

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101223\
 Data File : VU055762.D
 Acq On : 12 Oct 2023 13:29
 Operator : MD/SY
 Sample : 04792-09
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VHBLK001

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055762.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	88	96	113	rBV	185818	217744	12.05%	1.573%
2	1.837	141	170	178	rBV9	35134	153035	8.47%	1.106%
3	1.888	179	186	201	rVB	150170	218700	12.10%	1.580%
4	2.509	377	379	382	rVB	649	347	0.02%	0.003%
5	2.560	382	395	414	rBV	321889	529362	29.30%	3.825%
6	2.705	438	440	441	rBV2	698	284	0.02%	0.002%
7	2.737	447	450	452	rBV3	674	325	0.02%	0.002%
8	2.782	459	464	465	rBV	967	635	0.04%	0.005%
9	2.853	482	486	488	rBV2	429	387	0.02%	0.003%
10	2.866	488	490	495	rVB3	425	349	0.02%	0.003%
11	2.943	512	514	518	rVB2	688	361	0.02%	0.003%
12	2.972	518	523	525	rBV3	669	530	0.03%	0.004%
13	3.042	534	545	554	rBV5	4744	8740	0.48%	0.063%
14	3.116	563	568	573	rBV2	409	405	0.02%	0.003%
15	3.174	573	586	599	rBV2	17670	41804	2.31%	0.302%
16	3.274	615	617	622	rVB	622	406	0.02%	0.003%
17	3.348	635	640	647	rVV2	479	598	0.03%	0.004%
18	3.512	686	691	693	rBV2	369	309	0.02%	0.002%
19	3.808	780	783	786	rBV2	427	311	0.02%	0.002%
20	3.843	790	794	795	rBV	424	273	0.02%	0.002%
21	3.914	813	816	820	rBV2	337	295	0.02%	0.002%
22	3.956	825	829	833	rVB2	391	283	0.02%	0.002%
23	3.978	833	836	841	rBV	314	347	0.02%	0.003%
24	4.049	852	858	861	rBV3	425	410	0.02%	0.003%
25	4.113	873	878	881	rBV	336	348	0.02%	0.003%
26	4.190	894	902	904	rBV2	235	303	0.02%	0.002%
27	4.222	910	912	915	rBV2	384	269	0.01%	0.002%
28	4.390	960	964	972	rVB3	312	367	0.02%	0.003%
29	4.570	1012	1020	1023	rBV3	422	558	0.03%	0.004%
30	4.615	1023	1034	1074	rBV	147578	416033	23.03%	3.006%
31	4.904	1120	1124	1125	rBV3	603	462	0.03%	0.003%
32	5.055	1153	1171	1195	rBV	335170	744480	41.20%	5.379%
33	5.319	1248	1253	1254	rBV3	569	463	0.03%	0.003%
34	5.380	1269	1272	1276	rVB2	347	257	0.01%	0.002%
35	5.605	1337	1342	1345	rBV2	397	349	0.02%	0.003%
36	5.718	1356	1377	1404	rBV2	646575	1806865	100.00%	13.056%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

37	5.962	1450	1453	1457	rBV4	789	751	0.04%	0.005%
38	6.091	1490	1493	1497	rBV3	454	425	0.02%	0.003%
39	6.145	1507	1510	1514	rVB2	422	324	0.02%	0.002%
40	6.245	1527	1541	1562	rBV	509263	987560	54.66%	7.136%
41	6.441	1600	1602	1607	rVB4	581	380	0.02%	0.003%
42	6.470	1609	1611	1616	rVB4	433	344	0.02%	0.002%
43	6.528	1616	1629	1641	rBV3	21574	43068	2.38%	0.311%
44	6.685	1663	1678	1704	rBV	422225	833405	46.12%	6.022%
45	6.801	1710	1714	1717	rBV4	1372	1087	0.06%	0.008%
46	6.853	1728	1730	1734	rVB2	444	265	0.01%	0.002%
47	6.972	1764	1767	1771	rBV2	393	350	0.02%	0.003%
48	7.042	1783	1789	1793	rVB2	408	464	0.03%	0.003%
49	7.164	1824	1827	1828	rBV	585	279	0.02%	0.002%
50	7.193	1828	1836	1847	rVV8	3375	6116	0.34%	0.044%
51	7.380	1890	1894	1898	rVB2	398	362	0.02%	0.003%
52	7.560	1936	1950	1986	rBV	222182	407410	22.55%	2.944%
53	7.795	2018	2023	2026	rBV4	463	490	0.03%	0.004%
54	7.894	2040	2054	2082	rBV	753295	1324875	73.32%	9.573%
55	8.110	2118	2121	2125	rVB3	585	438	0.02%	0.003%
56	8.177	2130	2142	2161	rBV	155803	271337	15.02%	1.961%
57	8.270	2169	2171	2176	rVB3	895	769	0.04%	0.006%
58	8.299	2176	2180	2184	rBV4	666	531	0.03%	0.004%
59	8.460	2228	2230	2238	rVB3	429	278	0.02%	0.002%
60	8.550	2251	2258	2269	rVB6	5425	9680	0.54%	0.070%
61	8.634	2269	2284	2321	rBV3	408190	1040057	57.56%	7.515%
62	8.865	2353	2356	2361	rVB6	840	461	0.03%	0.003%
63	8.930	2374	2376	2380	rVB2	475	272	0.02%	0.002%
64	9.341	2502	2504	2512	rVB2	492	606	0.03%	0.004%
65	9.415	2512	2527	2560	rBV	755842	1291650	71.49%	9.333%
66	9.576	2574	2577	2583	rVB4	824	969	0.05%	0.007%
67	9.698	2609	2615	2624	rBV4	1214	1815	0.10%	0.013%
68	9.756	2629	2633	2638	rVB3	417	303	0.02%	0.002%
69	10.074	2729	2732	2735	rBV	333	268	0.01%	0.002%
70	10.100	2737	2740	2744	rBV2	452	348	0.02%	0.003%
71	10.168	2758	2761	2763	rBV	459	252	0.01%	0.002%
72	10.290	2796	2799	2801	rBV2	459	329	0.02%	0.002%
73	10.450	2844	2849	2853	rBV3	387	506	0.03%	0.004%
74	10.753	2930	2943	2965	rBV	653302	1064236	58.90%	7.690%
75	10.933	2991	2999	3005	rVB2	602	1021	0.06%	0.007%
76	10.971	3005	3011	3014	rBV2	427	451	0.02%	0.003%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

77	11.020	3023	3026	3030	rBV2	248	265	0.01%	0.002%
78	11.097	3047	3050	3054	rVB2	509	405	0.02%	0.003%
79	11.293	3108	3111	3119	rVB2	492	475	0.03%	0.003%
80	11.389	3137	3141	3143	rBV	860	667	0.04%	0.005%
81	11.627	3212	3215	3219	rVV2	499	266	0.01%	0.002%
82	11.811	3259	3272	3299	rBV	706134	1158906	64.14%	8.374%
83	11.958	3316	3318	3322	rVB2	859	542	0.03%	0.004%
84	12.052	3342	3347	3350	rBV4	413	423	0.02%	0.003%
85	12.113	3363	3366	3369	rBV2	409	270	0.01%	0.002%
86	12.190	3376	3390	3422	rBV	742050	1229455	68.04%	8.884%
87	12.412	3456	3459	3460	rBV2	555	293	0.02%	0.002%
88	12.698	3546	3548	3552	rBV2	333	263	0.01%	0.002%
89	12.720	3552	3555	3559	rVV3	446	432	0.02%	0.003%
90	12.827	3584	3588	3592	rVB2	715	576	0.03%	0.004%
91	13.074	3662	3665	3669	rBV2	377	398	0.02%	0.003%
92	13.155	3687	3690	3692	rBV2	574	351	0.02%	0.003%
93	13.315	3737	3740	3745	rVB2	902	588	0.03%	0.004%
94	13.338	3745	3747	3751	rBV	339	278	0.02%	0.002%
95	13.409	3765	3769	3772	rBV4	472	390	0.02%	0.003%
96	13.476	3788	3790	3793	rVB3	584	342	0.02%	0.002%
97	13.872	3907	3913	3914	rBV2	1004	950	0.05%	0.007%
98	14.370	4066	4068	4071	rVB2	878	464	0.03%	0.003%
99	14.386	4071	4073	4076	rBV2	716	445	0.02%	0.003%
100	14.521	4113	4115	4119	rBV2	553	324	0.02%	0.002%

Sum of corrected areas: 13839294

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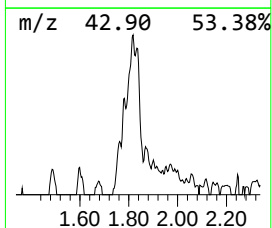
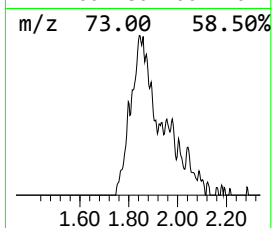
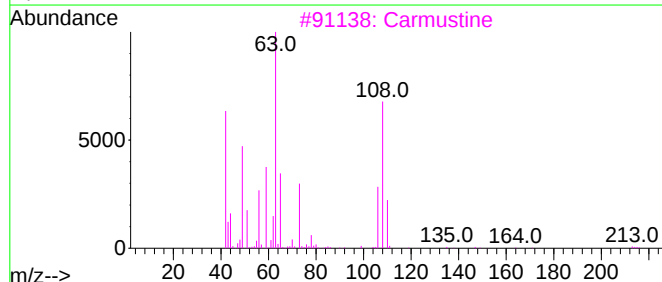
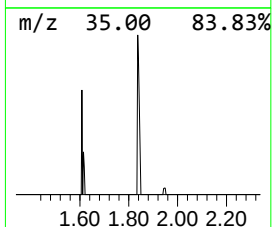
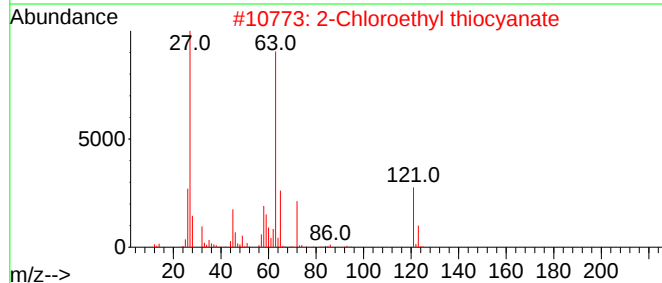
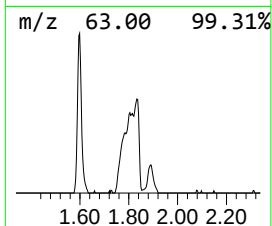
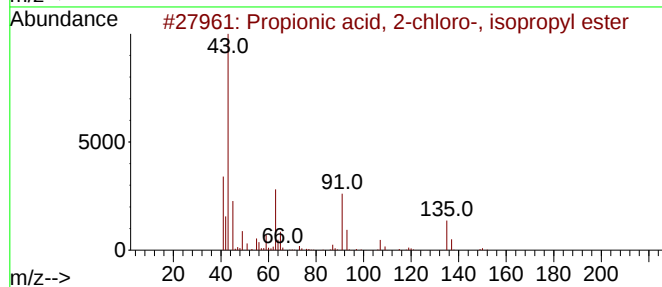
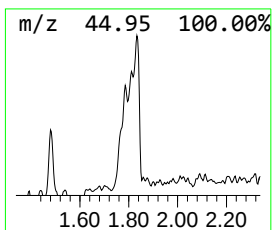
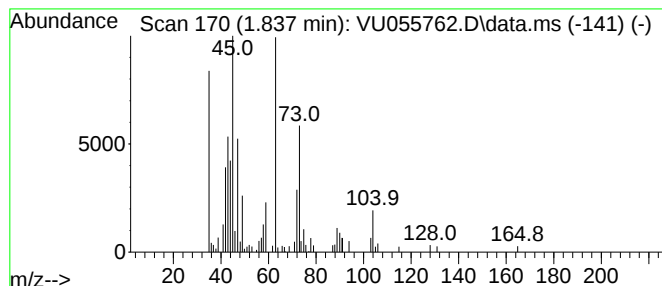
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
1.837	7.75 ug/L	153035	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propionic acid, 2-chloro-, isopr...	150	C6H11ClO2	040058-87-5	40
2			2-Chloroethyl thiocyanate	121	C3H4ClNS	1000342-25-2	12
3			Carmustine	213	C5H9Cl2N3O2	000154-93-8	9
4			ethane-1,2-diyl diethyl dicarbonate	206	C8H14O6	1000456-16-7	9
5			Diethyl pyrocarbonate	162	C6H10O5	001609-47-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.837	7.8	ug/L	153035	1	6.245	987560	50.0