

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
 Data File : VU053637.D
 Acq On : 11 Apr 2023 16:01
 Operator : JC/MD
 Sample : 02251-08DL 200X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COMC6DL

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: VU053637.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	33	40	52	rBV	17581	31540	1.86%	0.357%
2	1.597	74	80	96	rVB	97400	112250	6.60%	1.270%
3	1.909	170	177	196	rVB	80398	112904	6.64%	1.277%
4	2.565	369	381	397	rBV	154489	247748	14.58%	2.802%
5	2.777	445	447	449	rBV	447	267	0.02%	0.003%
6	3.041	518	529	550	rVB2	28961	55008	3.24%	0.622%
7	3.491	666	669	675	rVB	438	392	0.02%	0.004%
8	3.523	675	679	681	rBV2	280	203	0.01%	0.002%
9	3.617	705	708	709	rBV2	204	97	0.01%	0.001%
10	3.793	761	763	766	rVB	205	67	0.00%	0.001%
11	3.964	814	816	819	rVB2	211	117	0.01%	0.001%
12	4.067	845	848	852	rVB2	210	148	0.01%	0.002%
13	4.131	864	868	872	rBV2	270	261	0.02%	0.003%
14	4.289	914	917	919	rBV	214	123	0.01%	0.001%
15	4.414	950	956	959	rBV2	343	412	0.02%	0.005%
16	4.549	996	998	1000	rBV	155	79	0.00%	0.001%
17	4.565	1001	1003	1004	rBV	174	56	0.00%	0.001%
18	4.613	1005	1018	1049	rBV	66796	161447	9.50%	1.826%
19	4.983	1130	1133	1135	rBV2	337	152	0.01%	0.002%
20	5.057	1140	1156	1182	rBV2	146229	330797	19.46%	3.742%
21	5.211	1201	1204	1206	rBV2	302	178	0.01%	0.002%
22	5.298	1229	1231	1232	rBV2	115	53	0.00%	0.001%
23	5.327	1238	1240	1241	rBV2	256	83	0.00%	0.001%
24	5.340	1241	1244	1246	rBV2	169	116	0.01%	0.001%
25	5.391	1258	1260	1262	rBV	217	116	0.01%	0.001%
26	5.440	1273	1275	1277	rVB	230	63	0.00%	0.001%
27	5.465	1280	1283	1285	rBV	194	165	0.01%	0.002%
28	5.555	1307	1311	1313	rBV2	261	193	0.01%	0.002%
29	5.607	1325	1327	1330	rBV	294	137	0.01%	0.002%
30	5.719	1341	1362	1370	rBV2	278299	766771	45.11%	8.673%
31	5.999	1446	1449	1454	rVB2	302	229	0.01%	0.003%
32	6.108	1481	1483	1485	rVB	204	76	0.00%	0.001%
33	6.118	1485	1486	1488	rBV	351	111	0.01%	0.001%
34	6.160	1496	1499	1501	rBV	187	127	0.01%	0.001%
35	6.244	1511	1525	1551	rBV	288652	549037	32.30%	6.210%
36	6.530	1603	1614	1622	rVB3	2270	4240	0.25%	0.048%

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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	6.581	1625	1630	1632	rBV2	303	242	0.01%	0.003%
38	6.684	1649	1662	1684	rBV	173419	342197	20.13%	3.870%
39	6.842	1709	1711	1712	rBV	169	74	0.00%	0.001%
40	7.057	1776	1778	1780	rBV	157	90	0.01%	0.001%
41	7.186	1812	1818	1823	rBV3	913	1156	0.07%	0.013%
42	7.433	1892	1895	1899	rBV2	269	213	0.01%	0.002%
43	7.562	1923	1935	1954	rBV2	96036	170962	10.06%	1.934%
44	7.784	2001	2004	2009	rBV2	287	233	0.01%	0.003%
45	7.825	2014	2017	2021	rVB2	358	236	0.01%	0.003%
46	7.893	2025	2038	2056	rBV	360434	621936	36.59%	7.034%
47	8.173	2114	2125	2144	rBV2	67875	116136	6.83%	1.314%
48	8.311	2166	2168	2170	rBV	274	124	0.01%	0.001%
49	8.539	2236	2239	2240	rBV	220	152	0.01%	0.002%
50	8.552	2240	2243	2246	rVB	432	259	0.02%	0.003%
51	8.626	2255	2266	2297	rBV	199761	363859	21.41%	4.115%
52	8.874	2340	2343	2345	rBV	267	184	0.01%	0.002%
53	8.999	2378	2382	2385	rBV2	271	227	0.01%	0.003%
54	9.137	2422	2425	2427	rBV2	330	235	0.01%	0.003%
55	9.269	2462	2466	2467	rBV	184	130	0.01%	0.001%
56	9.359	2492	2494	2495	rBV	195	95	0.01%	0.001%
57	9.414	2498	2511	2514	rBV	422492	630792	37.11%	7.135%
58	9.658	2585	2587	2591	rBV2	355	291	0.02%	0.003%
59	10.012	2693	2697	2703	rBV2	335	306	0.02%	0.003%
60	10.105	2723	2726	2731	rBV2	339	309	0.02%	0.003%
61	10.128	2731	2733	2737	rBV	270	201	0.01%	0.002%
62	10.208	2756	2758	2760	rBV	172	99	0.01%	0.001%
63	10.394	2813	2816	2819	rVB	192	102	0.01%	0.001%
64	10.751	2915	2927	2948	rVB	261364	423277	24.90%	4.788%
65	11.279	3088	3091	3092	rBV	223	101	0.01%	0.001%
66	11.613	3192	3195	3196	rBV	273	150	0.01%	0.002%
67	11.742	3224	3235	3245	rBV	117602	184892	10.88%	2.091%
68	11.829	3245	3262	3286	rVB2	633462	1662075	97.79%	18.799%
69	12.205	3362	3379	3399	rBV2	758456	1699666	100.00%	19.224%
70	12.407	3440	3442	3448	rBV	216	234	0.01%	0.003%
71	12.452	3453	3456	3461	rBV	226	168	0.01%	0.002%
72	13.044	3638	3640	3643	rBV2	319	119	0.01%	0.001%
73	13.095	3653	3656	3657	rBV2	339	200	0.01%	0.002%
74	13.208	3686	3691	3698	rBV5	2153	2962	0.17%	0.034%
75	13.500	3779	3782	3783	rBV	327	204	0.01%	0.002%
76	13.536	3791	3793	3794	rBV	232	84	0.00%	0.001%

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Instrument :
MSVOA_U
ClientSampleId :
C0MC6DL

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	13.835	3875	3886	3903	rBV	105796	175777	10.34%	1.988%
78	13.918	3910	3912	3915	rVB2	372	187	0.01%	0.002%
79	13.938	3915	3918	3919	rBV	425	283	0.02%	0.003%
80	14.037	3946	3949	3952	rBV2	367	296	0.02%	0.003%
81	14.327	4029	4039	4050	rBV2	39757	63958	3.76%	0.723%

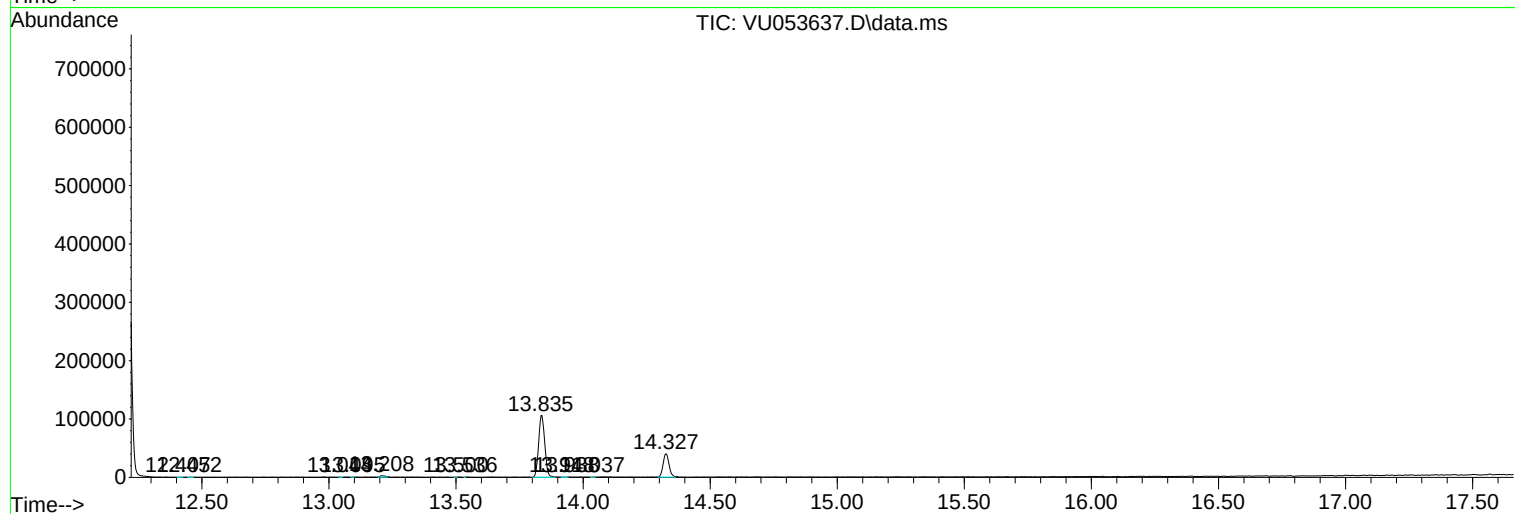
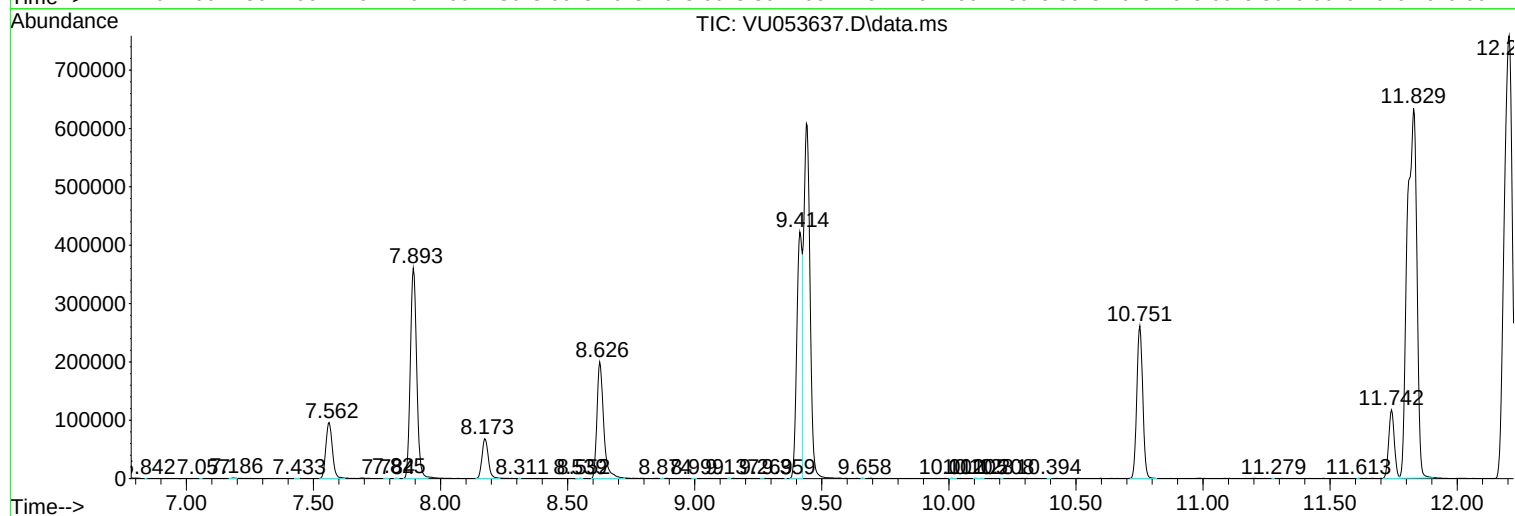
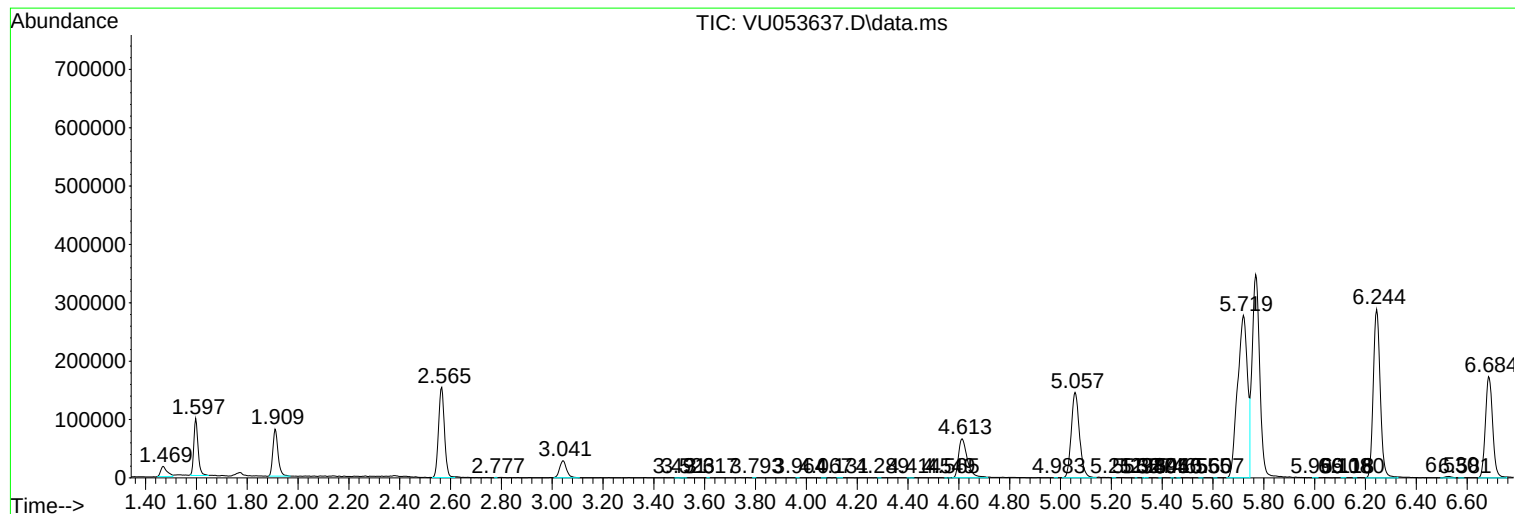
Sum of corrected areas: 8841236

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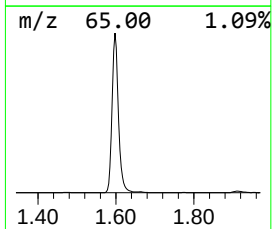
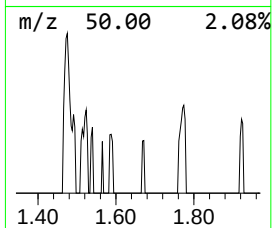
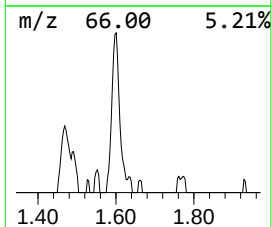
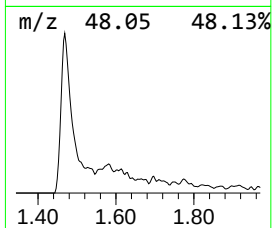
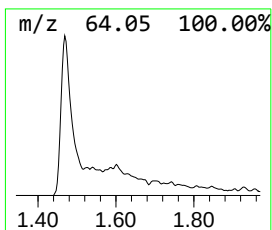
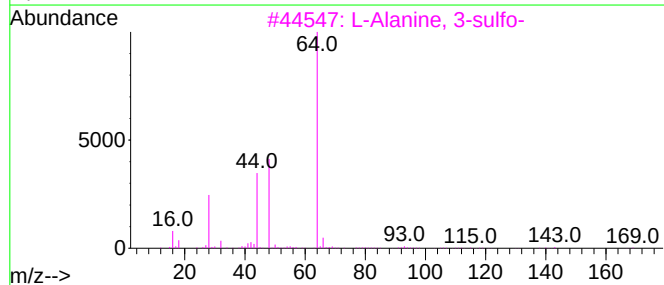
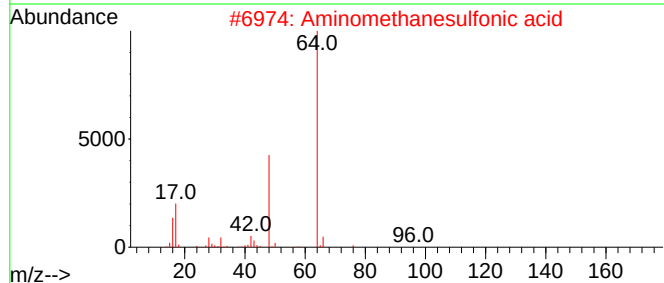
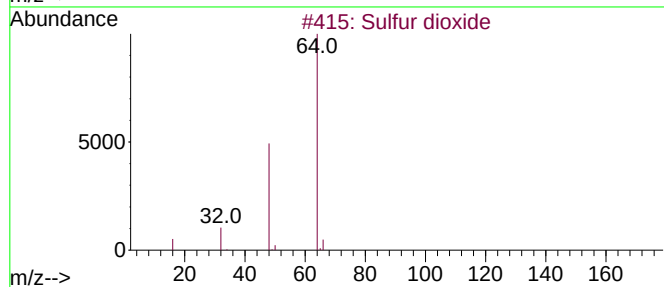
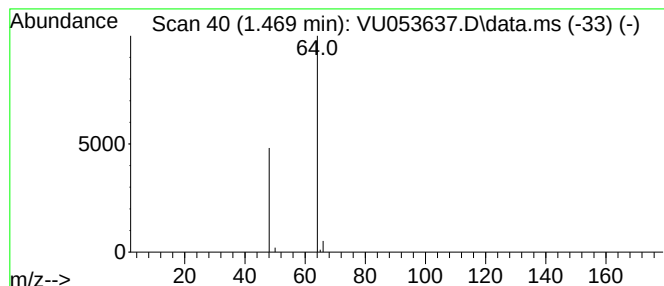
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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	2.87 ug/L	31540	1,4-Difluorobenzene	6.244

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			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	2.9	ug/L	31540	1	6.244	549037	50.0