

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121623\
 Data File : VX039293.D
 Acq On : 16 Dec 2023 16:16
 Operator : JC/MD
 Sample : 05845-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 64 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 YCHE6

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_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039293.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	15	rVB3	2389	3194	0.32%	0.036%
2	1.240	23	25	28	rBV	3855	4895	0.48%	0.056%
3	1.368	41	46	56	rVB	119827	139712	13.79%	1.585%
4	1.666	91	95	110	rVB	66887	101205	9.99%	1.148%
5	2.319	194	202	208	rBV2	552787	1012794	100.00%	11.492%
6	2.374	208	211	225	rVB	68619	112672	11.12%	1.278%
7	2.532	230	237	254	rBV	349062	634309	62.63%	7.198%
8	2.959	298	307	319	rVB2	7778	18503	1.83%	0.210%
9	3.105	325	331	340	rVB6	2684	7787	0.77%	0.088%
10	3.172	340	342	344	rBV	278	304	0.03%	0.003%
11	3.312	364	365	367	rBV	338	203	0.02%	0.002%
12	3.404	378	380	383	rBV2	261	260	0.03%	0.003%
13	3.526	398	400	402	rVV2	301	264	0.03%	0.003%
14	3.550	402	404	405	rVV2	460	293	0.03%	0.003%
15	3.611	406	414	426	rVB	41581	99157	9.79%	1.125%
16	3.892	456	460	462	rVB	190	244	0.02%	0.003%
17	3.953	466	470	471	rBV2	167	220	0.02%	0.002%
18	4.459	544	553	564	rBV2	88566	366525	36.19%	4.159%
19	5.056	633	651	672	rBV	121851	390534	38.56%	4.431%
20	5.276	685	687	690	rVB3	411	491	0.05%	0.006%
21	5.385	696	705	717	rVB2	12310	35322	3.49%	0.401%
22	5.532	727	729	731	rBV	308	260	0.03%	0.003%
23	5.970	789	801	816	rBV2	300015	896554	88.52%	10.173%
24	6.239	843	845	847	rBV2	373	388	0.04%	0.004%
25	6.373	864	867	870	rBV	212	254	0.03%	0.003%
26	6.434	874	877	878	rBV2	336	214	0.02%	0.002%
27	6.605	903	905	906	rBV	263	201	0.02%	0.002%
28	6.653	912	913	919	rVB3	305	396	0.04%	0.004%
29	6.763	922	931	950	rBV	224101	539007	53.22%	6.116%
30	7.129	982	991	1002	rBV3	9292	21967	2.17%	0.249%
31	7.306	1010	1020	1036	rBV	183684	407737	40.26%	4.627%
32	7.568	1059	1063	1064	rBV	163	207	0.02%	0.002%
33	7.678	1076	1081	1087	rVV2	1173	2689	0.27%	0.031%
34	7.915	1115	1120	1123	rVV4	740	1493	0.15%	0.017%
35	8.324	1181	1187	1199	rBV	126312	208392	20.58%	2.365%
36	8.580	1225	1229	1234	rVB2	450	692	0.07%	0.008%

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 Title : VOC Analysis

37	8.647	1234	1240	1251	rBV	445184	705350	69.64%	8.004%
38	8.879	1275	1278	1281	rVB2	320	407	0.04%	0.005%
39	8.952	1284	1290	1300	rBV	89727	135886	13.42%	1.542%
40	9.086	1310	1312	1314	rBV3	253	214	0.02%	0.002%
41	9.220	1332	1334	1336	rVB2	431	297	0.03%	0.003%
42	9.275	1336	1343	1349	rBV3	1558	2997	0.30%	0.034%
43	9.385	1355	1361	1379	rBV	384292	559711	55.26%	6.351%
44	9.805	1428	1430	1434	rBV	352	259	0.03%	0.003%
45	10.055	1465	1471	1490	rBV	481967	666512	65.81%	7.563%
46	10.262	1503	1505	1509	rBB2	201	226	0.02%	0.003%
47	10.305	1509	1512	1516	rBV4	816	1298	0.13%	0.015%
48	10.366	1520	1522	1523	rBV2	315	230	0.02%	0.003%
49	10.555	1552	1553	1556	rBV	320	264	0.03%	0.003%
50	10.646	1565	1568	1570	rBV2	680	787	0.08%	0.009%
51	10.750	1583	1585	1589	rVB2	221	278	0.03%	0.003%
52	10.787	1589	1591	1593	rBV	242	214	0.02%	0.002%
53	10.964	1617	1620	1624	rVV3	432	537	0.05%	0.006%
54	11.012	1624	1628	1635	rVV2	1989	3188	0.31%	0.036%
55	11.085	1637	1640	1645	rVB3	724	1210	0.12%	0.014%
56	11.189	1652	1657	1666	rBV	332899	433716	42.82%	4.921%
57	11.311	1673	1677	1682	rVB4	1334	2156	0.21%	0.024%
58	11.421	1691	1695	1698	rVB2	231	316	0.03%	0.004%
59	11.451	1698	1700	1703	rBV3	493	520	0.05%	0.006%
60	11.634	1727	1730	1732	rBV2	203	219	0.02%	0.002%
61	11.719	1740	1744	1745	rVV	204	248	0.02%	0.003%
62	11.756	1746	1750	1752	rVV2	509	553	0.05%	0.006%
63	11.854	1764	1766	1770	rVB2	183	202	0.02%	0.002%
64	11.969	1783	1785	1788	rVB2	365	264	0.03%	0.003%
65	12.024	1788	1794	1809	rBV	496794	663280	65.49%	7.526%
66	12.225	1823	1827	1837	rBV3	1488	2374	0.23%	0.027%
67	12.317	1837	1842	1850	rBV	474336	605525	59.79%	6.871%
68	12.573	1882	1884	1886	rBV2	261	264	0.03%	0.003%
69	12.640	1893	1895	1897	rBV	273	226	0.02%	0.003%
70	12.762	1911	1915	1919	rVV3	571	918	0.09%	0.010%
71	13.018	1955	1957	1963	rVB2	174	209	0.02%	0.002%
72	13.225	1985	1991	1992	rBV2	176	321	0.03%	0.004%
73	13.274	1997	1999	2001	rVB	309	255	0.03%	0.003%
74	13.305	2001	2004	2007	rBV2	394	572	0.06%	0.006%
75	13.433	2021	2025	2030	rVB3	1037	1398	0.14%	0.016%
76	13.591	2046	2051	2054	rBV4	1003	1291	0.13%	0.015%

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Integration Parameters: LSCINT.P

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

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 Title : VOC Analysis

77	13.646	2057	2060	2061	rVB	296	245	0.02%	0.003%
78	13.792	2079	2084	2087	rBV3	486	961	0.09%	0.011%
79	13.963	2108	2112	2115	rVB3	348	495	0.05%	0.006%
80	14.207	2149	2152	2156	rVB2	234	359	0.04%	0.004%
81	14.249	2156	2159	2162	rBV2	269	395	0.04%	0.004%
82	14.304	2166	2168	2171	rVB2	287	254	0.03%	0.003%
83	14.329	2171	2172	2176	rBV2	255	279	0.03%	0.003%
84	14.506	2199	2201	2204	rVB	310	274	0.03%	0.003%
85	14.603	2214	2217	2224	rBV3	934	1537	0.15%	0.017%
86	14.713	2232	2235	2236	rVB2	415	312	0.03%	0.004%
87	14.749	2239	2241	2243	rBV	355	204	0.02%	0.002%
88	14.816	2249	2252	2254	rBV3	167	255	0.03%	0.003%
89	15.036	2284	2288	2290	rBV3	237	349	0.03%	0.004%
90	15.140	2304	2305	2307	rBV	346	204	0.02%	0.002%
91	15.188	2311	2313	2315	rVB	378	260	0.03%	0.003%
92	15.207	2315	2316	2319	rBV	225	238	0.02%	0.003%
93	15.292	2326	2330	2331	rVB	341	329	0.03%	0.004%
94	15.347	2338	2339	2341	rBV	300	205	0.02%	0.002%
95	15.511	2363	2366	2368	rBV2	298	205	0.02%	0.002%
96	15.542	2368	2371	2376	rVB2	294	371	0.04%	0.004%
97	15.609	2381	2382	2385	rVB2	346	268	0.03%	0.003%
98	16.146	2467	2470	2472	rBV2	351	376	0.04%	0.004%
99	16.176	2472	2475	2476	rBV2	292	226	0.02%	0.003%
100	16.194	2476	2478	2480	rVB2	287	234	0.02%	0.003%

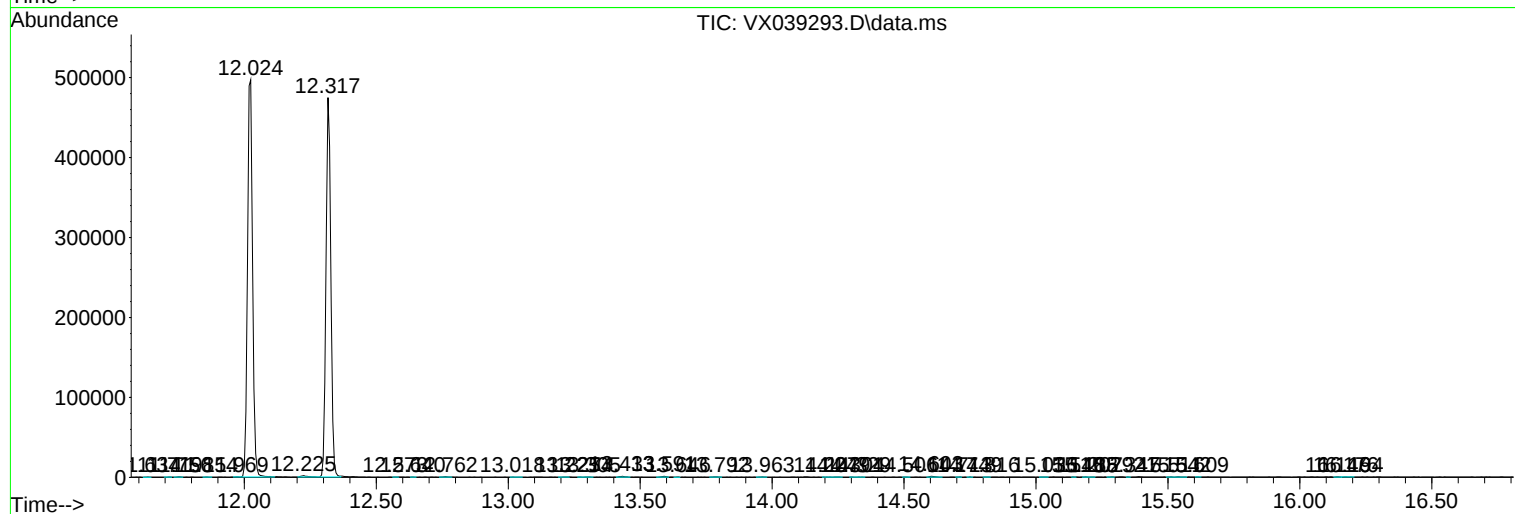
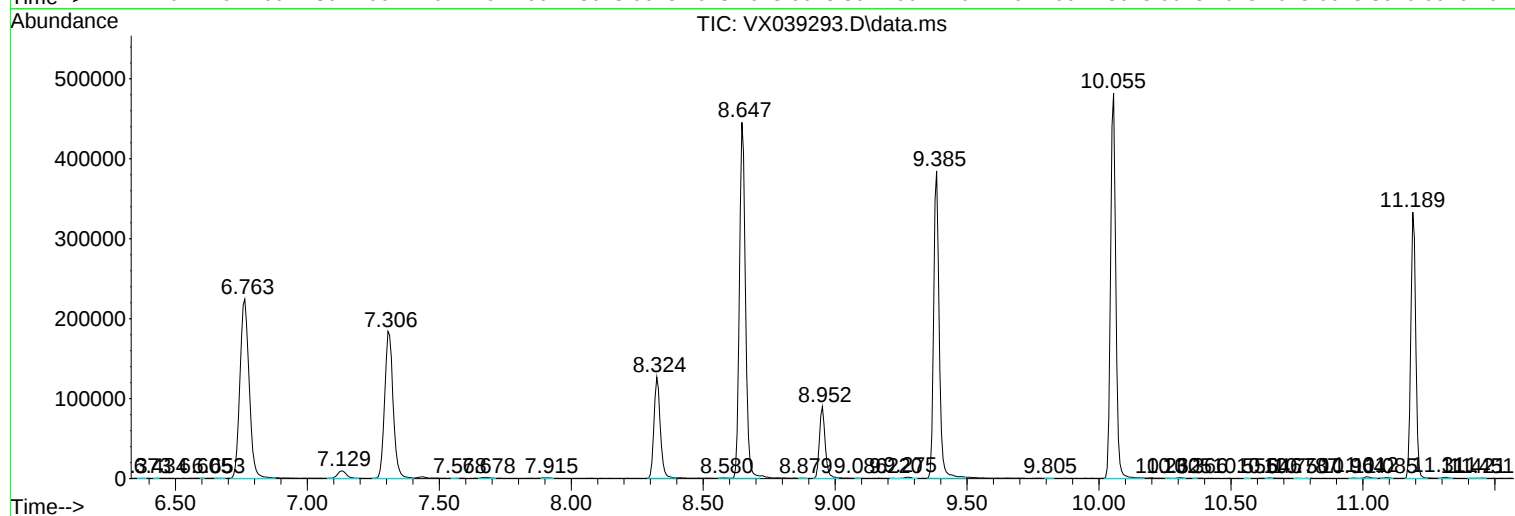
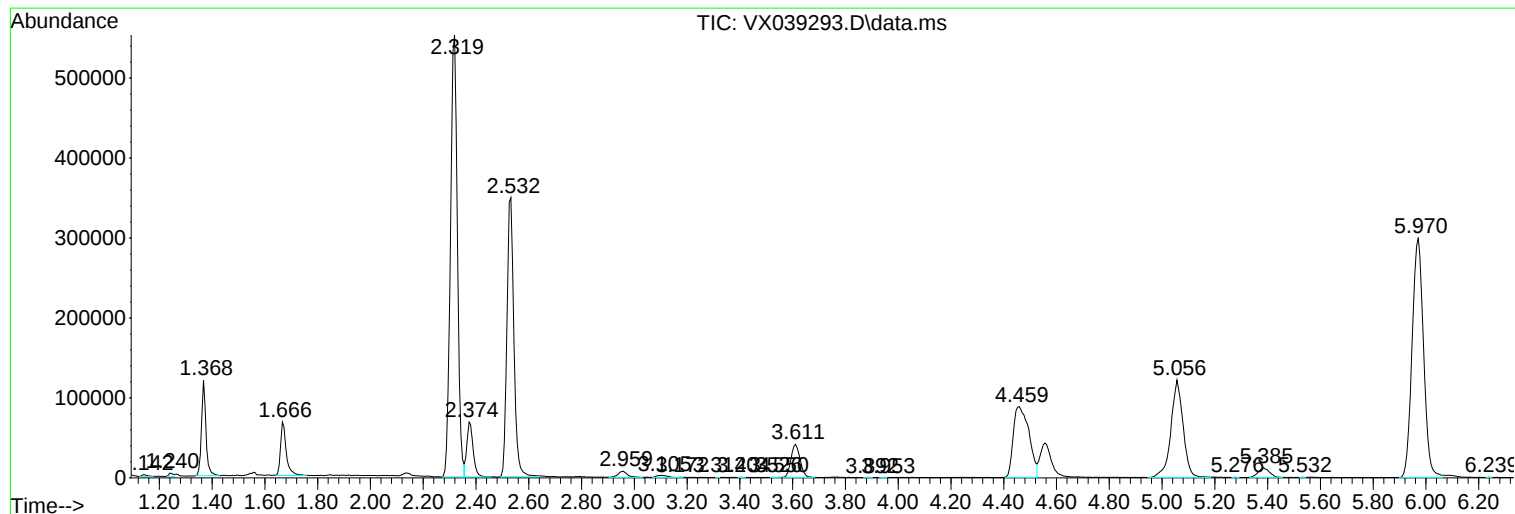
Sum of corrected areas: 8812866

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

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



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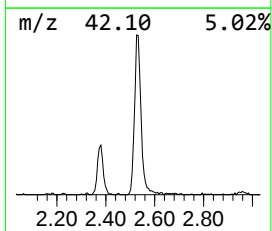
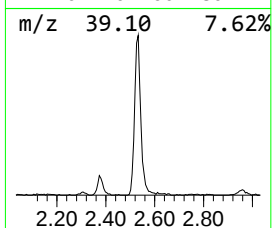
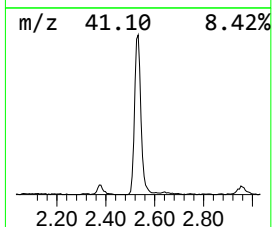
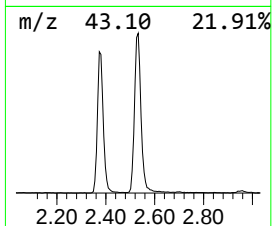
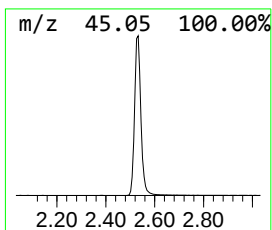
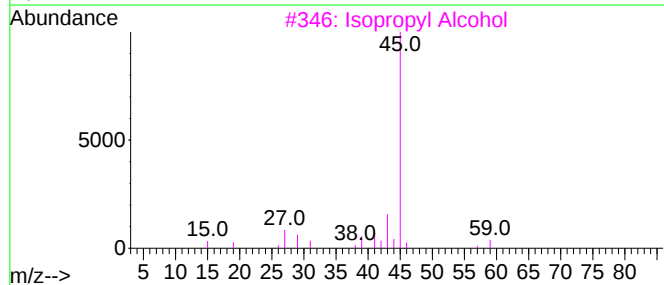
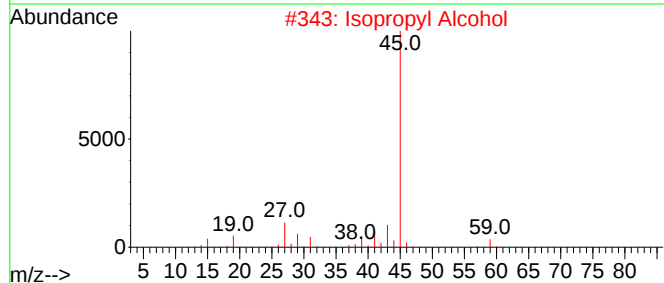
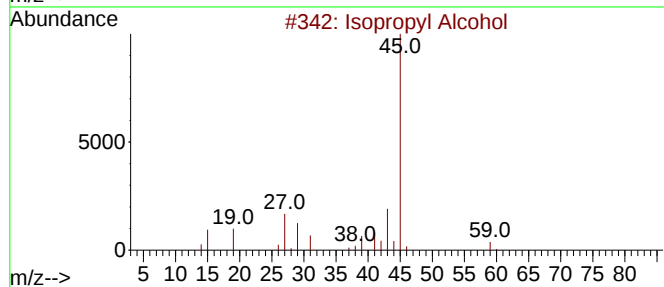
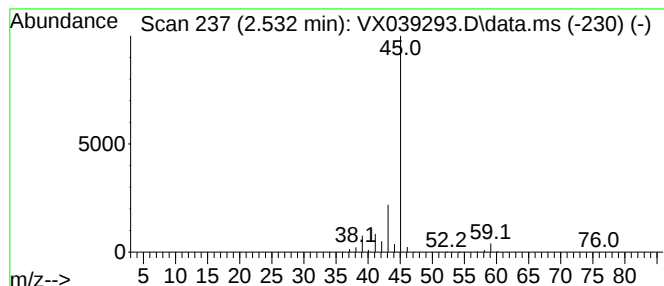
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.532	58.84 ug/L	634309	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
5			Isopropyl Alcohol	60	C3H8O	000067-63-0	9



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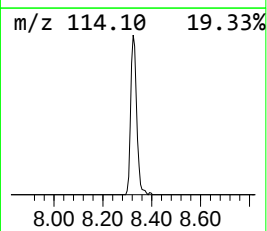
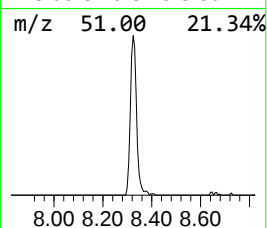
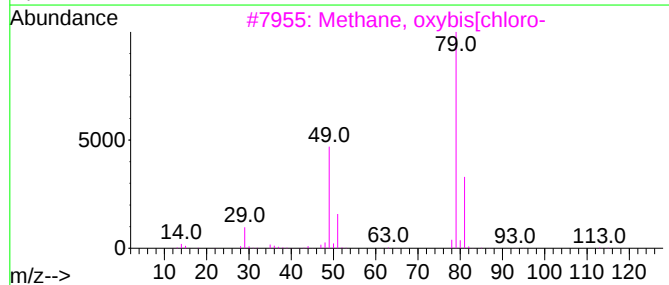
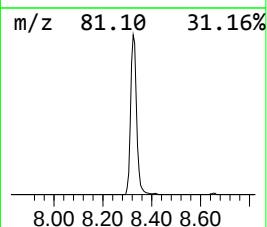
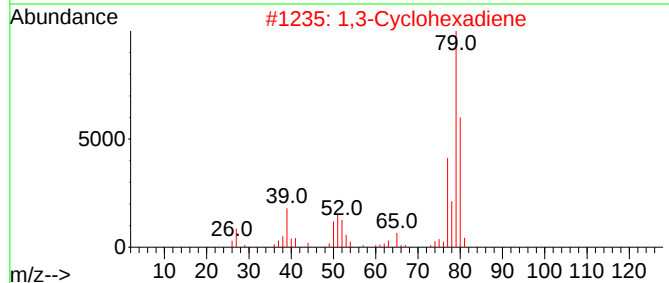
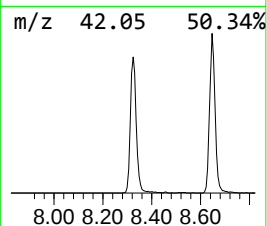
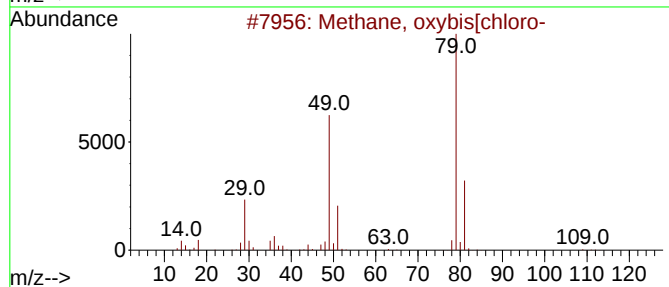
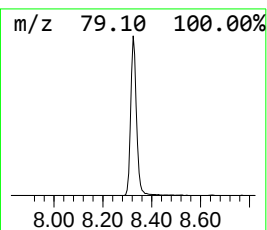
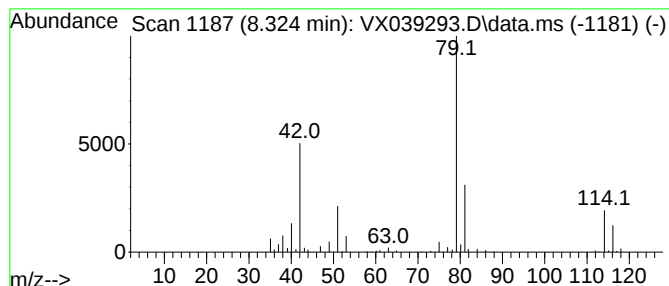
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.324	19.33 ug/L	208392	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	47
2			1,3-Cyclohexadiene	80	C6H8	000592-57-4	25
3			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	25
4			.alpha.,.alpha.-Dichloromethyl m...	114	C2H4Cl2O	004885-02-3	25
5			1,3-Cyclohexadiene	80	C6H8	000592-57-4	25



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.532	58.8	ug/L	634309	1	6.763	539007	50.0
unknown-01	8.324	19.3	ug/L	208392	1	6.763	539007	50.0