# Characterization and Comparison of Aroma Profiles and Aroma-Active Compounds Between Traditional and Modern Sichuan Vinegars by Molecular Sensory Science

Sam Al-Dalali[1,2], Fuping Zheng[1,3*], Baoguo Sun[1], Feng Chen[4]

[1] Beijing Advanced Innovation Center for Food Nutrition and Human Health, Beijing Technology and Business University, Beijing 100048, China

[2] Department of Food Science and Technology, Ibb University, Ibb, Yemen

[3] Beijing Laboratory of Food Quality and Safety, Beijing Technology and Business University

[4] Department of Food, Nutrition and Packaging Sciences, Clemson University, South Carolina, USA

* Corresponding authors:

Dr. Fuping Zheng

E-mail: zhengfp@btbu.edu.cn

Tel: 0086-10-68985413

**Table S1.** General Information about the Collected Vinegar Samples

| Collected samples | | | | |
|---|---|---|---|---|
| Batches | STV | No. of samples | SMV | No. of samples |
| Batch 1 | 10/1/2018 | 3 | 10/1/2018 | 3 |
| Batch 2 | 23/11/2018 | 2 | 16/2/2019 | 2 |
| Batch3 | 31/1/2019 | 2 | 18/2/2019 | 2 |

**Table S2.** Identification of Volatile Compounds in STV and SMV Samples

| Compounds | CAS | RI[a] | | Identification[b] | STV | SMV |
|---|---|---|---|---|---|---|
| | | HP-5 | DB-Wax | | | |
| (E)-3-(furan-2-yl)-2-methylprop-2-enal[c] | 874-66-8 | 1173 | 1893 | RI, MS, S | NBF | NBF |
| (*E*)-4-(furan-2-yl)but-3-en-2-one | 623-15-4 | 1184 | | RI, MS, S | NBF | n.d |
| 1-(4-hydroxy-3-methoxyphenyl)-ethanone[c] | 498-02-2 | 1486 | | RI, MS, S | AF | AF |
| 1-(furan-2-yl)-2-hydroxyethanone[c] | 17678-19-2 | 1082 | 2034 | RI, MS[d] | WS, NBF, AF | WS, NBF |
| 1-(furan-2-yl)ethanone | 1192-62-7 | | 1515 | RI, MS, S | WS, NBF, AF | NBF |
| 1,3-thiazole[c] | 288-47-1 | | 1248 | RI, MS, S | n.d | NBF |
| 1-butanol | 71-36-3 | | 1149 | RI, MS[d] | NBF | NBF |
| 1H-pyrrole-2-carboxaldehyde | 1003-29-8 | 1024 | 2048 | RI, MS, S | WS, NBF, AF | NBF, AF |
| 1-hydroxy-2-butanone[c] | 5077-67-8 | | 1380 | RI, MS[d] | NBF, AF | NBF, AF |
| 1-hydroxypropan-2-one | 116-09-6 | | 1302 | RI, MS, S | WS, NBF, AF | WS, AF |
| 1-hydroxypropan-2-yl acetate | 6214-01-3 | 906 | 1626 | RI, MS[d] | WS, AF | WS, NBF, AF |
| 1-phenylethanone | 98-86-2 | 1069 | 1666 | RI, MS, S | AF | AF |
| 1-propanol | 71-23-8 | | 1050 | RI, MS, S | WS, NBF, AF | WS, NBF,AF |
| 2(5H)-furanone[c] | 497-23-4 | | 1770 | RI, MS, S | WS, NBF | WS, NBF |
| 2,3-butanediol | 513-85-9 | 816 | 1549 | RI, MS, S | WS, AF | WS, AF |
| 2,3-butanedione | 431-03-8 | | 983 | RI, MS[d] | WS, NBF, AF | NBF, AF |
| 2,3-pentanedione[c] | 600-14-6 | | 1060 | RI, MS, S | NBF | WS, NBF |
| 2,4,5-trimethyl-1,3-dioxolane | 3299-32-9 | 748 | 980 | RI, MS, S | WS, NBF | WS, NBF |
| 2,5-dimethylbenzaldehyde[c] | 5779-94-2 | 1216 | 1832 | RI, MS, S | AF | n.d |
| 2,6-dimethylpyrazine | 108-50-9 | | 1337 | RI, MS, S | WS, NBF | WS, NBF |
| 2-acetyl-5-methylfuran | 1193-79-9 | 1036 | | RI, MS, S | NBF | n.d |
| 2-acetyloxypropyl acetate[c] | 623-84-7 | | 1521 | RI, MS[d] | WS, NBF | WS, NBF |
| 2-acetylpyrrole | 1072-83-9 | 1071 | 1990 | RI, MS, S | WS, NBF | WS, NBF |
| 2-butanol | 78-92-2 | | 1031 | RI, MS, S | WS, NBF, AF | WS, NBF,AF |
| 2-ethyl-1-hexanol | 104-76-7 | 1032 | 1498 | RI, MS, S | AF | NBF |
| 2-ethyl-3-hydroxyhexyl 2-methylpropanoate[c] | 74367-31-0 | 1374 | | RI, MS[d] | n.d | NBF |
| 2-furanmethanol | 98-00-0 | 869 | | RI, MS, S | WS, NBF, AF | WS, NBF, AF |
| 2-hydroxy-3-butanone | 513-86-0 | 715 | 1291 | RI, MS, S | WS, NBF, AF | WS, NBF, AF |
| 2-hydroxy-3-pentanone[c] | 5704-20-1 | | 1368 | RI, MS[d] | WS, NBF, AF | WS, NBF, AF |
| 2-hydroxypropyl acetate[c] | 627-69-0 | 890 | 1581 | RI, MS[d] | WS, NBF, AF | WS, NBF, AF |
| 2-methoxy-4-methylphenol | 93-51-6 | 1188 | 1974 | RI, MS, S | WS, NBF | WS, NBF, AF |
| 2-methoxyphenol | 90-05-1 | 1086 | 1876 | RI, MS, S | WS, NBF, AF | WS, NBF, AF |
| 2-methyl-1,3-dioxane | 626-68-6 | | 1068 | RI, MS[d] | NBF, AF | WS, NBF |
| 2-methylbutanoic acid | 116-53-0 | 925 | | RI, MS, S | AF | AF |
| 2-methyloxolan-3-one | 3188-00-9 | | 1263 | RI, MS, S | NBF | WS, NBF |
| 2-methylpropan-1-ol | 78-83-1 | | 1096 | RI, MS[d] | WS, NBF, AF | WS, NBF,AF |
| 2-methylpropanoic acid | 79-31-2 | 809 | 1572 | RI, MS, S | WS, AF | WS, AF |
| 2-methyl-*γ*-butyrolactone[c] | 1679-47-6 | | 1601 | RI, MS[d] | NBF | NBF |
| 2-phenethyl acetate | 103-45-7 | 1254 | 1832 | RI, MS, S | WS, NBF | NBF |
| 2-phenyl-2-butenal | 4411-89-6 | 1270 | 1953 | RI, MS, S | WS, NBF | WS, NBF |
| 2-phenyl-3-(2-furyl)-propenal | 57568-60-2 | 1684 | | MS, S | WS, NBF | WS, NBF |
| 2-phenylacetaldehyde | 122-78-1 | 1047 | 1656 | RI, MS, S | NBF | NBF |
| 2-phenylacetic acid | 103-82-2 | 1260 | | RI, MS[d] | AF | WS, AF |
| 2-phenylethanol | 60-12-8 | 1116 | 1932 | RI, MS, S | WS, NBF, AF | WS, NBF, AF |
| 2-propen-1-ol[c] | 107-18-6 | | 1120 | RI, MS, S | WS, AF | WS |
| 2-propyl-1,3-benzodioxane[c] | 56182-51-5 | 1422 | | RI, MS[d] | NBF | n.d |
| 3-(methylthio)-1-propanol | 505-10-2 | 983 | 1731 | RI, MS, S | NBF, AF | NBF, AF |
| 3-(methylthio)propyl acetate | 16630-55-0 | 1124 | | RI, MS, S | n.d | NBF |
| 3-acetyloxypropyl acetate[c] | 628-66-0 | 1102 | 1666 | RI, MS[d] | WS, NBF | WS, NBF |
| 3-ethoxypropanol | 111-35-3 | | 1386 | RI, MS, S | NBF, AF | NBF, AF |
| 3-hydroxy-3-methylbutan-2-one | 115-22-0 | | 1242 | RI, MS[d] | n.d | NBF |
| 3-hydroxy-4,4-dimethyloxolan-2-one | 79-50-5 | 1046 | | RI, MS[d] | AF | AF |
| 3-methyl-2-butenoic acid[c] | 541-47-9 | | 1807 | RI, MS, S | AF | AF |
| 3-methylbutan-1-ol | 123-51-3 | | 1212 | RI, MS, S | NBF | WS, NBF,AF |
| 3-methylbutanal | 590-86-3 | 652 | | MS, S | NBF | NBF |
| 3-methylbutanoic acid | 503-74-2 | 900 | 1675 | RI, MS, S | WS, AF | WS, AF |
| 3-methylpentane-2,4-dione[c] | 815-57-6 | | 1215 | RI, MS[d] | WS, NBF | WS |
| 3-oxobutan-2-yl acetate | 4906-24-5 | 895 | 1396 | RI, MS, S | WS, NBF | WS, NBF |
| 4-ethyl-2-methoxyphenol | 2785-89-9 | 1276 | 2030 | RI, MS, S | n.d | WS, NBF |

**Table S2** Continued

| Compounds | CAS | RI[a] | | Identification[b] | STV | SMV |
|---|---|---|---|---|---|---|
| | | HP-5 | DB-Wax | | | |
| 4-methyl-4-heptanol[c] | 598-01-6 | 1004 | | RI, MS[d] | NBF | n.d |
| 4-methylpentanoic acid | 646-07-1 | 973 | 1813 | RI, MS, S | AF | AF |
| 5-acetoxymethyl-2-furaldehyde | 10551-58-3 | 1302 | 2158 | RI, MS[d] | n.d | NBF |
| 5-hydroxymethylfurfural | 67-47-0 | 1224 | 2496 | RI, MS, S | WS, NBF, AF | NBF, AF |
| 5-methyl-2(3H)-furanone | 591-12-8 | | 1438 | RI, MS, S | n.d | AF |
| 5-methyl-2-phenyl-2-hexenal | 21834-92-4 | 1486 | 2096 | RI, MS, S | WS, NBF | WS, NBF |
| 5-methylfuran-2-carbaldehyde | 620-02-0 | 963 | 1582 | RI, MS, S | NBF | NBF |
| 5-methyloxolan-2-one | 108-29-2 | 959 | | RI, MS, S | n.d | NBF |
| acetic acid | 64-19-7 | | 1445 | RI, MS, S | WS, AF | WS, AF |
| benzaldehyde | 100-52-7 | | 1534 | RI, MS, S | WS, NBF | WS, NBF |
| benzoic acid | 65-85-0 | 1185 | | RI, MS, S | AF | AF |
| benzothiazole | 95-16-9 | 1228 | | RI, MS, S | NBF | n.d |
| benzyl alcohol | 100-51-6 | 1039 | 1892 | RI, MS, S | WS, NBF | WS, NBF, AF |
| butanoic acid | 107-92-6 | 875 | 1632 | RI, MS, S | WS, AF | WS, AF |
| butyrolactone | 96-48-0 | 922 | 1642 | RI, MS, S | WS, NBF | WS, NBF, AF |
| decanal | 112-31-2 | 1203 | | RI, MS, S | AF | n.d |
| diethyl butanedioate | 123-25-1 | | 1683 | RI, MS, S | n.d | NBF |
| ethyl 2-hydroxy-4-methylpentanoate | 10348-47-7 | 1061 | 1553 | RI, MS, S | WS, NBF | WS, NBF |
| ethyl 3-hydroxybutanoate | 5405-41-4 | 937 | | RI, MS, S | n.d | AF |
| ethyl lactate | 97-64-3 | 816 | 1357 | RI, MS, S | WS, NBF, AF | NBF, AF |
| ethyl pyridine-3-carboxylate[c] | 614-18-6 | 1214 | | RI, MS, S | n.d | NBF |
| furan-2-carbaldehyde | 98-01-1 | 858 | 1480 | RI, MS, S | WS, NBF, AF | WS, NBF, AF |
| furan-2-ylmethyl acetate | 623-17-6 | 993 | 1546 | RI, MS, S | NBF | NBF |
| heptanoic acid | 111-14-8 | 1090 | | RI, MS, S | n.d | AF |
| hexanal | 66-25-1 | | 1089 | RI, MS, S | AF | NBF |
| hexanoic acid | 142-62-1 | 1010 | 1854 | RI, MS, S | WS, AF | WS, AF |
| methyl 2-hydroxypropanoate[c] | 2155-30-8 | | 1326 | RI, MS[d] | WS, NBF | WS |
| methylpyrazine | 109-08-0 | | 1267 | RI, MS, S | NBF | WS, NBF |
| nonanal | 124-19-6 | 1092 | 1398 | RI, MS, S | n.d | AF |
| octanoic acid | 124-07-2 | 1179 | 2072 | RI, MS, S | AF | AF |
| oxepan-2-one[c] | 695-06-7 | | 1719 | RI, MS, S | WS, NBF | WS, NBF |
| pentanoic acid | 109-52-4 | 928 | 1746 | RI, MS, S | AF | AF |
| phenol | 108-95-2 | 984 | 2019 | RI, MS, S | AF | AF |
| propanoic acid | 79-09-4 | 787 | 1535 | RI, MS, S | WS, AF | WS, AF |
| pyridin-3-ylmethanol[c] | 100-55-0 | 1132 | | RI, MS[d] | NBF | n.d |
| tetramethylpyrazine | 1124-11-4 | 1085 | 1492 | RI, MS, S | WS, NBF | WS, NBF |
| trimethyloxazole | 20662-84-4 | | 1200 | RI, MS, S | WS, NBF | WS, NBF |
| trimethylpyrazine | 14667-55-1 | | 1415 | RI, MS, S | NBF | NBF |
| vanillin | 121-33-5 | 1397 | 2568 | RI, MS, S | WS, AF | WS, AF |
| $\gamma$-nonalactone | 104-61-0 | 1360 | 2055 | RI, MS, S | WS, NBF | WS, NBF |

[a] Retention indices; [b] Identification method was done for each compound based on the following: RI, retention indices, MS, mass spectrometry, S, injection of the standard compound, odor, compare the odor descriptions for the analytes with its corresponding standards, and also with the literature; [c] compounds that identified for the first time in vinegar; [d] Compounds that tentatively identified; n.d, not detected; WS, whole extracted sample without fractionations; NBF, neutral base fraction; AF, acid fraction.