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# Aprendendo a usar o Chemsketch

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Prof. Dr. Márcio Marques Martins



digimarcio

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## Onde encontrar o software?

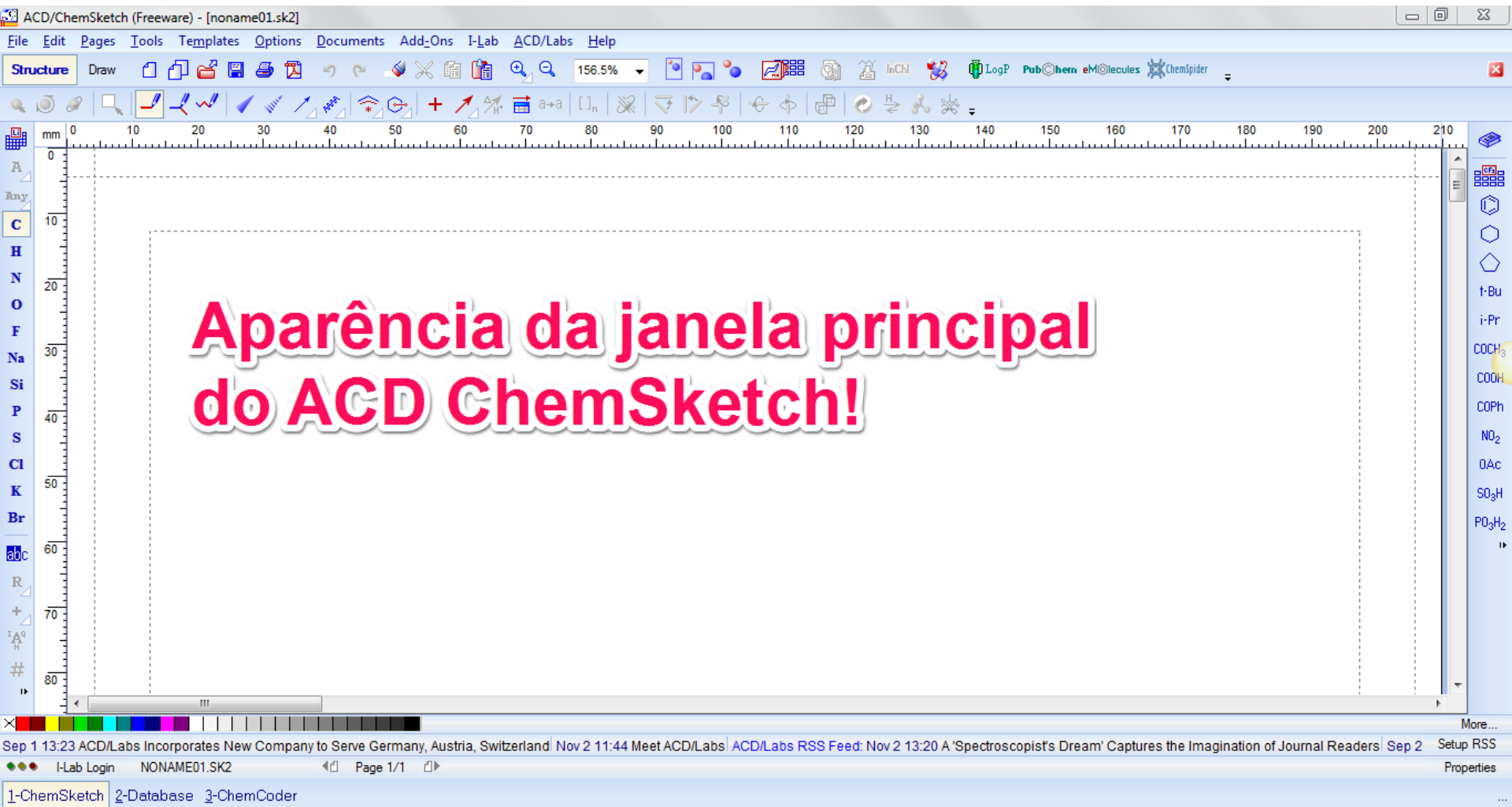
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O ChemSketch pode ser baixado de forma gratuita no endereço <http://goo.gl/XX9Q8j>.

É necessário fazer um cadastro.

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# Janela principal



# Barra de desenho

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**SELECIONAR/MOVER**

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# Barra de desenho

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**SELECIONAR/MOVER/REDIMENSIONAR**

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# Barra de desenho

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**ROTAÇÃO 3D**

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# Barra de desenho

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**LAÇO ON/OFF**

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# Alternando entre modos de desenho

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

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# Alternando entre modos de desenho

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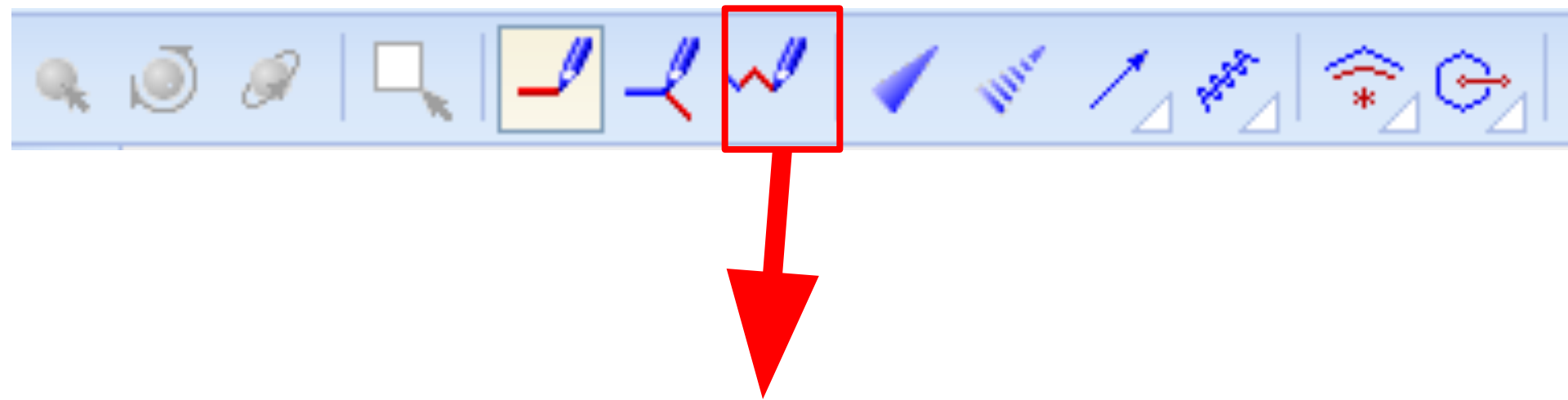


**DESENHAR CONTÍNUO - SIMILAR AO MODO NORMAL**

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# Alternando entre modos de desenho

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

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# Tipos de ligações químicas

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**LIGAÇÕES ESTEREOQUÍMICAS**

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# Tipos de ligações químicas

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**VÁRIOS TIPOS DE LIGAÇÕES  
COORDENADAS**

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# Tipos de ligações químicas

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**LIGAÇÕES ESTÉREO INDEFINIDAS**

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# Tipos de ligações químicas

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**LIGAÇÕES DESLOCALIZADAS**

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# Tipos de ligações químicas

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**LIGAÇÕES DE MARKUSH  
LIGANTES EM POSIÇÕES INDEFINIDAS**

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# 1º exemplo: desenho modo normal

The screenshot displays the ACD/ChemSketch (Freeware) interface. The title bar reads "ACD/ChemSketch (Freeware) - [noname01.sk2]". The menu bar includes "File", "Edit", "Pages", "Tools", "Templates", "Options", "Documents", "Add-Ons", "I-Lab", "ACD/Labs", and "Help". The "Structure" tab is active, and the "Draw" menu is open, showing various drawing tools. A blue box highlights the "Normal" drawing mode icon. A red box highlights the periodic table in the left sidebar, and a pink box highlights the chemical symbols bar. A blue text box with a white border contains the following text: "A tabela periódica (em vermelho), a barra de símbolos químicos (em rosa) e o modo normal de desenho (em azul) serão utilizadas nesse exemplo." The interface also shows a ruler at the top, a status bar at the bottom, and a taskbar at the very bottom.

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

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

Structure Draw

mm 0 20 30 40 50 60 70 80 90 1

Any

C

H

N

O

F

Na

Si

P

S

Cl

K

Br

abc

R

+

A

#

156.5%

Sep 1 13:23 ACD/Labs Incorporates New Company to Serve Germany, Austria, Switzerland Nov 2 11:44 Meet ACD/Lab

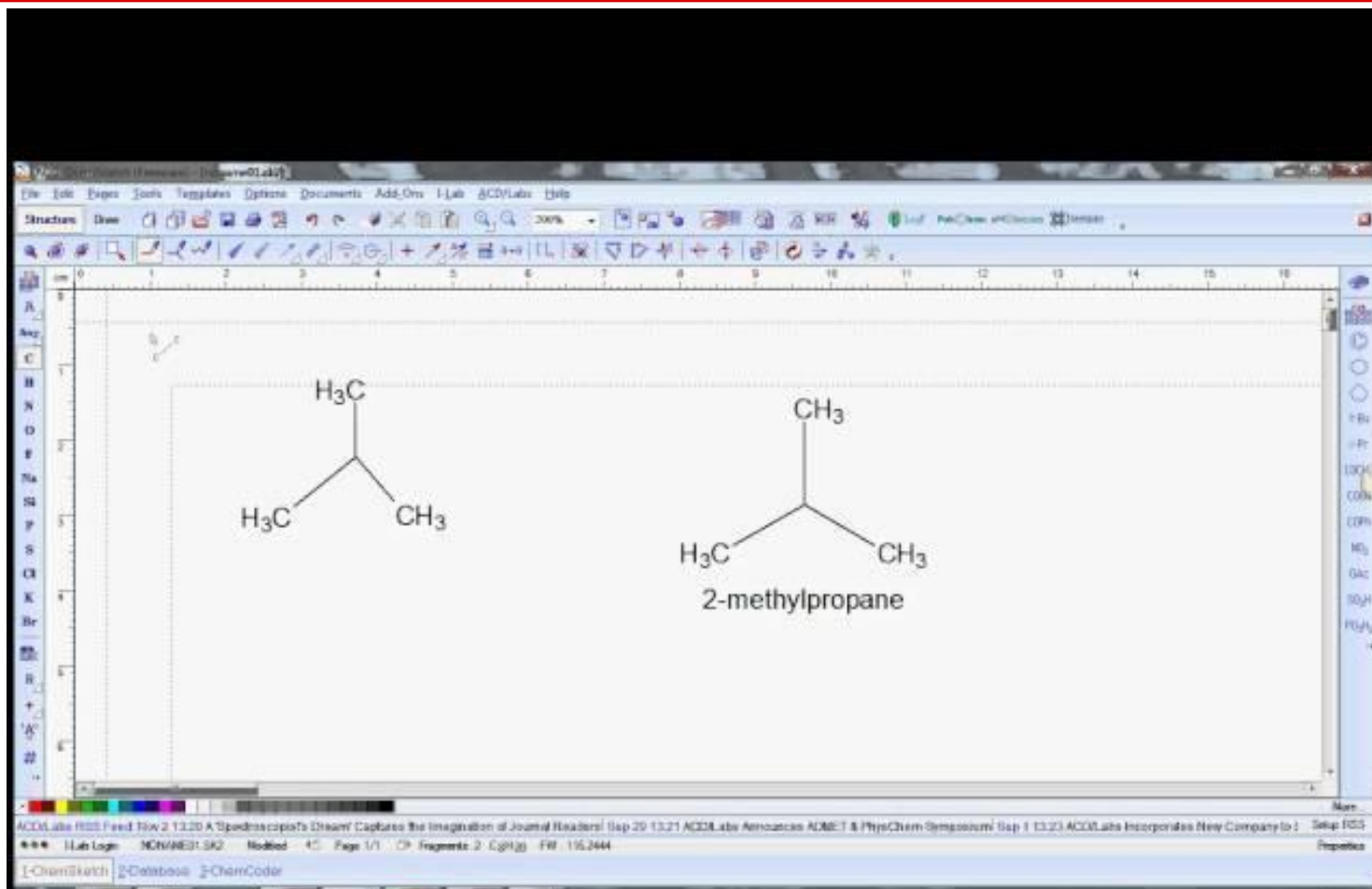
I-Lab Login NONAME01.SK2 Modified Page 1/1

1-ChemSketch 2-Database 3-ChemCoder

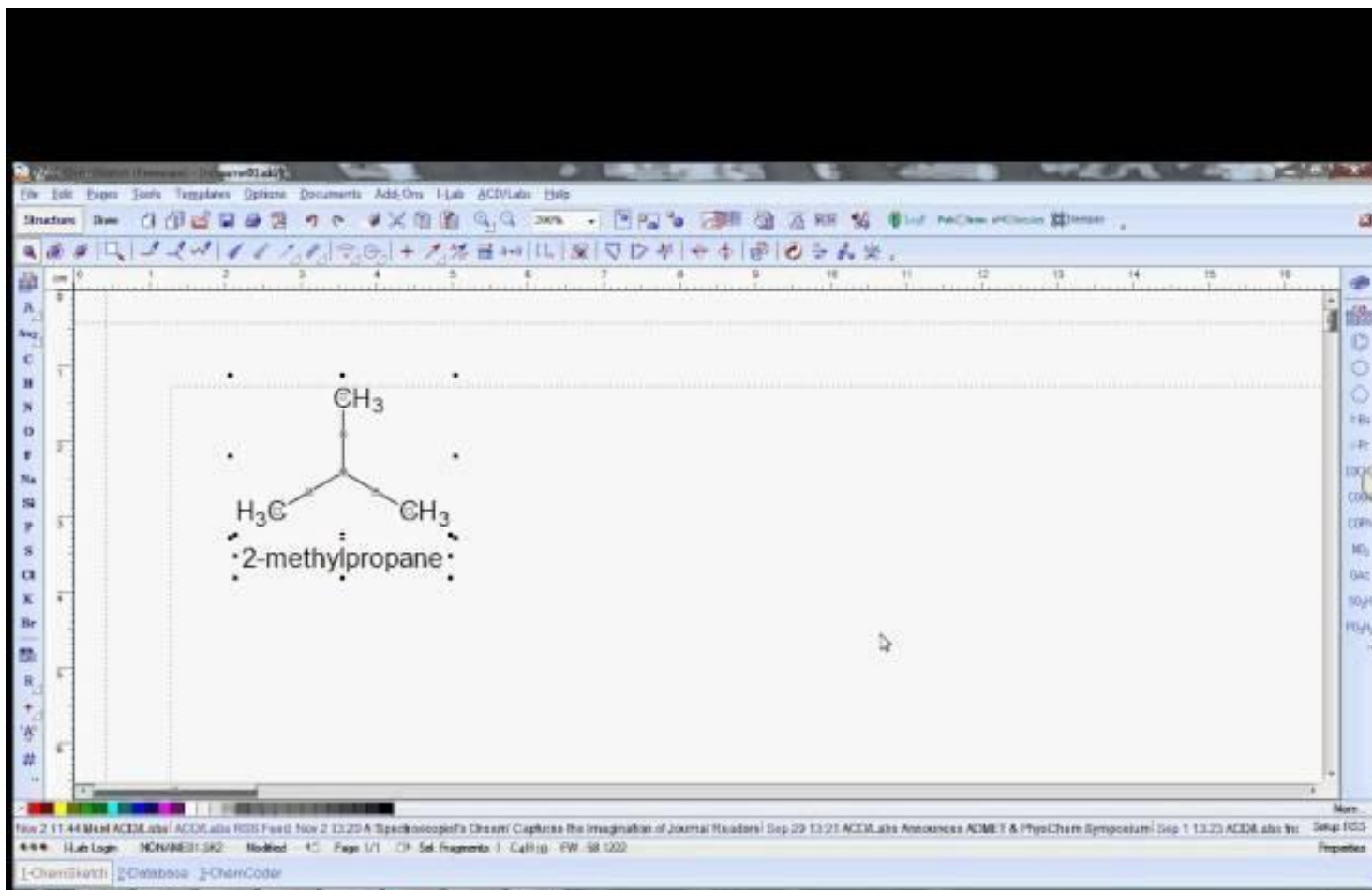
A tabela periódica (em vermelho), a barra de símbolos químicos (em rosa) e o modo normal de desenho (em azul) serão utilizadas nesse exemplo.



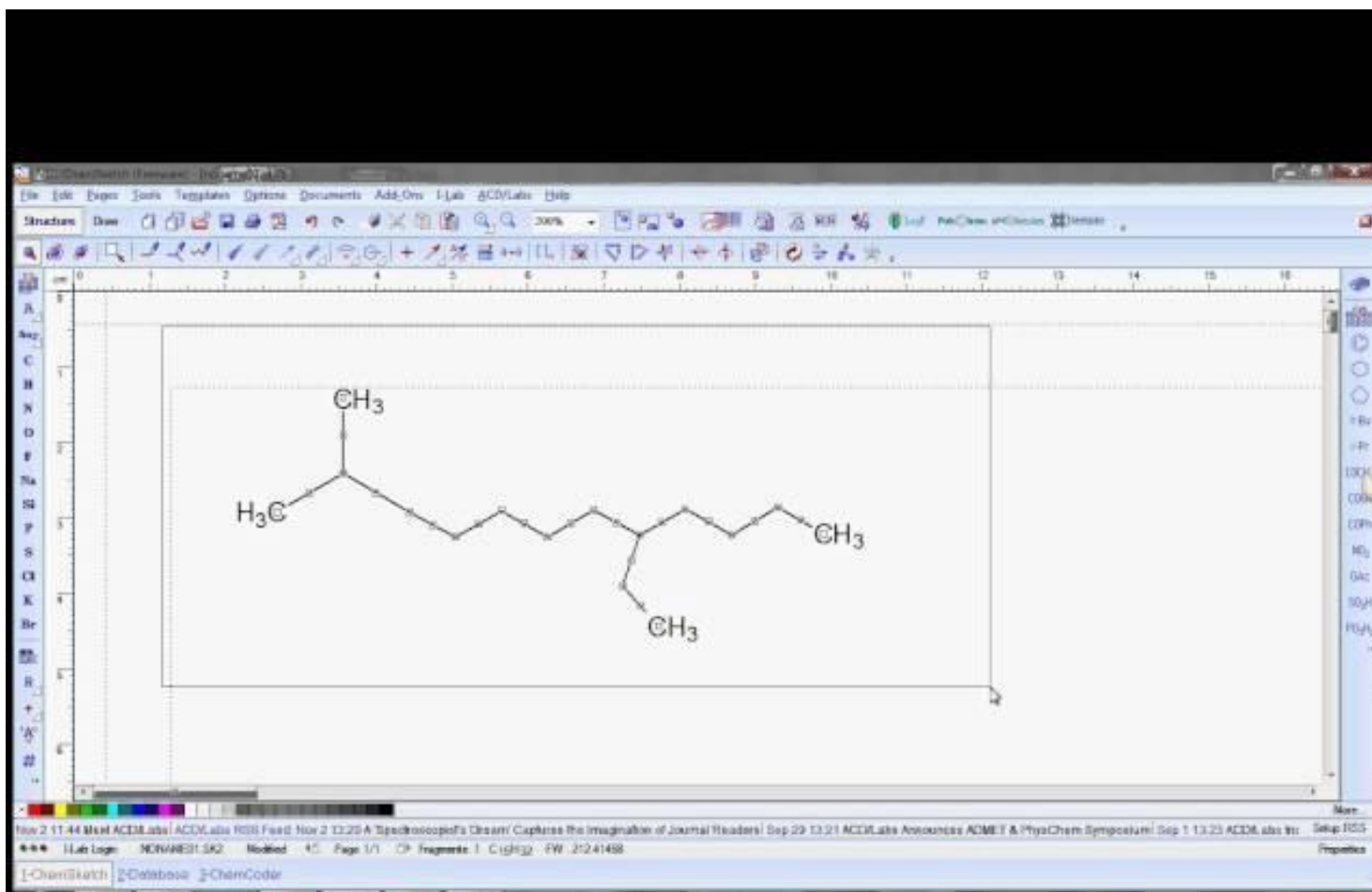
# 1. desenhando o 2-metilpropano



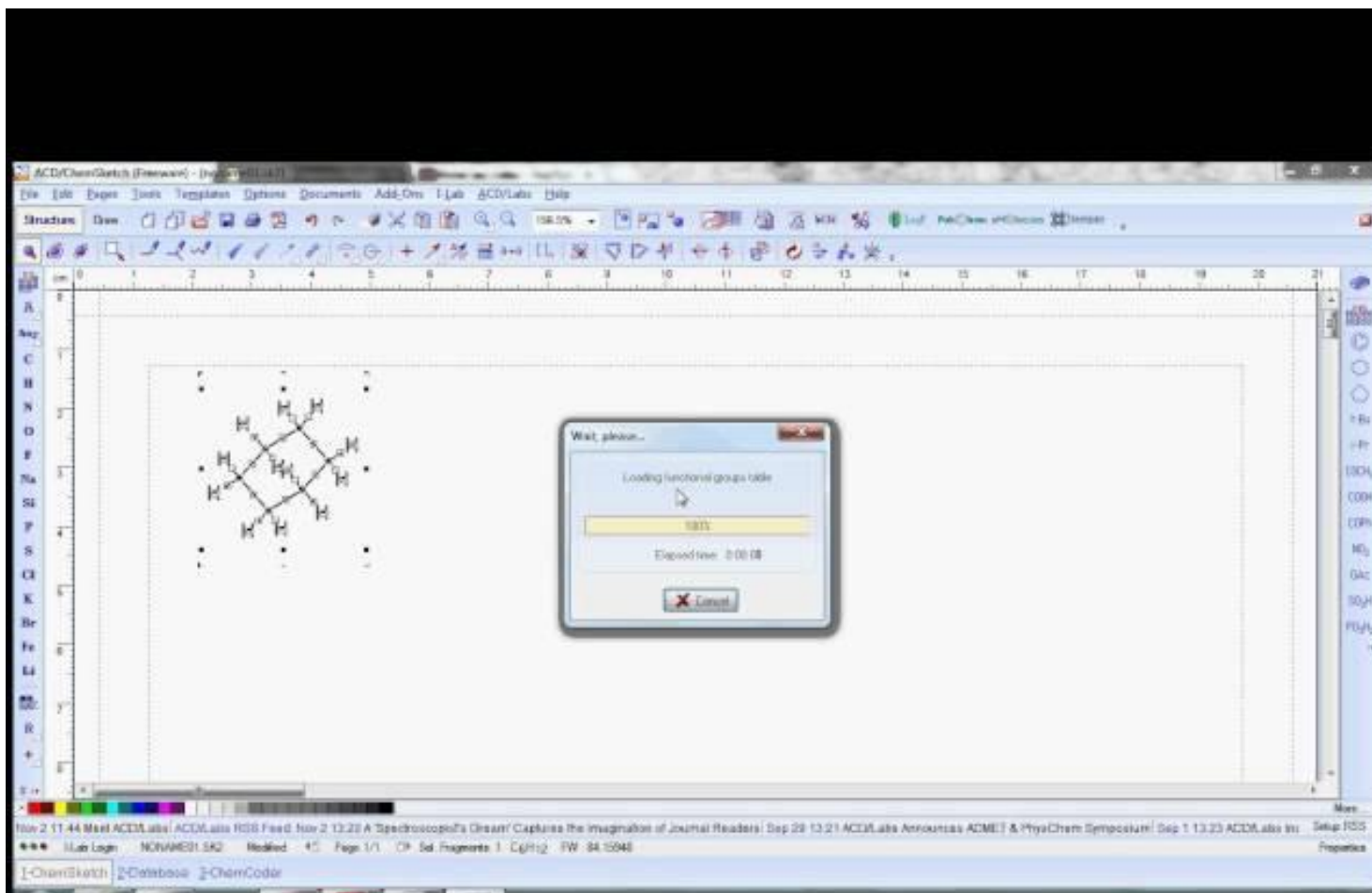
# 2-obtendo info sobre o 2- metilpropano



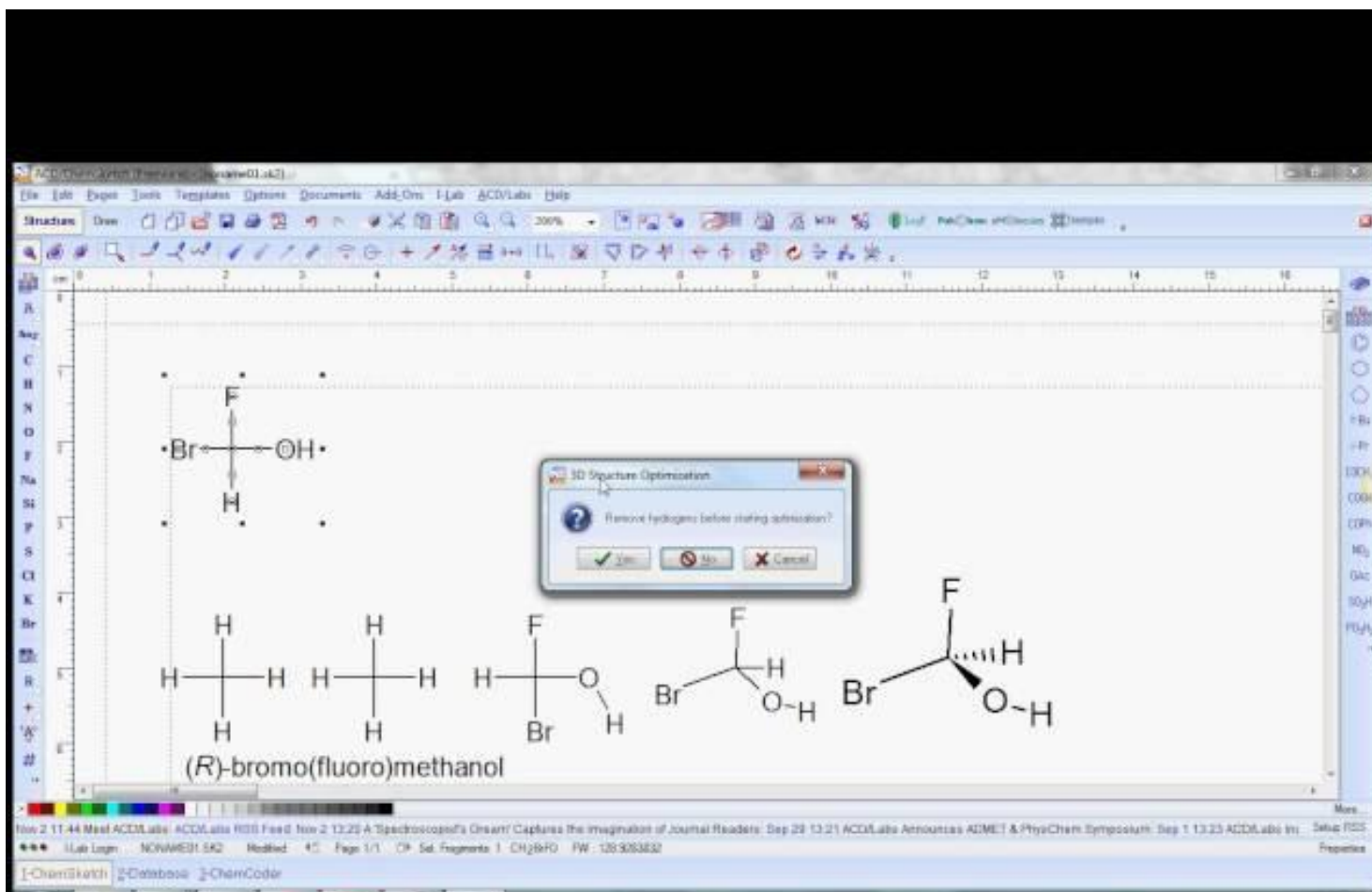
# 3. desenhando no modo cadeias



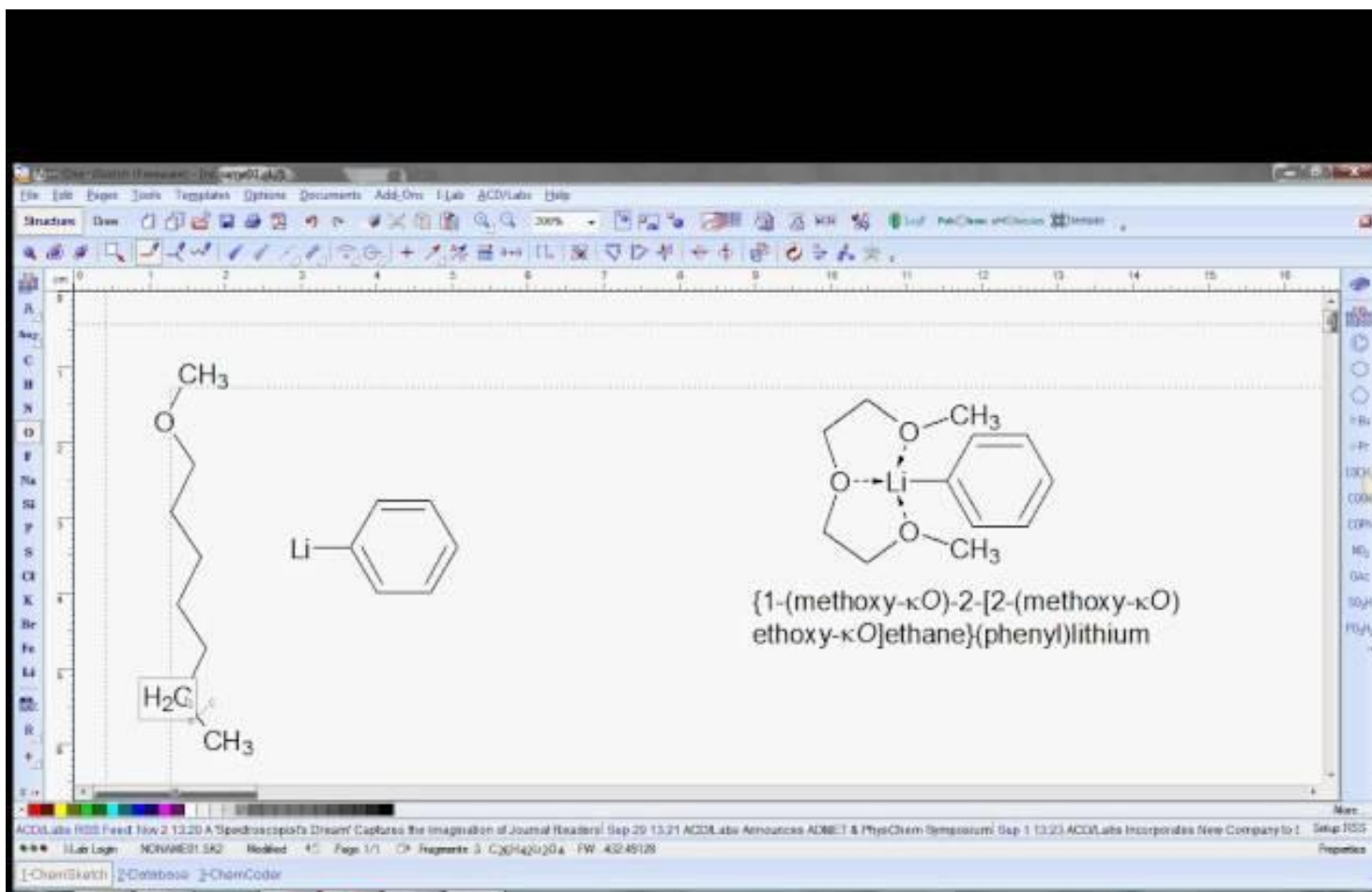
# 4. desenhando ciclohexano (modo contínuo)



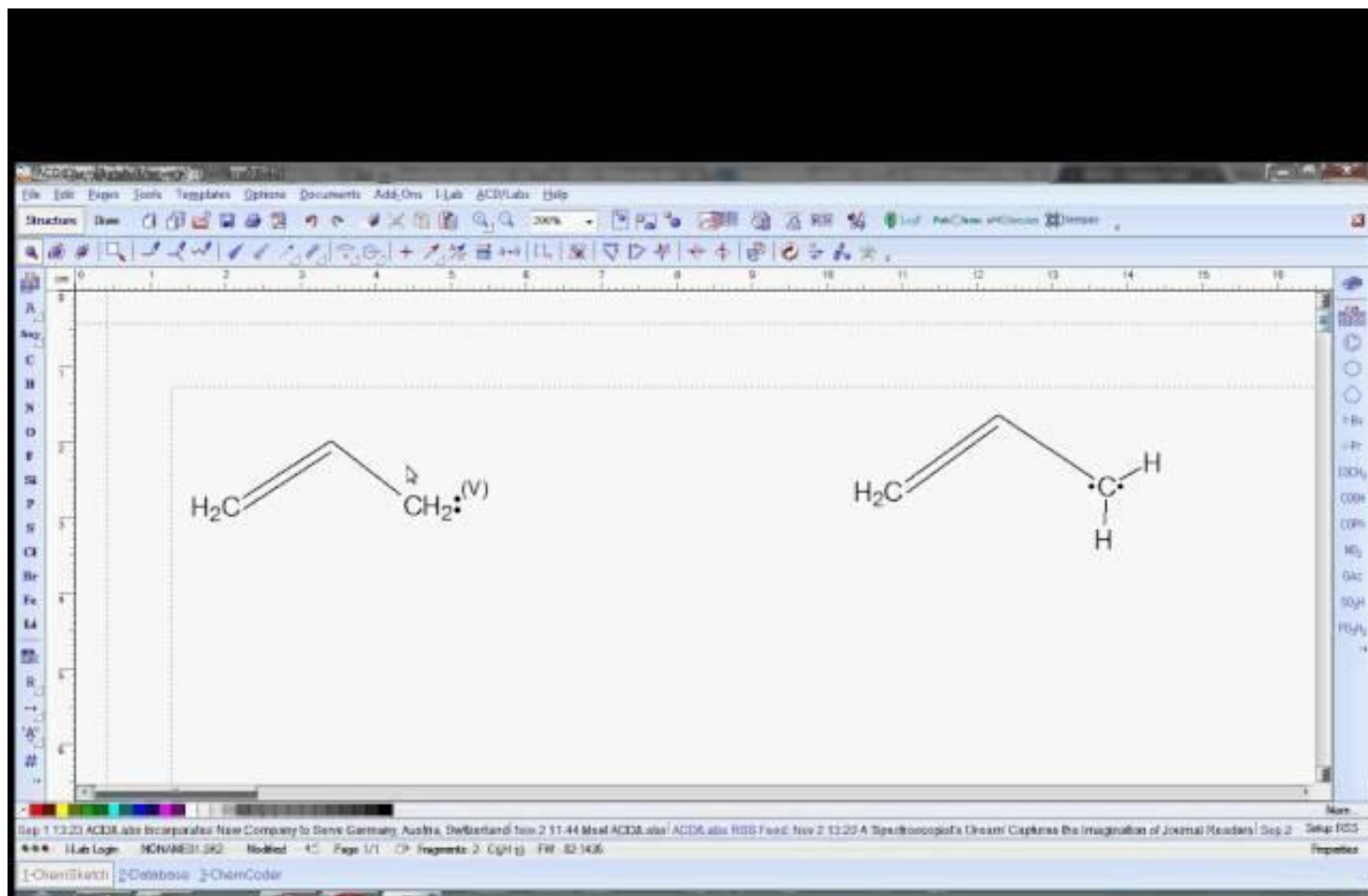
# 5. desenhando isômeros



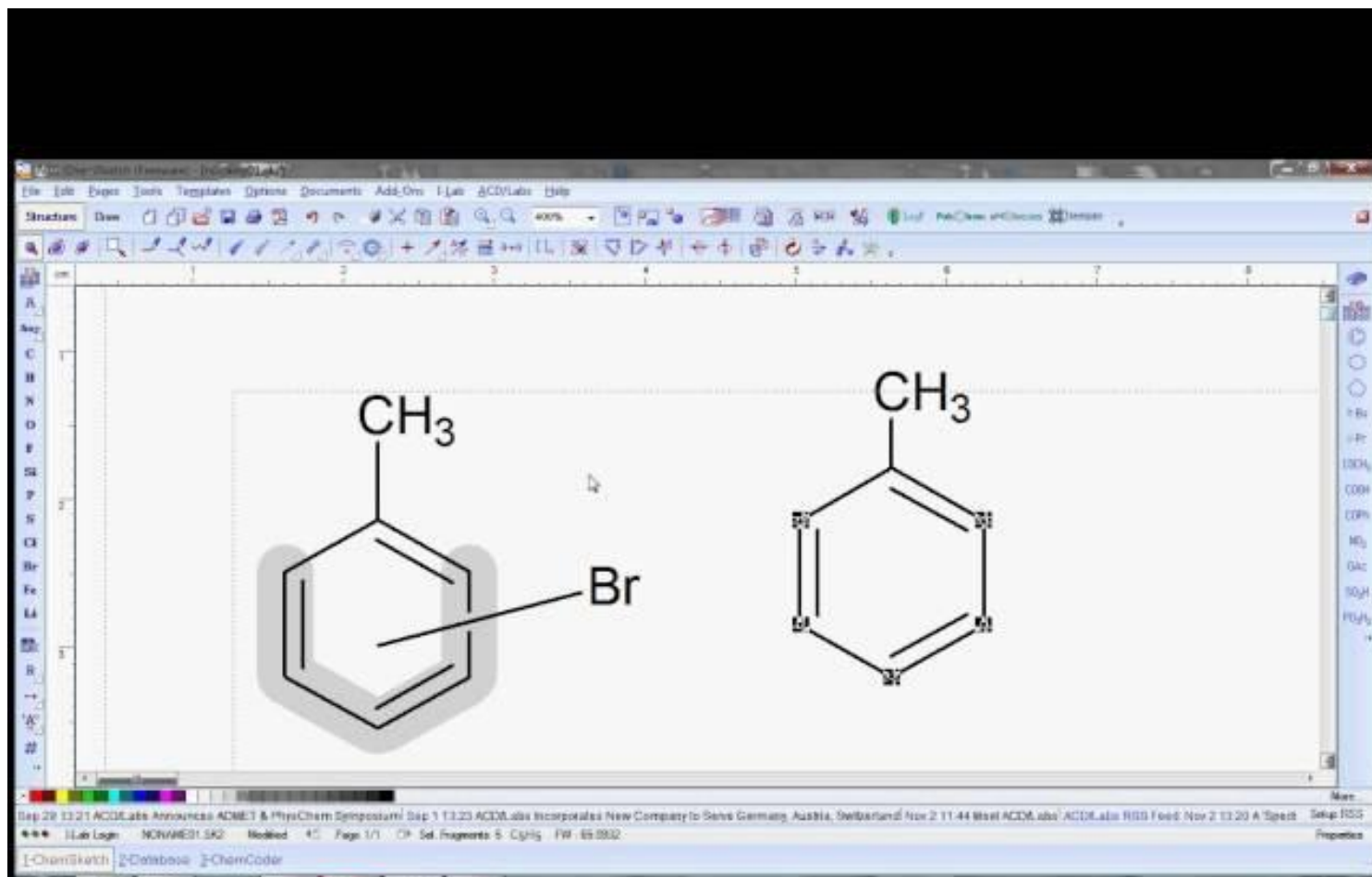
# 6. ligações coordenadas



# 7. desenhando um radical alila

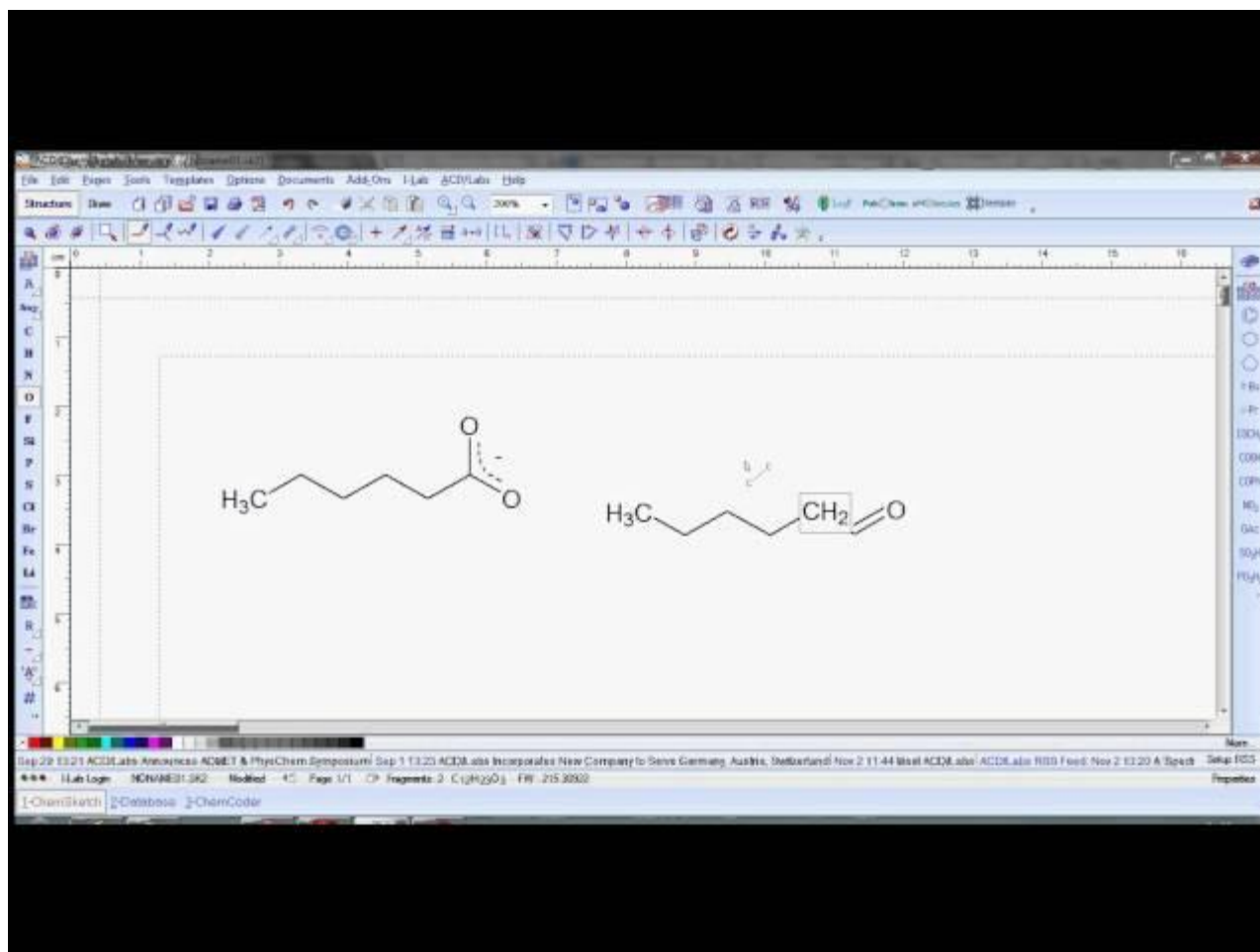


# 8. ligações de Markush

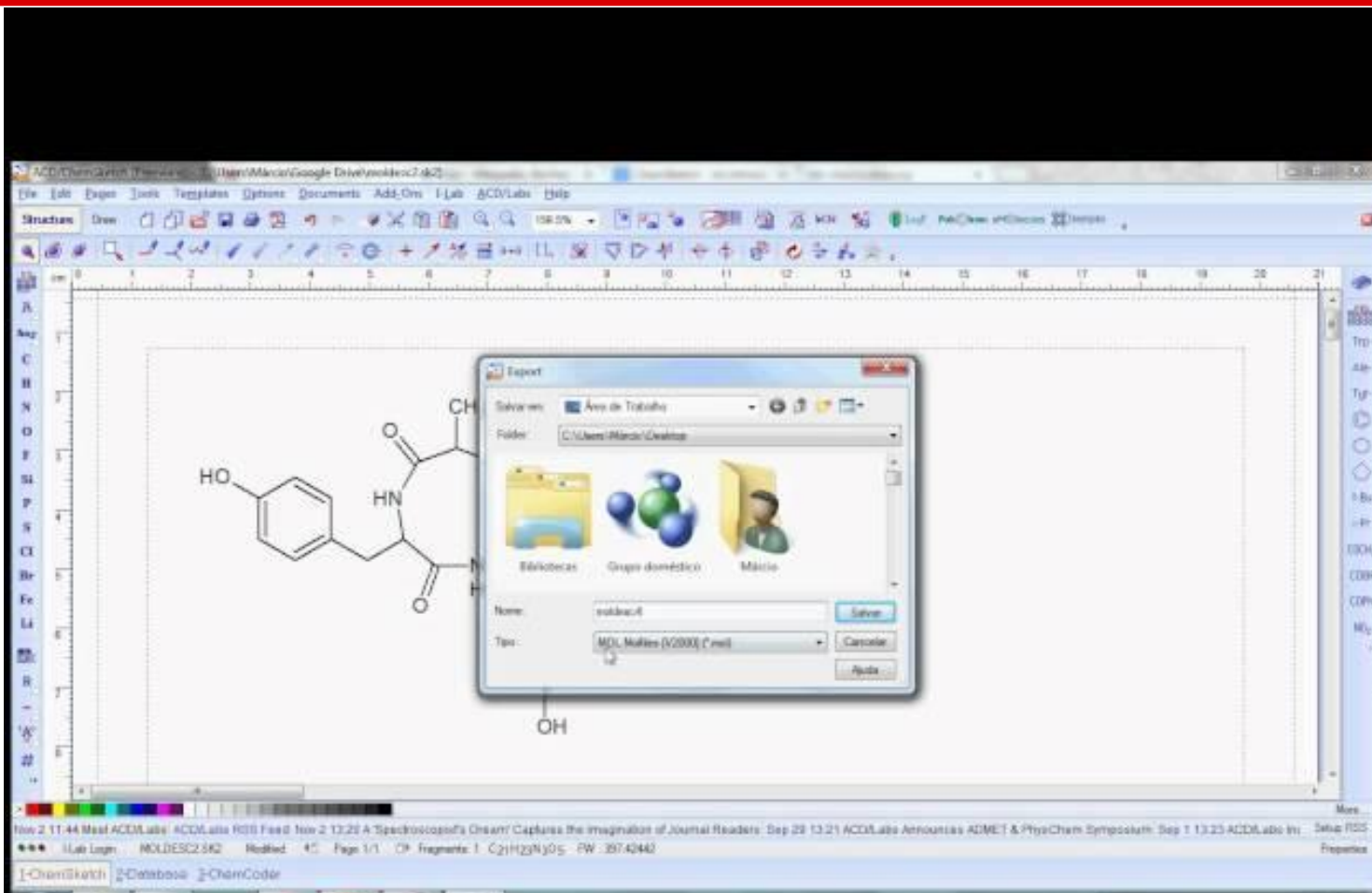




# 9. ligações deslocalizadas - íon hexanoato



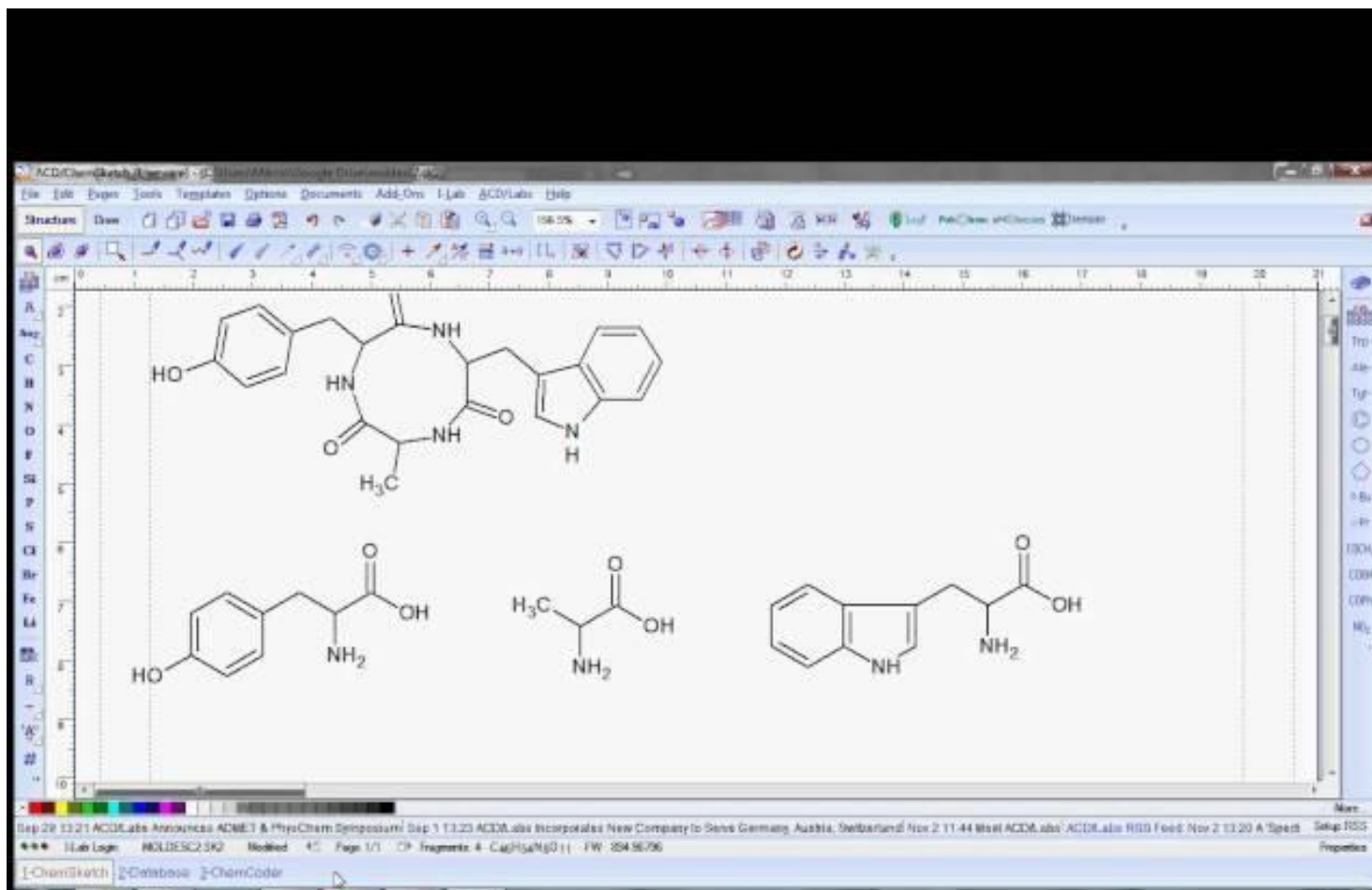
# 10. desenhando um peptídeo



# Utilizando templates

The screenshot shows the ChemSpider software interface. The main window is titled "Template Window" and has a dropdown menu set to "Amino Acids" and a sub-menu set to "1(4) Acids". The word "Templates" is written in large, pink, stylized letters across the top of the window. A red box highlights the template icon in the top toolbar, and a red arrow points from it to the "Trp-Ala-Tyr" text. A blue box highlights the "Amino Acids" dropdown. A green box highlights the "Trp-Ala-Tyr" text, with a green arrow pointing to the Tryptophan (Trp) structure. Another green box highlights the Tryptophan (Trp) and Tyrosine (Tyr) structures. The window displays a grid of 20 amino acid structures, each with its chemical structure and name in red text: Alanine (Ala), Aminobutyric Acid (Abu), Arginine (Arg), Asparagine (Asn), Aspartic Acid (Asp), Cysteine (Cys), Glutamic Acid (Glu), Glutamine (Gln), Glycine (Gly), Histidine (His), Homocysteine (Hcy), Isoleucine (Ile), Leucine (Leu), Lysine (Lys), Methionine (Met), Norleucine (Nle), Norvaline (Nva), Proline (Pro), Serine (Ser), Threonine (Thr), Tryptophan (Trp), Tyrosine (Tyr), and Valine (Val).

# 11.desenhando peptideo a partir de templates



# Exercício do detetive químico

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Que molécula é essa?



# Dica

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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.

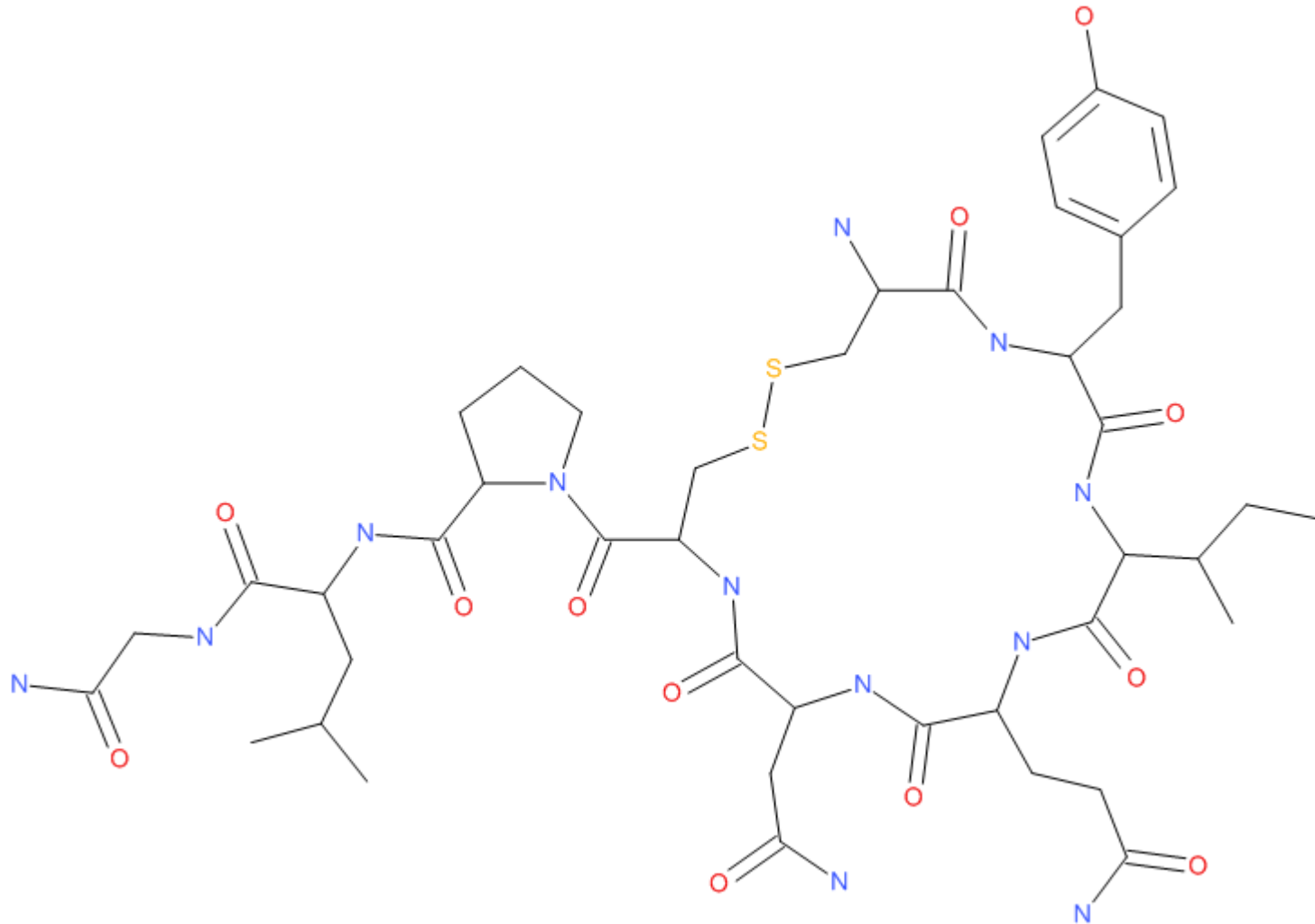
<http://goo.gl/4Twcw6> (formato mol)

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

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# Molécula misteriosa

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

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About More Searches Web APIs Help  Search

Simple search Structure search Advanced search

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

Search

8+1 97

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*ChemSpider* is a free chemical structure database providing fast text and structure search access to over 29 million structures from hundreds of

- Systematic names
- Synonyms
- Trade names
- Database identifiers


- Create structure-based queries
- Draw structures in the web page
- Use structure files from your

- Literature references
- Physical properties
- Interactive spectra
- Chemical suppliers

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




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# ChemSpider

Search and share chemistry



About More Searches Web APIs Help  Search

Simple search **Structure search** Advanced search

*eg. Aspirin*

Systematic names	Synonyms	Trade names	Registry number	SMILES	InChI
1,2-dihydroxybenzene	AIBN	Aspirin	7732-18-5	<chem>O=C(O)C</chem>	<chem>C1=CC=CC=C1C(=O)O</chem>

**Clique aqui para buscar a estrutura da molécula misteriosa!**

 97    

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## What is ChemSpider?

ChemSpider is a free chemical structure database providing fast text and structure search access to over 29 million structures from hundreds of

## Search by chemical names

- Systematic names
- Synonyms
- Trade names
- Database identifiers

## Search by chemical structure

- Create structure-based queries
- Draw structures in the web page
- Use structure files from your

## Find important data

- Literature references
- Physical properties
- Interactive spectra
- Chemical suppliers



THE SCIENCE  
WHAT'S POSSIBLE

Give Feedback 

Generate Leads

# 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).

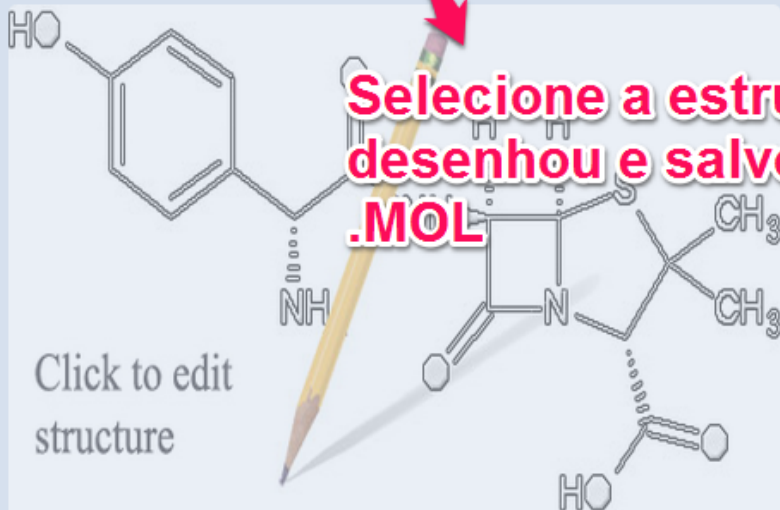
Escolher arquivo Nenhum arquivo selecionado

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

Convert

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

### 2. Edit molecule



Exact  
 Substructure

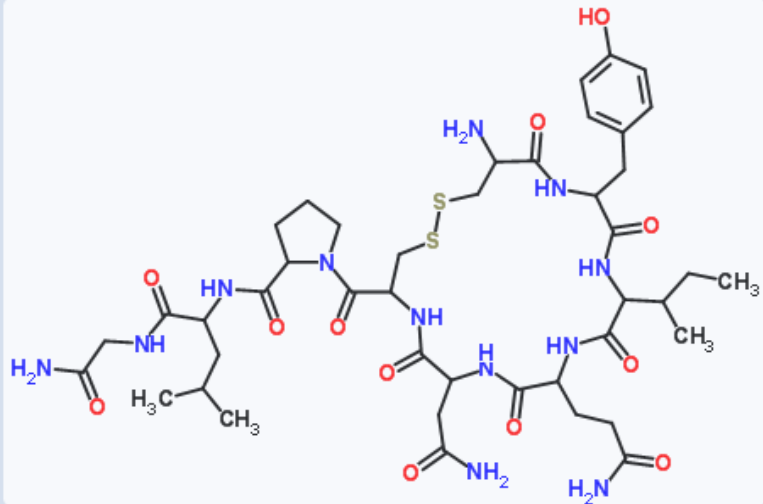
**Selecione a estrutura que você desenhou e salvou em formato .MOL**

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

# 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

Options

**Clique para buscar estruturas semelhantes.**

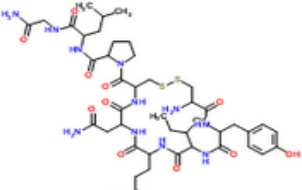
 Search Clear form Search Hits Limit: 100

# Mistério resolvido: ocitocina

Search and share chemistry

About | More Searches | Web APIs | Help |  **Search**

Search term: **Structure Search - Exact**



**2D 3D Save Zoom**

**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: C<sub>43</sub>H<sub>66</sub>N<sub>12</sub>O<sub>12</sub>S<sub>2</sub>  
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  
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**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] IACD/IUPAC Name

**E isso encerra nosso curso...**

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