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Fuzzy Divisive Hierarchical Clustering of Solvents According to Their Experimentally and Theoretically Predicted Descriptors

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Received: 5 September 2020; Accepted: 22 October 2020; Published: 24 October 2020



Abstract: The present study describes a simple procedure to separate into patterns of similarity a large group of solvents, 259 in total, presented by 15 specific descriptors (experimentally found and theoretically predicted physicochemical parameters). Solvent data is usually characterized by its high variability, different molecular symmetry, and spatial orientation. Methods of chemometrics can usefully be used to extract and explore accurately the information contained in such data. In this order, advanced fuzzy divisive hierarchical-clustering methods were efficiently applied in the present study of a large group of solvents using specific descriptors. The fuzzy divisive hierarchical associative-clustering algorithm provides not only a fuzzy partition of the solvents investigated, but also a fuzzy partition of descriptors considered. In this way, it is possible to identify the most specific descriptors (in terms of higher, smallest, or intermediate values) to each fuzzy partition (group) of solvents. Additionally, the partitioning performed could be interpreted with respect to the molecular symmetry. The chemometric approach used for this goal is fuzzy c-means method being a semi-supervised clustering procedure. The advantage of such a clustering process is the opportunity to achieve separation of the solvents into similarity patterns with a certain degree of membership of each solvent to a certain pattern, as well as to consider possible membership of the same object (solvent) in another cluster. Partitioning based on a hybrid approach of the theoretical molecular descriptors and experimentally obtained ones permits a more straightforward separation into groups of similarity and acceptable interpretation. It was shown that an important link between objects' groups of similarity and similarity groups of variables is achieved. Ten classes of solvents are interpreted depending on their specific descriptors, as one of the classes includes a single object and could be interpreted as an outlier. Setting the results of this research into broader perspective, it has been shown that the fuzzy clustering approach provides a useful tool for partitioning by the variables related to the main physicochemical properties of the solvents. It gets possible to offer a simple guide for solvents recognition based on theoretically calculated or experimentally found descriptors related to the physicochemical properties of the solvents.

Keywords: solvents; fuzzy hierarchical clustering; fuzzy associative-clustering; physicochemical descriptors

1. Introduction

The large number of different solvents used for many important chemical processes and technologies need special attention since their properties depend on a range of specific chemical and physical parameters such as melting and boiling point, water solubility, polarity, vapor pressure, density, viscosity, and even toxicity and many others.

Solvents can be separated by one of four basic methods: by solvent power (solubility polarity, acidity/basicity, properties/parameters), evaporation rate/boiling point, chemical structure, and hazard classification. Within the latter, this evaluation identifies both physical hazards (e.g., flash point, flammability, or reactivity) and toxicity, etc. The partitioning based on chemical structure groups used three groups: hydrocarbons, and oxygenated and chlorinated solvents [1–3].

Parker [1] divides them into: protic, aprotic, and inert according to the dipolarity of the solvent molecules and their ability to act as hydrogen bond donors. One disadvantage of a classification scheme such as this is that the groups are not restraining.

Partitioning of solvents based on physicochemical properties proved to be a significant and challenging problem [2–6]. Special interest provides a new study [7] where a new solvent similarity index is introduced, aiding in discovering the most suitable solvent for specific purposes. The solvent similarity index was calculated based on 261 pure solvents at 298 K, and classification was done for the solvents according to their solvation properties. Pushkarova et al. [8] used, as empirical characteristics of solvent-solute interactions via Taft-Kamlet-Abboud, polarity functions to determine the solvatochromic polarity. The practice of solvatochromic probing is growing rapidly but classification of media based on these values can be difficult. The paper focuses on the artificial neural networks (ANN) for the classification of solvent on the basis of their solvatochromic characteristics. Also, the influence of data variation on the stability of classification has been studied.

In the study of Gramatica et al. [9] a neuron nets approach was used for solvent separation. In general, many other chemometric methods contributed to proper solvent selection for practical needs like regression analysis, factor analysis, or partial least square regression [3–5].

Bradley et al. [10] used the Abraham general solvation model to predict the solvent coefficients for all organic solvents. The models were used to propose sustainable solvent replacements for commonly used solvents.

Recent efforts are concentrated on the application of chemometric strategies as suitable tools for classification of solvents (as objects of the analysis) characterized by many properly selected variables (chemical, structural, and physicochemical descriptors [11–15]). The majority of the methodologies are well developed and widely used for classification, interpretation, and modeling purposes like cluster analysis, principal components and factor analysis, artificial neural networks, partial least square regression, and discriminant analysis. A limited number of applications are related to fuzzy analysis [16,17].

Fuzzy clustering and partitioning also finds application in solvents characterization [18].

Fuzzy clustering analysis offers unique opportunities for decomposition of a large data set into a fixed number of similarity groups or clusters. Indeed, the classical cluster analysis (hierarchical or non-hierarchical) could achieve similar results but the strong advantage of the fuzzy partitioning strategy is the opportunity to locate a certain object (or variable) not to a single group of similarity but to calculate a function of membership for each object. Thus, a single object could be attributed to more than one cluster. This makes the interpretation efforts more loosely allowing considering specific distribution of objects into clusters with respective degree of membership. It eliminates ambiguity in interpretation or often unavoidable overlapping of clusters.

The major goal of the present study is to achieve a reliable partitioning of a large number of solvents with broad practical use by application of fuzzy partitioning methodology.

In this study, the fuzzy divisive hierarchical clustering and the powerful fuzzy divisive hierarchical associative-clustering method, which offer an excellent possibility to associate each fuzzy partition of samples to a fuzzy set of characteristics (descriptors), were successfully applied for the characterization

of 259 solvents, according to their 15 specific descriptors (experimentally found and theoretically predicted). What is quite new is the partitioning of solvents and their association with different descriptors with high, moderate, and low values. The obtained results clearly demonstrated the efficiency and information power of the advanced fuzzy clustering method in solvents characterization and clustering.

2. Materials and Methods

2.1. Fuzzy Clustering Methods

The application of fuzzy logic for various scientific and technical goals has been commented on for decades [19]. This approach differs from the classical hard clustering where each object of the data set finds its own cluster. Thus, an object either belongs to a defined cluster or is out of it. The application of Fuzzy theory to the problem of finding similarity between objects of interest leads to the conclusion that a particular object can belong simultaneously to more than one cluster, but with different degrees of membership (DOMs) between 0 and 1 [20,21]. In one of the possible approaches to so-called fuzzy c-means clustering (FCM), each cluster is replaced by a cluster prototype [22,23] with a respective center, which contains information about the size and the shape of the cluster. The degrees of membership are computed from the distances of the data point to the cluster centers. These distances are responsible for the value of DOM and determine the cluster properties and shape (point, line, etc.) [24].

There are different algorithms in fuzzy clustering applications, the most used being the binary divisive algorithm and the generalized fuzzy c-means algorithm (GFCM). The fuzzy methods briefly described above and the corresponding software were clearly described and efficiently applied in previous papers [25–30].

2.2. Data Set

The dataset consists of 269 solvents. Each solvent was described by 15 variables (molecular descriptors and experimentally obtain properties) shown below in Table 1.

Table 1. Molecular descriptors and experimentally obtained properties.

No.	Variable Name	Code
1	Melting point (experimental)	MPe
2	Melting point (calculated)	MPc
3	Boiling point (experimental)	BPe
4	Boiling point (calculated)	BPc
5	Density	Dens
6	Water solubility (experimental)	WSe
7	Water solubility (calculated)	WSc
8	Vapor pressure (experimental)	VPe
9	Vapor pressure (calculated)	VPc
10	Henry Law constant (experimental)	HLe
11	Henry Law constant (calculated)	HLc
12	Octanol/water coefficient (experimental)	logKOWe
13	Octanol/water (calculated)	logKOWc
14	Octanol/Air (calculated)	logKOAc
15	Bioconcentration Factor	log BCF

In the present study, the following set of subprograms implemented in the EPI Suite™ version 4.10 were used: MPBPWIN™, WATERNT™, HENRYWIN™, KOAWIN™, KOWWIN™, and BCFBAF™.

The melting point (MP), boiling point (BP), and vapor pressure (VP) within the MPBPWIN™ module in EPI Suite™ were applied to predict the properties of our interests. The MPBPWIN™ estimates melting point by the two methods: (1) the Joback Method (a group contribution method); (2) the Gold and Ogle method $MP = 0.5839 * BP$ (in °K). Boiling point is valued by an adaptation of the Stein and Brown (1994) method, which is also a group contribution method. Vapor pressure is predictable as well by the methods: (1) Antoine, (2) Modified Grain method, and (3) the Mackay method. WATERNT™ estimates water solubility directly using a “fragment constant” method similar to that used in the KOWWIN™ program.

The Henry’s law constant is estimated by the subprogram HENRYWIN™, which calculates (air/water partition coefficient) using both the group contribution and the bond contribution methods.

This KOAWIN™ program evaluates the logarithm of the octanol-air partition coefficient (KOA) of an organic compound with the compound’s octanol–water partition coefficient (Kow) and Henry’s law constant (HLC). For the KOAWIN only a chemical structure was needed for estimation of KOA. In the KOAWIN structures are implemented by the SMILES codes (Simplified Molecular Input Line Entry System). The KOA is possible to be predicted from the octanol–water partition coefficient (KOW) and Henry’s law constant (H) by the subsequent equation:

$$KOA = KOW(RT)/H$$

where R is the ideal gas constant and T is the absolute temperature. KOA and KOW are unitless values. H/RT is the unit less Henry’s law constant, also known as the air–water partition coefficient (KAW).

Therefore, the equation to estimate KOA is:

$$KOA = KOW/KAW$$

The KOWWIN™ program is for the octanol–water partition coefficient prediction. The basis of prediction in KOWWIN is a “fragment constant” methodology. In this “fragment constant” method, the starting structure is divided and then evaluated.

The comparison with the available experimental data shows a high level of correlation. In such a way, missing data in the large data set could be replaced.

3. Results and Discussion

3.1. Fuzzy Divisive Hierarchical Clustering of Descriptors

The fuzzy clustering of the variables (15 in total) aims to check the following:

- If the experimental values of the respective variables conform with the calculated one (i.e. if they fall within a fuzzy cluster with high membership function);
- If the partitioning procedure could determine stable groups of similarity between the variables with high DOM;
- The procedure is important for revealing information about possible descriptors for classification of the solvents in interest.

In the supplemental information section (Supplement T1) the fuzzy partitioning results for 15 variables are presented. In total, 28 groups are considered. The summary of the final partitioning is shown below:

A1—only HLC is included (a typical outlier)

A2—MPe MPc BPe BPc Dens WSe WSc VPe VPc HLe logKOWe LogKOWc logKOAc logBCF (the rest of the variables show a high level of similarity with a distinct difference from HLC).



In the next steps of fuzzy partitioning respective groups of similarity based on DOM will be sought.

A21—MPe MPc BPe BPc Dens VPe VPc HLe logKOWe LogKOWc logKOAc logBCF

A22—WSe WSc

In this partitioning stage, the experimentally found and theoretically calculated values of water solubility are extracted as a group of similarity different from the rest of variables in subgroup A21.

A211—BPe BPc

A212—MPe MPc Dens VPe VPc HLe logKOWe LogKOWc logKOAc logBCF

A2111—BPe

A2112—BPc

A2121—Dens

At this level of fuzzy partitioning, one finds separation between the experimentally and theoretically found values of boiling points and density. According to the DOM values the differences are small and the similarity between these three variables is significant,

A2122—MPe MPc VPe VPc HLe logKOWe LogKOWc logKOAc logBCF

A21221—VPe VPc HLe logKOWe LogKOWc logKOAc logBCF

A21222—MPe MPc

A212211—VPe VPc

The separation of two other groups of similarity is indicated melting point (experimental and theoretical values) and vapor pressure (experimental and theoretical values).

A212212—HLe logKOWe LogKOWc logKOAc logBCF

A2122111—VPc

A2122112—VPe

A2122121—logBCF

This stage of fuzzy partitioning reveals a slight difference between vapor pressure (theoretical and experimental values), and a more specific role of logBCF as compared to the stable group of logKOW (experimental and theoretical values) and logKOAc (calculated values).

A2122122—HLe logKOWe LogKOWc logKOAc

A21221221—HLe logKOWe LogKOWc

A21221222—logKOAc

A212212211—LogKOWc

A212212212—HLe logKOWe

A2122122121—logKOWe

A21221221212—HLe

A212221—MPe

A212222—MPc

A221—WSc

A222—Wse

The fuzzy partitioning carried out for 15 variables characterizing a set of solvents revealed the following fuzzy linkage of the variables:

- Very good coincidence between experimentally determined and theoretically calculated values of the variables characterizing the solvents; this means that if experimental values of some solvents are missing, calculation substitutes could be successfully used for classification and interpretation goals;

- HLc was defined as a typical outlier;
- The group of variables characterizing the distribution between different media (important for toxicity properties determination) is very compact;
- The parameters characterizing physicochemical properties (MP, BP, WS, and VP) indicate various type of similarity with the other parameters—water solubility is the most distant to the rest of parameters, followed by BP and MP; density is closest to BP; logBCF is slightly different as compared to the rest of “toxicity esteems.”

Additional material could be found in Supplement

3.2. Fuzzy Divisive Hierarchical Clustering of Solvents

To compare the partitions, and the similarity and differences of the investigated solvents, we have to analyze both the characteristics of the prototypes corresponding to the partitions hierarchy obtained by applying fuzzy divisive hierarchical clustering and DOMs of solvents corresponding to all fuzzy partitions. The results presented in Table 2 clearly illustrate the most specific characteristics of each fuzzy partition and their similarity and differences.

The initial two clusters A1 and A2 indicate that one typical outlier is present in the list of solvents—perfluorooctane, whose properties are completely different from those of the other 268 solvents. The further divisive fuzzy clustering indicates the level of the membership function of each solvent into each of the next groups included (22 in total).

Next, Table 2 shows the final fuzzy partitioning with the prototypes of the partitions, ranked solvents for each group and the range of DOM.

Table 2. Final fuzzy partitioning.

Final Fuzzy Partitions	Prototypes of Fuzzy Partitions		Solvents (Ranked in Decreasing Order)	DOMs Range
	Parameters of Prototype			
A111111	−24.06; −54.87; 233.98; 203.55; 21.61; 8685.76; 1293.07; 1.39; 0.83; 0.00; 0.03 1.20; 1.94; 6.05; 0.98		19	0.6348
A111112	−14.24; 188.97; 186.54; 2.09; 18.27; 9376.14; 42.79; 2.64; 0.31; 0.00; 1.53; 0.75; 5.65; 0.58; −77.87		202, 259, 217, 162,	0.7181–0.4695
A11112	−65.36; −50.74; 131.11; 132.12; 43.49; 7923.34; 3573.41; 21.71; 20.30; 0.00; 0.02; 1.75; 1.88; 3.84; 0.39		102, 117	0.6730–0.2889
A11121	−60.21; −53.00; 142.95; 135.46; 42.30; 5004.94; 2542.52; 83.02; 78.23; 0.00; 0.03; 1.84; 1.84; 4.05; 0.59		54, 38, 52, 53, 9, 134	0.7262–0.2825
A11122	−71.27; −76.34; 107.00; 147.22; 122.42; 3417.29; 4425.60; 198.31; 70.84; 0.01; 0.03; 1.78; 1.53; 4.90; 0.33		118, 104, 57, 96	0.8062–0.8062
A11211	80.41; −23.42; 319.82; 112.29; 573.17; 4808.29; 3389.89; 6.06; 92.03; 0.00; 0.31; 1.33; 9.59; 0.80; −114.19		157, 223	0.9574–0.9491
A11212	−24.89; 76.99; 154.75; 8.68; 2427.15; 2994.14; 647.18; 53.07; 7.58; 0.00; 1.52; 1.23; 4.64; 0.93; −35.57		260, 188, 231	0.7190–0.2987
A11221	−58.62; 121.52; 135.12; 1.73; 7497.75; 6004.92; 136.19; 103.68; 0.21; 0.00; 1.44; 1.69; 3.73; 0.63; −78.32		233, 145, 179, 144	0.5978–0.3376
A11222	−47.51; 136.10; 138.25; 2.50; 6432.46; 3613.26; 122.45; 59.46; 0.38; 0.00; 1.70; 1.71; 3.92; 0.62; −42.74		200, 218, 234, 227	0.5407–0.2093

Table 2. Cont.

Final Fuzzy Partitions	Prototypes of Fuzzy Partitions	Solvents (Ranked in Decreasing Order)	DOMs Range
	Parameters of Prototype		
A12111	−18.28; −10.51; 184.30; 150.65; 12.53; 31.27; 28.06; 20.28; 13.51; 0.19; 0.83; 1.56; 2.13; 4.38; −3.25	136, 129, 115, 55, 17, 110, 6, 67, 80, 49, 97, 112, 26, 109, 124, 86, 44, 23, 193, 68, 87, 135, 58, 45, 5, 75, 50, 37, 46, 33, 114, 133, 65, 29, 18, 149, 197, 254, 11, 238, 95, 84, 81, 88, 22, 100, 28, 77, 94, 56, 31, 121, 122, 32, 208, 41, 30, 1, 90, 240, 36, 111, 47, 89, 185, 216	0.9956–0.2976
A12112111	16.28; 89.97; 337.65; 355.25; 3.90; 97.01; 4.08; 1.86; 5.41; 0.02; 0.03; 6.00; 7.21; 8.30; 2.05	99 103 35 43 116 27 92 78 101 64 119 268	0.6005–0.0600
A12112112	10.77; 55.33; 305.37; 309.65; 2.75; 95.45; 9.19; 1.95; 1.25; 0.02; 0.03; 5.99; 6.11; 7.37; 2.08	123, 8, 24, 25, 71, 66, 105, 130	0.6368–0.1414
A121121211	18.65; 29.24; 273.01; 219.70; 8.12; 125.43; 5.96; 5.76; 0.99; 0.03; 0.02; 1.72; −0.08; 6.95; −0.20	48, 21, 152	0.6432–0.0937
A121121212	2.70; 30.76; 269.06; 258.53; 3.06; 123.06; 4.16; 2.48; 0.42; 0.03; 0.01; 5.05; 2.10; 7.25; 0.81	73, 120, 113, 2	0.7989–0.3787
A12112122	4.40; −7.63; 243.97; 239.15; 4.24; 134.37; 21.91; 3.45; 1.32; 0.03; 0.03; 3.57; 3.47; 5.96; 1.12	98, 126, 108, 61, 60, 93, 76	0.7381–0.1055
A121122	−14.32; 16.36; 184.44; 149.07; 117.55; 465.95; 353.89; 34.18; 24.34; 0.02; 0.40 2.88; 4.28; 3.77; −5.09	253, 13, 106, 170, 34, 125, 62, 10, 42, 132, 15, 40, 69	0.5034–0.0892
A1212111	18.33; 218.26; 232.00; 5.49; 20.77; 18.76; 16.13; 3.73; 4.80; 0.02; 1.99; 1.41; 6.44; 1.22; −48.90	248, 177, 261, 137, 148, 163, 225, 138, 158, 181, 265, 147, 207, 269, 205, 150, 256, 161, 171, 155, 143, 186, 235, 250, 239	0.5992–0.1036
A1212112	−19.64; 169.10; 172.41; 7.39; 15.19; 17.95; 15.96; 8.17; 3.94; 0.05; 1.51; 1.24; 5.20; 1.14; −52.63	201, 262, 212, 198, 139, 190, 183, 222, 173, 266, 214, 246	0.5090–0.1133
A1212121	−61.90; 89.25; 97.95; 11.00; 8.68; 14.72; 46.64; 47.82; 5.89; 0.07; 0.48; 0.66; 3.55; 0.87; −25.63	156, 264, 169, 224, 182, 154, 153, 219, 141, 164, 180, 210	0.5958–0.1890
A1212122	−45.95; 126.62; 125.31; 4.78; 6.59; 9.59; 14.37; 13.52; 1.99; 0.06; 0.66; 0.77; 4.30; 0.78; −29.46	213, 142, 196, 242, 236, 151, 192, 175, 176, 178, 165, 191, 252, 251, 160, 263, 203, 189, 226, 204, 241, 194, 249	0.7261–0.1019
A12122	−43.23; 50.28; 135.60; 63.69; 61.31; 128.10; 130.95; 86.49; 35.51; 0.11; 0.90; 1.75; 3.55; 2.46; −17.62	232, 159, 211, 195, 168, 187, 245, 172, 174, 237, 199, 228, 74, 167, 85, 267, 51, 14, 230, 91, 39, 12, 3, 255, 63, 131, 79, 140, 257, 244, 127	0.9979–0.1005
A1221	−45.95; 126.62; 125.31; 4.78; 6.59; 9.59; 14.37; 13.52; 1.99; 0.06; 0.66; 0.77; 4.30; 0.78; −29.46	215, 258, 221, 243, 166, 146, 247, 206, 209, 220	0.6506–0.3753
A1222	−45.48; 37.33; 145.26; 205.85; 747.83; 1979.16; 1053.58; 52.32; 18.56; 0.01; 0.39; 2.23; 2.41; 6.05; −4.47	4, 82, 16, 70, 229, 7, 59, 184, 128, 83, 107, 72	0.9676–0.1448
A2	42.00; −58.65; 105.90; 102.10; 1.73; 3371.80; 0.00; 57.84; 33.90; 0.04; 2,450,000.00; 1.62; 6.17; −1.15; 3.74	20	1.0000

3.3. Fuzzy Divisive Hierarchical Associative-Clustering of Solvents and Descriptors

To compare the partitions, and the similarity and differences of solvents, we have to analyze the DOMs corresponding to all fuzzy partitions for both the samples and characteristics (descriptors). The results obtained by applying the fuzzy divisive hierarchical associative-clustering method using the descriptor data are presented in Table 3. By carefully analyzing the fuzzy partitions at each level

(partition history/hierarchy) in parallel with the descriptor considered data, the following remarks may be taken. The fuzzy partitioning of the solvents with indication of the descriptors related to each fuzzy partition (cluster) is depicted in Table 3.

Table 3. The fuzzy partitioning of the solvents and variables (descriptors).

Solvents	Variables	DOM Solvents	DOM Variables
A1 244 15 10 257 125 132 106 42 140 4 62 220 40 82 34 267 79 131 268 209 92 27 255 230 74 239 167 155 63 170 90 71 76 205 269 130 8 199 25 111 185 105 250 89 216 13 207 159 228 150 101 119 2 69 214 120 152 95 246 11 78 81 240 249 21 137 93 18 116 221 22 181 98 258 253 208 172 174 235 126 245 99 51 148 85 265 114 103 36 87 35 261 24 47 161 43 64 229 45 66 68 147 49 194 41 211 123 138 238 256 186 97 188 225 254 158 171 67 109 26 237 124 143 5 180 23 112 195 44 37 160 183 222 113 80 262 210 139 198 73 169 33 166 135 252 251 197 29 65 176 168 133 88 50 46 86 48 75 164 190 189 60 212 175 108 187 248 61 58 151 213 193 192 149 156 236 153 17 201 178 263 163 196 84 14 100 191 16 142 129 154 6 94 39 173 3 177 264 242 55 224 115 241 182 266 110 165 91 121 122 1 56 32 219 141 30 31 77 28 204 226 203 12 59 136 232 260 70 243 127 215 7 247 206 118 134 157 184 223 146 9 96 231 128 83 52 104 227 53 54 38 72 107 162 202 217 218 259 19 234 200 102 57 233 179 144 145 117	1–10 12–15	1.000	1.000–0.9957
A2 20	11	1.000	1.000
A11 218 162 259 234 38 217 202 72 107 54 19 200 53 102 57 233 179 144 145 227 117 104 52 83 9 231 128 96 223 157 184	5–7	0.9991–0.5167	0.8819–0.7767
A12 111 13 199 152 214 76 246 89 150 228 18 174 172 245 239 253 159 170 114 47 255 211 41 256 194 137 74 195 237 180 66 23 210 238 230 181 186 49 68 161 126 254 171 45 97 98 143 169 124 87 138 235 109 26 67 261 158 112 5 208 225 147 37 265 44 93 22 85 240 160 222 148 80 164 21 123 139 198 262 36 183 33 64 197 252 251 135 43 65 81 24 187 35 60 103 29 113 46 176 73 133 75 50 86 189 248 88 11 167 190 51 168 212 249 95 99 175 108 48 213 61 78 58 120 151 156 193 149 192 2 116 153 267 236 201 178 163 263 90 17 196 84 100 216 14 191 207 154 142 129 94 6 264 119 177 39 173 3 242 224 101 185 55 130 241 115 182 105 266 165 110 91 121 25 122 250 1 56 32 219 30 141 31 8 77 28 204 226 82 203 12 71 269 205 136 155 232 4 27 92 63 34 268 106 131 62 79 140 257 125 42 10 244 132 15 209 40 220 258 69 221 229 166 16 188 70 59 243 260 127 215 206 247 7 118 146 134	8 9 2 13 14 12 10 15 1 4	0.9999–0.5020	0.9996–0.8953
A111 19 162 217 202 259 53 102 54 179 38 117 223 52 157 9	6	0.9607–0.3961	0.8819
A112 218 234 200 72 107 227 144 145 57 233 83 104 128 231 96 184	5 7	0.9967–0.3022	0.9–0.3022
A1121 72 107 57 83 128 104 96	7	0.8–0.2718	0.7987
A1122 218 234 200 227 144 145 233 231 184	5	0.9–0.2123	0.7709
A121 106 82 119 105 8 90 71 25 120 2 11 95 101 78 229 81 92 216 221 268 130 125 27 4 257 166 21 116 132 185 69 93 260 22 258 244 10 98 155 220 269 205 59 209 126 16 240 70 243 36 99 250 215 207 7 40 255 127 247 103 239 206 79 131 87 63 118 134 146	13 14 12 10 9 15 1 8 2	0.9–0.3475	0.9–0.6356

Table 3. Cont.

Solvents	Variables	DOM Solvents	DOM Variables
A122 253 88 212 48 228 190 198 61 262 47 252 251 159 197 256 17 248 222 175 263 151 201 213 139 6 108 29 73 236 193 129 60 210 176 100 94 178 113 55 183 196 142 173 58 149 242 115 156 254 163 133 191 195 110 3 192 241 264 39 14 169 224 122,121 164 266 194 1 33 165 160 238 158 167 177 32 37 30 56 154 170 211 189 31 225 219 182 153 168 204 187 5 180 141 91 84 50 65 226 203 12 138 152 171 80 214 28 77 237 86 230 135 41 246 46 174 124 111 89 136 44 232 143 245 42 109 172 75 147 140 66 26 114 23 112 186 123 150 161 97 18 261 15 265 62 13 67 34 199 148 85 68 137 51 45 24 249 49 235 43 188 74 208 76 64 35 267 181	4 3	0.9–0.5186	0.9–0.8369
A1211 258 269 205 155 257 215 209 250 207 247 243 166 40 7 255 206 63 131 79 146	8 9 2	0.7318–0.2235	0.8666–0.5420
A1212 8 105 90 71 25 120 11 82 95 119 2 106 4 130 125 21 78 116 69 132 81 92 27 98 101 93 10 260 59 22 126 99 70 16 216 127 240 36 103 185 87 268 244 229 221 118 220 134 239	12 10 13 14 1 15	0.9382–0.2880	0.9–0.9379
A12121 106 81 240 216 185 260 101 268	1		
A12122 90 120 25 8 82 2 119 105 4 130 78 95 116 71 125 11 27 69 132 98 93 10 126 59 21 99 22 127 16 70 103 36 229 118 221 92 87 134 244 220 239	12 13 10 14 15	0.8–0.3352	0.9408
A121221 119 11 95 93 22 21 98 10 126 87 221 244 220	13 14 12	0.9–0.2867	0.9–0.8168
A121222 25 8 82 105 2 120 130 78 71 90 116 27 132 4 69 99 59 103 16 70 36 127 125 92 118 239 134 229	10 15	0.8–0.2226	0.9–0.7336
A1212221 1 119 11 95 22 21 87	14	0.7–0.3422	0.9207
A1212222 2 98 10 126 93 221 220 244	13 12	0.5–0.1733	0.9–0.5802
A1212221 8 25 132 69 105 71 27 59 127 16 70 118 92 239 134	15	0.8–0.1720	0.7326
A1212222 2 120 78 4 82 130 90 116 99 36 103 125 229	10	0.7–0.1169	0.8960
A1221 48 61 17 47 73 60 108 113 6 129 55 115 42 140 110 111 89 66 15 62 123 34 37 13 114 88 18 5 267 26 24 188 50 109 80 97 124 112 43 135 35 64 76 49 68 74	4	0.9–0.3307	0.9159
A1222 252 251 263 175 212 151 213 190 139 176 173 183 222 228 198 236 242 256 266 241 160 178 196 142 62 253 210 201 156 192,191 264 169 194 226 248 165 219 224 189 163 246 177 225 193 197 149 138 203 158 214 180 170 254 154 141 164 153 182 238 147 159 33 195 204 211 30 94 84 152 237 121 167 91 122 65 171 12 32 3 39 31 58 14 100 28 1 168 265 56 187 143 150 261 77 249 230 161 186 29 148 136 232 137 41 174 245 75 172 86 235 85 208 181 51 67 199 45	3	0.9–0.3509	0.8366

For the final goal of fuzzy partitioning of the objects (solvents) was performed by the use of 10 variables (only the experimentally found ones) (Table 4).

Table 4. Solvents included in each class and the respective class descriptor.

Class	Solvents	Variables
1	9 19 38 52 53 54 102 117 157 162 179 202 217 223 259 57 72 83 96 104 107 128	WSe
2	144 145 184 200 218 227 231 233 234	Dens
3	7 40 63 79 131 146 155 166 205 206 207 209 215 243 247 250 255 257 258 269	VPe
4	81 101 106 185 216 240 260 268	MPe
5	11 21 22 87 95 119	logKOA
6	10 93 98 126 220 221 244	logKOWe
7	8 16 25 27 59 69 70 71 92 105 118 127 132 134 239	logBCF
8	2 4 36 78 82 90 99 103 116 120 125 130 229	HLe
9	5 6 13 15 17 18 23 24 26 34 35 37 42 43 44 46 47 48 49 50 55 60 61 62 64 66 68 73 74 76 80 88 89 97 108 109 110 111 112 113 114 115 123 124 129 133 135 140 188 267 1 3 12 14 28 29 30 31 32 33 39 41 45 51 56 58 65 67 75 77 84 85 86 91 94 100 121 122 136 137 138 139 141 142 143 147 148 149 150 151 152 153 154 156 158 159 160 161 163 164 165 167 168 169 170 171 172 173 174 175 176 177 178 180 181 182 183 186 187 189 190 191 192 193 194 195 196 197 198 199 201 203 204 208 210 211 212 213 214 219 222 224 225 226 228 230 232 235 236 237 238 241 242 245 246 248 249 251 252 253 254 256 261 262 263 264 265 266	BPe
10	20	HLc

The fuzzy partitioning performed reveals the following classes of solvents:

Class 1 (WSe): 9 19 38 52 53 54 102 117 157 162 179 202 217 223 259 57 72 83 96 104 107 128

Iodoethane Diethyl glutarate 1,1-dichloroethane Dimethyl phthalate quinoline 2,4-dimethyl-3-pentanone n-butyl acetate 1,2-dichloroethane Glycerol-1,3-Dibutyl ether m-cresol Dimethyl adipate Glycerol-1,2,3-triethyl ether diethyl carbonate Caprylic acid diethanolamide DMEU 1-hexanol 4-methyl-2-pentanone Butylacetate 1-chloropropane 2-chloropropane 2-Methyltetrahydrofuran Diethyl succinate.

Mainly chlorinated solvents and similar ones except for diethyl carbonate and buthylacetate (CHLORINATED SOLVENTS CLASS) with major descriptor WSe (experimental water solubility value; calculated water solubility gives the same separation).

Class 2 (Dens): 144 145 184 200 218 227 231 233 234

Bromoethane Di-isopropyl ether Benzonitrile Acetophenone Isobutyl acetate Di-n-propyl ether Carbon disulfide Benzaldehyde Chloroform.

Nonpolar and volatile solvents except for isobutyl acetate (NON-POLAR AND VOLATILE SOLVENTS CLASS) major descriptor DENS (density).

Class 3 (VPe): 7 40 63 79 131 146 155 166 205 206 207 209 215 243 247 250 255 257 258 269

Benzene 1,1,1-trichloroethane Dichloromethane Methyl formate Diethyl ether 1,1-dichloroethylene Oleyl alcohol Fluorobenzene Tetraethylene glycol Ricinoleic acid Triethylene glycol Butyl stearate Methyl benzoate 1,1,2,2-tetrachloroethane 1,8-Cineole gamma-Valerolactone Nopol alpha-Terpineol beta-Terpineol PolyEthyleneGlycol 200.

This is a mixture of polar solvents—acids and esters with non-polar ones such as benzene or 1,1,1-TCA (POLAR AND NON-POLAR SOLVENTS MIXED CLASS separated mainly by descriptor vapor pressure experimental values; the calculated value gives the same results).

Class 4 (MPe): 81 101 106 185 216 240 260 268

Glycerol triacetate Oleic acid Menthanol Diisooctylsuccinat Dioctylsuccinate Isosorbide dioctanoate DPMU PolyEthyleneGlycol 600.

POLAR SOLVENTS CLASS I defined by descriptor melting point I.

Class 5 (logKOA): 11 21 22 87 95 119

2-Pyrrolidone Sulfolane Propylene carbonate N-methylacetamide Glycerol Water

POLAR SOLVENTS CLASS II defined by descriptor logKOA.

Class 6 (logKOWe): 10 93 98 126 220 221 244

Phenetole Diisobutyl adipate Geranyl acetate Menthanyl acetate Trichloroethylene Pentyl acetate 1-Octanol.

The grouping was defined properly as a polar solvent except trichloroethylene POLAR SOLVENTS CLASS III defined by logKOW (experimental or theoretical).

Class 7 (logBCF): 8 16 25 27 59 69 70 71 92 105 118 127 132 134 239

Ethyl myristate Isoamyle acetate Butyl laurate Methyl abietate 2,6-dimethyl-4-heptanone N,N-dimethylaniline Nitrobenzene Benzyl benzoate Methyl stearate Methyl myristate Dimethyl 2-methylglutarate 1,1,3,3-tetramethyl urea Diethyl phthalate Diethyl adipate Glycerol-1,2,3-tributyl ether.

The group of polar ones, except for nitrobenzene—POLAR SOLVENTS CLASS IV defined by logBCF.

Class 8 (HLe): 2 4 36 78 82 90 99 103 116 120 125 130 229

Ethyl laurate Glycerol-1,2-dibutyl ether Acetyltributyl citrate Diisoamylsuccinate N,N-Diethylolcapramide Dibenzyl ether Butyl palmitate Methyl linolenate Methyl ricinoleate Methyl laurate Ethyl benzoate Dibutyl sebacate Anisole.

The group defined by a HIGH MOLECULAR WEIGHT POLAR SOLVENTS defined by HLe (experimental).

Class 9 (BPe): 5 6 13 15 17 18 23 24 26 34 35 37 42 43 44 46 47 48 49 50 55 60 61 62 64 66 68 73 74 76 80 88 89 97 108 109 110 111 112 113 114 115 123 124 129 133 135 140 188 267

1 3 12 14 28 29 30 31 32 33 39 41 45 51 56 58 65 67 75 77 84 85 86 91 94 100 121 122 136 137 138 139 141 142 143 147 148 149 150 151 152 153 154 156 158 159 160 161 163 164 165 167 168 169 170 171 172 173 174 175 176 177 178 180 181 182 183 186 187 189 190 191 192 193 194 195 196 197 198 199 201 203 204 208 210 211 212 213 214 219 222

224 225 226 228 230 232 235 236 237 238 241 242 245 246 248 249 251 252 253 254 256 261 262 263 264 265 266

This group is quite large. Most of the solvents are polar except for: carbon tetrachloride, xylenes, and bromobenzene.

Cyclohexanol Isododecane Di-n-butyl acetate 1-chlorobutane Glycerol-2-methyl monoether m-dichlorobenzene p-Cymene Methyl palmitate Isopropylacetate chlorobenzene Isopropyl palmitate 2,6-dimethylpyridine 1-bromobutane Butyl myristate Furfurylic alcohol 1-2,4-dimethylpyridine Dihydromyrcenol 3-Hydroxypropionic acid Benzyl alcohol Cyclohexanone 1,3-Dioxan-5-ol Diisobutyl succinate Glycerol-2-ethyl monoether Toluen Methyl Linoleate.

N,N-Dimethyldecanamide N-methylformamide Cyclopentane Propylene glycol Iodobenzene Glycerol-1,3-dimethyl ether Piperidine o-xylene Aniline Diisobutyl glutarate Tetrahydrofurfurylic alcohol 3-Methoxy-3-methyl-1-butanol p-xylene cis-decaline Dimethylisoborbide mesitylene Glycerol-1,2-dimethyl ether Isopropyl myristate d-Limonene 1,3-Dioxolane-4-methanol Propionic acid

N-decane Carbon tetrachloride Cyclopentyl methyl ether N-pentane Triethylamine Propyl formate Ethanol Ethyl acetate 1-Butanol 4-picoline 3-methyl-2-butanone n-Propyl acetate propionitrile Dimethyl sulfoxide 1,3-Dioxolane Cyclohexane Formamide Diethylamine Iso-octane Glycerol-1,2,3-trimethyl ether Dimethyl succinate 1,3-Propanediol Propylene glycol Butyronitrile N,N-dimethylformamide Ethyl formate β -Pinene 2,2,2-trifluoroethanol 3-pentanone Pyridine 2-pentanone n-heptane 3-Butyl-1-methylimidazolium tetrafluoroborate 1-Decanol N-methyl-pyrrolidin-2-one α -Pinene 1,2-dimethoxyethane 2-methoxyethanol Methyl oleate Decamethylcyclopentasiloxane Diethylene glycol Glycerol-2-butyl monoether Tributylamine 1-pentanol EthylHexyllactate Nitromethane.

Tert-butyl alcohol 1,4-dioxane Glycerol-1-ethyl monoether Cyclohexene N,N-dimethylacetamide Ethyl palmitate 5-(Hydroxymethyl)furfural 2-butanone 2-methyl-2-butanol styrene Methyl acetate Pyrrolidine N,N-Dimethyloctanamide Glycerol carbonate Acetone 2-aminoethanol tert-butyl methyl ether Acetylacetone 3-picoline Dipropylenglycol.

2-pentanol n-butylamine Diphenyl ether 2-propanol Ethylene glycol Ethyl linolenate Methanol Cyclopentyl methyl ether Nitroethane Phenol Isobutyl alcohol Ethylenediamine.

β -Farnesen Tetrachloroethylene Tetrahydrofuran 3-pentanol Methyl 5-(dimethylamino) 2-methyl-oxopentanoate 2,4,6-trimethylpyridine Glycerol-1,3-diethyl ether 2-butanol Acetic anhydride Ethyl linoleate trifluoroacetic acid n-hexane Ethyl lactate Cyclopentanone o-dichlorobenzene 3,3-dimethyl-2-butanone Dimethyl glutarate 1-propanol Glycerol-1-methyl monoether n-octane m-xylene Bromobenzene Choline acetate Ethyl oleate Acetic acid.

Acetonitrile Glycerol-1,2,3-tributyl ether morpholine 3-methyl-1-butanol Acetone 1,4-Cineole Terpeneol acetate 2-Furfuraldehyde beta-Myrcene Terpinolene Cyclademol Glycofurof (n = 2) Solketal HMPTA DEGDEE DEGDME Ethyl propionate TEGDME Dimethylsulfoxide.

Class 10 (HLc): *Outlier Perfluorooctane 20*

The solvents underlined above do not strictly belong to logical formation of similarity classes and seem more to be rather odd than reasonable as members of the respective class (polar, non-polar, or volatile solvents determined by specific variables). A careful check of the position of these 12 solvents into the fuzzy partitioning groups indicates that all of them have quite low maximal value of DOM as determined by fuzzy analysis (this values is shown next to the name of the solvent).

The few exceptions found (only 9 out of 259 solvents), namely:

(diethyl carbonate, benzene, nitrobenzene);(o-, m-, p-xylene) and (carbon tetrachloride, bromobenzene, trichloroethylene), are resultant to their low maximal DOM, so their position into one group of similarity is not stable and they could be considered either as members of the group with low probability, or members of a different class.

In Table 5 summarized results according to obtained classes are presented.

The table could be used as a practical guide for selection of type of solvents based on their physicochemical properties.

Table 5. Defined classes of solvents with the descriptors.

Name	Class	Polar	Non-Polar	Volatile	Polar-Volatile	Descriptor
Iodoethane 9	1			x		Wsol
Diethyl glutarate 19	1	x				Wsol
1,1-dichloroethane 38	1			x		Wsol
2,4-dimethyl-3-pentanone 54	1			x		Wsol
1-hexanol 57	1		x			Wsol
4-methyl-2-pentanone 72	1			x		Wsol
1-chloropropane 96	1			x		Wsol
n-butyl acetate 102	1				x	Wsol
2-chloropropane 104	1			x		Wsol
2-Methyltetrahydrofuran 107	1				x	Wsol
1,2-dichloroethane 117	1			x		Wsol
Diethyl succinate 128	1	x				Wsol
Glycerol-1,3-Dibutyl ether 157	1	x				Wsol
m-cresol 162	1		x			Wsol
Dimethyl adipate 179	1	x				Wsol
Glycerol-1,2,3-triethyl ether 202	1	x				Wsol
diethyl carbonate 217	1				x	Wsol
Caprylic acid diethanolamide 223	1	x				Wsol
Benzaldehyde 233	1		x			Wsol
Chloroform 234	1			x		Wsol
DMEU 259	1	x				Wsol
Dimethyl phthalate 52	1		x			Wsol
Quinoline 53	1		x			Wsol
Butylacetate 83	1		x			Wsol
Bromoethane 144	2			x		Dens
di-isopropyl ether 145	2			x		Dens
Benzonitrile 184	2		x			Dens
Isobutyl acetate 218	2				x	Dens
di-n-propyl ether 227	2			x		Dens
carbon disulfide 231	2			x		Dens



Table 5. Cont.

Name	Class	Polar	Non-Polar	Volatile	Polar-Volatile	Descriptor
Benzene 7	3			x		VPe
1,1,1-trichloroethane 40	3			x		VPe
Dichloromethane 63	3			x		VPe
methyl formate 79	3				x	VPe
diethyl ether 131	3			x		VPe
1,1-dichloroethylene 146	3			x		VPe
Oleyl alcohol 155	3		x			VPe
Fluorobenzene 166	3			x		VPe
tetraethylene glycol 205	3	x				VPe
Ricinoleic acid 206	3		x			VPe
triethylene glycol 207	3	x				VPe
Butyl stearate 209	3		x			VPe
methyl benzoate 215	3		x			VPe
1,8-Cineole 247	3		x			VPe
gamma-Valerolactone 250	3		x			VPe
alpha-Terpineol 257	3		x			VPe
beta-Terpineol 258	3		x			VPe
1,1,2,2-tetrachloroethane 243	3			x		VPe
Nopol 255	3		x			VPe
PolyEthyleneGlycol 200 269	3	x				VPe
Diocylsuccinate 216	4		x			MPe
Isosorbide dioctanoate 240	4		x			MPe
Glycerol triacetate 81	4	x				MPe
Oleic acid 101	4		x			MPe
Menthanol 106	4		x			MPe
Diisooctylsuccinate 185	4		x			MPe
DPMU 260	4	x				MPe
PolyEthyleneGlycol 600 268	4	x				MPe
2-Pyrrolidone 11	5		x			logKOA
Sulfolane 21	5	x				logKOA
Propylene carbonate 22	5	x				logKOA
N-methylacetamide 87	5	x				logKOA
Glycerol 95	5	x				logKOA
Water 119	5				x	logKOA



Table 5. Cont.

Name	Class	Polar	Non-Polar	Volatile	Polar-Volatile	Descriptor
Phenetole 10	6		x			logKOW
Diisobutyl adipate 93	6		x			logKOW
Geranyl acetate 98	6		x			logKOW
1-Octanol 244	6		x			logKOW
Menthanyl acetate 126	6		x			logKOW
Trichloroethylene 220	6			x		logKOW
pentyl acetate 221	6		x			logKOW
Ethyl myristate 8	7	x				logBCF
Isoamyle acetate 16	7				x	logBCF
Methyl abietate 27	7		x			logBCF
Methyl myristate 105	7		x			logBCF
Butyl laurate 25	7		x			logBCF
2,6-dimethyl-4-heptanone 59	7		x			logBCF
N,N-dimethylaniline 69	7		x			logBCF
Nitrobenzene 70	7		x			logBCF
Benzyl benzoate 71	7		x			logBCF
Methyl stearate 92	7		x			logBCF
Geraniol 239	7		x			logBCF
Dimethyl 2-methylglutarate 118	7	x				logBCF
1,1,3,3-tetramethyl urea 127	7	x				logBCF
Diethyl phthalate 132	7		x			logBCF
Diethyl adipate 134	7		x			logBCF
Ethyl laurate 2	8	x				HLe
Glycerol-1,2-dibutyl ether 4	8	x				HLe
dibenzyl ether 90	8		x			HLe
Methyl linolenate 103	8		x			HLe
Methyl ricinoleate 116	8		x			HLe
Methyl laurate 120	8		x			HLe
ethyl benzoate 125	8		x			HLe
Dibutyl sebacate 130	8		x			HLe
Acetyltributyl citrate 36	8		x			HLe
Diisoamylsuccinate 78	8		x			HLe
N,N-Diethylolcapramid 82	8		x			HLe
Butyl palmitate 99	8		x			HLe
Anisole 229	8		x			HLe



Table 5. Cont.

Name	Class	Polar	Non-Polar	Volatile	Polar-Volatile	Descriptor
Triethylamine 1	9				x	BPe
propyl formate 3	9				x	BPe
Cyclohexanol 5	9	x				BPe
Ethanol 12	9				x	BPe
di-n-butyl acetate 13	9				x	BPe
Ethyl acetate 14	9				x	BPe
1-chlorobutane 15	9			x		BPe
Glycerol-2-methyl monoether 17	9	x				BPe
m-dichlorobenzene 18	9		x			BPe
p-Cymene 23	9		x			BPe
Methyl palmitate 24	9		x			BPe
Isopropylacetate 26	9	x				BPe
1-Butanol 28	9				x	BPe
4-picoline 29	9				x	BPe
3-methyl-2-butanone 30	9				x	BPe
n-Propyl acetate 31	9				x	BPe
Propionitrile 32	9				x	BPe
Dimethyl sulfoxide 33	9	x				BPe
Chlorobenzene 34	9			x		BPe
Isopropyl palmitate 35	9		x			BPe
2,6-dimethylpyridine 37	9	x				BPe
1,3-Dioxolane 39	9				x	BPe
Cyclohexane 41	9			x		BPe
1-bromobutane 42	9			x		BPe
Butyl myristate 43	9		x			BPe
Furfurylic alcohol 44	9	x				BPe
Formamide 45	9	x				BPe
2,4-dimethylpyridine 46	9		x			BPe
Dihydromyrcenol 47	9		x			BPe
3-Hydroxypropionic acid 48	9	x				BPe
Benzyl alcohol 49	9		x			BPe
Cyclohexanone 50	9		x			BPe
Diethylamine 51	9				x	BPe
1,3-Dioxan-5-ol 55	9		x			BPe



Table 5. Cont.

Name	Class	Polar	Non-Polar	Volatile	Polar-Volatile	Descriptor
iso-octane 56	9			x		BPe
Glycerol-1,2,3-trimethyl ether 58	9	x				BPe
Glycerol-2-ethyl monoether 61	9	x				BPe
Toluene 62	9			x		BPe
1,3-Propanediol 67	9	x				BPe
N-methylformamide 68	9	x				BPe
Glycerol-1-butyl monoether 73	9	x				BPe
Cyclopentane 74	9			x		BPe
Propylene glycol 75	9	x				BPe
Iodobenzene 76	9		x			BPe
Butyronitrile 77	9				x	BPe
Glycerol-1,3-dimethyl ether 80	9	x				BPe
N,N-dimethylformamide 84	9	x				BPe
ethyl formate 85	9				x	BPe
β -Pinene 86	9		x			BPe
Piperidine 88	9				x	BPe
o-xylene 89	9			x		BPe
2,2,2-trifluoroethanol 91	9				x	BPe
3-pentanone 94	9				x	BPe
Aniline 97	9	x				BPe
Pyridine 100	9				x	BPe
Diisobutyl glutarate 108	9		x			BPe
Tetrahydrofurfurylic alcohol 109	9	x				BPe
3-Methoxy-3-methyl-1-butanol 110	9	x				BPe
p-xylene 111	9			x		BPe
cis-decaline 112	9		x			BPe
Dimethylisosorbide113	9	x				BPe
Mesitylene 114	9		x			BPe
Glycerol-1,2-dimethyl ether 115	9	x				BPe
2-pentanone 121	9				x	BPe
n-heptane 122	9			x		BPe
Isopropyl myristate 123	9		x			BPe
d-Limonene 124	9		x			BPe
1,3-Dioxolane-4-methanol 129	9	x				BPe
Propionic acid 133	9				x	BPe



Table 5. Cont.

Name	Class	Polar	Non-Polar	Volatile	Polar-Volatile	Descriptor
n-decane 135	9		x			BPe
3-Butyl-1-methylimidazolium tetrafluoroborate 136	9		x			BPe
1-Decanol 137	9		x			BPe
N-methyl-pyrrolidin-2-one 138	9	x				BPe
α -Pinene 139	9		x			BPe
carbon tetrachloride 140	9			x		BPe
1,2-dimethoxyethane 141	9				x	BPe
2-methoxyethanol 142	9				x	BPe
Methyl oleate 143	9		x			BPe
Decamethylcyclopentasiloxane 147	9		x			BPe
diethylene glycol 148	9	x				BPe
Glycerol-2-butyl monoether 149	9	x				BPe
Tributylamine 150	9		x			BPe
1-pentanol 151	9	x				BPe
EthylHexyllactate 152	9		x			BPe
Nitromethane 153	9				x	BPe
tert-butyl alcohol 154	9				x	BPe
1,4-dioxane 156	9				x	BPe
Glycerol-1-ethyl monoether 158	9	x				BPe
Cyclohexene 159	9			x		BPe
N,N-dimethylacetamide 160	9	x				BPe
Ethyl palmitate 161	9		x			BPe
5-(Hydroxymethyl)furfural 163	9		x			BPe
2-butanone 164	9			x		BPe
2-methyl-2-butanol 165	9				x	BPe
Styrene 167	9		x			BPe
Methyl acetate 168	9				x	BPe
Pyrrolidine 169	9				x	BPe
N,N-Dimethyloctanamide 170	9		x			BPe
Glycerol carbonate 171	9	x				BPe
Acetone 172	9				x	BPe
2-aminoethanol 173	9	x				BPe
tert-butyl methyl ether 174	9				x	BPe
Acetylacetone 175	9	x				BPe



Table 5. Cont.

Name	Class	Polar	Non-Polar	Volatile	Polar-Volatile	Descriptor
3-picoline 176	9	x				BPe
Dipropyleneglycol 177	9	x				BPe
2-pentanol 178	9				x	BPe
n-butylamine 180	9				x	BPe
diphenyl ether 181	9		x			BPe
2-propanol 182	9				x	BPe
Ethylene glycol 183	9	x				BPe
Ethyl linolenate 186	9		x			BPe
Methanol 187	9				x	BPe
Cyclopentyl methyl ether 188	9				x	BPe
Nitroethane 189	9				x	BPe
Phenol 190	9	x				BPe
isobutyl alcohol 191	9				x	BPe
Ethylenediamine 192	9				x	BPe
β -Farnesen 193	9		x			BPe
Tetrachloroethylene 194	9			x		BPe
Tetrahydrofuran 195	9				x	BPe
3-pentanol 196	9				x	BPe
Methyl 5-(dimethylamino)	9					BPe
2-methyl-oxopentanoate 197	9	x				BPe
2,4,6-trimethylpyridine 198	9		x			BPe
n-propylamine 199	9				x	BPe
Acetophenone 200	9				x	BPe
Glycerol-1,3-diethyl ether 201	9	x				BPe
2-butanol 203	9				x	BPe
acetic anhydride 204	9	x				BPe
Ethyl linoleate 208	9		x			BPe
trifluoroacetic acid 210	9				x	BPe
n-hexane 211	9			x		BPe
Ethyl lactate 212	9	x				BPe
Cyclopentanone 213	9	x				BPe
o-dichlorobenzene 214	9		x			BPe
3,3-dimethyl-2-butanone 219	9				x	BPe
Dimethyl glutarate 222	9	x				BPe
1-propanol 224	9				x	BPe



Table 5. Cont.

Name	Class	Polar	Non-Polar	Volatile	Polar-Volatile	Descriptor
Glycerol-1-methyl monoether 225	9	x				BPe
n-octane 226	9			x		BPe
m-xylene 228	9			x		BPe
Bromobenzene 230	9		x			BPe
Choline acetate 232	9		x			BPe
Ethyl oleate 235	9		x			BPe
Acetic acid 236	9				x	BPe
Acetonitrile 237	9				x	BPe
Morpholine 241	9				x	BPe
3-methyl-1-butanol 242	9				x	BPe
Acetone 245	9				x	BPe
2-Furfuraldehyde 249	9	x				BPe
Glycofurol (n = 2) 254	9	x				BPe
Solketal 256	9	x				BPe
HMPTA 261	9	x				BPe
DEGDEE 262	9	x				BPe
DEGDME 263	9	x				BPe
ethyl propionate 264	9				x	BPe
TEGDME 265	9	x				BPe
Dimethylsulfoxide 266	9	x				BPe
n-pentane 267	9			x		BPe
Isododecane 6	9		x			BPe
Diisobutyl succinate 60	9		x			BPe
Methyl Linoleate 64	9		x			BPe
Dimethyl succinate 65	9		x			BPe
N,N-Dimethyldecanamide 66	9		x			BPe
Glycerol-1,2,3-tributyl ether 238	9		x			BPe
1,4-Cineole 246	9		x			BPe
Terpineol acetate 248	9		x			BPe
beta-Myrcene 251	9		x			BPe
Terpinolene 252	9		x			BPe
Cyclademo 253	9		x			BPe



4. Conclusions

The fuzzy hierarchical clustering of a large group of solvents into 10 classes of similarity made it possible to find patterns of the chemicals with specific properties divided by important descriptors. The fuzzy partitioning method applied helped in finding relationships between solvents of various nature (polar, non-polar, volatile etc.) and the physicochemical variables used. Additionally, the chemometric analysis has proven that if there are missing data of specific descriptors the theoretical calculation of them is possible with very high level of approximate to the experimentally observed and established physicochemical indicators.

Thus, the present study offers a simple methodological approach to the complex problem of solvent partitioning.

In order to understand the similarity and differences of various solvents, fuzzy divisive hierarchical clustering and fuzzy divisive hierarchical associative-clustering were successfully applied. The fuzzy partition hierarchy of solvents and descriptors associated allowed identifying partitions (groups) of solvents with more or less similar characteristics in terms of higher, smallest, or intermediate values of considered descriptors.

Supplementary Materials: The following are available online at <http://www.mdpi.com/2073-8994/12/11/1763/s1>.

Author Contributions: Conceptualization, M.N.; methodology, C.S.; M.N.; software C.S.; M.N.; validation, M.N., V.S. formal analysis, M.N., M.T., C.S., V.S.; investigation, M.N.; resources, M.N.; data curation, C.S., M.N.; writing—original draft preparation, M.N., C.S., M.T., V.S.; writing—review and editing, M.N., V.S.; visualization, M.N. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by Information and Communication Technologies for a Single Digital Market in Science, Education and Security” of the Scientific Research Center, grant number NIS-3317 and National roadmaps for research infrastructures (RIs) grant number [NIS-3318]. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

Acknowledgments: The author M.N. is grateful for the additional support by the project “Information and Communication Technologies for a Single Digital Market in Science, Education and Security” of the Scientific Research Center, NIS-3317 and National roadmaps for research infrastructures (RIs) grant number [NIS-3318].

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Parker, A. Protic-dipolar aprotic solvent effects on rates of bimolecular reactions. *Chem. Rev.* **1967**, *69*, 1–32. [[CrossRef](#)]
2. Tobiszewski, M.; Nedyalkova, M.; Madurga, M.; Pena-Pereira, F.; Namieśnik, J.; Simeonov, V. Pre-selection and assessment of green organic solvents by clustering chemometric tools. *Ecotoxicol. Environ. Saf.* **2018**, *147*, 292–298. [[CrossRef](#)] [[PubMed](#)]
3. Katritzky, A.; Fara, D.; Kuanar, M.; Hur, E.; Karelson, M. The Classification of Solvents by Combining Classical QSPR Methodology with Principal Component Analysis. *J. Phys. Chem. A.* **2005**, *109*, 10323–10341. [[CrossRef](#)] [[PubMed](#)]
4. Molnar, M.; Komar, M.; Brahmabhatt, H.; Babić, J.; Jokić, S.; Rastija, V. Deep Eutectic Solvents as Convenient Media for Synthesis of Novel Coumarinyl Schiff Bases and Their QSAR Studies. *Molecules* **2017**, *22*, 1482. [[CrossRef](#)]
5. Chastrette, M.; Rajzmann, M.; Chanon, M.; Purcell, K. Approach to a general classification of solvents using a multivariate statistical treatment of quantitative solvent parameters. *J. Am. Chem. Soc.* **1985**, *107*, 1–11. [[CrossRef](#)]
6. Laurence, C.; Legros, J.; Chantzis, A.; Planchat, A.; Jacquemin, D. A Database of Dispersion-Induction DI, Electrostatic ES, and Hydrogen Bonding α_1 and β_1 Solvent Parameters and Some Applications to the Multiparameter Correlation Analysis of Solvent Effects. *J. Phys. Chem. B* **2015**, *119*, 3174–3184. [[CrossRef](#)]
7. Driver, M.; Hunter, C. Solvent similarity index. *PCCP* **2020**, *22*, 11967–11975. [[CrossRef](#)]
8. Pushkarova, Y.; Kholin, Y. The classification of solvents based on solvatochromic characteristics: The choice of optimal parameters for artificial neural networks. *Cent. Eur. J. Chem.* **2010**, *10*, 1318–1327. [[CrossRef](#)]

9. Sahigara, F.; Ballabio, D.; Todeschini, R.; Consonni, V. Defining a novel k-nearest neighbors approach to assess the applicability domain of a QSAR model for reliable predictions. *J. Cheminform.* **2013**, *5*, 27. [[CrossRef](#)]
10. Bradley, J.-C.; Abraham, M.H.; Acree, W.E.; Lang, A.S.I.D. Predicting Abraham model solvent coefficients. *Chem. Cent. J.* **2015**, *12*, 2–10. [[CrossRef](#)]
11. Johnson, A.R.; Vitha, M.F. Chromatographic Selectivity Triangles. *J. Chromatogr. A* **2011**, *1218*, 556–586. [[CrossRef](#)] [[PubMed](#)]
12. Katritzky, A.R.; Tamm, T.; Wang, Y.; Sild, S.; Karelson, M. A Unified Treatment of Solvent Properties. *J. Chem. Inf. Comput. Sci.* **1999**, *39*, 692–698. [[CrossRef](#)]
13. Poole, C.F.; Karunasekara, T. Solvent Classification for Chromatography and Extraction. *J. Planar Chromatogr.* **2012**, *25*, 190–199. [[CrossRef](#)]
14. Lesellier, E. Spider Diagram: A Universal and Versatile Approach for System Comparison and Classification: Application to Solvent Properties. *J. Chromatogr. A* **2015**, *1389*, 49–64. [[CrossRef](#)]
15. Wypych, G. *Handbook of Solvents*, 2nd ed.; Chem Tec Publishing: Toronto, ON, Canada, 2001.
16. Sarbu, C.; Pop, H.F. Fuzzy Soft-Computing Methods and Their Applications in Chemistry. In *Reviews in Computational Chemistry*; Lipkowitz, K.B., Larter, R., Cundari, T.R., Eds.; Wiley-VCH: Hoboken, NJ, USA, 2004; Chapter 5, pp. 249–332.
17. Halgamuge, S.K.; Wang, L. (Eds.) *Classification and Clustering for Knowledge Discovery*; Springer: Berlin/Heidelberg, Germany, 2005.
18. Guidea, A.; Sarbu, C. Fuzzy characterization and classification of solvents according to their polarity and selectivity. A comparison with the Snyder approach. *J. Liq. Chromatogr. Relat. Technol.* **2020**, *43*, 336–343. [[CrossRef](#)]
19. Kaufman, L.; Rousseeuw, P.J. *Finding Groups in Data: An Introduction to Cluster Analysis*; John Wiley & Sons: New York, NY, USA, 2009.
20. Zadeh, L.A. Fuzzy sets. *Inf. Control* **1965**, *8*, 338–353. [[CrossRef](#)]
21. Rouvray, D. *Fuzzy Logic in Chemistry*; Academic Press: San Diego, CA, USA, 1997; p. 364.
22. Sarbu, C.; Pop, H.F. Fuzzy Soft-Computing Methods and Their Applications in Chemistry. *Rev. Comput. Chem.* **2004**, *20*, 249–332.
23. Bezdek, J.C. *Pattern Recognition with Fuzzy Objective Function Algorithms*; Plenum Press: New York, NY, USA, 1987; p. 272.
24. Hoppner, F.; Klawonn, R.K.; Kruse, R.; Runkler, T. *Fuzzy Cluster Analysis: Methods for Classification, Data Analysis and Image Recognition*; John Wiley & Sons: Chichester, UK, 1999; p. 300.
25. Sârbu, C.; Zehl, K.; Einax, J.W. Fuzzy divisive hierarchical clustering of soil data using gustafson-kessel algorithm. *Chemom. Intell. Lab. Syst.* **2007**, *87*, 121–129. [[CrossRef](#)]
26. Sârbu, C.; Moț, A.C. Ecosystem discrimination and fingerprinting of Romanian propolis by hierarchical fuzzy clustering and image analysis of TLC patterns. *Talanta* **2011**, *85*, 1112–1117. [[CrossRef](#)]
27. Pop, H.; Dumitrescu, D.; Sârbu, C. A Study of Roman Pottery (terra sigillata) Using Hierarchical Fuzzy Clustering. *Anal. Chim. Acta* **1995**, *310*, 269–279. [[CrossRef](#)]
28. Pop, H.; Sârbu, C. The fuzzy hierarchical cross-clustering algorithm. Improvements and comparative study. *J. Chem. Inf. Comput. Sci.* **1997**, *37*, 510–516. [[CrossRef](#)]
29. Dumitrescu, D.; Pop, H.; Sârbu, C. Fuzzy Hierarchical Cross-Classification of Greek Muds. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 851–857. [[CrossRef](#)]
30. Sârbu, C.; Horovitz, O.; Pop, H. A Fuzzy Cross-Classification of Chemical Elements, Based on Their Physical, Chemical and Structural Features. *J. Chem. Inf. Comput. Sci.* **1996**, *36*, 1098–1108. [[CrossRef](#)]

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