

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW081423\
 Data File : VW026731.D
 Acq On : 14 Aug 2023 13:17
 Operator : SY/MD
 Sample : 03968-27
 Misc : 4.85g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A48P4

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: VW026731.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.149	40	43	44	rBV3	3132	3358	0.12%	0.018%
2	2.357	71	77	93	rVB	103102	247170	8.78%	1.288%
3	2.893	158	165	178	rBV	76766	218621	7.76%	1.140%
4	3.192	212	214	217	rBV4	1467	1556	0.06%	0.008%
5	3.381	242	245	249	rBV5	2012	3074	0.11%	0.016%
6	3.466	257	259	263	rBV5	1338	1427	0.05%	0.007%
7	3.527	263	269	274	rBV5	4164	10677	0.38%	0.056%
8	3.771	306	309	314	rBV6	1012	1604	0.06%	0.008%
9	4.015	337	349	364	rBV	233844	801273	28.45%	4.177%
10	4.332	399	401	405	rBV4	1664	1719	0.06%	0.009%
11	4.612	443	447	448	rBV4	1278	1524	0.05%	0.008%
12	4.753	466	470	473	rBV5	1115	1376	0.05%	0.007%
13	4.783	473	475	478	rVB3	1415	1558	0.06%	0.008%
14	4.917	484	497	506	rBV2	19973	80285	2.85%	0.418%
15	5.149	531	535	537	rBV5	1274	1629	0.06%	0.008%
16	5.466	585	587	589	rVB3	1779	1507	0.05%	0.008%
17	5.557	600	602	605	rBV4	1076	1449	0.05%	0.008%
18	5.673	618	621	623	rBV2	1174	1339	0.05%	0.007%
19	5.941	656	665	675	rBV5	9840	30938	1.10%	0.161%
20	6.057	682	684	689	rVB6	1464	2375	0.08%	0.012%
21	6.094	689	690	693	rBV3	1163	1336	0.05%	0.007%
22	6.380	736	737	742	rVB4	1181	1455	0.05%	0.008%
23	6.551	763	765	770	rVB6	1641	2342	0.08%	0.012%
24	6.710	786	791	793	rBV5	962	1589	0.06%	0.008%
25	6.978	832	835	838	rBV5	1037	1618	0.06%	0.008%
26	7.021	838	842	843	rVV4	1292	1479	0.05%	0.008%
27	7.075	843	851	876	rVV2	87144	296344	10.52%	1.545%
28	7.240	876	878	882	rVV5	1491	2409	0.09%	0.013%
29	7.648	934	945	959	rBV	459242	1136173	40.34%	5.922%
30	8.087	1016	1017	1022	rBV5	944	1497	0.05%	0.008%
31	8.276	1035	1048	1063	rBV2	952519	2816408	100.00%	14.681%
32	8.569	1093	1096	1097	rBV3	1746	1942	0.07%	0.010%
33	8.691	1114	1116	1118	rBV3	2089	2519	0.09%	0.013%
34	8.843	1132	1141	1153	rBV	860106	1701558	60.42%	8.870%
35	9.038	1169	1173	1176	rBV6	2766	4571	0.16%	0.024%
36	9.270	1201	1211	1223	rBV	666245	1356816	48.18%	7.073%

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

37	9.416	1234	1235	1238	rVB3	1790	1390	0.05%	0.007%
38	9.514	1249	1251	1254	rVB4	1540	1574	0.06%	0.008%
39	9.660	1271	1275	1279	rBV7	3109	4573	0.16%	0.024%
40	9.764	1287	1292	1295	rVB7	1267	2414	0.09%	0.013%
41	9.801	1295	1298	1302	rVB6	1122	1391	0.05%	0.007%
42	9.977	1324	1327	1329	rBV4	1431	1552	0.06%	0.008%
43	10.032	1329	1336	1347	rBV	313734	575344	20.43%	2.999%
44	10.203	1360	1364	1367	rVB5	1583	2414	0.09%	0.013%
45	10.325	1373	1384	1392	rBV	1236031	2177853	77.33%	11.352%
46	10.575	1417	1425	1435	rBV	220035	392022	13.92%	2.043%
47	10.703	1440	1446	1451	rVV3	12485	21905	0.78%	0.114%
48	10.819	1462	1465	1466	rBV3	1316	1619	0.06%	0.008%
49	10.843	1466	1469	1475	rBV7	3171	6534	0.23%	0.034%
50	10.922	1476	1482	1493	rBV	236628	413635	14.69%	2.156%
51	11.026	1494	1499	1503	rBV	29376	47623	1.69%	0.248%
52	11.172	1519	1523	1528	rVV5	6082	10162	0.36%	0.053%
53	11.239	1532	1534	1538	rVB5	1873	2037	0.07%	0.011%
54	11.325	1546	1548	1551	rBV4	1286	1292	0.05%	0.007%
55	11.398	1556	1560	1566	rBV7	4615	8506	0.30%	0.044%
56	11.629	1590	1598	1607	rBV	1238202	2036817	72.32%	10.617%
57	11.715	1608	1612	1619	rVB3	5643	10956	0.39%	0.057%
58	11.837	1628	1632	1635	rVB6	2247	3962	0.14%	0.021%
59	11.867	1635	1637	1640	rVB4	1517	1825	0.06%	0.010%
60	11.904	1640	1643	1645	rBV4	1325	1729	0.06%	0.009%
61	12.160	1683	1685	1687	rVV3	2661	2515	0.09%	0.013%
62	12.306	1707	1709	1711	rBV2	1515	1295	0.05%	0.007%
63	12.343	1711	1715	1718	rBV6	1270	2469	0.09%	0.013%
64	12.465	1730	1735	1737	rBV5	2196	3177	0.11%	0.017%
65	12.605	1751	1758	1765	rBV	17385	34164	1.21%	0.178%
66	12.690	1765	1772	1779	rBV	548738	886986	31.49%	4.624%
67	12.830	1790	1795	1796	rBV4	1618	2292	0.08%	0.012%
68	12.885	1799	1804	1806	rVV5	3787	4829	0.17%	0.025%
69	12.928	1809	1811	1813	rBV3	2442	1718	0.06%	0.009%
70	13.038	1824	1829	1832	rVB6	3048	4709	0.17%	0.025%
71	13.080	1832	1836	1838	rBV4	3447	4337	0.15%	0.023%
72	13.154	1843	1848	1851	rBV3	6156	11399	0.40%	0.059%
73	13.208	1851	1857	1866	rVV	188724	305972	10.86%	1.595%
74	13.282	1866	1869	1878	rVB4	15220	29164	1.04%	0.152%
75	13.495	1902	1904	1907	rBV4	2631	3321	0.12%	0.017%
76	13.556	1907	1914	1925	rVV	1128165	1805353	64.10%	9.411%

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

77	13.641	1926	1928	1933	rVB6	7213	11123	0.39%	0.058%
78	13.702	1936	1938	1941	rVB4	2670	2968	0.11%	0.015%
79	13.733	1941	1943	1944	rBV2	1991	1895	0.07%	0.010%
80	13.757	1944	1947	1950	rVB4	4770	5706	0.20%	0.030%
81	13.794	1950	1953	1955	rBV4	2511	2077	0.07%	0.011%
82	13.849	1955	1962	1969	rBV	936254	1483453	52.67%	7.733%
83	14.068	1994	1998	2012	rVB3	9844	24387	0.87%	0.127%
84	14.257	2024	2029	2033	rBV7	3293	5512	0.20%	0.029%
85	14.324	2033	2040	2043	rVV9	7477	13772	0.49%	0.072%
86	14.379	2047	2049	2053	rVB5	1515	1653	0.06%	0.009%
87	14.513	2063	2071	2076	rVB10	4930	12108	0.43%	0.063%
88	14.568	2076	2080	2081	rVB3	1513	1892	0.07%	0.010%
89	14.623	2086	2089	2090	rBV3	1488	1374	0.05%	0.007%
90	14.690	2096	2100	2101	rBV4	5501	6451	0.23%	0.034%
91	14.714	2101	2104	2109	rVB5	10570	15814	0.56%	0.082%
92	14.787	2114	2116	2120	rVB5	1806	1796	0.06%	0.009%
93	14.873	2126	2130	2132	rBV5	1751	1990	0.07%	0.010%
94	15.086	2163	2165	2166	rBV2	1934	1814	0.06%	0.009%
95	15.123	2169	2171	2173	rVV3	1435	1469	0.05%	0.008%
96	15.312	2200	2202	2204	rBV2	1203	1342	0.05%	0.007%
97	15.470	2226	2228	2230	rVV3	1646	1528	0.05%	0.008%
98	15.787	2278	2280	2282	rBV3	1398	1401	0.05%	0.007%
99	16.025	2317	2319	2321	rVB3	2124	1834	0.07%	0.010%
100	16.476	2392	2393	2398	rVB5	2545	3498	0.12%	0.018%

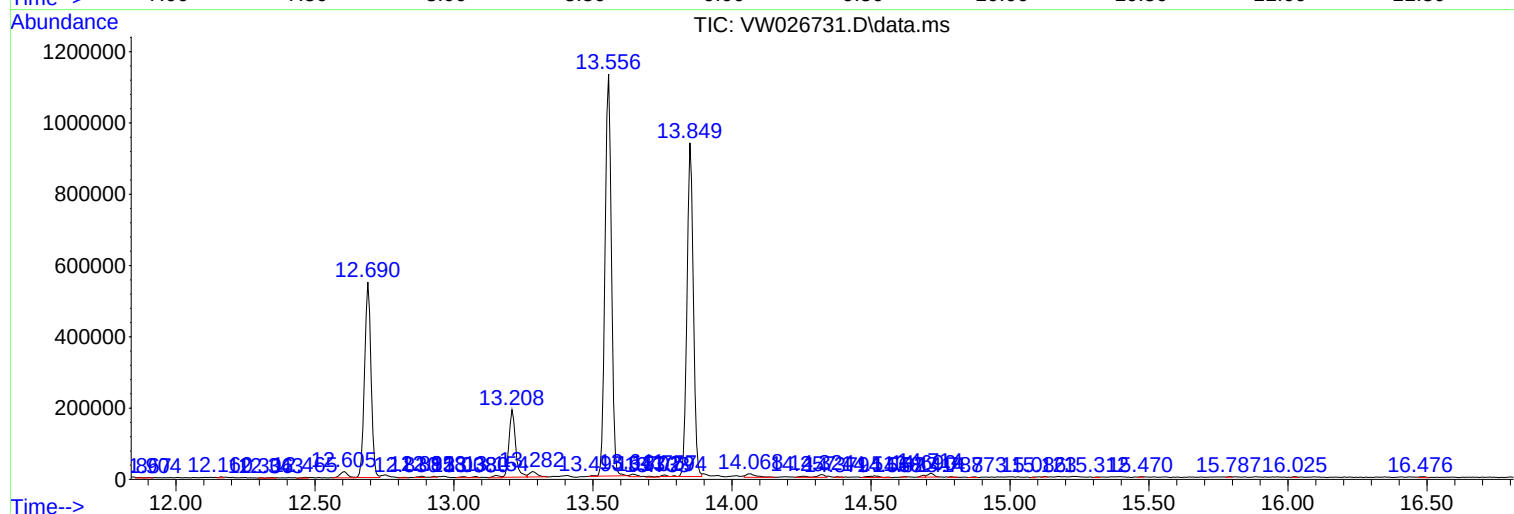
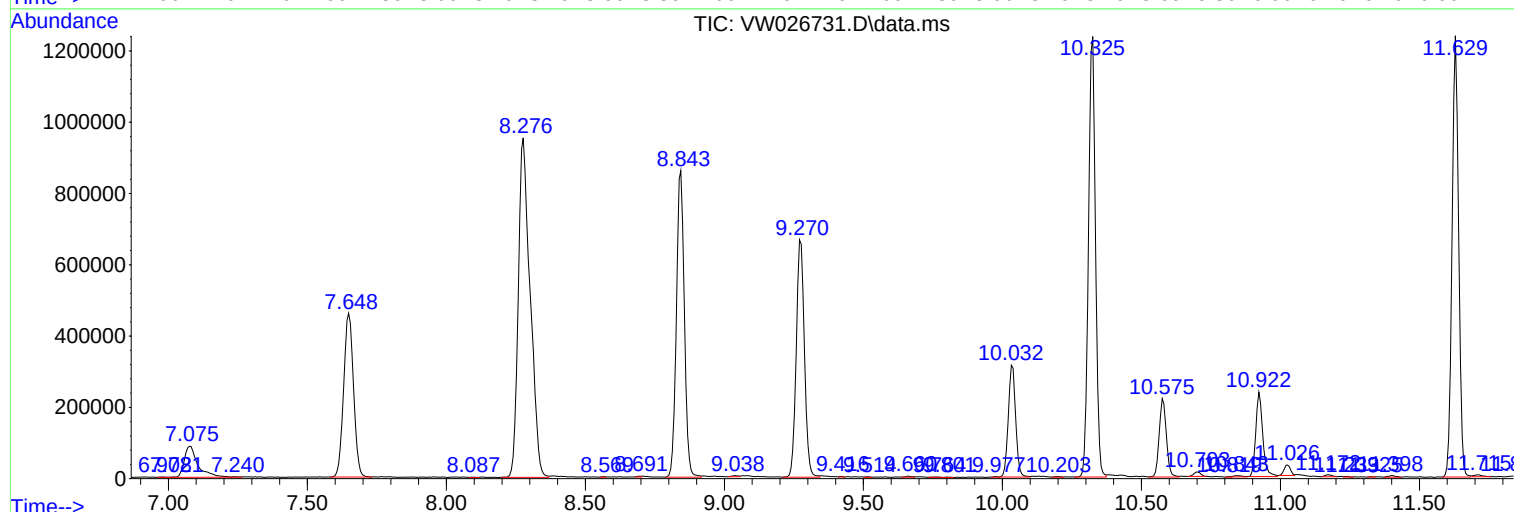
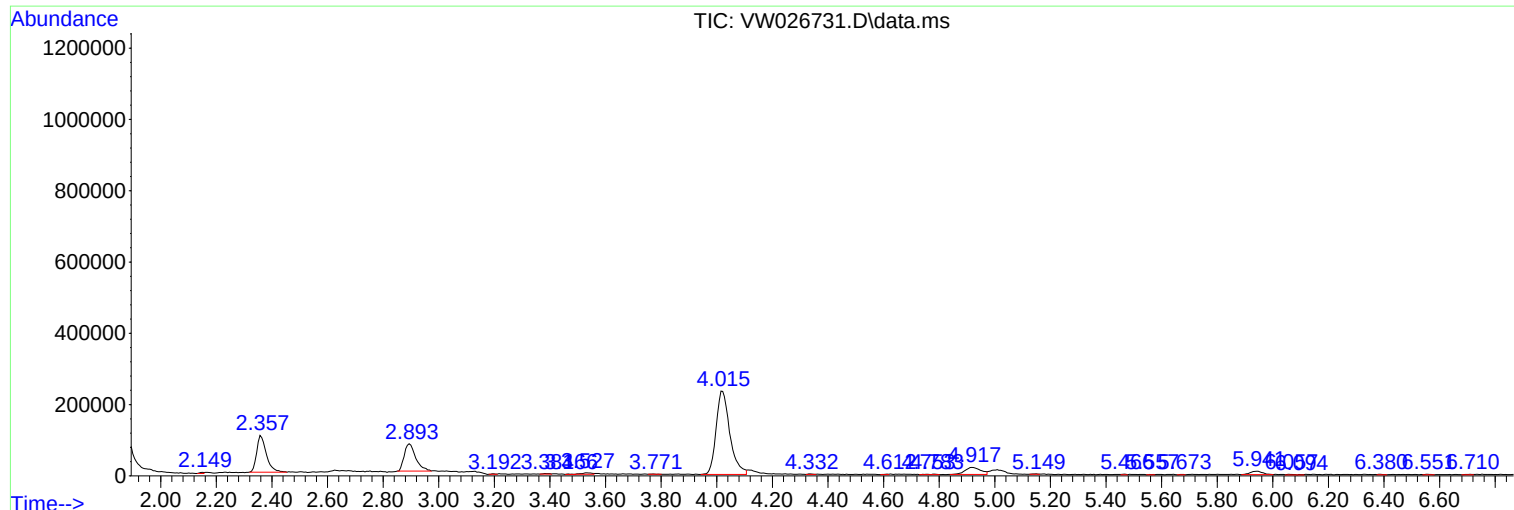
Sum of corrected areas: 19184201

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A48P4

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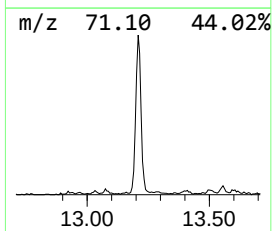
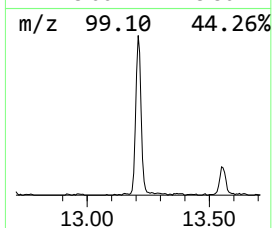
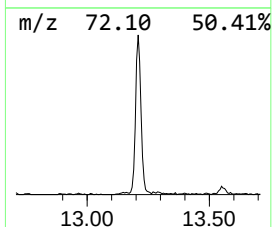
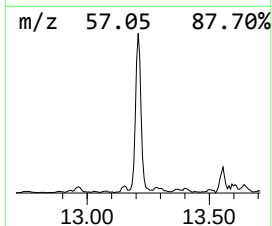
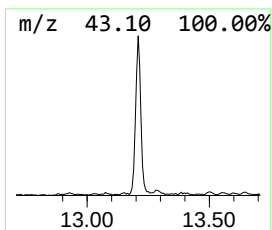
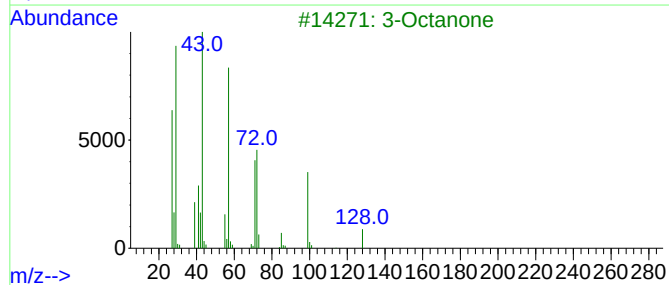
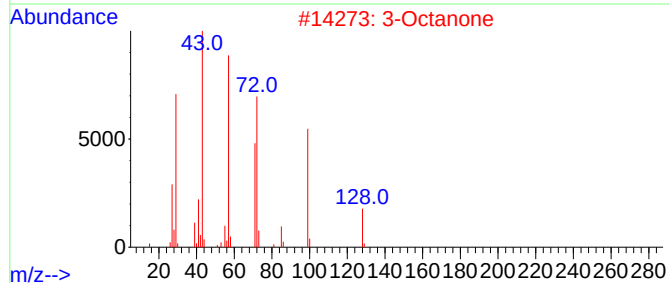
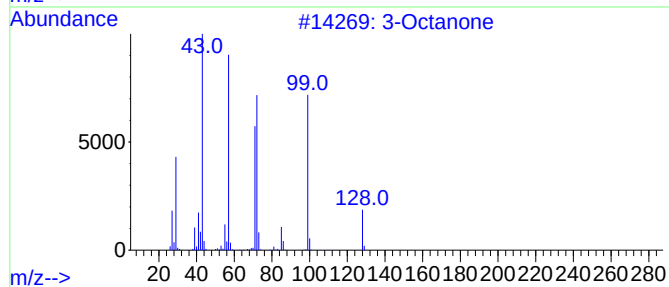
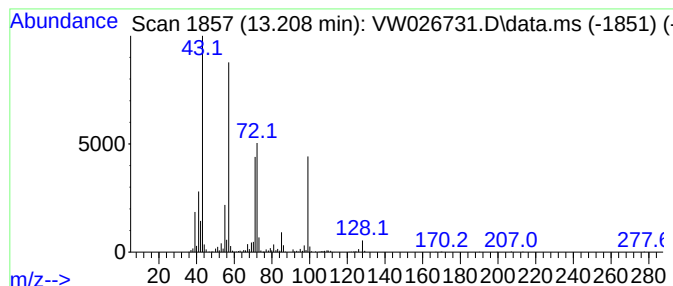
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM081023SMA.M
Quant Title : SFAM01.0

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.
13.209	4.24 ug/L	305972	1,4-Dichlorobenzene-d4	13.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Octanone	128	C8H16O	000106-68-3	93
2		3-Octanone	128	C8H16O	000106-68-3	68
3		3-Octanone	128	C8H16O	000106-68-3	64
4		Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	52
5		2,3-Octanedione	142	C8H14O2	000585-25-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Octanone	13.209	4.2	ug/L	305972	3	13.556	1805350	25.0