

# **AN INTEGRATED COMPUTING PLATFORM PROTOTYPE SUPPORTING IN SILICO DRUG DISCOVERY ACTIVITIES**

*Authors:*

Ari Wibisono, Muhammad H. Hilman, Alhadi  
Bustamam,  
Arry Yanuar, Kevin Burrage, Xue Li, and Heru  
Suhartanto

Presented at : PRAGMA26, Tainan, Taiwan  
by Heru Suhartanto and Arry Yanuar

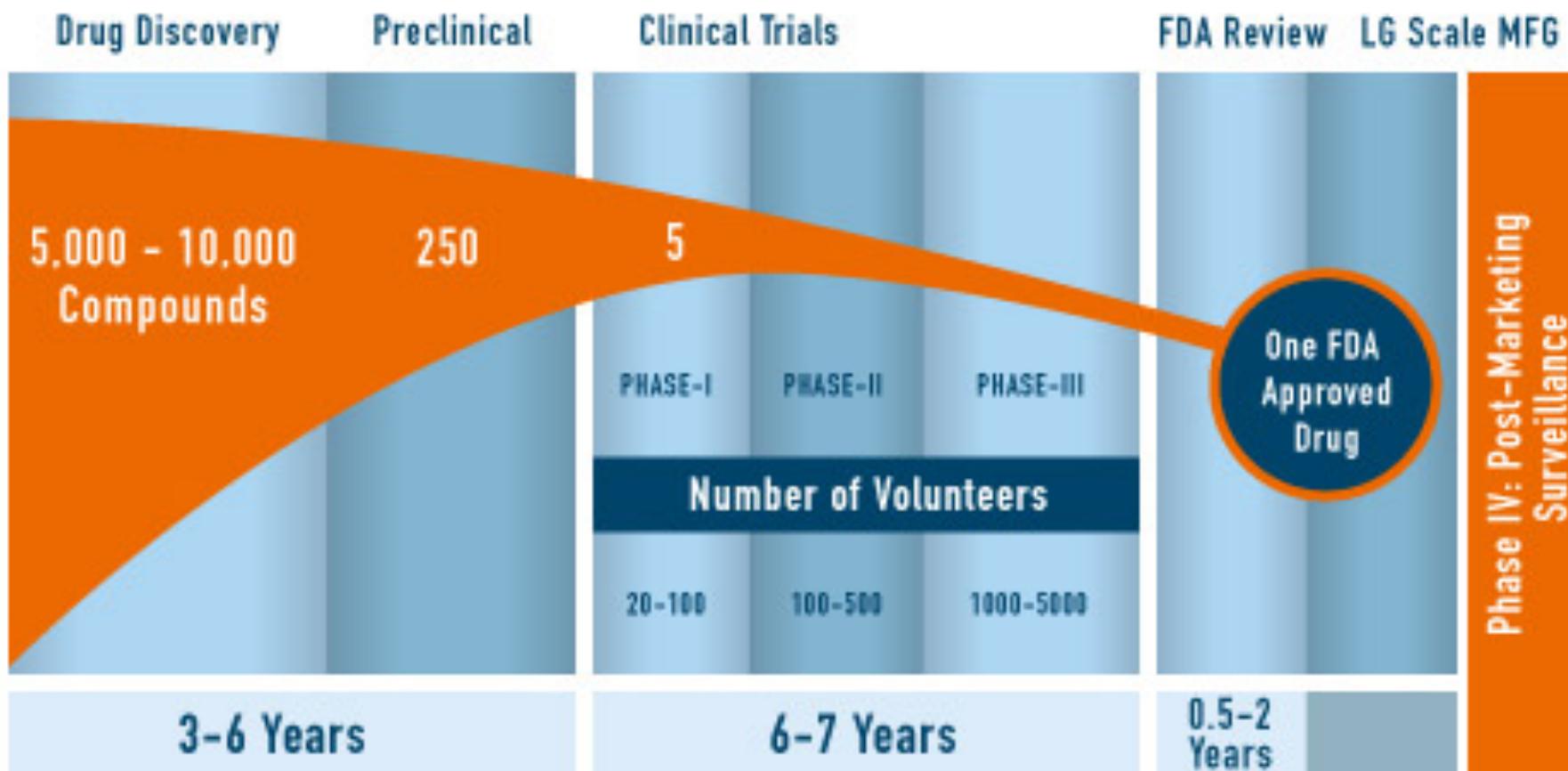
---

# background

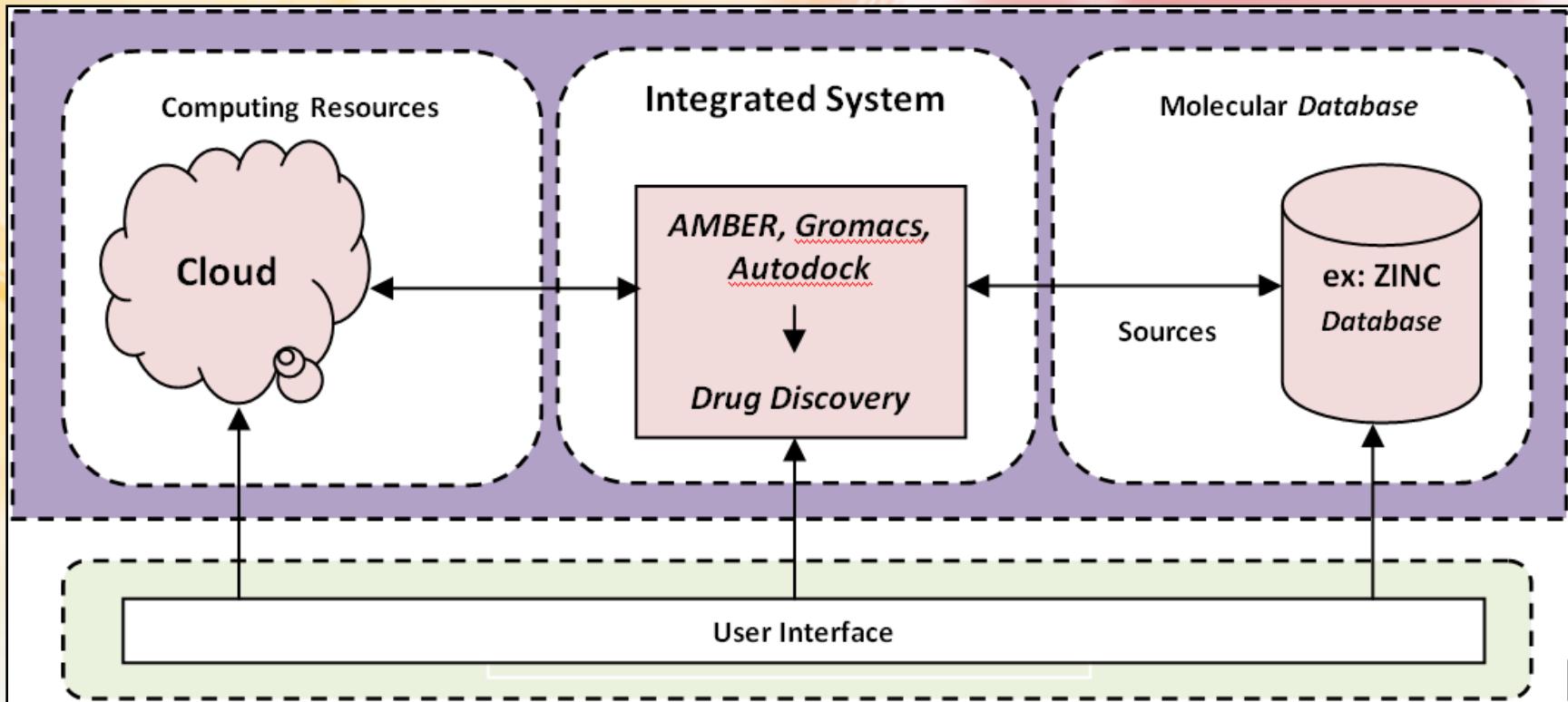
---

- In our world, there are about 40,000 species of plants, of which 30,000 species live in the islands of Indonesia. Among the 30,000 species of plants that live on the islands of Indonesia, it is known that there are at least 9600 species of medicinal plants. [Braz, 2010, Cotelle, 2006]. Focus -> insilico drug discovery based on medical plants.
- Succesfull facts:
  - Computational Based Drug Design accelerates the process of discovery of new drugs. Raltegravir, an antiretroviral drug to HIV-1 infection, was identified through a process using computational docking program AutoDock in 2004 by Prof. McCammon (Schames et al., 2004).
  - It has obtained a license for clinical use by the FDA on October 12, 2007 (merck.com, 2007). Raltegravir acts as integrase inhibitor, where integrase is an enzyme that presents only in viruses that play a role in the introduction of genetic material (DNA) into host cell DNA (human).
- Challenges
  - Reliable, achievable, easy to use preparation environment, high performance computing resources integrated with medical plant database

# ANOTHER TARGET: SPEEDING UP DRUG DEVELOPMENT PROCESS



# THE DESIGN



# Previous Results

**DATABASE OF INDONESIAN MEDICINAL PLANTS**

Database Senyawa Aktif Tanaman Obat Indonesia

**Mengkudu (pace)**  
Keistimewaan buah ini adalah mempunyai kandungan scopoletin, serotonin, damnacantal, athraquinon,dll. Buah pace sangat efisien untuk mengobati diabetes, penyakit jantung, strooke, memperbaiki tekanan darah bahkan dapat menyehatkan kelenjar throid, meningkatkan kekebalan tubuh.

**<http://herbaldb.farmasi.ui.ac.id/>**

## Previous Results : Infrastructure and user acceptance tests

**Table 1.** Specifications cluster of four scenarios

Parameter	SCluster	LCLuster	XLCluster	Cluster05
Memory	1.7GB	7.5GB	15GB	4GB
Compute Unit/Processors	1 1.2GHz	4 1.2GHz	8 1.2GHz	Quad Core 2.8GHz
Platform	32-bit	64-bit	64-bit	32-bit
Cost/Hour	\$0.085	\$0.34	\$0.68	-

**Table 2.** SCloud System Testing

No	Parameter	Result
1	All Feature Operation	100 %
2	Average time of Feature Operation	1569 second
3	Average of user's mistake	Twice on each features
4	Level of easiness	4.92 of 5
5	Level of user satisfaction	4.7 of 5

**Table 3.** Manual System Testing

No	Parameter	Result (second)
1	Average execution time of the user establishment	3600 (s)
2	Average time user configuration	1800 (s)
3	Average time of user's script writing	500 (s)
	Total time	5900 (s)

## Previous Results : Virtual Screening of Indonesian Herbal Database as HIV-1 Reverse Transcriptase Inhibitor

---

Rezi Riadhi Syahdi, Abdul Mun'im,  
Heru Suhartanto, Arry Yanuar, Bioinformation 8(24), 2012:

top ten compounds were  
mulberrin, plucheoside A, vitexilactone, brucine N-oxide,  
cyanidin 3-arabinoside, alpha-mangostin, guaijaverin,  
erycristagallin, morusin and sanggenol N.

## Recent Results : Virtual Screening of Indonesian Herbal Database as HIV-1 Protease Inhibitor

---

Arry Yanuar<sup>1\*</sup>, Heru Suhartanto<sup>2</sup>, Abdul Mun'im<sup>1</sup>, Bram Hik Anugraha<sup>1</sup> & Rezi Riadhi Syahdi<sup>1</sup>, Bioinformation 10(2), 2014:

top ten compounds were  
8-Hydroxyapigenin 8-(2",4"-disulfatoglucuronide),  
Isoscutellarein 4'-methyl ether, Amaranthin, Torvanol A,  
Ursonic acid, 5-Carboxypyranocyanidin 3-O-(6"-O-  
malonyl-beta-glucopyranoside), Oleoside, Jacoumaric  
acid, Platanic acid and 5-Carboxypyranocyanidin 3-O-  
beta-glucopyranoside.

# FUTURE WORKS

---

- Accomodating GPUs into the infrastructure,
- Building automated workflow of drug discovery activities.
- Improving user interface of the molecular database system.
- Analyzing the performance of commercial cloud as computational resource.
- Bridging each entities with interfaces to provide access,
- Continuing with in vitro activities....