ANALYTICAL CHALLENGE

Solution to the wing-giving challenge

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Accepted: 1 August 2023 / Published online: 11 October 2023 © The Author(s), under exclusive licence to Springer-Verlag GmbH, DE part of Springer Nature 2023

The winner of the Wing-giving challenge (published in volume 415 issue 9) is:

Charlotte A. Corbett, Dulles, VA 20166, USA.

The award entitles the winner to select a Springer book of their choice up to a value of $\in 100$,-.

Our Congratulations!

The molecule described in the Wing-giving Challenge [1] is 2-aminoethanesulfonic acid, commonly known as taurine.

Taurine takes its name from a bull or ox in Latin (taurus) or Ancient Greek (taûros) because it was first isolated from ox bile by German scientists Friedrich Tiedemann and Leopold Gmelin in 1827 [2]. In 1846, taurine was discovered by Edmund Ronalds also in a human bile.

Because of the low p K_a of the sulfonic acid, taurine is typically ionized into a zwitterion ${}^{-}O_3S$ -CH₂-CH₂-NH₃⁺. (Note that taurine is not to be confused with "taurin" (C₁₅H₂₀O₃) which also goes by the names gracilin or berrelierin.) Taurine is an ingredient in various dietary supplements and helps to maintain skin hydration in cosmetics. Above all, taurine is component of some energy drinks, containing up to one gram per serving.

The relatively simple structure of taurin leads to rather simple spectra. Nevertheless, the assignment of the NMR signals is often incorrect. A simple reason for this might be the incorrect assignment of the two methylene groups in an open-source spectral database of organic compounds [3]. The correct NMR assignment given below is based on the experimental spectra and ¹³C-NMR shift calculation using the CSEARCH robot referee service [4].

$$^{13}C_{calc} = 50.2 \text{ ppm}$$

NH₂

HO

 $^{13}C_{calc} = 37.6 \text{ ppm}$

$$^{1}H_{exp} = 2.72 \text{ ppm}$$
 $^{1}H_{exp} = 3.05 \text{ ppm}$ $^{13}C_{exp} = 47.5 \text{ ppm}$ $^{13}C_{exp} = 36.1 \text{ ppm}$ $^{13}C_{calc} = 51.9 \text{ ppm}$ $^{13}C_{calc} = 37.8 \text{ ppm}$

O
$$NH_3^+$$

 $O^ NH_3^+$
 $O^ O^ O^-$

This article is the solution to the Analytical Challenge to be found at https://doi.org/10.1007/s00216-023-04561-6

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Declarations

Conflict of interest The author declares no competing interests.

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