

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042783.D
 Acq On : 31 Jul 2024 19:08
 Operator : JC/MD
 Sample : P3361-22ME
 Misc : 10.57g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20Q2ME

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: VX042783.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	22	28	37	rBV2	13312	25639	5.89%	0.807%
2	1.374	43	47	49	rBV2	12009	19608	4.51%	0.617%
3	2.270	189	194	212	rBV	57807	110909	25.49%	3.492%
4	2.782	271	278	283	rBV3	2087	4629	1.06%	0.146%
5	3.056	321	323	326	rBV	176	211	0.05%	0.007%
6	3.081	326	327	330	rVB	221	154	0.04%	0.005%
7	3.142	334	337	338	rBV	170	177	0.04%	0.006%
8	3.215	347	349	354	rBB	118	189	0.04%	0.006%
9	3.507	395	397	400	rBB	248	227	0.05%	0.007%
10	3.666	420	423	425	rBB	118	138	0.03%	0.004%
11	3.715	427	431	433	rBV	200	214	0.05%	0.007%
12	3.861	452	455	456	rBB	149	128	0.03%	0.004%
13	3.892	457	460	464	rBB	160	183	0.04%	0.006%
14	3.952	468	470	472	rBV	205	191	0.04%	0.006%
15	4.038	482	484	488	rBB	140	183	0.04%	0.006%
16	4.081	488	491	492	rBV	223	237	0.05%	0.007%
17	4.263	520	521	524	rBB	200	207	0.05%	0.007%
18	4.391	541	542	544	rBV	189	153	0.04%	0.005%
19	4.501	551	560	576	rBV2	22648	81349	18.70%	2.561%
20	5.056	640	651	668	rBV	55406	173918	39.97%	5.475%
21	5.208	675	676	678	rVB	514	290	0.07%	0.009%
22	5.318	692	694	695	rBB	183	131	0.03%	0.004%
23	5.355	695	700	703	rBB	197	320	0.07%	0.010%
24	5.391	703	706	707	rBV	280	213	0.05%	0.007%
25	5.519	725	727	731	rBV2	335	386	0.09%	0.012%
26	5.550	731	732	733	rVV2	262	128	0.03%	0.004%
27	5.611	739	742	745	rBV2	243	384	0.09%	0.012%
28	5.696	753	756	757	rBV	186	186	0.04%	0.006%
29	5.763	764	767	769	rBV	254	277	0.06%	0.009%
30	5.873	782	785	786	rBV	131	137	0.03%	0.004%
31	5.964	789	800	813	rBV2	154750	435102	100.00%	13.698%
32	6.172	833	834	837	rBV	222	203	0.05%	0.006%
33	6.202	837	839	840	rBV	168	134	0.03%	0.004%
34	6.379	862	868	875	rBV3	981	2831	0.65%	0.089%
35	6.470	881	883	888	rVB2	333	343	0.08%	0.011%
36	6.568	898	899	901	rBB2	240	163	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042783.D
 Acq On : 31 Jul 2024 19:08
 Operator : JC/MD
 Sample : P3361-22ME
 Misc : 10.57g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20Q2ME

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	6.678	915	917	920	rBV	198	279	0.06%	0.009%
38	6.757	922	930	943	rBV	109357	263154	60.48%	8.285%
39	7.050	976	978	979	rBV	208	151	0.03%	0.005%
40	7.110	985	988	989	rBV	530	505	0.12%	0.016%
41	7.220	998	1006	1007	rBV3	1929	2515	0.58%	0.079%
42	7.306	1013	1020	1039	rBV	86833	194629	44.73%	6.127%
43	7.482	1045	1049	1051	rBV	325	426	0.10%	0.013%
44	7.549	1057	1060	1061	rVB2	173	144	0.03%	0.005%
45	7.641	1073	1075	1076	rBV	205	173	0.04%	0.005%
46	7.720	1085	1088	1091	rBV2	220	324	0.07%	0.010%
47	7.866	1110	1112	1114	rBV	193	188	0.04%	0.006%
48	8.043	1138	1141	1146	rBV2	283	521	0.12%	0.016%
49	8.263	1173	1177	1181	rBV2	265	513	0.12%	0.016%
50	8.324	1182	1187	1198	rVV	49454	85339	19.61%	2.687%
51	8.433	1202	1205	1209	rBV2	362	475	0.11%	0.015%
52	8.647	1234	1240	1253	rBV	217033	346869	79.72%	10.920%
53	8.885	1277	1279	1281	rBV	254	261	0.06%	0.008%
54	8.903	1281	1282	1285	rBV2	344	235	0.05%	0.007%
55	8.952	1285	1290	1304	rBV	34372	56201	12.92%	1.769%
56	9.171	1324	1326	1327	rBV	237	187	0.04%	0.006%
57	9.281	1340	1344	1348	rBV	397	705	0.16%	0.022%
58	9.397	1357	1363	1381	rBV	94900	203517	46.77%	6.407%
59	9.714	1412	1415	1420	rVB3	911	1349	0.31%	0.042%
60	9.775	1424	1425	1427	rBV3	280	196	0.05%	0.006%
61	9.964	1455	1456	1459	rVB	179	165	0.04%	0.005%
62	10.000	1459	1462	1465	rBV	180	202	0.05%	0.006%
63	10.055	1465	1471	1486	rBV	221780	311937	71.69%	9.821%
64	10.488	1539	1542	1545	rBV	261	324	0.07%	0.010%
65	10.555	1549	1553	1554	rBV	214	232	0.05%	0.007%
66	10.592	1558	1559	1562	rBV	207	230	0.05%	0.007%
67	10.909	1608	1611	1613	rVB	202	197	0.05%	0.006%
68	11.055	1632	1635	1638	rVB	251	360	0.08%	0.011%
69	11.085	1638	1640	1645	rBV2	225	408	0.09%	0.013%
70	11.195	1652	1658	1666	rBV	175671	231247	53.15%	7.280%
71	11.415	1692	1694	1696	rBV	209	211	0.05%	0.007%
72	11.439	1696	1698	1700	rBV	285	293	0.07%	0.009%
73	11.597	1722	1724	1726	rBV2	295	194	0.04%	0.006%
74	11.762	1748	1751	1755	rBV	386	571	0.13%	0.018%
75	11.860	1765	1767	1770	rBV	187	210	0.05%	0.007%
76	11.982	1783	1787	1788	rBV	263	247	0.06%	0.008%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042783.D
 Acq On : 31 Jul 2024 19:08
 Operator : JC/MD
 Sample : P3361-22ME
 Misc : 10.57g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20Q2ME

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	12.024	1788	1794	1804	rBV	218037	282877	65.01%	8.906%
78	12.250	1827	1831	1832	rBV	265	339	0.08%	0.011%
79	12.323	1837	1843	1853	rBV	235733	315886	72.60%	9.945%
80	12.567	1881	1883	1888	rVB	141	155	0.04%	0.005%
81	12.640	1894	1895	1896	rBV	278	138	0.03%	0.004%
82	12.762	1911	1915	1919	rBV2	539	662	0.15%	0.021%
83	12.878	1931	1934	1935	rBV2	176	200	0.05%	0.006%
84	12.939	1942	1944	1945	rBV	189	134	0.03%	0.004%
85	13.201	1985	1987	1989	rBV	250	160	0.04%	0.005%
86	13.225	1989	1991	1994	rBV	270	271	0.06%	0.009%
87	13.365	2011	2014	2016	rBV2	283	336	0.08%	0.011%
88	13.457	2027	2029	2031	rBV	237	134	0.03%	0.004%
89	13.481	2031	2033	2035	rBV	207	157	0.04%	0.005%
90	13.500	2035	2036	2040	rBV	178	160	0.04%	0.005%
91	13.530	2040	2041	2043	rBV	192	135	0.03%	0.004%
92	13.634	2054	2058	2060	rBV2	250	245	0.06%	0.008%
93	13.701	2065	2069	2070	rBV2	294	302	0.07%	0.010%
94	13.780	2078	2082	2092	rBV2	4310	6781	1.56%	0.213%
95	14.006	2117	2119	2120	rBV	244	130	0.03%	0.004%
96	14.042	2123	2125	2129	rVB2	451	371	0.09%	0.012%
97	14.445	2189	2191	2195	rBV2	311	271	0.06%	0.009%
98	14.536	2205	2206	2207	rBV2	260	145	0.03%	0.005%
99	14.585	2210	2214	2215	rBV2	461	415	0.10%	0.013%
100	14.615	2217	2219	2220	rBV	324	212	0.05%	0.007%

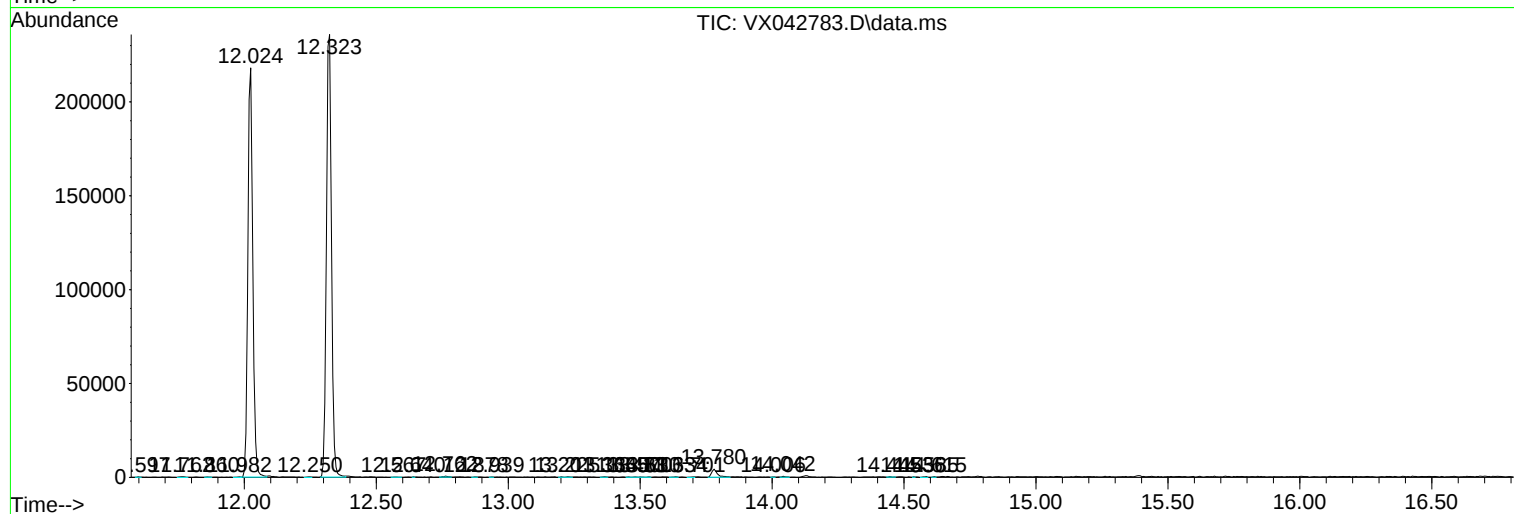
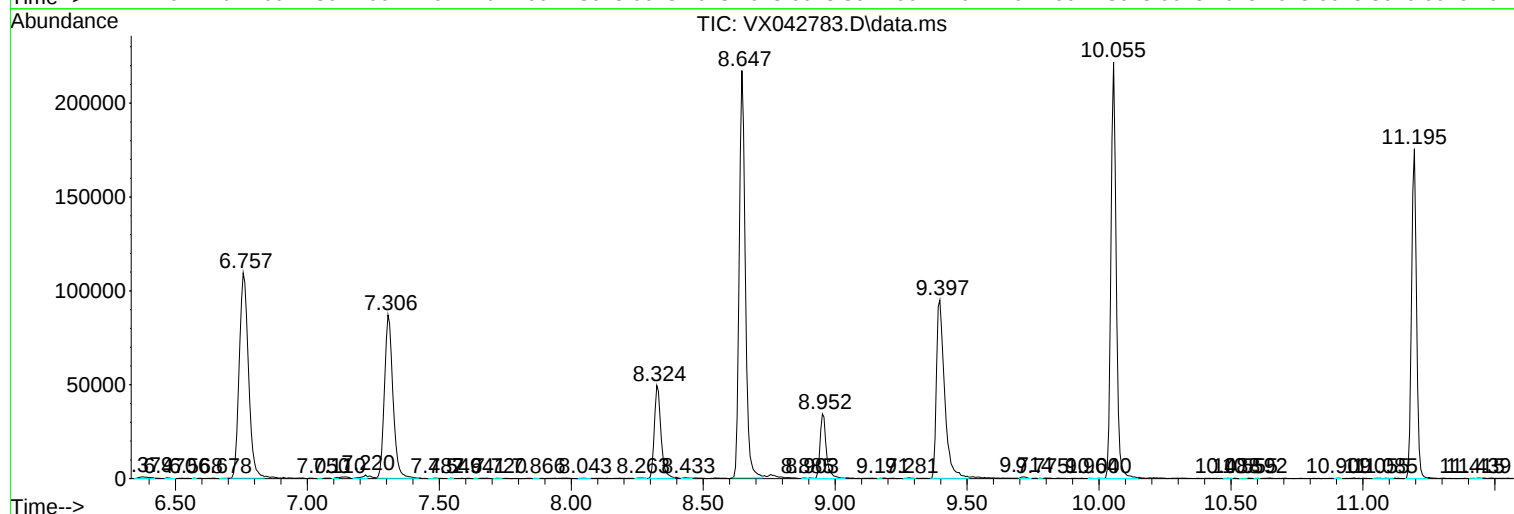
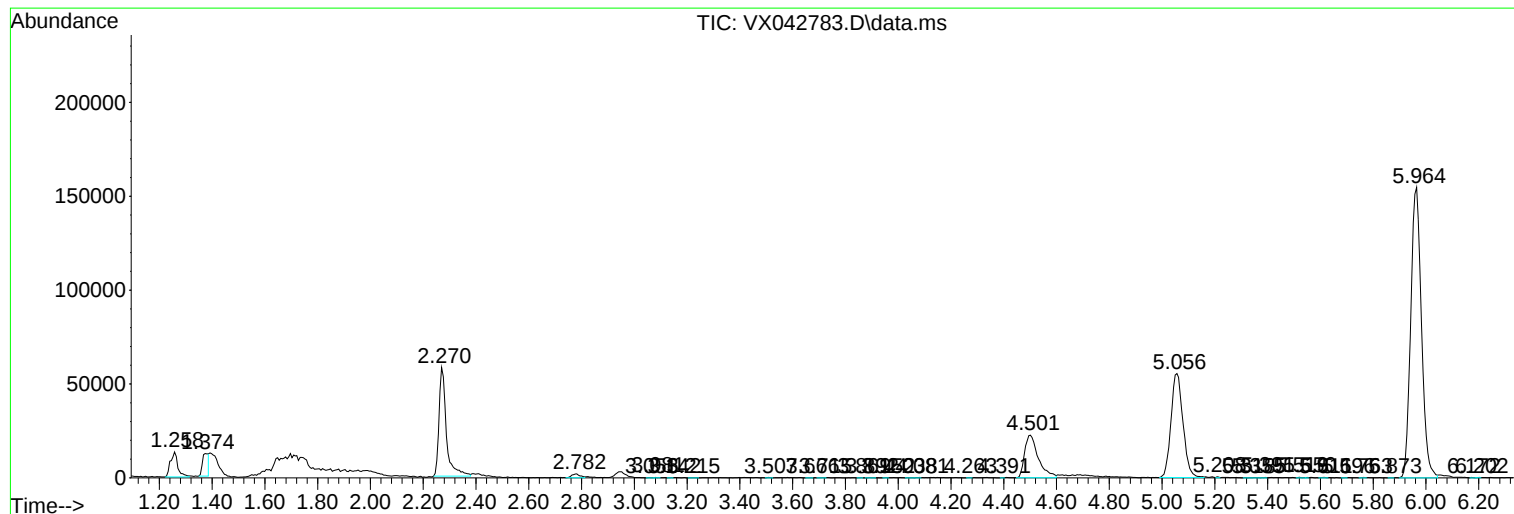
Sum of corrected areas: 3176372

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042783.D
Acq On : 31 Jul 2024 19:08
Operator : JC/MD
Sample : P3361-22ME
Misc : 10.57g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20Q2ME

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 : VX042783.D
Acq On : 31 Jul 2024 19:08
Operator : JC/MD
Sample : P3361-22ME
Misc : 10.57g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20Q2ME

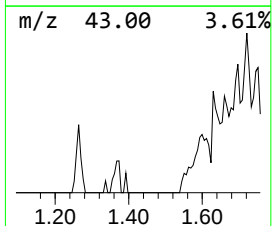
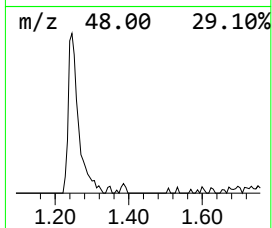
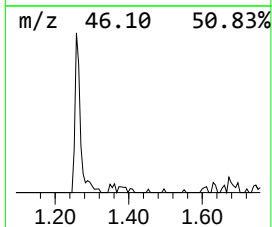
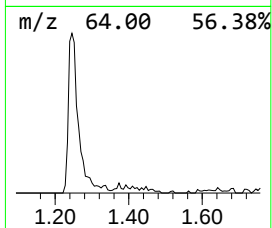
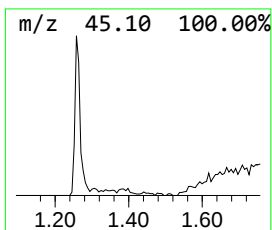
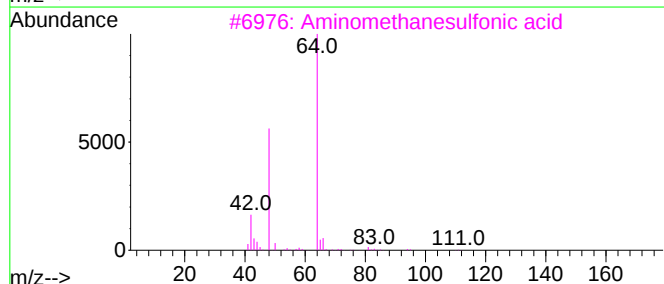
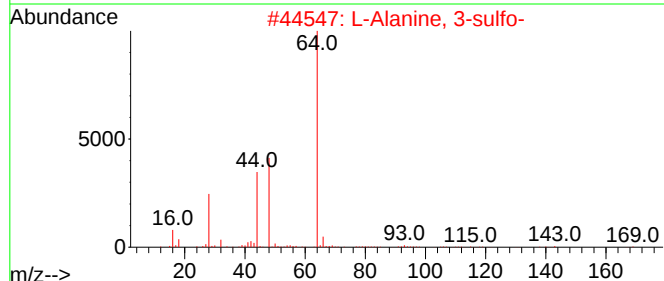
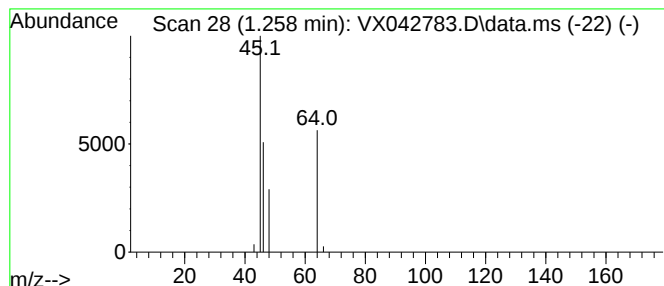
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	4.87 ug/L	25639	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	38
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			Dimethyl ether	46	C2H6O	000115-10-6	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042783.D
Acq On : 31 Jul 2024 19:08
Operator : JC/MD
Sample : P3361-22ME
Misc : 10.57g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E20Q2ME

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
unknown-01	1.258	4.9	ug/L	25639	1	6.757	263154	50.0