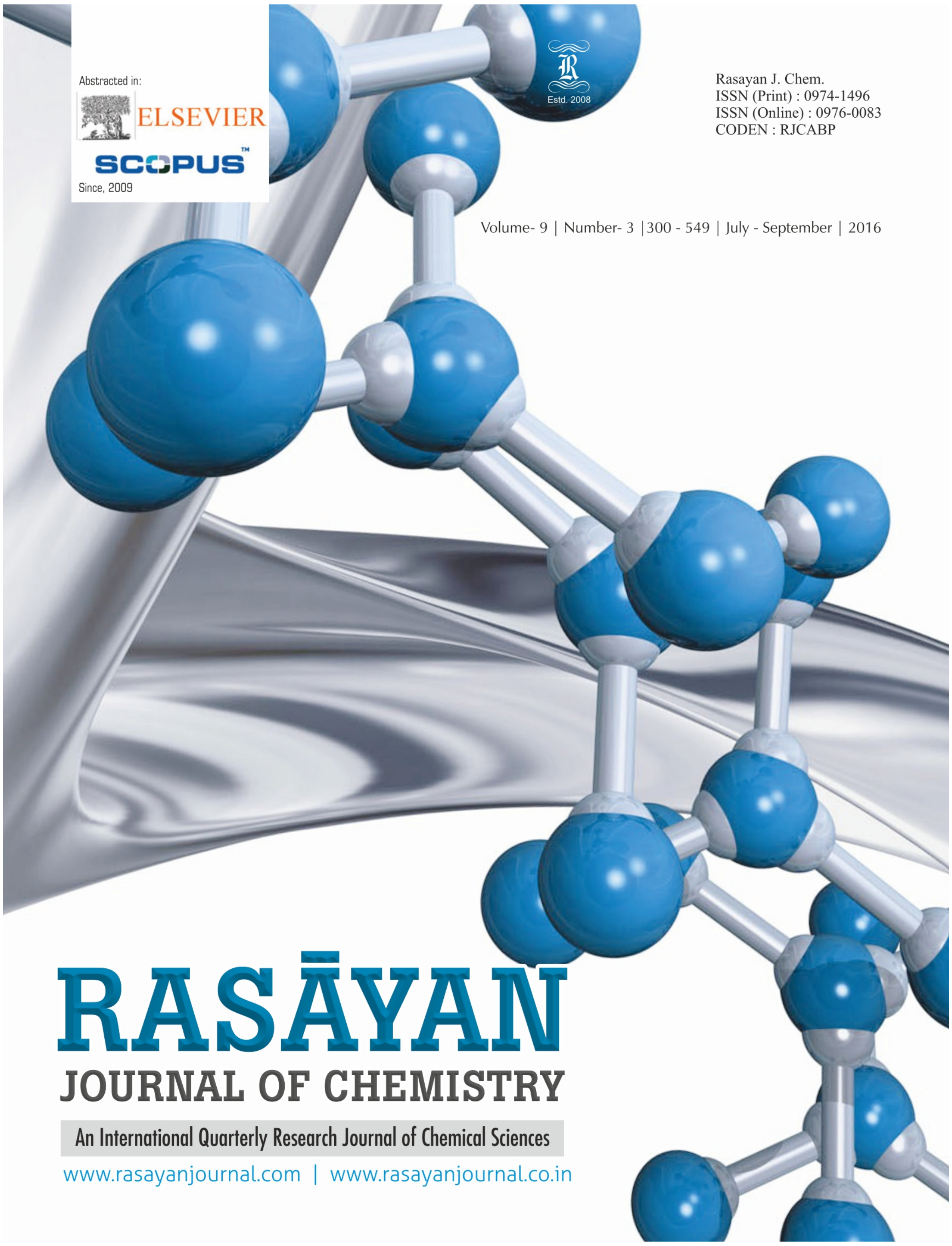
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# SYNTHESIS OF SOME CHALCONE DERIVATIVES, IN VITRO AND IN SILICO TOXICITY EVALUATION

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**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).

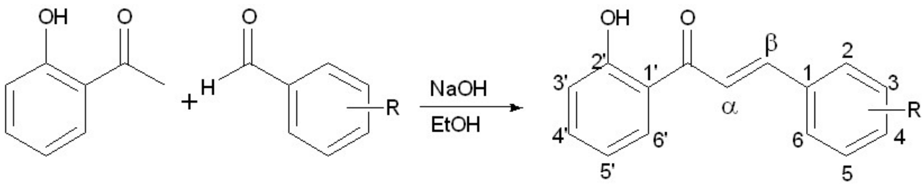


Fig.-1: Synthesis Reaction for Chalcone Derivatives Using Claisen Schmidt Condensation


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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-di$CH_3$) | 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) $\lambda_{max}$ (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, $H_\beta$); 7.92 (1H, dd, *J*=1.7 & 8.1 Hz, H-6′); 7.78 (1H, d, *J*=15.6 Hz, $H_\alpha$); 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) $\lambda_{max}$ (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, $H_\beta$); 7.91 (1H, dd, *J*=1.3 & 8.0 Hz, H-6´); 7.62 (1H, d, *J*=15.5 Hz, $H_\alpha$); 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) $\lambda_{max}$ (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) $\lambda_{max}$ (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, $CDCl_3$) $\delta_H$ (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, $CDCl_3$) $\delta_c$ (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) $\lambda_{max}$ (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, $CDCl_3$) $\delta_H$ (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, $CDCl_3$) $\delta_c$ (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) $\lambda_{maks}$ (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, $CDCl_3$) $\delta_H$ (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, $CDCl_3$) $\delta_c$ (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 (2$CH_3$). HRMS : 290.11583 (M+Na) suitable for molecular formula of $C_{17}H_{17}NO_2$

**4-fluoro-2'-hydroxychalcone (7)**

UV(EtOH) $\lambda_{maks}$ (nm), (log $\varepsilon$): 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, $CDCl_3$) $\delta_H$ (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, $^4J_{H-F}$ = 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, $^3J_{H-F}$ = 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, $CDCl_3$) $\delta_C$ (ppm): 193.7 (C, C=O); 164.4 (d, $^1J_{C-F}$ = 252.6 Hz, C-4); 163.7 (C, C-2'); 144.3 (CH, C-β); 136.6 (CH, C-4'); 131.0 (d, $^4J_{C-F}$ = 3.4 Hz, C-1); 130.8 (d, $^3J_{C-F}$ = 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, $^2J_{C-F}$ = 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) $\lambda_{maks}$ (nm), (log $\varepsilon$): 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, $CDCl_3$) $\delta_H$ (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, $CDCl_3$) $\delta_C$ (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

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

$IC_{50}$ 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

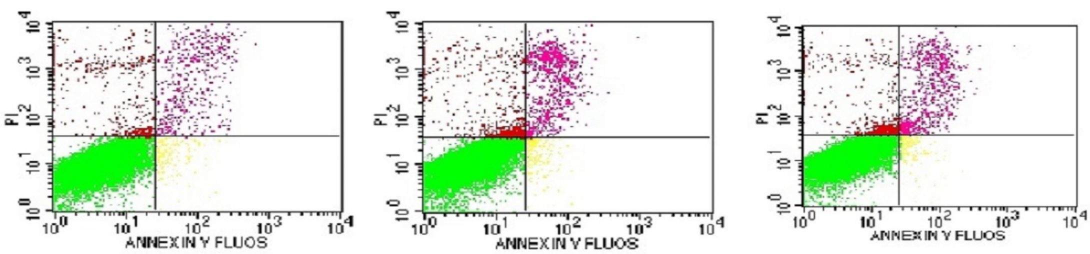
To evaluate the cytotoxic activity, synthesized compounds were incubated with cervical cancer cells (HeLa). The result of cytotoxicity assay ($IC_{50}$) is presented in Table-2.

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.




Control (HeLa cell without active compound) | HeLa cell + $IC_{50}$ of 4-chloro-2'-hydroxychalcone | HeLa cell + $IC_{50}$ of 2,5-dimethoxy-2´-hidroxychalcone

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.

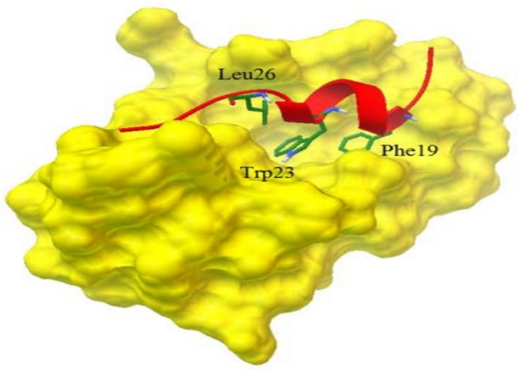
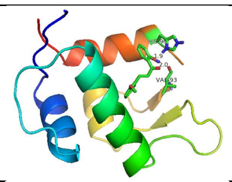
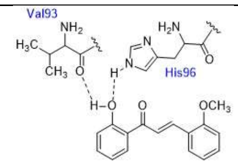
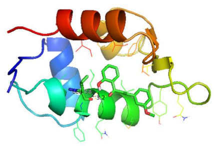
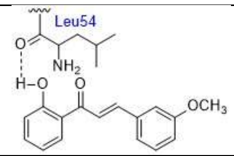
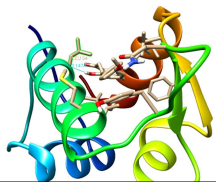
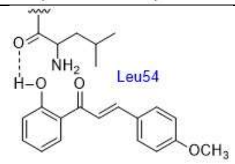
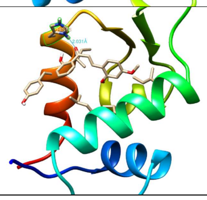
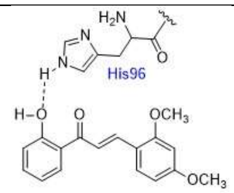
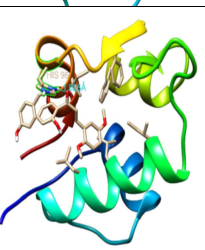
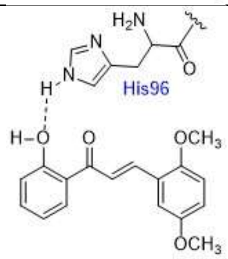
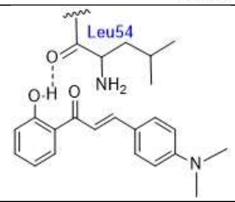
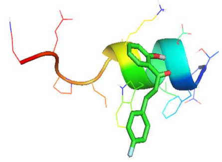
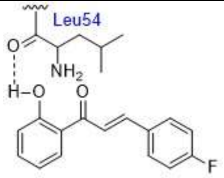
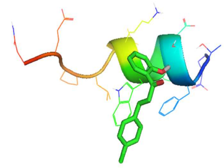
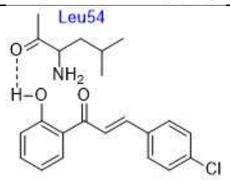



Fig.-3: Complex of MDM2 (Yellow) – p53 (Red)

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).

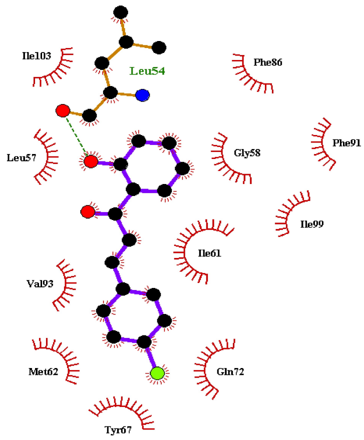



Fig.-4: Vander Waals Interaction between 4-Chloro 2’-hydroxycalkon with MDM2

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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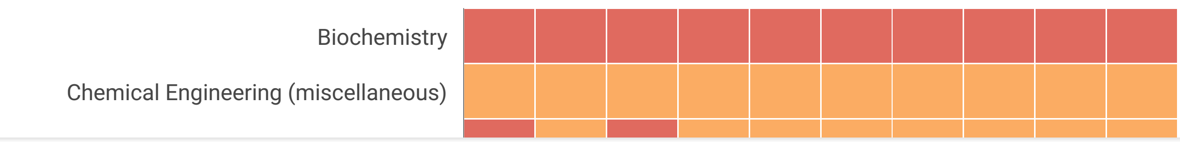


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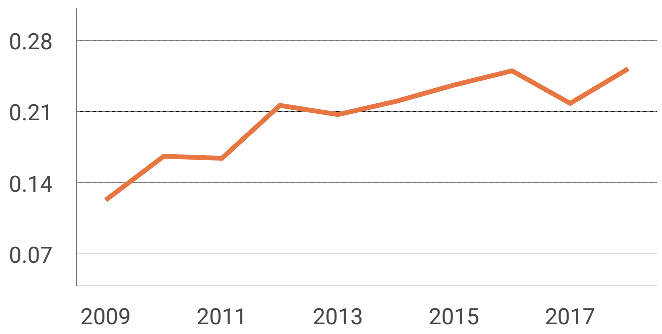


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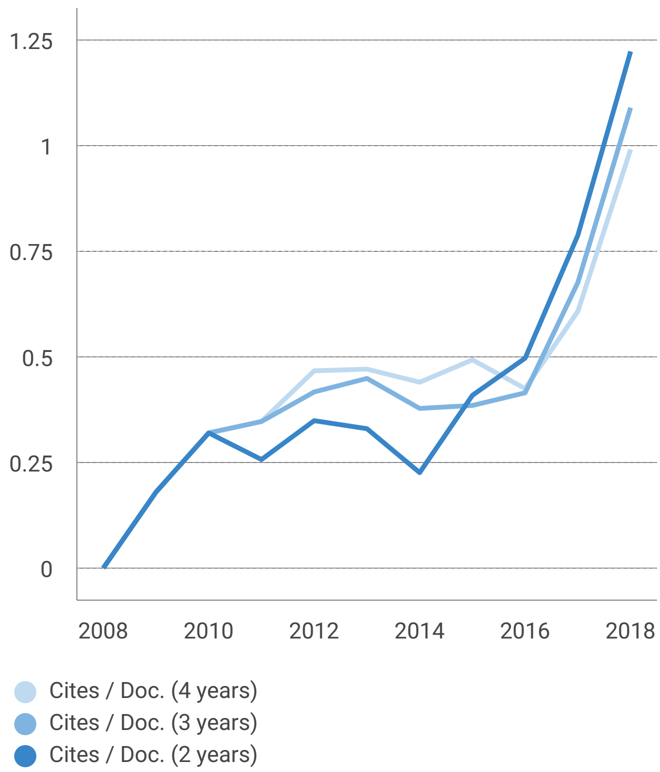


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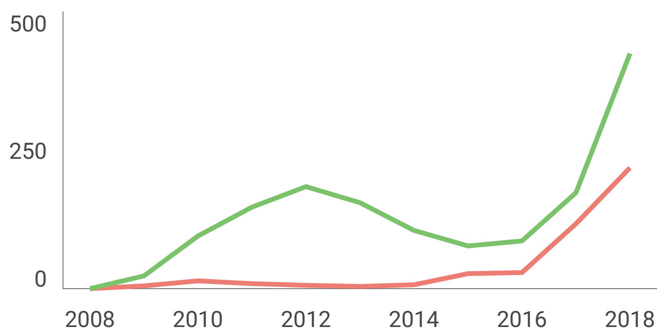


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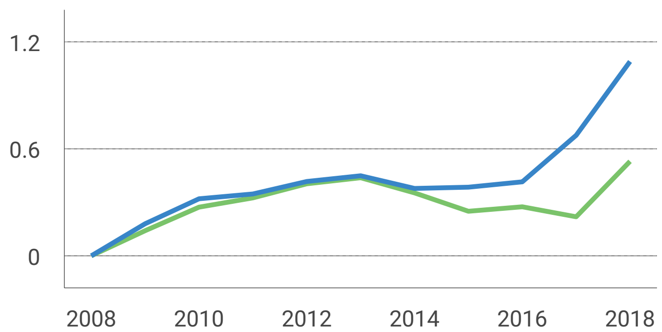


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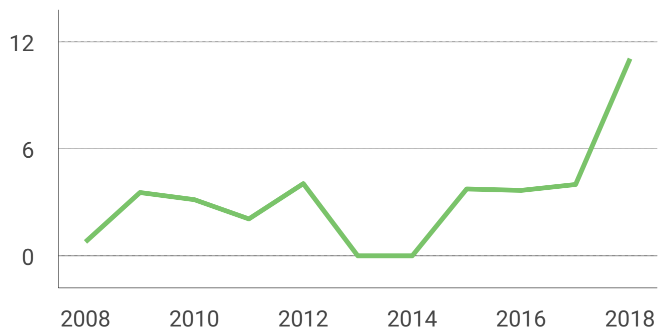


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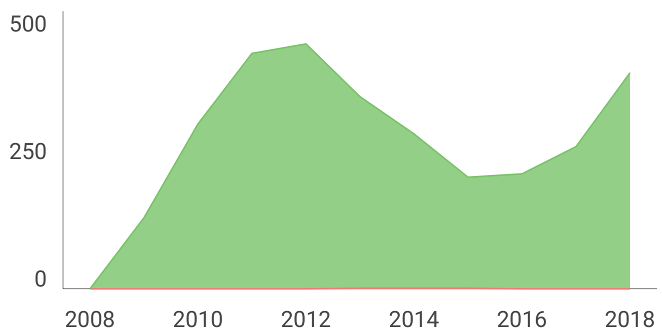


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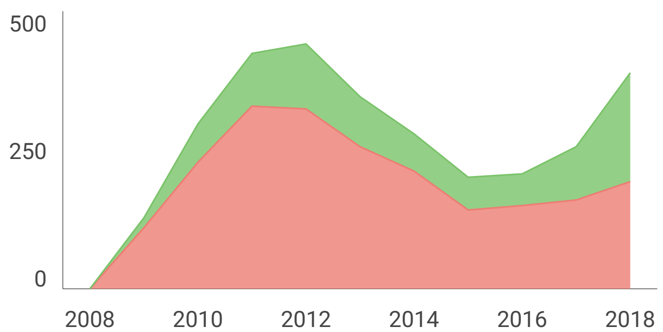


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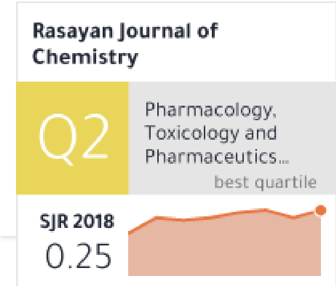


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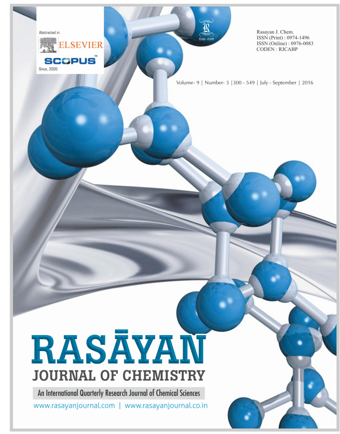


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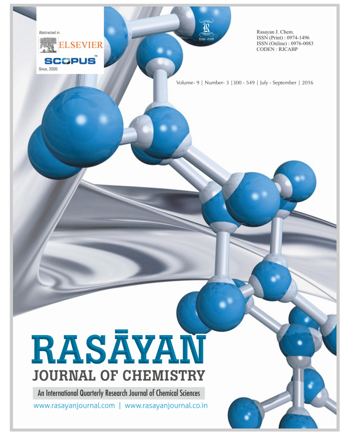


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DETERMINATION OF HEAVY METALS IN PRISTIPOMA FURCATUS AND ACANTHURUS STRIGOSUS FISH SPECIES COLLECTED FROM PULICAT LAKE, CHENNAI

*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

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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

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315570

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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

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

*Shaik. John Saida, A. Manikandan , V.V.S.R.N. Anji Karun Mutha , Muralidharan Kaliyaperumal , Chidananda Swamy Rumalla , Ramulu Yanaka and S. Venkat Rao*

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

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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315579

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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

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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

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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

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315496

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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

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315615

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315492

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315532

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315593

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315497

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315596

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315484

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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

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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

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

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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

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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.

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315539

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315512

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315502

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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.

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315343

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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

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315523

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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

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315551

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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.

**DOI:** http://dx.doi.org/10.31788/RJC.2020.1315197

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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

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

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

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

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

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

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MICROWAVE-ASSISTED SYNTHESIS OF TETRAZOLE BASED BIPHENYLS DERIVATIVES AND THEIR ANTIMICROBIAL ACTIVITY

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

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

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

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

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

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OPTIMIZATION SYNTHESIS FATTY ACID ETHYL ESTER AS BIODIESEL FROM PALM FATTY ACID DISTILLATE USING SO4²?/ TIO2 CATALYST SUPPORTED BY MESOPOROUS SILICA

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

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

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ENHANCEMENT OF ANTIBACTERIAL ACTIVITY OF SUEDE LEATHER THROUGH COATING SILVER NANOPARTICLES SYNTHESIZED USING PIPER BETLE

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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SYNTHESIS OF NOVEL PYRAZOLINES AND THEIR ANTIMICROBIAL ACTIVITY

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

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

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

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

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

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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

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

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

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

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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.

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