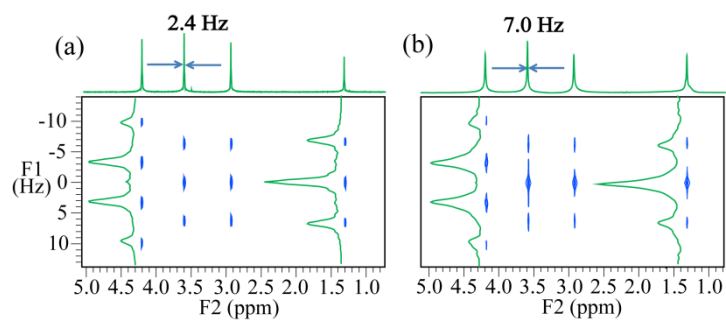


## Supporting Information

### A single-scan method for NMR 2D *J*-resolved spectroscopy

Liangjie Lin, Zhiliang Wei, Yanqin Lin\*, Zhong Chen

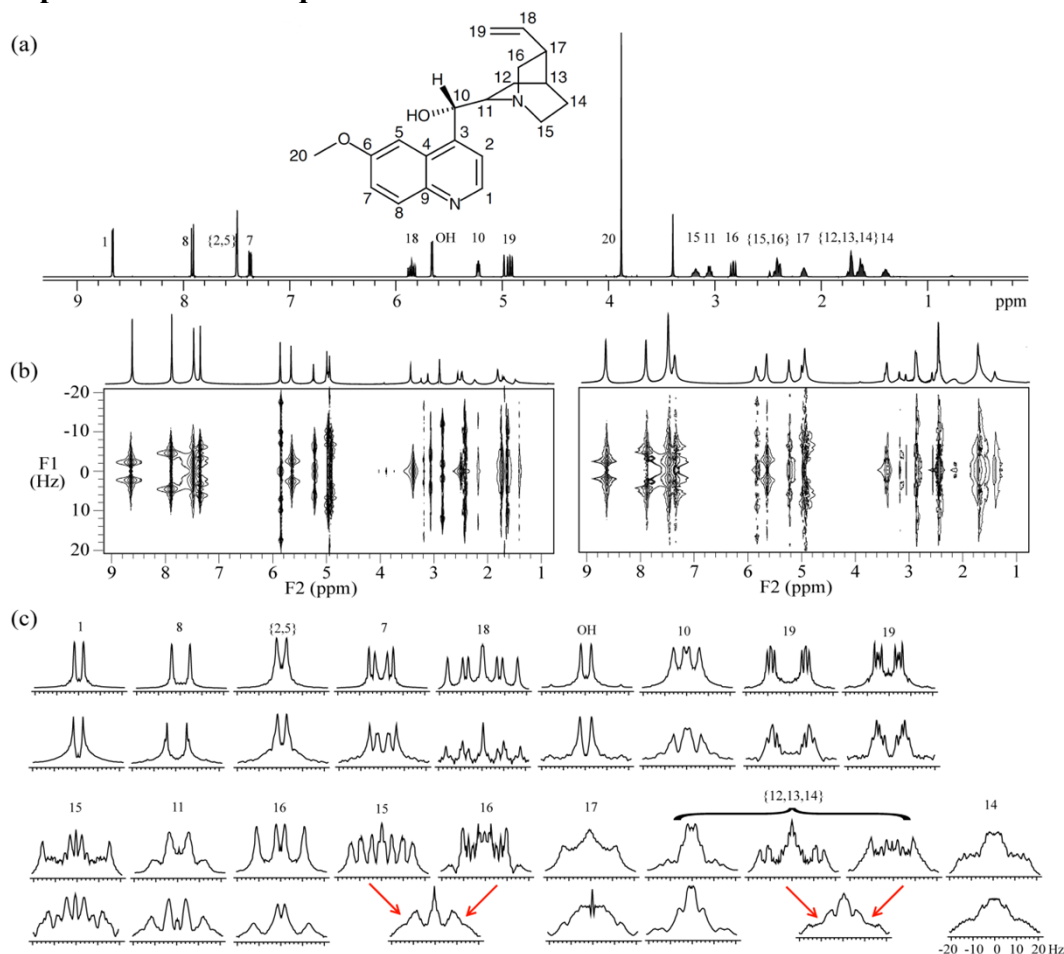
#### I. Spectra of a low-concentration sample (5 mM ethyl 3-bromopropionate in CDCl<sub>3</sub>)



**Figure S1.** (a) Conventional 2D *J*-resolved spectrum and (b) SSJ spectrum of the 5 mM ethyl 3-bromopropionate solution. The F2 projections are given on the top of the boxed diagrams, and F1 projections for resonances located at 1.3 and 4.2 ppm are also given inside the boxed diagrams.

The performance of SSJ is acceptable on a 5 mM ethyl 3-bromopropionate solution. Linewidths in the F2 dimension for the conventional 2D *J*-resolved and SSJ spectra are 2.4 and 7.0 Hz, respectively.

## II. Spectra of 200 mM quinine in DMSO-d6



**Figure S2.** (a) Molecular structure and conventional 1D spectrum of quinine, (b) conventional 2D *J*-resolved (left) and SSJ spectra (right) of quinine, (c) F1 projections of conventional 2D *J*-resolved (odd rows) and SSJ (even rows) spectra. The red arrows indicate that resonances are separated in the conventional 2D *J*-resolved spectrum, and overlapped in the SSJ spectrum.

Resonances from the aromatic and vinyl region of quinine are located in the spectral range from 4.5 to 9.0 ppm, and resonances from the aliphatic region in the spectral range from 1.0 to 4.0 ppm. In addition, two peaks of DMSO-d<sub>6</sub> (solvent) are located at 3.4 and 2.5 ppm. The methyl signal at 3.9 ppm was suppressed in both conventional 2D *J*-resolved and SSJ experiments for better spectral performances. The SSJ proves effective in providing fine structures of most the resonances in the quinine molecule, especially in the aromatic and vinyl region, and its performance degenerates in dealing with several crowded resonances in the aliphatic region. Resonances {15, 16} (around 2.4 ppm), which are distinguishable in the Con-*J* spectrum, become overlapped in the SSJ spectrum because of the small chemical-shift difference (about 10 Hz). Similarly, resonances {12, 13, 14} (around 1.7 ppm), exhibiting three chemical shifts in the Con-*J* spectrum, can narrowly show two chemical shifts in the SSJ spectrum.

### III. Pulse sequence code, reconstruction macro, and detailed description of data construction

#### 1. The core code of SSJ sequence:

```
#include <standard.h>
#include <chempack.h>
pulsesequence()
{
    //variables definition
    double np2=getval("np2");//'np2': double the number of complex data point in F2 dimension
    double np1=getval("np1");//'np1': number of data point in the F1 dimension.
    double i=1;
    double retdly=getval("retdly");//'retdly': time delay for controlling the sampling interval.

    rgpulse(pw,0,rof1,rof2);//the first exciting pulse. 'pw': the duration of the  $\pi/2$  pulse.
    delay(5e-6);
    for(i=1;i<np1/2+1;i++)//cyclic sampling.
    {
        //Phases of repeated 180° pulses are altered by reference to (x, x, -x, -x) for alleviating pulse
        //imperfections.
        rcvron();
        delay(5e-6);
        acquire(np2,1/sw);
        delay(5e-6);
        rcvroff();
        delay((retdly-2*pw)/2);
        rgpulse(2*pw,zero,rof1,rof2);
        delay((retdly-2*pw)/2);

        rcvron();
        delay(5e-6);
        acquire(np2,1/sw);
        delay(5e-6);
        rcvroff();
        delay((retdly-2*pw)/2);
        rgpulse(2*pw,zero,rof1,rof2);
        delay((retdly-2*pw)/2);

        rcvron();
        delay(5e-6);
        acquire(np2,1/sw);
        delay(5e-6);
        rcvroff();
    }
}
```

```

delay((retddy-2*pw)/2);
rgpulse(2*pw,two,rof1,rof2);
delay((retddy-2*pw)/2);

rcvron();
delay(5e-6);
acquire(np2,1/sw);
delay(5e-6);
rcvroff();
delay((retddy-2*pw)/2);
rgpulse(2*pw,two,rof1,rof2);
delay((retddy-2*pw)/2);
}
}

```

**2. Data of SSJ are processed with the vendor-provided software (VnmrJ 3.2), and the post-processing procedures are performed as follows:**

First, because VnmrJ 3.2 cannot process original SSJ data as 2D data directly, we need to create a blank 2D data container. This container can be reused for data of different samples.

Second, we move the acquired SSJ data to the aforementioned container. This task can be quickly (less than one second) accomplished with the aid of a macro command. The macro command codes are given as:

```

//N1: data points in F1 dimension; N2: data points in F2 dimension
//exp1: source data (original SSJ data); exp2: destination data (data container)
$ii=1
$jj=0
while ($ii <= N1) do
mfddata(exp1,1,(0+$jj*N2),exp2,$ii,0,N2)
$ii = $ii+1
$jj = $jj+2
endwhile

```

Third, parameters for LP calculation need to be set prior to the 2D DFT. Details for linear prediction include: 1. linear prediction (LP) coefficients should be greater than the number of sinusoidal signals contained in that FID; 2. data points available for calculating the LP coefficients should be greater than, or equal to, double the coefficient number; 3. data points of SSJ in the F2 dimension can usually be extrapolated by tenfold with the aid of suitable weighting functions.

Finally, implement the 2D DFT.