

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU030520\
 Data File : VU037097.D
 Acq On : 05 Mar 2020 20:43
 Operator : JC/MD
 Sample : L1784-14
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0B02

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.613	78	85	97	rBV	116238	121039	0.09%	0.081%
2	1.928	175	183	197	rVB	110109	140345	0.10%	0.094%
3	2.597	376	391	406	rBV3	331595	704845	0.50%	0.472%
4	2.787	438	450	468	rBV2	17662	33566	0.02%	0.022%
5	3.076	533	540	552	rVB3	1625	2731	0.00%	0.002%
6	3.221	573	585	601	rVB2	4366	9167	0.01%	0.006%
7	3.353	620	626	630	rBV	295	291	0.00%	0.000%
8	3.375	630	633	635	rBV	498	329	0.00%	0.000%
9	3.446	649	655	658	rBV2	283	278	0.00%	0.000%
10	3.533	679	682	687	rBV	209	199	0.00%	0.000%
11	3.562	687	691	695	rBV2	246	218	0.00%	0.000%
12	3.604	698	704	710	rVB2	199	261	0.00%	0.000%
13	3.661	716	722	724	rBV2	259	213	0.00%	0.000%
14	3.768	750	755	757	rBV	232	232	0.00%	0.000%
15	3.893	787	794	795	rBV	511	439	0.00%	0.000%
16	3.912	795	800	804	rVV3	980	1075	0.00%	0.001%
17	4.253	901	906	908	rBV	222	204	0.00%	0.000%
18	4.581	1005	1008	1011	rBV	220	206	0.00%	0.000%
19	4.668	1020	1035	1071	rBV2	108002	363173	0.26%	0.243%
20	5.031	1144	1148	1152	rBV2	664	589	0.00%	0.000%
21	5.102	1154	1170	1195	rVV	172246	392073	0.28%	0.262%
22	5.192	1195	1198	1203	rVB3	372	330	0.00%	0.000%
23	5.356	1231	1249	1280	rVV	453274	1024392	0.73%	0.686%
24	5.517	1295	1299	1300	rBV3	328	219	0.00%	0.000%
25	5.558	1300	1312	1326	rVV3	11898	25461	0.02%	0.017%
26	5.613	1327	1329	1332	rVB	354	221	0.00%	0.000%
27	5.761	1352	1375	1403	rVV2	368177	998640	0.71%	0.668%
28	6.015	1450	1454	1457	rBV	327	279	0.00%	0.000%
29	6.079	1468	1474	1480	rVB2	280	334	0.00%	0.000%
30	6.134	1487	1491	1493	rBV2	330	287	0.00%	0.000%
31	6.150	1493	1496	1499	rVV2	439	344	0.00%	0.000%
32	6.198	1502	1511	1521	rVB2	1143	1983	0.00%	0.001%
33	6.282	1521	1537	1558	rBV	324636	619176	0.44%	0.414%
34	6.594	1608	1634	1637	rBV6	71469970	140188416	100.00%	93.843%

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 Title : VOC Analysis

35	6.996	1756	1759	1763	rBV4	1146	1106	0.00%	0.001%
36	7.060	1775	1779	1783	rBV4	561	574	0.00%	0.000%
37	7.137	1796	1803	1814	rVB3	1464	2150	0.00%	0.001%
38	7.208	1814	1825	1833	rBV6	4093	7869	0.01%	0.005%
39	7.594	1932	1945	1961	rVV	127309	216905	0.15%	0.145%
40	7.710	1977	1981	1990	rVB5	1480	2051	0.00%	0.001%
41	7.745	1990	1992	1994	rBV2	494	273	0.00%	0.000%
42	7.922	2033	2047	2064	rBV	433492	740102	0.53%	0.495%
43	8.201	2123	2134	2148	rBV	88228	146764	0.10%	0.098%
44	8.423	2191	2203	2214	rBV	42592	71440	0.05%	0.048%
45	8.513	2217	2231	2243	rBV	127126	223923	0.16%	0.150%
46	8.574	2243	2250	2259	rVB2	15649	26056	0.02%	0.017%
47	8.658	2264	2276	2320	rVV	283346	529037	0.38%	0.354%
48	8.848	2327	2335	2349	rVB4	2378	5021	0.00%	0.003%
49	9.308	2475	2478	2483	rVB3	231	243	0.00%	0.000%
50	9.362	2483	2495	2506	rBV2	7241	12046	0.01%	0.008%
51	9.436	2506	2518	2550	rVV	464206	779513	0.56%	0.522%
52	9.549	2550	2553	2558	rVV3	887	858	0.00%	0.001%
53	9.587	2562	2565	2571	rVB4	587	606	0.00%	0.000%
54	9.671	2581	2591	2608	rBV4	9044	16648	0.01%	0.011%
55	9.793	2612	2629	2653	rVB	110256	259050	0.18%	0.173%
56	9.896	2659	2661	2665	rBV3	337	253	0.00%	0.000%
57	10.002	2685	2694	2703	rVB3	1330	1917	0.00%	0.001%
58	10.073	2709	2716	2720	rBV2	360	448	0.00%	0.000%
59	10.099	2720	2724	2728	rBV2	556	544	0.00%	0.000%
60	10.121	2728	2731	2737	rVB3	755	544	0.00%	0.000%
61	10.304	2779	2788	2799	rVB3	1788	3179	0.00%	0.002%
62	10.352	2799	2803	2805	rBV2	301	300	0.00%	0.000%
63	10.500	2836	2849	2861	rVB6	4866	9156	0.01%	0.006%
64	10.568	2867	2870	2876	rVB3	1001	884	0.00%	0.001%
65	10.619	2881	2886	2888	rBV	244	235	0.00%	0.000%
66	10.680	2902	2905	2907	rBV	466	319	0.00%	0.000%
67	10.774	2920	2934	2951	rVB	302660	491154	0.35%	0.329%
68	10.877	2960	2966	2969	rBV2	461	389	0.00%	0.000%
69	11.005	3003	3006	3010	rVV4	253	225	0.00%	0.000%
70	11.057	3016	3022	3027	rBV3	366	517	0.00%	0.000%
71	11.082	3027	3030	3034	rBV2	284	272	0.00%	0.000%

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72	11.217	3069	3072	3074	rVV2	298	203	0.00%	0.000%
73	11.488	3154	3156	3166	rVB3	545	645	0.00%	0.000%
74	11.542	3170	3173	3176	rBV2	284	215	0.00%	0.000%
75	11.693	3214	3220	3223	rBV3	288	368	0.00%	0.000%
76	11.761	3238	3241	3244	rBV3	405	280	0.00%	0.000%
77	11.828	3248	3262	3282	rBV	363605	609704	0.43%	0.408%
78	12.082	3339	3341	3344	rVB3	527	276	0.00%	0.000%
79	12.140	3356	3359	3364	rBV3	269	240	0.00%	0.000%
80	12.208	3365	3380	3396	rBV	349721	584322	0.42%	0.391%
81	12.510	3471	3474	3477	rBV2	260	221	0.00%	0.000%
82	12.616	3503	3507	3516	rVB3	329	447	0.00%	0.000%
83	12.655	3516	3519	3524	rVB2	346	299	0.00%	0.000%
84	12.703	3531	3534	3536	rBV2	277	203	0.00%	0.000%
85	12.828	3572	3573	3577	rVB2	393	226	0.00%	0.000%
86	12.857	3577	3582	3584	rBV2	345	257	0.00%	0.000%
87	13.050	3638	3642	3644	rVV	227	211	0.00%	0.000%
88	13.140	3667	3670	3674	rVB2	443	404	0.00%	0.000%
89	13.163	3674	3677	3682	rBV3	293	310	0.00%	0.000%
90	13.204	3683	3690	3691	rBV2	283	306	0.00%	0.000%
91	13.243	3698	3702	3703	rBV	378	253	0.00%	0.000%
92	13.362	3736	3739	3742	rBV2	349	254	0.00%	0.000%
93	13.385	3742	3746	3749	rBV2	293	330	0.00%	0.000%
94	13.523	3786	3789	3793	rBV3	250	229	0.00%	0.000%
95	13.973	3926	3929	3931	rBV2	361	241	0.00%	0.000%
96	14.307	4029	4033	4035	rBV3	306	220	0.00%	0.000%
97	14.378	4052	4055	4056	rBV	372	259	0.00%	0.000%
98	14.664	4142	4144	4148	rBV3	345	323	0.00%	0.000%
99	14.764	4171	4175	4180	rVB4	349	431	0.00%	0.000%
100	15.265	4324	4331	4334	rBV2	495	699	0.00%	0.000%

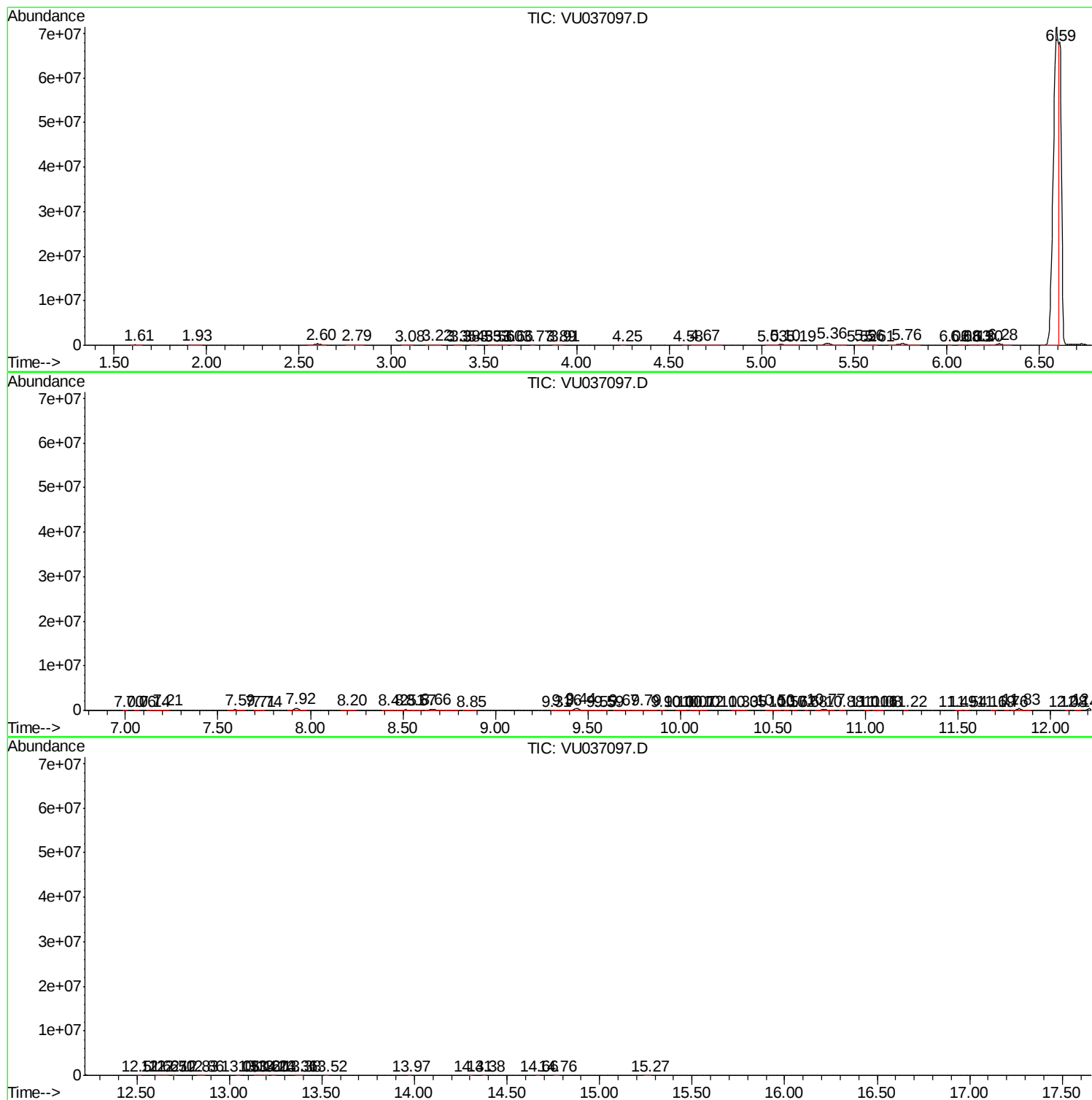
Sum of corrected areas: 149386502

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
Quant Title : VOC Analysis

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



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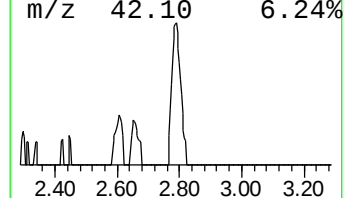
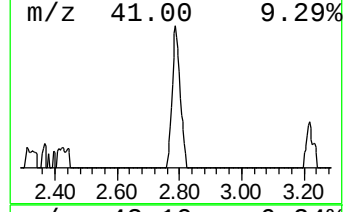
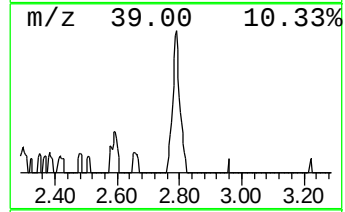
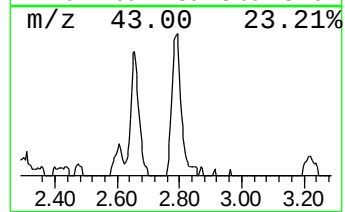
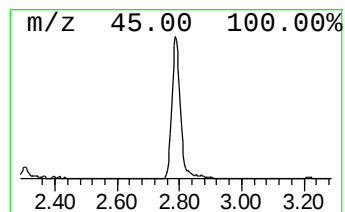
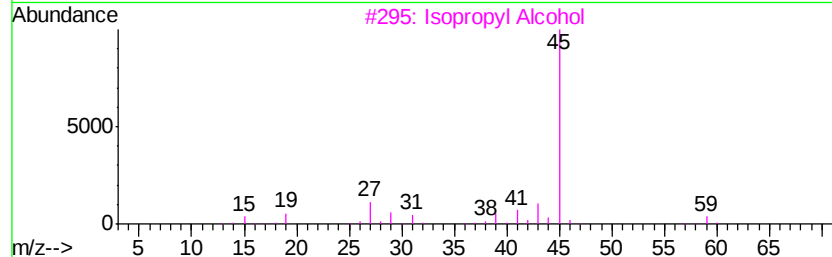
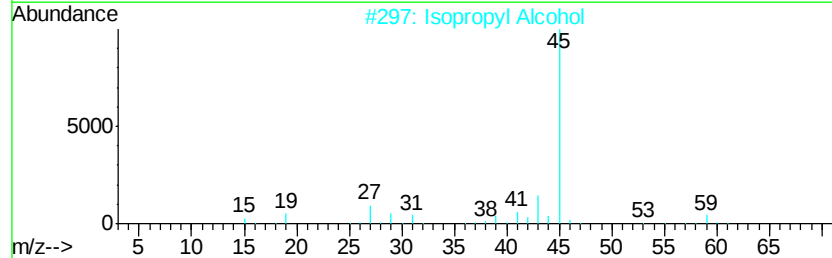
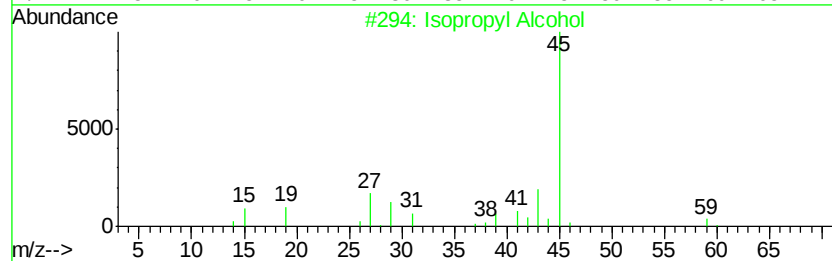
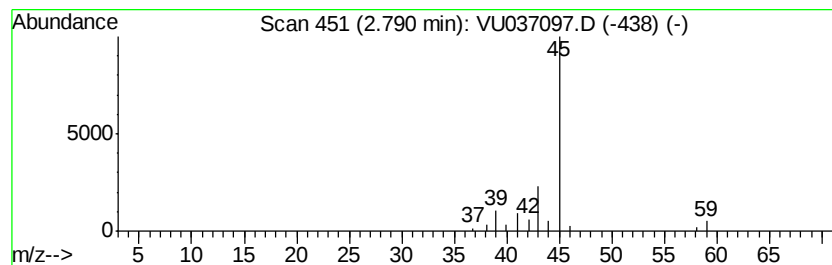
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	2.71 ug/L	33566	1,4-Difluorobenzene	6.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			4-Penten-2-ol	86	C5H10O	000625-31-0	9
5			Ethylamine	45	C2H7N	000075-04-7	5



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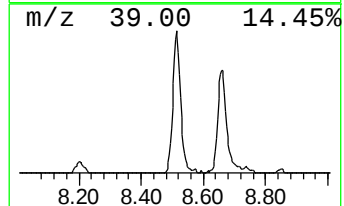
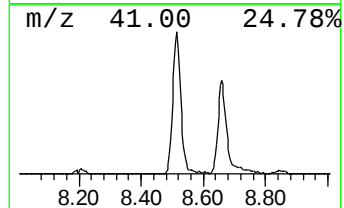
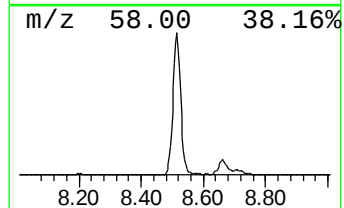
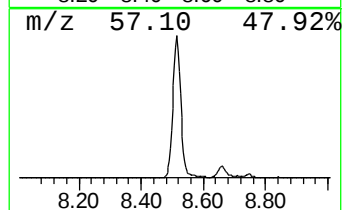
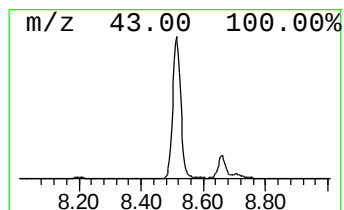
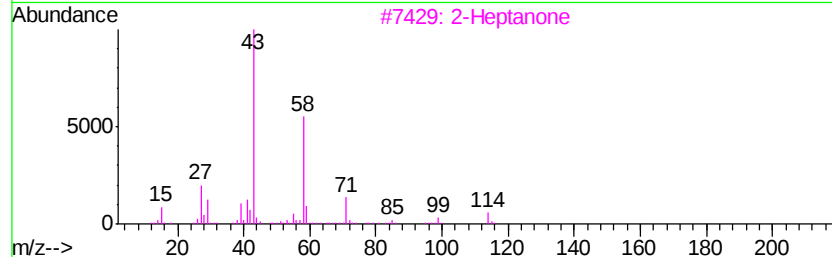
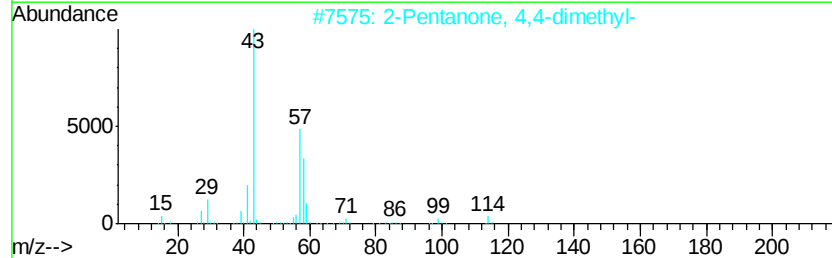
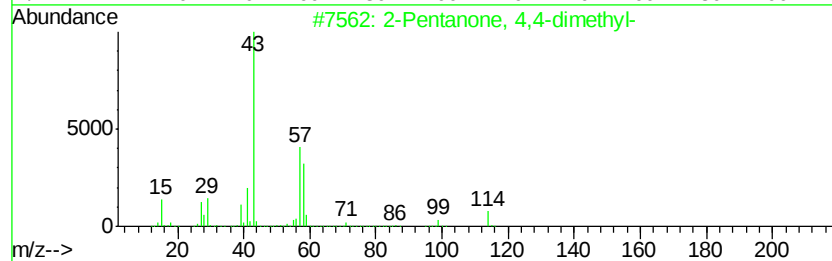
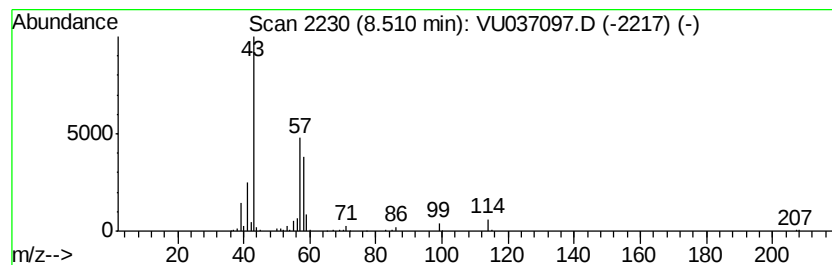
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 2-Pentanone, 4,4-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.51	14.36 ug/L	223923	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	91
2		2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	86
3		2-Heptanone	114	C7H14O	000110-43-0	64
4		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	56
5		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	56



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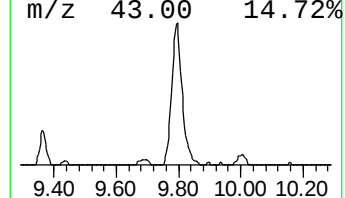
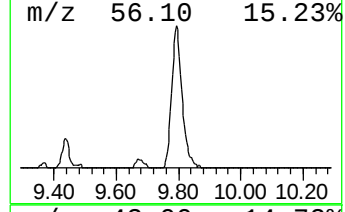
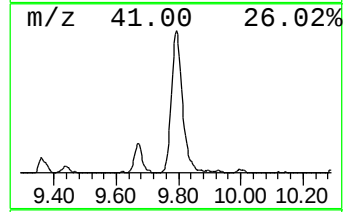
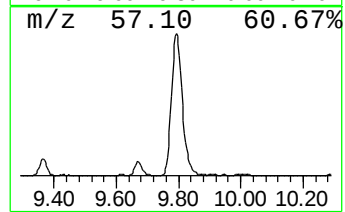
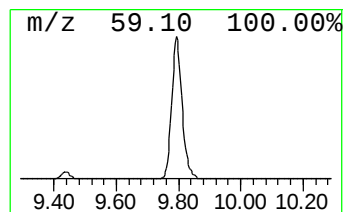
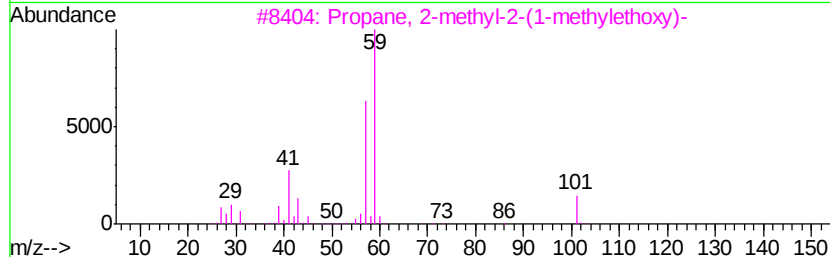
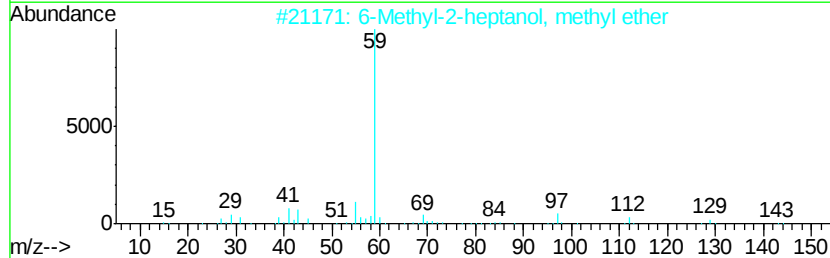
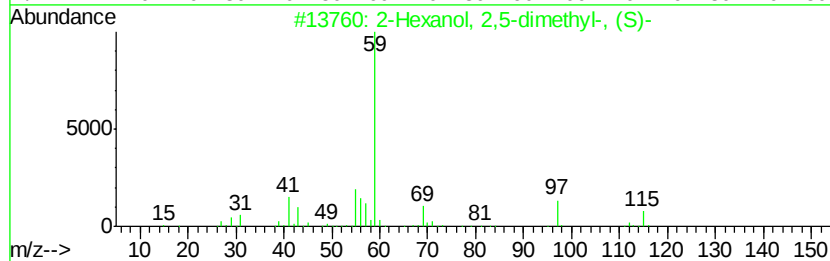
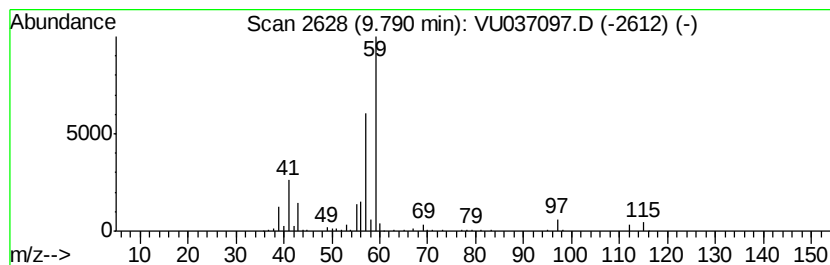
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Quant Title : VOC Analysis

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

Peak Number 4 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.79	16.62 ug/L	259050	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	64
2		6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	59
3		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	50
4		3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	50
5		Acetic acid, cyano-, 1,1-dimethyl-	141	C7H11NO2	001116-98-9	45



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU030520\
Data File : VU037097.D
Acq On : 05 Mar 2020 20:43
Operator : JC/MD
Sample : L1784-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0B02

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM022420WMA.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
Isopropyl Alcohol	2.79	2.7	ug/L	33566	1	6.29	619176	50.0
2-Pentanone, 4,4-...	8.51	14.4	ug/L	223923	2	9.44	779513	50.0
2-Hexanol, 2,5-di...	9.79	16.6	ug/L	259050	2	9.44	779513	50.0