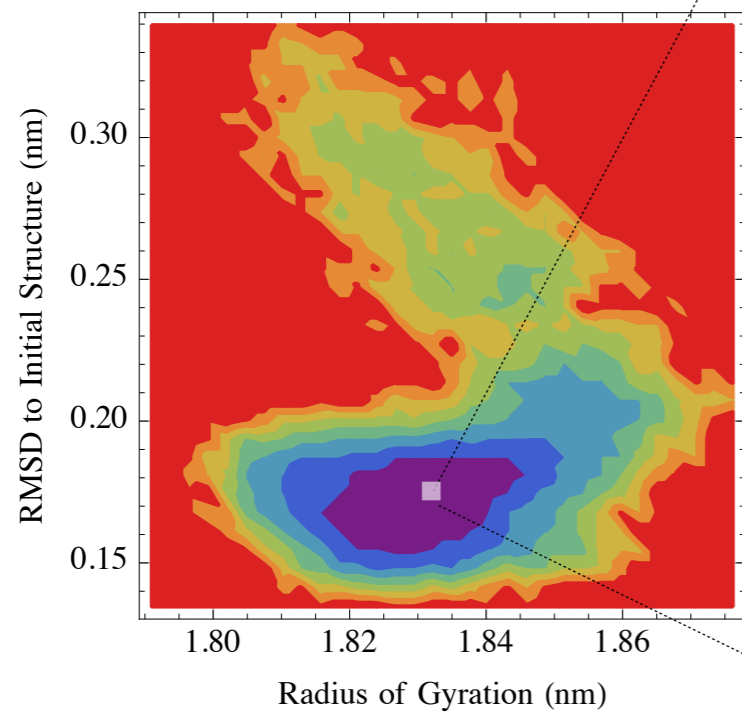
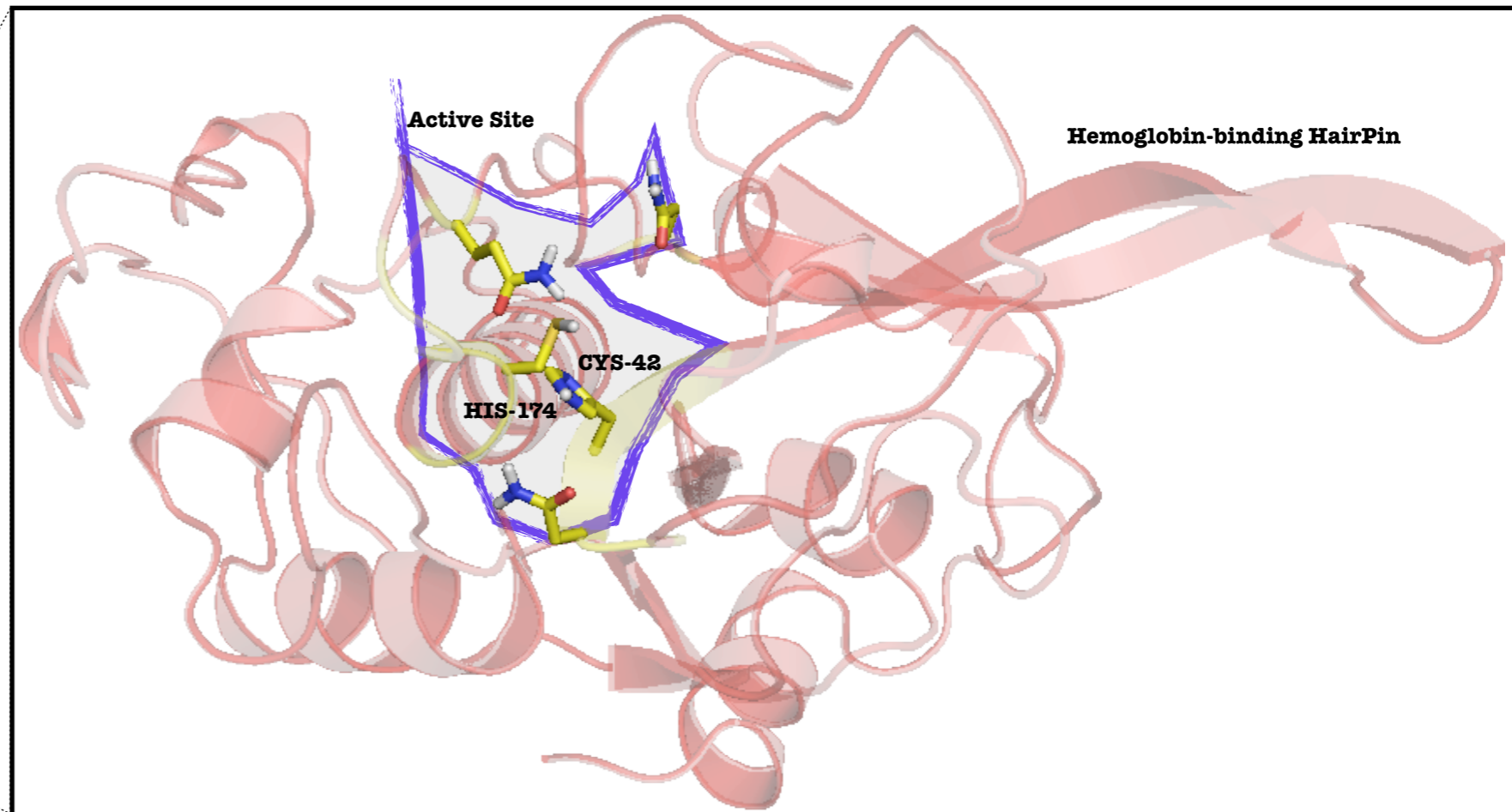


# Supplementary figures

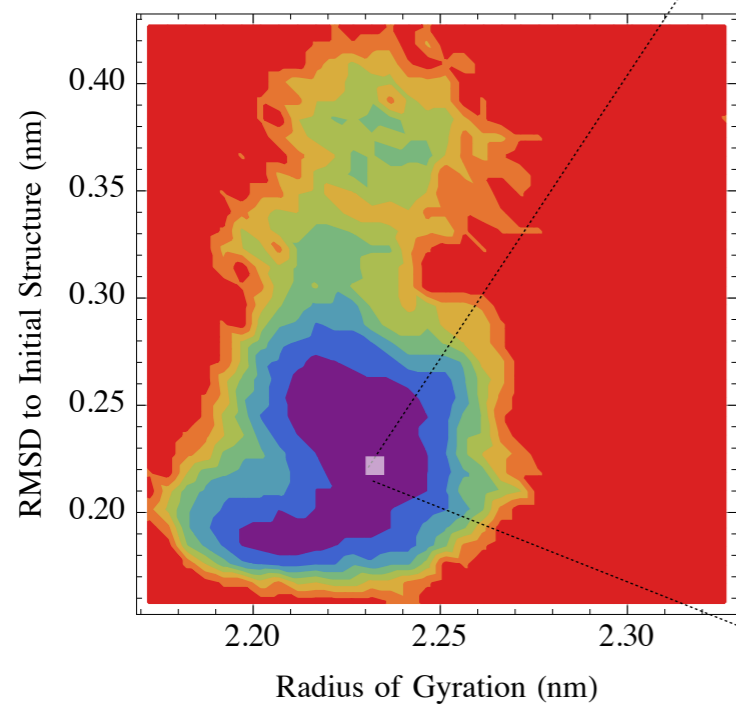
**Supplementary figure  
1A**



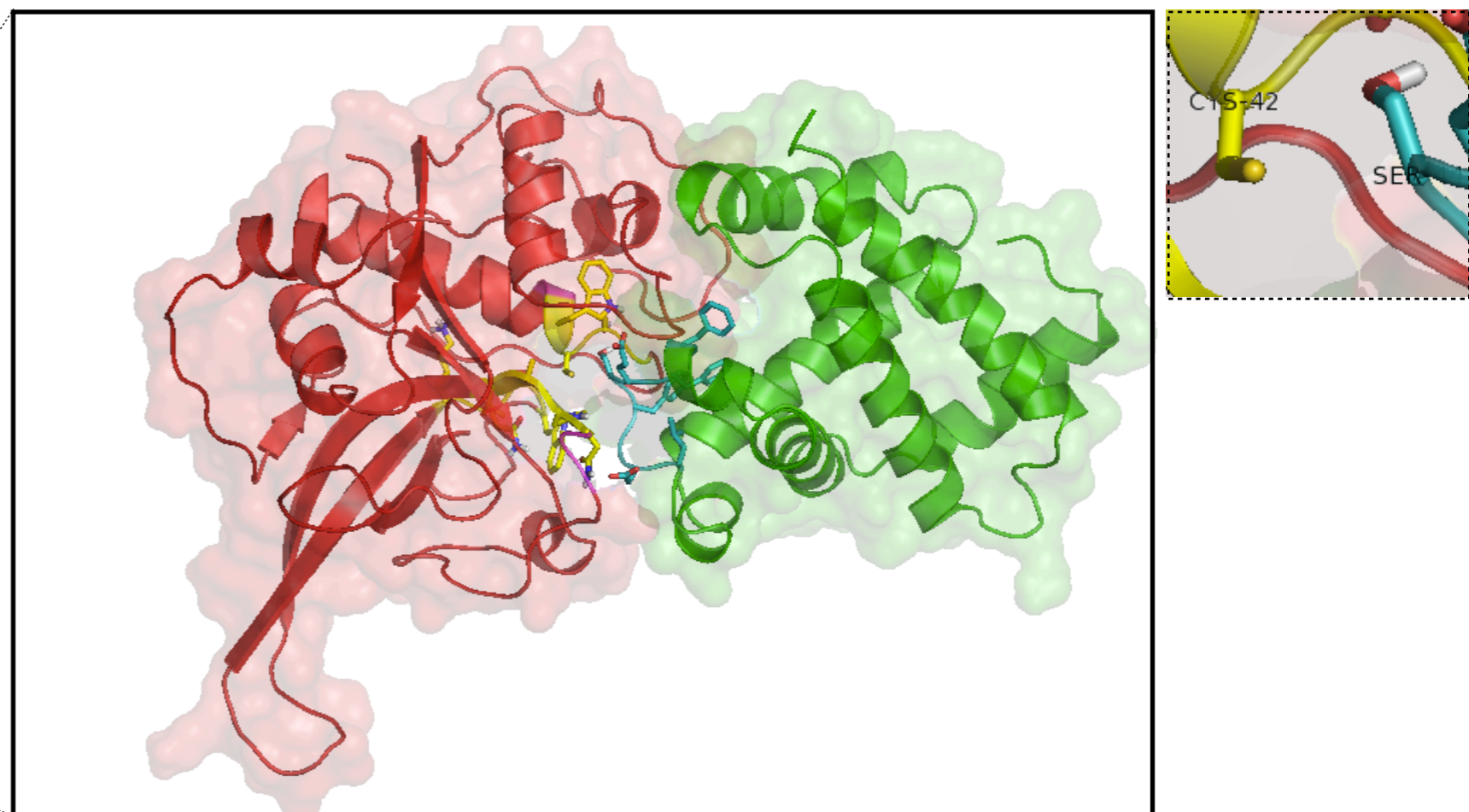
**1B**



**1C**



**1D**



The summary of molecular dynamics simulation and quantum mechanical calculation in this study

Suppl. Table 1.0

| S/N  | BioSystem                      | Simulation Type                  | No. of runs | TIME (ns) |
|------|--------------------------------|----------------------------------|-------------|-----------|
| I    | (E64-less) - FP-2              | Heavy Atom Restrained Simulation | 1           | 500       |
| II   | FP-2*                          | Production                       | 2           | 250       |
| III  | E64-FP-2                       | Production                       | 2           | 250       |
| IV   | docked Hemoglobin-FP2*(tight)* | Heavy Atom Restrained Simulation | 1           | 500       |
| V    | Hemoglobin-FP2*(tight)         | Production                       | 2           | 250       |
| VI   | Hemoglobin-E64-FP2 (loose)     | Production                       | 2           | 250       |
| VII  | Hemoglobin-FP2 (loose)         | Production                       | 2           | 250       |
| VIII | Heme-Heamoglobin               | Production                       | 2           | 250       |
| IX   | Heamoglobin                    | Production                       | 2           | 250       |
| X    | Hemoglobin-FP2*(tight)         | Pulling simulation               | 1           | 0.5       |
| XI   | Hemoglobin-FP2*(tight)         | Quantum mechanic SCF calculation | 50          | N/A       |