

CELEBRATING
COMMERCIALISATION
YEAR 2014

iiindex 2014

AN INTERNATIONAL EXPOSITION ON RESEARCH AND INNOVATION

invention
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exposition 2014

INNOVATEUR
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2014

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UNIVERSITI TEKNOLOGI MARA
MALAYSIA

*Bridging
the valley of death :
advancing the
commercialisation
of research*

RESEARCH BOOK

iiindex2014

AN INTERNATIONAL EXPOSITION ON RESEARCH AND INNOVATION

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RESEARCH INNOVATION BUSINESS UNIT
UiTM-MTDC Technopreneur Centre, Universiti Teknologi MARA
40450 Shah Alam, Selangor Darul Ehsan, MALAYSIA
Tel : +603-5544 2747/2748/2750
Fax : +603-5544 2790

Web : www.iiindex.com.my
Email : iiindexuitm@gmail.com



FOREWORD

The Honourable Minister of Science, Technology and Innovation (MOSTI) has launched 2014 as Malaysia Commercialisation Year 2014 (MCY2014) with the theme Science Technology and Innovation (STI) for Wealth Creation. In line with this theme, Invention, Innovation, Design & Exposition 2014 (iidex2014) is an annual exposition organized by UiTM and is the ultimate platform to highlight and commercialise new inventions and innovations. Researchers and inventors will exhibit their products which cater to the needs and wants of the community and the country.

The iidex2014 creates a new dimension by fusing two competitive concepts, a competition among innovative products and a competition to invite Innovateur Wannabes to perform live pitching of their products to the audience. The iidex2014 focuses on comprehensive commercialization and creating opportunities for entrepreneurs to carry out R&D as well as to provide avenue to commercialise their products. Through expositions such as iidex2014, MOSTI hopes to inculcate the culture of commercialisation of new technology designed and created by Malaysians.

I wish to congratulate all the participants of the iidex2014 and this is the opportunity for all researchers to show their ideas and exhibits their products and creativity. Apart from showcasing their products, innovators will have the opportunity to provide a window to the industry for business matching during the exposition.

Tan Sri Dato' Sri Sallehuddin Mohamed
Pro-Chancellor, Universiti Teknologi MARA

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DETERMINATION OF ABSOLUTE CONFIGURATION OF CLERODANE-TYPE DITERPENES USING EXPERIMENTAL AND THEORETICAL ELECTRONIC CIRCULAR DICHROISM TECHNIQUES

Ahmad Nazif Bin Aziz, Nor Hadiani ismail, Khalijah Awang, Rohaya Ahmad, Norizan Ahmat
Atta-Ur-Rahman Institute for Natural Product Discovery, UiTM Puncak alam, Selangor.
Email: nazif_umt@yahoo.com

Clerodane-type diterpenes isolated from plants are chiral compounds with specific stereochemistry. The compounds have complex structure with many stereo centres which gives them unique 3 dimensional features, not uncommonly found for natural products. These 3 dimensional (3D) features are in fact what makes natural product compounds unique and in many cases contributes to their biological functions. In exhibiting their biological properties, the natural product compounds very often bind with enzymes and proteins, which take place in lock and key manner. Stereochemistry of the compounds becomes crucial and may help explain important questions in the mechanism of action for a particular biological activity. In this project, absolute configurations of these compounds were determined using Electronic Circular Dichroism spectroscopy (ECD) techniques. Circular Dichroism (CD) may be regarded as one of the most powerful techniques for stereochemical analysis. It is sensitive to the absolute configuration as well as to conformational features, which are often completely obscured in the ordinary absorption spectrum. CD is a measurement of how an optically active compound absorbs right- and left-handed circularly polarized light. Optically active compounds containing chromophores exhibit different extinction coefficients for R and L circularly polarized light waves produced characteristic absorption bands. Electronic Circular Dichroism (ECD) spectroscopy exploits this phenomenon to probe the handedness of the environment of the chromophores. ECD is a very sensitive diagnostic tool for determining not only absolute configuration and conformation, but also for monitoring intermolecular interactions where chiral systems are involved. The experimental ECD spectra were verified by predicting the theoretical CD spectra using a semi-empirical ab initio calculations employing time-dependent density functional theory (TD-DFT) using Gaussian09 software. The conformational analysis of the compounds was implemented prior to the TD-DFT calculations, using the Boltzmann method. This method will find all possible minimum structures which are populated at the room temperature. The structures within 3 kcal mol⁻¹ energy cut-off were taken into consideration. Boltzmann method is also useful in uncovering any errors in the assignment of absolute configuration by experimental ECD. The assignments of absolute configuration of the natural diterpenoids were finalized by comparing the experimental and theoretical ECD data. The developments of the density functional theory (DFT) method have revolutionized the determination of the absolute configurations of chiral molecules using these chiroptical properties. This method is applicable for other chiral compounds with suitable chromophores since it is measured within the Ultraviolet (UV) range wavelength. A multi stereo centred clerodane- type diterpenoid namely crovatin were selected for the determination of its absolute configurations. This compound was isolated from the dichloromethane extracts of *Croton laevifolius* collected from Dungun, Terengganu, Malaysia. The experimental CD was done in HPLC grade acetonitrile solvent. Conformational analysis resulted with five conformers within 3 kcal mol⁻¹ energy cut-off. TDDFT calculations were done at B3LYP/6-31G+(d, p) level, by considering the normal and end configurations of this clerodane diterpene. The comparison of the experimental and calculated ECD spectra of crovatin has resulted in the conclusion that this compound follows the normal clerodane configuration and its absolute configurations were successfully determined.