

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120921\
 Data File : VU046217.D
 Acq On : 09 Dec 2021 14:03
 Operator : SY/MD
 Sample : M4887-14MEDL 10X
 Misc : 3.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 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: VU046217.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	75	81	95	rVB	85788	95233	11.40%	1.197%
2	1.919	172	180	191	rVB	69073	87754	10.51%	1.103%
3	2.208	267	270	273	rVB	208	117	0.01%	0.001%
4	2.224	273	275	277	rBV	215	87	0.01%	0.001%
5	2.237	277	279	281	rBV	138	76	0.01%	0.001%
6	2.285	292	294	297	rBV	172	95	0.01%	0.001%
7	2.311	298	302	304	rVB2	244	176	0.02%	0.002%
8	2.327	304	307	311	rVB2	218	139	0.02%	0.002%
9	2.359	311	317	320	rBV	316	399	0.05%	0.005%
10	2.440	339	342	343	rBV	396	218	0.03%	0.003%
11	2.452	343	346	351	rVV	530	501	0.06%	0.006%
12	2.571	371	383	416	rBV	140725	241188	28.88%	3.031%
13	3.054	523	533	543	rBV5	2006	3743	0.45%	0.047%
14	3.559	687	690	695	rBB2	344	262	0.03%	0.003%
15	3.983	819	822	825	rVB	494	325	0.04%	0.004%
16	4.224	893	897	901	rBV2	514	583	0.07%	0.007%
17	4.259	906	908	911	rVV	414	240	0.03%	0.003%
18	4.636	1009	1025	1060	rBV	103268	297365	35.61%	3.737%
19	5.066	1144	1159	1185	rVB	153992	357256	42.78%	4.490%
20	5.613	1326	1329	1330	rBV	283	144	0.02%	0.002%
21	5.729	1343	1365	1384	rBV2	298052	835129	100.00%	10.497%
22	6.015	1451	1454	1456	rBV	383	234	0.03%	0.003%
23	6.250	1513	1527	1552	rBV	310281	585168	70.07%	7.355%
24	6.546	1605	1619	1639	rBV	273338	515293	61.70%	6.477%
25	6.693	1651	1665	1683	rBV	203070	396215	47.44%	4.980%
26	6.851	1711	1714	1721	rBV	375	448	0.05%	0.006%
27	7.105	1784	1793	1802	rBV	828	1813	0.22%	0.023%
28	7.568	1925	1937	1953	rVB	121827	207783	24.88%	2.612%
29	7.722	1983	1985	1988	rBV	349	242	0.03%	0.003%
30	7.774	1997	2001	2002	rBV	553	405	0.05%	0.005%
31	7.899	2027	2040	2056	rBV	356525	615966	73.76%	7.742%
32	8.179	2116	2127	2143	rBV	84325	139529	16.71%	1.754%
33	8.401	2190	2196	2205	rVB4	6270	8844	1.06%	0.111%
34	8.500	2225	2227	2229	rBV	262	117	0.01%	0.001%
35	8.520	2229	2233	2235	rBV2	385	323	0.04%	0.004%
36	8.555	2235	2244	2253	rVB2	9752	15991	1.91%	0.201%

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 Title : VOC Analysis

37	8.635	2257	2269	2304	rVB	320163	590473	70.70%	7.421%
38	9.417	2498	2512	2535	rBV	443018	741027	88.73%	9.314%
39	9.687	2591	2596	2598	rBV4	1436	1328	0.16%	0.017%
40	9.742	2609	2613	2615	rBV2	334	225	0.03%	0.003%
41	9.835	2637	2642	2646	rBV2	413	453	0.05%	0.006%
42	9.893	2657	2660	2662	rBV	238	123	0.01%	0.002%
43	9.906	2662	2664	2669	rVB	319	227	0.03%	0.003%
44	10.034	2701	2704	2706	rBV	298	206	0.02%	0.003%
45	10.288	2779	2783	2784	rBV	220	163	0.02%	0.002%
46	10.394	2812	2816	2818	rBV2	498	365	0.04%	0.005%
47	10.449	2830	2833	2834	rBV2	358	211	0.03%	0.003%
48	10.465	2834	2838	2847	rVV6	1436	1938	0.23%	0.024%
49	10.606	2879	2882	2883	rBV	441	252	0.03%	0.003%
50	10.758	2916	2929	2945	rBV	373482	598915	71.72%	7.528%
51	10.947	2983	2988	2995	rVB2	341	433	0.05%	0.005%
52	11.012	2999	3008	3014	rVB6	1318	2200	0.26%	0.028%
53	11.073	3024	3027	3028	rBV2	273	160	0.02%	0.002%
54	11.118	3038	3041	3046	rBV	549	461	0.06%	0.006%
55	11.291	3092	3095	3099	rVB2	448	306	0.04%	0.004%
56	11.417	3131	3134	3140	rBV3	930	776	0.09%	0.010%
57	11.767	3239	3243	3245	rBV	407	299	0.04%	0.004%
58	11.812	3245	3257	3273	rVV	490559	778407	93.21%	9.784%
59	11.886	3278	3280	3281	rBV	398	174	0.02%	0.002%
60	12.012	3316	3319	3321	rBV	214	146	0.02%	0.002%
61	12.195	3363	3376	3390	rBV	460280	747526	89.51%	9.395%
62	12.298	3404	3408	3411	rBV2	463	417	0.05%	0.005%
63	12.404	3438	3441	3442	rBV	192	113	0.01%	0.001%
64	12.639	3512	3514	3516	rBV	227	107	0.01%	0.001%
65	12.655	3516	3519	3524	rVB	401	302	0.04%	0.004%
66	12.700	3529	3533	3536	rBV2	372	310	0.04%	0.004%
67	12.815	3562	3569	3575	rVB5	2748	3719	0.45%	0.047%
68	13.166	3675	3678	3683	rVB3	884	759	0.09%	0.010%
69	13.249	3701	3704	3708	rVB	366	252	0.03%	0.003%
70	13.272	3708	3711	3715	rBV	297	220	0.03%	0.003%
71	13.510	3775	3785	3795	rBV2	48896	71615	8.58%	0.900%
72	13.700	3840	3844	3851	rVB4	2318	2251	0.27%	0.028%

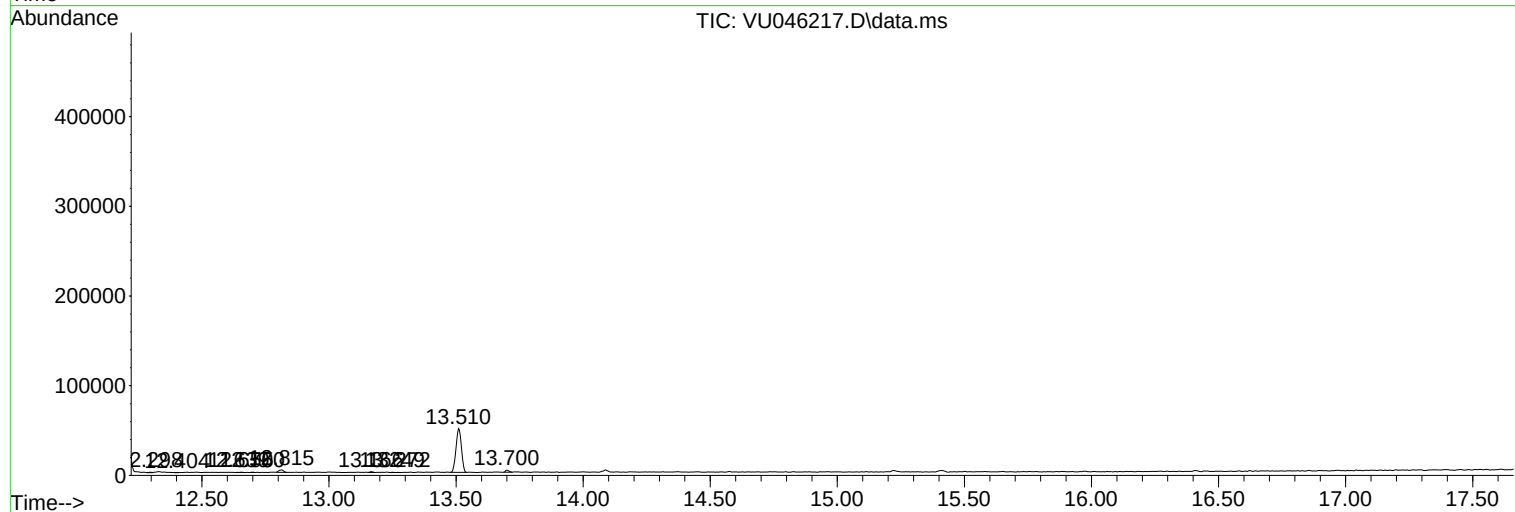
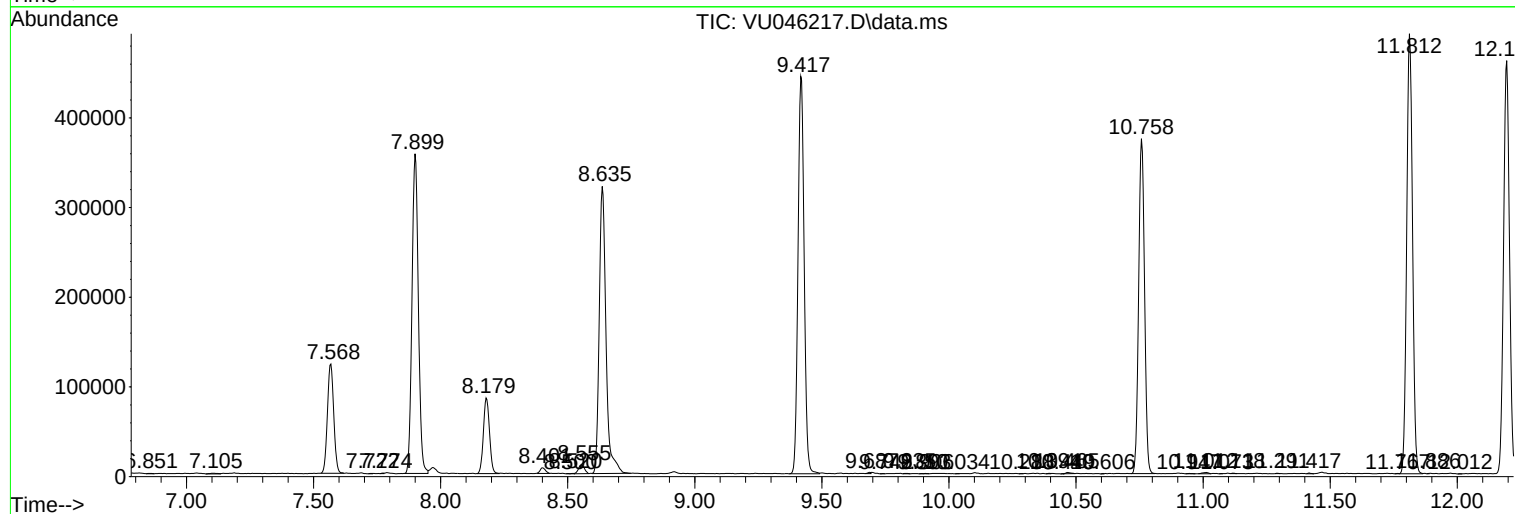
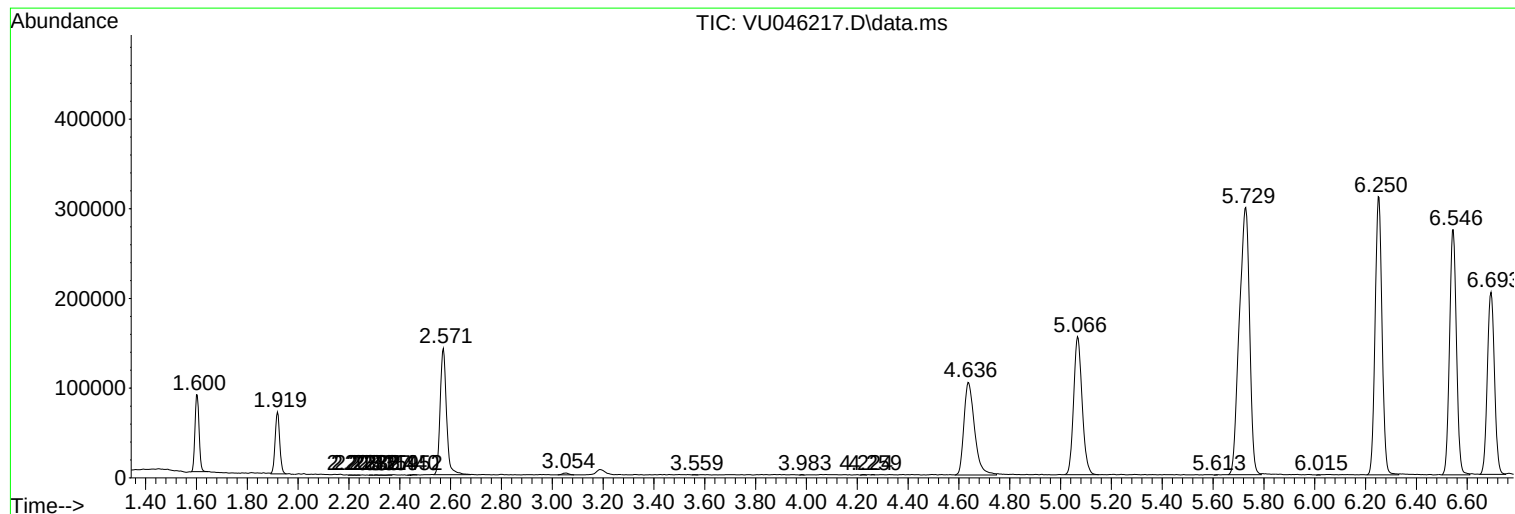
Sum of corrected areas: 7956260

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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



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

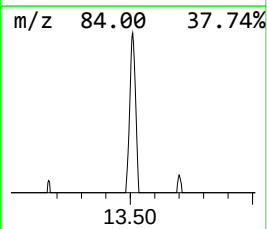
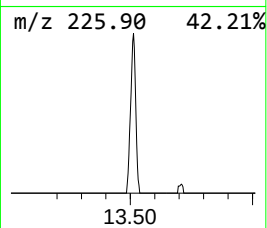
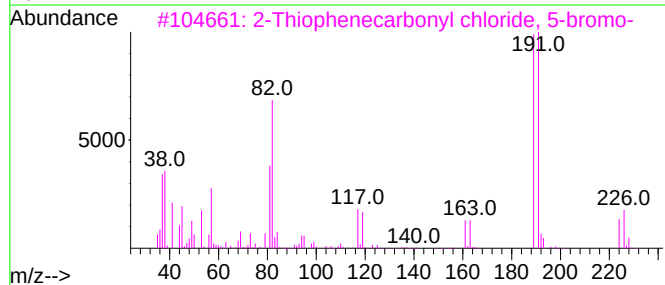
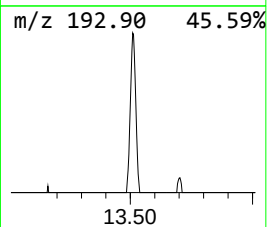
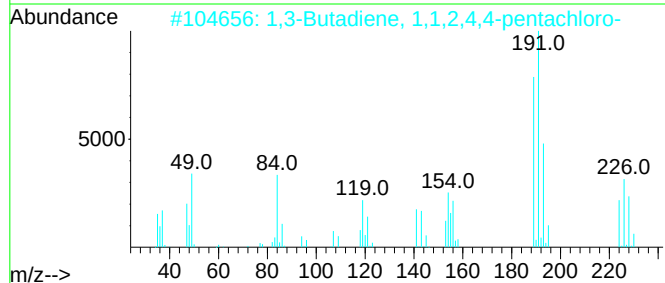
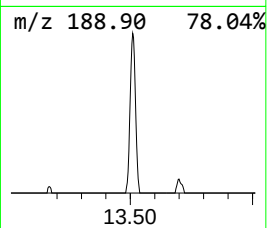
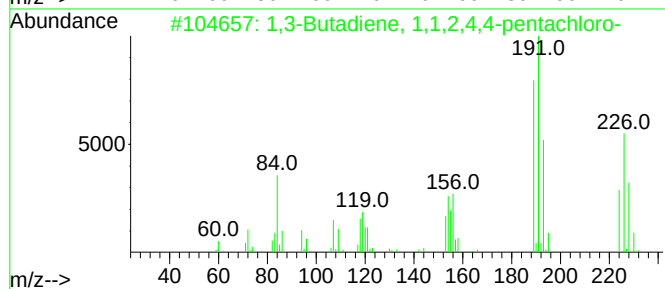
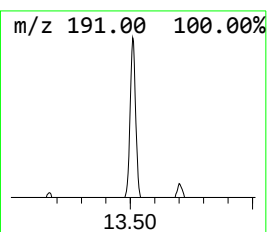
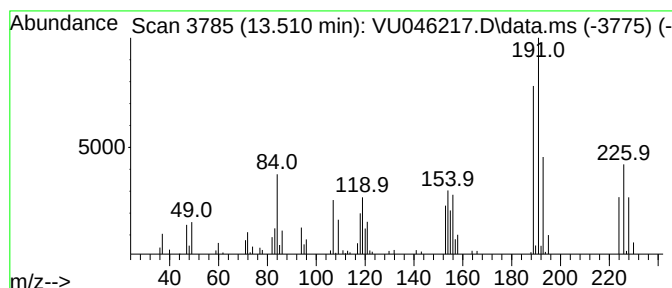
TIC Library : C:\Database\NIST20.L

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	4.60 ug/L	71615	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	2-Thiophenecarbonyl chloride, 5-...	224	C5H2BrClO5	031555-60-9	38		
4	4-Bromo-2-furamide	189	C5H4BrNO2	957345-95-8	32		
5	5-Bromopyridine-2,3-diol	189	C5H4BrNO2	034206-49-0	30		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Butadiene, ...	13.510	4.6	ug/L	71615	3	11.812	778407	50.0