

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042571.D
 Acq On : 25 Jul 2024 16:58
 Operator : JC/MD
 Sample : P3334-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20E6

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: VX042571.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	22	25	41	rBV	43626	55299	13.33%	1.924%
2	1.368	43	46	57	rVB	28569	37024	8.93%	1.288%
3	1.648	89	92	101	rVB	30292	36850	8.89%	1.282%
4	2.294	193	198	208	rBV	58384	90943	21.93%	3.165%
5	2.392	208	214	222	rBV	4170	8356	2.01%	0.291%
6	2.569	237	243	253	rBV2	5651	11084	2.67%	0.386%
7	2.782	274	278	286	rBV2	1606	3306	0.80%	0.115%
8	2.861	289	291	294	rVB	213	153	0.04%	0.005%
9	2.886	294	295	297	rBV	136	112	0.03%	0.004%
10	2.947	297	305	320	rVB	7436	17568	4.24%	0.611%
11	3.062	322	324	325	rBV	259	180	0.04%	0.006%
12	3.093	327	329	331	rBV2	304	187	0.05%	0.007%
13	3.184	341	344	347	rBV	104	163	0.04%	0.006%
14	3.239	351	353	354	rVB	178	115	0.03%	0.004%
15	3.264	354	357	358	rBV	144	165	0.04%	0.006%
16	3.337	365	369	374	rBV2	308	511	0.12%	0.018%
17	3.422	380	383	384	rBV2	168	153	0.04%	0.005%
18	3.556	403	405	407	rVV2	143	128	0.03%	0.004%
19	3.599	409	412	414	rBV	133	146	0.04%	0.005%
20	3.623	414	416	419	rBV	119	129	0.03%	0.004%
21	3.703	428	429	432	rVB	114	114	0.03%	0.004%
22	3.727	432	433	436	rBV2	132	158	0.04%	0.005%
23	3.782	441	442	444	rBV2	100	91	0.02%	0.003%
24	3.849	451	453	455	rBV2	71	73	0.02%	0.003%
25	3.879	455	458	459	rBV2	112	88	0.02%	0.003%
26	4.196	508	510	512	rVB	101	79	0.02%	0.003%
27	4.355	534	536	539	rVB	128	103	0.02%	0.004%
28	4.465	546	554	571	rBV	42650	131046	31.60%	4.561%
29	4.739	597	599	600	rVB	177	84	0.02%	0.003%
30	4.867	618	620	621	rVB	189	95	0.02%	0.003%
31	4.977	636	638	639	rBV	114	72	0.02%	0.003%
32	5.062	639	652	668	rBV2	56369	175161	42.24%	6.096%
33	5.391	705	706	709	rVV2	107	110	0.03%	0.004%
34	5.452	714	716	717	rBV	141	87	0.02%	0.003%
35	5.556	731	733	739	rBV	209	332	0.08%	0.012%
36	5.660	748	750	752	rBV2	108	115	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042571.D
 Acq On : 25 Jul 2024 16:58
 Operator : JC/MD
 Sample : P3334-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20E6

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

37	5.721	757	760	761	rBV	87	85	0.02%	0.003%
38	5.769	766	768	770	rBV2	134	145	0.03%	0.005%
39	5.964	788	800	820	rBV2	138664	414700	100.00%	14.432%
40	6.269	848	850	854	rBV2	149	215	0.05%	0.007%
41	6.324	857	859	862	rBV	99	107	0.03%	0.004%
42	6.355	862	864	865	rBV	88	75	0.02%	0.003%
43	6.580	898	901	902	rBV2	145	154	0.04%	0.005%
44	6.666	911	915	916	rBV	162	232	0.06%	0.008%
45	6.763	922	931	942	rBV	100111	239959	57.86%	8.351%
46	7.043	976	977	979	rBV	92	86	0.02%	0.003%
47	7.129	986	991	997	rBV5	1444	3133	0.76%	0.109%
48	7.202	1002	1003	1006	rBV	203	249	0.06%	0.009%
49	7.312	1012	1021	1037	rBV	85023	193281	46.61%	6.726%
50	7.489	1049	1050	1053	rBV2	193	127	0.03%	0.004%
51	7.873	1112	1113	1115	rBV	161	144	0.03%	0.005%
52	7.952	1121	1126	1134	rBV4	614	1367	0.33%	0.048%
53	8.116	1151	1153	1155	rBV2	82	77	0.02%	0.003%
54	8.226	1168	1171	1172	rBV2	109	135	0.03%	0.005%
55	8.330	1182	1188	1196	rBV	38749	67117	16.18%	2.336%
56	8.446	1205	1207	1209	rVB	133	70	0.02%	0.002%
57	8.513	1213	1218	1220	rBV	422	776	0.19%	0.027%
58	8.647	1234	1240	1249	rBV	148942	241089	58.14%	8.390%
59	8.952	1285	1290	1300	rBV	27811	42503	10.25%	1.479%
60	9.104	1313	1315	1318	rVB	122	97	0.02%	0.003%
61	9.275	1338	1343	1348	rVB3	1717	2117	0.51%	0.074%
62	9.385	1356	1361	1376	rBV	162686	252409	60.87%	8.784%
63	9.592	1394	1395	1397	rBV2	347	287	0.07%	0.010%
64	10.006	1461	1463	1465	rBV	99	83	0.02%	0.003%
65	10.055	1465	1471	1486	rBV	172016	240316	57.95%	8.363%
66	10.201	1493	1495	1501	rVB2	731	773	0.19%	0.027%
67	10.256	1501	1504	1506	rBV3	174	191	0.05%	0.007%
68	10.305	1509	1512	1519	rVV3	890	1479	0.36%	0.051%
69	10.372	1521	1523	1524	rBV	155	111	0.03%	0.004%
70	10.470	1537	1539	1540	rVB	155	80	0.02%	0.003%
71	10.500	1540	1544	1545	rBV2	124	116	0.03%	0.004%
72	10.653	1565	1569	1577	rBV4	739	1759	0.42%	0.061%
73	10.768	1586	1588	1592	rVV2	167	136	0.03%	0.005%
74	10.872	1604	1605	1607	rBV2	93	73	0.02%	0.003%
75	10.957	1617	1619	1624	rVB3	178	257	0.06%	0.009%
76	11.116	1643	1645	1647	rBV	99	72	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042571.D
 Acq On : 25 Jul 2024 16:58
 Operator : JC/MD
 Sample : P3334-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20E6

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	11.195	1652	1658	1664	rBV	183953	248424	59.90%	8.646%
78	11.311	1675	1677	1684	rVB2	297	404	0.10%	0.014%
79	11.415	1692	1694	1696	rBV	164	97	0.02%	0.003%
80	11.451	1698	1700	1704	rVB2	357	430	0.10%	0.015%
81	11.561	1716	1718	1720	rBV	130	114	0.03%	0.004%
82	11.756	1747	1750	1754	rVB	466	458	0.11%	0.016%
83	11.896	1772	1773	1776	rBV	105	86	0.02%	0.003%
84	11.982	1782	1787	1789	rBV3	315	440	0.11%	0.015%
85	12.024	1789	1794	1802	rBV	124254	158056	38.11%	5.501%
86	12.219	1822	1826	1833	rVB3	2434	3741	0.90%	0.130%
87	12.274	1833	1835	1836	rVB2	135	96	0.02%	0.003%
88	12.317	1837	1842	1856	rBV	136812	182836	44.09%	6.363%
89	12.811	1921	1923	1924	rBV	150	128	0.03%	0.004%
90	12.908	1938	1939	1940	rBV	176	111	0.03%	0.004%
91	12.988	1950	1952	1953	rBV	146	103	0.02%	0.004%
92	13.426	2023	2024	2026	rBV	104	73	0.02%	0.003%
93	13.548	2042	2044	2046	rBV2	108	127	0.03%	0.004%
94	13.689	2064	2067	2069	rBV	167	182	0.04%	0.006%
95	14.030	2121	2123	2125	rBV	125	89	0.02%	0.003%
96	14.414	2184	2186	2188	rBV2	138	138	0.03%	0.005%
97	14.457	2192	2193	2196	rVB2	257	150	0.04%	0.005%
98	14.634	2221	2222	2223	rBV	274	131	0.03%	0.005%
99	14.719	2234	2236	2237	rBV2	240	181	0.04%	0.006%
100	16.652	2551	2553	2555	rBV	325	284	0.07%	0.010%

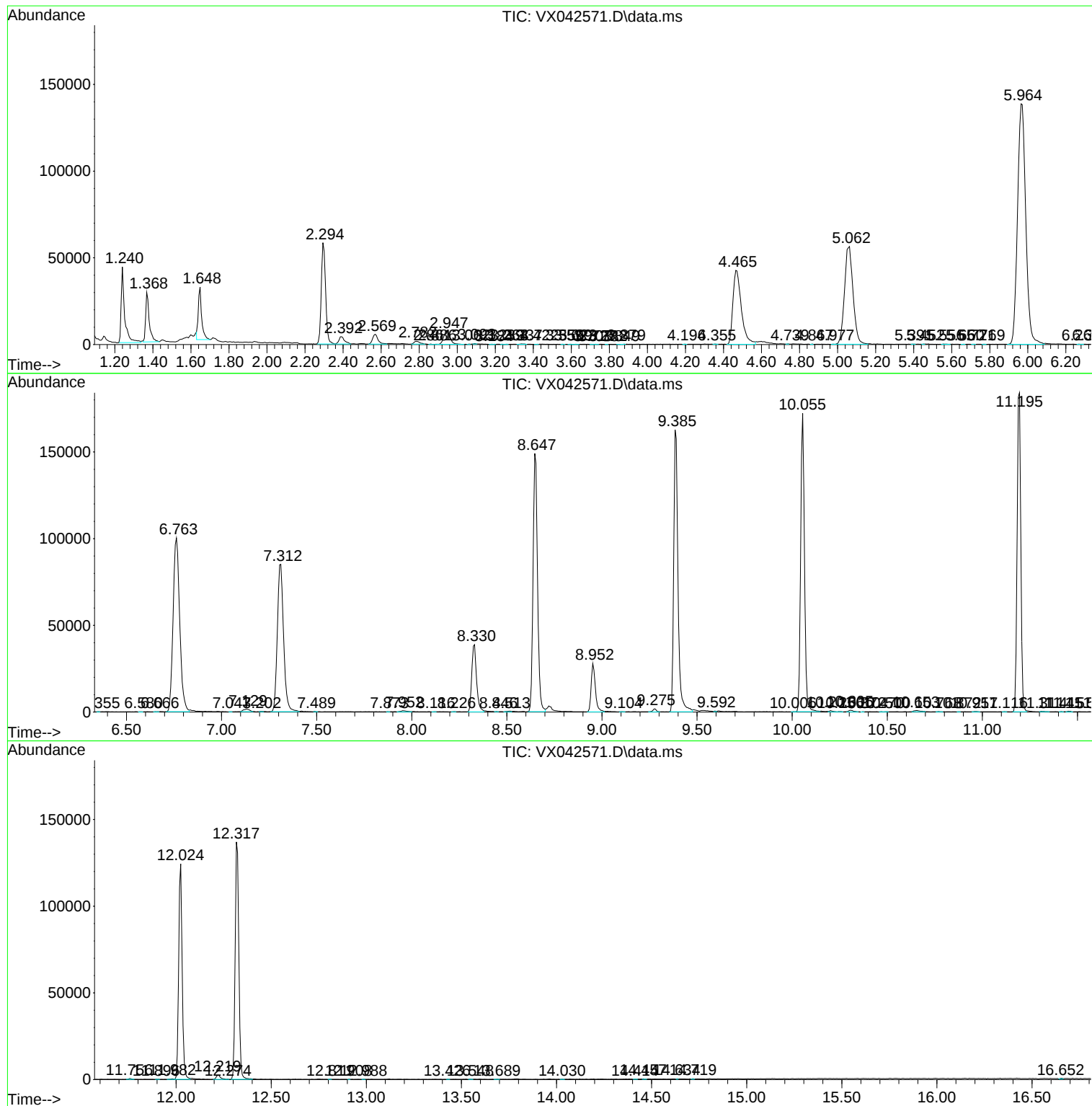
Sum of corrected areas: 2873441

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042571.D
Acq On : 25 Jul 2024 16:58
Operator : JC/MD
Sample : P3334-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20E6

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042571.D
Acq On : 25 Jul 2024 16:58
Operator : JC/MD
Sample : P3334-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20E6

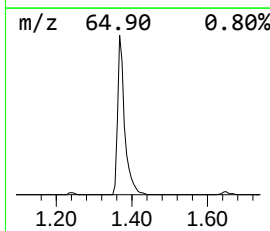
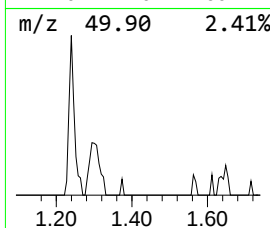
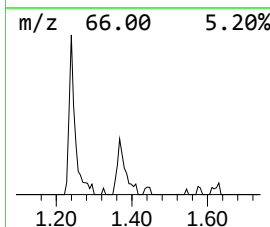
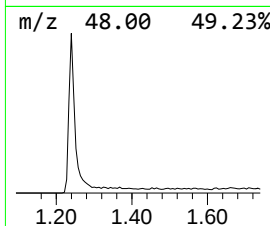
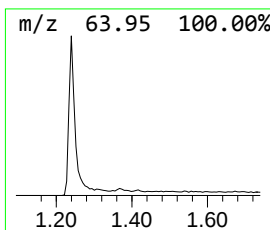
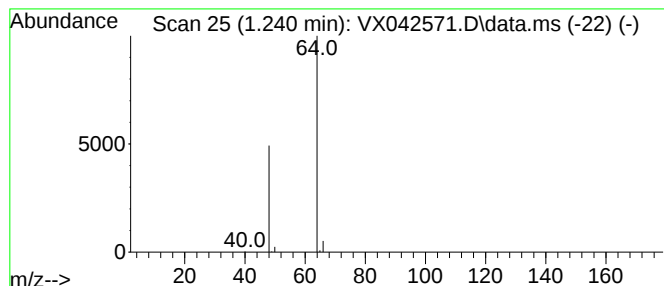
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	11.52 ug/L	55299	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042571.D
Acq On : 25 Jul 2024 16:58
Operator : JC/MD
Sample : P3334-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20E6

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	11.5	ug/L	55299	1	6.763	239959	50.0