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Short Report

Solubility Prediction of Solutes in Non-Aqueous Binary Solvent Mixtures

Abolghasem Jouyban,*,[a] Maryam Khoubnasabjafari,[b] Somaieh Soltani,[c] Shahla Soltanpour,[d] Elnaz Tamizi[e] and William E. Acree Jr.[f]

[a]*Faculty of Pharmacy and Drug Applied Research Center, Tabriz University of Medical Sciences, 51664, Iran*

[b]*Kimia Research Institute, P.O. Box 51665-171, Iran*

[c]*Research Center for Pharmaceutical Nanotechnology, Tabriz University of Medical Sciences, 51664, Iran*

[d]*Biotechnology Research Centre, Tabriz University of Medical Sciences, 51664, Iran*

[e]*Student Research Center, Tabriz University of Medical Sciences, 51664, Iran*

[f]*Department of Chemistry, University of North Texas, Denton, TX 76203-5070, USA*

Foi investigada a possibilidade de substituir os parâmetros de Abraham calculados teoricamente pelos parâmetros experimentais, na previsão da solubilidade de solutos não-aquoso em misturas de solventes binários, utilizando-se o modelo de Jouyban-Acree. As solubilidades de 90 conjuntos de dados, coletados a partir da literatura, foram preditas utilizando-se estes parâmetros, os coeficientes de solventes e também as solubilidades de sistemas mono-solventes. A precisão das solubilidades previstas foi avaliada calculando-se a média percentual do desvio (MPD) e também dos desvios percentuais (IPDs) individuais. O MPD global para a análise utilizando os parâmetros de Abraham, experimentais e teóricos, foram os mesmos e <14%. Uma boa distribuição (IPD) foi obtida por estas análises numéricas. Os conjuntos de dados investigados neste trabalho foram coletados a várias temperaturas e os resultados confirmaram a possibilidade de previsão da solubilidade em solventes binários a diferentes temperaturas. Explorou-se a possibilidade de cálculos *ab initio* nesta previsão utilizando as solubilidades calculadas em sistemas mono-solventes. No entanto, a diferença entre os valores previstos e observados, para os coeficientes dos solventes, aumentou para aproximadamente 60% e 200% quando usou-se gás e água, respectivamente. Estes, são valores muito grandes para várias aplicações de previsão.

The possibility of replacing theoretically computed Abraham parameters with the experimental Abraham parameters in solubility prediction of solutes in non-aqueous binary solvent mixtures using the Jouyban-Acree model was investigated. The solubilities of 90 data sets collected from the literature were predicted using their Abraham parameters, the solvent coefficients and also the solubilities in mono-solvent systems. The accuracy of the predicted solubilities was evaluated by calculating the mean percentage deviation (*MPD*) and also individual percentage deviations (*IPD*s). The overall *MPD* for the analysis using experimental and computed Abraham parameters were the same and was < 14%. A favoured *IPD* distribution was obtained for these numerical analyses. The data sets investigated in this work were collected at various temperatures and the results confirmed the possibility of solubility prediction in binary solvents at various temperatures. We did explore the possibility of *ab initio* solubility prediction of solutes in binary mixtures using the calculated solubilities in mono-solvent systems, however, the difference between the predicted and observed values increased to *ca.* 60% for gas-to-solvent coefficients and *ca.* 200% for water-to-solvent coefficients, which is too large for many predictive applications.

Keywords: solubility, prediction, non-aqueous mixed solvents, Abraham model, Jouyban-Acree model

Introduction

Solubility of a solute is affected by solvent's and solute's chemical structures and could be mathematically represented using meaningful parameters like Abraham solvation parameters. The Abraham solvation parameter models provided numerical methods for prediction of solutes' solubility in a wide variety of neat organic solvents.[1-6] The

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*e-mail: ajouyban@hotmail.com

Abraham models employ five parameters for each solute and six solvent coefficients that were computed for a number of common solvents.[3-4] The basic models proposed for process within condensed phases is:

$$\log\left(\frac{C_S}{C_W}\right) = c + e\cdot E + s\cdot S + a\cdot A + b\cdot B + v\cdot V \qquad (1)$$

and for process involving gas-to-condensed phase transfer is:

$$\log\left(\frac{C_S}{C_G}\right) = c + e\cdot E + s\cdot S + a\cdot A + b\cdot B + l\cdot L \qquad (2)$$

where C_S and C_W are the solute solubility in the organic solvent and water (in mole per liter), respectively, C_G is the gas phase concentration of the solute, E is the excess molar refraction, S is dipolarity/polarizability of solute, A denotes the solute's hydrogen-bond acidity, B stands for the solute's hydrogen-bond basicity, V is the McGowan volume of the solute, and L is the logarithm of the solute gas-hexadecane partition coefficient at 298.15 K. In equations (1) and (2) the coefficients *c, e, s, a, b, v* and *l* are the model constants (i.e. solvent's coefficients), which depend upon the solvent system under consideration. Numerical values of the model constants have been reported in the literature[3-4] for several water-to-organic solvent and gas-to-organic solvent systems.

Solvent mixing or cosolvency is the most common method to alter the solubility of a solute. There is an infinite number of solvent compositions for a given binary solvent, and for some compounds, both linear and non-linear solubility behavior have been reported in mixed solvent systems. The most accurate model to represent the solubility data in mixed solvent systems is the Jouyban-Acree model.[7-9] Its general form is:

$$\ln X_m = f_1 \ln X_1 + f_2 \ln X_2 + f_1 f_2 \sum_{j=0}^{2} B_j \left(f_1 - f_2\right)^j \qquad (3)$$

where X is the mole fraction solubility of the solute, f denotes the mole fraction of the solvents 1 and 2 in the solvent mixture, subscripts m, 1 and 2 are the mixed solvent and solvents 1 and 2, respectively, B_j is the model constant which represent various solute-solute, solvent-solvent and solute-solvent interactions. In a previous study,[10] QSPR models were proposed to calculate the numerical values of the B_j terms using the Abraham coefficients for 22 solvents and solute descriptors for 5 solutes.

The QSPR models proposed in an earlier work using water-to-solvent coefficients were:

$$B_0 = 0.028 + 2.123(c_1 - c_2)^2 - 0.160E(e_1 - e_2)^2 + 0.282S(s_1 - s_2)^2 + 1.713B(b_1 - b_2)^2 + 2.006V(v_1 - v_2)^2 \qquad (4)$$

$$B_1 = 0.033 + 0.670(c_1 - c_2)^2 - 0.477E(e_1 - e_2)^2 + 0.051S(s_1 - s_2)^2 + 0.476B(b_1 - b_2)^2 - 0.234V(v_1 - v_2)^2 \qquad (5)$$

$$B_2 = 0.022 + 2.024(c_1 - c_2)^2 - 0.204E(e_1 - e_2)^2 + 0.034S(s_1 - s_2)^2 + 0.243B(b_1 - b_2)^2 + 0.848V(v_1 - v_2)^2 \qquad (6)$$

and the QSPR models using gas-to-solvent coefficients were:

$$B_0 = 0.062 + 0.118(c_1 - c_2)^2 - 0.332E(e_1 - e_2)^2 + 0.410S(s_1 - s_2) + 2.399B(b_1 - b_2)^2 + 15.715L(l_1 - l_2)^2 \qquad (7)$$

$$B_1 = 0.103 - 1.864(c_1 - c_2)^2 - 1.590E(e_1 - e_2)^2 + 0.119S(s_1 - s_2)^2 + 1.010B(b_1 - b_2)^2 - 9.493L(l_1 - l_2)^2 \qquad (8)$$

$$B_2 = -0.008 + 1.075(c_1 - c_2)^2 + 0.053E(e_1 - e_2)^2 + 0.084S(s_1 - s_2)^2 + 0.414B(b_1 - b_2)^2 + 7.727L(l_1 - l_2)^2 \qquad (9)$$

The applicability of the proposed method was checked using 194 solubility data sets of five different solutes in various non-aqueous binary solvents. In this work, the possibility of replacing experimentally obtained Abraham parameters with the computed parameters is examined. The prediction capability of the previously developed QSPR models is checked using 90 solubility data sets[11-24] of solutes which were not used in training process of the QSPR models. The applicability of the proposed method is also shown for predicting solubility at various temperatures. The main limitation of the Abraham model is that solute solvational parameters are known for only 4,000 organic compounds. In a recently released software[25], this limitation is overcome and one is able to compute *E, S, A, B, V* and *L* parameters.

Computational Methods and Experimental Data

The solubilities of the solutes in binary solvent mixtures were collected from the literature.[11-24] Table S1 listed details of the experimental solubility data. The numerical values of the solvents' coefficients were listed in Table S2. In addition to the experimental database of solute's parameters, commercial software is also available to compute the parameters.[25] Table S3 lists the experimental and computed values of solute's parameters. Since the numerical values of A term for the solutes studied in the previous paper[10] were equal to zero, the corresponding terms have been omitted from the QSPR models.

The B_j constants of the Jouyban-Acree model were computed using equations (4)-(6) and (7)-(9), and these model constants were then used to predict the solubilities

Table 1. Details of various numerical analyses carried out using experimental and computed Abraham parameters

Method No.	B_j terms computed by	Solubility in mono-solvents
I	Water-to-solvent coefficients (equations (4)-(6))	Experimental data
II	Gas-to-solvent coefficients (equations (7)-(9))	Experimental data
III	Water-to-solvent coefficients (equations (4)-(6))	Computed by equation (1)
IV	Gas-to-solvent coefficients (equations (7)-(9))	Computed by equation (2)

of solutes in binary solvents. The predictions still required numerical values of the solute solubility in each pure solvent, *i.e.* X_1 and X_2. In order to provide a predictive model (without any experimentally determined data), C_S values of the solutes in the neat solvents under consideration were computed using Abraham models (using experimental values of C_W or C_G). The calculated molar solubilities, C_S, were converted to the mole fraction solubilities using density of the pure organic solvent. The calculated X_1 and X_2 values were then substituted into equation (3), along with the B_j values from equations (4)-(6) (or equations (7)-(9)) to predict the solubility in binary solvents by the Jouyban-Acree model. The density of pure organic solvents has been used to convert the molar solubility to mole fraction solubility and the effect of solute on density of the solution has been ignored. Table 1 summarizes the various numerical methods discussed in this work.

The predicitve ability of each computational method was assessed in terms of the mean percentage deviation (*MPD*) of observed ($(X_m)_{obs.}$) and calculated ($(X_m)_{cal.}$) solubilities, defined by equation (10):

$$MPD = \frac{100}{N}\sum \frac{|(X_m)_{cal.} - (X_m)_{obs.}|}{(X_m)_{obs.}} \quad (10)$$

where *N* is the number of data points. In addition, we also calculated the individual percentage deviation (*IPD*):

$$IPD = 100\left\{\frac{|(X_m)_{cal.} - (X_m)_{obs.}|}{(X_m)_{obs.}}\right\} \quad (11)$$

for each solubility data point.

Results and Discussion

Validation of the previously derived coefficients for solubility predictions using computed Abraham solute descriptors

The solubilities of the solutes in 194 different binary solvent mixtures (for details see Table 1 of a previous paper[10]) were predicted using the Jouyban-Acree model and calculated B_j values based on equations (4)-(6) and (7)-(9). Both experimental and computed Abraham solute descriptors were used in the B_j calculationss. Table 2 gives the overall *MPD* (± SD) values for the four predictive methods employed. There are no significant differences between *MPD*s for methods I and II that used experimental or computed Abraham parameters and experimental values of X_1 and X_2 (*t*-test, $p > 0.05$). This observation is important in that it is possible to use computed solute descriptors instead of experimentally based values for predicting B_j constants of the Jouyban-Acree model. However, significant differences are observed using predicted X_1 and X_2 by equations (1) and (2) for the same set of data and the coefficients ($p < 0.0005$), revealing that the computed Abraham parameters using PharmaAlgorithm software produced less accurate solubility predictions in mono-solvent systems in comparison with the experimental Abraham parameters. To confirm this hypothesis, readers could refer to the predicted solubilities using equations (1) and (2) employing experimental Abraham parameters. As examples, the *IPD*s of the predicted solubilities of anthracene using equation (1) in various solvents were listed in Table S4 where the differences between predicted solubilities using experimental and computed Abraham parameters were statistically significant (paired t-test, $p < 0.001$ or $p < 0.0005$, for details see footnote of

Table 2. Overall *MPD* (±SD) for solubility prediction of 194 sets from a previous work,[10] and this work using experimental and computed Abraham solute parameters

Numerical method	Experimental parameters	Computed parameters	Significance
194 data set from a previous work			
I	4.6 ± 3.9	4.6 ± 4.0	Not significant
II	11.3 ± 13.3	10.5 ± 13.0	Not significant
III	33.0 ± 20.6	52.0 ± 32.2	$p < 0.0005$
IV	23.9 ± 21.5	118 ± 258.4	$p < 0.0005$
This work			
I	13.7 ± 14.0	13.6 ± 13.8	Not significant
II	12.7 ± 13.9	12.5 ± 13.7	Not significant
III	228.4 ± 337.7	168.8 ± 325.4	Not significant
IV	53.5 ± 30.0	62.7 ± 43.6	$p < 0.016$

Table S4). A possible reason for such deviations could be the non-ideally adjusted water-to-solvent coefficients of some solvents as it was reported slightly different *c, e, s, a, b* and *v* values for cyclohexane in an earlier report[1] and a recent one[5] in which the *IPD* of anthracene solubility in cyclohexane predicted by equation (1) using earlier[1] and amended[5] *c, e, s, a, b* and *v* values were 213.2 and 148.4%, respectively. We have computed the *IPD* of anthracene in cyclohexane using amended[5] *c, e, s, a, b* and *v* values equal to 149.6%. The second reason for very large deviations between theoretically derived and experimentally determined solubility values could be any error in the solute's parameter calculations. The third reason could be the temperature effects on X_1 and X_2 values which did not considered in the equations (1) and (2).

It is possible to improve our *ab initio* prediction approach by developing better methods to predict the solubility in mono-solvent systems. It is difficult to guesstimate the error that one could reasonably expect from employing predictive methods to estimate the solubility in the neat organic solvents as the published methods have been tested on relatively few of the many possible solute-solvent combinations. Based on our review of the published comparisons, we do not think that it would be unreasonable to assign an expected error in the range of 0.1 to 0.3 log units to solubilities predicted by group contribution and linear free energy correlations for many of the simpler systems.

Predictions using water-to-solvent process and experimental solubility data in mono-solvents

The predictive calculations discussed in the preceding section concerned solubility data used in generating equations (4)-(9). A more stringent test of any predictive solubility method is its ability to accurately predict solubilities of additional solute molecules, or solubilities of solutes dissolved in additional binary solvent mixtures. To better assess the applications and limitations of methods I-IV, we have compiled from the published literature experimental solubility data for 90 additional data sets (see Table S1). In the first set of calculations on the new data set, we computed the B_j coefficients using equations (4)-(6) and experimentally-based Abraham solute descriptors. The calculated B_j values were then combined with experimentally measured solubility data in the mono-solvents to predict the mole fraction solubility $\ln X_m$ values for the 90 additional data sets (numerical method I of Table 1) using equation (3). The prediction accuracy of the data was evaluated using *MPD* values for this analysis and reported in column 2 of Table S5. The minimum (0.2%) and maximum (61.6%) *MPD*s were observed for p-benzoquinone in 2, 2, 4-trimethylpentane + cyclohexane and benzophenone in carbon tetrachloride + dodecane mixtures both at 25 °C. The overall *MPD* (± SD) was 13.7 ± 14.0%. A similar set of calculations were performed using computed Abraham parameters by PharmaAlgorithm software (see column 6 of Table S5). The minimum (0.2%) and maximum (61.8%) *MPD*s were observed for the same data sets and the overall *MPD* (± SD) was 13.6 ± 13.8%. There was no significant difference between 13.7 and 13.6% (paired *t*-test, p > 0.05). Figures 1 and 2 showed the relative frequencies of *IPD*s sorted in three subgroups, *i.e.* ≤ 4, 4-30 and > 30%, for various numerical methods employing experimental and computed Abraham parameters. There was no significant difference between frequencies of *IPD*s of both parameters for numerical method I. Figure S1 depicted the overall *MPD*s for various solutes and there was no difference between *MPD*s calculated using experimental and computed Abraham parameters. These findings confirm the above results using 194 data sets from a previous work[10] and reveal that it is possible to replace the experimentally determined Abraham parameters with the computationally obtained parameters for solubility prediction in mixed solvent system using method I.

The equations (4)-(6) were obtained employing the B_j terms calculated using solubility data of solutes at 25 and 26 °C, however, the equations were able to predict the solubility a wider temperature range (20-50 °C) as is evident (as examples) from set numbers 1-7 or 8-14 of Table S1. This is an oversimplification on the constants of the Jouyban-Acree model where it has been assumed that

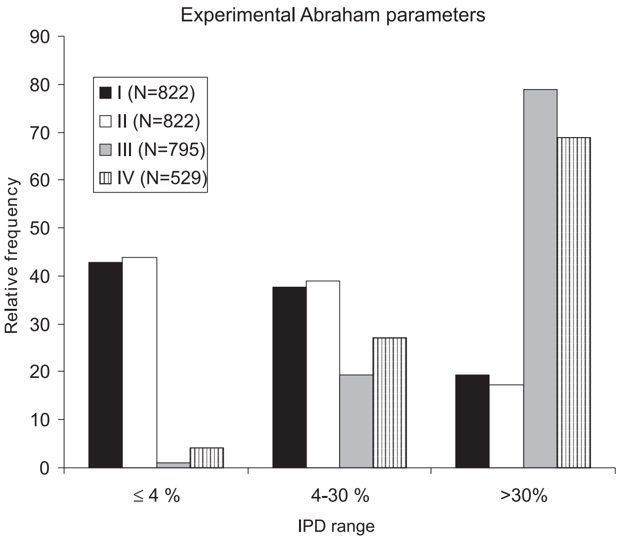

Figure 1. The relative frequency of the individual percentage deviations (*IPD*) for various numerical analysis employing experimental Abraham parameters.

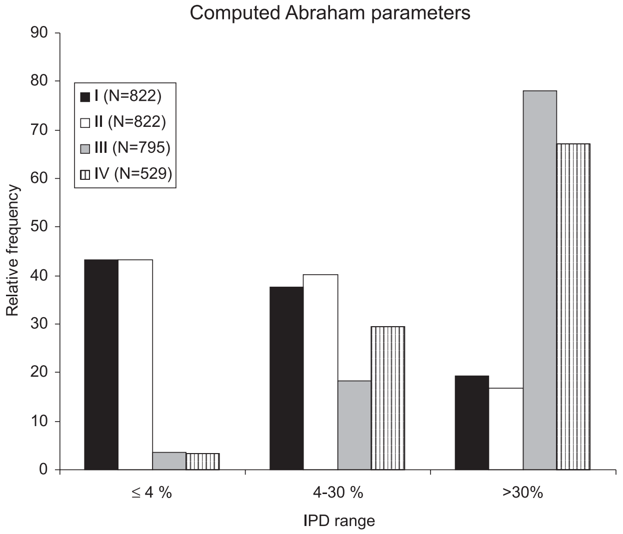

Figure 2. The relative frequency of the individual percentage deviations (*IPD*) for various numerical analysis employing computed Abraham parameter.

the Jouyban-Acree model constants are not temperature dependent. The reason for this simplification was the shortage of the solubility data of solutes in non-aqueous binary solvents at various temperatures. The capability of the Jouyban-Acree model for calculating the solubility of solutes in binary solvents at various temperatures has been shown earlier.[26]

Predictions using gas-to-solvent process and experimental solubility data in mono-solvents

In the second set of calculations on the new data set, we computed the B_j coefficients using equations (7)-(9) and experimentally-based Abraham solute descriptors. The calculated B_j values were then combined with experimental $\ln X_1$ and $\ln X_2$ data to predict the mole fraction solubility $\ln X_m$ values for the 90 additional data sets (numerical method II of Table 1) using equation (3). The obtained *MPD* values are reported in column 3 of Table S5. The minimum (0.2%) and maximum (67.3%) *MPD*s were observed for p-benzoquinone in heptane + cyclohexane and for benzophenone in carbon tetrachloride + dodecane mixtures both at 25 °C. The overall *MPD* (± SD) was 12.7 ± 13.9%. The same calculations were carried out using the computed Abraham parameters by PharmaAlgorithm software and the *MPD*s were listed in the column 7 of Table S5). The minimum (0.2%) and maximum (68.4%) *MPD*s were observed for p-benzoquinone in heptane + cyclohexane and benzophenone in carbon tetrachloride + dodecane mixtures and the overall *MPD* (± SD) was 12.5 ± 13.7%. There were i) no significant difference between 12.7 and 12.5% (paired *t*-test, p >0.05), ii) the same frequency pattern for both *IPD*s and iii) no difference between overall *MPD*s for various solutes (see Figure S2) employing experimental and computed Abraham parameters, revealing that one can employ solute parameters computed by PharmaAlgorithm instead of their experimentally obtained values. Full agreement was observed from the results of the 90 and 194 data sets (see Table 2) and the relative frequency of *IPDs* was favorable.

Ab initio predictions using water-to-solvent process and computed solubility data in mono-solvents

In the third set of predictive calculations we again calculated the B_j terms using equations (4)-(6) and the experimentally-based Abraham solute descriptors; however, in equation (3) the experimental mole fraction solubilities in the two mono-solvents were replaced with estimated X_1 and X_2 values based on equation (1). Results of these calculations are summarized in the fourth column of Table S5 for 86 of the 90 data sets considered. Predictions could not be made for the four p-tolylacetic acid systems because the molar solubility of p-tolylacetic acid in water, C_w, was not known. The molar solubility of the solute in water is a required input parameter in the estimation of solute's solubility in mono-solvents through equation (1). A minimum *MPD* of 11.2% was observed for naphthalene in benzene + toluene at 25 °C, and a maximum *MPD* of 1811.2% was obtained for carbazole in octane + cyclohexane at 25 °C. The overall average *MPD* was 228.7%. The largest *MPD*s were observed for data set numbers 15-22 (benzoic acid), 29-44 (carbazole) and 77-82 (phenylacetic acid). Similar computations were performed using computed Abraham parameters for predicting X_1, X_2 and B_j terms using the relevant equations. The *MPD* values of these computations are listed in column 8 of Table S5. A nearly identical *MPD* pattern was observed for data predicted by the experimental and computed parameters. The overall *MPD* was 168.9%. Figure S3 showed overall *MPD* for various solutes studied for experimental and computed parameters. This particular estimational scheme (method III) requires a prior knowledge of the solute's aqueous molar solubility, and based on the relatively large IPD and MPD between predicted and observed values the method did not provide a very reasonable prediction of the observed solubility behavior.

Ab initio predictions using gas-to-solvent process and computed solubility data in mono-solvents

Numerical method IV (see Table 1) involved using B_j coefficiens based on equations (7)-(9), and estimated values for the solubility of the solute in both mon-solvents computed from equation (2). The minimum and maximum *MPD* for method IV (see column 5 of Table S5) were 3.6 and 101.5%, respectively, for naphthalene dissolved in benzene + toluene at 25 °C and for pyrene dissolved in toluene + heptane at 20 °C using experimentally-based Abraham solute descriptors. The overall *MPD* was 53.5 (± 30.0)%. A slightly larger minimum *MPD* of 5.6% (for naphthalene in carbon tetrachloride + hexane) and larger maximum *MPD* of 197.5% (for pyrene in toluene + heptane at 20 °C) were obtained using computed Abraham solute descriptors. The overall *MPD* was also larger, *MPD* = 62.7%, for the method IV predictions that used computed solute descriptors as input values (see column 9 of Table S5). As discussed above, the large deviations in binary solvents result mostly from the high *IPD*s of the solutes in mono-solvents (see Table S6 for details). It is difficult to accurately predict solubility in binary solvent mixtures when the inputted solubility data for the mono-solvents that make up the binary solvent mixtures is poorly predicted. Better estimation methods for solute solubility in mono-solvents should allow one to reduce these deviations significantly.

Conclusions

Published methods for estimating the B_j constants of the Jouyban-Acree model were applied successfully to a data set containing experimental solubility data for 90 additional solute-binary solvent-temperature combinations. None of the binary solvent solubility data was used in the regression analyses used to develop the predictive B_j correlations. The predicted B_j constants, when combined with experimental solubility data for the solute dissolved in the mono-solvents, enabled one to estimate the solubility of crystalline organic solutes in binary solvents using the Jouyban-Acree model. The expected prediction errors were < 14 and < 13%, respectively for water-to-solvent and gas-to-solvent coefficients employing both experimentally determined and theoretically calculated Abraham solute descriptors. The relatively small prediction errors indicate that it is possible to predict the solubility in binary solvents with minimum experimental efforts. Experimental solubility data exists in the published literature for many organic solutes in mono-solvents, and the Jouyban-Acree model allows one to quantitively estimate the extent to which cosolvency increases or decreases solute solubility. Such predictions are important in both solubilization and crystallization processes. Moreover, predictive methods, such as the Jouyban-Acree model, provide a convenient means to screen compiled experimental solubility data in order to detect possible outliers for re-determination. For any solubility datum with very high *IPD*, the re-measurement is recommended. The proposed methods could also be extended to predict the solubility in mixed solvents at various temperatures. We tried to develop an *ab initio* prediction method employing C_W or C_G data of the solute (numerical methods III and IV); however, the obtained *MPD*s were *ca.* 200 and 60%.

As a practical conclusion, there are a number of possible solutions depending on the availability of the required input data: *i*) If the experimental solubility data of the solute in mono-solvent systems, *i.e.* X_1 and X_2, are available, the best solution to predict the solubility in mixed solvents is the numerical methods I or II and the expected prediction error is *ca.* 14%. *ii*) If X_1 and X_2 are not available and the aqueous solubility of the solute is known, one could use the numerical method III and the expected prediction error is relatively high (170%) for computed Abraham parameters. *iii*) If X_1 and X_2 are not available and C_G of the solute is known, the numerical method IV could be a solution and the expected prediction error is slightly high (*ca.* 60%) for computed Abraham parameters.

Supplemenatry Information

Supplementary data are available free of charge at http://jbcs.sbq.org.br, as PDF file.

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Solubility Prediction of Solutes in Non-Aqueous Binary Solvent Mixtures

***Abolghasem Jouyban,*[,a] Maryam Khoubnasabjafari,[b] Somaieh Soltani,[c] Shahla Soltanpour,[d]
Elnaz Tamizi[e] and William E. Acree Jr.[f]***

[a]Faculty of Pharmacy and Drug Applied Research Center, Tabriz University of Medical Sciences, 51664, Iran

[b]Kimia Research Institute, P.O. Box 51665-171, Iran

[c]Research Center for Pharmaceutical Nanotechnology, Tabriz University of Medical Sciences, 51664, Iran

[d]Biotechnology Research Centre, Tabriz University of Medical Sciences, 51664, Iran

[e]Student Research Center, Tabriz University of Medical Sciences, 51664, Iran

[f]Department of Chemistry, University of North Texas, Denton, TX 76203-5070, USA

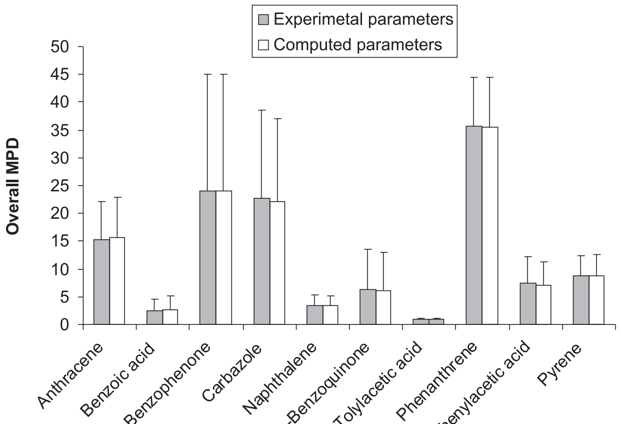

Figure S1. The overall *MPD* (± SD) for numerical method I for various solutes

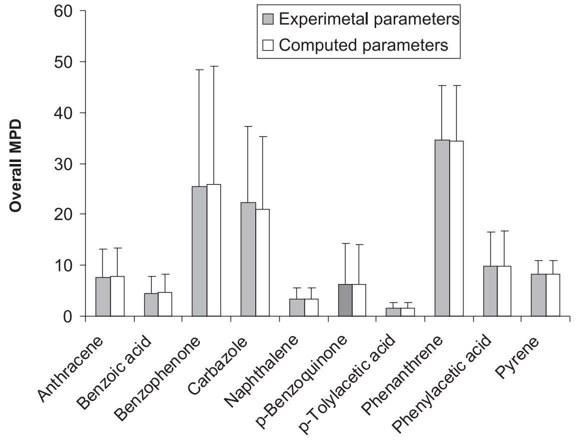

Figure S2. The overall *MPD* (± SD) for numerical method II for various solutes

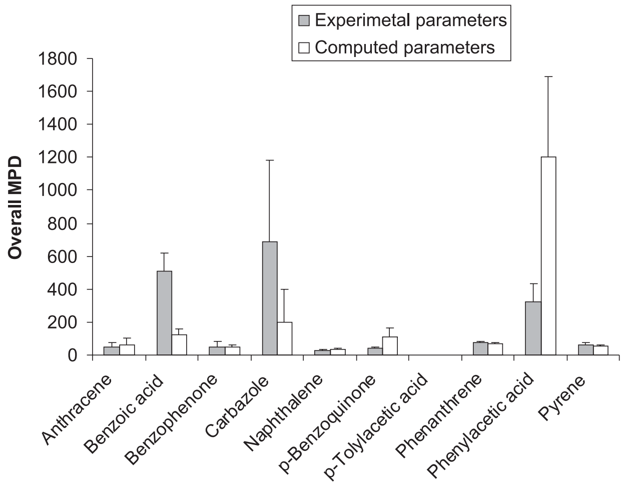

Figure S3. The overall *MPD* (± SD) for numerical method III for various solutes

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*e-mail: ajouyban@hotmail.com

Table S1. Details of solutes and solvents names, the references of experimental data sets, logarithms of solubility in mono-solvents (lnX_1 and lnX_2) and temperature (T)

No.	Solute	Solvent 1	Solvent 2	N	Reference	lnX_1	lnX_2	T (°C)
1	Anthracene	Toluene	2-Propanol	11	11	-5.10	-8.57	20
2	Anthracene	Toluene	2-Propanol	11	11	-4.92	-7.90	25
3	Anthracene	Toluene	2-Propanol	11	11	-4.77	-7.76	30
4	Anthracene	Toluene	2-Propanol	11	11	-4.55	-7.46	35
5	Anthracene	Toluene	2-Propanol	11	11	-4.49	-7.21	40
6	Anthracene	Toluene	2-Propanol	11	11	-4.25	-7.22	45
7	Anthracene	Toluene	2-Propanol	11	11	-4.14	-6.82	50
8	Anthracene	Toluene	Heptane	10	11	-5.05	-6.72	20
9	Anthracene	Toluene	Heptane	10	11	-4.94	-6.61	25
10	Anthracene	Toluene	Heptane	10	11	-4.77	-6.29	30
11	Anthracene	Toluene	Heptane	10	11	-4.62	-6.34	35
12	Anthracene	Toluene	Heptane	10	11	-4.51	-6.05	40
13	Anthracene	Toluene	Heptane	10	11	-4.25	-5.72	45
14	Anthracene	Toluene	Heptane	10	11	-4.23	-5.68	50
15	Benzoic acid	Carbon tetrachloride	Cyclohexane	7	12	-3.01	-4.47	25
16	Benzoic acid	Carbon tetrachloride	Heptane	10	12	-3.01	-4.47	25
17	Benzoic acid	Carbon tetrachloride	Heptane	6	12	-2.82	-4.22	30
18	Benzoic acid	Carbon tetrachloride	Hexane	7	12	-3.01	-4.61	25
19	Benzoic acid	Carbon tetrachloride	Hexane	7	12	-2.82	-4.37	30
20	Benzoic acid	Cyclohexane	Heptane	7	12	-4.47	-4.47	25
21	Benzoic acid	Cyclohexane	Hexane	7	12	-4.47	-4.61	25
22	Benzoic acid	Cyclohexane	Hexane	7	12	-4.23	-4.37	30
23	Benzophenone	Carbon tetrachloride	Decane	11	13	-0.60	-3.03	25
24	Benzophenone	Carbon tetrachloride	Dodecane	11	13	-0.60	-3.54	25
25	Benzophenone	Carbon tetrachloride	Heptane	11	13	-0.60	-3.16	25
26	Benzophenone	Carbon tetrachloride	Hexane	9	13	-0.60	-3.75	25
27	Benzophenone	Carbon tetrachloride	Nonane	11	13	-0.60	-2.81	25
28	Benzophenone	Carbon tetrachloride	Octane	11	13	-0.60	-2.66	25
30	Carbazole	Cyclohexane	2,2,4-Trimethylpentane	11	14	-8.61	-8.98	25
31	Carbazole	Cyclohexane	Heptane	9	14	-8.61	-8.66	25
32	Carbazole	Cyclohexane	Hexane	9	14	-8.61	-8.88	25
29	Carbazole	Dibutylether	2,2,4-Trimethylpentane	9	15	-5.30	-8.98	25
33	Carbazole	Dibutylether	Cyclohexane	11	16	-5.30	-8.61	25
34	Carbazole	Dibutylether	Heptane	11	16	-5.30	-8.66	25
35	Carbazole	Dibutylether	Hexadecane	11	17	-5.30	-7.79	25
36	Carbazole	Dibutylether	Hexane	11	16	-5.30	-8.88	25
37	Carbazole	Dibutylether	Methylcyclohexane	11	15	-5.30	-8.54	25
38	Carbazole	Dibutylether	Methylcyclohexane	11	16	-5.30	-8.54	25
39	Carbazole	Dibutylether	n-Heptane	11	15	-5.30	-8.66	25
40	Carbazole	Dibutylether	n-Hexane	11	15	-5.30	-8.88	25
41	Carbazole	Dibutylether	n-Octane	11	15	-5.30	-8.53	25
42	Carbazole	Dibutylether	Octane	11	16	-5.30	-8.53	25
43	Carbazole	Methylcyclohexane	Cyclohexane	9	14	-8.54	-8.61	25
44	Carbazole	Octane	Cyclohexane	9	14	-8.53	-8.61	25
45	Naphthalene	Benzene	Carbon tetrachloride	6	18	-1.22	-1.35	25

Table S1. continuation

No.	Solute	Solvent 1	Solvent 2	N	Reference	lnX_1	lnX_2	*T* (°C)
46	Naphthalene	Benzene	Cyclohexane	8	18	-1.22	-1.91	25
47	Naphthalene	Benzene	Hexadecane	6	18	-1.22	-1.59	25
48	Naphthalene	Benzene	Hexane	8	18	-1.22	-2.15	25
49	Naphthalene	Benzene	Toluene	7	18	-1.22	-1.23	25
50	Naphthalene	Carbon tetrachloride	Cyclohexane	6	19	-1.35	-1.91	25
51	Naphthalene	Carbon tetrachloride	Hexadecane	6	19	-1.35	-1.59	25
52	Naphthalene	Carbon tetrachloride	Hexane	8	19	-1.35	-2.15	25
53	Naphthalene	Cyclohexane	Hexane	6	19	-1.91	-2.15	25
54	Naphthalene	Hexadecane	Cyclohexane	7	19	-1.59	-1.91	25
55	Naphthalene	Hexadecane	Hexane	6	19	-1.59	-2.15	25
56	Naphthalene	Toluene	Carbon tetrachloride	6	20	-1.23	-1.35	25
57	Naphthalene	Toluene	Cyclohexane	6	20	-1.23	-1.91	25
58	Naphthalene	Toluene	Hexadecane	6	20	-1.23	-1.59	25
59	Naphthalene	Toluene	Hexane	6	20	-1.23	-2.15	25
60	p-Benzoquinone	2,2,4-Trimethylpentane	Cyclohexane	7	21	-5.01	-5.03	25
61	p-Benzoquinone	Carbon tetrachloride	Heptane	8	21	-3.37	-5.01	25
62	p-Benzoquinone	Carbon tetrachloride	Octane	7	21	-3.37	-4.89	25
63	p-Benzoquinone	Dodecane	Heptane	7	21	-4.74	-5.01	25
64	p-Benzoquinone	Heptane	Cyclohexane	7	21	-5.01	-5.03	25
65	p-Tolylacetic acid	Cyclohexane	2,2,4-Trimethylpentane	7	22	-4.32	-4.83	25
66	p-Tolylacetic acid	Cyclohexane	Heptane	7	22	-4.30	-4.78	25
67	p-Tolylacetic acid	Cyclohexane	Hexane	8	22	-4.32	-4.85	25
68	p-Tolylacetic acid	Cyclohexane	Octane	7	22	-4.32	-4.75	25
69	Phenanthrene	Toluene	2,2,4-Trimethylpentane	7	23	-0.77	-3.96	20
70	Phenanthrene	Toluene	2,2,4-Trimethylpentane	7	23	-0.70	-3.32	30
71	Phenanthrene	Toluene	2,2,4-Trimethylpentane	7	23	-0.55	-2.44	40
72	Phenanthrene	Toluene	2,2,4-Trimethylpentane	7	23	-0.50	-1.98	50
73	Phenanthrene	Toluene	Heptane	11	23	-0.77	-4.17	20
74	Phenanthrene	Toluene	Heptane	11	23	-0.70	-3.70	30
75	Phenanthrene	Toluene	Heptane	11	23	-0.55	-3.32	40
76	Phenanthrene	Toluene	Heptane	11	23	-0.50	-2.96	50
77	Phenylacetic acid	Carbon tetrachloride	2,2,4-Trimethylpentane	11	24	-1.75	-4.40	25
78	Phenylacetic acid	Carbon tetrachloride	Cyclohexane	11	24	-1.75	-3.70	25
79	Phenylacetic acid	Carbon tetrachloride	Heptane	11	24	-1.75	-4.31	25
80	Phenylacetic acid	Carbon tetrachloride	Octane	11	24	-1.75	-4.24	25
81	Phenylacetic acid	Cyclohexane	2,2,4-Trimethylpentane	9	24	-3.70	-4.40	25
82	Phenylacetic acid	Cyclohexane	Heptane	8	24	-3.70	-4.31	25
83	Pyrene	Toluene	2,2,4-Trimethylpentane	12	20	-2.87	-4.72	20
84	Pyrene	Toluene	2,2,4-Trimethylpentane	12	20	-2.41	-4.47	30
85	Pyrene	Toluene	2,2,4-Trimethylpentane	12	20	-2.21	-4.37	40
86	Pyrene	Toluene	2,2,4-Trimethylpentane	12	20	-1.57	-3.94	50
87	Pyrene	Toluene	Heptane	11	20	-2.87	-4.47	20
88	Pyrene	Toluene	Heptane	11	20	-2.41	-4.17	30
89	Pyrene	Toluene	Heptane	11	20	-2.21	-3.63	40
90	Pyrene	Toluene	Heptane	11	20	-1.57	-3.01	50

Table S2. Coefficients in equations (1) and (2) for water-to-solvent and gas-to-solvent processes of the solvents used in this study[a]

No.	Water-to-solvent coefficients	c	e	s	a	b	v
1	2,2,4-Trimethylpentane	0.288	0.382	-1.668	-3.639	-5.000	4.461
2	2-Propanol	0.063	0.320	-1.024	0.445	-3.824	4.067
3	Benzene	0.142	0.464	-0.588	-3.099	-4.625	4.491
4	Carbone tetrachloride	0.260	0.573	-1.254	-3.558	-4.558	4.589
5	Cyclohexane	0.159	0.784	-1.678	-3.740	-4.929	4.577
6	Decane	0.160	0.585	-1.730	-3.440	-5.080	4.582
7	Dibutyl ether	0.203	0.369	-0.954	-1.488	-5.426	4.508
8	Dodecane	0.114	0.668	-1.640	-3.550	-5.010	4.459
9	Heptane	0.325	0.670	-2.061	-3.317	-4.733	4.543
10	Hexadecane	0.087	0.667	-1.620	-3.59	-4.870	4.433
11	Hexane	0.361	0.579	-1.723	-3.599	-4.764	4.344
12	Methylcyclohexane	0.246	0.782	-1.982	-3.517	-4.293	4.528
13	Nonane	0.240	0.619	-1.710	-3.530	-4.920	4.482
14	Octane	0.223	0.642	-1.647	-3.480	-5.067	4.526
15	Toluene	0.143	0.527	-0.720	-3.010	-4.824	4.545
No.	Gas-to-solvent coefficients	c	e	s	a	b	l
1	2,2,4-Trimethylpentane	0.275	–0.244	0.000	0.000	0.000	0.972
2	2-Propanol	-0.060	-0.335	0.702	4.017	1.040	0.893
3	Benzene	0.107	–0.313	1.053	0.457	0.169	1.020
4	Carbone tetrachloride	0.282	–0.303	0.460	0.000	0.000	1.047
5	Cyclohexane	0.163	-0.110	0.000	0.000	0.000	1.013
6	Decane	0.156	-0.140	0.000	0.000	0.000	0.989
7	Dibutyl ether	0.165	–0.421	0.760	2.102	–0.664	1.002
8	Dodecane	0.053	0.000	0.000	0.000	0.000	0.986
9	Heptane	0.275	–0.162	0.000	0.000	0.000	0.983
10	Hexadecane	0.000	0.000	0.000	0.000	0.000	1.000
11	Hexane	0.292	–0.169	0.000	0.000	0.000	0.979
12	Methylcyclohexane	0.318	–0.215	0.000	0.000	0.000	1.012
13	Nonane	0.200	-0.145	0.000	0.000	0.000	0.980
14	Octane	0.215	–0.049	0.000	0.000	0.000	0.967
15	Toluene	0.121	–0.222	0.938	0.467	0.099	1.012

[a] Data taken from a reference.[5]

Table S3. The experimental and computed Abraham parameters along with the input properties for solutes studied in this work and their references

Solute	E	S	*A*	*B*	*V*	*L*	log C_W	log C_G	Reference
	Experimental Abraham parameters								
Anthracene	2.290	1.34	0.000	0.280		7.568	-6.430	-9.460	2
Benzoic acid	0.730	0.90	0.590	0.400		4.395	-1.550	-6.690	27
Benzophenone	1.447	1.50	0.000	0.500		6.852	-3.120[28]	-[a]	25
Carbazole	1.787	2.01	0.180	0.080		7.982	-5.270[28]	-[a]	25
Naphthalene	1.340	0.92	0.000	0.200		5.161	-3.610[29]	-5.340	30
p-Benzoquinone	0.750	0.55	0.000	0.810		3.492	-0.880[31]	-[a]	25
p-Tolylacetic acid	0.730	0.97	0.600	0.640		5.480	-[a]	-[a]	25
Phenanthrene	2.055	1.29	0.000	0.290		7.632	-5.170	-7.970	2
Phenylacetic acid	0.730	1.01	0.590	0.610		4.933	-0.890[28]	-7.562[b]	25
Pyrene	2.808	1.71	0.000	0.280		8.833	-6.150	-9.650	5
	Computed Abraham parameters								
Anthracene	1.99	1.34	0.000	0.23	1.454	7.706			25
Benzoic acid	0.75	1.08	0.570	0.44	0.932	4.533			25
Benzophenone	1.37	1.59	0.000	0.51	1.481	7.308			25
Carbazole	1.94	1.43	0.310	0.39	1.315	7.869			25
Naphthalene	1.27	1.02	0.000	0.17	1.085	5.332			25
p-Benzoquinone	0.90	0.43	0.000	0.76	0.791	3.500			25
p-Tolylacetic acid	0.77	1.02	0.570	0.45	1.214	5.499			25
Phenanthrene	1.99	1.34	0.000	0.23	1.454	7.706			25
Phenylacetic acid	0.75	1.08	0.570	0.45	1.073	5.028			25
Pyrene	2.60	1.52	0.000	0.25	1.585	9.110			25

[a] The data was not available.

[b] $\log C_G$ of phenylacetic acid was calculated using the extrapolated vapor pressure data from a reference[32] as: $\log C_G = \dfrac{6.796\times10^{-2}\ (vapor\ \ pressure)}{298.15\times0.08206\times101325}$.

Table S4. The individual percentage deviations (*IPD*s) of solubilities of solutes[10] in some of the solvents predicted by equations (1) and (2) employing experimental and computed Abraham parameters

Solute[a]	Solvent[a]	*T* (°C)	Experimental parameters		Computed parameters	
			Equation (1)	Equation (2)	Equation (1)	Equation (2)
Anthracene	1,4-Dioxane	25	20.5	20.0	64.4	36.1
Anthracene	1-Butanol	25	25.5	1.0	45.6	43.7
Anthracene	1-Octanol	25	17.0	23.9	35.7	8.8
Anthracene	1-Pentanol	25	34.4	21.9	47.0	13.5
Anthracene	2,2,4-Trimethylpentane	25	40.3	36.3	18.5	2.6
Anthracene	2-Butanol	25	21.2	24.0	55.6	22.8
Anthracene	2-Methyl-1-propanol	25	37.7	11.7	64.8	34.1
Anthracene	2-Propanol	25	28.5	5.4	60.0	40.4
Anthracene	Acetonitrile	25	14.6	6.3	80.0	70.1
Anthracene	Benzene	25	97.7	52.7	143.6	155.2
Anthracene	Carbon tetrachloride	25	49.3	3.3	69.7	65.7
Anthracene	Cyclohexane	25	149.6	7.7	156.1	37.3
Anthracene	Dibutyl ether	25	11.5	32.4	61.2	33.8
Anthracene	Heptane	25	16.7	28.2	9.6	9.7
Anthracene	Hexane	25	12.0	26.2	2.0	13.2
Anthracene	Methanol	25	3.2	1.8	24.0	27.9
Anthracene	Methyl tert-buthyl ether	25	22.6	24.6	82.0	44.6
Anthracene	Methylcyclohexane	25	66.8	17.8	59.4	31.4
Anthracene	Octane	25	46.8	18.7	68.8	14.3
Anthracene	Toluene	25	132.9	78.7	181.0	182.0
Benzil	1-Butanol	25	5.3	15.8	94.8	1599.5
Benzil	1-Octanol	25	60.1	29.0	91.8	1540.8
Benzil	1-Pentanol	25	10.9	95.6	95.1	1421.3
Benzil	1-Propanol	25	5.7	25.1	94.9	1146.8
Benzil	2,2,4-Trimethylpentane	25	38.2	29.4	99.0	375.6
Benzil	2-Butanol	25	46.5	32.3	91.0	2172.1
Benzil	2-Propanol	25	25.4	14.0	92.6	1882.9
Benzil	Carbon tetrachloride	25	38.6	51.6	97.8	337.6
Benzil	Cyclohexane	25	4.2	36.7	98.0	373.9
Benzil	Heptane	25	34.2	10.9	99.1	521.9
Benzil	Octane	25	25.6	14.2	97.7	498.8
Pyrene	1-Butanol	26	33.8	42.0	17.2	115.8
Pyrene	1-Octanol	26	39.8	1.9	0.0	45.3
Pyrene	1-Pentanol	26	34.0	43.1	18.1	16.8
Pyrene	1-Propanol	26	21.2	13.8	35.0	26.1
Pyrene	2,2,4-Trimethylpentane	26	75.4	23.1	40.1	59.7
Pyrene	2-Butanol	26	36.8	2.8	11.0	50.2
Pyrene	2-Methyl-1-propanol	26	26.4	21.0	29.4	77.3
Pyrene	2-Propanol	26	27.7	41.5	26.2	100.7
Pyrene	Benzene	26	64.4	210.3	124.4	300.3
Pyrene	Cyclohexane	26	59.5	38.1	215.3	173.6
Pyrene	Dibutyl ether	26	32.0	9.7	23.6	86.4
Pyrene	Heptane	26	66.0	5.7	16.1	88.8
Pyrene	Hexane	26	57.4	0.0	5.2	100.7
Pyrene	Methylcyclohexane	26	25.8	1.2	61.5	105.9
Pyrene	Octane	26	23.5	8.7	62.1	103.4
Thianthrene	2,2,4-Trimethylpentane	25	45.2	27.1	71.1	112.5
Thianthrene	Cyclohexane	25	53.1	22.9	29.4	121.9
Thianthrene	Heptane	25	12.3	3.1	56.2	176.4
Thianthrene	Hexane	25	17.7	12.6	58.4	149.3
Thianthrene	Methylcyclohexane	25	8.3	31.8	45.5	103.9

Table S4. continuation

Solute[a]	Solvent[a]	*T* (°C)	Experimental parameters		Computed parameters	
			Equation (1)	Equation (2)	Equation (1)	Equation (2)
Thianthrene	Octane	25	57.1	7.7	25.1	189.8
Trans-Stilbene	1-Propanol	25	23.4	10.8	33.9	57.4
Trans-Stilbene	2,2,4-Trimethylpentane	25	22.2	9.5	16.7	63.0
Trans-Stilbene	2-Butanol	25	53.2	28.5	79.9	32.5
Trans-Stilbene	Cyclohexane	25	32.2	14.5	22.7	67.7
Trans-Stilbene	Heptane	25	6.0	5.4	23.9	62.6
Trans-Stilbene	Hexane	25	17.7	8.7	22.0	63.7
Trans-Stilbene	Methylcyclohexane	25	21.4	4.3	8.8	62.5
Trans-Stilbene	Octane	25	27.2	11.9	27.5	65.9
Anthracene	1,4-Dioxane	25	20.5	20.0	64.4	36.1
		All	36.3[b]	24.4[c]	59.7[b]	262.8[c]
		25	34.6[d]	22.2[e]	64.5[d]	319.4[e]

[a] Details of the references of data were reported in an earlier work.[10]; [b] The difference was statistically significant (paired t-test, p<0.0005); [c] The difference was statistically significant (paired t-test, p<0.0005); [d] The difference was statistically significant (paired t-test, p<0.0005); [e] The difference was statistically significant (paired t-test, p>0.001).

Table S5. The mean percentage deviation (*MPD*) of various numerical analyses employing the experimental and computed Abraham parameters of the solutes and the overall (± SD) of *MPD*s

Numerical method No.[a]	I	II	III	IV	I	II	III	IV
	Experimental Abraham parameters				Computed Abraham parameters			
1	30.3	18.2	95.8	72.9	31.0	18.7	138.0	161.3
2	18.3	3.6	45.2	28.8	19.1	4.1	76.4	94.8
3	17.7	4.5	27.1	17.6	18.6	5.0	53.5	69.8
4	16.9	1.6	23.0	21.1	17.8	1.9	22.5	32.3
5	15.9	3.8	29.5	28.9	16.7	4.1	24.3	24.2
6	22.2	7.3	33.2	37.5	23.0	8.0	26.2	20.8
7	16.5	2.2	43.3	48.5	17.3	2.5	36.0	30.0
8	16.9	14.8	112.2	68.2	16.9	14.8	145.8	160.0
9	11.6	9.7	79.3	44.0	11.6	9.7	106.8	119.1
10	16.1	14.2	52.7	27.3	16.1	14.2	74.8	81.5
11	2.7	2.2	34.2	23.1	2.7	2.2	47.8	49.6
12	5.7	4.4	32.0	26.9	5.7	4.4	41.3	39.9
13	16.0	13.9	26.2	31.9	16.0	14.0	31.5	27.9
14	7.6	5.9	28.5	38.8	7.6	6.0	31.1	27.1
15	0.8	0.7	493.7	94.4	0.7	0.6	135.8	91.5
16	6.5	10.0	460.9	93.4	7.2	10.5	115.4	90.0
17	5.1	8.4	357.9	94.6	5.6	8.8	69.6	92.0
18	2.1	5.3	510.0	93.5	2.3	5.7	141.0	90.3
19	2.6	5.2	386.3	94.8	2.8	5.5	91.8	92.2
20	1.0	1.5	626.6	92.9	0.8	1.5	138.3	90.3
21	0.5	1.7	697.2	92.9	0.5	1.7	176.4	90.3
22	0.7	2.1	527.9	94.4	0.7	2.1	117.5	92.3
23	6.9	8.9	23.9	-	7.0	9.5	43.5	-
24	61.6	67.3	114.6	-	61.8	68.4	43.1	-
25	15.0	13.9	37.9	-	14.9	13.8	62.4	-
26	34.8	36.8	37.4	-	34.9	37.2	25.1	-
27	7.4	10.7	25.8	-	7.4	11.2	47.9	-
28	18.1	15.4	38.4	-	18.0	15.4	59.2	-
29	34.9	31.7	324.3	-	34.8	29.8	53.1	-
30	0.9	4.5	1291.2	-	0.9	4.4	370.3	-
31	0.9	0.8	1011.5	-	0.9	0.8	409.3	-
32	1.7	0.8	1355.5	-	1.9	0.8	461.7	-
33	41.4	39.4	596.9	-	41.1	38.0	118.1	-
34	28.2	29.8	231.9	-	27.7	27.9	50.6	-
35	16.7	14.3	528.2	-	15.6	11.9	65.3	-

Table S5. Cont.

Numerical method	I	II	III	IV	I	II	III	IV
No.[a]	Experimental Abraham parameters				Computed Abraham parameters			
36	35.5	34.5	348.6	-	34.4	32.9	61.1	-
37	36.2	37.2	282.8	-	32.2	35.8	87.7	-
38	35.6	36.6	268.2	-	31.0	35.0	87.3	-
39	28.2	29.8	231.9	-	27.7	27.9	50.6	-
40	35.5	34.5	349.0	-	34.3	32.8	61.2	-
41	32.2	28.3	581.9	-	32.3	26.4	83.7	-
42	32.2	28.3	581.9	-	32.3	26.4	83.7	-
43	2.2	0.6	1208.1	-	5.3	0.6	602.1	-
44	1.3	3.3	1811.2	-	1.1	3.3	547.9	-
45	2.4	3.5	23.1	16.3	2.6	3.7	21.3	30.7
46	4.7	3.5	26.5	31.5	4.3	3.1	28.6	22.7
47	1.9	4.1	26.8	12.8	2.2	4.6	29.5	26.8
48	5.4	4.2	36.7	27.6	5.0	3.8	38.0	18.2
49	1.1	1.3	11.2	3.6	1.1	1.4	4.7	48.6
50	1.9	0.7	32.4	39.1	2.0	0.5	39.3	11.2
51	6.0	8.4	30.3	17.5	6.0	8.5	36.9	18.4
52	2.0	1.1	42.0	33.2	2.0	1.4	47.7	5.6
53	1.1	0.3	37.6	41.7	1.1	0.3	46.5	15.1
54	6.4	6.2	28.3	25.7	6.4	6.2	37.4	11.0
55	4.7	2.6	36.7	25.6	4.7	2.7	44.7	7.5
56	2.1	3.4	18.7	12.3	2.1	3.6	17.9	34.2
57	5.1	3.3	22.3	27.5	4.7	3.0	25.0	23.5
58	2.1	3.6	23.1	9.9	2.3	4.0	26.4	29.2
59	5.2	5.1	32.7	24.7	4.8	4.7	34.7	18.2
60	0.2	1.1	45.5	-	.2	1.1	88.3	-
61	10.0	12.7	42.0	-	9.5	12.5	96.1	-
62	17.2	17.0	52.5	-	16.6	16.7	51.4	-
63	3.3	0.3	28.9	-	3.1	0.3	160.3	-
64	1.0	0.2	27.7	-	.9	0.2	167.5	-
65	1.1	0.7	-	-	1.1	0.7	-	-
66	1.1	0.5	-	-	1.0	0.5	-	-
67	0.9	2.6	-	-	1.0	2.6	-	-
68	0.5	2.3	-	-	0.5	2.3	-	-
69	36.0	33.4	70.1	40.3	35.9	33.3	54.8	35.2
70	31.2	28.3	77.3	49.9	31.1	28.1	65.8	39.0
71	26.5	23.3	84.5	66.9	26.4	23.1	76.7	59.8
72	20.3	16.7	86.1	70.8	20.2	16.4	79.1	64.4
73	42.2	43.0	61.7	55.2	42.1	42.9	52.4	53.0
74	45.1	45.8	71.3	56.0	44.9	45.7	59.6	50.4
75	43.3	44.1	77.1	58.2	43.1	43.9	67.4	53.1
76	40.5	41.4	80.3	61.9	40.3	41.2	71.8	54.0
77	11.4	16.5	274.9	98.3	10.4	16.8	994.3	97.9
78	6.4	6.6	158.9	99.0	6.9	6.5	620.2	98.8
79	6.1	9.3	263.2	98.4	6.2	9.5	901.2	97.9
80	14.7	19.3	323.8	98.3	13.4	19.5	1096.2	97.9
81	2.1	4.0	439.8	97.9	2.1	4.0	1823.2	97.4
82	3.7	3.0	458.7	97.8	3.6	3.0	1769.7	97.3
83	8.1	11.3	58.9	80.5	8.1	10.4	55.9	166.5
84	6.7	4.8	60.1	50.1	7.0	5.0	46.7	70.7
85	16.8	12.5	66.0	49.1	17.3	13.1	51.7	40.8
86	8.6	7.1	78.3	48.0	8.8	7.3	61.9	25.0
87	6.7	6.8	50.0	101.5	6.5	7.4	70.9	197.5
88	11.0	9.6	43.9	65.1	10.2	9.0	43.7	119.7
89	7.9	8.1	54.0	48.4	7.9	8.3	40.5	59.6
90	4.7	5.3	74.9	48.9	4.9	5.8	58.3	34.4
Overall:	13.7	12.7	228.7	53.5	13.6	12.5	168.9	62.7
SD	14.0	13.9	337.7	30.0	13.8	13.7	325.4	43.6

[a] Details of the data is the same as Table S1.

Table S6. The individual percentage deviations (*IPD*s) of solubilities of solutes in some of the solvents of this work predicted by equations (1) and (2) employing experimental and computed Abraham parameters

Solute	Solvent	*T* (°C)	Experimental parameters		Computed parameters	
			equation (1)	equation (2)	equation (1)	equation (2)
Anthracene	2-Propanol	20	180.1	105.3	248.7	204.8
Anthracene	2-Propanol	25	43.1	4.9	78.1	55.7
Anthracene	2-Propanol	30	24.3	8.9	54.7	35.2
Anthracene	2-Propanol	35	7.9	32.5	14.6	0.2
Anthracene	2-Propanol	40	28.5	47.6	10.9	22.2
Anthracene	2-Propanol	45	27.8	47.1	10.1	21.4
Anthracene	2-Propanol	50	51.5	64.5	39.7	47.2
Anthracene	Heptane	20	8.9	6.5	18.2	42.9
Anthracene	Heptane	25	2.9	16.7	5.4	27.3
Anthracene	Heptane	30	29.3	39.3	23.3	7.3
Anthracene	Heptane	35	25.8	36.3	19.5	2.7
Anthracene	Heptane	40	44.1	52.0	39.4	26.7
Anthracene	Heptane	45	59.8	65.5	56.4	47.3
Anthracene	Heptane	50	61.8	67.2	58.5	49.9
Anthracene	Toluene	20	181.9	115.5	240.1	239.9
Anthracene	Toluene	20	169.4	105.9	225.0	224.8
Anthracene	Toluene	25	136.4	80.7	185.2	185.0
Anthracene	Toluene	25	139.4	83.0	188.9	188.7
Anthracene	Toluene	30	102.3	54.7	144.1	144.0
Anthracene	Toluene	35	63.4	24.9	97.1	97.0
Anthracene	Toluene	35	74.8	33.6	110.9	110.8
Anthracene	Toluene	40	53.7	17.5	85.5	85.4
Anthracene	Toluene	40	57.1	20.0	89.5	89.4
Anthracene	Toluene	45	20.9	7.6	45.8	45.8
Anthracene	Toluene	50	8.1	17.3	30.5	30.4
Anthracene	Toluene	50	18.5	9.4	43.0	42.9
Benzoic acid	Carbon tetrachloride	25	336.2	95.2	100.8	92.1
Benzoic acid	Carbon tetrachloride	30	258.9	96.1	65.2	93.5
Benzoic acid	Cyclohexane	25	690.6	93.4	176.6	90.9
Benzoic acid	Cyclohexane	30	522.7	94.8	117.8	92.9
Benzoic acid	Heptane	25	569.9	92.1	101.2	89.3
Benzoic acid	Heptane	30	419.5	93.9	56.0	91.7
Benzoic acid	Hexane	25	708.0	92.1	177.1	89.2
Benzoic acid	Hexane	30	541.2	93.7	119.9	91.5
Benzophenone	Carbon tetrachloride	25	49.2	-	64.4	-
Benzophenone	Decane	25	28.7	-	25.9	-
Benzophenone	Dodecane	25	182.0	-	64.7	-
Benzophenone	Heptane	25	7.6	-	51.1	-
Benzophenone	Hexane	25	87.7	-	8.3	-
Benzophenone	Nonane	25	15.4	-	33.2	-
Benzophenone	Octane	25	15.7	-	32.3	-
Carbazole	2,2,4-Trimethylpentane	25	761.8	-	158.0	-
Carbazole	Cyclohexane	25	1967.8	-	661.6	-
Carbazole	Dibutyl ether	25	391.4	-	57.4	-
Carbazole	Heptane	25	333.7	-	193.8	-
Carbazole	Hexadecane	25	1017.3	-	280.2	-
Carbazole	Hexane	25	835.7	-	282.4	-
Carbazole	Methyl cyclohexane	25	557.4	-	470.5	-
Carbazole	Heptane	25	333.7	-	193.8	-
Carbazole	Hexane	25	835.7	-	282.4	-
Carbazole	Octane	25	1692.0	-	445.9	-

Table S6. continuation

Solute	Solvent	T (°C)	Experimental parameters		Computed parameters	
			equation (1)	equation (2)	equation (1)	equation (2)
Naphthalene	Benzene	25	16.5	8.7	9.4	43.0
Naphthalene	Carbon tetrachloride	25	33.6	29.8	37.1	8.7
Naphthalene	Cyclohexane	25	28.7	46.1	39.0	21.6
Naphthalene	Hexadecane	25	34.7	20.5	42.4	9.3
Naphthalene	Hexane	25	46.6	37.3	54.1	8.7
Naphthalene	Toluene	25	6.6	0.4	0.9	51.1
p-Benzoquinone	2,2,4-Trimethylpentane	25	54.8	-	44.4	-
p-Benzoquinone	Carbon tetrachloride	25	68.0	-	8.8	-
p-Benzoquinone	Cyclohexane	25	37.6	-	126.9	-
p-Benzoquinone	Dodecane	25	47.5	-	83.3	-
p-Benzoquinone	Heptane	25	16.7	-	215.2	-
p-Benzoquinone	Octane	25	45.7	-	89.6	-
Phenanthrene	2,2,4-Trimethylpentane	20	46.7	41.8	17.6	72.5
Phenanthrene	2,2,4-Trimethylpentane	30	71.9	25.2	56.5	9.0
Phenanthrene	2,2,4-Trimethylpentane	40	88.4	69.2	82.1	62.5
Phenanthrene	2,2,4-Trimethylpentane	50	92.7	80.4	88.6	76.2
Phenanthrene	Heptane	20	20.5	173.4	64.2	228.3
Phenanthrene	Heptane	30	24.9	70.5	2.4	104.7
Phenanthrene	Heptane	40	48.5	17.0	29.8	40.4
Phenanthrene	Heptane	50	64.3	18.9	51.3	2.6
Phenanthrene	Toluene	20	59.1	29.2	39.7	14.2
Phenanthrene	Toluene	30	62.1	34.5	44.2	20.7
Phenanthrene	Toluene	40	67.3	43.4	51.7	31.4
Phenanthrene	Toluene	50	68.7	45.9	53.9	34.5
Phenyl acetic acid	2,2,4-Trimethylpentane	25	561.6	97.1	2363.6	96.5
Phenyl acetic acid	Carbon tetrachloride	25	76.9	99.3	283.1	99.0
Phenyl acetic acid	Cyclohexane	25	339.2	98.6	1405.1	98.2
Phenyl acetic acid	Heptane	25	574.0	96.9	2107.4	96.2
Phenyl acetic acid	Octane	25	701.5	97.2	2677.3	96.6
Pyrene	2,2,4-Trimethylpentane	20	80.2	37.8	51.7	29.3
Pyrene	2,2,4-Trimethylpentane	30	84.5	51.4	62.3	0.9
Pyrene	2,2,4-Trimethylpentane	40	86.1	56.4	66.2	9.4
Pyrene	2,2,4-Trimethylpentane	50	90.9	71.5	77.9	40.7
Pyrene	Heptane	20	67.2	8.8	19.2	82.6
Pyrene	Heptane	30	75.7	32.5	40.2	35.2
Pyrene	Heptane	40	85.8	60.6	65.1	21.1
Pyrene	Heptane	50	92.5	79.0	81.4	57.9
Pyrene	Toluene	20	105.4	284.4	188.8	394.2
Pyrene	Toluene	30	30.2	143.6	83.0	213.2
Pyrene	Toluene	40	6.4	99.2	49.6	156.1
Pyrene	Toluene	50	43.8	5.2	21.0	35.2
		All	207.2[a]	59.1[b]	188.0[a]	73.6[b]
		25	343.6[c]	62.6[d]	331.1[c]	76.2[d]

[a] The difference was not statistically significant (paired t-test, p>0.05); [b] The difference was statistically significant (paired t-test, p<0.008); [c] The difference was not statistically significant (paired t-test, p>0.05); [d] The difference was not statistically significant (paired t-test, p>0.05).