



The „Health Wonder“ That Wasn't: Fake Sample Exposed by IR Analysis

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Introduction

The global market for dietary supplements, herbal preparations, and alternative health products has expanded rapidly in recent decades. This growth has also created significant problems; some with serious health risks. Unlike authorized pharmaceuticals, many supplements are not strictly regulated, and manufacturers may provide incomplete, misleading, or incorrect information about product composition. Substances sold under familiar names may actually contain unrelated chemicals, cheap fillers, or harmful substitutes. Similar issues are known from counterfeit medicines, where undeclared or substituted ingredients pose severe dangers.

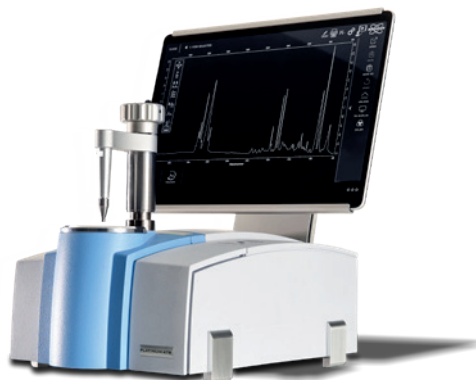
The consequences are wide-ranging: Consumers may experience ineffective treatment, unexpected pharmacological effects, allergic reactions, or harmful interactions with prescribed drugs. Healthcare providers can be misled when patients unknowingly ingest undeclared substances. Economically, fraudulent products can damage corporate reputation and lead to costly claims.

Fourier Transform Infrared (FT-IR) spectroscopy offers a fast and reliable tool to address these challenges. With minimal sample preparation and the ability to confirm chemical identity via characteristic spectral fingerprints, FT-IR enables rapid screening of diverse materials, making it valuable for pharmacies, quality-control labs, and regulatory bodies confronting potentially falsified or mislabeled supplements.

Instrumentation

The ALPHA II is a compact and highly robust FT-IR spectrometer designed for ease of use and reliability. It is operated using the intuitive OPUS TOUCH software interface. Typically, the ALPHA II is equipped with an Attenuated Total Reflection (ATR) accessory. The sample to be tested is simply placed on the measuring crystal. No further sample preparation is required, and cleaning is very easy. The resulting spectrum is like a chemical fingerprint of the sample and can be used for fully automated evaluation.

Fig. 1
ALPHA II spectrometer equipped with touch operated Microsoft Surface computer in tablet holder.



Example Cases

Pangamic Acid

Pangamic acid is a compound frequently referenced in alternative medicine literature, yet it has never been conclusively shown to exist in an isolated, well characterized chemical form. The term was introduced by Ernst T. Krebs, Sr. and Ernst T. Krebs, Jr. as the name for an ester derived from D gluconic acid and dimethylglycine (see Figure 2). In 1949, they obtained a patent for this proposed substance and later published papers in which they claimed to have synthesized it and to have isolated the compound from apricot seeds. However, subsequent investigations have shown that the substance itself was never synthesized and is thus not commercially available. Instead, a variety of unrelated compounds are marketed under the name "pangamic acid" such as diisopropylamine dichloroacetate, calcium gluconate and lactose.

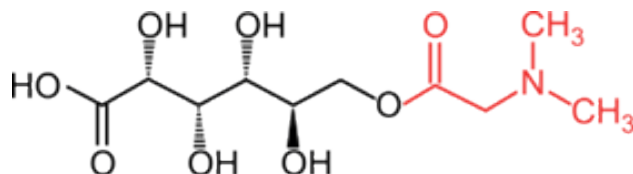


Fig. 2
Structure of pangamic acid.
Red: Dimethylglycine part.
Black: D-gluconic acid part.

We have obtained two different spectra for verification from pharmacies. They were recorded from samples that were labeled as pangamic acid sodium salt and pangamic acid, respectively. The data analysis was performed using Bruker's new machine learning based identification function "Composition-A.I.D.": It evaluates all feasible explanations for a spectrum based on single and combined reference spectra and automatically selects the best match, while still allowing experts to review alternatives when needed.

Figure 3 shows the search result for the sample labeled as pangamic acid sodium salt with an excellent hit-quality of 979 (out of max 1000) points. The spectrum clearly demonstrates that the material is actually sodium D-gluconate, which corresponds to the sodium salt of the gluconic acid moiety highlighted in black in Figure 2. Sodium D-gluconate is commonly used as a chelating agent and also as a food additive. It is considered safe, but it has no known health benefits in the context of the claims associated with pangamic acid.

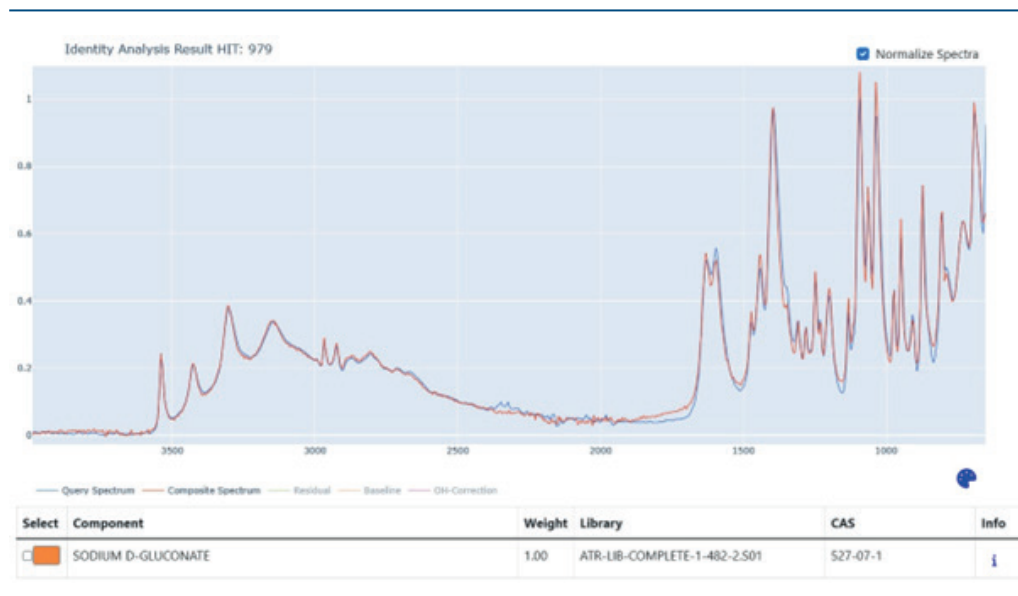


Fig. 3
A.I.D. search result of pangamic acid sodium salt.
Blue: Query spectrum,
Orange: Library spectrum.

The search result of the second substance is shown in Figure 4 with a very good hit quality value of 971. Interestingly, we found N,N-dimethylglycine hydrochloride in this sample which is basically the HCl-salt of the other part of the ester (shown in Figure 2, Red part). Dimethylglycine is classified as 'harmful if swallowed', but it has relatively low toxicity and may exhibit some positive biological activity.

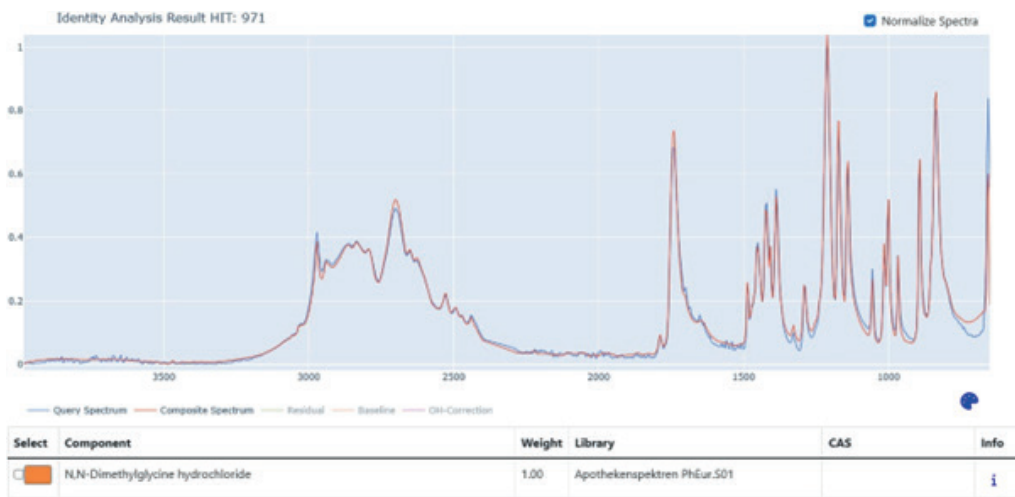


Fig. 4
A.I.D. search result of pangamic acid sodium salt.
Blue: Query spectrum,
Orange: Library spectrum.

Summary

Two products marketed as “pangamic acid” were analyzed using the ALPHA II ATR FT-IR spectrometer and evaluated with Composition A.I.D. Although pangamic acid has never been shown to exist as a defined chemical substance, both samples were sold under this name. FT-IR analysis revealed that one sample was sodium D gluconate, while the other contained N,N dimethylglycine hydrochloride. These results highlight the strong variability and mislabeling associated with such products and demonstrate how FT-IR spectroscopy enables rapid and reliable detection of incorrectly labeled dietary supplements and pharmaceutical APIs.

