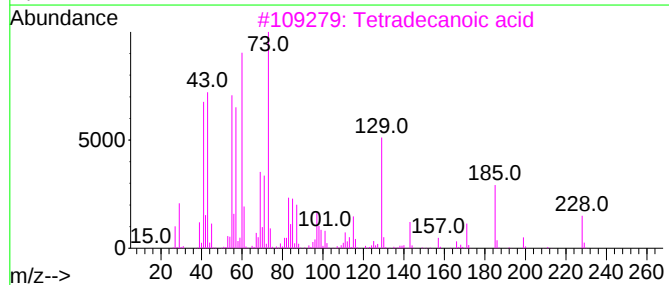
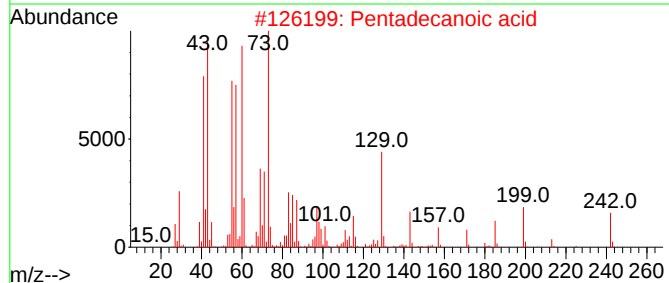
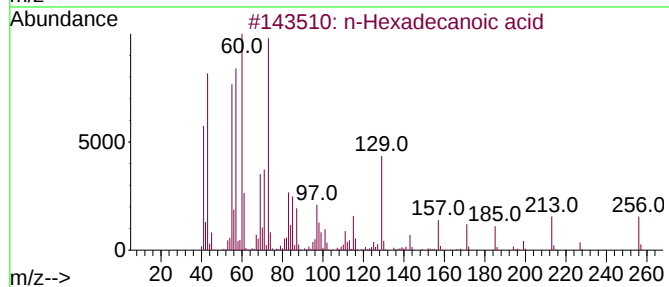
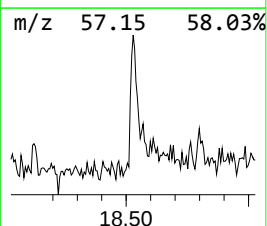
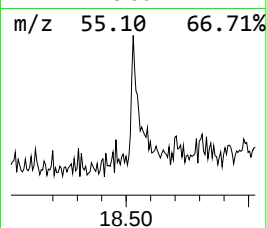
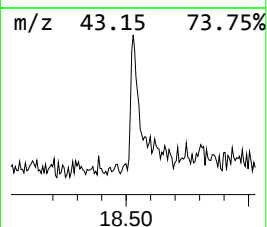
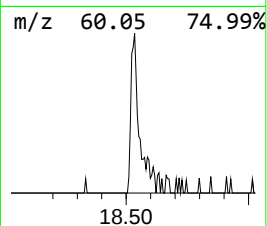
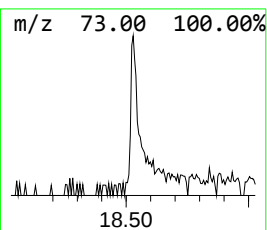
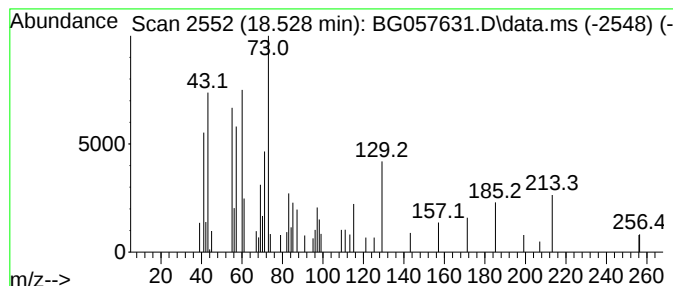
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.528	2.41 ng	51338	Phenanthrene-d10	17.688

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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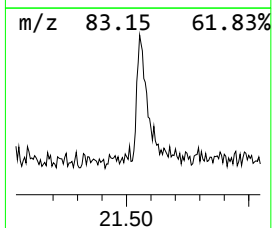
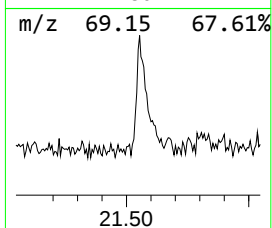
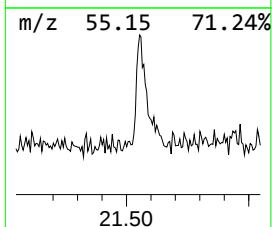
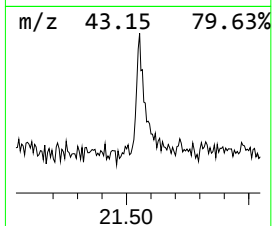
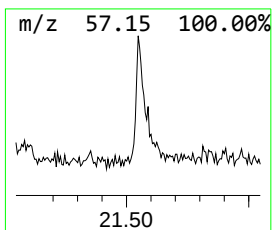
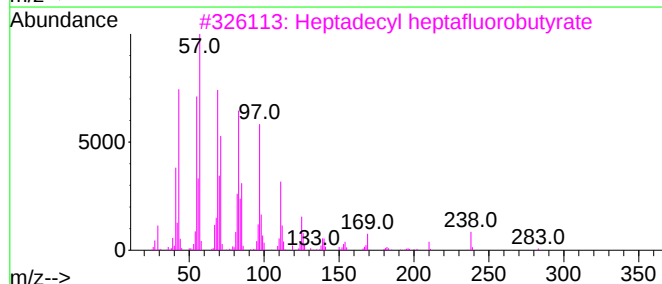
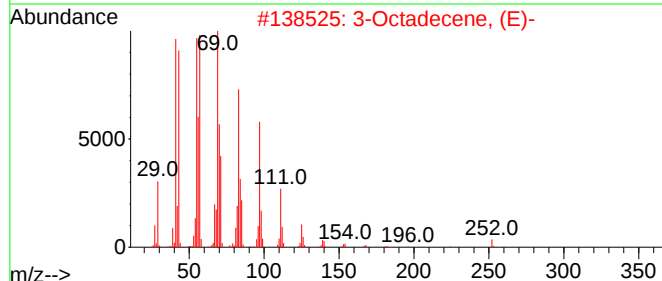
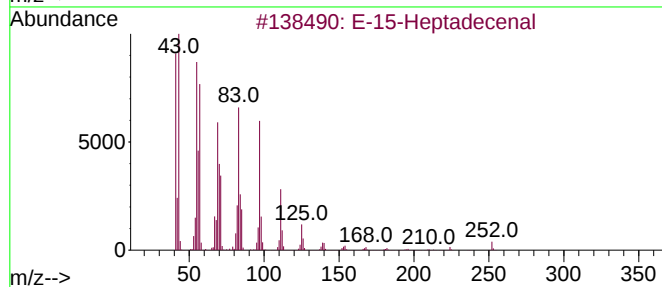
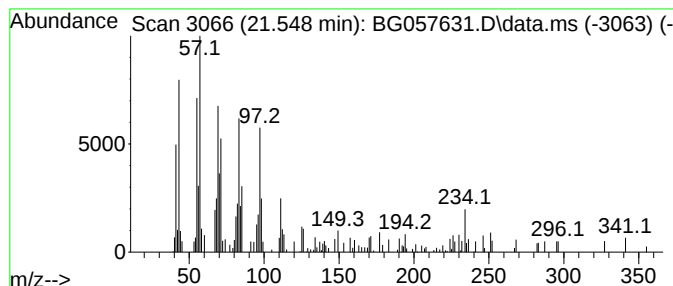
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Peak Number 3 E-15-Heptadecenal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.548	3.96 ng	85830	Chrysene-d12	21.994

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	E-15-Heptadecenal			252	C17H32O	1000130-97-9	91
2	3-Octadecene, (E)-			252	C18H36	007206-19-1	90
3	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	90
4	1-Octadecene			252	C18H36	000112-88-9	83
5	E-7-Octadecene			252	C18H36	1000130-92-0	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.370	2.2	ng	18879	1	8.336	173333	20.0
n-Hexadecanoic ...	18.528	2.4	ng	51338	4	17.688	426230	20.0
E-15-Heptadecenal	21.548	4.0	ng	85830	5	21.994	433903	20.0