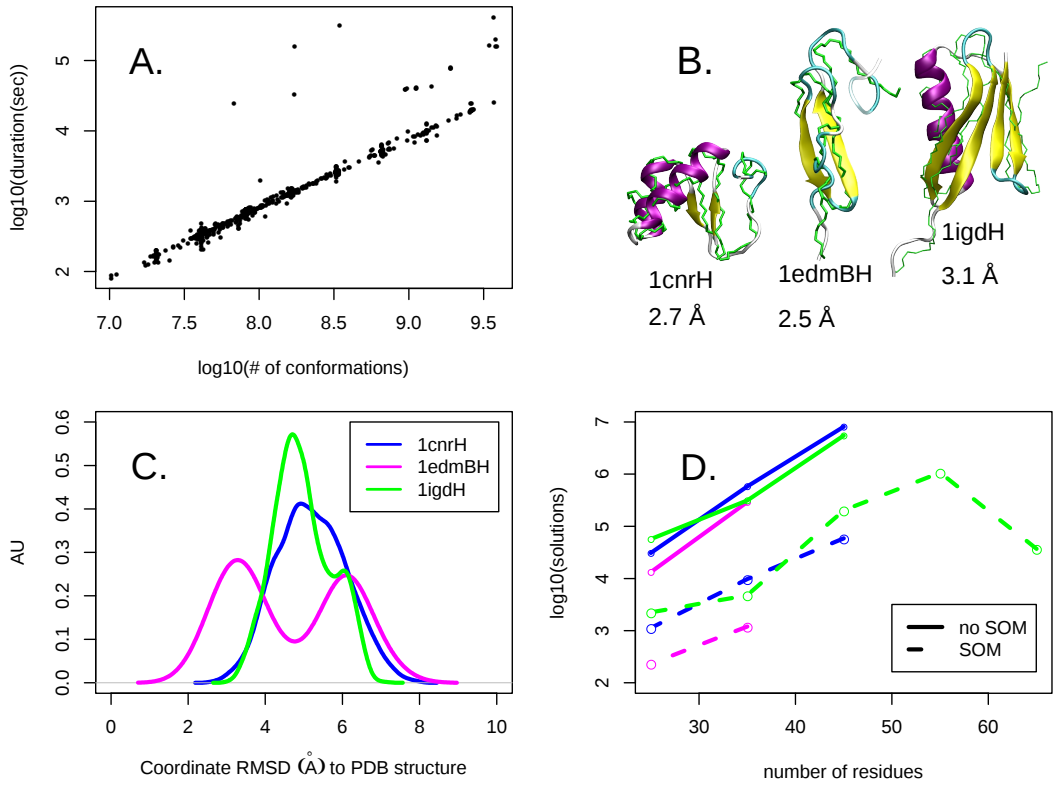


Figure 1: **Exploration of conformational space using iBP. A.** The implementation of iBP [1] (github.com/geekysuavo/ibp-ng) is able to generate $10^7$ up $10^{9.6}$ conformations of 753 15-residues peptides spanning proteins up to 100 residues. The durations of calculations are from few minutes up to two days. These calculations were performed using single processors, and some orders of magnitude can be gained using threading, GPU or supercomputing architecture. **B.** PDB-closest protein conformation obtained using iBP on three examples. The PDB structure is drawn in cartoon, the trace of iBP conformation in green, and the coordinate RMSD (Å) between the C$\alpha$ of two conformations are given along with the PDB entries. The distance restraints between peptide extremities had uncertainties of $\pm$ 1 Å whereas the long-range distance restraints had uncertainties of $\pm$ 3-6 Å. **C.** Distribution of coordinate RMSD (Å) with respect to the PDB structure along all conformations generated by iBP: 3235 conformations for 1cnrH, 56 conformations for 1edmBH, 2103 conformations for 1igdH. **D.** Number of intermediate conformations along the protein intermediate lengths. The curve colors correspond to the legend of panel C. The curves are given in the absence (solid line) and in presence of a clustering (self-organizing map [2]) of intermediate conformations. The use of clustering reduces the number of conformations by at least one order of value.

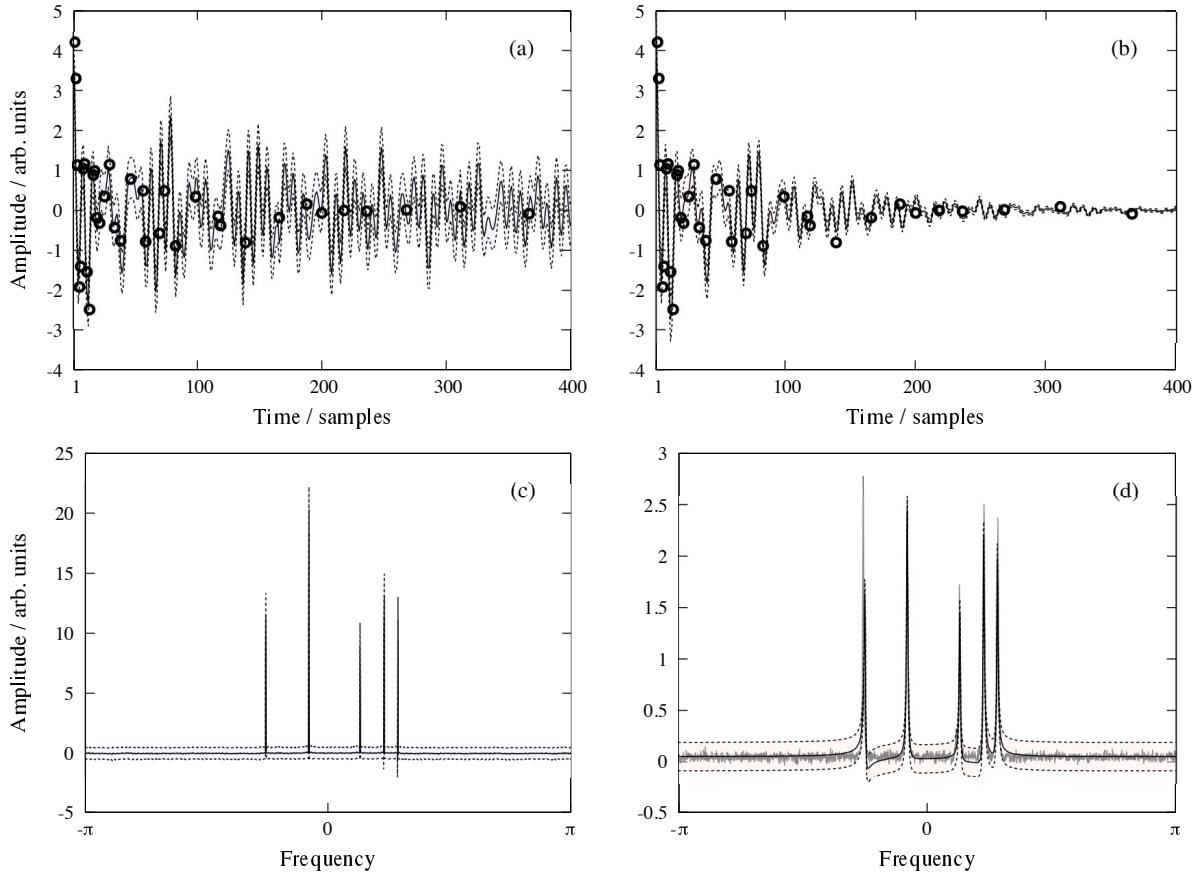


Figure 2: **Variational Bayesian (VB) processing of a single indirect-dimension slice of an N-HSQC.** Two VB models of the same data in the left and right sides. On the left is vbCS, and on the right is a parametric model. Top and bottom are time- and frequency-domain, respectively.

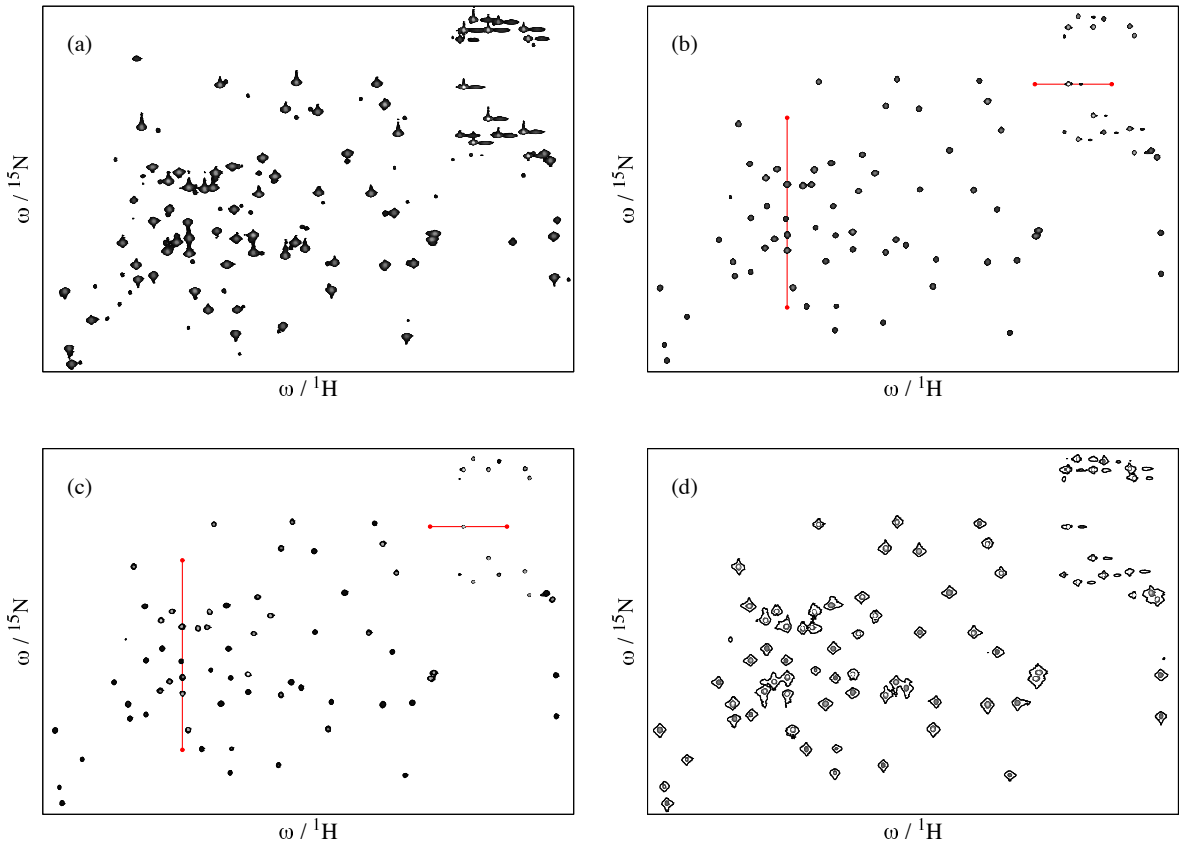


Figure 3: **Variational Bayesian (VB) processing of the corresponding 2D HSQC.** In (a), the complete-data (uniformly sampled) spectrum is shown. The NESTA reconstruction is shown in (b), and the vbCS mean and standard deviation are shown in (c) and (d), respectively.

# References

[1] **Worley B**, Delhommel F, **Cordier F**, **Malliavin T**, **Bardiaux B**, **Wolff N**, Nilges M, Lavor C, **Liberti L**. Tuning interval Branch-and-Prune for protein structure determination. *Journal of Global Optimization* pages accepted. https://doi.org/10.1007/s10898–018–0635–0 (2018).

[2] Bouvier G, Duclert-Savatier N, Desdouits N, Meziane-Cherif D, Blondel A, Courvalin P, Nilges M, **Malliavin TE**. Functional motions modulating VanA ligand binding unraveled by self-organizing maps. *Journal of chemical information and modeling* 54:289–301 (2014).