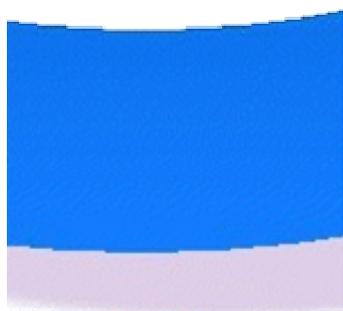


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... *Linear prediction processing technique can double the sensitivity and resolution of the spectra ...*

NMR PROCESSING TECHNIQUE "LINEAR PREDICTION"

KWANCHAI KHONGWATTANANON

Talking about Linear Prediction processing technique, I have to admit that it should have been introduced to our NMR users earlier. Linear Prediction can double the sensitivity and the resolution of the spectra. This technique is time-saving and, above all, it provides better results.

Linear Prediction (LP) is a mathematic processing tool, like other processing tools we are familiar with, such as window function or zero filling. As its name already implies, linear prediction is applied to the FID to predict and add more data points. This is very useful for 2D-NMR, by which our collected series of FID on F1 dimension are never premium

enough, for instance, at 1024 rows (td1). It helps much to gain the better F1 resolution and sensitivity from a limited number of td1, especially in inverse experiments, e.g. HMQC, HSQC, HMBC, where the F1 dimension is ¹³C.

As a matter of fact, there are two types of Linear Prediction which are useful for our works. The first one is "Backward Linear Prediction" used in correcting distorted first data points, but with the digital filter, it might not be that beneficial. The second type is "Forward Linear Prediction", by calculating the data at the end of FID in a 2D experiment, where the acquisition data

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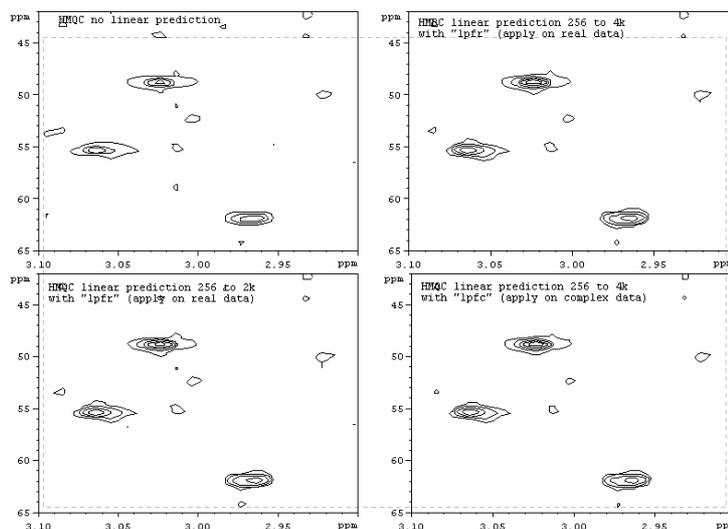


Figure 1: Contour plot of expanded HMQC spectra; (a) upper-left: without forward linear prediction, (b) lower-left: with forward linear prediction on real data to 2048 [8-fold], (c) upper-right: with forward linear prediction on real data to 4096 [16-fold], (d) lower-right: linear prediction on complex data to 4096 [16-fold]. All spectra are plotted with the same scale and threshold.

Linear Prediction

or increment data is short. And this proves to be a real potential advantage, when applying forward linear prediction on F1 dimension, which is mainly discussed here.

As a matter of fact, there are two types of Linear Prediction which are useful for our works. The first one is “Backward Linear Prediction” used in correcting distorted first data points, but with the digital filter, it might not be that beneficial. The second type is “Forward Linear Prediction”, by calculating the data at the end of FID in a 2D experiment, where the acquisition data or increment data is short. And this proves to be a real potential advantage, when applying forward linear prediction on F1 dimension, which is mainly discussed here.

Let’s start with a real experiment. As

shown on figure 1, 4 HMQC spectra are compared, each of which was different from one another only by different processing techniques, i.e. with and without *forward F1 Linear Prediction* {original time domain on F1 (td1) is 256}. One can easily realize the better sensitivity and resolution on contour plots of the spectra with linear prediction, compared to the spectra without linear prediction. There is no major difference between the 8-fold and the 16-fold linear prediction, as well as between linear prediction method applied with real data and with complex data.

We further investigate the ^{13}C cross-sectional spectra (projection as summation of columns) from HMQC experiments, as shown on figure 2, clearly illustrating the higher sensitiv-

ity and resolution for the experiment with linear prediction. It also shows that the spectrum with the 16-fold linear prediction has an averagely better signal-to-noise and resolution than the 8-fold linear prediction.

The last experiment is illustrated on figure 4. The ^1H cross-sectional spectra from a COSY experiment clearly confirm that the 16-fold forward linear prediction gives us the best resolution and sensitivity. The signal-to-noise measurement at the signal of 3 ppm over noise range from 3.5 to 4 ppm (0.5 ppm) shows that the spectra with the 16-fold linear prediction has approximately 20 times better than the spectra without the linear prediction.

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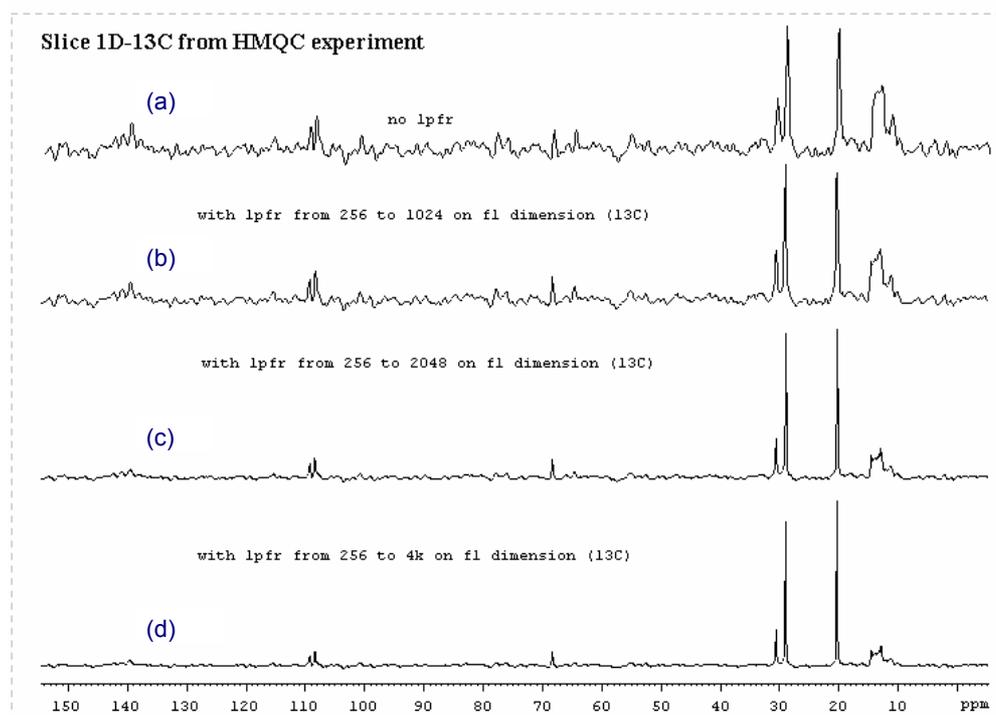


Figure 2: Cross-sectional ^{13}C spectra from 2D-HMQC experiment, (a) no linear prediction, (b) 4-fold linear prediction from 256 to 1024, (c) 8-fold linear prediction from 256 to 2048, (d) 16-fold linear prediction from 256 to 4096

“And this proves to be a real potential advantage, when applying forward linear prediction on F1 dimension, ...”

‘Linear Prediction’

Applying forward linear prediction involves a few set up on processing parameters. *ME-mod* is a linear prediction mode, if set to ‘LPfr’ meaning the forward linear prediction on real data, if to ‘LPfc’ meaning the forward linear prediction on complex data. *NCOEF* is a number of linear prediction coefficients, typically set to 2-3 times the number of expected peaks. *LPBIN* is a number of points for linear prediction. $LPBIN = 0$ means $LPBIN = td$ (2-fold linear prediction). *SI*, the number of points for Fourier transformations, has to be high enough to enable adding of points.

By default (see also figure 2), *ME_mod* is set to LPfr mode, *NCOEF* is set to 32 and *LPBIN* is set to zero (2-fold LP). But to our illustrated examples, the 8-fold or even the 16-fold gives the better

result! Nevertheless, please note that predicting too much points can severely change the lineshape of the signal. We recommend LPBIN at 4-fold ($3 \cdot td$) or 8-fold ($7 \cdot td$). *SI* must be set to be more than $(TD+LPBIN)/2$ for phase sensitive spectra.

Now, you might want to add more points for better resolution and sensitivity by this forward linear prediction to your 2D-NMR spectra. You just simply change some processing parameters as mentioned above and re-process (Fourier transform, xfb) it without losing any data. You also might find out that your default setup for processing parameters already had the forward linear prediction applied.

Enjoy prediction!

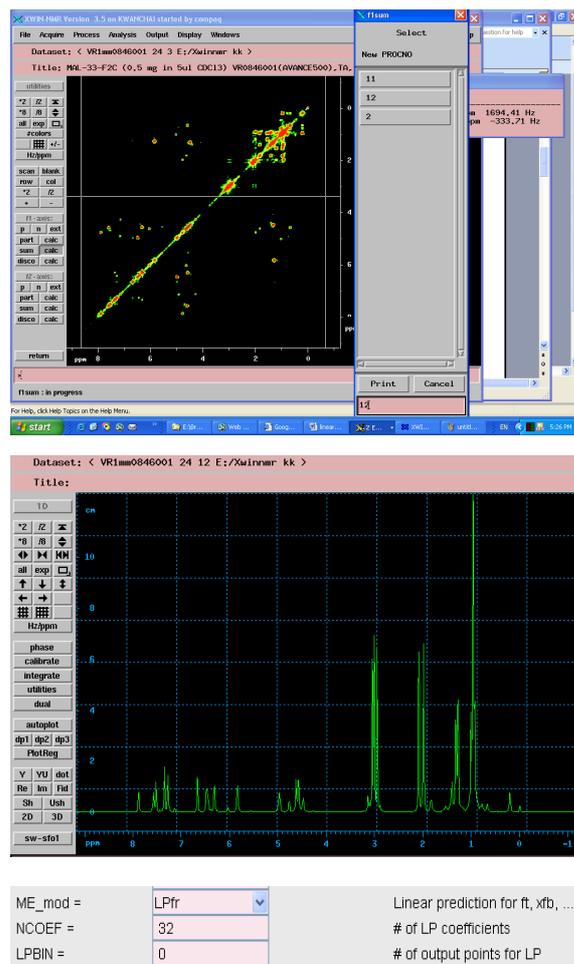


Figure 3: Upper left window shows the “Utilities” page of XWINNMR software, to project 1D as cross-sectional spectra. Upper right window shows the saved cross-sectional spectra. Lowest window shows the important parameters for applying the forward linear prediction.

Slice on f1 dimension from 2D-COSY Experiment

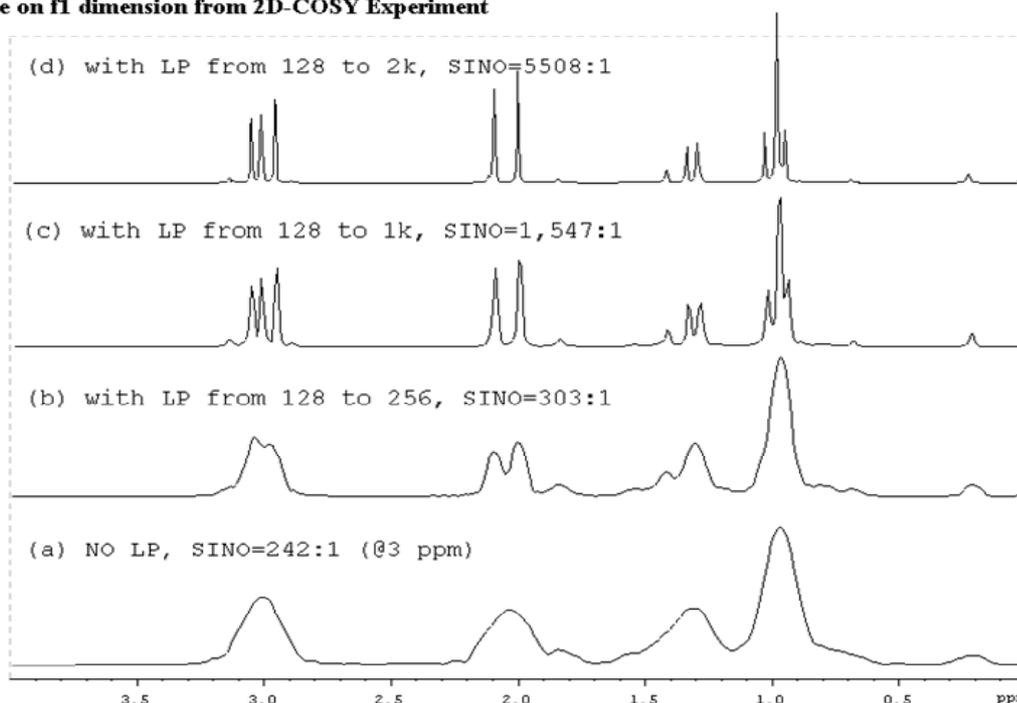


Figure 4: Cross-sectional 1H spectra from 2D-COSY experiment.

- (a) without forward linear prediction, signal-to-noise is 242:1
- (b) with 2-fold (from 128 to 256) forward linear prediction, signal-to-noise is 303:1
- (c) with 8-fold forward linear prediction from 128 to 1024 points, signal-to-noise is 1,547:1
- (d) with 16-fold forward linear prediction from 128 to 2048 points, signal-to-noise is 5,508:1

All spectra have a measurement of signal-to-noise at 3 ppm over noise range 0.5 ppm (from 3.5 to 4 ppm).

Our NMR service meeting on 29th October 2004, at Pathumwan Princess hotel was another successful event. Thanks to 16 Ajarns from almost all universities/institutes who attended this meeting. We had a great discus-



sion among us about the service and maintenance issues. We will maintain the quality of service and always seek ways to make it better, as one of our main missions. Thank you very much again for your contribution!

Photos from the NMR service meeting 29oct2004



Visit your NMR LAB Year 2005

As some of you may know, Bruker Thailand was established in February 1996 by Peter Sprenger as the first Bruker office in this Southeast Asian region. Year 2005 is the next full step to the 10th year anniversary of our business operation here. Without your trust in our products and services, we would not have come this far. To show our appreciation of your continued support, we would like to take this opportunity to thank all of you with a very special way, that is, we are pleased to offer a free-of-charge visit to your NMR laboratory. This proposal includes a one full-day visit for service and a talk in any NMR topics. Also, you can specify your requirements, as you see appropriate for your research works. This offer is to emphasize our main long-term mission

as your research partner contributing as much as possible to the Thai scientific and research community.

Please feel free to sign-up for this complimentary offer. On next page you can find the sign-up form.

MERRY CHRISTMAS AND
HAPPY NEW YEAR

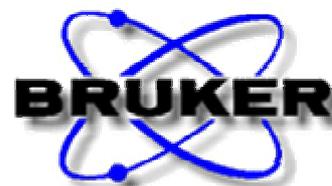


WE WISH YOU ALL THE BEST
FOR THE COMING YEAR!

... as our main long
term business mission
in Thailand as your
partner contributing
to ...

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