

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
 Data File : VX042384.D
 Acq On : 18 Jul 2024 20:51
 Operator : JC/MD
 Sample : P3238-18ME
 Misc : 5.98g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CG8ME

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: VX042384.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	42	rBV2	17391	27104	3.05%	0.412%
2	1.368	42	46	60	rVV	36411	88679	9.99%	1.347%
3	1.532	71	73	75	rBV3	1262	1400	0.16%	0.021%
4	1.648	89	92	107	rVB	23524	69270	7.80%	1.052%
5	2.282	189	196	213	rBV	127256	242990	27.36%	3.690%
6	2.593	245	247	250	rVB2	133	133	0.01%	0.002%
7	2.721	262	268	274	rBV	9584	19862	2.24%	0.302%
8	2.928	301	302	303	rBV	276	196	0.02%	0.003%
9	3.050	320	322	323	rBV	174	143	0.02%	0.002%
10	3.117	332	333	336	rBV	115	113	0.01%	0.002%
11	3.325	365	367	370	rBV	131	161	0.02%	0.002%
12	3.477	391	392	398	rBV2	141	168	0.02%	0.003%
13	3.721	431	432	434	rVV2	151	111	0.01%	0.002%
14	3.825	448	449	451	rBV	160	112	0.01%	0.002%
15	3.843	451	452	455	rVB2	173	129	0.01%	0.002%
16	3.879	455	458	459	rVB2	156	136	0.02%	0.002%
17	3.910	459	463	468	rBV	243	266	0.03%	0.004%
18	3.953	468	470	471	rBV2	150	123	0.01%	0.002%
19	4.111	493	496	499	rVB2	199	252	0.03%	0.004%
20	4.257	516	520	521	rBV2	99	134	0.02%	0.002%
21	4.379	539	540	544	rVB2	146	158	0.02%	0.002%
22	4.489	549	558	579	rBV	57069	210522	23.71%	3.197%
23	4.916	626	628	630	rVB2	192	148	0.02%	0.002%
24	5.056	639	651	672	rBV	111393	349646	39.37%	5.309%
25	5.324	694	695	700	rBV	136	159	0.02%	0.002%
26	5.379	700	704	705	rBV2	292	428	0.05%	0.006%
27	5.483	720	721	723	rBV2	125	112	0.01%	0.002%
28	5.562	727	734	735	rBV3	477	918	0.10%	0.014%
29	5.672	750	752	754	rBV2	137	117	0.01%	0.002%
30	5.690	754	755	758	rVB	232	124	0.01%	0.002%
31	5.958	789	799	828	rBV2	304511	888001	100.00%	13.484%
32	6.275	848	851	853	rBV2	162	176	0.02%	0.003%
33	6.434	876	877	881	rBV2	144	109	0.01%	0.002%
34	6.666	911	915	916	rBV2	219	203	0.02%	0.003%
35	6.757	921	930	956	rBV	189978	465256	52.39%	7.065%
36	7.111	982	988	996	rVB4	1937	4769	0.54%	0.072%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

37	7.172	996	998	1000	rVB	186	134	0.02%	0.002%
38	7.220	1000	1006	1007	rBV3	434	640	0.07%	0.010%
39	7.306	1011	1020	1041	rVV	184043	403051	45.39%	6.120%
40	7.470	1045	1047	1049	rBV	290	318	0.04%	0.005%
41	7.592	1066	1067	1068	rBV	249	126	0.01%	0.002%
42	7.732	1087	1090	1091	rBV2	136	111	0.01%	0.002%
43	7.836	1105	1107	1109	rBV	110	111	0.01%	0.002%
44	7.927	1119	1122	1123	rBV2	180	139	0.02%	0.002%
45	7.958	1123	1127	1132	rBV5	707	1552	0.17%	0.024%
46	8.196	1162	1166	1169	rBV2	112	148	0.02%	0.002%
47	8.232	1170	1172	1175	rBV	159	119	0.01%	0.002%
48	8.324	1181	1187	1203	rBV	101244	173010	19.48%	2.627%
49	8.647	1233	1240	1257	rBV	449575	709951	79.95%	10.781%
50	8.952	1285	1290	1305	rBV	74583	115092	12.96%	1.748%
51	9.275	1341	1343	1347	rVB2	671	545	0.06%	0.008%
52	9.391	1357	1362	1382	rBV	248161	479353	53.98%	7.279%
53	9.720	1414	1416	1419	rBV	266	300	0.03%	0.005%
54	9.811	1428	1431	1435	rBV3	219	262	0.03%	0.004%
55	9.891	1440	1444	1445	rVB2	134	178	0.02%	0.003%
56	9.927	1448	1450	1452	rVB2	183	134	0.02%	0.002%
57	9.945	1452	1453	1456	rBV2	158	135	0.02%	0.002%
58	10.055	1465	1471	1486	rBV	391279	540246	60.84%	8.204%
59	10.305	1509	1512	1516	rBV3	556	811	0.09%	0.012%
60	10.421	1529	1531	1532	rBV3	145	120	0.01%	0.002%
61	10.451	1535	1536	1540	rBV	140	117	0.01%	0.002%
62	10.573	1554	1556	1559	rBV2	131	153	0.02%	0.002%
63	10.610	1559	1562	1563	rVB	179	172	0.02%	0.003%
64	10.646	1565	1568	1569	rBV2	308	339	0.04%	0.005%
65	10.738	1582	1583	1585	rBV2	137	126	0.01%	0.002%
66	10.927	1612	1614	1616	rBV2	132	122	0.01%	0.002%
67	10.970	1618	1621	1624	rVV3	965	935	0.11%	0.014%
68	11.079	1637	1639	1641	rBV2	118	113	0.01%	0.002%
69	11.104	1641	1643	1649	rVB2	247	314	0.04%	0.005%
70	11.189	1652	1657	1670	rBV	367179	509253	57.35%	7.733%
71	11.384	1687	1689	1692	rVB2	146	158	0.02%	0.002%
72	11.457	1697	1701	1702	rBV2	297	291	0.03%	0.004%
73	11.713	1740	1743	1744	rBV2	240	163	0.02%	0.002%
74	11.762	1747	1751	1756	rVB4	832	1502	0.17%	0.023%
75	11.902	1770	1774	1775	rBV2	180	124	0.01%	0.002%
76	11.939	1778	1780	1783	rVB2	289	298	0.03%	0.005%

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 ClientSampleId :
 A4CG8ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

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

77	11.982	1783	1787	1788	rBV2	890	971	0.11%	0.015%
78	12.024	1788	1794	1810	rVB	399563	531869	59.90%	8.076%
79	12.189	1820	1821	1825	rBV4	242	232	0.03%	0.004%
80	12.225	1825	1827	1832	rVB	444	561	0.06%	0.009%
81	12.317	1837	1842	1856	rBV	539164	715894	80.62%	10.871%
82	12.573	1883	1884	1886	rVB2	178	129	0.01%	0.002%
83	12.762	1911	1915	1919	rVB3	748	993	0.11%	0.015%
84	12.811	1921	1923	1926	rBV	154	165	0.02%	0.003%
85	12.872	1929	1933	1939	rBV2	4095	5850	0.66%	0.089%
86	13.018	1956	1957	1959	rBV	224	127	0.01%	0.002%
87	13.164	1979	1981	1983	rBV	201	182	0.02%	0.003%
88	13.268	1996	1998	1999	rVB	210	134	0.02%	0.002%
89	13.280	1999	2000	2004	rBV2	169	203	0.02%	0.003%
90	13.323	2004	2007	2009	rBV2	113	153	0.02%	0.002%
91	13.402	2017	2020	2025	rBV2	2511	3491	0.39%	0.053%
92	13.683	2062	2066	2072	rVV4	1302	2198	0.25%	0.033%
93	13.780	2078	2082	2089	rBV2	1690	2853	0.32%	0.043%
94	14.128	2134	2139	2143	rBV2	771	1219	0.14%	0.019%
95	14.189	2147	2149	2150	rBV2	201	136	0.02%	0.002%
96	14.213	2150	2153	2154	rVB2	168	111	0.01%	0.002%
97	14.268	2160	2162	2164	rBV	233	246	0.03%	0.004%
98	14.426	2184	2188	2196	rVB2	2457	3595	0.40%	0.055%
99	14.646	2221	2224	2228	rBV2	727	868	0.10%	0.013%
100	14.731	2236	2238	2239	rBV	245	134	0.02%	0.002%

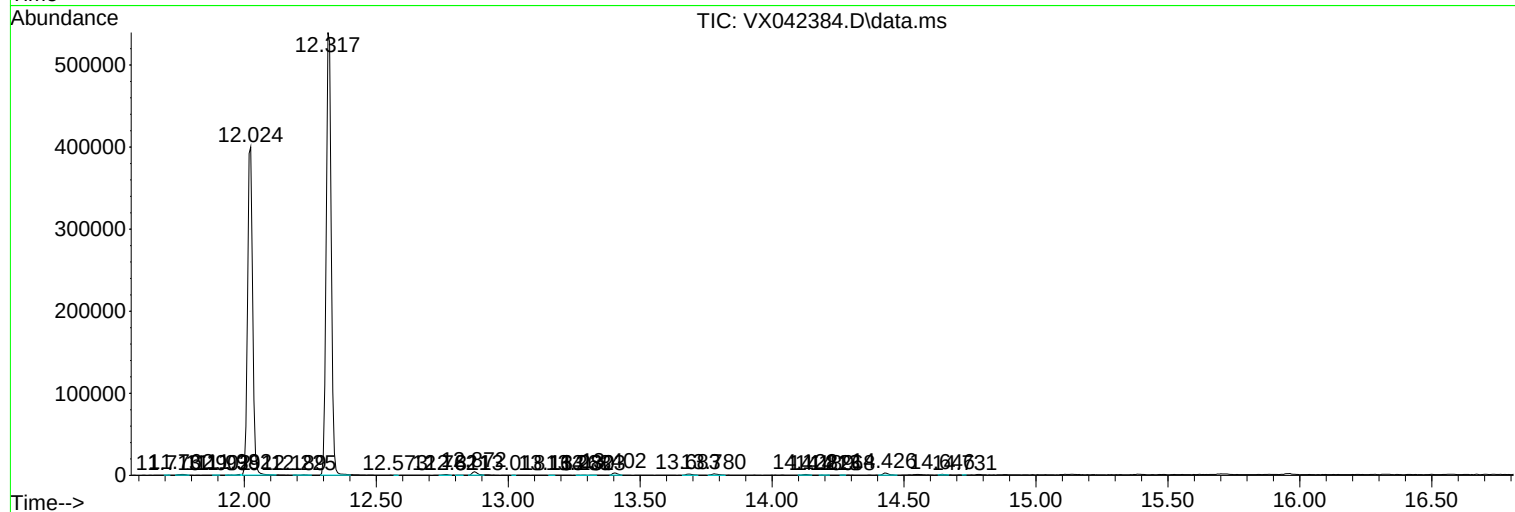
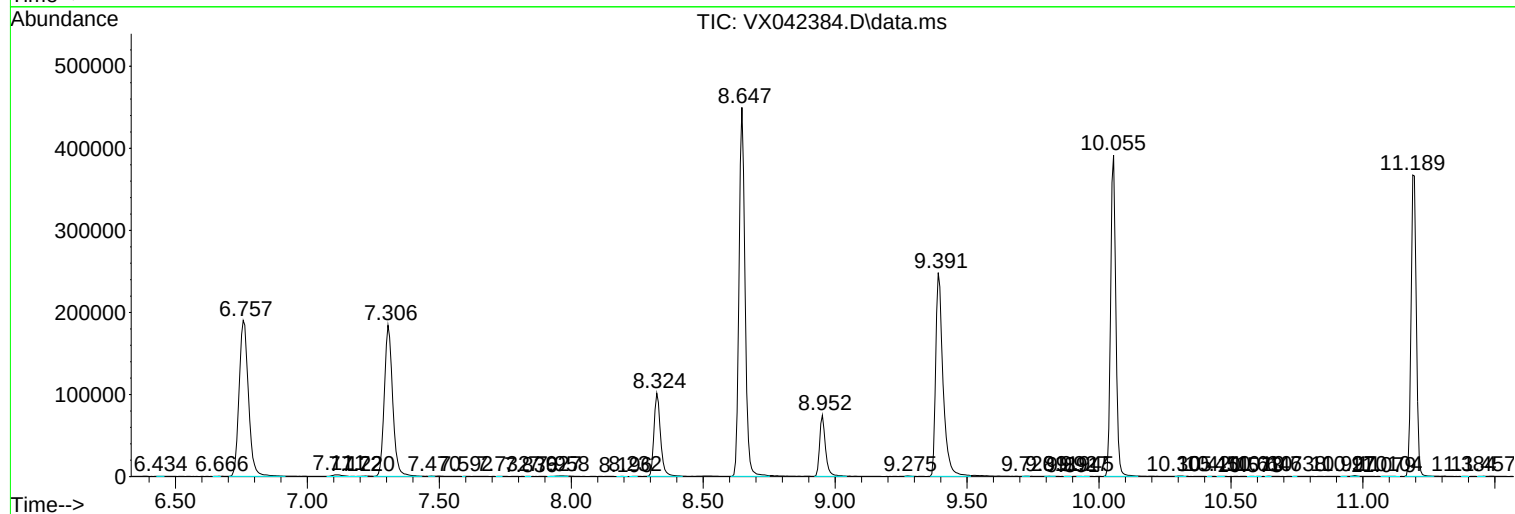
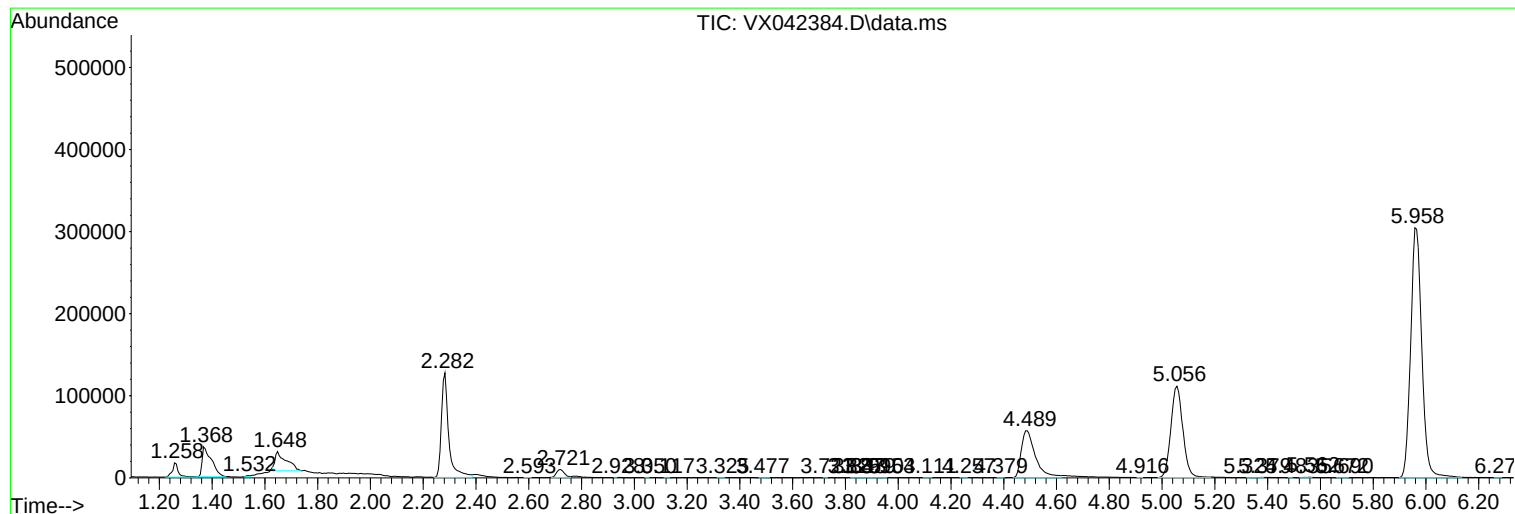
Sum of corrected areas: 6585408

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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4CG8ME

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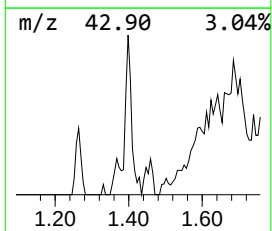
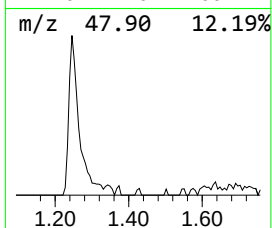
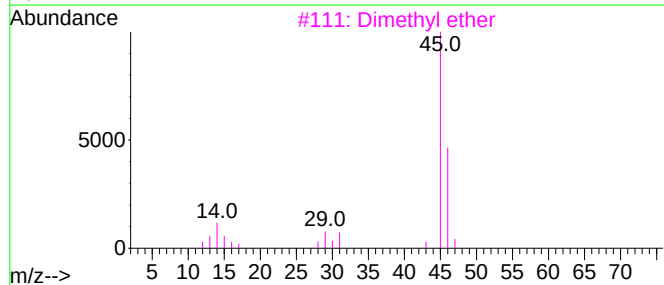
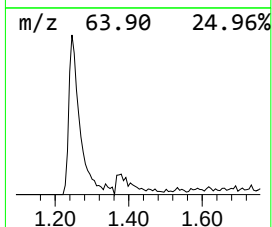
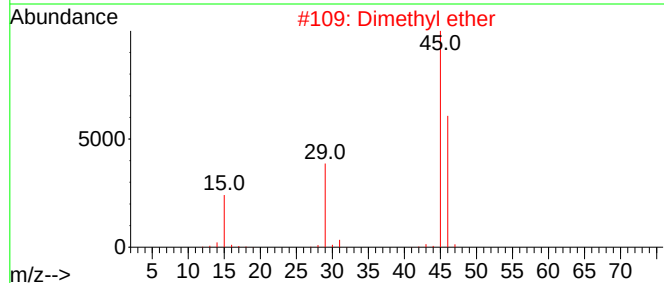
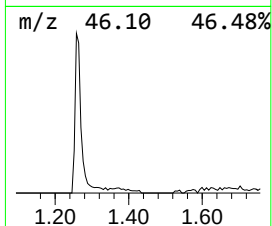
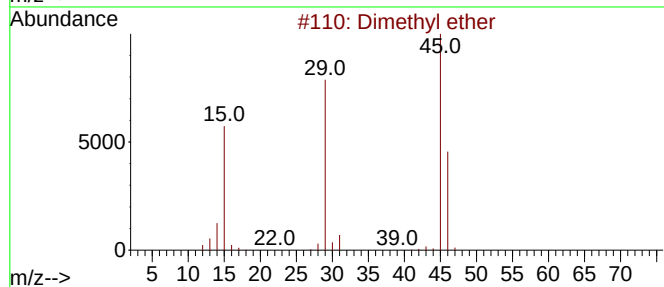
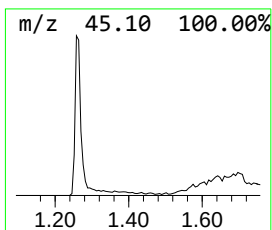
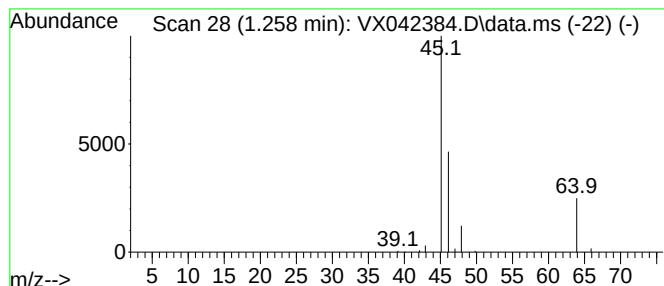
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	2.91 ug/L	27104	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	45
2			Dimethyl ether	46	C2H6O	000115-10-6	9
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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.258	2.9	ug/L	27104	1	6.757	465256	50.0