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## **Supplementary Material**



**Figure S1** The Radius of gyration of Met-Enkephalin using AMBER-99SB (A) and AMBER-FB15 (B) Forcefield.



**Figure S2** shows the number of unique clusters per bin of  $2^n$ , where n stands for number of bins equivalent to number of bits used.



**Figure S3** shows the variation in the number of minima found using DNCS method as a function of Number of torsions.



**Figure S4** shows the comparison of the distribution of radius of gyration between DNCS method (A) and NMR structures (B).