Biosciences Working Group Break Out Sessions Update

Habibah Wahab, Ph.D., USM, Malaysia

Wilfred W. Li, Ph.D., UCSD, USA

Seok Jong Yu, Ph.D., KISTI, Korea

Hosted by Kasetsart University

Bangkok, Thailand March 20-22, 2012

Breakout Sessions

- Day 1 3:00-4:30 pm
  - CLB+/OPAL
    - Kevin Dong, CNIC
    - Wilfred, SDSC
  - Daun5000
    - Habibah Wahab, USM
  - Active Folder
    - Suntae Huang, Kookmin U.

- Day 2 11:00 – 12:30 pm
  - Shahir Shamsir, UTM
  - Seok Jong Yu, KISTI

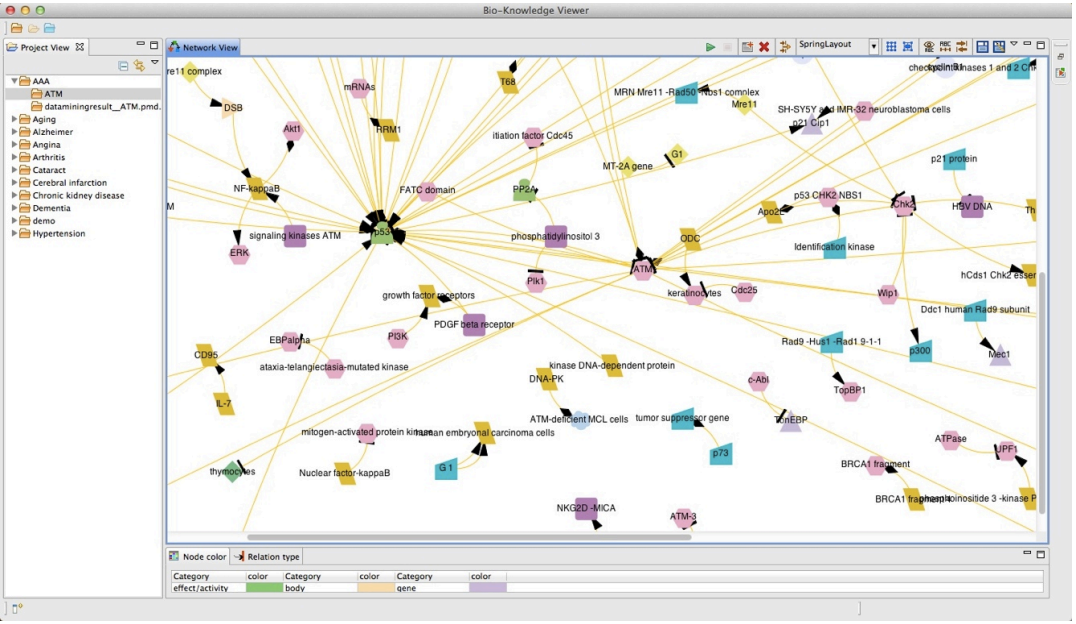
- Day 2 14:30 pm -16:00 pm

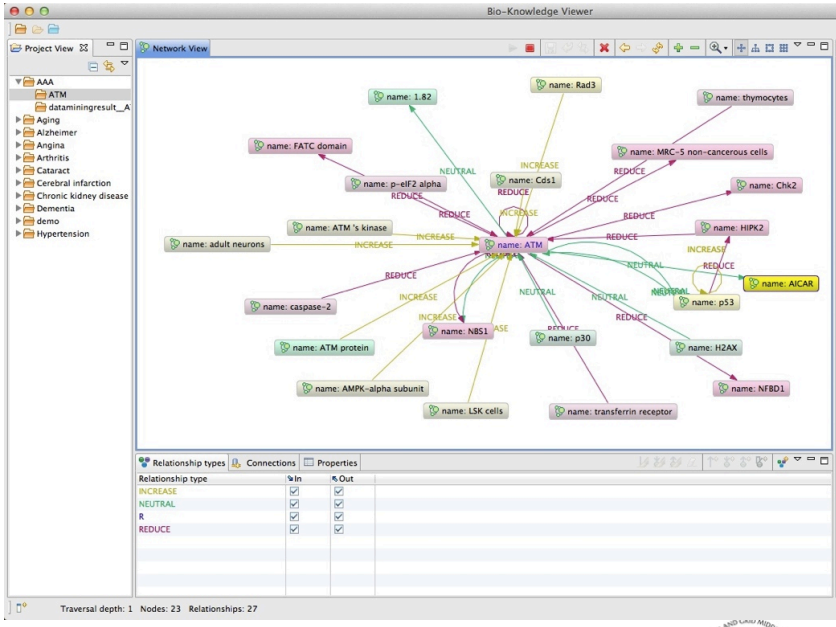
  Kwan, HKU
  - Seok Jong Yu, KISTI

  - Discussion on potential collaboration

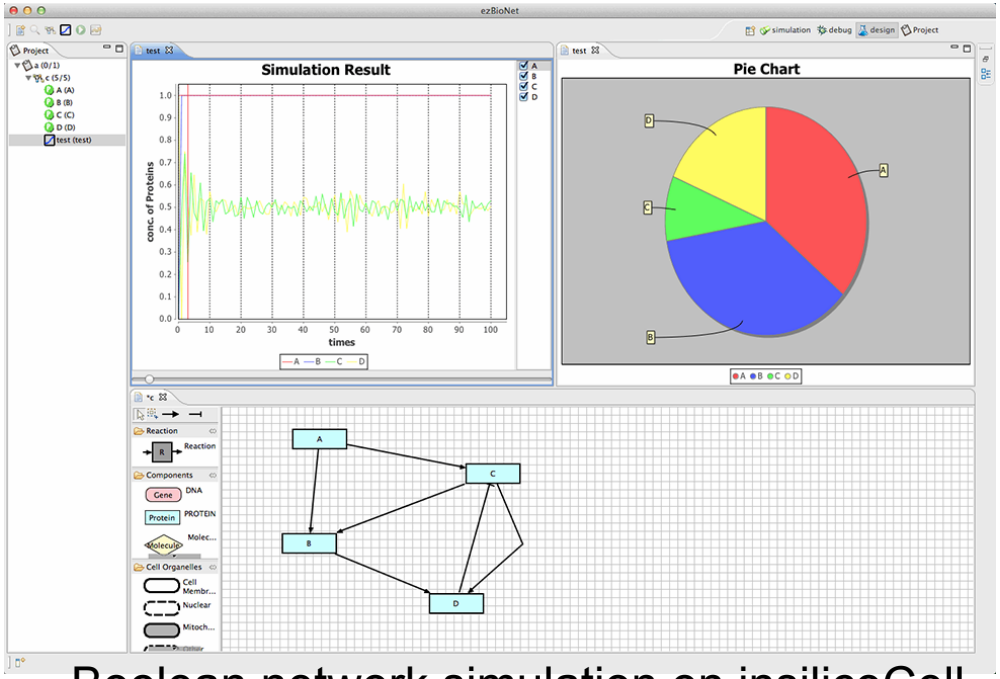
Development of insilicoCell - KISTI

- KISTI – Dr. Seok Jong Yu
  - Text-mining Tool (BioKnowledge Viewer)
    - is enhanced by adding a new visualization and navigation system.



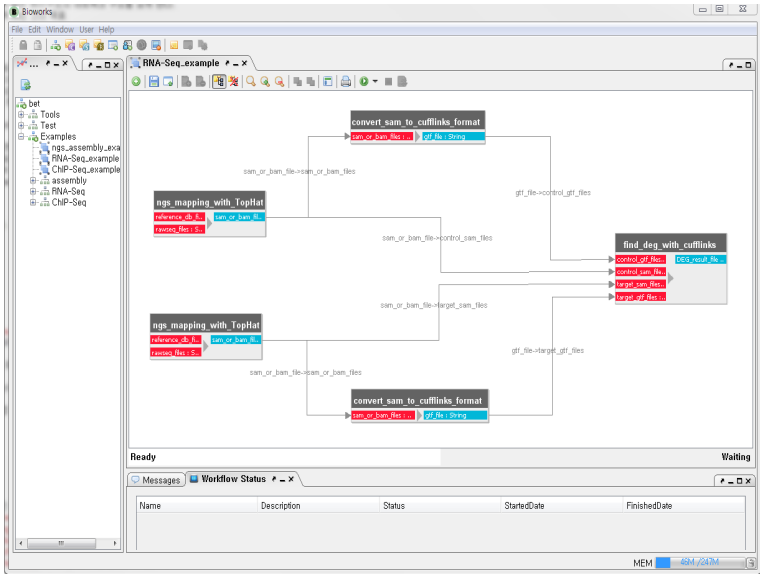


- Simulation tools is expanded by adding the Boolean network analysis tool.
- OPAL was setup and enhanced the job monitoring module.

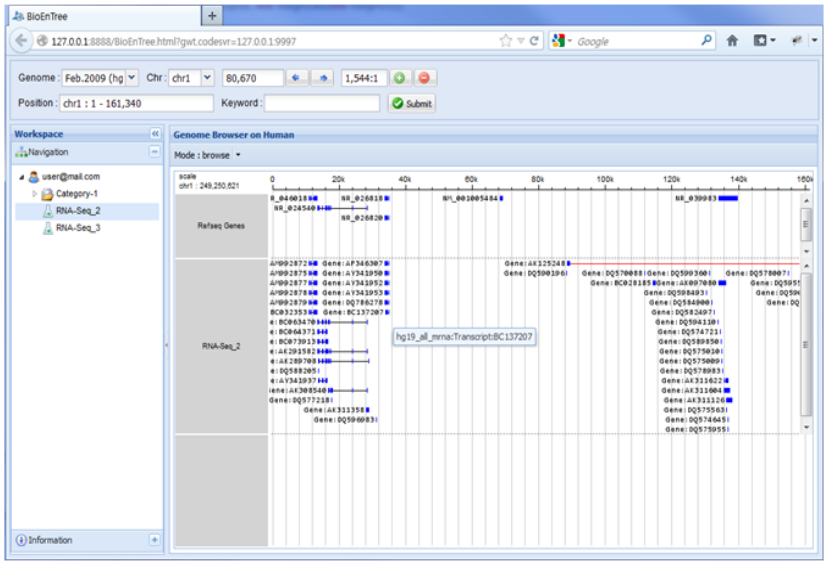


Boolean network simulation on insilicoCell

- Bioworks for NGS analysis
  - Developing a workflow system for NGS analysis process
  - Currently, have made a workflow for RNA-seq analysis.



Bioworks



Genome map Viewer

- Bio-Cloud service using Galaxy on PRAGMA Cloud
  - Creating a virtual image for NGS analysis on Galaxy system.

University of Indonesia Bio-WG

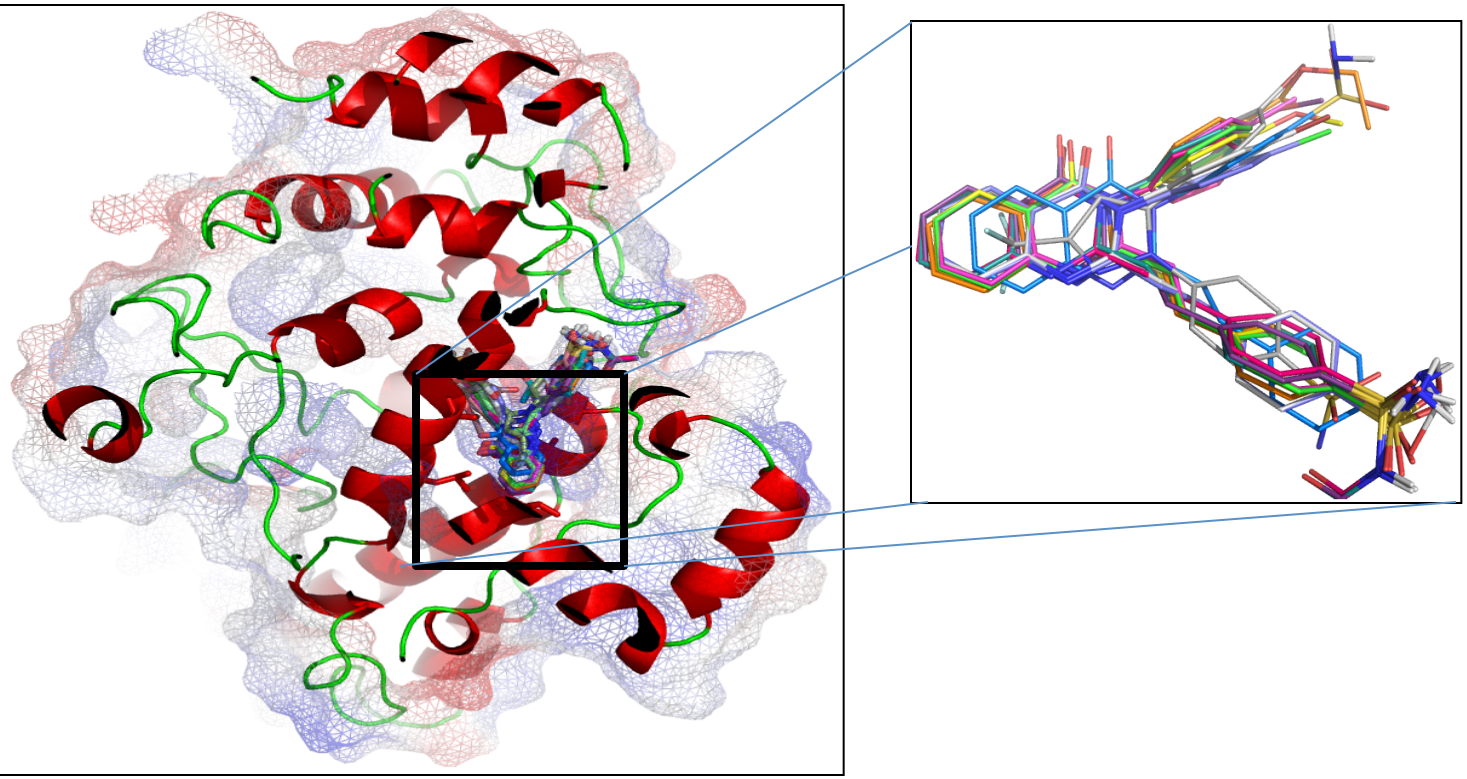
- **Member :**
  - Prof. Heru Suhartanto, Ph.D (High Performance and Numerical Computing)
  - Dr. Arry Yanuar (Pharmaceutical Chemistry)
  - Alhadi Bustamam, Ph.D. (GPU Computing)
  - Dr. Abdul Mun'im (Phytochemistry)
- **Student:**
  - Rezi Riadhi Syahdi, MSc.

University of Indonesia Bio-WG

- **On progress Research Activities**
  - High performance computing Simulation process as part of infectious disease drug discovery based on Indonesian grown medical plants,
  - Virtual Screening and *invitro* activity of Compounds from Medicinal Plants Database in Indonesia for targeting HIV-1 and Malaria.

Molecular Docking and Molecular Dynamics of Cyclooxygenase-2 complex with several quinazolinone series compound

M.A. Setiajid, Hayun, Arry Yanuar
Faculty of Pharmacy, University of Indonesia



2a (green);
2b (red);
2c (yellow);
2d (white);
2e (bluish purple) ;
2f (orange);
2i (blue);
2aa (cyan);
2ba (pink);
2ca (purple);
SC-558 (grey)

Very selective	Selective	Non-selective
SC-558 (ΔG -10.13 kcal/mol)	Celecoxib (ΔG -10 kcal/mol)	Aspirin (ΔG -4.9 kcal/mol)
2i (ΔG -10,56 kcal/mol)	2f (ΔG -9.21 kcal/mol)	2aa (ΔG -5.87 kcal/mol)
2e (ΔG -9.95 kcal/mol)	2b (ΔG -8.86 kcal/mol)	2ba (ΔG -6.22 kcal/mol)
2d (ΔG -9.73 kcal/mol)	2c (ΔG -8.79 kcal/mol)	2ca (ΔG -6.01 kcal/mol)
	2a (ΔG -8.39 kcal/mol)	

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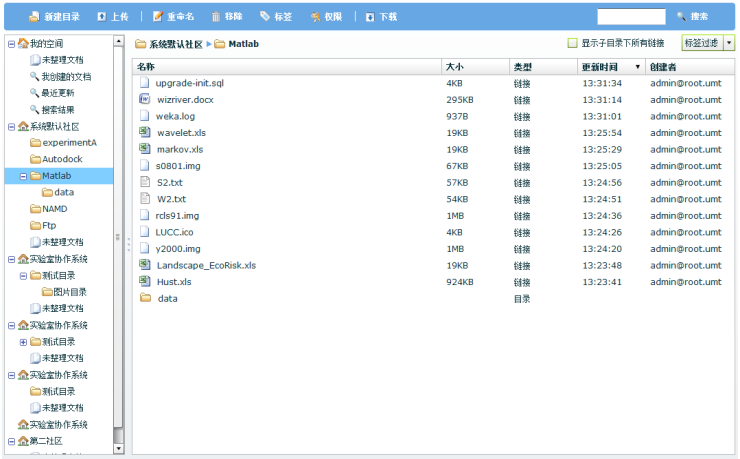
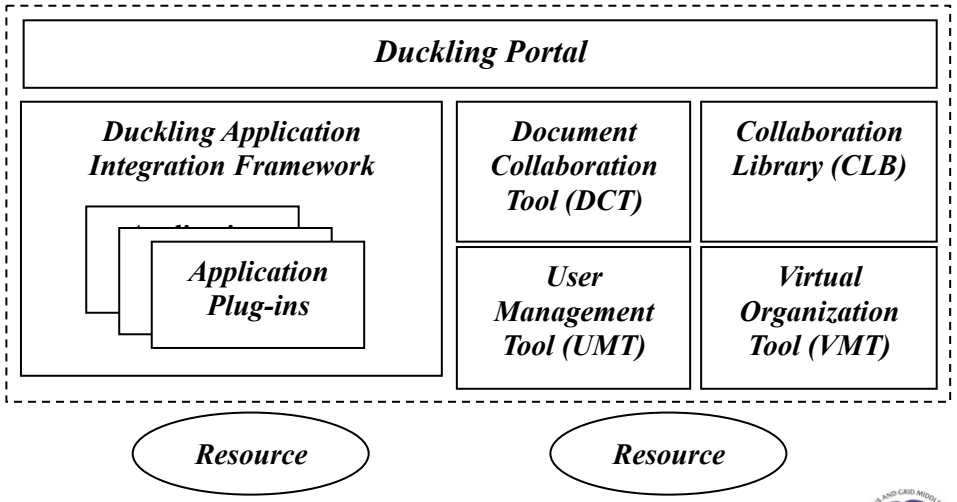
- **Publication**
  - Hayun; Hudiyono, S. , Hanafi, M., and **Yanuar, A.**, **Synthesis and COX-2 Inhibitory Activity of 4-[(E)-2-(4-Oxo-3-phenyl-3, 4-dihydroquinazolin-2-yl) ethenyl] benzene-1-sulfonamide and Its Analogs**, Pharmaceuticals 2012, 5(12) 1282-1290; doi:10.3390/ph5121282
  - Syahdi, RR., Mun'im, A., Suhartanto, H., **Yanuar, A**. **Virtual Screening of Indonesian Herbal Database as HIV-1 Reverse Transcriptase Inhibitor**, Bioinformation 2012, 8(24) 1201-1210,

CNIC – Duckling Collaboration Library

- CLB - Collaboration Library
  - A component of Duckling, an open-source toolkit developed by the CNIC, Chinese Academy of Sciences (CAS)
  - Used by all Duckling applications as the Data Repository

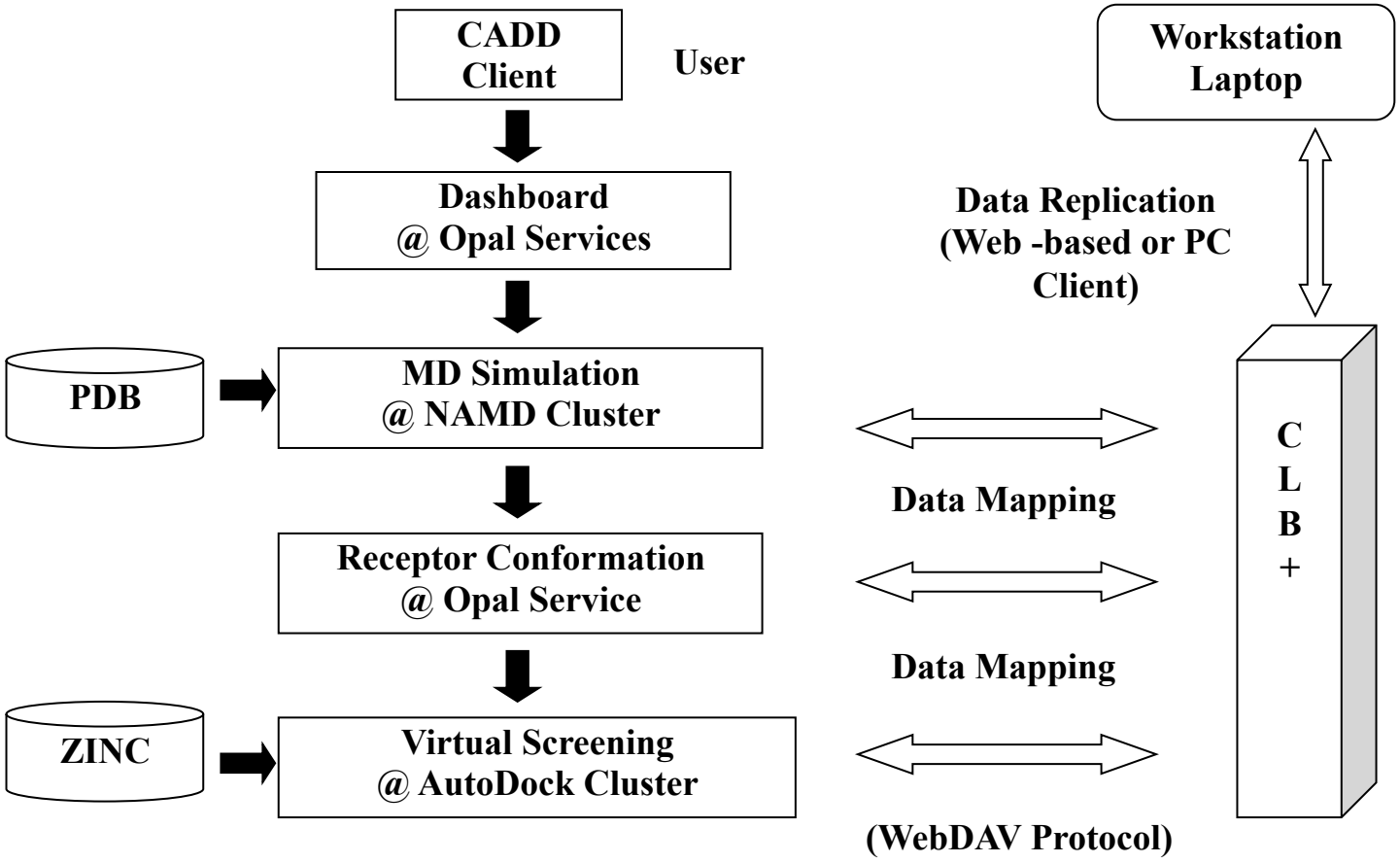




Key Features

- Cloud-based Data Repository
  - Means offering a robust and scalable data cloud service. Researchers do not need to worry about where the data is stored or whether it is backed up or not.
- Ease of Access
  - Stands for the data accessibility from most experimental environments. Scientists can access the data from their desktop, servers and mobile devices on demand.
- Data Life Cycle Management
  - Indicates that the cloud repository can be used to store and track all processes and data generated by experiments, especially for workflow-based jobs, by the means of data versioning, which is crucial for experimental data collaboration.

Use Case Scenario



Report on some of the status of BioSciences research in HKU(Kwan)

- (1) More HKU researchers involvement in BioSc. Research
  - Zoology / Botany / Statistics
  - BioChem / Community Medicine / Pediatrics / Pathology
  - Civil Engin. (Waste water treatment)
  - Genomic Sciences Centre (recently change the name)
- (2) Big Data and its handling due to disparity of low cost large storage devices
  - e.g. for mainframe type: 10K HK$/TB for EMC Epsilon
  - but 60K HK$ NAS equipped with 8*3 TB hardisk ->3K$/TB
- (3) More recognizable project involvement with large funding
  - local HK Government - UGC/RGC/ITF projects
  - Shenzhen SAR projects
  - China 863 projects

HKU

(4) Computing Environment

- HPC vs HTC
- HPC vs cloud
- How to help users in adapting VM cloud migration for HTC type application (large data set docking, MD simulation over a range of parameter, Gromacs ...)
- How to work in a public cloud but demands for more computing resources from pre-arranged designated resources suppliers (say a well developed application, wants to extend the scale of computation, due to sudden availability of government funding, or due to sudden natural disaster)

•(5) Researchers' concern and challenge for large scale Bioinformatics computing

- hierachy:
  - personal/group pilot development
  - departmental facility
  - central computer centre computing
  - regional/national computer centre computing
  - Big data migration/computation/ownership-concern
  - Information-security/data-privacy in during migration

- (6) Others
  - more incoming collaborations with overseas/China
  - Jessie Bao in Tianjin Inst. of Biotech
  - KISTI
  - SZ
- * During visit last Friday, NSCCSZ deputy director
- Dr. Fiona HUANG mentioned that while all 1.2 bil RMB hardware budget has been used up, around .1 bil RMB software package budget is still available for the THIRD batch of software purchase. She would like to have advice from HKU researchers, and of course international experts.

PRAGMA Updates and Spin Offs from Universiti Teknologi Malaysia

- Publish the bats scanning result in Nature Scientific Reports 2012 – presented in PRAGMA 22 Taiwan
- **Geoportal – Reed Beaman (University of Florida) + Aimee Stewart (Kansas University)**
  - Member of PRAGMA biodiversity team
  - Metadata host for Mt Kinabalu flora
  - Part of pragma grid for ultramafic environment studies
- **Phyknome – Prof Heru/Dr Arry (University of Indonesia) + Prof Habibah (Universiti Sains Malaysia)**
  - Ethnobotanical & Phytochemical Knowledge DB
  - 20,000 species of Malaysian plants
  - http://mapping.fbb.utm.my/phyknome
- **GBIF**
  - 1st and only node in M'sia (thanks ACB)
  - 6 datasets (Amphibians, Reptiles, Moss, Fern, Mangrove)
  - http://birg4.fbb.utm.my:8080/ipt

UTM
UNIVERSITI TEKNOLOGI MALAYSIA

http://mapping.fbb.utm.my/phyknome/

SCIENTIFIC REPORTS | ARTICLE OPEN

Counting in the dark: Non-intrusive laser scanning for population counting and identifying roosting bats

Suzanna Noor Azmy, Shahrul Anuar Mohd Sah, Nur Juliani Shafie, Azman Ariffin, Zulkepli Majid, Muhamad Nor Akmal Ismail & Mohd Shahir Shamsir

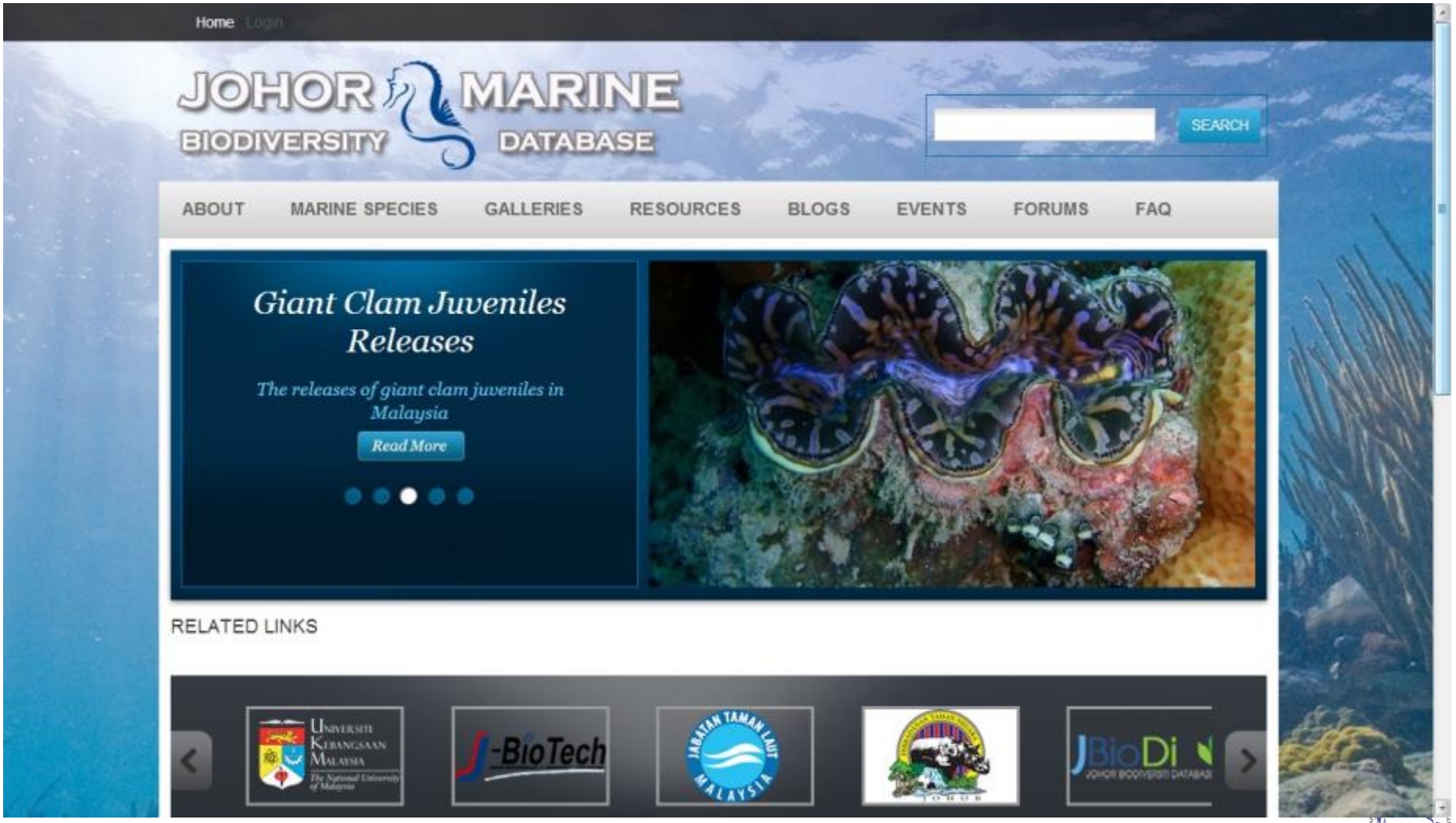
Affiliations | Contributions | Corresponding author

Scientific Reports **2**, Article number: 524 | doi:10.1038/srep00524

Received 23 February 2012 | Accepted 04 July 2012 | Published 23 July 2012

Population surveys and species recognition for roosting bats are either based on capture, sight or optical-mechanical count methods. However, these methods are intrusive, are tedious and, at best, provide only statistical estimations. Here, we demonstrated the successful use of a terrestrial Light Detection and Ranging (LIDAR) laser scanner for remotely identifying and determining the exact population of roosting bats in caves. LIDAR accurately captured the 3D features of the roosting bats and their spatial distribution patterns in minimal light. The high-resolution model of the cave enabled an exact count of the visibly differentiated *Hipposideros larvatus* and their roosting pattern within the 3D topology of the cave. We anticipate that the development

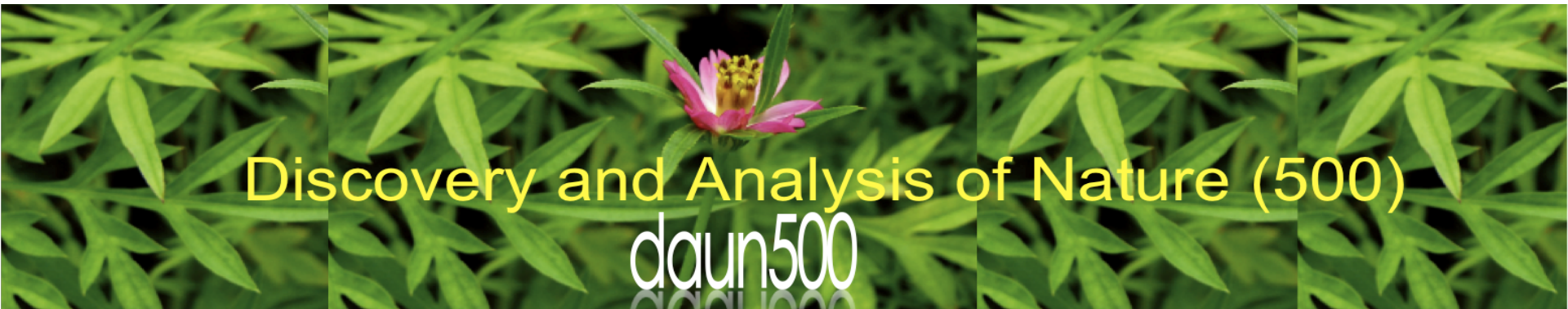
http://mapping.fbb.utm.my/jmarine/



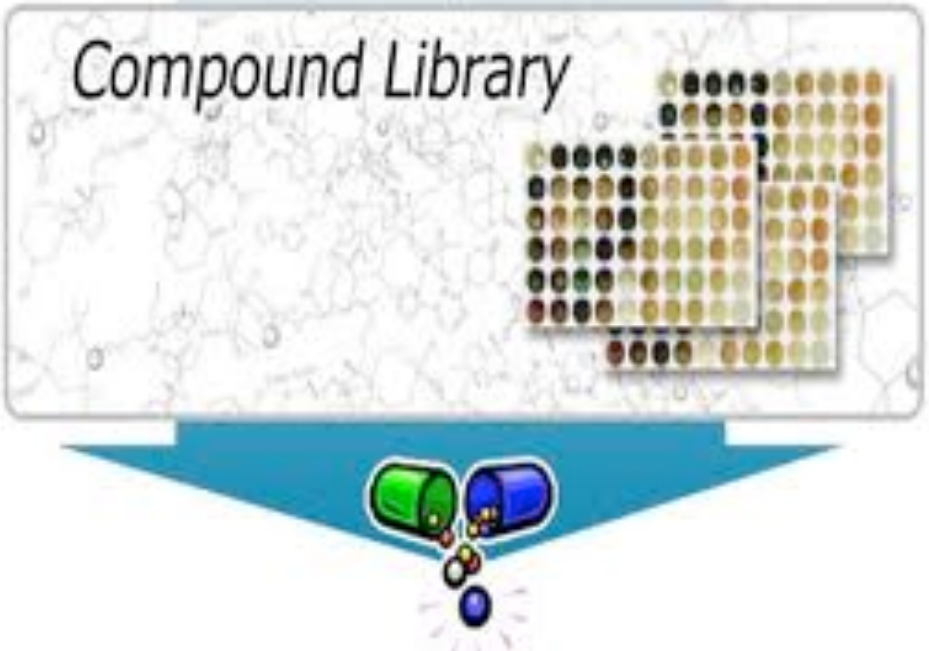
http://johorbotanicalgarden.johordt.gov.my/

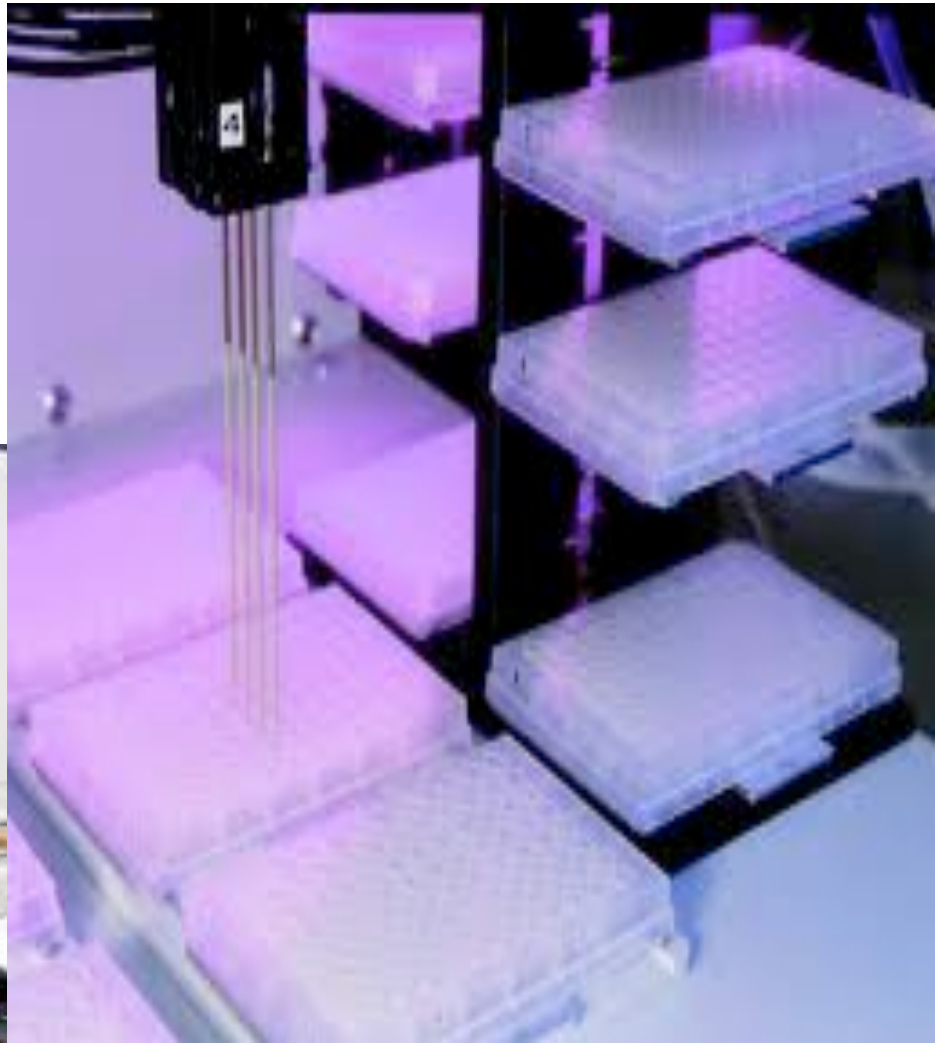
Daun500

- profile the chemical compositions of 500 Malaysian plants
- analyse the toxicity of the 500 Malaysian plants
- screen the 500 Malaysian plants on 50 bioassays (of selected diseases)
- 500 Malaysian plants on 5 HTS assays
- library of Malaysian Plants Natural Product containing at least 10,000 extracts/fractions/ compounds



Output: National Natural Product Repository & HTS





Output: Knowledge Based of Malaysian Natural Product Discovery

Safari File Edit View History Bookmarks Window Help (2:39) Tue 8:28 AM

Daun500: Natural Remedies

http://202.170.57.56/Daun500/detail_data.php?code=9

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Detail : Bioassay Result and Activities

Bioassay (commonly used shorthand for biological assay), or biological standardization is a type of scientific experiment.

1 Search 2 Result 3 Detail

Common name: Phaleria macrocarpa
Local name: Mahkota dewa

Bioassays Legend :
YES NO Positive activity Negative activity

Source	Toxicity	SRB1	NAH1	NAHTS	NAH5	NAH3	XO	NS3	NSHTS	EP	ACE	BACE	PI
Phaleria macrocarpa	✓	+	−	+	+	+	−	+	−	−	−	−	
Source	Toxicity	SRB1	NAH1	NAHTS	NAH5	NAH3	XO	NS3	NSHTS	EP	ACE	BACE	PI

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NADI-Chem

User friendly interface,search substructure, formula, Log P and molecular ranges,structures for cheminfo

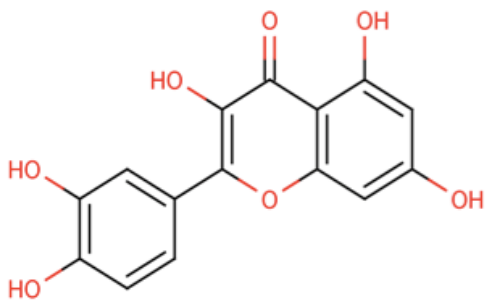
1 Search 2 Advance Search 3 Result 4 Detail

Dashboard

Note:To view and download data , please refer detail chemical data

Chemical Compound Structure

NADI Code: MSC427



Similiar Chemical Structure

Chemical Compound | Similiar Substructure

Similiar Chemical Structure

Chemical Compound | Similiar Substructure

Description

Chemical Name	Quercetin
Synonyms	Xanthaurine; Sophoretin; Meletin; 3,3â€™,4â€™,5, Pentahydroxyflavone; Sophoretin;
InChI	1S/C15H10O7 /c16-7-4-10(19)12-11(5-7)22-15(14(2 2-8(17)9(18)3-6/h1-5,16-19,21H
Chemical Formula	C15H10O7
SMILES	Oc1ccc(cc1O)C=3Oc2cc(O)cc(O)c2C(=O)(
Log.P (approx.)	-2.83
Weight	302.24
H-Bond Acceptors	7
H-Bond Donors	5
Chemotype	Flavanol

Plant Source

1. Common name: Ageratum conyzoides
   Local Names: Rumput Tahi Ayam
   Plant Parts:

References

O., Adewole, (2002). Ageratum conzoides L.(Asteraceae). Journal of Fitoterapia, 73, p. 1.

2. Common name: Allium cepa
   Local Names: Bawang besar
   Plant Parts:

Local Names: Koko
Plant Parts: Bean, Leaf, Flower

References

F., Sanchez-Rabaneda, et. al., (2003). Liquid chromatographic/electrospray ionization tandem mass spectrometric study of the phenolic composition of cocoa (Theobroma cacao). J. Mass Spectrom., 38, p. 35â€"42

L.A., Griffiths, (1958). Phenolic Acids and Flavonoids of Theobroma cacao L. Separation and Identification by Paper Chromatography. J. Biochem., 70(1), p. 120â€"125.

51. Common name: Trichosanthes anguina
    Local Names: Petola ular
    Plant Parts: Fruit

References

- *KH Mlean & S. Mohamed, (2001) Flavonoid (Myrcetin, Quercetin, Luteolin, and Apigenin) Content of Edible Tropical Plants, J Agric Food Chem., 49, p. 3106-3112*

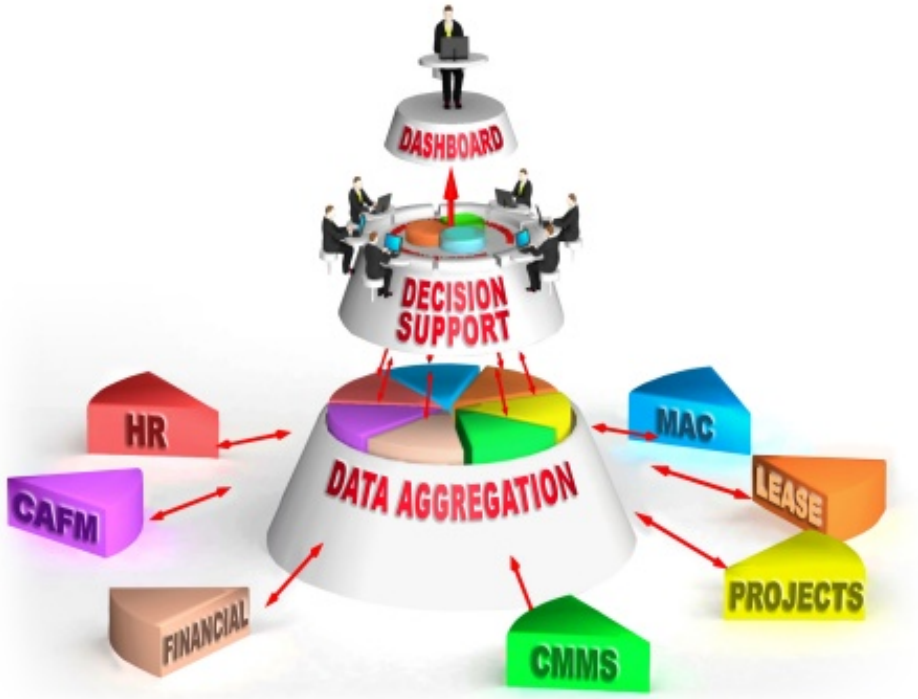
Plant Source [+]

Investigated Activities

1: Anti-oxidant (1, 4, 5)
2: Anti-tumor effects of lavonoids (2)
3: Inhibition o lung cancer cell growth via G2/M arrest and induction of apoptosis (3)
4: Anticancer
5: Antiplatelets, Anti-hypertensive

1) *Subramaniam, et. al., (2003). Natural Antioxidants: Piper sarmentosum (Kadok) and Morinda elliptica (Mengkudu). Malaysian Journal of Nutrition, 9(1), p.41-51*
2) *Kanadaswami et al., (2005). The antitumor activities of flavonoids, In Vivo, 19, P.895â€"909*
3) *Yang et al., (2006). Inhibition of lung cancer cell growth by quercetin glucuronides via G2/M arrest and induction of apoptosis, Drug Metabolism and Disposition: The Biological Fate of Chemicals, 34, P.296â€"304*
4) *F., Nessa, et. al., (2004). Free radical-scavenging activity of organic extracts and of pure flavonoids of Blumea balsamifera DC leaves. Food Chemistry, 88, p. 243â€"252.*
5) *L. C. Hong et. al., (2007). Extraction and Characterization of Antioxidant Compositions From Fermented Fruit Juice of Morinda citrifolia (Noni). Agricultural Sciences in China, 6(12), p. 1494-1501.*

Data from Family and Community Assessment Program (FAP)



- Tools for the executive of Sub-district Administration Organization Network (SAON) to improve decision-making

Puangrat Jinpon, Center of Excellence for Ecoinformatics, and Computational Science Graduate Program, School of Science, Walailak University

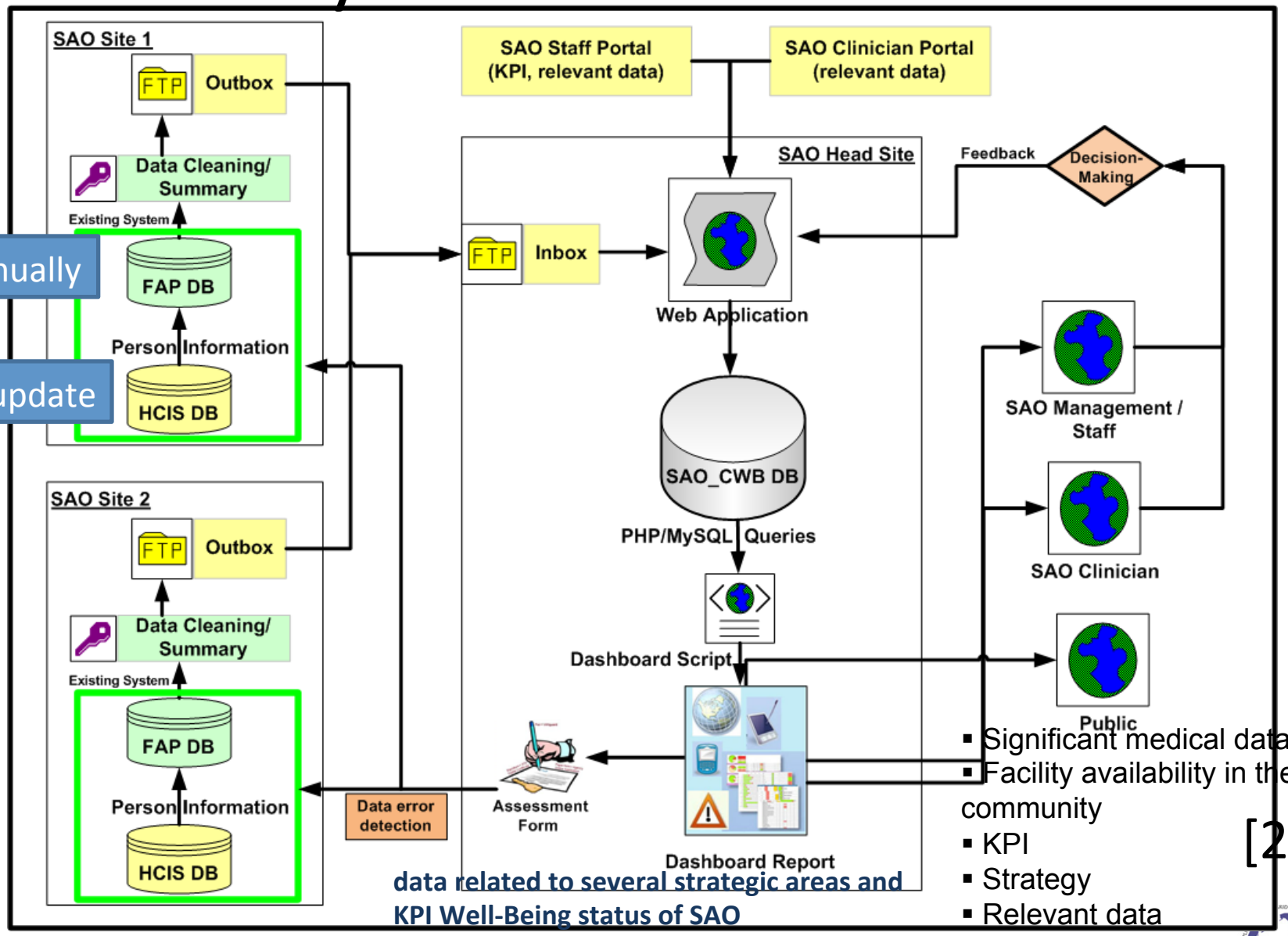
Study Sites

Available data

- 8 sites as 2009 and 1 site as 2011;
- 51,976 Persons;
- 13,345 Families.

The data from 2 sites are in the process

System architecture



data related to several strategic areas and KPI Well-Being status of SAO

- Significant medical data
- Facility availability in the community
- KPI
- Strategy
- Relevant data

[27]

Home Page: English Version
http://webserver.sct.ac.th/communitywellbeing

Future Collaborations

- U. Indonesia and Kookmin University, ActiveFolder
- USM, UTM, UI, with KISTI on Bioknowledge Visualiser

Future Collaborations

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- USM, UTM, UI, with KISTI on Bioknowledge Visualiser