

Supplementary Materials for

***Anti-Helicobacter pylori* Compounds from *Oliveria decumbens* Vent. through
Urease Inhibitory *In-vitro* and *In-silico* Studies**

Mahdieh Eftekhari, Mohammad Reza Shams Ardekani, Mohsen Amin, Mahboubeh Mansourian,
Mina Saeedi, Tahmineh Akbarzadeh and Mahnaz Khanavi*

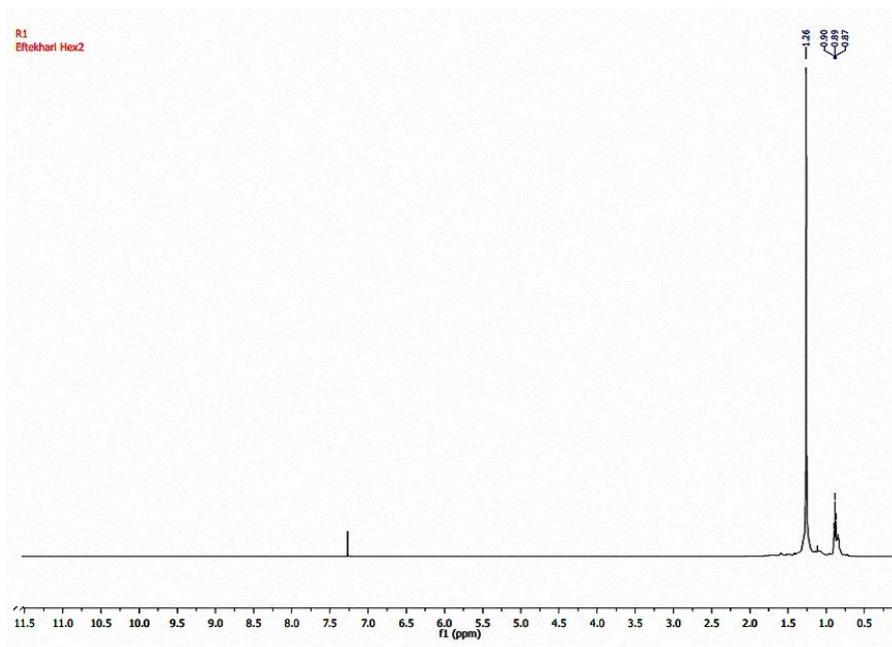
*To whom correspondence should be addressed. E-mail: khanavim@tums.ac.ir

Volume 20, Issue 3 (Summer 2021)

This PDF file includes:

Figures S1-S18

(a)



(b)

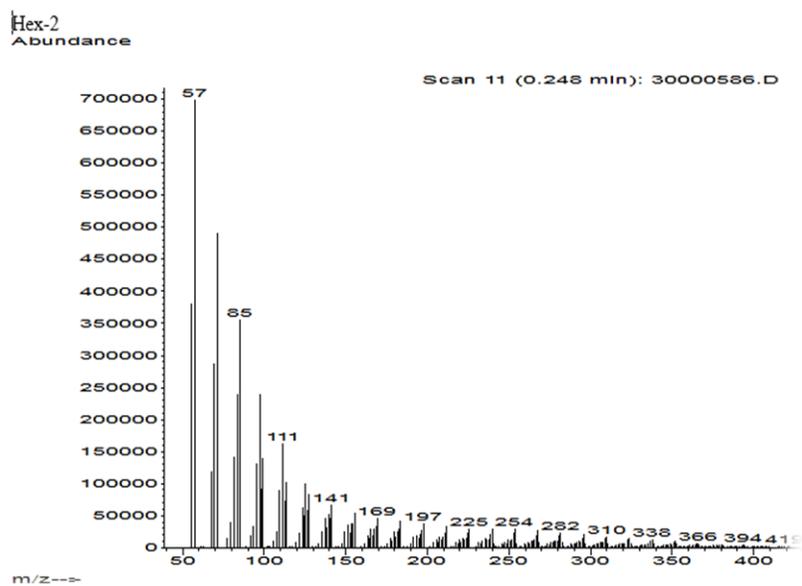


Figure S1. (a) ^1H NMR 500 MHz, in CDCl_3 : Octacosane, (b) EI-MASS :Octacosane

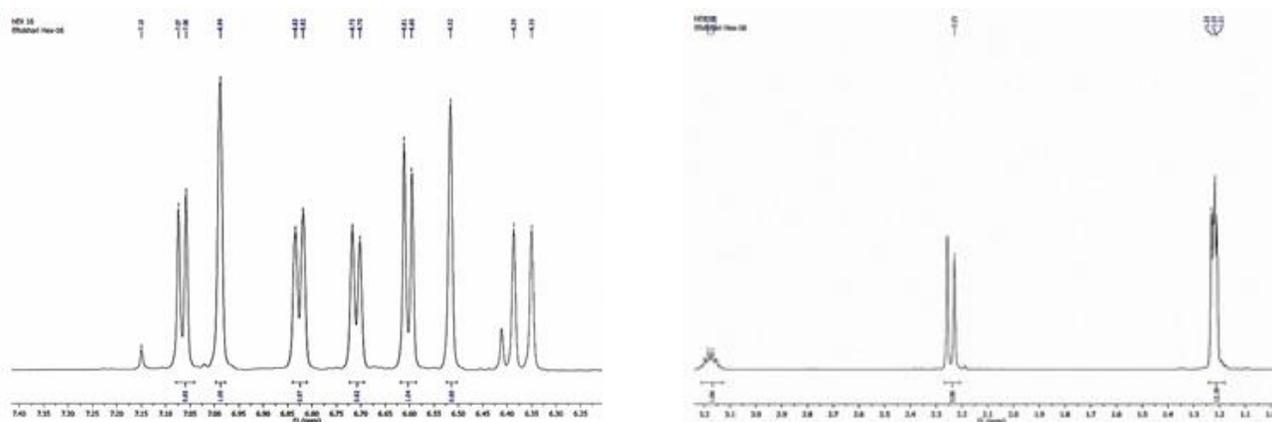


Figure S2. ¹H NMR 500 MHz, in CDCl₃: Mixture of thymol and carvacrol

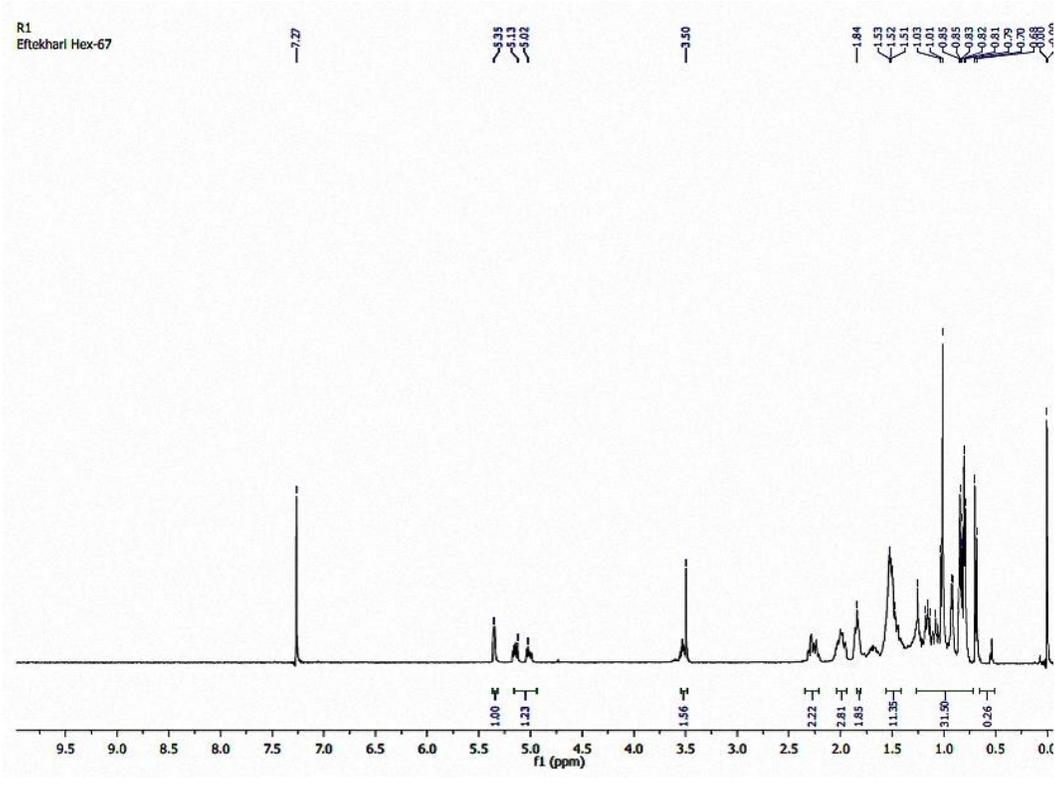


Figure S3¹HNMR 500 MHz, in CDCl₃: Stigmasterol

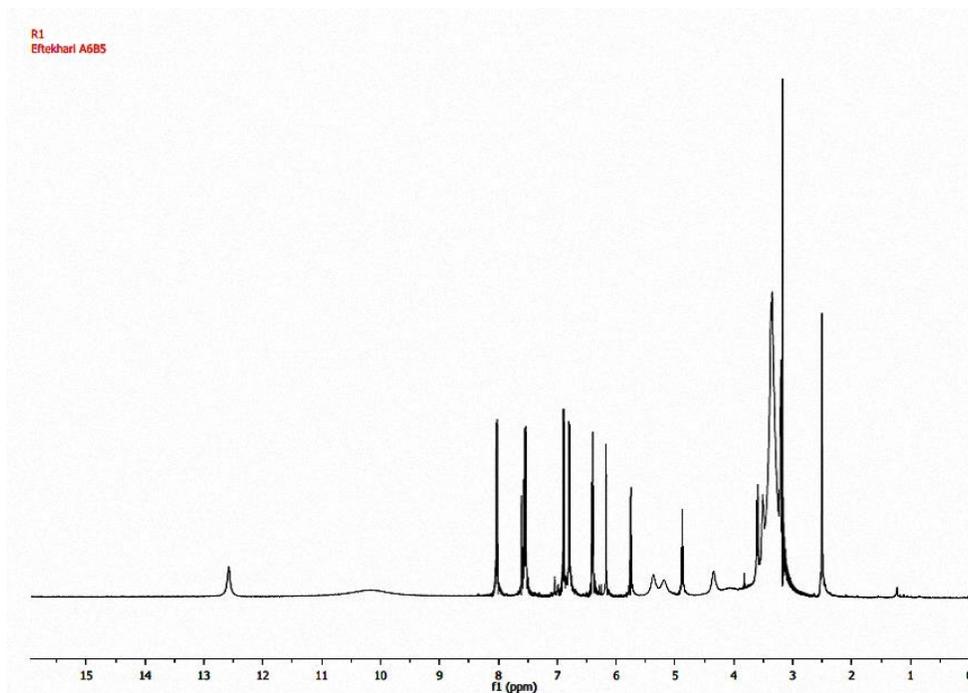


Figure S4. ^1H NMR 500 MHz, in DMSO-d_6 : Kaempferol-3-O-(6''-O-trans-coumaryl)glucoside

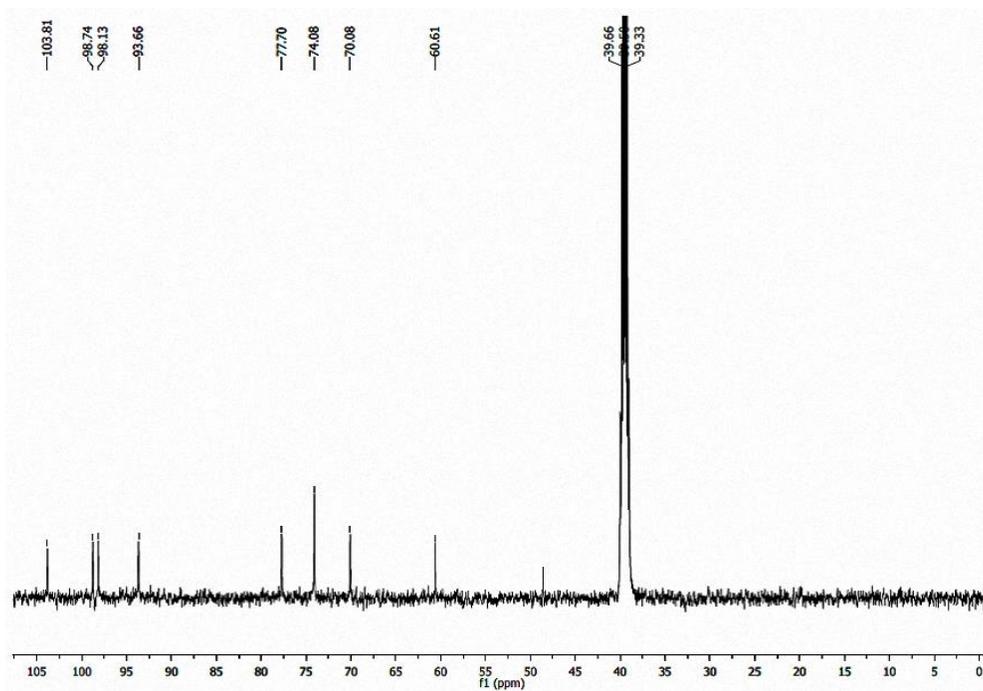


Figure S5. ^{13}C NMR 125 MHz, in DMSO-d_6 : Kaempferol-3-O-(6''-O-trans-coumaryl)glucoside

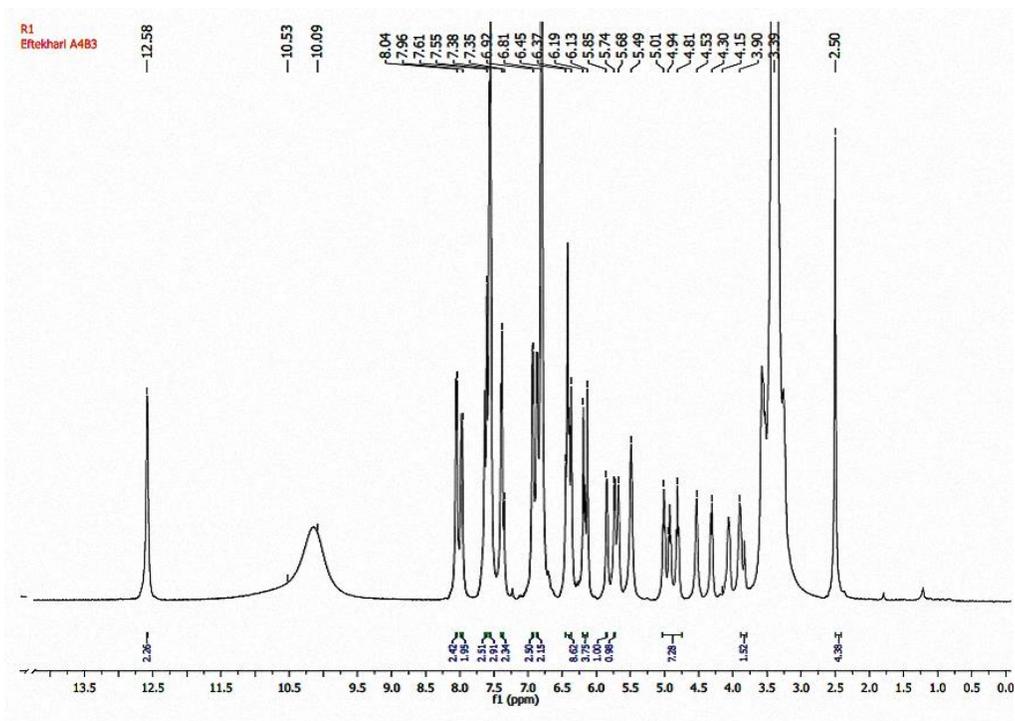


Figure S6. ^1H NMR 500 MHz, in DMSO-d_6 : Kaempferol 3-O-(6''-O-trans-coumaryl)glucoside 7-O-(6'''-O-trans-coumaryl) glucoside.

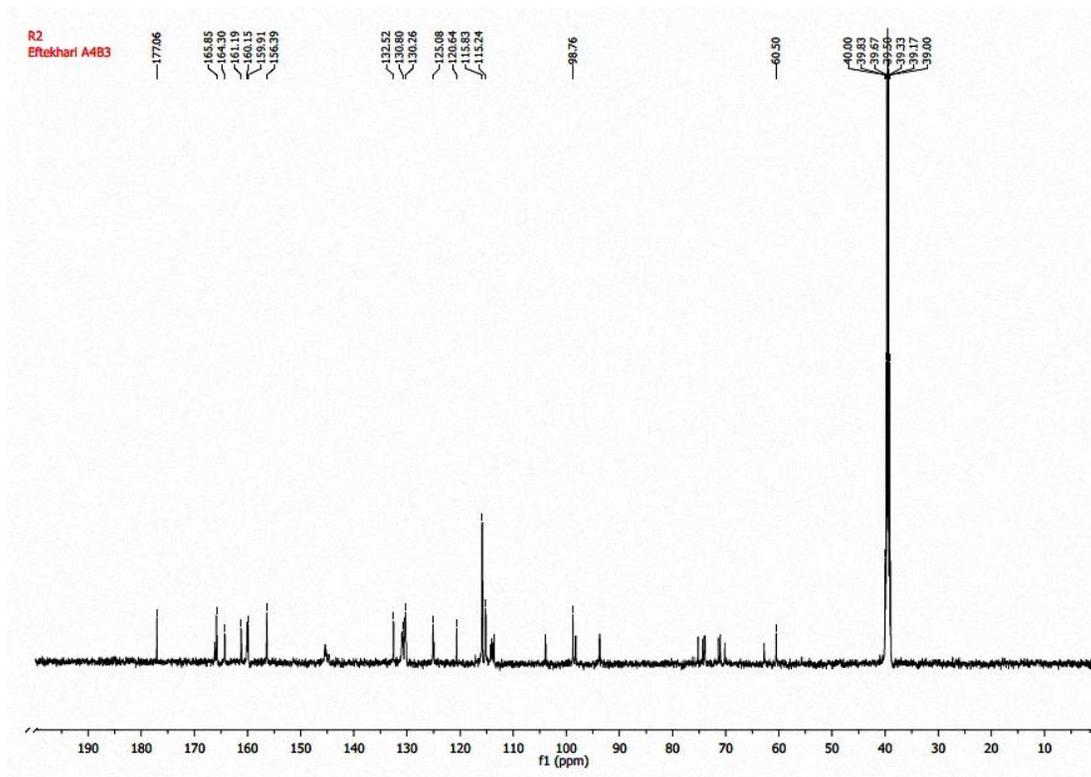


Figure S7. ^{13}C NMR 125, in DMSO-d_6 , Kaempferol 3 -O-(6''-O-trans-coumaryl)glucoside 7-O-(6''-O-trans-coumaryl) glucoside.

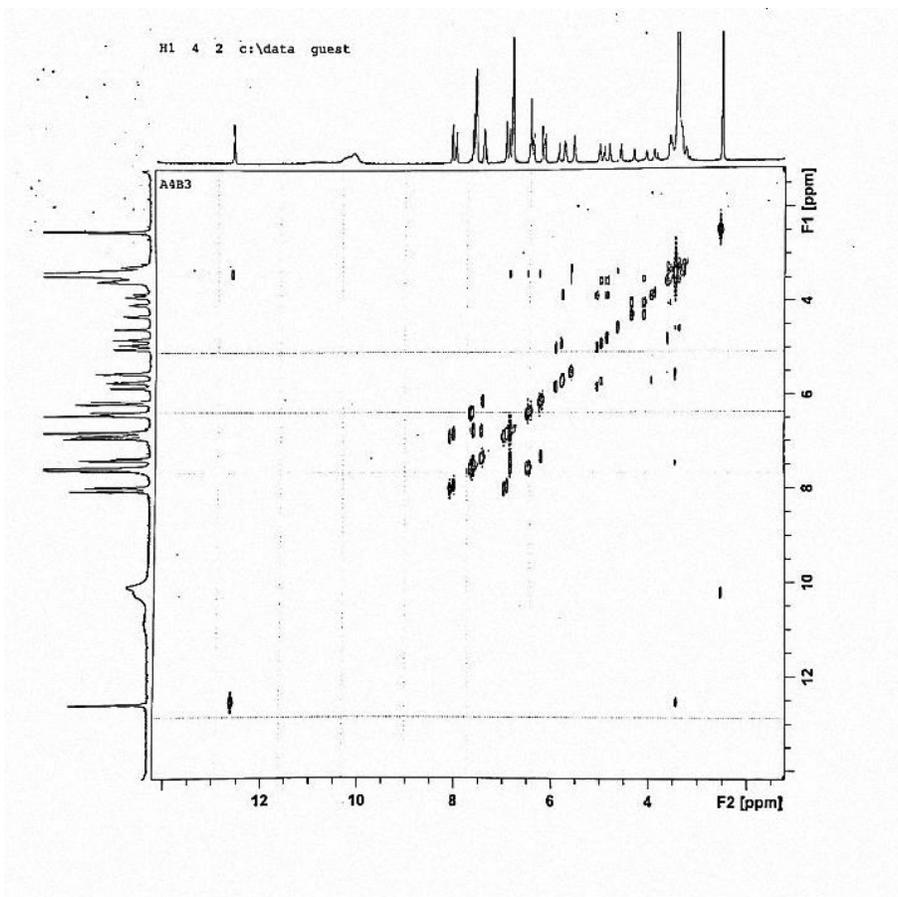


Figure S8. COSY, in DMSO-d₆, Kaempferol 3 -O-(6''-O-trans-coumaryl)glucoside 7-O-(6'''-O-trans-coumaryl) glucoside

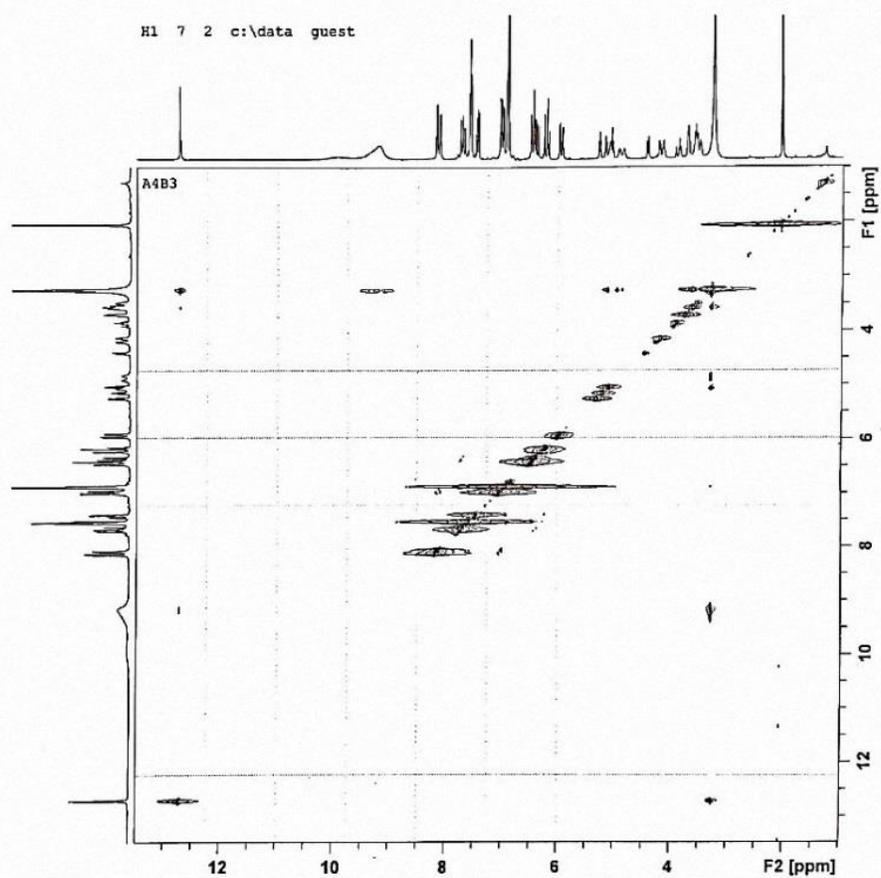


Figure S9. NOSEY, in Acetone- d_6 , Kaempferol 3 -O-(6''-O-trans-coumaryl)glucoside 7-O-(6'''-O-trans-coumaryl) glucoside

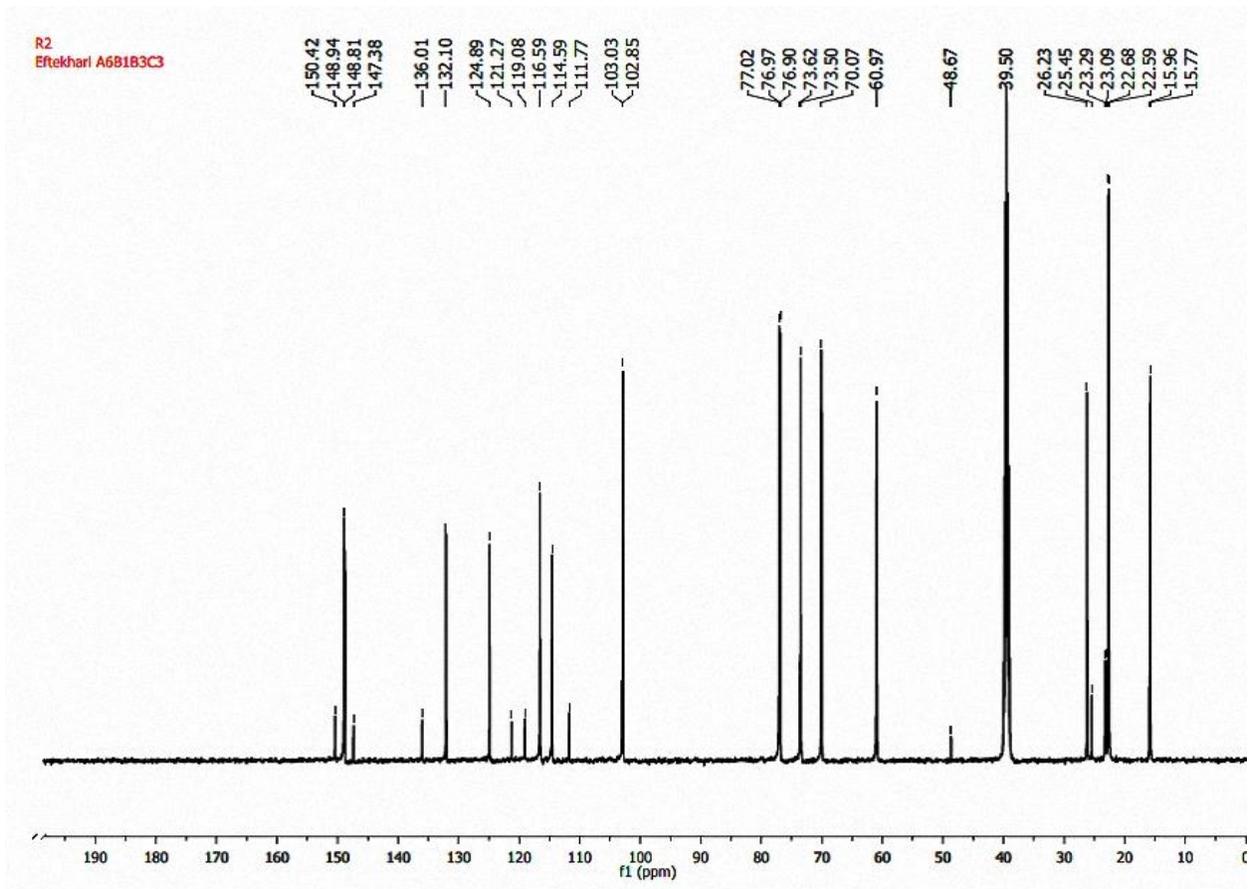


Figure S10. ^{13}C NMR 125 MHz, in DMSO-d_6 : 3-Hydroxythymol-6-O-D-Glucopyranoside- & 6-Hydroxythymol-3-O-D-Glucopyranoside

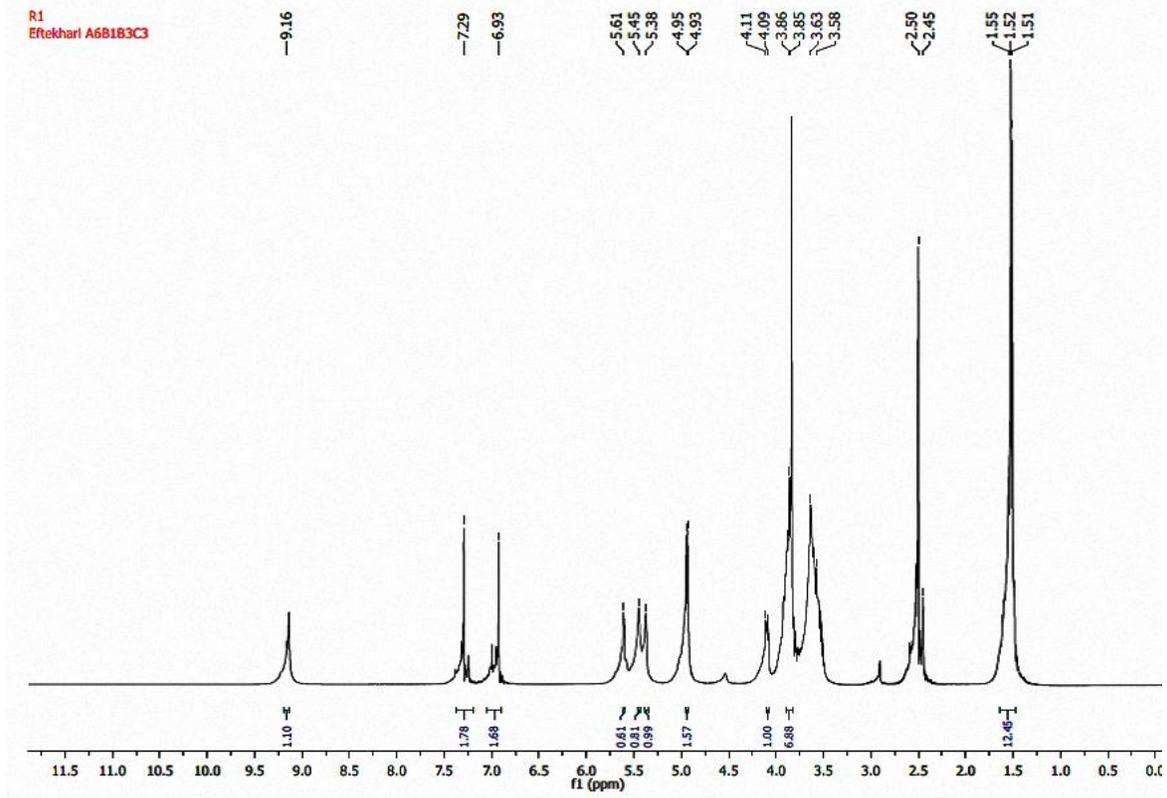


Figure S11. ^1H NMR 500 MHz, in DMSO-d_6 , 3-Hydroxythymol-6-O-D-Glucopyranoside- & 6-Hydroxythymol-3-O-D-Glucopyranoside

R1
Eftekhari A4B4C3

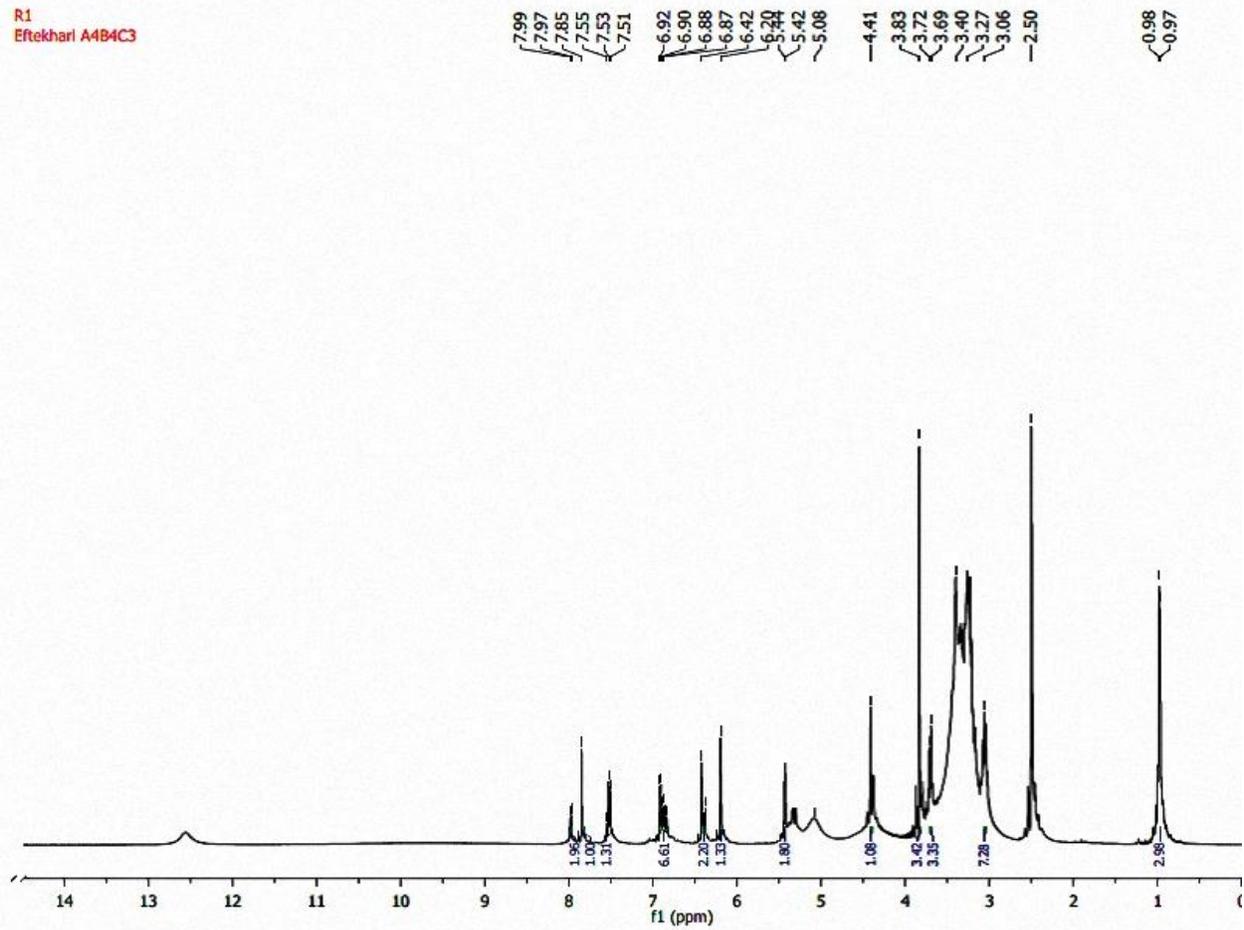


Figure S12. ^1H NMR 500 MHz, in DMSO-d_6 : : kaempferol 3-O-neohesperidoside-7-O-[2-O-(cis-feruloyl)]-D-glucopyranoside

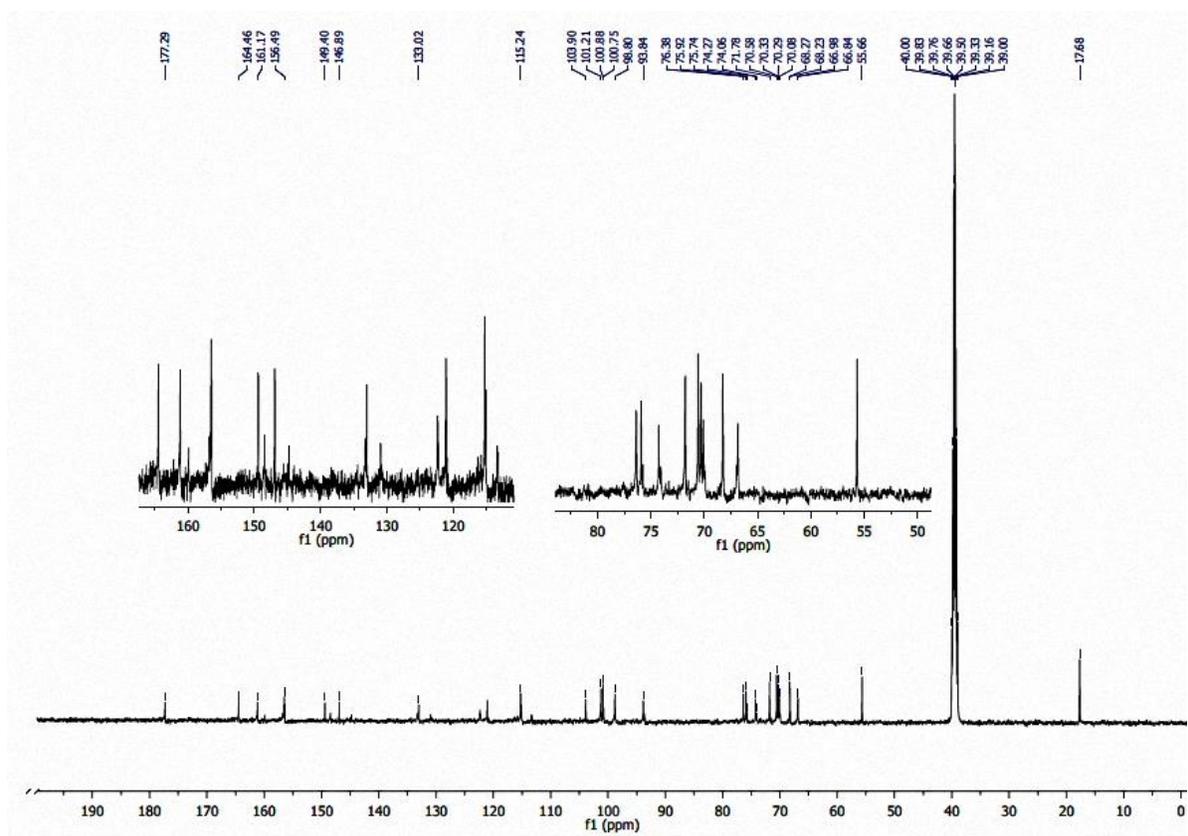


Figure S13. ^{13}C NMR 125 MHz, in DMSO-d_6 : kaempferol 3-O-neohesperidoside-7-O-[2-O-(cis-feruloyl)]-D-glucopyranoside

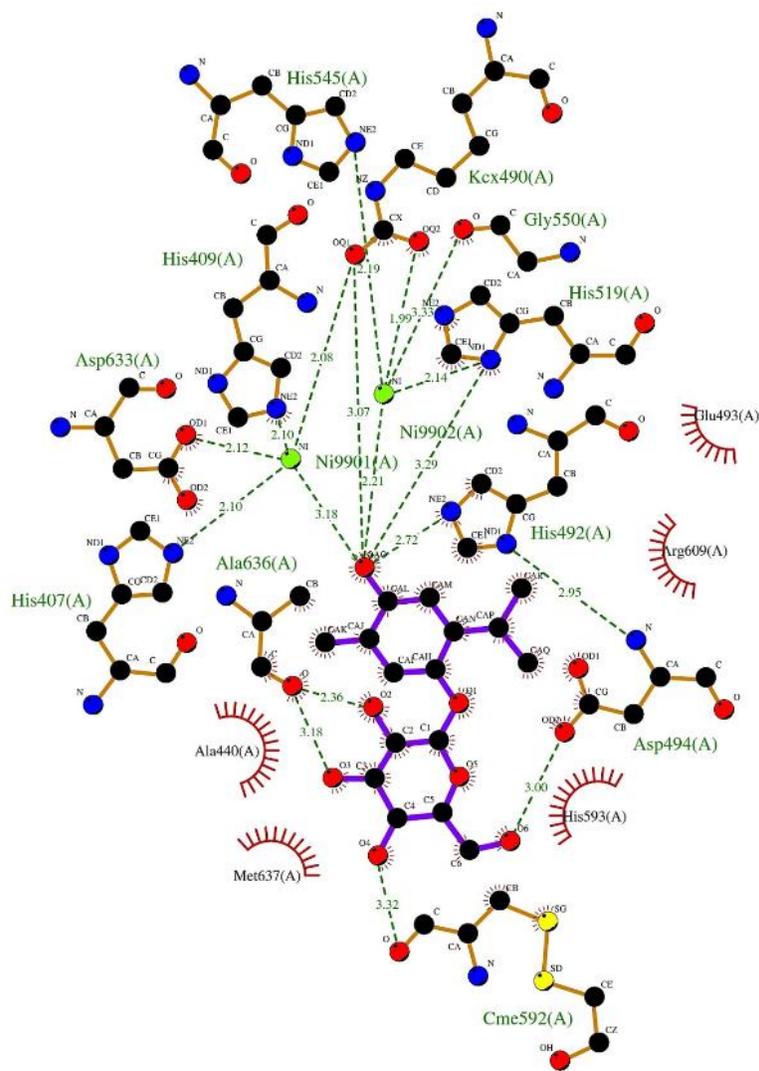


Figure S15. Schematic interaction of the best docking resulting from AutoDock software presented by LigPlot software for compound 7. In this figure, the compound exposure is highlighted in blue. Hydrogen bonding is in green and van der Waals interactions are in red circulars.

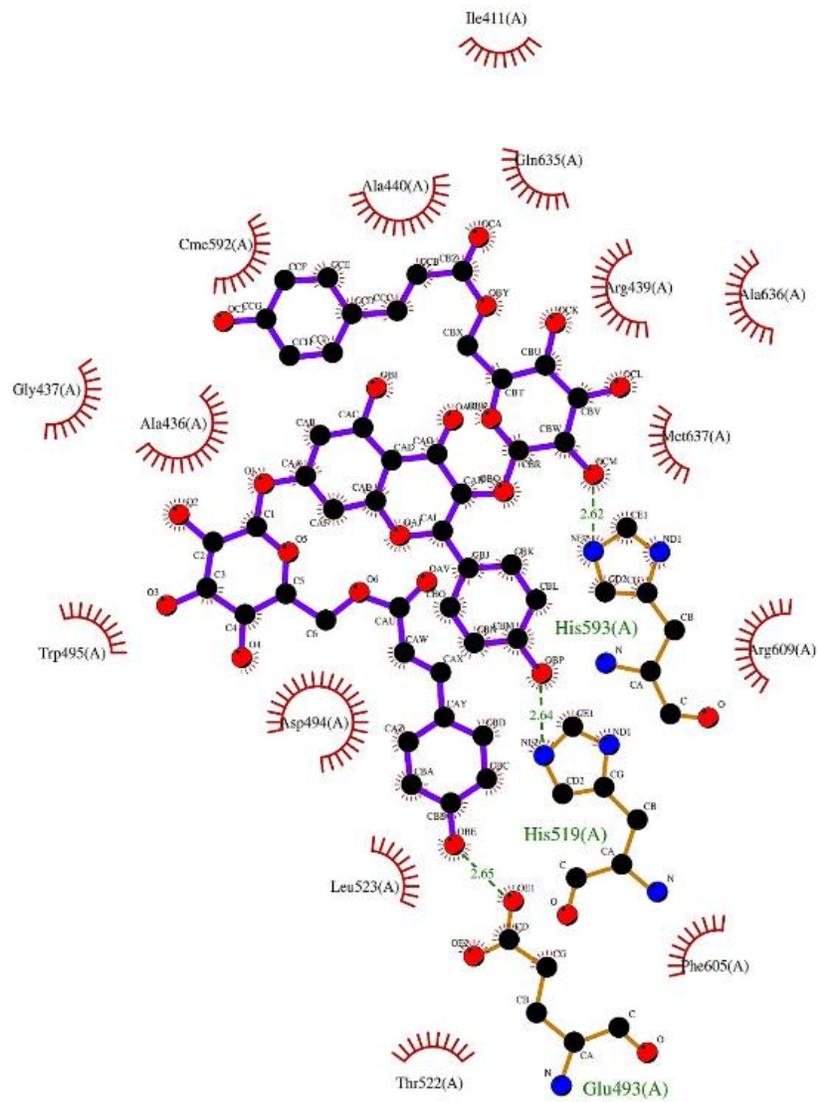


Figure S16. Schematic interaction of the best docking resulting from AutoDock software presented by LigPlot software for compound 8. In this figure, the compound exposure is highlighted in blue. Hydrogen bonding is in green and van der Waals interactions are in red circulars.

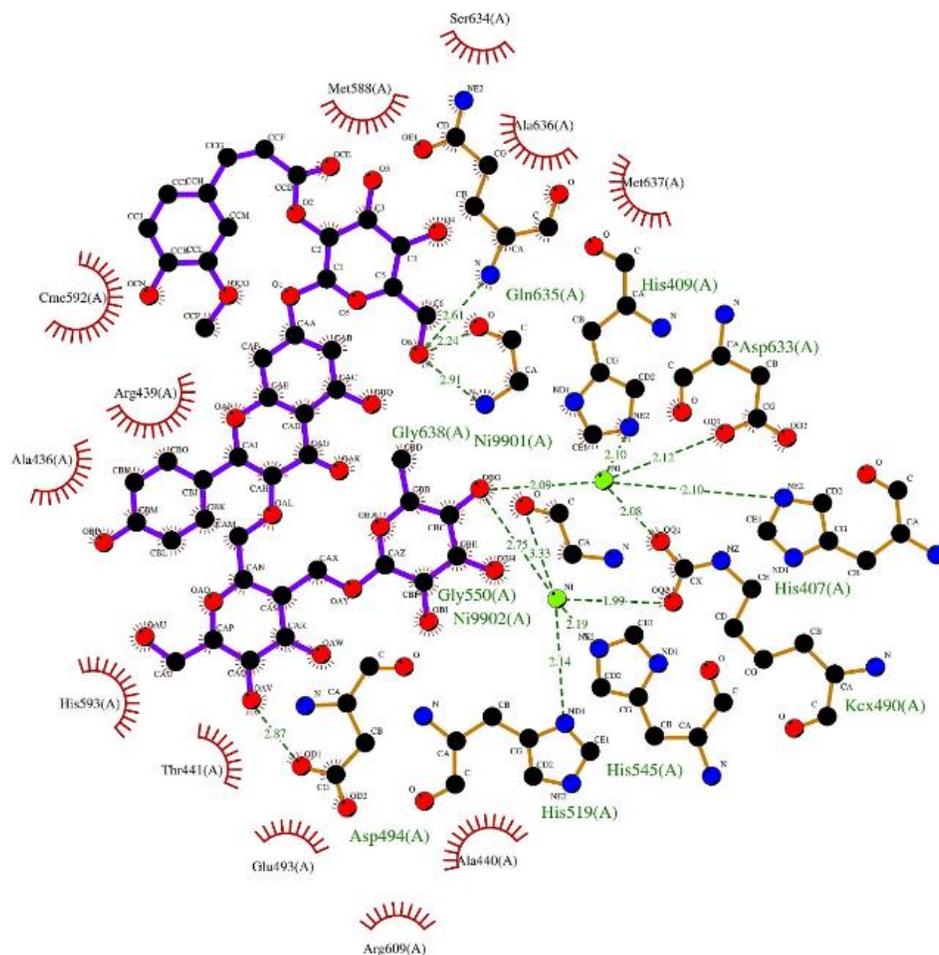


Figure S17. Schematic interaction of the best docking resulting from AutoDock software presented by LigPlot software for compound 6. In this figure, the compound exposure is highlighted in blue. Hydrogen bonding is in green and van der Waals interactions are in red circulars.

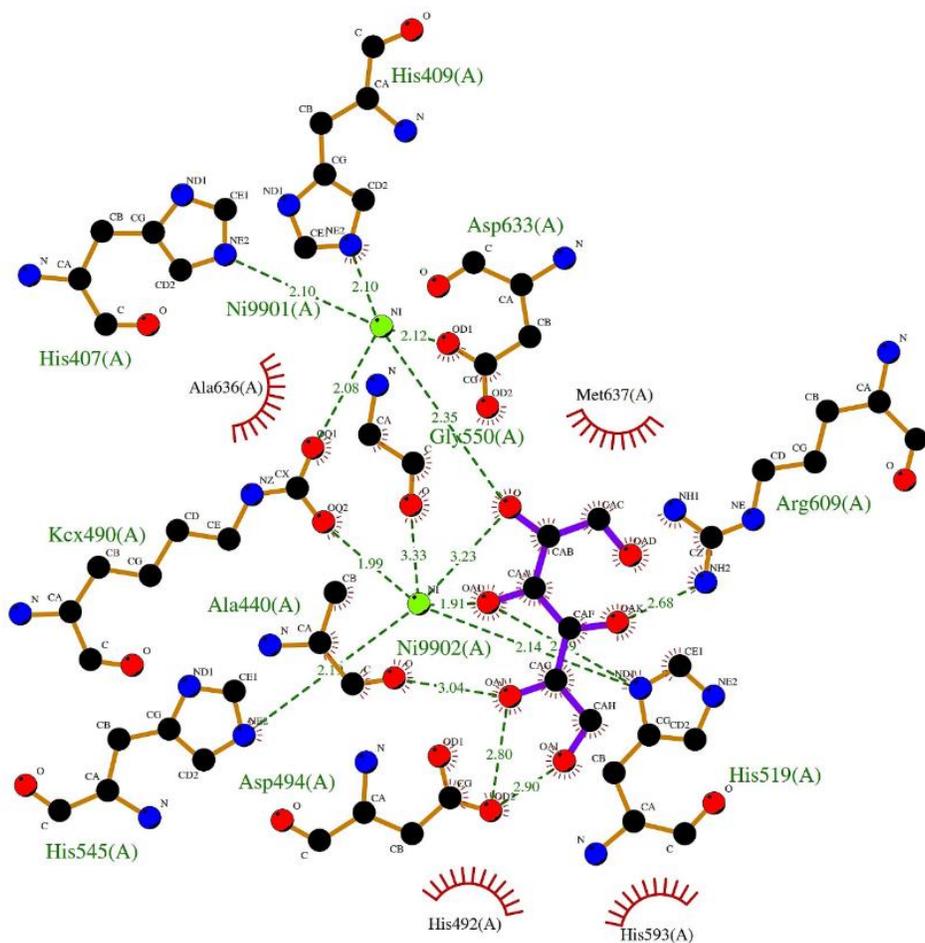


Figure S18. Schematic interaction of the best docking resulting from AutoDock software presented by LigPlot software for compound 9. In this figure, the compound exposure is highlighted in blue. Hydrogen bonding is in green and van der Waals interactions are in red circulars.