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Synthesis, Biological Activity and Molecular Docking Study of Some New Chalcones, 5,6-dihydropyrimidin-2-ol and 5,6-dihydropyrimidin-2-thiol Derivatives Bearing 1,2,3- Triazoline

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RESEARCH ARTICLE

Synthesis, Biological Activity and Molecular Docking Study of Some New Chalcones, 5,6-Dihydropyrimidin-2-Ol and 5,6-Dihydropyrimidin-2-Thiol Derivatives Bearing 1,2,3-Triazoline

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ABSTRACT

Many new chemicals, including chalcones, derivatives of 5,6-dihydropyrimidin-2-ol and 5,6-dihydropyrimidin-2-thiol, are synthesized in this work. The starting materials are substituted acetophenone derivatives involving 1,2,3-triazoline (**1**). Chalcone derivatives (**2a-h**) were obtained by condensing compound (**1**) with some substituted aromatic aldehydes in the presence of 40% potassium hydroxide KOH. The process of producing pyrimidin-2-ol derivatives (**3a–e**) by cyclizing produced chalcone derivatives (**2a–e**) urea in the presence of sodium hydroxide. Equivalent pyrimidin-2-thiol derivatives (4a-d) were produced when chalcone derivatives (**2a-d**) reacted with thiourea in the presence of sodium hydroxide. The target compounds are characterized using ^{1}H-NMR, ^{13}C-NMR, and FT-IR. The findings demonstrate the target compounds' strong biological activity, including their antioxidant and antibacterial properties. The studies on molecular docking.

Keywords: Antibacterial, Antioxidants, Chalcone, Molecular docking, Pyrimidine

Introduction

Heterocyclic compounds are those that have atoms other than carbon in their complicated toroidal component. Sulfur, oxygen, and nitrogen are the most prevalent heterogeneous atoms. These substances are significant since nature contains a number of biologically active natural products.[1] One of the flavonoid familial subcategories, chalcones are flavonoids but open-chain with two aromatic rings linked to an α, β-unsaturated enone.[2] Because chalcones are utilized as intermediates in the synthesis of numerous heterocyclic chemicals, their manufacture is crucial to industry.[3] There are numerous ways to synthesize chalcones. Chalcones were often made by benzaldehyde derivatives acting as electrophiles and acetophenone derivatives acting as a nucleophiles by a Claisen-Schmidt condensation reaction with bases such as NaOH, KOH, and $Ba(OH)_2$.[4] The biological activities of chalcones and their derivatives were observed, such as antibacterial,[5] antiflammatory,[6] antiulcer,[7] antidepression,[8] antioxidant,[9] and anticancer.[10] Pyrimidine is an important six-membered diazaheterocycle, wherein two nitrogen atoms occupy 1 and 3 positions in the ring.[11] Nitrogen-based heterocycles such as pyrimidines constitute a fundamental class of NLO (nonlinear optical allows us to change the color of a light beam, to change its

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shape in space and time, and to create the shortest events ever made by humans) materials because nitrogen atom in pyrimidine plays role of the electron acceptor group in a π-conjugated structure. Furthermore, the lone pair of nitrogen increases its basic character, protonation ability, chelation, and hydrogen bond formation.[12] Pyrimidine nucleobases includes: uracil, thymine and cytosine.[13] The structural diversity and biological importance of pyrimidines have made them attractive targets for synthesis over many years.[14] Condensed heterocyclic compounds with pyrimidine ring are of interest since they include valuable pharmacological substances.[15] Pyrimidine derivatives are found to have a wide range of chemotherapeutic effects including angiogenic, enzyme inhibitory effects and anti-leishmanial activity.[16] Heterocyclic compounds containing nitrogen atoms have a great benefits within the field of drugs and industrial chemistry due to their strong and selective probability to occur hydrogen bonds with protein/enzyme Parts, which are responsible for important biological activities such as antibacterial,[17] anti-proliferative,[18] antitubercular.[19] and antifungal activity.[20] In the present paper, we report the synthesis of some new chalcones, 5,6-dihydropyrimidin-2-ol and 5,6-dihydropyrimidin-2-thiol derivatives bearing 1,2,3-triazoline and investigating their practical and theoretical biological activities.

Materials and methods

Experimental methods

All Chemicals were purchased from BDH, Merck, and Fluka. A recorder called M.P. was used to makes use of an electrothermal (m.P.) device. A Shimadzu FT-IR8400S spectrophotometer in the Chemistry Department, College, University of Kerbala, was used to record the FT-IR spectrum data. The ^{1}H-NMR and ^{13}C-NMR spectra are recorded at 500 MHz in Tehran University's central laboratory, with DMSO-d6 and (TMS) serving as interior standards.

General method for chalcone derivatives synthesis (2a-h)[21]

Benzaldehydes Such as *m*-hydroxy, *p*-hydroxy, *p*-chloro, *p*-bromo, *p*-nitro, *p*-N,N-dimethyl, and 2,4-dimethoxy benzaldehyde (12 mmol, 0.00014 mg) and Substituted acetophenone involving 1,2,3-triazoline (**1**) (12 mmol, 0.0046 mg) were dissolved in ethanol (10 mL), and 40% potassium hydroxide solution (10 mL) was added dropwise while stirring at room temperature over a period of 30 minutes and refluxed for eight to ten hours. The progress of the reaction was monitored by TLC. The solvent was removed on a rotary evaporator under reduced pressure, the residue was poured into ice water, and the product was filtered off and recrystallized from methanol (**2a–h**), as shown in Scheme 1. Physical properties of compounds **(2a–h)** are listed in Table 1.

2-(N-((1-(4-(3-phenylacryloyl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl)benzoic acid (2a)

FT-IR (KBr), ν(cm^{-1}): 3286(N-H and O-H vib. Coupling) 3059(C-H)Ar, 2924 and 2862(C-H aliph) 1708(C=O)acid, 1651(C=O)ketone, 1599(C=C), 1529(N=N), 1336(SO_2)Asym, 1168(SO_2)Sym, 1224(C-O)Asym, 1118(C-O)Sym. ^{1}H-NMR (DMSO-d_6), (δppm): 2.43 (d, 2H, C$\underline{H}_2$ triazoline), 3.67(t, 2H, C$\underline{H}_2$-NH), 4.77–4.86 (m, 1H, C$\underline{H}$ triazoline), 6.76–7.00(m, 2H, CH=C-$\underline{H}$), 7.12–7.99 (m, 14H Ar-H and N$\underline{H}$-CH_2), 12.35 (s, 1H,-O-H). ^{13}C-NMR (δ ppm): 44.91(C$\underline{H}_2$-NH), 54.39(C$\underline{H}_2$triazoline), 75.05(C$\underline{H}$-N), 119.03(O=C-C$\underline{=}$C), 124–145 (C$\underline{\text{-}}$Ar), 147.78(C=C$\underline{}$), 163.92 (O=C$\underline{}$-O-H), 195, 45(C$\underline{}$=O).

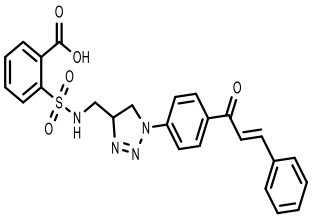
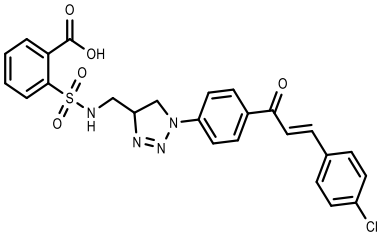
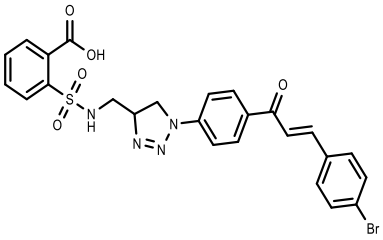
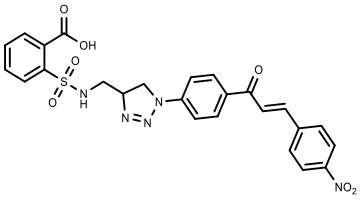
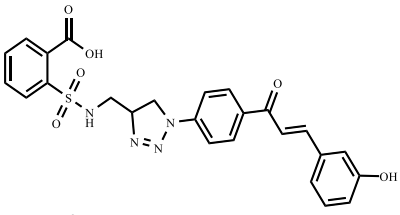
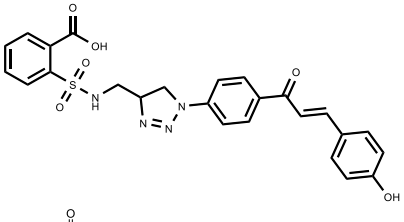
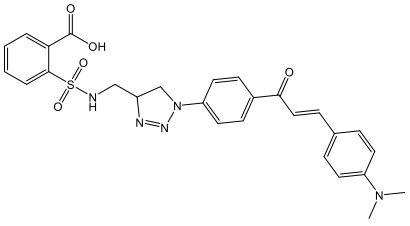
2-(N-((1-(4-(3-(4-chlorophenyl)acryloyl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl) benzoic acid (2b)

FT-IR (KBr), ν(cm^{-1}): 3375(O-H), 3302(N-H), 3061(C-H)Ar, 2928 and 2858(C-H aliph), 1689(C=O)acid, 1633(C=O)ketone, 1599(C=C), 1529(N=N), 1327(SO_2)Asym, 1170(SO_2)Sym, 1230(C-O)Asym, 1120(C-O)sym.

(Z)-2-(N-((1-(4-(3-(4-bromophenyl)acryloyl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl) benzoic acid (2c)

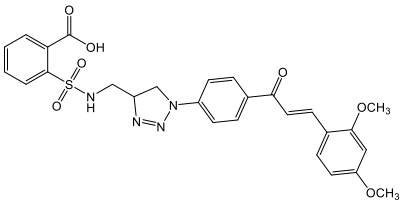
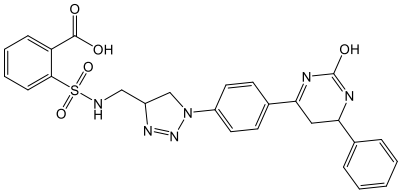
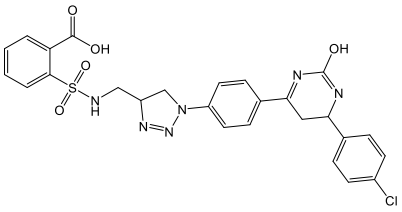
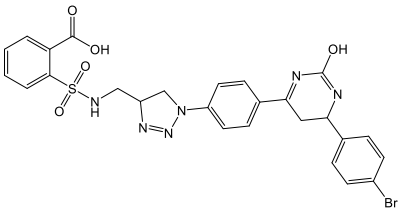
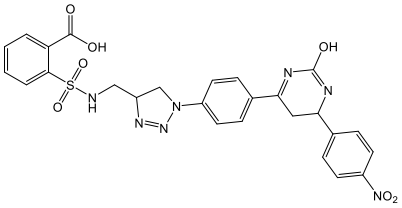
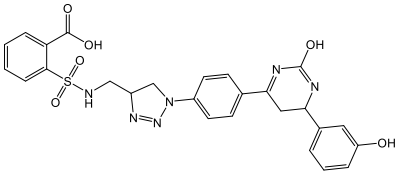
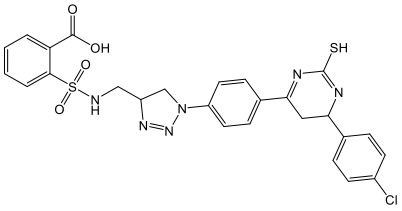
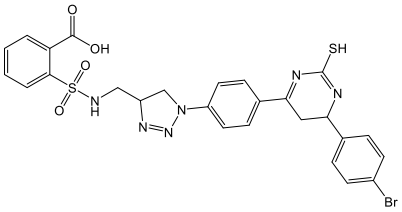
FT-IR (KBr), ν(cm^{-1}): 3373(O-H), 3271(N-H), 3088(C-H)Ar, 2926 and 2858(C-H aliph) 1681(C=O)acid, 1637(C=O)ketone, 1593(C=C), 1529(N=N), 1325(SO_2)Asym, 1168(SO_2)Sym, 1236(C-O), 1120(C-O)Sym. ^{1}H-NMR(DMSO-d_6): 2.50 (d, 2H, C$\underline{H}_2$ triazoline), 3.47(t, 2H, C$\underline{H}_2$-NH), 4.29–4.34 (m, 1H, C$\underline{H}$ triazoline), 6.31–6.70(m, 2H, C$\underline{H}$=C-$\underline{H}$), 7.76–8.08 (m, 13H Ar-H and N$\underline{H}$-CH_2), 12.69 (s,1H,-O-H). ^{13}C-NMR (δ ppm): 45.19(C$\underline{H}_2$ -NH), 55.85(C$\underline{H}_2$ triazoline), 73.99(C$\underline{H}$-N), 119.09(O=C-C$\underline{=}$C), 121.08–145.05 (C$\underline{}$-Ar), 151.42(C=C$\underline{}$), 176.14 (O=C$\underline{}$-O-H), 197, 13(C$\underline{}$=O).

Table 1. Physical properties of compounds (2a-h), (3a-e) and (4a-d).

No.	Chemical structure	Chemical formula	M.W. g/mol	M.P. °C	Yield %	Color
2a		$C_{25}H_{22}N_4O_5S$	490.53	108–111	87	Brown
2b		$C_{25}H_{21}ClN_4O_5S$	524.98	112–113	77	Deep Brown
2c		$C_{25}H_{21}BrN_4O_5S$	569.43	116–117	80	Brown
2d		$C_{25}H_{21}N_5O_7S$	535.53	125–127	73	Brown
2e		$C_{25}H_{22}N_4O_6S$	506.53	118–120	68	Pale Brown
2f		$C_{25}H_{22}N_4O_6S$	506.53	105–106	76	Pale Brown
2g		$C_{27}H_{27}N_5O_5S$	533.60	122–126	82	Pale Green

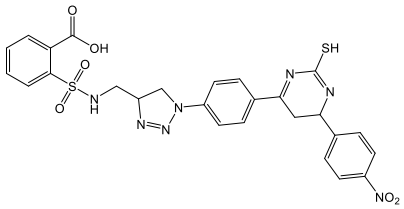
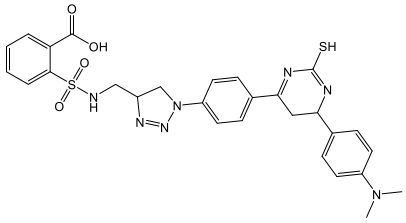
(Continued)

Table 1. Continued.

No.	Chemical structure	Chemical formula	M.W. g/mol	M.P. °C	Yield %	Color
2h		$C_{27}H_{26}N_4O_7S$	550.59	128–129	72	Redish Brown
3a		$C_{26}H_{24}N_6O_5S$	532.58	172–174	54	red
3b		$C_{26}H_{23}ClN_6O_5S$	567.02	176–178	65	Deep Red
3c		$C_{26}H_{23}BrN_6O_5S$	611.47	184–186	56	Pale Brown
3d		$C_{26}H_{23}N_7O_7S$	577.57	196–198	73	Pale Brown
3e		$C_{26}H_{24}N_6O_6S$	548.57	191–193	61	Green
4a		$C_{26}H_{23}ClN_6O_4S_2$	583.08	203–204	70	Green
4b		$C_{26}H_{23}BrN_6O_4S_2$	627.53	211–212	59	Brown

(Continued)

Table 1. Continued.

No.	Chemical structure	Chemical formula	M.W. g/mol	M.P. °C	Yield %	Color
4c		$C_{26}H_{23}N_7O_6S_2$	593.63	219–220	76	Pale yellow
4d		$C_{28}H_{29}N_7O_4S_2$	591.71	193–194	75	Pale Brown

2-(N-((1-(4-(3-(4-nitrophenyl)acryloyl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl) benzoic acid (2d)

FTIR(KBr), $\nu(cm^{-1})$: 3452(O-H), 3377(N-H), 3076 (C-H)Ar, 2929 and 2870(C-H aliph), 1714(C=O) acid, 1651(C=O)ketone, 1593(C=C), 1516(N=N), 1450(NO_2)Assyn, 1338(NO_2)Sym, 1390(SO_2)Asym, 1168(SO_2)Sym, 1220(C-O)Asym, 1136(C-O) Sym.

2-(N-((1-(4-(3-(3-hydroxyphenyl)acryloyl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl) benzoic acid (2e)

FT-IR (KBr), $\nu(cm^{-1})$: 3365(O-H), 3267(N-H), 3064(C-H)Ar, 2926 and 2872(C-H aliph), 1718(C=O)acid, 1651(C=O)ketone, 1595(C=C), 1529(N=N), 1332(SO_2)Asym, 1165(SO_2)Sym, 1273(C-O)Asym, 1122(C-O)Sym.

2-(N-((1-(4-(3-(4-hydroxyphenyl)acryloyl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl) benzoic acid (2f)

FT-IR (KBr), $\nu(cm^{-1})$: 3363(O-H), 3217(N-H) 3068(C-H)Ar, 2928 and 2858(C-H aliph), 1718(C=O)acid, 1651(C=O)ketone, 1595(C=C), 1514(N=N), 1332(SO_2)Asym, 1165(SO_2)Sym, 1222(C-O)Asym, 1064(C-O)Sym.

2-(N-((1-(4-(3-(4-(dimethylamino)phenyl)acryloyl) phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl) sulfamoyl)benzoic acid (2g)

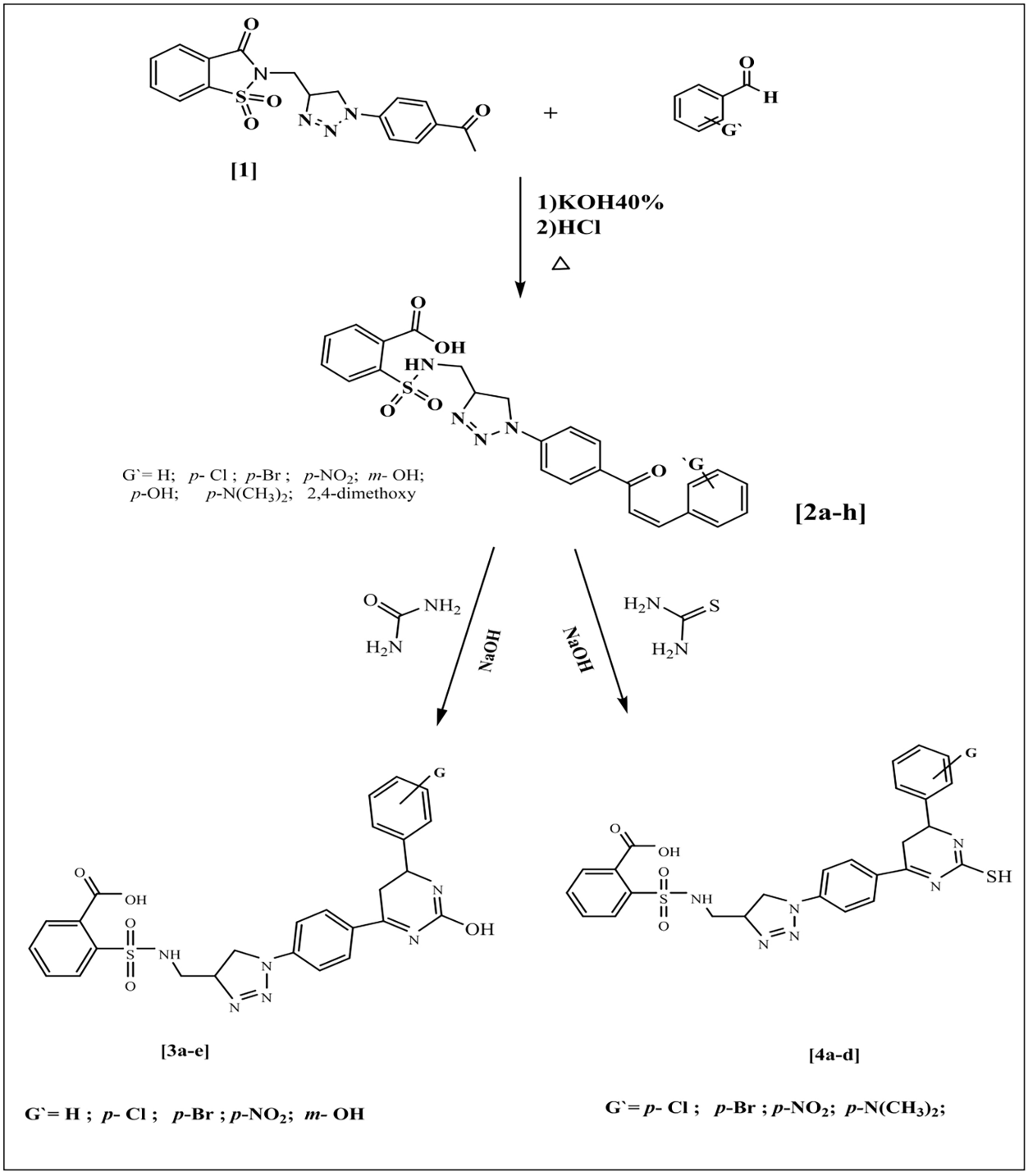
FT-IR (KBr), $\nu(cm^{-1})$: 3392(O-H), 3286(N-H), 3036(C-H)Ar, 2922 and 2858(C-H aliph), 1724(C=O)acid, 1649(C=O)ketone, 1595(C=C), 1525(N=N), 1336(SO_2)Asym, 1180(SO_2)Sym, 1230(C-O)Asym, 1124(C-O)Sym. ^{1}H-NMR: 2.67 (d, 2H, C$\underline{H}_2$ triazoline), 3.03(s, 6H, CH_3), 3.50(t, 2H, C$\underline{H}_2$-NH), 4.91–4.95 (m, 1H, C$\underline{H}$ triazoline), 5.74–5.86(m, 2H, C$\underline{H}$=C-$\underline{H}$), 6.10–7.90 (m, 13H Ar-H and N$\underline{H}$-CH_2), 12.76 (s,1H,-O-H). ^{13}C-NMR (δ ppm): 30.01($\underline{C}H_3$), 42.72($\underline{C}H_2$-NH), 52.69($\underline{C}H_2$ triazoline), 71.51($\underline{C}$H-N), 112.06(O=C-$\underline{C}$=C), 119.09–136.71($\underline{C}$-Ar), 153.56(C=$\underline{C}$), 176.92 (O=$\underline{C}$-O-H), 196,48($\underline{C}$=O).

2-(N-((1-(4-(3-(2,4-dimethoxyphenyl)acryloyl) phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl) sulfamoyl)benzoic acid (2h)

FT-IR (KBr), $\nu(cm^{-1})$: 3433(O-H), 3371(N-H), 3066(C-H)Ar, 2937 and 2847(C-H aliph), 1674(C=O)acid, 1649(C=O)ketone, 1600(C=C), 1510(N=N), 1301(SO_2)Asym, 1165(SO_2)Sym, 1213(C-O)Asym, 1114(C-O)Sym.

General method for 5,6-dihydropyrimidin-2-ol derivatives synthesis of (3a-e)[22]

A mixture of chalcone (**2a-h**) (0.01 mol), urea (0.01 mol, 0.6 g) was dissolved in ethanol (10 mL). To this, 40% aqueous potassium hydroxide solution (10 mL) was added slowly with constant stirring. The reaction mixture was allowed to reflux on water bath for 8 hours. TLC was monitored to check the completion of reaction. After completion of reaction, the reaction mixture was cooled to room temperature and then poured into ice cold water and neutralized by adding dilute HCl. The obtained precipitate (**3a-e**), as shown in Scheme 1, was filtered, washed with water and dried. The product was recrystallized from ethanol. Physical properties of compounds **(3a-e)** are listed in Table 1.



Scheme 1. Route synthesized compounds (2a-h), (3a-e) and (4a-d).

2-(N-((1-(4-(2-oxo-6-phenyl-1,2,5,6-tetrahydropyrimidin-4-yl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl)benzoic acid (3a)

FT-IR (KBr), ν(cm^{-1}): 3389(O-H), 3271(NH), 3095(C-H)Ar, 2949 and 2883(C-H aliph), 1716(C=O)acid, 1653(C=N) pyrimidine, 1606(C=C), 1533(N=N), 1315(SO_2)Asym, 1180(SO_2)Sym. ^{1}H-NMR: 2.49 (d, 2H, C$\underline{H}_2$ pyrimidine), 3.25(d, 2H, C$\underline{H}_2$-NH), 3.74 (d, 2H, C$\underline{H}_2$ triazoline), 4.28(t, 1H, C$\underline{H}$ pyrimidine), 4.68–4.74 (m, 1H, C$\underline{H}$ triazoline), 6.54–8.32 (m, 14H Ar-H and

NH-CH_2), 10.59 (s,1H,-O-H), 12.45(s,1H,O=C-O-H) carboxyl. ^{13}C-NMR (δ ppm): 39.26(CH_2-NH), 44.44(CH_2 pyrimidine), 52.11(CH_2 triazoline), 55.08(CH pyrimidine), 76.35(CH triazoline), 110.03–152.52(C-Ar), 165.24(C=N pyrimidine), 173, 50(O=C-O-H).

2-(N-((1-(4-(6-(4-chlorophenyl)-2-oxo-1,2,5,6-tetrahydropyrimidin-4-yl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl)benzoic acid (3b)

FT-IR (KBr), ν(cm^{-1}): 3373(O-H), 3296(NH), 3063(C-H)Ar, 2926 and 2860(C-H aliph),1687(C=O)acid, 1653(C=N) 1595(C=C), 1529(N=N), 1329(SO_2)Asym, 1180(SO_2)Sym, 819(C-Cl).

2-(N-((1-(4-(6-(4-bromophenyl)-2-oxo-1,2,5,6-tetrahydropyrimidin-4-yl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl)benzoic acid (3c)

FT-IR (KBr), ν(cm^{-1}): 3373(O-H), 3327(NH), 3028(C-H)Ar, 2920 and 2862(C-H aliph), 1691(C=O)acid, 1649(C=N), 1591(C=C), 1514(N=N), 1323(SO_2)Asym, 1170(SO_2)Sym, 758(C-Br).

2-(N-((1-(4-(6-(4-nitrophenyl)-2-oxo-1,2,5,6-tetrahydropyrimidin-4-yl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl)benzoic acid (3d)

FT-IR (KBr), ν(cm^{-1}): 3373(O-H), 3227(N-H), 3066(C-H)Ar, 2926 and 2860(C-H aliph), 1708(C=O)acid, 1631(C=N)pyrimidine,1593(C=C), 1516(N=N and Asym NO_2 vib. Coupling), 1327(SO_2 and NO_2 sym vib. Coupling), 1168(SO_2) Sym.

2-(N-((1-(4-(6-(3-hydroxyphenyl)-2-oxo-1,2,5,6-tetrahydropyrimidin-4-yl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl)benzoic acid (3e)

FT-IR (KBr), ν(cm^{-1}): 3381(O-H), 3236(N-H), 3066(C-H)Ar, 2924 and 2858(C-H aliph), 1674(C=O)acid, 1647(C=N)pyrimidine, 1593(C=C), 1518(N=N), 1317(SO_2)Asym, 1165(SO_2)Sym. ^{1}H-NMR: 2.53 (d, 2H, CH_2 pyrimidine), 3.25(d, 2H, CH_2-NH), 3.29 (d, 2H, CH_2 triazoline), 4.50(t, 1H, CH pyrimidine), 4.71–4.77 (m, 1H, CH triazoline), 6.54–8.32 (m, 13H Ar-H and NH-CH_2), 11.31 (d,2H,-O-H), 12.75(s,1H,O=C-O-H) carboxyl. ^{13}C-NMR (δ ppm): 34.47(CH_2-NH), 44.07(CH_2 pyrimidine), 51.35(CH_2 triazoline), 55.08(CH pyrimidine), 81.10(CH triazoline), 116.52–151.85(C-Ar), 165.61(C=N pyrimidine), 174, 16(O=C-O-H).

General method for 5,6-dihydropyrimidin-2-thiol derivatives synthesis of (4a-d)[22]

A mixture of chalcone (**2b**, **2c**, **2d**, and **2g**) (0.01 mol), thiourea (0.01 mol, 0.6 g) were dissolved in ethanol (10 mL). To this, 40% aqueous potassium hydroxide solution (10 mL) was added slowly with constant stirring. The reaction mixture was allowed to reflux on water bath for 8 h. TLC was monitored to check the completion of reaction. After completion of reaction, the reaction mixture was cooled to room temperature and then poured into ice cold water and neutralized by adding dilute HCl. The precipitate (**4a–d**) as shown in Scheme 1. obtained was filtered, washed with water and dried. The product was recrystallized from ethanol. Physical properties of compounds **(4a-d)** are listed in Table 1.

2-(N-((1-(4-(6-(4-chlorophenyl)-2-thioxo-1,2,5,6-tetrahydropyrimidin-4-yl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl)benzoic acid (4a)

FT-IR (KBr), ν(cm^{-1}): 3483(O-H), 3285(N-H) 3061(C-H)Ar, 2926 and 2848(C-H aliph), 2569(S-H), 1687(C=O)acid, 1653(C=N) pyrimidine, 1593(C=C), 1519(N=N), 1321(SO_2)Asym, 1168(SO_2)Sym, 1242(C=S)Asym, 823 ν(C-Cl).

2-(N-((1-(4-(6-(4-bromophenyl)-2-thioxo-1,2,5,6-tetrahydropyrimidin-4-yl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl)benzoic acid (4b)

FT-IR (KBr), ν(cm^{-1}): 3369(O-H), 3255(N-H), 3063(C-H)Ar, 2924 and 2858(C-H aliph), 2569(S-H), 1681(C=O acid and C=N pyrimidine vib. Overlap), 1593(C=C), 1527(N=N), 1325(SO_2)Asym, 1168(SO_2)Sym, 758 ν(C-Br), 1274 (C=S).

2-(N-((1-(4-(6-(4-nitrophenyl)-2-thioxo-1,2,5,6-tetrahydropyrimidin-4-yl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl)benzoic acid (4c)

FT-IR (KBr), ν(cm^{-1}): 3458(O-H), 3379(N-H), 3070(C-H)Ar, 2926 and 2850(C-H aliph), 2534(S-H), 1693(C=O)acid, 1654(C=N)pyrimidine, 1595(C=C), 1518(N=N and NO_2 vib. coupling), 1290(SO_2)Asym, 1166(SO_2)Sym, 1253(C=S). ^{1}H-NMR: 2.04(s, 1H,

SH), 2.48(d, 2H, CH_2 pyrimidine), 3.04 (d, 2H, CH_2 triazoline), 3.77(d, 2H, CH_2-NH), 4.38(t, 1H, CH pyrimidine), 4.61–4.69 (m, 1H, CH triazoline), 6.54–8.18 (m, 13H Ar-H and NH-CH_2), 12.09(s,1H,O=C-O-H). ^{13}C-NMR (δ ppm): 31.71(CH_2-NH), 43.76(CH_2 pyrimidine), 52.32(CH_2 triazoline), 64.37(CH pyrimidine), 84.60(CH triazoline), 120.05–146.34(C-Ar), 156.68(C=N pyrimidine), 165, 91(O=C-O-H), 174.54 (C=S).

2-(N-((1-(4-(6-(4-(dimethylamino)phenyl)-2-thioxo-1,2,5,6-tetrahydropyrimidin-4-yl)phenyl)-4,5-dihydro-1H-1,2,3-triazol-4-yl)methyl)sulfamoyl)benzoic acid (4d)

FT-IR (KBr), ν(cm^{-1}): 3356(O-H),3255(N-H), 3061(C-H)Ar, 2912 and 2808(C-H aliph), 2602(S-H), 1670(C=O)acid, 1651 (C=N) pyrimidine, 1595(C=C), 1521(N=N), 1338(SO_2)Asym, 1165(SO_2)Sym, 1230(C=S). ^{1}H-NMR: 2.06(s, 1H, SH), 2.48(d, 2H, CH_2 pyrimidine), 3.02(s, 6H, CH_3), 3.27 (d, 2H, CH_2 triazoline), 3.53(d, 2H, CH_2-NH), 4.31(t, 1H, CH pyrimidine), 4.64–4.72 (m, 1H, CH triazoline), 6.54–8.04 (m, 13H Ar-H and NH-CH_2), 13.53(s,1H,O=C-O-H).

Results and discussion

Substituted acetophenone involved 1, 2, 3-triazoline (**1**). By using N-allyl saccharin[23] to cyclize p-acetyl azido benzene, compound (**1**) was created as a starting material. The synthesis of chalcone derivatives involved the condensation of several benzaldehydes, in the presence of potassium hydroxide 40%. The new bands arise at the range (1651 to 1633) and (1600 to1593) cm^{-1} are because of the (C=O) and (C=C), correspondingly. On the other hand, 5.74 to 7.00 (m, 2H, CH=C–H) and 12.35 to12.76 (s, 1H,–O–H) were found using ^{1}H- and ^{13}C-NMR. and 163.92–176.92 (O=C-O-H), 147.78–153.56 (C=C), and 112.06–119.03 (O=C-C=C). The reaction cyclization of chalcones with urea and thiourea correspondingly, in the presence of aqueous potassium hydroxide solutions,[22] afforded the corresponding 5,6-dihydropyrimidin-2-ol. The results showed the disappearance of ν(C=O) acetophenone group at (1651 to 1633) cm^{-1}. And the appearance of new bands is attributed to the ν(C=N) at (1683 to 1647) cm^{-1}. The results of ^{1}H-NMR and ^{13}C-NMR indicated the 3.74–3.29 (d, 2H, CH_2 pyrimidin-2-ol), 4.28–4.50 (t, 1H, CH pyrimidin-2-ol), 10.59–11.31(s,1H,OH), and 44.44–44.07 (CH_2 pyrimidine), 55.08 (CH 5,6-dihydropyrimidin-2-ol), (151.85 COH5,6-dihydropyrimidin-2-ol), 165.42–165.61(C=N 5,6-dihydropyrimidin-2-ol)and appeared 3.27–3.04 (d, 2H, CH_2 pyrimidin-2-thiol), 4.31–4.38 (t, 1H, CH 5, 6-dihydropyrimidin-2-thiol), and 43.76(CH_2 5, 6-dihydropyrimidin-2-ol), 64.37(5, 6-dihydropyrimidin-2-ol), 156.68(C=N 5,6-dihydropyrimidin-2-ol) and 174.54 (C=S). Scheme 1. Shows the route synthesized compounds (2a-h), (3a-e) and (4a-d).

Table 2. Biological activity of some prepared compounds and the control drug.

Comp.	*S. aureus* (Gram-positive)	*E. coli* (Gram-negative)
2d	-	19
2e	-	18
2g	-	17
3a	13	12
4c	21	18
4d	12	19
Ceftriaxone	12	16
Control	-	-

[Control]: mL at 100μg; dimethylsulfoxide is the solvent.
(-) No inhibition; (12–16) moderate; and (17–20) high inhibition Zone.

Biological activity

The disk diffusion method[24] was followed in the execution of the test. One strain of *S. aureus*, a Gram-positive bacterium, and one strain of *E. coli*, a Gram-negative bacterium, were used to evaluate the produced compounds. Petri dishes and prepared agar were autoclaved for 15 minutes at 121 degrees Celsius to sterilize them. The examined microorganisms' broth culture was uniformly injected into the agar plates. Appropriately spaced 6 mm diameter holes were created in the solidified medium, and 100μl of the produced compounds 1 milligram of the chemical diluted in 1 milliliter of DMSO solvent were placed inside. For 24 hours, these plates were incubated at 37 degrees Celsius. We looked at the inhibitory zones that the different chemicals produced on the bacterium. The results indicated that the newly synthesized derivatives (compounds **2d**, **2e**, **2g**, **4c** and **4d**) showed enhanced activity against Gram-negative bacteria when compared with that of the control drug (Ceftriaxone), while compound **4c** showed enhanced activity against Gram-positive bacteria when compared with that of the control drug (Ceftriaxone) because contain electron with drawing group (NO_2) which increase biological activity[25–27] illustrated in the Table 2.

Electrochemical oxidation effect

Measurement of the electrochemical index, evaluation of antioxidant capacity, and exploration of antioxidant substances are all highly promising applications of electrochemical methods. The instruments, which are based on potentiostatic analysis and either cyclic or differential pulse voltammetry, can be flow-through or stationary. The techniques are well-known for their applicability to food control and for tracking antioxidant capacity levels in various biological matrices and samples. Several researchers have looked into the use of electrochemical techniques that uses to the investigations clinical and botanical patterns in order to determine their antioxidant qualities. [28] As seen in Table 1, some of the new derivatives in this

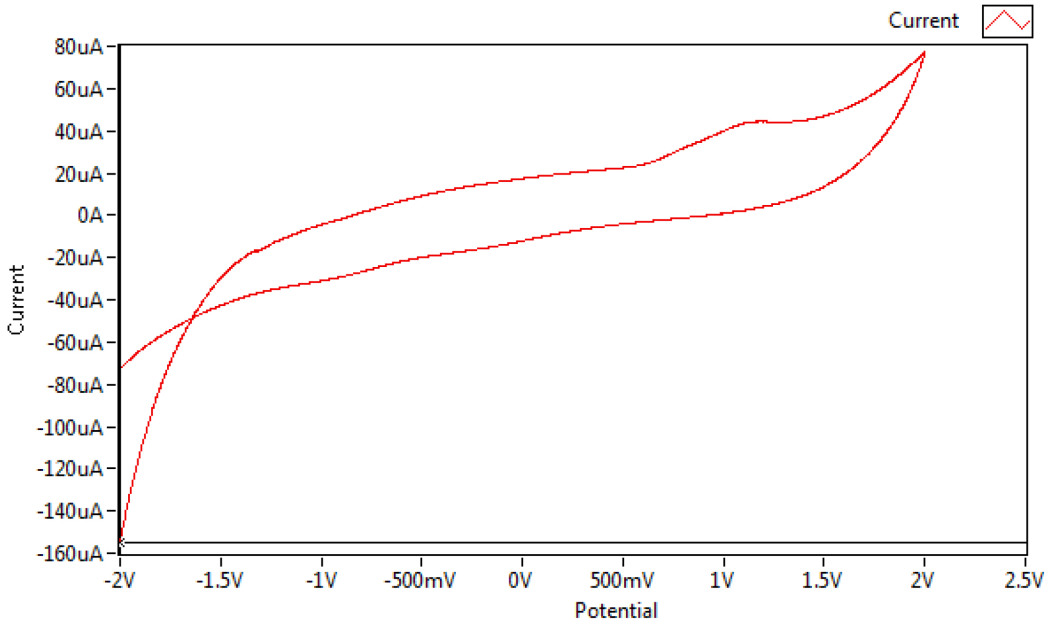


Fig. 1. Shows a decrease the peak of current in the cyclic voltammogram at (+1) v of chemical [2d] at 1000 μ/L con. within the blood serum medium via GCE/CNT and Silver/Silver chloride as reference electrodes.

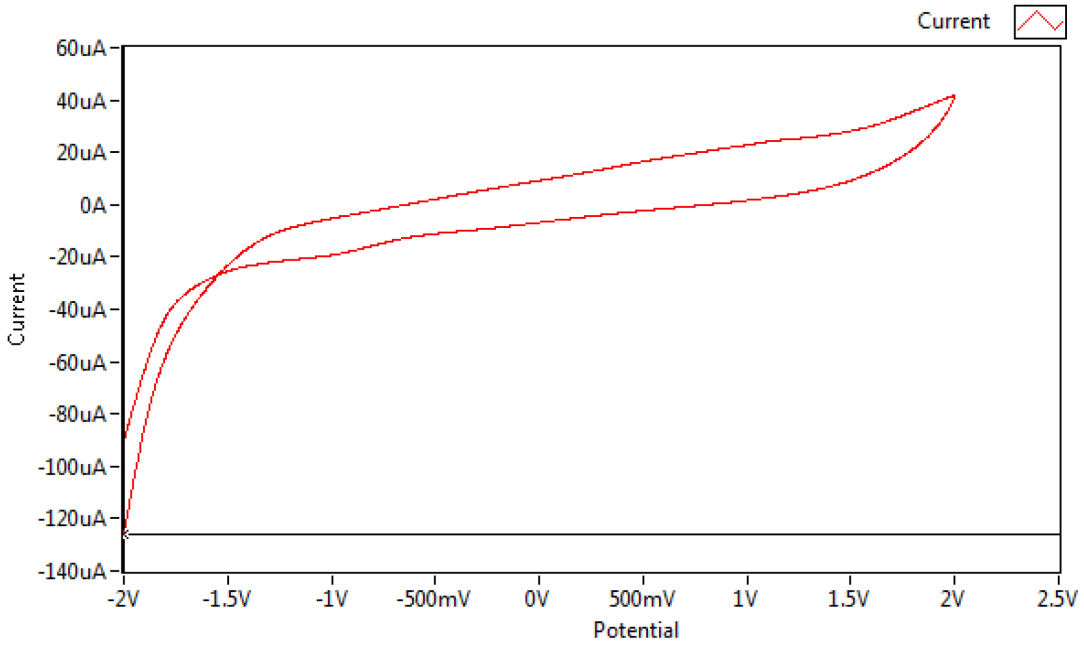


Fig. 2. The CV of chemical [4b] at 1000 μ/L conc. Within the blood serum medium, with an oxidation current peak at (+1.2) v, using GCE/CNT and Silver/Silver chloride as reference electrodes.

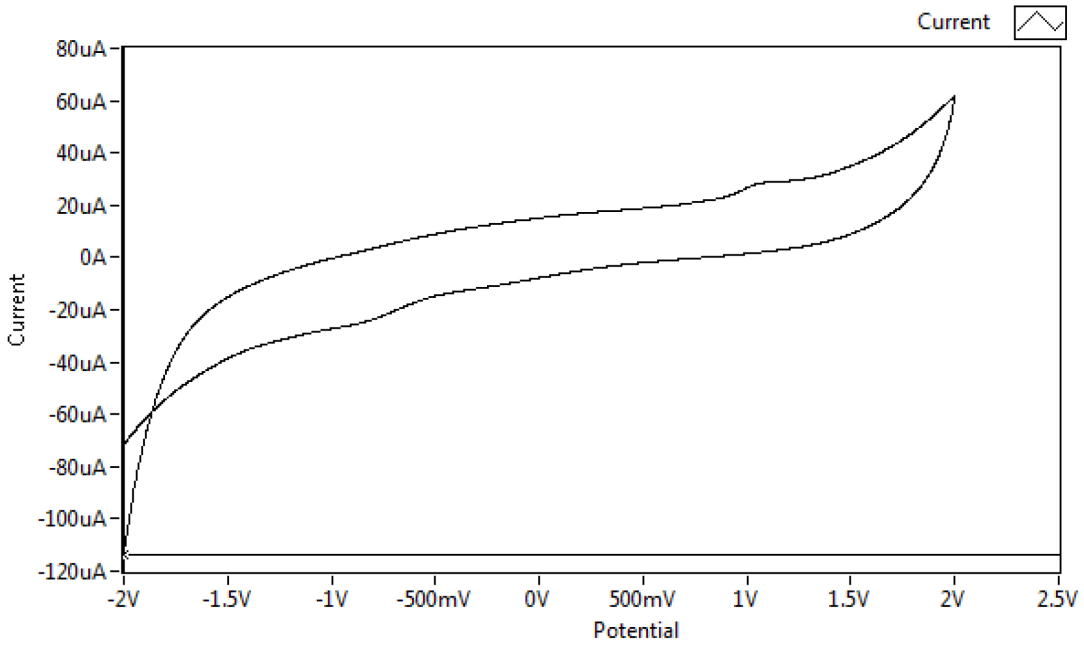


Fig. 3. CV of chemical [2g] in blood serum medium at 1000 μ/L concentration, with Ag/AgCl and GCE/CNT serving as reference electrodes. revealed two peaks for the current rate of oxidation at (-0.2) and (+1.2) volts.

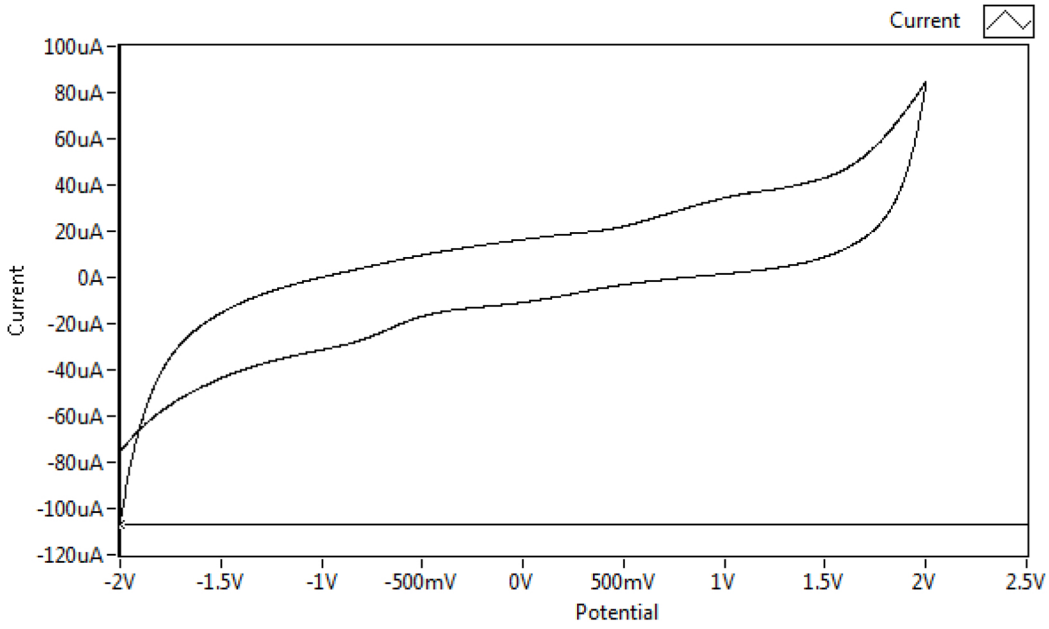


Fig. 4. CV of chemical [3b] in blood serum medium at 1000 μ/L concentration, with Ag/AgCl and GCE/CNT serving as reference electrodes.

investigation [**2d**, **2e**, **2g**, **4c**, and **4d**] possess strong antimicrobial properties. While some of them had a modest degree and were good antioxidants than the others.

2g > 4d > 3b > 4b > 3d > 2d

The results are arranged in terms of their effectiveness as antioxidant from high antioxidant to low antioxidant respectively. The results showed that compounds (**2g)** that having donating group (N,N-dimethyl) in para position and (**4d)** having donating group (2,4-dimethoxy) are a good antioxidant with medical uses because they contain one oxidation beak, compounds (**3b)** and (**4b)** are actual average against oxidation stress because they have two oxidation peaks, while compounds (**3d)** and (**2d)** that having electron withdrawn in position para (*p*-nitro)

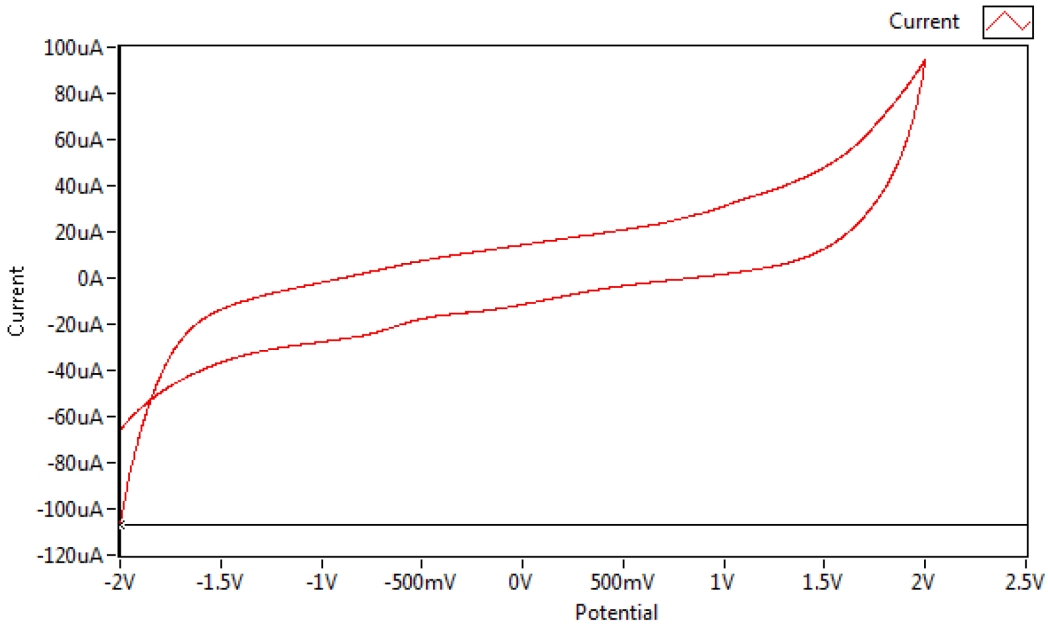


Fig. 5. GCE/CNT and Ag/AgCl as reference electrodes, CV of chemical [3d] at 1000 μ/L conc. Within the blood serum medium.

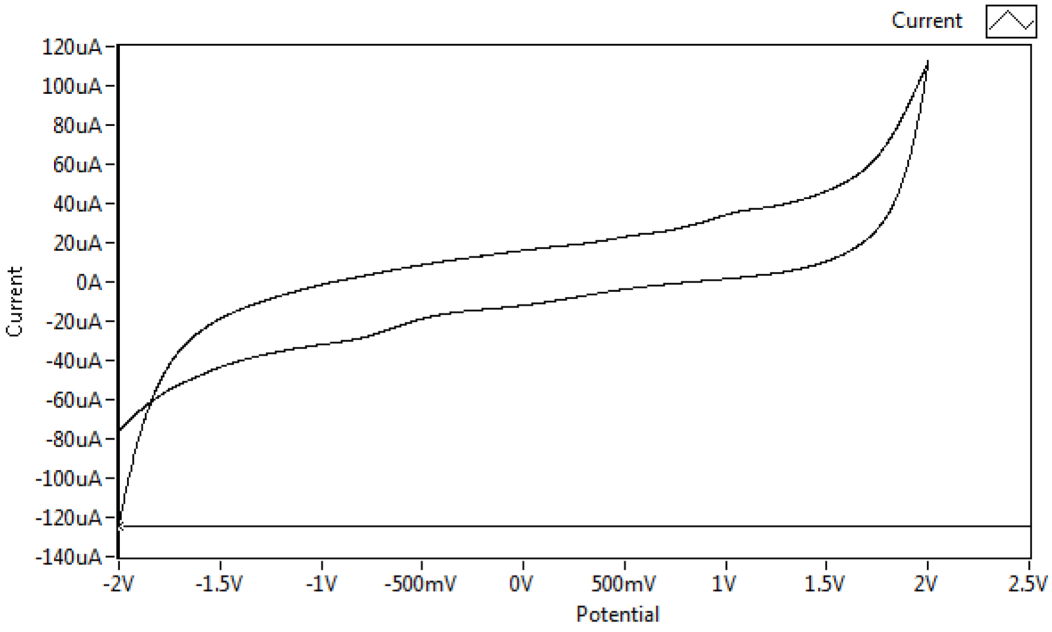


Fig. 6. GCE/CNT and Silver/Silver chloride as reference electrodes, CV of chemical [4d] at 1000 μ/L conc. Within the blood serum medium.

are highly toxic and are not recommended to be used as an antioxidant in the therapeutic processes because there are four oxidation peaks as shown in Figs. 1 to 6.

Molecular docking studies

The molecular docking studies were performed using PyRx and Biovia Discovery Studio 2021 client for the current studies, the target X- ray structure of *E. coli* as receptor (PDB ID: 6ul7) was taken from protein data bank(PDB) website (https://www.rcsb.org/). The ligand and the protein were converted to the PDBQT format using PyRx, the water molecules and the hate atom were removed. The docking were carried out by using Biovia Discovery Studio 2021 client software and we found specific and non-specific interaction through the linked. The binding energy,

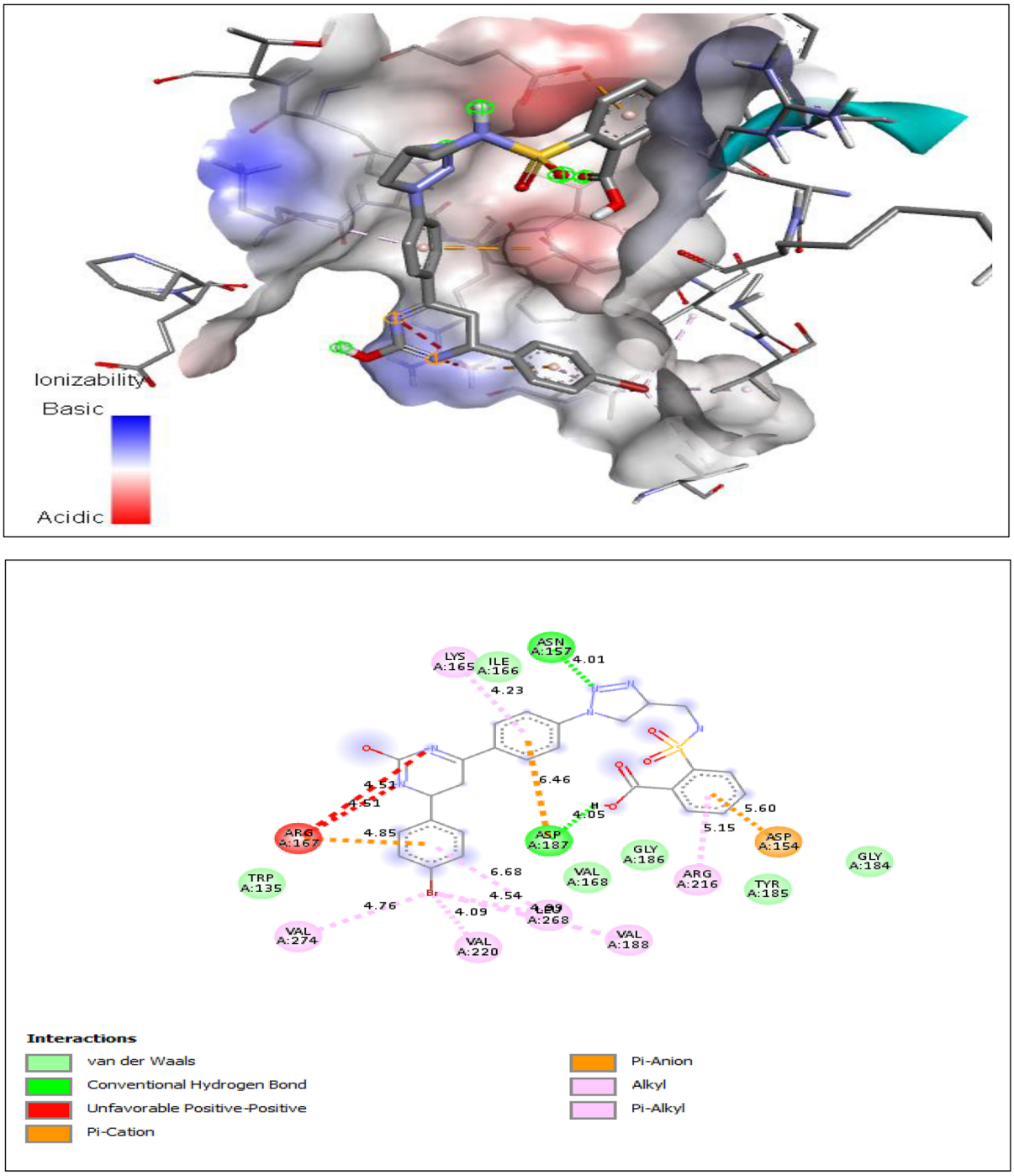


Fig. 7. The binding interaction of receptor (PDB ID: 6ul7) with the ligand (3c) with 2D and 3D shape.

bond length and type of interaction between ligand and protein were measured.[29–32] Tables 3 and 5 show the estimated free energy in (kcal/mol) for the prepared compounds with targets proteins. Tables 4 and 6 show docking scores estimated binding energy (kcal/mol), Bonds length (Å) and interaction types with target *E. coli* as receptor (PDB ID: 6ul7).[33]

All seventeen prepared compounds were studied for their molecular docking using the (PyRx and Biovia Discovery Studio 2021 client) program against one type of target, *E. coli*. The results showed that the prepared derivatives **3c** and **4b** give a higher activity than the other derivatives. Figs. 7 and 8 show the 2D and 3D of ligands **3c** and **4b** with receptor (PDB ID: 6uI7).

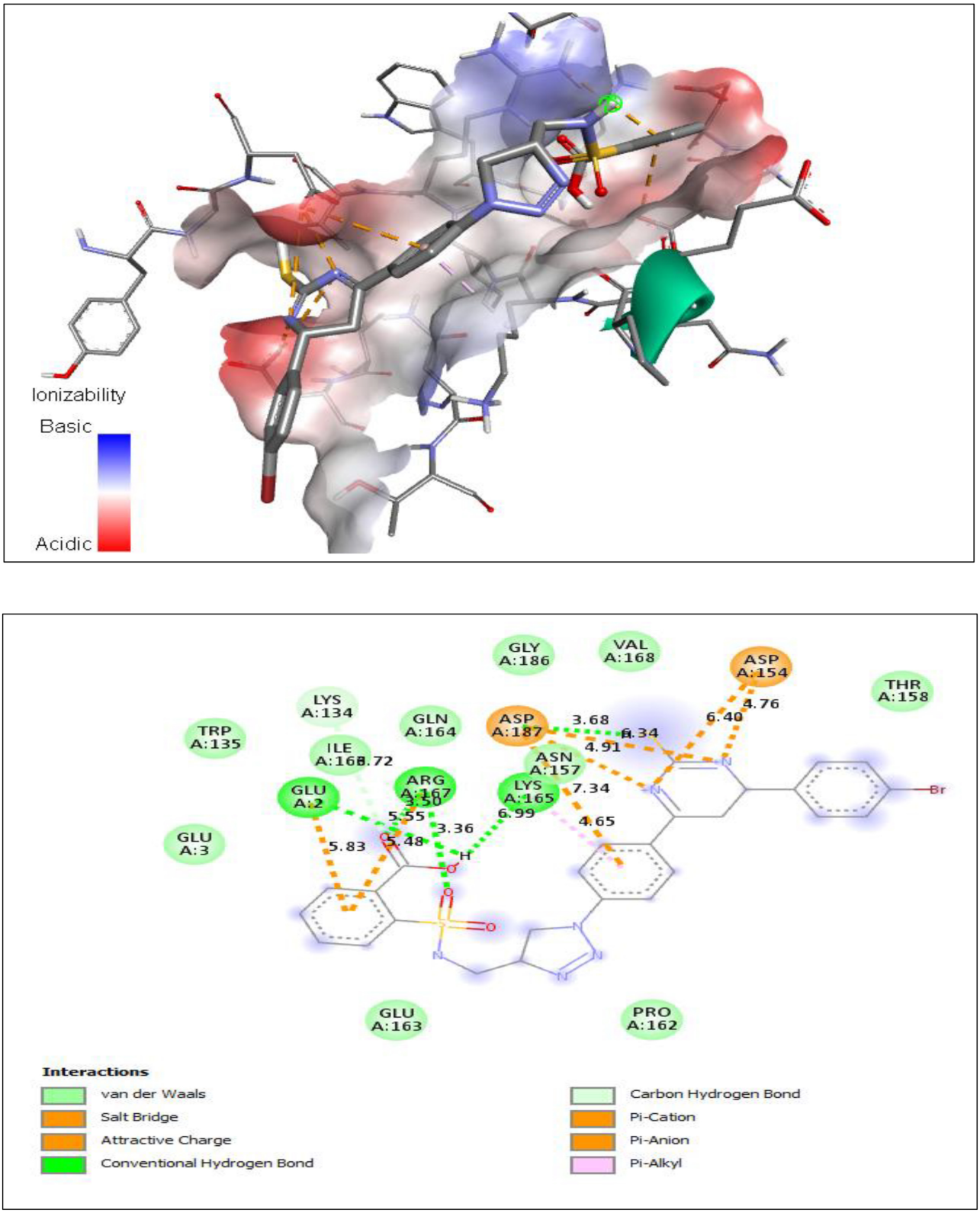


Fig. 8. The binding interaction of receptor (PDB ID: 6ul7) with the ligand (4b) with 2D and 3D shape.

Table 3. Compounds (3a-e) docking scores with the receptor (PDB ID: 6ul7).

Comp.	Estimated energy (kcal/mol)
3a	–8.4
3b	–7.9
3c	–8.8
3d	–8.5
3e	–8.5

Table 4. Compound 3c bond length and interaction type with receptor.

Length of Bond (Å)	Interaction type
4.01	Conventional hydrogen bond
4.05	Conventional hydrogen bond
5.60	Pi-Cation
4.85	Pi-Cation
6.46	Pi-Cation
4.23	Pi-Alkyl
5.15	Pi-Alkyl
4.09	Pi-Alkyl
4.74	Pi-Alkyl
4.54	Pi-Alkyl
6.68	Pi-Alkyl
4.59	Pi-Alkyl
4.61	Unfavourable Positive - positive
4.51	Unfavourable Positive - positive

Table 5. Compounds (4a-d) docking scores with the receptor (PDB ID: 6ul7).

Comp.	Estimated energy (kcal/mol)
4a	–8.3
4b	–8.8
4c	–8.3
4d	–6.7

Table 6. Compound 4b bond length and interaction type with receptor.

Length of Bond (Å)	Interaction type
6.99	Conventional hydrogen bond
3.36	Conventional hydrogen bond
5.48	Conventional hydrogen bond
5.55	Conventional hydrogen bond
3.68	Conventional hydrogen bond
6.72	Van der waals
4.65	Pi-Alkyl
5.83	Pi-Cation
5.55	Pi-Cation
7.34	Pi-Cation
4.91	Pi-Cation
6.34	Pi-Cation
6.40	Pi-Cation
4.76	Pi-Cation

Conclusion

The following series of (compounds **3a-e**) and (**4a-d**) produced derivatives were utilized to use Pyrex - virtual Screening Toll and BIOVIO Discovery Studio to dock to the putative binding site of *E. coli*. They all demonstrated encouraging binding affinities, which may indicate a robust binding association. Compounds **2f**, **3c**, and **4b** showed the highest potential binding affinity among them. In comparison to Gram-positive bacteria, the synthetic chalcone, pyrimidin-2-ol, and pyrimidin-2-thiol seemed to have a greater effect on *E. coli* bacteria. Compounds **3a** and **4c** of Pyrimidin-2-ol were shown to have greater activity versus *S. aureus* than Ceftriaxone, while the derivatives **2d**, **2e**, **2g**, **4c**, and **4d** were discovered to have superior activity against Gram-negative bacteria than Ceftriaxone. Compound **2d** showed reduction activity whereas the other prepared selected compounds demonstrated antioxidant activity.

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Authors' declaration

- Conflicts of Interest: None.
- We hereby confirm that all the figures and tables in the manuscript are ours. Furthermore, figures and images, that are not ours, have been included with the necessary permission for re-publication, which is attached to the manuscript.
- No animal studies are present in the manuscript.
- No human studies are present in the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at University of Baghdad.

Authors' contribution statement

All the chemical aspects including compounds synthesis, characterization and antioxidant activity measurements were performed by H. R. A. and A. W. N. The molecular docking study including docking procedure and 2D and 3D visualization were done by H. R. A.

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تحضير و دراسة الفعالية البيولوجية والالتحام الجزيئي لبعض الجالكونات الجديدة ومشتقات 5,6-ثنائي هايدرو بيريميدين-2-أول و5,6-ثنائي هايدرو بيريميدين-2-ثايول الحاملة 1،2،3-تريازولين

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المستخلص

في هذا العمل تم تحضير انوع مختلفة من المركبات الجديدة مثل الجالكونات، بريميدين-2-اول و بريميدين-2-ثايول الحاوية على حلقة 1,2,3-ترايازولين. حيث تم استخدام المركب (1) كبادئ حيث تم تكثيفه مع مجموعة من الالديهايدات الاروماتية وهي البنزلديهايد، بارا-كلورو بنزلديهايد، بارا-برومو بنزلديهايد، بارا-نايترو بنزلديهايد، ميتا-نايترو بنزلديهايد، بارا-N,N-ثنائي مثيل بزلديهايد و 2,4-ثنائي ميثوكسي بنزلديهايد بوجود قاعدة KOH%40 لتعطي مشتقات الجالكونات (a-h2). وتم تفاعل بعض الجالكونات (a-e2) مع اليوريا بوجود هيدروكسيد الصوديوم لتعطي مشتقات بريميدين-2-اول (a-e3). وأيضا تم تفاعل بعض الجالكونات (a-d2) مع الثايوريا بوجود قاعدة هيدروكسيد البوتاسيوم للحصول على مشتقات بريميدين-2-ثايول (4a-d). تم تشخيص المركبات المحضرة طيفيا بواسطة تقنيات (الاشعة تحت الحمراء وطيف الرنين النووي المغناطيسي للبروتون والكاربون). أظهرت المركبات المحضرة فعالية بيولوجية جيدة كمضادات للبكتيريا ومضادات للأكسدة. وقد أظهرت دراسات الالتحام الجزيئي بواسطة برنامج (PyRx و Discovery studio 2021 client) باستخدام البروتين 6uI7 مع المركبات المحضرة الجديدة مواقع التحام جيدة وقد أظهرت النتائج الحالية ان المركبات المحضرة تمتلك فعالية بيولوجية افضل مع البكتيريا السالبة لصبغة كرام (Escherichia Coli).

الكلمات المفتاحية: مضادات البكتيريا، مضادات الأكسدة، جالكون، الالتحام الجزيئي، بيريميدين.