Supplementary Data

Modern in silico molecular docking perspective for investigation of *Rindera lanata* Bunge var. *lanata* targeting: phytochemical profile, phytotoxicity and bioactivity assays

Hadi Ghanbari ^{1,2}, Sanaz Hamedeyazdan ¹, Reza Ghanbari ³, Mostafa Alilou ⁴ Abbas Delazar ^{1,7}, Samad Nejad Ebrahimi ⁵, Amirreza Nazemiyeh¹, Mohammad Yousef Memar ⁶, Hossein Nazemiyeh ^{1*}

¹ Department of Pharmacognosy, Faculty of Pharmacy, Tabriz University of Medical Sciences, Tabriz, Iran.

² Student Research Committee, Tabriz University of Medical Sciences, Tabriz, Iran.

³ Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC, USA.

⁴ Department of Pharmacognosy, Institute of Pharmacy, Center for Molecular Biosciences Innsbruck, University of Innsbruck, Innrain 80/82, 6020 Innsbruck, Austria.

⁵ Department of Phytochemistry, Medicinal Plants and Drugs Research Institute, Shahid Beheshti University, Evin, Tehran, Iran.

⁶ Infectious and Tropical Diseases Research Center, Tabriz University of Medical Sciences, Tabriz, Iran.

⁷ Drug Applied Research Center, Tabriz University of Medical Sciences, Tabriz, Iran.

Running title: Phytochemical constituents from Rindera lanata extracts

Corresponding Authors:

*Hossein Nazemiyeh: Department of Pharmacognosy, Faculty of Pharmacy, Tabriz University of Medical Sciences, Tabriz, Iran. E-mail: <u>nazemiyehh@yahoo.com</u>

Telephone: +984133341315, Fax: +984133334798.

Antioxidants, total phenol and total flavnoid standad curve



Figure S1:DPPH antioxidant test of Quercetin standard



Figure S2: Hydrogen peroxide scavenging of Ascorbic acid



Figure S3: Ferric reducing power of Quercetin standard



Figure S4: The standard curve of total flavonoids content as quercetin



Figure S5: The standard curve of total phenolics content as gallic acid



Figure S6: H-NMR compound 1



Figure S7: HMBC compound 1



Figure S8: HSQC compound 1



Figure S9: COSY compound 1



Figure S10: HNMR compund-2-Apigenin



Figure S11: HSQC compund-2-Apigenin



Figure S12: COSY compund-2-Apigenin



Figure S13: HMBC compund-2-Apigenin



Figure S14: HNMR compund-3Chrysoeriol



Figure S15: HMBC compund-3Chrysoeriol



Figure S16: HSQC compund-3Chrysoeriol



Figure S17: COSY compund-3Chrysoeriol



Figure S18: HNMR compund-4-luteulin-7glycoside



Figure S19: HMBC compund-4-luteulin-7glycoside



Figure S20: HSQC compund-4-luteulin-7glycoside



Figure S21: COSY compund-4-luteulin-7glycoside



Figure S22: HNMR compound 5rutin



Figure S23: CNMR compound 5rutin



Figure S24: HMBC compound 5rutin



Figure S25: HSQC compound 5rutin