HelmholtzZentrum münchen
German Research Center for Environmental Health

Bayerisches NMR Zentrum

Protokoll G-NMR-Treffen "Pulsprogramme", BNMRZ, Garching, 15.01.2014

Protokollführer: G. Gemmecker, BNMRZ/TUM

I. Participants

Monika Beerbaum (FMP Berlin)

Wolfgang Bermel (Bruker BioSpin; Rheinstetten)
Dirk Bockelmann (MPI Göttingen)
Jörg Fohrer (Uni Hannover)
Gerd Gemmecker (TU München)
Steffen Glaser (TU München)
Donghan Lee (MPI Göttingen)
Frank Löhr (Goethe Universität Frankfurt)
Tobias Madl
Senada Nozinovic (Uni Bonn)
Bernd Reif (TUM)
Christian Richter (Goethe Universität Frankfurt)
Michael Sattler (TU München)
Peter Schmieder (FMP Berlin)

II. Presentations

a) Gerd Gemmecker/BNMRZ, TU München

Local "M*" programs use (mostly) PROSOL definitions, spectrometer set-ups include regularly updated temp. calibrations and PROSOL pulse lengths (^{1}H: separate for organic / aqueous solvents)

> *Hint: PULSECAL command sets ALL ^{1}H pulses new (hard & decoupling & soft pulses); call "getprosol nucleus_name Pulse_length" to selectively update e.g. all ^{1}H pulses*
>
> *e.g. "Getprosol 1H P90 PL90" copies pulses of all relevant nuclei and recalculates those for ^{1}H*

Problem: put different versions (TROSY, 2H decoupled, SE, CT, ^{13}C/^{15}N and all combinations) as separate pulse programs – or as ONE with many switching options (=unreadable)?

"Mseq" macro:

Problem: transfer of experiments between different spectrometers:

- adjust frequencies, sweep widths; pulse widths (by PROSOL!)
- depending on hard/software (DRX/AV I / AV II etc.):, powercheck, pre/after shape delays

Hint: PARACON command helps transfer experiments between spectrometers (adjust SFO1s) for Bruker / user-defined parameters sets.

Which file(s) are required to transfer a functional experiment between NMR centers?

- just pulse programs? (then COMPLETE descriptions of all parameters are required!)
- PPs &additional files (specific pulse shapes etc.)
- PPS plus complete data sets / parameters sets?

Organisation of pulse programs on the spectrometers:

- situation at BNMRZ: ONE user ("guest" etc.) – everything accessible, but very long list of "user PPS" - difficult to search …
- alternative: individual users - "separate worlds" (pulse programs, data sets etc.)

b) Monika Beerbaum/FMP Berlin-Buch

The FMP NMR installation relies on a unique set-up and definition of parameters (proprietary PROSOL, relations files).

Definitions use specific and unique parameter names, so few (ca. 50) dataset/parameter files are needed for ca. 260 different pulse programs, exclusively for AV III consoles.

For these pre-defined sequences, little additional user support is needed: everything is self-explaining and well described &set-up (including tables showing available experiments and macros and *au* programs for set-up)

Limitations: users are (more or less) restricted to the existing library.

Hint: Topspin allows switching between PROSOL (standard) and USERPROSOL (user defined) tables, to use proprietary and Bruker library PPs parallel ("getprosol", "getuserprosol")

Hint: a script is available from W. Bermel on request to convert "old"mc syntax PPs to "new" (TS3.x) syntax (ca. 98% perfect, manual check required)

c) Frank Löhr/BMRZ Univ. Frankfurt

Schwalbe group: uses Bruker release sequences (protein, RNA) plus own experiments (mostly PROSOL compatible)

Dötsch group: uses proprietary set of "fl*" pulse programs, not PROSOL compatible nor extensively commented; users copy existing "template" data sets.

Heterogeneous hard- and software (DRX, AV I, AVIII consoles)

Example for own improved pulse sequences:

a) BEST TROSY release sequence (order of REBURP /REBURPtr reversed) thereby the sequence can be corrected and still stays PROSOL compatible
b) (HB)CB(CGCCTOCSY)Har

Hint: PFGs have limited rise times (ca. 40 us from 0-100%), so very short gradients (≤250 us) might not scale linearly and need manual calibration

d) Dirk Bockelmann/MPI Göttingen

Bruker library PPs are used, but PROSOL generally not maintained on the various spectrometers

Group leaders act as "group memory" for PPs etc., Bruker library is used as back-up. This means of course that important new developments should be incorporated in the official releases ASAP (requires common effort from users and manufacturers!).

Bruker library PPS are automatically updated upon Topspin installations. Can be updated manually (by copying from the PP directories), but new PP implementations might actually require the new program version for proper performance!

Wolfgang Bermel/Bruker Biospin

Files supplied with new TOPSPIN releases:

- Update.info changes in new TOPSPION versions (including new / corrected PPs!)
- Param.info standard parameter definitions used by library PPS and PROSOL
- Relations.info "translation" used by PROSOL

Jörg Föhrer/Uni Hannover

Mostly small molecules / natural compounds (organic & inorganic chemistry)

1 DRX / 1 AV III console; PROSOL / standard parameters sets used extensively

Analog spectrometer log book to track spectrometer usage

III. Discussion

How can we make new pulse sequences available to the community fast?

- Have manufacturers provide it?
  - Yes, but time frame will depend on new program releases (typically ≥6 months)

- G-NMR could provide a faster distribution of new / improved experiments
  - Exchange could be easily set-up via the G-NMR webpage (probably log-in required)
  - Should we communicate via Facebook? (with "likes" / "dislikes"???)
  - or have a blog to communicate?
  - or a Wiki?
  - or a new "G-NMR pulse program mailing list"?

Opinions vary; potential problems might be: who has time to use yet another … (there are already so many other NMR blogs / mailing lists)? Who will contribute? Won't people prefer to just write a quick e-mail to a colleague instead?

Which experiments should be "deposited" there:

- New experiments that have been described/used in a publication could be "deposited" like PDB structures etc. – test this within G-NMR first, if it works could be expanded beyond G-NMR
- Many "small" improvements will never make it into a separate publication, - but help for good practice within the G-NMR community

IV. Next steps

1. **Set-up a web page/exchange platform to up-/download pulse sequences**
   - BMRZ/Frankfurt and BNMRZ/TUM should contribute some "good examples" as a starting point
   - Information that should be provided: pulse sequence, example dataset, short description, author/submitter (contact e-mail), date, hard-/software requirements (Bruker/Agilent; hardware/software version), publication (doi link), results (pdf)
   - Start as a simple HTML table; if it is being recognized by G-NMR users, a blog can be implemented
   - Implement by Feb. 2014 (BNMRZ/TUM)

2. **Next meeting: ca. 6 months after implementation/ fall 2014**