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Identification and structure elucidation of cleomiscosins using spectroscopy

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Abstract

Characterisation of isolated compounds has always been crucial in natural drug discovery. Spectroscopy is highly useful in exploring the exact structure of phytochemicals. Majority of the bioactive secondary metabolites of plants exist as isomers whose structure determination is a most challenging task.

The scope of this presentation is primarily to demonstrate the usefulness of various spectroscopic techniques like UV, IR, MS and NMR, to elucidate the structure of cloemiscosins, which generally exist as regioisomeric pairs. Cleomiscosin A - D are the major biologically active compounds of coumarinolignans. Cleomiscosins are formed by fusion between a coumarin moiety and a phenyl propanoid unit. Cliv 92, a preparation of cleomiscosins is used for hepatoprotective properties.

In UV spectra, coumarin and substituted benzene chromophore exhibit λ_{max} at 315-325 nm with shoulders around 288 and 230 nm. The presence of lactone carbonyl and phenolic hydroxyl groups can be verified by IR spectroscopy. The important fragmentation of cleomiscosins is retro-*Diels-Alder* cleavage of dioxane bridge under EIMS. The coumarinolignan skeleton can be identified through detailed analysis of ^{1}H and ^{13}C NMR spectra. However, these conventional techniques will not differentiate the two possible regioisomers. The determination of exact mode of linkage of the phenyl propanoid unit to the coumarin nucleus can be successful by heteronuclear decoupling NMR experiment and SINEPT NMR technique. Observation of enhancements induced in the spectra through the irradiation of particular proton provides the clear structure determination of the two isomers. Structural ambiguity between the positional isomers may be settled by HMBC technique as well.

Biography

Sajeli Begum completed her Ph.D. at the age of 26 from Banaras Hindu University. She is a recipient of Deutscher Akademischer Austausch Dienst (DAAD) Fellowship (2004) to pursue part of her doctoral research at *Eberhard Karls Universitat, Tuebingen*, Germany. Currently, she is an Assistant Professor in BITS-Pilani Hyderabad Campus. Her research interest is focused on identification of lead molecules for treatment of cancer through isolation, structure elucidation and pharmacological screening of natural products. She has published 20 papers in reputed journals. She has authored a chapter in vol. 93 of book series, “Progress in the Chemistry of Organic Natural Products”.