

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012623\
 Data File : VU052820.D
 Acq On : 26 Jan 2023 16:52
 Operator : JC/MD
 Sample : 01316-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44H5

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\SFAMULM012623WMA.M
 Title : VOC Analysis

Signal : TIC: VU052820.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	40	44	49	rVB3	1589	1518	0.07%	0.006%
2	1.600	71	81	97	rBV2	205293	273588	12.60%	1.130%
3	1.793	135	141	147	rBV2	1535	1757	0.08%	0.007%
4	1.912	169	178	179	rBV	96289	89763	4.13%	0.371%
5	2.343	309	312	315	rBV2	398	295	0.01%	0.001%
6	2.433	331	340	344	rBV3	508	727	0.03%	0.003%
7	2.565	366	381	396	rBV3	328210	642575	29.60%	2.654%
8	2.787	437	450	469	rBV	219102	369242	17.01%	1.525%
9	2.944	488	499	516	rBV	100585	194033	8.94%	0.801%
10	3.041	516	529	558	rVB	134881	277563	12.78%	1.147%
11	3.179	558	572	592	rBV2	12229	29022	1.34%	0.120%
12	3.359	611	628	653	rVB	241843	554375	25.53%	2.290%
13	3.472	660	663	668	rVB2	320	213	0.01%	0.001%
14	3.694	729	732	734	rBV2	354	238	0.01%	0.001%
15	3.861	765	784	802	rBV2	70087	166731	7.68%	0.689%
16	3.967	815	817	820	rVB2	425	242	0.01%	0.001%
17	3.989	820	824	828	rBV2	448	560	0.03%	0.002%
18	4.147	868	873	879	rVB	276	359	0.02%	0.001%
19	4.192	882	887	893	rVB3	436	449	0.02%	0.002%
20	4.366	937	941	944	rBV	297	271	0.01%	0.001%
21	4.510	981	986	988	rBV2	343	283	0.01%	0.001%
22	4.655	1006	1031	1059	rBV2	112677	410872	18.93%	1.697%
23	4.915	1106	1112	1115	rBV2	314	406	0.02%	0.002%
24	5.057	1140	1156	1183	rVV2	194412	431224	19.86%	1.781%
25	5.160	1185	1188	1194	rVB2	318	272	0.01%	0.001%
26	5.311	1218	1235	1262	rBV	192831	431270	19.86%	1.781%
27	5.443	1272	1276	1280	rBV2	255	320	0.01%	0.001%
28	5.520	1294	1300	1304	rBV2	391	401	0.02%	0.002%
29	5.719	1339	1362	1374	rBV2	400413	1075171	49.52%	4.441%
30	5.787	1374	1383	1403	rVB	227860	452635	20.85%	1.870%
31	5.877	1409	1411	1415	rVB3	677	355	0.02%	0.001%
32	5.935	1426	1429	1432	rVB2	438	304	0.01%	0.001%
33	6.079	1466	1474	1482	rVB3	751	1172	0.05%	0.005%
34	6.118	1483	1486	1488	rVB2	325	201	0.01%	0.001%
35	6.150	1488	1496	1501	rBV	317	412	0.02%	0.002%
36	6.189	1504	1508	1510	rBV2	241	203	0.01%	0.001%

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37	6.243	1510	1525	1548	rBV	328656	613096	28.24%	2.532%
38	6.452	1588	1590	1593	rVB2	354	225	0.01%	0.001%
39	6.478	1594	1598	1601	rBV	289	272	0.01%	0.001%
40	6.536	1601	1616	1641	rBV	457884	848731	39.09%	3.506%
41	6.684	1649	1662	1680	rBV	247231	473908	21.83%	1.958%
42	6.784	1680	1693	1709	rVB	142398	268341	12.36%	1.108%
43	7.031	1750	1770	1799	rVB3	14307	56617	2.61%	0.234%
44	7.150	1803	1807	1810	rBV3	349	301	0.01%	0.001%
45	7.185	1810	1818	1821	rBV3	1973	2450	0.11%	0.010%
46	7.279	1842	1847	1851	rBV2	223	271	0.01%	0.001%
47	7.436	1893	1896	1898	rBV	272	216	0.01%	0.001%
48	7.562	1922	1935	1956	rVV	137765	242731	11.18%	1.003%
49	7.713	1967	1982	1995	rBV2	9058	17888	0.82%	0.074%
50	7.793	1995	2007	2026	rVV2	170993	389620	17.95%	1.609%
51	7.893	2026	2038	2050	rVV	527115	900930	41.50%	3.721%
52	7.964	2050	2060	2084	rVB	378175	644692	29.69%	2.663%
53	8.176	2114	2126	2131	rBV	101531	174720	8.05%	0.722%
54	8.269	2149	2155	2165	rVB4	3894	6226	0.29%	0.026%
55	8.311	2165	2168	2174	rVB	341	252	0.01%	0.001%
56	8.340	2174	2177	2182	rVB2	345	290	0.01%	0.001%
57	8.394	2182	2194	2215	rVB	289947	504551	23.24%	2.084%
58	8.549	2229	2242	2256	rBV	289088	477291	21.98%	1.972%
59	8.642	2258	2271	2279	rBV	225650	458779	21.13%	1.895%
60	8.918	2345	2357	2376	rVV	148550	249450	11.49%	1.030%
61	9.263	2461	2464	2467	rBV	278	266	0.01%	0.001%
62	9.414	2498	2511	2515	rBV	490263	776757	35.78%	3.209%
63	9.565	2545	2558	2578	rBV	865140	1361960	62.73%	5.626%
64	9.687	2583	2596	2621	rVB	588777	926026	42.65%	3.825%
65	9.857	2645	2649	2652	rBV4	438	370	0.02%	0.002%
66	9.944	2671	2676	2679	rBV2	201	214	0.01%	0.001%
67	10.105	2711	2726	2749	rBV4	552541	1121151	51.64%	4.631%
68	10.230	2762	2765	2772	rVB5	841	868	0.04%	0.004%
69	10.288	2772	2783	2797	rBV2	85753	145484	6.70%	0.601%
70	10.388	2808	2814	2818	rBV3	297	325	0.01%	0.001%
71	10.481	2829	2843	2867	rBV	601426	948860	43.71%	3.919%
72	10.568	2867	2870	2873	rVB3	387	252	0.01%	0.001%
73	10.626	2884	2888	2895	rVB4	534	614	0.03%	0.003%
74	10.658	2895	2898	2903	rBV	275	233	0.01%	0.001%
75	10.780	2915	2936	2960	rBV3	990938	2171052	100.00%	8.968%
76	11.459	3142	3147	3148	rBV2	535	356	0.02%	0.001%

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77	11.533	3168	3170	3175	rVB	318	232	0.01%	0.001%
78	11.742	3223	3235	3245	rBV	222884	343193	15.81%	1.418%
79	11.809	3245	3256	3260	rBV	559868	907375	41.79%	3.748%
80	11.976	3304	3308	3312	rBV3	278	285	0.01%	0.001%
81	12.044	3326	3329	3331	rBV	316	214	0.01%	0.001%
82	12.143	3356	3360	3362	rBV2	333	286	0.01%	0.001%
83	12.205	3362	3379	3401	rVV2	862016	1972490	90.85%	8.148%
84	12.340	3415	3421	3424	rBV3	365	344	0.02%	0.001%
85	12.468	3457	3461	3467	rBV3	1309	1556	0.07%	0.006%
86	12.513	3473	3475	3480	rBV3	229	200	0.01%	0.001%
87	12.716	3534	3538	3540	rBV2	252	239	0.01%	0.001%
88	12.992	3612	3624	3647	rVB	239310	381556	17.57%	1.576%
89	13.076	3647	3650	3652	rBV2	368	217	0.01%	0.001%
90	13.214	3681	3693	3711	rBV	545440	845010	38.92%	3.490%
91	13.340	3729	3732	3736	rVV2	398	236	0.01%	0.001%
92	13.365	3736	3740	3743	rBV3	321	290	0.01%	0.001%
93	13.674	3833	3836	3839	rBV3	329	270	0.01%	0.001%
94	13.758	3857	3862	3864	rBV2	612	522	0.02%	0.002%
95	13.841	3882	3888	3898	rVB4	1855	2592	0.12%	0.011%
96	13.925	3911	3914	3915	rBV	346	201	0.01%	0.001%
97	14.086	3959	3964	3972	rVB3	2735	3256	0.15%	0.013%
98	14.327	4024	4039	4056	rBV	335852	552257	25.44%	2.281%
99	14.909	4217	4220	4221	rBV	419	227	0.01%	0.001%
100	15.169	4299	4301	4307	rVB2	643	439	0.02%	0.002%

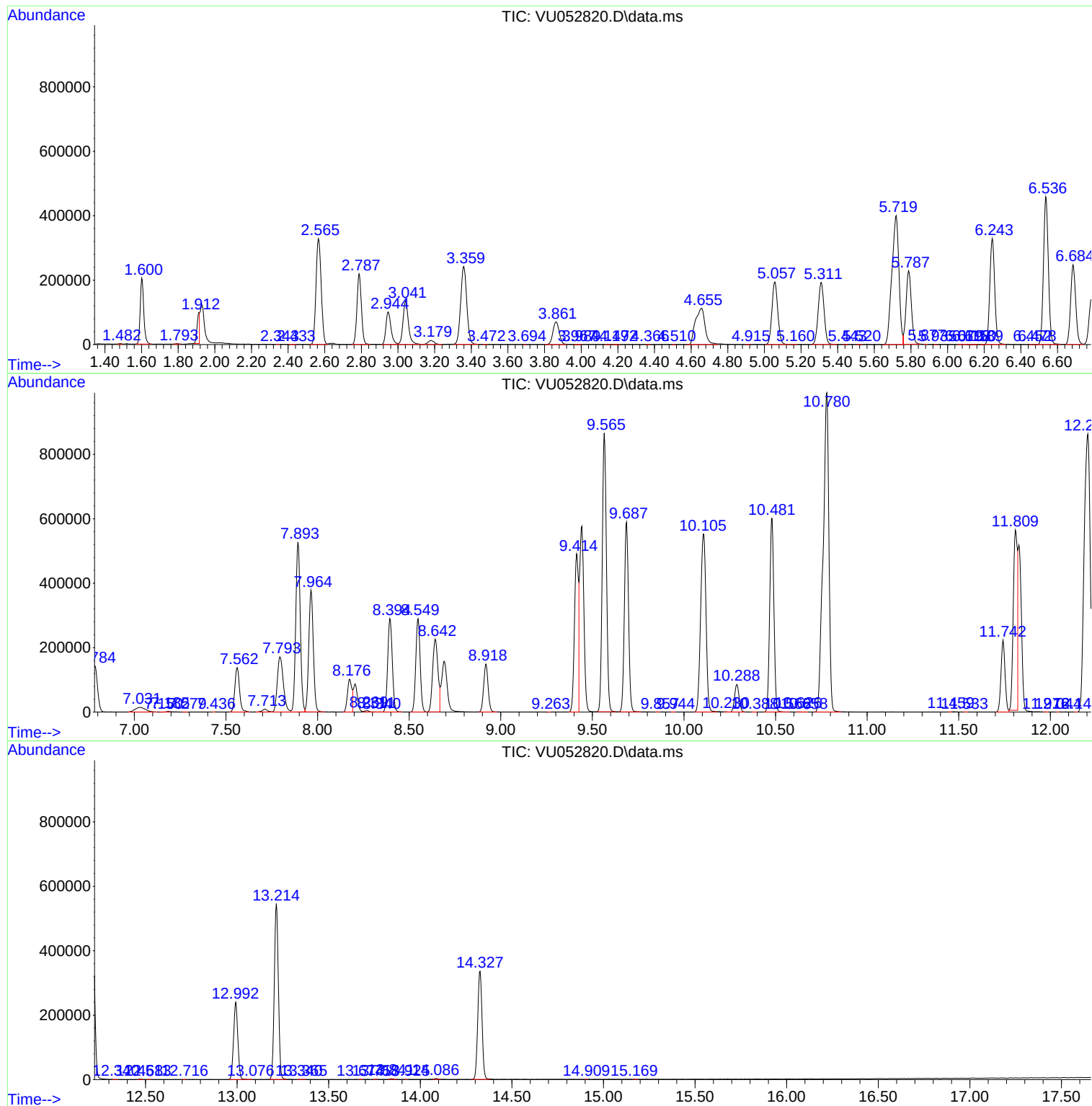
Sum of corrected areas: 24209145

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.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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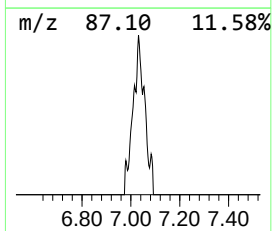
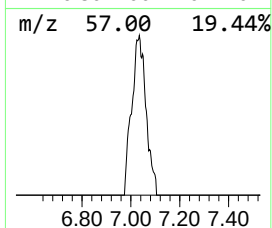
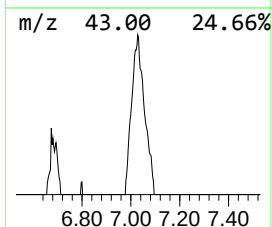
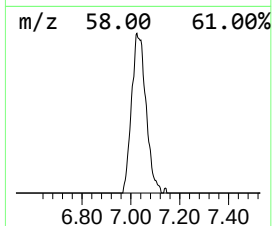
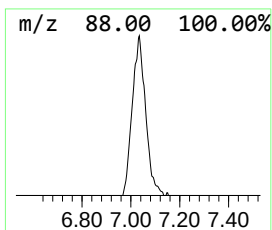
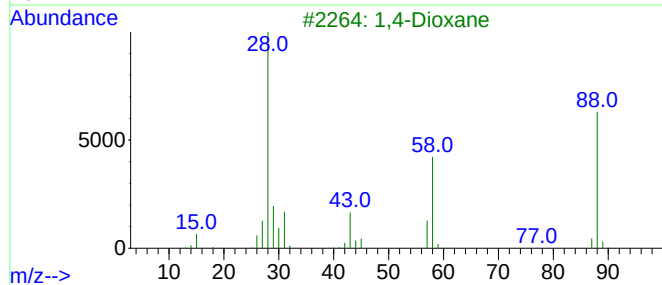
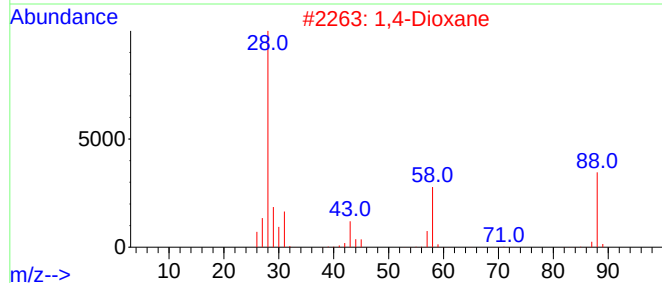
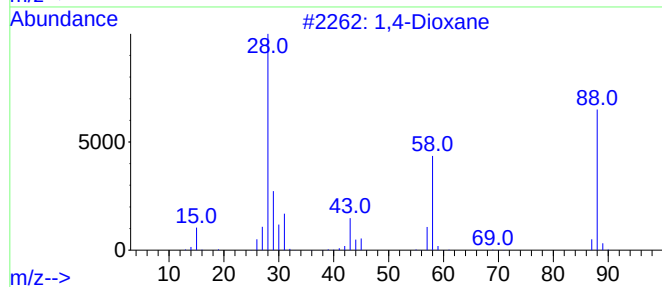
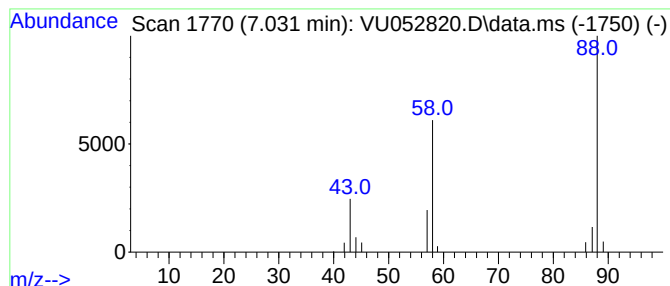
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 1,4-Dioxane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.031	4.62 ug/L	56617	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxane			88	C4H8O2	000123-91-1	86
2	1,4-Dioxane			88	C4H8O2	000123-91-1	83
3	1,4-Dioxane			88	C4H8O2	000123-91-1	83
4	1,4-Dioxane			88	C4H8O2	000123-91-1	83
5	1,4-Dioxane			88	C4H8O2	000123-91-1	78



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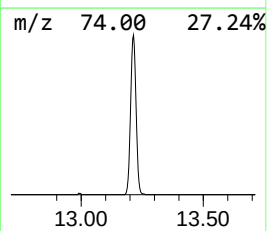
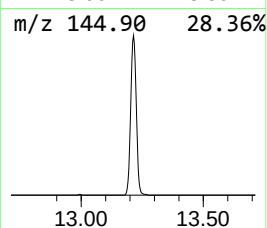
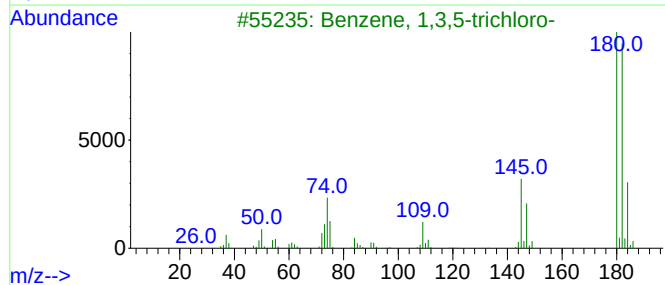
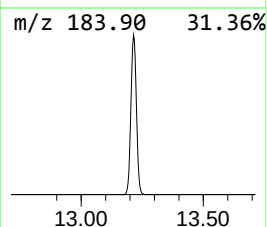
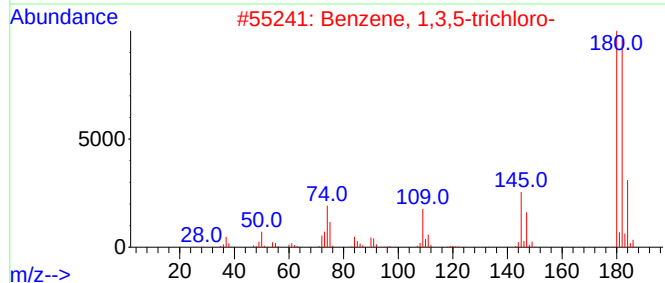
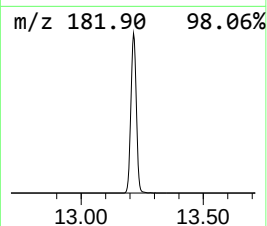
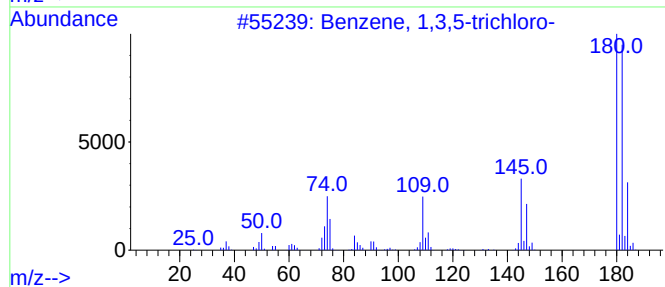
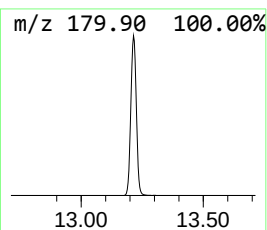
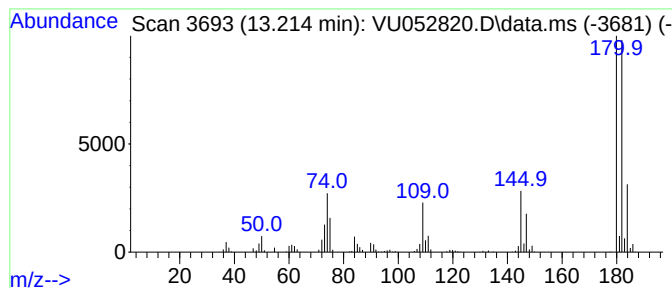
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1,3,5-trichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.214	46.56 ug/L	845010	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
2			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
3			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	97
4			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	96
5			Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	96



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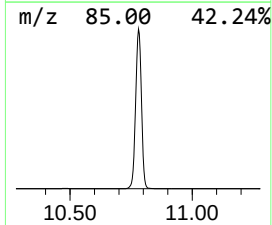
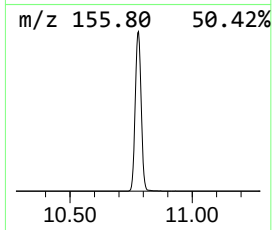
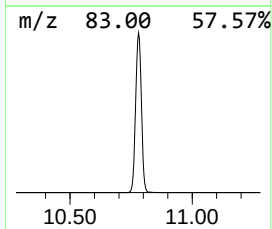
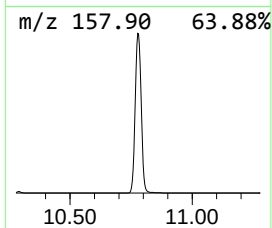
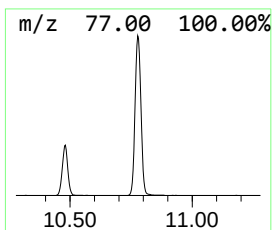
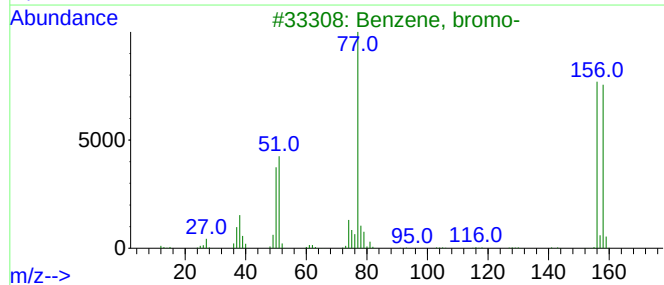
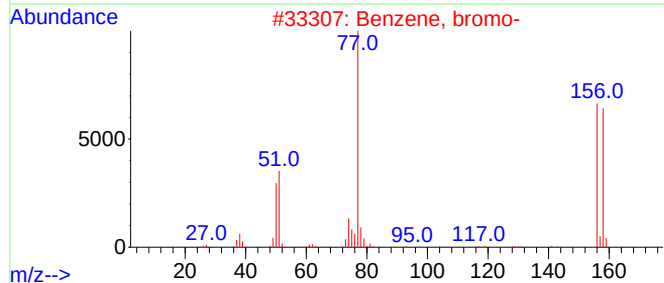
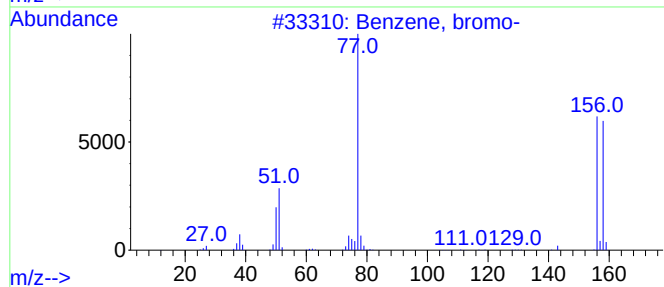
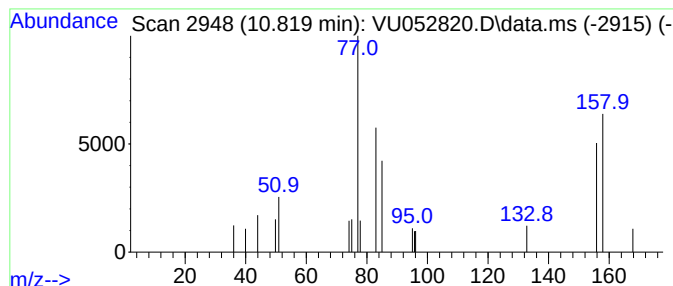
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Benzene, bromo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.780	119.63 ug/L	2171050	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, bromo-	156	C6H5Br	000108-86-1	46
2			Benzene, bromo-	156	C6H5Br	000108-86-1	43
3			Benzene, bromo-	156	C6H5Br	000108-86-1	43
4			Benzene, bromo-	156	C6H5Br	000108-86-1	35
5			2,4'-Bipyridine	156	C10H8N2	000581-47-5	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012623\
Data File : VU052820.D
Acq On : 26 Jan 2023 16:52
Operator : JC/MD
Sample : 01316-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44H5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.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
1,4-Dioxane	7.031	4.6	ug/L	56617	1	6.243	613096	50.0
Benzene, 1,3,5-...	13.214	46.6	ug/L	845010	3	11.809	907375	50.0
Benzene, bromo-	10.780	119.6	ug/L	2171050	3	11.809	907375	50.0