**Supporting Information**

**Structure-based virtual screening and molecular dynamics of phytochemicals derived from Saudi medicinal plants to identify potential COVID-19 therapeutics**

**Mubarak A. Alamri\*, Ali A. Altharawi, Alhumaidi B. Alabbas, Manal A. Alossaimi, Safar M. Alqahtani**

Department of Pharmaceutical Chemistry, College of Pharmacy, Prince Sattam Bin Abdulaziz University, P.O. Box 173, Al-Kharj 11942, Saudi Arabia

\***Corresponding author**: [m.alamri@psau.edu.sa](mailto:m.alamri@psau.edu.sa)

**Table S1:** Example of top five chemical classes from the designed in-house phytochemical database.

|  |  |  |
| --- | --- | --- |
| **Chemical class** | **Phytochemicals** | **Natural Occurrence** |
| Terpenes  (monoterpenoid, diterpenoid, triterpenoid and sesquiterpenoid) | Veridiflorene, alantolactone, cadalene, β- amyrenone, friedelin curcusone A-D, psydrin, cucurnitacin B, anagallisins A, B, D & E | Psidium guajava [1]  Pulicaria crispa [2]  Euphoria hirta [3]  Jatropha curas [4]  Juniperus procera [5]  Anagallis arvensis [6] |
| Flavonoids  (flavonol, flavanone, isoflavone, flavone, and biflavonoid) | Quercetin, isokaempferoside, kaempferol-3β-rutinoside, eriodicytol, genistein, cupressuflavone, luteolin 7-rutinoside | Delonix elata [7]  Dodonea angustifolia [8]  Eruca sativa [9]  Euphoria tirucalli [10]  Fiscus benghalensis [11]  Juniperus phonicea [12]  Mrrrubium vulgare [13] |
| Alkaloids  (tropane, quinoline, isoquinoline, indole, pyrrolidine, and protoberberine) | (+)- Bicuculine, adlumidiceine, tetrahydroharman, haplotubinone, solanocapsine, solamargine | Fumaria prrviflora [14]  Guiera senegalensis [15]  Haplophyllum tuberculum [16]  Solanum surattense [17] |
| Phenol and Polyphenols | 2,4-Bis (1-phenylethyl) phenol, rosmarinic acid, chlonergic acid, methyl gallate | Jatropha curas [4]  Mrrrubium vulgare [18]  Ricinus communis [19]  Indigofera caerulea [20] |
| Steroids | Withanolide A, dinoxin B, 17-α-hydroxypregnenolone, stigmasta-7,25-diene-3β-ol, calonysterone | Daturia innoxi [21]  Jatropha curas [4]  Senna [22] |

**References**

1. Weli, A., Al-Kaabi, A., Al-Sabahi, J., Said, S., Hossain, M.A. and Al-Riyami, S., *Chemical composition and biological activities of the essential oils of Psidium guajava leaf.* Journal of King Saud University-Science, 2019. **31**(4): 993-998.

2. Alo Yahya, M., El-Sayed, A., Mossa, J., Kozlowski, J., Antoun, M., Ferin, M., Baird, W. and Cassady, J., *Potential cancer chemopreventive and cytotoxic agents from Pulicaria crispa.* Journal of natural products, 1988. **51**(3): 621-624.

3. Al-Snafi, A.E., *Pharmacology and therapeutic potential of Euphorbia hirta (Syn: Euphorbia pilulifera)-A review.* IOSR Journal of Pharmacy, 2017. **7**(3): 7-20.

4. Abdelgadir, H. and Van Staden, J., *Ethnobotany, ethnopharmacology and toxicity of Jatropha curcas L.(Euphorbiaceae): A review.* South African Journal of Botany, 2013. **88**: 204-218.

5. Alqasoumi, S.I., Farraj, A.I. and Abdel-Kader, M.S., *Study of the hepatoprotective effect of Juniperus phoenicea constituents.* Pak. J. Pharm. Sci, 2013. **26**(5): 999-1008.

6. Mahato, S.B., Sahu, N.P., Roy, S.K. and Sen, S., *Structure elucidation of four new triterpenoid oligoglycosides from Anagallis arvensis.* Tetrahedron, 1991. **47**(28): 5215-5230.

7. Jahan, I., Rahman, M., Rahman, M., Kaisar, M., Islam, M., Wahab, A. and Rashid, M., *Chemical and biological investigations of Delonix regia (Bojer ex Hook.) Raf.* Acta Pharmaceutica, 2010. **60**(2): 207-215.

8. Omosa, L.K., Amugune, B., Ndunda, B., Milugo, T.K., Heydenreich, M., Yenesew, A. and Midiwo, J.O., *Antimicrobial flavonoids and diterpenoids from Dodonaea angustifolia.* South African journal of botany, 2014. **91**: 58-62.

9. Rizwana, H., Alwhibi, M.S., Khan, F. and Soliman, D., *Chemical composition and antimicrobial activity of Eruca sativa seeds against pathogenic bacteria and fungi.* The J. Anim. Plant Sci, 2016. **26**(6): 1859-1871.

10. Le, D.T.K., Bui, H.X., Nguyen, T.T.A., Pham, T.N.K. and Duong, H.T., *Chemical constituents of Euphorbia tirucalli L.* Science and Technology Development Journal-Natural Sciences, 2018. **2**(5): 76-82.

11. Verma, V.K., Sehgal, N. and Prakash, O., *Characterization and screening of bioactive compounds in the extract prepared from aerial roots of Ficus benghalensis.* International Journal of Pharmaceutical Sciences And Research, 2015. **6**(12): 5056.

12. Alqasoumi, S.I. and Abdel-Kader, M.S., *Terpenoids from Juniperus procera with hepatoprotective activity.* Pakistan journal of pharmaceutical sciences, 2012. **25**(2).

13. Neamah, S.I., Sarhan, I.A. and Al-Shayeʼa, O.N., *Bioactive Compounds from Marrubium Vulgare L. based on in vitro Antioxidant Activity.* 2009.

14. Al-Snafi, A.E., *Fumaria parviflora-A review.* INDO AMERICAN JOURNAL OF PHARMACEUTICAL SCIENCES, 2018. **5**(3): 1728-1738.

15. Fiot, J., Sanon, S., Azas, N., Mahiou, V., Jansen, O., Angenot, L., Balansard, G. and Ollivier, E., *Phytochemical and pharmacological study of roots and leaves of Guiera senegalensis JF Gmel (Combretaceae).* Journal of ethnopharmacology, 2006. **106**(2): 173-178.

16. Al-Rehaily, A.J., Al-Howiriny, T.A., Ahmad, M.S., Al-Yahya, M.A., El-Feraly, F.S., Hufford, C.D. and McPhail, A.T., *Alkaloids from Haplophyllum tuberculatum.* Phytochemistry, 2001. **57**(4): 597-602.

17. Tekuri, S.K., Pasupuleti, S.K., Konidala, K.K., Amuru, S.R., Bassaiahgari, P. and Pabbaraju, N., *Phytochemical and pharmacological activities of Solanum surattense Burm. f.–A review.* Journal of Applied Pharmaceutical Science, 2019. **9**(03): 126-136.

18. Lodhi, S., Vadnere, G.P., Sharma, V.K. and Usman, M., *Marrubium vulgare L.: A review on phytochemical and pharmacological aspects.* Journal of Intercultural Ethnopharmacology, 2017. **6**(4): 429.

19. Abdul, W.M., Hajrah, N.H., Sabir, J.S., Al-Garni, S.M., Sabir, M.J., Kabli, S.A., Saini, K.S. and Bora, R.S., *Therapeutic role of Ricinus communis L. and its bioactive compounds in disease prevention and treatment.* Asian Pacific Journal of Tropical Medicine, 2018. **11**(3): 177.

20. Rahman, T.U., Zeb, M.A., Liaqat, W., Sajid, M., Hussain, S. and Choudhary, M.I., *Phytochemistry and pharmacology of genus indigofera: A review.* Records of Natural Products, 2018. **12**(1): 1-13.

21. Maheshwari, N.O., Khan, A. and Chopade, B.A., *Rediscovering the medicinal properties of Datura sp.: A review.* Journal of Medicinal Plants Research, 2013. **7**(39): 2885-2897.

22. Li, S.F., Di, Y.T., Wang, Y.H., Tan, C.J., Fang, X., Zhang, Y., Zheng, Y.T., Li, L., He, H.P. and Li, S.L., *Anthraquinones and lignans from Cassia occidentalis.* Helvetica Chimica Acta, 2010. **93**(9): 1795-1802.