



**ACD/Labs**

Visionary Software



Advancing Research



**ACD/Percepta**



New Platform incorporating ACD/Labs prediction tools for:

- PhysChem
- ADME
- Toxicity



# ACD/Labs and Pharma Algorithms: Analogous Paths



- Chemistry software for pharma
- A market leader in PhysChem prediction
- Offerings include pKa, LogD, Sol<sub>aq</sub>
- Trainable algorithms
- Scientific leadership
- Geography:



Pharma Algorithms

- Chemistry software for pharma
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# ACD/Percepta

- In 2009 ACD/Labs acquired predictive software technology from Pharma Algorithms
- New software included ADME and Toxicity



# Components of ACD/Labs PhysChem Puzzle

## ACD/Labs Software

PhysChem Modules  
LogP, LogD, pKa, Sol, etc

Structure Designer

Structure Design Suite

## Pharma Algorithms Software

PhysChem Modules  
LogP, LogD, pKa, Sol

ADME Modules

Tox Modules

**The challenge: Two different interfaces, duplication of some modules**



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# ADME and Toxicity Property Predictors

ADME
Blood Brain Barrier
P-gp specificity
Oral bioavailability
Absolv
Passive absorption
Distribution
PK Explorer
P450 Inhibitors, Substrates, Regioselectivity

Toxicity
hERG Inhibition
Genotoxicity
Acute Toxicity
Aquatic Toxicity
Irritation
Endocrine System Disruption
Health Effects

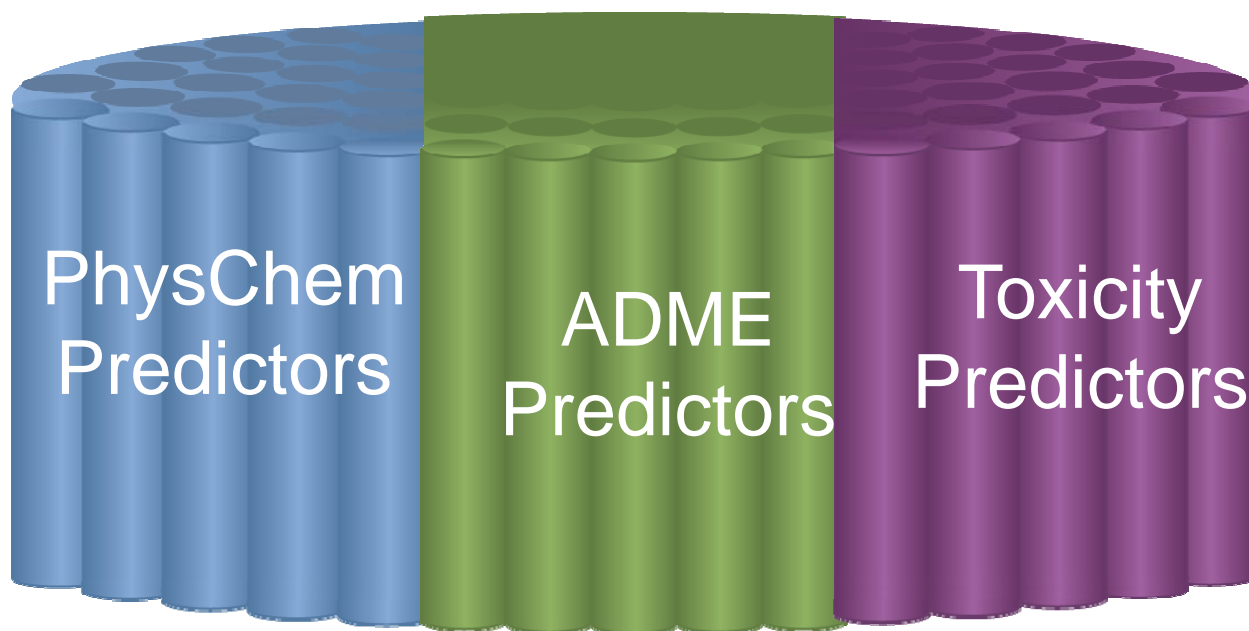


# Development Approach

- One unified platform for all predictive models
- Adoption of a new interface
- Modular design
- Maintain “Expert” and “Casual” user tiers
- Integration



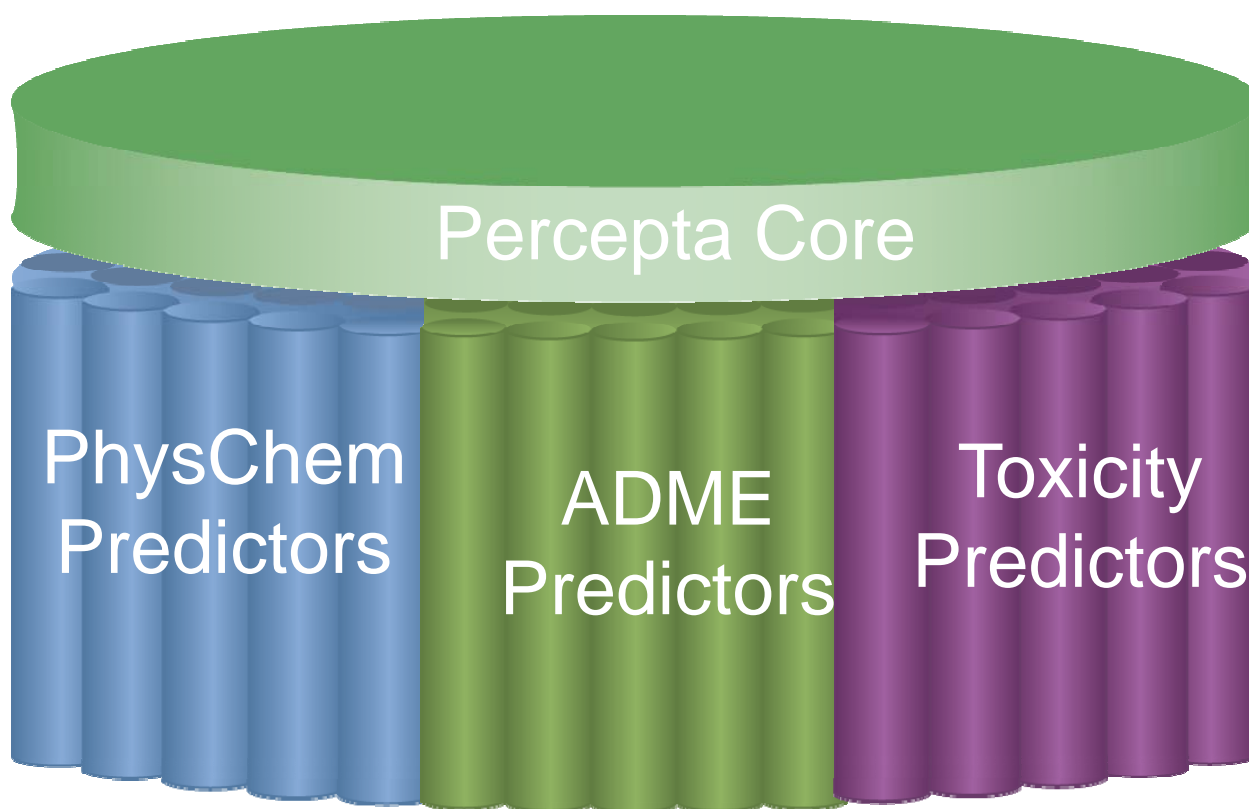
# Percepta Platform



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# Percepta Platform



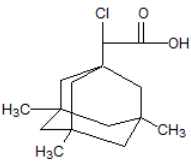
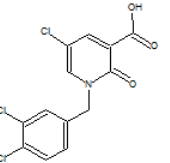
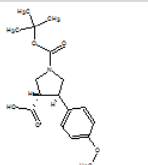
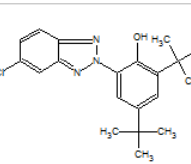
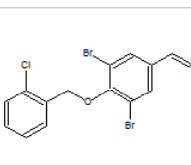
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# Percepta Core

ACD/ADME Suite Module View Spreadsheet View

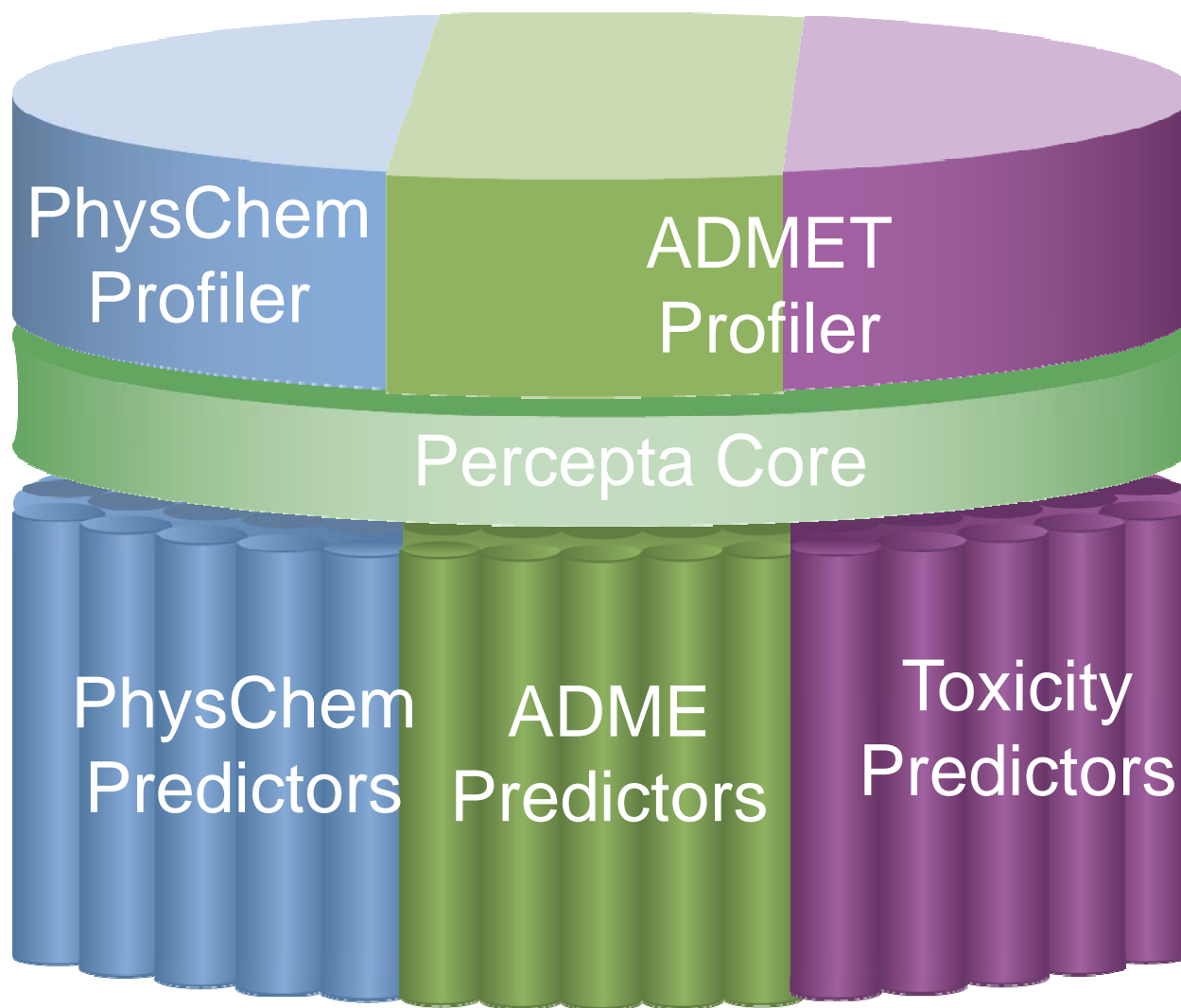
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Structure	McGowan Volume (V)	%PPB	LogKa(HSA)	Vd (L/kg)	pKa(Acid) (ACD/Labs)	pKa(Base) (ACD/Labs)	CNS categories	PgP Substrat...	Ames ...	I ibinski ...
	2.0931	83.3971	4.8284	0.2783	2.8665	No pKa	Good	Good	Good	Good
	2.0652	97.8277	5.2769	0.3137	2.2314	-3.5508	Bad	Good	Unknown	Good
	2.4650	84.4470	4.9680	0.3004	4.3260	-3.0425	Bad	Good	Unknown	Good
	2.7803	97.6146	5.1240	6.2277	9.2308	-0.7629	Good	Unknown	Unknown	Average
	2.1528	99.6847	4.4269	3.3519	No pKa	No pKa	Bad	Good	Good	Average



# Percepta Platform

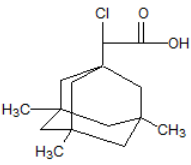
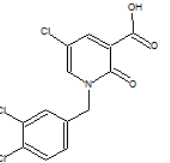
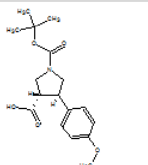
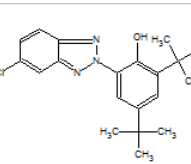
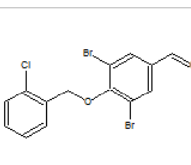


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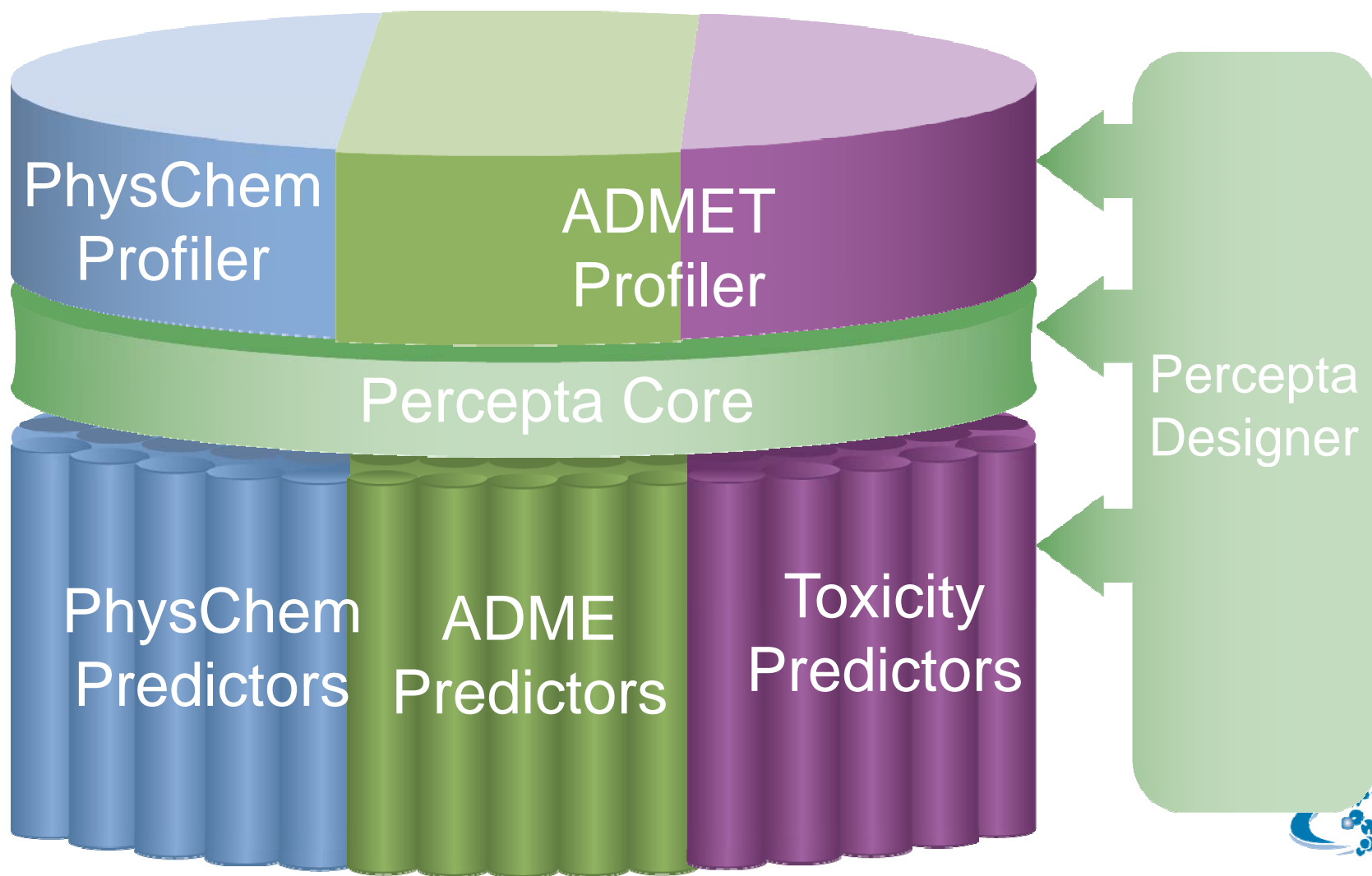
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# Percepta Platform



# Benefits

- All ADME, Tox and PhysChem predictors in one interface
- Meets the needs of both the Advanced Users and Casual Users
- Improved PhysChem prediction accuracy via consensus (logP, logD, Solubility)
- Percepta Core an excellent productivity tool
- Percepta Designer - Structure Designer on steroids





**ACD/Percepta**

**Release Date:  
Late 2011**



**ACD/Labs**