

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012623\
 Data File : VU052819.D
 Acq On : 26 Jan 2023 16:30
 Operator : JC/MD
 Sample : 01314-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A44Q4

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: VU052819.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.520	51	56	65	rBV3	1308	1664	0.08%	0.007%
2	1.600	72	81	100	rVB2	208189	274032	12.57%	1.115%
3	1.793	137	141	148	rVB2	1839	1659	0.08%	0.007%
4	1.861	156	162	163	rBV5	1160	1079	0.05%	0.004%
5	1.928	169	183	205	rBV2	123077	280742	12.88%	1.142%
6	2.141	245	249	251	rBV2	548	425	0.02%	0.002%
7	2.218	271	273	274	rBV2	470	222	0.01%	0.001%
8	2.430	337	339	343	rBV	379	247	0.01%	0.001%
9	2.568	367	382	396	rBV3	324704	640882	29.40%	2.608%
10	2.639	400	404	415	rVB2	3541	5604	0.26%	0.023%
11	2.787	436	450	468	rBV	229196	382984	17.57%	1.558%
12	2.944	486	499	516	rBV	103037	199744	9.16%	0.813%
13	3.041	517	529	555	rVB	136043	278515	12.78%	1.133%
14	3.179	558	572	583	rBV2	10934	24390	1.12%	0.099%
15	3.256	592	596	598	rBV2	392	266	0.01%	0.001%
16	3.359	611	628	650	rVB	249968	567869	26.05%	2.311%
17	3.629	709	712	715	rBV2	275	212	0.01%	0.001%
18	3.861	768	784	809	rBB2	71577	168863	7.75%	0.687%
19	4.076	847	851	855	rVV2	279	294	0.01%	0.001%
20	4.153	870	875	878	rBV2	429	442	0.02%	0.002%
21	4.520	981	989	992	rBV2	525	616	0.03%	0.003%
22	4.655	1007	1031	1064	rBV2	109219	402998	18.48%	1.640%
23	4.832	1084	1086	1091	rVB2	357	225	0.01%	0.001%
24	4.906	1107	1109	1114	rBV3	412	362	0.02%	0.001%
25	5.057	1139	1156	1175	rBV	187556	413507	18.97%	1.683%
26	5.150	1183	1185	1189	rVB2	443	231	0.01%	0.001%
27	5.179	1192	1194	1198	rVB	464	301	0.01%	0.001%
28	5.202	1198	1201	1204	rBV2	303	274	0.01%	0.001%
29	5.311	1215	1235	1254	rBV	198940	447092	20.51%	1.819%
30	5.536	1302	1305	1308	rVB2	359	243	0.01%	0.001%
31	5.719	1340	1362	1374	rBV2	377686	1026502	47.08%	4.177%
32	5.787	1374	1383	1405	rVB	229875	457816	21.00%	1.863%
33	6.041	1457	1462	1465	rBV	220	238	0.01%	0.001%
34	6.083	1467	1475	1481	rBV4	830	1236	0.06%	0.005%
35	6.115	1481	1485	1489	rVB3	362	389	0.02%	0.002%
36	6.192	1503	1509	1510	rBV2	329	289	0.01%	0.001%

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 Title : VOC Analysis

37	6.243	1510	1525	1547	rBV	340302	635709	29.16%	2.587%
38	6.536	1602	1616	1634	rBV	473724	869538	39.88%	3.538%
39	6.684	1649	1662	1680	rBV	232748	451117	20.69%	1.836%
40	6.787	1681	1694	1712	rVB2	144839	271635	12.46%	1.105%
41	7.025	1747	1768	1790	rVV3	14413	55021	2.52%	0.224%
42	7.189	1810	1819	1826	rVV4	1774	2837	0.13%	0.012%
43	7.353	1868	1870	1874	rVB	376	256	0.01%	0.001%
44	7.430	1891	1894	1895	rBV	499	302	0.01%	0.001%
45	7.446	1895	1899	1905	rVV3	355	405	0.02%	0.002%
46	7.491	1909	1913	1916	rBV2	386	266	0.01%	0.001%
47	7.562	1923	1935	1960	rBV2	132124	232932	10.68%	0.948%
48	7.713	1967	1982	1994	rBV2	8923	18040	0.83%	0.073%
49	7.793	1994	2007	2026	rVV	180179	398067	18.26%	1.620%
50	7.893	2026	2038	2050	rVV	505041	862543	39.56%	3.510%
51	7.964	2050	2060	2082	rVB	386879	659854	30.27%	2.685%
52	8.176	2111	2126	2131	rBV	95737	166804	7.65%	0.679%
53	8.394	2182	2194	2214	rBV	300944	511632	23.47%	2.082%
54	8.549	2227	2242	2258	rBV	289673	488884	22.42%	1.989%
55	8.642	2258	2271	2279	rBV	212673	431023	19.77%	1.754%
56	8.918	2344	2357	2379	rVB	154015	257775	11.82%	1.049%
57	9.414	2498	2511	2515	rBV	493200	800816	36.73%	3.259%
58	9.565	2545	2558	2578	rBV	880715	1387472	63.64%	5.646%
59	9.687	2583	2596	2619	rVB	595564	949553	43.55%	3.864%
60	9.835	2638	2642	2646	rVB3	329	353	0.02%	0.001%
61	10.050	2704	2709	2710	rBV2	348	293	0.01%	0.001%
62	10.108	2710	2727	2746	rBV4	575566	1145265	52.53%	4.660%
63	10.217	2758	2761	2764	rBV3	538	432	0.02%	0.002%
64	10.234	2764	2766	2771	rVV2	481	439	0.02%	0.002%
65	10.288	2771	2783	2799	rVB2	87091	148378	6.81%	0.604%
66	10.481	2830	2843	2859	rBV	620143	972316	44.60%	3.957%
67	10.590	2875	2877	2886	rVB2	503	473	0.02%	0.002%
68	10.632	2886	2890	2892	rBV2	883	641	0.03%	0.003%
69	10.780	2915	2936	2954	rBV2	1040003	2180151	100.00%	8.872%
70	11.079	3024	3029	3030	rBV	496	340	0.02%	0.001%
71	11.333	3105	3108	3112	rBV2	266	230	0.01%	0.001%
72	11.475	3146	3152	3153	rBV3	722	583	0.03%	0.002%
73	11.536	3168	3171	3175	rVB2	388	341	0.02%	0.001%
74	11.561	3175	3179	3181	rBV	300	271	0.01%	0.001%
75	11.606	3189	3193	3196	rBV2	273	253	0.01%	0.001%
76	11.742	3223	3235	3245	rBV	223807	352128	16.15%	1.433%

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77	11.809	3245	3256	3260	rBV	590607	942620	43.24%	3.836%
78	12.066	3333	3336	3342	rBV2	253	239	0.01%	0.001%
79	12.205	3361	3379	3408	rBV2	847084	1965410	90.15%	7.998%
80	12.442	3449	3453	3456	rBV	288	285	0.01%	0.001%
81	12.471	3456	3462	3467	rVV4	1237	1472	0.07%	0.006%
82	12.828	3570	3573	3578	rBV2	406	457	0.02%	0.002%
83	12.992	3612	3624	3646	rVB	239908	386336	17.72%	1.572%
84	13.076	3646	3650	3655	rVB2	313	277	0.01%	0.001%
85	13.214	3681	3693	3715	rBV	562581	867996	39.81%	3.532%
86	13.616	3813	3818	3822	rVB3	481	516	0.02%	0.002%
87	13.700	3841	3844	3848	rBV3	408	296	0.01%	0.001%
88	13.841	3883	3888	3895	rVB4	2275	2712	0.12%	0.011%
89	14.028	3943	3946	3949	rBV	305	228	0.01%	0.001%
90	14.089	3957	3965	3973	rBV2	2640	3492	0.16%	0.014%
91	14.198	3995	3999	4001	rBV2	275	248	0.01%	0.001%
92	14.224	4004	4007	4013	rVV	495	454	0.02%	0.002%
93	14.282	4022	4025	4026	rBV2	345	219	0.01%	0.001%
94	14.323	4026	4038	4059	rVV	351601	561528	25.76%	2.285%
95	14.455	4076	4079	4082	rBV2	418	320	0.01%	0.001%
96	14.513	4094	4097	4098	rBV	408	256	0.01%	0.001%
97	14.558	4108	4111	4113	rBV2	398	291	0.01%	0.001%
98	14.992	4244	4246	4250	rVB2	724	397	0.02%	0.002%
99	15.481	4396	4398	4400	rBV2	678	358	0.02%	0.001%
100	15.973	4549	4551	4556	rBV4	786	484	0.02%	0.002%

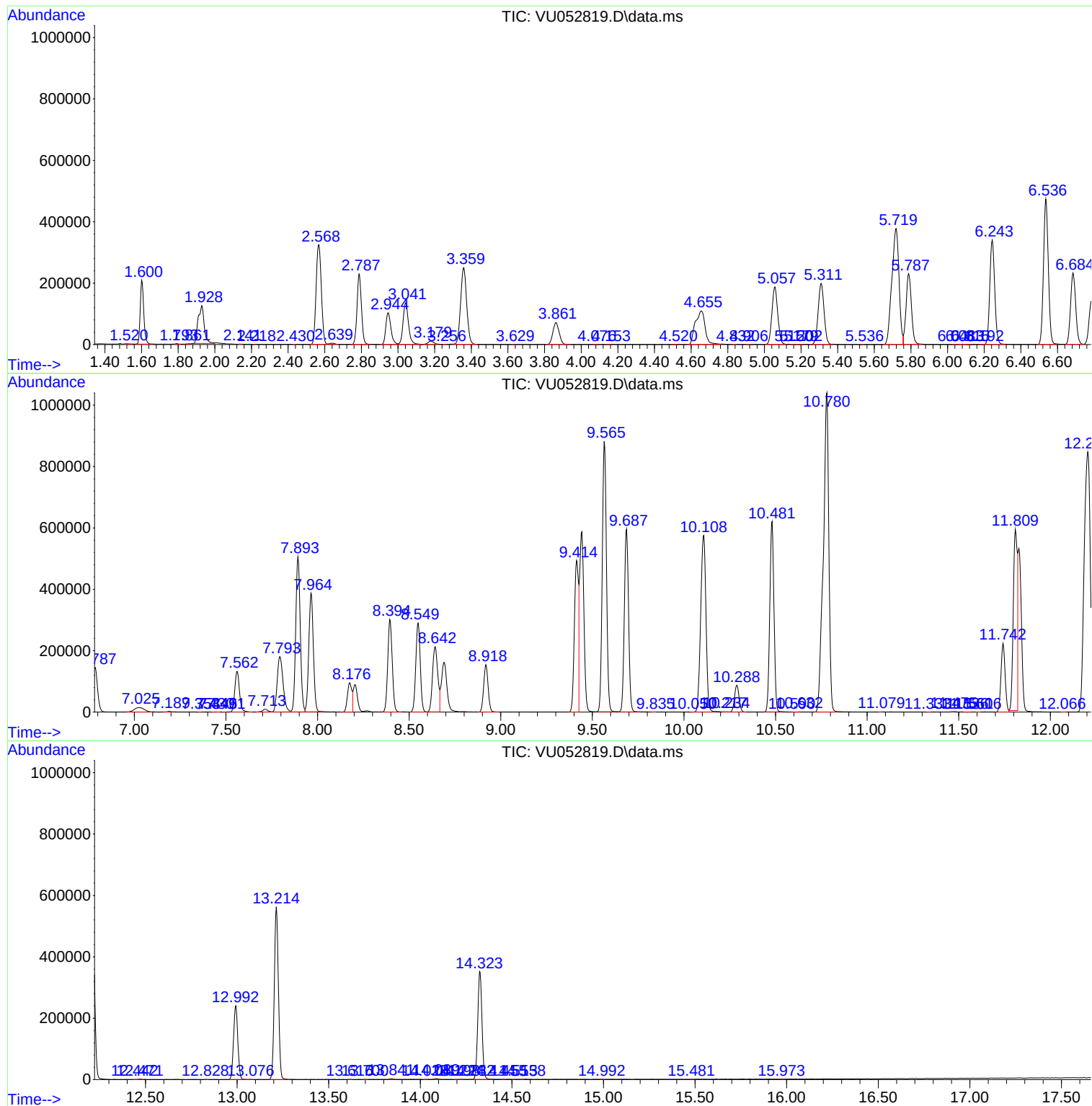
Sum of corrected areas: 24574713

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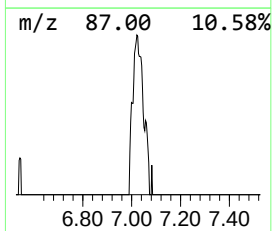
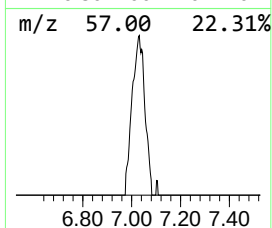
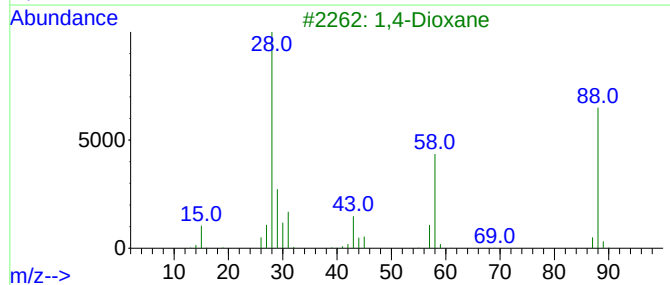
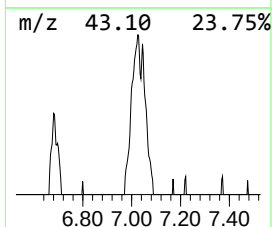
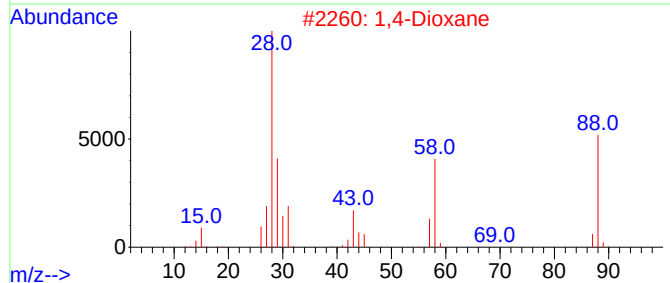
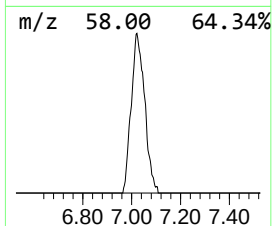
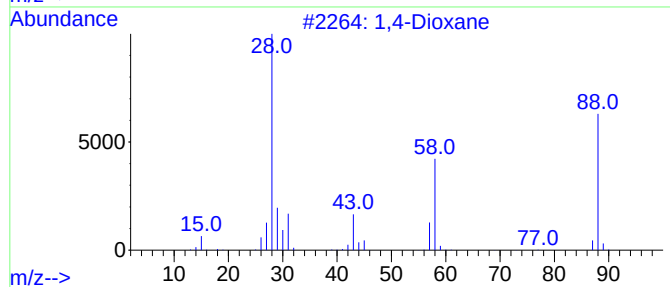
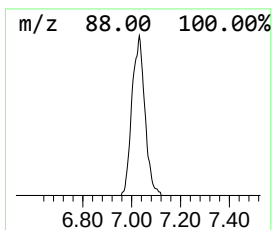
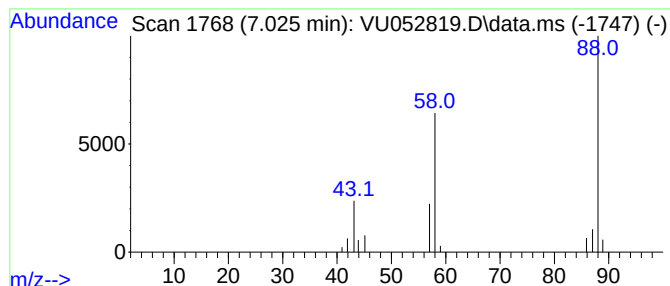
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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.
7.025	4.33 ug/L	55021	1,4-Difluorobenzene	6.243

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



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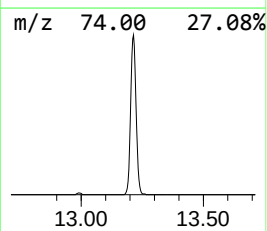
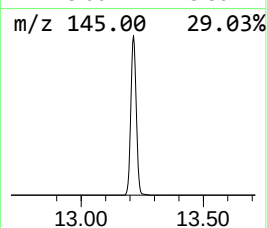
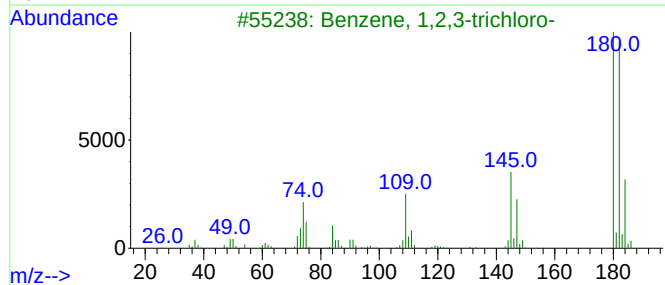
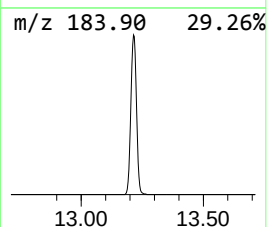
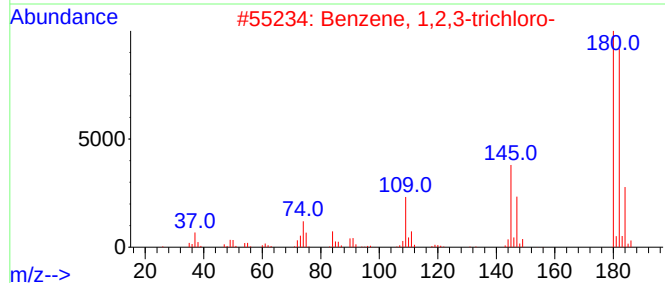
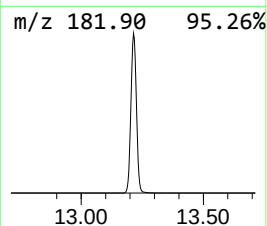
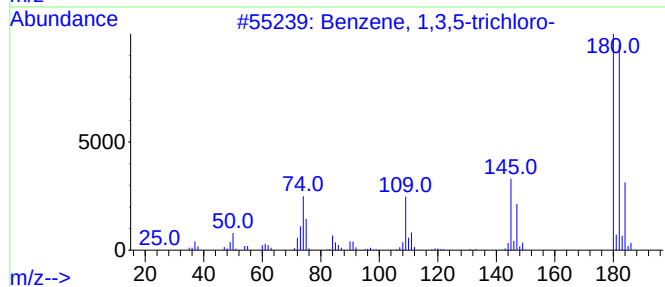
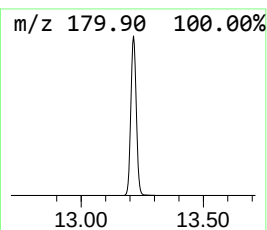
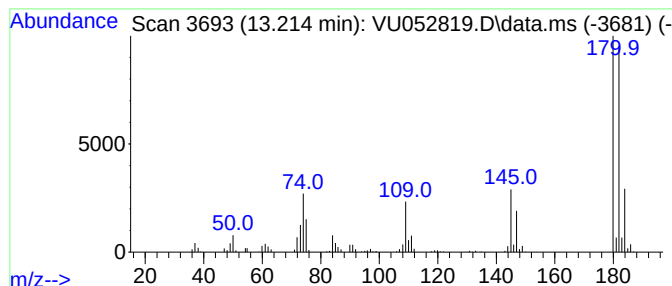
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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	46.04 ug/L	867996	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, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
3			Benzene, 1,2,3-trichloro-	180	C6H3Cl3	000087-61-6	98
4			Benzene, 1,3,5-trichloro-	180	C6H3Cl3	000108-70-3	98
5			Benzene, 1,2,4-trichloro-	180	C6H3Cl3	000120-82-1	97



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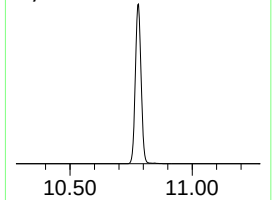
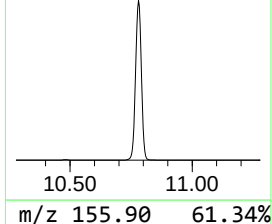
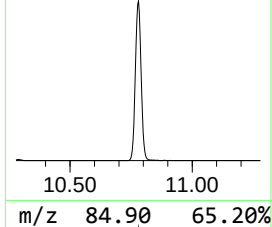
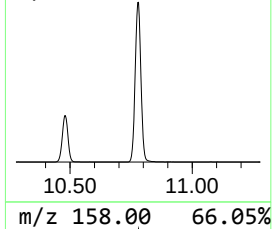
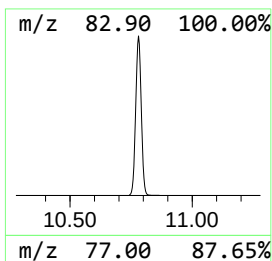
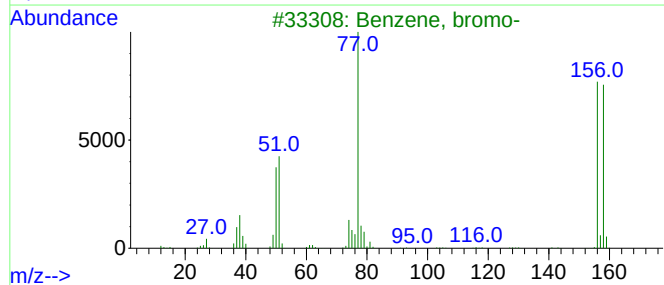
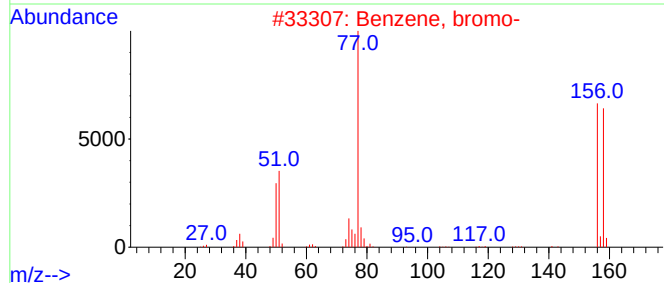
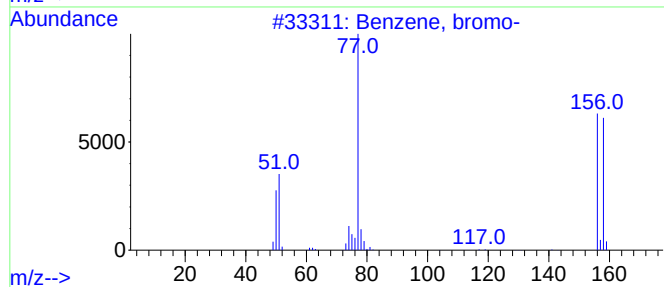
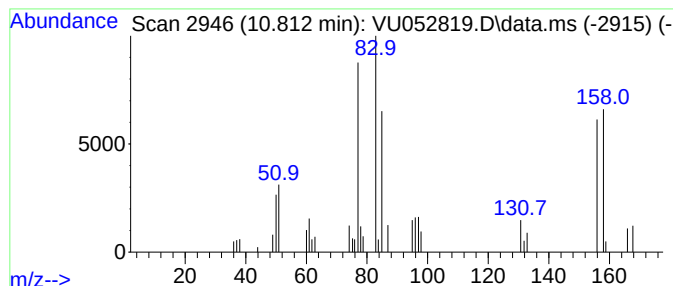
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM012623WMA.M
Quant Title : VOC Analysis

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	115.64 ug/L	2180150	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, bromo-	156	C6H5Br	000108-86-1	83
2			Benzene, bromo-	156	C6H5Br	000108-86-1	83
3			Benzene, bromo-	156	C6H5Br	000108-86-1	53
4			Ethane, 1,1,2,2-tetrachloro-	166	C2H2Cl4	000079-34-5	50
5			Benzene, bromo-	156	C6H5Br	000108-86-1	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012623\
Data File : VU052819.D
Acq On : 26 Jan 2023 16:30
Operator : JC/MD
Sample : 01314-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A44Q4

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	7.025	4.3	ug/L	55021	1	6.243	635709	50.0
Benzene, 1,3,5-...	13.214	46.0	ug/L	867996	3	11.809	942620	50.0
Benzene, bromo-	10.780	115.6	ug/L	2180150	3	11.809	942620	50.0