

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071824\
 Data File : VX042366.D
 Acq On : 18 Jul 2024 13:58
 Operator : JC/MD
 Sample : P3215-03ME
 Misc : 5.69g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4C00ME

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: VX042366.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	13321	28939	4.82%	0.574%
2	1.367	43	46	58	rBV	26431	63103	10.51%	1.253%
3	2.282	190	196	212	rBV	90247	166012	27.66%	3.295%
4	2.617	249	251	252	rBV	207	161	0.03%	0.003%
5	2.654	255	257	260	rBV2	245	288	0.05%	0.006%
6	2.715	260	267	274	rBV	63919	124481	20.74%	2.471%
7	3.233	350	352	354	rBV	141	118	0.02%	0.002%
8	3.343	364	370	377	rVB4	515	1184	0.20%	0.024%
9	3.422	380	383	384	rBV2	169	155	0.03%	0.003%
10	3.910	461	463	466	rVV	125	141	0.02%	0.003%
11	3.971	469	473	474	rBV	154	210	0.03%	0.004%
12	4.019	479	481	484	rBV2	154	170	0.03%	0.003%
13	4.087	489	492	494	rVV2	114	147	0.02%	0.003%
14	4.117	496	497	502	rVB2	140	151	0.03%	0.003%
15	4.251	517	519	522	rBV2	133	132	0.02%	0.003%
16	4.483	547	557	576	rBV	36461	126688	21.11%	2.515%
17	4.903	624	626	628	rVB2	176	150	0.02%	0.003%
18	4.928	628	630	631	rBV	189	122	0.02%	0.002%
19	5.056	639	651	670	rBV	71411	223074	37.17%	4.428%
20	5.239	680	681	684	rBV2	193	205	0.03%	0.004%
21	5.385	701	705	706	rBV2	291	423	0.07%	0.008%
22	5.537	728	730	731	rBV	253	188	0.03%	0.004%
23	5.763	765	767	770	rBV2	197	262	0.04%	0.005%
24	5.818	774	776	779	rVB2	175	187	0.03%	0.004%
25	5.854	779	782	784	rBV2	129	135	0.02%	0.003%
26	5.964	789	800	820	rBV2	198577	572340	95.36%	11.361%
27	6.281	850	852	855	rVB2	179	172	0.03%	0.003%
28	6.373	862	867	868	rBV2	317	330	0.05%	0.007%
29	6.421	873	875	877	rBV	223	206	0.03%	0.004%
30	6.446	877	879	883	rBV2	167	187	0.03%	0.004%
31	6.549	890	896	899	rBV3	230	433	0.07%	0.009%
32	6.623	907	908	910	rBV	199	147	0.02%	0.003%
33	6.678	915	917	921	rVV2	352	278	0.05%	0.006%
34	6.757	921	930	950	rVV	211795	512279	85.36%	10.169%
35	7.116	984	989	997	rVB4	1163	2580	0.43%	0.051%
36	7.226	999	1007	1011	rBV4	620	1347	0.22%	0.027%

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Integrator: RTE

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Peak separation: 5

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

37	7.305	1011	1020	1038	rBV	116148	256362	42.72%	5.089%
38	7.482	1046	1049	1050	rBV	215	223	0.04%	0.004%
39	7.513	1052	1054	1055	rVB	292	160	0.03%	0.003%
40	7.690	1081	1083	1086	rBV2	153	150	0.02%	0.003%
41	7.720	1086	1088	1091	rBV	178	190	0.03%	0.004%
42	7.769	1094	1096	1099	rVB	181	163	0.03%	0.003%
43	7.799	1099	1101	1102	rBV2	173	130	0.02%	0.003%
44	7.964	1122	1128	1143	rBV2	8863	19245	3.21%	0.382%
45	8.324	1181	1187	1201	rBV	63584	110274	18.37%	2.189%
46	8.445	1205	1207	1211	rBV3	242	385	0.06%	0.008%
47	8.506	1215	1217	1218	rBV	165	144	0.02%	0.003%
48	8.592	1229	1231	1234	rBV	135	111	0.02%	0.002%
49	8.647	1234	1240	1255	rBV	295263	459960	76.64%	9.130%
50	8.854	1272	1274	1275	rBV	278	120	0.02%	0.002%
51	8.897	1279	1281	1284	rBV2	142	146	0.02%	0.003%
52	8.951	1285	1290	1300	rBV	46371	73211	12.20%	1.453%
53	9.116	1315	1317	1321	rVB	174	203	0.03%	0.004%
54	9.275	1339	1343	1350	rVB5	1109	1791	0.30%	0.036%
55	9.390	1357	1362	1377	rBV	148114	285217	47.52%	5.662%
56	9.720	1414	1416	1417	rBV	539	317	0.05%	0.006%
57	10.055	1465	1471	1489	rBV	438026	600167	100.00%	11.914%
58	10.311	1509	1513	1518	rBV2	795	1067	0.18%	0.021%
59	10.652	1565	1569	1576	rVB3	269	464	0.08%	0.009%
60	10.768	1585	1588	1589	rBV	180	181	0.03%	0.004%
61	10.799	1592	1593	1596	rBV	169	141	0.02%	0.003%
62	10.835	1596	1599	1603	rVB2	112	156	0.03%	0.003%
63	10.878	1603	1606	1608	rVB	159	150	0.02%	0.003%
64	10.915	1608	1612	1613	rBV2	119	147	0.02%	0.003%
65	10.939	1614	1616	1618	rVV	849	919	0.15%	0.018%
66	10.969	1618	1621	1627	rVV	2151	2996	0.50%	0.059%
67	11.097	1638	1642	1646	rVB3	476	650	0.11%	0.013%
68	11.128	1646	1647	1649	rBV	194	133	0.02%	0.003%
69	11.195	1652	1658	1670	rVV	236604	317123	52.84%	6.295%
70	11.323	1674	1679	1682	rVB2	289	438	0.07%	0.009%
71	11.707	1737	1742	1744	rBV3	726	1074	0.18%	0.021%
72	11.738	1744	1747	1748	rVV2	1106	1370	0.23%	0.027%
73	11.762	1748	1751	1760	rVB3	6063	9264	1.54%	0.184%
74	11.975	1783	1786	1788	rBV2	1611	1855	0.31%	0.037%
75	12.024	1788	1794	1803	rVB	457120	585895	97.62%	11.630%
76	12.225	1824	1827	1833	rVB4	986	1350	0.22%	0.027%

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Instrument :
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 ClientSampleId :
 A4C00ME

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	12.323	1837	1843	1858	rBV	339243	448002	74.65%	8.893%
78	12.573	1880	1884	1887	rVB3	413	559	0.09%	0.011%
79	12.689	1901	1903	1906	rVB	172	121	0.02%	0.002%
80	12.762	1912	1915	1918	rVB3	483	728	0.12%	0.014%
81	12.804	1918	1922	1923	rBV2	111	138	0.02%	0.003%
82	12.872	1929	1933	1937	rBV	4905	6000	1.00%	0.119%
83	13.085	1967	1968	1971	rBV2	134	123	0.02%	0.002%
84	13.115	1971	1973	1976	rVV2	196	195	0.03%	0.004%
85	13.402	2016	2020	2029	rBV3	3350	4435	0.74%	0.088%
86	13.597	2049	2052	2054	rBV3	277	301	0.05%	0.006%
87	13.682	2063	2066	2073	rBV3	1389	1791	0.30%	0.036%
88	13.756	2075	2078	2079	rBV	149	146	0.02%	0.003%
89	13.780	2079	2082	2085	rBV	520	817	0.14%	0.016%
90	13.810	2085	2087	2093	rVB2	928	1394	0.23%	0.028%
91	13.896	2099	2101	2103	rVB2	149	125	0.02%	0.002%
92	14.012	2118	2120	2122	rVB	187	128	0.02%	0.003%
93	14.042	2124	2125	2128	rBV	271	236	0.04%	0.005%
94	14.127	2136	2139	2143	rBV2	662	878	0.15%	0.017%
95	14.170	2143	2146	2149	rVV3	459	468	0.08%	0.009%
96	14.231	2154	2156	2158	rBV	385	300	0.05%	0.006%
97	14.432	2185	2189	2195	rBV	2110	2682	0.45%	0.053%
98	14.670	2226	2228	2230	rBV	245	180	0.03%	0.004%
99	14.889	2260	2264	2269	rBV6	951	1567	0.26%	0.031%
100	15.956	2434	2439	2445	rBV4	3357	5184	0.86%	0.103%

Sum of corrected areas: 5037665

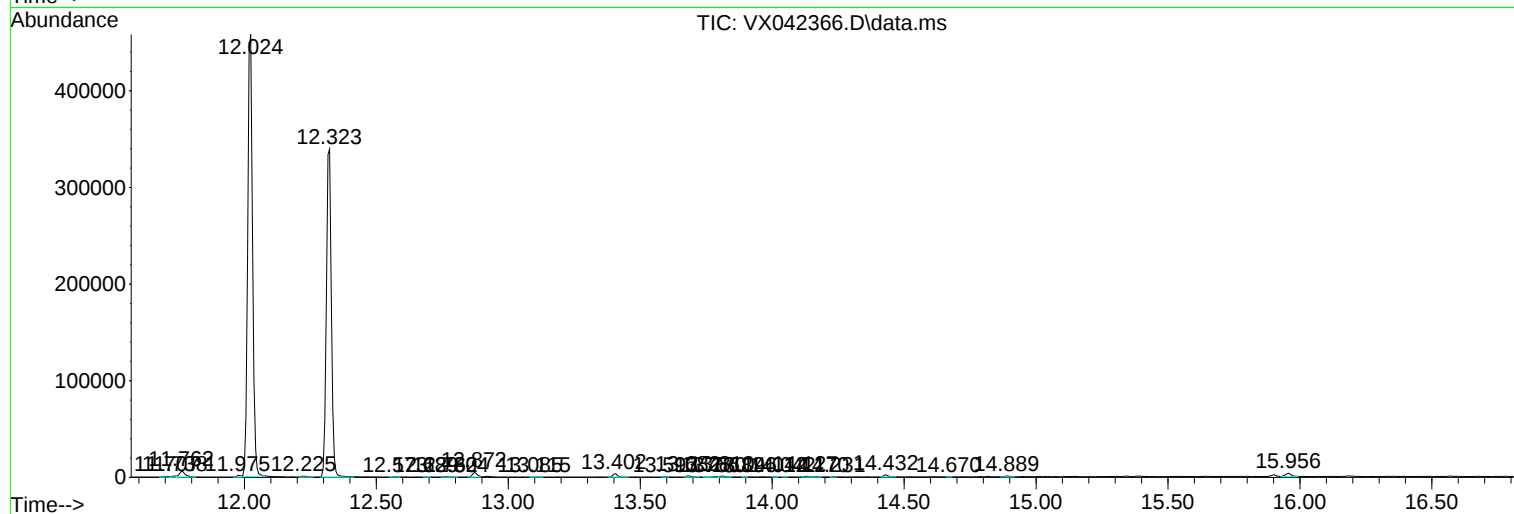
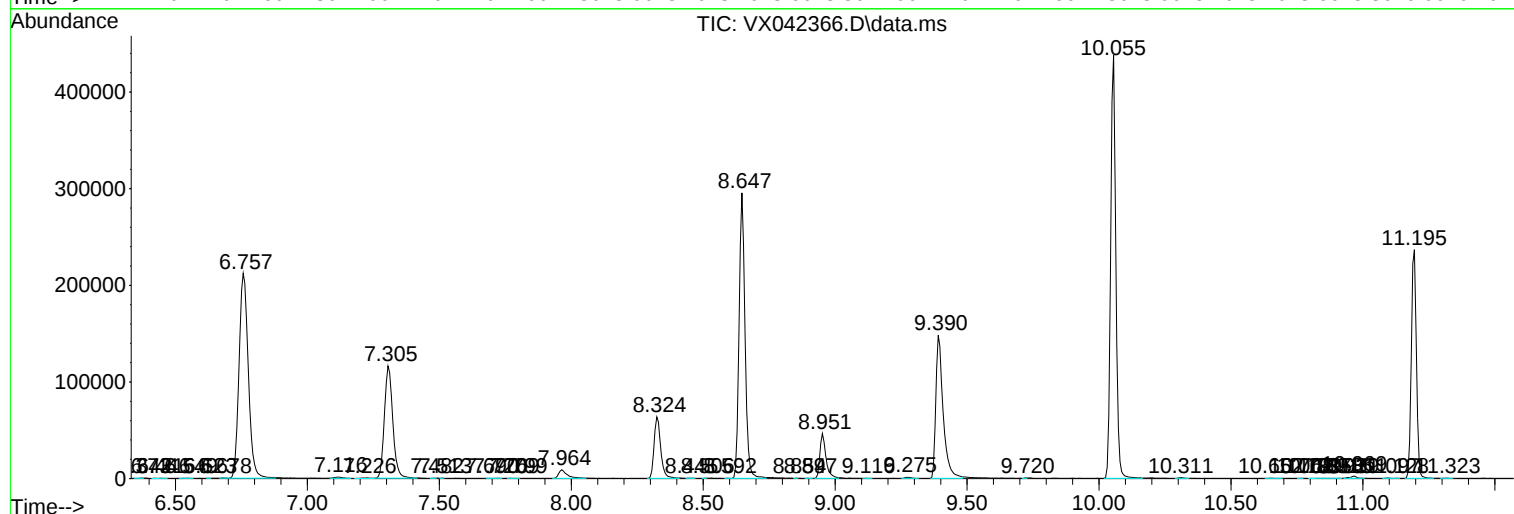
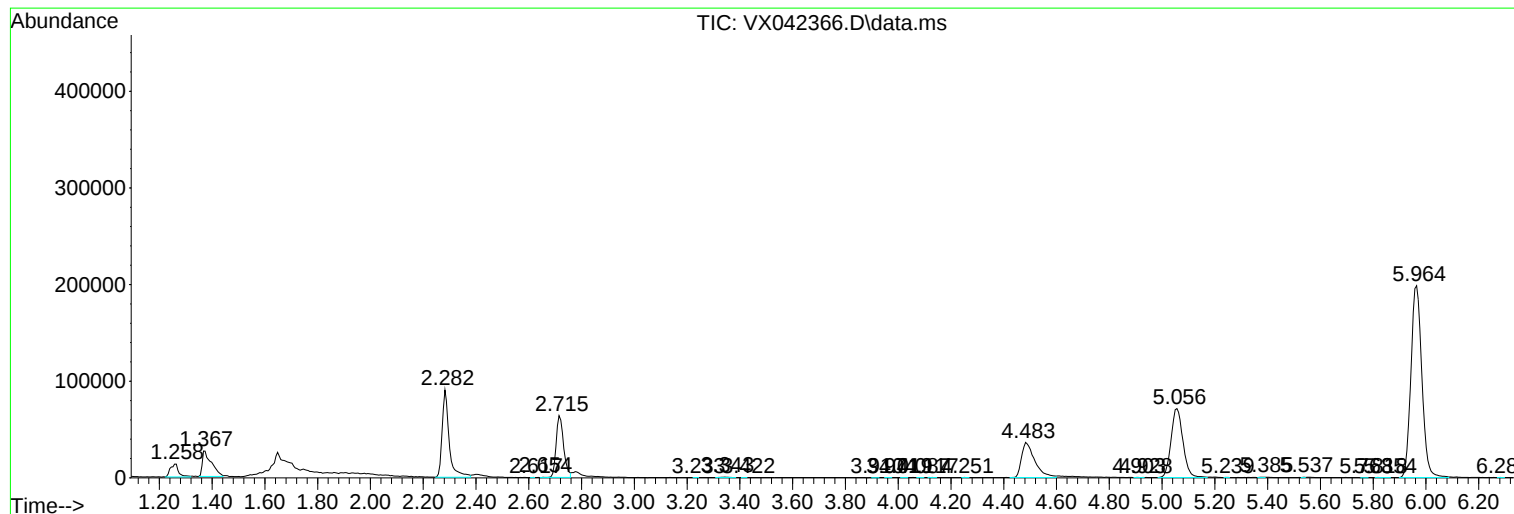
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4C00ME

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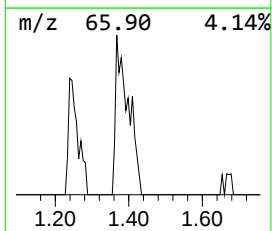
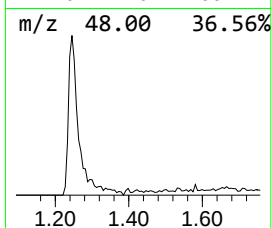
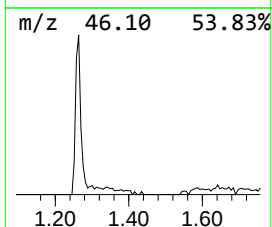
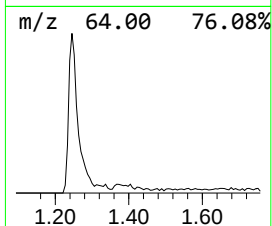
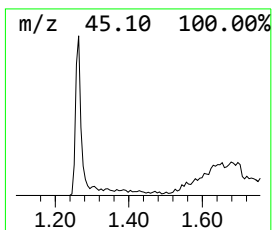
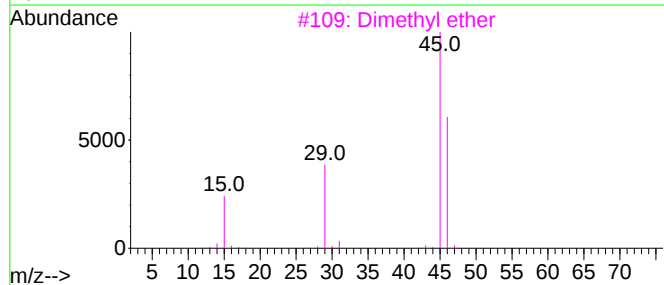
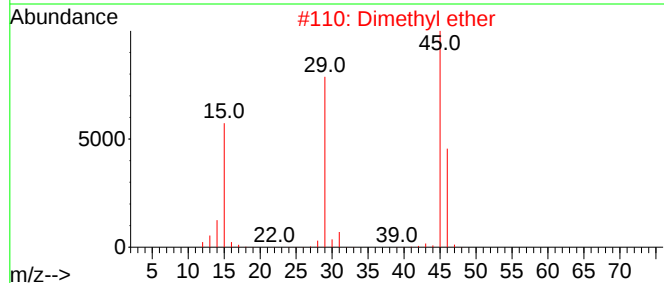
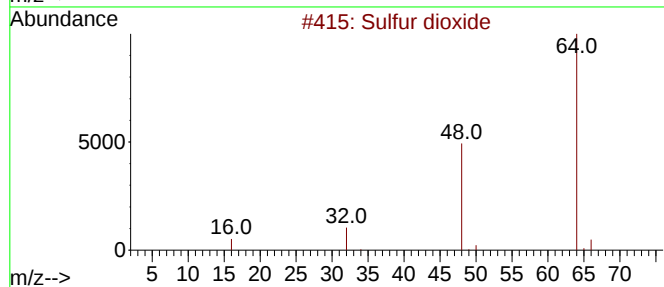
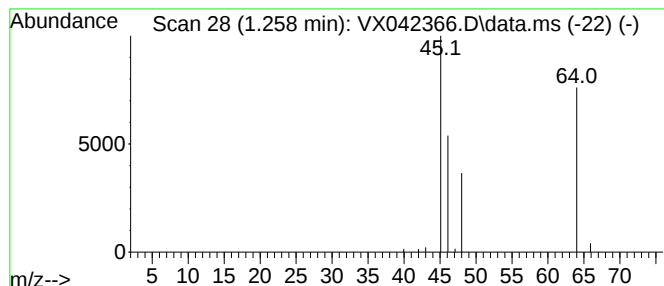
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	2.82 ug/L	28939	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	42
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Dimethyl ether	46	C2H6O	000115-10-6	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.258	2.8	ug/L	28939	1	6.757	512279	50.0