ChemAxon

ChemAxon Usermeeting 2019

22-23. May 2019 Budapest

Transforming AnalytiCon‘s Database Infrastructure

Lars Ole Haustedt, Director Projects & Innovation

AnalytiCon discovery

The Natural Product Company

Agenda

1 Introduction AnalytiCon Discovery GmbH

2 Database Infrastructure

3 Plexus Connect

4 Library Enumeration

5 Computational Chemistry

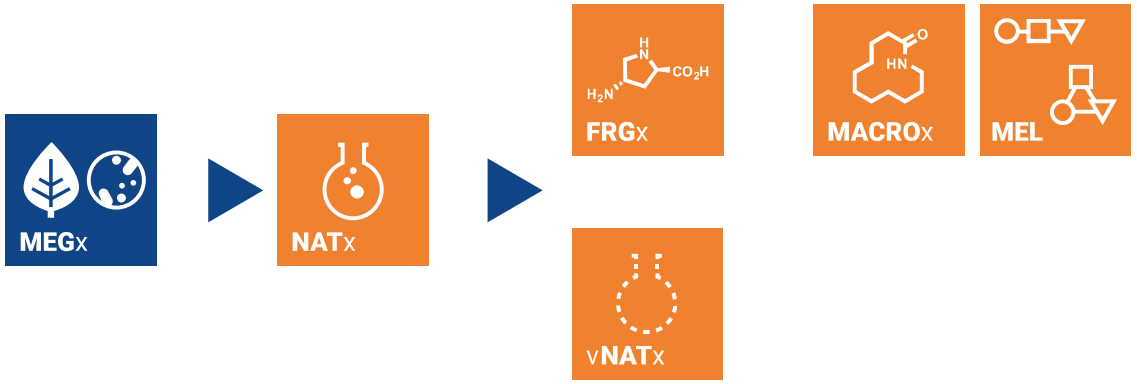
AnalytiCon Discovery GmbH

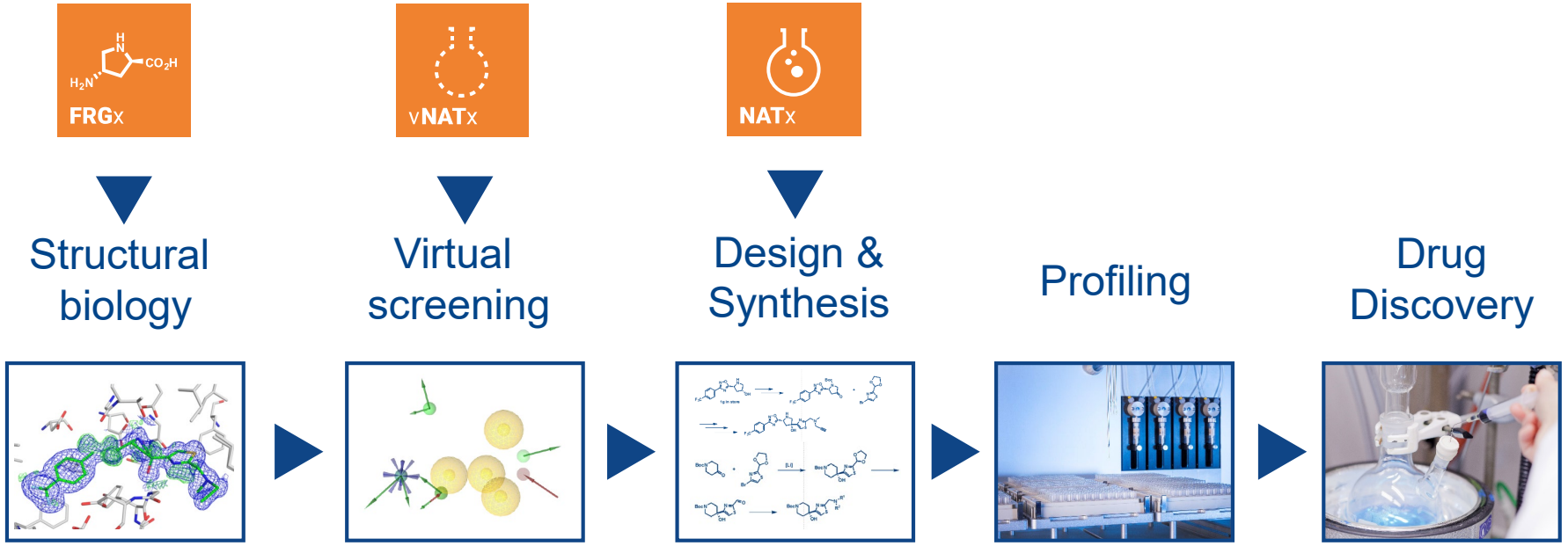
- Headquarters: **Potsdam, Germany**
- Subsidiary: **Rockville** (MD), **USA**
- Privat company founded **2000**
- **65 employees** (17 PhD)

- Microbiology
- Discovery Biology
- Library Design & Generation
- Separation & Analytical Chemistry
- Discovery Chemistry & Medicinal Chemistry
- Structural Biology & Computational Chemistry

AnalytiCon‘s Chemical EcoSystem

AnalytiCon‘s Chemical Space





AnalytiCon discovery

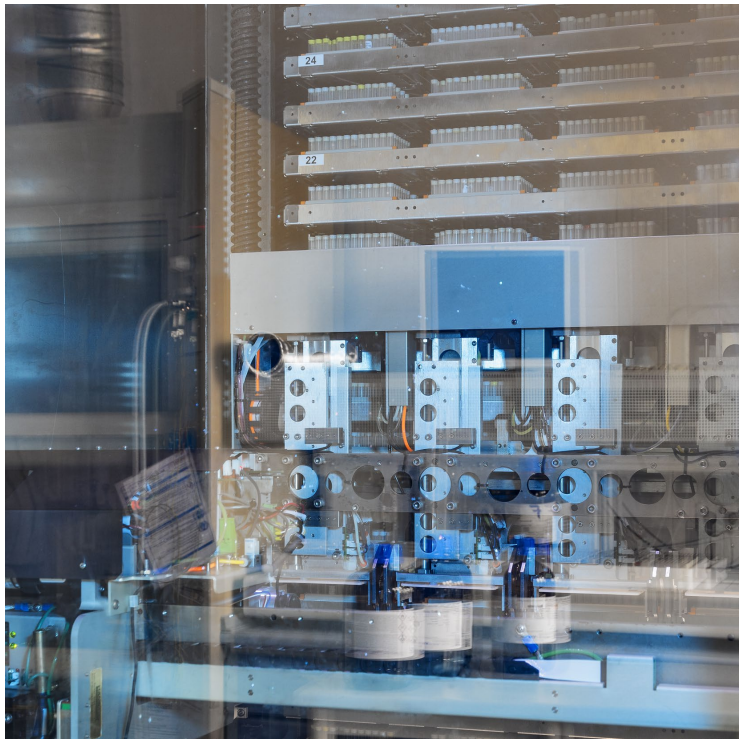
Transformation of Data Managementand Storage

Company Legacy

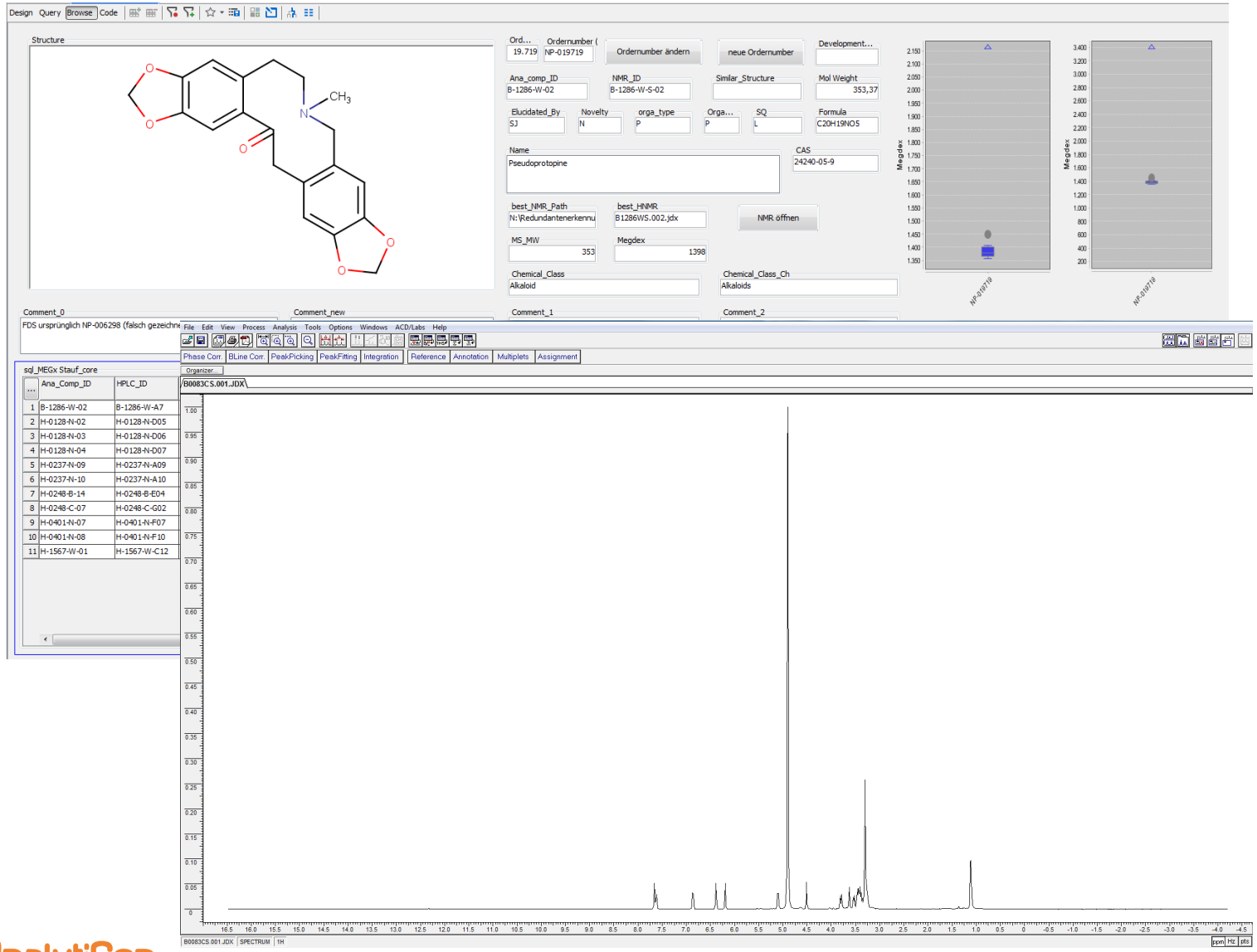
- Complex Interactions of Structural data, Analytical data and Biological data
- Large LCMS and NMR data sets (> 5TB)
- Medium sized structural datasets (< 10GB, 200,000 structure records)
- ChemFinder, Access and Excel based (ISIS Base)
- Tedious maintenance

Perspective

- Relational data base
- MySQLand IJChem based
- Browser based viewing and editing
- Registration, inventory, relation to QC (analytical) data
- Integration of medicinal chemistry & computational chemistry



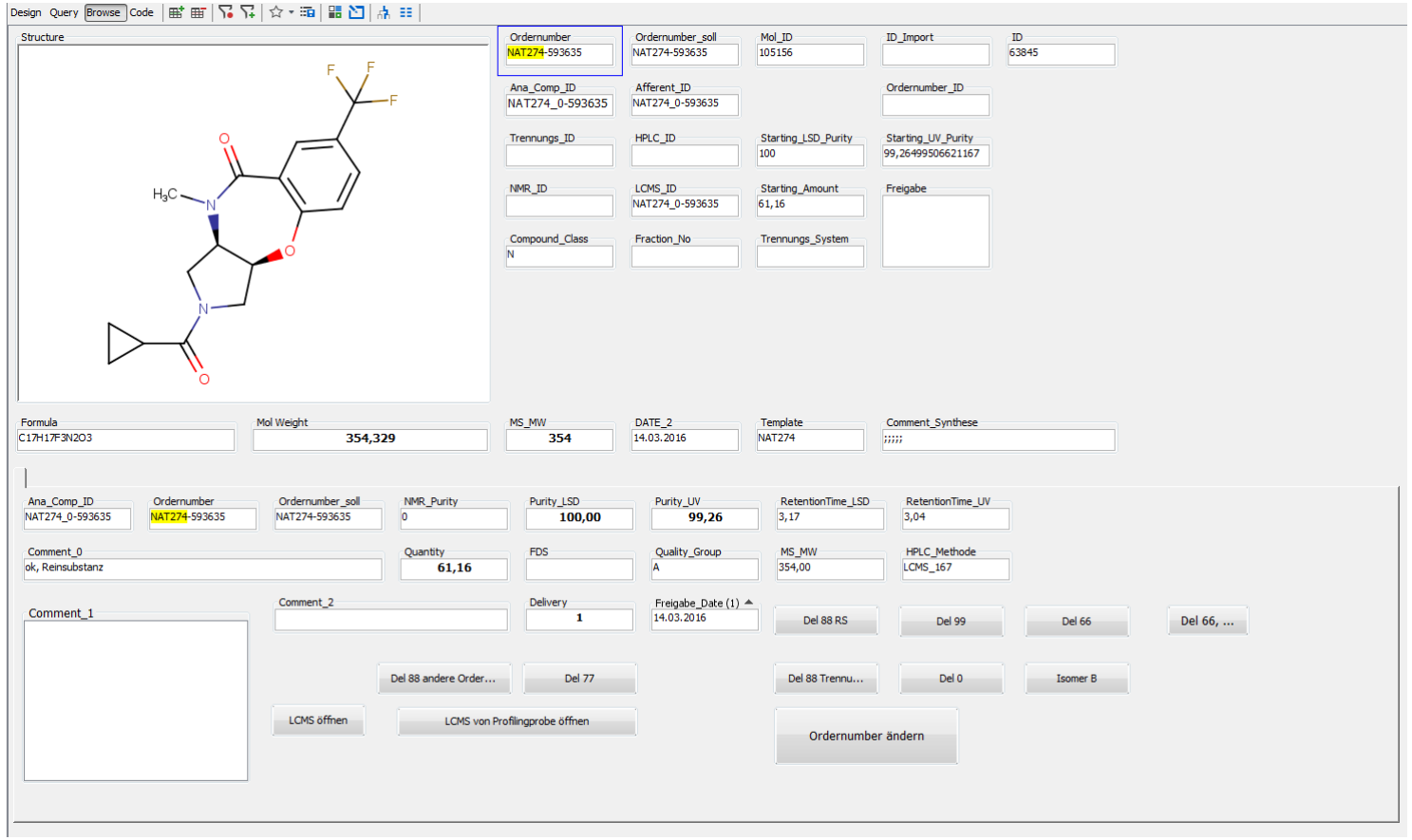
IJChem MySQL



Natural Product Database

- Storage of Chemical Structure
- Relational table with all batches
- Direct link to NMR data (JCAMP-DX,)
- Direct link to LCMS pdf
- Polarity Indicator

IJChem MySQL



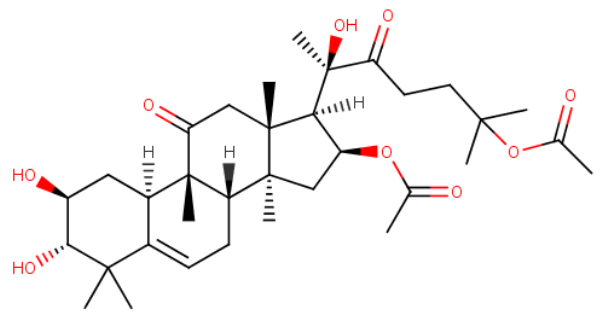
Synthetic Cpd Database

- Storage of Chemical Structure
- Direct link to LCMS pdf
- Synthetic Synthon
- Compound Management / Storage

Plexus Connect

MEGx_Stauf _Plexus

Structure



Ordernumber	Development_ID	Mol Weight	Formula
NP-019961		604,8	C34H52O9

Ana_comp_ID	NMR_ID	Similar_Struct...	Chemical_Clas...
C-1878-E-15	C-1878-E-S-17		Terpenoids

CAS	Novelty	orga_t...	Orga_type_V
586960-44-3	N	P	P

Name

Hemslecin D

best_NMR_Path	best_HNMR	Megd...	MS_MW
N:\Jcamp\	C1878ES.017.dx	2330	604

Comment_0	Comment_new	Comment_1	Comment_2

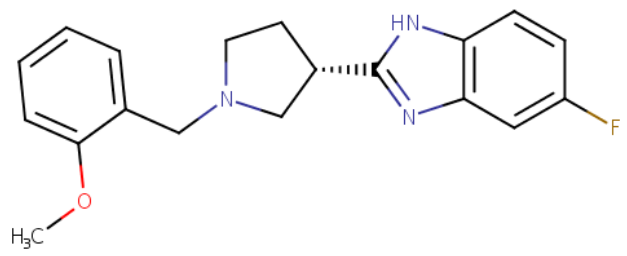
sql_MEGx Stauf_core

Ana_Co...	HPLC_ID	NMR_ID	Fraction_No	MS...	Meg...	NMR_P...	Purity	Quant...	Formiat	Orga_...	Ana Orga ID	Analyticon ID	Genus	Species	Comment Material	Comment Profiling
C-1878-E-14	C-1878-E-E12	C-1878-E-S-16	69+70	604	2330	2	99,8	146,5		P	15687-1	ACD-V-21978-W-0	Hemsleya	carnosiflora		
C-1878-E-15	C-1878-E-F01	C-1878-E-S-17	71+72+73	604	2332	1	99,3	212,7		P	15687-1	ACD-V-21978-W-0	Hemsleya	carnosiflora		
C-1878-E-16	C-1878-E-F02	C-1878-E-S-18	74+75+76	604	2331	2	94,7	73,3		P	15687-1	ACD-V-21978-W-0	Hemsleya	carnosiflora		
C-1878-D-26	C-1878-D-D08	C-1878-D-S-29	94+95+96+97	604	2329	3	90,3	9,1		P	15687-1	ACD-V-21978-W-0	Hemsleya	carnosiflora		
C-1878-D-26		C-1878-D-26_L	94+95+96+97	604	2329	3	90,3	8,1	1	P	15687-1	ACD-V-21978-W-0	Hemsleya	carnosiflora		
C-1878-E-14		C-1878-E-14_L	69+70	604	2330	2	99,8	131,7	1	P	15687-1	ACD-V-21978-W-0	Hemsleya	carnosiflora		
C-1878-E-15		C-1878-E-15_L	71+72+73	604	2332	1	99,3	198,7	1	P	15687-1	ACD-V-21978-W-0	Hemsleya	carnosiflora		
C-1878-E-16		C-1878-E-16_L	74+75+76	604	2331	2	94,7	67,8	1	P	15687-1	ACD-V-21978-W-0	Hemsleya	carnosiflora		
C-2049-H-11	C-2049-H-A11	C-2049-H-S-12	57+58+59+60	604	2345	1	97,8	6,0	0	P	15685-9	ACD-V-21976-W-0	Phlomis	betonicoides		
C-2049-H-12	C-2049-H-A12	C-2049-H-S-13	62+63+64+65	604	2349	4	50,4	4,7	0	P	15685-9	ACD-V-21976-W-0	Phlomis	betonicoides		

Plexus Connect

NATx_Production_Plexxus

Structure



Ordernumber	Ordernumber_...	Mol_ID	ID_Import	ID
NAT31-457216	NAT31-457216	30846		45014

Ana_Comp_ID	Afferent_ID	Ordernumber_ID
NAT31 1-457216	NAT31 1-457216	

Trennungs_ID	HPLC_ID	Starting_LSD_...	Starting_UV_P...
	NAT31 1-457216	98,482	98,454

NMR_ID	LCMS_ID	Starting_Amount	Freigabe
		106,50	

Compound_Class	Fraction_No	Trennungs_Sys...
B		

Formula	Mol Weight	MS_MW	DATE_2	Template	Comment_Synthese
C19H20FN3O	325,387	325	22.09.2009	123	;;;;

Ana_Comp_ID	Ordernumber	Ordernumber_...	NMR_Purity	Purity_LSD	Purity_UV	RetentionTime...	RetentionTime...
NAT31_1-457216	NAT31-457216	NAT31-457216	0	98,48	98,45	7,22	7,01

Comment_0	Quantity	FDS	Quality_Group	MS_MW	HPLC_Methode
ok, Reinsubstanz	106,50		A	325,00	B31

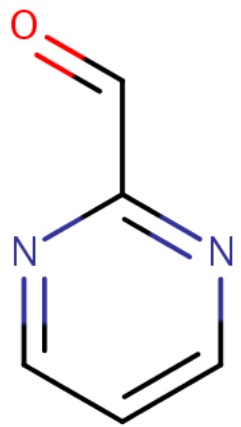
Comment_1	Comment_2	Delivery	Freigabe_Date
		1	22.09.2009

Unbound	Unbound

AnalytiCon discovery

Plexus Connect

Chemikalien-DB_Plexus

Structure	Name
	Pyrimidine-2-carboxaldehyde

CAS	Größe	Einheit	Reinheit
27427-92-5	1	g	

Anbieter	Best.-Nr.	Preis	Währung
Manchester Organics	D45360	184,00	Euro

Raum	Ablage	Entleiher	Kuehlung
EG8	KS1		

Bestellt	Datum erstellt	Erhalten	Geöffnet am
Am	2019-03-26	Ras	

CdId	Formel	Mol Weight	Dichte
7600	C5H4N2O	108,100	

Kommentar

Brennbar	Lagerklasse	H-Sätze
		H315-H317-H319-H335

P-Sätze
P233-P260-P261-P264-P271-P272-P280-P302+P352-P304+P340-P312-P321-P332+P313

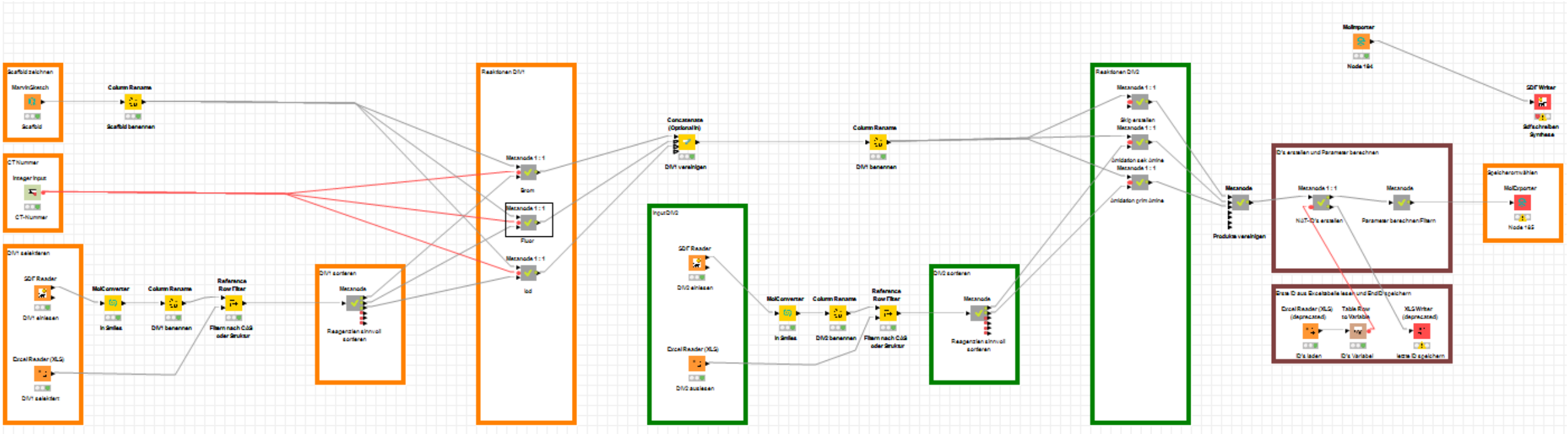
ReagentDatabase

- Storage of chemical structure
- Provider / price Info
- Inventory information
- Browser access for lab staff
- User friendly selection of reagent sets

Feature Requests Plexus Connect

- Implementation of scripts and buttons in form view
- Pull down menus in form view
- Import functionality (SD- file)
- Adding records in form view
- Definition of mandatory fields in form view

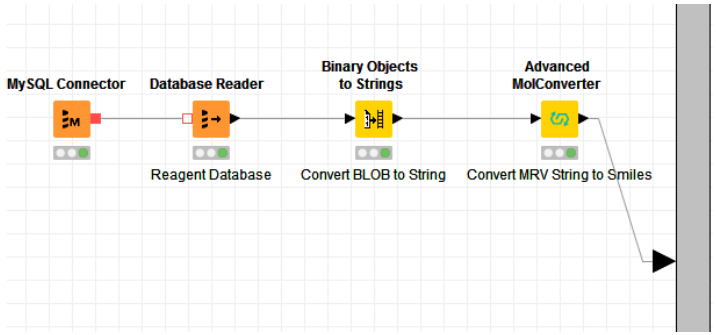
ChemAxon Knime Nodes: Library Enumeration



Knime Workflow

- Library Enumeration
- Generation of unique compound identifier
- Tractable synthon information
- Property calculation (TPSA, clogP)
- Generation of conformers (Inteligand)
- Export: MySQL, SDF, Table of SMILES

Library Enumeration



File Hilite Navigation View

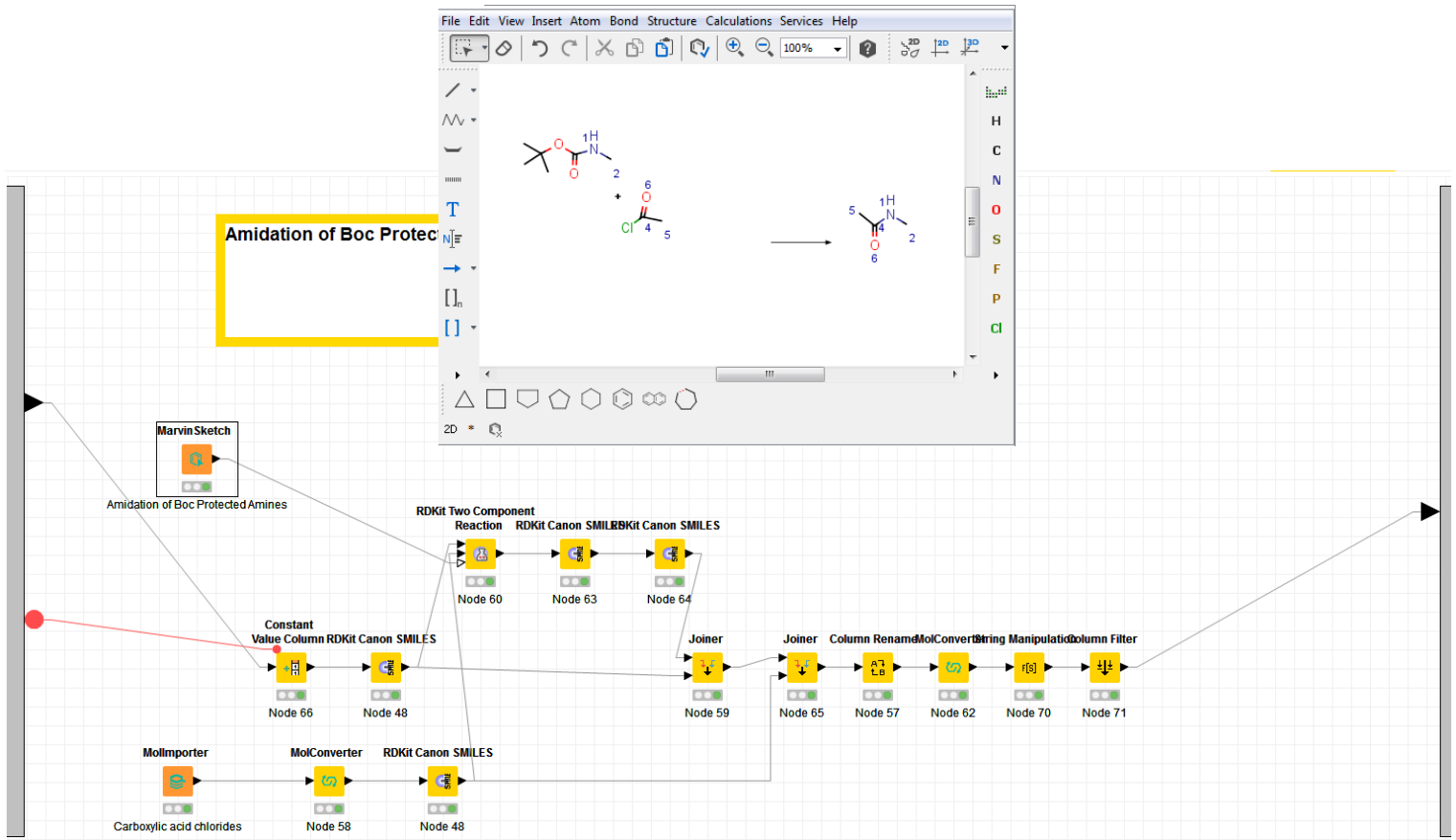
Table "default" - Rows: 7229 | Spec - Columns: 2 | Properties | Flow Variables

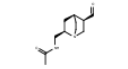
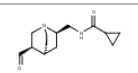
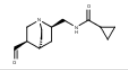
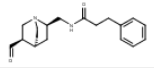
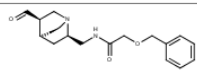
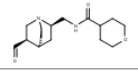
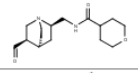
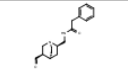
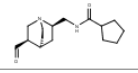
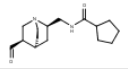
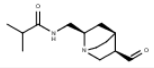
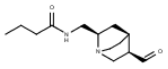
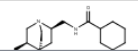
Row ID	cd_structure	CAS
Row0		25016-11-9
Row1		3034-50-2
Row2		123-08-0
Row3		1074-86-8
Row4		10200-59-6
Row5		1196-69-6
Row6		35344-95-7
Row7		65873-72-5
Row8		10070-92-5
Row9		27258-33-9
Row10		4649-09-6
Row11		487-89-8
Row12		112758-40-4
Row13		123-11-5

ReagentDatabase

- Direct import from MySQL reagent database
- Import of Sub Selections
- No redundant storage of information

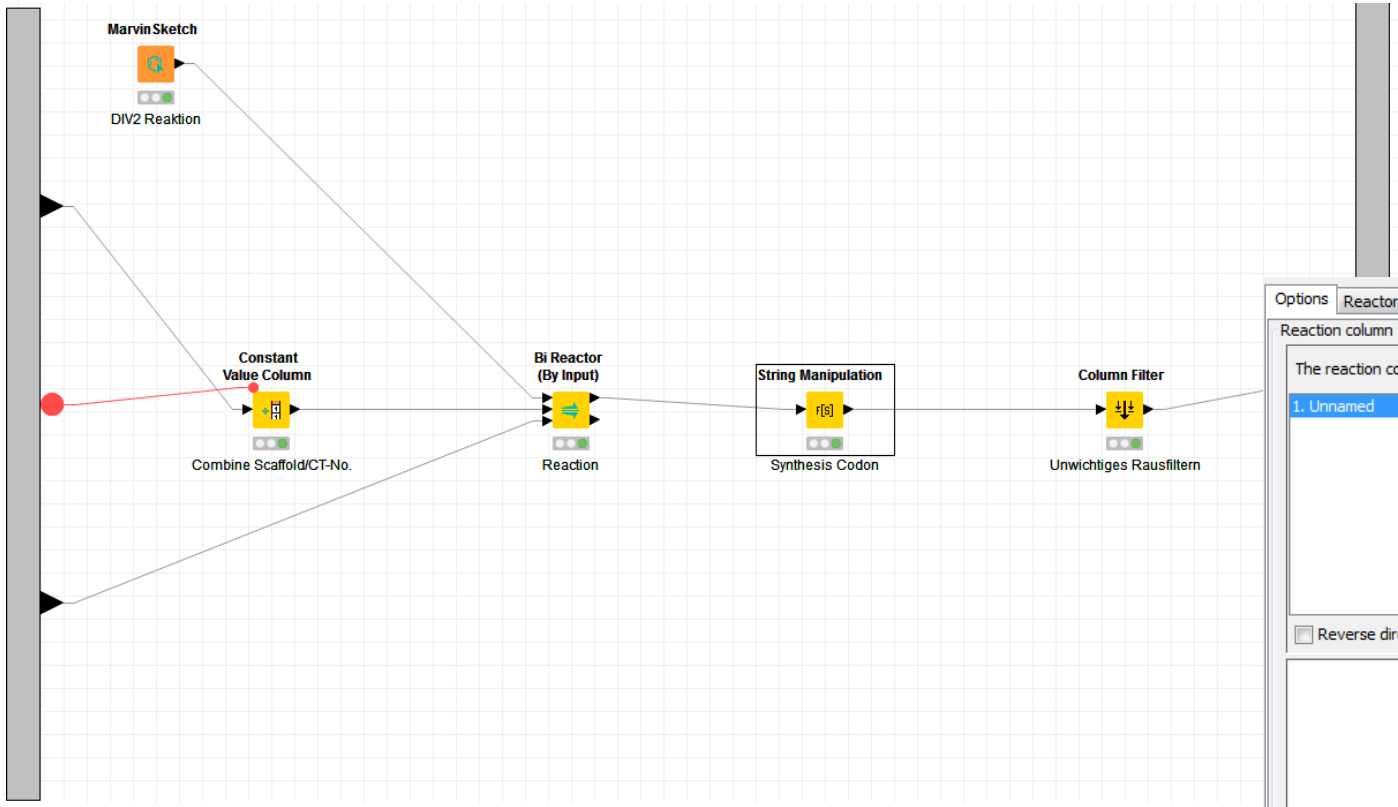
Workflow without JChem Knime Nodes

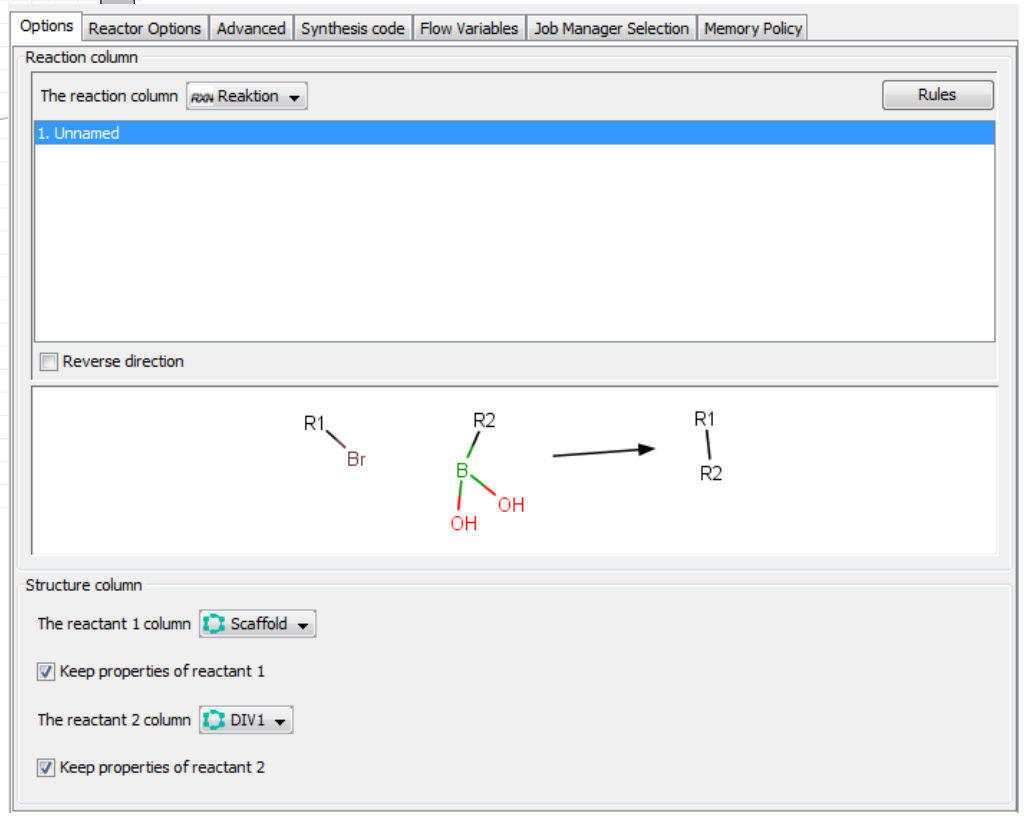


Row ID	Alkyne	Library_Intermediates-1	DIV1-ID
0_0_0_0_Ro...			31--CAS-75-36-5
0_1_0_0_Ro...			31--CAS-4023-34-1
0_1_0_0_Ro...			31--CAS-4023-34-1
0_2_0_0_Ro...			31--CAS-645-45-4
0_3_0_0_Ro...			31--CAS-19810-31-2
0_4_0_0_Ro...			31--CAS-40191-32-0
0_4_0_0_Ro...			31--CAS-40191-32-0
0_5_0_0_Ro...			31--CAS-103-80-0
0_6_0_0_Ro...			31--CAS-4524-93-0
0_6_0_0_Ro...			31--CAS-4524-93-0
0_7_0_0_Ro...			31--CAS-79-30-1
0_8_0_0_Ro...			31--CAS-141-75-3
0_9_0_0_Ro...			31--CAS-2719-27-9

- Traction of synthon information more tedious
- Careful inspection (filtering) of results necessary

Workflow Making Use of JChem Knime Nodes

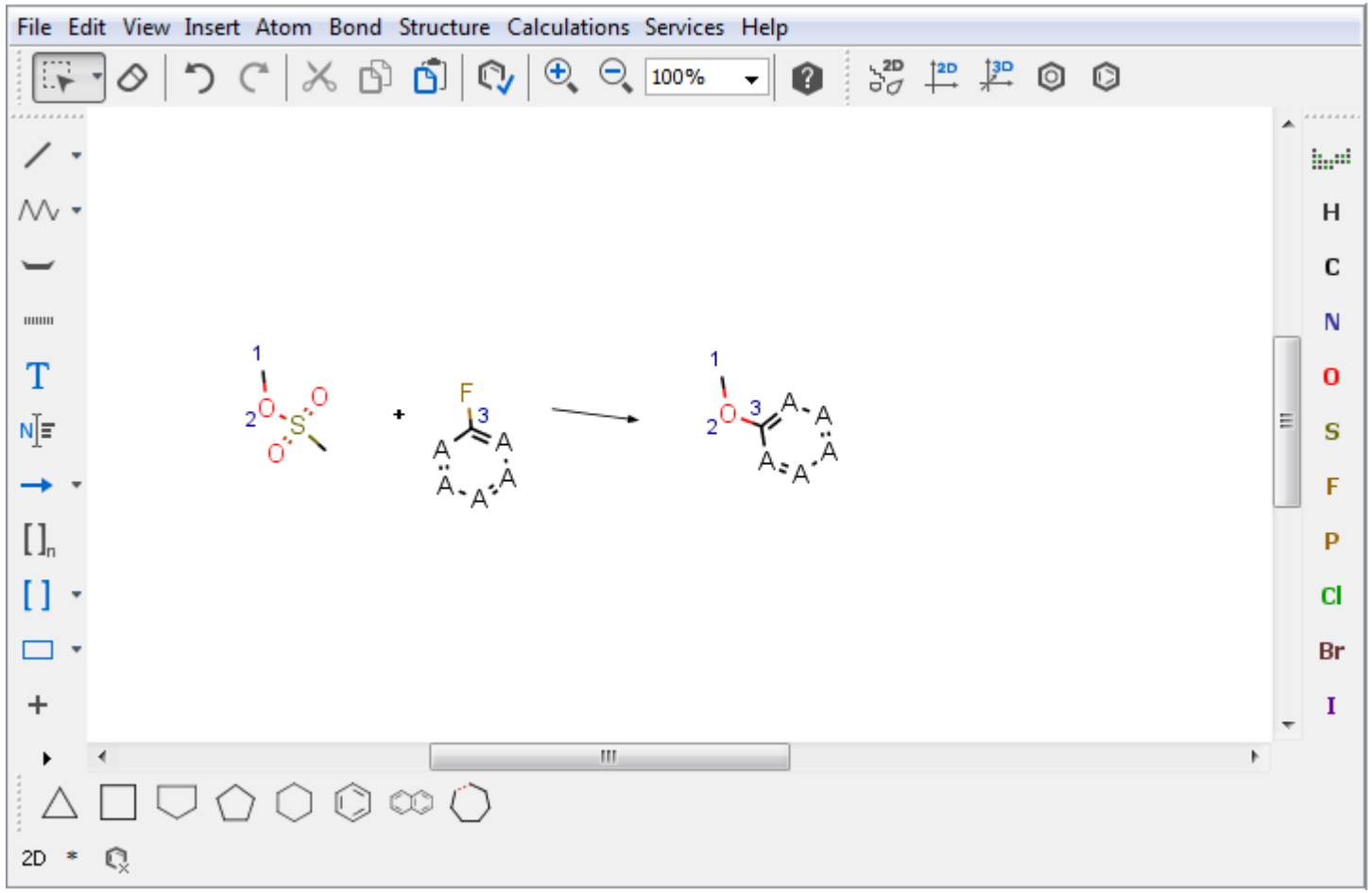




- User friendly traction of reagent properties
- Better control on reaction products

AnalytiCon discovery

Definition of Reactions for Enumeration



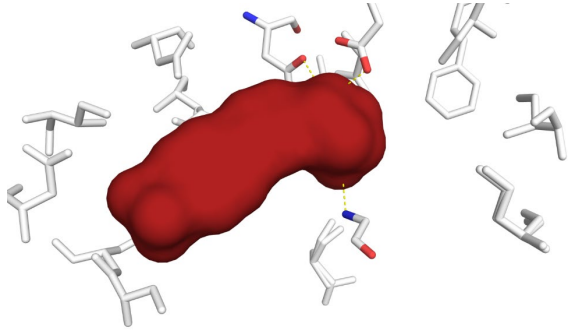
Definition of Reactions with Marvin

- Very flexible
- Chemical support by Marvin (SMARTS)
- Good atom mapping
- Intuitive no need for non chemical hacks

Computational Chemistry

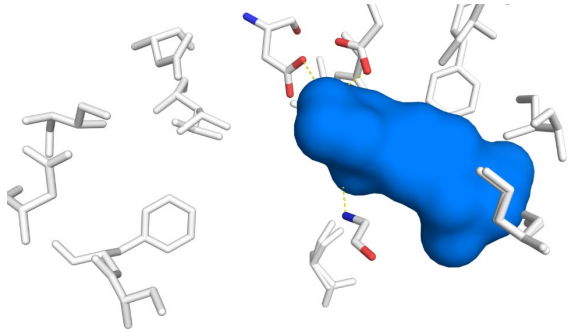
Virtual Libraries

- Design of virtual libraries based on pharmacophores or established scaffolds
- Virtual Library Enumeration
- Calculation of properties; calculation of conformations , calculation of fingerprints



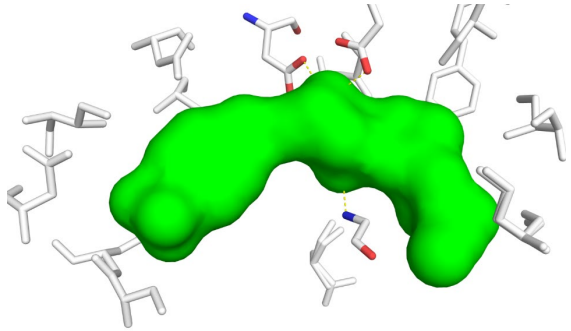
Virtual Screening

- Pharmacophore Search(LigandScout)
- Docking (SeeSAR, LeadIT)



Compound Selection

- Results from virtual screening
- Property based selection (similarity or diversity)
- Fingerprint based selection (similarity or diversity)



Summary

Achievements

- Sustainable, stable high performance relational structural database (MySQL,IJChem)
- Less complex more reliable infrastructure
- Company wide access via Plexus Connect
- Library enumeration integrated (reagent database, synthesis selection, JChem Knime nodes)
- Better integration with compound storage system
- Better integration into Microsoft Office (JChem for Office, Marvin)

Requests

- More functionality and customizable dynamic content in Plexus Connect
- Even more intuitive format menue (color, superscript, subscript) in Marvin

Thank you.

AnalytiCon Discovery GmbH

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AnalytiCon discovery

The Natural Product Company