

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041822\
 Data File : VU048118.D
 Acq On : 18 Apr 2022 14:07
 Operator : SY/MD
 Sample : N2374-02ME
 Misc : 4.72g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFD5ME

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\SFAMULM032422WMA.M

Title : VOC Analysis

Signal : TIC: VU048118.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	110	rVB	98758	214836	10.55%	1.406%
2	1.877	163	167	175	rBV	34923	42408	2.08%	0.277%
3	2.539	361	373	385	rBV	297844	516464	25.36%	3.379%
4	2.851	467	470	476	rVB2	264	274	0.01%	0.002%
5	2.883	476	480	484	rBV3	313	273	0.01%	0.002%
6	3.035	520	527	534	rBV5	2260	3865	0.19%	0.025%
7	3.115	550	552	556	rVB3	320	187	0.01%	0.001%
8	3.179	556	572	588	rBV	37518	94651	4.65%	0.619%
9	3.375	630	633	634	rBV2	560	363	0.02%	0.002%
10	3.465	655	661	665	rBV2	445	614	0.03%	0.004%
11	3.530	676	681	689	rVB2	304	434	0.02%	0.003%
12	3.575	691	695	700	rVB3	245	234	0.01%	0.002%
13	3.620	704	709	711	rBV2	378	348	0.02%	0.002%
14	3.684	727	729	731	rBV	400	203	0.01%	0.001%
15	3.703	731	735	741	rVB3	342	442	0.02%	0.003%
16	3.742	741	747	752	rBV2	343	492	0.02%	0.003%
17	3.806	763	767	769	rBV2	354	235	0.01%	0.002%
18	3.819	769	771	775	rVB	479	228	0.01%	0.001%
19	3.845	775	779	783	rBV2	292	319	0.02%	0.002%
20	3.871	783	787	793	rVB3	304	402	0.02%	0.003%
21	4.057	843	845	849	rVB2	278	189	0.01%	0.001%
22	4.096	849	857	860	rBV2	886	1131	0.06%	0.007%
23	4.218	889	895	896	rBV2	307	253	0.01%	0.002%
24	4.305	916	922	925	rBV	266	319	0.02%	0.002%
25	4.375	939	944	947	rBV3	314	305	0.01%	0.002%
26	4.440	961	964	967	rVB2	301	196	0.01%	0.001%
27	4.552	994	999	1002	rBV2	238	209	0.01%	0.001%
28	4.633	1010	1024	1087	rBV	200159	697032	34.22%	4.561%
29	5.063	1139	1158	1185	rVV	357124	833333	40.91%	5.453%
30	5.202	1196	1201	1204	rBV3	541	499	0.02%	0.003%
31	5.279	1220	1225	1228	rBV3	606	575	0.03%	0.004%
32	5.340	1235	1244	1254	rBV5	2255	4707	0.23%	0.031%
33	5.719	1340	1362	1389	rBV2	783313	2036775	100.00%	13.327%
34	5.977	1430	1442	1456	rBV4	13207	30161	1.48%	0.197%
35	6.102	1478	1481	1484	rVV3	387	252	0.01%	0.002%
36	6.247	1511	1526	1554	rBV	340102	680976	33.43%	4.456%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

37	6.436	1583	1585	1589	rVB2	243	184	0.01%	0.001%
38	6.459	1589	1592	1595	rBV	367	309	0.02%	0.002%
39	6.526	1602	1613	1626	rVV6	6230	13540	0.66%	0.089%
40	6.597	1626	1635	1649	rVV4	5882	13799	0.68%	0.090%
41	6.690	1649	1664	1690	rVV	465682	963229	47.29%	6.303%
42	6.800	1694	1698	1701	rBV3	1094	890	0.04%	0.006%
43	6.906	1728	1731	1735	rBV	355	247	0.01%	0.002%
44	6.973	1746	1752	1755	rBV2	353	358	0.02%	0.002%
45	7.054	1768	1777	1779	rBV2	1319	1684	0.08%	0.011%
46	7.185	1807	1818	1849	rVV7	14960	45381	2.23%	0.297%
47	7.295	1849	1852	1853	rBV3	383	181	0.01%	0.001%
48	7.388	1878	1881	1886	rBV3	246	212	0.01%	0.001%
49	7.497	1908	1915	1923	rBV2	494	611	0.03%	0.004%
50	7.568	1923	1937	1960	rBV	228374	449977	22.09%	2.944%
51	7.690	1967	1975	1994	rVB2	4381	9934	0.49%	0.065%
52	7.790	1994	2006	2025	rVB2	18297	38267	1.88%	0.250%
53	7.899	2025	2040	2056	rBV	861577	1561721	76.68%	10.219%
54	8.182	2115	2128	2154	rBV	148459	316851	15.56%	2.073%
55	8.349	2174	2180	2181	rBV4	1207	918	0.05%	0.006%
56	8.558	2240	2245	2247	rBV2	338	279	0.01%	0.002%
57	8.655	2256	2275	2311	rBV	681110	1476675	72.50%	9.662%
58	8.931	2353	2361	2365	rBV5	1410	2140	0.11%	0.014%
59	9.102	2411	2414	2417	rBV2	281	225	0.01%	0.001%
60	9.218	2447	2450	2453	rVB2	348	236	0.01%	0.002%
61	9.343	2485	2489	2492	rVB4	307	233	0.01%	0.002%
62	9.423	2497	2514	2540	rBV	475413	926600	45.49%	6.063%
63	9.581	2558	2563	2568	rVV3	740	825	0.04%	0.005%
64	9.697	2592	2599	2605	rBV4	1200	1702	0.08%	0.011%
65	10.057	2709	2711	2717	rVB2	223	194	0.01%	0.001%
66	10.394	2813	2816	2819	rVB2	298	192	0.01%	0.001%
67	10.472	2831	2840	2849	rVB5	2386	4038	0.20%	0.026%
68	10.526	2854	2857	2860	rBV2	460	332	0.02%	0.002%
69	10.549	2860	2864	2866	rBV3	576	414	0.02%	0.003%
70	10.597	2876	2879	2881	rBV3	523	418	0.02%	0.003%
71	10.652	2890	2896	2898	rBV4	2558	2235	0.11%	0.015%
72	10.764	2916	2931	2948	rBV	916647	1489217	73.12%	9.745%
73	10.864	2959	2962	2965	rBV3	370	192	0.01%	0.001%
74	10.883	2965	2968	2970	rBV2	746	502	0.02%	0.003%
75	10.996	3001	3003	3006	rBV2	428	282	0.01%	0.002%
76	11.118	3028	3041	3049	rBV6	4587	7306	0.36%	0.048%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

77	11.179	3056	3060	3064	rBV2	235	251	0.01%	0.002%
78	11.234	3073	3077	3082	rBV2	209	274	0.01%	0.002%
79	11.314	3099	3102	3107	rVB4	948	741	0.04%	0.005%
80	11.375	3115	3121	3128	rVB5	1054	1359	0.07%	0.009%
81	11.410	3128	3132	3133	rBV	786	443	0.02%	0.003%
82	11.462	3141	3148	3151	rBV3	1707	2164	0.11%	0.014%
83	11.571	3180	3182	3190	rVB3	795	748	0.04%	0.005%
84	11.693	3217	3220	3230	rVB4	1622	1633	0.08%	0.011%
85	11.754	3233	3239	3242	rBV4	742	728	0.04%	0.005%
86	11.816	3245	3258	3282	rBV	620713	996634	48.93%	6.521%
87	11.918	3284	3290	3297	rVV6	5359	7125	0.35%	0.047%
88	11.970	3302	3306	3314	rVB4	2101	2774	0.14%	0.018%
89	12.034	3323	3326	3331	rBV3	411	345	0.02%	0.002%
90	12.063	3331	3335	3338	rBV2	395	265	0.01%	0.002%
91	12.195	3361	3376	3397	rBV	1065599	1761602	86.49%	11.527%
92	12.452	3452	3456	3459	rVB4	389	297	0.01%	0.002%
93	12.606	3500	3504	3506	rBV2	265	242	0.01%	0.002%
94	12.764	3547	3553	3556	rBV4	573	722	0.04%	0.005%
95	12.954	3609	3612	3614	rBV2	291	207	0.01%	0.001%
96	12.986	3619	3622	3628	rVB3	403	384	0.02%	0.003%
97	13.844	3882	3889	3899	rVB4	2794	4645	0.23%	0.030%
98	14.098	3961	3968	3976	rBV2	836	1597	0.08%	0.010%
99	14.401	4059	4062	4068	rBV2	505	345	0.02%	0.002%
100	15.131	4286	4289	4291	rBV2	544	317	0.02%	0.002%

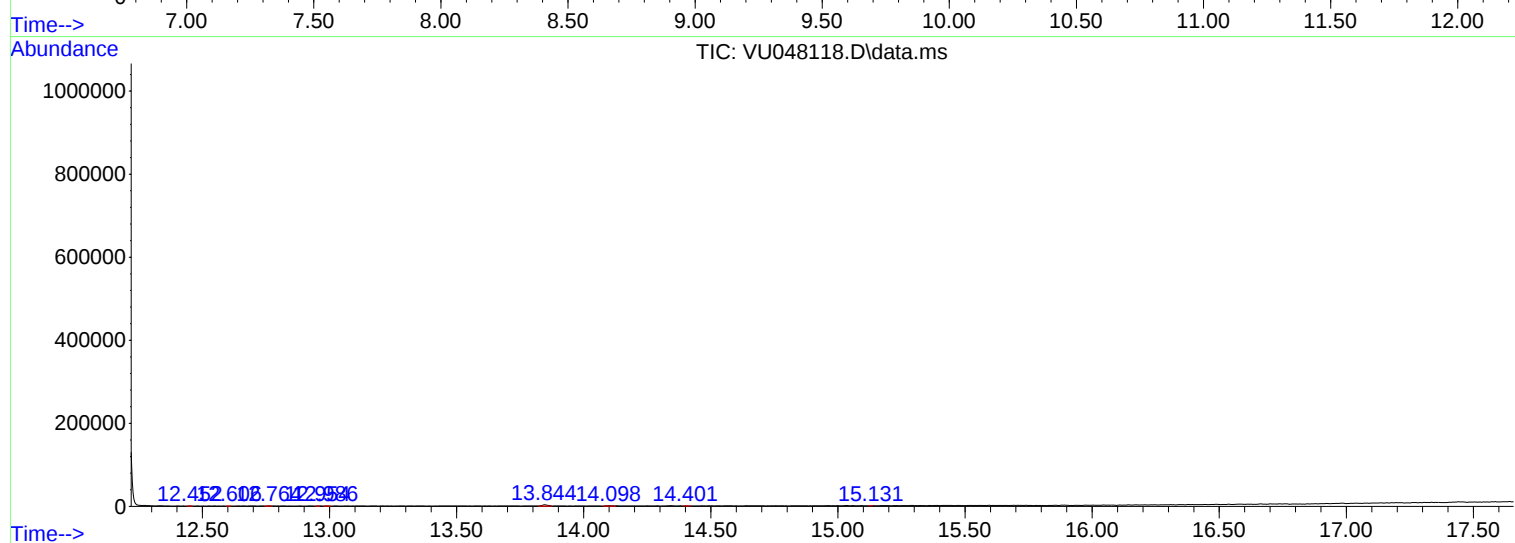
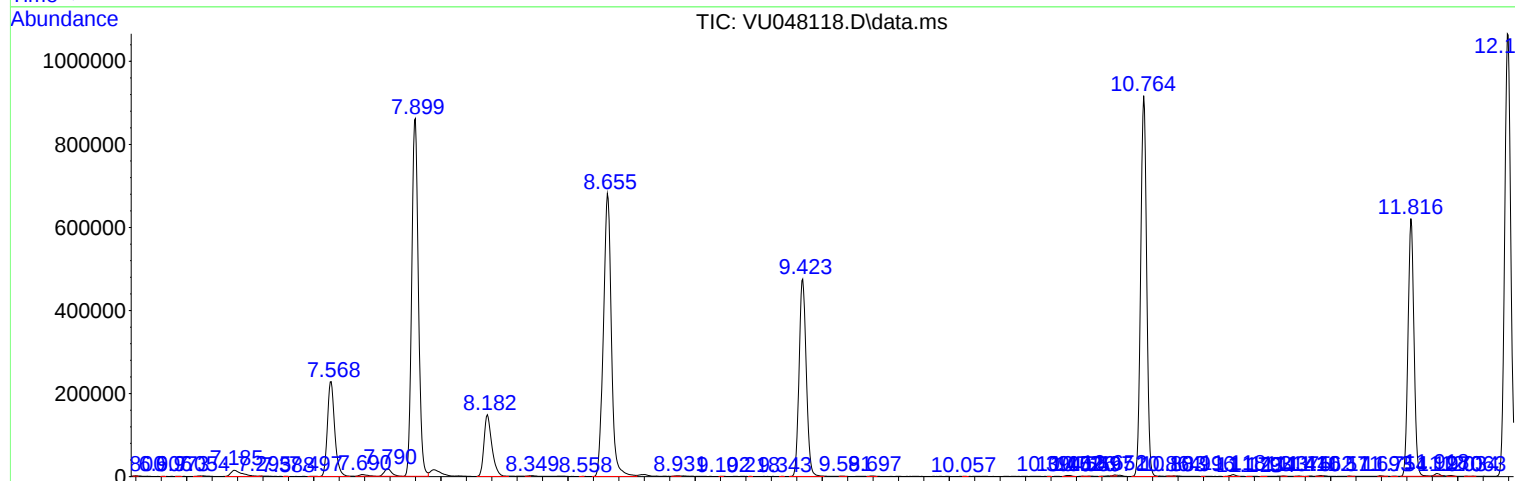
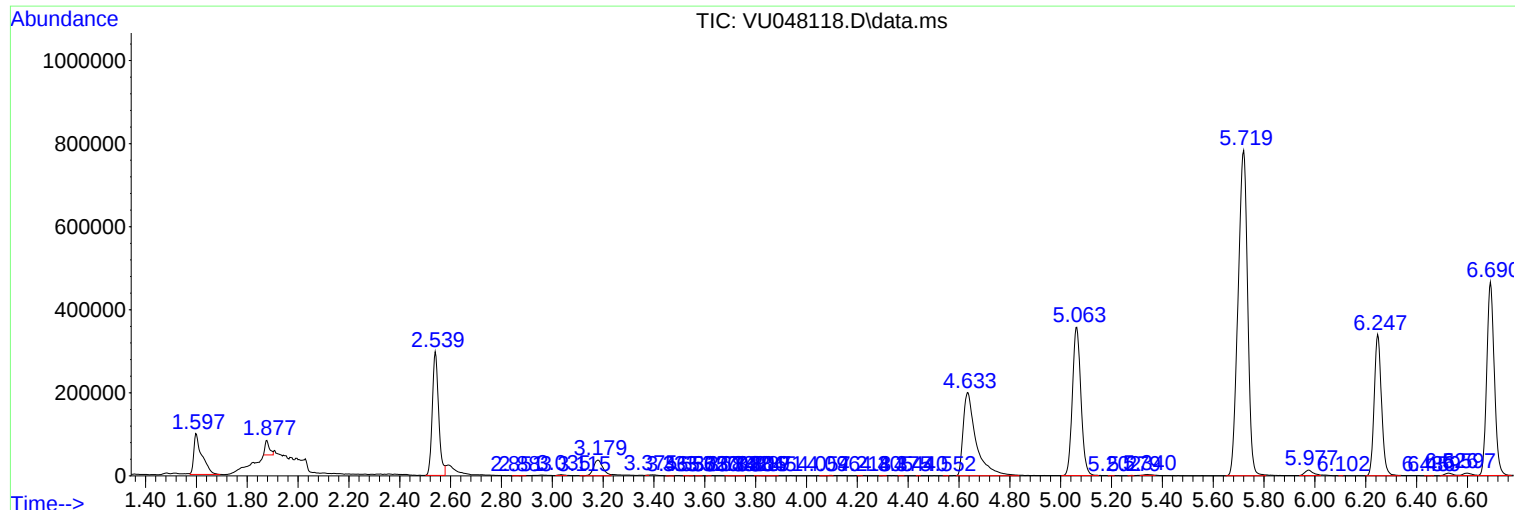
Sum of corrected areas: 15282556

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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BFFD5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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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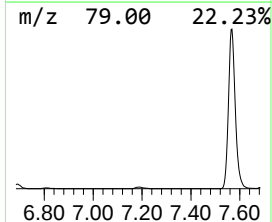
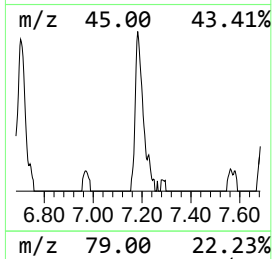
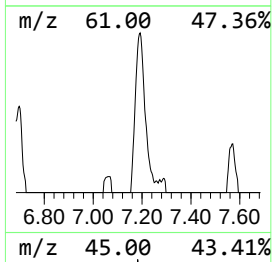
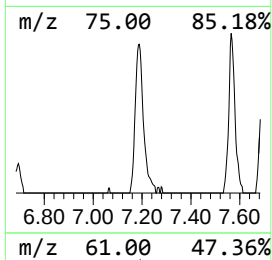
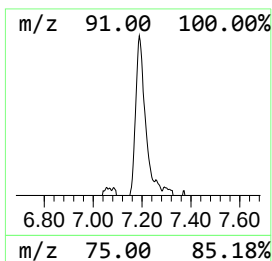
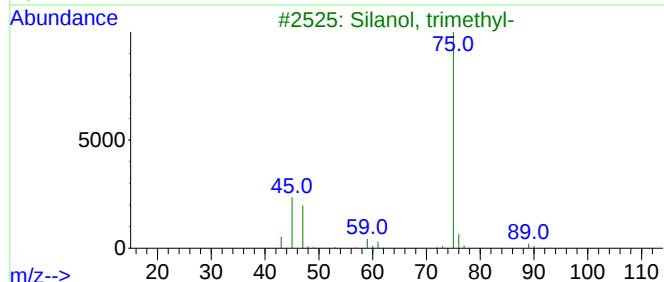
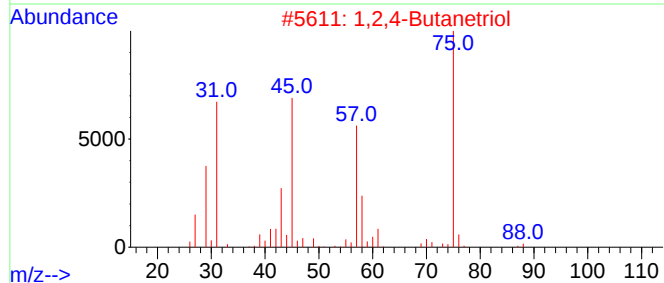
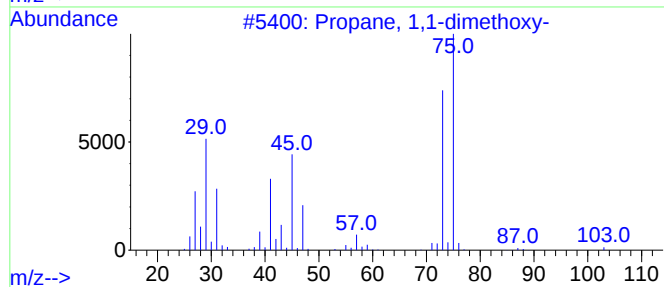
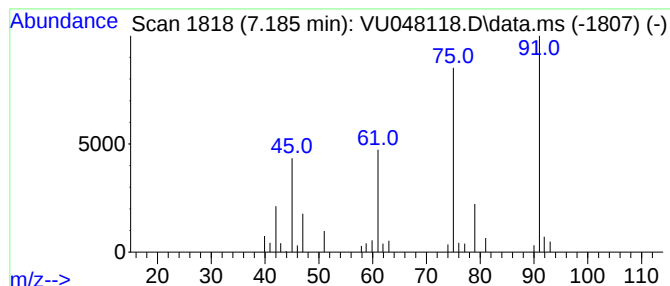
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.185	3.33 ug/L	45381	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	37
2			1,2,4-Butanetriol	106	C4H10O3	003068-00-6	25
3			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	17
4			Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	17
5			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	7.185	3.3	ug/L	45381	1	6.247	680976	50.0