

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040423\
 Data File : VU053567.D
 Acq On : 04 Apr 2023 17:31
 Operator : JC/MD
 Sample : 02158-23
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 20 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: VU053567.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	97	rVB	104807	121901	15.55%	1.646%
2	1.909	170	177	196	rVB	82216	112347	14.34%	1.517%
3	2.372	312	321	333	rVB2	45666	71356	9.10%	0.964%
4	2.565	370	381	395	rBV	147586	243356	31.05%	3.287%
5	3.015	515	521	522	rBV	340	224	0.03%	0.003%
6	3.025	522	524	525	rBV	719	331	0.04%	0.004%
7	3.134	555	558	560	rBV2	450	270	0.03%	0.004%
8	3.350	616	625	638	rVB2	5126	10014	1.28%	0.135%
9	3.610	702	706	709	rBV	240	217	0.03%	0.003%
10	3.639	712	715	719	rVV2	271	260	0.03%	0.004%
11	3.864	769	785	807	rBV2	53446	127606	16.28%	1.723%
12	3.960	811	815	816	rBV2	360	280	0.04%	0.004%
13	3.973	816	819	820	rBV2	641	388	0.05%	0.005%
14	4.079	846	852	855	rBV2	304	300	0.04%	0.004%
15	4.305	918	922	928	rVB2	213	298	0.04%	0.004%
16	4.613	1006	1018	1027	rBV	71501	164645	21.01%	2.224%
17	4.909	1106	1110	1115	rBV4	335	223	0.03%	0.003%
18	5.057	1139	1156	1176	rBV	150339	325171	41.49%	4.391%
19	5.247	1210	1215	1220	rVB2	368	288	0.04%	0.004%
20	5.372	1248	1254	1255	rBV3	979	844	0.11%	0.011%
21	5.719	1342	1362	1376	rBV2	278891	783712	100.00%	10.584%
22	5.983	1441	1444	1447	rBV2	320	259	0.03%	0.003%
23	6.105	1479	1482	1488	rBV2	247	245	0.03%	0.003%
24	6.243	1512	1525	1547	rBV	289330	554977	70.81%	7.495%
25	6.485	1596	1600	1603	rBV	260	224	0.03%	0.003%
26	6.536	1605	1616	1631	rVB6	12217	24262	3.10%	0.328%
27	6.603	1633	1637	1641	rVB	316	241	0.03%	0.003%
28	6.687	1649	1663	1678	rBV	181243	352376	44.96%	4.759%
29	6.857	1713	1716	1723	rVB2	268	231	0.03%	0.003%
30	6.964	1743	1749	1756	rVV4	791	1120	0.14%	0.015%
31	7.156	1800	1809	1815	rBV6	1522	2403	0.31%	0.032%
32	7.562	1923	1935	1957	rBV	100866	181403	23.15%	2.450%
33	7.681	1970	1972	1980	rVB3	527	571	0.07%	0.008%
34	7.767	1996	1999	2003	rBV2	249	233	0.03%	0.003%
35	7.893	2026	2038	2058	rBV	358951	624698	79.71%	8.437%
36	8.173	2114	2125	2140	rBV	75535	123999	15.82%	1.675%

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Integrator: RTE

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

37	8.455	2209	2213	2215	rVV2	452	359	0.05%	0.005%
38	8.472	2216	2218	2221	rVV2	568	376	0.05%	0.005%
39	8.549	2235	2242	2251	rVB5	4751	7306	0.93%	0.099%
40	8.626	2255	2266	2304	rBV	211155	391757	49.99%	5.291%
41	8.755	2304	2306	2311	rBV2	339	219	0.03%	0.003%
42	8.796	2316	2319	2323	rBV2	273	250	0.03%	0.003%
43	8.857	2329	2338	2339	rBV3	1352	1239	0.16%	0.017%
44	9.012	2383	2386	2390	rVB3	356	276	0.04%	0.004%
45	9.089	2404	2410	2411	rBV2	288	277	0.04%	0.004%
46	9.269	2458	2466	2468	rBV2	362	490	0.06%	0.007%
47	9.414	2497	2511	2532	rBV	405923	729266	93.05%	9.849%
48	9.565	2552	2558	2568	rVB2	2529	3756	0.48%	0.051%
49	9.671	2580	2591	2594	rBV6	2114	3277	0.42%	0.044%
50	9.883	2654	2657	2661	rVB2	288	217	0.03%	0.003%
51	9.973	2682	2685	2689	rBV2	278	246	0.03%	0.003%
52	10.034	2701	2704	2706	rBV2	350	218	0.03%	0.003%
53	10.070	2712	2715	2717	rVB2	461	258	0.03%	0.003%
54	10.099	2717	2724	2733	rBV6	1012	1698	0.22%	0.023%
55	10.269	2772	2777	2782	rBV4	695	619	0.08%	0.008%
56	10.481	2834	2843	2855	rVB4	5140	7593	0.97%	0.103%
57	10.587	2870	2876	2879	rBV2	218	249	0.03%	0.003%
58	10.639	2889	2892	2897	rBV2	345	304	0.04%	0.004%
59	10.751	2914	2927	2947	rBV	284767	451564	57.62%	6.098%
60	10.822	2947	2949	2950	rVV2	600	216	0.03%	0.003%
61	10.902	2964	2974	2982	rBV4	2069	3493	0.45%	0.047%
62	11.002	3000	3005	3006	rBV	460	359	0.05%	0.005%
63	11.086	3022	3031	3041	rBV	4906	7333	0.94%	0.099%
64	11.253	3079	3083	3085	rVB	668	453	0.06%	0.006%
65	11.288	3085	3094	3112	rVB2	7893	14049	1.79%	0.190%
66	11.465	3141	3149	3159	rBV	10481	15476	1.97%	0.209%
67	11.606	3187	3193	3196	rBV2	1428	1630	0.21%	0.022%
68	11.742	3227	3235	3243	rVV2	6412	8356	1.07%	0.113%
69	11.809	3243	3256	3273	rVV	460790	747245	95.35%	10.092%
70	11.889	3275	3281	3295	rVB3	11496	17801	2.27%	0.240%
71	12.002	3310	3316	3324	rBV5	2531	3756	0.48%	0.051%
72	12.092	3333	3344	3360	rVB3	32645	52112	6.65%	0.704%
73	12.188	3360	3374	3390	rBV	409021	675406	86.18%	9.121%
74	12.375	3423	3432	3440	rBV	3592	5602	0.71%	0.076%
75	12.462	3449	3459	3464	rBV3	7659	11267	1.44%	0.152%
76	12.565	3483	3491	3499	rBV2	4347	7085	0.90%	0.096%

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 Title : VOC Analysis

77	12.610	3499	3505	3515	rVB4	7769	11642	1.49%	0.157%
78	12.677	3515	3526	3546	rBV3	16956	36336	4.64%	0.491%
79	12.806	3558	3566	3575	rBV5	1326	2137	0.27%	0.029%
80	12.860	3575	3583	3599	rVB7	6454	12641	1.61%	0.171%
81	13.021	3625	3633	3643	rVB2	13515	20552	2.62%	0.278%
82	13.108	3652	3660	3667	rBV5	3861	5723	0.73%	0.077%
83	13.185	3682	3684	3687	rBV	407	245	0.03%	0.003%
84	13.291	3710	3717	3742	rVB7	6965	13959	1.78%	0.189%
85	13.397	3744	3750	3756	rVV5	2192	3071	0.39%	0.041%
86	13.446	3756	3765	3782	rVV4	33167	56207	7.17%	0.759%
87	13.520	3782	3788	3794	rVB7	1889	2458	0.31%	0.033%
88	13.619	3811	3819	3832	rVB3	14602	23255	2.97%	0.314%
89	13.667	3832	3834	3839	rBV	312	228	0.03%	0.003%
90	13.835	3877	3886	3896	rBV6	15677	27545	3.51%	0.372%
91	13.989	3932	3934	3939	rBV	362	319	0.04%	0.004%
92	14.082	3946	3963	3982	rBV	36690	67717	8.64%	0.915%
93	14.188	3987	3996	4011	rVV4	8930	14322	1.83%	0.193%
94	14.282	4019	4025	4034	rVB2	14769	21431	2.73%	0.289%
95	14.481	4080	4087	4093	rBV4	4899	7024	0.90%	0.095%
96	14.680	4138	4149	4161	rVB7	9184	20837	2.66%	0.281%
97	14.806	4181	4188	4196	rVB5	2526	3527	0.45%	0.048%
98	15.015	4244	4253	4264	rBV7	10035	17260	2.20%	0.233%
99	15.410	4368	4376	4386	rVB4	18458	30972	3.95%	0.418%
100	15.751	4480	4482	4484	rBV	812	449	0.06%	0.006%

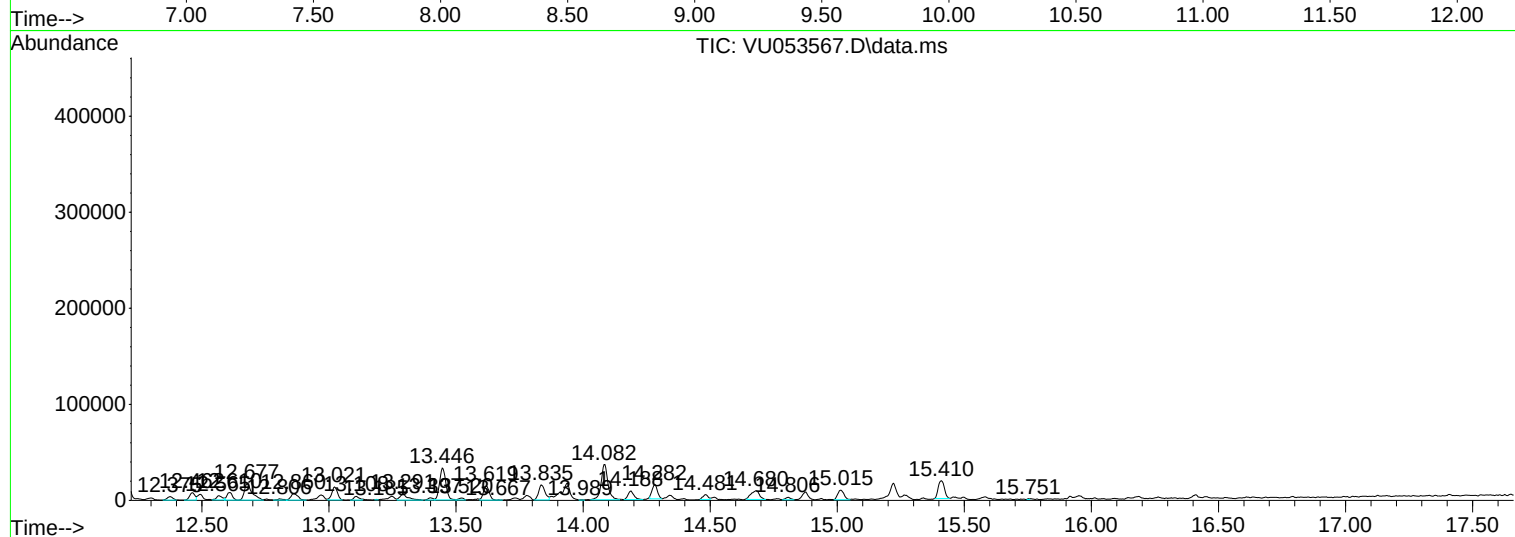
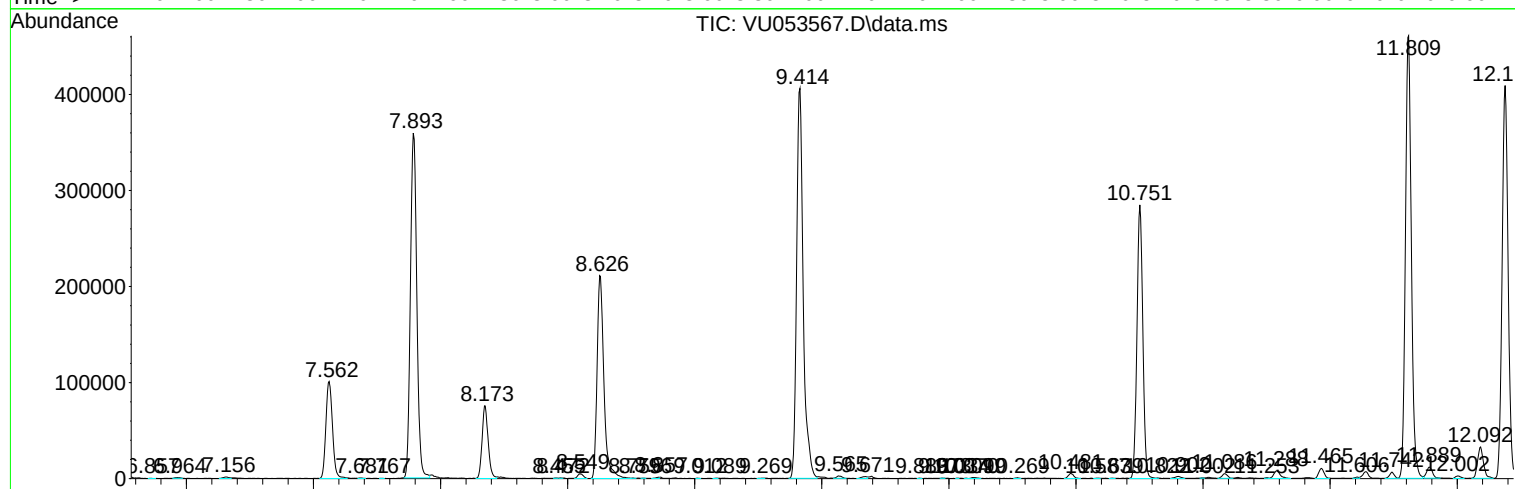
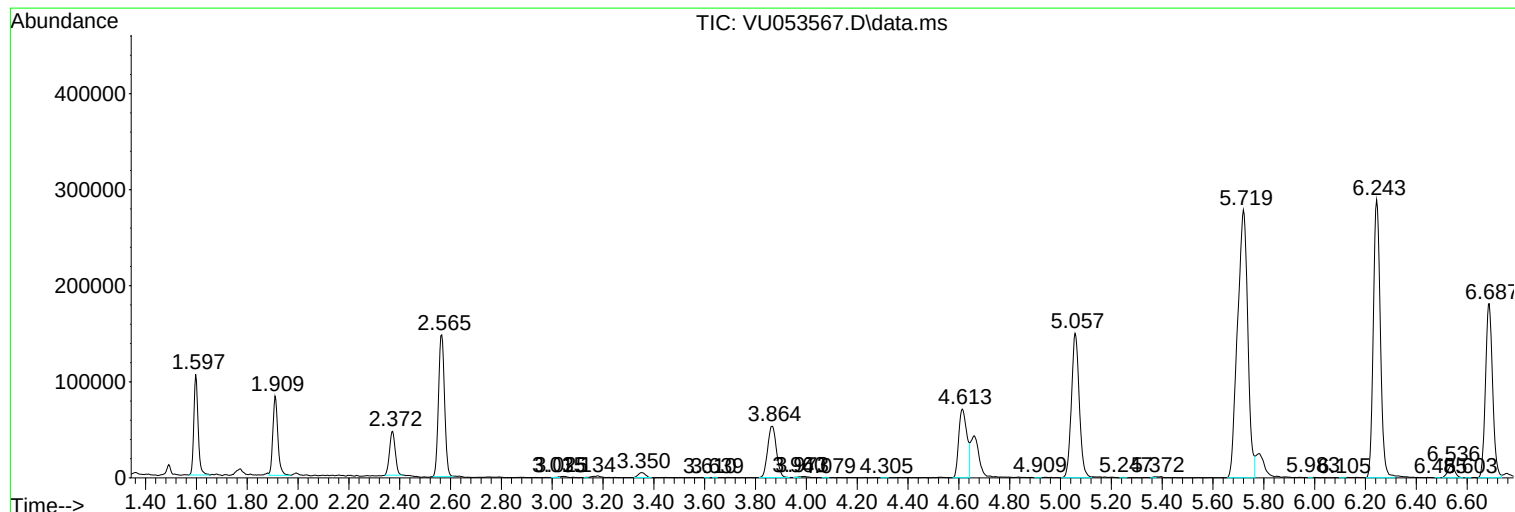
Sum of corrected areas: 7404583

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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040423\
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Instrument :
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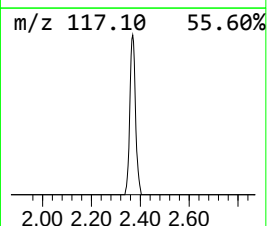
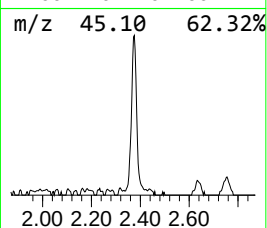
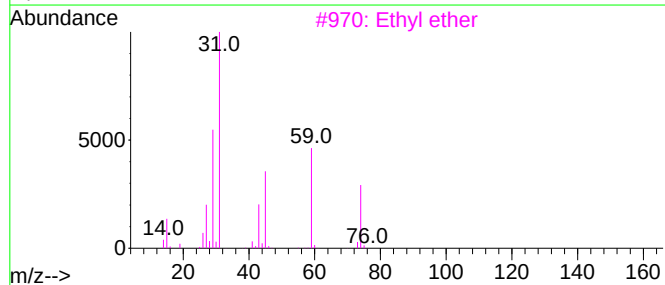
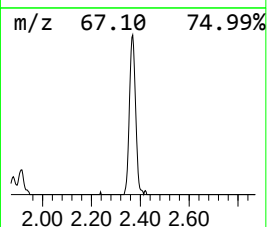
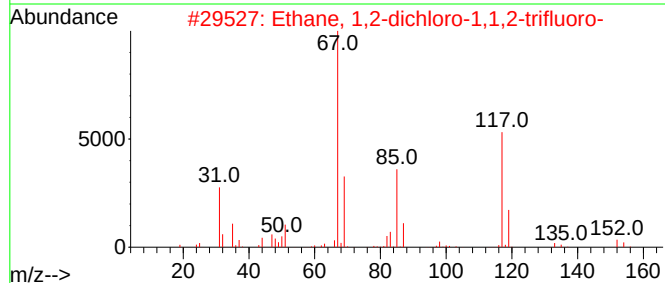
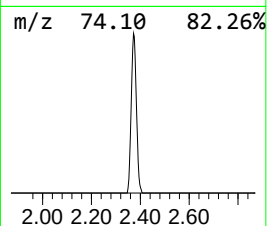
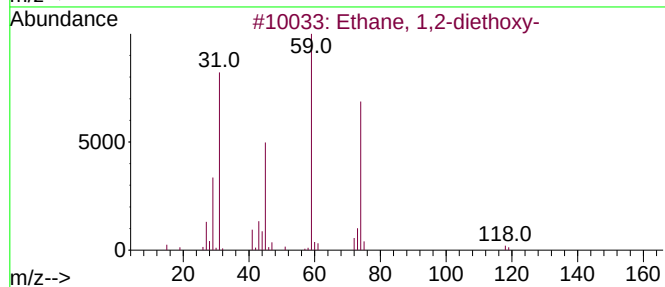
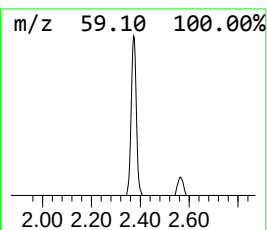
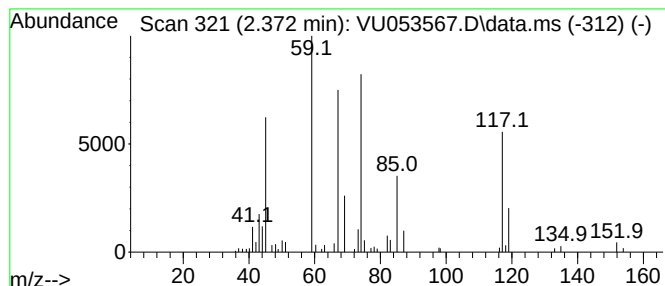
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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	6.43 ug/L	71356	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,2-diethoxy-	118	C6H14O2	000629-14-1	49
2			Ethane, 1,2-dichloro-1,1,2-trifl...	152	C2HC12F3	000354-23-4	46
3			Ethyl ether	74	C4H10O	000060-29-7	46
4			Ethyl ether	74	C4H10O	000060-29-7	46
5			Ethyl ether	74	C4H10O	000060-29-7	46



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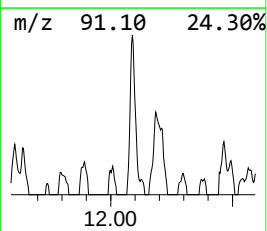
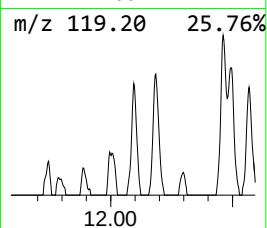
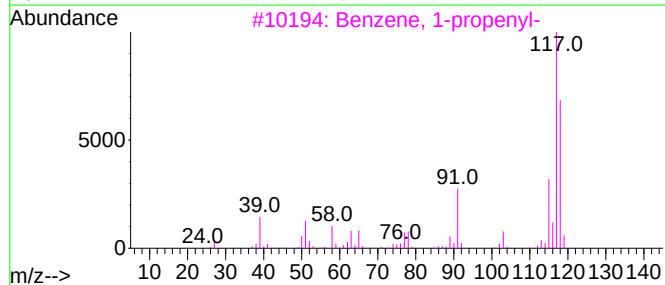
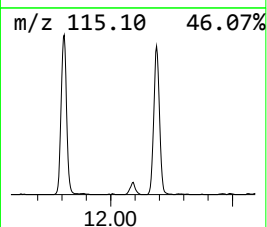
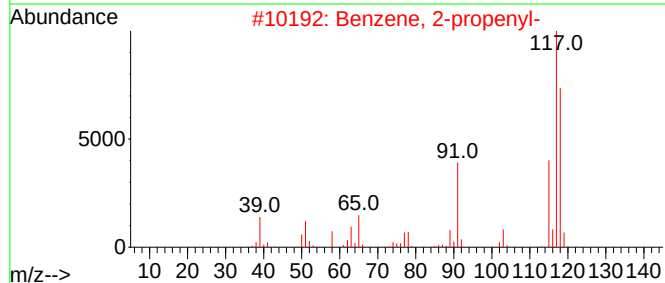
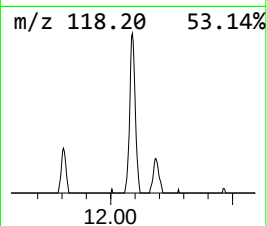
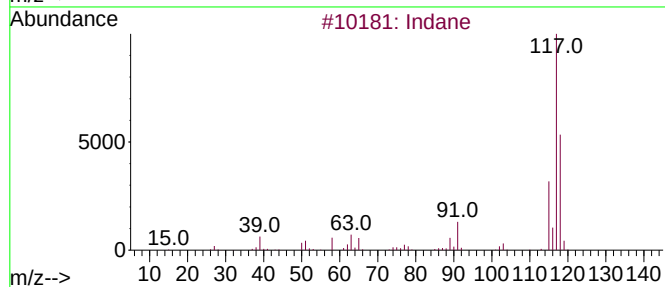
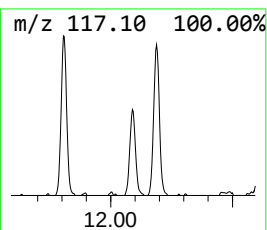
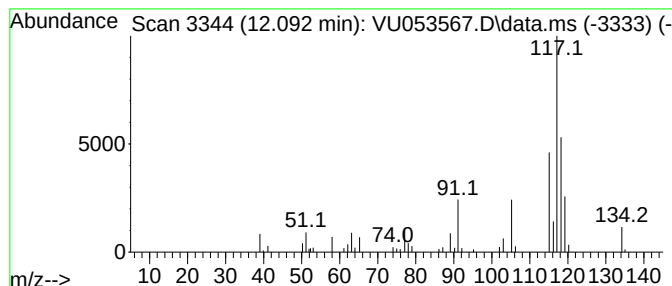
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	3.49 ug/L	52112	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	91
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	60
4			Indane	118	C9H10	000496-11-7	53
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	53



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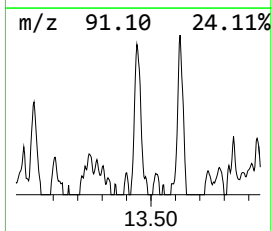
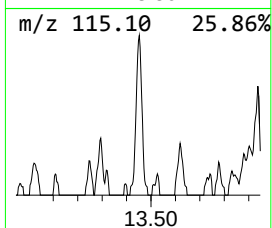
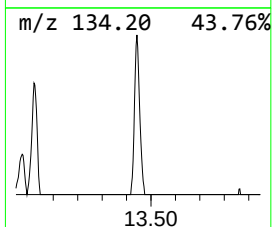
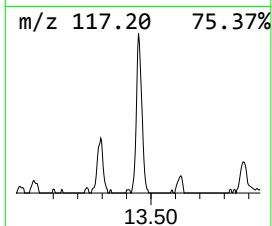
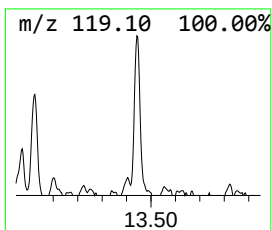
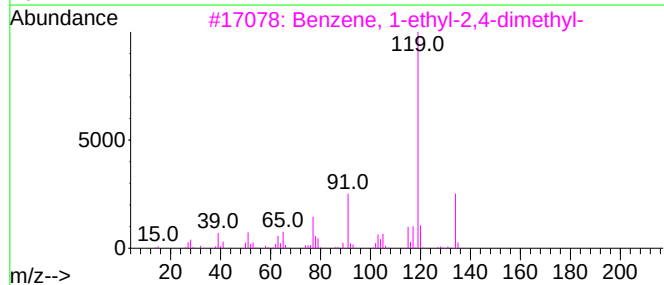
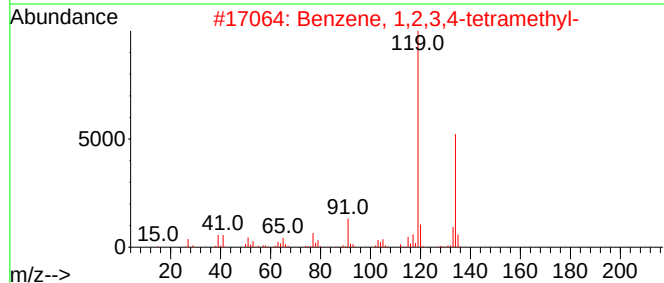
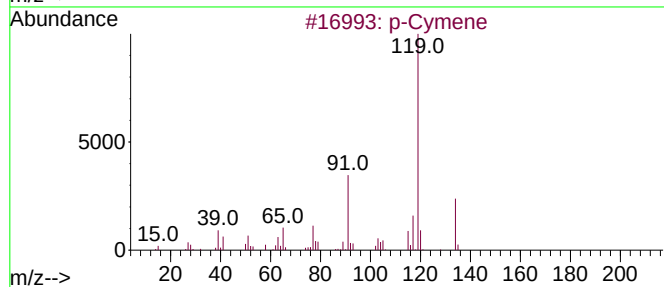
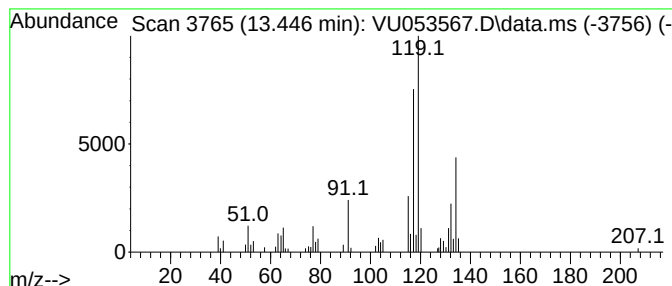
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 p-Cymene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.446	3.76 ug/L	56207	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Cymene	134	C10H14	000099-87-6	55
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	55
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	55
4			o-Cymene	134	C10H14	000527-84-4	55
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040423\
Data File : VU053567.D
Acq On : 04 Apr 2023 17:31
Operator : JC/MD
Sample : 02158-23
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
PMW-3(20230331)

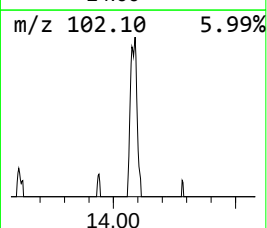
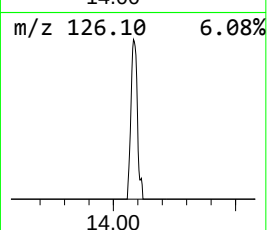
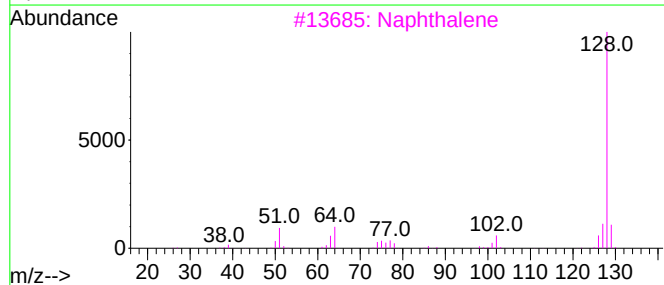
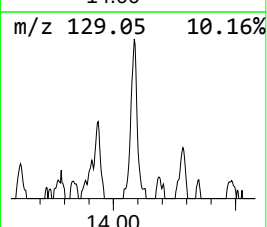
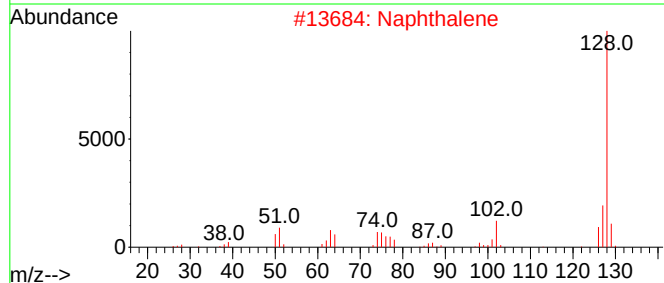
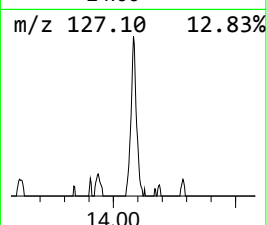
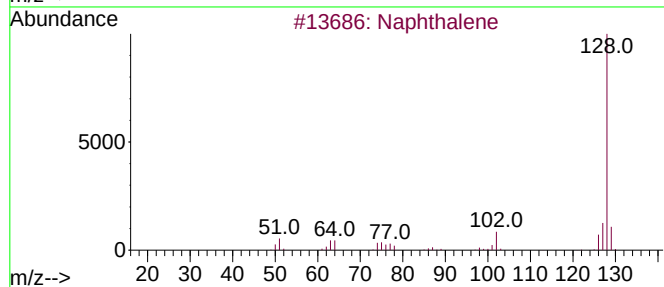
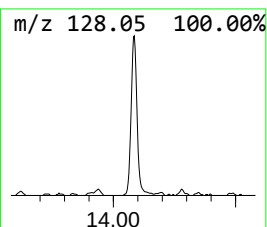
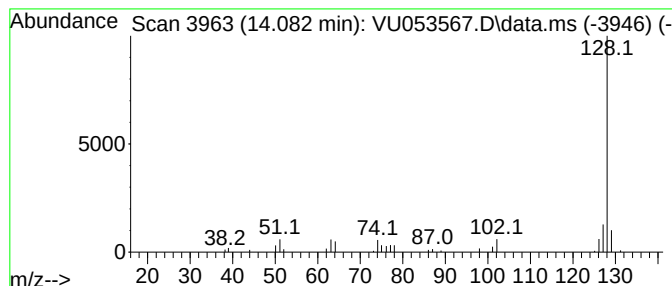
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Quant Title : VOC Analysis

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

Peak Number 5 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.082	4.53 ug/L	67717	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	91
3			Naphthalene	128	C10H8	000091-20-3	90
4			Azulene	128	C10H8	000275-51-4	90
5			Naphthalene	128	C10H8	000091-20-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040423\
Data File : VU053567.D
Acq On : 04 Apr 2023 17:31
Operator : JC/MD
Sample : 02158-23
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 20 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	6.4	ug/L	71356	1	6.243	554977	50.0
Indane	12.092	3.5	ug/L	52112	3	11.809	747245	50.0
p-Cymene	13.446	3.8	ug/L	56207	3	11.809	747245	50.0
Azulene	14.082	4.5	ug/L	67717	3	11.809	747245	50.0