

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
 Data File : VX042221.D
 Acq On : 05 Jul 2024 19:13
 Operator : JC/MD
 Sample : P3100-21ME
 Misc : 4.86g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D38ME

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\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042221.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	37	rBV	25015	30243	6.38%	0.809%
2	1.398	43	51	67	rVB	13231	55480	11.70%	1.483%
3	1.557	70	77	78	rBV3	3183	5847	1.23%	0.156%
4	2.270	189	194	208	rBV	66534	120474	25.41%	3.221%
5	2.721	263	268	274	rBV	12620	26869	5.67%	0.718%
6	2.940	298	304	315	rVB	6074	14746	3.11%	0.394%
7	3.142	335	337	339	rVB2	183	136	0.03%	0.004%
8	3.288	359	361	365	rVB2	211	223	0.05%	0.006%
9	3.343	369	370	373	rBV2	133	128	0.03%	0.003%
10	3.416	379	382	384	rBV	294	332	0.07%	0.009%
11	3.574	407	408	411	rVV2	116	122	0.03%	0.003%
12	3.635	415	418	419	rVB	128	117	0.02%	0.003%
13	3.660	419	422	426	rVB2	89	133	0.03%	0.004%
14	3.727	431	433	436	rVV	135	99	0.02%	0.003%
15	3.959	468	471	472	rBV	144	99	0.02%	0.003%
16	3.983	474	475	478	rVV	188	124	0.03%	0.003%
17	4.227	514	515	517	rBV	172	128	0.03%	0.003%
18	4.306	526	528	529	rVB	170	105	0.02%	0.003%
19	4.361	534	537	538	rBV	151	125	0.03%	0.003%
20	4.501	552	560	576	rBV	22677	79187	16.70%	2.117%
21	5.056	640	651	668	rBV2	50590	161046	33.97%	4.305%
22	5.385	702	705	707	rBV2	254	308	0.06%	0.008%
23	5.501	722	724	726	rBV2	116	109	0.02%	0.003%
24	5.538	726	730	731	rBV	322	273	0.06%	0.007%
25	5.599	739	740	744	rVB2	125	121	0.03%	0.003%
26	5.659	747	750	753	rBV	195	197	0.04%	0.005%
27	5.739	758	763	764	rBV2	111	165	0.03%	0.004%
28	5.824	776	777	780	rBB	180	102	0.02%	0.003%
29	5.958	789	799	815	rBV2	151340	441123	93.04%	11.793%
30	6.342	861	862	865	rBV2	102	105	0.02%	0.003%
31	6.385	865	869	875	rVV3	412	703	0.15%	0.019%
32	6.513	885	890	891	rBV	156	233	0.05%	0.006%
33	6.531	891	893	896	rVV	163	142	0.03%	0.004%
34	6.574	896	900	902	rVB2	161	224	0.05%	0.006%
35	6.665	911	915	916	rBV2	112	138	0.03%	0.004%
36	6.757	921	930	945	rBV	166763	415842	87.71%	11.117%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
 Title : VOC Analysis

37	7.104	983	987	996	rVB5	931	2110	0.45%	0.056%
38	7.220	1001	1006	1010	rBV3	605	1158	0.24%	0.031%
39	7.306	1012	1020	1037	rBV	85085	195370	41.21%	5.223%
40	7.482	1046	1049	1051	rBV3	175	204	0.04%	0.005%
41	7.647	1074	1076	1078	rVB2	141	106	0.02%	0.003%
42	7.690	1080	1083	1085	rBV2	130	169	0.04%	0.005%
43	7.787	1098	1099	1101	rBV2	126	103	0.02%	0.003%
44	7.964	1126	1128	1129	rBV	176	112	0.02%	0.003%
45	7.982	1129	1131	1133	rVV2	253	230	0.05%	0.006%
46	8.098	1146	1150	1154	rBV	141	219	0.05%	0.006%
47	8.281	1177	1180	1181	rBV2	97	108	0.02%	0.003%
48	8.324	1181	1187	1206	rVV	43599	78841	16.63%	2.108%
49	8.452	1206	1208	1209	rBV2	189	123	0.03%	0.003%
50	8.525	1217	1220	1221	rBV	170	172	0.04%	0.005%
51	8.647	1232	1240	1250	rBV	222798	355645	75.01%	9.508%
52	8.952	1285	1290	1307	rBV	30943	50197	10.59%	1.342%
53	9.067	1307	1309	1312	rVB	148	109	0.02%	0.003%
54	9.275	1338	1343	1349	rVB	4177	6140	1.30%	0.164%
55	9.397	1357	1363	1381	rBV	89168	199085	41.99%	5.322%
56	9.714	1411	1415	1423	rVB2	2530	4187	0.88%	0.112%
57	9.872	1439	1441	1445	rVB2	172	189	0.04%	0.005%
58	9.909	1445	1447	1449	rBV2	127	130	0.03%	0.003%
59	10.055	1465	1471	1485	rBV	340046	474111	100.00%	12.675%
60	10.244	1498	1502	1510	rBV	5536	7590	1.60%	0.203%
61	10.305	1510	1512	1518	rVB3	903	1437	0.30%	0.038%
62	10.360	1518	1521	1522	rVB2	160	101	0.02%	0.003%
63	10.384	1522	1525	1527	rBV2	112	176	0.04%	0.005%
64	10.457	1533	1537	1538	rBV2	117	105	0.02%	0.003%
65	10.665	1568	1571	1580	rVB4	662	1339	0.28%	0.036%
66	10.726	1580	1581	1583	rVV	186	114	0.02%	0.003%
67	10.774	1586	1589	1593	rVV3	545	716	0.15%	0.019%
68	10.811	1593	1595	1596	rVB	248	136	0.03%	0.004%
69	10.854	1601	1602	1607	rBV	165	155	0.03%	0.004%
70	10.939	1614	1616	1620	rBV3	346	403	0.09%	0.011%
71	11.012	1627	1628	1630	rBV	149	113	0.02%	0.003%
72	11.091	1639	1641	1644	rBV3	405	512	0.11%	0.014%
73	11.195	1652	1658	1667	rBV	168531	222393	46.91%	5.945%
74	11.311	1673	1677	1682	rVB	8734	11624	2.45%	0.311%
75	11.561	1717	1718	1721	rBV2	131	117	0.02%	0.003%
76	11.719	1743	1744	1747	rVB2	212	158	0.03%	0.004%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
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77	12.024	1788	1794	1804	rBV	342858	439017	92.60%	11.737%
78	12.177	1818	1819	1820	rBV	242	131	0.03%	0.004%
79	12.323	1837	1843	1859	rBV	237135	315563	66.56%	8.436%
80	12.707	1904	1906	1907	rBV	189	142	0.03%	0.004%
81	12.768	1910	1916	1920	rVB2	2055	2884	0.61%	0.077%
82	12.865	1930	1932	1935	rVB3	112	117	0.02%	0.003%
83	13.024	1956	1958	1959	rBV	172	129	0.03%	0.003%
84	13.103	1969	1971	1976	rVB3	195	296	0.06%	0.008%
85	13.256	1994	1996	1999	rBV2	118	113	0.02%	0.003%
86	13.286	1999	2001	2004	rVV2	126	138	0.03%	0.004%
87	13.335	2008	2009	2011	rBV	142	121	0.03%	0.003%
88	13.353	2011	2012	2015	rBV	160	141	0.03%	0.004%
89	13.445	2026	2027	2029	rBV	145	125	0.03%	0.003%
90	13.469	2029	2031	2032	rVB	244	116	0.02%	0.003%
91	13.591	2049	2051	2053	rBV2	124	101	0.02%	0.003%
92	13.774	2072	2081	2083	rBV4	1085	2020	0.43%	0.054%
93	13.920	2103	2105	2106	rBV2	169	151	0.03%	0.004%
94	14.073	2129	2130	2133	rVB3	244	197	0.04%	0.005%
95	14.134	2136	2140	2144	rVB2	676	941	0.20%	0.025%
96	14.286	2164	2165	2167	rBV2	204	137	0.03%	0.004%
97	14.432	2185	2189	2192	rBV2	1154	1541	0.33%	0.041%
98	14.481	2196	2197	2199	rBV	256	113	0.02%	0.003%
99	14.554	2200	2209	2216	rVB7	1536	4547	0.96%	0.122%
100	15.213	2316	2317	2318	rBV	446	224	0.05%	0.006%

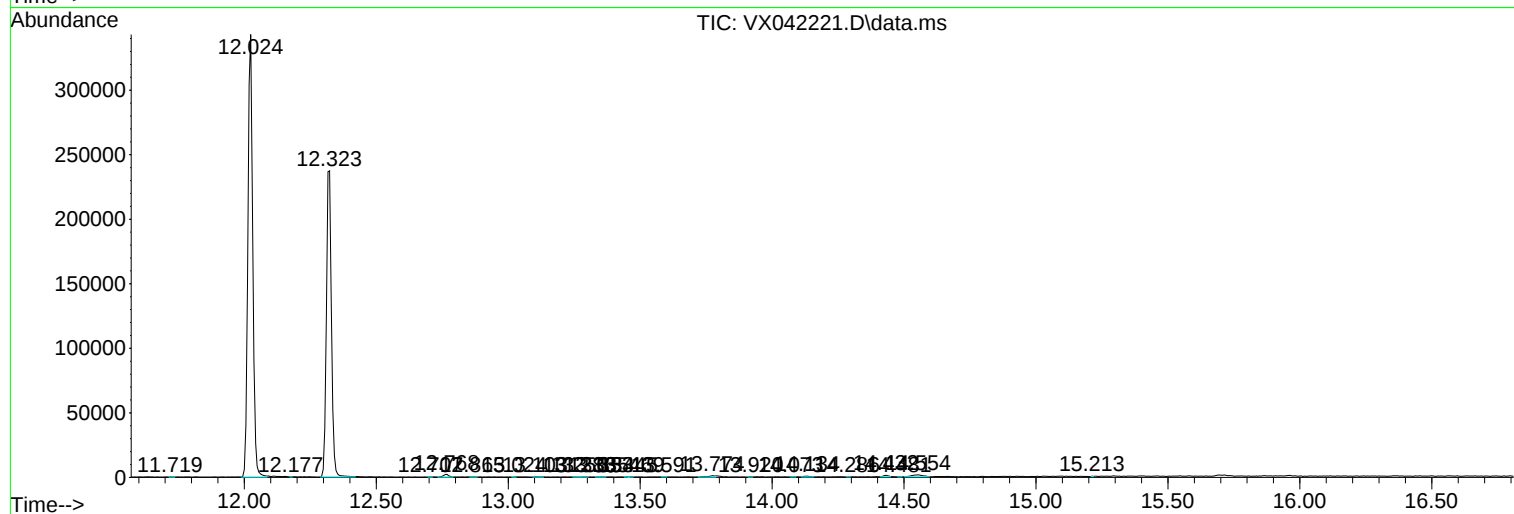
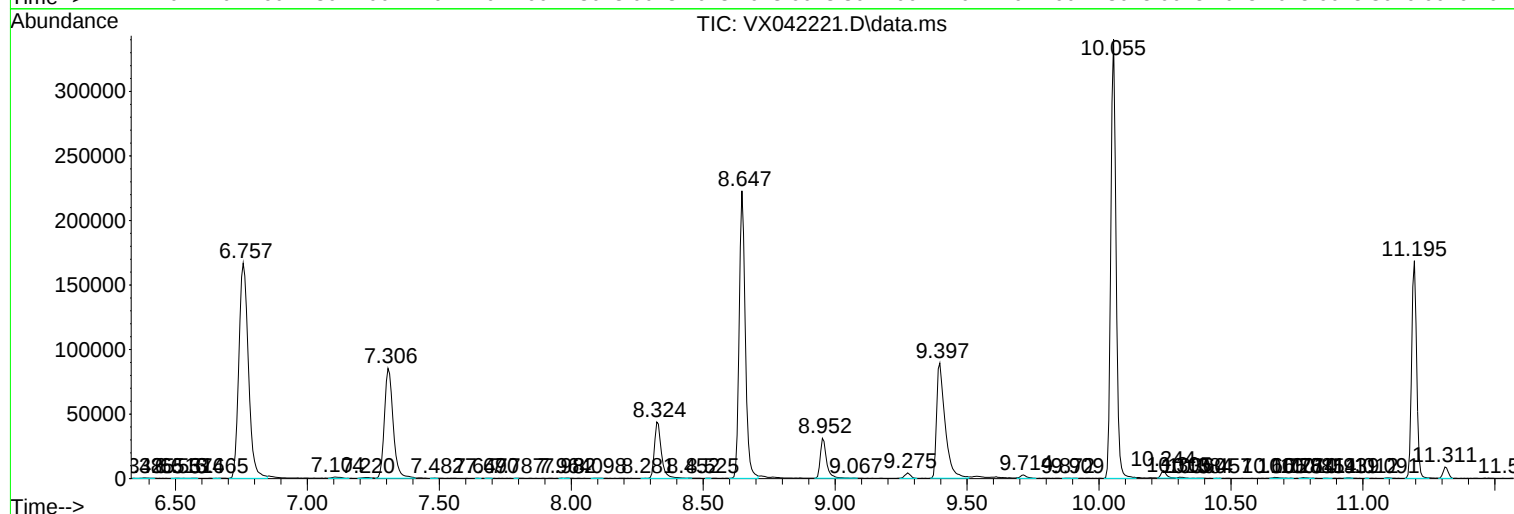
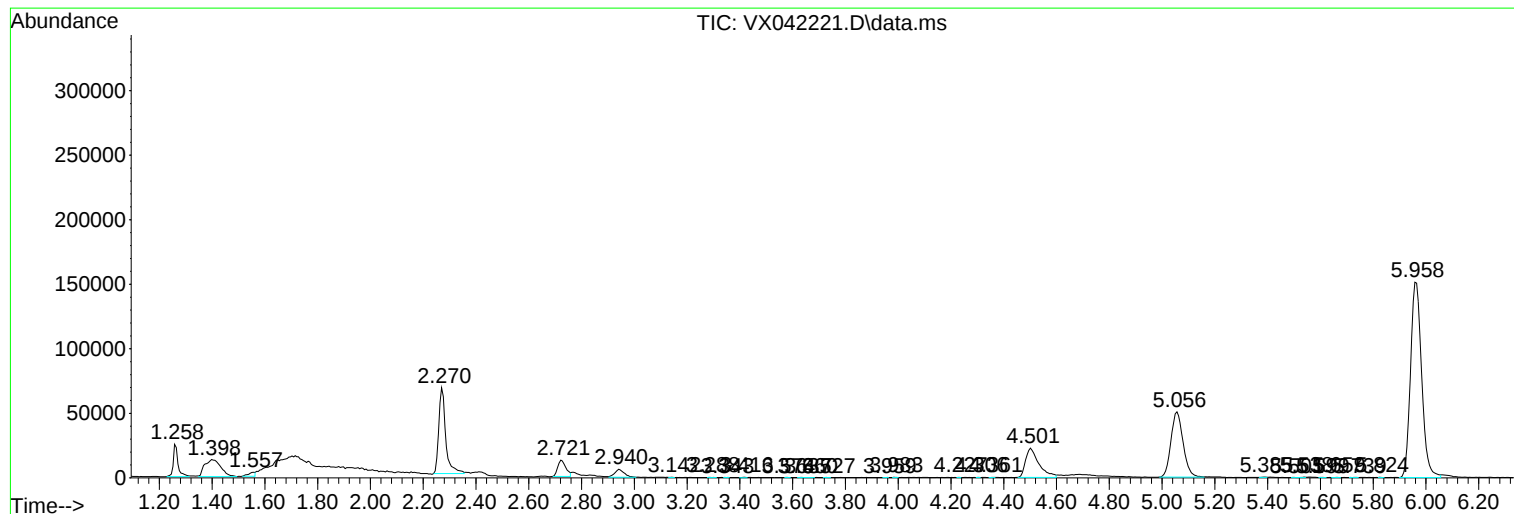
Sum of corrected areas: 3740560

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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D38ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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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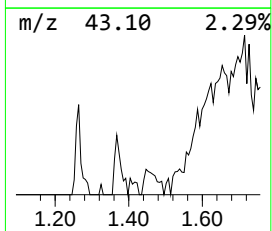
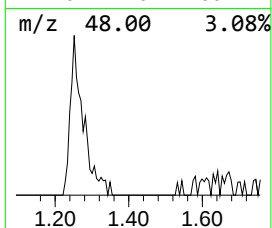
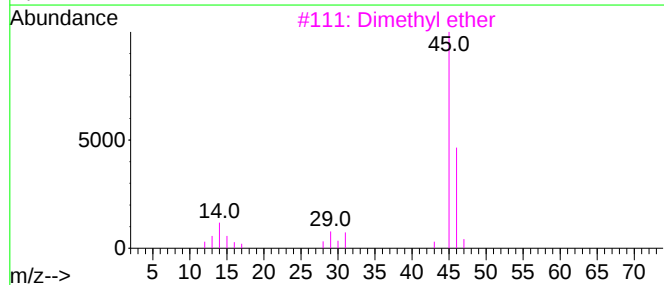
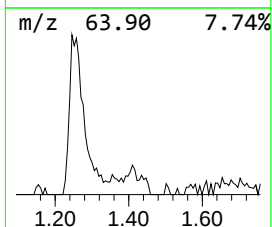
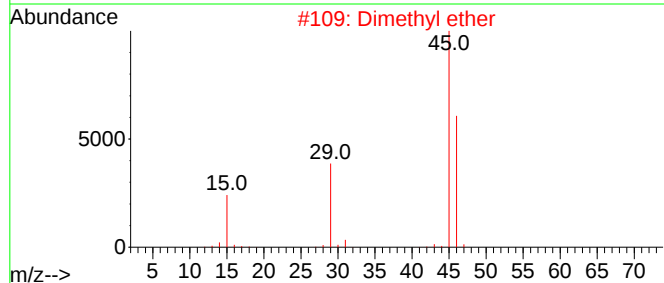
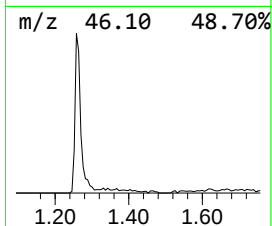
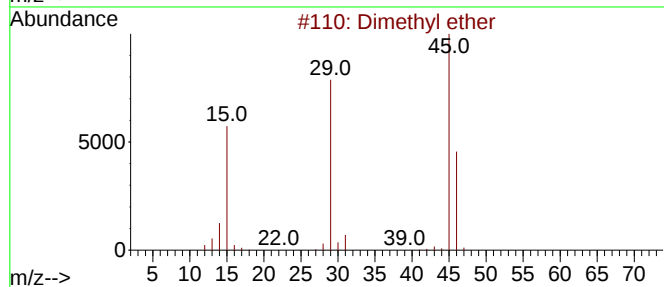
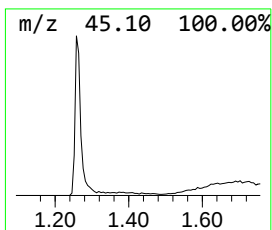
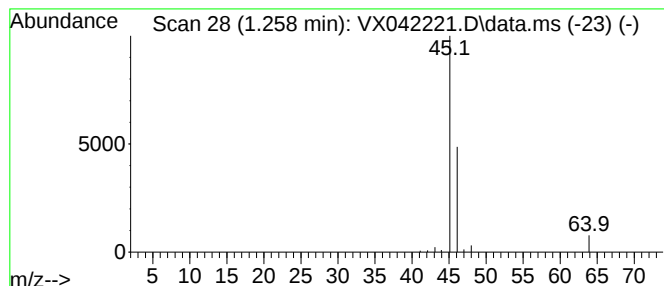
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Dimethyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	3.64 ug/L	30243	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	90
2			Dimethyl ether	46	C2H6O	000115-10-6	74
3			Dimethyl ether	46	C2H6O	000115-10-6	7
4			Ethanol	46	C2H6O	000064-17-5	7
5			Ethanol	46	C2H6O	000064-17-5	7



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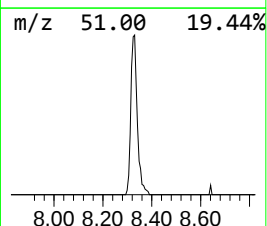
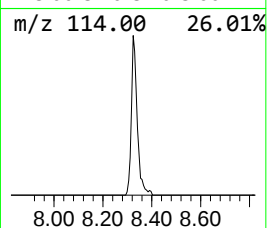
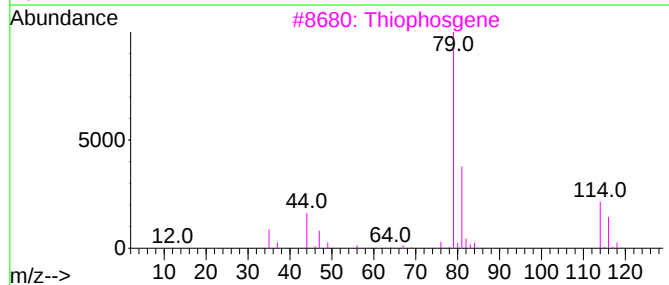
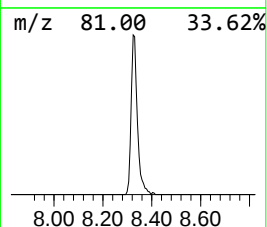
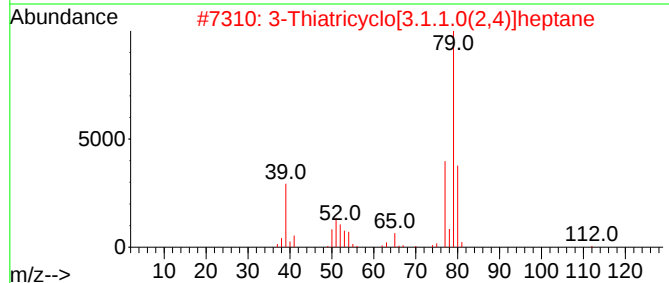
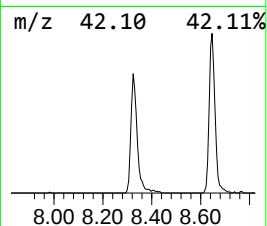
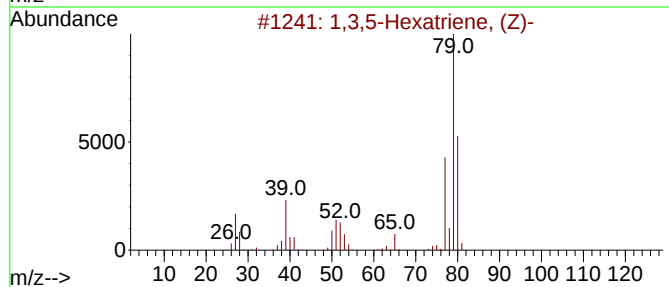
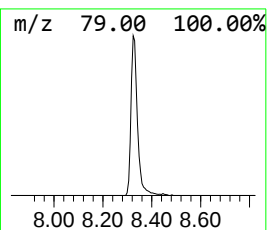
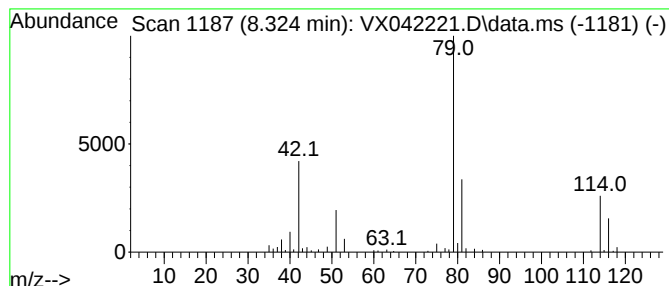
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.324	9.48 ug/L	78841	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Hexatriene, (Z)-	80	C6H8	002612-46-6	37
2			3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	37
3			Thiophosgene	114	CCl2S	000463-71-8	28
4			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	25
5			1,3-Cyclohexadiene	80	C6H8	000592-57-4	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl ether	1.258	3.6	ug/L	30243	1	6.757	415842	50.0
unknown-01	8.324	9.5	ug/L	78841	1	6.757	415842	50.0