

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU080518\
 Data File : VU025875.D
 Acq On : 04 Aug 2018 15:47
 Operator : MD/SY
 Sample : J4261-19ME
 Misc : 6.29g/5mL/100uL/5.00mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E5FA4ME

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\SOMULM072018WMA.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	0.628	9	12	20	rVB3	446	681	0.07%	0.007%
2	0.709	33	37	44	rVB2	437	559	0.06%	0.006%
3	1.082	138	153	173	rBV	790167	867709	86.61%	8.584%
4	1.288	214	217	224	rVB2	2657	2551	0.25%	0.025%
5	1.394	244	250	270	rVB	78288	113364	11.32%	1.121%
6	1.590	289	311	312	rBV	19485	44057	4.40%	0.436%
7	1.641	323	327	341	rVB	51292	60993	6.09%	0.603%
8	2.236	502	512	527	rVB	199891	302110	30.16%	2.989%
9	2.471	582	585	588	rBV4	525	389	0.04%	0.004%
10	2.529	600	603	606	rBV4	417	368	0.04%	0.004%
11	2.612	626	629	631	rBV2	575	380	0.04%	0.004%
12	2.680	644	650	653	rBV4	2563	2991	0.30%	0.030%
13	2.831	684	697	715	rBV2	12527	29580	2.95%	0.293%
14	2.895	715	717	723	rVB3	830	669	0.07%	0.007%
15	2.969	729	740	741	rBV3	1116	1472	0.15%	0.015%
16	3.275	828	835	838	rVV3	1407	1670	0.17%	0.017%
17	3.304	842	844	847	rVV2	578	362	0.04%	0.004%
18	3.333	850	853	858	rBV3	439	369	0.04%	0.004%
19	3.435	881	885	890	rBV2	408	359	0.04%	0.004%
20	3.638	943	948	953	rBV3	420	544	0.05%	0.005%
21	4.079	1072	1085	1095	rVB4	2021	4578	0.46%	0.045%
22	4.194	1105	1121	1163	rBV	64629	218349	21.80%	2.160%
23	4.400	1181	1185	1188	rBV2	623	481	0.05%	0.005%
24	4.416	1188	1190	1195	rVB3	486	402	0.04%	0.004%
25	4.648	1244	1262	1284	rBV2	166182	407974	40.72%	4.036%
26	4.796	1302	1308	1312	rBV4	491	587	0.06%	0.006%
27	4.882	1332	1335	1339	rVB2	532	358	0.04%	0.004%
28	4.982	1355	1366	1379	rVB10	3276	7856	0.78%	0.078%
29	5.201	1426	1434	1438	rBV3	579	547	0.05%	0.005%
30	5.332	1451	1475	1503	rBV2	349774	1001826	100.00%	9.911%
31	5.548	1536	1542	1550	rVB6	925	1074	0.11%	0.011%
32	5.609	1554	1561	1563	rBV3	3324	4114	0.41%	0.041%
33	5.667	1575	1579	1583	rBV4	522	464	0.05%	0.005%
34	5.776	1606	1613	1619	rBV6	1347	1825	0.18%	0.018%

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Integration Parameters: LSCINT.P

Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
 Title : VOC Analysis

35	5.886	1632	1647	1673	rBV	364400	734734	73.34%	7.268%
36	6.066	1700	1703	1707	rVB2	499	375	0.04%	0.004%
37	6.101	1707	1714	1718	rBV2	576	637	0.06%	0.006%
38	6.181	1727	1739	1747	rVV8	2602	5053	0.50%	0.050%
39	6.249	1751	1760	1771	rVV4	1764	3776	0.38%	0.037%
40	6.332	1771	1786	1803	rVV	214338	449551	44.87%	4.447%
41	6.410	1803	1810	1821	rVV6	10694	20721	2.07%	0.205%
42	6.644	1881	1883	1890	rVB4	830	650	0.06%	0.006%
43	6.747	1911	1915	1922	rVB4	548	535	0.05%	0.005%
44	6.799	1928	1931	1935	rVB	463	380	0.04%	0.004%
45	6.837	1937	1943	1945	rBV2	352	353	0.04%	0.003%
46	6.857	1945	1949	1952	rBV2	689	638	0.06%	0.006%
47	6.873	1952	1954	1956	rBV2	721	448	0.04%	0.004%
48	7.024	1997	2001	2005	rBV2	471	459	0.05%	0.005%
49	7.175	2043	2048	2049	rBV	874	716	0.07%	0.007%
50	7.230	2052	2065	2085	rVV	123291	232201	23.18%	2.297%
51	7.336	2096	2098	2104	rVB3	642	605	0.06%	0.006%
52	7.490	2133	2146	2153	rBV4	4870	8778	0.88%	0.087%
53	7.567	2157	2170	2185	rVV	453122	803014	80.16%	7.944%
54	7.641	2187	2193	2207	rVB2	10260	17256	1.72%	0.171%
55	7.853	2243	2259	2275	rBV	89675	163233	16.29%	1.615%
56	8.043	2313	2318	2321	rBV4	661	613	0.06%	0.006%
57	8.162	2348	2355	2356	rBV	297	355	0.04%	0.004%
58	8.229	2362	2376	2393	rBV	405191	688427	68.72%	6.810%
59	8.326	2393	2406	2433	rVB	279281	517966	51.70%	5.124%
60	8.490	2455	2457	2461	rVB2	858	588	0.06%	0.006%
61	8.545	2467	2474	2482	rBV5	1886	2649	0.26%	0.026%
62	8.606	2489	2493	2496	rBV3	679	482	0.05%	0.005%
63	8.705	2521	2524	2528	rVB2	490	392	0.04%	0.004%
64	8.943	2591	2598	2606	rVB3	600	1129	0.11%	0.011%
65	9.037	2621	2627	2629	rBV3	548	460	0.05%	0.005%
66	9.094	2631	2645	2666	rBV	546773	922348	92.07%	9.124%
67	9.258	2687	2696	2704	rVB3	2225	3255	0.32%	0.032%
68	9.329	2714	2718	2721	rBV2	460	446	0.04%	0.004%
69	9.377	2721	2733	2742	rVV3	5839	9972	1.00%	0.099%
70	9.442	2748	2753	2763	rVB6	2412	3363	0.34%	0.033%
71	9.487	2763	2767	2771	rBV3	472	493	0.05%	0.005%

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Integration Parameters: LSCINT.P

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
 Title : VOC Analysis

72	9.786	2851	2860	2868	rVV3	4485	7035	0.70%	0.070%
73	9.918	2896	2901	2902	rBV2	592	456	0.05%	0.005%
74	10.049	2934	2942	2944	rBV4	1213	1440	0.14%	0.014%
75	10.065	2944	2947	2952	rVB2	696	584	0.06%	0.006%
76	10.168	2971	2979	2988	rBV3	1197	2190	0.22%	0.022%
77	10.229	2992	2998	3004	rVV5	663	886	0.09%	0.009%
78	10.438	3049	3063	3079	rBV	345343	552238	55.12%	5.463%
79	10.496	3079	3081	3087	rVB3	461	367	0.04%	0.004%
80	10.586	3104	3109	3111	rBV3	1185	948	0.09%	0.009%
81	10.699	3134	3144	3151	rBV5	860	1547	0.15%	0.015%
82	10.815	3175	3180	3189	rVB4	1989	2163	0.22%	0.021%
83	11.152	3281	3285	3293	rVB4	1473	1937	0.19%	0.019%
84	11.281	3318	3325	3326	rBV2	427	505	0.05%	0.005%
85	11.406	3360	3364	3366	rBV2	679	523	0.05%	0.005%
86	11.487	3376	3389	3405	rBV	626195	984469	98.27%	9.739%
87	11.644	3436	3438	3442	rVB3	616	366	0.04%	0.004%
88	11.670	3443	3446	3450	rBV3	421	434	0.04%	0.004%
89	11.866	3493	3507	3525	rBV	530844	861593	86.00%	8.523%
90	12.027	3551	3557	3565	rBV4	2183	2436	0.24%	0.024%
91	12.699	3758	3766	3770	rBV3	599	799	0.08%	0.008%
92	12.766	3784	3787	3791	rBV3	399	370	0.04%	0.004%
93	12.950	3840	3844	3848	rBV2	377	381	0.04%	0.004%
94	13.757	4088	4095	4101	rBV3	2057	2817	0.28%	0.028%
95	13.827	4114	4117	4123	rBV3	538	479	0.05%	0.005%
96	14.027	4175	4179	4183	rBV3	409	395	0.04%	0.004%
97	14.589	4350	4354	4356	rBV2	575	463	0.05%	0.005%
98	15.052	4495	4498	4501	rBV2	943	618	0.06%	0.006%
99	15.136	4522	4524	4527	rBV2	671	444	0.04%	0.004%
100	15.757	4713	4717	4720	rBV4	1229	1073	0.11%	0.011%

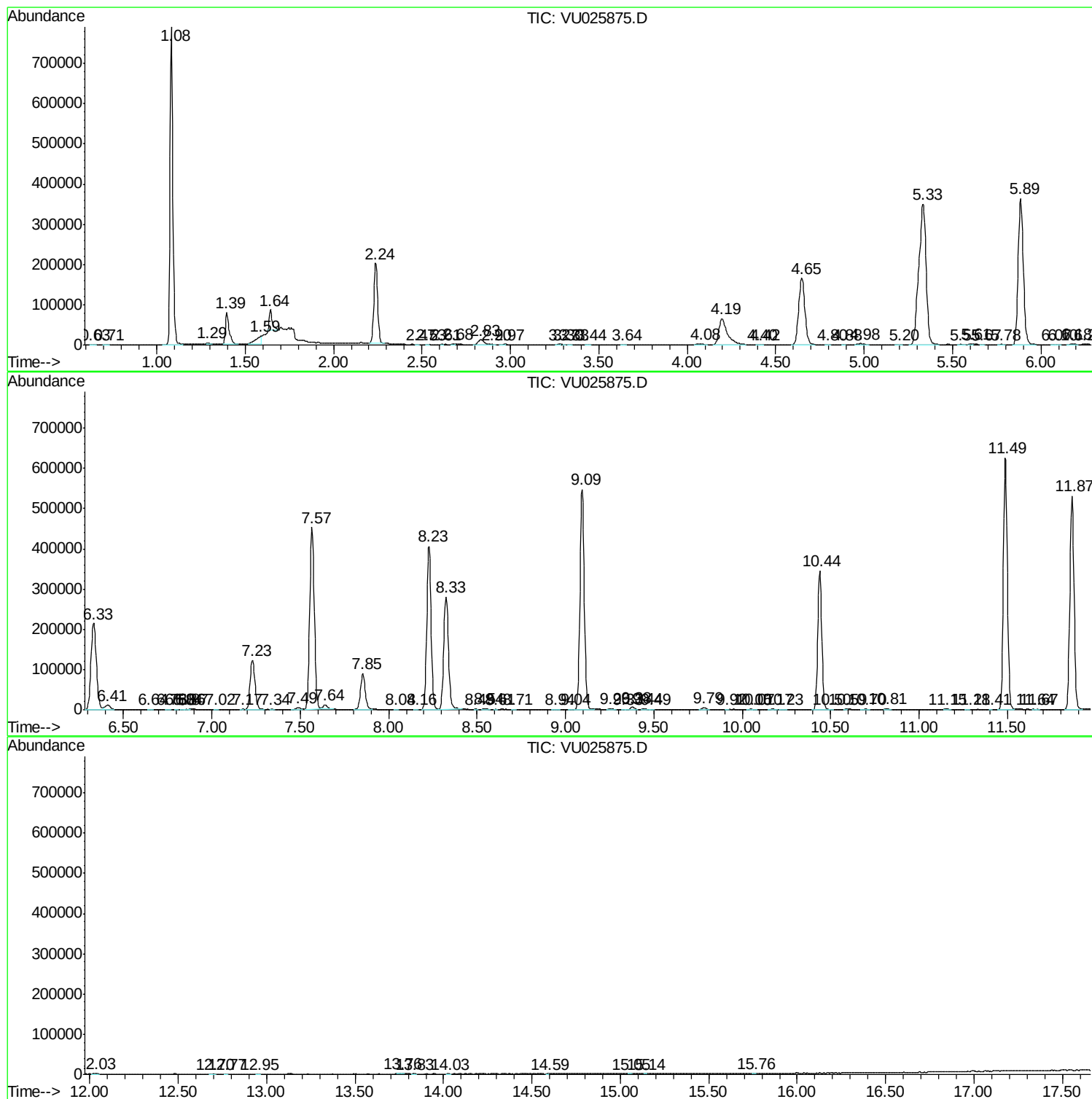
Sum of corrected areas: 10108619

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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



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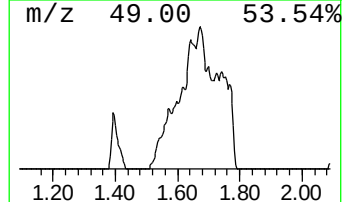
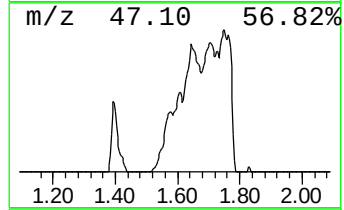
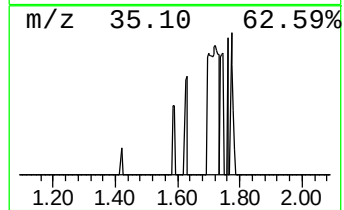
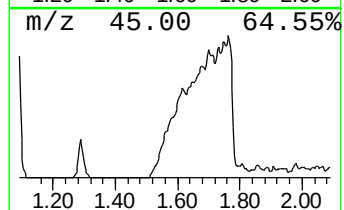
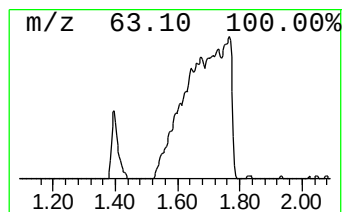
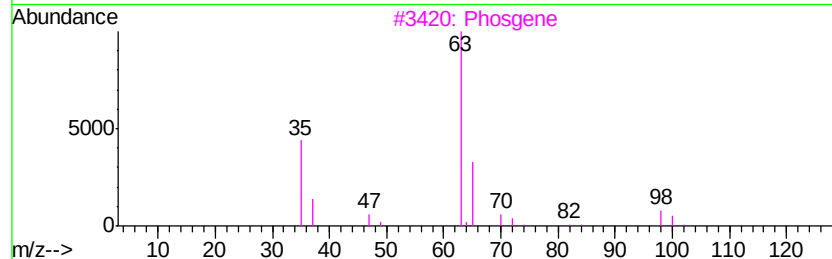
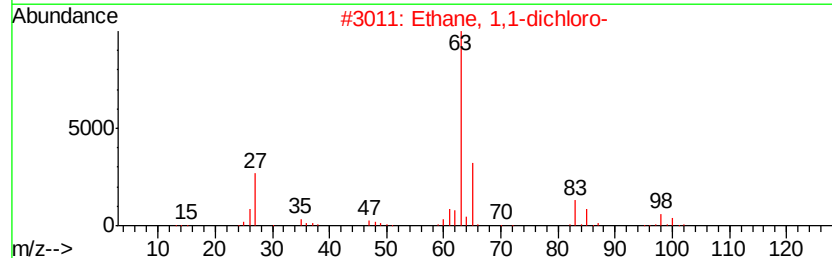
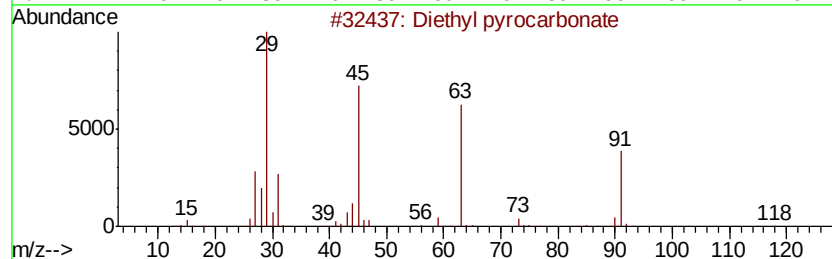
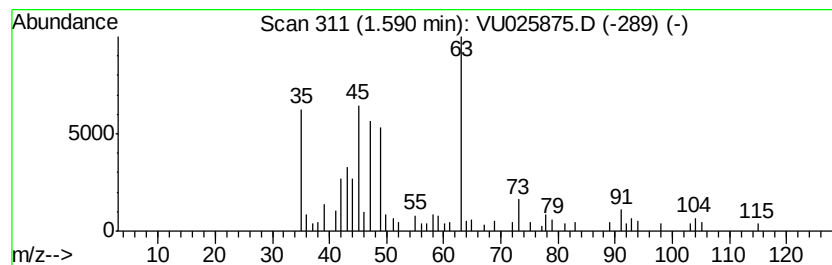
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.59	3.00 ug/L	44057	1,4-Difluorobenzene	5.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl pyrocarbonate	162	C6H10O5	001609-47-8	17
2	Ethane, 1,1-dichloro-	98	C2H4Cl2	000075-34-3	9
3	Phosgene	98	CCl2O	000075-44-5	9
4	Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	017639-93-9	9
5	Phosgene	98	CCl2O	000075-44-5	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.59	3.0	ug/L	44057	1	5.89	734734	50.0