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Molecular docking of neohesperidin dihydrochalcone with the main components of SARS-CoV-2

Qassim Hassan Aubais Aljelehawy

Department of Chemistry, College of Education, University of Al-Qadisiyah, Iraq

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ABSTRACT

Neohesperidin dihydrochalcone is an artificial sweetener with remarkable antioxidant activity, stable to basic or acidic conditions and elevated temperatures. This bioactive compound has demonstrated antiviral, antibacterial, antifungal, and anti-inflammatory effects. Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) causes coronavirus disease 2019 (COVID-19), a highly contagious viral infection. Main proteases (M^{pro}), papain-like protease (PL^{pro}), RNA-dependent RNA polymerase (RdRp), and helicase are the main components of this virus suitable for targeting. In this way, molecular docking of neohesperidin dihydrochalcone was performed against these receptors by CB-Dock. This study showed the best binding affinity was found for neohesperidin dihydrochalcone towards helicase with a Vina score of -9.1 kcal/mol. Future investigations should be focused on *in vitro* and *in vivo* studies based on this metabolite compared to other natural and synthetic antiviral compounds.

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1. Introduction

Flavonoid metabolites are phytochemical compounds having potential medicinal applications including antibacterial, antiviral, antifungal, anti-inflammatory, anticancer, and antioxidant activities [1]. Neohesperidin dihydrochalcone ($C_{28}H_{36}O_{15}$ with a molar mass of 612.58 g/mol) is an artificial sweetener (a sugar substitute providing sweetness with low-calorie or zero-calorie) isolated from citrus [2]. This hydrogenated flavonoid derivative has significant antioxidant activity [3]. This artificial sweetener in contrast to aspartame is stable to basic or acidic conditions and elevated temperatures. Antibacterial, antifungal, and anti-inflammatory activities of this compound have been reported previously [4-6]. Drug repurposing approaches can be employed for the therapy of viral infections based on reviving conventional antiviral drugs [7]. There are about 61 direct-acting antiviral agents (DAA) in clinical trials and many of these drugs have been screened and evaluated by molecular docking studies after the emergence of coronavirus disease 2019 (COVID-19) [8, 9]. In addition, presenting novel and effective antiviral agents isolated from natural sources is the critical issue [10-13]. Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) causes COVID-19, a contagious respiratory viral infection with common symptoms of fever, loss of taste/smell, and cough [14]. Helicase, RNA-dependent RNA polymerase (RdRp), papain-like protease (PL^{pro}), and main proteases (M^{pro}) have been found as the main components of SARS-CoV-2 [15-17]. In the present study, molecular docking of neohesperidin dihydrochalcone with helicase, RdRp, PL^{pro}, and M^{pro} of SARS-CoV-2 has been evaluated by CB-Dock as a protein-ligand docking method.

2. Materials and methods

Viral receptors were helicase (PDB code: 6ZSL, resolution: 1.94 Å), M^{pro} (PDB code: 6LU7, resolution: 2.16 Å), PL^{pro} (PDB code: 3E9S, resolution: 2.50 Å), and RdRp (PDB code: 6M71, resolution: 2.90 Å) have been extracted from protein data bank (PDB) (Figures 1a-d). The chemical structure of neohesperidin dihydrochalcone was obtained from the PubChem database and optimized

*Corresponding author. E-mail: qassim.hassan@qu.edu.iq

by the UCSF Chimera1.12 program (Figure 1e). CB-Dock server (http://clab.labshare.cn/cb-dock/php/index.php) was employed to evaluate the docking of neohesperidin dihydrochalcone with each receptor [18, 19].

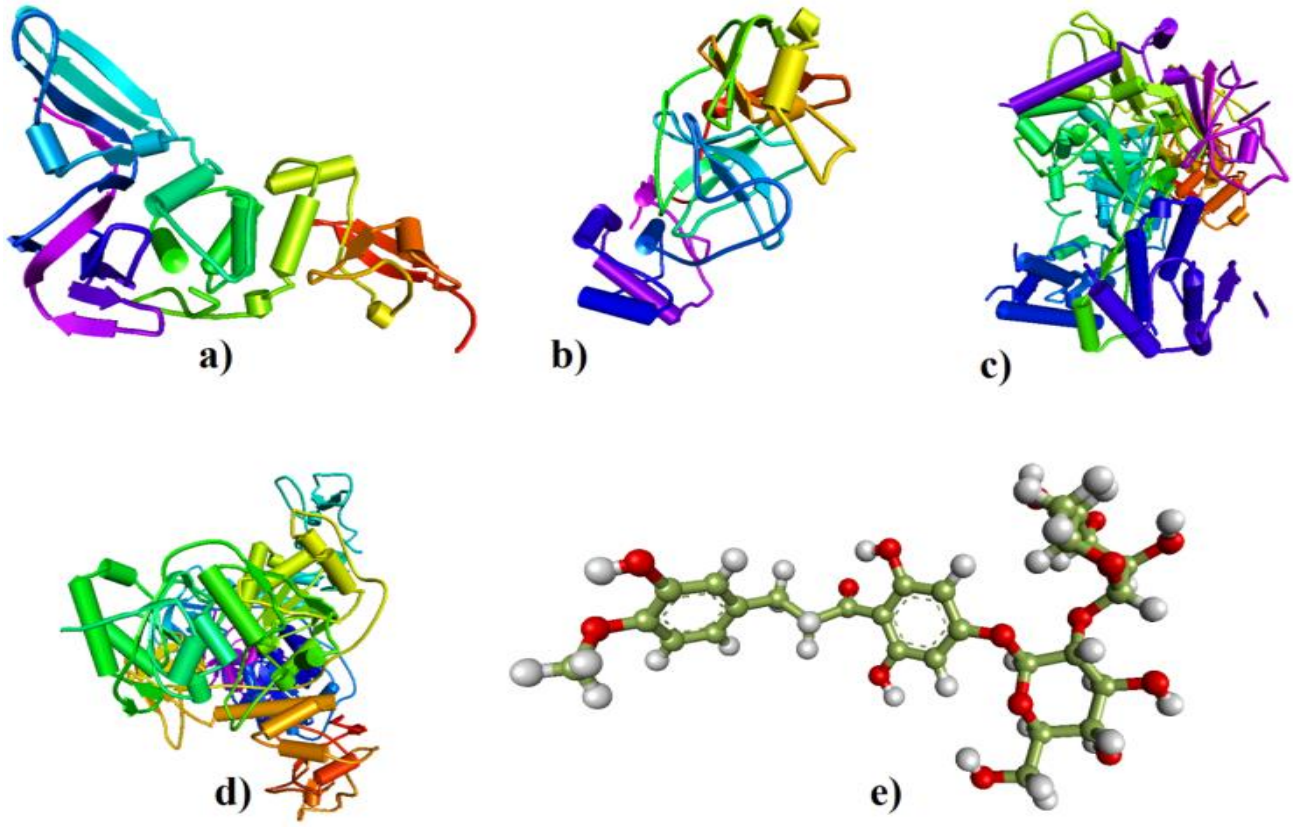

Fig. 1. Molecular structures of a) 3E9S, b) 6LU7, c) 6M71, d) 6ZSL, and chemical structure of e) neohesperidin dihydrochalcone.

3. Results and discussion

As presented in tables 1-4, docking results of CB-Dock showed that neohesperidin dihydrochalcone can interact with helicase, RdRp, PL^{pro}, and M^{pro} by best Vina scores of -9.1, -8.3, -8.1, and -7.6 kcal/mol with cavity volumes of 2984, 724, 243, and 258 $Å^3$, respectively. Best binding affinity was found for neohesperidin dihydrochalcone -helicase by Vina score of -9.1 kcal/mol and interacting amino acids of chain B including PRO175, ASN177, ARG178, ASN179, TYR180, LEU405, PRO406, ALA407, PRO408, ARG409, THR410, LEU412, GLY415, THR416, LEU417, SER485, SER486, PRO514, TYR515, ASN516, SER517, THR532, ASP534, ALA553, HIS554, SER555, ASN557, and ARG560 (Table 1). Docking interaction of neohesperidin dihydrochalcone with the SARS-CoV-2 NSP13 helicase as the best-docked pose with related interacting amino acids has been demonstrated in Figure 2. Docking scores were −8.3 and −8.4 kcal/mol against M^{pro}, for epigallocatechin gallate related to green tea and theaflavin-3,3′-digallate related to black tea, respectively. In addition, theaflavin-3,3′-digallate showed binding energies of −11.3 and −6 kcal/mol towards PL^{pro} and RdRp, respectively [20]. In a comparative study, lopinavir, darunavir, amprenavir, rupintrivir, and sofosbuvir had docking scores of −9.918, −8.843, −8.655, −8.342, and −8.324 kcal/mol against M^{pro}, respectively [21]. Similarly, daclatasvir, cobicistat, remdesivir, simeprevir, and raltegravir antiviral drugs illustrated −7.2, −7.4, −7.8, −8.7, and −9.1 kcal/mol binding energies, respectively toward M^{pro} [22]. Docking interactions of 40 antiviral phytochemicals with M^{pro} were evaluated by GOLD suite and AutoDock Vina to indicate an antiviral candidate with the best binding affinities. The best

binding affinity values were found for cyanidin 3-glucoside, glabridin, hypericin, α-ketoamide-11r (alpha-Ketoamide inhibitor 11r), and baicalin with important interacting amino acids of His41 and Cys145 [23]. Antiviral peptides also may be employed significantly to hinder SARS CoV-2 [24-26]. Based on the Firedock score, among the 15 antiviral peptides, the lowest binding energy was found for S2P26 against the receptor-binding domain (RBD) of the spike protein of SARS-CoV-2 with a value of −63.1 kcal/mol [27]. In docking study via AutoDock Vina based on a Lamarckian genetic algorithm, lopinavir-ritonavir, tipranavir, raltegravir, α-Ketoamide13b, nelfinavir, dolutegravir, tenofovir-disoproxil, baloxavir-marboxil, letermovir, and maraviroc showed binding energies of −10.6, −8.7, −8.3, −8.3, −8.2, −8.1, −8.1, −8.1, −8.0, and −8.0 kcal/mol toward SAR-CoV-2 M^{pro}, respectively [28]. Similarly, drug-repurposing studies exhibited that raltegravir can interact with SAR-CoV-2 M^{pro} by the lowest binding energy value of -9 kcal/mol [29]. In another study, Autodock Vina and SwissDock have been utilized to dock and redock four compounds related to the genus *Arthrospira* including folic acid, phycourobilin, phycocyanobilin, and phycoerythrobilin against the SARS-CoV-2 spike receptor-binding domain. Based on Autodock Vina results, there were binding energies of -7, -7.1, -7.4, and -7.4 kcal/mol for folic acid, phycourobilin, phycocyanobilin, and phycoerythrobilin, respectively [30].

Table 1. CB-dock results for neohesperidin dihydrochalcone-6ZSL.

CurPocket ID	Vina score (kcal/mol)	Cavity volume (Å^3)	Center (x, y, z)	Docking size (x, y, z)	Contact residues
C3	-9.1	2984	-23, 20, -21	35, 28, 28	**Chain B**: PRO175 ASN177 ARG178 ASN179 TYR180 LEU405 PRO406 ALA407 PRO408 ARG409 THR410 LEU412 GLY415 THR416 LEU417 SER485 SER486 PRO514 TYR515 ASN516 SER517 THR532 ASP534 ALA553 HIS554 SER555 ASN557 ARG560
C1	-8.2	4329	-32, 20, -49	28, 28, 28	**Chain B**: LEU147 TYR185 SER191 LYS192 VAL193 GLN194 VAL226 LEU227 THR228 SER229 HIS230 THR231 **Chain A**: ILE334 PRO335 ALA336 ALA338 VAL340 GLU341 CYS342 ASP344 VAL348 ASN349 SER350
C4	-8.2	2136	-16, 35, -64	28, 28, 28	**Chain A**: LYS139 GLU142 GLU143 PHE145 LYS146 TYR149 ASN179 TYR180 VAL181 LEU227 THR228 CYS309 SER310 HIS311 ARG339 THR359 ASN361 MET378 THR380 TYR382 ASP383 ALA407 PRO408 ARG409 THR410 LEU411
C2	-7.7	3723	-11, 20, -69	28, 28, 35	**Chain A**: LYS139 GLU142 GLU143 LYS146 ASN179 TYR180 VAL181 GLU197 LEU227 THR228 CYS309 SER310 HIS311 ARG339 THR359 ASN361 MET378 THR380 TYR382 ASP383 PRO408 THR410
C5	-7.7	2002	-32, 29, -75	28, 28, 28	**Chain A**: PHE145 TYR149 PRO172 ARG173 PRO174 PRO175 ASN177 ASN179 TYR180 PRO408 ARG409 THR410 LEU411 LEU412 THR413 SER485 SER486 ALA487 PRO514 TYR515 ASN516 THR532 ASP534 SER535 HIS554 ARG560

Table 2. CB-dock results for neohesperidin dihydrochalcone-6M71.

CurPocket ID	Vina score (kcal/mol)	Cavity volume ($Å^3$)	Center (x, y, z)	Docking size (x, y, z)	Contact residues
C3	-8.3	724	120, 120, 136	28, 28, 28	**Chain A**: ASP164 LYS551 ARG553 GLY616 TRP617 ASP618 TYR619 PRO620 LYS621 CYS622 ASP623 ASN691 SER759 ASP760 ASP761 ALA762 PHE793 MET794 SER795 LYS798 TRP800 GLU811 PHE812 CYS813 SER814 GLN815
C4	-7.7	574	146, 132, 82	28, 28, 28	**Chain A**: ARG33 ALA34 PHE35 ASP36 ILE37 TYR38 ASN39 VAL71 VAL72 LYS73 ASN79 ARG116 THR123 VAL204 THR206 ASP208 ASN209 TYR217 ASP218 ASP221 PHE222
C2	-7.4	775	127, 135, 127	28, 28, 28	**Chain A**: LEU172 THR246 LEU247 THR248 ARG249 THR252 SER318 THR319 VAL320 PHE321 PRO323 ARG349 THR394 CYS395 PHE396 TYR456 ARG457 TYR458 ASN459 LEU460 PRO461 PRO677
C1	-6.7	1089	122, 139, 100	28, 28, 28	**Chain A**: ARG197 SER229 GLY230 VAL231 PRO232 LEU280 LYS281 PHE283 ASP284 PHE287 LYS288 TYR289 TRP290 ASP291 GLN292 THR293 TYR294
C5	-5.4	549	121, 96, 146	28, 28, 28	**Chain A**: GLU431 GLY432 GLU436 LEU437 LYS438 PHE440 **Chain C**: LYS2 MET3 SER4 LYS7 LYS43 ASP44 THR45

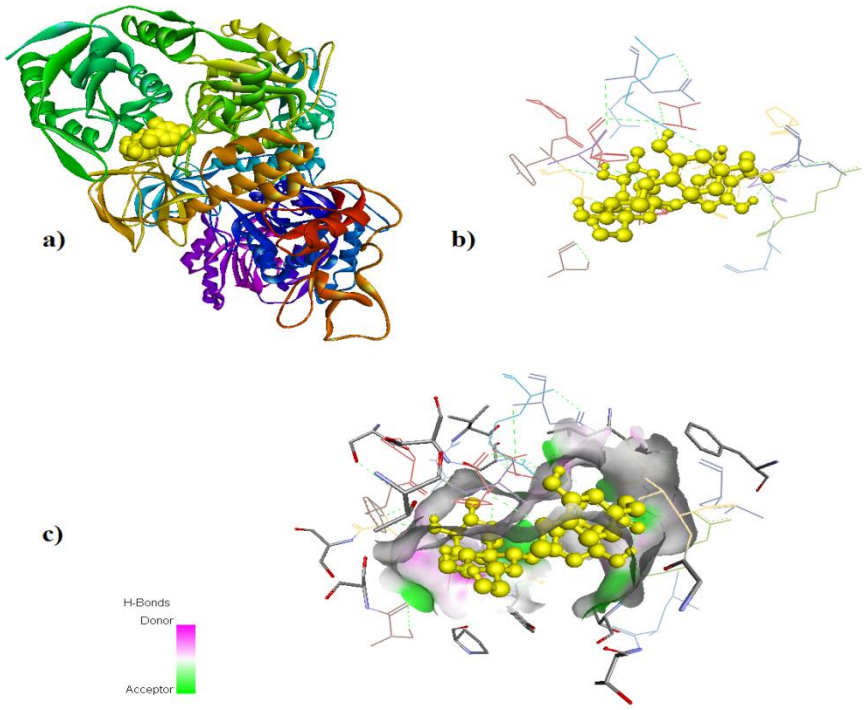

Fig. 2. The best model of docking active site prepared by CB-Dock (a), the interaction of amino acids of helicase with the neohesperidin dihydrochalcone (b), and the surface around ligand of neohesperidin dihydrochalcone (c).

Table 3. CB-dock results for neohesperidin dihydrochalcone-6LU7.

CurPocket ID	Vina score (kcal/mol)	Cavity volume (Å^3)	Center (x, y, z)	Docking size (x, y, z)	Contact residues
C3	-7.6	258	-14, 11, 72	28, 28, 28	**Chain A**: HIS41 CYS44 MET49 TYR54 PHE140 LEU141 ASN142 GLY143 SER144 CYS145 HIS163 HIS164 MET165 GLU166 LEU167 PRO168 GLY170 HIS172 ASP187 ARG188 GLN189 THR190 ALA191 GLN192
C1	-7.2	688	-24, 1, 56	28, 28, 28	**Chain A**: ARG131 LYS137 ASP197 THR198 THR199 LYS236 TYR237 ASN238 TYR239 LEU271 LEU272 GLY275 MET276 ALA285 LEU286 LEU287 GLU288 ASP289
C2	-6.9	548	-14, 34, 56	28, 28, 28	**Chain A**: GLU14 GLY15 CYS16 MET17 VAL18 GLN19 TRP31 GLN69 ALA70 GLY71 ASN72 VAL73 ASN95 PRO96 LYS97 ASN119 GLY120 SER121 PRO122
C5	-6.8	212	-34, 16, 54	28, 28, 28	**Chain A**: PHE8 LYS102 VAL104 ARG105 ILE106 GLN107 GLN110 THR111 ASN151 ILE152 ASP153 SER158 ASP248 ILE249 LEU250 PRO252 THR292 PRO293 PHE294 VAL297
C4	-6.7	239	-37, 5, 58	28, 28, 28	**Chain A**: PHE8 VAL104 ARG105 ILE106 GLN107 GLN110 THR111 ASN151 ASP153 ASP245 ILE249 LEU250 PRO252 THR292 PRO293 PHE294 VAL297

Table 4. CB-dock results for neohesperidin dihydrochalcone-3E9S.

CurPocket ID	Vina score (kcal/mol)	Cavity volume (Å^3)	Center (x, y, z)	Docking size (x, y, z)	Contact residues
C3	-8.1	243	-5, 26, 15	28, 28, 28	**Chain A**: PRO34 TYR36 LEU59 PRO60 LEU65 ARG66 SER67 ALA69 PHE70 THR75 LEU76 ASP77 GLU78 SER79 PHE80 LEU81 GLY82 ARG83
C2	-7.3	647	-28, 21, 28	28, 28, 28	**Chain A**: LYS158 LEU163 GLY164 ASP165 ARG167 GLU168 MET209 ALA247 PRO248 PRO249 TYR265 ASN268 TYR269 GLN270 CYS271 TYR274 THR302 ASP303
C1	-6.9	712	-8, 12, 9	28, 28, 28	**Chain A**: ASN14 TYR36 LEU37 ASP38 GLY39 THR55 PHE56 PHE57 LEU88 THR91 LYS92 LYS93 TRP94 LYS95 PHE96 ARG139 GLY143 ASP144 ALA145 ALA146 ASN147
C5	-6.4	203	-40, 11, 10	28, 28, 28	**Chain A**: GLY100 GLY101 LEU102 LEU121 GLN122 GLN123 LEU124 GLU125 VAL126 TYR137 ARG141 LEU260 THR278 ALA279 LYS280 TYR284 LYS307
C4	-5.2	212	-28, 8, 27	28, 28, 28	**Chain A**: LYS106 TRP107 ASN110 LEU163 THR266 GLY267 CYS271 GLY272 HIS273 ARG285 ASP287 HIS290

4. Conclusions

In silico study can provide predicting approach for designing effective antiviral compounds. Compared to M^{pro}, RdRp, and PL^{pro}, neohesperidin dihydrochalcone showed higher binding affinity toward the SARS-CoV-2 helicase. Although, the binding affinity of this compound is lower than antiviral peptides such as S2P26, the biocompatibility of neohesperidin dihydrochalcone is considerable. In a better strategy, combination treatment or novel drug design can be promising therapeutic. This molecular docking study illustrated that neohesperidin dihydrochalcone can be regarded for more therapeutic investigations, which can be employed for drug design based on chemical structure. Experimental studies including *in vitro* and *in vivo* should be regarded to better understand the antiviral activity of neohesperidin dihydrochalcone.

Study Highlights

- Neohesperidin dihydrochalcone showed higher binding affinity toward the SARS-CoV-2 helicase compared to M^{pro}, RdRp, and PL^{pro}.
- Although, the binding affinity of neohesperidin dihydrochalcone is lower than antiviral peptides such as S2P26, the biocompatibility of neohesperidin dihydrochalcone is considerable.
- Experimental studies including in vitro and in vivo should be regarded to better understand the antiviral activity of neohesperidin dihydrochalcone.

Abbreviations

ACE2: Angiotensin-converting enzyme 2
COVID-19: Coronavirus disease 2019
M^{pro}: Main proteases
PL^{pro}: Papain-like protease
RBD: The receptor-binding domain
RdRp: RNA-dependent RNA polymerase
SARS-CoV-2: Severe acute respiratory syndrome coronavirus 2
DAA: Direct-acting antiviral agents

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Conflict of interest

Not applicable.

Ethical approval

This article does not contain any studies with animals or human participants performed by any of the authors.

Author contributions

Not applicable.

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