

# Ligand Efficiency Indices for Drug Discovery

## Ligand Efficiency Indices for Drug Discovery Towards an Atlas-Guided Paradigm

**Celerino Abad-Zapatero**, PhD, Adjunct Professor to the Graduate Faculty, Center for Pharmaceutical Biotechnology, University of Illinois at Chicago, Chicago, IL



*A guided 'mini-atlas' of the content of Chemico-Biological Space with snapshots, postcards and views of the chemistry and biology related to pharmacology, medicine and drug-discovery*

### DESCRIPTION

The purpose of *Ligand Efficiency Indices for Drug Discovery: Towards an Atlas-Guided Paradigm* is to introduce in a concise and self-contained form the concepts, ideas, applications and some examples of efficiency-driven drug discovery to the biomedical community at large. Available in full color, this book emphasizes the use of a graphical representation and objective numerical methods to drive drug discovery more rapidly and effectively. It presents the definition of Ligand Efficiency Indices (LEIs) and the corresponding efficiency planes within an atlas-like environment to provide a robust graphical and numerical framework for medicinal chemists, students and those pharmaceutical scientists who are active in drug discovery.

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#### Prologue

#### Introduction

#### PART 1: The Elements: Data, Variables, Concept and the Server

A numerical framework and a tool are introduced to represent the content of structure-activity databases and in doing so allows a mapping of chemico-biological space in efficiency planes.

#### PART 2: Conceptual Applications of the AtlasCBS: A New Paradigm

The algebraic framework introduced previously is used to illustrate a new graphical depiction of medicinal-chemistry data and its drug discovery applications.

#### PART 3: Exploring CBS: Practical Examples Using the AtlasCBS Server

A few snapshots, vistas and postcards of the resulting atlas-like representation of chemico-biological space are presented to illustrate its power and to pique the curiosity of the future user.

#### References

#### Epilogue

#### Appendix A

#### Appendix B

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