

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061822\
 Data File : VU049280.D
 Acq On : 18 Jun 2022 14:48
 Operator : SY/MD
 Sample : VU0618WBL01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK143

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\SFAMULM061022WMA.M
 Title : VOC Analysis

Signal : TIC: VU049280.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.491	39	47	62	rBV3	14688	42332	3.94%	0.455%
2	1.597	73	80	91	rBV	132337	145459	13.54%	1.563%
3	1.909	170	177	192	rVB	103412	135062	12.57%	1.451%
4	2.565	369	381	397	rBV	212496	344095	32.02%	3.697%
5	2.793	446	452	460	rBV2	1354	1842	0.17%	0.020%
6	2.871	474	476	480	rBV2	283	241	0.02%	0.003%
7	2.990	510	513	515	rBV2	375	294	0.03%	0.003%
8	3.009	517	519	524	rVV2	523	406	0.04%	0.004%
9	3.047	527	531	537	rVB5	883	883	0.08%	0.009%
10	3.182	562	573	585	rBV3	1722	3627	0.34%	0.039%
11	3.350	620	625	627	rBV2	311	227	0.02%	0.002%
12	3.488	664	668	672	rBV2	213	227	0.02%	0.002%
13	3.594	693	701	704	rVB2	347	510	0.05%	0.005%
14	3.617	704	708	715	rBV3	460	716	0.07%	0.008%
15	3.996	822	826	827	rBV	300	229	0.02%	0.002%
16	4.144	863	872	875	rBV3	204	298	0.03%	0.003%
17	4.205	887	891	894	rVV2	285	249	0.02%	0.003%
18	4.440	960	964	968	rVB2	278	253	0.02%	0.003%
19	4.469	968	973	977	rBV3	233	290	0.03%	0.003%
20	4.623	1008	1021	1050	rBV	133908	337851	31.44%	3.630%
21	4.948	1119	1122	1128	rBV3	222	249	0.02%	0.003%
22	4.980	1128	1132	1137	rVB2	351	279	0.03%	0.003%
23	5.063	1141	1158	1181	rBV	195056	433797	40.37%	4.661%
24	5.182	1192	1195	1197	rBV3	636	433	0.04%	0.005%
25	5.195	1197	1199	1204	rVB3	457	325	0.03%	0.003%
26	5.295	1224	1230	1233	rVB4	408	464	0.04%	0.005%
27	5.372	1237	1254	1276	rBV	242809	501730	46.69%	5.390%
28	5.533	1301	1304	1309	rVV4	392	366	0.03%	0.004%
29	5.726	1339	1364	1397	rBV2	399230	1074512	100.00%	11.544%
30	5.845	1397	1401	1405	rVB2	419	381	0.04%	0.004%
31	5.919	1420	1424	1427	rBV3	423	313	0.03%	0.003%
32	5.944	1427	1432	1435	rVV4	379	419	0.04%	0.005%
33	5.983	1440	1444	1447	rBV3	516	420	0.04%	0.005%
34	6.247	1512	1526	1552	rBV	365059	695011	64.68%	7.467%
35	6.359	1558	1561	1567	rVB3	435	326	0.03%	0.004%
36	6.440	1583	1586	1591	rBV3	377	283	0.03%	0.003%

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 Title : VOC Analysis

37	6.520	1606	1611	1613	rBV2	1479	1314	0.12%	0.014%
38	6.626	1641	1644	1647	rBV3	295	244	0.02%	0.003%
39	6.690	1650	1664	1686	rBV	263989	513362	47.78%	5.515%
40	6.803	1693	1699	1707	rBV5	628	1114	0.10%	0.012%
41	7.099	1786	1791	1798	rVV2	524	654	0.06%	0.007%
42	7.134	1799	1802	1810	rVV2	542	516	0.05%	0.006%
43	7.185	1810	1818	1830	rVV4	1706	2966	0.28%	0.032%
44	7.292	1848	1851	1855	rVB	464	379	0.04%	0.004%
45	7.565	1924	1936	1954	rBV	145168	253457	23.59%	2.723%
46	7.690	1968	1975	1985	rVB4	1162	1963	0.18%	0.021%
47	7.751	1990	1994	1997	rBV2	322	324	0.03%	0.003%
48	7.787	2000	2005	2008	rBV2	753	730	0.07%	0.008%
49	7.896	2026	2039	2061	rBV	486869	855597	79.63%	9.192%
50	8.063	2089	2091	2099	rVB3	337	255	0.02%	0.003%
51	8.179	2111	2127	2150	rBV	98543	170464	15.86%	1.831%
52	8.465	2213	2216	2218	rBV2	348	252	0.02%	0.003%
53	8.632	2255	2268	2315	rBV	400079	739680	68.84%	7.947%
54	9.176	2435	2437	2440	rVB	558	298	0.03%	0.003%
55	9.195	2440	2443	2447	rBV2	396	345	0.03%	0.004%
56	9.218	2447	2450	2455	rVB3	315	271	0.03%	0.003%
57	9.301	2470	2476	2479	rBV2	290	339	0.03%	0.004%
58	9.417	2498	2512	2538	rBV	504673	836149	77.82%	8.983%
59	9.571	2555	2560	2564	rVB3	702	671	0.06%	0.007%
60	9.661	2586	2588	2594	rVB	778	575	0.05%	0.006%
61	9.693	2594	2598	2602	rBV2	612	590	0.05%	0.006%
62	9.751	2611	2616	2618	rBV2	364	278	0.03%	0.003%
63	9.796	2623	2630	2633	rVB3	264	309	0.03%	0.003%
64	10.115	2726	2729	2737	rVB5	983	938	0.09%	0.010%
65	10.192	2748	2753	2755	rBV	272	235	0.02%	0.003%
66	10.754	2915	2928	2949	rVV	363650	587312	54.66%	6.310%
67	10.832	2949	2952	2955	rVV	551	403	0.04%	0.004%
68	10.861	2959	2961	2964	rVV2	433	262	0.02%	0.003%
69	10.996	2995	3003	3008	rVB3	322	518	0.05%	0.006%
70	11.095	3024	3034	3039	rBV3	642	866	0.08%	0.009%
71	11.147	3044	3050	3053	rBV2	354	324	0.03%	0.003%
72	11.172	3055	3058	3062	rVB	346	250	0.02%	0.003%
73	11.356	3112	3115	3120	rVB2	361	278	0.03%	0.003%
74	11.404	3125	3130	3135	rVB3	371	388	0.04%	0.004%
75	11.443	3138	3142	3146	rBV4	270	229	0.02%	0.002%
76	11.475	3147	3152	3156	rBV4	605	605	0.06%	0.006%

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 Title : VOC Analysis

77	11.517	3162	3165	3172	rVB3	273	309	0.03%	0.003%
78	11.690	3214	3219	3223	rVB3	454	540	0.05%	0.006%
79	11.716	3223	3227	3231	rBV2	291	303	0.03%	0.003%
80	11.748	3231	3237	3240	rBV3	1380	1482	0.14%	0.016%
81	11.812	3244	3257	3273	rBV	486937	777116	72.32%	8.349%
82	12.150	3359	3362	3363	rBV2	355	231	0.02%	0.002%
83	12.192	3363	3375	3395	rVV	482994	780176	72.61%	8.382%
84	12.430	3444	3449	3453	rBV3	231	234	0.02%	0.003%
85	12.774	3551	3556	3563	rVV3	401	515	0.05%	0.006%
86	12.967	3613	3616	3619	rBV2	453	324	0.03%	0.003%
87	13.224	3690	3696	3703	rVB3	2086	2275	0.21%	0.024%
88	13.671	3830	3835	3841	rBV3	310	426	0.04%	0.005%
89	13.844	3881	3889	3898	rBV6	4608	6298	0.59%	0.068%
90	14.089	3955	3965	3984	rBV	15132	25514	2.37%	0.274%
91	14.282	4022	4025	4032	rBV3	294	332	0.03%	0.004%
92	14.330	4032	4040	4051	rVV4	5513	8270	0.77%	0.089%
93	14.404	4060	4063	4067	rBV2	289	280	0.03%	0.003%
94	14.635	4131	4135	4139	rBV3	409	488	0.05%	0.005%
95	14.889	4211	4214	4220	rBV2	320	341	0.03%	0.004%
96	15.021	4250	4255	4257	rBV2	501	430	0.04%	0.005%
97	15.237	4319	4322	4324	rBV	460	289	0.03%	0.003%
98	15.555	4419	4421	4425	rBV2	602	378	0.04%	0.004%
99	16.073	4577	4582	4584	rBV4	864	831	0.08%	0.009%
100	16.449	4696	4699	4701	rBV3	762	409	0.04%	0.004%

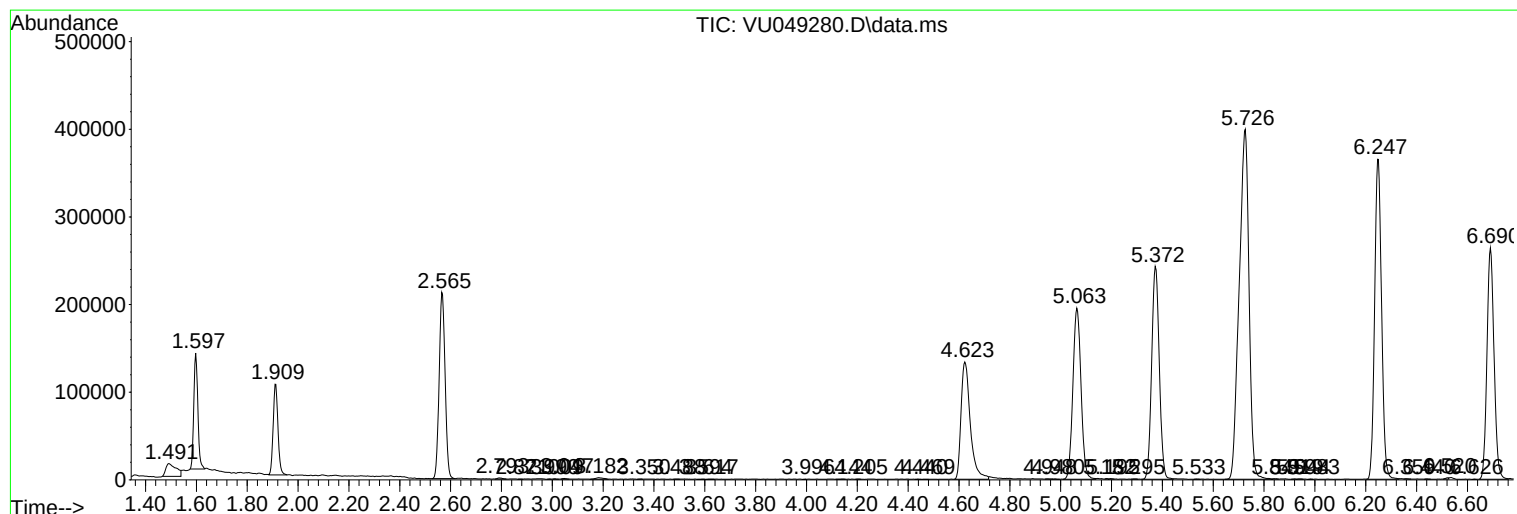
Sum of corrected areas: 9307894

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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



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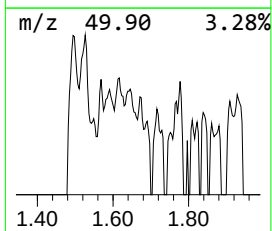
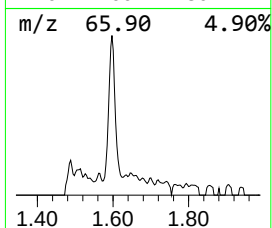
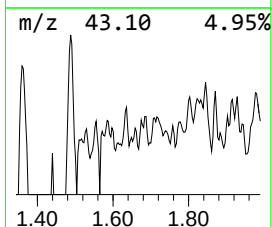
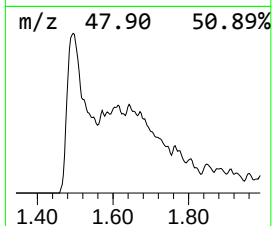
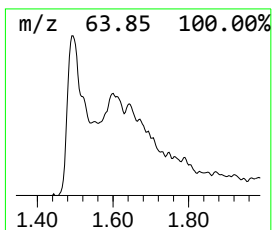
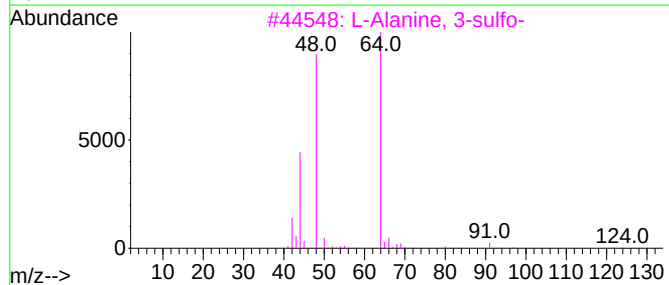
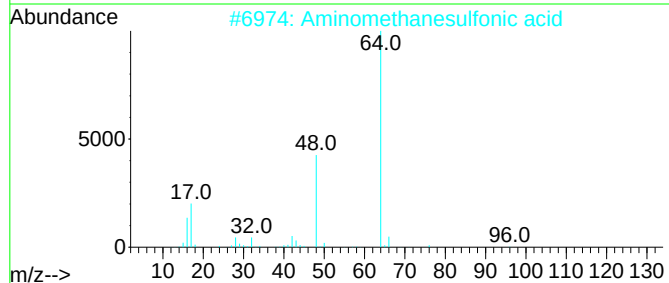
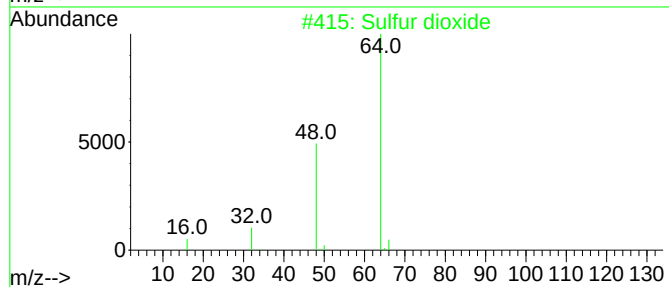
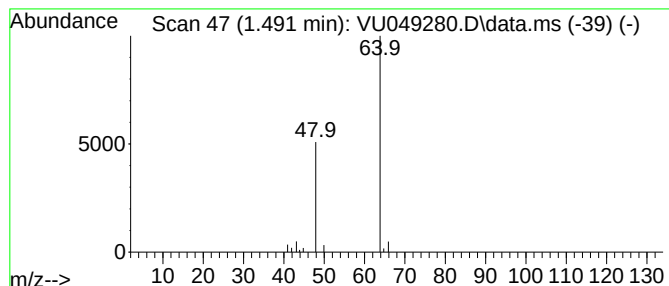
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM061022WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.491	3.05 ug/L	42332	1,4-Difluorobenzene	6.250

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	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	64
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.491	3.0	ug/L	42332	1	6.250	695011	50.0