

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071322\
 Data File : VW023671.D
 Acq On : 14 Jul 2022 02:16
 Operator : SY/VA
 Sample : VW0713SBL02
 Misc : 5.00g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 VBLK544

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\SFAMWLM071322SMA.M
 Title : SFAM01.0

Signal : TIC: VW023671.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	48	58	59	rBV3	13330	35722	4.06%	0.545%
2	2.343	68	72	80	rBV	147690	246982	28.09%	3.769%
3	2.879	155	160	169	rVB	76401	155336	17.67%	2.370%
4	3.672	288	290	293	rVB4	1792	1672	0.19%	0.026%
5	3.702	293	295	298	rBV3	1193	1282	0.15%	0.020%
6	3.739	298	301	302	rBV3	1096	1368	0.16%	0.021%
7	3.928	330	332	334	rVB3	1565	1271	0.14%	0.019%
8	4.013	334	346	357	rBV2	74841	243044	27.65%	3.709%
9	4.355	399	402	403	rBV3	1258	1317	0.15%	0.020%
10	4.397	405	409	410	rBV4	1982	1836	0.21%	0.028%
11	4.568	435	437	440	rVB4	1359	1179	0.13%	0.018%
12	4.598	440	442	443	rBV2	1292	1323	0.15%	0.020%
13	4.672	451	454	455	rBV3	1185	951	0.11%	0.015%
14	4.702	457	459	462	rBV4	1564	1550	0.18%	0.024%
15	4.806	474	476	478	rBV3	1133	1050	0.12%	0.016%
16	4.915	488	494	503	rVB3	8109	24976	2.84%	0.381%
17	5.117	518	527	531	rBV7	3994	11751	1.34%	0.179%
18	5.421	574	577	578	rBV3	1126	1208	0.14%	0.018%
19	5.659	614	616	618	rVB2	1276	918	0.10%	0.014%
20	6.031	675	677	680	rVB4	1470	1136	0.13%	0.017%
21	6.214	705	707	712	rBV4	1318	1412	0.16%	0.022%
22	6.501	752	754	757	rVB4	1387	1197	0.14%	0.018%
23	6.555	761	763	765	rBV2	1449	1306	0.15%	0.020%
24	6.580	765	767	770	rVB4	1206	1111	0.13%	0.017%
25	6.769	796	798	799	rBV2	1478	1197	0.14%	0.018%
26	6.866	812	814	817	rBV4	1153	1056	0.12%	0.016%
27	6.897	817	819	821	rVB3	1546	1169	0.13%	0.018%
28	6.952	826	828	833	rBV6	1292	1571	0.18%	0.024%
29	7.080	841	849	855	rBV	24742	67080	7.63%	1.024%
30	7.275	879	881	884	rVB4	1206	1138	0.13%	0.017%
31	7.305	884	886	888	rBV3	1110	1260	0.14%	0.019%
32	7.647	934	942	952	rVB	149008	362763	41.26%	5.535%
33	7.872	976	979	982	rVB6	1484	1630	0.19%	0.025%
34	8.275	1035	1045	1058	rBV2	290096	879151	100.00%	13.415%
35	8.659	1106	1108	1110	rBV2	1666	1252	0.14%	0.019%
36	8.842	1130	1138	1147	rBV	241918	474662	53.99%	7.243%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
 Title : SFAM01.0

37	9.024	1167	1168	1171	rBV3	1382	1393	0.16%	0.021%
38	9.274	1201	1209	1218	rBV	197446	395169	44.95%	6.030%
39	9.634	1265	1268	1269	rBV3	1016	1034	0.12%	0.016%
40	9.677	1273	1275	1279	rVV5	1412	1690	0.19%	0.026%
41	9.823	1297	1299	1301	rBV2	1351	1249	0.14%	0.019%
42	9.878	1307	1308	1311	rVB3	1352	1106	0.13%	0.017%
43	9.976	1323	1324	1326	rBV2	1558	1456	0.17%	0.022%
44	10.036	1326	1334	1343	rVV	94474	178666	20.32%	2.726%
45	10.268	1370	1372	1373	rBV2	1388	1047	0.12%	0.016%
46	10.323	1374	1381	1391	rVV	422141	729047	82.93%	11.125%
47	10.482	1406	1407	1410	rBV3	1077	916	0.10%	0.014%
48	10.579	1415	1423	1430	rBV	67484	117780	13.40%	1.797%
49	10.701	1437	1443	1449	rBV2	29958	54422	6.19%	0.830%
50	10.835	1463	1465	1466	rBV2	1321	1047	0.12%	0.016%
51	10.927	1473	1480	1490	rBV	105640	184235	20.96%	2.811%
52	11.067	1497	1503	1509	rVB2	34598	61103	6.95%	0.932%
53	11.256	1532	1534	1537	rBV4	1270	1359	0.15%	0.021%
54	11.359	1547	1551	1553	rBV5	1068	1217	0.14%	0.019%
55	11.384	1553	1555	1556	rVV2	1496	1080	0.12%	0.016%
56	11.433	1560	1563	1569	rVB2	13356	21380	2.43%	0.326%
57	11.628	1588	1595	1604	rBV	375514	638216	72.59%	9.739%
58	12.115	1672	1675	1678	rBV5	964	889	0.10%	0.014%
59	12.396	1716	1721	1722	rBV4	1287	1929	0.22%	0.029%
60	12.414	1722	1724	1726	rVB3	1126	1020	0.12%	0.016%
61	12.542	1744	1745	1748	rVB3	1287	1123	0.13%	0.017%
62	12.603	1749	1755	1761	rVB3	18019	31871	3.63%	0.486%
63	12.688	1761	1769	1777	rVB2	168232	284433	32.35%	4.340%
64	12.743	1777	1778	1781	rBV3	1161	1217	0.14%	0.019%
65	12.877	1796	1800	1801	rVV4	911	1436	0.16%	0.022%
66	12.926	1803	1808	1814	rVV2	8487	14968	1.70%	0.228%
67	13.079	1832	1833	1836	rBV3	974	866	0.10%	0.013%
68	13.243	1856	1860	1863	rVB5	998	1533	0.17%	0.023%
69	13.280	1864	1866	1868	rBV3	1838	1547	0.18%	0.024%
70	13.383	1880	1883	1884	rBV3	1387	873	0.10%	0.013%
71	13.402	1884	1886	1890	rBV5	2421	2862	0.33%	0.044%
72	13.475	1896	1898	1899	rBV	1552	1291	0.15%	0.020%
73	13.554	1905	1911	1924	rVB	366263	593784	67.54%	9.061%
74	13.713	1935	1937	1939	rBV2	901	1101	0.13%	0.017%
75	13.853	1953	1960	1967	rBV	394423	626089	71.22%	9.554%
76	14.060	1990	1994	2000	rVB2	6722	12707	1.45%	0.194%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
 Title : SFAM01.0

77	14.322	2034	2037	2042	rVB6	2407	4558	0.52%	0.070%
78	14.450	2055	2058	2060	rVB4	1150	1226	0.14%	0.019%
79	14.487	2060	2064	2066	rBV4	1213	1913	0.22%	0.029%
80	14.725	2101	2103	2105	rVB4	1543	1182	0.13%	0.018%
81	14.859	2123	2125	2128	rBV3	1056	1441	0.16%	0.022%
82	14.987	2142	2146	2149	rVB6	1380	2171	0.25%	0.033%
83	15.023	2149	2152	2153	rBV2	1335	1375	0.16%	0.021%
84	15.103	2162	2165	2166	rBV3	1370	1373	0.16%	0.021%
85	15.346	2202	2205	2207	rBV4	946	1218	0.14%	0.019%
86	15.365	2207	2208	2211	rVB2	1490	934	0.11%	0.014%
87	15.432	2215	2219	2223	rVV5	3318	4604	0.52%	0.070%
88	15.633	2250	2252	2255	rVB4	923	873	0.10%	0.013%
89	15.664	2255	2257	2260	rBV4	1112	1325	0.15%	0.020%
90	15.962	2302	2306	2307	rBV4	1480	2179	0.25%	0.033%
91	16.066	2319	2323	2325	rBV5	1449	2064	0.23%	0.031%
92	16.109	2329	2330	2333	rBV3	957	934	0.11%	0.014%
93	16.291	2357	2360	2363	rBV5	1240	1621	0.18%	0.025%
94	16.316	2363	2364	2371	rVV7	1607	1807	0.21%	0.028%
95	16.383	2371	2375	2376	rVV4	967	1262	0.14%	0.019%
96	16.401	2376	2378	2381	rVV4	1184	1538	0.17%	0.023%
97	16.444	2383	2385	2387	rVB3	1038	884	0.10%	0.013%
98	16.480	2387	2391	2393	rBV4	1640	2378	0.27%	0.036%
99	16.517	2393	2397	2399	rVV5	1239	1932	0.22%	0.029%
100	16.639	2413	2417	2421	rVB6	1374	1715	0.20%	0.026%

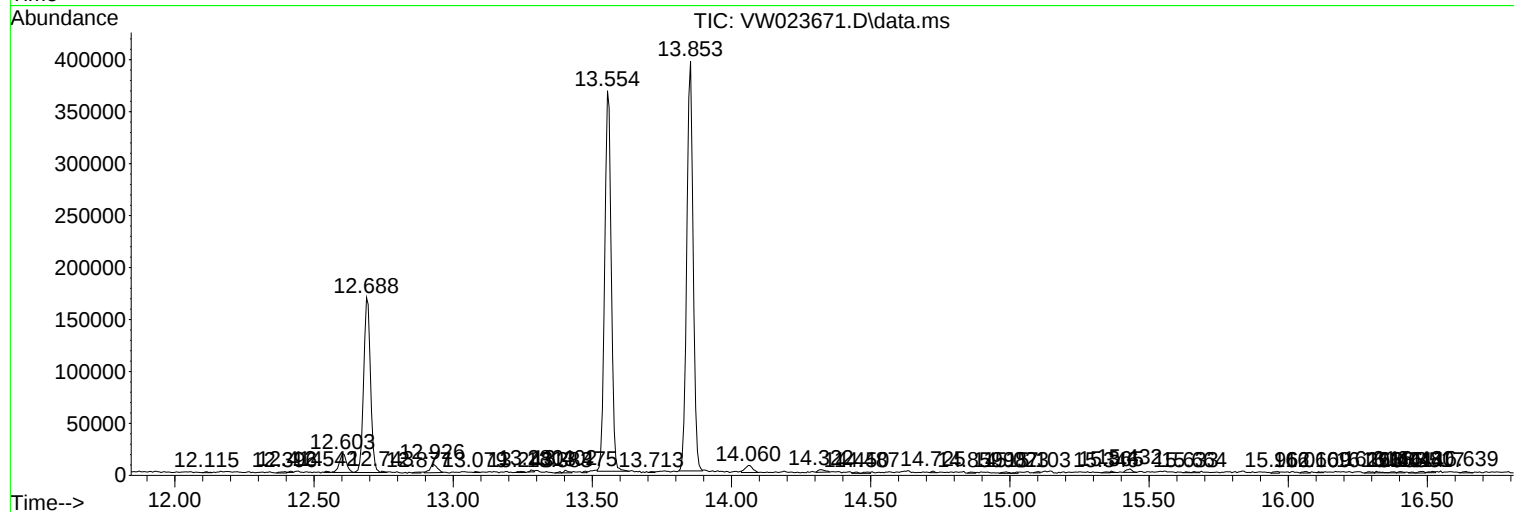
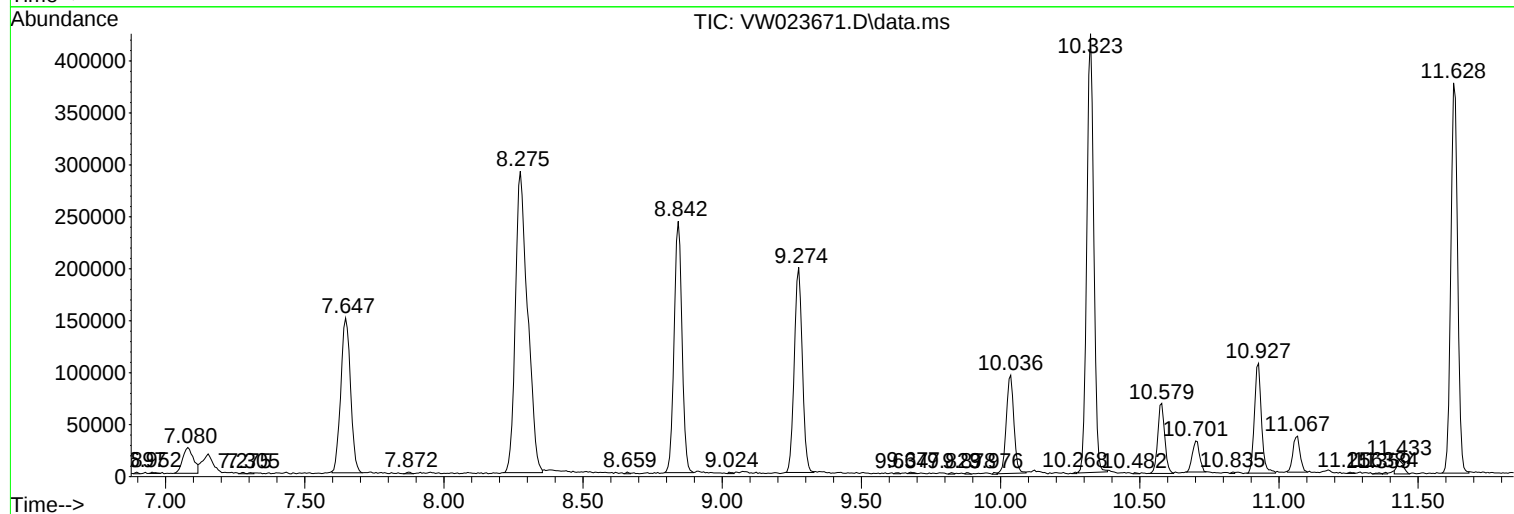
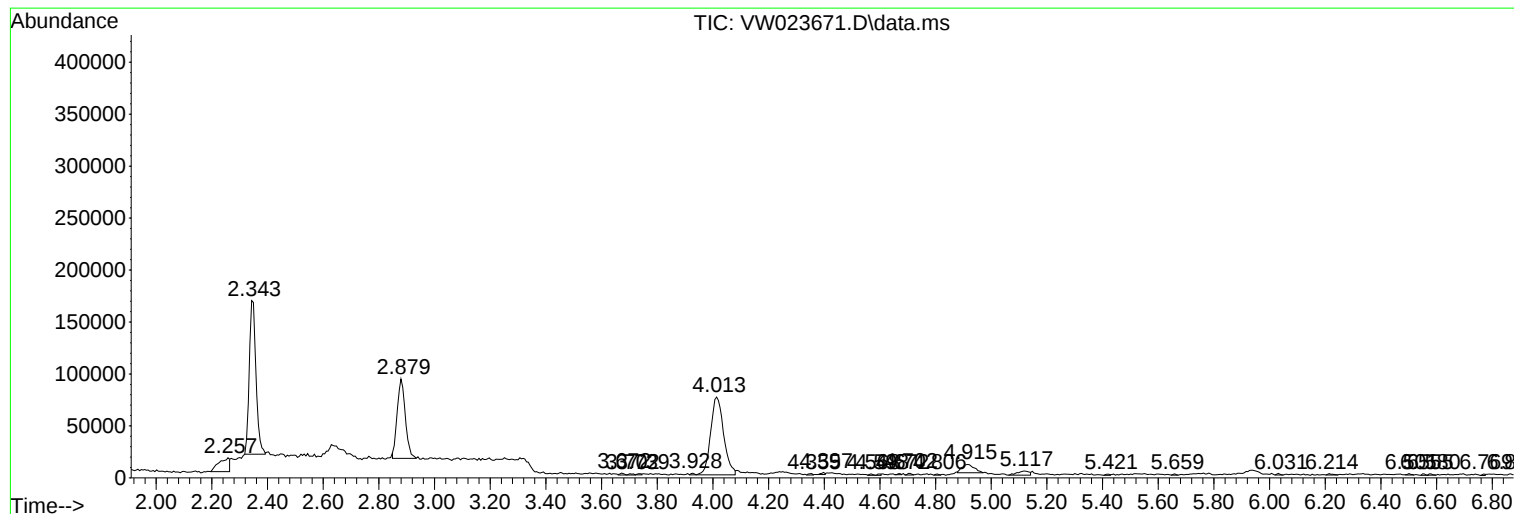
Sum of corrected areas: 6553485

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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_W
ClientSampleId :
VBLK544

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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



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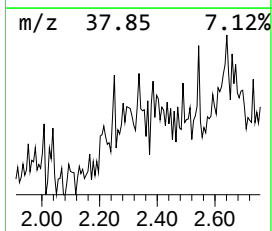
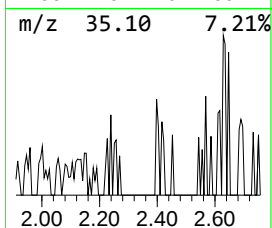
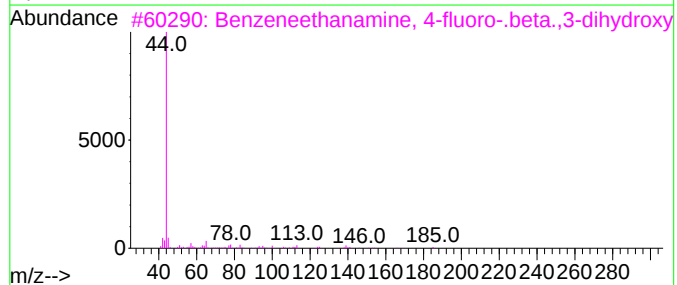
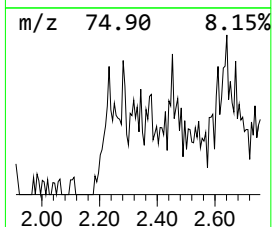
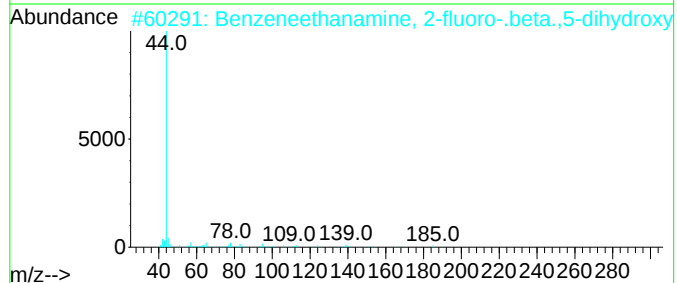
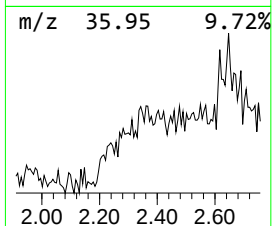
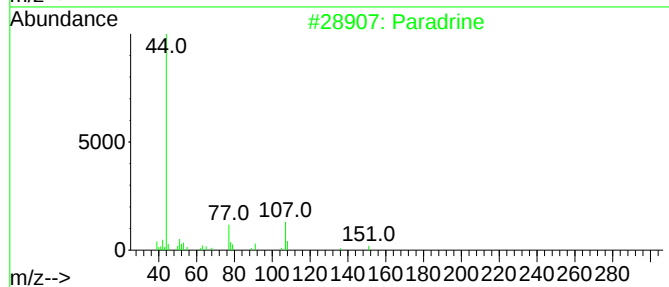
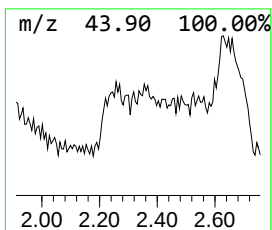
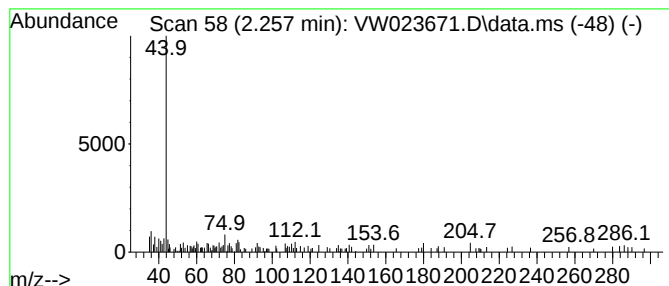
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Paradrine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	1.88 ug/L	35722	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Paradrine	151	C9H13NO	000103-86-6	64
2			Benzeneethanamine, 2-fluoro-.bet...	185	C9H12FN02	103439-07-2	64
3			Benzeneethanamine, 4-fluoro-.bet...	185	C9H12FN02	103439-06-1	64
4			8-[N-Aziridylethylamino]-2,6-dim...	224	C14H28N2	1000256-01-2	64
5			Paradrine	151	C9H13NO	000103-86-6	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Paradrine	2.257	1.9	ug/L	35722	1	8.842	474662	25.0