Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Classical molecular dynamics and metadynamics simulations decipher the mechanism of CBP30 selectively inhibiting CBP/p300 bromodomains

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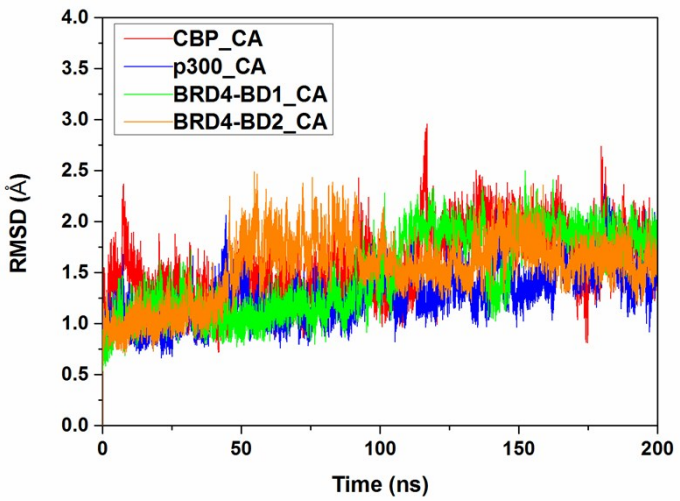

Fig. S1. Root mean square deviations (RMSD) of protein Cα atoms for four systems as a function of time in MD simulations.

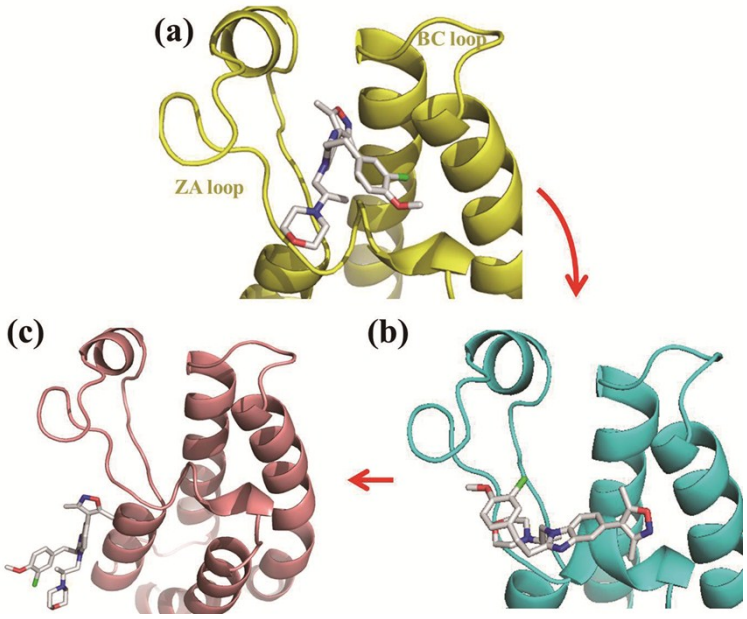

Fig. S2. Representative structures of (a) binding state ("B"), (b) transition state ("T"), and (c) unbinding state ("U") of p300-CBP30 complex during the unbinding process.

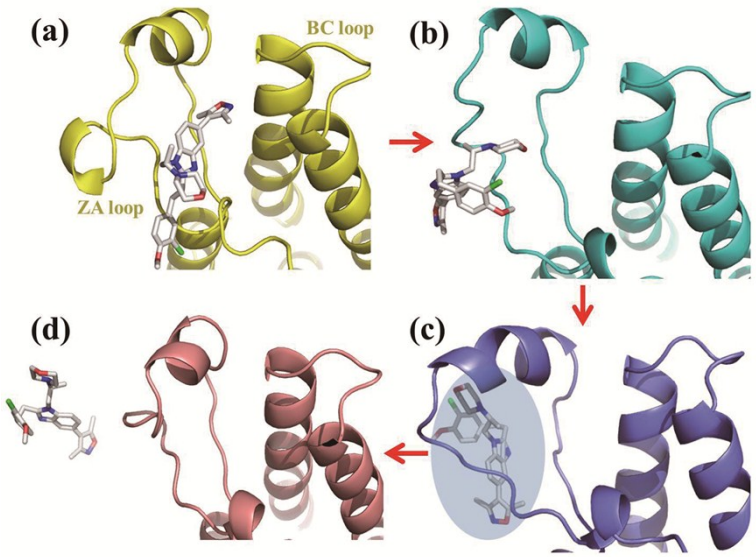

Fig. S3. Representative structures of (a) binding state (“B”), (b) transition state (“T”), (c) temporary intermediate state (“I”), and (d) unbinding state (“U”) of BRD4-BD2-CBP30 complex during the unbinding process.