Computer-Based Drug Design and Synthesis of Various Thiazole Derivatives Having Potential Anti-HCV Activity

Thesis

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ولم يجزوا ابدا بما يستحقون

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List of Abbreviations

% Max: The maximum percentage inhibition of virus replication.

[ ] Max: The concentration at which maximum inhibition of virus replication.

2D: 2-Dimensional

A°: Angstrom

BG: Background

C: Core protein

CC: Cell control

CsA: Cyclosporin A

Cyp A: Cyclophilin A

Cyp B: Cyclophilin B

DIEA: Diisopropylethyl amine

DMEM: Dublecco's modified Eagle's medium

DMF: Dimethyl formamide

E1: Envelope glycoprotein1

E2: Envelope glycoprotein2

EC_{50}: Effective concentration 50

EC_{70}: Effective concentration 70

EC_{90}: Effective concentration 90

EDHS: Egyptian Demographic and Health Survey

EDTA: Ethylenediaminetetraacetic acid

ELISA: Enzyme linked immunosorbent assay

ER: Endoplasmic reticulum

FACS: Fluoresence-activated cell sorting

FCS: Fetal calf serum

FDA: Food and Drug Administration

FT-IR: Fourier transform-Infrared

GB/SA: Generalized born surface area implicit solvent model

GDD: Gly 317, Asp 318, Asp 319

Glide SP: Glide Standard Precision

Glide: Grid-based ligand docking with energetics

HCC: Hepatocellular carcinoma

HCV: Hepatitis C Virus

Huh: Human hepatoma

IC_{50}: Inhibitory concentration 50

IFN: Interferon

IRES: Internal ribosomal entry site

IUPAC: International union of pure and applied chemistry

Luc: Luciferase

MENA: Middle East and North Africa

MHz: Mega hertz

MS: Mass spectroscopy

MTS: (3-(4,5-dimethylthiazol-2-yl)-5-(3-carboxymethoxyphenyl)-2-(4-sulfophenyl)-2H-tetrazolium

Neo: Neomycin phosphotransferase

NIs: Nucleoside inhibitors

NMR: Nuclear magnetic resonance

NNIs: Non-nucleoside inhibitors

NS: Non structural

NTP: Nucleoside triphosphate

OPLS: Optimized potential for liquids simulation

ORF: Open reading frame

PBS: Phosphate buffered saline

PCR: Polymerase chain reaction

PDB: Protein data bank

Peg-IFN-α: Pegylated interferon-α

PMS: Phenazine monophosphate

PPi: Pyrophosphate group

PPIase: Peptidyl-prolyl cis-trans isomerase

RBV: Ribavirin

RdRp: RNA dependent RNA polymerase

RMSD: root mean square deviation

RNA: Ribonucleic acid

rt: Room temperature

RT-PCR: Reverse transcriptase-polymerase chain reaction

SI: Selectivity index

SoC: Standard of care

SS: Selectivity surface

SVR: Sustained virological response

TCT: 2,4,6-trichloro-1,3,5-triazine

TEA: Triethylamine

THF: Tetrahydrofuran

TLC: Thin layer chromatography