

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046155.D
 Acq On : 07 Dec 2021 21:26
 Operator : SY/MD
 Sample : M4887-11ME
 Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046155.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	72	81	98	rVB	161711	207504	14.26%	2.135%
2	1.861	157	162	167	rBV2	806	930	0.06%	0.010%
3	1.919	170	180	197	rVV	93425	154915	10.65%	1.594%
4	2.549	364	376	391	rBV	220092	365343	25.11%	3.759%
5	3.179	559	572	591	rBV	9011	23823	1.64%	0.245%
6	3.472	659	663	666	rBV	157	185	0.01%	0.002%
7	3.517	673	677	686	rBV	177	343	0.02%	0.004%
8	3.678	724	727	730	rBV	148	146	0.01%	0.002%
9	3.909	795	799	801	rBV	155	157	0.01%	0.002%
10	4.012	827	831	834	rBV	144	146	0.01%	0.002%
11	4.137	867	870	875	rBV	182	226	0.02%	0.002%
12	4.208	890	892	895	rVB	257	145	0.01%	0.001%
13	4.330	928	930	935	rBV	148	171	0.01%	0.002%
14	4.655	1013	1031	1083	rBV2	70475	337935	23.22%	3.477%
15	5.063	1142	1158	1186	rVB	229000	558592	38.39%	5.748%
16	5.189	1194	1197	1199	rBV	248	170	0.01%	0.002%
17	5.295	1226	1230	1233	rBV2	266	221	0.02%	0.002%
18	5.327	1237	1240	1245	rBB	170	190	0.01%	0.002%
19	5.388	1256	1259	1262	rBV	197	179	0.01%	0.002%
20	5.440	1270	1275	1278	rBB	167	166	0.01%	0.002%
21	5.469	1281	1284	1286	rBV	229	157	0.01%	0.002%
22	5.588	1315	1321	1324	rBV	183	227	0.02%	0.002%
23	5.723	1341	1363	1390	rBV2	567898	1455153	100.00%	14.973%
24	5.829	1393	1396	1399	rVV	232	173	0.01%	0.002%
25	5.890	1412	1415	1417	rBV	325	217	0.01%	0.002%
26	5.980	1431	1443	1458	rBV4	5723	14627	1.01%	0.151%
27	6.125	1486	1488	1494	rVB	180	201	0.01%	0.002%
28	6.250	1509	1527	1557	rVV	191982	395756	27.20%	4.072%
29	6.359	1559	1561	1566	rVB	344	221	0.02%	0.002%
30	6.536	1603	1616	1628	rVV7	8871	19596	1.35%	0.202%
31	6.604	1631	1637	1650	rVV4	2313	5256	0.36%	0.054%
32	6.690	1650	1664	1691	rVB	315031	641503	44.08%	6.601%
33	6.803	1696	1699	1706	rVB3	474	476	0.03%	0.005%
34	6.890	1723	1726	1730	rBV	153	173	0.01%	0.002%
35	6.961	1745	1748	1751	rBV	186	172	0.01%	0.002%
36	7.060	1776	1779	1786	rVB2	363	444	0.03%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046155.D
 Acq On : 07 Dec 2021 21:26
 Operator : SY/MD
 Sample : M4887-11ME
 Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	7.150	1802	1807	1809	rBV	163	196	0.01%	0.002%
38	7.182	1812	1817	1820	rVV	231	294	0.02%	0.003%
39	7.234	1828	1833	1837	rVB3	647	673	0.05%	0.007%
40	7.305	1849	1855	1858	rBV	340	386	0.03%	0.004%
41	7.362	1870	1873	1877	rBB2	278	210	0.01%	0.002%
42	7.568	1923	1937	1968	rBV	172717	347359	23.87%	3.574%
43	7.690	1971	1975	1977	rVV2	281	241	0.02%	0.002%
44	7.703	1977	1979	1986	rVB3	488	419	0.03%	0.004%
45	7.793	1997	2007	2020	rVB4	2951	5401	0.37%	0.056%
46	7.899	2025	2040	2057	rBV	660414	1242327	85.37%	12.783%
47	8.186	2116	2129	2159	rBV	100903	235078	16.15%	2.419%
48	8.292	2159	2162	2167	rVB	187	195	0.01%	0.002%
49	8.378	2181	2189	2193	rBV	207	355	0.02%	0.004%
50	8.472	2211	2218	2224	rBV	242	391	0.03%	0.004%
51	8.552	2235	2243	2254	rVB3	9213	15361	1.06%	0.158%
52	8.681	2259	2283	2316	rBV2	231217	741253	50.94%	7.627%
53	8.854	2333	2337	2341	rBV2	259	217	0.01%	0.002%
54	8.957	2359	2369	2377	rVB	855	1529	0.11%	0.016%
55	9.423	2500	2514	2542	rVB	223095	498011	34.22%	5.124%
56	9.575	2556	2561	2570	rVB3	544	721	0.05%	0.007%
57	9.697	2592	2599	2600	rBV	924	918	0.06%	0.009%
58	10.671	2894	2902	2910	rBV2	3637	5346	0.37%	0.055%
59	10.771	2918	2933	2949	rBB	444992	748938	51.47%	7.706%
60	10.838	2950	2954	2956	rBV2	255	158	0.01%	0.002%
61	10.870	2957	2964	2965	rBV2	564	616	0.04%	0.006%
62	10.925	2977	2981	2984	rVB	387	363	0.02%	0.004%
63	11.002	2999	3005	3007	rBV2	254	283	0.02%	0.003%
64	11.092	3029	3033	3036	rBV2	299	250	0.02%	0.003%
65	11.118	3036	3041	3045	rVV4	651	668	0.05%	0.007%
66	11.140	3046	3048	3050	rVB2	275	145	0.01%	0.001%
67	11.205	3065	3068	3071	rBV	185	166	0.01%	0.002%
68	11.298	3092	3097	3101	rVV3	371	375	0.03%	0.004%
69	11.452	3137	3145	3160	rVB4	2636	5196	0.36%	0.053%
70	11.578	3179	3184	3192	rVB3	590	707	0.05%	0.007%
71	11.693	3214	3220	3230	rBV4	1843	2505	0.17%	0.026%
72	11.819	3246	3259	3271	rBV	326336	519922	35.73%	5.350%
73	11.944	3284	3298	3301	rBV4	1495	2511	0.17%	0.026%
74	11.970	3303	3306	3315	rVV3	2792	3508	0.24%	0.036%
75	12.012	3315	3319	3324	rVB	274	282	0.02%	0.003%
76	12.076	3333	3339	3342	rBV	215	186	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046155.D
 Acq On : 07 Dec 2021 21:26
 Operator : SY/MD
 Sample : M4887-11ME
 Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF Filtering: 5
 Sampling : 1 Min Area: 0 % 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:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

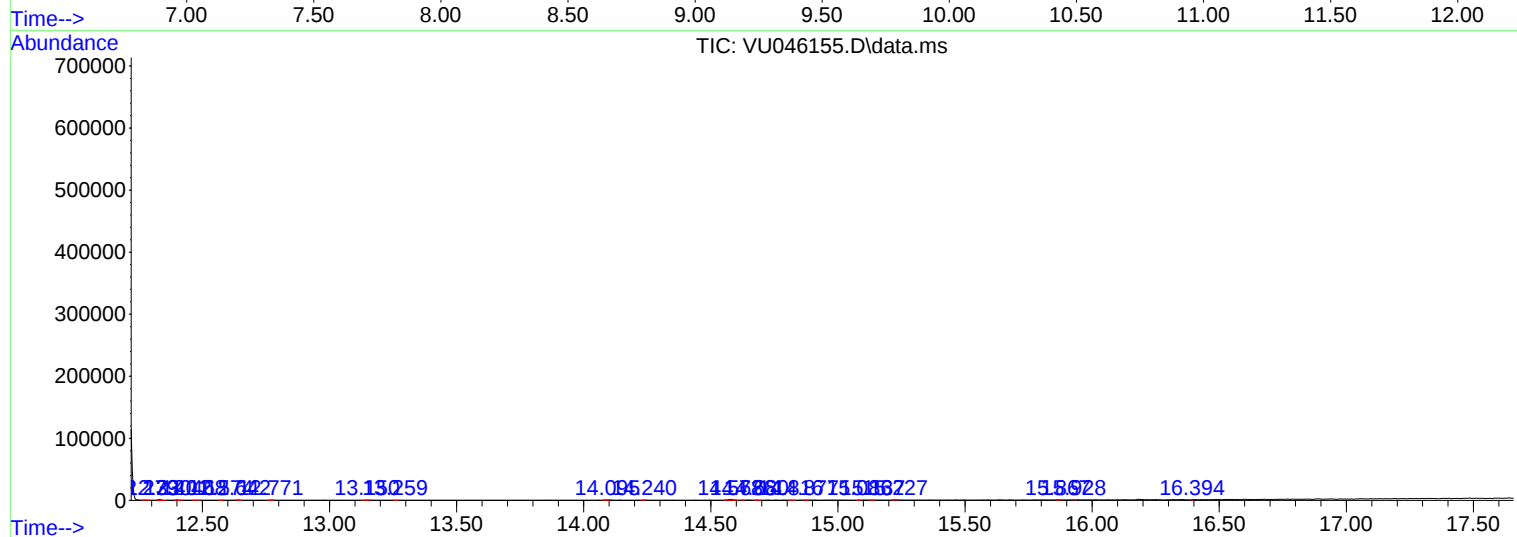
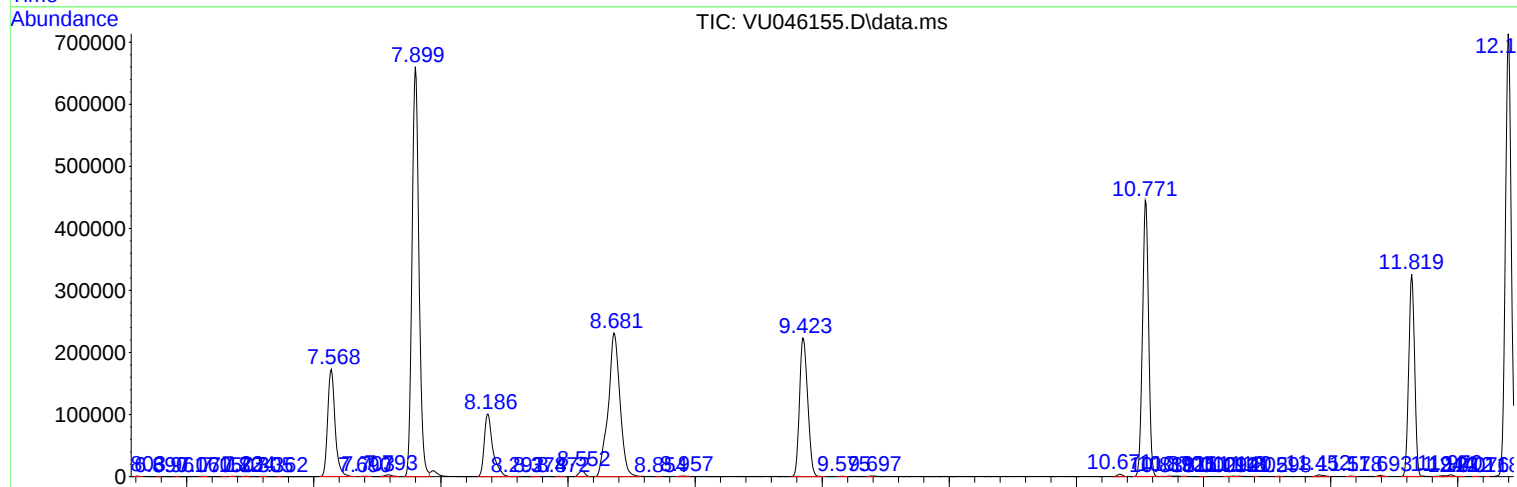
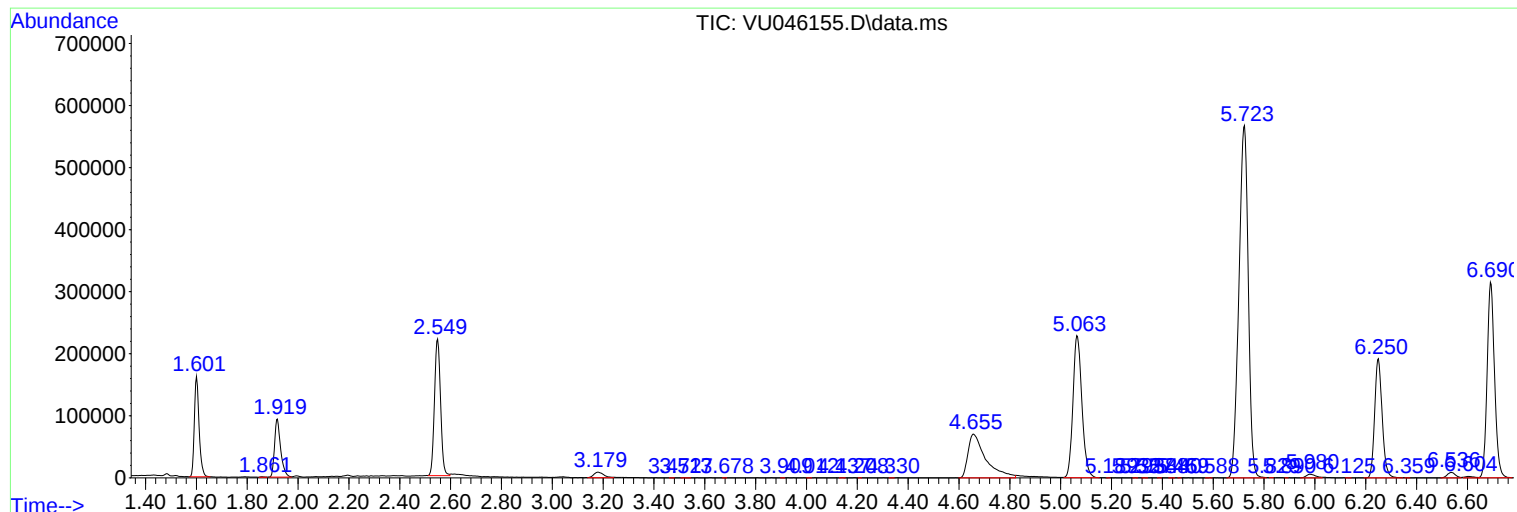
77	12.118	3349	3352	3355	rBV2	218	164	0.01%	0.002%
78	12.198	3358	3377	3397	rVV	713488	1139593	78.31%	11.726%
79	12.279	3397	3402	3407	rVB4	415	471	0.03%	0.005%
80	12.330	3414	3418	3425	rVB2	1101	1193	0.08%	0.012%
81	12.401	3436	3440	3448	rVB3	506	562	0.04%	0.006%
82	12.468	3458	3461	3468	rBV	139	166	0.01%	0.002%
83	12.574	3490	3494	3496	rBV	157	149	0.01%	0.002%
84	12.642	3512	3515	3520	rVB2	488	389	0.03%	0.004%
85	12.771	3550	3555	3558	rBV2	358	381	0.03%	0.004%
86	13.150	3665	3673	3676	rBV3	444	634	0.04%	0.007%
87	13.259	3704	3707	3711	rBV	152	156	0.01%	0.002%
88	14.095	3960	3967	3968	rBV2	545	568	0.04%	0.006%
89	14.240	4007	4012	4013	rBV	201	164	0.01%	0.002%
90	14.578	4109	4117	4127	rVB3	1177	1749	0.12%	0.018%
91	14.626	4130	4132	4134	rBV	225	148	0.01%	0.002%
92	14.680	4146	4149	4154	rVB2	207	152	0.01%	0.002%
93	14.816	4188	4191	4197	rBV	189	149	0.01%	0.002%
94	14.877	4205	4210	4212	rBV	301	243	0.02%	0.003%
95	15.086	4271	4275	4277	rBV	405	299	0.02%	0.003%
96	15.137	4287	4291	4293	rBV	192	196	0.01%	0.002%
97	15.227	4314	4319	4322	rBV2	454	466	0.03%	0.005%
98	15.867	4515	4518	4522	rBV	437	349	0.02%	0.004%
99	15.928	4535	4537	4540	rBV2	358	238	0.02%	0.002%
100	16.394	4679	4682	4684	rBV3	411	328	0.02%	0.003%

Sum of corrected areas: 9718406

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046155.D
Acq On : 07 Dec 2021 21:26
Operator : SY/MD
Sample : M4887-11ME
Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 29 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046155.D
Acq On : 07 Dec 2021 21:26
Operator : SY/MD
Sample : M4887-11ME
Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 29 Sample Multiplier: 1

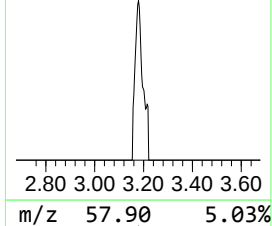
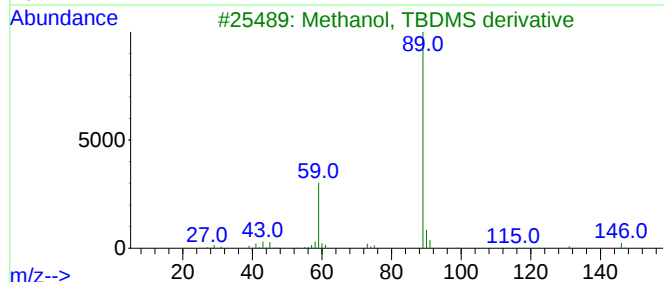
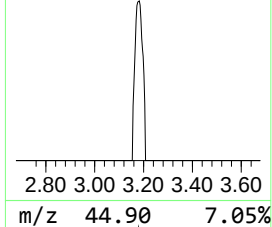
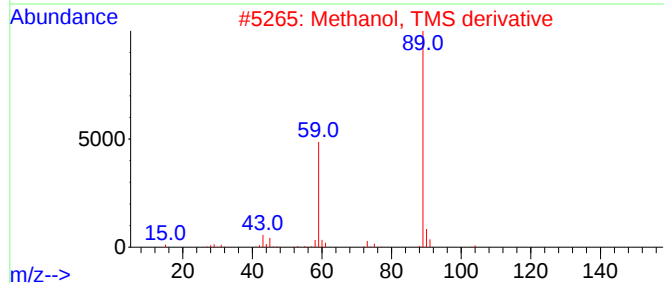
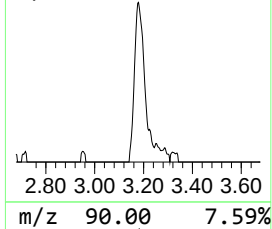
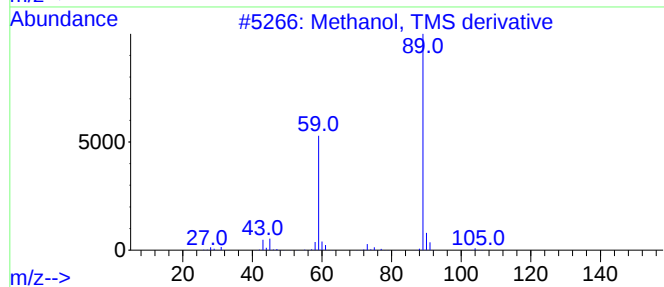
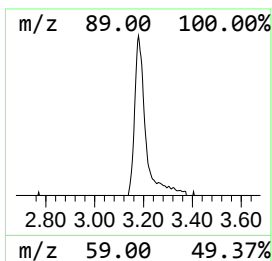
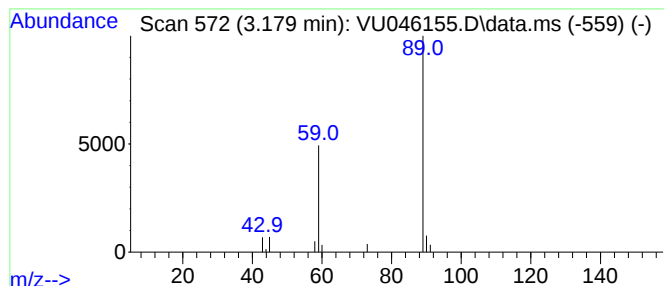
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methanol, TMS derivative Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.179	3.01 ug/L	23823	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
2			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
3			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	74
4			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	43
5			Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046155.D
Acq On : 07 Dec 2021 21:26
Operator : SY/MD
Sample : M4887-11ME
Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 29 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanol, TMS d...	3.179	3.0	ug/L	23823	1	6.250	395756	50.0