

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW011322\
 Data File : VW021884.D
 Acq On : 13 Jan 2022 12:14
 Operator : SY/VA
 Sample : N1114-20
 Misc : 5.86g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 BGLR2

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\SFAMWLM011122SMA.M
 Title : SFAM01.0

Signal : TIC: VW021884.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.349	68	73	83	rVB	38713	66296	0.09%	0.075%
2	2.489	94	96	106	rVB	4570	9208	0.01%	0.010%
3	2.879	154	160	169	rVB	24707	52800	0.07%	0.060%
4	3.306	228	230	237	rVB3	762	1518	0.00%	0.002%
5	3.373	239	241	242	rBV2	430	329	0.00%	0.000%
6	3.446	247	253	261	rVB2	5115	11389	0.02%	0.013%
7	3.580	273	275	279	rVB4	352	340	0.00%	0.000%
8	3.678	287	291	298	rVB3	555	1226	0.00%	0.001%
9	3.788	298	309	315	rBV4	1372	3811	0.01%	0.004%
10	4.038	335	350	362	rBV	335901	1005136	1.36%	1.137%
11	4.385	396	407	416	rBV2	2915	9544	0.01%	0.011%
12	4.483	422	423	426	rBV	187	219	0.00%	0.000%
13	4.538	428	432	433	rBV2	227	216	0.00%	0.000%
14	4.580	433	439	441	rBV2	197	335	0.00%	0.000%
15	4.660	450	452	455	rBV	194	219	0.00%	0.000%
16	4.702	455	459	460	rBV2	176	253	0.00%	0.000%
17	4.903	486	492	494	rBV4	1512	2549	0.00%	0.003%
18	5.172	532	536	539	rBV3	214	342	0.00%	0.000%
19	5.202	539	541	546	rVB2	176	246	0.00%	0.000%
20	5.422	570	577	588	rVB2	3615	10589	0.01%	0.012%
21	5.562	598	600	602	rBV	204	241	0.00%	0.000%
22	5.769	631	634	635	rBV2	239	266	0.00%	0.000%
23	5.861	646	649	652	rBV2	240	330	0.00%	0.000%
24	5.928	652	660	662	rBV3	684	1311	0.00%	0.001%
25	6.001	670	672	673	rVB	369	235	0.00%	0.000%
26	6.062	679	682	685	rBV2	238	323	0.00%	0.000%
27	6.214	695	707	724	rVV	315434	976036	1.32%	1.104%
28	6.452	744	746	753	rVV3	282	461	0.00%	0.001%
29	6.531	757	759	763	rVB2	280	278	0.00%	0.000%
30	6.617	770	773	775	rBV2	229	326	0.00%	0.000%
31	6.988	832	834	837	rVV2	498	580	0.00%	0.001%
32	7.080	841	849	855	rVV2	13735	38016	0.05%	0.043%
33	7.171	856	864	877	rVB	55790	149384	0.20%	0.169%
34	7.366	893	896	897	rVB3	310	228	0.00%	0.000%
35	7.385	897	899	900	rBV	265	253	0.00%	0.000%
36	7.647	932	942	952	rVV	81688	202054	0.27%	0.228%

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 Title : SFAM01.0

37	7.775	958	963	965	rBV	277	348	0.00%	0.000%
38	7.915	979	986	991	rBV3	369	898	0.00%	0.001%
39	8.275	1034	1045	1060	rBV2	151265	465003	0.63%	0.526%
40	8.695	1111	1114	1117	rVB2	444	445	0.00%	0.001%
41	8.842	1128	1138	1148	rBV	141205	277250	0.38%	0.313%
42	8.921	1148	1151	1153	rVB2	310	321	0.00%	0.000%
43	9.092	1168	1179	1196	rBV	5199238	9750742	13.23%	11.026%
44	9.275	1201	1209	1219	rVB	98802	200856	0.27%	0.227%
45	9.506	1244	1247	1249	rVV2	354	436	0.00%	0.000%
46	9.592	1256	1261	1266	rBV3	328	691	0.00%	0.001%
47	9.634	1266	1268	1271	rBV	273	279	0.00%	0.000%
48	9.665	1271	1273	1277	rVV3	517	626	0.00%	0.001%
49	9.726	1277	1283	1292	rVB4	1795	3925	0.01%	0.004%
50	9.884	1304	1309	1314	rVB4	4354	7372	0.01%	0.008%
51	10.037	1326	1334	1343	rVB	51171	96163	0.13%	0.109%
52	10.171	1353	1356	1358	rBV2	254	328	0.00%	0.000%
53	10.207	1359	1362	1365	rVV4	307	506	0.00%	0.001%
54	10.323	1373	1381	1388	rBV	217233	379351	0.51%	0.429%
55	10.390	1388	1392	1401	rVB	8960	16264	0.02%	0.018%
56	10.463	1402	1404	1407	rBV3	265	318	0.00%	0.000%
57	10.579	1416	1423	1430	rBV	31274	55433	0.08%	0.063%
58	10.707	1439	1444	1447	rVV2	1174	1949	0.00%	0.002%
59	10.756	1447	1452	1455	rBV4	1317	1976	0.00%	0.002%
60	10.872	1460	1471	1478	rBV2	33737919	73727584	100.00%	83.367%
61	11.286	1535	1539	1543	rVB2	1469	2100	0.00%	0.002%
62	11.549	1577	1582	1584	rVB4	925	1356	0.00%	0.002%
63	11.628	1586	1595	1607	rVV	161173	280277	0.38%	0.317%
64	11.731	1607	1612	1618	rVB	7261	11173	0.02%	0.013%
65	11.835	1623	1629	1637	rVV	16907	29849	0.04%	0.034%
66	11.981	1651	1653	1656	rVV3	316	384	0.00%	0.000%
67	12.164	1677	1683	1689	rVB	15122	25067	0.03%	0.028%
68	12.359	1711	1715	1719	rVB3	2535	3831	0.01%	0.004%
69	12.469	1729	1733	1734	rBV3	389	456	0.00%	0.001%
70	12.603	1749	1755	1761	rVB	23041	36245	0.05%	0.041%
71	12.689	1762	1769	1778	rVB	77732	128822	0.17%	0.146%
72	13.073	1829	1832	1833	rVB	315	247	0.00%	0.000%
73	13.103	1833	1837	1842	rBV3	563	918	0.00%	0.001%
74	13.182	1845	1850	1857	rBV4	910	1829	0.00%	0.002%
75	13.243	1857	1860	1864	rBV3	850	1155	0.00%	0.001%
76	13.402	1879	1886	1890	rVB4	1430	2400	0.00%	0.003%

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 Title : SFAM01.0

77	13.469	1890	1897	1899	rBV5	1045	1566	0.00%	0.002%
78	13.554	1902	1911	1923	rBV	113685	185840	0.25%	0.210%
79	13.737	1939	1941	1942	rBV	495	400	0.00%	0.000%
80	13.853	1952	1960	1967	rBV	105350	175509	0.24%	0.198%
81	13.908	1967	1969	1971	rVB3	418	301	0.00%	0.000%
82	14.060	1990	1994	1999	rBV2	1778	2909	0.00%	0.003%
83	14.103	1999	2001	2003	rBV	356	341	0.00%	0.000%
84	14.310	2033	2035	2037	rBV	387	352	0.00%	0.000%
85	14.511	2065	2068	2074	rBV4	472	980	0.00%	0.001%
86	14.670	2092	2094	2097	rVB3	386	345	0.00%	0.000%
87	14.719	2100	2102	2104	rVV	367	352	0.00%	0.000%
88	14.767	2107	2110	2112	rBV	278	303	0.00%	0.000%
89	15.011	2149	2150	2152	rVB2	366	232	0.00%	0.000%
90	15.145	2170	2172	2175	rBV2	305	265	0.00%	0.000%
91	15.347	2204	2205	2207	rBV2	406	336	0.00%	0.000%
92	15.432	2214	2219	2224	rBV3	1050	1974	0.00%	0.002%
93	15.877	2289	2292	2293	rBV2	367	393	0.00%	0.000%
94	15.944	2301	2303	2309	rVB	580	686	0.00%	0.001%
95	15.993	2309	2311	2313	rVB2	344	305	0.00%	0.000%
96	16.011	2313	2314	2317	rBV2	360	389	0.00%	0.000%
97	16.115	2330	2331	2333	rBV	240	216	0.00%	0.000%
98	16.426	2378	2382	2383	rBV2	378	413	0.00%	0.000%
99	16.724	2429	2431	2435	rVB3	581	462	0.00%	0.001%
100	16.773	2435	2439	2440	rBV2	345	472	0.00%	0.001%

Sum of corrected areas: 88437401

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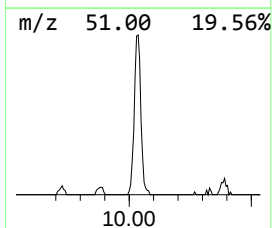
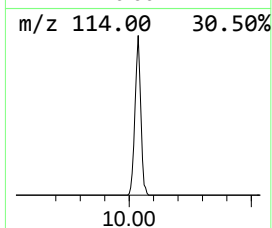
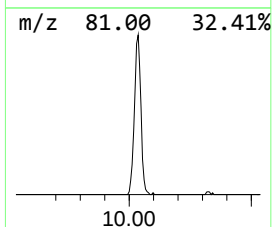
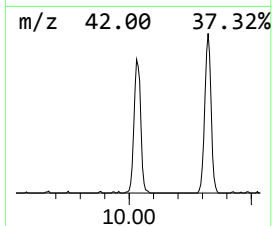
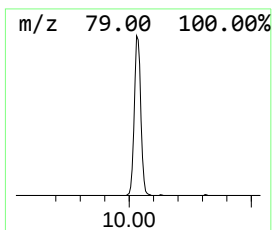
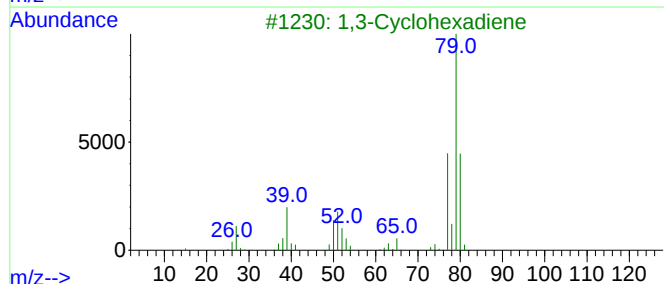
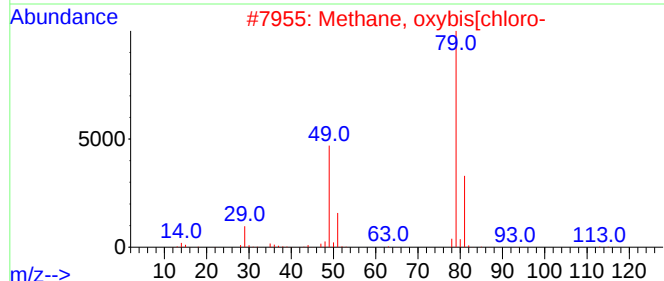
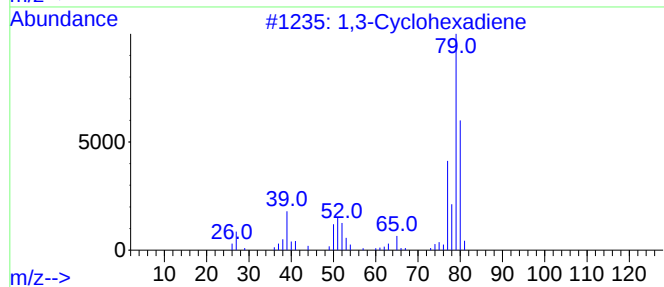
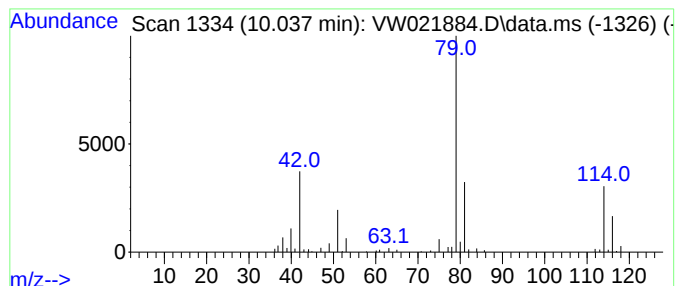
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM011122SMA.M
Quant Title : SFAM01.0

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.
10.037	8.67 ug/L	96163	1,4-Difluorobenzene	8.842

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Cyclohexadiene	80	C6H8	000592-57-4	38
2		Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	33
3		1,3-Cyclohexadiene	80	C6H8	000592-57-4	28
4		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	25
5		Cyclopropene, 3-methyl-3-vinyl-	80	C6H8	071153-30-5	9



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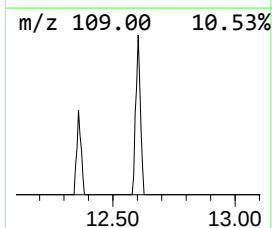
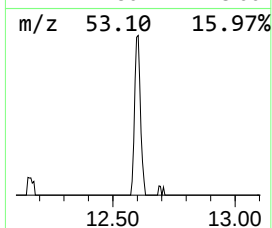
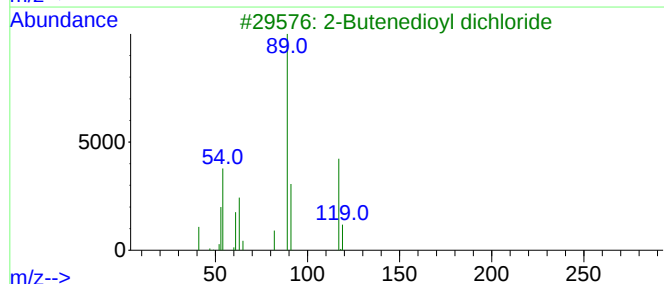
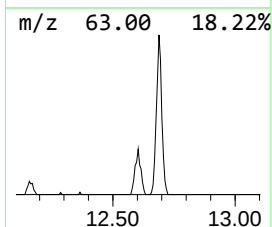
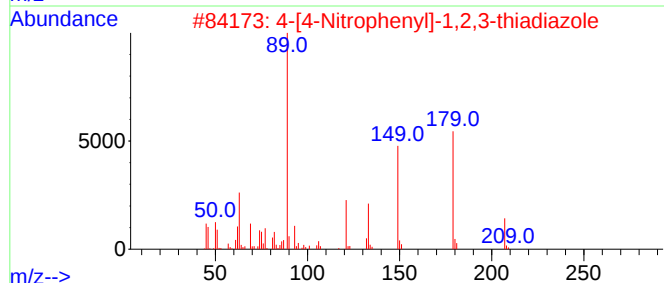
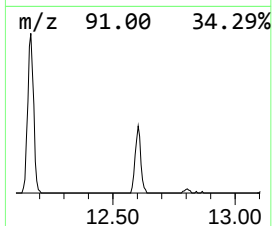
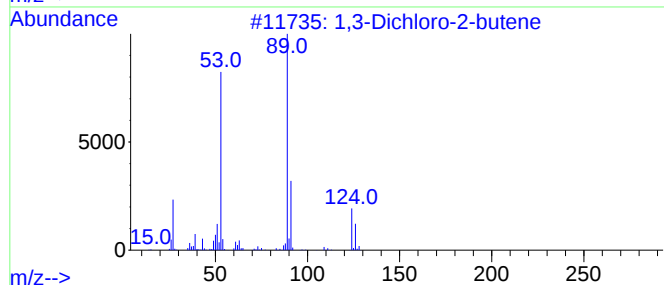
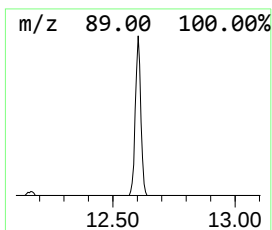
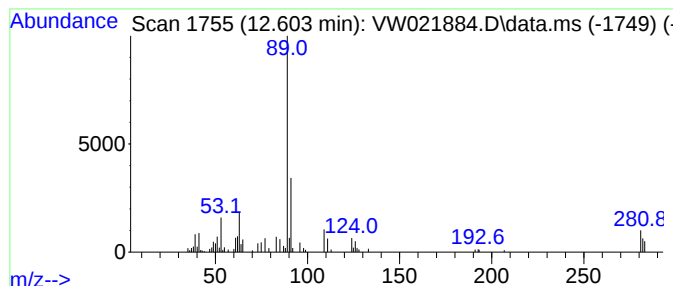
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM011122SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 1,3-Dichloro-2-butene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.603	4.88 ug/L	36245	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dichloro-2-butene	124	C4H6Cl2	000926-57-8	64
2			4-[4-Nitrophenyl]-1,2,3-thiadiazole	207	C8H5N3O2S	082894-98-2	56
3			2-Butenedioyl dichloride	152	C4H2Cl2O2	016769-97-4	56
4			Diglycolic acid, hexyl 3-methylp...	308	C17H24O5	1000382-10-3	43
5			Methyl 2-(methylthio)butyrate	148	C6H12O2S	051534-66-8	43



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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	10.037	8.7	ug/L	96163	1	8.842	277250	25.0
1,3-Dichloro-2-...	12.603	4.9	ug/L	36245	3	13.554	185840	25.0