Supporting information:

Insights into the interaction of discodermolide and docetaxel with tubulin. Mapping the binding sites of microtubule-stabilizing agents by using an integrated NMR and computational approach.

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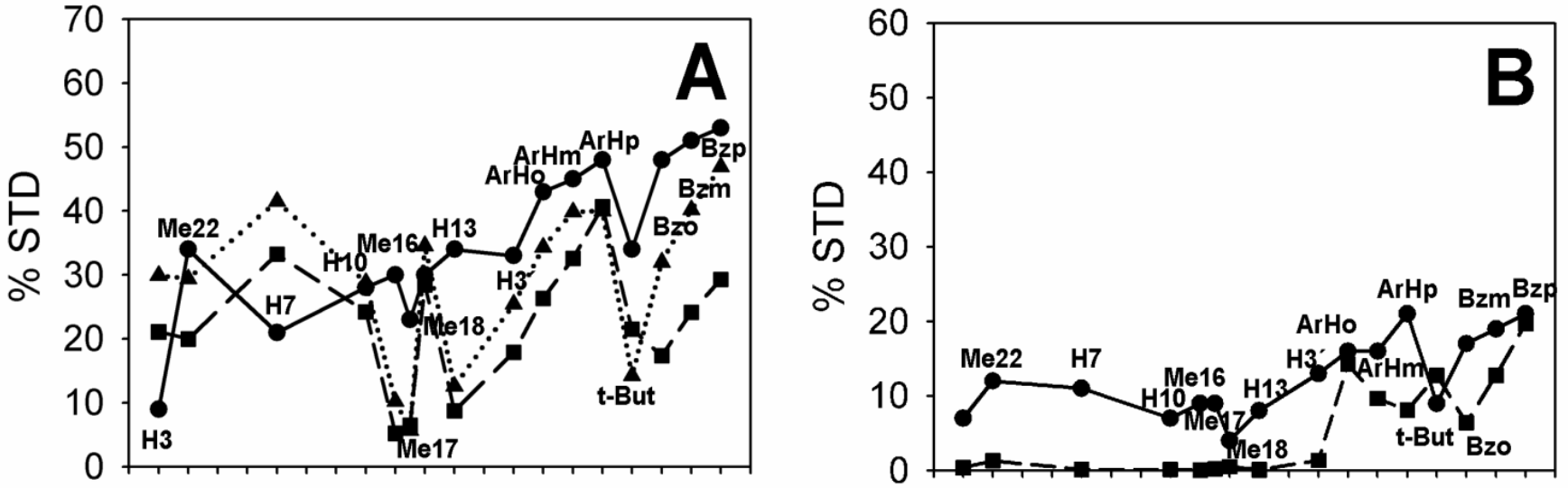
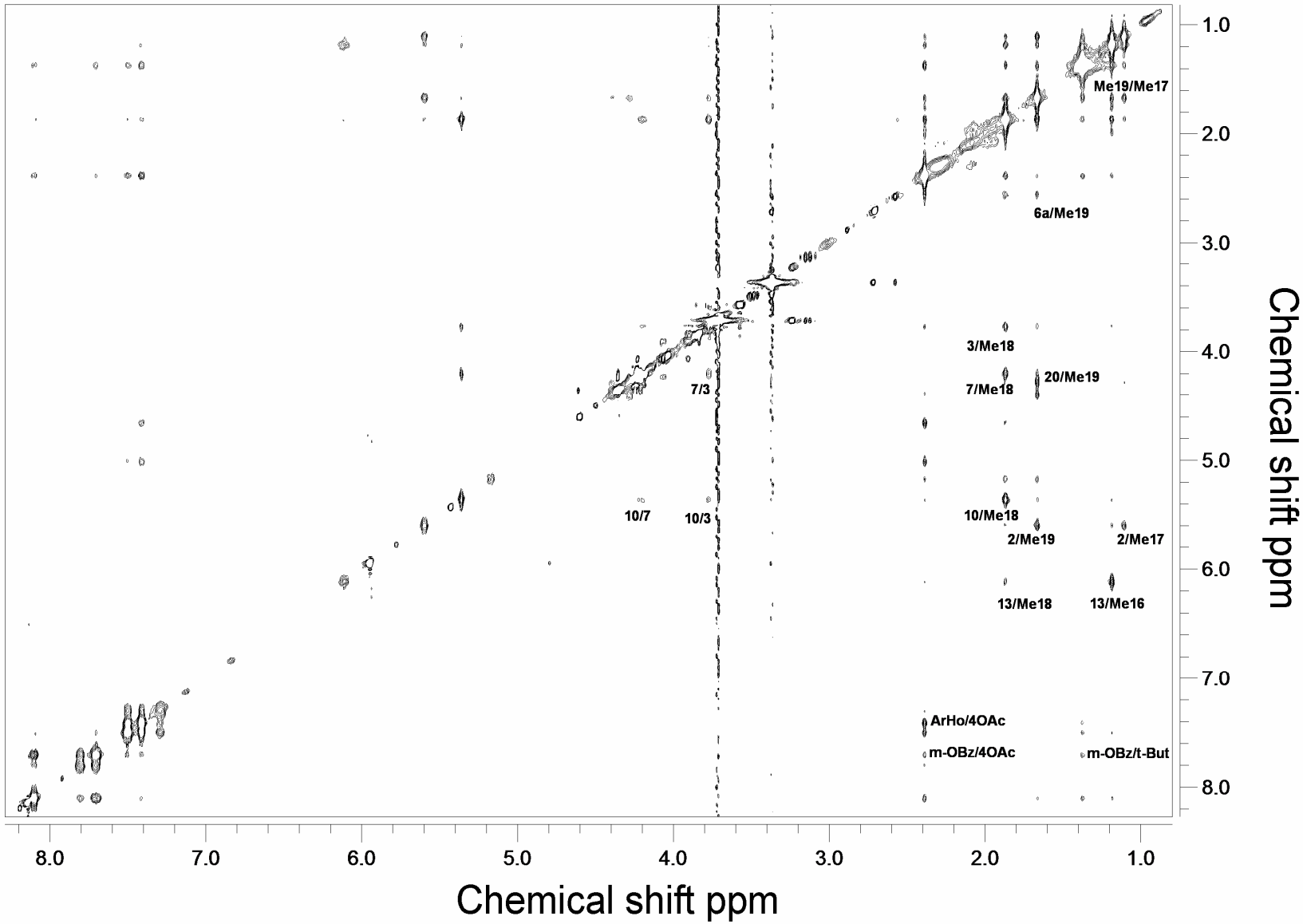
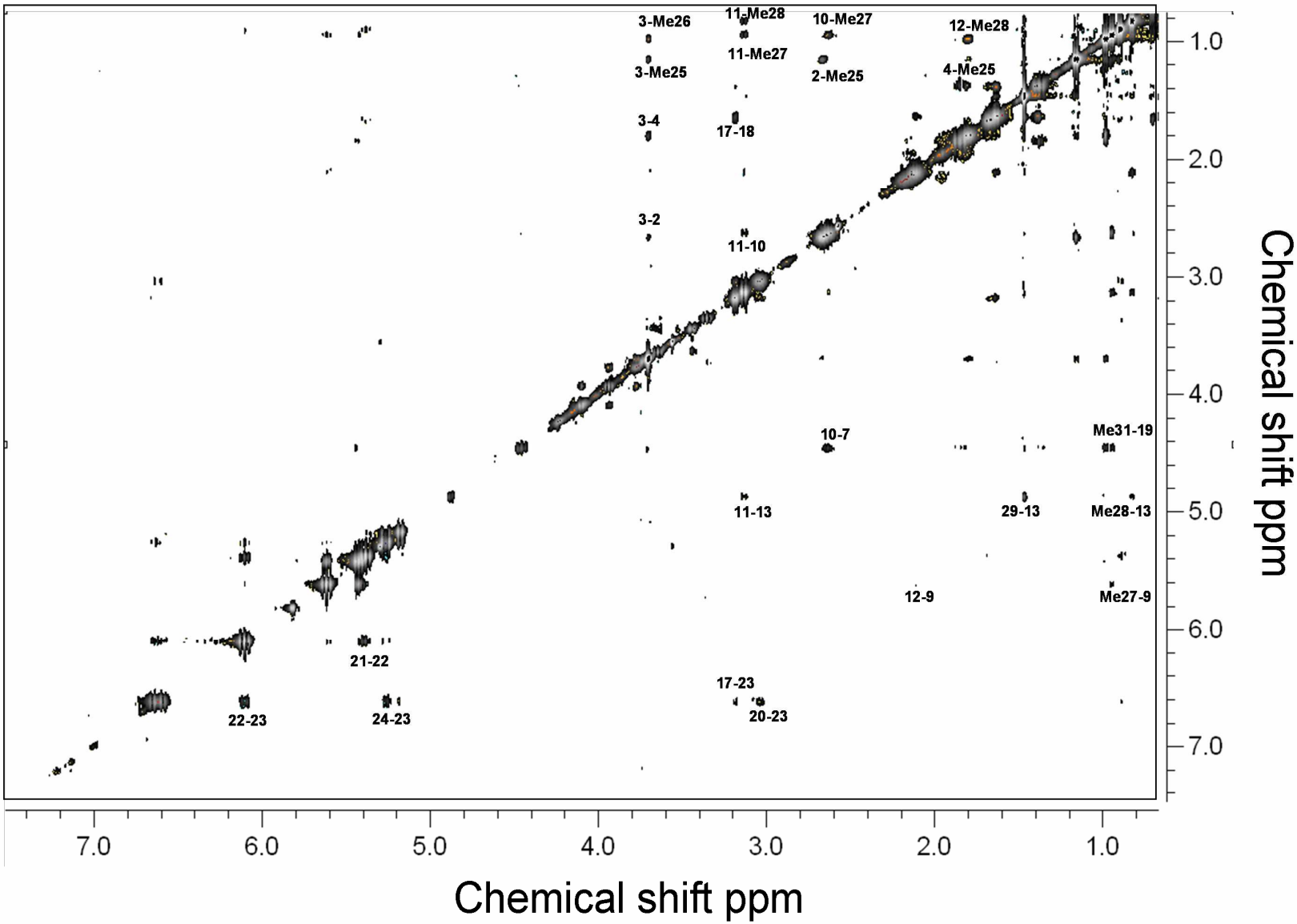


Supplementary Figure 1.- A. Solid line and circles denote docetaxel experimental STD effects when bound to microtubules. Dashed line and squares denote CORCEMA-STD calculation with the coordinates of the docetaxel at the pore of microtubules (pink structure, figure 5A). Dotted line and triangles denote CORCEMA-STD calculation with the coordinates of the docetaxel at the luminal site of microtubules. B. Solid line and circles denote docetaxel experimental STD effects when bound to dimers. Dashed line and squares denote CORCEMA-STD calculation with the coordinates of the docetaxel at the semisite pore (with only β4 present) of microtubules (pink structure, figure 5A).



Supplementary figure 2.- Expansion of TR-NOESY spectra (mixing time: 300 ms) of docetaxel (Figure 2A) in the presence of non-polymerized tubulin α/β-heterodimer (D_2O, 298 K).



Supplementary figure 3.- Expansion of TR-NOESY spectra (mixing time: 300 ms) of discodermolide (Figure 2B) in the presence of non-polymerized tubulin α/β-heterodimer (D_2O, 298 K).