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Configuration of complex traditional Chinese medicine prescriptions using digit topology circles

Yi LU[a*], Bo PENG[b, c], Saimei LI[c]

a. College of Mechanical Engineering, Yanshan University, Qinhuangdao, Hebei 066004, China

b. Guangzhou Deyi Jingcheng Traditional Chinese Medicine Clinic Co. Ltd., Guangzhou, Guangdong 510260, China

c. The First Affiliated Hospital of Guangzhou University of Chinese Medicine, Guangzhou, Guangdong 510405, China

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ABSTRACT

Objective To configure the complex traditional Chinese medicine (TCM) prescription using digit topology circle and to derive digit topology circle.

Methods The basic digit topology circles were constructed. Different digit topology circles were derived using basic digit topology circle, the character strings, and the digit groups. Different digit topology circles with ternary Chinese medicine were derived by adding ternary Chinese medicine into digit topology circles. The valuable TCM prescriptions were configured using the derived digit topology circles.

Results Nine simple basic digit topology circles were constructed from the character strings. Multiple digit topology circles and some digit topology circles with ternary Chinese medicine were derived using basic digit topology circles, the character strings, and the digit groups. Four complex TCM prescriptions were configured using four derived digit topology circles digit topology circles, respectively.

Conclusion The digit topology circles can be used to configure some existing TCM prescriptions and many novel TCM prescriptions. It has been verified that some existing TCM prescriptions have been used successfully to treat patients with diseases. Some novel valuable TCM prescriptions configured by digit topology circles may be used to treat patients with diseases.

1 Introduction

Traditional Chinese medicine (TCM) has accumulated rich resources and clinical experience through research aimed at exploring the prevention and treatment of various diseases. However, current medicine lacks in-depth research and validation regarding the established protocols and mechanisms of prescribed TCM at both macro and micro levels [1].

ZHAI et al. [2] summarized the key databases commonly used in network pharmacology, including those focused on herbs, components, diseases, as well as dedicated platforms for network pharmacology analysis. Mining data from TCM prescriptions is one of the important methods for inheriting the clinical experience of eminent physicians and developing novel therapeutic drugs [3]. Topology diagram of TCM prescriptions is a visual model that employs complex systematic thinking to analyze the

*Corresponding author: Yi LU, E-mail: luyi@ysu.edu.cn.

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structural relationships within prescriptions, thereby revealing the dynamic connections and overall efficacy in medicinal materials. Its core lies in revealing the dynamic connections and overall efficacy between these medicinal materials. In this aspect, CHEN et al. [4] applied network pharmacology and molecular docking techniques to clarify the molecular mechanisms of two TCM prescriptions of climacteric syndrome, and used topology analysis to explore the core targets and action pathways of Erzhi Pill (二至丸)-Erxian Decoction (二仙汤) for treating climacteric syndrome with a strategy of same disease treated differently. ZHANG et al. [5] examined the decoction mechanisms through network pharmacology analysis, and constructed a network diagram illustrating the relationships between active components and intersection targets. CHEN et al. [6] explored the mechanism by which compound Hongginshen Decoction (红极参汤) in improving pulmonary fibrosis through network pharmacology, and constructed the network diagram of the TCM component-disease target interaction for compound Hongginshen Decoction and analyzed the results. JI et al. [7] constructed the target protein-protein interaction (PPI) network to identify the key target proteins with network topology parameters. YU et al. [8] imported intersection targets of herbal medicine and disease into the Search Tool for the Retrieval of Interacting Genes/Proteins (STRING) database to construct PPI network, and subsequently screened key targets by network topology algorithms. CHU et al. [9] explored the potential mechanisms of Danzhi Xiaoyao Pills (丹栀逍遥丸) in treating depression by integrating network pharmacology and molecular docking techniques based on existing literature reports. REN et al. [10] proposed an integrated method combining serum pharmacochemistry, network pharmacology, and pharmacokinetics to screen and determine bioactive ingredients of Gushudan (骨疏丹) for osteoporosis treatment. LIU et al. [11] discovered the mechanisms of Liuwei Dihuang Pills (六味地黄丸) in treating parkinson's disease based on network pharmacology and molecular docking. ZHANG et al. [12] conducted a clinical observation study on the combined therapy of Hegu (LI14) acupuncture of Guizhi Shaoyao Decoction (桂枝芍药汤) for myofascial pain syndrome treatment. HU et al. [13] completed an experience-based analysis of Guizhi Qu Shaoyao Decoction (桂枝去芍药汤) in treating viral myocarditis. The results of the aforementioned studies have provided foundational technological support for the digit TCM. However, up to now, most TCM prescriptions are proposed by practitioners based on empirical knowledge and human intelligence. Generally, various valuable complex TCM prescriptions remain to be further developed to effectively treat diverse diseases. Topology graph (TG) is an effective tool for constructing complex mechanisms [14, 15]. In fact, the configuration of the TCM prescriptions is similar to the TG-based mechanisms. Let (*b*, *t*, *q*, *p*, *h*, ...) be (binary, ternary, quaternary, pentagonal, hexagonal, ...) link in mechanism. A digit topological circle with *n* (*q*, *p*, *h*, ...) excluding (*b*, *t*) was proposed for the type synthesis of complex closed robotic mechanisms because it is simpler than TG [16]. Therefore, it is a significant and challenging issue to configure the valuable complex TCM prescriptions using the digit topological circle. For this reason, several studies are conducted as follows.

(i) Discover the relationships between TCM and digit topological circle, and construct basic digit topology circles.

(ii) Derive different digit topological circles using basic digit topology circles, the character strings, and the digit groups.

(iii) Configure the valuable complex TCM prescriptions with digit topology circles.

2 Discover of conceptions of digit topology circles and its deviation rules

2.1 Relation among topology graph, prescription of TCM, and digit topology circle

In the topological graph TG, vertices denoted by *b*, *t*, *q*, *p*, *h* corresponded to binary, ternary, quaternary, pentagonal, hexagonal links, respectively. Each type (*b*, *t*, *q*, *p*, *h*) was represented by a dot v_u to connect with other (2, 3, 4, 5, 6) links, respectively [14, 15]. Generally, the complex TG included numerous edges that interconnect all dots. Any pair of dots is connected by several parallel edges. Each edge can be formed by several serial-connecting binary links, thereby forming various serial kinematic pairs or actuators. Let $C_{n(k)i}$ represent a basic digit topology circle. Let $C_{n(k)i,j}$ represent a digit topology circle.

A digit topology circle $C_{n(k)i,j}$ included *n* (*q*, *p*, *h*, ...) links, represented by *n* dots. $C_{n(k)i,j}$ was formed by a circle, *n* dots on circle, and several lines and *n* arcs. Each line or arc in $C_{n(k)i,j}$ was formed by a group parallel edge for two dots links. The digit marked on the line or the arc was the edge number of every group parallel edges. One or more *t* can be added in $C_{n(k)i,j}$ to derive $C_{n(k)i,j}$ with *n* (*t*, *q*, *p*, *h*, ...). In order to configure the TCM prescriptions with $C_{n(k)i,j}$, some symbols and subscripts are presented in Table 1.

The medicinal materials in the TCM prescriptions categorized as ternary *t*, quaternary *q*, pentagonal *p*, hexagonal *h*, etc., which were formed from the TCM rationale and the TCM experts or practitioners. Here, some medicinal materials (*t*, *q*, *p*, *h*) in the TCM prescriptions can be configured with other medicinal materials (3, 4, 5, 6), respectively. In fact, any medicinal materials may be categorized as one of the (*t*, *q*, *p*, *h*, ...) types when divided into (3, 4, 5, 6, ...) parts based on the dose, strength, and the therapeutic efficacy, respectively. Through rational combination and medicinal materials (*t*, *q*, *p*, *h*, ...) efficacy,

Table 1 Symbols and subscripts of TCM prescriptions and $C_{n(k)i,j}$

Symbol	Description
TCM	Traditional Chinese medicine
v_u	Dot in digit topology circle, $u = 1, ..., n$
e	Edge (single curve) in TG
b, n_b	Binary medicinal material, its number
t, n_t	Ternary medicinal material, its number
q, n_q	Quaternary medicinal material, its number
p, n_p	Pentagonal medicinal material, its number
h, n_h	Hexagonal medicinal material, its number
$C_{n(k)i}$	Basic digit topology circle
$C_{n(k)i,j}$	Digit topology circle with n (q, p, h, ...)
n	The number of dots or the number of digit arcs in $C_{n(k)i,j}$, $n = n_q + n_p + n_h + ...$
k	The number of valid character strings
i	The order number of different basic $C_{n(k)i}$
j	The sub-order number of different $C_{n(k)i,j}$
n_e	The number of edges in $C_{n(k)i,j}$, $n_e = (4n_q + 5n_p + 6n_h + ...)/2$
n_u	The number of e adjacent to v_u, n_u is (3, 4, 5, 6, ...) as (t, q, p, h, ...) in $C_{n(k)i,j}$
e_d	Line or arc formed by d parallel edges for connecting two dots and marked by digit d

diverse valuable TCM prescriptions can be configured to address various diseases.

Given that complex TCM prescriptions may include n (t, q, p, h, ...) medicinal materials combined with other medicinal materials (3, 4, 5, 6, ...), their configuration and isomorphism identification become highly complicated. Thus, a digit topological circle $C_{n(k)i,j}$ with n (q, p, h, ...), excluding (b, t) was proposed for configuring diverse valuable complex TCM prescriptions. By excluding $C_{n(k)i,j}$ (b, t) links, $C_{n(k)i,j}$ can be represented with fewer labeled lines and arcs, simplifying its derivation compared to complex TG. Therefore, it is easy to configure complex TCM prescriptions using $C_{n(k)i,j}$.

Let n_e donated the number of edges. The n_e can be calculated using formula: $n_e = (2n_b + 3n_t + 4n_q + 5n_p + 6n_h + ...)/2$. The basic $C_{n(k)i}$ is valid if n_e is a integral number, otherwise, it is invalid. Generally, n (q, p, h, ...) in the basic $C_{n(k)i}$ can be represented by distinct character strings in valid orders. Multiple basic $C_{n(k)i}$ configurations can be derived from the same characteristics string. Here, valid orders of the character string excluded repetitive, cyclic, and reversed sequences to minimize symmetric isomorphism of $C_{n(k)i}$. A single character string of n (q, p, h, ...) may correspond to multiple valid orders for deriving different basic $C_{n(k)i}$. The subscript k donates the number of distinct valid character strings for n (q, p, h, ...), while the subscript i increments from 1.

Examples of valid basic $C_{n(k)i}$ configurations, including n (q, p, h, ...) (n = 2, ..., 6; k = 1, ..., 6), and the valid character strings for $n \leqslant 6$ (q, p, h) in the basic $C_{n(k)i}$ are given in Table 2. For instance, $C_{6(k)6}$ included {n = 6, 3q + 2p + h, $n_e = (4n_4 + 5n_5 + 6n_6)/2 = (4 \times 3 + 5 \times 2 + 6 \times 1)/2$ = 14}. (3q, 2p, h) in $C_{6(k)6}$ has 5 distinct valid character strings (hpqqqp, hppqqq, ppqhqq, pqphqq, ppqhqq) as k = 1, ..., 5, respectively, see Table 2. Each of these strings can be used to derive 5 distinct basic $C_{6(k)6}$ (k = 1, ..., 5). Additionally, the nine simple basic digit topology circles, including $C_{2(1)i}$ (i = 3, 4, 5) and $C_{3(1)i}$ (i = 1, ..., 6), are constructed, see Figure 1 (a1, ..., a9), where, digits on arcs represented the number of edges.

For instance, the digits (2, 2) in $C_{2(1)3}$ represent that q_1 is connected with q_2 via two edges of 2e each. Similarly, the digits (3, 1, 3) in $C_{3(1)3}$ represent that h is connected to q_1 via a 3e edge, q_1 to q_2 via a 1e edge, and h to q_2 via another 3e edge. When deriving a TCM prescription from $C_{n(k)i}$, the digit marked on the line or arc in $C_{n(k)i}$ is the frequency number of the two configured medicinal materials compatibility. Thus, to derive a TCM prescription using $C_{2(k)3}$, (2, 2) in $C_{2(k)3}$ represent that the frequency number of two configured quaternary medicinal materials q_1 and q_2 are 4 times. For deriving other TCM prescriptions by $C_{3(1)3}$, (3, 1, 3) in $C_{3(1)3}$ represent that the frequency number of configured the hexagonal medicinal material h and the quaternary medicinal material q_1 are 3 times, the frequency number of configured two quaternary medicinal materials q_1 and q_2 are 1 time, the frequency number of configured the same h and the quaternary medicinal material q_2 are 3 times.

Generally, the more frequently two medicinal materials are used in combination, the greater their mutual efficacy is. In the light of the medicinal material (h, p, q, t) efficacy in TCM prescriptions, implying that the efficacy of q is larger than that of t, the efficacy of p is larger than that of q, the efficacy of h is larger than that of p. Therefore, the relationships of (h, p, q, t) medicinal materials in $C_{n(k)i,j}$ is similar to the relationships of (monarch, minister, assistant, and messenger) medicinal materials in the TCM combinations.

2.2 Construction of basic $C_{n(k)i}$ and rules of digits marked in $C_{n(k)i}$

A basic digit topology circle $C_{n(k)i}$ with n (q, p, h, ...) is constructed by a circle, n dots v_u (u = 1, ... , n), n_l lines $n_l = n(n-3)/2$ marked by digit, and n arcs marked by digit. The n dots v_u are arranged uniformly on the circle in counter-clockwise for representing n (q, p, h, ...).

The basic $C_{n(k)i}$ n = (3, 4, 5, 6, 7) are constructed, see Figure 2. The rules of digits marked in $C_{n(k)i}$ are given in Table 3.

Each dot v_u had a sub-digit group including n – 1 digits $\{d_{u1}d_{u2} ... d_{u(n-1)}\}$ in clockwise for representing the connection relations between dot v_u and other n – 1 dots. The v_u and $\{d_{u1}d_{u2} ... d_{u(n-1)}\}$ in $C_{n(k)i}$ satisfy 4 conditions as follows.

(i) The v_u was represented (q, p, h, ...), indicating $n_u = d_{u1} + d_{u2} ... + d_{u(n-1)}$ = (4, 5, 6, ...).

Table 2 Basic $C_{n(k)i}$ (n = 2, 3, ..., 6) including $n \leqslant 6$ (b, t, q, p, h) and their valid characteristics strings

$C_{n(k)i}$	n = 2, ..., 5	n_e	Valid characteristics string
$C_{2(k)1}$	$2b$	2	bb
$C_{2(k)2}$	$2t$	3	tt
$C_{2(k)3}$	$2q$	4	qq
$C_{2(k)4}$	$2p$	5	pp
$C_{2(k)5}$	$2h$	6	hh
$C_{3(k)1}$	$3q$	6	qqq
$C_{3(k)2}$	$q + 2p$	7	qpp
$C_{3(k)3}$	$2q + h$	7	qqh
$C_{3(k)4}$	$q + 2h$	8	qhh
$C_{3(k)5}$	$2p + h$	8	pph
$C_{3(k)6}$	$3h$	9	hhh
$C_{4(k)1}$	$4q$	8	qqqq
$C_{4(k)2}$	$3q + h$	9	qqqh
$C_{4(k)3}$	$2q + 2p$	9	qqpp, qpqp
$C_{4(k)4}$	$2q + 2h$	10	qqhh, qhqh
$C_{4(k)5}$	$4p$	10	pppp
$C_{4(k)6}$	$q + 2p + h$	10	qpph, qphp
$C_{4(k)7}$	$2p + 2h$	11	pphh, phph
$C_{4(k)8}$	$q + 3h$	11	qhhh
$C_{4(k)9}$	$4h$	12	hhhh
$C_{5(k)1}$	$5q$	10	qqqqq
$C_{5(k)2}$	$3q + 2p$	11	qqqpp, qpqpq
$C_{5(k)3}$	$4q + h$	11	qqqqh
$C_{5(k)4}$	$q + 4p$	12	qpppp
$C_{5(k)5}$	$3q + 2h$	12	qqqhh, qhqqh
$C_{5(k)6}$	$2q + 2p + h$	12	qqpph, qpqph, qhqpp, qqphp
$C_{5(k)7}$	$4p + h$	13	pppph
$C_{5(k)8}$	$q + 2p + 2h$	13	qpphh, qhphp, pqphh, pphqh,
$C_{5(k)9}$	$2q + 3h$	13	qqhhh, qhqhh
$C_{5(k)10}$	$q + 4h$	14	qhhhh
$C_{5(k)11}$	$5h$	15	hhhhh
$C_{6(k)1}$	$6q$	12	qqqqqq
$C_{6(k)2}$	$4q + 2p$	13	ppqqqq, qpqqqp, pqqpqq
$C_{6(k)3}$	$5q + h$	13	hqqqqq
$C_{6(k)4}$	$2q + 4p$	14	qqpppp, qpqppp, qppqpp
$C_{6(k)5}$	$4q + 2h$	14	hhqqqq, hqhqqq, hqqhqq
$C_{6(k)6}$	$3q + 2p + h$	14	hpqqqp, hppqqq, ppqhqq, pqphqq, ppqhqq
$C_{6(k)7}$	$q + 4p + h$	15	qhpppp, ppqpph, pqpppp
$C_{6(k)8}$	$2q + 2p + 2h$	15	qqpphh, qqphhp, qqphph, qphqph, pphqhh, qphqph
$C_{6(k)9}$	$3q + 3h$	15	qqqhhh, qhqhqh, qhqqhh, qqhqhh
$C_{6(k)10}$	$6p$	15	pppppp
$C_{6(k)11}$	$q + 2p + 3h$	16	qphhhp, qpphhh, ppqhhh
$C_{6(k)12}$	$2q + 4h$	16	qqhhhh, qhqhhh, qhhqhh
$C_{6(k)13}$	$4p + 2h$	16	hhpppp, hphppp,hpphpp
$C_{6(k)14}$	$2p + 4h$	17	pphhhh, phphhh, phhphh
$C_{6(k)15}$	$q + 5h$	17	qhhhhh
$C_{6(k)16}$	$6h$	18	hhhhhh

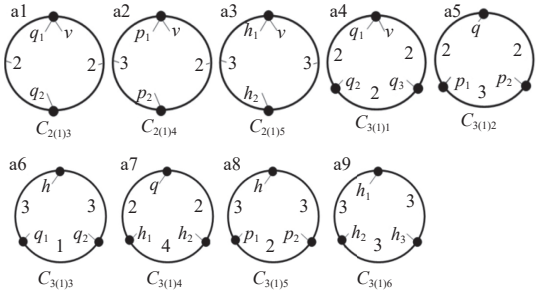

Figure 1 The nine simple basic digit topology circles $C_{n(k)i}$

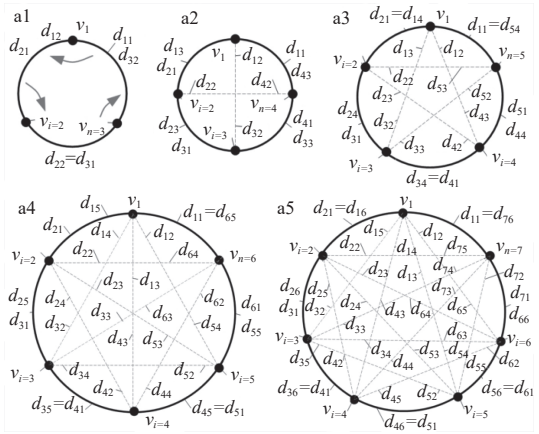

Figure 2 Basic digit topology circles $C_{n(k)i}$ with n dots v_u (u = 1, ..., n) as n = 3, ..., 7

(ii) $\sum_{u=1}^{n} n_u = 2n_e$.

(iii) The v_u was connected with v_{u+1} by $[d_{u(n-1)} = d_{(u+1)1} \geqslant 1]e$; v_n is connected with v_1 by $[d_{n(n-1)} = d_{11} \geqslant 1]e$.

(iv) As u = constant $\geqslant$ 1, m = 1, ..., $\leqslant (n - u - 1)$, v_u is connected with v_{u+m+1} by $[d_{u(n-m-1)} = d_{(u+m+1)(m+1)}]e$.

It is known from Table 2 that each of $C_{n(k)i}$ including n (q, p, h, ...) may have k distinct character strings. Each character string included n (q, p, h) represented by n dots v_u (u = 1, ..., n).

Each digit marked in $C_{n(k)i}$ as (n = 3, 4, 5, 6, 7) represented the number of parallel edges for connecting two dots. The digit arc was marked by digit $d \geqslant 1$. The digit solid line was marked by a digit $d \geqslant 1$. The digit dotted line was marked by 0. All these indicated that two Chinese medicines connected by dotted line do not configure each other. Generally, each character strings of the basic $C_{n(k)i}$ with n (q, p, h, ...) can be represented by diverse digit groups. Each digit group included n sub-digit groups of v_u (u = 1, ..., n). For deriving valid digit groups from the same character string, the sub-digit group of v_u in the different digit groups was placed from the minimum to the maximum. If the sub-digit group of v_u in the different digit groups are same, then the sub-digit group of v_{u+1} was placed from the minimum to the maximum. The order of valid digit groups excluded repetitive, circulated reversing order to reduce the symmetric isomorphism basic $C_{n(k)i}$.

Table 3 Rules of digits marked in basic $C_{n(k)i}$

n, n_l	u	m	n_l lines $v_u \to v_{u+m+1}$, $n_l = n(n-3)/2$, $m \leqslant n-u-1$	Marked by digits $d_{u(n-m-1)} = d_{(u+m+1)(m+1)}$	u	n arcs $v_u \to v_{u+1}$, $v_n \to v_1$	Marked by digits $d_{g(n-1)} = d_{(g+1)1} \geqslant 1$
3, 0			0	No	1	$v_1 \to v_2$	$d_{12} = d_{21} \geqslant 1$
					2	$v_2 \to v_3$	$d_{22} = d_{31} \geqslant 1$
					3	$v_3 \to v_1$	$d_{32} = d_{11} \geqslant 1$
4, 2	1	1	$v_1 \to v_3$	$d_{12} = d_{32}$	1	$v_1 \to v_2$	$d_{13} = d_{21} \geqslant 1$
	2	1	$v_2 \to v_4$	$d_{22} = d_{42}$	2	$v_2 \to v_3$	$d_{23} = d_{31} \geqslant 1$
					3	$v_3 \to v_4$	$d_{33} = d_{41} \geqslant 1$
					4	$v_4 \to v_1$	$d_{43} = d_{11} \geqslant 1$
5, 5	1	1	$v_1 \to v_3$	$d_{13} = d_{32}$	1	$v_1 \to v_2$	$d_{14} = d_{21} \geqslant 1$
	1	2	$v_1 \to v_4$	$d_{12} = d_{43}$	2	$v_2 \to v_3$	$d_{24} = d_{31} \geqslant 1$
	2	1	$v_2 \to v_4$	$d_{23} = d_{42}$	3	$v_3 \to v_4$	$d_{34} = d_{41} \geqslant 1$
	2	2	$v_2 \to v_5$	$d_{22} = d_{53}$	4	$v_4 \to v_5$	$d_{44} = d_{51} \geqslant 1$
	3	1	$v_3 \to v_5$	$d_{33} = d_{52}$	5	$v_5 \to v_1$	$d_{54} = d_{11} \geqslant 1$
	1	1	$v_1 \to v_3$	$d_{14} = d_{32}$			
6, 9	1	2	$v_1 \to v_4$	$d_{13} = d_{43}$	1	$v_1 \to v_2$	$d_{15} = d_{21} \geqslant 1$
	1	3	$v_1 \to v_5$	$d_{12} = d_{54}$	2	$v_2 \to v_3$	$d_{25} = d_{31} \geqslant 1$
	2	1	$v_2 \to v_4$	$d_{24} = d_{42}$	3	$v_3 \to v_4$	$d_{35} = d_{41} \geqslant 1$
	2	2	$v_2 \to v_5$	$d_{23} = d_{53}$	4	$v_4 \to v_5$	$d_{45} = d_{51} \geqslant 1$
	2	3	$v_2 \to v_6$	$d_{22} = d_{64}$	5	$v_5 \to v_6$	$d_{55} = d_{61} \geqslant 1$
	3	1	$v_3 \to v_5$	$d_{34} = d_{52}$	6	$v_6 \to v_1$	$d_{65} = d_{11} \geqslant 1$
	3	2	$v_3 \to v_6$	$d_{33} = d_{63}$			
	4	1	$v_4 \to v_6$	$d_{44} = d_{62}$			
	1	1	$v_1 \to v_3$	$d_{15} = d_{32}$			
7, 14	1	2	$v_1 \to v_4$	$d_{14} = d_{43}$	1	$v_1 \to v_2$	$d_{16} = d_{21} \geqslant 1$
	1	3	$v_1 \to v_5$	$d_{13} = d_{54}$	2	$v_2 \to v_3$	$d_{26} = d_{31} \geqslant 1$
	1	4	$v_1 \to v_6$	$d_{12} = d_{65}$	3	$v_3 \to v_4$	$d_{36} = d_{41} \geqslant 1$
	2	1	$v_2 \to v_4$	$d_{25} = d_{42}$	4	$v_4 \to v_5$	$d_{46} = d_{51} \geqslant 1$
	2	2	$v_2 \to v_5$	$d_{24} = d_{53}$	5	$v_5 \to v_6$	$d_{56} = d_{61} \geqslant 1$
	2	3	$v_2 \to v_6$	$d_{23} = d_{64}$	6	$v_6 \to v_7$	$d_{66} = d_{71} \geqslant 1$
	2	4	$v_2 \to v_7$	$d_{22} = d_{75}$	7	$v_7 \to v_1$	$d_{76} = d_{11} \geqslant 1$
	3	1	$v_3 \to v_5$	$d_{35} = d_{52}$			
	3	2	$v_3 \to v_6$	$d_{34} = d_{63}$			
	3	3	$v_3 \to v_7$	$d_{33} = d_{74}$			
	4	1	$v_4 \to v_6$	$d_{45} = d_{62}$			
	4	2	$v_4 \to v_7$	$d_{44} = d_{73}$			
	5	1	$v_5 \to v_7$	$d_{55} = d_{72}$			

3 Derivation of $C_{n(k)i,j}$ from basic $C_{n(k)i}$

3.1 Derivation of $C_{n(k)i,j}$ using character string and digit groups

Table 2 presents the basic $C_{4(1)1}$ $4q$ with only one character string qqqq. Based on the $C_{n(k)i}$ rules and the digit group of the basic $C_{n(k)i}$ in Section 2.2, the relations of v_u (u = 1, ..., 4) and $d_{u1}d_{u2}d_{u3}$ in $C_{4(1)1}$ with $4q$ are represented by a digit group as below.

$C_{4(1)1}$	$v_1 = q$	$v_2 = q$	$v_3 = q$	$v_4 = q$
digit group	$d_{11}d_{12}d_{13}$	$d_{21}d_{22}d_{23}$	$d_{31}d_{32}d_{33}$	$d_{41}d_{42}d_{43}$
	103	301	103	301

Similarly, the deriving character strings and the digit groups of the basic $C_{n(k)i}$ (n = 4, 5; k = 1, 2) are given in

Table 4. $C_{n(k)i,j}$ (n = 4, 5; k = 1, 2) are constructed using derived digit groups in Table 4 and Figure 3. Here, j is the sub-order number of $C_{n(k)i,j}$.

Table 4 The 9 character strings and the 45 digit groups of $C_{n(k)i,j}$ (n = 4, 5; k = 1, 2)

$C_{n(k)i,j}$	j	Digit group	Character string
$C_{4(1)1,j}$	1	103, 301, 103, 301	*q*, *q*, *q*, *q*
	2	112, 211, 112, 211	
	3	121, 121, 121, 121	
	4	202, 202, 202, 202	
	5	211, 112, 211, 112	
	6	301, 103, 301, 103	
$C_{4(1)2,j}$	1	112, 202, 212, 301	*q*, *q*, *h*, *q*
	2	121, 112, 222, 211	
$C_{4(1)3,j}$	1	103, 301, 104, 401	*q*, *q*, *p*, *p*
	2	112, 211, 113, 311	
	3	121, 121, 122, 221	
	4	202, 202, 203, 302	
	5	211, 112, 212, 212	
	6	301, 103, 302, 203	
$C_{4(2)3,j}$	1	103, 311, 103, 311	*q*, *p*, *q*, *p*
	2	121, 131, 121, 131	
	3	202, 212, 202, 212	
$C_{4(1)4,j}$	1	103, 301, 105, 501	*q*, *q*, *h*, *h*
	2	112, 211, 114, 411	
	3	121, 121, 123, 321	
	4	202, 202, 204, 402	
	5	301, 103, 303, 303	
$C_{4(2)4,j}$	1	103, 321, 103, 321	*q*, *h*, *q*, *h*
	2	112, 231, 112, 231	
	3	121, 141, 121, 141	
	4	202, 222, 202, 222	
$C_{5(1)1,j}$	1	1 003, 3 001, 1 012, 2 002, 2 101	*q*, *q*, *q*, *q*, *q*
	2	1 012, 2 011, 1 111, 1 102, 2 101	
	3	1 012, 2 101, 1 102, 2 002, 2 011	
	4	1 021, 1 111, 1 201, 1 102, 2 011	
	5	1 111, 1 111, 1 111, 1 111, 1 111	
	6	1 111, 1 102, 2 101, 1 012, 2 011	
	7	1 111, 1 201, 1 102, 2 011, 1 021	
	8	1 201, 1 102, 2 011, 1 021, 1 111	
	9	2 002, 2 002, 2 002, 2 002, 2 002	
	10	2 002, 2 011, 1 012, 2 101, 1 102	
	11	2 002, 2 101, 1 003, 3 001, 1 012	
$C_{5(1)2,j}$	1	1 003, 3 001, 1 013, 3 002, 2 101	*q*, *q*, *p*, *p*, *q*
	2	1 012, 2 002, 2 102, 2 003, 3 001	
	3	1 012, 2 011, 1 112, 2 102, 2 101	
$C_{5(2)2,j}$	1	1 111, 1 211, 1 111, 1 111, 1 121	*q*, *p*, *q*, *q*, *p*
	2	1 111, 1 301, 1 102, 2 011, 1 031	
	3	2 002, 2 102, 2 002, 2 002, 2 012	
	4	2 002, 2 111, 1 012, 2 101, 1 112	
	5	2 002, 2 201, 1 003, 3 001, 1 022	

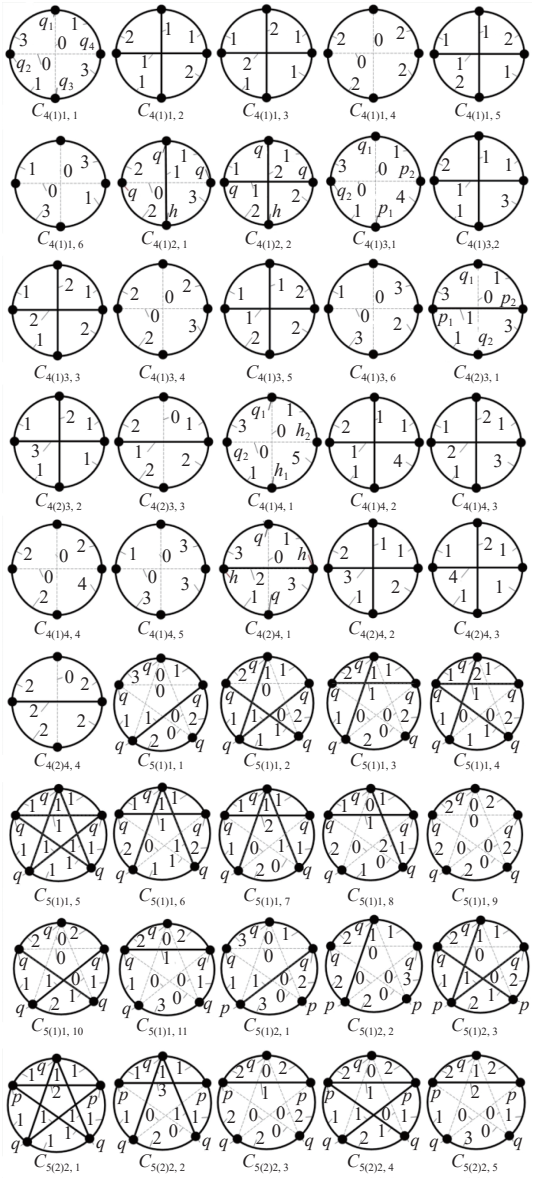

Figure 3 The 45 digit topology circles $C_{n(k)i,j}$ (n = 4, 5; k = 1, 2)

Using the rules in Section 2, the 46 digit groups of the character string qqqqqq are derived for deriving $C_{6(1)1,j}$ (n = 6; k = 1; j = 1, ..., 46) (Table 5).

(i) One character string qqqqqq of $C_{6(k)1,j}$ (n = 6; k = 1; j = 1, ..., 46) can be represented by 46 digit groups. Each digit group includes 6 sub-digit groups of v_u (u = 1, ..., 6).

(ii) The first sub-digit group in the 46 digit groups was placed from the minimum value 10 003 to the maximum value 20 002. When the first and the second sub-digit groups in the different digit groups of $C_{6(k)1,j}$ (n = 6; k = 1; j = 1, ..., 5) are constant 10 003 and constant 30 001, respectively, then the values of the third sub-digit group were placed from the minimum 10 003 to the maximum 10 201. When the first sub-digit group in the different digital groups of $C_{6(k)1,j}$ (n = 6; k = 1; j = 6, ..., 12) were increased from to 10 012, then the values of the second sub-digit group were placed from the minimum 20 002 to the maximum 21 001.

Table 5 The 46 digit groups for deriving $C_{6(1)1,j}$ (j = 1, ..., 46) with character string qqqqqq

j	q_1	q_2	q_3	q_4	q_5	q_6
1	10003	30001	10003	30001	10003	30001
2	10003	30001	10012	20011	11002	21001
3	10003	30001	10102	20002	20002	20101
4	10003	30001	10111	10012	21001	11101
5	10003	30001	10201	10003	30001	10201
6	10012	20002	21001	10012	20002	21001
7	10012	20011	11002	21001	10003	30001
8	10012	20011	11011	11011	11002	21001
9	10012	20101	11002	20011	11002	21001
10	10012	20101	11011	10021	11101	12001
11	10012	21001	11002	20002	20002	20011
12	10012	21001	11011	10012	21001	11011
13	10021	10021	12001	12001	10003	30001
14	10021	10201	12001	10021	10201	12001
15	10021	11011	12001	11002	20002	20011
16	10021	11101	12001	10012	20101	11011
17	10102	20002	20002	20101	10003	30001
18	10102	20011	10111	11101	11002	20101
19	10102	20101	10111	10111	11101	11101
20	10102	21001	10012	20101	11002	20011
21	10111	10012	21001	11101	10003	30001
22	10111	10111	11101	11101	10102	20101
23	10111	10201	11101	10111	10201	11101
24	10111	11011	11011	11101	11002	20011
25	10111	12001	11011	10102	21001	10021
26	10201	10102	20011	10201	10102	20101
27	10201	10201	10201	10201	10201	10201
28	10201	11002	20011	10201	11002	20011
29	10201	11101	10111	10201	11101	10111
30	10201	12001	10021	10201	12001	10021
31	11002	20011	10102	21001	10012	20101
32	11002	20011	10111	11011	10111	11101
33	11002	20011	10201	11002	20011	10201
34	11002	20101	10102	20011	10111	11101
35	11002	21001	10102	20002	20011	10111
36	11011	10021	11101	12001	10012	20101
37	11011	10111	11101	11011	10111	11101
38	11011	11002	21001	10012	20011	11011
39	11011	11011	11011	11011	11011	11011
40	11011	11101	11002	20011	10111	11011
41	11011	12001	11002	20002	20011	10021
42	20002	20002	20002	20002	20002	20002
43	20002	20011	10012	21001	11002	20002
44	20002	20011	10111	11002	21001	10102
45	20002	20101	10102	20002	20101	10102
46	20002	21001	10012	20002	21001	10012

(iii) The order of valid digit groups excluded repetitive, circulated, and reverse order.

(iv) When the values of the first sub-digit group from 20011 to 30001 were used to derive the different digit groups of qqqqqq of $C_{6(k)1,j}$ (n = 6; k = 1; j = 1, ..., 46), some mirror symmetry isomorphisms of $C_{n(k)i,j}$ can be derived.

Based on approach in Section 2, the 46 different $C_{6(k)1,j}$ (n = 6; k = 1; j = 1, ..., 46) are constructed using the 46 derived digit groups in Table 5 and Figure 4.

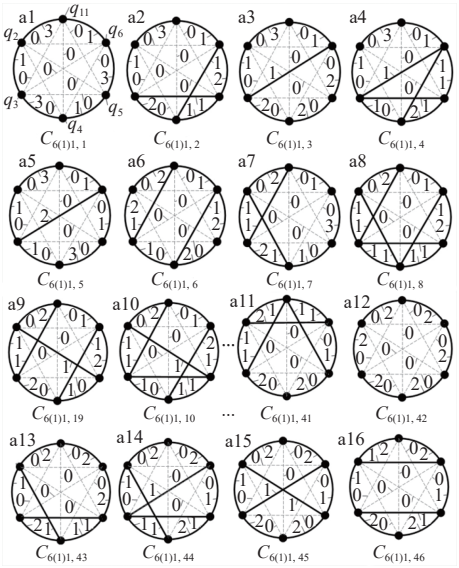

Figure 4 The digit topology circles $G_{6(k)1,j=1,...,46}$ with $6q$

3.2 Derivation of $C_{6(1)6,j}$ from basic $C_{6(1)6}$ with $3q + 2p + h$ and hpqqqp

The 104 different digit groups were derived for $C_{6(1)6,j}$ (n = 6; k = 1; i = 6, j = 1, ..., 104), see Table 6. Based on the approach in Section 2, the 4 distinct digit topology circles $C_{6(1)6,j}$ (j = 1, 2, 103, 104) are constructed using the derived (j = 1, 2, 103, 104) digit groups in Table 6 and Figure 5.

Table 6 The 10^4 different digit groups for $C_{6(1)6,j}$ with $3q + 2p + h$ and hpqqqp

j	h	p_1	q_1	q_2	q_3	p_2
1	10014	40001	11002	20011	10003	31001
2	10014	40001	11011	10021	11002	22001
...	...	...	...	...	...	...
103	30003	30101	10102	20002	20101	10103
104	30003	31001	10012	20002	21001	10013

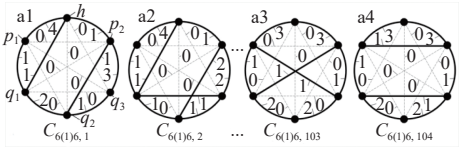

Figure 5 The 4 different digit topology circles $C_{6(1)6,j=1,...,104}$

4 Derivation of digit topology circles $t + C_{n(k)i,j}$

In order to configure the TCM prescriptions, including a ternary medicinal material t, the distinct digit topology circles $t + C_{n(k)i,j}$ can be derived by adding t into $C_{n(k)i,j}$.

When a t is added into $C_{n(k)i,j}$ with n (q, p, h, ...), the digit topology circle with $(n + 1)$ v_u (u = 1, ..., n, n + 1) can derive $t + C_{n(k)i,j}$ with $t + n$ (q, p, h, ...). The processes are explained as follows.

(i) Use one of v_u (u = 1, ..., n, n + 1) to represent t. (ii) Connect a dot of t with other one dot of n (q, p, h, ...) by a digit line or digit arc, respectively. (iii) Replace connected one of n (q, p, h, ...) by n (p, h, ...), respectively. (iv) Derive the valid character strings using $t + n9$ (q, p, h, ...). (v) Construct $t + C_{n(k)i,j}$ by the valid character strings of $t + n$ (q, p, h, ...).

For instance, when t is added into $C_{4(2)3,j}$ with qpqp to derive $t + C_{4(2)3,j}$, the 4 valid character strings (tppqp, tqppp, tqhqp, tqpqh) and their digit groups were constructed and listed in Table 7. Following the 20 distinct digit topology circles $t + C_{4(2)3,j}$ (n = 5; k = 2; j = 1, ..., 20) were derived and constructed with valid digit groups, see Figure 6.

Table 7 Valid character strings and digit groups of $t + C_{4(2)3,j}$ with (qpqp; n = 4; k = 2; i = 3; j = 1, ..., 20)

j	t	$q \rightarrow p$	p	q	p	Character string
1	1 002	2003	3 011	1 003	3 101	
2	1 002	2012	2021	1 102	2 201	
3	1 002	2021	1 031	1 201	2 201	tppqp
4	1 002	2 111	1 022	2 101	1 211	
5	1 002	2 201	1 013	3 001	1 121	
j	t	q	$p \rightarrow h$	q	p	Character string
6	1 011	1 003	3 111	1 003	3 101	
7	1 011	1 012	2 121	1 102	2 201	
8	1 011	1 021	1 131	1 201	1 301	tqhqp
9	1 011	1 111	1 122	2 101	1 211	
10	1 011	1 201	1 113	3 001	1 121	
j	t	q	$p \rightarrow h$	q	p	Character string
11	1 101	1 003	3 011	1 013	3 101	
12	1 101	1 012	2021	1 112	2 201	
13	1 101	1 021	1 031	1 211	1 301	tqhqp
14	1 101	1 111	1 022	2 111	1 211	
15	1 101	1 201	1 013	3 011	1 121	
j	t	q	$p \rightarrow h$	q	p	Character string
16	2001	1 003	3 011	1 003	3 102	
17	2001	1 012	2021	1 102	2 202	
18	2001	1 021	1 031	1 201	1 302	tqpqh
19	2001	1 111	1 022	2 101	1 212	
20	2001	1 201	1 013	3 001	1 122	

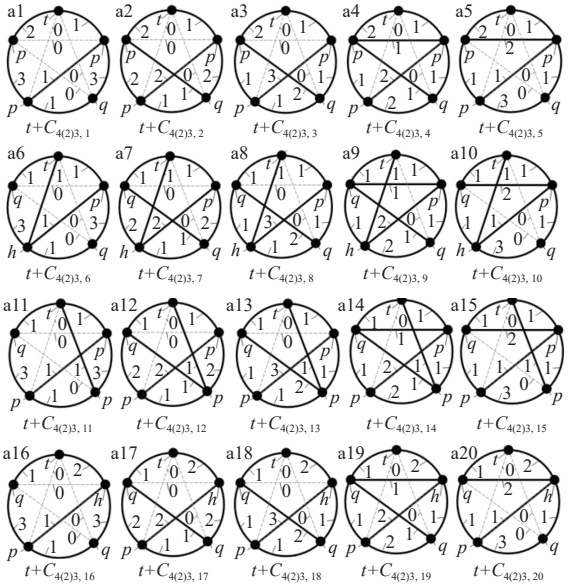

Figure 6 The 20 different digit topology circles $t + C_{4(2)3,j}$ with (qpqp; n = 4; k = 2; i = 3; j = 1, ..., 20)

Similarly, the more $t + C_{n(k)i,j}$ and the valid character strings of more $t + n$ (q, p, h, ...) can be derived using above method. After that, the complex TCM prescriptions with t can be derived using $t + C_{j(k)i,j}$.

5 Creation examples of complex TCM prescription using several digit topology circles

Four examples of complex TCM prescriptions were configured with the 4 $C_{4(1)1,3}$, $C_{5(2)2,9}$, $t + C_{4(2)3,10}$, and $C_{6(1)1,103}$, respectively, see Figure 7. After that, the TCM prescriptions for treating some diseases can be configured easily by TCM experts.

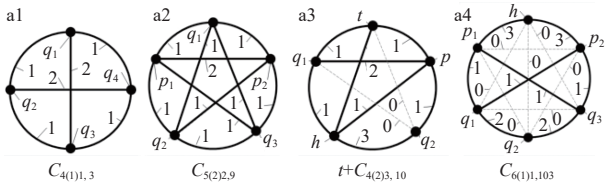

Figure 7 The 4 distinct digit topology circles $C_{n(k)i,j}$

(i) Example 1. A specific TCM prescription derived from $C_{4(1)1,3}$ with 4q, 8e (Figure 7, a1) and its properties are explained as follows.

Here, q_1 is Guizhi (Cinnamomi Ramulus), q_2 is Shaoyao (Paeoniae Radix Alba), q_3 is Shengjiang (Zingiberis Rhizoma Recens), q_4 is Renshen (Ginseng Radix et Rhizoma). Based on their medicinal efficacy and dose, (q_1, q_2, q_3, q_4) can be divided into (4, 4, 4, 4) parts. The 4 parts of q_1 are configured with (1 part of q_2, 2 parts of q_3, 1 part of q_4) , respectively; the 4 parts of q_2 are configured with (1 part of q_1, 1 part of q_3, 2 parts of q_4) , respectively; 4 parts of q_3 are configured with (1 part of q_2, 2 parts of q_1, 1 part of q_4) , respectively; the 4 parts of q_4 are configured with (1 part of q_1, 2 parts of q_2, 1 part of q_4) , respectively.

This TCM prescription can be used to cure body aches, pulse weak after sweating [1, 11-13].

(ii) Example 2. A specific TCM prescription derived from $C_{5(2)2,\ 9}$ with $2p + 3q$, $11e$ (Figure 7, a2) and its properties are explained as follows.

Here, q_1 is Guizhi (Cinnamomi Ramulus), q_2 is Renshen (Ginseng Radix et Rhizoma), q_3 is Gancao (Glycyrrhizae Radix et Rhizoma), p_1 is Shaoyao (Paeoniae Radix Alba), p_2 is Daozao (Jujubae Fructus). (q_1, q_2, q_3, p_1, p_2) can be divided into (4, 4, 4, 5, 5) parts based on their medicinal efficacy and dose.

The 4 parts of q_1 are configured with (1 part of p_1, 1 part of q_2, 1 part of q_3, 1 part of p_2), respectively; the 5 parts of p_1 are configured with (1 part of q_1, 1 part of q_2, 1 part of q_3, 2 parts of p_2), respectively; the 4 parts of q_2 are configured with (1 part of p_1, 1 part of q_1, 1 part of q_3, 1 part of p_2), respectively; the 4 parts of q_3 are configured with (1 part of q_2, 1 part of p_1, 1 part of q_1, 1 part of p_2), respectively; the 5 parts of p_2 are configured with (1 part of q_1, 2 parts of p_1, the 1 part of q_2, 1 part of q_3), respectively. This TCM prescription can cure lose one's breath and body aches after sweating [1, 11-13].

(iii) Example 3. A complex TCM prescription derived from $t + C_{4(2)3,\ 10}$ with $2q + p + h + t$, $11e$ (Figure 7, a3) and its properties are explained as follows.

A total of 5 different compatible medicinal materials (t, q_1 q_2, p, h) were divided into (3, 4, 4, 5, 6) parts, respectively, based on their medicinal efficacy and dose. h is configured with (1 part of t, 1 part of q_1, 1 part of p, 3 parts of q_2), respectively; p is configured with (1 part of t, 2 parts of q_1, 1 part of h, 1 part of q_2), respectively; q_1 is configured with (1 part of h, 2 parts of p, 1 part of t), respectively; q_2 is configured with (1 part of p, 3 parts of h), respectively; t is configured with (1 part of q_1, 1 part of h, 1 part of p), respectively.

When (t, q_1 q_2, p, h) are replaced by 5 specific compatible medicinal materials, respectively, some TCM prescriptions can be derived from $t + C_{4(2)3,\ 10}$.

(iv) Example 4. A complex TCM prescription derived from $C_{6(1)1,\ 103}$ with $3q + 2p + h$, $14e$ (Figure 7, a4) and its properties are explained as follows.

Based on their medicinal efficacy and dose, 6 different compatible medicinal materials (q_1 q_2, q_3, p_1, p_1, h) were divided into (4, 4, 4, 5, 5, 6) parts.

h is configured with (3 parts of p_1, 3 parts of p_2), respectively; p_1 is configured with (3 parts of h, 1 part of q_1, 1 part of q_3), respectively; q_1 is configured with (1 part of p_1, 2 parts of q_2, 1 part of p_2), respectively; q_2 is configured with (2 parts of q_1, 2 parts of q_3), respectively; q_3 is configured with (2 parts of q_2, 1 part of p_1, 1 part of p_2), respectively; p_2 is configured with (3 parts of h, 1 part of q_1, 1 part of q_3), respectively.

When (q_1 q_2, q_3, p_1, p_1, h) were replaced by 6 specific compatible medicinal materials, some TCM prescriptions can be derived from $C_{6(1)1,\ 103}$.

If all lines of $C_{n(k)i,\ j}$ I, such as $C_{4(1)1,\ 3}$ and $C_{5(2)2,\ 9}$ in Figure 7, are marked by 1 or more, then all medicinal materials in the TCM prescription I derived from $C_{n(k)i,\ j}$ I can be configured with each other. Generally, it is easy to identify the TCM prescription I from existing TCM prescriptions constructed by TCM experts or practitioners. If several digit lines of a $C_{n(k)i,\ j}$ II, such as $t + C_{4(2)3,\ 10}$ and $C_{6(1)1,\ 103}$ in Figure 7, are marked by 0, then several medicinal materials in the TCM prescription II derived from $C_{n(k)i,\ j}$ II cannot be configured mutually. Generally, it is difficult to find the TCM prescription II from existing TCM prescriptions constructed by medical experts or practitioners.

Since most $C_{n(k)i,\ j}$ includes 0 marked on the lines, numerous and valuable TCM prescriptions can be derived from various $C_{n(k)i,\ j}$ where lines are marked with 0. In this case, several sub-configurations of medicinal materials can be constructed respectively, from the medicinal materials configured each other in the TCM prescription II. A novel valuable TCM prescription can be formed by several sub-configurations of medicinal materials.

It is acknowledged that $C_{n(k)i,\ j}$ allows arbitrary connections between medicinal materials, including incompatible pairs such as those defined in the "Eighteen Counteractions" [e.g., Banxia (Pinelliae Rhizoma) and Chuanwu (Aconiti Radix), should not be paired]. Therefore, based on the medicine knowledge and TCM experience, TCM experts or practitioners must manually evaluate the incompatible medicinal materials, such as those outlined in the "Eighteen Counteractions", in any TCM prescriptions derived from $C_{n(k)i,\ j}$, thereby ensuring adherence to fundamental pharmaceutical principles.

Finally, each edge in $C_{n(k)i,\ j}$ can be formed by several serial-connecting binary medicinal materials, with the formation of these edges guided by TCM-specific properties, including the four natures and five flavors, and meridian tropism.

6 Conclusion

The digit topology circle is an effective tool for configuring complex TCM prescriptions. Many different digit topology circles $C_{n(k)i,\ j}$ with n (q, p, h) Chinese medicinal materials can be derived by integrating the basic digit topology circle, character strings, and digital groups. This structured derivation process enables the generation of a diverse array of topology-based representations for TCM prescriptions, forming a foundation for both existing and novel formulation strategies.

Some existing TCM prescriptions and many novel valuable TCM prescriptions can be configured using the derived $C_{n(k)i,\ j}$. Existing TCM prescriptions have been clinically validated to show their effects in treating various diseases across patient populations. The predictive potential of $C_{n(k)i,\ j}$-based novel TCM prescriptions is supported by preliminary evidence, suggesting their capacity to address diverse clinical conditions.

Some novel TCM prescriptions with $t + n$ (q, p, h, ...) Chinese medicine can be derived by adding a ternary Chinese medicinal material t into $C_{n(k)i,j}$ with n (q, p, h, ...) Chinese medicinal materials. Multiple novel TCM prescriptions with more ternary Chinese medicines can be derived by adding more t into $C_{n(k)i,j}$.

Four complex TCM prescriptions are configured using derived $C_{4(1)1,3}$, $C_{5(2)2,9}$, $t + C_{4(2)3,10}$, and $C_{6(1)1,103}$, respectively. Based on the TCM experts' experiences and the configured TCM prescriptions, TCM experts or practitioners can configure several valuable TCM prescriptions using $C_{n(k)i,j}$ easily for treating some diseases.

It is also a significant and challenging issue to judge the incompatible medicinal materials and to construct each edge in $C_{n(k)i,j}$ by serial-connecting binary Chinese medicines. Future research should be focused on these aspects.

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Competing interests

The authors declare no conflict of interest.

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使用数字拓扑圆配置复杂中药处方

路懿[a*], 彭博[b, c], 李赛美[c]

a. 燕山大学机械工程学院, 河北 秦皇岛 066004, 中国
b. 德医精诚中医诊疗所有限公司, 广东 广州 510260, 中国
c. 广州中医药大学第一附属医院, 广东 广州 510405, 中国

【摘要】目的 使用数字拓扑圆配置复杂的中药处方并推导不同的数字拓扑圆。**方法** 构建基本数字拓扑圆，用基本数字拓扑圆、字符串和数字组推导不同数字拓扑圆，通过在数字拓扑圆中添加三元中药推导不同含三元中药的数字拓扑圆，使用推导的数字拓扑圆配置有价值中药处方。**结果** 用字符串构建了 9 个简单的基本数字拓扑圆。用基本数字拓扑圆、字符串和数字组推导出许多不同的数字拓扑圆和一些含三元中药的数字拓扑圆；用 4 个推导的数字拓扑圆配置出 4 个复杂中药处方。**结论** 用数字拓扑圆可配置一些现有的中药处方，也可配置许多新型中药处方。已证实一些现有的中药处方可成功治愈患者的疾病，数字拓扑圆还可能配置一些新颖的有价值的中药处方用于治疗患者的某些疾病。

【关键词】数字拓扑圆；拓扑图；药方；中医药；配置