# Covariance NMR

## Eric Johnson

Symposium on Frontiers in Biomolecular NMR
Vanderbilt University
May 4, 2012

Bruker BioSpin

# Covariance NMR

- Resolution enhancement along indirect dimension

- "Transfer" resolution of direct dimension to indirect dimension

  - Result: Fully symmetric spectrum

- Singular value decomposition (SVD) of matrix square-root

  - Computationally efficient

- Amenable to wide range of solids and liquids applications

# Covariance NMR

Principle:

After FT in direct dimension:

- Compare all columns (indirect dimension)

- For columns which are similar:
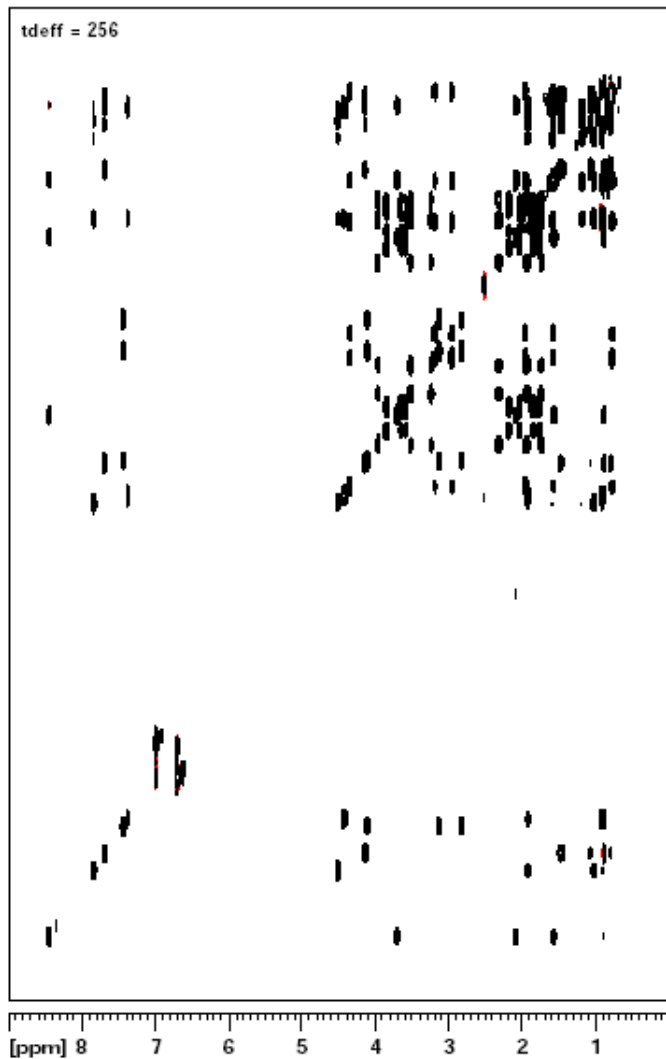  - transfer info of frequency in direct dimension to the indirect dimension

No further FT applied

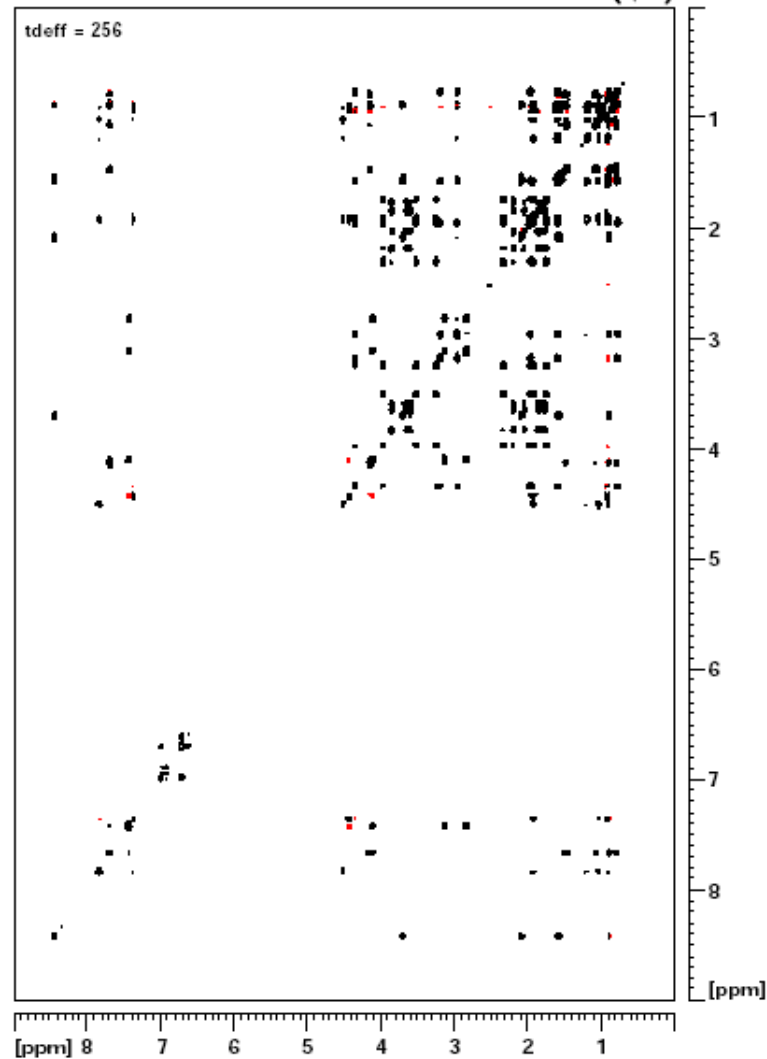Advantage: enhanced resolution in indirect dimension

# Covariance NMR

# Covariance NMR
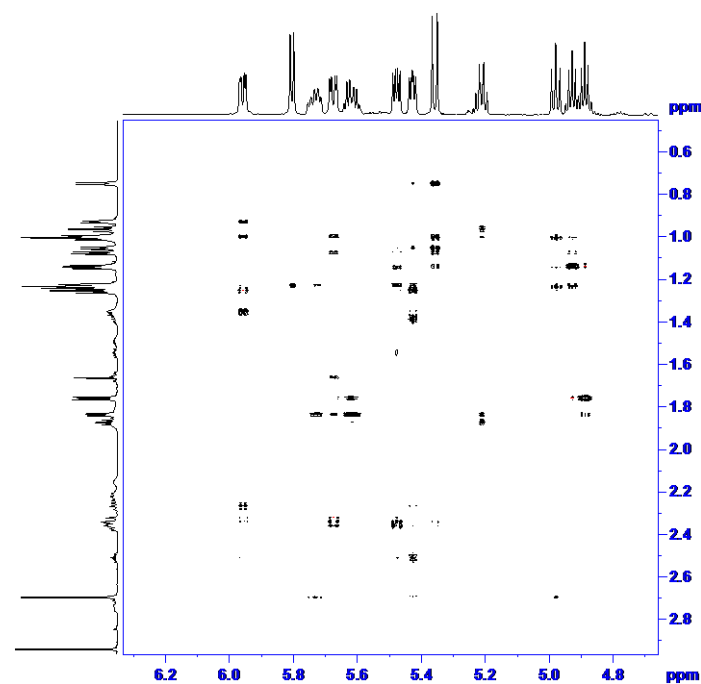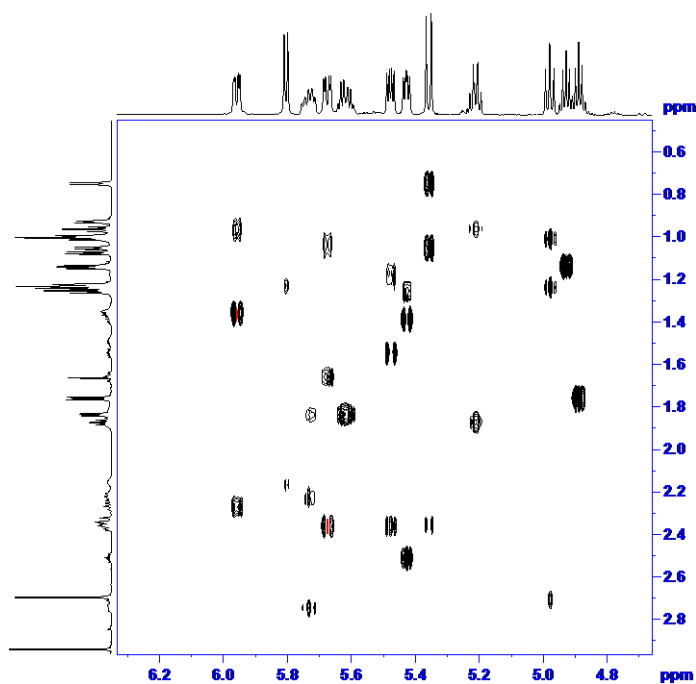
Application: Resolution enhancement

Example: Cyclosporine

TOCSY  TD (f1) = 128 $\rightarrow$ SI = 2kx2k

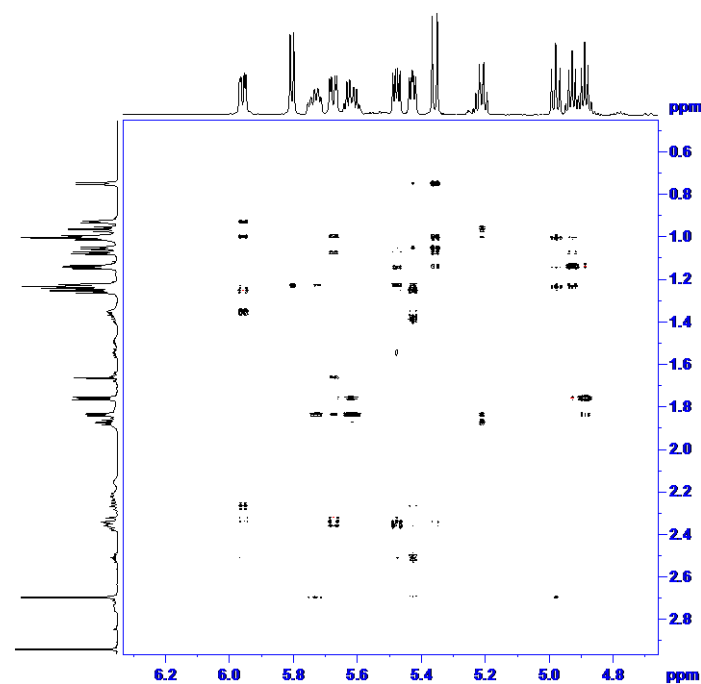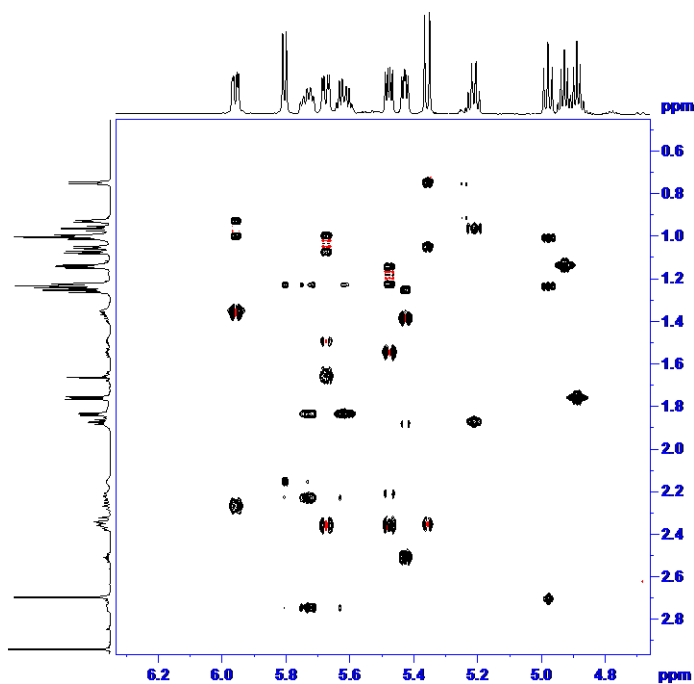FT                                                    Covariance

# Covariance NMR

Application: Resolution enhancement

Example: Cyclosporine

TOCSY  TD (f1) = 512  $\rightarrow$ SI = 2kx2k

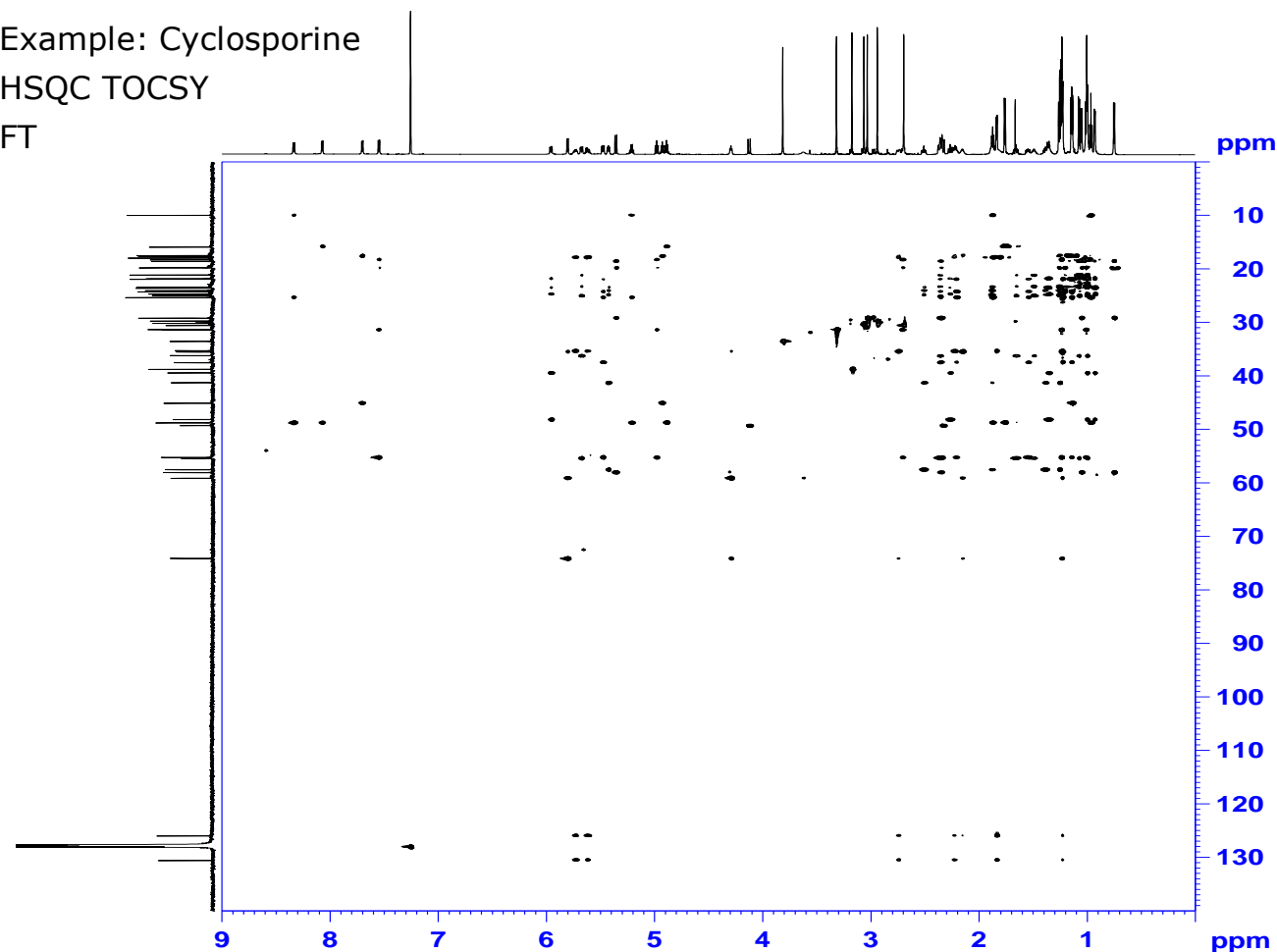FT                                                    Covariance

# Covariance NMR

Application: Inverse spectroscopy

Example: Cyclosporine
HSQC TOCSY
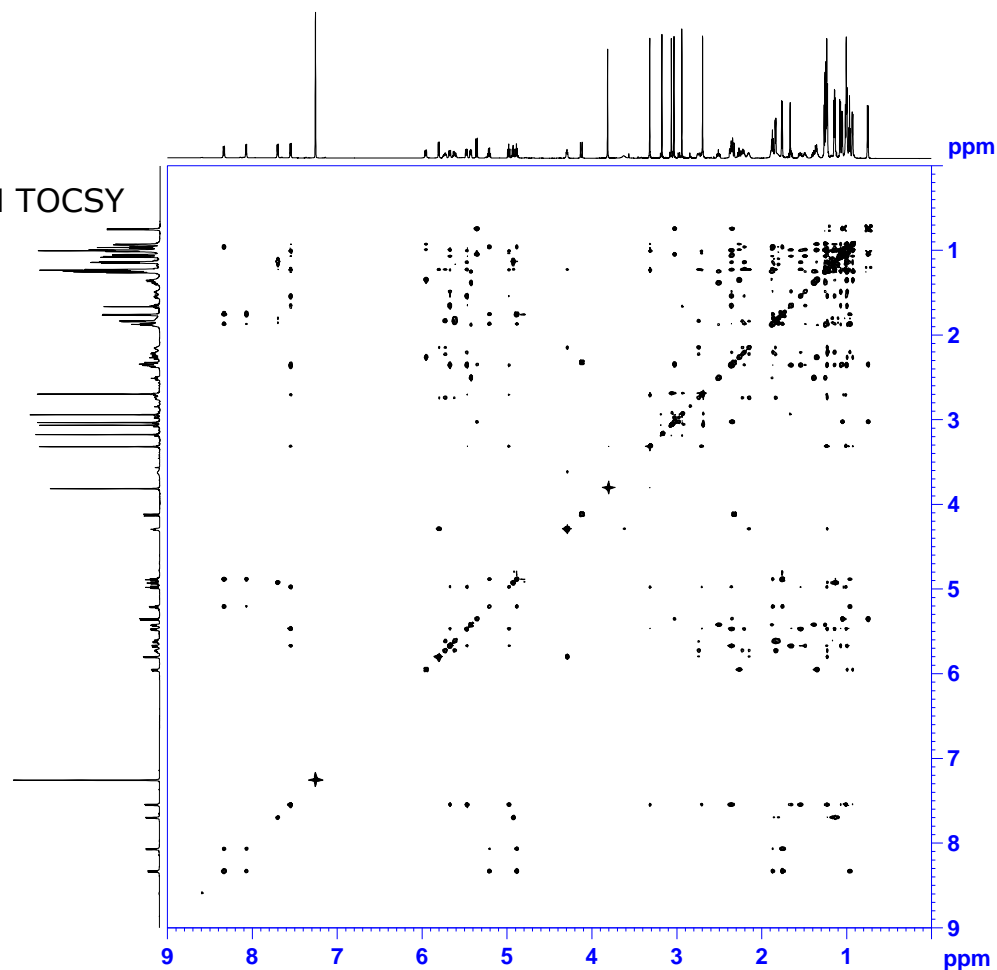FT

# Covariance NMR

Application: Inverse spectroscopy

Example: Cyclosporine

HSQC TOCSY

Covariance with FT in f2 → H,H TOCSY
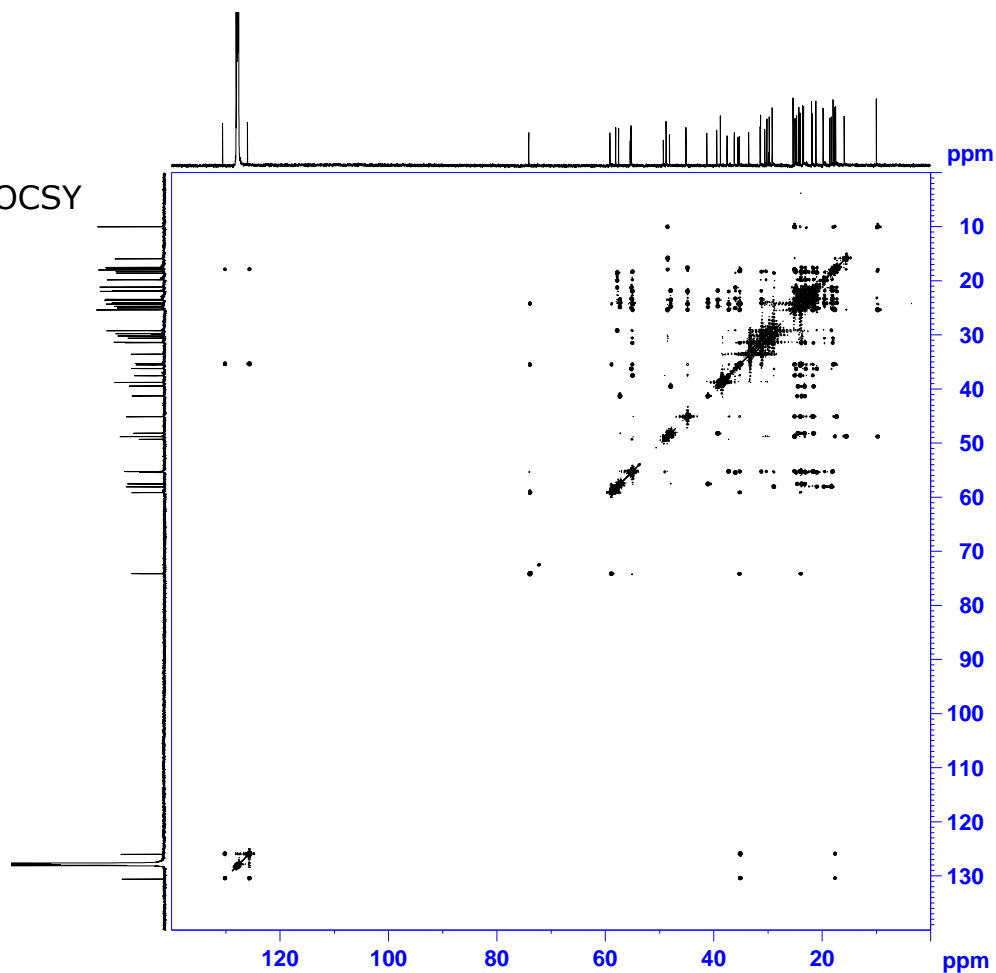
# Covariance NMR

Application: Inverse spectroscopy

Example: Cyclosporine

HSQC TOCSY

Covariance with FT in f1  → C,C TOCSY

# Implementation in Topspin

Data Processing

Process with fourier transform and phase correct.
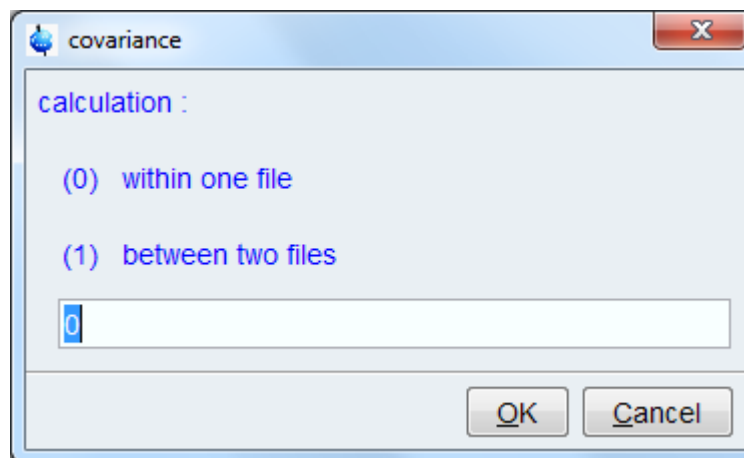
Start AU program:

*covariance* (with no argument for default options)

*covariance man* (for interactive mode)
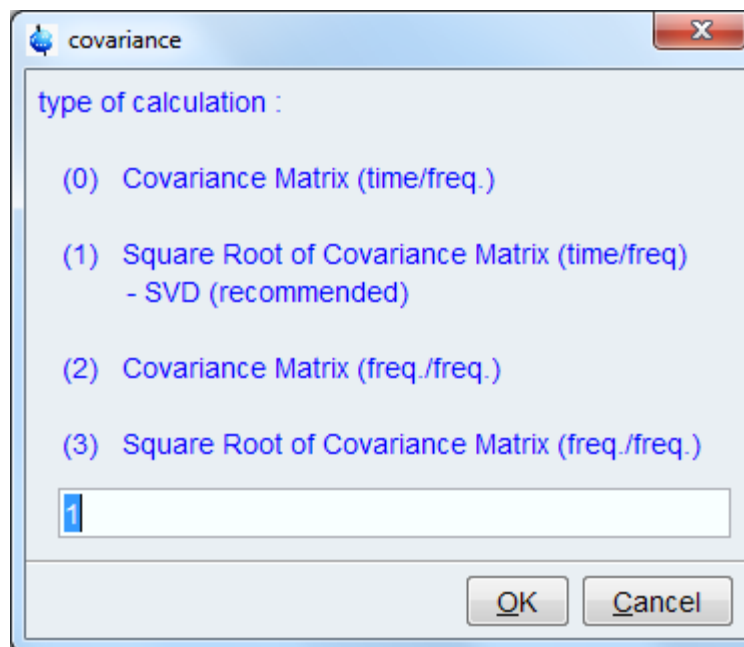
# Implementation in Topspin
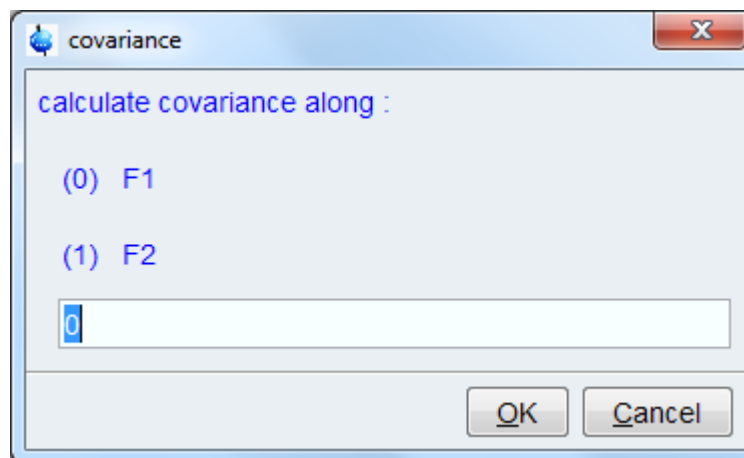
*covariance man*

# Implementation in Topspin

*covariance man*
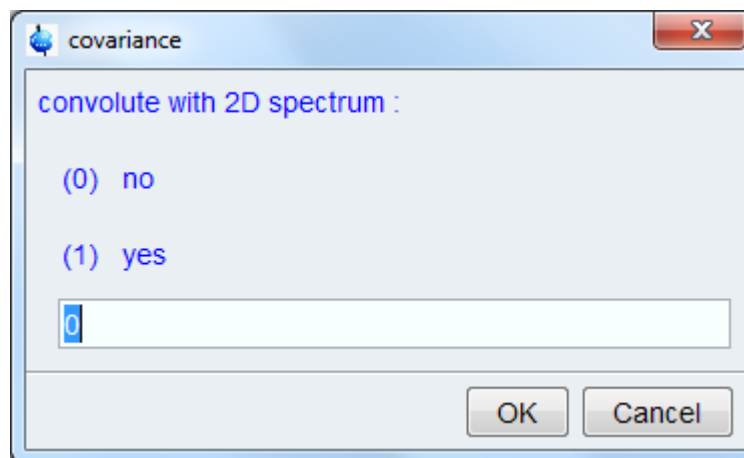
# Implementation in Topspin

*covariance man*
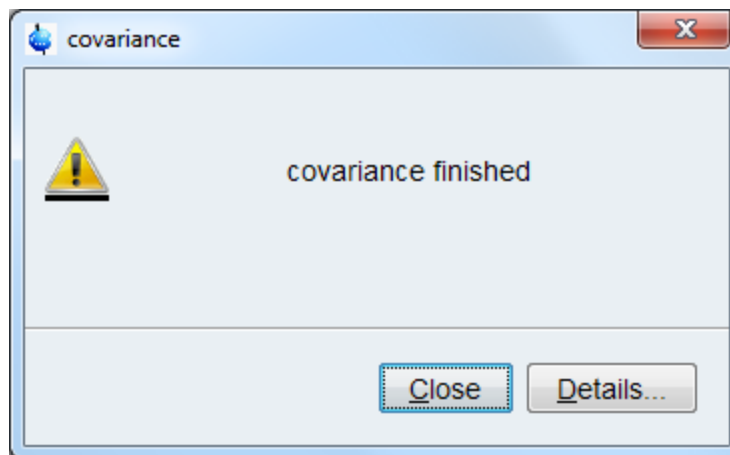
# Implementation in Topspin

*covariance man*

# Implementation in Topspin

*covariance man*

Wait until



Can take seconds or minutes, depending on processor speed and data set size.

# Availability

AU program is included as part of Topspin3.0 and newer

For Topspin2:

http://spin.magnet.fsu.edu/software/covNMR/covNMR.html

# Covariance NMR
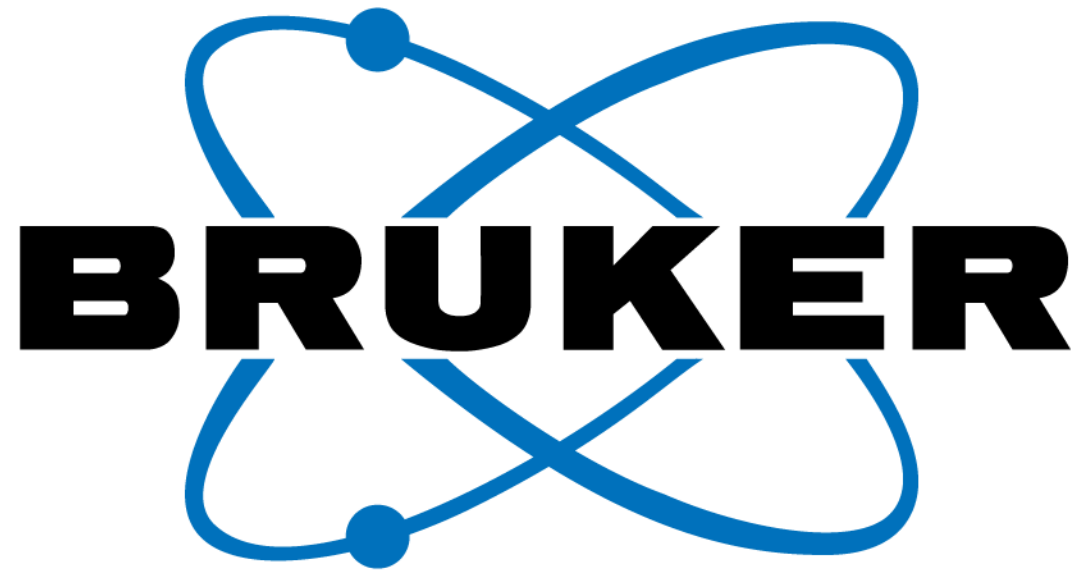
Literature

[1] R. Bruschweiler and F. Zhang, Covariance nuclear magnetic resonance spectroscopy
J. Chem. Phys. 120, 5253-5260 (2004)

[2] N. Trbovic, S. Smirnov, F. Zhang, and R. Bruschweiler, Covariance NMR spectroscopy by singular value decomposition
J.Magn. Reson. 171, 277-283 (2004)

[3] F. Zhang and R. Bruschweiler, Indirect covariance NMR spectroscopy
J. Am. Chem. Soc. 126, 13180-13181 (2004)

www.bruker-biospin.com