Pulse sequence editing by symbolic calculation — Sample diagrams

Michael P. Barnett*and Istvàn Pelczer†

January 30, 2010

Construction of Figure 2.1

```
draw[pulseSeq[HETCOR, refocused] =
 {channels[H1, C13], {pulse[90], }, delay[t1/2], {, pulse[180]}, delay[t1/2],
   delay[1/(2J)], pulse[90], delay[1/(3J)], {decouple, acquire}[taq]}]
```

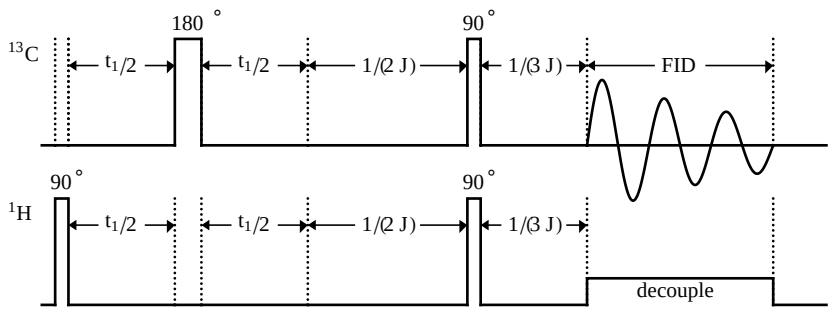

Figure 2.1. Refocused HETCOR.

*Meadow Lakes, Hightstown, NJ 08520, michaelb@princeton.edu
†Department of Chemistry, Princeton University, Princeton NJ 08544, ipelczer@princeton.edu

Construction of Figure 2.2

```
draw[pulseSeq[INEPT, gradientAssisted] =
  {channels[H1, C13, Gz], {pulse[90], }, delay[1/(4J)], pulse[180, x],
   delay[1/(4J)] , {pulse[90, x],}, gradientPulse[5 s], {, pulse[90, y]},
   {, acquire}[taq]}]
```

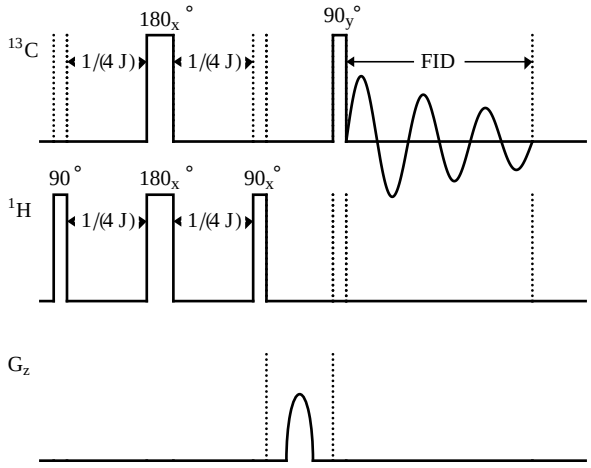

Figure 2.2. Gradient assisteded INEPT.

Construction of Figure 2.3

```
draw[pulseSeq[2D, TOCSY] =
 {channels[H1], pulse[90], delay[t1], spinLock[taum], acquire[t2]}]
```

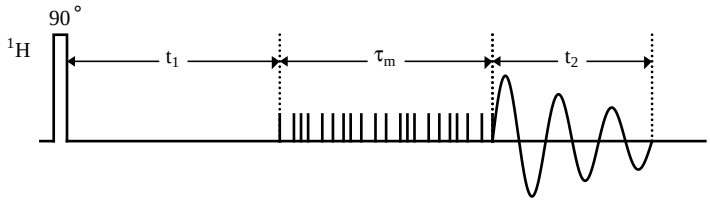

Figure 2.3. 2D basic TOCSY.

Construction of Figure 2.4

```
pulseSeq[2D, HSQC, basic] =
 {channels[H1, N15], {pulse[90], } , delay[Delta], pulse[180],
   delay[Delta], pulse[90], delay[t1/2], {pulse[180], }, delay[t1/2],
   pulse[90], delay[Delta], pulse[180], delay[Delta],
  {acquire, decouple}[t2]}

drawPulseSequence[2D, HSQC, basic, notes[ "Delta = 1/(4J),   J = J[1, NH]"]]
```

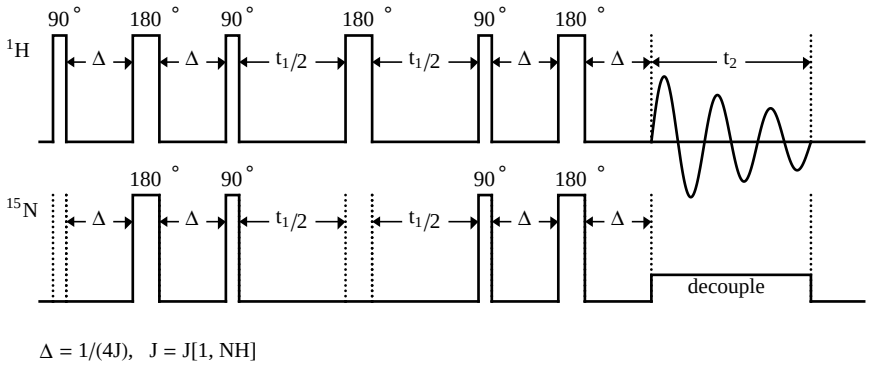

Figure 2.4. 2D basic HSQC.

Phase cycling

```
phaseList = "phi = x, y, -x, -y; receiver = -y, x, y, -x"

phaseCycled[explanatory] = phaseCycle[phaseList][pulseSeq[short]]

phaseCycled[explanatory] // expand[]
=>
{channels[H1], pulse[90, " x"], delay[t], acquire[taq], pulse[90, " y"],
 delay[t], acquire[taq], pulse[90, " -x"], delay[t], acquire[taq],
 pulse[90, " -y"], delay[t], acquire[taq]}

forCTHSQC = "phi1 = x, -x; phi2 = 8(x), 8(-x); phi3 = 2(x), 2(y), 2(-x), 2(-y);
 phi4 = 16(y), 16(-y); receiver = 2(x, -x, -x, x), 2(-x, x, x, -x)"

cyclingReplacementRules[forCTHSQC]
=>
{{phi1 -> " x", phi2 -> x, phi3 -> x, phi4 -> y, receiver -> x},
 {phi1 -> " -x", phi2 -> x, phi3 -> x, phi4 -> y, receiver -> -x},
                  <<28 cycles >>
 {phi1 -> " x", phi2 -> -x, phi3 -> -y, phi4 -> -y, receiver -> x},
 {phi1 -> " -x", phi2 -> -x, phi3 -> -y, phi4 -> -y, receiver -> -x}}
```

Construction of Figure 3.1

```
pulseSeq[2D, HSQC, basic, TOCSY] =
  pulseSeq[2D, HSQC, basic] // insert[spinLock[taum], on[H1], before[acquire]]

drawPulseSequence[2D, HSQC, basic, TOCSY,
  notes["Delta = 1/(4J),  J = J[1, NH]"]]
```

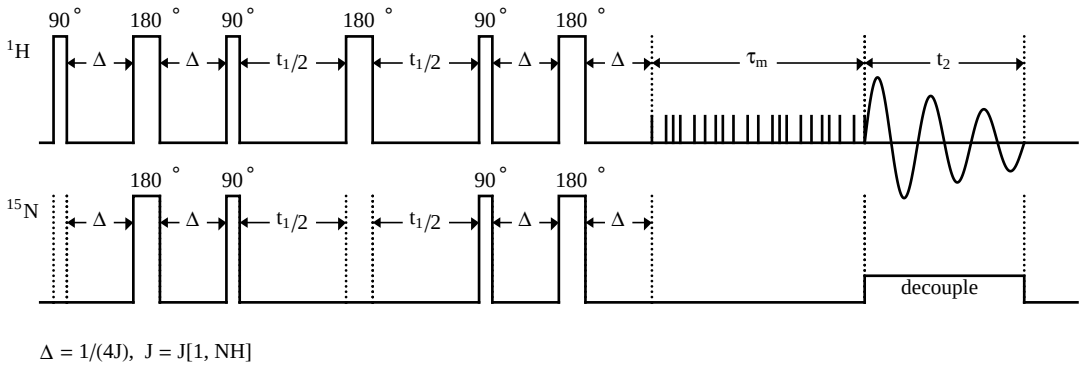

Figure 3.1. 2D basic HSQC TOCSY.

Construction of Figure 3.2

```
pulseSeq[2D, HSQC, gradientSelected] =
 pulseSeq[2D, HSQC, basic] //
  pipe[
    insert[gradientPulse[10], in[delay[t1/2], 2]],
    insert[gradientPulse[-1], in[delay[Delta], 3]]]

drawPulseSequence[2D, HSQC, gradientSelected, notes["t1/2 > gradient pulse"]]
```

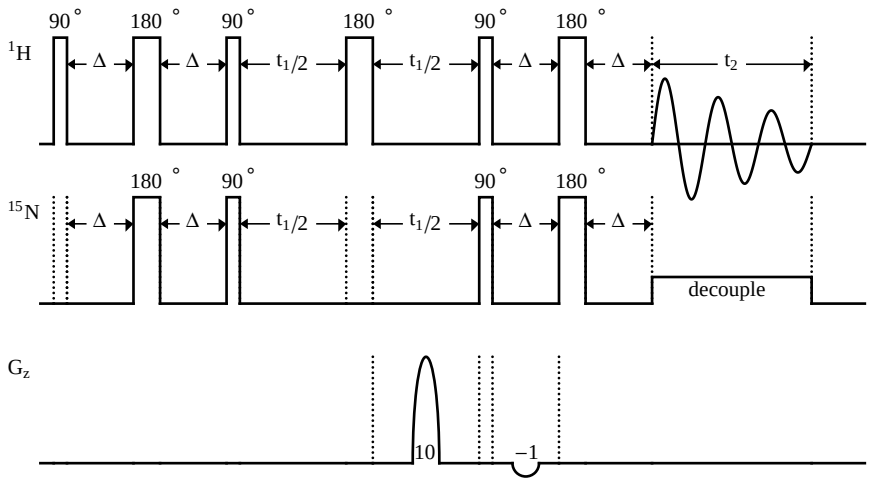

Figure 3.2. 2D gradient selected HSQC.

Construction of Figure X.1

```
pulseSeq[2D, HSQC, editedGradientSelected] =
 pulseSeq[2D, HSQC, basic] //
  pipe[
   insert[spinEcho, on[N15], after[delay[t1/2], 2]] ,
   insert[gradientPulse[10], in[delay[te/2], 2]],
   insert[gradientPulse[1], in[delay[Delta], 3]]]

drawPulseSequence[2D, HSQC, editedGradientSelected,
  notes["te/2 >gradient pulse duration"]];
```

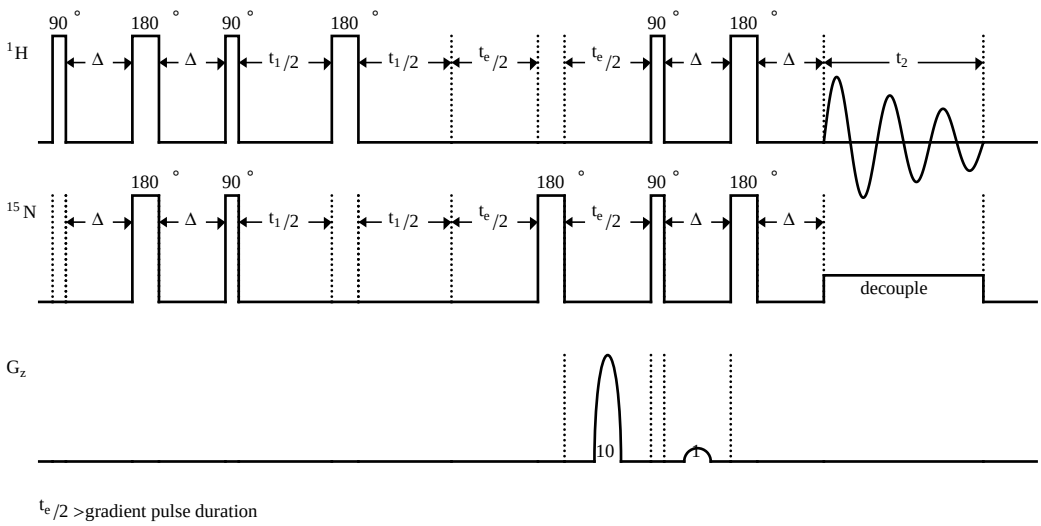

Figure X.1. 2D edited gradient selected HSQC.

Construction of Figure X.2

```
pulseSeq[2D, HSQC, gradientEnhanced] =
 pulseSeq[2D, HSQC, basic] //
  pipe[insert[gradientChannel],
   numberThePulses,
   pulse[3][_] -> Sequence[{pulse[90], }, gradientPulse[7s], {, pulse[90]}] ,
   pulse[5][__] -> Sequence[{, pulse[90]}, gradientPulse[10], {pulse[90], },
   gradientPulse[-1]],
   unnumberThePulses]

drawPulseSequence[2D, HSQC, gradientEnhanced]
```

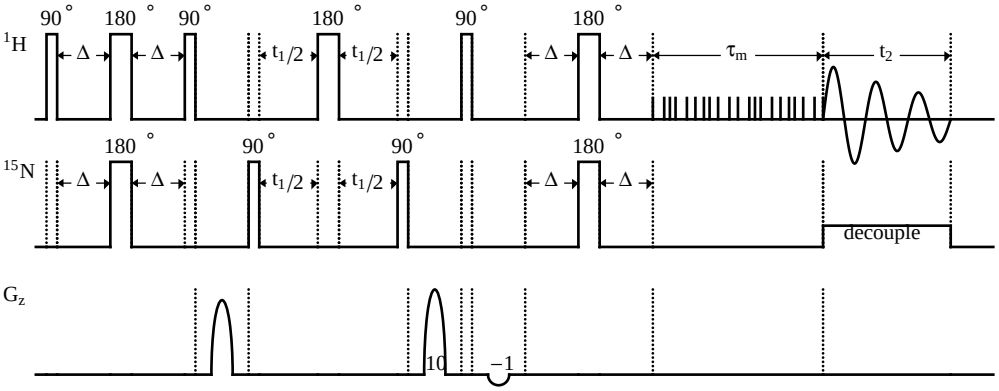

Figure X.2. 2D gradient enhanced HSQC.

Composite pulses

```
RRRbRb = {R} // attachCopy // attachInverse
=>
{R, R, -R, -R}

waltz4 = RRRbRb /. R -> {1, -2, 3} //Flatten
=>
{1, -2, 3, 1, -2, 3, -1, 2, -3, -1, 2, -3}
=>
{-2, 4, -2, 3, -1, 2, -4, 2, -3, 1}

waltz8 = Rp // attachInverse
=>
{-2, 4, -2, 3, -1, 2, -4, 2, -3, 1, 2, -4, 2, -3, 1, -2, 4, -2, 3, -1}

waltz16 = waltz8 // RotateRight // attachInverse // coalesce
=>
{-3, 4, -2, 3, -1, 2, -4, 2, -3, 3, -4, 2, -3, 1, -2, 4, -2, 3,
   3, -4, 2, -3,  1, -2, 4, -2, 3, -3, 4, -2, 3, -1, 2, -4, 2, -3}
```

Construction of Figures 4.1, X3, X4

```
adaptAssignmentOfPulse[2D, HSQC, basic, TOCSY, by[basic -> gradientSelected]]
```

This produces the following intermediate result, and the statement after it produces Figure 4.1.

```
{channels[H1, N15, Gz], {pulse[90], Null}, delay[Delta], pulse[180],
 delay[Delta], pulse[90], delay[t1/2], {pulse[180], Null},
 {delay, delay, gradientPulse[10]}[t1/2], pulse[90],
 {delay, delay, gradientPulse[-1]}[Delta], pulse[180], delay[Delta],
 {spinLock, Null, Null}[taum], {acquire, decouple}[t2]}

drawPulseSequence[2D, HSQC, gradientSelected, TOCSY]
```

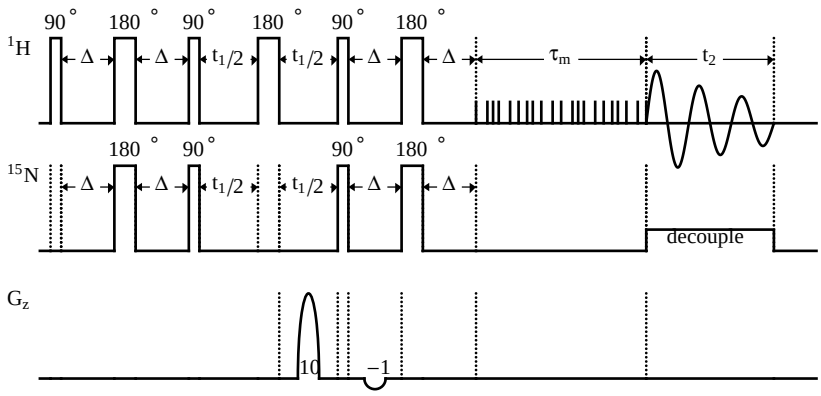

Figure 4.1. 2D gradient selected HSQC TOCSY.

Reconstruct Figure 4.1 and construct Figures X.3, X.4:

```
(adaptAssignmentOfPulse[2D, HSQC, basic, TOCSY,
  by[basic -> #]];
 drawPulseSequence[2D, HSQC, #, TOCSY])& /@
 {gradientSelected, editedGradientSelected, gradientEnhanced};
```

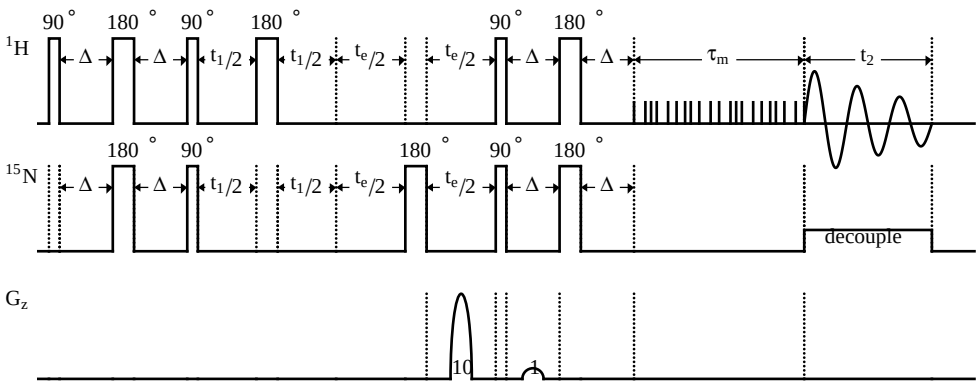

Figure X.3. 2D edited gradient selected HSQC TOCSY .

See `nmr.dta` for the intermediate expressions that reconstruct Figure 4.1, and (re)construct the further diagrams in this note.

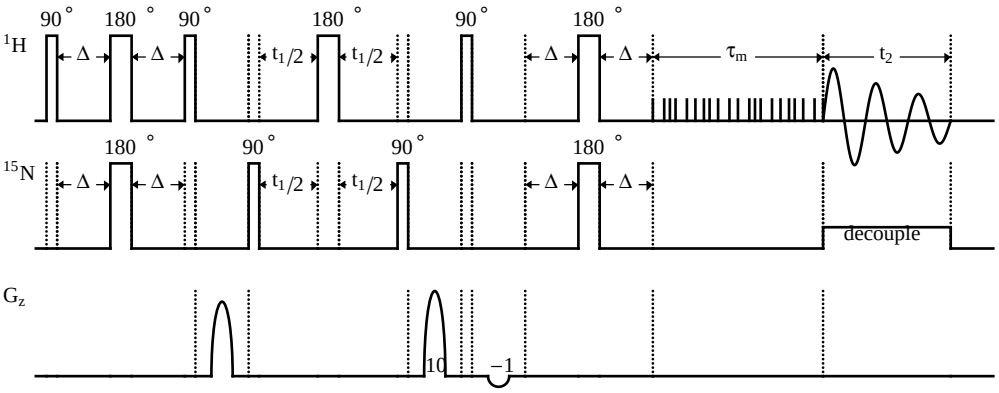

Figure X.4. 2D gradient enhanced HSQC TOCSY.

Construction of Figures 4.2, X.5, X.6, X.7

```
hsqcList =
 {basic, gradientSelected, editedGradientSelected, gradientEnhanced}

(pulseSeq[2D, TOCSY, HSQC, #] =
  pulseSeq[2D, HSQC, #] //
   insert[spinLock[taum], on[H1], before[delay[Delta], 1] ];
drawPulseSequence[2D, TOCSY, HSQC, #])& /@ hsqcList
```

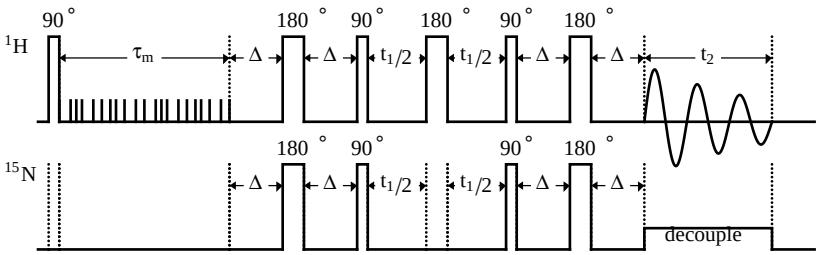

Figure 4.2. 2D basic TOCSY HSQC.

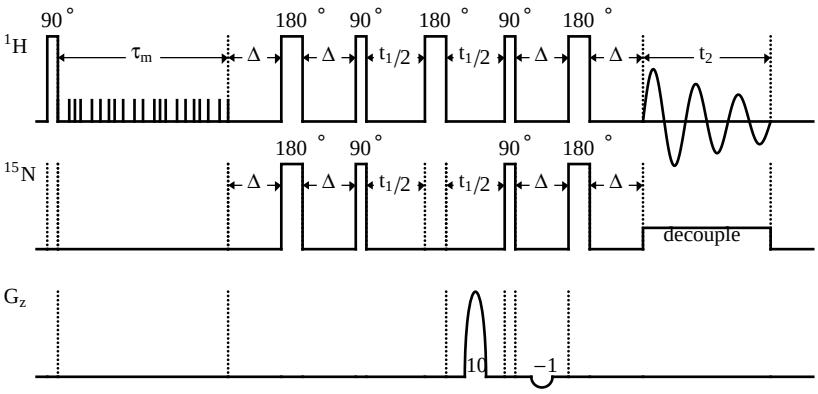

Figure X.5. 2D gradient selected TOCSY HSQC.

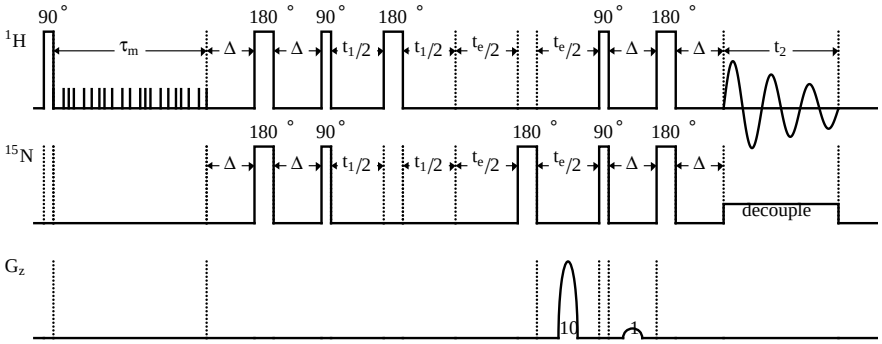

Figure X.6. 2D edited gradient selected TOCSY HSQC.

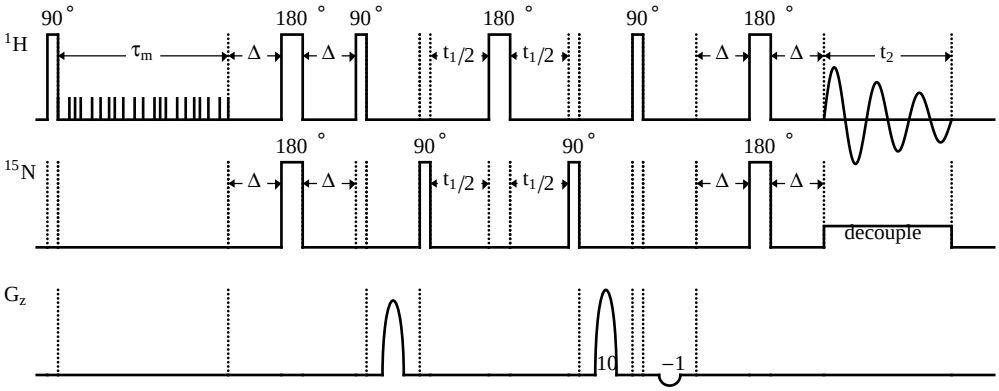

Figure X.7. 2D gradient enhanced TOCSY HSQC.

Construction of Figures 4.3, X8, X9, X10

```
list[3D, HSQC, TOCSY] =
(pulseSeq[3D, HSQC, #, TOCSY] = pulseSeq[2D, HSQC, #, TOCSY] //
  pipe[insert[spinEcho, on[N15], before[spinLock]], t2 -> t3, te -> t2];
  drawPulseSequence[3D, HSQC, #, TOCSY])&  /@ hsqcList
```

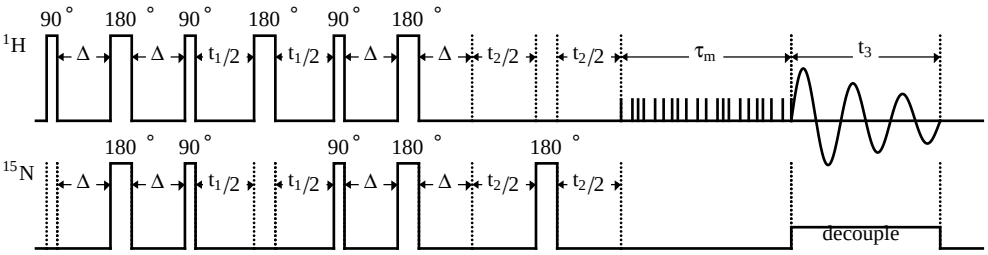

Figure 4.3. Basic 3D HSQC TOCSY.

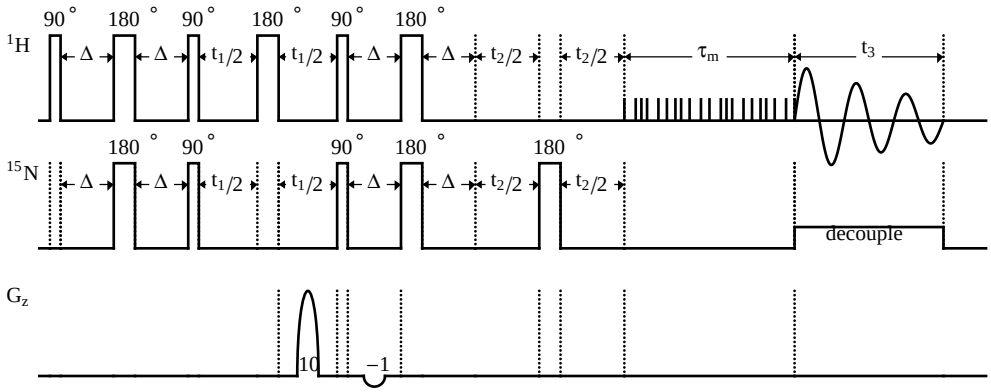

Figure X.8. 3D gradient selected HSQC TOCSY.

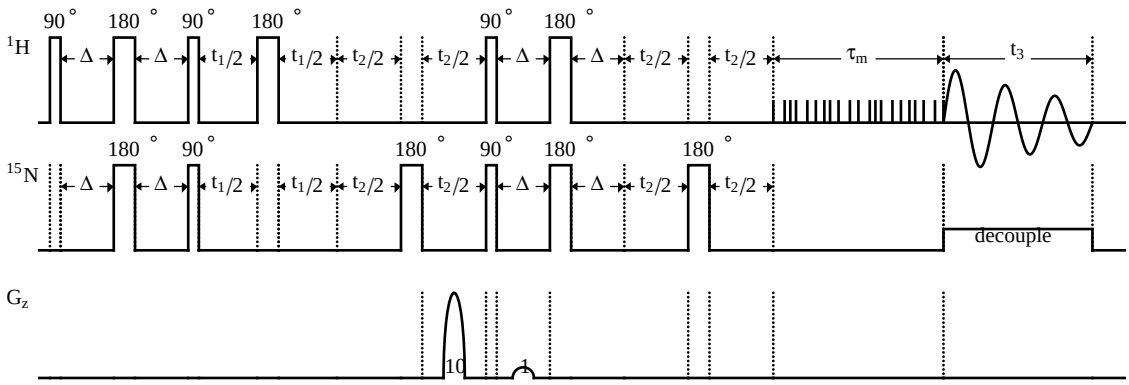

Figure X.9. 3D edited gradient selected HSQC TOCSY.

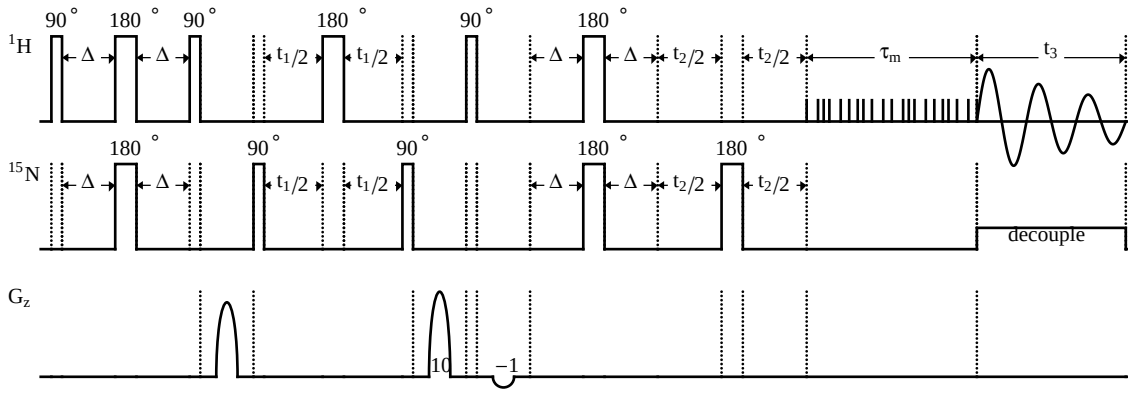

Figure X.10. 3D gradient enhanced HSQC TOCSY.

Construction of Figures 4.4, X11, X12, X13

```
list[3D, TOCSY, HSQC] = adaptAssignmentOf[ list[3D, HSQC, TOCSY],
   by[sequence[HSQC, #, TOCSY] -> sequence[TOCSY, HSQC, #]  ] ]
=>
list[3D, TOCSY, HSQC] =
(pulseSeq[3D, TOCSY, #, HSQC] = pulseSeq[2D, TOCSY, #, HSQC] //
  pipe[insert[spinEcho, on[N15], before[spinLock]], t2 -> t3, te -> t2];
  drawPulseSequence[3D, TOCSY, #, HSQC])&  /@ hsqcList
```

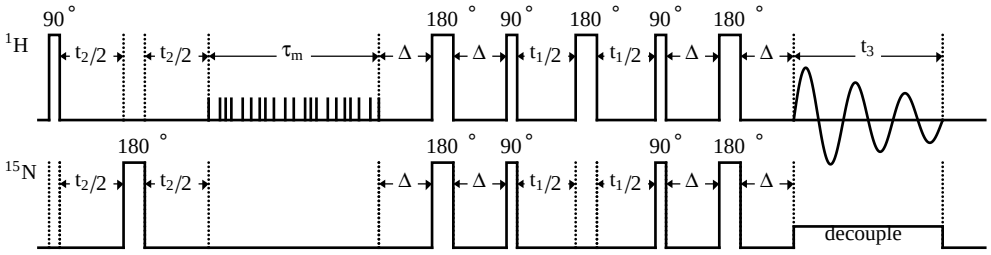

Figure 4.4. 3D basic TOCSY HSQC.

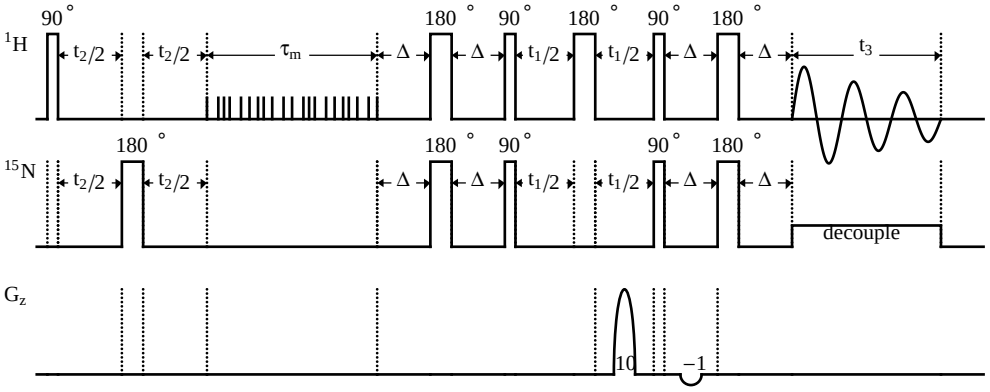

Figure X.11. 3D gradient selected TOCSY HSQC.

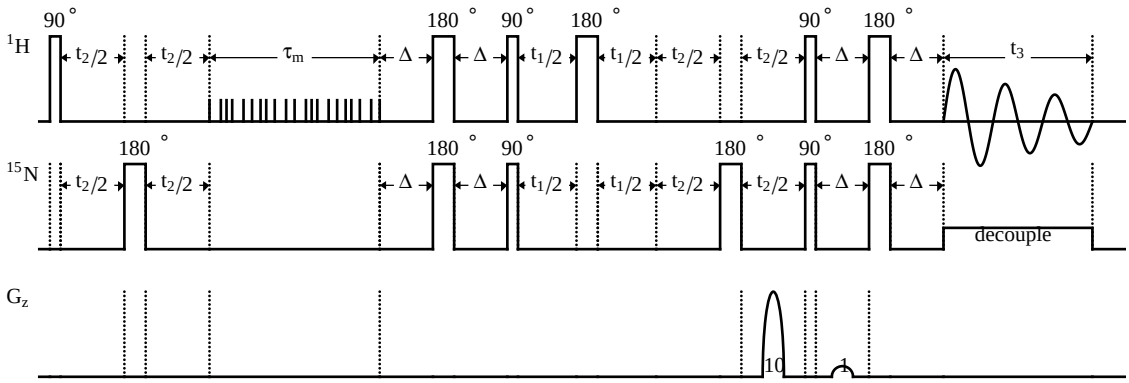

Figure X.12. 3D edited gradient selected TOCSY HSQC.

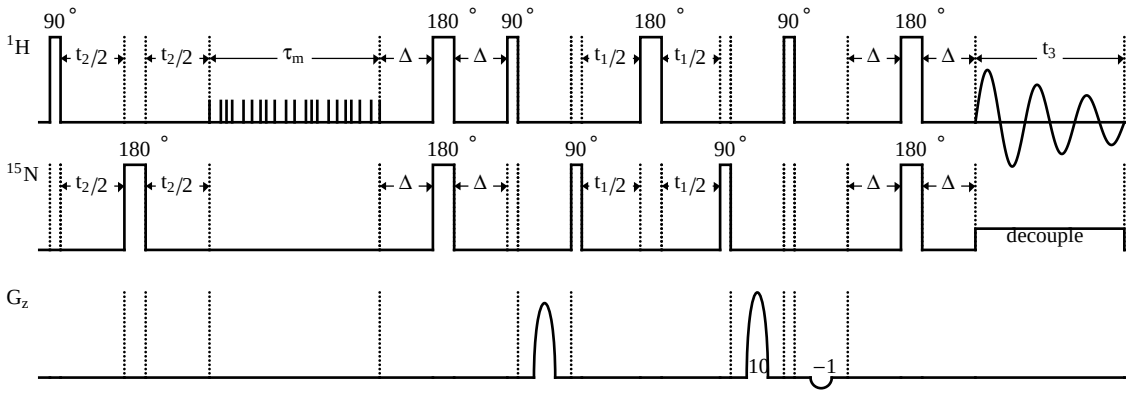

Figure X.13. 3D gradient enhanced TOCSY HSQC.

Acknowledgements

This work could not have been done without the expertize and patience of the computer experts to whom the authors have turned on an almost daily basis. In particular, we thank Dan Nordlund in the Chemistry Department, Neal Bituin, Greg Blaha, Tom Byrne, Dan Candeto, Mark Giannullo, Tom McStravock, Jesse Saunders, Eric Swingle, Donna Sy and Brad Wells in the Help Desk team of the Office of Information Technology, accessible 24/7, and Tom Francais, Becky Goodman, Paula Hulick and Mark Talarick, in other OIT groups.