

PINMRF

Bruker Avance / ARX NMR Spectrometers - Training Supplement for Advanced 1D NMR Spectroscopy

INCLUDING:

- Avance DRX500-1 w/ 5mm TXI Cryoprobe – 367 WTHR**
- Avance DRX500-2 w/ 5mm TXI or BBO Probes – G43 RHPH**
- ARX400 w/ 5mm QNP Probe – 369 WTHR**
- ARX300 w/ 5mm QNP Probe – G43 RHPH**
- Avance DPX300 w/ 5mm QNP Probe – 408 HANS**

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Advanced 1D Spectra using Standard Acquisition Macros - Overview

This booklet provides the information necessary to run some advanced 1D NMR spectra on routine samples using PINMRF's Bruker Avance and ARX-series NMR Spectrometers. These experiments require a minimum of operator intervention or optimization, and as such they are appropriate for the non-expert NMR user to carry out. Note that not all experiments are available for every instrument or probe. These experiments are set up using customized setup macros designed to work with PINMRF's dedicated parameter sets. These should provide good results, with minimal operator effort, for normal organic and organometallic samples in typical organic solvents or D₂O. However, if the ultimate in sensitivity or resolution is required in your work, or your sample is unusual or demanding in some way, please contact PINMRF staff for assistance with more highly specialised experiments.

The experiments presented here include the following:

1. The ¹³C DEPT experiment;
2. ¹H homonuclear decoupling;
3. ¹H nOe-difference spectroscopy;
4. peak suppression in ¹H NMR using presaturation.

Each experiment section includes all relevant instructions so that each one can be followed without referring to another experiment in this booklet. Note that some of these experiments require that probe tuning should be carried out on all relevant nuclei. See pp. 12-15 of the PINMRF manual [Bruker Avance / ARX NMR Spectrometers - Training Guide for Basic 1D NMR Spectroscopy](#) for information regarding probe tuning. These notes assume that the reader is already checked out for basic 1D operation on PINMRF's Bruker Spectrometers.

NOTE – DRX500-1:

Prior to acquiring any data using the cryoprobe, please check through the instructions on the yellow sheet to make sure that you know how to operate the system correctly!! If you are using a non-standard experiment, you must also check the Bruker publication [Typical Pulses for the 5mm Cryoprobe](#), a copy of which is in the binder, to ensure that you will not exceed the probe's power limits.

Bruker Avance / ARX NMR Spectrometers - ¹³C DEPT Instructions

For an overview of the DEPT experiment, see NOTE a) at the end of the instructions.

1. Run the conventional proton spectrum using the standard parameters as described elsewhere.
2. Process and phase the proton spectrum as normal.
3. If the proton spectrum is OK, it is advantageous to run the carbon-13 spectrum prior to running the DEPT spectrum. If time permits, run the carbon-13 spectrum using the standard parameters.

NOTE – DRX500-1:

3a. **Before** starting C13 or DEPT spectra, type **crplock** to set the cryoprobe preamplifiers correctly for C13 observation. Then proceed as outlined above. NOTE: when you want to observe H1 again, you will need to type **crpon** prior to starting the proton acquisition.

4. Process and phase the carbon-13 spectrum as normal.
5. Type **wrpa** followed by a new experiment number to copy the current dataset to a new dataset with the requested experiment number. For example, if the current dataset has the name "smellythiol" and the experiment number "2", typing **wrpa 3** will copy "smellythiol / 2" to "smellythiol / 3".
6. Type **re** followed by the new experiment number to go to the new dataset. Following the example above, type **re 3** to go to experiment number 3.
7. If you are using a 500 MHz spectrometer, check the tuning of both the proton and carbon-13 coils as described elsewhere.
8. Run the experiment with sample spinning ON.
9. In the new dataset, type **deptjsh** to convert the current experiment into the DEPT experiment. NOTE: if you did not run the carbon-13 spectrum as described above, you must read the correct C13 parameter set (using **rpar**) in the current experiment before executing the

deptjsh command. A reminder message will show, click OK if you are ready to start. At this point, a dialog begins, and you should enter the following:

- a) Enter type of DEPT experiment (45, 90 or 135): 135 (see NOTE a) below)
- e) Enter number of scans: 16 (or any multiple of 8)
- f) Enter number of dummy scans: 4
- g) Enter average J value: 150 (default value, see NOTE c))

The data will be acquired automatically after the parameter input is complete (there is no need to type zg).

10. After the acquisition completes process the data in the normal fashion. Keep in mind that the DEPT-135 will have both positive and negative peaks (see NOTE a)).

11. **COMPARING SPECTRA USING THE DUAL DISPLAY MODE:** Go to the expno of the DEPT spectrum (e.g., re 3). To set up the dual display function, type edc2 to enter the dataset info. In the edc2 menu enter the following values:

expno2:	expno of standard ¹³ C spectrum (in our current example, <u>2</u>)
procno2	<u>1</u>
expno3	DEPT expno (<u>3</u> in our example)
procno3	<u>2</u>

Then click the SAVE button on the lower left of the pop-up window.

To compare the reference and decoupled spectra, type dual to enter the dual display mode. The spectrum display will now have the DEPT spectrum (expno 3) in green and the standard ¹³C spectrum (expno 2) in purple displayed together. The buttons on the upper left can be used to expand and manipulate the display. To exit the dual display mode, click the RETURN button on the bottom of the left side of the window.

12. Repeat steps 5, 6 and 9, above, to acquire other DEPT spectra.

NOTES - DEPT:

a) The DEPT (Distortionless Enhancement by Polarization Transfer) experiment is a multipulse experiment that allows the determination of the different types of carbon atoms present in a molecule. The number at the end of the DEPT string (e.g. DEPT-45, DEPT-135) refers to the

duration in degrees of the last ^1H pulse in the pulse sequence, which is the part of the pulse sequence which actually differentiates between the types of carbon atoms. The DEPT-45 experiment shows all of the protonated carbons with positive phase. The DEPT-90 experiment shows only the $-\text{CH}-$ carbons, with positive phase. The DEPT-135 experiment shows $-\text{CH}_3$ and $-\text{CH}-$ carbons with positive phase and $-\text{CH}_2-$ carbons with negative phase. Quaternary carbons do not appear in any DEPT spectrum. Appropriate combinations of the different DEPT spectra on a given molecule can provide for subspectra of each different type of carbon atom to be generated.

b) The sensitivity of the DEPT experiment is higher than that of a normal ^1H -decoupled ^{13}C spectrum, up to a factor of two. DEPT spectra by default are also ^1H -decoupled.

c) Other than the ^1H pulse duration, the only other variable in the DEPT pulse sequence is the one-bond ^1H - ^{13}C J-coupling. Usually an approximate average value is used, which for most small organic molecules is on the order of 130 - 160 Hz.

Bruker Avance / ARX NMR Spectrometers - Proton Homonuclear Decoupling Instructions

21. Run the conventional proton spectrum using the standard parameters as described elsewhere.

22. Process and phase the proton spectrum as normal.

23. Type `wrpa` followed by a new experiment number to copy the current dataset to a new dataset with the requested experiment number. For example, if the current dataset has the name "smellythiol" and the experiment number "1", typing `wrpa 2` will copy "smellythiol / 1" to "smellythiol / 2".

24. Type `re` followed by the new experiment number to go to the new dataset. Following the example above, type `re 2` to go to experiment number 2.

25. **SET THE DECOUPLER FREQUENCY:** Expand the spectrum about the peak you want to decouple. Click with the left mouse button on the UTILITIES button to the left of the spectrum. Then click on the O2 button with the left mouse button. Then move the mouse pointer to the spectrum area (the pointer will jump to the spectrum) and place the cursor on the center of the multiplet you want to decouple. Click the middle mouse button to define this

frequency as the decoupler frequency (parameter O2). Then click the RETURN button on the lower left of the screen to return to the normal spectrum display.

26. If you are using a 500 MHz spectrometer, check the tuning of the proton coil as described elsewhere.

27. Run the experiment with sample spinning ON.

28. In the new dataset, type `homodecjsh` to convert the current experiment into the homodecoupling experiment. A reminder message will show, click OK if you are ready to start. Enter/confirm the parameters that are requested – usually the default values will work fine. The data will be acquired automatically after the parameter input is complete (i.e., there is no need to type ZG).

29. After the acquisition completes process the data in the normal fashion.

30. Expand the decoupled peak to check for complete decoupling. If decoupling is not complete, adjust the decoupler power. To do this, type `pl14` (Avance spectrometers) or `dl2` (ARX spectrometers) and enter a new value that is 3 - 6 units lower numerically than the current value (i.e., if the current value is 45, enter 42 or 39). Do not enter a pl14/dl2 value less (numerically lower) than 30! Repeat the experiment by re-running it using the `zg` command, then re-check for complete decoupling.

31. **COMPARING SPECTRA USING THE DUAL DISPLAY MODE:** Go to the expno of the spectrum with the peak that has been decoupled (e.g., `re 2`). To set up the dual display function, type `edc2` to enter the dataset info. In the `edc2` menu enter the following values:

expno2: expno of reference spectrum (in our current example, 1)

procno2 1

expno3 current expno (2 in our example)

procno3 2

Then click the SAVE button on the lower left of the pop-up window.

To compare the reference and decoupled spectra, type `dual` to enter the dual display mode. The spectrum display will now have the decoupled spectrum (expno 2) in green and the reference spectrum (expno 1) in purple displayed together. The buttons on the upper left can be used to

expand and manipulate the display. To exit the dual display mode, click the RETURN button on the bottom of the left side of the window.

32. Repeat steps 3, 4 and 5, above, followed by the command `ZG`, to acquire spectra with other peaks decoupled.

Bruker Avance / ARX NMR Spectrometers - Proton nOe-Difference Experiment Instructions

Please read the notes at the end of these instructions for some discussion and hints regarding this experiment.

41. Run the conventional proton spectrum using the standard parameters as described elsewhere.

42. Process and phase the proton spectrum as normal.

43. Type `wrpa` followed by a new experiment number to copy the current dataset to a new dataset with the requested experiment number. For example, if the current dataset has the name "smellythiol" and the experiment number "1", typing `wrpa 2` will copy "smellythiol / 1" to "smellythiol / 2".

44. Type `re` followed by the new experiment number to go to the new dataset. Following the example above, type `re 2` to go to experiment number 2.

45. **PUT THE IRRADIATION FREQUENCIES INTO A FREQUENCY LIST:** Expand the spectrum about the peak(s) you want to irradiate. Click with the left mouse button on the UTILITIES button to the left of the spectrum. Then click on the FRQLIST button with the left mouse button. At this point, a dialog begins, and you should enter the following (user input is underlined - terminate input with the return key):

- | | |
|--|--|
| a) Please enter type of list (f1, f2, f3): | <u>f1</u> (Avance spectrometers) or
<u>f2</u> (ARX spectrometers) |
| b) Please enter name of f1/f2 list: | <u>usernoediff</u>
(where "user" = your login ID) |
| c) Write name of f1/f2 list to acqu parameters?: | <u>y</u> |
| d) Freq. list exists, append, overwrite or quit: | <u>o</u> (this question may not appear) |

Now move the mouse pointer to the spectrum area (the pointer will jump to the spectrum) and place the cursor in an area of the spectrum close to the peak(s) you want to irradiate, but not on any peak (i.e., in a baseline region). Click the middle mouse button to define this frequency - an arrow will show up above the spectrum at this point. This frequency will be used to define the reference spectrum that the other irradiated spectra will be compared to when generating the difference spectra. Now move the mouse pointer to the center of a peak you want to irradiate then click the middle button again to add this frequency to the list. Repeat this process for all the peaks of interest. When you have added all the peaks you want irradiated, click the left mouse button to terminate the frequency list input. Then, click the RETURN button on the lower left of the screen to return to the normal spectrum display. See NOTE a), below, for more information.

46. If you are using a 500 MHz spectrometer, check the tuning of the proton coil as described elsewhere.

47. Turn off sample spinning. Turn on the VT controller if your data acquisition will last longer than ca. 30 minutes.

48. In the new dataset (expno 2, in our example), type `noediffjsh` to convert the current experiment into the nOe difference experiment. A reminder message will show, click OK if you are ready to start. At this point, another dialog begins, and you should enter the following:

- | | |
|---------------------------------------|---|
| a) Name of frequency list: | <u>usernoediff</u> (as above)
(where “user” = your login ID) |
| b) Irradiation time in seconds (=d1): | <u>4</u> (default should be OK) |
| c) Irradiation power level | <u>60</u> - <u>39</u> (see NOTE b) below) |
| d) # of irradiation points: | <u>2</u> or more - check it's correct |
| e) # of scans: | <u>8</u> |
| f) # of dummy scans: | <u>4</u> |
| g) # of time average cycles: | <u>1</u> (or more, see NOTE c) below) |

The data will be acquired automatically after the parameter input is complete (there is no need to type ZG). Various informational messages will show on the screen. Each irradiation frequency will be acquired in a new, sequential, expno.

49. After the acquisition completes process the data in the first expno in the normal fashion.

Unless you have specifically moved between different expno's, this will be the current expno.

50. Type `multiefp` to start the processing macro. When requested, enter the current expno and the number of expno's to process (this should be the same as the number of irradiation points, above). The macro will carry out Fourier transformation and phase correction on all of the spectra in sequential expno's.

51. Go to the expno of one of the spectra with a peak that has been irradiated (e.g., `re 3`) Expand the irradiated peak to check for complete saturation (i.e., the selected peak should be gone). If saturation is not complete, you will need to go back to the first expno of the nOe difference series (e.g. `re 2`) and re-run the experiment. When the "Irradiation power level:" question appears, enter a new value that is 3 - 6 units lower numerically than the initial value (i.e., if the current value is 60, enter 57 or 54). Do not enter a value less (numerically lower) than 30! Repeat the experiment to check the completeness of saturation. See NOTE b) for further discussion.

52. COMPARING SPECTRA USING THE DUAL DISPLAY MODE: Go to the expno of the first spectrum with a peak that has been irradiated (e.g., `re 3`). To set up the dual display function, type `edc2` to enter the dataset info. In the edc2 menu enter the following values:

expno2: expno of reference spectrum (in our current example, 2)

procno2 1

expno3 current expno (3 in our example)

procno3 2

Then click the SAVE button on the lower left of the edc window.

To compare the reference and irradiated spectra, type `dual` to enter the dual display mode. The spectrum display will now have the irradiated spectrum (expno 3) in green and the reference spectrum (expno 2) in purple displayed together. The buttons on the upper left can be used to expand and manipulate the display. To exit the dual display mode, click the RETURN button on the bottom of the left side of the window.

53. OBTAINING THE DIFFERENCE SPECTRUM: While still in the dual display mode, click the DIFF button on the left to subtract the spectrum in EXPNO2 from that in EXPNO1 - i.e., the purple spectrum is subtracted from the green one. This spectrum should show the irradiated peak with full negative intensity, and any peaks that show a nOe to this peak will show

up as weak positive peaks. Peaks that are dispersive (up and down) are subtraction artifacts and cannot reliably be considered to be the result of a nOe interaction. If these are present they sometimes can be minimized by left-clicking on the HOR. SHIFT button on the left menu and moving the mouse left to right. This shifts the spectra relative to one another and sometimes can improve the quality of the subtraction. If you want to save the difference spectrum, click the RETURN button on the bottom of the left side of the window, followed by SAVE & RETURN in the pop-up menu that will appear. A new pop-up will appear asking you to confirm the target expno and procno of the difference spectrum. Check that this is the same as what was entered above, and if so, click OK. If not, click CANCEL, and the software will open the edc2 menu again to allow changes.

54. The difference spectrum can be manipulated like any spectrum. The dataset title is not stored with it so that information will have to be re-entered (`setti`) prior to printing. The difference spectrum can be integrated, and I recommend setting the value of the integral of the irradiated peak to be -100 for peaks comprising one proton, -200 for those from two protons and -300 for those from three protons (e.g. methyl groups). The remaining integrals can then be read as percentages. This spectrum can be printed, but the plot settings in `edg` will need to be checked and/or adjusted.

55. To go back to one of the other spectra of the nOe difference series the correct procno must be specified. Thus, to go back to expno 2, enter `re 2 1` (read expno 2 procno 1). The `edc` command also can be used to enter the desired dataset's information. See NOTE d), below, for more about moving between datasets when multiple procno's are in use.

NOTES:

- a) In general, an nOe difference measurement will require at least two, ideally more, irradiation frequencies: the reference (off-resonance) frequency, and the peak of interest and its nOe partner(s). It is usually beneficial to obtain difference spectra with irradiation of all nOe-interacting partners.
- b) When setting the irradiation power, keep in mind the following. Broader peaks require more power than do narrow ones, and peaks that are very close to another resonance should be irradiated with a minimum amount of power in order to reduce the possibility of partly irradiating another peak. In this case a longer irradiation time may be beneficial.

- c) The nOe difference experiment set up presented in this discussion allows the entire series of irradiations to be repeated for signal averaging. For example, if you needed to run 64 scans for each irradiation, it could be done in one of two ways: the number of scans could be set to 64 (step 8e), and the number of cycles set to one (step 8g), or the number of scans could be set to eight (step 8e) and the number of cycles set to eight (step 8g). The latter setup (8 x 8) is recommended, as it will reduce the effects of any drifting or instability that might be present.
- d) When working with datasets that have multiple expno's and multiple procno's within each expno, keep in mind that when using the `re` or `edc` commands to move between datasets, the correct procno for the target dataset must be set. My recommendation is to always use procno 1 for the target (e.g., type `re 3 1` instead of just `re 3`), which will guarantee that you will end up in the correct target expno.
- e) The sample quality is particularly important for nOe-based experiments. For more information on this, please see pp. 11-12 of the PINMRF manual [Bruker Avance / ARX NMR Spectrometers - Routine/Survey 2D Spectra using Standard Parameter Sets.](#)

Bruker Avance / ARX NMR Spectrometers - Proton Presaturation

61. Run the conventional proton spectrum using the standard parameters as described elsewhere.
62. Process and phase the proton spectrum as normal.
63. Type `wrpa` followed by a new experiment number to copy the current dataset to a new dataset with the requested experiment number. For example, if the current dataset has the name "smellythiol" and the experiment number "1", typing `wrpa 2` will copy "smellythiol / 1" to "smellythiol / 2".
64. Type `re` followed by the new experiment number to go to the new dataset. Following the example above, type `re 2` to go to experiment number 2.
65. **SET THE IRRADIATION FREQUENCY:** Expand the spectrum about the peak you want to irradiate. Click with the left mouse button on the UTILITIES button to the left of the spectrum. Then click on the O2 button with the left mouse button. Then move the mouse pointer to the spectrum area (the pointer will jump to the spectrum) and place the cursor on the center of the peak you want to remove (saturate). Click the middle mouse button to define this

frequency as the decoupler frequency (parameter O2). Then click the RETURN button on the lower left of the screen to return to the normal spectrum display.

66. If you are using a 500 MHz spectrometer, check the tuning of the proton coil as described elsewhere.

67. Turn off sample spinning.

68. In the new dataset, type `presatjsh` to convert the current experiment into the presaturation experiment. A reminder message will show, click OK if you are ready to start. Enter/confirm the parameters that are requested – usually the default values will work fine. The data will be acquired automatically after the parameter input is complete (i.e., there is no need to type Zg).

69. After the acquisition completes process the data in the normal fashion.

70. Expand the irradiated peak to check for complete saturation. If saturation is not complete (enough), adjust the decoupler power. To do this, type `pl14` (Avance spectrometers) or `dl2` (ARX spectrometers) and enter a new value that is 3 units lower numerically than the current value (i.e., if the current value is 45, enter 42). Do not enter a pl14/dl2 value less (numerically lower) than 30! Repeat the experiment by re-running it using the `Zg` command, then re-check the saturation efficiency.

71. Repeat steps 3, 4 and 5, above, followed by the command `Zg`, to acquire spectra with other peaks irradiated.

XWINNMR

Commonly Used Keyboard Commands

NOTE THAT ALMOST ALL COMMANDS ARE AVAILABLE FROM THE PULL-DOWN MENUS AT THE TOP OF THE SPECTRUM DISPLAY

Parameter Setup

edc - edit current dataset - reads existing and/or creates new datasets
eda - edit acquisition parameters
ased, edasp - edit acquisition parameters - pulse program driven or nucleus-related
gpro - update current experiment with current probe's pulse calibration parameters
edte - set up temperature controller parameters
edp - edit processing parameters
edg - edit graphics parameters - controls plot output attributes
wrpa - copy current dataset to a new one - specify new name and experiment number
re - read new dataset - specify new name and experiment number

Data Acquisition

lockdisp - display lock window
lock - start autolocking routine using Bruker default parameters
rpar - read parameter set
rsh - read shim set
wsh - save shim set - enter a unique name in the menu
ii - initialize interfaces
acqu - display acquisition window - shows FID on screen
wobb - start wobble routine for probe tuning
rga - set receiver gain automatically
ns - number of scans
2s ns - display number of scans stored with current dataset
zg - zero current data and start acquisition
go - start data acquisition
tr - transfer FID to disk for processing
halt - halt data acquisition after next scan
stop - stop data acquisition immediately
standard - set up spectrometer for CDCl₃ standard sample

Data Acquisition - DRX500-1 - Cryoprobe Specific

crpon - enable cold preamplifier for H1 observation
crplock - enable warm preamplifier for C13 observation
cwobb - start wobble routine for cryoprobe tuning

Custom Acquisition AU Programs for Advanced 1D Spectra

deptjsh – turn current C13 dataset into DEPT experiment and acquire

homodecjsh – turn current H1 dataset into a homodecoupling experiment and acquire

noediffjsh – turn current H1 dataset into a 1D nOe-difference experiment and acquire

presatjsh – turn current H1 dataset into a presaturation experiment and acquire

Data Processing and Plotting

setti - enter title for plot

ft - Fourier transformation

ef - exponential multiplication and Fourier transformation

efp - carry out “ef” plus apply existing phase corrections to spectrum

multiefp - carry out “efp” on multiple spectra in sequential experiment numbers

lb - controls amount of exponential multiplication

sref – set chemical shift scale reference using TMS or default parameters

nzp - number of data points to zero at start of FID

zp - zero nzp points at start of FID

basl - enter baseline correction routine

pscal - define plot vertical scaling method

cy - plot vertical scaling

cx - plot horizontal scaling

mi - threshold for peak picking

pps - peak picking with output on screen

pp - peak picking with output on paper

view - view plot output on screen

plot - plot spectrum on paper

dual - enter dual display mode - EXPNO2 and PROCNO2 parameters must be correct in the menu

xwinplot - start XwinPlot standalone program using current dataset

xwp - start XwinPlot standalone program using current plot region

Data Handling

dir – show a listing of your experiment names

dirf – show a listing of all 1D FID files (includes experiment names and numbers)

dirser – show a listing of all 2D SER files (includes experiment names and numbers)

dirs – show a listing of all 1D spectra (includes experiment names and numbers)

dir2d – show a listing of all 2D spectra (includes experiment names and numbers)

dels – delete 1D processed spectra (FID’s are not deleted)

del2d – delete 2D processed spectra (SER files are not deleted)

Notes

Bruker Avance / ARX Spectrometer Parameter Sets - 11-01-2006

NOTE: “solv” = solvent = acet, cdcl, d2o, dmsu, or meth (for C₆D₆ use cdcl).

NOTE: some parameter sets do not include a “solv” field in their filename.

Parameter Sets

DRX-500-1 (cryoprobe)

h1.cryo.solv
presat.cryo.d2o
c13.cryo.solv
c13dept.cryo.solv
cosy.cryo.solv
tocsy.cryo.solv
noesy.cryo.solv
hmqc.cryo.solv
hmbc.cryo.solv

DRX-500-2 (bbo or txi probe)

h1.bbo.solv	h1.txi.solv
presat.bbo.d2o	presat.txi.d2o
c13.bbo.solv	c13.txi.solv
c13dept.bbo.solv	c13dept.txi.solv
cosy.bbo.solv	cosy.txi.solv
tocsy.bbo.solv	tocsy.txi.solv
noesy.bbo.solv	noesy.txi.solv
hetcor.bbo.solv	hmqc.txi.solv
p31.bbo	hmbc.txi.solv
p31nd.bbo	
si29.bbo	
ga69.bbo	
ga71.bbo	
n15.bbo	

ARX-400, DPX-300, ARX-300 (qnp probe)

h1.qnp.solv
c13.qnp.solv
c13dept.qnp.solv
f19.qnp.cdcl
p31.qnp.cdcl
p31nd.qnp.cdcl
cosy.qnp.solv
tocsy.qnp.solv
noesy.qnp.solv
hetcor.qnp.solv

Shim Files

DRX-500-1 (cryoprobe)

shims.cryo

DRX-500-2 (bbo or txi probe)

shims.bbo	shims.txi
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ARX-400, DPX-300, ARX-300 (qnp probe)

shims.qnp

