

# FKPPL Project application (2012)

*Red info should be replaced by the appropriate text in black*

<b>ID: Title</b>	<b>WISDOM, grid enabled in silico drug discovery</b>					
<b>Members</b>	<b>French Group</b>			<b>Korean Group</b>		
	<b>Name</b>	<b>Title</b>	<b>Affiliation</b>	<b>Name</b>	<b>Title</b>	<b>Affiliation</b>
	Leader Breton Vincent	Dr.	LPC CF -IN2P3	<u>Leader:</u> Kim, Doman	Dr.	Chonnam Natl Univ
	Bui The Quang	PhD student	LPC	Hwang, Soonwook	Dr.	KISTI
				Hanh, Than	Res. Associate	Chonnam Natl Univ
				Kim, Seok-Kyoo	Dr.	KISTI
				Kim, Sangwan	Res. Associate	KISTI
				Rho, Seungwoo	Res. Associate	KISTI
<b>Requested LIA specific funding from France</b>						
<b>Description</b>		<b>Euro/unit</b>	<b>Nb of units</b>	<b>Total (euros)</b>	<b>Requested to: *</b>	
Visit to Korea						
Travels						
Total						
<b>Requested funding from Kprea</b>						
<b>Description</b>		<b>Won/Unit</b>	<b>Nb of units</b>	<b>Total (Won)</b>	<b>Requested to: **</b>	
Travel		4000000	4 travel	16000000	Korean Government	
Visit to France		200000/day	days			
Total				16000000		
<b>Additional funding</b>	<b>Funding from France</b>			<b>Funding from Korea</b>		
	<b>Provided by or requested to ***</b>	<b>Type</b>	<b>Euro</b>	<b>Provided by or requested to</b>	<b>Type</b>	<b>Won</b>
	ANR	Postdoc & PhD student		Korean Gov	Materials & Equipment	20000000

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\* For example: IN2P3, CEA. \*\* Korean University or Institute. \*\*\* French Embassy, CNRS Egide,.....

<b>Summary of Project</b>	<p>The goal of the project is to explore novel techniques for drug discovery. The WISDOM collaboration uses <i>in silico</i> docking techniques, where researchers use computing systems to compute the probability that potential drugs will dock with a target protein. This lets researchers rule out the vast majority of potential drugs, so that they can concentrate on the most promising compounds in laboratory tests. This speeds up the screening process and reduces the cost of new drug development to treat diseases such as malaria.</p> <p>In 2011, collaboration between CNU, KISTI and LPC Clermont-Ferrand focused on a potential drug target, the 3CLpro protein, to fight SARS. Data challenges were deployed by LPC Clermont-Ferrand and KISTI while CNU contributed to the analysis of the results.</p> <p>For 2012, we will pursue on the Korean side the work on the protease Dengue virus target. For this target, a number of compounds selected <i>in silico</i> will be tested <i>in vitro</i> at CNU. During this work, researchers from CNU will also select the relevant enzyme targets, preparation for docking for parameter and proceed with <i>in vitro</i> testing of the most promising compounds selected <i>in silico</i>. CNU will start collaboration with Vietnam Institute of Natural Products and Chemistry for new ligand libraries.</p> <p>On the French side, efforts will focus on improving the virtual screening pipeline on the grid. This effort will take place in collaboration with both Korean and Vietnamese engineers within FKPPL and FVPPL LIAs.</p>
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