Dataset of potential Rhizoma Polygonati compound-druggable targets and partial pharmacokinetics for treatment of COVID-19

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\textbf{A B S T R A C T}

Rhizoma Polygonati (Chinese name as 黄精, pinyin as huangjing), as medicine and food homology of Traditional Chinese Medicine, has been recently applied for the complex prescriptions of alternative medicine for treatment of COVID-19 but the mechanisms are largely unclear. Here using public database search and filtering the potential chemical compound based drug targets with COVID-19 targets mapped, the list of data were provided and suggested pharmacokinetic tolerating dose of selected natural compounds were further collected from database. The data provided is the supplementary as a reference showing the intersections of Rhizoma

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Abbreviations: COVID-19, corona virus disease-2019; TCMSp, Chinese Medicine System Pharmacology Database and Analysis Platform; OB, Oral bioavailability; DL, drug-like.

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Specifications Table

| Subject | Biochemistry |
|---------|--------------|
| Specific subject area | Chemical biological binding; Traditional Chinese Medicine; Medicinal plant; Food Biochemistry |

**Type of data**

| How data were acquired | The data were acquired from TC MSP (Chinese Medicine System Pharmacology Database and Analysis Platform) and Swiss Target Prediction databases to sort out the potential targets of the main chemical components of the Rhizoma Polygonati. NCBI, GenCLiP3, and GeneCard were databases used to search COVID-19 related targets. Finally, the common targets were obtained by the Venny2.1.0 mapping. The tolerated doses of the compounds in human were obtained from the pharmacokinetic pkCSM database. |

**Data format**

| Parameters for data collection | The data were acquired from TC MSP (Chinese Medicine System Pharmacology Database and Analysis Platform) with the filtering out by the herbal medicine name “Huangjing” and bioavailability ("Oral" bioavailability) more than 30% and drug-like (DL) more than 0.18 as screening parameters for Rhizoma Polygonati. The rationale is that DL representing the chemical properties and biological properties including distribution, or toxicity related to the best clinical efficacy. OB resembles the absorption of the drug by circulation. DL≥0.18 and OB≥30% are usually used for screening conditions for active compounds in Traditional Chinese Medicine [1]. The intersection-targets of the Rhizoma Polygonati targeting COVID-19 were obtained by Venny2.1.0 based mapping. |

**Description of data collection**

| Data source location | Primary data sources: TC MSP (Chinese Medicine System Pharmacology Database and Analysis Platform); NCBI, GenCLiP3, GeneCard, GEPIA, pkCSM databases. |
| Data accessibility | With the article Mu C, Sheng Y, Wang Q, Amin A, Li X, Xie Y. Potential compound from herbal food of rhizoma polygonati for treatment of COVID-19 analyzed by network pharmacology and molecular docking technology. J Funct Foods. 2020 Aug 14:104149. doi: 10.1016/j.jff.2020.104149. Epub ahead of print. PMID: 32837538; PMCID: PMC7427583. |

**Value of the Data**

- The data are important for developing new COVID-19 drugs using Traditional Chinese Medicine derived natural products.
- Researcher, Clinician and pharmacist can benefit from the database by applying potential anti-COVID-19 drugs using herbal medicine.
- The data provide the potential chemical compound from an herb for further experimental testing in anti-COVID-19.

**1. Data Description**

Table 1 described the data obtained from the database of TC MSP (Chinese Medicine System Pharmacology Database and Analysis Platform) that drug targets of corresponding chemical
Table 1
The targets of the Rhizoma Polygonati

| Uniport ID | Gene description | Gene symbol |
|------------|------------------|-------------|
| Q02880     | DNA topoisomerase II | TOP2B       |
| P03372     | Estrogen receptor | ESR1        |
| P07900     | Heat shock protein HSP 90 | HSP90AA1   |
| P23219     | Prostaglandin G/H synthase 1 | PTGS1     |
| P35354     | Prostaglandin G/H synthase 2 | PTGS2     |
| P37238     | Amine oxidase [flavin-containing] B | MAOB      |
| P19793     | Retinoic acid receptor RXR-alpha | RXRA      |
| P48539     | Calmodulin | PC4         |
| Q14432     | CGMP-inhibited 3',5'-cyclic phosphodiesterase | PDE3A     |
| P61925     | cAMP-dependent protein kinase inhibitor alpha | PDEA1     |
| P07550     | Beta-2 adrenergic receptor | ADRB2     |
| P31645     | Sodium-dependent serotonin transporter | SLC6A4    |
| P14867     | Gamma-aminobutyric acid receptor subunit alpha-1 | GABRA1    |
| P10275     | Androgen receptor | AR          |
| Q16539     | Mitogen-activated protein kinase 14 | MAPK14    |
| P49841     | Prostaglandin G/H synthase 2 | PTGS2     |
| P24941     | Cell division protein kinase 2 | CDK2      |
| P37231     | Peroxisome proliferator activated receptor | PPARG     |
| P07477     | Trypsin-1 | PRSS1       |
| O14757     | Serine/threonine-protein kinase Chk1 | CHEK1     |
| Q15788     | Nuclear receptor coactivator 1 | NCOA1     |
| P20248     | Cyclin-A2 | CCNA2       |
| P35228     | Nitric oxide synthase, inducible | NOS2      |
| Q92731     | Estrogen receptor beta | ESR2      |
| P27487     | Dipetidyl peptidase IV | DPP4      |
| P99999     | Cytochrome c | CYCS       |
| P05164     | Myeloperoxidase | MPO         |
| P06493     | Cell division control protein 2 homolog | CDK1      |
| P15692     | Vascular endothelial growth factor A | VEGFA     |
| P10415     | Apoptosis regulator Bcl-2 | BCL2      |
| Q9GZT9     | Egl nine homolog 1 | EGLN1     |
| P04637     | Cellular tumor antigen p53 | TP53      |
| P35896     | Aryl hydrocarbon receptor | AHR       |
| Q15596     | Nuclear receptor coactivator 2 | NCOA2     |
| Q04206     | Transcription factor p65 | RELA      |
| P31749     | RAC-alpha serine/threonine-protein kinase | AKT1      |
| P01100     | Proto-oncogene c-Fos | FOS       |
| Q07812     | Apoptosis regulator BAX | BAX       |
| P14780     | Matrix metalloproteinase-9 | MMP9      |
| P42574     | Caspase-3 | CASP3       |
| Q16665     | Hypoxia-inducible factor 1-alpha | HIF1A     |
| P15407     | Fos-related antigen 1 | FOSL1     |
| P15408     | Fos-related antigen 2 | FOSL2     |
| P14635     | G2/mitotic-specific cyclin-B1 | CCNB1     |
| P01344     | Insulin-like growth factor II | IGF2      |
| P18054     | Arachidonate 12-lipoxygenase, 12S-type | ALOX12    |
| O95644     | Nuclear factor of activated T-cells, cytoplasmic 1 | NFATC1    |
| Q8NHU6     | Tudor domain-containing protein 7 | TDRD7     |
| Q96PH1     | NADPH oxidase 5 | NOX5       |
| P01469     | Fatty acid-binding protein, epidermal | FABP5     |
| P05090     | Apolipoprotein D | APOD       |
| Q12809     | Potassium voltage-gated channel subfamily H member 2 | KCNH2     |
| P11229     | Muscarinic acetylcholine receptor M1 | CHRM1     |
| P27169     | Serum paraoxonase/arylesterase 1 | PON1      |
| P05412     | Transcription factor AP-1 | JUN       |
| P11137     | Microtubule-associated protein 2 | MAP2      |
| Q14524     | Sodium channel protein type 5 subunit alpha | SCN5A     |

(continued on next page)
| Uniport ID | Gene description                              | Gene symbol |
|-----------|-----------------------------------------------|-------------|
| P21728    | Dopamine D1 receptor                          | DRD1        |
| P08173    | Muscarinic acetylcholine receptor M4          | CHRM4       |
| P28223    | 5-hydroxytryptamine 2A receptor               | HTR2A       |
| P20309    | Muscarinic acetylcholine receptor M3          | CHRM3       |
| P25100    | Alpha-1A adrenergic receptor                  | ADRA1D      |
| P06401    | Progesterone receptor                         | PGR         |
| P08172    | Muscarinic acetylcholine receptor M2          | CHRM2       |
| P35368    | Alpha-1B adrenergic receptor                  | ADRA1B      |
| Q15822    | Neuronal acetylcholine receptor subunit alpha-2| CHRNA2      |
| P35372    | Mu-type opioid receptor                       | OPRM1       |
| P55211    | Caspase-9                                     | CASP9       |
| Q14790    | Caspase-8                                     | CASP8       |
| P17252    | Protein kinase C alpha type                   | PRKCA       |
| P01137    | Transforming growth factor beta-1             | TGFBI       |
| A8MY62    | Beta-lactamase                                | LACTBL1     |
| P49327    | Fatty acid synthase                           | FASN        |
| P04040    | Catalase                                      | CAT         |
| P42345    | Serine/threonine-protein kinase mTOR          | MTOR        |
| P00441    | Superoxide dismutase [Cu-Zn]                 | SOD1        |
| P47712    | Cytosolic phospholipase A2                   | PLA2G4A     |
| P08235    | Mineralocorticoid receptor                    | NR3C2       |
| P38936    | Cyclin-dependent kinase inhibitor 1           | CDKN1A      |
| Q075469   | Nuclear receptor subfamily 1 group I member 2 | NR1I2       |
| Q92887    | Canalicular multispecific organic anion transporter 1 | ABCC2 |
| P40763    | Signal transducer and activator of transcription 3 | STAT3       |
| P60568    | Interleukin-2                                  | IL2         |
| P25105    | Platelet activating factor receptor           | PTAFR       |
| Q07817    | Apoptosis regulator Bcl-X                     | BCL2L1      |
| Q07688    | Protein phosphatase 2C beta                  | PPM1B       |
| P18031    | Protein-tyrosine phosphatase 1B              | PTPN1       |
| P36873    | Serine/threonine protein phosphatase          | PPP1CC      |
| P67775    | Serine/threonine protein phosphatase 2A, catalytic subunit, alpha isoform | PPP2CA     |
| Q15172    | Serine/threonine protein phosphatase 2A, 56 kDa regulatory subunit, alpha isoform | PPP2RSA      |
| P80365    | 11-beta-hydroxysteroid dehydrogenase 2       | HSD11B2     |
| P28845    | 11-beta-hydroxysteroid dehydrogenase 1       | HSD11B1     |
| P05230    | Acidic fibroblast growth factor               | FGF1        |
| P09038    | Basic fibroblast growth factor                | FGF2        |
| Q9Y251    | Heparanase                                    | HPSE        |
| P00734    | Thrombin                                      | F2          |
| Q9UHC9    | Niemann-Pick C1-like protein 1                | NPC1L1      |
| Q13133    | LXR-alpha                                     | NR1H3       |
| P51449    | Nuclear receptor ROR-gamma                   | RORC        |
| P05093    | Cytochrome P450 17A1                         | CYP17A1     |
| P04035    | HMG-CoA reductase                             | HMGC       |
| Q16850    | Cytochrome P450 51                           | CYP5A1      |
| P04278    | Testis-specific androgen-binding protein      | SHBG        |
| Q12772    | Sterol regulatory element-binding protein 2   | SREBF2      |
| P35398    | Nuclear receptor ROR-alpha                   | RORA        |
| P11511    | Cytochrome P450 19A1                         | CYP19A1     |
| P23975    | Cytochrome P450 2C19                         | CYP2C19     |
| P08185    | Norepinephrine transporter                    | SLC6A2      |
| P11413    | Corticosteroid binding globulin              | SERPINA6    |
| P06276    | Glucose-6-phosphate 1-dehydrogenase          | G6PD        |
| P22303    | Butyrylcholinesterase                        | BCHE        |
| P31645    | Acetylcholinesterase                         | ACHE        |
| P55055    | Nuclear receptor subfamily 1 group I member 3 | NR1I3       |
| P34995    | LXR-beta                                     | NR1H2       |
Table 1 (continued)

| Uniport ID | Gene description                                      | Gene symbol |
|------------|-------------------------------------------------------|-------------|
| P43116     | Prostanoid EP1 receptor                                | PTGER1      |
| P11473     | Prostanoid EP2 receptor                                | PTGER2      |
| O00748     | Vitamin D receptor                                     | VDR         |
| P23141     | Carboxylesterase 2                                     | CES2        |
| O14684     | Prostaglandin E synthase                               | PTGES       |
| Q9UBM7     | Anti-estrogen binding site                             | DHCR7       |
| Q07869     | Peroxisome proliferator-activated receptor alpha       | PPARA       |
| Q03181     | Peroxisome proliferator-activated receptor delta       | PPARD       |
| Q14534     | Squalene monoxygenase                                  | SQLE        |
| P29350     | Protein-tyrosine phosphatase 1C                        | PTPN6       |
| P17706     | T-cell protein-tyrosine phosphatase                    | PTPN2       |
| P23415     | Glycine receptor subunit alpha-1                       | GLRA1       |
| P37268     | Squalene synthetase                                    | FDT1        |
| P16662     | UDP-glucuronosyltransferase 2B7                        | UGT2B7      |
| P06746     | DNA polymerase beta                                    | POLB        |

Table 2

Maximum tolerated dose numeric in human obtained from pkCSM website of database [http://biosig.unimelb.edu.au/pkcsmprediction]

| Compound name                                      | Dose (mg/kg/day) |
|----------------------------------------------------|------------------|
| 3′-Methoxydaidzein                                  | 1.333            |
| 4′,5-Dihydroxyflavone                               | 1.104            |
| Baicalein                                          | 3.147            |
| (2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one     | 0.445            |
| Diosgenin                                          | 0.276            |
| (+)-Syringaresinol-O-beta-D-glucoside               | 0.595            |
| DFV                                                | 0.446            |

The compound of Rhizoma Polygonati. Table 2 is the Pharmacokinetic tolerated dose of the selected compound in human from database.

2. Experimental Design, Materials and Methods

Database of Chinese Medicine System Pharmacology Database and Analysis Platform (TCMSP, https://tcmspw.com/tcmsp.php) was applied for the collecting of chemical compound of Rhizoma Polygonati by inputting key word “Huangjing”. Based on pharmacokinetic information, oral bioavailability (OB) and drug-like (DL) with at least 30% and 0.18 respectively were used as sorting out parameters for Rhizoma Polygonati [2-5]. The corresponding drug targets were obtained from the same database of TCMSP and Swiss Target Prediction databases which are listed in Table 1. Finally the Rhizoma Polygonati targets were mapped to the COVID-19 targets by the Venny2.1.0 (https://bioinfogp.cnb.csic.es/tools/venny/) and the intersection-targets were obtained [6-9].

Pharmacokinetic properties of the selected chemical compounds were obtained by searching pkCSM website of database (http://biosig.unimelb.edu.au/pkcsmprediction) by inputting SMILES files.

Ethics Statement

Not Applicable.
Credit Author Statement

Chenglin Mu: Data curation. Yifan Sheng: Writing- Original draft preparation. Qian Wang: Visualization, Investigation. Amr Amin: Supervision, Conceptualization. Xugang Li: Methodology, Supervision, Writing- Reviewing. Yingqiu Xie: Writing- Original draft preparation, Conceptualization.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships which have, or could be perceived to have, influenced the work reported in this article.

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