



Formula: C₂₀H₁₆N₂O₄

MW: 348.36

CAS: 2114-45-4, 7689-03-4

TNP NUMBER: TNP00113

MDL NUMBER: MFCD00058538

IUPAC: (4S)-4-ethyl-4-hydroxy-4,12-dihydro-1H-pyrano[3,4-f]quinolino[2,3-a]indolizine-3,14-dione

Smiles: n12c(c3nc4cccc4cc3C2)cc2C(C(=O)OCc2c1=O)(O)CC

THERAPEUTIC CATEGORY: Antitumor alkaloid; prototype DNA topoisomerase I inhibitor.

REFERENCE: Reference Fan, Y., et al., Molecular modeling studies of the DNA-topoisomerase I ternary cleavable complex with camptothecin. *J. Med. Chem.* 41, 2216-2226, (1998) abstract Morris. E.J., and Geller, H.M., Induction of neuronal apoptosis by camptothecin, an inhibitor of DNA topoisomerase-I: evidence for cell cycle-independent toxicity. *J. Cell Biol.* 134, 757-770, (1996) abstract Kaufmann, S. H., Cell death induced by topoisomerase-targeted drugs: more questions than answers. *Biochim. Biophys. Acta* 1400, 195-211, (1998) abstract Borovitskaya, A.E., and D-Arpa, P., Replication-dependent and -independent camptothecin cytotoxicity of seven human colon tumor cell lines. *Oncol. Res.* 10, 271-276, (1998) abstract Pommier, Y., et al., Mechanism of action of eukaryotic DNA topoisomerase I and drugs targeted to the enzyme. *Biochim. Biophys. Acta* 1400, 83-105, (1998) abstract Desai, S. D., et al., Ubiquitin-dependent destruction of topoisomerase I is stimulated by the antitumor drug camptothecin. *J. Biol. Chem.* 272, 24159-24164, (1997) abstract Beidler, D.R., and Cheng, Y.C., Camptothecin induction of a time- and concentration-dependent decrease of topoisomerase I and its implication in camptothecin

activity. Mol. Pharmacol. 47, 907-914, (1994) Merck Merck 13,1743 reference FT-IR 2 (3), 4267:D / Structure Index 1, 462:C:1

SOURCE: Isolation from stem wood of the Chinese tree, *Camptotheca acuminata* Decsne., Nyssaceae

ACCEPTORS: 4

DONORS: 1

ROTATION BONDS: 1

N+O: 6

Chiral Centers: 1

LogP: 3.07

LogS: -4.47

LIPINSKI: 4

Monograph Number: 0001743

Title: Camptothecin

CAS Registry Number: 7689-03-4

CAS Name: (S)-4-Ethyl-4-hydroxy-1H-pyrano[3