

# **INCT-INOFAR**

[www.inct-inofar.ccs.ufrj.br](http://www.inct-inofar.ccs.ufrj.br)



1st International symposium on challenges & new technologies in drug discovery & pharmaceutical production – Copacabana Mar Hotel, Rio de Janeiro, R.J., Brazil - 04-05 May, 2010

## **A Brazilian network for RD&I in pharmaceutical sciences**

# Summary

## ● Prologue

- ▀ Contemporary scientific research;
- ▀ Interdisciplinarity of drug discovery process;
- ▀ Pharmaceutical & therapeutic innovation;

## ● Conception & mission of INCT-INOFAR

- ▀ Innovation in drug discovery & design: the search of new lead-compounds as novel drug candidates (NCE's);
- ▀ Incremental innovation: new opportunities in synthetic generic drugs;
- ▀ *Portal dos Fármacos* : the observatory to divulgation & propagation of Pharmaceutical Sciences in Web;

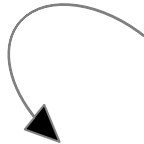




# The scientific research through the ages...



**Galileo, Newton, Darwin, & Einstein**



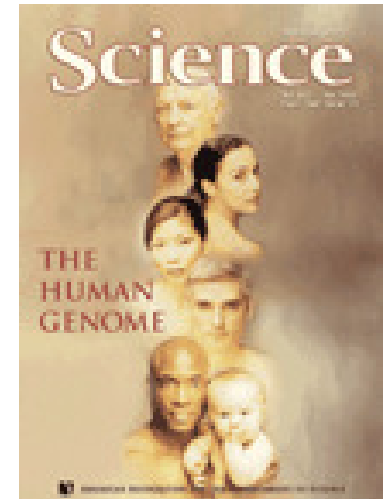
**The physical Crick & the biologist Watson**



**The human genome team**

## The Sequence of the Human Genome

J. Craig Venter, Mark D. Adams, Eugene W. Myers, Peter W. Li, Richard J. Mural, Granger G. Sutton, Hamilton O. Smith, Mark Yandell, Cheryl A. Evans, Robert A. Holt, Jeannine D. Gocayne, Peter Amanatides, Richard M. Ballew, Daniel H. Huson, Jennifer Russo Wortman, Qing Zhang, Chinnappa D. Kodira, Xiangqun H. Zheng, Lin Chen, Marian Skupski, Gangadharan Subramanian, Paul D. Thomas, Jinghui Zhang, George L. Gabor Miklos, Catherine Nelson, Samuel Broder, Andrew G. Clark, Joe Nadeau, Victor A. McKusick, Norton Zinder, Arnold J. Levine, Richard J. Roberts, Mel Simon, Carolyn Slayman, Michael Hunkapiller, Randall Bolanos, Arthur Delcher, Ian Dew, Daniel Fasulo, Michael Flanigan, Liliana Florea, Aaron Halpern, Sridhar Hannenhalli, Saul Kravitz, Samuel Levy, Clark Mobarry, Knut Reinert, Karin Remington, Jane Abu-Threideh, Ellen Beasley, Kendra Biddick, Vivien Bonazzi, Rhonda Brandon, Michele Cargill, Ishwar Chandramouliswaran, Rosane Charlab, Kabir Chaturvedi, Zuoming Deng, Valentina Di Francesco, Patrick Dunn, Karen Eilbeck, Carlos Evangelista, Andrei E. Gabrielian, Weiniu Gan, Wangmao Ge, Fangcheng Gong, Zhiping Gu, Ping Guan, Thomas J. Heiman, Maureen E. Higgins, Rui-Ru Ji, Zhaoxi Ke, Karen A. Ketchum, Zhongwu Lai, Yiding Lei, Zhenya Li, Jiayin Li, Yong Liang, Xiaoying Lin, Fu Lu, Gennady V. Merkulov, Natalia Milshina, Helen M. Moore, Ashwinikumar K Naik, Vaibhav A. Narayan, Beena Neelam, Deborah Nusskern, Douglas B. Rusch, Steven Salzberg, Wei Shao, Bixiong Shue, Jingtao Sun, Zhen Yuan Wang, Aihui Wang, Xin Wang, Jian Wang, Ming-Hui Wei, Ron Wides, Chunlin Xiao, Chunhua Yan, Alison Yao, Jane Ye, Ming Zhan, Weiqing Zhang, Hongyu Zhang, Qi Zhao, Liansheng Zheng, Fei Zhong, Wenyan Zhong, Shiaoping C. Zhu, Shaying Zhao, Dennis Gilbert, Suzanna Baumhueter, Gene Spier, Christine Carter, Anibal Cravchik, Trevor Woodage, Feroze Ali, Huijin An, Aderonke Awe, Danita Baldwin, Holly Baden, Mary Barnstead, Ian Barrow, Karen Beeson, Dana Busam, Amy Carver, Angela Center, Ming Lai Cheng, Liz Curry, Steve Danaher, Lionel Davenport, Raymond Desilets, Susanne Dietz, Kristina Dodson, Lisa Doup, Steven Ferriera, Neha Garg, Andres Gluecksmann, Brit Hart, Jason Haynes, Charles Haynes, Cheryl Heiner, Suzanne Hladun, Damon Hostin, Jarrett Houck, Timothy Howland, Chinyere Ibegwam, Jeffery Johnson, Francis Kalush, Lesley Kline, Shashi Koduru, Amy Love, Felecia Mann, David May, Steven McCawley, Tina McIntosh, Ivy McMullen, Mee Moy, Linda Moy, Brian Murphy, Keith Nelson, Cynthia Pfannkoch, Eric Pratts, Vinita Puri, Hina Qureshi, Matthew Reardon, Robert Rodriguez, Yu-Hui Rogers, Deanna Romblad, Bob Ruhfel, Richard Scott, Cynthia Sitter, Michelle Smallwood, Erin Stewart, Renee Strong, Ellen Suh, Reginald Thomas, Ni Ni Tint, Sukyee Tse, Claire Vech, Gary Wang, Jeremy Wetter, Sherita Williams, Monica Williams, Sandra Windsor, Emily Winn-Deen, Keriellen Wolfe, Jayshree Zaveri, Karena Zaveri, Josep F. Abril, Roderic Guigó, Michael J. Campbell, Kimmen V. Sjolander, Brian Karlak, Anish Kejariwal, Huaiyu Mi, Betty Lazareva, Thomas Hatton, Apurva Narechania, Karen Diemer, Anushya Muruganujan, Nan Guo, Shinji Sato, Vineet Bafna, Sorin Istrail, Ross Lippert, Russell Schwartz, Brian Walenz, Shibu Yooseph, David Allen, Anand Basu, James Baxendale, Louis Blick, Marcelo Caminha, John Carnes-Stine, Parris Caulk, Yen-Hui Chiang, My Coyne, Carl Dahlke, Anne Deslattes Mays, Maria Dombroski, Michael Donnelly, Dale Ely, Shiva Esparham, Carl Fosler, Harold Gire, Stephen Glanowski, Kenneth Glasser, Anna Glodek, Mark Gorokhov, Ken Graham, Barry Gropman, Michael Harris, Jeremy Heil, Scott Henderson, Jeffrey Hoover, Donald Jennings, Catherine Jordan, James Jordan, John Kasha, Leonid Kagan, Cheryl Kraft, Alexander Levitsky, Mark Lewis, Xiangjun Liu, John Lopez, Daniel Ma, William Majoros, Joe McDaniel, Sean Murphy, Matthew Newman, Trung Nguyen, Ngoc Nguyen, Marc Nodell, Sue Pan, Jim Peck, Marshall Peterson, William Rowe, Robert Sanders, John Scott, Michael Simpson, Thomas Smith, Arlan Sprague, Timothy Stockwell, Russell Turner, Eli Venter, Mei Wang, Meiyuan Wen, David Wu, Mitchell Wu, Ashley Xia, Ali Zandieh, and Xiaohong Zhu



*Science* 2001 291, 1304-1351 [DOI: 10.1126/science.1058040]





NEWS FEATURE

NATURE | Vol 455 | 9 October 2008

## What makes a successful team?

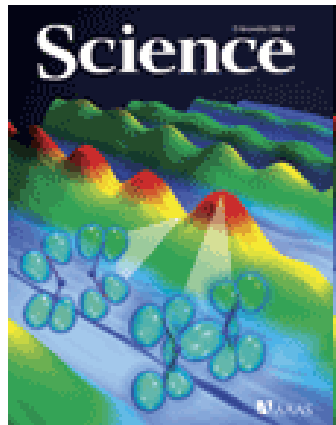


What makes a successful team? **John Whitfield** looks at research that uses massive online databases and network analysis to come up with some rules of thumb for productive collaborations.

# Multi-University Research Teams: Shifting Impact, Geography, and Stratification in Science



Benjamin F. Jones,<sup>1,2\*</sup> Stefan Wuchty,<sup>3\*</sup> Brian Uzzi<sup>1,3,4\*</sup>



SCIENCE VOL 322 21 NOVEMBER 2008 1259

<sup>1</sup>Kellogg School of Management, Northwestern University, Evanston, IL 60208, USA. <sup>2</sup>National Bureau of Economic Research, Cambridge, MA 02138, USA. <sup>3</sup>Northwestern Institute on Complexity (NICO), Northwestern University, Evanston, IL 60208, USA. <sup>4</sup>Haas School of Business, University of California at Berkeley, Berkeley, CA 94720, USA.



.....  
 "This paper demonstrates that teamwork in *science* increasingly spans university boundaries, a dramatic shift in knowledge production that generalizes across virtually all fields of *science*"

## Slide 6

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### EJB4

Para completude em sua atuação com plena formação de M&D,I a PG precisa interagir além de sua própria arena, sem ir de lado mas com decisão.

Eliezer J. Barreiro; 04/03/2010

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- ▶ **Interdisciplinarity of drug discovery process;**
- ▶ **Pharmaceutical & therapeutic innovation;**



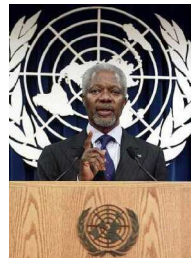
## ● Conception & mission of INCT-INO FAR

- ▶ **Innovation in drug discovery & design: the search of new lead-compounds as novel drug candidates (NCE's);**
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**"Science has contributed immensely to human progress and to the development of modern society.**

**The application of scientific knowledge continues to furnish powerful means for solving many of the challenges facing humanity...."**



**Kofi Annan**

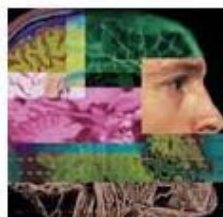
**U.N. – Secretary-General**

**A Challenge to the World's Scientists**



**Science**

*Science, 2003, 299, 1485*



# the Pharmaceutical Century

ACS PUBLICATION  
HIGH QUALITY. HIGH IMPACT

TEN DECADES OF DRUG DISCOVERY

[Analytical Chemistry](#) | [Chemical & Engineering News](#) | [Modern Drug Discovery](#)  
| [Today's Chemist at Work](#) | [E-Mail Us](#) | [Electronic Readers Service](#)

1800s to 1919

We live today in a world of drugs. Drugs for pain, drugs for disease, drugs for allergies, drugs for pleasure, and drugs for mental health. Drugs that have been rationally designed; drugs that have been synthesized in the factory or purified from nature. Drugs fermented and drugs engineered. Drugs that have been clinically tested. Effective. Safe.



zoom



"We live today in a world of **drugs**. Drugs for **pain**, drugs for **disease**, drugs for **allergies**, drugs for **pleasure**, and drugs for **mental health**. Drugs that have been **rationally designed**; drugs that **have been synthesized** or **purified from nature**. Drugs **fermented** and drugs **engineered**. Drugs that have been clinically tested. Effective. Safe."

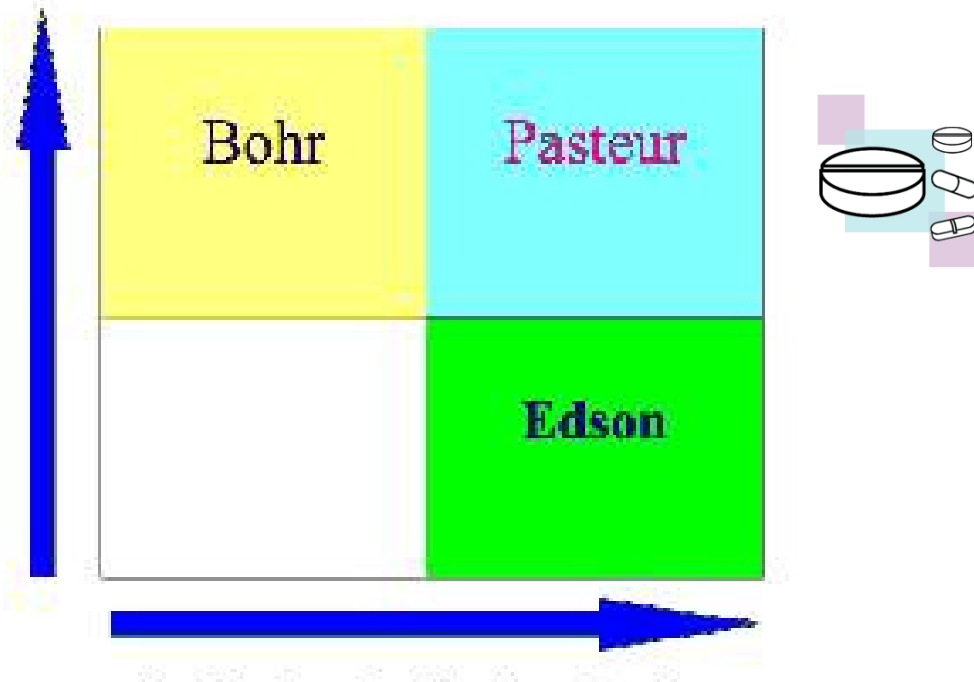
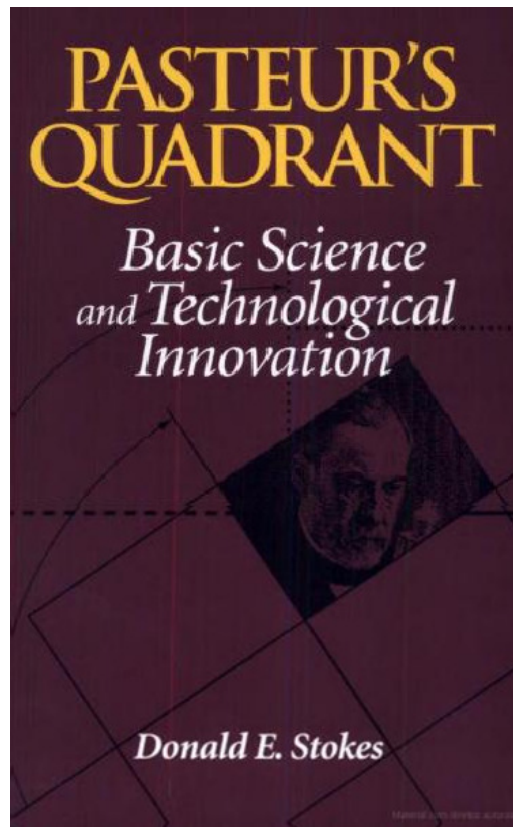
**Slide 9**

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**EJB7**

Eliezer J Barreiro; 02/05/2010

# The production of knowledge



D. E. Stokes; *Pasteur's Quadrant: Basic Science and Technological Innovation*, Book News, Inc., Portland, EUA, 1999.

M. Gibbons *et al.*, *The new production of knowledge: the dynamics of science & research in contemporary societies*, SAGE, London, 1994.

**Slide 10**

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**EJB6**

**The production of knowlegde**

Eliezer J Barreiro; 02/05/2010





# Nobel Prize, 1959

“for their discovery of the mechanisms in the biological synthesis of RNA and DNA”



“We have the paradox of the two cultures,

chemistry and biology,

growing further apart even as they discover more common ground...

Pharmaceutical chemistry was until recently the bastion of organic chemistry...

...in the search for alternative or superior drugs for the treatment of various diseases.”

Interdisciplinarity



Arthur Kornberg

Biochemistry 1987, 26, 6888-6891

**Slide 11**

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**EJB6**

Rio de Janeiro, 05 de março de 2010, Prof. Eliezer J. Barreiro, LASSBio, UFRJ.  
Eliezer J. Barreiro; 04/03/2010



**nature**

- MRI shows best for tumours
- Search to bedside and back
- Organizing for innovation
- New tactic for drug discovery

**TRANSLATIONAL RESEARCH**

# CROSSING THE VALLEY OF DEATH

A chasm has opened up between biomedical researchers and the patients who need their discoveries. **Declan Butler** asks how the ground shifted and whether the US National Institutes of Health can bridge the gap.

D. Butler, *Nature* 2008, 453, 840

**Slide 12**

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**EJB5**

**Nature 2008, 453, 840**

Eliezer J Barreiro; 02/05/2010

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# INCT-INO FAR

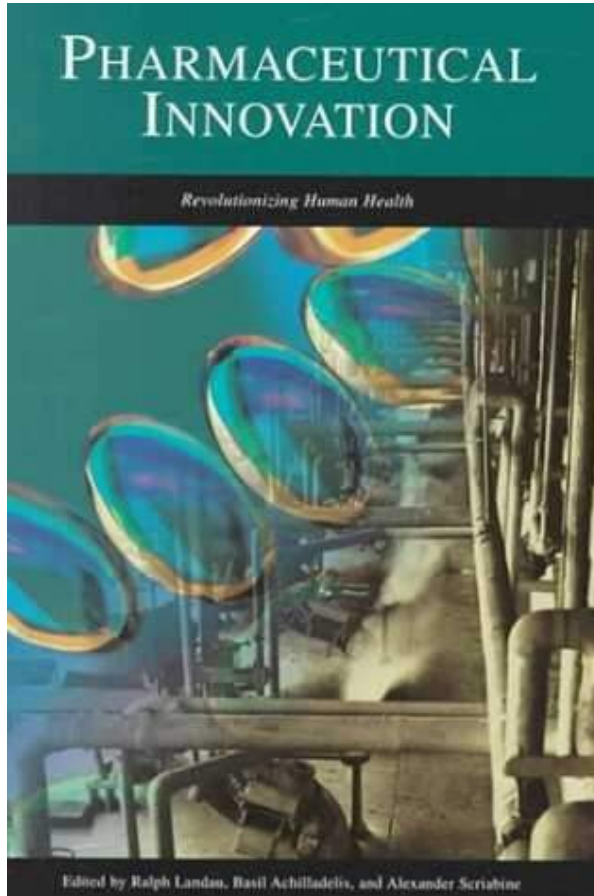
Technological innovation is a dynamic process  
perhaps the most dynamic of all  
industrial activities;



The dynamism of technological innovation  
dependent of the interaction  
of Science & Technology;



The technological innovation is the principal  
driving-force of pharmaceutical industry ;

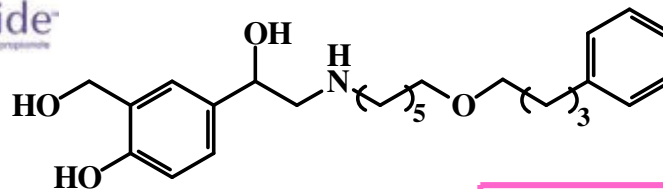
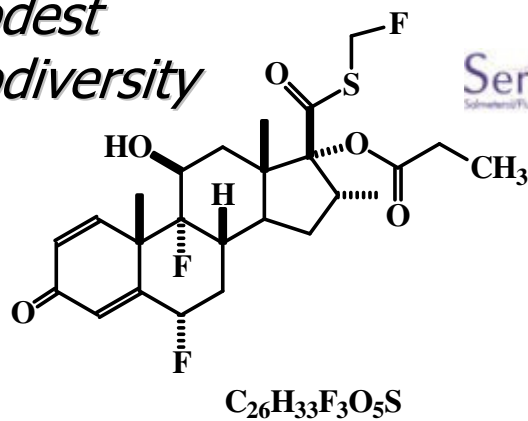


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The drug world market, in 2008: ca. US\$ 785 bi

# Top-5 drugs in world market (2009)\*

modest  
chemodiversity



Clopidogrel (BMS, 2011)

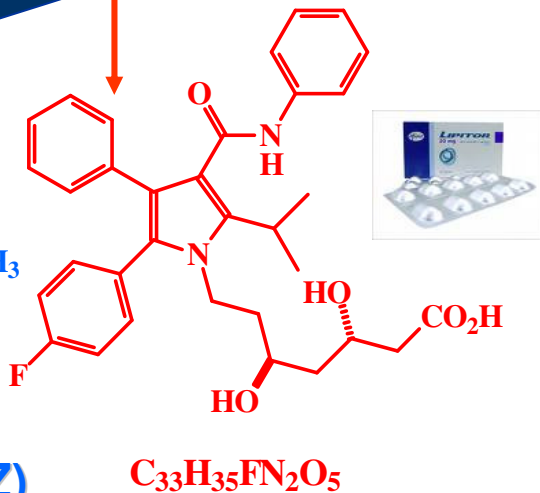
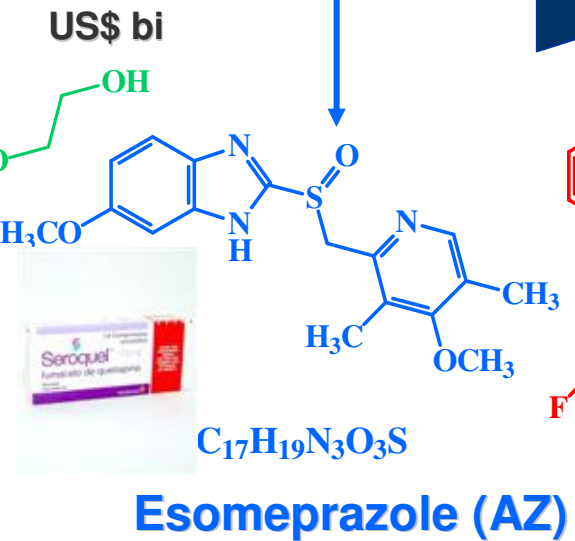
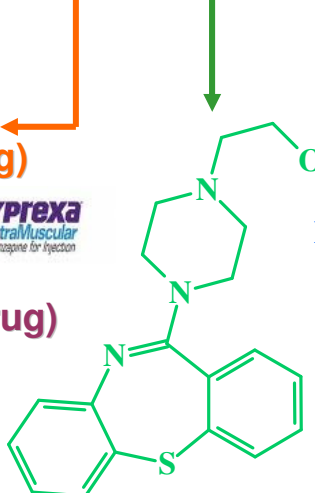


**Etanercept**  
(Enbrel<sup>®</sup>, biotech-drug)

**Olanzapine**  
**Infliximab**  
(Remicade<sup>®</sup>, biotech-drug)

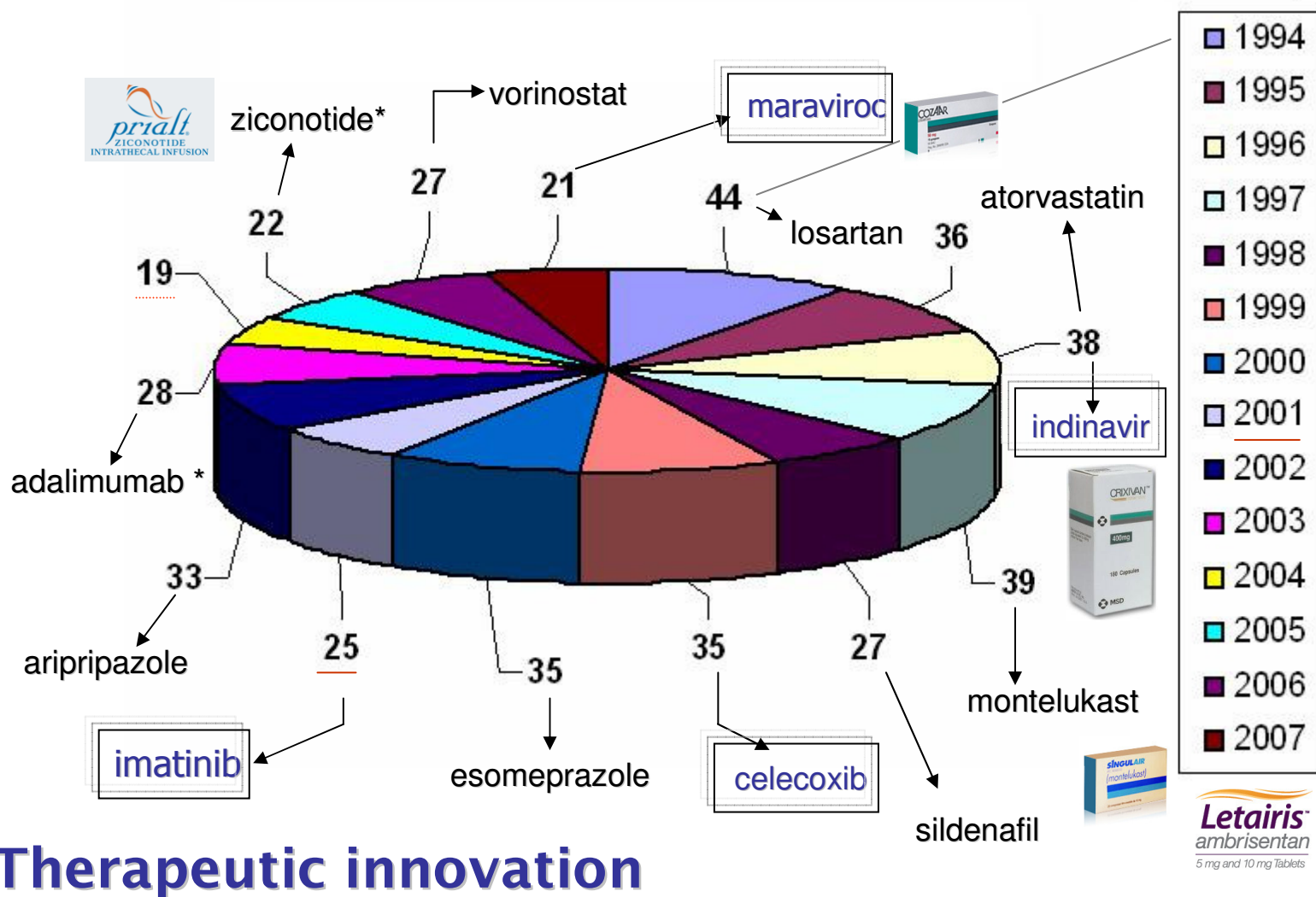
**Montelukast**  
(Singulair<sup>®</sup>, Merck)

**Rosuvastatin**  
(Crestor<sup>®</sup>, AZ)  
**68,1**  
(8,2%)



\* SJ Ainsworth, C&EN 2009 (07/12) 13-21

# New drugs launched between 1994 to 2007

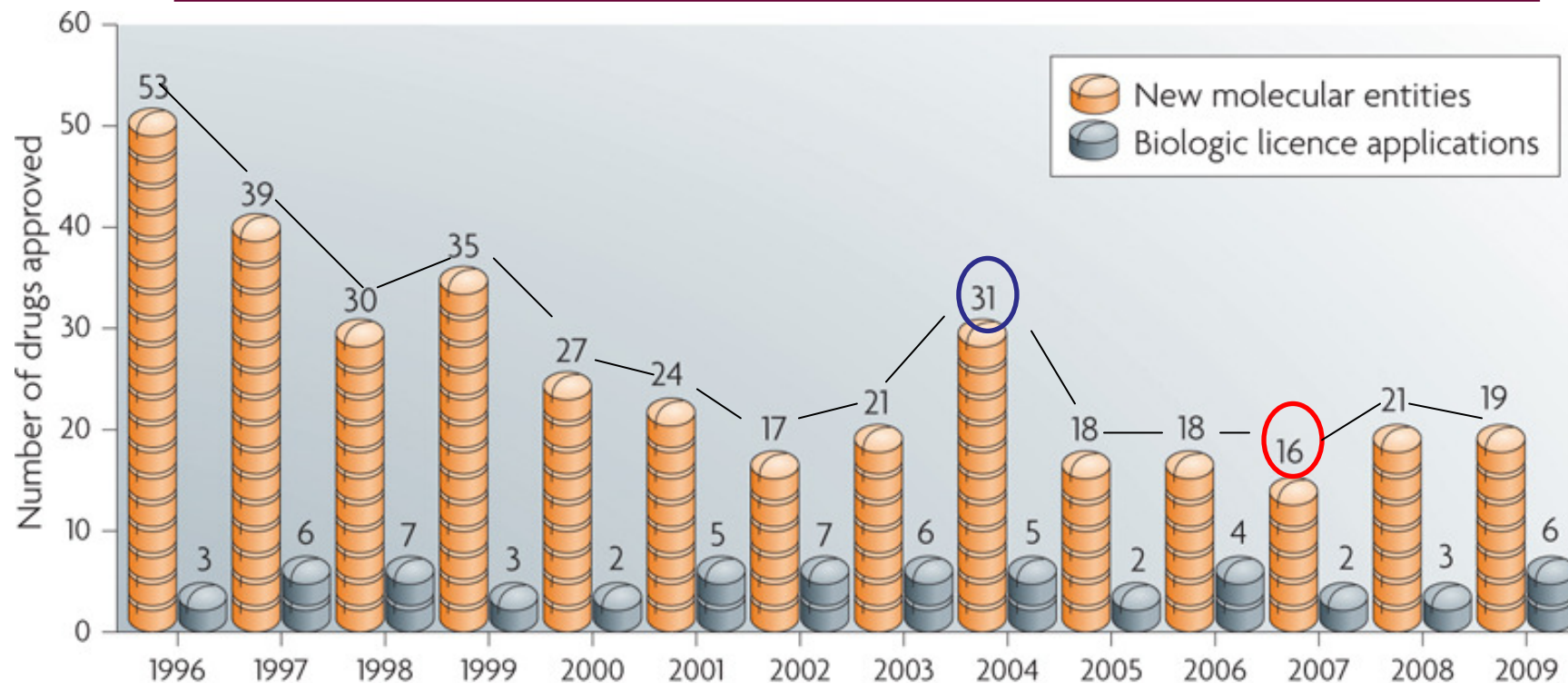


## Therapeutic innovation

ca. 30 new drugs are launched each year



# New molecular entities...



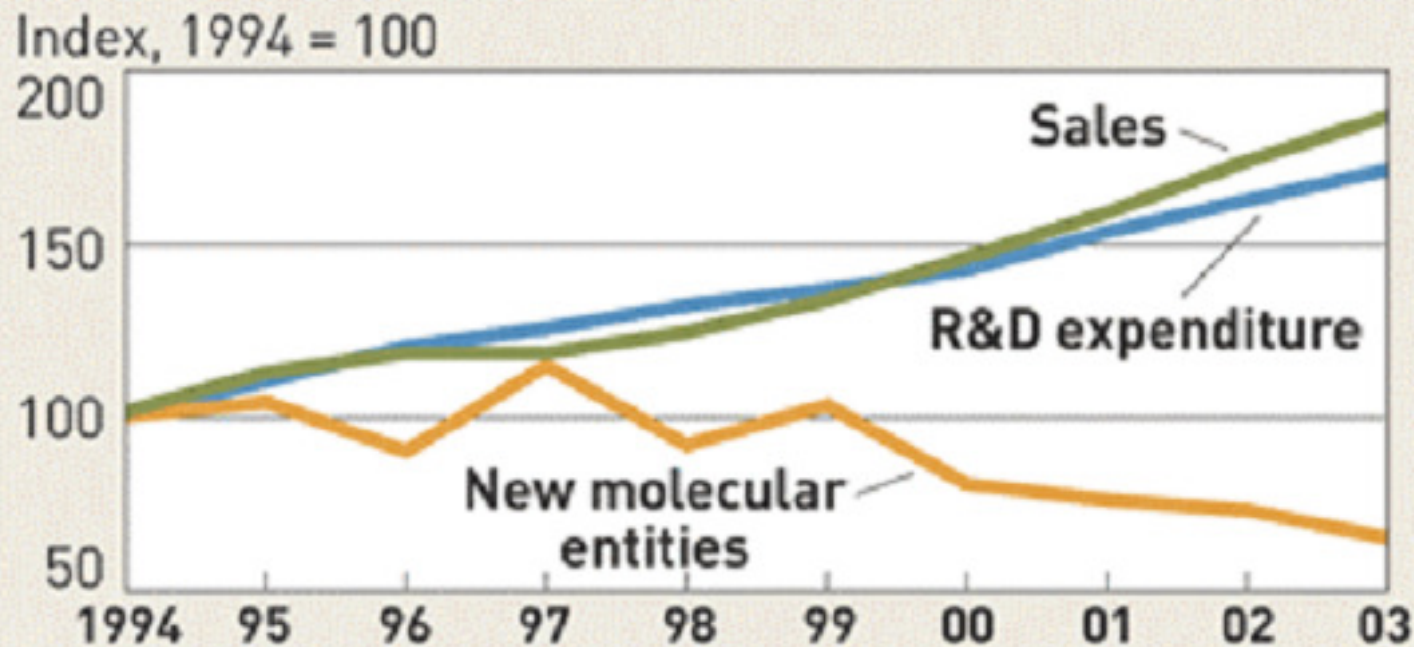
Nature Reviews | Drug Discovery

B. Hughes, 2009 FDA drug approvals, *Nature Rev. Drug Discov.* **2010**, 9, 89-92 [doi:10.1038/nrd3101](https://doi.org/10.1038/nrd3101)



# The creativity crisis in Bigpharma

## DIMINISHING RETURNS



SOURCES: Center for Medicines Research International, IMS Health

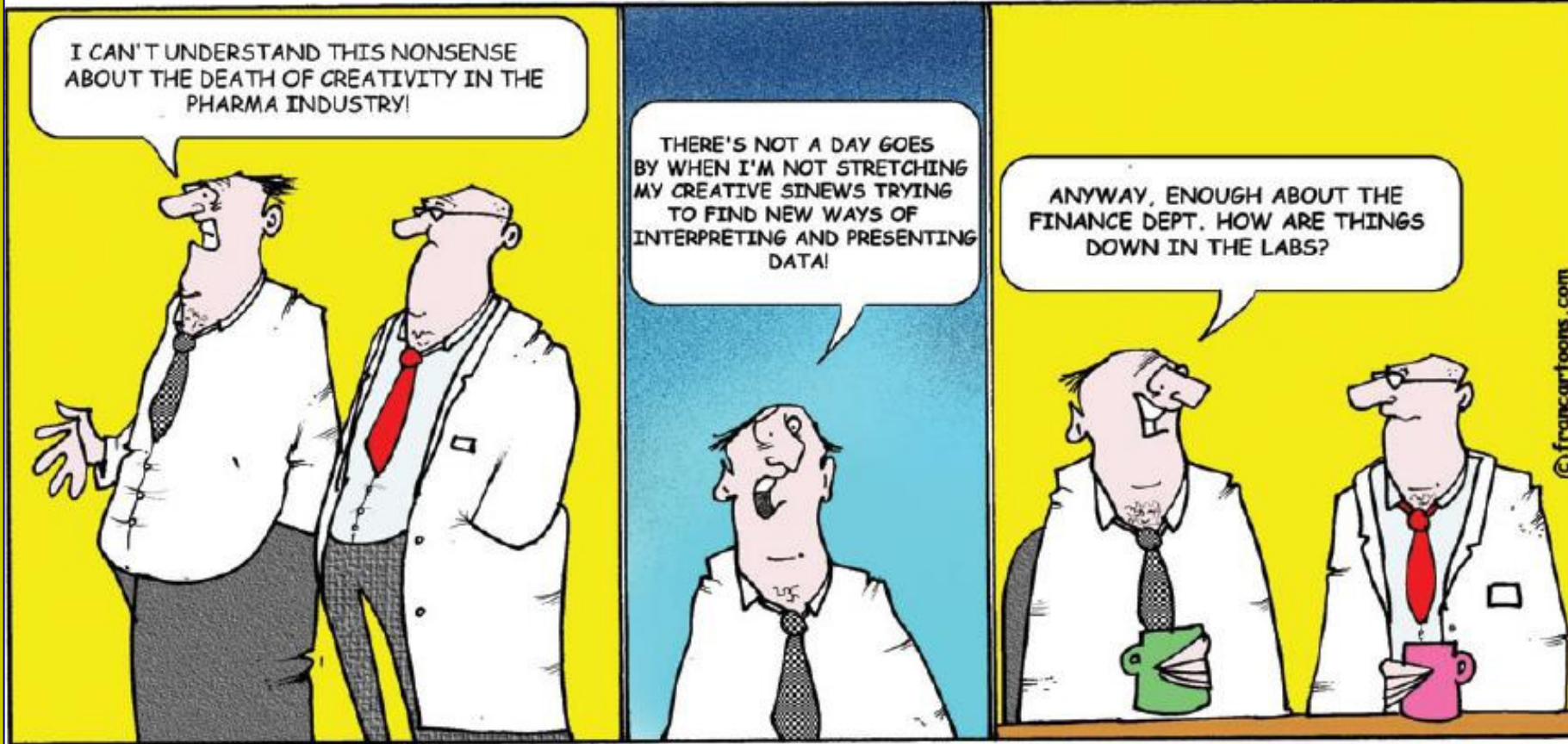


C&EN 2005, Feb. 28, vol. 83, pp. 29



## The blockbuster-drug syndrome

# About the creativity crisis...



File supplied with permission of © PJB Publications 2003

[www.scripmag.com](http://www.scripmag.com)

Scrip Magazine October 2003



# Discoveries & invention

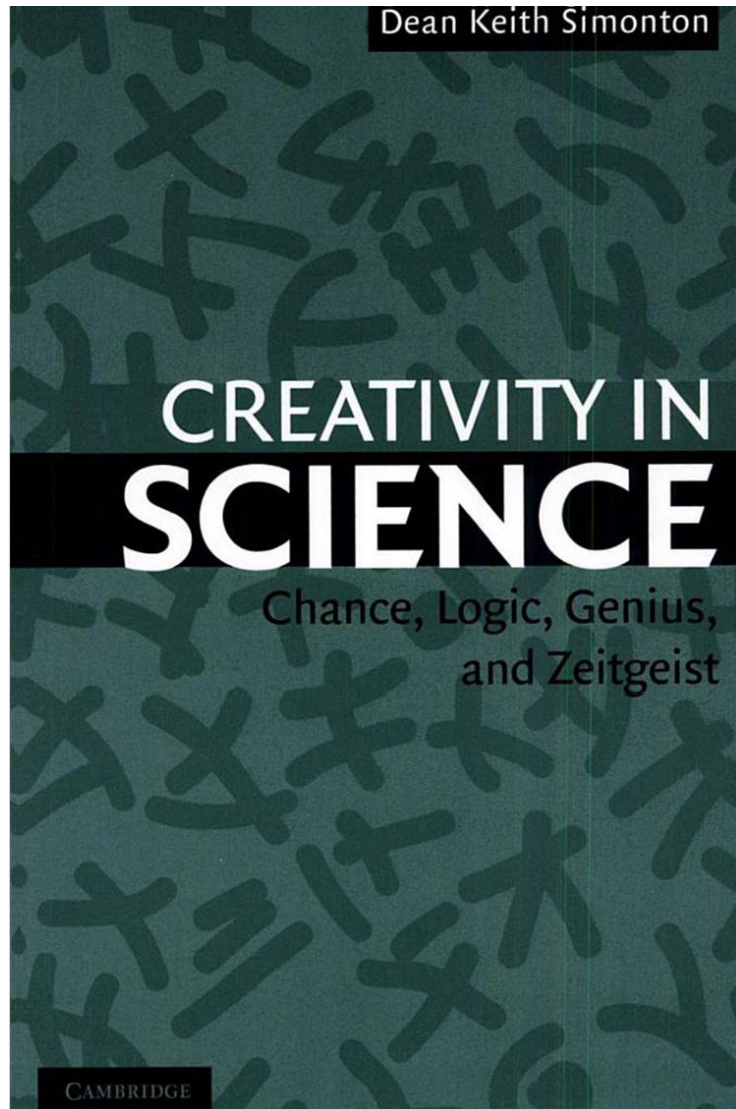


*zeitgeist* or "spirit of the times"

"discoveries and inventions become virtually inevitable (1) as prerequisite kinds of knowledge accumulate in man's cultural store; (2) as the attention of a sufficient number of investigators is focused on a problem – by emerging social needs, or by developments internal to the particular science, or by both"

Robert K. Merton (1961)

The role of genius in scientific advance. *New Scientist*, 12, 306-308



Drug Discovery Today • Volume 14, Numbers 1/2 • January 2009

REVIEWS



Reviews • POST SCREEN

## Drug discovery: new models for industry–academic partnerships

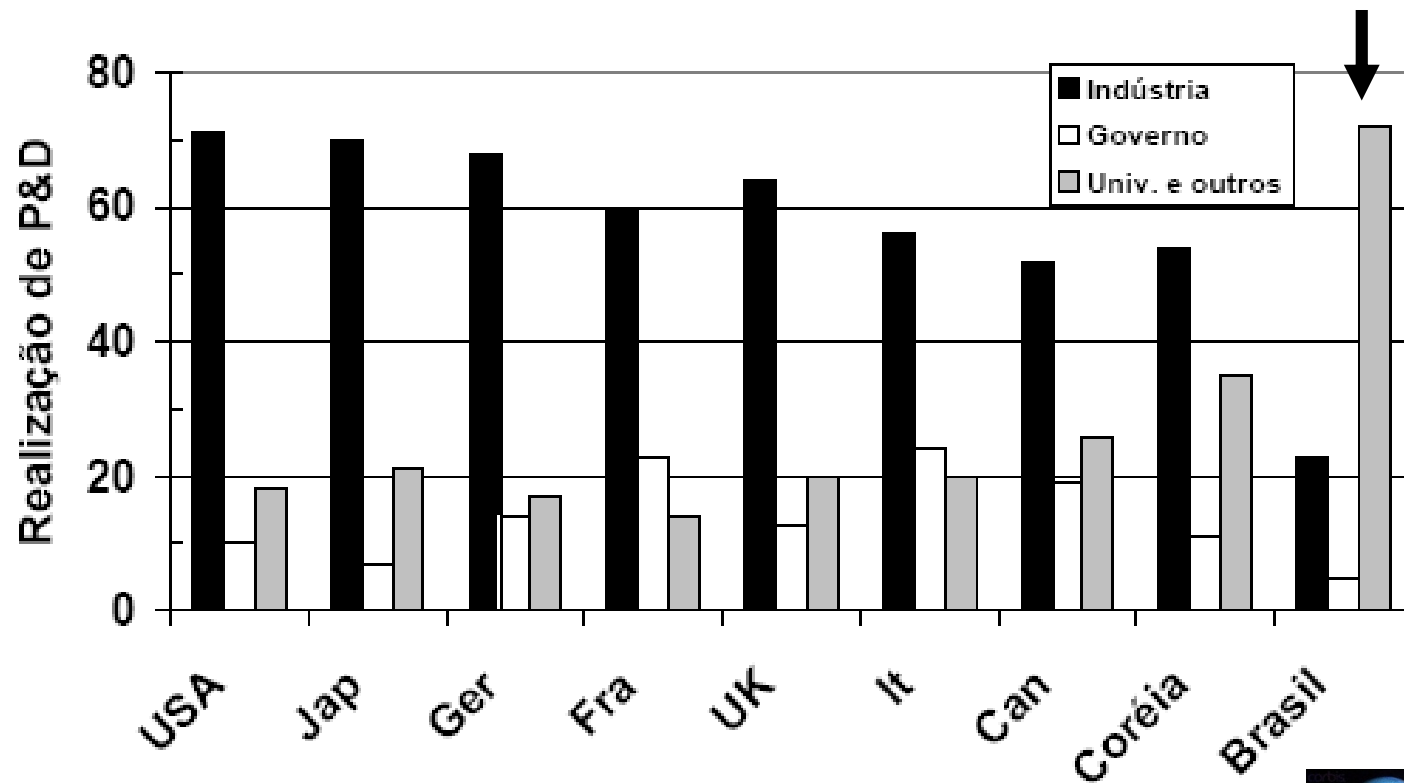
**Cathy J. Tralau-Stewart, Colin A. Wyatt, Dominique E. Kleyn and Alex Ayad**

Drug Discovery Centre and Business Development, Imperial College London SW7 2AZ, UK

The re-focusing of pharmaceutical industry research away from early discovery activities is stimulating the development of novel models of drug discovery, notably involving academia as a 'front end'. In this article the authors explore the drivers of change, the role of new entrants (universities with specialised core facilities) and novel partnership models. If they are to be sustainable and deliver, these new models must be flexible and properly funded by industry or public funding, rewarding all partners for contributions. The introduction of an industry-like process and experienced management teams signals a revolution in discovery that benefits society by improving the value gained from publicly funded research.



# The scientific mainpower



Adopted from C. H. Brito Cruz & C. A. Pacheco, "Conhecimento & Inovação: Desafios do Brasil no Século XXI", em [www.inovacao.unicamp.br/report/intc-pacheco-brito.pdf](http://www.inovacao.unicamp.br/report/intc-pacheco-brito.pdf) (2/01/2009)





# Summary

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- ▶ ***Portal dos Fármacos* : the observatory to divulgation & propagation of Pharmaceutical Sciences in Web;**



**inct**  
institutos nacionais  
de ciência e tecnologia



- Apresentação
- Institutos
- Notícias
- Contato

Um dos maiores  
programas  
de Ciência  
e Tecnologia  
do Brasil



### Notícias

[Pesquisadores do IICT de Astrofísica publicam 100 artigos em oito meses](#)

[UFMG faz pesquisa pioneira para tratamento da dengue](#)

[IICT de Fixação Biológica de Nitrogênio promove simpósio internacional em setembro](#)

### Instituto em Destaque

[Instituto Nacional de Ciência e Tecnologia de Nanodispositivos Semicondutores](#)

O tema do Instituto engloba o estudo e o desenvolvimento de nanoestruturas semicondutoras



Program budget: R\$ 608 million (392 FG + 216 RSF's)



Saturday, 01 de May de 2010



Project CNPq 573.564/2008-6

Home

INCT-INOFAR

Team

Scientific adviser board  
(SAB)

Research groups

Research people

Useful articles

Publications

Meetings

Videos

## The Mission

- Organize the Brazilian scientific capacity in an effective drug discovery network;
- Support multi-institutional research projects in drug discovery & design;
- Contribute to Brazilian radical & incremental innovation in new & generic drugs;
- Studies in total synthesis of generic drugs & advanced synthetic intermediates and starting materials;
- Contribute to continuous high qualification of students in medicinal chemistry & pharmacology;



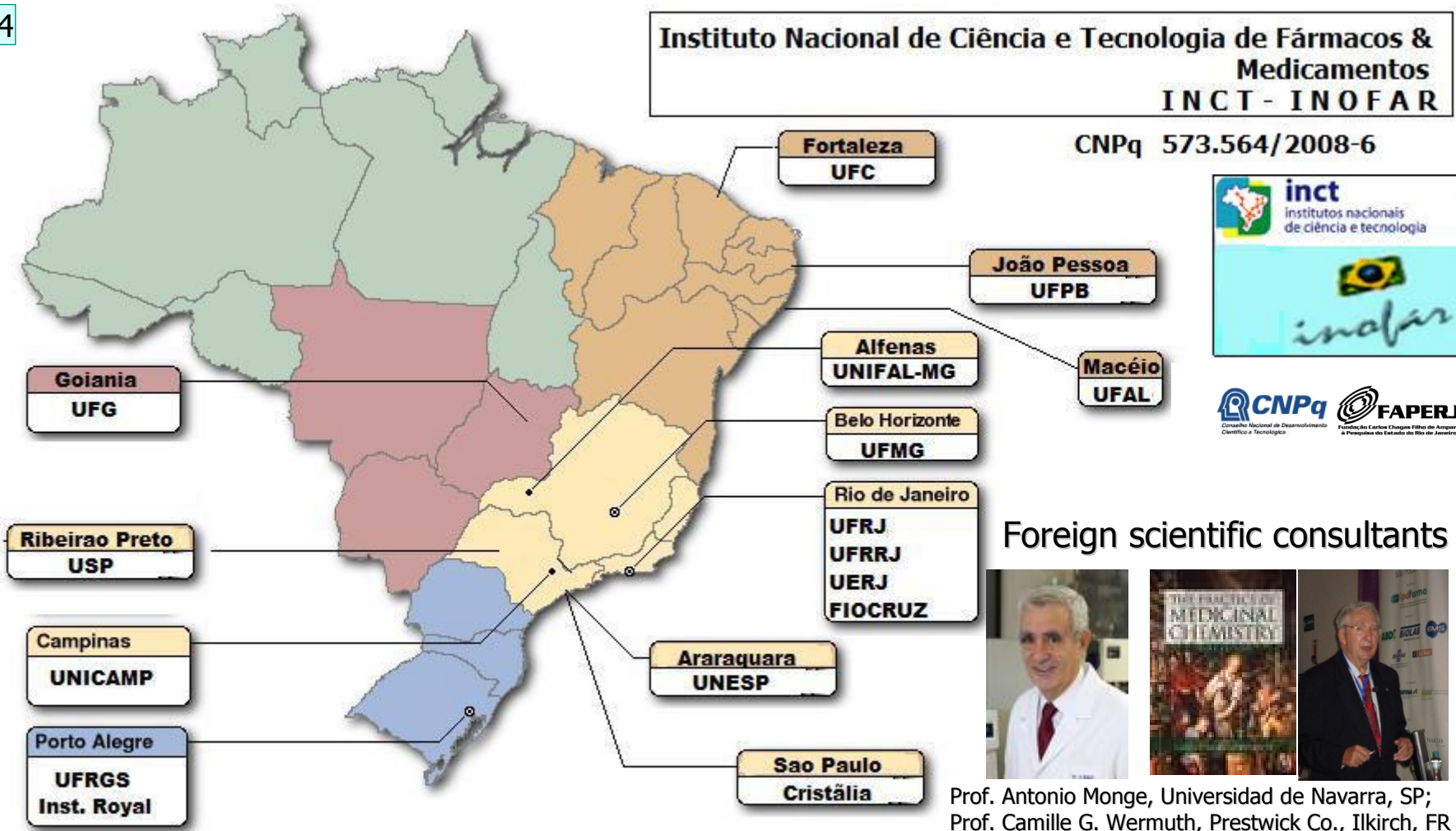
# Governance committee

**2nd Coordinator: Prof. Fernando Q. Cunha,  
School of Medicine, Un. Sao Paulo-RP, SP;**

**Members: Prof. Vanderlan S. Bolzani,  
Institute of Chemistry, UNESP, Araraquara,  
SP; Prof. Heloisa O. Beraldo, Institute  
of Chemistry, UFMG, MG; Prof. Angelo C.  
Pinto, Institute of Chemistry, UFRJ, RJ;  
Prof. Luis Carlos Dias, Institute of Chemistry,  
UNICAMP, SP.**







Prof. Antonio Monge, Universidad de Navarra, SP;  
Prof. Camille G. Wermuth, Prestwick Co., Ilkirch, FR

**Research teams (27):** UFC: Manoel Odorico de Moraes Filho (FM); Ronaldo de Albuquerque Ribeiro (FM); UFPB: Margareth de Fátima Formiga Melo Diniz (LTF); UFAL: João Xavier Jr. (DF); Magna Suzana Alexandre Moreira (PPGCB); UNIFAL: Claudio Viegas Jr. (IQ); UFMG: Heloisa de Oliveira Beraldo (DQ); UFRJ: Adelaide Maria de Souza Antunes (EQ); Angelo da Cunha Pinto; (IQ); Carlos Alberto Manssour Fraga (LASSBio); Francisco Radler de Aquino Neto (IQ); François Germain Noël (ICB); Gisele Zapata Sudo (ICB); Lidia Moreira Lima (LASSBio); Patrícia Rieken Macedo Rocco (IBCCF); Roberto Takashi Sudo (ICB); UFRRJ: Carlos Maurício Rebello de Santana (IQ); UERJ: Theresa Christina Barja-Fidalgo (IB); FIOCRUZ-RJ: Francisco José R. Paumgarten; Marco Aurélio Martins; Patrícia Silva; UNESP: Vanderlan da Silva Bolzani (IQ); CRISTÁLIA: Roberto Debon Moreira (Cristália Prod. Farmacêuticos Ltda); UFG: Valéria de Oliveira (FF); Ricardo Menegatti (FF); USP: Fernando Queiroz Cunha (FM-RP); UNICAMP: Luiz Carlos Dias (IQ); UFRGS: Stela Maris Kuze Rates (FF); João Antonio Pegas Henriques (Inst. Royal.).





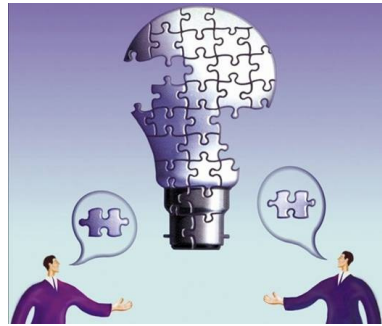


# innovation

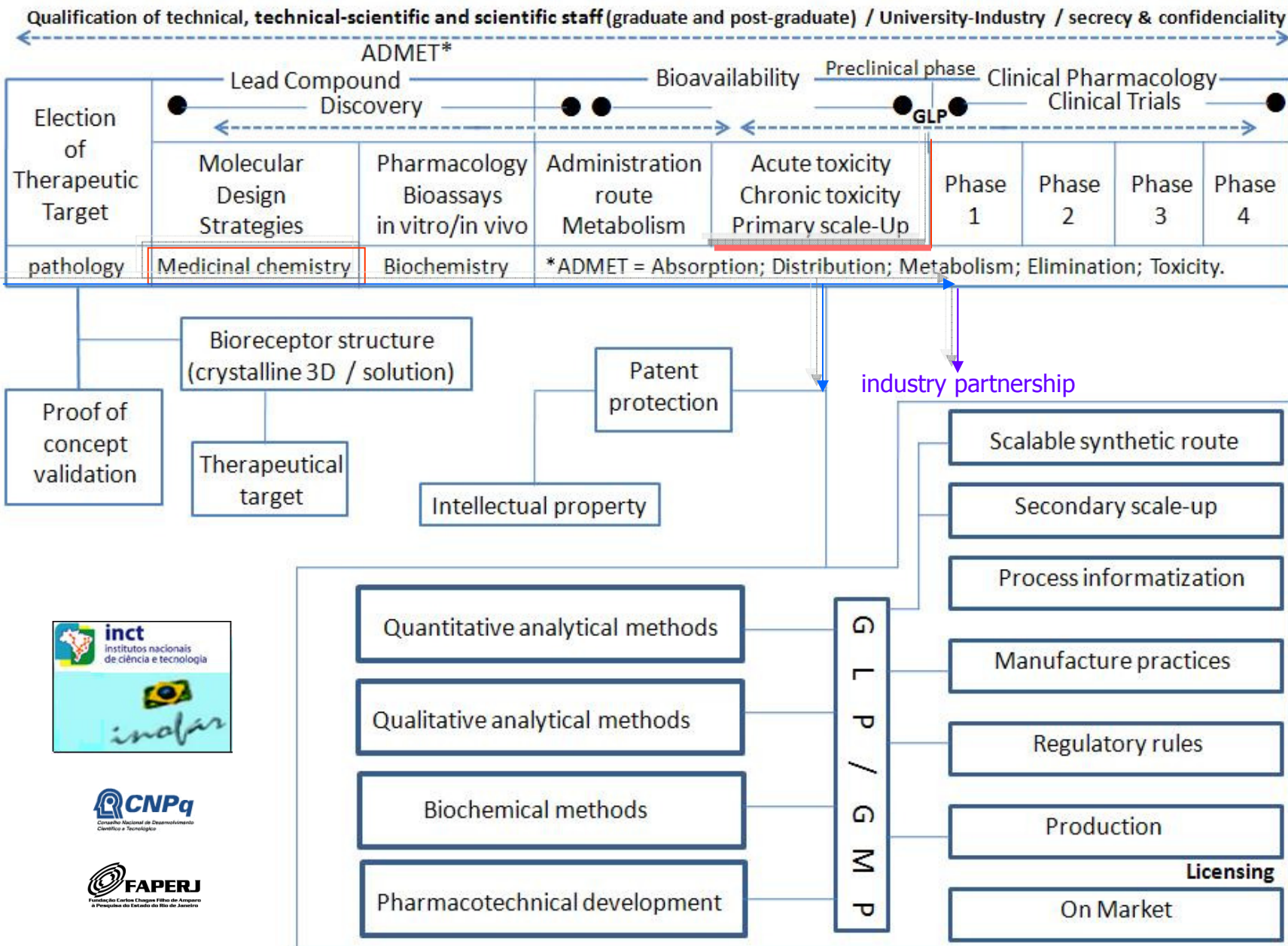
Why ?

Can we?

How ?



**The drug discovery & design process**



**Slide 30**

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**EJB3**

The innovation chain of DD process

Eliezer J Barreiro; 02/05/2010



# New lead-compound for asthma

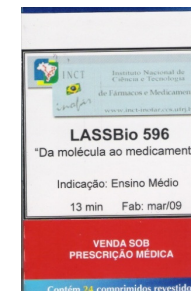


## 2010

### LASSBio-596



Pre-clinic studies



PIBR 0208767-7 - 08/11/2002  
PIBR 0401660-2 - 27/04/2004

## C O P D

L. M. Lima *et al.*, *Bioorg. Med. Chem. Lett.*, **12**, 1533, 3067 (2002) ; P. R. M. Rocco *et al.*, *Eur. Respir. J.*, **22**, 20 (2003) ; L. M. Lima *et al.*, *Antii-nflamatory & Anti-allergy Agents in Medicinal Chemistry*, **3**, 9 (2004) ; J. V. Bevilaqua *et al.*, *Applied Biochem. Biotechnol.*, **121**, 117 (2005); M. S. Alexandre-Moreira *et al.*, *International Immunopharmacology*, **5**, 485 (2005); H. S. Campos *et al.*, *Braz. J. Med. Biol. Res.*, **39**, 283 (2006) ; L.M. Lima *et al.*, *Anti-inflammatory & Anti-allergy Agents in Medicinal Chemistry*, **5**, 79 (2006)

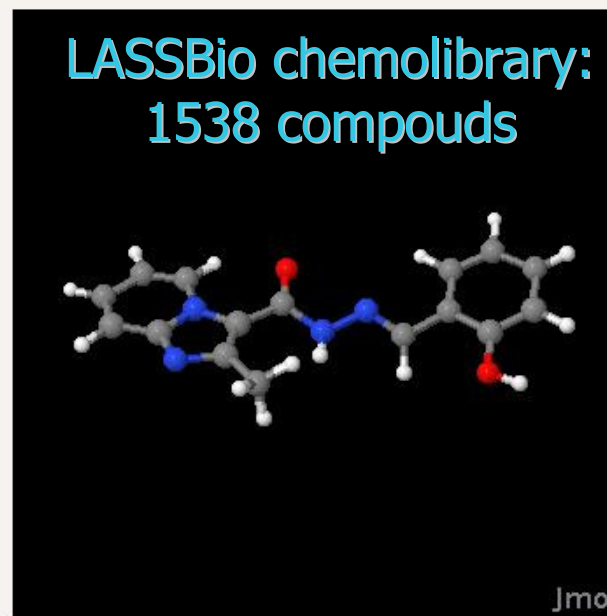


# New lead-compounds for treatment of neglected tropical diseases



Molecular Form:	C16H14N4O2
IUPAC Nomenclature :	???????? ? ? ? ?
Fantasy Name :	Teste
Number of Quiral Centers :	0
Number of H-Bond Donors	2
Number of H-Bond Acceptors	4
Number of Free Bonds	4
Log P	2.0
Fusion Point	100
Functional Group:	Acylhydrazone

**LASSBio**  
Laboratório de Avaliação e Síntese de Substâncias Bioativas



Wireframe Ball-and-Stick Space Fill  
To return for initial orientation  
Rotacionar

UdelaR, UBA, ULP



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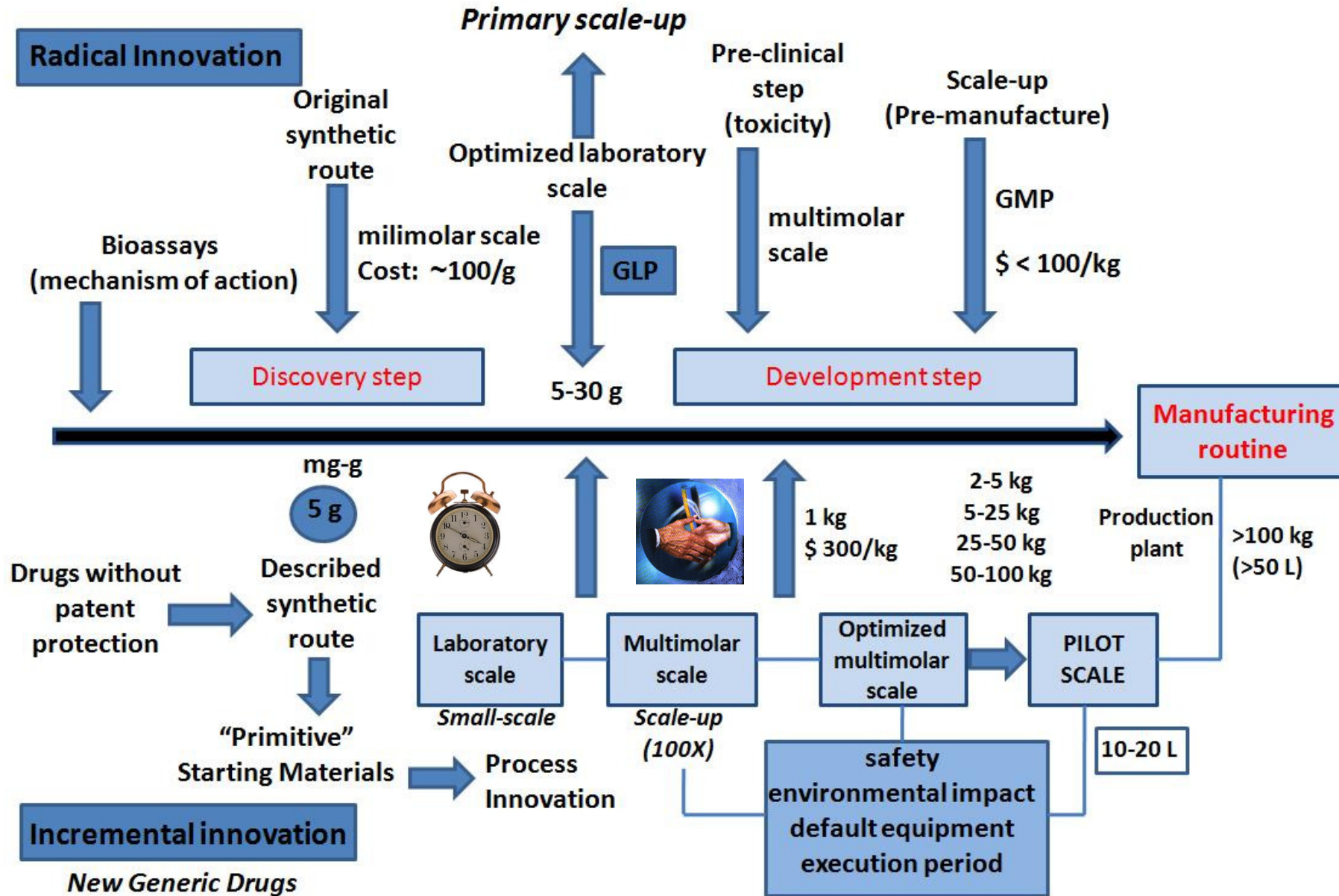


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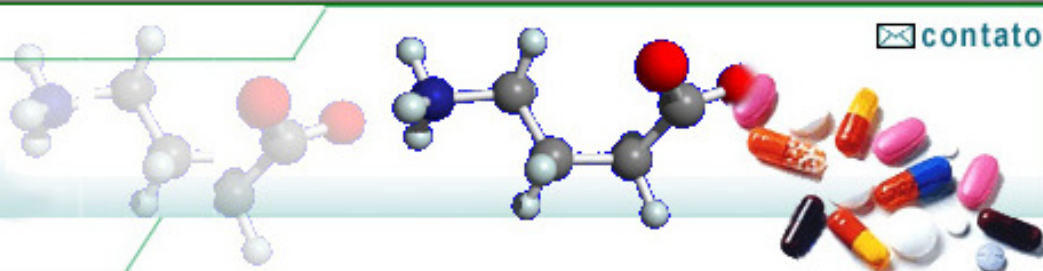
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- ▶ ***Portal dos Fármacos* : the observatory to divulgation & propagation of Pharmaceutical Sciences in Web;**



# Incremental *Innovation*







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*Este Portal é o observatório do Instituto Nacional de Ciência e Tecnol*

Domingo, 27 de Setembro de 2009

## The observatory to divulgation of Pharmaceutical Sciences in Web

Parceiros:



A construção deste Portal foi possível graças ao apoio da FAPERJ através de seu programa de - *Edital FAPERJ 04/2007*.

**Conheça os projetos contemplados**

### AGENDA

XVI  
Escola de Verão em  
Química Farmacêutica



Inscrições:  
01/set. a 30/nov./2009

25 a 29 de janeiro de 2010

Inscrições: de 01 de  
setembro a  
30 de novembro de 2009

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