ChemAxon

David Malatinszky

USER GROUP MEETING

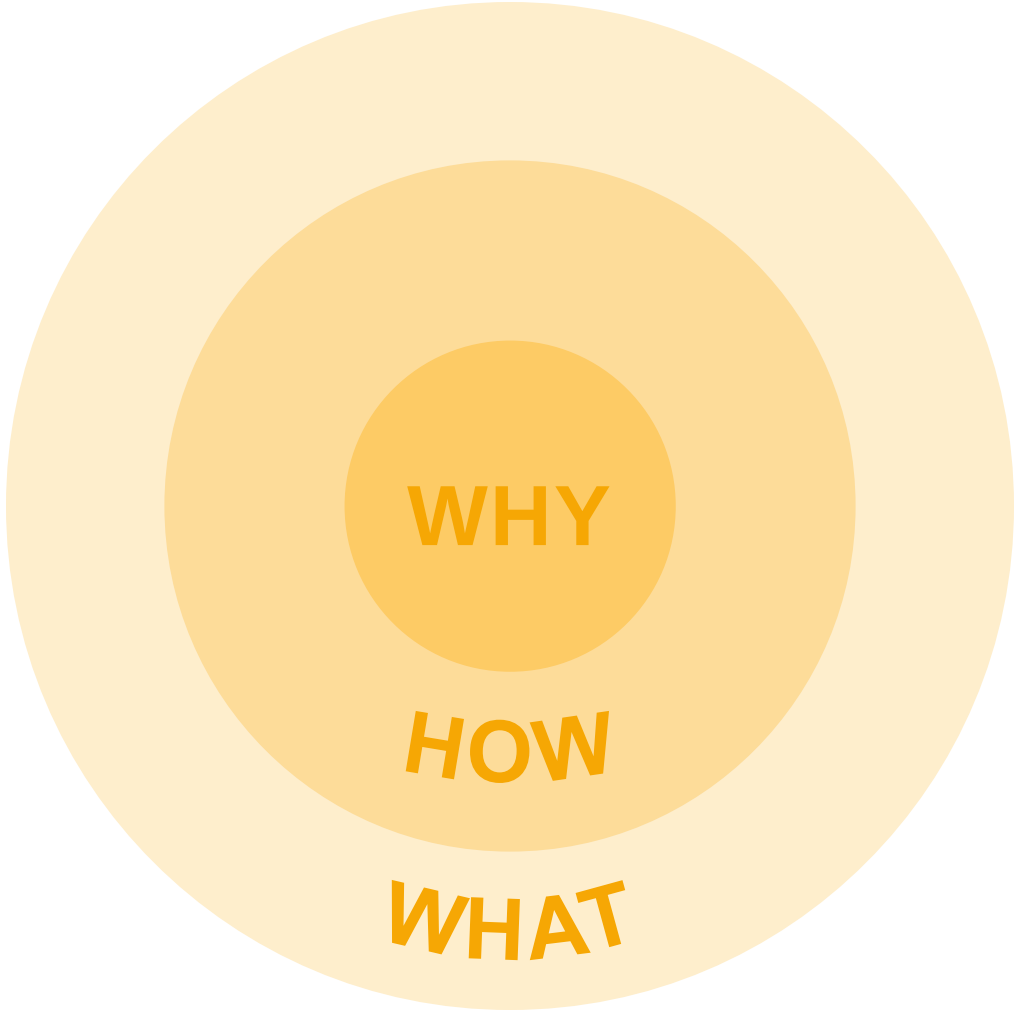
Budapest, Hungary

„I would like to draw a synthesis scheme.”

„When optimizing a lead I am
testing my ideas by trial and error.”

„I would like to go with ChemAxon.
Are you compatible with my favourite ELN?”

ChemAxon



The "golden circle" from Simon Sinek
(author of Start With Why: How Great Leaders Inspire Everyone to Take Action)

ChemAxon

VISION

No boundaries

in chemistry drawing

ChemAxon

ENHANCING YOUR DRAWING EXPERIENCE

Insert images, shapes and custom arrows

Create multi-step reaction schemes

Benefit from a built-in Structure Checker

Stay tuned for
Efi Hoffmann’s talk
(coming up next)

VISION

ChemAxon

Fast thinking requires fast responses

ChemAxon

CHASING NEW CHALLENGES...

NEO4J CARTRIDGE Chemical search for graph databases

DISTRIBUTED SEARCH Chemical search in very large datasets

Get the details from
Andras Volford's talk
in the afternoon

VISION

ChemAxon

Ideas and inspiration come anytime, anywhere

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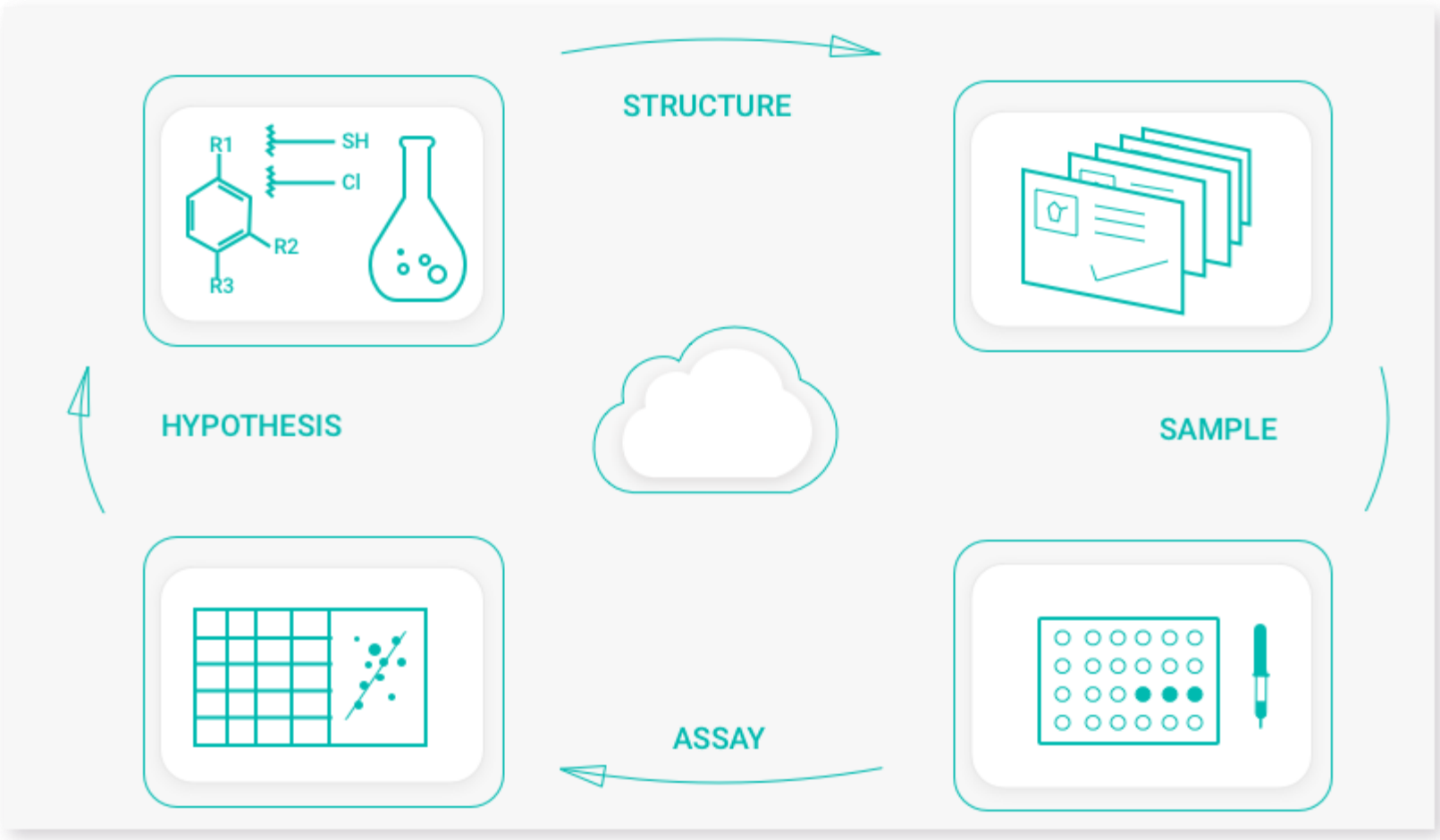

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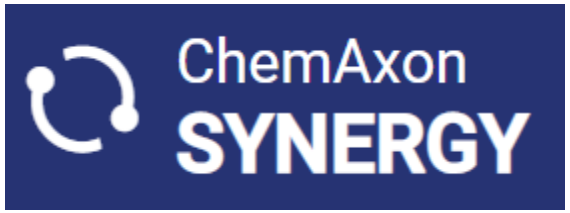

ChemAxon

Cloud platform for application integration
Encoura[illegible]ndor best of breed system
Combine with Consultancy Service

ChemAxon SYNERGY

Find Csaba Peltz for a word on Synergy and our cloud solutions

VISION

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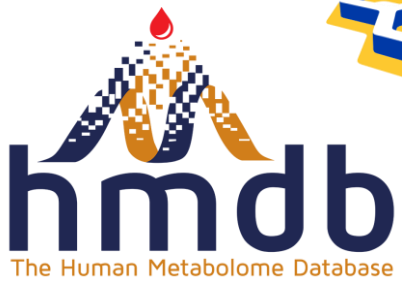
Information should enable and not overwhelm

ChemAxon

Available Chemicals Directory

CompTox



What if we could search an arbitrary volume of chemical data using a single interface?

To find out more,
stay tuned for
Ivan Solt's talk

VISION

ChemAxon

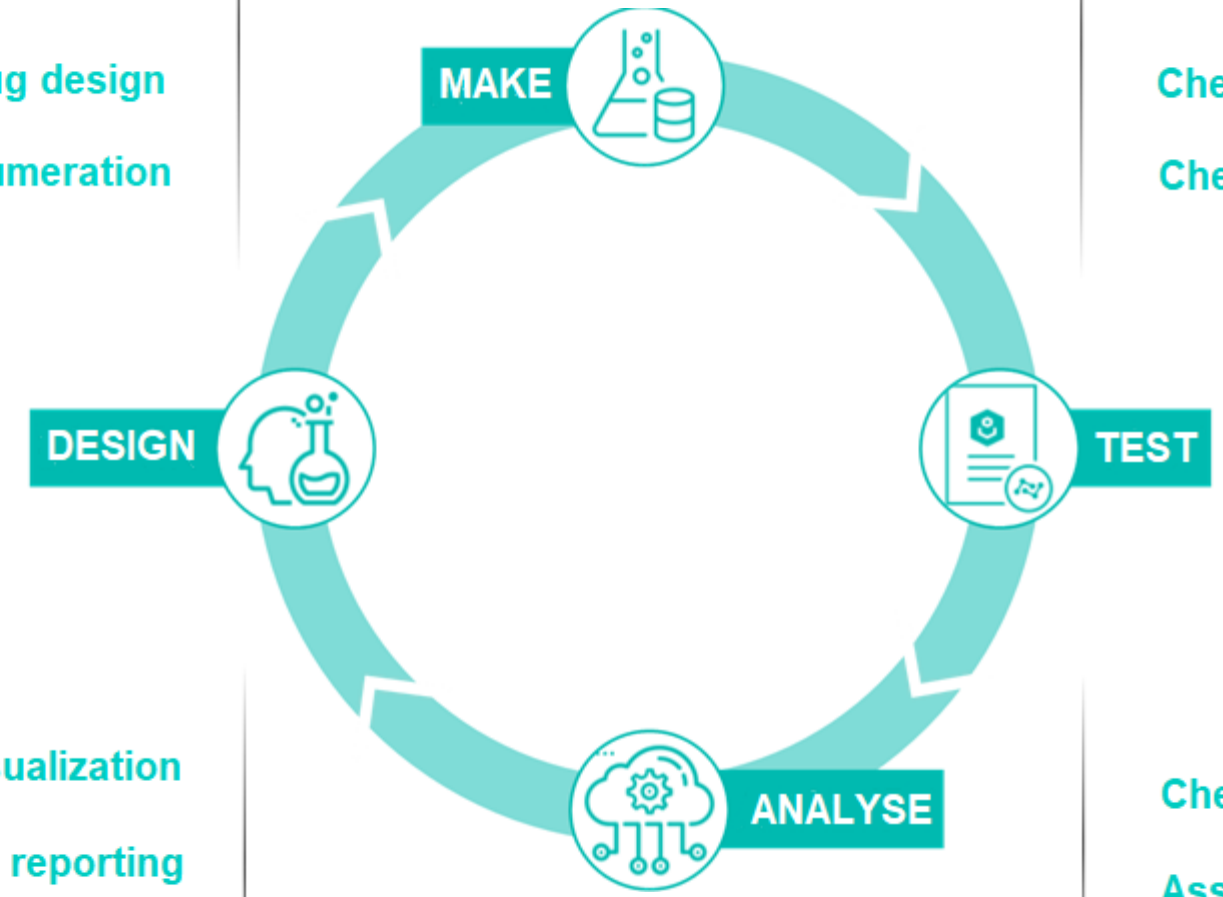
PORTFOLIO

Structure sketchers

Property calculators

Live drug design

Library enumeration



Small molecule registration

Biologics registration toolkit

Chemical compliance

Chemical text mining

Data visualization

Analysis and reporting

Collaboration and sharing

Chemical search engines

Assay data management

ChemAxon

S	Structure search
D	Drug design and discovery
C	Chemistry in documents
M	Markush technologies
O	Online education

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STRUCTURE SEARCH

THE JCHEM FAMILY

S
D
C
M
O

JCHEM BASE	Industry-standard structure search
JCHEM POSTGRESQL CARTRIDGE *CHORAL ORACLE CARTRIDGE	Fast, relevance-sorted structure search
*JCHEM MICROSERVICES	Scalable, modular web cheminformatics

*New product

ChemAxon

EXPLORATORY SEARCH

S
D
C
M
O

MADFAST SIMILARITY SEARCH Ultra fast similarity search

Have a discussion with Gabor Imre about MadFast

ChemAxon

DRUG DESIGN AND DISCOVERY

CHEMISTRY DRAWING

S
D
C
M
O

MARVINSKETCH	Publication-quality drawing on desktop
MARVIN JS	Browser component for chemical drawing

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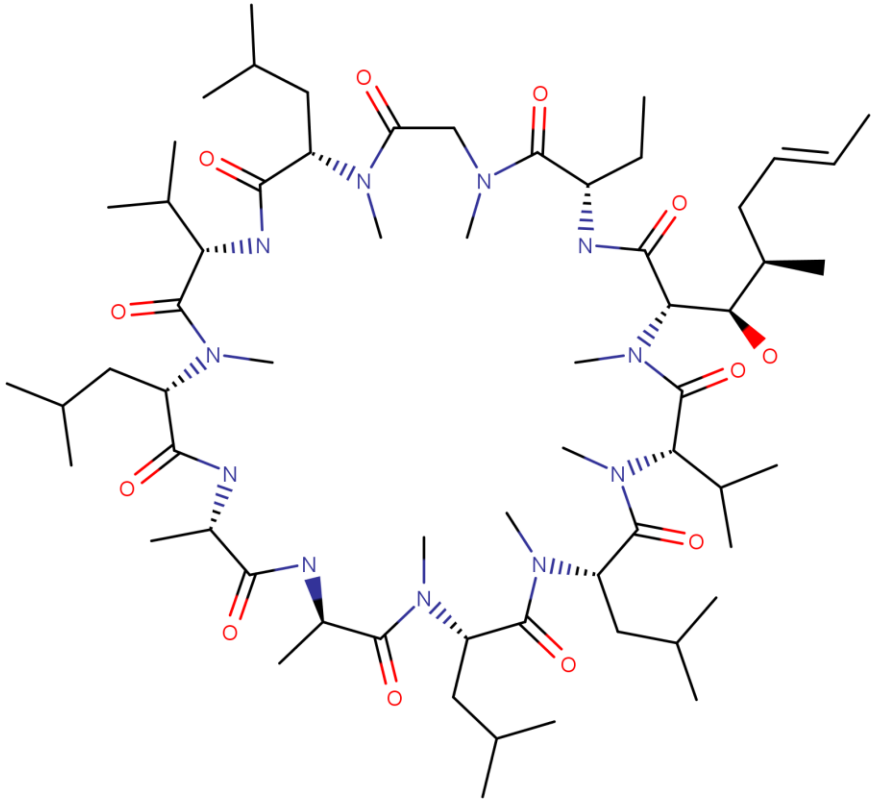
What about macromolecules?

ChemAxon

Cyclosporin



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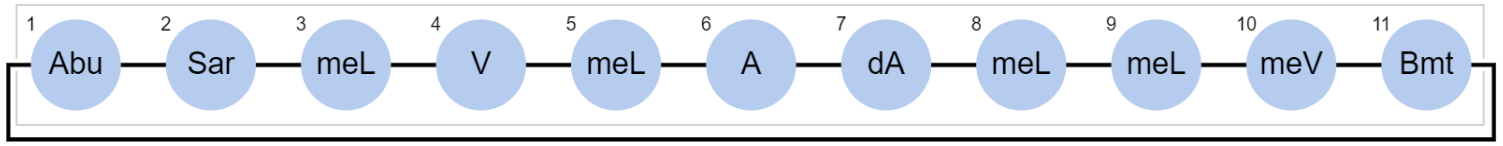
Cyclosporin



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MACROMOLECULE EDITING

S
D
C
M
O

BIOEDDIE Monomer-based large molecule editor

AGNOSTIC REGISTRATION One size does not always fit all.

Find Roland Knispel for a chat on a new registration system

ChemAxon

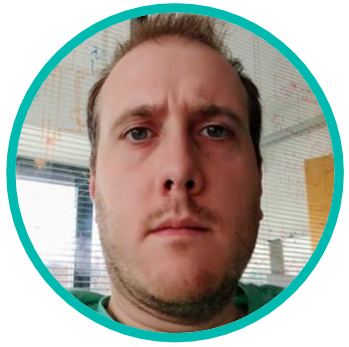
MOLECULE DESIGN

S
D
C
M
O

MARVIN LIVE Live drug design and ideation platform

PHYS-CHEM CALCULATORS Structure-based property prediction

PLEXUS DESIGN Scaffold- and reaction-based enumeration



Ask Andras Stracz about the future of Marvin Live

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COMPOUND AND ASSAY DATA HANDLING

S
D
C
M
O

COMPOUND REGISTRATION	Standardized compound repository
***CHEMAXON ASSAY**	Standardized assay data uploader
PLEXUS CONNECT WITH CHARTS	Visualization and SAR reporting tool

*New product

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CHEMISTRY IN DOCUMENTS

FINDING CHEMISTRY

SDCMO

CHEMLOCATOR Extract and find chemical names in text

Locate Jozsef David
with questions about
ChemLocator

ChemAxon

INSERTING CHEMISTRY

S D C M O

JCHEM FOR OFFICE — Create rich chemistry content in MS Office

JCHEM FOR OFFICE ONLINE — Enable chemistry in Office Online

JCHEM FOR OFFICE LITE — Invisible, vendor-independent chemistry in Word, PowerPoint and Outlook

Discuss your expectations of JChem for Office with Akos Papp

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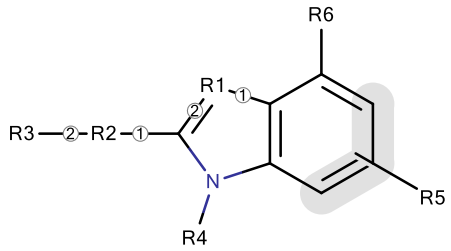
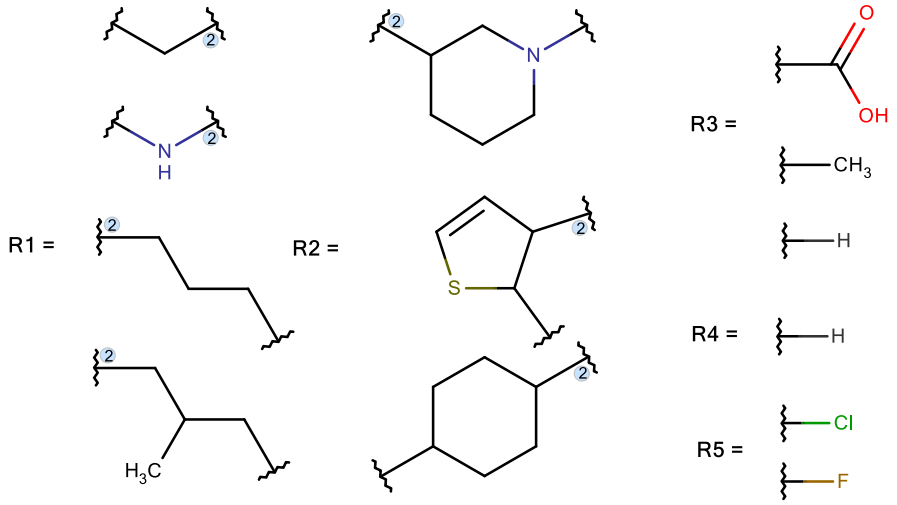
MARKUSH TECHNOLOGIES

WHAT IS A MARKUSH STRUCTURE?



Markush structure (scaffold)



Markush definition

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IP AND LEGAL COMPLIANCE

S
D
C
M
O

CHEMCURATOR	Patent analysis and Markush search
COMPLIANCE CHECKER	Detection of controlled substances

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ONLINE EDUCATION

INTERACTIVE CONTENT PUBLISHING

SDCMO

*ZOSIMOS Content-independent quiz framework

*New product

Meet Erika Biro and
find out more about
the Zosimos framework

ChemAxon

Continuously improving chemical search

Intuitive cloud applications for drug discovery

Flexible Consultancy Service for customization

ChemAxon

We know chemistry.
We are integrable.

It’s you.

ChemAxon

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