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Data Article

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

Chenglin Mu[1,6], Yifan Sheng[2], Qian Wang[3], Amr Amin[4], Xugang Li[1,6,*], Yingqiu Xie[5,*]

[1] State Key Laboratory of Crop Biology, College of Life Sciences, Shandong Agricultural University, Daizong Street 61, Tai'an, 271018, China
[2] College of Life Science, Northeast Agricultural University, Harbin, 150030, China
[3] Tai'an Xianlu Food Co. Ltd., Tai'an, China
[4] Biology Department, UAE University, Al Ain 15551, UAE
[5] Department of Biology, School of Sciences and Humanities, Nazarbayev University, Nur-Sultan, 010000, Republic of Kazakhstan
[6] Sino German Joint Research Center for Agricultural Biology, College of Life Sciences, Shandong Agricultural University, Daizong Street 61, Tai'an, 271018, China

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ABSTRACT

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

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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* Corresponding authors.
E-mail addresses: Chenglinmusdau@163.com (C. Mu), shengyf317@126.com (Y. Sheng), 18953811122@163.com (Q. Wang), a.amin@uaeu.ac.ae (A. Amin), xgli@sdau.edu.cn (X. Li), yingqiu.xie@nu.edu.kz (Y. Xie).

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Polygonati druggable targets of lists from current database and potentially related ones targeting COVID-19.

Specifications Table

Subject	Biochemistry
Specific subject area	Chemical biological binding; Traditional Chinese Medicine; Medicinal plant; Food Biochemistry
Type of data	Table
How data were acquired	The data were acquired from TCMSP (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	Raw
Parameters for data collection	The data were acquired from TCMSP (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	Secondary Data.
Data source location	Primary data sources: TCMSP (Chinese Medicine System Pharmacology Database and Analysis Platform); NCBI, GenCLiP3, GeneCard, GEPIA, pKCSM databases.
Data accessibility	With the article
Related research 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 TCMSP (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*
P27338	Amine oxidase [flavin-containing] B	*MAOB*
P19793	Retinoic acid receptor RXR-alpha	*RXRA*
P48539	Calmodulin	*PCP4*
Q14432	CGMP-inhibited 3′,5′-cyclic phosphodiesterase A	*PDE3A*
P61925	cAMP-dependent protein kinase inhibitor alpha	*PKIA*
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	Glycogen synthase kinase-3 beta	*GSK3B*
P24941	Cell division protein kinase 2	*CDK2*
P37231	Peroxisome proliferator activated receptor gamma	*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	Dipeptidyl 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*
P35869	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*
Q01469	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*)

Table 1 (*continued*)

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	*TGFB1*
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*
O75469	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*
O75688	Protein phosphatase 2C beta	*PPM1B*
P18031	Protein-tyrosine phosphatase 1B	*PTPN1*
P36873	Serine/threonine protein phosphatase PP1-gamma catalytic subunit	*PPP1CC*
P67775	Serine/threonine protein phosphatase 2A, catalytic subunit, alpha isoform	*PPP2CA*
Q15172	Serine/threonine protein phosphatase 2A, 56 kDa regulatory subunit, alpha isoform	*PPP2R5A*
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	*HMGCR*
Q16850	Cytochrome P450 51	*CYP51A1*
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*

(*continued on next page*)

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 monooxygenase	*SQLE*
P29350	Protein-tyrosine phosphatase 1C	*PTPN6*
P17706	T-cell protein-tyrosine phosphatase	*PTPN2*
P23415	Glycine receptor subunit alpha-1	*GLRA1*
P37268	Squalene synthetase	*FDFT1*
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/pkcsm/prediction)

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

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/pkcsm/prediction) 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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