

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW042723\
 Data File : VW025730.D
 Acq On : 27 Apr 2023 17:36
 Operator : SY/MD
 Sample : 02499-22
 Misc : 5.82g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCCC0

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\SFAMWLM042723SMA.M
 Title : SFAM01.0

Signal : TIC: VW025730.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.363	72	78	94	rBV	78071	211645	9.18%	1.026%
2	2.497	94	100	111	rBV	108657	305698	13.26%	1.481%
3	2.893	159	165	183	rVB2	72603	215992	9.37%	1.047%
4	3.344	236	239	243	rBV6	1312	2319	0.10%	0.011%
5	3.527	262	269	271	rBV6	3169	6242	0.27%	0.030%
6	3.679	292	294	296	rBV3	1562	1312	0.06%	0.006%
7	3.722	296	301	304	rBV4	3580	7793	0.34%	0.038%
8	3.923	331	334	335	rBV3	1148	1285	0.06%	0.006%
9	4.027	338	351	358	rBV	193728	647818	28.11%	3.139%
10	4.112	358	365	384	rVB	608634	1690836	73.36%	8.194%
11	4.387	405	410	412	rBV5	2629	5167	0.22%	0.025%
12	4.563	436	439	442	rBV4	1671	2063	0.09%	0.010%
13	4.600	442	445	446	rBV2	1409	1646	0.07%	0.008%
14	4.795	475	477	480	rVB4	2131	2046	0.09%	0.010%
15	4.826	480	482	485	rBV4	1295	1918	0.08%	0.009%
16	4.923	487	498	515	rBV2	22831	98003	4.25%	0.475%
17	5.149	533	535	537	rVV3	1443	1370	0.06%	0.007%
18	5.191	540	542	545	rVB4	1870	1784	0.08%	0.009%
19	5.222	545	547	552	rBV5	2161	3056	0.13%	0.015%
20	5.551	599	601	604	rBV4	1096	1288	0.06%	0.006%
21	5.777	634	638	639	rBV3	5007	6121	0.27%	0.030%
22	5.947	659	666	673	rVB7	5712	15790	0.69%	0.077%
23	6.069	682	686	688	rBV5	1050	1385	0.06%	0.007%
24	6.088	688	689	691	rBV2	1398	1366	0.06%	0.007%
25	6.533	760	762	767	rVB4	1577	1953	0.08%	0.009%
26	6.728	791	794	798	rVB5	1362	2214	0.10%	0.011%
27	6.783	798	803	806	rBV7	1080	2362	0.10%	0.011%
28	6.905	816	823	826	rBV7	2986	6399	0.28%	0.031%
29	6.935	826	828	831	rVB4	1819	1780	0.08%	0.009%
30	6.990	831	837	838	rBV6	2619	4126	0.18%	0.020%
31	7.075	842	851	859	rVV	99874	277106	12.02%	1.343%
32	7.173	860	867	881	rVB	74561	210625	9.14%	1.021%
33	7.648	933	945	959	rBV	382476	938657	40.73%	4.549%
34	7.837	973	976	980	rBV6	1171	1859	0.08%	0.009%
35	7.923	986	990	993	rVV6	1397	2643	0.11%	0.013%
36	7.947	993	994	1004	rVB9	2869	6760	0.29%	0.033%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM042723SMA.M
 Title : SFAM01.0

37	8.020	1004	1006	1007	rBV2	1545	1345	0.06%	0.007%
38	8.160	1026	1029	1032	rBV5	1287	1999	0.09%	0.010%
39	8.276	1034	1048	1065	rBV2	774101	2304805	100.00%	11.169%
40	8.551	1085	1093	1103	rVV3	53965	120924	5.25%	0.586%
41	8.709	1109	1119	1126	rBV2	14975	35711	1.55%	0.173%
42	8.843	1132	1141	1154	rBV	884769	1740549	75.52%	8.435%
43	9.093	1177	1182	1187	rVB4	8960	19936	0.86%	0.097%
44	9.270	1202	1211	1228	rVV	546436	1143191	49.60%	5.540%
45	9.666	1271	1276	1282	rBV9	3385	6502	0.28%	0.032%
46	9.758	1287	1291	1298	rVB8	2495	6240	0.27%	0.030%
47	9.892	1307	1313	1317	rBV7	3973	8907	0.39%	0.043%
48	10.032	1326	1336	1347	rBV	281241	516395	22.41%	2.502%
49	10.203	1362	1364	1367	rBV3	2055	2215	0.10%	0.011%
50	10.239	1368	1370	1374	rVB5	2647	3068	0.13%	0.015%
51	10.319	1375	1383	1391	rBV	1025577	1810123	78.54%	8.772%
52	10.575	1419	1425	1435	rBV	184617	326139	14.15%	1.580%
53	10.703	1441	1446	1452	rVB	10554	19449	0.84%	0.094%
54	10.861	1464	1472	1477	rBV	299751	519257	22.53%	2.516%
55	10.922	1477	1482	1497	rVB	358999	622584	27.01%	3.017%
56	11.074	1505	1507	1514	rVB8	3563	4198	0.18%	0.020%
57	11.398	1556	1560	1566	rVB7	2035	4112	0.18%	0.020%
58	11.471	1569	1572	1574	rBV4	1178	1319	0.06%	0.006%
59	11.629	1588	1598	1610	rBV	1209433	2026456	87.92%	9.820%
60	11.830	1626	1631	1641	rBV8	6101	16054	0.70%	0.078%
61	12.111	1673	1677	1679	rVV5	1993	2867	0.12%	0.014%
62	12.166	1681	1686	1693	rVB5	7852	15522	0.67%	0.075%
63	12.239	1694	1698	1701	rBV6	2392	3430	0.15%	0.017%
64	12.373	1717	1720	1721	rBV3	1305	1304	0.06%	0.006%
65	12.458	1730	1734	1739	rBV6	2684	4586	0.20%	0.022%
66	12.605	1750	1758	1764	rVV2	40746	79239	3.44%	0.384%
67	12.690	1765	1772	1779	rVV	481143	780459	33.86%	3.782%
68	12.757	1779	1783	1787	rVV5	8038	15437	0.67%	0.075%
69	12.934	1808	1812	1820	rVB8	5720	11906	0.52%	0.058%
70	13.001	1820	1823	1824	rBV3	1937	1683	0.07%	0.008%
71	13.111	1836	1841	1844	rBV7	2181	3414	0.15%	0.017%
72	13.184	1850	1853	1858	rVB4	5408	8030	0.35%	0.039%
73	13.245	1861	1863	1864	rBV2	3792	3292	0.14%	0.016%
74	13.397	1882	1888	1894	rBV3	10820	20288	0.88%	0.098%
75	13.464	1894	1899	1902	rBV4	9335	14871	0.65%	0.072%
76	13.556	1907	1914	1925	rVV	1211483	1953218	84.75%	9.465%

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 Title : SFAM01.0

77	13.641	1925	1928	1936	rVB2	13287	23313	1.01%	0.113%
78	13.757	1941	1947	1951	rBV7	4248	10056	0.44%	0.049%
79	13.848	1955	1962	1975	rVV	956356	1534397	66.57%	7.436%
80	14.001	1984	1987	1988	rBV3	1983	2226	0.10%	0.011%
81	14.062	1992	1997	2003	rVV	37353	62188	2.70%	0.301%
82	14.196	2016	2019	2021	rBV4	1556	2177	0.09%	0.011%
83	14.324	2035	2040	2045	rVB9	7232	12401	0.54%	0.060%
84	14.495	2064	2068	2069	rBV4	1573	1658	0.07%	0.008%
85	14.623	2083	2089	2094	rBV9	4428	9421	0.41%	0.046%
86	14.714	2102	2104	2107	rVB4	1769	1519	0.07%	0.007%
87	14.775	2112	2114	2119	rBV6	1666	2462	0.11%	0.012%
88	14.995	2148	2150	2152	rVB3	1468	1276	0.06%	0.006%
89	15.123	2169	2171	2175	rBV5	2830	4041	0.18%	0.020%
90	15.177	2175	2180	2186	rBV9	3858	7872	0.34%	0.038%
91	15.360	2206	2210	2213	rVV3	4139	7675	0.33%	0.037%
92	15.427	2216	2221	2226	rVV2	18789	34815	1.51%	0.169%
93	15.482	2226	2230	2236	rVB	14257	23999	1.04%	0.116%
94	15.543	2236	2240	2243	rBV6	2991	4610	0.20%	0.022%
95	15.629	2252	2254	2258	rBV5	1472	1947	0.08%	0.009%
96	15.787	2275	2280	2284	rBV8	4049	7166	0.31%	0.035%
97	15.933	2302	2304	2305	rBV2	1591	1518	0.07%	0.007%
98	16.086	2325	2329	2333	rBV6	2298	3937	0.17%	0.019%
99	16.311	2364	2366	2369	rVB4	1675	1629	0.07%	0.008%
100	16.531	2400	2402	2406	rBV5	1257	1729	0.08%	0.008%

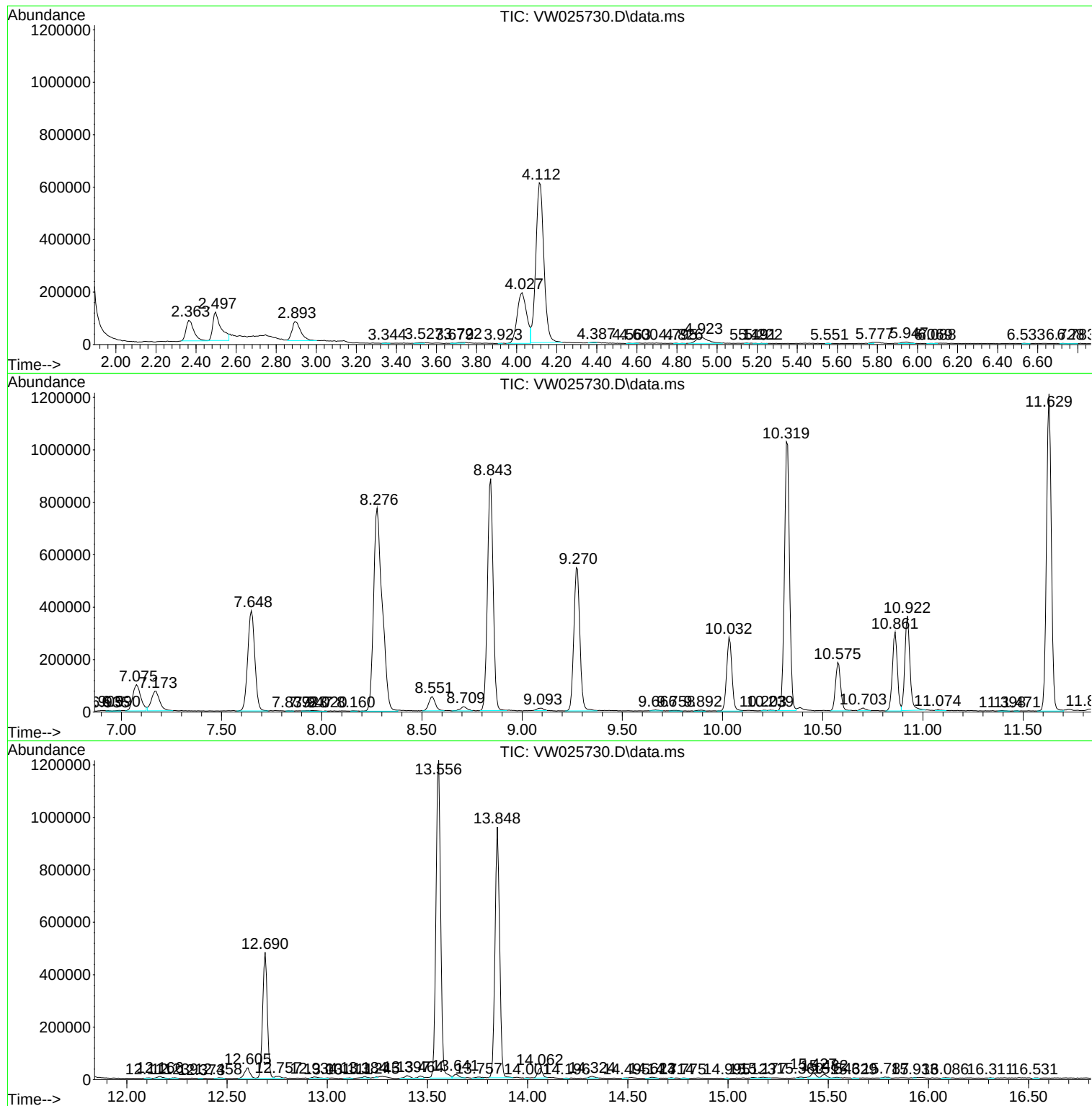
Sum of corrected areas: 20635483

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM042723SMA.M
Quant Title : SFAM01.0

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



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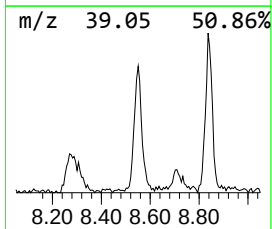
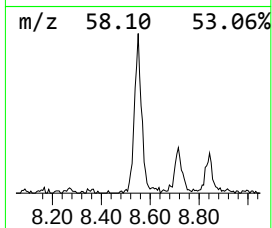
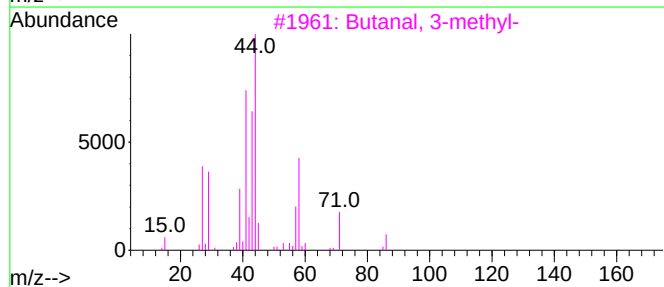
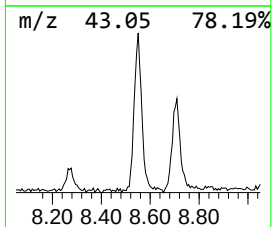
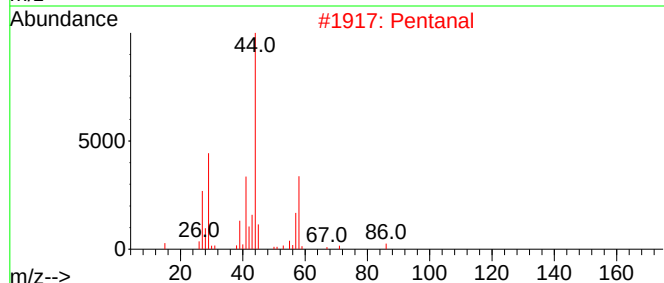
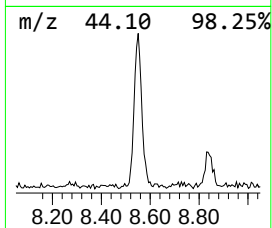
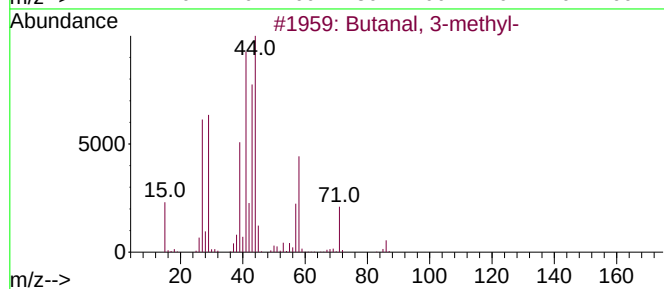
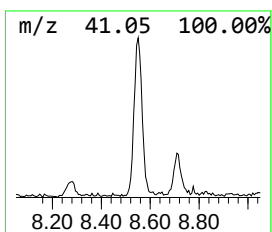
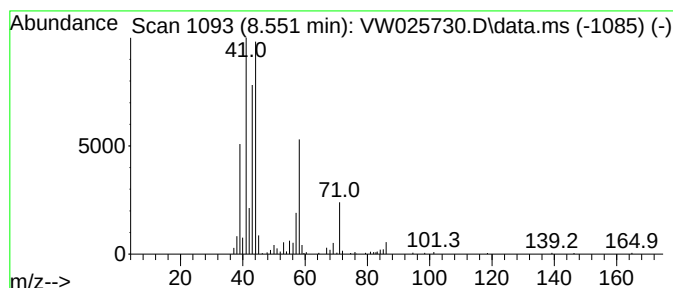
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM042723SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 Butanal, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.551	1.74 ug/L	120924	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 3-methyl-	86	C5H10O	000590-86-3	91
2			Pentanal	86	C5H10O	000110-62-3	47
3			Butanal, 3-methyl-	86	C5H10O	000590-86-3	45
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	43
5			Butanal, 3-methyl-	86	C5H10O	000590-86-3	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal, 3-methyl-	8.551	1.7	ug/L	120924	1	8.843	1740550	25.0