Supporting Information for:

A Method to Selectively Observe a Desired Linear Combination of Chemical Shifts in GFT Projection NMR Spectroscopy

Monalisa Swain[a,b] and Hanudatta S. Atreya*[,b]

[a]*Solid State and Structural Chemistry Unit and* [b]*NMR Research Centre, Indian Institute of Science, Bangalore-560012, India*

Table S1. Selection of Linear Combinations of Chemical Shifts Using Phase Cycling for Experiments Shown in Figs. (1-3).

Notes:

1. The r.f. phases (Φ_i) shown below correspond to those in Figs. (**1-2**). In these r.f. pulse sequences, the phase '*x*' selects cosine modulation of the signals and phase '*y*' selects the sine modulation. An 180^0 shift of phase results in inversion of the signals.

2. In experiments employing the sensitivity enhanced mode of data acquisition, an r.f. pulse exciting the ^{15}N spin immediately before its chemical shift evolution is chosen for phase cycling (e.g., r.f. phase Φ_4 in Fig. **2**). However, unlike the data acquired with the States method (Tables **1** and **2**), the phase Φ_4 is not incremented by 90^0 for acquiring the imaginary part. Instead, phase of another appropriate r.f. pulse (marked with phases Φ_6 in Fig. **2**) is changed by 180^0 simultaneously with inversion of a gradient (G2) used for coherence selection. This results in a *phase shift of* 90^0 for the ^{15}N chemical shift.

Experiment	FID	Scan	r.f Phases	Signal	Rec. Phase	Net Result
			Φ_1 Φ_2		Φ_{rec}	
(3,2)D HACA(CON)HN $\Omega(^{13}C^{\alpha}) + \Omega(^{1}H^{\alpha})$	Real	1	x x	$\cos(\Omega(^{1}H^{\alpha})t)*\cos(\Omega(^{13}C^{\alpha})t)$	0^0	Scan 1 – Scan 2 $\cos((\Omega(^{13}C^{\alpha})+\Omega(^{1}H^{\alpha}))t)$
		2	y y	$\sin(\Omega(^{1}H^{\alpha})t)*\sin(\Omega(^{13}C^{\alpha})t)$	180^0	
	Imag Φ_2+90^0	1	x y	$\cos(\Omega(^{1}H^{\alpha})t)*\sin(\Omega(^{13}C^{\alpha})t)$	0^0	Scan 1 – Scan 2 $\sin((\Omega(^{13}C^{\alpha}) + \Omega(^{1}H^{\alpha}))t)$
		2	y $-x$	$-\sin(\Omega(^{1}H^{\alpha})t)*\cos(\Omega(^{13}C^{\alpha})t)$	180^0	
(3,2)D HACA(CON)HN $\Omega(^{13}C^{\alpha}) - \Omega(^{1}H^{\alpha})$	Real	1	x x	$\cos(\Omega(^{1}H^{\alpha})t)*\cos(\Omega(^{13}C^{\alpha})t)$	0^0	Scan 1 – Scan 2 $\cos((\Omega(^{13}C^{\alpha}) - \Omega(^{1}H^{\alpha}))t)$
		2	y $-y$	$-\sin(\Omega(^{1}H^{\alpha})t)*\sin(\Omega(^{13}C^{\alpha})t)$	180^0	
	Imag Φ_2+90^0	1	x y	$\cos(\Omega(^{1}H^{\alpha})t)*\sin(\Omega(^{13}C^{\alpha})t)$	0^0	Scan 1 – Scan 2 $\sin((\Omega(^{13}C^{\alpha}) - \Omega(^{1}H^{\alpha}))t)$
		2	y x	$\sin(\Omega(^{1}H^{\alpha})t)*\cos(\Omega(^{13}C^{\alpha})t)$	180^0	
			Φ_1 Φ_4		Φ_{rec}	
(3,2)D HNNCO(CA) $\Omega(^{15}N) + \Omega(^{13}C')$	Real	1	x x	$\cos(\Omega(^{13}C')t)*\cos(\Omega(^{15}N)t)$	0^0	Scan 1 – Scan 2 $\cos((\Omega(^{15}N) +\Omega(^{13}C'))t)$
		2	y y	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{15}N)t)$	180^0	
	Imag Invert G2 & Φ_6	1	x x $+90^0$	$\cos(\Omega(^{13}C')t)*\sin(\Omega(^{15}N)t)$	0^0	Scan 1 – Scan 2 $\sin((\Omega(^{15}N) + \Omega(^{13}C'))t)$
		2	y y $+90^0$	$-\sin(\Omega(^{13}C')t)*\cos(\Omega(^{15}N)t)$	180^0	

(Table S1). Contd…...

(3,2)D HN<u>NCO</u>(CA) $\Omega(^{15}N) - \Omega(^{13}C')$	Real	1	$x \quad x$	$\cos(\Omega(^{13}C')t)*\cos(\Omega(^{15}N)t)$	0^0	Scan 1 – Scan 2 $\cos((\Omega(^{15}N) - \Omega(^{13}C'))t)$
		2	$y \quad -y$	$-\sin(\Omega(^{13}C')t)*\sin(\Omega(^{15}N)t)$	180^0	
	Imag Invert G2 & Φ_6	1	$x \quad x \quad +90^0$	$\cos(\Omega(^{13}C')t)*\sin(\Omega(^{15}N)t)$	0^0	Scan 1 – Scan 2 $\sin((\Omega(^{15}N) - \Omega(^{13}C'))t)$
		2	$y \quad -y \quad +90^0$	$\sin(\Omega(^{13}C')t)*\cos(\Omega(^{15}N)t)$	180^0	
(4,2)D HN<u>NCO</u>(CA) $\Omega(^{15}N) + \Omega(^{13}C') + \Omega(^{13}C^{\alpha})$	Real	1	$\Phi_1 \quad \Phi_2 \quad \Phi_4$ $x \quad x \quad x$	$\cos(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	Φ_{rec} 0^0	Scan 1 – Scan 2 + Scan 3 - Scan 4 $\cos((\Omega(^{15}N) + \Omega(^{13}C') + \Omega(^{13}C^{\alpha}))t)$
		2	$y \quad y \quad x$	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	180^0	
		3	$-x \quad y \quad y$	$-\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	0^0	
		4	$-y \quad -x \quad y$	$\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	180^0	
	Imag Invert G2 & Φ_6	1	$\Phi_1 \quad \Phi_2 \quad \Phi_4$ $x \quad x \quad x \quad +90^0$	$\cos(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	Φ_{rec} 0^0	Scan 1 – Scan 2 + Scan 3 - Scan 4 $\sin((\Omega(^{15}N) + \Omega(^{13}C') + \Omega(^{13}C^{\alpha}))t)$
		2	$y \quad y \quad x \quad +90^0$	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	180^0	
		3	$-x \quad y \quad y \quad +90^0$	$\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	0^0	
		4	$-y \quad -x \quad y \quad +90^0$	$-\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	180^0	
(4,2)D HN<u>NCO</u>(CA) $\Omega(^{15}N) + \Omega(^{13}C') - \Omega(^{13}C^{\alpha})$	Real	1	$\Phi_1 \quad \Phi_2 \quad \Phi_4$ $x \quad -x \quad x$	$-\cos(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	Φ_{rec} 0^0	Scan 1 – Scan 2 + Scan 3 - Scan 4 $-\cos((\Omega(^{15}N) + \Omega(^{13}C') - \Omega(^{13}C^{\alpha}))t)$
		2	$y \quad y \quad x$	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	180^0	
		3	$-x \quad y \quad y$	$-\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	0^0	

(Table S1). Contd…..

		4	$-y \quad x \quad y$	$-\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	180^0	
	Imag Invert G2 & Φ_6	$\Phi_1 \quad \Phi_2 \quad \Phi_4$ 1	$x \quad -x \quad x \quad +90^0$	$-\cos(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	Φ_{rec} 0^0	Scan 1 – Scan 2 + Scan 3 - Scan 4 $-\sin((\Omega(^{15}N)+\Omega(^{13}C') - \Omega(^{13}C^{\alpha}))t)$
		2	$y \quad y \quad x \quad +90^0$	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	180^0	
		3	$-x \quad y \quad y \quad +90^0$	$\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	0^0	
		4	$-y \quad x \quad y \quad +90^0$	$\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	180^0	
(4,2)D HNNCO(CA) $\Omega(^{15}N) - \Omega(^{13}C') + \Omega(^{13}C^{\alpha})$	Real	$\Phi_1 \quad \Phi_2 \quad \Phi_4$ 1	$x \quad -x \quad x$	$-\cos(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	Φ_{rec} 0^0	Scan 1 – Scan 2 + Scan 3 - Scan 4 $-\cos((\Omega(^{15}N) - \Omega(^{13}C') + \Omega(^{13}C^{\alpha}))t)$
		2	$y \quad y \quad x$	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	180^0	
		3	$-x \quad y \quad -y$	$\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	0^0	
		4	$-y \quad x \quad -y$	$\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	180^0	
	Imag Invert G2 & Φ_6	$\Phi_1 \quad \Phi_2 \quad \Phi_4$ 1	$x \quad -x \quad x \quad +90^0$	$-\cos(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	Φ_{rec} 0^0	Scan 1 – Scan 2 + Scan 3 - Scan 4 $-\sin((\Omega(^{15}N) - \Omega(^{13}C') + \Omega(^{13}C^{\alpha}))t)$
		2	$y \quad y \quad x \quad +90^0$	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	180^0	
		3	$-x \quad y \quad -y \quad +90^0$	$-\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	0^0	
		4	$-y \quad x \quad -y \quad +90^0$	$-\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	180^0	

(Table S1). Contd…...

(4,2)D HNNCO(CA) $\Omega(^{15}N)$ -$\Omega(^{13}C')$ - $\Omega(^{13}C^{\alpha})$	Real		Φ_1 Φ_2 Φ_4		Φ_{rec}	
		1	x x x	$\cos(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	0^0	Scan 1 – Scan 2 + Scan 3 - Scan 4
		2	y y x	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	180^0	$\cos((\Omega(^{15}N) -\Omega(^{13}C') - \Omega(^{13}C^{\alpha}))t)$
		3	$-x$ y $-y$	$\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	0^0	
		4	$-y$ $-x$ $-y$	$-\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	180^0	
	Imag Invert G2 & Φ_6		Φ_1 Φ_2 Φ_4		Φ_{rec}	
		1	x x x $+90^0$	$\cos(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	0^0	Scan 1 – Scan 2 + Scan 3 - Scan 4
		2	y y x $+90^0$	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	180^0	$\sin((\Omega(^{15}N) -\Omega(^{13}C')t - \Omega(^{13}C^{\alpha})t)$
		3	$-x$ y $-y$ $+90^0$	$-\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	0^0	
		4	$-y$ $-x$ $-y$ $+90^0$	$\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	180^0	