

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090722\
 Data File : VU050666.D
 Acq On : 07 Sep 2022 17:26
 Operator : SY/MD
 Sample : N4372-02RE
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY184RE

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\SFAMULM090222WMA.M

Title : VOC Analysis

Signal : TIC: VU050666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	41	45	52	rVB5	2273	2738	0.28%	0.040%
2	1.597	73	80	100	rBV	66107	85616	8.89%	1.261%
3	1.810	129	146	154	rVB8	11865	24787	2.57%	0.365%
4	1.900	165	174	185	rBV	61833	84428	8.77%	1.244%
5	2.038	213	217	218	rBV	439	308	0.03%	0.005%
6	2.163	254	256	258	rBV	453	282	0.03%	0.004%
7	2.292	284	296	304	rBV3	5153	10512	1.09%	0.155%
8	2.356	314	316	318	rBV2	304	223	0.02%	0.003%
9	2.491	354	358	363	rVB2	448	356	0.04%	0.005%
10	2.562	368	380	394	rBV	140626	230575	23.95%	3.397%
11	2.694	417	421	424	rVB2	345	267	0.03%	0.004%
12	2.758	431	441	464	rBV	6074	14953	1.55%	0.220%
13	3.044	523	530	534	rBV3	598	725	0.08%	0.011%
14	3.118	550	553	559	rVB2	333	355	0.04%	0.005%
15	3.147	559	562	564	rBV2	496	321	0.03%	0.005%
16	3.186	564	574	583	rVV5	2324	5147	0.53%	0.076%
17	3.617	705	708	713	rBV	312	267	0.03%	0.004%
18	3.748	747	749	754	rVV2	203	186	0.02%	0.003%
19	4.086	850	854	856	rBV2	376	314	0.03%	0.005%
20	4.166	876	879	887	rVB2	207	210	0.02%	0.003%
21	4.459	967	970	971	rBV	276	190	0.02%	0.003%
22	4.527	989	991	995	rVB	337	220	0.02%	0.003%
23	4.552	995	999	1001	rBV2	274	219	0.02%	0.003%
24	4.620	1008	1020	1067	rBV	106496	305201	31.70%	4.497%
25	4.826	1082	1084	1088	rVB2	405	209	0.02%	0.003%
26	4.864	1094	1096	1099	rBV3	443	254	0.03%	0.004%
27	5.060	1142	1157	1180	rBV	175523	387352	40.23%	5.707%
28	5.224	1206	1208	1211	rVB2	347	202	0.02%	0.003%
29	5.240	1211	1213	1218	rVB2	487	300	0.03%	0.004%
30	5.276	1221	1224	1227	rBV3	915	801	0.08%	0.012%
31	5.340	1241	1244	1247	rBV	300	202	0.02%	0.003%
32	5.366	1248	1252	1253	rBV	492	318	0.03%	0.005%
33	5.578	1314	1318	1321	rBV	364	355	0.04%	0.005%
34	5.617	1325	1330	1333	rBV2	439	445	0.05%	0.007%
35	5.723	1342	1363	1393	rBV2	340887	962888	100.00%	14.186%
36	6.018	1452	1455	1458	rBV3	206	199	0.02%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
 Title : VOC Analysis

37	6.157	1493	1498	1502	rBV2	310	374	0.04%	0.006%
38	6.247	1513	1526	1548	rBV	242337	475435	49.38%	7.005%
39	6.417	1574	1579	1580	rBV2	424	202	0.02%	0.003%
40	6.475	1592	1597	1599	rBV2	292	299	0.03%	0.004%
41	6.536	1606	1616	1617	rBV3	1761	2115	0.22%	0.031%
42	6.578	1626	1629	1633	rBV4	570	393	0.04%	0.006%
43	6.626	1641	1644	1648	rVB4	351	229	0.02%	0.003%
44	6.690	1648	1664	1684	rBV	232687	452267	46.97%	6.663%
45	6.813	1698	1702	1708	rVB3	855	898	0.09%	0.013%
46	6.848	1711	1713	1719	rVB3	639	483	0.05%	0.007%
47	7.166	1807	1812	1813	rBV	498	306	0.03%	0.005%
48	7.176	1813	1815	1817	rBV2	534	285	0.03%	0.004%
49	7.314	1856	1858	1862	rVV2	318	208	0.02%	0.003%
50	7.475	1903	1908	1913	rBV2	276	307	0.03%	0.005%
51	7.565	1923	1936	1962	rBV	113889	205717	21.36%	3.031%
52	7.655	1962	1964	1970	rVB2	629	417	0.04%	0.006%
53	7.690	1970	1975	1979	rBV4	830	942	0.10%	0.014%
54	7.752	1991	1994	2002	rVB2	558	487	0.05%	0.007%
55	7.896	2025	2039	2066	rBV	370601	657741	68.31%	9.691%
56	8.179	2116	2127	2148	rBV	81900	141065	14.65%	2.078%
57	8.298	2161	2164	2165	rBV2	346	196	0.02%	0.003%
58	8.443	2203	2209	2211	rBV	406	431	0.04%	0.006%
59	8.636	2256	2269	2278	rBV3	190287	411260	42.71%	6.059%
60	8.854	2334	2337	2341	rBV	245	233	0.02%	0.003%
61	8.915	2353	2356	2360	rVB2	315	221	0.02%	0.003%
62	8.954	2365	2368	2372	rVB2	362	212	0.02%	0.003%
63	9.005	2380	2384	2388	rBV2	333	328	0.03%	0.005%
64	9.105	2413	2415	2421	rVB3	342	215	0.02%	0.003%
65	9.356	2490	2493	2497	rBV2	214	190	0.02%	0.003%
66	9.417	2499	2512	2533	rBV	366141	616850	64.06%	9.088%
67	9.694	2594	2598	2606	rVB2	469	524	0.05%	0.008%
68	9.748	2613	2615	2621	rVV2	243	206	0.02%	0.003%
69	9.787	2624	2627	2631	rBV	284	208	0.02%	0.003%
70	10.067	2708	2714	2718	rBV2	268	404	0.04%	0.006%
71	10.105	2722	2726	2732	rVB3	495	459	0.05%	0.007%
72	10.468	2836	2839	2842	rBV	261	190	0.02%	0.003%
73	10.488	2842	2845	2848	rVB2	454	295	0.03%	0.004%
74	10.571	2861	2871	2877	rBV2	332	552	0.06%	0.008%
75	10.755	2915	2928	2952	rBV	385460	625813	64.99%	9.220%
76	11.295	3092	3096	3098	rBV	241	206	0.02%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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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\SFAMULM090222WMA.M
 Title : VOC Analysis

77	11.375	3119	3121	3128	rVB2	287	239	0.02%	0.004%
78	11.411	3128	3132	3135	rBV2	269	225	0.02%	0.003%
79	11.475	3148	3152	3157	rVB2	554	485	0.05%	0.007%
80	11.510	3158	3163	3165	rBV	270	279	0.03%	0.004%
81	11.694	3217	3220	3225	rVB2	257	187	0.02%	0.003%
82	11.748	3234	3237	3241	rBV3	579	424	0.04%	0.006%
83	11.812	3244	3257	3277	rBV	289724	474484	49.28%	6.991%
84	12.063	3331	3335	3338	rBV2	845	704	0.07%	0.010%
85	12.192	3362	3375	3403	rBV	349639	584142	60.67%	8.606%
86	12.636	3510	3513	3519	rBV2	287	334	0.03%	0.005%
87	12.899	3593	3595	3599	rVB2	480	248	0.03%	0.004%
88	12.928	3599	3604	3605	rBV	300	274	0.03%	0.004%
89	13.115	3659	3662	3667	rVB2	452	318	0.03%	0.005%
90	13.365	3737	3740	3744	rVB	409	243	0.03%	0.004%
91	13.491	3776	3779	3783	rBV2	332	276	0.03%	0.004%
92	14.108	3969	3971	3975	rBV2	394	244	0.03%	0.004%
93	14.333	4039	4041	4045	rVB2	505	274	0.03%	0.004%
94	14.436	4071	4073	4076	rBV2	444	208	0.02%	0.003%
95	14.761	4171	4174	4180	rBV5	818	751	0.08%	0.011%
96	14.790	4181	4183	4187	rVB3	646	405	0.04%	0.006%
97	15.102	4275	4280	4282	rBV4	551	553	0.06%	0.008%
98	15.144	4290	4293	4294	rBV	352	205	0.02%	0.003%
99	15.156	4294	4297	4298	rBV	561	308	0.03%	0.005%
100	15.243	4322	4324	4327	rBV4	886	525	0.05%	0.008%

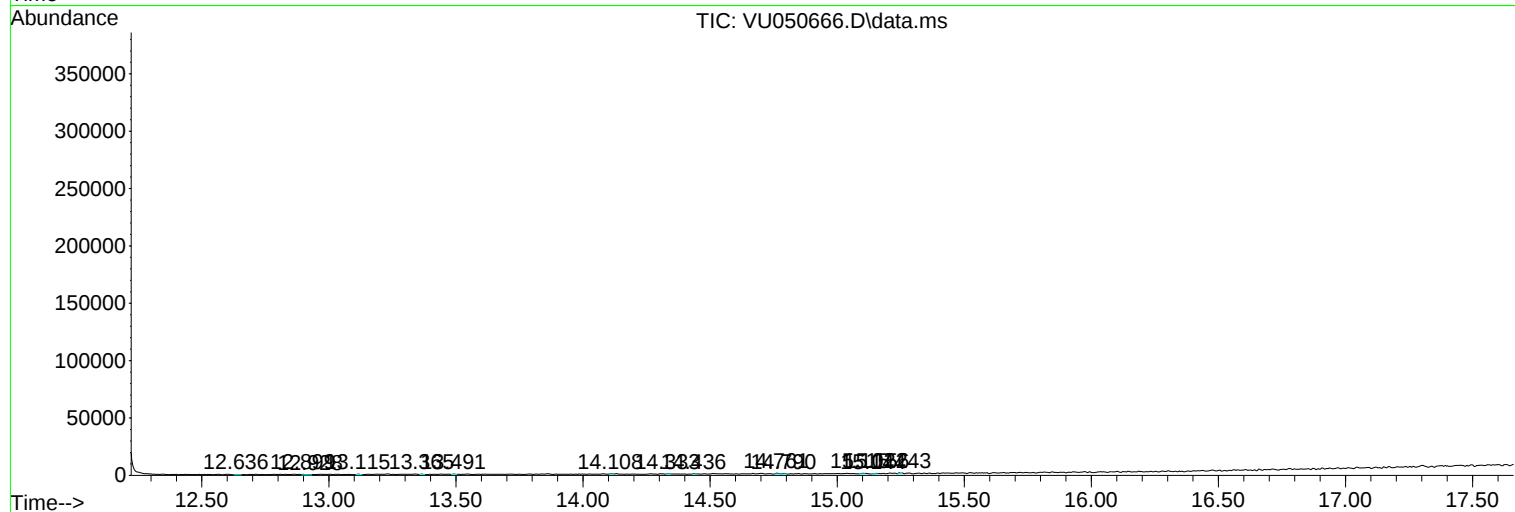
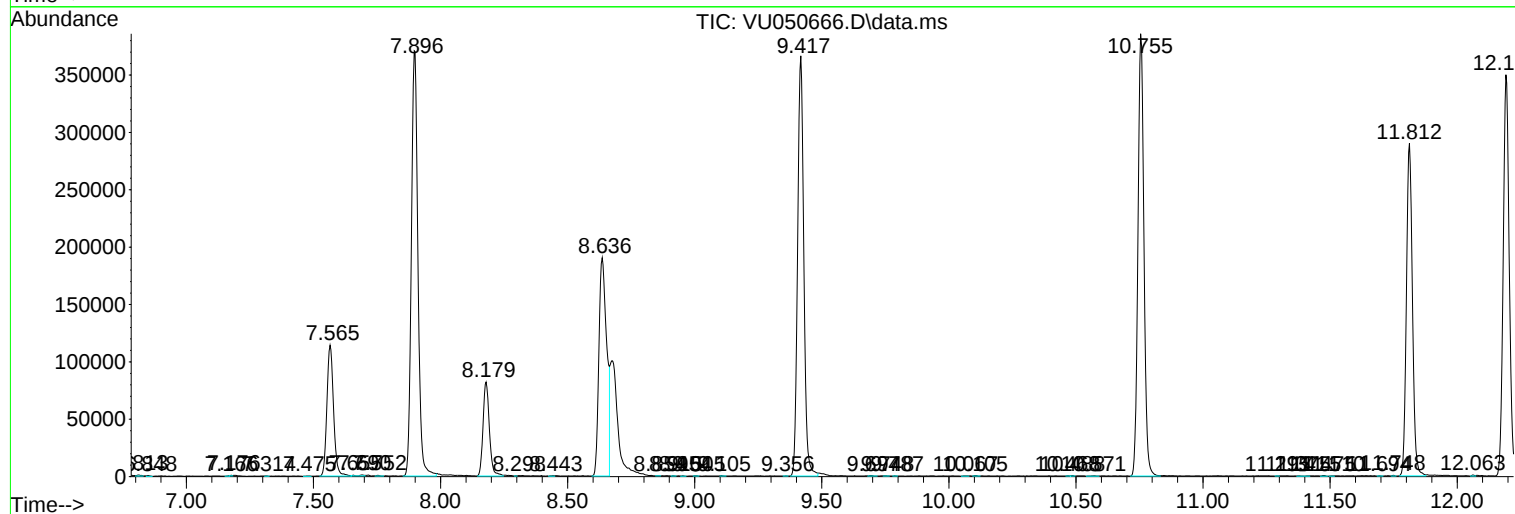
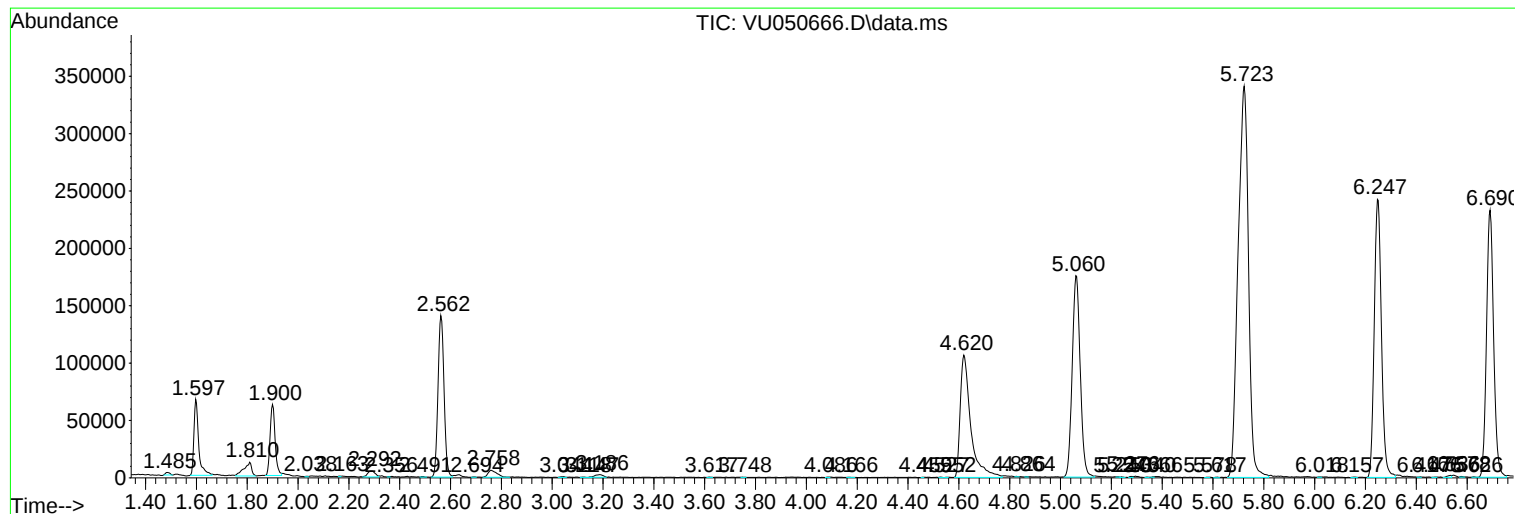
Sum of corrected areas: 6787423

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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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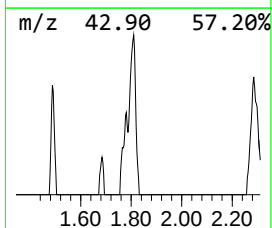
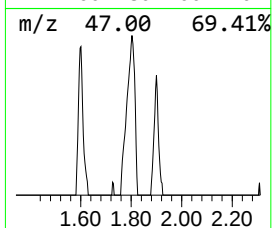
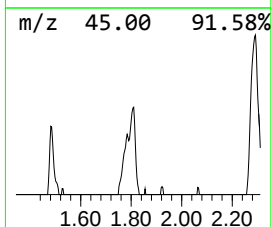
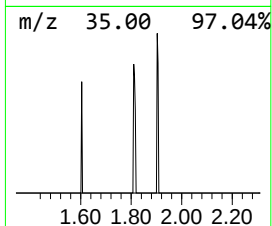
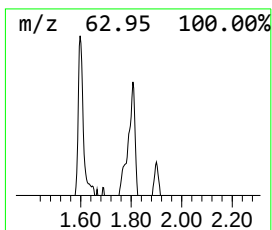
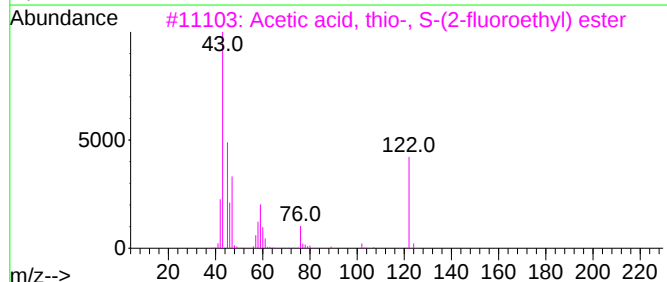
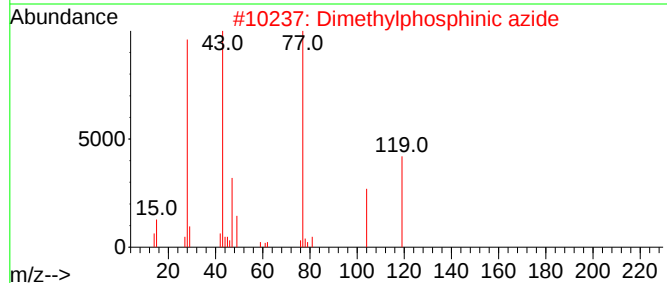
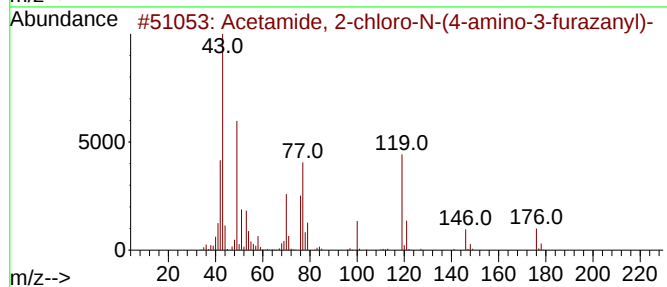
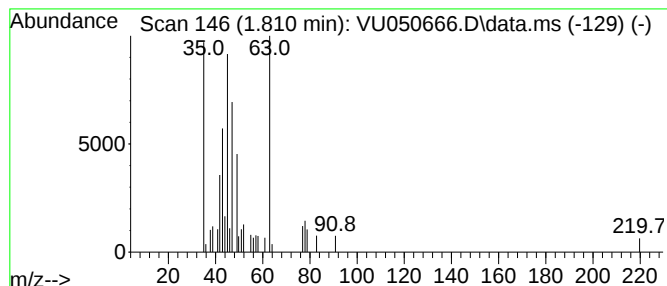
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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.
1.810	2.61 ug/L	24787	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, 2-chloro-N-(4-amino-3...	176	C4H5ClN4O2	101140-12-9	9
2			Dimethylphosphinic azide	119	C2H6N3OP	058347-13-0	9
3			Acetic acid, thio-, S-(2-fluoroe...	122	C4H7FOS	000462-31-7	9
4			trans-2-Chlorovinylacetate	120	C4H5ClO2	1000288-27-5	9
5			Methan-d3-ol	35	CHD3O	001849-29-2	4



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.810	2.6	ug/L	24787	1	6.250	475435	50.0