

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
 Data File : VU059263.D
 Acq On : 14 Jun 2024 21:12
 Operator : MD/SY
 Sample : P2798-06ME
 Misc : 4.63g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB17ME

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: VU059263.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.483	56	60	65	rVB3	2269	1993	0.29%	0.039%
2	1.592	87	94	114	rVB	22407	36928	5.35%	0.729%
3	1.824	135	166	167	rBV4	49830	165851	24.01%	3.272%
4	2.541	378	389	406	rVB	58417	95192	13.78%	1.878%
5	2.631	413	417	422	rVB3	966	989	0.14%	0.020%
6	2.730	442	448	451	rBV2	432	350	0.05%	0.007%
7	2.763	452	458	459	rBV2	772	593	0.09%	0.012%
8	2.891	493	498	501	rBV3	964	1025	0.15%	0.020%
9	3.029	530	541	556	rBV3	5203	10808	1.56%	0.213%
10	3.171	571	585	605	rBV2	9947	26871	3.89%	0.530%
11	3.348	635	640	644	rBV3	520	445	0.06%	0.009%
12	3.644	726	732	735	rBV2	261	282	0.04%	0.006%
13	3.669	738	740	744	rVV2	291	181	0.03%	0.004%
14	3.750	762	765	771	rVB	165	179	0.03%	0.004%
15	3.878	798	805	808	rBV2	250	259	0.04%	0.005%
16	4.377	956	960	964	rBV2	233	202	0.03%	0.004%
17	4.647	1025	1044	1068	rBV3	98022	357812	51.81%	7.059%
18	4.859	1106	1110	1113	rVB2	324	263	0.04%	0.005%
19	5.052	1155	1170	1193	rBV	86080	192587	27.88%	3.800%
20	5.312	1249	1251	1256	rVB2	308	209	0.03%	0.004%
21	5.338	1256	1259	1262	rBV	258	181	0.03%	0.004%
22	5.531	1313	1319	1321	rBV2	235	210	0.03%	0.004%
23	5.711	1354	1375	1399	rBV2	152873	420639	60.90%	8.299%
24	5.872	1422	1425	1430	rVB3	250	230	0.03%	0.005%
25	5.904	1430	1435	1438	rBV2	278	220	0.03%	0.004%
26	5.975	1451	1457	1467	rVV3	725	1366	0.20%	0.027%
27	6.242	1526	1540	1561	rBV	270883	527895	76.43%	10.415%
28	6.534	1617	1631	1643	rBV6	10168	20714	3.00%	0.409%
29	6.589	1645	1648	1649	rBV2	569	347	0.05%	0.007%
30	6.682	1664	1677	1696	rBV2	107604	216833	31.39%	4.278%
31	6.849	1723	1729	1733	rVB2	192	213	0.03%	0.004%
32	7.097	1802	1806	1813	rVB2	282	281	0.04%	0.006%
33	7.168	1825	1828	1830	rBV2	242	184	0.03%	0.004%
34	7.203	1830	1839	1843	rBV3	951	1363	0.20%	0.027%
35	7.222	1843	1845	1852	rVB4	816	699	0.10%	0.014%
36	7.422	1901	1907	1910	rBV3	202	198	0.03%	0.004%

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 ClientSampleId :
 BHB17ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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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\SFAMULM052924WMA.M
 Title : VOC Analysis

37	7.483	1923	1926	1936	rVB2	228	317	0.05%	0.006%
38	7.560	1939	1950	1970	rBV	48714	91138	13.20%	1.798%
39	7.708	1992	1996	1999	rBV3	608	563	0.08%	0.011%
40	7.740	2004	2006	2013	rVB2	293	218	0.03%	0.004%
41	7.775	2014	2017	2022	rVB3	372	300	0.04%	0.006%
42	7.804	2023	2026	2030	rVB2	300	253	0.04%	0.005%
43	7.891	2042	2053	2075	rBV	150705	267960	38.80%	5.287%
44	8.049	2098	2102	2105	rBV2	273	213	0.03%	0.004%
45	8.177	2132	2142	2162	rBV3	31863	59865	8.67%	1.181%
46	8.267	2167	2170	2174	rBV2	293	200	0.03%	0.004%
47	8.367	2198	2201	2211	rVB2	238	393	0.06%	0.008%
48	8.434	2216	2222	2226	rBV2	370	534	0.08%	0.011%
49	8.476	2230	2235	2239	rVB3	371	386	0.06%	0.008%
50	8.547	2246	2257	2272	rVB3	39943	68482	9.92%	1.351%
51	8.640	2273	2286	2323	rBV	156273	386200	55.92%	7.619%
52	8.991	2391	2395	2400	rVV3	209	192	0.03%	0.004%
53	9.129	2435	2438	2444	rVB2	389	362	0.05%	0.007%
54	9.174	2444	2452	2455	rBV	283	327	0.05%	0.006%
55	9.216	2463	2465	2469	rBV2	274	225	0.03%	0.004%
56	9.415	2514	2527	2562	rBV	381517	690663	100.00%	13.626%
57	9.573	2572	2576	2585	rVB4	1191	1487	0.22%	0.029%
58	9.659	2601	2603	2606	rVV2	315	198	0.03%	0.004%
59	9.704	2606	2617	2622	rVV3	1141	2061	0.30%	0.041%
60	9.730	2622	2625	2628	rVV2	246	224	0.03%	0.004%
61	9.823	2648	2654	2659	rBV2	174	205	0.03%	0.004%
62	9.865	2659	2667	2669	rBV2	225	302	0.04%	0.006%
63	10.052	2722	2725	2728	rVB2	239	207	0.03%	0.004%
64	10.138	2748	2752	2757	rBV3	307	268	0.04%	0.005%
65	10.167	2757	2761	2764	rVV2	256	184	0.03%	0.004%
66	10.248	2782	2786	2797	rBV5	628	772	0.11%	0.015%
67	10.386	2826	2829	2834	rVB2	298	244	0.04%	0.005%
68	10.437	2838	2845	2848	rBV	275	334	0.05%	0.007%
69	10.457	2848	2851	2854	rVB2	288	181	0.03%	0.004%
70	10.614	2898	2900	2902	rBV2	537	369	0.05%	0.007%
71	10.646	2906	2910	2915	rVB2	620	581	0.08%	0.011%
72	10.675	2915	2919	2921	rBV2	258	215	0.03%	0.004%
73	10.753	2931	2943	2968	rBV	227246	385101	55.76%	7.598%
74	10.881	2980	2983	2984	rBV2	486	279	0.04%	0.006%
75	11.042	3030	3033	3038	rBB2	207	209	0.03%	0.004%
76	11.225	3087	3090	3092	rBV	309	211	0.03%	0.004%

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 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB17ME

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

77	11.415	3139	3149	3153	rBV4	1374	1905	0.28%	0.038%
78	11.730	3244	3247	3251	rBV2	215	217	0.03%	0.004%
79	11.753	3251	3254	3260	rBV2	383	365	0.05%	0.007%
80	11.810	3260	3272	3300	rBV	388546	636091	92.10%	12.549%
81	11.987	3325	3327	3332	rVB2	402	316	0.05%	0.006%
82	12.013	3332	3335	3337	rBV3	390	193	0.03%	0.004%
83	12.064	3349	3351	3355	rBV2	200	181	0.03%	0.004%
84	12.190	3378	3390	3417	rBV	208493	354291	51.30%	6.990%
85	12.312	3426	3428	3431	rVB2	649	362	0.05%	0.007%
86	12.698	3543	3548	3551	rBV	249	264	0.04%	0.005%
87	12.759	3562	3567	3571	rBV3	906	1090	0.16%	0.022%
88	12.936	3619	3622	3627	rVB	290	212	0.03%	0.004%
89	13.055	3656	3659	3663	rBV	311	193	0.03%	0.004%
90	13.659	3845	3847	3851	rVB	335	199	0.03%	0.004%
91	14.097	3974	3983	4002	rBV3	9672	20770	3.01%	0.410%
92	14.280	4038	4040	4044	rVB	276	201	0.03%	0.004%
93	14.495	4103	4107	4109	rBV	386	319	0.05%	0.006%
94	14.572	4123	4131	4137	rVB4	1236	1979	0.29%	0.039%
95	14.605	4137	4141	4144	rVB2	432	318	0.05%	0.006%
96	14.698	4168	4170	4174	rBV3	273	204	0.03%	0.004%
97	14.942	4242	4246	4251	rBV	430	547	0.08%	0.011%
98	14.990	4259	4261	4268	rVB2	385	350	0.05%	0.007%
99	15.064	4279	4284	4285	rBV2	408	368	0.05%	0.007%
100	16.074	4592	4598	4600	rBV4	843	771	0.11%	0.015%

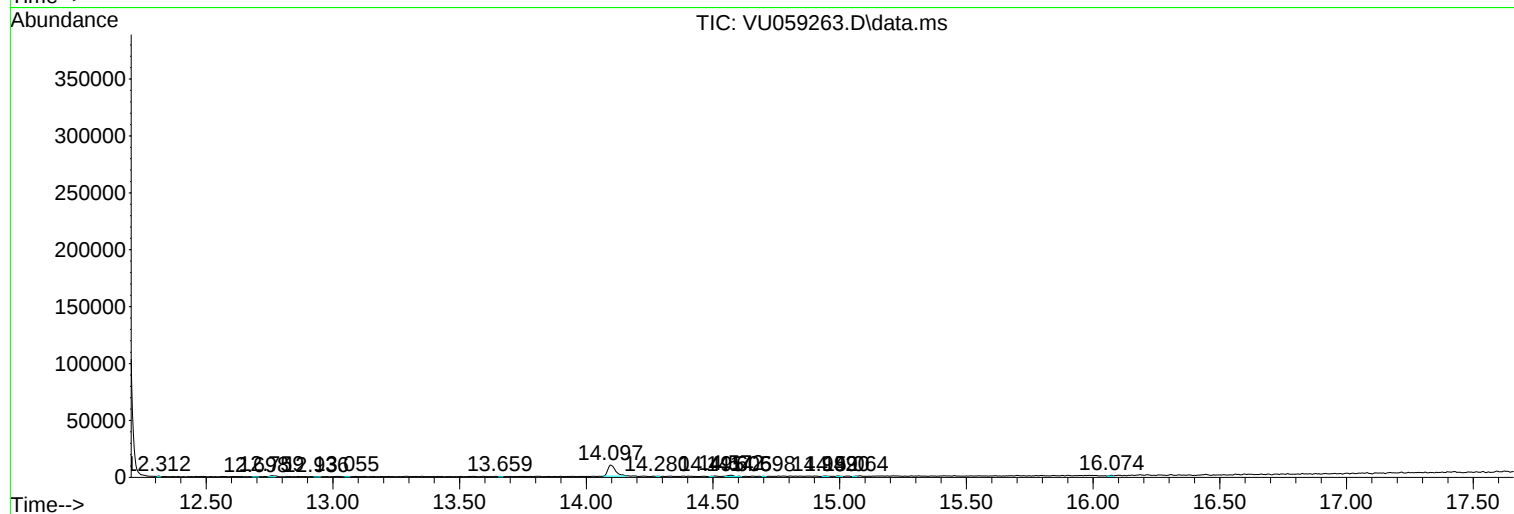
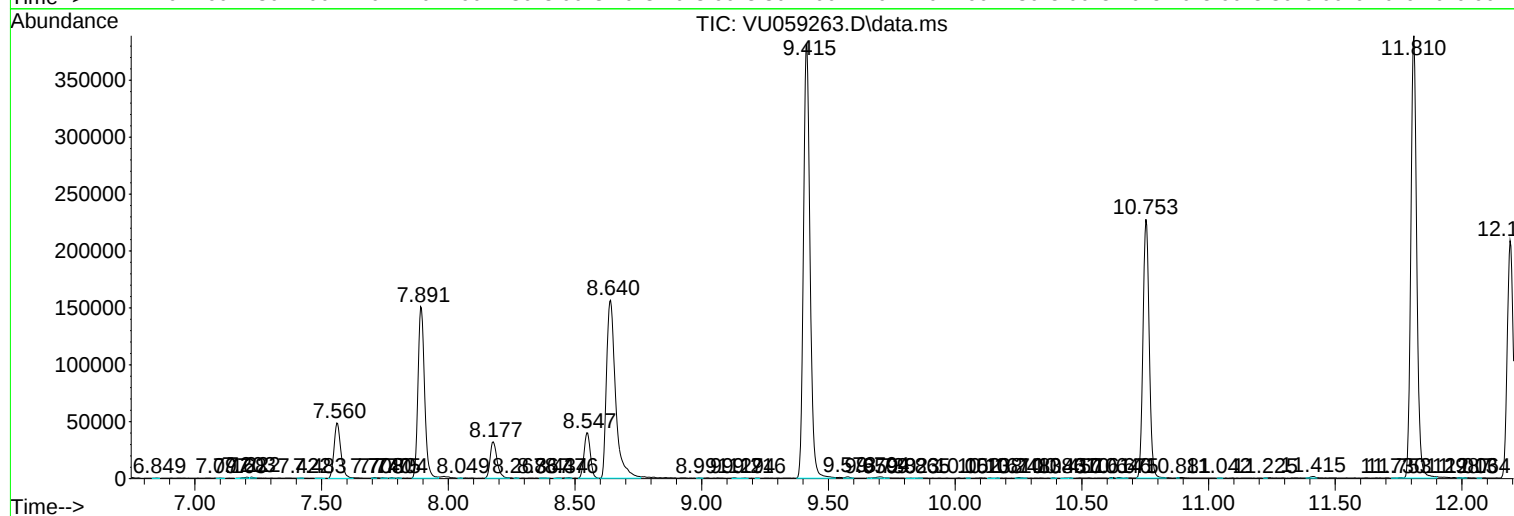
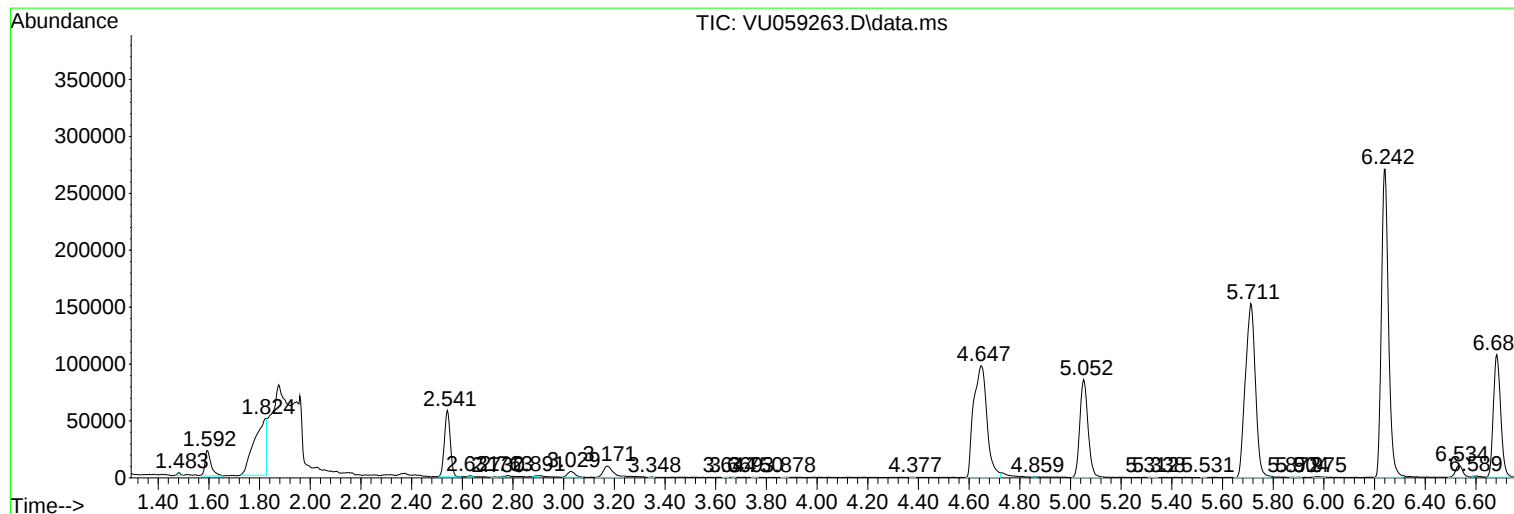
Sum of corrected areas: 5068721

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
Data File : VU059263.D
Acq On : 14 Jun 2024 21:12
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Sample : P2798-06ME
Misc : 4.63g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB17ME

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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Instrument :
MSVOA_U
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BHB17ME

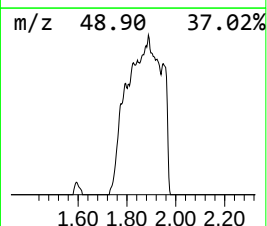
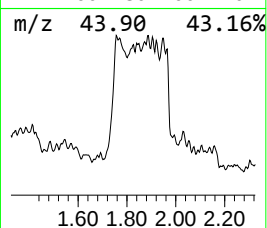
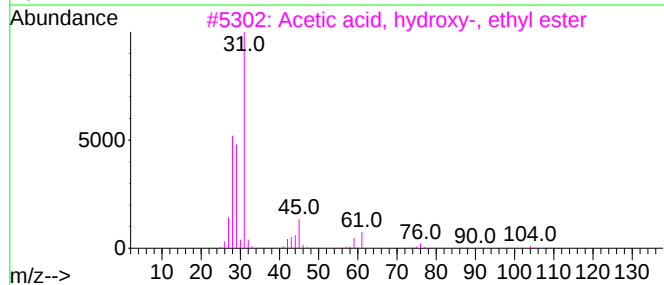
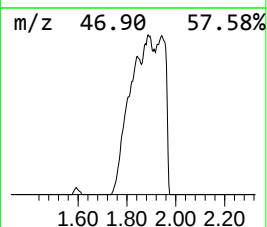
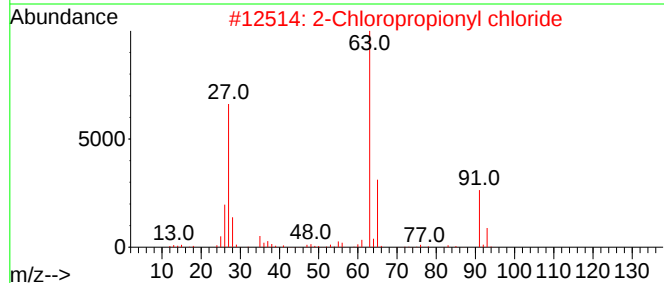
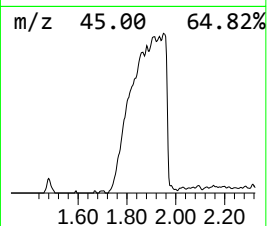
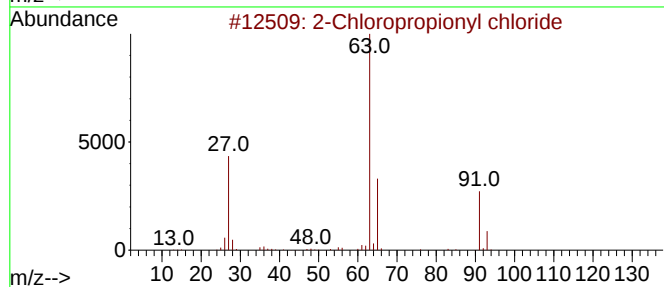
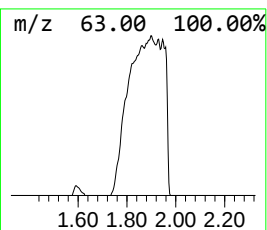
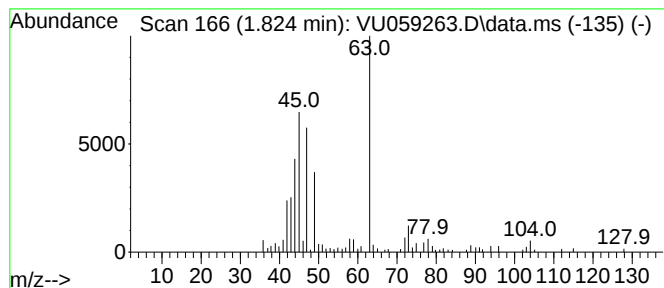
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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.
1.824	15.71 ug/L	165851	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloropropionyl chloride	126	C3H4Cl2O	007623-09-8	25
2			2-Chloropropionyl chloride	126	C3H4Cl2O	007623-09-8	25
3			Acetic acid, hydroxy-, ethyl ester	104	C4H8O3	000623-50-7	9
4			Ethane, 1,2-bis(2-chloroethoxy)-	186	C6H12Cl2O2	000112-26-5	9
5			Phosgene	98	CCl2O	000075-44-5	9



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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	1.824	15.7	ug/L	165851	1	6.242	527895	50.0