**Supporting Information**

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

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

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|  **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] |

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