

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
 Data File : VU053635.D
 Acq On : 11 Apr 2023 15:11
 Operator : JC/MD
 Sample : 02251-19
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMD7

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_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053635.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	32	40	54	rBV	36560	64887	8.22%	1.014%
2	1.597	74	80	94	rBV	98084	112879	14.30%	1.763%
3	1.909	171	177	192	rVB	81694	111950	14.18%	1.749%
4	2.565	369	381	395	rBV	153305	250849	31.78%	3.918%
5	2.777	445	447	450	rBV2	735	567	0.07%	0.009%
6	3.038	523	528	533	rBV4	885	1057	0.13%	0.017%
7	3.629	709	712	717	rBV2	254	242	0.03%	0.004%
8	3.665	721	723	727	rVB	233	140	0.02%	0.002%
9	3.729	741	743	745	rBV	186	89	0.01%	0.001%
10	3.771	753	756	760	rBV2	225	212	0.03%	0.003%
11	4.112	859	862	868	rVB	318	205	0.03%	0.003%
12	4.163	874	878	879	rBV	212	174	0.02%	0.003%
13	4.430	959	961	963	rVB	149	77	0.01%	0.001%
14	4.520	987	989	990	rBV	226	105	0.01%	0.002%
15	4.610	1006	1017	1043	rBV	68499	163134	20.67%	2.548%
16	4.931	1114	1117	1122	rVB2	423	313	0.04%	0.005%
17	5.054	1141	1155	1175	rBV	141134	312727	39.62%	4.885%
18	5.282	1223	1226	1228	rBV2	404	281	0.04%	0.004%
19	5.346	1243	1246	1248	rBV	221	147	0.02%	0.002%
20	5.610	1324	1328	1334	rVB2	255	248	0.03%	0.004%
21	5.719	1341	1362	1388	rBV2	279822	789278	100.00%	12.329%
22	6.005	1445	1451	1456	rBV3	419	461	0.06%	0.007%
23	6.243	1511	1525	1545	rBV	273010	519861	65.87%	8.121%
24	6.497	1601	1604	1607	rBV2	452	345	0.04%	0.005%
25	6.571	1624	1627	1629	rVB	257	127	0.02%	0.002%
26	6.594	1631	1634	1636	rBV2	173	144	0.02%	0.002%
27	6.684	1648	1662	1683	rBV	174974	343560	43.53%	5.367%
28	6.941	1739	1742	1745	rBV	145	104	0.01%	0.002%
29	7.012	1762	1764	1766	rVB	130	32	0.00%	0.000%
30	7.189	1812	1819	1827	rVB4	1222	1503	0.19%	0.023%
31	7.269	1840	1844	1847	rBV2	350	342	0.04%	0.005%
32	7.317	1857	1859	1863	rBV	263	102	0.01%	0.002%
33	7.340	1863	1866	1867	rBV2	193	112	0.01%	0.002%
34	7.404	1884	1886	1888	rBV	200	98	0.01%	0.002%
35	7.562	1922	1935	1959	rBV	99423	171965	21.79%	2.686%
36	7.674	1966	1970	1971	rBV2	352	272	0.03%	0.004%

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Integrator: RTE

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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_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

37	7.748	1990	1993	1995	rBV	219	150	0.02%	0.002%
38	7.893	2025	2038	2056	rBV	353782	618836	78.41%	9.667%
39	8.076	2092	2095	2102	rVB3	255	321	0.04%	0.005%
40	8.108	2102	2105	2108	rBV	244	139	0.02%	0.002%
41	8.176	2115	2126	2144	rBV2	67424	116129	14.71%	1.814%
42	8.340	2173	2177	2179	rBV	285	200	0.03%	0.003%
43	8.407	2196	2198	2200	rBV	252	131	0.02%	0.002%
44	8.436	2204	2207	2209	rBV	207	152	0.02%	0.002%
45	8.510	2228	2230	2232	rBV2	211	115	0.01%	0.002%
46	8.549	2238	2242	2247	rBV2	391	351	0.04%	0.005%
47	8.574	2248	2250	2251	rBV2	158	47	0.01%	0.001%
48	8.626	2254	2266	2300	rBV	200222	372432	47.19%	5.818%
49	8.819	2324	2326	2330	rVB2	434	279	0.04%	0.004%
50	8.896	2347	2350	2352	rBV	190	116	0.01%	0.002%
51	9.028	2389	2391	2398	rVV2	264	220	0.03%	0.003%
52	9.060	2398	2401	2403	rVB	209	96	0.01%	0.001%
53	9.414	2498	2511	2533	rBV	381190	695612	88.13%	10.866%
54	9.613	2571	2573	2576	rVB2	222	125	0.02%	0.002%
55	9.690	2595	2597	2602	rVB2	500	264	0.03%	0.004%
56	9.748	2612	2615	2617	rBV2	239	146	0.02%	0.002%
57	10.124	2728	2732	2735	rBV	495	440	0.06%	0.007%
58	10.208	2756	2758	2760	rBV	242	124	0.02%	0.002%
59	10.417	2821	2823	2826	rBV	219	115	0.01%	0.002%
60	10.449	2830	2833	2834	rBV	181	85	0.01%	0.001%
61	10.565	2867	2869	2873	rBV2	273	196	0.02%	0.003%
62	10.668	2899	2901	2903	rBV	160	57	0.01%	0.001%
63	10.751	2915	2927	2946	rBV	269877	431142	54.62%	6.735%
64	11.272	3087	3089	3090	rBV	237	102	0.01%	0.002%
65	11.314	3100	3102	3105	rBV	187	97	0.01%	0.002%
66	11.442	3140	3142	3143	rBV	142	45	0.01%	0.001%
67	11.475	3149	3152	3156	rVB2	383	270	0.03%	0.004%
68	11.745	3227	3236	3242	rBV3	1765	2205	0.28%	0.034%
69	11.806	3243	3255	3278	rBV	406444	676563	85.72%	10.568%
70	12.188	3361	3374	3396	rBV	377234	629734	79.79%	9.837%
71	12.372	3427	3431	3434	rBV	348	238	0.03%	0.004%
72	12.391	3434	3437	3440	rVV2	317	210	0.03%	0.003%
73	12.529	3475	3480	3483	rBV	294	273	0.03%	0.004%
74	12.549	3483	3486	3491	rBV	341	310	0.04%	0.005%
75	12.767	3552	3554	3557	rVB	261	117	0.01%	0.002%
76	13.024	3632	3634	3635	rBV	326	80	0.01%	0.001%

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C0MD7

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_U\Method\SFAMULM033123WMA.M
Title : VOC Analysis

77	13.632	3819	3823	3827	rBV2	425	468	0.06%	0.007%
78	13.848	3883	3890	3899	rVB4	2355	3834	0.49%	0.060%
79	14.581	4114	4118	4121	rBV3	664	559	0.07%	0.009%

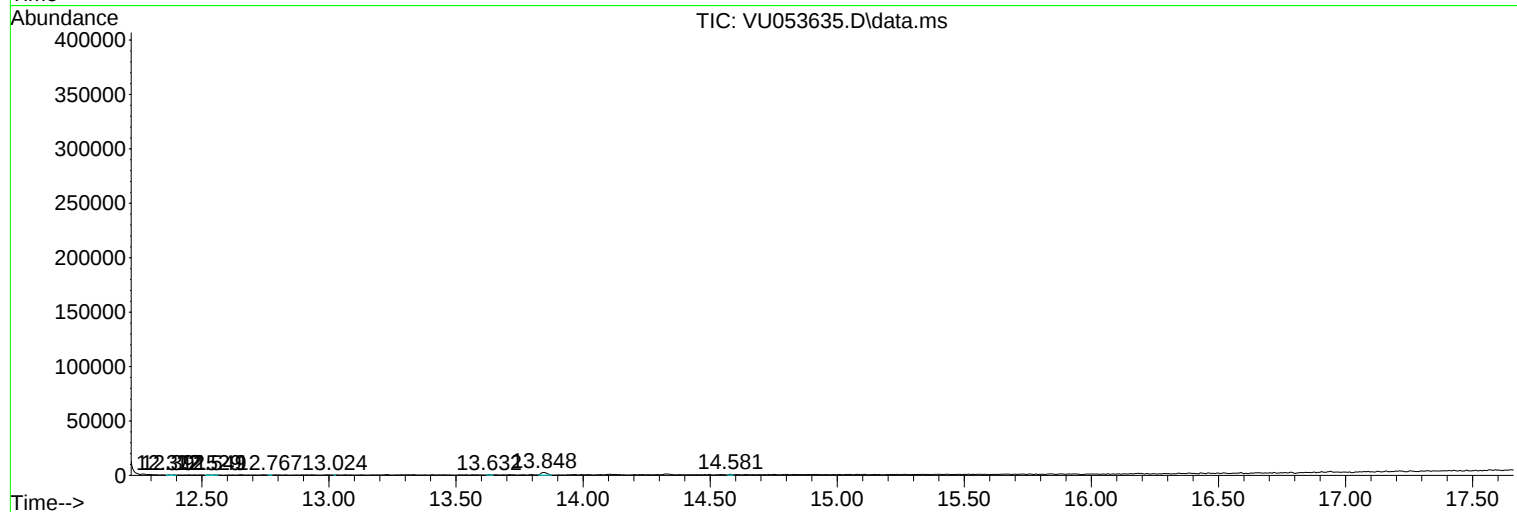
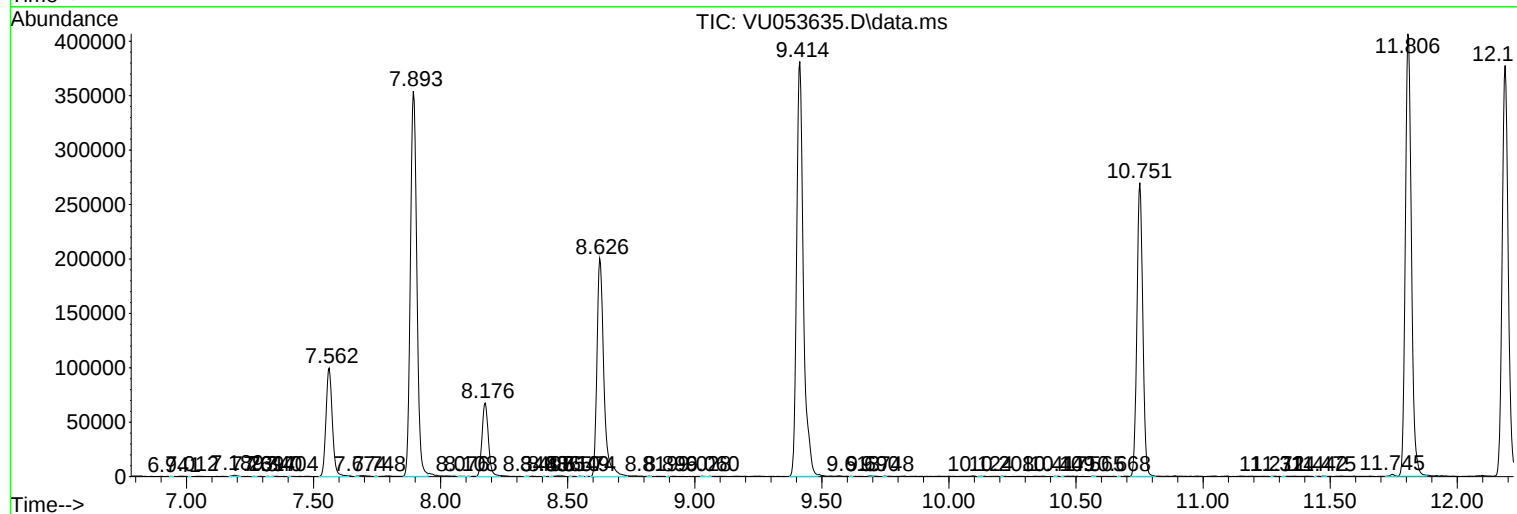
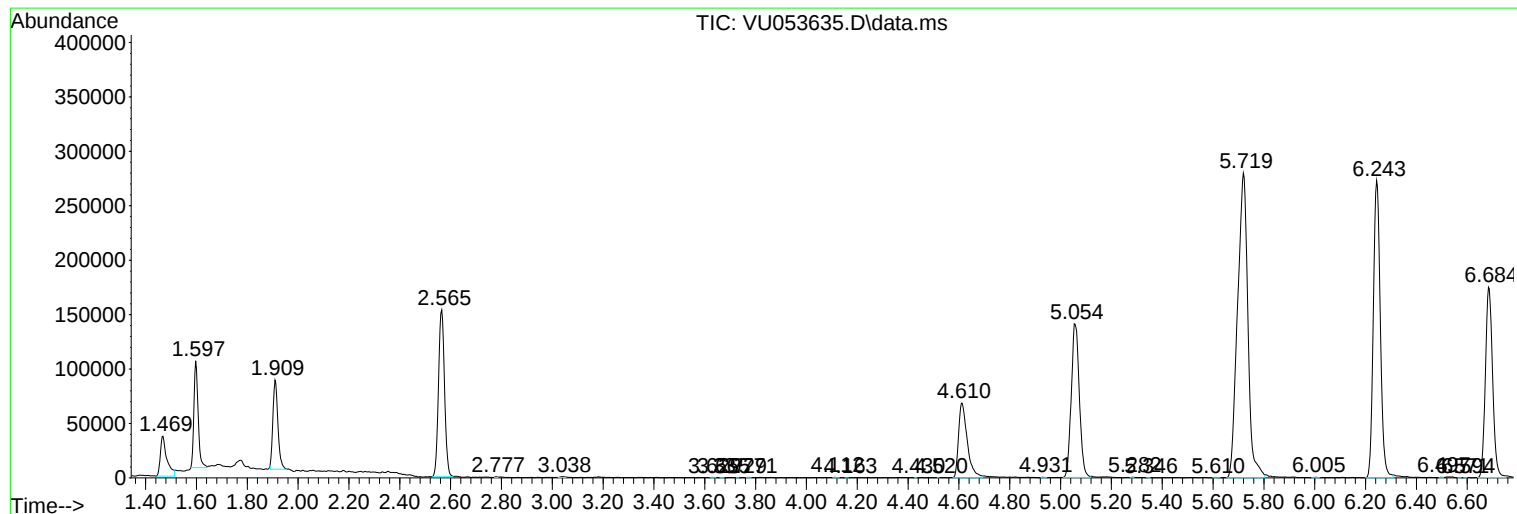
Sum of corrected areas: 6401714

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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MSVOA_U
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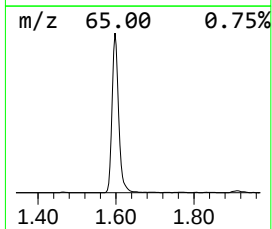
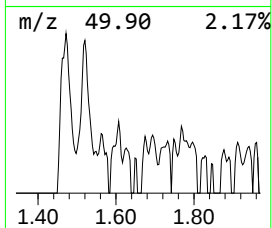
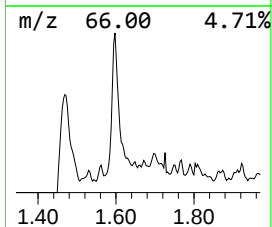
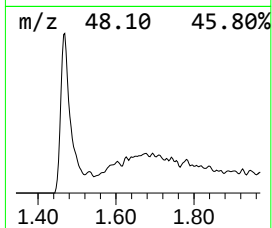
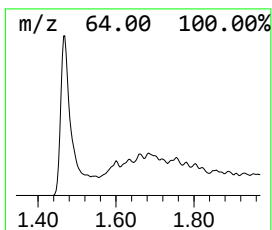
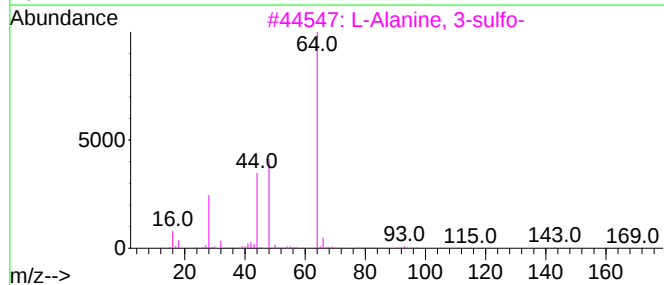
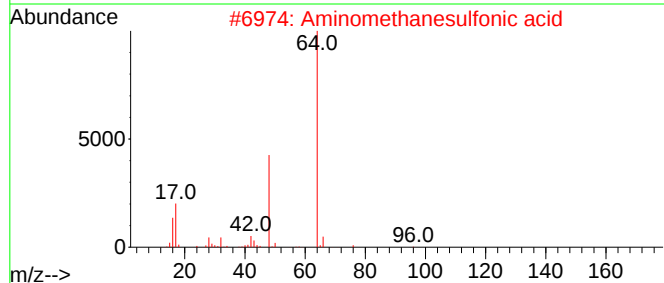
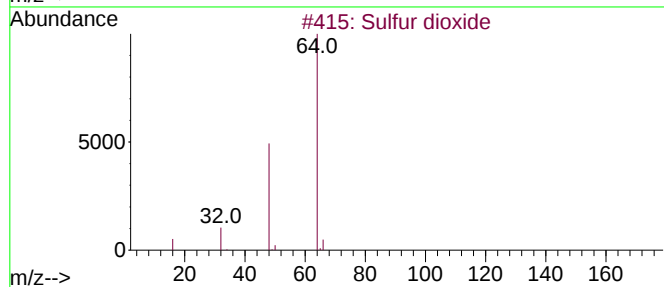
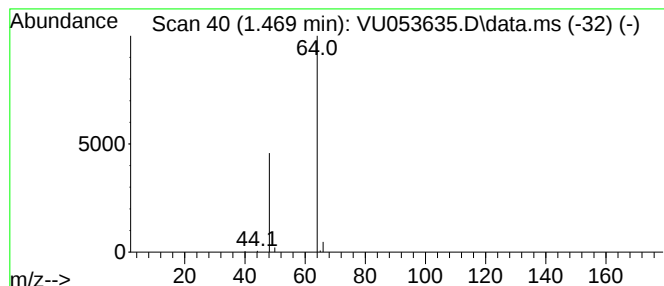
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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.
1.469	6.24 ug/L	64887	1,4-Difluorobenzene	6.243

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



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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	1.469	6.2	ug/L	64887	1	6.243	519861	50.0