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Noise Suppression in NMR Spectrum by Using Wavelet Transform Analysis

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Abstract: Wavelet transforms are introduced as a new tool to distinguish real peaks from the noise contaminated NMR data in this paper. New algorithms of two wavelet transforms including Daubechies wavelet transform as a discrete and orthogonal wavelet transform (DWT) and Morlet wavelet transform as a continuous and nonorthogonal wavelet transform(CWT) were developed for noise elimination. DWT and CWT method were successfully applied to the noise reduction in spectrum. The inevitable distortion of NMR spectral baseline and the imperfection in noise elimination were observed in DWT method while CWT method gives a better baseline shape and a well noise suppressed spectrum.

INTRODUCTION

Fourier transform (FT) is most widely used in the conversion of time domain multinuclear multidimensional NMR signals or free induction decay into a frequency domain spectrum. After the introduction of wavelet transform by Morlet and his coworkers in 1984,[1,2] applications of wavelet transform have been received a great attention from researchers in many different areas. Two types of wavelet transform including discrete wavelet transform (DWT) and continuous wavelet transform(CWT) have shown a promising result in such diverse fields as image compression, noise suppression of image, signal processing, computer graphics, and pattern recognition, etc.

Some efforts have been made in the analysis of spectral lines and possible applications to NMR spectroscopy.[3,4]. The application of wavelet transform was successfully achieved in the extraction of dynamic behavior in NMR signal at the beginning with DWT method[5]. For the convenience, orthogonal wavelet transform that can easily return to original domain has been used to eliminate noise signal in image processing and other

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signals in processing areas. As a general orthogonal wavelet transform method of DWT, Daubechies developed useful wavelet transform method in which an operational matrix is applied to the data to make a wavelet coefficients and multiply a transverse matrix of previously used matrix to return to original domain, in 1988.[6] Mallat developed a fast algorithm that can be used with orthogonal wavelet transform.[7] Using Daubechies wavelet transform and Mallat's fast algorithm, a new NMR data processing method were developed.

Morlet wavelet transform using a continuous wavelet transform is categorized to nonorthogonal wavelet transform. Mallat's algorithm used in DWT cannot be used because of nonorthogonal property of Morlet wavelet transform. The inverse wavelet transform of Morlet has to be performed by more complex equation. CWT has not been used specially in NMR because of mathematical complexity. A successful attempt of CWT to NMR spectroscopy was made with an approximate CWT method.[8] If the CWT algorithm is well developed, it can be used in extraction of useful information in NMR signals, dynamic phase correction and large peak suppression.

The most interesting and characteristic of this method is the great improvement of S/N ratio with fast processing time and high resolution. For the purpose of noise elimination, three steps of operation such as wavelet transform, noise elimination in wavelet space, and inverse wavelet transform are basically required.[9] Therefore, forward and backward (inverse) wavelet transform must be considered simultaneously. In order to utilize the advantage of wavelet transform, new algorithms and techniques of DWT and CWT for noise elimination were developed in this current work. Theoretical background of wavelet transforms and noise elimination with wavelet transform are discussed for mathematical simplification of coding and application to NMR signals in following section.

THEORETICAL BACKGROUND

Continuous Wavelet Transform (CWT)

Morlet suggested a definition of the wavelet transform of signal $x(t)$ as Eq. (1).

$$W(a,b) = \langle \Psi_{a,b}(t), x(t) \rangle = |a|^{-1/2} \int x(t) \Psi^{*}_{a,b} dt \quad (1)$$

where Eq. (2) is called as baby wavelet denoting of (*) complex conjugate.

$$\Psi_{a,b}(t) = \Psi\left(\frac{t-b}{a}\right) \quad (2)$$

a and b stand for the scale factor and the time location, respectively[10]. Various functions can be used as mother wavelet $\Psi(t)$ to make a baby wavelet $\Psi_{a,b}(t)$. The transform coefficients $W(a,b)$ can be considered as functions of translation b for each fixed scale a which give the information of $x(t)$ at different levels of resolution.

Classical inversion formula of the signal $x(t)$ from these wavelet coefficients $W(a,b)$ is

$$x(t) = C_{\Psi}^{-1} \int\int W(a,b) \Psi_{a,b}(t) \frac{1}{a^2} da db \tag{3}$$

where
$$C_{\Psi} = \int \left|\hat{\Psi}(\omega)\right|^2 / |\omega| d\omega \tag{4}$$

$$\hat{\Psi}(\omega) = \int \Psi(t) \exp(-j\omega t) dt \tag{5}$$

Another simple inversion formula used by Morlet function is given by Eq. (6)[11]

$$x(t) = C_{1\Psi}^{-1} \int W(a,b) \frac{da}{a^{3/2}} \tag{6}$$

where

$$C_{1\Psi} = \int_{-\infty}^{\infty} \hat{\Psi}^*(\omega) / |\omega| \, d\omega \tag{7}$$

Discrete Wavelet Transform (DWT)

The terminology of "discrete" used in DWT is from the "discretized from CWT". There are three types of discretized wavelet transform.[12] The first type of DWT is given by following Eq. (8)

$$W(m,n) = a_o^{-\frac{m}{2}} \int x(t) \Psi(a_o^{-m} t - n b_o) dt \tag{8}$$

Where the parameters a, b are discretized to $a = a_o^m$ and $b = n b_o a_o^m$ with sampling intervals a_o, b_o and integers m, n. Even though a discretization is made, $x(t)$ and $\Psi(a_o^{-m} t)$ are still continuous for time domain. The second type of DWT is given by the following Eq. (9).

$$W(m,n) = a_0^{-\frac{m}{2}} \sum_k x(k)\Psi(a_o^{-m}k - nb_o) \tag{9}$$

The Eq. (9) is a time discretization of (8) with $t=kT$ and the sampling interval $T=1$. And this is similar to the discrete fourier series where both time and frequency are discrete. The third type of DWT is given by the following Eq. (10).

$$W(m,n) = 2^{-\frac{m}{2}} \sum_k x(k)\Psi(2^{-m}k - n) \tag{10}$$

Here the discrete wavelet $\Psi(k)$ can be a sampled version of continuous counterpart. The Eq. (10) is derived from the Eq. (9) when $\Psi(k)$ is a discretization of $\Psi(t)$, and a_o and b_o are fixed to 2 and 1. Discrete wavelet transform generally refers to the third type of Eq. (10).

Noise Elimination Methods

Signals distinguished from the noisy time domain data in a wavelet space can be more efficiently treated. Therefore, the efficiency of noise elimination increases when a proper noise elimination step is applied in a wavelet space. Two types of noise elimination method including filtering method and threshold method are widely used.

There are several types of filtering method have been used in many applicable areas. The Wiener filter method, is only described in detail in this paper for our algorithm development. Wavelet coefficient W_i is a value of the ith at a given scale and position resulting from a noisy process with a gaussian distribution as follow,

$$P(W_i/\widetilde{W}_i) = \frac{1}{\sqrt{2\pi}B_i}\exp\left[-\frac{(W_i - \widetilde{W}_i)^2}{2B_i^2}\right] \tag{11}$$

where a mathematical expectation is given by $\widetilde{W}_i$, and a standard deviation is given by B_i. Now, the set of expected coefficients W_i for a given scale is assumed to follow a gaussian distribution with a null mean and a standard deviation S_i

$$P(\widetilde{W}_i) = \frac{1}{\sqrt{2\pi}S_i}\exp\left[-\frac{\widetilde{W}_i^2}{2S_i^2}\right] \tag{12}$$

The null mean value results from the wavelet property.

$$\int_{-\infty}^{\infty} \Psi^*(x)dx = 0 \tag{13}$$

The following equations (14) and (15) are derived with an estimation of $\widetilde{W}_i$ from known W_i Bayes' theorem,

$$P(\widetilde{W}_i / W_i) = \frac{P(\widetilde{W}_i)P(W_i / \widetilde{W}_i)}{P(W_i)} \tag{14}$$

$$P(\widetilde{W}_i / W_i) = \frac{1}{\sqrt{2\pi}\beta_i} \exp\left[-\frac{(\widetilde{W}_i - \alpha_i W_i)^2}{2\beta_i^2} \right] \tag{15}$$

where

$$\alpha_i = \frac{S_i^2}{S_i^2 + B_i^2} \tag{16}$$

The probability $P(\widetilde{W}_i / W_i)$ follows a gaussian distribution with mean

$$m = \alpha_i W_i \tag{17}$$

and variance, and is given by Eq. (18)

$$\beta_i^2 = \frac{S_i^2 B_i^2}{S_i^2 + B_i^2} \tag{18}$$

The mathematical expectation of $\widetilde{W}_i$ refers to $\alpha_i W_i$. B_i values can be estimated from the standard deviation of W_i and the variation of a white gaussian noise. S_i values are obtained from $S_i^2 = s_i^2 - B_i^2$, where s_i^2 is the variance of W_i.

Threshold methods are very simple and effective in a wavelet space. Soft threshold and hard threshold method using in many applicable area are described here in detail[13]. Wavelet coefficient smaller than a determined threshold value from the standard deviation of noise is simply discarded in hard threshold method as shown in Eq. (19).

$$W_i = \begin{cases} W_i & \text{if } |W_i| \geq \text{threshold} \\ 0 & \text{if } |W_i| \leq \text{threshold} \end{cases} \tag{19}$$

Wavelet coefficient values smaller than a threshold value are discarded like the hard threshold, and wavelet coefficients greater than the threshold value are shrunken at the same time in soft threshold method.

$$W_i = \begin{cases} \text{sign}(W_i)(|W_i| - \text{threshold}) & \text{if } |W_i| \geq \text{threshold} \\ 0 & \text{if } |W_i| \leq \text{threshold} \end{cases} \tag{20}$$

CODING of WAVELET TRANSFORM and EXPERIMENTS

Specially designed orthogonal or biorthogonal wavelet transforms easily going back to the original domain can be simply applied to the noise elimination method. However, nonorthogonal wavelet transform carrying a complex inversion mechanism similar to equations (3)~(7) are generally complicate and not easy to apply for noise elimination. Detail computational procedure and noise suppression methods are described in detail as follow.

Discrete Wavelet Transform

Discrete wavelet transforms were coded with pyramidal algorithm and Daubechies filter coefficients and suppress noises by utilizing a threshold method. Because of asymmetric shape of the Daubechies wavelet shown in Figure 1, the baseline of the reconstructed signals after the application of threshold in the wavelet space is always distorted. For the purpose of the correction of this distortion, two procedures to compensate distortion were also developed. The first method is shown in Figure 2.

A given NMR time domain signal containing noises is transformed into frequency domain signal. DWT with a given soft threshold value is applied to this signal to reach wavelet space. The treatment of the inverse DWT results in the noise eliminated frequency domain signal. The obtained spectrum always gives a distorted spectral baseline. To correct or compensate this distortion of baseline, same procedure is repeated with the 180° phase shifted signal. The soft threshold value was adjusted to the smaller value than the standard deviation value of noise in a second iteration for the more ideal compensation.

As shown in Figure 3 for the second method, two sets of original and 180° phase shifted data are simultaneously processed and finally two data sets are added at the last step. There are not much differences in the results of procedure 1 and 2, but second procedure is

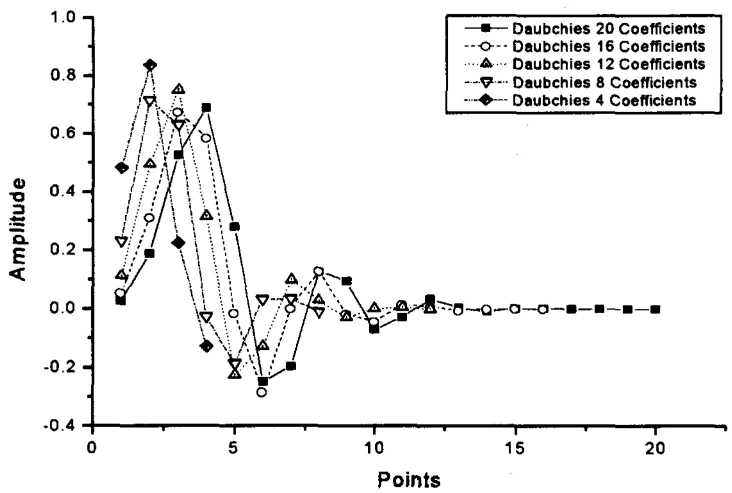

Fig. 1. The shape of the selected sets of the Daubchies wavelet coefficients.

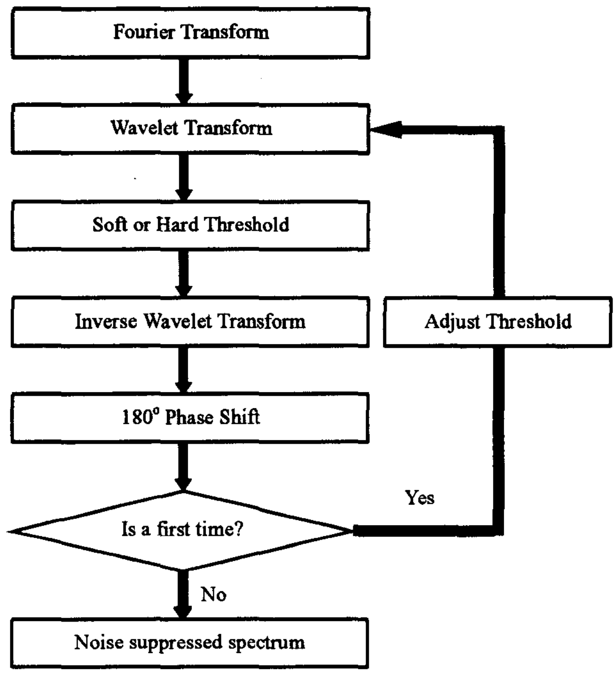

Fig. 2. Flow diagram of the first noise elimination scheme using discrete wavelet transform

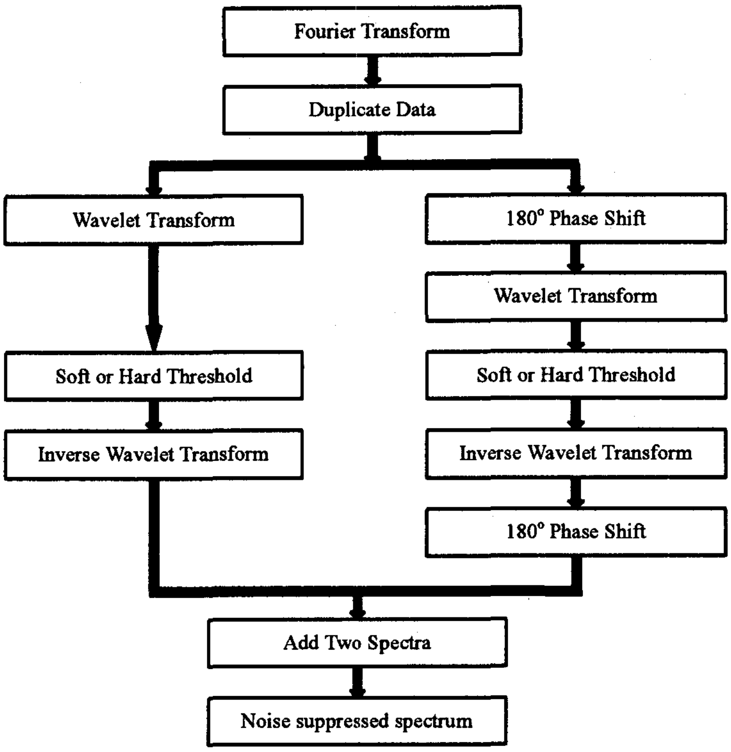

Fig. 3. Flow diagram of the second noise elimination scheme using discrete wavelet transform

more convenient since there are not necessary to determine the threshold-adjusting weight of the second iteration of procedure 1. Real threshold values are calculated by multiplication of user provided threshold value and standard deviation of noise. Therefore, the threshold value given in the procedure implies that the real threshold is the same as the standard deviation of noise.

Continuous Wavelet Transform

Morlet function as shown in Figure 4 and Eq. (21) is given by real cosine function and imaginary sine function, respectively. Real part has to be chosen as mother wavelet function[5] from the Morlet wavelet function.

$$\Psi(t) = \exp^{j\omega t} \exp^{-\beta^2 t^2/2} \quad (21)$$

$$\Psi(t) = \exp^{-\beta^2 t^2/2} \cos(\pi t) \quad (22)$$

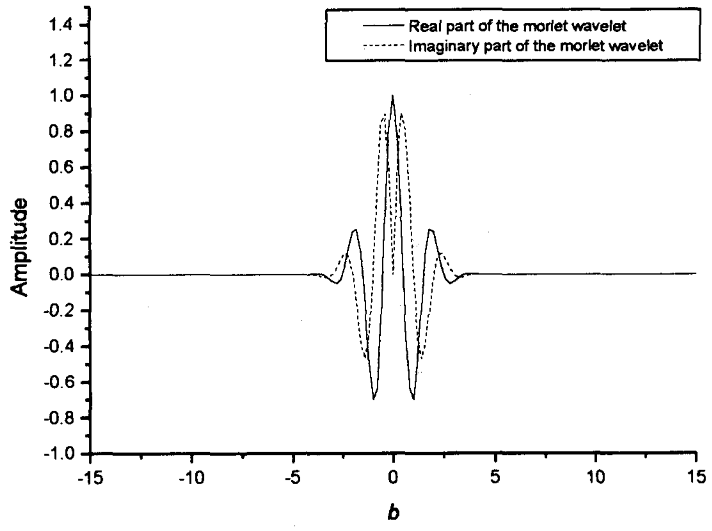

Fig. 4. The shape of the Morlet wavelet function with real and imaginary part.

Baby wavelets can be derived to Eq. (23) with Eq. (2) and real wavelet functions.

$$\Psi_{a,b}(t) = \exp\left[-\frac{\beta^2(t-b)^2}{a^2}\right]\cos\left[\frac{\pi(t-b)}{a}\right] \tag{23}$$

Detail explanations of each procedure are shown in the flow chart of Figure 5.

After the frequency domain dilation factor a and the time domain location factor b are initially set, Morlet baby wavelets are generated by Eq. (23). The resulting baby wavelets are convoluted with noise containing NMR signal by Eq. (1). A series of time location b values are generated with the variation of a from -15 to 15 and with an increment of 0.1. Continuous wavelet transforms are accomplished at this point, and a soft threshold are subsequently applied to each time location slice for noise elimination. Mother coefficients calculated from Eq. (22) are applied to Eq. (5) in order to resolve the frequency domain coefficients. Results are then plugged into Eq. (7) to get a constant $C_{1\Psi}$ adjusting the magnitude in the reconstruction procedure. The reconstructions of the noise eliminated signal carried out by using Eq. (6) give rise to the noise suppressed final frequency domain NMR signal.

All C/C++ codes are programmed on SGI Octane workstation. ^1H coupled ^{13}C-NMR data of the alanine was used as a test data. Sample purchased from Cambridge Isotope Co. was prepared by dissolving ^{13}C labeled alanine in D_2O solvent. All NMR spectra were

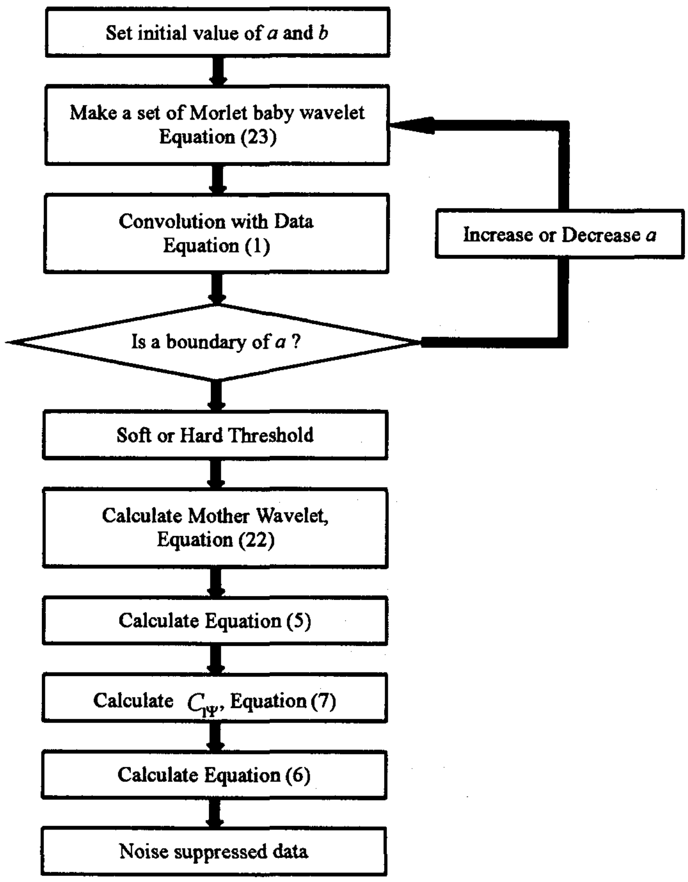

Fig. 5. Flow diagram of the noise elimination scheme using continuous wavelet transform

on a Varian Mercury 300 spectrometer with 64 k data points. This data was converted into HyNMR™(Hanyang NMR, multidimensional NMR data processor) data format and was processed with currently developed methods for wavelet transform and noise reduction procedure.

RESULT and DISCUSSION

Noise reductions have been attempted to NMR data with currently developed DWT method implemented with four different Daubechies filter coefficients (4, 8, 12, 20) exhibiting different curves in Figure 1. As the number of Daubechies filter coefficients increase from 4 to 20, the efficiency of noise reduction decrease, and even it gives a severe distortion of spectral baseline. Two DWT noise elimination methods of **1** and **2** shown in Figure 2 and Figure3, respectively, have been successfully applied to correct the serious

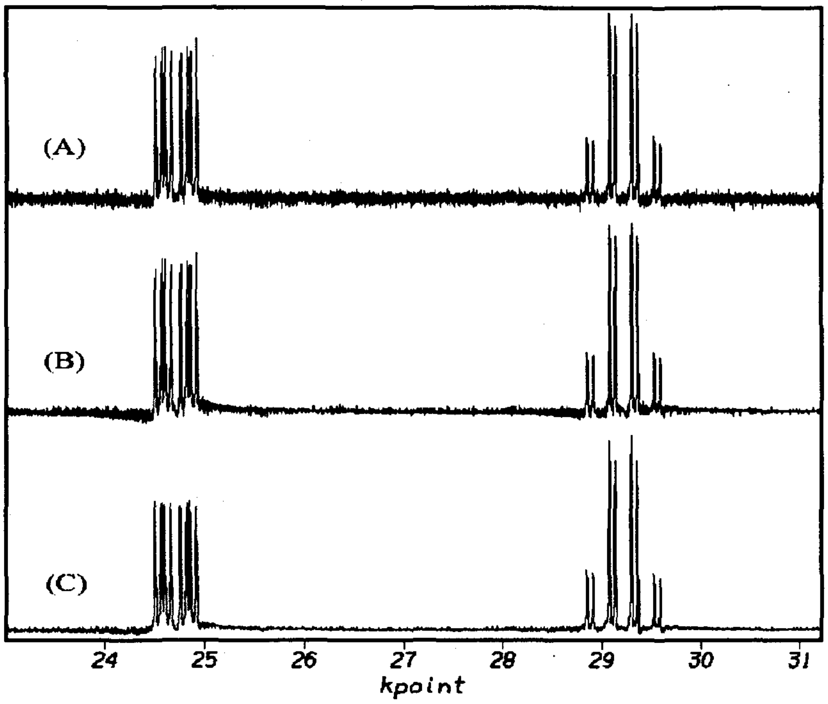

Fig. 6. Comparison of the noise level in a frequency domain between original spectrum (A) and After noise elimination treatment by discrete wavelet transform (B) and continuous wavelet transform (B).

distortion problems on the baseline of NMR spectrum after wavelet transform as shown in Figure 6(B). However, the distribution of residual noise obtained from two DWT methods is not impartial, and the spectral baseline slightly distorted yet. These faults arising from the usage of asymmetric Daubechies filter coefficients can be minimized in phase correction and baseline correction before application of the noise elimination routines.

Morlet wavelet transform (CWT) gives a better results in better S/N ratio and more flat baseline as shown in Figure 6 (C). Because of the symmetric shape of the Morlet wavelet transform as shown in Figure 4, it may be more appropriate to NMR spectrum that are usually exhibited as a symmetric gaussian function. Symmetric forms of functions are still retained in a wavelet space and soft threshold does not give a distortion of peaks as shown in Figure 7. Comparison of the noise reduction level for various threshold variations are illustrated in Figure 7. A slice of wavelet coefficient at a=0.6 in a wavelet space is shown in Figure 7(B), and subsequent soft threshold can eliminate the noise without reduction of real NMR signals as shown in Figure 7(C,D,E). In summary, both DWT and CWT methods were successfully applied to noise reduction of noise contaminated NMR signal. Although two procedures to compensate the inevitable distortion of NMR spectral

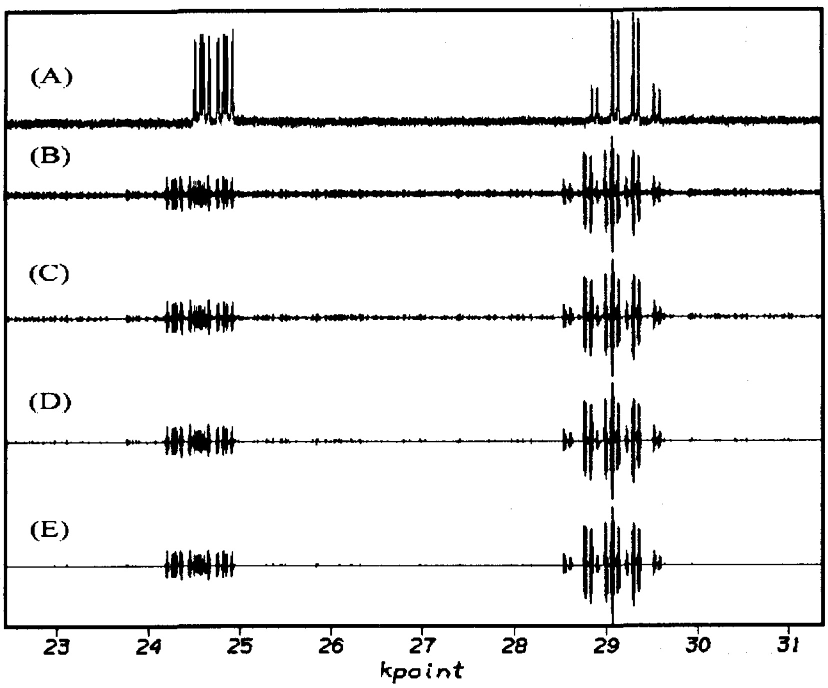

Fig. 7. A comparison of the noise elimination level according to threshold variation. The original noise contaminated ^{1}H coupled ^{13}C NMR signal of α and β carbon of the ^{13}C labeled alanine dissolved in D_2O (A). After applying the continuous wavelet transform using Morlet wavelet, A slice of wavelet coefficients at a=0.6 in a wavelet space (B), and after applying soft threshold with the threshold value of 1 (C); 2 (D); and 3 (E).

baseline arising from DWT method were successful to NMR spectrum, the spectral baseline is still distorted. Further studies are necessary in the imperfection in noise elimination procedures. Although the reconstruction procedure is more complicate, but CWT method gives a better spectral baseline and noise suppressed spectrum. There are still a necessity of the development of mother wavelet functions optimized to NMR signal processing.

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