

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV041621\
 Data File : VV021044.D
 Acq On : 16 Apr 2021 13:51
 Operator : SY/MD
 Sample : M2067-02
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG599

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\SFAMVLM041421WMA.M

Title : VOC Analysis

Signal : TIC: VV021044.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	78	83	99	rVB	150296	167197	10.77%	1.296%
2	1.571	158	165	182	rVB	130352	160113	10.32%	1.241%
3	2.108	323	332	349	rVB	338175	486653	31.36%	3.772%
4	2.404	421	424	428	rVB2	480	308	0.02%	0.002%
5	2.519	452	460	467	rBV6	1412	2185	0.14%	0.017%
6	2.577	473	478	481	rBV3	592	354	0.02%	0.003%
7	2.622	483	492	496	rBV4	2810	4290	0.28%	0.033%
8	2.770	527	538	543	rBV6	2177	2928	0.19%	0.023%
9	2.899	574	578	580	rBV	314	278	0.02%	0.002%
10	2.931	585	588	593	rVB2	251	266	0.02%	0.002%
11	2.976	594	602	608	rBV3	932	1360	0.09%	0.011%
12	3.050	615	625	635	rBV7	4474	9390	0.61%	0.073%
13	3.127	646	649	654	rVB2	459	327	0.02%	0.003%
14	3.191	666	669	673	rBV	478	415	0.03%	0.003%
15	3.217	673	677	678	rBV	482	286	0.02%	0.002%
16	3.394	729	732	735	rVV2	342	280	0.02%	0.002%
17	3.494	758	763	765	rBV2	593	488	0.03%	0.004%
18	3.545	776	779	786	rBV2	450	619	0.04%	0.005%
19	3.770	838	849	863	rBV7	5216	11458	0.74%	0.089%
20	3.863	871	878	880	rBV2	429	366	0.02%	0.003%
21	3.915	881	894	930	rBV	70456	283638	18.28%	2.198%
22	4.355	1014	1031	1063	rBV2	271418	683457	44.04%	5.297%
23	4.535	1082	1087	1093	rVB4	922	927	0.06%	0.007%
24	4.648	1120	1122	1124	rBV2	735	477	0.03%	0.004%
25	4.744	1146	1152	1157	rVB4	629	915	0.06%	0.007%
26	4.776	1157	1162	1167	rBV3	479	508	0.03%	0.004%
27	4.818	1172	1175	1179	rBV2	420	380	0.02%	0.003%
28	4.889	1193	1197	1202	rVB2	376	343	0.02%	0.003%
29	5.050	1231	1247	1275	rBV2	605708	1551761	100.00%	12.027%
30	5.432	1364	1366	1368	rBV	562	303	0.02%	0.002%
31	5.490	1378	1384	1386	rBV4	793	701	0.05%	0.005%
32	5.622	1413	1425	1450	rBV	513400	1024531	66.02%	7.941%
33	5.828	1486	1489	1492	rBV2	632	470	0.03%	0.004%
34	5.921	1510	1518	1528	rVB7	2228	3866	0.25%	0.030%
35	6.002	1536	1543	1545	rBV3	829	717	0.05%	0.006%
36	6.075	1549	1566	1595	rBV	338714	684566	44.12%	5.306%

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 Title : VOC Analysis

37	6.346	1645	1650	1654	rBV4	830	628	0.04%	0.005%
38	6.397	1661	1666	1668	rBV3	733	508	0.03%	0.004%
39	6.436	1676	1678	1679	rBV	547	263	0.02%	0.002%
40	6.677	1751	1753	1757	rVB2	691	365	0.02%	0.003%
41	6.744	1769	1774	1775	rBV2	421	280	0.02%	0.002%
42	6.770	1779	1782	1788	rVB3	493	516	0.03%	0.004%
43	6.796	1788	1790	1795	rBV2	395	358	0.02%	0.003%
44	6.992	1840	1851	1873	rBV	197015	359717	23.18%	2.788%
45	7.320	1941	1953	1973	rBV	725960	1266783	81.64%	9.818%
46	7.625	2038	2048	2076	rBV2	143493	251107	16.18%	1.946%
47	7.789	2097	2099	2104	rVB4	910	518	0.03%	0.004%
48	7.825	2107	2110	2114	rVB3	797	527	0.03%	0.004%
49	7.944	2132	2147	2163	rBV	108889	205835	13.26%	1.595%
50	8.046	2176	2179	2181	rBV2	423	266	0.02%	0.002%
51	8.095	2184	2194	2222	rBV	366470	650458	41.92%	5.041%
52	8.336	2266	2269	2272	rBV2	921	630	0.04%	0.005%
53	8.522	2320	2327	2329	rBV	542	595	0.04%	0.005%
54	8.583	2343	2346	2349	rVB	752	471	0.03%	0.004%
55	8.603	2349	2352	2355	rBV	468	350	0.02%	0.003%
56	8.638	2360	2363	2371	rVB3	909	742	0.05%	0.006%
57	8.673	2371	2374	2378	rBV2	477	363	0.02%	0.003%
58	8.857	2419	2431	2460	rBV	778597	1260795	81.25%	9.772%
59	9.056	2491	2493	2496	rVB2	763	400	0.03%	0.003%
60	9.152	2518	2523	2525	rBV3	1888	1488	0.10%	0.012%
61	9.230	2544	2547	2552	rBV2	584	623	0.04%	0.005%
62	9.304	2566	2570	2575	rVB2	490	499	0.03%	0.004%
63	9.336	2575	2580	2582	rBV2	364	364	0.02%	0.003%
64	9.445	2610	2614	2616	rBV2	418	351	0.02%	0.003%
65	9.551	2644	2647	2652	rBV2	631	614	0.04%	0.005%
66	9.689	2686	2690	2692	rBV	461	379	0.02%	0.003%
67	9.744	2703	2707	2710	rBV4	431	404	0.03%	0.003%
68	10.133	2820	2828	2836	rBV4	3229	4506	0.29%	0.035%
69	10.220	2844	2855	2873	rBV	550842	860494	55.45%	6.669%
70	10.323	2885	2887	2894	rVB	579	553	0.04%	0.004%
71	10.387	2894	2907	2922	rVB	182392	311553	20.08%	2.415%
72	10.461	2927	2930	2933	rVB2	812	469	0.03%	0.004%
73	10.487	2933	2938	2946	rBV2	551	567	0.04%	0.004%
74	10.561	2954	2961	2966	rBV3	816	1079	0.07%	0.008%
75	10.587	2966	2969	2972	rBV3	858	623	0.04%	0.005%
76	10.657	2989	2991	2995	rBV3	555	357	0.02%	0.003%

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 Title : VOC Analysis

77	10.776	3022	3028	3030	rBV2	431	447	0.03%	0.003%
78	10.808	3035	3038	3044	rVB3	606	563	0.04%	0.004%
79	10.860	3051	3054	3055	rBV	785	397	0.03%	0.003%
80	10.921	3067	3073	3075	rBV4	2938	3311	0.21%	0.026%
81	11.082	3120	3123	3128	rVB2	501	352	0.02%	0.003%
82	11.104	3128	3130	3133	rBV	438	275	0.02%	0.002%
83	11.146	3139	3143	3144	rBV2	1292	978	0.06%	0.008%
84	11.255	3165	3177	3196	rBV	762027	1204450	77.62%	9.335%
85	11.429	3228	3231	3240	rVB5	2267	2476	0.16%	0.019%
86	11.464	3240	3242	3244	rBV2	493	298	0.02%	0.002%
87	11.513	3255	3257	3262	rBV3	654	467	0.03%	0.004%
88	11.632	3282	3294	3311	rBV	828808	1288483	83.03%	9.987%
89	11.828	3352	3355	3359	rVB3	863	634	0.04%	0.005%
90	11.850	3359	3362	3365	rBV	620	524	0.03%	0.004%
91	11.937	3387	3389	3391	rBV	486	338	0.02%	0.003%
92	12.024	3412	3416	3422	rVB	937	773	0.05%	0.006%
93	12.056	3422	3426	3430	rBV	629	651	0.04%	0.005%
94	12.258	3478	3489	3501	rVB2	71871	114313	7.37%	0.886%
95	12.541	3576	3577	3582	rVB2	564	277	0.02%	0.002%
96	12.657	3611	3613	3615	rBV	622	299	0.02%	0.002%
97	12.873	3677	3680	3684	rBV2	491	352	0.02%	0.003%
98	13.072	3740	3742	3745	rVB	638	318	0.02%	0.002%
99	13.455	3858	3861	3862	rBV	589	320	0.02%	0.002%
100	14.046	4034	4045	4052	rBV3	3550	6296	0.41%	0.049%

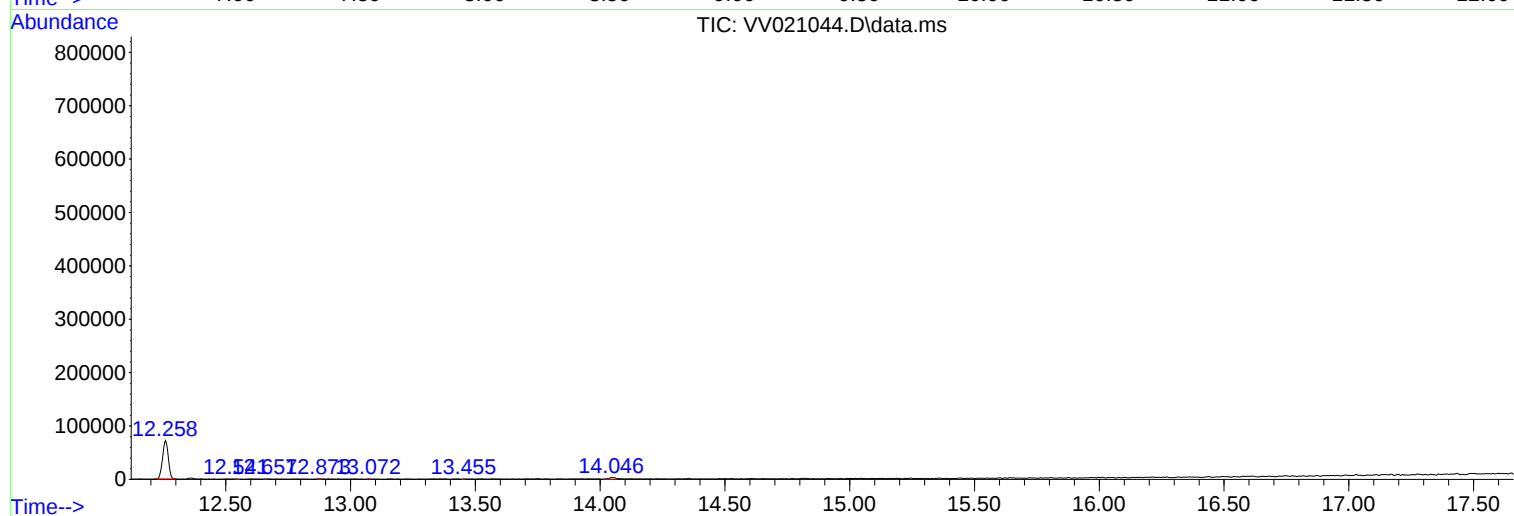
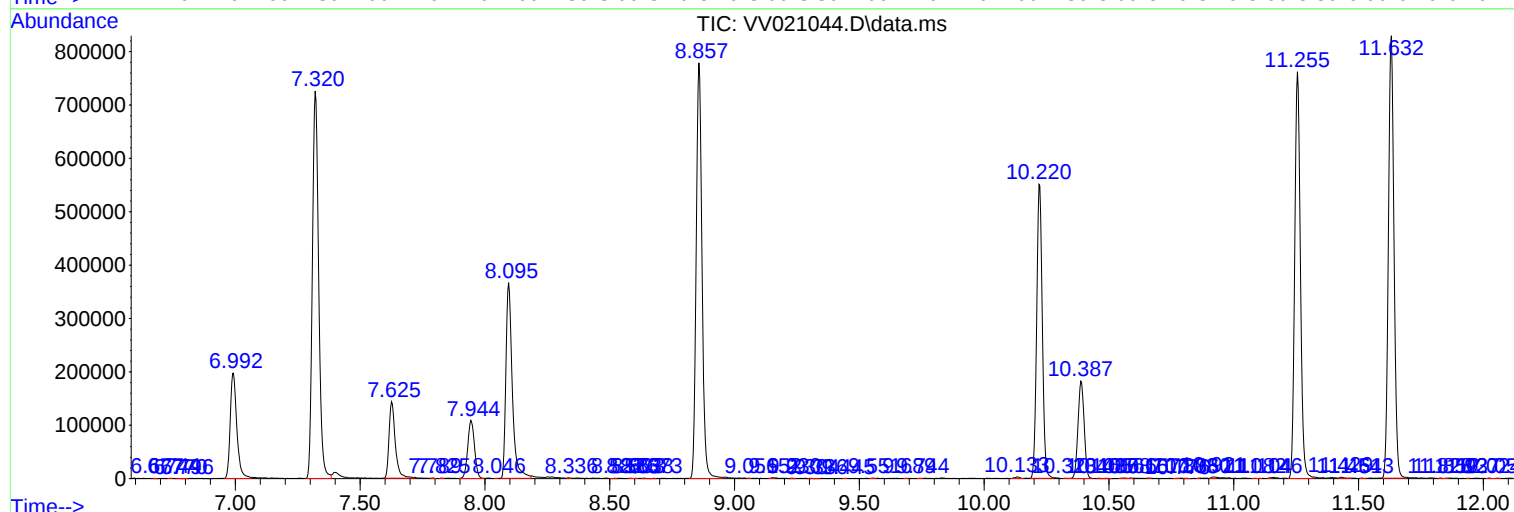
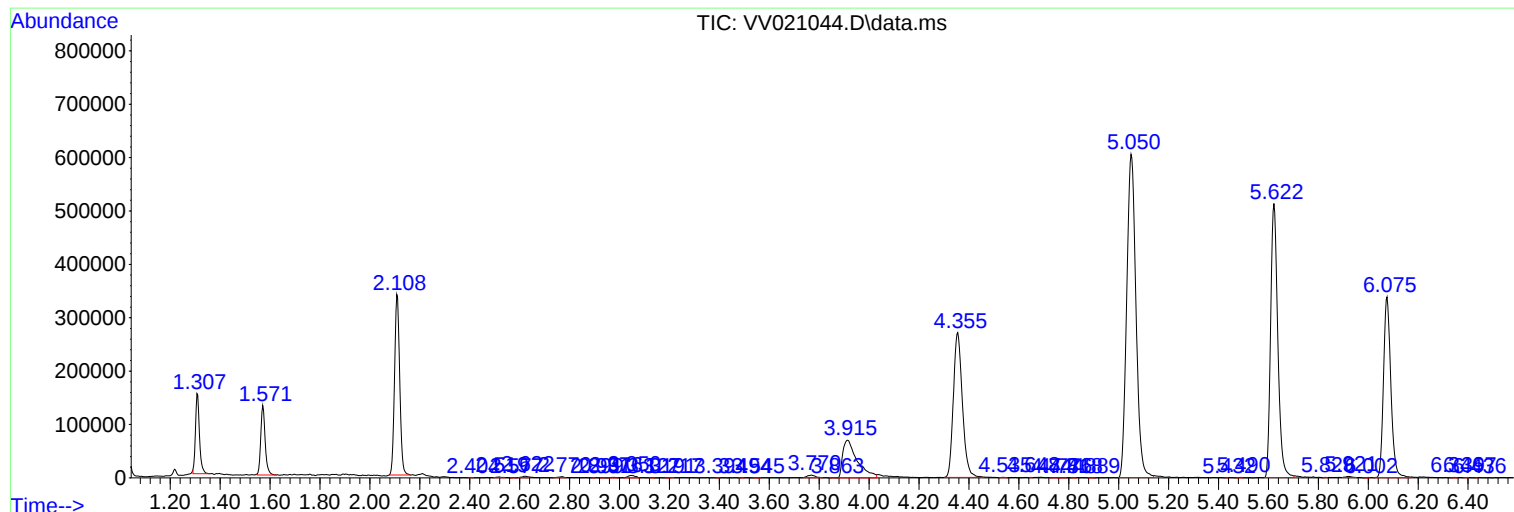
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041421WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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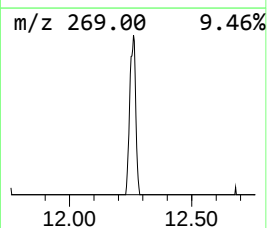
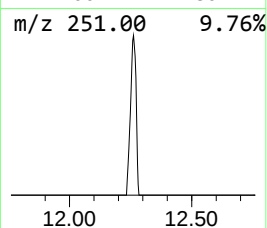
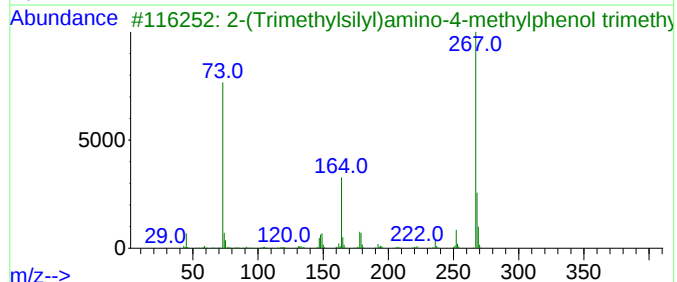
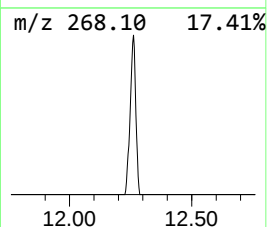
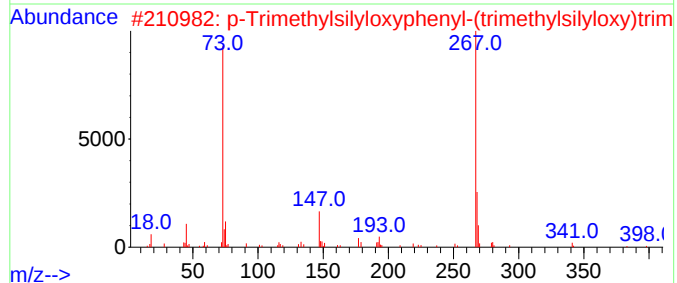
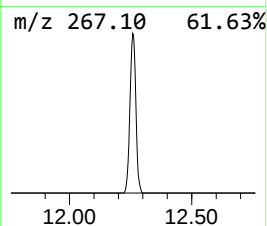
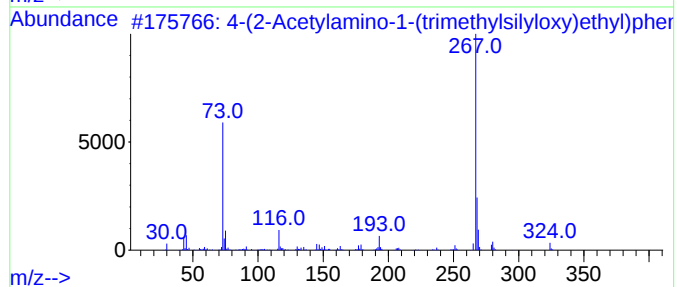
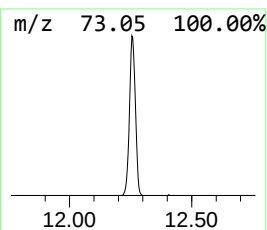
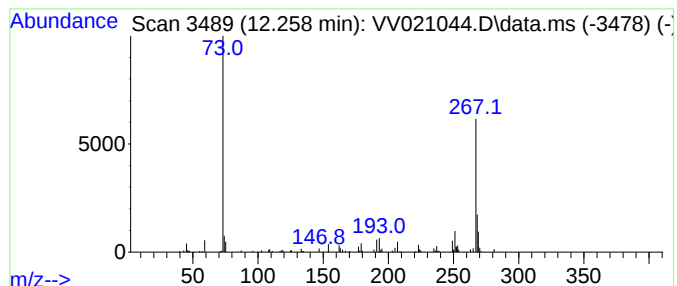
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM041421WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4-(2-Acetylamino-1-(trimeth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.259	4.75 ug/L	114313	1,4-Dichlorobenzene-d4	11.255

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-(2-Acetylamino-1-(trimethylsil...	339	C16H29NO3Si2	1000373-43-5	64
2			p-Trimethylsilyloxyphenyl-(trime...	398	C18H34O4Si3	1000079-05-1	59
3			2-(Trimethylsilyl)amino-4-methyl...	267	C13H25NOSi2	1000373-28-1	53
4			4-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-53-3	50
5			Benzeneethanamine, N-butyl-.beta...	353	C18H35NO2Si2	040629-66-1	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-(2-Acetylamin...	12.259	4.8	ug/L	114313	3	11.255	1204450	50.0