

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059306.D
 Acq On : 18 Jun 2024 12:53
 Operator : MD/SY
 Sample : P2798-03ME
 Misc : 5.39g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB14ME

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: VU059306.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	87	94	117	rVB	31135	57452	11.02%	1.421%
2	1.808	139	161	162	rBV3	34816	92172	17.68%	2.279%
3	2.357	329	332	333	rBV3	1303	750	0.14%	0.019%
4	2.534	375	387	404	rVB	88489	143454	27.52%	3.547%
5	2.679	429	432	436	rBV2	324	272	0.05%	0.007%
6	2.753	451	455	459	rBV3	475	453	0.09%	0.011%
7	3.029	528	541	554	rBV2	6719	14100	2.70%	0.349%
8	3.377	645	649	651	rBV	324	261	0.05%	0.006%
9	3.470	673	678	685	rBV	328	451	0.09%	0.011%
10	3.566	702	708	712	rVB2	331	400	0.08%	0.010%
11	3.627	723	727	731	rBV2	254	268	0.05%	0.007%
12	3.840	789	793	797	rVV2	177	207	0.04%	0.005%
13	3.962	829	831	838	rVB	338	279	0.05%	0.007%
14	4.068	859	864	866	rBV2	209	204	0.04%	0.005%
15	4.113	875	878	883	rVV2	207	204	0.04%	0.005%
16	4.338	944	948	951	rBV2	218	202	0.04%	0.005%
17	4.425	971	975	981	rVB	230	230	0.04%	0.006%
18	4.454	981	984	989	rBV2	223	219	0.04%	0.005%
19	4.627	1026	1038	1076	rBV2	39077	142948	27.42%	3.535%
20	4.853	1104	1108	1111	rBV2	333	307	0.06%	0.008%
21	4.901	1120	1123	1129	rVB2	358	332	0.06%	0.008%
22	4.975	1144	1146	1150	rVB2	322	205	0.04%	0.005%
23	5.052	1155	1170	1192	rBV2	79394	180663	34.66%	4.467%
24	5.132	1192	1195	1197	rVB2	356	208	0.04%	0.005%
25	5.174	1203	1208	1211	rBV3	375	293	0.06%	0.007%
26	5.480	1300	1303	1308	rVB2	259	221	0.04%	0.005%
27	5.557	1322	1327	1329	rBV	262	207	0.04%	0.005%
28	5.711	1358	1375	1399	rBV3	169723	447581	85.87%	11.067%
29	5.852	1418	1419	1426	rVB3	294	251	0.05%	0.006%
30	5.923	1437	1441	1446	rVB2	286	340	0.07%	0.008%
31	5.971	1450	1456	1457	rBV4	634	580	0.11%	0.014%
32	6.100	1490	1496	1503	rBV2	319	455	0.09%	0.011%
33	6.242	1527	1540	1564	rBV	205737	403222	77.36%	9.970%
34	6.534	1620	1631	1642	rVB7	4821	9793	1.88%	0.242%
35	6.595	1642	1650	1652	rBV4	1145	1361	0.26%	0.034%
36	6.682	1665	1677	1699	rBV2	101097	201717	38.70%	4.988%

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 ClientSampleId :
 BHB14ME

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	6.894	1740	1743	1748	rVB	307	264	0.05%	0.007%
38	7.164	1821	1827	1830	rBV2	274	337	0.06%	0.008%
39	7.203	1830	1839	1848	rVV5	1254	2298	0.44%	0.057%
40	7.306	1868	1871	1877	rVB2	312	265	0.05%	0.007%
41	7.405	1897	1902	1905	rBV2	198	214	0.04%	0.005%
42	7.563	1939	1951	1972	rBV	49548	90653	17.39%	2.241%
43	7.701	1990	1994	1995	rBV2	673	384	0.07%	0.009%
44	7.759	2009	2012	2015	rBV	269	229	0.04%	0.006%
45	7.891	2041	2053	2074	rBV	193815	340561	65.33%	8.421%
46	8.020	2090	2093	2100	rVB4	524	396	0.08%	0.010%
47	8.097	2114	2117	2121	rBV2	292	269	0.05%	0.007%
48	8.177	2131	2142	2162	rVV2	33757	60314	11.57%	1.491%
49	8.254	2162	2166	2170	rVB3	278	263	0.05%	0.007%
50	8.457	2225	2229	2230	rBV2	410	234	0.04%	0.006%
51	8.505	2241	2244	2250	rBV2	245	341	0.07%	0.008%
52	8.553	2250	2259	2267	rVV2	5125	8343	1.60%	0.206%
53	8.640	2274	2286	2320	rBV	97645	231031	44.32%	5.712%
54	8.907	2364	2369	2375	rBV2	273	300	0.06%	0.007%
55	9.312	2492	2495	2498	rVV2	333	244	0.05%	0.006%
56	9.348	2498	2506	2509	rVV2	140	207	0.04%	0.005%
57	9.415	2515	2527	2553	rBV	297221	521257	100.00%	12.889%
58	9.560	2569	2572	2575	rBV2	263	212	0.04%	0.005%
59	9.576	2575	2577	2586	rVB3	437	522	0.10%	0.013%
60	9.698	2608	2615	2618	rBV3	1060	1234	0.24%	0.031%
61	9.975	2697	2701	2703	rBV2	228	202	0.04%	0.005%
62	10.142	2747	2753	2754	rBV2	227	247	0.05%	0.006%
63	10.473	2852	2856	2858	rBV2	285	211	0.04%	0.005%
64	10.589	2888	2892	2896	rBV	272	246	0.05%	0.006%
65	10.756	2928	2944	2962	rBV	160617	267097	51.24%	6.604%
66	10.830	2962	2967	2975	rVB4	392	432	0.08%	0.011%
67	10.891	2981	2986	2988	rBV2	417	356	0.07%	0.009%
68	10.991	3014	3017	3020	rBV2	243	202	0.04%	0.005%
69	11.171	3070	3073	3080	rBV2	278	433	0.08%	0.011%
70	11.270	3102	3104	3108	rBV2	218	210	0.04%	0.005%
71	11.431	3147	3154	3157	rBV	268	254	0.05%	0.006%
72	11.505	3174	3177	3180	rVV2	280	207	0.04%	0.005%
73	11.547	3184	3190	3194	rBV	248	287	0.06%	0.007%
74	11.704	3236	3239	3243	rBV2	273	265	0.05%	0.007%
75	11.765	3255	3258	3260	rVB2	382	210	0.04%	0.005%
76	11.810	3260	3272	3295	rBV	301229	487431	93.51%	12.052%

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 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB14ME

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	12.010	3330	3334	3337	rBV	449	352	0.07%	0.009%
78	12.145	3371	3376	3379	rBV2	182	212	0.04%	0.005%
79	12.193	3379	3391	3413	rBV	184718	315680	60.56%	7.805%
80	12.669	3537	3539	3544	rBV2	221	206	0.04%	0.005%
81	12.730	3555	3558	3564	rBV2	363	354	0.07%	0.009%
82	12.762	3564	3568	3571	rBV2	499	489	0.09%	0.012%
83	12.884	3604	3606	3608	rBV	371	247	0.05%	0.006%
84	12.929	3617	3620	3624	rBV2	267	247	0.05%	0.006%
85	13.180	3694	3698	3703	rBV2	220	268	0.05%	0.007%
86	13.254	3719	3721	3727	rVB2	321	242	0.05%	0.006%
87	13.508	3796	3800	3806	rBV2	228	322	0.06%	0.008%
88	13.621	3831	3835	3837	rBV	344	287	0.06%	0.007%
89	13.669	3848	3850	3855	rVB	356	280	0.05%	0.007%
90	13.711	3856	3863	3866	rBV2	328	389	0.07%	0.010%
91	13.878	3912	3915	3917	rVB2	474	257	0.05%	0.006%
92	14.080	3974	3978	3983	rBV3	301	262	0.05%	0.006%
93	14.447	4086	4092	4093	rBV2	450	426	0.08%	0.011%
94	14.537	4115	4120	4122	rBV3	408	358	0.07%	0.009%
95	14.566	4126	4129	4130	rBV2	703	435	0.08%	0.011%
96	14.646	4152	4154	4156	rBV2	318	212	0.04%	0.005%
97	14.794	4197	4200	4202	rBV	409	246	0.05%	0.006%
98	14.990	4252	4261	4263	rBV2	441	612	0.12%	0.015%
99	15.125	4299	4303	4309	rBV3	395	573	0.11%	0.014%
100	15.244	4337	4340	4346	rBV3	346	474	0.09%	0.012%

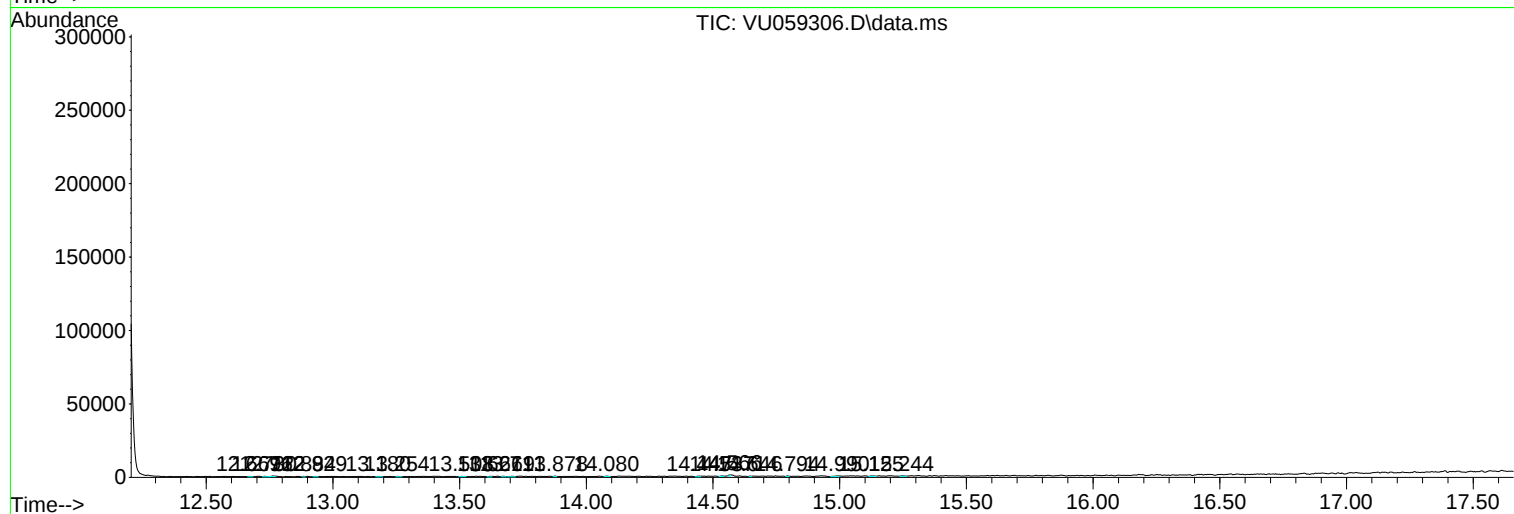
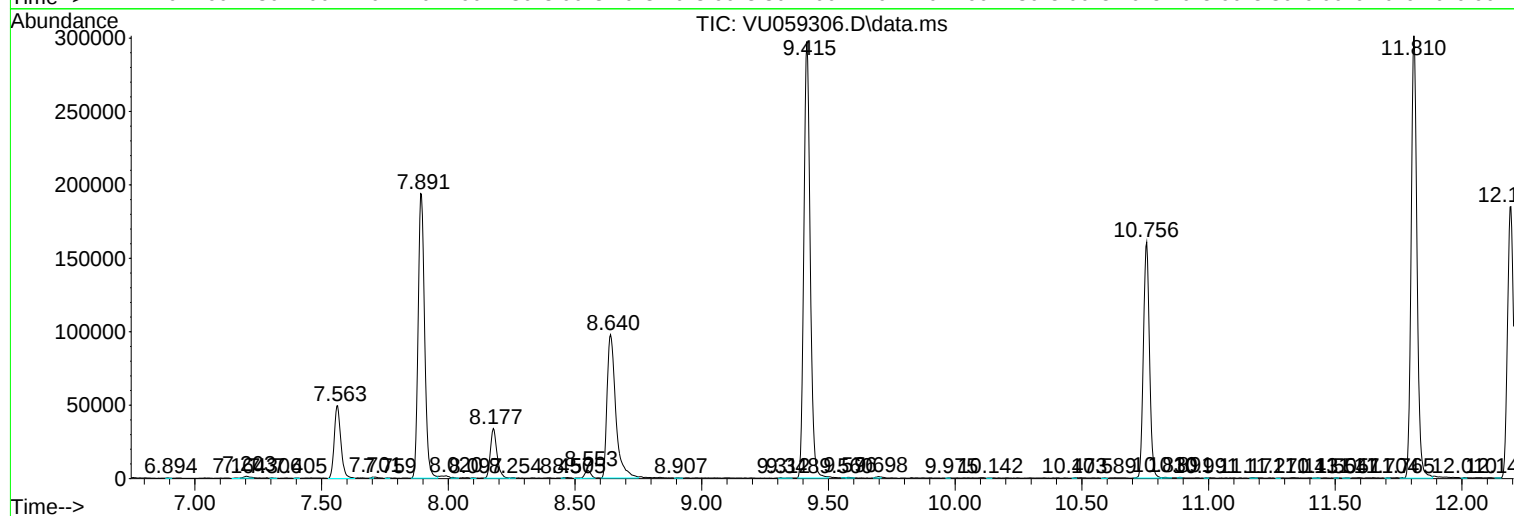
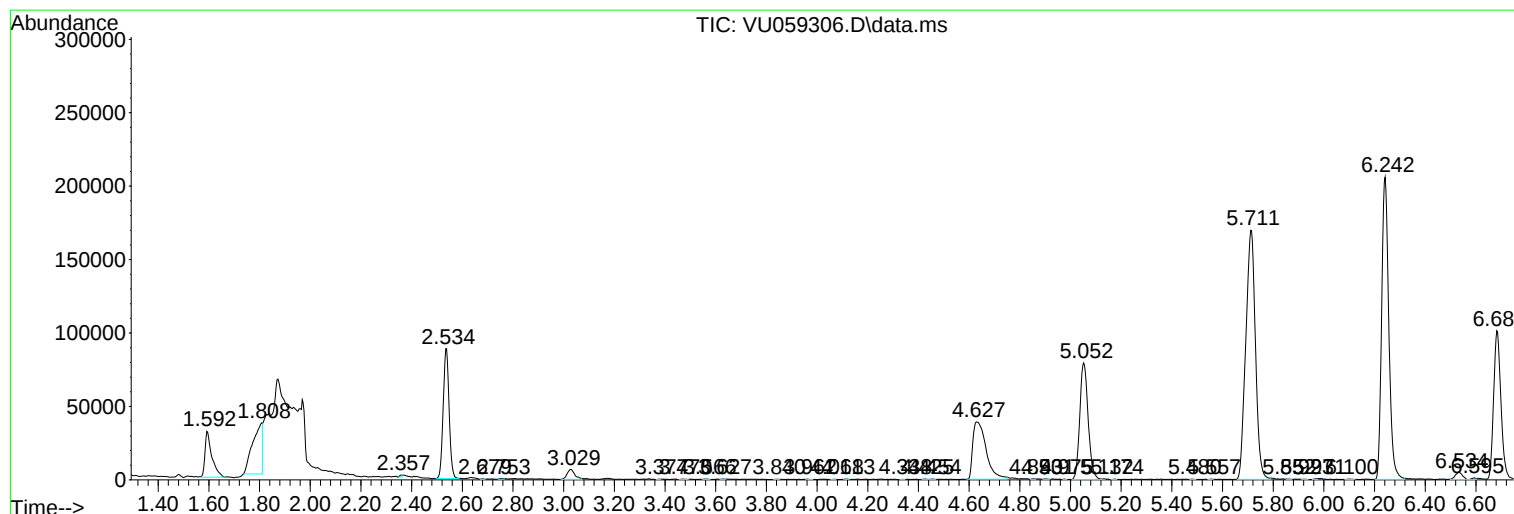
Sum of corrected areas: 4044354

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059306.D
Acq On : 18 Jun 2024 12:53
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Misc : 5.39g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB14ME

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 : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
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BHB14ME

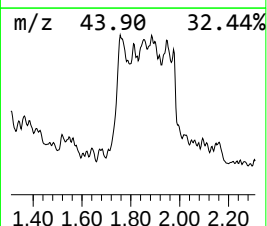
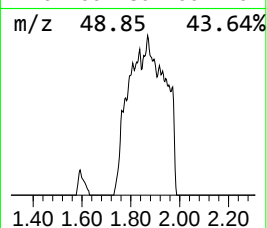
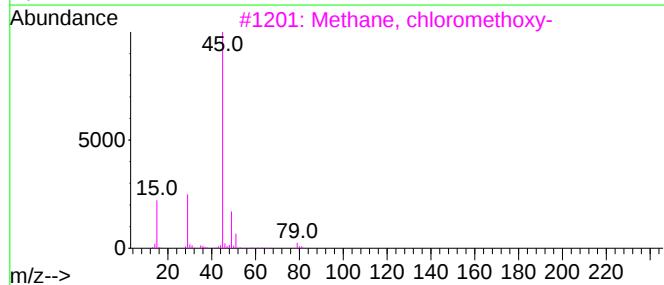
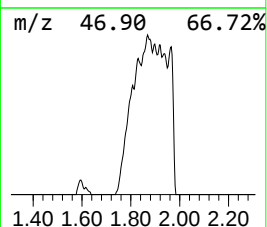
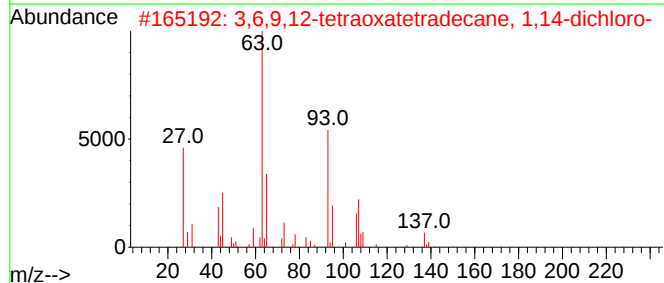
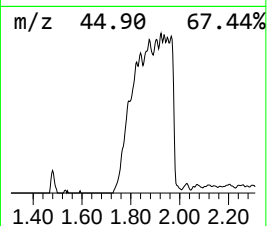
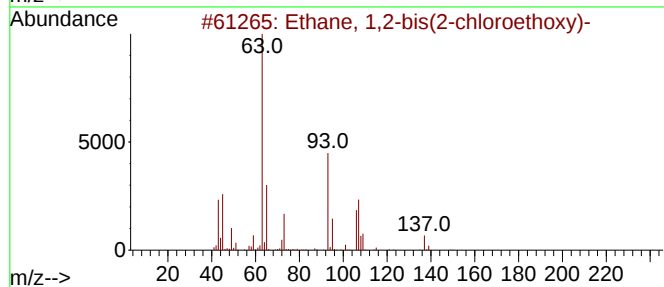
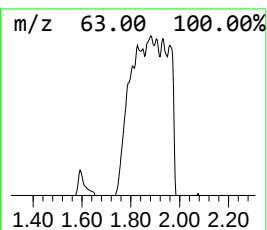
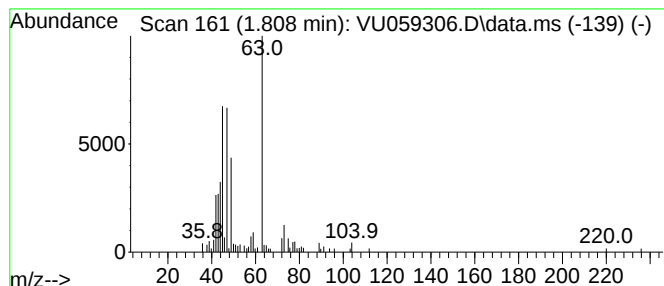
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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.
1.808	11.43 ug/L	92172	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	36
2			3,6,9,12-tetraoxatetradecane, 1,...	274	C10H20Cl2O4	1000401-80-9	25
3			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
4			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
5			2-Propanol, 1-chloro-3-fluoro-	112	C3H6ClFO	189937-18-6	9



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.808	11.4	ug/L	92172	1	6.242	403222	50.0