

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012424\
 Data File : VV033846.D
 Acq On : 24 Jan 2024 12:21
 Operator : SY/MD
 Sample : P1191-13
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMQ3

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_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

Signal : TIC: VV033846.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.169	32	40	53	rBV	35711	43133	5.11%	0.642%
2	1.281	68	75	93	rBV2	157164	178458	21.13%	2.656%
3	1.532	146	153	166	rVV	104575	125126	14.82%	1.862%
4	1.597	167	173	186	rVB	17781	23992	2.84%	0.357%
5	2.063	307	318	345	rVB	219590	332616	39.39%	4.951%
6	2.188	353	357	358	rBV2	433	324	0.04%	0.005%
7	2.240	364	373	378	rBV4	666	1268	0.15%	0.019%
8	2.297	387	391	392	rBV	165	131	0.02%	0.002%
9	2.445	428	437	449	rBV5	1397	2725	0.32%	0.041%
10	2.516	449	459	470	rVV4	2779	5409	0.64%	0.081%
11	2.558	470	472	484	rVB2	201	249	0.03%	0.004%
12	2.703	506	517	524	rVB5	1534	2543	0.30%	0.038%
13	3.101	636	641	647	rBV2	193	289	0.03%	0.004%
14	3.352	716	719	726	rVB2	179	178	0.02%	0.003%
15	3.574	781	788	791	rBV2	151	193	0.02%	0.003%
16	3.674	808	819	833	rBV5	1765	4377	0.52%	0.065%
17	3.783	845	853	883	rBV	49919	143867	17.04%	2.141%
18	4.014	922	925	929	rVB	287	167	0.02%	0.002%
19	4.249	982	998	1023	rBV2	129999	331096	39.21%	4.928%
20	4.455	1059	1062	1066	rBV2	367	325	0.04%	0.005%
21	4.506	1073	1078	1081	rVB3	290	226	0.03%	0.003%
22	4.529	1081	1085	1087	rBV2	262	172	0.02%	0.003%
23	4.590	1093	1104	1114	rVB3	1875	4065	0.48%	0.061%
24	4.696	1134	1137	1142	rBV2	181	182	0.02%	0.003%
25	4.815	1171	1174	1177	rVB	198	151	0.02%	0.002%
26	4.838	1177	1181	1189	rVB2	254	381	0.05%	0.006%
27	4.956	1202	1218	1246	rBV2	319408	844434	100.00%	12.569%
28	5.111	1264	1266	1269	rBV4	338	212	0.03%	0.003%
29	5.329	1330	1334	1337	rVB3	273	233	0.03%	0.003%
30	5.407	1356	1358	1362	rVB	223	179	0.02%	0.003%
31	5.429	1362	1365	1369	rBV2	203	171	0.02%	0.003%
32	5.532	1386	1397	1432	rBV	268713	551502	65.31%	8.209%
33	5.796	1476	1479	1481	rBV2	199	164	0.02%	0.002%
34	5.837	1485	1492	1501	rVB3	1217	2231	0.26%	0.033%
35	5.918	1513	1517	1520	rBV2	226	230	0.03%	0.003%
36	5.989	1524	1539	1564	rBV	182621	375801	44.50%	5.594%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012424\
 Data File : VV033846.D
 Acq On : 24 Jan 2024 12:21
 Operator : SY/MD
 Sample : P1191-13
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMQ3

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_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

37	6.143	1584	1587	1589	rBV3	351	164	0.02%	0.002%
38	6.249	1615	1620	1622	rVB2	207	145	0.02%	0.002%
39	6.452	1677	1683	1685	rBV2	180	202	0.02%	0.003%
40	6.554	1711	1715	1720	rBV2	179	178	0.02%	0.003%
41	6.583	1720	1724	1729	rBV2	203	231	0.03%	0.003%
42	6.735	1765	1771	1779	rVB2	322	453	0.05%	0.007%
43	6.828	1795	1800	1803	rBV	288	354	0.04%	0.005%
44	6.911	1816	1826	1857	rBV	109153	204286	24.19%	3.041%
45	7.243	1918	1929	1971	rBV	393639	691419	81.88%	10.292%
46	7.471	1997	2000	2005	rBV3	294	300	0.04%	0.004%
47	7.554	2017	2026	2049	rBV	73054	130351	15.44%	1.940%
48	7.677	2061	2064	2069	rVB3	324	281	0.03%	0.004%
49	7.754	2086	2088	2090	rVB	316	134	0.02%	0.002%
50	7.773	2090	2094	2101	rVB3	402	425	0.05%	0.006%
51	7.825	2107	2110	2111	rBV	212	137	0.02%	0.002%
52	7.870	2122	2124	2130	rVB3	262	245	0.03%	0.004%
53	8.024	2163	2172	2209	rBV	175392	345523	40.92%	5.143%
54	8.336	2264	2269	2270	rBV2	198	180	0.02%	0.003%
55	8.783	2397	2408	2439	rBV	414250	674595	79.89%	10.041%
56	9.005	2472	2477	2479	rBV2	436	302	0.04%	0.004%
57	9.525	2634	2639	2645	rBV2	182	218	0.03%	0.003%
58	9.619	2666	2668	2671	rVB2	248	156	0.02%	0.002%
59	10.056	2797	2804	2807	rBV2	192	228	0.03%	0.003%
60	10.152	2822	2834	2857	rBV	233452	362663	42.95%	5.398%
61	10.323	2883	2887	2891	rVB2	339	278	0.03%	0.004%
62	10.445	2920	2925	2930	rVB2	221	240	0.03%	0.004%
63	10.477	2930	2935	2937	rBV	141	144	0.02%	0.002%
64	10.657	2987	2991	2995	rBV	140	133	0.02%	0.002%
65	10.731	3012	3014	3022	rVB2	199	191	0.02%	0.003%
66	11.024	3098	3105	3110	rVB2	137	194	0.02%	0.003%
67	11.127	3135	3137	3143	rVB	269	146	0.02%	0.002%
68	11.185	3144	3155	3182	rBV	438237	684908	81.11%	10.195%
69	11.516	3254	3258	3260	rVV2	802	736	0.09%	0.011%
70	11.561	3260	3272	3294	rVB	397025	628473	74.43%	9.355%
71	11.686	3309	3311	3314	rVB2	369	193	0.02%	0.003%
72	12.297	3496	3501	3502	rBV	917	750	0.09%	0.011%
73	12.381	3521	3527	3532	rBV2	316	320	0.04%	0.005%
74	12.413	3533	3537	3541	rVB	267	258	0.03%	0.004%
75	12.876	3676	3681	3685	rBV2	537	524	0.06%	0.008%
76	13.001	3717	3720	3725	rVB2	163	138	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012424\
 Data File : VV033846.D
 Acq On : 24 Jan 2024 12:21
 Operator : SY/MD
 Sample : P1191-13
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCMQ3

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_V\Method\SFAMVLM011024WMA.M
 Title : VOC Analysis

77	13.043	3727	3733	3737	rVV3	214	213	0.03%	0.003%
78	13.381	3831	3838	3846	rBV4	1194	1821	0.22%	0.027%
79	13.455	3854	3861	3867	rBV5	736	1145	0.14%	0.017%
80	13.554	3889	3892	3897	rVB2	305	206	0.02%	0.003%
81	13.580	3897	3900	3902	rBV2	247	153	0.02%	0.002%
82	13.808	3968	3971	3974	rVB2	444	225	0.03%	0.003%
83	13.911	4001	4003	4006	rBV2	192	132	0.02%	0.002%
84	14.043	4041	4044	4046	rVB2	232	131	0.02%	0.002%
85	14.062	4048	4050	4054	rVB3	243	184	0.02%	0.003%
86	14.178	4083	4086	4088	rBV3	246	150	0.02%	0.002%
87	14.226	4099	4101	4106	rVB3	280	215	0.03%	0.003%
88	14.262	4110	4112	4116	rBV	183	162	0.02%	0.002%
89	14.483	4178	4181	4183	rBV2	238	133	0.02%	0.002%
90	14.516	4187	4191	4193	rBV2	228	175	0.02%	0.003%
91	14.606	4216	4219	4221	rBV	243	142	0.02%	0.002%
92	14.789	4272	4276	4279	rBV2	296	308	0.04%	0.005%
93	14.837	4288	4291	4296	rBV2	270	241	0.03%	0.004%
94	15.004	4340	4343	4344	rBV2	233	135	0.02%	0.002%
95	15.120	4373	4379	4381	rBV4	511	489	0.06%	0.007%
96	15.197	4401	4403	4406	rBV2	336	205	0.02%	0.003%
97	15.278	4426	4428	4431	rBV3	268	190	0.02%	0.003%
98	15.454	4481	4483	4486	rBV2	375	267	0.03%	0.004%
99	15.535	4506	4508	4514	rBV3	447	522	0.06%	0.008%
100	16.249	4725	4730	4736	rBV4	2981	3167	0.38%	0.047%

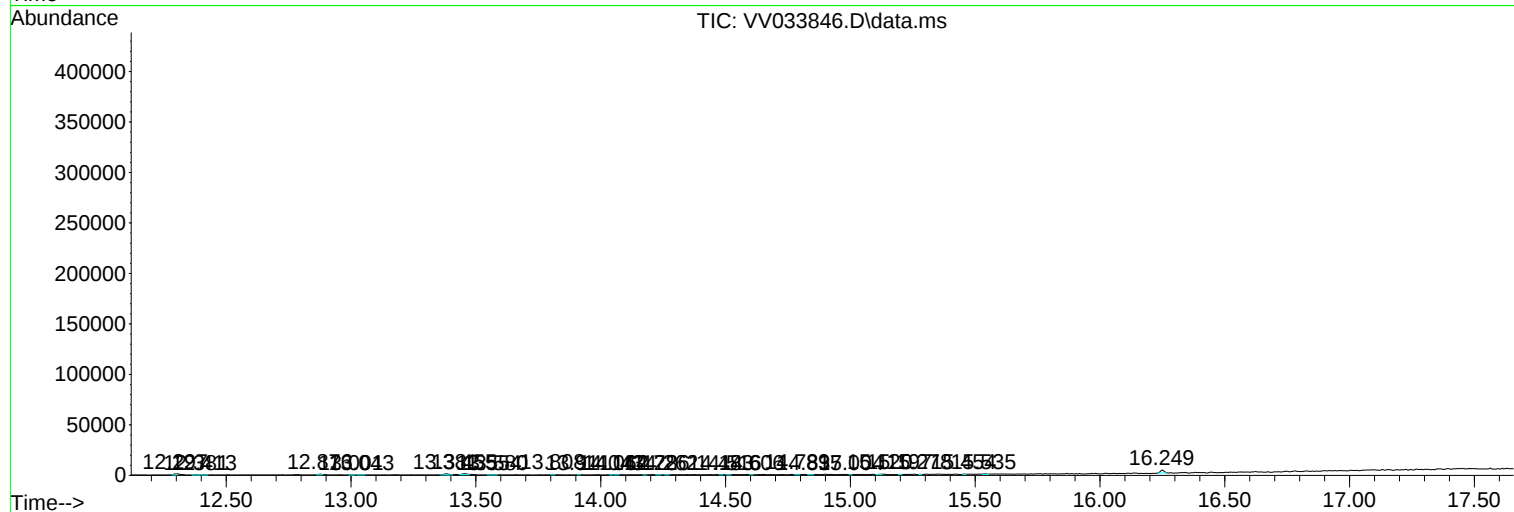
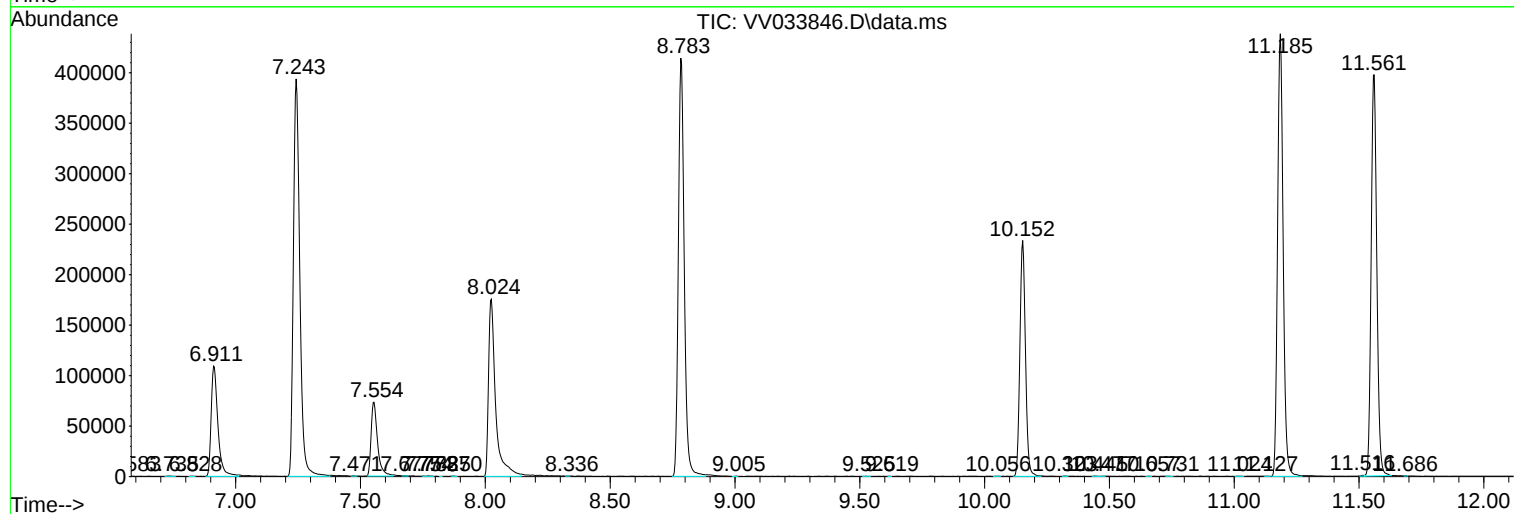
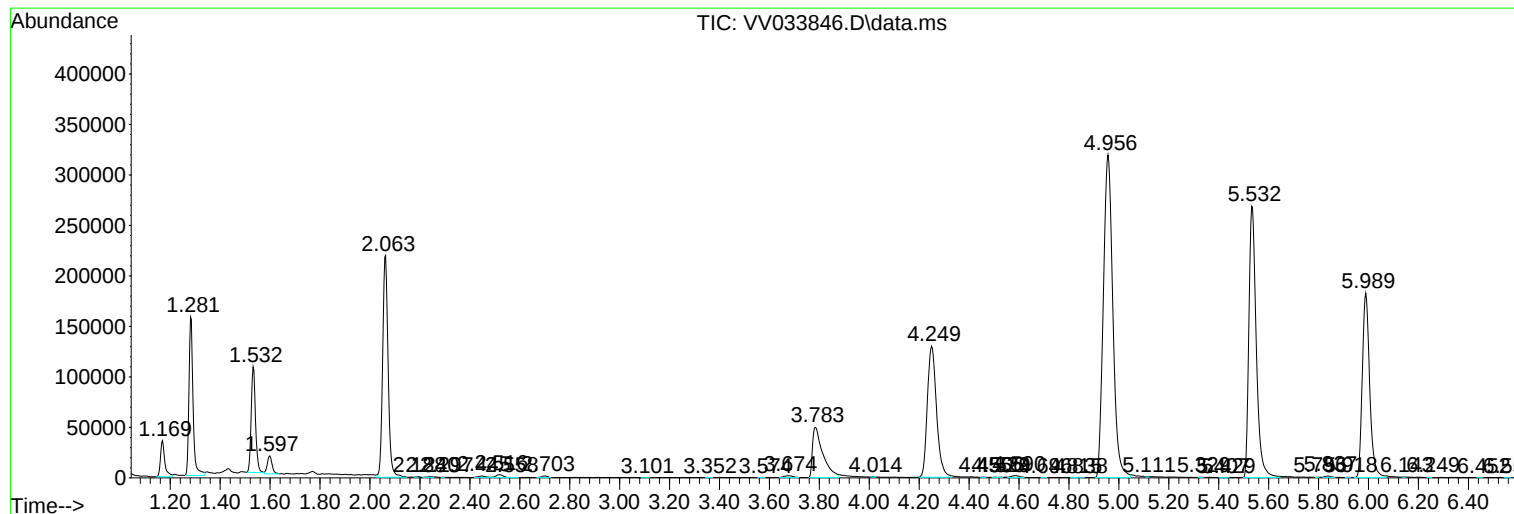
Sum of corrected areas: 6718307

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012424\
Data File : VV033846.D
Acq On : 24 Jan 2024 12:21
Operator : SY/MD
Sample : P1191-13
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMQ3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012424\
Data File : VV033846.D
Acq On : 24 Jan 2024 12:21
Operator : SY/MD
Sample : P1191-13
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMQ3

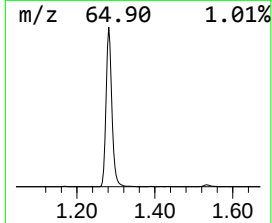
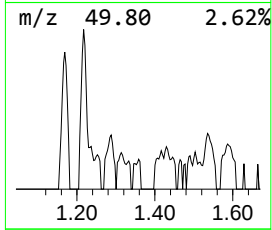
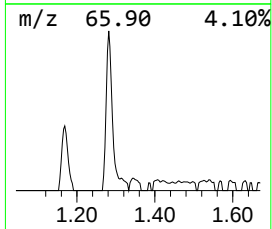
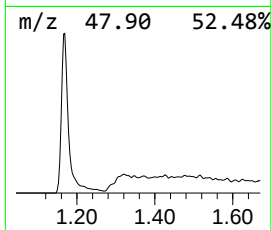
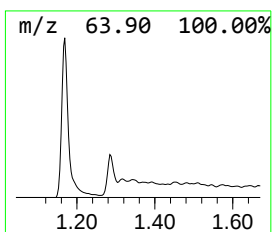
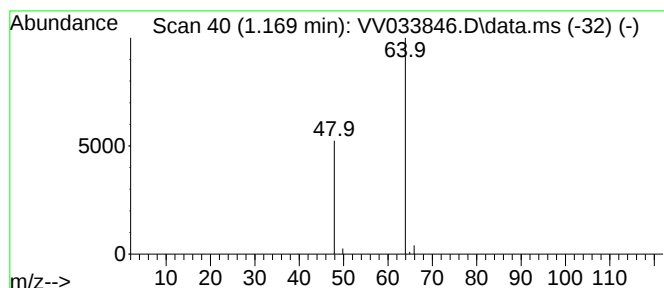
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.M
Quant Title : VOC Analysis

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.
1.169	3.91 ug/L	43133	1,4-Difluorobenzene	5.535

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV012424\
Data File : VV033846.D
Acq On : 24 Jan 2024 12:21
Operator : SY/MD
Sample : P1191-13
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DCMQ3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM011024WMA.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	1.169	3.9	ug/L	43133	1	5.535	551502	50.0