

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041222\
 Data File : VU047946.D
 Acq On : 12 Apr 2022 11:37
 Operator : SY/MD
 Sample : N2293-05ME
 Misc : 6.63g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 7 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: VU047946.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	105	rBV	49287	93084	9.26%	1.157%
2	1.784	120	138	139	rBV6	20734	45146	4.49%	0.561%
3	2.543	362	374	385	rBV	124655	213171	21.20%	2.651%
4	2.774	438	446	457	rVB4	1315	2380	0.24%	0.030%
5	3.035	522	527	538	rVB7	1411	2617	0.26%	0.033%
6	3.080	538	541	544	rVB2	391	239	0.02%	0.003%
7	3.163	561	567	568	rBV3	548	460	0.05%	0.006%
8	3.215	581	583	588	rBV4	464	337	0.03%	0.004%
9	3.314	610	614	618	rBV2	265	214	0.02%	0.003%
10	3.453	654	657	661	rBV	349	310	0.03%	0.004%
11	3.851	776	781	786	rBV2	410	438	0.04%	0.005%
12	3.928	802	805	810	rBV2	269	209	0.02%	0.003%
13	4.018	830	833	837	rBV2	281	234	0.02%	0.003%
14	4.034	837	838	843	rVB2	377	210	0.02%	0.003%
15	4.163	874	878	882	rBV2	269	259	0.03%	0.003%
16	4.411	949	955	959	rVB2	361	422	0.04%	0.005%
17	4.436	959	963	967	rBV2	283	201	0.02%	0.002%
18	4.459	967	970	972	rBV2	265	190	0.02%	0.002%
19	4.571	1001	1005	1007	rBV2	293	231	0.02%	0.003%
20	4.633	1010	1024	1068	rBV	94035	307883	30.61%	3.828%
21	5.063	1140	1158	1180	rBV	167559	385924	38.37%	4.799%
22	5.205	1199	1202	1205	rVB	459	321	0.03%	0.004%
23	5.234	1205	1211	1212	rBV	219	224	0.02%	0.003%
24	5.285	1223	1227	1229	rBV3	455	412	0.04%	0.005%
25	5.446	1274	1277	1282	rVB2	370	282	0.03%	0.004%
26	5.504	1288	1295	1298	rBV3	304	314	0.03%	0.004%
27	5.552	1307	1310	1315	rVB2	399	355	0.04%	0.004%
28	5.581	1315	1319	1327	rVB2	280	364	0.04%	0.005%
29	5.626	1327	1333	1337	rBV2	303	356	0.04%	0.004%
30	5.719	1341	1362	1395	rBV2	350358	987421	98.18%	12.278%
31	5.861	1401	1406	1409	rVB3	367	348	0.03%	0.004%
32	5.886	1409	1414	1421	rBV2	335	391	0.04%	0.005%
33	5.980	1439	1443	1447	rBV3	430	338	0.03%	0.004%
34	5.999	1447	1449	1453	rVB3	614	350	0.03%	0.004%
35	6.028	1453	1458	1459	rBV2	657	510	0.05%	0.006%
36	6.247	1511	1526	1550	rBV	333730	657528	65.38%	8.176%

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 Title : VOC Analysis

37	6.427	1579	1582	1585	rVB3	331	183	0.02%	0.002%
38	6.530	1607	1614	1616	rBV4	1021	1126	0.11%	0.014%
39	6.690	1649	1664	1687	rVV	219115	447775	44.52%	5.568%
40	6.809	1700	1701	1706	rVB	391	210	0.02%	0.003%
41	6.973	1744	1752	1755	rBV2	298	429	0.04%	0.005%
42	7.057	1768	1778	1781	rBV3	836	1403	0.14%	0.017%
43	7.189	1805	1819	1838	rBV3	8941	20065	2.00%	0.249%
44	7.317	1855	1859	1863	rVB3	415	233	0.02%	0.003%
45	7.340	1863	1866	1868	rBV2	232	198	0.02%	0.002%
46	7.485	1905	1911	1917	rBV4	439	592	0.06%	0.007%
47	7.568	1924	1937	1954	rBV	100547	193351	19.22%	2.404%
48	7.697	1969	1977	1980	rBV5	1111	1556	0.15%	0.019%
49	7.735	1987	1989	1993	rVB3	505	297	0.03%	0.004%
50	7.899	2024	2040	2055	rBV	333570	602750	59.93%	7.495%
51	8.054	2084	2088	2091	rVB	358	307	0.03%	0.004%
52	8.182	2115	2128	2149	rBV2	64818	134837	13.41%	1.677%
53	8.266	2150	2154	2157	rBV3	428	342	0.03%	0.004%
54	8.472	2212	2218	2220	rBV4	350	339	0.03%	0.004%
55	8.584	2250	2253	2256	rBV3	258	241	0.02%	0.003%
56	8.652	2259	2274	2312	rBV	369040	758935	75.46%	9.437%
57	8.835	2329	2331	2334	rBV2	416	254	0.03%	0.003%
58	9.089	2407	2410	2413	rVB2	369	208	0.02%	0.003%
59	9.214	2446	2449	2453	rBV2	265	222	0.02%	0.003%
60	9.295	2471	2474	2477	rVB2	300	189	0.02%	0.002%
61	9.420	2500	2513	2542	rBV2	459246	1005756	100.00%	12.506%
62	9.693	2591	2598	2608	rVB3	1464	2559	0.25%	0.032%
63	9.751	2613	2616	2620	rBV2	251	232	0.02%	0.003%
64	9.796	2624	2630	2634	rVB3	318	462	0.05%	0.006%
65	9.851	2642	2647	2653	rVB3	353	411	0.04%	0.005%
66	9.893	2653	2660	2661	rBV2	374	401	0.04%	0.005%
67	9.989	2687	2690	2693	rBV2	255	211	0.02%	0.003%
68	10.060	2710	2712	2715	rVB	329	212	0.02%	0.003%
69	10.102	2719	2725	2728	rBV3	923	904	0.09%	0.011%
70	10.211	2757	2759	2764	rBV	216	195	0.02%	0.002%
71	10.253	2770	2772	2778	rVB3	244	188	0.02%	0.002%
72	10.401	2814	2818	2820	rBV2	322	250	0.02%	0.003%
73	10.668	2898	2901	2905	rVB2	539	265	0.03%	0.003%
74	10.764	2918	2931	2948	rBV	432997	692000	68.80%	8.604%
75	10.848	2955	2957	2963	rVB2	454	315	0.03%	0.004%
76	10.886	2963	2969	2970	rBV2	511	402	0.04%	0.005%

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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

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

77	10.976	2992	2997	2999	rBV3	282	315	0.03%	0.004%
78	11.063	3017	3024	3027	rBV2	445	468	0.05%	0.006%
79	11.082	3027	3030	3031	rBV	319	179	0.02%	0.002%
80	11.144	3044	3049	3052	rBV3	348	333	0.03%	0.004%
81	11.208	3064	3069	3072	rVB3	229	205	0.02%	0.003%
82	11.349	3109	3113	3117	rBV2	280	280	0.03%	0.003%
83	11.475	3143	3152	3161	rVB5	1024	1923	0.19%	0.024%
84	11.526	3165	3168	3170	rBV2	218	187	0.02%	0.002%
85	11.578	3179	3184	3185	rBV	353	230	0.02%	0.003%
86	11.751	3229	3238	3246	rBV7	3440	5154	0.51%	0.064%
87	11.816	3246	3258	3276	rBV	500721	799233	79.47%	9.938%
88	11.883	3277	3279	3282	rVB3	576	322	0.03%	0.004%
89	11.970	3304	3306	3309	rBV2	329	221	0.02%	0.003%
90	12.076	3337	3339	3344	rBV3	215	216	0.02%	0.003%
91	12.195	3361	3376	3395	rBV	377868	632131	62.85%	7.860%
92	12.291	3404	3406	3409	rVB3	536	245	0.02%	0.003%
93	12.674	3522	3525	3530	rBV	316	357	0.04%	0.004%
94	12.748	3545	3548	3550	rBV	300	218	0.02%	0.003%
95	12.976	3610	3619	3633	rVB3	8262	13891	1.38%	0.173%
96	13.333	3724	3730	3739	rVB4	1758	2653	0.26%	0.033%
97	13.848	3883	3890	3898	rBV2	1899	2350	0.23%	0.029%
98	14.095	3959	3967	3976	rBV2	2508	4442	0.44%	0.055%
99	14.330	4037	4040	4049	rVB5	1459	2122	0.21%	0.026%
100	14.475	4083	4085	4087	rBV2	383	198	0.02%	0.002%

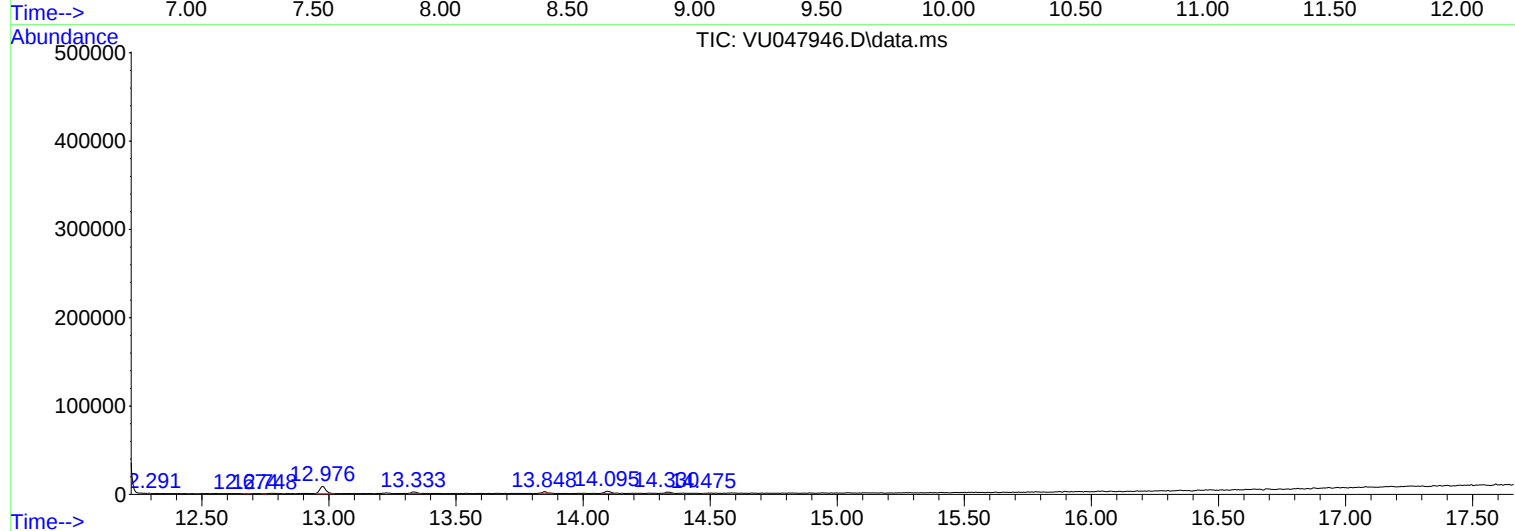
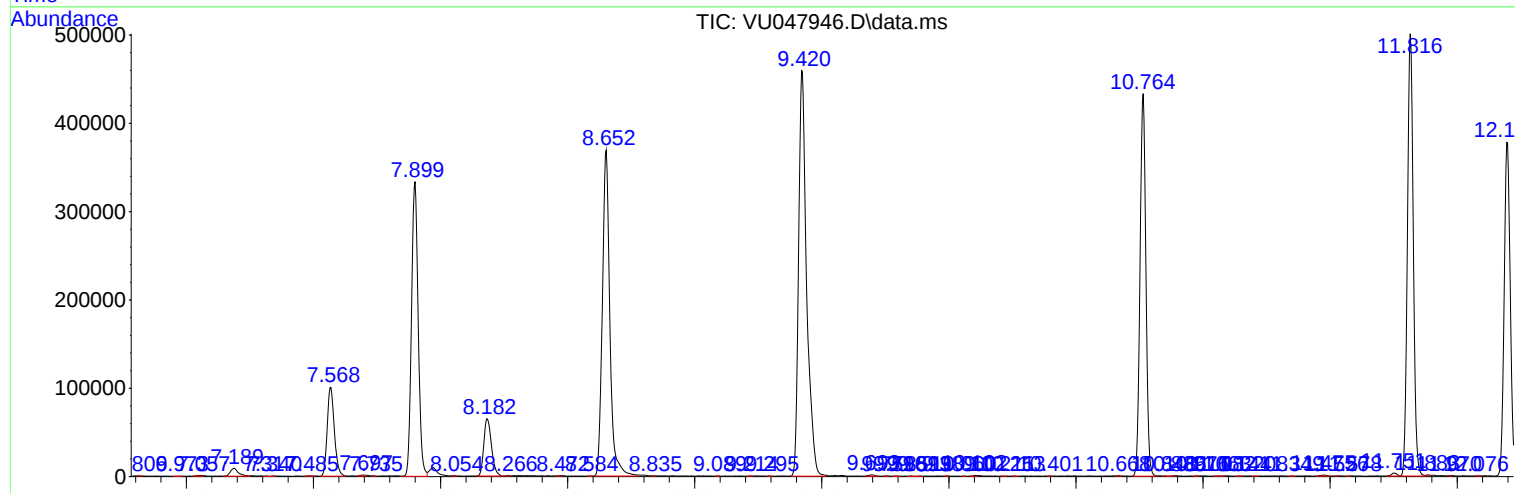
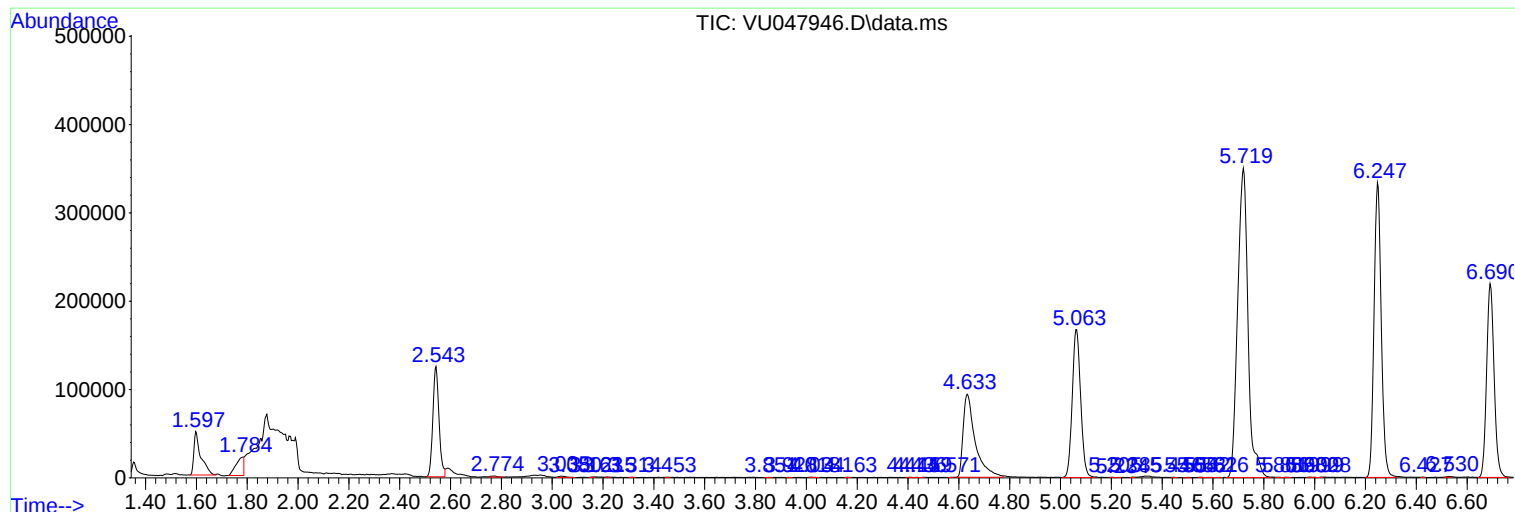
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ALS Vial : 7 Sample Multiplier: 1

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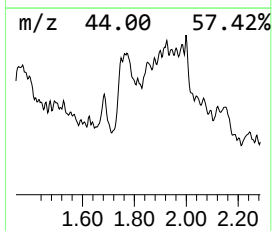
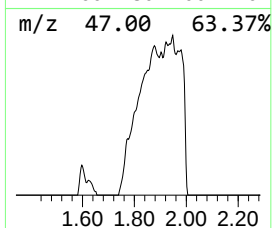
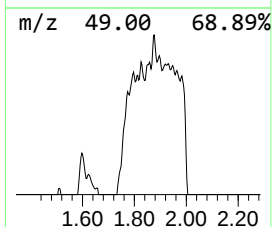
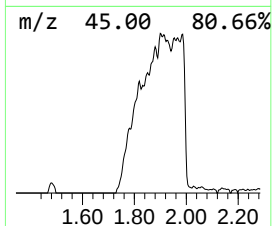
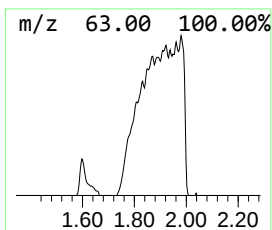
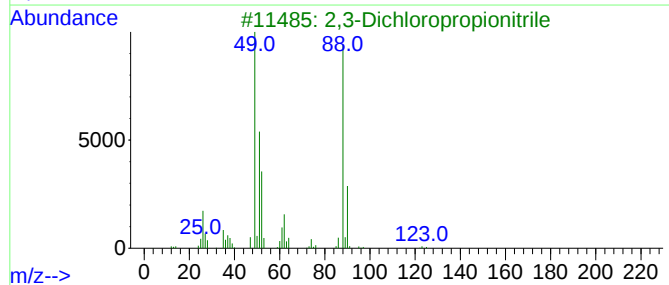
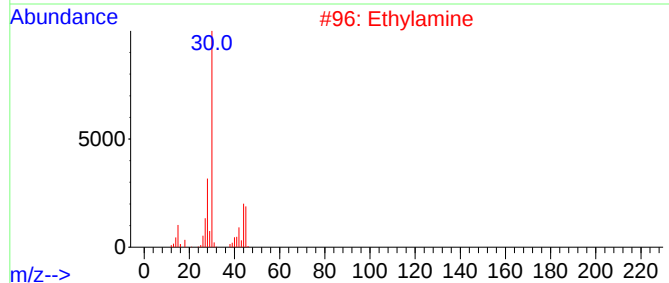
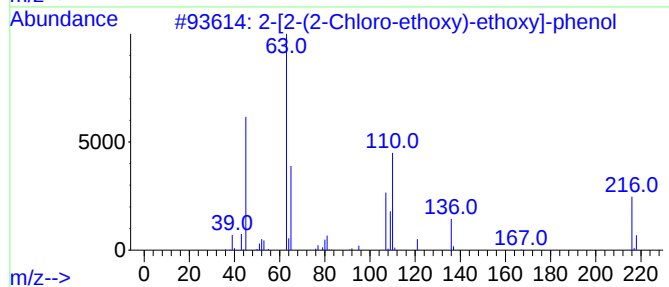
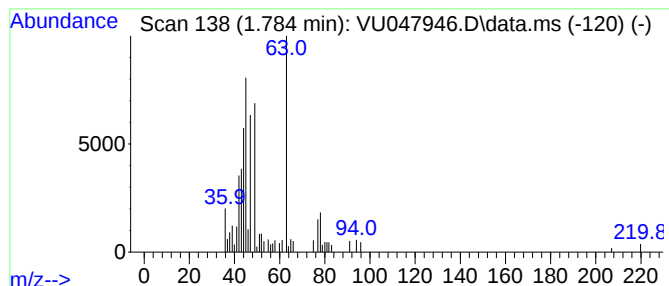
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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.
1.784	3.43 ug/L	45146	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2	-	[2-(2-Chloro-ethoxy)-ethoxy]-p...	216	C10H13ClO3	1000317-46-1	25
2	Ethylamine			45	C2H7N	000075-04-7	9
3	2,3-Dichloropropionitrile			123	C3H3Cl2N	002601-89-0	9
4	Chlorodibromoacetic acid			250	C2HBr2ClO2	005278-95-5	9
5	m-Dioxan-4-ol, 2,6-dimethyl-			132	C6H12O3	004740-77-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.784	3.4	ug/L	45146	1	6.247	657528	50.0