PULSE PROGRAM CATALOGUE:
I. 1D & 2D NMR EXPERIMENTS

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TOPSPIN v2.0
NMRGuide
## VOLUME I: 1D & 2D NMR EXPERIMENTS

- Table of Contents ................................................................. 1-2  
- Introduction ........................................................................... 3-6  

- Standard Pulse Schemes
  1. Basic 1D pulse sequences .................................................. 7  
  2. T1 & T2 Relaxation .............................................................. 13  
  3. Selective Excitation & Selective 1D Experiments ............... 15  
  4. 1D Solvent suppression
     - Presaturation  
     - Jump and Return  
     - Watergate  
     - Excitation Sculpting  
     - WET .......................................................... 21  
  5. 19F specific experiments .................................................. 27  
  6. 2H specific experiments .................................................. 29  
  7. Basic 1D Gradients ............................................................. 31

- Homonuclear Experiments
  8. 2D COSY ................................................................. 33  
  9. 2D COSY-DQF ............................................................ 37  
 10. 2D SECSY ................................................................. 41  
 11. 2D RELAY ................................................................. 43  
 12. 2D TOCSY ................................................................. 47  
 13. 2D ROESY ................................................................. 53  
 14. 2D NOESY ................................................................. 57  
 15. 1D & 2D Double-Quantum ............................................. 63  
 16. 2D J-Resolved ............................................................. 67

- Heteronuclear 1D & 2D X-detected experiments
  17. Decoupler Pulse Calibration ........................................... 69  
 18. 1D DEPT & INEPT ........................................................ 73  
 19. 2D HETCOR ............................................................. 81  
 20. 2D COLOC ................................................................. 87  
 21. 2D Heteronuclear J-resolved ........................................ 89  
 22. 2D HOESY ................................................................. 91  
 23. 1D & 2D INADEQUATE ............................................. 93

- 2D Inverse Experiments
  24. Basic 1D Inverse .......................................................... 97  

**Direct 2D Correlations**
  25. HMQC ................................................................. 101  
 26. DEPT-HMQC ............................................................. 111  
 27. HSQC ................................................................. 113  
 28. Multiplicity-edited HSQC ............................................. 127  
 29. Constant-time correlations .......................................... 133  
     - CT-HSQC  
     - CT-HMQC
 30. Inverse-INEPT ............................................................ 137  
 31. Spin-edited HSQC for J(XH) determination ..................... 139  
     - 2D HSQC-α,β  
     - 2D IPAP-HSQC  
     - 2D J-modulated CT-HSQC
 32. TROSY ................................................................. 145  
 33. CRINEPT ............................................................... 151  

**2D HMQC hybrids**
  34. HMQC-COSY .......................................................... 153  
     - H2BC .............................................................. 157
36. HMQC-ROESY................................................................. 163
37. HMQC-NOESY............................................................. 167

2D HSQC hybrids
38. HSQC-TOCSY ........................................................... 171
39. HSQC-ROESY ........................................................... 179
40. HSQC-NOESY ........................................................... 183

2D Long-Range Correlations
41. HMBC ................................................................. 187
42. Measurement of long-range proton-carbon coupling constants .......... 193

Phase-sensitive HMBC
CT-HMBC
J-HMBC
Long-range HSQC (HSQMBC)
EXSIDE
HETLOC
HSQC-HECADE

43. ADEQUATE ................................................................. 201
  1,1-ADEQUATE
  1,n-ADEQUATE
  n,1-ADEQUATE
  n,n-ADEQUATE

• Miscellaneous Experiments
44. 1D, 2D & 3D Diffusion/DOSY............................................ 207
  STE
  STEBP
  DSTE
  DSTE BP
  LED
  LEDBP
  DOSY-COSY
  DOSY-TOCSY
  DOSY-NOESY

45. 1D & 2D Saturation Transfer Difference (STD)............................ 213
  STD-TOCSY
  STD-NOESY
  STD-HSQC

46. 1D & 2D Experiments using CLEANEX.................................. 223
  CLEANEX-HSQC
  CLEANEX-TROSY

47. 1D & 2D LC-NMR Experiments........................................... 227
48. Basic Solid-State NMR Experiments.......................................... 235

• Appendix 1. Pulse Program Info......................................... 237
• Appendix 2. Pulse Program Parameters ................................. 241
• Appendix 3. Relations with edprosol/getprosol ......................... 246

VOLUME II: BIOMOLECULAR NMR EXPERIMENTS..................... 250
This catalogue presents the pulse sequence diagram for all standard pulse programs included in TOPSPIN v2.0. This information is part of NMRGuide 4.1, also available for BRUKER AVANCE spectrometers.

These pulse programs are located in the

/TOPSPINHOME/pp/stand/nmr/lists/pp

directory after conventional installation using expinstall and they can be visualized directly into the TOPSPIN program from the PulsProg section. Otherwise, alternative pulse program sequence representation is also available using the showpp program.

For more details on pulse programs, parameter sets, tutorials, experiment descriptions, bibliographic references and other related information, please refer to the electronic version of NMRGuide 4.1.
### Pulse Programs

<table>
<thead>
<tr>
<th>1D Experiments</th>
<th>2D Homonuclear</th>
<th>2D Heteronuclear</th>
<th>2D Inverse and Gradients</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isotope</td>
<td>Homonuclear</td>
<td>X-detected</td>
<td>from f3 ch.ann.el</td>
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<tr>
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<td>ln vuse</td>
<td>from f3 ch.ann.el</td>
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<td>from f2 clwmel</td>
<td>2DIROSY</td>
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<tr>
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<td>X-d)</td>
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### 3D Experiments

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AVAILCB-f'ILLlrlia/s

NMR Assistance

Step 1: Is the Spectrometer Ready?
- Installation & Configuration (cf & expinstall)
- Tests & Calibrations (edprosol)
- Defining the probe (edbead)

Step 2: Preliminary Set-up
- About Sample Preparation
- Insert the sample (ij/ej)
- Select the solvent (lock)
- Tuning & Matching ... (wobb)
- Shimrlng ... (rsh ...)

Step 3: Data Acquisition (eda)
- Create a new file (edc)
- Read Parameter Set (rpar ...)
- Set Pulses (getprosol)
- Modify parameters (ased)
- Start Acquisition (rga & zg)

Step 4: Data Processing (edp)
- Transforming the data (ft, xfb ...)
- Phase correction (apk)
- Baseline correction (abs)
- Plot (edg, xwi.nplot)

Step 5: Automation ...
- Using macros ... (edmac)
- Using icomum ... (Biotool)
- buttumlum & butschmtr
- AU Programs (xau)

Step 6: Deciding what to do?
- Which experiments can I do ...
- Starting Parameter Set...
- Routine IDAR experiments
- Interpreting the spectra...
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BASIC 1D PULSE SEQUENCES
• **Standard Experiments:**

Conventional ¹H spectrum (zg30 / zg / zg0 | PROTON)
Acquired as 2D (zg2d)

1D ¹H Homodecoupling (zg0hd / zghd / zghd.2 | PROHOMODEC)
1D ¹H Band-selective homodecoupling (zghe / zghe.2)

NOEDIFF experiment:
  Single irradiation (zgf2pr)
  Using frequency list (noediff / noediff.2 / noedif.2 | NOEDIFF)
  Irradiation multiplet frequencies within one multiplet (noemul)

¹³C spectrum with selective ¹H decoupling using CW (zgcw30 / zgcw / zg0cw)
¹H-decoupled ¹³C spectrum (zgdc30 / zgdc / zg0dc | C13CPD)
¹H-coupled ¹³C spectrum (zgdc30 / zgdc / zg0dc | C13GD)
¹H-decoupled ¹³C spectrum without NOE (zgig30 / zgig / zg0ig | C13IG)
¹H,¹⁰P-decoupled ¹³C spectrum without NOE (zgfbig)

Antiring sequence (aring, aring2)
1D sequence for suppression of background signals using composite pulse (zgbs)

• **Examples:**

  ³¹P-decoupled ¹H spectrum (zgig30 / zgig | PROP31DEC)
  ³¹B-decoupled ¹H spectrum (zgig30 / zgig | PROB11DEC)

  ¹H-decoupled ¹⁵N spectrum without NOE (zgig / zgf3ig | N15IG)
  ¹H-coupled ¹⁵N spectrum without NOE (zg | N15)
  ¹H-decoupled ³¹P spectrum (zgpg30 | P31CPD)
  ¹H-coupled ³¹P spectrum (zg | P31)

• **Standard BRUKER parameter sets available for other nuclei:**

  ¹⁹F spectrum ( zg | F19ZG)
  ¹⁷O spectrum ( zg | O17ZG)
  ²³Na spectrum ( zg | NA23ZG)
  ²⁷Al spectrum ( zg | AL27ND)
  ¹H-decoupled ²⁹Si spectrum (zgig | S29IG)
  ¹⁸Cl spectrum ( zg | CL35ZG)
  ³¹Cl spectrum ( zg | CL37ZG)
  ³¹Ga spectrum ( zg | GA71ZG)
  ³¹Ga spectrum ( zg | SE77ZG)
  ¹⁸Rh spectrum ( zg | RH103ZG)
  ¹⁹Cd spectrum ( zg | CD111ZG)
  ¹⁰Cd spectrum ( zg | CD113ZG)
  ¹H-decoupled ¹¹Sn spectrum (zgig | SN119G)
  ¹⁹Pt spectrum ( zg | PT195ZG)
  ¹⁹Hg spectrum (zgpg | HG199CPD)
d1 is pre-scan delay
p1 is read pulse
aq is acquisition time
td is time domain
dw is dwell time
ns is number of scans

\[ aq = td \times dw = \frac{td}{2 \times sw} \]
**Pulse Program Catalogue**

*NMRGuide 4.1 - Topspin 2.0*

---

**zghc**

**zghc.2**

**zghd.2**

**zghd**

- **pl1**
  - Homodecoupling
  - **pl24**

**zg0hd**

- **pl24**

**zgadchd**

- **pl24**

---

**d1** = 3  **pl24** = 40

**o2p** = 1.29(H-13)

**pulprog** = **zghd.2**

---

**zcw**

- **pl1**
  - CW
  - **pl26**

**zg0cw**

- **pl26**

**zgcw30**

- 30°

---

- **noedif.2**
- **noediff**
- **noediff.2**

---

Also see: solvent suppression

(***zgf2pr***)

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T1 & T2 RELAXATION
$^1$H T$_2$ measurements
- As 1D acquisition (cpmg1d)
- As 2D acquisition (cpmg)
- As 1D acquisition with presaturation (cpmgpr1d)

$^1$H T$_1$ measurements:
- As 1D acquisition (t1ir1d)
- As 2D acquisition (t1ir || PROTON1)

T$_1$ 13C measurements (t1irpg)

Also see: 2D HSQC for Backbone Dynamics

\[ I_z = I_0(1 - 2\exp(-d_7/T_1)) \]
\[ \ln(I_0-I_z) = \ln(2I_0)-d_7/T_1 \]
\[ t_{null} = T_1*\ln2 \]
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SELECTIVE EXCITATION &
SELECTIVE 1D EXPERIMENTS
- **Phase-Cycled:**
  - Using a shaped 90° pulse (selzg | SELZG1H)
  - Selective 1D COSY experiment (selco | SELCO1H)
  - Selective 1D RELAY experiment (selcorl)
  - Selective 1D TOCSY experiment (selmlzf | SELMLZF1H)
  - Selective 1D NOESY experiment (selno | SELNO1H)
  - Selective 1D ROESY experiment (selro | SELRO1H)

- **Gradient-based:**
  - Using selective pulsed-field-gradient spin-echo or SPFGE (selgpse | SELGPSE)
  - Selective ge-1D COSY experiment (selcogp | SELCOGP)
  - Selective ge-1D TOCSY experiment:
    - using MLEV (selmlgp | SELMLGP)
    - using MLEV With ZQ suppression (selmlgp.2)
    - using DIPSI-2 (seldgp)
  - Selective ge-1D NOESY experiment (selnogp | SELNOGP)
  - Selective ge-1D ROESY experiment (selrogp | SELROGP)
  - Selective ge-1D T-ROESY experiment (selrogp.2)

- **13C Selective:**
  - 13C Selective excitation using a shaped 90° pulse (selzgpg)
  - Selective 1D X-X COSY experiment (selcogp)
  - Selective 1D INADEQUATE experiment (selina)

- **Miscellaneous:**
  - 2-2-6-2-2 DANTE-z scheme (dazzg)
  - 3-6-3 DANTE-z scheme (daz363zg)
  - 1-1 DANTE-z scheme (daz11zg)
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1D SOLVENT SUPPRESSION
1D Solvent suppression

Classical:

1D water presaturation:
   Conventional (zgpr / zg0pr | ZGPR)
   Using composite pulses (zgcpr | ZGCPR)
   Using spoil gradient (zggppr)
   Using composite pulse and spoil gradient (zgcpgppr)
   From f2 channel (zgf2pr / zg0f2pr)
   Using shaped pulse for off-resonance presaturation (zgps)

Jump and return:
   1-1 scheme (p11)
   1-3-3-1 scheme (p1331)

Gradient-based:

1D WATERGATE:
   Using 3-9-19 scheme (p3919gp | P3919GP)
   Using 3-9-19 and flip back pulse (p3919fpgp)
   Using 90° water-selective pulses (zggpwg | ZGGPWG)

1D Excitation Sculpting:
   Using 180° water-selective pulses (zgesgp)
   Using 180° water-selective and flip back pulse (zgesfpgp)
   Using W5 pulse train (zggpw5)

1D WET scheme:
   Conventional (wet)
   With 13C decoupling on f2 during WET and AQ (wetdc | LC1DWTDC)
   With 13C decoupling on f2 during WET (wetdw)

Related Experiments:

- All these 1D experiments can be incorporated in any multidimensional NMR experiment. Please refer to each chapter to check the different possibilities for 2D and 3D solvent-suppressed experiments
- LC-NMR Experiments
Pulse Program Catalogue
NMRGuide 4.1 - Topspin 2.0

Also see: LC-NMR experiments

Also see: noediff

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$^{19}$F SPECIFIC EXPERIMENTS
### $^{19}$F Experiments

#### 1D spectra:

- $^1$H-decoupled $^{19}$F spectrum (zgfhigqn / zgfhigqn.2 | F19CPD)
- $^1$H-coupled $^{19}$F spectrum (zgfqn | F19)
- $^{19}$F-homodecoupled $^{19}$F spectrum (zhflhdqn)

- $^{19}$F-decoupled 1D $^1$H spectrum (zghfigqn / zghfigqn30 | PROF19DEC)
- $^1$H spectrum with $^{19}$F-presaturation (zgf2hfpr)

#### 2D spectra:

- 2D $^{19}$F-$^1$H HETCOR experiment (hfcoqfqn)
- 2D $^{19}$F-$^1$H HOESY experiment (hoesyhfqfqrn)

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2H SPECIFIC EXPERIMENTS
• **1D spectra:**
  
  1D \(^2\)H spectrum (zg2h)
  1D X-decoupled \(^2\)H spectrum (zgig2h, zgig2hf4)

• **2D spectra:**
  
  Magnitude-mode 2D HETCOR with \(^2\)H-decoupling (hxcoq2h)

• **Miscellaneous:**
  
  High-power 90° \(^2\)H decouple pulse calibration (decp902h, decp902hf4)

Related Experiments:

- Also see: 2H-decoupled 3D triple-resonance experiments
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BASIC 1D GRADIENTS
• **Standard:**
  
  Gradient-enhanced 1D Echo experiment (zggegp)
  Gradient-enhanced 1D Spin-Echo experiment (zgpse)

• **Gradient Calibration:**
  
  Gradient Strength Calibration (calibgp)
  Gradient Preemphasis Adjustment. Gradient Recovery Test (preempgp2)

• **Gradient Shimming:**
  
  1D Gradient Echo for gradshim-procedure (imgegp1d)
  1D Gradient Echo for gradshim-procedure using 2H (imgegp1d2h)
  1D Gradient Echo for gradshim-procedure using selective pulse (imgegps1d)

  3D Gradient Echo for gradshim-procedure (imgegp3d)
  3D Gradient Echo for gradshim-procedure with BSMS RCB board (imrchgegp3d)
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2D COSY EXPERIMENTS
**Phase-cycled:**

- Magnitude-mode 2D COSY (cosyqf | COSY45SW / COSY90SW)
- Magnitude-mode 2D COSY using a 45 pulse (cosyqf45 | COSY45SW)
- Magnitude-mode 2D COSY using a 90 pulse (cosyqf90 | COSY90SW)
- Magnitude-mode 2D COSY using purge pulses before d1 (cosyppqf)
- Phase-sensitive 2D COSY (cosyph)
  - Magnitude-mode Long-Range optimized 2D COSY (cosylrqf)
  - Constant-Time 2D COSY (cosyjdqf)

**Phase-cycled and solvent suppression:**

- Magnitude-mode 2D COSY with presaturation (cosyprqf)
- Phase-sensitive 2D COSY with presaturation (cosyphpr | COSYPHPR)

**Gradient-based:**

- Magnitude-mode ge-2D COSY (cosygpqf | COSYGPSW)
- Magnitude-mode ge-2D COSY using purge pulses before d1 (cosygpqppqf)
- Phase-sensitive ge-2D COSY using echo-antiecho (cosyetgp)

**Miscellaneous:**

- Phase-sensitive w1-region-selective 2D COSY (scosyph)
- Phase-sensitive w1-region-selective 2D COSY with refocusing (scosyphrd)

- Phase-sensitive 2D COSY with off-resonance single or multiple presaturation (cosycwphps | COSYCWHPS)
  - Magnitude-mode 2D 13C-13C COSY (cosydcqf)
  - Magnitude-mode long-range optimized 2D 13C-13C COSY (cosydcrlrqf)
  - Phase-sensitive 2D 13C-13C COSY (cosydcph)
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2D COSY-DQF EXPERIMENTS
• **Phase-cycled:**
  - Magnitude-mode 2D COSY with DQF (cosydfqf)
  - Magnitude-mode 2D COSY with TQF (cosyqttf)
  - Phase-sensitive 2D COSY with DQF (cosydfph | COSYDQFPHSW)
  - Phase-sensitive 2D COSY with TQF (cosyphqtf)
  - Phase sensitive 2D E.COSY - KcMAX=3 (ecos3nph)
  - Complementary Phase sensitive 2D E.COSY - KcMAX=3 (ecos3cph)

• **Phase-cycled and solvent suppression:**
  - Phase-sensitive 2D COSY with DQF & presaturation (cosydfphpr)

• **Gradient-based:**
  - Magnitude-mode ge-2D COSY with multiple-quantum filter (cosygpmfqf | COSYGPMFSW)
  - Phase-sensitive ge-2D COSY with multiple-quantum filter (cosygpmfph | COSYGPDFPHSW)
  - Phase-sensitive ge-2D COSY with DQF using echo-antiecho (cosydfetgp.1)
  - Phase-sensitive ge-2D COSY with gradient-based DQF using echo-antiecho (cosydfetgp.2)
  - Gradient E.COSY (ecosygpph)

• **Gradient-based and solvent suppression:**
  - Phase-sensitive 2D COSY-DQF with WATERGATE using 3-9-19 (cosydfgpph19)
  - Phase-sensitive 2D COSY-DQF with Excitation Sculpting using 180 water-selective pulse (ES element) (cosydfeesgpph)
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2D SECSY EXPERIMENTS
Magnitude-mode 2D SECSY (secsyqf)
Magnitude-mode long-range optimized 2D SECSY (secsylrfqf)
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2D RELAYED EXPERIMENTS
Magnitude-mode one-step 2D RELAY (cosyqfrl)
Magnitude-mode one-step 2D RELAY with incremented mixing times (cosyimqfrl)
Magnitude-mode two-step 2D RELAY (cosyqfr2)
Magnitude-mode two-step 2D RELAY with incremented mixing times (cosyimqfr2)
Magnitude-mode three-step 2D RELAY (cosyqfr3)
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2D TOCSY EXPERIMENTS
Phase-cycled

Phase-sensitive 2D TOCSY using MLEV (mlevph | MLEVPHSW)
Phase-sensitive 2D TOCSY using MLEV with purge pulses before d1 (mlevphpp)
Phase-sensitive 2D TOCSY using DIPSI-2 (dipsi2ph)

Phase-cycled and solvent suppression

Phase-sensitive 2D TOCSY with presaturation using MLEV (mlevphpr | MLEVPHPR )
Phase-sensitive 2D TOCSY with presaturation using MLEV only using first trim pulse (mlevphpr.2 | H2OSUPMLEV)
Phase-sensitive 2D TOCSY with presaturation using DIPSI-2 (dipsi2phpr)
Phase-sensitive 2D Clean-TOCSY with presaturation using MLEV (clmlevphpr)

Gradient-based

Phase-sensitive ge-2D TOCSY with MLEV using echo-antiecho (mlevetgp)
Phase-sensitive ge-2D TOCSY with DIPSI-2 using echo-antiecho (dipsi2etgp)
Phase-sensitive ge-2D TOCSY with DIPSI-2 using PEP (dipsi2etgpsi)

Gradient-based and solvent suppression

Phase-sensitive 2D TOCSY with WATERGATE (3-9-19) using MLEV (mlevgpph19 | MLEVGP19HGW)
Phase-sensitive 2D TOCSY with WATERGATE (3-9-19) using DIPSI-2 (dipsi2gpph19)
Phase-sensitive sensitivity-improved 2D TOCSY with WATERGATE (3-9-19) and using DIPSI-2 (dipsi2etgpsi19)
Phase-sensitive 2D Adiabatic TOCSY with WATERGATE (3-9-19) using X_M16 sequence (atocsygpph19)

Phase-sensitive 2D TOCSY with excitation sculpting (W5) using MLEV (mlevgpphw5)
Phase-sensitive 2D TOCSY with excitation sculpting (180 water-selective pulse-ES element) using MLEV (mlevesgpph)
Phase-sensitive 2D TOCSY with excitation sculpting (180 water-selective pulse-ES element) using DIPSI-2 (dipsi2esgpph)

Related Experiments:

- LC-NMR Experiments
mlevetgp

I  d1  d0  d9
Gz

MLEV-17
p6
pl10

G1
G2

dipsi2etgp

I  d1  d0  d9
Gz

DIPSI-2 (y)
p6
pl10

G1
G2

G21 < rec

dipsi2etgpsi

I  d1  d0  d9
Gz

DIPSI-2 (y)
p6
pl10

G1
G2

G21 < rec

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2D ROESY EXPERIMENTS
Phase-cycled:

- Phase-sensitive 2D ROESY (roesyph | ROESYPHSW)
- Phase-sensitive 2D ROESY using purgue pulses before d1 (roesyphpp)
- Phase-sensitive 2D T-ROESY (roesyph.2)
- Phase-sensitive 2D T-ROESY using purgue pulses before d1 (roesyphpp.2)
- Phase-sensitive 2D ROESY with compensation (croesyph)
- Phase-sensitive off-resonance 2D ROESY (troesyph)

Phase-cycled and solvent suppression:

- Phase-sensitive 2D ROESY with presaturation (roesyphpr | ROESYPHPR)
- Phase-sensitive 2D T-ROESY with presaturation (roesyphpr.2)
- Phase-sensitive 2D ROESY with compensation and presaturation (croesyphpr)
- Phase-sensitive off-resonance 2D ROESY with presaturation (trosesyphpr)

Gradient-based:

- Phase-sensitive ge-2D ROESY using echo-antiecho (roesyetgp)
- Phase-sensitive ge-2D ROESY with T-ROESY using echo-antiecho (roesyetgp.2)

Gradient-based and solvent suppression:

- Phase-sensitive 2D ROESY with WATERGATE using 3-9-19 (roesygpph19)
- Phase-sensitive 2D T-ROESY with WATERGATE using 3-9-19 (roesygpph19.2)
- Phase-sensitive 2D ROESY with excitation sculpting using 180 water-selective pulse (ES element) (roesyesgpph)

Related Experiments:

- Selective 1D ROESY Experiments
- 2D NOESY Experiments
- 2D HSQC-ROESY Experiments
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2D NOESY EXPERIMENTS
2D NOESY Experiments

1D Version:

1D NOESY with presaturation (noesypr1d)
1D NOESY with presaturation and spoil gradients (noesygppr1d)

Phase-cycled:

Phase-sensitive 2D NOESY (noesyph | NOESYPH|SW)
Phase-sensitive 2D NOESY using purge pulses before d1 (noesyphpp)
Phase-sensitive 2D NOESY using random mixing time (noesyphrv)

Phase-cycled and solvent suppression:

Phase-sensitive 2D NOESY with presaturation (noesyphpr | H2OSUPNOESY)
Phase-sensitive 2D NOESY with presaturation using random mixing time (noesyphprrv)
Phase-sensitive 2D NOESY with 1-1 solvent suppression (noesyph11)

Gradient-based:

Phase-sensitive ge-2D NOESY (noesygph)
Phase-sensitive ge-2D NOESY using purge pulses before d1 (noesygpphpp)
Phase-sensitive ge-2D NOESY with z-spoil (noesygphzs)
Phase-sensitive ge-2D NOESY using echo-antiecho (noesyetgp)

Gradient-based and solvent suppression:

Phase-sensitive 2D NOESY using jump-and-return and optional $^{13}$C and $^{15}$N decoupling during acquisition (noesygpphjrrs)

Phase-sensitive 2D NOESY with WATERGATE: Using
3-9-19 (noesygpph19 | NOESYGPPH19SW) Using
water flip-back and 3-9-19 (noesyfpgpph19)
Using water flip-back and water-selective 90 pulses (noesyfpgpphmg)
Using water flip-back, 3-9-19 and PFG in t$_1$ (noesyfpgpphrs19)
Using water flip-back, water-selective 90 pulses and PFG in t$_1$ (noesyfpgpphrswg)

Phase-sensitive 2D NOESY with excitation sculpting:
Using W5 (noesygpph5)
Using 180 water-selective pulse (ES element) (noesyesgpph)

Related experiment:

Phase-sensitive 2D NOESY with RELAY and DQF (NOESY-RELAY experiment) (noesydfphr1)

Related experiments:

- Selective 1D NOESY
- 2D ROESY Experiments
- 2D HSQC-NOESY & 2D HMOC-NOESY
- 3D NOESY-HSQC & 2D HSQC-NOESY-HSQC
- 2D & 3D X-filtered NOESY experiments
noesypr1d

$^1\text{H}$

$\text{d}_1$ || $\text{d}_8$

presat || presat

$\text{p}_1\text{v}$

Gz

noesygppr1d

presat

$\text{p}_1\text{v}$

$G_z$

G1 || G2

NOE

H

H

xy

$\text{d}_1$

$\text{d}_0$

$\text{d}_8$

$\text{p}_1\text{v}$

$\text{p}_1\text{v}$

noesyph

noesyphrv

H

$\text{d}_1$

$\text{d}_0$

$\text{d}_8$

noesyphpp

H

xy

$\text{d}_1$

$\text{d}_0$

$\text{d}_8$

$\text{p}_1\text{v}$

$\text{p}_1\text{v}$

noesyphpr

noesyphrrv

H

$\text{d}_1$

$\text{d}_0$

$\text{d}_8$

noesyph11

H

$\text{d}_1$

$\text{d}_0$

$\text{d}_8$

$\text{d}_{19}$

noesydfphrl

H

$\text{d}_1$

$\text{d}_0$

$\text{d}_8$

$\text{d}_4$

$\text{d}_4$
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1D & 2D DOUBLE-QUANTUM EXPERIMENTS
• **1D Double-Quantum (DQ)**
  
  1D Double-Quantum experiments (dqs1d)  
  1D Multiple Quantum Filter (mqsgp1d | mqsgp1d2)

• **2D Phase-cycled Double-Quantum (DQ)**
  
  Magnitude-mode 2D Double-Quantum (DQ) (dqsqf)  
  Phase-sensitive Double-Quantum (DQ)(dqsph)  
  Phase-sensitive 2D Double-Quantum (DQ) with presaturation (dqsphpr)

• **2D Gradient-based Double-Quantum (DQ)**
  
  Phase-sensitive ge-2D Double-quantum using echo-antiecho, 45/135 degree conversion pulse for better sensitivity and remote peak minimisation (dqseagp135)  
  Phase-sensitive ge-2D Double-quantum using echo-antiecho (dqseagp90)

Related Experiments:

  o 1D & 2D INADEQUATE
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2D J-RESOLVED EXPERIMENTS
• **Classical:**
  
  Magnitude-mode 2D J-Resolved (jresqf)
  Magnitude-mode 2D J-Resolved with f2 decoupling (jresdcqf)

• **With solvent suppression:**
  
  2D J-Resolved with presaturation (lcjresprqf)
  2D J-Resolved with presaturation using shape pulse (lcjrespsqf)

Also see:

LC-NMR Experiments
DECOUPLER PULSE CALIBRATION
Calibration of the 90 decoupler pulse (decp90, decp90f3)
Calibration of the 90 decoupler shaped pulse (decp90sp)

Calibration of the 180 decoupler pulse (dec180)
Calibration of the shaped 180 decoupler pulse (dec180sp)
Calibration of the 180 decoupler pulse using presaturation (dec180pr, dec180f3pr)
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1D DEPT & INEPT EXPERIMENTS
• **DEPT Experiments:**

  - DEPT (dept)
  - DEPT-45 (dept45 | C13DEPT45)
  - DEPT-90 (dept90 | C13DEPT90)
  - DEPT-135 (dept135 | C13DEPT135)
  - DEPT-45 with adiabatic pulses (deptsp45 / deptsp)
  - DEPT-90 with adiabatic pulses (deptsp90)
  - DEPT-135 with adiabatic pulses (deptsp135)
  - DEPT with composite pulses (deptcp)
  - DEPT-45 with composite pulses (deptcp45)
  - DEPT-90 with composite pulses (deptcp90)
  - DEPT-135 with composite pulses (deptcp135)

  - DEPT without $^1$H-decoupling (deptnd)
  - DEPT++ without $^1$H-decoupling (deptppnd)

• **INEPT Experiments:**

  - INEPT without refocusing (ineptnd)
  - Refocused INEPT with decoupling (ineptrd)
  - Refocused INEPT with decoupling using adiabatic pulses (ineptrdsp)
  - INEPT+ without decoupling (ineptpnd)

  - Non-refocused $^1$H-coupled $^{15}$N spectrum using INEPT (ineptnd)
  - $^1$H-decoupled $^{15}$N spectrum using INEPT (ineptrd | N15INEPT)
  - Refocused $^1$H-coupled $^{15}$N spectrum using INEPT+ (ineptpnd)

  - 1D X-relayed H,X-COSY (ineptrl1 / ineptrl2)

• **Other editing experiments:**

  - Spin-Echo or SEFT (jmod)
  - Conventional APT (apt | C13APT)
  - APT with J-compensation (aptjc)

  - Quaternary-carbons with decoupling (quatd)
  - Quaternary-carbons without decoupling (quat)
ineptrl1

I d1 d21 d21 d3 CPD
    pl12

S d4 d4

ineptrl2

I d1 d21 d21 d3 CPD CPD
    pl12 pl12

S d4 d4 d2
DEPT-90
only CH

DEPT-135
CH + CH3
CH2

160 140 120 100 80  60  40 ppm

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2D X-DETECTED HETCOR
EXPERIMENTS
• INEPT-Based HETCOR
  o Magnitude-mode 2D HETCOR (hxcoqf | hccosw)
  o Magnitude-mode 2D HETCOR with 2H-decoupling (hxcoqf2h)
  o Magnitude-mode 2D HETCOR using composite pulses (hxcoqcqf)
  o Magnitude-mode 2D HETCOR with $^1$H-$^1$H decoupling in F1 using BIRD (hxcobiqf)
  o Magnitude-mode 2D HETCOR with $^1$H-$^1$H decoupling in F1 using BIRD and composite pulses (hxcobicpqf)
  o Magnitude-mode 2D HETCOR with refocusing of chemical shifts (hxinepqf)
  o Phase-sensitive 2D HETCOR with refocusing of chemical shifts (hxinepph)

• DEPT-based HETCOR
  o Magnitude-mode DEPT-based 2D HETCOR (hxdeptqf)
  o Phase-sensitive DEPT-based 2D HETCOR (hxdeptph)
  o Magnitude-mode DEPT-based 2D HETCOR with $^1$H-$^1$H decoupling in F1 using BIRD (hxdeptbqf)
  o Phase-sensitive DEPT-based 2D HETCOR with $^1$H-$^1$H decoupling in F1 using BIRD (hxdeptbpqf)
  o Phase-sensitive DEPT-based TOCSY-HETCOR experiment (hxdeptmlph)

• 2D H-relayed HETCOR experiment
  o Magnitude-mode 2D H-relayed HETCOR (hhxcoqf / hhxcoqf.2)

• 2D X-relayed HETCOR experiment
  o Magnitude-mode 2D X-relayed HETCOR (hxxcoqf)

Related Experiments:

• 2D HMQC
• 2D HSQC
**Pulse Program Catalogue**

NMRGuide 4.1 - Topspin 2.0

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**Pulse Programs**

- **hxdeptph**
  - Hxdeptph
  - Hxdeptqf

- **hxdeptbiph**
  - Hxdeptbiph
  - Hxdeptbiqf

- **hxdeptmlph**
  - Hxdeptmlph

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2D COLOC EXPERIMENT
• Magnitude-mode 2D COLOC (colocqf | HCCOLOCSW)

Related Experiments:

• 2D HETCOR
• 2D HMBC
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2D HETERONUCLEAR
J-RESOLVED EXPERIMENT
Magnitude-mode 2D Heteronuclear J-Resolved (hjresqf)
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2D HOESY EXPERIMENTS
Magnitude-mode 2D $^1$H-$^{13}$C HOESY (hoesyqfrv)
Phase-sensitive 2D $^1$H-X HOESY (hoesyph)

Also see 19F experiments
(hoesyfhqfqnrv)
• **1D INADEQUATE**

  1D INADEQUATE without refocusing (inad1d)
  1D INADEQUATE using composite pulses (inadcp1d)
  1D INADEQUATE with refocusing (inadr1d)
  1D INADEQUATE using initial INEPT (inepin)

• **2D INADEQUATE**

  Magnitude-mode 2D INADEQUATE (inadqf, inadqf.2 | INAD)
  Phase sensitive 2D INADEQUATE (inadph)
  Magnitude-mode symmetric 2D INADEQUATE (inadqfsy)

Also see 1D & 2D DQ Experiments
inad1d

\[ ^1H \quad \text{CPD} \quad \text{pL12} \]
\[ ^{13}C \quad \text{d1} \quad \text{d4} \quad \text{d4} \]

inadrd1d

\[ ^1H \quad \text{CPD} \quad \text{pL12} \]
\[ ^{13}C \quad \text{d1} \quad \text{d4} \quad \text{d4} \quad \text{d4} \quad \text{d4} \]

inadcp1d

\[ ^1H \quad \text{CPD} \quad \text{pL12} \]
\[ ^{13}C \quad \text{d1} \quad \text{d4} \quad \text{d4} \quad \text{d4} \]

inepin

\[ ^1H \quad \text{CPD} \quad \text{pL12} \]
\[ ^1J_{CH} \]
\[ ^1J_{CC} \]

Also see ineptr1l
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1D INVERSE EXPERIMENTS
• **Phase-Cycled:**

  1D inverse DEPT with refocusing and no decoupling (ideptnd)
  1D inverse INEPT without refocusing and without decoupling (iineptnd)
  1D inverse INEPT with refocusing and decoupling (iineptrd)

  1D HMQC with refocusing but not decoupling (hmqcndrd1d | HMQC1D)
  1D HMQC without refocusing and without decoupling (inv3nd1d/ hmqcn1d)
  1D HMQC with refocusing and decoupling (hmqcrd1d)
  1D HMQC using BIRD without refocusing and without decoupling (hmqcbind1d)
  1D HMQC using BIRD with refocusing and without decoupling (hmqcbindrd1d)
  1D HMQC using BIRD with refocusing and decoupling (hmqcbird1d)

  1D DEPT-HMQC with refocusing and decoupling (indecord1d)
  1D DEPT-HMQC using BIRD with refocusing and decoupling (indecobird1d)

• **Gradient-based:**

  ge-1D HMQC with refocusing but not decoupling (hmqcgpnd1d)
  ge-1D HSQC with refocusing and no decoupling (hsqcgpnd1d)

Any 2D or 3D pulse sequence can be used for 1D acquisition (mc commands)
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2D HMQC EXPERIMENTS
Phase-cycled:

Magnitude-mode 2D HMQC (hmqcfqf | HMQC)
Magnitude-mode 2D HMQC without decoupling (hmqcndqf)
Magnitude-mode 2D HMQC using BIRD (hmqcbiqf | HMQCBI)
Magnitude-mode 2D HMQC using BIRD without decoupling (hmqcbindqf)
Phase-sensitive 2D HMQC (hmqcpm | HMQCPh)
Phase-sensitive 2D HMQC without decoupling (hmqcpmdqf)
Phase-sensitive 2D HMQC using BIRD (hmqcbipm | HMQCBIPM)
Phase-sensitive 2D HMQC using BIRD without decoupling (hmqcbindpm)

Phase-cycled and solvent suppression

From f2 channel:
Phase-sensitive 2D HMQC with presaturation (hmqcpmpfr | HMQCPHPR)
Phase-sensitive 2D HMQC using BIRD and presaturation (hmqcbipmpfr)
Phase-sensitive 2D HMQC with 1-1 water suppression (hmqcpmp11)

From f3 channel:
Phase-sensitive 2D \textsuperscript{1}H-\textsuperscript{15}N HMQC (hmqcf3pm)
Phase-sensitive 2D \textsuperscript{1}H-\textsuperscript{15}N HMQC using presaturation (hmqcf3pmfr)
Phase-sensitive 2D \textsuperscript{1}H-\textsuperscript{15}N HMQC using BIRD (hmqcbif3pm)
Phase-sensitive 2D \textsuperscript{1}H-\textsuperscript{15}N HMQC using decoupling in a third f2 channel (hmqcf3pm)

Gradient-based:

From f2 channel:
Magnitude-mode ge-2D HMQC (hmqcgpqf | HMQCGP)
Phase-sensitive ge-2D HMQC using z-filter (hmqcgpph)
Phase-sensitive ge-2D HMQC using echo-antiecho (hmqchetgp)
Phase-sensitive ge-2D HMQC using echo-antiecho with adiabatic refocusing (hmqchetgp.2)
Phase-sensitive ge-2D HMQC using PEP (hmqchetgpsi)
Phase-sensitive ge-2D HMQC using PEP and shorter overall timing (hmqchetgpsi.2)

From f3 channel:
Phase-sensitive ge-2D \textsuperscript{1}H-\textsuperscript{15}N HMQC using echo-antiecho (hmqcf3gpm)
Phase-sensitive ge-2D \textsuperscript{1}H-\textsuperscript{15}N HMQC using PEP (hmqcf3gpsi)
Phase-sensitive ge-2D \textsuperscript{1}H-\textsuperscript{15}N HMQC using PEP and shorter overall timing (hmqcf3gpsi.2)

Gradient-based and solvent suppression

Phase-sensitive ge-2D \textsuperscript{1}H-\textsuperscript{15}N HMQC using WATERGATE (3-9-19) (hmqcf3gpph19)
hmqcetgpsi

\[ ^1H \quad d_1 \quad d_2 \quad <l \quad <\text{lrec} \quad y \quad d_2 \quad d_2 \quad d_2 \quad 8 \quad 8 \quad 8 \quad 8 \quad <\text{lrec} \]

\[ ^1^3C \quad d_0 \quad d_0 \quad 8 \quad 8 \quad 8 \quad 8 \quad <\text{lrec} \quad y \quad <\text{GARP} \quad \text{pl12} \]

\[ ^1^5N \quad \text{optional} \quad \text{sp}3 \quad \text{sp}3 \quad \text{Gz} \quad \text{G2} \]

Gz

G1 G1

G2

hmqcetgpsi.2

\[ ^1H \quad d_1 \quad d_4 \quad d_4 \quad <l \quad <\text{lrec} \quad y \quad d_4 \quad d_4 \quad d_4 \quad d_4 \quad 8 \quad 8 \quad 8 \quad 8 \quad <\text{lrec} \]

\[ ^1^3C \quad d_0 \quad d_0 \quad 8 \quad 8 \quad 8 \quad 8 \quad <\text{lrec} \quad y \quad <\text{GARP} \quad \text{pl12} \]

\[ ^1^5N \quad \text{optional} \quad \text{sp}3 \quad \text{sp}3 \quad \text{Gz} \quad \text{G2} \]

Gz

G1 G1

G2
2D DEPT-HMQC EXPERIMENTS
Phase-sensitive 2D DEPT-HMQC (indecoph)
Phase-sensitive 2D DEPT-HMQC using BIRD (indecobiph)
Phase-sensitive 2D DEPT-HMQC-TOCSY using BIRD (indecobimlph)
Pulse Program Catalogue
NMRGuide 4.1 - Topspin 2.0

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2D HSQC EXPERIMENTS
FROM F2 CHANNEL

• **Phase-cycled:**

  - Phase-sensitive 2D HSQC (hsqcph)

• **Phase-cycled and solvent suppression:**

  - Phase-sensitive 2D HSQC with presaturation (hsqcphpr)
  - Phase-sensitive 2D HSQC with off-resonance presaturation (hsqcphps)

• **Gradient-based:**

  - Phase-sensitive ge-2D HSQC using z-filter and selection before t1 (hsqcgp | HSOCGP)
  - Phase-sensitive ge-2D HSQC using z-filter and selection after t1 (hsqcgp2)
  - Phase-sensitive ge-2D HSQC using echo-antiecho (hsqctgp | HSQCETGP)
  - Phase-sensitive ge-2D HSQC using echo-antiecho and adiabatic pulses for inversion (hsqctgpsh)
  - Phase-sensitive ge-2D HSQC using echo-antiecho and adiabatic pulses for inversion and refocusing (hsqctgpsh2)
  - Phase-sensitive ge-2D HSQC using PEP (hsqcetgpsi)
  - Phase-sensitive ge-2D HSQC using PEP with gradients in back-inent (hsqcetgpsi2)
  - Phase-sensitive ge-2D HSQC using PEP and adiabatic pulses for inversion (hsqcetgpsisp | HSQCETGPSISP)
  - Phase-sensitive ge-2D HSQC using PEP and adiabatic pulses for inversion with gradients in back-inent (hsqcetgpsisp2)
  - Phase-sensitive ge-2D HSQC using PEP and adiabatic pulses for inversion and refocusing (hsqcetgpsisp2 | HSQCETGPSISP.2)
  - ge-2D 'H-X HSQC experiment with X-Y-decoupling during acquisition and with selective Cb/C=O decoupling. (hsqcdhetgpsh)
FROM F3 CHANNEL

• Phase-cycled:

  Phase-sensitive 2D $^1$H-$^{15}$N HSQC (hsqc3f3ph)

• Phase-cycled and solvent suppression:

  Phase-sensitive 2D $^1$H-$^{15}$N HSQC using presaturation (hsqc3f3phpr)

• Gradient-based:

  Phase-sensitive ge-2D $^1$H-$^{15}$N HSQC using echo-antiecho (hsqcetf3gp | HSQCETF3GP)
  Phase-sensitive ge-2D $^1$H-$^{15}$N HSQC using PEP (hsqcetf3gpsi | HSQCETF3GPSI)
  Phase-sensitive ge-2D $^1$H-$^{15}$N HSQC using PEP with gradients in back-inept (hsqcetf3gpsi2)
  Phase-sensitive ge-2D $^1$H-$^{15}$N HSQC using XY16-CPMG(hsqcetf3gpxy, hsqcetf3gpxy.2)

• Gradient-based and solvent suppression

  Phase-sensitive ge-2D $^1$H-$^{15}$N HSQC using water flip-back and echo-antiecho (hsqcetfpf3gp | HSQCETFP3GP)
  Phase-sensitive ge-2D $^1$H-$^{15}$N HSQC using water flip-back and PEP (hsqcetfpf3gpsi | HSQCETFP3GPSI)
  Phase-sensitive ge-2D $^1$H-$^{15}$N HSQC using water flip-back and PEP with gradients in back-inept (hsqcetfpf3gpsi2)
  Phase-sensitive ge-2D $^1$H-$^{15}$N HSQC using WATERGATE (3-9-19) (hsqc3gpph19)
  Fast-HSQC, Phase-sensitive ge-2D $^1$H-$^{15}$N HSQC using WATERGATE (3-9-19) (hsqc3gpph | FHSQC3GPPH)
  Phase-sensitive ge-2D $^1$H-$^{15}$N HSQC using water flip-back and WATERGATE (selective pulse) (hsqcetfpf3gpphwg | HSQCETFP3GPPHWG)
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hsqcetgp

\[ ^1H \quad d_1 \quad d_4 \quad d_4 \quad p_{2\phi} \quad d_4 \quad d_4 \quad \rightarrow \\
^1C \quad \rightarrow \quad d_0 \quad d_0 \quad \left(\text{GARP} \quad p_{112}\right) \]

\[ ^1N \quad \text{optional} \quad \quad \quad \quad \quad \quad \quad \quad \quad \]

\[ G_1 \quad G_2 \]

hsqcetgosp

\[ ^1H \quad d_1 \quad d_4 \quad d_4 \quad p_{2\phi} \quad d_4 \quad d_4 \quad \rightarrow \\
^1C \quad \rightarrow \quad d_0 \quad d_0 \quad \left(\text{GARP} \quad p_{112}\right) \]

\[ ^1N \quad \text{optional} \quad \quad \quad \quad \quad \quad \quad \quad \quad \]

\[ G_1 \quad G_2 \]

hsqcetgosp.2

\[ ^1H \quad d_1 \quad d_4 \quad d_4 \quad p_{2\phi} \quad d_4 \quad d_4 \quad \rightarrow \\
^1C \quad \rightarrow \quad d_0 \quad d_0 \quad \left(\text{GARP} \quad p_{112}\right) \]

\[ ^1N \quad \text{optional} \quad \quad \quad \quad \quad \quad \quad \quad \quad \]

\[ G_1 \quad G_2 \]
hsqcetf3gp

^{1}H  d_{1}  d_{26}  d_{26}  p_{26}  d_{26}  d_{26}  
^{15}N  
^{13}C  optional  
G_{x}  p_{14}  sp_{3}  
G_{1}  G_{2}  G_{3}  

^{1}J_{NH}  

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hsqcetf3gpsi

$^1H$ \(d_1\) \(d_{26}\) \(d_{26}\) \(p_{28}\) \(d_{24}\) \(d_{24}\) \(d_{26}\) \(d_{26}\) $<\text{rec}$

$^1H$ $^1N$ $^3C$

$G_1$ $G_2$ $G_3$

optional

GARP

hsqcetf3gpsi2

$^1H$ \(d_1\) \(d_{26}\) \(d_{26}\) \(p_{28}\) \(d_{24}\) \(d_{24}\) \(d_{26}\) \(d_{26}\) $<\text{rec}$

$^1H$ $^1N$ $^3C$

$G_1$ $G_2$ $G_4$ $G_4$ $G_5$ $G_5$ $G_3$

optional

GARP

$^1H-15N$ HSQC列表outlying line
in doubly-labeled proteins

zgopns -DLABEL_CN in eda
hsqcetf3gpxy

$^1$H  $^1$N  $^{13}$C

$^1$H  $^1$N  $^{13}$C

G$_x$

hsqcetf3gpxy.2

$^1$H  $^1$N  $^{13}$C

$^1$H  $^1$N  $^{13}$C

G$_x$
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2D MULTIPLICITY-EDITED
HSQC EXPERIMENTS
Gradient-enhanced form \( f_2 \) channel

- Phase-sensitive ge-2D multiplicity-edited HSQC using \( z \)-filter (hsqcedgpph | HSQCEDGPPH)
- Phase-sensitive ge-2D multiplicity-edited HSQC using echo-antiecho and adiabatic pulses (hsqcedetgp)
- Phase-sensitive ge-2D multiplicity-edited HSQC using echo-antiecho and adiabatic pulses with gradients (hsqcedetgpsp)
- Phase-sensitive ge-2D multiplicity-edited HSQC using echo-antiecho and inversion and matched sweep adiabatic pulses (hsqcedetgpsi.3)
- Phase-sensitive ge-2D multiplicity-edited HSQC using PEP and adiabatic inversion pulses (hsqcedetgpsisp)
- Phase-sensitive ge-2D multiplicity-edited HSQC using PEP and adiabatic inversion and refocusing pulses (hsqcedetgpsisp2)
- Phase-sensitive ge-2D multiplicity-edited HSQC using PEP and adiabatic inversion pulses with gradients in back-inept (hsqcedetgpsisp2)
- Phase-sensitive ge-2D multiplicity-edited HSQC using PEP and adiabatic inversion and refocusing pulses with gradients in back-inept (hsqcedetgpsisp2.2)
- Phase-sensitive ge-2D multiplicity-edited HSQC using PEP and inversion, refocusing and matched sweep adiabatic pulses with gradients in back-inept (hsqcedetgpsisp2.3)

Gradient-enhanced form \( f_3 \) channel

- Phase-sensitive ge-2D \(^1\text{H} \cdot ^{15}\text{N}\) HSQC-edited using PEP (hsqcedetf3gpsi)
- Phase-sensitive ge-2D \(^1\text{H} \cdot ^{15}\text{N}\) HSQC-edited using PEP with gradients in back-inept (hsqcedetf3gpsi2)
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2D CONSTANT-TIME HSQC AND HMQC EXPERIMENTS
2D Constant-time Correlations

Phase-sensitive Constant-time ge-2D HSQC

- Using adiabatic pulses (hsqcctetgsp)
- Using adiabatic pulses without CO refocusing (hsqcctetgsp.2)
- Using adiabatic pulses and PEP (hsqcctetgspisip)

Phase-sensitive Constant-time ge-2D HMQC

- Using adiabatic pulses (hmqcctetgp)
- For correlating CH2 groups (hsqcctetgp.2)

Also see hsqctetgpjc and hsqctetgpcjcl

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2D INVERSE-INEPT EXPERIMENT
Phase-sensitive ge-2D Inverse INEPT using echo-antiecho (xhcoetgp)
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2D SPIN-EDITED
HSQC EXPERIMENTS
One-bond $^1$H-$^{15}$N Couplings

- ge-2D $^1$H-$^{15}$N a,¢-HSQC (hsqcetf3gpss)
- ge-2D $^1$H-$^{15}$N HSQC-IPAP using watergate (hsqcf3gpiaphwg)
- ge-2D $^1$H-$^{15}$N HSQC-IPAP using watergate and sensitivity improvement (hsqcf3gpiaphsiwg)

One-bond $^1$H-$^{13}$C Couplings

- 2D H-1/C-13 CT-HSQC (hsqectetgpjc)
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2D TROSY EXPERIMENTS

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2D TROSY Experiments

From f2 channel:

Phase-sensitive ge-2D TROSY with presaturation (trosygpphp)
ge-2D TROSY for aromatic residues with WATERGATE (trosyargphwg)

From f3 channel:

Phase-sensitive ge-2D $^1$H-$^{15}$N TROSY

- Using echo-antiecho (trosyetf3gpsi | TROSYETF3GPSI)
- Using echo-antiecho and different phase cycling (trosyetf3gpsi2)
- Using echo-antiecho and different phase cycling to give IPAP TROSY (trosyetf3gpiasi)
- Using WATERGATE (3-9-19) (trosyf3gpph19 | TROSYF3GPPH19)
- Using WATERGATE and improved sensitivity (trosyf3gpphsi19 | TROSYF3GPPHSI19)

Phase-sensitive ge-2D $^1$H-$^{15}$N ZQ-TROSY using WATERGATE (trosyzqgpphgw)
trosyef3gpsi

$^1$H  d1  d26  d26  

$^1$N  d24  d24  d26  d26  8  8  <ll

$^1$C  optional

Gz  G1  G1  G2  G2  G3  G3  G4  G4  G5

2D HSQC  2D TROSY  2D half-TROSY
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2D CRINEPT EXPERIMENT
ge-2D \(^1\)H-\(^{15}\)N CRINEPT using flip-back (crineptgpph)
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2D HMQC-COSY EXPERIMENTS
2D HMQC-COSY Experiments

Phase cycled:

- Magnitude-mode 2D HMQC-COSY using BIRD (hmqcbindqfrl)
- Phase-sensitive 2D HMQC-COSY using BIRD with decoupling (hmqcbiphrl)
- Phase-sensitive 2D HMQC-COSY using BIRD without decoupling (hmqcbindphrl)
- Phase-sensitive 2D HMQC-COSY-DQF using BIRD (hmqcbidphrl)

Gradient-enhanced:

- Magnitude-mode ge-2D HMQC-COSY (hmqcgpqfrl)
- H2BC experiment with a three-low-pass filter (h2bcetgpl3)

Also see HMQC and HMQC-TOCSY experiments
hmqcbindqrl

hmqcbinthrl

hmqcbindphrl

- \( x \)

\( d_1 \)
\( d_2 \)
\( d_2 \)
\( d_7 \)
\( d_2 \)
\( d_2 \)
\( y \)

\( d_0 \)
\( d_0 \)

GARP

pl12

hmqcbiphrl

- \( x \)

\( d_1 \)
\( d_2 \)
\( d_2 \)
\( d_7 \)
\( d_2 \)
\( d_2 \)
\( y \)

\( d_0 \)
\( d_0 \)

GARP

pl12

hmqcbidpfrl

- \( x \)

\( d_1 \)
\( d_2 \)
\( d_2 \)
\( d_7 \)
\( d_2 \)
\( d_2 \)
\( y \)

\( d_0 \)
\( d_0 \)

GARP

pl12
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2D HMQC-TOCSY EXPERIMENTS
• **Phase-cycled:**
  
  Phase-sensitive 2D HMQCTOCSY (hmqcmlph)
  Phase-sensitive 2D HMQCTOCSY without decoupling (hmqcmldndph)
  Magnitude-mode 2D HMQCTOCSY using BIRD (hmqcbirmqf)
  Magnitude-mode 2D HMQCTOCSY using BIRD without decoupling (hmqcbirmqndqf)
  Phase-sensitive 2D HMQCTOCSY using BIRD (hmqcbirmqf)
  Phase-sensitive 2D HMQCTOCSY using BIRD without decoupling (hmqcbirmqndqf)

• **Phase-cycled and solvent suppression:**
  
  Phase-sensitive 2D HMQCTOCSY with presaturation (hmqcmphpr)
  Phase-sensitive 2D HMQCTOCSY with presaturation and without decoupling (hmqcmldphpr)

• **Gradient-enhanced from f2 channel:**
  
  Magnitude-mode ge-2D HMQCTOCSY with MLEV (hmqcgpmqf | HMQCPML)
  Phase-sensitive ge-2D HMQCTOCSY with DIPSI-2 using echo-antiecho (hmqcdietgp)
  Phase-sensitive ge-2D HMQCTOCSY with DIPSI-2 using PEP (hmqcdietgpsi)
  Phase-sensitive ge-2D HMQCTOCSY with DIPSI-2 using PEP using shorter overall timing (hmqcdietgpsi.2)

• **Gradient-enhanced from f3 channel:**
  
  Phase sensitive ge-2D ¹H-¹⁵N HMQCTOCSY with DIPSI-2 using echo-antiecho (hmqcdietf3gp)
  Phase sensitive ge-2D ¹H-¹⁵N HMQCTOCSY with DIPSI-2 using PEP (hmqcdietf3gpsi)
  Phase sensitive ge-2D ¹H-¹⁵N HMQCTOCSY with DIPSI-2 using PEP and shorter overall timing (hmqcdietf3gpsi.2)
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hmqcgpmlqf

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hmqcdietgp

\[ ^1\text{H} \quad \text{d1} \quad \text{d2} \quad \text{d2} \quad \text{d2} \quad \text{d9} \quad \text{DIPSI-2} \text{y} \quad \text{y} \quad \text{\textless lrec} \]

\[ ^{13}\text{C} \quad \text{d0} \quad \text{d0} \quad \text{8} \quad \text{8} \quad \text{8} \quad \text{p6} \quad \text{p110} \quad \text{GARP} \]

\[ ^{15}\text{N} \quad \text{optional} \quad \text{d2} \quad \text{d2} \quad \text{d2} \quad \text{d2} \quad \text{y} \quad \text{p6} \quad \text{p110} \quad \text{GARP} \]

\[ G_z \text{ optional} \quad \text{G1 G1} \quad \text{G2} \]

hmqcdietgpsi

\[ ^1\text{H} \quad \text{d1} \quad \text{d2} \quad \text{d2} \quad \text{d2} \quad \text{d2} \quad \text{d9} \quad \text{DIPSI-2} \text{y} \quad \text{y} \quad \text{\textless lrec} \]

\[ ^{13}\text{C} \quad \text{d0} \quad \text{d0} \quad \text{8} \quad \text{8} \quad \text{8} \quad \text{p6} \quad \text{p110} \quad \text{GARP} \]

\[ ^{15}\text{N} \quad \text{optional} \quad \text{d2} \quad \text{d2} \quad \text{d2} \quad \text{d2} \quad \text{y} \quad \text{p6} \quad \text{p110} \quad \text{GARP} \]

\[ G_z \quad \text{G1 G1} \quad \text{G2} \]

hmqcdietgpsi.2

\[ ^1\text{H} \quad \text{d1} \quad \text{d4} \quad \text{d4} \quad \text{d4} \quad \text{d4} \quad \text{d9} \quad \text{DIPSI-2} \text{y} \quad \text{y} \quad \text{\textless lrec} \]

\[ ^{13}\text{C} \quad \text{d0} \quad \text{d0} \quad \text{8} \quad \text{8} \quad \text{8} \quad \text{p6} \quad \text{p110} \quad \text{GARP} \]

\[ ^{15}\text{N} \quad \text{optional} \quad \text{d2} \quad \text{d2} \quad \text{d2} \quad \text{d2} \quad \text{y} \quad \text{p6} \quad \text{p110} \quad \text{GARP} \]

\[ G_z \quad \text{G1 G1} \quad \text{G2} \]
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2D HMQC-ROESY EXPERIMENTS
• Gradient-enhanced from the f2 channel

Phase-sensitive ge-2D HMQC-ROESY using echo-antiecho (hmqctgpro)
Phase-sensitive ge-2D HMQC-ROESY with T-ROESY using echo-antiecho (hmqctgpro.2)

• Gradient-enhanced from the f3 channel

Phase-sensitive ge-2D 1H-15N HMQC-ROESY using echo-antiecho (hmqctf3gpro)
Phase-sensitive ge-2D 1H-15N HMQC-ROESY with T-ROESY using echo-antiecho (hmqctf3gpro.2)
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hmqctf3gpro

hmqctf3gpro.2
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2D HMQC-NOESY EXPERIMENTS
• Phase cycled:

- Phase-sensitive 2D HMQC-NOESY with presaturation (hmqcnophpr)
- Phase-sensitive 2D HMQC-NOESY using BIRD (hmqcbinoph)

• Gradient-enhanced from the f2 channel:

- Phase-sensitive ge-2D HMQC-NOESY using echo-antiecho (hmqctgpno)

• Gradient-enhanced from the f3 channel:

- Phase-sensitive ge-2D $^1$H-$^1$N HMQC-NOESY using echo-antiecho (hmqctf3gpno)
hmqctgpn0

$^1$H  d1  d2  
$^3$C  
$^{15}$N  optional  sp3  
$G_z$

hmqctf3gpno

$^1$H  d1  d21  
$^{15}$N  
$^{13}$C  optional  
$G_z$

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2D HSQC-TOCSY EXPERIMENTS
Gradient-enhanced from the $f_2$ channel

Phase sensitive ge-2D HSQC-TOCSY with MLEV using z-filter (hsqcgpmlph | HSQCgpmlph)
Phase-sensitive ge-2D HSQC-TOCSY with MLEV using echo-antiecho (hsqcetgpml | HSQCETgpml)
Phase-sensitive ge-2D HSQC-TOCSY with DIPSI-2 using PEP (hsqcdietgpsisp)
Phase-sensitive ge-2D HSQC-TOCSY with PEP and adiabatic inversion pulses (hsqcdietgpsisp | HSQCDIETgpsisp)
Phase-sensitive ge-2D HSQC-TOCSY with DIPSI-2 using PEP and adiabatic inversion and refocusing pulses (hsqcdietgpsisp.2)

Gradient-enhanced with editing from the $f_2$ channel

Phase sensitive ge-2D HSQC-TOCSY using PEP with editing of multiplicity (hsqcdiedetgpsisp.1)
Phase sensitive ge-2D HSQC-TOCSY using PEP with editing of direct responses (hsqcdiedetgpsisp.2)
Phase sensitive ge-2D HSQC-TOCSY using PEP with editing of multiplicity and direct responses (hsqcdiedetgpsisp.3)

Gradient-enhanced from the $f_3$ channel

Phase sensitive ge-2D $^{1}H-^{15}N$ HSQC-TOCSY with MLEV using echo-antiecho (hsqctef3gpml)
Phase sensitive ge-2D $^{1}H-^{15}N$ HSQC-TOCSY with DIPSI-2 using PEP (hsqcdietf3gpsi | HSQCDIETf3gpsi)

Also see HSQC-TOCSY type experiments for $^{3}J_{CH}$ measurements
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2D HSQC-ROESY EXPERIMENTS
• **Gradient-enhanced from the \( f_2 \) channel**

  Phase-sensitive ge-2D HSQC-ROESY using echo-antiecho and adiabatic pulses
  (hsqcetgprosp | HSQCETGPROSP)
  Phase-sensitive ge-2D HSQC-ROESY using echo-antiecho and adiabatic pulses with T-ROESY(hsqcetgprosp.2)

• **Gradient-enhanced from the \( f_3 \) channel**

  Phase-sensitive ge-2D \(^1^H\)\(^{15}^N\) HSQC-ROESY using echo-antiecho (hsqcetf3gpro)
  Phase-sensitive ge-2D \(^1^H\)\(^{15}^N\) HSQC-ROESY with T-ROESY using echo-antiecho (hsqcetf3gpro.2)
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hsqctgprosp

\[ 1^H \quad d_1 \quad d_4 \quad d_4 \quad d_4 \quad p_{28} \quad d_4 \quad d_4 \quad p_{15} \quad p_{111} \quad \text{cw} \quad \angle \text{free} \]

\[ ^{13}C \quad \text{p}_{14} \quad \text{sp}^3 \quad \text{d}_0 \quad \text{d}_0 \]

\[ ^{15}N \quad \text{optional} \quad \text{p}_{14} \quad \text{sp}^3 \]

\[ G_x \]

G1

G2

hsqctgprosp.2

\[ 1^H \quad d_1 \quad d_4 \quad d_4 \quad d_4 \quad d_4 \quad d_4 \quad d_4 \quad d_4 \quad p_{28} \quad p_{25} \quad p_{127} \quad \text{cw} \quad \angle \text{free} \]

\[ ^{13}C \quad \text{p}_{14} \quad \text{sp}^3 \quad \text{d}_0 \quad \text{d}_0 \quad \text{t-rosy} \]

\[ ^{15}N \quad \text{optional} \quad \text{p}_{14} \quad \text{sp}^3 \]

\[ G_x \]

G1

G2

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2D HSQC-NOESY EXPERIMENTS
• Gradient-enhanced from the \( f_2 \) channel

Phase-sensitive ge-2D HSQC-NOESY using echo-antiecho and adiabatic pulses (hsqctgpnosp | HSQCETGPNOSP)

• Gradient-enhanced from the \( f_3 \) channel

Phase-sensitive ge-2D \(^1H-^{15}N\) HSQC-NOESY using echo-antiecho (hsqctf3gpno | HSQCETF3GPNO)
Phase-sensitive ge-2D \(^1H-^{15}N\) HSQC-NOESY using XY16 and WATERGATE (hsqcf3gpnowgxy)
hsqcetf3gpno

hsqcf3gpnowgxy
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2D HMBC EXPERIMENTS
Phase cycled:

Magnitude-mode 2D HMBC using low-pass J-filter (hmbclpndqf | HMBCLPND)
Magnitude-mode 2D HMBC with presaturation (hmbendprqf)
Magnitude-mode 2D HMBC with off-resonance presaturation (hmbcndpsqf)

Gradient-based:

Magnitude-mode ge-2D HMBC (hmbcgpndqf | HMCGBPND)
Magnitude-mode ge-2D HMBC using low-pass J-filter (hmbcgplpndqf | HMCGBGPLPND)
Magnitude-mode ge-2D HMBC using double low-pass J-filter (hmbcgpl2ndqf)

Magnitude-mode band-selective ge-2D HMBC without decoupling (shmbcgpndqf)

Magnitude-mode CIGAR-HMBC without decoupling (hmbcacgpndqf)
Magnitude-mode CIGAR-HMBC with decoupling (hmbcacgplpqf)
ge-2D 2J,3J HMBC, STAR-HMBC (hmbcacbigpl2ndqf)
ge-2D HSMC (hmscetgpnd)

Also see:

- Measurement of long-range proton-carbon coupling constants
- 2D COLOC Experiment
- ADEQUATE Experiments
3J_{CH} 2J_{CH}

hmbclpndqf

H d1 d2 ∅rec
X d6 d0 d0

hmbcnmdprqf

H d1 d6 ∅rec
presat p19
X d0 d0

hmbcnmdpsqf

H d1 d6 ∅rec
off-reson. presat p18 sp6
X d0 d0
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2D EXPERIMENTS TO MEASURE
LONG-RANGE PROTON-CARBON
COUPLING CONSTANTS
ge-2D HMBC-type experiments

Phase-sensitive ge-2D HMBC using echo-antiecho (hmbcetgpnnd)
Phase-sensitive ge-2D HMBC using a two-fold low-pass J-filter (hmbcetgpl2nd)
Phase-sensitive ge-2D CT-HMBC using echo-antiecho (hmbcctetgpnnd)

ge-2D J-HMBC using a two-fold low-pass J-filter (hmbcetgpjl2nd)

Long-range optimized ge-2D HSQC

Phase-sensitive ge-2D long-range optimized HSQC (HSQMBC) (hsqcetgplrsp)
Phase-sensitive ge-2D long-range optimized HSQC using G-BIRD (GBIRD-HSQMBC) (hsqcetgpjlrd)
ge-2D long-range optimized J-HSQC (EXSIDE) (hsqcetgpljcsip)

ge-2D HSQC-TOCSY type experiments

ge-2D w1-filtered TOCSY using DIPSI-2 (HETLOC) (dipsi2etgpjcsix1)
Phase-sensitive ge-2D HSQC-HECADE (hsqcietgpjcsisp)

Also see 2D HMBC and 2D HSQC-TOCSY experiments

HSQC-TOCSY

HMBC

Others: HMQC-TOCSY, HECADE, HETLOC
Two steps: \(^{1}J_{CH} + {J_{HH}}\)
Only for protonated carbons
In-phase Magnetization

Others: HSQMBC, EXSIDE, J-HMBC
A single step: \(^{2}J_{CH}\)
For all carbons
Anti-phase Magnetization
J-scaling factor of N

\[ N^* nJ(HA-CB) \]

hmbcetgpjcl2nd

\[ ^1H \quad d1 \quad d6/2-d0 \]

\[ X \]

\[ G_j \]

\[ G3 \quad G4 \quad G5 \]

\[ p14 \quad sp3 \]

\[ p24 \quad sp7 \]

\[ G1 \quad G1 \]

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J-scaling factor of N

\[ N \times nJ(\text{HA-CB}) \]

hsqcetgplrcsp

<table>
<thead>
<tr>
<th></th>
<th>( ^1H )</th>
<th>( ^13C )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 135^\circ )</td>
<td>d1</td>
<td>p12 sp3</td>
</tr>
<tr>
<td>( 45^\circ )</td>
<td>d2</td>
<td>p14 sp3</td>
</tr>
<tr>
<td>0</td>
<td>d6/4+ n*d0</td>
<td>p14 sp3</td>
</tr>
<tr>
<td>d6/4+ n*d0</td>
<td>d6/4+ n*d0</td>
<td>p14 sp3</td>
</tr>
<tr>
<td>d6/4+ n*d0</td>
<td>0</td>
<td>p14 sp3</td>
</tr>
<tr>
<td>d6/4+ n*d0</td>
<td>d6/4</td>
<td>p14 sp3</td>
</tr>
<tr>
<td>d6/4</td>
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<td>p14 sp3</td>
</tr>
<tr>
<td>d6/4</td>
<td>d6/4</td>
<td>p14 sp3</td>
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<td>d6/4</td>
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<td>p14 sp3</td>
</tr>
<tr>
<td>d6/4</td>
<td>d6/4</td>
<td>p14 sp3</td>
</tr>
</tbody>
</table>

\( \phi_{\text{rec}} \)

GARP

\[ \text{pp1144, sp3} \]

\[ \text{pp1122, sp2} \]

\[ \text{pp2244, sp7} \]

\[ \text{pp1122, sp2} \]

\[ \text{pp1144, sp3} \]

\[ \text{pp1122, sp2} \]

\[ \text{pp1144, sp3} \]

\[ \text{pp1122, sp2} \]

\[ \text{pp1144, sp3} \]

\[ \text{pp1122, sp2} \]
The document contains diagrams of pulse sequences labeled as \textit{hsqcetgplrsp} and \textit{hsqcetgpjclmd}. These sequences involve proton (\textsuperscript{1}H) and carbon (\textsuperscript{13}C) nuclei, with applications in NMR spectroscopy. The sequences include elements such as \text{p14 sp3}, \text{p24 sp7}, and a series of Gz pulses. The diagrams illustrate the timing and phase relationships between these elements, essential for understanding the pulse program's functionality.
J-scaling factor of $N$

$J(\text{HA-CA})$, $J(\text{HB-CA})$

$dipsi2etgpjcsix1$

$^1H$, $^1C$

$G_z$

ppm

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2D ADEQUATE EXPERIMENTS
• **1,1-ADEQUATE:**

  Phase-sensitive 1,1 ADEQUATE ( adeq11etgp )
  Phase-sensitive 1,1 ADEQUATE using adiabatic pulse ( adeq11etgpsp )
  Phase-sensitive 1,1 ADEQUATE with refocusing ( adeq11etgprd )
  Phase-sensitive 1,1 ADEQUATE with refocusing using adiabatic pulse ( adeq11etgprdsp )

• **1,n-ADEQUATE:**

  Phase-sensitive 1,n ADEQUATE ( adeq1netgp )

• **n,1-ADEQUATE:**

  Phase-sensitive n,1 ADEQUATE ( adeqn1etgp )

• **n,n-ADEQUATE:**

  Phase-sensitive n,n ADEQUATE ( adeqnnetgp )
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adeq11etgprd

\[ ^{1}H \quad ^{13}C \]

\[ d_1 \quad d_4 \quad d_4 \quad d_2 \quad d_4 \quad d_4 \quad d_2 \quad d_4 \]

\[ ^{1}H \quad ^{13}C \]

\[ d_2 \quad d_2 \quad d_0 \quad d_0 \quad d_2 \quad d_2 \quad d_0 \quad d_0 \]

\[ G_z \quad G_z \quad G_z \]

GARP

adeq11etgprdsq

\[ ^{1}H \quad ^{13}C \]

\[ d_1 \quad d_4 \quad d_4 \quad d_2 \quad d_4 \quad d_4 \quad d_2 \quad d_4 \]

\[ ^{1}H \quad ^{13}C \]

\[ d_2 \quad d_2 \quad d_0 \quad d_0 \quad d_2 \quad d_2 \quad d_0 \quad d_0 \]

\[ G_z \quad G_z \quad G_z \]

GARP

\[ ^{1}H \]

\[ d_1 \quad d_4 \quad d_4 \quad d_2 \quad d_4 \quad d_4 \quad d_2 \quad d_4 \]

\[ ^{13}C \]

\[ d_2 \quad d_2 \quad d_0 \quad d_0 \quad d_2 \quad d_2 \quad d_0 \quad d_0 \]

\[ G_z \quad G_z \quad G_z \]

GARP

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DIFFUSION/DOSY
EXPERIMENTS
Conventional 1D:

1D Stimulated Echo experiment (STE) (stegp1s1d)
1D Stimulated Echo experiment using bipolar gradients (stebpgp1s1d)
1D LED experiment (ledgp2s1d)
1D LED experiment using bipolar gradients (ledbpgp2s1d)
1D Double-Stimulated Echo Experiment (DSTE) (dstegp3s1d)
1D Double-Stimulated Echo Experiment (DSTE) using bipolar gradients (dstebpgp3s1d)

1D Stimulated Echo experiment using bipolar gradients and WATERGATE (stebpgp1s191d)
1D STE-INEPT experiment (stebpgpin1s1d)

2D DOSY maps:

2D Stimulated Echo experiment (STE) (stegp1s)
2D Stimulated Echo experiment using bipolar gradients (stebpgp1s)

2D Double-Stimulated Echo Experiment (DSTE) (dstegp3s)
2D Double-Stimulated Echo Experiment (DSTE) using bipolar gradients (dstebpgp3s)
2D LED experiment (ledgp2s)
2D LED experiment using bipolar gradients (ledbpgp2s)

2D Stimulated Echo experiment using bipolar gradients and WATERGATE (stebpgp1s19)
2D STE-INEPT experiment (stebpgpin1s)

2D & 3D DOSY related experiments:

3D DOSY-COSY using LED with bipolar gradients (ledbpcco2s3d)
2D DOSY-TOCSY with LED using bipolar gradients (ledbpgpml2s2d)
2D DOSY-TOCSY with LED using bipolar gradients and WATERGATE (ledbpgpml2s192d)
3D DOSY-TOCSY using LED with bipolar gradients (ledbpgpml2s3d)
3D DOSY-NOESY using LED with bipolar gradients (ledbpgpno2s3d)
\[ I = I_0 \exp\left(-D\gamma^2 g^2 \left( -\frac{2}{3}\right)\right) \]

\[ \ln(I/I_0) = -D\gamma^2 g^2 \left( -\frac{2}{3}\right) \]

Stokes-Einstein Equation

\[ D = \frac{K T}{6 \pi \eta R_H} \]

- \( I \): Initial Peak intensity
- \( I_0 \): Initial Peak intensity
- \( D \): Diffusion Coefficient
- \( \gamma \): Gyromagnetic Constant
- \( g \): Applied Gradient
- \( G_{\text{max}} \): Maximum Gradient
- \( p30 \): Gradient Duration
- \( d20 \): Diffusion Time
- \( K \): Boltzmann Constant
- \( T \): Temperature
- \( \eta \): Viscosity
- \( R_H \): Hydrodynamic radius
- \( \pi \): Pi

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1D & 2D SATURATION TRANSFER DIFFERENCE (STD) EXPERIMENTS
• 1D STD:
  
  1D STD (stddiff)
  1D STD with spoil (stddiff.2)
  1D STD with spoil and T2 filter (stddiff.3)

• 1D STD with solvent suppression:
  
  1D STD using 3-9-19 WATERGATE (stddiffgp19)
  1D STD with spoil using 3-9-19 WATERGATE (stddiffgp19.2)
  1D STD with spoil and T2 filter using 3-9-19 WATERGATE (stddiffgp19.3)
  1D STD using excitation sculpting (stddiffesgp)
  1D STD with spoil using excitation sculpting (stddiffesgp.2)
  1D STD with spoil and T2 filter using excitation sculpting (stddiffesgp.3)

• 2D STD-TOCSY:
  
  2D STD-TOCSY (stdmlevph)
  2D STD-TOCSY using 3-9-19 WATERGATE (stdmlevgpph19)
  2D STD-TOCSY using excitation sculpting (stdmlevesgpph)

• 2D STD-NOESY:
  
  2D STD-NOESY with T2 filter in F2 (stdnoesygpph)
  2D STD-NOESY with T2 filter in F1 and F2 (stdnoesygpph.2)
  2D STD-NOESY using 3-9-19 WATERGATE with T2 filter in F2 (stdnoesygpph19)
  2D STD-NOESY using 3-9-19 WATERGATE with T2 filter in F1 and F2 (stdnoesygpph19.2)
  2D STD-NOESY using excitation sculpting with T2 filter in F2 (stdnoesyesgpph)
  2D STD-NOESY using excitation sculpting with T2 filter in F1 and F2 (stdnoesyesgpph.2)

• 2D STD-HSQC:
  
  2D STD-HSQC using echo-antiecho (stdhsqetgpsp)
  2D STD-HSQC with sensitivity-improvement (stdhsqetgpsisp)
Pulse Program Catalogue
NMRGuide 4.1 - Topspin 2.0

stddiffgp19

f2 channel

Selective 90°

f1 channel

d1

Gz

G1 G1

stddiffgp19.2

f2 channel

Selective 90°

f1 channel

y d1

Gz

G1 G2 G2

stddiffgp19.3

f2 channel

Selective 90°

f1 channel

y d1

Gz

G1 G2 G2

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stdmlevph

f2 channel

f1 channel

Selective saturation

Gz

G1

d0

d9

MLEV-17

p17 p110

90º

p13

sp3

l5

d1

90º

d20

stdmlevgpph19

f2 channel

f1 channel

Selective saturation

Gz

G1

d0

d9

MLEV-17

p17 p110

90º

p13

sp3

l5

d1

90º

d20

stdmlevesgpph

f2 channel

f1 channel

Selective saturation

Gz

G1

d0

d9

MLEV-17

p17 p110

90º

p13

sp3

l5

d1

90º

d20

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stdnoesygpph

f2 channel

Selective saturation
90°
saturation time
d20

f1 channel

y d1

G1

G2

stdnoesygpph.2

f2 channel

Selective saturation
90°
saturation time
d20

f1 channel

y d1

G1

G2

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stdnoesygpph19

f2 channel

Selective saturation time d20

f1 channel

p13 p13
15 15
90º 90º
d0 d0
d8 d8

G1 G2 G3 G3

stdnoesygpph19.2

f2 channel

Selective saturation time d20

f1 channel

p13 p13
15 15
90º 90º
d0 d0
d8 d8

G1 G2 G3 G3

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Selective 90º

stdhsqetgpsp

$^1H$

\[ \text{d1} \text{ d4} \text{ d4} \text{ y} \text{ d4} \text{ d4} \text{ <rec}}

$^1C$

\[ \text{p13} \text{ sp3} \text{ y} \text{ y} \text{ l5} \text{ <l} \text{ rec} \text{ p28} \text{ d24} \text{ d24} \text{ d4} \text{ d4} \text{ d4} \text{ 13C} \text{ Gz} \text{ pp1144} \text{ sp3} \text{ 1} \text{ d0} \text{ d0} \text{ pp2244} \text{ sp7} \text{ pp2244} \text{ sp7} \text{ 'I' pp1144} \text{ sp3} \text{ GARP pl12} \text{ G2} \text{ G1} \]

GARP

\[ \text{G1} \text{ G2} \]
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CATALOGUE

NMRGuide

CLEANEX EXPERIMENTS
1D CLEANEX using 3-9-19 WATERGATE (zgcxgp19)
1D CLEANEX using excitation sculpting (zgcxesgp)
2D CLEANEX-Fast HSQC using 3-9-19 WATERGATE (fhsqccxf3gpph)
2D CLEANEX-TROSY using 3-9-19 WATERGATE (trosycxf3gpphsi19)
**Pulse Program Catalogue**

**NMRGuide 4.1 - Topspin 2.0**

---

### fhsqccxf3gpph

- **$^1H$**
  - $d_1$: Selective
  - H2O 180°
- $d_26$: $p_7$, sp21
- $d_26$: p10, p127, d31
- $d_26$: p14, sp3

### trosycxf3gpphsi19

- **$^1H$**
  - $d_1$: Selective
  - H2O 180°
- $d_26$: $p_7$, sp21
- $d_26$: p10, p127, d31
- $d_26$: p14, sp3

---

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1D ¹H spectrum

- 1D ¹H with double presaturation (lc1prf2 | LC1D12)
- 1D ¹H with triple presaturation (lc1prft)
- 1D ¹H with WET (wet)
- 1D ¹H with WET and CW decoupling on f2 during WET and ACQ (wetdc | LC1DWTDCC)
- 1D ¹H with WET and CW decoupling on f2 during WET (wetdw)
- 1D ¹H WET solvent suppression with shape pulse and C-13 decoupling on f2 during WET and AQ for LC isocratic runs (lc2wetdc)
- 1D ¹H WET solvent suppression with shape pulse and C-13 decoupling on f2 during WET and AQ with intermediate preparation scan into second dataset for LC gradient runs with updated shapes (lc2wetdcus | LC2DWTUS)

1D NOESY

- 1D NOESY with presaturation (noesypr1d)
- 1D NOESY with presaturation and CW decoupling on f2 (lc1pncw)
- 1D NOESY with double presaturation and CW decoupling on f2 (lc1pncwfd)
- 1D NOESY with presaturation using shaped pulse and CW decoupling on f2 (lc1pncwps)
- 1D NOESY with double presaturation (lc1pnf2)
- 1D NOESY with multiple presaturation (lc1pnfr)
- 1D NOESY with triple presaturation (lc1pnft)
- 1D NOESY with presaturation using shaped pulse (lc1pnps)

Pseudo-2D-sequence

- Pseudo-2D-sequence for lc-nmr on flow detection (lc2)
- Pseudo-2D-sequence for lc-nmr on flow detection with power-gated decoupling (lc2pg)
- Pseudo-2D-sequence for lc-nmr on flow detection with presaturation (lc2pn)
- Pseudo-2D-sequence for lc-nmr on flow detection with double presaturation (lc2pnf2)
- Pseudo-2D-sequence for lc-nmr on flow detection with solvent gradients (lc2pnpl)
- Pseudo-2D-sequence for lc-nmr on flow detection with solvent gradients (lc2pnul)
- Pseudo-2D-sequence for lc-nmr on flow detection with presaturation (lc2pr)
- Pseudo-2D-sequence for lc-nmr on flow detection with double presaturation (lc2prf2)
- Pseudo-2D-sequence for lc-nmr on flow detection with presaturation using shape pulse (lc2ps)

2D homonuclear J-resolved

- 2D J-resolved with double presaturation and CW decoupling on f2 (lcjrescwfdprqf)
- 2D J-resolved with presaturation and CW decoupling on f2 (lcjrescwprqf)
- 2D J-resolved with presaturation using shape pulse and CW decoupling on f2 (lcjrescwpsqf)
- 2D J-resolved with double presaturation (lcjresf2prqf)
- 2D J-resolved with presaturation (lcjresprqf)
- 2D J-resolved with presaturation using shape pulse (lcjrespsqf)

2D TOCSY

- 2D TOCSY with double presaturation and CW decoupling on f2 (lcmllevcwfdpcph)
- 2D TOCSY with presaturation and CW decoupling on f2 (lcmllevcwpcphps)
- 2D TOCSY with double presaturation using composite pulse (lcmllevf2pcph)
- 2D TOCSY with double presaturation (lcmllevf2phpr | LCML12)
2D TOCSY with presaturation using shape pulse and composite pulse (lcmlevpcphps)
2D TOCSY with presaturation using composite pulse (lcmlevpcph)

2D Experiments using WET

2D COSY using WET (cosydcphwt | COSYDCPHT)
2D TOCSY using WET (mlevdcphwt | MLEVDCPHT)
2D HSQC using WET (hsqctegpsiw | HSQCETGPSWT)

2D Experiments using single/multiple presaturation using shape pulse

Phase-sensitive 2D COSY using using single/multiple presaturation (cosycwphps | COSYCWPHT)
Phase-sensitive 2D HSQC using using single/multiple presaturation (hsqcphps)
2D HMBC using using single/multiple presaturation (hmbcndpsqf)

Related experiments:

Also see 1D Solvent suppression
lcjrescwprqf

\(^{13}\text{C}\)

\[^{1}\text{H}\]

\(\text{presat}\)

\(d_1\) \(d_0\) \(d_0\)

\(\text{CW}\)

\(\text{pl21}\)

lcjrescwpqsf

\(^{13}\text{C}\)

\[^{1}\text{H}\]

\(\text{presat}\)

\(d_1\) \(d_0\) \(d_0\)

\(\text{off-reson.}\)

\(\text{pl21}\)

lcjresf2prqf

channel f2\(^{1}\text{H}\)

\(\text{presat}\)

\(\text{pl21}\)

\[^{1}\text{H}\]

\(d_1\) \(d_0\) \(d_0\)

\(\text{pl19}\)

lcjrescfdpqrf

\(^{13}\text{C}\)

channel f3\(^{1}\text{H}\)

\(\text{presat}\)

\(\text{pl22}\)

\[^{1}\text{H}\]

\(d_1\) \(d_0\) \(d_0\)

\(\text{pl19}\)
icmlevpcph

\[ ^1H \]
\[ \text{presat} \]
\[ p_{19} \]
\[ d_1 \rightarrow d_9 \]
\[ \text{MLEV-17} \]
\[ p_{6}, p_{110} \]

icmlevpcphps

\[ ^1H \]
\[ \text{presat} \]
\[ \text{off-reson.} \]
\[ d_1 \rightarrow d_9 \]
\[ \text{MLEV-17} \]
\[ p_{6}, p_{110} \]

icmlevf2phpr

\[ \text{channel f2} \]
\[ ^1H \]
\[ \text{presat} \]
\[ p_{121} \]
\[ d_1 \rightarrow d_9 \]
\[ \text{MLEV-17} \]
\[ p_{6}, p_{110} \]

icmlevf2pcph

\[ \text{channel f2} \]
\[ ^1H \]
\[ \text{presat} \]
\[ p_{121} \]
\[ d_1 \rightarrow d_9 \]
\[ \text{MLEV-17} \]
\[ p_{6}, p_{110} \]

icmlevcwpcphps

\[ ^13C \]
\[ \text{CW} \]
\[ d_1 \rightarrow d_9 \]
\[ p_{121} \]

icmlevcwfdpcph

\[ ^13C \]
\[ \text{CW} \]
\[ d_1 \rightarrow d_9 \]
\[ p_{121} \]
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BASIC SOLID-STATE
NMR EXPERIMENTS
1D one-pulse High power decoupling (hpdec)
1D CP (cp)
1D CP (cpnqs)
1D Sideband suppression with SELTICS (cpseltics)
1D CPMAS with total sideband suppression using TOSS (cptossa)
1D CPMAS with total sideband suppression using TOSS (cptossb)
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NMRGuide

APPENDIX
For a pulse program the first characters (usually up to 6, but sometimes more) specify the type of experiment, e.g. DEPT, COSY, NOESY etc. Further properties of the pulse program are indicated by a two-character code, which is added to the name in alphabetical order. For 2D experiments the mode (absolute value, phase sensitive or echo-antischo) is always indicated. H- or X-decoupling is assumed to be default for heteronuclear experiments, but not for homonuclear ones (except inad).

In case of redundant information some two-character codes may be omitted.

The two-character codes used are the following:

;ar experiment for aromatic residues
;at adiabatic TOCSY
;bi with bird pulse for homonuclear J-decoupling
;bp using bipolar gradients
;cc cross correlation experiment
;cp with composite pulse
;ct constant time
;cw decoupling using cw command
;cx using CLEANEX_PM
;dc decoupling using cpd command
;df double quantum filter
;di with DIPSI mixing sequence
;dh homonuclear decoupling in indirect dimension
;dw decoupling using cpd command only during wet sequence
;dq double quantum coherence
;ea phase sensitive using Echo/Antiecho method
;ec with E.COSY transfer
;ed with multiplicity editing
;es excitation sculpting
;et phase sensitive using Echo/Antiecho-TPPI method
;fb using f2- and f3- channel
;fd using f1- and f3- channel (for presaturation)
;fr with presaturation using a frequency list
;fp using f1-, f2- and f3- channel (for presaturation)
;fh F-19 observe with H-1 decoupling
;fp using a flip-back pulse
;fl for F-19 ecoupler
;f2 using f2- channel (for presaturation)
;f3 using f3- instead of f2- channel
;f4 using f4- instead of f2- channel
;gd gated decoupling using cpd command
;ge gradient echo experiment
;gp using gradients with ":gp" syntax
;gr using gradients
;gs using shaped gradients
;hb hydrogen bond experiment
;hc homodecoupling of a region using a cpd-sequence
;hd homodecoupling
;hf H-1 observe with F-19 decoupling
;hs with homospoil pulse
;ia InPhase-AntiPhase (IPAP) experiment
;ig inverse gated
;il using inverse (invI/HSQC) sequence
;im with incremented mixing time
;ir using inverse (inv4/HMQC) sequence
;jc for determination of J coupling constant
;jd homonuclear J-decoupled
;jr with jump-return pulse
;lp with low-pass J-filter
;lq with Q-switching (low Q)
;lr for long-range couplings
;l2 with two-fold low-pass J-filter
;mf multiple quantum filter
;ml with MLEV mixing sequence
Pulse Program Catalogue
NMRGuide4.1 – Topspin 2.0

;mq using multiple quantum
;nd no decoupling
;no with NOESY mixing sequence
;pc with presaturation and composite pulse
;pg power-gated
;ph phase sensitive using States-TPPI, TPPI, States or QSEC
;pl preparing a frequency list
;pn with presaturation using a 1D NOESY sequence
;pp using purge pulses
;pr with presaturation
;ps with presaturation using a shaped pulse
;qf absolute value mode
;qn for QNP-operation
;qs phase sensitive using qseq-mode
;rd focussed
;rl with relay transfer
;ru with radiation damping suppression using gradients
;rv with radiation damping compensation unit
;r2 with 2 step relay transfer
;r3 with 3 step relay transfer
;se spin echo experiment
;sh phase sensitive using States et al. method
;si sensitivity improved
;sm simultaneous evolution of X and Y chemical shift
;sp using a shaped pulse
;sq using single quantum
;ss spin-state selective experiment
;st phase sensitive using States-TPPI method
;sy symmetric sequence
;tf triple quantum filter
;tp phase sensitive using TPPI
;tr using TROSY sequence
;tz zeroquantum (ZQ) TROSY
;ul using a frequency list
;us updating shapes
;wg watergate using a soft-hard-soft sequence
;wt with WET watersuppression
;w5 watergate using W5 pulse
;xf x-filter experiments
;xy with XY CPMG sequence
;xl x-filter in F1
;x2 x-filter in F2
;x3 x-filter in F3
;zf with z-filter
;zq zero quantum coherence
;zs using a gradient/rf spoil pulse
;1d 1D version
;ls using 1 spoil gradients
;11 using 1-1 pulse
;45 using a 45 degree flip angle
;90 using a 90 degree flip angle
;135 using a 135 degree flip angle

;Typical experiment names would be:
; 2-dimensional, dept, dipsi2, hmbc, hmqc, hoesy, hsqc, inad, inept,
; 30 using a 30 degree flip angle
; 45 using a 45 degree flip angle
; 90 using a 90 degree flip angle
; 135 using a 135 degree flip angle

;Inverse correlations are denoted as hmbc, hmqc or hsqc.
; Experiments with a BIRD sequence in the beginning
; also contain a bi in the name.

;1D experiments, which are analogues of 2D experiments by virtue of
; a selective pulse, start with sel.
; Semiselective 2D experiments have the same name as the unselective
A phase-sensitive (States-TPPI, TPPI etc.) NOESY experiment with presaturation would then be:

\[ \text{noesy + ph + pr = noesymphpr.} \]

In the other direction the pulseprogram \texttt{hmbcgplpndqf} would be:

\[ \text{hmbc + gp + lp + nd + qf} \]

and therefore an:

inverse correlation for long-range couplings (HMBC) with coherence selection using gradients with ":gp" syntax,

\[ \text{low-pass J-filter, no decoupling in absolute value mode.} \]

The nomenclature of parameters is described in \texttt{Pulprog.info}.

Comments like:

\[ ;\text{avance-version} \]
\[ ;\text{begin} \]
\[ ;\text{end} \]
\[ ;\text{with (} = \text{MLEV17, DIPSI2, ...} \]

are evaluated by \texttt{NMRSIM} for the pulseprogram display and should therefore not be removed. The syntax for begin/end statements allows characters, numbers and ".". Arithmetic operators must not be used.

The comments:

\[ ;\text{preprocessor-flags-start} \]
\[ ;\text{preprocessor-flags-end} \]

are also evaluated to identify flags used in the pulseprogram and must also not be removed.

\[ @Id: \$ \]
The following convention is used for power levels, pulses, delays and loop counters throughout the microprograms:

The following convention is used for power levels, pulses, delays and loop counters throughout the microprograms:

<table>
<thead>
<tr>
<th>PL Code</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>pl0</td>
<td>f1 channel - power level for pulse (default) {all, PL90[F1]}</td>
</tr>
<tr>
<td>pl1</td>
<td>f2 channel - power level for pulse (default) {all, PL90[F2]}</td>
</tr>
<tr>
<td>pl2</td>
<td>f3 channel - power level for pulse (default) {all, PL90[F3]}</td>
</tr>
<tr>
<td>pl3</td>
<td>f4 channel - power level for pulse (default) {all, PL90[F4]}</td>
</tr>
<tr>
<td>pl4</td>
<td>f5 channel - power level for pulse (default) {}</td>
</tr>
<tr>
<td>pl5</td>
<td>f6 channel - power level for pulse (default) {}</td>
</tr>
<tr>
<td>pl6</td>
<td>f7 channel - power level for pulse (default) {}</td>
</tr>
<tr>
<td>pl7</td>
<td>f8 channel - power level for pulse (default) {}</td>
</tr>
<tr>
<td>pl8</td>
<td>f9 channel - power level for pulse (default) {}</td>
</tr>
<tr>
<td>pl9</td>
<td>f1 channel - power level for presaturation {default+lcnmr+triple+triple2+triple_na, PLCW[F1]}</td>
</tr>
<tr>
<td>pl10</td>
<td>f1 channel - power level for TOCSY-spinlock {all, PLTOC[F1]}</td>
</tr>
<tr>
<td>pl11</td>
<td>f1 channel - power level for ROESY-spinlock {all, PLROE[F1]}</td>
</tr>
<tr>
<td>pl12</td>
<td>f2 channel - power level for CPD/BB decoupling {all, PLCPDP[F2]}</td>
</tr>
<tr>
<td>pl13</td>
<td>f2 channel - power level for second CPD/BB decoupling {default+lcnmr+triple_c, PLCPDP2[F2]}</td>
</tr>
<tr>
<td>pl14</td>
<td>f2 channel - power level for CW saturation {triple+triple2, PLSH2[F2]}</td>
</tr>
<tr>
<td>pl15</td>
<td>f2 channel - power level for low power decoupling {lcnmr, PLUSER1[F2]}</td>
</tr>
<tr>
<td>pl16</td>
<td>f3 channel - power level for CPD/BB decoupling {all, PLCPDP[F3]}</td>
</tr>
<tr>
<td>pl17</td>
<td>f4 channel - power level for CPD/BB decoupling {all, PLCPDP[F4]}</td>
</tr>
<tr>
<td>sp0</td>
<td>f1 channel - shaped pulse 180 degree (adiabatic TOCSY) {}</td>
</tr>
<tr>
<td>sp1</td>
<td>f1 channel - shaped pulse 180 degree (two-fold modulated) {triple, PLSH8U[F1]}</td>
</tr>
<tr>
<td>sp2</td>
<td>f1 channel - shaped pulse for selective excitation {triple+triple2+triple_na, PLSH8[F1]}</td>
</tr>
<tr>
<td>sp3</td>
<td>f2 channel - shaped pulse 180 degree (adiabatic) {triple+triple2+triple_na, PLSH8[F1]}</td>
</tr>
</tbody>
</table>

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; or f2 channel - shaped pulse 180 degree (on resonance) {triple_na, PLSH3U[F2]}
; sp4 : f2 channel - shaped pulse 90 degree (off resonance) {triple+triple2, PLSH4[F2]}
; sp5 : f2 channel - shaped pulse 180 degree (off resonance) {triple+triple2, PLSH6[F2]}
; or f2 channel - shaped pulse 180 degree (on resonance) {triple_na, PLSH3U[F2]}
; sp6 : f1 channel - shaped pulse for presaturation {default+lcnmr+triple2+triple_na, PLSH7[F1]}
; sp7 : f1 channel - shaped pulse for wet {lcnmr, PLSH3[F1]+0.87}
; or f1 channel - shaped pulse 180 degree (adiabatic) {triple_c, PLSH13[F1]}
; or f2 channel - shaped pulse 180 degree (adiabatic) {default, PLSH2[F2]}
; or f2 channel - shaped pulse 180 degree (off resonance2) {triple+triple2, PLSH6[F2]}
; or f2 channel - shaped pulse 180 degree (off resonance2) {triple_na, PLSH3U[F2]}
; sp8 : f1 channel - shaped pulse for wet {lcnmr, PLSH3[F1]-1.04}
; or f2 channel - shaped pulse 90 degree (on res., time reversed) {triple+triple2, PLSH5[F2]}
; or f2 channel - shaped pulse 90 degree (on res., time reversed) {triple+triple2, PLSH8U[F2]}
; or f1 channel - shaped pulse for water flipback {default, PLSH8[F1]}
; or f1 channel - shaped pulse for water flipback2 {triple+triple2+triple_na, PLSH9[F1]}
; or f2 channel - shaped pulse for water flipback {triple_c, PLSH6[F2]}
; or f2 channel - shaped pulse 90 degree (higher selectivity) {triple+triple2, PLSH6U[F2]}
; sp10 : f1 channel - shaped pulse for tilted ROESY
; or f1 channel - shaped pulse for wet {lcnmr, PLSH3[F1]-5.05}
; or f2 channel - shaped pulse 90 degree (higher selectivity) {triple+triple2, PLSH7[F2]}
; or f2 channel - shaped pulse 90 degree (higher selectivity) {triple+triple2, PLSH9[F2]}
; or f2 channel - shaped pulse 90 degree (adiabatic) {triple, PLSH16[F2]}
; sp11 : f1 channel - shaped pulse for wet2
; or f1 channel - shaped pulse 90 degree (higher selectivity) {triple+triple2, PLSH4U[F2]}
; or f2 channel - shaped pulse 90 degree (higher selectivity) {triple+triple2, PLSH5[F2]}
; or f2 channel - shaped pulse 90 degree (adiabatic) {triple, PLSH12[F1]}
; or f2 channel - shaped pulse 180 degree (adiabatic) {default+triple, PLSH15[F2]}
; or f3 channel - shaped pulse 180 degree (adiabatic) {triple, PLSH14[F2]}
; sp12 : f1 channel - shaped pulse for wet2
; or f2 channel - shaped pulse 90 degree (higher sel., time rev.) {triple+triple2, PLSH8[F2]}
; or f2 channel - shaped pulse 90 degree (higher sel., time rev.) {triple+triple2, PLSH14[F2]}
; or f1 channel - shaped pulse for wet2 {lcnmr, PLSH5U[F2]}
; or f1 channel - shaped pulse 180 degree (adiabatic) {triple_c, PLSH12[F1]}
; or f2 channel - shaped pulse 180 degree (adiabatic) {triple, PLSH16[F2]}
; sp13 : f1 channel - shaped pulse for wet2
; or f2 channel - shaped pulse 180 degree (adiabatic) {triple, PLSH16[F2]}
; or f2 channel - shaped pulse 180 degree (adiabatic) {triple, PLSH14[F2]}
; sp14 : f1 channel - shaped pulse for wet2
; or f2 channel - shaped pulse 180 degree (adiabatic bive decoupling) {default+triple2, PLSH12[F2]}
; or f3 channel - shaped pulse 180 degree (adiabatic) {triple, PLSH14[F2]}
; or f2 channel - shaped pulse 90 degree (NH) {triple, PLSH14[F2]}
; or f3 channel - shaped pulse 90 degree (NH, adiabatic ramp up) {triple2, PLSH13[F3]}
; sp15 : f1 channel - shaped pulse 180 degree for decoupling (Ca or CO)
; or f2 channel - shaped pulse 180 degree for decoupling (Cbeta) {triple2, PLSH13[F2]}
; or f2 channel - shaped pulse 180 degree for decoupling ('C') {triple, PLSH6U[F2]}
; sp16 : f1 channel - shaped pulse 180 degree (higher sel., off res.) {triple+triple2, PLSH9[F2]}
; or f2 channel - shaped pulse 180 degree (higher sel., off res.) {triple, PLSH14[F2]}
; sp17 : f2 channel - shaped pulse 180 degree (higher sel., off res.) {triple+triple2, PLSH9[F2]}
; sp18 : f2 channel - shaped pulse 180 degree (adiabatic matched sweep) {default+triple, PLSH15[F2]}
; or f1 channel - shaped pulse for wet {lcnmr, PLSH3[F1]+0.87}
; or f2 channel - shaped pulse 90 degree (NH) {triple, PLSH14[F2]}
; or f3 channel - shaped pulse 90 degree (TRho, adiabatic ramp up) {triple2, PLSH13[F3]}
; sp19 : f1 channel - shaped pulse for wet {default, PLSH3[F1]-1.04}
; or f2 channel - shaped pulse 90 degree (NH, time reversed) {triple, PLSH14[F2]}
; or f3 channel - shaped pulse 90 degree (TRho, adiabatic ramp down) {default, PLSH3[F1]+2.27}
; or f1 channel - shaped pulse 180 degree (cleanex, H2O) {triple2, PLSH11[F1]}
; sp20 : f1 channel - shaped pulse for wet {default, PLSH3[F1]-5.05}
; or f1 channel - shaped pulse 90 degree (cleanex, H2O) {triple2, PLSH10[F1]}
; or f1 channel - shaped pulse 180 degree (off resonance) {triple, PLSH10[F1]}
; or f1 channel - shaped pulse 180 degree (off resonance) {triple, PLSH6[F1]}
; or f1 channel - shaped pulse 180 degree (off resonance) {triple, PLSH4[F1]}
; or f1 channel - shaped pulse 180 degree (off resonance) {triple, PLSH6U[F2]}
; sp21 : f1 channel - shaped pulse 180 degree (adiabatic sweep: z-spoil)
; or f1 channel - shaped pulse 180 degree (adiabatic sweep: z-spoil) {default, PLSH16[F1]}

Pulse Program Catalogue
NMRGuide4.1 – Topspin 2.0

;p30: f1 channel - shaped pulse 180 degree (sim. Ca + CO) {triple_c, PLSH15[F1]}
; or f2 channel - shaped pulse 180 degree for decoupling (sim. Ca + CO) {triple2, PLSH14[F2]}
p31: f2 channel - shaped pulse 180 degree (adiabatic bilevel decoupling)
{default+triple+triple2+triple_na, PLSH11[F2]}

;p0 : {all, P90[F1]}
p1 : f1 channel - 90 degree high power pulse {all, P90[F1]}
p2 : f1 channel - 180 degree high power pulse {all, P90[F1]^2}
p3 : f2 channel - 90 degree high power pulse {all, P90[F2]}
p4 : f2 channel - 180 degree high power pulse {all, P90[F2]^2}
p5 : f1 channel - 60 degree low power pulse {all, PTOC[F1]*0.66}
p6 : f1 channel - 90 degree low power pulse {all, PTOC[F1]}
p7 : f1 channel - 180 degree low power pulse
{default+lcnmr+triple+triple_c, PLSH3[F1]};
 or f2 channel - 90 degree shaped pulse (cleanex sel. H2O) {triple2, PSH11[F1]}
; or f2 channel - 180 degree shaped pulse (adiabatic bilevel) {default+lcnmr+triple+triple2+triple_na, PSH3[F2]}
p8 : f2 channel - 60 degree low power pulse{}
; or f1 channel - 90 degree shaped pulse (wet) {default, P90[F1]}
; or f1 channel - 180 degree shaped pulse (adiabatic) {default+lcnmr+triple+triple2+triple_na, PSH3[F2]}
p9 : f2 channel - 90 degree low power pulse (TOCSY) {all, PTOC[F2]}
p10: f1 channel - 90 degree low power pulse (cleanex spinlock) {triple2, PUSER1[F1]}
; or f2 channel - 180 degree low power pulse
{default+lcnmr+triple+triple2+triple_na, PTOC[F2]^2}
; or f2 channel - 180 degree shaped pulse (higher selectivity) {triple2, PSH4U[F2]}
p11: f1 channel - 90 degree shaped pulse (selective excitation) {default+lcnmr, PSH1[F1]}
; or f1 channel - 90 degree shaped pulse (selective excitation) {triple_c, PSH4[F1]}
; or f1 channel - 90 degree shaped pulse (wet) {lcnmr, PSH3[F1]}
; or f1 channel - 90 degree shaped pulse (water flipback/watergate)
{default+lcnmr+triple+triple2+triple_na, PSH8[F1]}
p12: f1 channel - 180 degree shaped pulse (H, selective) {default+lcnmr, PSH2[F1]}
; or f1 channel - 180 degree shaped pulse (C, adiabatic) {default+lcnmr, PSH2[F1]}
; or f1 channel - 180 degree shaped pulse (C, selective) {triple, PSH4[F1]}
; or f1 channel - 180 degree shaped pulse (excitation sculpting) {default+lcnmr, PSH8[F1]^2}
; or f1 channel - 180 degree shaped pulse (H, selective) {triple2, PSH1U[F1]}
p13: f2 channel - 90 degree shaped pulse {triple2, PSH4[F2]}
; or f2 channel - 90 degree shaped pulse {triple2, PSH1U[F2]}
; or f2 channel - 90 degree shaped pulse (H, selective) {triple, PSH4[F1]}
p14: f2 channel - 180 degree shaped pulse (adiabatic) {default+lcnmr, PSH3[F2]}
; or f2 channel - 180 degree shaped pulse (selective) {default+lcnmr, PSH6[F2]}
; or f2 channel - 180 degree shaped pulse (selective) {triple, PSH3U[F2]}
p15: f1 channel - pulse for ROESY spinlock
{default+lcnmr, PTOE[F1]}
; or f2 channel - 180 degree shaped pulse (cleanex sel. H2O) {triple2, PSH10[F1]}
; or f2 channel - 180 degree shaped pulse (adiabatic matched sweep) {triple2, PSH15[F2]}
; or f2 channel - 90 degree shaped pulse (higher selectivity) {triple2, PSH4U[F2]}
p16: homospoil/gradient pulse
{all, P_grad1}
p17: f1 channel - trim pulse at pl10 or pl15
{all, P_mlev}
p18: f1 channel - shaped pulse (off resonance presaturation)
{default+lcnmr+triple+triple2+triple_na, PSH7[F1]}
p19: homospoil/gradient pulse 2
{all, P_grad2}
p20: f2 channel - trim pulse
{all, P_mlev}
p21: f3 channel - 90 degree high power pulse
{all, P90[F3]}
p22: f3 channel - 180 degree high power pulse
{all, P90[F3]^2}
p23: f2 channel - 90 degree shaped pulse (higher selectivity) {triple2, PSH7[F2]}
; or f2 channel - 90 degree shaped pulse (twofold modulated)
{default+lcnmr, PSH7[U,F2]}
p24: f1 channel - 90 degree high power pulse {default, P90[F4]}
p25: f1 channel - 90 degree high power pulse
{default+lcnmr, P90[F4]^2}
p26: f1 channel - 90 degree shaped pulse (adiabatic) {default+lcnmr, PSH9[F1]}
; or f2 channel - 90 degree shaped pulse (selective) {triple2, PSH9[F2]}
p27: f1 channel - 90 degree pulse at pl12 (TOCSY, higher sel.)
{triple2, PUSER4[F3]}
; or f1 channel - 90 degree shaped pulse (higher selectivity)
{triple2, PUSER3[F3]}
p28: f1 channel - trim pulse at pl1
{all, P_hsqc}
p29: f1 channel - 90 degree shaped pulse (water flipback)
{default+lcnmr, PSH8[F1]}
; or f1 channel - 90 degree shaped pulse (water flipback2)
{default+lcnmr+triple+triple2+triple_na, PSH9[F1]}
Pulse Program Catalogue
NMRGuide4.1 – Topspin 2.0

; or f2 channel – 90 degree shaped pulse (water flipback) {triple_c, PSH16[F2]}
; or f3 channel – 90 degree shaped pulse (T1rho adiabatic ramp) {triple2, PSH1[F3]}
; or homospoil/gradient pulse 3 {pp}
; p30: f1 channel – 180 degree shaped pulse (sim. Ca + CO) {triple_c, PSH15[F1]}
; or f2 channel – 180 degree shaped pulse (sim. Ca + CO decoupling) {triple2, PSH14[F2]}
; or f3 channel – 180 degree pulse at pl23 {triple_na, PSH1U[F3]}
; or homospoil/gradient pulse 4 {pp}
; or gradient pulse for diffusion (dosy) {};
; p31: f2 channel – 180 degree shaped pulse (adiabatic matched sweep) {default, PSH15[F2]}
; or f2 channel – 180 degree shaped pulse (sel. Ca or CO decoupling) {triple, PSH10[F2]}
; or f2 channel – 180 degree shaped pulse (Cbeta decoupling) {triple2, PSH13[F2]}
; or f2 channel – 180 degree pulse at pl23 {triple_na, PSH1U[F2]}
; or homospoil/gradient pulse 5 {pp}
; p32: f1 channel – 180 degree shaped pulse (adiabatic sweep: z-spoil) {default, PSH16[F1]}
; or f3 channel – 180 degree shaped pulse (adiabatic) {triple_na, PSH2U[F3]}
; p33: f3 channel – trim pulse {triple_na, P_mlev}
; p34: f2 channel – 180 degree shaped pulse (adiabatic bilev sweep)
  {default+triple+triple2+triple_na, PSH11[F2]}

;d0 : incremented delay (2D or 3D) [3 usec]
; d1 : relaxation delay; 1-5 * T1
; d2 : 1/(2J)
; d3 : 1/(3J) or 1/(6J)
; d4 : 1/(4J)
; d5 : DE/2
; d6 : delay for evolution of long range couplings
; d7 : delay for inversion recovery
; d8 : NOESY mixing time
; d9 : TOCSY mixing time {all, TT0C[F1]}
; d10: incremented delay (3D)
; d11: delay for disk I/O [30 msec]
; d12: delay for power switching [2D usec]
; d13: short delay [4 usec]
; d14: delay for evolution after shaped pulse
; d15: TOCSY mixing time (CC) {triple*, TT0C[F2]}
; d16: delay for homospoil/gradient recovery {all, D_grad}
; d17: delay for DANTE pulse-train
; d18: delay for evolution of long range couplings
; d19: delay for binomial water suppression
; d20: for different applications
; d21: for different applications
; d22: 1/(2J(XY))
; d23: 1/(4J(XY)) or 1/(2J(XY))
; d24: for different applications
; d25: 1/(6J(XH)) or 1/(8J(XY))
; d26: 1/(4J(YH))
; d27: for different applications
; d28: for different applications
; d29: for different applications
; d30: for different applications
; d31: for different applications

; cnst0 : for protein experiments - N chemical shift (offset, in ppm)
; or for na experiments - calculated chemical shift (offset, in ppm)
; or for na experiments - N(aro) chemical shift (offset, in ppm) [195 ppm]
; cnst1 : J (HH)
; cnst2 : J (XH)
; cnst3 : J (XX)
; cnst4 : J (YH)
; cnst5 : J (XY)
; cnst6 : J (XH)min
; cnst7 : J (XH)max
; cnst8 : bandwidth of excitation for Dante-z pulse
; cnst9 : for different applications as J
; cnst10: for different applications as J
; cnst11: for multiplicity selection
; cnst12: for multiplicity selection
; cnst13: J (XH) long range
; cnst14: J (XH) long range (min)
; cnst15: J (XH) long range (max)
; cnst16: J-scale factor
Pulse Program Catalogue
NMRGuide4.1 – Topspin 2.0

;cnst17: factor to compensate for coupling evolution during a pulse
; or for na experiments - H1' chemical shift (offset, in ppm)
;cnst18: for protein experiments - H2O chemical shift (offset, in ppm)
; or for na experiments - H2O chemical shift (offset, in ppm)
;cnst19: for protein experiments - H(N) chemical shift (offset, in ppm)
; or for na experiments - H(N) chemical shift (offset, in ppm)
;cnst20: for protein experiments - Haliphatic chemical shift (offset, in ppm)
;cnst21: for na experiments - C1' chemical shift (offset, in ppm) [90 ppm]
; or for protein experiments - CO chemical shift (offset, in ppm)
;cnst22: for protein experiments - Calpha chemical shift (offset, in ppm)
; or for na experiments - C6/8 chemical shift (offset, in ppm) [137 ppm]
;cnst23: for protein experiments - Caliphatic chemical shift (offset, in ppm)
; or for na experiments - C2' chemical shift (offset, in ppm) [72 ppm]
;cnst24: for protein experiments - Caromatic chemical shift (offset, in ppm)
; or for na experiments - C4 (C/U) chemical shift (offset, in ppm) [169 ppm]
;cnst25: for protein experiments - flag for cross peak / reference experiments
; or for na experiments - C6 (A) chemical shift (offset, in ppm) [160 ppm]
;cnst26: for protein experiments - Call chemical shift (offset, in ppm)
; or for na experiments - C5 (G) chemical shift (offset, in ppm) [119 ppm]
;cnst27: for protein experiments - ( Cgamma chemical shift (offset, in ppm) )
; or for na experiments - C2/4 chemical shift (offset, in ppm) [152 ppm]
;cnst28: for protein experiments - Haromatic chemical shift (offset, in ppm)
; or for na experiments - C5 (C/U) chemical shift (offset, in ppm) [105 ppm]
;cnst29: for protein experiments - N(H) chemical shift (offset, in ppm)
; or for na experiments - C(aro) chemical shift (offset, in ppm) [145 ppm]
;cnst30: for protein experiments - Cbeta chemical shift (offset, in ppm)
; or for na experiments - N(H2) chemical shift (offset, in ppm) [151 ppm]
;cnst31: scaling factor
; or for na experiments - N(H2) chemical shift (offset, in ppm) [81 ppm]

;vc : variable loop counter, taken from vc-list
;vd : variable delay, taken from vd-list
;l1 : loop for spinlock cycle
;l2 : loop for GARP cycle: 12 * 31.75 * 4 * p9 => AQ
;l3 : loop for phase sensitive 2D or 3D using
; States et al. or States-TPPI method: l3 = td1/2
;l4 : for different applications
;l5 : for different applications
;l6 : loop for shaped pulse presaturation during relaxation delay
;l7 : loop for shaped pulse presaturation during mixing time
;l8 : number of frequencies for multiple presaturation
;l11: loop for spinlock cycle 2
The following convention is used for power levels, pulses, delays and loop counters in the different relation files for prosol:

- all = default + lcnmr + triple + triple2 + triple_c + triple_na
- triple* = triple + triple2 + triple_c + triple_na
- ! = except

**prosol par. rel. file pulseprogram parameter**

- **D_grad** all d16: delay for homospoil/gradient recovery
- **P90[F1]** all p0: f1 channel - 90 degree high power pulse
- **P90[F1]** all(!triple_c) p27: f1 channel - 90 degree pulse at pl18 (3-9-19 watergate)
- **P90[F1]*2** all p2: f1 channel - 180 degree high power pulse
- **P90[F2]** all p3: f2 channel - 90 degree high power pulse
- **P90[F2]*2** all p4: f2 channel - 180 degree high power pulse
- **P90[F3]** all p21: f3 channel - 90 degree high power pulse
- **P90[F3]*2** all p22: f3 channel - 180 degree high power pulse
- **P90[F4]** default p23: f4 channel - 90 degree high power pulse
- **PCPDP[F1]** triple+triple2+triple_c p26: f1 channel - 90 degree pulse at pl19
- **PL90[F1]** all pl1: f1 channel - power level for pulse (default)
- **PL90[F1]** all(!triple_c) pl18: f1 channel - power level for 3-9-19-pulse (watergate)
- **PL90[F2]** all pl2: f2 channel - power level for pulse (default)
- **PL90[F3]** all pl3: f3 channel - power level for pulse (default)
- **PL90[F4]** all pl4: f4 channel - power level for pulse (default)
- **PLCPDP[F1]** all(!triple_c) pl19: f1 channel - power level for CPD/BB decoupling
- **PLCPDP[F2]** all pl12: f2 channel - power level for CPD/BB decoupling
- **PLCPDP[F2]** default+triple+triple2 pl30: f2 channel - power level for CPD/BB decoupling +triple_na
- **PLCPDP[F2]-18** lcnmr pl26: f2 channel - power level for cw decoupling
- **PLCPDP[F2] default** f2 channel - power level for second CPD/BB decoupling
- **PLCW[F1]** all(!triple_c) pl9: f1 channel - power level for presaturation
- **PLCW[F2]** default+lcnmr pl21: f2 channel - power level for presaturation
- **PLCW[F2]** triple+triple2 pl14: f2 channel - power level for cw saturation
- **PLHD[F2]** all pl24: f2 channel - power level for hd/hc decoupling
- **PLSH1[F1]** default sp1: f1 channel - shaped pulse for selective excitation
- **PLSH1[F1]** lcnmr sp2: f1 channel - shaped pulse for wet
- **PLSH1[F1]+0.87** lcnmr sp2: f1 channel - shaped pulse for wet
- **PLSH1[F1]+0.87** default sp7: f1 channel - shaped pulse for wet
- **PLSH1[F1]-1.04** lcnmr sp8: f1 channel - shaped pulse for wet
- **PLSH1[F1]-1.04** default sp9: f1 channel - shaped pulse for wet
- **PLSH1[F1]+2.27** lcnmr sp9: f1 channel - shaped pulse for wet
- **PLSH1[F1]+2.27** default sp21: f1 channel - shaped pulse for wet
- **PLSH1[F1]-5.05** lcnmr sp10: f1 channel - shaped pulse for wet
- **PLSH1[F1]-5.05** default sp22: f1 channel - shaped pulse for wet
Pulse Program Catalogue
NMRGuide4.1 – Topspin 2.0

;PLSH1U[F1] triple_na sp23: f1 channel - shaped pulse 180 degree (NA: H)
;PLSH1U[F1] triple_na sp24: f1 channel - shaped pulse 180 degree (NA: H)
;PLSH1U[F2] triple_na sp2: f2 channel - shaped pulse 90 degree (NA: C)
;PLSH1U[F3] triple_na sp9: f3 channel - shaped pulse 180 degree (NA: N)
;PLSH2U[F2] triple_na sp14: f2 channel - shaped pulse 90 degree (NA: C, tr)
;PLSH2U[F3] triple_na sp10: f2 channel - shaped pulse 180 degree (NA: C, adiabatic)
;PLSH3U[F2] triple_na sp3: f2 channel - shaped pulse 180 degree (NA: C)
;PLSH3U[F2] triple_na sp5: f2 channel - shaped pulse 180 degree (NA: C)
;PLSH4U[F2] triple_na sp12: f2 channel - shaped pulse 90 degree (NA: C, higher sel.)
;PLSH4U[F2] triple_na sp25: f2 channel - shaped pulse 180 degree (NA: C, higher sel.)
;PLSH5U[F2] triple_na sp12: f2 channel - shaped pulse 90 degree (NA: C, tr)
;PLSH5U[F2] triple_na sp25: f2 channel - shaped pulse 180 degree (NA: C, tr)
;PLSH6U[F2] triple_na sp15: f2 channel - shaped pulse 180 degree (NA: C, decoupling)
;PLSH6U[F2] triple_na sp25: f2 channel - shaped pulse 180 degree (NA: C, higher sel.)
;PLSH6U[F2] triple_na pl28: f2 channel - shaped pulse 180 degree (NA: C, decoupling)
;PLSH7U[F2] triple_na sp0: f2 channel - shaped pulse 180 degree (NA: C, twofold mod)

;PLTOC[F1] all pl10: f1 channel - power level for TOCSY-spinlock
;PLTOC[F2] all pl15: f2 channel - power level for TOCSY-spinlock
;PLTOC[F3] all(!triple2+triple_na) pl23: f3 channel - power level for TOCSY-spinlock

;PLUSER1[F1] triple2 p127: f1 channel - power level for CLEANEX spinlock
;PLUSER1[F2] lcnmr p114: f2 channel - power level for low power decoupling
;PLUSER1[F3] triple* p125: f3 channel - power level for T1rho spinlock
;PLUSER2[F2] default+triple2 p131: f2 channel - power level for bilev dec. (cw part)
;PLUSER2[F3] triple2 p123: f3 channel - power level for Rexchange
;PLUSER3[F1] triple2 p125: f1 channel - power level for hetero TOCSY
;PLUSER3[F2] triple2 p126: f2 channel - power level for hetero TOCSY
;PLUSER4[F2] triple2 p127: f2 channel - power level for hetero TOCSY higher sel.
;PLUSER5[F3] triple2 p122: f3 channel - power level for hetero TOCSY higher sel.
;PLUSER5[F2] p120: f2 channel - power level for TOCSY higher sel.

;PROE[F1]*2 default+lcnmr p25: f1 channel - 90 degree pulse at pl27 (pulsed ROESY)

;PSH1[F1] default p11: f1 channel - 90 degree shaped pulse (selective excitation)
;PSH1[F1] triple2 p29: f3 channel - shaped pulse for adiabatic ramping
;PSH1[F2] default+1cnnmr p12: f1 channel - 180 degree shaped pulse (C, adiabatic)
;PSH2[F1] default+1cnnmr p12: f1 channel - 180 degree shaped pulse (H, selective)
;PSH3[F1] lcnmr p11: f1 channel - 90 degree shaped pulse (H2O)
;PSH3[F1] default p8 : f1 channel - 90 degree shaped pulse (H2O)
;PSH3[F2] default+1cnnmr p14: f2 channel - 180 degree shaped pulse (adiabatic)
;PSH3[F2] triple2+triple2+triple_na p8 : f2 channel - 180 degree shaped pulse (adiabatic)
;PSH4[F1] triple_c p11: f1 channel - 90 degree shaped pulse
;PSH4[F2] triple2+triple2 p13: f2 channel - 90 degree shaped pulse
;PSH6[F1] triple_c p12: f1 channel - 180 degree shaped pulse (selective)
;PSH6[F2] triple2+triple2 p14: f2 channel - 180 degree shaped pulse (selective)
;PSH7[F1] all(!triple_c) p18: f1 channel - shaped pulse (off resonance presaturation)
;PSH7[F2] triple2+triple2 p23: f2 channel - 90 degree shaped pulse (higher selectivity)
;PSH8[F1] triple2+triple2+triple_na p11: f1 channel - 90 degree shaped pulse (water flipback/watergate)
;PSH8[F1]*2 triple2+triple2+triple_na p11: f1 channel - 90 degree shaped pulse (water sculpting)
;PSH9[F1] default p29: f1 channel - 90 degree shaped pulse (water flipback)
;PSH9[F1] triple2+triple2+triple_na p29: f1 channel - 90 degree shaped pulse (water flipback2)
;PSH9[F2] triple2+triple2 p24: f2 channel - 180 degree shaped pulse (higher selectivity)
;PSH10[F1] triple2 p15: f1 channel - 90 degree shaped pulse (H2O on resonance)
;PSH10[F2] p12: f1 channel - 180 degree shaped pulse (sel. Ca or CO decoupling)
Pulse Program Catalogue
NMRGuide4.1 – Topspin 2.0

<table>
<thead>
<tr>
<th>Program</th>
<th>Description</th>
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