

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047964.D
 Acq On : 12 Apr 2022 18:27
 Operator : SY/MD
 Sample : N2293-05ME
 Misc : 6.63g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNN5ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU047964.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	102	rVB	72041	120641	8.63%	1.151%
2	1.790	121	140	141	rBV6	22013	48994	3.50%	0.468%
3	2.543	362	374	398	rBV	179754	325962	23.31%	3.110%
4	2.813	455	458	461	rVB3	603	393	0.03%	0.004%
5	2.829	461	463	465	rBV2	511	259	0.02%	0.002%
6	3.038	519	528	542	rVB5	1912	4085	0.29%	0.039%
7	3.247	591	593	596	rVB2	453	263	0.02%	0.003%
8	3.318	613	615	625	rVB3	592	766	0.05%	0.007%
9	3.404	638	642	646	rVV	329	373	0.03%	0.004%
10	3.440	650	653	658	rBV2	314	341	0.02%	0.003%
11	3.465	658	661	664	rVV3	295	247	0.02%	0.002%
12	3.504	669	673	681	rBV2	354	498	0.04%	0.005%
13	3.626	706	711	712	rBV	366	317	0.02%	0.003%
14	3.723	738	741	747	rBV3	239	203	0.01%	0.002%
15	3.781	756	759	762	rVB2	299	223	0.02%	0.002%
16	3.874	785	788	792	rBV2	237	197	0.01%	0.002%
17	3.941	802	809	812	rBV	340	384	0.03%	0.004%
18	4.096	849	857	859	rBV2	401	418	0.03%	0.004%
19	4.498	980	982	991	rVB2	262	239	0.02%	0.002%
20	4.633	1010	1024	1065	rBV	106199	334138	23.90%	3.188%
21	4.980	1126	1132	1135	rBV	379	350	0.03%	0.003%
22	4.999	1135	1138	1141	rVV	327	285	0.02%	0.003%
23	5.060	1141	1157	1182	rVV	198771	448846	32.10%	4.283%
24	5.333	1232	1242	1245	rBV4	1927	3006	0.21%	0.029%
25	5.633	1333	1335	1338	rVB	348	194	0.01%	0.002%
26	5.719	1338	1362	1396	rBV2	418239	1156679	82.73%	11.037%
27	6.025	1454	1457	1462	rVB	276	223	0.02%	0.002%
28	6.051	1463	1465	1470	rVB	398	259	0.02%	0.002%
29	6.112	1477	1484	1487	rBV2	534	540	0.04%	0.005%
30	6.247	1512	1526	1547	rBV	421778	824896	59.00%	7.871%
31	6.446	1586	1588	1592	rVB2	376	261	0.02%	0.002%
32	6.488	1596	1601	1605	rBV3	336	372	0.03%	0.004%
33	6.530	1608	1614	1615	rBV3	905	856	0.06%	0.008%
34	6.597	1630	1635	1636	rBV3	467	354	0.03%	0.003%
35	6.607	1636	1638	1645	rVB2	464	446	0.03%	0.004%
36	6.690	1649	1664	1687	rBV	253719	511081	36.55%	4.877%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

37	6.787	1692	1694	1698	rBV2	438	212	0.02%	0.002%
38	6.806	1698	1700	1703	rBV2	315	216	0.02%	0.002%
39	7.041	1766	1773	1778	rBV2	1074	1538	0.11%	0.015%
40	7.186	1805	1818	1836	rVV2	7548	16967	1.21%	0.162%
41	7.247	1836	1837	1842	rVB2	560	327	0.02%	0.003%
42	7.288	1847	1850	1853	rVV2	393	246	0.02%	0.002%
43	7.311	1853	1857	1860	rVV	330	243	0.02%	0.002%
44	7.488	1905	1912	1913	rBV3	468	455	0.03%	0.004%
45	7.568	1923	1937	1956	rBV	128431	242268	17.33%	2.312%
46	7.694	1969	1976	1985	rBV5	1460	2487	0.18%	0.024%
47	7.806	2006	2011	2012	rBV2	396	306	0.02%	0.003%
48	7.816	2012	2014	2018	rVB2	312	203	0.01%	0.002%
49	7.899	2025	2040	2054	rBV	465625	835243	59.74%	7.970%
50	8.182	2115	2128	2148	rBV	84560	167195	11.96%	1.595%
51	8.366	2179	2185	2190	rVB5	736	826	0.06%	0.008%
52	8.391	2190	2193	2196	rBV3	344	214	0.02%	0.002%
53	8.433	2203	2206	2209	rVV2	327	290	0.02%	0.003%
54	8.475	2210	2219	2235	rVB2	2392	4684	0.34%	0.045%
55	8.648	2258	2273	2311	rBV	427338	841396	60.18%	8.029%
56	8.874	2341	2343	2345	rBV	368	266	0.02%	0.003%
57	9.282	2468	2470	2474	rBV2	306	190	0.01%	0.002%
58	9.420	2498	2513	2544	rBV2	652323	1398200	100.00%	13.342%
59	9.578	2556	2562	2569	rVB3	1557	2226	0.16%	0.021%
60	9.610	2569	2572	2577	rBV2	347	292	0.02%	0.003%
61	9.645	2577	2583	2586	rBV3	215	259	0.02%	0.002%
62	9.700	2590	2600	2610	rVV5	2677	4404	0.31%	0.042%
63	9.925	2667	2670	2674	rVB3	334	291	0.02%	0.003%
64	10.102	2719	2725	2736	rVB5	1840	2844	0.20%	0.027%
65	10.282	2778	2781	2786	rBV2	277	216	0.02%	0.002%
66	10.417	2820	2823	2828	rBV	293	240	0.02%	0.002%
67	10.481	2839	2843	2845	rBV	489	420	0.03%	0.004%
68	10.668	2893	2901	2908	rVV4	1487	2253	0.16%	0.021%
69	10.764	2915	2931	2949	rBV	481105	787006	56.29%	7.510%
70	10.893	2963	2971	2981	rVB3	3763	5625	0.40%	0.054%
71	10.980	2996	2998	3001	rVV2	487	322	0.02%	0.003%
72	10.996	3001	3003	3008	rVB3	390	305	0.02%	0.003%
73	11.208	3066	3069	3073	rVB3	299	212	0.02%	0.002%
74	11.279	3087	3091	3092	rBV	296	189	0.01%	0.002%
75	11.298	3095	3097	3100	rBV2	308	220	0.02%	0.002%
76	11.417	3131	3134	3136	rVV	295	193	0.01%	0.002%

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Instrument :
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 ClientSampleId :
 ETNN5ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

77	11.468	3141	3150	3161	rVV4	2801	4500	0.32%	0.043%
78	11.517	3161	3165	3168	rVB2	411	306	0.02%	0.003%
79	11.578	3181	3184	3187	rBV3	438	342	0.02%	0.003%
80	11.697	3216	3221	3230	rVB6	734	1262	0.09%	0.012%
81	11.751	3230	3238	3246	rBV6	3695	6286	0.45%	0.060%
82	11.816	3246	3258	3276	rBV	824476	1292704	92.45%	12.335%
83	12.034	3324	3326	3329	rVB2	555	261	0.02%	0.002%
84	12.054	3329	3332	3334	rBV2	456	282	0.02%	0.003%
85	12.066	3334	3336	3337	rBV	417	188	0.01%	0.002%
86	12.195	3360	3376	3396	rBV	584421	972909	69.58%	9.284%
87	12.774	3550	3556	3566	rVB5	1663	2740	0.20%	0.026%
88	12.899	3590	3595	3599	rBV2	321	370	0.03%	0.004%
89	12.973	3608	3618	3631	rBV3	18248	29603	2.12%	0.282%
90	13.333	3722	3730	3738	rBV3	4451	7270	0.52%	0.069%
91	13.378	3738	3744	3755	rVB5	4653	6992	0.50%	0.067%
92	13.619	3816	3819	3821	rBV2	337	211	0.02%	0.002%
93	13.851	3888	3891	3897	rVB3	1177	1081	0.08%	0.010%
94	13.922	3910	3913	3917	rBV2	423	384	0.03%	0.004%
95	14.095	3963	3967	3979	rVB2	930	1634	0.12%	0.016%
96	14.365	4043	4051	4059	rVB3	3278	4346	0.31%	0.041%
97	14.578	4112	4117	4123	rBV3	1153	1695	0.12%	0.016%
98	15.545	4411	4418	4427	rVB6	10206	15427	1.10%	0.147%
99	15.722	4471	4473	4475	rBV3	757	460	0.03%	0.004%
100	16.388	4673	4680	4689	rBV5	12495	19267	1.38%	0.184%

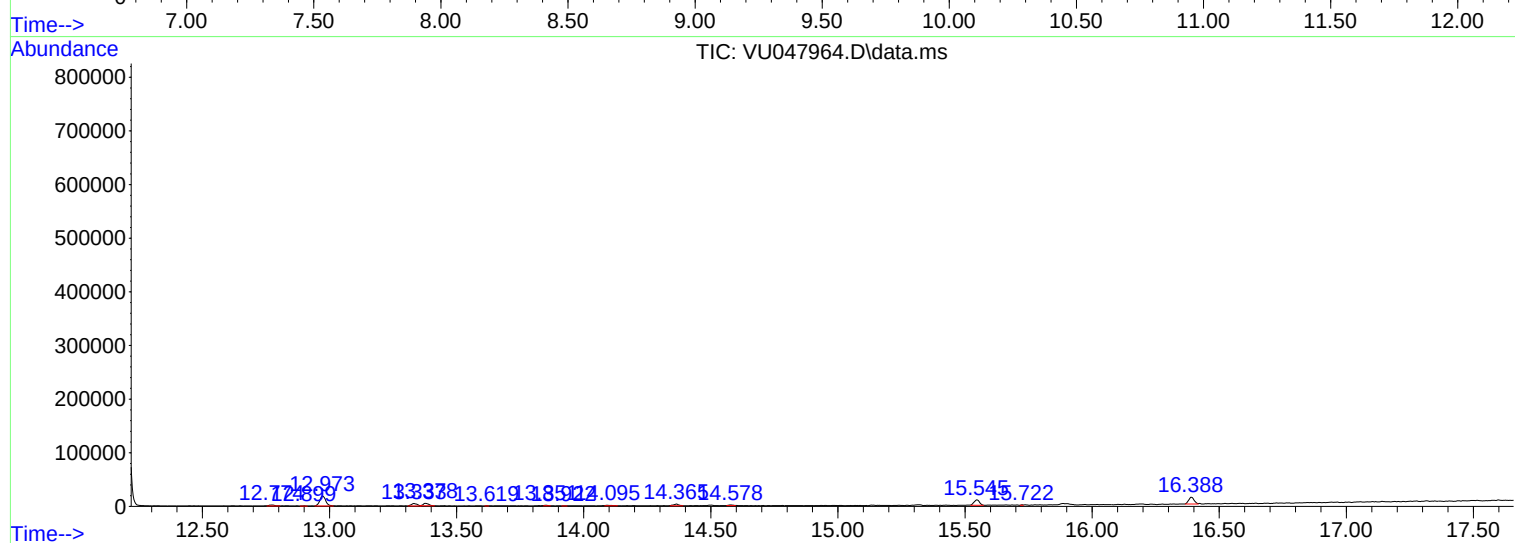
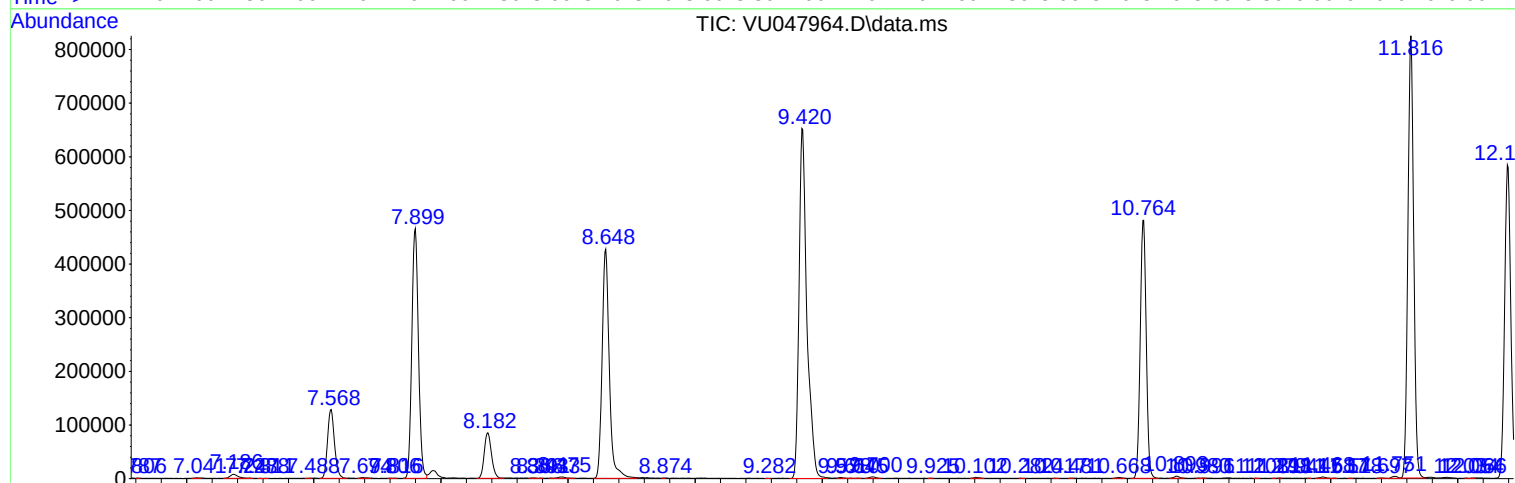
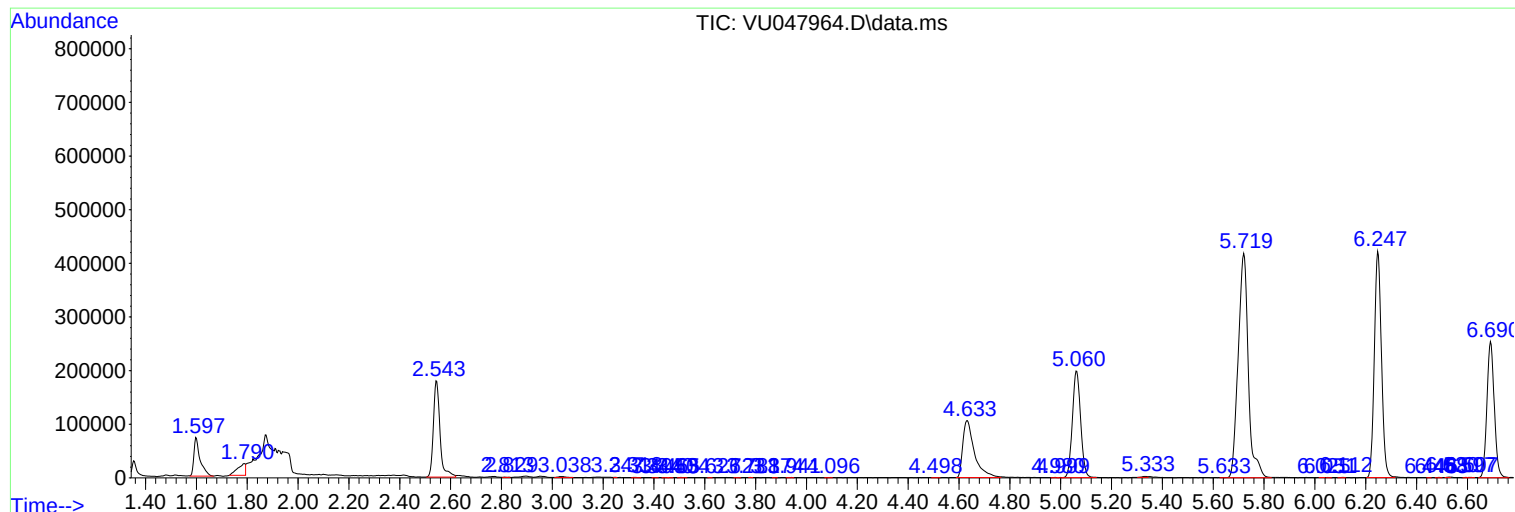
Sum of corrected areas: 10479598

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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNN5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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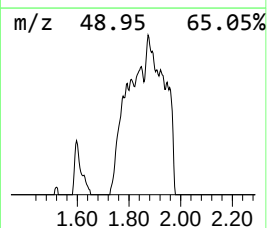
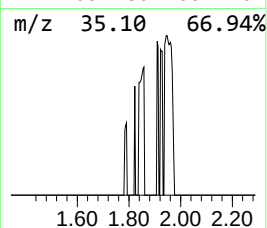
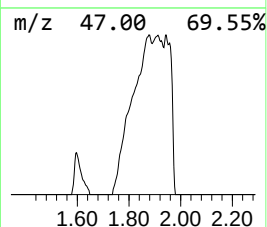
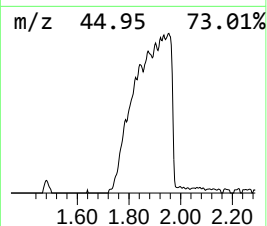
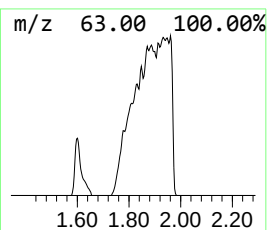
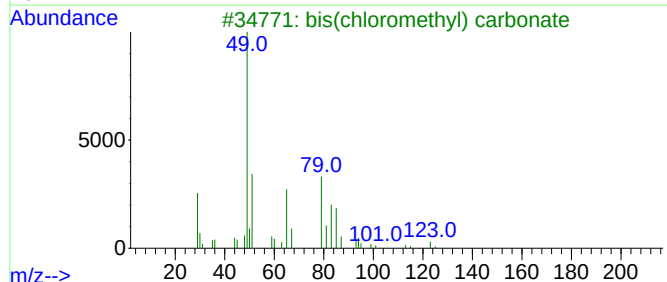
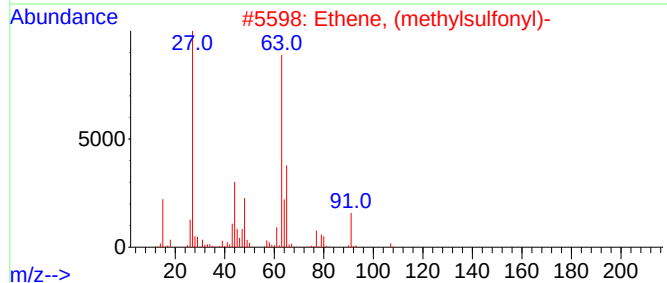
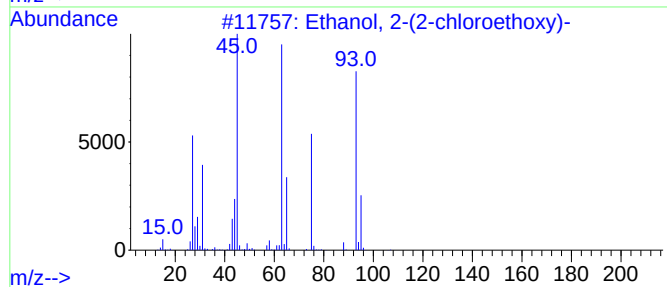
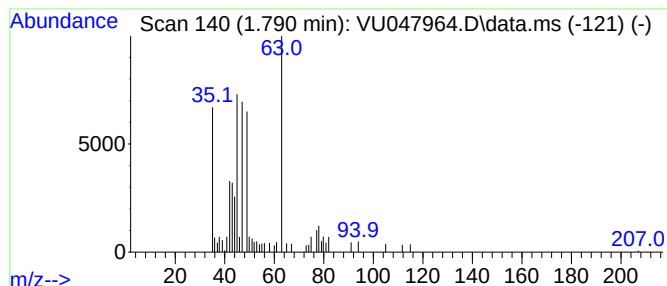
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.790	2.97 ug/L	48994	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-chloroethoxy)-	124	C4H9ClO2	000628-89-7	23
2			Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	9
3			bis(chloromethyl) carbonate	158	C3H4Cl2O3	1000404-37-0	9
4			Ethanol, 2-(2-chloroethoxy)-	124	C4H9ClO2	000628-89-7	9
5			Methan-d3-ol	35	CHD3O	001849-29-2	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.790	3.0	ug/L	48994	1	6.247	824896	50.0