

6th Asian Association of Schools of Pharmacy Conference

PROCEEDINGS ● ● ●

6th Asian Association of Schools of Pharmacy Conference

*Integrating Science, Technology and Practice
for Sustained Excellence in Pharmacy Education*



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Results & Discussion

The docking results revealed that *curculigoside* A can interact with the binding sites of the studied cancer receptors. Interaction of *curculigoside* A with CDK-2 and CDK-6 are better binding interactions than those of other receptors as shown by their free binding energy of -7.59 kcal/mol and -7.83 kcal/mol, respectively. Upon interaction with CDK-2, *curculigoside* A forms hydrogen bonds to Glu12, Thr14, Lys33, Asp86, Asn144. With CDK-6 interaction are with Ile19, Lys43, Glu61, Val101, Gln149 and Asp163 residues. Moreover, they have the same pattern of hydrogen bonds with the known binding ligands (*roscovitine* and *fisetin*) for CDK-2 and CDK-6, respectively.

Conclusion

Curculigoside A has a comparable binding mode to the known binder roscovitine upon interaction with CDK-2, and of fisetin upon interaction with CDK-6.

THE AFFINITY PREDICTION OF ASIATIC ACID DERIVATIVES ON INDUCIBLE NITRIC OXIDE SYNTHASE BY MOLECULAR DOCKING

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Introduction

Asiatic acid (AA) is a pentacyclic triterpenoid compound isolated from pegagan (*Centella asiatica*). Anti-inflammatory activities of asiatic acid include acting as an inducible nitric oxide synthase (iNOS) inhibitor, an isoenzyme responsible for catalysis of nitric oxide formation, using *in vitro* and *in vivo* methods have been reported before. The aim of the present study was to obtain the affinity properties of AA and its derivatives using a docking method.

Experimental

Molecular docking simulations were performed using the AutoDock 3.0 (3). All water molecules and hetero-atoms attached to the proteins were removed. Hydrogen atoms were removed from the protein structure but later added only for polar hydrogen atoms using the program protonation and charges assigned using the kolla-amber option of AutoDock 3.0.5. The grid map of $40 \times 40 \times 40$ points with a spacing of 0.375 \AA were set for AutoGrid computation with grid centred at (x) 9.740; (y) 64.640; (z) 15.986 to cover important residues in the binding site.

Results & Discussion

The results showed that 2,3,23-triacetoxy-12-ene asiatic acid, 2,3-dioxo-11,13 diene-23-carboxy asiatic acid methylester, 2,3-dioxo-11,13 diene-23-carboxy asiatic acid and 2,3-dioxo-12-ene-23-carboxy asiatic acid methylester have the free energy binding (FEB) values of -10.17 kcal/mol, -11.30 kcal/mol, -11.33 kcal/mol, and -10.93 kcal/mol, respectively. These affinity values were higher than that of AA which was -9.79 kcal/mol.

Conclusion

Based on these results, it was predicted that the four asiatic acid derivatives show better anti-inflammatory activities than AA.

HPTLC FINGERPRINT PROFILE OF PIPER BETTLE FOLIUM FROM BANDUNG- BOGOR-SOLO INDONESIA

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Introduction

HPTLC is common used as the first line analytical tool for the quantification of plant

used as a reference for the identification and quality control of the herbal drug.

COSTUS SPECIOSUS LEAF WATER EXTRACT REDUCES THE ATHEROGENIC RISK IN HIGH-FAT-DIET INDUCED INSULIN RESISTANT RATS.

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Introduction

Insulin resistance (IR) is due to abnormalities of the insulin signalling pathway. IR has been identified as a major cause of type 2 diabetes and many cardiovascular diseases. It is evident that atherosclerosis is associated with down regulation of the insulin signalling pathway and thereby with IR. Previous studies have shown that *Costus speciosus* (CS) leaves significantly improved IR in high-fat diet fed, experimental rats. Therefore, this study was designed to assess the effects of CS leaves on atherogenesis in insulin resistant rats.

Experimental

Eight week old Male Wistar rats (170–250g) were used for this study. Rats were divided into six groups (n = 6) and fed with a high-fat diet for three months to induce IR. Then they were treated orally with different doses of *Costus speciosus*-leaf-water-extract (cslwex) for twelve weeks. Group 1: Distilled water (control), Group 2: 1500mg/kg/d, Group 3: 2000mg/kg/d, Group 4: 2500mg/kg/d, Group 5: 3000mg/kg/d, Group 6: 20mg/kg Proglitazone. Fasting Triglyceride, HDL-Cholesterol and Total Cholesterol were measured at the baseline and after the therapy.

HPTLC fingerprint has better resolution and estimation of active compounds. Chromatographic fingerprint is a rational option to meet the need for more effective and powerful quality assessment to herbal drugs. Statistical chemometric analysis can be a method for the analysis for similarity between obtained chromatograms of herbal drug. For this study, we reported the HPTLC fingerprint profiles of *Piper bettle* L. leaves obtained from central herbal gardens of Manoko-Bandung, Bogor and Tawang-Mangu-Solo of Indonesia.

Experimental

0.1 gram of each powdered *Piper bettle* Folium samples were added to 1 mL methanol and extraction aided by immersing into an ultrasonic bath at 60°C for 5 minutes. 5 μL extract was spotted on a HPTLC plate. For each sample, spotting was carried out over 6 replicates and plate was eluted by toluene-ethyl acetate (7: 3 v/v). Developed spots were detected under UV-lamp at 254 and 366 nm. Each chromatogram was scanned at 210 nm under TLC-Scanner 3 Camag. *In situ* spectrum of each peak was scanned between 200–400 nm. Eugenol was spotted as reference. The similarity of chromatograms was obtained through multi-variance PCA and HCA analyses.

Results & Discussion

The mobile phase had provided a good separation of the phytochemical constituents of *Piper bettle*. HPTLC produced good similarity chromatogram peaks pattern between the samples. *Piper bettle* samples from Bandung and Bogor showed similarities in phytochemical contents but not the sample from Solo. HPTLC-fingerprint profiles could provide a means to distinguish samples from different areas of cultivation.

Conclusion

The results obtained from the qualitative evaluation of HPTLC fingerprint images and chromatograms had shown good information of the phytochemical constituents of *Piper bettle* Folium. HPTLC analysis of *Piper bettle* can provide the standard fingerprint that can be



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CERTIFICATE OF PARTICIPATION

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President, Asian Association of Schools of Pharmacy

Celine V Liew
Chairperson, Organizing Committee

HPTLC FINGERPRINT PROFILE OF PIPER BETTLE FOLIUM FROM BANDUNG-BOGOR- SOLO INDONESIA

by Gelgel Wirasuta

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Introduction

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Conclusion

The results obtained from the qualitative evaluation of HPTLC fingerprint images and chromatograms had shown good information of the phytochemical constituents of *Piper bettle Folium*. HPTLC analysis of *Piper bettle* can provide the standard fingerprint that can be used as a reference for the identification and quality control of the herbal drug.

HPTLC FINGERPRINT PROFILE OF PIPER BETTLE FOLIUM FROM BANDUNG-BOGOR-SOLO INDONESIA

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