nmrdb.org
Tools for NMR spectroscopists

Universidad del Valle

ME

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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 molfile ! 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.

Paste or drop a molfile or SMILES

Help

Simulate spectrum

Advanced options

Frequency:	400	
From:	0	ppm
To:	11	ppm
Line width:	1	Hz
Number points:	32k	

Draw a chemical structure and click on "Calculate spectrum".
You may also DRAG / DROP a molfile !
You will get an interactive NMR spectrum.

Labile protons like OH, NH, CO_2H are not predicted !

Chemical structure with hydrogen exploded

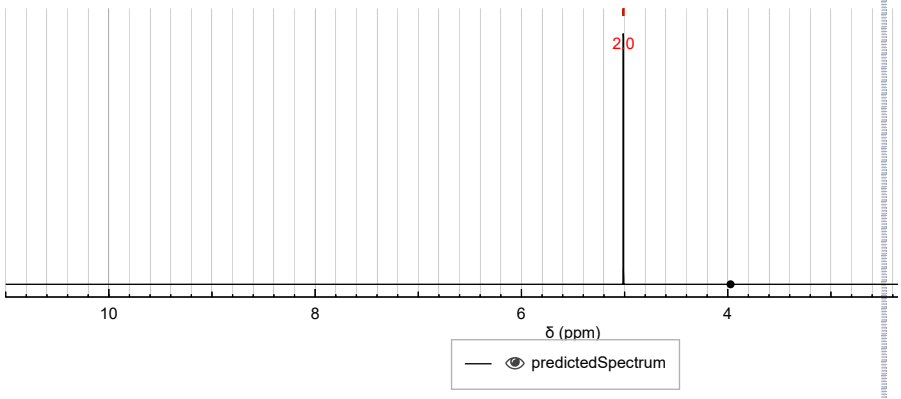
List of signals

Assignm…	Delta	N…	Mult	J (Hz)	…
3,4	5.011	2	s		

^{1}H NMR: δ 5.01 (2H, s).

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

3.97 ppm



References

- Banfi, D.; Patiny, L. **www.nmrdb.org: Resurrecting and processing NMR spectra on-line** *Chimia*, **2008**, 6
- Fast and Accurate Algorithm for the Simulation of NMR spectra of Large Spin Systems. Andrés M. Castillo, L *of Magnetic Resonance* **2011.** **10.1016/j.jmr.2010.12.008**
- Aires-de-Sousa, M. Hemmer, J. Gasteiger, "**Prediction of 1H NMR Chemical Shifts Using Neural Network** *74*(1), 80-90 most of the proton descriptors are explained. In that work they were used for the prediction of 1H counterpropagation neural networks. Y. Binev, J. Aires-de-Sousa, "**Structure-Based Predictions of 1H NMR Forward Neural Networks**",