## **Supporting Information for:**

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

Monalisa Swain<sup>a,b</sup> and Hanudatta S. Atreya<sup>\*,b</sup>

<sup>a</sup>Solid State and Structural Chemistry Unit and <sup>b</sup>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 ( $\Phi_i$ ) 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<sup>0</sup> 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 <sup>15</sup>N spin immediately before its chemical shift evolution is chosen for phase cycling (e.g., r.f. phase  $\Phi_4$  in Fig. 2). However, unlike the data acquired with the States method (Tables 1 and 2), the phase  $\Phi_4$  is not incremented by 90<sup>0</sup> for acquiring the imaginary part. Instead, phase of another appropriate r.f. pulse (marked with phases  $\Phi_6$  in Fig. 2) is changed by 180<sup>0</sup> simultaneously with inversion of a gradient (G2) used for coherence selection. This results in a *phase shift of 90<sup>0</sup>* for the <sup>15</sup>N chemical shift.

Experiment	FID	Scan	r.f Phases	Signal	Rec. Phase	Net Result
			$\mathbf{\Phi}_1  \mathbf{\Phi}_2$		$\Phi_{ m rec}$	Scan 1 - Scan 2
	Real	1	x x	$\cos(\Omega({}^{1}\mathrm{H}^{\alpha})t) * \cos(\Omega({}^{13}\mathrm{C}^{\alpha})t)$	$0^{0}$	Scall I – Scall 2
						$\cos((\Omega(^{13}C^{\alpha})+\Omega(^{1}H^{\alpha}))t)$
(3,2)D HACA(CON)HN		2	у у	$\sin(\Omega(^{1}\mathrm{H}^{\alpha})t)^{*}\sin(\Omega(^{13}\mathrm{C}^{\alpha})t)$	$180^{0}$	
	Imag					Scan 1 – Scan 2
$\Omega(^{13}C^{\alpha}) + \Omega(^{1}H^{\alpha})$		1	x y	$\cos(\Omega(^{1}\mathrm{H}^{\alpha})t)*\sin(\Omega(^{13}\mathrm{C}^{\alpha})t)$	00	
	$\Phi_{2}$ +90 <sup>0</sup>					$\sin((\Omega(^{13}C^{\alpha}) + \Omega(^{1}H^{\alpha}))t)$
		2	y -x	$-\sin(\Omega({}^{1}\mathrm{H}^{\alpha})t)*\cos(\Omega({}^{13}\mathrm{C}^{\alpha})t)$	$180^{0}$	
(3,2)D <u>HA-</u>		1	<i>x x</i>	$\cos(\Omega(^{1}\mathrm{H}^{a})t)*\cos(\Omega(^{13}\mathrm{C}^{a})t)$	00	Scan 1 – Scan 2
<u>CA</u> (CON)HN	Real					$((\Omega)^{13}C^{(0)}, \Omega)^{(111^{(0)})}$
$\Omega(^{13}C^{\alpha}) - \Omega(^{1}H^{\alpha})$		2	у -у	$-\sin(\Omega({}^{1}\mathrm{H}^{\alpha})t)*\sin(\Omega({}^{13}\mathrm{C}^{\alpha})t)$	1800	$\cos((\Omega((\Omega((C^*) - \Omega(H^*))t)$
						Scan 1 – Scan 2
	Imag	1	х у	$\cos(\Omega(^{1}\mathrm{H}^{\alpha})t) * \sin(\Omega(^{13}\mathrm{C}^{\alpha})t)$	00	
	$\Phi_{+}90^{0}$					$\sin((\Omega({}^{*}C^{*}) - \Omega({}^{*}H^{*}))t)$
	$\Phi_2 + 90$	2	y x	$\sin(\Omega(^{1}\mathrm{H}^{\alpha})t)^{*}\cos(\Omega(^{13}\mathrm{C}^{\alpha})t)$	$180^{0}$	
			$\mathbf{\Phi}_1  \mathbf{\Phi}_4$		$\Phi_{ m rec}$	
						Scan 1 – Scan 2
(3,2)D	Real	1	x x	$\cos(\Omega(^{13}\mathrm{C'})t)^*\cos(\Omega(^{15}\mathrm{N})t)$	00	
HN <u>NCO</u> (CA)						$\cos((\Omega(^{15}N) + \Omega(^{13}C'))t)$
$O(^{15}N) + O(^{13}C')$		2	у у	$\sin(\Omega(^{13}\mathrm{C}')t)*\sin(\Omega(^{15}\mathrm{N})t)$	$180^{0}$	
22( 14) ⊤ 22( C )	Imag					
		1	$x = x + 90^{\circ}$	$\cos(\Omega(^{13}\mathrm{C'})t)*\sin(\Omega(^{15}\mathrm{N})t)$	00	Scan 1 – Scan 2
	Invert G2 &					
	$\Phi_6$	2	<i>y y</i> +90 <sup>0</sup>	$-\sin(\Omega(^{13}\mathrm{C'})t)^*\cos(\Omega(^{15}\mathrm{N})t)$	$180^{0}$	$\sin((\Omega(^{15}\mathrm{N}) + \Omega(^{13}\mathrm{C'}))t)$

(Table S1). Contd.....

						Scan 1 – Scan 2
		1	<i>x x</i>	$\cos(\Omega(^{13}\mathrm{C'})t)*\cos(\Omega(^{15}\mathrm{N})t)$	00	15 12
(3,2)D HN <u>NCO</u> (CA)	Real	2	у -у	$-\sin(\Omega(^{13}\mathrm{C}')t)*\sin(\Omega(^{15}\mathrm{N})t)$	$180^{0}$	$\cos((\Omega(^{13}\mathrm{N}) - \Omega(^{13}\mathrm{C}^{*}))t)$
$\Omega(^{15}N) - \Omega(^{13}C')$	Imag	1	$x = x + 90^{\circ}$	$\cos(\Omega(^{13}\mathrm{C}')t)*\sin(\Omega(^{15}\mathrm{N})t)$	00	Scan 1 – Scan 2
	Invert G2 &					$\sin((\Omega(^{15}N) - \Omega(^{13}C'))t)$
	$\Phi_6$	2	<i>y</i> - <i>y</i> +90 <sup>0</sup>	$\sin(\Omega(^{13}\mathrm{C'})t)^*\cos(\Omega(^{15}\mathrm{N})t)$	$180^{0}$	
			$\Phi_1  \Phi_2  \Phi_4$		$\Phi_{ m rec}$	
(4,2)D H <u>NNCO(</u> CA)		1	<i>x x x</i>	$\cos(\Omega(^{13}\mathrm{C}')t)*\cos(\Omega(^{13}\mathrm{C}'')t)$ $*\cos(\Omega(^{15}\mathrm{N})t)$	00	Scan 1 – Scan 2 + Scan 3 - Scan 4
$\begin{split} \Omega(^{15}\mathrm{N}) + \Omega(^{13}\mathrm{C}^{*}) \\ + \Omega(^{13}\mathrm{C}^{\alpha}) \end{split}$	Real	2	y y x	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C')t)$ $*\cos(\Omega(^{15}N)t)$	1800	$\cos((\Omega(^{15}N) + \Omega(^{13}C') + \Omega(^{13}C'))$
		3	-х у у	$-\cos(\Omega(^{13}\mathrm{C}')t)*\sin(\Omega(^{13}\mathrm{C}'')t)$ $*\sin(\Omega(^{15}\mathrm{N})t)$	00	
		4	-y -x y	$\sin(\Omega(^{13}\text{C}')t)*\cos(\Omega(^{13}\text{C}^{\alpha})t)$ $*\sin(\Omega(^{15}\text{N})t)$	1800	
			$\Phi_1  \Phi_2  \Phi_4$		$\Phi_{ m rec}$	
		1	$x x x +90^{0}$	$\cos(\Omega(^{13}C')t)*\cos(\Omega(^{13}C')t)$ $*\sin(\Omega(^{15}N)t)$	00	Scan 1 – Scan 2 + Scan 3 - Scan 4
I Inve	Imag	2	$y y x +90^{\circ}$	$\sin(\Omega(^{13}\text{C}')t)*\sin(\Omega(^{13}\text{C}^{\alpha})t)$ $*\sin(\Omega(^{15}\text{N})t)$	180 <sup>0</sup>	$\sin((\Omega(^{15}N) + \Omega(^{13}C'))$
	Invert G2 & $\Phi_6$	3	$-x  y  y + 90^{0}$	$\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	00	$+ \Omega(\mathcal{C}^{*})t)$
		4	$-y$ $-x$ $y$ $+90^{0}$	$-\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	$180^{0}$	
			$\Phi_1  \Phi_2  \Phi_4$		$\Phi_{ m rec}$	
(4,2)D H <u>NNCO(</u> CA)		1	x -x x	$-\cos(\Omega(^{13}C')t)^*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	00	Scan 1 – Scan 2 + Scan 3 - Scan 4
$\Omega(^{15}N) + \Omega(^{13}C')$ $- \Omega(^{13}C^{\alpha})$	Real	2	y y x	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	1800	$-\cos((\Omega(^{15}N) + \Omega(^{13}C') - \Omega(^{13}C'))t)$
		3	-х у у	$-\cos(\Omega(^{13}\text{C}^{*})t)*\sin(\Omega(^{13}\text{C}^{\alpha})t)$ $*\sin(\Omega(^{15}\text{N})t)$	00	

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		4	-y x y	$-\sin(\Omega(^{13}\mathrm{C}')t)*\cos(\Omega(^{13}\mathrm{C}^{\alpha})t)$ $*\sin(\Omega(^{15}\mathrm{N})t)$	180 <sup>0</sup>	
			$\Phi_1  \Phi_2  \Phi_4$		$\Phi_{ m rec}$	
				$-\cos(\Omega(^{13}\mathrm{C}')t)*\cos(\Omega(^{13}\mathrm{C}^{\alpha})t)$		
	Imag Invert G2 & Φ <sub>6</sub>	1	$x -x x +90^{\circ}$	$sin(\Omega(^{15}N)t)$	00	Scan 1 – Scan 2
		2	$y y x + 90^{0}$	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C')t)$ $*\sin(\Omega(^{15}N)t)$	1800	+ Scan 3 - Scan 4 -sin(( $\Omega(^{15}N) + \Omega(^{13}C')$ - $\Omega(^{13}C^{\alpha}))t$ )
		3	$-x  y  y + 90^{0}$	$\cos(\Omega(^{13}\text{C}')t)*\sin(\Omega(^{13}\text{C}^{\alpha})t)$ $*\cos(\Omega(^{15}\text{N})t)$	00	
		4	$-y  x  y  +90^{\circ}$	$\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C')t)$ $*\cos(\Omega(^{15}N)t)$	1800	
			$\Phi_1  \Phi_2  \Phi_4$		$\Phi_{ m rec}$	
(4,2)D H <u>NNCO(</u> CA)		1	x -x x	$-\cos(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	00	Scan 1 – Scan 2 + Scan 3 - Scan 4
$\Omega(^{15}N) - \Omega(^{13}C')$ + $\Omega(^{13}C^{\alpha})$	Real	2	y y x	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C')t)$ $*\cos(\Omega(^{15}N)t)$	180 <sup>0</sup>	$-\cos((\Omega(^{15}N) - \Omega(^{13}C^{*})))$
		3	-х у -у	$\cos(\Omega(^{13}\text{C}')t)*\sin(\Omega(^{13}\text{C}^{\alpha})t)$ $*\sin(\Omega(^{15}\text{N})t)$	00	+ <u>s</u> z( C <i>j</i> ),
		4	-y x -y	$\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	1800	
			$\Phi_1  \Phi_2  \Phi_4$		$\Phi_{ m rec}$	
			220	$-\cos(\Omega(^{13}\mathrm{C}')t)*\cos(\Omega(^{13}\mathrm{C}^{\alpha})t)$		
		1	$x -x + 90^{\circ}$	$sin(\Omega(^{15}N)t)$	00	Scan 1 – Scan 2
	Imag Invert G2 & Φ <sub>6</sub>	2	$y y x +90^{0}$	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	1800	+ Scan 3 - Scan 4
		3	$-x$ y $-y$ $+90^{0}$	$-\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	00	$-\sin((\Omega(N) - \Omega(TC)) + \Omega(TC)) + \Omega(TC)$
		4	$-y  x  -y  +90^{0}$	$-\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	180 <sup>0</sup>	

### (Table S1). Contd......

			$\Phi_1  \Phi_2  \Phi_4$		$\Phi_{ m rec}$	
(4,2)D H <u>NNCO</u> (CA)		1	<i>x x x</i>	$\cos(\Omega(^{13}C')t)^*\cos(\Omega(^{13}C^a)t)$ $*\cos(\Omega(^{15}N)t)$	00	Scan 1 – Scan 2 + Scan 3 - Scan 4
$Ω(^{15}N) - Ω(^{13}C')$ - $Ω(^{13}C^{\alpha})$	Real	2	y y x	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	$180^{0}$	$\cos((\Omega(^{15}N) - \Omega(^{13}C'))$
		3	-x y -y	$\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C')t)$ $*\sin(\Omega(^{15}N)t)$	00	$- \Omega(C^{(m)})t)$
		4	-y -x -y	$-\sin(\Omega(^{13}C')t)*\cos(\Omega(^{13}C^{a})t)$ $*\sin(\Omega(^{15}N)t)$	$180^{0}$	
			$\Phi_1  \Phi_2  \Phi_4$		$\Phi_{ m rec}$	
		1	<i>x x x</i> +90 <sup>0</sup>	$\begin{aligned} \cos(\Omega(^{13}\mathrm{C}')t) &* \cos(\Omega(^{13}\mathrm{C}^{\alpha})t) \\ &* \sin(\Omega(^{15}\mathrm{N})t) \end{aligned}$	00	Scan 1 – Scan 2
	Imag	2	y y x +90 <sup>0</sup>	$\sin(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\sin(\Omega(^{15}N)t)$	$180^{0}$	+ Scan 3 - Scan 4
	Invert G2 & $\Phi_6$	3	-x y $-y$ +90 <sup>0</sup>	$-\cos(\Omega(^{13}C')t)*\sin(\Omega(^{13}C^{\alpha})t)$ $*\cos(\Omega(^{15}N)t)$	00	$\sin((\Omega({}^{15}\mathrm{N}) - \Omega({}^{15}\mathrm{C}')t) - \Omega({}^{15}\mathrm{C}'')t)$ $- \Omega({}^{13}\mathrm{C}'')t)$
		4	$-y$ $-x$ $-y$ $+90^{\circ}$	$\sin(\Omega(^{13}C')t)^*\cos(\Omega(^{13}C^a)t)$ $*\cos(\Omega(^{15}N)t)$	180 <sup>0</sup>	