

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW091323\
 Data File : VW027088.D
 Acq On : 13 Sep 2023 13:14
 Operator : SY/MD
 Sample : 04330-12RE
 Misc : 6.32g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 EZYF8RE

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\SFAMWLM090523SMA.M
 Title : SFAM01.0

Signal : TIC: VW027088.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.820	151	153	154	rBV2	1684	882	0.85%	0.144%
2	2.899	161	166	172	rVB2	7974	14861	14.30%	2.419%
3	3.210	215	217	219	rBV3	1495	1203	1.16%	0.196%
4	3.375	242	244	245	rBV2	1962	1002	0.96%	0.163%
5	3.582	276	278	280	rBV3	1075	906	0.87%	0.148%
6	3.728	300	302	304	rBV3	1922	1496	1.44%	0.244%
7	3.826	316	318	320	rVB3	1926	1483	1.43%	0.241%
8	3.893	326	329	330	rBV3	1987	1701	1.64%	0.277%
9	4.027	343	351	358	rBV4	11361	33272	32.01%	5.417%
10	4.082	358	360	362	rVB3	2003	1259	1.21%	0.205%
11	4.344	400	403	404	rBV3	1729	1359	1.31%	0.221%
12	4.387	409	410	411	rBV	1401	754	0.73%	0.123%
13	4.448	419	420	422	rBV2	1428	1026	0.99%	0.167%
14	4.582	439	442	444	rBV3	1397	1354	1.30%	0.220%
15	4.704	460	462	465	rVB4	1610	1576	1.52%	0.257%
16	4.795	475	477	478	rBV2	1987	1666	1.60%	0.271%
17	5.051	518	519	520	rBV	1506	706	0.68%	0.115%
18	5.137	531	533	536	rBV4	2875	2522	2.43%	0.411%
19	5.216	545	546	548	rBV2	942	718	0.69%	0.117%
20	5.240	548	550	552	rVB3	2321	1534	1.48%	0.250%
21	5.258	552	553	554	rBV	1310	791	0.76%	0.129%
22	5.350	566	568	569	rBV2	1774	1177	1.13%	0.192%
23	5.386	572	574	577	rBV4	1993	1394	1.34%	0.227%
24	5.447	582	584	585	rBV2	2036	2017	1.94%	0.328%
25	5.722	627	629	631	rBV3	1263	1283	1.23%	0.209%
26	5.844	646	649	651	rBV4	1558	1889	1.82%	0.308%
27	5.935	661	664	665	rBV3	1831	1935	1.86%	0.315%
28	6.033	678	680	681	rVB2	1307	873	0.84%	0.142%
29	6.051	681	683	684	rBV2	1051	970	0.93%	0.158%
30	6.124	694	695	697	rVV2	1203	693	0.67%	0.113%
31	6.167	699	702	703	rBV3	1276	811	0.78%	0.132%
32	6.228	708	712	715	rVB6	1354	1842	1.77%	0.300%
33	6.478	750	753	757	rVB5	1898	2797	2.69%	0.455%
34	6.520	757	760	761	rBV3	2158	1823	1.75%	0.297%
35	6.557	764	766	773	rVB8	2394	3868	3.72%	0.630%
36	6.868	815	817	818	rBV2	1472	1173	1.13%	0.191%

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 Title : SFAM01.0

37	6.929	826	827	830	rBV3	1146	853	0.82%	0.139%
38	7.051	845	847	849	rVB3	2527	2073	1.99%	0.338%
39	7.094	849	854	856	rBV6	3596	7232	6.96%	1.177%
40	7.222	873	875	877	rBV3	1556	1146	1.10%	0.187%
41	7.331	891	893	894	rBV2	831	611	0.59%	0.099%
42	7.417	905	907	910	rBV4	1616	1542	1.48%	0.251%
43	7.459	912	914	916	rVB3	1356	1203	1.16%	0.196%
44	7.581	932	934	935	rBV2	1176	599	0.58%	0.098%
45	7.654	935	946	954	rVV2	18756	53611	51.58%	8.728%
46	7.837	973	976	978	rVB4	2091	1864	1.79%	0.303%
47	7.874	978	982	983	rBV4	1041	1427	1.37%	0.232%
48	7.929	990	991	992	rBV	1182	569	0.55%	0.093%
49	8.026	1005	1007	1008	rBV2	1068	741	0.71%	0.121%
50	8.093	1017	1018	1019	rVB	872	319	0.31%	0.052%
51	8.118	1019	1022	1023	rBV3	1244	1302	1.25%	0.212%
52	8.227	1037	1040	1041	rBV3	1799	1742	1.68%	0.284%
53	8.282	1041	1049	1065	rVV4	29806	103935	100.00%	16.921%
54	8.496	1082	1084	1087	rVB4	1883	1727	1.66%	0.281%
55	8.532	1087	1090	1091	rBV3	2263	2654	2.55%	0.432%
56	8.575	1094	1097	1101	rVV5	1931	2727	2.62%	0.444%
57	8.697	1116	1117	1119	rVB3	1544	1002	0.96%	0.163%
58	8.746	1123	1125	1126	rBV2	901	465	0.45%	0.076%
59	8.788	1126	1132	1135	rBV8	2003	3241	3.12%	0.528%
60	8.843	1135	1141	1149	rBV	30358	64823	62.37%	10.554%
61	8.947	1155	1158	1163	rBV7	2354	4111	3.96%	0.669%
62	9.008	1167	1168	1170	rBV2	1119	668	0.64%	0.109%
63	9.032	1170	1172	1173	rVB2	1896	1164	1.12%	0.190%
64	9.075	1173	1179	1180	rBV5	4257	6521	6.27%	1.062%
65	9.209	1200	1201	1203	rBV2	1597	1175	1.13%	0.191%
66	9.276	1203	1212	1220	rVV3	23569	53435	51.41%	8.700%
67	9.392	1229	1231	1234	rBV4	1668	1625	1.56%	0.265%
68	9.465	1241	1243	1244	rVB2	1505	859	0.83%	0.140%
69	9.502	1245	1249	1250	rBV4	1504	2049	1.97%	0.334%
70	9.624	1266	1269	1270	rBV3	2273	1913	1.84%	0.311%
71	9.800	1296	1298	1300	rVB3	1683	1216	1.17%	0.198%
72	9.819	1300	1301	1303	rBV2	1632	1380	1.33%	0.225%
73	10.038	1331	1337	1342	rBV3	9055	19209	18.48%	3.127%
74	10.251	1367	1372	1373	rBV5	2158	3558	3.42%	0.579%
75	10.325	1379	1384	1389	rBV	22046	41880	40.29%	6.818%
76	10.526	1415	1417	1419	rVB3	2531	1540	1.48%	0.251%

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Title : SFAM01.0

77	10.550	1419	1421	1422	rBV2	1476	1293	1.24%	0.211%
78	10.581	1423	1426	1431	rVB7	4641	8392	8.07%	1.366%
79	10.703	1441	1446	1450	rBV7	2369	3911	3.76%	0.637%
80	11.117	1512	1514	1515	rVB2	1897	915	0.88%	0.149%
81	11.251	1534	1536	1538	rBV3	1944	1938	1.86%	0.316%
82	11.629	1593	1598	1605	rVB2	26256	46102	44.36%	7.506%
83	12.593	1754	1756	1759	rVB4	2522	2318	2.23%	0.377%
84	12.690	1769	1772	1780	rVB2	13921	25002	24.06%	4.071%
85	13.556	1910	1914	1923	rVB3	12954	28023	26.96%	4.562%

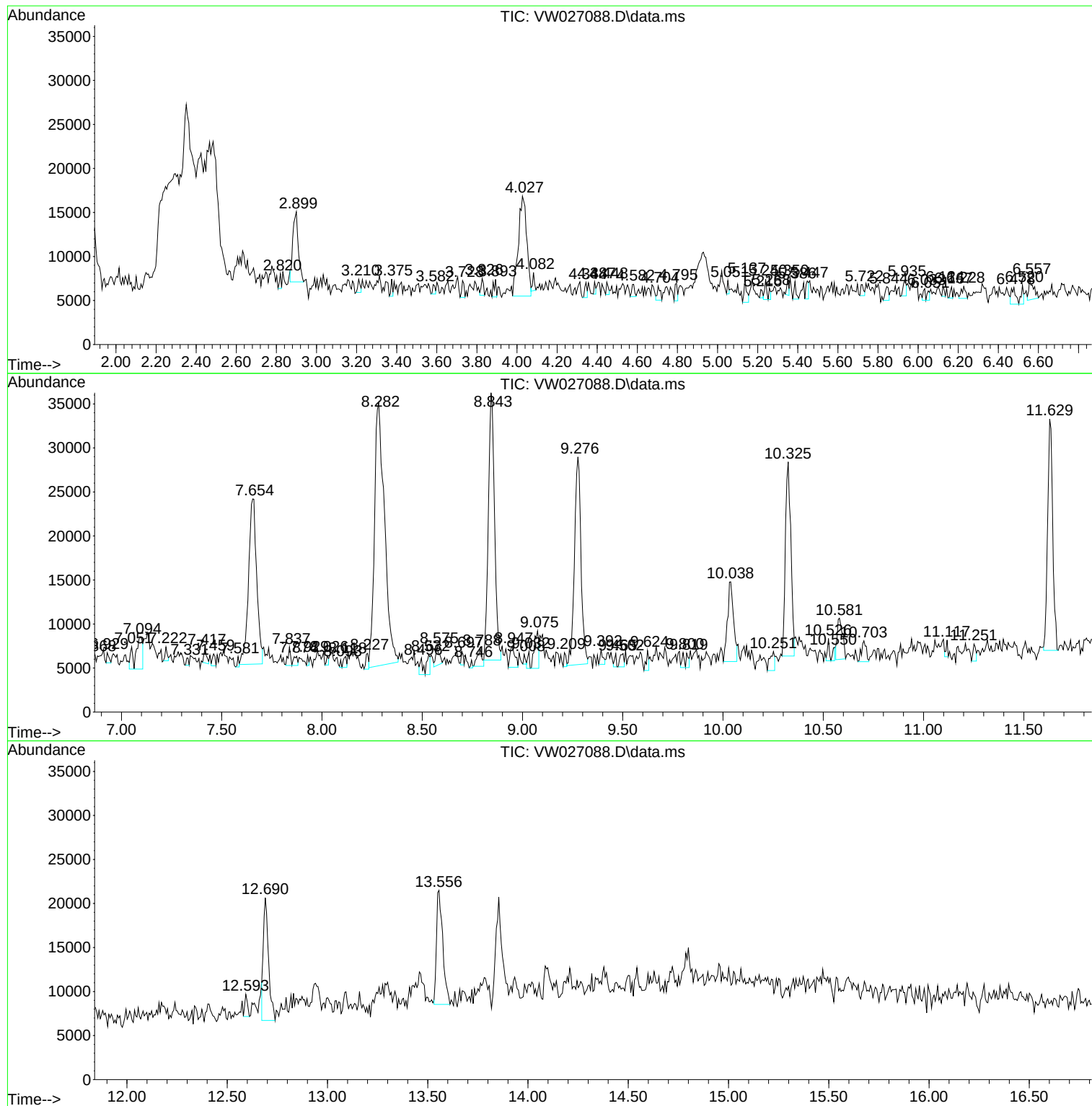
Sum of corrected areas: 614221

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM090523SMA.M
Quant Title : SFAM01.0

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



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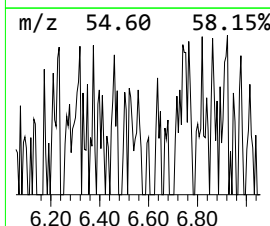
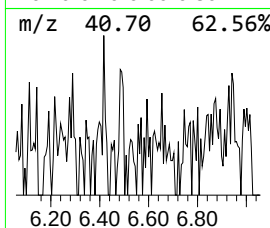
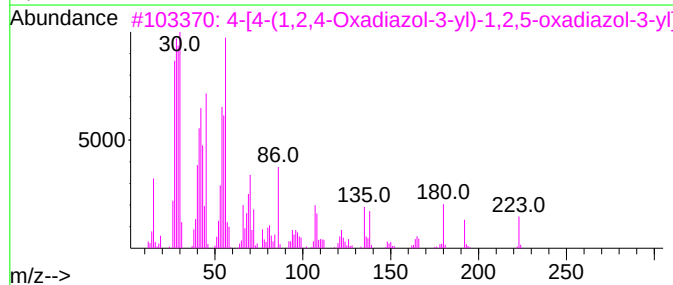
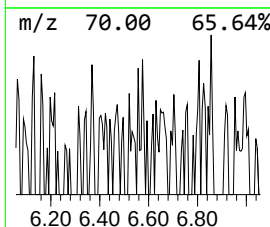
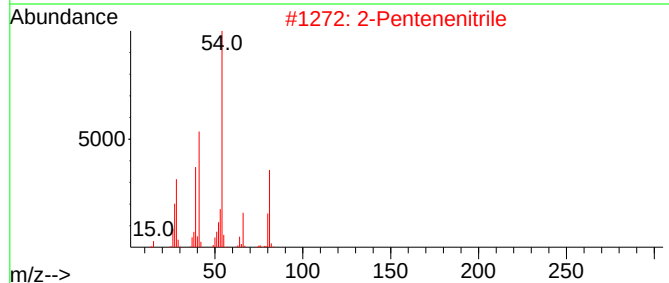
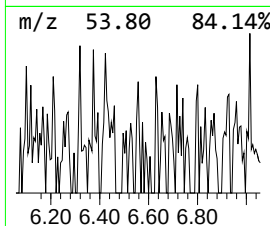
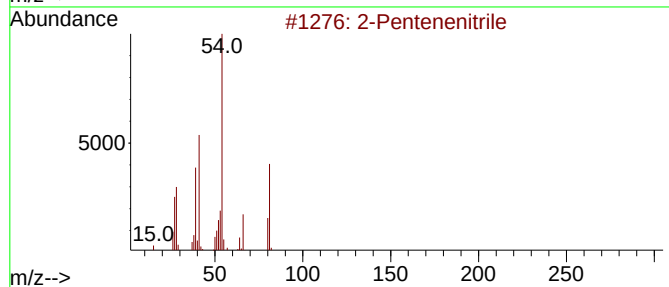
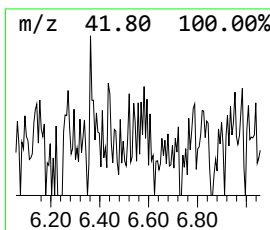
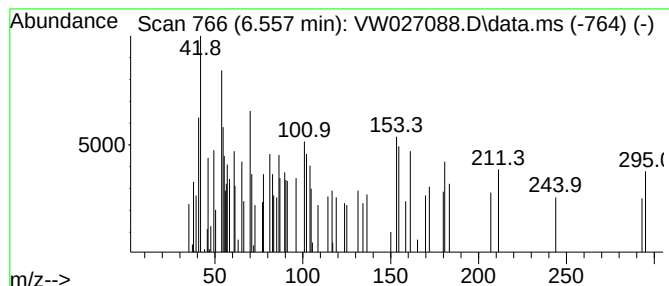
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM090523SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.557	1.49 ug/L	3868	1,4-Difluorobenzene	8.849

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentenenitrile	81	C5H7N	013284-42-9	30
2			2-Pentenenitrile	81	C5H7N	013284-42-9	27
3			4-[4-(1,2,4-Oxadiazol-3-yl)-1,2,...	223	C8H9N5O3	1000436-50-3	16
4			2-Pentenenitrile	81	C5H7N	013284-42-9	16
5			(E)-2-Pentenenitrile	81	C5H7N	026294-98-4	12



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Quant Title : SFAM01.0

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	6.557	1.5	ug/L	3868	1	8.849	64823	25.0