

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046149.D
 Acq On : 07 Dec 2021 19:11
 Operator : SY/MD
 Sample : M4887-03ME
 Misc : 5.34g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 23 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: VU046149.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	99	rVB	168211	223221	14.40%	2.136%
2	1.864	159	163	170	rVB3	1539	1500	0.10%	0.014%
3	1.916	170	179	198	rBV	94376	164797	10.63%	1.577%
4	2.060	222	224	225	rBV2	621	297	0.02%	0.003%
5	2.549	364	376	390	rBV	230831	378485	24.42%	3.621%
6	3.041	520	529	539	rBV4	1665	3170	0.20%	0.030%
7	3.112	547	551	553	rVB2	257	162	0.01%	0.002%
8	3.182	558	573	592	rBV	12197	31507	2.03%	0.301%
9	3.334	618	620	624	rVB2	345	220	0.01%	0.002%
10	3.401	638	641	646	rBV	155	209	0.01%	0.002%
11	3.491	663	669	670	rBV	156	182	0.01%	0.002%
12	3.668	721	724	727	rBV2	235	154	0.01%	0.001%
13	3.732	740	744	748	rBV	216	252	0.02%	0.002%
14	3.819	766	771	776	rBV	146	216	0.01%	0.002%
15	3.880	786	790	794	rBB	168	190	0.01%	0.002%
16	3.925	801	804	806	rBV	158	140	0.01%	0.001%
17	4.015	830	832	836	rVB	228	174	0.01%	0.002%
18	4.070	846	849	855	rBV	184	233	0.02%	0.002%
19	4.224	890	897	900	rBB	175	255	0.02%	0.002%
20	4.658	1013	1032	1089	rBV2	75279	371440	23.96%	3.554%
21	5.067	1142	1159	1186	rVV	238311	598827	38.63%	5.730%
22	5.321	1233	1238	1241	rBV	166	188	0.01%	0.002%
23	5.362	1249	1251	1256	rVB	165	156	0.01%	0.001%
24	5.723	1342	1363	1393	rBV2	606945	1550031	100.00%	14.831%
25	5.851	1401	1403	1409	rVB2	301	257	0.02%	0.002%
26	5.877	1409	1411	1413	rVV	266	138	0.01%	0.001%
27	5.906	1417	1420	1423	rVB2	278	215	0.01%	0.002%
28	5.983	1432	1444	1459	rBV5	4980	13595	0.88%	0.130%
29	6.092	1474	1478	1481	rBV	278	198	0.01%	0.002%
30	6.250	1512	1527	1563	rVV	211257	431516	27.84%	4.129%
31	6.385	1567	1569	1572	rVB2	253	183	0.01%	0.002%
32	6.465	1591	1594	1598	rBB	130	137	0.01%	0.001%
33	6.494	1599	1603	1605	rBV	156	156	0.01%	0.001%
34	6.530	1605	1614	1625	rBV6	4885	10393	0.67%	0.099%
35	6.604	1632	1637	1649	rVB3	1821	3074	0.20%	0.029%
36	6.690	1649	1664	1693	rVB	330525	684760	44.18%	6.552%

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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	6.800	1693	1698	1699	rBV3	667	469	0.03%	0.004%
38	6.838	1707	1710	1718	rVB3	261	315	0.02%	0.003%
39	6.919	1732	1735	1741	rBB	161	208	0.01%	0.002%
40	6.957	1744	1747	1750	rBV	188	169	0.01%	0.002%

41	7.054	1774	1777	1779	rVV2	233	155	0.01%	0.001%
42	7.095	1789	1790	1795	rBB	220	144	0.01%	0.001%
43	7.189	1812	1819	1826	rBV2	582	841	0.05%	0.008%
44	7.269	1837	1844	1846	rBV2	245	296	0.02%	0.003%
45	7.452	1896	1901	1904	rBV	170	220	0.01%	0.002%

46	7.568	1923	1937	1964	rBV	184087	370620	23.91%	3.546%
47	7.684	1970	1973	1978	rVB3	314	196	0.01%	0.002%
48	7.793	1996	2007	2021	rBV3	3189	6371	0.41%	0.061%
49	7.899	2025	2040	2058	rBV	700559	1326000	85.55%	12.687%
50	8.044	2084	2085	2089	rVB2	311	149	0.01%	0.001%

51	8.112	2101	2106	2109	rBV	205	225	0.01%	0.002%
52	8.182	2115	2128	2159	rBV	109183	251850	16.25%	2.410%
53	8.388	2189	2192	2194	rBV	183	153	0.01%	0.001%
54	8.472	2214	2218	2225	rVB2	364	544	0.04%	0.005%
55	8.555	2230	2244	2256	rVB2	45532	78820	5.09%	0.754%

56	8.681	2259	2283	2314	rBV2	246333	796639	51.40%	7.622%
57	8.944	2358	2365	2367	rBV	1264	1208	0.08%	0.012%
58	9.427	2498	2515	2537	rVV	237969	541901	34.96%	5.185%
59	9.578	2554	2562	2570	rVV2	490	717	0.05%	0.007%
60	9.697	2591	2599	2616	rVB3	1403	2595	0.17%	0.025%

61	9.806	2631	2633	2637	rVB	204	167	0.01%	0.002%
62	9.832	2638	2641	2643	rBV	172	145	0.01%	0.001%
63	10.115	2724	2729	2733	rVB4	329	371	0.02%	0.004%
64	10.234	2763	2766	2770	rVB2	187	153	0.01%	0.001%
65	10.488	2841	2845	2853	rVB2	303	326	0.02%	0.003%

66	10.671	2892	2902	2911	rVV2	3989	5767	0.37%	0.055%
67	10.774	2916	2934	2950	rBV	462682	793495	51.19%	7.592%
68	10.870	2958	2964	2969	rBV2	627	1034	0.07%	0.010%
69	10.922	2977	2980	2987	rVB3	412	418	0.03%	0.004%
70	11.002	3002	3005	3007	rBV	260	188	0.01%	0.002%

71	11.108	3028	3038	3039	rBV4	686	856	0.06%	0.008%
72	11.205	3062	3068	3071	rVB	200	225	0.01%	0.002%
73	11.459	3137	3147	3162	rVB5	2899	6046	0.39%	0.058%
74	11.578	3179	3184	3190	rVB2	517	677	0.04%	0.006%
75	11.697	3213	3221	3227	rVB3	1853	2498	0.16%	0.024%

76	11.754	3236	3239	3242	rVB	451	259	0.02%	0.002%
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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

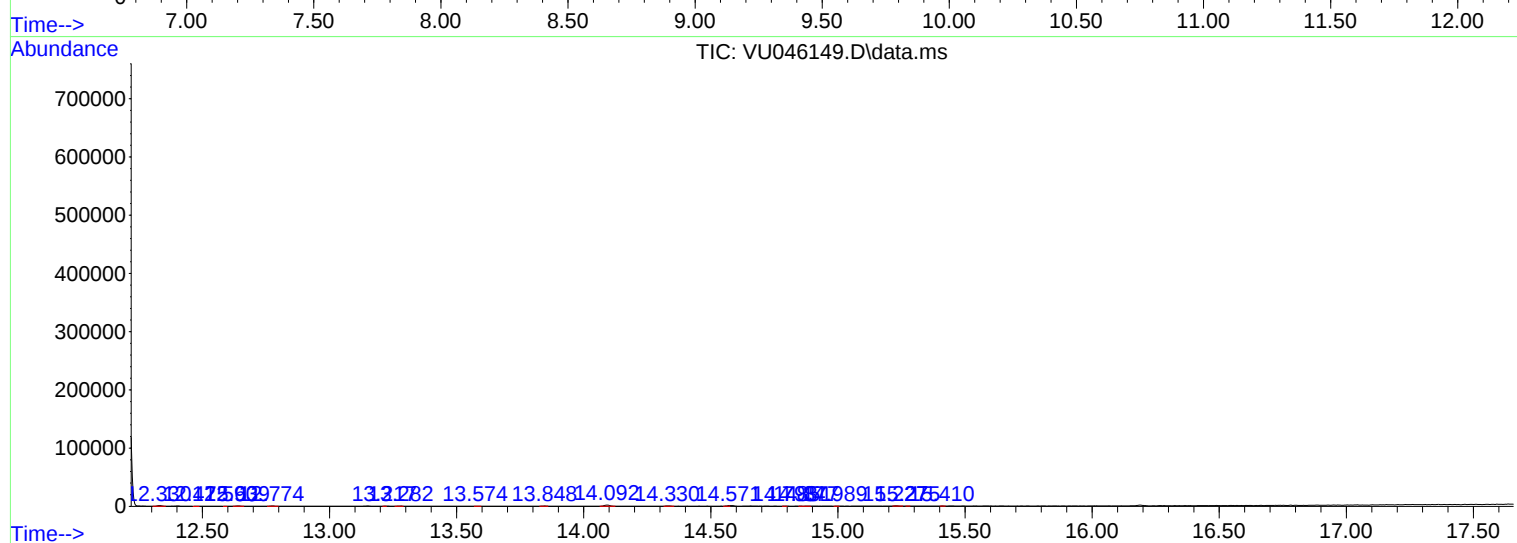
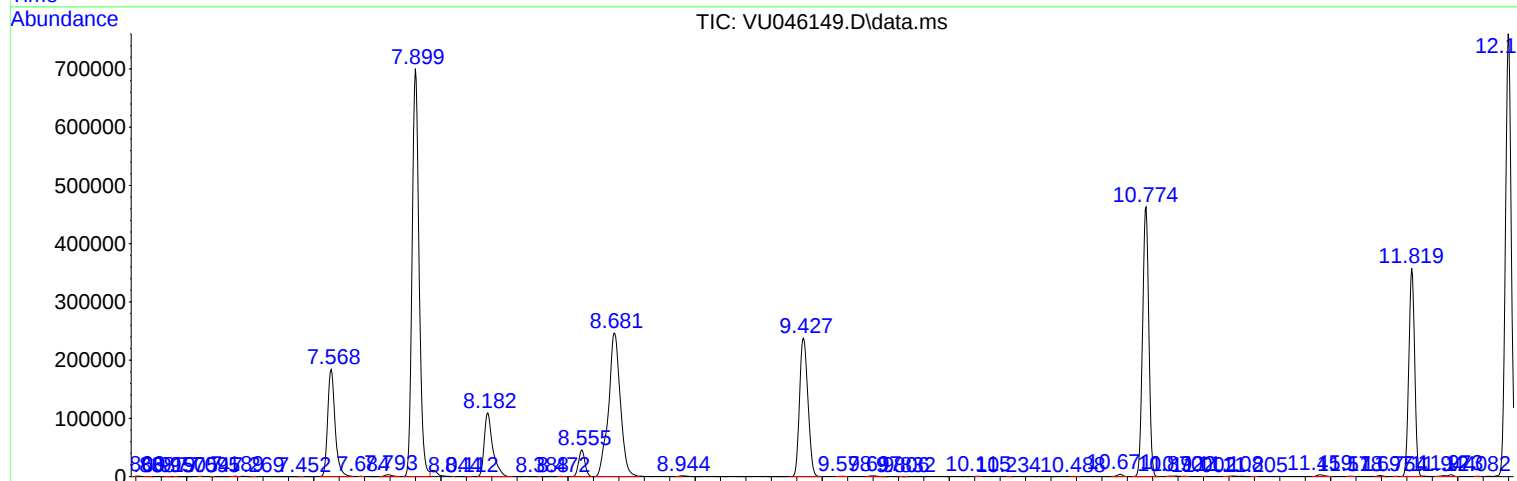
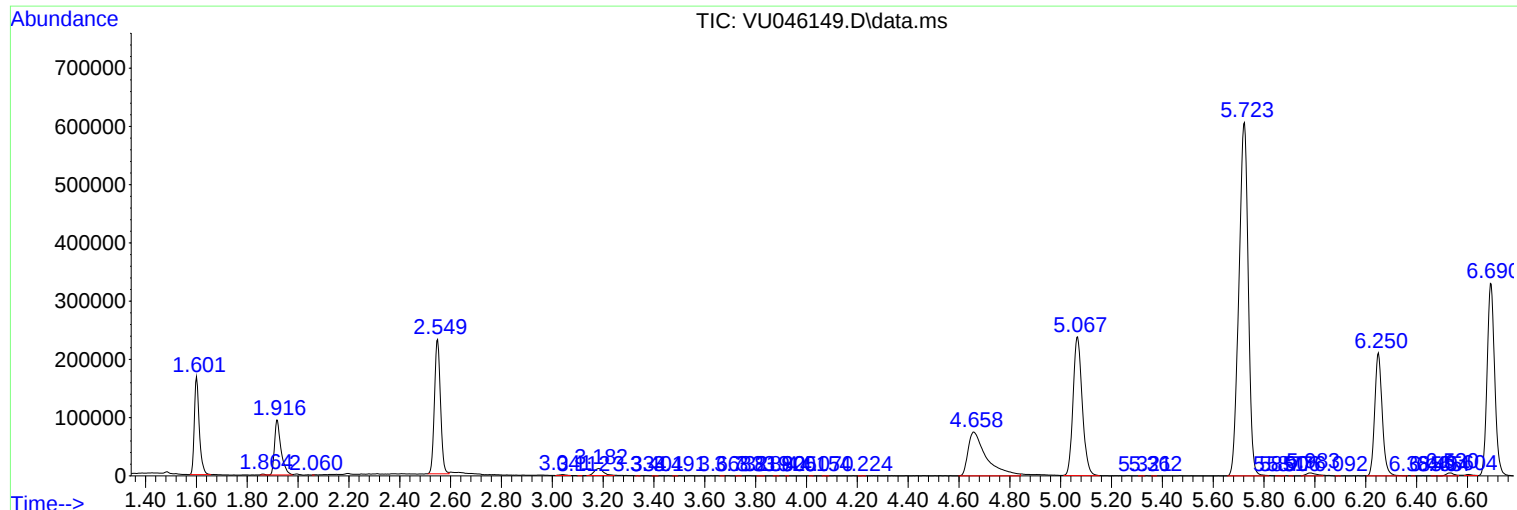
77	11.819	3245	3259	3272	rBV	357898	564882	36.44%	5.405%
78	11.944	3287	3298	3302	rBV4	1549	2461	0.16%	0.024%
79	11.973	3303	3307	3317	rVB3	3063	3690	0.24%	0.035%
80	12.082	3335	3341	3344	rBV3	351	411	0.03%	0.004%
81	12.198	3358	3377	3392	rBV	760136	1204007	77.68%	11.520%
82	12.330	3410	3418	3426	rVB5	1169	1672	0.11%	0.016%
83	12.475	3459	3463	3467	rBV	148	145	0.01%	0.001%
84	12.590	3496	3499	3501	rBV	204	148	0.01%	0.001%
85	12.639	3508	3514	3522	rBV3	643	882	0.06%	0.008%
86	12.774	3550	3556	3564	rBV3	626	898	0.06%	0.009%
87	13.217	3691	3694	3696	rBV2	306	220	0.01%	0.002%
88	13.282	3706	3714	3717	rBV3	509	601	0.04%	0.006%
89	13.574	3803	3805	3812	rVB	174	136	0.01%	0.001%
90	13.848	3883	3890	3894	rBV2	577	641	0.04%	0.006%
91	14.092	3957	3966	3976	rVB	1924	2935	0.19%	0.028%
92	14.330	4035	4040	4048	rVB3	504	766	0.05%	0.007%
93	14.571	4108	4115	4116	rBV3	1116	911	0.06%	0.009%
94	14.793	4180	4184	4186	rBV2	267	224	0.01%	0.002%
95	14.851	4200	4202	4207	rVB2	264	175	0.01%	0.002%
96	14.877	4207	4210	4215	rBV	205	253	0.02%	0.002%
97	14.989	4243	4245	4250	rBV2	168	175	0.01%	0.002%
98	15.227	4315	4319	4328	rVV2	637	721	0.05%	0.007%
99	15.275	4331	4334	4337	rBV	210	140	0.01%	0.001%
100	15.410	4373	4376	4380	rBV	287	218	0.01%	0.002%

Sum of corrected areas: 10451370

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ALS Vial : 23 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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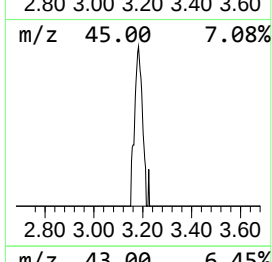
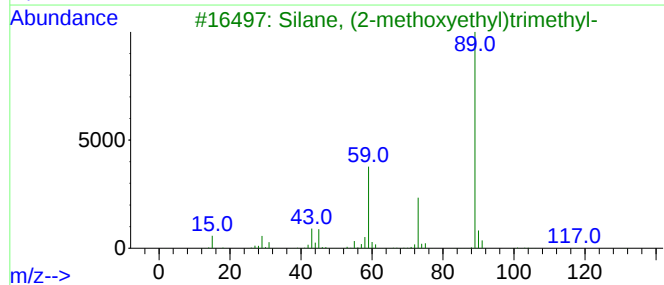
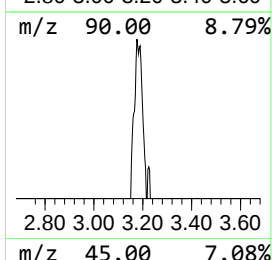
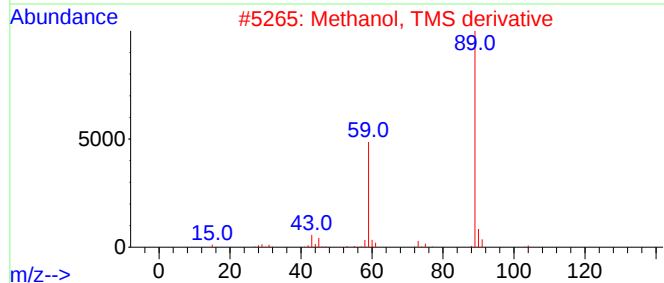
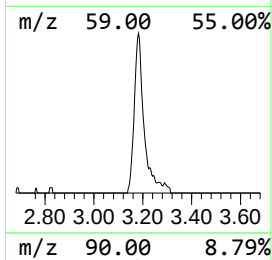
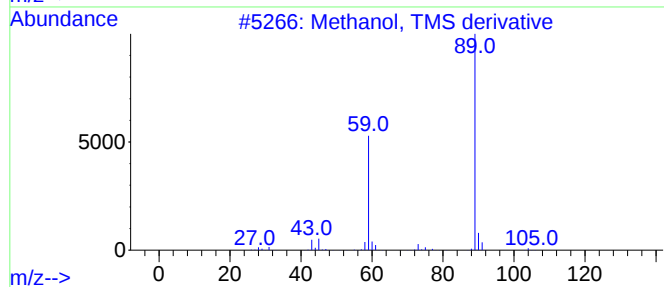
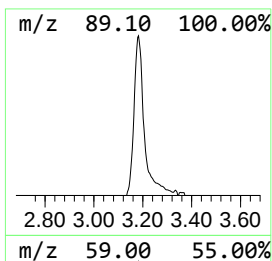
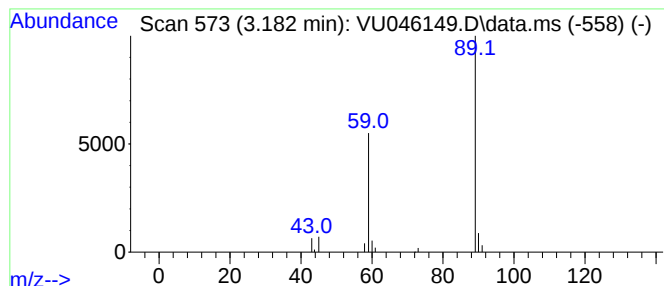
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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.
3.182	3.65 ug/L	31507	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	74
4			Methanol, TBDMS derivative	146	C7H18OSi	1000364-10-7	43
5			Tricyclo[5.2.2.0(2,6)]undecan-11...	352	C18H24O7	1000155-17-7	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...	3.182	3.6	ug/L	31507	1	6.250	431516	50.0