

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
 Data File : VV021275.D
 Acq On : 04 May 2021 17:13
 Operator : SY/MD
 Sample : M2209-18ME 400X
 Misc : 6.27g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG7F3ME

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_V\Method\SFAMVLM050321WMA.M

Title : VOC Analysis

Signal : TIC: VV021275.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	77	83	91	rBV	175704	169007	7.14%	0.834%
2	1.568	158	164	174	rVB	186068	198644	8.40%	0.980%
3	2.108	323	332	344	rBV	447199	623866	26.37%	3.078%
4	2.400	419	423	426	rBV4	1377	964	0.04%	0.005%
5	2.442	430	436	438	rBV6	1706	1728	0.07%	0.009%
6	2.474	441	446	448	rBV4	1439	1476	0.06%	0.007%
7	2.510	451	457	459	rBV4	5556	6336	0.27%	0.031%
8	2.587	477	481	486	rVB8	1773	1701	0.07%	0.008%
9	2.622	486	492	495	rBV5	2989	3126	0.13%	0.015%
10	2.754	526	533	534	rBV5	1225	1125	0.05%	0.006%
11	2.851	558	563	566	rVB4	947	809	0.03%	0.004%
12	2.947	589	593	596	rBV5	1223	1082	0.05%	0.005%
13	2.979	600	603	606	rBV2	1369	1031	0.04%	0.005%
14	3.034	615	620	624	rBV7	1452	1312	0.06%	0.006%
15	3.056	624	627	630	rVB5	1682	1144	0.05%	0.006%
16	3.220	674	678	681	rBV5	1353	1295	0.05%	0.006%
17	3.236	681	683	686	rVB4	1510	920	0.04%	0.005%
18	3.365	718	723	726	rVB4	1558	1142	0.05%	0.006%
19	3.764	838	847	849	rBV7	1604	1838	0.08%	0.009%
20	3.844	867	872	875	rBV4	1304	1145	0.05%	0.006%
21	3.905	879	891	922	rBV2	116599	430520	18.20%	2.124%
22	4.352	1015	1030	1054	rBV2	394424	931684	39.38%	4.597%
23	4.600	1105	1107	1110	rVV4	1289	845	0.04%	0.004%
24	4.670	1127	1129	1136	rVB5	1677	1666	0.07%	0.008%
25	4.754	1153	1155	1159	rBV3	1272	915	0.04%	0.005%
26	4.818	1173	1175	1180	rVB5	1416	1112	0.05%	0.005%
27	4.867	1185	1190	1193	rBV7	1124	1055	0.04%	0.005%
28	5.050	1230	1247	1271	rBV3	810389	2103732	88.92%	10.381%
29	5.362	1341	1344	1348	rBV5	1353	1246	0.05%	0.006%
30	5.449	1367	1371	1372	rBV3	1270	918	0.04%	0.005%
31	5.567	1403	1408	1411	rBV5	1616	1492	0.06%	0.007%
32	5.622	1413	1425	1451	rBV	837517	1680935	71.05%	8.294%
33	5.908	1504	1514	1530	rBV2	46911	102372	4.33%	0.505%
34	6.008	1542	1545	1548	rBV5	1510	1130	0.05%	0.006%
35	6.075	1551	1566	1592	rBV2	451999	939421	39.71%	4.635%
36	6.362	1651	1655	1656	rVV3	1442	1043	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
 Data File : VV021275.D
 Acq On : 04 May 2021 17:13
 Operator : SY/MD
 Sample : M2209-18ME 400X
 Misc : 6.27g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG7F3ME

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_V\Method\SFAMVLM050321WMA.M
 Title : VOC Analysis

37	6.436	1672	1678	1681	rBV6	1900	2014	0.09%	0.010%
38	6.545	1708	1712	1715	rVB5	1223	1138	0.05%	0.006%
39	6.564	1715	1718	1723	rVB3	1119	861	0.04%	0.004%
40	6.609	1730	1732	1740	rVB8	1038	1011	0.04%	0.005%
41	6.722	1762	1767	1769	rBV5	1086	844	0.04%	0.004%
42	6.812	1792	1795	1798	rVV4	1665	1160	0.05%	0.006%
43	6.844	1802	1805	1809	rBV2	1993	1219	0.05%	0.006%
44	6.866	1809	1812	1815	rBV5	1297	965	0.04%	0.005%
45	6.992	1840	1851	1867	rBV2	283735	520675	22.01%	2.569%
46	7.320	1940	1953	1973	rBV	981410	1699794	71.85%	8.387%
47	7.516	2010	2014	2020	rBV6	2279	2664	0.11%	0.013%
48	7.551	2023	2025	2027	rVB2	2185	944	0.04%	0.005%
49	7.587	2033	2036	2039	rBV4	1818	1406	0.06%	0.007%
50	7.625	2039	2048	2066	rBV2	204759	366830	15.51%	1.810%
51	7.825	2105	2110	2113	rBV5	2582	2680	0.11%	0.013%
52	7.979	2143	2158	2175	rBV	1447222	2365864	100.00%	11.674%
53	8.095	2185	2194	2228	rBV2	503815	969385	40.97%	4.783%
54	8.468	2308	2310	2312	rBV3	1570	876	0.04%	0.004%
55	8.583	2342	2346	2349	rBV5	1922	1787	0.08%	0.009%
56	8.670	2369	2373	2375	rVB4	1558	1137	0.05%	0.006%
57	8.709	2381	2385	2387	rBV4	1414	862	0.04%	0.004%
58	8.783	2406	2408	2414	rVB5	2227	1578	0.07%	0.008%
59	8.857	2418	2431	2450	rBV	1242636	2039728	86.21%	10.065%
60	9.027	2479	2484	2488	rVB6	2559	2098	0.09%	0.010%
61	9.111	2505	2510	2513	rBV6	1557	1440	0.06%	0.007%
62	9.188	2532	2534	2539	rVB5	1920	1129	0.05%	0.006%
63	9.249	2550	2553	2557	rBV4	1090	991	0.04%	0.005%
64	9.394	2593	2598	2604	rBV5	1350	1570	0.07%	0.008%
65	9.429	2604	2609	2615	rVV9	1698	2154	0.09%	0.011%
66	9.574	2652	2654	2659	rVB5	2026	1155	0.05%	0.006%
67	9.677	2682	2686	2688	rBV4	1420	835	0.04%	0.004%
68	9.693	2688	2691	2694	rVV4	1436	1113	0.05%	0.005%
69	9.722	2698	2700	2705	rVB5	1385	1116	0.05%	0.006%
70	10.008	2787	2789	2795	rVB4	1303	922	0.04%	0.005%
71	10.046	2795	2801	2803	rBV5	1141	959	0.04%	0.005%
72	10.127	2821	2826	2828	rBV5	2386	2365	0.10%	0.012%
73	10.223	2844	2856	2873	rVV2	709940	1089320	46.04%	5.375%
74	10.442	2921	2924	2927	rVB4	2093	1244	0.05%	0.006%
75	10.477	2930	2935	2937	rBV5	1931	1488	0.06%	0.007%
76	10.542	2950	2955	2957	rBV6	2276	1784	0.08%	0.009%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
 Data File : VV021275.D
 Acq On : 04 May 2021 17:13
 Operator : SY/MD
 Sample : M2209-18ME 400X
 Misc : 6.27g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG7F3ME

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_V\Method\SFAMVLM050321WMA.M
 Title : VOC Analysis

77	10.580	2962	2967	2970	rVV7	1938	1653	0.07%	0.008%
78	10.921	3068	3073	3074	rBV4	3992	2859	0.12%	0.014%
79	11.255	3166	3177	3199	rBV	1329436	2074206	87.67%	10.235%
80	11.632	3281	3294	3311	rBV	1159012	1841900	77.85%	9.089%
81	11.796	3339	3345	3349	rBV6	1919	2010	0.08%	0.010%
82	11.931	3383	3387	3393	rBV7	1144	1442	0.06%	0.007%
83	12.059	3424	3427	3429	rBV4	1310	814	0.03%	0.004%
84	12.114	3440	3444	3445	rVV3	1263	966	0.04%	0.005%
85	12.127	3445	3448	3453	rVB5	1697	1361	0.06%	0.007%
86	12.230	3477	3480	3483	rBV4	1709	1584	0.07%	0.008%
87	12.468	3552	3554	3558	rVV4	2033	1291	0.05%	0.006%
88	12.529	3570	3573	3575	rBV3	1753	976	0.04%	0.005%
89	12.664	3612	3615	3620	rVB4	2331	2160	0.09%	0.011%
90	12.702	3623	3627	3630	rBV5	1458	1405	0.06%	0.007%
91	12.783	3648	3652	3655	rBV5	1805	1433	0.06%	0.007%
92	13.127	3757	3759	3763	rBV3	1887	961	0.04%	0.005%
93	13.628	3912	3915	3917	rBV5	1617	1035	0.04%	0.005%
94	13.712	3939	3941	3944	rBV3	1659	898	0.04%	0.004%
95	13.831	3975	3978	3980	rBV3	2041	1070	0.05%	0.005%
96	13.934	4008	4010	4013	rBV4	1702	805	0.03%	0.004%
97	14.021	4034	4037	4043	rBV7	1834	1697	0.07%	0.008%
98	14.123	4066	4069	4072	rBV3	1491	946	0.04%	0.005%
99	14.390	4149	4152	4158	rBV7	2575	3268	0.14%	0.016%
100	14.937	4319	4322	4326	rBV4	2335	2516	0.11%	0.012%

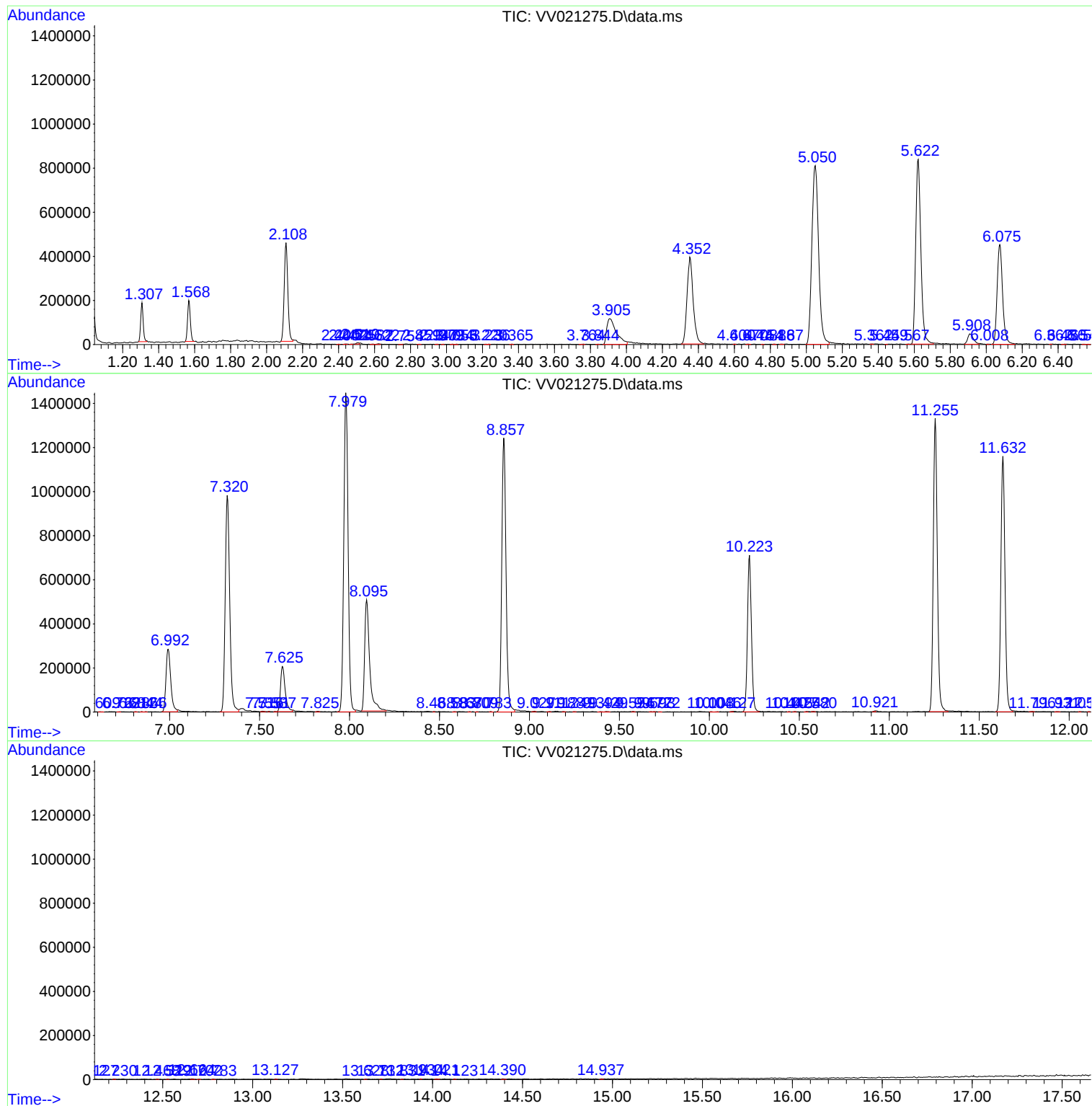
Sum of corrected areas: 20266138

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
Data File : VV021275.D
Acq On : 04 May 2021 17:13
Operator : SY/MD
Sample : M2209-18ME 400X
Misc : 6.27g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG7F3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
Data File : VV021275.D
Acq On : 04 May 2021 17:13
Operator : SY/MD
Sample : M2209-18ME 400X
Misc : 6.27g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG7F3ME

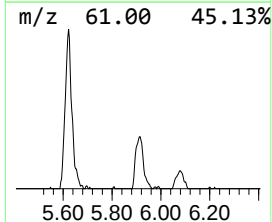
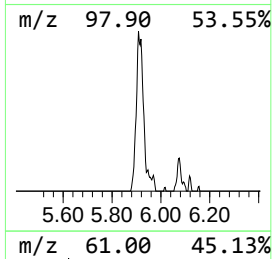
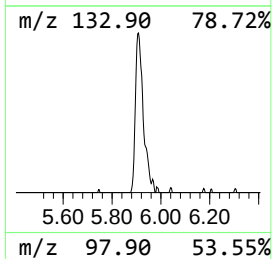
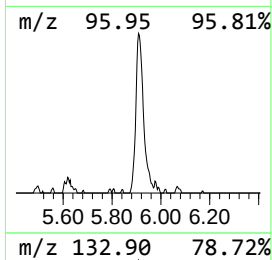
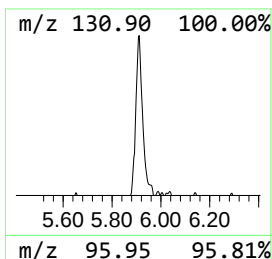
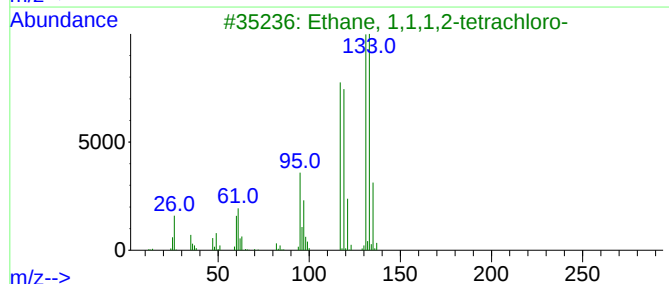
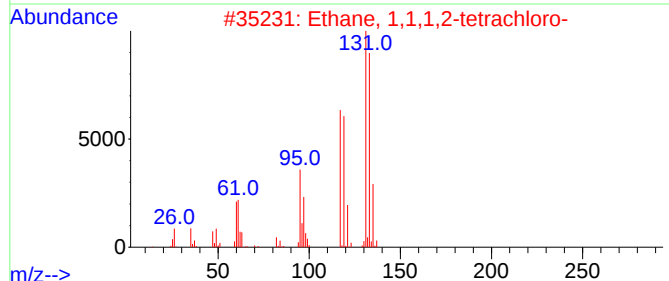
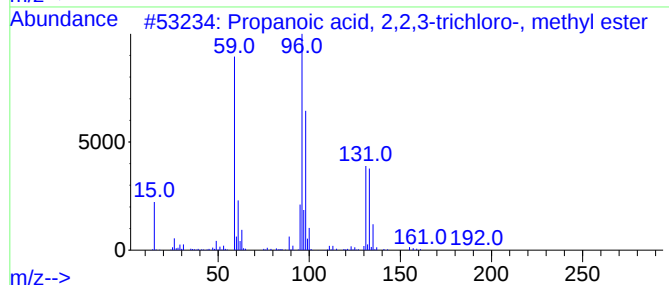
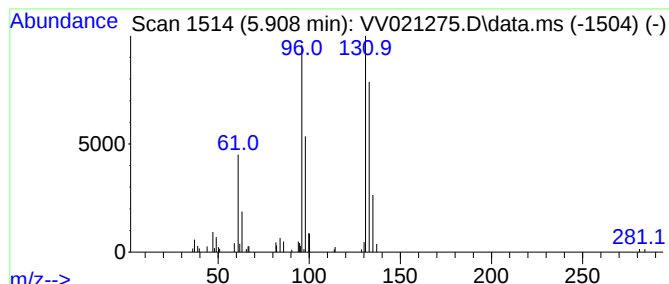
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	3.05 ug/L	102372	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25
4			Clorethate	322	C5H4Cl6O3	005634-37-7	25
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050421\
Data File : VV021275.D
Acq On : 04 May 2021 17:13
Operator : SY/MD
Sample : M2209-18ME 400X
Misc : 6.27g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG7F3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.908	3.0	ug/L	102372	1	5.622	1680940	50.0