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OINTERNATIONAL

BAU DRUG DESIGN CONGRESS

NOVEL METHODS AND EMERGING TARGETS IN

DRUG DISCOVERY & PATENTED DRUG DEVELOPMENT

BOUSLAH MOKHNACHI NAIMA

FERROUKHI Ouassila

Verda Begüm Tezcan

Photodynamic Therapy Agent

dynamics-based features

hepatocellular carcinoma

Structural studies of IDH1

Development Of Novel Fluorescent Tyrosinase Enzyme Sensor And Tyrosinase Activable

In silico discovery of potential azole containing mPGES 1 inhibitors by virtual screening,

Tacrine-Hydrazone Compound as Multi-Target Agent for The Treatment of Alzheimer's

Pathogenicity prediction of cancer-related variants with protein sequence, structure,

Quantum Chemical, Molecular Docking, Molecular Dynamics and ADMET Studies of

Computational approach for inhibition of ATPases acting antagonistically in Type IV Pilus of

Novel Antipyrine Derivatives As Antioxidant Reagents: Synthesis, In-Silico Pharmacokinetics,

Molecular Docking Studies, An Implication In Identifying The Nitric Oxide Synthase Inhibition

Disease and Type II Diabetes Mellitus: Design, Synthesis and Bioactivity Studies

Creation Of Homology Models Of Some Hiv-1 Integrase Mutations And

The Degradation Reaction Mechanism of Ampicilin with Hydroxyl Radical

In Silico Determination of Potential Candidates as AXL Kinase Inhibitors

{In-silico} Study on the Effect of Pro 120 Ser Mutation on NPC-2 Protein

The combinatorial drug repurposing strategy enhances cytotoxicity in

Transcriptional regulation of YY1 with a novel G-quadruplex stabilizer

Discovery of HDAC6 selective inhibitors by deep machine learning methods

Prediction of CYP450—related pharmacokinetic drug-drug interactions using

Towards Selective Stabilization of G-Quadruplex DNA/RNA Structures with

Mutant Forms Of MutsA Heterodimer With Molecular Dynamic Simulations

New Hexahydroquinoline Derivatives And Their Cytotoxic Properties On HePG2 Cells

Design and Synthesis of New Coumarin-Bistriazole Hybrids as Potential Drug Candidates

Synthesis, Purification and Application of Isotopic Derivatives of Various Pharmaceutical Active

Investigation of Breast Cancer Cell Responses to the Fullerenol-Dexamethasone Dual Therapy

Trace Levels in Blood and Urine of Colchicine Active Substance Used in the Treatment of Goutand

Behçet's Disease, Also Used in the Treatment of COVID-19, with the HPLC system determination to the contract of the contract o

Synthesis, pharmacokinetic and biological evaluation of 5-aminoquinoline-triazole hybrid derivatives

Development of a new generation and high-throughput detection kit for monkeypox virus infection

Dissecting the Effect of Viscosity of Deep Eutectic Solvents on the Structure and

Development new generation of imatinib using structural biology techniques at

The Development of Antagonists for Knockdown of Axl Overexpression

Synthesis of Bisindolylmaleimide Based Potential Antitumor Compounds

An in Silico study of the Antiviral Activity of Mediterranean Herbs and Spices

Molecular Docking Studies Reveal Toxin Binding Differences That Enable

A Qsar Study On Novel 2,4-diaminoquinazoline Derivatives Toward Designing

New Lead Compounds For The Potential Treatment Of Spinal Muscular Atrophy

Synthesis and human monoamine oxidase inhibitory activity of novel C2-, C3- and

Development of Novel Diagnostic and Therapeutic Agents for Use in Hypoxic Cancer

Investigation of Tomentosin β -Amino Alcohol Derivatives Interactions with Topoisomerase

{Aspergillus Carneus} Metabolite Averufanin induced cell cycle arrest and apoptotic cell

Synthesis of Various Organic Molecules and Smart Liquid-Liquid Microextraction Method Together with Slotted Quartz Tube

Accelerated MD simulations elucidate that conformational preference of AR antiandrogens

Regulating the Expression of Oncogenes or Genes Associated With Cancer Energy Metabolic

Investigation of Reaction Mechanism of Human Lysosomal Cathepsin A Enzyme in silico

N-succinyltransferase (Dapd) Enzyme And Identification Of Novel Antimicrobials Via High-throughput Screening

Affinity determination of antisense oligonucleotides specifically designed for conserved

Elaboration of pH-sensitive Calcium alginate/poly(vinyl alcohol) hydrogel beads Study of

Deep learning approach to predict selectivity of bioactive compounds retention time of

Discovering Anti-Cancer Molecules Targeting p53-MDM2 Interaction by Drug Repurposing

Discovery of new small molecules as RET tyrosine kinase inhibitor to stop the tumor growth of Thyroid cancers

Identification Of Therapeutic Molecules That Will Interact Covalently Against Sars-cov2 Main Protease, Spike /ace2,

Tmprss2 And Rdrp Target Structures Using Structure And Ligand-based In Silico Approaches And In Vitro Tests

Inhibition of c-MET interactions with downstream proteins for the treatment of cancer

Screening of small molecule libraries using combined text mining, ligand- and target- driven

IN SILICO SCREENING OF THE APPROVED DRUGS, PEPTIDOMIMETICS AND DESIGNING OF

Investigation of the role of CLDNs and TRPs proteins and their associated proteins in peritumoral brain edema (PTBE)

Bahçeşehir University

by evaluating gliovascular unit (GVU) in disrupted blood brain barrier in glioma IDH 1 mutant vs IDH 1 wild type.

and non-small cell lung cancers occurring by RET protein mutations with minimum resistance to inhibitors

Flame Atomic Absorption Spectrophotometer for the Determination of Trace Amounts of Metals in Biological Systems and Wastewater

Deep Learning Based Drug Repurposing Study for JAK2 Inhibitors

Molecular Docking and in Silico ADMET Analyses of Novel Fedratinib Derivatives as

Investigation Of The Structural Differences Between Wild-type And

Alphafold Based Pathogenicity Prediction of Missense Variants

Investigation of OXA enzyme inhibitors using computational tools

R448Q Mutation In The Transcription Factor CTCF: Novel Insight Into Structure - Function

pharmacophore modeling and molecular dynamics simulations

Neisseria meningitidis by FDA-approved natural drugs

Potent Anticancer Diimine-Dioxime Agents

Graph Convolutional Neural Network

Relationship From In Silico Analysis

Dynamics of Thermostable Lipases

Ingredients in Analytical Determination Methods

Against Multiple Targets of SARS-CoV-2

Selectivity For Sodium Channels

C4-substituted phthalonitriles

Synthesis and Evaluation of Functionalised Polycyclic

death on cancer cell lines via inducing DNA Damage

The Mechanism and Energetics of the Dynein Priming Stroke

An Overview of Bioanalytical Assays and Techniques Used at

regions of the SARS-CoV-2 genome by in-silico analyses

The antioxidant activity and antibacterial properties

Virtual Screening of Small Molecule Libraries Against

ERCC1-XPF for the Identification of Potent Inhibitors

Discovery of novel Allatostatin type-c receptor agonists

Virtual Screening of Large-Scale Small Molecule Libraries Against

Bruton Tyrosine Kinase Effective in Chronic Lymphotic Leukemia

Marin Exopolysacharides and Their Application in Dermocosmetics

based approaches for identification of novel granzyme H inhibitors

Construction of new hERG blocker models based on heteroatom

numbers from ultra large ligand libraries

NEW PEPTIDES AGAINST AXL-GAS6 TARGET

In Silico Characterization Of The Klebsiella Pneumoniae Tetrahydrodipicolinate

A DFT Study On The Mechanism Of Catalytic Asymmetric Synthesis Of

Small Molecular inhibitors of Aurora kinase B; From Structural Insight to

Ph-responsive hydrogel beads for controlled drug delivery of indomethacin

Antibody-Drug Conjugate (ADC) Characterization

Switching Through Tissue/Site Specific DNA Alkylation and Stabilization

Benzo[4,5]-Imidazo[1,2-a]-Pyrimidin-4-yl Structure

II Enzyme Using Molecular Docking Method

contributes to agonism/antagonism

Chiral Amines As Drug Building Blocks

Mechanism Based Design

a new RP-HPLC column

Structurally Optimized Ligand

Potent JAK2 Inhibitors

ambient temperature

Investigation Of Their Relationship With Cabotegravir By In Silico Methods

Molecular Docking Study of Some Nitro-Substituted Benzamide Compounds as

Cyclin-Dependent Kinase Inhibitors and The Anticancer Activity in TNBC cells