

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW101521\
 Data File : VW020541.D
 Acq On : 15 Oct 2021 18:11
 Operator : SY/VA
 Sample : M4210-22
 Misc : 2.88g/10mL/MSVOA_W/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 JDGG1

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\SFAMWLM100821SMA.M

Title : SFAM01.0

Signal : TIC: VW020541.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	67	73	81	rVB	64964	108820	13.34%	1.969%
2	2.879	154	160	168	rVB	35544	68815	8.44%	1.245%
3	3.379	235	242	251	rVB2	5333	12254	1.50%	0.222%
4	3.721	293	298	302	rBV3	577	1051	0.13%	0.019%
5	3.800	308	311	313	rBV3	117	132	0.02%	0.002%
6	4.019	335	347	357	rBV2	82907	246858	30.26%	4.466%
7	4.129	358	365	379	rVB	45960	123804	15.18%	2.240%
8	4.550	431	434	435	rVB2	160	103	0.01%	0.002%
9	4.696	452	458	461	rVV3	244	511	0.06%	0.009%
10	4.916	483	494	507	rBV	15984	51753	6.34%	0.936%
11	5.135	528	530	533	rBV2	114	112	0.01%	0.002%
12	5.940	654	662	671	rVV4	2430	7627	0.93%	0.138%
13	6.074	682	684	686	rBV2	87	108	0.01%	0.002%
14	6.159	696	698	700	rBV	99	106	0.01%	0.002%
15	6.293	716	720	724	rBV2	141	252	0.03%	0.005%
16	6.805	802	804	808	rBV2	72	118	0.01%	0.002%
17	6.921	822	823	826	rBV	116	103	0.01%	0.002%
18	7.086	841	850	858	rBV	20237	56878	6.97%	1.029%
19	7.366	893	896	901	rBV3	138	276	0.03%	0.005%
20	7.519	913	921	928	rVV2	563	1458	0.18%	0.026%
21	7.653	932	943	957	rVV	144097	353145	43.29%	6.389%
22	7.793	962	966	967	rVB2	141	126	0.02%	0.002%
23	8.037	1004	1006	1011	rVB2	81	104	0.01%	0.002%
24	8.141	1021	1023	1026	rVB2	85	91	0.01%	0.002%
25	8.275	1035	1045	1061	rBV2	274671	815798	100.00%	14.760%
26	8.714	1110	1117	1123	rVB3	952	2137	0.26%	0.039%
27	8.842	1130	1138	1150	rBV	262655	515478	63.19%	9.326%
28	9.079	1171	1177	1181	rBV2	690	1223	0.15%	0.022%
29	9.153	1187	1189	1193	rBV	331	434	0.05%	0.008%
30	9.275	1200	1209	1219	rBV	203996	404804	49.62%	7.324%
31	9.439	1234	1236	1242	rVV2	651	718	0.09%	0.013%
32	9.506	1245	1247	1254	rVB3	157	317	0.04%	0.006%
33	9.659	1268	1272	1278	rBV4	542	1109	0.14%	0.020%
34	9.774	1289	1291	1293	rVB2	121	104	0.01%	0.002%
35	9.890	1308	1310	1312	rVB2	170	139	0.02%	0.003%
36	10.037	1326	1334	1345	rVV	92027	163536	20.05%	2.959%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
 Title : SFAM01.0

37	10.128	1345	1349	1355	rVB4	588	1029	0.13%	0.019%
38	10.177	1355	1357	1358	rVB	203	122	0.01%	0.002%
39	10.220	1360	1364	1368	rVB4	598	854	0.10%	0.015%
40	10.256	1368	1370	1371	rBV2	133	128	0.02%	0.002%
41	10.323	1373	1381	1388	rBV	349622	606485	74.34%	10.973%
42	10.390	1388	1392	1400	rVB	6138	10978	1.35%	0.199%
43	10.445	1400	1401	1407	rVB2	218	191	0.02%	0.003%
44	10.500	1407	1410	1411	rBV2	225	209	0.03%	0.004%
45	10.579	1415	1423	1431	rBV	58892	100814	12.36%	1.824%
46	10.671	1436	1438	1439	rBV2	192	145	0.02%	0.003%
47	10.701	1439	1443	1451	rVB	5341	8751	1.07%	0.158%
48	10.823	1462	1463	1466	rBV	200	162	0.02%	0.003%
49	10.854	1466	1468	1469	rVV2	213	161	0.02%	0.003%
50	10.927	1472	1480	1498	rVV	75447	131510	16.12%	2.379%
51	11.067	1499	1503	1511	rVV2	1859	3498	0.43%	0.063%
52	11.341	1545	1548	1550	rBV2	91	103	0.01%	0.002%
53	11.402	1554	1558	1561	rBV3	184	282	0.03%	0.005%
54	11.634	1588	1596	1605	rBV	325463	544897	66.79%	9.859%
55	11.768	1616	1618	1621	rBV	102	117	0.01%	0.002%
56	11.890	1635	1638	1639	rBV	89	113	0.01%	0.002%
57	11.927	1642	1644	1647	rVB3	152	136	0.02%	0.002%
58	12.006	1656	1657	1659	rBV	157	105	0.01%	0.002%
59	12.024	1659	1660	1663	rVB	136	93	0.01%	0.002%
60	12.061	1663	1666	1668	rBV2	151	154	0.02%	0.003%
61	12.122	1673	1676	1679	rVB2	131	139	0.02%	0.003%
62	12.164	1679	1683	1686	rBV3	297	443	0.05%	0.008%
63	12.231	1690	1694	1696	rBV	265	289	0.04%	0.005%
64	12.603	1748	1755	1763	rVV2	3703	6679	0.82%	0.121%
65	12.695	1763	1770	1777	rVV	109792	181121	22.20%	3.277%
66	12.756	1777	1780	1787	rVB3	690	1249	0.15%	0.023%
67	12.853	1795	1796	1800	rBV2	194	214	0.03%	0.004%
68	12.890	1800	1802	1805	rVV2	266	315	0.04%	0.006%
69	12.939	1805	1810	1817	rVB4	949	1862	0.23%	0.034%
70	13.048	1823	1828	1830	rVB3	186	264	0.03%	0.005%
71	13.091	1834	1835	1838	rBV2	125	94	0.01%	0.002%
72	13.158	1838	1846	1849	rBV2	5712	10475	1.28%	0.190%
73	13.213	1849	1855	1863	rVV	128502	197067	24.16%	3.565%
74	13.286	1863	1867	1879	rVB2	9078	16854	2.07%	0.305%
75	13.481	1893	1899	1900	rBV3	642	1083	0.13%	0.020%
76	13.554	1905	1911	1918	rBV	247069	400335	49.07%	7.243%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
 Title : SFAM01.0

77	13.768	1942	1946	1950	rVB5	928	1347	0.17%	0.024%
78	13.798	1950	1951	1953	rBV	248	231	0.03%	0.004%
79	13.853	1953	1960	1971	rVV	209908	336667	41.27%	6.091%
80	14.066	1988	1995	2000	rBV	4376	7043	0.86%	0.127%
81	14.213	2017	2019	2028	rVB5	557	1127	0.14%	0.020%
82	14.322	2028	2037	2041	rBV4	820	1728	0.21%	0.031%
83	14.396	2047	2049	2050	rBV2	258	207	0.03%	0.004%
84	14.420	2050	2053	2057	rVB3	635	787	0.10%	0.014%
85	14.542	2072	2073	2076	rBV	175	169	0.02%	0.003%
86	14.591	2078	2081	2085	rVV2	269	401	0.05%	0.007%
87	14.621	2085	2086	2088	rVB	205	129	0.02%	0.002%
88	14.713	2098	2101	2104	rBV2	220	349	0.04%	0.006%
89	14.896	2129	2131	2136	rBV2	159	248	0.03%	0.004%
90	15.402	2212	2214	2215	rBV2	282	276	0.03%	0.005%
91	15.432	2215	2219	2223	rVV2	1241	1915	0.23%	0.035%
92	15.487	2224	2228	2235	rVB	1535	2741	0.34%	0.050%
93	15.786	2275	2277	2284	rBV4	389	788	0.10%	0.014%
94	16.103	2327	2329	2330	rBV2	228	162	0.02%	0.003%
95	16.194	2342	2344	2345	rBV2	133	96	0.01%	0.002%
96	16.414	2378	2380	2383	rVB3	209	228	0.03%	0.004%
97	16.450	2383	2386	2388	rBV2	180	207	0.03%	0.004%
98	16.554	2401	2403	2405	rBV	175	107	0.01%	0.002%
99	16.700	2425	2427	2431	rBV3	170	140	0.02%	0.003%
100	16.749	2434	2435	2437	rVV	228	125	0.02%	0.002%

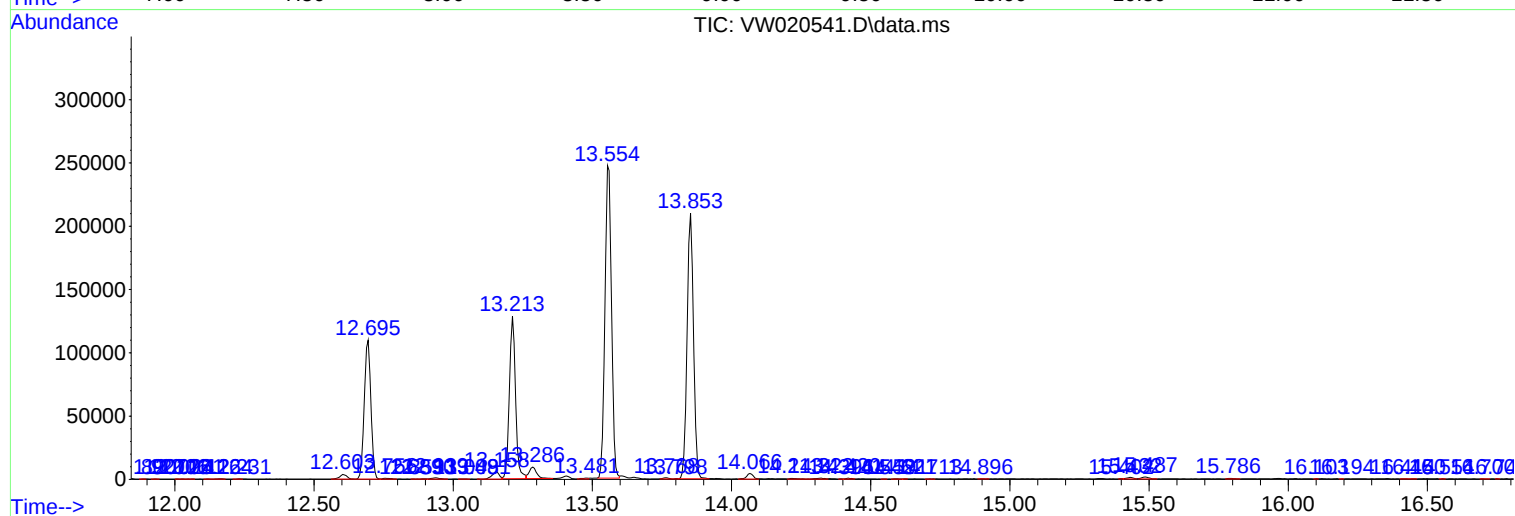
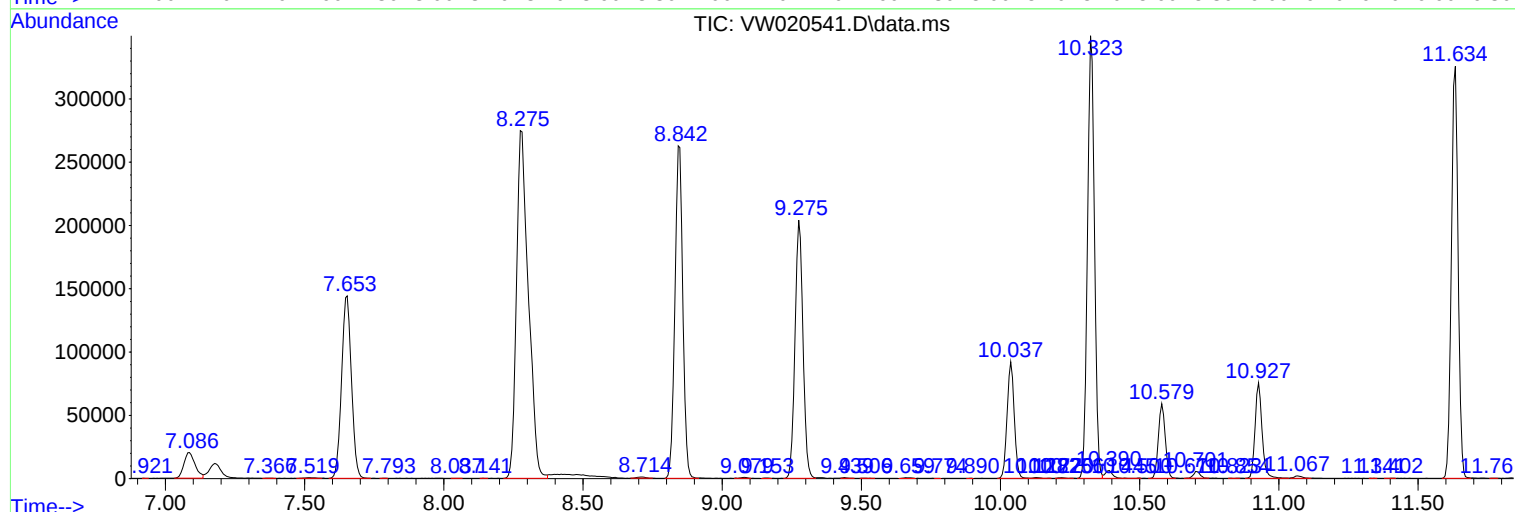
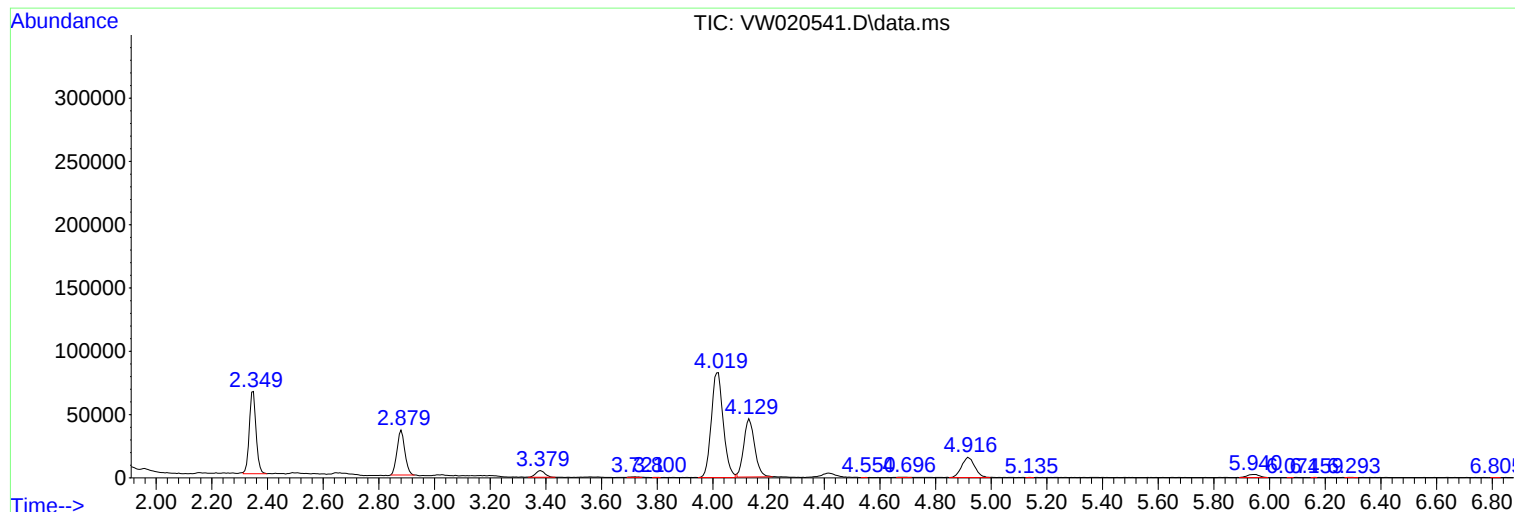
Sum of corrected areas: 5527140

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
Quant Title : SFAM01.0

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



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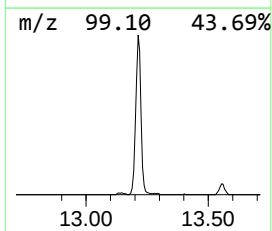
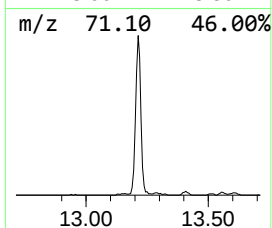
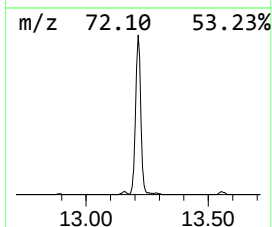
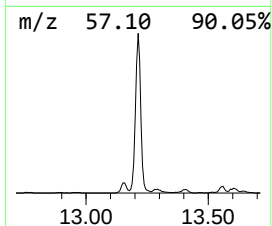
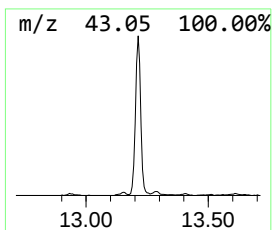
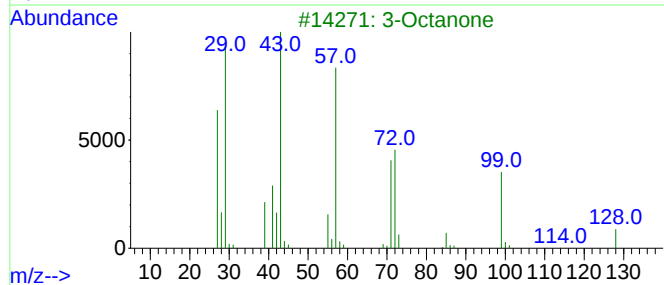
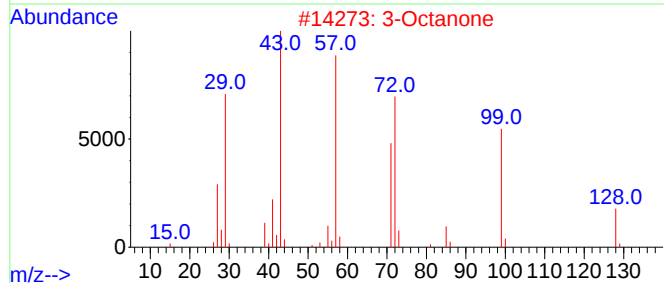
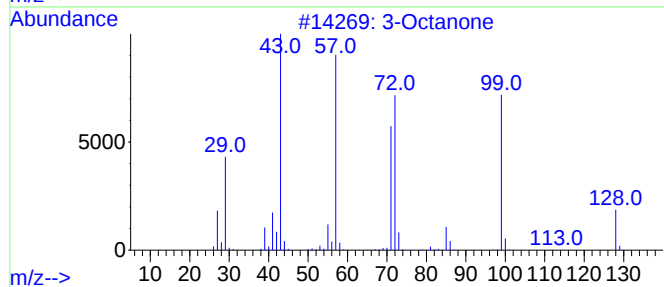
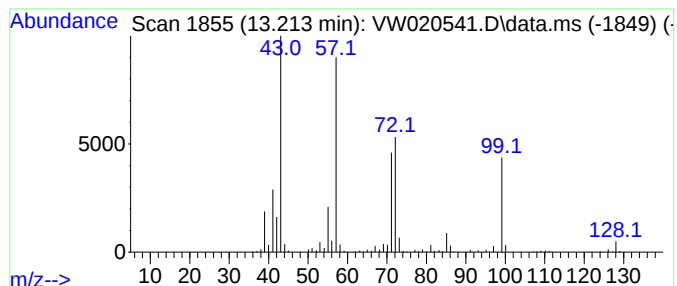
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 3-Octanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.213	12.31 ug/L	197067	1,4-Dichlorobenzene-d4	13.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octanone	128	C8H16O	000106-68-3	90
2			3-Octanone	128	C8H16O	000106-68-3	78
3			3-Octanone	128	C8H16O	000106-68-3	74
4			4-Oxononanal	156	C9H16O2	1000314-10-4	50
5			3-Octanone	128	C8H16O	000106-68-3	40



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Octanone	13.213	12.3	ug/L	197067	3	13.560	400335	25.0