Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Two-dimensional proton-detected $^{35}Cl/^{1}H$ correlation solid-state NMR experiment under fast magic angle sample spinning: Application to pharmaceutical compounds

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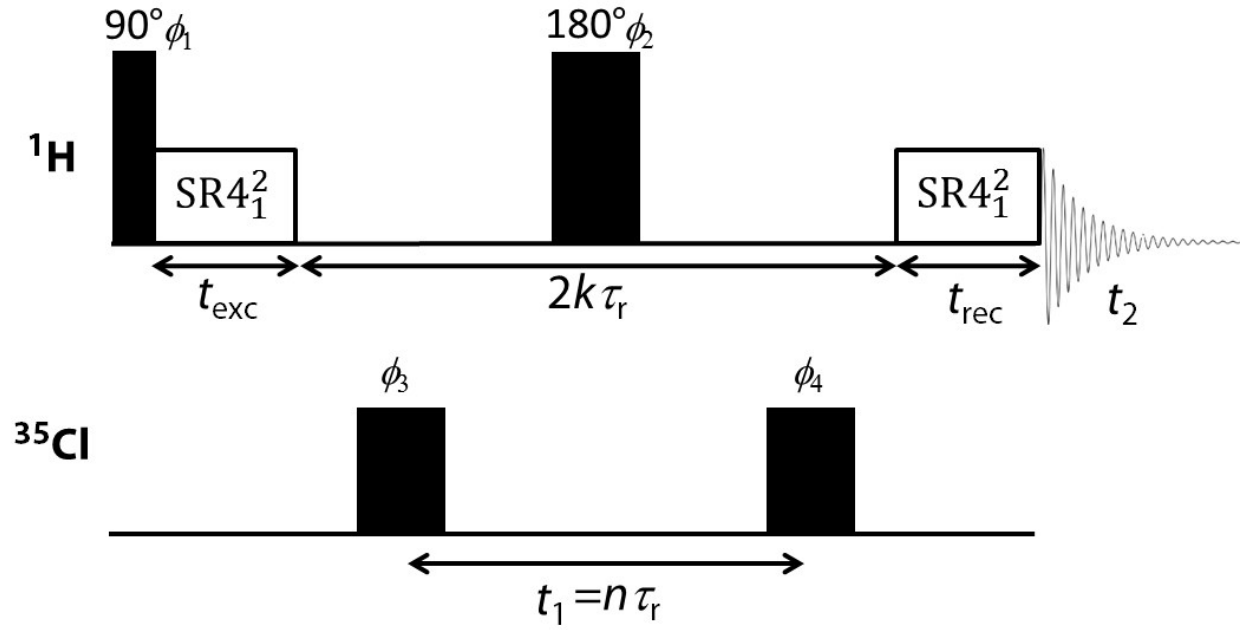

Figure S1. Two-dimensional heteronuclear dipolar coupling based D-HMQC pulse sequence to accomplish ^{35}Cl/^{1}H correlations in the present study. Rotor-synchronized heteronuclear dipolar recoupling sequence $SR4_1^2$ is applied during the excitation and reconversion periods. To maximize the formation of rotational echoes, the time intervals between $SR4_1^2$ and 180°pulse on ^{1}H channel are rotor-synchronized. The phase cycling scheme used for the pulse sequence shown is as follows: ϕ_1 = {2(0), 2(180), 2(90), 2(270)}, ϕ_2 = {0}, ϕ_3={0, 180}, ϕ_4={0}, ϕ_{aqc} = {0, 180, 180, 0, 270, 90, 90, 270}.

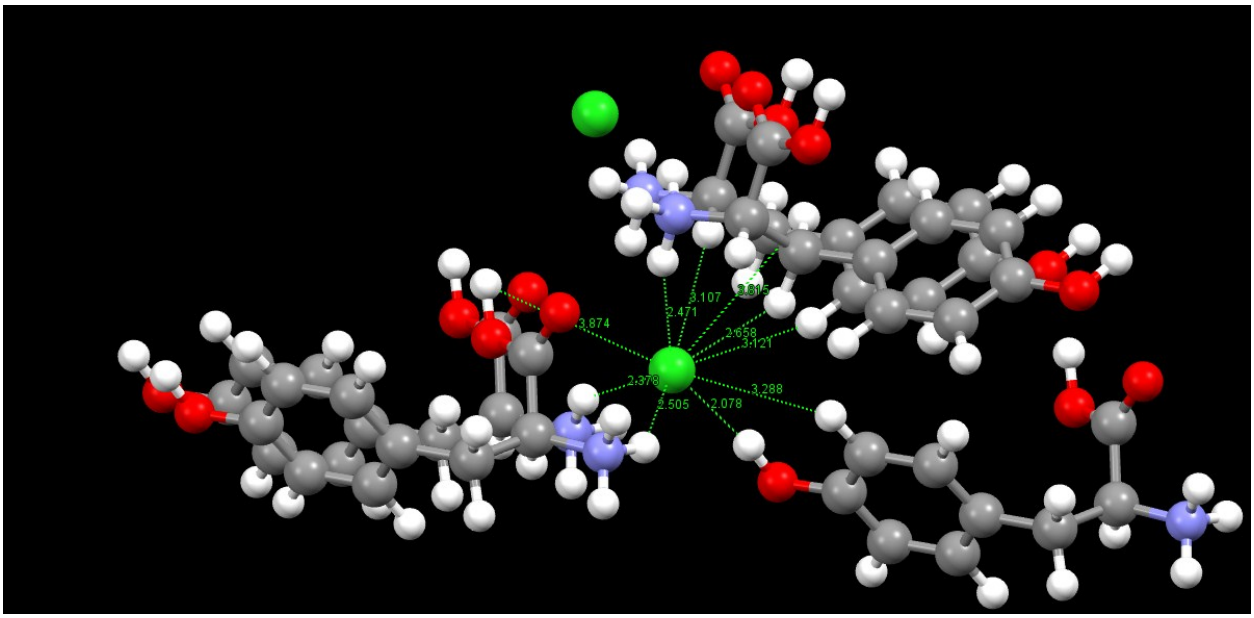

Figure S2. ^{35}Cl (green sphere) to ^{1}H (white sphere) distances from the crystal structure of L-Tyrosine.HCl. All distances shorter than 3.784 Å are shown.

Aminoguanidine HCl (Amin)

Procainamide HCl (Proc)

Figure S3. Molecular structures of Amonoguanidine HCl (Amin) and Procainamide HCl (Proc).

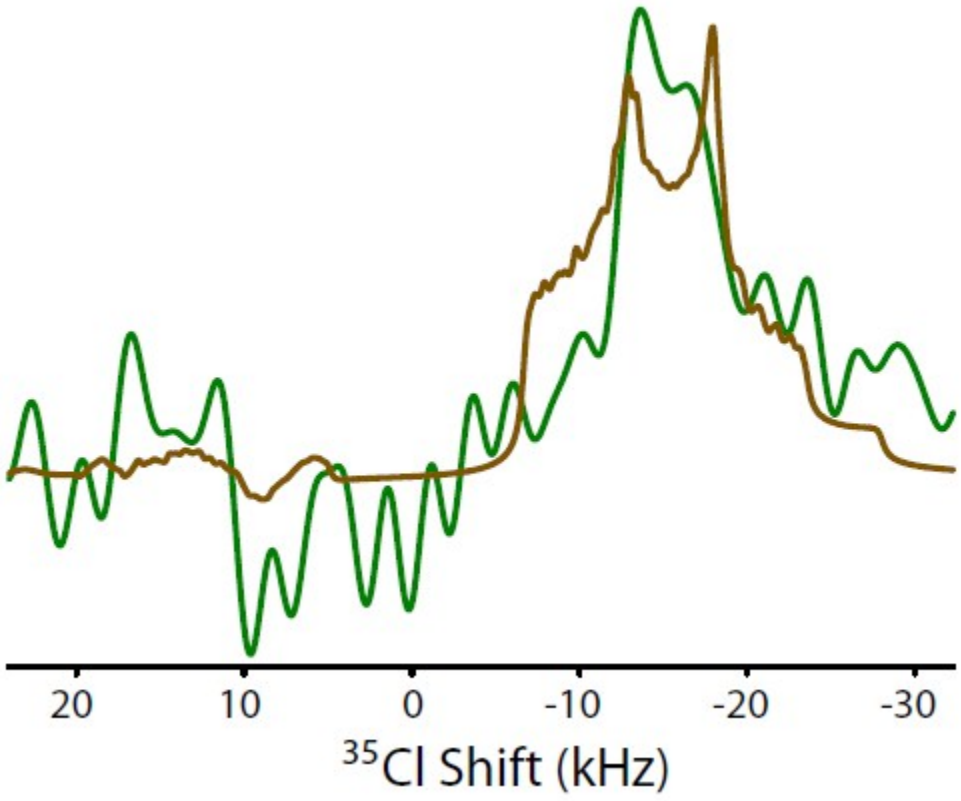

Figure S4. ^{35}Cl experimental lineshape (green) extracted parallel to the indirect frequency dimension of the 2D ^{35}Cl/^{1}H correlation spectrum at 10.4 ppm ^{1}H chemical shift of Amin and the corresponding simulated lineshape (brown).