Data Article

Dataset on the total phenolic contents and total anti-oxidants capacity in commercially available whiskey

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ARTICLE INFO

Article history:
Received 26 July 2022
Revised 11 September 2022
Accepted 13 September 2022
Available online 8 October 2022

Dataset link: Dataset on the total phenolic contents and total anti-oxidants capacity in naturally distilled whiskey (Original data)

Keywords:
Whiskey
Total phenolic content
Total anti-oxidants capacity
Aged whiskey

ABSTRACT

Data in this article are acquired from 46 naturally distilled whiskey. Whiskey samples were produced in the United Kingdom, United States, Ireland, Scotland, and Canada. Samples differ with their type of distillery including (Blended, finest blended, Malted, single Malted, rye, straight Rye, special blended, and special reserved), years of aging, and ethanol percentages. The contents of beneficial bioactive components including total phenolic contents and total anti-oxidants activity and the correlation between them were addressed.

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https://doi.org/10.1016/j.dib.2022.108608
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Specifications Table

| Subject                          | Total phenolic content and total anti-oxidant capacity in aged Whiskey |
|---------------------------------|------------------------------------------------------------------------|
| Specific subject area           | Food science                                                           |
| Type of data                    | Coulometric analyzer EXPERT-006 (Econix-Expert, Russia)                |
| How the data were acquired      | Spectrophotometer (Shimadzu UV 2401pc, Japan)                          |
|                                 | Sodium carbonate, powder, ≥99.5%, ACS reagent (Sigma-Aldrich, st. louis, USA) |
|                                 | Ascorbic acid 99% (Sigma-Aldrich, st. louis, USA)                      |
|                                 | Folin-Ciocalteu’s phenol reagent (Sigma-Aldrich, st. louis, USA)       |
|                                 | Gallic acid reference substance ≥98.0% (Sigma-Aldrich, st. louis, USA) |
|                                 | Potassium bromide ACS Reagent (Supelco, Pennsylvania, USA)             |
| Data format                     | Raw data provided in Microsoft Excel Worksheet                          |
| Description of data collection  | 46 samples of naturally distilled whiskey were purchased from the supermarket (Perekrostok, Moscow, Russia). Whiskey samples were produced in the United Kingdom, United States, Ireland, Scotland, and Canada. Samples differ with their type of distillery including (Blended, finest blended, Malted, single Malted, rye, straight Rye, special blended, and special reserved), years of aging, and ethanol percentages. The data on total phenolic content were obtained by the colorimetric method of Folin–Ciocalteu using gallic acid as a standard [1]. The data on total antioxidants capacity was obtained by coulometric analysis method using electrogenerated bromine radicals as described by Lapin A. [2,3] with modifications. Microsoft Excel Worksheet containing mean values of total phenolic contents and total anti-oxidants capacity, years of aging, type of distillery, and alcohol percentages of 46 sorts of Whiskey. |
| Data source location            | Institution: Plekhanov Russian University of Economics                  |
|                                 | City/Town/Region: Moscow                                               |
|                                 | Country: Russian Federation                                            |
|                                 | Whiskey samples were produced in Scotland, Ireland, Canada, The United States, and United Kingdom. |
| Data accessibility              | With the article                                                       |
|                                 | Repository name: https://data.4tu.nl/                                  |
|                                 | Data identification number: 10.4121/20337516(/13:underline)             |

Value of the Data

- These data can add an additional information regarding the content of total phenolic content and anti-oxidant capacity of 46 common whisky commodity
- This dataset is necessary as a qualification approach to the systematic identification of whiskey products
- The method of determination of total anti-oxidants capacity described in this manuscript is precise, relevant, and short time consuming that can be used by oenologists and whiskey researchers

1. Data Description

This dataset contains analyzed data obtained by galvanostatic coulometric analyzer and spectrophotometer from freshly opened whiskey bottles obtained from the supermarket. Whiskey samples were produced in the United Kingdom, United States, Ireland, Scotland, and Canada. Samples differ with their type of distillery including (Blended, finest blended, Malted, single Malted, rye, straight Rye, special blended, and special reserved), years of aging, and ethanol percentages. Dataset provided about total phenolics content and total anti-oxidants capacity is displayed in Table 1. Data on years of distillation was obtained from the labelling of each bottle. Correlations between total phenolic contents, total anti-oxidants capacity, and distillation years are shown in Table 2.
Table 1
Distillery type, percentage of alcohol, distillation years, total phenolic contents, and total anti-oxidant capacity of 46 whiskey samples.

| No | Name of Whiskey                                      | Distillery type | Alcohol, % | Aged | Total phenolic contents, (mg GAE/mL) | Total Anti-oxidant capacity, (mg AA/100mL) |
|----|------------------------------------------------------|----------------|------------|------|-------------------------------------|------------------------------------------|
| 1  | JAMESON Crested x Eight Degrees Brewing              | Blended        | 43         | *    | 4.24 ± 0.01                         | 32.92 ± 0.88                             |
| 2  | JAMESON IRISH WHISKEY                                | Blended        | 40         | 4    | 4.26 ± 0.07                         | 21.6 ± 0.09                              |
| 3  | JAMESON Black Barrel                                | Blended        | 40         | 12   | 4.58 ± 0.08                         | 28.2 ± 0.60                              |
| 4  | JIM BEAM BOURBON WHISKEY                            | Blended        | 40         | 4    | 3.27 ± 0.03                         | 47.3 ± 0.87                              |
| 5  | JIM BEAM BOURBON WHISKEY - Honey                    | Blended        | 35         | 4    | 3.09 ± 0.14                         | 66.4 ± 0.50                              |
| 6  | JIM BEAM BOURBON WHISKEY Black                      | Blended        | 43         | 8    | 3.62 ± 0.06                         | 60.0 ± 0.03                              |
| 7  | JACK DANIEL'S Straight Rye Tennessee Whiskey        | Rye            | 45         | 5    | 4.38 ± 0.11                         | 59.5 ± 0.58                              |
| 8  | JACK DANIEL'S Old No. 7                             | Blended        | 40         | 5    | 4.43 ± 0.08                         | 48.9 ± 0.15                              |
| 9  | JACK DANIEL'S Tennessee Honey Whiskey               | Blended        | 35         | 5    | 7.59 ± 0.14                         | 76.4 ± 0.48                              |
| 10 | JACK DANIEL'S GENTLEMAN JACK Whiskey                | Double         | 40         | 10   | 6.55 ± 0.27                         | 70.8 ± 0.53                              |
|    | Ballantine's finest blended Scotch whisky           |                |            |      |                                     |                                          |
| 11 | Ballantine's 17 Year Old Whisky                     | Blended        | 40         | 18   | 5.64 ± 0.02                         | 78.6 ± 0.41                              |
| 12 | Ballantine's 12 Year Old Whisky                     | Blended        | 40         | 12   | 4.60 ± 0.21                         | 79.4 ± 0.24                              |
| 13 | Ballantine's 30 Year Old Whisky                     | Blended        | 40         | 30   | 6.45 ± 0.18                         | 83.0 ± 0.40                              |
| 14 | Ballantine's Glenburgie 15 Year Old Whisky          | Blended        | 40         | 15   | 5.54 ± 0.42                         | 71.3 ± 0.29                              |
| 15 | Buchanan Scotch Whisky (De luxe)                    | Finest blended | 40         | 12   | 12.16 ± 0.19                        | 33.26 ± 0.60                             |
| 16 | Buchanan Scotch Whisky                              | Blended        | 40         | 12   | 6.93 ± 0.14                         | 73.8 ± 0.52                              |
| 17 | Buchanan Scotch Whisky (special reserved)           | Single Malted  | 40         | 15   | 15.186 ± 0.12                       | 51.98 ± 0.72                             |
| 18 | Buchanan Scotch Whisky                              | Single Malted  | 40         | 18   | 7.80 ± 0.11                         | 64.7 ± 0.90                              |
| 19 | Buchanan Scotch Whisky                              | Blended        | 40         | 21   | 21.21 ± 0.00                        | 73.21 ± 0.40                             |
| 20 | Loch Lomond Single Malt Scotch Whisky Highland      | Single Malted  | 40         | 12   | 7.39 ± 0.09                         | 77.7 ± 0.54                              |
| 21 | Loch Lomond Single Malt Scotch Whisky Highland      | Single Malted  | 40         | 18   | 7.64 ± 0.09                         | 53.9 ± 0.42                              |
| 22 | Loch Lomond Single Malt Scotch Whisky Highland      | Single Malted  | 40         | 21   | 7.08 ± 0.04                         | 63.6 ± 0.41                              |
| 23 | Johnnie Walker Green Label blended malt Scotch whisky | Malted        | 43         | 15   | 6.48 ± 0.25                         | 54.7 ± 0.01                              |
| 24 | Johnnie Walker Blue Label blended Scotch whisky     | Malted         | 43         | 28   | 7.49 ± 0.02                         | 71.4 ± 0.26                              |
| 25 | Johnnie Walker Red Label blended Scotch whisky      | Blended        | 40         | 12   | 7.12 ± 0.10                         | 32.6 ± 0.12                              |
| 26 | Glenfiddich Special Reserve single malt Scotch whisky| Single Malted | 43         | 12   | 5.59 ± 0.06                         | 33.9 ± 0.34                              |
| 27 | Glenfiddich Special Reserve single malt Scotch whisky| Single Malted | 43         | 12   | 5.59 ± 0.06                         | 33.9 ± 0.34                              |

(continued on next page)
**Table 1 (continued)**

| No | Name of Whiskey                          | Distillery type | Alcohol, % | Aged | Total phenolic contents, (mg GAE/mL) | Total Anti-oxidant capacity, (mg AA/100mL) |
|----|------------------------------------------|-----------------|------------|------|--------------------------------------|--------------------------------------------|
| 28 | Glenfiddich Special Reserve single malt Scotch whisky | Single Malted    | 40         | 12   | 5.81 ± 0.06                          | 36.8 ± 0.03                                |
| 29 | Glenfiddich Special Reserve single malt Scotch whisky | Single Malted    | 40         | 15   | 6.50 ± 0.05                          | 52.9 ± 0.12                                |
| 30 | Chivas Regal blended Scotch whisky        | Blended         | 40         | 12   | 6.69 ± 0.20                          | 40.2 ± 0.70                                |
| 31 | Chivas Regal blended Scotch whisky        | Blended         | 40         | 18   | 7.11 ± 0.23                          | 57.5 ± 0.48                                |
| 32 | Clontarf Irish whiskey reserve           | Blended         | 40         | *    | 3.26 ± 0.17                          | 21.76 ± 0.16                               |
| 33 | Clontarf Irish whiskey reserve           | Blended         | 40         | *    | 6.81 ± 0.09                          | 22.6 ± 0.17                                |
| 34 | Clontarf 1014 Black Label Classic Blend  | Single Malted    | 40         | 4    | 4.40 ± 0.08                          | 19.9 ± 0.32                                |
| 35 | Clontarf 1014 Irish whisky               | Single Malted    | 40         | 3    | 3.48 ± 0.05                          | 19.1 ± 0.11                                |
| 36 | Clan Denny blended malt Scotch whisky from speyside | Malted         | 46.7       | 3    | 2.65 ± 0.02                          | 17.2 ± 0.33                                |
| 37 | Glenkinchie malt lowland Scotch whisky   | Malted          | 43         | 10   | 3.62 ± 0.06                          | 49.9 ± 0.11                                |
| 38 | Glenfiddich Special Reserve single malt Scotch whisky | Single Malted    | 40         | 18   | 7.71 ± 0.07                          | 78.9 ± 0.17                                |
| 39 | Dewar's                                  | Blended         | 40         | 12   | 4.25 ± 0.05                          | 35.5 ± 0.33                                |
| 40 | GlenClyde                                | Blended         | 40         | 12   | 4.33 ± 0.08                          | 30.1 ± 0.14                                |
| 41 | Crown Royal Canadian Whisky              | Blended         | 40         | 13   | 6.14 ± 0.10                          | 36.7 ± 0.15                                |
| 42 | The Girvan Patent Still No4              | Blended         | 42         | 25   | 7.60 ± 0.30                          | 75.93 ± 0.19                               |
| 43 | The Girvan Patent Still                  | Blended         | 42         | 10   | 5.69 ± 0.08                          | 45.65 ± 0.07                               |
| 44 | Grant’s Triple Wood                     | Blended         | 40         | 3    | 2.38 ± 0.12                          | 19.23 ± 0.13                               |
| 45 | Monkey Shoulder                         | Blended         | 40         | *    | 4.71 ± 0.05                          | 30.81 ± 1.33                               |
| 46 | Glenfiddich                              | Single malted   | 40         | 12   | 5.64 ± 0.34                          | 19.23 ± 0.14                               |

* no-age-statement whisky

**Table 2**

Correlations between total phenolic contents, total anti-oxidants capacity, and distillation years.

| Total Phenolic Contents | Total Anti-oxidants Capacity | Aged |
|-------------------------|------------------------------|------|
| Total Phenolic Contents  | .516**                       | .707** |
| Total Anti-oxidants Capacity | .516**                      | .568** |
| Aged                    | .707**                       | .568** |

** Correlation is significant at the 0.01 level (2-tailed).
2. Experimental Design, Materials and Methods

2.1 Total phenols content

This method is based on the oxidation of phenolic compounds with a Folin-Chocalteu reagent. The reagent is a mixture of phosphoric-tungsten H3PW12O40 and phosphoric-molybdenum H3PMo12O40 acids, which are reduced by oxidation due to the existence of phenols into a mixture of oxides including blue tungsten (W8O23) and molybdenum (Mo8O23). Blue staining makes it possible to measure the maximum absorption of the solution. It is proportional to the content of phenolic compounds.

Sample preparation comprises the preparation of a reaction mixture including 30 ml of whiskey, 2220 mL distilled water, 150 mL of Folin-Chocalteu reagent, 600 ml of a 20% solution of sodium carbonate (Na2CO3).

A control sample was also prepared, where distilled water was used instead of whiskey. Thus, the composition of the control sample was as follows: 2250 μl distilled water, 150 μl of Folin-Chocalteu reagent, 600 μl of a 20% solution of sodium carbonate (Na2CO3).

Further, the obtained solutions were kept for 90 min at room conditions until the complete completion of the oxidation reaction of phenolic compounds, when the optical density practically did not change during subsequent measurements, which made it possible to reduce the error several times.

Optical density measurements were carried out at a wavelength of 750 nm using (Shimadzu UV 2401pc, Japan) spectrophotometer. Measurements were carried out in 1 cm thick cuvettes. Total phenolic content was expressed as mg gallic acid equivalents (GAE) per milliliter of Whiskey using gallic acid calibration curve (R2=0.989). For this purpose, a calibration graph was constructed. The average value of triplicate measurements for each sample was used for calculation.

2.2 Total anti-oxidant capacity

The principle of determination of AOC in whiskey samples is based on Faraday’s law where the mass of the analyte is determined by the amount of electricity spent on the reaction. The method was described by Lapin A. and Othman A.J. [2,3] and slightly modified as the following:

Exactly 1 mL of whiskey sample was transferred into the electrochemical cell containing 50 mL of buffer solution (0.2 M potassium bromide and 0.1 M sulfuric dioxide) with continuous stirring for 1 min. The electrolysis process begins when electric current generates Bromine anions at a constant current of 50 mA from the buffer solution.

The electrolysis begins at 40 millivolts, the initial, and the end value of the electrical titration were adjusted on 150 millivolts.

The initial and end values of electro-titration were set on 200 mV electrical current. Bromine anions were generated under 50 mA electrical current where all compounds with anti-Oxidants properties would react with the excessive bromine anions. The electrolysis process initiated at 40 mV. Total anti-oxidants capacity expressed as mg ascorbic acid equivalents per 100 mL of whiskey.

2.3 Statistical Analysis

Pearson’s correlation coefficient, means, and standard deviations were performed using SPSS
Ethics Statements

There is no funding for the present effort. There is no conflict of interest. The data is available in public domain.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data Availability

Dataset on the total phenolic contents and total anti-oxidants capacity in naturally distilled whiskey (Original data) (4tu.researchdata).

CRediT Author Statement

Ali J. Othman: Conceptualization, Methodology, Software, Formal analysis, Writing – original draft; Sarah G. Saker: Software, Formal analysis, Writing – original draft.

Acknowledgments

This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Supplementary Materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.dib.2022.108608.

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