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# Communication Implementation equations for HS<sub>n</sub> RF pulses

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#### ABSTRACT

Implementation equations for the family of stretched hyperbolic secant (HS<sub>n</sub>) pulses are derived in the linear adiabatic range for inversion of spins. These master equations provide convenience relations for relating the peak amplitude  $RF_{max}$  of the pulse to the frequency sweep (*bwdth*) range of the pulse and its duration  $T_p$ . The bandwidth of the pulse can also be related to the effective coverage (*bw<sub>eff</sub>*) of the pulse to a defined or chosen spectral region. The choice of pulse determined by the use of these derived expressions guarantees uniform inversion to a prescribed efficiency across the selected spectral region. The performance of HS<sub>n</sub> pulses in determining the cut-off region between spectral regions was also examined. It is found that beyond a unique  $T_p bwdth$  product no additional gain may be obtained by extending pulse durations for a chosen *bwdth* of pulse. An example of practical implementation of the inversion pulses is presented for adiabatic decoupling using HS<sub>7</sub> and HS<sub>8</sub> pulses. It is shown that despite added  $B_1$  inhomogeneity in the form of additional amplifier power to 400% from optimal, these pulses can still yield reproducible decoupled spectra.

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#### 1. Introduction

The hyperbolic secant (HS) amplitude/frequency waveform [1] is widely used in NMR and MRI for adiabatic broadband or selective inversion or decoupling. Unfortunately a criticism of the pulse is the large peak amplitude (RF<sub>max</sub>) often required to achieve the desired rotation/s. Modulation functions such as constant/linear (or CHIRP) [2], WURST [3], tanh/tan [4] and numerous others [5] were developed to overcome these limits. All are useful in one manner or another but direct and fair comparison is usually not possible. For example, selectivity profiles defining the cut-off region between two peaks say, may be less than satisfactory and are not readily realized particularly in narrow-band applications. The latter is important in homo-decoupling applications and spectral region selection in crowded spectra as well as slab selection in 3D magnetic resonance imaging applications. While due consideration should be given to all pulses touted to behave adiabatically, complete, accurate and generally applicable methods of implementation into pulse sequence programs still remains a problem because of the difficulty in solving the Bloch equations analytically for any arbitrary input function. Numerical solution of the Bloch equations for an arbitrary waveform during execution of a pulse sequence program may also be feasible. However, when the number of digitization points np, in a waveform is large (e.g. >1000 points) calculation may take the order of seconds or more. Moreover, target efficiencies such as the level of inversion have to be determined usually requiring recursive algorithms and in these cases more programming effort is required for failsafe operation. An alternative strategy is the creation of a database of numerically optimized pulses [6,7] but the draw-back is that tables are discrete increments of some parameter of the pulse and so general applicability becomes a problem of finding the closest match from prebuilt input waveforms. Having available a set of simple equations relating the operating parameters of the pulse to the NMR spectrum or image, that are easily programmed for a family of pulses, seems a better approach. The HS<sub>n</sub> family [8] meets this criterion. But, there are no implementation equations nor analytical solutions readily realized for the plethora of applications nor combinations of duration, spectral coverage, peak amplitudes, or exponent where these pulse may be used.

In previous work [9], universal implementation equations were derived for sech/tanh pulses, where it was shown that linear master equations of the form  $(RF_{max}T_p)^2 = m_{RF}T_pbwdth + c_{RF}$  could be derived empirically. Relevant pulse parameters of peak amplitude,  $RF_{max}$  (kHz), duration  $T_p$  (ms), and nominal pulse frequency sweep *bwdth* (kHz) could be determined and easily implemented in pulse sequence programs for error free use of these inversion pulses. The coefficients  $m_{RF}$  and  $c_{RF}$  are fitting constants. Likewise the parameter relating the chosen spectral bandwidth *bw*<sub>eff</sub> to *bwdth* was also found to be linearly proportional and so implementation only really required the spectral width to be set. Equations were also provided for the tanh/tan pulse and a similar strategy could also be used for determining the relevant parameters for other amplitude and frequency swept schemes such as WURST and the like. These pulses were further categorized as "linearly" or "partially"

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adiabatic and the  $T_pbwdth$  product of each was determined to further limit the use of the pulse to be in the linearly adiabatic range.

In this article, numerically derived master equations for the  $HS_n$ family are provided, where *n* is an integer exponent of time in the modulation functions driving the RF pulse. These pulses (or rather these waveforms) have been used extensively, particularly in applications for  $T_{1\rho}$  [10], and  $T_{2\rho}$  [11,12], contrast generation [13,14], localized spectroscopy [15] and more recently in frequency swept imaging [16]. The latter, however, is a special application of these pulses where variable spin flips are generated in the linear portion of the peak amplitude profile and may be described as the product operator transform of  $I_z \rightarrow I_{\pm(x,y)}$  depending on the phase of the pulse. An excellent treatment has been provided for this promising application [17]. It is also possible to use the equations derived here to arrive at the optimal peak amplitude and this is briefly discussed later in the article. Here only the inversion  $I_{z} \rightarrow -I_{z}$  is treated. It follows that in the absence of any influence of the coupling mechanism between two spins, the transforms,  $2I_zS_z \rightarrow -2I_zS_z$ ,  $2I_zS_{\pm(x,y)} \rightarrow -2I_zS_{\pm(x,y)}$  may also be treated with the derived equations. This operating bound is sometimes called the "high power limit". Evolution of spin states due to a reduced coupling constant may be safely neglected for  $T_{\rm p} \leq (1/2I)$  ms and  $B_1 >> I$  as has been shown previously [18] for HS<sub>1</sub>. HS<sub>n</sub> can be applied for short durations without violating peak amplitude or duty cycle requirements. The advantage of  $HS_n$  pulses is that with increasing n the peak amplitude of the pulse is reduced and so imaging and spectroscopic applications need not be limited by such things as coil/probe limits. In spectroscopy applications, where it is often thought that only short duration pulses lead to efficient excitations relative to longitudinal and spin-spin relaxation, these pulses also can be of short duration. For ease of implementation, universal master equations guaranteeing consistent performance are required.

#### 2. Results and discussion

#### 2.1. Derivation of peak amplitude master equation

The HS<sub>n</sub> amplitude  $B_1$ , and phase  $\varphi$  functions, were implemented according to [8]

$$B_1(\tau) = \mathsf{RF}_{\mathsf{max}}\mathsf{sech}(\beta\tau^n) \tag{1}$$

$$\varphi(\tau) = (360T_p bwdth/np) \int_0^\tau \int_0^\tau B_1^2(\tau) d\tau$$
(2)

with  $\tau = 2t/T_p$  (ms) and  $-1.0 \le t \le 1.0$ . Here *bwdth* is the extent of frequency sweep in kilohertz, *np* is the number of digitized points, *n* is an integer exponent in the range 2–8, the truncation factor  $\beta = 5.23^n$  and RF<sub>max</sub> is the peak amplitude of the pulse in units of kilohertz. To ensure high fidelity of each pulse,  $np \ge 1024$ . Simulations were carried out with the 3 × 3 rotation matrix of the Bloch equations as described in [19] in the following fashion.

First, the cut-off for partial adiabaticity was determined by searching for the minimum *bwdth* where the wobbles disappeared from the RF<sub>max</sub> profile for  $T_p = 1.0$  ms. That is the  $T_pbwdth$  product (or *R* factor) was varied. The maximum range for the RF<sub>max</sub> sweep was determined by considering the potential applications of the pulse. In a proton spectrum it is not unusual to find on-resonance square pulse durations of a few micro-seconds. Of course there are a number of variables to consider but maximum peak amplitudes up to ~60 kHz for protons is feasible for some high resolution probes. For higher gyromagnetic nuclei the maximum is usually quite less. To complete the initial search for  $T_pbwdth$  range the maximum limit was found so that the operation  $I_z \rightarrow -I_z$  was achieved. The limits of simulation vary with *n*.

Second,  $RF_{max}$  was determined by continuous application of the rotation matrix to initial unit magnetization  $I_z = 1.0$  in 2048  $RF_{max}$  steps. Third, an interpolating polynomial of the profile was created using Mathematica software (Wolfram Scientific, Champaign, Illinois) and then solved for chosen inversion numbers  $\iota_0$ , where the inversion number represents the percentage inversion as described previously (9). The inversion numbers chosen were in the range  $0.90 \leq \iota_0 \leq 0.99$  providing an extra variable to ensure guaranteed performance of a chosen pulse. The product  $T_p bwdth$  was plotted against  $(RF_{max}T_p)^2$  to yield linear plots from which the intercept and slope were determined and plotted against  $\iota_0$  to yield the auxiliary equations of [9].

Shown in Fig. 1 are the  $RF_{max}$  profiles of  $HS_n$  pulses for a constant  $T_p bwdth$  product. It is easy to note that there is a significant improvement in the peak amplitude required to achieve inversion for a chosen exponent. More importantly though, if amplifier



**Fig. 1.** Peak amplitude profiles for HS<sub>n</sub> inversion pulses with  $T_pbwdth = 40.0$  ( $T_p = 1.0$  ms and bwdth = 40.0). An expansion of the region where RF<sub>max</sub> = 4.0 and 6.25 kHz is plotted showing the lower power required by the various HS<sub>n</sub> pulses with increasing *n* as labeled.

power settings are kept constant such that  $\text{RF}_{\text{max}} \ge 8$  kHz, any of the 8 pulses could be used to achieve the same rotation. In addition, the profiles for n > 5 only offer marginal improvements in peak amplitude reduction for the same rotation and so in the first instance one would be hard pressed to find any use for HS pulses with n > 5. Nevertheless peak amplitudes of this family of pulses may be calculated according to,

$$RF_{max} = T_p^{-1} \sqrt{m_{RF} T_p bwdth} + c_{RF}$$
(3)

with

$$m_{\rm RF} = \sqrt{\left(a_0 + a_1 \iota - a_2/(1-\iota)\right)^{-1}} \tag{4}$$

and

$$c_{\rm RF} = (b_0 + b_1 \iota - b_2 / (1 - \iota))^{-1}$$
(5)

Curve fitting parameters for each of the HS<sub>n</sub> pulses is given in Table 1 and may be substituted into the appropriate equations of [7]. It must be noted that the simulation limits were set in such a way as to reflect the operation of the RF pulse in the linearly adiabatic range. These limits are such that  $20 \le T_p bwdth \le 1000$ . Thus if a user chooses to operate over a very narrow bandwidth of frequencies,  $T_p bwdth$  must be greater than or equal to 20 for the relations given by the fitting parameters of Table 1 to hold. In the case

of partially adiabatic pulses, universal relations are even more difficult to establish even with numerical simulation and are outside the scope of this article.

#### 2.2. Determining excitation profile characteristics

Since the inversion profile is symmetric around the chosen RF transmitter frequency, only the point where  $i_0$  met the chosen setting was recorded. Accordingly the effective bandwidth  $bw_{eff}$  is twice the value determined for a pulse of chosen frequency sweep *bwdth*. Effective bandwidth profiles were determined as described for the peak amplitude profiles above using the  $3 \times 3$  rotation matrix. The relationship between  $bw_{eff}$  and bwdth is also linear. Determination of an auxiliary function with respect to  $i_0$  completes the derivation of all functions necessary to define a master equation in terms of the variables, RF<sub>max</sub>, *bwdth*, *bw*<sub>eff</sub>, and  $T_p$ .

The response of magnetization inversion across the spectral bandwidth is shown in Fig. 2. Here this is labeled as effective bandwidth (or  $bw_{\text{eff}}$ ) as this is a property of the pulse rather than the chosen spectral bandwidth that may be set by the user in normal operation of a spectrometer. The effective bandwidth coverage is excellent over a large range of frequency offsets except at the edges where deflections from  $i_0$  are evident. In further simulations for deriving a relationship between *bwdth* and *bw*<sub>eff</sub> measurements of *bw*<sub>eff</sub> were made in increments of 0.01 from  $i_0 = 0.900$  to 0.980 but RF<sub>max</sub> was calculated for  $i_0 = 0.990$ . The difference is called

Table 1

Curve fitting parameters for Eqs. (4) and (5) for calibration of peak amplitude given arbitrary bandwidth and duration  $HS_n$  pulses.

п	m <sub>RF</sub>			C <sub>RF</sub>					
	<i>a</i> <sub>0</sub>	<i>a</i> <sub>1</sub>	<i>a</i> <sub>2</sub>	$b_0$	$b_1$	<i>b</i> <sub>2</sub>			
1	2.809	-2.695	0.00015	-2.999	2.885	-0.00014			
2	13.1721	-12.5443	0.00164557	73.1919	-72.059	-0.000124453			
3	23.1589	-22.0563	0.00289193	76.7873	-73.0955	0.00946038			
4	30.967	-29.4931	0.00386602	105.994	-100.91	0.0134375			
5	36.9702	-35.2109	0.00461509	126.321	-120.215	0.0157604			
6	41.6564	-39.6743	0.00519944	146.154	-139.394	0.019002			
7	45.3921	-43.2323	0.00566627	148.37	-141.223	0.0167866			
8	48.4283	-46.1244	0.00000000	156.039	-147.382	0.0216615			



**Fig. 2.** Effective bandwidth profiles for the  $HS_n$  pulses as annotated in the inset for the same pulses used in Fig. 1. With increasing *n*, there is a loss of effective bandwidth coverage at the edge of the effective bandwidth caused by the steeper rise in peak amplitude. Pulses may be truncated at less than 1% of the peak amplitude to overcome the poor response at the edge but at the expense of increased  $RF_{max}$ . In broadband applications these losses are of little or no consequence.

 $\Delta i$ . This ensures greater than 96% inversion across the entire spectral bandwidth with 99.5% inversion on-resonance. The plots of Fig. 3 show the intercepts  $c_{\rm bw}$ , and slopes  $m_{\rm bw}$  of the linear  $T_{\rm p}bw_{\rm eff}$  versus  $T_{\rm p}bwdth$  plots fitted to,

$$m_{\rm bw} = c_0 + c_1/c_2 \cdot \Delta \iota \tag{6}$$

$$c_{\rm bw} = d_0 + d_1/d_2 \cdot \Delta \iota \tag{7}$$

Curve fitting parameters  $c_n$  and  $d_n$  of Fig. 3 are presented in Table. 2. Determination of the fitting coefficients then enables use of the peak amplitude master Eq. (3) and *bwdth* may be determined by Eq. (8), for a chosen  $\Delta t$ .

$$bwdth = (T_p bw_{\rm eff} - c_{\rm bw})/m_{\rm bw}T_p \tag{8}$$

It is well known that with increasing  $T_p$  the selectivity of the inversion profile is inversely proportional. For the simulation results of Fig. 4, the *bwdth* of the RF pulse was set at 40.0 kHz and  $T_p$  incremented from 1.0 to 40.0 ms for each of the HS<sub>n</sub> pulses. The peak amplitude was calculated using Eq. (3) and the effective bandwidth profile simulated. Interpolating functions were used to calculate the slope of the profile positive edge at the roots of  $t_0 = 0.5$  and  $t_0 = -0.5$ . Previously, selectivity was defined as  $\Delta bw = bwdth-bw_{eff}$ . Here a new definition is given where selective

ity is redefined as the slope in the range  $-0.5 \ge \iota_0 \le 0.5$ . Thus, for better selectivity  $\Delta bw \to \infty$ , or rather approaches the asymptote of chosen  $bw_{\text{eff}}$  because perfectly rectangular profiles across a spectral width are simply not possible. Interestingly, it is observed that beyond a particular  $T_p bwdth$  product, no additional gain in selectivity can be achieved. These are plotted as points on Fig. 4. No general relation has been incorporated into Eq. (8) for selectivity but the limits shown in Fig. 4 can be easily incorporated into a pulse sequence program to guide the user in selecting an appropriate

Table 2

Curve fitting parameters of Eqs. (6) and (7) relating the frequency sweep extent of the pulse and its efficiency of response.

п	m <sub>bw</sub>			Cbw			
	<i>c</i> <sub>0</sub>	<i>c</i> <sub>1</sub>	<i>c</i> <sub>2</sub>	$d_0$	$d_1$	$d_2$	
1	n/a	n/a	n/a	n/a	n/a	n/a	
2	1.16703	0.148477	34.7343	4.91443	-2.69978	32.2359	
3	1.09462	0.163382	72.6164	5.63907	-2.33021	33.9993	
4	1.06553	0.00328039	2.88295	6.52165	-0.16007	4.48865	
5	1.06	0.0605982	136.186	6.90398	0.00331353	56.2083	
6	1.05332	0.000368677	7.62293	6.91054	63.5322	1908.44	
7	1.07979	-0.00148105	0.891319	3.60916	1.99132	8.28099	
8	1.08354	-0.172168	74.0155	3.27327	31.722	98.17	



**Fig. 3.** Plots of the slope  $m_{bw}$  (a), and intercept  $c_{bw}$  (b) as a function of  $\Delta \iota$ . The slope and the intercept for each HS<sub>n</sub> pulse was determined by curve fitting plots of  $T_p bw_{eff}$  versus  $T_p bw dth$  by simulating  $bw_{eff}$  profiles with the Bloch equations. These are plotted as symbols on the curve fitted lines of Eq. (3). The coefficients of fitting are given in Table 2. The abscissa of the plots are  $\Delta \iota = \iota_0 - \iota_{bw}$ , where  $\iota_0$  is the target inversion number for a desired inversion efficiency (i.e. the number at which RF<sub>max</sub> was calculated) and  $\iota_{bw}$  is the inversion number at which  $bw_{eff}$  was measured.



**Fig. 4.** The behavior of  $HS_n$  pulses as a function of increasing duration for constant *bwdth* characterizes a selectivity that is optimal only to certain  $T_p bwdth$  limits. The  $T_p bwdth$  limit for each of the pulses annotated is shown in brackets. Better selectivity can be achieved with  $HS_2$  than with  $HS_8$  but at the expense of a larger  $T_p bwdth$  product. This translates to longer duration pulses in practice.

RF pulse for selective applications. In practical applications selectivity is critical in determining the level of separation between inverted and non-inverted spins.

The accuracy of derived Eqs. (3) and (8) was tested as follows. The effective bandwidth was set at 20.0 kHz. RF pulse bwdth was calculated using Eq. (8) for  $T_p$  ranging from 1.0 to 10.0 ms. It must be noted here that the first pulse falls in the partially adiabatic range and while the Bloch equation estimate is in error using the automated method with interpolating functions, peak amplitudes may be calculated with Eq. (3). The accuracy will, however, be poor because this represents extrapolation rather than operation within the bounds of numerical simulations. Nevertheless, peak amplitudes calculated for partially adiabatic pulses may be used with caution. With *bwdth* calculated, the resulting  $HS_n$  pulses were then used to calculate RF<sub>max</sub> for a desired level of inversion (in this case  $i_0$  = 0.990). Since Eq. (3) is compact the calculation takes a negligible amount of time and is ideally suited for "on-the-fly" decision making in pulse sequence programs. For comparison with Eq. (3), Bloch equations were used to generate RF<sub>max</sub> profiles with peak amplitudes calculated as described in methods section using interpolating functions. Such an operation can take a number of seconds depending on the processor type, np and the number of RF<sub>max</sub> increments etc. The comparison of Eqs. (3) and (8) with Bloch equation simulations are presented in Fig. 5a. Calculated peak amplitudes are in excellent agreement with Bloch equation simulations only deviating by less than 1% for the  $T_{\rm p}bwdth$  range chosen. The correlation coefficient of the straight line fit is 0.9997. As the  $T_{\rm p}$  bwdth product increases, RF<sub>max</sub> deviation of that calculated from Eq. (3) decreases as well. But as  $T_{\rm p}bwdth$  approaches the partially adiabatic limit, accuracy diminishes. In general the master equation yields highly accurate peak amplitudes for any given T<sub>p</sub>bwdth product in the linearly adiabatic range.

In the next test, effective bandwidth profiles were generated using the Bloch equations and compared with the nominal  $bw_{eff}$ of 20.0 kHz. Again there is excellent agreement between the chosen effective bandwidth and that calculated using Eq. (8) with deviations less than 1% for  $T_pbwdth$  products greater than 20 for all HS<sub>n</sub> pulses. These are presented in Fig. 5b. It is also worth noting that the RF pulse is determined by the effective bandwidth. In other words, the spectral width determines the extent of frequency sweep (*bwdth*) for the pulse. Thus comparing Fig. 2 where  $T_p bwdth = 40$  with Fig. 5b where  $T_p bw_{eff} = 20$  it is clear that having available a set of master equations guarantees practical performance – given that the spectral coverage is similar (i.e. ~20 kHz).

The most common use of adiabatic inversion is in broadband decoupling. Presented in Fig. 6 are spectra from one slice of a <sup>15</sup>N HSQC (Fig. 6a) with decoupling of <sup>15</sup>N accomplished with HS<sub>8</sub> and HS<sub>7</sub> pulses. An effective bandwidth of 10.0 kHz was chosen and  $T_p = 3.0$  ms, thus ensuring an RF pulse operating in the linearly adiabatic range. The frequency sweep extent bwdth, was calculated using Eq. (8) yielding 12.0 and 11.9 kHz for HS<sub>7</sub> and HS<sub>8</sub>, respectively. Optimal RF<sub>max</sub> was calculated using Eq. (3), which are 1.68 and 1.65 kHz, respectively. An additional 5–20% of  $RF_{max}$  was added to the peak amplitude for HS<sub>8</sub> and HS<sub>7</sub> pulses. Decoupling performance is not compromised even up to 20% increase in RF<sub>max</sub>. However, the user must be cautioned that adding more power into the sample simply results in sample heating and while line-width increases are not observed for the short acquisition time used for this sample, long acquisition runs on the same sample may lead to decreased performance. This will be true for all such pulses, however.

In Fig. 6c, extreme abuse of amplifier power setting is demonstrated for the HS<sub>7</sub> pulse used for decoupling in <sup>15</sup>N HSQC. The decibel units shown here are from that used in Topspin 2.5 software supplied by the instrument manufacturer (Bruker Biospin, GmBH). It is understood that these will be different for the various spectrometers in use. Here a 500 W amplifier was used with -6.0 dB representing full power. In the absence of any peak power checks or duty cycle limits, inadvertent miss-setting of power levels is possible. Thus at 0 dB (~250 W) the user may still observe decoupled peaks in spectra with about 25% loss in signal amplitude from the optimal setting (<9 dB).

#### 3. Experimental

All RF pulses were created using Eqs. (1) and (2), and implemented as either a C program or a Mathematica script for use with Bruker format waveform files. Gradient coherence selected HSQC experiments with sensitivity enhancement [20] were conducted



**Fig. 5.** Accuracy comparison between numerically derived Eq. (3) for (a) effective bandwidth and (b) for  $RF_{max}$  and Bloch equation simulations for the HS<sub>8</sub> pulse as an example. In the inset of plot (a) the effective bandwidth determined by Bloch equation simulation are plotted as points at  $t_{bw}$  = 0.990. The profiles beginning with  $T_p$  = 1.0 (right most dashed line) to 10.0 ms (left most plot) in 1.0 ms increments were determined by Bloch equations after calculating the *bwdth* of pulse required for chosen  $bw_{eff}$  = 20.0 (solid vertical line) and with  $RF_{max}$  determined by Eq. (3). Thus the divergence of the points from the vertical line represents the divergence of Eqs. (3) and (8) and the approach to partial adiabaticity. Similar plots can be derived for the other HS<sub>n</sub> pulses. In addition, the complete plot shows the usual selectivity improvement with increasing  $T_p$  and this is the case for any RF pulse. In plot (b), the excellent correspondence of Eq. (3) or by simulation is admonstrated for all HS<sub>n</sub> pulses. Here *bwdth* was determined for a target  $t_{bw}$  = 0.990 from Eq. (8), and RF<sub>max</sub> calculated with Eq. (3) or by simulation. Individual results are plotted as indicated.

on a Bruker 500 MHz NMR spectrometer with a triple resonance XYZ gradient 5 mm probe. The sample used was recombinant ubiquitin (Isotec), 2.5 mg dissolved in 0.5 mL, pH 7.4 buffered H<sub>2</sub>O/D<sub>2</sub>O (90:10 v/v) solution with a trace amount of NaN<sub>3</sub>. The sample was maintained at 295 K for all experiments. The hard 90 degree proton pulse duration for this sample was determined to be 8.3 µs at an amplifier setting of 2.3 dB. The hard 90 degree pulse duration  $pw_N$  for <sup>15</sup>N spins was determined to be 35.0 µs at 2.0 dB. All other conversions were calculated using the following expression;

$$dB = 20\log_{10}(B_{1(\text{ref})}/B_{1(\text{unknown})}) + dB_{\text{ref}}$$
(9)

Here  $B_{1(ref)} = 1000/4pw_N$  and  $B_{1(unknown)} \equiv RF_{max}$  calculated from Eq. (3). A STUD 112 [21] step phase cycle was directly written into the pulse sequence. In the *F*1 dimension 256 increments were col-

lected and 2048 F2 points of the free induction decay. The recycle delay was 1 s and spectra were collected in just over 10 min. All spectra were zero – filled to  $4096 \times 1024$  with sine-bell shifted window functions applied in both dimensions prior to Fourier transform.

#### 4. Conclusion

Adiabatic inversions are of value in NMR spectroscopy and imaging. A major limit of the use of these pulses has been the availability of general relations collecting the variables of such pulses into a closed form expression so that pulse sequence programming and decisions are made easily in some intuitive fashion and realistically related to the spin-system. With the availability of separable



**Fig. 6.** (a) <sup>15</sup>N HSQC spectrum collected with HS<sub>7</sub> used for decoupling with STUD112 cycle showing good decoupling over the entire spectral region. In (b), the decoupled boxed peak is shown with decoupling accomplished with a 3.0 ms HS<sub>8</sub> pulse of *bwdth* = 11.9 kHz, with  $l_0 = 0.990$  and  $l_{bw} = 0.900$ . RF<sub>max</sub> was calculated using Eq. (3) yielding 1.65 (optimal) and 1.73 (+5%) kHz. For HS<sub>7</sub>, the same inversion efficiency target was used and *bwdth* = 12.0 kHz. The increases in RF<sub>max</sub> correspond to 1.76, 1.85, 1.93 and 2.02 kHz from 5% to 20% of optimal RF<sub>max</sub>. Clearly decoupling performance is not compromised. The abuse of extreme power miss-setting is demonstrated in (c) with units given in dB units with 0 dB corresponding to ~250 W for the 500 W amplifier used here. With insufficient RF<sub>max</sub> *J*-coupling is only partially decoupled. The increase from 18 to 0 dB corresponds to RF<sub>max</sub> = 1.13, 2.26, 3.19, 4.51, 6.37, 8.99 kHz, i.e. ranging from a 33% underestimate to 435% over estimate.

expressions for  $RF_{max}$ ,  $T_p$ , *bwdth* and *bw*<sub>eff</sub> optimal parameters can be determined very quickly with these expressions embedded into pulse sequence programs.

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