

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046179.D
 Acq On : 08 Dec 2021 16:34
 Operator : SY/MD
 Sample : M4887-14ME
 Misc : 3.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8C8ME

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: VU046179.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	74	81	98	rVB	73477	96360	1.81%	0.730%
2	1.916	172	179	197	rVB	45698	76398	1.43%	0.579%
3	1.993	199	203	213	rVB5	2783	3386	0.06%	0.026%
4	2.189	256	264	265	rBV4	1117	1315	0.02%	0.010%
5	2.549	360	376	388	rBV	137536	229339	4.31%	1.737%
6	3.044	521	530	531	rBV5	2122	3079	0.06%	0.023%
7	3.186	561	574	589	rVV	8562	20784	0.39%	0.157%
8	4.514	979	987	988	rBV2	1176	1139	0.02%	0.009%
9	4.658	1014	1032	1067	rBV2	39126	173427	3.26%	1.313%
10	5.067	1143	1159	1189	rVB	115831	296204	5.56%	2.243%
11	5.385	1247	1258	1267	rBV6	1608	3194	0.06%	0.024%
12	5.723	1343	1363	1393	rVB2	291999	750686	14.09%	5.685%
13	5.983	1433	1444	1458	rVV6	6068	14669	0.28%	0.111%
14	6.250	1512	1527	1553	rBV	233388	478597	8.98%	3.624%
15	6.542	1601	1618	1647	rBV	2781101	5327142	100.00%	40.340%
16	6.694	1651	1665	1680	rBV	161149	329506	6.19%	2.495%
17	7.070	1772	1782	1793	rBV5	1925	4062	0.08%	0.031%
18	7.234	1825	1833	1839	rBV5	1486	2209	0.04%	0.017%
19	7.497	1906	1915	1921	rVV4	1642	2436	0.05%	0.018%
20	7.568	1924	1937	1960	rVV	88377	177113	3.32%	1.341%
21	7.793	1998	2007	2014	rBV4	3030	5781	0.11%	0.044%
22	7.899	2020	2040	2056	rBV	324813	618763	11.62%	4.686%
23	8.128	2107	2111	2117	rVB2	1737	1977	0.04%	0.015%
24	8.182	2117	2128	2157	rVB2	53279	126256	2.37%	0.956%
25	8.404	2187	2197	2228	rVB3	34302	89813	1.69%	0.680%
26	8.555	2231	2244	2260	rVB	92102	161210	3.03%	1.221%
27	8.681	2260	2283	2312	rBV	123934	401514	7.54%	3.040%
28	8.867	2332	2341	2349	rBV3	3977	6078	0.11%	0.046%
29	8.925	2351	2359	2369	rBV5	5897	9561	0.18%	0.072%
30	9.121	2411	2420	2427	rBV4	3838	5908	0.11%	0.045%
31	9.166	2427	2434	2442	rVB8	1477	2379	0.04%	0.018%
32	9.211	2442	2448	2456	rBV3	1659	2202	0.04%	0.017%
33	9.340	2483	2488	2494	rVB6	1474	1788	0.03%	0.014%
34	9.427	2494	2515	2536	rBV	269687	604899	11.36%	4.581%
35	9.574	2555	2561	2569	rBV4	1526	2682	0.05%	0.020%
36	9.652	2580	2585	2588	rBV3	1293	1437	0.03%	0.011%

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

37	9.700	2591	2600	2609	rBV2	6305	11997	0.23%	0.091%
38	10.021	2693	2700	2708	rVV6	2012	3709	0.07%	0.028%
39	10.108	2718	2727	2738	rVB3	6277	11549	0.22%	0.087%
40	10.253	2760	2772	2773	rBV5	5383	8468	0.16%	0.064%
41	10.320	2787	2793	2798	rBV5	3019	3657	0.07%	0.028%
42	10.472	2826	2840	2855	rBV4	15456	29603	0.56%	0.224%
43	10.658	2892	2898	2899	rBV4	2118	1823	0.03%	0.014%
44	10.703	2909	2912	2918	rVB6	1697	1873	0.04%	0.014%
45	10.771	2918	2933	2959	rVB	240289	443309	8.32%	3.357%
46	10.912	2965	2977	2984	rBV9	2514	5606	0.11%	0.042%
47	11.015	2999	3009	3021	rVB2	19393	32660	0.61%	0.247%
48	11.115	3029	3040	3050	rVB5	12023	21423	0.40%	0.162%
49	11.301	3087	3098	3106	rBV8	3665	6379	0.12%	0.048%
50	11.378	3115	3122	3125	rBV6	1132	1220	0.02%	0.009%
51	11.417	3126	3134	3141	rVV4	7624	11474	0.22%	0.087%
52	11.471	3142	3151	3165	rVB4	9448	19167	0.36%	0.145%
53	11.574	3178	3183	3185	rBV3	1448	1156	0.02%	0.009%
54	11.648	3201	3206	3214	rVB3	3303	3876	0.07%	0.029%
55	11.703	3218	3223	3224	rBV4	1811	1582	0.03%	0.012%
56	11.819	3246	3259	3272	rBV	411069	654793	12.29%	4.958%
57	11.902	3278	3285	3294	rVV4	5379	8055	0.15%	0.061%
58	12.124	3348	3354	3360	rVB6	1494	2094	0.04%	0.016%
59	12.198	3364	3377	3388	rBV	368430	604703	11.35%	4.579%
60	12.327	3408	3417	3426	rVV2	20227	30573	0.57%	0.232%
61	12.378	3429	3433	3448	rVB2	4630	8707	0.16%	0.066%
62	12.449	3450	3455	3456	rBV3	1693	1242	0.02%	0.009%
63	12.465	3456	3460	3463	rBV2	1627	1586	0.03%	0.012%
64	12.664	3517	3522	3528	rBV3	1411	1569	0.03%	0.012%
65	12.716	3531	3538	3539	rBV5	2357	2590	0.05%	0.020%
66	12.774	3549	3556	3559	rBV6	2153	3166	0.06%	0.024%
67	12.812	3559	3568	3582	rVB2	38507	59112	1.11%	0.448%
68	12.934	3600	3606	3609	rBV5	1760	2470	0.05%	0.019%
69	13.047	3633	3641	3651	rVB8	4377	8313	0.16%	0.063%
70	13.127	3657	3666	3667	rBV3	1259	1603	0.03%	0.012%
71	13.169	3672	3679	3693	rVB4	12845	19171	0.36%	0.145%
72	13.285	3710	3715	3716	rBV3	1516	1268	0.02%	0.010%
73	13.356	3732	3737	3740	rBV3	1476	1659	0.03%	0.013%
74	13.433	3748	3761	3773	rBV3	15783	28090	0.53%	0.213%
75	13.513	3774	3786	3798	rVB	520592	797650	14.97%	6.040%
76	13.584	3801	3808	3815	rBV4	4557	6167	0.12%	0.047%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

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Sampling : 1

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Peak Location: TOP

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 Title : VOC Analysis

77	13.703	3836	3845	3852	rBV2	32164	48383	0.91%	0.366%
78	13.741	3853	3857	3871	rVB5	11288	15804	0.30%	0.120%
79	13.838	3875	3887	3894	rBV8	3985	8104	0.15%	0.061%
80	14.089	3957	3965	3973	rVB	17530	25941	0.49%	0.196%
81	14.192	3985	3997	4004	rBV6	4903	8321	0.16%	0.063%
82	14.275	4018	4023	4032	rVV8	2206	3575	0.07%	0.027%
83	14.372	4050	4053	4060	rVB3	1101	1383	0.03%	0.010%
84	14.452	4067	4078	4090	rBV4	9707	16152	0.30%	0.122%
85	14.520	4094	4099	4102	rBV7	2023	2400	0.05%	0.018%
86	14.645	4132	4138	4143	rBV6	1759	2313	0.04%	0.018%
87	15.044	4260	4262	4265	rVV2	1505	1246	0.02%	0.009%
88	15.066	4265	4269	4280	rVB7	3324	4606	0.09%	0.035%
89	15.221	4307	4317	4327	rBV	19899	30800	0.58%	0.233%
90	15.272	4327	4333	4341	rVB7	2659	4141	0.08%	0.031%
91	15.410	4361	4376	4386	rBV2	21498	38651	0.73%	0.293%
92	15.500	4397	4404	4412	rVB5	16133	22742	0.43%	0.172%
93	15.918	4529	4534	4537	rBV5	1402	1432	0.03%	0.011%
94	16.153	4600	4607	4612	rVV7	3282	4686	0.09%	0.035%
95	16.185	4612	4617	4626	rVB9	3151	4694	0.09%	0.036%
96	16.262	4631	4641	4656	rBV3	8083	16169	0.30%	0.122%
97	16.362	4669	4672	4677	rVB5	1277	1232	0.02%	0.009%
98	16.410	4678	4687	4693	rBV2	15234	23537	0.44%	0.178%
99	16.446	4694	4698	4708	rVB3	9840	12395	0.23%	0.094%
100	16.719	4777	4783	4793	rVB7	6163	8489	0.16%	0.064%

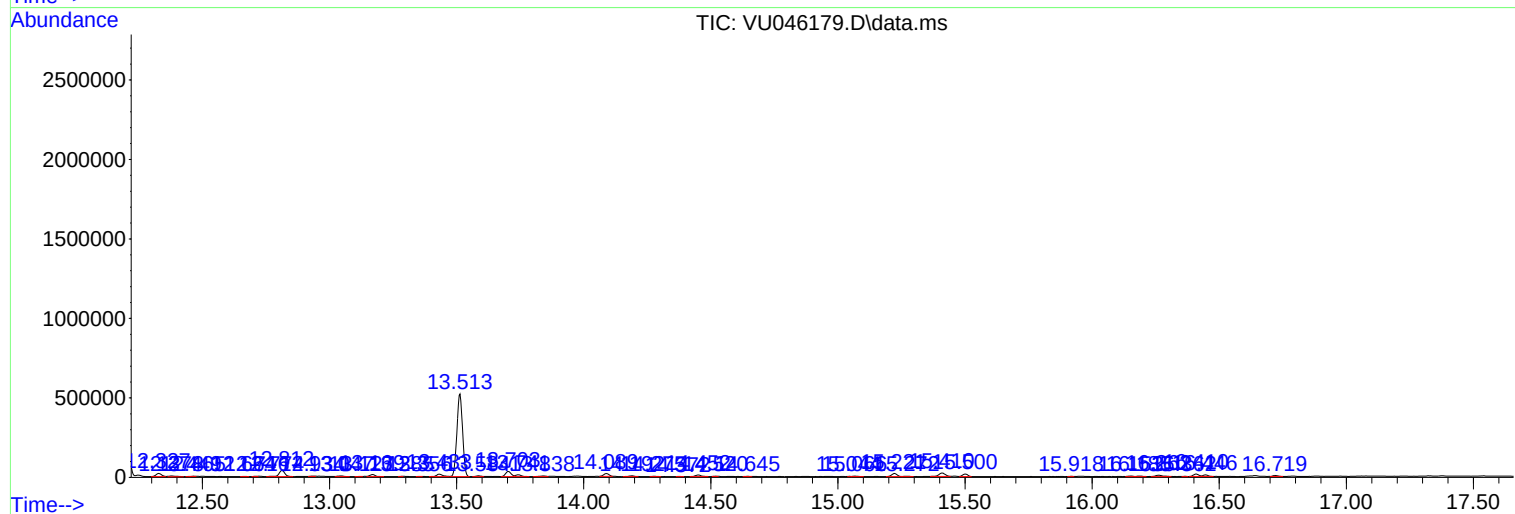
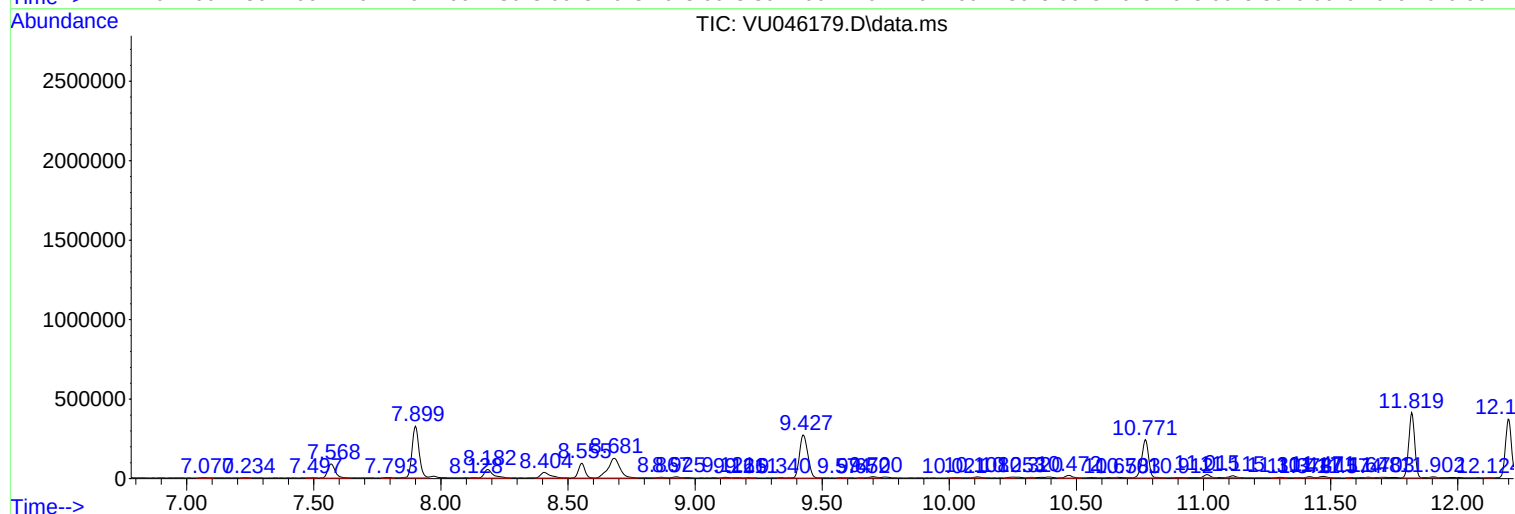
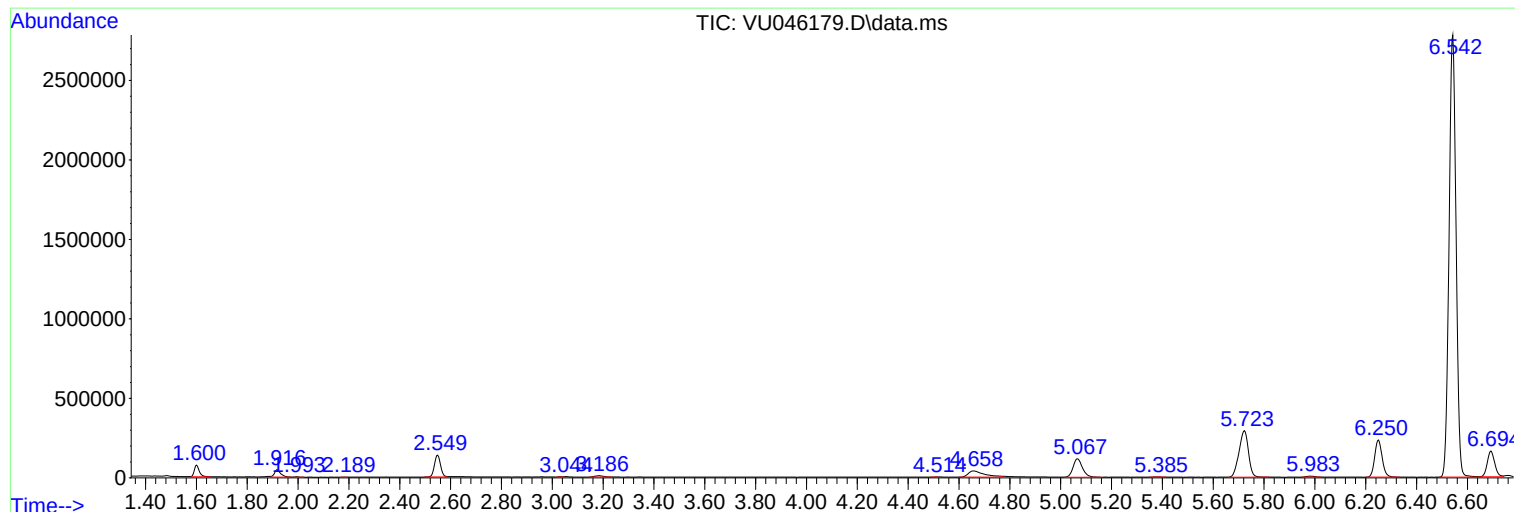
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Instrument :
MSVOA_U
ClientSampleId :
EX8C8ME

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 : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8C8ME

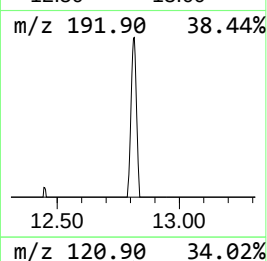
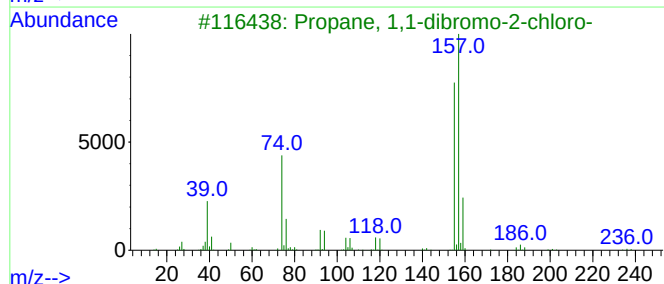
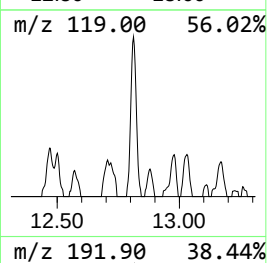
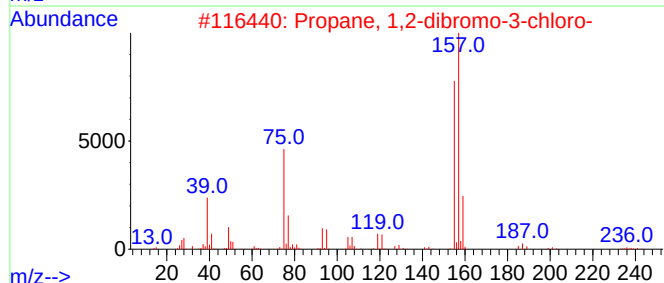
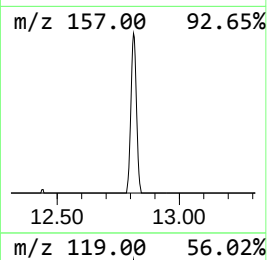
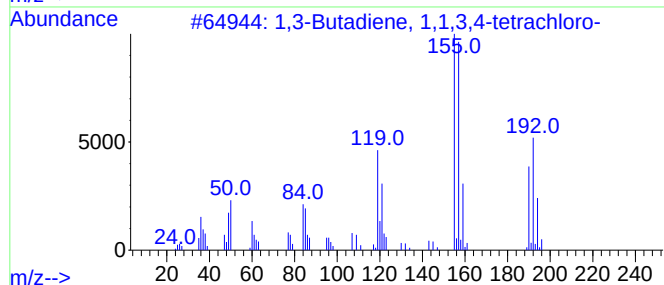
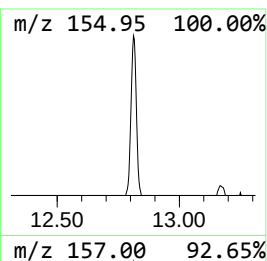
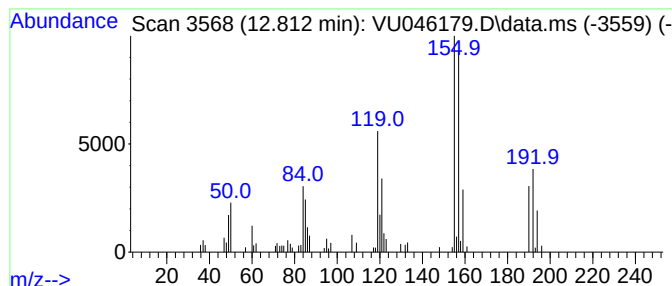
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.812	4.51 ug/L	59112	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Butadiene, 1,1,3,4-tetrachloro-	190	C4H2Cl4	042769-38-0	95
2			Propane, 1,2-dibromo-3-chloro-	234	C3H5Br2Cl	000096-12-8	38
3			Propane, 1,1-dibromo-2-chloro-	234	C3H5Br2Cl	055162-35-1	23
4			3-Pyridinecarboxylic acid, 2-chl...	157	C6H4ClNO2	002942-59-8	10
5			4-Pyridinol 3-chloro-2,6-dimethyl-	157	C7H8ClNO	088545-07-7	10



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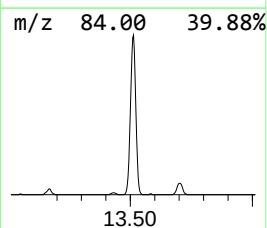
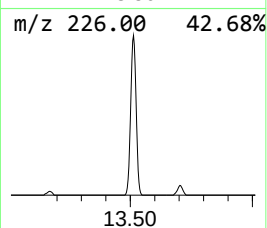
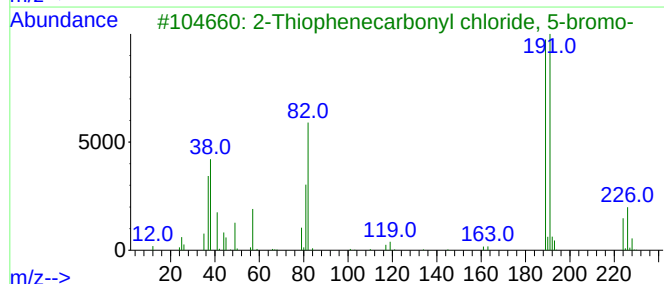
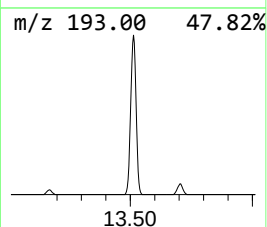
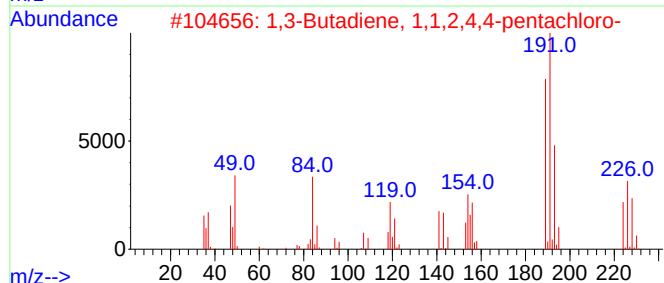
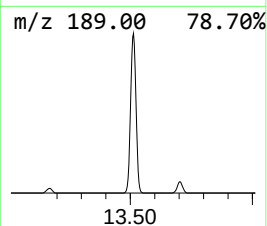
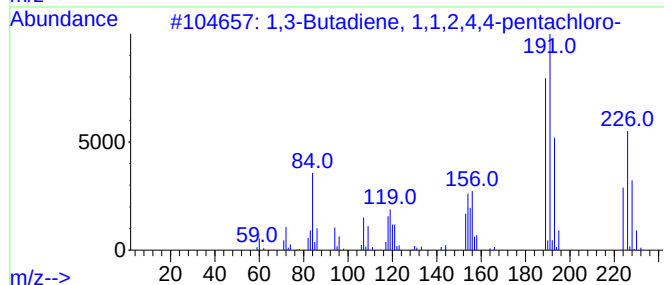
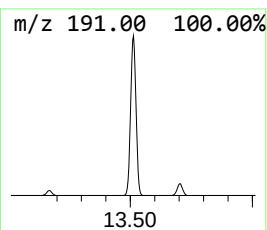
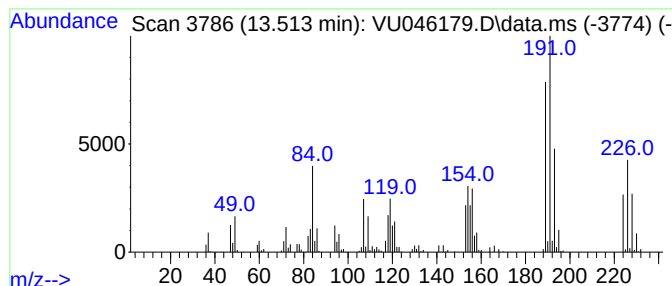
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.513	60.91 ug/L	797650	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	C4HCl5	021400-41-9	99		
2	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HCl5	021400-41-9	94		
3	2-Thiophenecarbonyl chloride, 5-...	224	C5H2BrClO5	031555-60-9	52		
4	4-Bromo-2-furamide	189	C5H4BrNO2	957345-95-8	38		
5	2-Thiophenecarbonyl chloride, 5-...	224	C5H2BrClO5	031555-60-9	38		



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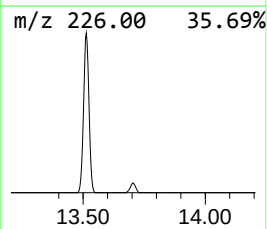
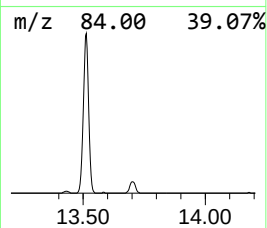
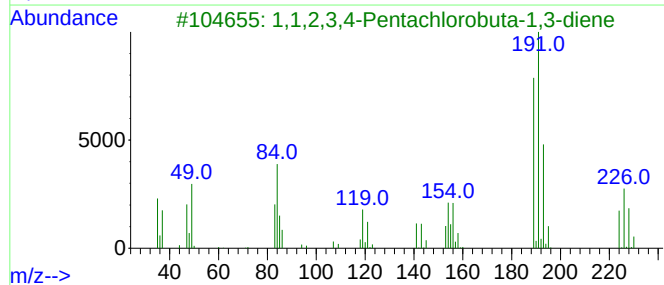
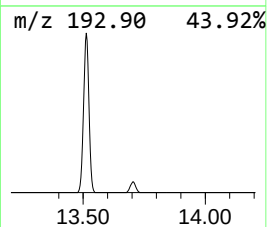
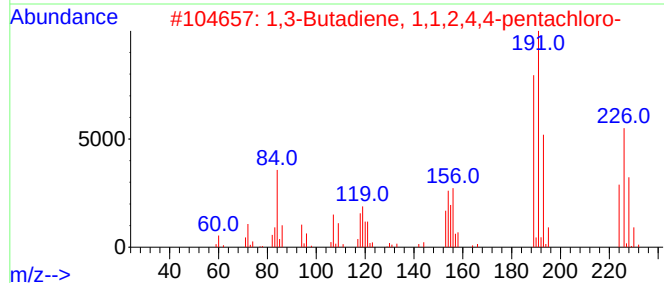
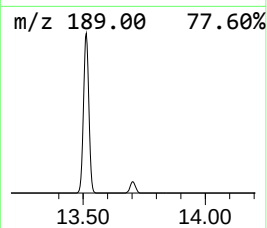
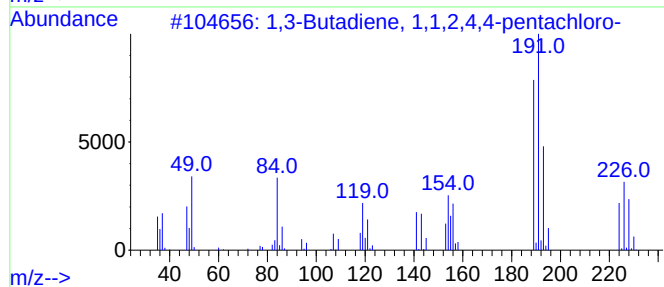
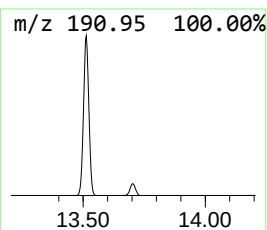
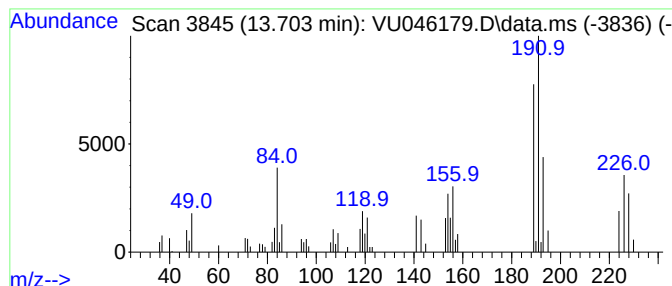
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1,1,2,3,4-Pentachlorobuta-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.703	3.69 ug/L	48383	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	97		
3	1,1,2,3,4-Pentachlorobuta-1,3-diene	224	C4HC15	1010487-10-4	94		
4	4-Bromo-2-furamide	189	C5H4BrNO2	957345-95-8	38		
5	Thiophene-3-carbonyl chloride, 4...	224	C5H2BrClO5	072899-51-5	28		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
Data File : VU046179.D
Acq On : 08 Dec 2021 16:34
Operator : SY/MD
Sample : M4887-14ME
Misc : 3.64g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8C8ME

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, ...	12.812	4.5	ug/L	59112	3	11.819	654793	50.0
1,3-Butadiene, ...	13.513	60.9	ug/L	797650	3	11.819	654793	50.0
1,1,2,3,4-Penta...	13.703	3.7	ug/L	48383	3	11.819	654793	50.0