



CURSO

**Búsqueda, análisis, representación y
visualización de información química
 contenida en bases de datos moleculares**

Grupo DIFACQUIM



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Luis Rivera



Armando Rufino



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DIFACQUIM

Diseño de Fármacos Asistido por Computadora en la Facultad de Química



Información de contacto:

Facultad de Química, U.N.A.M. Edificio F, cubículo 309

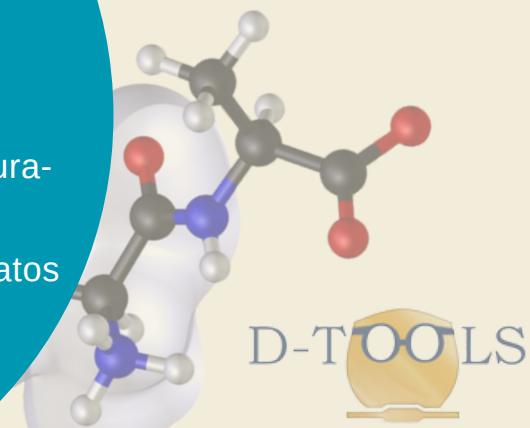
Teléfono: +52(55)-56223899, ext. 44458

Email: medinajl@unam.mx



INVESTIGACIÓN

- Modelado molecular de compuestos con actividad biológica.
 - Quimiogenómica computacional y reposicionamiento de fármacos.
 - Relaciones: estructura-actividad, estructura-múltiple actividad (SAR, SmAR)
 - Análisis quimioinformático de bases de datos moleculares (productos naturales)



CONSULTORIA Y COLABORACIÓN



CURSOS/ **DOCENCIA**

- Talleres de Químioinformática
 - Escritura de artículos científicos

DESARROLLO DE HERRAMIENTAS DIGITALES

- PUMA: Platform for Unified Molecular Analysis
 - Epigenetic Target Profiler
 - D-Peptide Builder
 - Activity Landscape Plotter
 - Consensus Diversity Plots

DIFUSIÓN Y DIVULGACIÓN DE LA CIENCIA

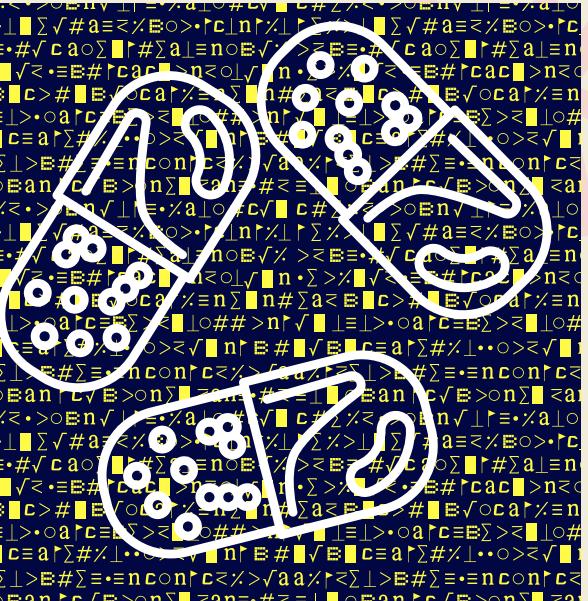
- Organización y participación en simposios y congresos
 - Artículos de divulgación

Quimioinformática

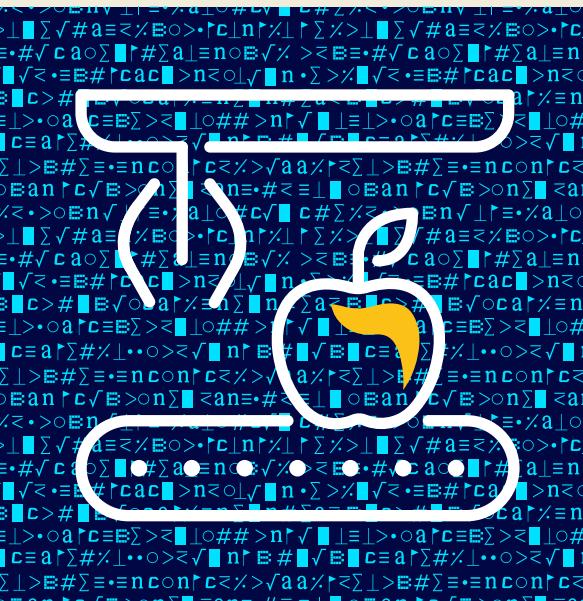
“La aplicación de métodos informáticos para resolver problemas químicos.”

Gasteiger, J. & Engel, T. Chemoinformatics: A Textbook, Wiley, 2003.

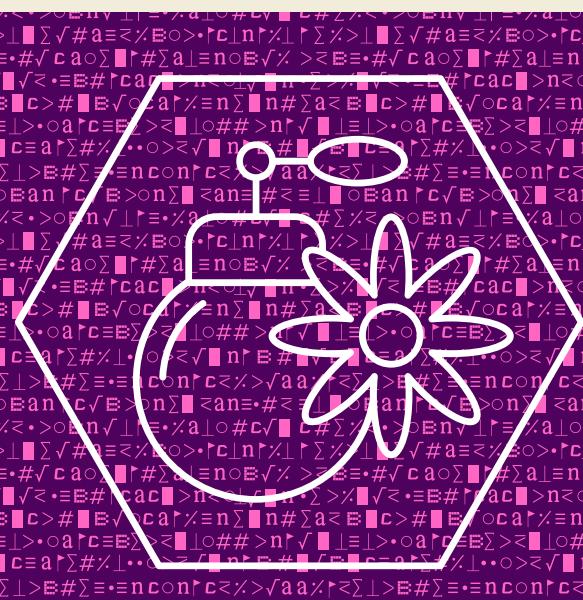
Aplicaciones de la quimioinformática



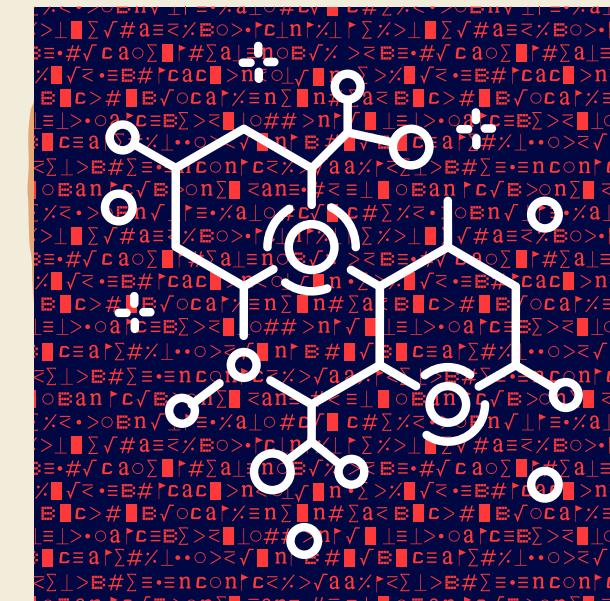
Diseño de fármacos asistido por computadora (DiFAC)



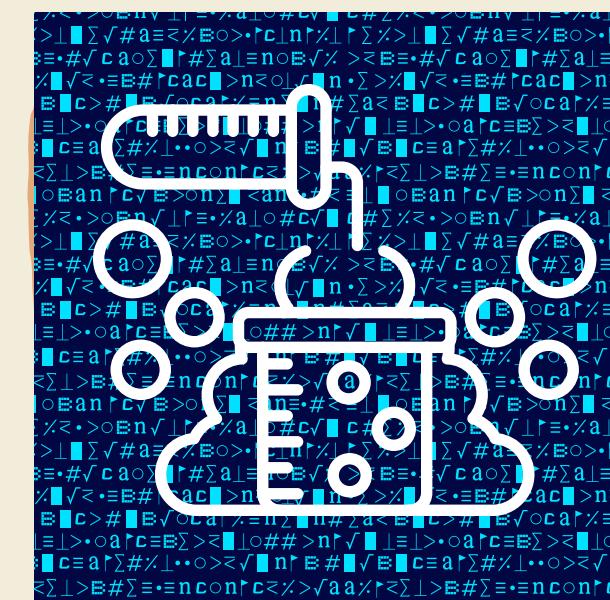
FoodInformatics



Cosméticos



Ciencia de materiales



Química Orgánica



Productos Naturales

Literatura recomendada



Educación Química (2017) 28, 51-58

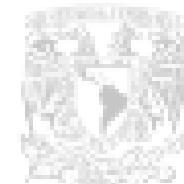


educación
Química
www.educacionquimica.info



COMUNICACIÓN

Descubrimiento y desarrollo de fármacos: un enfoque computacional



Fernanda Saldivar-González, Fernando D. Prieto-Martínez y José L. Medina-Franco*

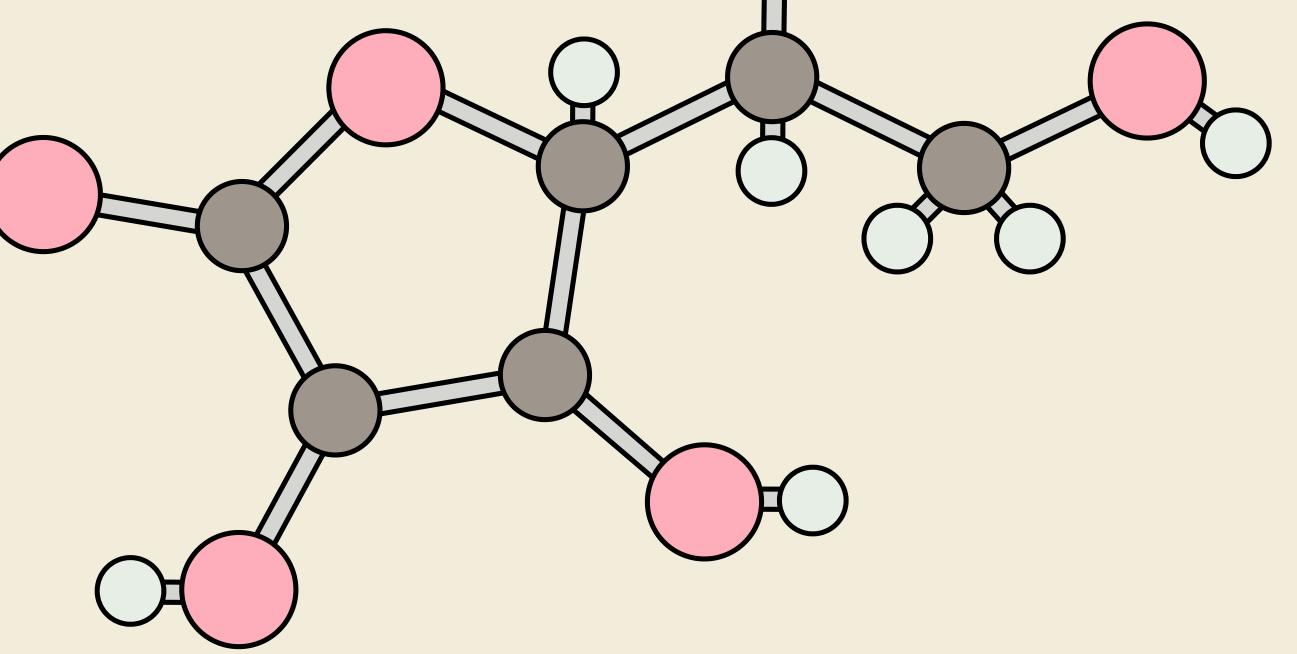
Departamento de Farmacia, Facultad de Química, Universidad Nacional Autónoma de México, Ciudad de México, México

Recibido el 5 de abril de 2016; aceptado el 20 de junio de 2016
Disponible en Internet el 12 de septiembre de 2016

Inteligencia artificial en el diseño de fármacos: hacia la inteligencia aumentada

Artificial intelligence in drug design: towards augmented intelligence

Fernanda I. Saldivar-González¹, Eli Fernández-de Gortari² y José L. Medina-Franco¹



Temario

9-13 octubre 2023

18:00 - 20:00 (hora CDMX)

Introducción a Python

Lunes 9

Bases de datos moleculares

SciFINDER®
A CAS SOLUTION

ChEMBL

PubChem

Martes 10

Jueves 12

Viernes 13

Representación molecular

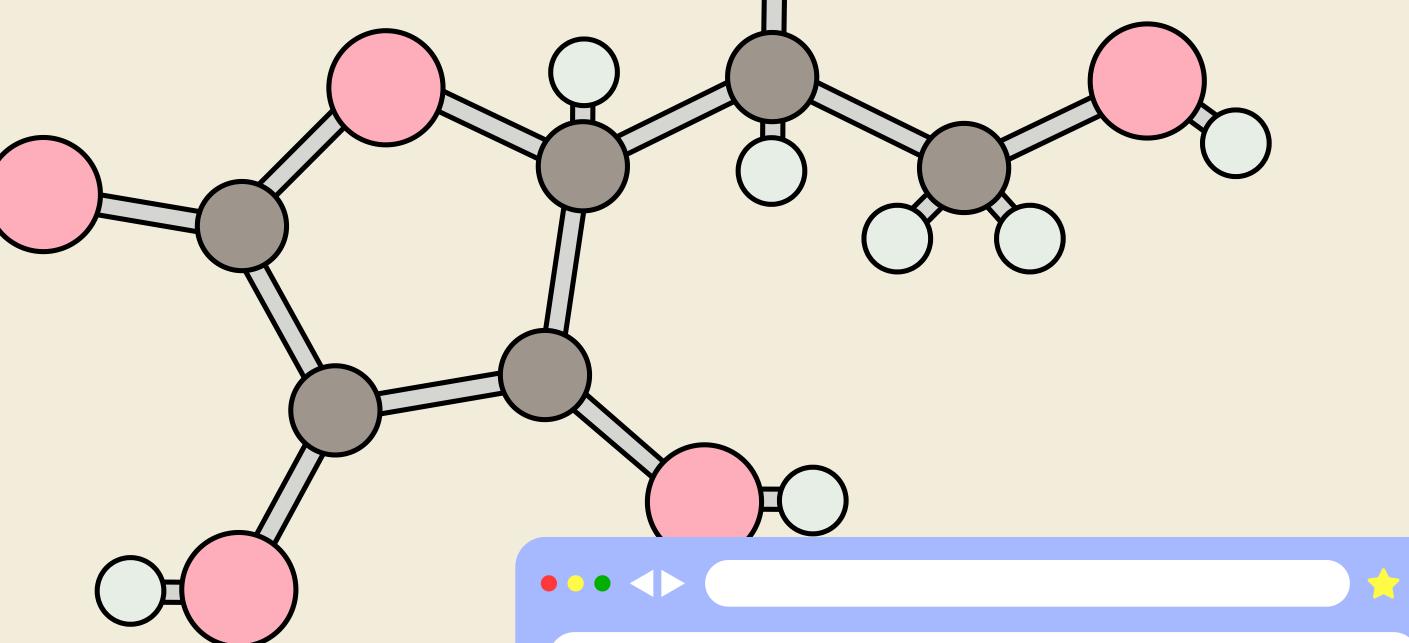
```
#Find substructures in a list of molecules
smiles_list = ['CC1CCC2(CC3CC(=O)CC=C(C(C=C=C4COCSC4(C=C(CS(=O)(=O)O)C)C(=O)O)O)C)O'
mol_list = []
for smiles in smiles_list:
    mol = Chem.MolFromSmiles(smiles)
    mol_list.append(mol)

pattern = Chem.MolFromSmarts('[*]-1-[*]-[*]C2([*]-[*]-[*][*]2)[#8]-[#6]-[#6]-1')

img = Draw.MolsToGridImage( mol_list, subImgSize=(300,300), molsPerRow=2, highlight=mol_list[0])
img
```

CC1CCC2(CC3CC(=O)CC=C(C(C=C=C4COCSC4(C=C(CS(=O)(=O)O)C)C(=O)O)O)C)O

*C1=CC=C2=C1C(=O)C3=C2C=C4=C3C=C5=C4C=C6=C5C=C7=C6C=C8=C7C=C9=C8C=C10=C9C=C11=C10C=C12=C11C=C13=C12C=C14=C13C=C15=C14C=C16=C15C=C17=C16C=C18=C17C=C19=C18C=C20=C19C=C21=C20C=C22=C21C=C23=C22C=C24=C23C=C25=C24C=C26=C25C=C27=C26C=C28=C27C=C29=C28C=C30=C29C=C31=C30C=C32=C31C=C33=C32C=C34=C33C=C35=C34C=C36=C35C=C37=C36C=C38=C37C=C39=C38C=C40=C39C=C41=C40C=C42=C41C=C43=C42C=C44=C43C=C45=C44C=C46=C45C=C47=C46C=C48=C47C=C49=C48C=C50=C49C=C51=C50C=C52=C51C=C53=C52C=C54=C53C=C55=C54C=C56=C55C=C57=C56C=C58=C57C=C59=C58C=C60=C59C=C61=C60C=C62=C61C=C63=C62C=C64=C63C=C65=C64C=C66=C65C=C67=C66C=C68=C67C=C69=C68C=C70=C69C=C71=C70C=C72=C71C=C73=C72C=C74=C73C=C75=C74C=C76=C75C=C77=C76C=C78=C77C=C79=C78C=C80=C79C=C81=C80C=C82=C81C=C83=C82C=C84=C83C=C85=C84C=C86=C85C=C87=C86C=C88=C87C=C89=C88C=C90=C89C=C91=C90C=C92=C91C=C93=C92C=C94=C93C=C95=C94C=C96=C95C=C97=C96C=C98=C97C=C99=C98C=C100=C99C=C101=C100C=C102=C101C=C103=C102C=C104=C103C=C105=C104C=C106=C105C=C107=C106C=C108=C107C=C109=C108C=C110=C109C=C111=C110C=C112=C111C=C113=C112C=C114=C113C=C115=C114C=C116=C115C=C117=C116C=C118=C117C=C119=C118C=C120=C119C=C121=C120C=C122=C121C=C123=C122C=C124=C123C=C125=C124C=C126=C125C=C127=C126C=C128=C127C=C129=C128C=C130=C129C=C131=C130C=C132=C131C=C133=C132C=C134=C133C=C135=C134C=C136=C135C=C137=C136C=C138=C137C=C139=C138C=C140=C139C=C141=C140C=C142=C141C=C143=C142C=C144=C143C=C145=C144C=C146=C145C=C147=C146C=C148=C147C=C149=C148C=C150=C149C=C151=C150C=C152=C151C=C153=C152C=C154=C153C=C155=C154C=C156=C155C=C157=C156C=C158=C157C=C159=C158C=C160=C159C=C161=C160C=C162=C161C=C163=C162C=C164=C163C=C165=C164C=C166=C165C=C167=C166C=C168=C167C=C169=C168C=C170=C169C=C171=C170C=C172=C171C=C173=C172C=C174=C173C=C175=C174C=C176=C175C=C177=C176C=C178=C177C=C179=C178C=C180=C179C=C181=C180C=C182=C181C=C183=C182C=C184=C183C=C185=C184C=C186=C185C=C187=C186C=C188=C187C=C189=C188C=C190=C189C=C191=C190C=C192=C191C=C193=C192C=C194=C193C=C195=C194C=C196=C195C=C197=C196C=C198=C197C=C199=C198C=C200=C199C=C201=C200C=C202=C201C=C203=C202C=C204=C203C=C205=C204C=C206=C205C=C207=C206C=C208=C207C=C209=C208C=C210=C209C=C211=C210C=C212=C211C=C213=C212C=C214=C213C=C215=C214C=C216=C215C=C217=C216C=C218=C217C=C219=C218C=C220=C219C=C221=C220C=C222=C221C=C223=C222C=C224=C223C=C225=C224C=C226=C225C=C227=C226C=C228=C227C=C229=C228C=C230=C229C=C231=C230C=C232=C231C=C233=C232C=C234=C233C=C235=C234C=C236=C235C=C237=C236C=C238=C237C=C239=C238C=C240=C239C=C241=C240C=C242=C241C=C243=C242C=C244=C243C=C245=C244C=C246=C245C=C247=C246C=C248=C247C=C249=C248C=C250=C249C=C251=C250C=C252=C251C=C253=C252C=C254=C253C=C255=C254C=C256=C255C=C257=C256C=C258=C257C=C259=C258C=C260=C259C=C261=C260C=C262=C261C=C263=C262C=C264=C263C=C265=C264C=C266=C265C=C267=C266C=C268=C267C=C269=C268C=C270=C269C=C271=C270C=C272=C271C=C273=C272C=C274=C273C=C275=C274C=C276=C275C=C277=C276C=C278=C277C=C279=C278C=C280=C279C=C281=C280C=C282=C281C=C283=C282C=C284=C283C=C285=C284C=C286=C285C=C287=C286C=C288=C287C=C289=C288C=C290=C289C=C291=C290C=C292=C291C=C293=C292C=C294=C293C=C295=C294C=C296=C295C=C297=C296C=C298=C297C=C299=C298C=C2100=C299C=C2101=C2100C=C2102=C2101C=C2103=C2102C=C2104=C2103C=C2105=C2104C=C2106=C2105C=C2107=C2106C=C2108=C2107C=C2109=C2108C=C2110=C2109C=C2111=C2110C=C2112=C2111C=C2113=C2112C=C2114=C2113C=C2115=C2114C=C2116=C2115C=C2117=C2116C=C2118=C2117C=C2119=C2118C=C2120=C2119C=C2121=C2120C=C2122=C2121C=C2123=C2122C=C2124=C2123C=C2125=C2124C=C2126=C2125C=C2127=C2126C=C2128=C2127C=C2129=C2128C=C2130=C2129C=C2131=C2130C=C2132=C2131C=C2133=C2132C=C2134=C2133C=C2135=C2134C=C2136=C2135C=C2137=C2136C=C2138=C2137C=C2139=C2138C=C2140=C2139C=C2141=C2140C=C2142=C2141C=C2143=C2142C=C2144=C2143C=C2145=C2144C=C2146=C2145C=C2147=C2146C=C2148=C2147C=C2149=C2148C=C2150=C2149C=C2151=C2150C=C2152=C2151C=C2153=C2152C=C2154=C2153C=C2155=C2154C=C2156=C2155C=C2157=C2156C=C2158=C2157C=C2159=C2158C=C2160=C2159C=C2161=C2160C=C2162=C2161C=C2163=C2162C=C2164=C2163C=C2165=C2164C=C2166=C2165C=C2167=C2166C=C2168=C2167C=C2169=C2168C=C2170=C2169C=C2171=C2170C=C2172=C2171C=C2173=C2172C=C2174=C2173C=C2175=C2174C=C2176=C2175C=C2177=C2176C=C2178=C2177C=C2179=C2178C=C2180=C2179C=C2181=C2180C=C2182=C2181C=C2183=C2182C=C2184=C2183C=C2185=C2184C=C2186=C2185C=C2187=C2186C=C2188=C2187C=C2189=C2188C=C2190=C2189C=C2191=C2190C=C2192=C2191C=C2193=C2192C=C2194=C2193C=C2195=C2194C=C2196=C2195C=C2197=C2196C=C2198=C2197C=C2199=C2198C=C2200=C2199C=C2201=C2200C=C2202=C2201C=C2203=C2202C=C2204=C2203C=C2205=C2204C=C2206=C2205C=C2207=C2206C=C2208=C2207C=C2209=C2208C=C2210=C2209C=C2211=C2210C=C2212=C2211C=C2213=C2212C=C2214=C2213C=C2215=C2214C=C2216=C2215C=C2217=C2216C=C2218=C2217C=C2219=C2218C=C2220=C2219C=C2221=C2220C=C2222=C2221C=C2223=C2222C=C2224=C2223C=C2225=C2224C=C2226=C2225C=C2227=C2226C=C2228=C2227C=C2229=C2228C=C2230=C2229C=C2231=C2230C=C2232=C2231C=C2233=C2232C=C2234=C2233C=C2235=C2234C=C2236=C2235C=C2237=C2236C=C2238=C2237C=C2239=C2238C=C2240=C2239C=C2241=C2240C=C2242=C2241C=C2243=C2242C=C2244=C2243C=C2245=C2244C=C2246=C2245C=C2247=C2246C=C22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Construcción y curado de bases de datos moleculares

Enumeración de bibliotecas químicas

[N;O;S]:1

Temario

16-20 octubre 2023

Lunes 16

Martes 17

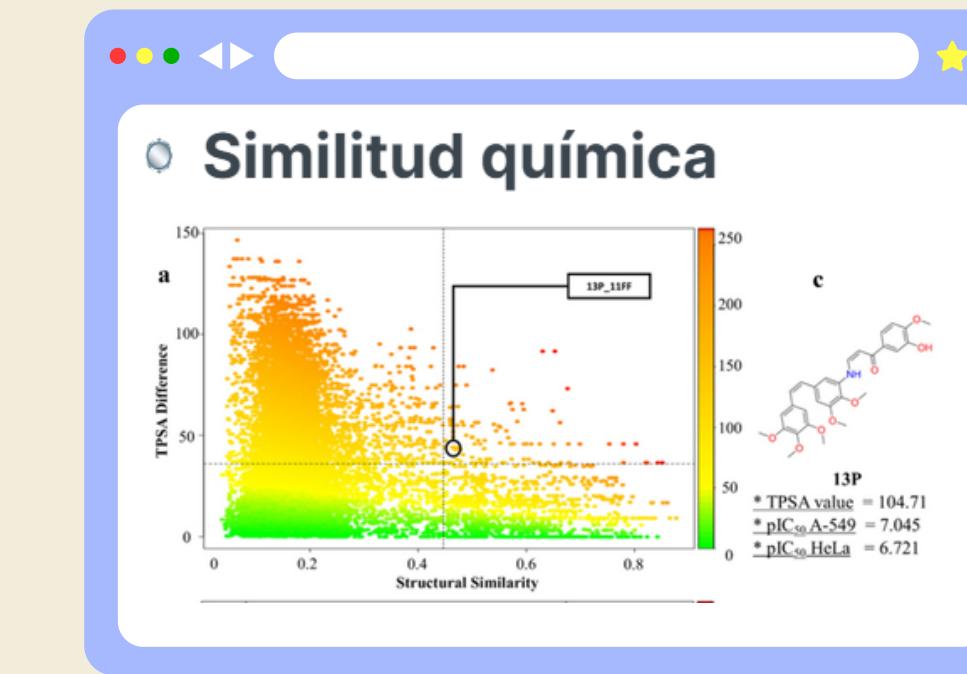
Miércoles 18

18:00 - 20:00

(hora CDMX)

Jueves 19

Viernes 20



Materiales del curso

The screenshot shows a GitBook page titled "Quimioinformática aplicada al diseño de fármacos". The left sidebar contains a table of contents with sections like "Introducción a Python y a Google Colab", "Fundamentos de programación", "Limpieza de datos", "Representación molecular", "SMILES", and "SMARTS". The main content area displays several 3D molecular models and logos, including the DIFACQUIM logo and the UNAM seal. At the bottom, it says "GitBook elaborado por el grupo DIFACQUIM-UNAM".

[https://difacquim.gitbook.io/
quimioinformatica](https://difacquim.gitbook.io/quimioinformatica)



[https://github.com/
DIFACQUIM](https://github.com/DIFACQUIM)