

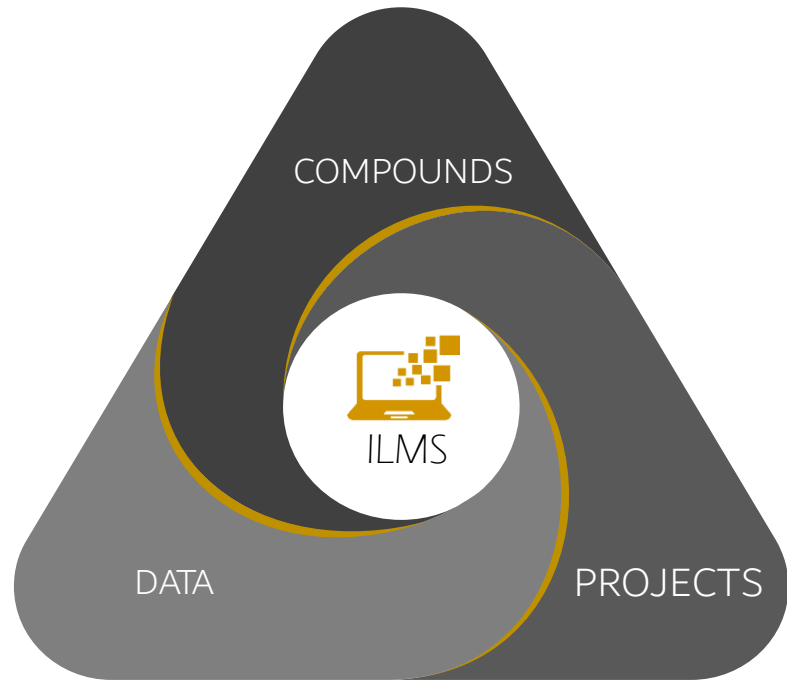
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Biotech.

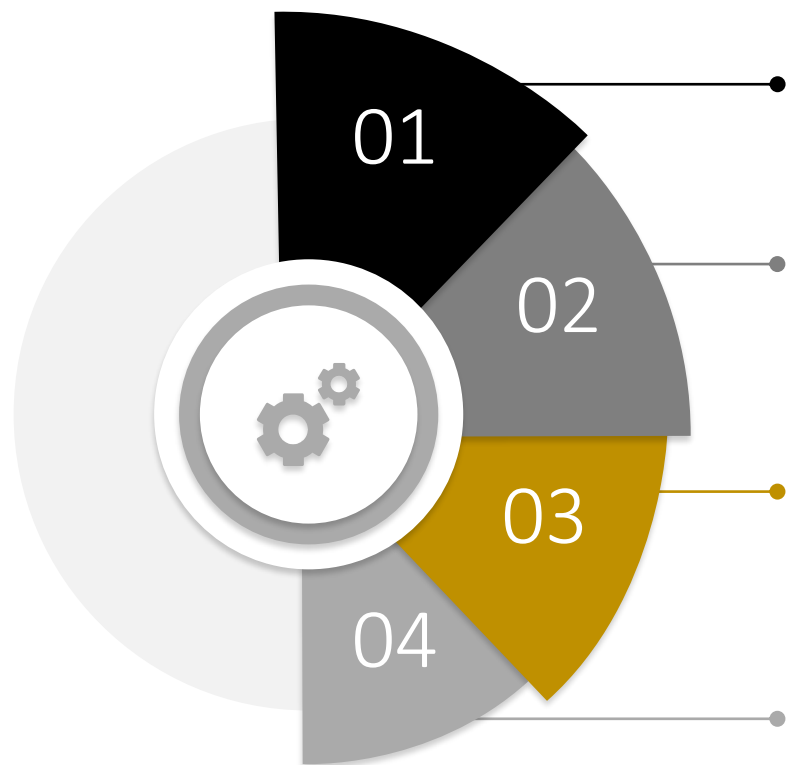
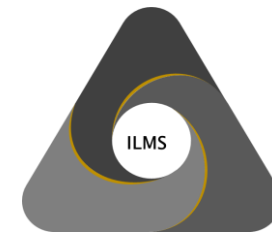
- Build Together -

Bruno Sargueil INEON Biotech
Chemaxon user meeting –Budapest 21-03-2018

INEON Lab Management Software



Compound Management



Manual design

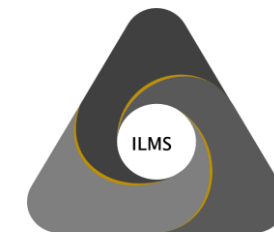
Sd file import (.sdf)

Intuitive field mapping interface

Sub-library organization (provider – research results – series ...)

Multiparametric search (structure, properties results ...)

Compound management – ID



CONTAINER INFO

BATCHES INFO

ATTACHED DOCS

POWERED BY ChemAxon

INEON - BDD IDV - [Composé: TIK000001]

Fichier Composé Import Plaque Projet Trace Test Affichage Administration Fenêtre ?

Banques Opérations

Hierarchie des banques

- [Auto] Globale (4555)
- [Auto] EvaCorporation (0)
- [Auto] Prestwick (4555)

Composé

Nom 10,13-diméthyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tétradécahydro-1H-cyclopenta[a]phénanthrène-3-yl acetate

Code TIK000001

Code secondaire 1

Code secondaire 2

Code secondaire 3

Commentaires

Propriétés

Stereochimie

LogP 4,61

LogS -5,017

H donneurs

H accepteurs

Sel

Etat [P] Poudre

Formule C21H30O3

Masse mol (g/M) 330,468

Couleur Yellow

Fluorescence ex 342 - Em 418

Solubilité 3,0000000000

Chemical structure: CC(=O)OC12CC3=C(C)CC4=C(C)C(=O)CC5=C4C=CC=C3C51

Opérations

Projet

Documents

Projet

Conditionnement

Enregistrer Enregistrer et fermer

code 1 Ancien code 2 Ancien code 3

Informations sur le lot sélectionné

Propriété	Valeur
Quantité achetée (mg)	50,00000
Quantité en solution (mg)	50,00000
Quantité en solution (mg)	0,00000
Quantité totale restante (mg)	0,00742

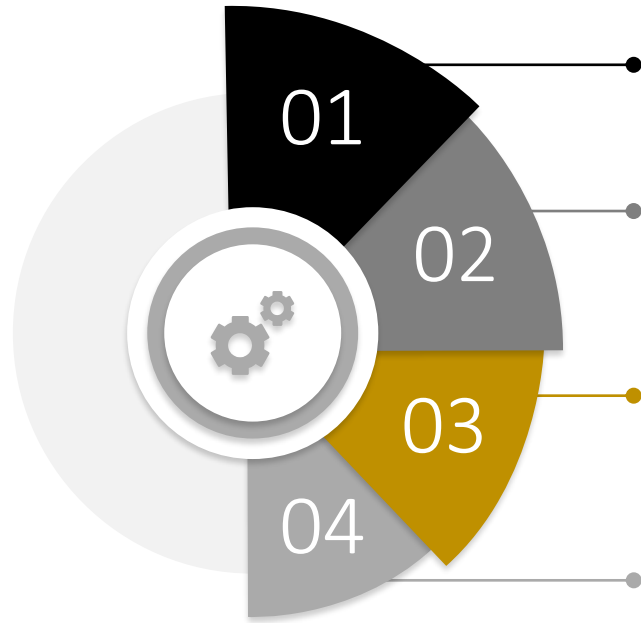
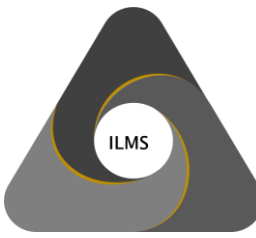
Code Nom Ancien code 1 Ancien code 2 Ancien code 3 Série Formule

Code	Nom	Ancien code 1	Ancien code 2	Ancien code 3	Série	Formule
TIK000001	10,13-diméthyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tétradécahydro-1H-cyclopenta[a]phénanthrène-3-yl acetate					C21H30O3
TIK000002	N-(4,6-dipropoxy-2-pyridinylethyl)acétamide					C17H24N2O5
TIK000003	4-nitro-N-(2-pyridinylethyl)acetamide					C11H12N2O4
TIK000004	4-chloro-3,5-diméthylbenzamide					C11H12ClN2O

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Designations – Structure – Physicochemical properties

Library management – Robotic jobs



Reformatting 96 ↔ 384

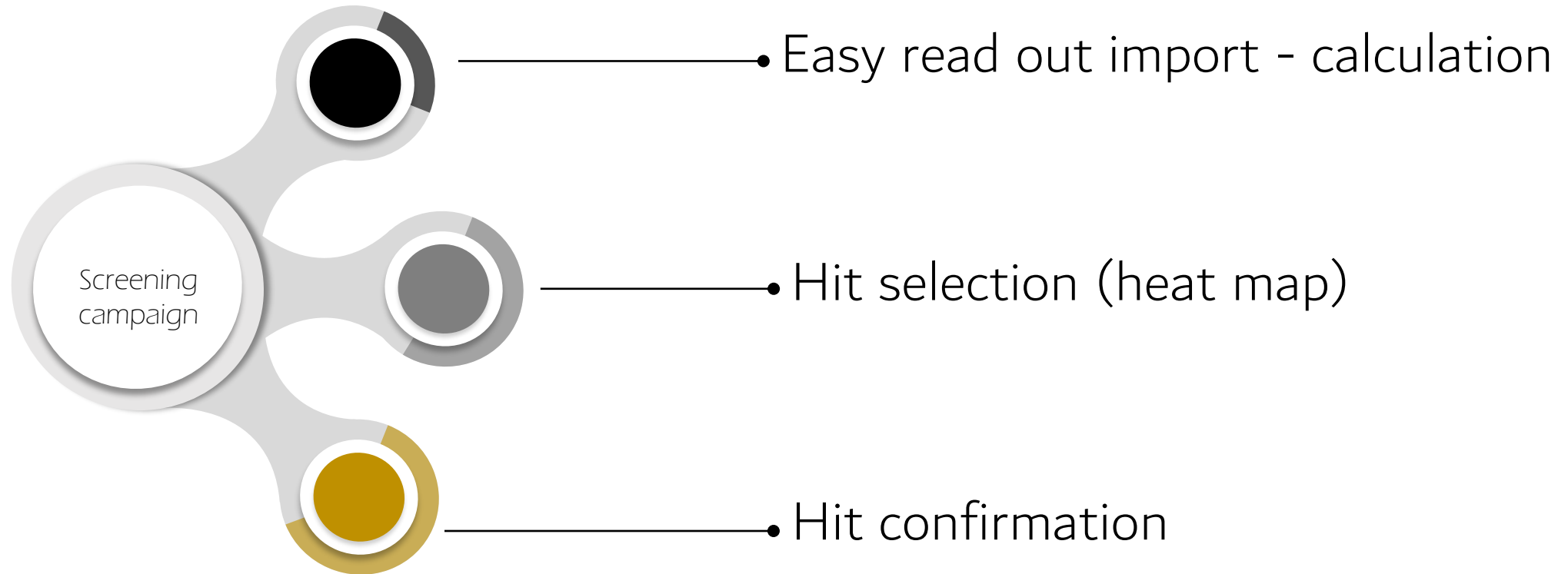
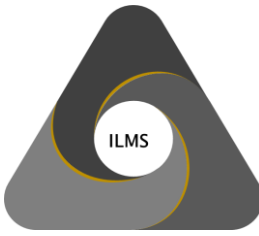
Replication

Dilution

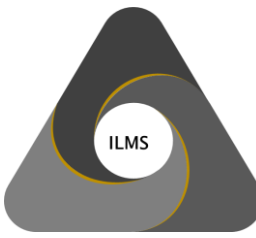
Cherry Picking

Generates worklists for robotic platforms – Job tracking through robotic exports

Screening campaign



Screening follow-up



INEON - BDD IDV - [Projet :]

Fichier Composé Import Plaque Projet Trace Test Affichage Administration Fenêtre ?

Opérations Projets

Tous les projets

- En cours
 - [Alpha] Alpha
 - IC50
 - Screening I
 - Screening II
- Terminés

Composé	Structure	Série	Z	Z'	% inhibition	IC50	Quantité restante (mg)
TIK002151		CYD 3206	0,816908	0,488257	0,4589855980		0,000000
TIK002181		CK 137	0,816908	0,488257	0,3880192027	16,1000000000	0,000000
TIK002280		CYD 3206	0,816908	0,488257	0,9215195158	16,1000000000	0,000000
TIK002551			0,816908	0,488257	0,3892715508	16,3000000000	0,000000

19 composé(s) / 95 résultat(s)

Supprimer Enregistrer Enregistrer et Fermer Sortir

Banque : 1-1000 / 4555 (Tous) [1/5]

Code	Nom	Ancien code 1	Ancien code 2	Ancien code 3	Série	Formule
TIK000001	10,13-diméthyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tétradécahydro-1H-cyclopenta[a]phénanthrène-3-yl acétate					C21H30O3
TIK000002	N-(4,6-dipropoxy-2-pyrimidinyl)-4-nitrobenzamide					C17H20N4O5
TIK000003	4-nitro-N-[(2-phényl-2H-1,2,3-triazol-4-yl)méthylène]benzohydrazide					C16H12N6O3
TIK000004	4-chloro-3,5-diméthylphényl 3-(2-nitrophényl)acrylate					C17H14ClNO4

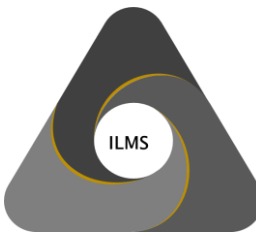
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bsargueil - Bruno SARGUEIL

- Hit ranking
- Multiparametric search
- Series definition

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Series optimization



INEON - BDD IDV - [Projet :]

Fichier Composé Import Plaque Projet Trace Test Affichage Administration Fenêtre ?

Opérations Projets

Tous les projets

- En cours
 - [Alpha] Alpha
 - IC50
 - Screening I
 - Screening II
- Terminés

Général Équipe Tests primaires Tests secondaires

Cc1ccc(cc1)CN(Cc2ccc(cc2)C)OC3=CC=CC=C3C

18 composé(s) / 18 résultat(s)

Code composé: TIK000050

Série:

Voir Document lié Fichier Date

Lot	Test	Résultat	Unité	Autre valeur	Plaque	Expérimentateur	Date	Quantité restante (mg)
000001	Screening II			Oui	TOK000001	Val	09/02/2018	0.000000
000001	Screening II			Oui	TOK000001	Val	09/02/2018	0.000000
000001	Screening II			Fébrile	TOK000001	Val	09/02/2018	0.000000
000001	Screening II			Mort	TOK000001	Val	09/02/2018	0.000000
000001	Screening II			Chétif	TOK000001	Val	09/02/2018	0.000000
000001	Screening II			Ok	TOK000001	Val	09/02/2018	0.000000
000001	Screening II			Valide	TOK000001	Val	09/02/2018	0.000000
000001	Screening II			Aveugle	TOK000001	Val	09/02/2018	0.000000
000001	Screening II			Gonflé à bloc	TOK000001	Val	09/02/2018	0.000000
000001	Screening II			Toujours en vie	TOK000001	Val	09/02/2018	0.000000
000001	Screening II	12.000000	UI		TOK000001	Val	09/02/2018	0.000000
000001	Screening II	15.000000	UI		TOK000001	Val	09/02/2018	0.000000
000001	Screening II	18.000000	UI		TOK000001	Val	09/02/2018	0.000000
000001	Screening II	5.000000	UI		TOK000001	Val	09/02/2018	0.000000
000001	Screening II	1.000000	UI		TOK000001	Val	09/02/2018	0.000000
000001	Screening II	22.000000	UI		TOK000001	Val	09/02/2018	0.000000
000001	Screening II	13.000000	UI		TOK000001	Val	09/02/2018	0.000000

Ajouter Enlever Filtrer Série

Supprimer Enregistrer Enregistrer et Fermer Sortir

Banque : 1-1000 / 4555 (Tous) [1/5]

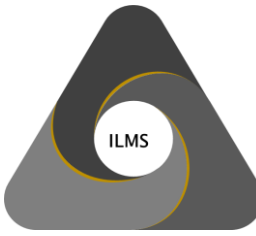
Code	Nom	Ancien code 1	Ancien code 2	Ancien code 3	Série	Formule
TIK000001	10.13-dimethyl-17-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl acetate					C21H30O3
TIK000002	N-(4,6-dipropoxy-2-pyrimidinyl)-4-nitrobenzamide					C17H20N4O5
TIK000003	4-nitro-N-([2-phenyl-2H-1,2,3-triazol-4-yl]methylene)benzohydrazide					C16H12N6O3
TIK000004	4-chloro-3,5-dimethylphenyl 3-(2-nitrophenyl)acrylate					C17H14ClNO4

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- Multiple results management
- Multiparametric search
- Reporting

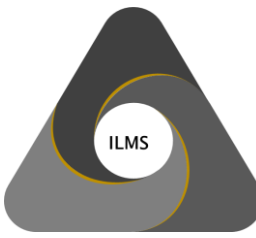
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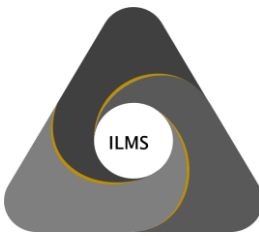
- All in one
- Intuitive
- Collaborative (profiles with authorizations)
- Strict tracking
- Easy customization

Pricing



Users	Company		Academics	
	SAAS	On-Premise	SAAS	On-Premise
1	500 €	50 000 €	350 €	33 000 €
2	475 €		333 €	
3	450 €		315 €	
4	425 €		298 €	
5	400 €		280 €	
>5	Contact us			

INEON - facts



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Scientific
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