**NEO 900 solution NMR infosheet**

*NEO || CP2.1 5mm TCI 1H/15N/13C/2H Z-GRAD z168416 /0002 || Topspin 4.1.4*/opt/nmrdata/user

**Temperature**

* flow 535 l/h, BCU medium for 298-308 K: correction implemented
* flow 535 l/h, BCU maximum for 288-298 K: correction implemented

**Sample loading**

* via the sampleCase changer: *sx* # (*sx ej* to only eject sample)
* sampleCase cooling via *vtudisp*, or via *edte*

**Shimming**

* use *ts1dz6* or *ts3d* macro for shimming, *ts1dc*/*ts3dc* for small molecule shimming (z1-correction +16 applied); report: QF ~ 0.4 for good shim

**Tuning/matching**

* use *atma high* for automatic, *atmm* for manual (*atma f1* for only 1H channel)

**Maximum pulse powers and typical pulse lengths**

1H @ –11 dB / 12.6 W = 6-15 us (depending on salt level, 3 vs 5 mm tubes)

13C @ –22.3 dB / 135 W = 13 us

13C @ –3.5 dB / 2.2 W = 100 us (decouple pulse for aliphatic 13C w/ GARP)

15N @ –24.3 dB / 270 W = 36.5 us

15N @ –4.7 dB / 3 W = 320 us (decouple pulse)

2H @ 34.8 W = 74 us

2H @ 11 W = 172us (decouple pulse)

**Protocol:**

* set temperature: *edte* (select appropriate correction)
* load sample via sampleCase: *sx #*, where # is the holder number
* use *hvi\_setup* macro to create dataset, fill out your sample and conditions details
* follow step-by-step instructions in the created dataset
* lock your sample: *lock* (select your solvent, i.e. 90%H2O+10%D2O)
* tuning/matching: *atma high* (or e.g *atma f1 exact*; *atma f2 coarse*; *atma f3 exact*)
* shimming: *ts1dz6,* quality factor in report should be =< 0.4-0.5
* *re 1*: 1H pulse calibration (*pulsecalTCI*); determine H2O offset
* *re 2*; 15N pulse calibration
* *re 3*; 13C pulse calibration
* *re 4*; inspect 1D w/o decoupling
* *re 5*; inspect 1D w/ 15N/13C decoupling
* *re 6*; record 15N TROSY (always TROSY at 900, also small proteins!)
* *re 7*; record 13C HSQC (CT)
* *i* or *edc* to create new expnos
* rpar *experiment\_of\_interest*
* save parameter-sets whenever appropiate (*wpar*)