

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050489.D
 Acq On : 29 Aug 2022 17:11
 Operator : SY/MD
 Sample : N4399-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVA3

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\SFAMULM082422WMA.M

Title : VOC Analysis

Signal : TIC: VU050489.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.372	6	10	31	rVB2	6502	11768	0.77%	0.109%
2	1.684	102	107	119	rVB	8196	10351	0.67%	0.096%
3	1.903	168	175	197	rVB	149741	204514	13.31%	1.900%
4	2.562	368	380	394	rBV	59374	94833	6.17%	0.881%
5	2.639	394	404	421	rVV2	13955	27358	1.78%	0.254%
6	2.874	473	477	480	rBV2	475	404	0.03%	0.004%
7	2.960	501	504	507	rBV	384	286	0.02%	0.003%
8	3.006	514	518	522	rBV2	377	329	0.02%	0.003%
9	3.041	522	529	541	rVB5	1492	2742	0.18%	0.025%
10	3.115	549	552	555	rBV2	238	191	0.01%	0.002%
11	3.176	565	571	576	rBV3	469	739	0.05%	0.007%
12	3.385	632	636	639	rVB2	366	227	0.01%	0.002%
13	3.584	691	698	708	rVV5	1031	1950	0.13%	0.018%
14	3.652	712	719	723	rBV2	321	282	0.02%	0.003%
15	3.903	794	797	802	rVV2	179	159	0.01%	0.001%
16	4.099	852	858	866	rBV2	251	294	0.02%	0.003%
17	4.147	870	873	881	rVV2	207	209	0.01%	0.002%
18	4.276	909	913	917	rBV2	540	608	0.04%	0.006%
19	4.378	939	945	949	rVB	267	285	0.02%	0.003%
20	4.462	967	971	975	rBV3	298	256	0.02%	0.002%
21	4.629	1000	1023	1067	rBV	152727	438634	28.54%	4.075%
22	5.063	1140	1158	1184	rBV	266926	589421	38.35%	5.476%
23	5.292	1222	1229	1237	rBV3	1306	1601	0.10%	0.015%
24	5.369	1248	1253	1256	rBV3	742	792	0.05%	0.007%
25	5.726	1342	1364	1395	rBV2	532774	1450193	94.36%	13.473%
26	5.976	1435	1442	1457	rVB5	970	1613	0.10%	0.015%
27	6.054	1460	1466	1469	rBV2	159	200	0.01%	0.002%
28	6.121	1481	1487	1490	rBV2	340	422	0.03%	0.004%
29	6.166	1497	1501	1503	rBV	505	347	0.02%	0.003%
30	6.250	1513	1527	1550	rBV	364282	696156	45.30%	6.468%
31	6.388	1568	1570	1574	rBV5	295	162	0.01%	0.002%
32	6.523	1606	1612	1613	rBV5	904	807	0.05%	0.007%
33	6.587	1628	1632	1638	rVB3	268	238	0.02%	0.002%
34	6.690	1649	1664	1685	rBV	350153	680916	44.31%	6.326%
35	6.819	1701	1704	1707	rVB2	540	325	0.02%	0.003%
36	6.886	1719	1725	1730	rBV4	1294	1792	0.12%	0.017%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

37	6.992	1753	1758	1763	rBV2	324	485	0.03%	0.005%
38	7.018	1763	1766	1771	rVV2	168	187	0.01%	0.002%
39	7.073	1779	1783	1787	rBV2	382	382	0.02%	0.004%
40	7.163	1806	1811	1814	rBV4	304	300	0.02%	0.003%
41	7.436	1892	1896	1899	rBV2	275	267	0.02%	0.002%
42	7.491	1910	1913	1916	rBV	272	212	0.01%	0.002%
43	7.578	1932	1940	1946	rVB2	477	559	0.04%	0.005%
44	7.613	1946	1951	1954	rBV	444	270	0.02%	0.003%
45	7.655	1961	1964	1970	rVB2	214	187	0.01%	0.002%
46	7.800	2001	2009	2013	rBV4	999	1279	0.08%	0.012%
47	7.899	2025	2040	2062	rBV	465586	815817	53.08%	7.580%
48	8.073	2092	2094	2100	rVB2	336	332	0.02%	0.003%
49	8.195	2129	2132	2137	rBV2	272	258	0.02%	0.002%
50	8.230	2137	2143	2146	rBV2	229	260	0.02%	0.002%
51	8.253	2146	2150	2159	rBV2	354	580	0.04%	0.005%
52	8.478	2214	2220	2222	rBV4	381	335	0.02%	0.003%
53	8.491	2222	2224	2228	rVB	404	193	0.01%	0.002%
54	8.552	2229	2243	2258	rBV	905485	1536848	100.00%	14.278%
55	8.639	2259	2270	2308	rVB2	389764	857882	55.82%	7.970%
56	8.896	2346	2350	2351	rBV2	345	205	0.01%	0.002%
57	8.989	2377	2379	2384	rVB2	381	342	0.02%	0.003%
58	9.015	2384	2387	2389	rBV2	317	236	0.02%	0.002%
59	9.082	2405	2408	2416	rVB	245	269	0.02%	0.002%
60	9.166	2429	2434	2439	rBV3	261	277	0.02%	0.003%
61	9.227	2450	2453	2455	rBV	290	172	0.01%	0.002%
62	9.269	2462	2466	2470	rVB2	421	284	0.02%	0.003%
63	9.317	2478	2481	2485	rVV2	193	177	0.01%	0.002%
64	9.417	2499	2512	2540	rBV	514091	868761	56.53%	8.071%
65	9.533	2544	2548	2555	rVB5	3044	4066	0.26%	0.038%
66	9.658	2583	2587	2592	rVV3	287	318	0.02%	0.003%
67	9.722	2601	2607	2615	rBV3	1671	2047	0.13%	0.019%
68	9.819	2635	2637	2641	rBV2	207	176	0.01%	0.002%
69	9.979	2683	2687	2692	rBV2	219	284	0.02%	0.003%
70	10.060	2709	2712	2715	rBV	312	198	0.01%	0.002%
71	10.098	2720	2724	2728	rBV	239	217	0.01%	0.002%
72	10.143	2731	2738	2742	rBV2	777	823	0.05%	0.008%
73	10.217	2757	2761	2763	rBV2	217	172	0.01%	0.002%
74	10.291	2772	2784	2796	rBV	43279	72918	4.74%	0.677%
75	10.349	2796	2802	2812	rVB4	6345	9748	0.63%	0.091%
76	10.397	2812	2817	2820	rBV2	201	209	0.01%	0.002%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

77	10.443	2827	2831	2834	rBV2	187	168	0.01%	0.002%
78	10.610	2880	2883	2887	rBV2	172	176	0.01%	0.002%
79	10.758	2916	2929	2947	rBV	506488	827413	53.84%	7.687%
80	10.906	2968	2975	2978	rBV4	1851	2116	0.14%	0.020%
81	11.018	3007	3010	3014	rVB	347	200	0.01%	0.002%
82	11.053	3016	3021	3025	rBV	648	716	0.05%	0.007%
83	11.314	3098	3102	3104	rBV2	421	248	0.02%	0.002%
84	11.487	3145	3156	3164	rBV4	1055	2297	0.15%	0.021%
85	11.696	3213	3221	3231	rVB5	2331	2922	0.19%	0.027%
86	11.812	3244	3257	3279	rBV	382749	620654	40.38%	5.766%
87	12.066	3327	3336	3338	rBV4	3541	3834	0.25%	0.036%
88	12.114	3343	3351	3363	rVB2	24803	39647	2.58%	0.368%
89	12.195	3363	3376	3406	rBV	480558	856499	55.73%	7.957%
90	12.430	3445	3449	3451	rBV2	443	316	0.02%	0.003%
91	12.542	3480	3484	3487	rBV2	489	401	0.03%	0.004%
92	12.616	3503	3507	3509	rBV3	338	237	0.02%	0.002%
93	12.706	3532	3535	3537	rVB2	332	180	0.01%	0.002%
94	12.725	3537	3541	3543	rBV	303	240	0.02%	0.002%
95	12.751	3546	3549	3554	rVB3	376	283	0.02%	0.003%
96	12.815	3566	3569	3572	rBV2	446	341	0.02%	0.003%
97	12.896	3586	3594	3601	rBV4	2393	3186	0.21%	0.030%
98	13.249	3701	3704	3708	rBV	801	694	0.05%	0.006%
99	13.352	3734	3736	3738	rVB	352	169	0.01%	0.002%
100	14.108	3966	3971	3975	rBV4	439	554	0.04%	0.005%

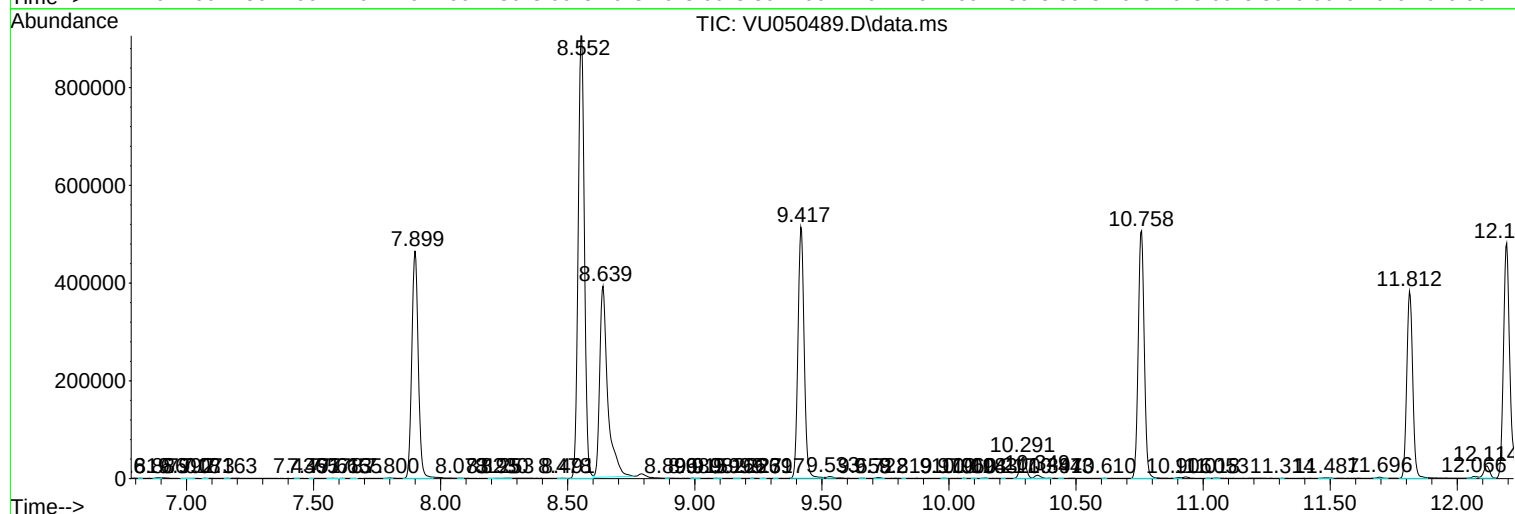
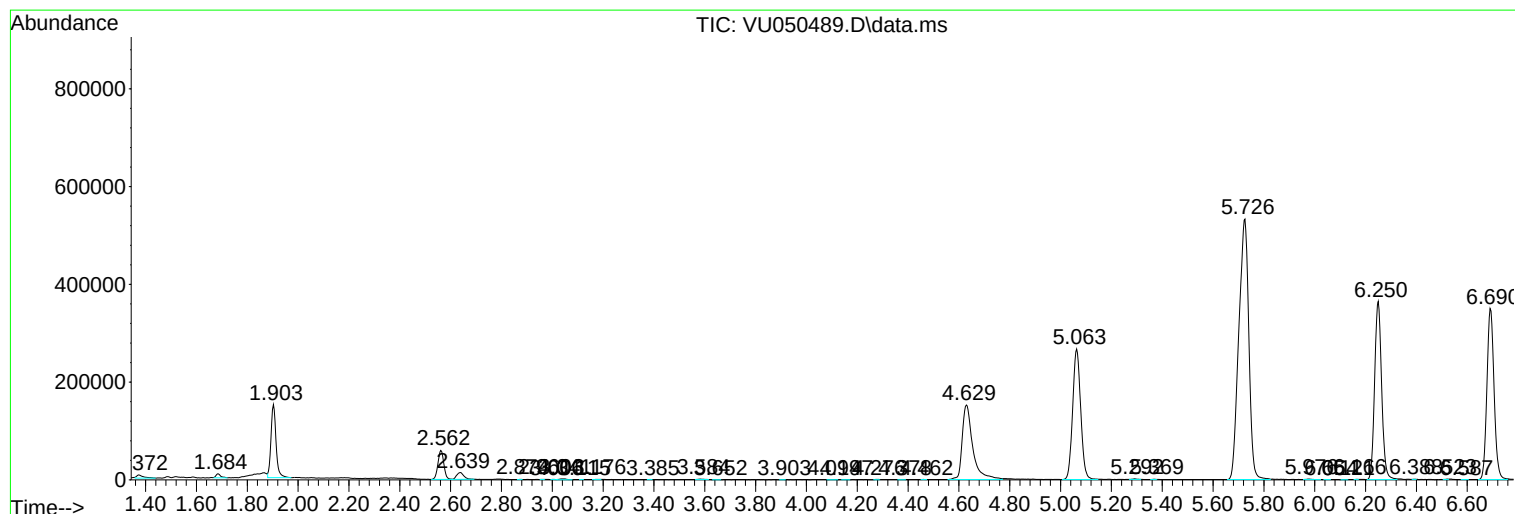
Sum of corrected areas: 10763427

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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



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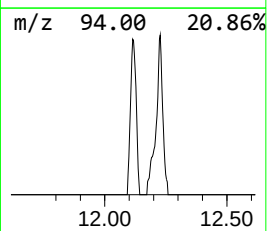
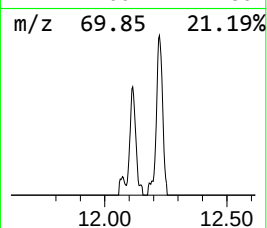
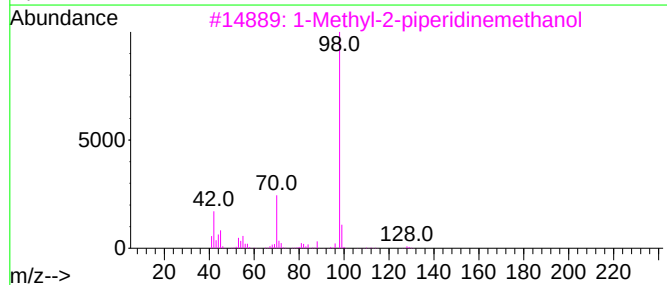
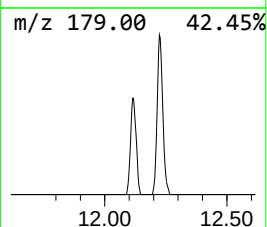
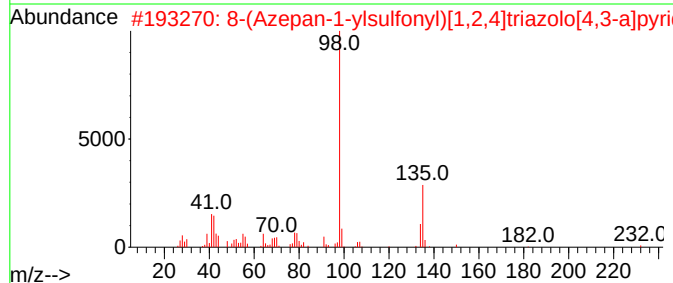
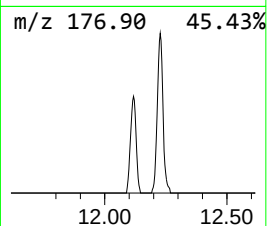
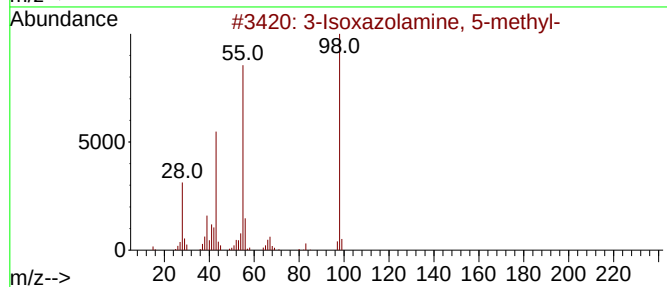
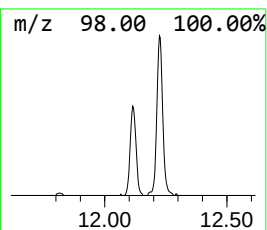
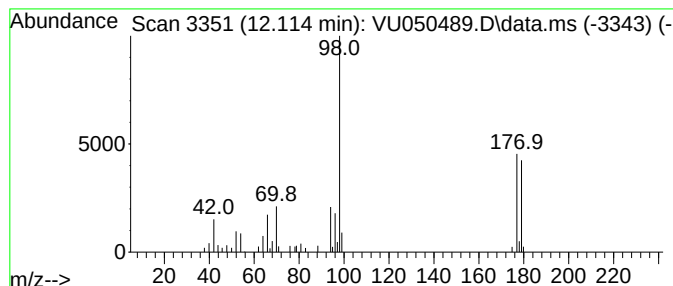
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.115	3.19 ug/L	39647	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Isloxazolamine, 5-methyl-		98	C4H6N2O	001072-67-9	27	
2	8-(Azepan-1-ylsulfonyl)[1,2,4]tr...		296	C12H16N4O3S	1291486-98-0	27	
3	1-Methyl-2-piperidinemethanol		129	C7H15NO	020845-34-5	25	
4	N-Methyl-1-(1-methylpiperidin-2-...		142	C8H18N2	1000484-42-5	25	
5	Benzen-d5-amine		98	C6H2D5N	004165-61-1	23	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	12.115	3.2	ug/L	39647	3	11.812	620654	50.0