

# The IUPAC International Chemical Identifier and Mass Spectrometry

Linstrom, P.J.<sup>1</sup>, Heller, S.R.<sup>1</sup>, McNaught, A.D.<sup>2</sup>, Mirokhin, Y.A.<sup>1</sup>, Stein, S.E.<sup>1</sup>, Tchekhovskoi, D.V.<sup>1</sup>, Pletnev, I.V.<sup>3</sup>

<sup>1</sup> NIST, Gaithersburg, MD; <sup>2</sup> Cambridge, U.K.; <sup>3</sup> Moscow State University, Moscow, Russia



## What is the IUPAC Identifier?

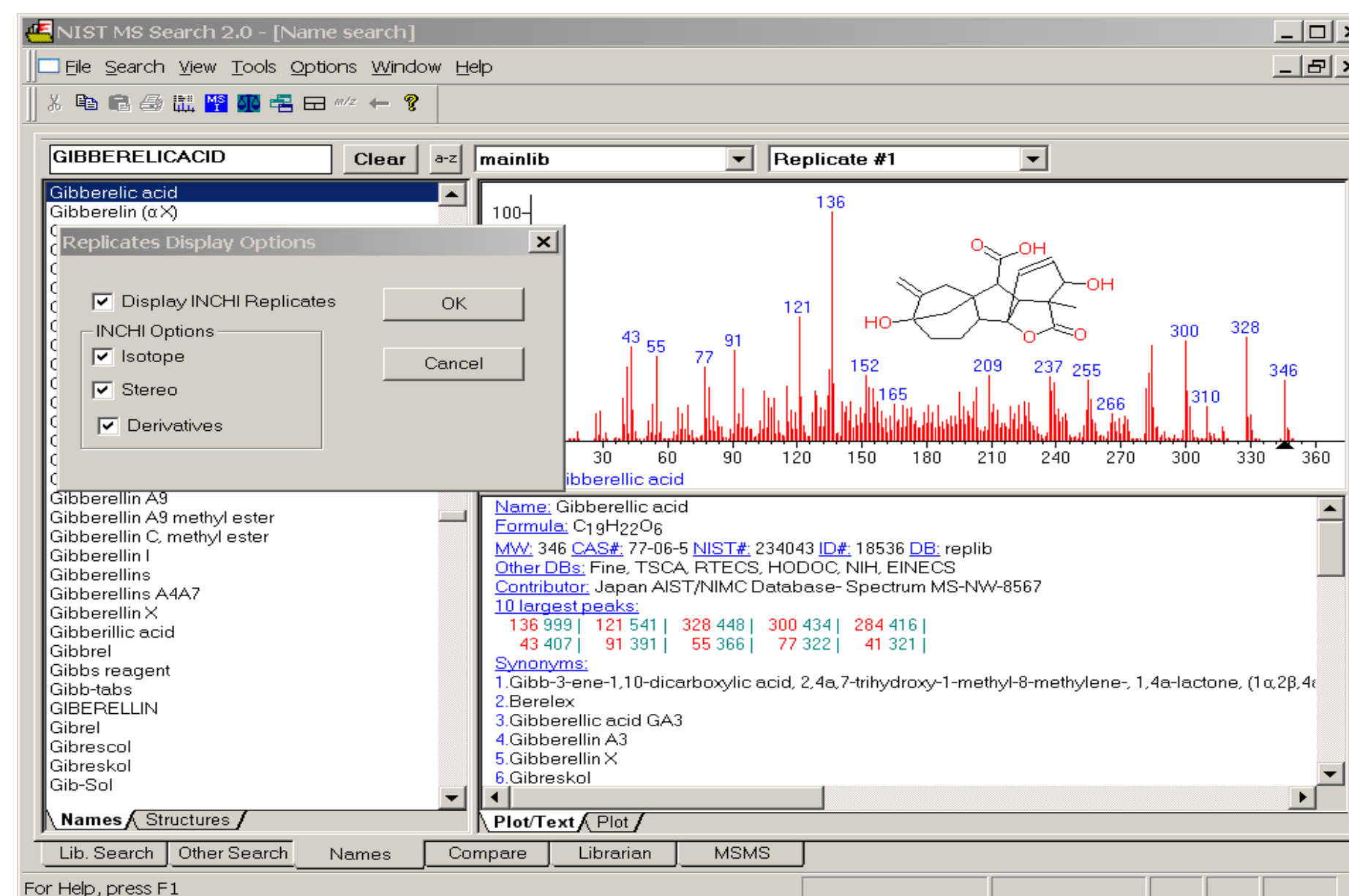
The IUPAC International Chemical Identifier (InChI) is an IUPAC standard for identifying chemical species. It is a unique text string which is derived from the chemical structure of a species.

## Advantages of InChI

- Constructed solely from structure
  - Avoids the need for third parties
  - No complicated nomenclature rules
  - Less chance for human error (processing is done by standardized open-source software)
- Modular design allows for “partial matches”
  - Geometric and optical isomers
  - Isotopomers
  - Species with the same atomic connectivity
- Fixed length hash (InChIKey) speeds searching
  - InChIKey is designed to be compatible with Internet search engines

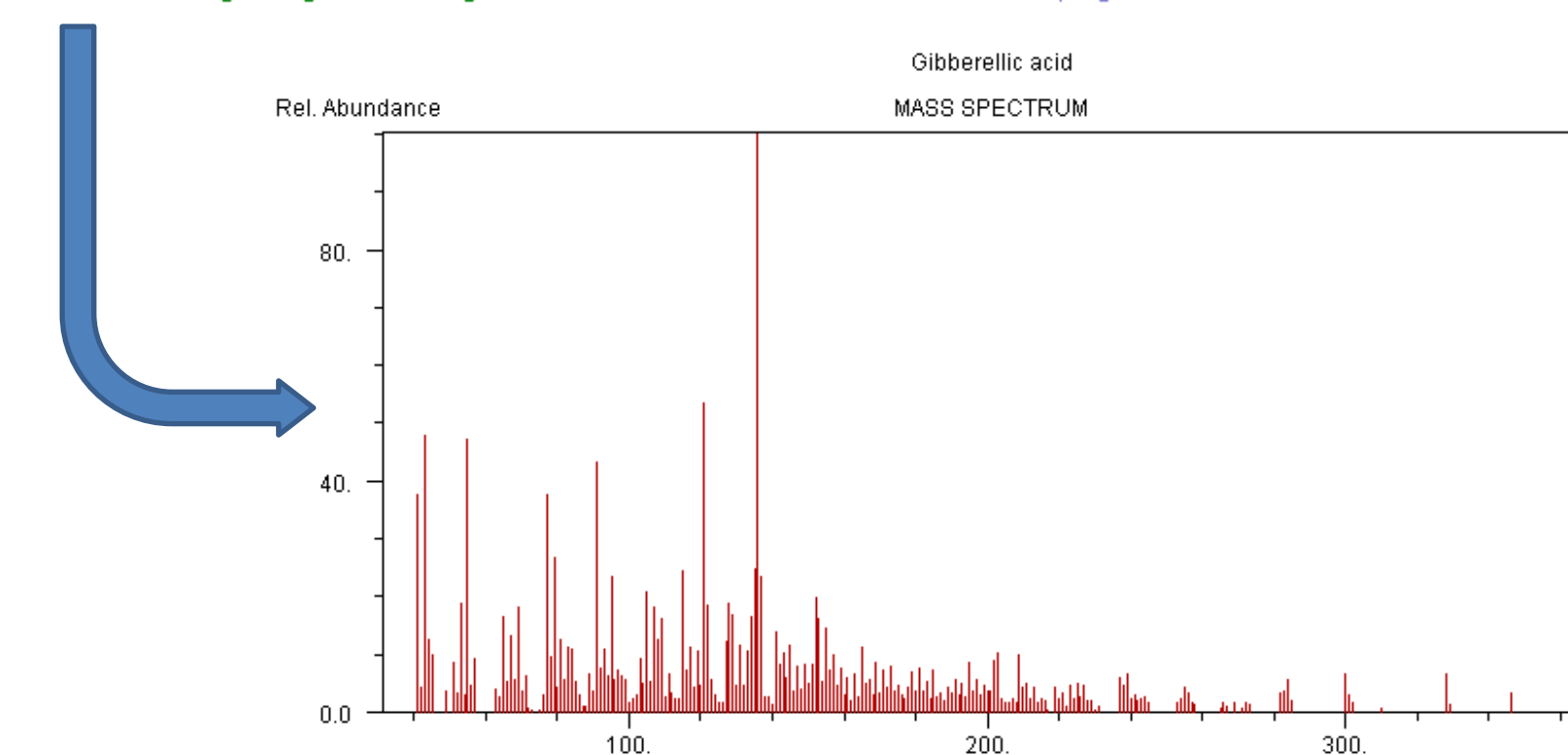
## InChI in NIST MS Search

InChI is used in the NIST MS Search program to identify replicate spectra. The modular nature of InChI provides options for matching structures. In particular, InChI can cope well with the case where geometric stereochemistry (cis/trans, E/Z) is not known with certainty.



## Data Discovery

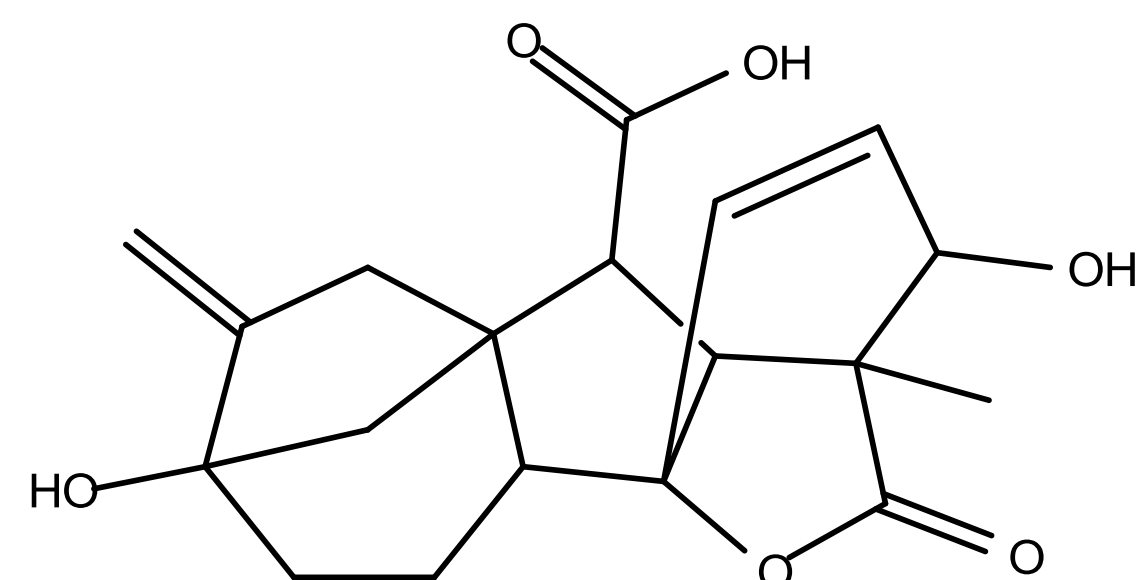
IXORZMNAPKEEDV-UHFFFAOYSA-N mass spectrum Search  
InChIKey  
**Gibberellic acid**  
IUPAC Standard InChIKey: IXORZMNAPKEEDV-UHFFFAOYSA-N; CAS Registry Number: 77-06-5; Chemical structure: ... Mass spectrum (electron ionization).  
Options: ...  
[webbook.nist.gov/cgi/cbook.cgi?ID=77-06-5-8k](http://webbook.nist.gov/cgi/cbook.cgi?ID=77-06-5-8k) - Cached - Similar pages



## For More Information

<http://www.iupac.org/inchi/>

## How Is InChI / InChIKey Made?



Structure

Canonicalization  
Normalization  
Open Source Software

InChI=1S/C19H22O6/c1-9-7-17-8-  
18(9,24)5-3-10(17)19-6-4-  
11(20)16(2,15(23)25-  
19)13(19)12(17)14(21)22/h4,6,10-  
13,20,24H,1,3,5,7-8H2,2H3,(H,21,22)

InChI

Hash computation  
Open Source Software

IXORZMNAPKEEDV-  
UHFFFAOYSA-N

InChIKey