

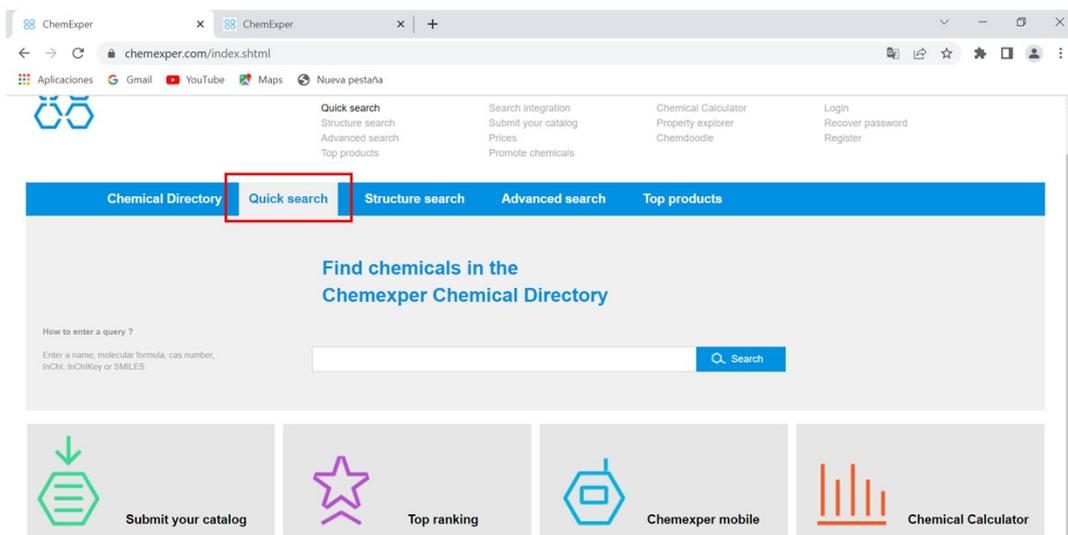
DEPARTAMENTO DE QUÍMICA INORGÁNICA

Tutorial sobre **ChemExper**
<https://www.chemexper.com/>

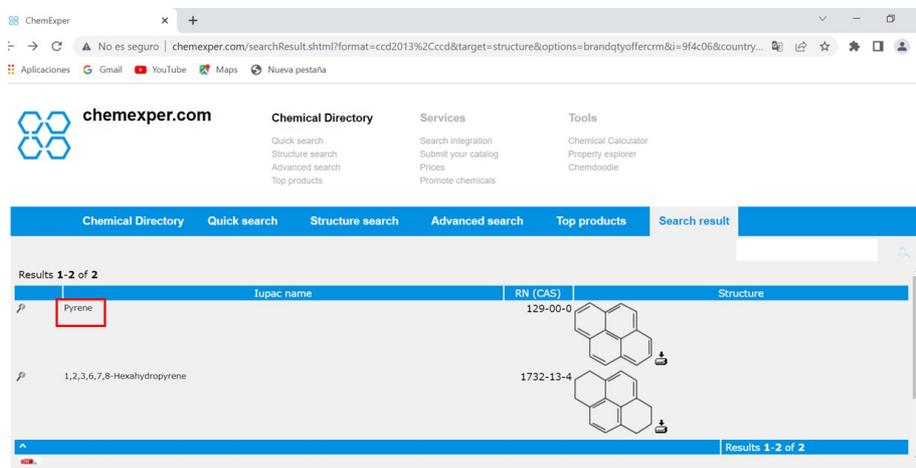
Natalia Cutillas Aulló

La aplicación contiene información sobre propiedades físicas y químicas, estructura, datos de seguridad, etc., de un gran número de sustancias. También es posible simular los espectros de RMN, tanto mono como bidimensionales, de los compuestos, porque redirige a *rmndb.org*

En la página principal se puede hacer una búsqueda rápida seleccionando **Quick Search** e introduciendo el nombre (en inglés), CAS o su fórmula molecular o SMILES, InChI o InChIKey.



Por ejemplo, si introducimos pyrene y seleccionamos **Search**, nos aparece la siguiente pantalla en la que elegiremos la molécula que nos interesa:



Iupac name	RN (CAS)	Structure
pyrene	129-00-0	
1,2,3,6,7,8-Hexahydropyrene	1732-13-4	

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Pyrene

C16H10

RN: 129-00-0
MF: C16H10 (1)
MW: 202.2554
bp (°C): 393
mp (°C): 148

InChI: 1S/C16H10/c1-3-11-7-9-13-5-2-6-14-10-8-12(4-1)15(11)16(13)14/h1-10H
InChIKey: BBEAQIROQSPTKN-UHFFFAOYSA-N

H donor: 0
H acceptor: 0
Rotatable bond: 0
Stereocenter: 0

cLogP: 5.033
cLogS: -6.072
Polar surface: 0
NEW: 3D model: Show (2)
 Report error(s)

Permanent link: <http://www.chemexper.com/search/cas/129000.html>

Click on a product name to get more information on that compound, on a supplier name to get more information on that supplier.

A continuación, si presionamos en la **fórmula empírica (1)** obtenemos su composición centesimal y datos de distribución isotópica. Si lo hacemos en **3D model (Show) (2)** aparece una pantalla en la que se visualiza un modelo tridimensional de la molécula que podemos girar libremente y, finalmente, en **Predict NMR spectrum (3)** tenemos la posibilidad de simular espectros de NMR. En este caso, como es un programa diferente, hay que introducir de nuevo los datos de la especie que nos interesa.

Trabajemos con las tres opciones. Presionamos en la fórmula empírica (**C₁₆H₁₀**) y nos lleva a una nueva pantalla con la información indicada.

ChemCalc

You entered: **C₁₆H₁₀**
 The formula is: C₁₆H₁₀
 Molecular weight: 202.2554
 Monoisotopic mass: 202.07825

Elemental analysis of C₁₆H₁₀:

Element	Number	Percentage
C	16	95.016499
H	10	4.983501

Isotopic distribution

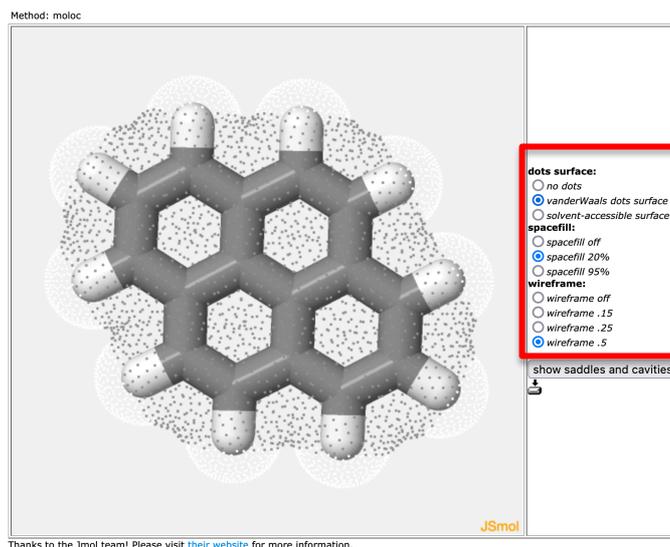
Your browser does not support applets.

Size: x

[Download jcamp file](#)

En esta pantalla también nos podemos descargar el fichero jcamp de la molécula (puede servir para otras aplicaciones).

Presionando en **3D model Show**, llegamos a una pantalla interactiva donde se muestra la estructura de la molécula. Podemos dibujarla de acuerdo con diversas opciones que se muestran en una tabla, a la derecha de la imagen.



Finalmente, si seleccionamos **Predict NMR spectrum**, nos lleva a la página de nmrdb.org.

Try the new HTML5 only predictor that works also on iPad, Android, ... and does not require JAVA (only HTML5)!!!
 This page allows to predict the spectrum from the chemical structure based on "Spinus". You may find more information on the authors website.

References

- Banfi, D.; Patiny, L. *www.nmrdb.org: Resurrecting and processing NMR spectra on-line* *Chimia*, **2008**, *62*(4), 280-281.
- Andrés M. Castillo, Luc Patiny and Julien Wist. *Fast and Accurate Algorithm for the Simulation of NMR spectra of Large Spin Systems*. *Journal of Magnetic Resonance* **2011**.
- Aires-de-Sousa, M. Hemmer, J. Gasteiger. "Prediction of 1H NMR Chemical Shifts Using Neural Networks", *Analytical Chemistry*, **2002**, *74*(1), 80-90 most of the proton descriptors are explained. In that work they were used for the prediction of 1H NMR chemical shifts by counterpropagation neural networks.

How to proceed ?

If you are really in hurry, just click here to get a predicted spectrum of ethylvinylether.

1. Draw a molecule or test with ethylvinylether.

Moffile:

You need to install Java 1.4 or later to see this applet.

2. You are now ready to predict the NMR spectrum. Just click here to proceed.
3. You may also copy the ACS assignment

Or a tab-delimited assignment

You have a fast computer (or plenty of time), just try our new real spectrum simulator. It will calculate the same spectrum but taking into account the second order effects.

We thank Molecular Networks for providing the predicting engine.

Tutorial

nmrdb.org
 Tools for NMR spectroscopists

ABOUT PREDICT 1H NMR PREDICT 13C NMR PREDICT 2D TOOLS EXERCISES WEB SERVICES CONTACT

NMR Predict

You may also try the old Applet version
 Draw a chemical structure and click on "Calculate spectrum". You may also DRAG / DROP a moffile ! You will get an interactive NMR spectrum.

References

- Banfi, D.; Patiny, L. *www.nmrdb.org: Resurrecting and processing NMR spectra on-line* *Chimia*, **2008**, *62*(4), 280-281.
- Andrés M. Castillo, Luc Patiny and Julien Wist. *Fast and Accurate Algorithm for the Simulation of NMR spectra of Large Spin Systems*. *Journal of Magnetic Resonance* **2011**.
- Aires-de-Sousa, M. Hemmer, J. Gasteiger. "Prediction of 1H NMR Chemical Shifts Using Neural Networks", *Analytical Chemistry*, **2002**, *74*(1), 80-90.

Chemical structure with hydrogen exploded

Paste or drop a moffile or SMILES

Assignment	Delta	Nb at...	Mult	J (Hz)
18.20	7.657	2	s	0.06-0.47
16.17-21.23	7.7625	4	ddd	0.06-2.69-2.71-0.31
10.20-24.25	7.9325	4	ddd	0.25-2.71-0.49

¹H NMR: 8.758-7.83 (8H, 7.64 (t, J = 8.1, 0.5 Hz), 7.76 (ddd, J = 8.1, 2.9, 2.7, 0.5 Hz), 7.93 (8H, dd, J = 8.3, 2.7, 0.5 Hz)

1H NMR spectra - Double click to zoom out, SHIFT + double click to zoom out by step, SHIFT + drag to move spectrum

Advanced options
 Spectrometer frequency: 400 MHz
 P1: 0 s
 T1: 10 s
 Line width: 1 Hz
 Number points: 64k

A toda esta información se puede acceder también eligiendo en el menú principal **Structure search** y dibujando la correspondiente molécula.

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How to enter a query ?
This applet allows you to draw the substructure you are looking for and search for all the products containing this structure.

Keyboard shortcuts:
• bonds ~#
• rings S,B,Pn (n=1)
• atoms C,N,O,P,S,F,I,B,I
• Esc - return to the standard state (C, single bond)

Molecules may be moved by "dragging" free space and rotated by pressing concurrently also the shift key

This Java Applet was realized by Peter Ertl and Bruno Bienfait

JSMIE Molecular Editor by Peter Ertl and Bruno Bienfait

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Por otro lado, la herramienta **Chemical calculator** (en la página de inicio) calcula la masa molecular, la masa exacta, el análisis elemental y traza el gráfico de distribución isotópica. Sólo hay que introducir una fórmula en el cuadro, hacer clic en el botón y ver los resultados. Puede introducir átomos, isótopos y grupos.

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MF ANALYSIS

MOLECULAR FORMULA: $H_6C_2N_2P_1$ MOLECULAR WEIGHT: 300.05
 MONOISOTOPIC MASS: 298.95560 ISOTOPOGRAPHY: -
 MZ: CHANGE: 0

ELEMENT	MASS	PERCENT
H	6	2.00%
C	2	23.60%
N	2	33.34%
P	1	61.02%

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