

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD042823\
 Data File : VD075890.D
 Acq On : 28 Apr 2023 16:20
 Operator : KP/SY
 Sample : 02525-19
 Misc : 5.39G/10.00ml/MSVOA_D/SOIL
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 DCCM2

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_D\Method\SFAMDLM042023SMA.M
 Title : SFAM01.0

Signal : TIC: VD075890.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.734	14	25	36	rBV	164676	297659	17.23%	1.983%
2	2.152	91	96	98	rBV4	2554	4506	0.26%	0.030%
3	2.276	111	117	125	rBV	245453	359844	20.82%	2.397%
4	2.417	135	141	152	rBV	147966	258114	14.94%	1.719%
5	2.599	167	172	174	rBV3	2677	4753	0.28%	0.032%
6	2.799	200	206	214	rVB	208007	377044	21.82%	2.511%
7	3.317	291	294	295	rBV2	717	629	0.04%	0.004%
8	3.511	325	327	328	rBV2	809	527	0.03%	0.004%
9	3.628	339	347	355	rBV3	8855	21014	1.22%	0.140%
10	3.764	366	370	373	rBV2	802	1028	0.06%	0.007%
11	3.805	375	377	378	rVB	1027	550	0.03%	0.004%
12	3.917	385	396	405	rBV	205048	542638	31.40%	3.614%
13	4.023	405	414	431	rVB	253804	700182	40.52%	4.663%
14	4.340	466	468	470	rVB2	1097	825	0.05%	0.005%
15	4.381	473	475	477	rVB	800	578	0.03%	0.004%
16	4.399	477	478	479	rBV	907	554	0.03%	0.004%
17	4.564	505	506	508	rVB	801	561	0.03%	0.004%
18	4.622	513	516	518	rVB	499	479	0.03%	0.003%
19	4.664	522	523	525	rBV	655	439	0.03%	0.003%
20	4.681	525	526	530	rVB2	855	826	0.05%	0.006%
21	4.793	536	545	546	rBV3	20168	33020	1.91%	0.220%
22	4.899	561	563	567	rBV2	514	784	0.05%	0.005%
23	5.011	579	582	584	rBV2	490	527	0.03%	0.004%
24	5.475	658	661	662	rBV	429	417	0.02%	0.003%
25	5.517	666	668	671	rVB2	442	448	0.03%	0.003%
26	5.634	686	688	690	rVV2	729	521	0.03%	0.003%
27	5.811	715	718	719	rBV	730	690	0.04%	0.005%
28	5.828	719	721	722	rBV2	1385	1295	0.07%	0.009%
29	5.893	730	732	736	rVB2	767	888	0.05%	0.006%
30	5.934	736	739	741	rBV2	621	754	0.04%	0.005%
31	6.058	758	760	761	rBV2	570	551	0.03%	0.004%
32	6.164	775	778	779	rVB	597	421	0.02%	0.003%
33	6.187	779	782	783	rBV2	512	461	0.03%	0.003%
34	6.399	816	818	822	rBV	537	621	0.04%	0.004%
35	6.464	828	829	832	rBV2	456	412	0.02%	0.003%
36	6.616	854	855	857	rBV	641	435	0.03%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM042023SMA.M
 Title : SFAM01.0

37	6.805	883	887	888	rBV2	992	1046	0.06%	0.007%
38	6.905	903	904	906	rBV	700	623	0.04%	0.004%
39	6.987	909	918	927	rBV2	39292	108786	6.30%	0.725%
40	7.364	981	982	984	rBV	583	514	0.03%	0.003%
41	7.422	989	992	994	rBV2	808	800	0.05%	0.005%
42	7.440	994	995	997	rBV2	699	527	0.03%	0.004%
43	7.564	1006	1016	1033	rBV	285988	789188	45.67%	5.256%
44	7.828	1059	1061	1065	rVB2	700	879	0.05%	0.006%
45	7.863	1065	1067	1068	rBV	574	569	0.03%	0.004%
46	7.899	1070	1073	1074	rBV2	562	491	0.03%	0.003%
47	7.934	1078	1079	1082	rBV2	480	450	0.03%	0.003%
48	8.205	1112	1125	1143	rBV2	585826	1728019	100.00%	11.509%
49	8.458	1166	1168	1169	rBV2	861	712	0.04%	0.005%
50	8.546	1182	1183	1185	rBV	882	668	0.04%	0.004%
51	8.599	1190	1192	1193	rBV	613	444	0.03%	0.003%
52	8.634	1194	1198	1199	rBV2	1004	1060	0.06%	0.007%
53	8.687	1205	1207	1209	rVB	559	415	0.02%	0.003%
54	8.775	1213	1222	1233	rBV	645511	1305570	75.55%	8.696%
55	9.016	1254	1263	1273	rBV	125658	256665	14.85%	1.709%
56	9.152	1285	1286	1287	rBV	644	423	0.02%	0.003%
57	9.210	1287	1296	1309	rVV	402567	830308	48.05%	5.530%
58	9.346	1317	1319	1321	rVB2	1162	575	0.03%	0.004%
59	9.599	1361	1362	1365	rVV2	1162	927	0.05%	0.006%
60	9.622	1365	1366	1367	rVV	1047	415	0.02%	0.003%
61	9.834	1400	1402	1406	rVB2	1082	1322	0.08%	0.009%
62	9.899	1411	1413	1416	rVB2	665	570	0.03%	0.004%
63	9.981	1419	1427	1434	rBV	203180	374937	21.70%	2.497%
64	10.152	1451	1456	1461	rBV3	6908	12138	0.70%	0.081%
65	10.269	1468	1476	1485	rBV	849782	1504838	87.08%	10.023%
66	10.440	1502	1505	1507	rBV2	1103	1443	0.08%	0.010%
67	10.481	1510	1512	1513	rBV2	815	735	0.04%	0.005%
68	10.528	1513	1520	1528	rVV	132228	232185	13.44%	1.546%
69	10.622	1533	1536	1537	rVV	774	934	0.05%	0.006%
70	10.663	1538	1543	1549	rVV	8611	15898	0.92%	0.106%
71	10.722	1551	1553	1555	rBV	943	663	0.04%	0.004%
72	10.810	1564	1568	1572	rBV3	3875	4639	0.27%	0.031%
73	10.875	1573	1579	1587	rBV	141083	252632	14.62%	1.683%
74	11.128	1620	1622	1625	rBV2	766	621	0.04%	0.004%
75	11.352	1658	1660	1668	rVB4	1707	2657	0.15%	0.018%
76	11.581	1691	1699	1711	rBV	979778	1677913	97.10%	11.175%

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77	11.681	1714	1716	1717	rBV	809	426	0.02%	0.003%
78	11.757	1727	1729	1730	rBV	1083	884	0.05%	0.006%
79	11.840	1741	1743	1745	rVB2	698	436	0.03%	0.003%
80	12.057	1779	1780	1782	rVB	1189	684	0.04%	0.005%
81	12.081	1782	1784	1785	rBV	768	411	0.02%	0.003%
82	12.199	1800	1804	1808	rBV3	1753	2808	0.16%	0.019%
83	12.228	1808	1809	1812	rVB2	620	492	0.03%	0.003%
84	12.487	1852	1853	1856	rVB2	922	545	0.03%	0.004%
85	12.522	1856	1859	1860	rBV	860	914	0.05%	0.006%
86	12.581	1861	1869	1874	rVB2	11492	21299	1.23%	0.142%
87	12.651	1874	1881	1889	rBV	258414	435075	25.18%	2.898%
88	13.087	1952	1955	1956	rBV2	1280	1308	0.08%	0.009%
89	13.228	1973	1979	1985	rBV2	11156	18954	1.10%	0.126%
90	13.410	2008	2010	2011	rBV	693	435	0.03%	0.003%
91	13.434	2011	2014	2017	rBV3	4176	4731	0.27%	0.032%
92	13.522	2021	2029	2038	rBV	924540	1532659	88.69%	10.208%
93	13.604	2042	2043	2044	rBV	2321	1522	0.09%	0.010%
94	13.722	2061	2063	2066	rVB2	1964	1907	0.11%	0.013%
95	13.816	2071	2079	2091	rVB	759709	1226630	70.98%	8.170%
96	14.051	2114	2119	2124	rVB2	12399	19252	1.11%	0.128%
97	14.251	2152	2153	2154	rBV	915	490	0.03%	0.003%
98	14.269	2154	2156	2158	rVV2	1601	1624	0.09%	0.011%
99	14.393	2175	2177	2178	rBV2	1057	657	0.04%	0.004%
100	15.404	2347	2349	2356	rVB4	7285	10949	0.63%	0.073%

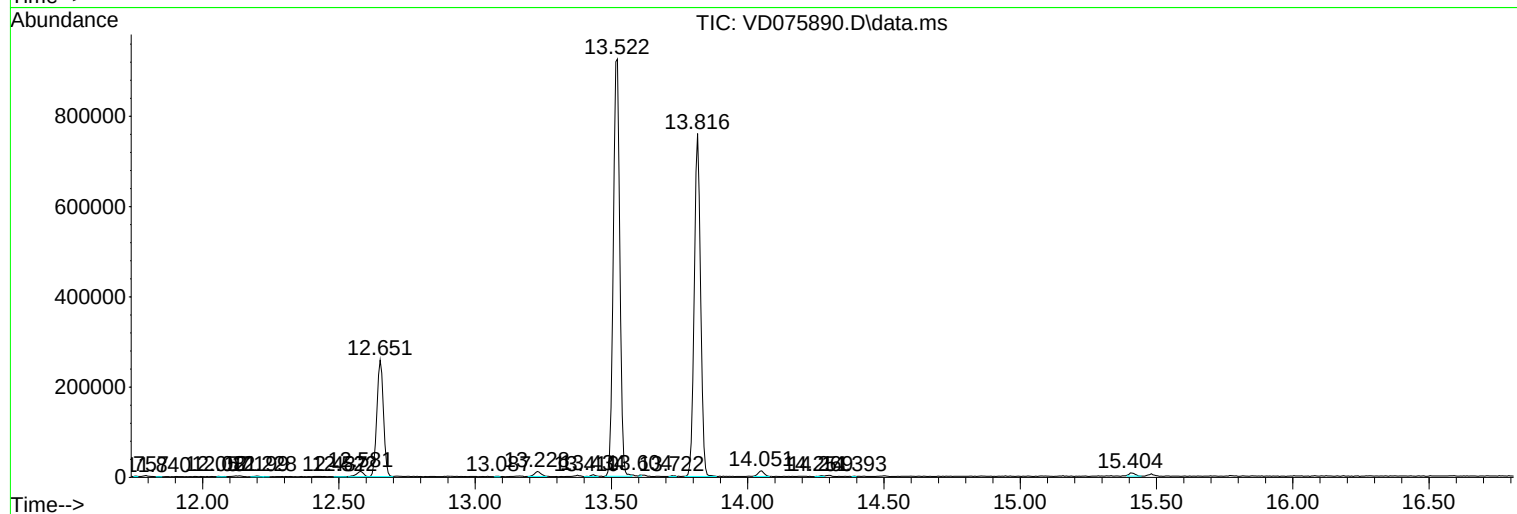
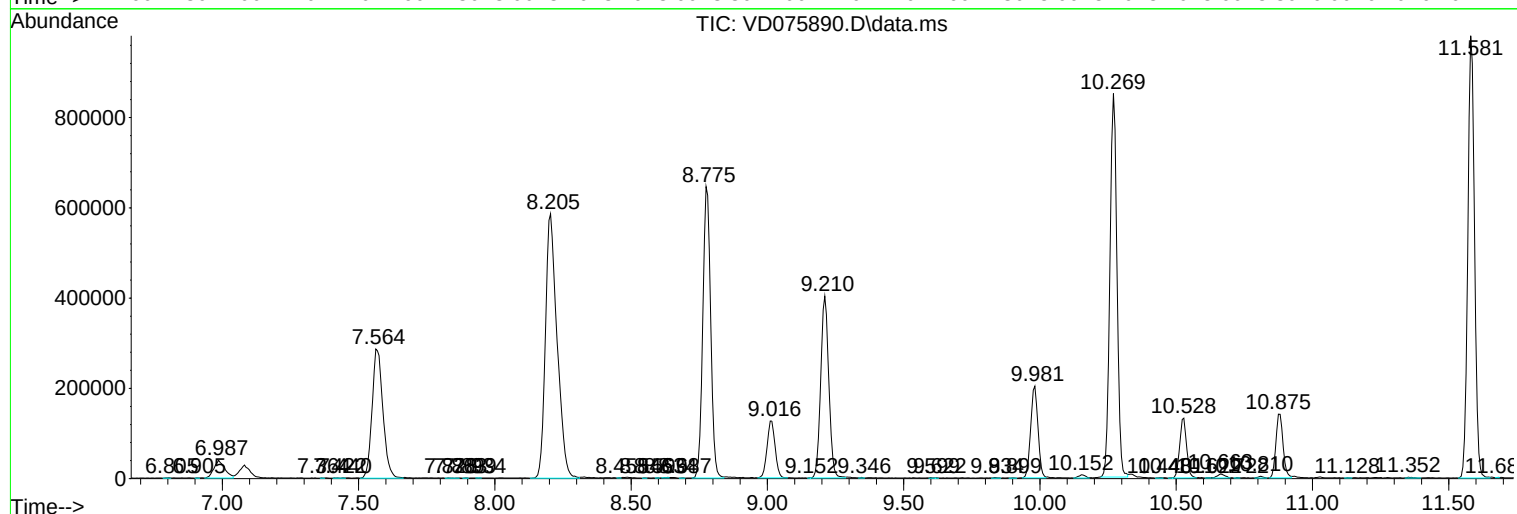
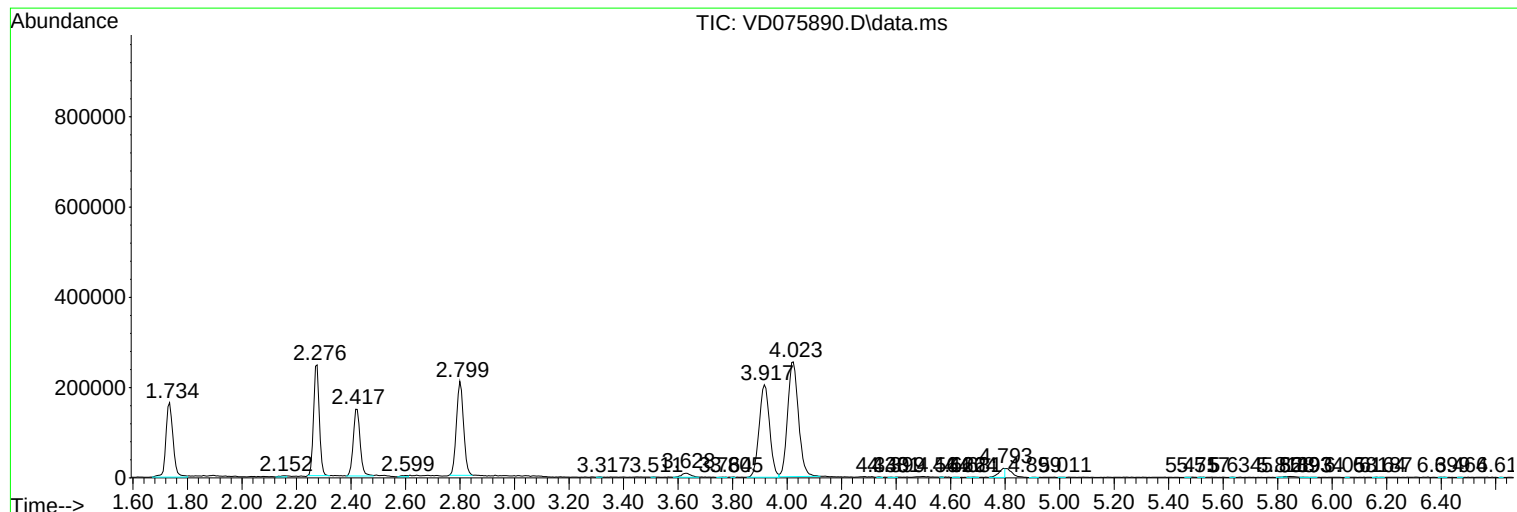
Sum of corrected areas: 15014286

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM042023SMA.M
Quant Title : SFAM01.0

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



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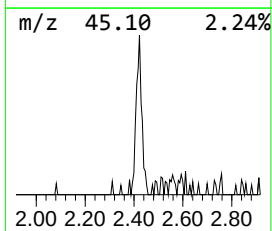
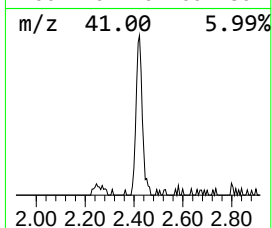
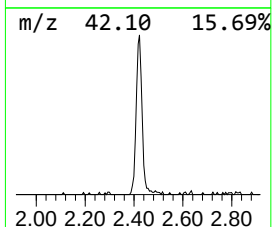
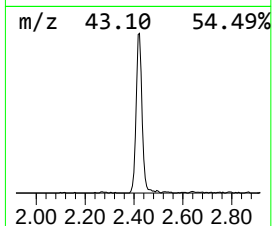
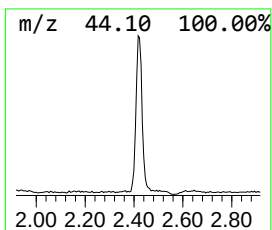
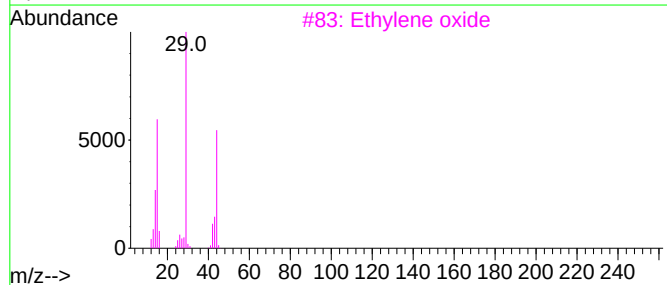
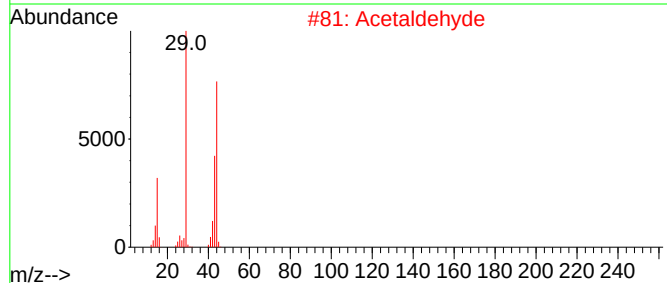
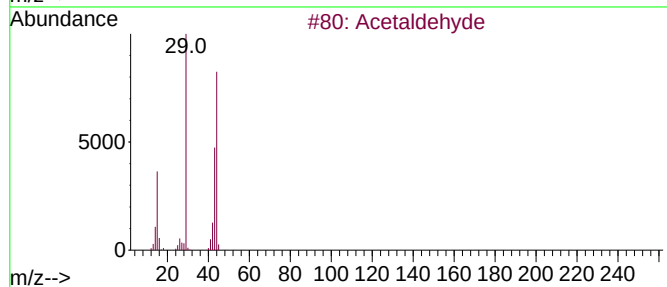
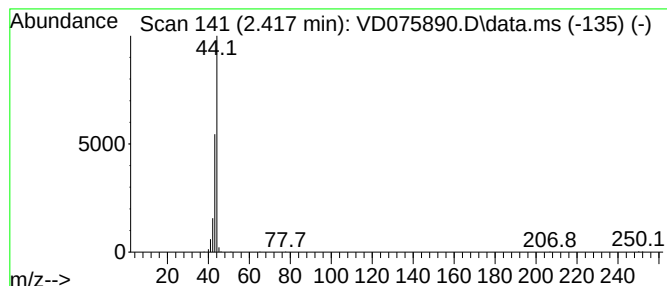
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM042023SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.417	4.94 ug/L	258114	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	64
2			Acetaldehyde	44	C2H4O	000075-07-0	64
3			Ethylene oxide	44	C2H4O	000075-21-8	5
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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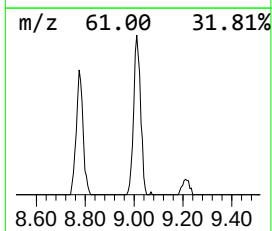
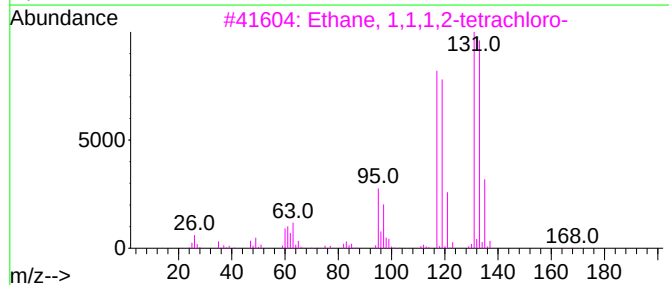
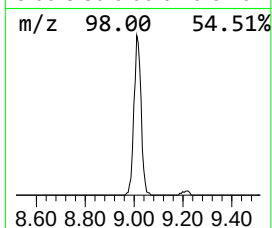
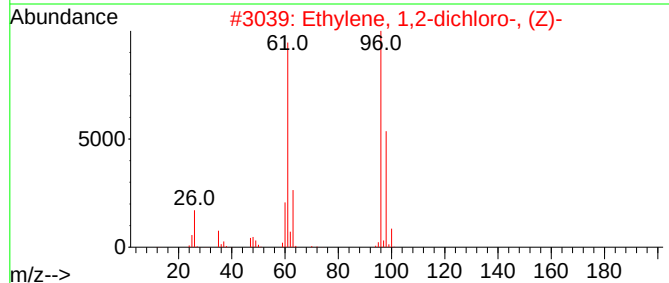
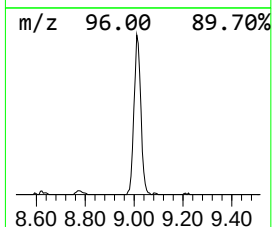
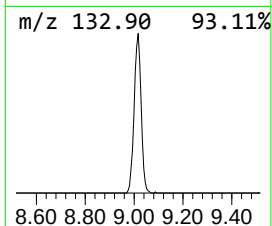
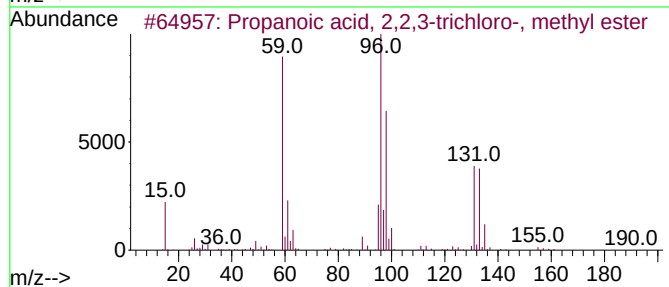
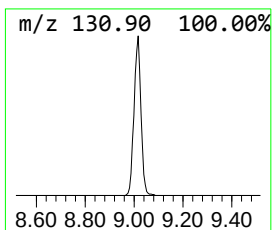
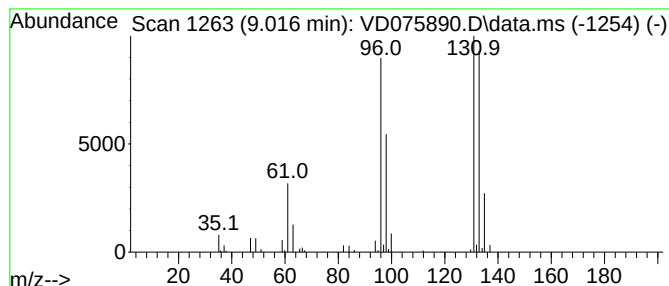
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM042023SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Propanoic acid, 2,2,3-trich... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.016	4.91 ug/L	256665	1,4-Difluorobenzene	8.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	30
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25
4			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	25
5			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	16



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Quant Title : SFAM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.417	4.9	ug/L	258114	1	8.775	1305570	25.0
Propanoic acid,...	9.016	4.9	ug/L	256665	1	8.775	1305570	25.0