

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
 Data File : VX042381.D
 Acq On : 18 Jul 2024 19:41
 Operator : JC/MD
 Sample : P3238-09ME
 Misc : 5.41g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4BF4ME

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: VX042381.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	22	28	37	rBV2	17836	27758	3.10%	0.419%
2	1.368	43	46	64	rVB	37538	91231	10.17%	1.376%
3	1.648	86	92	96	rBV2	28338	57724	6.44%	0.870%
4	2.282	189	196	214	rBV	126817	245203	27.35%	3.697%
5	2.557	240	241	243	rVB2	218	138	0.02%	0.002%
6	2.624	251	252	255	rBV2	139	148	0.02%	0.002%
7	2.672	257	260	261	rBV2	165	203	0.02%	0.003%
8	2.721	261	268	274	rBV	9162	18092	2.02%	0.273%
9	2.953	300	306	313	rVB3	345	798	0.09%	0.012%
10	3.270	357	358	361	rVB2	156	127	0.01%	0.002%
11	3.294	361	362	365	rBV2	144	182	0.02%	0.003%
12	3.355	368	372	374	rVV2	227	259	0.03%	0.004%
13	3.447	383	387	388	rVV2	174	167	0.02%	0.003%
14	3.556	402	405	407	rBV2	107	115	0.01%	0.002%
15	3.971	469	473	474	rVV2	113	134	0.01%	0.002%
16	3.995	474	477	479	rVB	148	180	0.02%	0.003%
17	4.050	485	486	490	rBV2	120	114	0.01%	0.002%
18	4.196	508	510	512	rVB	162	128	0.01%	0.002%
19	4.233	514	516	523	rBV2	159	338	0.04%	0.005%
20	4.489	549	558	584	rBV	60051	219515	24.48%	3.310%
21	4.946	631	633	636	rVB2	168	154	0.02%	0.002%
22	5.056	640	651	667	rVV	115464	354579	39.54%	5.347%
23	5.276	686	687	690	rBV	166	129	0.01%	0.002%
24	5.385	701	705	706	rBV	463	407	0.05%	0.006%
25	5.452	714	716	718	rBV2	127	135	0.02%	0.002%
26	5.538	727	730	732	rBV2	368	460	0.05%	0.007%
27	5.964	788	800	816	rBV2	315883	896689	100.00%	13.521%
28	6.275	849	851	852	rBV2	138	115	0.01%	0.002%
29	6.379	864	868	869	rBV	222	255	0.03%	0.004%
30	6.397	869	871	875	rVB3	154	203	0.02%	0.003%
31	6.470	881	883	885	rBV	232	153	0.02%	0.002%
32	6.501	885	888	889	rVB	135	131	0.01%	0.002%
33	6.653	911	913	914	rBV	428	262	0.03%	0.004%
34	6.757	921	930	949	rBV	188059	457599	51.03%	6.900%
35	7.111	983	988	996	rVB4	1768	4241	0.47%	0.064%
36	7.214	1001	1005	1012	rBV3	502	1151	0.13%	0.017%

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Instrument :
MSVOA_X
ClientSampleId :
A4BF4ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

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

37	7.306	1012	1020	1036	rBV	180625	407967	45.50%	6.152%
38	7.592	1064	1067	1069	rBV2	157	195	0.02%	0.003%
39	7.763	1094	1095	1098	rBV	239	139	0.02%	0.002%
40	7.873	1112	1113	1118	rVB	161	119	0.01%	0.002%
41	7.970	1122	1129	1136	rVV6	913	2708	0.30%	0.041%
42	8.025	1137	1138	1141	rVB	269	151	0.02%	0.002%
43	8.275	1175	1179	1181	rBV	202	245	0.03%	0.004%
44	8.324	1181	1187	1206	rVV	102347	178431	19.90%	2.690%
45	8.513	1214	1218	1223	rVB5	519	1046	0.12%	0.016%
46	8.586	1228	1230	1234	rBV2	264	476	0.05%	0.007%
47	8.647	1234	1240	1252	rBV	462231	723729	80.71%	10.913%
48	8.897	1279	1281	1284	rBV2	195	200	0.02%	0.003%
49	8.952	1285	1290	1303	rVV	77152	116940	13.04%	1.763%
50	9.080	1309	1311	1313	rVB3	329	215	0.02%	0.003%
51	9.220	1333	1334	1337	rVV2	106	135	0.02%	0.002%
52	9.281	1340	1344	1346	rVB3	417	538	0.06%	0.008%
53	9.336	1352	1353	1355	rBV	113	115	0.01%	0.002%
54	9.391	1357	1362	1380	rBV	254721	487094	54.32%	7.345%
55	9.732	1416	1418	1426	rVB5	337	494	0.06%	0.007%
56	9.848	1435	1437	1439	rBV	122	127	0.01%	0.002%
57	9.945	1451	1453	1457	rVB	292	317	0.04%	0.005%
58	9.988	1457	1460	1461	rBV	134	141	0.02%	0.002%
59	10.055	1465	1471	1487	rBV	381903	532524	59.39%	8.030%
60	10.305	1509	1512	1517	rVB3	554	827	0.09%	0.012%
61	10.537	1547	1550	1552	rBV	140	126	0.01%	0.002%
62	10.598	1555	1560	1562	rBV	123	147	0.02%	0.002%
63	10.640	1564	1567	1569	rBV3	249	298	0.03%	0.004%
64	10.665	1569	1571	1574	rVB3	218	228	0.03%	0.003%
65	10.823	1595	1597	1600	rBV2	157	207	0.02%	0.003%
66	10.933	1614	1615	1617	rBV	131	130	0.01%	0.002%
67	10.964	1617	1620	1626	rVV2	2282	3485	0.39%	0.053%
68	11.098	1639	1642	1646	rVB2	303	315	0.04%	0.005%
69	11.195	1652	1658	1667	rBV	391267	515723	57.51%	7.776%
70	11.311	1675	1677	1680	rBV2	495	503	0.06%	0.008%
71	11.494	1703	1707	1712	rVB3	503	732	0.08%	0.011%
72	11.768	1748	1752	1755	rBV4	1067	1450	0.16%	0.022%
73	11.848	1763	1765	1769	rVB2	204	251	0.03%	0.004%
74	11.927	1777	1778	1780	rBV2	163	120	0.01%	0.002%
75	11.982	1784	1787	1789	rBV3	1407	1648	0.18%	0.025%
76	12.024	1789	1794	1809	rVB	408713	522555	58.28%	7.879%

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 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4BF4ME

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

77	12.226	1824	1827	1832	rBV4	600	778	0.09%	0.012%
78	12.323	1837	1843	1856	rBV	546366	721897	80.51%	10.885%
79	12.567	1881	1883	1887	rVB2	181	150	0.02%	0.002%
80	12.762	1910	1915	1919	rBV4	828	1213	0.14%	0.018%
81	12.829	1924	1926	1928	rBV2	159	195	0.02%	0.003%
82	12.872	1929	1933	1944	rVB2	4748	7101	0.79%	0.107%
83	13.110	1969	1972	1974	rBV2	120	189	0.02%	0.003%
84	13.164	1979	1981	1984	rVV2	220	206	0.02%	0.003%
85	13.329	2006	2008	2009	rBV	163	139	0.02%	0.002%
86	13.359	2011	2013	2016	rBV2	110	140	0.02%	0.002%
87	13.408	2016	2021	2025	rBV2	4109	6769	0.75%	0.102%
88	13.573	2047	2048	2053	rVV	257	236	0.03%	0.004%
89	13.634	2057	2058	2062	rVV2	154	158	0.02%	0.002%
90	13.683	2062	2066	2072	rVV4	1120	1849	0.21%	0.028%
91	13.780	2080	2082	2090	rVB4	1076	1821	0.20%	0.027%
92	13.890	2096	2100	2102	rVV3	188	286	0.03%	0.004%
93	14.085	2130	2132	2135	rVB2	282	244	0.03%	0.004%
94	14.134	2136	2140	2142	rVV3	764	1075	0.12%	0.016%
95	14.176	2145	2147	2149	rBV	210	158	0.02%	0.002%
96	14.432	2186	2189	2195	rVB3	1061	1931	0.22%	0.029%
97	14.756	2241	2242	2244	rBV2	349	207	0.02%	0.003%
98	14.884	2261	2263	2270	rVB3	1364	2002	0.22%	0.030%
99	15.140	2304	2305	2311	rVB5	964	1012	0.11%	0.015%
100	15.213	2316	2317	2318	rVB	426	156	0.02%	0.002%

Sum of corrected areas: 6631920

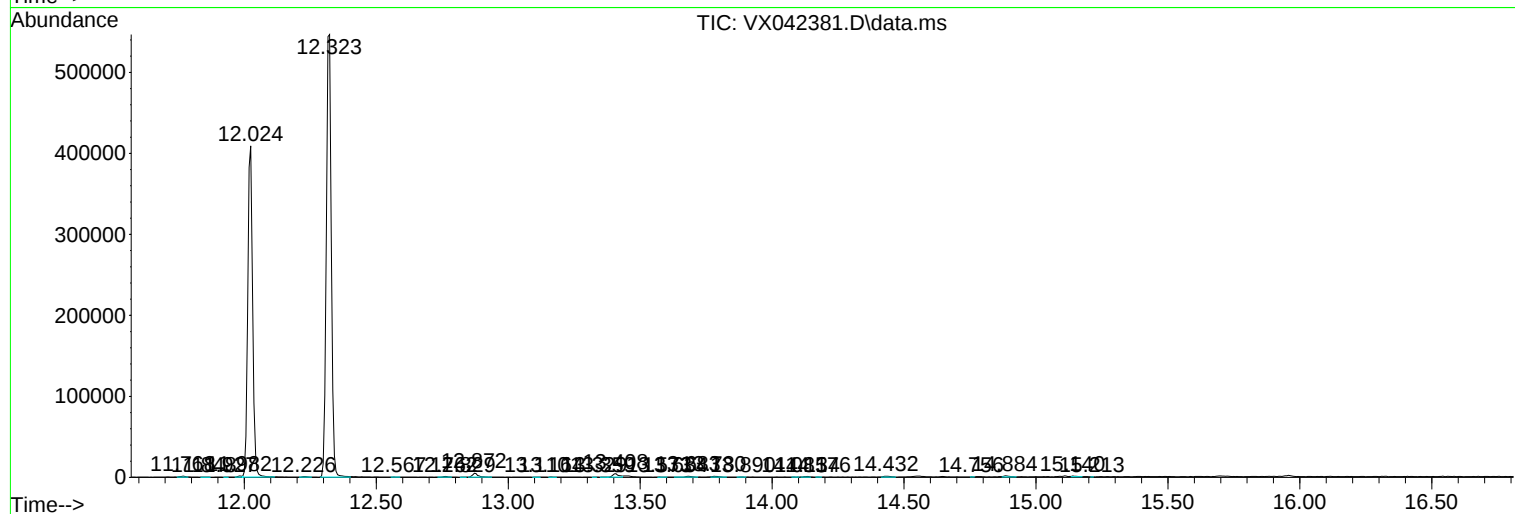
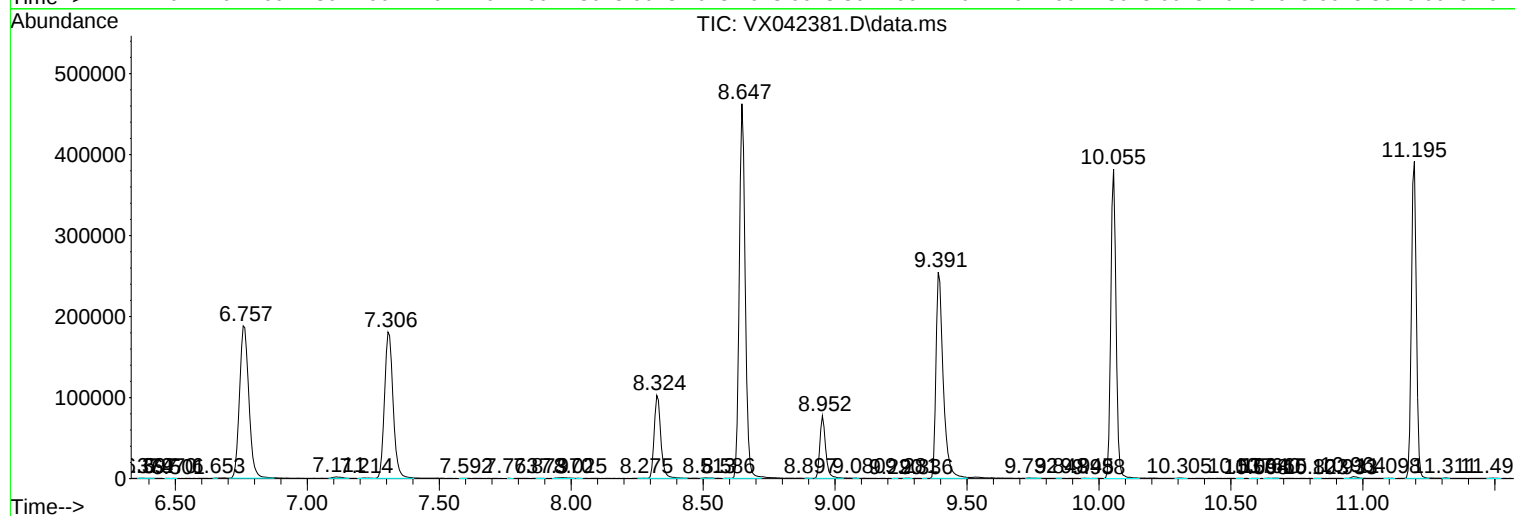
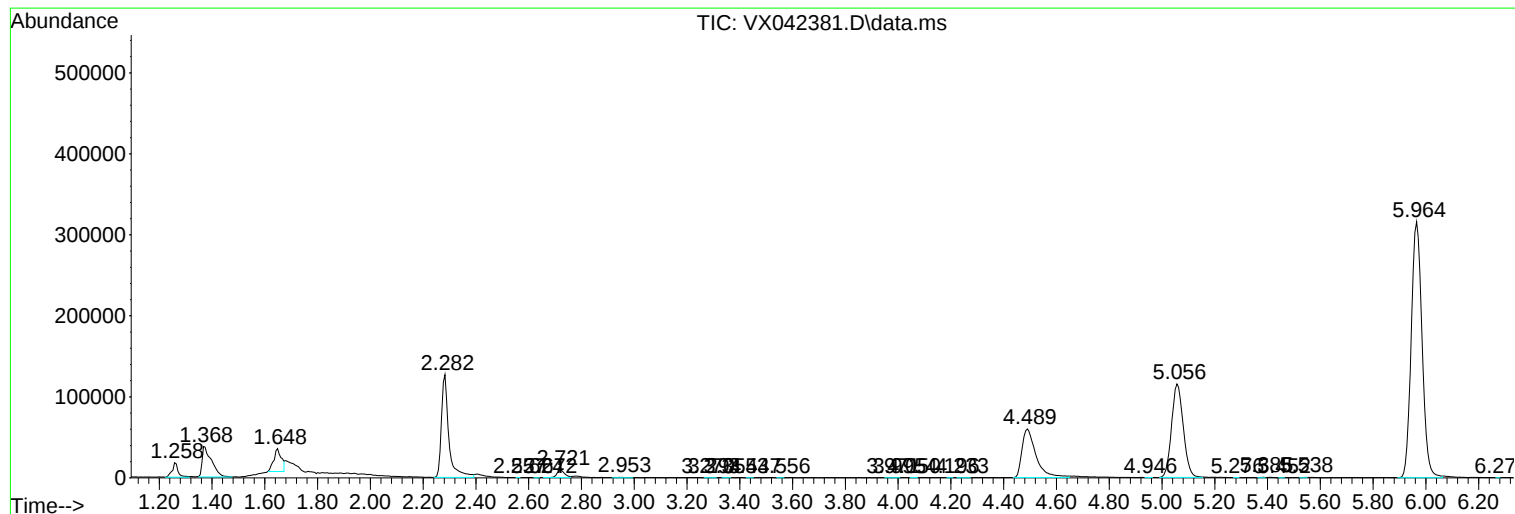
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BF4ME

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 :
MSVOA_X
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A4BF4ME

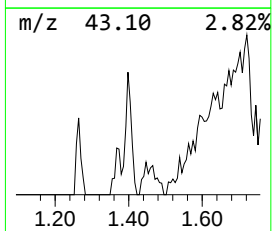
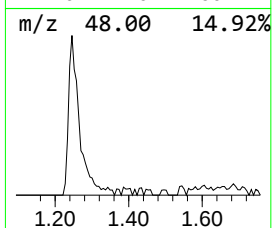
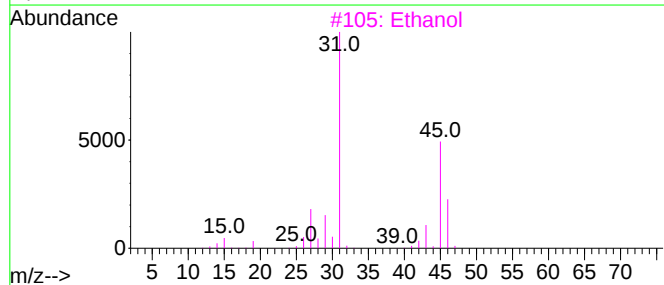
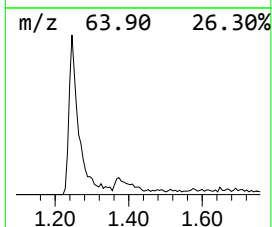
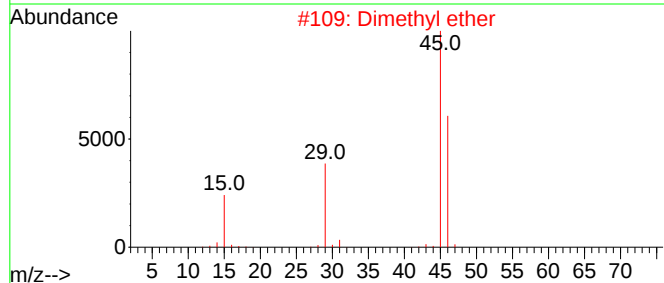
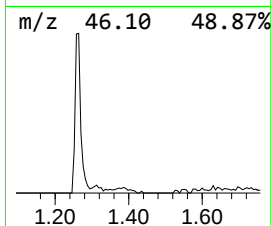
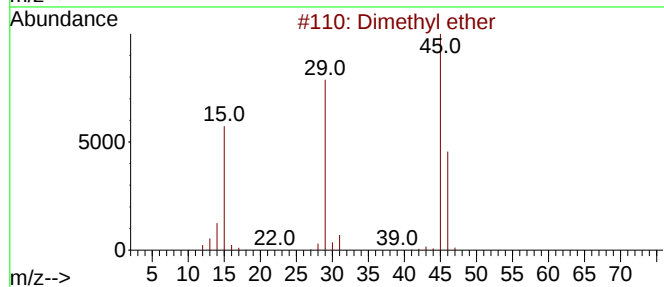
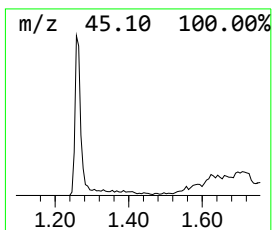
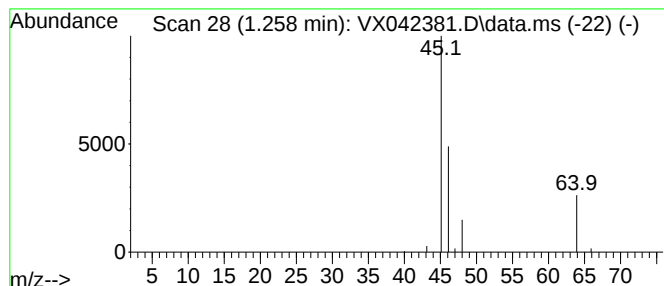
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	3.03 ug/L	27758	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	9
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Ethanol	46	C2H6O	000064-17-5	7
4			Ethanol	46	C2H6O	000064-17-5	7
5			Ethanol	46	C2H6O	000064-17-5	7



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.258	3.0	ug/L	27758	1	6.757	457599	50.0