

## LC-MS Identification and Effects of *Diplotaxis acris* Metabolites Against SARS-CoV-2 Main Protease Supported by *In Silico* Computational Studies

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**SUMMARY.** Covid-19 was announced as a pandemic in March 2020, since then scientists are trying to find out effective therapeutics as treatment. Many medicinal herbs contain antiviral compounds, such as rutin, and flavonoid glycosides that are efficient against viruses. *Diplotaxis acris* is a famous plant traditionally used to prepare rocket salad. LC-MS of methanol extract revealed the presence of 12 compounds, quercetin 3-O- $\beta$ -rhamnoside, isorhamnetin 7-O- $\beta$ -glucoside, kaempferol 3,7- diglucoside, apigenin 7-rhamnoside, and apigenin 7-O- $\beta$ - glucoside as major compounds. The computational studies showed that all flavonoids form strong interaction with SARS-CoV-2 main protease with good CDOCKER interaction energy (Kcal/mol) of -53.1, -51.7, -44.1, -48.0, and -49.7, respectively, which are apigenin 7-rhamnoside as a suitable contender for oral administration. Results suggest that *Diplotaxis acris* have potential against SARS-CoV-2 and could be a good source of lead compounds against the novel coronavirus.

**RESUMEN.** Covid-19 se anunció como una pandemia en marzo de 2020; desde entonces los científicos están tratando de encontrar terapias efectivas como tratamiento. Muchas hierbas medicinales contienen compuestos antivirales, como la rutina, y glucósidos flavonoides que son eficaces contra los virus. *Diplotaxis acris* es una famosa planta utilizada tradicionalmente para preparar ensalada de rúcula. La LC-MS del extracto de metanol reveló la presencia de 12 compuestos, quercetina 3-O- $\beta$ -ramnósido, isorramnetina 7-O- $\beta$ -glucósido, kaempferol 3,7-diglucósido, apigenina 7-ramnósido y apigenina 7-O-  $\beta$ -glucósido como compuestos mayoritarios. Los estudios computacionales mostraron que todos los flavonoides forman una fuerte interacción con la proteasa principal del SARS-CoV-2 con una buena energía de interacción CDOCKER (Kcal/mol) de -53,1, -51,7, -44,1, -48,0 y -49,7, respectivamente, que son apigenina 7-ramnósido como un competidor adecuado para la administración oral. Los resultados sugieren que *Diplotaxis acris* tiene potencial contra el SARS-CoV-2 y podría ser una buena fuente de compuestos de plomo contra el nuevo coronavirus.

**KEY WORDS:** apigenin 7-rhamnoside, *in silico*, LC-MS, SARS-CoV-2.

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