



The 1st Kamphaengsaen International Natural Products Symposium

The Relationship Between Living Organisms and Environment
October 23-24, 2010 Swissôtel Le Concorde Hotel, Bangkok, Thailand

Proceeding Book

The first Kamphaengsaen International **Natural Products Symposium**
The Relationship Between Living Organisms and Environment



BRUKER



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มหาวิทยาลัยเกษตรศาสตร์ วิทยาเขตกำแพงแสน

Introductory Remarks

To the Vice Secretary of the Higher Education Commission, Thailand, the President of Kasetsart University, the Organizing Committee, distinguished guests, ladies and gentlemen, a warm greeting to all of you.

The Research Promotion and Technology Transfer Center of Faculty of Liberal Arts and Science, Kasetsart University at Kamphaengsaen is hosting the first Kamphaengsaen International Natural Products Symposium (KINS2010) jointly with the coorganizers namely the Japan Korea Thailand China Agricultural Science Research Group (JKTC'Group), Academic Service Center, Kasetsart University at Krabi Province, Thailand and the Weed Science Society of Thailand.

The symposium brings together scientists, especially graduate students from around the world to exchange experimental information on the Natural Products Science with the theme: "The Relationships between Living Organisms and Environment."

The objectives of KINS2010 are to motivate graduate students and young scientists in Natural Products Science and related fields; to engage in the international collaborative research; to stimulate young scientists to meet with the authorities in the fields; to allow the passing-on of research experiences from generation to generation and to promote Natural Products Science research activities in Thailand

KINS2010 is an international symposium on natural products science and its associated disciplines. Three sessions have been preliminarily assigned with 8 topics namely;

Session 1: Natural Products Chemistry which is divided into two categories:

- Isolation and Structural Elucidation.
- Natural Products Synthesis and Synthetic Methodology

Session 2: Utilization of Natural Products consisting of the following related areas:

- Pharmaceutical Science
- Agricultural Science
- Environmental Science
- Food Science and Biotechnology
- Bioenergy

Session 3: The JKTC research group meeting with emphasis on the theme "The Relationship between Plants and Environment"

A total of 120 participants from 15 countries have registered in this symposium. They will discuss and share their research results either by oral or poster presentation. They will also have an opportunity to collaborate with other researchers both from academe and industries.

Plenary and invited speakers are drawn from noted researchers within the area of natural products science. A total of 6 plenary lectures will be given by Prof. Dr. Pichaet Wiriyachitra, CEO, Asian Phytochemicals Public Co., Ltd.; Prof. Dr. Stephen G. Pyne from the University of

Wollongong, Australia; Prof. Dr. T. Randall Lee from University of Houston, USA; Dr. Lukas Oberer from Novartis Pharma AG, Switzerland; Professor Dr. Prakash Naraiyan Kalla from University, Bikaner, Campus - Jaipur, India and Dr. Gilbert Sigua from Sub Tropical Agricultural Research Station (USDA), USA. Moreover, there are 34 oral and 44 poster presentations in this symposium. All of which are surely interesting, informative and worth attending.

It will be an opportunity for the international community to exchange ideas and develop a common vision for the future of World Natural Products Science. The organizing committee has been working to make KINS2010 a truly memorable experience for all participants.

I would also like to recognize the sponsors of this conference. Without their support, this symposium will not be possible. I would like to thank especially the Asian Phytochemicals Public Co., Ltd., Kasetsart University, Econmicline newspaper, Bruker and all sponsors which are shown in the abstract book .

I also have to thank every member of the Faculty of Liberal Arts and Science, Kasetsart University at Kamphaengsaen and to our friends from the Philippines. And, I would like to give my special thanks to my symposium secretary, Dr. Prapa Sohsalam, for her hard work and patience in communication and management tasks.



Assoc. Prof. Weerachai Phutdhawong, Ph.D
KINS2010 Chairman

Welcome Address

To the respectable Vice Secretary of the Higher Education Commission of Thailand, to the hardworking members and head of the Organizing Committee, distinguished guests and participants from all over the world, it is with great honour and pleasure to welcome you all to the 1st Kamphangsaeen International Natural Products Symposium (KINS 2010).

Let me take this opportunity to share with you one of the major policies of Kasertsart University in line with this event, that is, internationalization. Hosting international symposium like this strongly supports our great vision to see KU as a leading research university in agriculture, food, technology, and innovation. Kasertsart University is a public university where bodies of knowledge and research potential have been continually accumulated for nearly seven decades. Now, as a national research university endorsed by the Commission on Higher Education of Thailand, KU is ready to drive to our major goal as a leading university and to deploy networks for the accomplishment to be a world class university in the near future.

Symposium in natural products is probably not a new event for most of us here. International gatherings and meetings of experts in natural products chemistry have been conducted elsewhere before. But there are things that make differences in this two-day conference.

First, this conference is initiated by one of the campuses of Kasertsart University, which is the Kamphangsaeen Campus. Indeed, I would like to congratulate our staff and officials at the Kamphangsaeen Campus for such a remarkable effort to support the university's advocacy for internationalization. Hosting international conference like this shows our commitment to the global academic society. This is the first and surely will not be the last.

Second, the conference theme which is "The relationship between living organisms and environment" encompasses diverse topics in natural products science with emphasis on environmental issues and concerns. Man as one of the living organisms and being part of the environment has to maintain a balance relationship between the two.

Lastly, this conference is also a joint effort of four countries: Japan, Korea, Thailand and China which make the JKTC Agricultural Science Group. Thus, this conference is truly worth your effort and time.

I am looking forward to the success of this two-day event. This will be an opportunity to exchange scientific information on natural products. To our reputable guest speakers, thank you for sharing your expertise. To our budding researchers, take this as a chance to meet and collaborate with our natural product experts worldwide. Let this symposium be an avenue of sharing and learning. Again, on behalf of Kasetsart University, once again I warmly welcome all of you to KINS 2010. I am hoping that this conference will be memorable to each and every one of us. Through this conference, may you also feel the warmth of the traditional Thai hospitality.



Assoc. Prof. Vudtechai Kapilakanchana
President of Kasetsart University

Opening Remarks

In behalf of the Higher Education Commission of Thailand, let me extend a warm greeting and appreciation to all our distinguished guests, delegates, colleagues and friends who despite their busy schedule travel all the way here to participate in the “1st Kamphangsaeen International Natural Products Symposium” or KINS 2010.

I would like to open this program by giving insights on this conference theme: “The relationship between living organisms and environment”. There are three notable words that make this theme important in my view. These are relationship, living organisms, and environment.

When we talk about relationship it could mean association, connection, correlation, bond or link between two things. Living organisms as everyone knows include human beings, plants, animals, and other microorganisms that are not visible to our naked eyes. All the living organisms together with abiotic elements like air, soil, water and others make up the environment. That is, we are part of the environment. Any harm or damage we inflicted to our environment greatly affects us. We are all related to each other.

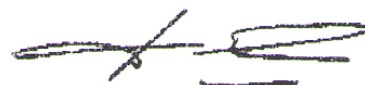
With the advent of Science and Technology, man has gained a lot from his environment. The clothes we wear, the shelter we live on, the food we eat, the medicines and vitamins we take, the cosmetics we use, the fuel that runs our vehicles and many other things that have turned the lives of man comfortable are all products of Science and Technology, of which the raw materials come from the environment. Indeed, we have gained a lot from our environment. But have we given something in return to our environment?

Through this symposium, I am certain we would once again be reminded that the relationship between living organisms and the environment must be mutual. It must be balanced so that our environment can sustain life for the future generation.

With this, I would like to give my commendation to the organizers of this event. Not only they support one of the goals of the Higher Education Commission of Thailand which is global competitiveness of Thai Universities, but they also address one of the pressing issues man is facing today: our relationship with our environment.

As I look around this hall, I am pleased to see faces from many parts of the world, gathered here for the next two days to meet, collaborate and learn from our distinguished speakers and each other.

Without further adieu and in behalf of the Higher Education Commission of Thailand, I formally open this conference. Thank you for joining us. I wish everyone success in this two-day affair. I also hope everyone will enjoy their stay in Thailand, which is known to be the “Land of Smiles”.



Assoc. Prof. Piniti Rattananukul, Ph. D
Vice Secretary of the Higher Education Commission, Thailand

Message from KINS2010 Secretary

On behalf of the symposium staff, I would like to welcome you all again to Thailand. For your convenience, I would like to recommend a travel guide during your vacation.

Upon arrival at Suvarnabhumi International Airport airport, there are 4 ways to go to Swissotel Le Concorde Hotel at 204 Ratchadapisek Road, Huai Khwang, Bangkok.

By car rental. To get a rental car, contact "Car Rental" service counter at the Arrivals level (2nd floor) or take a Shuttle Bus (Express Route) to the Transport Center to pick your rental car.

By public taxi. To get a taxi, contact Taxi Counter, Level 1 - Ground Level, near entrances 3, 4, 7 and 8. Upon arrangement, proceed to the pickup area at the Taxi Stand Level 1 - Ground Level. Taxi fare includes the metered taxi fare plus 50 Baht airport surcharge and expressway fees.

By public bus. Take the free shuttle bus (Express route) to the Transport Center. 24-hour public bus service is provided from the Bus Terminal at the Transport Center. Take the bus which connects Suvarnabhumi Airport to the On-Nut sky train station via Bangna-Bangpakong Road, taking a right turn to Sukhumvit Road until the On-Nut sky train station. Bus fare is 35 baht. Then, ride the BTS which connects to MRT to Huai Khwang Station. The hotel is just 5-min walk from the Huai Khwang Station.

By Airport Express. Airport Express provides air-conditioned bus service between Suvarnabhumi Airport and first-class Bangkok hotels. Airport Express operates 4 bus routes to downtown. The cost is ~150 baht for entire route. Airport Express service operates from 5:00 am to midnight. To take the Airport Express, contact Airport Express Counter Level 1, near Entrance 8. Choose (bus number, AE 1-4). Inform the in-charged to drop you off at (BTS station). Ride the BTS, then, transfer to MRT to Huai Khwang Station.

For further information, please avail of free Bangkok Maps upon your arrival at any BTS or MRT station. For reference, visit:

<http://map.top-travel-bangkok.com/bts.htm>

<http://www.bangkokairportonline.com/node/56>

<http://www.bangkokairportonline.com/node/55>

Let me extend a warm greeting and appreciation to all our distinguished guests, delegates, colleagues and friends



Dr. Prapa Sohsalam
KINS2010 Secretariat

KINS 2010 schedule

October 23, 2010 (Salon B, 2 nd floor)						
8.00-9.00	Registration					
9.00-9.30	Opening Ceremony + Thank you sponsor					
9.30-10.45	Assoc.Prof.Dr.Pichaet Wiriyachitra (Asian Phytochemical Public Co.,Ltd.): From the Lab Bench to Balancing Immune					
10.45-11.00	Coffee Break					
11.00-11.30	Prof.Dr.Stephen G.Pyne (University of Wollongong, Australia): Stemona alkaloids and derivatives with potential agricultural and medicinal application					
11.30-12.00	Dr.Kimberly Colson (Bruker Biospin, USA): Strategies for Structure Elucidation of Unknown Natural Products					
12.00-13.00	Lunch (G floor at fountain room)					
	Salon B (2nd floor)		Jamjuee (2nd floor)		Sakhong (2nd floor)	
	Chairman: Dr.Nantanit Wanichacheva and Dr.Suwatthai Jarussophon		Chairman: Dr.Sravut Klorvuttimontara and Ms.Melisa B. Augustin		Chairman: Asst.Prof.Dr.Thitaya Pung and Dr.Veeramol Vaikhit	
13.00-13.15	IS001	Isolation and Structural Elucidation of the Antitubercular Constituents From Ampalaya (<i>Momordica charantia</i> Linn.) - B.G. Panillo, S. Franzblau, W.Z. Qing, R. Pascual, G. Dietmar, K. Simeon, K. Karsten and A.M. Aguinaldo	PS002	Introduction of drought resistant medical plants (Case study: Ardakan) - S.Y. Kazemi, S.H. Zali, M. Kargar and F.F. Shokrian	ES003	Bioremediation / Biodegradation of Oil and Herbicides Spoilage by Natural Microorganisms - S. Somporn and L. Jureerat
13.15-13.30	IS003	A New Cyclohexylethanoid from <i>Dolichandrone serrulata</i> - P. Orasa and K. Rossukon	PS006	Antifungal Activity of <i>Cassia Surattensis</i> Flower Against <i>Aspergillus niger</i> - V. Sumathy, S. Sasidharan and Z. Zakaria	ES008	Pretreatment of Rice Straw Using Physicochemical Hydrolysis for Ethanol Production - T. Chanbarjong, K. Simakahn and R. Pawongrat
13.30-13.45	IS005	Chemical Constituents from <i>Cassia alata</i> , Antibacterial and Antioxidation Properties - T. Promgool, S. Techa and S. Deachathai	PS007	Influence of Desertification on New Current Issue of Toxic Diseases in Magnolia - G. Oyuntsetseg, A. Altanchimeg, A. Shimada, B. Baymunkh, Mungun-Ochir, D. Khurebaatar and Y. Ganbold	AG002	Effect of Dietary Pantothenic Acid Supplemental on Culturing of Green Catfish (<i>Mystus nemurus</i> , Valenciennes, 1840) - D.V. Hien, S. Doolindachaporn
13.45-14.00	IS008	Chemical Constituents from the Root of <i>Sesbania grandiflora</i> (L.) pers - Noviany, H. Osman, and K.C. Wibng	PS011	Chemical Profiling and Antioxidant Activity of Selected Medicinal Herbs Used in Malaysian Diet - J.R. Naidu, C. Yeng and R.B. Ismail	AG003	Effects of Neem leaves powder on groundnuts termites, <i>Microtermes thoracalis</i> and white curbs, <i>Phyllophaga crinita</i> and on Yield in Gedarif State - E.N.H. Suliman
14.00-14.15	IS009	Isolation and Identification zederone as a Marker Compound of <i>curcuma aeruginosa</i> roxb. Rhizome - I. Nasrullah, S. Astuti, L. Yarni, S. Murhandini and W.P. Rahayu	FSB001	Transformation Efficiency studies in <i>E.coli</i> strains (DH5a and JM101) using Calcium Chloride & Electroporation Methods - S. Tharannum, P. Smriti, K. Swapna, K. Yashaswini, A. Sahana, R. Ranjitha and N.M. Gangamma	AG004	Effects of Tannin contents of several varieties of sorghum on the damage caused by the African bollworm, <i>Helicoverpa armigera</i> (Hub.) (Lepidoptera: Noctuidae) in Sudan - E.N.H. Suliman, R.M. Khafagi and E.M. Etamin
14.15-14.30	IS014	Antiplasmodial from <i>Phoebe tavoyana</i> - O. Hanita, E. Berna, A.N. Mohd, A. Khalijah, R.M. Mat and A.H.A. Hadi	FSB003	Investigated the quality and effects of processing on organic and conventional okra - A. Arlai, R. Nakkong, N. Samjamin, B. Sithipaisarnkun, P. Sirakaew, P. Boonsompang and P. Jamjournrat	AG005	Efficacy of biopesticides at field level against white fly (<i>Bemisia tabaci</i> Genn.) infesting ladyfinger (<i>Abelmoschus esculentus</i> L.) - S.K. Ghosh and G. Chakraborty
14.30-14.45	Coffee Break					
	Chairman: Dr.Suwatthai Jarussophon and Dr.Nongpanga Jarussophon		Chairman: Mr. Wilhelm Josef Holzschuh and Dr.Sutthidej Precharum		Chairman: Prof.Dr.T.Randall Lee and Dr.Piched Anurugodom	
14.45-15.00	IS015	Oxoporphine Alkaloids from <i>Pseuduvaria</i> Species (Anonaceae) - T. Hairin, N.A. Ibrahim, M. Khalit and A.H.A. Hadi	FSB007	Effect of Fortification of Soy Flour on Nutrition, Texture and Sensory of Steamed Stuffed Buns - N. Panjoyai	AG006	Ethnobotanical study of Alpine ranges plants in northern Alborz of Iran - Q.A. Heydari and S.H. Zali
15.00-15.15	IS016	New N-2-Hydroxypropyl aporphines from <i>Lauraceae</i> species - A.H.A. Hadi, R. Tiah, O. Hanita, A.N. Mohd, R.M. Mat and A. Khalijah	FSB008	Changes of GABA Content in Industrial Production of KDML 105 Parboiled Germinated Rice - P. Yupakanit and K. Wasana	AG007	Effect of organic farming system on pest management in watermelon crop - J.M. Mari, M.A. Rustamani and M.K. Lohar
15.15-15.30	IS017	Selection of Xylanase Cellulase and Phytase Producing Isolate of Natural Microorganisms - P. Kittibouch and L. Jureerat	FSB010	The Microbiological safety of ready-to-eat food "Toh chine" from nakhon pathom province - A. Innun, S. Thepsuwan, P. Yenbunroong and S. Tirawattanapichat	AG009	Investigation of root growth in Initial three-year seedling of <i>Prunus avium</i> (North Iran) - G.H. Bibalani
15.30-15.45	PS001	Ethno Medicinal Usage of Plants in Biosphere Caches of Iran Case Study: Miankaleh Protected Zone - S.H. Zali	ES002	Determination of Biochemical Parameters of Plant Species in Shivamogga City Environment, India - M.P. Adamsab, K. Hina, M.H. Sirajuddin and M. Ravichandran	AG012	Boassay on Allelopathic Potentialities of <i>Duranta repens</i> L. and <i>Muntingia calabura</i> L - D.A. Antesa
15.45-16.00	IS030	Isolation and partial characterization of antifungal compounds from environmental bacterias - Thongsri Y., Pariyachitgul C., Puapermpoonsiri S., Aromdee C.	ES006	Utilization of chitosan bead with titanium dioxide for dye removal - R. Aparatikul, S. Krissana, T. Patjaneenat, H. Patcharida	AG013	Effect on Cadmium Uptake by <i>Brassica chinensis</i> Seedling of g-Polyglutamic Acid from <i>Bacillus subtilis</i> - O. Chunnachart, N. Kotabin, K. Issakul, A. Morita and Y. Tahara
16.00-16.15	Break					
16.15-17.30	Poster Presentation (3 rd floor)					
17.30-20.00	KINS2010 Welcome Party (3 rd floor)					

October 24, 2010 (Salon B, 2nd floor)					
9.30-10.00	Prof.Dr.T.Randall Lee (University of Houston, USA): Shell/Core Nanoparticles for Diagnostics, Therapeutics and Photo-Induced Delivery of Natural Products				JKTC Presentation - Jamjuee room
10.00-10.30	David J. Harding (Walailak University, Thailand): Redox-Coupled Spin Crossover in [Co(Beta-dkt)2(N-N)]0/+ Redox Pairs: Structural, Electrochemical and DFT Insights and Relevance to Biological Enzymes				
10.30-10.45	Coffee Break				
10.45-11.30	Assoc.Prof.Dr.Pichaet Wiriyachitra (Asian Phytochemical Public Co.,Ltd.): From the lab bench to figure trimming				JKTC Presentation - Jamjuee room
11.30-12.00	Closing Ceremony				
12.00-13.00	Lunch (G floor at fountain room)				

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Acknowledgement

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Chemical Constituents from the Root of *Sesbania grandiflora* (L.) Pers

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Abstract: *Sesbania grandiflora* (L.) Pers (Leguminosae) is a small erect and sparsely branched tree. It is a member of the subfamily Faboideae and tribe Robinieae. The Malay names of this plant are turi and geti. This plant is native to tropical Asia and is widespread in Malaysia, Indonesia, Philippines, and India. The root, bark, leaves, flowers, and fruits of the plant are used to treat various diseases in folkloric medicines. A variety of compounds such as sterols, saponins and tannins exhibits many interesting effects such as hypotensive, oedema, and diuretic. Due to the above mentioned biological activities, root of the *Sesbania grandiflora* was selected for phytochemical investigation. Three isoflavonoids, 3-hydroxy-9-methoxypterocarpan, 7,4'-dihydroxy-2'-methoxyisoflavan, and 7-hydroxy-2',4'-dimethoxyisoflavan, were isolated from the root of *S. grandiflora*. This is the first report on the occurrence of isoflavonoids in this plant. Their structures were elucidated on the basis of spectroscopic data and by comparison with the known compounds.

Keywords: *Sesbania grandiflora* (L.) Pers., Leguminosae, Isoflavanoids, 3-hydroxy-9-methoxypterocarpan, 7,4'-dihydroxy-2'-methoxyisoflavan, 7-hydroxy-2',4'-dimethoxyisoflavan.

Introduction

Sesbania grandiflora (family: Leguminosae; subfamily Faboideae; tribe Robinieae) is native to tropical Asia and is widely distributed in Malaysia, Indonesia, Philippines, and India. The Malay names of this plant are turi and geti. *S. grandiflora* is a small erect, quick-growing, and sparsely branched plant with 10 m in height. Different parts of this plant are used as a traditional remedy in folk medicine to treat various diseases such as catarrh, dysentery, fevers, headaches, smallpox, sores, sore throat, and stomatitis [1,2]. A previous study by Fojas, *et al.* [3] revealed that the crude extracts of *S. grandiflora* could produce a variety of compounds such as sterols, saponins and tannins. Several studies have been conducted with regards to the phytochemical and

pharmacological properties of various parts of *S. grandiflora*. Kasture et al.[4], Pari and Uma [5], Ramesh *et al.* [6,7] and Doddola *et al.*[8] have found that *S. grandiflora* leaves exhibited a variety of pharmacological activities, including the anticonvulsant effect, anxiolytic activity, protective effect against erythromycin estolate-induced hepatotoxicity, antioxidant activity, and antiurolithiatic activity against calcium oxalate-type stones. Recently, another study revealed that supplementation of *S. grandiflora* leaves could also afford a significant hypolipidemic effect against triton induced hyperlipidemia in rats [9]. As far as we know, even though their pharmacological properties have been conducted for this species, no systematical studies on chemical constituents have been performed from the root of *S. grandiflora*. Therefore, we started to study the constituents of *S. grandiflora* root. In the present study, we report the isolation of the three isoflavonoid, 3-hydroxy-9-methoxypterocarpan (**1**), 7-hydroxy 2',4'-dimethoxyisoflavan (**2**), and 7,4'-dihydroxy-2'-methoxyisoflavan (**3**) from the root of *S. grandiflora*. Their chemical structures were determined by comparison of their spectroscopic of MS, 1D-NMR, and 2DNMR with those earlier reported in the literatures. All of these compounds have not been previously isolated in the plant.

Materials and methods

General experimental procedures

Optical rotation was determined on a Digital Polarimeter (JASCO, DIP-370) with a 0.5 cm microcell. A Bruker Avance 300 spectrometer, operating at 300 MHz for ¹H and ¹³C and at 400 MHz were used for 2D-experiments with Me₄Si as internal standard. HRESIMS spectra were recorded using a Micro TOF-Q mass spectrometer in positive-ion mode. IR spectra were recorded using a Perkin-Elmer system 2000 FT-IR Spectrometer, in a range from 4000 to 650 cm⁻¹. UV spectra were recorded using a Perkin-Elmer Lambda 25 Spectrometer. TLC was performed on pre-coated Merck plastic sheets (silica gel 60 PF254, 0.25 mm) and the plates were sprayed with Ce (SO₄)₂.H₂O. Preparative plates [20x20 cm, Kieselgel F254 (0.5 mm)] were air dried and used without prior activation. Column chromatography was done on silica gel Merck Kieselgel 60 (230-400 mesh ASTM).

Plant material

Sesbania grandiflora roots were collected in September 2008 in the village of Sidosari, in South Lampung, Indonesia. The identity of the plant specimen was authenticated and a voucher specimen was deposited at the Bogoriense Herbarium, Bogor, Indonesia.

Extraction and isolation

The dried and powdered roots of *S. grandiflora* (1.5 kg) were extracted three times with methanol (90%) by maceration for 2 x 24 h. Removal of solvent *in vacuo* yielded a methanolic extract (19 g). The methanolic extract was partitioned with *n*-hexane to afford hexane fraction (1.9 g). The residual MeOH fraction was suspended in H₂O and partitioned subsequently with CHCl₃, EtOAc, and acetone which yielded three corresponding fractions: CHCl₃ fraction (0.9 g), EtOAc fraction (2.3 g), and acetone fraction (1.7 g). The ethyl acetate and acetone fractions were combined on the basis of TLC analysis and then it was called acetone fraction. Acetone fraction was fractionated by extensive column chromatography over silica gel using *n*-hexane and *n*-hexane-EtOAc gradient and obtained seven major fractions (fr. 1-7). Among these fractions, fr. 2 was selected for further purification by using preparative TLC method which gave compound **2** (20 mg). CHCl₃ fraction was also repeatedly chromatographed over silica gel column and eluted with gradient of *n*-hexane and acetone to yield eight fractions (fr.1-8). Among them, fraction 5 afforded compounds **1** (18.5 mg) and **3** (7 mg) by additional purification step on preparative thin layer chromatography (TLC) (silica gel, toluene/ ethyl acetate 99:1). All isolated compounds were characterized by NMR spectroscopy and also by comparing their observed and reported physical data [10-14]. Compounds **1**, **2**, and **3** were identified as 3-hydroxy-9-methoxypterocarpan; 7,4'-dihydroxy-2'-methoxyisoflavan; and 7-hydroxy-2',4'-dimethoxyisoflavan respectively. Their molecular structures are shown in Figure 1.

3-hydroxy-9-methoxypterocarpan (1): amorphous powder (18.5 mg); m.p 129-131°C. UV (MeOH) λ_{\max} nm (log ϵ): 210 (4.72), 229 *sh* (4.26), 286 (4.07). HRESI-MS, *m/z* 269.0816 [M-H]⁺ (calcd for C₁₆H₁₄O₄, 269.0819). IR λ_{\max} (KBr) cm⁻¹: 3411, 2924, 2853, 1622, 1599, 1497, 1277, and 1155. ¹H-NMR (acetone-d₆, 400 MHz) and ¹³C-NMR (acetone-d₆, 300 MHz) spectral data are given in Table 2.

7,4'-dihydroxy-2'-methoxyisoflavan (2): amorphous powder (20 mg); $[\alpha]_D^{20}$: -66.6 (c. 0.1 MeOH); m.p 166-167°C. UV (MeOH) λ_{\max} nm (log ϵ): 207 (4.58), 227 *sh* (4.09), 284 (3.70). FAB-MS, *m/z* 273.1 [M+H]⁺ (calcd for C₁₆H₁₆O₄). IR λ_{\max} (KBr) cm⁻¹: 3361, 2941, 1624, 1593, 1455, 1269, 1142. ¹H-NMR (acetone-d₆, 400 MHz) and ¹³C-NMR (acetone-d₆, 300 MHz) spectral data are given in Table 2.

7-hydroxy-2',4'-dimethoxyisoflavan (3): amorphous powder (7 mg), m.p 124-126°C. UV (MeOH) λ_{\max} nm (log ϵ): 208 (4.69), 228 *sh* (4.32), 283 (3.92). HRESI-MS, *m/z* 285.1119 [M-H]⁺ (calcd for C₁₇H₁₈O₄, 285.1132). IR λ_{\max} (KBr) cm⁻¹: 3365, 2938, 1614, 1591, 1506, 1461, 1279, 1208, 1160 and 1115. ¹H-NMR (acetone-d₆, 400 MHz) and ¹³C-NMR (acetone-d₆, 300 MHz) spectral data are given in Table 1.

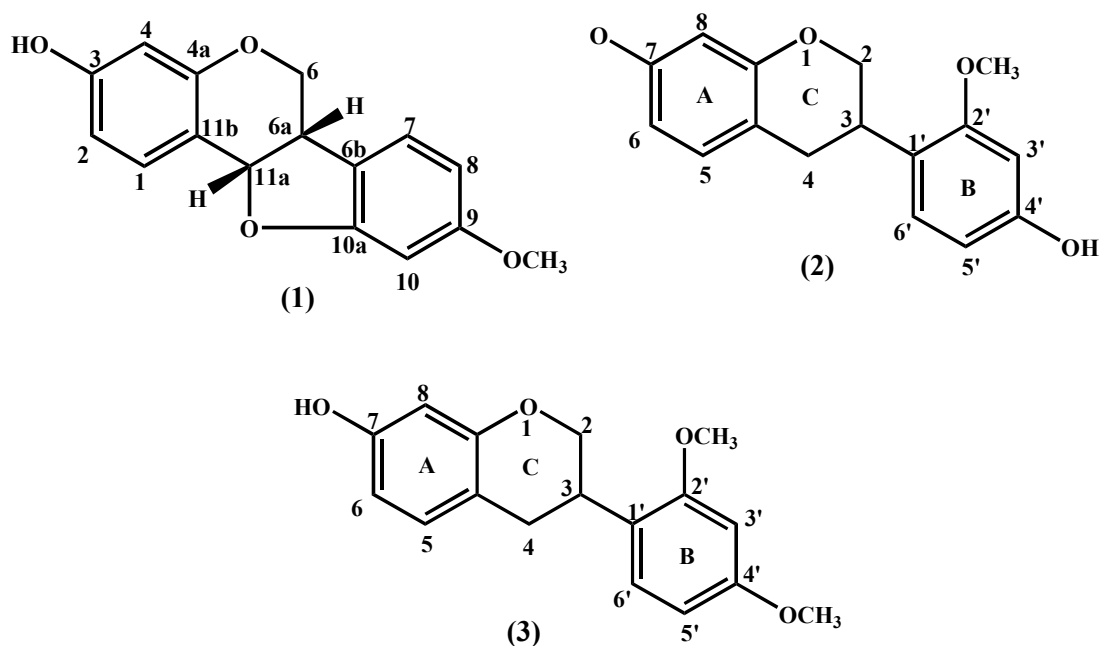


Figure 1. Molecular structures of compounds **1** (3-hydroxy-9-methoxypterocarpan), **2** (7,4'-dihydroxy-2'-methoxyisoflavan) and **3** (7-hydroxy-2',4'-dimethoxyisoflavan).

Results and Discussion

The crude methanol extract of the roots of *S. grandiflora* was fractionated by extensive column chromatography over silica gel to obtain three compounds, **1-3**. Compound **1** was obtained as an amorphous powder and its molecular formula was assigned as $C_{16}H_{14}O_4$ ($[M-H]^+$ m/z 269.0816) from the HRESI mass spectrum. This compound was found to be an isoflavanoid on the basis of its characteristic spectral data; λ_{max} 227 and 284 nm in the UV. The 1H -NMR spectrum of compound **1** revealed four proton signals, [δ_H 3.61 (d, $J = 6$ Hz, H-6 \square), 4.28 (*br* d, $J = 6$ Hz, H-6 \square), 3.61 (d, $J = 6$ Hz, H-6a), and 5.52 (*br* d, $J = 6$ Hz, H-11a)], due to hydrogen at C-6 (δ_C 66.6, CH_2), C-6a (δ_C 39.9), and C-11a (δ_C 78.9), respectively. This suggested that compound **1** has a pterocarpan skeleton. The aromatic region of the 1H -NMR spectrum (Table 1) of compound **1** displayed two sets of the AMX type aromatic protons (δ 6.37, 6.57, and 7.33; and 6.39, 6.46, and 7.24). These data indicated a similarity in the basic structural features of those previously reported of **1**. The location of the methoxyl group at C-9 and the hydroxyl group at C-3 position were established on the basis of the ^{13}C NMR spectrum and HMBC experiment. The HMBC spectrum of compound **1** indicated a correlation between the proton at C-1 (δ_C 132.6) and carbon at C-3 (δ 159.2), and correlation between the proton C-7 (δ_C 125.3) and C-9 (δ 161.6). Homo-COSY, HMQC, and HMBC spectral data showed that the methoxyl group of **1** is attached at C-9, while the hydroxyl group is attached at C-3. The structure of compound **1** was identified by detailed analysis of 1H and ^{13}C NMR data aided by 2D NMR experiments (COSY, HMQC,

HMBC, and NOESY) and identified as 3-hydroxy-9-methoxypterocarpan or medicarpin (Figure 1). Further support for the structure was achieved by comparison of spectral data with those reported earlier for **1** [10,11].

Table 1. ¹H-NMR and ¹³C-NMR spectral data for compounds isolated (**1-3**) from *S.grandiflora* root (at 400 MHz for ¹H, 300 MHz for ¹³C in acetone-*d*₆; δ in ppm, *J* in Hz)

Position	Compound 1		Compound 2		Compound 3	
	δ ¹ H	δ ¹³ C	δ ¹ H	δ ¹³ C	δ ¹ H	δ ¹³ C
5	-	6.90, <i>d</i> (8.2)	130.49	6.90, <i>d</i> (8.2)	130.47	
6	H _α , 4.28, <i>br d</i> (6) H _β , 3.61, <i>d</i> (6)	66.6	6.38, <i>dd</i> (8.2 & 2.4)	108.28	6.38, <i>dd</i> (8.2 & 2.5)	108.00
7	7.24, <i>d</i> (8.2)	125.3	-	157.03	-	157.08
8	6.46, <i>dd</i> (8.2 & 2.3)	106.4	6.29, <i>d</i> (2.4)	103.99	6.29, <i>d</i> (2.5)	103.21
9	-	161.6	-	156.23	-	155.59
10	6.39, <i>d</i> (2.3)	96.8	-	113.83	-	113.00
1'	-	-	-	120.49	-	122.11
2'	-	-	-	159.64	-	158.71
3'	-	-	6.51, <i>d</i> (2.5)	102.08	6.59, <i>d</i> (2.5)	98.88
4'	-	-	-	155.64	-	160.33
5'	-	-	6.43, <i>dd</i> (8.5 & 2.5)	105.24	6.50, <i>dd</i> (8.4 & 2.5)	105.04
6'	-	-	7.06, <i>d</i> (8.5)	128.24	7.10, <i>d</i> (8.4)	127.92
1	7.33, <i>d</i> (8.4)	132.6	-	-	-	-
2	6.57, <i>dd</i> (8.2 & 2.4)	110.0	H _α , 3.99, <i>t</i> (10)	70.01	H _α , 3.95, <i>t</i> (10)	70.07
	-	-	H _β , 4.25, <i>br d</i> (10; 3; & 2)	-	H _β , 4.20, <i>ddd</i> (10; 3; & 2)	-
3	-	159.2	3.49, <i>m</i> (8; 5; & 3)	33.69	3.47, <i>m</i>	31.97
4	6.37, <i>d</i> (2.4)	103.5	H _α , 2.81, <i>dd</i> (10; 5 & 2)	32.19	H _α , 2.78, <i>br d</i> (7; 5 & 2)	30.68
	-	-	H _β , 2.98, <i>dd</i> (16, 5)	-	H _β , 2.81, <i>br d</i> (7; 5 & 2)	-
4a	-	157.3	-	-	-	-
6a	3.61, <i>d</i> (6)	39.9	-	-	-	-
6b	-	119.9	-	-	-	-
10a	-	161.3	-	-	-	-
11a	5.52, <i>br d</i> (6)	78.9	-	-	-	-

11b	-	112.4	-	-	-	-
3-OH	8.66, <i>br s</i>	-	-	-	-	-
2'-OCH ₃	-	-	3.73, <i>s</i> , 3H	54.89	3.80, <i>s</i> , 3H	55.07
4'-OH	-	-	8.14, <i>br s</i>	-	-	-
4'-OCH ₃	-	-	-	-	3.86, <i>s</i> , 3H	55.36
7-OH	-	-	8.59, <i>br s</i>	-	8.15, <i>br s</i>	-
9-OCH	3.76, <i>s</i> , 3H	55.2	-	-	-	-

Even though compound **1** is new to *S. grandiflora*, it has previously been isolated from plants of the family Leguminosae frequently [11]. However, two isoflavans (compounds **2** and **3**) are less common, and their spectroscopic data were reported many years ago. In this study, ¹³C and ¹H-NMR data of compound **2** and **3** have been assigned on the basis of modern 2D NMR techniques. Compound **2** and **3** were found to be isoflavans on the basis of its characteristic spectral data; λ_{max} 227-228 dan 283-284 nm in the UV spectrum. The ¹H-NMR spectra of **2** and **3** showed the characteristic signals of isoflavan: H-2, H-3, and H-4 [(δ 2.81, 2.98, 3.49, 3.99, and 4.25 in compound **2**; δ 2.78, 2.81, 3.47, 3.95, and 4.20 in compound **3**], which indicated the presence of an isoflavan-type C-ring. These compounds were identified as 7,4'-dihydroxy-2'-methoxyisoflavan (**2**) and sativan (7-hydroxy-2',4'-dimethoxyisoflavan) (**3**) by comparison of their spectroscopic data (UV, IR, ¹H and ¹³C NMR, and ESIMS) with those reported in the literature [10-14].

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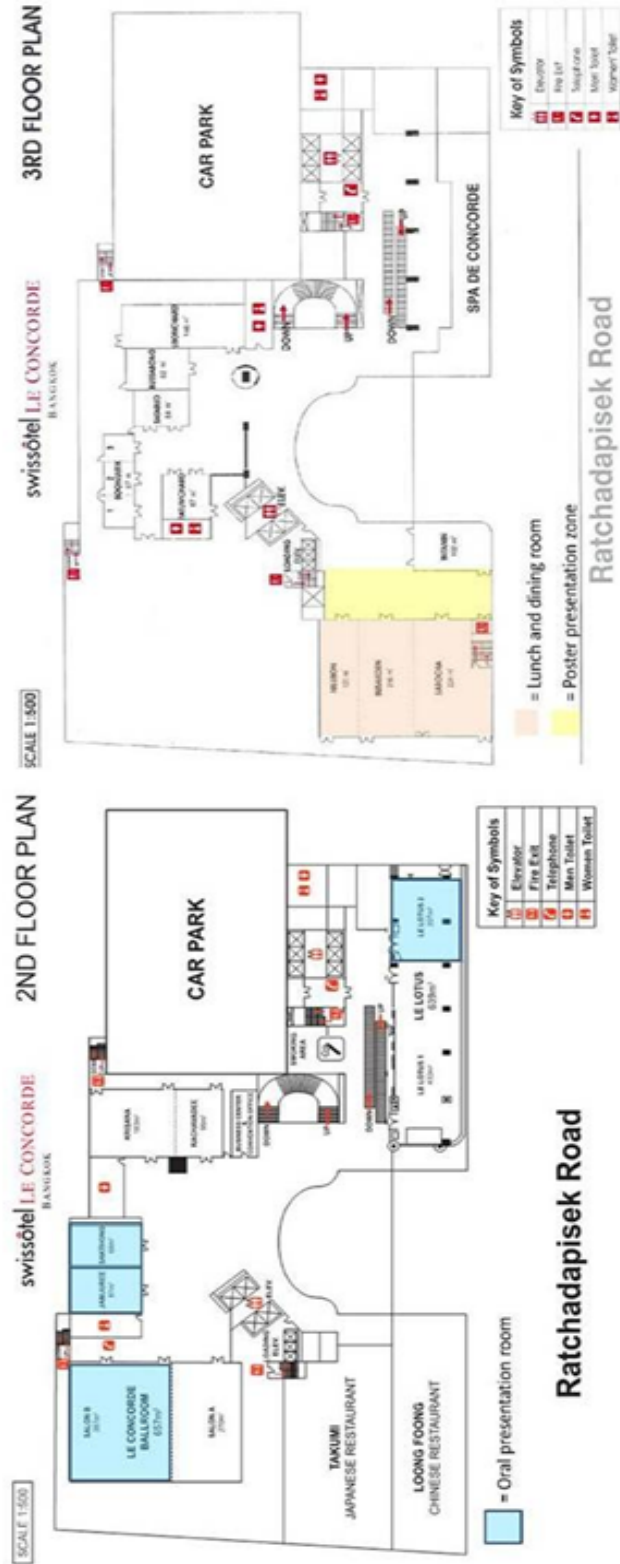
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Swissotel Floor Plan

Swissotel Floor Plan (2nd and 3rd floor)



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