

## Characterising the role of water in sildenafil citrate by NMR crystallography: Supplementary Information

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### Data bundle information

**Table S6:** Summary of data contained in associated data bundle.

Data bundle	Results presented	Comments
Sildenafil_citrate_AJR.zip	Figure 1	Varian .fid files containing 75 MHz $^{13}\text{C}$ spectra as a function of temperature: ajr19Mar0701.fid ... ajr20Mar0714.fid
Sildenafil-citrate-HETCOR.zip	Figure 6	Varian .fid files containing $^{13}\text{C}/^1\text{H}$ HETCOR data (see contained README for details)
sildenafil-citrate-2HVT.tar	Figure 2	Spinsight files containing $^2\text{H}$ VT data (see contained README for further information)
sildenafil-citrate-2HEXSY.tar	Figures 3 & 4	Raw (Spinsight) and processed data for $^2\text{H}$ DQ/SQ EXSY experiments (see contained README for further information)
sildenafil-citrate-CASTEP.tar	Figures 5 & 6	CASTEP results and analysis spreadsheet
sild13dvs0015.xls	Figure S1	Dynamic Vapour Sorption results (Excel spreadsheet)
SildenafilCitrateTGA.zip	(Not shown)	TGA results for “wet” and “dry” sample as Excel spreadsheets.