

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
 Data File : VX042383.D
 Acq On : 18 Jul 2024 20:28
 Operator : JC/MD
 Sample : P3238-16ME
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4BZ6ME

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: VX042383.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	38	rBV2	15815	25294	2.82%	0.377%
2	1.368	43	46	64	rVB	37822	94215	10.51%	1.403%
3	1.648	89	92	107	rVB	25006	68103	7.60%	1.014%
4	2.282	189	196	214	rBV	130280	249748	27.86%	3.720%
5	2.575	242	244	248	rBB2	120	119	0.01%	0.002%
6	2.611	248	250	252	rVB	281	197	0.02%	0.003%
7	2.660	256	258	262	rBV2	172	229	0.03%	0.003%
8	2.721	262	268	273	rBV	4443	8515	0.95%	0.127%
9	2.916	298	300	301	rBV2	144	118	0.01%	0.002%
10	2.940	301	304	309	rVB2	386	676	0.08%	0.010%
11	3.270	354	358	361	rVB2	229	303	0.03%	0.005%
12	3.501	394	396	400	rBV2	99	128	0.01%	0.002%
13	3.623	414	416	419	rBV	146	128	0.01%	0.002%
14	3.672	421	424	426	rVB2	108	144	0.02%	0.002%
15	3.879	455	458	459	rBV2	117	118	0.01%	0.002%
16	4.111	494	496	497	rBV	113	109	0.01%	0.002%
17	4.178	504	507	510	rVB2	146	195	0.02%	0.003%
18	4.294	524	526	530	rBV2	178	200	0.02%	0.003%
19	4.483	548	557	574	rBV	57853	206173	23.00%	3.071%
20	5.056	639	651	665	rBV	114881	352671	39.34%	5.253%
21	5.379	702	704	706	rBV2	329	387	0.04%	0.006%
22	5.568	727	735	737	rVV3	419	1046	0.12%	0.016%
23	5.617	740	743	745	rBV2	104	131	0.01%	0.002%
24	5.653	745	749	751	rBV	136	170	0.02%	0.003%
25	5.672	751	752	756	rVV2	129	137	0.02%	0.002%
26	5.727	759	761	764	rVB	159	157	0.02%	0.002%
27	5.757	764	766	768	rBV2	113	139	0.02%	0.002%
28	5.964	788	800	814	rBV2	310624	896420	100.00%	13.352%
29	6.190	835	837	839	rBV2	231	216	0.02%	0.003%
30	6.318	856	858	859	rVB	183	120	0.01%	0.002%
31	6.361	863	865	867	rBV	213	238	0.03%	0.004%
32	6.550	893	896	898	rVV2	186	206	0.02%	0.003%
33	6.659	911	914	917	rVV	108	140	0.02%	0.002%
34	6.757	921	930	950	rBV	193547	476904	53.20%	7.104%
35	7.110	982	988	996	rBV4	1922	4655	0.52%	0.069%
36	7.171	996	998	1001	rVB	221	172	0.02%	0.003%

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Integrator: RTE

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Peak Location: TOP

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Peak separation: 5

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 Title : VOC Analysis

37	7.214	1001	1005	1007	rBV2	454	710	0.08%	0.011%
38	7.306	1011	1020	1042	rBV	184812	414033	46.19%	6.167%
39	7.482	1045	1049	1051	rBV3	394	568	0.06%	0.008%
40	7.702	1079	1085	1086	rBV2	170	263	0.03%	0.004%
41	7.775	1096	1097	1100	rVB	173	111	0.01%	0.002%
42	7.812	1100	1103	1105	rBV2	97	119	0.01%	0.002%
43	7.836	1105	1107	1111	rVV2	131	120	0.01%	0.002%
44	7.952	1122	1126	1131	rBV4	732	1557	0.17%	0.023%
45	8.135	1155	1156	1158	rBV	137	120	0.01%	0.002%
46	8.324	1181	1187	1205	rVV	101015	179186	19.99%	2.669%
47	8.507	1214	1217	1218	rBV3	499	485	0.05%	0.007%
48	8.647	1233	1240	1257	rBV	454017	728186	81.23%	10.846%
49	8.854	1273	1274	1277	rBV3	225	131	0.01%	0.002%
50	8.952	1285	1290	1308	rVB	75722	117438	13.10%	1.749%
51	9.202	1328	1331	1333	rBV2	130	147	0.02%	0.002%
52	9.226	1333	1335	1337	rBV2	240	186	0.02%	0.003%
53	9.275	1341	1343	1346	rVB2	482	388	0.04%	0.006%
54	9.317	1346	1350	1352	rBV	106	157	0.02%	0.002%
55	9.391	1356	1362	1385	rBV	259235	484656	54.07%	7.219%
56	9.640	1401	1403	1406	rBV4	305	315	0.04%	0.005%
57	9.775	1423	1425	1429	rBV2	218	245	0.03%	0.004%
58	9.988	1458	1460	1465	rBV2	177	197	0.02%	0.003%
59	10.055	1465	1471	1487	rBV	405387	559599	62.43%	8.335%
60	10.311	1509	1513	1519	rVB	734	995	0.11%	0.015%
61	10.652	1565	1569	1572	rVB2	345	465	0.05%	0.007%
62	10.750	1583	1585	1587	rBV2	83	110	0.01%	0.002%
63	10.811	1592	1595	1597	rBV2	169	211	0.02%	0.003%
64	10.848	1599	1601	1602	rVB	182	115	0.01%	0.002%
65	10.872	1602	1605	1608	rBV2	148	164	0.02%	0.002%
66	10.915	1610	1612	1615	rVB2	129	133	0.01%	0.002%
67	10.969	1615	1621	1627	rBV3	979	1642	0.18%	0.024%
68	11.067	1636	1637	1639	rBV	144	128	0.01%	0.002%
69	11.098	1639	1642	1644	rBV2	327	248	0.03%	0.004%
70	11.195	1652	1658	1667	rBV	394501	521789	58.21%	7.772%
71	11.311	1673	1677	1682	rVB	7924	10777	1.20%	0.161%
72	11.451	1698	1700	1702	rBV	254	217	0.02%	0.003%
73	11.482	1704	1705	1709	rVB2	267	230	0.03%	0.003%
74	11.555	1715	1717	1720	rVB2	158	139	0.02%	0.002%
75	11.677	1733	1737	1738	rVB2	139	162	0.02%	0.002%
76	11.707	1740	1742	1744	rBV	208	226	0.03%	0.003%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Sampling : 1

Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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

77	11.750	1748	1749	1752	rBV2	287	224	0.02%	0.003%
78	11.902	1770	1774	1776	rVV2	109	145	0.02%	0.002%
79	11.982	1784	1787	1788	rBV2	294	335	0.04%	0.005%
80	12.024	1789	1794	1810	rVB	422496	546773	61.00%	8.144%
81	12.219	1824	1826	1833	rBV5	480	793	0.09%	0.012%
82	12.317	1837	1842	1852	rBV	545469	724467	80.82%	10.791%
83	12.762	1911	1915	1920	rBV2	4194	5668	0.63%	0.084%
84	12.872	1929	1933	1944	rVB	3508	4668	0.52%	0.070%
85	13.311	2003	2005	2006	rBV2	126	114	0.01%	0.002%
86	13.408	2017	2021	2026	rVV5	2116	3122	0.35%	0.047%
87	13.463	2029	2030	2033	rVB2	160	116	0.01%	0.002%
88	13.530	2039	2041	2045	rBV	152	165	0.02%	0.002%
89	13.695	2063	2068	2070	rBV3	543	749	0.08%	0.011%
90	13.780	2078	2082	2090	rVV3	1373	2315	0.26%	0.034%
91	13.835	2090	2091	2093	rVB	203	117	0.01%	0.002%
92	14.024	2118	2122	2123	rBV	203	309	0.03%	0.005%
93	14.036	2123	2124	2126	rVB	280	146	0.02%	0.002%
94	14.054	2126	2127	2130	rBV	193	152	0.02%	0.002%
95	14.127	2135	2139	2145	rVV	2244	2963	0.33%	0.044%
96	14.176	2145	2147	2149	rBV2	192	120	0.01%	0.002%
97	14.432	2185	2189	2197	rVB2	1638	2410	0.27%	0.036%
98	14.548	2204	2208	2209	rBV2	534	780	0.09%	0.012%
99	14.646	2222	2224	2229	rVB4	656	792	0.09%	0.012%
100	15.139	2302	2305	2309	rVB4	734	873	0.10%	0.013%

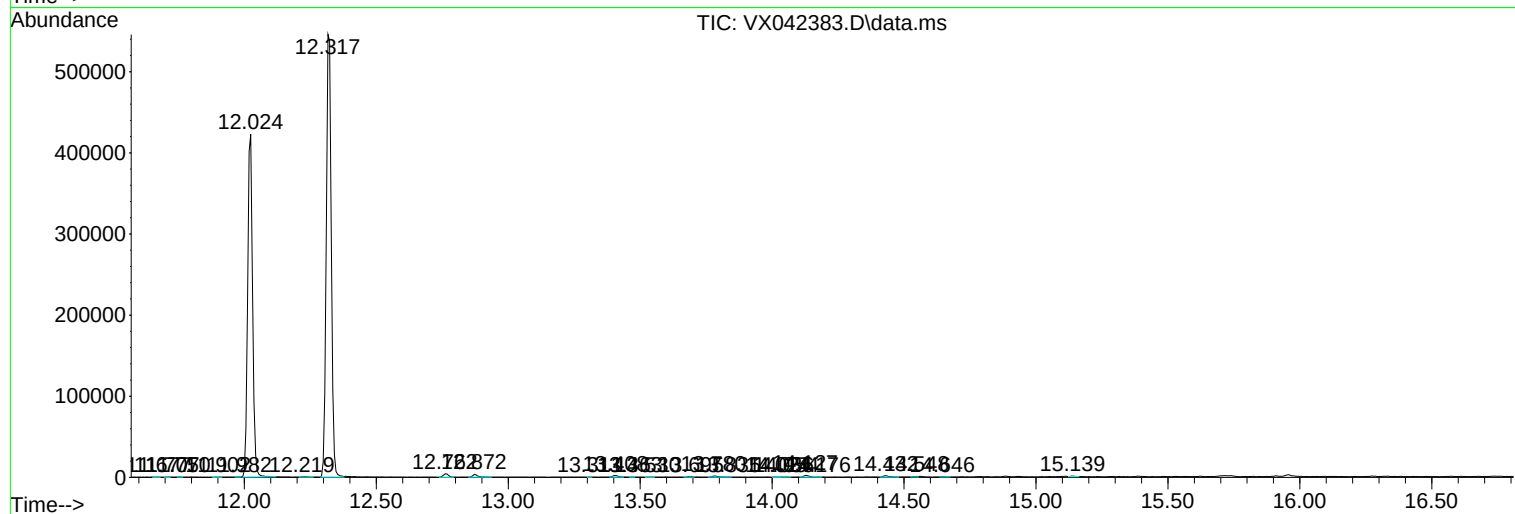
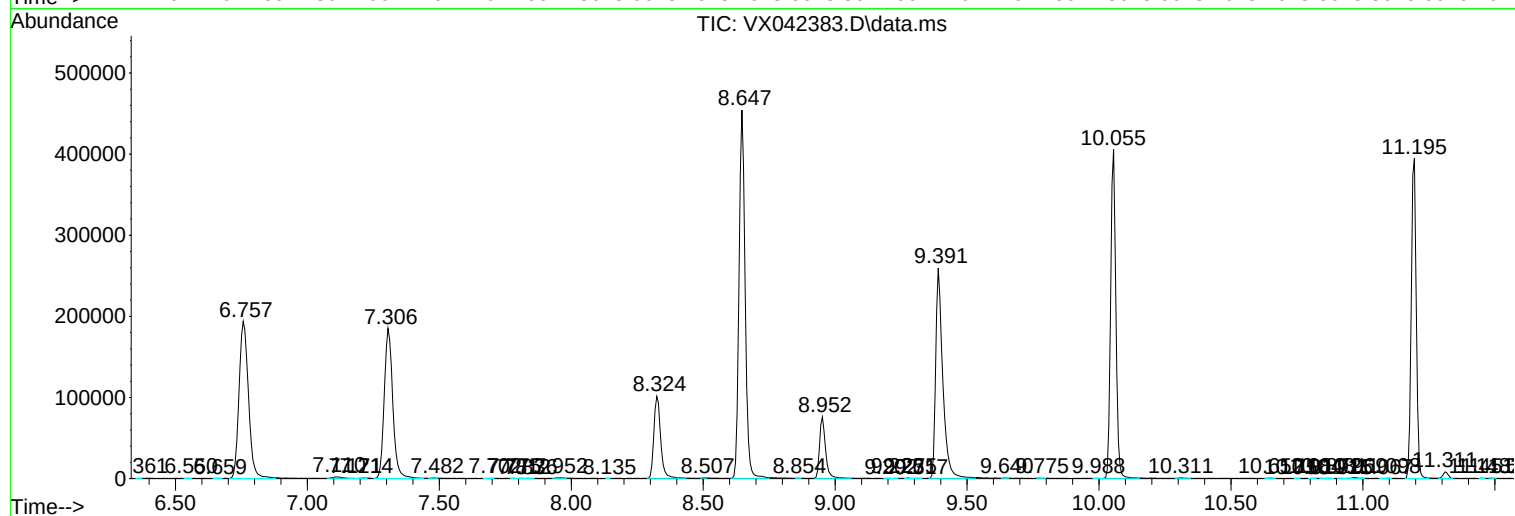
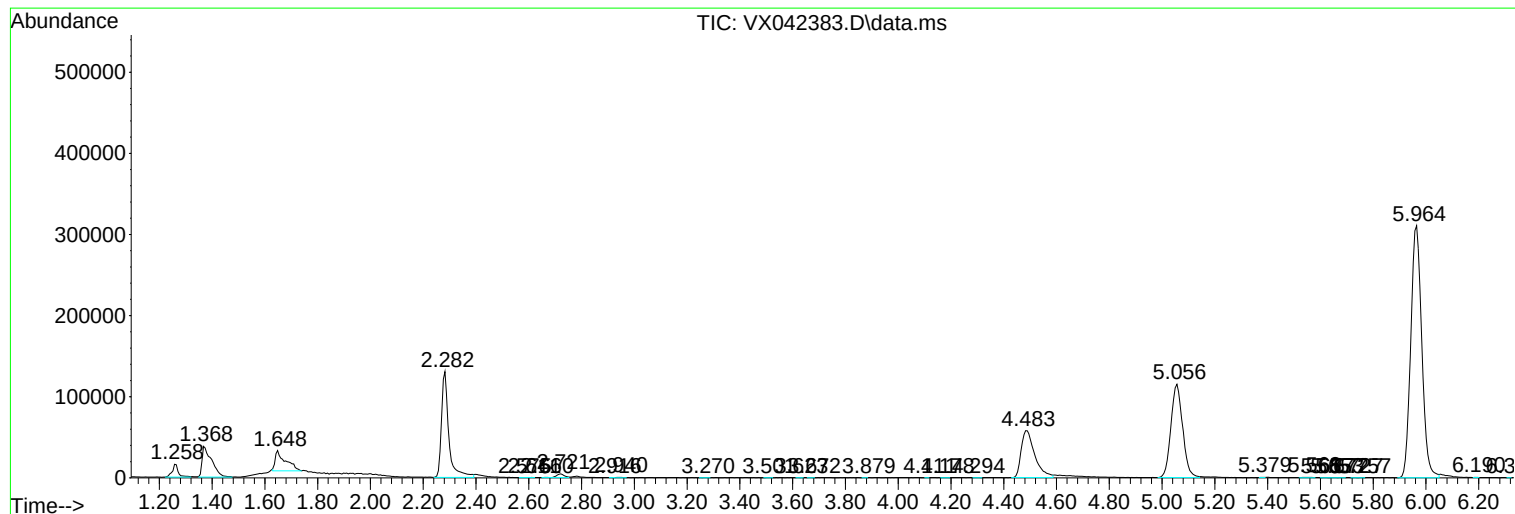
Sum of corrected areas: 6713605

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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BZ6ME

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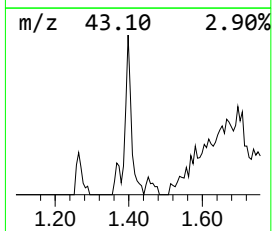
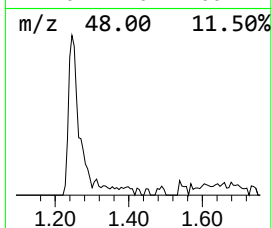
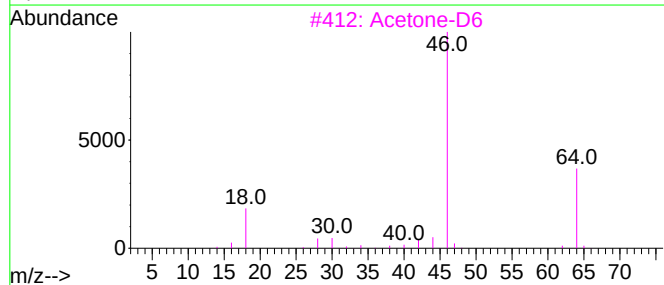
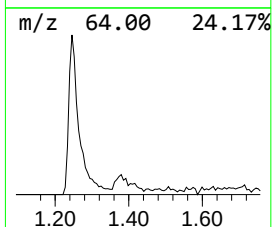
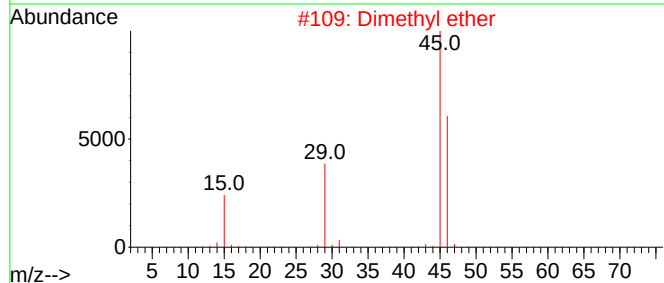
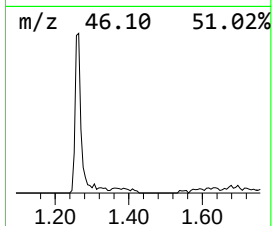
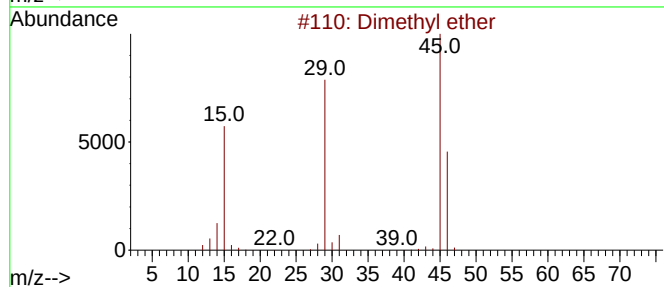
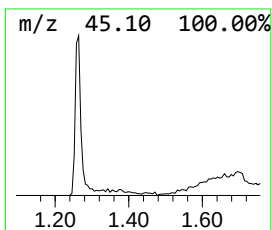
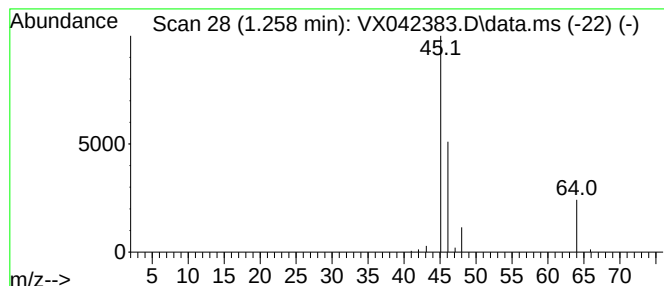
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	2.65 ug/L	25294	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	50
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Acetone-D6	64	C3D6O	000666-52-4	9
4			Ethanol	46	C2H6O	000064-17-5	7
5			Dimethyl ether	46	C2H6O	000115-10-6	7



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Dimethyl ether	1.258	2.6	ug/L	25294	1	6.757	476904	50.0