

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042409.D
 Acq On : 19 Jul 2024 18:05
 Operator : JC/MD
 Sample : P3238-07ME
 Misc : 5.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4BF0ME

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: VX042409.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	37	rBV2	52166	89058	18.49%	2.159%
2	1.374	43	47	59	rBV	31093	68637	14.25%	1.664%
3	1.648	85	92	112	rVB2	19981	75624	15.70%	1.834%
4	2.197	180	182	185	rBV2	212	207	0.04%	0.005%
5	2.282	190	196	212	rBV	75755	141762	29.44%	3.437%
6	2.624	249	252	255	rVB2	141	217	0.05%	0.005%
7	2.721	258	268	273	rBV	6826	13683	2.84%	0.332%
8	2.782	274	278	288	rVV2	1969	4184	0.87%	0.101%
9	2.947	293	305	315	rBV	6212	16178	3.36%	0.392%
10	3.337	366	369	374	rVB4	252	303	0.06%	0.007%
11	3.465	386	390	392	rVB2	177	270	0.06%	0.007%
12	3.495	392	395	398	rBV2	126	194	0.04%	0.005%
13	4.489	549	558	575	rBV	24802	90466	18.79%	2.193%
14	5.056	639	651	668	rBV	58328	181083	37.60%	4.391%
15	5.397	702	707	709	rBV2	314	462	0.10%	0.011%
16	5.489	720	722	726	rVB2	176	208	0.04%	0.005%
17	5.550	726	732	738	rBV2	570	1323	0.27%	0.032%
18	5.800	770	773	776	rBV	160	228	0.05%	0.006%
19	5.964	789	800	824	rBV2	169057	480653	99.82%	11.654%
20	6.129	825	827	829	rVB3	304	266	0.06%	0.006%
21	6.342	857	862	864	rBV	228	325	0.07%	0.008%
22	6.379	864	868	876	rBV2	317	727	0.15%	0.018%
23	6.757	922	930	945	rBV	98312	234658	48.73%	5.689%
24	7.001	968	970	973	rVB2	255	206	0.04%	0.005%
25	7.037	973	976	979	rBV3	263	426	0.09%	0.010%
26	7.117	984	989	994	rVB3	866	1637	0.34%	0.040%
27	7.196	997	1002	1003	rBV2	155	201	0.04%	0.005%
28	7.220	1003	1006	1007	rBV2	290	339	0.07%	0.008%
29	7.306	1012	1020	1039	rVV	95351	214219	44.49%	5.194%
30	7.897	1115	1117	1119	rBV	246	201	0.04%	0.005%
31	7.970	1124	1129	1132	rBV2	685	1283	0.27%	0.031%
32	8.324	1181	1187	1203	rBV	63287	110482	22.94%	2.679%
33	8.452	1206	1208	1211	rVB3	246	265	0.06%	0.006%
34	8.519	1218	1219	1221	rBV2	254	249	0.05%	0.006%
35	8.647	1231	1240	1248	rBV	307550	481541	100.00%	11.675%
36	8.720	1248	1252	1266	rVB	17170	33520	6.96%	0.813%

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Integrator: RTE

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

37	8.866	1274	1276	1278	rBV2	352	241	0.05%	0.006%
38	8.903	1280	1282	1284	rBV2	253	228	0.05%	0.006%
39	8.952	1284	1290	1302	rBV	45268	71741	14.90%	1.739%
40	9.177	1325	1327	1329	rVB2	194	195	0.04%	0.005%
41	9.208	1329	1332	1333	rBV	187	213	0.04%	0.005%
42	9.275	1339	1343	1347	rVB2	704	883	0.18%	0.021%
43	9.391	1357	1362	1383	rBV	135528	266111	55.26%	6.452%
44	9.598	1393	1396	1398	rBV3	308	408	0.08%	0.010%
45	9.708	1409	1414	1419	rBV	2110	2932	0.61%	0.071%
46	9.842	1434	1436	1438	rVV	194	200	0.04%	0.005%
47	9.866	1438	1440	1443	rVV2	242	247	0.05%	0.006%
48	10.055	1465	1471	1490	rVV	236395	329228	68.37%	7.982%
49	10.195	1492	1494	1499	rVV3	759	978	0.20%	0.024%
50	10.305	1508	1512	1520	rVV	1071	1948	0.40%	0.047%
51	10.647	1564	1568	1572	rVB2	374	548	0.11%	0.013%
52	10.884	1604	1607	1610	rBV2	476	590	0.12%	0.014%
53	10.964	1616	1620	1625	rBV3	1322	2144	0.45%	0.052%
54	11.025	1628	1630	1633	rVB2	232	259	0.05%	0.006%
55	11.092	1637	1641	1643	rBV3	470	604	0.13%	0.015%
56	11.122	1643	1646	1649	rVB2	675	822	0.17%	0.020%
57	11.195	1652	1658	1667	rBV	221147	296084	61.49%	7.179%
58	11.311	1673	1677	1681	rBV4	544	775	0.16%	0.019%
59	11.390	1685	1690	1693	rBV3	420	597	0.12%	0.014%
60	11.433	1693	1697	1698	rBV2	495	489	0.10%	0.012%
61	11.482	1698	1705	1709	rVB6	1192	2464	0.51%	0.060%
62	11.561	1716	1718	1720	rBV3	308	309	0.06%	0.007%
63	11.634	1726	1730	1734	rBV5	677	981	0.20%	0.024%
64	11.689	1734	1739	1741	rBV3	608	865	0.18%	0.021%
65	11.713	1741	1743	1745	rBV3	607	515	0.11%	0.012%
66	11.744	1745	1748	1753	rBV3	1579	2491	0.52%	0.060%
67	11.835	1761	1763	1767	rBV3	678	923	0.19%	0.022%
68	11.890	1770	1772	1775	rVB3	777	593	0.12%	0.014%
69	11.933	1775	1779	1783	rBV2	2864	4002	0.83%	0.097%
70	11.976	1784	1786	1789	rBV2	865	455	0.09%	0.011%
71	12.024	1789	1794	1805	rVB	250126	322658	67.01%	7.823%
72	12.122	1805	1810	1813	rBV4	2404	3670	0.76%	0.089%
73	12.226	1824	1827	1829	rBV3	763	905	0.19%	0.022%
74	12.250	1829	1831	1836	rVV5	988	1544	0.32%	0.037%
75	12.323	1837	1843	1855	rVB	330413	449330	93.31%	10.894%
76	12.433	1856	1861	1863	rBV6	1447	2350	0.49%	0.057%

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Instrument :
 MSVOA_X
 ClientSampleId :
 A4BF0ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

77	12.573	1876	1884	1890	rBV6	1539	4285	0.89%	0.104%
78	12.683	1897	1902	1907	rVB7	1529	2744	0.57%	0.067%
79	12.732	1907	1910	1913	rBV5	841	1162	0.24%	0.028%
80	12.762	1913	1915	1917	rBV3	565	668	0.14%	0.016%
81	12.817	1920	1924	1928	rVB4	4079	5989	1.24%	0.145%
82	12.878	1929	1934	1936	rBV3	3432	5735	1.19%	0.139%
83	12.981	1948	1951	1957	rVB7	2676	4789	0.99%	0.116%
84	13.049	1957	1962	1966	rVB7	2130	3899	0.81%	0.095%
85	13.085	1966	1968	1970	rBV3	969	956	0.20%	0.023%
86	13.292	1998	2002	2006	rVB5	3778	5681	1.18%	0.138%
87	13.390	2014	2018	2019	rBV2	2700	3511	0.73%	0.085%
88	13.609	2047	2054	2058	rBV8	2226	6379	1.32%	0.155%
89	13.701	2061	2069	2072	rBV8	3304	7559	1.57%	0.183%
90	13.798	2077	2085	2089	rVB4	4102	9652	2.00%	0.234%
91	13.841	2089	2092	2099	rBV3	7186	9982	2.07%	0.242%
92	14.067	2125	2129	2131	rBV5	2123	3349	0.70%	0.081%
93	14.615	2216	2219	2221	rBV3	3587	4465	0.93%	0.108%
94	14.786	2245	2247	2255	rVB8	3062	3888	0.81%	0.094%
95	14.847	2255	2257	2260	rBV4	2190	2290	0.48%	0.056%
96	15.091	2293	2297	2299	rBV5	2674	4957	1.03%	0.120%
97	15.957	2435	2439	2443	rBV6	2115	3605	0.75%	0.087%
98	16.091	2457	2461	2466	rVB8	2983	5097	1.06%	0.124%
99	16.274	2487	2491	2495	rBV6	2717	4120	0.86%	0.100%
100	16.694	2557	2560	2561	rBV3	1709	1846	0.38%	0.045%

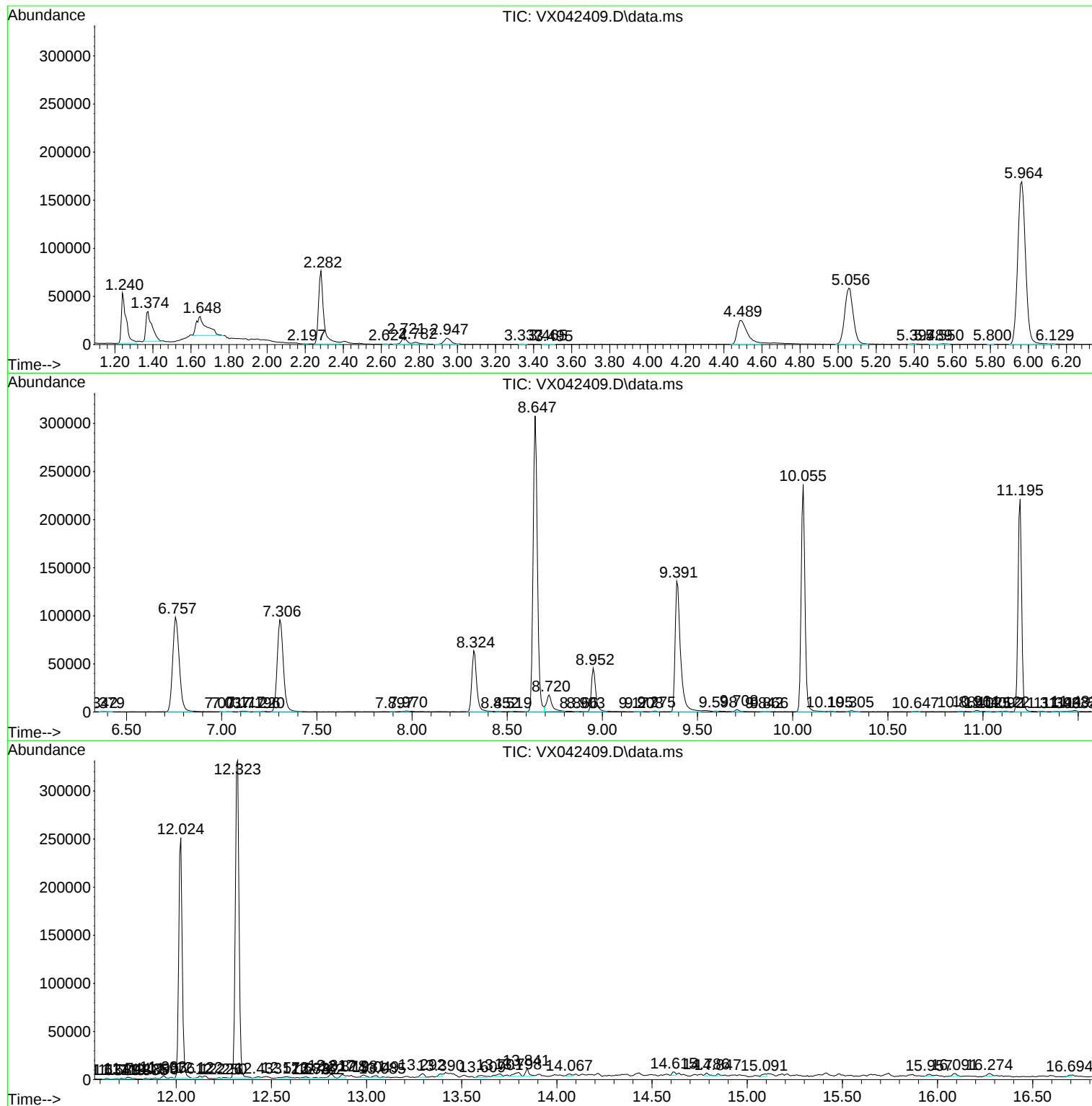
Sum of corrected areas: 4124413

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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BF0ME

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
ClientSampleId :
A4BF0ME

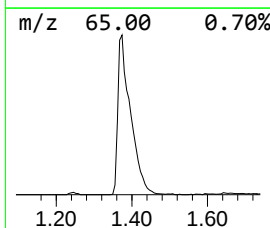
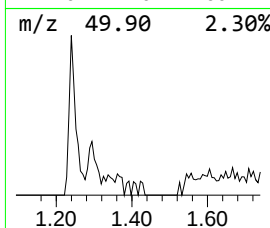
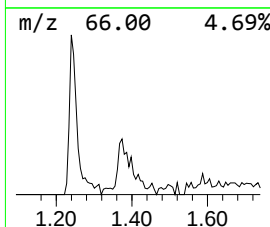
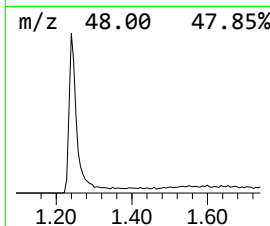
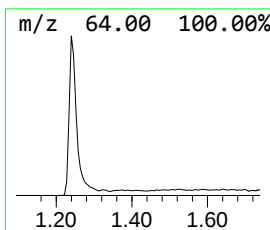
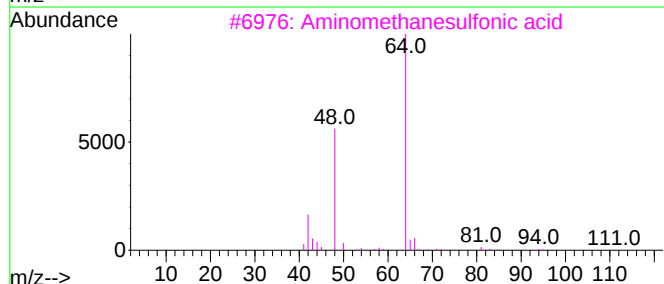
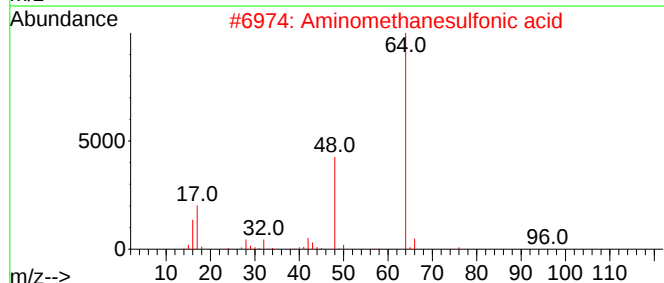
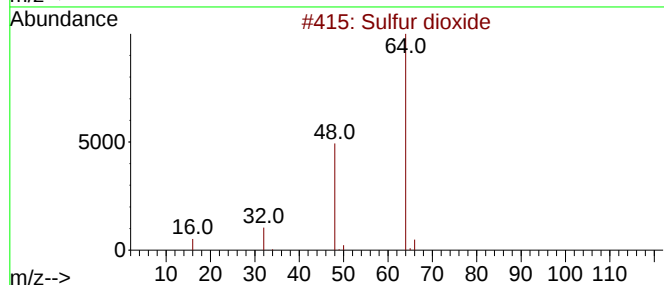
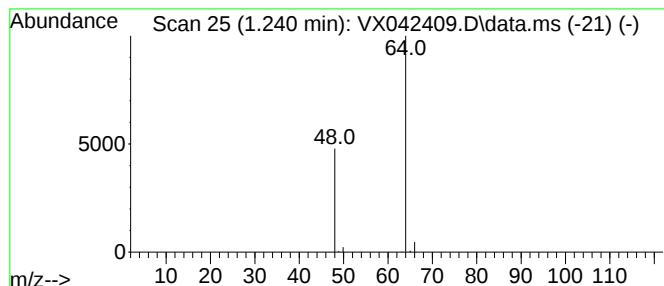
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	18.98 ug/L	89058	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	19.0	ug/L	89058	1	6.757	234658	50.0