

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112122\
 Data File : VU052036.D
 Acq On : 22 Nov 2022 11:43
 Operator : JC/MD
 Sample : N5716-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 52 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A0B26

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\SFAMULM112122WMA.M
 Title : VOC Analysis

Signal : TIC: VU052036.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.385	7	14	31	rVB	92942	108709	2.77%	0.238%
2	1.482	37	44	50	rBV	93580	100466	2.56%	0.220%
3	1.524	50	57	70	rVV	224583	295181	7.51%	0.645%
4	1.598	72	80	95	rVV	233488	283479	7.21%	0.620%
5	1.829	147	152	164	rVB	127685	157962	4.02%	0.345%
6	1.893	164	172	186	rVB	166185	236592	6.02%	0.517%
7	2.131	235	246	261	rBV	209928	310593	7.90%	0.679%
8	2.565	367	381	390	rBV2	536389	1088313	27.70%	2.379%
9	2.620	391	398	425	rVB	826483	1395494	35.52%	3.050%
10	2.942	487	498	517	rVV	362103	651762	16.59%	1.424%
11	3.044	518	530	558	rVV	176551	377864	9.62%	0.826%
12	3.183	562	573	589	rVB2	14746	35173	0.90%	0.077%
13	3.260	594	597	601	rVB	457	304	0.01%	0.001%
14	3.360	606	628	661	rBV	1044860	2378706	60.54%	5.199%
15	3.649	716	718	723	rVB2	479	356	0.01%	0.001%
16	3.678	723	727	729	rBV3	456	317	0.01%	0.001%
17	3.993	818	825	831	rVB4	853	1072	0.03%	0.002%
18	4.327	926	929	936	rVB2	228	273	0.01%	0.001%
19	4.617	1007	1019	1035	rBV	174997	420715	10.71%	0.919%
20	4.697	1036	1044	1077	rVB	113215	274166	6.98%	0.599%
21	5.060	1140	1157	1178	rBV	321553	706417	17.98%	1.544%
22	5.289	1221	1228	1233	rBV2	923	1232	0.03%	0.003%
23	5.385	1238	1258	1278	rBV2	206934	470156	11.97%	1.028%
24	5.491	1289	1291	1296	rVB2	680	397	0.01%	0.001%
25	5.520	1296	1300	1303	rBV2	537	389	0.01%	0.001%
26	5.720	1341	1362	1374	rBV2	680077	1819429	46.31%	3.976%
27	5.790	1375	1384	1408	rVB	475481	945020	24.05%	2.065%
28	6.035	1453	1460	1463	rBV5	759	885	0.02%	0.002%
29	6.125	1484	1488	1493	rVB	537	507	0.01%	0.001%
30	6.247	1507	1526	1548	rBV	573769	1085200	27.62%	2.372%
31	6.466	1592	1594	1599	rVB2	364	271	0.01%	0.001%
32	6.539	1601	1617	1646	rBV	410008	775950	19.75%	1.696%
33	6.687	1649	1663	1674	rBV	418931	815913	20.77%	1.783%
34	6.758	1674	1685	1708	rVB	815493	1608351	40.93%	3.515%
35	6.964	1737	1749	1774	rVV2	36521	73213	1.86%	0.160%
36	7.176	1807	1815	1816	rBV2	1284	1151	0.03%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
 Title : VOC Analysis

37	7.359	1869	1872	1876	rBV2	325	269	0.01%	0.001%
38	7.482	1902	1910	1914	rVB2	306	378	0.01%	0.001%
39	7.562	1923	1935	1958	rBV	217689	381882	9.72%	0.835%
40	7.694	1972	1976	1977	rBV3	499	352	0.01%	0.001%
41	7.787	1992	2005	2026	rVV	1304648	2296888	58.46%	5.020%
42	7.896	2027	2039	2050	rVV	880778	1530708	38.96%	3.345%
43	7.967	2050	2061	2083	rVB	1395829	2387328	60.76%	5.217%
44	8.176	2115	2126	2147	rVB	153998	261392	6.65%	0.571%
45	8.276	2155	2157	2160	rVB3	984	515	0.01%	0.001%
46	8.334	2172	2175	2178	rBV3	695	510	0.01%	0.001%
47	8.424	2201	2203	2209	rVB3	559	505	0.01%	0.001%
48	8.459	2209	2214	2217	rBV3	343	290	0.01%	0.001%
49	8.549	2230	2242	2256	rBV	242116	406342	10.34%	0.888%
50	8.633	2256	2268	2276	rBV	549547	973921	24.79%	2.128%
51	8.681	2276	2283	2312	rVB	801938	1379999	35.12%	3.016%
52	9.018	2382	2388	2389	rBV2	601	551	0.01%	0.001%
53	9.115	2413	2418	2421	rBV2	615	700	0.02%	0.002%
54	9.414	2498	2511	2517	rBV	868365	1479820	37.66%	3.234%
55	9.568	2546	2559	2575	rBV	724345	1149227	29.25%	2.512%
56	9.687	2583	2596	2629	rVB	2144374	3341203	85.04%	7.302%
57	9.825	2636	2639	2644	rVB4	1265	1161	0.03%	0.003%
58	9.848	2644	2646	2647	rBV2	585	288	0.01%	0.001%
59	9.944	2672	2676	2680	rVB3	419	389	0.01%	0.001%
60	10.108	2710	2727	2758	rBV4	1984158	3929202	100.00%	8.587%
61	10.481	2829	2843	2866	rBV	1368058	2127632	54.15%	4.650%
62	10.591	2874	2877	2881	rVB3	993	733	0.02%	0.002%
63	10.629	2886	2889	2893	rVB3	1040	713	0.02%	0.002%
64	10.694	2906	2909	2913	rBV3	546	382	0.01%	0.001%
65	10.758	2913	2929	2930	rBV	742201	958885	24.40%	2.096%
66	10.899	2971	2973	2977	rVV4	939	675	0.02%	0.001%
67	10.983	2991	2999	3011	rVB9	2271	3911	0.10%	0.009%
68	11.057	3017	3022	3026	rBV2	329	339	0.01%	0.001%
69	11.089	3026	3032	3038	rVB4	1286	1605	0.04%	0.004%
70	11.179	3054	3060	3063	rBV2	285	323	0.01%	0.001%
71	11.324	3098	3105	3108	rBV3	726	789	0.02%	0.002%
72	11.407	3128	3131	3133	rBV	495	302	0.01%	0.001%
73	11.469	3146	3150	3154	rBV2	764	845	0.02%	0.002%
74	11.594	3185	3189	3193	rBV	382	294	0.01%	0.001%
75	11.748	3231	3237	3243	rBV5	1453	2043	0.05%	0.004%
76	11.809	3243	3256	3288	rBV2	807053	1814423	46.18%	3.965%

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 Title : VOC Analysis

77	11.948	3298	3299	3305	rVB4	1124	758	0.02%	0.002%
78	11.977	3305	3308	3312	rVV2	654	472	0.01%	0.001%
79	11.999	3312	3315	3317	rVV3	440	281	0.01%	0.001%
80	12.015	3318	3320	3322	rVV	458	264	0.01%	0.001%
81	12.028	3322	3324	3330	rVB4	875	732	0.02%	0.002%
82	12.089	3341	3343	3347	rVB2	526	353	0.01%	0.001%
83	12.137	3354	3358	3361	rBV	567	418	0.01%	0.001%
84	12.192	3361	3375	3404	rVV3	904917	1964828	50.01%	4.294%
85	12.391	3433	3437	3440	rBV	616	397	0.01%	0.001%
86	12.526	3474	3479	3480	rBV	393	280	0.01%	0.001%
87	12.819	3565	3570	3576	rBV3	576	813	0.02%	0.002%
88	12.993	3620	3624	3630	rBV4	479	480	0.01%	0.001%
89	13.153	3671	3674	3677	rBV2	409	361	0.01%	0.001%
90	13.214	3680	3693	3716	rBV	811877	1269361	32.31%	2.774%
91	13.324	3724	3727	3733	rVB3	474	423	0.01%	0.001%
92	13.446	3760	3765	3768	rBV3	508	448	0.01%	0.001%
93	13.838	3874	3887	3908	rBV	228744	371812	9.46%	0.813%
94	14.057	3951	3955	3956	rBV3	593	421	0.01%	0.001%
95	14.211	4000	4003	4005	rBV2	384	274	0.01%	0.001%
96	14.247	4011	4014	4017	rBV2	351	267	0.01%	0.001%
97	14.327	4025	4039	4065	rVV	775926	1281926	32.63%	2.802%
98	14.893	4213	4215	4219	rBV3	448	321	0.01%	0.001%
99	15.269	4329	4332	4334	rBV3	683	398	0.01%	0.001%
100	15.472	4392	4395	4399	rBV3	590	442	0.01%	0.001%

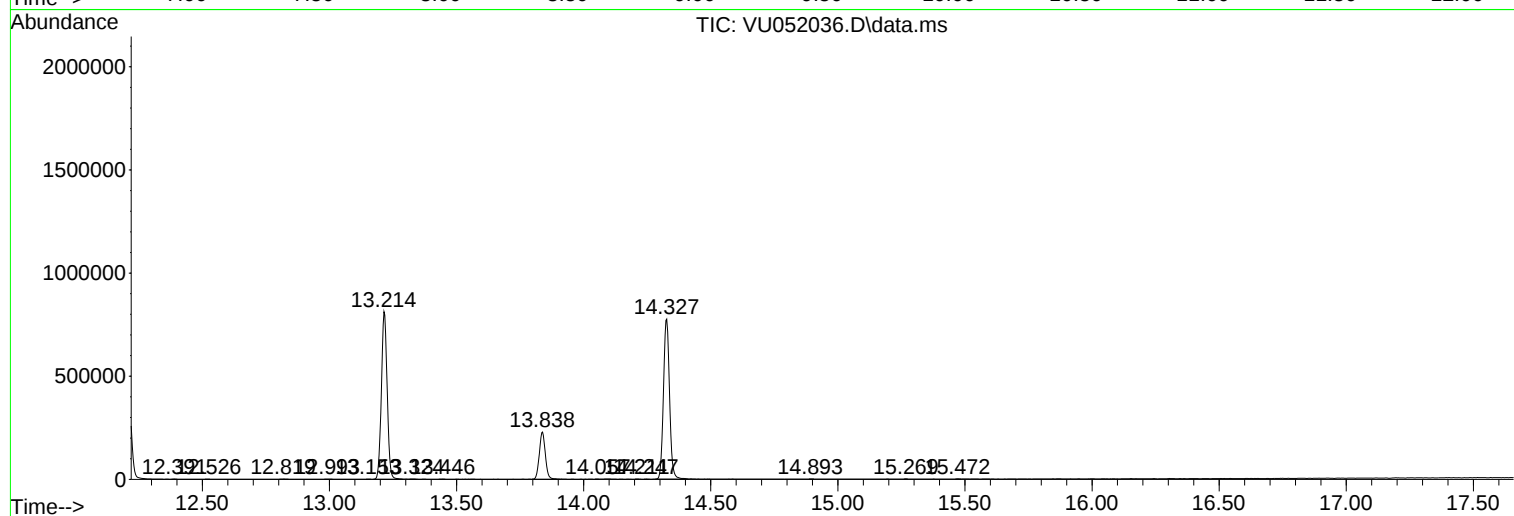
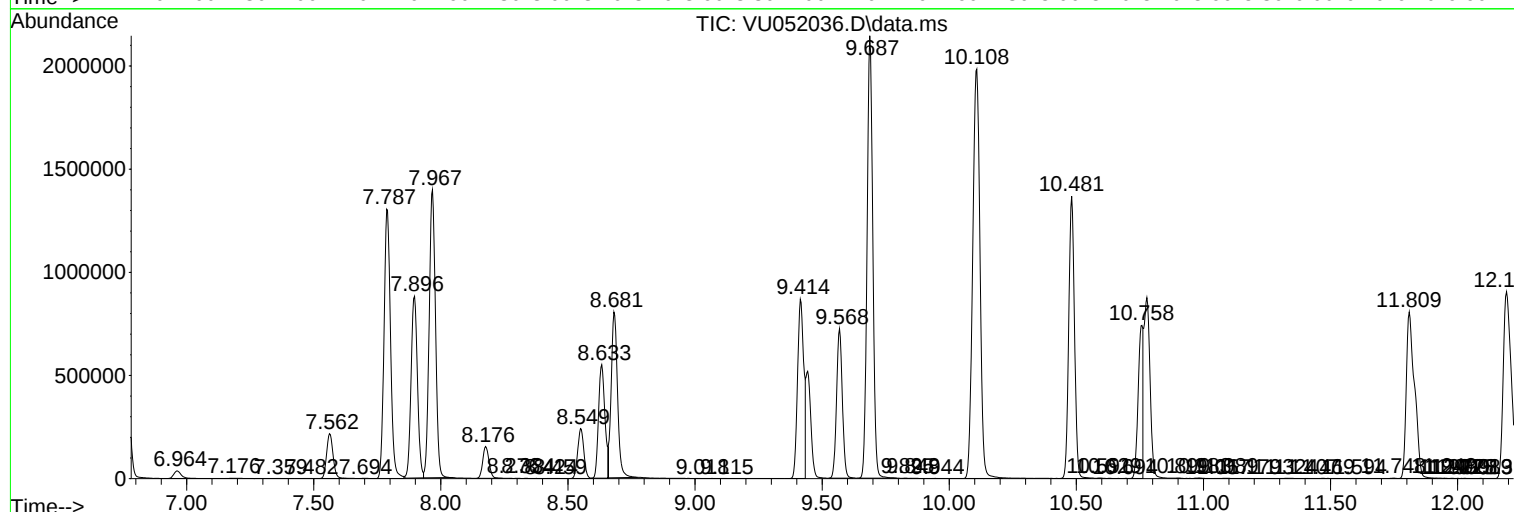
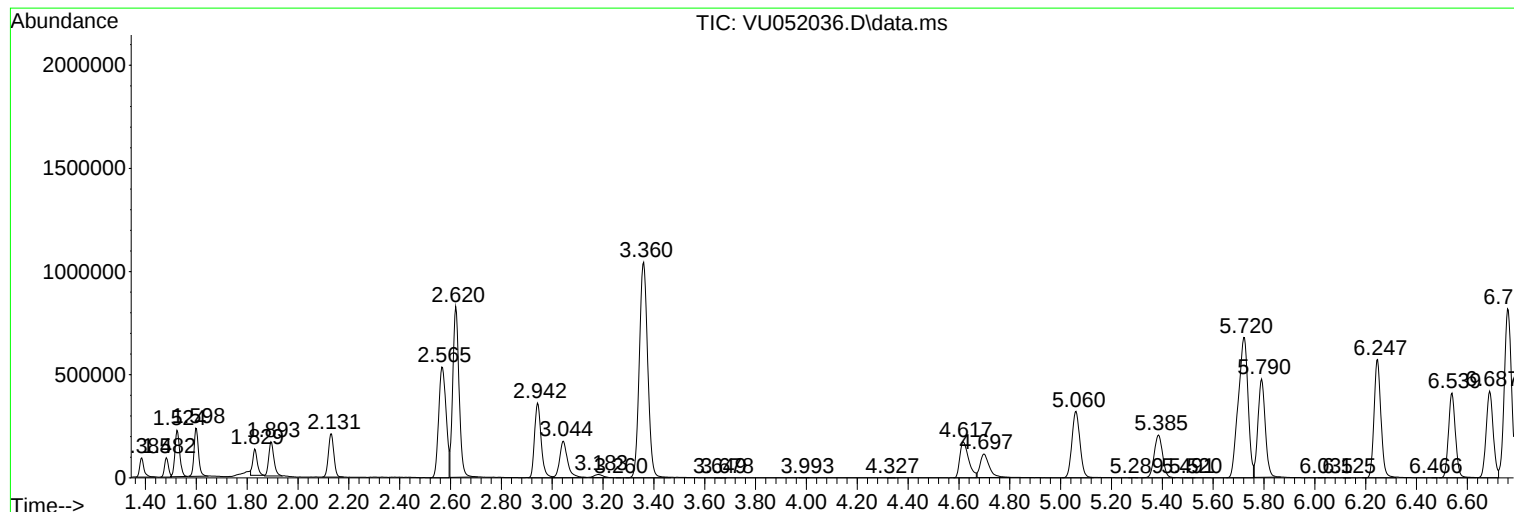
Sum of corrected areas: 45756222

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.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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ClientSampleId :
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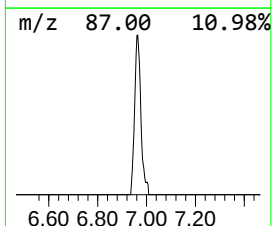
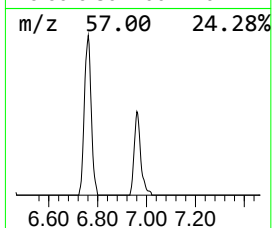
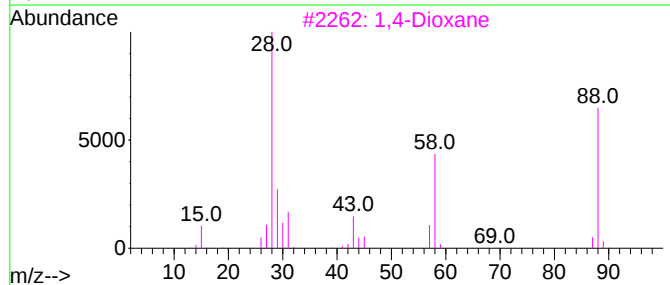
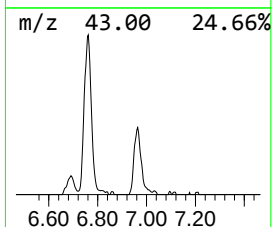
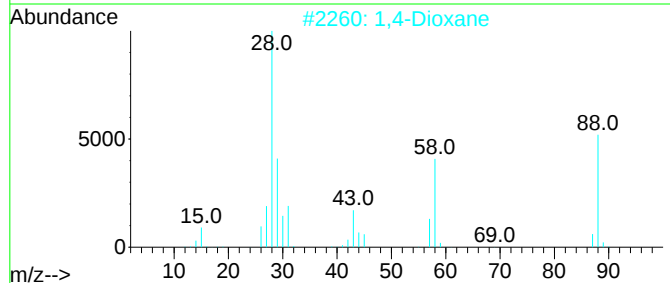
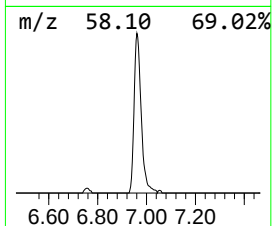
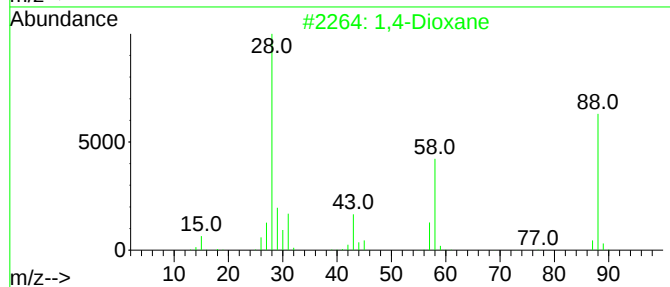
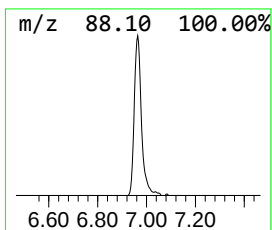
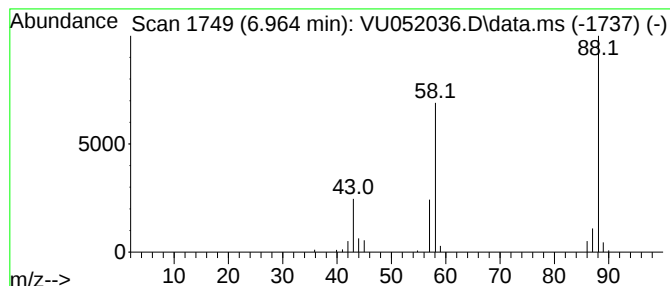
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

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.
6.964	3.37 ug/L	73213	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxane			88	C4H8O2	000123-91-1	90
2	1,4-Dioxane			88	C4H8O2	000123-91-1	86
3	1,4-Dioxane			88	C4H8O2	000123-91-1	86
4	1,4-Dioxane			88	C4H8O2	000123-91-1	83
5	1,4-Dioxane			88	C4H8O2	000123-91-1	64



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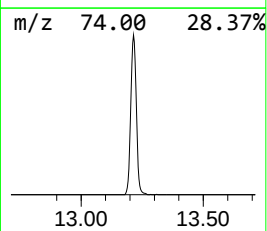
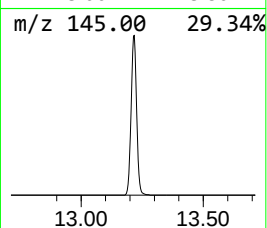
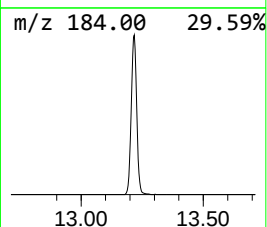
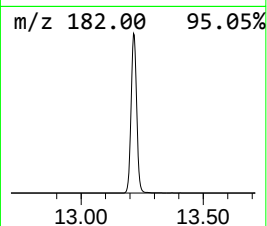
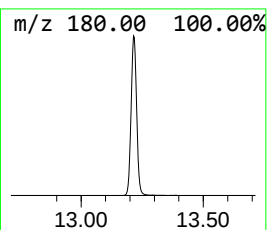
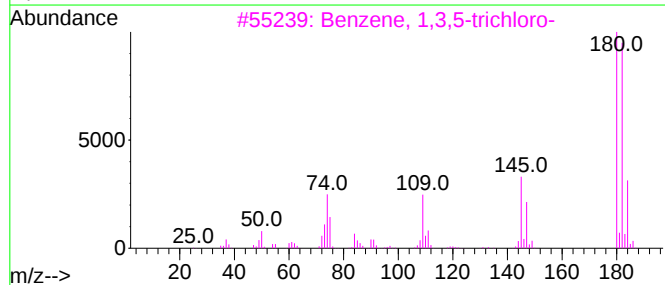
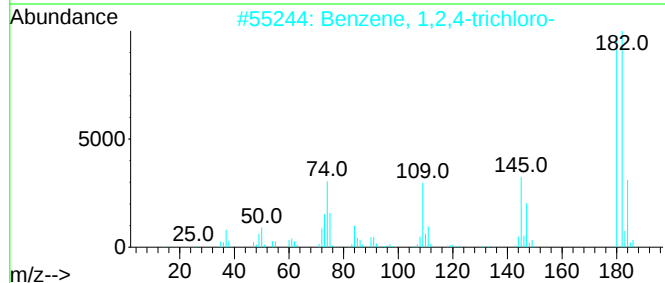
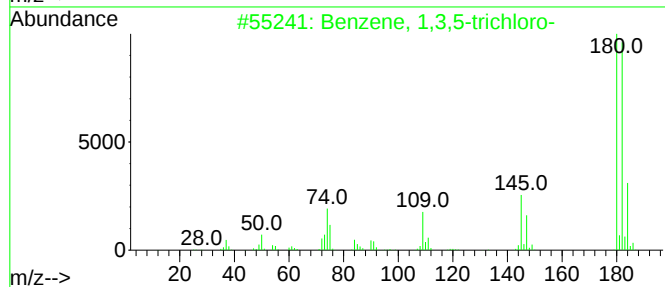
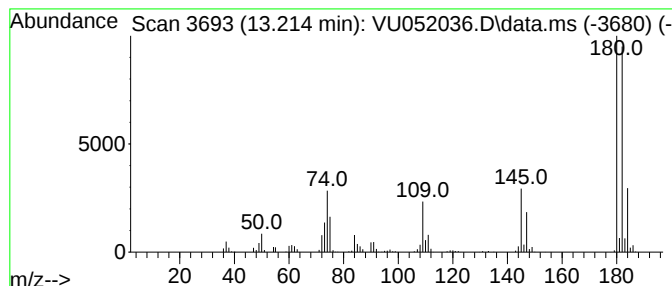
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

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	34.98 ug/L	1269360	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	97
2			Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	97
3			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	97
4			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	97
5			Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	95



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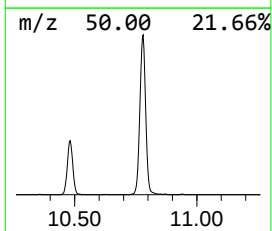
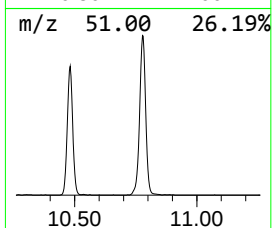
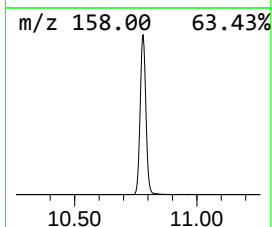
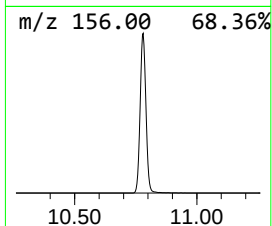
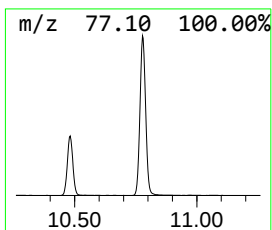
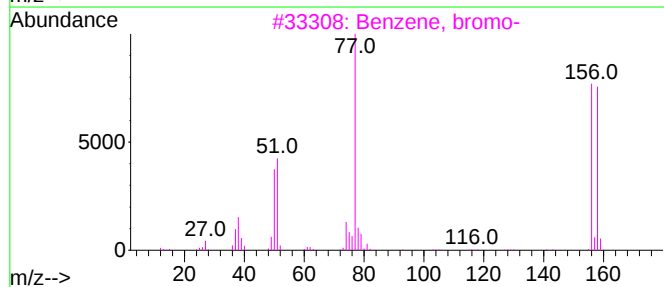
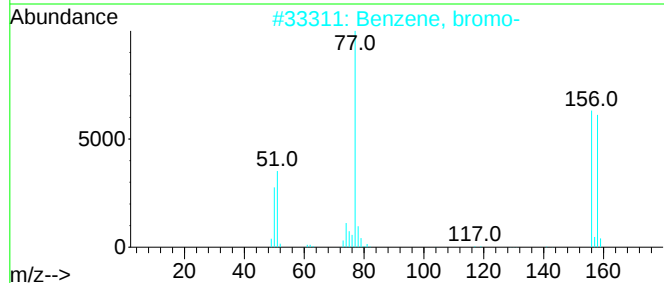
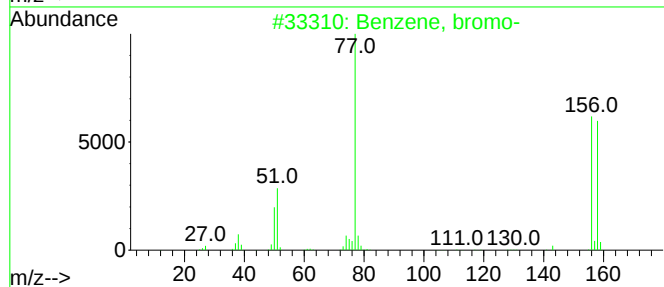
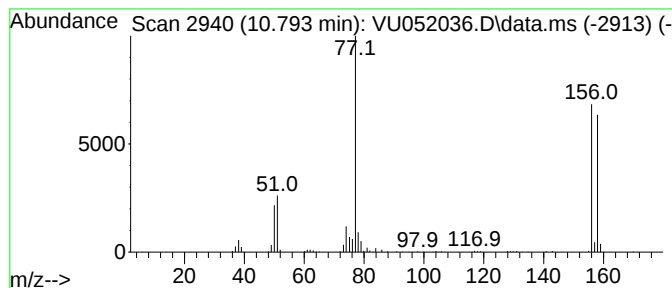
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.M
Quant Title : VOC Analysis

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.
10.758	26.42 ug/L	958885	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, bromo-	156	C6H5Br	000108-86-1	97
2			Benzene, bromo-	156	C6H5Br	000108-86-1	96
3			Benzene, bromo-	156	C6H5Br	000108-86-1	94
4			Benzene, bromo-	156	C6H5Br	000108-86-1	94
5			Benzene, bromo-	156	C6H5Br	000108-86-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112122\
Data File : VU052036.D
Acq On : 22 Nov 2022 11:43
Operator : JC/MD
Sample : N5716-06
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 52 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A0B26

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112122WMA.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	6.964	3.4	ug/L	73213	1	6.247	1085200	50.0
Benzene, 1,3,5-...	13.214	35.0	ug/L	1269360	3	11.809	1814420	50.0
Benzene, bromo-	10.758	26.4	ug/L	958885	3	11.809	1814420	50.0