NMR Spectroscopy Database and Searching System

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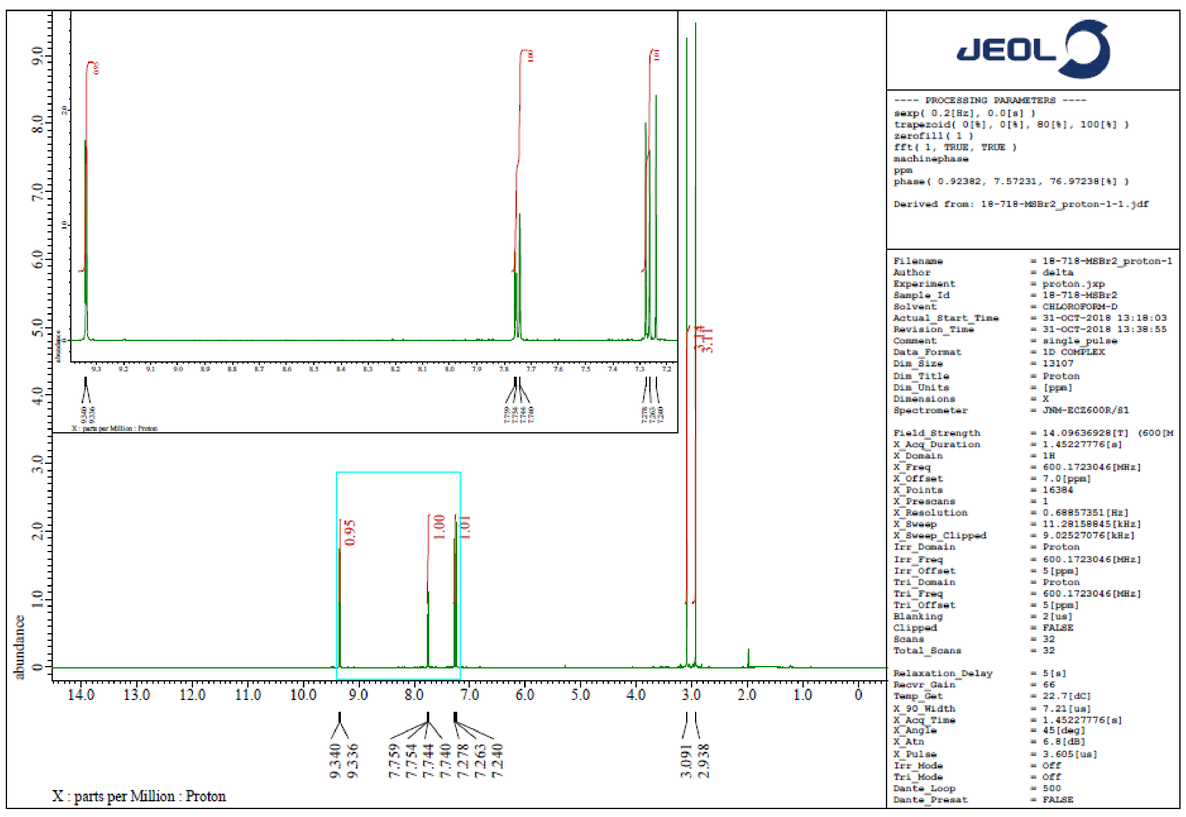
Abstract

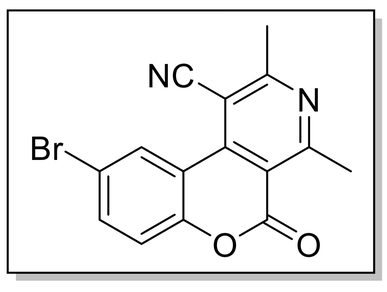
NMR spectroscopy is the most important analytical technology for organic compounds and plays the key role for the chemical characterizations and identifications in chemistry, pharmacy, materials science, environments, biology, and many related fields. In most cases, a NMR spectrum is compared with the known spectra to check if the sample contains a known chemical or is a new product. However, the current comparison process relayed on human beings and waste a lot of time and efforts. A new database and searching system is thus in need.

Typical Presentation Methods for a NMR Spectrum

A. Graphic Presentation: Good for human reading



B. Numerical Description: Good for digital searching



9-bromo-2,4-dimethyl-5-oxo-5*H*-chromeno[3,4-*c*]pyridine-1-carbonitrile

^{1}H NMR ($CDCl_3$, 600 MHz): δ 2.94 (s, 3H), 3.09 (s, 3H), 7.27 (d, 1H, *J* = 8.9 Hz), 7.75 (dd, 1H, *J* = 8.9 Hz, 2.0 Hz), 9.34 (d, 1H, *J* = 2.0 Hz). ^{13}C{^{1}H} NMR ($CDCl_3$, 150 MHz): δ 25.2, 27.9, 100.0, 113.2, 116.5, 117.1, 117.8, 119.6, 128.4, 137.1, 142.6, 151.5, 157.6, 167.8, 168.0.

Current Databases and Literature

- Databases: Mostly in graphic; some in both. Only Searching by names and formula. Contains common chemicals only.
- Literatures: Mostly in numerical; some has graphics in supporting information.
- Researchers need to search and compare by themselves. No convenient or quick searching methods.

Database Facilitated Screening and Chemical Identification Process