

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW081123\
 Data File : VW026704.D
 Acq On : 11 Aug 2023 12:46
 Operator : SY/MD
 Sample : 03968-05
 Misc : 5.20g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A48N7

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: VW026704.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	95	rVB	131246	359819	11.47%	1.862%
2	2.893	158	165	181	rBV	112570	340011	10.84%	1.759%
3	3.271	225	227	230	rVB4	1511	1337	0.04%	0.007%
4	3.387	240	246	253	rVB3	3715	7454	0.24%	0.039%
5	3.533	268	270	275	rVB5	2214	1969	0.06%	0.010%
6	3.740	302	304	307	rVV3	1347	1146	0.04%	0.006%
7	4.021	339	350	379	rBV	265539	981534	31.30%	5.078%
8	4.356	403	405	406	rVB2	2182	1216	0.04%	0.006%
9	4.399	408	412	415	rBV6	1276	1428	0.05%	0.007%
10	4.600	442	445	447	rBV4	1257	2045	0.07%	0.011%
11	4.862	484	488	489	rBV4	1488	1800	0.06%	0.009%
12	4.917	489	497	505	rBV2	16261	57238	1.83%	0.296%
13	5.167	537	538	543	rVB5	1231	1722	0.05%	0.009%
14	5.313	558	562	563	rVB4	1039	1192	0.04%	0.006%
15	5.344	563	567	570	rBV5	1268	1596	0.05%	0.008%
16	5.435	580	582	586	rVB5	1229	1024	0.03%	0.005%
17	5.539	597	599	602	rBV4	1266	1284	0.04%	0.007%
18	5.594	605	608	611	rBV5	1081	1715	0.05%	0.009%
19	5.850	649	650	654	rBV4	819	1143	0.04%	0.006%
20	5.947	655	666	674	rBV4	8325	25837	0.82%	0.134%
21	6.179	700	704	705	rVB2	1263	1664	0.05%	0.009%
22	6.368	733	735	738	rBV4	1329	1422	0.05%	0.007%
23	6.527	758	761	763	rVB3	885	1018	0.03%	0.005%
24	6.612	772	775	777	rVB3	1197	1259	0.04%	0.007%
25	6.795	801	805	807	rVB5	921	1257	0.04%	0.007%
26	6.825	807	810	814	rBV6	1492	2413	0.08%	0.012%
27	6.911	823	824	829	rBV4	1420	1476	0.05%	0.008%
28	7.002	836	839	841	rBV4	1396	1381	0.04%	0.007%
29	7.075	841	851	870	rBV2	85131	294690	9.40%	1.525%
30	7.258	879	881	883	rVB3	1557	1049	0.03%	0.005%
31	7.301	886	888	890	rVB3	1455	1098	0.04%	0.006%
32	7.532	922	926	932	rVV7	1361	2418	0.08%	0.013%
33	7.648	932	945	959	rBV	511903	1266483	40.38%	6.552%
34	7.825	972	974	977	rBV4	1374	2017	0.06%	0.010%
35	7.929	986	991	992	rBV4	1285	2122	0.07%	0.011%
36	8.136	1022	1025	1029	rBV5	774	1316	0.04%	0.007%

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

37	8.276	1035	1048	1063	rBV2	1088993	3136247	100.00%	16.226%
38	8.544	1090	1092	1094	rVB4	1517	1193	0.04%	0.006%
39	8.685	1112	1115	1116	rBV3	1163	1379	0.04%	0.007%
40	8.703	1116	1118	1121	rVB4	1810	1379	0.04%	0.007%
41	8.843	1130	1141	1156	rBV	1002974	1980082	63.14%	10.244%
42	9.038	1171	1173	1174	rBV2	1629	1158	0.04%	0.006%
43	9.081	1178	1180	1187	rVB8	4567	8306	0.26%	0.043%
44	9.136	1187	1189	1191	rBV2	1556	1385	0.04%	0.007%
45	9.270	1201	1211	1221	rBV	719199	1485208	47.36%	7.684%
46	9.514	1249	1251	1255	rVB5	1077	1307	0.04%	0.007%
47	9.569	1258	1260	1262	rBV3	1200	1152	0.04%	0.006%
48	9.605	1265	1266	1269	rVV3	1645	1634	0.05%	0.008%
49	9.666	1272	1276	1279	rVV4	2292	3922	0.13%	0.020%
50	9.819	1299	1301	1304	rVB4	1443	1200	0.04%	0.006%
51	9.983	1323	1328	1329	rBV4	4105	5175	0.17%	0.027%
52	10.032	1329	1336	1350	rVB	349770	630589	20.11%	3.263%
53	10.325	1375	1384	1392	rBV	1288980	2290661	73.04%	11.851%
54	10.575	1418	1425	1437	rVV	233395	406477	12.96%	2.103%
55	10.703	1440	1446	1452	rVB	22931	39222	1.25%	0.203%
56	10.843	1463	1469	1476	rBV2	8597	17476	0.56%	0.090%
57	10.922	1476	1482	1495	rBV	217862	389188	12.41%	2.014%
58	11.172	1518	1523	1528	rVB2	15372	24461	0.78%	0.127%
59	11.337	1546	1550	1555	rBV8	2353	3986	0.13%	0.021%
60	11.404	1555	1561	1566	rBV	11829	20151	0.64%	0.104%
61	11.520	1577	1580	1583	rVB5	1085	1654	0.05%	0.009%
62	11.629	1590	1598	1606	rBV	1200296	2023322	64.51%	10.468%
63	11.709	1608	1611	1615	rVB	6382	10462	0.33%	0.054%
64	11.837	1626	1632	1640	rVB	2483	7037	0.22%	0.036%
65	11.971	1651	1654	1657	rVB4	1551	2098	0.07%	0.011%
66	12.123	1675	1679	1680	rBV4	1152	1370	0.04%	0.007%
67	12.184	1683	1689	1694	rBV10	2114	5493	0.18%	0.028%
68	12.233	1695	1697	1701	rVB5	1317	1257	0.04%	0.007%
69	12.306	1705	1709	1710	rBV5	1266	1925	0.06%	0.010%
70	12.379	1719	1721	1724	rBV4	730	1065	0.03%	0.006%
71	12.599	1750	1757	1764	rBV3	18862	38835	1.24%	0.201%
72	12.690	1764	1772	1778	rBV	478583	785547	25.05%	4.064%
73	12.751	1780	1782	1789	rVB3	11254	16553	0.53%	0.086%
74	12.885	1796	1804	1807	rBV5	7458	14588	0.47%	0.075%
75	12.928	1807	1811	1813	rBV5	4570	5903	0.19%	0.031%
76	13.031	1824	1828	1832	rVV4	5317	8212	0.26%	0.042%

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 Title : SFAM01.0

77	13.074	1832	1835	1841	rVB6	5177	7193	0.23%	0.037%
78	13.208	1850	1857	1866	rBV2	39750	74086	2.36%	0.383%
79	13.397	1886	1888	1895	rVB7	4952	7404	0.24%	0.038%
80	13.446	1895	1896	1898	rBV2	1189	1151	0.04%	0.006%
81	13.464	1898	1899	1901	rVV2	2286	2097	0.07%	0.011%
82	13.501	1901	1905	1907	rVV4	5567	8924	0.28%	0.046%
83	13.556	1907	1914	1926	rVV	833328	1336599	42.62%	6.915%
84	13.641	1926	1928	1933	rVB4	6548	10743	0.34%	0.056%
85	13.751	1942	1946	1950	rBV6	8921	14929	0.48%	0.077%
86	13.848	1955	1962	1969	rBV	594663	973947	31.05%	5.039%
87	13.940	1975	1977	1981	rVB5	5579	6729	0.21%	0.035%
88	14.062	1993	1997	2013	rVB4	12505	39261	1.25%	0.203%
89	14.178	2014	2016	2017	rBV2	2539	1953	0.06%	0.010%
90	14.257	2025	2029	2034	rVB7	5799	10428	0.33%	0.054%
91	14.318	2034	2039	2043	rBV8	8134	15917	0.51%	0.082%
92	14.464	2060	2063	2064	rBV3	1888	1801	0.06%	0.009%
93	14.495	2064	2068	2070	rBV5	6168	9621	0.31%	0.050%
94	14.617	2086	2088	2089	rBV2	1841	1277	0.04%	0.007%
95	14.684	2096	2099	2102	rBV5	11407	18416	0.59%	0.095%
96	14.714	2102	2104	2112	rVB	15743	22715	0.72%	0.118%
97	15.177	2178	2180	2181	rBV2	2218	1642	0.05%	0.008%
98	15.446	2222	2224	2227	rBV4	2073	2471	0.08%	0.013%
99	16.202	2346	2348	2354	rVB7	2908	3771	0.12%	0.020%
100	16.439	2385	2387	2388	rBV2	1772	1455	0.05%	0.008%

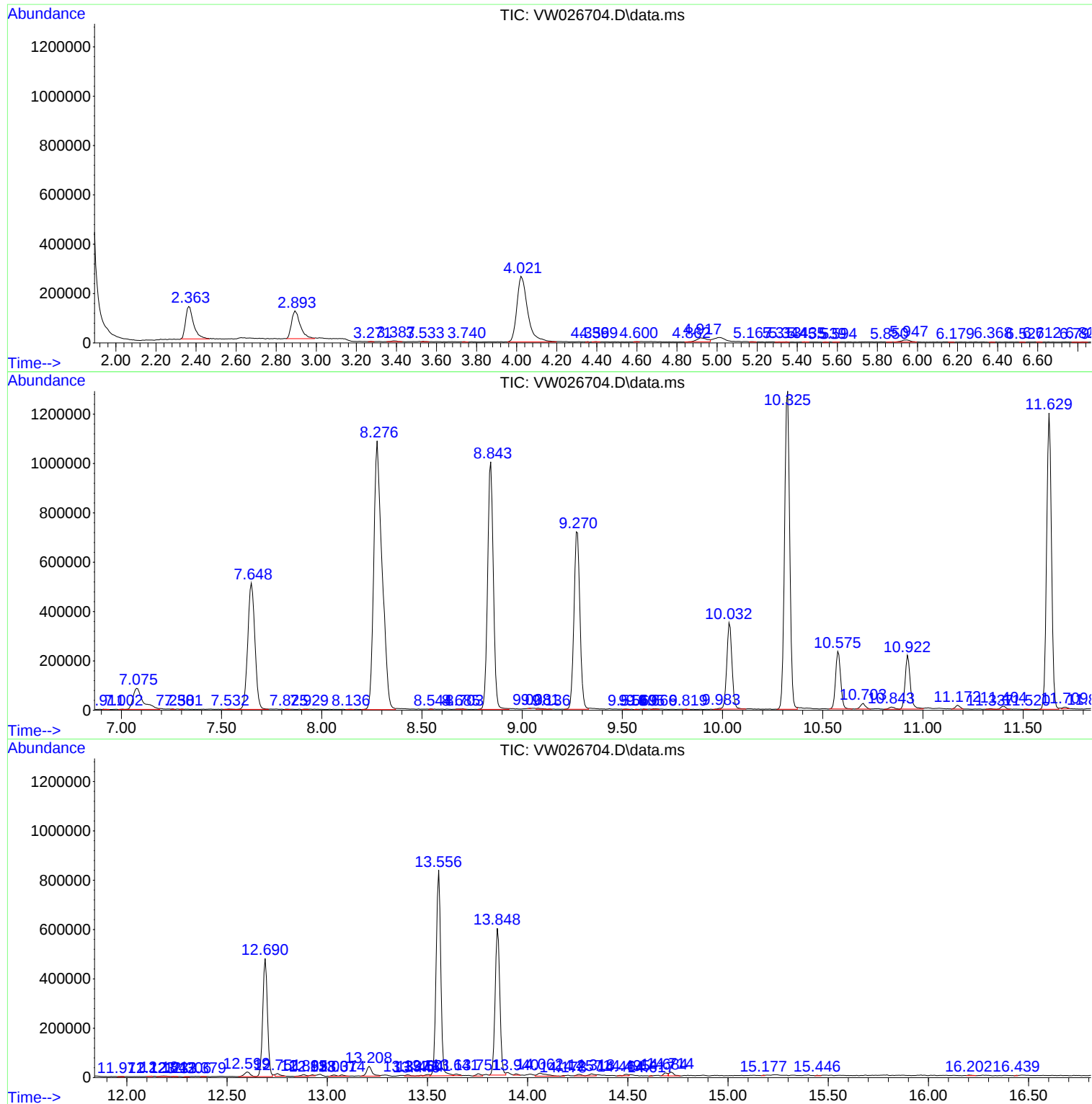
Sum of corrected areas: 19328382

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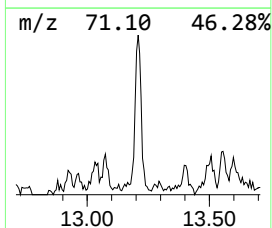
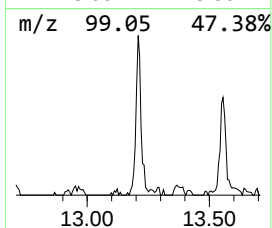
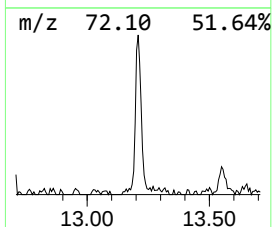
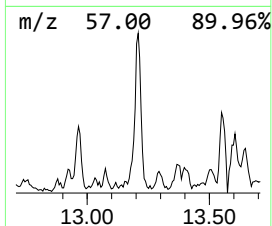
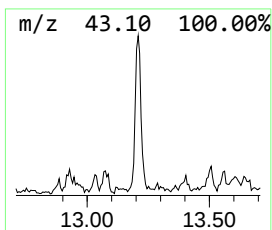
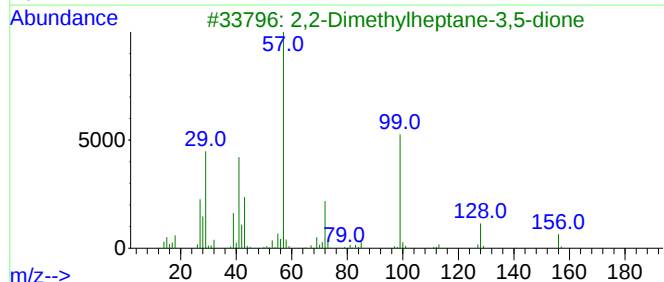
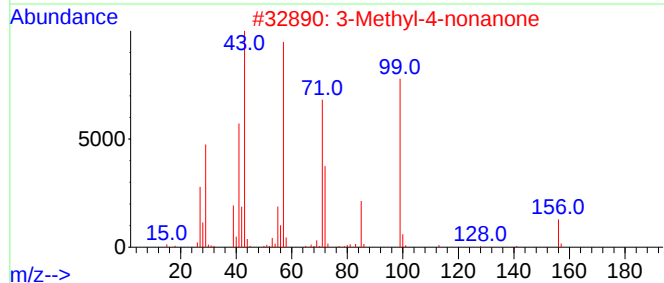
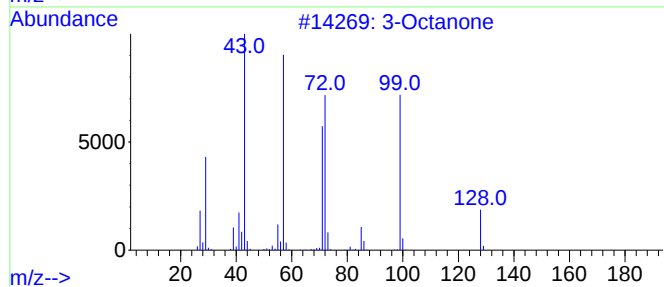
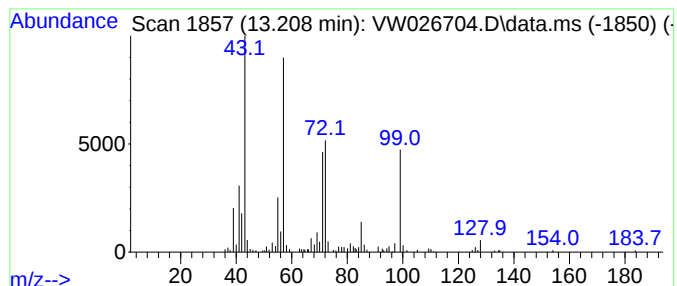
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.M
Quant Title : SFAM01.0

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	1.39 ug/L	74086	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octanone	128	C8H16O	000106-68-3	74
2			3-Methyl-4-nonanone	156	C10H20O	035778-39-3	53
3			2,2-Dimethylheptane-3,5-dione	156	C9H16O2	020734-29-6	43
4			Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	38
5			1-Iodo-2-methylnonane	268	C10H21I	1000101-47-9	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Octanone	13.208	1.4	ug/L	74086	3	13.556	1336600	25.0