

SUPPLEMENTARY DATA

In Silico Study of Bioactive Compounds from Some Tropical Trees as Inhibitors of Papain-Like Protease SARS-COV-2

Syamsul Falah*, Shobiroh Nuur'Alimah, Laksmi Ambarsari

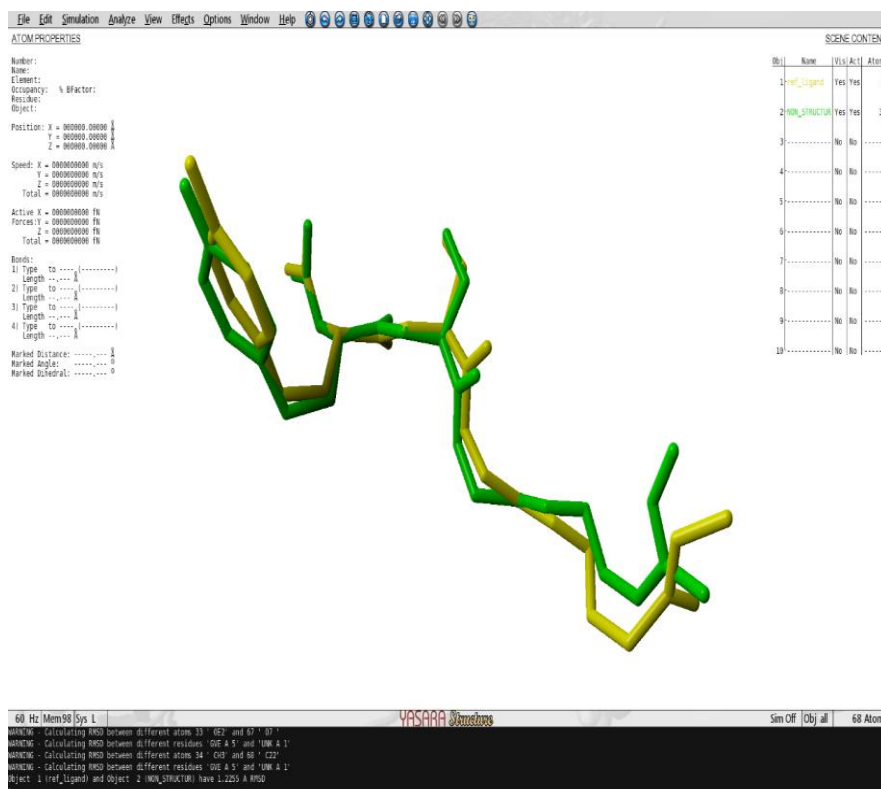
Department of Biochemistry, Faculty of Mathematics and Natural Sciences, IPB University,
Bogor 16680, Indonesia 16680

*Corresponding author email: syamsulfa@apps.ipb.ac.id

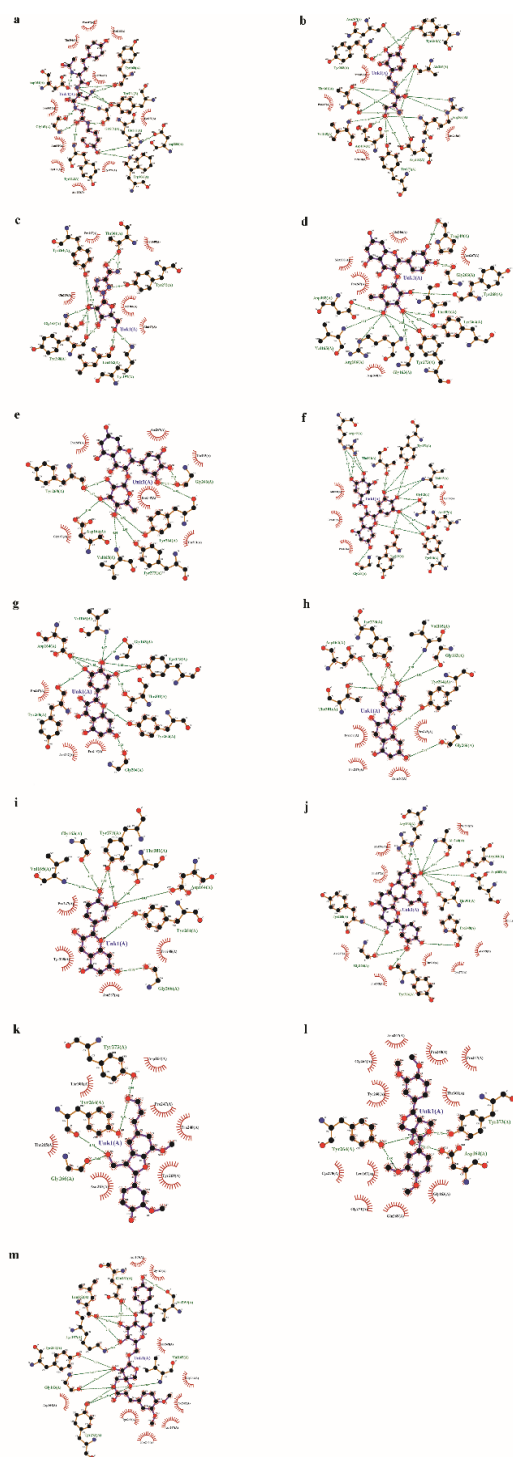
Appendix 1. Active compounds of *Syzygium polyanthum* leaf, *Swietenia macrophylla* bark, *Gmelina arborea* bark

Ligands	Source
<i>Syzygium polyanthum</i> leaf	
Quercitrin	Muthmainah (2016)
Myricitrin	Syabana <i>et al.</i> (2021b)
Epigallocatechin-3-gallate	Syabana <i>et al.</i> (2021a)
Myricetin	Dewijanti (2020)
Quercetagetin	Dewijanti <i>et al.</i> (2020)
Quercetin	Hasan <i>et al.</i> (2020)
Retusin	Alwie <i>et al.</i> (2021)
Phloretin	
Malvidin	
Delphinidin	
Flavan-3-ol	
<i>Swietenia macrophylla</i> bark	
Catechin	Falah <i>et al.</i> (2008)
Epicatechin	
Swietemacrophyllanin	
<i>Gmelina arborea</i> Roxb. bark	
Balanophonin	
Gmelinol	
(-)-p-hydroxyphenylethyl[5"-O-(3,4-dimethoxysinamoyl)- β -D-apiofuranosyl(1" $\rightarrow$ 6')]- β -D-glucopyranoside	Falah <i>et al.</i> (2008)
2-(4-hydroxyphenyl) ethanol	
2,6-dimethoxy-p-benzokuinon	
3,4,5-trimethoxyfenol	

Appendix 2. Image of the measurement of RMSD native ligand VIR251 of 1.2255Å



Appendix 3. 2D visualization results



Appendix 3. Visualization of 2D binding pocket PLpro SARS-CoV-2 with (a) native ligand VIR251, (b) Benserazide, (c) Ribavirin, (d) Quercitrin, (e) Myrcitrin, (f) Epigallocatechin-3-gallate, (g) Myrcetin, (h) Catechin, (i) Epicatechin, (j) Swietemacrophyllanin, (k) Balanophonin (l) Gmelinol, (m) (-)-p-hydroxyphenyl ethyl [5'''-O-(3,4-dimethoxysinamoyl)-β-D-apiofuranosyl(1''' → 6')]-β-D-glucopiranosida