“INTEGRATED CONCEPT”
for
INSILICO SCREENING & DRUG DESIGN

ACTIVITY, ADME, TOXICITY, PROPERTY ANALYSIS AND PREDICTION

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In Silico Data
Miracles by the KY-methods

1 *"Integrated" concept*

2 *Application pattern of integrated concept*
"Integrated in silico screening"
"Integrated in silico drug design"

3 *Multivariate and pattern recognition*
From pattern analysis to scientific analysis

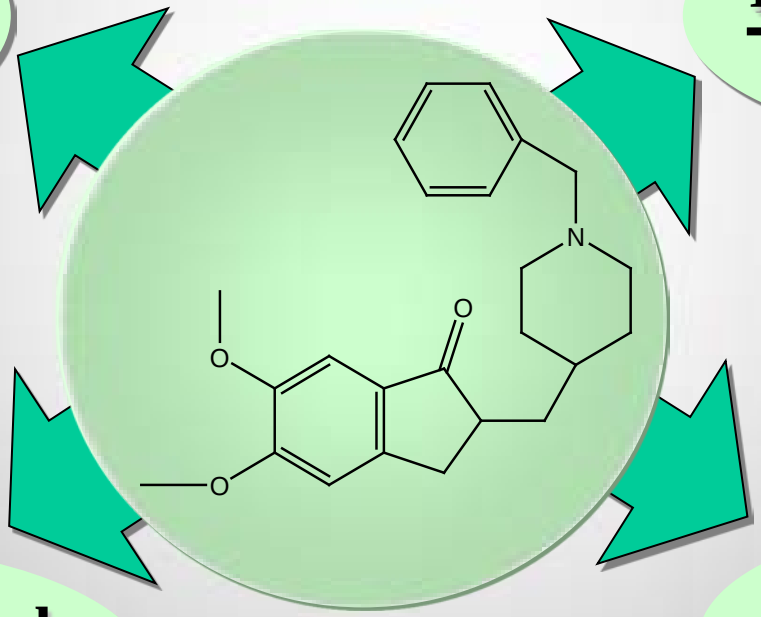
High classification and prediction rate
by
KY-methods and Tailor made modeling

"*Integrated*" concept

Drug properties and compound structure

ADME properties

Pharmacological activity



Physico chemical properties

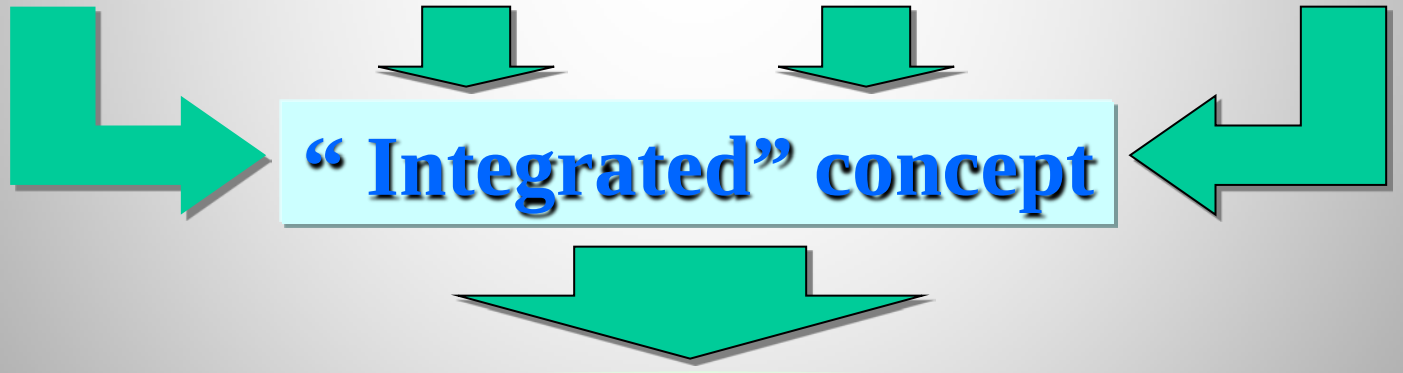
Toxicity

“*Integrated*” concept

“Integrated” concept for drug development

Activity + ADME + Toxicity + Property

All drug properties shall be considered at the same time



“ Integrated” in silico screening & drug design

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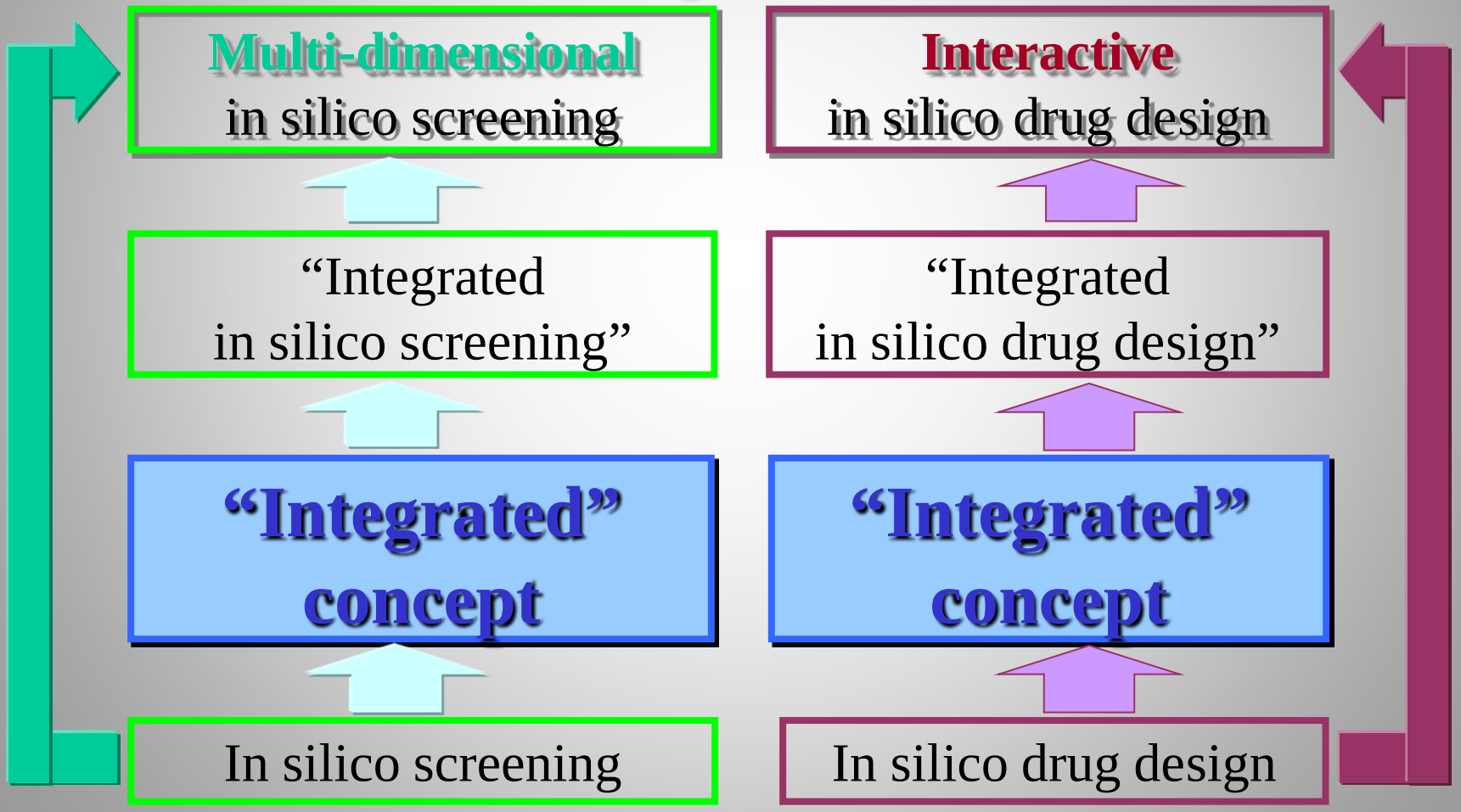
Application pattern of integrated concept

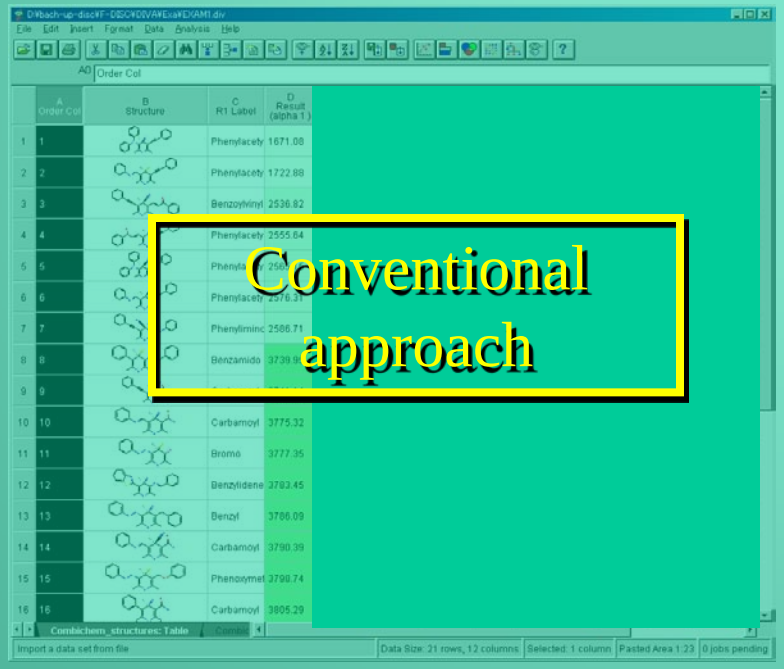
Two application style of "Integrated"



"Integrated" in silico screening

One-dimensional screening

one activity／compound



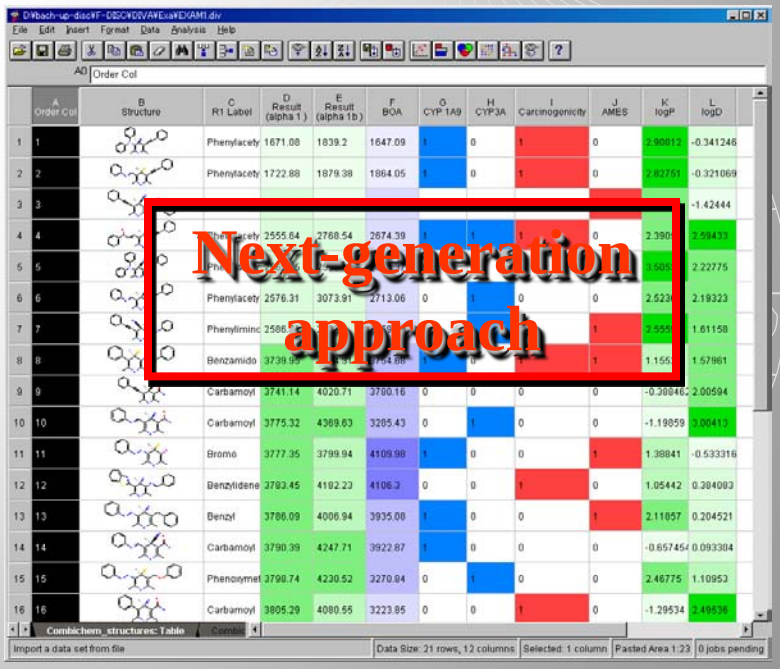
Conventional approach

Multi-dimensional screening

multiple activities

- **" ADME**
- **" toxicities**
- **" properties**

／ compound



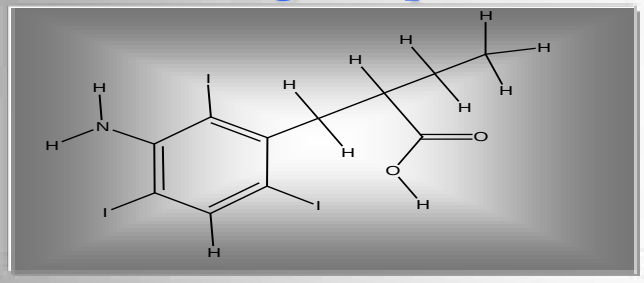
Next-generation approach

Application pattern of integrated concept

"Interactive and real-time" drug design

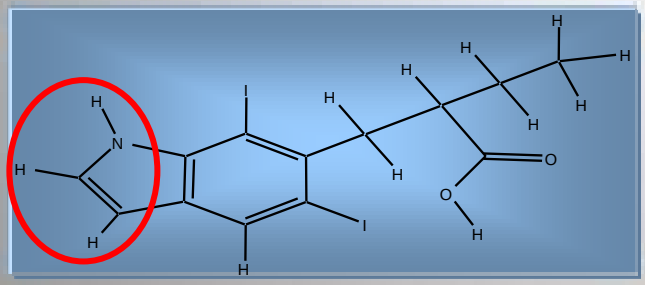
* Check the effects of structure modifications on compound properties real-time

Starting compound



modification

activity
ADME
toxicity
property



Modified compound

antibacterial	Anti-inflammatory	anticancer	・・・・・	pesticide
carcinogenicity	Ames test	LD50	・・・・・	others

ADME and properties

Caco－2	BBB	CYP
LogP	pKa	$LogD_{7.4}$

antibacterial	Anti-inflammatory	anticancer	・・・・・	pesticide
carcinogenicity	Ames test	LD50	・・・・・	others

Information on different properties of different compounds is available anytime

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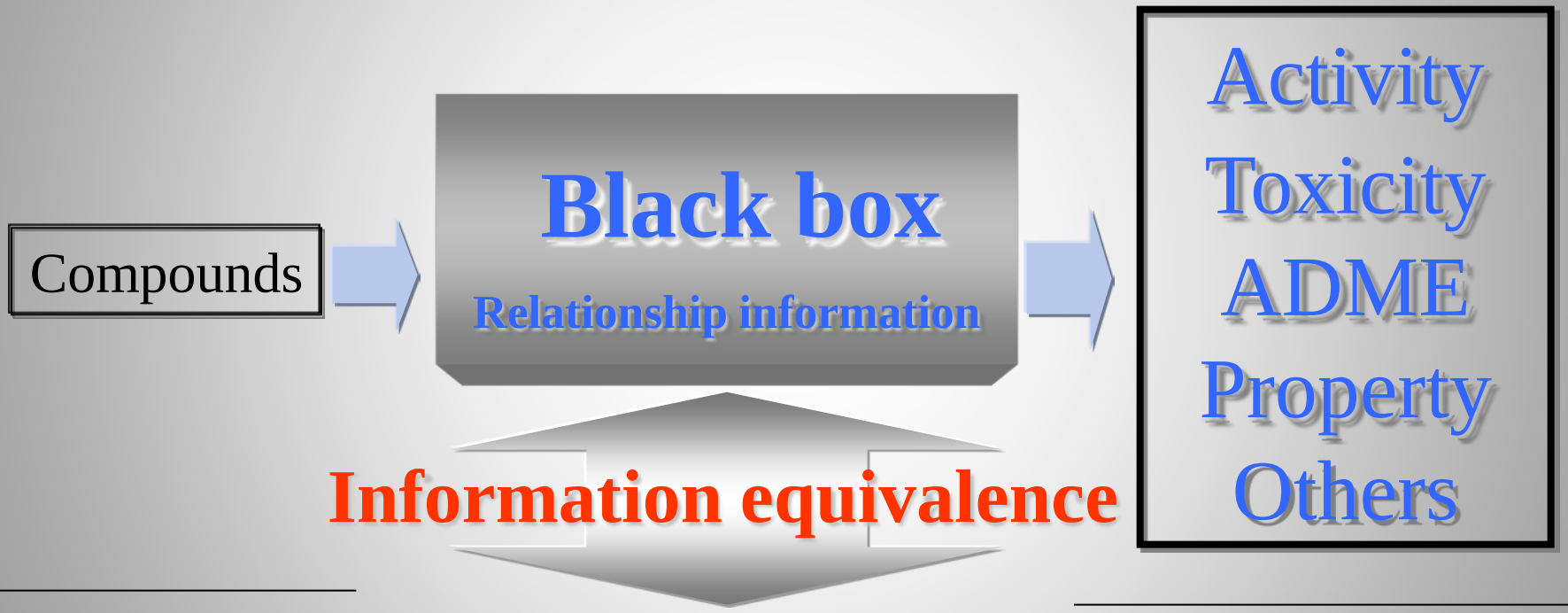
Multivariate and pattern recognition

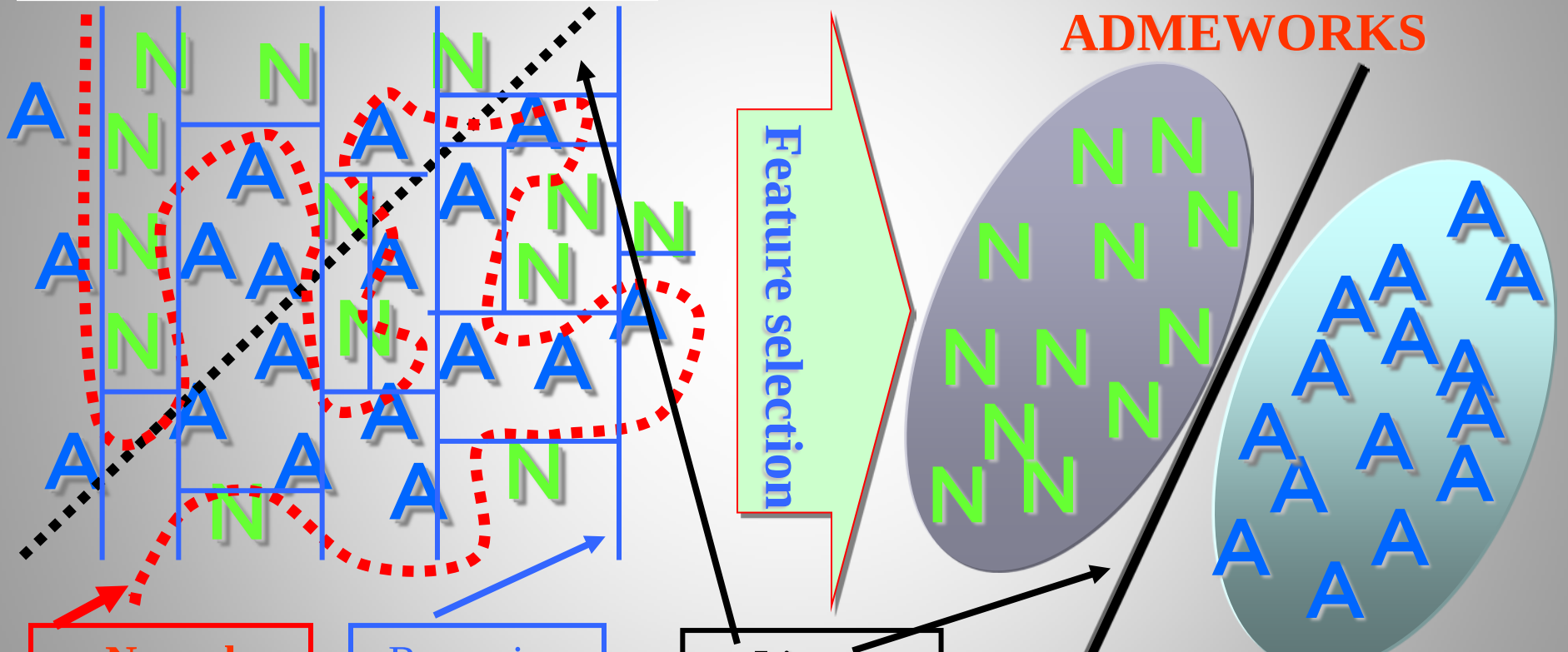
Basic priniciple of data analysis by MVA & PR



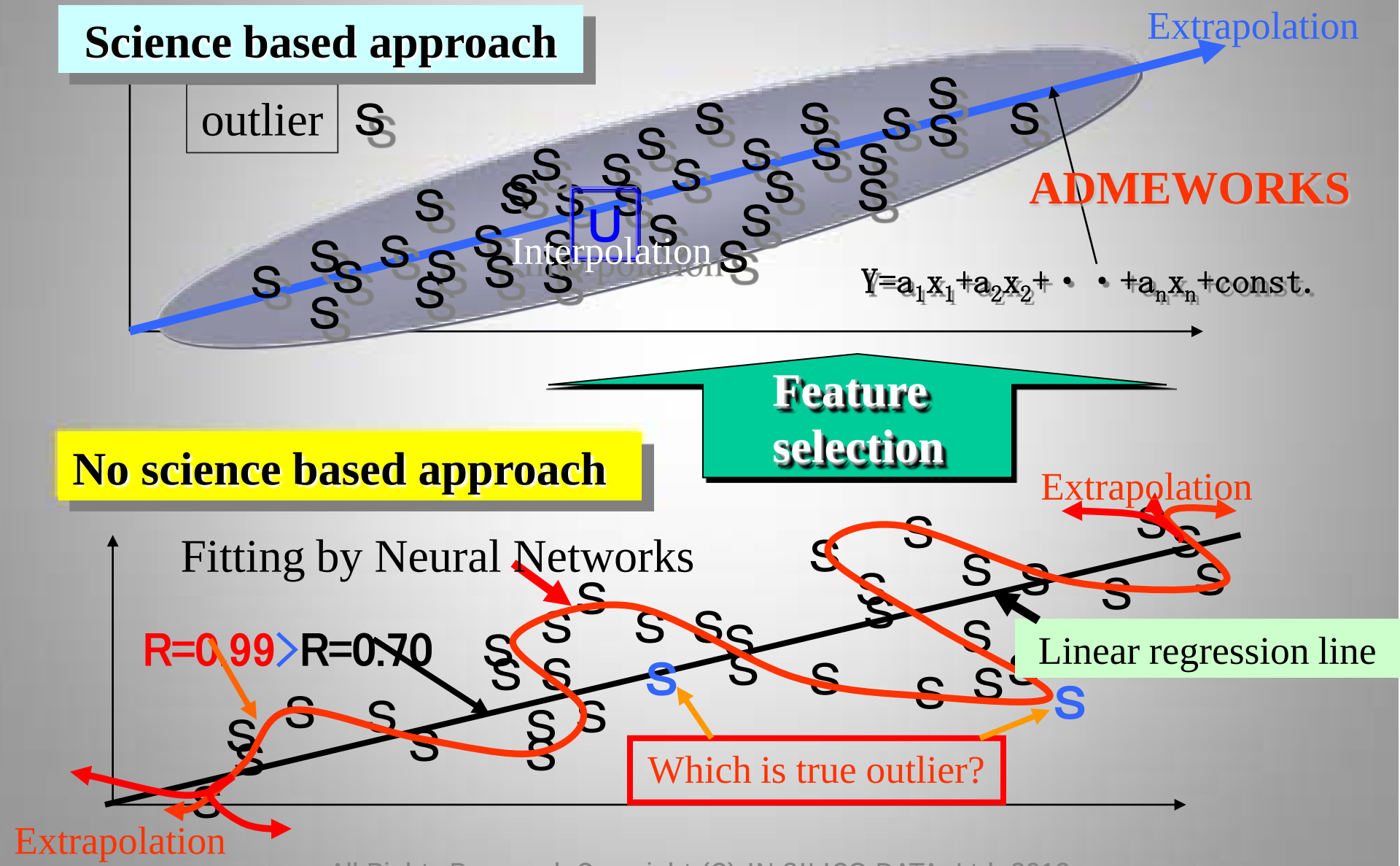
Simple classification and scientific classification

Pattern space impossible to be classified by linear discriminant

Pattern space classified by linear discriminant



Simple fitting and scientific fitting



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