

Supplementary material

UHPLC-MS Phytochemical Profiling and Insight into Bioactivity of Rabelera holostea (Greater Stitchwort) Extract

Jelena S. Katanić Stanković ^{1,*}, Jelena Đorović Jovanović ¹, Danijela Mišić ², Uroš Gašić ², Stefanie Nikles ³, Zoran Marković ¹, Rudolf Bauer ^{3,*}

¹ *University of Kragujevac, Institute for Information Technologies Kragujevac, Department of Science, Jovana Cvijića bb, 34000 Kragujevac, Serbia*

² *University of Belgrade, Institute for Biological Research "Siniša Stanković" – National Institute of Republic of Serbia, Department of Plant Physiology, Bulevar Despota Stefana 142, 11060 Belgrade, Serbia*

³ *University of Graz, Institute for Pharmaceutical Sciences, Department of Pharmacognosy, Bethovenstrasse 8, 8010 Graz, Austria*

Correspondence: jkatanic@kg.ac.rs (J.S.K.S.); rudolf.bauer@uni-graz.at (R.B.)

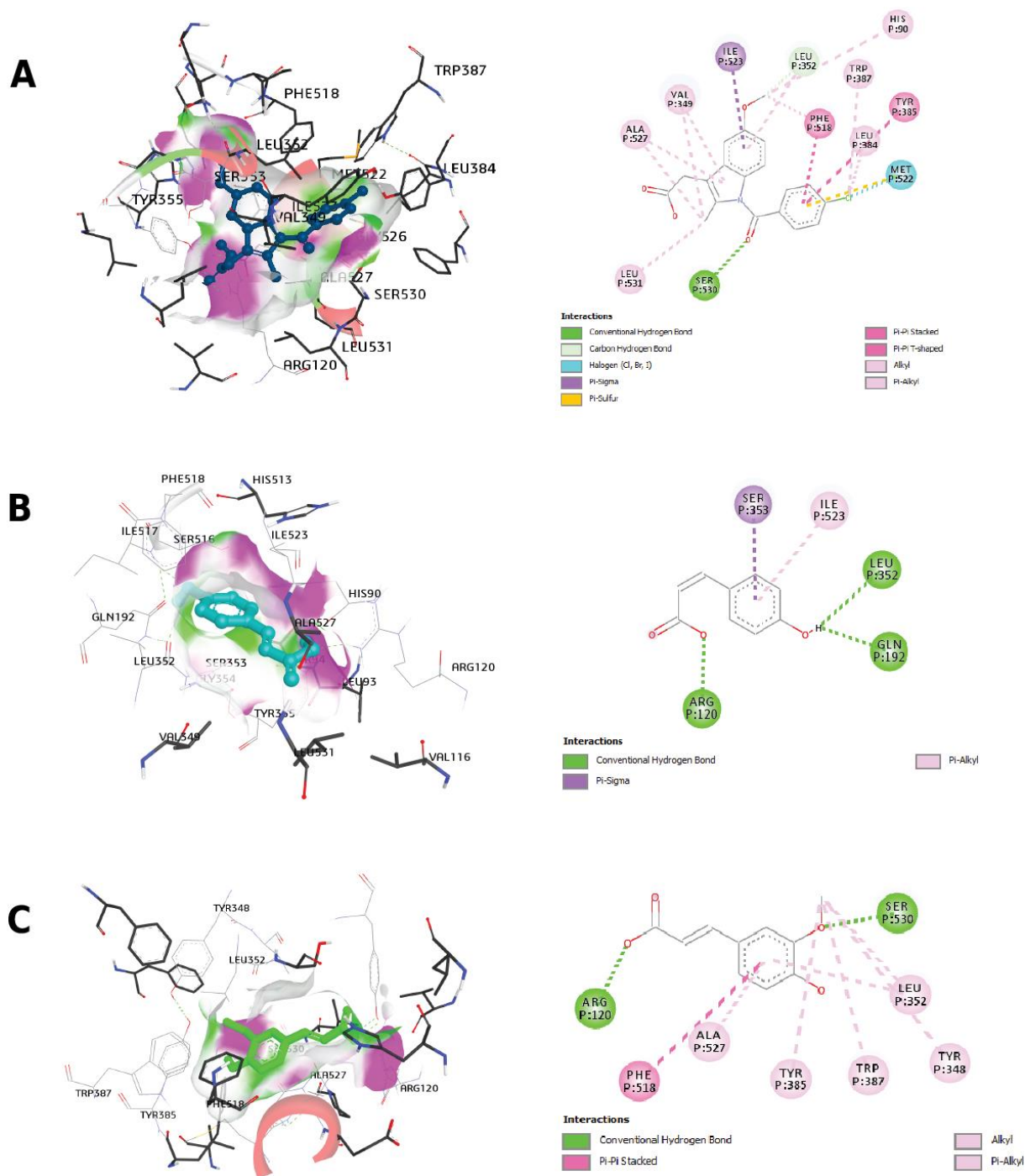


Figure S1. The established interactions of the most stable conformations of protein-ligand complex structures of: A – indomethacin (IND), B – *p*-coumaric acid (*p*-CA), and C – ferulic acid (FA) and COX-1.

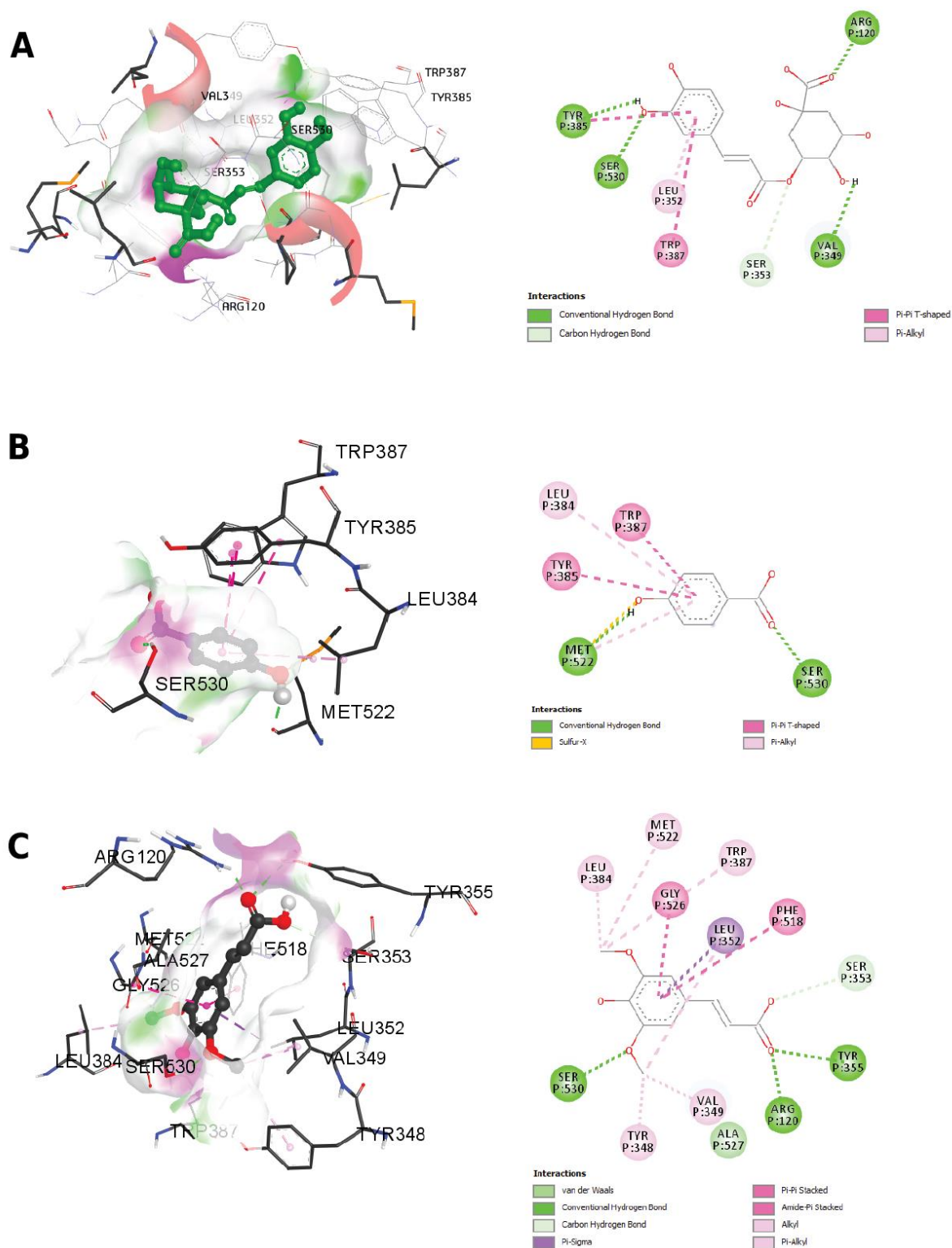


Figure S2. The established interactions of the most stable conformations of protein-ligand complex structures of: A – chlorogenic acid (CA), B – *p*-hydroxybenzoic acid (*p*-HBA), and C – synapic acid (SYN) and COX-1.

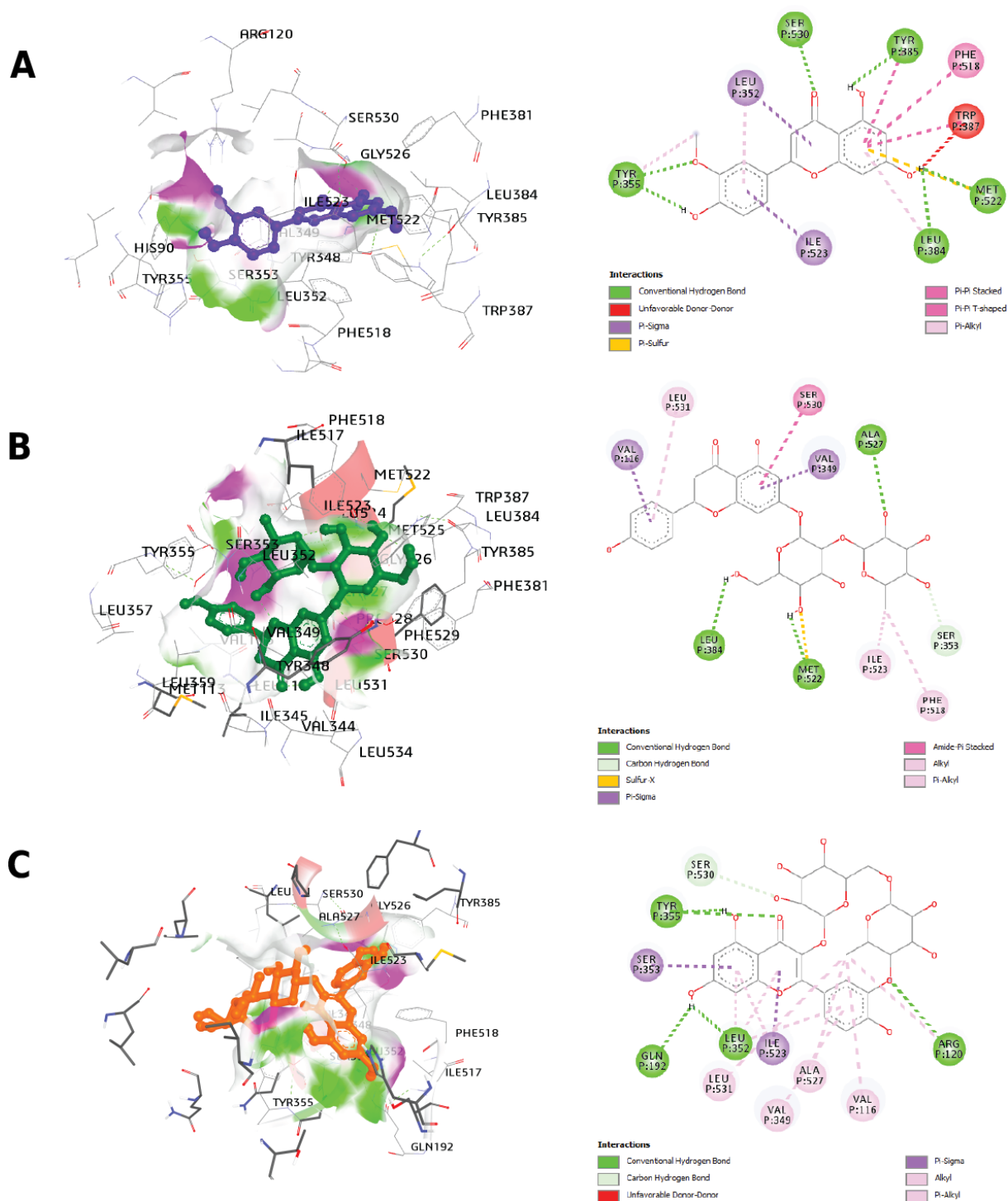


Figure S3. The established interactions of the most stable conformations of protein-ligand complex structures of: A – chrysoeriol (CHR), B – naringin (NAR), and C – rutin (RU) and COX-1.

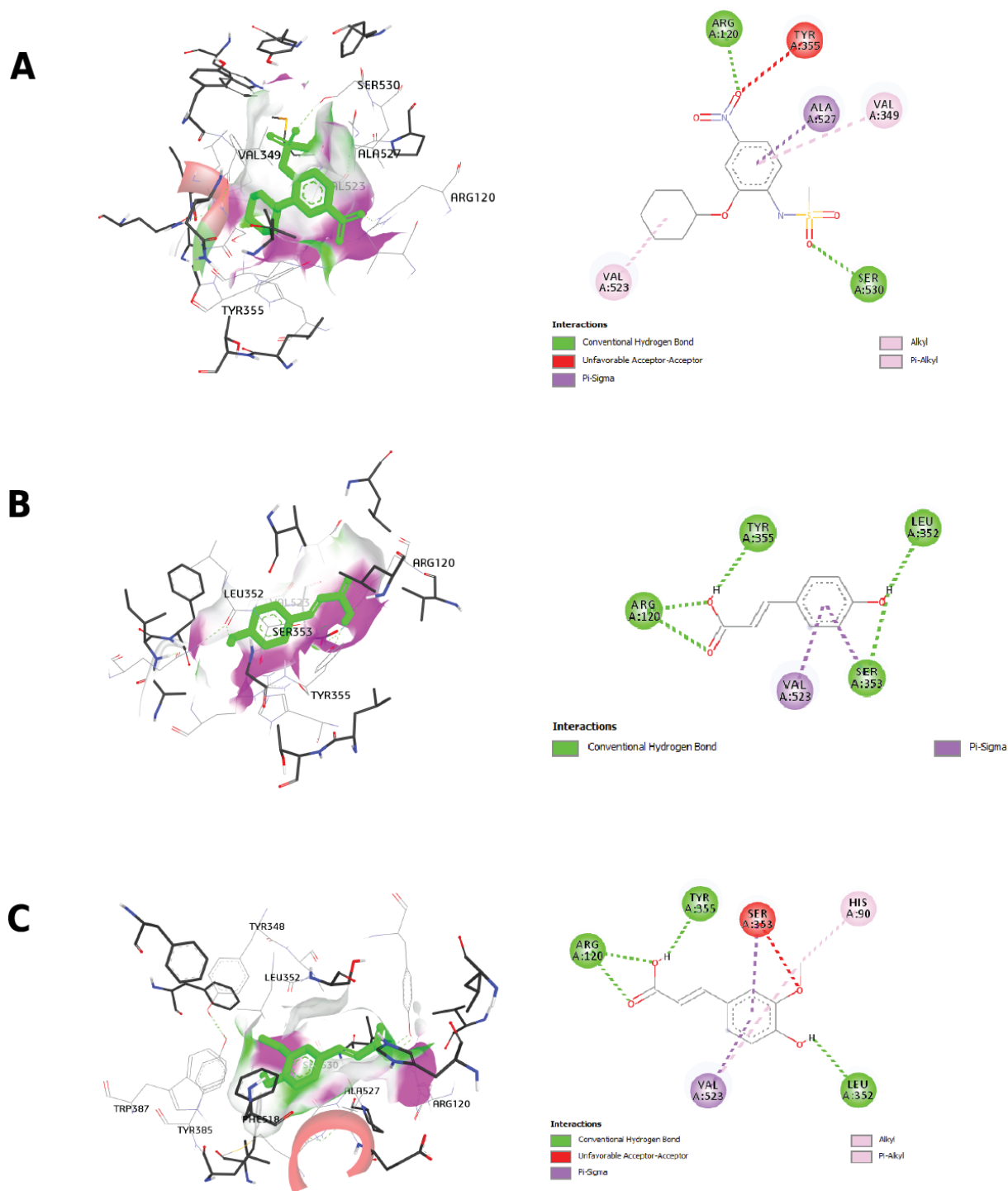


Figure S4. The established interactions of the most stable conformations of protein-ligand complex structures of: A – NS398, B – *p*-coumaric acid (*p*-CA), and C – ferulic acid (FA) and COX-2.

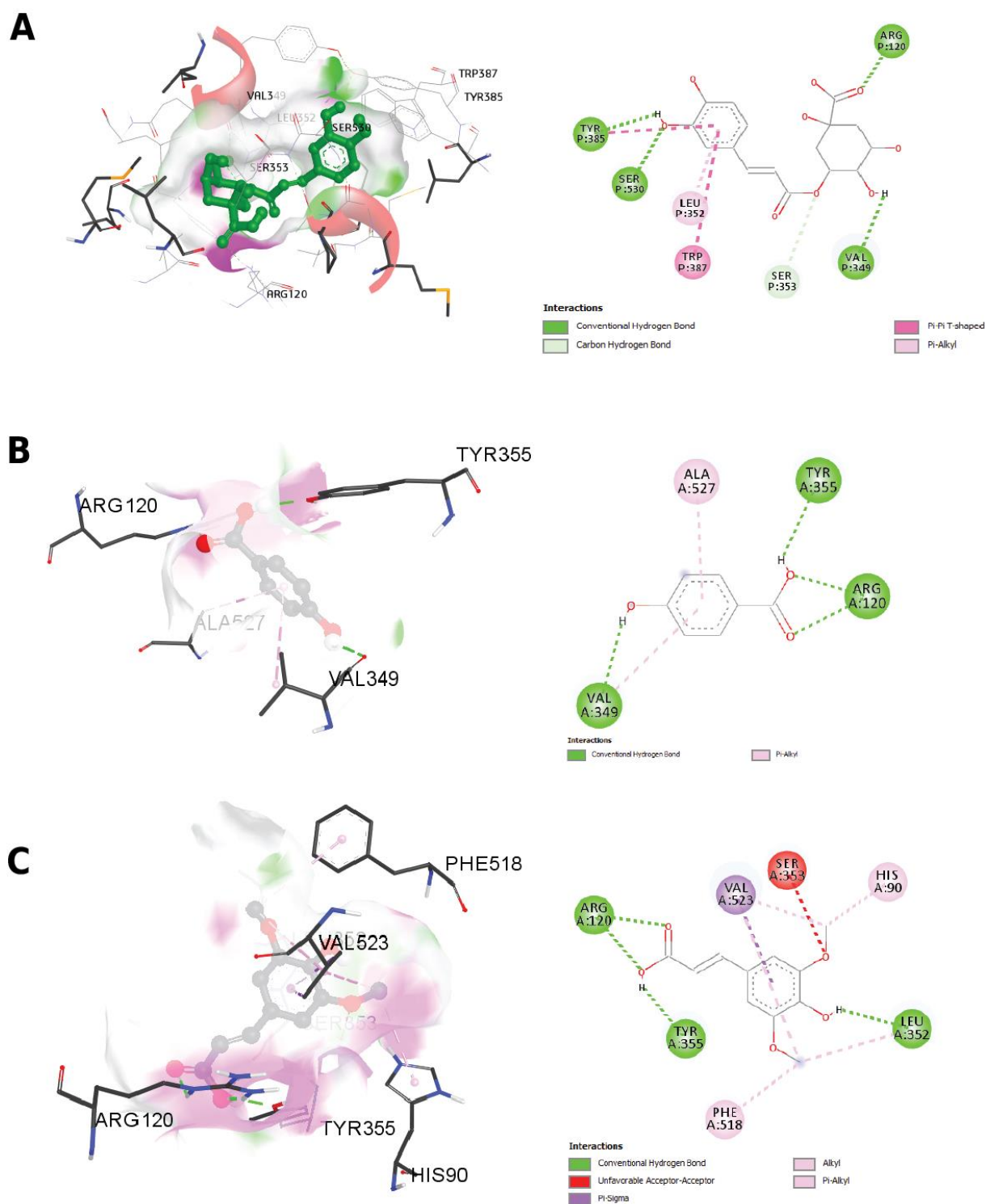


Figure S5. The established interactions of the most stable conformations of protein-ligand complex structures of: A – chlorogenic acid (CA), B – *p*-hydroxybenzoic acid (*p*-HBA), and C – synapic acid (SYN) and COX-2.

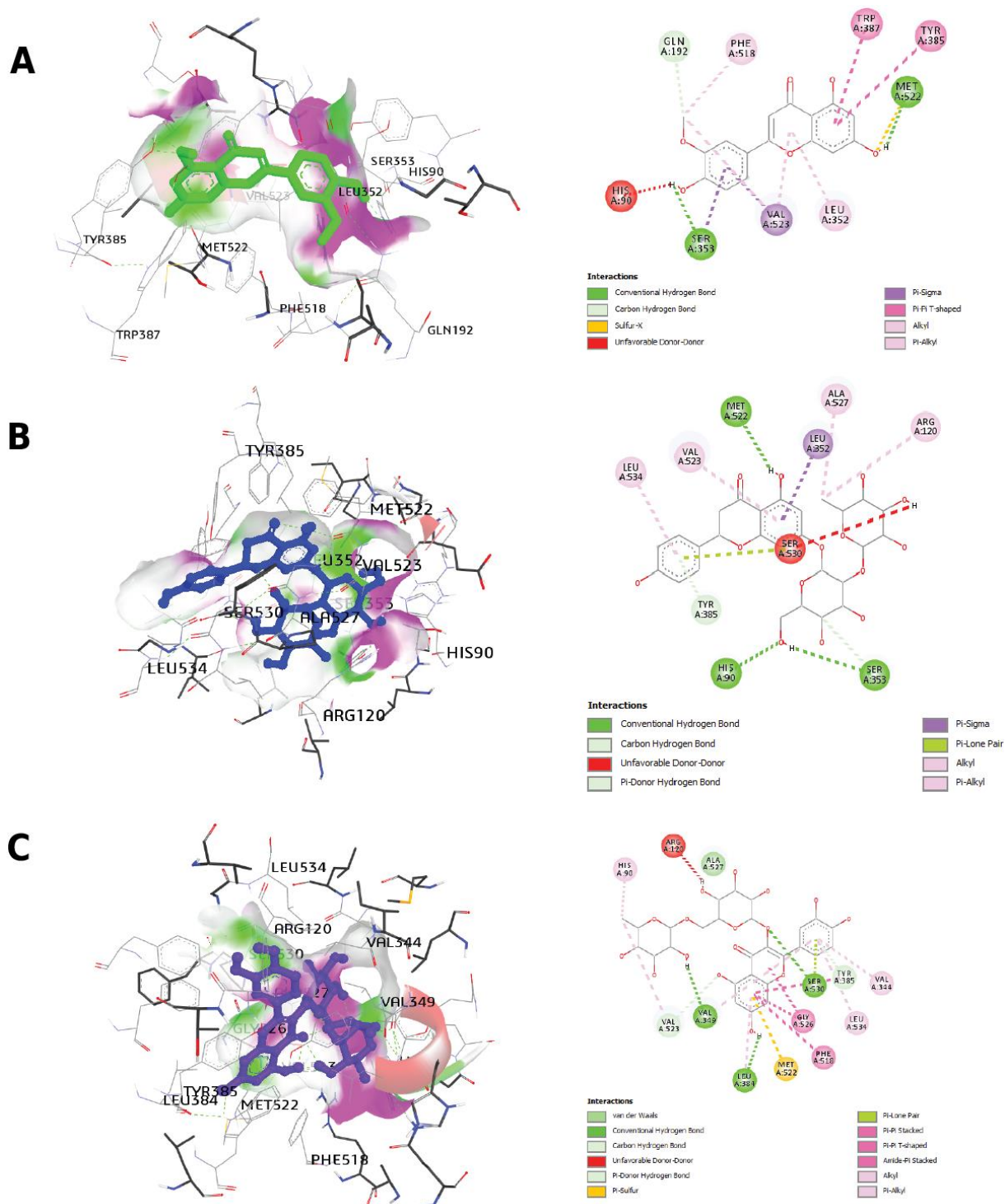


Figure S6. The established interactions of the most stable conformations of protein-ligand complex structures of: A – chrysoeriol (CHR), B – naringin (NAR), and C – rutin (RU) and COX-2.