Non-Covalent Interactions of a Drug Molecule Encapsulated in a Hybrid Silica Gel

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Supplementary information

Table 1. Relative molar ratios, pH and stirring time (t_s) for hybrid gel formulations

Gel	*TEOS*	*MTS*	*H_2O*	*Ethanol*	*HCl*	*PP*	*t_s (h)/pH*
TEOS:MTS(1:1)	*1*	*1.00*	*9.79*	*3.90*	*0.0039*	*0.058*	*24 / 2.2*
TEOS:MTS(3:1)	*1*	*0.33*	*6.53*	*2.60*	*0.0026*	*0.039*	*24 / 2.2*
TEOS:MTS(5:1)	*1*	*0.20*	*5.88*	*2.34*	*0.0023*	*0.035*	*24 / 2.2*

Table 2: 2D ^{29}Si-^{1}H FSLG HETCOR and ^{13}C-^{1}H FSLG HETCOR NMR experimental parameters.

	^{29}Si-^{1}H HETCOR	^{13}C-^{1}H HETCOR
Number of t_1 increments	80	76
Relaxation delay /s	2	2
Number of scans	72	400
MAS rate /kHz	12.5	12.5
^{1}H RF field /kHz	104	104
^{1}H LG offset frequency /kHz	+1.0	+1.0
FSLG decoupling power /kHz	127	127
Positive offset frequency (+ΔLG) /kHz	+74.680	+74.680
Negative offset frequency (–ΔLG) /kHz	–72.680	–72.680
CP Contact time /ms	2.0	1.0

In theory, under FSLG decoupling, the proton chemical shift is scaled by $1/\sqrt{3}$ (0.577) and the proton chemical shift scale has been corrected for this scaling in all of the 2D spectra. The ^{1}H chemical shift scale and the scaling factors were determined by comparing the 1D ^{1}H spectra recorded under fast MAS. The scaling factors obtained for all the 2D spectra were well within the range of the theoretical value. ^{13}C and ^{29}Si chemical shifts are reported using the δ scale and are externally referenced to adamantane and Q^8M^8, respectively. In addition, ^{13}C{^{1}H} and ^{29}Si{^{1}H} CPMAS experiments were performed with a CP contact time of 2.0 and 7.0 ms, respectively.

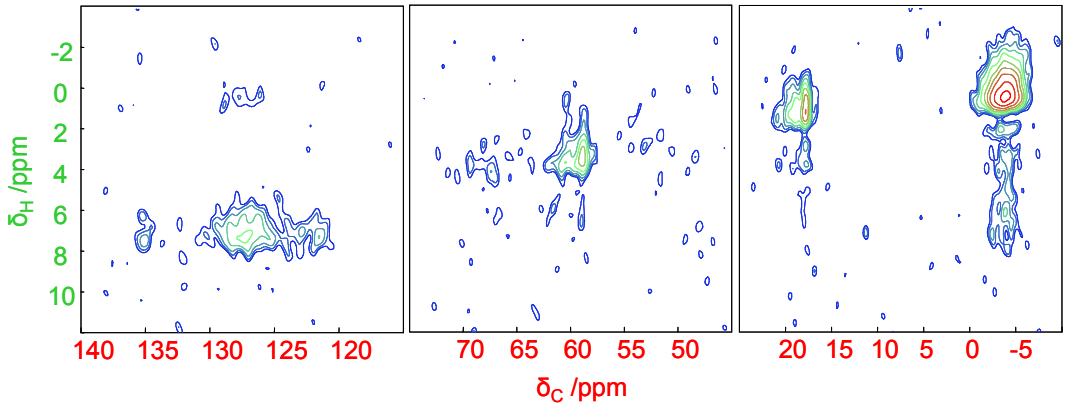

Fig. S1: The 2D ^{13}C-^{1}H FSLG HETCOR NMR spectra of hybrid gel (TEOS:MTS 3:1) at MAS of 12.5 kHz and a contact time of 0.8 ms.