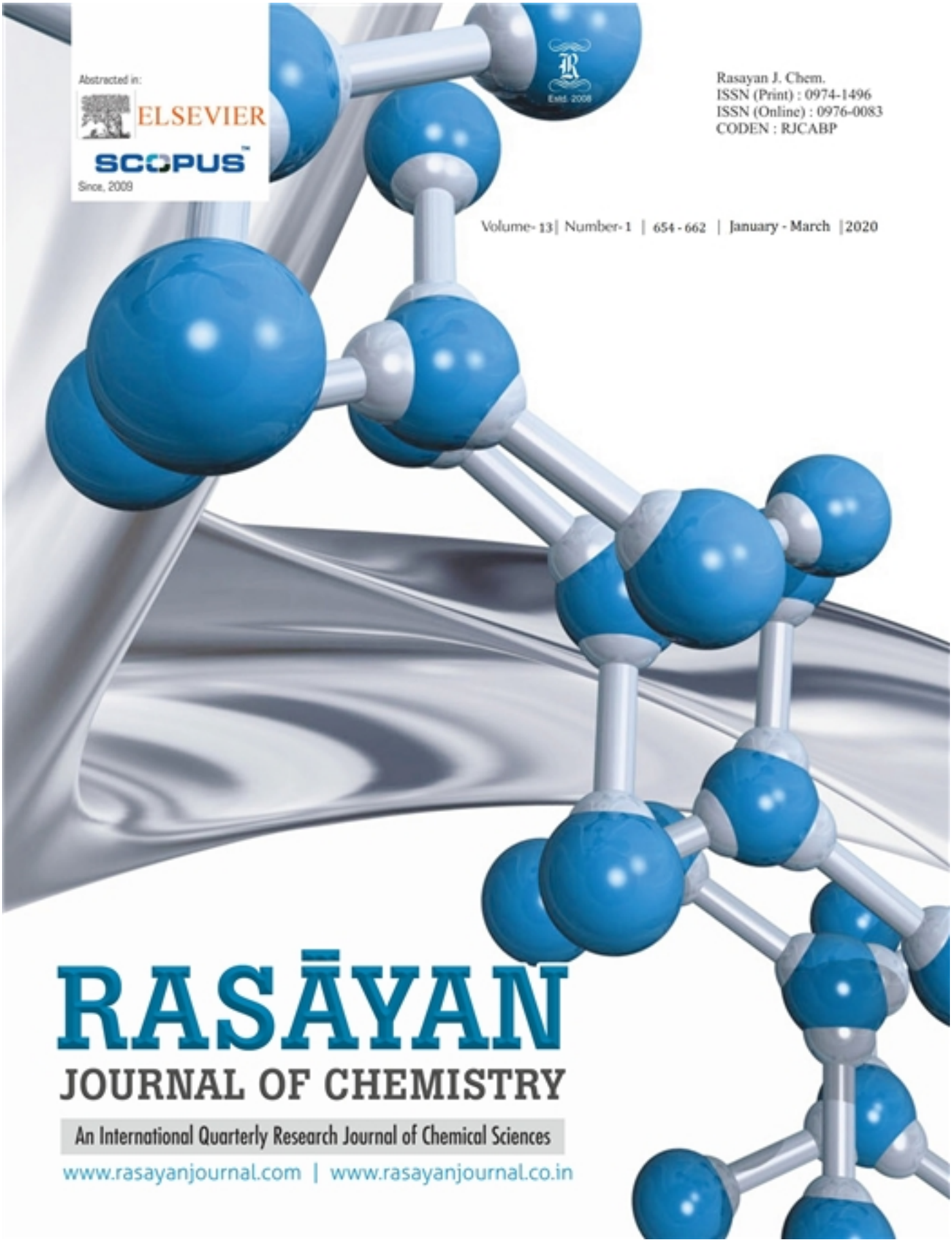

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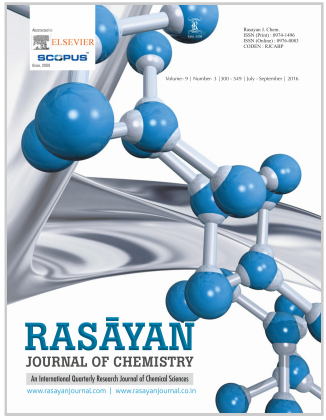

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Deswati, Amelliza Deviona , Ella Intan Sari , Yulizar Yusuf and Hilfi Pardi

Rasayan J. Chem, 13 (1), 1- 10 (2020)

Keywords: Aquaponic, Modified Conventional Aquaculture, Ammonia, Nitrite, Nitrate

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UPDATES ON 4-HYDROXYDERRICIN AND XANTHOANGELOL OF ANGELICA PLANTS: EXTRACTION AND PHARMACOLOGICAL ACTIVITIES

D. L. Aulifa, I. K. Adnyana , Sukrasno and J. Levita

Rasayan J. Chem, 13 (1), 11- 17 (2020)

Keywords: Angelica keiskei, Chalcones, 4-Hydroxyderricin, Xanthoangelol

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IDENTIFICATION OF SECONDARY METABOLITE OF LABAN LEAF EXTRACT (VITEX PINNATA L) FROM GEOTHERMAL AREAS AND NON-GEOTHERMAL OF AGAM MOUNTAINS IN ACEH BESAR, ACEH PROVINCE, INDONESIA

Cut Nuraskin, Marlina , R. Idroes , C. Soraya and Djufri

Rasayan J. Chem, 13 (1), 18- 23 (2020)

Keywords: Identification, Secondary Metabolites, Laban leaves, Geothermal Areas, and Non-geothermal

DOI: http://dx.doi.org/10.31788/RJC.2020.1315434

A STRAIGHT FORWARD, FAST, SENSITIVE, EPI- HPLCMS/MS METHOD FOR THE SIMULTANEOUS ESTIMATION OF CLOZAPINE AND AMITRIPTYLINE IN HUMAN PLASMA

Muni Krishnaiah A , C. Rama Chandraiah, M. Srinivas and N. Devanna

Rasayan J. Chem, 13 (1), 24- 37 (2020)

Keywords: Amitriptyline, Clozapine, LC-MS/MS, Simultaneous Estimation, Gradient Technique.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315466

DYE-SENSITIZED SOLAR CELLS PROPERTIES FROM NATURAL DYE AS LIGHT-REAPING MATERIALS EXTRACTED FROM GAYO ARABICA COFFEE HUSKS

Hasby, Nurhafidhah , Gawang Pamungkas , and Said Ali Akbar

Rasayan J. Chem, 13 (1), 38- 43 (2020)

Keywords: Waste of Coffee Husks, Computational Studies, Energy Gap, DSSC.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315576

VAPOUR GENERATION CHEMILUMINESCENCE DETECTION SYSTEM FOR DETERMINATION OF DIMETHYLSULPHONIOPROPIONATE AND DIMETHYLSULPHIDE IN TROPICAL SEAWATER

A. E. Adedapo, N. U. Benson, A. B. Williams and K. Toda

Rasayan J. Chem, 13 (1), 44- 50 (2020)

Keywords: Dimethylsulphide, Dimethylsulphoniopropionate, Seawater, Vapour Generation Chemiluminescence Detection

DOI: http://dx.doi.org/10.31788/RJC.2020.1315432

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Rasayan J. Chem, 13 (1), 51- 63 (2020)

Keywords: Greywater, Novel Equipment, Adsorbent, Wood Apple Shell, Flushing, Irrigation

DOI: http://dx.doi.org/10.31788/RJC.2019.1245354

BIOPROSPECTING CELLULOLYTIC FUNGI ASSOCIATED WITH TEXTILE WASTE AND INVITRO OPTIMIZATION OF CELLULASE PRODUCTION BY Aspergillus flavus NFCCI-4154

Priya Sutaoney, Rachana Choudhary and A.K. Gupta

Rasayan J. Chem, 13 (1), 64- 84 (2020)

Keywords: Aspergillus, Fungal Diversity, CMCase, Submerged Fermentation, Textile

DOI: http://dx.doi.org/10.31788/RJC.2020.1315536

PREPARATION AND CHARACTERIZATION OF GOATSKIN GELATIN AS HALAL ALTERNATIVE TO BOVINE GELATIN

A. Bahar , N. Kusumawati and S. Muslim

Rasayan J. Chem, 13 (1), 85- 98 (2020)

Keywords: Collagen, Gelatin, Goatskin, Base Curing, Extraction.

DOI: http://dx.doi.org/10.31788/RJC.2019.1245409

CHARACTERISTIC OF HYDROXYAPATITE-SUPPORTED Ni, Ce, Cu CATALYST PREPARED BY DEPOSITIONPRECIPITATION AND IMPREGNATION METHOD FOR GLYCEROLAQUEOUS PHASE REFORMING PROCESS

L. Hakim, H. Husin, R. Sari, R. Dewi and Meriatna

Rasayan J. Chem, 13 (1), 99- 104 (2020)

Keywords: Hydroxyapatite, Glycerol, Aqueous-phase reforming, Catalyst, Deposition-precipitation, Impregnation

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SYNTHESIS, CHARACTERIZATION, SURFACE FUNCTIONALIZATION OF MAGNETITE NANOPARTICLES AND THEIR ANTIBACTERIAL STUDIES

Jaiveer Singh, Arti Jangra, Jai Kumar, Keerti Rani and Ramesh Kumar

Rasayan J. Chem, 13 (1), 105- 111 (2020)

Keywords: Nanoparticles, Surface Functionalization, Antibacterial Activity, Ciprofloxacin, Fourier Transform Infrared Spectroscopy.

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KINETICS AND MECHANISM OF THE AQUEOUS PHASE OXIDATION OF HYDROGEN SULFIDE BY OXYGEN: CATALYZED BY HYDROQUINONE

Deepak Singh Rathore and C. P. Singh Chandel

Rasayan J. Chem, 13 (1), 112- 120 (2020)

Keywords: Hydrogen sulfide, Hydroquinone, Oxygen, Oxidation, Catalysis.

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THE MODIFICATION OF CYANIDIN BASED DYES TO IMPROVE THE PERFORMANCE OF DYE-SENSITIZED SOLAR CELLs (DSSCs)

Imelda , Emriadi, Hermansyah Aziz, Adlis Santoni and Nofitri Utami

Rasayan J. Chem, 13 (1), 121- 130 (2020)

Keywords: Cyanidin, D-Ï€-A Type, DFT, DSSCs

DOI: http://dx.doi.org/10.31788/RJC.2019.1245449

SYNTHESIS AND ANTIOXIDANT ACTIVITY STUDY OF NEW MANNICH BASES DERIVED FROM VANILLIC ACID

H. Hayun, I. Gavrila, S. Silviana, A.E.K. Siahaan, R.F. Vonna and M.I. Latifah

Rasayan J. Chem, 13 (1), 131- 138 (2020)

Keywords: Vanillic Acid, Mannich Bases, Synthesis, Antioxidant, DPPH, FRAP.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315300

REMOVAL OF CO, SO2 AND HC GASES FROM INCINERATOR USING DIATOMACEOUS EARTH AND COMPOST-MODIFIED SORBENT IN FIXED BED ABSORPTION REACTOR

Mariana, F. Mulana and L. Juniar

Rasayan J. Chem, 13 (1), 139- 145 (2020)

Keywords: Modified Sorbent, Gas Sorption, Fixed Bed Reactor, Diatomaceous Earth, Compost.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315377

ASSESSMENT OF WATER QUALITY OF SITNICA RIVER BY USING WATER QUALITY INDEX (WQI)

A. M. Shala Abazi , B. H. Durmishi , F. S. Sallaku , H. S. Ã‡adraku , O. B. Fetoshi, P. H. Ymeri and P. S. BytyÃ§i

Rasayan J. Chem, 13 (1), 146- 159 (2020)

Keywords: Assessment, Water Quality Index, Physico-chemical parameters, Pollutant, Sitnica River.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315344

UNSYMMETRIC COMPARTMENTAL LIGANDS FOR METALLOBIOSITE MODELLING: A MINI REVIEW

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Rasayan J. Chem, 13 (1), 160- 167 (2020)

Keywords: Bridging ligands, Bimetallic Complexes, Metallobiosites, Metalloenzymes, Dinucleating Ligands, Transition Metals.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315586

PHYSICOCHEMICAL AND BIOLOGICAL WATER QUALITY ASSESSMENT OF THE GUEBLI RIVER, NORTHEASTERN ALGERIA

K. Boudeffa, F. Fekrache and N. Bouchareb

Rasayan J. Chem, 13 (1), 168- 176 (2020)

Keywords: River, Water Quality, Physicochemical Parameters, Pollution, Algeria.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315255

ISOLATION AND CHARACTERISATION OF CELLULOSE NANOCRYSTAL OBTAINED FROM SUGARCANE PEEL

C. V. Abiaziem, A. B. williams , A. I. Inegbenebor , C. T. Onwordi , C. O. Ehi-Eromosele and L. F. Petrik

Rasayan J. Chem, 13 (1), 177- 187 (2020)

Keywords: Sugarcane Peel, Cellulose, Cellulose Nanocrystal, Acid Hydrolysis, Characterization

DOI: http://dx.doi.org/10.31788/RJC.2020.1315328

BIOSYNTHESIS OF FUNCTIONALIZED GOLD NANOPARTICLES BY USING METHYL COMMATE C IN Scoparia dulcis LEAF EXTRACT AS REDUCING AGENT

J. Mary Joselin, V. Ganesh Kumar, T. Selvaraj, K. Govindaraju and V. Karthick

Rasayan J. Chem, 13 (1), 188- 194 (2020)

Keywords: Spectroscopy, Nanomaterials, Scoparia dulcis, Gold nanoparticles, Methyl commate C

DOI: http://dx.doi.org/10.31788/RJC.2020.1315515

DETERMINATION OF HEAVY METALS IN PRISTIPOMA FURCATUS AND ACANTHURUS STRIGOSUS FISH SPECIES COLLECTED FROM PULICAT LAKE, CHENNAI

B. Prabhu Dass Batvari and D. Saravanan

Rasayan J. Chem, 13 (1), 195- 201 (2020)

Keywords: Heavy Metals, Pristipoma furcatus, Acanthurus strigosus, Aquatic Ecosystem, Sediment

DOI: http://dx.doi.org/10.31788/RJC.2020.1315474

POLYANILINE (PANI)-SENSITIZED Fe3O4/SiO2/TiO2 NANOCOMPOSITES AS PHOTOCATALYST FOR THE REDUCTION OF Au(III) IONS

I. S. Budi, S. J. Santosa and E. S. Kunarti

Rasayan J. Chem, 13 (1), 202- 209 (2020)

Keywords: Polyaniline, Fe3O4, SiO2, TiO2, Au(III), Photoreduction

DOI: http://dx.doi.org/10.31788/RJC.2020.1315509

ASSESSMENT OF TOXIC METALS IN COMMON FOOD GRAINS GROWN IN JODHPUR CITY

Pallavi Mishra, Rajshri Soni, Vandana Kachhwaha and Naresh Giri

Rasayan J. Chem, 13 (1), 210- 214 (2020)

Keywords: Jojari River, Industrial Effluents, Heavy Metals, AAS, CETP

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SYNTHESIS, CHARACTERIZATION AND ANTIMICROBIAL ACTIVITY OF Mn(II),Fe(II), Ni(II),Co(II) AND Zn(II) COMPLEXES OF SCHIFF BASE DERIVED FROM 2,2- DIMETHYLPROPANE 1, 3-DIAMINE AND 5-CHLORO ISATIN

N. P. Singh, K. Kumar , A. Kumar and U. Agarwal

Rasayan J. Chem, 13 (1), 215- 221 (2020)

Keywords: Schiff Base, Metal(II) Complexes, 2,2 Dimethylpropane-1,3-diamine, 5-Chloroisatin, Octahedral Geometry, Antimicrobial activity.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315571

DEGRADATION STUDYOF PIMAVANSERIN: IDENTIFICATION, ISOLATION AND STRUCTURAL CHARACTERIZATION OF DEGRADANTS

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Rasayan J. Chem, 13 (1), 222- 229 (2020)

Keywords: Pimavanserin, Degradation Products, UPLC-MS, NMR.

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Mangifera odorata GRIFF SEED EXTRACT AS CORROSION INHIBITOR OF MILD STEEL IN HYDROCHLORIC ACID MEDIUM

Y. Stiadi, Rahmayeni, L. Rahmawati, M. Efdi, H. Aziz and Emriadi

Rasayan J. Chem, 13 (1), 230- 239 (2020)

Keywords: Mild Steel, Mangifera odorata Griff, Corrosion Inhibitor, Potentiodynamic Polarization.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315325

OPTIMIZATION OF ENCAPSULATION EFFICIENCY AND LACTIC ACID BACTERIA VIABILITY THROUGH A COMBINATION BETWEEN CAPSULE AGENTS AND TOFU WASTE PREBIOTIC

Virna Muhardina, Putri Meutia Sari , Yuliani Aisyah , Sri Haryani and Said Ali Akbar

Rasayan J. Chem, 13 (1), 240- 244 (2020)

Keywords: Alginate, Carrageenan, Tofu, Lactic Acid Bacteria, Encapsulation

DOI: http://dx.doi.org/10.31788/RJC.2020.1315569

THEORETICAL VALIDATION OF MEDICINAL PROPERTIES OF Curcuma longa Linn

Sampat Suryawanshi and Pramod Kulkarni

Rasayan J. Chem, 13 (1), 245- 248 (2020)

Keywords: Molinspiration, Curcuma longa Linn, Bioactivity Score, Lipinskiâ€™s Rule

DOI: http://dx.doi.org/10.31788/RJC.2020.1315581

SILICA EXTRACTION FROM BEACH SAND FOR DYES REMOVAL: ISOTHERMS, KINETICS AND THERMODYNAMICS

M. Lutfi Firdaus, Fitri E. Madina , Sasti Yulia F., Rina Elvia , Soraya N. Ishmah , Diana R. Eddy, Abigail P. Cid-Andres

Rasayan J. Chem, 13 (1), 249- 254 (2020)

Keywords: Silica, Remazol Blue, Congo Red, Adsorption, Isotherms, Kinetic, Thermodynamics

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GROWTH CONTROL OF ZnO-TiO2/CHITOSAN NANOROD ON COTTON TEXTILE FIBER BASED ON DIFFERENT CHLORO ACETIC MOLAR COMPOSITION AS CROSS LINKER

Yetria Rilda, Dyah Rahayu Ratyaningsih , Yulia Eka Putri , Refinel Syukri , Anthoni Agustien and Hilfi Pardi

Rasayan J. Chem, 13 (1), 255- 263 (2020)

Keywords: Nanorods, ZnO-TiO2/chitosan, Chloroacetic Acid, Mechanics, B. subtilis (ATCC 6633)

DOI: http://dx.doi.org/10.31788/RJC.2020.1315673

STUDY OF ACOUSTICAL PARAMETERS OF MONOMETHYLAMMONIUM PERCHLORATE IN SOME NON-AQUEOUS SOLVENTS AT DIFFERENT TEMPERATURES USING ULTRASONIC TECHNIQUE

Vivek Pathania , Shrutila Sharma, Shashi Kiran Vermani and B.K.Vermani

Rasayan J. Chem, 13 (1), 264- 274 (2020)

Keywords: Apparent Molal Volume, Specific Acoustic Impedance, Intermolecular Free Lengths, Acetonitrile, Dimethylacetamide, Dimethylsulfoxide

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MECHANICAL PROPERTIES OF BIOPLASTICS JANENG STARCH (Dioscorea hispida) FILM WITH GLYCEROL AND ZINC OXIDE AS REINFORCEMENT

Chairul Amni , Ismet , Sri Aprilia , Mariana and Said Ali Akbar

Rasayan J. Chem, 13 (1), 275- 281 (2020)

Keywords: Bioplastics, Janeng (Dioscorea hispida), Plasticizers, Tensile Strength

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SYNTHESIS OF NEW SULPHANILAMIDE BASED SCHIFF BASE NICKEL COMPLEXES WITH STUDY OF ITS ANTIBACTERIAL ACTIVITY AND NANOPARTICLE SYNTHESIS

R. R. Surve and S. T. Sankpal

Rasayan J. Chem, 13 (1), 282- 290 (2020)

Keywords: Sulphanilamide, Schiff Base, Square Planar, Antibacterial Activity, Nanoparticles

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SYNTHESIS OF FEW 1,3,4-OXADIAZOLE DERIVATIVES BLENDED WITH DIFFERENT HETEROCYCLES AND THEIR IN-VITRO ANTIBACTERIAL ACTIVITIES

M. Idrees, Y.G. Bodkhe , N. J. Siddiqui and S. Kola

Rasayan J. Chem, 13 (1), 291- 297 (2020)

Keywords: 1,3,4-Oxadiazole, Quinoline, Benzofuran, Pyrazole, p-Tolyloxy, Carbohydrazide

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SYNTHESIS OF MgFe2O4-MgO NANOCOMPOSITE: INFLUENCE OF MgO ON THE CATALYTIC ACTIVITY OF MAGNESIUM FERRITE IN BIODIESEL PRODUCTION

Helmiyati , G.H. Abbas, Y. Budiman and S. Ramadhani

Rasayan J. Chem, 13 (1), 298- 305 (2020)

Keywords: Biodiesel, Catalyst, Magnesium Ferrite, Nanocomposite, Oleic Acid

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PHYTOCHEMICAL GINKGOLIDE B PROTECTS CULTURED NEUROBLASTOMA SH-SY5Y CELLS AGAINST Aβ(25-35) INDUCED OXIDATIVE STRESS RESPONSES BY MAINTAINING THE MITOCHONDRIAL INTEGRITY

Navrattan Kaur , Sharanjot Kaur , Meenu Saini , Monisha Dhiman and Anil K. Mantha

Rasayan J. Chem, 13 (1), 306- 321 (2020)

Keywords: ROS/RNS, Oxidative Stress, Amyloid Beta, Ginkgolide B, Alzheimerâ€™s Disease, AP Endonuclease 1, BER-pathway

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TWO FLAVANONES FROM FINGER-ROOT (Curcuma rotunda) AND ITS ANTIBACTERIAL ACTIVITIES

Purwantiningsih, N. Jannah and D. U. C. Rahayu

Rasayan J. Chem, 13 (1), 322- 326 (2020)

Keywords: Antibacterial, Curcuma rotunda, Finger-root, Flavanone, Pinocembrin, Pinostrobin

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BIOACTIVE COMPOUND FROM THE MANGROVE PLANT ENDOPHYTIC FUNGUS Diaporthe amygdali SgKB4

D. Handayani, T. Wahyuningsih , Rustini , M.A. Artasasta , A. E. Putra and P. Proksch

Rasayan J. Chem, 13 (1), 327- 332 (2020)

Keywords: Diaporthe amygdali, Endophytic fungus, Sonneratia griffithii, Cytochalasin H, Antibacterial Activity, MRSA

DOI: http://dx.doi.org/10.31788/RJC.2020.1315589

SYNTHESIS AND CHARACTERIZATION OF CROSS-LINKED TRI-POLYMERS OF POLY ACRYLIC ACID AS WATER THICKENING AGENTS

Zalak J. Patel, Mukesh C. Patel , Parimal M. Chatrabhuji , Viral A. Patel and Dharmesh R. Patel

Rasayan J. Chem, 13 (1), 333- 338 (2020)

Keywords: Poly allyl tris buffer, Di-vinyl Benzene, Acrylic Acid, Water-absorbing Agent, Copolymer Composition

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DETERMINATION OF THE CONDITIONS OF PHOSPHATE COATINGS FORMATION ON IRON BY VOLTAMMETRIC METHOD

V. N. Statsyuk, A. Bold, L. A. Fogel, U. Sultanbek and Zh. Tilepbergen

Rasayan J. Chem, 13 (1), 339- 345 (2020)

Keywords: Phosphate Coatings, Cyclic Voltammetry, Akimovâ€™s Method, Optimal Conditions, Hydroxylamine.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315460

RESULTS OF THE STUDY OF FILMS OBTAINED BY ADDING VARIOUS IMPURITIES TO THE SOLUTION OF NICKEL PHOSPHIDE

P. Abdurazova, Sh. Koshkarbayeva, M. Sataev, N. Dzhakipbekova and Y. Raiymbekov

Rasayan J. Chem, 13 (1), 346- 353 (2020)

Keywords: Chemical Films, Nickel Phosphide, Chemical Method, Solution, Metal.

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ELECTROPHORETIC DEPOSITION OF ZIRCONIA ON ALUMINA FOR MOLTEN SALT APPLICATIONS

A. Sheik Mideen, G. Venkatasubramanian , T.M. Sridhar and S. Vasudevan

Rasayan J. Chem, 13 (1), 354- 362 (2020)

Keywords: Electrophoretic Deposition, Zirconia Deposits, Alumina Crucibles, Sintering, XRD, FTIR, SEM

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SYSTEMATIC LC-MS/MS METHOD FOR QUANTIFICATION OF 2,3-DIMETHYL-2H-INDAZOLE-6-AMINE CONTENT IN PAZOPANIB HYDROCHLORIDE

Pikkili Viswanath, Doddipalli Venkata Ramana Reddy and Nagaraju Chamarthi

Rasayan J. Chem, 13 (1), 363- 369 (2020)

Keywords: Genotoxic Impurity, Pazopanib Hydrochloride, ICH, LC/MS/MS, LOD, LOQ

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GREEN ROUTE FOR THE SYNTHESIS OF OXADIAZOLE DERIVATIVE CONTAINING BENZIMIDAZOLE MOIETY AND ITS MANNICH BASES: IN-VITRO ANTIMICROBIAL ACTIVITY

Samrin Naz and Mahendra B. Bagade

Rasayan J. Chem, 13 (1), 370- 376 (2020)

Keywords: Mannich Bases, Oxadiazole, Benzimidazole, Microwave Irradiation, Antibacterial Activity.

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ANTIMICROBIAL METABOLITE FROM THE ENDOPHYTIC FUNGI Aspergillus flavus ISOLATED FROM Sonneratia alba, A MANGROVE PLANT OF TIMOR-INDONESIA

Antonius R. B. Ola, Christina A. P. Soa, YosephSugi , Theo Da Cunha, Henderiana L. L. Belli and Herianus J. D. Lalel

Rasayan J. Chem, 13 (1), 377- 381 (2020)

Keywords: Mangrove, Sonneratia alba, Timor, Endophytic Fungi, Kojic Acid, Antibacterial.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315585

PHYSICOCHEMICAL CHARACTERIZATION OF NATURAL KAOLIN FROM JABOI INDONESIA

R. Dewi, H. Agusnar, Z. Alfian and Tamrin

Rasayan J. Chem, 13 (1), 382- 388 (2020)

Keywords: DSC/TGA, FTIR, Jaboi, Kaolin, Physicochemical, XRF, SEM EDX, XRD

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THE ENCAPSULATION OF METFORMIN ON CHITOSAN MATRIX AS DIABETES MELLITUS DRUG SLOW RELEASE SYSTEM

S. E.Cahyaningrum , N. Herdyastuti, W. Imroni and A. Sholikhah

Rasayan J. Chem, 13 (1), 389- 394 (2020)

Keywords: Encapsulation, Metformin, Diabetes Mellitus, Chitosan, Slow-release System

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GROWTH, CHARACTERIZATION OF Mn(II) DOPED Zn(II) L-HISTIDINE HYDROCHLORIDE MONOHYDRATE COMPLEX CRYSTALS

V. Parvathi, J. Sai Chandra , Y. Sunandamma and H.Ananda Lakshmi

Rasayan J. Chem, 13 (1), 395- 404 (2020)

Keywords: L-Histidine, EPR, XRD, Microhardness.

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ADSORPTION CORROSION INHIBITIVE BEHAVIOR OF PEELS EXTRACT OF Theobroma cacao ON MILD STEEL AS A CORROSION INHIBITOR IN HCl MEDIA

Y. Yetri, R. Hidayat, R. Sumiati and N. P. Tissos

Rasayan J. Chem, 13 (1), 405- 416 (2020)

Keywords: Theobroma cacao Peels, Essential Compound, Mild Steel, XPS, XRD

DOI: http://dx.doi.org/10.31788/RJC.2020.1315550

BIOACTIVE METABOLITE FROM MARINE SPONGEDERIVED FUNGUS Cochliobolus geniculatus WR12

D. Handayani, R. A. Putri , F. Ismed , T. Hertiani N. P. Ariantari and P. Proksch

Rasayan J. Chem, 13 (1), 417- 422 (2020)

Keywords: Antibacterial Activity, Cochliobolus geniculatus, Cytotoxic Activity, Haliclona fascigera, Marine Sponge-derived fungi, Radicinin

DOI: http://dx.doi.org/10.31788/RJC.2020.1315517

Teedia lucida ROOT EXTRACTS BY ULTRASONICATION AND MACERATION TECHNIQUES: PHYTOCHEMICAL SCREENING, ANTIMICROBIAL AND ANTIOXIDANT POTENTIALS

P.T. Motsumi , T. Qwebani-Ogunleye , I.P. Ejidike , F.M. Mtunzi and Z. Nate

Rasayan J. Chem, 13 (1), 423- 433 (2020)

Keywords: Teedia lucida, Phenolic, Roots, Tannins, Total Flavonoids, Antioxidant, Antibacterial

DOI: http://dx.doi.org/10.31788/RJC.2020.1315594

EFFECTIVE METHODS OF PYRIDOXINE SUPPLEMENTATION IN LAYING HENS TO ALBUMIN AND GLOBULIN LEVELS

S. Silaban, B. Sinaga , M. Damanik and P. M. Silitonga

Rasayan J. Chem, 13 (1), 434- 438 (2020)

Keywords: Albumin, Globulin, Egg, Laying Hens, Supplementation of pyridoxine

DOI: http://dx.doi.org/10.31788/RJC.2020.1315506

POROSITY EFFECT OF Ag DOPED ZnO NANOCRYSTALLITES

M. Giruba, J. Christina Rhoda , S. Chellammal and K. Ravichandran

Rasayan J. Chem, 13 (1), 439- 447 (2020)

Keywords: ZnO Nanocrystallites, Capping Agent, Co-precipitation, Porosity, Strain, Geometrical Parameter

DOI: http://dx.doi.org/10.31788/RJC.2020.1315501

COMPARATIVE STUDY ON ADSORPTION OF CATIONIQUE DYE ONTO EXPANDED PERLITE AND NATURAL CLAY

B. Damiyine, A. Guenbour and R. Boussen

Rasayan J. Chem, 13 (1), 448- 463 (2020)

Keywords: Adsorption Isotherm, Natural Moroccan Clay, Expanded Perlite, Kinetics Studies, Rhodamine B.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315588

IDENTIFICATION, CHARACTERIZATION AND ANTIBACTERIAL POTENTIAL OF PROBIOTIC LACTIC ACID BACTERIA ISOLATED FROM NANIURA (A TRADITIONAL BATAK FERMENTED FOOD FROM CARP) AGAINST Salmonella typhi

G. Haro , I. Iksen, and N. Nasri

Rasayan J. Chem, 13 (1), 464- 468 (2020)

Keywords: Probiotic, Lactic Acid Bacteria, Naniura, Antibacterial, Salmonella typhi

DOI: http://dx.doi.org/10.31788/RJC.2020.1315530

MOLECULAR DOCKING ANALYSIS OF GOSSYPOL ANALOGUES AS HUMAN NEUTROPHIL ELASTASE (HNE), MATRIX METALLOPROTEINASES (MMP 2 AND 9) AND TYROSINASE INHIBITORS

Vishnu Ragavan , Aishwarya Ramesh and Radhakrishnan Narayanaswamy

Rasayan J. Chem, 13 (1), 469- 475 (2020)

Keywords: Molecular Docking, Gossypol Analogues, Human Neutrophil Elastase, Matrix Metalloproteinase, Tyrosinase.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315541

PHYTOCHEMICAL SCREENING AND TOXICITY OF ETHANOLIC EXTRACT OF MANGROVE (Rhizophora mucronata) LEAVES FROM LANGSA, ACEH TIMUR

Gimelliya Saragih, Tamrin , Marpongahtun , Darwin Yunus Nasution and Abdillah

Rasayan J. Chem, 13 (1), 476- 480 (2020)

Keywords: Mangrove, Rhizophora mucronata, Phytochemical, FTIR, UV-Vis, Toxicity

DOI: http://dx.doi.org/10.31788/RJC.2020.1315524

WETTING ABILITY OF A PHYTOPREPARATION AND THEIR ASSOCIATES WITH POLYELECTROLYTES

O. Yessimova , S. Kumargaliyeva , M. Kerimkulova , K. Mussabekov and Zh. Toktarbay

Rasayan J. Chem, 13 (1), 481- 487 (2020)

Keywords: Polyhexamethylene Guanidine Hydrochloride, Polyelectrolyte, Phytopreparation, Adsorption, Wetting

DOI: http://dx.doi.org/10.31788/RJC.2020.1315566

NOVEL HETEROPOLYACID SALT: TITANIUM (IV) MOLYBDOTUNGSTATE

N. Sharma, H.K. Sharma and P. Dogra

Rasayan J. Chem, 13 (1), 488- 493 (2020)

Keywords: Titanium Molybdotungstate, Synthesis, Heteropolyacid, Ion-exchange, IR

DOI: http://dx.doi.org/10.31788/RJC.2020.1315355

SYNTHESIS OF 4-CHLORO-PIPERIDINE DERIVATIVES VIA NbCl5 MEDIATED AZA-PRINS TYPE CYCLIZATION OF EPOXIDES AND HOMOALLYLIC AMINES

K. Kamesu, G. V. Krishna Mohan and K. Rajasekhar

Rasayan J. Chem, 13 (1), 494- 498 (2020)

Keywords: Aza Prins, Epoxides, Homoallylic Amines, Piperidines, Niobium Pentachloride

DOI: http://dx.doi.org/10.31788/RJC.2020.1315392

EVALUATION OF TETRA-n-BUTYLAMMONIUM BROMIDE AS CORROSION INHIBITOR FOR MILD STEEL IN 1N HCl MEDIUM: EXPERIMENTAL AND THEORETICAL INVESTIGATIONS

N. Subasree, J. Arockia Selvi, M. Arthanareeswari, and Renjith S. Pillai

Rasayan J. Chem, 13 (1), 499- 513 (2020)

Keywords: Corrosion Inhibition, Weight Loss Method, Polarization Sudy, XRD, AFM

DOI: http://dx.doi.org/10.31788/RJC.2020.1315485

EFFECTS OF PYROLYSIS TEMPERATURE ON THE COMPOSITION OF LIQUID SMOKE DERIVED FROM OIL PALM EMPTY FRUIT BUNCHES

M. Faisal , Asri Gani, Farid Mulana, Hera Desvita and S. Kamaruzzaman

Rasayan J. Chem, 13 (1), 514- 520 (2020)

Keywords: Liquid Smoke, Oil Palm Empty Fruit Bunches, Pyrolysis, Phenol, Acetic Acid

DOI: http://dx.doi.org/10.31788/RJC.2020.1315507

BINUCLEAR TRANSITION METAL COMPLEXES DERIVED FROM 3, 3'-DIHYDROXY BENZIDIENE AND 2-AMINO THIO PHENOL: SPECTROSCOPIC, THERMOGRAVIMETRIC, DNA CLEAVAGE, AND ANTIMICROBIAL STUDIES

Kuttiyapillai Sivakumar and Venkatachalam Chandrasekaran

Rasayan J. Chem, 13 (1), 521- 528 (2020)

Keywords: Binuclear, 3, 3'-Dihydroxy benzidiene, 2-Amino thiophenol, Infrared, Electronic Spectra, DNA Cleavage Study, Antimicrobial Study

DOI: http://dx.doi.org/10.31788/RJC.2020.1315538

FORMULA COMPARISON OF NANOEMULSION AND CREAM CONTAINING MICONAZOLE NITRATE: PENETRATION TEST USING FRANZ DIFFUSION CELLS AND ANTIFUNGAL ACTIVITY TEST ON Tricophyton mentagrophytes, Microsporum canis AND Candida albicans

H. L. Maha, and Masfria

Rasayan J. Chem, 13 (1), 529- 534 (2020)

Keywords: Nanoemulsion, Cream, Miconazole Nitrate, Franz Diffusion Cell, Antifungal.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315553

RAPID DETECTION OF ASHITABA (Angelica keiskei) HERBAL MEDICINE ADULTERATION USING FTIR AND PRINCIPAL COMPONENT ANALYSIS METHOD

Anne Yuliantini , Fenti Salafiah , Aiyi Asnawi

Rasayan J. Chem, 13 (1), 535- 540 (2020)

Keywords: Adulteration, Ashitaba, Celery, FTIR, PCA

DOI: http://dx.doi.org/10.31788/RJC.2020.1315557

NANOGRAM DETERMINATION OF MNII CATALYST IN THE DEGRADATION OF P-BROMOANILINE BY PERIODATE ION

R. D. Kaushik, Jaspal Singh , Malvika Chawla and Kavita Rawat

Rasayan J. Chem, 13 (1), 541- 547 (2020)

Keywords: Nanogram Determination, Sodium Metaperiodate, p-Bromoaniline, MnII Catalysed, 4-Methyl-1,2- benzoquinone.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315578

SYNTHESIS, CHARACTERISATION AND CATALYTIC STUDIES OF NANO ZINC OXIDE-ALUMINA FOR DISPLACEMENT REACTION ON CARBONYLDIIMIDAZOLE

S. Sumathi , M. Balaganesh and K.K. Balasubramanian

Rasayan J. Chem, 13 (1), 548- 555 (2020)

Keywords: Nano zinc oxide, alumina, SEM, XRD, carbonyldiimidazole, amines, disubstituted ureas.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315487

ANTIOXIDANT AND ANTI-MICROBIAL ACTIVITY STUDY OF SYNTHESIZED COPPER, NICKEL AND ZINC METALS SCHIFF BASE DERIVATIVE OF SALICYLALDEHYDE

J. Panda, L. Adhikari , A.Pal , S.S. Rout , S. Pattanaik and P. Pradhan

Rasayan J. Chem, 13 (1), 556- 561 (2020)

Keywords: Organometallic, Schiff Base, DPPH, Metal Complexes, Antioxidant.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315477

DEVELOPMENT OF TWO-DIMENSIONAL Mg DOPED ZnO NANO HYBRIDS AS ELECTRODE MATERIALS FOR ELECTROCHEMICAL SUPERCAPACITOR APPLICATIONS

Abisheik John Samuel , A. Deepi , G. Srikesh and A. Samson Nesaraj

Rasayan J. Chem, 13 (1), 562- 569 (2020)

Keywords: Supercapacitors, Electrode Materials, Mg-doped ZnO, Characterization

DOI: http://dx.doi.org/10.31788/RJC.2020.1315528

ANTI-DIABETIC PROPERTY OF GREEN SYNTHESIZED ZINC-OXIDE NANOPARTICLES FROM LEAF EXTRACT OF Chrysanthemum indicum PLANT

Neha Silas, and Reena S. Lawrence

Rasayan J. Chem, 13 (1), 570- 573 (2020)

Keywords: Diabetic Mellitus, Diabetic Activity, Zinc Oxide Nanoparticles, Anti-diabetic Agent.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315417

PHOTOCATALYTIC ACTIVITY OF TiO2/SiO2 PREPARED FROM SILICA CONTAINED IN VOLCANIC ASH FOR AMMONIA REMOVAL

E.T. Wahyuni, S. Suherman , D. Setyawati , R. Puspita , and M.Mudasir

Rasayan J. Chem, 13 (1), 574- 584 (2020)

Keywords: Volcanic Ash, Silica Source, TiO2/SiO2, Nanoparticles, Ammonia

DOI: http://dx.doi.org/10.31788/RJC.2020.1315464

SYNTHESIS, MOLECULAR DOCKING AND ANTITUBERCULAR ACTIVITY OF NEW BI HETEROCYCLIC COMPOUNDS ON BENZIMIDAZOLE MOIETY

Dhanaja Kotte , Kumaraswamy Gullapelli , Ravichandar Maroju Ramchander Merugu Brahmeshwari Gavaji

Rasayan J. Chem, 13 (1), 585- 592 (2020)

Keywords: Synthesis, Molecular Docking, Antitubercular Activity, Benzimidazole Derivatives

DOI: http://dx.doi.org/10.31788/RJC.2020.1315465

THE EXFOLIATION PROCESS OF SAWAHLUNTO COAL INTO GRAPHENE THROUGH THE MODIFIED HUMMER METHOD

V. Purwandari , S. Gea, B. Wirjosentono , A. Haryono , S. Rahayu and Y. A. Hutapea

Rasayan J. Chem, 13 (1), 593- 600 (2020)

Keywords: Sawahlunto Coal, Exfoliation Process, Graphene, Modified Hummer Method

DOI: http://dx.doi.org/10.31788/RJC.2020.1315473

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D. Ashok, Nalaparaju Nagaraju , M. Ram Reddy , Ravinder Dharavath, K. Ramakrishna and M. Sarasija

Rasayan J. Chem, 13 (1), 601- 609 (2020)

Keywords: Aromatic Boronic Acid, Suzuki Cross-coupling Reaction, Microwave Irradiation, Antimicrobial Activity

DOI: http://dx.doi.org/10.31788/RJC.2020.1315490

PREPARATION OF ANTIBACTERIAL IRON-BASED NANOPARTICLES USING Ruellia tuberosa L. ROOT EXTRACTS AS BIOREDUCTOR

A. Safitri, M. Ramadhan , and A. Sabarudin

Rasayan J. Chem, 13 (1), 610- 620 (2020)

Keywords: Iron Nanoparticles, Antibacterial Agent, Ruellia tuberosa L., SEM-EDS

DOI: http://dx.doi.org/10.31788/RJC.2020.1315511

OPTIMIZATION SYNTHESIS FATTY ACID ETHYL ESTER AS BIODIESEL FROM PALM FATTY ACID DISTILLATE USING $SO4^{2}$?/ TIO2 CATALYST SUPPORTED BY MESOPOROUS SILICA

J. Manga, A. Ahmad , P. Taba , and Firdaus

Rasayan J. Chem, 13 (1), 621- 627 (2020)

Keywords: Palm Fatty Acid Distillate, Ethyl Ester, Esterification, Heterogeneous catalyst, Biodiesel, Esterification

DOI: http://dx.doi.org/10.31788/RJC.2020.1315494

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E. Rohaeti, E. Kasmudjiastuti , R. S. Murti , and D. Irwanto

Rasayan J. Chem, 13 (1), 628- 635 (2020)

Keywords: Antibacterial Activity, Piper Betle, Suede Leather, Silver Nanoparticle, SEM.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315516

LEAF EXTRACT OF Artocarpus altilis [Park.] Fosberg HAS POTENCY AS ANTIINFLAMMATORY, ANTIOXIDANT, AND IMMUNOSUPPRESSANT

D. H. S. Palupi, D. S. Retnoningrum , M. I. Iwo , and A. A. Soemardji

Rasayan J. Chem, 13 (1), 636- 646 (2020)

Keywords: Artocarpus altilis, Complete Freund's Adjuvant, Anti-inflammatory, Antioxidants, Immunosuppressant, Traditional Medicines

DOI: http://dx.doi.org/10.31788/RJC.2020.1315519

SYNTHESIS OF (E)-4-METHYL-2-((PHENETHYLIMINO (PHENYL)METHYL)PHENOL AND ITS TRANSITION METAL COMPLEXES, CHARACTERIZATION AND ELECTRICAL CONDUCTIVITY STUDY OF COMPLEXES

A. B. Sahare and R. B. Mohod

Rasayan J. Chem, 13 (1), 647- 653 (2020)

Keywords: Schiff Base, FTIR, Diffuse Reflectance, Electrical Conductivity, Transition Metal Complexes, Metal Chelates

DOI: http://dx.doi.org/10.31788/RJC.2020.1315525

SYNTHESIS OF SOME CHALCONE DERIVATIVES, IN VITRO AND IN SILICO TOXICITY EVALUATION

A. N. Kristanti , H. Suwito, N.S. Aminah, K.U. Haq, H. D. Hardiyanti, H. Anggraeni, N. Faiza, R.S. Anto and S. Muharromah

Rasayan J. Chem, 13 (1), 654- 662 (2020)

Keywords: 2-Hydroxychalcone Derivatives, Claisen-Schmidt Condensation, HeLa Cell, Apoptosis, MDM2 Protein.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315534

QUANTUM MECHANICAL STUDIES ON THE EFFECT OF INTERMOLECULAR ROTATION OF THE STACKING INTERACTION OF DIAZINE ISOMERS

Mahasweta Choudhury, Shruti Sharma, Benzir Ahmed and Bipul Bezbaruah

Rasayan J. Chem, 13 (1), 663- 671 (2020)

Keywords: MPn, Diazine, Dihedral Angle, ?-? Stacking etc.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315535

A NOVEL MICROBIAL FUEL CELL TECHNOLOGY FOR ENERGY GENERATION AND COMPARISON OF POWER DENSITIES FOR DIFFERENT ELECTRODES USING NANOTECHNOLOGY

Samatha Singh and S. Suresh

Rasayan J. Chem, 13 (1), 672- 675 (2020)

Keywords: Electrodes, Microbial Fuel Cell(MFC), Power Density, Silver Nanoparticles (SNP)

DOI: http://dx.doi.org/10.31788/RJC.2020.1315556

SYNTHESIS OF NOVEL PYRAZOLINES AND THEIR ANTIMICROBIAL ACTIVITY

S. Sathiya , A. Keerthika ,B. S. Krishnamoorthy, S. Nandhabala , S. Aravind , N. Hari and R. Ravikumar

Rasayan J. Chem, 13 (1), 676- 683 (2020)

Keywords: Chalcones, Pyrazolines, XRD, Antimicrobial activity. 4-nitro aniline derived triazoles, electronegativity, extend of conjugation.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315568

TOTAL PHENOLIC CONTENT AND ANTIOXIDANT ACTIVITIES OF BUNI FRUIT (ANTIDESMA BUNIUS L.) IN MONCONGLOE MAROS DISTRICT EXTRACTED USING ULTRASOUND-ASSISTED EXTRACTION

M. Yasser, M. Rafi , W.T. Wahyuni , S.E. Widiyanti and A.M.I.A Asfar

Rasayan J. Chem, 13 (1), 684- 689 (2020)

Keywords: Buni Fruit, Ultrasound-Assisted Extraction, Total Phenolic Content, Antioxidant Activities, Ethanol

DOI: http://dx.doi.org/10.31788/RJC.2020.1315584

MOLECULAR DOCKING AND MOLECULAR DYNAMIC SIMULATION OF THE AGLYCONE OF CURCULIGOSIDE A AND ITS DERIVATIVES AS ALPHA GLUCOSIDASE INHIBITORS

Nursamsiar, M. Siregar , A. Awaluddin , N. Nurnahari , S. Nur , E. Febrina and A. Asnawi

Rasayan J. Chem, 13 (1), 690- 698 (2020)

Keywords: Aglycone Curculigoside A, Alpha Glucosidase, Chalcone, Docking, MD

DOI: http://dx.doi.org/10.31788/RJC.2020.1315577

IMPROVEMENT OF CORROSION BY MOLTEN SALTS IN COATING POWDERS MIXED IN DIFFERENT COMPOSITIONS OF YSZ–Al2O3

J. Bautista-Ruiz , A. Chaparro and J.C. Caicedo

Rasayan J. Chem, 13 (1), 699- 706 (2020)

Keywords: Alumina (Al2O3), Zirconia stabilized with Itria, Coatings, Corrosion.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315591

THERMO-PHYSICAL, SPECTRAL EVALUATION OF MOLECULAR INTERACTIONS IN LIQUID BINARIES OF DIETHYL MALONATE AND AMIDES AT TEMPERATURES (303.15, 308.15, 313.15, 318.15) K

Ch. Udayalakshmi , Shaik Beebi , P.B. Sandhya Sri ,V.N.S.R. Venkateswararao, G. Lakshmana Rao, and C. Rambabu

Rasayan J. Chem, 13 (1), 707- 722 (2020)

Keywords: Diethyl Malonate, Ultrasonic Velocity, Density, Acoustical, Molecular Interactions.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315595

SYNTHESIS OF Co-NH2/MESOPOROUS SILICA BIFUNCTIONAL CATALYST USING SIDOARJO MUD AND BOVINE BONE GELATIN TEMPLATE FOR CONVERSION OF USED COOKING OIL INTO BIOFUEL

W. Trisunaryanti, Triyono and D. A. Fatmawati

Rasayan J. Chem, 13 (1), 723- 732 (2020)

Keywords: Bifunctional Catalyst, Biofuel, Gelatin, Mesoporous Silica, Sidoarjo Mud

DOI: http://dx.doi.org/10.31788/RJC.2020.1315514

DEVELOPMENT OF COMPLEX FERTILIZER TECHNOLOGY WITH IMPROVED AGROCHEMICAL PROPERTIES USING HYDROGEL

Raikhan ZH. Omirova, Aidar A. Bolysbek , Shavkat D. Shirinov and Abdulakhat T. Dzhalilov

Rasayan J. Chem, 13 (1), 733- 738 (2020)

Keywords: Hydrogel, Macro and Microelement Containing Fertilizers, Water Solution, Soil, Fertilizer Properties.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315651

EFFECT OF OKRA (Abelmoschus esculentus L.) FRUIT EXTRACT IN IMPROVING INSULIN SENSITIVITY BY MODIFYING GLUCOSE-REGULATING GENE EXPRESSION

W. Aligita, S. Muhsinin , K.T. Wijaya , A. Artarini and I.K. Adnyana

Rasayan J. Chem, 13 (1), 739- 746 (2020)

Keywords: Diabetes Mellitus, Abelmoschus esculentus L., Okra Fruit, Insulin Resistance, PPAR- ?

DOI: http://dx.doi.org/10.31788/RJC.2020.1315555

ZnO INCORPORATED ON NATURAL ZEOLITE FOR PHOTODEGRADATION OF METHYLENE BLUE

N. P. Diantariani, I. Kartini , A. Kuncaka , and E. T. Wahyuni

Rasayan J. Chem, 13 (1), 747- 756 (2020)

Keywords: ZnO, Natural Zeolites, Photocatalysts, Photodegradation, Methylene Blue.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315597

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Adiansyah, I. Elisabeth Purba , M. Tarigan , Lisnadiyanti , Yusnaidar and I.P. Mahendra

Rasayan J. Chem, 13 (1), 757- 760 (2020)

Keywords: TiO2, Doping process, Sulfur, Photocatalyst, Reactive Black 05.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315461

EXTRACTION OF Co(II) AND Cu(II) FROM WASTE MATERIALS WITH SEMICARBAZONE OF 4-NITROBENZALDEHYDE

Jaspal Singh, R. D. Kaushik, Payal Devi and Preeti Das

Rasayan J. Chem, 13 (1), 761- 766 (2020)

Keywords: Solvent Extraction, 4 Nitrobenzaldehydesemicarbozone, Semicarbazone, Thiosemicarbazones.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315563

INFLUENCE OF THE DIFFERENT FORMS OF CRUM RUBBER PARTICLE IN NAO BRAKE PAD MATERIALS

Adnan Ibrahim Shihab

Rasayan J. Chem, 13 (1), 767- 771 (2020)

Keywords: Waste Crumb Rubber, Chase Test, Tribological Properties, Brake Pad.

DOI: http://dx.doi.org/10.31788/RJC.2020.1315542

THE EFFECT OF NICKEL CONTENT IMPREGNATED ON ZEOLITE TOWARD CATALYTIC ACTIVITY AND SELECTIVITY FOR HYDROTREATING OF CASHEW NUT SHELL LIQUID OIL

M. L. Permata, W. Trisunaryanti , I. I. Falah, M. T. Hapsari and D. A. Fatmawati

Rasayan J. Chem, 13 (1), 772- 779 (2020)

Keywords: Cashew Nut Shell Liquid Oil, Gasoline, Hydrotreating, Mordenite, Nickel

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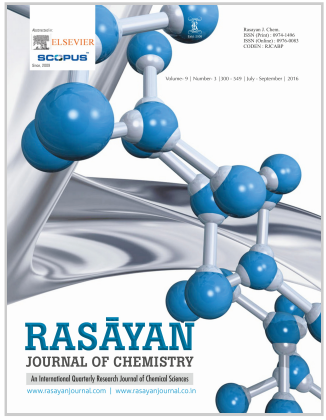

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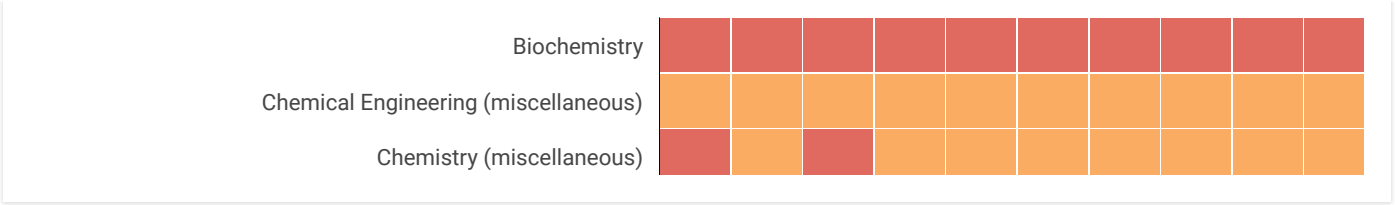

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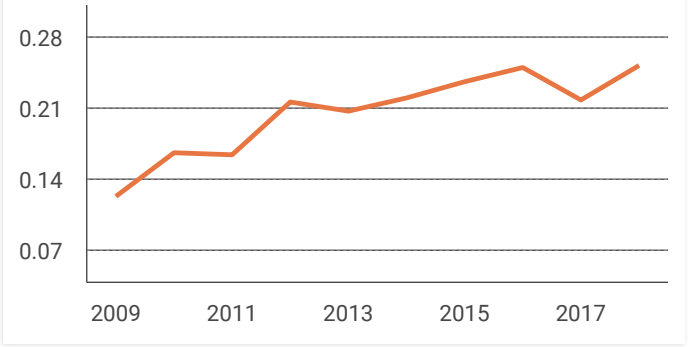

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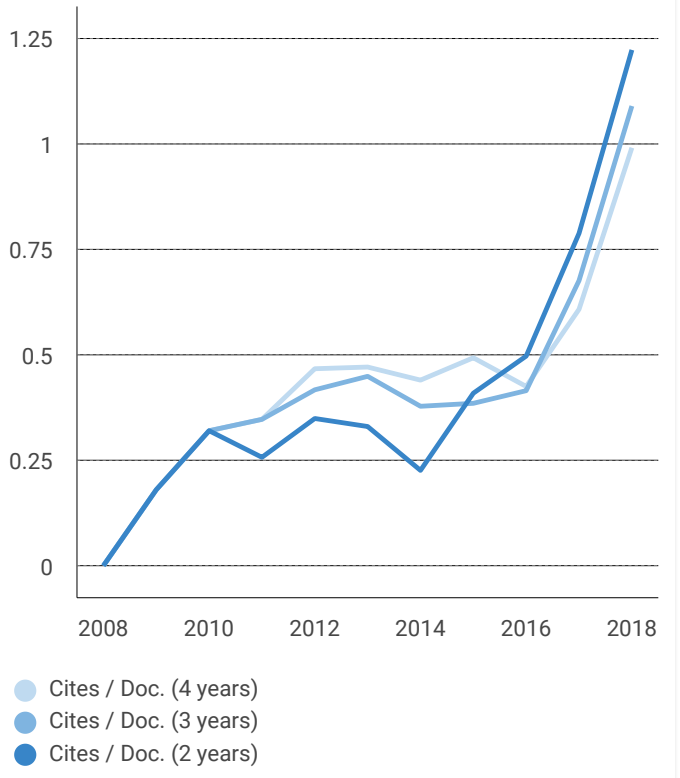

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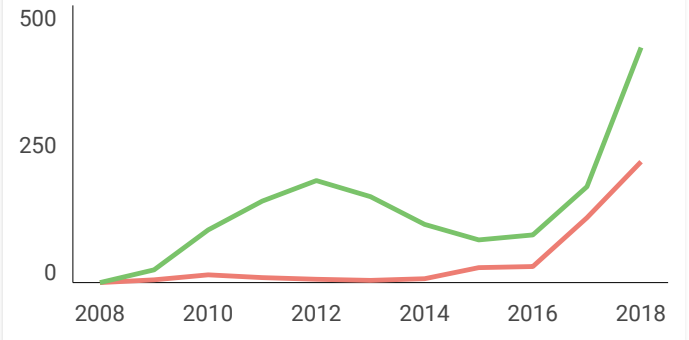

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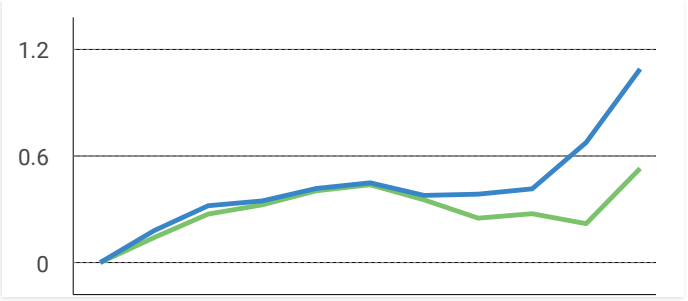

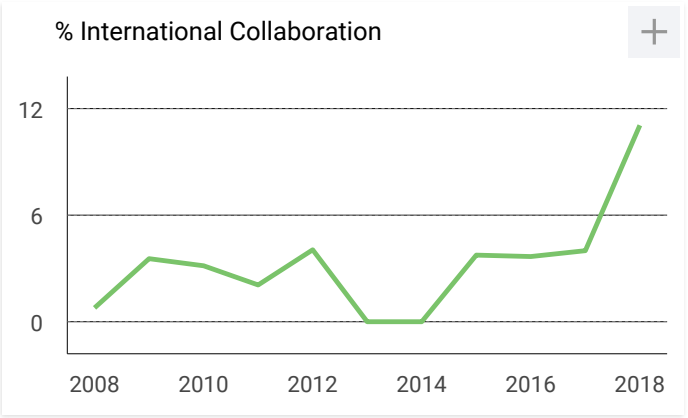

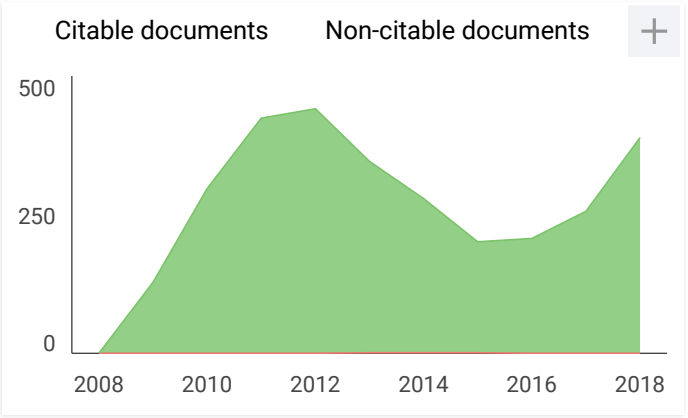

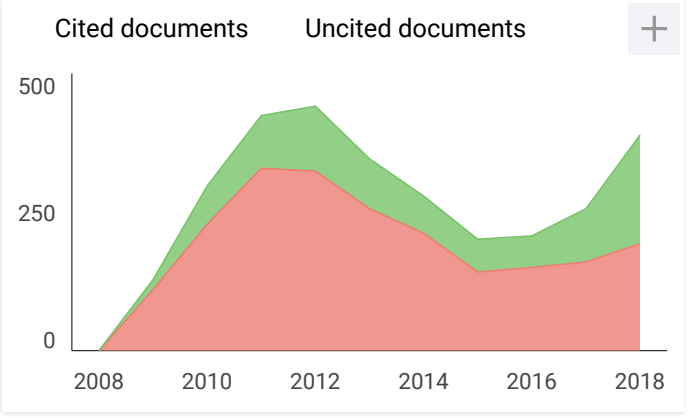

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SYNTHESIS OF SOME CHALCONE DERIVATIVES, IN VITRO AND IN SILICO TOXICITY EVALUATION

A. N. Kristanti*, H. Suwito, N.S. Aminah, K.U. Haq, H. D. Hardiyanti, H. Anggraeni, N. Faiza, R.S. Anto and S. Muharromah
Department of Chemistry, Faculty of Science and Technology, Universitas Airlangga, Surabaya-60115, Indonesia
*E-mail: alfinda-n-k@fst.unair.ac.id

ABSTRACT
Chalcone can be synthesized using some methods, but conventional Claisen-Schmidt condensation is still the best method. The objevtives of this study were to synthesize some chalcone derivatives using conventional Claisen-Schmidt condensation by reacting 2-hydroxyacetophenone and some substituted benzaldehydes using NaOH 40%, followed by evaluating their cytotoxicity in vitro against HeLa cancer cells line using MTT method and analyzing molecular docking on p53 and MDM2 interaction. Cytotoxicity test exhibited that 2,5-dimethoxy-2′-hydroxychalcone and 4-chloro-2'-hydroxychalcone gave very low IC_{50}, but both did not show potential apoptosis activity, while in docking analysis 4-chloro-2'-hydroxychalcone showing the best results.
Keywords: 2-Hydroxychalcone Derivatives, Claisen-Schmidt Condensation, HeLa Cell, Apoptosis, MDM2 Protein.

INTRODUCTION

Chalcones belong to one of secondary metabolites produced by plants showing various pharmacological activities, such as antimicrobial and antifungal[1], anti-tumor and anti-angiogenic[2], antiinflamation, cytotoxic and antioxidant[3], anticancer[4], antileishmanial[5], antibacterial[6], antimalarial[7], and antidiabetic.[1-8] Chalcone can be synthesized using some organic reactions, such as Claisen-Schmidt, Suzuki, Wittig, Friedel-Craft acylation of cinnamoyl chloride and phenyl cinammic acid *photo*-Fries rearrangement. Various catalysts and reagents have been used in chalcone synthesis, for example $SOCl_2$, natural phosphat, lithium nitrate, *amino grafted zeolite*, ZnO, Na_2CO_3, PEG-400, silica sulfate, $ZrCl_4$, and ionic liquid.[9] To date, conventional Claisen-Schmidt condensation is still the best method to synthesize chalcone. This method is carried out using alkali solution as catalyst, microwave or ultrasound irradiation. Almost 75% of chalcone synthesis is performed using alkali solution.[10] Synthesis using microwave irradiation takes a shorter time which can be more effective, faster, and energy efficient in addition[11]. Nevertheless, some researcher found that in this methode difficult to control the reaction, so that many by-products are formed. As a consequence, further separation is necessary.[12] Chalcones synthesis was observed under ultrasound irradiation for a notable enhancing effect on the time of reaction and yield.[13]
In this study, some chalcone derivatives (compound **1**-**8**) were succesfully synthesized using classical Claisen-Schmidt condensation by reacting 2-hydroxyacetophenone and some substituted benzaldehydes using NaOH 40% (Fig.-1 and Table-1).

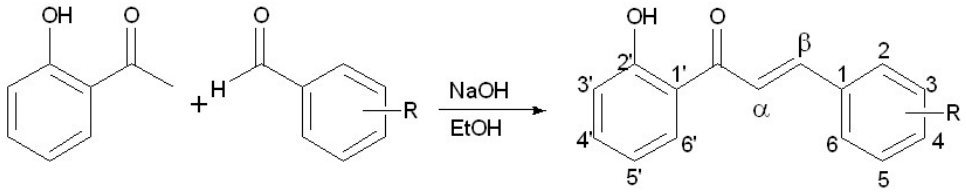

Fig.-1: Synthesis Reaction for Chalcone Derivatives Using Claisen Schmidt Condensation

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Table-1: The Synthezised Chalcones

Compounds	R	Compound's Name
1	2-OMe	2-methoxy-2'-hydroxychalcone
2	3-OMe	3-methoxy-2'-hydroxychalcone
3	4-OMe	4-methoxy-2'-hydroxychalcone
4	2,4-diOMe	2,4-dimethoxy-2'-hydroxychalcone
5	2,5-diOMe	2,5-dimethoxy-2'-hydroxychalcone
6	4-(N,N-diCH_3)	4-N,N-dimethyl-2'-hydroxychalcone
7	4-F	4-fluro-2'-hydroxychalcone
8	4-Cl	4-chloro-2'-hydroxychalcone

In cancer cases, overexpression of oncoprotein MDM2, as well as inactivation of p53 gene is observed. As a result, the tumor supressor protein p53 was inhibited by the oncoprotein MDM2 that was bound to the transactivation domain of p53.[14,15] Therefore reactivation of p53 activity through inhibition of MDM2/p53 interaction is a promising mechanism to find anticancer agents. As reported by Stoll et al, some chalcone derivatives were found to show anticancer activity through this mechanism with moderate activity.[16] Based on this report, we studied the cytotoxicity of some hydroxychalcone derivatives attaching substituents that withdraw and donate electrons.

Cytotoxic activity against HeLa cancer cells of the prepared chalcones were determined by MTT assay, while their apoptosis mechanism test was determined using flow cytometry experiment. Furthermore, molecular interaction between MDM2 and the prepared chalcones was studied by molecular docking experiment

EXPERIMENITAL

Material and Methods

All chemicals were provided from E.Merck in Darmstadt, Germany and Sigma-Aldrich in St. Louis, the United States and used directly without prior purification. Melting-point determination was conducted using Fisher-Johns *melting point apparatus* (Fisher Scientific Serial 40400075) and it was uncorrected. Each type of spectrum was recorded using different instruments : UV-Vis spectrophotometer Shimadzu UV-1800 was used to record UV-Vis spectra, *Fourier Transform Infrared spectroscopy* (FTIR) Shimadzu IRTracer-100 was used to record IR spectra, whereas *Nuclear Magnetic Resonance* (NMR) JEOL JNM-ECS 400 was used to record ^{1}H and ^{13}C NMR spectra.

General Procedure

The Synthesis Of Chalcones (1-8)

This procedure refered to Suwito et al.[17] A solution of 2'-hydroxyacetophenone (6 mmol) and benzaldehyde derivatives (6 mmol) in 30 mL of ethanol was stirred and refluxed at 5-10^{o}C until the mixture formed a homogenous solution. Then 6 mL of NaOH 40% solution was added dropwise and the reaction mixture was kept under 10^{o}C under stirring for 1 hour. The stirring was then kept on going at room temperature for one night. The mixture of reaction was transferred into crush ice and under stirring, then 15 mL of H_2SO_4 4N solution was added dropwise. The precipitate was filtered off, dried and recrystallized using ethanol yielding 40%-90%.

2-methoxy-2'-hydroxychalcone (1)

UV-Vis (EtOH) λ_{max} (nm) **:** 366 (0.521); 308 (0.353); 250 (0.249). FTIR (KBr) $\tilde{\nu}$ (cm^{-1}) : 3300 (OH phenolic); 3047 (C-H aromatic); 2964 (C-H sp^3); 1691 (C=O conjugated); 1643 (C=C conjugated); 1581 (C=C aromatic); 1251 (C-O phenolic); 1205 (C-O methoxy). ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) : 12.95 (1H, s, OH); 8.22 (1H, d, *J*=15.6 Hz, H_β); 7.92 (1H, dd, *J*=1.7 & 8.1 Hz, H-6′); 7.78 (1H, d, *J*=15.6 Hz, H_α); 7.64 (1H, dd, *J*=8.6 & 1.7 Hz, H-3′); 7.48 (1H, td, *J*=8.6; 7.2; 1.7 Hz, H-4′); 7.40 (1H, td, *J*=8.1; 7.2; 1.7 Hz, H-5′); 7.04-6.91 (4H, m, H-3, H-4, H-5, H-6); 3.93 (3H, s, OCH_3). ^{13}C-NMR (100.5 MHz, $CDCl_3$) δ (ppm) : 194.4 (C, C=O); 163.7 (C, C-2′); 159.1 (C, C-2); 141.2 (CH, Cβ); 136.3 (CH, C-4′); 132.3 (CH, C-4); 129.8 (CH, C-6′); 129.8 (CH, C-6); 123.7 (C, C1); 120.9 (CH; Cα); 120.8 (CH, C-5); 120.3 (C, C-1′); 118.9 (CH, C-5′); 118.6 (CH, C-3′); 114.4 (CH, C-3); 55.7 (CH_3, OCH_3). HRMS : 277.08336 (M+Na) suitable for molecular formula of $C_{16}H_{14}O_3$

3-methoxy-2´-hydroxychalcone (2)
UV-Vis (EtOH) λ_{max} (nm) **:** 312 (0.761); 254 (0.419). FTIR (KBr) $\tilde{\nu}$ (cm^{-1}) : 3300 (OH phenolic); 3012 (C-H aromatic); 2966 (C-H sp^3); 1637 (C=O conjugated); 1602 (C=C conjugated); 1577 (C=C aromatic); 1259 (C-O phenolic); 1209 (C-O methoxy). ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) : 12.81 (1H, s, OH); 7.87 (1H, d, *J*=15.5 Hz, H_β); 7.91 (1H, dd, *J*=1.3 & 8.0 Hz, H-6´); 7.62 (1H, d, *J*=15.5 Hz, H_α); 7.64 (1H, dd, *J*=8.6 & 1.7 Hz, H-3´); 7.49 (1H, td, *J*=8.4; 7.1; 1.3 Hz, H-4´); 7.40 (1H, td, *J*=8.1; 7.2; 1.7 Hz, H-5´); 7.34 (1H, m, H-5); 7.25 (1H, m, H-4); 7.16 (1H, m, H-2); 7.05-6.91 (3H, m, H-3', H-5', H-6); 3.86 (3H, s, OCH_3). ^{13}C-NMR (100.5 MHz, $CDCl_3$) δ (ppm) : 193.8 (C, C=O); 163.7 (C, C-2´); 160.1 (C, C-3); 145.5 (CH, Cβ); 136.6 (C, C-1); 136.0 (CH, C-4'); 130.1 (CH, C-6´); 129.7 (CH, C-5); 121.4 (CH, C6); 120.5 (CH; Cα); 120.8 (CH, C-5); 120.1 (C, C-1´); 119.0 (CH, C-5´); 118.7 (CH, C-4); 116.7 (CH, C-3'); 113.8 (CH, C-2); 55.5 (CH_3, OCH_3). HRMS : 277.08301 (M+Na) suitable for molecular formula of $C_{16}H_{14}O_3$

4- methoxy -2´- hydroxychalcone (3)
UV-Vis (EtOH) λ_{max} (nm) **:** 362 (0.888). FTIR (KBr) $\tilde{\nu}$ (cm^{-1}) : 3300 (OH phenolic); 3024 (C-H aromatic); 2970 (C–H sp^3); 1637 (C=O conjugated); 1606 (C=C conjugated); 1562 (C=C aromatic); 1233 (C-O phenolic); 1211 (C-O methoxy). ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) : 12.95 (1H, s, OH); 7.87-7.92 (2H, m, H-4', H-6'); 7.62 (2H, d, *J*=15 Hz, Hα, Hβ); 7.45-7.55 (2H, m, H-3', H-5'); 6.94 (3H, m, H-2, H-3, H-5). ^{13}C-NMR (100.5 MHz, $CDCl_3$) δ (ppm) : 194.8 (C, C=O); 163.6 (C, C-2'); 162.1 (C-C-4); 145.5 (CH, Cβ); 136.3 (CH, C-4'); 130.7 (2CH, C-2, C-6); 129.9 (CH, C-6'); 127.4 (C, C-1); 120.2 (C, C-1'); 118.9 (CH, Cα); 118.7 (CH, C-5'); 117.6 (CH, C-3'); 114.6 (2CH, C-3, C-5); 55.55 (OCH_3). HRMS : 277.08526 (M+Na) suitable for molecular formula of $C_{16}H_{14}O_3$

2,4- dimethoxy-2'-hydroxychalcone (4)
UV-Vis (EtOH) λ_{max} (nm) : 385 (0.583); 254 (0.288)**,** FTIR (KBr) $\tilde{\nu}$ (cm^{-1}) : 3300 (OH phenolic); 3072 (C-H aromatic); 2950 (C-H sp^3); 1635 (C=O conjugated), 1608 (C=C conjugated); 1550 (C=C aromatic); 1228 (C-O phenolic), 1228 (C-O methoxy). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H (ppm): 13.10 (s, OH); 8.15 (d, 1H, *J* = 15.5 Hz); 7.90 (d, 1H, *J* = 8.0 Hz); 7.68 (d, 1H, *J* = 15.4 Hz); 7.57 (d, 1H, *J* = 8.6 Hz); 7.46 (t, 1H, *J* = 7.8 Hz); 3.85 (s, 3H); 7.00 (d, 1H, *J* = 8.4 Hz); 6.91 (t, 1H, *J* = 7.6 Hz); 6.53 (dd, 1H, *J* = 8.6; 2.0 Hz); 6.47 (d, 1H, *J* = 1.8 Hz); 3.91 (s, 3H). ^{13}C-NMR (100.5 MHz, $CDCl_3$) δ_c (ppm) : 194.4 (C, C=O); 163.6 (C, C-2'); 163.5 (C, C-4); 160.8 (C, C-2); 141.4 (CH, C-β); 136.0 (CH, C-4'); 131.6 (CH, C-6); 129.7 (CH, C-6'); 120.4 (C, C-1'); 118.8 (CH, C-5'); 118.6 (CH, C-α); 118.1 (CH, C-3'); 116.9 (C, C-1); 105.7 (CH, C-5); 98.5 (CH, C-C-3); 55.7 (OCH_3); 55.6 (OCH_3). HRMS : 307.09543 (M+Na) suitable for molecular formula of $C_{17}H_{16}O_4$

2,5- dimethoxy -2'-hydroxychalcone (5)
UV-Vis (EtOH) λ_{max} (nm) : 310 (0.789). FTIR (KBr) $\tilde{\nu}$ (cm^{-1}) : 3300 (OH phenolic); 3068 (C-H aromatic); 2962 (C-H sp^3); 1639 (C=O conjugated); 1610 (C=C conjugated); 1500 (C=C aromatic); 1222 (C-O phenolic); 1220 (C-O methoxy);. ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H (ppm) : 12.92 (1H, s, OH); 8.18 (1H, d, *J*=15.6 Hz, Hβ); 7.91 (1H, dd, *J*=1.8 & 7.5 Hz; H-6'); 7.74 (1H, d, H-4', H-6'); 7.62 (2H, d, *J*=15.6 Hz, Hα); 7.48 (1H, m, H-4'); 7.15 (1H, d, *J*=3 Hz, H-6); 7.01 (1H, d, *J*=7.9 Hz, H-3); 6.88-6.97 (2H, m, H-3', H-5'); 6.94 (1H, dd, *J*=3.0 & 7.9 Hz, H-4); 3.88 (3H, s, OCH_3); 3.82 (3H, s, OCH_3). ^{13}C-NMR (100.5 MHz, $CDCl_3$) δ_c (ppm) : 194.3 (C, C=O); 163.6 (C, C-2'); 153.7 (C-C-2); 153.6 (CH, C-5); 141.0 (CH, Cβ); 136.3 (CH, C-4'); 129.9 (CH, C-6'); 127.4 (C, C-1'); 124.3 (CH, Cα); 121.1 (CH, C-5'); 120.3 (C, C-1); 118.9 (CH, C-1'); 118.7 (CH, C-3); 117.8 (CH, C-3'); 114.3 (CH, C-4); 112.6 (CH, C-6); 56.2 (OCH_3); 56.0 (OCH_3). HRMS : 307.09460 (M+Na) suitable for molecular formula of $C_{17}H_{16}O_4$

4-N,N-dimethyl-2'-hydroxychalcone (6)
UV-Vis (EtOH) λ_{maks} (nm) : 437 (57.043); 275 (24.259). FTIR (KBr) $\tilde{\nu}$ (cm^{-1}) : 3300 (OH phenolic); 2940 (C-H sp^3); 1620 (C=O conjugated), 1598 (C=C conjugated); 1580 (C=C aromatic); 1342 (C-N); 1207 (C-O phenolic). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H (ppm): 13.22 (s, OH); 7.91 (d, 1H, *J* = 15.4 Hz); 7.90 (dd, 1H, *J* = 7.2 & 1.2 Hz); 7.56 (d, 2H, *J* = 8.9 Hz); 7.45 (td, 1H, *J* = 8.4; 7.2; 1.6 Hz); 7.44 (d, 1H, *J* = 15.4

Hz); 7.00 (dd, 1H, *J* = 9.4; & 1.2 Hz); 6.91 (td, 1H, *J* = 8.4; 7.2; 1.2 Hz); 6.68 (d, 2H, *J* = 8.9 Hz); 3.04 (s, 6H). ^{13}C-NMR (100.5 MHz, $CDCl_3$) δ_c (ppm): 193.6 (C, C=O); 163.6 (C, C-2'); 152.4 (C, C-4); 146.7 (CH, C-β); 135.8 (CH, C-4'); 131.0 (2CH, C-2 & C-6); 129.5 (CH, C-6'); 122.4 (C, C-1); 120.5 (C, C-1'); 118.7 (CH, C-α); 118.6 (CH, C-5'); 114.3 (CH, C-3'); 111.9 (2CH, C-3 & C-5); 40.2 ($2CH_3$). HRMS : 290.11583 (M+Na) suitable for molecular formula of $C_{17}H_{17}NO_2$

4-fluoro-2'-hydroxychalcone (7)
UV(EtOH) λ_{maks} (nm), (log ε): 317.9 (4.1); 223.9 (4.0). FTIR (KBr) $\tilde{\nu}$ (cm^{-1}): 3300 (OH phenolic); 3035 (C-H aromatic); 1638 (C=O conjugated), 1580 (C=C conjugated); 1493 (C=C aromatic); 1209 (C-O phenolic). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H (ppm): 12.80 (s, OH); 7.91 (dd, 1H, *J* = 8.1 & 1.7 Hz); 7.88 (d, 1H, *J* = 15.6 Hz); 7.66 (dd, 2H, *J* = 8.7 Hz, $^4J_{H\text{-}F}$ = 5.4 Hz); 7.58 (d, 1H, *J* = 15.6 Hz); 7.51 (td, 1H, *J* = 8.5; 7.2; 1.7 Hz); 7.13 (t, 2H, *J* = 8.7 Hz, $^3J_{H\text{-}F}$ = 8.7 Hz); 7.03 (dd, 1H, *J* = 8.5 & 1.2 Hz); 6.95 (td, 1H, *J* = 8.1; 7.2; 1.2 Hz). ^{13}C-NMR (100.53 MHz, $CDCl_3$) δ_C (ppm): 193.7 (C, C=O); 164.4 (d, $^1J_{C\text{-}F}$ = 252.6 Hz, C-4); 163.7 (C, C-2'); 144.3 (CH, C-β); 136.6 (CH, C-4'); 131.0 (d, $^4J_{C\text{-}F}$ = 3.4 Hz, C-1); 130.8 (d, $^3J_{C\text{-}F}$ = 8.6 Hz, C-2 & C-6); 129.7 (CH-C-6'); 120.1 (C, C-1'); 119.9 (CH, C-α); 119.0 (CH, C-5'); 118.8 (CH, C-3'); 116.4 (d, $^2J_{C\text{-}F}$ = 22.0 Hz, C-3 & C-5). HRMS : 265.06225 (M+Na) suitable for molecular formula of $C_{15}H_{11}FO_2$

4-chloro-2'-hydroxychalcone (8)
UV(EtOH) λ_{maks} (nm), (log ε): 320.0 (4.2); 221.0 (4.2). FTIR (KBr) $\tilde{\nu}$ (cm^{-1}): 3300 (OH phenolic); 3059 (C-H aromatic); 1641 (C=O conjugated); 1578 (C=C conjugated); 1487 (C=C aromatic); 1206 (C-O phenolic). ^{1}H-NMR (400 MHz, $CDCl_3$) δ_H (ppm): 12.76 (s, OH); 7.91 (dd, 1H, *J* = 8.0 & 1.8 Hz); 7.86 (d, 1H, *J* = 15.4 Hz); 7.62 (d, 1H, *J* = 15.4 Hz); 7.59 (d, 2H, *J* = 8.5 Hz); 7.51 (td, 1H, *J* = 8.6; 7.2; 1.8 Hz); 7.41 (d, 2H, *J* = 8.5 Hz); 7.03 (dd, 1H, *J* = 8.6 & 1.3 Hz); 6.95 (td, 1H, *J* = 8.0; 7.2; 1.3 Hz). ^{13}C-NMR (100.53 MHz, $CDCl_3$) δ_C (ppm): 193.6 (C, C=O); 163.7 (C, C-2'); 144.1 (CH, C-β); 137.0 (C, C-1); 136.7 (CH, C-4'); 133.2 (C, C-4); 129.9 (CH, C-6'); 129.7 (2CH, C-2 & C-6); 129.5 (2CH, C-3 & C-5); 120.7 (CH, C-α); 120.0 (C, C-1'); 119.0 (CH, 5'); 118.8 (CH, 3'). HRMS : 281.03307 (M+Na) suitable for molecular formula of $C_{15}H_{11}ClO_2$

Cytotoxic Assay
HeLa cells were cultured in a 96-well plate at 213.4 x 10^4 cell/well density. The cells were then treated with 100 µL of the prepared compounds with various concentrations (1.5625; 3.125; 6.25; 12.5; 25; 50; ~~dan~~ and 100 µg/mL) for 24 hours. MTT (3-[4,5-dimethylthiazol-2-yl]-2,5-diphenyltetrazolium bromide solution (50 mg MTT in 10 mL of PBS) 100 µL was added, followed by incubation in CO_2 incubator for 4 hours. The amount of viable cells was visualized by the formation of purple color due to formation of formazan crystals. The formed formazan that was proportionate to the total of viable cells was calculated using spectrophotometer at 560 nm. The number of viable cells was calculated using following formula

$$\%\ \text{Viable Cells} = \frac{\text{Treatment Absorbance} - \text{Control Medium Absorbance}}{\text{Negative Control Absorbance} - \text{Control Medium Absorbance}}\ \text{x}\ 100\%$$

IC_{50} was obtained after statistical analysis using SPSS program. Doxorubicin was used as a positive control in this assay. The test was conducted in triplicate.

Cell Apoptosis Induction Test Using Flowcytometry Method
The next step was testing the cell apoptosis induction of the most potential prepared compound (compound **5** and **8**) using a flowcytometer. This procedure refered to Roihatul et al.[18]

Computational Docking
The docking experiment was carried out on Toshiba Satellite Pro C640, Intel(R) Core(TM) i3-2330M CPU @ 2.20 GHz, 4.00 GB *memory* (RAM) 32-bit system type, Windows 7 Ultimate Operation System. Docking experiment was performed using AutodockTools and Autodock4. Program ChemDraw Ultra

12.0 was used to draw ligand. Ligand optimation was carried out using Program HyperChem 8.0.8 and UCSF Chimera 1.11.2. Program PyMOL 1.3, UCSF Chimera 1.11.2 and LigPlot+ v.2.1 were used to analyze the *docking* results. The 3D structure of p53 and MDM2 protein was taken from *Protein Data Bank* (PDB) with the access code 1YCR.

RESULTS AND DISCUSSION

Organic Synthesis

The synthesized compounds were obtained according to Claisen-Schmidt condensation as presented in Fig.-1. The IR spectra of compound **1**-**8** displayed a vibration band at 1691-1620 cm^{-1} corresponding to conjugated carbonyl which gave a signal at δ 193.6-194.8 ppm in ^{13}C NMR. ^{1}H NMR spectra of compound **1**-**8** showed a double signal with *J*= 15.4 Hz at 8.22-7.14 ppm for *trans* ethylenic group.

Cytotoxic Assay

To evaluate the cytotoxic activity, synthesized compounds were incubated with cervical cancer cells (HeLa). The result of cytotoxicity assay (IC_{50}) is presented in Table-2.

Table-2: The Result of Cytotoxicity Assay using MTT Method

Compound's Number	Compounds	IC_{50}(μM)
1	2-methoxy-2′- hydroxychalcone	0.052
2	3-methoxy-2′- hydroxychalcone	0,029
3	4-methoxy-2′- hydroxychalcone	0,050
4	2,4-dimethoxy-2′- hydroxychalcone	0,074
5	2,5- dimethoxy-2′- hydroxychalcone	0,015
6	4-N,N-dimethyl-2′- hydroxychalcone	62,667
7	4-fluoro-2′- hydroxychalcone	0,054
8	4-chloro-2′- hydroxychalcone	0,016
9	Doxorubicin	0,002

These results showed that there are two compounds possessing potential IC_{50} that are 2,5-dimethoxy-2′-hydroxychalcone (0.015 μM) and 4-chloro-2'-hydroxychalcone (0.016 μM). All the prepared chalcones exhibited lower activity compared to doxorubicin as positive control.

The apoptosis effect of the two most active prepared chalcones (2,5-dimethoxy-2′-hydroxychalcone and 4-chloro-2'-hydroxychalcone) against HeLa cancer cells line was investigated with a methode of double staining conjugated with Annexin V and Propidium iodide. The result of flow cytometry is presented in Fig.-2 and Table-3 respectively.

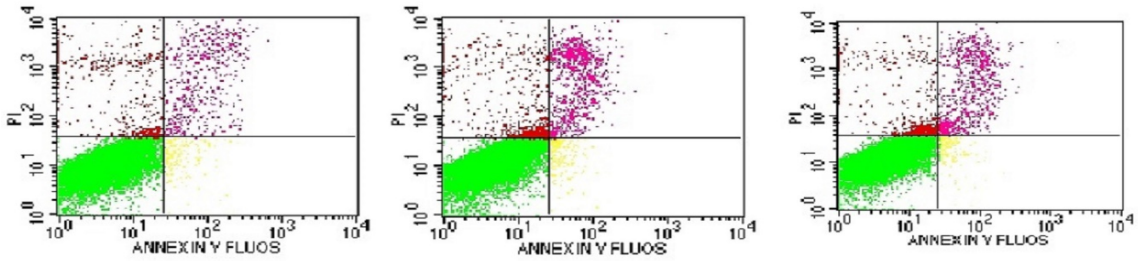


Fig.-2: The Result of Flow Cytometry Test (a) Control (HeLa Cell without Active Compound), (b) HeLa cell + IC_{50} of 4-chloro-2'-hydroxychalcone, (c)HeLa Cell + IC_{50} of 2,5-dimethoxy-2′-hydroxychalcone

From the Fig.-2 and Table-3, it can be seen that the treatment of the tested compound at IC_{50} concentrations on HeLa cells (24-hour incubation) did not provide significant results compared with control. The treatment using 4-chloro-2'-hydroxychalcone and 2,5-dimethoxy-2′-hydroxychalcone caused 5.04% and 4.47% respectively HeLa cells undergo late apoptosis (control 2.75%). The treatment also

caused successively 4.75% and 4.56% of HeLa cells to experience necrosis (control 2.92%). The results listed in Table 3 illustrate that the synthesized chalcone derivatives did not show the potential apoptotis activity although based on MTT test results, two chalcones (2,5-dimethoxy-2′-hydroxychalcone and 4-chloro-2'-hydroxychalcone) showed very potential anticancer activity.

Table-3: The Result of Flow Cytometry Analysis of the Synthesized Compounds (**5** and **8**)

Treatment on HeLa Cell	Cell Population (%)			
	Viable Cells	Early Apoptosis	Late Apoptosis	Necrosis
Control	93.56	0.85	2.75	2.92
IC_{50} 4-chloro-2'-hydroxychalcone (8)	89.48	0.90	5.04	4.75
IC_{50} 2,5-dimethoxy-2′-hydroxychalcone (5)	90.30	0.83	4.47	4.56

The cell cycle inhibition that occurs could be observed by comparing the effects of the treatment with the synthesized compounds and control. The results of observations are listed in the Table-4. Based on the data obtained, it appears that there is no significant difference in results between tested compound and control. Even though the data obtained did not show high activity, it appeared that the inhibition of the HeLa cell cycle began at the G0-G1 phase, followed by the S phase and G2-M phase. 4-chloro-2'-hydroxychalcone (**8**) showed slightly better activity than 2,5-dimethoxy-2′-hydroxychalcone (**5**).

Table-4: Analysis of HeLa Cells Cycle Treated with Synthesized Compounds (5 and 8)

Treatment	Cell Population (%)				
	M_1	G_0-G_1	S	G_2-M	M_5
Control	1.99	57.92	7.99	22.56	10.12
IC_{50} of 4-chloro-2'-hydroxychalcone (8)	2.96	56.46	10.32	20.91	10.29
IC_{50} of 2,5-dimetoxy-2′-hydroxychalcone (5)	2.67	56.48	9.23	20.82	11.52

Docking Molecular

p53 is a tumor suppressor protein. As it is the human genome, protein p53 is a factor of transcription controlling the cellular response of cells to DNA damage through induction of cell-cycle cessation, reparation of DNA, apoptosis, or senescence. The p53 gene is deactivated in numerous human tumors, otherwise in cancer case it occurs an overexpression of MDM2. Therefore the disrupted MDM2-p53 interaction lead to greater levels of p53 and restoration of p53 transcriptional activity.[16]

In the MDM2-p53 complex structure, 2 intermolecular hydrogen bonds were found. One is in the middle of Phe-19 backbone amide of p53 and the Gln-72 side chain of MDM2 at the cleft entrance. Another is among nitrogen indole Trp-23 in p53 with the MDM2 Leu-54 backbone carbonyl, which is deep inside the cleft. The MDM2 cleft is positioned along with 14 preserved amino acids (hydrophobic and aromatic), which create many van der Waals contacts with p53. These 14 amino acids are Met-50, Leu-54, Leu-57, Gly-58, Ile-61, Met-62, Tyr-67, His-73, Val-75, Phe-91, Val-93, His-96, Ile-99, and Tyr-100[19]. Fig.-3 presents the MDM2-p53 interaction.

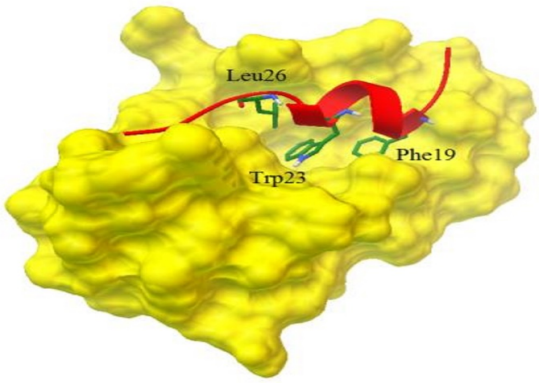
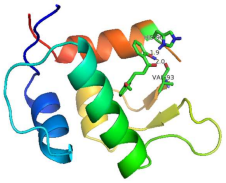
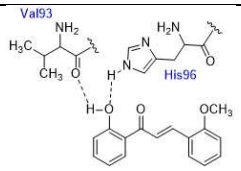
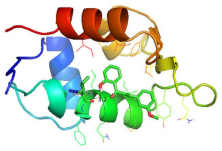
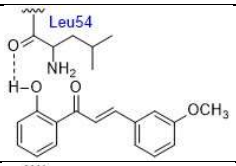
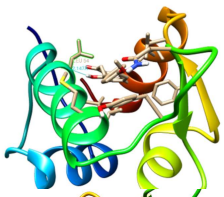
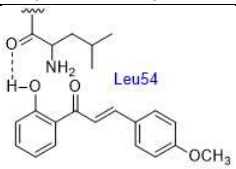
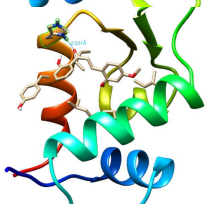
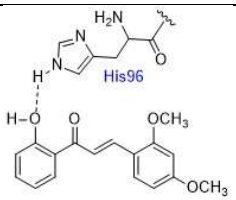
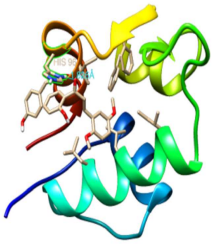
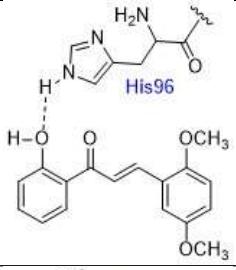
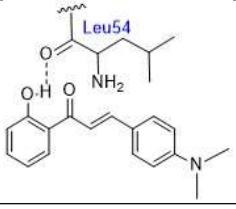
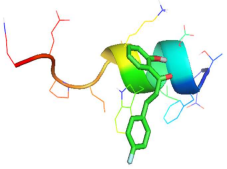
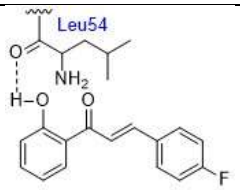
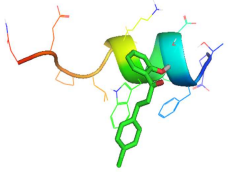
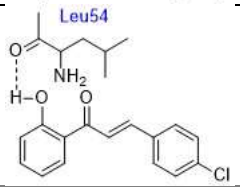


Fig.-3: Complex of MDM2 (Yellow) – p53 (Red)

Docking molecular exhibited the interaction between synthesized compound as ligand and MDM2 protein target as shown in Table-5. This interaction was represented by ΔG and K_i.[20] It can be seen in Table 5 that all chalcone compounds formed interactions with MDM-2. The hydrogen bond formed between chalcone and MDM2 mostly involved Leu-54 and His 96. Val-93 also formed interaction with one chalcone (Compound **1**). Kussie *et al* had stated that two amino acids on MDM 2 which formed hydrogen bond with p53 were Gln-72 and Leu-54.[19] Therefore, the presence of chalcone which could form hydrogen bonds with Leu-54 on MDM2 will disrupt the MDM2-p53 interaction, as showed by compound **2**, **3**, **6**, **7** and **8.** The interaction between 4-chloro-2'-hydroxychalcone (**8**) and MDM2 showed the smallest ΔG and Ki, even though only one hydrogen bond was formed with an amino acid residue (Leu-54).

Table-5: Resume of Docking Results of the Prepared Compounds on MDM2

Compound	Complex of Prepared Chalcones-MDM2			
	ΔG (kcal/ mol)	Inhibition Constant (μM)	Hydrogen Bond	Docking Pose and 2D Visualization
2-methoxy-2′-hydroxy chalcone	-6,27	25,36	His96, Val93	 
3- methoxy - 2′-hydroxychalcone	-6,37	21,26	Leu54	 
4- methoxy - 2'-hydroxychalcone	-6,29	24,61	Leu54	 
2,4-dimethoxy 2'-hydroxychalcone	-6,21	28,03	His96	 
2,5-dimethoxy 2'-hydroxychalcone	-5,99	40,72	His96	 
4-N,N-dimethyl-2'-hydroxychalcone	-5,91	46,49	Leu54	 

4-fluoro-2'-hydroxychalcone	-6,14	31,83	Leu54		
4-chloro-2'-hydroxychalcone	-6,51	16,91	Leu54		

Visualization of molecular docking using Ligplot program also showed that beside hydrogen bond, 4-chloro-2'- hydroxychalcone was also able to build van der Waals interaction with twelve amino acid residues at MDM2, that were Leu-54, Leu-57, Gly-58, Ile-61, Met-62, Tyr-67, Gln-72, Phe-86, Phe-91, Val-93, Ile-99, Ile-103 (Fig.-4).

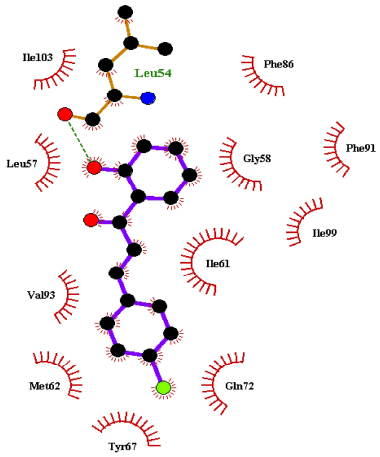


Fig.-4: Vander Waals Interaction between 4-Chloro 2'-hydroxycalkon with MDM2

Among the 12 amino acid residues in the MDM2 structure, there are 9 amino acid residues (hydrophobic and aromatic amino acids) which create many van der Waals contacts with p53. These 9 amino acids are Leu-54, Leu-57, Gly-58, Ile-61, Met-62, Tyr-67, Phe-91, Val-93, Ile-99. If the 9 amino acids form a van der Waals interaction with chalcone, then it can be ascertained that there will be interference with the interaction between MDM2-p53. So chalcone that could also form hydrophobic interactions with MDM2, in addition to hydrogen bonds, it will greatly disrupt in MDM2-p53 interaction.
The result of molecular docking was in accordance with the results of cytotoxicity test revealing that 4-chloro-2'- hydroxychalcone showed the highest activity.

CONCLUSION

Eight 2'hydroxychalcones (**1-8**) derivatives compounds have been synthesized with 4-chloro-2'-hydroxychalcone showing the best results in docking analysis while cytotoxicity test with MTT method exhibited that 2,5-dimethoxy-2'hydroxychalcone and 4-chloro-2'-hydroxychalcone gave very low IC_{50} of 0.15 and 0.16 μM respectively, but both did not show potential apoptosis activity

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Managing Editor, RASĀYAN Journal of Chemistry

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alfinda novi kristanti <alfinda-n-k@fst.unair.ac.id> Thu, Oct 31, 2019 at 3:51 PM
To: "RASĀYAN J. Chem." <rasayanjournal@gmail.com>

Dear Dr. Sanjay K. Sharma, FRSC
Editor of Rasayan Journal of Chemistry

Thank you very much for accepting our manuscript to publish in your journal, Rasayan Journal of Chemistry. Herewith I send you the APC Clearance Slip and the evidence of the payment through the Mandir Bank Indonesia as attachments. Thank you again for your kind attention

Best regards,
Dr. Alfinda Novi Kristanti
Dep. of Chemistry
Faculty of Science and Technology
Universitas Airlangga Indonesia

2 attachments

Mandiri.jpg
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RASĀYAN J. Chem. <rasayanjournal@gmail.com> Fri, Nov 1, 2019 at 10:59 AM
To: alfinda novi kristanti <alfinda-n-k@fst.unair.ac.id>

Acceptance Letter: RJC- 5543/2019

Dear Author,

Congratulations!
Your manuscript has been accepted for the publication in the latest issue of **RASĀYAN Journal of Chemistry,** i.e. **RJC, Vol.13, No.1, 2020.**

Herewith please find attached the **Acceptance Letter and Invoice**for your above-mentioned manuscript.

Also,find **Copyright Transfer Form**and **Letter of Original Work**attached. Please send these duly filled and signed docs as soon as possible.

Looking Forward.

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RASĀYAN_Accounts <rasayan.finance@gmail.com> Wed, Dec 18, 2019 at 8:18 PM
To: alfinda-n-k@fst.unair.ac.id

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Kunal Sharma

Assistant Executive, Accounts
RASĀYAN Journal of Chemistry.

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Assistant Executive, Accounts
RASĀYAN Journal of Chemistry.

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With best regards
Alfinda Novi Kristanti
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RASĀYAN J. Chem. <rasayanjournal@gmail.com> Sat, Dec 21, 2019 at 5:58 PM
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REVISION-2 :RJC-5534/2019

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We have received your mail regarding clearance of printing charges, thanks.

You are requested to revise your above-mentioned manuscript(As per the Template attached)once again in the light of the REVIEWER'S REPORT(S) and PLAGIARISM CHECK REPORT (Attached)and following points given below [Note:Points No. 6, 7, 8 and 9 are very important, without addressing these points, your manuscript will not be considered for publication process. All your revisions must be visible in the Revised Manuscript, therefore you are requested to useRed/Blueink for revisions.]:

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4. Check **Abstract** and **Keywords** once again.
5. References in the text should be cited as super-scripted and at the end of the sentence. Please rectify this mistake also, if there.
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On Sat, Nov 2, 2019 at 9:35 AM alfinda novi kristanti <alfinda-n-k@fst.unair.ac.id> wrote:
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Reviewer's Report, RJC-5534.pdf
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alfinda novi kristanti <alfinda-n-k@fst.unair.ac.id> Fri, Jan 3, 2020 at 2:34 PM
To: "RASĀYAN J. Chem." <rasayanjournal@gmail.com>

Dear Dr. Sanjay K. Sharma, FRSC
Editor, RASĀYAN Journal of Chemistry

Happy New Year 2020

Thank you to give us some suggestions for improving our manuscript. Herewith I send you the Revision-2 version of our manuscript (in word file). I also send you the file of "Answer to Reviewer's Comments" and the file of Plagiarism Check Report (pdf file). Improvements of the manuscript were written in red and green highlighter. I have all explained in the file of "Answer to Reviewer's Comments.

We hope the improvements that have been made, make our manuscript feasible to be published soon in Rasayan Journal of Chemistry. Thank you.

With best regards,
Dr. Alfinda Novi Kristanti

3 attachments

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RASĀYAN J. Chem. <rasayanjournal@gmail.com> Wed, Jan 8, 2020 at 4:57 PM
To: alfinda novi kristanti <alfinda-n-k@fst.unair.ac.id>

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As your manuscript has been accepted for publication in **RJC, Vol.13, No.1, January- March, 2020**, kindly note that this issue is still open and will be open till 30th March 2020.
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Regarding anything else, please feel free to write us back.

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Dear Author,

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Dear Editor of Rasayan J. Chem.

Herewith I send back the galley proof of our manuscript with some corrections completed with **verification text**.

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1. All textual changes were highlighted in red
2. Figure-3 was moved just after the paragraph that it is mentioned
3. I chose single piece on figure 4
4. Table -5 was made vertical

As attachment, I send you the revised manuscript and the Response on Author's Queries. Thank you very much for your attention.

Best regards,
Dr. Alfinda Novi Kristanti

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Your paper has been published Online First in RJC, Vol.13, No.1, January- March, 2020

RASĀYAN J. Chem. <rasayanjournal@gmail.com> Wed, Mar 18, 2020 at 2:17 PM
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