**Table S1.** Docking grid parameters for hTopo1B-DNA complex (1A36) with ligands.

| S.no | Protein-Ligand Complexes | Center | | | Size | | |
|---|---|---|---|---|---|---|---|
| | | X | Y | Z | X | Y | Z |
| 1 | Coptisine | -3.302 | -2.253 | 10.926 | 41.448 | 42.497 | 55.676 |
| 2 | Epiberberine | -0.052 | 0.997 | 14.176 | 38.198 | 39.247 | 52.426 |
| 3 | Berberastine | -6.302 | -5.253 | 7.926 | 44.448 | 45.497 | 58.676 |
| 4 | Berberine | -1.802 | -0.753 | 12.426 | 39.948 | 40.997 | 54.176 |
| 5 | Fetidine | 0.961 | 2.180 | 15.419 | 37.211 | 38.430 | 51.669 |
| 6 | Jatrorrhizine | -4.302 | -3.253 | 9.926 | 42.448 | 43.497 | 56.676 |
| 7 | Palmatine | -2.052 | -1.003 | 12.176 | 40.198 | 41.247 | 54.426 |

**Table S2**. The table demonstrated the distribution of residues based on their backbone dihedral angles φ(phi) and ψ(psi) as analyzed by PROCHECK.

| S. No | Regions | Number of Residues | Percentage |
|---|---|---|---|
| 1 | Residues in most Favored Regions (A, B, and L) | 437 | 87.6% |
| 2 | Residues in additional allowed regions (a, b, l, and p) | 59 | 11.8% |
| 3 | Residues in generously allowed regions (~a, ~b, and, ~p) | 3 | 0.6% |
| 4 | Residues in disallowed regions | 0 | 0.0% |
| 5 | Number of non-glycine and non-proline residues | **499** | **100%** |
| 6 | Number of end-residues (excl. Glycine and Proline) | 48 | |
| 7 | Number of glycine residues (shown as triangles) | 19 | |
| 8 | Number of proline residues | 22 | |
| | **Total number of residues** | **588** | |

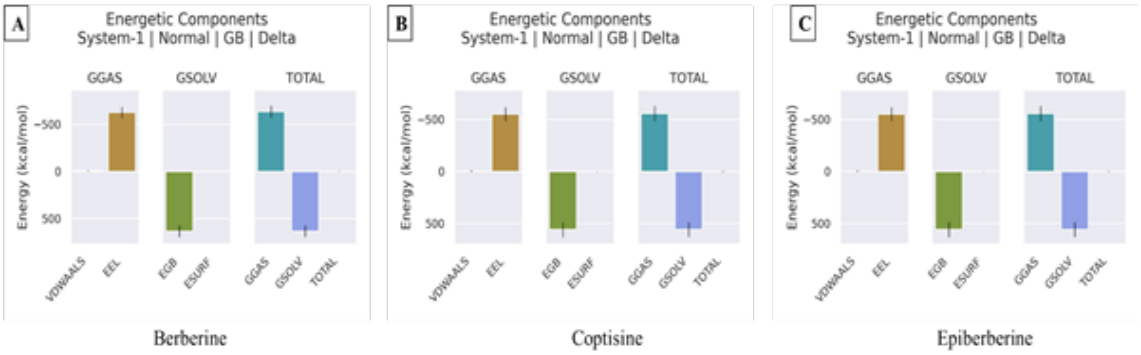



**Fig. S1. A**. MMGBSA

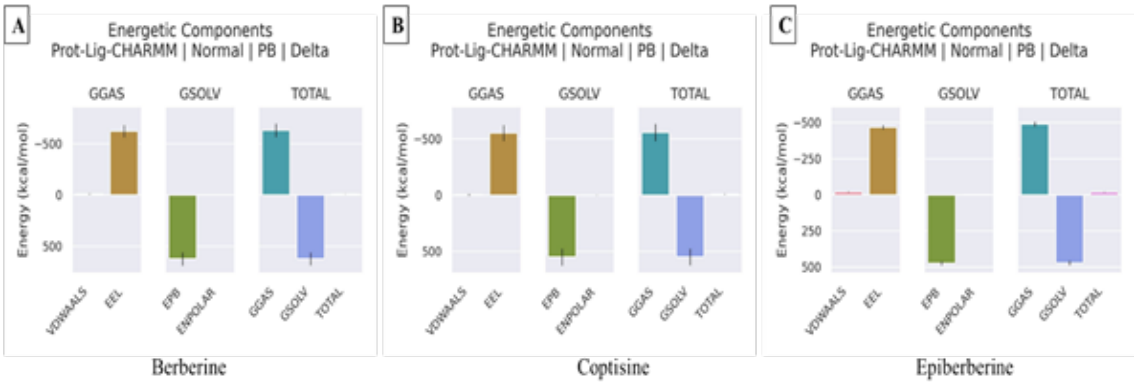



**Fig. S1. B.** MMGPSA

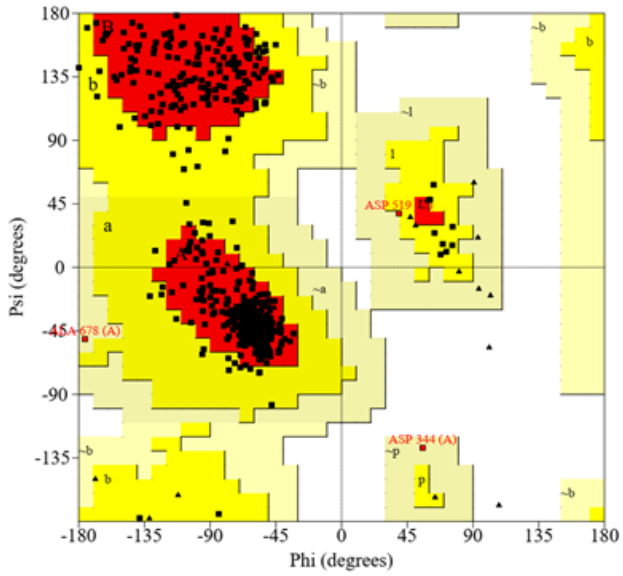



**Fig. S2.** Ramachandran plot of Human topoisomerase 1B (1A36) model generated by PROCHECK.