3wayPLS modeling of potentiometric multisensor system response for quantification of bitter taste in pharmaceuticals

Dmitry Kirsanov[1,3], *Yulia Blinova*[1], *Alisa Rudnitskaya*[2,3], *David Clapham*[4], *Andrey Legin*[1,3]
[1]*Chemistry Department, St. Petersburg State University, St. Petersburg, Russia*
[2]*CESAM/Chemistry Department, Aveiro University, Aveiro, Portugal*
[3]*Sensor Systems LLC, St. Petersburg, Russia*
[4]*GSK Pharmaceuticals, Park Road, Ware, UK*

In the present work the application of the artificial sensory system (Electronic Tongue, ET) for quantification of the bitter taste of various chemically dissimilar substances is reported. This approach to artificial quantification of bitterness is practically feasible and may be particularly useful on the early stages of development of novel API (active pharmaceutical ingredients) in pharmaceutical research and for flavour control of various pharmaceutical compositions, healthcare products and food ingredients [1].

The measurements were performed in a set of bitter substances provided by GlaxoSmithKline and assessed by human and rat sensory panels to produce bitterness intensity scores for each substance in different concentrations. The set consisted of 8 substances mostly used as API of various chemical nature, both inorganic and organic – potassium nitrate, quinine, caffeine, paracetamol, chlorhexidine, ibuprofen, etc. It must be pointed out that most of the substances studied belong to different classes and has got little in common both in composition and in properties of solution when dissolved. Furthermore, their behavior in water solutions is very different, some of them have acidic properties, and some of them are not ionized at neutral pH values. The latter issue is of crucial importance for potentiometric sensors as they respond to ionic species only. To circumvent this limitation we designed the experiment where all substances in all concentrations where studied at different pH levels ranging from 2 to 10, thus promoting their ionization. This experiment yielded 3 way data array (sensors X samples X pH). 3wayPLS regression models where constructed with reference data from rat sensory panel (% of inhibition values). These models where validated by various methods and were further applied for prediction of bitterness of unknown substances employed neither for calibration nor for validation. Predicted values were compared with rat panel estimates for these substances.

The details of experiment as well as results will be discussed in the presentation.

References

1. A. Legin, A. Rudnitskaya, D. Clapham, B. Seleznev, K. Lord, Yu. Vlasov, Analytical and Bioanalytical Chemistry, 2004, 380, 36-45, (2004)