

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042590.D
 Acq On : 26 Jul 2024 00:19
 Operator : JC/MD
 Sample : P3276-14ME
 Misc : 9.69g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20J3ME

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: VX042590.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	36	rBV2	13235	26089	0.55%	0.292%
2	1.374	43	47	65	rVB	18107	58482	1.22%	0.655%
3	2.276	190	195	214	rBV	76072	150773	3.16%	1.690%
4	2.562	240	242	244	rBV	92	74	0.00%	0.001%
5	2.672	259	260	263	rBV	128	129	0.00%	0.001%
6	2.782	271	278	293	rBV	10548	28333	0.59%	0.318%
7	2.934	301	303	313	rVB3	1188	2724	0.06%	0.031%
8	3.081	325	327	330	rVB	289	268	0.01%	0.003%
9	3.105	330	331	334	rBV	80	67	0.00%	0.001%
10	3.264	355	357	359	rBV2	91	77	0.00%	0.001%
11	3.367	371	374	375	rBV	96	94	0.00%	0.001%
12	3.434	383	385	386	rVB	170	95	0.00%	0.001%
13	3.459	386	389	391	rBV2	88	123	0.00%	0.001%
14	3.611	412	414	415	rBV2	127	124	0.00%	0.001%
15	3.672	422	424	427	rVB2	198	165	0.00%	0.002%
16	3.733	432	434	436	rBV	125	121	0.00%	0.001%
17	3.837	449	451	454	rBV	112	141	0.00%	0.002%
18	3.885	454	459	460	rBV2	134	240	0.01%	0.003%
19	3.934	463	467	470	rBV	126	144	0.00%	0.002%
20	3.971	472	473	474	rBV	143	82	0.00%	0.001%
21	3.989	474	476	477	rBV	83	62	0.00%	0.001%
22	4.202	509	511	515	rBV2	168	185	0.00%	0.002%
23	4.404	542	544	547	rBV2	140	138	0.00%	0.002%
24	4.495	550	559	582	rBV	30606	116323	2.43%	1.304%
25	4.971	635	637	640	rVB	184	115	0.00%	0.001%
26	5.056	640	651	665	rBV	67577	209779	4.39%	2.351%
27	5.275	686	687	689	rVB2	141	80	0.00%	0.001%
28	5.379	702	704	705	rBV	121	81	0.00%	0.001%
29	5.562	731	734	736	rBV2	137	166	0.00%	0.002%
30	5.708	754	758	760	rBV2	97	141	0.00%	0.002%
31	5.812	773	775	776	rBV	103	74	0.00%	0.001%
32	5.830	776	778	779	rVB	131	72	0.00%	0.001%
33	5.958	789	799	818	rBV2	187618	537537	11.25%	6.024%
34	6.239	844	845	846	rVB	171	63	0.00%	0.001%
35	6.269	846	850	853	rBV	164	207	0.00%	0.002%
36	6.336	857	861	862	rBV	176	150	0.00%	0.002%

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 Title : VOC Analysis

37	6.373	862	867	874	rBV3	1023	2528	0.05%	0.028%
38	6.489	885	886	889	rBV	100	112	0.00%	0.001%
39	6.556	894	897	899	rBV	152	116	0.00%	0.001%
40	6.757	921	930	955	rBV	161178	391561	8.19%	4.388%
41	7.049	976	978	980	rVB	194	169	0.00%	0.002%
42	7.123	980	990	1012	rBV	2166204	4778590	100.00%	53.550%
43	7.305	1013	1020	1039	rVB	108234	249371	5.22%	2.794%
44	7.519	1053	1055	1057	rVB2	261	210	0.00%	0.002%
45	7.555	1060	1061	1063	rVB2	158	63	0.00%	0.001%
46	7.574	1063	1064	1066	rBV2	167	114	0.00%	0.001%
47	7.976	1126	1130	1136	rVB4	461	951	0.02%	0.011%
48	8.037	1138	1140	1141	rBV	109	105	0.00%	0.001%
49	8.049	1141	1142	1145	rBV2	99	91	0.00%	0.001%
50	8.244	1172	1174	1179	rBV3	259	344	0.01%	0.004%
51	8.324	1182	1187	1201	rBV	59210	103569	2.17%	1.161%
52	8.513	1216	1218	1220	rBV2	154	160	0.00%	0.002%
53	8.549	1222	1224	1227	rVV	124	92	0.00%	0.001%
54	8.647	1234	1240	1255	rBV	271976	427260	8.94%	4.788%
55	8.952	1285	1290	1309	rBV	43213	66805	1.40%	0.749%
56	9.073	1309	1310	1313	rBV	197	168	0.00%	0.002%
57	9.110	1314	1316	1317	rBV	261	119	0.00%	0.001%
58	9.165	1323	1325	1327	rBV2	134	106	0.00%	0.001%
59	9.214	1331	1333	1335	rVB	130	102	0.00%	0.001%
60	9.275	1338	1343	1349	rBV2	6704	9736	0.20%	0.109%
61	9.390	1357	1362	1377	rBV	114159	241589	5.06%	2.707%
62	9.714	1410	1415	1422	rBV3	919	1580	0.03%	0.018%
63	9.890	1442	1444	1447	rBV2	164	138	0.00%	0.002%
64	10.055	1465	1471	1489	rBV	328200	445351	9.32%	4.991%
65	10.287	1507	1509	1510	rBV	96	72	0.00%	0.001%
66	10.311	1510	1513	1519	rBV2	430	574	0.01%	0.006%
67	10.531	1547	1549	1550	rBV2	87	64	0.00%	0.001%
68	10.646	1566	1568	1570	rVB	153	90	0.00%	0.001%
69	10.811	1592	1595	1598	rBV2	153	270	0.01%	0.003%
70	10.969	1619	1621	1627	rBV2	163	244	0.01%	0.003%
71	11.195	1652	1658	1671	rBV	211482	276046	5.78%	3.093%
72	11.311	1675	1677	1682	rVB2	234	217	0.00%	0.002%
73	11.439	1693	1698	1700	rBV2	163	298	0.01%	0.003%
74	11.488	1705	1706	1707	rBV	113	61	0.00%	0.001%
75	11.567	1716	1719	1722	rBV2	186	274	0.01%	0.003%
76	11.634	1727	1730	1735	rVB3	198	304	0.01%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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 >

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

77	11.756	1749	1750	1752	rVB	176	113	0.00%	0.001%
78	11.902	1772	1774	1776	rBV2	81	83	0.00%	0.001%
79	12.024	1789	1794	1812	rVB	314656	401231	8.40%	4.496%
80	12.183	1819	1820	1823	rVB2	200	135	0.00%	0.002%
81	12.317	1837	1842	1854	rBV	285706	384718	8.05%	4.311%
82	12.853	1928	1930	1932	rBV	109	100	0.00%	0.001%
83	12.920	1939	1941	1942	rVB	131	71	0.00%	0.001%
84	13.012	1953	1956	1957	rBV	148	151	0.00%	0.002%
85	13.268	1996	1998	2000	rVB	201	157	0.00%	0.002%
86	13.378	2015	2016	2019	rVV2	204	208	0.00%	0.002%
87	13.408	2019	2021	2022	rVV2	127	89	0.00%	0.001%
88	13.597	2050	2052	2054	rVV2	190	169	0.00%	0.002%
89	13.786	2082	2083	2086	rBV2	146	125	0.00%	0.001%
90	13.975	2112	2114	2115	rBV	207	141	0.00%	0.002%
91	13.993	2115	2117	2119	rVV2	206	166	0.00%	0.002%
92	14.018	2119	2121	2122	rVV	120	74	0.00%	0.001%
93	14.036	2122	2124	2130	rVB2	685	752	0.02%	0.008%
94	14.127	2136	2139	2143	rBV4	370	509	0.01%	0.006%
95	14.164	2143	2145	2146	rBV2	132	73	0.00%	0.001%
96	14.335	2171	2173	2175	rVB	254	156	0.00%	0.002%
97	14.353	2175	2176	2178	rBV	184	155	0.00%	0.002%
98	14.432	2187	2189	2190	rBV	225	131	0.00%	0.001%
99	14.755	2239	2242	2245	rVB2	699	801	0.02%	0.009%
100	14.871	2259	2261	2264	rVB2	324	244	0.01%	0.003%

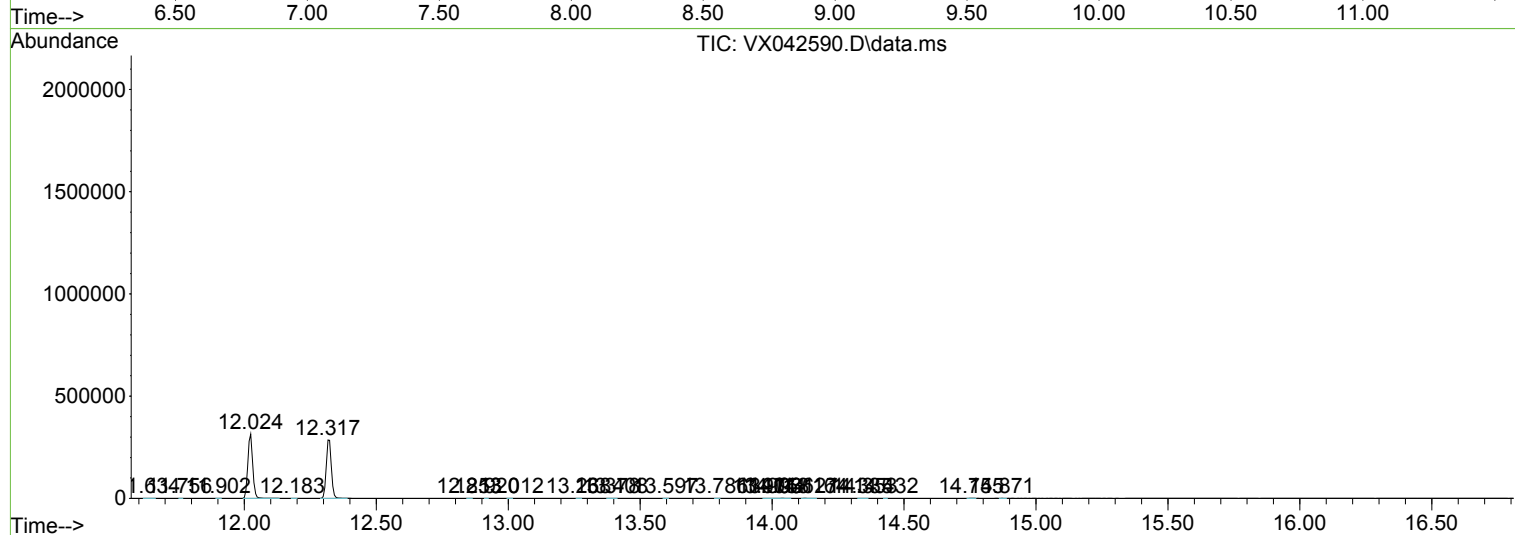
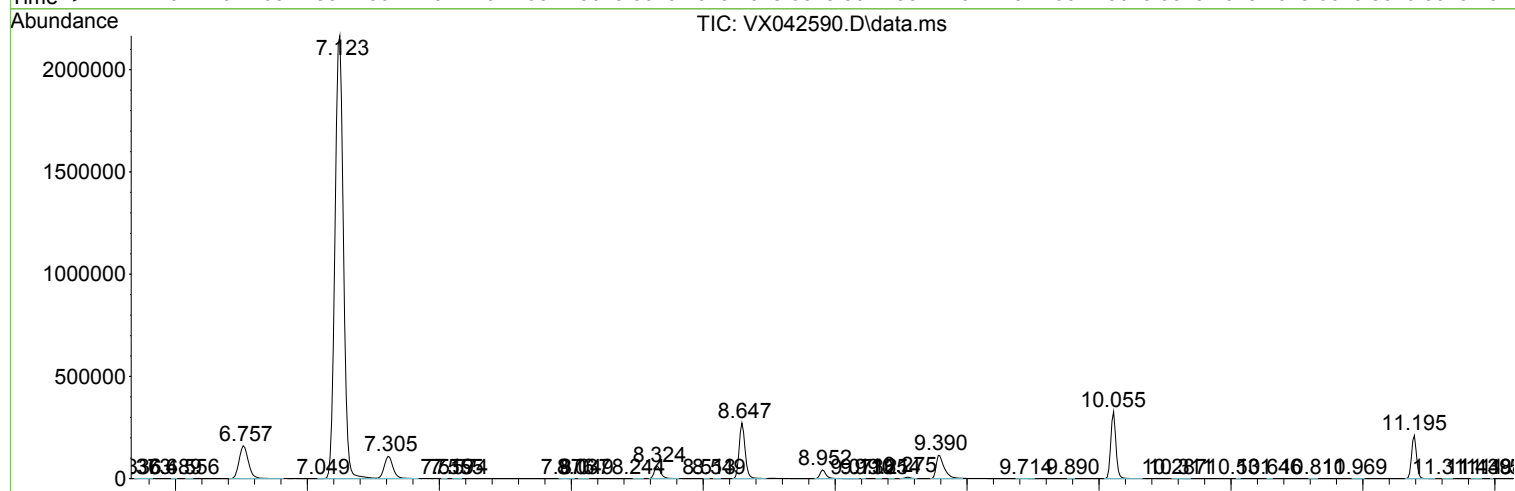
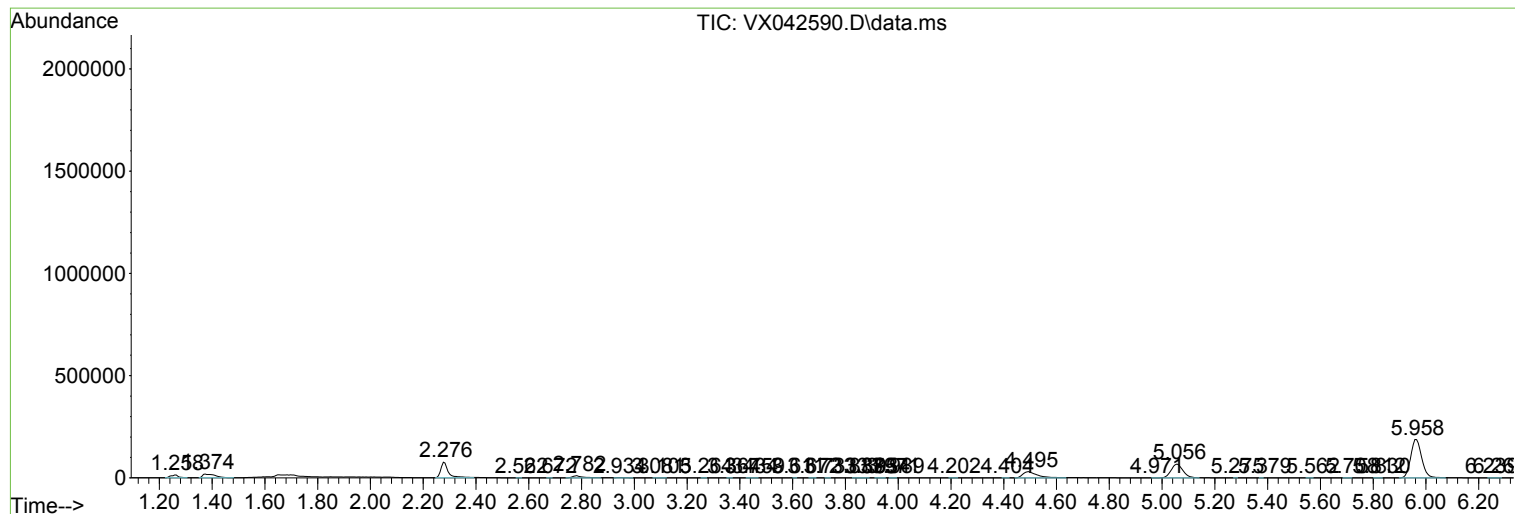
Sum of corrected areas: 8923684

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ALS Vial : 27 Sample Multiplier: 1

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



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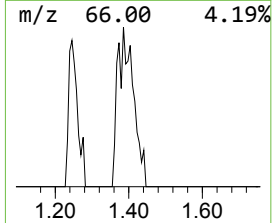
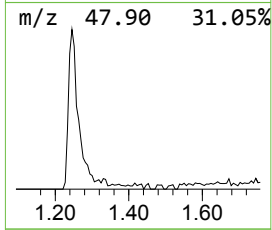
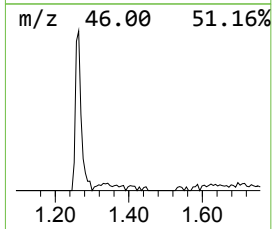
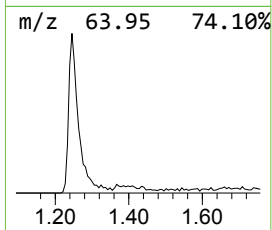
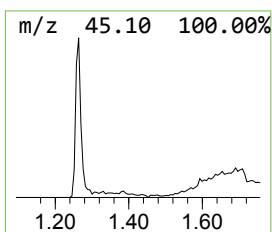
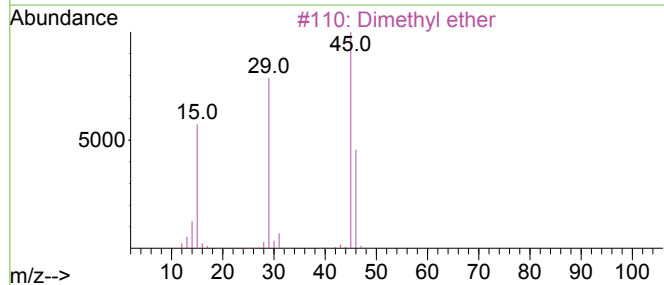
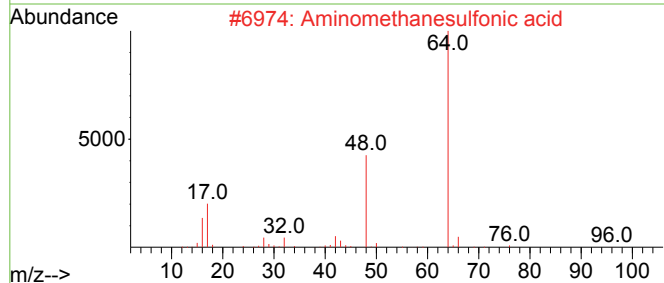
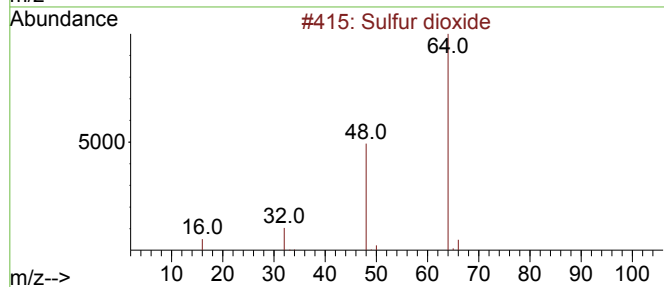
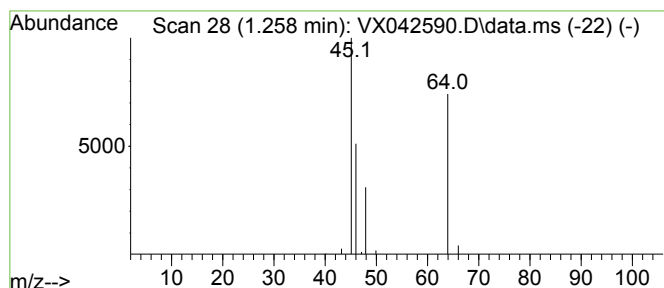
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	3.33 ug/L	26089	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	42
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	36
3			Dimethyl ether	46	C2H6O	000115-10-6	9
4			Dimethyl ether	46	C2H6O	000115-10-6	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.258	3.3	ug/L	26089	1	6.757	391561	50.0