

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW081023\
 Data File : VW026687.D
 Acq On : 10 Aug 2023 19:19
 Operator : SY/MD
 Sample : 03967-04
 Misc : 5.20g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A48K4

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\SFAMWLM081023SMA.M
 Title : SFAM01.0

Signal : TIC: VW026687.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.155	40	44	46	rBV	4678	6819	0.21%	0.034%
2	2.369	72	79	93	rBV	112772	358173	10.81%	1.809%
3	2.893	158	165	186	rVB	111200	347245	10.48%	1.754%
4	3.393	240	247	254	rBV4	10695	27389	0.83%	0.138%
5	3.582	268	278	279	rBV2	12395	27623	0.83%	0.140%
6	3.814	314	316	320	rBV4	953	1379	0.04%	0.007%
7	4.027	339	351	377	rVV	265224	1051639	31.74%	5.311%
8	4.381	406	409	412	rBV5	1296	1739	0.05%	0.009%
9	4.436	416	418	421	rVV4	1308	1328	0.04%	0.007%
10	4.570	437	440	442	rBV3	1386	1480	0.04%	0.007%
11	4.625	442	449	452	rBV5	2401	6291	0.19%	0.032%
12	4.759	470	471	473	rBV2	1343	1219	0.04%	0.006%
13	4.917	491	497	500	rBV7	3875	8322	0.25%	0.042%
14	5.106	522	528	533	rBV10	1319	2837	0.09%	0.014%
15	5.277	552	556	559	rVB6	1398	2272	0.07%	0.011%
16	5.313	559	562	564	rBV4	1012	1217	0.04%	0.006%
17	5.545	598	600	605	rVB5	835	1378	0.04%	0.007%
18	5.667	618	620	623	rVB4	1286	1377	0.04%	0.007%
19	5.746	631	633	634	rBV2	1458	1177	0.04%	0.006%
20	5.941	657	665	674	rBV2	3119	9091	0.27%	0.046%
21	6.130	693	696	699	rVB4	1209	1303	0.04%	0.007%
22	6.289	718	722	724	rBV4	991	1347	0.04%	0.007%
23	6.521	756	760	765	rVB7	920	1459	0.04%	0.007%
24	6.679	783	786	788	rBV4	1268	1329	0.04%	0.007%
25	6.813	806	808	814	rBV4	1481	2738	0.08%	0.014%
26	6.880	816	819	822	rBV5	1087	1289	0.04%	0.007%
27	6.917	824	825	831	rVB6	1029	1554	0.05%	0.008%
28	7.081	844	852	859	rBV	81467	233821	7.06%	1.181%
29	7.429	905	909	910	rBV4	1381	1257	0.04%	0.006%
30	7.447	910	912	916	rVB4	2137	2106	0.06%	0.011%
31	7.648	935	945	957	rBV	536948	1318396	39.80%	6.658%
32	7.807	968	971	974	rVB4	1196	1195	0.04%	0.006%
33	7.886	981	984	985	rBV3	1088	1279	0.04%	0.006%
34	8.039	1007	1009	1012	rBV4	1516	2170	0.07%	0.011%
35	8.130	1021	1024	1026	rVB4	1288	1231	0.04%	0.006%
36	8.276	1036	1048	1064	rBV2	1129667	3312804	100.00%	16.730%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.M
 Title : SFAM01.0

37	8.532	1086	1090	1091	rBV4	1914	2193	0.07%	0.011%
38	8.618	1102	1104	1110	rVB7	1642	2424	0.07%	0.012%
39	8.709	1112	1119	1128	rVB4	6835	17748	0.54%	0.090%
40	8.843	1132	1141	1157	rBV	949232	1871760	56.50%	9.453%
41	9.063	1169	1177	1178	rBV6	3975	7660	0.23%	0.039%
42	9.270	1202	1211	1222	rVV	739019	1532584	46.26%	7.740%
43	9.429	1235	1237	1247	rVB8	2785	6763	0.20%	0.034%
44	9.587	1259	1263	1265	rBV5	945	1377	0.04%	0.007%
45	9.654	1268	1274	1276	rBV7	2092	3685	0.11%	0.019%
46	10.032	1329	1336	1351	rBV	329017	592709	17.89%	2.993%
47	10.209	1361	1365	1368	rBV6	1161	1685	0.05%	0.009%
48	10.319	1375	1383	1392	rBV	1417250	2505554	75.63%	12.654%
49	10.428	1397	1401	1408	rVB6	10048	17071	0.52%	0.086%
50	10.502	1410	1413	1417	rBV6	3121	5091	0.15%	0.026%
51	10.575	1419	1425	1436	rVV	223193	387273	11.69%	1.956%
52	10.703	1440	1446	1453	rVB	16870	30781	0.93%	0.155%
53	10.751	1453	1454	1459	rBV5	1668	2347	0.07%	0.012%
54	10.849	1466	1470	1476	rBV7	3363	5139	0.16%	0.026%
55	10.922	1476	1482	1493	rBV	196727	347945	10.50%	1.757%
56	11.026	1494	1499	1515	rVB3	41994	87956	2.66%	0.444%
57	11.172	1520	1523	1529	rVB7	4239	7656	0.23%	0.039%
58	11.312	1541	1546	1547	rBV4	1365	1814	0.05%	0.009%
59	11.398	1553	1560	1566	rBV4	4228	9185	0.28%	0.046%
60	11.629	1588	1598	1608	rBV	1173964	1956137	59.05%	9.879%
61	11.837	1626	1632	1637	rBV8	3595	7582	0.23%	0.038%
62	11.922	1642	1646	1648	rBV5	1643	3141	0.09%	0.016%
63	12.172	1682	1687	1694	rVB9	4876	11095	0.33%	0.056%
64	12.337	1712	1714	1716	rBV3	1490	1442	0.04%	0.007%
65	12.379	1719	1721	1725	rVB5	1396	1828	0.06%	0.009%
66	12.452	1728	1733	1734	rBV5	2926	3164	0.10%	0.016%
67	12.605	1748	1758	1763	rBV2	19060	37270	1.13%	0.188%
68	12.690	1763	1772	1781	rBV	469842	773884	23.36%	3.908%
69	12.757	1781	1783	1790	rVB8	5141	7906	0.24%	0.040%
70	12.940	1808	1813	1816	rBV6	6117	12241	0.37%	0.062%
71	13.038	1822	1829	1833	rBV8	3894	7476	0.23%	0.038%
72	13.080	1833	1836	1838	rVB4	2038	2205	0.07%	0.011%
73	13.147	1843	1847	1851	rBV6	3534	6097	0.18%	0.031%
74	13.208	1851	1857	1866	rVV	187676	315796	9.53%	1.595%
75	13.282	1866	1869	1878	rVB2	22701	46992	1.42%	0.237%
76	13.501	1900	1905	1908	rBV6	11906	18844	0.57%	0.095%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.M
 Title : SFAM01.0

77	13.556	1908	1914	1925	rVB	765944	1212292	36.59%	6.122%
78	13.751	1943	1946	1950	rBV5	5239	8831	0.27%	0.045%
79	13.849	1955	1962	1968	rBV	603167	995424	30.05%	5.027%
80	13.946	1975	1978	1983	rVB4	6916	8795	0.27%	0.044%
81	14.062	1993	1997	2003	rVB	10160	15281	0.46%	0.077%
82	14.263	2025	2030	2034	rBV7	3621	6062	0.18%	0.031%
83	14.324	2036	2040	2047	rVB7	5940	10775	0.33%	0.054%
84	14.489	2064	2067	2070	rBV5	3364	4096	0.12%	0.021%
85	14.519	2070	2072	2075	rVB4	3668	3817	0.12%	0.019%
86	14.623	2084	2089	2096	rBV4	9955	19362	0.58%	0.098%
87	14.690	2096	2100	2102	rVV4	6846	10876	0.33%	0.055%
88	14.714	2102	2104	2108	rVV3	9017	11706	0.35%	0.059%
89	14.775	2112	2114	2117	rVB4	1801	1278	0.04%	0.006%
90	14.818	2117	2121	2122	rBV4	1239	1350	0.04%	0.007%
91	14.940	2139	2141	2146	rVB6	1844	2371	0.07%	0.012%
92	15.068	2157	2162	2166	rBV7	5234	9840	0.30%	0.050%
93	15.129	2166	2172	2180	rVV4	9145	20733	0.63%	0.105%
94	15.367	2203	2211	2214	rBV3	8691	19535	0.59%	0.099%
95	15.549	2236	2241	2248	rVB5	9879	18053	0.54%	0.091%
96	15.684	2256	2263	2265	rBV6	2649	5384	0.16%	0.027%
97	15.745	2271	2273	2274	rBV2	1984	1522	0.05%	0.008%
98	15.830	2285	2287	2291	rBV5	1714	2573	0.08%	0.013%
99	15.946	2303	2306	2308	rBV4	1815	2320	0.07%	0.012%
100	16.604	2411	2414	2417	rBV5	1778	2206	0.07%	0.011%

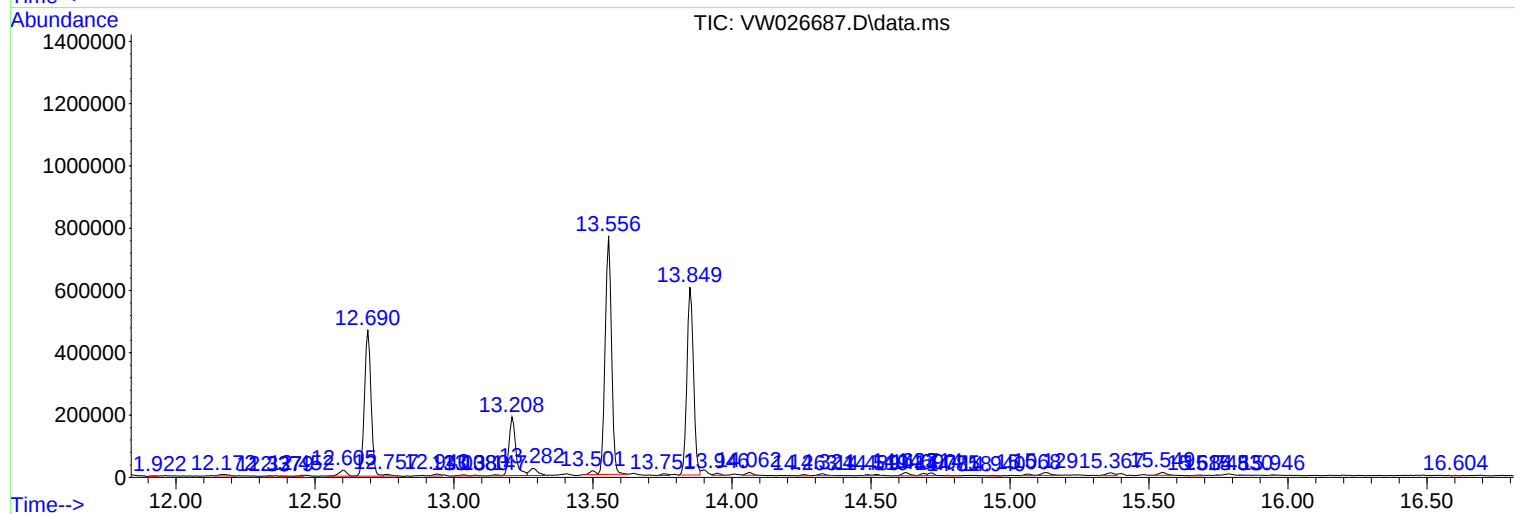
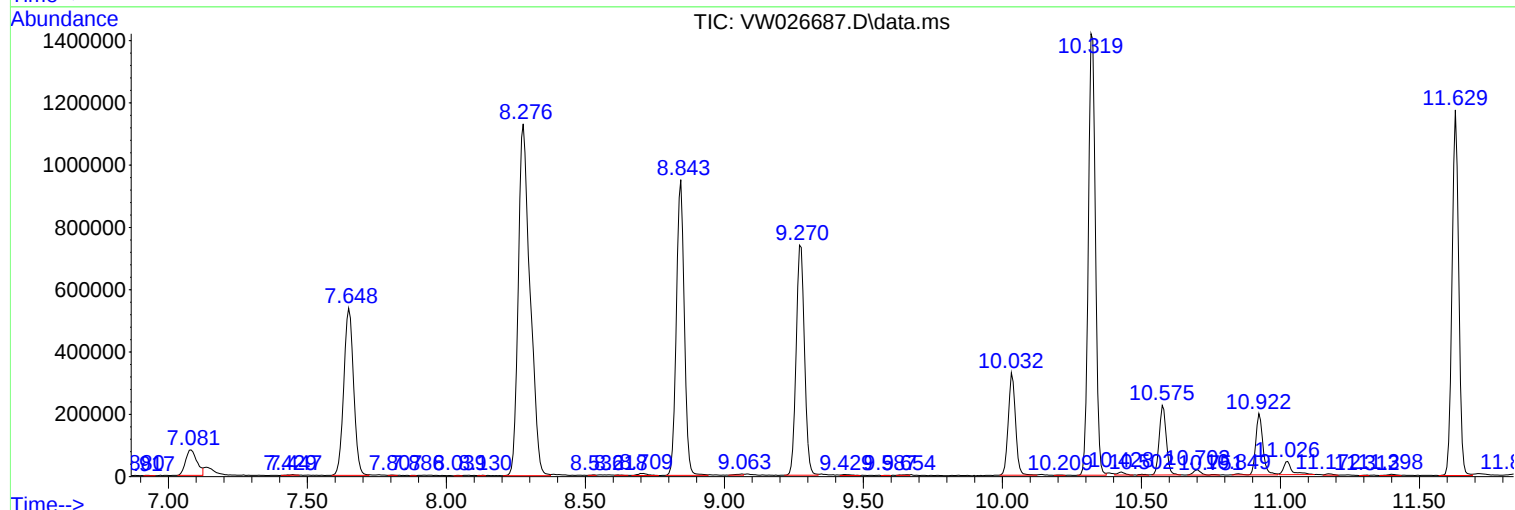
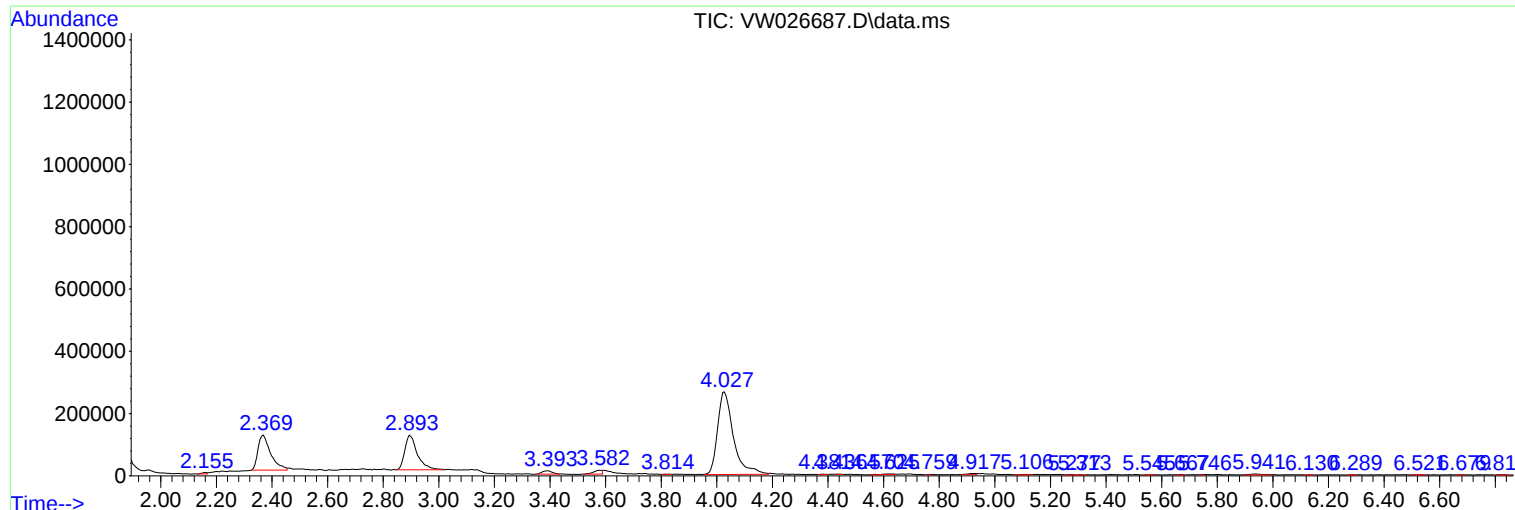
Sum of corrected areas: 19801255

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.M
Quant Title : SFAM01.0

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



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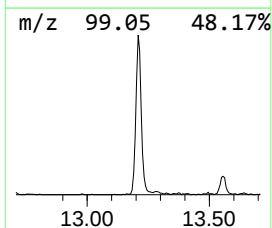
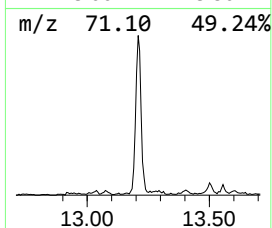
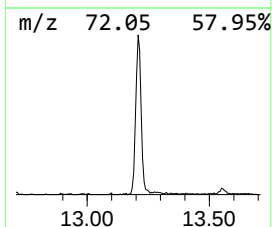
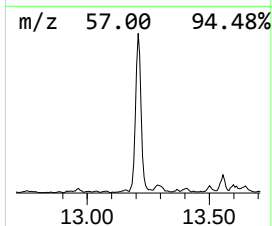
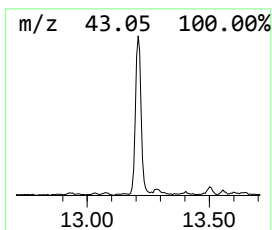
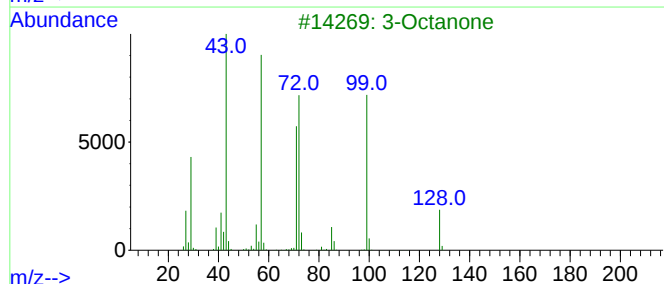
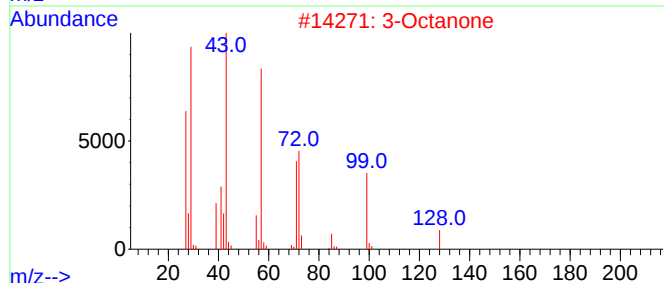
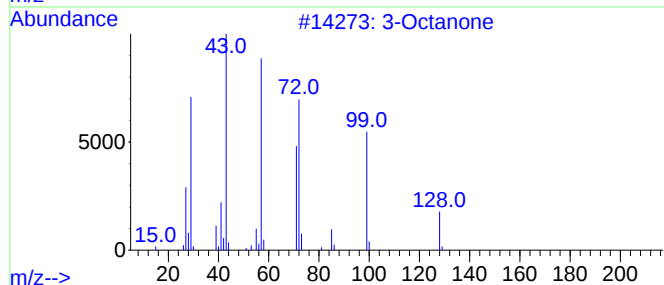
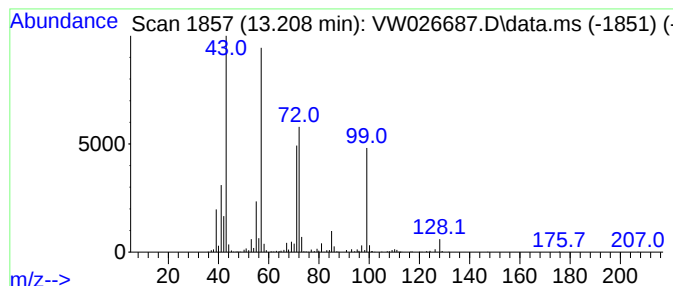
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 3-Octanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.208	6.51 ug/L	315796	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone			128	C8H16O	000106-68-3	91
2	3-Octanone			128	C8H16O	000106-68-3	83
3	3-Octanone			128	C8H16O	000106-68-3	78
4	3-Octanone			128	C8H16O	000106-68-3	50
5	1-Pyrrolidinecarboxaldehyde			99	C5H9NO	003760-54-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Octanone	13.208	6.5	ug/L	315796	3	13.556	1212290	25.0