

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW061224\
 Data File : VW029101.D
 Acq On : 12 Jun 2024 12:51
 Operator : SY/MD
 Sample : P2776-19
 Misc : 4.80g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A4C72

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\SFAMWLM060324SMA.M
 Title : SFAM01.0

Signal : TIC: VW029101.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	70	78	93	rBV	125713	279872	14.31%	2.021%
2	2.899	158	166	184	rBV	87464	252060	12.89%	1.820%
3	3.387	244	246	249	rVB3	604	693	0.04%	0.005%
4	3.472	257	260	263	rBV4	498	680	0.03%	0.005%
5	3.802	312	314	318	rVB2	652	710	0.04%	0.005%
6	3.844	318	321	323	rBV4	712	887	0.05%	0.006%
7	3.869	323	325	328	rVB	631	726	0.04%	0.005%
8	4.021	338	350	364	rBV	221233	647615	33.11%	4.676%
9	4.222	379	383	385	rVB4	771	818	0.04%	0.006%
10	4.393	404	411	414	rBV6	820	1802	0.09%	0.013%
11	4.515	429	431	434	rBV3	850	826	0.04%	0.006%
12	4.539	434	435	439	rVV2	660	693	0.04%	0.005%
13	4.753	467	470	475	rBV4	349	683	0.03%	0.005%
14	4.923	486	498	513	rBV3	22328	79835	4.08%	0.576%
15	5.131	530	532	533	rBV	753	574	0.03%	0.004%
16	5.582	603	606	609	rBV4	607	685	0.04%	0.005%
17	5.771	633	637	638	rBV2	555	574	0.03%	0.004%
18	5.941	657	665	666	rBV5	3319	6944	0.35%	0.050%
19	6.051	679	683	685	rVB2	571	635	0.03%	0.005%
20	6.100	689	691	694	rBV3	535	588	0.03%	0.004%
21	6.246	711	715	720	rBV5	597	824	0.04%	0.006%
22	6.417	740	743	745	rBV2	564	761	0.04%	0.005%
23	6.752	795	798	803	rVB4	788	1401	0.07%	0.010%
24	6.838	808	812	814	rBV3	680	706	0.04%	0.005%
25	6.874	814	818	820	rBV3	560	739	0.04%	0.005%
26	6.899	820	822	826	rBV2	578	808	0.04%	0.006%
27	7.075	841	851	875	rBV	53264	166222	8.50%	1.200%
28	7.392	898	903	905	rVB3	674	1059	0.05%	0.008%
29	7.472	915	916	921	rVB5	820	862	0.04%	0.006%
30	7.520	921	924	925	rBV3	762	573	0.03%	0.004%
31	7.539	925	927	934	rVB7	513	792	0.04%	0.006%
32	7.648	934	945	958	rBV	338142	825643	42.21%	5.961%
33	7.758	962	963	969	rVB4	936	1356	0.07%	0.010%
34	7.923	986	990	991	rBV3	752	897	0.05%	0.006%
35	8.002	999	1003	1006	rBV4	386	627	0.03%	0.005%
36	8.051	1009	1011	1017	rVB4	591	961	0.05%	0.007%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM060324SMA.M
 Title : SFAM01.0

37	8.148	1025	1027	1032	rVB5	737	980	0.05%	0.007%
38	8.276	1036	1048	1065	rBV2	659321	1956133	100.00%	14.123%
39	8.514	1086	1087	1091	rVB4	694	605	0.03%	0.004%
40	8.545	1091	1092	1095	rBV3	947	911	0.05%	0.007%
41	8.636	1105	1107	1110	rVB2	853	874	0.04%	0.006%
42	8.667	1110	1112	1114	rBV3	747	947	0.05%	0.007%
43	8.685	1114	1115	1122	rVB5	1556	2417	0.12%	0.017%
44	8.776	1126	1130	1131	rBV2	565	596	0.03%	0.004%
45	8.843	1131	1141	1155	rBV	697992	1394861	71.31%	10.071%
46	9.045	1167	1174	1177	rBV8	1909	4619	0.24%	0.033%
47	9.197	1196	1199	1200	rBV3	605	618	0.03%	0.004%
48	9.270	1200	1211	1236	rVV	456516	934542	47.77%	6.747%
49	9.429	1236	1237	1241	rVB3	789	566	0.03%	0.004%
50	9.502	1246	1249	1251	rBV4	535	572	0.03%	0.004%
51	9.672	1269	1277	1278	rBV5	1759	3267	0.17%	0.024%
52	10.032	1327	1336	1346	rBV	233860	419403	21.44%	3.028%
53	10.118	1348	1350	1360	rVB	1789	3594	0.18%	0.026%
54	10.319	1374	1383	1399	rBV	896218	1596700	81.63%	11.528%
55	10.575	1418	1425	1435	rBV	142831	244335	12.49%	1.764%
56	10.642	1435	1436	1439	rBV3	754	671	0.03%	0.005%
57	10.697	1440	1445	1451	rVB	13838	24490	1.25%	0.177%
58	10.837	1465	1468	1472	rBV4	909	1475	0.08%	0.011%
59	10.922	1475	1482	1494	rBV	192436	337321	17.24%	2.435%
60	11.020	1495	1498	1502	rVB5	2981	4607	0.24%	0.033%
61	11.172	1522	1523	1527	rVB4	1326	1152	0.06%	0.008%
62	11.398	1556	1560	1565	rBV5	661	1072	0.05%	0.008%
63	11.629	1589	1598	1607	rBV	905717	1531907	78.31%	11.060%
64	11.709	1607	1611	1620	rVV3	6310	13899	0.71%	0.100%
65	11.776	1620	1622	1626	rVV5	843	1171	0.06%	0.008%
66	11.837	1626	1632	1639	rVB7	4715	9793	0.50%	0.071%
67	12.093	1670	1674	1676	rBV4	761	1141	0.06%	0.008%
68	12.135	1679	1681	1682	rBV2	858	706	0.04%	0.005%
69	12.154	1682	1684	1685	rBV2	987	620	0.03%	0.004%
70	12.465	1730	1735	1743	rVB8	3091	6457	0.33%	0.047%
71	12.599	1746	1757	1765	rBV	25538	45193	2.31%	0.326%
72	12.690	1765	1772	1782	rBV	297895	494798	25.29%	3.572%
73	12.769	1783	1785	1788	rVB5	983	909	0.05%	0.007%
74	12.873	1800	1802	1803	rBV2	692	601	0.03%	0.004%
75	12.885	1803	1804	1807	rVB2	863	657	0.03%	0.005%
76	12.928	1807	1811	1813	rBV3	1075	1678	0.09%	0.012%

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 Title : SFAM01.0

77	13.154	1841	1848	1850	rBV6	2887	5101	0.26%	0.037%
78	13.208	1851	1857	1865	rBV	87098	141337	7.23%	1.020%
79	13.397	1882	1888	1893	rVB6	3563	6500	0.33%	0.047%
80	13.464	1894	1899	1902	rVV6	2399	4855	0.25%	0.035%
81	13.556	1906	1914	1924	rVV	774751	1267127	64.78%	9.149%
82	13.641	1924	1928	1940	rVB2	11262	21672	1.11%	0.156%
83	13.849	1954	1962	1973	rBV	638059	1036493	52.99%	7.483%
84	14.062	1992	1997	2002	rVB2	7916	12924	0.66%	0.093%
85	14.153	2011	2012	2015	rVB3	848	570	0.03%	0.004%
86	14.190	2015	2018	2020	rBV4	838	1153	0.06%	0.008%
87	14.318	2035	2039	2046	rBV4	3392	5971	0.31%	0.043%
88	14.446	2058	2060	2063	rBV4	739	976	0.05%	0.007%
89	14.519	2067	2072	2076	rVB6	3255	5266	0.27%	0.038%
90	14.690	2096	2100	2101	rBV4	652	863	0.04%	0.006%
91	14.800	2115	2118	2120	rBV4	543	628	0.03%	0.005%
92	15.068	2156	2162	2165	rBV7	895	1656	0.08%	0.012%
93	15.184	2177	2181	2182	rBV4	1295	1701	0.09%	0.012%
94	15.245	2188	2191	2196	rVB6	1266	1812	0.09%	0.013%
95	15.360	2205	2210	2215	rBV5	862	1369	0.07%	0.010%
96	15.714	2264	2268	2269	rVB2	557	715	0.04%	0.005%
97	15.934	2302	2304	2307	rBV3	537	563	0.03%	0.004%
98	16.031	2318	2320	2323	rBV4	541	630	0.03%	0.005%
99	16.184	2344	2345	2347	rBV2	634	580	0.03%	0.004%
100	16.561	2404	2407	2410	rBV3	788	954	0.05%	0.007%

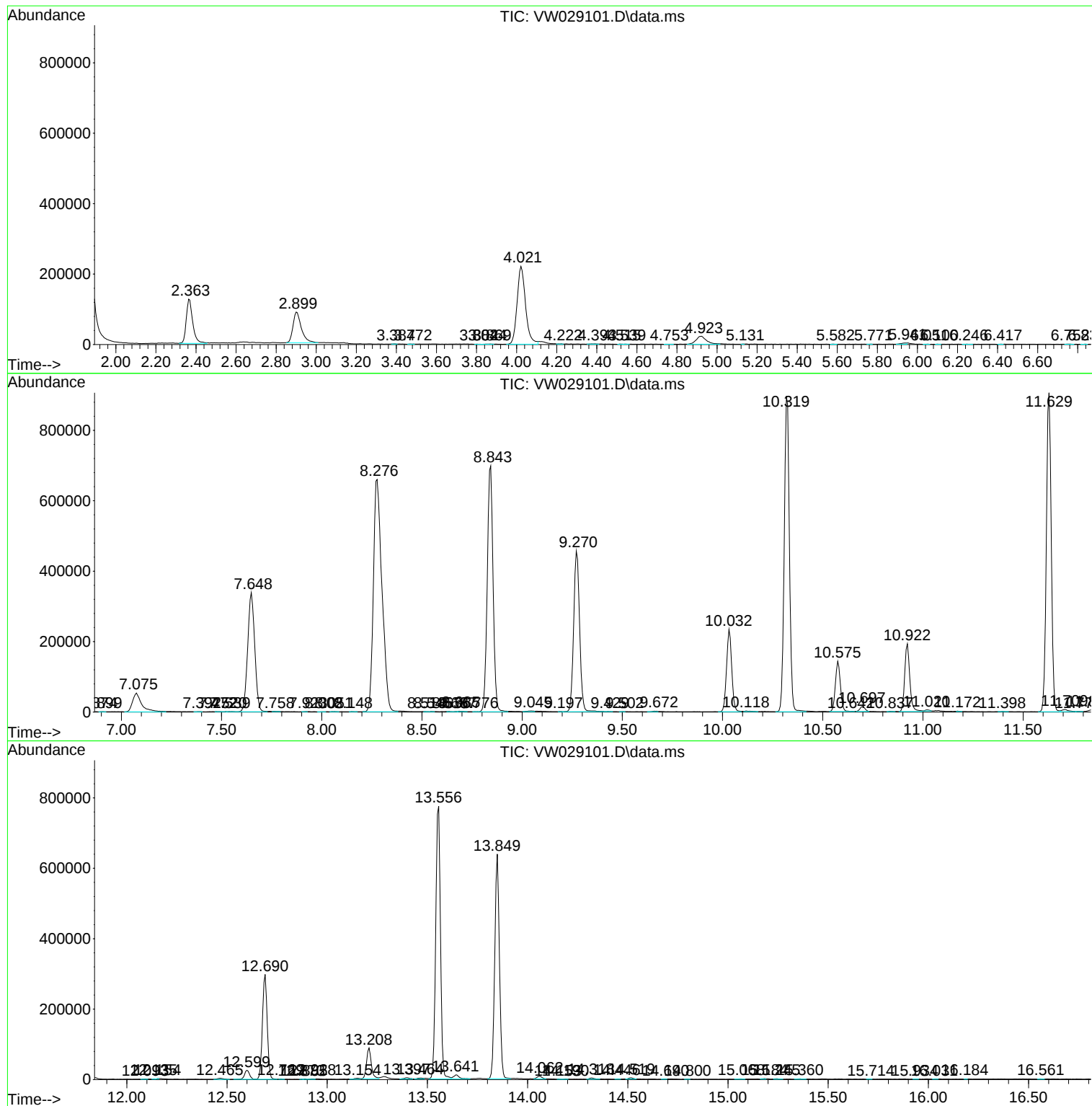
Sum of corrected areas: 13850405

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM060324SMA.M
Quant Title : SFAM01.0

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



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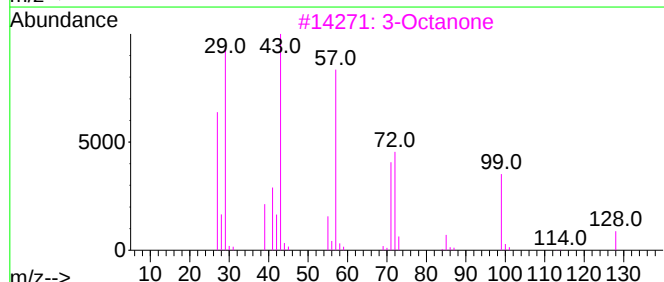
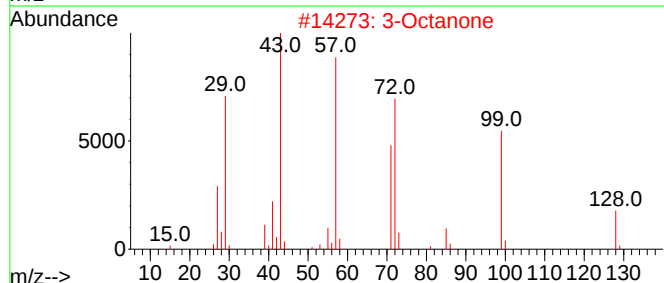
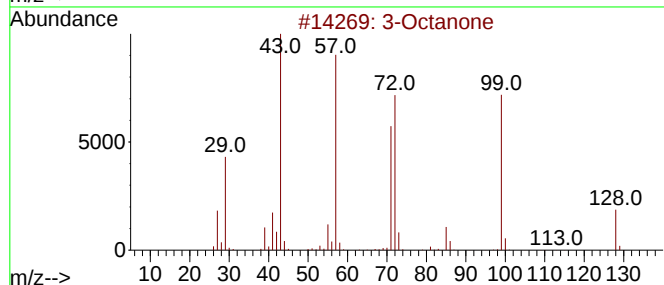
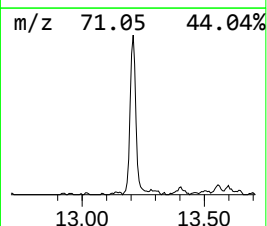
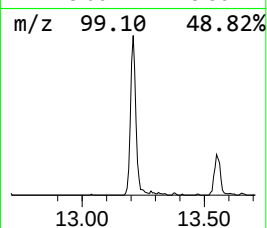
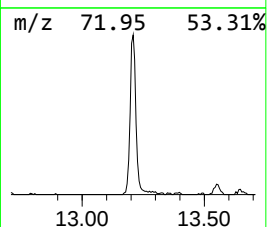
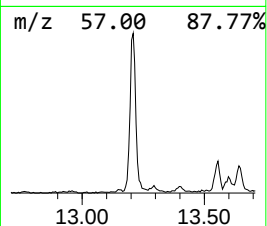
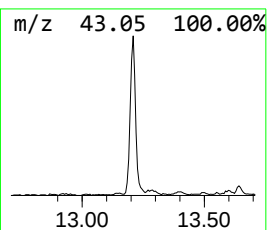
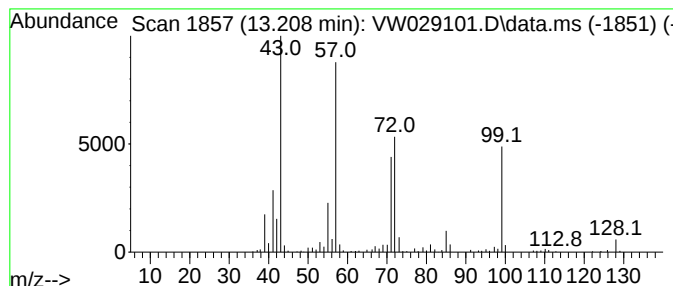
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM060324SMA.M
Quant Title : SFAM01.0

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	2.79 ug/L	141337	1,4-Dichlorobenzene-d4	13.556

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	87
3	3-Octanone			128	C8H16O	000106-68-3	59
4	3-Heptanone, 6-methyl-			128	C8H16O	000624-42-0	50
5	3-Heptanone, 6-methyl-			128	C8H16O	000624-42-0	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Octanone	13.208	2.8	ug/L	141337	3	13.556	1267130	25.0