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## Application of information theory and numerical taxonomy methods to thin-layer chromatographic investigations of *Hypericum perforatum* L.

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The efficiency of nine TLC systems for separating six main components of a methanolic extract of *Hypericum perforatum* L. (St. John's wort) was investigated. For this purpose, three mathematical approaches have been applied. The first approach was the calculation of the information content for each chromatographic system. Secondly, the discriminating power of the systems was measured individually and in diverse combinations. As a third approach the chromatographic systems were classified into dissimilar groups and of each group with similar separation characteristics the best system was selected according to the information content. The classification was carried out by the numerical taxonomy methods.

**Keywords:** *Hypericum perforatum* L., thin-layer chromatography, information content, discriminating power, numerical taxonomy

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In this study we used numerical taxonomy methods in order to evaluate the separating power of TLC systems for splitting a methanolic extract of *Hypericum perforatum* L. (St. John's wort) into six main compounds (flavonoid glycosides, chlorogenic acid, hypericin).

*Hypericum perforatum* is an aromatic perennial herb belonging to the family *Hypericaceae*, of widespread distribution in Europe, western Asia and throughout the United States. It is a ca. 60 cm tall herbaceous plant producing five-merous yellow flowers with many and prominent, long stamens and opposite, translucently dotted leaves. The drug

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\* Correspondence

(*Hyperici herba*) consists of the aerial parts (leaves and flowering tops). The herb is used internally for the treatment of psychogenic disturbances, depressive states and/or nervous excitements, and externally as oily preparations for the treatment and after-treatment of incised and contused wounds and first-degree burns (1).

Chemical investigations have detected a number of constituents including hypericin and hypericin-like substances (2), flavonoids (3, 4), the hyperforin antibiotic substance (2, 5, 6), essential oil, small amounts of procyanidins (7) and tannins. The structures of the flavonoid glycosides rutin, hyperoside, quercitrin, *iso*quercitrin, of chlorogenic acid and hypericin analysed in this paper are presented in Fig. 1.

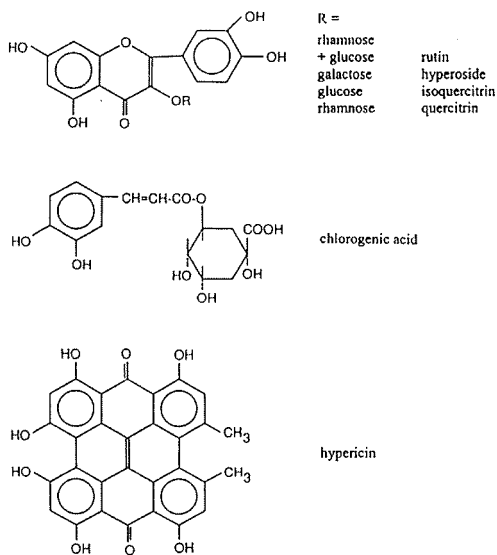


Fig. 1. Structural formulas of the investigated constituents of a methanolic *Hypericum* extract.

In our times, St. John's wort is widely used in Europe for its antidepressive effects as an alternative to medical synthetic drugs. For this reason numerous reports dealing with the drug and its preparations can be found in literature, *e.g.* a monograph edited by the German Commission E. Several authors propose analytical methods for investigating *Hypericum perforatum*. In this paper the efficiency of different TLC systems described in literature and own modifications of them are compared by numerical taxonomy methods.

The information content or equivocation can serve – with certain restrictions – as an important criterion for the evaluation, selection or optimization of analytical procedures (8). Information theory can be used to compare the quality of chromatographic systems as well as to optimize such systems (9). Shannon's formula was applied to calculate the information contents and the unit of information (bit), as it is used in binary-coded systems. The information theory approach is based on the combination of all chromatographic systems studied with an estimation for the average amount of information of the selected set of compounds (10, 11). The discriminating power (DP) is used

as a measure of the effectiveness of chromatographic systems. The DP of chromatographic system is the probability of separating two compounds selected at random from a specific substance population (12). The calculation of the DP values and their maximization can be more easily attained by the following conditions: an even distribution of  $hR_f$  values, reproducibility of results and no correlations between the chromatographic systems.

The methods of numerical taxonomy classify the chromatographic systems according to clusters (13, 14). The chromatographic systems are divided into groups with similar separation properties. The selection of the most efficient chromatographic system from each group is carried out by numerical taxonomy methods. The results obtained by applying those techniques were compared by using our computer search program KT 1 (10).

## EXPERIMENTAL

### Materials

*Test solution.* – 1.0 g air-dried, coarsely powdered drug was refluxed with 10.0 mL methanol for 10 minutes, filtered, the filtrate concentrated under reduced pressure, and the residue taken up in 5.0 mL methanol.

*Reference solution.* – 10 mg rutin and 5 mg hyperoside were dissolved in 10 mL methanol.

Precoated 20×20 cm TLC silica gel 60 F<sub>254</sub> sheets (thickness of layer 0.2 mm) were obtained from Merck (Darmstadt, Germany). The foils were prewashed twice with methanol, desiccated in stream of air and kept overnight at relative humidity of 40–45%. Sample application was performed with a Linomat IV apparatus (Camag, Muttenz, Switzerland). 5  $\mu$ L of the extract solutions were applied 20 mm from the bottom of the sheet as 10 mm wide bands at a delivery rate of 4 s  $\mu$ L<sup>-1</sup>. Developments were performed by the linear ascending mode at 20.5–22.0 °C room temperature and 40–45% relative humidity in a saturated (eluent system 1–6, 9) or unsaturated (eluent system 7, 8) twin-through 20×20 chamber (Camag). The solvent volume was 30 mL and the development distance 150 mm (single development). All solvents were of analytical grade, purchased from Merck. The foils were dried at room temperature in a stream of cold air. Visualization of the flavonoids was attained by spraying the sheets with 1% methanolic diphenylborylethylamine, followed by 5% ethanolic polyethylene glycol 4000. The chromatograms were evaluated in UV 366 nm light (flavonoids as orange-yellow, chlorogenic acid as blue and hypericin as red fluorescent bands).

### Methods

*Calculation of the information content.* – Extensive information has been calculated for nine TLC systems by Shannon's formula. The calculation of the information content will become possible if the uncertainties before and after the analysis can be expressed in a quantitative way.

The distribution of  $hR_f$  values into groups with an error factor  $E$  (e.g.,  $E = 0.05$  or  $E = 0.10$ ) with respect to  $hR_f$  units and the assumption of  $n_k hR_f$  values in the  $k$ -th groups, the average information content (entropy) is given by the following Shannon's equation (15–17):

$$I(X) = H(X) = -\sum_k [n_k/n] \text{ld} [n_k/n] [\text{bit}]$$

It is also assumed that the compounds with  $hR_f$  values within one group cannot be identified. It is obvious that the entropy is at its highest level if there is only one  $hR_f$  value, i.e.  $H_m(X) = \text{ld} n$  within each group.

*Determination of discriminating power (DP).* – The DP of a set of chromatographic systems is defined as the probability of identifying two randomly selected compounds in at least one of the systems (18–22). It must be possible to discriminate all pairs of  $N$  in order to compute the DP of  $k$  chromatographic systems in which  $N$  compounds are investigated. For the total number of matching pairs ( $M$ ) the probability of a random selection of chromatographically similar pairs is  $2M/N(N-1)$ . Therefore, the DP of  $k$  systems is:

$$DP_k = 1 - 2M/N(N-1)$$

The average number of chromatographically similar compounds ( $T$ ) for the chromatographic systems considered can be calculated from the equation:

$$T = 1 + (N-1)(1 - DP_k)$$

*Calculation of taxonomic distances, cluster formation and dendrogram.* – Taxonomy is defined as the theoretical study of classification including its elementary principles, procedures and rules (13). Numerical taxonomy deals with ways of classifying chromatographic systems into taxonomic groups based on characteristic values ( $hR_f$  values). The mathematical principle of this procedure is established on the formation of a matrix where the columns represent the solvent systems and the lines of the substances. Classification is carried out with respect to resemblances between the solvent systems. Dissimilarity expressed as the complement of similarity is proportional to the distances of the solvent systems in the given metric space. The greater the differences in properties of the solvent systems, the larger their spatial distances are. Taxonomic distance is inversely related to similarity. The distance  $d_{j,k}$  between the solvent systems  $j$  and  $k$  is defined as:

$$d_{j,k} = \left[ \sum_{i=1}^N (X_{i,j} - X_{i,k})^2 \right]^{1/2}$$

where  $X_{i,j}$  and  $X_{i,k}$  are the  $hR_f$  values of investigated compound  $i$  in the solvent systems  $j$  and  $k$ , and  $N$  is the number of  $hR_f$  values taken into account.

In the classification by taxonomy a resemblance matrix containing either the correlation coefficient or the taxonomic distance is constructed. The reduction of this matrix is carried out by a weighted pair group method using the arithmetic average (13). The smallest distance  $d_{i,k}$  or highest correlation coefficient is selected:  $i$  and  $k$  are the most similar solvent systems and are therefore considered to form one group  $p'$ . The similarity coefficient between the new group  $p'$  and all other phases (e.g.  $q$ ), is calculated e.g. for the distance, as follows:

$$d_{j,p'} = \frac{1}{2} (d_{j,p'} + d_{j,q})$$

The total number of rows and columns in the resemblance matrix is therefore reduced to one. This process is repeated until all chromatographic systems are comprised in one non-overlapping hierarchic system of groups and subgroups (clusters). The procedure for cluster formation is presented by a dendrogram (10, 23, 24).

## RESULTS AND DISCUSSION

Optimization procedures are widely used in the development of different analytical methods. Chromatographic methods, particularly TLC and HPLC, are procedures in which different chemometrical methods are used most frequently (25, 26).

The different times of development of the TLC sheets and the  $hR_f$  values of the compounds on which the calculations are based are listed in Table I. A data set of  $hR_f$  values for the separation of the main components of a methanolic extract of *Hypericum perforatum* into nine different chromatographic systems was analysed. An optimal combination of two or more systems was selected using two procedures:

- a) determination and comparison of the information content and DP for all possible combinations of chromatographic systems,
- b) division of chromatographic systems into groups with similar separation properties and selection of the most efficient chromatographic system from each group.

Table II gives the input and output data for the information content and the DP for each TLC system and for combined systems in a range of error factors. The error factors were 0.05 and 0.10, respectively.

Under the conditions frequently used in chromatographic analysis, i.e.  $E = 0.05$ , the most suitable systems for separating the compounds studied are the chromatographic systems 2 and 4 because they showed the largest DP values ( $DP = 1.000$ ) and a high information content ( $I = 2.585$ ). Systems 1, 3 and 5 are also suitable because of their slightly lower DP value ( $DP = 0.933$ ) and identical information content as systems 2 and 4.

The results made evident that at  $E = 0.10$  the most appropriate systems for separating the compounds are the systems 1 and 4 because of their high DP value and information content ( $DP = 0.933$ ,  $I = 2.585$ ). The systems 2 and 3 are also acceptable. Combining two chromatographic systems with the error  $E = 0.05$  or  $0.10$  all systems show very high DP values ( $DP = 1.000$  and  $0.933$ , respectively) and the number of compounds with similar chromatographic properties is at a minimum ( $T = 1.000$  and  $1.333$ , respectively).

Table 1. TLC-investigation of components of *Hypericum perforatum* in different eluents

| No | Eluent system   | Time of development (min) | Literature | <i>R<sub>f</sub></i> values of components |            |                 |            |                  |           |
|----|---|---------------------------|------------|---|------------|-----------------|------------|------------------|-----------|
|    |   |                           |            | Rutin                                     | Hyperoside | Iso-quericitrin | Quercitrin | Chlorogenic acid | Hypericin |
| 1  | Etac-EMK-HCOOH-H <sub>2</sub> O<br>50:30:10:10                          | 100                       | (27)       | 47  | 70         | 74              | 85         | 58               | 98        |
| 2  | Etac-HCOOH-H <sub>2</sub> O<br>30:2:3                                   | 105                       | (28)       | 12  | 37         | 43              | 63         | 30               | 82        |
| 3  | Etac-HCOOH-CH <sub>3</sub> COOH-H <sub>2</sub> O<br>100:11:11:27        | 141                       | (29)       | 46  | 70         | 74              | 86         | 54               | 95        |
| 4  | Etac-HCOOH-CH <sub>3</sub> COOH-EMK-H <sub>2</sub> O<br>50:7:3:30:10    | 108                       | (30)       | 44  | 69         | 75              | 87         | 55               | 99        |
| 5  | Ethylformate-acetone-H <sub>2</sub> O-CH <sub>3</sub> COOH<br>5:4:1:0:4 | 85                        | (31)       | 36  | 52         | 56              | 69         | 31               | 99        |
| 6  | n-BuOH-CH <sub>3</sub> COOH-H <sub>2</sub> O<br>12:3:5                  | 380                       | (32)       | 57  | 69         | 69              | 75         | 48               | 83        |
| 7  | Toluene-Etac-HCOOH<br>50:40:10  | 58                        | (33)       | 0   | 4          | 6               | 13         | 2                | 62        |
| 8  | Toluene-Etac-HCOOH<br>15:75:10  | 52                        | (33), var. | 6   | 18         | 25              | 45         | 18               | 78        |
| 9  | Acetone-tert. butylmethylether-HCOOH<br>40:50:10                        | 60                        | (34), var. | 24  | 48         | 57              | 78         | 47               | 97        |

System 4 can be found in the first ten combinations. In a series of three systems, regardless of the error factor  $E$ , the TLC system 4 is also found in the first ten combinations.

In order to obtain the optimal combination of systems according to the dendrogram (Fig. 2), irrespective of the error factor  $E$  and number of systems ( $K = 2$  or  $K = 3$ ), the

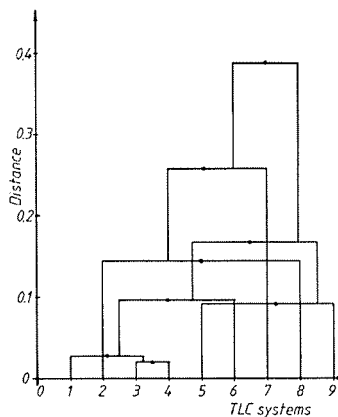


Fig. 2. Dendrogram for nine TLC systems.

Table II. Input and output data for the DP and cluster formation

Input data ( $hR_i$ -values of the main components of *Hypericum perforatum*)

| Compound            | Solvent system |    |    |    |    |    |    |    |    |
|---------------------|----------------|----|----|----|----|----|----|----|----|
|                     | 1              | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  |
| 1. Rutin            | 47             | 12 | 46 | 44 | 36 | 57 | 0  | 6  | 24 |
| 2. Hyperoside       | 70             | 37 | 70 | 69 | 52 | 69 | 4  | 18 | 48 |
| 3. Isoquercitrin    | 74             | 43 | 74 | 75 | 56 | 69 | 6  | 25 | 57 |
| 4. Quercitrin       | 85             | 63 | 86 | 87 | 69 | 75 | 13 | 45 | 78 |
| 5. Chlorogenic acid | 58             | 30 | 54 | 55 | 31 | 48 | 2  | 18 | 47 |
| 6. Hypericin        | 98             | 82 | 95 | 99 | 99 | 83 | 62 | 78 | 97 |

Systems

| TLC-system | $E = 0.05$ |        | $E = 0.10$ |        |
|------------|------------|--------|------------|--------|
|            | DP         | I(bit) | DP         | I(bit) |
| 1          | 0.933      | 2.585  | 0.933      | 2.585  |
| 2          | 1.000      | 2.585  | 0.867      | 2.585  |
| 3          | 0.933      | 2.585  | 0.800      | 2.585  |
| 4          | 1.000      | 2.585  | 0.933      | 2.585  |
| 5          | 0.933      | 2.585  | 0.867      | 1.918  |
| 6          | 0.933      | 2.252  | 0.667      | 2.252  |
| 7          | 0.667      | 1.792  | 0.467      | 1.252  |
| 8          | 0.933      | 2.252  | 0.800      | 2.252  |
| 9          | 0.933      | 2.252  | 0.800      | 2.252  |



Table II. Continued

Combined systems

| Combination sequence |            |           | E = 0.05 |       | E = 0.10 |       |
|----------------------|------------|-----------|----------|-------|----------|-------|
|                      |            |           | DP       | T     | DP       | T     |
| K = 2                | 1. system  | 6 - 9     | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 2. system  | 6 - 8     | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 3. system  | 5 - 9     | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 4. system  | 5 - 8     | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 5. system  | 4 - 9     | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 6. system  | 4 - 8     | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 7. system  | 4 - 7     | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 8. system  | 4 - 6     | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 9. system  | 4 - 5     | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 10. system | 3 - 9     | 1.000    | 1.000 | 0.933    | 1.333 |
| K = 3                | 1. system  | 6 - 8 - 9 | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 2. system  | 6 - 7 - 9 | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 3. system  | 6 - 7 - 8 | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 4. system  | 5 - 8 - 9 | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 5. system  | 5 - 7 - 9 | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 6. system  | 5 - 7 - 8 | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 7. system  | 5 - 6 - 9 | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 8. system  | 5 - 6 - 8 | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 9. system  | 4 - 8 - 9 | 1.000    | 1.000 | 0.933    | 1.333 |
|                      | 10. system | 4 - 7 - 9 | 1.000    | 1.000 | 0.933    | 1.333 |

| Cluster formation |         |         |          |
|-------------------|---------|---------|----------|
| Cluster           | Solvent | Solvent | Distance |
| 1                 | 3       | 4       | 0.0200   |
| 2                 | 1       | 3       | 0.0208   |
| 3                 | 3       | 7       | 0.0915   |
| 4                 | 1       | 4       | 0.0956   |
| 5                 | 2       | 5       | 0.1417   |
| 6                 | 1       | 3       | 0.1636   |
| 7                 | 2       | 3       | 0.2560   |
| 8                 | 1       | 2       | 0.3889   |

best systems in cluster 1 are the systems 4, 5 or 6, and in cluster 2 the systems 2, 7, or 8. Considering the best system to be the one with the largest DP and information content I, it is obvious that the most suitable system of cluster 1 is system 4 due to its high DP value (DP = 1.000 or 0.933) and the information content (I = 2.585).

The results obtained by applying these techniques are useful mathematical tools in the classification and combination of chromatographic systems. As far as the methods are concerned, it is clear that the combined use of mathematical tools such as information theory, pattern recognition, principal components analysis and numerical taxonomy permits the classification and combination of chromatographic techniques. They should

therefore be of value in comparative physicochemical studies of these systems and in the selection of sets of preferred solvent systems.

The proposed calculations point to the conclusion that for the TLC analysis of six main components of *Hypericum perforatum* chromatographic system 4, which is described by Wagner *et al.* (30) for *Crataegi* folium and flos and system 2 reported in Hager's Handbuch der Pharmazeutischen Praxis (28) are the most useful methods. The suggested solvent combinations proved an excellent reproducibility of the results and an even distribution of the  $hR_f$  values. Some of the TLC systems described, especially the one for *Hypericum perforatum* in papers or monographs (e.g. Deutscher Arzneimittel-Codex), did not give sufficient results.

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## S A Ž E T A K

### Primjena teorije informacije i metoda numeričke taksonomije u istraživanju gospine trave (*Hypericum perforatum* L.) tankoslojnom kromatografijom

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Metodom tankoslojne kromatografije istražen je metanolni ekstrakt gospine trave (*Hypericum perforatum* L.). Uspješnost devet kromatografskih razvijaa ispitana je matematičkim metodama: određivanjem srednjega vlastitog sadržaja informacije, koeficijenta DP, te formiranjem klastera i dendrograma. Svrstavanje kromatografski sličnih razvijaa u klastera provedeno je metodama numeričke taksonomije.

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