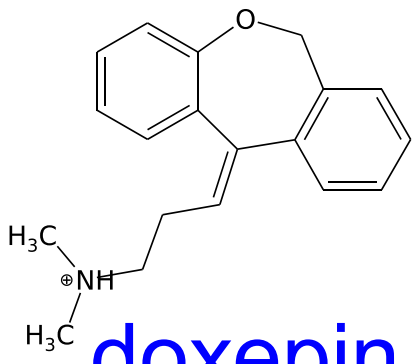
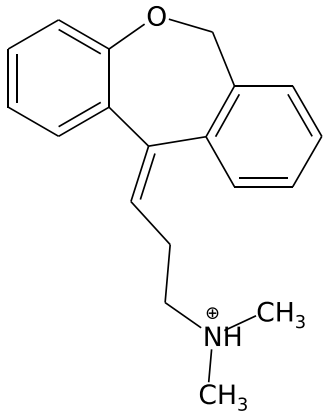
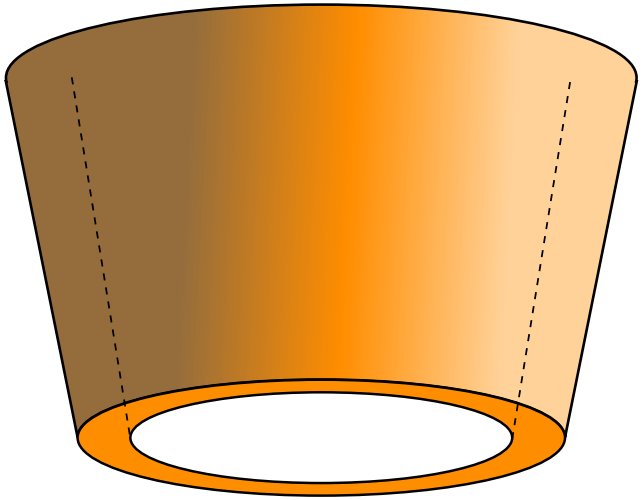
Introduction of reacting partners



doxepin ?





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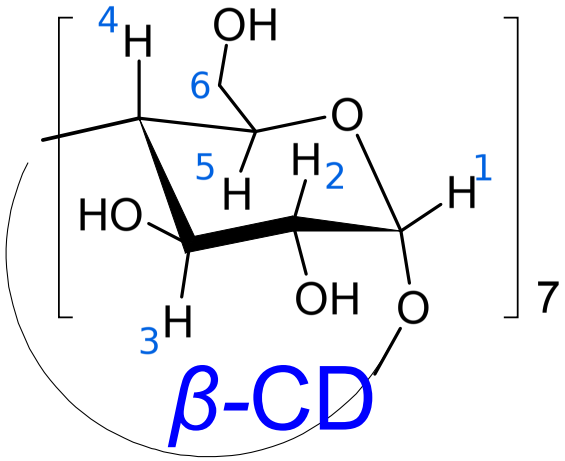
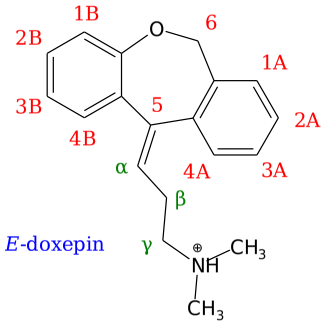
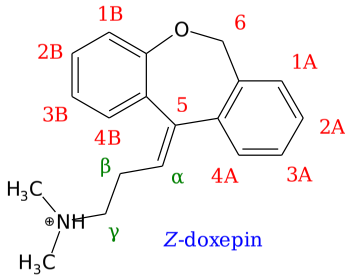


β-CD

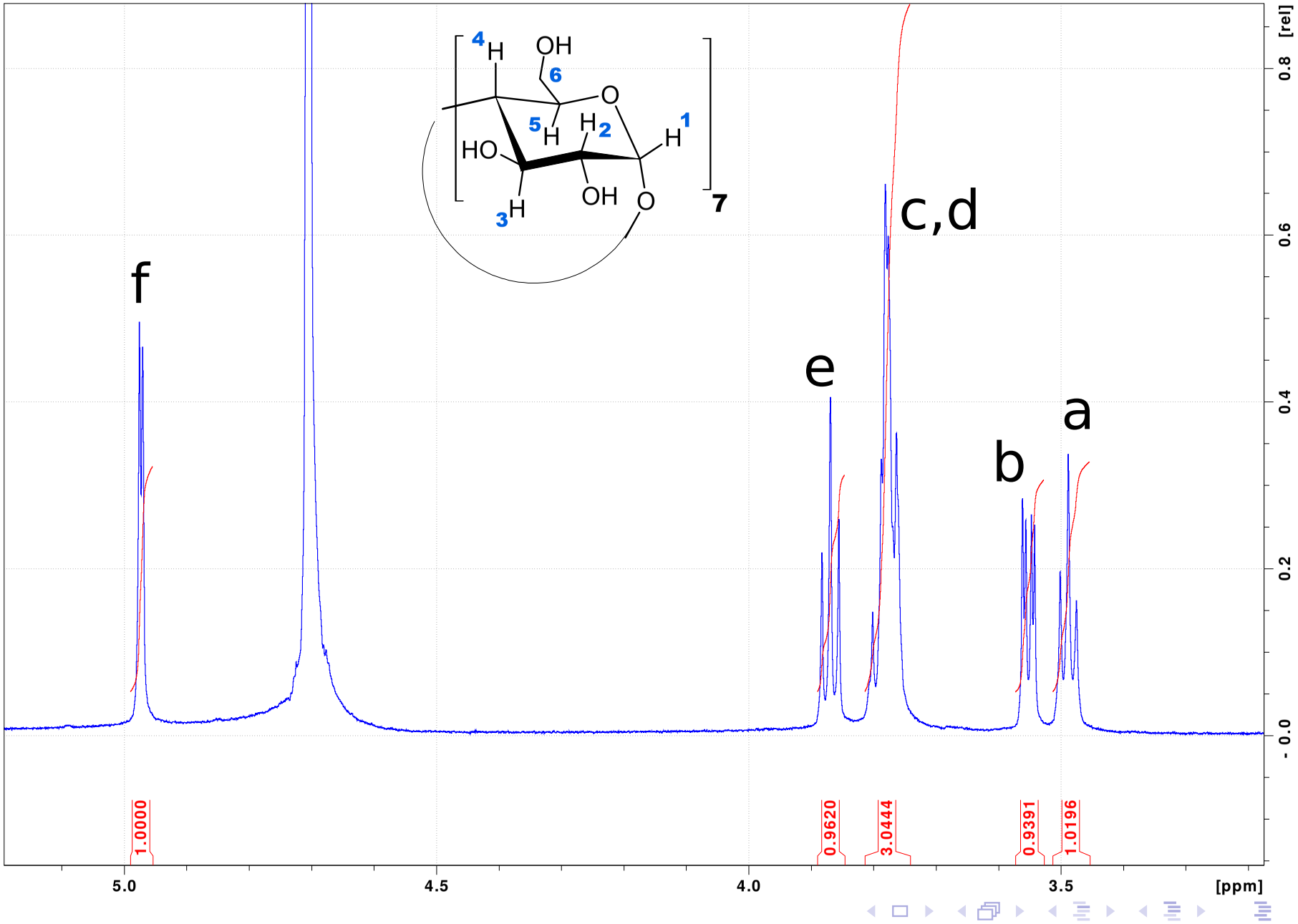
Recommended procedure

1. Assignment of free receptor: β-cyklodextrine (1D ^{1}H, DQF-COSY)
2. Assignment of free ligand: doxepine (1D ^{1}H, DQF-COSY, NOESY)
   - Identification of proton resonances of ring A and B
   - Determination of major and minor conformation of doxepin
3. 1D NMR titration: rearrangement of β-cyclodextrin resonaces upon interaction $\Rightarrow$ identification of inner protons
4. 1D NMR titration: rearrangement of doxepin resonaces upon complexation $\Rightarrow$ estimation of binding mode
5. ROESY spectrum of complex: ROE intermolecular contacts
6. Fitting the titration isotherm

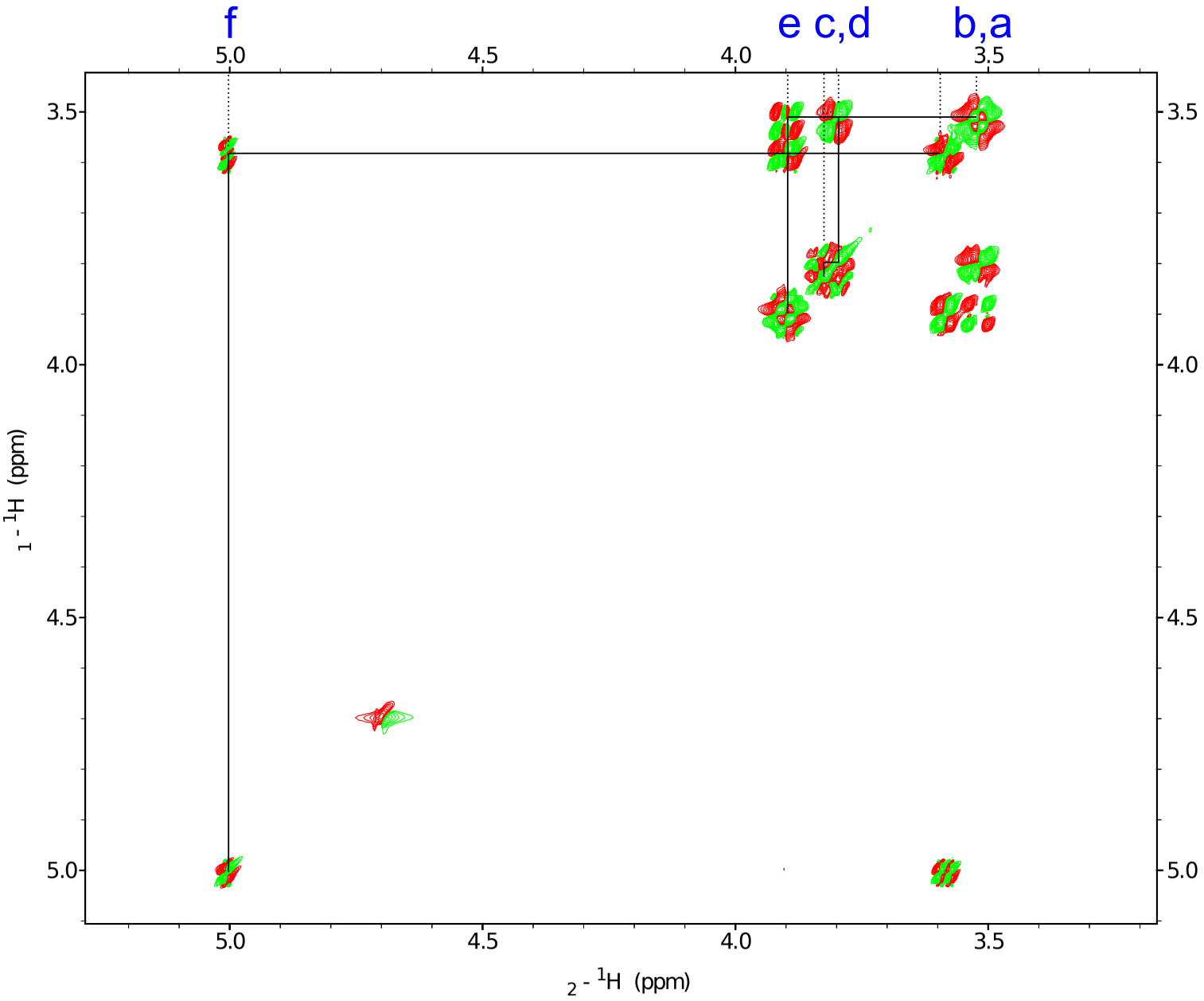




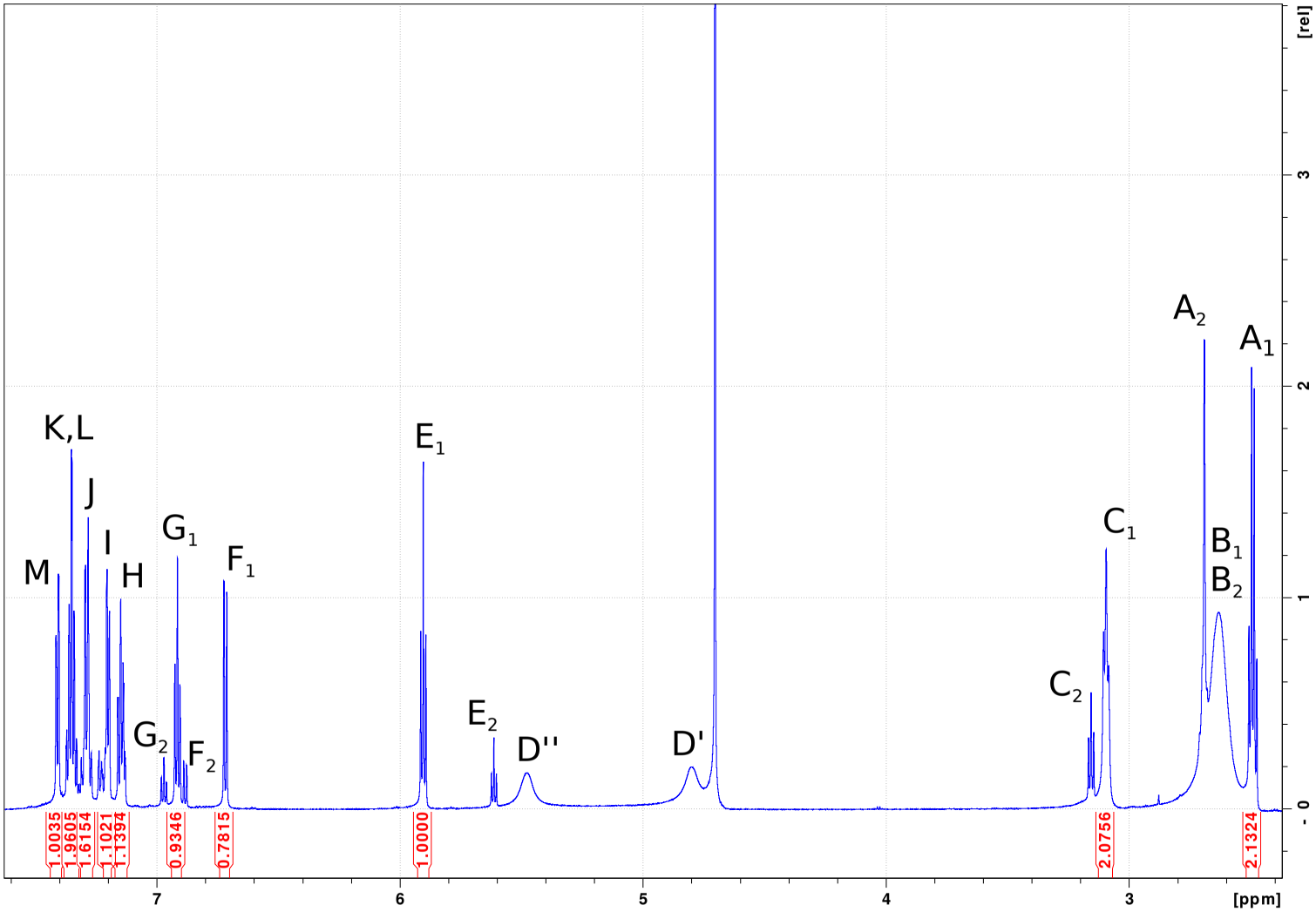
1D ^{1}H of β-cyclodextrin in D_2O



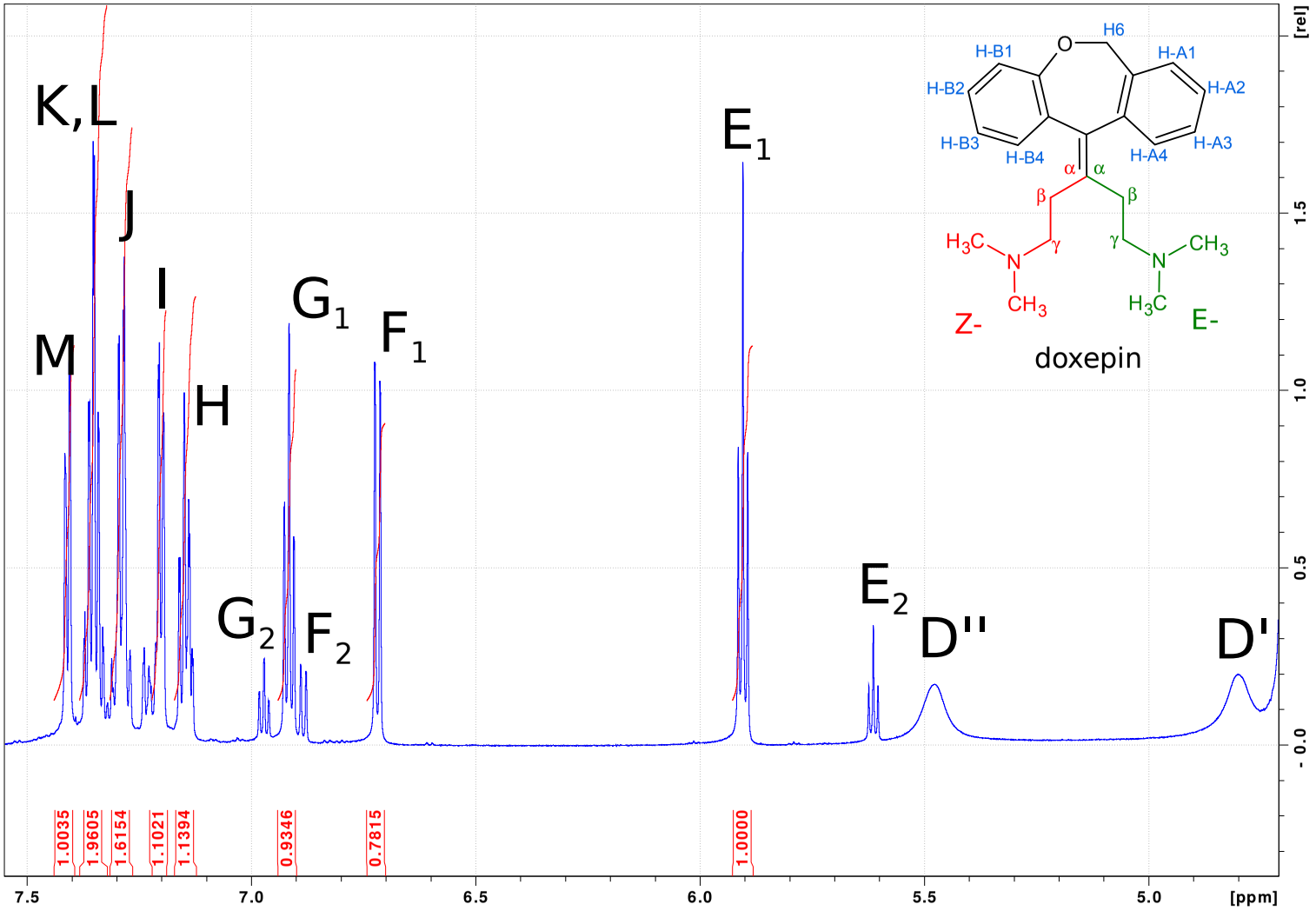
DQF-COSY of β-cyclodextrin in D_2O



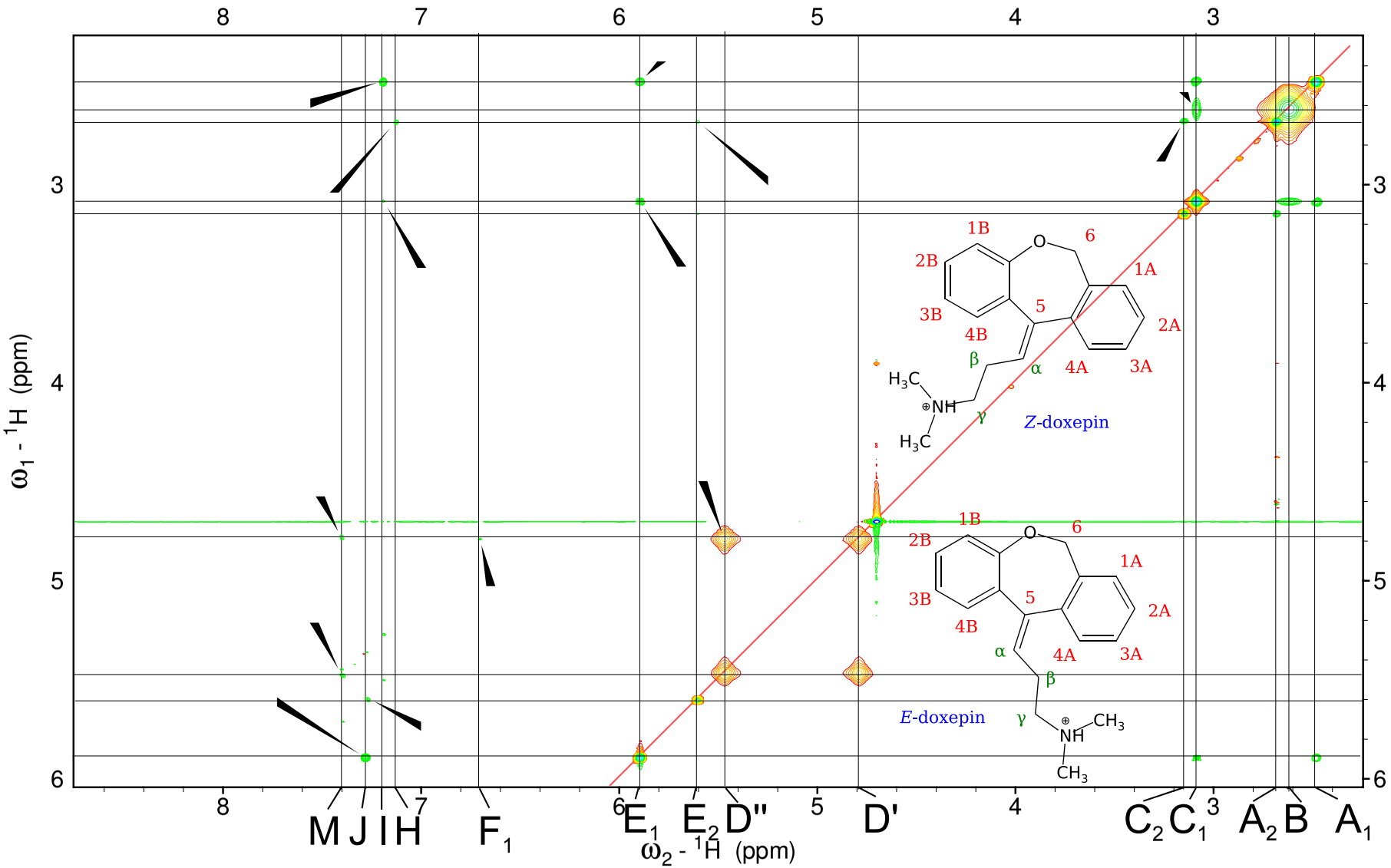
1D ^{1}H of doxepin in D_2O



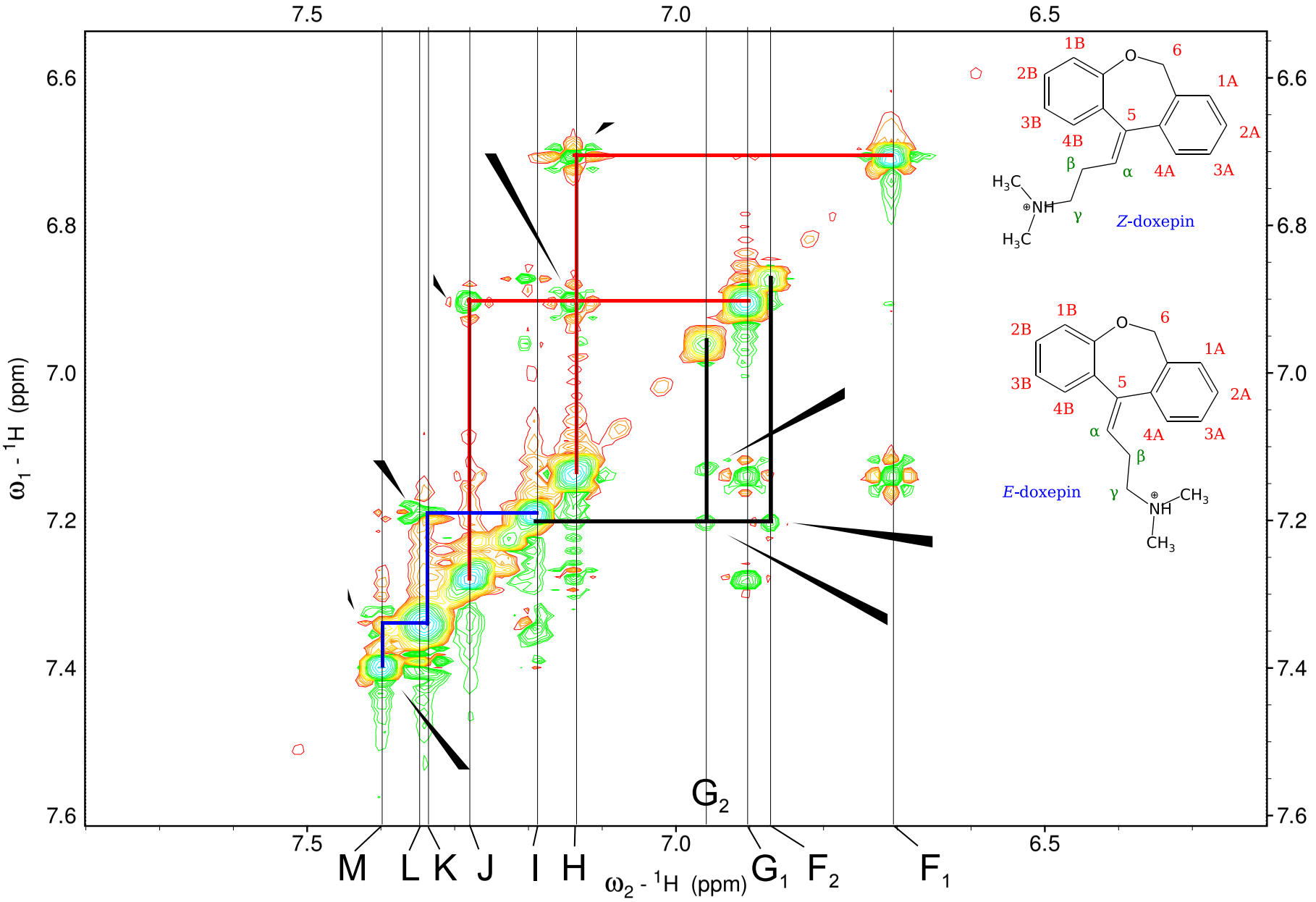
1D ^{1}H of doxepin in D_2O



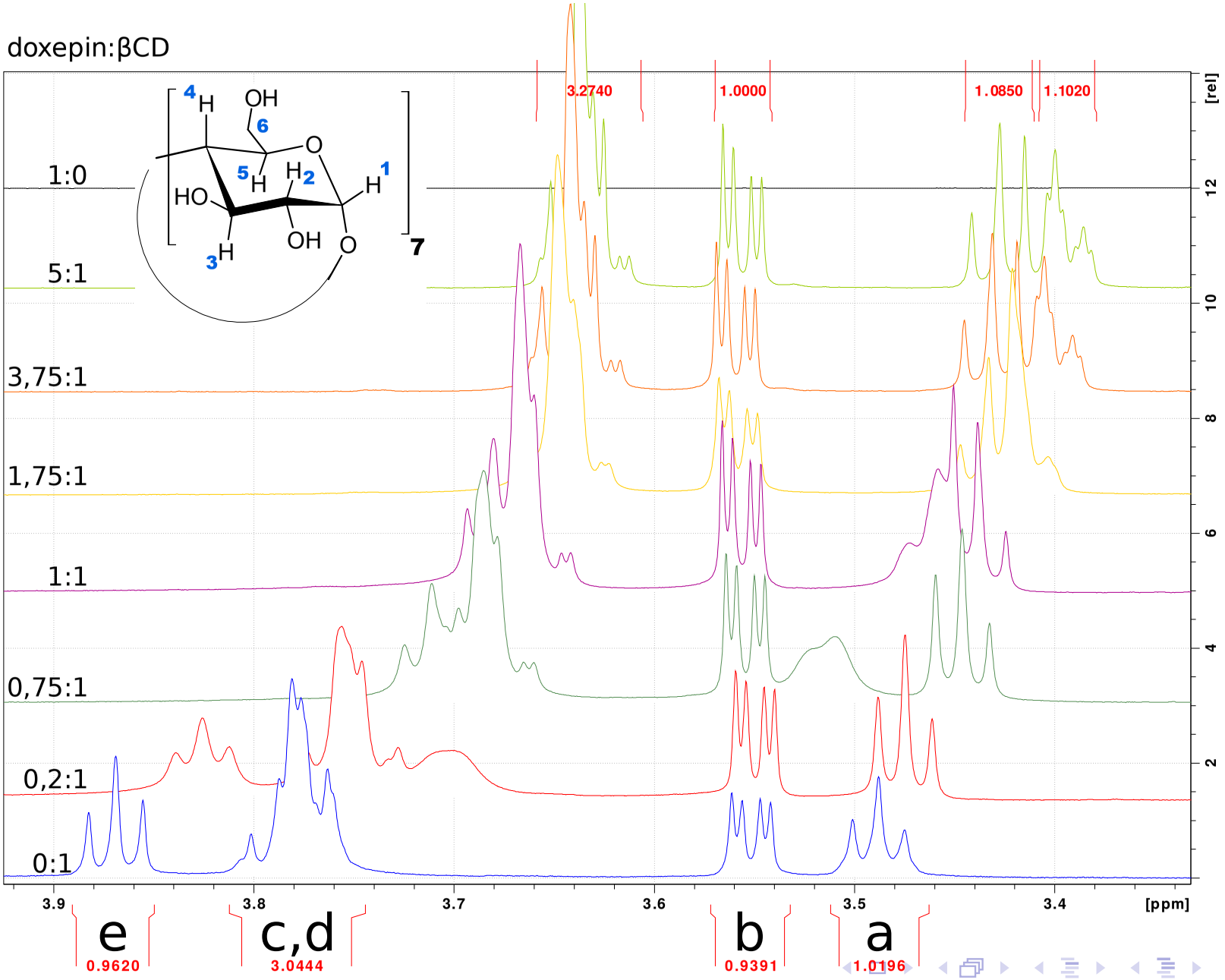
NOESY 700ms of doxepin in D_2O



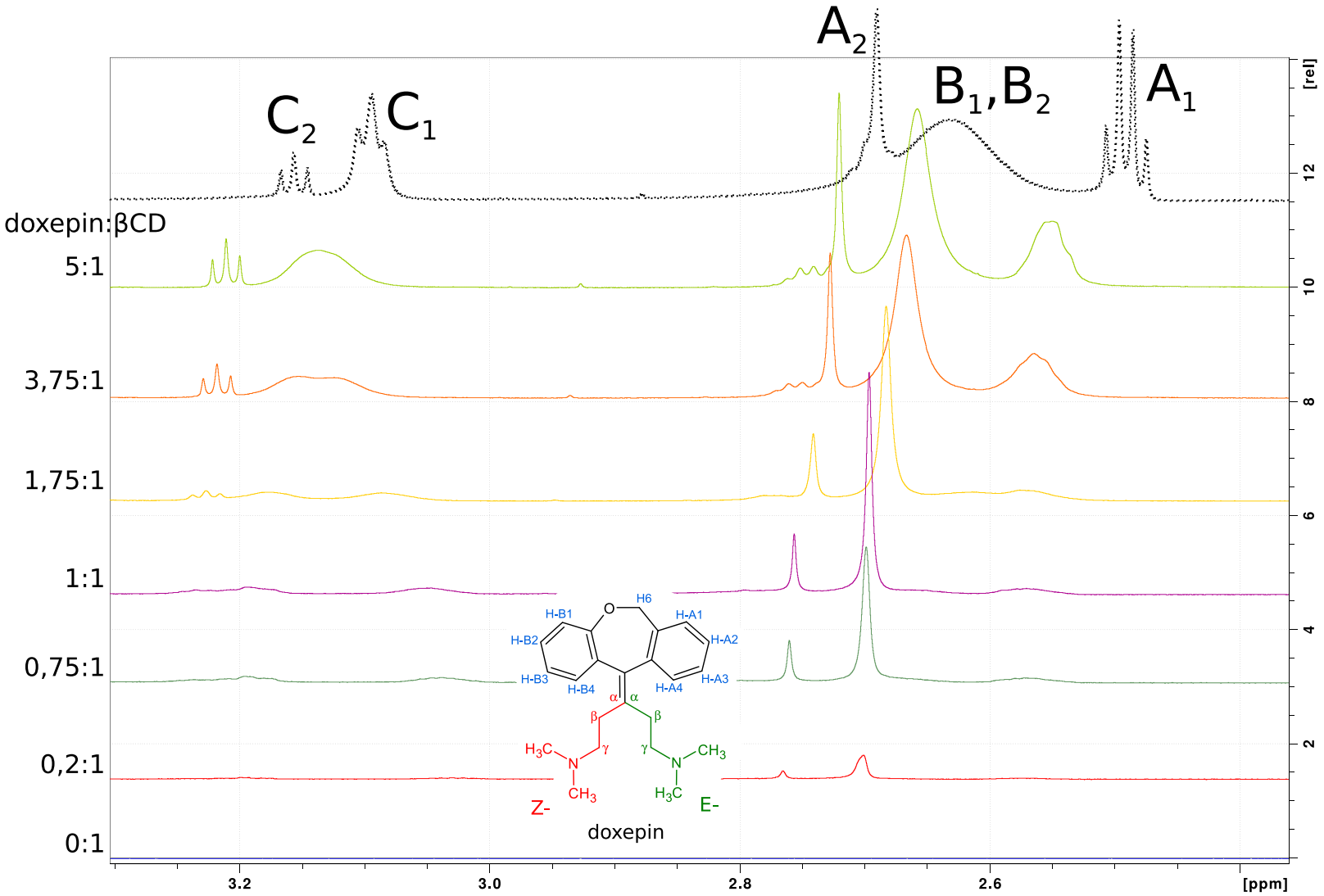
NOESY 700ms of doxepin in D_2O



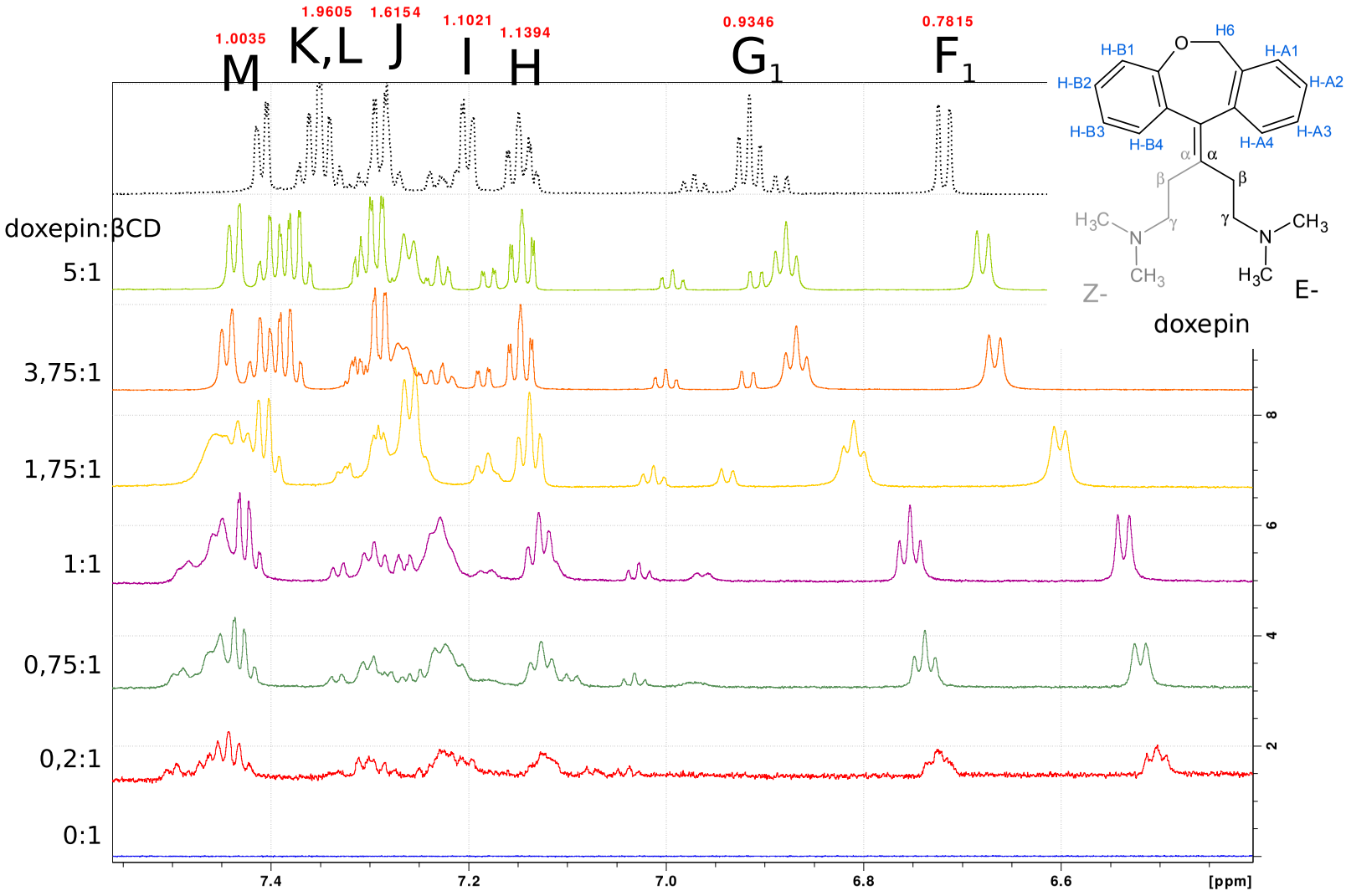
1D ^{1}H NMR titration: β-cyclodextrin



1D ^{1}H NMR titration: doxepin



1D ^{1}H NMR titration: doxepin



Find the most perturbed resonances and estimate the time regime of interaction:

ROESY 300ms - doxepin:βcyclodextrin=5:1