

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
 Data File : VU048311.D
 Acq On : 27 Apr 2022 13:54
 Operator : SY/MD
 Sample : N2562-02ME
 Misc : 7.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW462ME

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\SFAMULM042522WMA.M
 Title : VOC Analysis

Signal : TIC: VU048311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	39	44	50	rBV2	5728	7531	0.35%	0.049%
2	1.597	73	80	115	rVB	116803	320404	15.02%	2.087%
3	1.813	122	147	148	rBV6	26584	72591	3.40%	0.473%
4	2.536	359	372	421	rBV	356268	714112	33.47%	4.652%
5	2.867	472	475	477	rBV	314	212	0.01%	0.001%
6	2.909	485	488	490	rBV2	320	192	0.01%	0.001%
7	2.954	495	502	507	rBV3	1076	1283	0.06%	0.008%
8	3.035	516	527	537	rBV2	9421	20290	0.95%	0.132%
9	3.179	560	572	587	rVB	10919	24443	1.15%	0.159%
10	3.321	613	616	618	rBV2	431	251	0.01%	0.002%
11	3.382	631	635	636	rBV	307	214	0.01%	0.001%
12	3.504	669	673	680	rVB2	441	571	0.03%	0.004%
13	3.539	680	684	688	rVB2	263	270	0.01%	0.002%
14	3.568	688	693	697	rBV	268	328	0.02%	0.002%
15	3.601	700	703	705	rBV	310	190	0.01%	0.001%
16	3.729	738	743	745	rBV	256	241	0.01%	0.002%
17	3.816	767	770	772	rBV	355	234	0.01%	0.002%
18	3.925	801	804	809	rBV	392	344	0.02%	0.002%
19	3.951	810	812	816	rVV2	244	206	0.01%	0.001%
20	3.999	819	827	832	rBV	429	631	0.03%	0.004%
21	4.028	832	836	842	rBV2	196	254	0.01%	0.002%
22	4.154	871	875	878	rBV3	374	301	0.01%	0.002%
23	4.179	878	883	884	rBV2	277	189	0.01%	0.001%
24	4.301	918	921	928	rBV3	340	389	0.02%	0.003%
25	4.636	1010	1025	1048	rBV	147095	509368	23.88%	3.318%
26	4.970	1127	1129	1132	rVB2	462	240	0.01%	0.002%
27	5.063	1139	1158	1186	rBV	344306	829845	38.90%	5.406%
28	5.192	1196	1198	1202	rBV2	381	238	0.01%	0.002%
29	5.285	1220	1227	1232	rBV3	478	651	0.03%	0.004%
30	5.337	1234	1243	1258	rBV3	1978	4251	0.20%	0.028%
31	5.501	1291	1294	1299	rVV2	256	216	0.01%	0.001%
32	5.591	1317	1322	1326	rVB2	261	241	0.01%	0.002%
33	5.617	1326	1330	1336	rBV2	202	279	0.01%	0.002%
34	5.716	1340	1361	1389	rBV2	850055	2133450	100.00%	13.899%
35	5.871	1407	1409	1415	rVB3	385	306	0.01%	0.002%
36	5.973	1430	1441	1471	rVB3	13714	35694	1.67%	0.233%

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 ClientSampleId :
 EW462ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
 Title : VOC Analysis

37	6.102	1476	1481	1484	rBV2	237	267	0.01%	0.002%
38	6.141	1491	1493	1496	rBV2	409	300	0.01%	0.002%
39	6.166	1496	1501	1503	rBV3	706	779	0.04%	0.005%
40	6.247	1511	1526	1558	rBV	403116	831211	38.96%	5.415%
41	6.443	1582	1587	1588	rBV3	273	260	0.01%	0.002%
42	6.526	1600	1613	1621	rBV8	4841	9915	0.46%	0.065%
43	6.597	1626	1635	1648	rVV3	6096	13576	0.64%	0.088%
44	6.690	1648	1664	1691	rVV	452752	954965	44.76%	6.221%
45	6.928	1736	1738	1741	rVV2	345	255	0.01%	0.002%
46	7.054	1770	1777	1778	rBV2	637	627	0.03%	0.004%
47	7.192	1806	1820	1826	rBV2	8196	19320	0.91%	0.126%
48	7.298	1849	1853	1854	rBV2	754	591	0.03%	0.004%
49	7.385	1876	1880	1884	rBV2	212	190	0.01%	0.001%
50	7.430	1889	1894	1900	rBV2	178	262	0.01%	0.002%
51	7.459	1900	1903	1908	rVB2	234	201	0.01%	0.001%
52	7.491	1910	1913	1914	rBV	621	336	0.02%	0.002%
53	7.565	1923	1936	1961	rBV	233295	473728	22.20%	3.086%
54	7.649	1961	1962	1966	rVB3	452	303	0.01%	0.002%
55	7.690	1971	1975	1976	rBV3	532	399	0.02%	0.003%
56	7.787	1997	2005	2021	rVB4	4182	7834	0.37%	0.051%
57	7.896	2025	2039	2057	rBV	965396	1769420	82.94%	11.527%
58	8.182	2114	2128	2154	rBV	147439	323497	15.16%	2.107%
59	8.353	2173	2181	2184	rBV5	1375	1495	0.07%	0.010%
60	8.369	2184	2186	2190	rVB4	413	216	0.01%	0.001%
61	8.472	2211	2218	2220	rBV3	1267	1308	0.06%	0.009%
62	8.555	2240	2244	2246	rBV	359	206	0.01%	0.001%
63	8.658	2257	2276	2315	rBV	534613	1259963	59.06%	8.208%
64	8.903	2350	2352	2354	rBV	310	208	0.01%	0.001%
65	8.925	2357	2359	2360	rBV	446	202	0.01%	0.001%
66	8.954	2365	2368	2372	rVV3	707	527	0.02%	0.003%
67	8.996	2379	2381	2384	rVB2	510	262	0.01%	0.002%
68	9.163	2430	2433	2435	rBV2	278	214	0.01%	0.001%
69	9.195	2440	2443	2452	rVV3	387	497	0.02%	0.003%
70	9.237	2452	2456	2460	rVB2	337	285	0.01%	0.002%
71	9.423	2499	2514	2551	rVB	539948	1092888	51.23%	7.120%
72	9.697	2592	2599	2608	rVB5	928	1658	0.08%	0.011%
73	9.835	2636	2642	2646	rBV2	302	351	0.02%	0.002%
74	10.224	2760	2763	2773	rVB3	332	440	0.02%	0.003%
75	10.394	2812	2816	2820	rVB2	408	223	0.01%	0.001%
76	10.668	2893	2901	2910	rBV4	4231	6235	0.29%	0.041%

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 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW462ME

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\SFAMULM042522WMA.M

Title : VOC Analysis

77	10.764	2915	2931	2951	rBV	764484	1270215	59.54%	8.275%
78	10.893	2962	2971	2980	rVB4	2185	3693	0.17%	0.024%
79	11.115	3033	3040	3048	rBV4	4364	6590	0.31%	0.043%
80	11.369	3116	3119	3126	rBV3	590	613	0.03%	0.004%
81	11.420	3126	3135	3138	rVV3	1080	1385	0.06%	0.009%
82	11.456	3141	3146	3160	rVB5	2973	5267	0.25%	0.034%
83	11.568	3178	3181	3182	rBV	628	295	0.01%	0.002%
84	11.697	3214	3221	3229	rVB6	1353	2220	0.10%	0.014%
85	11.816	3245	3258	3281	rBV	638151	1024484	48.02%	6.674%
86	11.941	3291	3297	3300	rBV6	1423	1843	0.09%	0.012%
87	11.973	3303	3307	3315	rVB3	3218	4113	0.19%	0.027%
88	12.124	3347	3354	3358	rBV4	747	985	0.05%	0.006%
89	12.198	3359	3377	3395	rBV	955405	1556890	72.98%	10.143%
90	12.333	3413	3419	3426	rVB5	3079	4438	0.21%	0.029%
91	12.520	3474	3477	3480	rBV2	458	405	0.02%	0.003%
92	12.632	3508	3512	3515	rBV4	589	561	0.03%	0.004%
93	12.771	3551	3555	3566	rVB4	1771	2181	0.10%	0.014%
94	12.912	3597	3599	3602	rBV2	447	252	0.01%	0.002%
95	13.144	3667	3671	3680	rBV3	688	1150	0.05%	0.007%
96	13.433	3755	3761	3767	rBV5	1970	2342	0.11%	0.015%
97	13.587	3805	3809	3816	rVB6	1275	1290	0.06%	0.008%
98	13.848	3886	3890	3897	rBV4	714	936	0.04%	0.006%
99	14.192	3994	3997	4000	rVB3	488	297	0.01%	0.002%
100	15.397	4368	4372	4380	rBV7	1448	1734	0.08%	0.011%

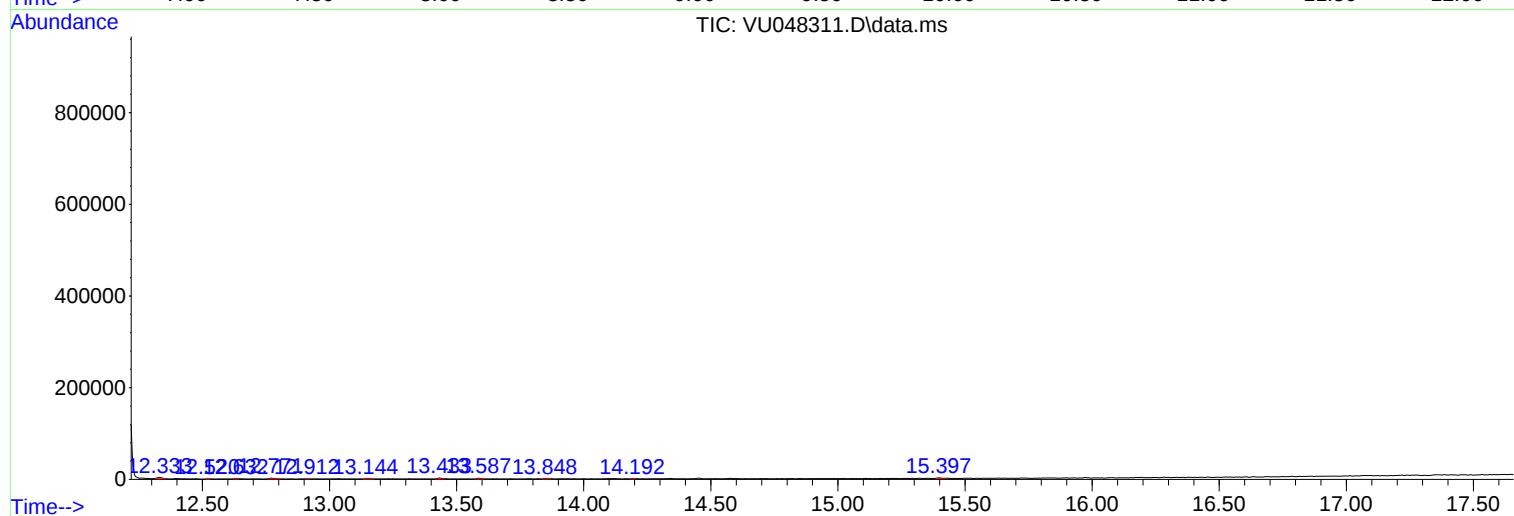
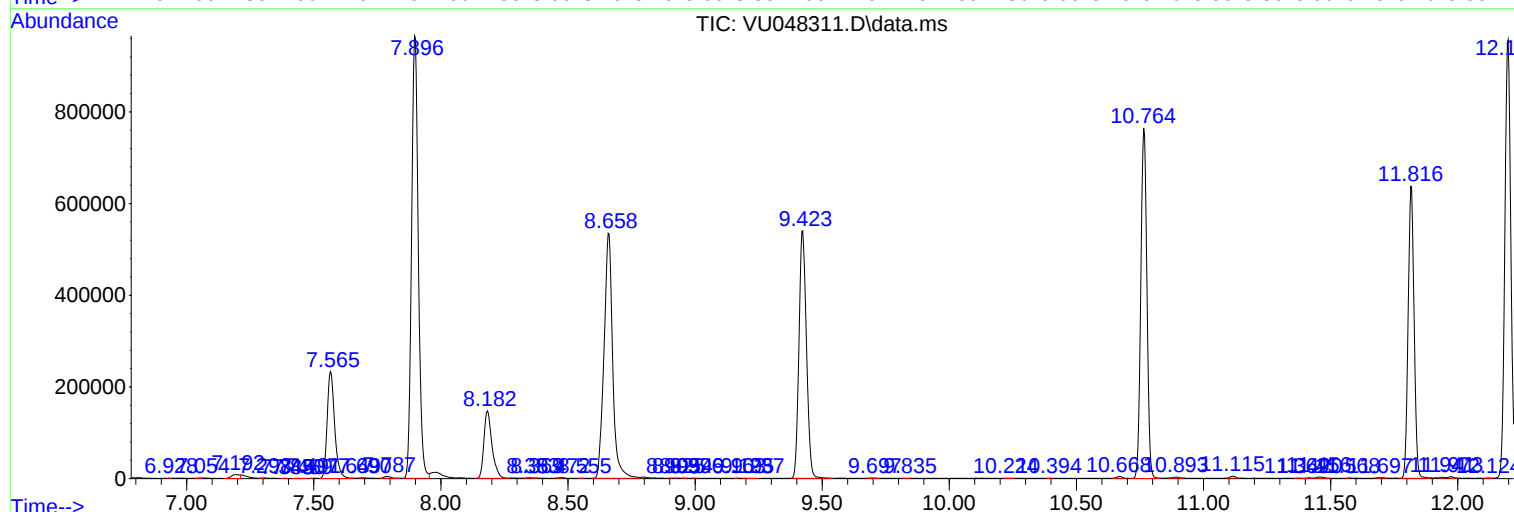
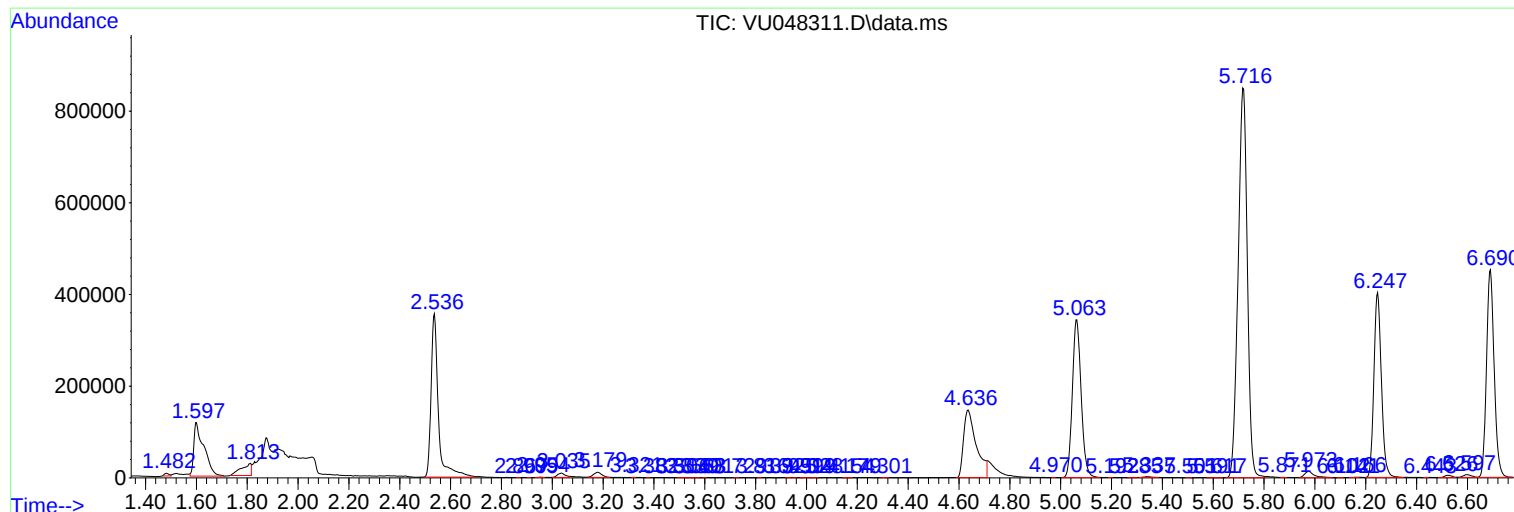
Sum of corrected areas: 15350043

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042722\
Data File : VU048311.D
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW462ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
ClientSampleId :
EW462ME

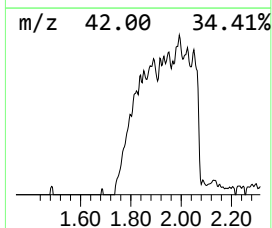
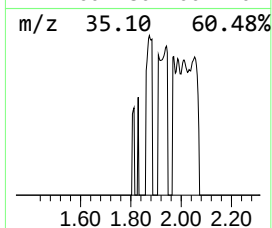
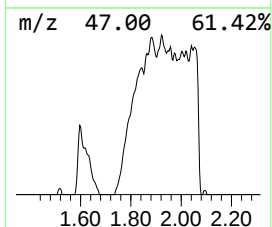
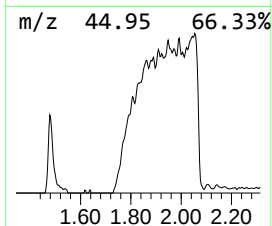
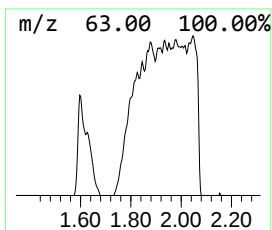
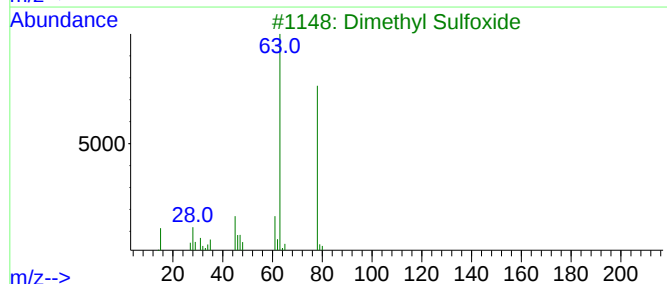
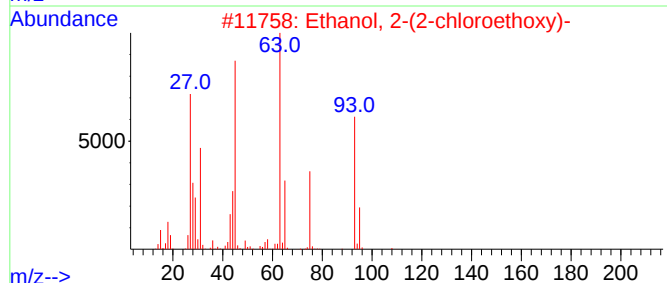
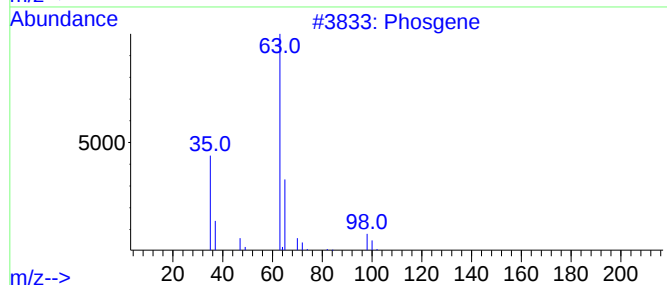
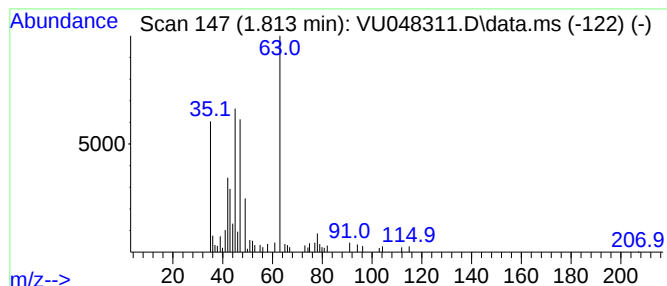
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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.
1.813	4.37 ug/L	72591	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phosgene	98	CCl2O	000075-44-5	4
2			Ethanol, 2-(2-chloroethoxy)-	124	C4H9ClO2	000628-89-7	4
3			Dimethyl Sulfoxide	78	C2H6OS	000067-68-5	4
4			Dimethyl Sulfoxide	78	C2H6OS	000067-68-5	4
5			Carbonic acid, octyl propyl ester	216	C12H24O3	1000314-53-5	4



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.813	4.4	ug/L	72591	1	6.247	831211	50.0