

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW042622\
 Data File : VW022624.D
 Acq On : 26 Apr 2022 15:02
 Operator : SY/VA
 Sample : N2562-04
 Misc : 7.95g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 EW464

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_W\Method\SFAMWLM040722SMA.M
 Title : SFAM01.0

Signal : TIC: VW022624.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.959	6	9	17	rVB2	28435	47335	4.97%	0.861%
2	2.355	69	74	82	rVB	119226	198715	20.86%	3.612%
3	2.891	156	162	171	rVB	63476	136666	14.35%	2.484%
4	3.934	331	333	335	rBV3	837	817	0.09%	0.015%
5	4.019	337	347	359	rVV2	95968	288319	30.27%	5.241%
6	4.391	397	408	418	rBV2	13166	41596	4.37%	0.756%
7	4.519	428	429	431	rVB2	981	637	0.07%	0.012%
8	4.568	435	437	438	rVV2	741	448	0.05%	0.008%
9	4.592	438	441	446	rVV5	995	1215	0.13%	0.022%
10	4.666	452	453	455	rVB2	1171	684	0.07%	0.012%
11	4.690	455	457	458	rBV	774	639	0.07%	0.012%
12	4.867	484	486	487	rBV	1420	1091	0.11%	0.020%
13	4.922	487	495	497	rBV3	7227	16759	1.76%	0.305%
14	5.208	541	542	544	rBV2	739	575	0.06%	0.010%
15	5.269	551	552	554	rVB2	928	409	0.04%	0.007%
16	5.293	554	556	560	rVB4	729	984	0.10%	0.018%
17	5.422	574	577	578	rBV2	934	907	0.10%	0.016%
18	5.495	588	589	593	rVB3	1052	773	0.08%	0.014%
19	5.635	609	612	615	rBV5	1275	1944	0.20%	0.035%
20	5.775	627	635	639	rBV9	1994	5894	0.62%	0.107%
21	5.854	645	648	650	rBV3	690	710	0.07%	0.013%
22	5.946	655	663	671	rVB8	4885	14657	1.54%	0.266%
23	6.031	675	677	678	rBV	896	726	0.08%	0.013%
24	6.184	700	702	703	rBV	1097	524	0.06%	0.010%
25	6.245	711	712	714	rBV2	913	429	0.05%	0.008%
26	6.275	715	717	721	rVB2	1084	1192	0.13%	0.022%
27	6.330	721	726	729	rBV7	1172	2473	0.26%	0.045%
28	6.397	734	737	743	rBV8	1277	2553	0.27%	0.046%
29	6.507	746	755	757	rBV5	1419	2555	0.27%	0.046%
30	6.653	777	779	780	rVB	812	472	0.05%	0.009%
31	6.671	780	782	784	rBV2	602	488	0.05%	0.009%
32	6.812	801	805	806	rBV3	1352	1425	0.15%	0.026%
33	6.866	812	814	815	rBV2	863	516	0.05%	0.009%
34	7.080	841	849	865	rBV	48334	148114	15.55%	2.693%
35	7.397	898	901	902	rVB3	842	746	0.08%	0.014%
36	7.433	905	907	908	rBV2	781	653	0.07%	0.012%

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 Title : SFAM01.0

37	7.647	933	942	952	rBV	187557	463291	48.64%	8.422%
38	7.744	956	958	961	rVB4	898	547	0.06%	0.010%
39	7.781	962	964	966	rVB3	1100	706	0.07%	0.013%
40	7.824	970	971	973	rVB2	850	567	0.06%	0.010%
41	8.025	998	1004	1006	rBV6	1653	2809	0.29%	0.051%
42	8.086	1012	1014	1016	rVB3	775	503	0.05%	0.009%
43	8.110	1016	1018	1021	rBV4	855	923	0.10%	0.017%
44	8.141	1021	1023	1025	rBV3	933	692	0.07%	0.013%
45	8.159	1025	1026	1029	rVB3	1618	932	0.10%	0.017%
46	8.275	1033	1045	1061	rBV2	294667	952481	100.00%	17.315%
47	8.689	1111	1113	1115	rBV3	1253	1304	0.14%	0.024%
48	8.744	1120	1122	1123	rBV2	691	458	0.05%	0.008%
49	8.842	1130	1138	1150	rBV	297863	589830	61.93%	10.723%
50	8.957	1156	1157	1160	rBV3	790	737	0.08%	0.013%
51	9.073	1173	1176	1177	rBV3	1849	2239	0.24%	0.041%
52	9.171	1190	1192	1196	rVB5	609	559	0.06%	0.010%
53	9.274	1200	1209	1217	rBV	228823	466079	48.93%	8.473%
54	9.591	1256	1261	1267	rVB10	1755	3945	0.41%	0.072%
55	9.665	1269	1273	1275	rBV4	1458	1901	0.20%	0.035%
56	9.823	1296	1299	1302	rBV6	1002	981	0.10%	0.018%
57	9.878	1305	1308	1310	rBV2	1044	1454	0.15%	0.026%
58	9.945	1317	1319	1322	rBV4	983	1435	0.15%	0.026%
59	10.037	1325	1334	1347	rBV	83772	163645	17.18%	2.975%
60	10.128	1347	1349	1352	rBV4	1353	1541	0.16%	0.028%
61	10.189	1357	1359	1362	rBV4	786	1053	0.11%	0.019%
62	10.323	1373	1381	1388	rBV	289987	503760	52.89%	9.158%
63	10.579	1417	1423	1430	rBV	43769	73331	7.70%	1.333%
64	10.701	1439	1443	1449	rVB3	5399	8602	0.90%	0.156%
65	10.805	1458	1460	1464	rBV4	894	1015	0.11%	0.018%
66	10.927	1472	1480	1495	rBV	137677	252139	26.47%	4.584%
67	11.280	1535	1538	1541	rBV4	896	1167	0.12%	0.021%
68	11.390	1554	1556	1559	rBV4	1012	1172	0.12%	0.021%
69	11.457	1566	1567	1569	rBV2	851	472	0.05%	0.009%
70	11.512	1574	1576	1579	rBV3	1147	1103	0.12%	0.020%
71	11.628	1588	1595	1606	rBV	232829	401618	42.17%	7.301%
72	12.036	1660	1662	1664	rVB3	682	465	0.05%	0.008%
73	12.109	1672	1674	1676	rVB3	722	424	0.04%	0.008%
74	12.128	1676	1677	1680	rBV3	1276	1560	0.16%	0.028%
75	12.164	1681	1683	1687	rVB3	1825	2107	0.22%	0.038%
76	12.335	1709	1711	1713	rBV2	1448	1550	0.16%	0.028%

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 Title : SFAM01.0

77	12.463	1729	1732	1735	rBV5	1463	1796	0.19%	0.033%
78	12.603	1750	1755	1762	rVB3	9570	16435	1.73%	0.299%
79	12.689	1762	1769	1778	rBV	179322	295776	31.05%	5.377%
80	12.926	1805	1808	1810	rBV4	3663	4288	0.45%	0.078%
81	13.170	1844	1848	1849	rBV4	1467	1788	0.19%	0.033%
82	13.554	1905	1911	1918	rBV	82542	138994	14.59%	2.527%
83	13.853	1953	1960	1967	rBV	85476	148970	15.64%	2.708%
84	14.066	1990	1995	2003	rVB2	12384	23622	2.48%	0.429%
85	14.231	2020	2022	2023	rVB2	764	447	0.05%	0.008%
86	14.261	2023	2027	2031	rBV7	1251	2332	0.24%	0.042%
87	14.322	2031	2037	2042	rBV8	4867	8900	0.93%	0.162%
88	14.597	2080	2082	2084	rBV3	973	624	0.07%	0.011%
89	14.706	2094	2100	2105	rBV9	1964	5600	0.59%	0.102%
90	14.999	2145	2148	2149	rBV3	863	1035	0.11%	0.019%
91	15.017	2149	2151	2153	rVV3	1014	916	0.10%	0.017%
92	15.084	2160	2162	2163	rBV2	877	742	0.08%	0.013%
93	15.609	2246	2248	2249	rBV2	1049	426	0.04%	0.008%
94	15.670	2255	2258	2261	rBV4	1163	1414	0.15%	0.026%
95	15.792	2274	2278	2281	rBV5	2963	4639	0.49%	0.084%
96	16.231	2348	2350	2354	rVB5	1393	1236	0.13%	0.022%
97	16.298	2359	2361	2363	rBV2	1388	1153	0.12%	0.021%
98	16.474	2388	2390	2396	rBV7	1311	2353	0.25%	0.043%
99	16.541	2399	2401	2402	rBV	989	868	0.09%	0.016%
100	16.669	2421	2422	2424	rBV2	907	771	0.08%	0.014%

Sum of corrected areas: 5500862

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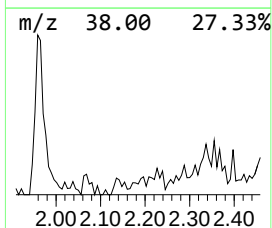
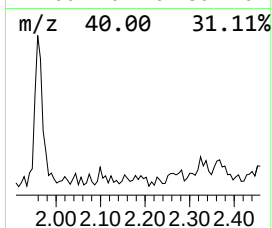
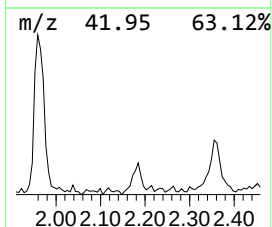
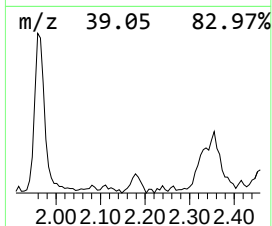
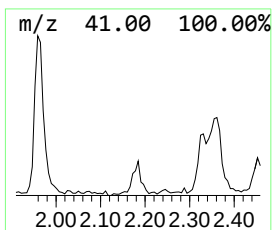
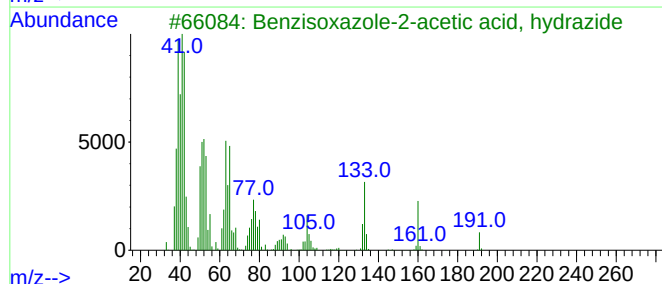
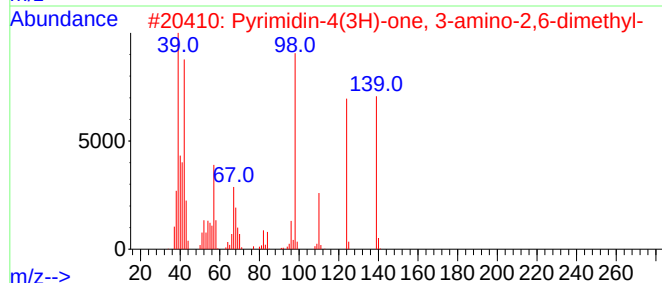
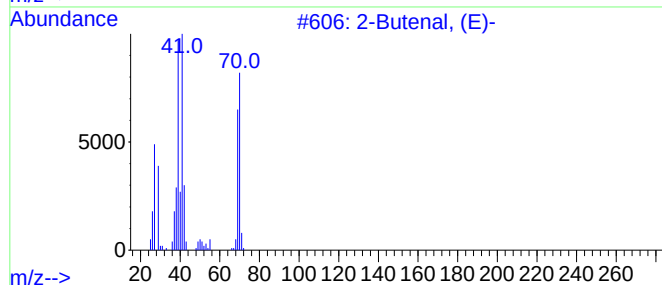
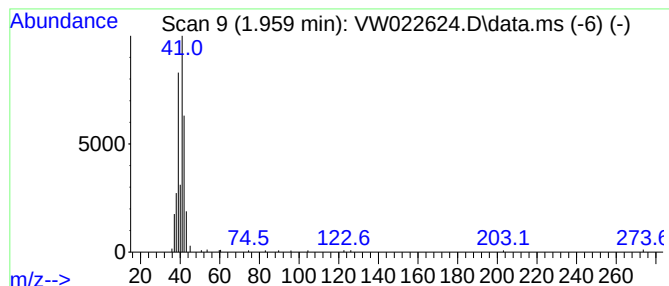
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040722SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 2-Butenal, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.959	2.01 ug/L	47335	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, (E)-		70	C4H6O	000123-73-9	78	
2	Pyrimidin-4(3H)-one, 3-amino-2,6...	139	C6H9N3O	093098-74-9	78		
3	Benzisoxazole-2-acetic acid, hyd...	191	C9H9N3O2	055244-10-5	74		
4	Propene	42	C3H6	000115-07-1	72		
5	5-Pyrimidinecarboxylic acid, hex...	214	C8H10N2O5	072088-02-9	64		



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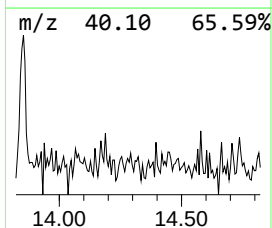
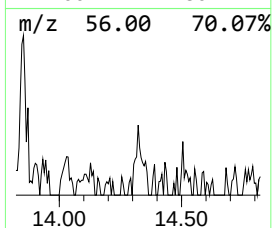
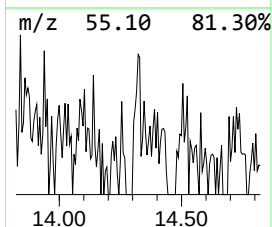
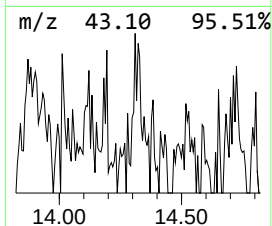
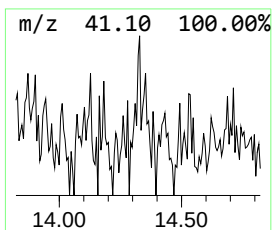
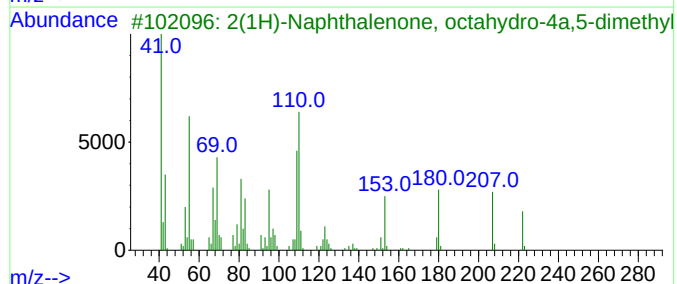
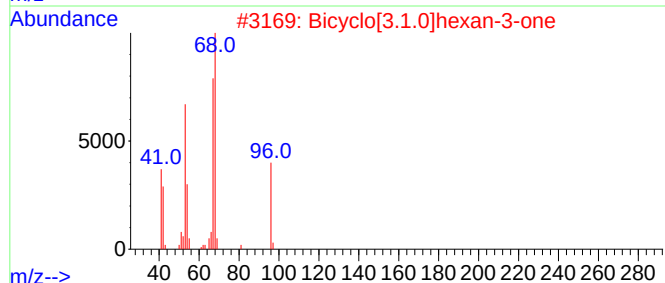
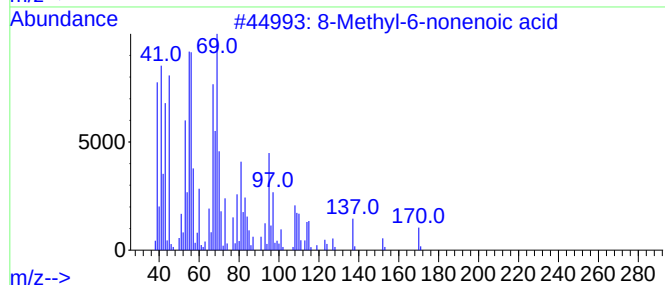
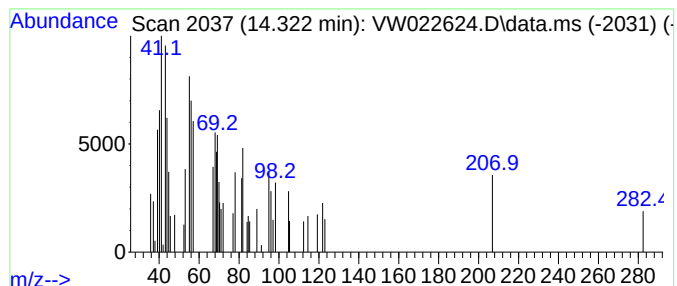
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM040722SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.322	1.60 ug/L	8900	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8-Methyl-6-nonenoic acid	170	C10H18O2	021382-25-2	38
2			Bicyclo[3.1.0]hexan-3-one	96	C6H8O	001755-04-0	38
3			2(1H)-Naphthalenone, octahydro-4...	222	C15H26O	055332-04-2	32
4			Bicyclo[5.2.0]nonane, 1,7-dimeth...	152	C11H20	020130-83-0	27
5			5-(3,7-Dimethylocta-2,6-dienyl)-...	268	C15H24O2S	1000305-61-4	22



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butenal, (E)-	1.959	2.0	ug/L	47335	1	8.842	589830	25.0
unknown-01	14.322	1.6	ug/L	8900	3	13.554	138994	25.0