

Water Peak Suppression: Time-Frequency vs Time-Scale Approach

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Wavelets are the most popular time-scale analysis tool. A well-known application of wavelets in nuclear magnetic resonance spectroscopy is water peak extraction/suppression. However, spectroscopists are more familiar with frequency than scale. So, from a spectroscopist point of view, a time-scale analysis tool (i.e., wavelets) is not natural and a time-frequency approach would be much more satisfactory. We explain a time-frequency solution to this problem based on Gabor analysis. As the two formalisms are closely linked together we continuously emphasize their similarities and differences. In particular we show that, here, the Gabor method is as efficient as the wavelet approach, and we give some examples. Those remarks also apply to other NMR problems solved previously with the continuous wavelet transform, such as quantification or dynamical phase correction. © 2000 Academic Press

Key Words: wavelets; Gabor transform; peak suppression; time-frequency analysis; time-scale analysis.

1. INTRODUCTION

The suppression of the strong signal from water is a prerequisite for observation of metabolites in biomedical spectroscopy and for the study of biomolecules in solutions.

Several *preacquisition* methods of peak suppression have been proposed (1–4). However, these techniques are not always easy to implement on biomedical spectroscopy and imaging systems. *Postacquisition* methods, based on time domain data processing, have also been proposed (5–11). These methods are easiest to apply when the peak to be suppressed is on resonance: The low frequency component is isolated and subtracted from the original signal. Recent techniques, such as oversampling combined with digital filtering (12, 13), provide extremely sharp filter cutoffs, flat magnitude response in the passband region, and near-ideal phase linearity. Together they effectively prevent the folding of undesirable peaks from outside the passband. Unfortunately these techniques are only available on the most recent equipment.

A different approach is to replace the standard Fourier technique by a combined time-frequency or time-scale representation of the signal, such as the wavelet or the Gabor formalism, and to perform the subtraction on the transformed

signal. Whereas this approach has become very common in general signal processing, its application to NMR spectroscopy is rather recent. In particular, the wavelet transform has been applied successfully to a number of standard problems, such as resonance subtraction, quantification, or spectrum rephasing (14–16) (we refer to these articles for a detailed description of the method). Among these, it yields a good water peak suppression. The method is fast and reliable, and the results do not depend on any modeling of the resonance peaks.

In the present paper, which can be seen as a sequel to Ref. (15), we intend to show that equally good results may be obtained with a time-frequency formalism, namely the Gabor transform. This is reassuring, in a sense, because the time-frequency approach is more natural and satisfactory from a spectroscopist point of view. Nevertheless, the two formalisms being very similar, it is instructive to pursue the analysis with both in parallel, and we shall do this in this sequel, emphasizing systematically throughout the paper the similarities and differences between the two.

We emphasize that the aim of the present approach is toward biomedical, even clinical, applications. Compared to high-resolution spectroscopy, this means, in general, very short relaxation time and equipment that is mostly automatic and not very flexible. As a consequence, time-frequency techniques are in a very good position, since they are much easier to implement (even on a PC) and do not require any sophisticated *preacquisition* sequence.

The paper is divided into three parts. First, we recall the basic theory of wavelet and Gabor transforms. Next, water peak suppression is described in the two approaches, and finally some examples are given.

2. THE CONTINUOUS WAVELET AND GABOR TRANSFORMS

In this sequel, we consider only signals of finite energy. The Fourier transform of a function $f \in L^2(\mathbb{R})$ will be denoted by \hat{f} , namely,

$$\hat{f}(\omega) = \int_{\mathbb{R}} f(x) e^{-i\omega x} dx \quad \omega \in \mathbb{R},$$

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where $\omega = 2\pi\nu$ with ν being the frequency (strictly speaking ω should be called the pulsation, but we shall stick to “frequency” throughout). The signal f can be recovered from its Fourier transform \hat{f} by the inversion formula,

$$f(x) = \frac{1}{2\pi} \int_{\mathbb{R}} \hat{f}(\omega) e^{i\omega x} d\omega.$$

In the present case, f will represent the NMR signal containing a broad peak to be subtracted. So f is either an FID or a spin echo.

Up to now, the problems of peak suppression or quantification and of dynamical phase correction have been addressed only with the continuous wavelet transform (CWT) (14, 15). However, as we shall show below, the same problems can be treated successfully with the Gabor transform. For the convenience of the reader, we shall thus begin by a quick review of the two transforms in parallel. Further information may be found in textbooks (17, 18).

Hereafter ψ denotes the wavelet and g the Gabor function. We suppose that $\psi \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ and $g \in L^2(\mathbb{R})$. So both ψ and g have finite energy.

In the wavelet context, $\psi_{b,a}$ ($a \in \mathbb{R}^*$, $b \in \mathbb{R}$) is a dilated and translated version of a single wavelet ψ :

$$\psi_{b,a}(x) = \frac{1}{a} \psi\left(\frac{x-b}{a}\right).$$

The continuous wavelet transform of f is simply the scalar product of f with the collection of $\psi_{b,a}$:

$$\begin{aligned} T_f(b, a) &= \langle \psi_{b,a}, f \rangle \\ &= \frac{1}{a} \int_{\mathbb{R}} \overline{\psi\left(\frac{x-b}{a}\right)} f(x) dx \end{aligned} \quad [1]$$

$$= \frac{\text{sign } a}{2\pi} \int_{\mathbb{R}} \overline{\hat{\psi}(a\omega) e^{-i\omega b}} \hat{f}(\omega) d\omega. \quad [2]$$

Relation [1] expresses the CWT in the time domain and [2] is its counterpart in the Fourier (frequency) domain.

If the wavelet ψ satisfies the so-called admissibility condition, that is,

$$0 < c_\psi = \int_{\mathbb{R}} |\hat{\psi}(u)|^2 \frac{du}{|u|} < \infty, \quad [3]$$

then the CWT may be inverted and the signal f can be recovered from its CWT coefficients:

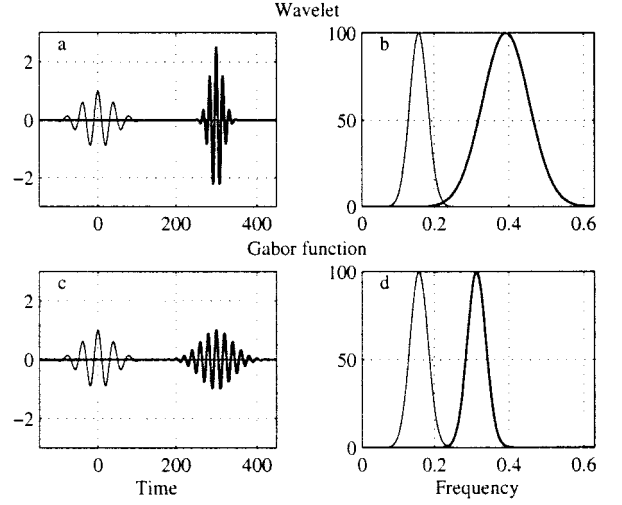


FIG. 1. Comparison between wavelet and Gabor functions. (a): Real part of two dilated and translated versions of the Morlet wavelet (thin line, $a = 1$; thick line, $a = 0.4$); (c): Real part of two modulated and translated versions of a Gaussian Gabor function (thin line, $\omega = \pi/20$; thick line, $\omega = \pi/10$). (b) (resp. (d)): The modulus of the Fourier transform of the wavelet of (a) (resp. Gabor function of (c)).

$$f(x) = \frac{1}{c_\psi} \int_{\mathbb{R}^* \times \mathbb{R}} T_f(b, a) \psi_{b,a}(x) \frac{da db}{a}. \quad [4]$$

Clearly, the admissibility condition [3] implies that $\hat{\psi}(0) = 0$, that is, the wavelet must have zero mean. While, strictly speaking, this weaker condition is only necessary, in practice it is also sufficient and usually taken as an admissibility condition. In addition, since $\psi \in L^2(\mathbb{R})$, $|\hat{\psi}(\omega)|$ tends to 0 when $\omega \rightarrow \infty$. So the Fourier transform of the wavelet ψ is a bandpass filter.

The well-known Morlet wavelet (see Figs. 1a and 1b),

$$\psi(x) = \exp(-x^2/(2\sigma_0^2)) \exp(i\omega_0 x) \quad [5]$$

$$\hat{\psi}(\omega) = \sqrt{2\pi}\sigma_0 \exp(-(\omega - \omega_0)^2 \sigma_0^2/2), \quad [6]$$

is not admissible, strictly speaking, but almost admissible. In general a correction term must be subtracted, but if $\omega_0 \sigma_0$ is sufficiently large ($\omega_0 \sigma_0 > 5.5$), this term is numerically negligible, and the wavelet [5] may safely be used. Now, $\hat{\psi}(\omega)$ is maximum at $\omega = \omega_0$, which means that $\hat{\psi}_{b,a}$ is maximum at the central frequency $\omega = \omega_0/a$. This suggests the identification of the frequency ω with the inverse scale $1/a = \omega/\omega_0$. Thus, the Morlet wavelet can be viewed as a linear bandpass filter whose bandwidth is proportional to $1/a$ or to the central frequency. As a wavelet must satisfy the admissibility condition, it cannot be maximum at $\omega = 0$. Thus the zero frequency or infinite scale is a limit or critical frequency, corresponding to an infinitely stretched wavelet.

In the Gabor context (18–20), the reference function, $g_{b,\omega}$, is a frequency modulated and time translated version of g ,

$$g_{b,\omega}(x) = g(x - b)e^{i\omega(x-b)} \quad b, \omega \in \mathbb{R}.$$

The Gabor transform of a signal f is the collection of scalar products of f with $g_{b,\omega}$:

$$G_f(b, \omega) = \int_{\mathbb{R}} \overline{g(x - b)e^{i\omega(x-b)}} f(x) dx \quad [7]$$

$$= \frac{1}{2\pi} \int_{\mathbb{R}} \overline{\hat{g}(\xi - \omega)e^{-i\xi b}} \hat{f}(\xi) d\xi. \quad [8]$$

Here again, the signal f can be recovered from its Gabor coefficients,

$$f(x) = \frac{1}{2\pi \|g\|^2} \int_{\mathbb{R} \times \mathbb{R}} G_f(b, \omega) g_{b,\omega}(x) db d\omega, \quad [9]$$

but now no admissibility condition on g is needed, i.e., any $L^2(\mathbb{R})$ function is admissible. The most common Gabor function is the Gaussian window (see Figs. 1c and 1d):

$$g(x) = \exp(-x^2/(2\sigma_0^2)) \quad [10]$$

$$\hat{g}(\omega) = \sqrt{2\pi}\sigma_0 \exp(-\omega^2\sigma_0^2/2). \quad [11]$$

Notice that, if g is the Gaussian window [10] and ψ the Morlet wavelet [5], then $G_f(b, \omega)$ and $T_f(b, a)$ coincide for $a = \omega_0/\omega$ (compare the two thin Gabor and wavelet functions in Figs. 1a and 1c).

As compared to the wavelet transform, the Gabor transform has several advantages:

1. This transform is covariant under frequency translation, i.e., modulation, whereas the wavelet transform is not. This means that if

$$f_1(x) = e^{i\xi_0 x} f(x), \quad \text{then } G_{f_1}(b, \omega) = G_f(b, \omega - \xi_0).$$

In other words, the Gabor transform of a modulated signal is equal to a frequency translation of the Gabor transform of the signal. This property is most welcome in the present context, since frequency translation is very common in NMR.

2. The bandwidth of the analyzing window $g_{b,\omega}$ does not depend on the analyzed frequency (compare the spectral widths of $\hat{\psi}$ and \hat{g} in Figs. 1b and 1d). The spectral width of $\hat{\psi}_{b,a}$ decreases when a increases, whereas that of $\hat{g}_{b,\omega}$ remains

constant, independently of ω . Hence, the zero frequency does not play any particular role in the Gabor transform. As there is no *a priori* reference frequency in NMR, this is exactly what a spectroscopist is expecting, too.

3. WATER PEAK SUPPRESSION

The theory of peak suppression with wavelets has been widely discussed in several papers (14, 15, 21, 22) (interestingly, the first real application of the CWT in spectroscopy was in the NMR context (21)).

Some of these authors, in particular those of Ref. (22), noticed that a time-frequency (Gabor) formalism is also an interesting solution. Here we will mainly focus on the advantages of this method from the spectroscopist's point of view. For better clarity, we treat complex and real signals separately.

3.1. Complex NMR Signals

Let us define, as usual, a spectral line by the complex function $S(x) = A(x)\exp(i(\omega_s x + \phi))$, with $A(x)$ a real and positive amplitude. We assume that $A(x)$ varies slowly and is analytic.

In the context of NMR, $A(x)$ could be a damped exponential, or a Gaussian, or a more complicated function if the disturbing peak was presaturated. In any case, the precise shape of the amplitude is irrelevant, and there is no need for a model.

The Gabor transform of the spectral line $S(x)$ reads

$$\begin{aligned} G_S(b, \omega) &= \frac{1}{2\pi} \int_{\mathbb{R}} \overline{\hat{g}(\xi - \omega)e^{-i\xi b}} \hat{A}(\xi - \omega_s) e^{i\phi} d\xi \\ &= \frac{1}{2\pi} e^{i(\omega b + \phi)} \int_{\mathbb{R}} \overline{\hat{g}(\zeta)e^{-i\xi b}} \hat{A}(\zeta + \omega - \omega_s) d\zeta. \end{aligned} \quad [12]$$

Using the Taylor expansion of \hat{g} around its maximum $\omega = 0$,

$$\hat{g}(\zeta) = \hat{g}(0) + \sum_{k=1}^{\infty} \frac{\zeta^k}{k!} \frac{d^k \hat{g}}{d\zeta^k}(0),$$

Expression [12] becomes

$$\begin{aligned} G_S(b, \omega) &= S(b) \overline{\hat{g}(\omega_s - \omega)} + e^{i(\omega_s b + \phi)} \sum_{k=1}^{\infty} \frac{(-i)^k}{k!} \\ &\quad \times \frac{d^k \bar{\hat{g}}}{d\omega^k}(\omega_s - \omega) \frac{d^k A}{db^k}(b). \end{aligned} \quad [13]$$

In the same manner, the CWT may be written as

$$T_S(b, a) = S(b) \overline{\hat{\psi}(a\omega_s)} + e^{i(\omega_s b + \phi)} \sum_{k=1}^{\infty} \frac{(-ia)^k}{k!} \times \frac{d^k \overline{\hat{\psi}}}{d\omega^k}(a\omega_s) \frac{d^k A}{db^k}(b). \quad [14]$$

The two Equations [13] and [14] are very similar, and in both cases the first order in the expansion is proportional to the spectral line. But the difference occurs in the higher order terms. In [13], these terms depend on the successive derivatives of g , at the same point, whereas in [14], in addition to ψ there is an additional explicit dependence on the scale variable a . Thus, from a spectroscopist point of view, handling [13] is much easier.

So the Gabor (resp. wavelet) coefficients along the line of maxima are a good approximation of the spectral line as long as $A(x)$ varies slowly and the derivative of \hat{g} (resp. $\hat{\psi}_{0,a}$) can be neglected:

$$S(b) \approx \frac{G_S(b, \omega_s)}{\hat{g}(0)}, \quad \text{resp.}, \quad S(b) \approx \frac{T_S(b, \omega_0/\omega_s)}{\hat{\psi}(\omega_0)}. \quad [15]$$

The iterative algorithm presented in (21, 22) for the wavelet case allows us to determine precisely the scale of the spectral line. Getting its time-frequency version is straightforward. Although this algorithm has been known for almost 10 years in the signal processing community, it may be worthwhile to summarize it here. It runs as follows.

- Initialization step: Set k to zero. Choose
 - a Gabor function (resp. wavelet) like a Gaussian (resp. a Morlet wavelet with reference frequency ω_0)
 - an initialization frequency ξ_0 (resp. an initialization scale α_0 with $\alpha_0 = \omega_0/\xi_0$) in the vicinity of the peak to suppress
 - a precision parameter ϵ
- Do
 - Compute $G_f(b, \xi_k)$ (resp. $T_f(b, \alpha_k)$) with a discretized version of [8] (resp. [2])
 - Use the regularization formula of the iterative algorithm,

$$\xi_{k+1} = \frac{1}{T} \int_T \frac{\partial \arg(G_f(b, \xi_k))}{\partial b} db.$$

In the wavelet case, replace $G_f(b, \xi_k)$ with $T_f(b, \alpha_k)$

and set $\alpha_{k+1} = \omega_0/\xi_{k+1}$

— $k = k + 1$

while $|\xi_k - \xi_{k-1}| > \epsilon$.

Then, the resulting function $G_f(b, \xi_k)$ (resp., $T_f(b, \alpha_k)$) is the spectral line to be subtracted to the signal.

If several spectral lines are involved and are sufficiently far from each other, they can be treated independently. Subtracting [15] from the full signal does not alter the phase of the signal. If the lines are very close, one can use a more sophisticated method based on the resolution of a linear system (21, 22).

3.2. Real NMR Signals

Now, assume that $S(x)$ is real,

$$S(x) = \Re\{A(x)\exp(i(\omega_s x + \phi))\} = A(x)\cos(\omega_s x + \phi),$$

with $A(x)$ a positive and low-pass function whose bandwidth lies within the interval $(-\omega_s, \omega_s)$. Its Gabor and wavelet transform are, respectively,

$$G_S(b, \omega) = \frac{1}{4\pi} \left(\int_{\mathbb{R}} \overline{\hat{g}(\xi - \omega)} e^{-i\xi b} \hat{A}(\xi - \omega_s) e^{i\phi} d\xi + \int_{\mathbb{R}} \overline{\hat{g}(\xi - \omega)} e^{-i\xi b} \hat{A}(\xi + \omega_s) e^{-i\phi} d\xi \right) \quad [16]$$

$$T_S(b, a) = \frac{\text{sign}(a)}{4\pi} \left(\int_{\mathbb{R}} \overline{\hat{\psi}(a\omega)} e^{-i\omega b} \hat{A}(\omega - \omega_s) e^{i\phi} d\omega + \int_{\mathbb{R}} \overline{\hat{\psi}(a\omega)} e^{-i\omega b} \hat{A}(\omega + \omega_s) e^{-i\phi} d\omega \right). \quad [17]$$

In order to extract the spectral line with the previous method, one requires the second integrals in [16] and [17] to be zero (or numerically negligible) around $\omega = \omega_s$.

Thus, the integrals will be equal to zero, if one imposes the additional admissibility conditions on g or ψ :

$$\hat{g}(\omega) = 0, \quad \text{for } \omega \leq -\omega_s,$$

$$\hat{\psi}(\omega) = 0, \quad \text{for } \omega \leq 0.$$

Then the spectral line is extracted from the time-frequency or time-scale representations:

$$S(b) \approx 2\Re\left\{\frac{G_S(b, \omega_s)}{\hat{g}(0)}\right\} \quad S(b) \approx 2\Re\left\{\frac{T_S(b, \omega_0/\omega_s)}{\hat{\psi}(\omega_0)}\right\}.$$

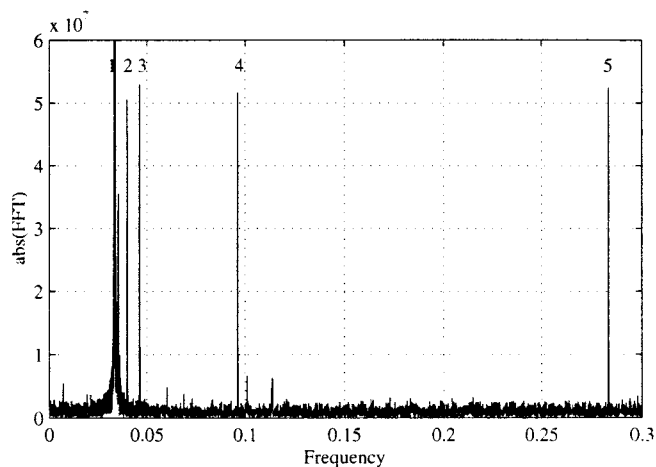


FIG. 2. Spectrum of the first signal.

4. EXAMPLES

The wavelet method is usually illustrated by FID examples (14, 15, 21, 22). One should notice, however, that the amplitude $A(x)$ of a FID is not a bandlimited low pass function and varies very rapidly around $x = 0$, growing from 0 to its maximum value. Hence both the Gabor transform and the CWT are prone to border effects around this transient point. To avoid this drawback, the first points of the water peak suppressed FID are usually omitted or set to zero.

In the sequel, we will treat instead spin echo sequences, which are much smoother and do not require any special trick.

The first example, Figs. 2 and 3, is a semi-synthetic spectrum obtained by taking the water signal at different offsets and different numbers of scans, in order to generate small lines about 0.25% of the main signal. The second example, Figs. 4 and 5, corresponds to a mixture of dioxane (line 2) and acetone

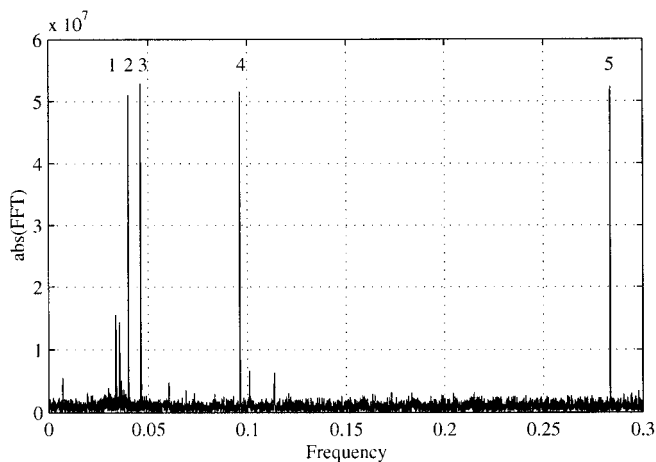


FIG. 3. Spectrum of the first signal after Gabor/wavelet water peak suppression.

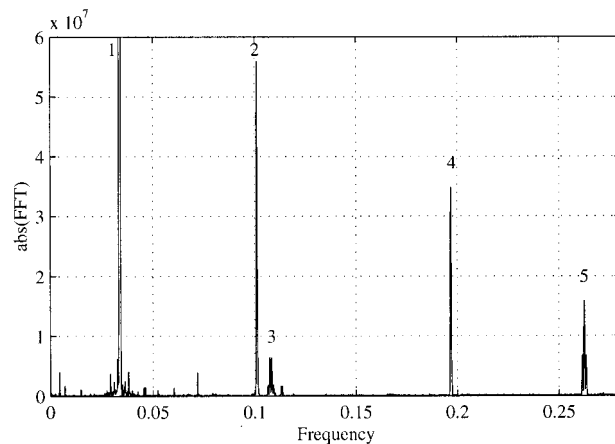


FIG. 4. Spectrum of the second signal.

(line 4) in water. Signals 3 and 5 correspond to impurities in the commercial grade chemicals used.

We emphasize that these are spectra obtained by direct Fourier transformation of time-domain signals, without any correction. The resolution is comparable to that obtained from a commercial machine (Bruker . . .), which in fact often tacitly incorporates various corrections (baseline . . .). Of course, for a purely synthetic spectrum such as the one given in (12), Fig. 1, any resolution or shape is possible by definition.

In fact, the results obtained in these examples are exactly the same with the Gabor and the wavelet suppression methods. Since the former is simpler, it becomes the first choice. As for the efficiency of the method, we display in Table 1 the area under each peak of the spectrum before and after water suppression. After Gabor/wavelet suppression, the water peaks are weak, whereas the shape and area of the peaks of interest remain the same. So both methods are very effective in subtracting unwanted large peaks.

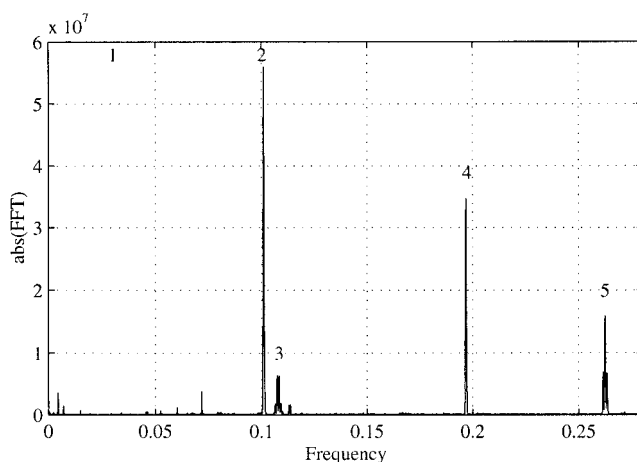


FIG. 5. Spectrum of the second signal after Gabor/wavelet water peak suppression.

TABLE 1
Area of the Spectral Line

Example	Line number				
	1	2	3	4	5
1	1000.00	2.34	2.80	2.22	2.33
1—water suppressed	4.19	2.27	2.79	2.23	2.33
2	1000.00	11.23	3.12	6.90	5.54
2—water suppressed	0.06	11.23	3.12	6.90	5.54

5. CONCLUSION

In conclusion, water peak suppression with the Gabor transform is as effective as with wavelets, and the two are closely linked. However, in this context, the Gabor transform and the underlying time-frequency formalism appears to be more suitable than a time-scale formalism.

As there are very few assumptions on the spectral line to be suppressed, this technique can also be applied to a signal acquired with a preacquisition water suppression sequence. This method could also be successfully applied to multidimensional experiments like COSY.

As a final remark, we may quote another application of wavelets in NMR spectroscopy, namely, dynamical phase correction (15). This problem too can easily be solved in the time-frequency formalism. Once again, the translation covariance (usually called shift invariance) of the method will please the spectroscopists, who are naturally more familiar with frequency translation than frequency dilation. This method will be implemented in the next release of EU software MRUI (Magnetic Resonance User Interface), to be found on the website (<http://www.mrui.uab.es/mrui/mruiHomePage.html>).

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