



Data Article

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

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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; TCMSPP, Chinese Medicine System Pharmacology Database and Analysis Platform; OB, Oral bioavailability; DL, drug-like.

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

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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. $DL \geq 0.18$ and $OB \geq 30\%$ 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. <i>J Funct Foods</i> . 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 1The 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	HSR90AA1
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
Q14757	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

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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 1 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 1 member 3	NR1I3
P34995	LXR-beta	NR1H2

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Table 1 (continued)

Uniport ID	Gene description	Gene symbol
P43116	Prostanoid EP1 receptor	<i>PTGER1</i>
P11473	Prostanoid EP2 receptor	<i>PTGER2</i>
O00748	Vitamin D receptor	<i>VDR</i>
P23141	Carboxylesterase 2	<i>CES2</i>
O14684	Prostaglandin E synthase	<i>PTGES</i>
Q9UBM7	Anti-estrogen binding site	<i>DHCR7</i>
Q07869	Peroxisome proliferator-activated receptor alpha	<i>PPARA</i>
Q03181	Peroxisome proliferator-activated receptor delta	<i>PPARD</i>
Q14534	Squalene monooxygenase	<i>SQLE</i>
P29350	Protein-tyrosine phosphatase 1C	<i>PTPN6</i>
P17706	T-cell protein-tyrosine phosphatase	<i>PTPN2</i>
P23415	Glycine receptor subunit alpha-1	<i>GLRA1</i>
P37268	Squalene synthetase	<i>FDFT1</i>
P16662	UDP-glucuronosyltransferase 2B7	<i>UGT2B7</i>
P06746	DNA polymerase beta	<i>POLB</i>

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://tcmssp.com/tcmssp.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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References

- [1] SS Ahmed, V. Ramakrishnan, Systems biological approach of molecular descriptors connectivity: optimal descriptors for oral bioavailability prediction, *PLoS One* 7 (7) (2012) e40654 Epub 2012 Jul 16 PMID:22815781 PMID: PMC3398012, doi:10.1371/journal.pone.0040654.
- [2] J. Ru, et al., TCMSP: a database of systems pharmacology for drug discovery from herbal medicines, *J Cheminform* 6 (2014) 13.
- [3] S.S. Ahmed, V. Ramakrishnan, Systems biological approach of molecular descriptors connectivity: optimal descriptors for oral bioavailability prediction, *PLoS One* 7 (7) (2012) e40654.
- [4] X. Xu, et al., A novel chemometric method for the prediction of human oral bioavailability, *Int J Mol Sci* 13 (6) (2012) 6964–6982.
- [5] A. Daina, O. Michielin, V. Zoete, Swiss target prediction: updated data and new features for efficient prediction of protein targets of small molecules, *Nucleic Acids Res* 47 (W1) (2019) W357–W364.
- [6] G. Stelzer, et al., The Gene cards suite: from gene data mining to disease genome sequence analyses, *Curr Protoc Bioinformatics* 54 (2016) 1301–13033.
- [7] J.H. Wang, et al., GenCLIP 3: mining human genes' functions and regulatory networks from PubMed based on co-occurrences and natural language processing, *Bioinformatics* (2019).
- [8] L. Sun, et al., DiVenn: an interactive and integrated web-based visualization tool for comparing gene lists, *Front Genet* 10 (2019) 421.
- [9] C Mu, Y Sheng, Q Wang, A Amin, X Li, Y Xie, 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) 104149 Epub ahead of print PMID:32837538 PMID: PMC7427583, doi:10.1016/j.jff.2020.104149.