

Advancing Personalized Medicine via Data Stewardship

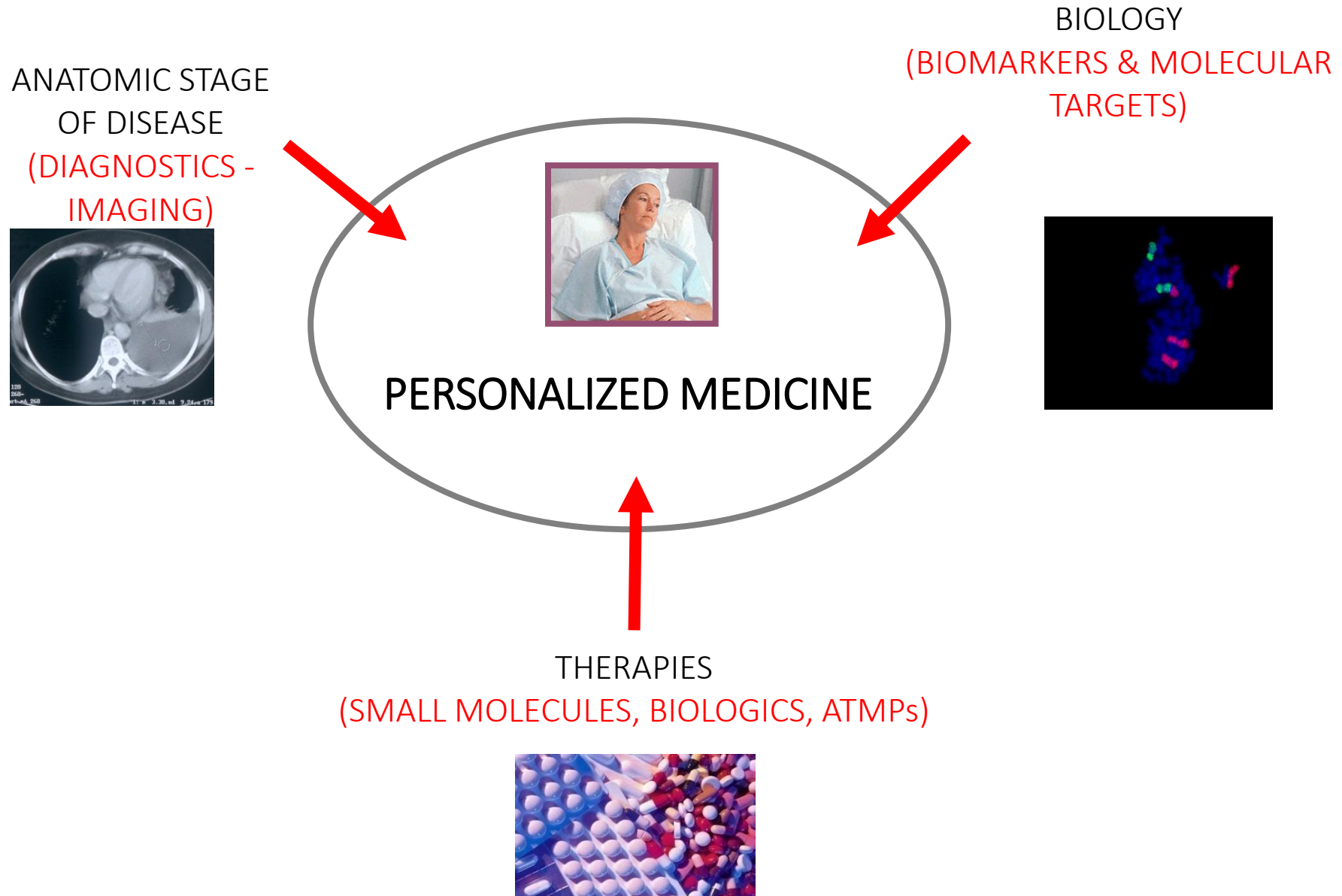
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Faculty of Medicine and Dentistry,
Palacky University Olomouc

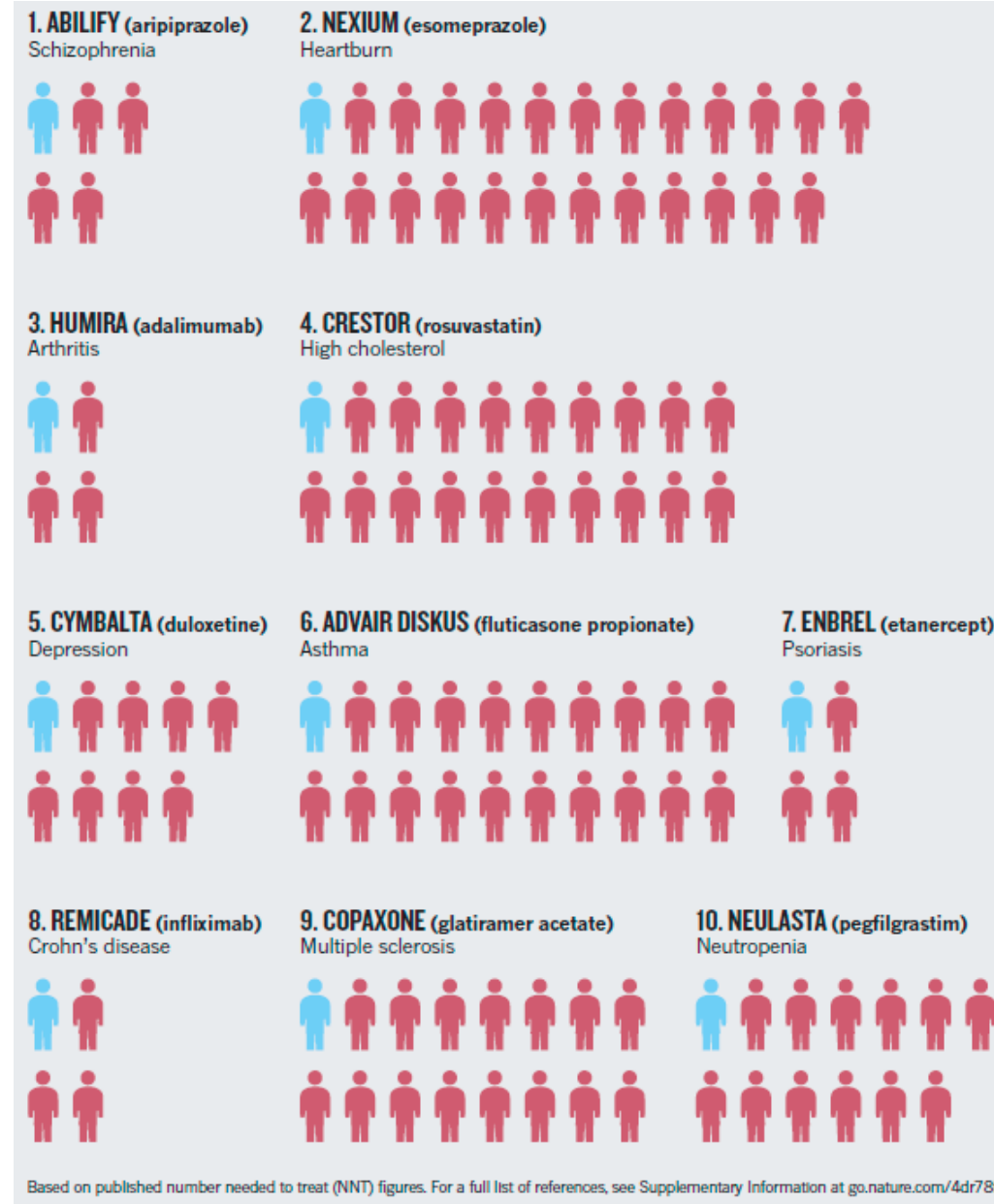
European Infrastructure For Translational Medicine (EATRIS-ERIC)

Info Day on EOSC – state of play, December 2, 2019

Major determinants of therapeutic outcome



Imprecision Medicine Era- Need for Personalization



Biomarker use in clinics

Prognostic

provides information about patient outcome, regardless of therapy

Predictive

estimates the response to a specific treatment before the advance of therapy

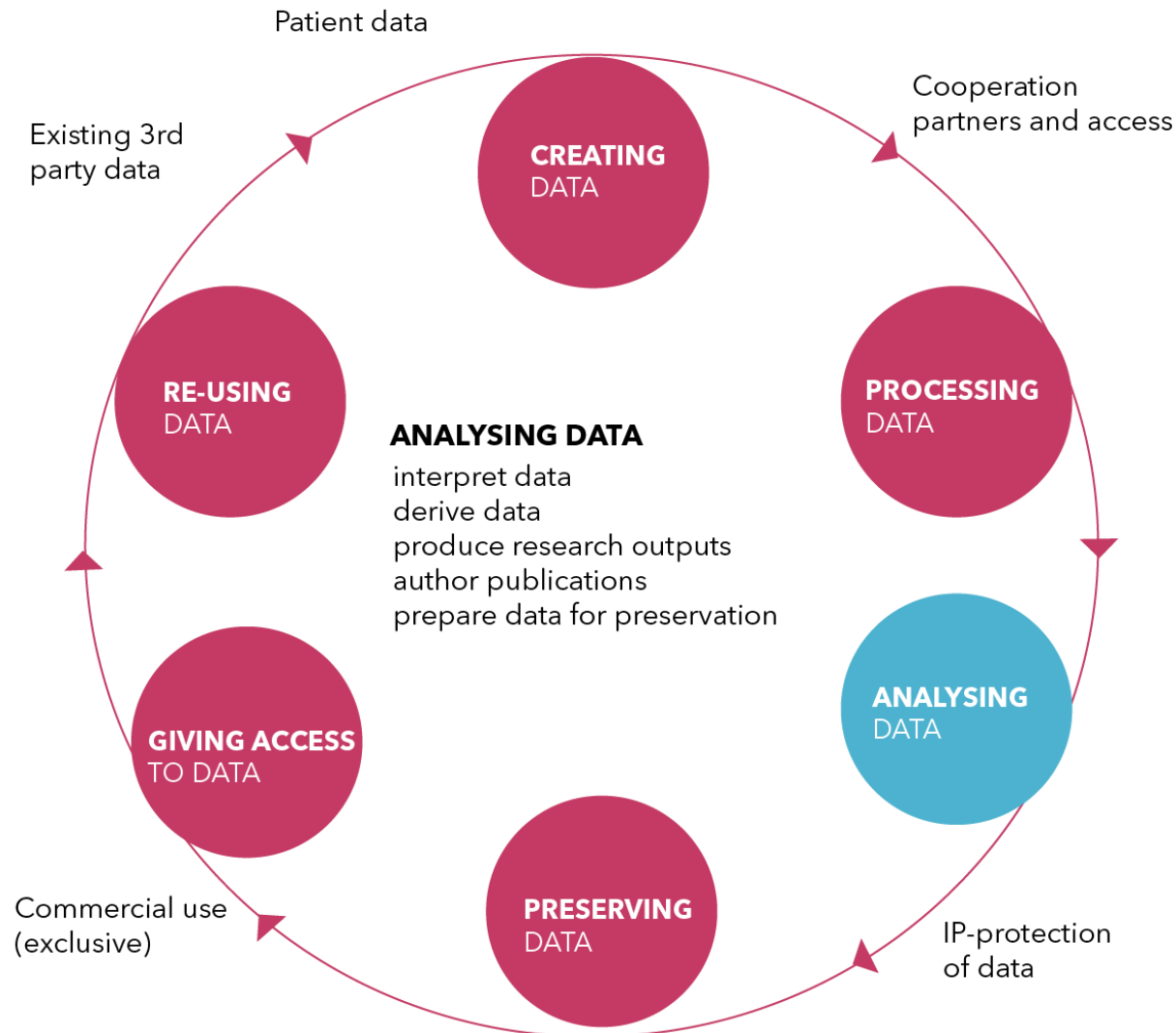
Pharmacological

estimates changes after treatment associated with target hit by therapy

Surrogate

substitutes a clinical endpoint

Data stewardship in medicine



IMTM data portal

Proprietary developed software



Clindata

Comprehensive information system for data stewardship in clinical trials, registries and other clinical/scientific databases.

<https://clindata.imtm.cz>



PreClinData

Comprehensive information system for data stewardship in pre-clinical trials and animal studies (GLP and non-GLP).

<https://preclindata.imtm.cz>



MedChemBio

Laboratory information and management system for medicinal chemistry, high-throughput screening and chemical biology: Compound registration and management, QA, in vitro biology, pharmacology, data analysis, storage, export and reporting.

<http://medchembio.imtm.cz>

<https://portal.imtm.cz>

Administration module

ClinData

PreClinData

MedChemBio Portal

MOLDIMED Pipeline

CLAIRE

others

Administration module

- **Authentication and Authorization** for all IMTM applications



Welcome to Central Authentication service of Institute of
Molecular and Translational Medicine

Login

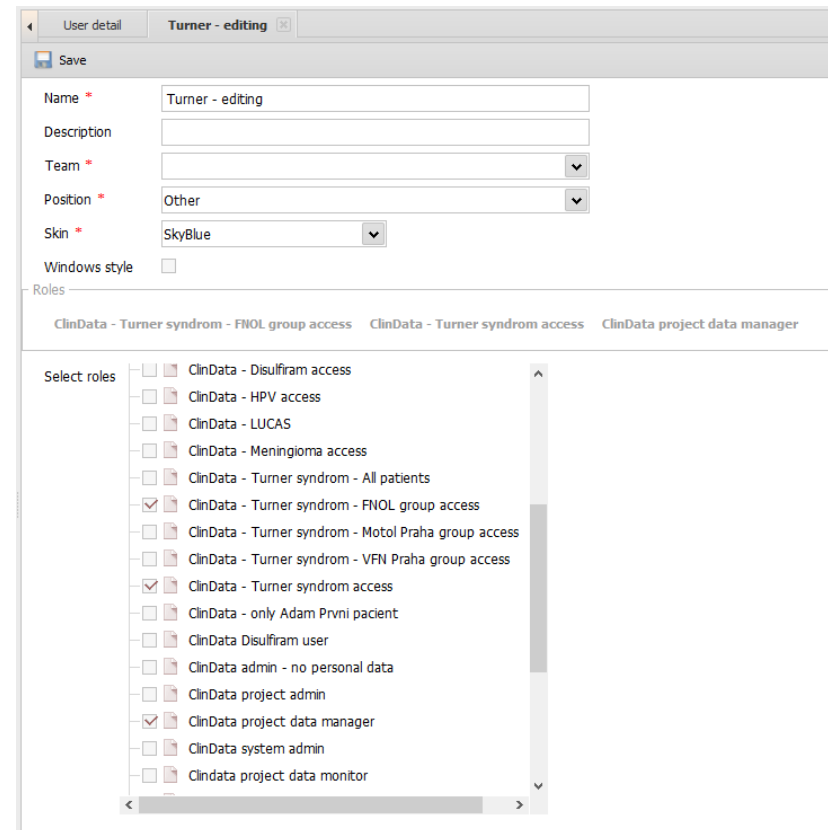
Email address

Password

LOGIN

Don't have an account? [Register here.](#)


Forgot your password?



The screenshot shows a web application interface for editing a user profile. The title bar indicates 'User detail' and 'Turner - editing'. Below the title bar is a 'Save' button. The form contains several fields: 'Name' (Turner - editing), 'Description' (empty), 'Team' (dropdown menu), 'Position' (Other), 'Skin' (SkyBlue), and 'Windows style' (checkbox). Below these fields is a 'Roles' section with a list of roles and checkboxes. The roles listed are: 'ClinData - Turner syndrom - FNOL group access', 'ClinData - Turner syndrom access', 'ClinData project data manager', 'ClinData - Disulfiram access', 'ClinData - HPV access', 'ClinData - LUCAS', 'ClinData - Meningioma access', 'ClinData - Turner syndrom - All patients', 'ClinData - Turner syndrom - FNOL group access' (checked), 'ClinData - Turner syndrom - Motol Praha group access', 'ClinData - Turner syndrom - VFN Praha group access', 'ClinData - Turner syndrom access' (checked), 'ClinData - only Adam Prvni pacient', 'ClinData Disulfiram user', 'ClinData admin - no personal data', 'ClinData project admin', 'ClinData project data manager' (checked), 'ClinData system admin', and 'ClinData project data monitor'.

Authentication

- CAS – central authentication server
- Single sign on
- 2 phase authentications support
 - Mobile
 - E-mail



Welcome to Central Authentication service of **Institute of Molecular and Translational Medicine**

Login

Email address

Password

LOGIN

Don't have an account? [Register here.](#)

[Forgot your password?](#)

Authorization

- User -> Profiles
- Profile -> Roles
- Role -> Privileges
-> Permissions (other profiles, specific data, whatever)

ClinData example:

Access **privileges** determine which ClinData objects a user can browse or edit. It has fine granularity. Every single item (menu item, button, field) can be controlled.

Roles are virtual entities which serve as a container for more privileges:

- ClinData system admin
- ClinData project admin
- ClinData principal investigator
- ClinData project data manager
- ClinData project data monitor
- ClinData project anonymized data browser

The screenshot shows the 'Turner - editing' user profile form. The form has a 'Save' button at the top left. The fields are as follows:

- Name: Turner - editing
- Description: (empty)
- Team: (dropdown menu)
- Position: Other
- Skin: SkyBlue
- Windows style: (checkbox)

Below the form is a 'Roles' section with a list of roles and checkboxes for selection:

- ClinData - Turner syndrom - FNOL group access
- ClinData - Turner syndrom access
- ClinData project data manager
- ClinData - Disulfiram access
- ClinData - HPV access
- ClinData - LUCAS
- ClinData - Meningioma access
- ClinData - Turner syndrom - All patients
- ClinData - Turner syndrom - FNOL group access
- ClinData - Turner syndrom - Motol Praha group access
- ClinData - Turner syndrom - VFN Praha group access
- ClinData - Turner syndrom access
- ClinData - only Adam Prvni pacient
- ClinData Disulfiram user
- ClinData admin - no personal data
- ClinData project admin
- ClinData project data manager
- ClinData system admin
- ClinData project data monitor

Admin new version

- Advanced settings
- Relevant information
- Profile & Role
 - > Roles
 - > Privileges
 - > Permissions

Profile(s) settings for selected Person

Profile list

+ new - delete reload evictCache

Name	Registered	Default
Institute of Molecular and Translational Medicine	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>

Profile details - edit

save cancel

Name * Institute of Molecular and Translational Medicine

Registered ☒

Description default profile

Team * IMTM31, IMTM, Puškinova 6, 775 20 Olomouc

Set this profile as default

Settings for selected Profile

Role (2) Privilege (84) Menu (25) Permission (3) Team (1) Profile (165)

Name	Selected	Subtree	Effective
ClinData project data monitor	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ClinData Disulfiram user	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ClinData admin - no personal data	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ClinData - All studies, No patient (only Adam Prvni testing)	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ClinData project data manager	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
PreclinData - access	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
ClinData project admin	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
assay Cell Cycle Analyses	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Admin - ROLE_CORE_ADMIN +	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
MBCH only	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Admin - ROLE_CORE_SITECONFIGURATION +	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Admin - basic user	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Admin - login/logout	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Admin - languages	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Supervisor	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input checked="" type="checkbox"/>
Laboratory head	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
Biologist investigator	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

checked: 2 0 2

Entities with access to the selected Profile

Profile (0) Role (0)

Email	Last name	First name	Profile name	Registered
				<input type="checkbox"/>

Administration module

ClinData

PreClinData

MedChemBio Portal

MOLDIMED Pipeline

CLAIRE

others

ClinData – software

- *<https://clindata.imtm.cz/>*
- Software solution designed for data management of clinical trials, registries, various healthcare or scientific databases
- Replacement of „Excel“ style of storing data
- The main programming language is Java 8. We use also String Framework, HTML, JavaScript, SQL and many others

ClinData - requirements

- The ClinData software is server-client application, web based. The only requirement for using it is Internet browser which supports HTML5 standard. The list of supported browsers:
 - Chrome: (Current - 1) and Current
 - Edge: (Current - 1) and Current
 - Firefox: (Current - 1) and Current
 - Internet Explorer: 11+
 - Safari: (Current - 1) and Current
 - Opera: Current

ClinData - hardware

- The ClinData software runs on computer cluster owned by Institute of Molecular and Translational Medicine (IMTM)
 - **Servers**
 - Blade chassis - BM Flex System Enterprise Chassis
 - 14x Compute node IBM Flex System x240 with 10 GB virtual fabric
 - 2x CPU Intel(R) Xeon(R) CPU E5-2650 0 @ 2.00GHz / 8C
 - 6x DDRIII SDRAM – 48GB
 - **Data Storages**
 - HP 3PAR data storage 700TB.
 - HP EML tape library
 - **Firewall**
 - HP F1000-S-EI VPN Firewall

ClinData - database

- The database used for storing data from the **ClinData** software is **Oracle Database** (commonly referred to as **Oracle RDBMS**)
- Version of database is 12.1. Standard edition.
- It runs on separated server which is firewalled from outside
- The operation system is RedHat.

ClinData – data backup

- Data are archived on **database level** and **operation system level**
- Database level backups
 - **RMAN** utility runs **every week**. The files are stored internally on database server and are copied to two independent backup sites.
 - **EXPDP/IMPDP** is data pump exporting data into text base backups every day. The backup files are stored to two independent backup sites.
 - **Redo Logs** are archived **every day** to filesystem.
- Operation system backups
 - **IBM Tivoli Storage Manager** (TSM Admin) is enterprise solution from IBM for backups and recovery of physical or virtual servers. It runs **every day** and the backup data is stored to disk array.

ClinData - secure connection

- Connection between server and client is secured by using **HTTPS** communication protocol which is encrypted using Transport Layer Security (**TLS**).
- **Security redirection**
 - All user requests coming via unsecured **HTTP** protocol are automatically **redirected** to secure **HTTPS** protocol.

ClinData - export and import

- **Import** Two ways how to insert new data into the ClinData software is to enter it manually via web forms or import via MS Excel format (.xlsx). The validity of data is controlled by in-build procedures.
- **Export** Exporting of data from the ClinData software is controlled by existing user's privileges/restrictions. Data is exported into MS Excel format (.xlsx).

ClinData - logging/auditing

- The ClinData software **records everything** happening in the system. There are two destinations for logging: files and database.
- **Software logging** is done on programming language level and is very detailed.
- **Access logging** is designed for controlling of user's activities. Every action of any user is written into logs.
- **Auditing** is focused to changes done in CRF forms.

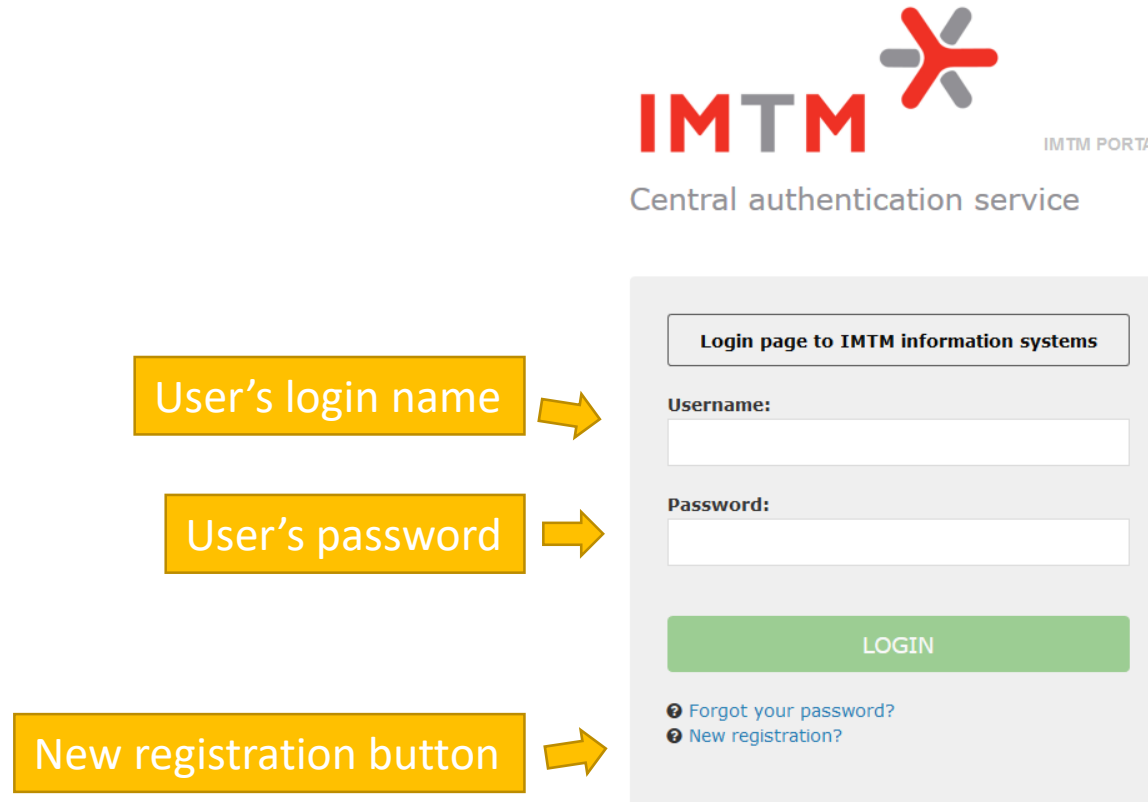


GDPR compliance

ClinData

**PROJECT: STANOVENI MULTIOMICKYCH PROFILU VE ZDRAVI A NEMOCI
A KORELACE S FENOTYPEM ONEMOCNENI: FAZE I ZDRAVI
DOBROVOLNICI**

ClinData – login page



The screenshot shows the login page for the IMTM PORTAL. At the top, the IMTM logo and 'IMTM PORTAL' text are displayed, followed by 'Central authentication service'. The main login form is titled 'Login page to IMTM information systems' and contains fields for 'Username:' and 'Password:'. A green 'LOGIN' button is positioned below these fields. At the bottom of the form, there are two links: 'Forgot your password?' and 'New registration?'. Three yellow callout boxes with arrows point to specific elements: 'User's login name' points to the username field, 'User's password' points to the password field, and 'New registration button' points to the 'New registration?' link.

IMTM PORTAL
Central authentication service

Login page to IMTM information systems

User's login name → Username:

User's password → Password:

LOGIN

[? Forgot your password?](#)
[? New registration?](#)

New registration button →

ClinData – home page

ClinData

Home

Patients



Study

CRF templates

Exports

Profiles

Logout (59:53)

ClinData

Server time December 13, 2018 12:28:54 PM CET

Search for patient

You can enter first name, second name, personal ID or address

Search

News

© 2018 IMTM

1.9.6-RELEASE

ClinData menu – access to all functions

Logout with timer

Search for patient

ClinData – list of patients

ClinData [Home](#) [Patients](#) [Study](#) [CRF templates](#) [Exports](#) [Profiles](#) [Logout \(59:57\)](#)

Patients in the study: STANOVENI MULTIMICKYCH PROFILU VE ZDRAVI A NEMOCI A KORELACE S FENOTYPEM ONEMOCNENI: FAZE I ZDRAVI DOBROVOLNICI

Filters

Search by id, name, a

Show rows



Sorting patients

Action buttons

Anonymized list of patients

ID	First name	Last name	Address	Sex	Birth date	Enrollment date	Last update	Action
2545	Patient 2545		n/a	M	1988/01/01	2018/09/26	2018/12/11	<input type="button" value="Open"/>
2546	Patient 2546				91/01/01	2018/09/26	2018/11/08	<input type="button" value="Open"/>
2547	Patient 2547		n/a	M	1978/01/01	2018/09/26	2018/11/08	<input type="button" value="Open"/>
2548	Patient 2548		n/a	M	1996/01/01	2018/09/26	2018/11/08	<input type="button" value="Open"/>
2549	Patient 2549		n/a	M	1988/01/01	2018/09/26	2018/11/08	<input type="button" value="Open"/>

ClinData – patient's tab

[ClinData](#)
[Home](#)
[Patients](#)
[Study](#)
[CRF templates](#)
[Exports](#)
[Profiles](#)
[Logout \(59:36\)](#)



Patient: Patient 2545 (id:2545) [Detailed identification data](#)

Patient in study: Patient 2545 [Enrollment data](#) [Back to list of patients](#)

Enrollment date

Control group

Informed consent files

[Export patient's data](#)

Forms in the study
STANOVENI MULTIMICKYCH PROFILU VE ZDRAVI A NEMOCI A KORELACE S FENOTYPEM
ONEMOCNENI: FAZE I ZDRAVI DOBROVOLNICI
[Export patient's data](#)

Overall completion of items on all forms

All: 74/171

Mandatory: 1/1

Action	Name	Last modification	Status	Completion ⓘ	
				All	Mandatory
Open	Identifikace dárce	24/10/2018	In progress	2/2	0/0
Open	Centrum		In progress	1/1	1/1
Open	Dotazník pro dárce krve		In progress	57/85	0/0
Open	Informovaný souhlas	11/12/2018	In progress	14/22	0/0
Open	Laboratoř		Not opened	0/27	0/0
Open	Rasa a etnická příslušnost		Not opened	0/34	0/0

List of CRFs (forms)


Form's status

Form's completion

ClinData – patient's CRF (form)

ClinData

[Home](#)
[Patients](#)
[Study](#)
[CRF templates](#)
[Exports](#)
[Profiles](#)

[Logout \(59:13\)](#)


Study

STANOVENI MULTIOMICKYCH PROFILU VE ZDRAVI A NEMOCI A KORELACE S
 FENOTYPEM ONEMOCNENI: FAZE I ZDRAVI DOBROVOLNICI

Status In progress
[Back to patient](#)

Form

Dotazník pro dárce krve (v.5)

[Open another form in the study](#)

Patient

Patient 2545 (id:2545)

Datum odběru

Datum odběru

Čas odběru

Údaje o dárci

Výška [cm]

Váha [kg]

Dotazník pro dárce krve

- Seznámil(a) jsem se s "Poučením dárce krve" a jeho obsahu rozumím.
- Považuji se za vhodného dárce bez rizikového chování, jehož krev neohrozí zdraví příjemce.
- Cítíte se zdrav(a)?
- Měl(a) jste v posledních měsících potíže (nachlazení, opar, průjem, zvracení)?
- Měl(a) jste někdy při odběru krve potíže (větší modřinu, slabost, mdloby, mravenčení)?

Header with location

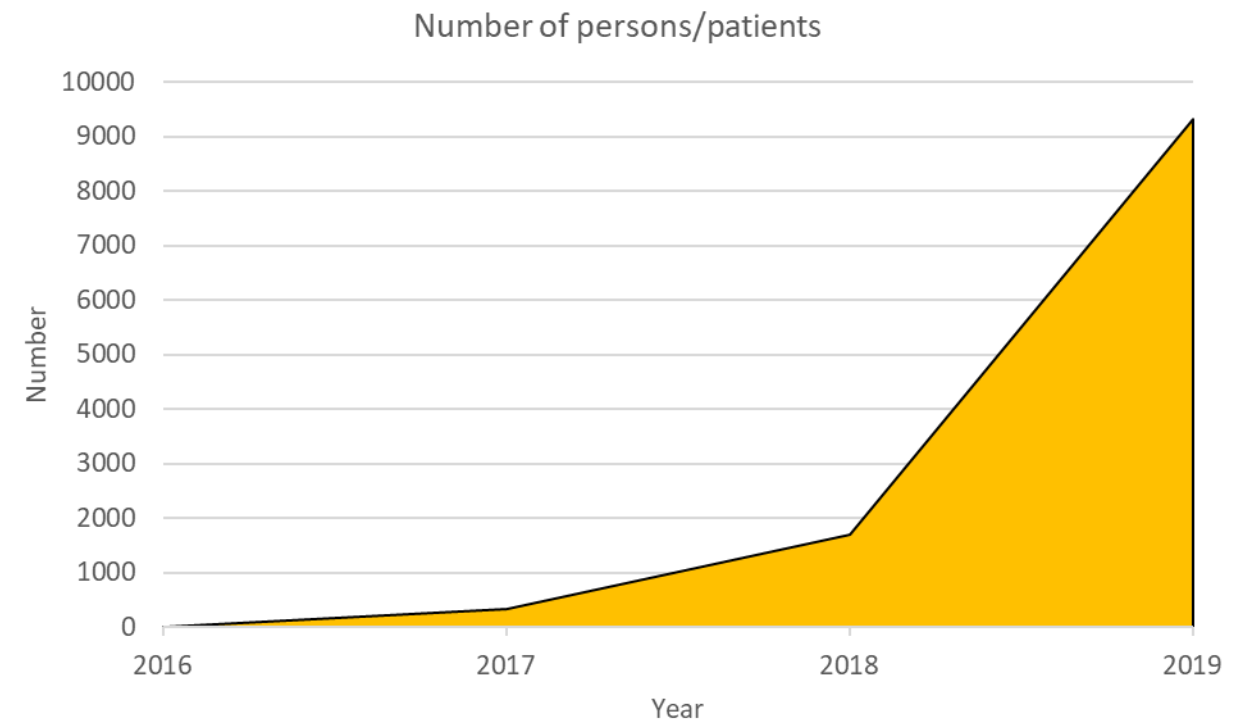
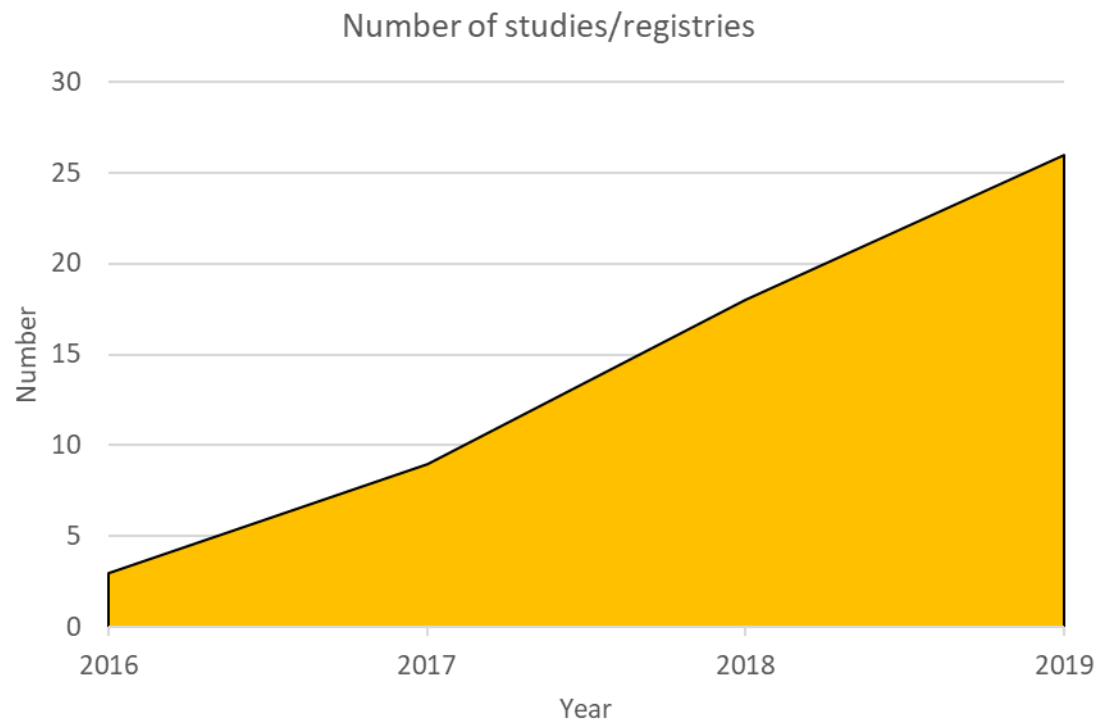
Form's status

Form's data

ClinData - exports

[illegible]

ClinData - statistics of usage



Mapping of the Czech Genome

- Target minimum 10.000 genomes, currently 2 funded projects (2x1.000):

ENIGMA (1000 genomes)

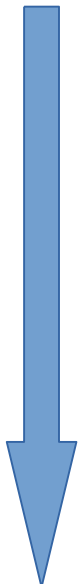
IAB, IMTM

A-C-G-T (1000 genomes)

CEITEC, UK, IMTM, CGB, Genomac



Bioinformatics – variant analysis

- 
- Reference genome: GRCh38/hg38 - primary assembly; without chromosomal anotation (ensembl)
 - Qualitative processing of FASTQ data using Trimmomatic software
 - alignment using BWA-MEM
 - Alignment optimization: labeling of PCR duplicates, recalibration of base quality (GATK)
 - QC of alignment using qualimap
 - Variants calling (VCF/gVCF) - GATK HaplotypeCaller

ENIGMA – current status

- 108 genomes sequenced
- Configuration of sequencing run: paired-end with length of 150 bases; NovaSeq
- Average size of files / sample:
- FASTQ 60 GB
- BAM 65 GB (to be archived)
- Object storage

Parameter	Experiment 1 (1x24)	Experiment 2 (1x12)
Yield [Gbp]	3010,58	3174,34
Cluster PF [%]	62,97	66,08
Average Q30 [%]	92	92,63
Number of Reads [Average]	2411762944	2530797696
Q30 [phred]		
Number of Reads per sample	401960491	421799616
Adapter Contamination	<1	<1
Coverage [Average]	min. 30x	min. 30x
Uniformity		

Multiomics study

- 1.000 healthy individuals as a reference
- **WGA**, epigenomics (PBMCs), transcriptomics (PBMCs), proteomics (plasma), **metabolomics** (plasma), **lipidomics** (plasma), miRNA profile (plasma)
- HORA – Human Omics Reference Atlas
- Disease cohorts to follow.

Administration module

ClinData

PreClinData

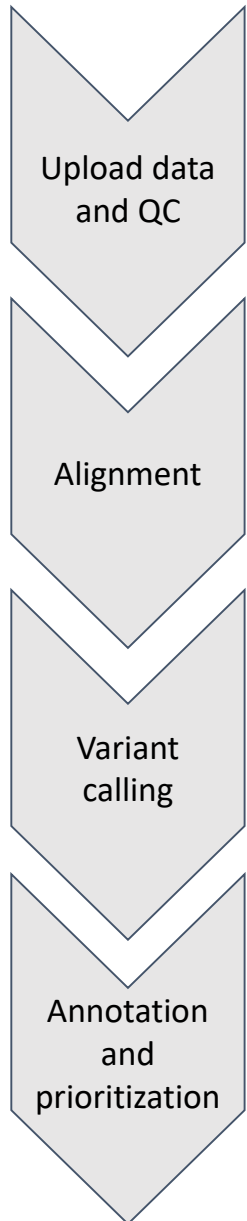
MedChemBio Portal

MOLDIMED Pipeline

CLAIRE

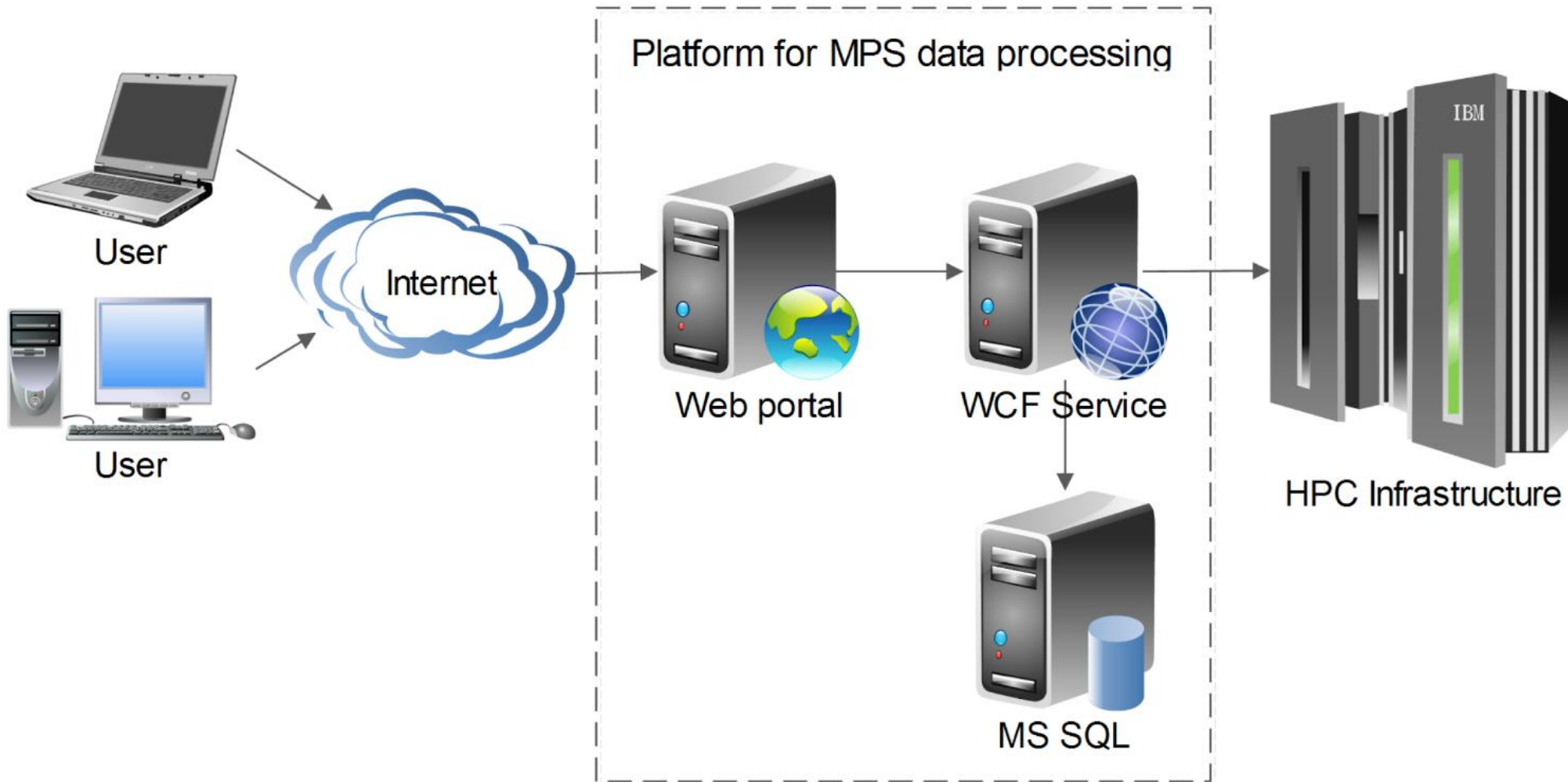
others

MOLDIMED Pipeline



- Integrated access for NGS data analysis
- Integration of 3rd party SWs and in house annotation SW (samtools, bcftools, FASTQC, BWA, GATK, VarScan2,...)
- GUI - web based access (“user-friendly”)
- Processing and analysis of WGS, WES, gene panels, CNVs in progress
- Gene variants annotation, integration of database resources, variants prioritization
- No need for internal computing capacity (HPC in Ostrava/Olomouc)

Implementation schema on HPC infrastructure



GUI

Home

Custom pipelines

Moldimed pipeline

Moldimed pipeline 2

Moldimed pipeline 3

Moldimed pipeline 5

NGS control

Visualization

Tools

File Upload

Feedback

Contact support

About

T A

Č R

Projekt č. TE02000058 Centrum kompetence pro molekulární diagnostiku a personalizovanou medicínu je řešen s finanční podporou TA ČR

11/6/2019, 7:58:04 PM

In case of any problem, please contact us on email: support.moldimed@it4i.cz

Adjustable parameters

Storage files

Input files

no files

Copy Files to Input

Delete Storage Files

Pipeline inputs

Input files

R2.fastq.gz

R1.fastq.gz

Sample Sheets

SaSh.csv

Copy to Single

Copy to Paired

Delete files

Single .fastq files

no files

Copy to Single root

Copy to Paired root

Delete Single files

Delete Paired files

Paired .fastq files

no files

Single-end project directories

no files

Delete Single files

Delete Paired files

Paired-end project directories

fastq_root

test_sample_01

test_sample_04

test_sample_02

test_sample_03

Delete Single files

Delete Paired files

Options

Remove duplicates

Assembly GRCH38.p10

VarScan2 settings

PHRED Mapping Quality

10

STRAND_FILTER

Create or edit SampleSheet

Service response

Starting pipelineFastq job ...

- Entry format: **FASTQ**

Key parameters are adjustable
(can be used for detection of somatic mutations just adjusting LOD)

- Parallel data processing (up to 3 clicks only)**

Imported annotated files

Imported annotated datasets

test_sample_01_NS_FM_CS_MD_MQ10.vcf_removedDuplicates_filtered_clin_pathogenic.csv (24/09/2018 08:56 Pipeline: 3)

View file

Export selection

Delete File

Saved filters

Filters

Load Filter

Delete Filter

Filters

Quality

=

Coverage

=

GO or HPO number

Common dbSNP

☒ All
 ☐ RS only
 ☐ without RS

Gene names (Import gene names from csv file and use semicolon (;) as a separator)

Choose File No file chosen

Parse CSV file

Filter results

Save filter

Reset Filters

Region

☐ gene
 ☐ non-genic
 ☐ chr not included

Structural variant

☐ SNV
 ☐ INDEL

Genotype

☐ non-reference heterozygous
 ☐ non-reference homozygous
 ☐ reference heterozygous

Transcript

☐ no duplicates

Feature

☐ NULL
 ☐ UTR5
 ☐ intron
 ☐ exon
 ☐ CDS
 ☐ spliceSite
 ☐ UTR3

Amino acid effect

☐ NULL
 ☐ INDEL
 ☐ synonymous
 ☐ nonsynonymous

Annotation and prioritization of variants is enabled via variant filtration using **gene ontology, population frequency and effect on protein translation**.

Frequency:

- dbSNP
- ExAC

Clinical effects:

- ClinVar

Functional predictors:

- Polyphen
- SIFT

Ontology:

- Human phenotype ontology (HPO)
- Gene ontology (GO)

Plus functional genes characterization, phenotypes, “drug-targeted” genes, etc.

MOLDIMED pipeline – current status

- Accredited according to ČSN EN ISO 15189:2013 for WES based diagnostics
- 13 users at the moment
- Implemented at IT4 and IMTM servers in Ostrava/Olomouc
- >120 WES analysed for routine diagnostic procedures
- Intended use for WGS in Czech Genomes project(s)

Administration module

ClinData

PreClinData

MedChemBio Portal

MOLDIMED Pipeline

CLAIRE

others

PreClinData – home page

Logout with timer

PreClinData [Studies](#) [Designers](#) [Profile](#) [Language](#) [Admin](#) [Logout](#) 29:01

[Create new study](#)

Protocol	Name	Start date	End date	Release date	Action
35-2019	Biodistribution study of RGD	2019-10-31	2019-10-31		Statistics Export
34-2019	Study of anticancer activity of compound PNH173 on subc...	2019-10-29	Not set	Not set	Open Statistics Export
33-2019	Study of anticancer activity of compound PNH173 on subc...	2019-10-29	Not set	Not set	Open Statistics Export
32-2019	Biodistribution study of siderophores.	2019-10-29	2019-10-29	Not set	Open Statistics Export
31-2019	Aspergillus infection therapy in rats	2019-10-17	2019-11-01	Not set	Open Statistics Export
30-2019	Biodistribution of radiolabelled ramucirumab in tumor mice	2019-10-11	Not set	Not set	Open Statistics Export
29-2019	Study of anticancer activity of compounds CuETAlb and irr...	2019-10-07	Not set	Not set	Open Statistics Export
28-2019	Animal Model Irradiation	2019-08-26	2019		Open Statistics Export
22-2019	Study of anticancer activity of compounds TZMB and CuET...	2019-05-29	2019-10-15	Not set	Open Statistics Export
20-2019	Animal Model Irradiation 6 Gy vs 8 Gy vs 10 Gy	2019-07-10	2019-08-19	Not set	Open Statistics Export

Showing 1 to 10 of 84 entries

Previous 1 2 3 4 5 ... 9 Next

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List of studies

Filtering and sorting

Available actions

PreClinData – Study details

Protocol number: **29-2019** | Study name: **Study of anticancer activity of compounds CuETAlb and irradiation on brain tumor.**

[Specifications](#)
[Drugs](#)
[Groups](#)
[Animals](#)
[Records](#)
[Statistics](#)
[Forms in study](#)
[Scheduler](#)

Study name:
 Study of anticancer activity of compounds CuETAlb and irradiation on brain tumor.
 Study components

Protocol number:
 29-2019

Reference number:
 41830/2018-7

Sponsors:
 IMTM

Aim:
 Study of anticancer activity of compounds CuETAlb and irradiation on brain tumor.
 Study parameters

Type of experiment:
 Study of anticancer activity

Species:
 Mice

Strains:
 × SCID

Vehicles:
 × H2O

Start date:
 2019-10-07

PreClinData – study components

[Specifications](#) [Drugs](#) [Groups](#) [Animals](#) [Records](#) [Statistics](#) [Forms in study](#) [Scheduler](#)

Drug name	LEM code	Description	Stock solution [mg/ml]	Action
<i>CuET albumin</i>	Not set	HSA+H2O+DTC+CuCl	1	Edit Delete
<i>RTG</i>			10	Edit Delete
<i>RTG + CuET albumin</i>	Not set	10Gy + 1 mg/ml	Not set	Edit Delete
<i>Control</i>	Not set	Not set	Not set	Edit Delete

[Save changes](#) [Discard changes](#) [+ Add new drug](#)

[Specifications](#) [Drugs](#) [Groups](#) [Animals](#) [Records](#) [Statistics](#) [Forms in study](#) [Scheduler](#)

Group name	Drug	Vehicle	Dose	Action
<i>Gr I.</i>	RTG + CuET albumin	H2O	10,1 + Gy,mg/kg	↑ ↓ Records Clone Edit Delete
<i>Gr II.</i>		H2O	1 mg/kg	↑ ↓ Records Clone Edit Delete
<i>Gr III.</i>	RTG	Not set	10 Gy	↑ ↓ Records Clone Edit Delete
<i>Gr IV.</i>	Control	Not set	mg/kg	↑ ↓ Records Clone Edit Delete

[Save changes](#) [Discard changes](#) [+ Create new group](#)

PreClinData – study records

Selection of groups

Selection of days

Drug, dose and vehicle

Gr I. [closed] Gr II. [closed] Gr III. [closed] Gr IV. [closed] D5 [closed] + New visit

Drug CuET albumin - 1 mg/ml Dose 1.0 mg/kg Edit Vehicle H2O

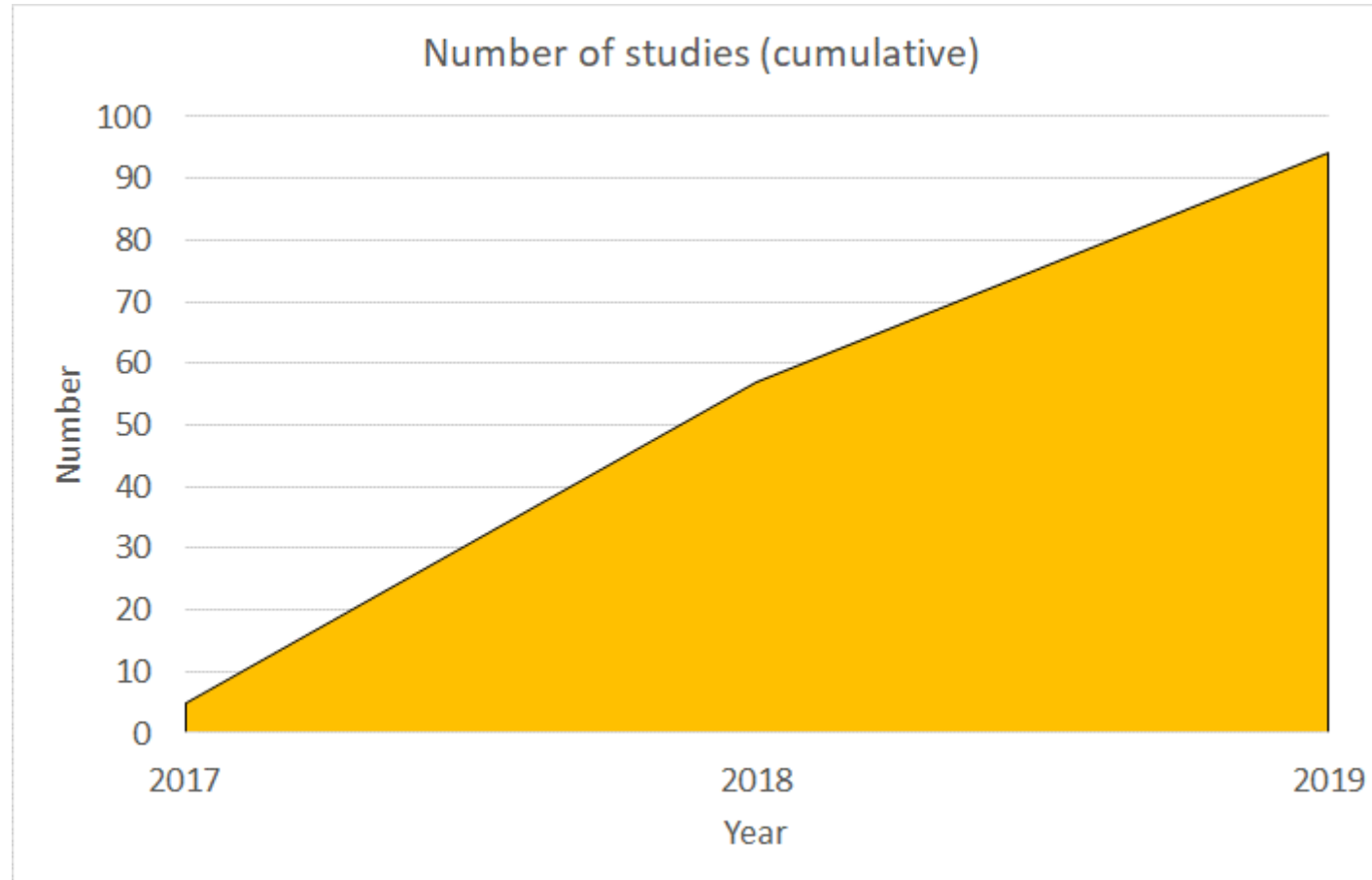
Animal	section				Action
	Weight	BSC	Adverse events description	Drug/vehicle [ul/g]	
Mouse_1 [alive]	16	BCS 3		16.0	Edit
Mouse_2 [alive]	21.1	BCS 3		21.1	Edit
Mouse_3 [alive]	22.6	BCS 3		22.6	Edit
Mouse_4 [alive]	21.8	BCS 3		21.8	Edit
Mouse_5 [alive]	22.4	BCS 3		22.4	Edit
Mouse_6 [alive]	21.3	BCS 3		21.3	Edit
Mouse_7 [alive]	20.8	BCS 3		20.8	Edit
Mouse_8 [alive]	21.2	BCS 3		21.2	Edit

Study records

PreClinData - statistics



PreClinData - statistics of usage



Administration module

ClinData

PreClinData

MedChemBio Portal

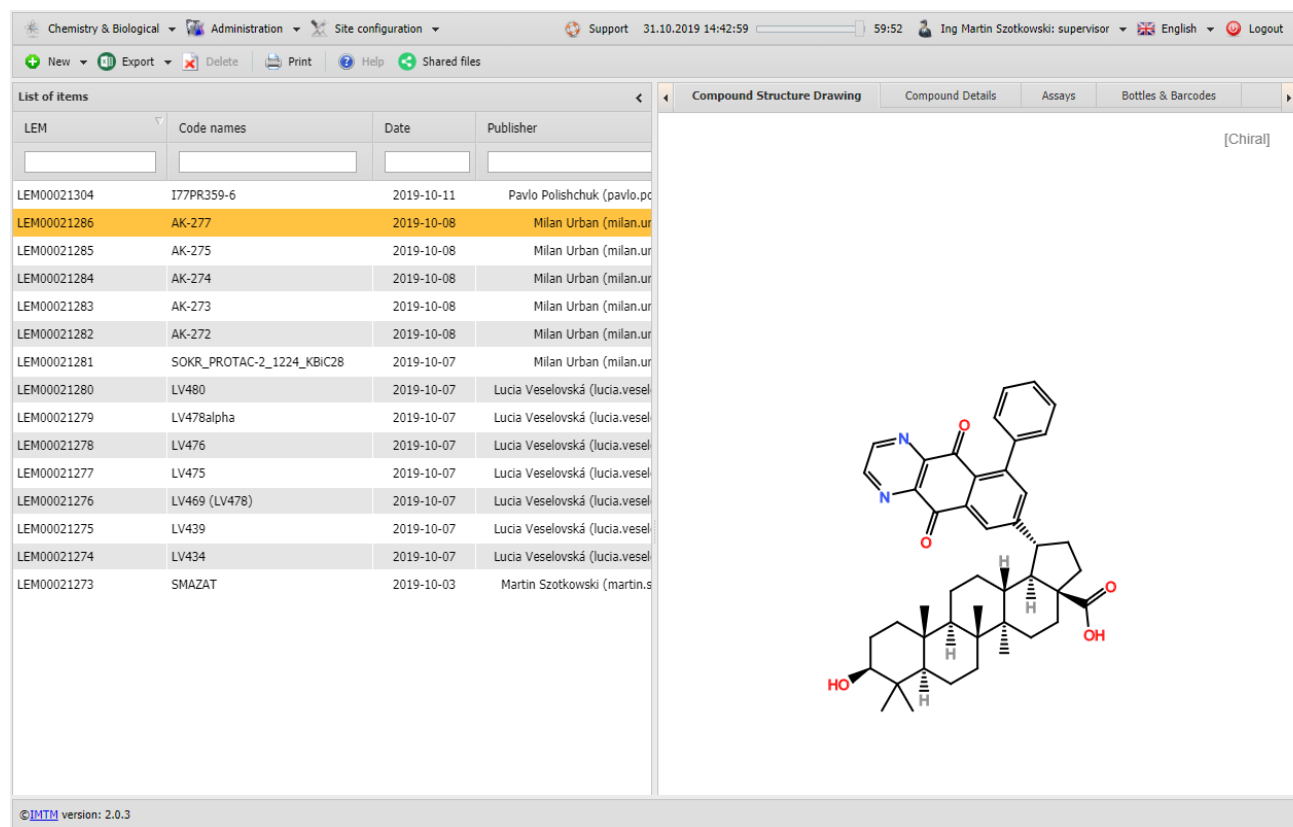
MOLDIMED Pipeline

CLAIRE

others

Portal MedChemBio

- Chemical portal
 - Compounds
 - Assays
 - Bottles & Barcodes
- Feature
 - Import, export
 - Edit
 - Search



The screenshot displays the Portal MedChemBio interface. The top navigation bar includes links for Chemistry & Biological, Administration, Site configuration, Support, and a user profile for Ing Martin Szotkowski. Below the navigation bar, there are tabs for New, Export, Delete, Print, Help, and Shared files. The main content area is divided into two sections: a table of items and a chemical structure drawing area.

LEM	Code names	Date	Publisher
LEM00021304	I77PR359-6	2019-10-11	Pavlo Polishchuk (pavlo.pc)
LEM00021286	AK-277	2019-10-08	Milan Urban (milan.ur)
LEM00021285	AK-275	2019-10-08	Milan Urban (milan.ur)
LEM00021284	AK-274	2019-10-08	Milan Urban (milan.ur)
LEM00021283	AK-273	2019-10-08	Milan Urban (milan.ur)
LEM00021282	AK-272	2019-10-08	Milan Urban (milan.ur)
LEM00021281	SOKR_PROTAC-2_1224_KBIC28	2019-10-07	Milan Urban (milan.ur)
LEM00021280	LV480	2019-10-07	Lucia Veselovská (lucia.vesel)
LEM00021279	LV478alpha	2019-10-07	Lucia Veselovská (lucia.vesel)
LEM00021278	LV476	2019-10-07	Lucia Veselovská (lucia.vesel)
LEM00021277	LV475	2019-10-07	Lucia Veselovská (lucia.vesel)
LEM00021276	LV469 (LV478)	2019-10-07	Lucia Veselovská (lucia.vesel)
LEM00021275	LV439	2019-10-07	Lucia Veselovská (lucia.vesel)
LEM00021274	LV434	2019-10-07	Lucia Veselovská (lucia.vesel)
LEM00021273	SMAZAT	2019-10-03	Martin Szotkowski (martin.s)

The chemical structure drawing area on the right shows a complex molecule with a steroid-like core and a fused ring system. The structure is labeled [Chiral] and includes stereochemical indicators. The bottom status bar indicates the version: © IMTM version: 2.0.3.

Compound registration

- Draw
- Single MDL MOL
- Multiple MDL SDF

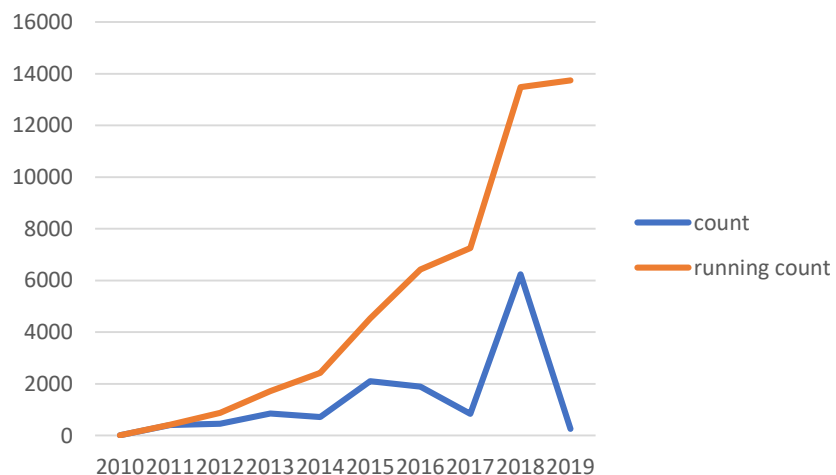
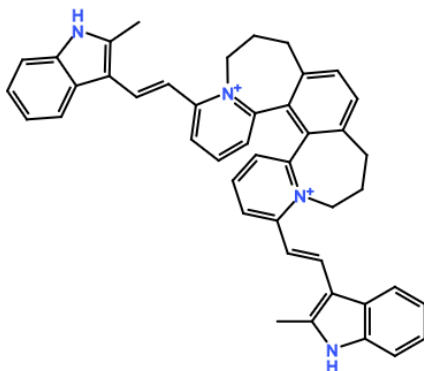
The screenshot displays three overlapping windows from a chemical software application:

- New item (Chemical Editor):** Shows a chemical structure of a complex molecule with an indole ring system connected to a polycyclic system. A vertical toolbar on the left lists elements: H, C, N, O, S, P, F, Cl, Br, and a bullet point. The top toolbar contains various drawing and editing tools.
- New item (MDL Molfile):** Displays the text representation of the structure. The text includes:

```
atoms 40 bonds 45
Portal of medicinal and biological chemistry
mol io
40 45 0 0 1 0 0 0 0 0999 V2000
-3.2383 -0.8972 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.2383 -1.7222 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
-2.5239 -2.1347 0.0000 C 0 0 1 0 0 0 0 0 0 0 0 0
-1.8094 -1.7222 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.8094 -0.8972 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0
-2.5239 -0.4847 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.0949 -2.1347 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.3804 -1.7222 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.3804 -0.8972 0.0000 C 0 0 2 0 0 0 0 0 0 0 0 0
-1.0949 -0.4847 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
0.3340 -0.4847 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
0.3340 0.3403 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
-0.3804 0.7528 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.0949 0.3403 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
1.0485 -0.8972 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0
```
- MDL SDF upload:** A dialog box titled "MDL SDF upload" with the subtitle "(SDF: <Code> -> Compound: Code name)". It features "Add files" and "Upload" buttons. Below, a file named "compounds.sdf (3.95 Kb)" is listed with a red 'X' icon.

Compounds

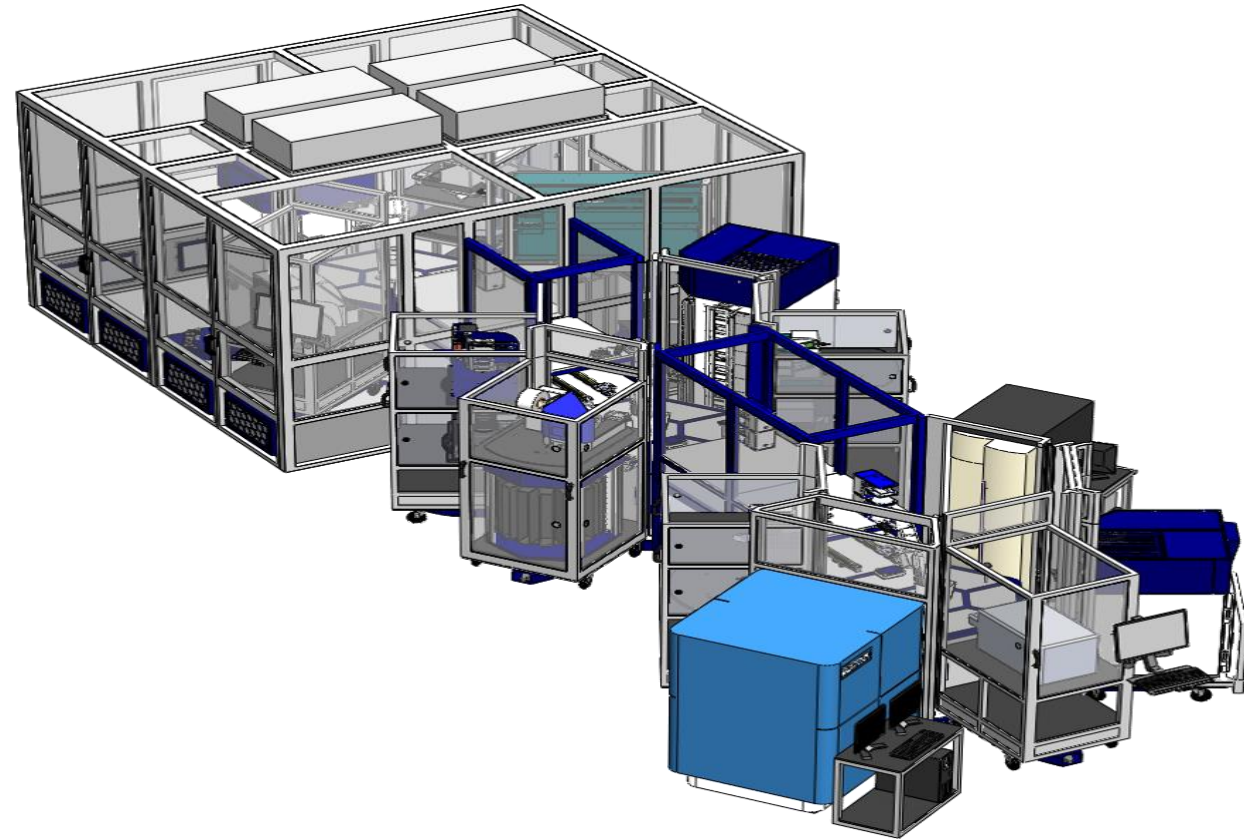
- Drawing
- LEM and Code name
- InChI, InChiKey, SMILES, MDL MOL
- ~20 000 compounds in IMTM proprietary collection



General information	
LEM Code	LEM00021304
Copyright (c)	© 2019 IMTM
Library	IMTM
Code name	I77PR359-6
InChI	InChI=1/C44H38N4.2CHF3O3S/c1-29-35(37-15-3-5-17-39(37)45-29)25-23-33-13-7-19-41-43-31(11-9-27-47(33)41)21-22-32-12-10-28-48-34(14-8-20-42(48)44(32)43)24-26-36-30(2)46-40-18-6-4-16-38(36)40;2*2-1(3,4)8(5,6)7/h3-
InChiKey	InChiKey=ICJJMJZRCUJXNU-UHFFFAOYNA-N
SMILES	CC1=C(C=CC2=CC=CC3=[N+]2CCCC4=CC=C5CCC[N+]6=C(C=CC=C6C=CC7=C(C)NC8=C7C=CC=C8)C5=C43)C9=C(C=CC=C9)N1.C(F)(F)(F)S(=O)(=O)[O-].C(F)(F)(F)S(=O)(=O)[O-]
Adding information	
Molecular formula	I77PR359-6
Molecular weight	922.9573131049: CAS Registry NO.
IUPAC Name	
Synonyms	
Chemical name / Description	
Files	
MDL Molfile	atoms 64 bonds 70 Portal of medicinal and biological chemistry mol io

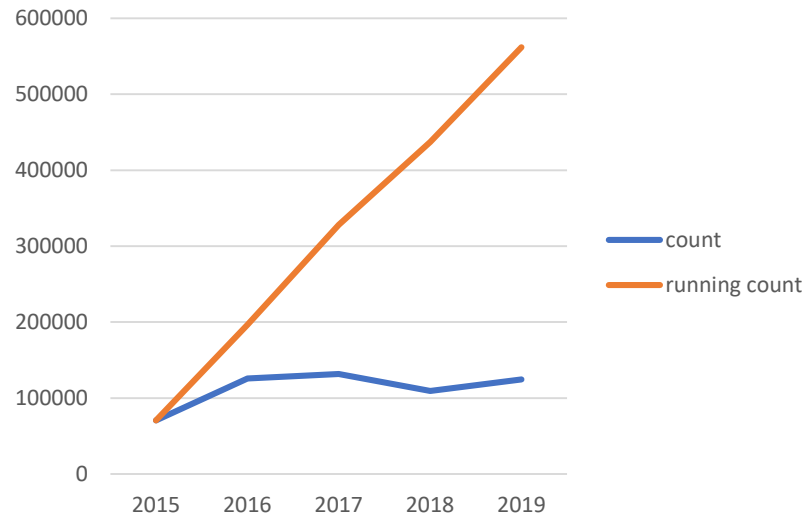
Assays

- Assays
 - Cytotoxicity (MTT + tMTT)
 - Antimicrobial Activity
 - Cell Cycle Analysis – Flow cytometry
 - Pharmacology in vitro
 - Kinase Activity
 - RAGE
- Source:
 - Dotmatics connection – HTS platform
 - Excel import + edit



Cytotoxicity

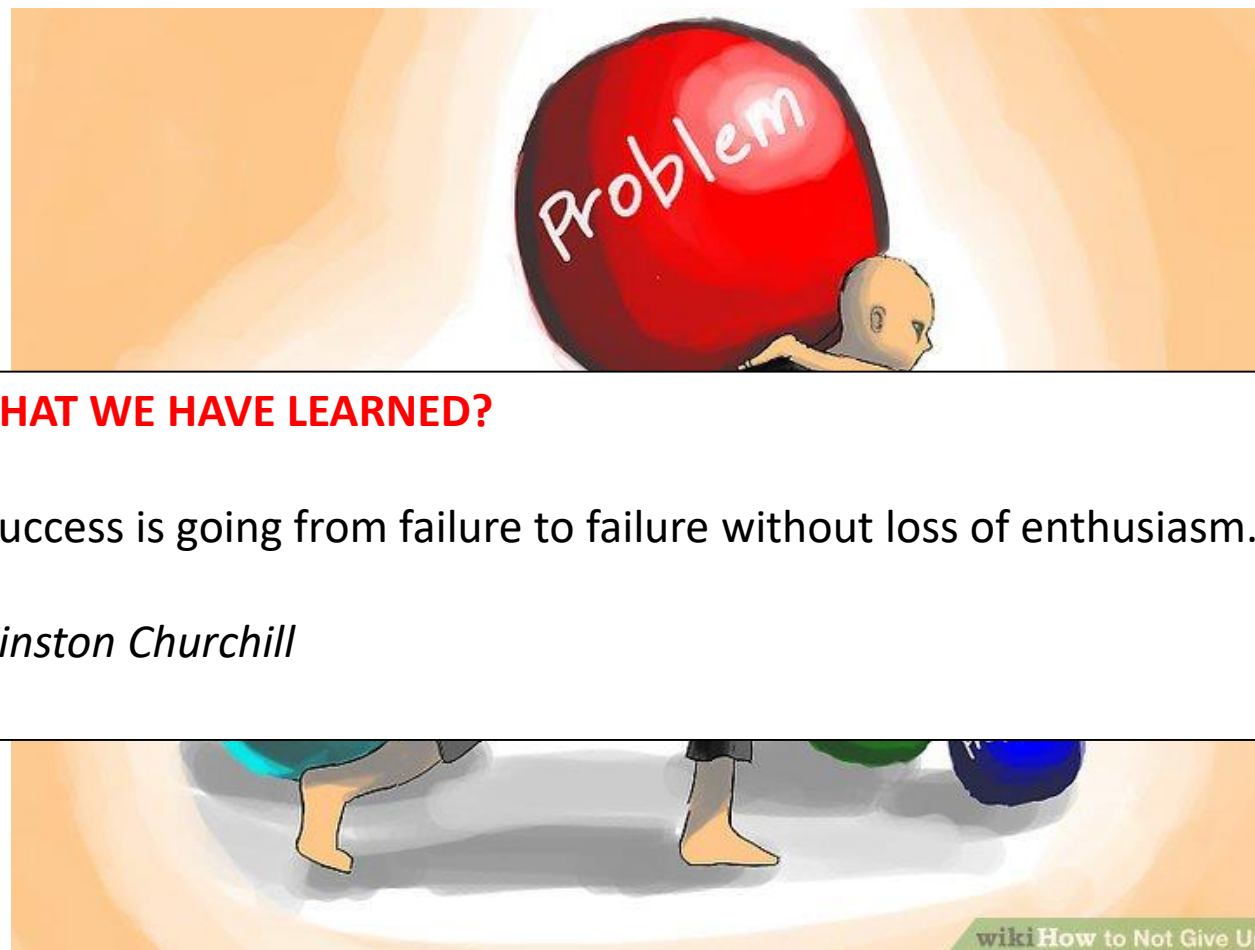
- Dotmatics
- ~600 000 experiments



MTT						
	Batch ID	Cell Line	IC50 (μM)	SD	Published	n
+	C11H9N3O2-001	A549	37.55	5.89	■ Yes	8
+	C11H9N3O2-001	BJ	>50	-	■ Yes	6
[-]	C11H9N3O2-001	CCRF-CEM	17.88	1.79	■ Yes	8
	Date	Experiment ID	X	Validated		
	2016-05-25	140657		18.09	■ Yes	
	2016-05-25	140657		15.17	■ Yes	
	2016-05-30	140705		19.74	■ Yes	
	2016-05-30	140705		19.60	■ Yes	
	2016-05-30	140704		19.56	■ Yes	
	2016-05-30	140704		18.17	■ Yes	
	2016-05-25	140656		17.09	■ Yes	
	2016-05-25	140656		15.62	■ Yes	
+	C11H9N3O2-001	CEM-DNR	25.65	2.09	■ Yes	7
+	C11H9N3O2-001	HCT116	20.15	0.72	■ Yes	6
+	C11H9N3O2-001	HCT116p53-	23.52	2.23	■ Yes	6
+	C11H9N3O2-001	K562	49.61	1.10	■ Yes	8
+	C11H9N3O2-001	K562-TAX	24.35	4.93	■ Yes	5
+	C11H9N3O2-001	MRC-5	>50	-	■ Yes	6
+	C11H9N3O2-001	U2OS	31.03	6.98	■ Yes	5

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- Authentication module: **Martin Szotkowski**, Petr Pavliš, Jan Lošťák, Marián Hajdúch, Petr Džubák
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WHAT WE HAVE LEARNED?

“Success is going from failure to failure without loss of enthusiasm.”

Winston Churchill

Thank you for attention!