

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091421\
 Data File : BF125477.D
 Acq On : 14 Sep 2021 16:42
 Operator : JU/CG
 Sample : PB139044BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB139044BL

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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125477.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.281	26	33	39	rVB	97844	137342	2.15%	0.348%
2	4.510	408	412	421	rBV	201600	231176	3.63%	0.585%
3	5.122	511	516	533	rBV	1008222	1537890	24.12%	3.893%
4	5.522	578	584	587	rBV	4288356	4936298	77.42%	12.496%
5	6.516	747	753	756	rBV	3909916	4797443	75.24%	12.144%
6	6.875	810	814	817	rBV	1294446	1083232	16.99%	2.742%
7	7.439	904	910	913	rBV	2724485	3347571	52.50%	8.474%
8	8.157	1027	1032	1038	rBV	1506010	1439679	22.58%	3.644%
9	9.239	1209	1216	1219	rBV	5145439	5773909	90.56%	14.616%
10	9.916	1325	1331	1342	rBV	1839280	1647950	25.85%	4.172%
11	10.710	1459	1466	1469	rBV	3792022	3821222	59.93%	9.673%
12	11.404	1579	1584	1592	rBV	1795954	1716508	26.92%	4.345%
13	12.998	1849	1855	1858	rBV	6530474	6375892	100.00%	16.140%
14	13.915	2007	2011	2018	rVB	119683	133051	2.09%	0.337%
15	14.051	2030	2034	2041	rVB	1560412	1376344	21.59%	3.484%
16	15.545	2282	2288	2304	rVB	841943	1148736	18.02%	2.908%

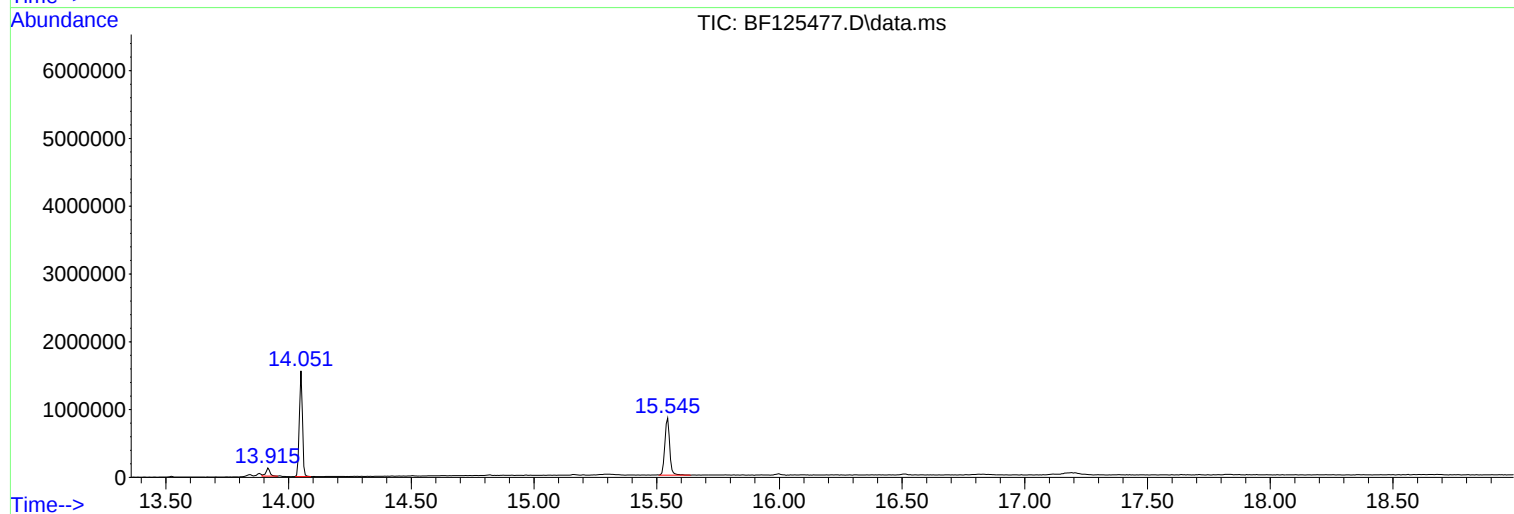
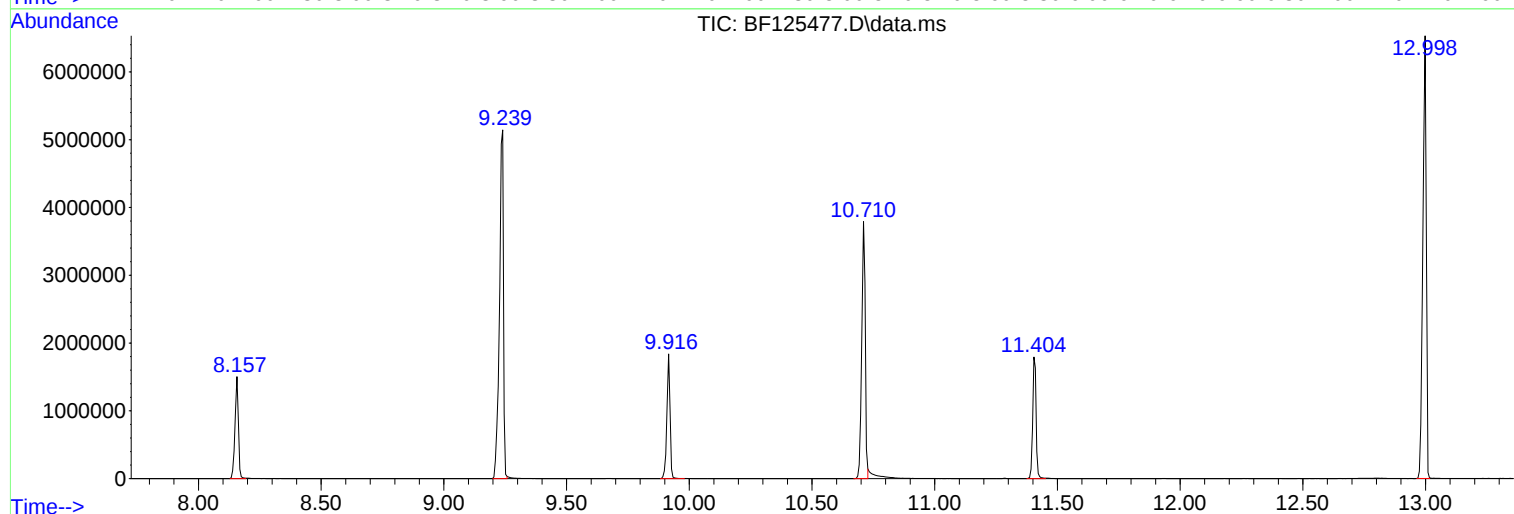
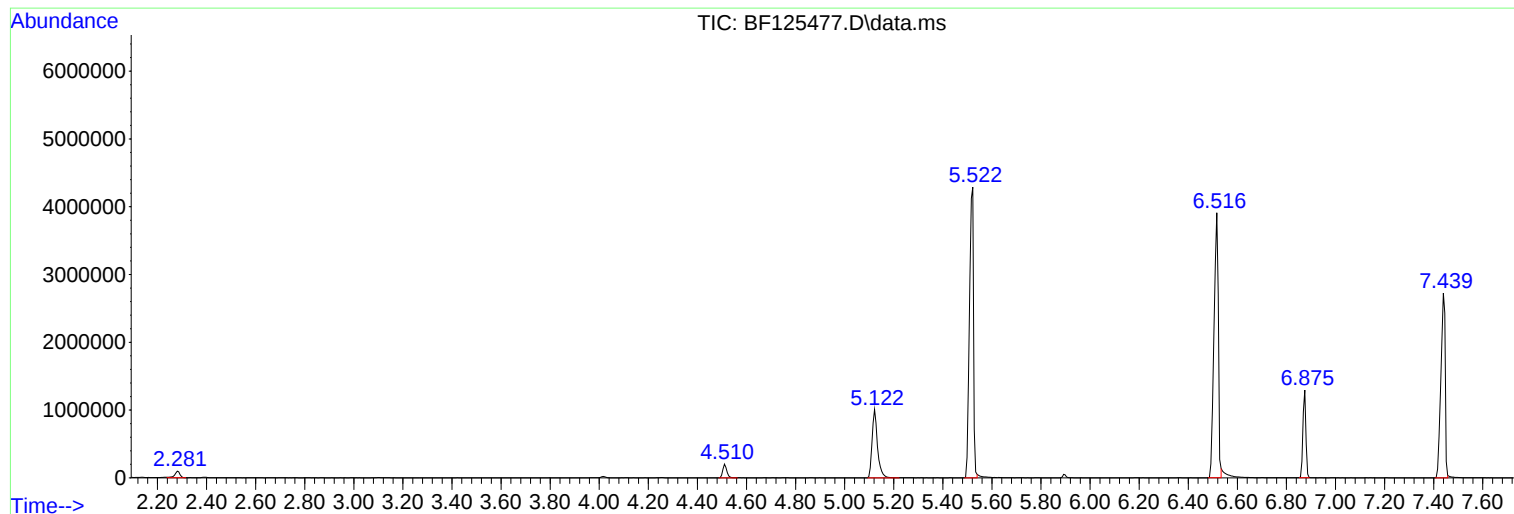
Sum of corrected areas: 39504243

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.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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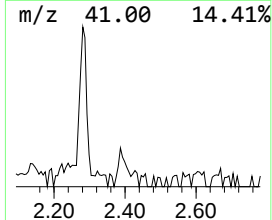
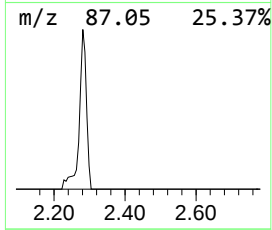
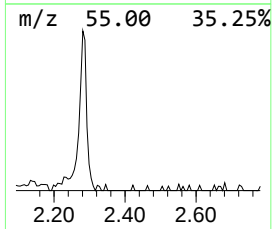
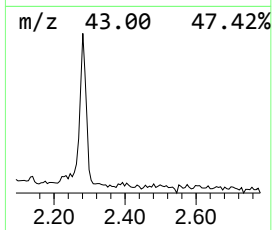
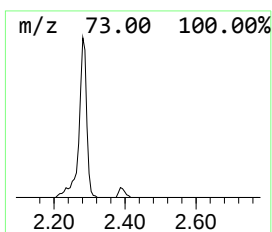
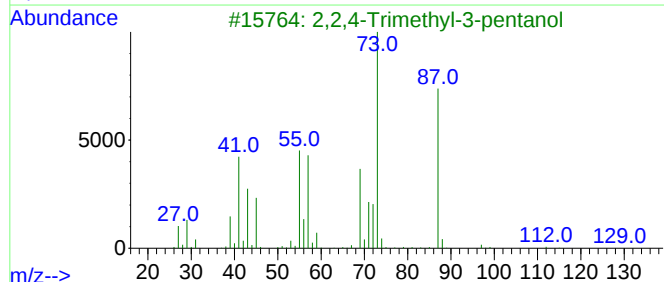
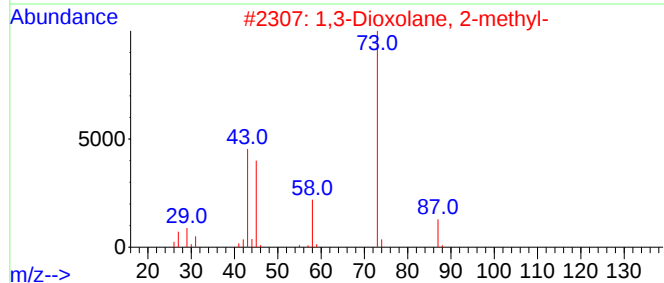
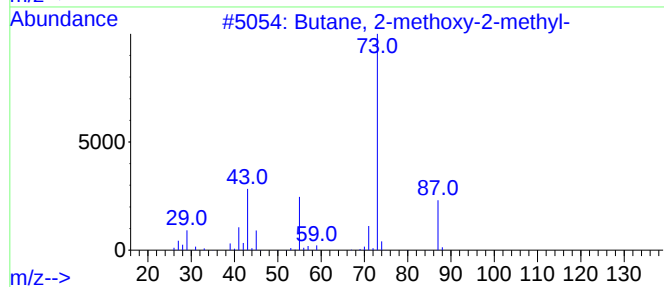
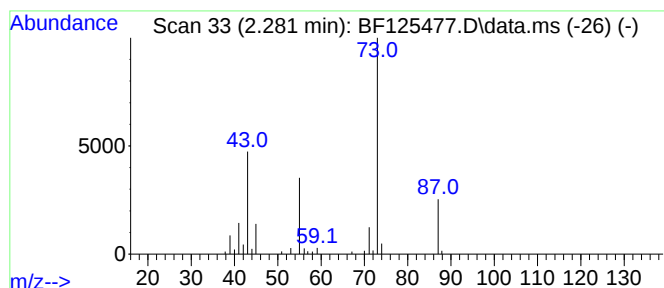
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.281	2.54 ng	137342	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	47
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	25
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25



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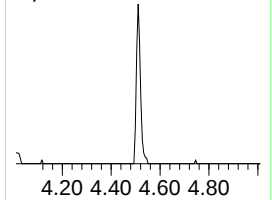
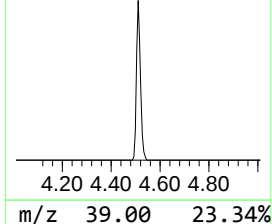
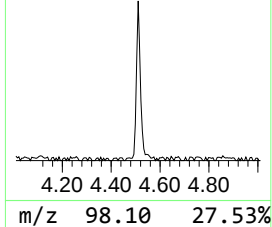
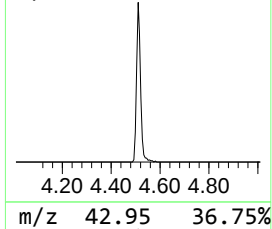
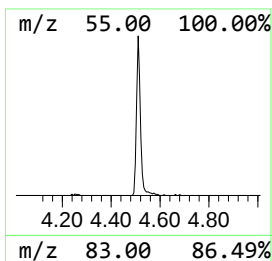
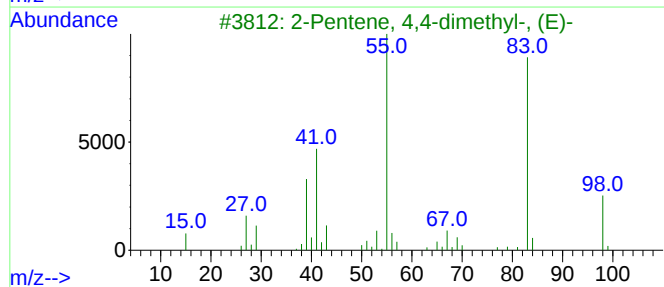
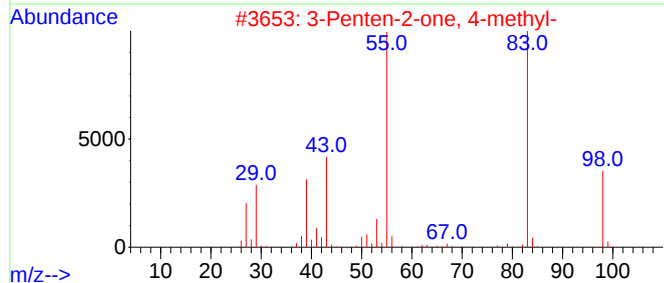
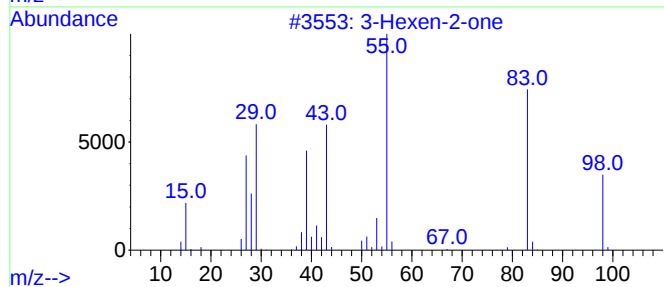
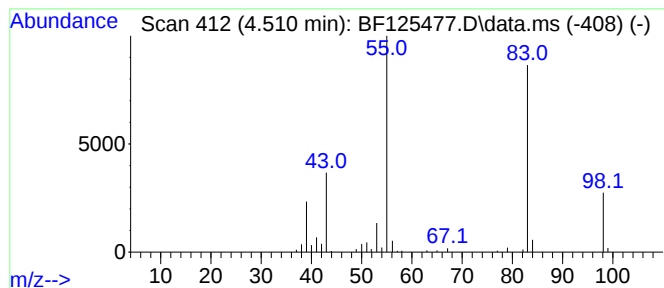
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Peak Number 2 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	4.27 ng	231176	1,4-Dichlorobenzene-d4	6.875

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
3			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	86



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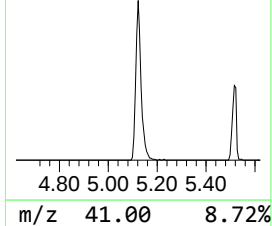
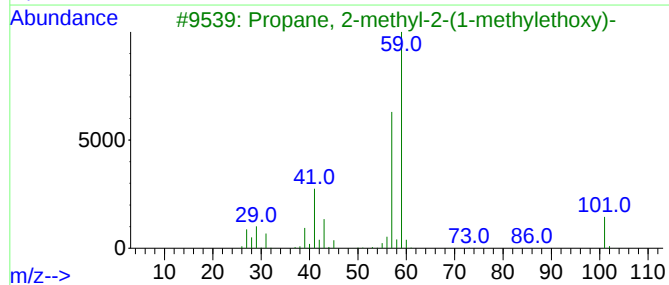
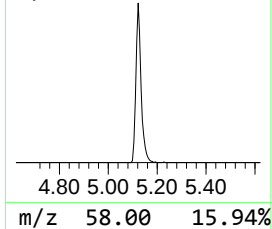
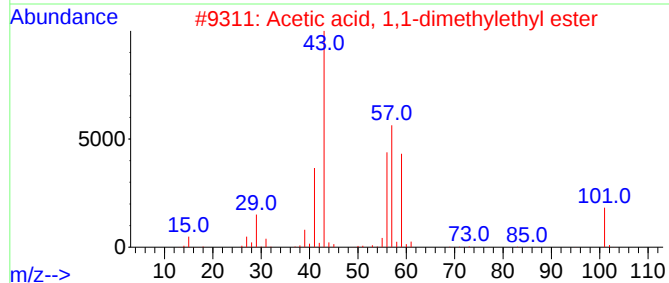
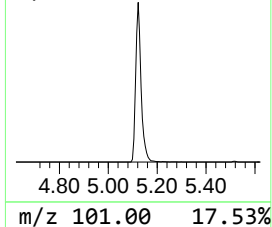
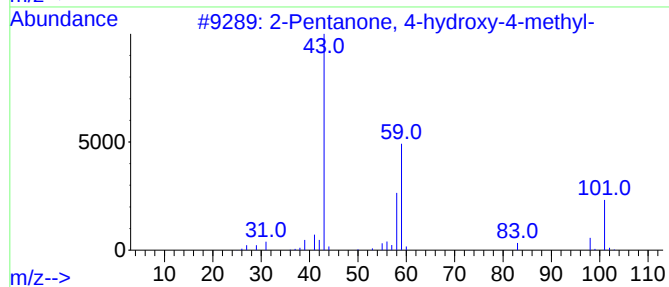
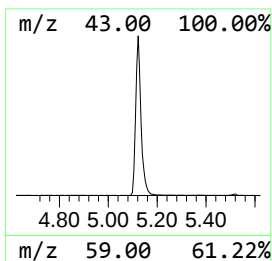
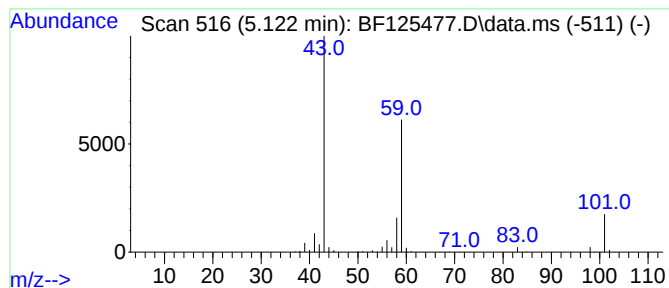
Instrument :
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.122	28.39 ng	1537890	1,4-Dichlorobenzene-d4	6.875	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.281	2.5	ng	137342	1	6.875	1083230	20.0
3-Hexen-2-one	4.510	4.3	ng	231176	1	6.875	1083230	20.0
2-Pentanone, 4-...	5.122	28.4	ng	1537890	1	6.875	1083230	20.0