

## Supplementary Materials

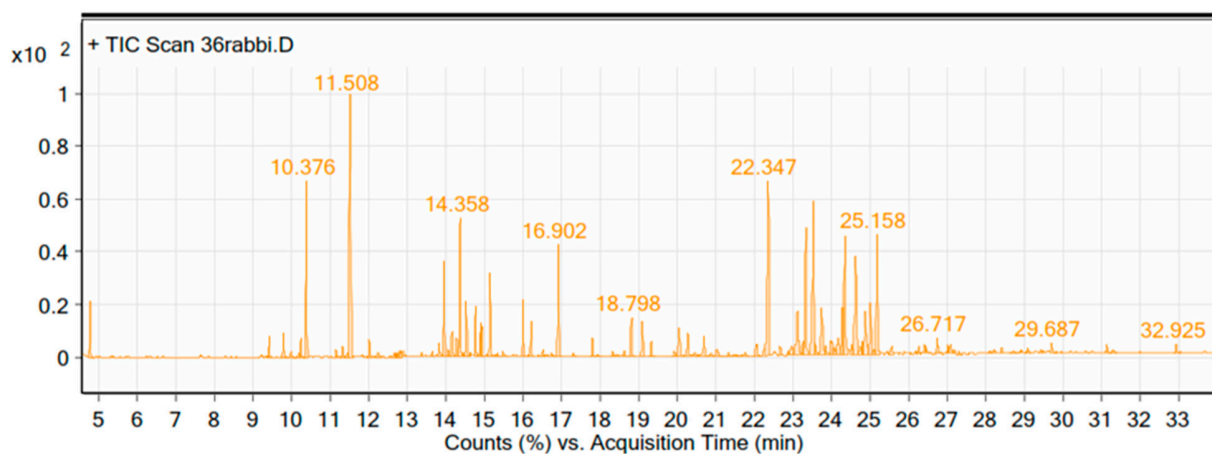
### Investigation on Essential Oils of *Achillea* Species: From Chemical Analysis to *In Silico* Uptake against SARS-CoV-2 Main Protease

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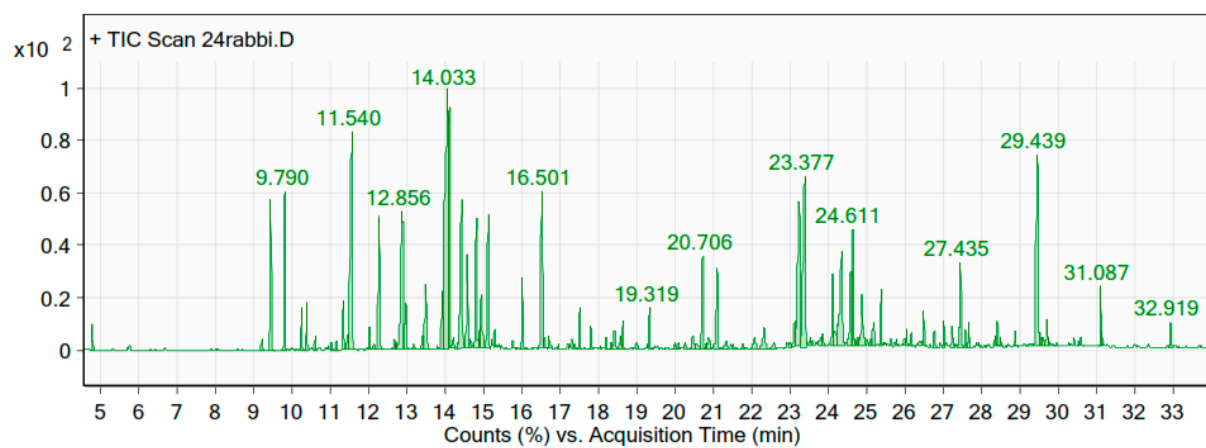
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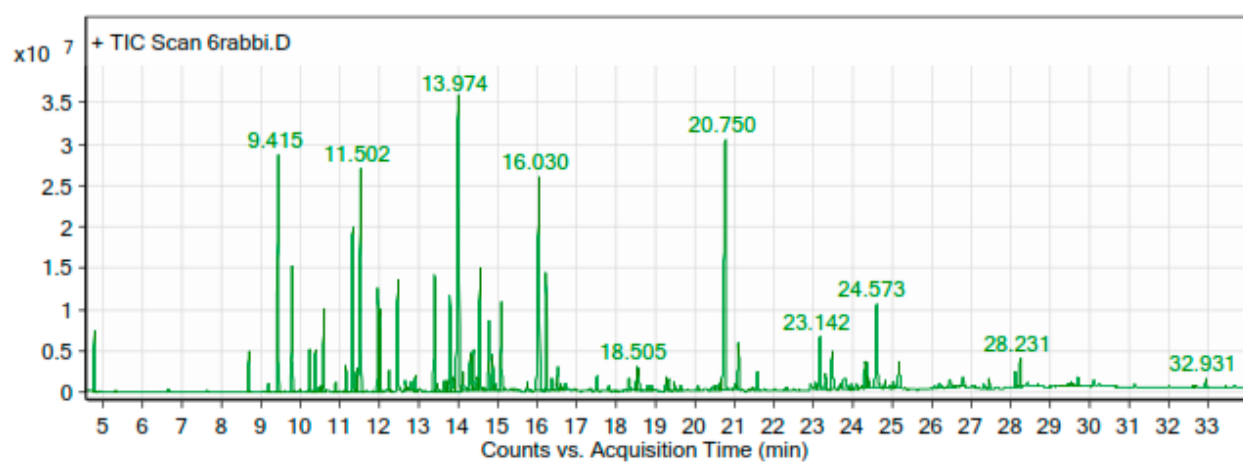
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**Figure S1.** Chromatogram of GC-MS analysis of essential oil of *Achillea millefolium* in Zanjan region



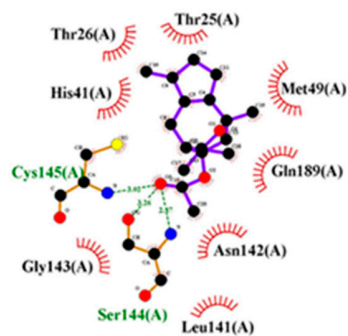
**Figure S2.** Chromatogram of GC-MS analysis of essential oil of *Achillea wilhelmsii* C. Koch in Zanzan region.



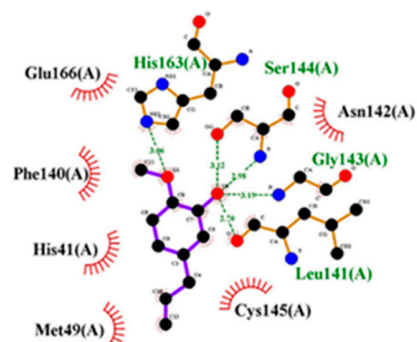
**Figure S3.** Chromatogram of GC-MS analysis of essential oil of vegetative body of *Achillea tenuifolia* Lam in Zanzan region

## I: SARS-CoV-2 3CL<sup>pro</sup>

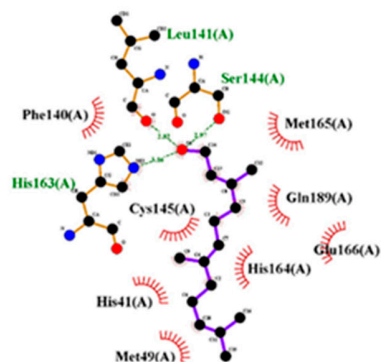
a)



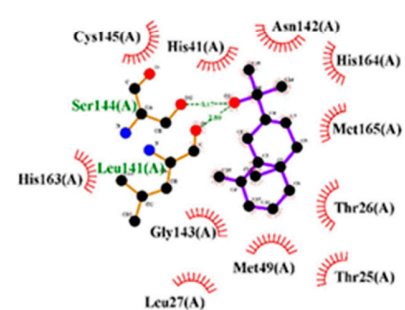
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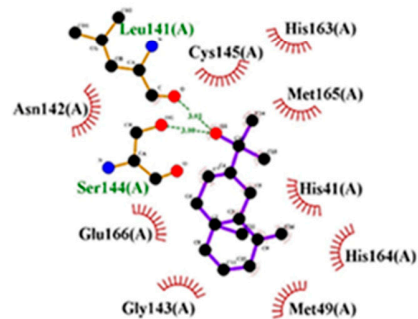
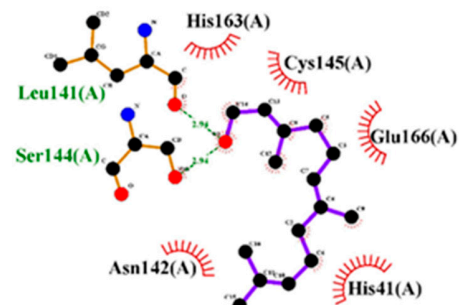
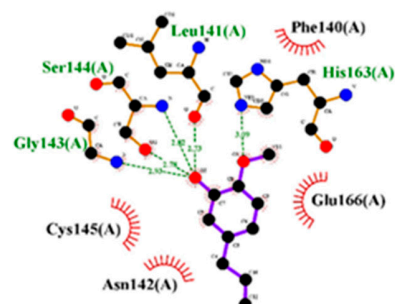
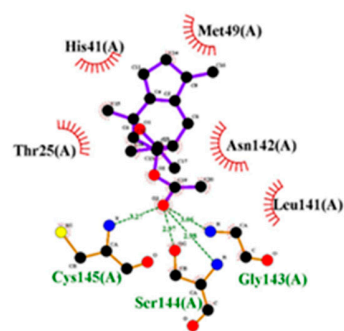
c)



d)



## II: SARS-CoV-1 3CL<sup>pro</sup>



**Figure S4.** 2D illustration of interactions between candidate compounds and viral polymerases; (I: SARS-CoV-2 3CL<sup>pro</sup>: 6NUR, II: SARS-CoV-2 3CL<sup>pro</sup>: 2H2Z): a) Kessanyl acetate, b) Chavibetol (m-Eugenol), c) Farnesol, d) 7-epi- $\beta$ -Eudesmol.