

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030657.D
 Acq On : 17 Aug 2022 14:05
 Operator : JC/MD
 Sample : N4221-20
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KP6

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\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030657.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	42	46	57	rVB	194087	199340	15.03%	1.995%
2	1.666	91	95	101	rBV	135973	162376	12.25%	1.625%
3	2.306	194	200	209	rBV	321989	489150	36.89%	4.895%
4	2.392	209	214	219	rVB2	4758	8095	0.61%	0.081%
5	2.489	229	230	233	rBV2	646	863	0.07%	0.009%
6	2.569	240	243	246	rBV2	739	814	0.06%	0.008%
7	2.642	252	255	256	rBV3	583	652	0.05%	0.007%
8	2.678	259	261	263	rVB2	624	449	0.03%	0.004%
9	2.794	276	280	284	rVB4	1095	1928	0.15%	0.019%
10	2.892	294	296	300	rBV2	318	339	0.03%	0.003%
11	2.928	300	302	304	rBV2	903	1008	0.08%	0.010%
12	3.001	313	314	317	rBV2	405	445	0.03%	0.004%
13	3.178	337	343	346	rBV2	383	843	0.06%	0.008%
14	3.270	355	358	359	rBV	543	594	0.04%	0.006%
15	3.300	361	363	366	rVB2	419	416	0.03%	0.004%
16	3.446	386	387	390	rVB	386	283	0.02%	0.003%
17	3.635	414	418	420	rBV	436	693	0.05%	0.007%
18	3.727	431	433	437	rVV2	486	497	0.04%	0.005%
19	3.879	457	458	461	rBV2	418	411	0.03%	0.004%
20	3.910	461	463	466	rVV2	318	352	0.03%	0.004%
21	3.989	473	476	478	rVV2	299	435	0.03%	0.004%
22	4.056	484	487	490	rVB2	448	610	0.05%	0.006%
23	4.190	505	509	512	rBV2	420	461	0.03%	0.005%
24	4.227	512	515	516	rBV	599	532	0.04%	0.005%
25	4.245	516	518	522	rBV2	380	530	0.04%	0.005%
26	4.465	545	554	571	rBV2	102630	298377	22.50%	2.986%
27	4.721	587	596	608	rBV	28945	83361	6.29%	0.834%
28	5.068	636	653	668	rBV	171474	549800	41.47%	5.502%
29	5.342	695	698	699	rBV2	401	501	0.04%	0.005%
30	5.470	717	719	723	rVB	581	699	0.05%	0.007%
31	5.525	726	728	729	rVV	765	669	0.05%	0.007%
32	5.562	730	734	742	rVB5	2519	5814	0.44%	0.058%
33	5.696	754	756	759	rBV2	341	337	0.03%	0.003%
34	5.976	790	802	817	rBV2	456390	1325901	100.00%	13.268%
35	6.172	830	834	836	rVV4	649	815	0.06%	0.008%
36	6.190	836	837	843	rVB2	909	927	0.07%	0.009%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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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\SFAMXML080422WMA.M
 Title : VOC Analysis

37	6.287	852	853	856	rBV2	418	479	0.04%	0.005%
38	6.354	861	864	866	rVV	542	387	0.03%	0.004%
39	6.617	903	907	908	rBV3	250	330	0.02%	0.003%
40	6.763	922	931	948	rBV	293721	712732	53.75%	7.132%
41	7.117	981	989	1001	rVB4	12162	29047	2.19%	0.291%
42	7.202	1001	1003	1005	rBV	484	465	0.04%	0.005%
43	7.232	1005	1008	1009	rBV2	415	334	0.03%	0.003%
44	7.312	1012	1021	1035	rBV2	272995	594341	44.83%	5.948%
45	7.482	1047	1049	1052	rBV3	600	745	0.06%	0.007%
46	7.586	1062	1066	1070	rBV3	1606	2684	0.20%	0.027%
47	7.781	1094	1098	1099	rVV2	349	394	0.03%	0.004%
48	7.940	1117	1124	1130	rBV4	1372	2578	0.19%	0.026%
49	7.988	1130	1132	1134	rBV2	342	354	0.03%	0.004%
50	8.330	1181	1188	1199	rBV	184922	297324	22.42%	2.975%
51	8.482	1206	1213	1215	rBV4	1013	1806	0.14%	0.018%
52	8.653	1234	1241	1250	rBV	689052	1066823	80.46%	10.676%
53	8.952	1285	1290	1299	rBV	130425	191650	14.45%	1.918%
54	9.183	1327	1328	1331	rBV2	356	397	0.03%	0.004%
55	9.281	1337	1344	1348	rBV4	3244	5660	0.43%	0.057%
56	9.384	1356	1361	1376	rBV	449544	665527	50.19%	6.660%
57	9.525	1380	1384	1390	rVB	26713	37264	2.81%	0.373%
58	9.640	1401	1403	1405	rVB2	532	339	0.03%	0.003%
59	9.671	1405	1408	1409	rBV2	403	478	0.04%	0.005%
60	9.903	1444	1446	1449	rBV2	407	518	0.04%	0.005%
61	10.055	1465	1471	1486	rBV	640999	853026	64.34%	8.536%
62	10.195	1491	1494	1496	rBV4	809	1067	0.08%	0.011%
63	10.268	1504	1506	1508	rVB	594	442	0.03%	0.004%
64	10.311	1508	1513	1515	rBV2	1075	1531	0.12%	0.015%
65	10.567	1553	1555	1557	rBV2	306	336	0.03%	0.003%
66	10.598	1558	1560	1564	rVB2	533	492	0.04%	0.005%
67	10.646	1564	1568	1575	rBV	7414	11325	0.85%	0.113%
68	10.768	1584	1588	1593	rBV3	1579	2622	0.20%	0.026%
69	10.860	1597	1603	1608	rVB3	3317	4603	0.35%	0.046%
70	10.945	1614	1617	1618	rBV	477	385	0.03%	0.004%
71	11.030	1625	1631	1636	rBV4	2129	3750	0.28%	0.038%
72	11.073	1636	1638	1640	rBV	838	804	0.06%	0.008%
73	11.195	1652	1658	1666	rBV	465792	600787	45.31%	6.012%
74	11.311	1674	1677	1683	rVB2	2034	3202	0.24%	0.032%
75	11.439	1696	1698	1699	rBV	483	353	0.03%	0.004%
76	11.622	1724	1728	1730	rBV3	855	870	0.07%	0.009%

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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\SFAMXMLM080422WMA.M
 Title : VOC Analysis

77	11.756	1747	1750	1759	rVB4	2871	5622	0.42%	0.056%
78	11.841	1762	1764	1771	rBV3	772	1453	0.11%	0.015%
79	11.933	1775	1779	1781	rBV2	2348	2766	0.21%	0.028%
80	12.024	1789	1794	1801	rBV	657668	784876	59.20%	7.854%
81	12.134	1810	1812	1814	rBV3	503	423	0.03%	0.004%
82	12.219	1821	1826	1836	rBV2	14222	23751	1.79%	0.238%
83	12.323	1837	1843	1853	rVV	712587	888578	67.02%	8.892%
84	12.512	1873	1874	1876	rVB	495	289	0.02%	0.003%
85	12.542	1876	1879	1880	rBV2	811	930	0.07%	0.009%
86	12.597	1883	1888	1893	rVV4	2498	4268	0.32%	0.043%
87	12.719	1904	1908	1909	rBV2	511	746	0.06%	0.007%
88	12.762	1912	1915	1921	rVV3	1615	2515	0.19%	0.025%
89	12.853	1925	1930	1936	rVV4	8599	10925	0.82%	0.109%
90	13.103	1967	1971	1976	rVB	12555	16802	1.27%	0.168%
91	13.591	2048	2051	2055	rVB4	1236	1676	0.13%	0.017%
92	13.774	2079	2081	2082	rBV	910	564	0.04%	0.006%
93	13.859	2093	2095	2098	rVB2	587	616	0.05%	0.006%
94	14.048	2124	2126	2129	rBV3	509	457	0.03%	0.005%
95	14.134	2137	2140	2145	rVB3	1816	2344	0.18%	0.023%
96	14.207	2150	2152	2156	rBV2	548	913	0.07%	0.009%
97	14.603	2213	2217	2218	rBV2	645	692	0.05%	0.007%
98	14.713	2233	2235	2236	rBV2	903	681	0.05%	0.007%
99	15.353	2336	2340	2343	rBV3	1378	2620	0.20%	0.026%
100	15.792	2410	2412	2414	rBV2	1075	1009	0.08%	0.010%

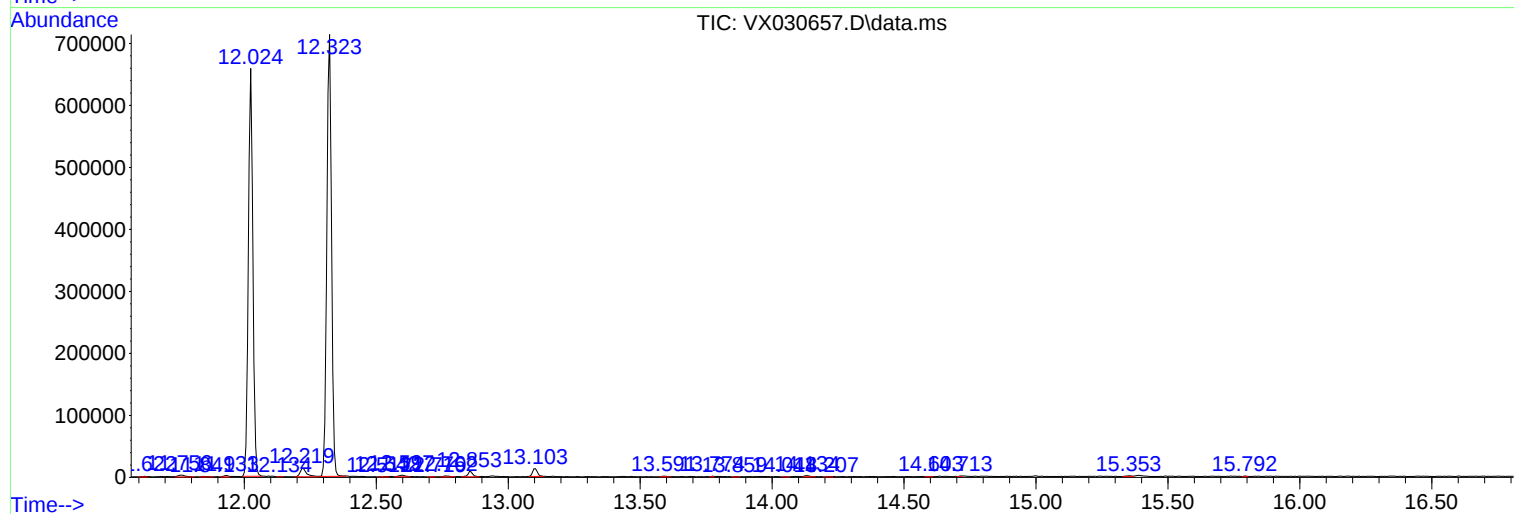
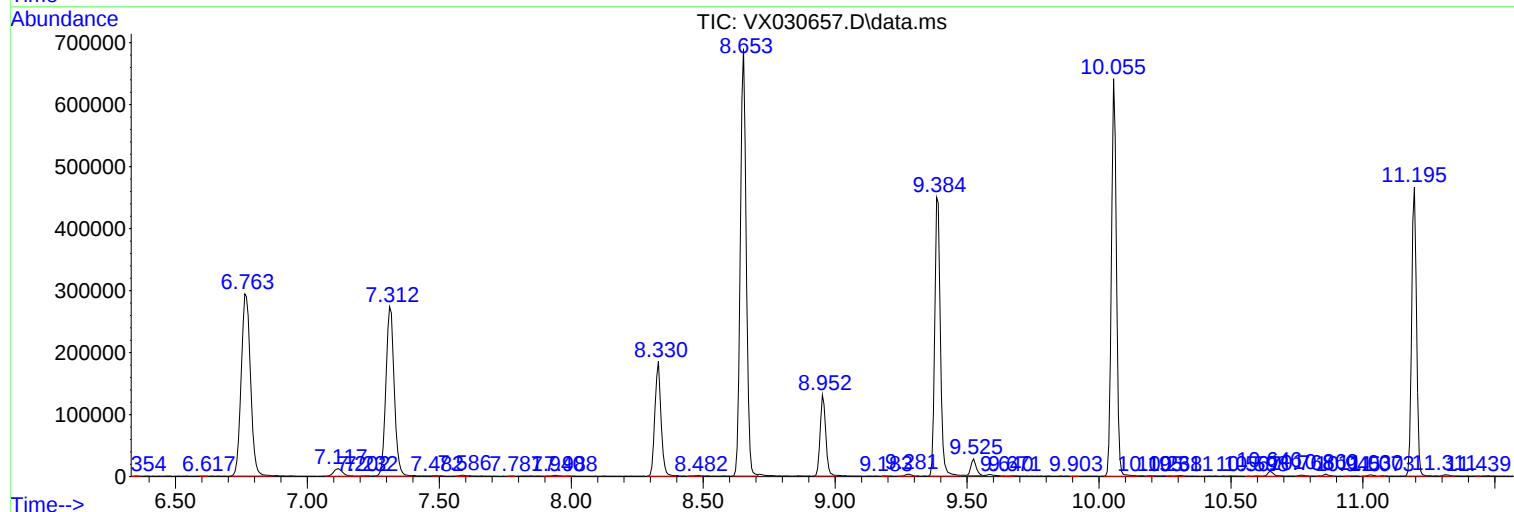
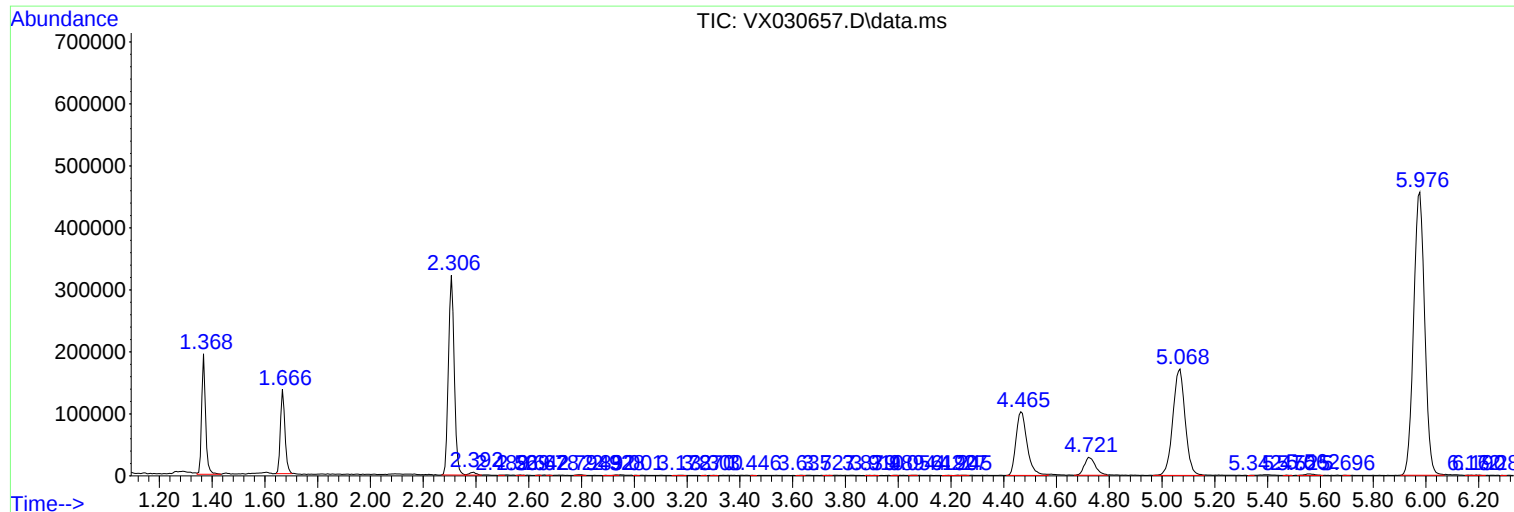
Sum of corrected areas: 9993084

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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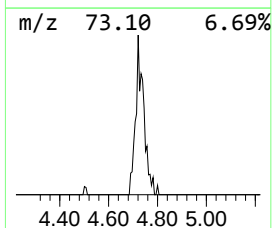
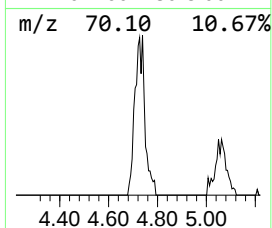
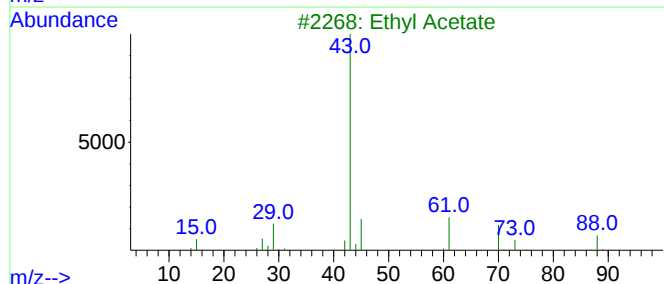
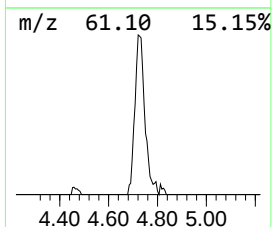
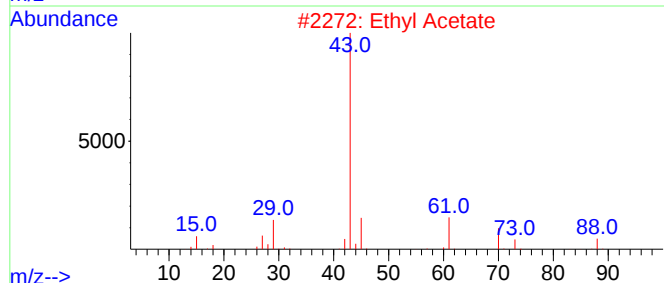
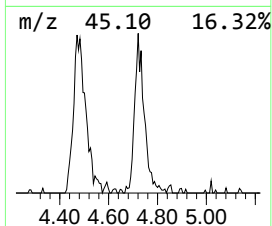
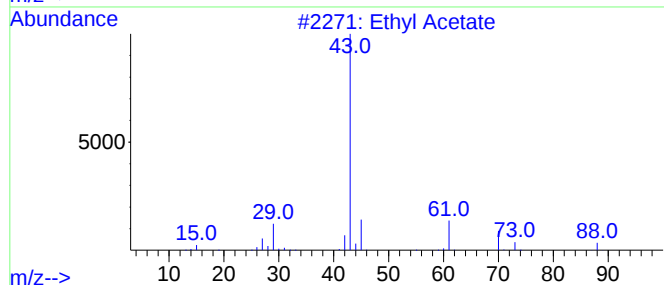
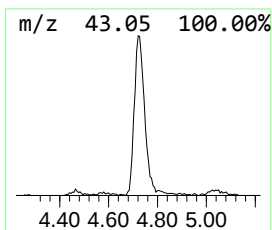
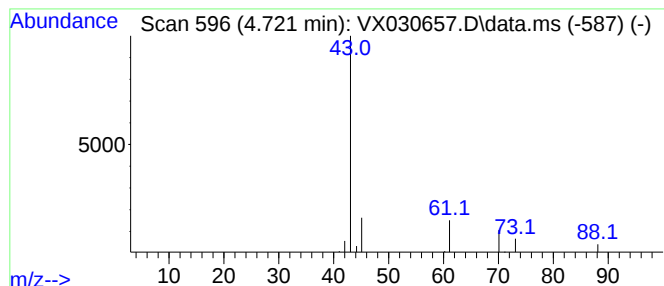
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.721	5.85 ug/L	83361	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	90
3			Ethyl Acetate	88	C4H8O2	000141-78-6	83
4			Ethyl Acetate	88	C4H8O2	000141-78-6	59
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.721	5.8	ug/L	83361	1	6.763	712732	50.0