

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042579.D
 Acq On : 25 Jul 2024 20:04
 Operator : JC/MD
 Sample : P3334-17
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20H4

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: VX042579.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	20	rVB	5985	8178	1.89%	0.234%
2	1.240	22	25	39	rVV	26268	37347	8.62%	1.069%
3	1.368	43	46	57	rVV2	33378	44871	10.35%	1.284%
4	1.447	57	59	65	rVB4	1093	1650	0.38%	0.047%
5	1.581	70	81	82	rBV3	2714	7040	1.62%	0.201%
6	1.648	88	92	101	rVB	29177	38032	8.78%	1.088%
7	1.721	101	104	112	rVB2	3261	4717	1.09%	0.135%
8	1.935	135	139	146	rVB3	1417	2263	0.52%	0.065%
9	2.087	161	164	168	rBV2	1268	1699	0.39%	0.049%
10	2.300	192	199	210	rBV2	90972	165852	38.27%	4.746%
11	2.386	210	213	225	rVB2	1888	4326	1.00%	0.124%
12	2.502	230	232	235	rVV3	173	191	0.04%	0.005%
13	2.569	238	243	251	rVB2	1018	2244	0.52%	0.064%
14	2.709	263	266	270	rBV	135	238	0.05%	0.007%
15	2.788	274	279	288	rVV7	1295	3060	0.71%	0.088%
16	2.855	288	290	294	rVB3	179	196	0.05%	0.006%
17	2.947	299	305	314	rVB	1931	4074	0.94%	0.117%
18	3.087	323	328	334	rBV4	447	870	0.20%	0.025%
19	3.209	346	348	350	rBV2	116	142	0.03%	0.004%
20	3.331	365	368	370	rBV3	316	421	0.10%	0.012%
21	3.428	382	384	387	rVV	252	331	0.08%	0.009%
22	3.648	416	420	422	rBV	125	150	0.03%	0.004%
23	3.697	427	428	431	rVB	191	179	0.04%	0.005%
24	3.782	436	442	443	rVB	159	253	0.06%	0.007%
25	3.800	443	445	448	rBV	152	163	0.04%	0.005%
26	3.837	448	451	452	rVB	204	163	0.04%	0.005%
27	3.959	468	471	473	rBV2	190	296	0.07%	0.008%
28	4.288	522	525	526	rBV2	305	356	0.08%	0.010%
29	4.477	547	556	573	rBV2	78076	253764	58.56%	7.261%
30	4.861	617	619	623	rVB	172	173	0.04%	0.005%
31	5.056	639	651	671	rVV	57433	177831	41.04%	5.089%
32	5.404	705	708	710	rBV3	158	154	0.04%	0.004%
33	5.458	713	717	719	rBV2	190	294	0.07%	0.008%
34	5.617	739	743	744	rBV	172	232	0.05%	0.007%
35	5.964	790	800	823	rBV2	146025	433337	100.00%	12.400%
36	6.257	847	848	850	rVB	208	142	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042579.D
 Acq On : 25 Jul 2024 20:04
 Operator : JC/MD
 Sample : P3334-17
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20H4

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	6.288	850	853	854	rBV2	209	192	0.04%	0.005%
38	6.580	899	901	903	rBV	169	178	0.04%	0.005%
39	6.605	903	905	909	rVB	102	138	0.03%	0.004%
40	6.763	922	931	943	rBV	112239	271479	62.65%	7.768%
41	7.123	982	990	1012	rBV	133948	296437	68.41%	8.482%
42	7.306	1013	1020	1038	rVB	90162	198178	45.73%	5.671%
43	7.921	1119	1121	1123	rBV2	140	146	0.03%	0.004%
44	7.952	1123	1126	1127	rVV2	438	508	0.12%	0.015%
45	7.964	1127	1128	1135	rVV3	561	729	0.17%	0.021%
46	8.330	1182	1188	1202	rBV	39166	69138	15.95%	1.978%
47	8.434	1204	1205	1208	rVB	310	181	0.04%	0.005%
48	8.647	1234	1240	1249	rBV	183692	290929	67.14%	8.325%
49	8.720	1249	1252	1263	rVB2	4028	8079	1.86%	0.231%
50	8.836	1270	1271	1277	rVB3	258	314	0.07%	0.009%
51	8.952	1285	1290	1307	rVV	27710	44046	10.16%	1.260%
52	9.281	1339	1344	1347	rVB3	936	1409	0.33%	0.040%
53	9.348	1351	1355	1356	rBV2	132	175	0.04%	0.005%
54	9.385	1356	1361	1380	rBV	146107	227601	52.52%	6.513%
55	9.610	1397	1398	1400	rVV2	189	167	0.04%	0.005%
56	9.921	1445	1449	1450	rBV2	131	179	0.04%	0.005%
57	10.055	1465	1471	1483	rVV	192800	273254	63.06%	7.819%
58	10.159	1486	1488	1493	rVV3	1237	2016	0.47%	0.058%
59	10.208	1493	1496	1500	rVV2	981	1418	0.33%	0.041%
60	10.244	1500	1502	1507	rVV2	228	341	0.08%	0.010%
61	10.305	1507	1512	1520	rVB2	1674	3000	0.69%	0.086%
62	10.366	1520	1522	1525	rVB2	166	200	0.05%	0.006%
63	10.397	1525	1527	1530	rBV2	161	234	0.05%	0.007%
64	10.647	1564	1568	1575	rBV4	717	1198	0.28%	0.034%
65	10.976	1620	1622	1623	rVB2	232	139	0.03%	0.004%
66	11.079	1637	1639	1641	rBV	181	207	0.05%	0.006%
67	11.189	1652	1657	1673	rVB	185033	243461	56.18%	6.967%
68	11.299	1673	1675	1677	rBV	156	186	0.04%	0.005%
69	11.378	1685	1688	1689	rBV2	200	203	0.05%	0.006%
70	11.457	1698	1701	1706	rBV2	346	506	0.12%	0.014%
71	11.622	1724	1728	1730	rBV2	143	193	0.04%	0.006%
72	11.756	1745	1750	1755	rBV	668	1039	0.24%	0.030%
73	11.915	1772	1776	1780	rBV2	171	319	0.07%	0.009%
74	11.976	1784	1786	1789	rBV2	141	148	0.03%	0.004%
75	12.024	1789	1794	1803	rBV	128508	163154	37.65%	4.669%
76	12.219	1822	1826	1837	rBV2	2512	3292	0.76%	0.094%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042579.D
Acq On : 25 Jul 2024 20:04
Operator : JC/MD
Sample : P3334-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20H4

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

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	12.317	1837	1842	1855	rBV	143871	189816	43.80%	5.432%
78	12.707	1903	1906	1910	rBV	139	259	0.06%	0.007%
79	12.744	1910	1912	1915	rVB	156	147	0.03%	0.004%
80	12.981	1949	1951	1955	rBV	125	159	0.04%	0.005%
81	13.341	2007	2010	2014	rBV2	144	283	0.07%	0.008%
82	13.780	2079	2082	2084	rBV2	310	409	0.09%	0.012%
83	13.939	2107	2108	2112	rVB	163	180	0.04%	0.005%
84	14.036	2121	2124	2126	rBV2	153	143	0.03%	0.004%
85	14.115	2135	2137	2140	rBV2	149	186	0.04%	0.005%
86	14.152	2142	2143	2147	rBV	120	188	0.04%	0.005%
87	14.182	2147	2148	2154	rVV2	143	277	0.06%	0.008%
88	14.457	2192	2193	2198	rBV2	134	179	0.04%	0.005%
89	14.499	2198	2200	2204	rBV	201	191	0.04%	0.005%
90	14.780	2244	2246	2248	rBV	238	202	0.05%	0.006%
91	15.213	2315	2317	2319	rVB	284	254	0.06%	0.007%
92	15.237	2319	2321	2322	rBV2	183	181	0.04%	0.005%
93	15.383	2344	2345	2348	rBV2	313	330	0.08%	0.009%
94	15.664	2389	2391	2393	rBV2	216	162	0.04%	0.005%
95	15.792	2410	2412	2417	rVB	258	303	0.07%	0.009%
96	15.835	2417	2419	2420	rBV2	236	143	0.03%	0.004%
97	15.938	2434	2436	2439	rVV2	230	169	0.04%	0.005%
98	16.420	2514	2515	2518	rVB2	308	160	0.04%	0.005%
99	16.560	2536	2538	2540	rBV2	205	192	0.04%	0.005%
100	16.609	2544	2546	2550	rVB3	306	240	0.06%	0.007%

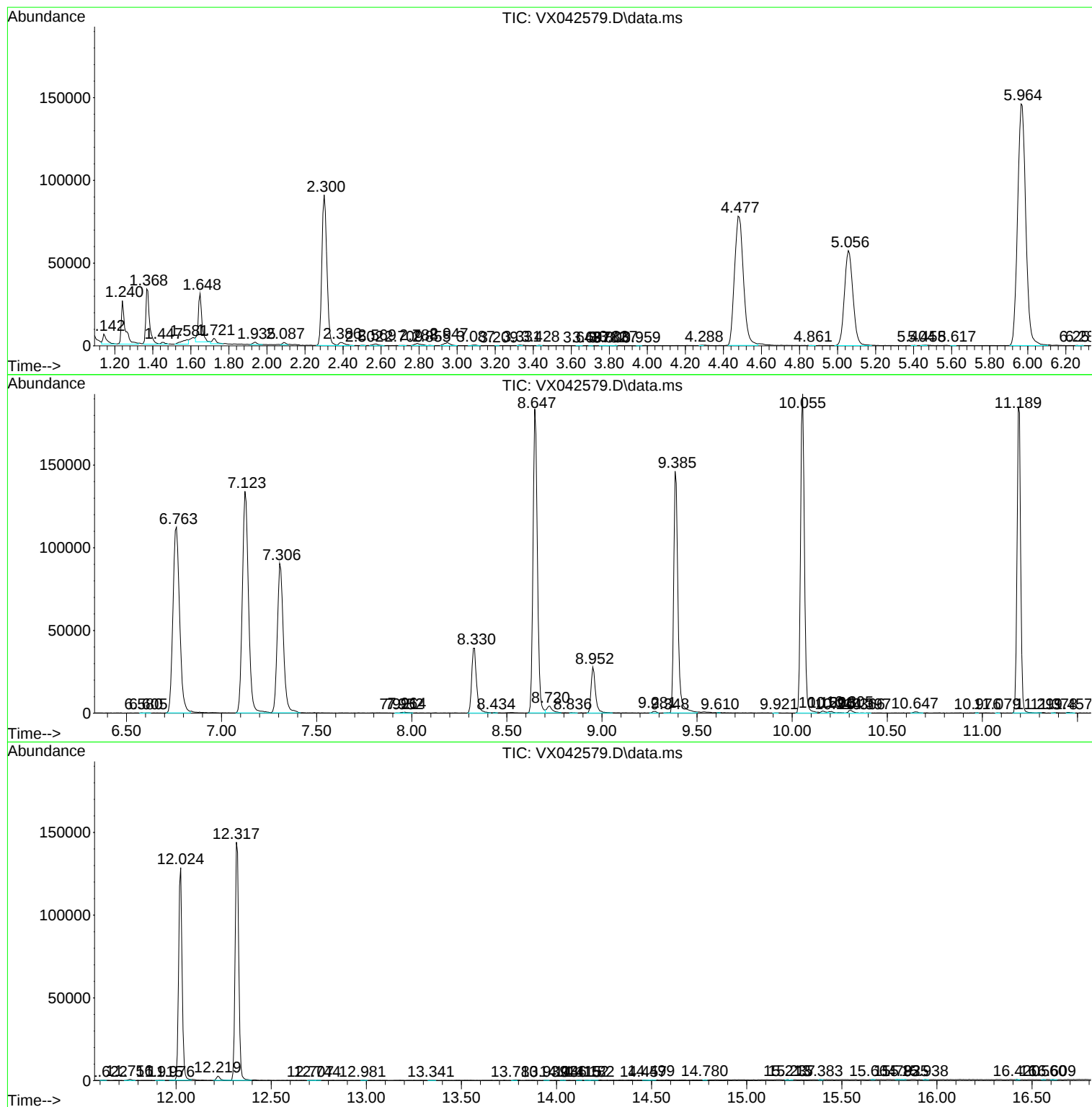
Sum of corrected areas: 3494693

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042579.D
Acq On : 25 Jul 2024 20:04
Operator : JC/MD
Sample : P3334-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20H4

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 : VX042579.D
Acq On : 25 Jul 2024 20:04
Operator : JC/MD
Sample : P3334-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20H4

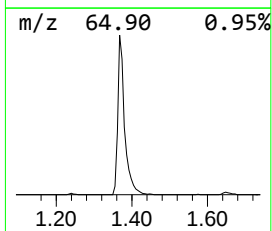
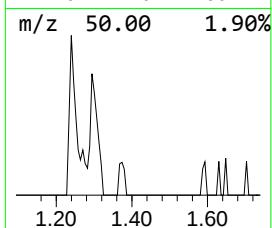
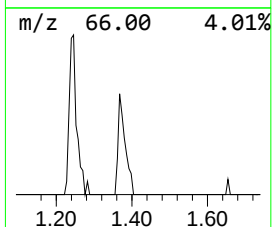
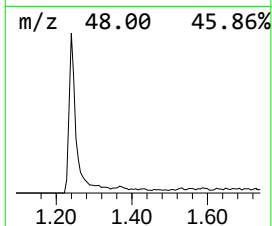
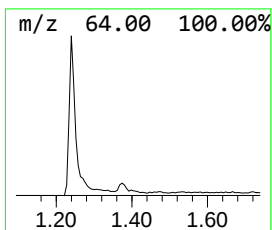
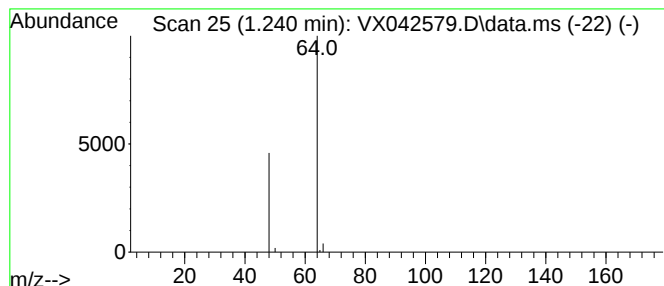
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	6.88 ug/L	37347	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042579.D
Acq On : 25 Jul 2024 20:04
Operator : JC/MD
Sample : P3334-17
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20H4

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	6.9	ug/L	37347	1	6.763	271479	50.0