

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042479.D
 Acq On : 23 Jul 2024 18:04
 Operator : JC/MD
 Sample : P3327-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E1ZW5

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: VX042479.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	6	9	20	rVB	9611	14611	2.00%	0.261%
2	1.239	22	25	28	rBV	34300	37462	5.14%	0.669%
3	1.367	43	46	57	rVB	76846	93523	12.83%	1.671%
4	1.648	88	92	100	rVB	51563	67313	9.24%	1.202%
5	1.721	101	104	110	rVB2	3961	5810	0.80%	0.104%
6	2.294	192	198	209	rVV	135903	216946	29.77%	3.875%
7	2.392	210	214	228	rVB2	3390	8360	1.15%	0.149%
8	2.501	228	232	237	rVB3	283	431	0.06%	0.008%
9	2.568	237	243	248	rBV	4513	7694	1.06%	0.137%
10	2.715	265	267	271	rVB	274	270	0.04%	0.005%
11	2.788	273	279	287	rVB3	1073	2132	0.29%	0.038%
12	2.946	295	305	317	rBV2	3338	7989	1.10%	0.143%
13	3.087	324	328	329	rBV	268	296	0.04%	0.005%
14	3.270	356	358	360	rBV2	129	137	0.02%	0.002%
15	3.727	432	433	437	rVB	135	139	0.02%	0.002%
16	4.026	481	482	485	rVB	192	134	0.02%	0.002%
17	4.050	485	486	490	rVB2	201	150	0.02%	0.003%
18	4.105	492	495	497	rVB	153	143	0.02%	0.003%
19	4.288	521	525	527	rVV2	196	246	0.03%	0.004%
20	4.355	534	536	540	rVB2	117	167	0.02%	0.003%
21	4.464	546	554	574	rBV	53053	160291	21.99%	2.863%
22	5.056	640	651	670	rBV2	91881	283608	38.91%	5.066%
23	5.269	684	686	690	rVB2	155	182	0.02%	0.003%
24	5.312	690	693	694	rBV	147	139	0.02%	0.002%
25	5.391	702	706	707	rBV	317	328	0.05%	0.006%
26	5.470	715	719	725	rVV2	423	686	0.09%	0.012%
27	5.562	728	734	740	rVB4	294	699	0.10%	0.012%
28	5.970	789	801	818	rBV2	248019	728817	100.00%	13.019%
29	6.373	862	867	870	rBV3	377	444	0.06%	0.008%
30	6.580	898	901	903	rVB2	187	218	0.03%	0.004%
31	6.610	903	906	909	rBV	104	135	0.02%	0.002%
32	6.763	921	931	947	rBV	189017	457983	62.84%	8.181%
33	6.952	960	962	963	rVB	259	169	0.02%	0.003%
34	6.964	963	964	970	rBV2	162	239	0.03%	0.004%
35	7.037	974	976	979	rBV2	113	153	0.02%	0.003%
36	7.123	984	990	996	rVB6	1057	2608	0.36%	0.047%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042479.D
 Acq On : 23 Jul 2024 18:04
 Operator : JC/MD
 Sample : P3327-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E1ZW5

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	7.208	1000	1004	1005	rBV	279	261	0.04%	0.005%
38	7.305	1012	1020	1039	rBV	144451	330468	45.34%	5.903%
39	7.476	1046	1048	1049	rBV2	250	186	0.03%	0.003%
40	7.696	1081	1084	1085	rBV	162	139	0.02%	0.002%
41	7.958	1124	1127	1132	rVV3	575	993	0.14%	0.018%
42	8.019	1135	1137	1140	rVB	199	139	0.02%	0.002%
43	8.080	1144	1147	1148	rBV2	158	151	0.02%	0.003%
44	8.324	1181	1187	1204	rBV	84328	145786	20.00%	2.604%
45	8.519	1216	1219	1220	rBV2	231	253	0.03%	0.005%
46	8.647	1234	1240	1250	rBV	358196	567493	77.86%	10.137%
47	8.799	1264	1265	1266	rBV	269	155	0.02%	0.003%
48	8.951	1285	1290	1299	rBV	60703	93188	12.79%	1.665%
49	9.275	1339	1343	1350	rVV2	4936	7237	0.99%	0.129%
50	9.384	1356	1361	1377	rBV	228412	352539	48.37%	6.297%
51	9.744	1419	1420	1423	rVV2	172	174	0.02%	0.003%
52	9.781	1423	1426	1429	rVB2	161	234	0.03%	0.004%
53	9.805	1429	1430	1435	rBV2	138	204	0.03%	0.004%
54	10.055	1465	1471	1488	rBV	382577	523621	71.85%	9.353%
55	10.207	1492	1496	1499	rVV2	637	986	0.14%	0.018%
56	10.232	1499	1500	1504	rVV2	207	305	0.04%	0.005%
57	10.311	1509	1513	1518	rVV	1098	1536	0.21%	0.027%
58	10.409	1526	1529	1532	rVB2	200	273	0.04%	0.005%
59	10.652	1565	1569	1572	rVB2	581	647	0.09%	0.012%
60	10.963	1618	1620	1624	rBV3	180	251	0.03%	0.004%
61	11.189	1652	1657	1668	rBV	312566	417339	57.26%	7.455%
62	11.311	1674	1677	1680	rVB3	270	362	0.05%	0.006%
63	11.457	1693	1701	1704	rVB3	413	622	0.09%	0.011%
64	11.536	1713	1714	1718	rVB2	173	166	0.02%	0.003%
65	11.628	1727	1729	1732	rBV2	126	151	0.02%	0.003%
66	11.756	1746	1750	1757	rVB3	500	787	0.11%	0.014%
67	11.981	1783	1787	1788	rBV2	199	204	0.03%	0.004%
68	12.024	1788	1794	1810	rBV	372434	491852	67.49%	8.786%
69	12.183	1817	1820	1821	rVB	184	153	0.02%	0.003%
70	12.219	1822	1826	1832	rBV3	2057	3062	0.42%	0.055%
71	12.317	1837	1842	1852	rBV	411449	540471	74.16%	9.654%
72	12.768	1912	1916	1920	rVB3	382	521	0.07%	0.009%
73	12.926	1939	1942	1943	rVV2	159	170	0.02%	0.003%
74	13.061	1960	1964	1967	rBV2	139	206	0.03%	0.004%
75	13.121	1972	1974	1976	rVV2	219	176	0.02%	0.003%
76	13.280	1998	2000	2003	rBV	219	258	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042479.D
 Acq On : 23 Jul 2024 18:04
 Operator : JC/MD
 Sample : P3327-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E1ZW5

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	13.688	2065	2067	2070	rBV2	144	168	0.02%	0.003%
78	13.725	2070	2073	2075	rBV	240	255	0.03%	0.005%
79	13.780	2079	2082	2084	rBV3	394	375	0.05%	0.007%
80	13.865	2094	2096	2102	rVB2	176	296	0.04%	0.005%
81	13.932	2106	2107	2109	rBV	174	141	0.02%	0.003%
82	14.066	2127	2129	2131	rBV2	183	191	0.03%	0.003%
83	14.127	2137	2139	2147	rVB2	849	1110	0.15%	0.020%
84	14.182	2147	2148	2151	rBV2	216	183	0.03%	0.003%
85	14.335	2171	2173	2174	rVV	259	169	0.02%	0.003%
86	14.353	2174	2176	2178	rVB2	252	198	0.03%	0.004%
87	14.408	2183	2185	2187	rVV2	144	135	0.02%	0.002%
88	14.554	2202	2209	2217	rBV6	1011	2900	0.40%	0.052%
89	14.615	2217	2219	2220	rBV2	226	151	0.02%	0.003%
90	14.749	2240	2241	2243	rBV	189	151	0.02%	0.003%
91	14.896	2263	2265	2268	rVB3	229	194	0.03%	0.003%
92	14.938	2271	2272	2275	rVV2	294	187	0.03%	0.003%
93	15.127	2299	2303	2305	rBV2	304	378	0.05%	0.007%
94	15.347	2337	2339	2341	rBV2	348	280	0.04%	0.005%
95	15.383	2341	2345	2352	rVV4	1211	2164	0.30%	0.039%
96	15.578	2375	2377	2379	rVB2	349	187	0.03%	0.003%
97	15.658	2388	2390	2391	rBV	376	248	0.03%	0.004%
98	15.700	2391	2397	2405	rVB6	1380	3260	0.45%	0.058%
99	16.212	2479	2481	2483	rBV2	344	304	0.04%	0.005%
100	16.755	2568	2570	2572	rBV	325	303	0.04%	0.005%

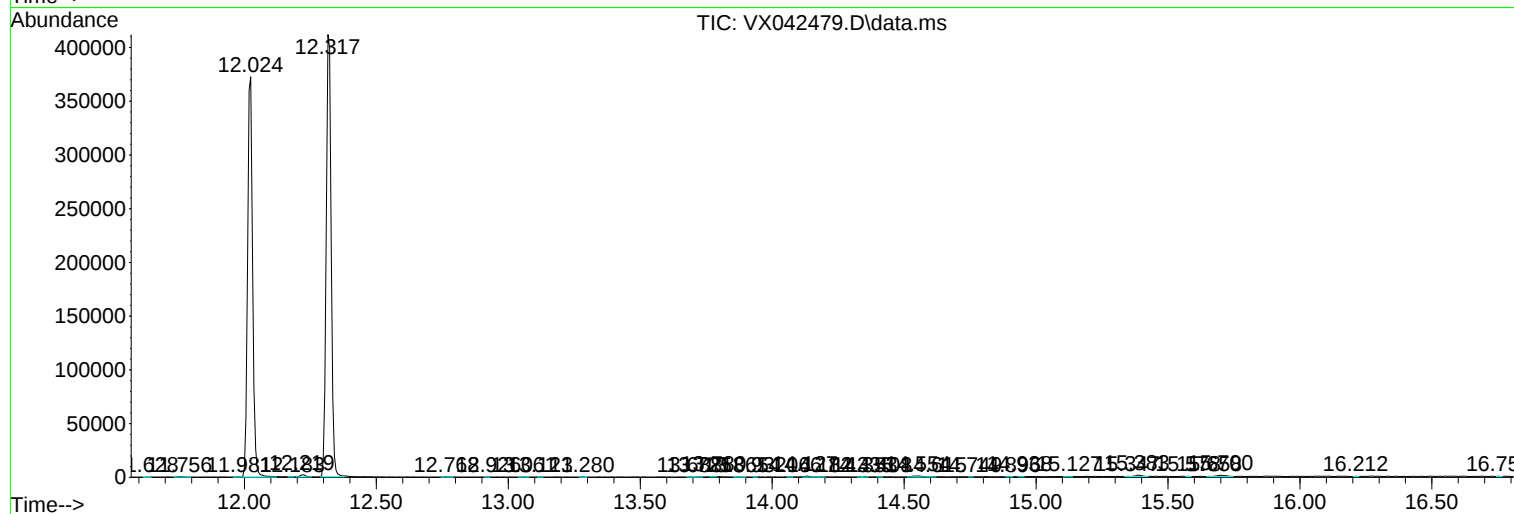
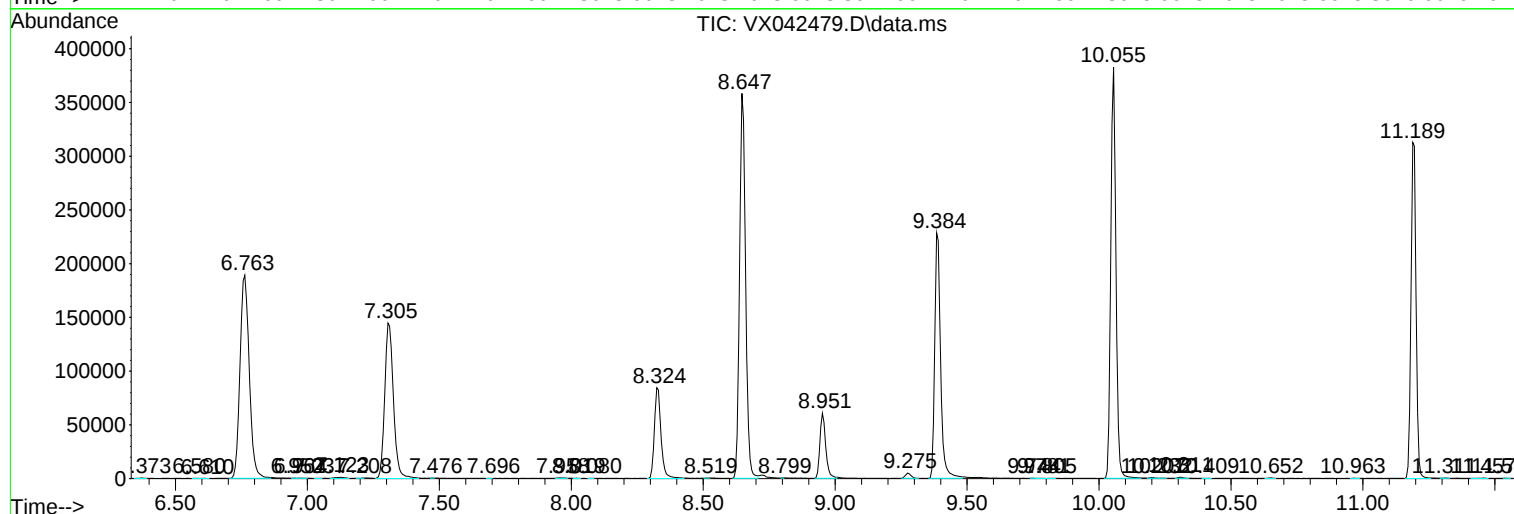
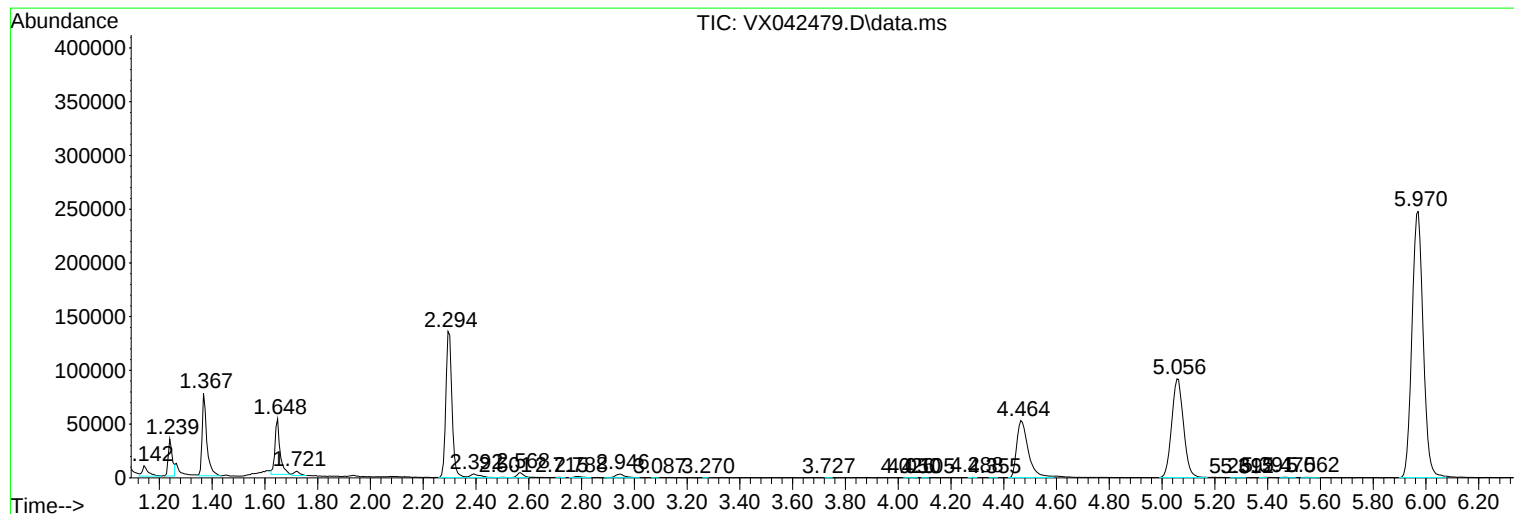
Sum of corrected areas: 5598299

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
Data File : VX042479.D
Acq On : 23 Jul 2024 18:04
Operator : JC/MD
Sample : P3327-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E1ZW5

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\VX072424\
Data File : VX042479.D
Acq On : 23 Jul 2024 18:04
Operator : JC/MD
Sample : P3327-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E1ZW5

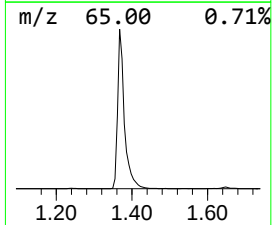
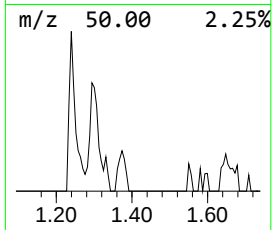
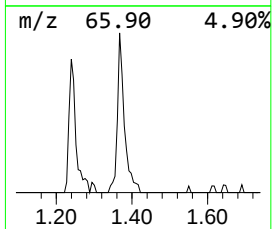
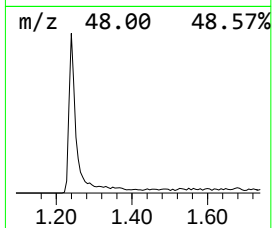
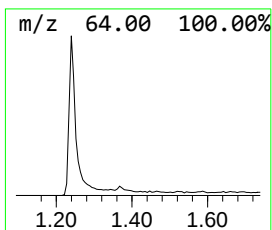
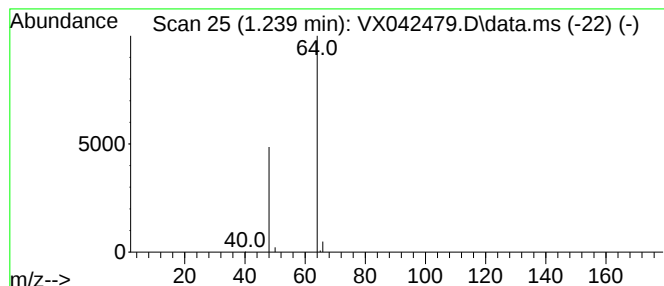
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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.
1.239	4.09 ug/L	37462	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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
Data File : VX042479.D
Acq On : 23 Jul 2024 18:04
Operator : JC/MD
Sample : P3327-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E1ZW5

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	1.239	4.1	ug/L	37462	1	6.763	457983	50.0