

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046154.D
 Acq On : 07 Dec 2021 21:03
 Operator : SY/MD
 Sample : M4887-10ME
 Misc : 5.11g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 28 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: VU046154.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	73	81	102	rVB	143170	184440	14.41%	2.032%
2	1.916	170	179	198	rBV	82774	134653	10.52%	1.483%
3	1.993	198	203	211	rVB6	1771	2438	0.19%	0.027%
4	2.028	211	214	216	rBV2	681	419	0.03%	0.005%
5	2.549	364	376	393	rBV	248018	411638	32.16%	4.534%
6	3.038	521	528	542	rVB5	1588	3178	0.25%	0.035%
7	3.115	550	552	556	rVB2	260	142	0.01%	0.002%
8	3.183	559	573	592	rBV	9785	26013	2.03%	0.287%
9	3.684	720	729	735	rBV	210	413	0.03%	0.005%
10	3.719	737	740	743	rBV	161	158	0.01%	0.002%
11	3.871	783	787	790	rBV	182	190	0.01%	0.002%
12	3.919	799	802	804	rBV	159	143	0.01%	0.002%
13	3.957	811	814	816	rBV	188	153	0.01%	0.002%
14	4.112	859	862	865	rBV	170	158	0.01%	0.002%
15	4.308	919	923	928	rBB	150	215	0.02%	0.002%
16	4.465	968	972	976	rBB	153	170	0.01%	0.002%
17	4.494	977	981	983	rBV	133	141	0.01%	0.002%
18	4.655	1014	1031	1096	rBV2	63657	303878	23.74%	3.347%
19	5.063	1142	1158	1190	rVB	203446	492992	38.52%	5.430%
20	5.173	1190	1192	1195	rVV	216	140	0.01%	0.002%
21	5.192	1195	1198	1204	rVV	284	301	0.02%	0.003%
22	5.279	1224	1225	1229	rVB	248	138	0.01%	0.002%
23	5.324	1236	1239	1241	rBV	153	130	0.01%	0.001%
24	5.369	1250	1253	1257	rBB	141	143	0.01%	0.002%
25	5.617	1326	1330	1333	rBB	162	156	0.01%	0.002%
26	5.723	1342	1363	1393	rBV2	504659	1279979	100.00%	14.099%
27	5.825	1394	1395	1399	rVV2	304	200	0.02%	0.002%
28	5.867	1403	1408	1410	rBV2	146	137	0.01%	0.002%
29	5.980	1430	1443	1457	rBV4	5518	14561	1.14%	0.160%
30	6.250	1511	1527	1554	rBV2	219789	451561	35.28%	4.974%
31	6.420	1577	1580	1584	rBV	153	177	0.01%	0.002%
32	6.530	1604	1614	1626	rBV4	4600	9758	0.76%	0.107%
33	6.597	1628	1635	1636	rBV3	1231	1277	0.10%	0.014%
34	6.694	1649	1665	1688	rVB	275982	563208	44.00%	6.204%
35	6.809	1694	1701	1708	rVB3	631	923	0.07%	0.010%
36	7.192	1812	1820	1823	rBV2	401	541	0.04%	0.006%

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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

37	7.227	1828	1831	1835	rVV3	282	243	0.02%	0.003%
38	7.301	1852	1854	1858	rVB2	248	169	0.01%	0.002%
39	7.362	1870	1873	1876	rBV	153	148	0.01%	0.002%
40	7.504	1913	1917	1920	rBV	176	184	0.01%	0.002%
41	7.568	1923	1937	1968	rVB	152743	303610	23.72%	3.344%
42	7.694	1972	1976	1979	rBV2	429	305	0.02%	0.003%
43	7.742	1987	1991	1995	rBV	282	242	0.02%	0.003%
44	7.790	1997	2006	2022	rVB3	3127	5793	0.45%	0.064%
45	7.899	2024	2040	2057	rBV	590036	1099364	85.89%	12.109%
46	8.047	2084	2086	2089	rVB	290	147	0.01%	0.002%
47	8.182	2116	2128	2155	rVV	90587	205472	16.05%	2.263%
48	8.404	2194	2197	2202	rBV	140	199	0.02%	0.002%
49	8.468	2214	2217	2222	rBV	343	367	0.03%	0.004%
50	8.552	2233	2243	2256	rVB2	29005	50073	3.91%	0.552%
51	8.681	2259	2283	2316	rBV2	209910	658200	51.42%	7.250%
52	8.944	2358	2365	2367	rBV2	798	1023	0.08%	0.011%
53	9.253	2456	2461	2463	rBV	177	210	0.02%	0.002%
54	9.423	2499	2514	2534	rBV	262180	571543	44.65%	6.296%
55	9.568	2555	2559	2562	rBV2	236	229	0.02%	0.003%
56	9.658	2576	2587	2591	rBV	154	239	0.02%	0.003%
57	9.700	2591	2600	2611	rVV2	902	1694	0.13%	0.019%
58	9.832	2636	2641	2644	rBV	211	268	0.02%	0.003%
59	10.108	2719	2727	2728	rBV2	214	252	0.02%	0.003%
60	10.546	2858	2863	2865	rBV	213	201	0.02%	0.002%
61	10.671	2893	2902	2910	rVB3	3600	4701	0.37%	0.052%
62	10.771	2919	2933	2949	rBV	396544	660395	51.59%	7.274%
63	10.867	2957	2963	2968	rBV2	718	922	0.07%	0.010%
64	10.890	2968	2970	2971	rBV2	325	150	0.01%	0.002%
65	10.925	2978	2981	2984	rVB	242	181	0.01%	0.002%
66	10.999	3001	3004	3006	rBV	181	140	0.01%	0.002%
67	11.099	3033	3035	3037	rVV	250	171	0.01%	0.002%
68	11.121	3040	3042	3048	rVB3	712	611	0.05%	0.007%
69	11.156	3048	3053	3058	rVB2	332	350	0.03%	0.004%
70	11.298	3093	3097	3103	rVB2	326	296	0.02%	0.003%
71	11.459	3138	3147	3158	rBV4	2532	4538	0.35%	0.050%
72	11.581	3179	3185	3191	rVB2	401	575	0.04%	0.006%
73	11.697	3213	3221	3231	rVB4	1543	2242	0.18%	0.025%
74	11.819	3245	3259	3271	rBV	373107	592475	46.29%	6.526%
75	11.899	3280	3284	3288	rBV3	233	199	0.02%	0.002%
76	11.941	3292	3297	3302	rVV6	1172	1804	0.14%	0.020%

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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

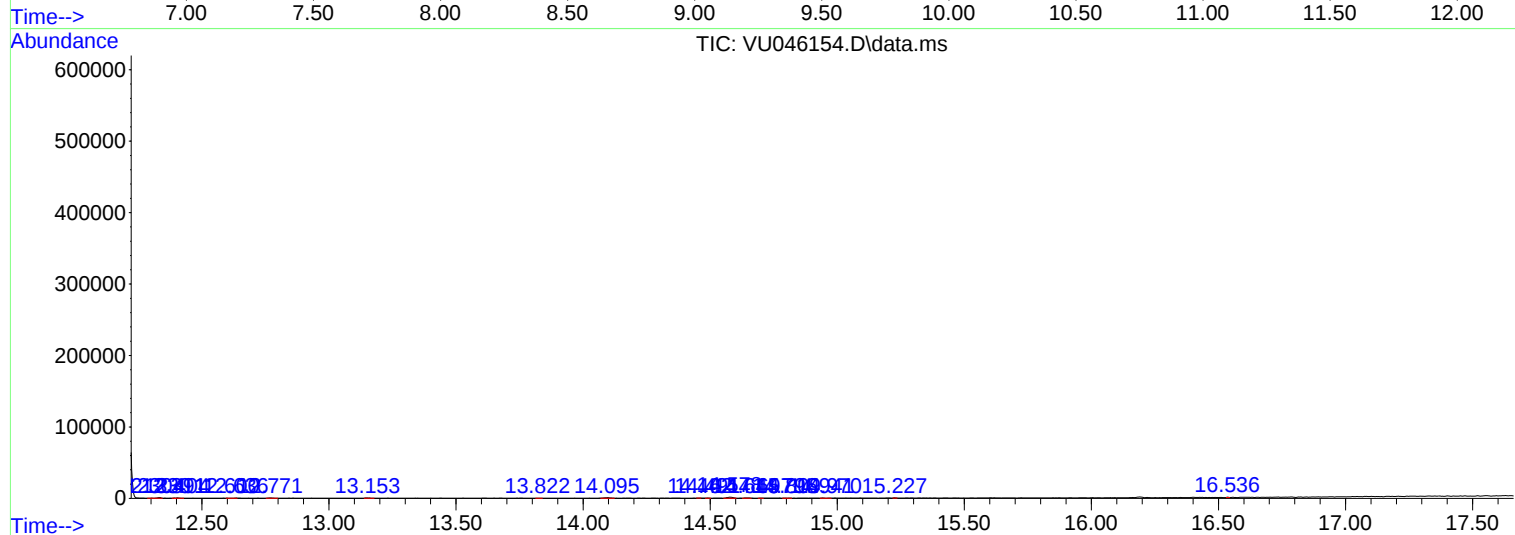
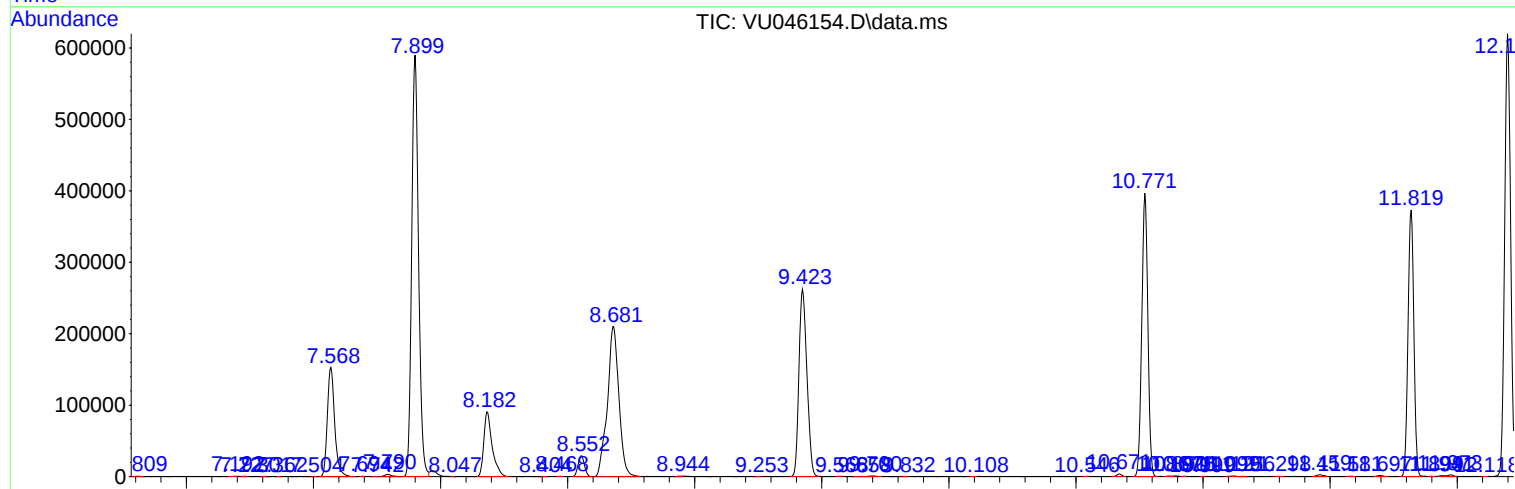
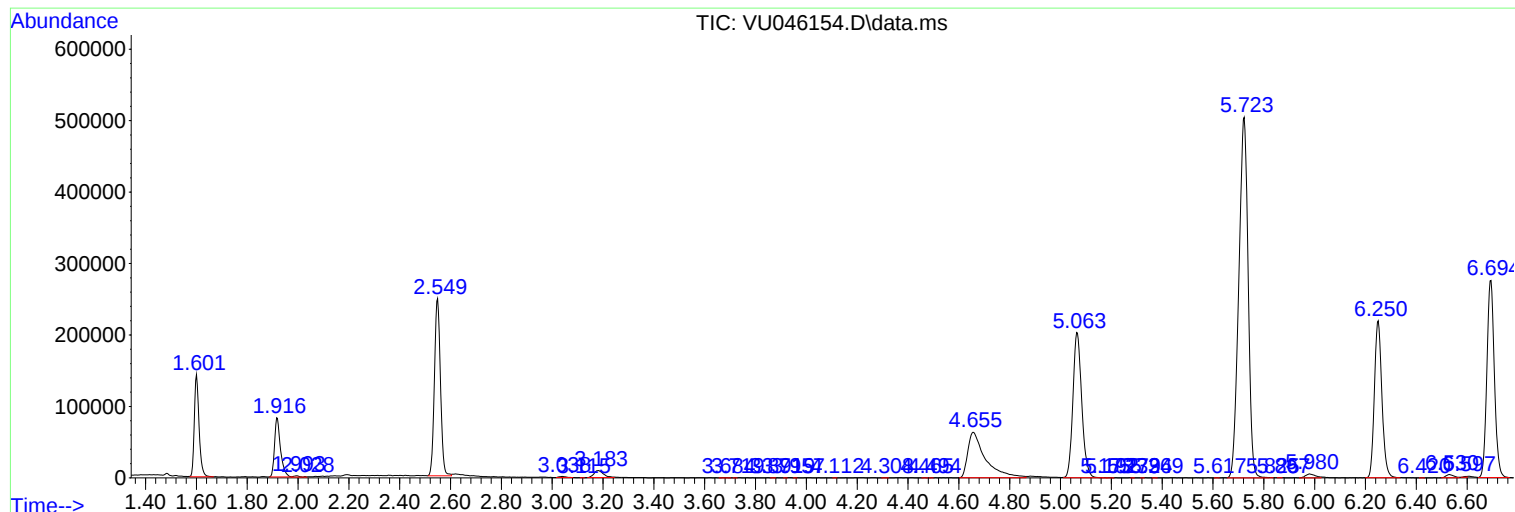
77	11.973	3302	3307	3315	rVB3	2092	2952	0.23%	0.033%
78	12.118	3346	3352	3353	rBV2	139	155	0.01%	0.002%
79	12.198	3359	3377	3395	rBV	619724	1010678	78.96%	11.133%
80	12.304	3404	3410	3413	rBV2	217	196	0.02%	0.002%
81	12.330	3413	3418	3423	rVV3	1041	1109	0.09%	0.012%
82	12.391	3434	3437	3438	rVV	392	212	0.02%	0.002%
83	12.404	3438	3441	3449	rVB2	620	539	0.04%	0.006%
84	12.600	3500	3502	3508	rVB2	204	155	0.01%	0.002%
85	12.636	3508	3513	3514	rBV	409	304	0.02%	0.003%
86	12.771	3549	3555	3564	rVB2	491	623	0.05%	0.007%
87	13.153	3669	3674	3682	rVB3	500	707	0.06%	0.008%
88	13.822	3879	3882	3888	rBV	130	140	0.01%	0.002%
89	14.095	3959	3967	3976	rVB	756	1217	0.10%	0.013%
90	14.462	4076	4081	4082	rBV	190	167	0.01%	0.002%
91	14.491	4087	4090	4094	rVB	270	147	0.01%	0.002%
92	14.578	4109	4117	4125	rBV3	1507	2309	0.18%	0.025%
93	14.645	4132	4138	4143	rBV2	397	578	0.05%	0.006%
94	14.697	4151	4154	4158	rBV2	212	224	0.02%	0.002%
95	14.796	4181	4185	4187	rBV2	267	214	0.02%	0.002%
96	14.809	4187	4189	4193	rVB	196	145	0.01%	0.002%
97	14.941	4227	4230	4235	rVB2	301	291	0.02%	0.003%
98	14.970	4235	4239	4241	rBV	167	152	0.01%	0.002%
99	15.227	4316	4319	4322	rVB	421	261	0.02%	0.003%
100	16.536	4724	4726	4729	rVB3	601	327	0.03%	0.004%

Sum of corrected areas: 9078589

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ALS Vial : 28 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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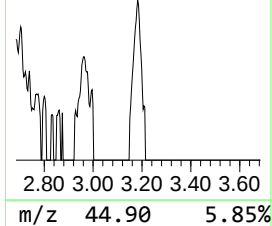
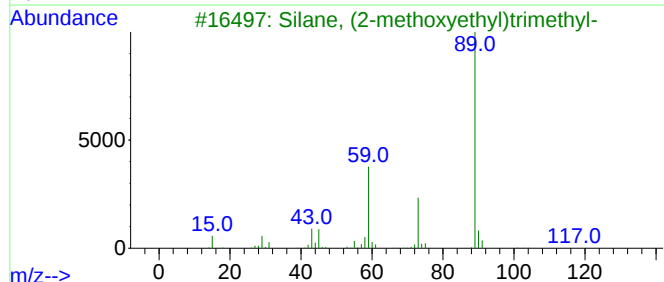
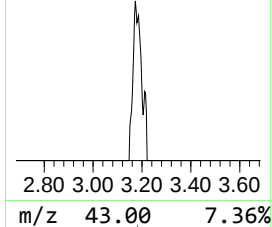
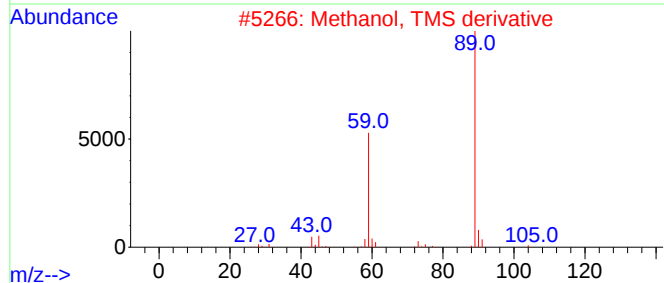
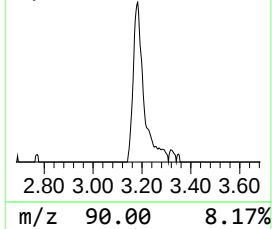
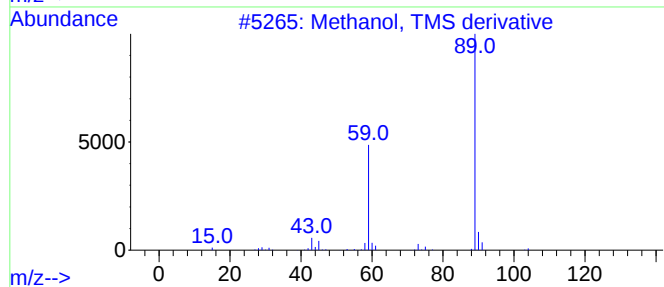
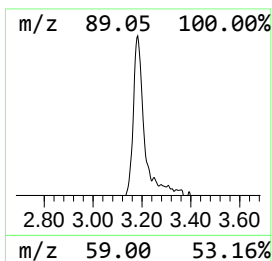
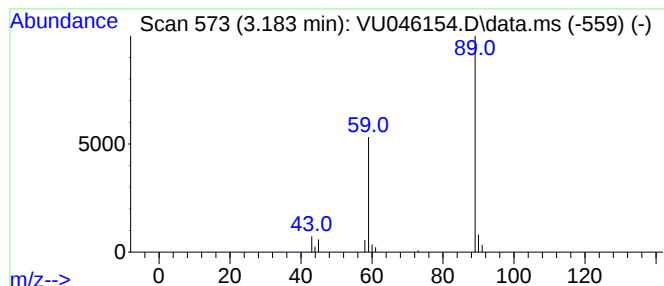
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Methanol, TMS derivative Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.183	2.88 ug/L	26013	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			Silane, (2-methoxyethyl)trimethyl-	132	C6H16OSi	018173-63-2	83
4			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	74
5			Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	7



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanol, TMS d...	3.183	2.9	ug/L	26013	1	6.250	451561	50.0