

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW122221\
 Data File : VW021595.D
 Acq On : 23 Dec 2021 04:54
 Operator : SY/VA
 Sample : M5214-04
 Misc : 6.05g/10.0mL/MSVOA_W/SOIL
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 BGLF1

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\SFAMWLM120921SMA.M
 Title : SFAM01.0

Signal : TIC: VW021595.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.349	68	73	80	rVB	37273	60647	13.43%	1.738%
2	2.879	155	160	170	rVB	22786	46612	10.33%	1.336%
3	3.727	296	299	301	rBV	96	134	0.03%	0.004%
4	4.013	335	346	363	rBV	49544	138819	30.75%	3.978%
5	4.269	385	388	389	rBV	80	101	0.02%	0.003%
6	4.349	398	401	402	rBV	102	127	0.03%	0.004%
7	4.403	407	410	412	rBV	84	116	0.03%	0.003%
8	4.464	419	420	422	rBV	84	83	0.02%	0.002%
9	4.538	430	432	435	rBB	109	116	0.03%	0.003%
10	4.568	435	437	439	rBB	101	81	0.02%	0.002%
11	4.623	442	446	447	rBB	86	108	0.02%	0.003%
12	4.684	454	456	458	rBB	125	112	0.02%	0.003%
13	4.751	464	467	468	rBV	99	103	0.02%	0.003%
14	4.916	483	494	505	rBV2	7177	21724	4.81%	0.623%
15	5.092	522	523	526	rVB2	147	124	0.03%	0.004%
16	5.226	543	545	546	rBV2	111	81	0.02%	0.002%
17	5.263	549	551	554	rBB	167	162	0.04%	0.005%
18	5.342	560	564	567	rBV	81	165	0.04%	0.005%
19	5.367	567	568	572	rVB	160	174	0.04%	0.005%
20	5.409	572	575	579	rBB	160	212	0.05%	0.006%
21	5.470	582	585	586	rBB	139	106	0.02%	0.003%
22	5.489	586	588	591	rBB	79	96	0.02%	0.003%
23	5.696	620	622	623	rBV	132	114	0.03%	0.003%
24	5.793	635	638	641	rBB	87	143	0.03%	0.004%
25	5.824	642	643	645	rBV	144	120	0.03%	0.003%
26	5.940	656	662	669	rVV4	810	2176	0.48%	0.062%
27	6.147	694	696	697	rBB4	115	79	0.02%	0.002%
28	6.184	698	702	704	rBB4	73	86	0.02%	0.002%
29	6.434	740	743	744	rBB4	136	103	0.02%	0.003%
30	6.482	749	751	755	rBB	104	131	0.03%	0.004%
31	6.562	763	764	767	rBB	114	85	0.02%	0.002%
32	6.623	773	774	777	rBV	60	86	0.02%	0.002%
33	6.665	779	781	783	rBB	130	93	0.02%	0.003%
34	6.781	796	800	804	rBV	147	262	0.06%	0.008%
35	6.885	816	817	819	rBB	141	78	0.02%	0.002%
36	7.086	842	850	866	rBV	9150	30346	6.72%	0.870%

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 Title : SFAM01.0

37	7.446	907	909	911	rBV	74	92	0.02%	0.003%
38	7.549	923	926	927	rBB	128	86	0.02%	0.002%
39	7.653	933	943	957	rBB	79676	197533	43.76%	5.661%
40	7.945	987	991	994	rBB2	179	271	0.06%	0.008%
41	8.159	1024	1026	1027	rBB2	144	79	0.02%	0.002%
42	8.189	1030	1031	1034	rBB2	141	90	0.02%	0.003%
43	8.275	1034	1045	1061	rBV2	149987	451432	100.00%	12.937%
44	8.708	1113	1116	1118	rBV	190	284	0.06%	0.008%
45	8.842	1130	1138	1150	rBV	156081	307499	68.12%	8.812%
46	9.067	1174	1175	1184	rVB3	251	467	0.10%	0.013%
47	9.214	1198	1199	1201	rBV	255	236	0.05%	0.007%
48	9.274	1201	1209	1218	rVV	104370	210061	46.53%	6.020%
49	9.659	1269	1272	1274	rBV	242	243	0.05%	0.007%
50	9.726	1282	1283	1285	rBV	87	85	0.02%	0.002%
51	9.890	1305	1310	1314	rBB2	1276	2171	0.48%	0.062%
52	9.957	1318	1321	1322	rBB2	118	84	0.02%	0.002%
53	10.037	1327	1334	1342	rBV	54153	95205	21.09%	2.728%
54	10.128	1347	1349	1352	rBB	125	131	0.03%	0.004%
55	10.226	1362	1365	1366	rBV	117	83	0.02%	0.002%
56	10.244	1366	1368	1373	rVB	473	667	0.15%	0.019%
57	10.323	1373	1381	1388	rBV	232368	403101	89.29%	11.552%
58	10.500	1407	1410	1413	rBB	199	202	0.04%	0.006%
59	10.579	1416	1423	1432	rBV	34735	58321	12.92%	1.671%
60	10.701	1438	1443	1451	rVB2	2671	4846	1.07%	0.139%
61	10.866	1464	1470	1474	rBV	3439	5759	1.28%	0.165%
62	10.927	1474	1480	1492	rVB	42945	71705	15.88%	2.055%
63	11.030	1495	1497	1499	rBV2	115	105	0.02%	0.003%
64	11.158	1516	1518	1520	rBV	75	92	0.02%	0.003%
65	11.628	1588	1595	1603	rBV	231364	393361	87.14%	11.273%
66	11.835	1624	1629	1637	rVB2	921	1707	0.38%	0.049%
67	11.920	1640	1643	1646	rBB2	108	148	0.03%	0.004%
68	12.073	1664	1668	1669	rBB2	116	128	0.03%	0.004%
69	12.164	1679	1683	1688	rBB2	336	470	0.10%	0.013%
70	12.463	1730	1732	1735	rVB	236	207	0.05%	0.006%
71	12.597	1748	1754	1763	rBB2	4259	8309	1.84%	0.238%
72	12.689	1763	1769	1777	rBV	85075	140870	31.21%	4.037%
73	12.749	1777	1779	1784	rVB	368	547	0.12%	0.016%
74	12.865	1795	1798	1800	rBV	202	266	0.06%	0.008%
75	12.938	1806	1810	1816	rBV5	684	1699	0.38%	0.049%
76	13.213	1843	1855	1860	rBV2	13228	24213	5.36%	0.694%

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 Title : SFAM01.0

77	13.408	1877	1887	1893	rBB4	2691	4847	1.07%	0.139%
78	13.469	1893	1897	1899	rBV2	519	658	0.15%	0.019%
79	13.554	1905	1911	1918	rBV	269464	427908	94.79%	12.263%
80	13.670	1928	1930	1932	rBB	174	124	0.03%	0.004%
81	13.701	1933	1935	1937	rBB	94	89	0.02%	0.003%
82	13.762	1940	1945	1952	rBV4	1651	2947	0.65%	0.084%
83	13.853	1953	1960	1970	rVB	224345	359911	79.73%	10.314%
84	14.066	1985	1995	2000	rBV2	2114	3710	0.82%	0.106%
85	14.188	2012	2015	2017	rBV	180	203	0.04%	0.006%
86	14.243	2022	2024	2027	rBV	139	196	0.04%	0.006%
87	14.298	2032	2033	2036	rBV	125	139	0.03%	0.004%
88	14.377	2044	2046	2049	rBB	92	102	0.02%	0.003%
89	14.402	2049	2050	2053	rBV	88	104	0.02%	0.003%
90	14.426	2053	2054	2055	rVV	151	80	0.02%	0.002%
91	14.463	2059	2060	2064	rBV	119	163	0.04%	0.005%
92	14.603	2080	2083	2085	rBV	160	173	0.04%	0.005%
93	14.658	2089	2092	2093	rBB	137	100	0.02%	0.003%
94	14.688	2094	2097	2098	rBV	104	86	0.02%	0.002%
95	14.780	2109	2112	2115	rBV	201	264	0.06%	0.008%
96	14.859	2121	2125	2127	rBV2	119	151	0.03%	0.004%
97	14.944	2137	2139	2140	rBV2	146	101	0.02%	0.003%
98	15.103	2160	2165	2166	rBV2	187	273	0.06%	0.008%
99	15.127	2167	2169	2173	rVV2	257	318	0.07%	0.009%
100	15.688	2260	2261	2262	rBV	244	109	0.02%	0.003%

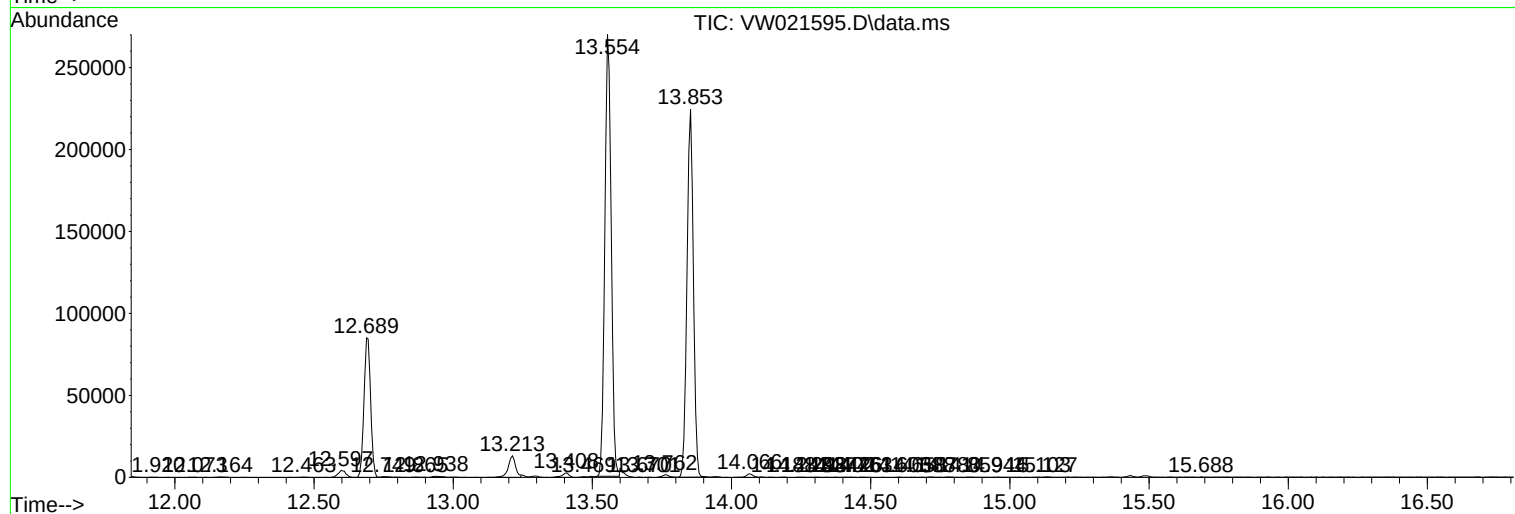
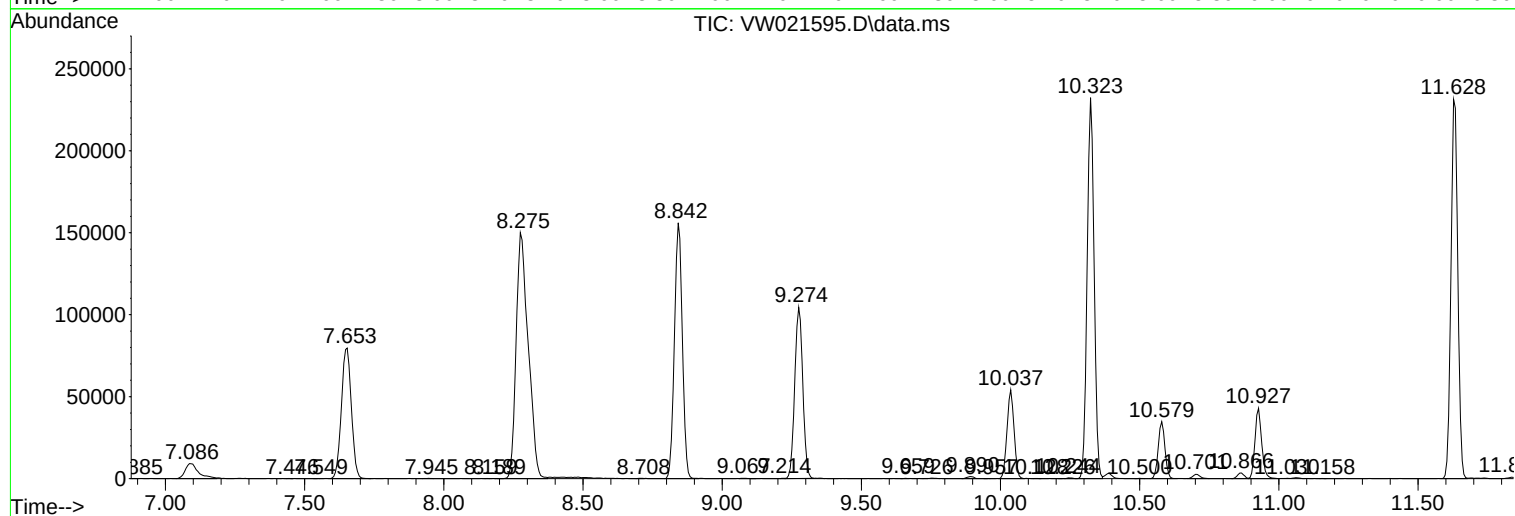
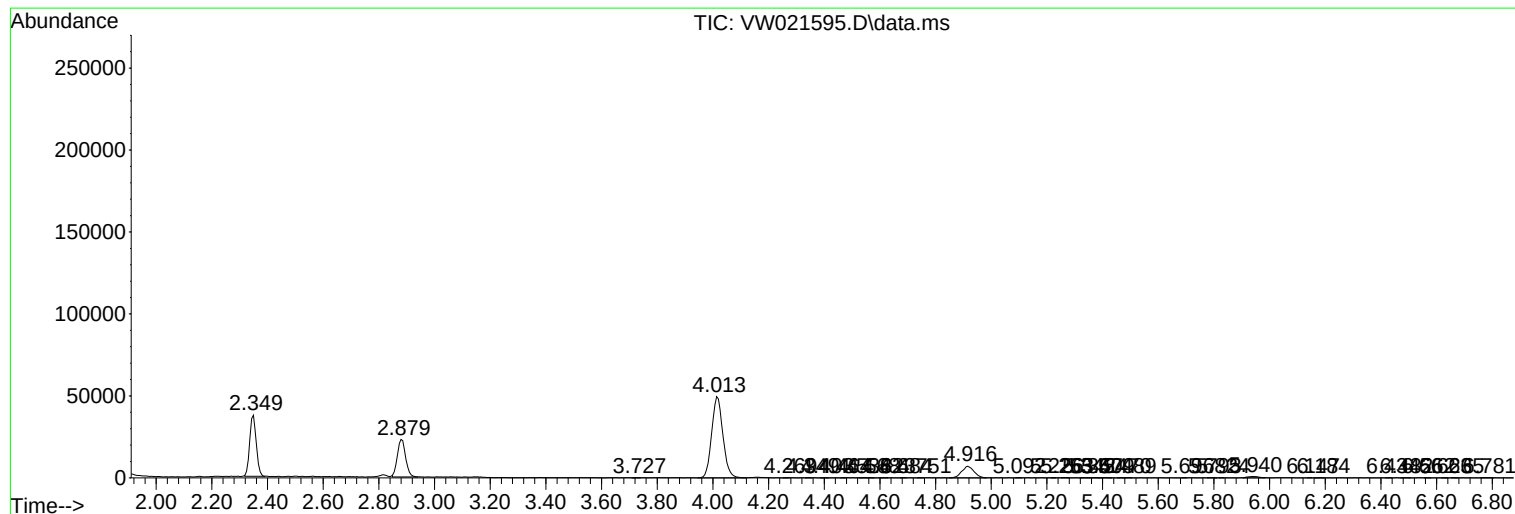
Sum of corrected areas: 3489516

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120921SMA.M
Quant Title : SFAM01.0

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



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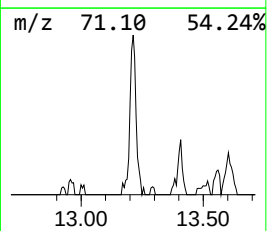
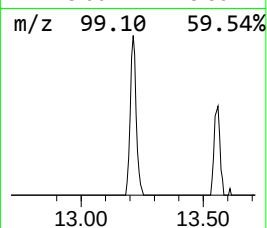
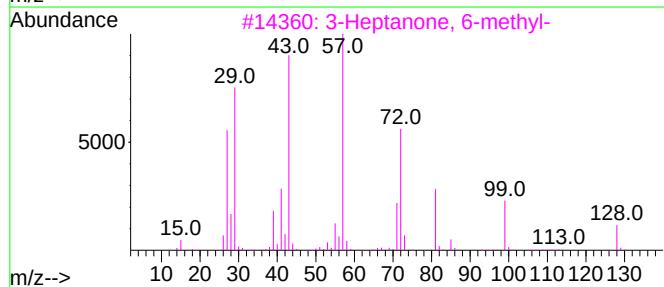
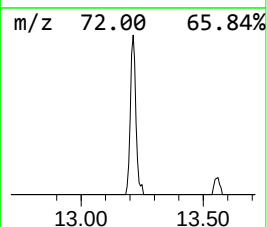
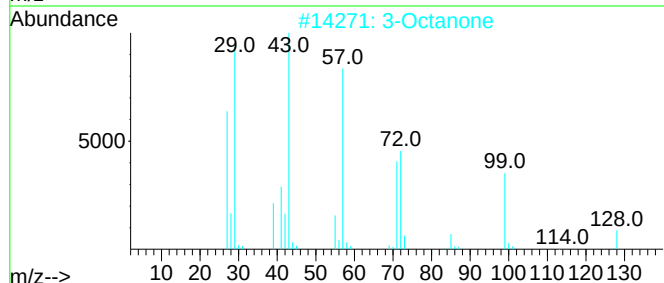
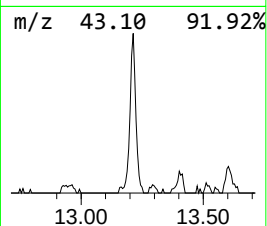
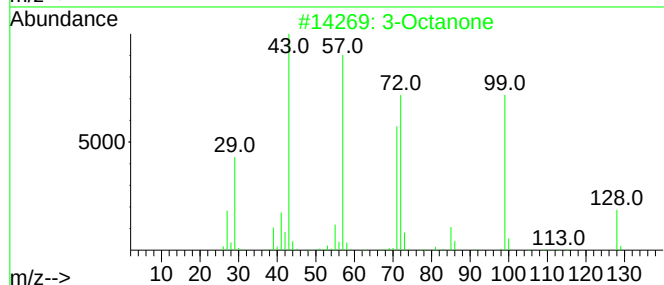
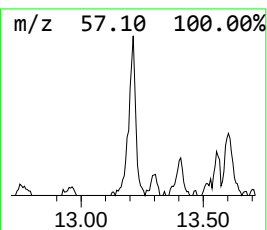
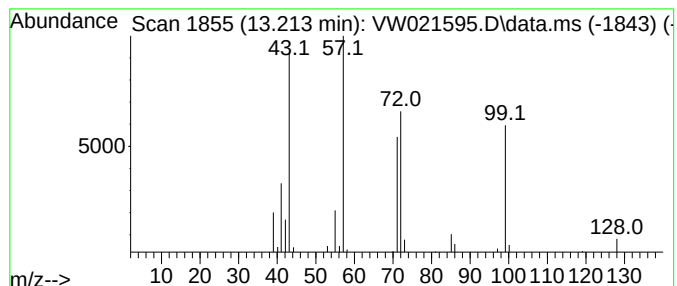
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM120921SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 3-Octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.213	1.41 ug/L	24213	1,4-Dichlorobenzene-d4	13.554

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone			128	C8H16O	000106-68-3	95
2	3-Octanone			128	C8H16O	000106-68-3	80
3	3-Heptanone, 6-methyl-			128	C8H16O	000624-42-0	58
4	3-Octanone			128	C8H16O	000106-68-3	53
5	3-Octanone			128	C8H16O	000106-68-3	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Octanone	13.213	1.4	ug/L	24213	3	13.554	427908	25.0