LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052021\
Data File : VU043858.D
Acq On : 20 May 2021 12:25
Operator : SY/MD
Sample : M2464-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : GB3Z4

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR051521WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU043858.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.494	43	48	54	rVB	10322	9549	1.31%	0.136%
2	1.588	69	77	101	rBV2	579520	705720	96.72%	10.083%
3	1.919	172	180	191	rVB	61123	75618	10.36%	1.080%
4	2.575	372	384	398	rBV	142869	233364	31.98%	3.334%
5	2.649	398	407	430	rVB	20462	49353	6.76%	0.705%
6	3.234	561	589	630	rBV3	25754	144322	19.78%	2.062%
7	4.452	949	968	988	rBV	25699	68054	9.33%	0.972%
8	4.642	1012	1027	1068	rBV2	113681	340491	46.67%	4.865%
9	5.076	1145	1162	1190	rBV3	133847	351168	48.13%	5.017%
10	5.735	1345	1367	1390	rBV2	261771	669278	91.73%	9.562%
11	6.256	1514	1529	1552	rBV	254152	475316	65.14%	6.791%
12	6.700	1651	1667	1688	rBV	162607	319029	43.72%	4.558%
13	7.137	1785	1803	1806	rBV3	15534	28250	3.87%	0.404%
14	7.176	1807	1815	1834	rVB2	43650	88709	12.16%	1.267%
15	7.575	1923	1939	1958	rBV	77672	136461	18.70%	1.950%
16	7.906	2027	2042	2057	rBV	301022	523220	71.71%	7.475%
17	7.976	2057	2064	2076	rVB	9360	15994	2.19%	0.229%
18	8.185	2118	2129	2147	rBV	48265	82299	11.28%	1.176%
19	8.481	2206	2221	2236	rVB7	5927	13160	1.80%	0.188%
20	8.645	2256	2272	2312	rBV	364887	729628	100.00%	10.424%
21	9.423	2501	2514	2548	rBV	373694	623354	85.43%	8.906%
22	10.764	2919	2931	2949	rBV	133103	213782	29.30%	3.054%
23	10.899	2962	2973	2985	rVB2	11896	19286	2.64%	0.276%
24	11.819	3245	3259	3277	rBV	363390	575276	78.85%	8.219%
25	12.070	3326	3337	3347	rBV3	8460	13833	1.90%	0.198%
26	12.198	3364	3377	3392	rBV	302595	494860	67.82%	7.070%

Sum of corrected areas: 6999374

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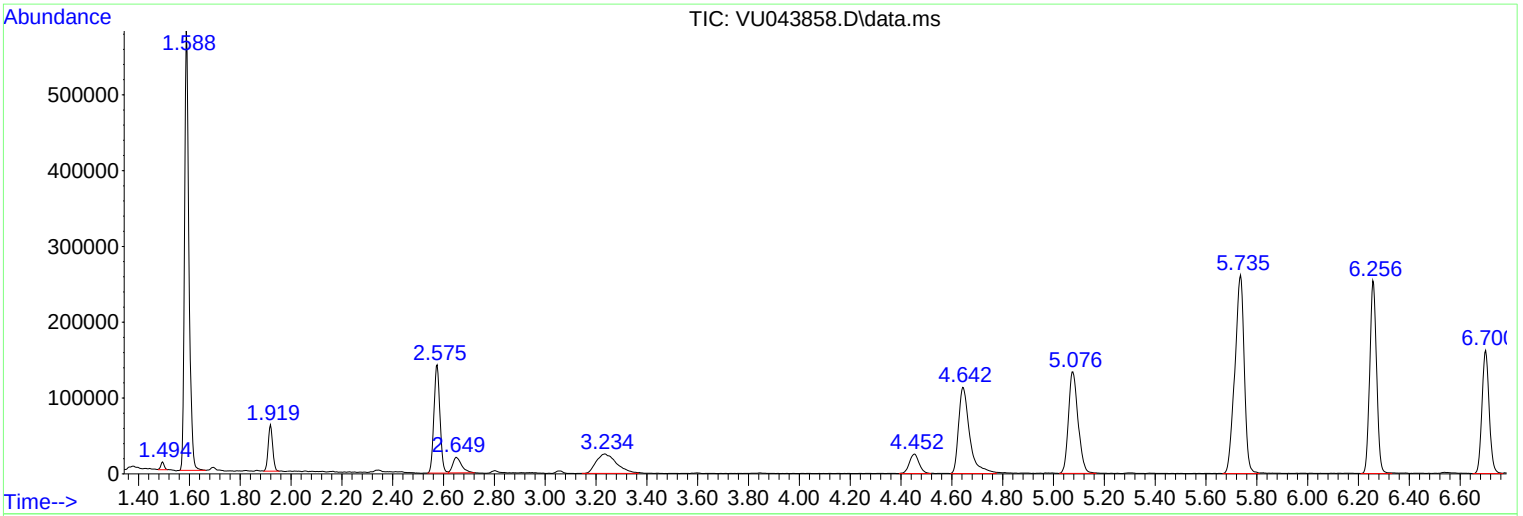
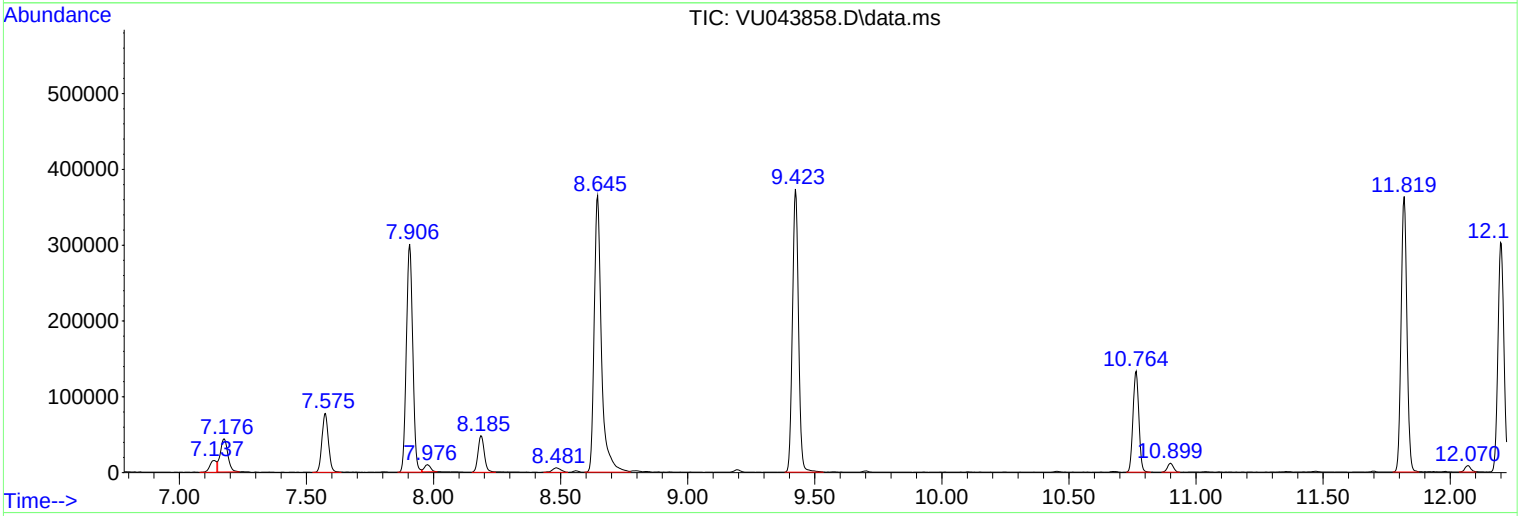
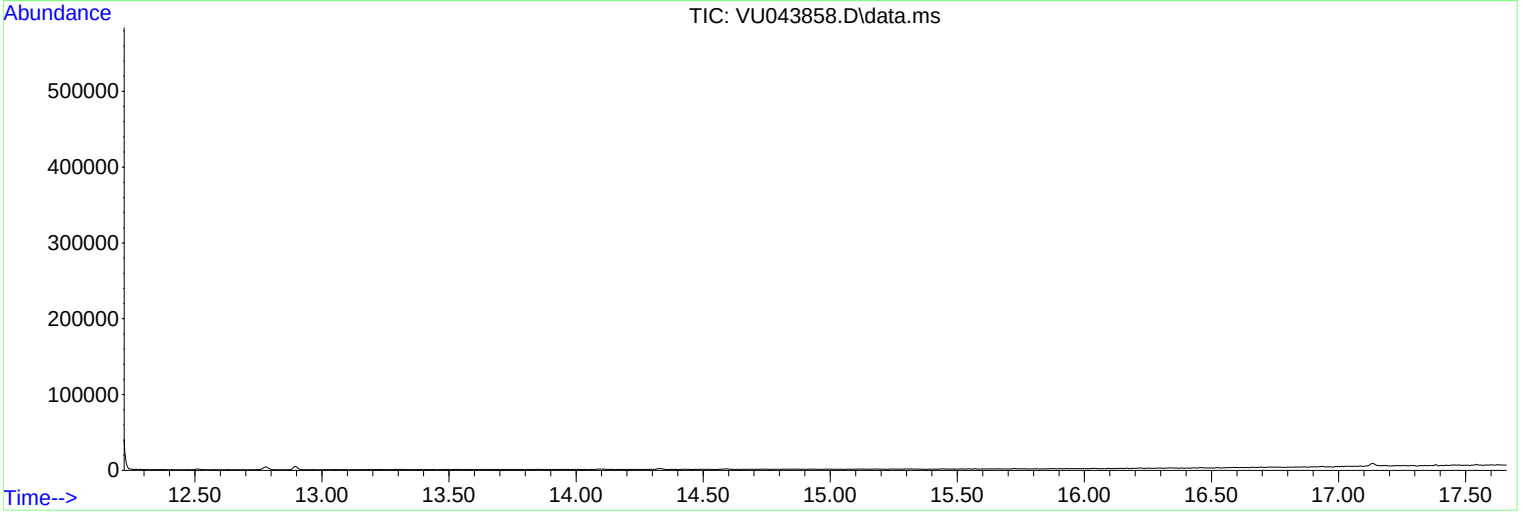
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR051521WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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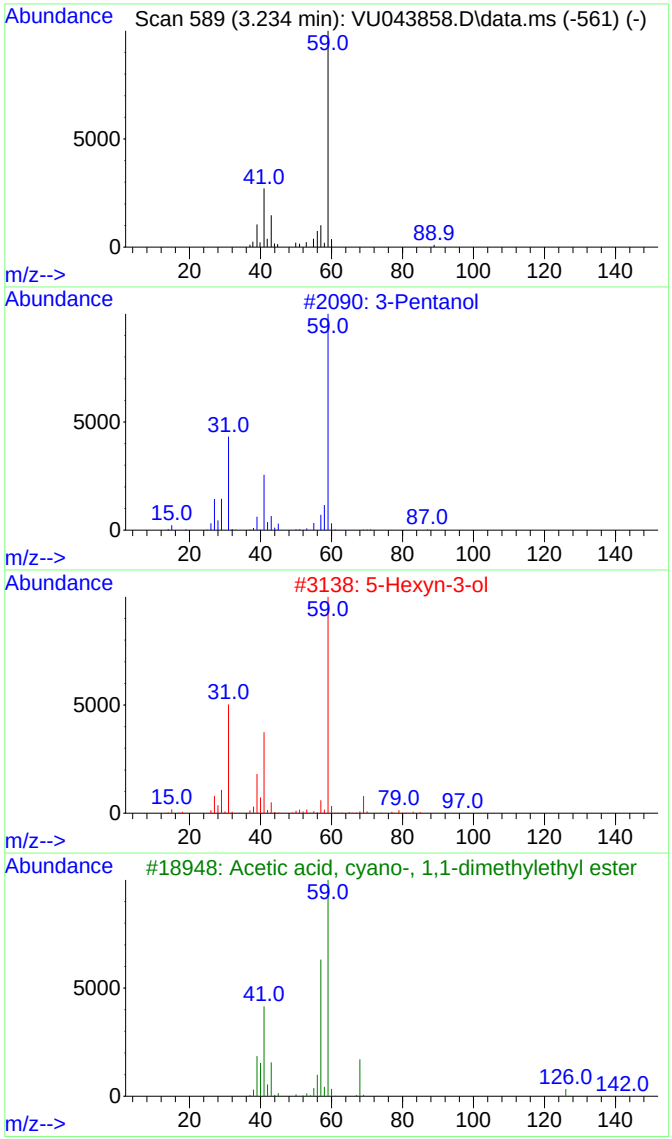
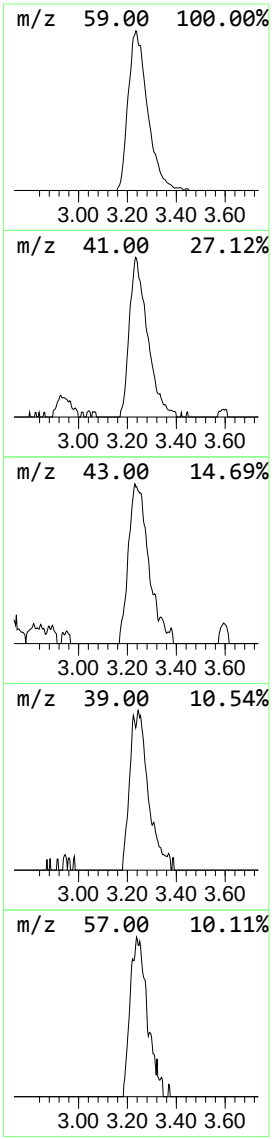
****

Peak Number 1 3-Pentanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.234	1.52 ug/L	144322	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol	88	C5H12O	000584-02-1	56
2	5-Hexyn-3-ol	98	C6H10O	019780-84-8	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	39
4	Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	38
5	Propane, 2-methoxy-	74	C4H10O	000598-53-8	9





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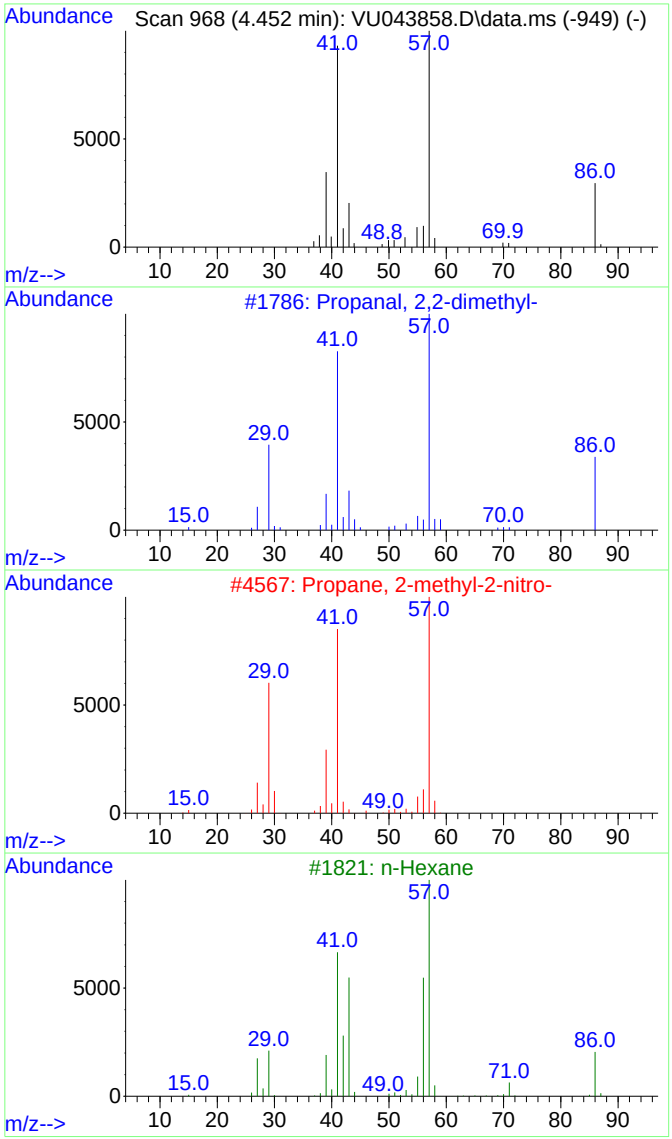
Quant Title : TRACE VOA SFAM1.0

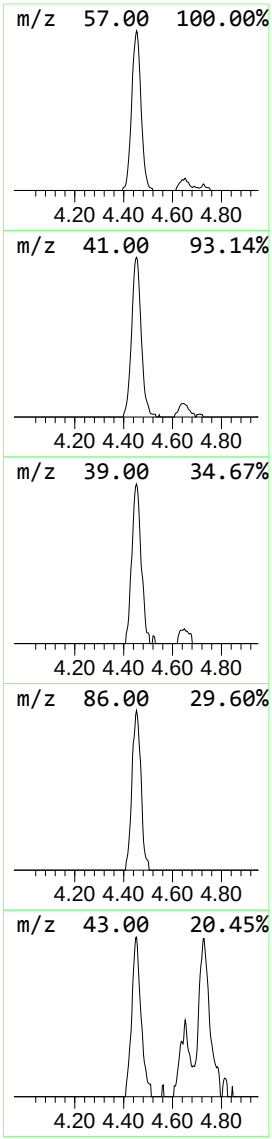
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propanal, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.452	0.72 ug/L	68054	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	64
2	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
3	n-Hexane	86	C6H14	000110-54-3	50
4	Butanal, 2-methyl-	86	C5H10O	000096-17-3	45
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	40





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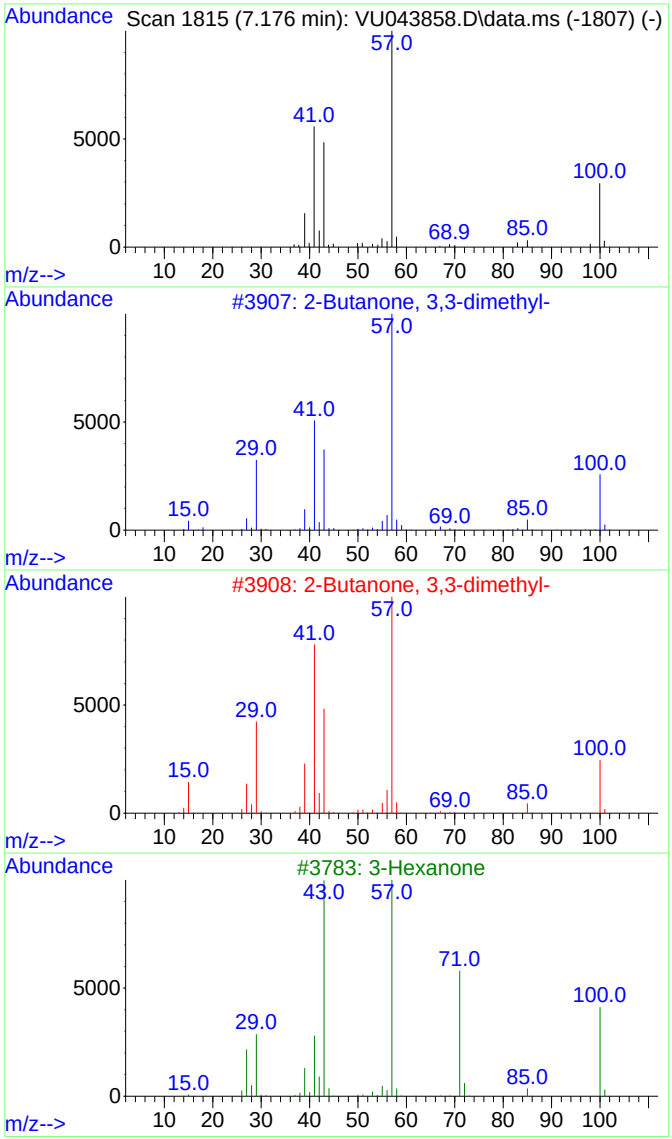
Quant Title : TRACE VOA SFAM1.0

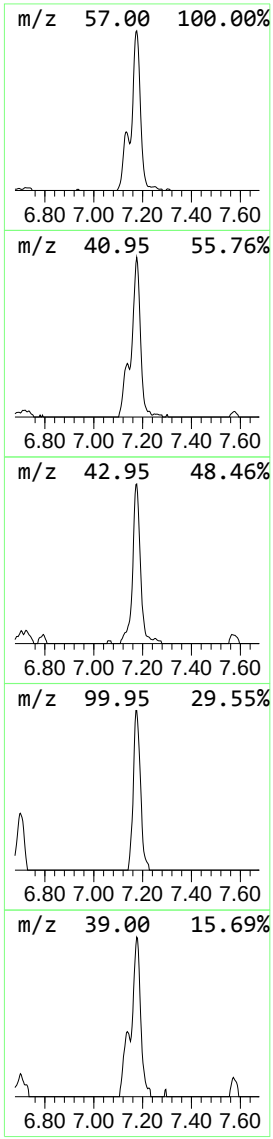
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.176	0.93 ug/L	88709	1,4-Difluorobenzene	6.256

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	86
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	72
3	3-Hexanone	100	C6H12O	000589-38-8	53
4	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	50
5	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	45





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Pentanol	3.234	1.5	ug/L	144322	1	6.256	475316	5.0
Propanal, 2,2-d...	4.452	0.7	ug/L	68054	1	6.256	475316	5.0
2-Butanone, 3,3...	7.176	0.9	ug/L	88709	1	6.256	475316	5.0