

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072823\
 Data File : VV031778.D
 Acq On : 28 Jul 2023 10:53
 Operator : SY/MD
 Sample : 03754-17
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH2Z3

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_V\Method\SFAMVLM072523WMA.M
 Title : VOC Analysis

Signal : TIC: VV031778.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.278	66	74	89	rVB	205073	226678	13.73%	1.767%
2	1.529	145	152	169	rVB	194245	237850	14.40%	1.854%
3	2.060	307	317	327	rBV	380373	551142	33.38%	4.296%
4	2.114	329	334	351	rVB	46203	75851	4.59%	0.591%
5	2.336	401	403	407	rVB5	1988	1360	0.08%	0.011%
6	2.362	407	411	418	rVB7	2198	2508	0.15%	0.020%
7	2.452	432	439	447	rBV7	3407	4971	0.30%	0.039%
8	2.574	466	477	488	rBV3	18454	39949	2.42%	0.311%
9	2.690	510	513	515	rBV4	1194	979	0.06%	0.008%
10	2.732	522	526	531	rVB6	1270	1386	0.08%	0.011%
11	2.796	543	546	550	rBV5	1716	1700	0.10%	0.013%
12	2.921	582	585	589	rVB4	1373	1046	0.06%	0.008%
13	3.066	628	630	633	rVB3	1311	904	0.05%	0.007%
14	3.089	633	637	639	rBV5	1671	1075	0.07%	0.008%
15	3.510	765	768	770	rBV3	1290	889	0.05%	0.007%
16	3.584	786	791	793	rBV5	1176	1052	0.06%	0.008%
17	3.658	811	814	817	rBV5	1571	1051	0.06%	0.008%
18	3.793	843	856	885	rBV	155173	464228	28.11%	3.618%
19	4.252	984	999	1032	rBV	291558	773873	46.87%	6.032%
20	4.468	1064	1066	1070	rVB5	1572	1066	0.06%	0.008%
21	4.645	1118	1121	1124	rVB5	1328	931	0.06%	0.007%
22	4.674	1124	1130	1131	rBV6	1259	1205	0.07%	0.009%
23	4.789	1162	1166	1168	rBV4	1663	1283	0.08%	0.010%
24	4.841	1178	1182	1184	rBV4	1536	1225	0.07%	0.010%
25	4.960	1202	1219	1242	rBV2	615187	1651225	100.00%	12.870%
26	5.326	1329	1333	1335	rVB5	1715	982	0.06%	0.008%
27	5.539	1387	1399	1421	rBV	374264	789207	47.80%	6.151%
28	5.825	1478	1488	1508	rVB2	68467	143598	8.70%	1.119%
29	5.912	1509	1515	1518	rBV7	6933	7531	0.46%	0.059%
30	5.992	1528	1540	1559	rBV	402538	820487	49.69%	6.395%
31	6.352	1650	1652	1657	rVB5	2711	1921	0.12%	0.015%
32	6.381	1657	1661	1664	rBV5	1953	2060	0.12%	0.016%
33	6.516	1695	1703	1711	rVB7	8438	15510	0.94%	0.121%
34	6.658	1744	1747	1750	rBV5	1992	1197	0.07%	0.009%
35	6.780	1782	1785	1789	rBV6	1539	1220	0.07%	0.010%
36	6.828	1796	1800	1804	rBV7	1500	1244	0.08%	0.010%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
 Title : VOC Analysis

37	6.918	1818	1828	1854	rBV	172855	327237	19.82%	2.550%
38	7.079	1876	1878	1883	rVB4	1654	1158	0.07%	0.009%
39	7.130	1890	1894	1895	rBV4	1384	1005	0.06%	0.008%
40	7.178	1905	1909	1911	rBV5	1560	1283	0.08%	0.010%
41	7.249	1919	1931	1962	rBV	575513	1060712	64.24%	8.267%
42	7.558	2016	2027	2055	rBV	133686	244016	14.78%	1.902%
43	7.886	2119	2129	2135	rBV4	5297	9666	0.59%	0.075%
44	7.911	2135	2137	2141	rVV5	1801	1214	0.07%	0.009%
45	8.030	2163	2174	2214	rBV3	444694	980603	59.39%	7.643%
46	8.420	2290	2295	2298	rVB6	1807	1642	0.10%	0.013%
47	8.513	2320	2324	2325	rBV4	1881	1132	0.07%	0.009%
48	8.789	2398	2410	2434	rBV	635392	1073422	65.01%	8.366%
49	9.005	2474	2477	2478	rBV3	1483	911	0.06%	0.007%
50	9.265	2556	2558	2562	rBV4	1323	1154	0.07%	0.009%
51	9.381	2592	2594	2599	rBV4	1192	1034	0.06%	0.008%
52	9.436	2608	2611	2615	rVB6	1809	1205	0.07%	0.009%
53	9.484	2621	2626	2628	rBV6	2087	1913	0.12%	0.015%
54	9.850	2736	2740	2745	rBV7	1172	1110	0.07%	0.009%
55	10.098	2813	2817	2820	rBV6	1444	1116	0.07%	0.009%
56	10.159	2824	2836	2859	rVV	532572	845987	51.23%	6.594%
57	10.259	2863	2867	2872	rBV7	2522	2429	0.15%	0.019%
58	10.329	2882	2889	2897	rBV6	7722	11909	0.72%	0.093%
59	10.410	2908	2914	2917	rBV6	1458	1659	0.10%	0.013%
60	10.474	2931	2934	2937	rVB5	1556	1038	0.06%	0.008%
61	10.551	2956	2958	2964	rBV6	1569	1555	0.09%	0.012%
62	10.718	3002	3010	3012	rBV7	2757	3320	0.20%	0.026%
63	10.799	3031	3035	3036	rBV4	1272	928	0.06%	0.007%
64	10.886	3060	3062	3066	rVB4	1267	887	0.05%	0.007%
65	10.992	3092	3095	3096	rBV3	2401	1151	0.07%	0.009%
66	11.104	3127	3130	3132	rBV4	1904	1088	0.07%	0.008%
67	11.133	3132	3139	3146	rVV6	11712	18016	1.09%	0.140%
68	11.191	3146	3157	3175	rVV	630620	979980	59.35%	7.638%
69	11.384	3212	3217	3218	rBV5	1856	1343	0.08%	0.010%
70	11.493	3242	3251	3262	rBV3	19303	42450	2.57%	0.331%
71	11.567	3263	3274	3290	rVB	732459	1152985	69.83%	8.986%
72	11.751	3328	3331	3333	rBV3	2202	1249	0.08%	0.010%
73	11.857	3362	3364	3370	rVB6	3217	1643	0.10%	0.013%
74	11.947	3383	3392	3404	rBV2	39317	64104	3.88%	0.500%
75	12.156	3452	3457	3461	rBV6	1618	1680	0.10%	0.013%
76	12.197	3463	3470	3477	rVV9	5446	8374	0.51%	0.065%

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 Title : VOC Analysis

77	12.252	3477	3487	3497	rVV9	23245	37858	2.29%	0.295%
78	12.294	3497	3500	3505	rBV6	2730	2243	0.14%	0.017%
79	12.368	3519	3523	3524	rBV4	1949	1425	0.09%	0.011%
80	12.593	3587	3593	3596	rBV5	2949	2845	0.17%	0.022%
81	12.696	3623	3625	3628	rVB4	2300	1302	0.08%	0.010%
82	12.921	3693	3695	3700	rVB6	1893	1007	0.06%	0.008%
83	12.947	3700	3703	3707	rBV5	1467	1132	0.07%	0.009%
84	13.294	3808	3811	3814	rVV4	2055	1572	0.10%	0.012%
85	13.339	3822	3825	3830	rBV5	2378	1926	0.12%	0.015%
86	13.429	3846	3853	3855	rBV7	2955	3348	0.20%	0.026%
87	13.567	3892	3896	3898	rBV4	1859	1228	0.07%	0.010%
88	13.586	3900	3902	3905	rVV4	1925	1189	0.07%	0.009%
89	13.619	3907	3912	3915	rBV6	1725	1413	0.09%	0.011%
90	13.693	3931	3935	3941	rVB7	2167	2633	0.16%	0.021%
91	13.873	3983	3991	4004	rBV2	43830	66686	4.04%	0.520%
92	13.992	4023	4028	4038	rVB9	4252	5812	0.35%	0.045%
93	14.349	4137	4139	4141	rBV3	1971	1040	0.06%	0.008%
94	14.596	4209	4216	4218	rBV8	2839	3114	0.19%	0.024%
95	14.776	4270	4272	4275	rBV5	1308	925	0.06%	0.007%
96	14.818	4282	4285	4289	rBV5	1885	1366	0.08%	0.011%
97	14.837	4289	4291	4294	rBV4	1826	1183	0.07%	0.009%
98	15.133	4381	4383	4386	rBV4	1687	928	0.06%	0.007%
99	15.165	4390	4393	4397	rBV5	1510	1574	0.10%	0.012%
100	15.799	4588	4590	4593	rBV4	1856	1021	0.06%	0.008%

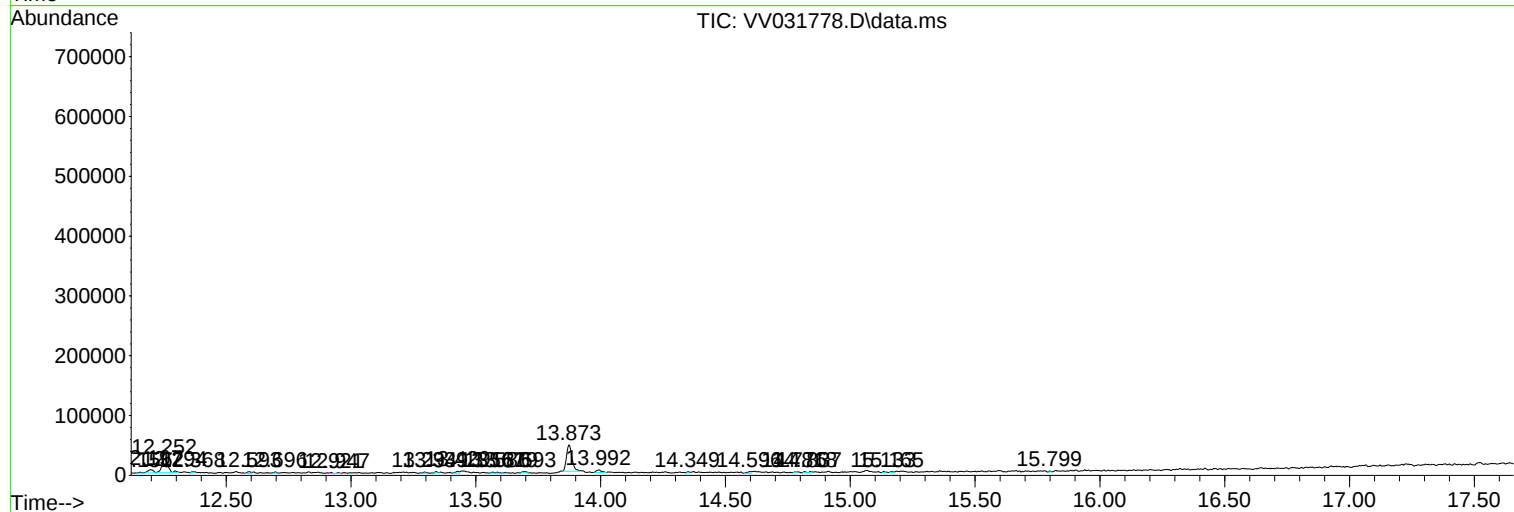
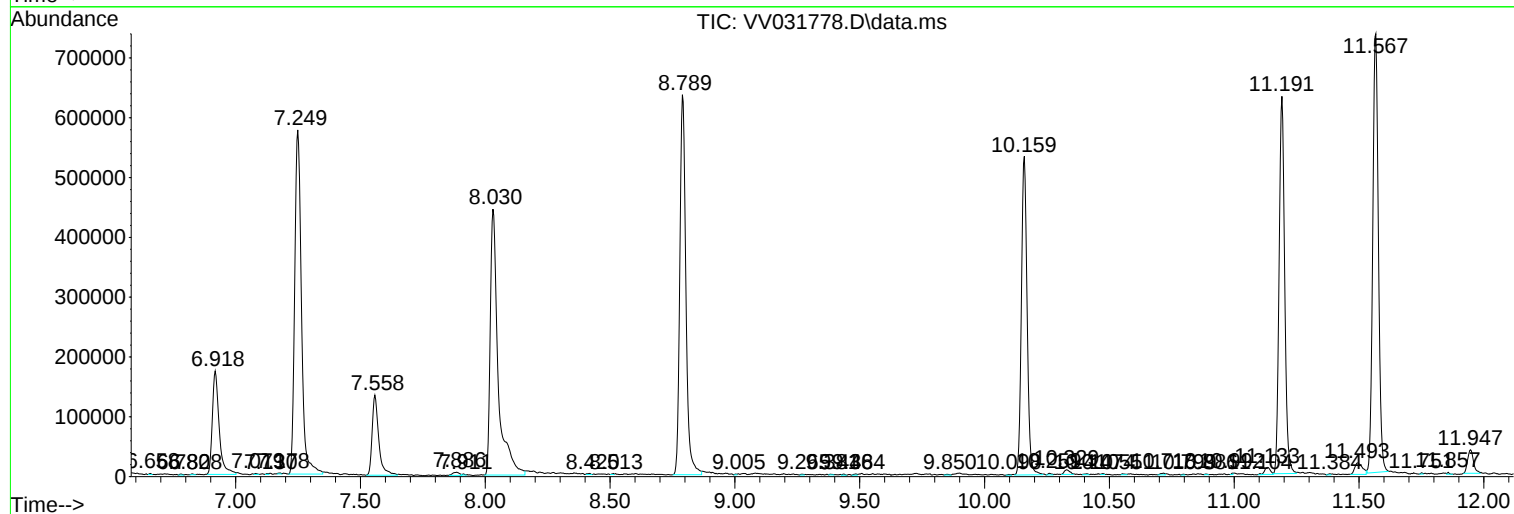
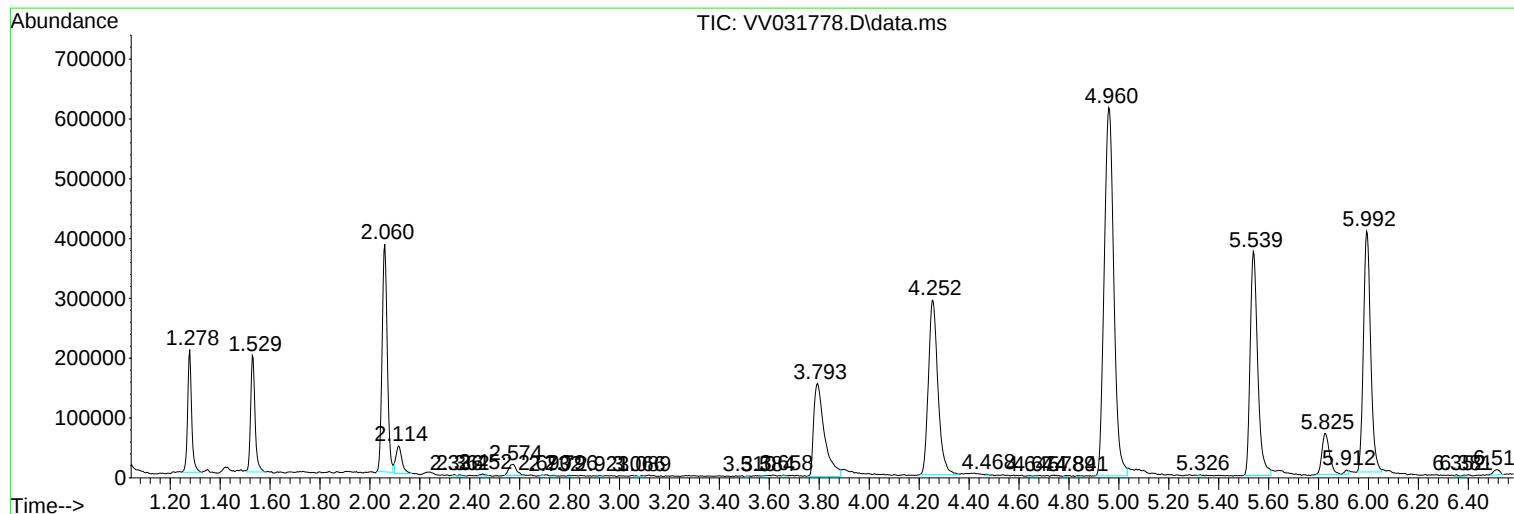
Sum of corrected areas: 12830462

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Instrument :
MSVOA_V
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.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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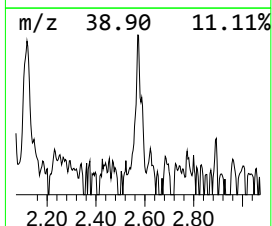
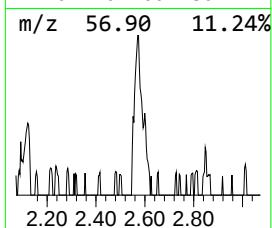
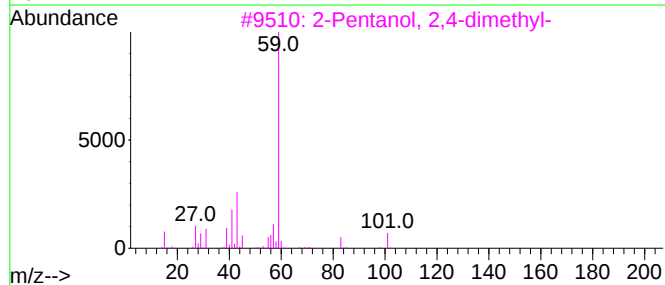
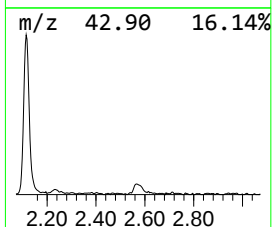
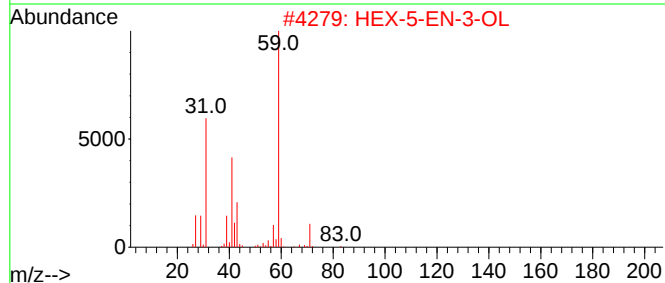
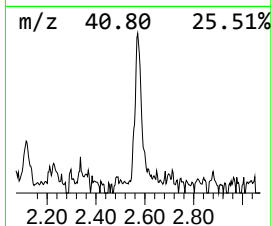
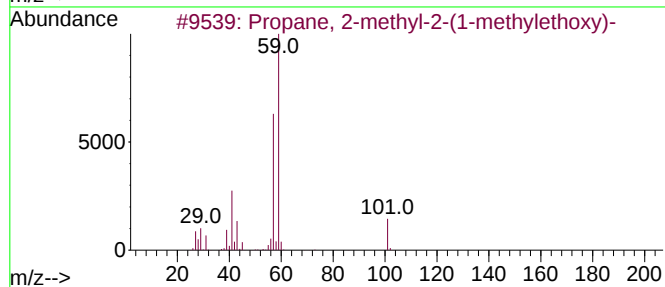
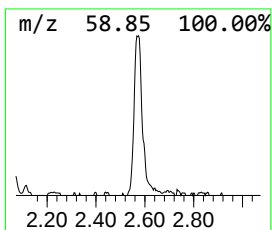
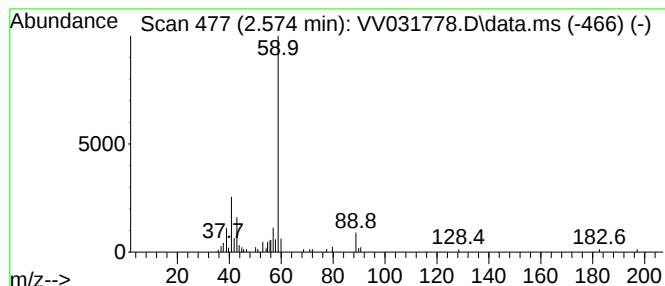
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.574	2.53 ug/L	39949	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2			HEX-5-EN-3-OL	100	C6H12O	000688-99-3	53
3			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	50
4			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	45
5			1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	45



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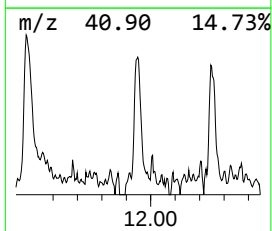
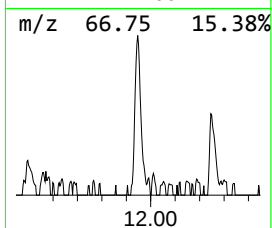
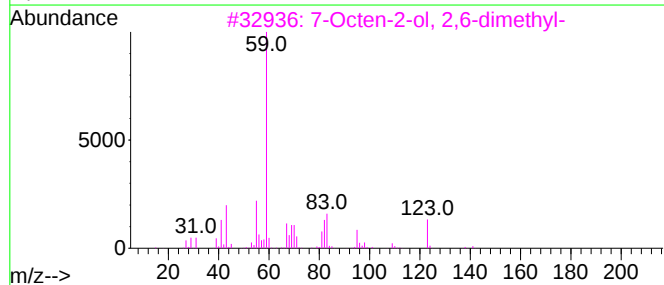
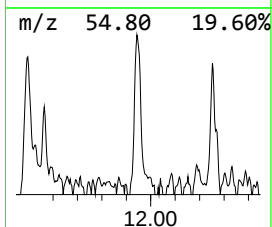
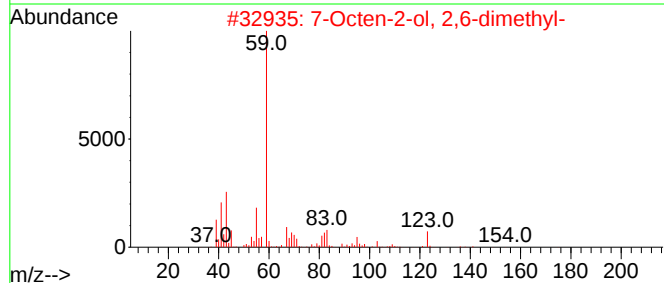
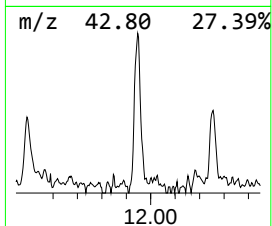
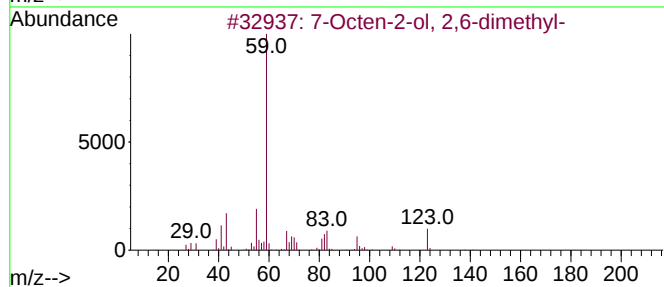
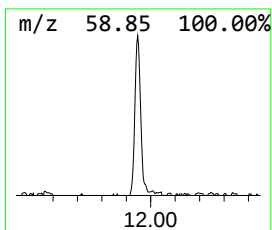
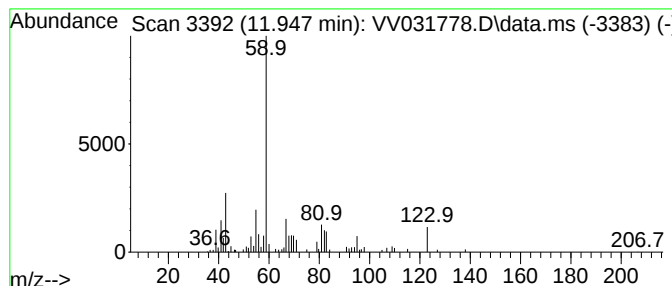
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.947	3.27 ug/L	64104	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	78
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
4			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
5			3-(2-Hydroxy-2-methyl-propyl)-cy...	168	C10H16O2	1000185-60-2	64



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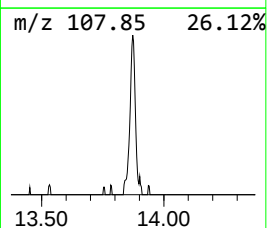
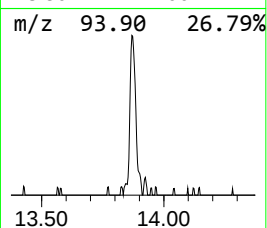
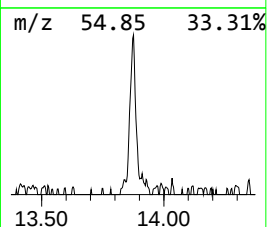
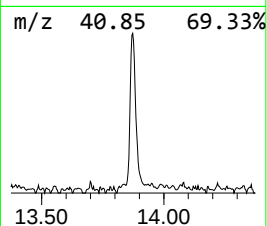
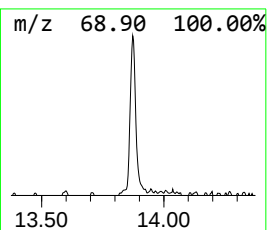
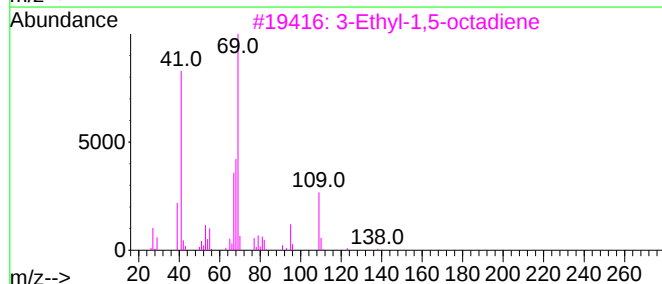
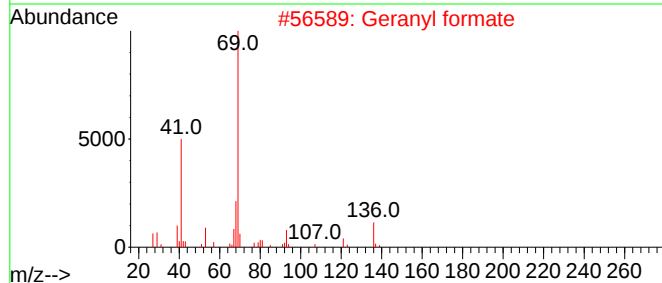
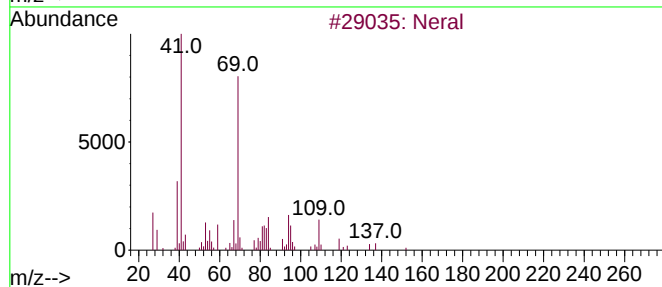
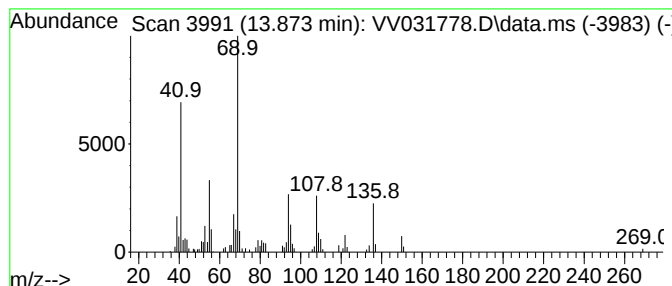
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.873	3.40 ug/L	66686	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Neral	152	C10H16O	000106-26-3	47
2			Geranyl formate	182	C11H18O2	000105-86-2	43
3			3-Ethyl-1,5-octadiene	138	C10H18	1000114-87-7	43
4			2,6-Octadien-1-ol, 3,7-dimethyl-...	196	C12H20O2	000141-12-8	38
5			6-Methyl-1,5-heptadiene	110	C8H14	007270-50-0	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072823\
Data File : VV031778.D
Acq On : 28 Jul 2023 10:53
Operator : SY/MD
Sample : 03754-17
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH2Z3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM072523WMA.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
Propane, 2-meth...	2.574	2.5	ug/L	39949	1	5.539	789207	50.0
7-Octen-2-ol, 2...	11.947	3.3	ug/L	64104	3	11.191	979980	50.0
unknown-01	13.873	3.4	ug/L	66686	3	11.191	979980	50.0