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Chemical composition of paracetamol determined by IR spectroscopy

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Abstract
In this article we determined the chemical composition of paracetamol using the ShemadzuIRPrestige-21 spectrophotometer. The IR spectrum of paracetamol contains the following bands of groups O-H, CH_3, C=O, C=C, N-H, C-H, C-C, C-N (aryl) and C-N (amide). Paracetamol (acetaminophen) is a widely used analgesic and antipyretic, structurally characterized by a para-aminophenol nucleus, which gives it a specific pharmacological profile. The active substance, N-acetyl-p-aminophenol, is formulated in various pharmaceutical presentations, from tablets and capsules to oral solutions or suppositories. In these forms, paracetamol is accompanied by excipients such as fillers, disintegrants, sweeteners, stabilizers or flavor correctors, which ensure stability, solubility and optimal bioavailability. Its relatively simple chemical composition, combined with a favorable tolerability profile, explains the use of paracetamol as a first-line drug in the management of pain and fever.

Keywords: Chemical composition, paracetamol, IR spectroscopy

Introduction

Paracetamol (or paraacetylaminophenol, acetaminophen) is a para-aminophenol derivative of the anilide class, with analgesic and antipyretic action. Its anti-inflammatory action is practically non-existent, but this does not mean that it cannot be used in pain caused by inflammation. Common trade names include Tylenol and Panadol. At a standard dose, paracetamol only slightly lowers body temperature; in this respect it is inferior to ibuprofen, and the benefits of its use in fever are unclear. Paracetamol can relieve pain in mild acute migraine, but only to a small extent in episodic tension headache [1-5].

It was synthesized in 1873 by the reduction of p-nitrophenol in acetic acid. Acetanilide (antifebrine) had already been discovered in 1866, and phenacetin in 1877, and were used as antipyretics and analgesics. The possible therapeutic properties of paracetamol were ignored at the time of its discovery. In 1893, paracetamol was detected in the urine of patients who had been given phenacetin, and in 1899 in that of patients who had taken acetanilide. In both cases, it was considered a pharmacologically unimportant metabolite of these drugs. In 1946, Bernard Brodie and Julius Axelrod were investigating the causal links between the analgesics phenacetin and acetanilide and methemoglobinemia. They discovered that the analgesic effect of acetanilide was actually due to its metabolite, paracetamol, and that when it was administered, methemoglobinemia was greatly reduced in incidence and magnitude.

Paracetamol has excellent bioavailability after oral administration, and for this reason its parenteral administration is extremely rarely used. In short, its therapeutic properties are explained by the inhibition of prostaglandin synthesis. This determines the analgesic effect (by blocking the formation of prostaglandins E2 in the central and peripheral nervous system) and the antipyretic effect (at the level of the thermoregulation center in the hypothalamus. The synthesis of prostaglandins is the result of the action of cyclooxygenase, which is indirectly inhibited by paracetamol.

It is rapidly and almost completely absorbed from the digestive tract, with the maximum plasma concentration occurring 40-60 minutes after ingestion. At a maximum of 4 hours, absorption is maximum. It diffuses into all tissues, including passing through the blood-brain barrier. The half-life is 1-3 hours, but increases to 5 hours in newborns and patients with liver or kidney failure. At therapeutic doses of 0.5-2 g, the binding to plasma proteins is a maximum of 25% and a minimum of 10%. At toxic doses or in case of liver failure, it reaches up to 50%. [6-12]

80-90% is metabolized in the liver by conjugation, resulting in glucurono- (mostly) and sulfoconjugates, then excreted in the urine. 2% to 4% is eliminated unchanged in the urine, and a small fraction takes the cytochrome P450 pathway in the liver mitochondria, being the source of a highly toxic metabolite, which is rapidly inactivated by conjugation with glutathione. This metabolite is then conjugated a second time with cysteine and mercapturic acid and eliminated renally. This 2-electron oxidation of acetaminophen to N-acetylbenzosemiquinonimine by PHS probably involves the formation of a 1-electron oxidation product, N-acetyl-benzosemiquinonimine, a free radical, both metabolites being involved in renal toxicity. There is controversy regarding the identity of this intermediate metabolite. A number of experimental evidence suggests that it is N-acetylimidoquinone. In addition to these inactivation pathways, paracetamol also undergoes cysteine conjugation and deacetylation (resulting in para-aminophenol) in the liver. As It is observed that activation in the presence of cytochromes P450 leads to hepatotoxicity, and activation by PHS leads to nephrotoxicity, this is because the renal medullary area has low levels of Cyt P450, but high levels of PHS [13-17].

Materials and methods

Paracetamol commercial samples were purified by recrystallization from an ethanol solution. The orthorhombic modification of paracetamol was obtained from a melt according to the procedure. IR spectra were recorded on a ShemadzuIRPrestige-21 with mid-near-far infrared

measurement range Fourier Transformed IR spectrometer (resolution 4 cm-1) for KBr pellets (2 mg sample with 500 mg KBr). Attempts were made to monitor the intermolecular interactions in solutions according to changes in the spectra.

FT-IR spectra were recorded on Shimadzu's Fourier transform infrared spectrometer (Japan) with frequency range of 4000-500 cm^{-1}. The FT-IR spectroscopic analysis of both control and treated samples of each drug paracetamol was carried out to evaluate the impact of biofield treatment at atomic level like bond strength (force constant) and stability of chemical structure.

Fig 1: ShemadzuIRPrestige-21 Spectofotometer

Results and discussions

Figure 2 shows the FTIR spectrum of paracetamol for wavelengths between 4000 and 500cm^{-1}.

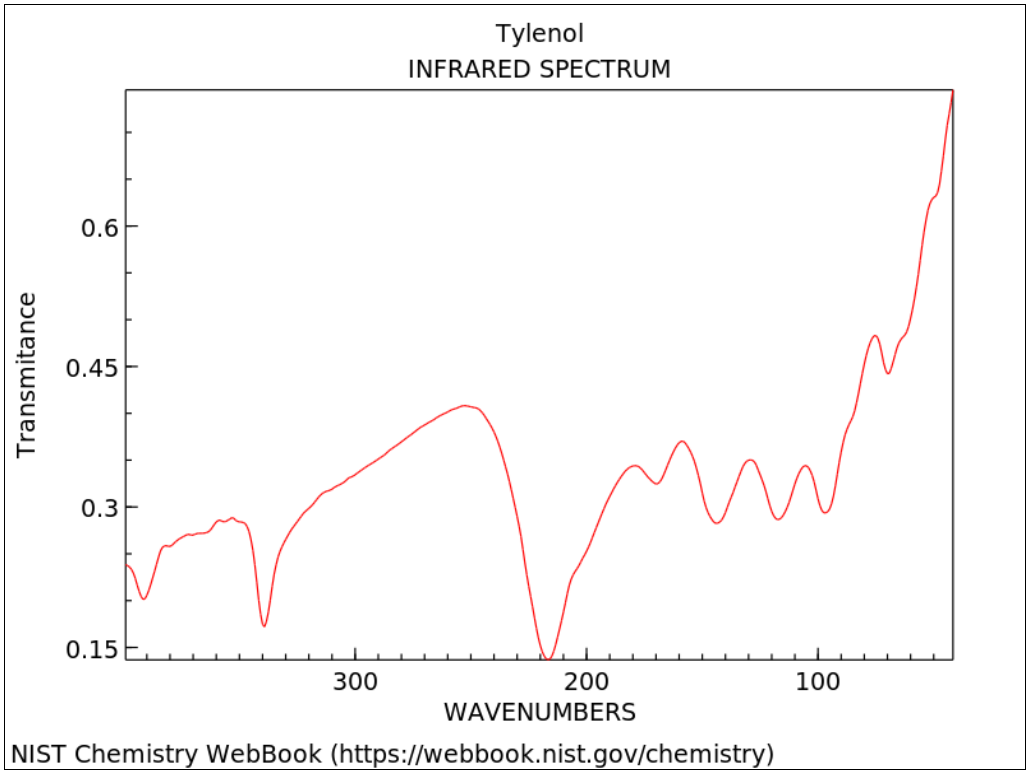

Fig 2: IR spectrum of paracetamol

The FT-IR spectra of both control and treated paracetamol are shown in (Figure 2). The spectrum of control sample of paracetamol (Figure 2) showed characteristic vibrational peak for O-H and CH_3 stretching at 3326 and 3162-3035 cm^{-1}, respectively. Vibrational peaks at 1654 and 1610 cm^{-1} were assigned to C=O and C=C stretching, respectively. The N-H amide II bending appeared at 1565 cm^{-1}. Asymmetrical bending in C-H bond appeared at 1507 cm^{-1}, and C-C stretching peak was appeared at 1443-1437 cm^{-1}. The absorption peaks at 1368-1328 and 1260-1227 cm^{-1} were assigned to symmetrical bending in C-H and C-N (aryl) stretching. Further, absorption peaks at 1171 and 965 cm^{-1} were assigned to C-O stretching and C-N (amide) stretching, respectively. Vibrational peaks at 838 and 514 cm^{-1} were assigned to para-disubstituted aromatic ring and out of plane ring deformation of phenyl ring, respectively. The observed FT-IR data of paracetamol was confirmed by the literature data [25].

Conclusions

The IR spectrum of paracetamol determined with the ShemadzuIRPrestige-21 spectrophotometer contains the following bands of the O-H, CH_3, C=O, C=C, N-H, C-H, C-C, C-N (aryl) and C-N (amide) groups. The composition of paracetamol, centered on its para-aminophenolic structure, is the basis of its analgesic and antipyretic properties. Its relatively simple chemical formula allows for good tolerability and efficient absorption, while the excipients used in the different pharmaceutical forms ensure the stability, solubility and easy administration of the active substance. Overall, the structural and pharmaceutical characteristics of paracetamol justify its essential role as a first-line drug in the treatment of mild-moderate pain and fever.

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