

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042780.D
 Acq On : 31 Jul 2024 17:57
 Operator : JC/MD
 Sample : P3398-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08L0

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\SFAMXML072624WMA.M
 Title : VOC Analysis

Signal : TIC: VX042780.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	32	rBV	14601	21087	3.42%	0.482%
2	1.367	43	46	57	rVB	41254	54016	8.77%	1.235%
3	1.648	88	92	100	rVB	29324	42296	6.87%	0.967%
4	2.136	170	172	173	rBV	335	209	0.03%	0.005%
5	2.227	184	187	191	rBV2	291	484	0.08%	0.011%
6	2.294	192	198	210	rBV	123397	197797	32.12%	4.524%
7	2.568	239	243	249	rVB2	914	1698	0.28%	0.039%
8	2.666	257	259	261	rVV	354	290	0.05%	0.007%
9	2.782	274	278	284	rBV3	1263	2430	0.39%	0.056%
10	2.843	287	288	290	rBV	307	198	0.03%	0.005%
11	2.940	299	304	312	rBV2	4528	10440	1.70%	0.239%
12	3.093	324	329	334	rVB3	829	1499	0.24%	0.034%
13	3.135	334	336	338	rBV	229	206	0.03%	0.005%
14	3.337	368	369	373	rVB2	272	298	0.05%	0.007%
15	3.385	373	377	380	rBV2	257	537	0.09%	0.012%
16	3.599	410	412	413	rBV	238	236	0.04%	0.005%
17	3.702	427	429	431	rBV	234	192	0.03%	0.004%
18	3.769	438	440	442	rVB	239	179	0.03%	0.004%
19	4.239	513	517	519	rBV2	247	308	0.05%	0.007%
20	4.312	527	529	535	rBV2	209	339	0.06%	0.008%
21	4.403	541	544	547	rBV	260	280	0.05%	0.006%
22	4.470	547	555	570	rBV	46145	138596	22.50%	3.170%
23	4.787	605	607	608	rBV2	337	180	0.03%	0.004%
24	4.946	630	633	636	rBV2	334	353	0.06%	0.008%
25	5.056	639	651	670	rVV	83926	255584	41.50%	5.845%
26	5.385	702	705	708	rBV3	351	519	0.08%	0.012%
27	5.507	721	725	727	rBV	406	497	0.08%	0.011%
28	5.604	739	741	744	rBV	310	348	0.06%	0.008%
29	5.635	744	746	749	rVV2	269	337	0.05%	0.008%
30	5.665	749	751	754	rVV	279	310	0.05%	0.007%
31	5.970	789	801	820	rBV2	207963	615864	100.00%	14.085%
32	6.434	875	877	879	rBV	193	210	0.03%	0.005%
33	6.586	899	902	905	rBV2	200	268	0.04%	0.006%
34	6.677	915	917	922	rVB2	343	342	0.06%	0.008%
35	6.763	922	931	944	rBV	152366	371553	60.33%	8.498%
36	7.019	971	973	977	rBV3	300	473	0.08%	0.011%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042780.D
 Acq On : 31 Jul 2024 17:57
 Operator : JC/MD
 Sample : P3398-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08L0

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\SFAMXML072624WMA.M
 Title : VOC Analysis

37	7.116	984	989	990	rBV4	1167	1346	0.22%	0.031%
38	7.202	1001	1003	1005	rBV2	254	201	0.03%	0.005%
39	7.305	1013	1020	1036	rBV	124254	276925	44.97%	6.333%
40	7.903	1116	1118	1125	rBV3	326	674	0.11%	0.015%
41	8.073	1145	1146	1149	rVB	335	233	0.04%	0.005%
42	8.330	1182	1188	1196	rBV	69613	117981	19.16%	2.698%
43	8.537	1220	1222	1224	rVB	393	224	0.04%	0.005%
44	8.561	1224	1226	1228	rBV	279	309	0.05%	0.007%
45	8.647	1234	1240	1250	rBV	273436	447915	72.73%	10.244%
46	8.872	1274	1277	1279	rBV2	338	372	0.06%	0.009%
47	8.951	1284	1290	1302	rBV	51280	80185	13.02%	1.834%
48	9.067	1307	1309	1312	rVV3	286	272	0.04%	0.006%
49	9.274	1340	1343	1347	rVB	2592	3510	0.57%	0.080%
50	9.390	1357	1362	1375	rBV	187201	293784	47.70%	6.719%
51	9.628	1399	1401	1404	rVB2	391	376	0.06%	0.009%
52	9.817	1430	1432	1436	rBV2	246	357	0.06%	0.008%
53	9.872	1440	1441	1444	rBV2	242	202	0.03%	0.005%
54	10.012	1462	1464	1465	rVB	369	248	0.04%	0.006%
55	10.055	1465	1471	1485	rBV	310113	418929	68.02%	9.581%
56	10.201	1494	1495	1497	rBV2	385	269	0.04%	0.006%
57	10.311	1509	1513	1517	rVV3	1210	1788	0.29%	0.041%
58	10.384	1521	1525	1526	rBV	168	206	0.03%	0.005%
59	10.402	1526	1528	1531	rVB2	266	298	0.05%	0.007%
60	10.646	1565	1568	1572	rBV	643	928	0.15%	0.021%
61	10.963	1619	1620	1622	rBV	244	192	0.03%	0.004%
62	11.042	1630	1633	1636	rVB2	616	793	0.13%	0.018%
63	11.195	1652	1658	1667	rBV	216309	291329	47.30%	6.663%
64	11.311	1673	1677	1682	rBV3	2036	3029	0.49%	0.069%
65	11.457	1699	1701	1703	rBV2	378	237	0.04%	0.005%
66	11.506	1707	1709	1711	rBV2	208	184	0.03%	0.004%
67	11.768	1747	1752	1753	rBV2	615	790	0.13%	0.018%
68	12.024	1788	1794	1803	rBV	264389	336892	54.70%	7.705%
69	12.158	1813	1816	1820	rVB2	365	489	0.08%	0.011%
70	12.243	1828	1830	1835	rVB2	624	654	0.11%	0.015%
71	12.323	1837	1843	1851	rBV	250242	342888	55.68%	7.842%
72	12.560	1881	1882	1883	rVB	511	187	0.03%	0.004%
73	12.609	1888	1890	1892	rVB	338	218	0.04%	0.005%
74	12.713	1905	1907	1910	rVB2	224	243	0.04%	0.006%
75	12.762	1910	1915	1918	rBV2	1083	1442	0.23%	0.033%
76	12.841	1924	1928	1929	rBV3	201	232	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042780.D
 Acq On : 31 Jul 2024 17:57
 Operator : JC/MD
 Sample : P3398-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08L0

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\SFAMXML072624WMA.M
 Title : VOC Analysis

77	13.060	1963	1964	1967	rBV2	245	234	0.04%	0.005%
78	13.146	1975	1978	1979	rBV2	319	296	0.05%	0.007%
79	13.396	2017	2019	2022	rBV	195	197	0.03%	0.005%
80	13.780	2076	2082	2091	rBV	6140	10252	1.66%	0.234%
81	14.127	2135	2139	2145	rVB2	1649	2522	0.41%	0.058%
82	14.389	2179	2182	2188	rBV2	375	652	0.11%	0.015%
83	14.853	2256	2258	2259	rVV	371	234	0.04%	0.005%
84	14.871	2259	2261	2268	rVV2	411	692	0.11%	0.016%
85	14.920	2268	2269	2272	rVB2	261	221	0.04%	0.005%
86	15.060	2289	2292	2295	rBV3	360	528	0.09%	0.012%
87	15.389	2341	2346	2351	rBV3	2286	3880	0.63%	0.089%
88	15.462	2357	2358	2360	rBV	371	242	0.04%	0.006%
89	15.511	2364	2366	2367	rBV	320	203	0.03%	0.005%
90	15.609	2380	2382	2385	rBV	323	384	0.06%	0.009%
91	15.712	2397	2399	2402	rBV3	448	672	0.11%	0.015%
92	15.767	2405	2408	2410	rBV2	433	606	0.10%	0.014%
93	15.889	2427	2428	2430	rBV	356	225	0.04%	0.005%
94	15.914	2430	2432	2433	rVV	309	192	0.03%	0.004%
95	15.950	2436	2438	2441	rBV2	486	428	0.07%	0.010%
96	16.176	2473	2475	2476	rBV2	319	233	0.04%	0.005%
97	16.218	2480	2482	2486	rBV4	406	434	0.07%	0.010%
98	16.304	2494	2496	2498	rBV	544	386	0.06%	0.009%
99	16.371	2505	2507	2508	rVB	380	214	0.03%	0.005%
100	16.694	2557	2560	2563	rBV2	526	785	0.13%	0.018%

Sum of corrected areas: 4372496

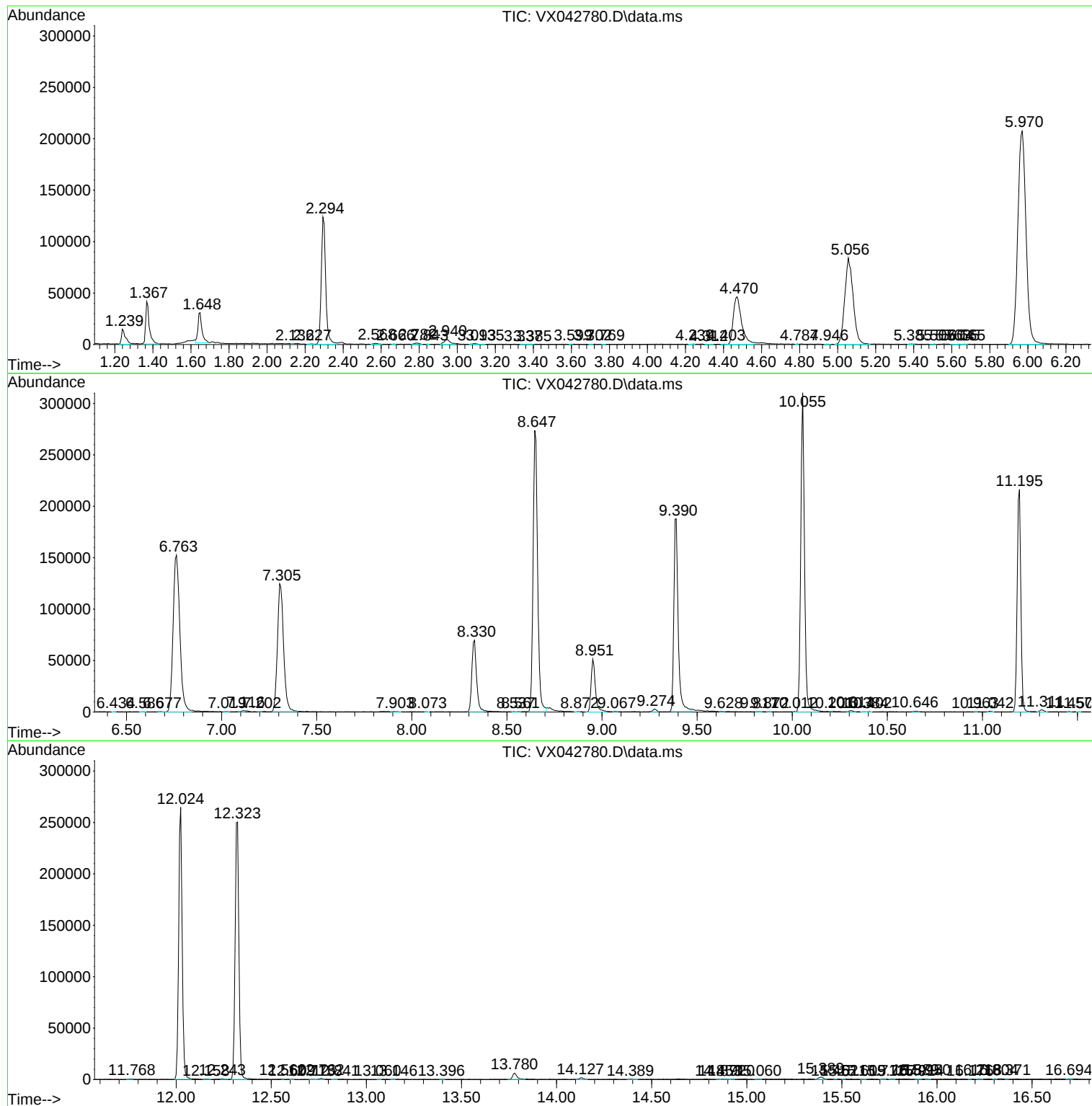
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042780.D
Acq On : 31 Jul 2024 17:57
Operator : JC/MD
Sample : P3398-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E08L0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042780.D
Acq On : 31 Jul 2024 17:57
Operator : JC/MD
Sample : P3398-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E08L0

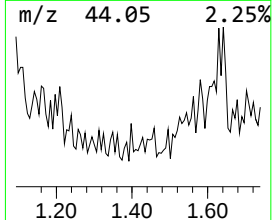
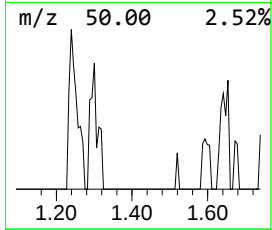
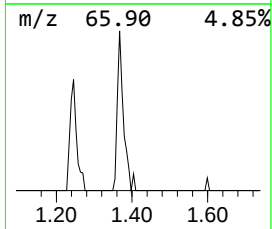
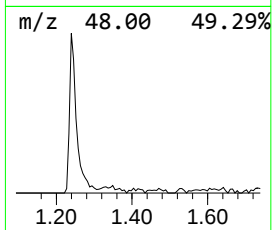
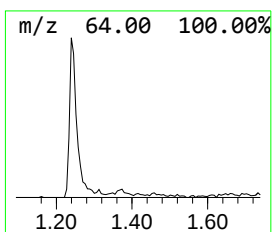
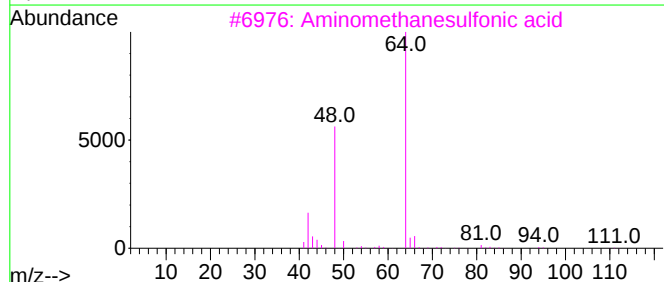
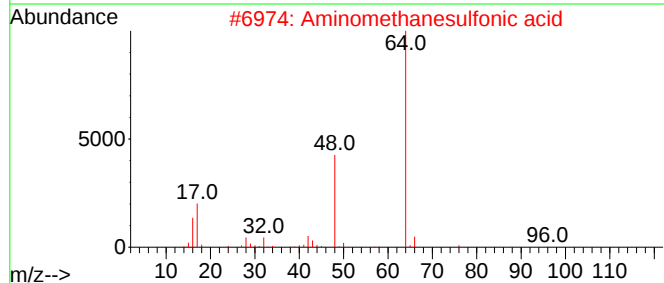
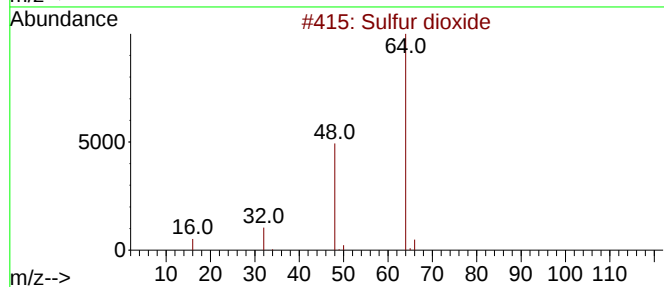
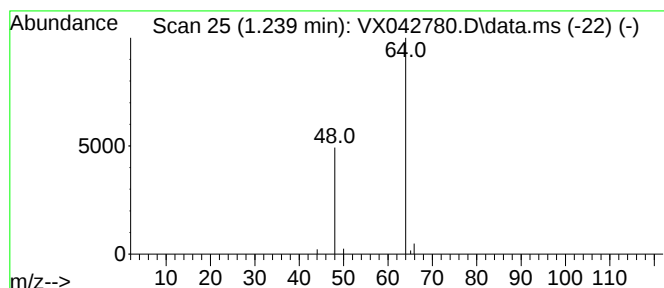
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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.
1.239	2.84 ug/L	21087	1,4-Difluorobenzene	6.763

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	64
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	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042780.D
Acq On : 31 Jul 2024 17:57
Operator : JC/MD
Sample : P3398-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E08L0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.239	2.8	ug/L	21087	1	6.763	371553	50.0