**Combining heteronuclear correlation NMR with spin-diffusion to detect relayed Cl-H-H and N-H-H proximities in molecular solids**

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**Abbreviations:**

DQ-SQ: Double Quantum-Single Quantum

SD: Spin Diffusion

RFDR: Radio Frequency Driven Recoupling

HMQC: Heteronuclear Multiple Quantum Coherence

**L-Histidine.HCl**

**Figure 3 #1 -** 1D single pulse experiment

**#2 -** 1D 1H{14N} HMQC spectrum

**#3 -** 1D 1H{14N} HMQC-RFDR spectrum

**#4 -** 1D 1H{35Cl} HMQC spectrum

**#5 -** 1D 1H{35Cl} HMQC-RFDR spectrum

**Figure 4 #6, #7 -** 2D 1H{14N} HMQC spectra

**#8, #9 -** 2D 1H{14N} HMQC-RFDR spectra

**Figure 5 #10, #11 -** 2D 1H{35Cl} HMQC spectrum

**#12, #13 -** 2D 1H{35Cl} HMQC-RFDR spectrum

**Figure S1 #14 -** 1D 1H-1H DQ-SQ correlation spectrum

**Figure S2 #15, #16 -** 2D 1H-1H SD

**Figure S3 #17, #18 -** 2D 1H-1H SD-RFDR

**Figure S4 #19-** 1D 35Cl Q-CPMG

DFT geometry optimized crystallography information file (cif)

Magres file for NMR shielding calculations

**Dopamine.HCl**

**Figure 6 #21 -** 1D single pulse experiment

**#22 -** 1D 1H{14N} HMQC spectrum

**#23 -** 1D 1H{14N} HMQC-RFDR spectrum

**#24 -** 1D 1H{35Cl} HMQC spectrum

**#25 -** 1D 1H{35Cl} HMQC-RFDR spectrum

**Figure 7 #26, #27 -** 2D 1H{14N} HMQC spectra

**#28, #29 -** 2D 1H{14N} HMQC-RFDR spectra

**Figure 8 #30 -** 2D 1H{35Cl} HMQC spectrum

**#31 -** 2D 1H{35Cl} HMQC-RFDR spectrum

**Figure S8 #32 -** 1D 1H-1H DQ-SQ correlation spectrum

**Figure S9 #33 -** 2D 1H-1H SD-RFDR

**Figure S10 #34 -** 1D 35Cl Q-CPMG

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