SIMPSON / SIMMOL
Demonstration

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5.000.000$

1.000$

Do as much as possible on the computer!

Triple-Resonance Pulse Sequences
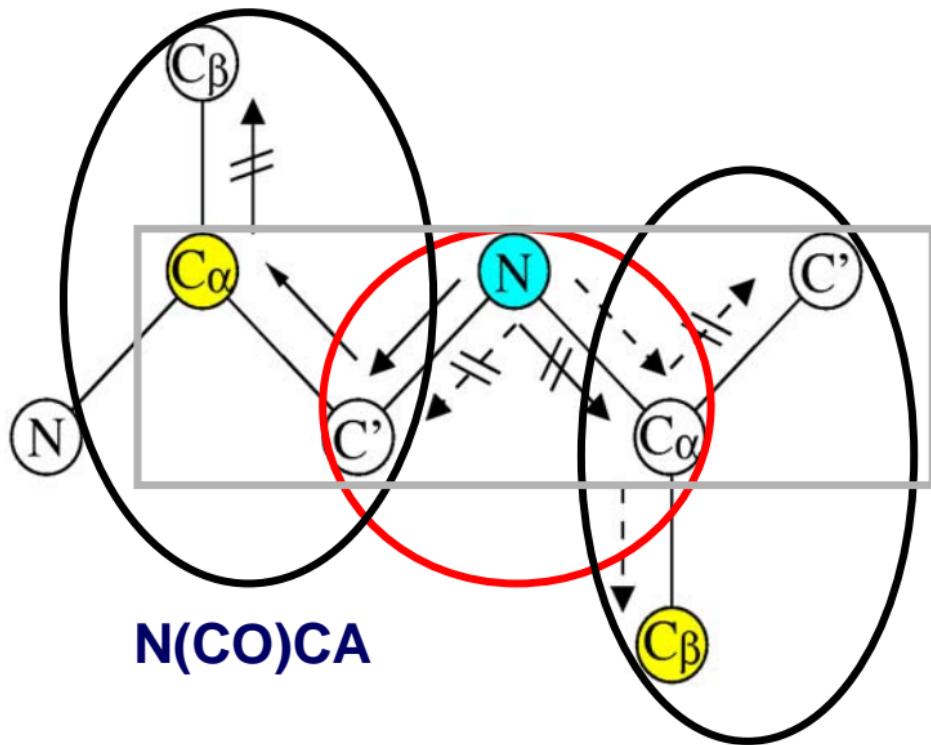
$^{15}N \rightarrow {}^{13}C'$: DCP

$^{13}C' \rightarrow {}^{13}C^{\alpha}$: C7

Many parameters to optimize!

SIMPSON input file

```
spinsys {
   channels 15N 13C
   nuclei   15N 13C 13C

   shift 1 ...
   dipole 1 2 ...
}

par {
   proton_frequency 400e6
   start_operator   I1x
   detect_operator  I3p
   sw               ...
}

proc pulseq {} {
   ...
}

proc main {} {
   ...
}
```

Setting Up the `spinsys` File
Introducing SIMMOL

SIMPSON's   "sample changer"
                               "peptide synthesizer"

"sample changer": mload "1C3W.pdb"
"peptide synthesizer": mmake 3 –65 –40

File: ncac.mol
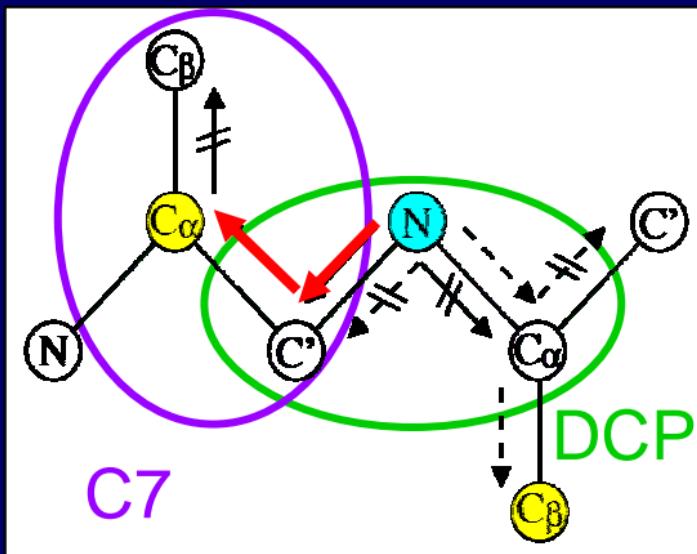
Strategy for Optimization of the DCP-C7 N(CO)CA Pulse Sequence

<u>$^{15}N \rightarrow {}^{13}C'$ DCP:</u>
- ^{15}N rf field strength 50 kHz
- Spinning frequency 5 kHz
- 9.4 T magnet

Optimize
- CP time
- ^{13}C carrier offset

<u>$^{13}C' \rightarrow {}^{13}C^{\alpha}$ C7:</u>
- Rf field strength 35 kHz

Optimize
- ^{13}C carrier offsets
- Mixing time

First Optimization: CP Time
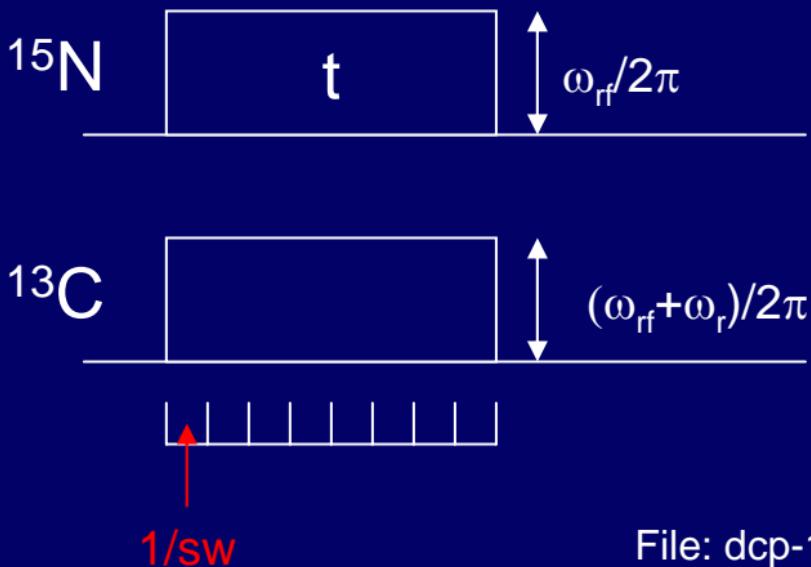
SLOW!!!

File: dcp-1.in

Reuse the Propagators

$$H = H(\alpha, \beta, \gamma, \omega_r t + \gamma)$$

t dependency: $e^{-m(\omega_r t + \gamma)}$

^{15}N t $\omega_{rf}/2\pi$

^{13}C $(\omega_{rf} + \omega_r)/2\pi$

t_r

1/sw
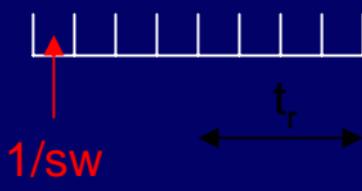
File: dcp-2.in

FASTER!!!

γ-COMPUTE BEST

File: dcp-3.in

Time-Offset Optimization

offset

3rd calculation ⟶

2nd calculation ⟶

1st calculation ⟶

t
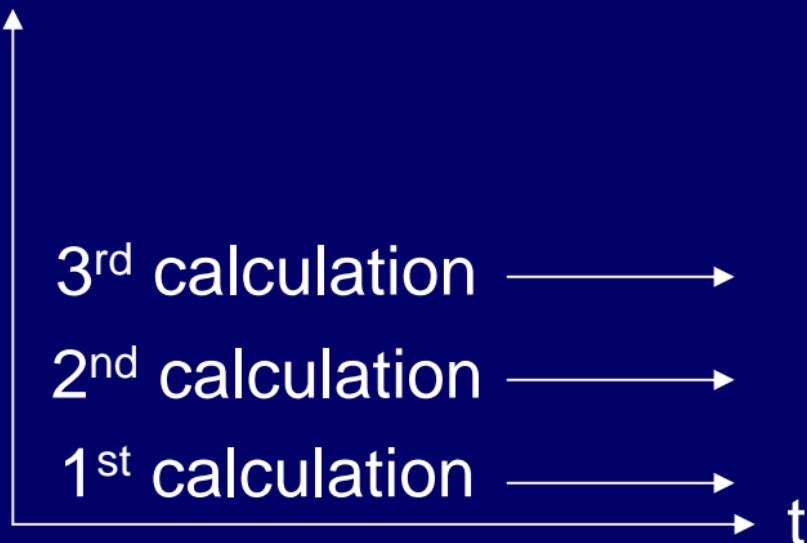
File: dcp-4.in

View 2D SIMPSON output
using nmrDraw/nmrPipe

# Setup C′-Cα-Cβ Spinsystem –
The `msetcoordsys` Command

File: ccacb.mol

-Defines a coordinate system
from atom positions

- X: from atom 2 to atom 1
- Z: perpenticular to the plane spanned
  by the three atoms
- Y: Z x X

1: H_i
2: N_i
3: C'_{i-1}
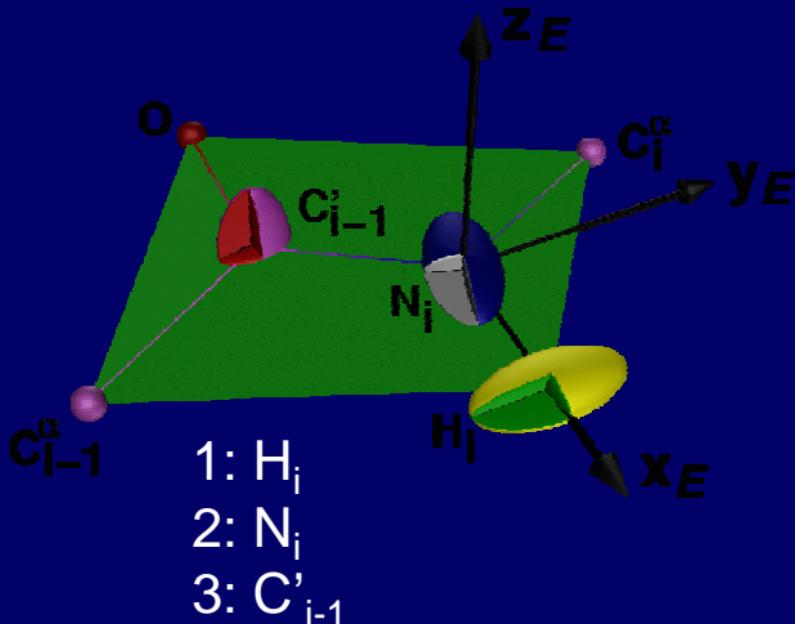
Offset profile of C7

$\delta_{iso}(1)$ →

$\delta_{iso}(2)$ →

C' − C$^\alpha$
C$^\alpha$ − C$^\beta$
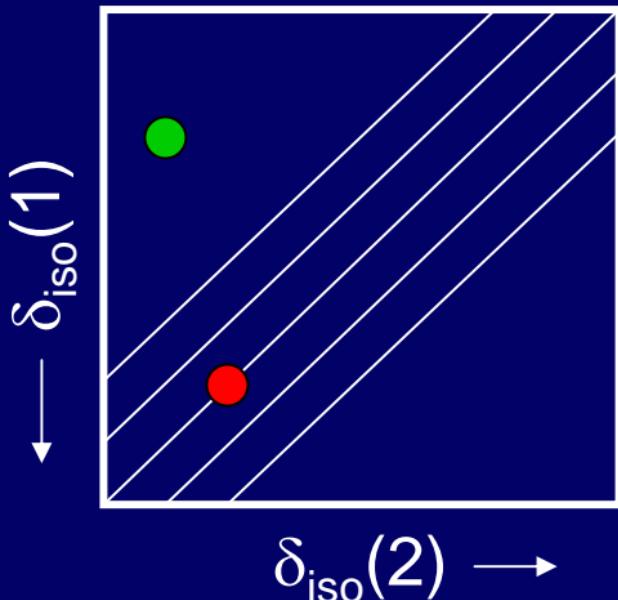
C7 Offset and Mixing Time Optimization

offset

3rd calculation ⟶

2nd calculation ⟶

1st calculation ⟶

t
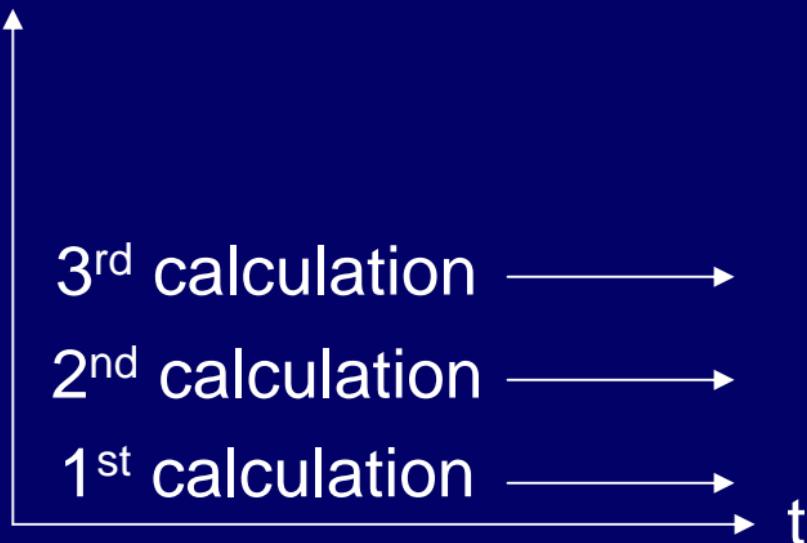
File: c7-1.in

How efficient is the transfer?
– map out intensity on C', C^α, and C^β

File: c7-2.in

Post C7

File: c7-3.in

DCP-C7 2D Simulation
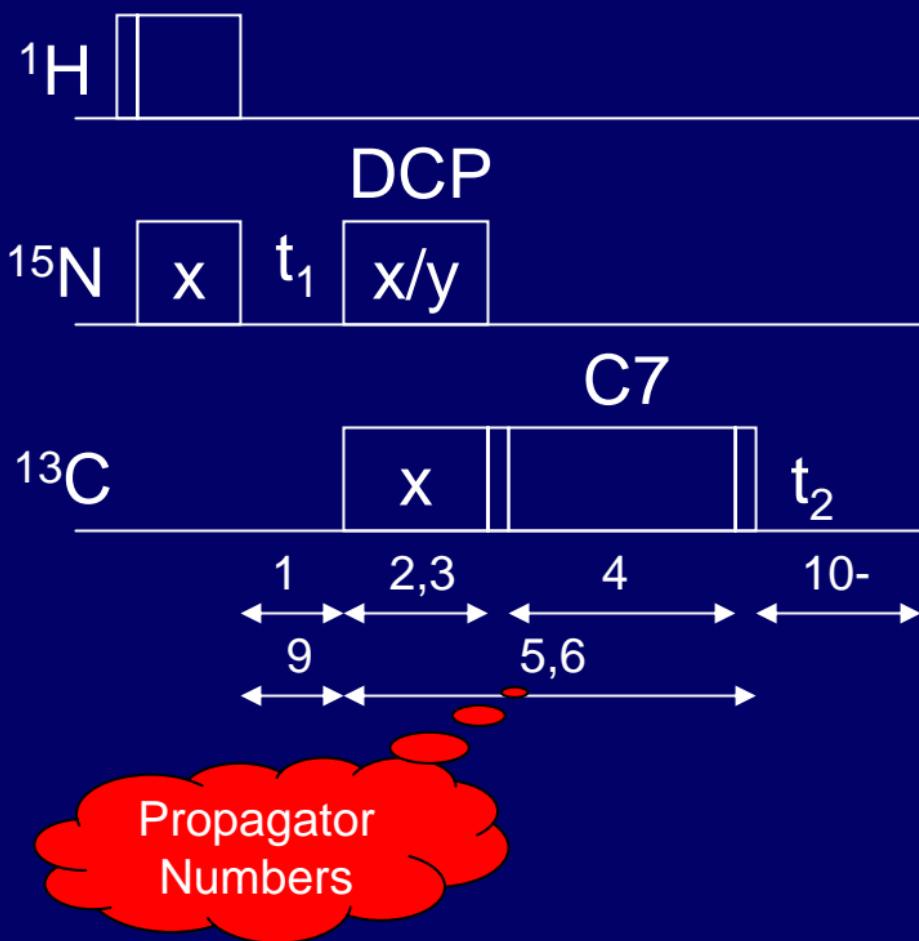
Fitting Experimental Spectra

Create "experimental" spectrum

```
fexpr $f "$re*rand()" ...
```

File: exp-1.in

```
proc minuit {} {
  global mn

  ...

  return $rms
}

proc main {} {
  global mn par

  ...
  mnpar iso   10   5
  mnpar aniso 20   5
  mnpar eta   0.5 0.1 0 1
  ...
}
```

File: fit-1.in

Initial value

Estimated error

Optional parameter limits