

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100621\
 Data File : VU045184.D
 Acq On : 06 Oct 2021 14:39
 Operator : SY/MD
 Sample : M3996-10
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A42

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU0451184.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.514	33	54	67	rBV	227208	1087263	83.50%	9.177%
2	1.600	77	81	118	rVB	276618	539405	41.43%	4.553%
3	1.899	168	174	201	rVB	152628	229149	17.60%	1.934%
4	2.565	368	381	400	rBV	275494	460129	35.34%	3.884%
5	2.687	414	419	428	rVB3	3289	4910	0.38%	0.041%
6	2.796	440	453	464	rBV2	5937	12895	0.99%	0.109%
7	3.192	563	576	595	rVB2	45556	106989	8.22%	0.903%
8	3.356	613	627	651	rVB	119910	239475	18.39%	2.021%
9	3.851	772	781	792	rBV3	1370	2909	0.22%	0.025%
10	4.031	834	837	841	rVB2	161	146	0.01%	0.001%
11	4.095	853	857	860	rBV	229	233	0.02%	0.002%
12	4.166	877	879	883	rBV	158	149	0.01%	0.001%
13	4.436	958	963	964	rBV2	216	153	0.01%	0.001%
14	4.568	994	1004	1008	rBV3	1690	2885	0.22%	0.024%
15	4.629	1009	1023	1032	rBV	144237	348362	26.76%	2.940%
16	4.935	1114	1118	1123	rVB2	236	202	0.02%	0.002%
17	4.960	1123	1126	1129	rBV3	176	158	0.01%	0.001%
18	5.012	1139	1142	1143	rBV	267	135	0.01%	0.001%
19	5.066	1143	1159	1184	rVV	228775	498323	38.27%	4.206%
20	5.185	1193	1196	1197	rBV	299	194	0.01%	0.002%
21	5.214	1201	1205	1208	rVV3	470	354	0.03%	0.003%
22	5.282	1222	1226	1228	rBV3	481	408	0.03%	0.003%
23	5.320	1236	1238	1245	rVB3	283	226	0.02%	0.002%
24	5.378	1249	1256	1261	rVB3	440	547	0.04%	0.005%
25	5.629	1329	1334	1336	rBV2	192	157	0.01%	0.001%
26	5.729	1343	1365	1385	rBV2	486836	1302037	100.00%	10.990%
27	5.986	1443	1445	1448	rBV2	211	170	0.01%	0.001%
28	6.005	1448	1451	1453	rVV3	321	198	0.02%	0.002%
29	6.018	1453	1455	1458	rVV	187	139	0.01%	0.001%
30	6.044	1460	1463	1470	rVB3	427	404	0.03%	0.003%
31	6.253	1512	1528	1545	rBV	379050	707004	54.30%	5.967%
32	6.546	1609	1619	1630	rVB3	12421	22344	1.72%	0.189%
33	6.697	1651	1666	1684	rBV	303220	590575	45.36%	4.985%
34	6.800	1696	1698	1700	rBV2	431	230	0.02%	0.002%
35	6.973	1747	1752	1756	rBV2	242	261	0.02%	0.002%
36	7.041	1768	1773	1776	rBV4	467	450	0.03%	0.004%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

37	7.144	1803	1805	1808	rVB	255	163	0.01%	0.001%
38	7.179	1808	1816	1817	rBV4	1184	1143	0.09%	0.010%
39	7.253	1833	1839	1840	rBV	171	160	0.01%	0.001%
40	7.279	1843	1847	1850	rBV	180	155	0.01%	0.001%
41	7.365	1871	1874	1876	rVB	239	149	0.01%	0.001%
42	7.381	1876	1879	1882	rBV2	163	151	0.01%	0.001%
43	7.420	1887	1891	1893	rBV	245	246	0.02%	0.002%
44	7.468	1902	1906	1909	rVB2	171	149	0.01%	0.001%
45	7.494	1909	1914	1915	rBV	220	188	0.01%	0.002%
46	7.568	1923	1937	1962	rBV	170396	294302	22.60%	2.484%
47	7.684	1969	1973	1981	rVB4	864	1116	0.09%	0.009%
48	7.719	1981	1984	1987	rBV	206	170	0.01%	0.001%
49	7.902	2026	2041	2056	rBV	600723	1017797	78.17%	8.591%
50	7.970	2057	2062	2074	rVB2	8397	13961	1.07%	0.118%
51	8.182	2114	2128	2143	rBV	119978	197065	15.14%	1.663%
52	8.327	2171	2173	2178	rVB2	172	151	0.01%	0.001%
53	8.468	2213	2217	2220	rBV3	376	386	0.03%	0.003%
54	8.555	2233	2244	2257	rBV2	119486	197848	15.20%	1.670%
55	8.635	2257	2269	2306	rVV	413055	713382	54.79%	6.021%
56	8.809	2317	2323	2326	rBV3	398	449	0.03%	0.004%
57	8.928	2355	2360	2362	rBV2	203	228	0.02%	0.002%
58	9.002	2381	2383	2386	rBV	167	133	0.01%	0.001%
59	9.111	2412	2417	2419	rBV2	143	132	0.01%	0.001%
60	9.420	2500	2513	2539	rBV	541950	883996	67.89%	7.461%
61	9.574	2555	2561	2569	rVB3	638	1031	0.08%	0.009%
62	9.693	2590	2598	2608	rBV4	1783	2838	0.22%	0.024%
63	9.777	2615	2624	2635	rVB2	7537	11674	0.90%	0.099%
64	10.105	2720	2726	2731	rVB3	469	469	0.04%	0.004%
65	10.233	2764	2766	2775	rVB3	265	212	0.02%	0.002%
66	10.468	2833	2839	2843	rBV2	171	254	0.02%	0.002%
67	10.532	2849	2859	2875	rVB2	5885	11114	0.85%	0.094%
68	10.613	2878	2884	2886	rBV	237	293	0.02%	0.002%
69	10.674	2895	2903	2912	rVB5	3413	5337	0.41%	0.045%
70	10.761	2917	2930	2949	rBV	418286	672252	51.63%	5.674%
71	10.902	2970	2974	2978	rVB3	319	284	0.02%	0.002%
72	11.002	3001	3005	3010	rVB2	201	251	0.02%	0.002%
73	11.124	3037	3043	3046	rBV3	717	665	0.05%	0.006%
74	11.140	3046	3048	3051	rVV3	493	347	0.03%	0.003%
75	11.208	3065	3069	3075	rBV2	173	214	0.02%	0.002%
76	11.385	3119	3124	3128	rBV2	306	336	0.03%	0.003%

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Integrator: RTE

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

77	11.465	3139	3149	3159	rBV5	1819	3438	0.26%	0.029%
78	11.587	3181	3187	3190	rVV4	346	436	0.03%	0.004%
79	11.700	3215	3222	3233	rVB4	1465	2253	0.17%	0.019%
80	11.767	3233	3243	3245	rBV2	321	556	0.04%	0.005%
81	11.815	3245	3258	3276	rBV	491819	784324	60.24%	6.620%
82	11.941	3292	3297	3302	rBV4	1062	1196	0.09%	0.010%
83	12.066	3331	3336	3337	rBV2	424	314	0.02%	0.003%
84	12.198	3357	3377	3396	rBV	528327	860344	66.08%	7.262%
85	12.336	3414	3420	3423	rVB2	523	519	0.04%	0.004%
86	12.401	3438	3440	3445	rBV2	275	162	0.01%	0.001%
87	12.532	3475	3481	3486	rBV2	286	405	0.03%	0.003%
88	12.680	3522	3527	3533	rBV	212	370	0.03%	0.003%
89	12.876	3583	3588	3590	rBV2	256	282	0.02%	0.002%
90	12.918	3598	3601	3603	rBV	241	175	0.01%	0.001%
91	13.143	3668	3671	3674	rBV2	255	149	0.01%	0.001%
92	13.330	3726	3729	3732	rBV2	191	134	0.01%	0.001%
93	13.719	3848	3850	3855	rBV	229	242	0.02%	0.002%
94	14.089	3961	3965	3966	rBV2	282	204	0.02%	0.002%
95	14.227	4006	4008	4011	rBV	199	139	0.01%	0.001%
96	14.455	4077	4079	4084	rBV2	243	166	0.01%	0.001%
97	14.658	4140	4142	4145	rBV2	233	179	0.01%	0.002%
98	14.709	4155	4158	4160	rVB2	274	144	0.01%	0.001%
99	14.944	4228	4231	4237	rVB2	261	281	0.02%	0.002%
100	14.973	4237	4240	4244	rBV3	363	404	0.03%	0.003%

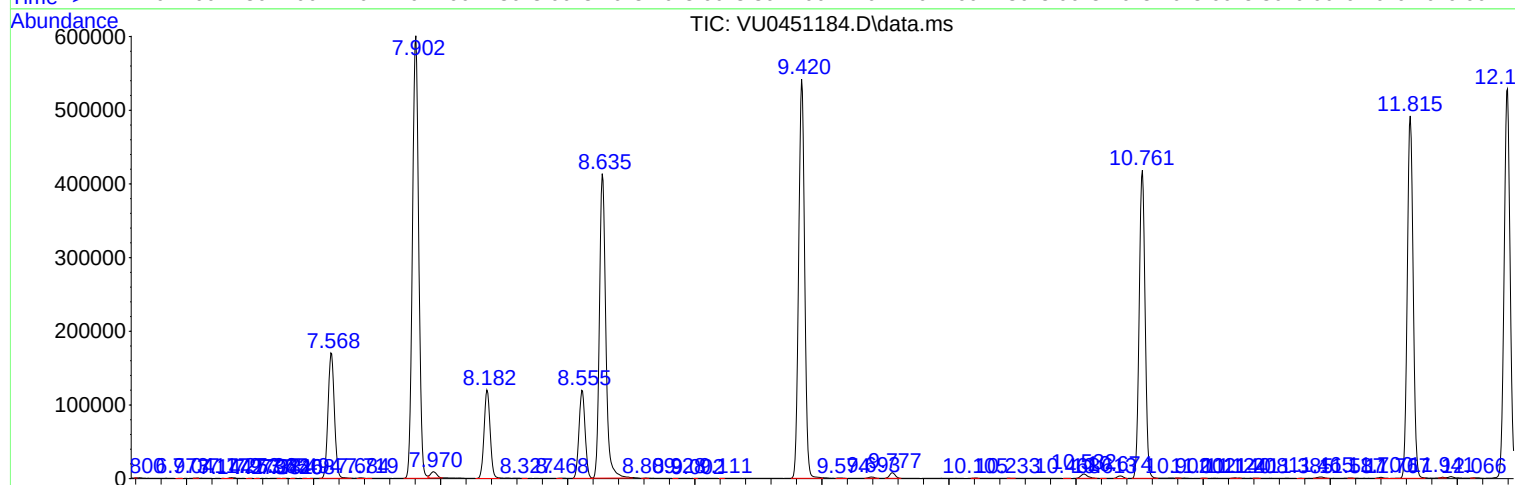
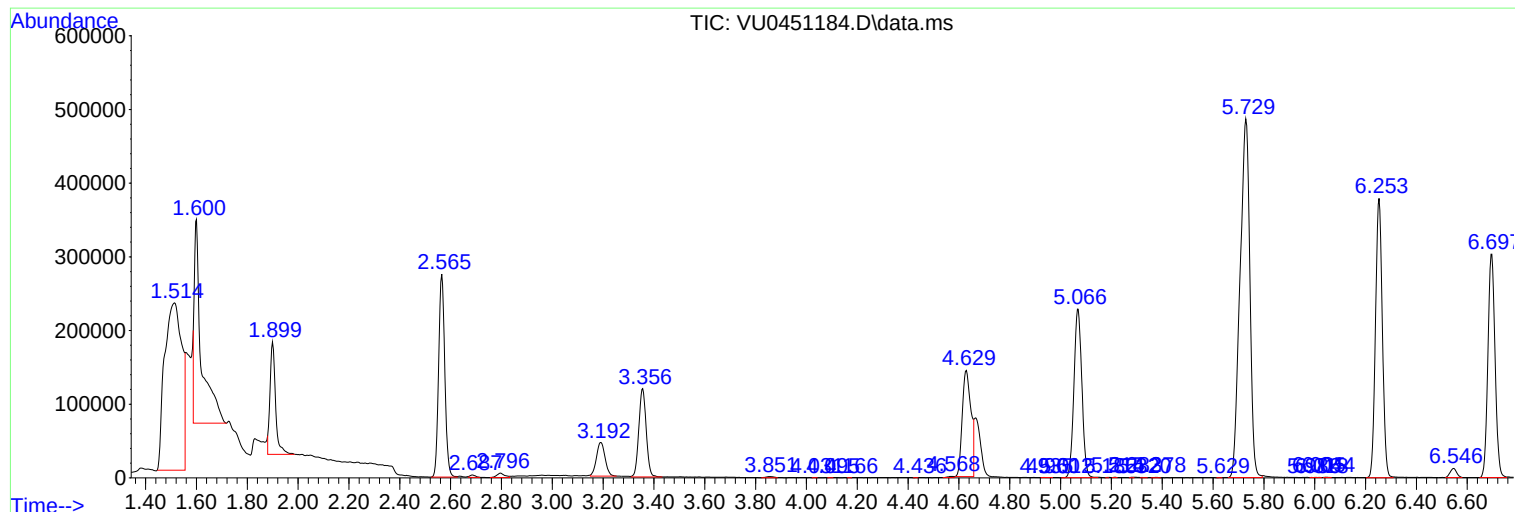
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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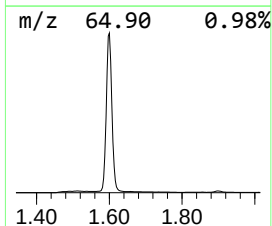
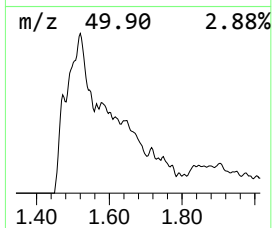
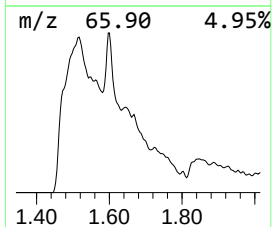
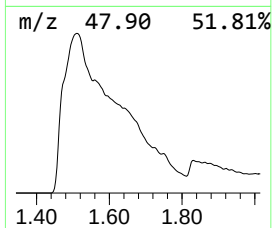
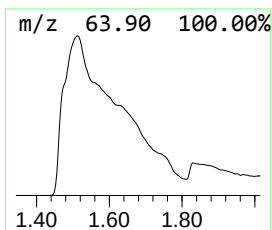
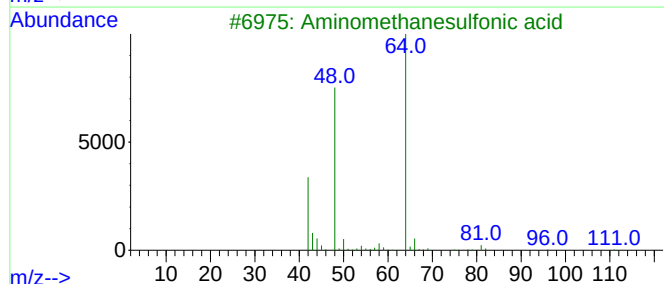
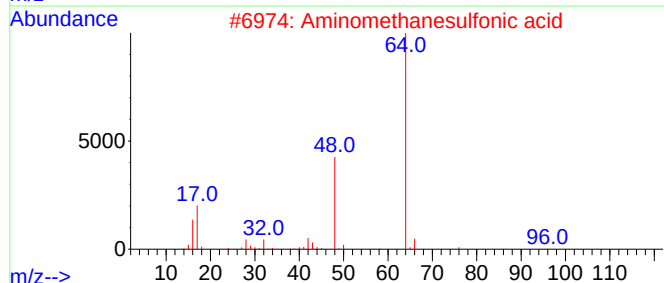
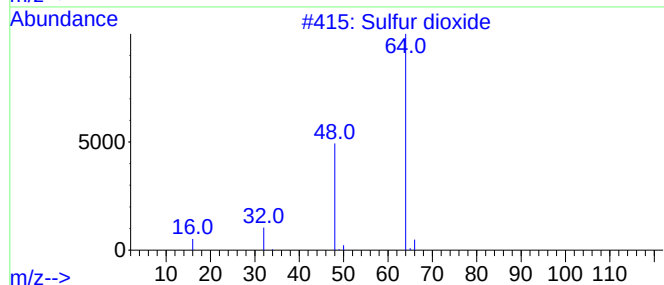
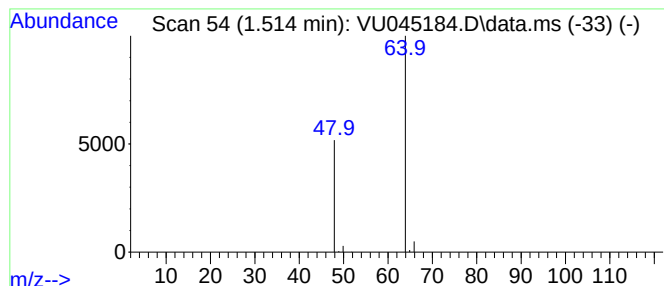
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.514	76.89 ug/L	1087260	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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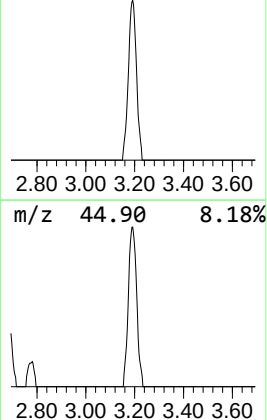
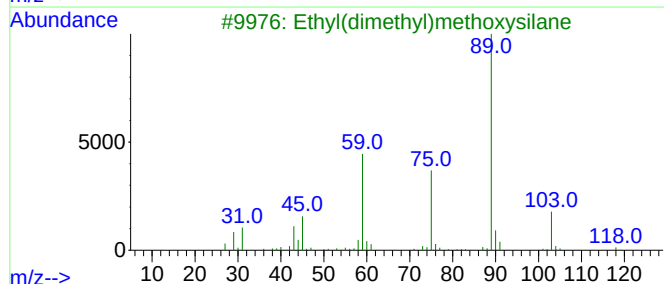
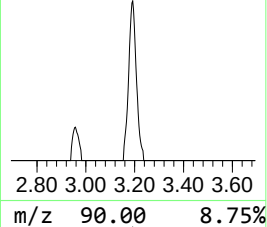
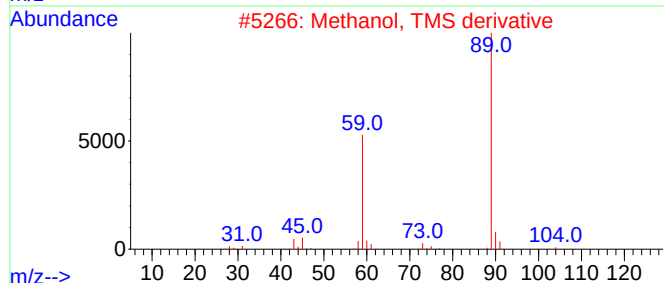
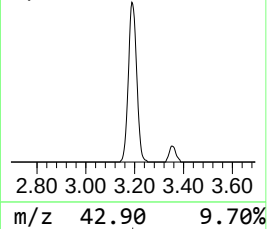
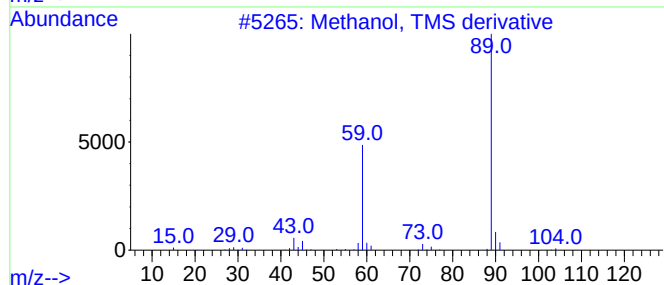
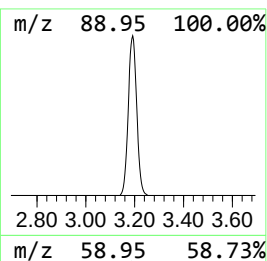
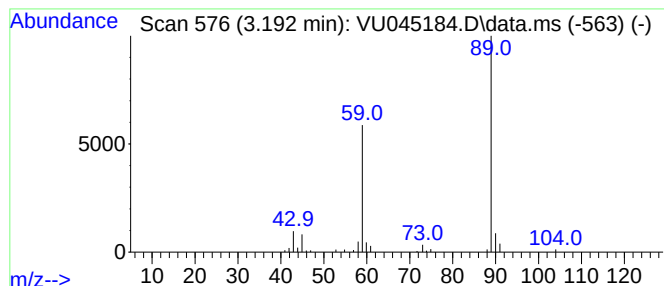
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Methanol, TMS derivative Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.192	7.57 ug/L	106989	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	91
2			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	91
3			Ethyl(dimethyl)methoxysilane	118	C5H14OSi	052686-75-6	74
4			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	74
5			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	64



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.514	76.9	ug/L	1087260	1	6.253	707004	50.0
Methanol, TMS d...	3.192	7.6	ug/L	106989	1	6.253	707004	50.0