

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046142.D
 Acq On : 07 Dec 2021 15:47
 Operator : SY/MD
 Sample : M4960-02 10X
 Misc : 5.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

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\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046142.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	97	rVB	160950	178965	15.12%	2.121%
2	1.919	170	180	198	rVB	110317	143940	12.16%	1.706%
3	1.986	198	201	206	rBV3	646	617	0.05%	0.007%
4	2.060	220	224	227	rBV2	422	389	0.03%	0.005%
5	2.199	264	267	273	rVB5	629	634	0.05%	0.008%
6	2.311	299	302	304	rBV2	288	228	0.02%	0.003%
7	2.572	370	383	421	rVB	260480	438538	37.05%	5.197%
8	2.797	450	453	458	rVV2	251	261	0.02%	0.003%
9	2.957	497	503	509	rBV2	399	473	0.04%	0.006%
10	3.051	524	532	542	rVB5	1386	2560	0.22%	0.030%
11	3.189	560	575	597	rVV2	11683	29931	2.53%	0.355%
12	3.346	619	624	626	rBV	169	201	0.02%	0.002%
13	3.488	661	668	671	rBB	165	237	0.02%	0.003%
14	3.662	718	722	729	rBV	192	325	0.03%	0.004%
15	3.713	735	738	744	rVV	161	208	0.02%	0.002%
16	3.755	748	751	757	rVB	280	250	0.02%	0.003%
17	3.838	772	777	781	rBV	143	208	0.02%	0.002%
18	3.912	796	800	803	rBB	178	170	0.01%	0.002%
19	3.990	821	824	828	rBV	143	171	0.01%	0.002%
20	4.221	893	896	900	rBV	151	172	0.01%	0.002%
21	4.282	911	915	919	rBB	206	205	0.02%	0.002%
22	4.453	964	968	971	rBV2	263	244	0.02%	0.003%
23	4.639	1010	1026	1064	rBV	100276	306433	25.89%	3.631%
24	4.935	1114	1118	1121	rVB2	270	265	0.02%	0.003%
25	4.970	1122	1129	1131	rBV2	332	304	0.03%	0.004%
26	5.067	1142	1159	1181	rBV	195269	450270	38.04%	5.336%
27	5.292	1226	1229	1232	rVB2	330	190	0.02%	0.002%
28	5.385	1255	1258	1263	rVB	226	229	0.02%	0.003%
29	5.475	1282	1286	1293	rBB	177	250	0.02%	0.003%
30	5.543	1304	1307	1312	rBB	164	175	0.01%	0.002%
31	5.655	1336	1342	1343	rBV	207	188	0.02%	0.002%
32	5.729	1343	1365	1382	rBV2	445053	1183609	100.00%	14.027%
33	6.250	1513	1527	1546	rBV	203213	381495	32.23%	4.521%
34	6.433	1581	1584	1587	rBV	357	283	0.02%	0.003%
35	6.530	1603	1614	1627	rVV2	2849	5873	0.50%	0.070%
36	6.607	1635	1638	1640	rBV	262	203	0.02%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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\SFAMULM112921WMA.M
 Title : VOC Analysis

37	6.694	1650	1665	1684	rBV	265055	513439	43.38%	6.085%
38	6.809	1697	1701	1705	rVB3	939	897	0.08%	0.011%
39	6.983	1753	1755	1761	rBV	156	210	0.02%	0.002%
40	7.041	1767	1773	1781	rVB2	665	911	0.08%	0.011%
41	7.089	1785	1788	1792	rBV	288	230	0.02%	0.003%
42	7.179	1811	1816	1819	rBV	361	394	0.03%	0.005%
43	7.237	1831	1834	1838	rVB	219	191	0.02%	0.002%
44	7.269	1838	1844	1846	rBV	170	214	0.02%	0.003%
45	7.565	1922	1936	1957	rBV	161474	275706	23.29%	3.267%
46	7.684	1969	1973	1977	rVV2	538	579	0.05%	0.007%
47	7.787	1998	2005	2008	rBV	1005	1230	0.10%	0.015%
48	7.899	2026	2040	2056	rBV	588393	1007167	85.09%	11.936%
49	8.179	2115	2127	2153	rVB	109337	183449	15.50%	2.174%
50	8.636	2256	2269	2299	rBV	354678	639589	54.04%	7.580%
51	8.835	2326	2331	2336	rVB	196	175	0.01%	0.002%
52	8.912	2349	2355	2367	rVB2	1446	2373	0.20%	0.028%
53	9.105	2411	2415	2418	rBV	168	179	0.02%	0.002%
54	9.417	2500	2512	2540	rBV	290399	480544	40.60%	5.695%
55	9.571	2553	2560	2567	rVV2	1087	1586	0.13%	0.019%
56	9.645	2580	2583	2586	rBV	172	174	0.01%	0.002%
57	9.697	2587	2599	2609	rVV2	3725	5672	0.48%	0.067%
58	10.102	2719	2725	2733	rBV2	891	1394	0.12%	0.017%
59	10.568	2865	2870	2875	rVB4	695	712	0.06%	0.008%
60	10.629	2884	2889	2894	rBV	238	222	0.02%	0.003%
61	10.671	2894	2902	2910	rBV4	3222	4437	0.37%	0.053%
62	10.758	2915	2929	2950	rVB	400175	636021	53.74%	7.537%
63	10.867	2958	2963	2967	rBV3	600	700	0.06%	0.008%
64	11.002	2998	3005	3008	rBV3	421	494	0.04%	0.006%
65	11.086	3027	3031	3035	rBV2	429	504	0.04%	0.006%
66	11.118	3035	3041	3047	rVB6	870	1256	0.11%	0.015%
67	11.156	3048	3053	3056	rBV3	359	372	0.03%	0.004%
68	11.295	3091	3096	3103	rBV	283	315	0.03%	0.004%
69	11.465	3138	3149	3159	rVB7	3484	6007	0.51%	0.071%
70	11.581	3178	3185	3191	rVB2	565	692	0.06%	0.008%
71	11.697	3215	3221	3228	rBV3	1378	1857	0.16%	0.022%
72	11.812	3245	3257	3271	rBV	334142	524857	44.34%	6.220%
73	11.922	3287	3291	3292	rBV	398	255	0.02%	0.003%
74	11.947	3292	3299	3301	rVV3	1345	1678	0.14%	0.020%
75	11.973	3303	3307	3316	rVB3	2723	3361	0.28%	0.040%
76	12.054	3326	3332	3333	rBV2	214	222	0.02%	0.003%

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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\SFAMULM112921WMA.M
 Title : VOC Analysis

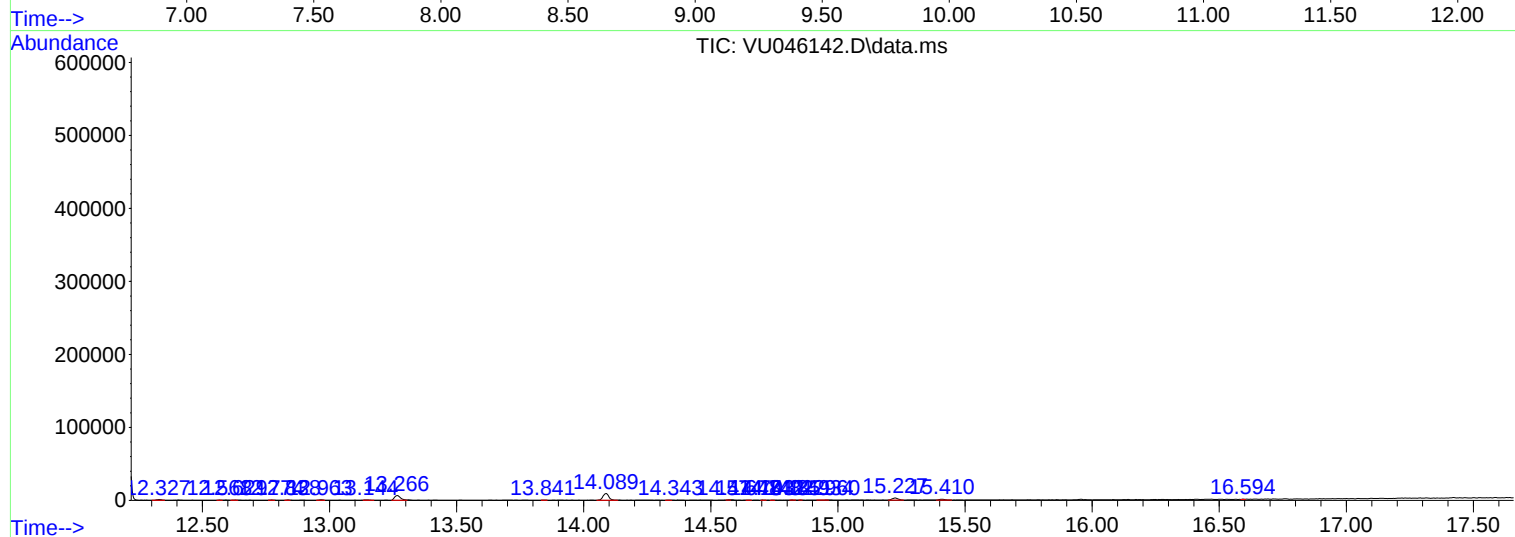
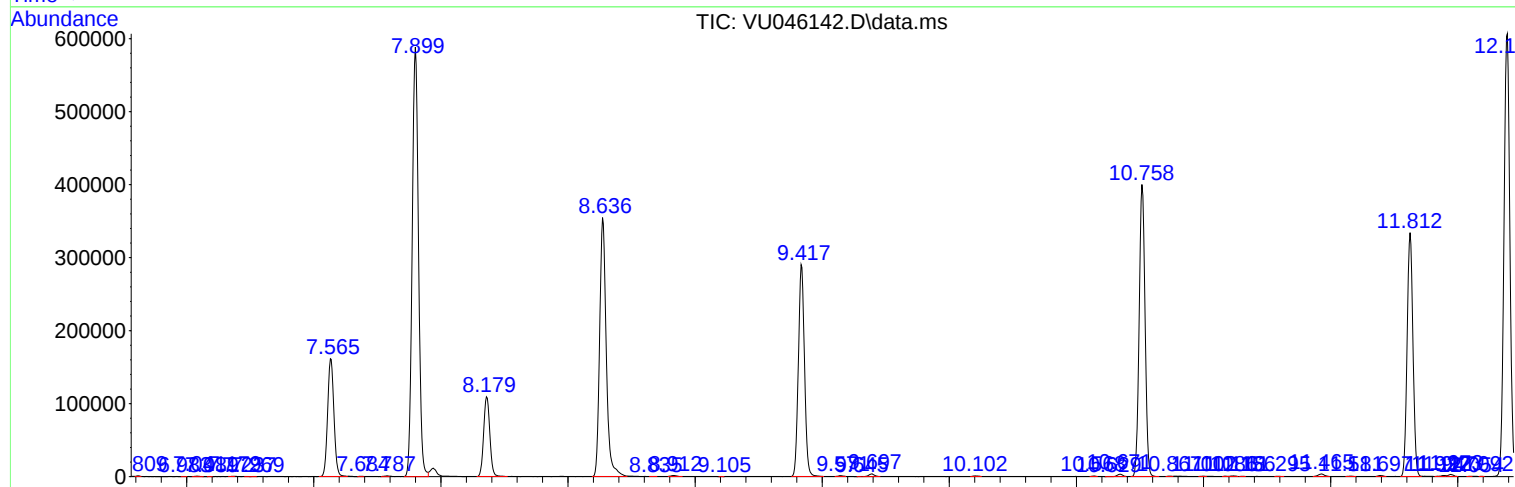
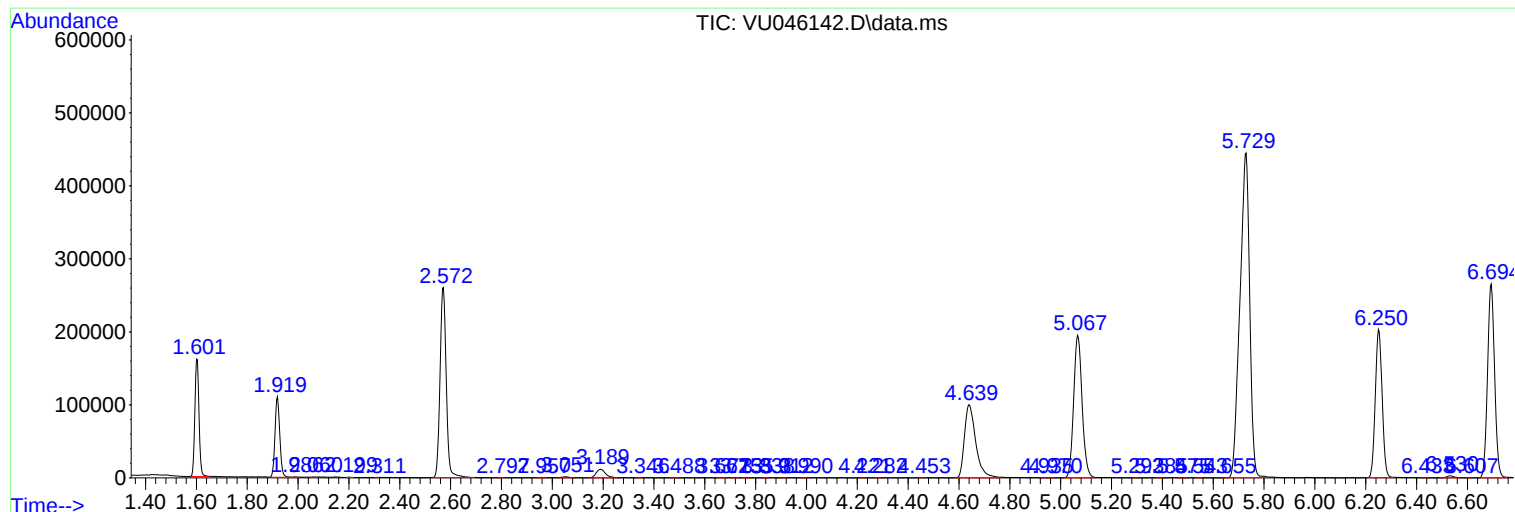
77	12.092	3341	3344	3348	rVB2	268	190	0.02%	0.002%
78	12.195	3356	3376	3394	rBV	606513	970502	82.00%	11.501%
79	12.327	3409	3417	3425	rBV5	887	1429	0.12%	0.017%
80	12.568	3488	3492	3495	rBV3	409	322	0.03%	0.004%
81	12.629	3505	3511	3514	rBV2	308	316	0.03%	0.004%
82	12.774	3551	3556	3559	rBV3	307	345	0.03%	0.004%
83	12.838	3571	3576	3578	rBV2	346	277	0.02%	0.003%
84	12.963	3610	3615	3621	rBV3	612	735	0.06%	0.009%
85	13.144	3667	3671	3681	rVB3	551	732	0.06%	0.009%
86	13.266	3702	3709	3721	rBV2	6464	10649	0.90%	0.126%
87	13.841	3885	3888	3893	rVB2	249	236	0.02%	0.003%
88	14.089	3953	3965	3979	rBV	9190	14706	1.24%	0.174%
89	14.343	4037	4044	4045	rBV	275	281	0.02%	0.003%
90	14.574	4111	4116	4117	rBV2	412	362	0.03%	0.004%
91	14.648	4136	4139	4143	rVB	242	215	0.02%	0.003%
92	14.703	4154	4156	4161	rVB	354	173	0.01%	0.002%
93	14.742	4165	4168	4171	rBV	223	179	0.02%	0.002%
94	14.822	4189	4193	4197	rVV2	233	212	0.02%	0.003%
95	14.851	4200	4202	4205	rVB	278	175	0.01%	0.002%
96	14.934	4222	4228	4231	rBV2	217	251	0.02%	0.003%
97	14.960	4231	4236	4237	rBV2	324	289	0.02%	0.003%
98	15.227	4310	4319	4329	rVB3	2916	4716	0.40%	0.056%
99	15.410	4369	4376	4388	rVB3	1096	1675	0.14%	0.020%
100	16.594	4741	4744	4747	rBV3	519	344	0.03%	0.004%

Sum of corrected areas: 8438270

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ALS Vial : 16 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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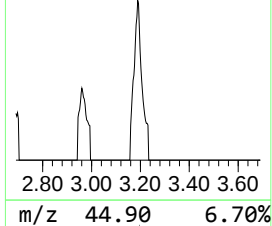
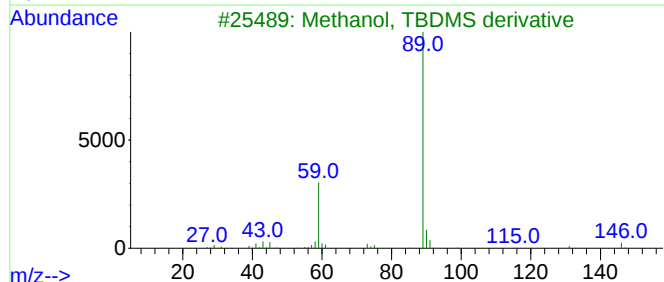
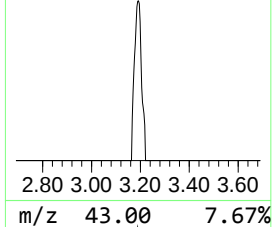
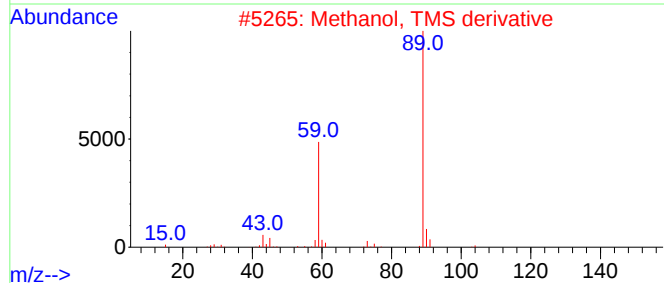
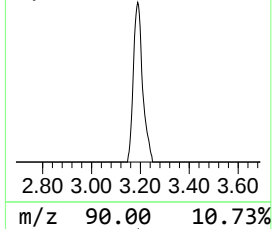
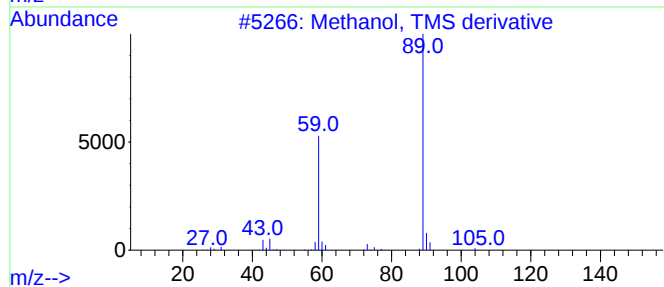
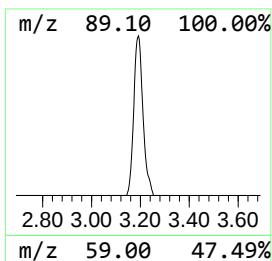
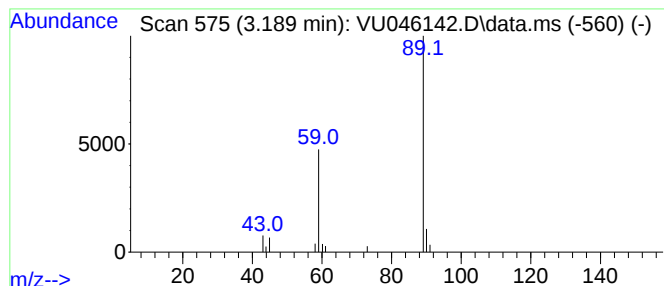
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Methanol, TMS derivative Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.189	3.92 ug/L	29931	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
2			Methanol, TMS derivative	104	C4H12OSi	001825-61-2	83
3			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	74
4			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	64
5			Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanol, TMS d...	3.189	3.9	ug/L	29931	1	6.250	381495	50.0