

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
 Data File : VV021921.D
 Acq On : 20 Aug 2021 18:13
 Operator : SY/MD
 Sample : M3458-19ME
 Misc : 4.91g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0B64ME

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\SFAMVLM081621WMA.M
 Title : VOC Analysis

Signal : TIC: VV021921.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	107	rBV	133532	183256	14.33%	1.766%
2	2.072	312	321	334	rBV	278109	391772	30.64%	3.776%
3	2.439	428	435	438	rBV4	2406	3283	0.26%	0.032%
4	2.667	504	506	510	rVB2	556	355	0.03%	0.003%
5	2.744	525	530	533	rBV2	410	393	0.03%	0.004%
6	2.825	550	555	556	rBV2	335	315	0.02%	0.003%
7	2.876	566	571	574	rBV3	417	409	0.03%	0.004%
8	3.018	607	615	617	rBV6	842	1152	0.09%	0.011%
9	3.063	627	629	632	rVB	516	257	0.02%	0.002%
10	3.105	640	642	645	rBV2	484	277	0.02%	0.003%
11	3.175	661	664	667	rBV	358	296	0.02%	0.003%
12	3.227	677	680	683	rBV3	411	251	0.02%	0.002%
13	3.339	711	715	717	rBV	458	300	0.02%	0.003%
14	3.725	832	835	836	rBV	290	180	0.01%	0.002%
15	3.825	859	866	869	rBV2	443	477	0.04%	0.005%
16	3.892	875	887	928	rBV2	65683	251777	19.69%	2.427%
17	4.346	1011	1028	1056	rBV	185454	491855	38.46%	4.741%
18	4.568	1095	1097	1099	rVB	570	286	0.02%	0.003%
19	4.580	1099	1101	1104	rBV2	311	217	0.02%	0.002%
20	4.629	1112	1116	1120	rBV2	580	534	0.04%	0.005%
21	4.670	1127	1129	1132	rVB4	564	313	0.02%	0.003%
22	4.690	1132	1135	1138	rVB3	412	305	0.02%	0.003%
23	4.751	1152	1154	1156	rBV2	291	183	0.01%	0.002%
24	4.822	1173	1176	1177	rBV2	537	245	0.02%	0.002%
25	4.847	1182	1184	1187	rBV	413	212	0.02%	0.002%
26	4.867	1187	1190	1195	rVB2	453	387	0.03%	0.004%
27	4.976	1218	1224	1226	rBV3	407	301	0.02%	0.003%
28	5.040	1227	1244	1276	rBV2	515647	1278782	100.00%	12.326%
29	5.339	1323	1337	1345	rBV8	5725	14439	1.13%	0.139%
30	5.532	1393	1397	1398	rBV	528	255	0.02%	0.002%
31	5.613	1407	1422	1455	rBV	465126	975483	76.28%	9.403%
32	5.805	1480	1482	1486	rBV2	554	404	0.03%	0.004%
33	5.905	1501	1513	1531	rBV2	24505	54380	4.25%	0.524%
34	6.069	1552	1564	1591	rVB	262101	556734	43.54%	5.366%
35	6.291	1630	1633	1636	rBV3	713	577	0.05%	0.006%
36	6.342	1645	1649	1650	rBV3	359	215	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
 Data File : VV021921.D
 Acq On : 20 Aug 2021 18:13
 Operator : SY/MD
 Sample : M3458-19ME
 Misc : 4.91g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0B64ME

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\SFAMVLM081621WMA.M
 Title : VOC Analysis

37	6.352	1650	1652	1656	rVB3	637	311	0.02%	0.003%
38	6.371	1656	1658	1661	rBV	404	272	0.02%	0.003%
39	6.426	1673	1675	1678	rBV	658	268	0.02%	0.003%
40	6.561	1714	1717	1722	rBV3	458	320	0.03%	0.003%
41	6.648	1735	1744	1754	rVV9	1456	2955	0.23%	0.028%
42	6.725	1766	1768	1772	rVB2	515	251	0.02%	0.002%
43	6.748	1772	1775	1776	rBV2	431	231	0.02%	0.002%
44	6.799	1789	1791	1795	rVB	332	199	0.02%	0.002%
45	6.915	1824	1827	1830	rVV2	340	180	0.01%	0.002%
46	6.989	1838	1850	1874	rBV	137139	272741	21.33%	2.629%
47	7.317	1939	1952	1972	rBV	590034	1061270	82.99%	10.230%
48	7.625	2037	2048	2074	rBV	90112	181093	14.16%	1.746%
49	7.751	2085	2087	2089	rBV	467	271	0.02%	0.003%
50	7.831	2110	2112	2115	rBV2	470	293	0.02%	0.003%
51	7.889	2127	2130	2133	rBV3	609	427	0.03%	0.004%
52	7.944	2144	2147	2151	rVB3	615	530	0.04%	0.005%
53	7.985	2156	2160	2164	rBV3	250	242	0.02%	0.002%
54	8.108	2183	2198	2223	rBV2	229305	532808	41.67%	5.136%
55	8.580	2342	2345	2346	rBV2	420	213	0.02%	0.002%
56	8.783	2406	2408	2413	rVB2	306	194	0.02%	0.002%
57	8.854	2418	2430	2458	rBV	676661	1197249	93.62%	11.540%
58	9.082	2498	2501	2506	rVB4	860	720	0.06%	0.007%
59	9.133	2511	2517	2518	rBV3	733	568	0.04%	0.005%
60	9.268	2557	2559	2562	rVB2	459	208	0.02%	0.002%
61	9.317	2573	2574	2578	rVB2	630	238	0.02%	0.002%
62	9.346	2578	2583	2585	rBV	248	234	0.02%	0.002%
63	9.561	2643	2650	2654	rBV4	660	862	0.07%	0.008%
64	9.648	2675	2677	2682	rVB3	350	273	0.02%	0.003%
65	9.677	2682	2686	2687	rBV	486	309	0.02%	0.003%
66	9.763	2710	2713	2714	rBV2	768	417	0.03%	0.004%
67	9.866	2737	2745	2750	rBV4	344	435	0.03%	0.004%
68	9.911	2752	2759	2763	rBV5	2603	3333	0.26%	0.032%
69	10.001	2782	2787	2789	rBV2	349	275	0.02%	0.003%
70	10.127	2818	2826	2834	rBV3	5476	8791	0.69%	0.085%
71	10.223	2843	2856	2880	rBV	376510	606370	47.42%	5.845%
72	10.471	2932	2933	2937	rBV2	505	372	0.03%	0.004%
73	10.522	2939	2949	2958	rVV6	4676	7361	0.58%	0.071%
74	10.580	2959	2967	2984	rVV10	2949	6870	0.54%	0.066%
75	10.661	2987	2992	3001	rVB5	1024	1435	0.11%	0.014%
76	10.702	3001	3005	3010	rBV3	509	415	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
 Data File : VV021921.D
 Acq On : 20 Aug 2021 18:13
 Operator : SY/MD
 Sample : M3458-19ME
 Misc : 4.91g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0B64ME

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\SFAMVLM081621WMA.M
 Title : VOC Analysis

77	10.879	3055	3060	3062	rBV2	903	702	0.05%	0.007%
78	10.921	3065	3073	3082	rVB7	4914	8677	0.68%	0.084%
79	11.037	3102	3109	3113	rBV4	1754	2036	0.16%	0.020%
80	11.153	3137	3145	3153	rVB7	2765	4244	0.33%	0.041%
81	11.191	3153	3157	3159	rBV3	1135	750	0.06%	0.007%
82	11.252	3165	3176	3194	rBV	798202	1241332	97.07%	11.965%
83	11.493	3249	3251	3253	rBV2	509	225	0.02%	0.002%
84	11.542	3258	3266	3271	rBV6	2424	3436	0.27%	0.033%
85	11.628	3281	3293	3313	rBV	637956	1004956	78.59%	9.687%
86	11.905	3377	3379	3381	rVB3	640	233	0.02%	0.002%
87	12.046	3420	3423	3425	rBV3	765	472	0.04%	0.005%
88	12.197	3467	3470	3473	rVV2	394	274	0.02%	0.003%
89	12.313	3504	3506	3510	rVB2	495	267	0.02%	0.003%
90	12.336	3510	3513	3516	rVB2	554	347	0.03%	0.003%
91	12.368	3519	3523	3527	rBV4	410	446	0.03%	0.004%
92	12.458	3545	3551	3553	rBV3	331	371	0.03%	0.004%
93	12.587	3585	3591	3593	rBV3	783	930	0.07%	0.009%
94	12.763	3644	3646	3649	rBV	327	237	0.02%	0.002%
95	12.841	3667	3670	3671	rBV	358	240	0.02%	0.002%
96	13.185	3772	3777	3779	rBV2	333	309	0.02%	0.003%
97	13.429	3850	3853	3855	rBV2	573	202	0.02%	0.002%
98	13.670	3925	3928	3930	rVB2	487	199	0.02%	0.002%
99	13.879	3991	3993	3996	rVB	681	337	0.03%	0.003%
100	13.902	3996	4000	4002	rBV3	636	553	0.04%	0.005%

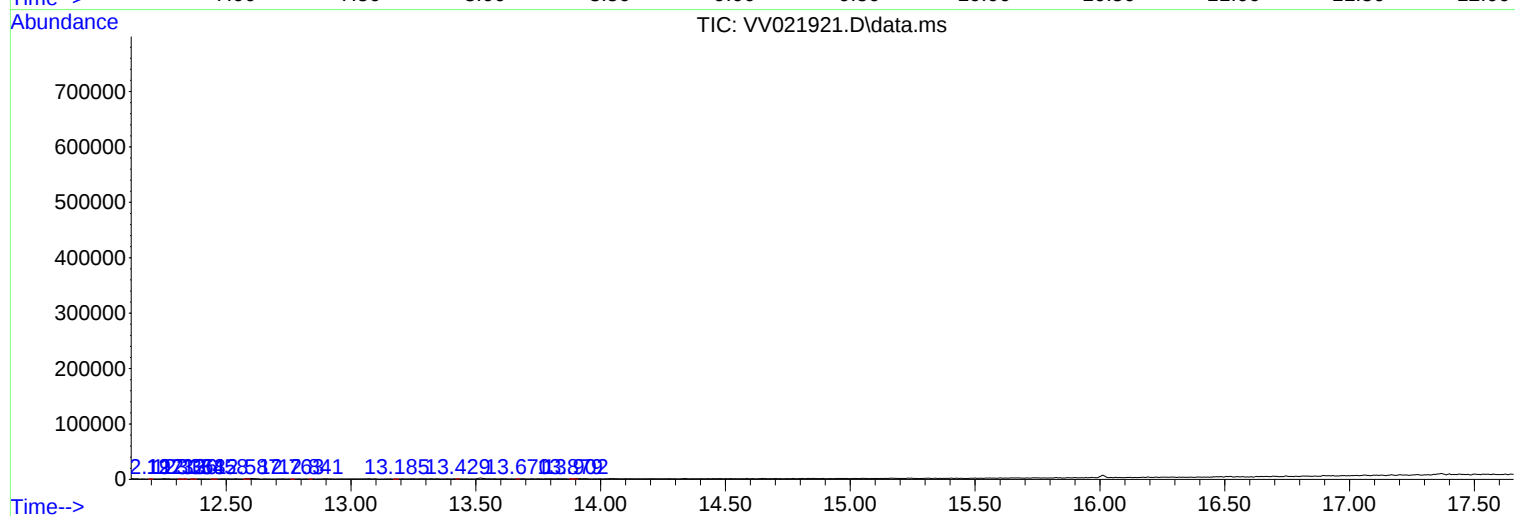
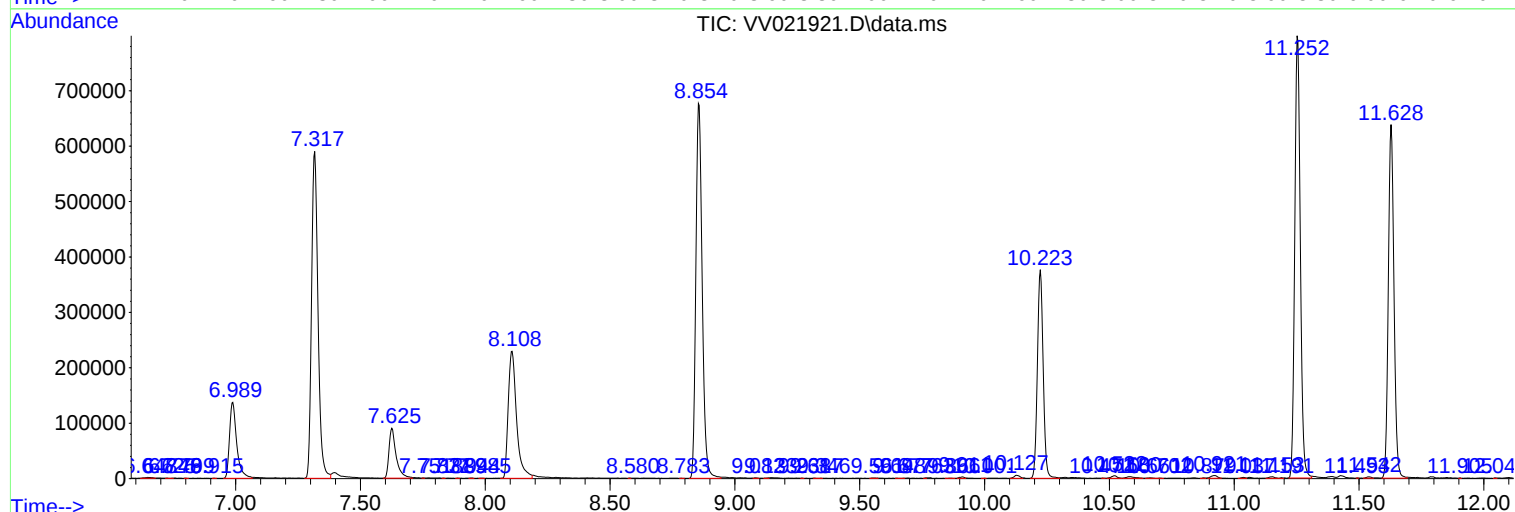
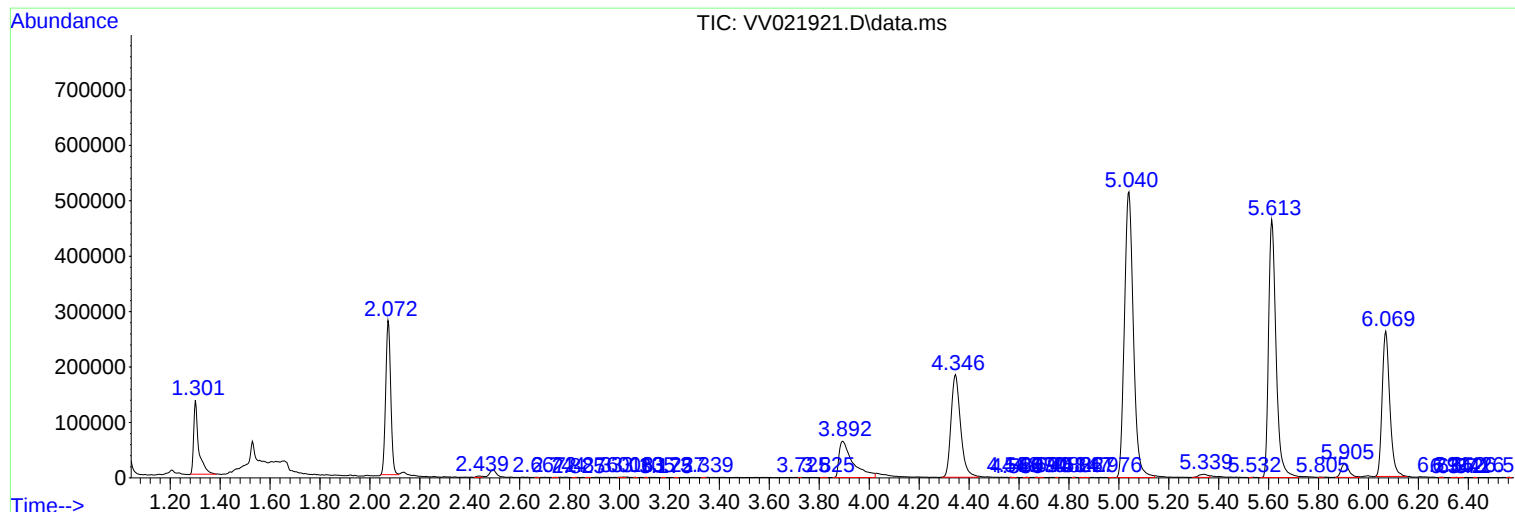
Sum of corrected areas: 10374436

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
Data File : VV021921.D
Acq On : 20 Aug 2021 18:13
Operator : SY/MD
Sample : M3458-19ME
Misc : 4.91g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0B64ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
Data File : VV021921.D
Acq On : 20 Aug 2021 18:13
Operator : SY/MD
Sample : M3458-19ME
Misc : 4.91g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0B64ME

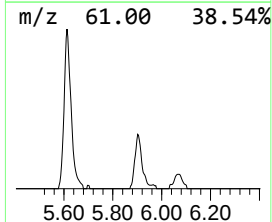
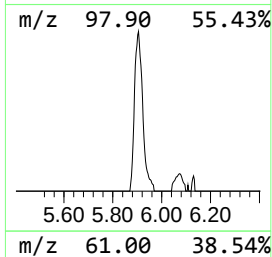
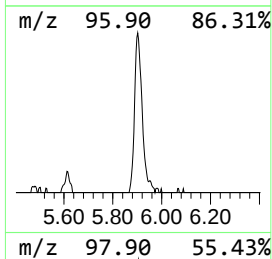
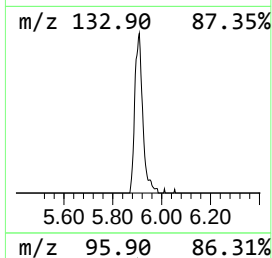
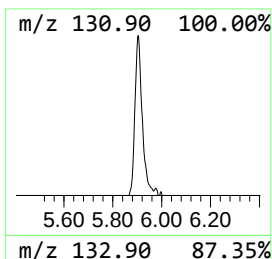
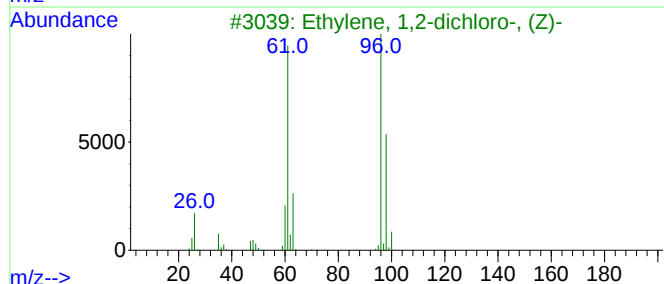
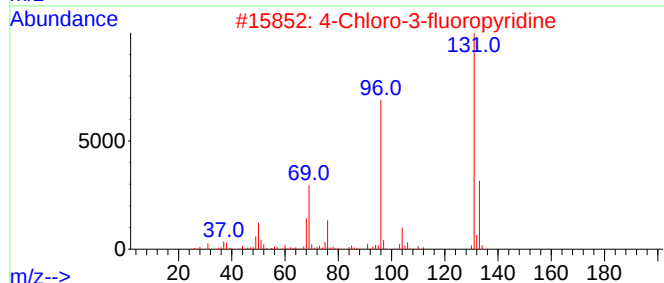
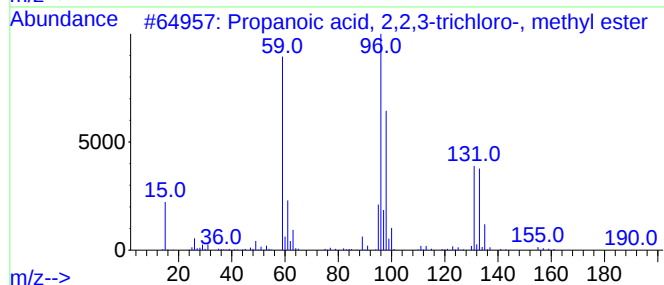
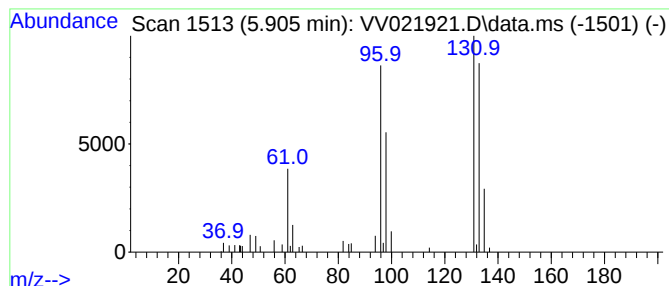
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.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.
5.905	2.79 ug/L	54380	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	72
2			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	38
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	35
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082021\
Data File : VV021921.D
Acq On : 20 Aug 2021 18:13
Operator : SY/MD
Sample : M3458-19ME
Misc : 4.91g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0B64ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM081621WMA.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
Propanoic acid,...	5.905	2.8	ug/L	54380	1	5.613	975483	50.0