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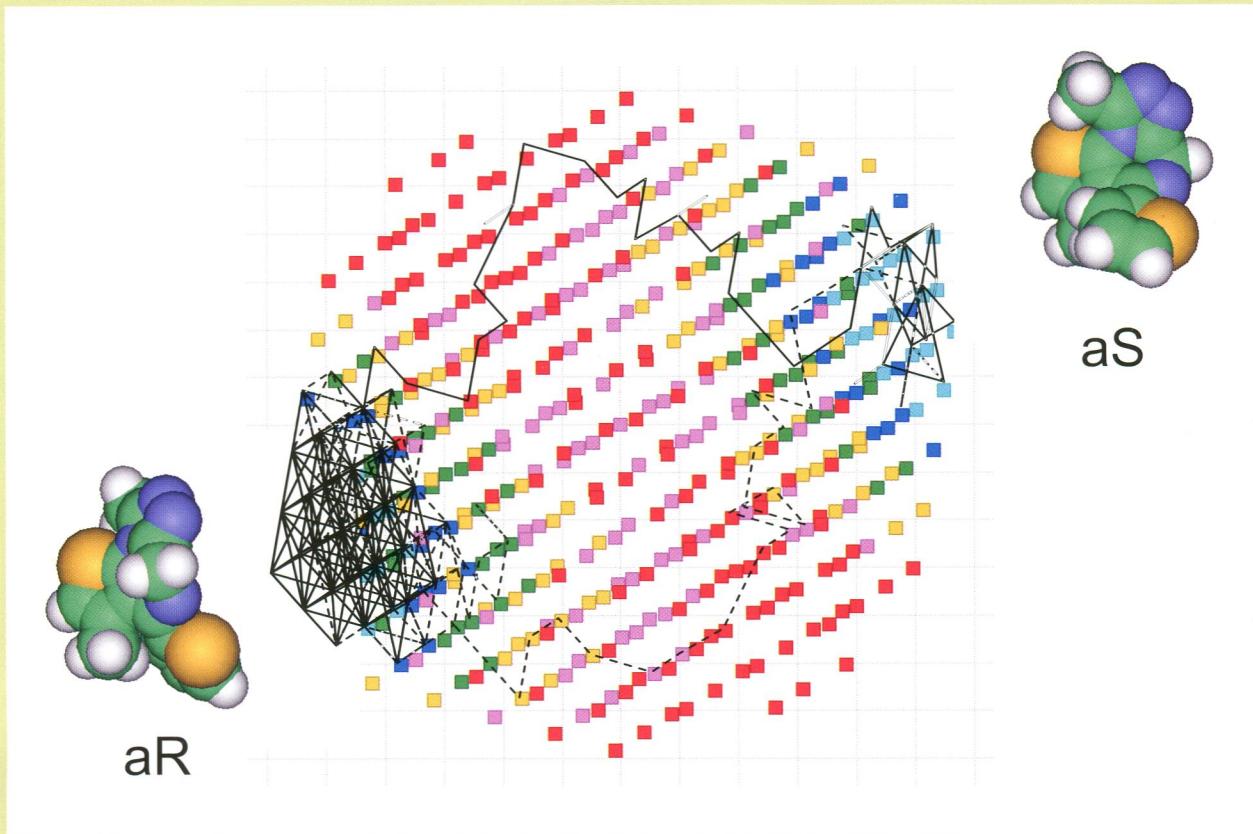
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# Chemical and Pharmaceutical Bulletin

March 2014

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Monte Carlo Simulations on Atropisomerism of Thienotriazolodiazepines  
Applicable to Slow Transition Phenomena Using Potential Energy  
Surfaces by *ab initio* Molecular Orbital Calculations

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# Chemical and Pharmaceutical Bulletin

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### Communication to the Editor

#### 4-Amino-pyrrolopyridine-5-carboxamide: A Novel Scaffold for JAK1-Selective Inhibitors

H. Shin, M. K. Kim, and Y. Chong

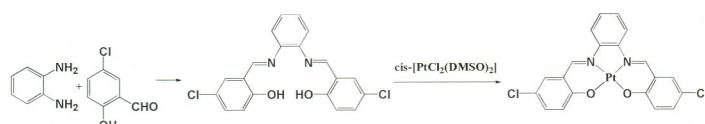
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Compd	IC <sub>50</sub> (μM)		Selectivity
	JAK1	JAK2	
2i	2.4	49.2	20.5
2j	2.2	54.4	24.7
2k	2.6	59.4	22.8

### Regular Articles

#### A Planar Schiff Base Platinum(II) Complex: Crystal Structure, Cytotoxicity and Interaction with DNA

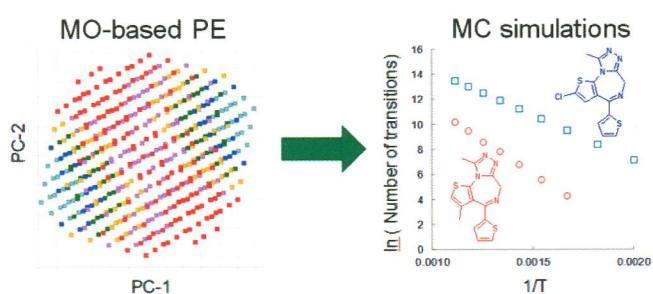
Y. Peng, H. Zhong, Z.-F. Chen, Y.-C. Liu, G.-H. Zhang, Q.-P. Qin, and H. Liang



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#### Monte Carlo Simulations on Atropisomerism of Thienotriazolodiazepines Applicable to Slow Transition Phenomena Using Potential Energy Surfaces by *ab initio* Molecular Orbital Calculations

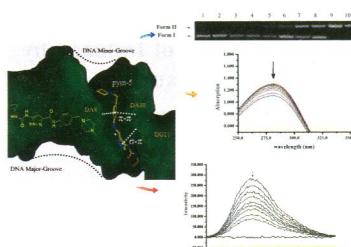
K. Morikami, Y. Itezono, M. Nishimoto, and M. Ohta



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#### Novel 1*H*-Pyrazole-3-carboxamide Derivatives: Synthesis, Anticancer Evaluation and Identification of Their DNA-Binding Interaction

Y. Lu, T. Ran, G. Lin, Q. Jin, J. Jin, H. Li, H. Guo, T. Lu, and Y. Wang

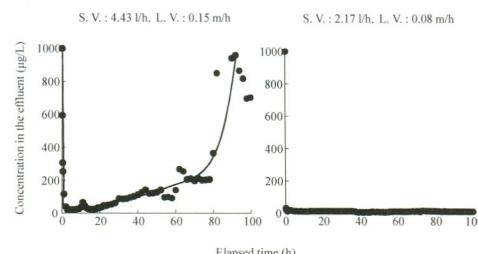


Four novel biologically active 1*H*-pyrazole-3-carboxamide derivatives have been synthesized and exhibit effective antitumor activities. The DNA interaction was investigated. Among them compound **pym-5** showed the most powerful DNA binding affinity.

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**A Study on the Adsorption of Heavy Metals by Using Raw Wheat Bran Bioadsorbent in Aqueous Solution Phase**

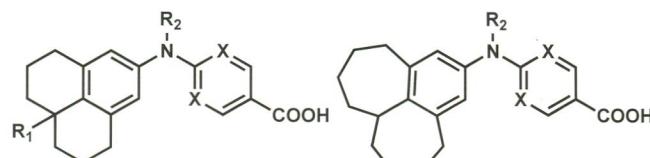
F. Ogata, M. Kangawa, Y. Iwata, A. Ueda, Y. Tanaka, and N. Kawasaki



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Y. Amano, M. Noguchi, and K. Shudo

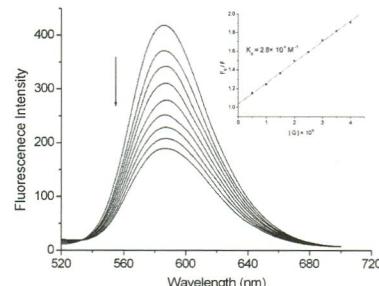


$R_1 = H$  or Methyl;  $R_2 = H$  or Alkyl;  $X = CH$  or  $N$

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**Cytotoxic Activity and DNA-Binding Properties of Isoeuxanthone Derivatives**

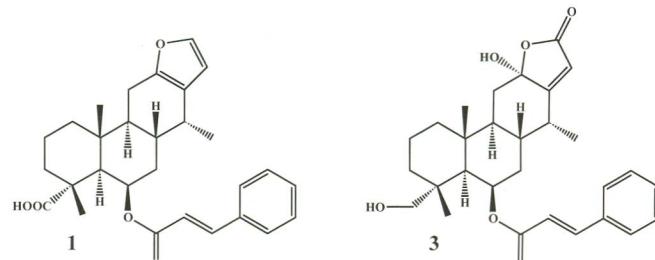
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**New Cassane-Type Diterpenoids of *Caesalpinia echinata* (Leguminosae) Exhibiting NF-κB Inhibitory Activities**

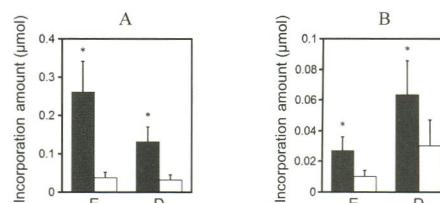
T. Mitsui, R. Ishihara, K. Hayashi, M. Sunadome, N. Matsuura, and H. Nozaki



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**Efficient Delivery and Distribution in Skin of Chlorogenic Acid and Resveratrol Induced by Microemulsion Using Sucrose Laurate**

R. Yutani, T. Kikuchi, R. Teraoka, and S. Kitagawa

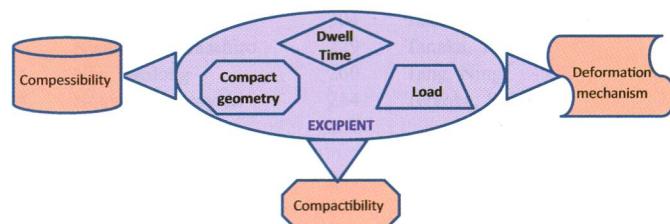


Incorporation Amount of Chlorogenic acid (A) and Resveratrol (B) in Epidermis (E) and Dermis (D) of Yucatan Micropig Skin at 40 h induced by Microemulsion using Sucrose Laurate (filled bars) and Microemulsion using Tween 80 (open bars)

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J. Rojas and S. Hernandez

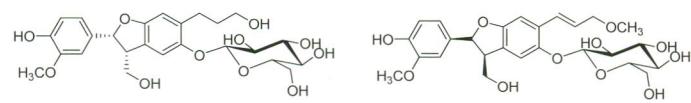


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### Three New Lignan Glycosides with IL-6 Inhibitory Activity from *Akebia quinata*

H.-G. Jin, A. R. Kim, H. J. Ko, S. K. Lee, and E.-R. Woo



1

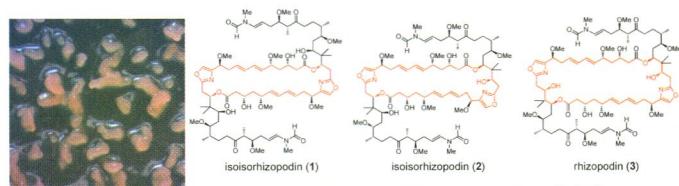
2

3

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### Two New Ring-Contracted Congeners of Rhizopodin Illustrate Significance of the Ring Moiety of Macrolide Toxins on the Actin Disassembly-Mediated Cytotoxicity

N. Oku, A. Matsumoto, T. Matsunaga, Y. Asano, H. Kasai, S. Matoba, and Y. Igarashi

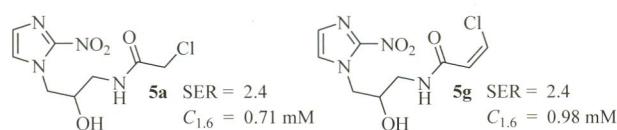


cytotoxicity against P388 murine leukemia cells: 1 < 2 < 3

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### Design and Synthesis of 2-Nitroimidazoles with Variable Alkyllating and Acylating Functionality

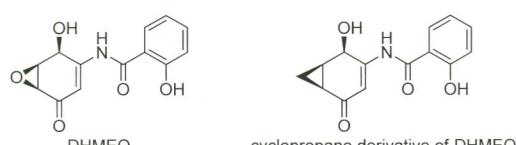
T. Winters, A. Sercel, C. Suto, W. Elliott, W. Leopold, J. Leopold, and H. Showalter



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