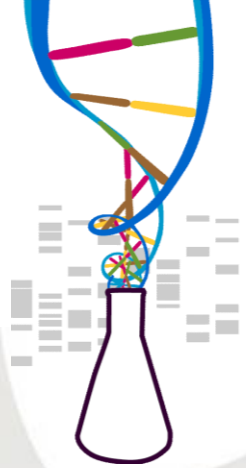


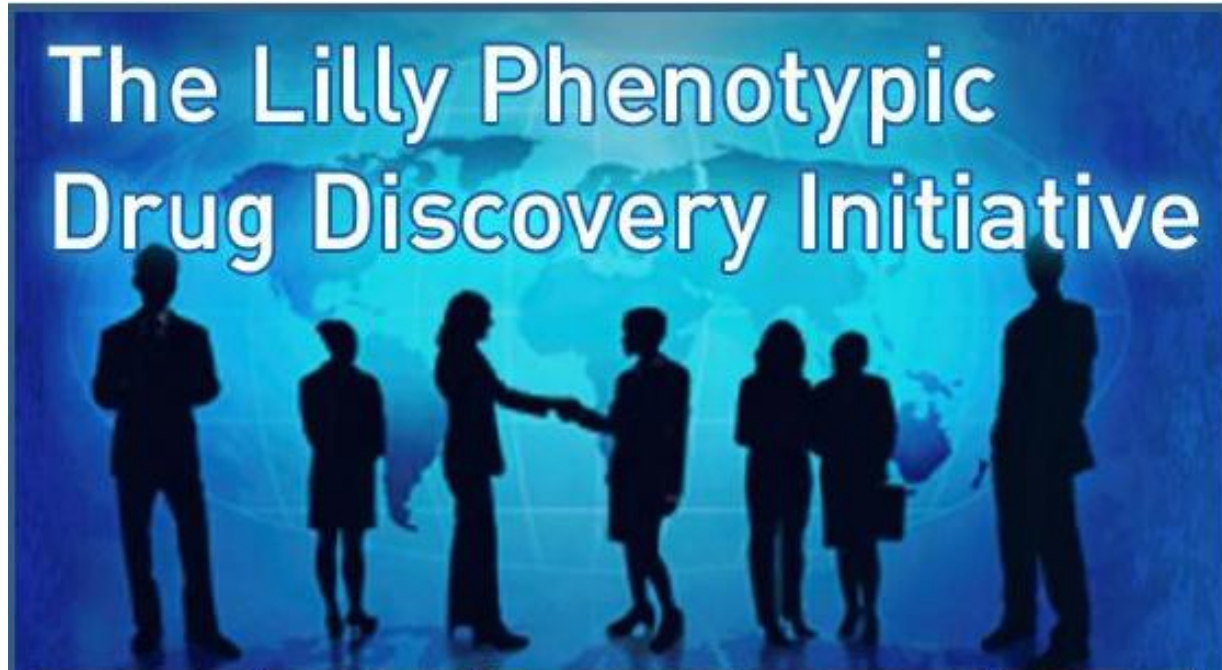
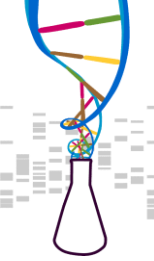
Ad Futurum: DEL XVII AL XXI: PROYECTANDO NUESTRA TRADICIÓN HACIA EL FUTURO



1608

2010

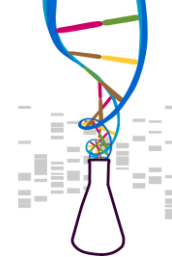
**1ª JORNADA
SECTORIAL: 16/02/11
L3: INVESTIGACIÓN EN
BIOMEDICINA Y DESARROLLO
DE FÁRMACOS**



Lilly

pd2.lilly.com

SÍNTESIS ORGÁNICA



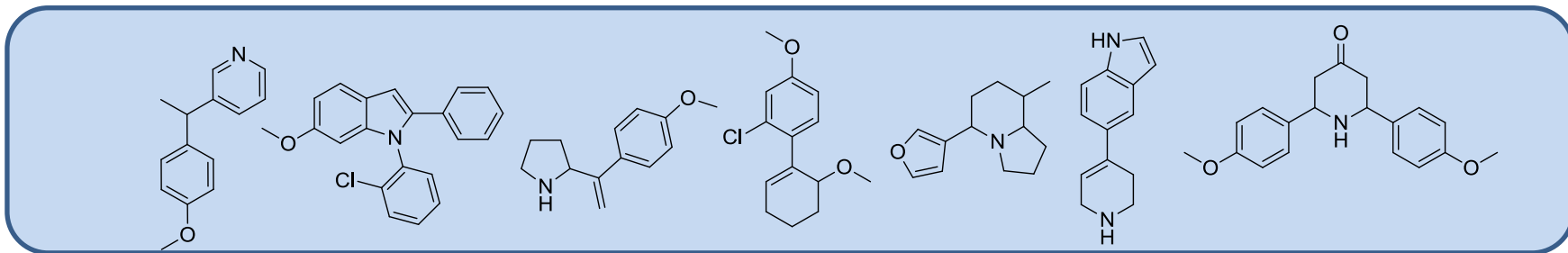
METODOLOGÍA SINTÉTICA

Nuevas reacciones
Nuevos reactivos
Nuevos procesos

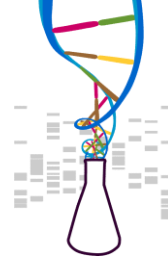
SÍNTESIS ORIENTADA A MOLECULAS OBJETIVO

Productos naturales
Fármacos
Quimiotecas

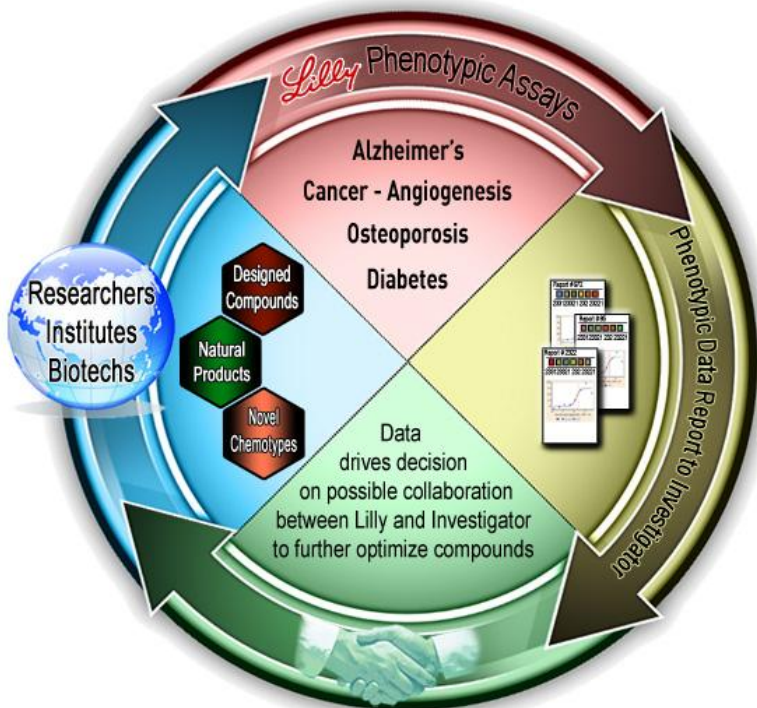
Diversidad molecular



¿Actividad biológica?



Lilly PD² Initiative



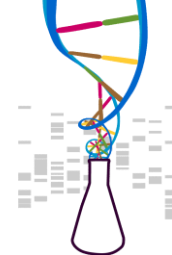
Acceso gratuito a un **panel de ensayos** fenotípicos de actividad de compuestos frente a diversas enfermedades

Proceso totalmente **confidencial**

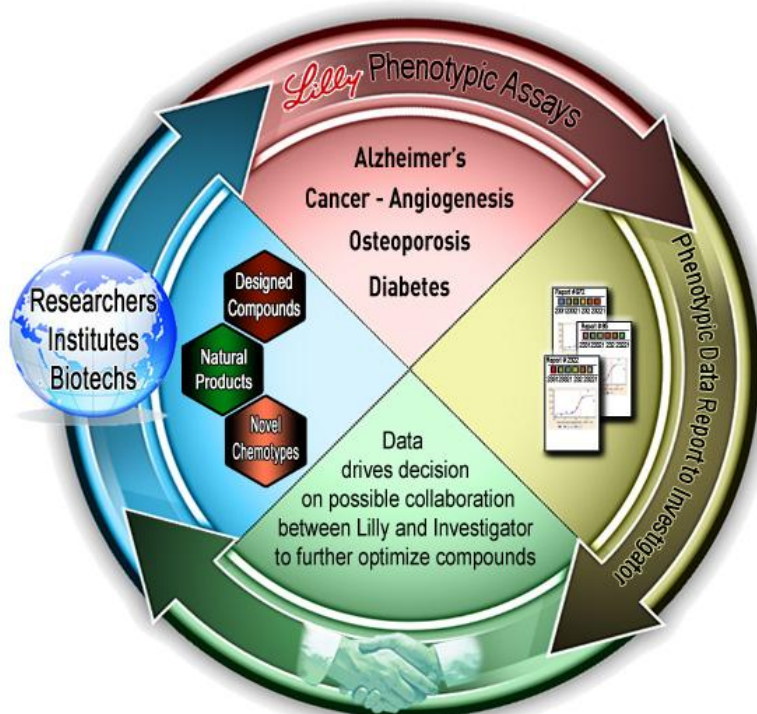
El investigador externo recibe todos los datos

El investigador mantiene la **propiedad intelectual**

Resultados prometedores podrían servir como base a **acuerdos de colaboración**



Lilly PD² Initiative



Beneficios

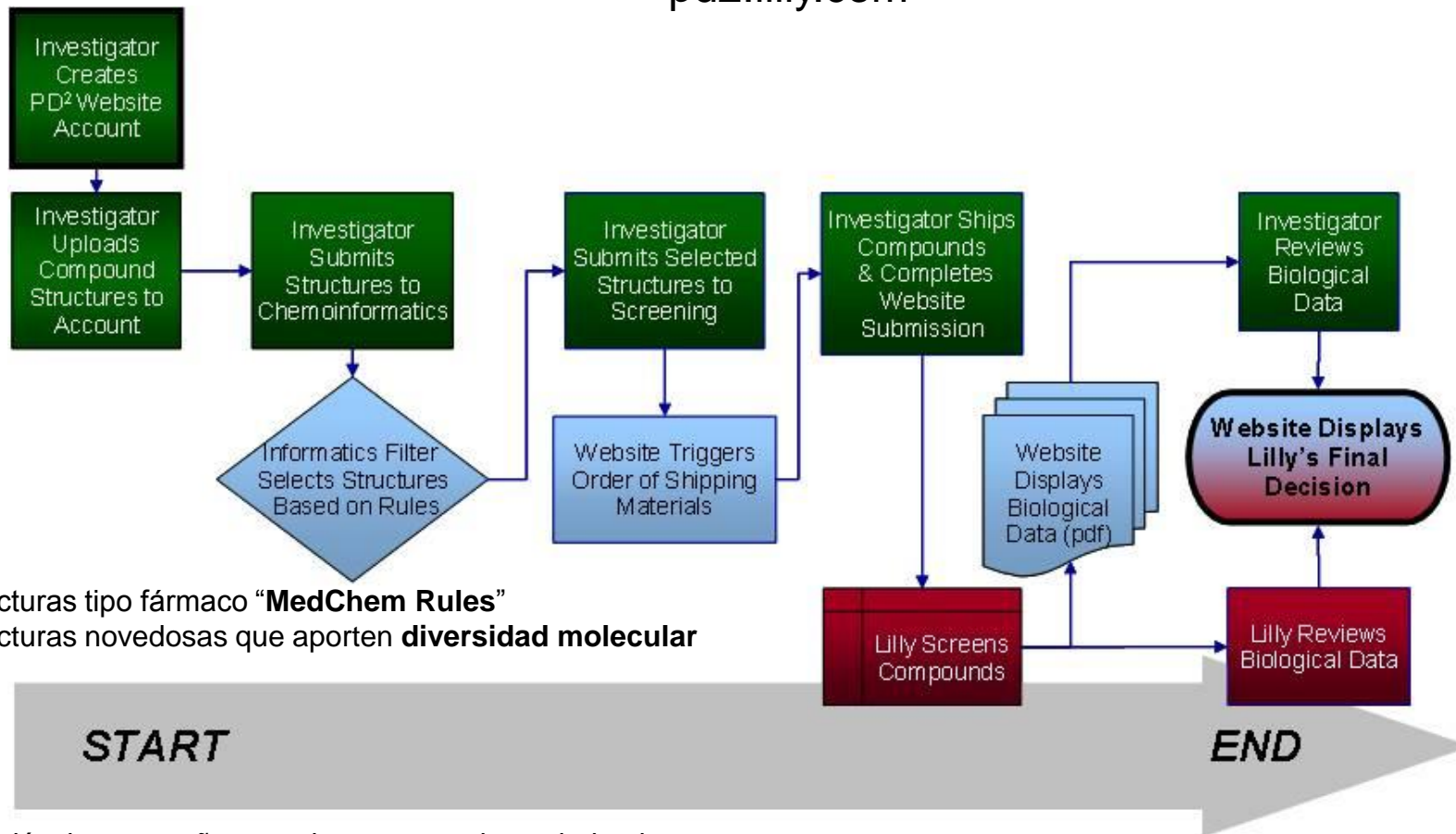
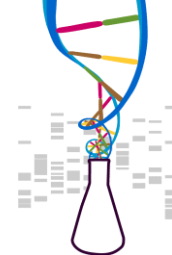
Lilly

Acceso a mayor *diversidad molecular* en sus programas de descubrimiento de fármacos

Investigadores Académicos

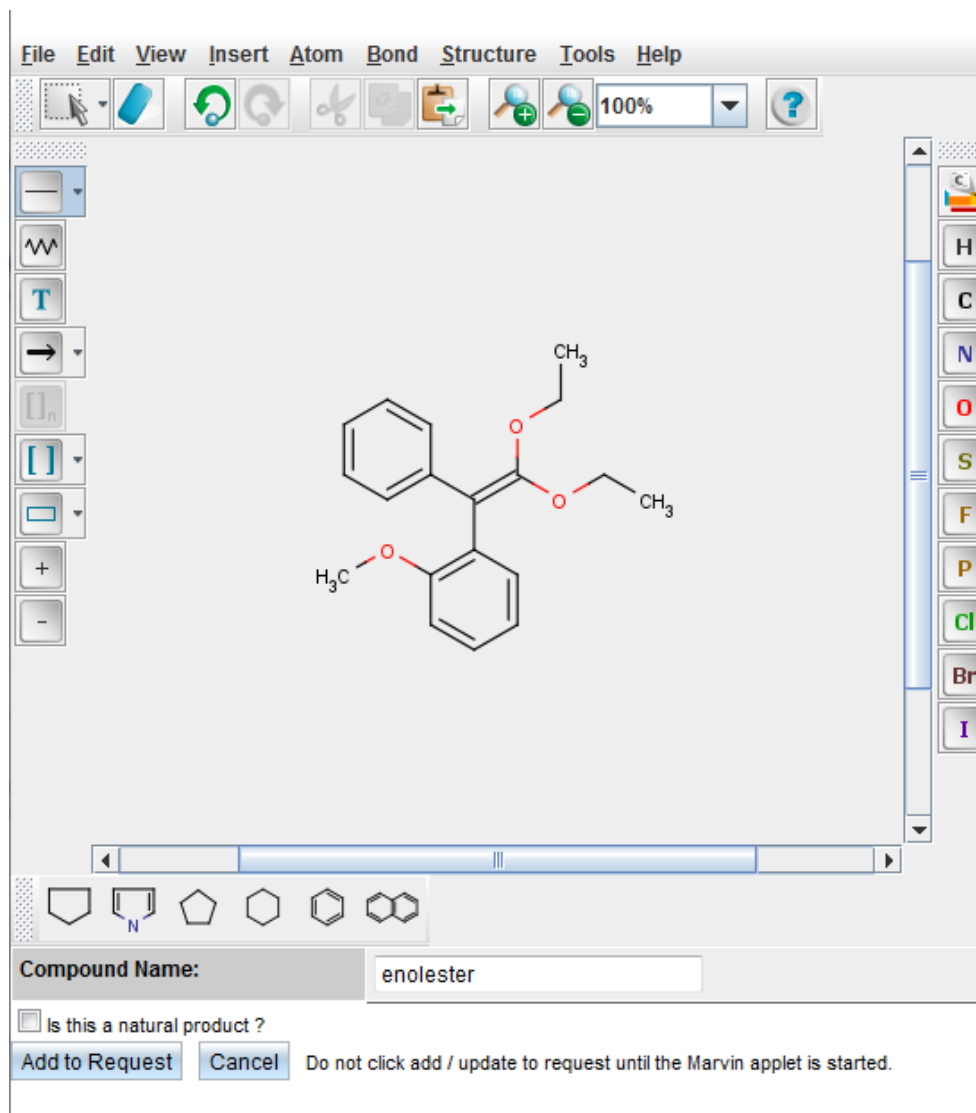
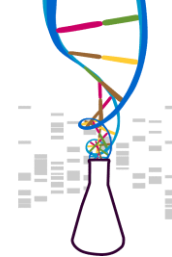
Acceso a *ensayos de actividad* relevantes para los compuestos desarrollados en el laboratorio

Posibilidad de establecer **colaboraciones**



Estructuras tipo fármaco “**MedChem Rules**”
Estructuras novedosas que aporten **diversidad molecular**

- SI: Moléculas pequeñas, productos naturales y derivados
- SI: Productos puros
- NO: Péptidos, proteínas, RNAs, oligonucleótidos antisentido
- NO: Mezclas de productos



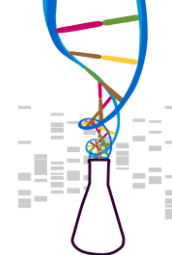
The screenshot shows the ChemDraw software interface. The main window displays the chemical structure of an enolester, which is a chalcone derivative. The structure consists of a central carbon-carbon double bond. One carbon is bonded to a phenyl ring and an ethoxy group (-OCH₂CH₃). The other carbon is bonded to a 4-methoxyphenyl ring and another ethoxy group (-OCH₂CH₃). The interface includes a menu bar (File, Edit, View, Insert, Atom, Bond, Structure, Tools, Help), a toolbar with various drawing tools, a vertical element palette on the right with buttons for H, C, N, O, S, F, P, Cl, Br, I, and a bottom panel with a "Compound Name" field containing "enolester", a checkbox for "Is this a natural product?", and "Add to Request" and "Cancel" buttons.

Compound Name: enolester

Is this a natural product ?

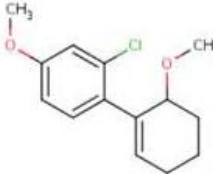
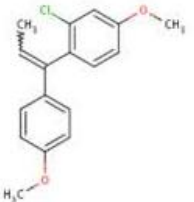
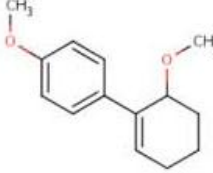
Add to Request Cancel Do not click add / update to request until the Marvin applet is started.

Applet para subir las estructuras tipo Chemdraw

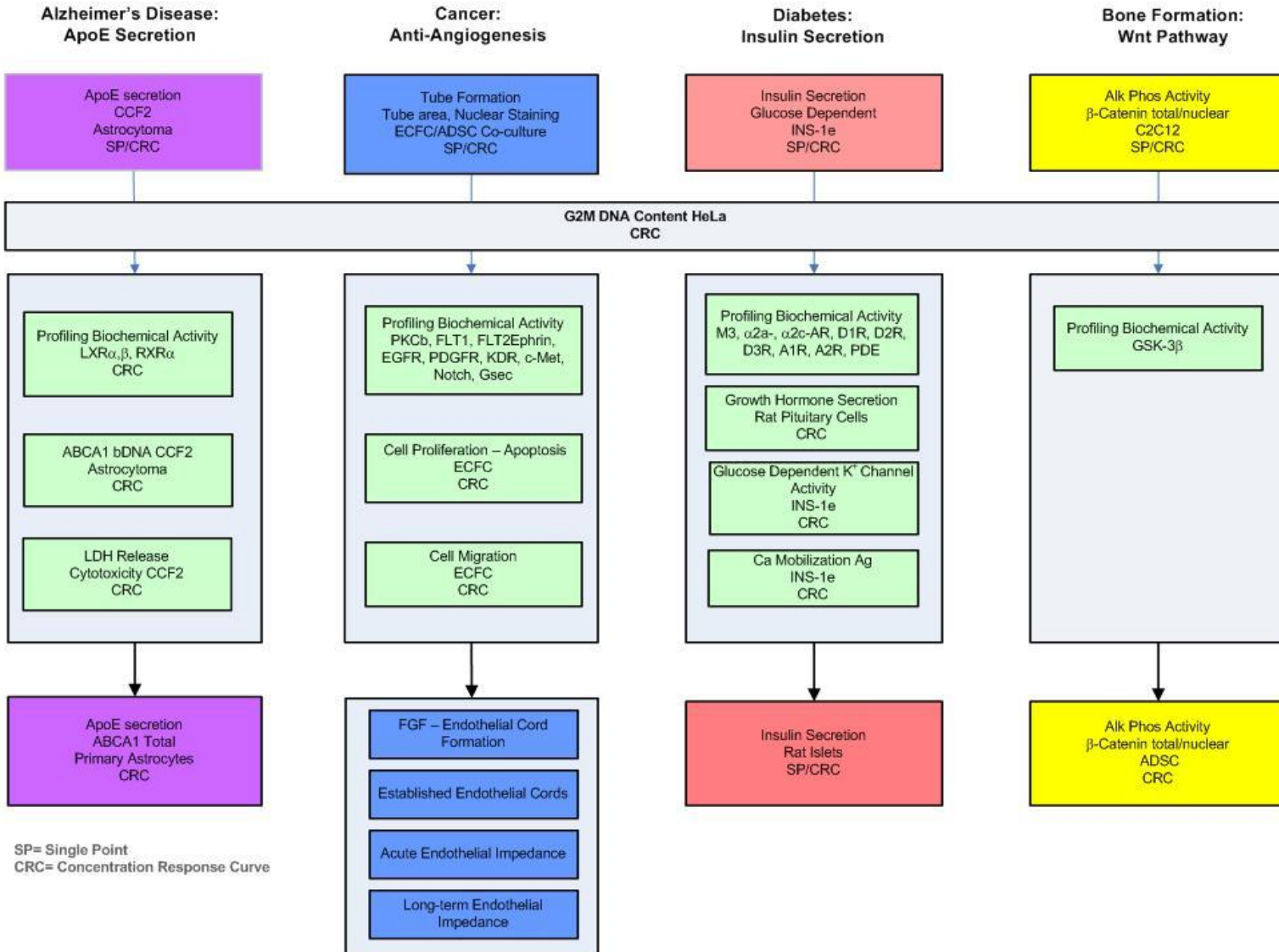


Current list of Compounds in Request (CV-nonaflates)

Number of rows: -- Select --

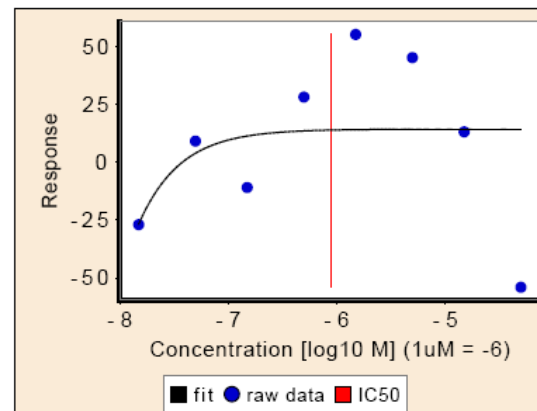
Compound ID	Compound Name	Compound Structure	Natural Products	Edit	Delete	Submit for Informatics	Submit for Screening	Barcode/Material Wt.(mg) <u>Shipment Instructions</u>	Screen Report	Data File
				<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>			
184079578	6l-nonaflates		Not a Natural Product	N/A	<input type="checkbox"/>	Passed on 12/20/2010	<input type="checkbox"/>	N/A	N/A	N/A
184079580	6p-nonaflates		Not a Natural Product	N/A	<input type="checkbox"/>	Failed on 12/20/2010	N/A	N/A	N/A	N/A
184079576	6j-nonaflates		Not a Natural Product	N/A	<input type="checkbox"/>	Passed on 12/20/2010	<input type="checkbox"/>	N/A	N/A	N/A

Ejemplo de respuesta quimioinformática

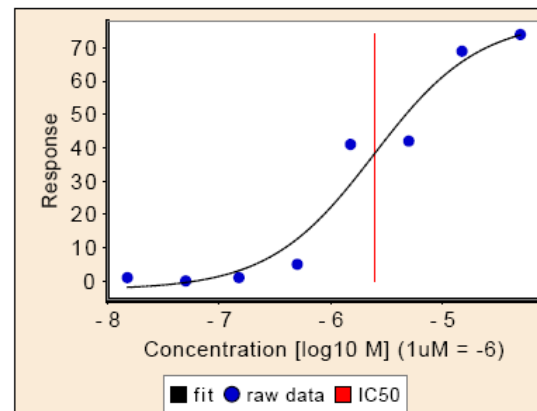


Dose Response Data for all Assays

Sample ID	Assay	IC50
cmpd_01	Assay 1	0.87933 μM



Sample ID	Assay	IC50
cmpd_01	Assay 2	2.50533 μM

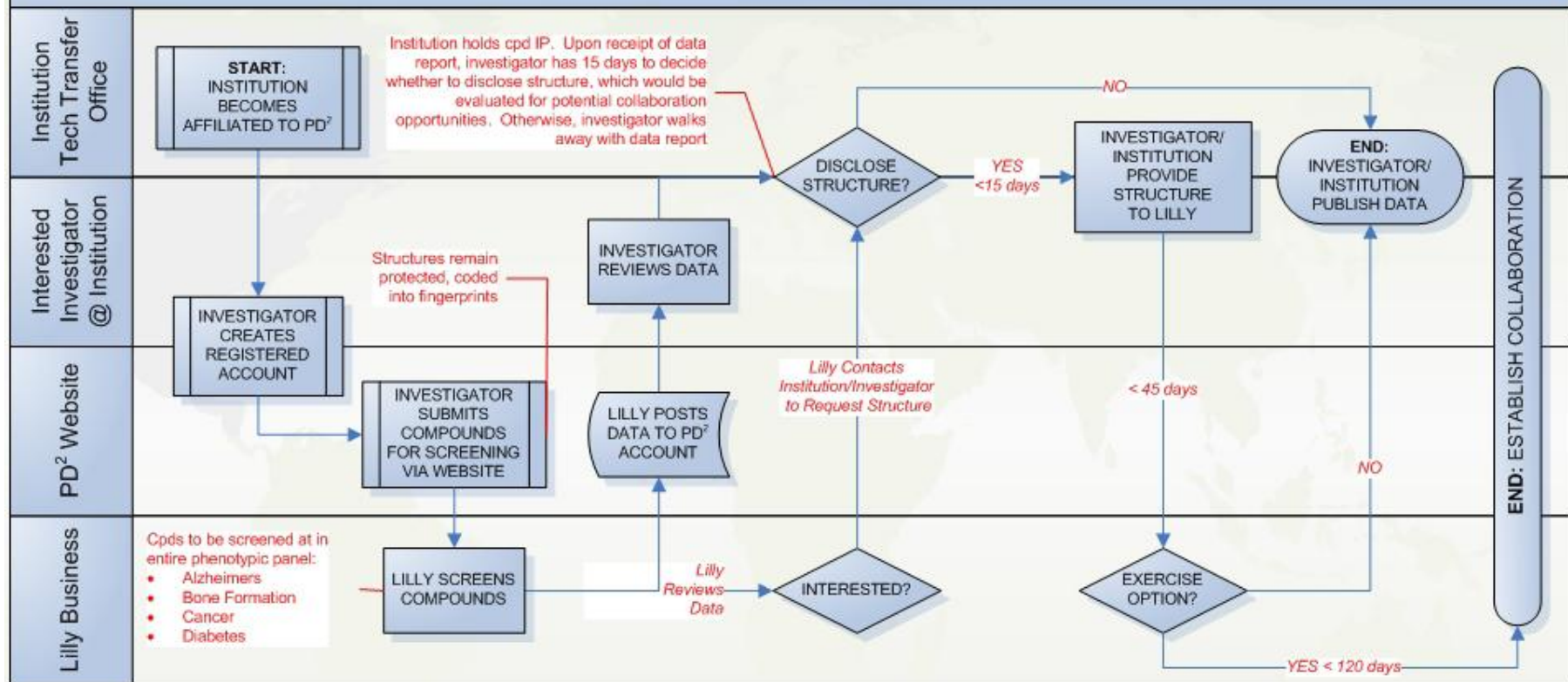


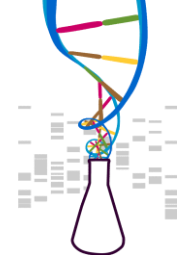
Lilly no conoce la identidad de los compuestos cuando recibe los datos de actividad. Para productos interesantes recaba esa información del investigador, y entonces puede proponer una colaboración – que el investigador puede o no aceptar.

What PD² Membership Means

Phenotypic Drug Discovery (PD²)

Membership in PD² is limited to investigators who work in an affiliated institution





Grupos de Investigación dedicados a ...

Síntesis Orgánica

Química Médica

Aislamiento de Productos Naturales

Modificación de Productos Naturales

Biosíntesis de Productos Naturales