

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU122018\
 Data File : VU028821.D
 Acq On : 20 Dec 2018 13:53
 Operator : MD/SY
 Sample : J6441-07
 Misc : 3.99g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE7Z6

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\SOMULM122018WMA.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	1.395	62	69	85	rVB	82649	93663	15.10%	1.702%
2	1.640	141	145	157	rVB	54988	56103	9.04%	1.019%
3	2.099	278	288	300	rBV	235044	327064	52.71%	5.942%
4	2.235	320	330	344	rBV	133894	204507	32.96%	3.715%
5	2.688	464	471	477	rVB3	987	1450	0.23%	0.026%
6	2.781	498	500	501	rBV	161	85	0.01%	0.002%
7	2.955	551	554	556	rBV2	343	167	0.03%	0.003%
8	3.035	576	579	582	rVB2	307	154	0.02%	0.003%
9	3.054	582	585	589	rBV	204	176	0.03%	0.003%
10	3.087	591	595	597	rBV2	256	225	0.04%	0.004%
11	3.157	612	617	618	rBV2	236	215	0.03%	0.004%
12	3.247	641	645	646	rBV	169	104	0.02%	0.002%
13	3.386	683	688	691	rBV2	201	178	0.03%	0.003%
14	3.405	691	694	696	rBV	161	132	0.02%	0.002%
15	3.501	722	724	731	rVB2	256	262	0.04%	0.005%
16	3.543	734	737	739	rBV	157	106	0.02%	0.002%
17	3.646	766	769	770	rBV	141	78	0.01%	0.001%
18	3.794	812	815	819	rBV2	249	191	0.03%	0.003%
19	3.826	823	825	831	rVB	218	118	0.02%	0.002%
20	3.861	831	836	838	rBV	186	164	0.03%	0.003%
21	3.903	845	849	851	rBV2	169	148	0.02%	0.003%
22	3.942	856	861	864	rBV	108	112	0.02%	0.002%
23	3.971	868	870	874	rVB	146	103	0.02%	0.002%
24	4.009	880	882	885	rBV	177	96	0.02%	0.002%
25	4.058	894	897	898	rBV2	138	75	0.01%	0.001%
26	4.112	912	914	916	rBV	289	103	0.02%	0.002%
27	4.189	925	938	974	rBV2	44875	152067	24.51%	2.763%
28	4.501	1033	1035	1039	rVB	262	204	0.03%	0.004%
29	4.546	1045	1049	1052	rBV	285	179	0.03%	0.003%
30	4.640	1062	1078	1106	rBV2	93376	229808	37.04%	4.175%
31	4.752	1111	1113	1116	rBV2	166	97	0.02%	0.002%
32	4.813	1130	1132	1133	rBV	157	90	0.01%	0.002%
33	4.836	1137	1139	1144	rVB2	155	114	0.02%	0.002%
34	4.884	1151	1154	1155	rBV	335	170	0.03%	0.003%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
 Title : VOC Analysis

35	4.906	1159	1161	1165	rVB	170	79	0.01%	0.001%
36	4.951	1170	1175	1178	rBV2	189	208	0.03%	0.004%
37	4.987	1185	1186	1193	rVB	257	121	0.02%	0.002%
38	5.096	1218	1220	1223	rBV	168	91	0.01%	0.002%
39	5.183	1241	1247	1250	rBV	97	106	0.02%	0.002%
40	5.241	1259	1265	1271	rBV	85	138	0.02%	0.003%
41	5.328	1271	1292	1321	rBV2	220578	620456	100.00%	11.272%
42	5.611	1375	1380	1383	rBV2	930	999	0.16%	0.018%
43	5.781	1430	1433	1439	rVB	246	195	0.03%	0.004%
44	5.881	1451	1464	1488	rBV	205104	419126	67.55%	7.614%
45	6.154	1539	1549	1551	rBV2	660	848	0.14%	0.015%
46	6.250	1568	1579	1587	rBV3	1196	2577	0.42%	0.047%
47	6.324	1589	1602	1623	rVV	134075	282955	45.60%	5.140%
48	6.459	1642	1644	1648	rBV	391	208	0.03%	0.004%
49	6.546	1666	1671	1675	rBV	145	128	0.02%	0.002%
50	6.646	1699	1702	1707	rBV	98	88	0.01%	0.002%
51	6.723	1723	1726	1730	rBV	100	79	0.01%	0.001%
52	6.826	1756	1758	1760	rVB	230	91	0.01%	0.002%
53	6.881	1768	1775	1778	rBV	577	626	0.10%	0.011%
54	7.057	1828	1830	1833	rVB2	137	77	0.01%	0.001%
55	7.141	1852	1856	1858	rBV	102	76	0.01%	0.001%
56	7.225	1870	1882	1903	rBV2	77251	150455	24.25%	2.733%
57	7.466	1951	1957	1959	rBV2	217	208	0.03%	0.004%
58	7.492	1963	1965	1970	rVB2	433	258	0.04%	0.005%
59	7.562	1971	1987	2005	rBV	271134	493539	79.54%	8.966%
60	7.852	2063	2077	2098	rBV	51612	100661	16.22%	1.829%
61	8.016	2125	2128	2131	rBV2	364	206	0.03%	0.004%
62	8.061	2138	2142	2145	rVB2	280	197	0.03%	0.004%
63	8.125	2160	2162	2166	rVB	144	126	0.02%	0.002%
64	8.241	2196	2198	2203	rVB	130	83	0.01%	0.002%
65	8.276	2206	2209	2211	rBV	153	85	0.01%	0.002%
66	8.324	2211	2224	2248	rBV	205116	394372	63.56%	7.165%
67	8.475	2270	2271	2272	rBV	231	78	0.01%	0.001%
68	8.601	2303	2310	2312	rBV2	410	501	0.08%	0.009%
69	8.729	2348	2350	2353	rVV	195	107	0.02%	0.002%
70	8.752	2354	2357	2362	rVB2	175	184	0.03%	0.003%
71	8.807	2371	2374	2375	rBV	177	98	0.02%	0.002%

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 Title : VOC Analysis

72	8.909	2400	2406	2411	rBV2	259	346	0.06%	0.006%
73	9.032	2438	2444	2447	rVB2	376	351	0.06%	0.006%
74	9.090	2448	2462	2499	rBV	303483	534993	86.23%	9.719%
75	9.382	2543	2553	2563	rBV5	944	2123	0.34%	0.039%
76	9.443	2568	2572	2576	rVB3	402	375	0.06%	0.007%
77	9.691	2647	2649	2650	rBV	256	112	0.02%	0.002%
78	9.790	2670	2680	2684	rBV	619	945	0.15%	0.017%
79	9.916	2716	2719	2721	rBV	360	195	0.03%	0.004%
80	9.951	2722	2730	2736	rVB3	2351	3385	0.55%	0.061%
81	10.012	2745	2749	2750	rBV2	531	303	0.05%	0.006%
82	10.086	2767	2772	2780	rVB5	2613	3784	0.61%	0.069%
83	10.154	2787	2793	2795	rBV2	617	562	0.09%	0.010%
84	10.221	2812	2814	2816	rBV2	201	109	0.02%	0.002%
85	10.299	2836	2838	2839	rBV	351	119	0.02%	0.002%
86	10.318	2840	2844	2845	rBV	1002	739	0.12%	0.013%
87	10.437	2867	2881	2894	rBV	226011	367768	59.27%	6.681%
88	10.520	2906	2907	2910	rBV	220	91	0.01%	0.002%
89	10.536	2910	2912	2915	rBV2	279	130	0.02%	0.002%
90	10.591	2924	2929	2935	rBV3	569	972	0.16%	0.018%
91	10.697	2955	2962	2970	rVB6	1737	2965	0.48%	0.054%
92	10.752	2972	2979	2991	rBV6	2804	4930	0.79%	0.090%
93	10.900	3019	3025	3029	rBV4	745	667	0.11%	0.012%
94	10.970	3043	3047	3053	rBV6	880	1180	0.19%	0.021%
95	11.112	3085	3091	3097	rBV2	5910	7849	1.27%	0.143%
96	11.263	3132	3138	3145	rBV5	1750	3074	0.50%	0.056%
97	11.485	3196	3207	3227	rVB	335196	523359	84.35%	9.508%
98	11.771	3289	3296	3297	rBV3	1785	1633	0.26%	0.030%
99	11.861	3311	3324	3345	rBV	303390	496624	80.04%	9.022%
100	12.607	3548	3556	3561	rBV6	3963	5857	0.94%	0.106%

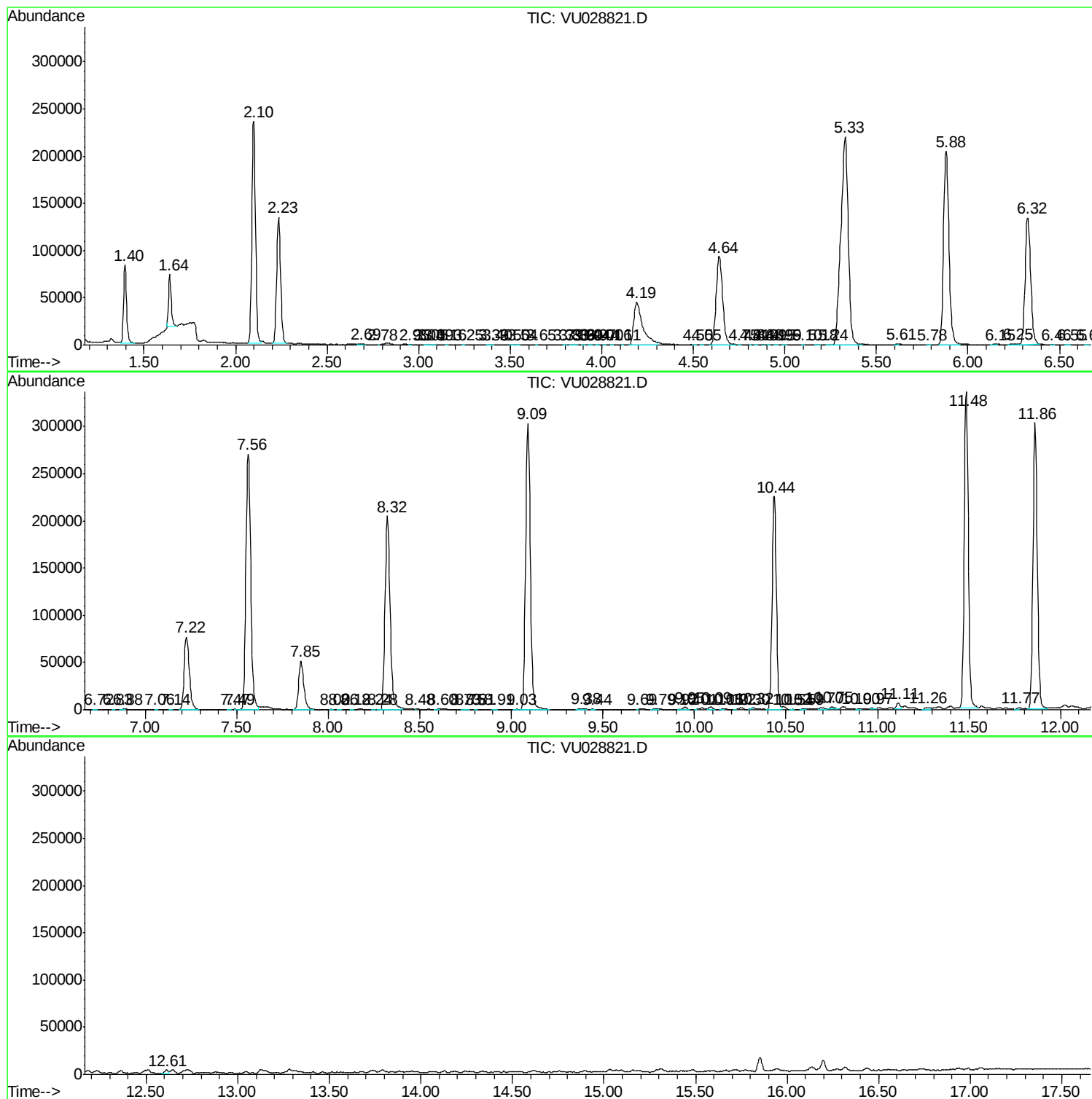
Sum of corrected areas: 5504478

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 13 Sample Multiplier: 1

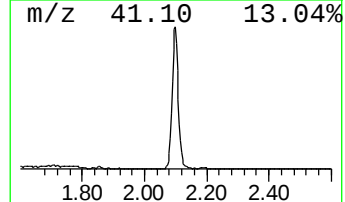
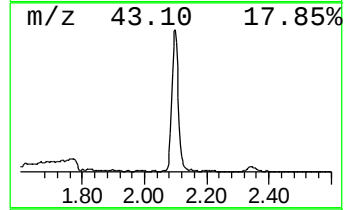
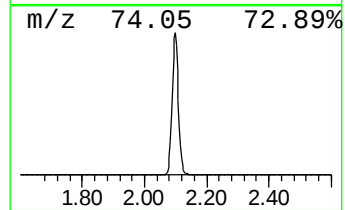
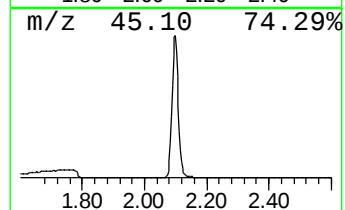
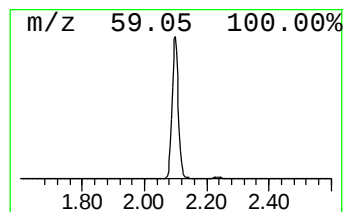
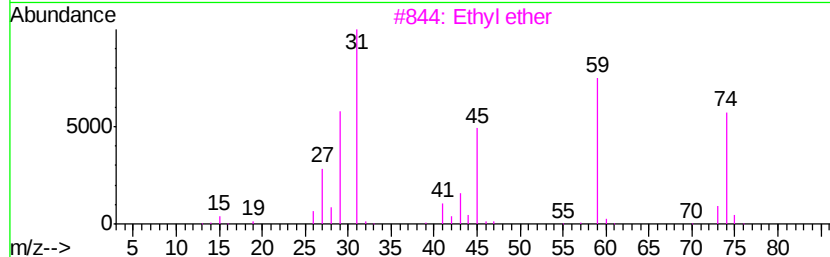
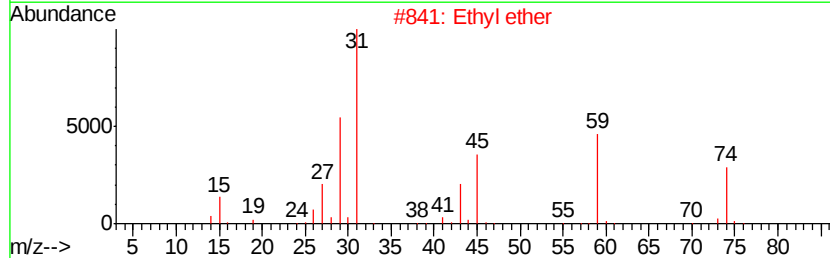
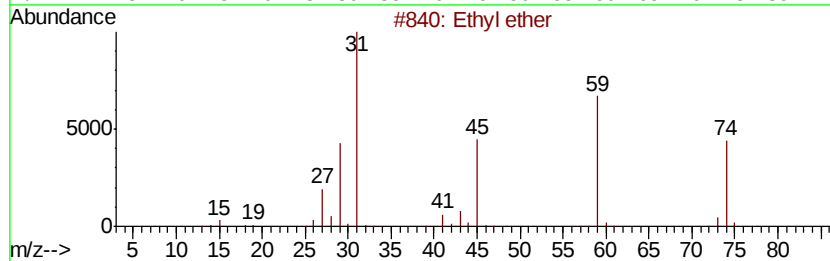
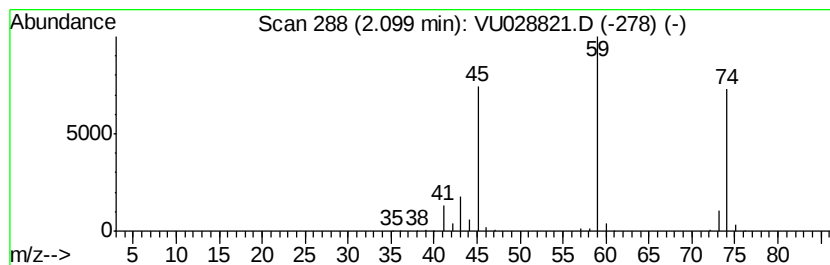
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.10	39.02 ug/L	327064	1,4-Difluorobenzene	5.88
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Ethyl ether	74	C4H100	000060-29-7 91
2	Ethyl ether	74	C4H100	000060-29-7 90
3	Ethyl ether	74	C4H100	000060-29-7 90
4	Ethyl ether	74	C4H100	000060-29-7 78
5	Ethyl ether	74	C4H100	000060-29-7 78



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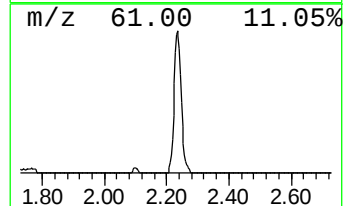
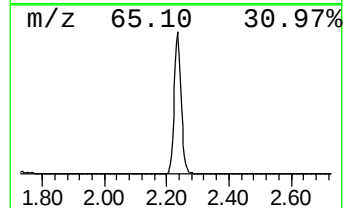
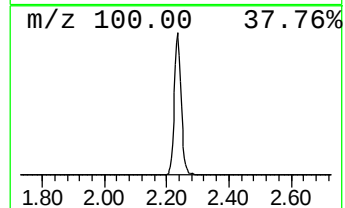
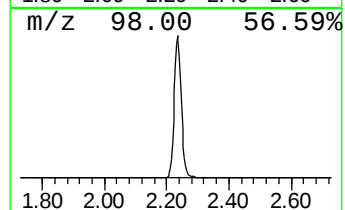
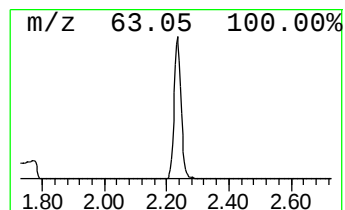
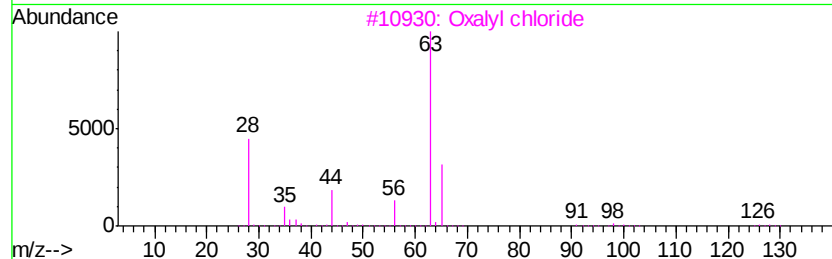
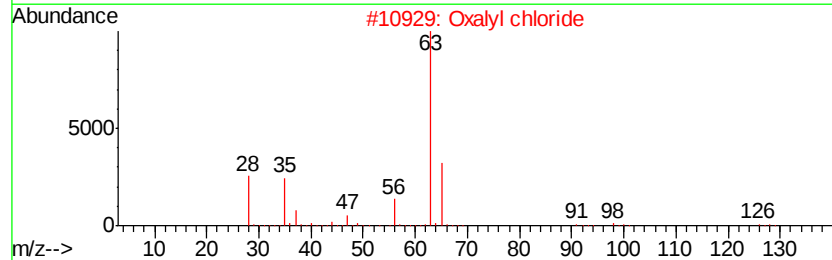
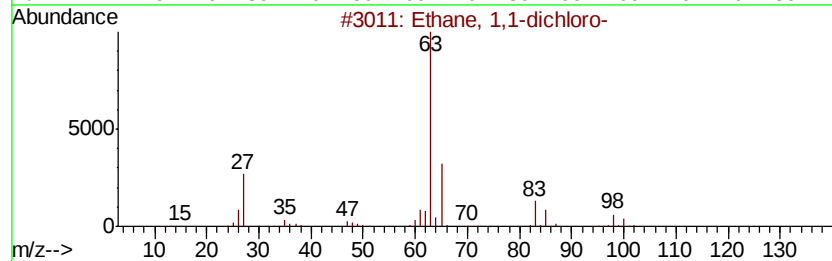
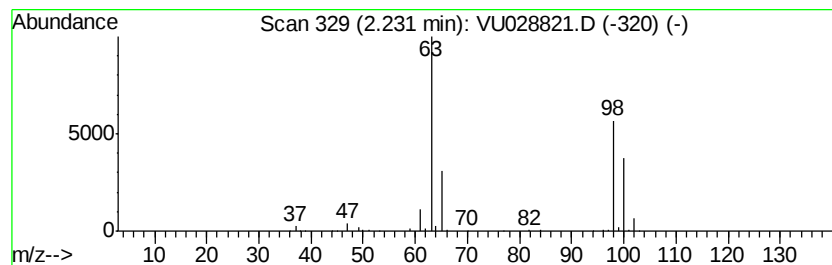
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Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	24.40 ug/L	204507	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethane, 1,1-dichloro-	98	C2H4Cl2	000075-34-3	39
2		Oxalyl chloride	126	C2Cl2O2	000079-37-8	38
3		Oxalyl chloride	126	C2Cl2O2	000079-37-8	9
4		2-Chloropropionyl chloride	126	C3H4Cl2O	007623-09-8	9
5		Propane, 1,2-dichloro-	112	C3H6Cl2	000078-87-5	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl ether	2.10	39.0	ug/L	327064	1	5.88	419126	50.0
unknown-01	2.23	24.4	ug/L	204507	1	5.88	419126	50.0