

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU092319\
 Data File : VU034734.D
 Acq On : 23 Sep 2019 15:30
 Operator : JC/SP
 Sample : K4982-05 10X
 Misc : 5.58g/5.0mL/100uL/10mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AW2

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\SOMULM091919WMA.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	1.392	87	94	108	rBV	360410	365794	2.43%	0.755%
2	1.579	133	152	161	rBV4	92548	247702	1.65%	0.511%
3	1.656	169	176	193	rVB	255503	338506	2.25%	0.699%
4	2.254	351	362	384	rVB	530161	842134	5.60%	1.739%
5	2.682	482	495	505	rBV4	9776	19460	0.13%	0.040%
6	2.768	519	522	524	rVV3	1285	825	0.01%	0.002%
7	2.784	524	527	530	rVB4	2416	1332	0.01%	0.003%
8	2.810	532	535	541	rBV7	2771	2550	0.02%	0.005%
9	2.862	549	551	555	rVB3	857	640	0.00%	0.001%
10	3.103	624	626	629	rVB3	1640	950	0.01%	0.002%
11	3.122	629	632	633	rBV2	1554	902	0.01%	0.002%
12	3.154	640	642	645	rBV3	1164	924	0.01%	0.002%
13	3.202	654	657	660	rVV4	1509	995	0.01%	0.002%
14	3.267	674	677	681	rBV4	1439	1126	0.01%	0.002%
15	3.334	696	698	704	rVB5	1502	1259	0.01%	0.003%
16	3.415	718	723	725	rBV4	2010	1617	0.01%	0.003%
17	3.547	761	764	767	rVB4	2225	1308	0.01%	0.003%
18	3.569	767	771	775	rBV5	2796	2409	0.02%	0.005%
19	3.711	811	815	818	rBV3	2068	1702	0.01%	0.004%
20	3.733	818	822	823	rVV3	1082	681	0.00%	0.001%
21	3.752	826	828	830	rBV2	1071	662	0.00%	0.001%
22	4.035	914	916	922	rVB6	1363	1146	0.01%	0.002%
23	4.064	922	925	927	rBV3	1340	895	0.01%	0.002%
24	4.106	935	938	939	rBV3	1079	758	0.01%	0.002%
25	4.148	939	951	979	rBV	232259	619285	4.12%	1.279%
26	4.337	1008	1010	1014	rBV4	1698	1269	0.01%	0.003%
27	4.495	1057	1059	1062	rVV3	1090	652	0.00%	0.001%
28	4.530	1068	1070	1074	rVB4	1117	671	0.00%	0.001%
29	4.556	1074	1078	1082	rBV8	1590	1546	0.01%	0.003%
30	4.620	1082	1098	1122	rBV	374252	914777	6.08%	1.889%
31	4.826	1159	1162	1166	rBV5	1971	1561	0.01%	0.003%
32	4.958	1199	1203	1206	rBV4	2326	2167	0.01%	0.004%
33	5.116	1248	1252	1255	rVB5	1075	827	0.01%	0.002%
34	5.145	1258	1261	1264	rBV3	1116	726	0.00%	0.001%

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Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
 Title : VOC Analysis

35	5.196	1264	1277	1282	rBV3	3900	6722	0.04%	0.014%
36	5.315	1290	1314	1345	rBV2	806878	2427150	16.13%	5.011%
37	5.649	1415	1418	1422	rBV5	1638	1156	0.01%	0.002%
38	5.723	1437	1441	1443	rBV5	1196	914	0.01%	0.002%
39	5.765	1443	1454	1467	rVB9	8044	16327	0.11%	0.034%
40	5.862	1470	1484	1509	rBV	660136	1301953	8.65%	2.688%
41	6.119	1562	1564	1568	rVB5	1682	831	0.01%	0.002%
42	6.154	1572	1575	1576	rBV3	2292	1261	0.01%	0.003%
43	6.225	1595	1597	1599	rBV4	1322	740	0.00%	0.002%
44	6.305	1606	1622	1644	rVV	552193	1123473	7.47%	2.319%
45	6.559	1696	1701	1703	rBV4	1643	1163	0.01%	0.002%
46	6.688	1739	1741	1744	rBV3	1382	923	0.01%	0.002%
47	6.739	1756	1757	1763	rVB5	1167	792	0.01%	0.002%
48	6.778	1765	1769	1771	rBV4	1023	733	0.00%	0.002%
49	6.845	1786	1790	1794	rBV6	1747	1757	0.01%	0.004%
50	6.874	1794	1799	1801	rVV6	1282	1238	0.01%	0.003%
51	6.977	1828	1831	1837	rVB6	1452	1322	0.01%	0.003%
52	7.006	1837	1840	1843	rBV3	1701	1195	0.01%	0.002%
53	7.064	1853	1858	1860	rBV5	1814	1552	0.01%	0.003%
54	7.083	1862	1864	1868	rVB3	1193	687	0.00%	0.001%
55	7.125	1874	1877	1879	rBV3	1321	887	0.01%	0.002%
56	7.167	1886	1890	1891	rBV3	1050	875	0.01%	0.002%
57	7.206	1891	1902	1921	rBV2	333589	610077	4.05%	1.260%
58	7.402	1959	1963	1966	rBV4	1628	1025	0.01%	0.002%
59	7.488	1987	1990	1993	rBV5	1291	982	0.01%	0.002%
60	7.543	1993	2007	2023	rBV	1124588	1955765	13.00%	4.038%
61	7.829	2082	2096	2118	rBV	235226	422149	2.81%	0.872%
62	8.000	2146	2149	2156	rVB8	1395	1287	0.01%	0.003%
63	8.125	2182	2188	2192	rBV8	1530	1795	0.01%	0.004%
64	8.151	2194	2196	2200	rBV4	1485	1282	0.01%	0.003%
65	8.215	2207	2216	2223	rVB4	6385	11328	0.08%	0.023%
66	8.244	2223	2225	2228	rVB2	1426	710	0.00%	0.001%
67	8.289	2228	2239	2271	rBV	800532	1465995	9.74%	3.027%
68	8.492	2300	2302	2307	rVB3	1683	840	0.01%	0.002%
69	8.643	2345	2349	2352	rBV5	1736	1407	0.01%	0.003%
70	8.701	2363	2367	2371	rVB5	1398	1215	0.01%	0.003%
71	8.784	2390	2393	2394	rBV3	1180	626	0.00%	0.001%

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Integration Parameters: LSCINT.P

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
 Title : VOC Analysis

72	8.816	2401	2403	2408	rBV5	1088	767	0.01%	0.002%
73	8.890	2421	2426	2432	rVV7	3765	4926	0.03%	0.010%
74	9.016	2460	2465	2468	rVV5	2538	2225	0.01%	0.005%
75	9.067	2468	2481	2508	rBV2	1044438	2168735	14.41%	4.477%
76	9.228	2520	2531	2547	rBV	395404	635745	4.23%	1.313%
77	9.350	2556	2569	2585	rBV	1339641	2186171	14.53%	4.513%
78	9.633	2652	2657	2661	rBV6	1901	1671	0.01%	0.003%
79	9.668	2664	2668	2670	rBV3	2415	1872	0.01%	0.004%
80	9.755	2684	2695	2714	rBV2	377755	628524	4.18%	1.298%
81	9.900	2736	2740	2742	rBV4	2855	2383	0.02%	0.005%
82	9.932	2742	2750	2759	rVB6	13291	22252	0.15%	0.046%
83	9.980	2759	2765	2768	rBV7	2517	3280	0.02%	0.007%
84	10.016	2771	2776	2778	rBV4	9137	8645	0.06%	0.018%
85	10.138	2806	2814	2826	rVB4	13525	27639	0.18%	0.057%
86	10.186	2826	2829	2830	rBV2	1914	931	0.01%	0.002%
87	10.196	2830	2832	2836	rVV5	1566	1161	0.01%	0.002%
88	10.408	2886	2898	2927	rVB	748760	1234508	8.21%	2.549%
89	10.569	2941	2948	2951	rBV6	5924	7365	0.05%	0.015%
90	10.652	2964	2974	2975	rBV6	15658	22540	0.15%	0.047%
91	10.794	3011	3018	3030	rVB2	76742	116399	0.77%	0.240%
92	11.022	3087	3089	3091	rBV3	2033	1216	0.01%	0.003%
93	11.093	3105	3111	3115	rBV5	11935	16542	0.11%	0.034%
94	11.125	3115	3121	3134	rVB2	37843	59932	0.40%	0.124%
95	11.247	3155	3159	3160	rBV3	3588	2927	0.02%	0.006%
96	11.392	3191	3204	3216	rBV	2893481	4620934	30.71%	9.540%
97	11.482	3216	3232	3248	rVB2	4356423	8269650	54.97%	17.073%
98	11.855	3332	3348	3375	rVB2	8755950	15045062	100.00%	31.061%
99	13.106	3730	3737	3750	rBV6	44120	80820	0.54%	0.167%
100	13.482	3845	3854	3871	rBV	295176	512290	3.41%	1.058%

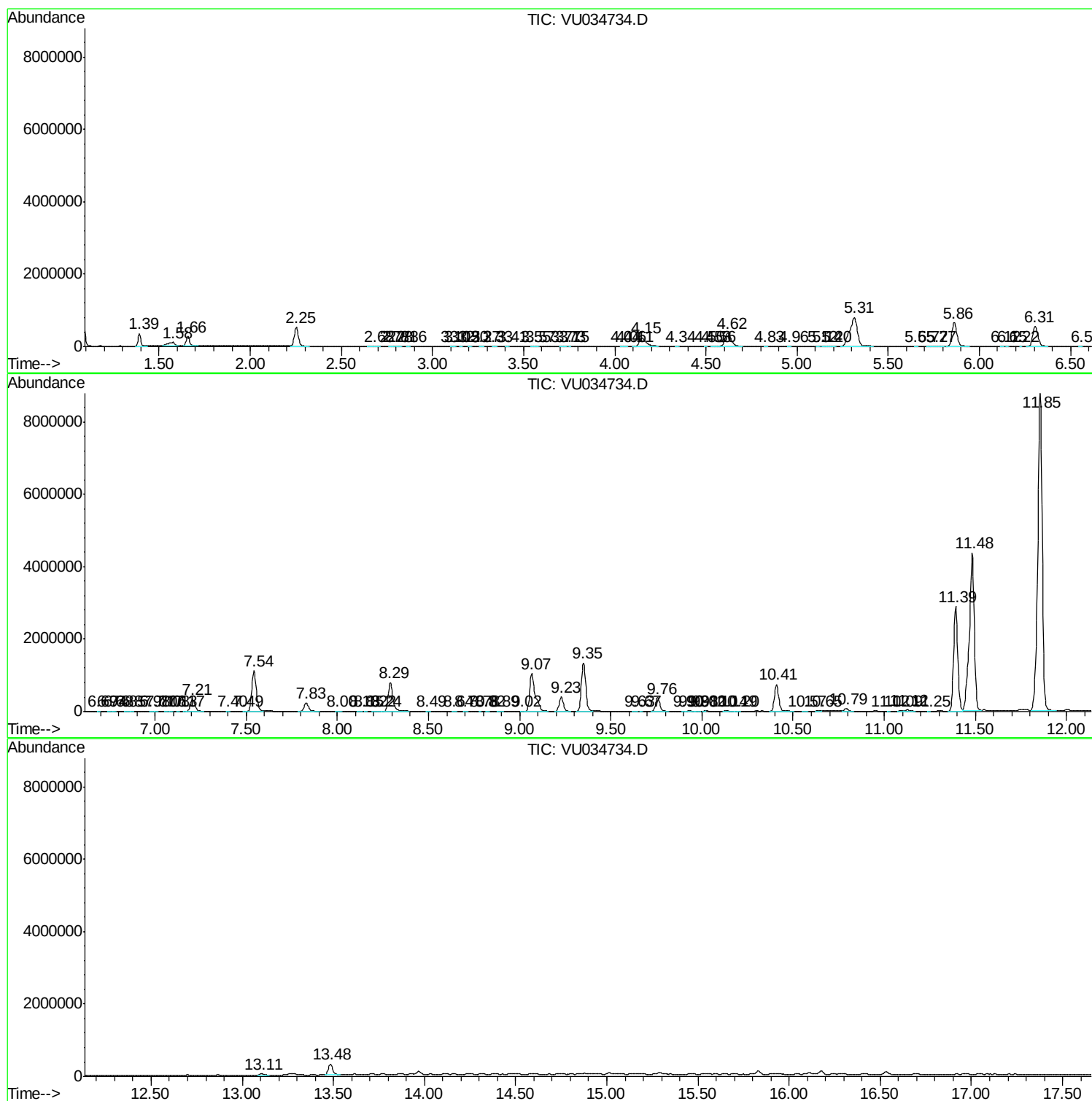
Sum of corrected areas: 48437004

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Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 10 Sample Multiplier: 1

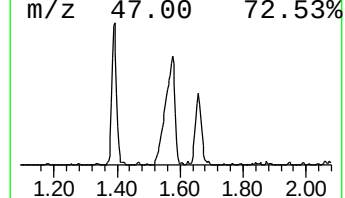
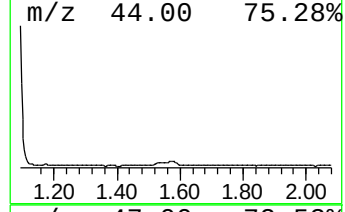
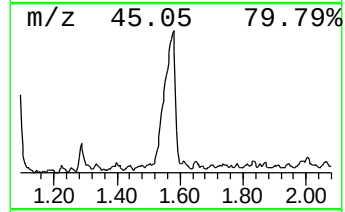
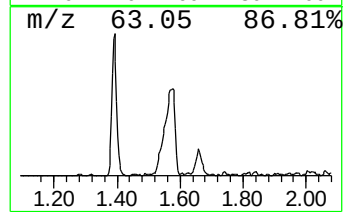
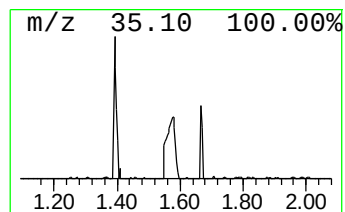
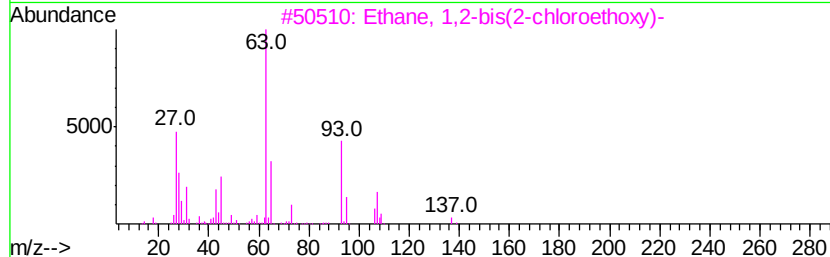
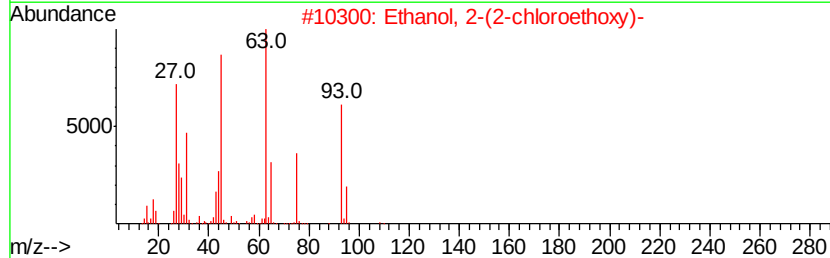
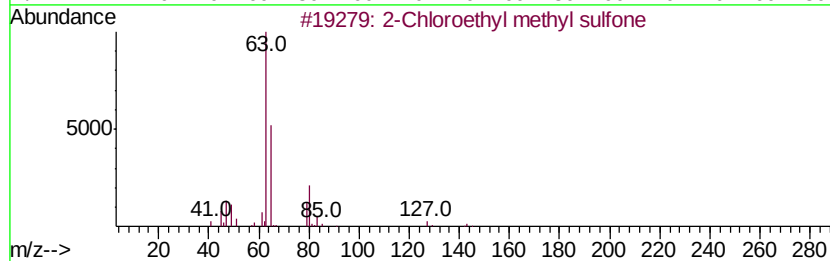
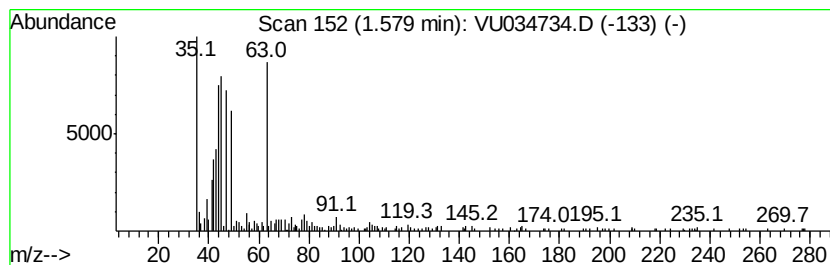
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091919WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.58	9.51 ug/L	247702	1,4-Difluorobenzene	5.86	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethyl methyl sulfone	142	C3H7ClO2S	050890-51-2	35
2	Ethanol, 2-(2-chloroethoxy)-	124	C4H9ClO2	000628-89-7	12
3	Ethane, 1,2-bis(2-chloroethoxy)-	186	C6H12Cl2O2	000112-26-5	10
4	Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	017639-93-9	10
5	Tris-(2-chloroethyl)orthoformate	250	C7H13Cl3O3	018719-58-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.58	9.5	ug/L	247702	1	5.86	1301950	50.0