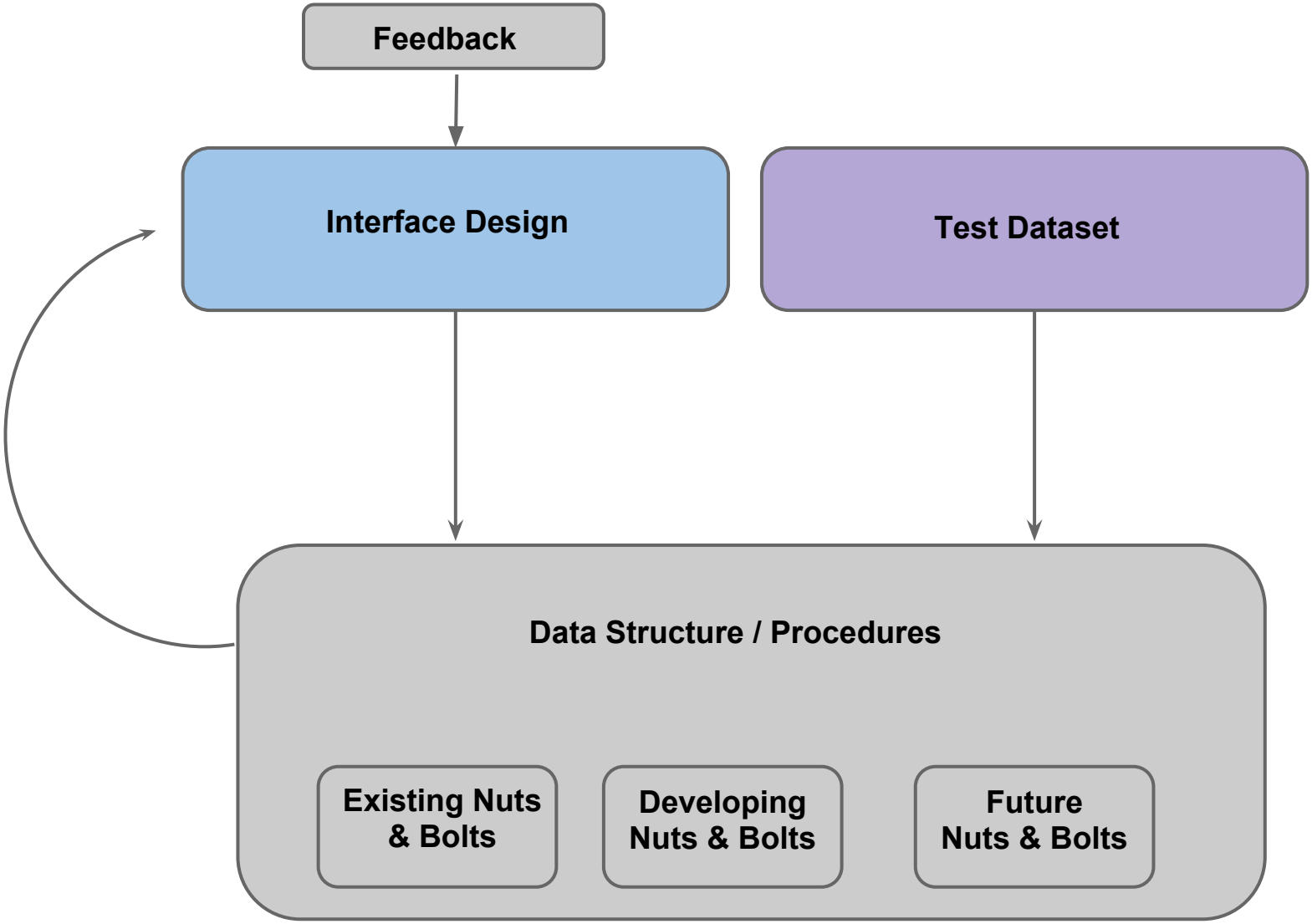
GINAS Software Development Update

- Frontend:
  - Web Interface / Form Design
- Backend:
  - Adapting / proving abstract Object Model based on:
    - Analysis of FDA test dataset
    - Necessary features of web interface
      - Registration
      - Display
      - Edit

Development Strategy



Web Interface Design

- Extremely Critical
  - A "Common Language" platform for development and discussion.
  - The main window into the system.
- Mock-ups Very Helpful
  - Registration Forms / Wizard (critical)
  - Record Displays
  - Search Interface
  - Login / Profile / Administration
    - Language / Jurisdiction

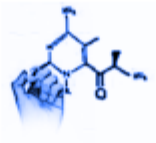
GINAS

Login Peryeat Password *********

Home Search Download Register Admin

Search GINAS Taxol

Chemical Structure Amino Acid Sequence Nucleic Acid Sequence



GINAS

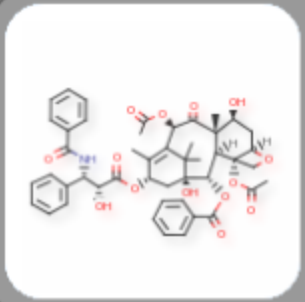
Peryeat logout

Home Search Download Register Admin

Taxol

Substances	2
Specified Substances	0
Products	0
Clinical Trials	0
Applications	0

Query:
Taxol



Paclitaxel UNII-P88XT4IS4D

Taxol (more)

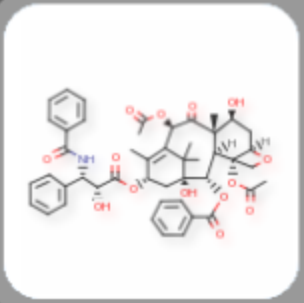
Definition:

Stereochemistry: Absolute, Chiral (more)

Classification:

Antineoplastic Agent : Taxanes [L01CD01] (more)

View Related(12) Full Record



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View Related(12) Full Record

(Previous) (Next)

FDA SRS - Test Migration (Chemical)

- Compiled test dataset from public domain FDA SRS
  - ~50,000 substances
  - ~500,000 names
  - ~80,000 products
  - Lots of other substance-related information

- Focus - Testing chemical object model:
  - Chemical Substances
  - Names

FDA SRS - Test Migration (Chemical)

- SRS dataset of 31,275 UNIIs with Chemical Structure
  - *1,665 substances not in chemical class*
  - 29,610 Chemical substance class
    - 145 with parsing errors (S-groups)
    - 29,465 Chemical substances loaded
    - 29,461 Unique Structure + Description
    - 29,222 Unique Chemical Structure

- Example apparent UNII 'clash'

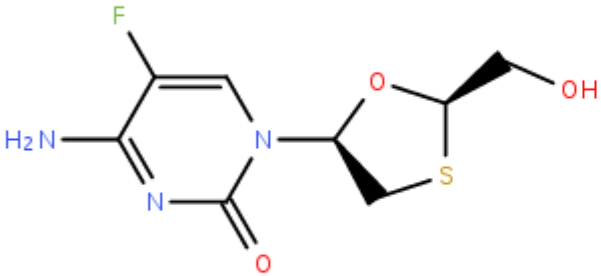
ULS8902U4O & ***G70B4ETF4S***

RACIVIR & EMTRICITABINE

Analyzing Test Data

ULS8902U4O

dqlKCa-YwkHIZ-HnfRNw



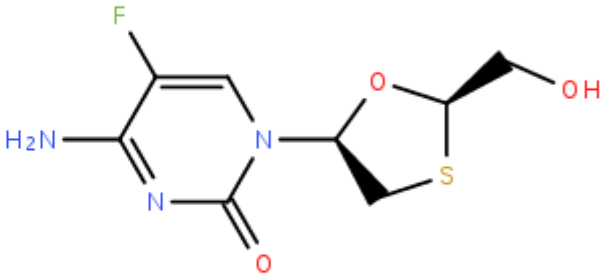
<NO FURTHER DESCRIPTION>

RACIVIR

(actually racemic)

G70B4ETF4S

dqlKCa-YwkHIZ-HnfRNw



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EMTRICITABINE