

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040521\
 Data File : VV020912.D
 Acq On : 05 Apr 2021 14:09
 Operator : SY/MD
 Sample : M1859-03
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG3G5

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\SOMVLM032321WMA.M

Title : VOC Analysis

Signal : TIC: VV020912.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	76	83	96	rVB	290276	285328	12.64%	1.632%
2	1.568	157	164	178	rVB	222696	253669	11.23%	1.451%
3	2.108	321	332	349	rBV	525038	760617	33.69%	4.351%
4	2.902	577	579	581	rBV2	546	261	0.01%	0.001%
5	2.941	588	591	592	rBV	703	436	0.02%	0.002%
6	3.043	612	623	637	rVB2	47068	90830	4.02%	0.520%
7	3.243	683	685	686	rBV	516	142	0.01%	0.001%
8	3.307	703	705	706	rBV	340	166	0.01%	0.001%
9	3.317	706	708	709	rBV	453	207	0.01%	0.001%
10	3.368	721	724	726	rBV3	524	334	0.01%	0.002%
11	3.397	729	733	735	rBV3	388	292	0.01%	0.002%
12	3.474	751	757	761	rBV2	847	685	0.03%	0.004%
13	3.494	761	763	765	rVV	718	309	0.01%	0.002%
14	3.510	765	768	771	rVV3	415	285	0.01%	0.002%
15	3.535	774	776	777	rBV3	256	118	0.01%	0.001%
16	3.555	777	782	784	rVV3	850	617	0.03%	0.004%
17	3.580	788	790	791	rBV3	246	127	0.01%	0.001%
18	3.590	791	793	798	rVB	669	426	0.02%	0.002%
19	3.629	803	805	806	rBV	130	56	0.00%	0.000%
20	3.642	806	809	811	rBV	465	289	0.01%	0.002%
21	3.680	815	821	825	rBV5	1093	1460	0.06%	0.008%
22	3.767	836	848	865	rVB3	85448	206917	9.16%	1.184%
23	3.899	874	889	918	rBV	108956	392522	17.38%	2.245%
24	4.352	1014	1030	1052	rBV	392080	955159	42.30%	5.464%
25	4.571	1096	1098	1099	rBV	509	189	0.01%	0.001%
26	4.886	1190	1196	1198	rBV4	505	488	0.02%	0.003%
27	4.899	1198	1200	1202	rVV2	453	231	0.01%	0.001%
28	4.976	1222	1224	1228	rVB2	581	370	0.02%	0.002%
29	5.050	1228	1247	1274	rBV3	887411	2257926	100.00%	12.917%
30	5.268	1313	1315	1317	rBV	727	332	0.01%	0.002%
31	5.362	1342	1344	1346	rBV3	786	370	0.02%	0.002%
32	5.413	1358	1360	1362	rBV3	763	345	0.02%	0.002%
33	5.439	1366	1368	1370	rBV	415	239	0.01%	0.001%
34	5.519	1391	1393	1395	rBV	642	296	0.01%	0.002%
35	5.619	1412	1424	1452	rBV	696638	1396061	61.83%	7.986%
36	5.908	1503	1514	1530	rBV3	50142	106948	4.74%	0.612%

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Integrator: RTE

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
 Title : VOC Analysis

37	6.072	1551	1565	1591	rBV	481085	984663	43.61%	5.633%
38	6.346	1647	1650	1651	rBV2	624	367	0.02%	0.002%
39	6.400	1664	1667	1668	rBV2	672	317	0.01%	0.002%
40	6.474	1686	1690	1693	rVB2	701	630	0.03%	0.004%
41	6.510	1695	1701	1705	rBV6	776	1098	0.05%	0.006%
42	6.625	1734	1737	1739	rBV3	576	341	0.02%	0.002%
43	6.641	1740	1742	1745	rVB2	684	340	0.02%	0.002%
44	6.744	1771	1774	1776	rVB3	998	447	0.02%	0.003%
45	6.773	1779	1783	1786	rBV2	888	687	0.03%	0.004%
46	6.799	1789	1791	1794	rVV3	454	325	0.01%	0.002%
47	6.828	1798	1800	1802	rVV2	1151	610	0.03%	0.003%
48	6.850	1805	1807	1810	rVB	497	199	0.01%	0.001%
49	6.899	1819	1822	1826	rBV	746	535	0.02%	0.003%
50	6.989	1839	1850	1874	rBV	281947	512588	22.70%	2.932%
51	7.217	1919	1921	1925	rVB	614	380	0.02%	0.002%
52	7.320	1941	1953	1971	rBV	1076097	1856665	82.23%	10.621%
53	7.625	2037	2048	2064	rBV	199129	347126	15.37%	1.986%
54	7.870	2122	2124	2125	rBV	536	159	0.01%	0.001%
55	7.899	2131	2133	2135	rBV2	319	150	0.01%	0.001%
56	7.918	2135	2139	2140	rBV4	985	731	0.03%	0.004%
57	8.095	2183	2194	2237	rBV2	452194	931836	41.27%	5.331%
58	8.526	2325	2328	2331	rBV2	414	286	0.01%	0.002%
59	8.661	2367	2370	2372	rBV	623	410	0.02%	0.002%
60	8.699	2379	2382	2386	rBV3	624	582	0.03%	0.003%
61	8.751	2393	2398	2402	rBV3	704	709	0.03%	0.004%
62	8.796	2410	2412	2414	rBV	719	353	0.02%	0.002%
63	8.857	2418	2431	2461	rBV	1050486	1689452	74.82%	9.665%
64	9.246	2549	2552	2555	rBV3	612	485	0.02%	0.003%
65	9.445	2609	2614	2618	rBV3	566	686	0.03%	0.004%
66	9.474	2621	2623	2627	rBV2	554	337	0.01%	0.002%
67	9.509	2632	2634	2636	rVB	524	143	0.01%	0.001%
68	9.529	2636	2640	2643	rBV2	721	503	0.02%	0.003%
69	9.558	2643	2649	2652	rBV3	1340	1450	0.06%	0.008%
70	9.773	2712	2716	2719	rBV2	1194	907	0.04%	0.005%
71	9.985	2779	2782	2785	rVB	473	233	0.01%	0.001%
72	10.005	2786	2788	2790	rBV2	465	220	0.01%	0.001%
73	10.130	2820	2827	2836	rBV6	5068	7350	0.33%	0.042%
74	10.220	2843	2855	2876	rBV	641460	1001444	44.35%	5.729%
75	10.381	2900	2905	2906	rBV3	2948	2387	0.11%	0.014%
76	10.580	2961	2967	2973	rBV5	1466	2115	0.09%	0.012%

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Title : VOC Analysis

77	10.651	2987	2989	2990	rBV2	664	293	0.01%	0.002%
78	10.808	3034	3038	3039	rBV2	412	218	0.01%	0.001%
79	10.853	3049	3052	3054	rBV3	1015	587	0.03%	0.003%
80	10.866	3054	3056	3059	rBV2	551	351	0.02%	0.002%
81	10.940	3065	3079	3091	rBV2	7958	22094	0.98%	0.126%
82	11.034	3104	3108	3109	rBV3	955	704	0.03%	0.004%
83	11.152	3137	3145	3146	rBV6	2419	2800	0.12%	0.016%
84	11.255	3165	3177	3197	rBV	1071089	1640706	72.66%	9.386%
85	11.632	3282	3294	3315	rBV	1113445	1742223	77.16%	9.967%
86	11.921	3382	3384	3386	rBV	661	346	0.02%	0.002%
87	12.037	3418	3420	3422	rBV2	584	341	0.02%	0.002%
88	12.156	3454	3457	3460	rBV2	811	509	0.02%	0.003%
89	12.197	3465	3470	3471	rBV	717	615	0.03%	0.004%
90	12.480	3554	3558	3559	rBV	825	513	0.02%	0.003%
91	12.615	3597	3600	3601	rBV2	870	467	0.02%	0.003%
92	12.857	3673	3675	3676	rBV2	391	131	0.01%	0.001%
93	13.014	3722	3724	3726	rBV2	631	301	0.01%	0.002%
94	13.123	3755	3758	3759	rBV	724	355	0.02%	0.002%
95	13.522	3879	3882	3885	rBV3	1136	717	0.03%	0.004%
96	13.593	3900	3904	3906	rBV2	732	683	0.03%	0.004%
97	13.921	4004	4006	4007	rBV	605	151	0.01%	0.001%

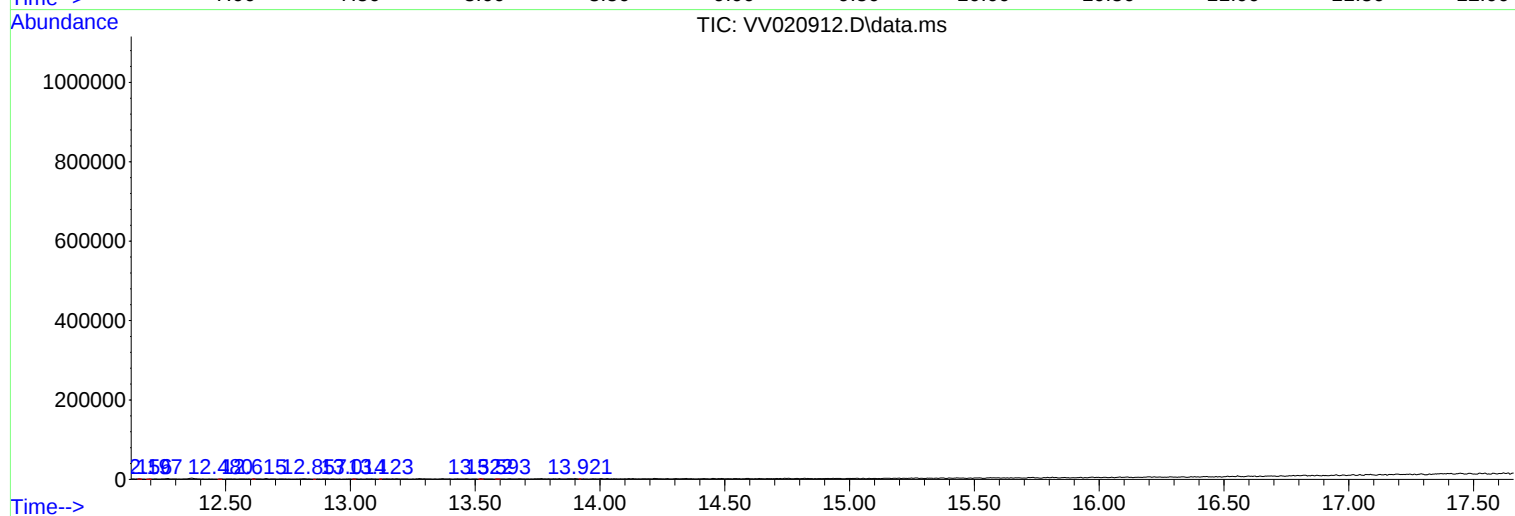
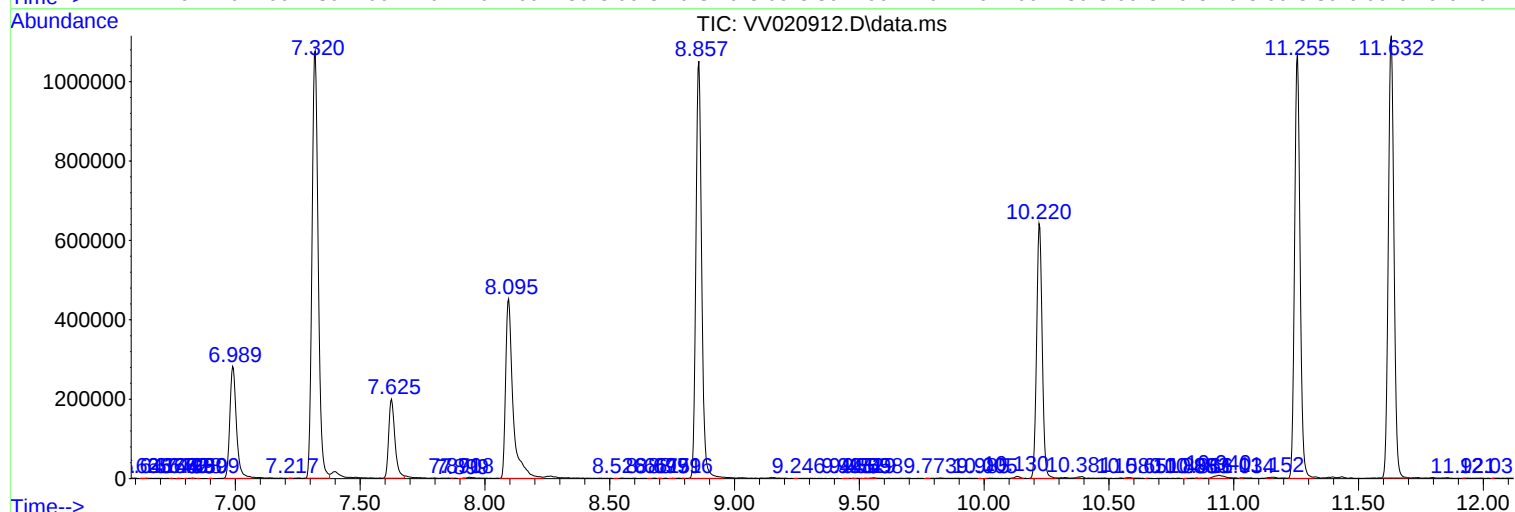
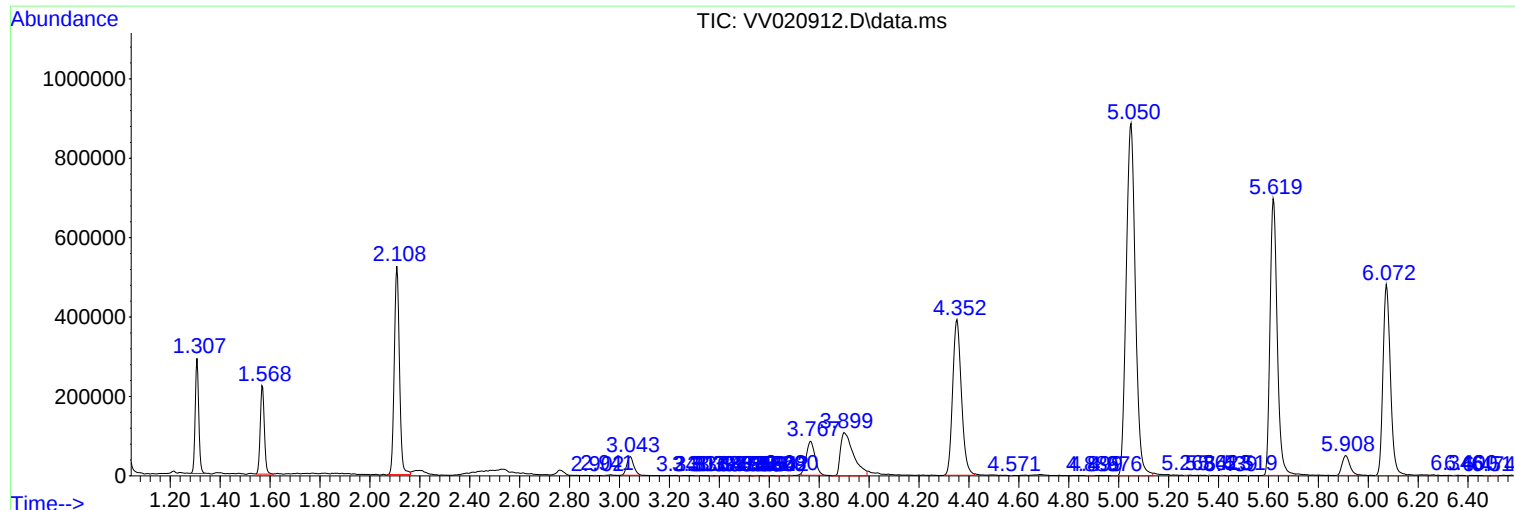
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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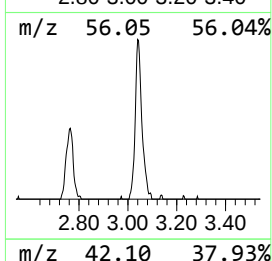
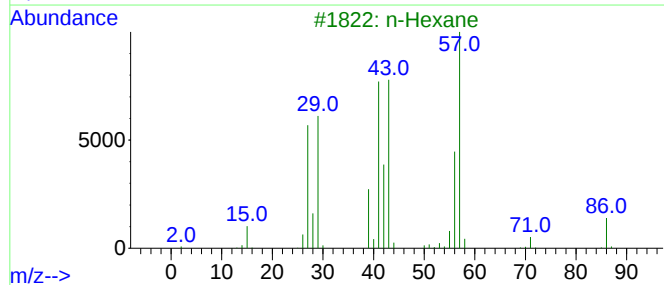
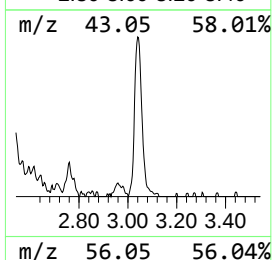
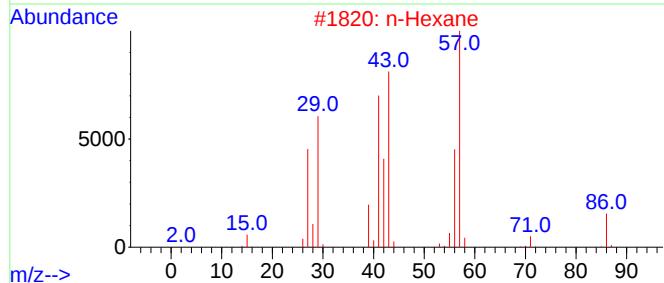
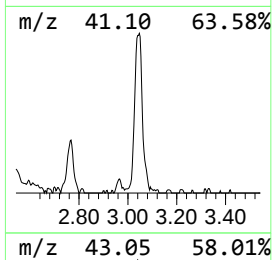
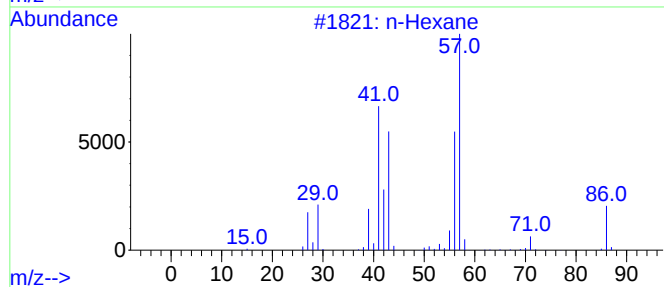
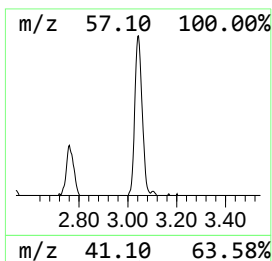
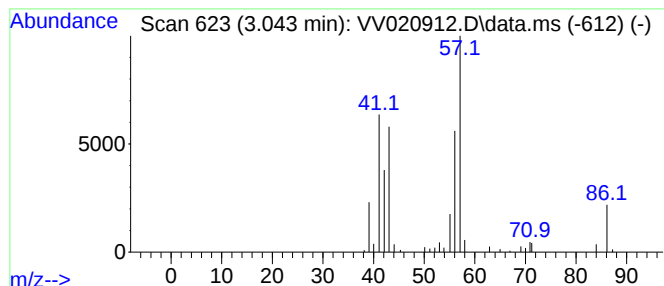
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.043	3.25 ug/L	90830	1,4-Difluorobenzene	5.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane		86	C6H14	000110-54-3	91
2	n-Hexane		86	C6H14	000110-54-3	64
3	n-Hexane		86	C6H14	000110-54-3	50
4	Furan, tetrahydro-3-methyl-		86	C5H10O	013423-15-9	47
5	Azetidine		57	C3H7N	000503-29-7	38



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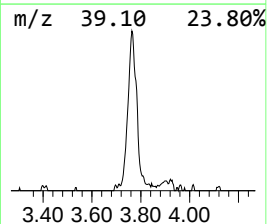
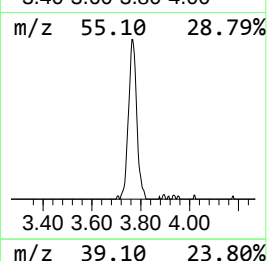
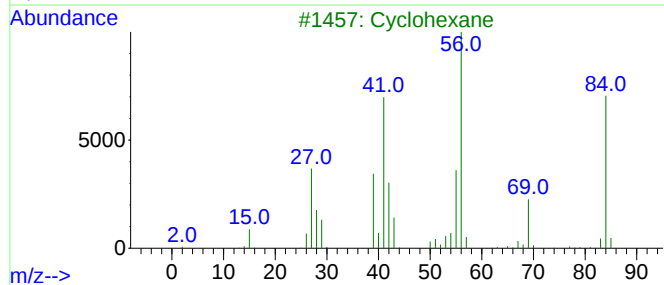
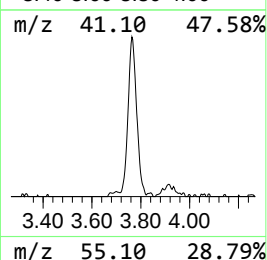
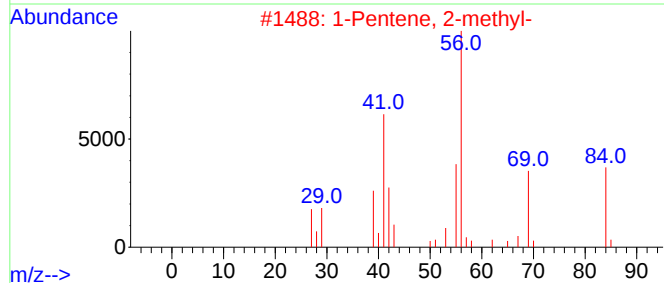
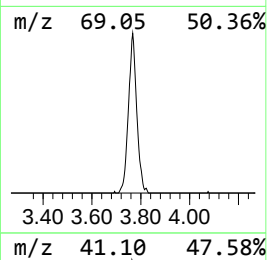
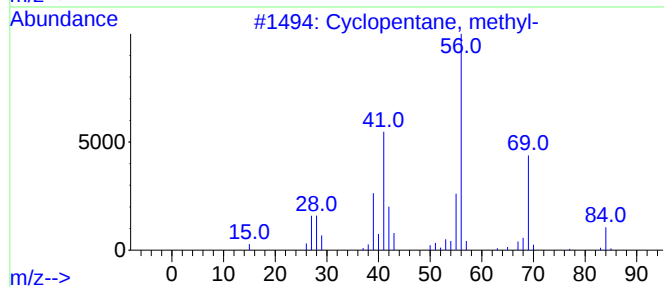
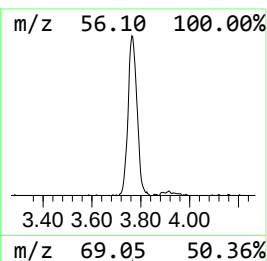
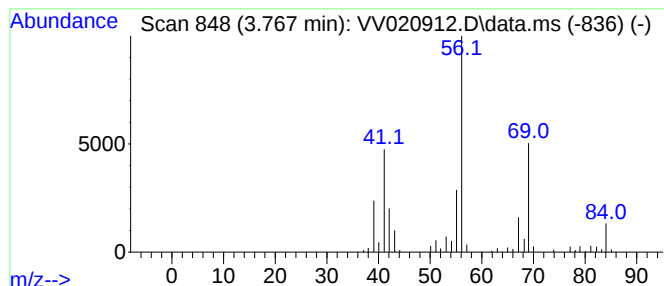
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Cyclic3.767 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.767	7.41 ug/L	206917	1,4-Difluorobenzene	5.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	83
3		Cyclohexane	84	C6H12	000110-82-7	83
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	80
5		Cyclohexane	84	C6H12	000110-82-7	72



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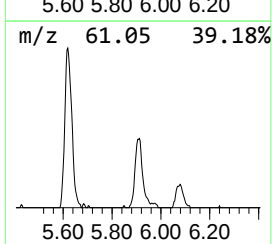
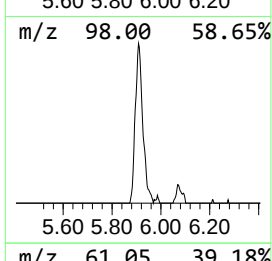
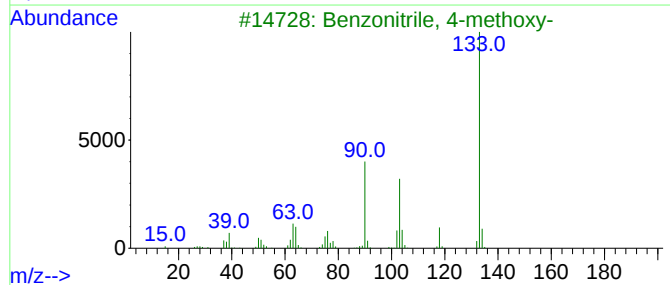
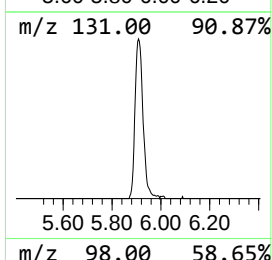
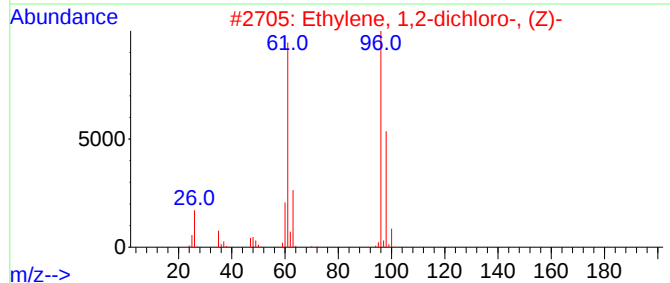
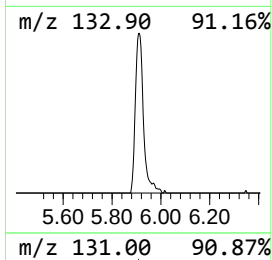
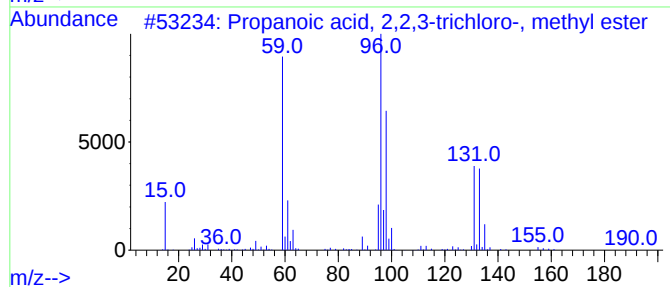
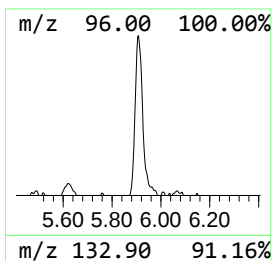
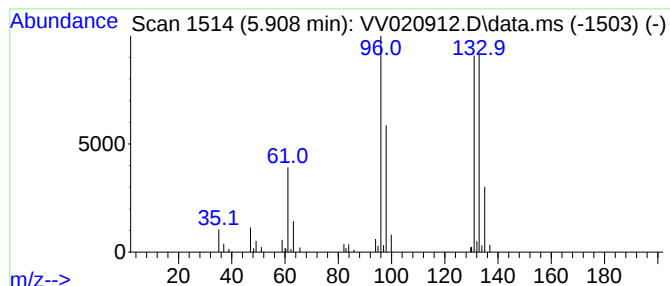
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 2,2,3-trich... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.908	3.83 ug/L	106948	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	50
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3			Benzonitrile, 4-methoxy-	133	C8H7NO	000874-90-8	9
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	9
5			2H-Benzotriazole, 2-methyl-	133	C7H7N3	016584-00-2	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV040521\
Data File : VV020912.D
Acq On : 05 Apr 2021 14:09
Operator : SY/MD
Sample : M1859-03
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BG3G5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SOMVLM032321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	3.043	3.3	ug/L	90830	1	5.619	1396060	50.0
(DEL) Alkane: C...	3.767	7.4	ug/L	206917	1	5.619	1396060	50.0
Propanoic acid,...	5.908	3.8	ug/L	106948	1	5.619	1396060	50.0