Filename Conventions for Unknown Samples in Chem. 636

raw filenames: **`IIIEESSS.FFN`** where

`III` – sample code (supplied on tube)

`EE` – experiment code:

- **`H1`** – standard 1d ^{1}H spectrum (including 1D setup-up for 2D spectra)
- **`HR`** – high-resolution 1d ^{1}H spectrum (increased AQ)
- **`HD`** – 1d ^{1}H homodecoupled spectrum
- **`CO`** – 2d ^{1}H standard COSY spectrum
- **`LR`** – 2d ^{1}H Long-Range COSY spectrum
- **`C3`** – standard 1d ^{13}C spectrum
- **`CQ`** – quaternary-enhanced 1d ^{13}C spectrum (increased RD/D1)
- **`GD`** – coupled 1d ^{13}C spectrum (GATEDEC)
- **`IG`** – quantitative 1d ^{13}C spectrum (INVGATE)
- **`D4`** – DEPT-45 1d ^{13}C spectrum
- **`D9`** – DEPT-90 1d ^{13}C spectrum
- **`D1`** – DEPT-135 1d ^{13}C spectrum
- **`I1`** – INEPT (-135-like) 1d ^{13}C spectrum
- **`CH`** – 2D $^{13}C\{^{1}H\}$ heterocorrelation (HETCOR)
- **`HC`** – 2D $^{1}H\{^{13}C\}$ inverse-heterocorrelation (HMQC)
- **`HS`** – 2D $^{1}H\{^{13}C\}$ inverse-heterocorrelation (HSQC)
- **`HB`** – 2D $^{1}H\{^{13}C\}$ inverse long-range heterocorrelation (HMBC)

`SSS` – student initials

`FF` – ^{1}H frequency in 10's of MHz:
- **25** for data acquired on Phoenix
- **28** for Athena, data acquired in automation
- **29** for Athena, data acquired manually
- **30** for data acquired on Homer

`N` – experiment number (somewhat arbitrary, 0-9)

NUTS filenames: **`IIIEESSS.FFN-nuts`**

For automation, the data set name is changed when saving the data as follows:

suppose the data was saved as:	SB190F.103 (see next page)
and the name code should be:	A16C3CGF.280
edit the PC name to:	A16C3CGF.280_SB190F.103

Filenames from Bruker Sample Automation (300MHz):