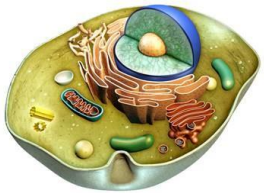
Sprint Bioscience

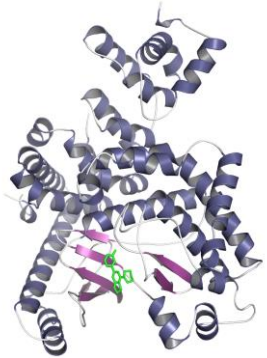
MANAGING PATENT APPLICATIONS USING CHEMCURATOR AND MARVIN LIVE

JENNY VIKLUND, CHEMAXON UGM MARCH 2018

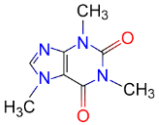
SPRINT BIOSCIENCE



Treat cancer

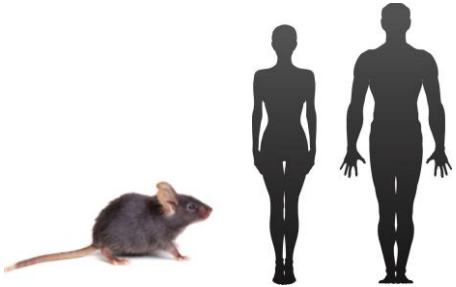


Select target



Find hits

Medicinal chemistry



Reduce tumor growth

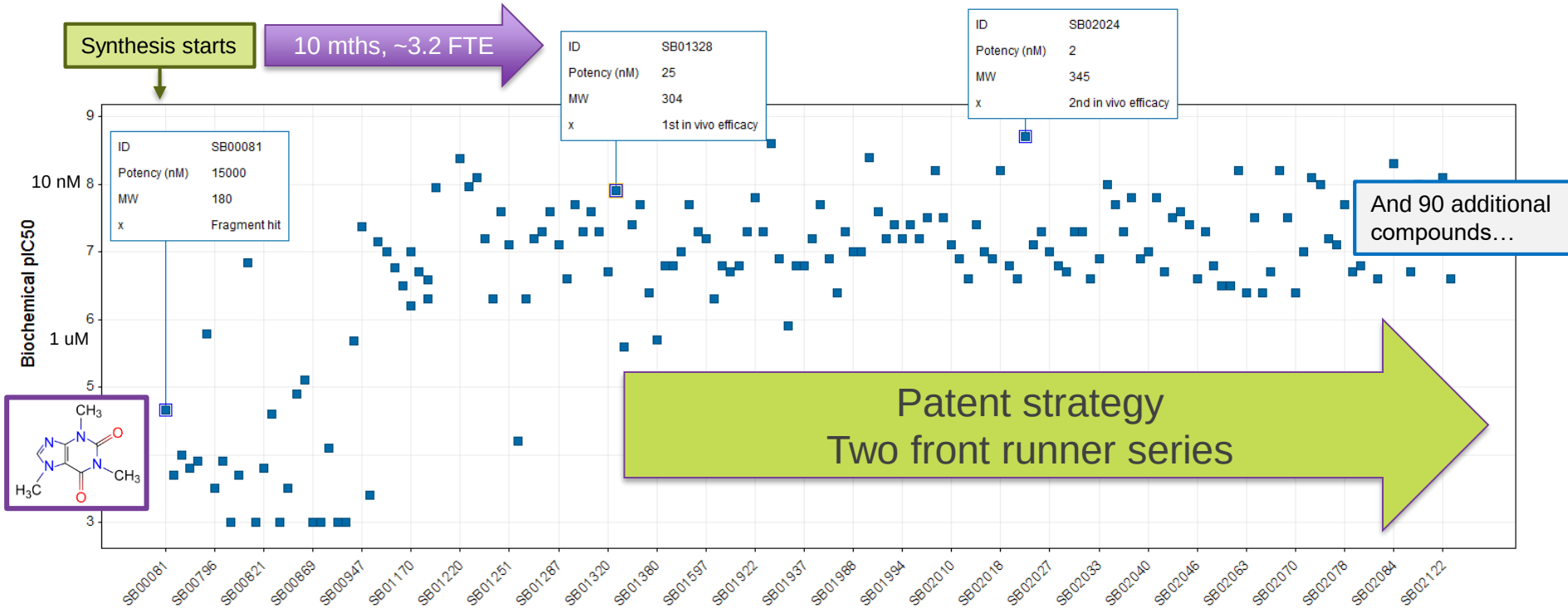
PiP4K2A

PETRA PHARMA

VPS34

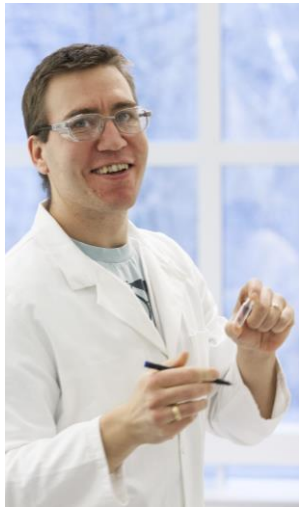
STK25

EFFECTIVE FBDD PROCESS TO CREATE SERIES

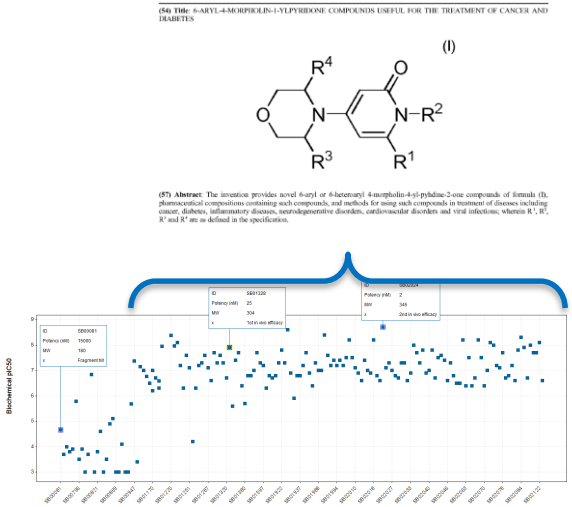


CHEMCURATOR TO DOUBLE CHECK CLAIMS

Synthesize the compounds



Write the claims:

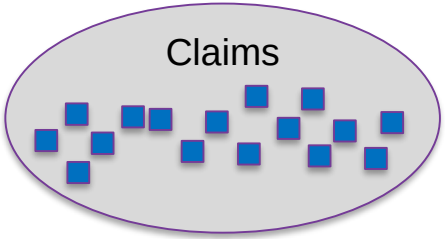


(54) Title: 6-ARYL-4-MORPHOLIN-1-YLPYRIDONE COMPOUNDS USEFUL FOR THE TREATMENT OF CANCER AND DIABETES

(I)

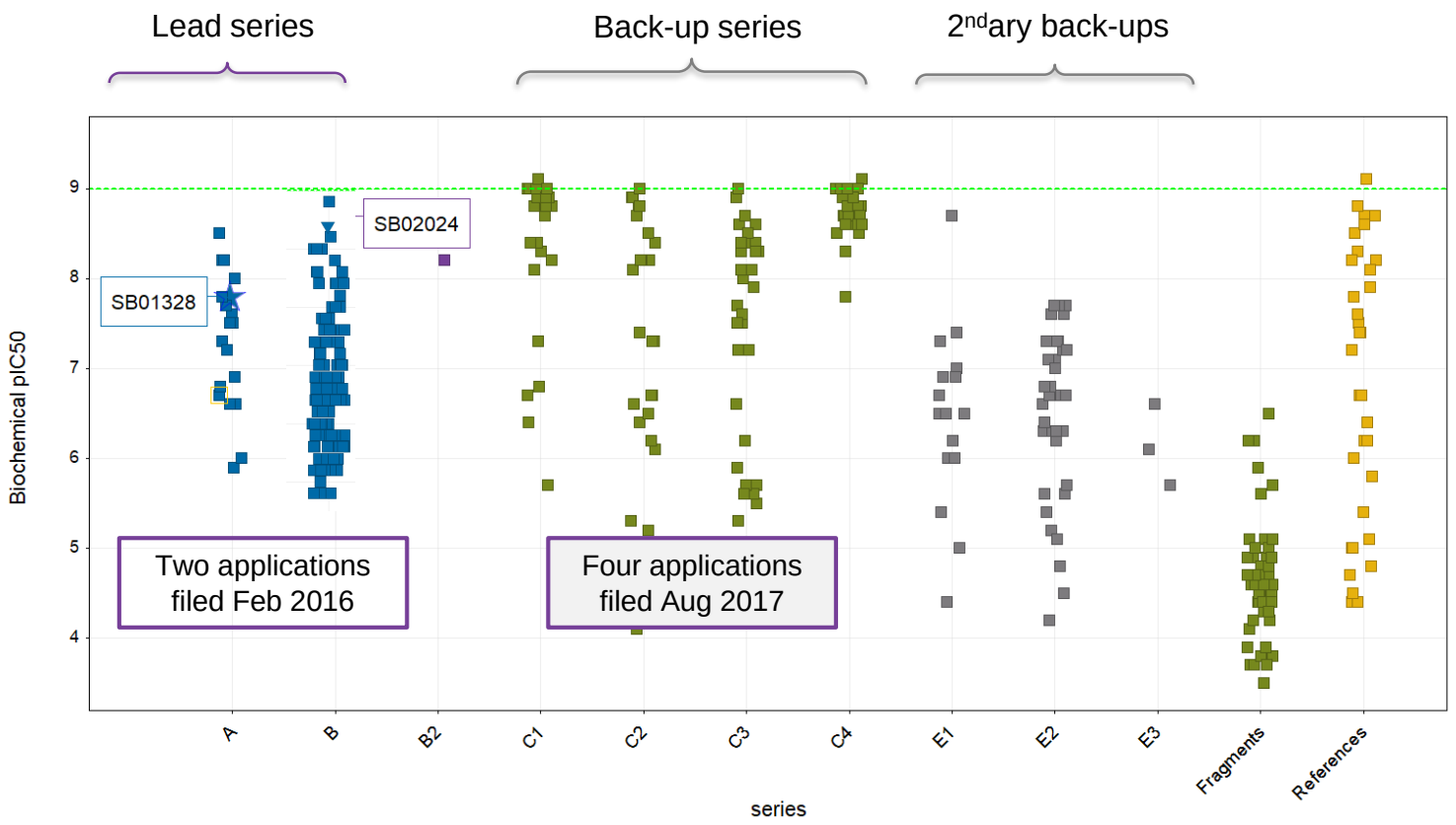
(57) Abstract: The invention provides novel 6-aryl or 6-heteroaryl 4-morpholin-4-yl-pyridine-2-one compounds of formula (I), pharmaceutical compositions containing such compounds, and methods for using such compounds in treatment of diseases including cancer, diabetes, inflammatory diseases, neurodegenerative disorders, cardiovascular disorders and viral infections; wherein R^1, R^2, R^3 and R^4 are as defined in the specification.

ChemCurator mission:
Double-check that the claims are covering all the exemplified structures:



Submit application

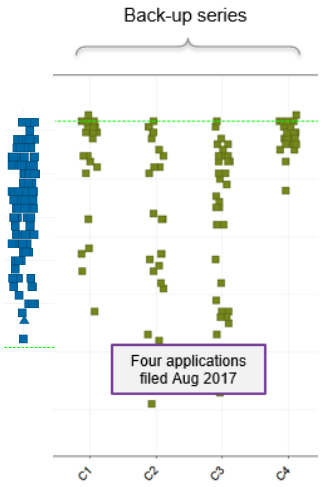
…AND FOUR BACK-UP SERIES!



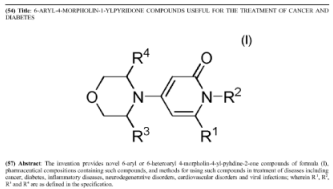
Assay wall: 1.5 nM

PROCESS FOR BACK-UP APPLICATIONS

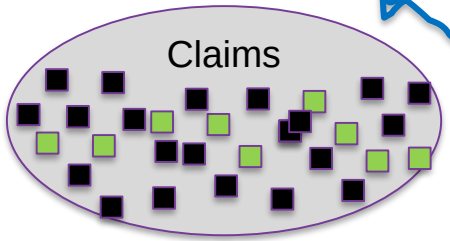
SOME compounds are synthesized



Imagine all compounds we want to synthesize and then write the claims:



ChemCurator mission: Double-check that claims are covering both **synthesized** and **ENUMERATED** structures:



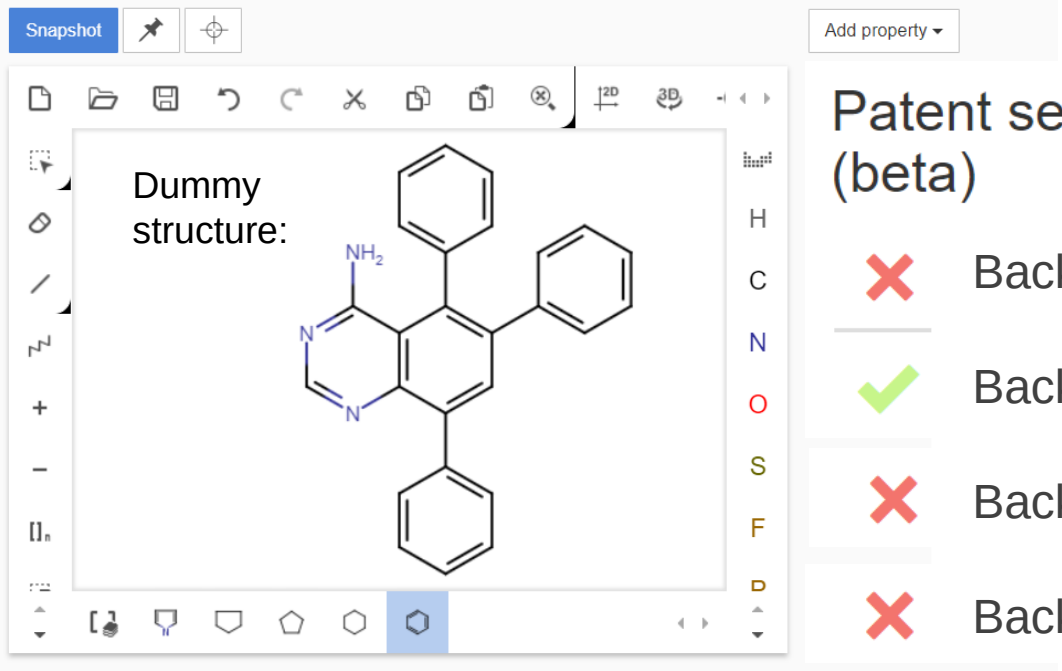
x 4

Double-check that claims are covering **new** compounds

SUBMIT

Synthesize additional compounds during priority year:

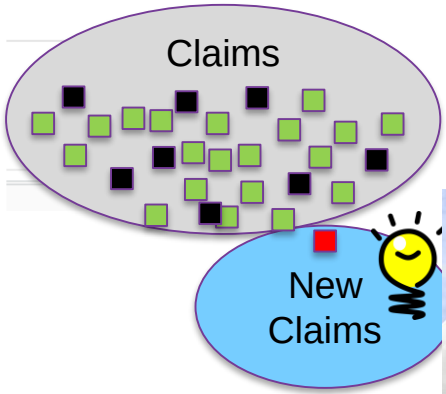
CHEMCURATOR INTEGRATED WITH MARVIN LIVE



Patent search (beta)

- ✗ Back-up A1
- ✓ Back-up A2
- ✗ Back-up A3
- ✗ Back-up A4

Double-check that claims are covering compounds synthesized within priority year



ACKNOWLEDGEMENTS

- Árpád Figyelmesi
- András Strácz
- Anna-Maria Kovacs

DREAM MODE

Idea for a program to facilitate
writing and double checking claims

TEDIOUS TO READ AND WRITE – BUT IMPORTANT

wherein
R^1 is aryl or heteroaryl, said aryl and said heteroaryl being mono- or bicyclic and optionally substituted with one or more of R^5, R^6, R^7 and R^8;
R^2, R^3 and R^4 are independently selected from hydrogen, C_1-C_3haloalkyl and C_1-C_3alkyl;
R^5, R^6, R^7 and R^8 are independently selected from halogen, C_1-C_6alkyl, C_1-C_6alkoxy, C_1-C_6haloalkyl, amino, $-NHSO_2R^9$, hydroxy, phenyl and a monocyclic heteroaryl;
R^9 is C_1-C_3haloalkyl or C_1-C_3alkyl;
and pharmaceutically acceptable salts, tautomers and stereoisomers thereof.

2. A compound according to claim 1, wherein R^4 is C_1-C_3alkyl.

3. A compound according to claim 1 or claim 2, wherein R^2 is selected from hydrogen and methyl.

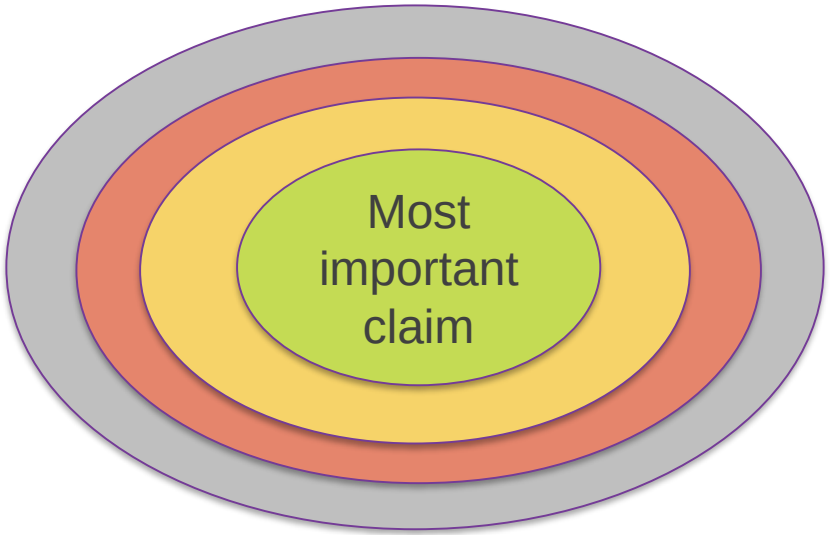
4. A compound according to any one of claims 1 to 3, wherein R^3 is hydrogen.

5. A compound according to any one of claims 1 to 4, wherein R^4 is methyl.

6. A compound according to any one of claims 1 to 5, wherein R^2 is hydrogen.

7. A compound according to any one of claims 1 to 6, wherein
R^1 is selected from phenyl, furyl, thienyl, pyridyl, pyrimidinyl, naphtyl, quinolinyl, indazolyl, indolyl, 4-azaindolyl, benzoxazolyl, benzimidazolyl, benzothiophenyl, each optionally substituted with one or more of R^5, R^6, R^7 and R^8; and

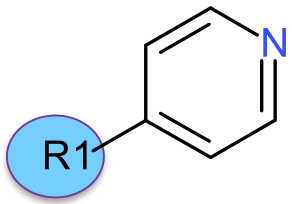
- Multi-dimensional onion structure

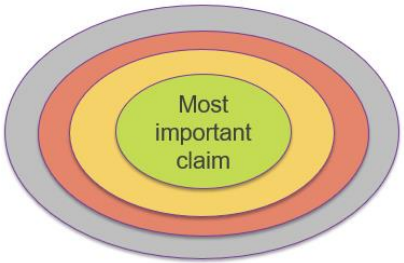


WHAT IS A PROGRAMMING FUNCTION?

- The Body Mass Index-function:
  - Input: length and weight (1.65 m and 70 kg)
  - Function calculates (weight/length^2) = 24

CREATE CLAIMS VIA ”SUBSTITUENT FUNCTIONS”:





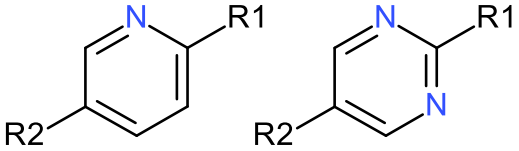
input	Name of the function
Cl Br Me tBu	– ”The most important substituents in R1”
F Et iPr	– ”Other substituents that we have synthesized but somewhat less promising”
H MeO cHexyl	– ”Additional substituents that we have not exemplified but it is reasonable to believe that they also will be active”

SUGGESTED WORKFLOW

1. Fill the ”functions” with input by drawing structures

2. Write and double check the claims, using the **name of the functions**.

3. Let the Dream Mode PROGRAM expand the functions into the usual patent lingo



”the core”

We want to claim…
The core, optionally substituted with one or more of the most important substituents in R1…

A compound according to claim 1, wherein R^1 is phenyl or a monocyclic 5-6 membered heteroaryl each optionally substituted with one or more substituents selected from C_1-C_6alkyl, C_1-C_6haloalkyl, C_1-C_6alkoxy, C_1-C_6haloalkoxy, amino, -N-C_1-C_3alkylamino, -N,N-di-C_1-C_3alkylamino or halogen;

BENEFITS OF DREAM MODE PROGRAM

- Easier and faster than plain writing
- Less errors
- Intuitive for Medicinal chemists
- Reduce cost when using patent attorneys

THANK YOU!

Questions?

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