

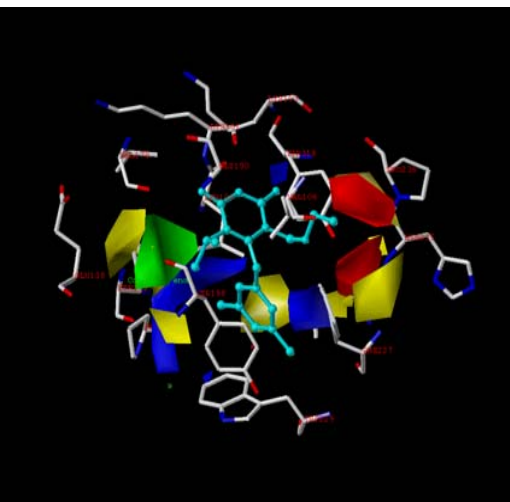
Cheminformatics Network in Thailand



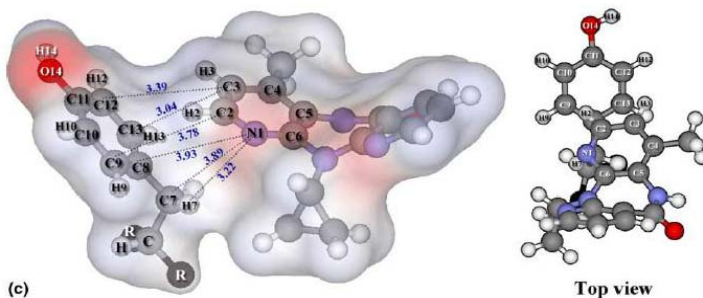
Cheminformatics has been started in Thailand since 1988 in term of Computational Chemistry research.

In 1997, Computational Science and Engineering network was initiated by NSTDA with collaboration of various Universities in Thailand. The strengthening forum can bring to Cheminformatics applications in the fields of

Quantitative Structure-Activity Relationships (QSAR)



- Calculation of Quantitative Structure Activity Relationship and Quantitative Structure Property Relationship values, used to predict the activity of compounds from their structures.



- In this context there is also a strong relationship to Chemometrics. In this context chemical expert systems are also highly important, since they represent parts of chemical knowledge as an in silico representation.

In silico Screening

- Creation of large in silico *virtual libraries* of compounds using Combinatorial chemistry techniques to increase the efficiency in mining the chemical space.
- *In silico* representation of chemical structures, using formats such as the XML based Chemical Markup Language, or SMILES. These representations are often used for storage in large chemical databases.

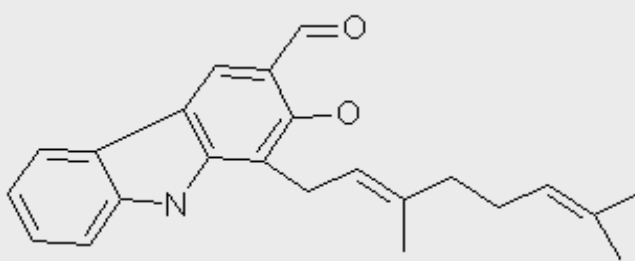
Molecular Database of Thai Natural Products

<http://chemiebase.ku.ac.th>

Home Menu Plant List Search Result Detail 3D Display

Output Format sdf Retrive

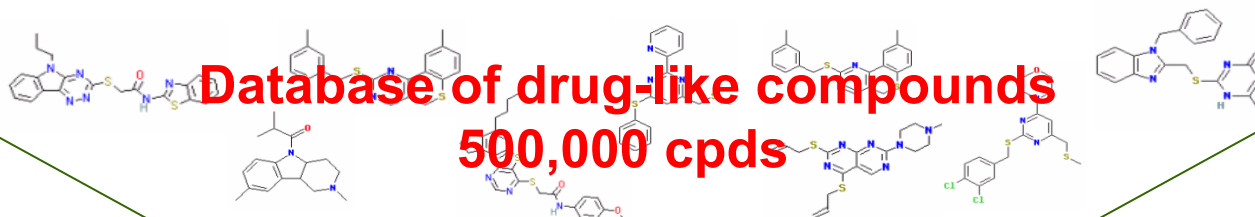
Detail			
ID Number:	1020005	CAS Number:	155519-82-7
Formula:	C ₂₃ H ₂₅ N O ₂	Weight:	347.45
H-Bond Acceptors:	3	Complexity:	-
H-Bond Donors:	2	Boiling Point:	551.1±40.0 °C
Rotatable Bond:	-	logP(cal.):	7.237±1.070
Enthalpy:	86.24±3.0 kJ/mol	other:	
SMILES:	<chem>C1[C@H]2[C@@H]([C@@H]3C[C@H](CO)[C@H](O)[C@@H](CC[C@@H](C)CCCC(C)C)[C@@H]3N2)CCC1</chem>		
Activity:			
Structure Name:	- 9H-Carbazole-3-carboxaldehyde - Clausenatine A - Mukoenine B - San sok (สันโสก) - Southeastern (thai) - Samat baiyai (สมัดใบใหญ่) - Phetchabun (thai) - Sam suea (สามเสื่อ) - Chon Buri (thai)		



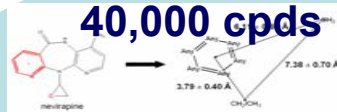
3D Display

The schematic of data searching in the system

In silico Screening



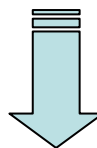
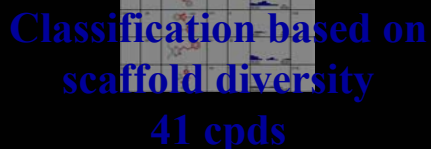
3D-database searching
40,000 cpds



Molecular Docking
6,000 cpds



Classification based on scaffold diversity
41 cpds



Biological testing

Data mining

- Typical computer science terms for data mining and machine learning topics are:
- Unstructured data
- Structured Data Mining, means mining Structured data
 - Database mining
 - Graph mining
 - Molecule mining
 - Sequence mining
- Tree mining

The past outcome

- **~ 100 international publications during the past 20 years coming out from this network.**
- **~ 20 Graduates at Ph.D. level and 50 for M.Sc. level.**

Univerisities networking

Kasetsart University	Department of Chemistry Cheminformatics Research Unit Computer Engineering	Associate Professor Dr.Supa Hannongbua Dr.Chak Sangma Assist.Prof.Dr.Puchong Utayopas Assist.Prof. Dr.Krisana Vaiyamai Chulalongkorn
Chulalongkorn University	Department of Chemistry Computational Chemistry Unit Cell Chemometrics	Prof.Dr.Supot Hannongbua Assoc.Prof.Dr.Sirirat Kokpol Assoc.Prof.Dr.Vudhichai Parasuk Assist.Prof.Dr.Pornthep Sompornpisut Assist.Prof.Dr.Somsak Pienvanich
Chiang-Mai University	Department of Chemistry Department of Mathematics	Dr.Vannachan Sanghiran Lee Dr.Piyarat Dr. Jeerayut Chaijaruwanich
Mahidol Univeristy	Department of Pharmaceutical Science	Assist.Prof.Dr.Jiraporn Ungvittayathorn
Khon-khane University	Department of Mathematics	Dr.Tawan Ruemsungnern
Thammasart University	Sirinthorn International Institute of Technology	Assist.Prof.Dr.Luckhana Lawtrakul
Ubonratchathanee University	Department of Chemistry	Dr.Pornpan Pungpo
Srinakharinwirot University	Department of Chemistry	Dr.Mayuso Kuno

Targeted-research on drug development for the Tropical Diseases in Thailand

- Anti AIDS drugs (HIV-1 RT, HIV-1 PR, HIV-1 INT)
- Anti malarial drugs (DHFR)
- Anti Dengue inhibitor (NS3 Proteinase)
- Anti SARS inhibitor (SARS CoV Proteinase)
- Anti Birdflu inhibitor (Neuraminidase)
- Anti TB inhibitor (Succinate dehydrogenase)
- Anti Alzheimer inhibitor (Acetylcholine esterase)
- Anti Inflammatory inhibitor (COX-II)
- Anti Cancer inhibitor (Topo-II)

Current activities

1. The Annual National Symposium on Computational Science and Engineering has been performed generally in March every year.
2. Workshop on Cheminformatics can be arranged for 1-2 times a year.
3. Exchange of graduate students and academic staffs between local Universities and international Universities

Expected output

1. New knowledge on Cheminformatics development methods
2. Lead compounds for drug development such as anti-HIV, anti-malaria, anti-TB, anti-Dengue, anti-infectious, anti-cancer, anti-H5N1 agents, etc.
3. Young potent Cheminformatics scientists.
4. International publications
5. Patent.

Supporting

- For conducting research in Cheminformatics, most of the grants have been supported by
 - individual Universities
 - The Thailand Research Funds
 - National Research Council of Thailand
 - NSTDA
 - Ministry of Education
 - Ministry of ICT
 - Ministry of Science and Technology.

Collaboration with foreign Institutions

Some Institutes from different countries have been close collaborated for many years, including

Malaysia

China

Korea

Japan

Austria

UK

USA,

Germany

France, etc.

Awards

- **Outstanding Scientist of Thailand**
- **NRCT Research Awards**
- **TRF Senior Research Scholar**
- **Young Scientist of Thailand**
- **Third World Academy of Science
Young Scientist Award**
- **Etc.**