

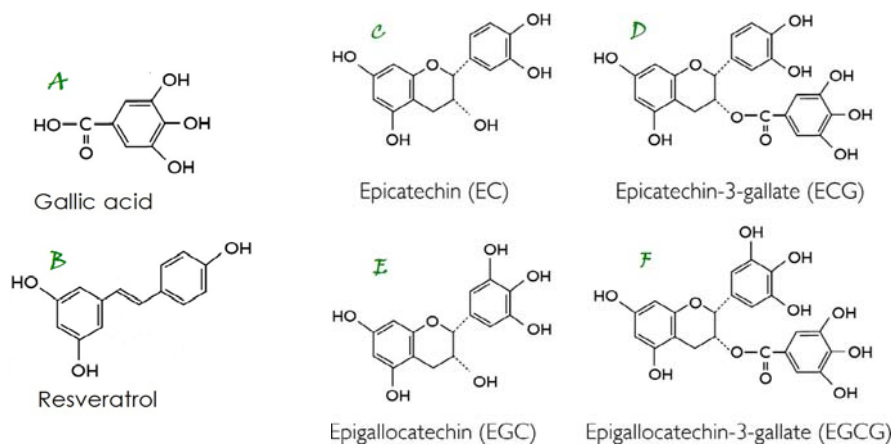
Evaluating the polyphenol content as quality attribute in green tea by NIR spectroscopy – selected examples

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Green tea has been consumed worldwide, almost as old as mankind. It is the handpicked and non-fermented young leaves of the evergreen plant, *Camellia sinensis* L. Its beneficial health effects are associated with the **antioxidant activity** mainly resulted from polyphenol compounds. These molecules cause also the characteristic astringent taste of green tea drink. Polyphenol content (predominantly catechins) may make up to 25-35% of the dry weight of green tea leaves. These phenols are mainly flavonols and their gallic acid derivatives (see [1]), namely (+)-catechin, **(-)-epicatechin**(C), (+)-gallocatechin, **(-)-epicatechin gallate** (D), **(-)-epigallocatechin** (E), and **(-)-epigallocatechin gallate** (F). It has been known that from structure-activity relationship studies, antioxidant activity of flavonoids depends substantially on the number and position of hydroxyl groups in the molecule [2].



The parent compound, the well-known **gallic acid** (A) was described from structural point of view by Billes et al [1,6]. Gallic acid is the basic building block of the green tea catechins (C, D, E, F) (see e.g. ref [7]). The antioxidative characteristics of food and drink increases their biological value, and thus enhances the biological quality of e.g. green tea. **Polyphenol content can be an important quality attribute in the lives of sapiental consumers.** A similar constituent of red berries and red wine is resveratrol (B), also a phenol-type molecule (see Molnár et al [8]).

An example for drug–green tea interaction

Bortezomib (marketed as Velcade) was developed as a potent, specific proteasome inhibitor for the treatment of relapsed and refractory multiple myeloma and currently it is still one of the most effective drugs available for treating multiple myeloma.

It was recently revealed that some flavonoids and vitamin C present in green leaves and green teas in the blood can neutralize bortezomib by directly interaction between two chemicals.

As a result the expression „**good quality**” is different in a the diet of a healthy consumer and that of a patient under treatment against myeloma.

Quality attributes in tea

In general, all of us may agree that judging tea quality and tasting is subjective and rather elusive. In fact, tea tasting has been used over centuries to evaluate tea quality; it is fast and affordable, which was necessary for the tea trade. Also tea tasting allows many samples to be evaluated quickly. However, a more objective method would serve with the opportunity to standardize the classification process. One of them could be the NIR spectroscopic method supported with suitable statistical processing of the measured data. NIR measurement is fast and non-destructive, serialization can be achieved easily (see e.g. ref [3]). The beneficial effect of the antioxidant content of green tea together with other important factors (amino acid content, enjoyment of the beverage, etc) increases the quality of green tea.

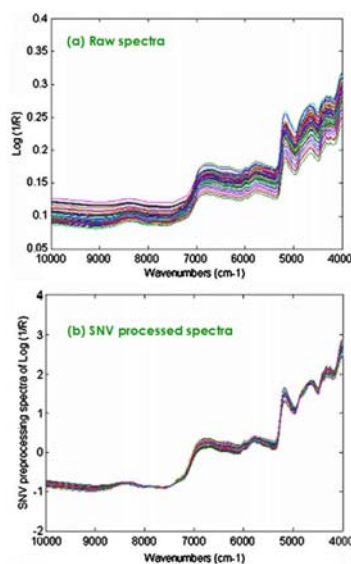
Another very important aspect of quality is the person who consumes a given product. As an example, the interaction of a modern effective anticancer drug, Bortezomib and green tea polyphenols illustrates the complex nature of quality and **thus the point of view of the consumer in assessing quality of a given product.**

References

- [1] Mohammed-Ziegler I., Billes F.: Vibrational spectroscopic calculations on pyrogallol and gallic acid, J. Mol. Struct.-THEOCHEM, 618(3), 259-265 (2002).
- [2] Farkas O., Jakus J., Heberger K.: Quantitative structure-antioxidant activity relationships of flavonoid compounds, Molecules, 9, 1079-1088 (2004).
- [3] Ziegler I., Csipor I., Billes F.: Changes of the European regulations of NIR spectroscopic methods and some applications, RITA tender summary, Oct. 2012, p. 1-9. (in Hungarian).
- [4] Chen, Q. Zhao, J., Chaitap, S., Guo, Z.: Simultaneous analysis of main catechins in green tea (*Camellia sinensis* L.), Food Chemistry, 113, 1272-1277 (2009).
- [5] Chen, Q. Zhao, J., Liu, M., Cai, J., Liu, J.: Determination of total phenols content in green tea using FT-NIR spectroscopy and different PLS algorithms, J. Pharm. Biomed. Anal., 46, 568-573 (2008).
- [6] Billes F., Mohammed-Ziegler I., Bombicz P: Vibrational Spectroscopy 43, 193–202 (2007).
- [7] Namal Senanayake, S.P.J.: Green tea extract: Chemistry, antioxidant properties and food application – A review, J. Functional Foods, 5, 1529-1541 (2013).
- [8] Molnár V., Billes F., Tyihák E., Mikosch H.: Spectrochimica Acta Part A 69, 542–558 (2008).
- [9] Jia, L., Liu, F.-T.: Why Bortezomib cannot go with „green”?, Cancer. Biol. Med., 10, 206-213 (2013).

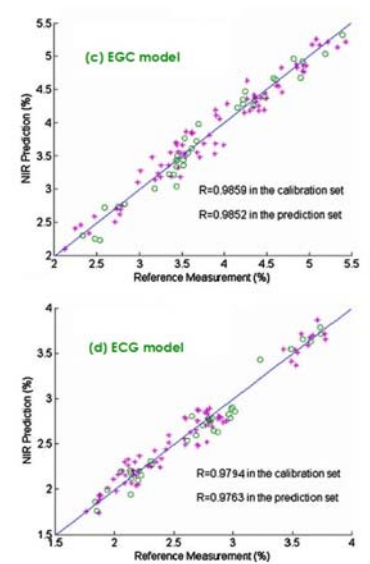
For the determination of these flavonoids various analytical methods are used but from quality assurance point of view the fast and non-destructive near infrared (NIR) spectroscopic methods have importance [3]. NIR methods require a reference method for calibration that can be e.g. reverse phase high performance liquid chromatography [4]. A suitable statistic evaluation method is also needed for which the well-known partial least squares (PLS) method was improved by Chen et al [4, 5]. Based on properly selected regions of the NIR spectra, the so-called synergy interval PLS method was found the best evaluation method [5].

NIR spectra of different green tea samples (based on ref [4])



Standard normal variate transformation (SNV) is a mathematical transformation method of the $\log(1/R)$ spectra to remove slope variation.

Correlation between reference measurement and NIR prediction (based on ref [4])



Reference method: reverse phase high performance liquid chromatography measurements. + denotes calibration and O NIR predicted values.