

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
 Data File : VU042282.D
 Acq On : 05 Feb 2021 16:45
 Operator : SY/MD
 Sample : M1327-01DL 50X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 X2Z60DL

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\SFAMULM020521WMA.M

Title : VOC Analysis

Signal : TIC: VU042282.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	92958	105950	10.26%	0.781%
2	1.916	171	179	197	rVB2	72469	122848	11.89%	0.905%
3	2.526	366	369	372	rBV2	241	179	0.02%	0.001%
4	2.578	372	385	416	rVV2	221658	432349	41.86%	3.187%
5	2.790	448	451	454	rBV	408	319	0.03%	0.002%
6	3.054	520	533	555	rVB	33480	63382	6.14%	0.467%
7	3.192	564	576	592	rVB2	2149	5613	0.54%	0.041%
8	3.253	592	595	597	rBV	175	132	0.01%	0.001%
9	3.372	616	632	652	rBV	97706	228877	22.16%	1.687%
10	3.539	678	684	688	rBV2	224	332	0.03%	0.002%
11	3.639	712	715	720	rBV	216	198	0.02%	0.001%
12	3.748	746	749	757	rVB	176	197	0.02%	0.001%
13	3.957	810	814	818	rVB	210	175	0.02%	0.001%
14	4.256	905	907	911	rVB	165	136	0.01%	0.001%
15	4.282	911	915	921	rBV2	242	215	0.02%	0.002%
16	4.639	1010	1026	1061	rBV	82163	237403	22.98%	1.750%
17	4.796	1072	1075	1079	rVB3	409	288	0.03%	0.002%
18	5.015	1139	1143	1145	rBV	171	142	0.01%	0.001%
19	5.073	1145	1161	1185	rBV2	154060	372085	36.02%	2.743%
20	5.221	1202	1207	1210	rBV2	299	242	0.02%	0.002%
21	5.327	1224	1240	1255	rBV2	34463	77706	7.52%	0.573%
22	5.533	1287	1304	1320	rBV2	63770	139487	13.50%	1.028%
23	5.735	1345	1367	1376	rBV2	295805	814407	78.84%	6.003%
24	5.973	1437	1441	1442	rBV	248	168	0.02%	0.001%
25	5.983	1442	1444	1446	rVB	315	129	0.01%	0.001%
26	6.018	1452	1455	1459	rBV2	181	168	0.02%	0.001%
27	6.256	1514	1529	1545	rBV	242174	456825	44.22%	3.367%
28	6.552	1606	1621	1640	rBV	157463	295882	28.64%	2.181%
29	6.700	1652	1667	1688	rBV	188043	364019	35.24%	2.683%
30	6.774	1688	1690	1692	rBV2	214	132	0.01%	0.001%
31	6.803	1697	1699	1702	rBV	284	180	0.02%	0.001%
32	6.838	1708	1710	1713	rVB2	159	110	0.01%	0.001%
33	6.928	1723	1738	1756	rBV	59083	113067	10.95%	0.833%
34	7.050	1765	1776	1785	rVV2	14796	27132	2.63%	0.200%
35	7.115	1785	1796	1812	rVV	67091	122615	11.87%	0.904%
36	7.189	1814	1819	1822	rVV3	383	429	0.04%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
 Title : VOC Analysis

37	7.224	1824	1830	1838	rVB2	1563	2389	0.23%	0.018%
38	7.574	1925	1939	1947	rBV	114450	203433	19.69%	1.499%
39	7.719	1975	1984	1997	rBV3	9037	18596	1.80%	0.137%
40	7.803	1998	2010	2028	rVV	191922	352869	34.16%	2.601%
41	7.906	2030	2042	2053	rVV	365593	628201	60.82%	4.630%
42	7.976	2053	2064	2091	rVB	381761	657595	63.66%	4.847%
43	8.189	2118	2130	2132	rBV	83666	114936	11.13%	0.847%
44	8.218	2135	2139	2166	rVB	195000	292754	28.34%	2.158%
45	8.407	2186	2198	2215	rBV	262357	448366	43.41%	3.305%
46	8.513	2230	2231	2234	rVB	389	147	0.01%	0.001%
47	8.562	2234	2246	2260	rBV	164660	279810	27.09%	2.062%
48	8.645	2260	2272	2280	rBV	273824	478578	46.33%	3.527%
49	8.697	2281	2288	2297	rVB	138480	215476	20.86%	1.588%
50	8.819	2315	2326	2350	rVB	76524	134334	13.00%	0.990%
51	8.931	2350	2361	2374	rVV2	12367	20334	1.97%	0.150%
52	8.996	2378	2381	2385	rVB	205	133	0.01%	0.001%
53	9.131	2420	2423	2431	rVB	263	225	0.02%	0.002%
54	9.169	2431	2435	2439	rBV2	218	198	0.02%	0.001%
55	9.221	2441	2451	2463	rBV2	16086	25369	2.46%	0.187%
56	9.295	2468	2474	2482	rBV	176	268	0.03%	0.002%
57	9.333	2482	2486	2491	rBV2	168	150	0.01%	0.001%
58	9.426	2502	2515	2521	rBV	334058	610334	59.09%	4.499%
59	9.542	2540	2551	2568	rVB	66905	110305	10.68%	0.813%
60	9.703	2586	2601	2622	rBV	363760	598013	57.89%	4.408%
61	10.121	2713	2731	2755	rBV2	360616	619699	59.99%	4.568%
62	10.298	2776	2786	2801	rBV	30727	49318	4.77%	0.364%
63	10.491	2839	2846	2851	rVB	469	615	0.06%	0.005%
64	10.603	2879	2881	2884	rBV	215	124	0.01%	0.001%
65	10.767	2918	2932	2936	rBV	263608	443486	42.93%	3.269%
66	10.896	2968	2972	2973	rBV	179	119	0.01%	0.001%
67	10.999	3000	3004	3008	rBV3	470	452	0.04%	0.003%
68	11.095	3021	3034	3049	rBV	422420	637429	61.71%	4.698%
69	11.388	3123	3125	3128	rBV	219	111	0.01%	0.001%
70	11.436	3134	3140	3146	rBV2	2580	2976	0.29%	0.022%
71	11.475	3146	3152	3160	rBV2	1941	2455	0.24%	0.018%
72	11.754	3227	3239	3248	rBV	108793	170300	16.49%	1.255%
73	11.822	3248	3260	3280	rVB2	369216	793393	76.81%	5.848%
74	12.111	3347	3350	3356	rVB	237	159	0.02%	0.001%
75	12.208	3365	3380	3398	rBV2	440627	1032961	100.00%	7.614%
76	12.295	3404	3407	3410	rBV2	179	129	0.01%	0.001%

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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

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 Peak separation: 5

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 Title : VOC Analysis

77	12.484	3460	3466	3474	rBV4	1709	1859	0.18%	0.014%
78	12.764	3550	3553	3555	rBV2	218	129	0.01%	0.001%
79	13.156	3673	3675	3681	rBV	193	193	0.02%	0.001%
80	13.365	3736	3740	3745	rBV	236	249	0.02%	0.002%
81	13.436	3760	3762	3766	rVB	231	141	0.01%	0.001%
82	13.790	3869	3872	3875	rBV	225	124	0.01%	0.001%
83	13.848	3878	3890	3904	rBV	203491	319071	30.89%	2.352%
84	14.031	3936	3947	3959	rBV2	201787	310098	30.02%	2.286%
85	14.143	3977	3982	3984	rBV2	239	193	0.02%	0.001%
86	14.179	3990	3993	4000	rVB2	287	253	0.02%	0.002%
87	14.343	4038	4044	4053	rVB3	1457	1936	0.19%	0.014%
88	14.446	4073	4076	4079	rVB2	335	224	0.02%	0.002%
89	14.577	4113	4117	4122	rBV	380	449	0.04%	0.003%
90	14.757	4170	4173	4175	rVB	291	152	0.01%	0.001%
91	14.799	4184	4186	4188	rVB	325	131	0.01%	0.001%
92	14.815	4188	4191	4193	rBV	356	236	0.02%	0.002%
93	14.970	4235	4239	4241	rBV2	338	242	0.02%	0.002%
94	15.217	4314	4316	4320	rBV3	334	248	0.02%	0.002%
95	15.343	4353	4355	4357	rBV	315	209	0.02%	0.002%
96	15.597	4432	4434	4436	rBV	271	116	0.01%	0.001%
97	15.648	4447	4450	4452	rBV2	310	203	0.02%	0.001%
98	15.732	4474	4476	4479	rBV2	372	218	0.02%	0.002%
99	15.966	4546	4549	4552	rBV2	368	290	0.03%	0.002%
100	16.179	4612	4615	4616	rBV2	505	278	0.03%	0.002%

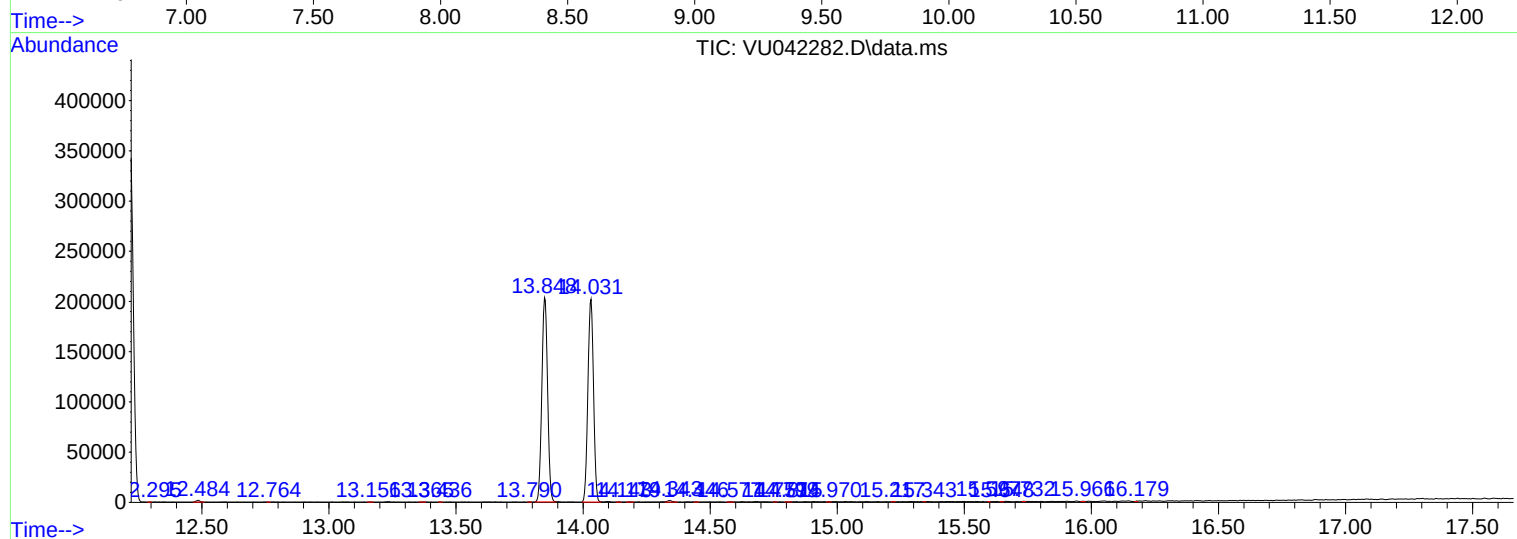
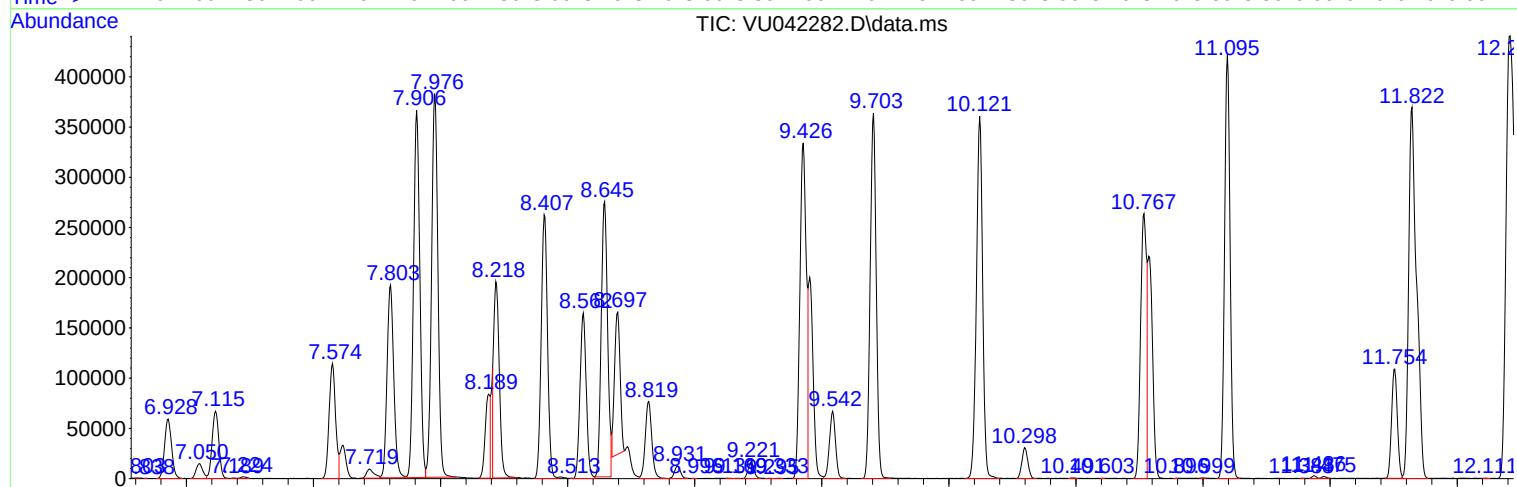
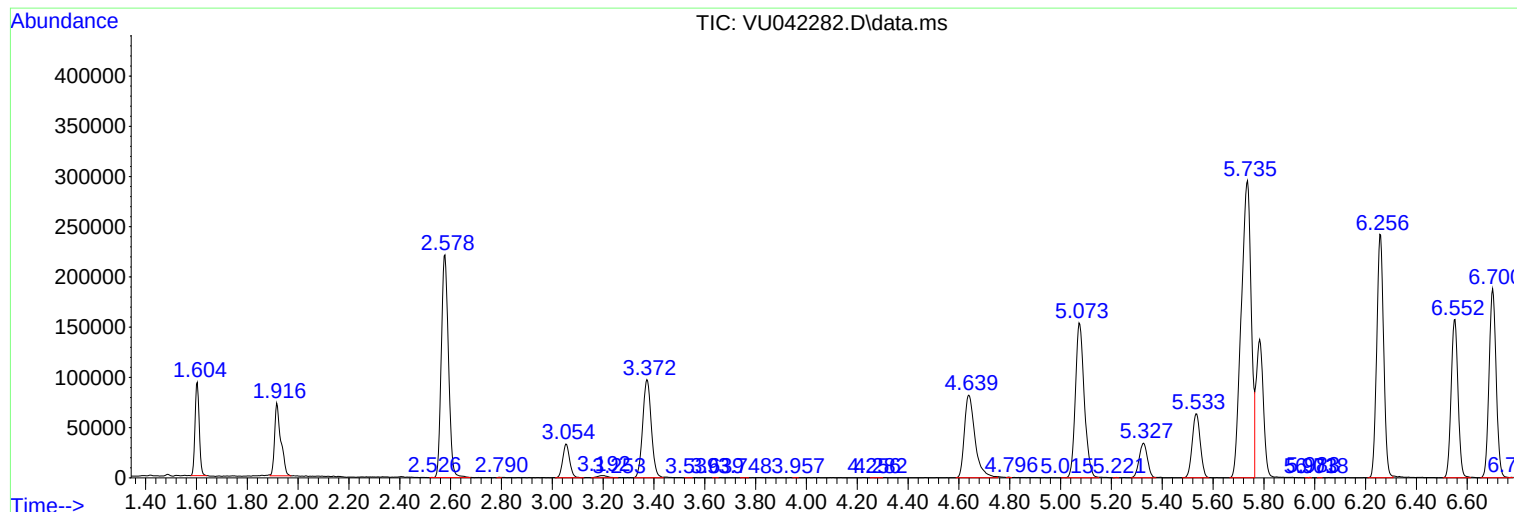
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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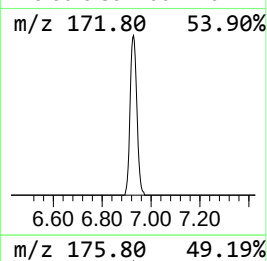
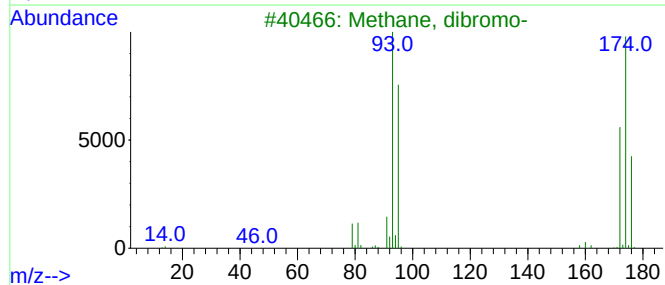
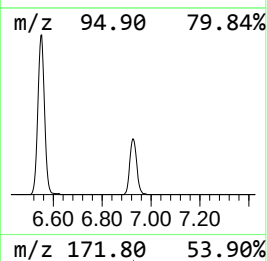
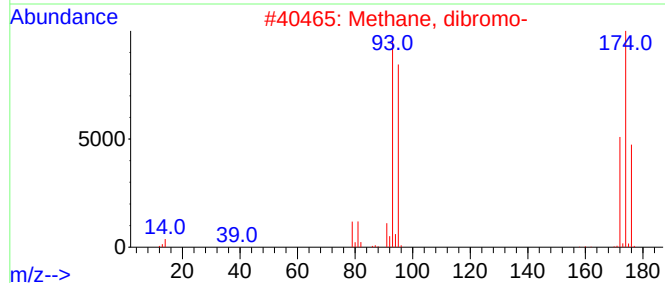
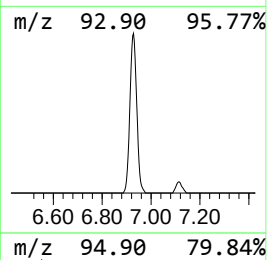
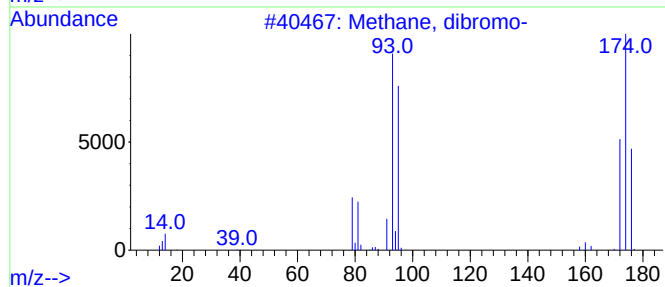
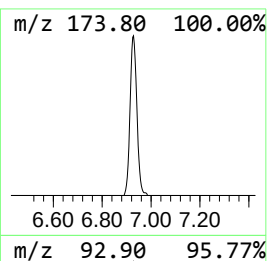
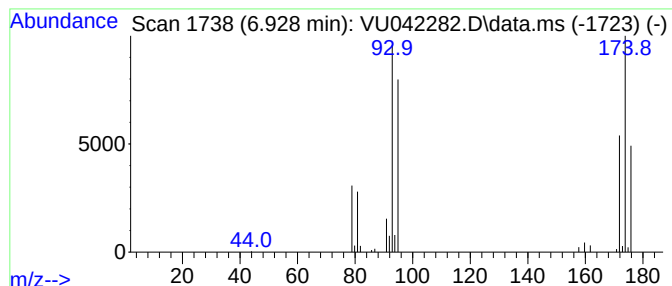
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Methane, dibromo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.928	12.38 ug/L	113067	1,4-Difluorobenzene	6.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, dibromo-	172	CH2Br2	000074-95-3	97
2			Methane, dibromo-	172	CH2Br2	000074-95-3	97
3			Methane, dibromo-	172	CH2Br2	000074-95-3	96
4			Bromine azide	121	BrN3	013973-87-0	9
5			(4-Methyl-cyclohex-3-enyl)-methanol	126	C8H14O	089690-46-0	9



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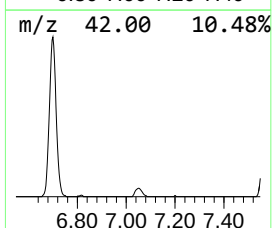
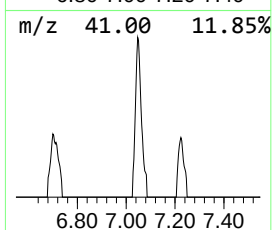
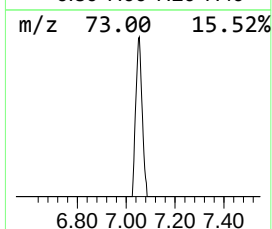
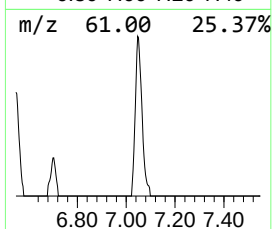
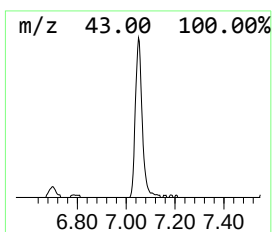
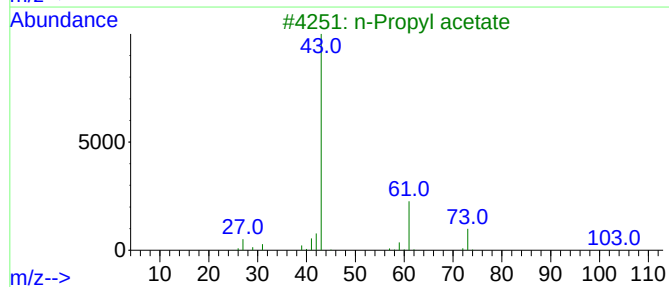
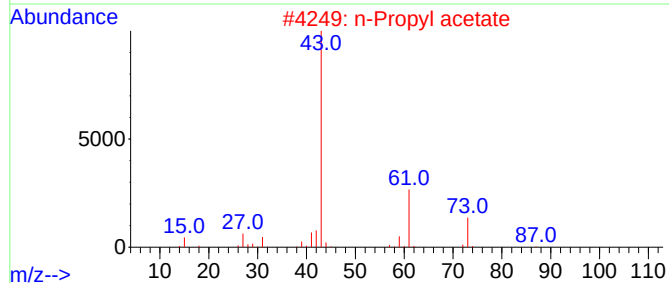
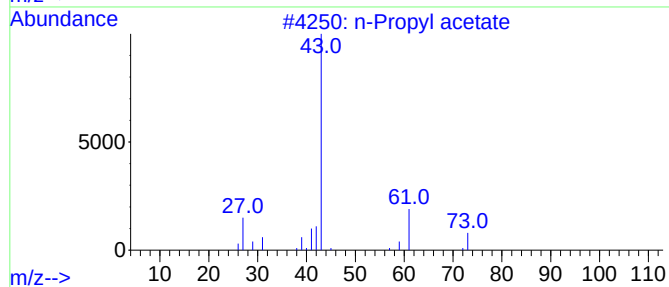
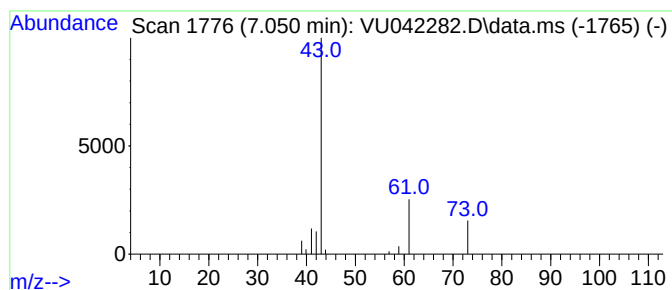
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Propyl acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.050	2.97 ug/L	27132	1,4-Difluorobenzene	6.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	74
2	n-Propyl acetate			102	C5H10O2	000109-60-4	39
3	n-Propyl acetate			102	C5H10O2	000109-60-4	9
4	Isobutylamine			73	C4H11N	000078-81-9	4
5	Isobutylamine			73	C4H11N	000078-81-9	4



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Instrument :
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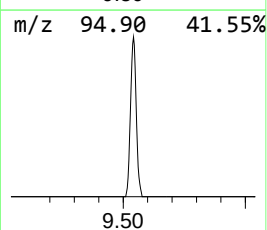
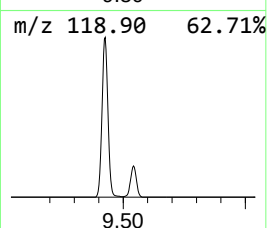
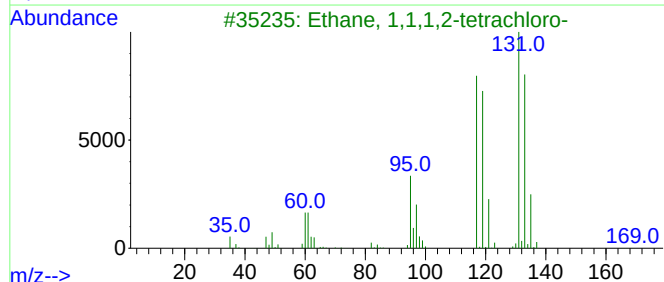
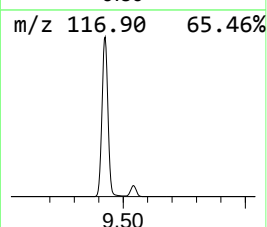
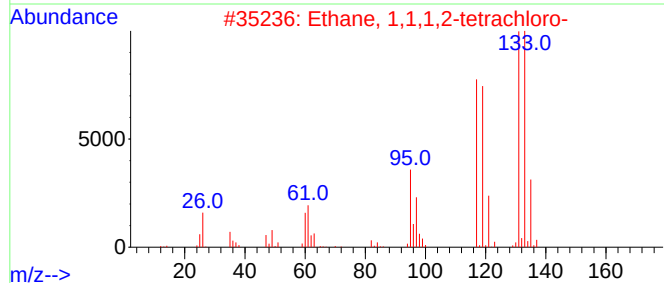
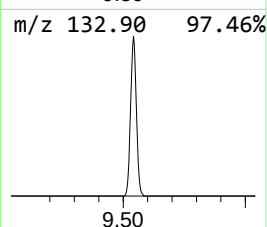
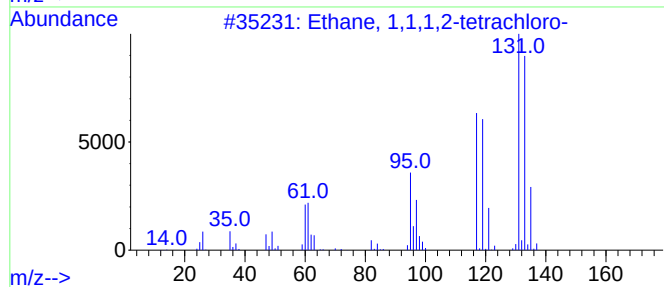
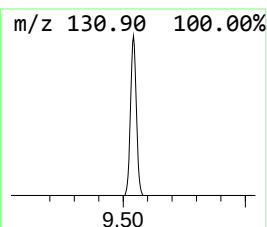
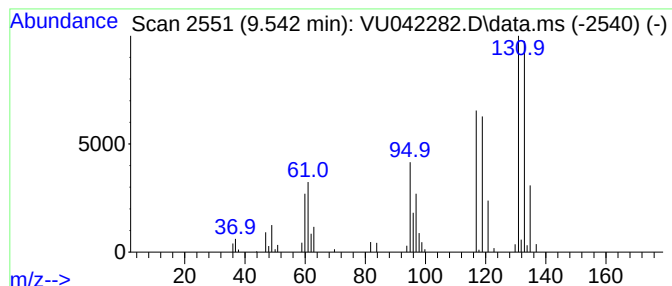
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethane, 1,1,1,2-tetrachloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.542	9.04 ug/L	110305	Chlorobenzene-d5	9.426

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	78
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	64
5			1,2,4-Triazolidin-3-one, 4-methy...	131	C3H5N3OS	022244-61-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042282.D
Acq On : 05 Feb 2021 16:45
Operator : SY/MD
Sample : M1327-01DL 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X2Z60DL

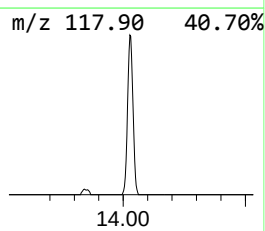
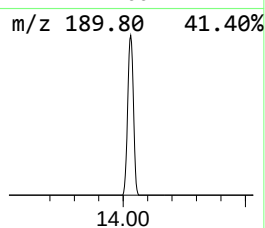
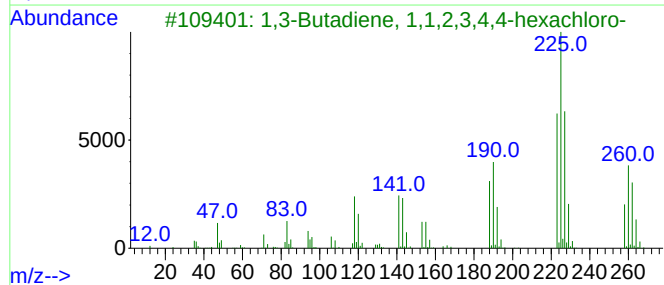
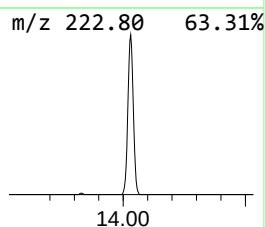
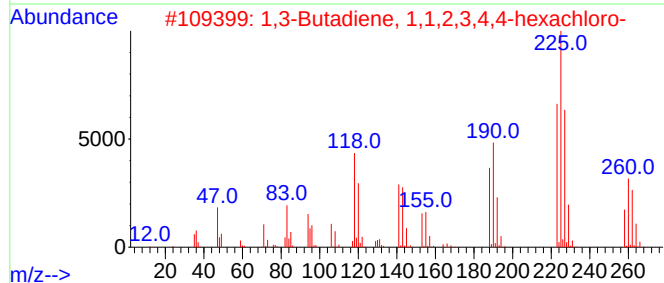
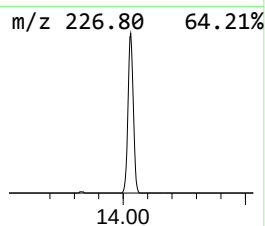
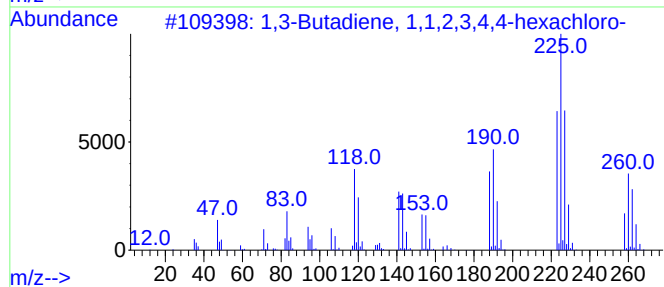
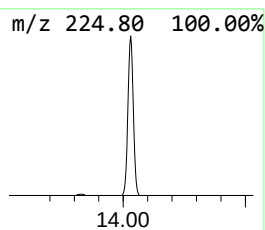
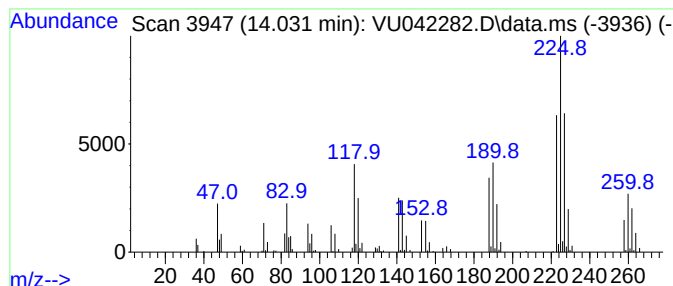
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.031	19.54 ug/L	310098	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
2			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
3			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
4			1,3-Butadiene, 1,1,2,3,4,4-hexac...	258	C4Cl6	000087-68-3	99
5			Stannane, trimethylphenyl-	242	C9H14Sn	000934-56-5	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020521\
Data File : VU042282.D
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Sample : M1327-01DL 50X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
X2Z60DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020521WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methane, dibromo-	6.928	12.4	ug/L	113067	1	6.259	456825	50.0
n-Propyl acetate	7.050	3.0	ug/L	27132	1	6.259	456825	50.0
Ethane, 1,1,1,2...	9.542	9.0	ug/L	110305	2	9.426	610334	50.0
1,3-Butadiene, ...	14.031	19.5	ug/L	310098	3	11.819	793393	50.0