

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053548.D
 Acq On : 04 Apr 2023 03:06
 Operator : JC/MD
 Sample : 02158-23
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 PMW-3(20230331)

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053548.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	91	rBV	130042	144413	16.34%	1.822%
2	1.909	170	177	191	rVB	95942	129822	14.69%	1.638%
3	2.372	311	321	347	rVB3	49603	84574	9.57%	1.067%
4	2.565	369	381	397	rBV	189106	303384	34.32%	3.828%
5	2.729	428	432	433	rBV	417	271	0.03%	0.003%
6	3.128	553	556	559	rBV2	436	303	0.03%	0.004%
7	3.173	562	570	582	rVB5	1467	3454	0.39%	0.044%
8	3.266	597	599	602	rBV	218	108	0.01%	0.001%
9	3.353	616	626	636	rVB3	5410	9668	1.09%	0.122%
10	3.549	684	687	690	rBV	283	155	0.02%	0.002%
11	3.867	770	786	806	rVB2	53867	129925	14.70%	1.640%
12	3.960	811	815	816	rBV3	416	328	0.04%	0.004%
13	4.128	865	867	873	rBV	166	173	0.02%	0.002%
14	4.417	953	957	960	rBV2	442	391	0.04%	0.005%
15	4.526	981	991	996	rBV2	879	1054	0.12%	0.013%
16	4.613	1003	1018	1026	rBV2	69945	153419	17.36%	1.936%
17	4.976	1127	1131	1140	rBV3	447	420	0.05%	0.005%
18	5.060	1140	1157	1179	rBV2	162832	359351	40.65%	4.535%
19	5.719	1342	1362	1378	rBV2	318635	883986	100.00%	11.155%
20	6.005	1449	1451	1453	rBV	240	124	0.01%	0.002%
21	6.031	1457	1459	1461	rVB	282	91	0.01%	0.001%
22	6.243	1511	1525	1543	rBV	297870	564888	63.90%	7.128%
23	6.462	1591	1593	1594	rBV	224	106	0.01%	0.001%
24	6.539	1602	1617	1631	rBV7	16933	34393	3.89%	0.434%
25	6.600	1633	1636	1637	rBV	205	120	0.01%	0.002%
26	6.684	1649	1662	1680	rBV	200371	387722	43.86%	4.893%
27	6.796	1694	1697	1699	rBV3	533	344	0.04%	0.004%
28	6.845	1710	1712	1717	rBV2	320	207	0.02%	0.003%
29	6.867	1717	1719	1722	rBV	241	105	0.01%	0.001%
30	6.960	1743	1748	1755	rBV4	830	1102	0.12%	0.014%
31	7.160	1800	1810	1813	rBV5	1117	1575	0.18%	0.020%
32	7.385	1878	1880	1881	rBV5	143	38	0.00%	0.000%
33	7.430	1890	1894	1897	rBV2	311	203	0.02%	0.003%
34	7.500	1913	1916	1919	rBV2	213	170	0.02%	0.002%
35	7.562	1922	1935	1952	rBV	111677	195310	22.09%	2.465%
36	7.783	2000	2004	2006	rBV2	267	210	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

37	7.893	2020	2038	2054	rBV	414308	721350	81.60%	9.103%
38	8.105	2101	2104	2107	rVB2	396	196	0.02%	0.002%
39	8.172	2115	2125	2141	rBV	77708	132501	14.99%	1.672%
40	8.552	2234	2243	2253	rVB5	7756	12288	1.39%	0.155%
41	8.626	2253	2266	2298	rBV	210978	391439	44.28%	4.940%
42	8.812	2322	2324	2327	rVB	257	103	0.01%	0.001%
43	8.848	2331	2335	2336	rBV	545	322	0.04%	0.004%
44	8.857	2336	2338	2345	rVB4	1088	1035	0.12%	0.013%
45	8.915	2354	2356	2358	rVB	385	198	0.02%	0.002%
46	8.931	2358	2361	2363	rBV2	217	123	0.01%	0.002%
47	9.298	2473	2475	2476	rBV2	179	63	0.01%	0.001%
48	9.349	2489	2491	2497	rBV	218	136	0.02%	0.002%
49	9.414	2497	2511	2534	rBV	413126	741443	83.87%	9.356%
50	9.571	2549	2560	2570	rBV4	2738	4348	0.49%	0.055%
51	9.632	2577	2579	2582	rBV	345	216	0.02%	0.003%
52	9.677	2583	2593	2602	rBV10	1992	5003	0.57%	0.063%
53	9.764	2619	2620	2622	rBV	205	99	0.01%	0.001%
54	9.825	2635	2639	2640	rBV	296	136	0.02%	0.002%
55	9.912	2665	2666	2667	rBV	144	46	0.01%	0.001%
56	10.098	2719	2724	2726	rBV2	1169	998	0.11%	0.013%
57	10.179	2747	2749	2752	rBB	242	113	0.01%	0.001%
58	10.262	2773	2775	2777	rBV	381	217	0.02%	0.003%
59	10.481	2835	2843	2854	rBV2	4946	7203	0.81%	0.091%
60	10.751	2915	2927	2943	rBV	286707	462369	52.31%	5.835%
61	10.832	2950	2952	2960	rBV2	335	309	0.03%	0.004%
62	10.902	2970	2974	2984	rVB2	2303	3194	0.36%	0.040%
63	11.086	3024	3031	3041	rVB3	5064	7403	0.84%	0.093%
64	11.185	3059	3062	3067	rVB3	810	578	0.07%	0.007%
65	11.243	3077	3080	3086	rBV4	614	642	0.07%	0.008%
66	11.288	3086	3094	3104	rVB2	8180	12064	1.36%	0.152%
67	11.333	3104	3108	3110	rBV2	285	188	0.02%	0.002%
68	11.414	3127	3133	3137	rBV2	970	1209	0.14%	0.015%
69	11.465	3141	3149	3163	rVB2	11434	16460	1.86%	0.208%
70	11.642	3196	3204	3213	rVB3	6861	10850	1.23%	0.137%
71	11.709	3222	3225	3227	rBV	264	168	0.02%	0.002%
72	11.741	3227	3235	3244	rVV3	12033	17567	1.99%	0.222%
73	11.809	3244	3256	3275	rVV	459891	786470	88.97%	9.925%
74	11.889	3275	3281	3291	rVB	11781	17177	1.94%	0.217%
75	12.005	3310	3317	3325	rVB4	2175	3145	0.36%	0.040%
76	12.092	3333	3344	3360	rVB2	33705	55042	6.23%	0.695%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

77	12.188	3360	3374	3392	rBV	453854	741914	83.93%	9.362%
78	12.327	3415	3417	3421	rVB	475	275	0.03%	0.003%
79	12.375	3426	3432	3442	rVB2	4474	6247	0.71%	0.079%
80	12.462	3450	3459	3464	rBV4	7136	11163	1.26%	0.141%
81	12.606	3499	3504	3516	rVB3	8422	12343	1.40%	0.156%
82	12.677	3516	3526	3545	rBV4	18194	38206	4.32%	0.482%
83	12.803	3562	3565	3568	rBV4	855	553	0.06%	0.007%
84	12.860	3577	3583	3585	rBV5	5793	6080	0.69%	0.077%
85	12.925	3601	3603	3604	rBV5	602	276	0.03%	0.003%
86	13.021	3627	3633	3643	rVB2	13028	19141	2.17%	0.242%
87	13.111	3653	3661	3669	rVB5	3338	4640	0.52%	0.059%
88	13.291	3710	3717	3724	rBV5	5339	7708	0.87%	0.097%
89	13.449	3758	3766	3782	rVB4	33955	56875	6.43%	0.718%
90	13.619	3812	3819	3830	rVB2	15145	23506	2.66%	0.297%
91	13.732	3846	3854	3860	rBV5	2747	3432	0.39%	0.043%
92	13.780	3862	3869	3876	rVB4	4542	6447	0.73%	0.081%
93	13.838	3877	3887	3898	rBV3	46340	78546	8.89%	0.991%
94	14.185	3988	3995	4009	rBV5	8740	14728	1.67%	0.186%
95	14.282	4018	4025	4034	rVB2	14445	21338	2.41%	0.269%
96	14.806	4183	4188	4198	rVB4	1870	2857	0.32%	0.036%
97	14.876	4202	4210	4220	rVB8	7377	12308	1.39%	0.155%
98	14.918	4220	4223	4224	rBV2	592	291	0.03%	0.004%
99	15.015	4244	4253	4266	rBV7	10337	18011	2.04%	0.227%
100	15.410	4369	4376	4389	rVB2	18553	31227	3.53%	0.394%

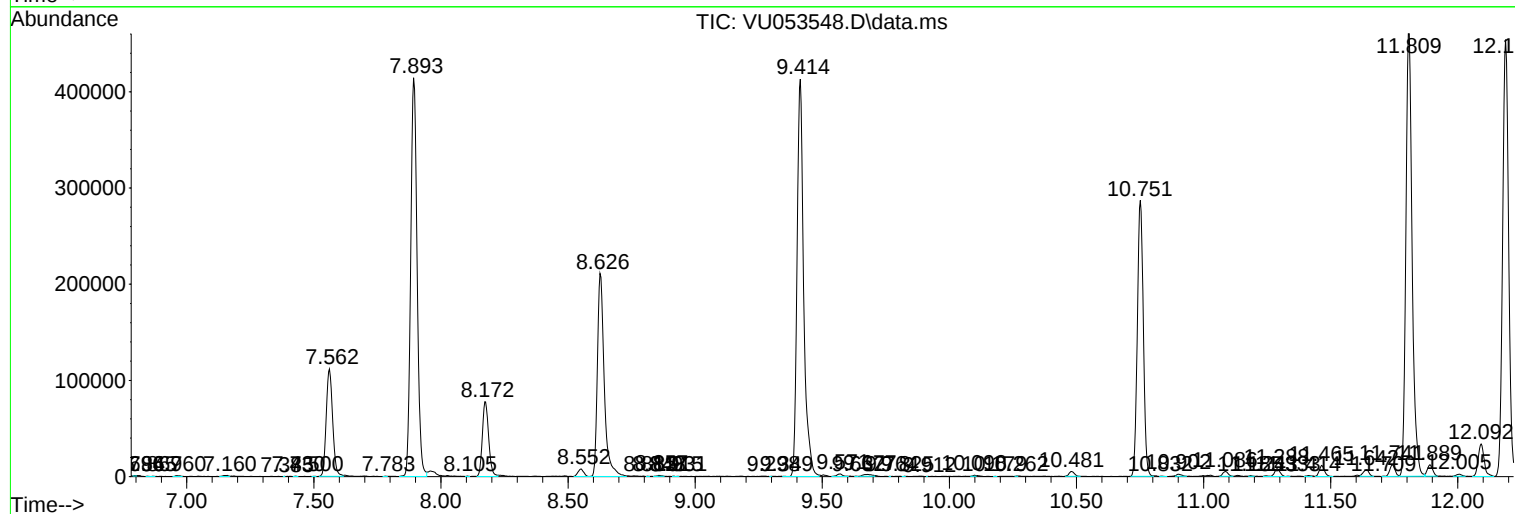
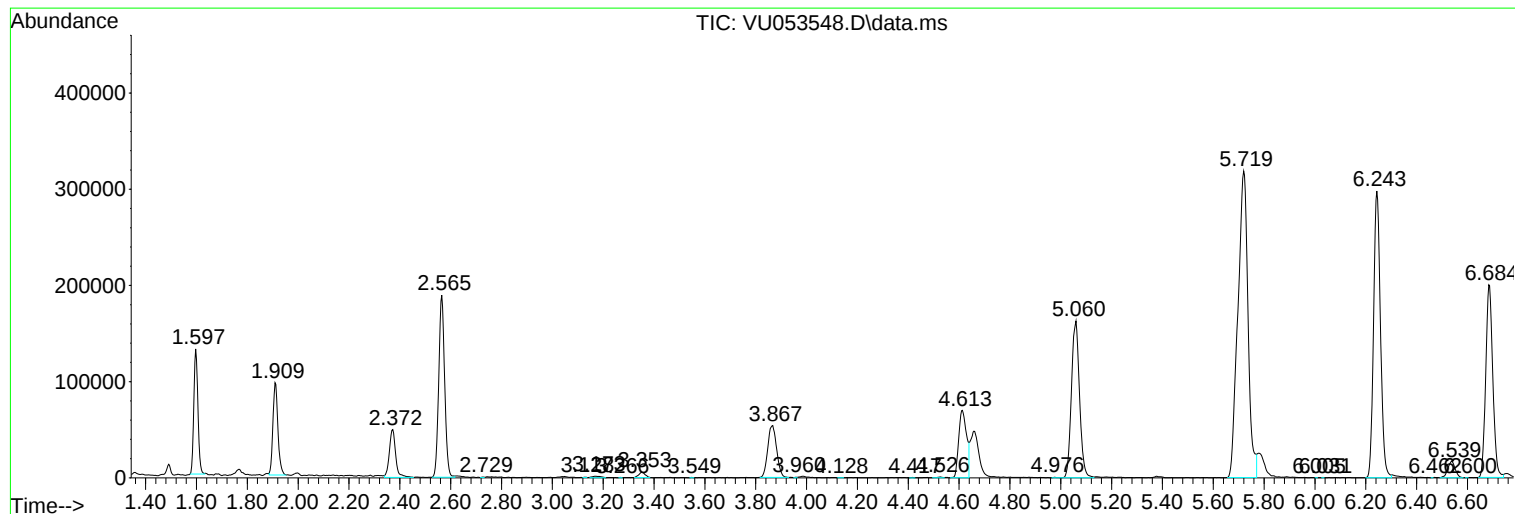
Sum of corrected areas: 7924430

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PMW-3(20230331)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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Misc : 5.0mL/MSVOA_U/WATER
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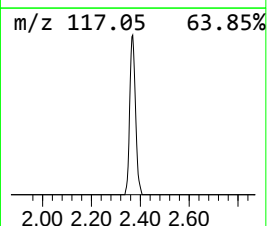
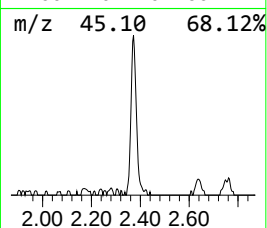
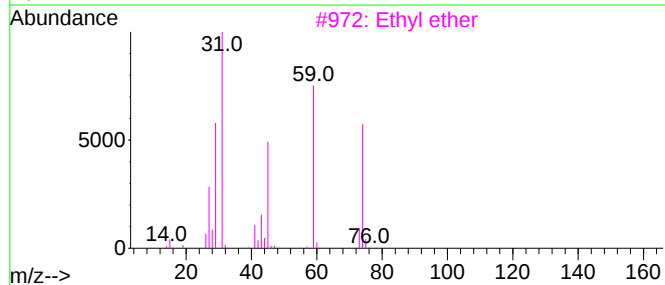
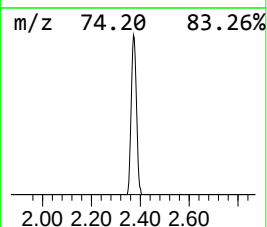
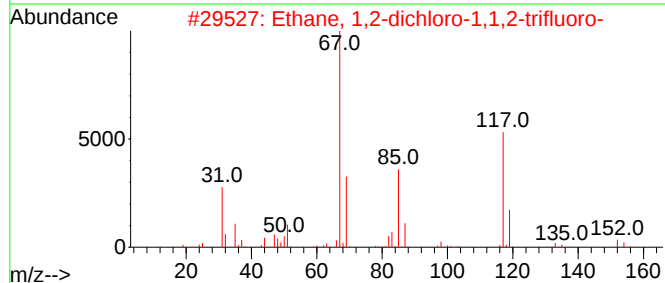
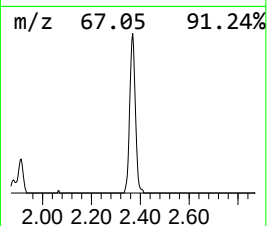
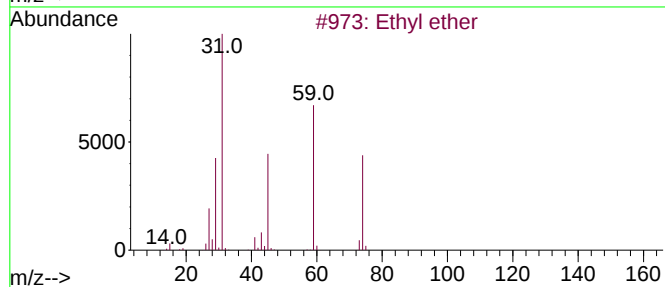
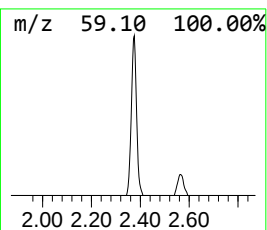
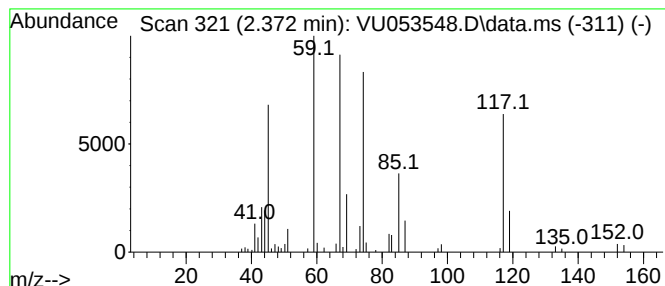
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.372	7.49 ug/L	84574	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl ether	74	C4H10O	000060-29-7	46
2			Ethane, 1,2-dichloro-1,1,2-trifl...	152	C2HCl2F3	000354-23-4	46
3			Ethyl ether	74	C4H10O	000060-29-7	46
4			Ethyl ether	74	C4H10O	000060-29-7	43
5			Boron trifluoride etherate	142	C4H10BF3O	000109-63-7	43



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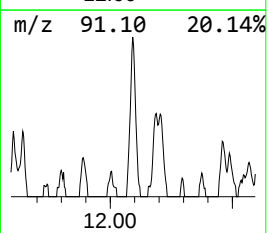
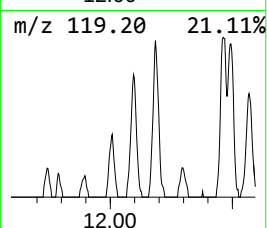
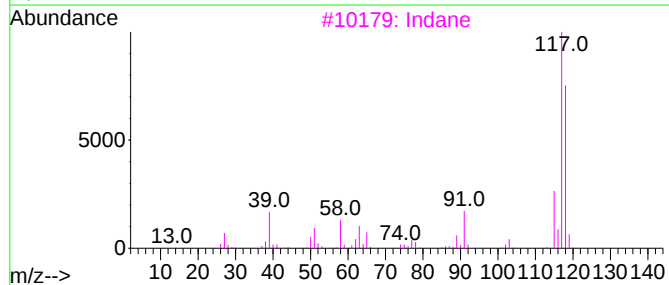
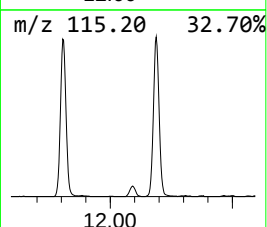
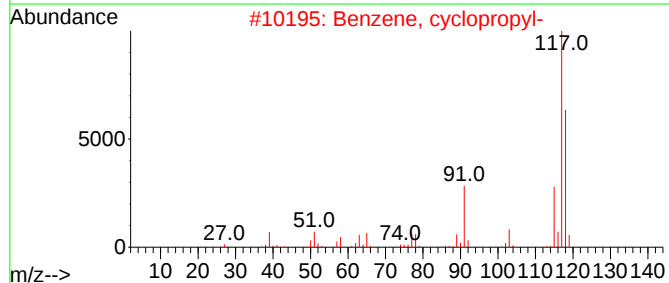
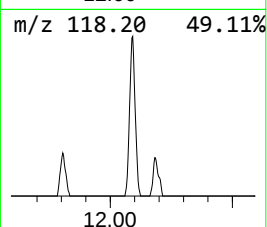
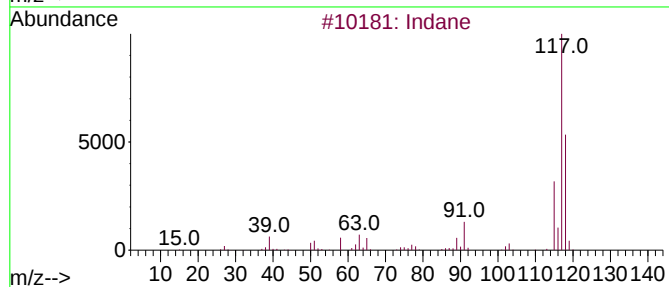
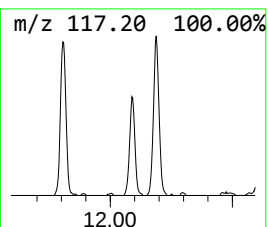
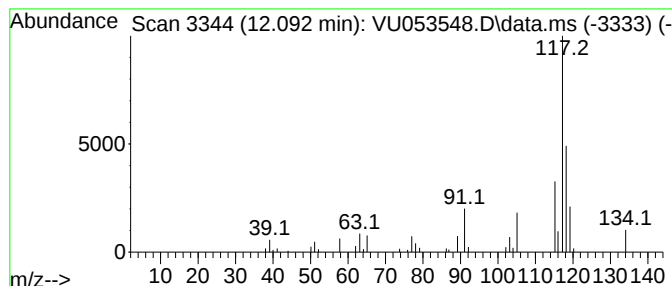
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	3.50 ug/L	55042	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	70
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
3			Indane	118	C9H10	000496-11-7	70
4			Indane	118	C9H10	000496-11-7	62
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	58



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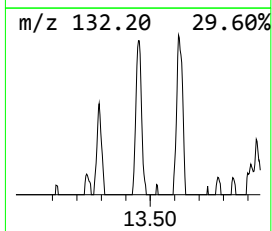
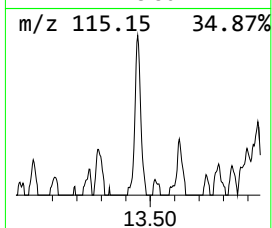
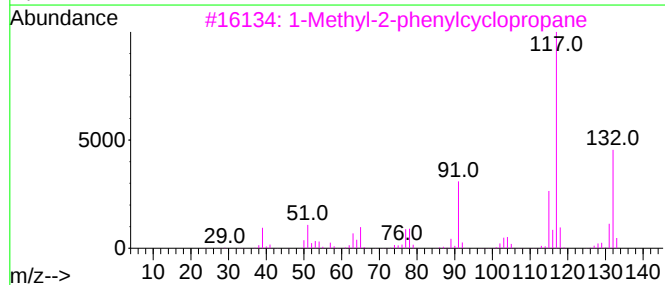
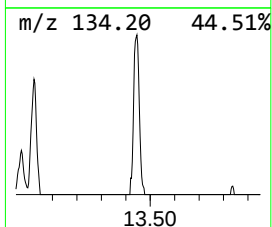
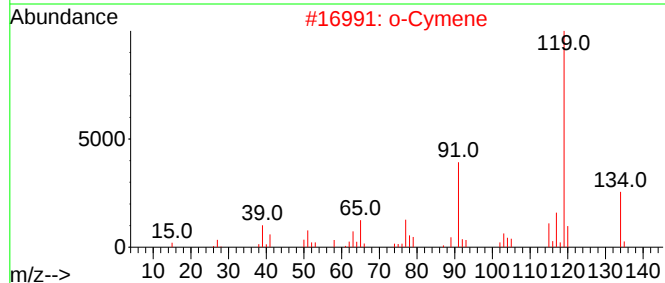
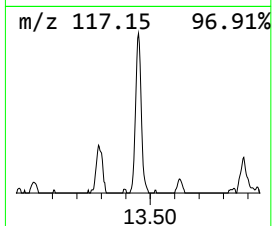
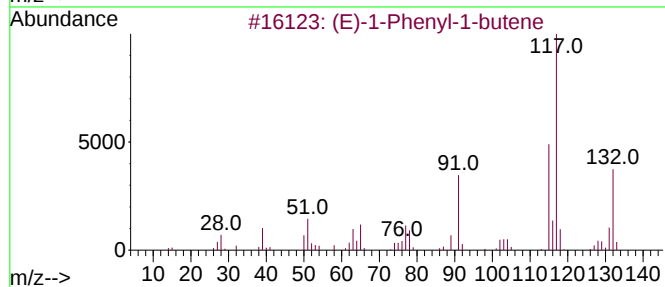
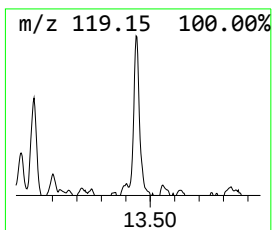
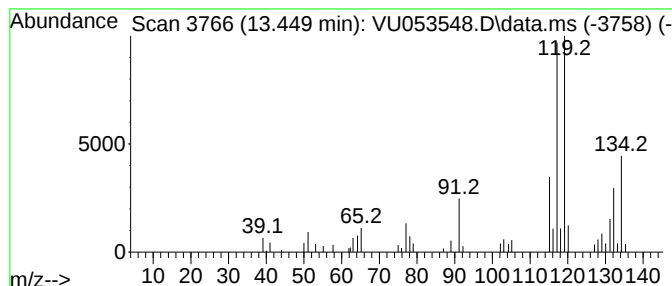
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (E)-1-Phenyl-1-butene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.449	3.62 ug/L	56875	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	64		
2	o-Cymene	134	C10H14	000527-84-4	55		
3	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	50		
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	50		
5	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	50		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053548.D
Acq On : 04 Apr 2023 03:06
Operator : JC/MD
Sample : 02158-23
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PMW-3(20230331)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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
unknown-01	2.372	7.5	ug/L	84574	1	6.243	564888	50.0
Indane	12.092	3.5	ug/L	55042	3	11.809	786470	50.0
(E)-1-Phenyl-1-...	13.449	3.6	ug/L	56875	3	11.809	786470	50.0