

Data Path : W:\HPCHEM1\MSVOA U\Data\VU121616\
 Data File : VU013915.D
 Acq On : 16 Dec 2016 16:45
 Operator : MD/SY
 Sample : H6036-18
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :

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 : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM121516WMA.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	0.645	10	17	19	rBV	465	469	0.002%	0.0002%
2	0.818	69	71	75	rBV2	400	311	0.001%	0.0001%
3	0.953	108	113	119	rBV2	337	401	0.001%	0.0002%
4	0.986	119	123	128	rBV2	451	396	0.001%	0.0002%
5	1.088	137	155	181	rBV	1940521	2644919	91.43%	10.185%
6	1.400	245	252	269	rVB	350307	376535	13.02%	1.450%
7	1.680	332	339	352	rVB	270435	339720	11.74%	1.308%
8	2.275	513	524	535	rBV	544775	824908	28.52%	3.177%
9	2.330	537	541	553	rVB	40849	59689	2.06%	0.230%
10	3.455	889	891	894	rBV3	1273	731	0.003%	0.0003%
11	3.619	940	942	945	rBV2	724	439	0.002%	0.0002%
12	4.024	1065	1068	1072	rBV3	490	359	0.001%	0.0001%
13	4.098	1087	1091	1094	rBV3	731	546	0.002%	0.0002%
14	4.114	1094	1096	1099	rVV	647	308	0.001%	0.0001%
15	4.217	1107	1128	1160	rBV3	250017	827363	28.60%	3.186%
16	4.661	1247	1266	1291	rBV	487324	1190438	41.15%	4.584%
17	4.844	1319	1323	1328	rVB3	869	888	0.003%	0.0003%
18	4.870	1328	1331	1332	rBV2	750	358	0.001%	0.0001%
19	4.892	1335	1338	1339	rBV2	661	431	0.001%	0.0002%
20	4.969	1359	1362	1364	rBV	636	406	0.001%	0.0002%
21	5.088	1396	1399	1404	rBV3	479	354	0.001%	0.0001%
22	5.169	1421	1424	1429	rVB3	693	465	0.002%	0.0002%
23	5.262	1451	1453	1455	rVB2	559	259	0.001%	0.0001%
24	5.345	1455	1479	1499	rBV2	1025843	2892819	100.00%	11.140%
25	5.509	1527	1530	1531	rBV2	521	272	0.001%	0.0001%
26	5.519	1531	1533	1541	rVB5	1600	1535	0.005%	0.0006%
27	5.554	1541	1544	1545	rBV	679	378	0.001%	0.0001%
28	5.628	1563	1567	1571	rBV6	659	693	0.002%	0.0003%
29	5.673	1575	1581	1583	rBV4	1371	1341	0.005%	0.0005%
30	5.741	1599	1602	1603	rBV	678	411	0.001%	0.0002%
31	5.754	1604	1606	1608	rVV	888	506	0.002%	0.0002%
32	5.767	1608	1610	1615	rVB2	807	487	0.002%	0.0002%
33	5.789	1615	1617	1619	rBV3	590	312	0.001%	0.0001%
34	5.895	1633	1650	1671	rBV	1034721	1999330	69.11%	7.699%

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 Title : VOC Analysis

35	6.181	1726	1739	1760	rBV4	49388	100814	3.48%	0.388%
36	6.259	1760	1763	1764	rBV3	480	266	0.01%	0.001%
37	6.342	1773	1789	1809	rBV	686762	1365172	47.19%	5.257%
38	6.509	1839	1841	1842	rBV2	645	352	0.01%	0.001%
39	6.545	1848	1852	1855	rBV4	506	430	0.01%	0.002%
40	6.677	1890	1893	1896	rBV2	384	262	0.01%	0.001%
41	6.731	1905	1910	1911	rBV3	582	458	0.02%	0.002%
42	6.770	1917	1922	1925	rBV4	800	748	0.03%	0.003%
43	6.786	1925	1927	1931	rBV2	473	310	0.01%	0.001%
44	6.821	1936	1938	1943	rBV2	401	267	0.01%	0.001%
45	6.860	1945	1950	1953	rBV4	1659	1781	0.06%	0.007%
46	7.017	1996	1999	2000	rBV2	805	408	0.01%	0.002%
47	7.088	2016	2021	2024	rBV2	409	412	0.01%	0.002%
48	7.236	2054	2067	2096	rBV	344253	608577	21.04%	2.344%
49	7.371	2106	2109	2112	rBV3	1332	1125	0.04%	0.004%
50	7.484	2142	2144	2148	rBV3	689	448	0.02%	0.002%
51	7.574	2156	2172	2191	rBV	1190813	2064958	71.38%	7.952%
52	7.808	2242	2245	2248	rVB4	784	634	0.02%	0.002%
53	7.857	2248	2260	2283	rBV	239801	412887	14.27%	1.590%
54	8.021	2306	2311	2314	rBV5	770	698	0.02%	0.003%
55	8.075	2323	2328	2329	rBV2	781	616	0.02%	0.002%
56	8.162	2352	2355	2359	rVB3	717	457	0.02%	0.002%
57	8.185	2359	2362	2365	rBV3	405	311	0.01%	0.001%
58	8.233	2369	2377	2391	rBV4	12507	19426	0.67%	0.075%
59	8.323	2392	2405	2443	rBV2	925940	1829046	63.23%	7.043%
60	8.705	2517	2524	2526	rBV5	1399	1602	0.06%	0.006%
61	8.767	2540	2543	2548	rVB3	892	739	0.03%	0.003%
62	8.805	2551	2555	2560	rBV4	984	676	0.02%	0.003%
63	8.831	2560	2563	2565	rBV2	879	582	0.02%	0.002%
64	8.902	2582	2585	2590	rBV3	755	507	0.02%	0.002%
65	8.985	2606	2611	2620	rBV4	1253	1787	0.06%	0.007%
66	9.033	2622	2626	2632	rBV3	800	767	0.03%	0.003%
67	9.095	2632	2645	2666	rBV	1515912	2494773	86.24%	9.607%
68	9.381	2728	2734	2737	rBV7	1701	1595	0.06%	0.006%
69	9.429	2747	2749	2751	rBV	908	480	0.02%	0.002%
70	9.442	2751	2753	2758	rVB2	1100	740	0.03%	0.003%
71	9.471	2759	2762	2763	rBV2	509	264	0.01%	0.001%

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Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM121516WMA.M
 Title : VOC Analysis

72	9.548	2783	2786	2789	rBV	651	430	0.01%	0.002%
73	9.651	2815	2818	2821	rVB	520	267	0.01%	0.001%
74	9.847	2878	2879	2883	rBV2	511	272	0.01%	0.001%
75	9.895	2892	2894	2897	rVB2	940	428	0.01%	0.002%
76	9.934	2901	2906	2910	rBV3	701	670	0.02%	0.003%
77	10.111	2958	2961	2964	rBV2	625	373	0.01%	0.001%
78	10.168	2974	2979	2981	rBV3	686	653	0.02%	0.003%
79	10.284	3012	3015	3019	rBV2	580	398	0.01%	0.002%
80	10.439	3049	3063	3081	rBV	930885	1483324	51.28%	5.712%
81	10.802	3171	3176	3181	rVB4	679	811	0.03%	0.003%
82	10.831	3181	3185	3187	rVB	588	388	0.01%	0.001%
83	10.844	3187	3189	3190	rBV2	571	276	0.01%	0.001%
84	10.979	3227	3231	3235	rBV3	840	753	0.03%	0.003%
85	11.091	3263	3266	3269	rBV3	893	647	0.02%	0.002%
86	11.120	3272	3275	3277	rBV2	438	274	0.01%	0.001%
87	11.490	3377	3390	3413	rBV	1399737	2257012	78.02%	8.691%
88	11.593	3420	3422	3423	rVB	1241	358	0.01%	0.001%
89	11.699	3453	3455	3458	rVB2	914	515	0.02%	0.002%
90	11.763	3464	3475	3492	rBV4	13312	29476	1.02%	0.114%
91	11.866	3493	3507	3529	rVV	1280304	2099357	72.57%	8.084%
92	12.030	3556	3558	3560	rBV	773	393	0.01%	0.002%
93	12.075	3570	3572	3575	rVB	1216	552	0.02%	0.002%
94	12.094	3575	3578	3582	rBV	1116	1112	0.04%	0.004%
95	12.139	3590	3592	3595	rVB2	1151	499	0.02%	0.002%
96	12.313	3643	3646	3650	rBV2	880	792	0.03%	0.003%
97	12.336	3650	3653	3656	rVV3	907	645	0.02%	0.002%
98	13.036	3868	3871	3872	rBV	837	437	0.02%	0.002%
99	14.001	4166	4171	4176	rBV3	2162	2457	0.08%	0.009%
100	14.326	4269	4272	4275	rBV2	1183	998	0.03%	0.004%

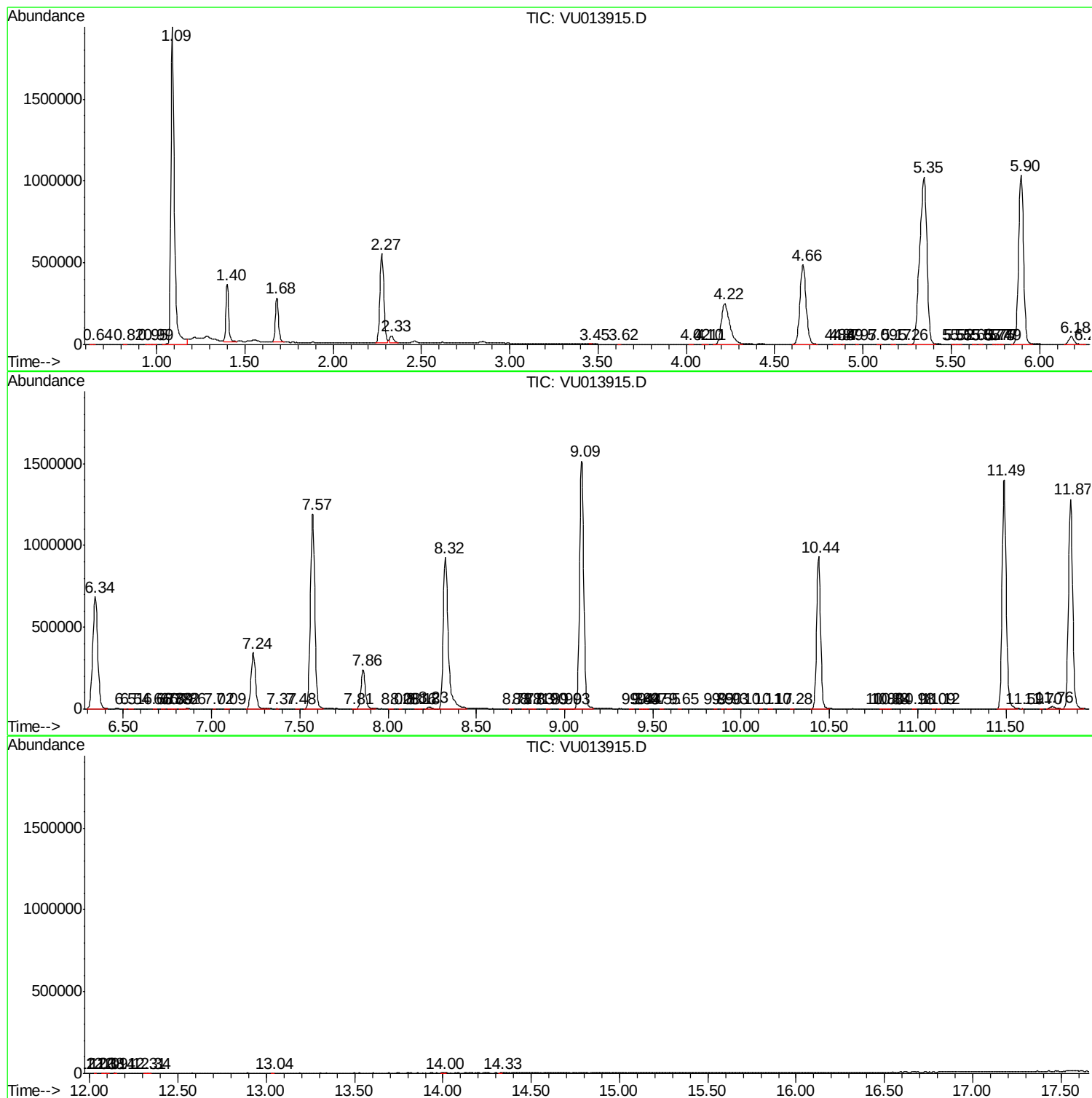
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Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM121516WMA.M
Quant Title : VOC Analysis

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



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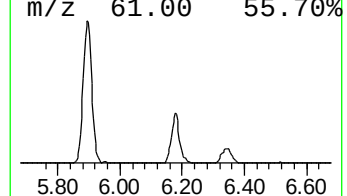
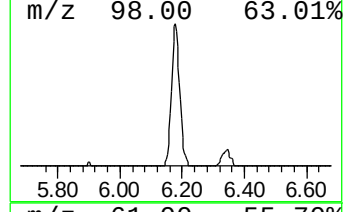
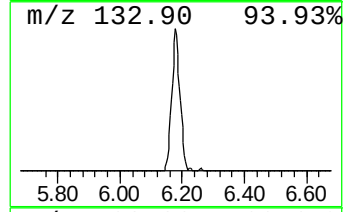
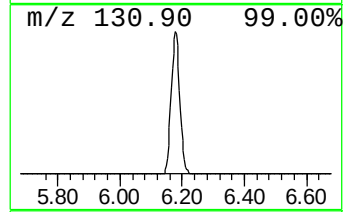
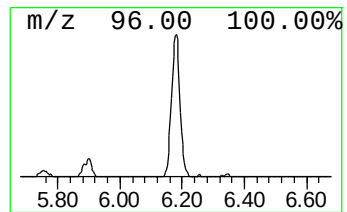
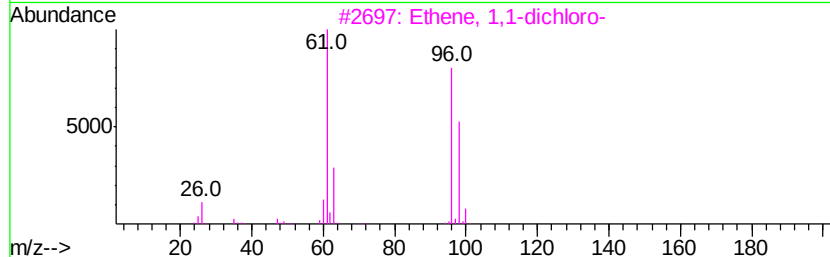
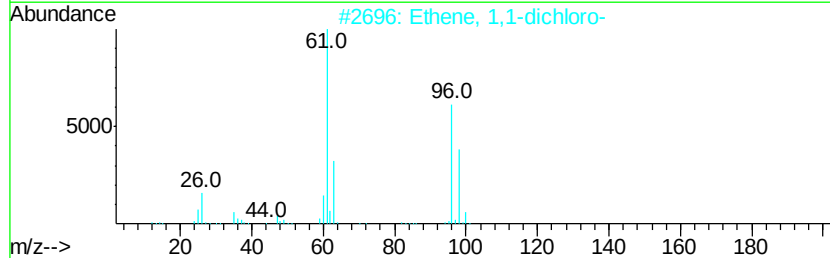
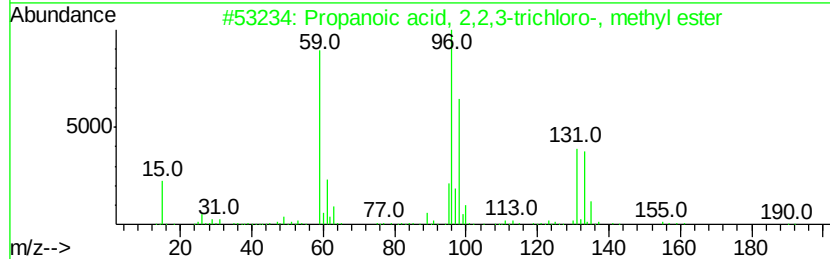
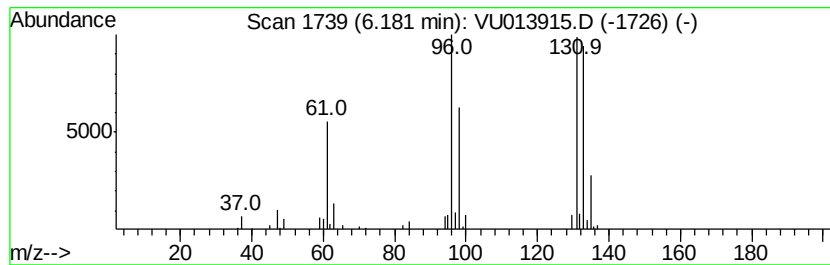
Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM121516WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	2.52 ug/L	100814	1,4-Difluorobenzene	5.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2		Ethene, 1,1-dichloro-	96	C2H2Cl2	000075-35-4	38
3		Ethene, 1,1-dichloro-	96	C2H2Cl2	000075-35-4	38
4		Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25
5		Ethene, 1,1-dichloro-	96	C2H2Cl2	000075-35-4	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid, 2...	6.18	2.5	ug/L	100814	1	5.90	1999330	50.0