

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046156.D
 Acq On : 07 Dec 2021 21:48
 Operator : SY/MD
 Sample : M4887-14ME
 Misc : 3.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 30 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: VU046156.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	100	rVB	172764	222124	14.63%	1.900%
2	1.919	170	180	198	rBV	100411	164161	10.81%	1.404%
3	2.028	212	214	216	rBV	490	290	0.02%	0.002%
4	2.549	364	376	389	rBV	301529	489440	32.23%	4.186%
5	3.038	521	528	540	rVB5	1566	2991	0.20%	0.026%
6	3.183	559	573	594	rBV	10456	26578	1.75%	0.227%
7	3.607	700	705	706	rBV	152	158	0.01%	0.001%
8	3.826	768	773	775	rVB	179	183	0.01%	0.002%
9	3.848	776	780	783	rBB	179	158	0.01%	0.001%
10	4.282	912	915	918	rBV	145	148	0.01%	0.001%
11	4.388	945	948	951	rBV	146	147	0.01%	0.001%
12	4.575	1001	1006	1011	rBB	173	248	0.02%	0.002%
13	4.655	1012	1031	1087	rBV2	77266	372107	24.50%	3.183%
14	5.063	1141	1158	1186	rVB	241658	584714	38.50%	5.001%
15	5.176	1191	1193	1197	rVB	317	180	0.01%	0.002%
16	5.723	1341	1363	1394	rBV2	595857	1518664	100.00%	12.989%
17	5.916	1420	1423	1427	rBV2	252	224	0.01%	0.002%
18	5.980	1432	1443	1456	rBV4	4933	12685	0.84%	0.108%
19	6.115	1481	1485	1492	rVB2	292	425	0.03%	0.004%
20	6.250	1512	1527	1554	rBV	264113	539814	35.55%	4.617%
21	6.343	1554	1556	1563	rVV	509	575	0.04%	0.005%
22	6.372	1563	1565	1568	rVV2	249	182	0.01%	0.002%
23	6.388	1568	1570	1574	rVV	263	207	0.01%	0.002%
24	6.411	1574	1577	1580	rVB	194	149	0.01%	0.001%
25	6.459	1590	1592	1596	rBV	150	152	0.01%	0.001%
26	6.539	1602	1617	1649	rBV	423166	813553	53.57%	6.958%
27	6.690	1650	1664	1693	rVV	328224	672937	44.31%	5.756%
28	6.793	1693	1696	1698	rVV2	296	221	0.01%	0.002%
29	6.809	1698	1701	1706	rVB2	546	565	0.04%	0.005%
30	7.044	1770	1774	1778	rBV2	273	286	0.02%	0.002%
31	7.092	1787	1789	1793	rVB2	180	143	0.01%	0.001%
32	7.186	1813	1818	1820	rBV	419	366	0.02%	0.003%
33	7.231	1830	1832	1836	rVB	485	302	0.02%	0.003%
34	7.253	1836	1839	1842	rBV	157	149	0.01%	0.001%
35	7.311	1854	1857	1861	rVB	297	247	0.02%	0.002%
36	7.359	1867	1872	1874	rBB	147	149	0.01%	0.001%

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 ALS Vial : 30 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

37	7.568	1922	1937	1966	rBV	182064	363518	23.94%	3.109%
38	7.687	1970	1974	1975	rBV	443	300	0.02%	0.003%
39	7.732	1986	1988	1994	rVB	214	181	0.01%	0.002%
40	7.793	1997	2007	2017	rBV3	3629	6776	0.45%	0.058%
41	7.899	2025	2040	2058	rBV	691983	1302449	85.76%	11.140%
42	8.182	2115	2128	2153	rVV	106571	245626	16.17%	2.101%
43	8.407	2191	2198	2205	rBV3	1781	2839	0.19%	0.024%
44	8.475	2212	2219	2225	rVB	349	554	0.04%	0.005%
45	8.552	2234	2243	2254	rBV4	12643	20954	1.38%	0.179%
46	8.677	2259	2282	2317	rBV	247124	797914	52.54%	6.825%
47	8.928	2355	2360	2361	rBV	401	300	0.02%	0.003%
48	8.944	2361	2365	2368	rVV3	368	404	0.03%	0.003%
49	9.423	2495	2514	2541	rVB	313604	680798	44.83%	5.823%
50	9.571	2554	2560	2566	rBV	304	466	0.03%	0.004%
51	9.703	2592	2601	2610	rVV2	1255	2241	0.15%	0.019%
52	10.108	2722	2727	2733	rVB2	527	683	0.04%	0.006%
53	10.224	2759	2763	2770	rVB	312	327	0.02%	0.003%
54	10.320	2790	2793	2800	rVB2	245	223	0.01%	0.002%
55	10.472	2833	2840	2845	rBV5	801	927	0.06%	0.008%
56	10.542	2856	2862	2869	rVB3	537	557	0.04%	0.005%
57	10.671	2893	2902	2912	rVB2	6303	9010	0.59%	0.077%
58	10.771	2919	2933	2952	rBV	476735	796283	52.43%	6.811%
59	10.864	2956	2962	2963	rBV	1150	838	0.06%	0.007%
60	11.012	3000	3008	3014	rBV3	995	1439	0.09%	0.012%
61	11.121	3026	3042	3048	rBV6	2024	3925	0.26%	0.034%
62	11.205	3064	3068	3071	rVB3	529	401	0.03%	0.003%
63	11.298	3094	3097	3099	rBV2	323	278	0.02%	0.002%
64	11.420	3129	3135	3139	rBV3	662	825	0.05%	0.007%
65	11.456	3139	3146	3161	rVB4	4917	8933	0.59%	0.076%
66	11.578	3177	3184	3191	rVB2	1078	1467	0.10%	0.013%
67	11.693	3213	3220	3232	rBV3	2883	4364	0.29%	0.037%
68	11.745	3232	3236	3238	rVB2	316	221	0.01%	0.002%
69	11.819	3246	3259	3273	rBV	456535	717119	47.22%	6.134%
70	11.902	3282	3285	3287	rBV2	332	246	0.02%	0.002%
71	11.944	3291	3298	3302	rVV4	2293	3808	0.25%	0.033%
72	11.970	3302	3306	3316	rVB2	4969	6901	0.45%	0.059%
73	12.086	3340	3342	3346	rVB2	291	199	0.01%	0.002%
74	12.198	3359	3377	3391	rBV	751565	1194281	78.64%	10.215%
75	12.266	3396	3398	3399	rBV	455	223	0.01%	0.002%
76	12.330	3409	3418	3428	rBV4	3450	4757	0.31%	0.041%

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 ALS Vial : 30 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

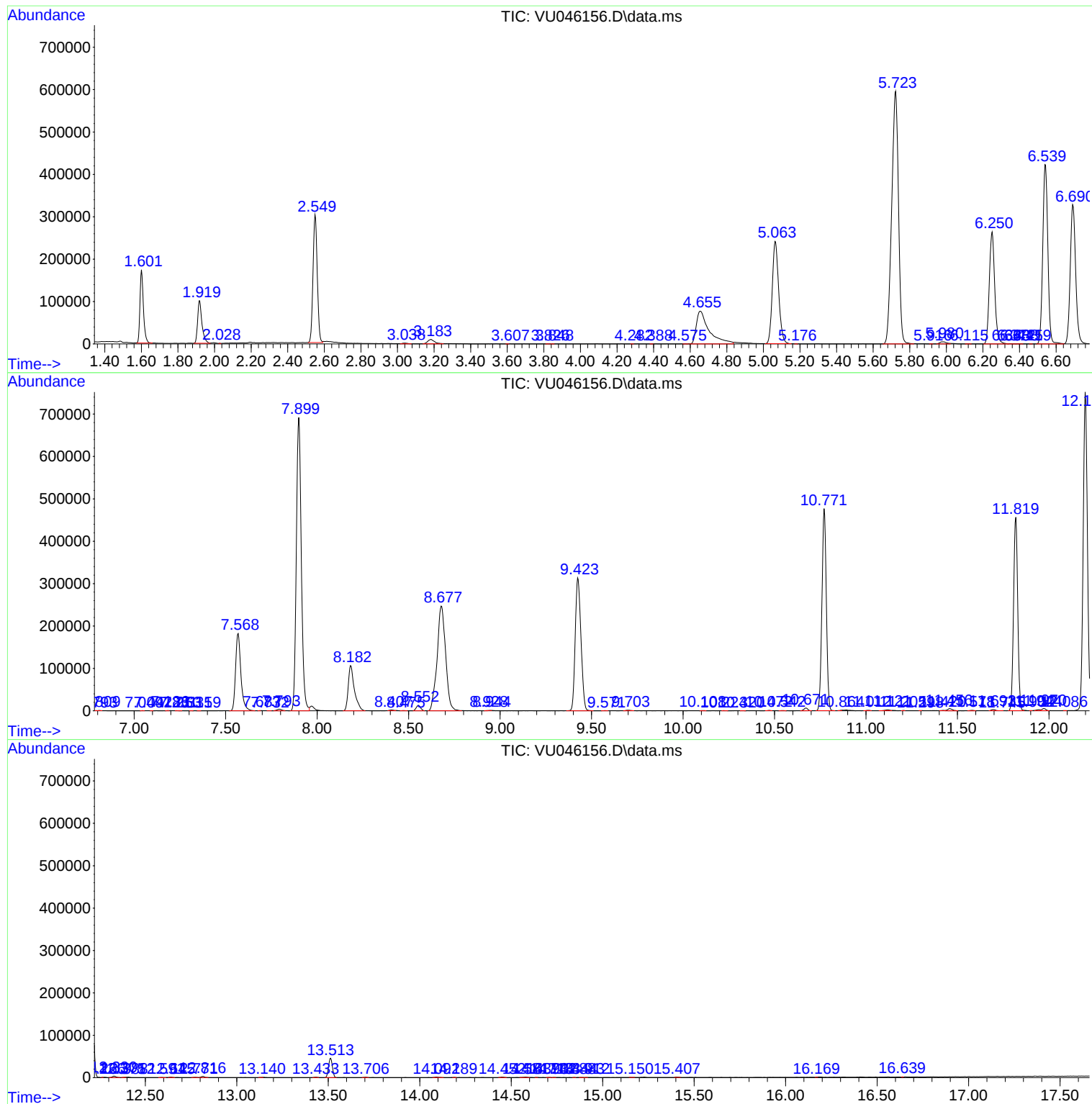
77	12.375	3430	3432	3434	rBV	343	201	0.01%	0.002%
78	12.388	3434	3436	3438	rBV	390	197	0.01%	0.002%
79	12.591	3493	3499	3506	rBV2	303	513	0.03%	0.004%
80	12.645	3510	3516	3521	rVB5	900	976	0.06%	0.008%
81	12.771	3549	3555	3561	rVV	559	807	0.05%	0.007%
82	12.816	3562	3569	3578	rVB3	2563	3401	0.22%	0.029%
83	13.140	3663	3670	3671	rBV2	621	543	0.04%	0.005%
84	13.433	3755	3761	3766	rVV3	923	1026	0.07%	0.009%
85	13.513	3776	3786	3796	rVB2	45632	65814	4.33%	0.563%
86	13.706	3839	3846	3851	rBV2	859	954	0.06%	0.008%
87	14.092	3959	3966	3978	rBV3	1196	1726	0.11%	0.015%
88	14.189	3993	3996	4000	rVB2	485	329	0.02%	0.003%
89	14.452	4071	4078	4085	rBV4	1054	1393	0.09%	0.012%
90	14.581	4107	4118	4124	rBV3	921	1633	0.11%	0.014%
91	14.639	4133	4136	4138	rBV2	317	218	0.01%	0.002%
92	14.713	4152	4159	4161	rBV2	198	237	0.02%	0.002%
93	14.732	4162	4165	4169	rVB2	239	201	0.01%	0.002%
94	14.844	4197	4200	4203	rVB	254	156	0.01%	0.001%
95	14.883	4208	4212	4217	rVB2	179	183	0.01%	0.002%
96	14.912	4217	4221	4223	rBV2	219	191	0.01%	0.002%
97	15.150	4293	4295	4303	rVB2	246	201	0.01%	0.002%
98	15.407	4370	4375	4381	rVB5	781	926	0.06%	0.008%
99	16.169	4609	4612	4614	rBV2	569	394	0.03%	0.003%
100	16.639	4756	4758	4760	rBV	595	249	0.02%	0.002%

Sum of corrected areas: 11691646

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ALS Vial : 30 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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ALS Vial : 30 Sample Multiplier: 1

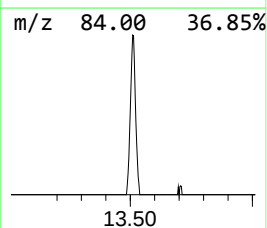
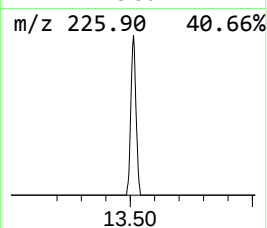
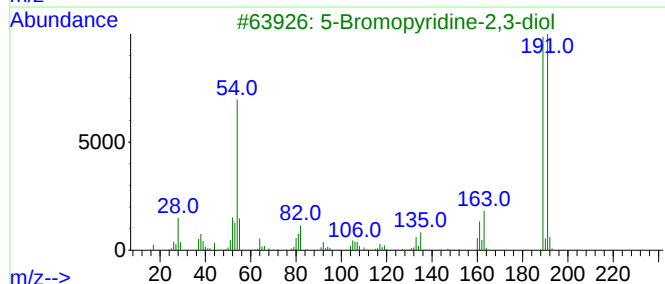
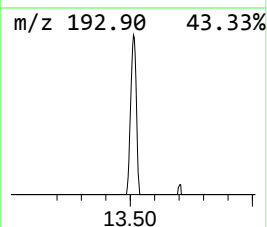
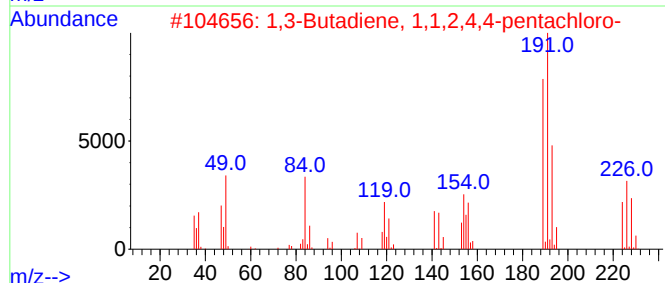
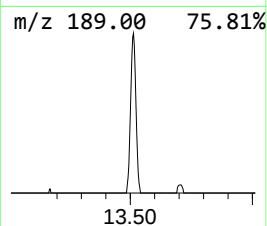
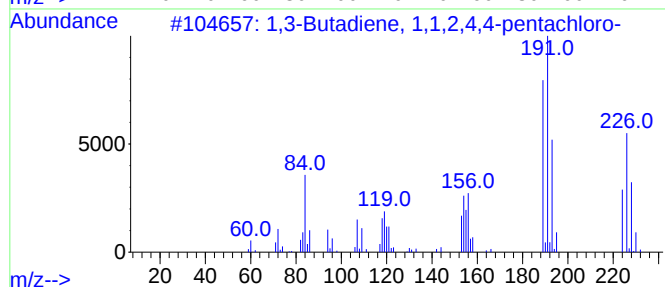
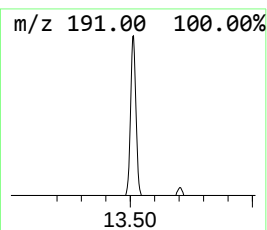
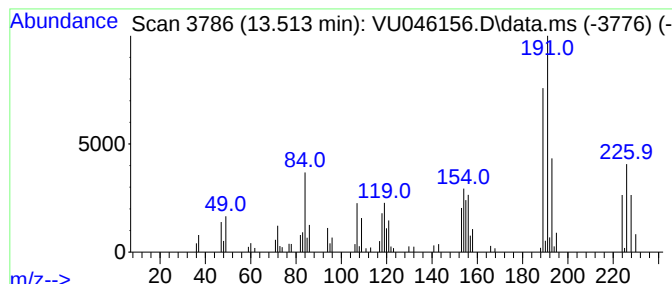
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.513	4.59 ug/L	65814	1,4-Dichlorobenzene-d4	11.819

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	51		
3	5-Bromopyridine-2,3-diol	189	C5H4BrNO2	034206-49-0	38		
4	1,1,2,3,4-Pentachlorobuta-1,3-diene	224	C4HC15	1010487-10-4	38		
5	4-Bromo-2-furamide	189	C5H4BrNO2	957345-95-8	35		



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Misc : 3.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 30 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Butadiene, ...	13.513	4.6	ug/L	65814	3	11.819	717119	50.0