

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120921\
 Data File : VU046213.D
 Acq On : 09 Dec 2021 12:33
 Operator : SY/MD
 Sample : M4887-14MEDL 10X
 Misc : 3.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8C8MEDL

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: VU046213.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	94	rVB	164401	182658	15.92%	2.032%
2	1.781	134	137	141	rBV2	680	610	0.05%	0.007%
3	1.864	159	163	167	rBV2	460	606	0.05%	0.007%
4	1.919	171	180	194	rVB	109504	140863	12.28%	1.567%
5	2.038	213	217	218	rBV2	462	338	0.03%	0.004%
6	2.112	236	240	247	rBV4	752	841	0.07%	0.009%
7	2.211	265	271	274	rBV3	382	388	0.03%	0.004%
8	2.314	299	303	306	rBV	489	321	0.03%	0.004%
9	2.334	306	309	318	rBV2	269	330	0.03%	0.004%
10	2.446	338	344	346	rBV2	741	754	0.07%	0.008%
11	2.571	367	383	412	rBV	259634	432103	37.67%	4.808%
12	2.687	417	419	422	rVV	696	452	0.04%	0.005%
13	2.793	445	452	454	rBV	721	582	0.05%	0.006%
14	2.854	468	471	475	rBV2	486	428	0.04%	0.005%
15	3.054	525	533	541	rVB3	2096	3269	0.28%	0.036%
16	3.192	563	576	588	rBV2	3926	9490	0.83%	0.106%
17	3.327	613	618	620	rBV	449	365	0.03%	0.004%
18	3.391	635	638	642	rVB2	365	319	0.03%	0.004%
19	3.424	645	648	654	rBV	363	426	0.04%	0.005%
20	3.571	692	694	702	rVB	523	431	0.04%	0.005%
21	3.803	762	766	769	rBV	460	365	0.03%	0.004%
22	3.829	771	774	779	rVB	628	553	0.05%	0.006%
23	4.150	869	874	877	rVB2	561	572	0.05%	0.006%
24	4.215	890	894	899	rVV	453	585	0.05%	0.007%
25	4.407	948	954	957	rVB	389	375	0.03%	0.004%
26	4.639	1007	1026	1069	rBV2	94080	291216	25.39%	3.240%
27	4.874	1094	1099	1103	rBV2	637	658	0.06%	0.007%
28	5.067	1143	1159	1182	rBV	190906	444137	38.72%	4.942%
29	5.298	1224	1231	1234	rBV2	540	518	0.05%	0.006%
30	5.729	1342	1365	1384	rBV2	428834	1147161	100.00%	12.764%
31	5.973	1437	1441	1453	rBV3	1053	1476	0.13%	0.016%
32	6.108	1479	1483	1485	rBV2	476	382	0.03%	0.004%
33	6.189	1503	1508	1510	rBV2	288	340	0.03%	0.004%
34	6.250	1514	1527	1547	rVV	221104	416779	36.33%	4.637%
35	6.369	1560	1564	1568	rBV3	625	565	0.05%	0.006%
36	6.404	1572	1575	1581	rVB2	528	450	0.04%	0.005%

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

37	6.546	1604	1619	1642	rBV	273634	522495	45.55%	5.814%
38	6.694	1650	1665	1683	rBV	259785	497438	43.36%	5.535%
39	6.928	1735	1738	1744	rBV	552	654	0.06%	0.007%
40	7.095	1787	1790	1795	rBV2	542	612	0.05%	0.007%
41	7.173	1810	1814	1815	rBV	700	516	0.04%	0.006%
42	7.362	1870	1873	1877	rBV	558	405	0.04%	0.005%
43	7.468	1903	1906	1912	rBV	375	330	0.03%	0.004%
44	7.568	1924	1937	1959	rBV	158589	274342	23.91%	3.053%
45	7.796	2002	2008	2014	rVB3	1481	1922	0.17%	0.021%
46	7.848	2021	2024	2026	rBV	451	347	0.03%	0.004%
47	7.899	2026	2040	2056	rBV	559577	968657	84.44%	10.778%
48	8.076	2091	2095	2103	rVB3	680	837	0.07%	0.009%
49	8.182	2116	2128	2144	rBV	105829	178484	15.56%	1.986%
50	8.401	2188	2196	2208	rVB4	6665	10743	0.94%	0.120%
51	8.472	2213	2218	2226	rVB4	1568	2211	0.19%	0.025%
52	8.555	2236	2244	2254	rVB3	10007	15478	1.35%	0.172%
53	8.639	2256	2270	2302	rVV	315898	593353	51.72%	6.602%
54	8.915	2349	2356	2357	rBV2	1925	1983	0.17%	0.022%
55	9.034	2390	2393	2396	rBV	548	375	0.03%	0.004%
56	9.163	2429	2433	2440	rBV2	832	1084	0.09%	0.012%
57	9.420	2499	2513	2532	rBV	320203	546391	47.63%	6.080%
58	9.578	2556	2562	2567	rVB2	1093	1257	0.11%	0.014%
59	9.697	2591	2599	2606	rVB3	2374	3556	0.31%	0.040%
60	9.883	2652	2657	2660	rBV	477	452	0.04%	0.005%
61	9.986	2686	2689	2692	rVB	600	359	0.03%	0.004%
62	10.089	2718	2721	2722	rVV	871	574	0.05%	0.006%
63	10.105	2723	2726	2734	rVB5	1578	1922	0.17%	0.021%
64	10.298	2782	2786	2790	rBV	723	726	0.06%	0.008%
65	10.468	2835	2839	2843	rBV	1151	1205	0.11%	0.013%
66	10.671	2896	2902	2910	rVB5	4003	5817	0.51%	0.065%
67	10.758	2917	2929	2946	rVB	386113	617906	53.86%	6.875%
68	10.838	2951	2954	2957	rBV2	715	493	0.04%	0.005%
69	10.870	2962	2964	2966	rVV2	980	656	0.06%	0.007%
70	10.896	2966	2972	2979	rVB4	2369	3464	0.30%	0.039%
71	10.967	2991	2994	2998	rBV	612	557	0.05%	0.006%
72	11.008	2999	3007	3014	rVV6	1273	2383	0.21%	0.027%
73	11.105	3035	3037	3039	rBV2	606	350	0.03%	0.004%
74	11.285	3089	3093	3095	rBV2	790	659	0.06%	0.007%
75	11.462	3141	3148	3162	rVB5	4391	7715	0.67%	0.086%
76	11.671	3209	3213	3214	rBV2	650	465	0.04%	0.005%

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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\SFAMULM112921WMA.M
 Title : VOC Analysis

77	11.693	3215	3220	3230	rVV5	1972	3215	0.28%	0.036%
78	11.751	3234	3238	3243	rVB2	1206	1003	0.09%	0.011%
79	11.812	3245	3257	3271	rBV	384276	607131	52.92%	6.755%
80	11.941	3292	3297	3300	rBV5	1024	1218	0.11%	0.014%
81	11.973	3303	3307	3315	rVB3	3395	4231	0.37%	0.047%
82	12.195	3360	3376	3391	rBV	571300	919503	80.15%	10.231%
83	12.301	3407	3409	3412	rVV	942	744	0.06%	0.008%
84	12.330	3413	3418	3425	rVB4	2135	2683	0.23%	0.030%
85	12.401	3437	3440	3447	rVB3	923	1001	0.09%	0.011%
86	12.809	3562	3567	3582	rVB4	3972	5536	0.48%	0.062%
87	12.983	3618	3621	3625	rBV	615	431	0.04%	0.005%
88	13.140	3667	3670	3673	rBV2	873	681	0.06%	0.008%
89	13.227	3692	3697	3703	rVB3	739	946	0.08%	0.011%
90	13.346	3732	3734	3739	rBV	386	414	0.04%	0.005%
91	13.510	3776	3785	3795	rBV2	50201	72574	6.33%	0.808%
92	13.703	3839	3845	3851	rVB4	1965	2134	0.19%	0.024%
93	13.844	3883	3889	3896	rBV3	1173	1556	0.14%	0.017%
94	14.089	3958	3965	3972	rBV3	2954	4311	0.38%	0.048%
95	15.159	4295	4298	4300	rBV2	486	383	0.03%	0.004%
96	15.227	4311	4319	4328	rBV4	2233	3695	0.32%	0.041%
97	16.005	4558	4561	4565	rBV	784	645	0.06%	0.007%
98	16.352	4666	4669	4671	rBV2	698	443	0.04%	0.005%
99	17.098	4898	4901	4906	rBV2	1004	1088	0.09%	0.012%
100	17.423	4998	5002	5005	rBV3	1019	909	0.08%	0.010%

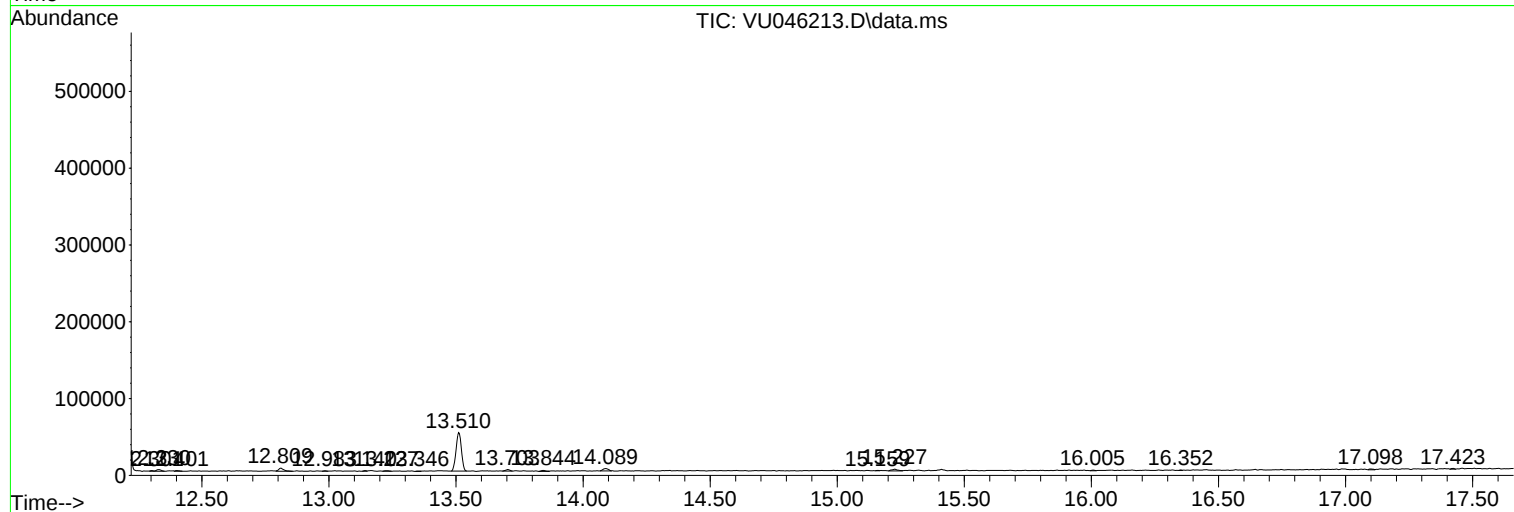
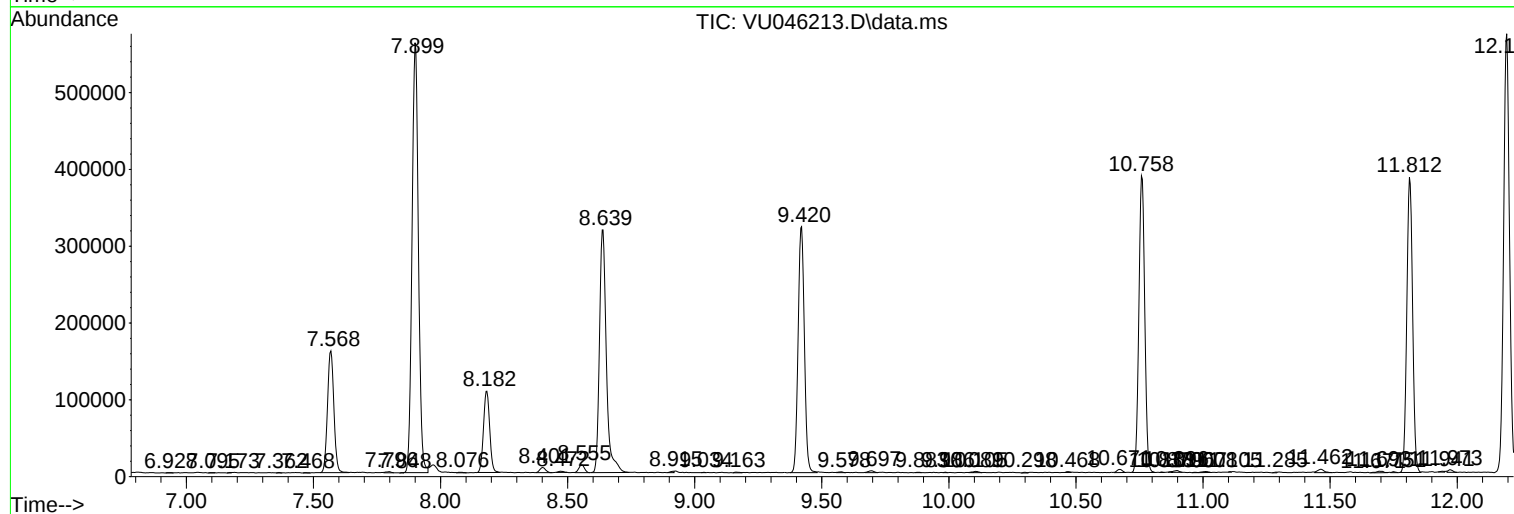
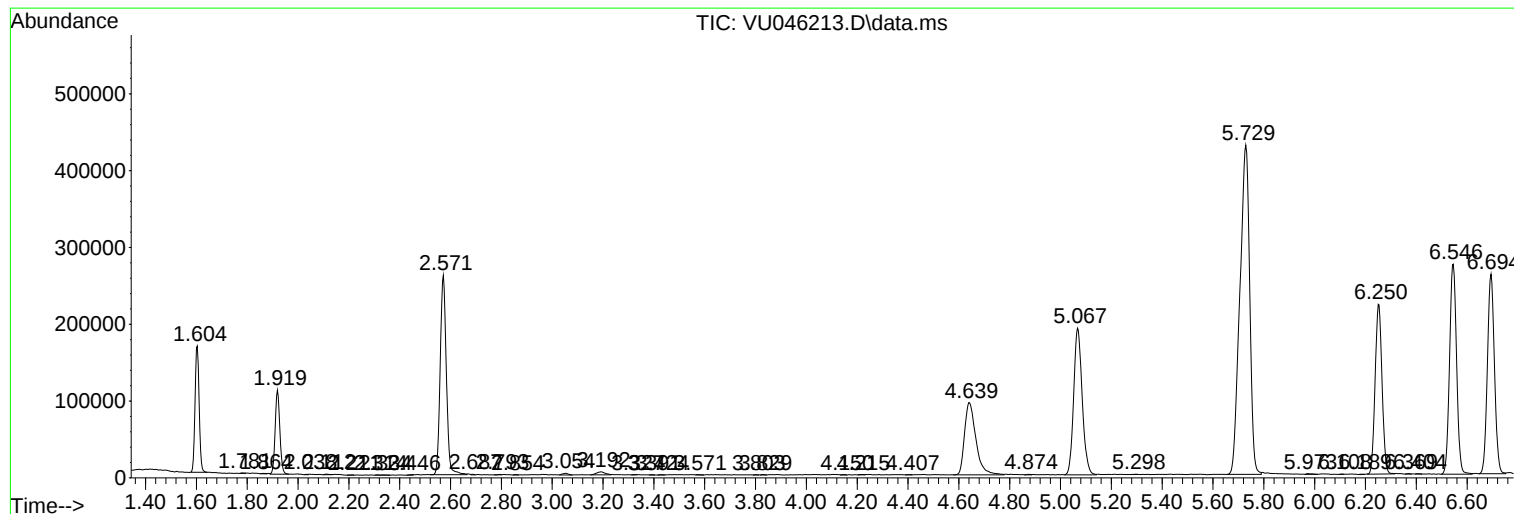
Sum of corrected areas: 8987354

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Instrument :
MSVOA_U
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EX8C8MEDL

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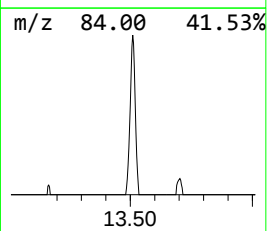
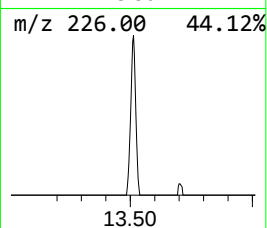
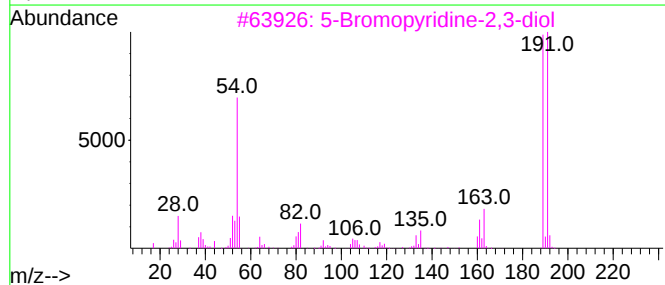
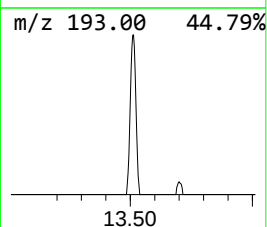
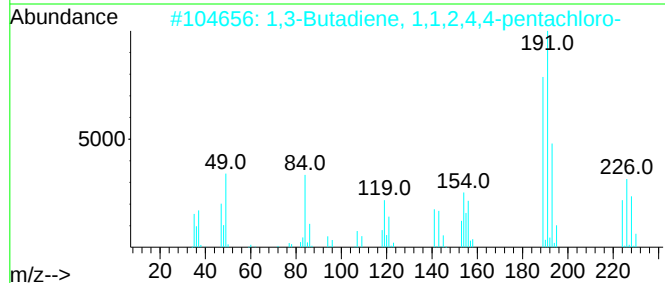
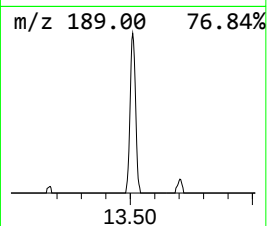
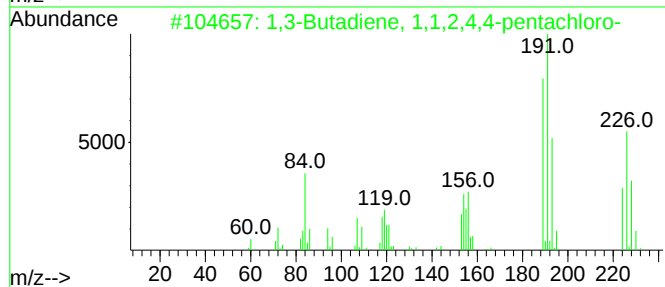
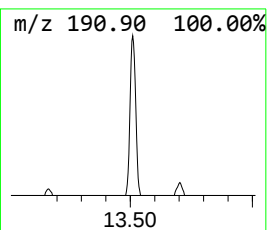
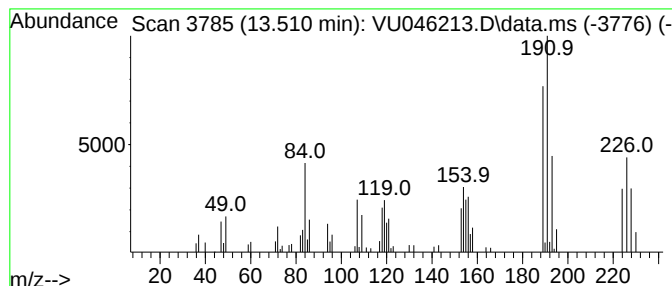
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 1,3-Butadiene, 1,1,2,4,4-pe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.510	5.98 ug/L	72574	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HC15	021400-41-9	99
2			1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HC15	021400-41-9	95
3			5-Bromopyridine-2,3-diol	189	C5H4BrNO2	034206-49-0	30
4			4-Bromo-2-furamide	189	C5H4BrNO2	957345-95-8	27
5			1,1,2,3,4-Pentachlorobuta-1,3-diene	224	C4HC15	1010487-10-4	18



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Butadiene, ...	13.510	6.0	ug/L	72574	3	11.812	607131	50.0