What is New in Chempack?

Varian User Conference
Burlington, VT
Sept. 10, 2006
Chempack Versions

Chempack 2.x  [userlib/chempack/CP.tgz]
  VNMR 6.1C/VNMRJ1.1B
  “classic” interface

Chempack 3.1  [userlib/chempack/CP3.tgz]
  VNMRJ 1.1D thru VNMRJ 2.1B
  “classic” and “java” interface

Chempack 4.0  [beta testing]
  VNMRJ 1.1D thru VNMRJ 2.1B
  “java” interface ONLY
What is new in Chempack?

Experiments
- Modular concept
- Features
- Customization

Chempack – Automation – StudyQ
[see me for details?]
Chempack 3.x [4.x]

Experiments

```
[cpwuser@sangeet psglib]$ ls
ADEQUATE.c  ECOSY.c  gHMBCme.c  gXHCAL.c  HSQCTOXY.c  selexcit.c
bsgHMBC.c  findz0.c  gHMQC.c  HETCOR.c  NOESY1D.c  TOCSY1D.c
bsgHSQCAD.c gCOSY.c  gHMQCTOXY.c  HMBC.c  NOESY.c  TOCSY.c
bsHSQCAD.c  gDQCOSY.c  gHSQCAD.c  HMQC.c  PRESAT.c  wet1D.c
CIGAR.c  gH2BCAD.c  gHSQCADTOXY.c  HMQCTOXY.c  PWXCAL.c  zTOCSY1D.c
COSY.c  gHETCOR.c  gHSQC.c  HSQCAD.c  ROESY1D.c  zTOCSY.c
DEPT.c  gHMBCAD.c  gHSQCTOXY.c  HSQCADTOXY.c  ROESY.c
DQCOSY.c  gHMBC.c  gmapz.c  HSQC.c  S2PUL.c
[cpwuser@sangeet psglib]$ 
```

Coming soon (?):
“relaxation” filters;
CRISIS²;  STEP;
Heteronuclear TOCSY filters
Steadystate()
    G-90-G or trim\_x-trim\_y
satpulse(duration,phase)
    off-resonance or on-resonance
purge(phases)
    off-resonance or on-resonance
shapedsatpulse(shapename,duration,phase)
    Multifrequency on-the-fly shaped pulse presaturation
shaped\_purge(phases)
    Multifrequency on-the-fly shaped purge
SpinLock(pattern,duration,pw90,phase)
    mlev16, mlev17, mlev17c, dispi2, dispi3, troesy, dante-roesy, cw

**PURGE**: A. Simpson, and S. Brown, JMR 175, 340-346 (2005)
if (satmode[0] == 'y')
{
    if ((d1-satdly) > 0.02)
        delay(d1-satdly);
    else
        delay(0.02);
    if (getflag("slpsat"))
    {
        shaped_satpulse("relaxD",satdly,v2);
        if (getflag("prgflg"))
            shaped_purge(v1,v2,v18,v19);
    }
    else
    {
        satpulse(satdly,v2,rof1,rof1);
        if (getflag("prgflg"))
            purge(v1,v2,v18,v19);
    }
} else
    delay(d1);
## Experiments – Modular approach

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Modular approach:
- Modules with "xoox_module" macro
- Modules in a file
- dpype in a file
- logo and macros
- Currently unused
Experiments – Modular approach

"ddrtc is set appropriately !!"

curpar → apptype → add newmodules → curpar

modules – parameter files in ~/vnmrsys/modules or /vnmr/modules

[May have an associated xxxxx_module macro]
Experiments – Modular approach

HSQCADTOXY

apptype = ‘hetero2D’
modules = ‘par2D wet presat gradients Dch_adiabatic spinlock zfilter’

PROTON

apptype=‘std1D’
modules =
  wet
  presat
  gradients

hetero2D
par2D
Dch_adiabatic
spinlock
zfilter

HSQCADTOXY

apptype=‘hetero2D’
modules =
  par2D
  wet
  presat
  gradients
  Dch_adiabatic
  spinlock
  zfilter
Experiments – Modular approach

HSQCADTOXY

apptype = ‘hetero2D’
modules = ‘par2D wet presat gradients Dch_adiabatic spinlock zfilter’

wet1D

apptype=‘lstd1D’
modules =
  wet
  presat
  gradients

hetero2D
par2D
Dch_adiabatic
spinlock
zfilter

HSQCADTOXY

apptype=‘hetero2D’
modules =
  par2D
  wet
  presat
  gradients
  Dch_adiabatic
  spinlock
  zfilter
Experiments – Modular approach

**HSQCADTOXY**

`apptype = 'hetero2D'
modules = 'par2D wet presat gradients Dch_adiabatic spinlock zfilter'

**PRESAT**

`apptype='lstd1D'
modules =
  wet
  presat
  gradients`

**hetero2D par2D Dch_adiabatic spinlock zfilter**

**HSQCADTOXY**

`apptype='hetero2D'
modules =
  par2D
  wet
  presat
  gradients
  Dch_adiabatic
  spinlock
  zfilter`
Experiments – Modular approach

HSQCADTOXY

apptype = ‘hetero2D’
modules = ‘par2D wet presat gradients Dch_adiabatic spinlock zfilter’

tn=19F dn=13C

FLUORINE

apptype=‘std1D’
modules =
  wet
  presat
  gradients

hetero2D
par2D
Dch_adiabatic
spinlock
zfilter

19F-13C

HSQCADTOXY

apptype=‘hetero2D’
modules =
  par2D
  wet
  presat
  gradients
  Dch_adiabatic
  spinlock
  zfilter
Experiments – Modular approach

**HSQCADTOXY**

*apptype = ‘hetero2D’*
*modules = ‘par2D wet presat gradients Dch_adiabatic spinlock zfilter’*

---

**apptype=‘std1D’**
*modules =*
  - wet
  - presat
  - gradients

---

**apptype=‘hetero2D’**
*modules =*
  - par2D
  - wet
  - presat
  - gradients
  - Dch_adiabatic
  - spinlock
  - zfilter
Experiments – Modular approach

HSQCADTOXY

apptype = ‘hetero2D’
modules = ‘par2D wet presat gradients Dch_adiabatic spinlock zfilter’

PROTON

apptype=‘std1D’
modules =
  wet
  presat
  gradients

hetero2D
par2D
Dch_adiabatic
spinlock
zfilter

HSQCADTOXY

apptype=‘hetero2D’
modules =
  par2D
  wet
  presat
  gradients
  Dch_adiabatic
  spinlock
  zfilter
Experiments – Modular approach

HSQC\textsubscript{ADTOXY}

\texttt{apptype = ‘hetero2D’}
\texttt{modules = ‘par2D wet presat gradients Dch\_adiabatic spinlock zfilter’}

\begin{itemize}
\item [\texttt{apptype=‘std1D’}]\texttt{modules =}
\begin{itemize}
\item wet
\item presat
\item gradients
\end{itemize}
\end{itemize}

\begin{itemize}
\item [\texttt{apptype=‘hetero2D’}]\texttt{modules =}
\begin{itemize}
\item par2D
\item wet
\item presat
\item gradients
\item Dch\_adiabatic
\item spinlock
\item zfilter
\end{itemize}
\end{itemize

\texttt{CRISIS: R. Boyer, R. Johnson, K. Krishnamurthy, JMR, 165, 253-259 (2003)}
**Experiments – Modular approach**

**HSQCADTOXY**

- `apptype` = 'hetero2D'
- `modules` = ‘par2D wet presat gradients Dch_adiabatic spinlock zfilter’

```
HSQCADTOXY
   apptype='hetero2D'
   modules =
       par2D
       wet
       presat
       gradients
       Dch_adiabatic
       spinlock
       zfilter
```

** Preserve:**
- `sw1`, `ni`, `dof`, `reference`, `jxh`, `adshapes`, etc.
Experiments – Modular approach

**HSQCADTOXY**

\[
\text{apptype} = \text{hetero2D'} \\
\text{modules} = \text{par2D wet presat gradients Dch\_adiabatic spinlock zfilter'}
\]

- **apptype='hetero2D'**
- **modules = 'par2D wet presat gradients Dch\_adiabatic spinlock zfilter'**

**Preserve:**
- sw1, ni, dof, reference, jxh, etc.
Experiments – Modular approach

HSQCADTOXY

apptype = ‘hetero2D’
modules = ‘par2D wet presat gradients Dch_adiabatic spinlock zfilter’

HSQCADTOCSY

apptype=‘homo2D’
modules =
par2D
wet
presat
gradients
Dch_adiabatic
spinlock
zfilter

hetero2D
par2D
Dch_adiabatic
spinlock
zfilter

HSQCADTOXOY

apptype=‘hetero2D’
modules =
par2D
wet
presat
gradients
Dch_adiabatic
spinlock
zfilter

Preserve:
spinlock pattern,
duration, etc.
PRESAT - Features

On-the-fly “multi-freq” PRESAT
On-the-fly “multi-freq” PURGE
[available in all chempack sequences]

- Predefine solvent (or)
- Suppress “n” tallest peaks
- 2-step or 4-step PURGE

Select presat peak(s) interactively
On-resonance
Off-resonance
Multi-frequency
2-step PURGE
4-step PURGE

On-resonance
Off-resonance
Multi-frequency
2-step PURGE
4-step PURGE

PRESAT

Delay 2.00 s
Offset (Hz) -173.0 4.65p
Power (dB) 0 46 Hz

Purge Cycle 2
Purge 200 200 µs
Gradient level 18660
Offset (Hz) -173
Chem. Shift ppm: 4.65p, 1.95p

Delay 2.00 s
Offset (Hz) -173.0 4.65p
Power (dB) 0 46 Hz

Purge Cycle 2
Purge 200 200 µs
Gradient level 18660
Offset (Hz) -173
Chem. Shift ppm: 4.65p, 1.95p
On-resonance PRESAT

Satpwr = 4

Satpwr = -6

On-resonance PURGE

Satpwr = 0

Off-resonance PURGE

Satpwr = 0

Multi-freq PURGE

5mM Glucose in 90% H2O/10% D2O
wet1D - Features

- Predefine solvents (or)
- Suppress “n” tallest peaks
- Optimize of wetpower (CF)

Select wet peaks interactively
- One at a time (or)
- “all” above a threshold
**TOCSY1D (dpfgse experiments)**

- Predefine peaks
- Predefine width or let the software estimate from 1D spectrum
- Or Select peak(s) interactively

**“Independent” echo pulses HEX Ready !!**

**HEX – Hadamard Excitation Sculpting**

HEX: K. Krishnamurthy, JMR 153, 144-150 (2001)
bsHSQCAD
(band-selective – dpfgse – 2D experiments)

Predefine selective band

Or Select band interactively
bsHSQCAD
(band-selective – dpfgse – 2D experiments)

“Independent” echo pulses
IMPRESS Ready!!

What if I want to **customize** the default parameters of an experiment?

[HSQCADTOXY]

```plaintext
apptype = 'hetero2D'
modules = 'par2D wet presat gradients Dch_adiabatic spinlock zfilter'
```

1. Experiment Level [CP4.x ONLY]:
   Use “MainMenu=>Edit=>Customize parlib…” tool
   i. PROTON HSQCADTOXY
   ii. nt=8 ni=384 mixT=0.06 slpatT='dipsi2'
   iii. MainMenu=>Tools=> Edit/Make parlib…
What if I want to customize the default parameters of an experiment?

[HSQCADTOXY]

- `apptype = 'hetero2D'`
- `modules = 'par2D wet presat gradients Dch_adibatic spinlock zfilter'`

- Save it as “myHSQCADTOXY”
- Macro/parlib/customizations are created from HSQCADTOXY
- myHSQCADTOXY macro is now available to do customized HSQCADTOXY

- Save it as “HSQCADTOXY”
- Macro/parlib/customizations are updated
- Customized HSQCADTOXY is now available
What if I want to **restore** the default parameters of an experiment?

**[HSQCADTOXY]**

- `apptype = 'hetero2D'`
- `modules = 'par2D wet presat gradients Dch_adiabatic spinlock zfilter'`

![Diagram showing the process of restoring default parameters.](image)
Customizations [Experiments]

What if I want to customize the default parameters of an experiment? [HSQCADTOXY]

- `apptype = 'hetero2D'`
- `modules = 'par2D wet presat gradients Dch_adiabatic spinlock zfilter'`

2. Module Level (One of the following):
   a. Modify `maclib/spinlock_module` [recommended]
      i. If not found, make a copy from `maclib/Generic_module`
   b. Modify `module/spinlock`
      i. `writeparam(userdir+'/modules/spinlock','mypar','current','add')`

Modifications are effective for ALL experiments with spinlock module
Q. Do I need to build my parameter set with modules?
A. No!! [But you must have a parlib entry]
Q. Should my experiment belong to one of “predefined” apptypes?
A. No !! When apptype="", the generic_apptype macro takes over. The generic_apptype macro does NOTHING but to add modules.
Q. Should my experiment belong to one of “predefined” apptypes?
A. No!! When apptype=“” and modules=“”, the \textit{generic\_apptype} macro takes over. The \textit{generic\_apptype} macro does NOTHING but do fread from procpar.
Q. Can I use my own macro/parameter set within chempack?
A. YES !! But…with a caveat: Replace ALL `psgset` with `Autopsgset`
Customizations

User Customization options –

usergo  
go_seqfil

userprocess  
pslabel_process

userplot  
pslabel_plot

user_cpsave  
pslabel_save

user_cpdone

user_auto_au

user_calibrate

user_rt

user_rtp

user_svf

user_svp

pslabel_setup
What is new in Chempack?

Experiments
Modular concept
Features
Customization

Chempack – Automation – StudyQ
[see me for details?]
Acknowledgement

Haitao Hu  
Eli Lilly

Charles Fry  
U. of Wisconsin

Charles Wandler  
U. of W. Washington

William Lenhart  
Kodak