

สารเคมีจากปะการังอ่อน *Cladiella tuberosa* Tixier-Durivault



นาย นิสิต พิศุทธานันท์

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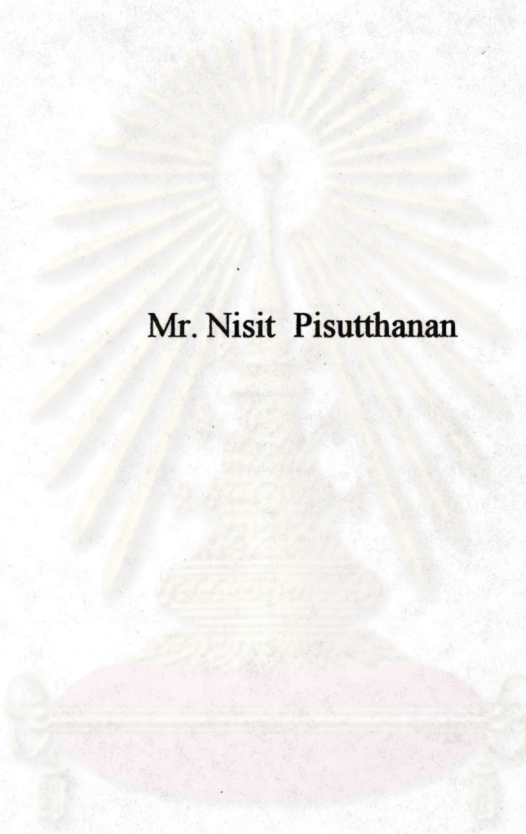
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**CHEMICAL CONSTITUENTS FROM THE SOFT CORAL  
*CLADIELLA TUBEROSA* TIXIER-DURIVAUT**



**Mr. Nisit Pisutthanan**

**A Thesis submitted in Partial Fulfillment of the Requirements  
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By                         Mr. Nisit Pisutthanan  
Department             Pharmacognosy  
Thesis Advisor         Mr. Khanit Suwanborirux, Ph.D.

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Accepted by the Graduate School, Chulalongkorn University in partial fulfillment of the Requirements for the Master's Degree.

*Santi Thoongsuwan*

..... Dean of Graduate School  
(Associate Professor Santi Thoongsuwan, Ph.D.)

Thesis Committee

*Chaiyo Chaichantipyuth*

..... Chairman  
(Associate Professor Chaiyo Chaichantipyuth, M.Sc.)

*Khanit Suwanborirux*

..... Thesis Advisor  
(Mr. Khanit Suwanborirux, Ph.D.)

*S. Amnuoypol*

..... Member  
(Associate Professor Surattana Amnuoypol, M.Sc.)

*Rutt Suttisri*

..... Member  
(Mr. Rutt Suttisri, Ph.D.)

พิมพ์ต้นฉบับบทคัดย่อวิทยานิพนธ์ภายในกรอบสี่เหลี่ยมนี้เพียงแผ่นเดียว

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จากการแยกสกัดสารควบคู่ไปกับการทดสอบฤทธิ์ทางชีวภาพ โดยการใช้ฤทธิ์ความเป็นพิษต่อเซลล์มะเร็งและฤทธิ์ฆ่าไรสีน้ำตาล ของสิ่งสกัดในชั้นไดคลอโรมีเทน จากปะการังอ่อน *Cladiella tuberosa* ทำให้สามารถแยกสารพวกยูนิซิลินไดเทอร์ปีน ได้ 4 ชนิด คือ สาร 3-deacetylpalmonin A ซึ่งเป็นสารอนุพันธ์ใหม่ที่ยังไม่มีการรายงานมาก่อน สาร deacetylcladiellin ซึ่งเป็นการค้นพบครั้งแรกในธรรมชาติ สาร sclerophytin A ซึ่งเป็นการรายงานครั้งแรกที่พบในปะการังอ่อนสกุล *Cladiella* และ สาร (1R, 2R, 3R, 6S, 9S, 10R, 14R)-cladiell-7(19),11(20)-dien-3,6-diol การพิสูจน์สูตรโครงสร้างทางเคมีและ relative stereochemistry ของสารทั้ง 4 ชนิดนี้ ทำโดยการวิเคราะห์ข้อมูลทางสเปกโทรสโกปี จาก IR, MS, <sup>1</sup>H และ <sup>13</sup>C NMR โดยเฉพาะอย่างยิ่ง 1-D และ 2-D NMR ร่วมกับการเปรียบเทียบข้อมูลกับสารอื่นที่มีสูตรโครงสร้างทางเคมีที่สัมพันธ์กัน นอกจากนี้ยังพบว่า สาร deacetylcladiellin แสดงความเป็นพิษต่อเซลล์มะเร็งหลายชนิด คือ P-388 โดยมี IC<sub>50</sub> 2 µg/ml HT-29, A-549 และ MEL-28 มี IC<sub>50</sub> 5 µg/ml และมีฤทธิ์ฆ่าไรสีน้ำตาลโดยมี LD<sub>50</sub> 0.6 µg/ml



ศูนย์วิทยทรัพยากร  
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ภาควิชา ..... เกสัชเวช  
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ลายมือชื่ออาจารย์ที่ปรึกษา .....  
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BIOACTIVITY

NISIT PISUTTHANAN : CHEMICAL CONSTITUENTS FROM THE SOFT CORAL

CLADIELLA TUBEROSA TIXIER-DURIVAUT. THESIS ADVISOR :

Mr. KHANIT SUWANBORIRUX, Ph.D., 171 pp. ISBN 974-632-990-1

The bioassay-directed fractionation, using cytotoxic and brine shrimp lethality activities, of the dichloromethane extract from the soft coral *Cladiella tuberosa* led to the isolation of four eunicellin diterpenoids : 3-deacetylpalmonin A which is a new eunicellin derivative, deacetylcladiellin which is reported for the first time as naturally occurring, sclerophytin A which has never been found in soft corals of the genus *Cladiella*, and (1R, 2R, 3R, 6S, 9S, 10R, 14R)-cladiell-7(19), 11(20)-dien-3,6-diol. The structures and relative stereochemistry of the compounds were elucidated through extensive analyses of their ir, ms, <sup>1</sup>H and <sup>13</sup>C nmr spectral data, especially 1D- and 2D-nmr, as well as comparison with known related compounds. Deacetylcladiellin showed cytotoxic activity against P-388 with IC<sub>50</sub> value of 2 µg/ml, whereas for HT-29, A-549, and MEL-28 the IC<sub>50</sub> was 5 µg/ml and also showed brine shrimp lethality activity with LD<sub>50</sub> of 0.6 µg/ml.

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## ABBREVIATIONS

br d	= Broad doublet
br s	= Broad singlet
br t	= Broad triplet
°C	= Degree celsius
<sup>13</sup> C-NMR	= Carbon-13 nuclear magnetic resonance
CDCl <sub>3</sub>	= Deuterated chloroform
CH <sub>2</sub> Cl <sub>2</sub>	= Dichloromethane
CHCl <sub>3</sub>	= Chloroform
cm	= Centimeter
COSY	= Correlated spectroscopy
δ	= Chemical shift
1-D	= One dimensional
2-D	= Two dimensional
d	= Doublet
dd	= Doublet of doublets
ddd	= Doublet of doublet of doublets
dddd	= Doublet of doublet of doublet of doublets
DEPT	= Distortionless enhancement by polarization transfer
dq	= Doublet of quartets
dt	= Doublet of triplets
EIMS	= Electron impact mass spectrum
FABMS	= Fast atom bombardment mass spectrum
g	= Gram
<sup>1</sup> H-NMR	= Proton nuclear magnetic resonance
HMBC	= <sup>1</sup> H-detected heteronuclear multiple bond coherence
HMQC	= <sup>1</sup> H-detected heteronuclear multiple quantum coherence
HSQC	= <sup>1</sup> H-detected high sensitive quantum coherence
Hz	= Hertz

IC <sub>50</sub>	= 50% Inhibition concentration
IR	= Infrared
<i>J</i>	= Coupling constant
kg	= Kilogram
l	= Liter
LD <sub>50</sub>	= 50% Lethality dose
M <sup>+</sup>	= Molecular ion
MeOH	= Methanol
MHz	= Megahertz
μg	= Microgram
mg	= Milligram
ml	= Milliliter
mm	= Millimeter
MS	= Mass spectrum
MTPA	= α-Methoxy-α-trifluoromethyl-α-phenylacetic acid
v <sub>max</sub>	= Wavenumber at maximum absorption
NA	= Nutrient agar
NMR	= Nuclear magnetic resonance
No.	= Number
NOE	= Nuclear Overhauser effect
NOEDS	= Nuclear Overhauser effect difference spectrum
NOESY	= Nuclear Overhauser effect correlated spectroscopy
ppm	= Part per million
q	= Quartet
s	= Singlet
SCUBA	= Self-contained underwater breathing apparatus
SDA	= Sabouraud dextrose agar
sp.	= Species
t	= Triplet
TLC	= Thin layer chromatography
TSA	= Trypticase soy agar