
DESENHO DE ESTRUTURAS QUÍMICAS

+

TÉCNICAS DE PESQUISA ONLINE

Prof. Dr. Márcio Marques Martins



digimarcio

<http://digichem.org>

<http://slideshare.net/marsjomm>

Dados físico-químicos

Podem ser obtidos com mais detalhes nos seguintes sites:

- 1) <http://chemicalize.org>
- 2) <http://webbook.nist.gov>

Saiba mais sobre o Chemicalize neste link:
<http://digichem.org/2012/03/12/dica-de-site-chemicalizeorg/>

Dados físico-químicos

No google, basta digitar o nome da molécula seguida de MSDS ou FISPQ.

MSDS: material safety data sheet

FISPQ: ficha de segurança de produtos químicos

Dados físico-químicos

Também é possível obter muita informação usando o site do NIST:

<http://webbook.nist.gov/chemistry>

Base de dados de Referência padrão do NIST número 69

Ver: [Opções de pesquisa](#), [Modelos e ferramentas](#), [Documentação](#), [Notas](#)

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O NIST reserva o direito de cobrar uma taxa pelo acesso a esta base de dados no futuro

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- [Propriedades termo-físicas de sistemas fluidos](#) Dados com elevada exactidão para um grupo seleccionado de fluidos.
 - [Estimativas baseadas na aditividade de grupos](#) Estimativas de propriedades termodinâmicas na fase gasosa feitas com base numa estrutura submetida.
-

[Documentação](#) [inicio](#)

- [questões frequentes \(faq\)](#)
- [história da base de dados](#)

Dicas para procurar em inglês

É sempre interessante conhecer alguns termos químicos em inglês para realizar uma busca mais elaborada:

Ponto de ebulição – boiling point

Ponto de fusão – melting point

Ponto de ignição - flash point

Entalpia – Enthalpy

Entropy – Entropia

Energia Livre de Gibbs – Gibbs Free Energy

Dicas para procurar em inglês

Quanto à forma de escrever os nomes de substâncias:

Alcano – alkane

Alceno – alkene

Alcino – alkyne

Álcool – alcohol/ Aldeído – aldehyde

Amina – Amine / Amida - Amide

Cetona - ketone

Ácido carboxílico – carboxylic acid

Éter – ether

Éster – esther

Hidro – hydro

Cloro – Chlorine

Cloreto – Chloride / Clorato – Chlorate / Clorito - Chlorite

Fluor – Fluorine / Fluoreto - Fluoride

Bromo – Bromine / Brometo - Bromide

Iodo – Iodine / Iodeto - Iodide

Silício – Silicon

Silicona - Silicone

Dicas para procurar em inglês

Quanto à forma de escrever os nomes de substâncias:

Oxigênio - Oxygen

Enxofre – Sulfur ou Tio

Selênio – Selenium

Telúrio – Telurium

Boro – Boron

Metais, em geral, ganham a terminação -ium

Alumínio – Aluminium

Cromo – Chromium

Platina – Platinum

Lítio – Lithium/Sódio- Sodium/Potássio – Potassium/Rubídio-Rubydium

Berílio - Ber

Ferro – Iron

Cobre – Copper

Níquel – Nickel

Ouro – Gold

Prata – Silver

Dicas para procurar em inglês

Quanto à forma de escrever os nomes de substâncias:

Hidrogênio – Hydrogen / Hidreto – Hydride / Hidrato - Hydrate

Etileno – Ethylene

Propileno – propylene

Metil – Methyl

Butil = butyl

Acetil – Acethyl

Alil – Allyl

Benzil – Benzyl

Infravermelho – Infrared (IR)

Ultravioleta – ultraviolet (UV)

Ressonância Magnética Nuclear (RMN) – Nuclear Magnetic Ressonance (NMR)

Espectroscopia – Spectroscopy

Especro – Spectrum (patronum?)

Cromatografia – Chromatography

Titulação – Tritration

Dicas para procurar em inglês

Tubo de ensaio – Test tube

Frasco de Erlenmeyer – Conical Flask

Placa de Petri – Petri Dish

Agitador Magnético – Magnetic Stirrer

Condensador/condensação – Condenser/condensation

Balão volumétrico – Volumetric flask

Vidro temperado – tempered glass

Pipeta graduada – pipette

Agitar/agitação – Stir/stirring

Verter ou derramar – Pour/pouring

Misturar/misturando – Mix/mixing

Aquecer/aquecimento – warm/warming

Ferver/fervente – boil/boiling

Resfriar/resfriamento – cool/cooling

Desenho de estruturas químicas

Online:

[JChemPaint](#)

[Engg Heads Chembox](#)

Offline:

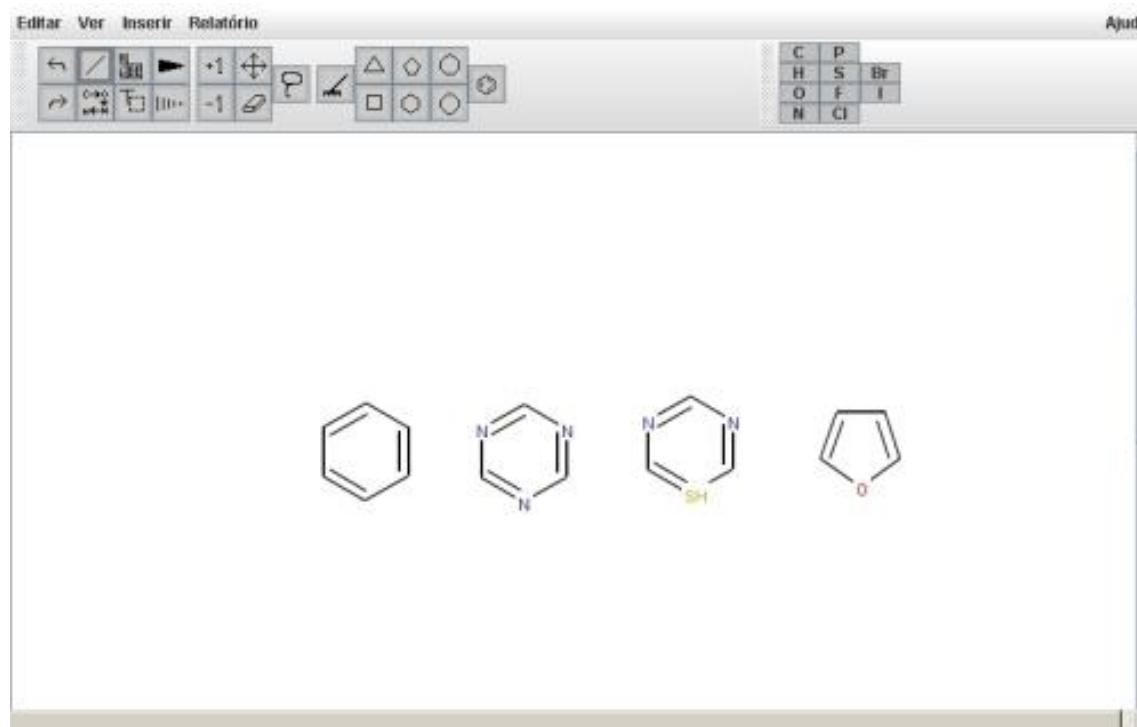
[SymyxDraw / Site](#)

[ChemSketch](#)

Desenho de estruturas químicas

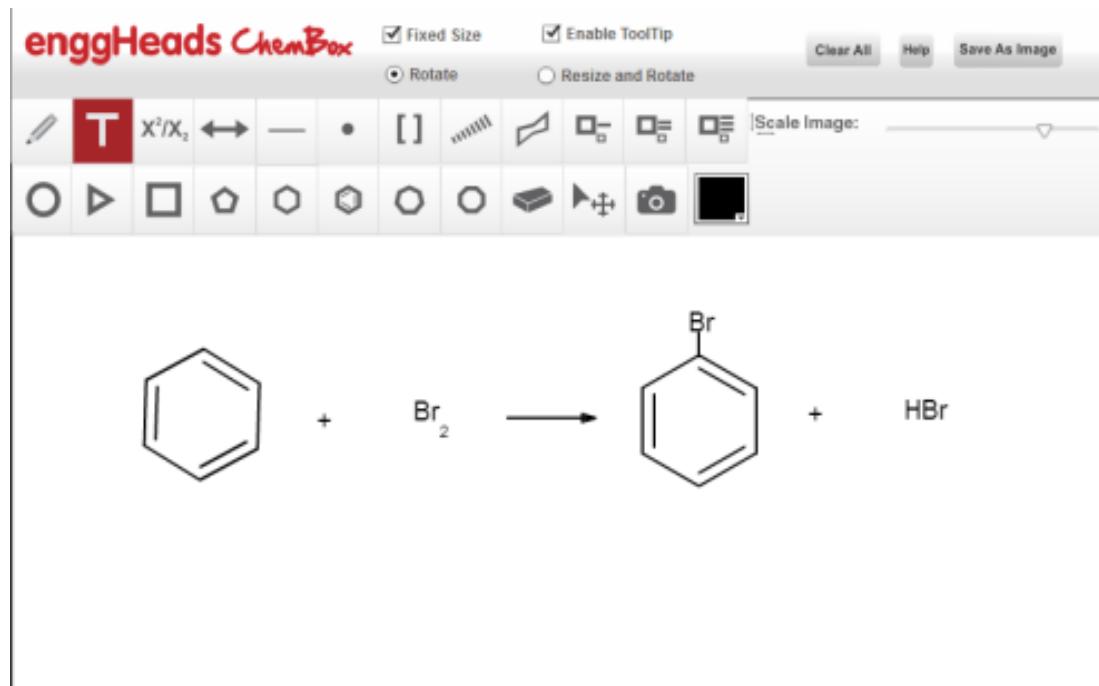
Online:

[JChemPaint](#)



Desenho de estruturas químicas

Online:
[Engg Heads Chembox](#)



Desenho de estruturas químicas

Offline:
[SymyxDraw / Site](#)



Tutoriais do Symyx Draw em Português *Tutoriais do Symyx Draw em Português*

[Download](#)
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Márcio Martins

Agora não quero escrever nada...

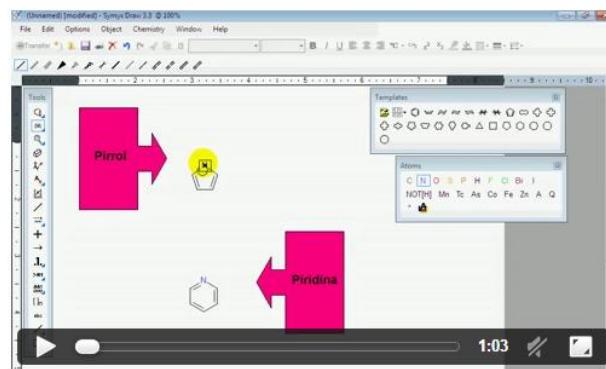


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Tags

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Exemplos - Pirrol e piridina



[Download 12.8-pirrol_e_piridina.avi](#)

Posted about 4 years ago

Como pesquisar em inglês?

O ChemSketch pode ser baixado de forma gratuita no endereço
<http://goo.gl/XX9Q8j>.

É necessário fazer um cadastro.

Janela principal

ACD/ChemSketch (Freeware) - [noname01.sk2]

File Edit Pages Tools Templates Options Documents Add-Ons I-Lab ACD/Labs Help

Structure Draw

156.5%

InChI LogP PubChem eMolecules ChemSpider

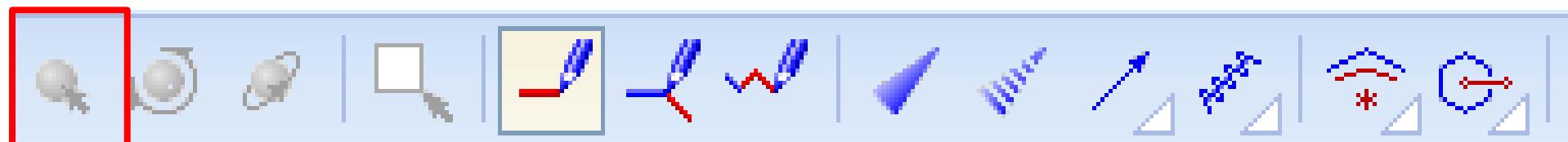
mm 0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200 210

A
Rny
C
H
N
O
F
Na
Si
P
S
Cl
K
Br
abc
R
+
#

Aparência da janela principal
do ACD ChemSketch!

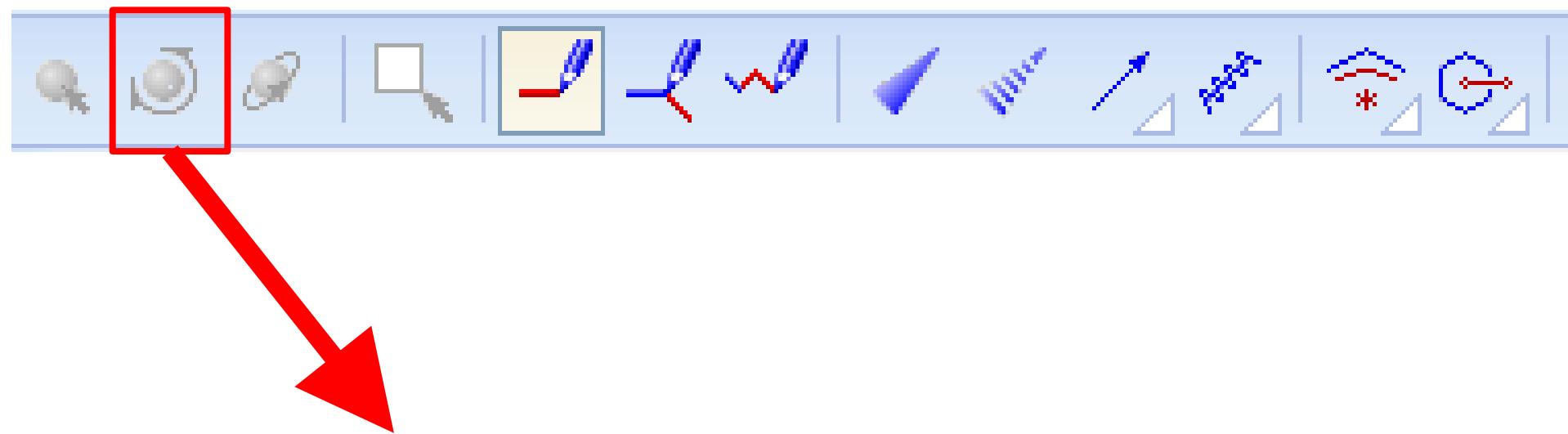
More...
Sep 1 13:23 ACD/Labs Incorporates New Company to Serve Germany, Austria, Switzerland | Nov 2 11:44 Meet ACD/Labs | ACD/Labs RSS Feed: Nov 2 13:20 A 'Spectroscopist's Dream' Captures the Imagination of Journal Readers | Sep 2 Setup RSS
I-Lab Login NONAME01.SK2 Page 1/1 Properties
1-ChemSketch 2-Database 3-ChemCoder

Barra de desenho



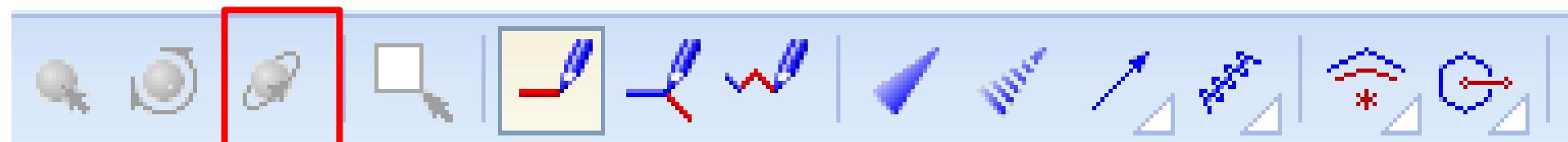
SELECCIONAR/MOVER

Barra de desenho



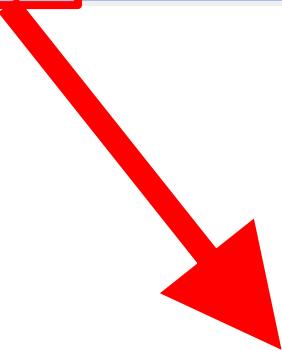
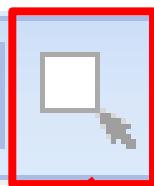
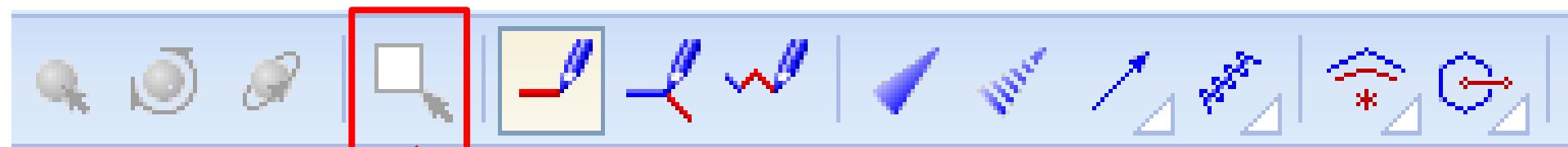
SELECCIONAR/MOVER/REDIMENSIONAR

Barra de desenho



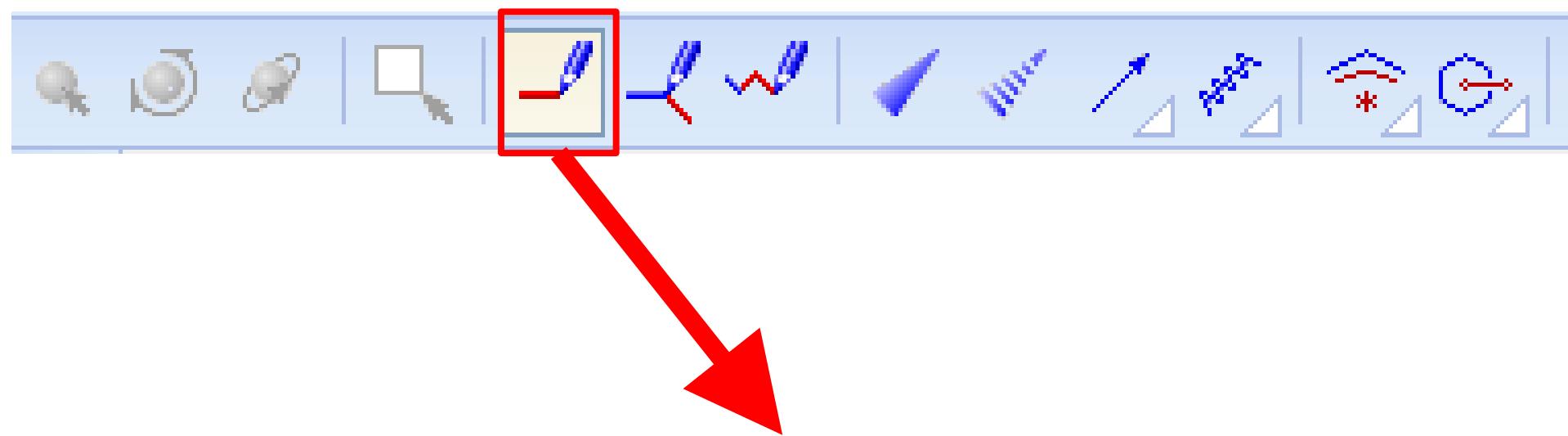
ROTAÇÃO 3D

Barra de desenho



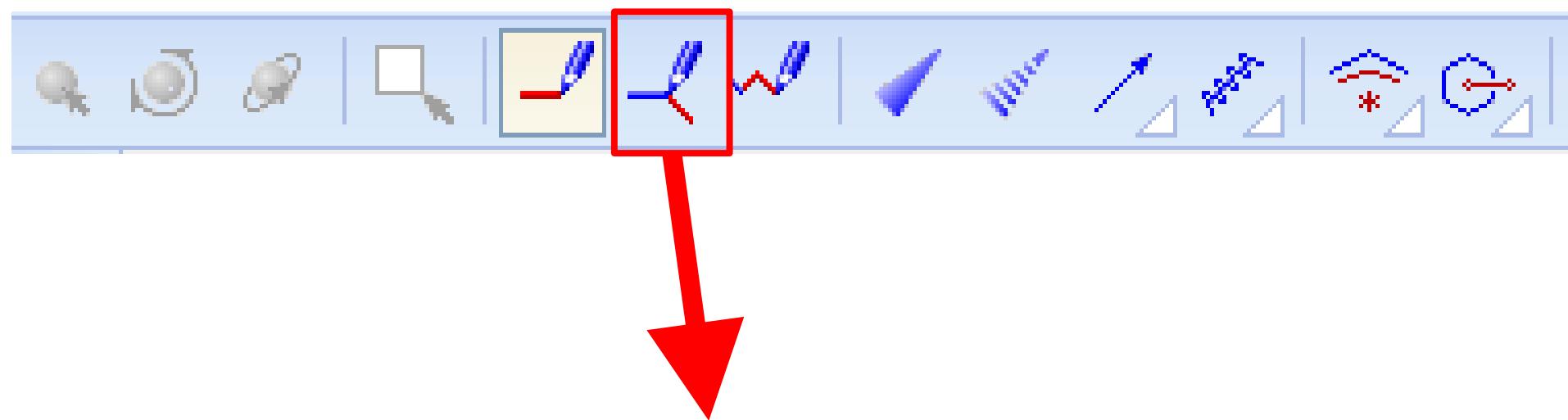
IAÇO ON/OFF

Alternando entre modos de desenho



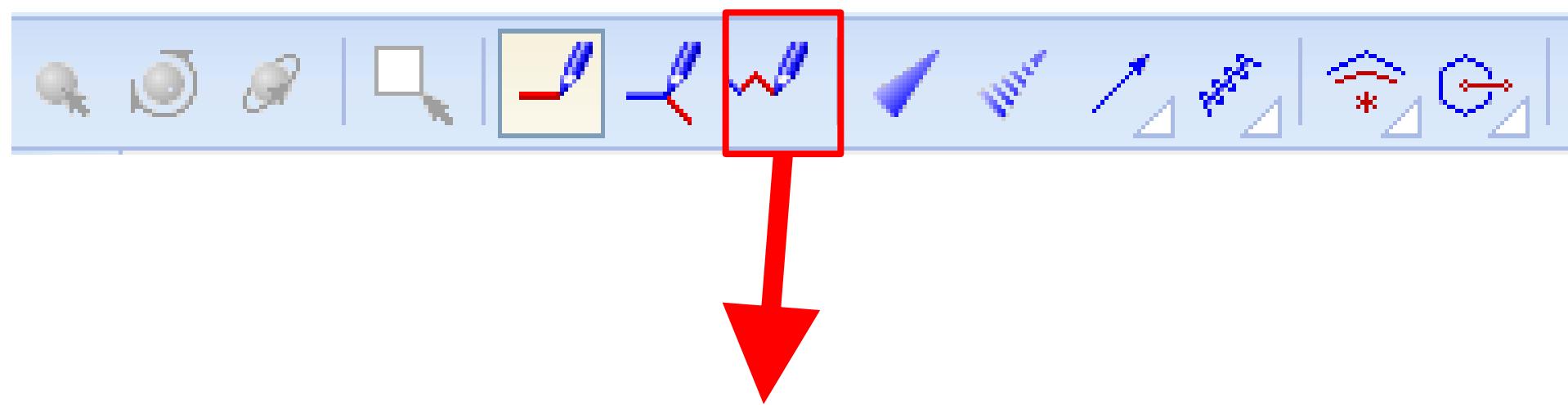
**DESENHAR NORMAL - PRODUZ MOLÉCULAS
COM BAIXA PRECISÃO
ESTRUTURAL**

Alternando entre modos de desenho



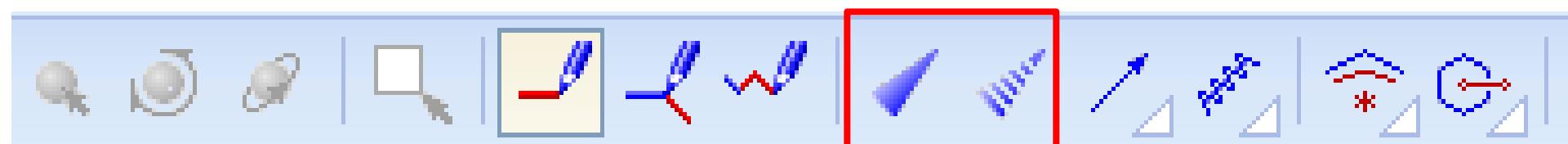
DESENHAR CONTÍNUO - SIMILAR AO MODO NORMAL

Alternando entre modos de desenho



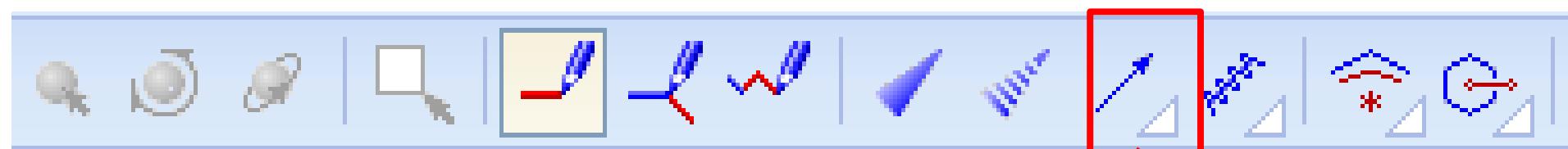
DESENHAR CADEIAS -
CLIQUE E ARRASTE O MOUSE E UMA CADEIA CARBÔNICA
SURGIRÁ COM O TAMANHO QUE VOCÊ QUISER.

Tipos de ligações químicas



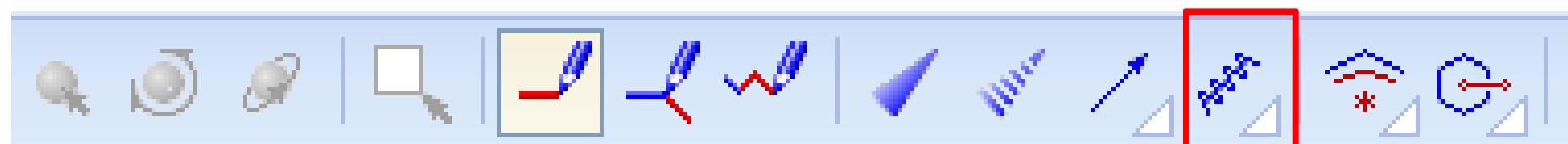
LIGAÇÕES ESTEREOQUÍMICAS

Tipos de ligações químicas



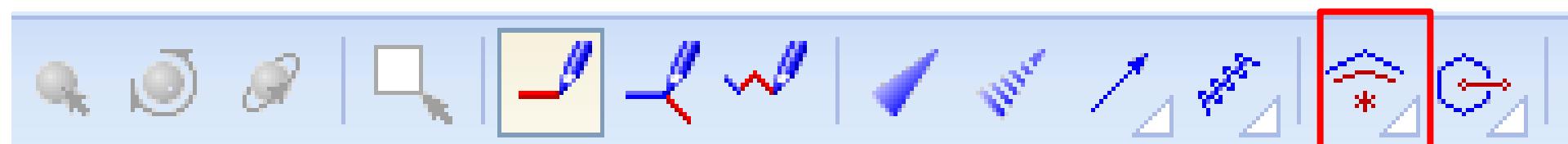
vÁRIOS TIPOS DE LIGAÇÕES COORDENADAS

Tipos de ligações químicas



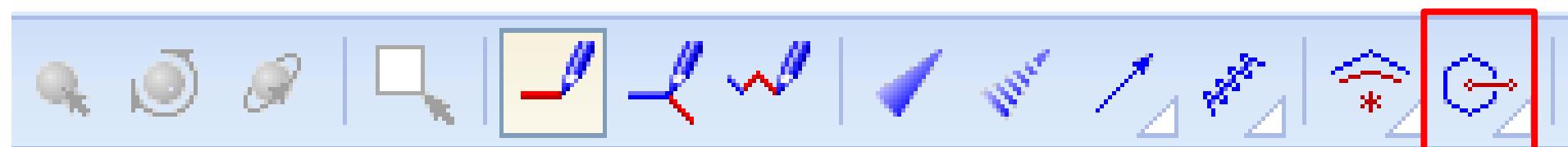
LIGAÇÕES ESTÉREO INDEFINIDAS

Tipos de ligações químicas



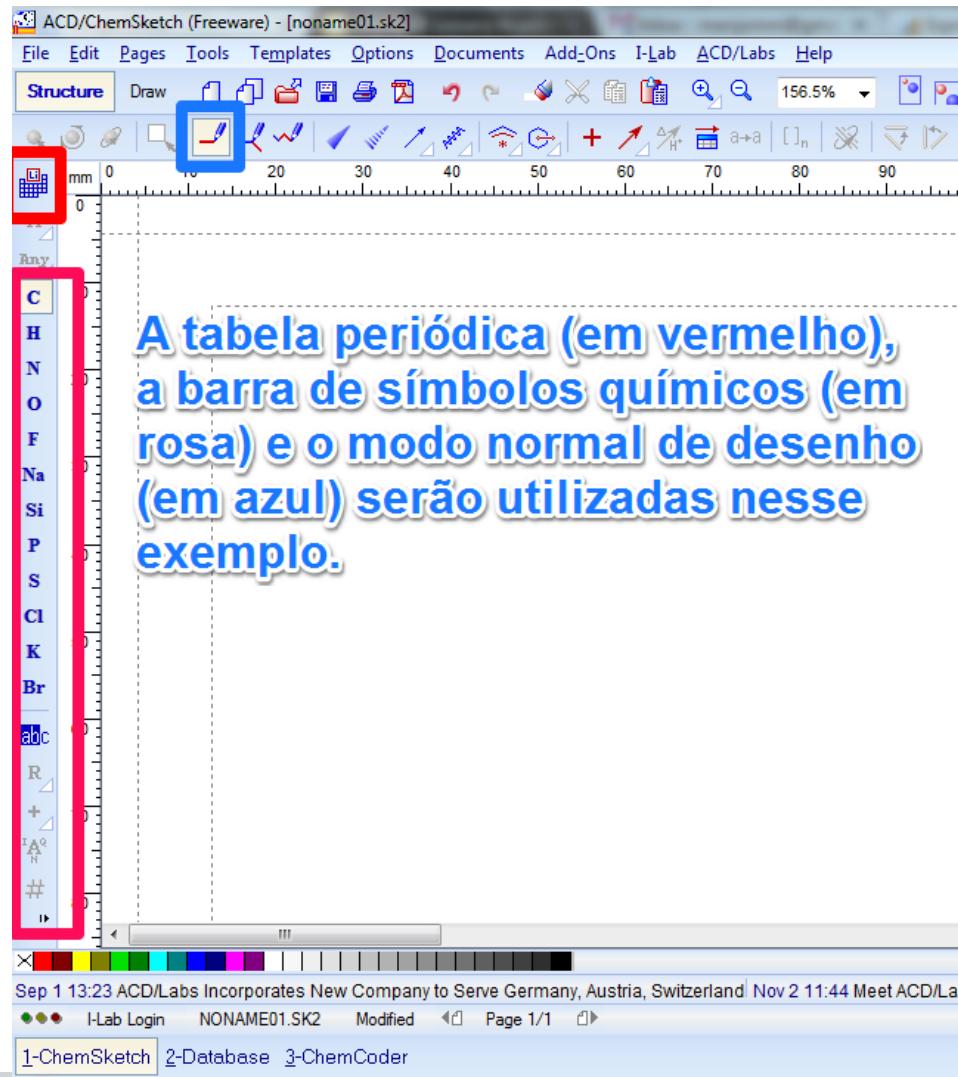
LIGAÇÕES DESLOCALIZADAS

Tipos de ligações químicas

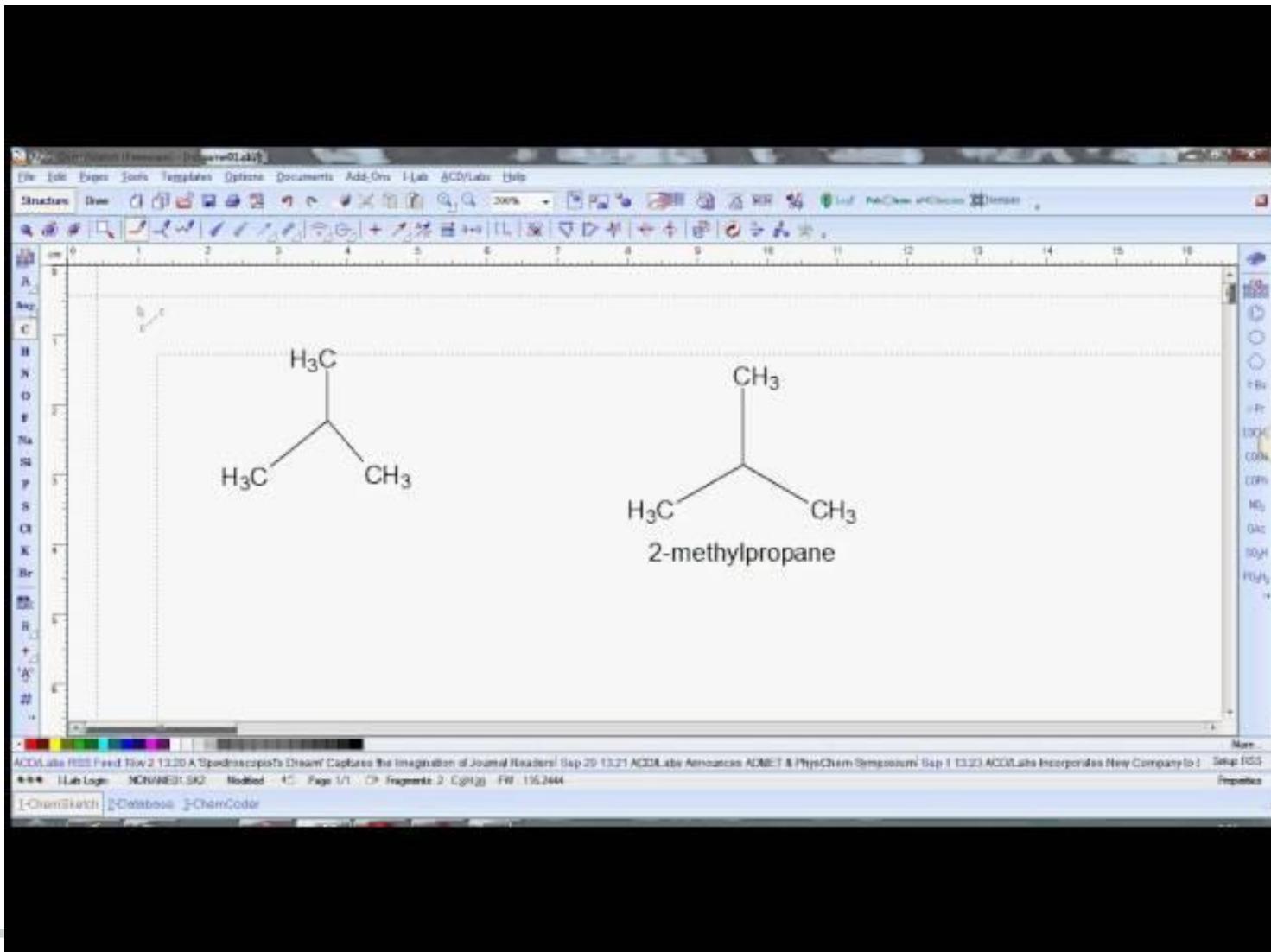


**LIGAÇÕES DE MARKUSH
LIGANTES EM POSIÇÕES INDEFINIDAS**

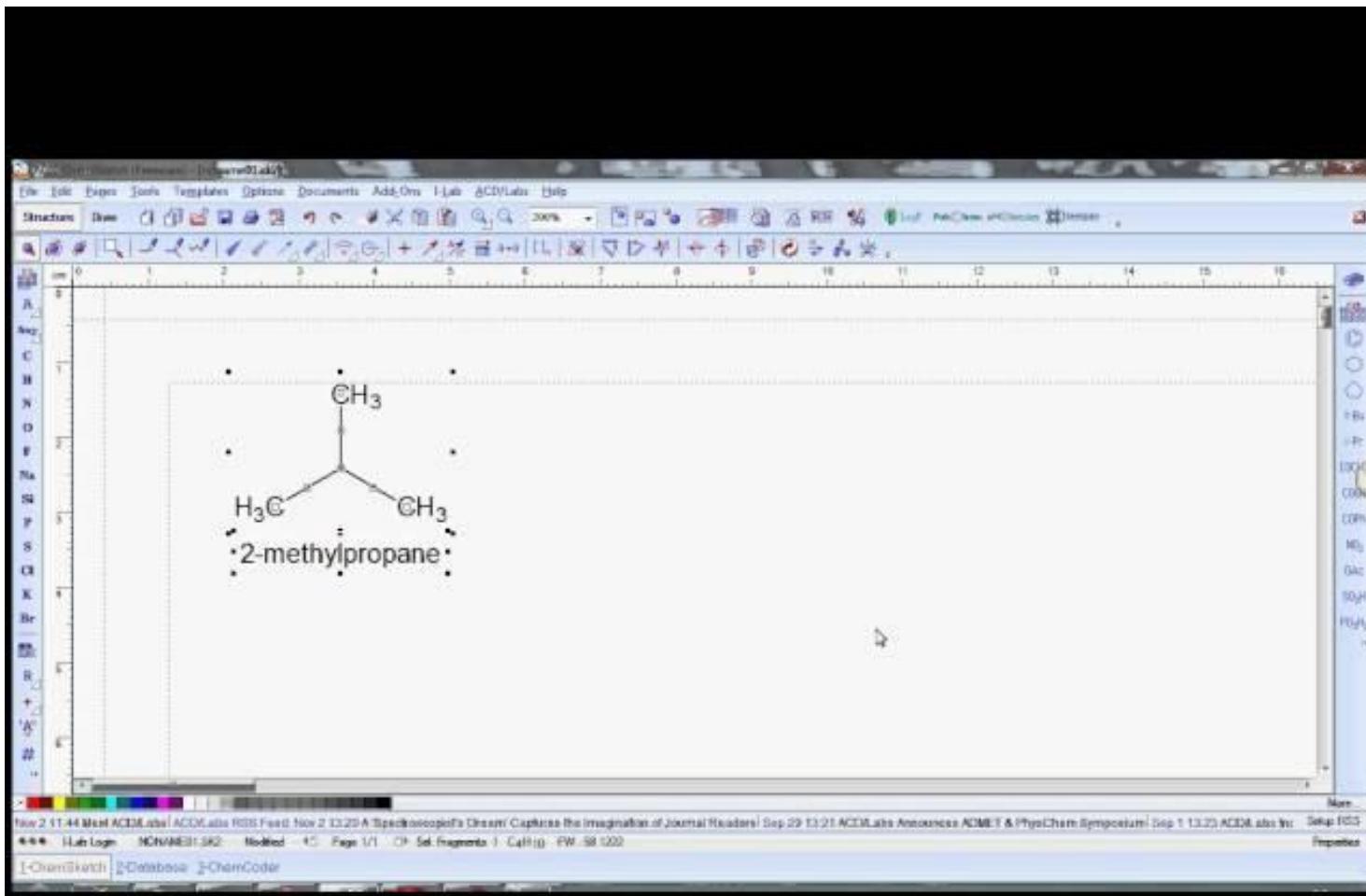
1º exemplo: desenho modo normal



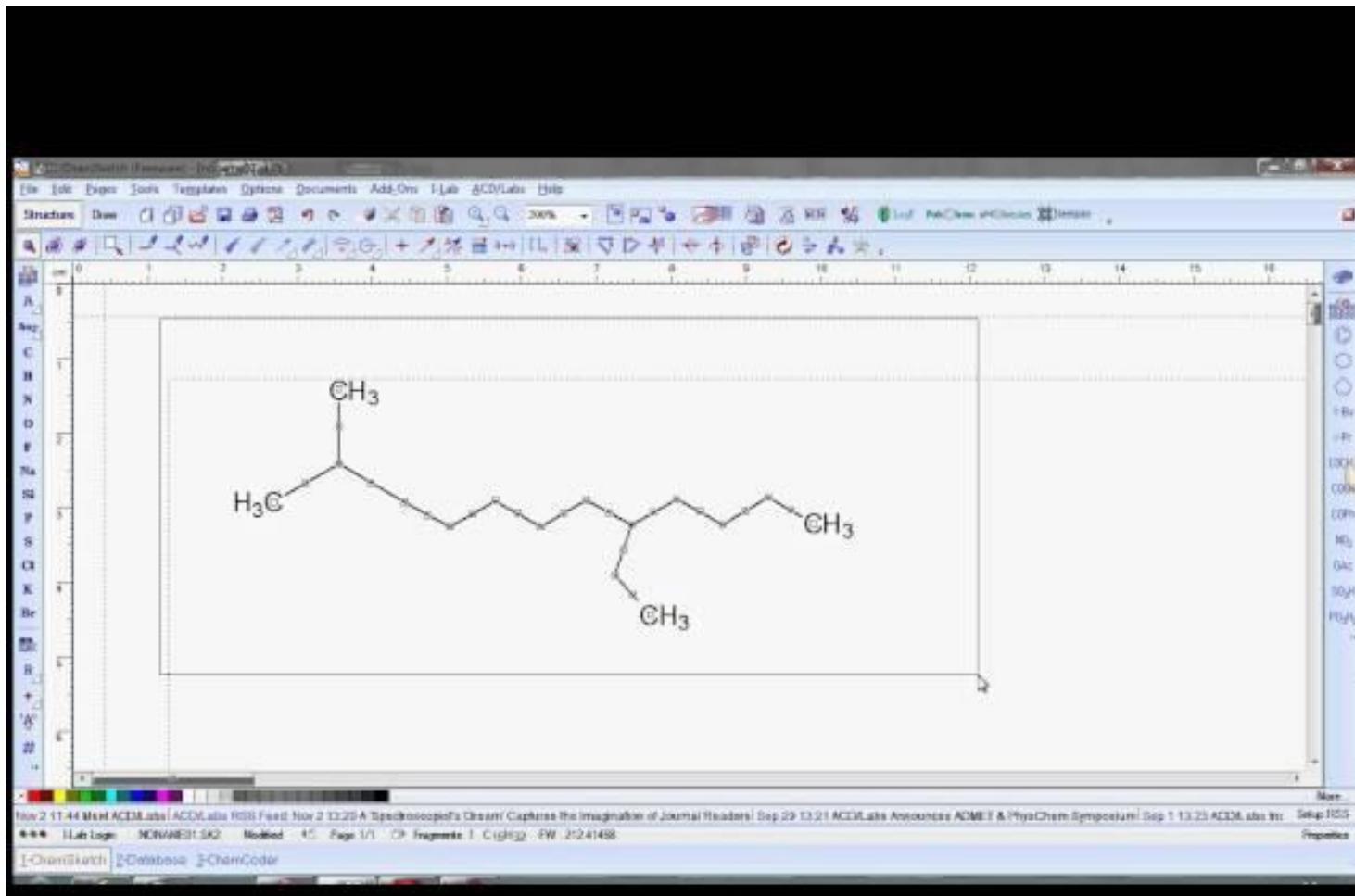
1. desenhando o 2-metilpropano



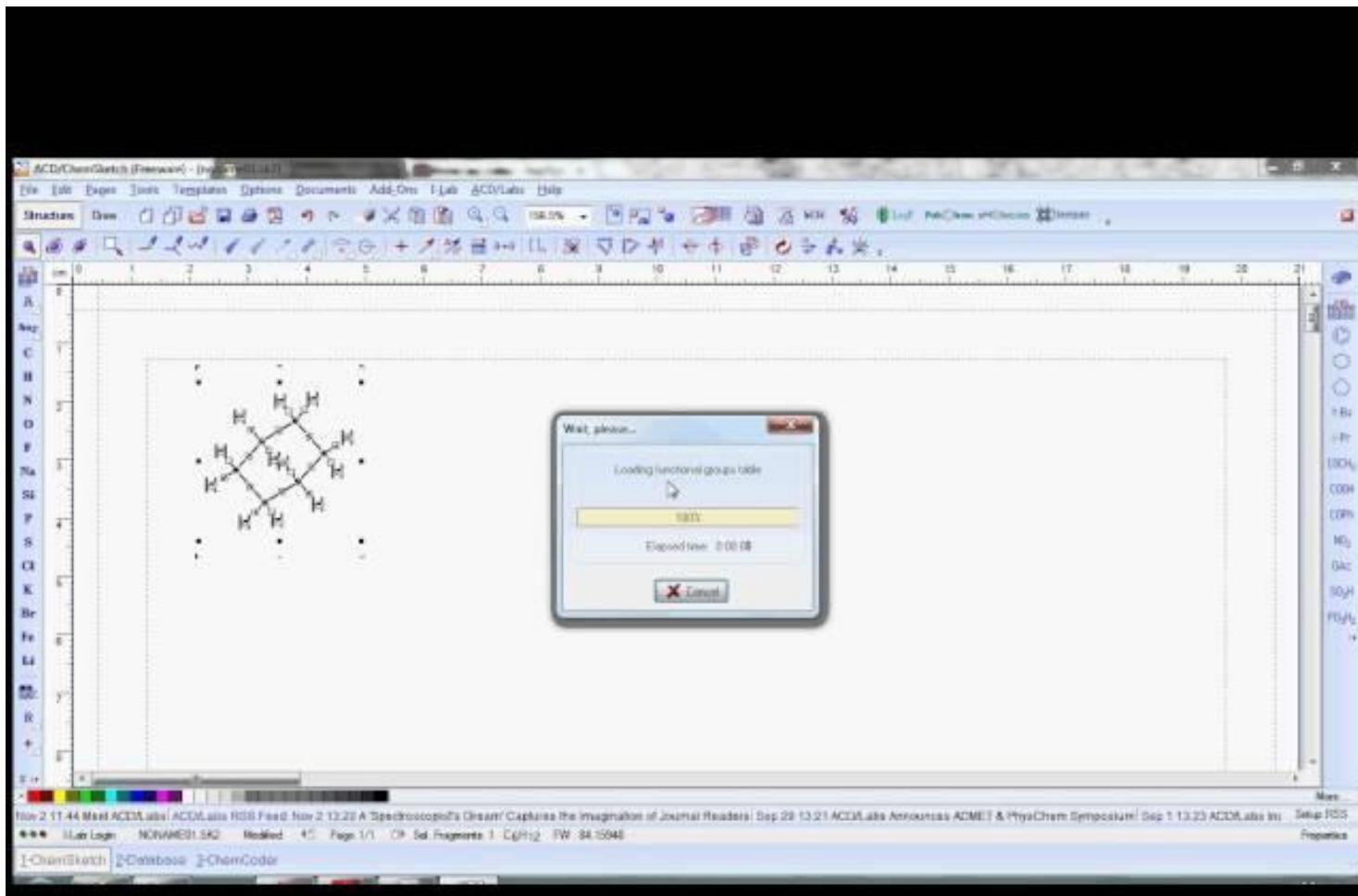
2-obtendo info sobre o 2- metilpropano



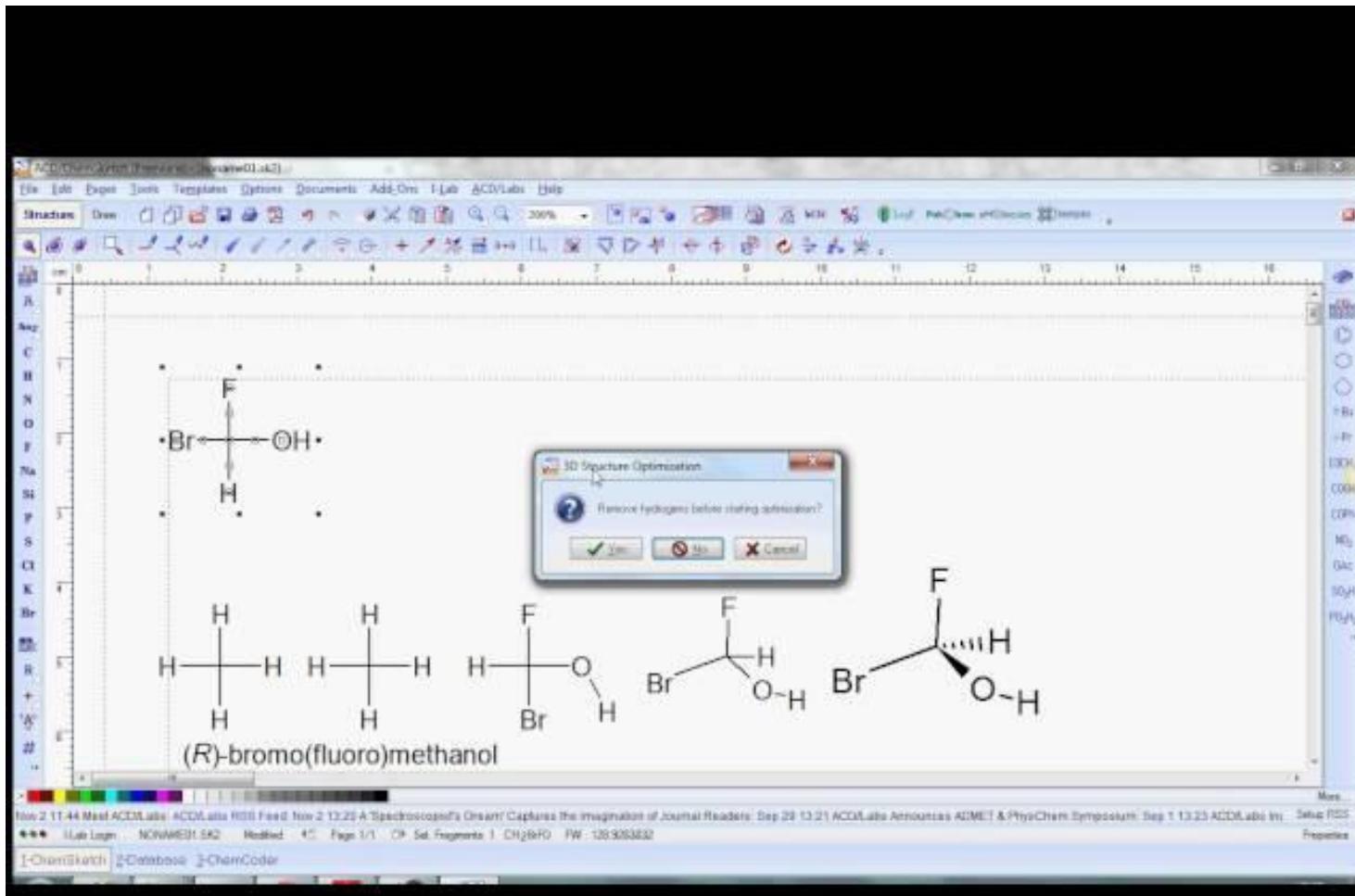
3.desenhando no modo cadeias



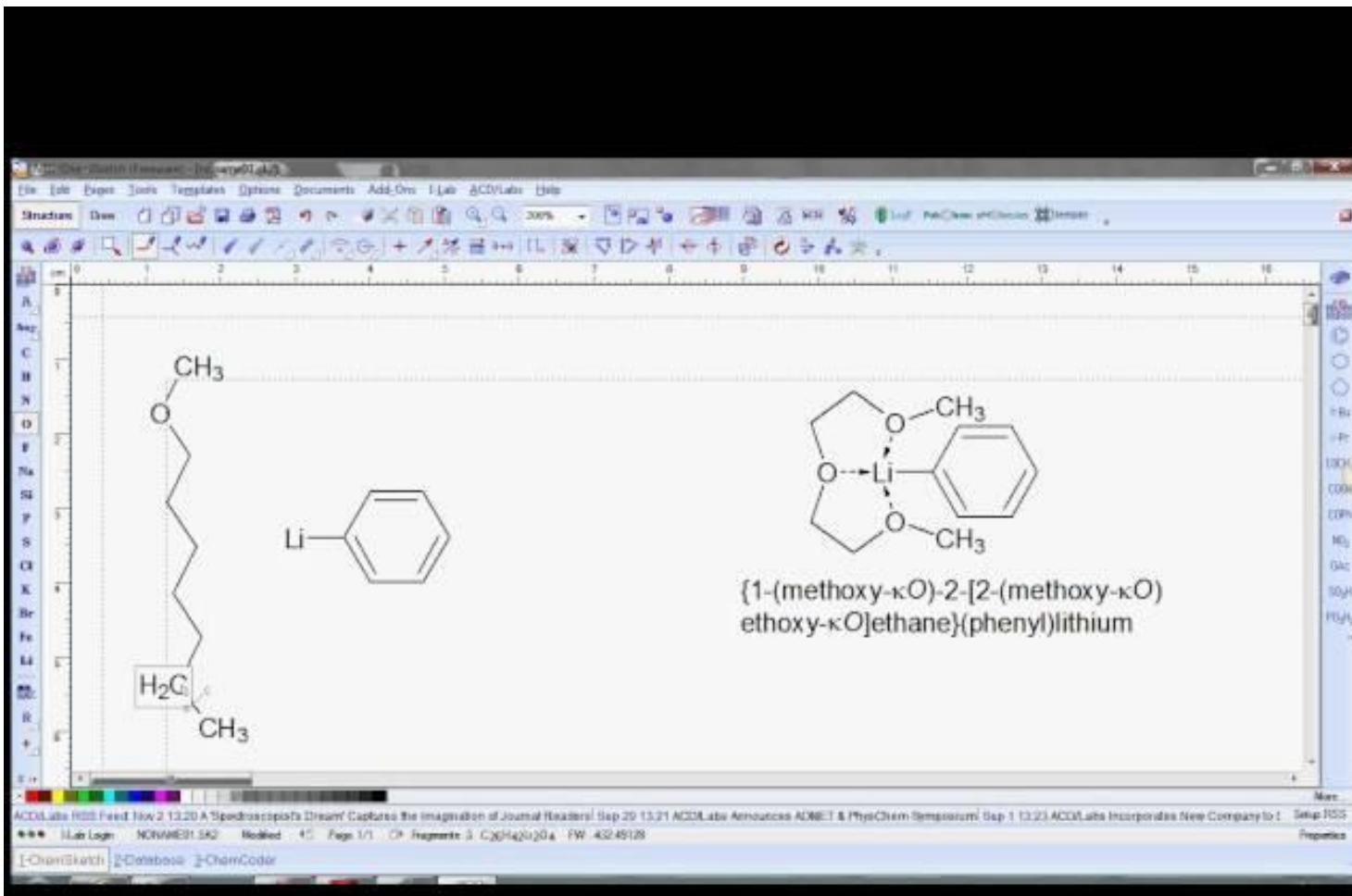
4.desenhando ciclohexano (modo contínuo)



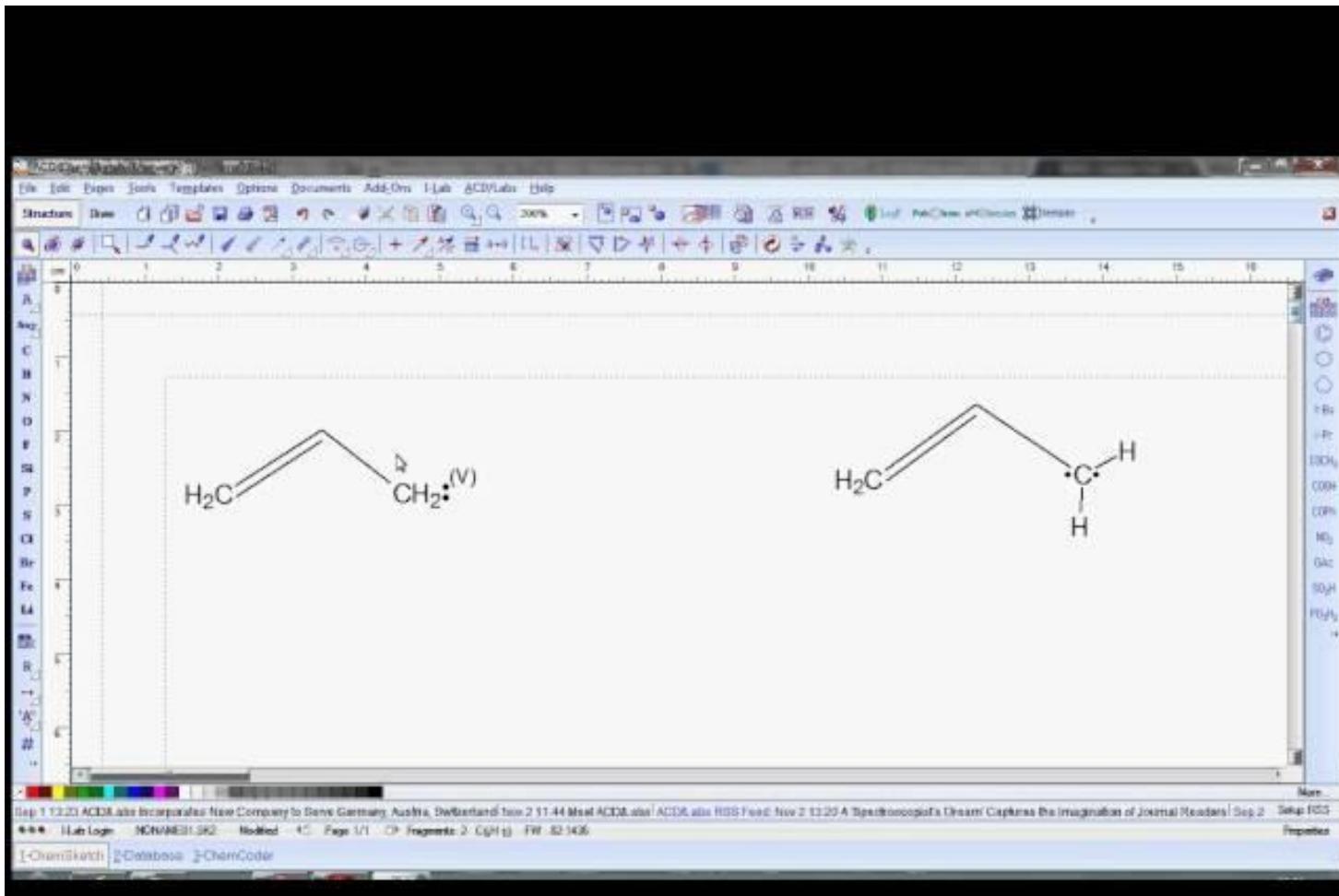
5. desenhando isômeros



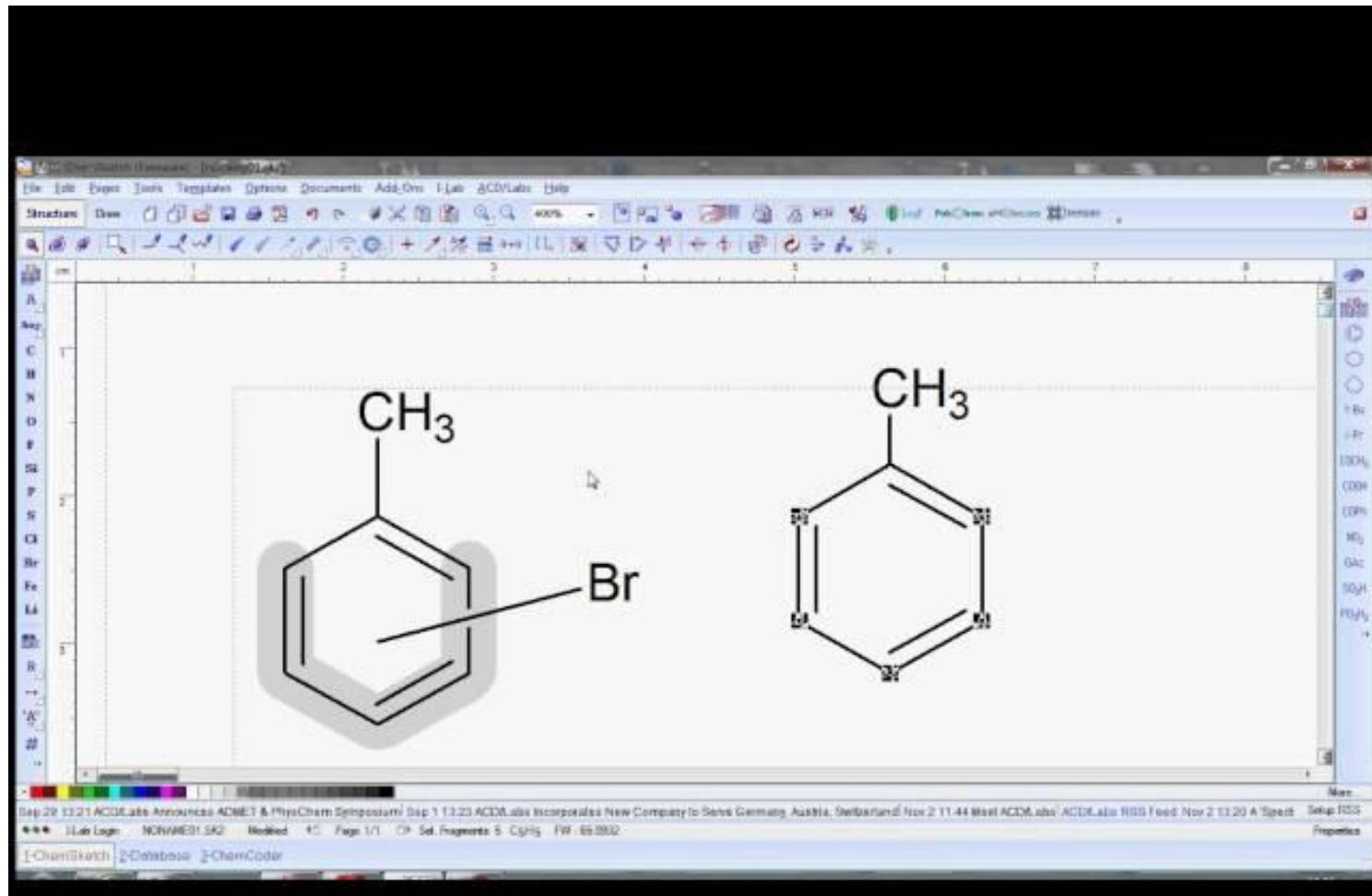
6.ligações coordenadas



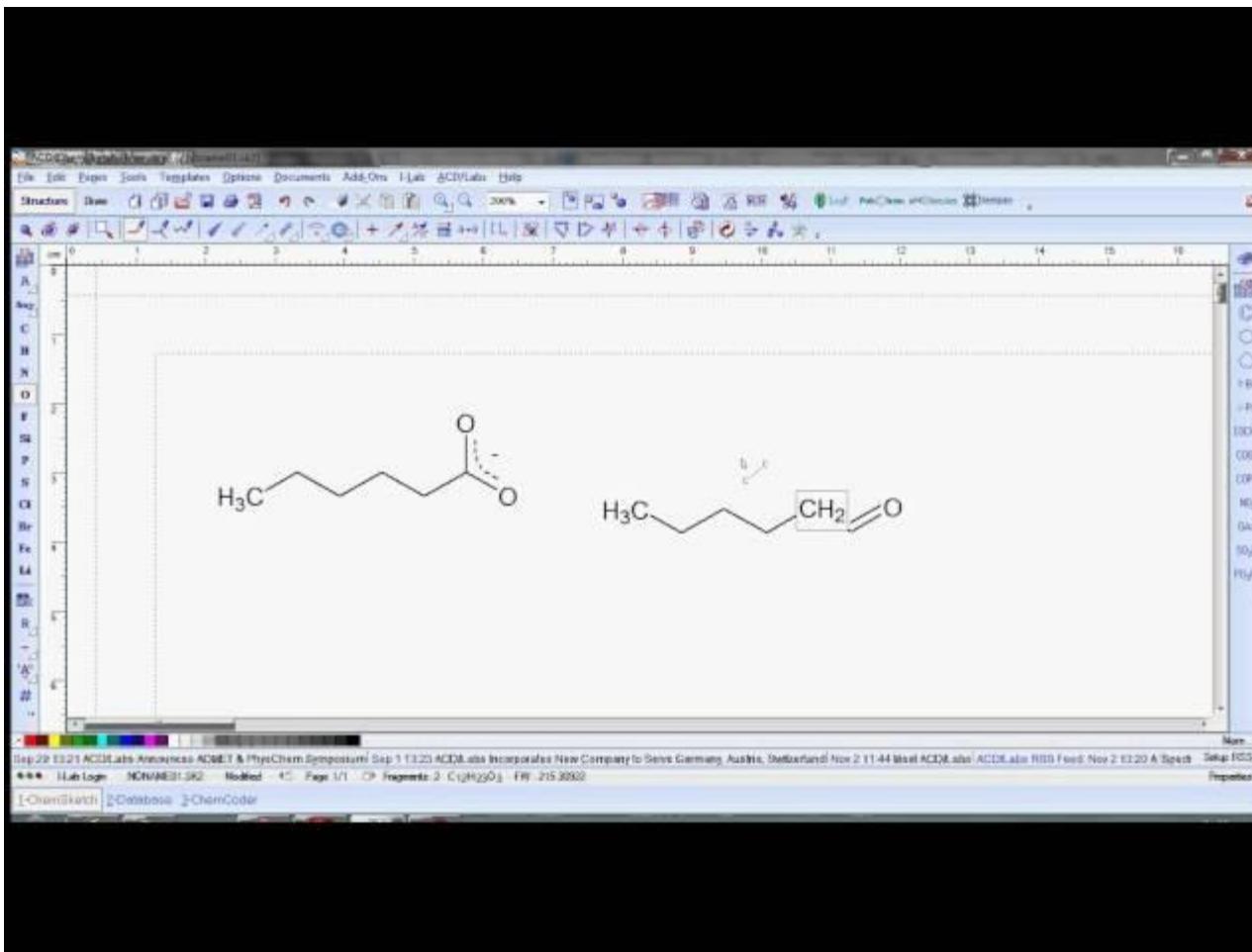
7.desenhando um radical alila



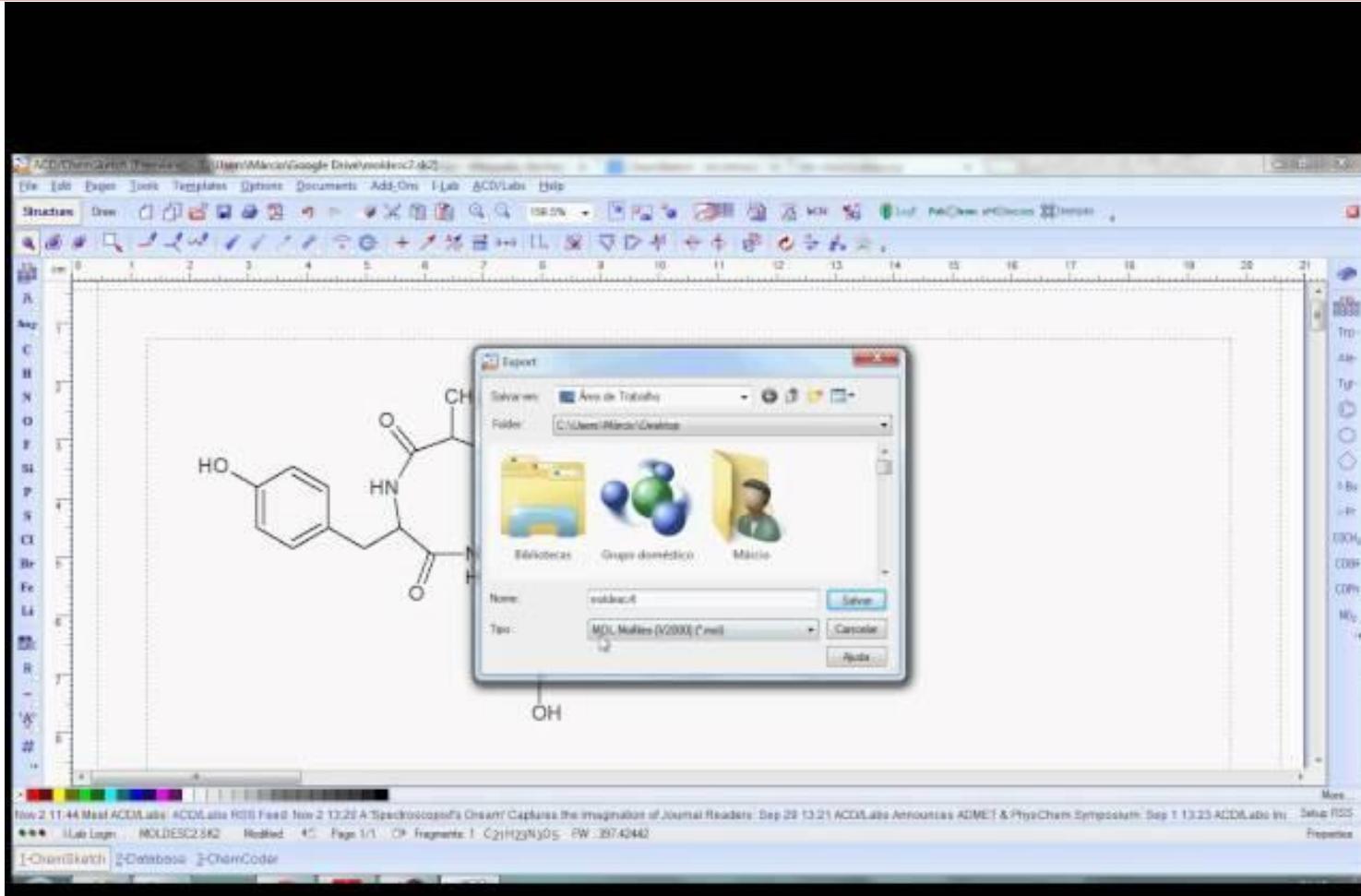
8.ligações de Markush



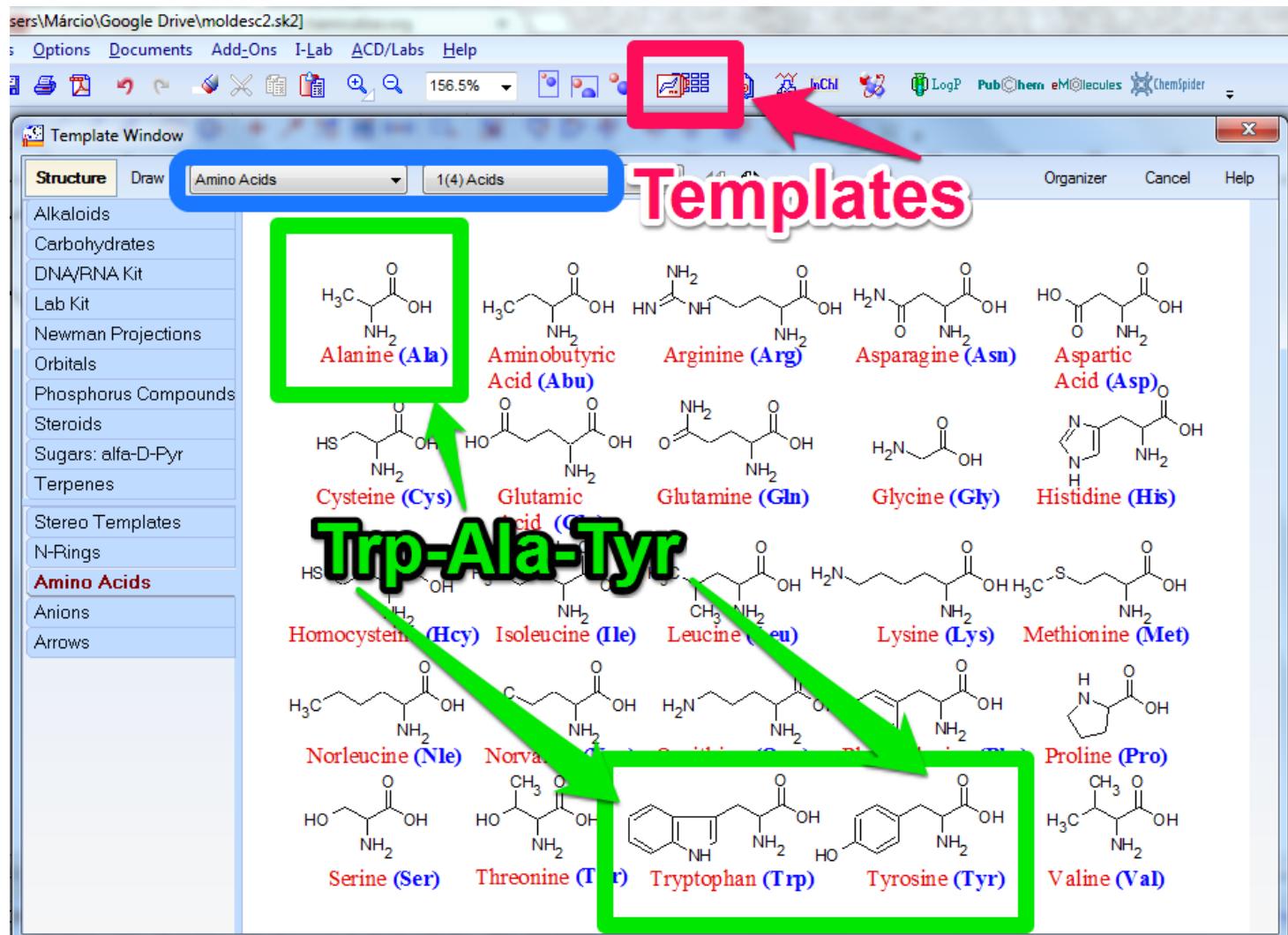
9.ligações deslocalizadas - íon hexanoato



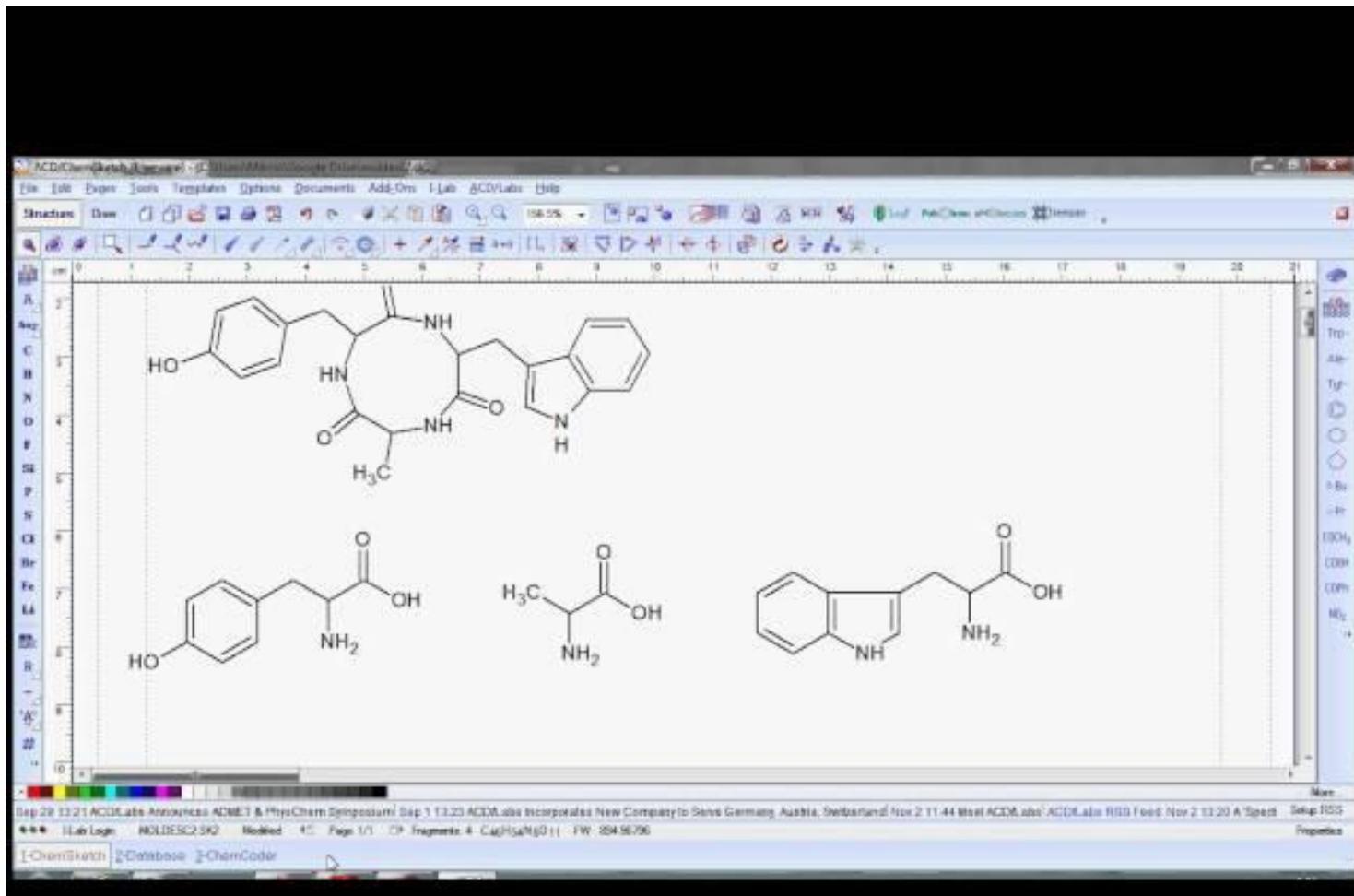
10. desenhando um peptídeo



Utilizando templates



11. desenhando peptídeo a partir de templates



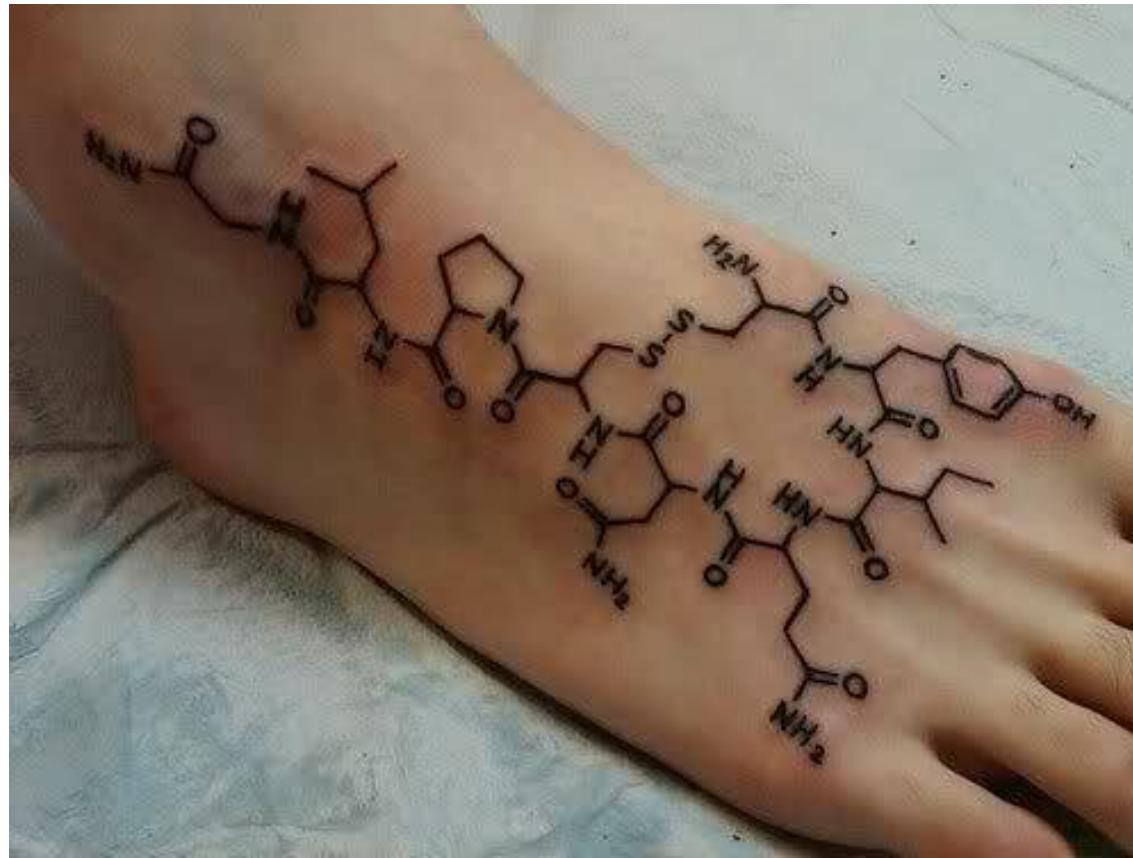
Exercitando técnicas de pesquisa online com o auxílio do ChemSketch

Vamos apresentar algumas moléculas encontradas na internet e vocês terão que desenhá-las.

Com o desenho pronto, vamos salvar e pesquisar dados físico-químicos online.

Molécula misteriosa 1

Que molécula é essa?



Dica

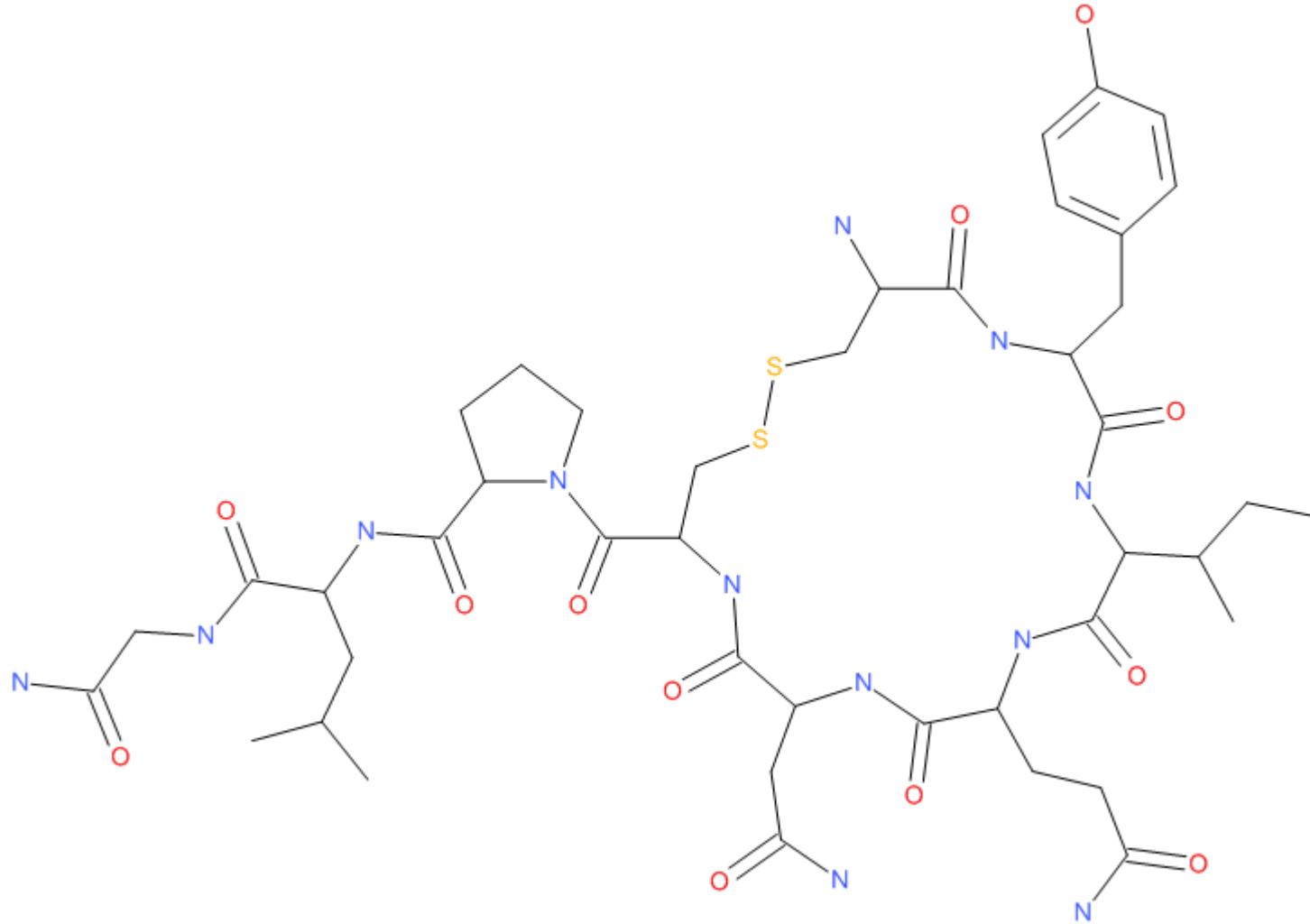
Desenhe a molécula no ChemSketch e salve-a em formato .MOL

Se você quiser facilitar as coisas, o link abaixo contém a estrutura já desenhada.

<http://goo.gl/4Twcw6> (formato mol)

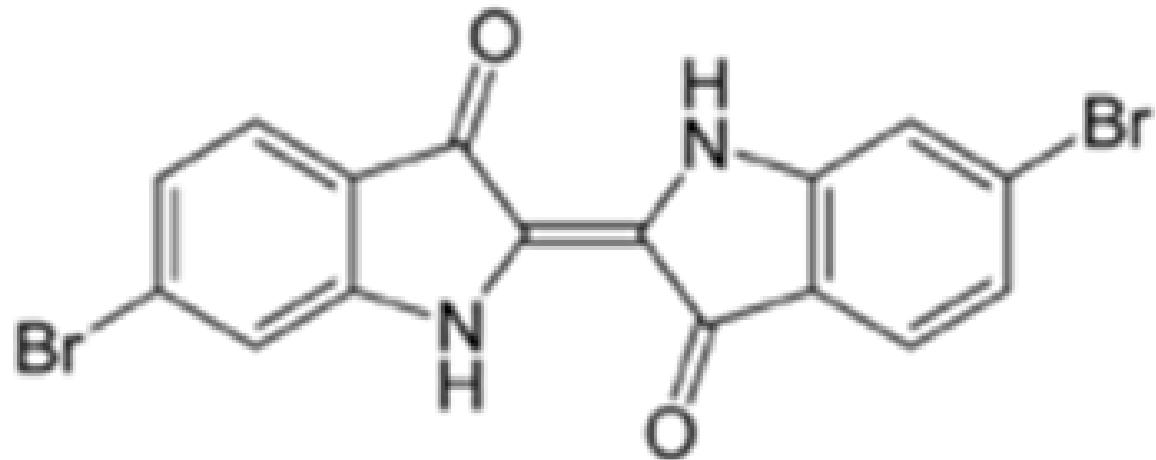
<http://goo.gl/nxapqo> (formato ChemSketch)

Molécula misteriosa 1



Molécula misteriosa 2

Que molécula é essa?



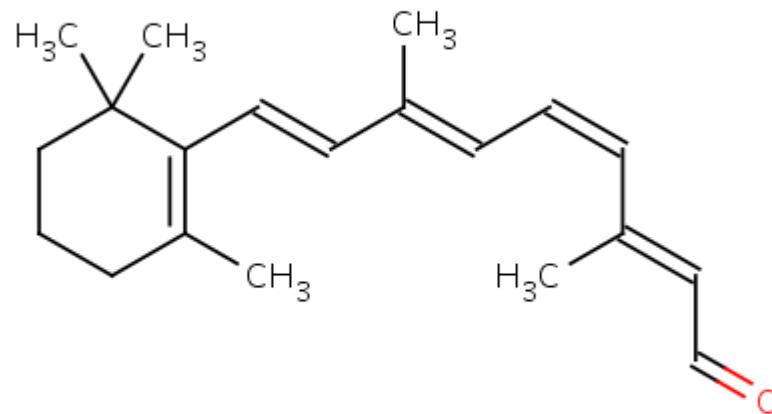
Molécula misteriosa 3

Que molécula é essa?



Molécula misteriosa 4

Que molécula é essa?



RESPONDA

- 1) Qual das moléculas misteriosas é a preferida do Bob Marley?
- 2) Qual das moléculas misteriosas é chamada “droga do amor”?
- 3) Qual é a molécula da visão?
- 4) Qual é a molécula preferida de reis e imperadores?

Como fazer para descobrir o nome?

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<http://www.chemspider.com/>

About More Searches Web APIs Help eg. Pyridine Search

Simple search Structure search Advanced search

eg. Aspirin

Systematic names 1,2-dihydroxybenzene	Synonyms AIBN	Trade names Aspirin	Registry numbers 7732-18-5	SMILES <chem>O=C(OCC)C</chem>	InChI <chem>InChI=1/CH4/h1H4</chem>
--	------------------	------------------------	-------------------------------	----------------------------------	--

Search

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- Interactive spectra
- Chemical suppliers

Waters THE SCIENCE OF WHAT'S POSSIBLE Give Feedback Generate Leads

<http://digichem.org/2011/10/24/dica-de-site-chemspider/>

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eg. Aspirin

Systematic names Synonyms Trade names
1,2-dihydroxybenzene AIBN Aspirin

Registry number SMILES InChI
7732-18-5 O=C(O)C(C)C [InChI]=1/CH4H1H4

Clique aqui para buscar a estrutura da molécula
Seamisteriosa!

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Usando a estrutura montada com ajuda do ChemSketch

▼ Search

Simple **Structure** Advanced ▾ More searches...

1. Input your structure (choose a, b or c)

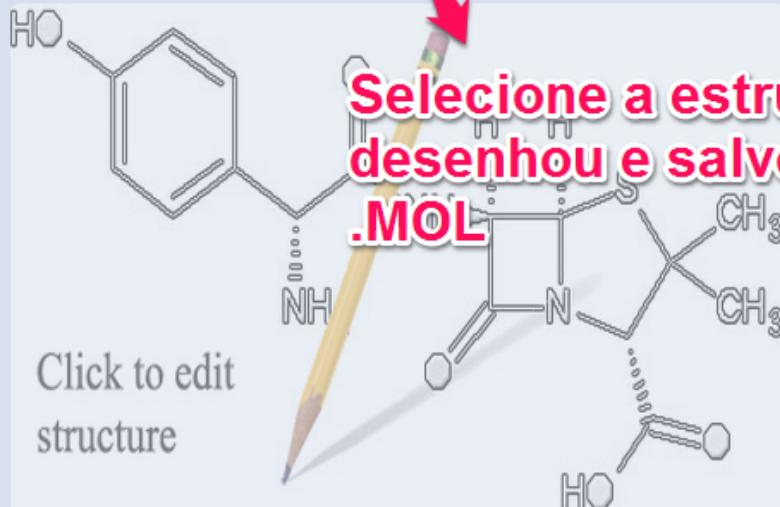
- a. Upload a structure file (MOL, SDF, CDX) or image file (PNG, JPG, GIF).

Nenhum arquivo selecionado

- b. Convert to structure using a name, SMILES, InChI or ChemSpider ID.

- c. Click the image to draw out the structure yourself.

2. Edit molecule



Buscando estruturas semelhantes

SDF, CDX) or image file (PNG, JPG, GIF).
Name, SMILES, InChI or ChemSpider ID.
Escolher arquivo Nenhum arquivo selecionado Convert

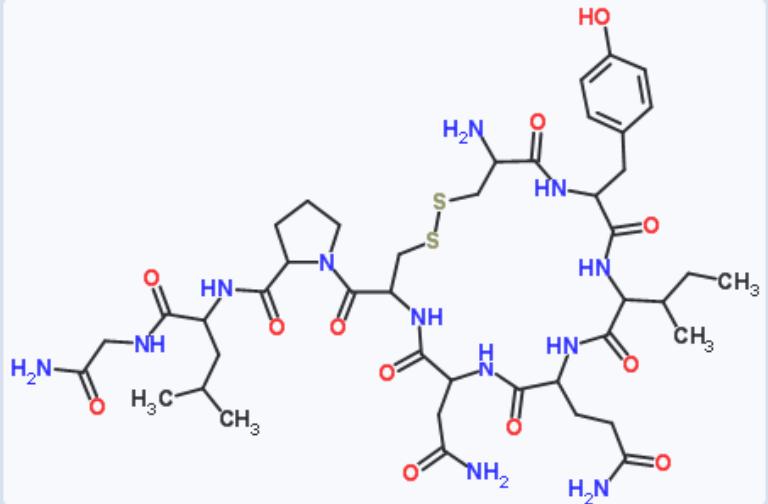
image to draw out the structure yourself.

2. Edit molecule

Exact
 Substructure
 Similarity

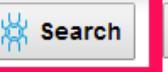
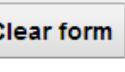
Search Options

Exact Match ?
 All Tautomers
 Same Skeleton (Including H)
 Same Skeleton (Excluding H)
 All Isomers



Clique para buscar estruturas semelhantes.

▶ Options

 Search  Clear form

Search Hits Limit: 100 ▾

Mistério 1 resolvido: ocitocina

Search and share chemistry

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Search term: Structure Search - Exact

8+ 0

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1-[19-Amino-7-(2-amino-2-oxoethyl)-10-(3-amino-3-oxopropyl)-13-sec-butyl-16-(4-hydroxybenzyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaazacycloicosan-4-yl]carbonyl]prolylleucylglycinamide

ChemSpider ID: 5567
Molecular Formula: C₄₃H₆₆N₁₂O₁₂S₂
Average mass: 1007.187317 Da
Monoisotopic mass: 1006.436462 Da

▼ Systematic name
1-[19-Amino-7-(2-amino-2-oxoethyl)-10-(3-amino-3-oxopropyl)-13-sec-butyl-16-(4-hydroxybenzyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaazacycloicosan-4-yl]carbonyl]prolylleucylglycinamide

► SMILES and InChIs
► Cite this record

Print

Name
Names an
Validated by...
... redirected by Users, Redirect Approved by Experts
Edit

É possível salvar a estrutura em 3D.

1-[19-Amino-7-(2-amino-2-oxoethyl)-10-(3-amino-3-oxopropyl)-13-sec-butyl-16-(4-hydroxybenzyl)-6,9,12,15,18-pentaoxo-1,2-dithia-5,8,11,14,17-pentaazacycloicosan-4-yl]carbonyl]prolylleucylglycinamide (German) (ACD/IUPAC Name)

Give Feedback

Generate Leads

Dados biológicos de moléculas

Se você quer encontrar artigos sobre estudos químicos e bioquímicos das moléculas em questão, entre no site PubChem.

<http://pubchem.ncbi.nlm.nih.gov/>

The screenshot shows the PubChem homepage. At the top, there is a navigation bar with links for Databases, Upload, Services, Help, and more. Below the navigation bar is the PubChem logo. A search bar contains the query "11-cis-retinal". To the right of the search bar is a "Go" button and an "Advanced Search" link. Below the search bar, there is a "Try the new PubChem Search" link. On the left side of the main content area, there are three buttons: BioAssay, Compound, and Substance. On the right side, there is a sidebar with various links and icons. The sidebar includes links for BioActivity Summary, BioActivity Datatable, BioActivity SAR, BioActivity structure-activity, Structure Search, 3D Conformer Tools, Structure Clustering, Classification, Upload, Download, and PubChem FTP. There are also social media sharing icons (Facebook, Twitter, Google+, RSS) and a "more ..." link.

Dados biológicos de moléculas

No exemplo, procurei por informações sobre o 11-cis-retinal.

NCBI Resources How To Sign in to NCBI

PubChem Compound "11-cis-retinal" Save search Limits Advanced

Display Settings: Summary, Sorted by Default order

Send to: Filters: [Manage Filters](#)

Results: 3

Clique aqui

1. [11-cis-Retinal: 11-cis-Vitamin A aldehyde; 11-cis-Retinene ...](#)

MW: 284.435720 g/mol MF: C₂₀H₂₈O
IUPAC name: (2E,4Z,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohexen-1-yl)...
CID: 5280490

[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [PubMed \(MeSH Keyword\)](#) [Active in 4 of 6 BioAssays](#)

2. [retinal: all-trans-Retinal: vitamin A aldehyde ...](#)

MW: 284.435720 g/mol MF: C₂₀H₂₈O
IUPAC name: (2E,4E,6E,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohexen-1-yl)...
CID: 638015

[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#)
Active in 89 of 275 BioAssays

3. [13-Cis retinal: Retinal, 9-cis-; 3,7-dimethyl-9-\(2,6,6-trimethylcyclohex-1-en-1-yl\)nona-2,4,6,8-tetraenal ...](#)

MW: 284.435720 g/mol MF: C₂₀H₂₈O
IUPAC name: 3,7-dimethyl-9-(2,6,6-trimethylcyclohexen-1-yl)nona-2,4,6,8-...

v.ncbi.nlm.nih.gov/pccompound?term="11-cis-retinal" #

Actions on your results

- [BioActivity Analysis](#)
Analyze the BioActivities of the compounds
- [Structure Clustering](#)
Cluster structures based on structural similarity
- [Structure Download](#)
Download the structures in various formats
- [Pathways](#)
Analyze pathways containing the compounds

Refine your results • What's this?

BioActivity Experiments

- [BioAssays, Active \(2\)](#)
- [BioAssays, Tested \(2\)](#)

Dados biológicos de moléculas

Clicando em *summary*, descobre-se a ficha completa da molécula.

Pode-se baixar um modelo 3D da molécula.

SHARE

Compound Summary for: CID 5280490

Retinaldehyde

Also known as: 11-cis-Retinal; 11-cis-Vitamin A aldehyde; 11-cis-Retinene; 11-cis-Retinaldehyde; CHEBI:16066; 564-87-4; Neoretinene b; cis-Retinal
Molecular Formula: C₂₀H₂₈O Molecular Weight: 284.43572 InChIKey: NCYCYZXNIZJOKI-IOUUIBBYSA-N

A carotenoid constituent of visual pigments. It is the oxidized form of retinol which functions as the active component of the visual cycle. It is bound to the protein opsin forming the complex rhodopsin. When stimulated by visible light, the retinal component of the rhodopsin complex undergoes isomerization at the 11-position of the double bond to the cis-form; this is reversed in "dark" reactions to return to the native trans-configuration. From: MeSH

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Classification

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PubChem Compound

Limits Advanced search

2D Structure 3D Conformer

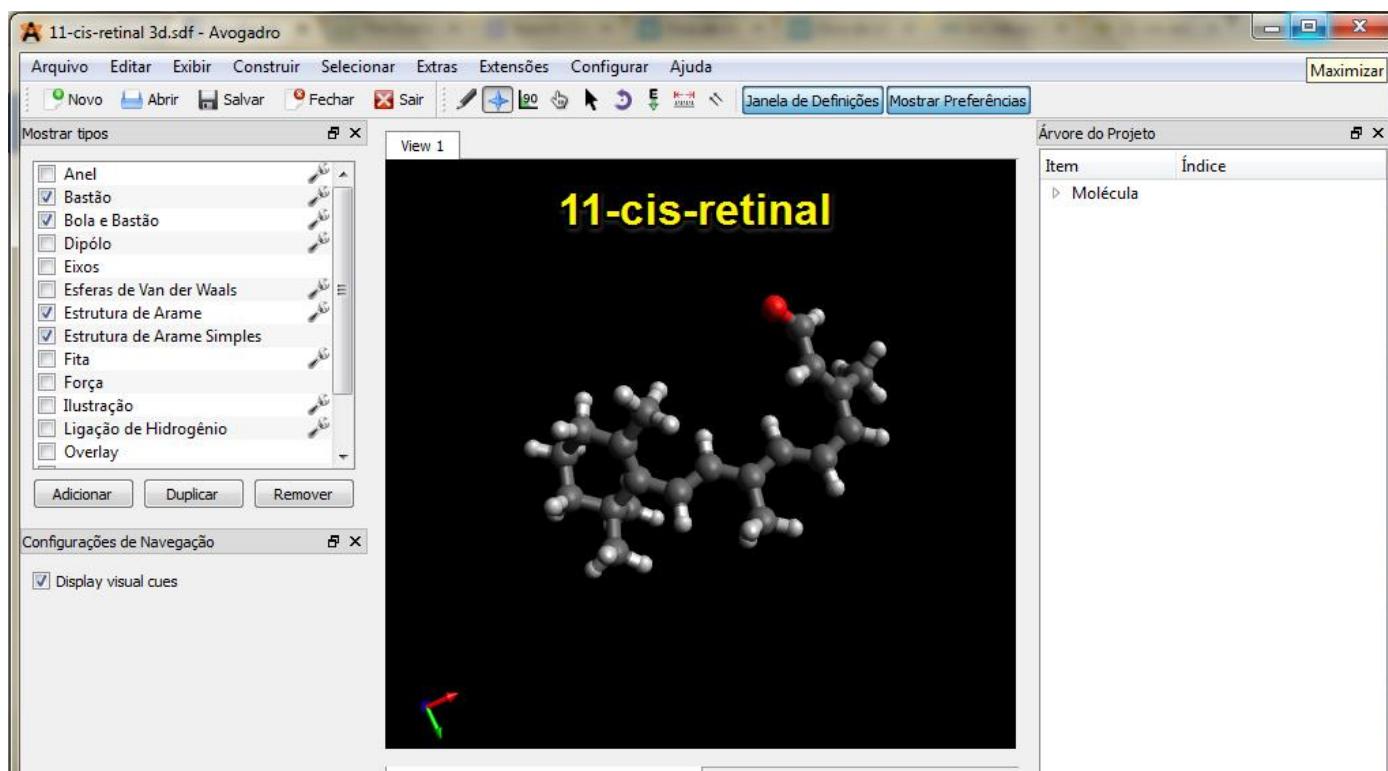
Chemical structure diagram of Retinaldehyde (11-cis-Retinal) showing its characteristic cis double bonds.

ASN.1 XML SDF

É possível obter um arquivo com a estrutura 3D da molécula.

Dados biológicos de moléculas

O formato é SDF, e pode ser aberto com o software Avogadro.



Dados biológicos de moléculas

Clicando no botão BioActivity summary, uma nova página com os dados biológicos surge.

NCBI

PubChem Compound

PubChem Compound Limits Advanced search Search Help

CID: CID 5280490

Retinal; 11-cis-Vitamin A aldehyde; 11-cis-Retinene; 11-cis-Retinaldehyde; CHEBI:16066; 564-87-4; Neoretinene b; cis-Retinal H₂₈O Molecular Weight: 284.43572 InChIKey: NCYCYZXKNIZJOKI-IOUUIBBYSA-N

of visual pigments. It is the oxidized form of retinol which functions as the active component of the visual cycle. It is bound to the protein opsin forming rhodopsin. When stimulated by visible light, the retinal component of the rhodopsin complex undergoes isomerization at the 11-position of the double bond to the "dark" reactions to return to the native trans-conformation.

Clicando nesse botão, o site buscará por atividade biológica da molécula

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2D Structure 3D Conform

Chemical structure diagram of Retinal (11-cis-Retinene).

Links and Related Information

Follow us on

Properties

Compound ID: 5280490
Molecular Weight: 284.43572 [g/mol]
Molecular Formula: C₂₀H₂₈O
H-Bond Donor: 0
H-Bond Acceptor: 1

BioActivity Data Links

This Compound with Similar Compounds

Dados biológicos de moléculas

Clicando no botão BioActivity summary, uma nova página com os dados biológicos surge.

Retinaldehyde (CID 5280490) - Compound BioActivity Data

A carotenoid constituent of visual pigments. It is the oxidized form of retinol which functions as the active component of the visual cycle. It is bound to the protein opsin forming the complex rhodopsin. When stimulated by visible light, the retinal component of the rhodopsin complex undergoes isomerization at the 11-position of the double bond to the cis-form; this is reversed in "dark" reactions to return to the native trans-configuration.

BioActivity Outcomes:

- Active(5)
- Unspecified(2)

Top Targets:

- Rhodopsin N(1)
- 7TM GPCR Srx(1)

BioAssay Types:

- Literature(7)

Target summary

Data download

Chemical Probe Active Inactive Inconclusive Unspecified

#	Substance	Activity	BioAssay	Target	Links	
#	Substance	Outcome	Type	Value [μM]		
1	3hx3 [SID170462749]	—	Kd	0.01	Experimentally measured binding affinity data (Kd) for protein-ligand complexes derived from PDB [AID977811, Type: Literature]	Chain A, Crystal Structure Of Cralbp Mutant R234w [gi:261824988] View
~	3hx3	—	Kd	~0.01	Experimentally measured binding affinity data (Kd) for protein-ligand complexes derived from PDB [AID977811, Type: Literature]	Chain A, Crystal Structure Of Cralbp Mutant R234w [gi:261824988] View

Respostas para os desafios

- 1) Oxitocina, também conhecida como droga do amor.
- 2) Púrpura de Tyrian, usada para tingir de púrpura as vestes de reis.
- 3) Tetrahidrocanabinol (THC), componente principal da maconha.
- 4) 11-cis-retinal, molécula envolvida na visão

E isso encerra nossa oficina...

