

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042574.D
 Acq On : 25 Jul 2024 18:08
 Operator : JC/MD
 Sample : P3334-11DL 1000X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20G6DL

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: VX042574.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	rBV	37005	45753	8.36%	0.991%
2	1.368	43	46	56	rVB	46643	58958	10.78%	1.277%
3	1.648	88	92	101	rVB	40643	51445	9.41%	1.114%
4	2.227	185	187	189	rBV	112	87	0.02%	0.002%
5	2.252	189	191	192	rVB	244	151	0.03%	0.003%
6	2.300	192	199	210	rBV	107648	172437	31.52%	3.735%
7	2.453	222	224	226	rVB	132	99	0.02%	0.002%
8	2.477	226	228	229	rVB	197	99	0.02%	0.002%
9	2.508	229	233	236	rBV2	341	542	0.10%	0.012%
10	2.709	263	266	267	rVB	100	71	0.01%	0.002%
11	2.721	267	268	270	rBV	113	88	0.02%	0.002%
12	2.745	270	272	273	rBV	151	86	0.02%	0.002%
13	2.788	273	279	291	rBV	15286	33420	6.11%	0.724%
14	2.940	299	304	312	rVB2	1040	2640	0.48%	0.057%
15	3.007	312	315	316	rVB	85	70	0.01%	0.002%
16	3.203	345	347	348	rVV	118	98	0.02%	0.002%
17	3.215	348	349	350	rVV	182	73	0.01%	0.002%
18	3.233	350	352	354	rVV	140	109	0.02%	0.002%
19	3.270	356	358	360	rVV	104	97	0.02%	0.002%
20	3.294	360	362	364	rVV2	86	80	0.01%	0.002%
21	3.312	364	365	367	rVB	155	73	0.01%	0.002%
22	3.367	370	374	376	rBV	117	152	0.03%	0.003%
23	3.422	381	383	386	rVB	99	111	0.02%	0.002%
24	3.471	389	391	394	rVB2	130	128	0.02%	0.003%
25	3.568	405	407	409	rBV	114	104	0.02%	0.002%
26	3.605	410	413	414	rVV	261	202	0.04%	0.004%
27	3.623	414	416	421	rVB2	203	212	0.04%	0.005%
28	3.770	438	440	441	rBV2	93	84	0.02%	0.002%
29	3.891	458	460	461	rVB	150	87	0.02%	0.002%
30	3.940	465	468	469	rBV2	79	83	0.02%	0.002%
31	4.062	486	488	491	rVB	124	105	0.02%	0.002%
32	4.141	499	501	502	rBV	87	78	0.01%	0.002%
33	4.160	502	504	505	rBV2	110	97	0.02%	0.002%
34	4.288	523	525	528	rVB	93	94	0.02%	0.002%
35	4.318	528	530	531	rBV	129	103	0.02%	0.002%
36	4.471	546	555	572	rBV	41292	127146	23.24%	2.754%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042574.D
 Acq On : 25 Jul 2024 18:08
 Operator : JC/MD
 Sample : P3334-11DL 1000X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20G6DL

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	4.666	586	587	588	rVB	207	76	0.01%	0.002%
38	4.751	600	601	603	rVB	203	135	0.02%	0.003%
39	4.794	603	608	612	rVB3	217	507	0.09%	0.011%
40	4.830	612	614	617	rBV2	177	248	0.05%	0.005%
41	4.910	625	627	629	rBV	131	73	0.01%	0.002%
42	4.952	633	634	637	rVB	182	126	0.02%	0.003%
43	5.056	639	651	671	rBV2	70418	218830	40.01%	4.740%
44	5.397	703	707	709	rBV3	229	224	0.04%	0.005%
45	5.635	743	746	747	rBV2	107	109	0.02%	0.002%
46	5.696	755	756	757	rBV	127	71	0.01%	0.002%
47	5.873	784	785	787	rVV	133	86	0.02%	0.002%
48	5.964	790	800	824	rBV3	184076	546987	100.00%	11.848%
49	6.373	865	867	869	rVB	197	128	0.02%	0.003%
50	6.409	871	873	875	rBV2	134	117	0.02%	0.003%
51	6.763	922	931	950	rBV	162051	384619	70.32%	8.331%
52	7.056	976	979	981	rBV2	191	173	0.03%	0.004%
53	7.123	981	990	1002	rBV	149025	333385	60.95%	7.221%
54	7.312	1012	1021	1042	rVB	108463	245069	44.80%	5.308%
55	7.452	1042	1044	1045	rBV	131	78	0.01%	0.002%
56	7.476	1045	1048	1049	rBV	184	163	0.03%	0.004%
57	7.519	1054	1055	1058	rBV2	80	78	0.01%	0.002%
58	7.915	1118	1120	1121	rBV	176	155	0.03%	0.003%
59	8.324	1181	1187	1200	rBV	66608	111368	20.36%	2.412%
60	8.647	1234	1240	1257	rBV	278505	438963	80.25%	9.508%
61	8.952	1285	1290	1306	rBV	48068	72227	13.20%	1.564%
62	9.275	1339	1343	1348	rVB2	1933	2421	0.44%	0.052%
63	9.384	1356	1361	1379	rBV	169371	259190	47.39%	5.614%
64	9.701	1409	1413	1417	rVB3	472	698	0.13%	0.015%
65	9.829	1432	1434	1437	rVB	186	178	0.03%	0.004%
66	9.860	1437	1439	1441	rBV	251	193	0.04%	0.004%
67	9.957	1453	1455	1457	rBV2	109	119	0.02%	0.003%
68	10.055	1465	1471	1490	rBV	323277	439461	80.34%	9.519%
69	10.311	1510	1513	1517	rBV2	218	327	0.06%	0.007%
70	10.402	1526	1528	1530	rBV	94	79	0.01%	0.002%
71	10.470	1537	1539	1542	rBV2	108	148	0.03%	0.003%
72	10.537	1547	1550	1554	rBV2	110	179	0.03%	0.004%
73	11.195	1652	1658	1673	rVV	211572	282450	51.64%	6.118%
74	11.311	1675	1677	1681	rVV	185	280	0.05%	0.006%
75	11.378	1684	1688	1690	rBV	157	188	0.03%	0.004%
76	11.421	1693	1695	1696	rBV	139	131	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042574.D
 Acq On : 25 Jul 2024 18:08
 Operator : JC/MD
 Sample : P3334-11DL 1000X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20G6DL

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	11.628	1727	1729	1735	rVB2	154	228	0.04%	0.005%
78	11.738	1743	1747	1750	rBV2	142	191	0.03%	0.004%
79	11.780	1752	1754	1757	rBV2	90	103	0.02%	0.002%
80	11.908	1773	1775	1776	rBV	117	101	0.02%	0.002%
81	12.024	1788	1794	1805	rBV	311312	394642	72.15%	8.548%
82	12.231	1824	1828	1831	rBV2	171	228	0.04%	0.005%
83	12.317	1837	1842	1853	rBV	285881	383059	70.03%	8.297%
84	12.475	1867	1868	1870	rBV	160	76	0.01%	0.002%
85	12.603	1887	1889	1891	rBV	124	154	0.03%	0.003%
86	12.670	1898	1900	1901	rBV	191	124	0.02%	0.003%
87	12.762	1913	1915	1917	rVB	281	144	0.03%	0.003%
88	13.201	1985	1987	1990	rBV2	106	121	0.02%	0.003%
89	13.402	2019	2020	2025	rBV2	159	241	0.04%	0.005%
90	13.634	2057	2058	2062	rBV2	150	215	0.04%	0.005%
91	13.786	2082	2083	2085	rBV	166	147	0.03%	0.003%
92	14.024	2120	2122	2124	rBV2	139	148	0.03%	0.003%
93	14.164	2144	2145	2146	rVB	239	87	0.02%	0.002%
94	14.194	2148	2150	2151	rVV2	196	118	0.02%	0.003%
95	14.231	2155	2156	2158	rBV	160	145	0.03%	0.003%
96	14.286	2163	2165	2169	rBV2	249	249	0.05%	0.005%
97	14.365	2175	2178	2179	rBV2	182	214	0.04%	0.005%
98	14.597	2215	2216	2218	rBV2	251	261	0.05%	0.006%
99	14.725	2234	2237	2242	rBV2	179	248	0.05%	0.005%
100	15.353	2338	2340	2342	rBV2	288	178	0.03%	0.004%

Sum of corrected areas: 4616721

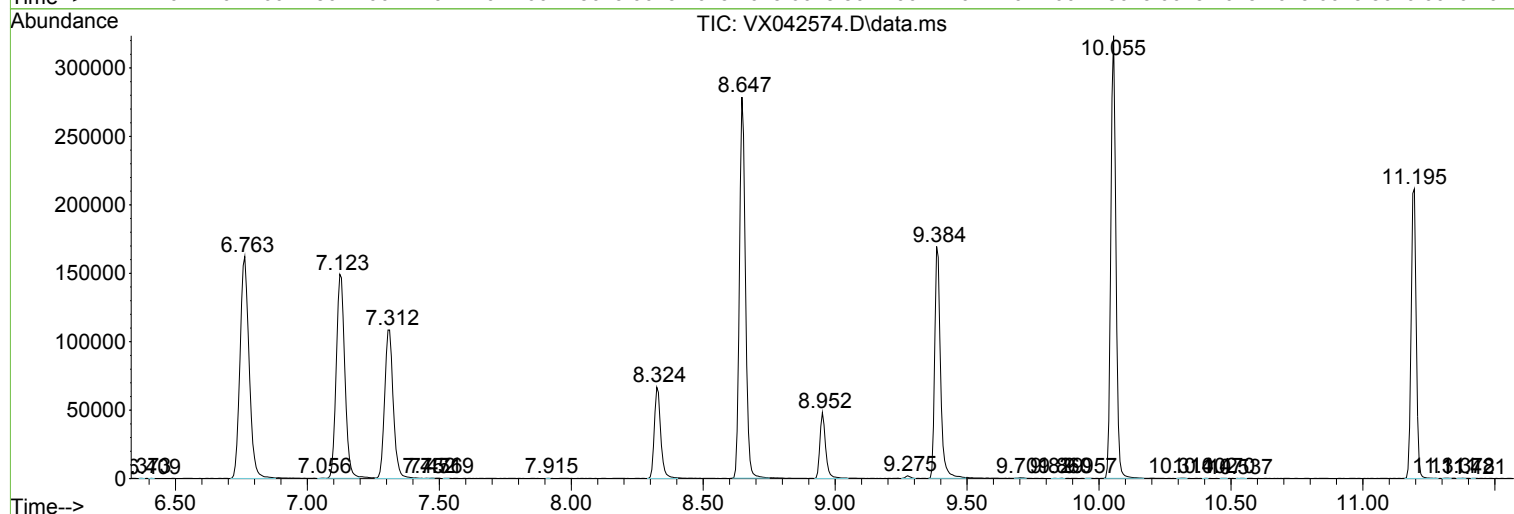
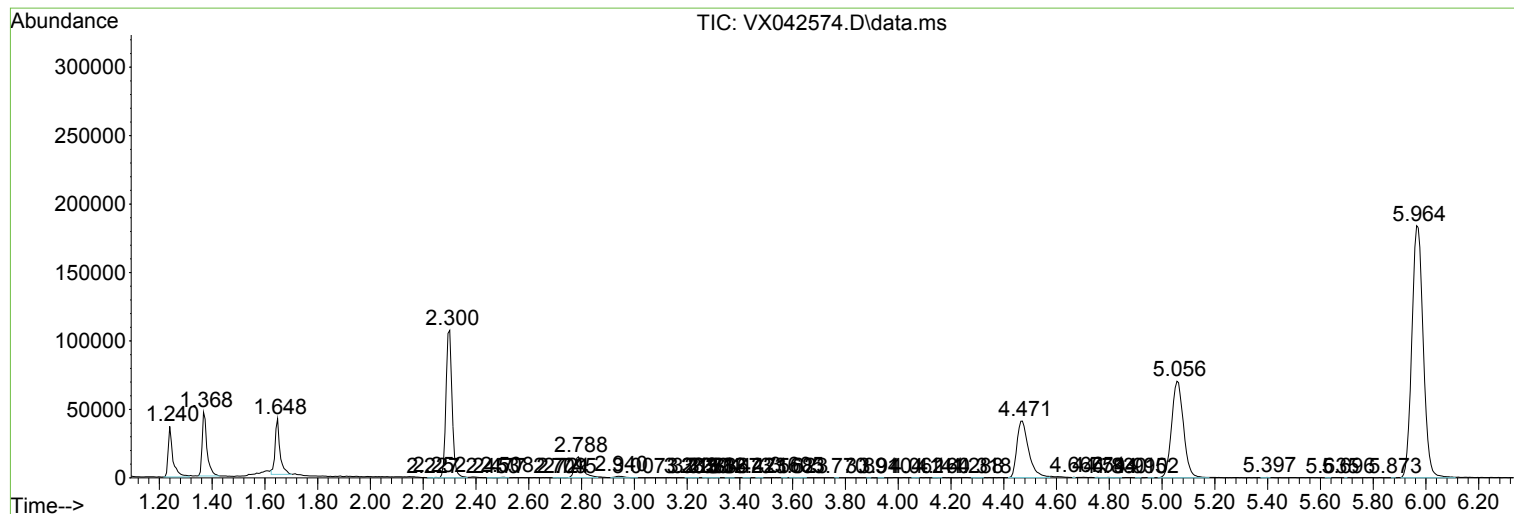
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042574.D
Acq On : 25 Jul 2024 18:08
Operator : JC/MD
Sample : P3334-11DL 1000X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20G6DL

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 : VX042574.D
Acq On : 25 Jul 2024 18:08
Operator : JC/MD
Sample : P3334-11DL 1000X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20G6DL

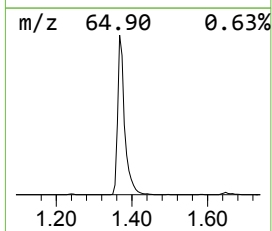
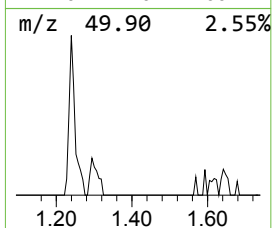
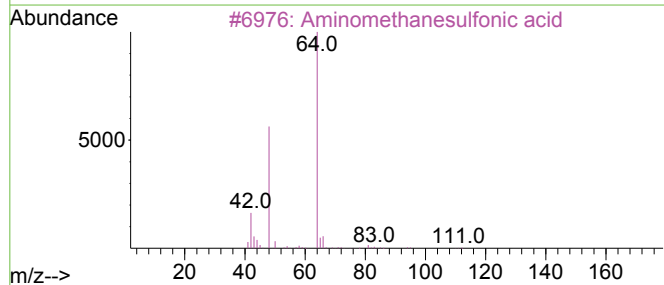
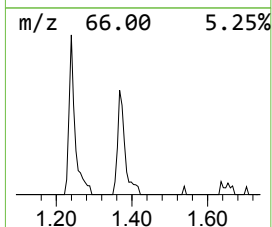
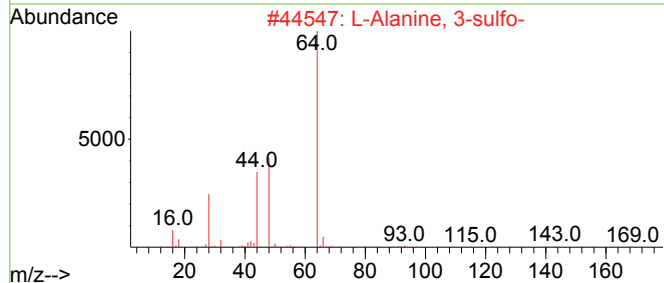
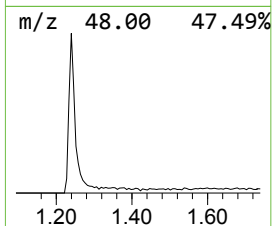
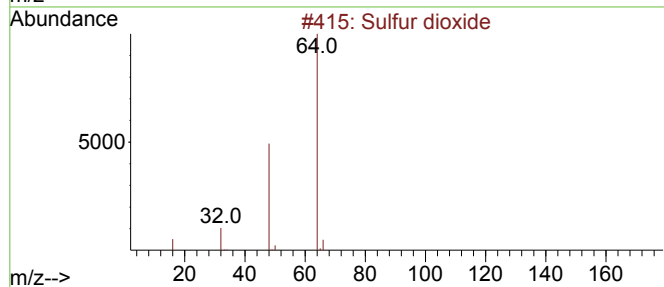
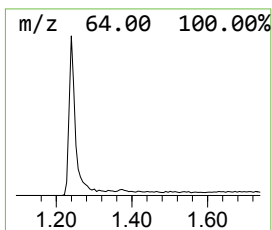
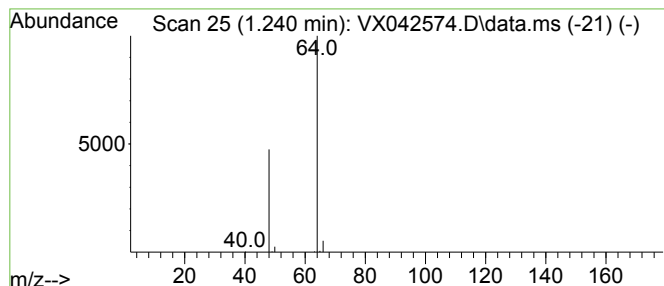
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	5.95 ug/L	45753	1,4-Difluorobenzene	6.763

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
Data File : VX042574.D
Acq On : 25 Jul 2024 18:08
Operator : JC/MD
Sample : P3334-11DL 1000X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20G6DL

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	6.0	ug/L	45753	1	6.763	384619	50.0