

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062424\
 Data File : VU059450.D
 Acq On : 24 Jun 2024 15:17
 Operator : MD/SY
 Sample : P2964-02ME
 Misc : 3.17g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4B49ME

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\SFAMULM052924WMA.M

Title : VOC Analysis

Signal : TIC: VU059450.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	86	94	116	rVB	30825	49703	7.63%	1.002%
2	1.817	136	164	165	rBV6	38448	120933	18.57%	2.439%
3	2.538	377	388	403	rVB	78281	124979	19.20%	2.520%
4	2.634	409	418	433	rVB4	2812	5701	0.88%	0.115%
5	2.946	506	515	531	rVB	16499	30497	4.68%	0.615%
6	3.026	533	540	549	rVV3	2384	3849	0.59%	0.078%
7	3.107	562	565	570	rVB2	557	385	0.06%	0.008%
8	3.174	570	586	602	rBV2	9955	25824	3.97%	0.521%
9	3.322	630	632	637	rVB2	240	206	0.03%	0.004%
10	3.570	706	709	710	rBV	337	173	0.03%	0.003%
11	3.666	736	739	740	rBV2	356	229	0.04%	0.005%
12	3.676	740	742	746	rVB2	623	439	0.07%	0.009%
13	3.695	746	748	749	rBV	185	58	0.01%	0.001%
14	3.795	776	779	782	rBV	266	233	0.04%	0.005%
15	4.329	943	945	950	rBV	166	141	0.02%	0.003%
16	4.464	984	987	991	rBV2	134	103	0.02%	0.002%
17	4.563	1017	1018	1019	rBV	141	36	0.01%	0.001%
18	4.621	1027	1036	1068	rBV	55664	164743	25.30%	3.322%
19	4.994	1150	1152	1155	rBV2	227	135	0.02%	0.003%
20	5.052	1155	1170	1193	rBV	95662	214186	32.90%	4.319%
21	5.152	1199	1201	1202	rBV	147	41	0.01%	0.001%
22	5.206	1214	1218	1220	rBV2	196	160	0.02%	0.003%
23	5.235	1224	1227	1230	rBV	317	213	0.03%	0.004%
24	5.557	1325	1327	1333	rVB2	434	497	0.08%	0.010%
25	5.611	1333	1344	1346	rBV2	451	902	0.14%	0.018%
26	5.711	1357	1375	1399	rBV2	187496	504690	77.52%	10.178%
27	5.904	1433	1435	1440	rBV2	271	162	0.02%	0.003%
28	5.939	1444	1446	1449	rVB	179	78	0.01%	0.002%
29	5.978	1451	1458	1459	rBV3	834	965	0.15%	0.019%
30	6.084	1486	1491	1497	rBV	289	425	0.07%	0.009%
31	6.129	1503	1505	1506	rVB	164	43	0.01%	0.001%
32	6.142	1506	1509	1513	rBV2	144	137	0.02%	0.003%
33	6.238	1526	1539	1563	rBV	255083	494372	75.93%	9.970%
34	6.525	1619	1628	1639	rVB4	3343	6529	1.00%	0.132%
35	6.566	1639	1641	1644	rBV2	145	103	0.02%	0.002%
36	6.599	1644	1651	1657	rBV3	1425	2258	0.35%	0.046%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

37	6.682	1664	1677	1701	rBV	120638	238792	36.68%	4.815%
38	6.930	1752	1754	1756	rBV	173	88	0.01%	0.002%
39	7.197	1828	1837	1842	rBV6	2028	3307	0.51%	0.067%
40	7.335	1877	1880	1888	rVB	239	243	0.04%	0.005%
41	7.367	1888	1890	1892	rBV	196	89	0.01%	0.002%
42	7.560	1939	1950	1969	rBV2	56900	103589	15.91%	2.089%
43	7.711	1988	1997	2000	rBV4	1262	1725	0.26%	0.035%
44	7.756	2009	2011	2013	rBV	212	110	0.02%	0.002%
45	7.808	2024	2027	2032	rVB2	250	214	0.03%	0.004%
46	7.891	2041	2053	2073	rBV	196292	347344	53.35%	7.005%
47	8.177	2131	2142	2162	rBV3	39063	71621	11.00%	1.444%
48	8.457	2226	2229	2230	rBV	369	157	0.02%	0.003%
49	8.534	2249	2253	2254	rBV	263	194	0.03%	0.004%
50	8.637	2273	2285	2315	rBV	159504	351160	53.94%	7.082%
51	8.814	2337	2340	2348	rVB3	460	420	0.06%	0.008%
52	8.933	2374	2377	2379	rBV2	271	170	0.03%	0.003%
53	9.010	2398	2401	2405	rVB3	311	193	0.03%	0.004%
54	9.062	2413	2417	2423	rBV	279	361	0.06%	0.007%
55	9.412	2514	2526	2556	rBV	372178	651061	100.00%	13.129%
56	9.566	2572	2574	2582	rBV2	762	839	0.13%	0.017%
57	9.640	2596	2597	2602	rVB2	342	140	0.02%	0.003%
58	9.695	2605	2614	2629	rVV3	7363	13075	2.01%	0.264%
59	10.103	2736	2741	2751	rVB4	1131	1488	0.23%	0.030%
60	10.476	2850	2857	2861	rBV3	947	1122	0.17%	0.023%
61	10.753	2931	2943	2966	rBV	231074	383424	58.89%	7.732%
62	10.869	2976	2979	2980	rBV	292	149	0.02%	0.003%
63	10.933	2994	2999	3000	rBV2	465	335	0.05%	0.007%
64	11.753	3249	3254	3257	rBV2	400	439	0.07%	0.009%
65	11.807	3259	3271	3293	rVV	382410	620954	95.38%	12.522%
66	11.959	3314	3318	3321	rBV	636	451	0.07%	0.009%
67	12.094	3356	3360	3363	rBV2	327	294	0.05%	0.006%
68	12.190	3378	3390	3416	rBV	245396	399368	61.34%	8.054%
69	12.595	3513	3516	3520	rBV3	317	227	0.03%	0.005%
70	12.762	3566	3568	3571	rBV	363	183	0.03%	0.004%
71	12.923	3609	3618	3639	rVB5	3136	6465	0.99%	0.130%
72	13.241	3714	3717	3719	rBV	270	129	0.02%	0.003%
73	13.624	3828	3836	3839	rBV3	1202	1382	0.21%	0.028%
74	13.659	3844	3847	3849	rBV	389	207	0.03%	0.004%
75	14.084	3976	3979	3983	rBV2	390	289	0.04%	0.006%
76	14.103	3983	3985	3986	rBV2	390	196	0.03%	0.004%

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Integrator: RTE

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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\SFAMULM052924WMA.M

Title : VOC Analysis

77	14.190	4009	4012	4015	rBV2	357	223	0.03%	0.004%
78	14.540	4118	4121	4123	rBV	318	208	0.03%	0.004%
79	14.971	4249	4255	4262	rBV7	1395	2277	0.35%	0.046%

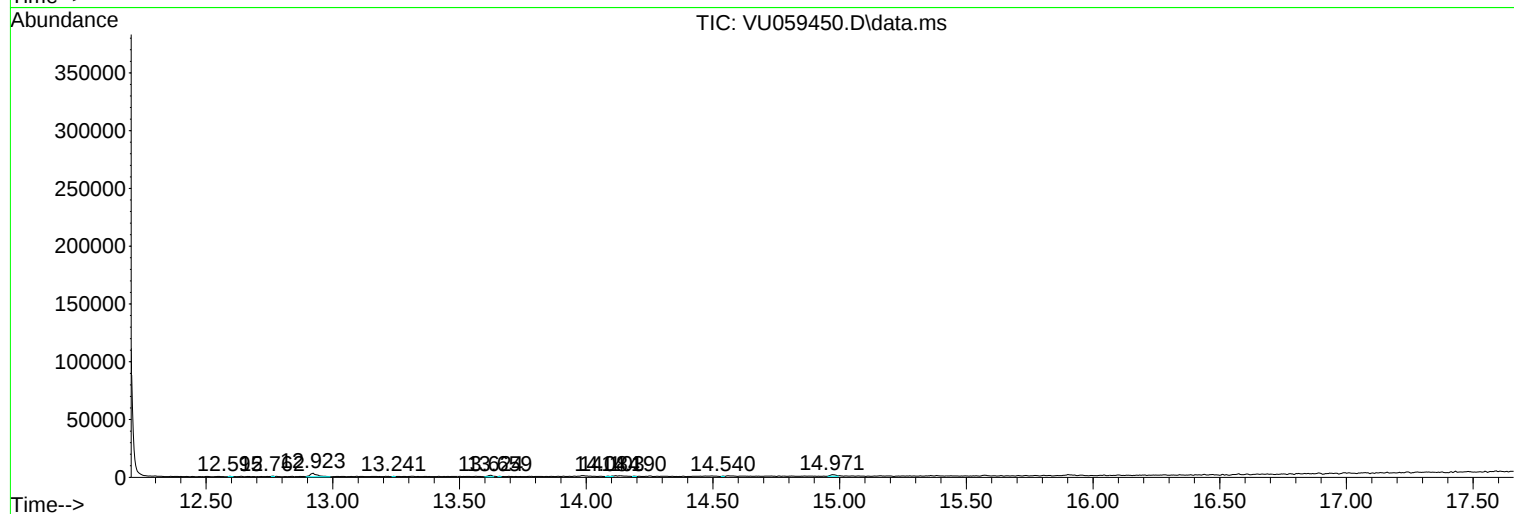
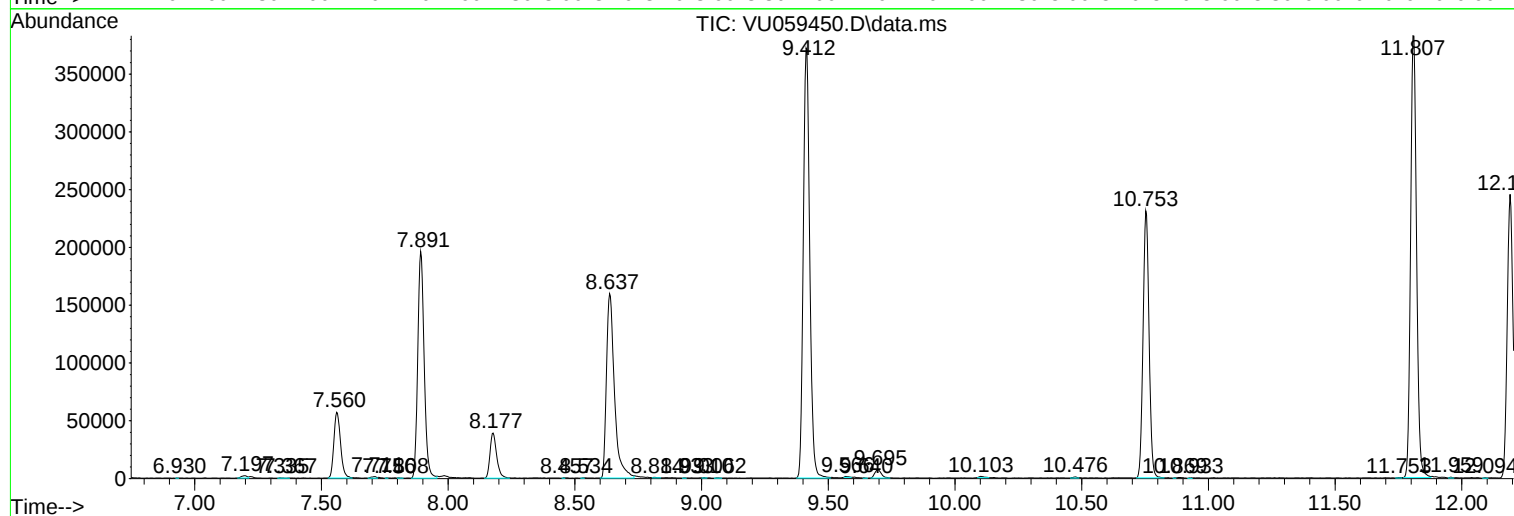
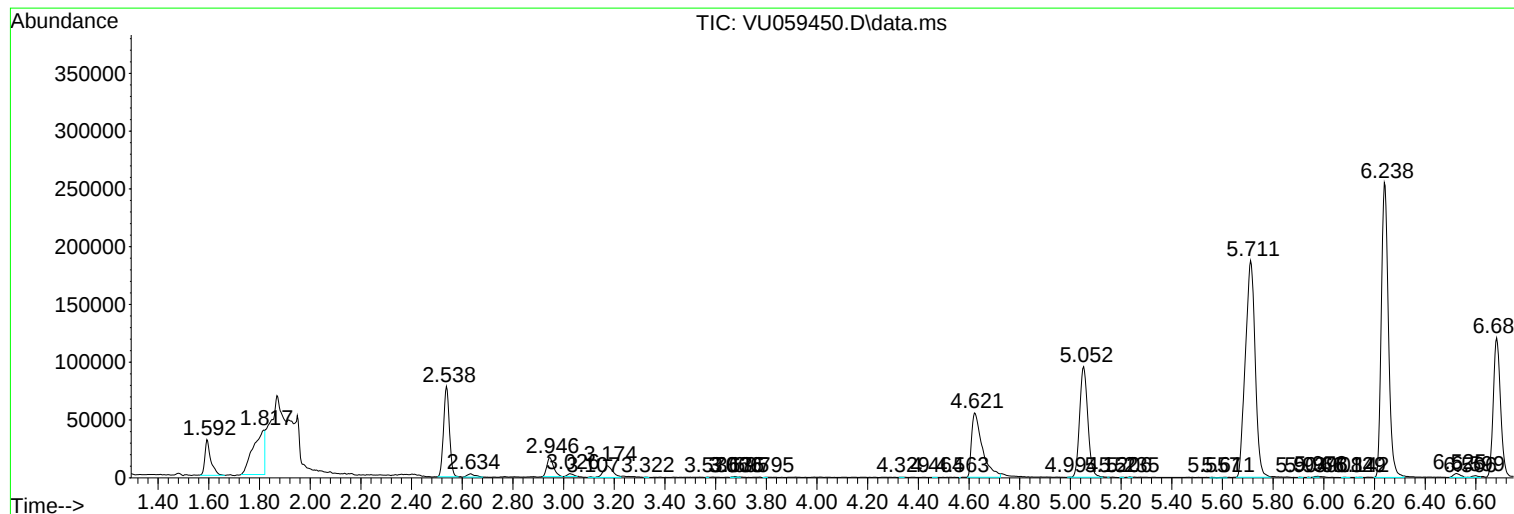
Sum of corrected areas: 4958830

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Instrument :
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ClientSampleId :
A4B49ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4B49ME

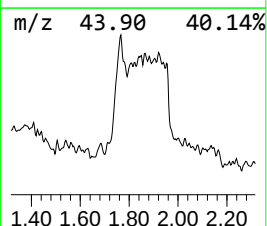
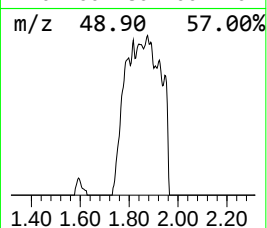
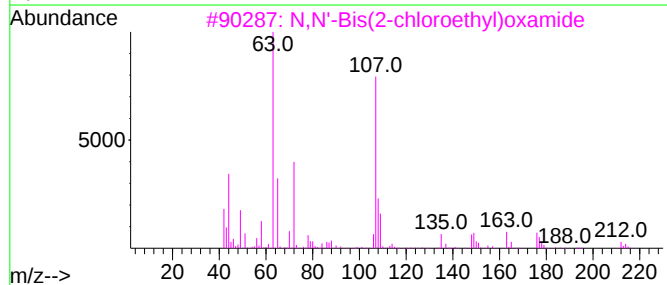
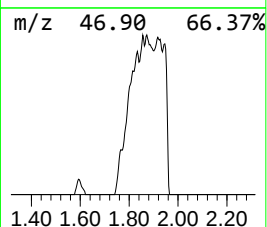
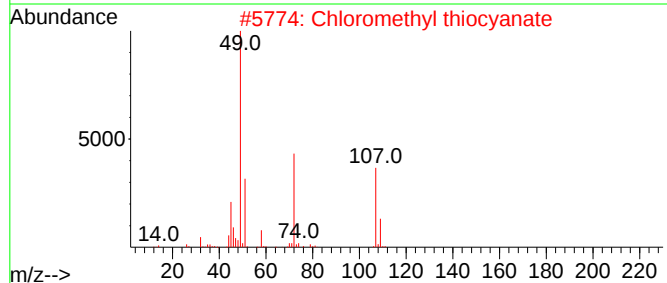
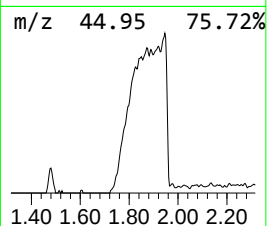
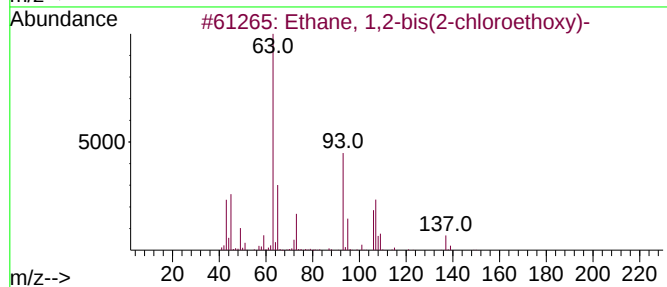
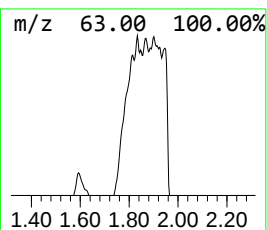
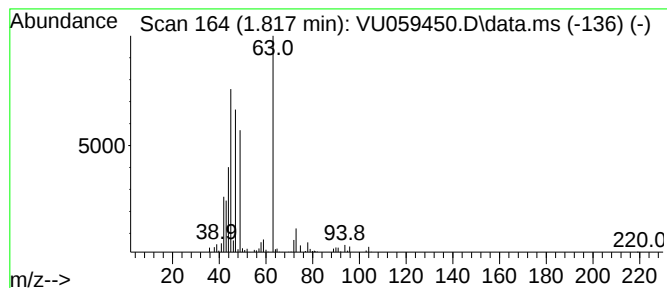
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.817	12.23 ug/L	120933	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,2-bis(2-chloroethoxy)-	186	C6H12Cl2O2	000112-26-5	23
2			Chloromethyl thiocyanate	107	C2H2ClNS	003268-79-9	9
3			N,N'-Bis(2-chloroethyl)oxamide	212	C6H10Cl2N2O2	016813-43-7	9
4			Bis(2-chloroethyl) sulfone	190	C4H8Cl2O2S	000471-03-4	9
5			Bis(2-(2-chloroethoxy)ethyl) ether	230	C8H16Cl2O3	000638-56-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.817	12.2	ug/L	120933	1	6.242	494372	50.0