Preferential Solvation Analysis of Moxidectin in Water/Alcohol Mixtures

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ABSTRACT

Preferential solvation analysis on experimental solubility data of moxidectin was performed by using the Inverse Kirkwood-Buff Integrals approach at 298.15 K. Local mole fraction of solvents in the solvation shell of moxidectin as well as the extent of preferential solvation by each of solvents were calculated as a function of the bulk mole fraction of binary mixtures of water with methanol, ethanol, isopropanol, and ethylene glycol. Results indicate that preferential solvation of moxidectin by water occurs in water-rich regions. Whereas, beyond water-rich regions, moxidectin was preferentially surrounded by alcohols in all binary mixtures studied.
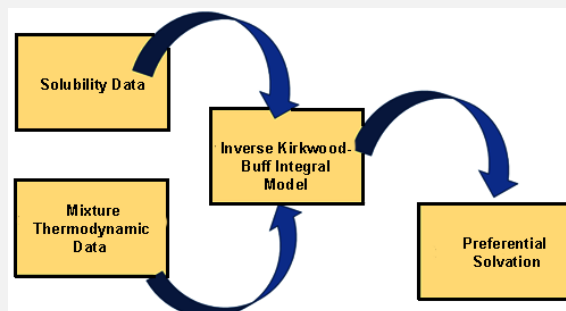
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1. Introduction

Investigation of intermolecular interactions in multicomponent systems and their relationship with the system structure has always been of interest to researchers [1-5]. As an attractive issue in solution chemistry, preferential solvation may occur in mixtures due to differences in interactions between components. In such cases, components experience different compositions in their solvation shell with respect to the bulk. The Inverse Kirkwood-Buff Integrals (IKBI) provides the best applicable approach for the analysis of preferential solvation of solutes in a mixture of two solvents [6]. In this method, the probability of finding a molecule of one solvent around a solute molecule is defined by the integrals of radial distribution functions for the pair of two molecules. With the help of statistical thermodynamics in an inverse way, KBI can be determined from some macroscopic thermodynamics data for mixed solvents and solutions. Analysis of obtained KBI over the mixture composition gives information on microscopic local composition of solvation shell of components and thus on the probability and extent of preferential solvation [1-6].

Solvent screening is the main step in process of optimization of synthesis, crystallization, extraction, and formulation of drugs in the pharmaceutical industry. In this regard, knowledge of solubility and dissolution mechanisms is critical. Most drugs because of their organic nature show low aqueous solubility that restricts their pharmacokinetics and pharmacodynamics. Co-solvency method in which miscible organic solvents are mixed with water is an advisable convenient and effective approach for solubility enhancement [7]. Despite of widely used co-solvency method in pharmacy, investigation on preferential solvation aimed to understand how a change in mixture composition improves the solubility has only been carried out in recent years [4, 8-11].

Moxidectin (with the molecular structure shown in **Figure 1**) is used as a drug in the treatment of various diseases in a veterinary clinics. Recently, the solubility of moxidectin has been determined in aqueous mixtures of alcohols including methanol, ethanol, isopropanol, and ethylene glycol over a temperature range of 278.15–323.15 K [12].
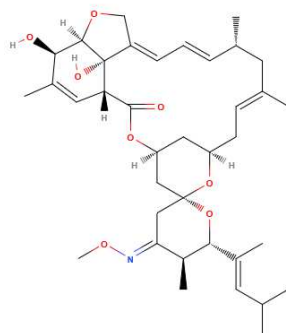
Figure 1. Molecular structure of moxidectin

Different co-solvency models have been used to correlate data to being used for the prediction of solubility over other compositions. However, no further analysis has been done on experimental data in the binary mixture in order to gain insight into solvation and enhance the effect of co-solvent on solubility. Most studies on drug solubility data in mixed solvents have been devoted to mathematical modeling and possibly predicting solubility from drug solubility in pure solvents. Depending kind of solvent mixtures, models such as Jouyban-Acree, NRTL, Wilson, and UNIQUAC have been developed [13-16]. Such models are successful to make a correlation between solubility data with mixture composition and temperature, but provide little detail on the actual molecular environment of the solute and the interactions leading to preferences between solute and each solvent in the mixture. The Inverse Kirkwood-Buff Integrals (IKBI) model is a powerful approach for providing insight into microscopic structures in mixed components based on thermodynamic data analysis [17-23]. Therefore, the aim of this work is preferential solvation analysis of solubility data of moxidectin in a binary mixture with the help of the IKBI approach to determine the local mole fractions of solvent in the solvation shell of moxidectin as well as the extent of preferential solvation over the mixture composition.

2. Theoretical considerations
2.1. IKBI model

The quantity $\delta x_{i,s} = x_{i,s}^L - x_i$ explains the preferential solvation of solute s by solvent i. Here, $x_{i,s}^L$ is the local mole fraction of solvent i around the solute s, and x_i is the mole fraction of solvent i in the bulk mixture of two solvents. According to Kirkwood-Buff Integrals, the extent of preferential solvation of can is calculated by Eq. (1) [17-23].

$$\delta x_{1,s} = \frac{x_1 x_2 \left(G_{1,s} - G_{2,3}\right)}{x_1 G_{1,s} + x_2 G_{2,s} + V_{cor}} \qquad (1)$$

In this equation, an affinity between components is defined by $G_{i,s}$ so-called Kirkwood-Buff integral. From point of view of statistical thermodynamics, $G_{i,s}$ can be readily determined by the following integration on the radial distribution function between solute and solvent, $g_{i,s}(r)$ as Eq. (2).

$$G_{i,s} = \int_0^{r_{cor}} (g_{i,s} - 1) 4\pi r^2 dr \qquad (2)$$

here, r is the distance between centers of molecules. However, $G_{i,s}$ can be accurately determined in an inverse approach from the macroscopic properties of the solution by using Eq. (3) and (4).

$$G_{1,s} = RT\kappa_T - V_s + \frac{x_2 V_2 D}{Q} \qquad (3)$$

$$G_{2,s} = RT\kappa_T - V_s + \frac{x_1 V_1 D}{Q} \qquad (4)$$

In these equations, isothermal compressibility κ_T molar volume for organic solvent (methanol, ethanol, isopropanol, and ethylene glycol) V_1, molar volume for water V_2, and molar volume for moxidectin V_s are needed to be known. R and T are the universal gas constant and temperature, respectively. Other functions D and Q are determined by thermodynamic functions including excess Gibbs free energy of mixing of two solvents in a binary mixture, G_{1+2}^{Exc}, and

the standard molar Gibbs energies of solute's transfer, $\Delta_{tr} G^o_{(s,2\to1+2)}$ from pure solvent 2 to binary mixture by using the following equations Eq. (5) and (6).

$$Q = RT + x_1 x_2 \left[\frac{\partial^2 G^{Exc}_{1+2}}{\partial x_2^2} \right]_{T,p} \tag{5}$$

$$D = \left(\frac{\partial \Delta_{tr} G^o_{(s,2\to1+2)}}{\partial x_1} \right)_{T,P} \tag{6}$$

Binary mixtures of two solvents $\Delta_{tr} G^o_{(s,2\to1+2)}$ can be readily determined by the mole fraction solubility of solute $x_{S,i}$ based on Eq. (7).

$$\Delta_{tr} G^o_{(s,2\to1+2)} = RT \ln \frac{x_{s,2}}{x_{s,2+1}} \tag{7}$$

Finally, in Eq. (1), the correlation volume V_{cor} is the area around the solute in which preferential solvation occurs. It is obvious that V_{cor} depends on the local composition. Eq. (10) is recommended for the calculation of V_{cor} by considering the first shell around the solute [4].

$$V_{cor} = 2522.5 \left[r_s + 0.1363 \left(x^L_{1,s} V_1 + x^L_{2,s} V_2 \right)^{1/3} - 0.085 \right]^3 \tag{8}$$

Therefore, one can analyze the preferential solvation by solving Eq. (1) by prior simultaneous solving of Eqs. (3)-(8) by knowledge of thermodynamic properties of solution [17-25].

3. Results and discussion

For calculation of function Q in Eq. (5), the excess Gibbs free energy of mixing water with methanol, ethanol, isopropanol, and ethylene glycol was extracted from the reference at 298.15 K [26]. Partial molar volume for solvents in mixtures was calculated from density data at 298.15 K available for the studied binary mixture from the literature [27, 28]. The isothermal compressibility for each aqueous binary mixture can be safely computed by $x_1 K_{T1} + x_2 K_{T2}$. for pure solvents, corresponding data was taken from the literature [29]. The standard Gibbs free energy of transfer of moxidectin from water to methanol (1) + water (2), ethanol (1) + water (2), isopropanol (1) + water (2), and ethylene glycol (1) + water (2) mixtures was determined by Eq. (7). Data for the mole fraction solubility of moxidectin in binary mixtures were taken from the literature [12]. In addition functions, D, Q, $G_{1,s}$, and $G_{2,s}$ were calculated by Eqs. (3)-(6) versus the bulk mole fractions and tabulated in **Table 1-4**. The correlation volume in Eq. (8) is a function of the local mole fractions. Therefore, in an iterative process, $\delta x_{1,s}$ and V_{cor} were computed by simultaneous solving of Eqs. (1) and (8) through iteration on the local mole fractions until a non-variant value was obtained.

Table 1. Kirkwood-Buff functions D, Q, $G_{2,s}$ and $G_{1,s}$ in methanol (1) + water (2) mixture at 298.15 K.

x_1	D (kJ·mol^{-1})	Q (kJ·mol^{-1})	$G_{1,s}$ (cm^3·mol^{-1})	$G_{2,s}$ (cm^3·mol^{-1})
0.00	-194.04	2.48	-1929	-516
0.05	-97.71	2.51	-1184	-589
0.10	-58.68	2.47	-902	-604
0.15	-39.10	2.38	-768	-608
0.20	-27.91	2.27	-693	-608
0.25	-20.91	2.14	-647	-608
0.30	-16.25	2.01	-616	-608
0.35	-12.99	1.90	-594	-608
0.40	-10.62	1.81	-577	-607
0.45	-8.85	1.74	-563	-605
0.50	-7.48	1.71	-552	-601
0.55	-6.41	1.72	-543	-597
0.60	-5.55	1.76	-536	-591
0.65	-4.86	1.83	-530	-584
0.70	-4.29	1.93	-525	-577
0.75	-3.81	2.04	-522	-571

0.80	-3.41	2.17	-519	-565
0.85	-3.07	2.29	-517	-560
0.90	-2.77	2.39	-516	-556
0.95	-2.52	2.46	-515	-554
1.00	-2.30	2.48	-514	-552

The affinity between alcohol and moxidectin, and between water and moxidectin are respectively determined by Kirkwood-Buff integrals $G_{1,s}$ and $G_{2,s}$. It is evident from **Tables 1-4** that $G_{1,s}$ and $G_{2,s}$ were negative in all compositions for all aqueous binary mixtures. It means that moxidectin show affinity for positive interaction with both solvents in all binary mixtures studied. However, a comparison of their values indicates that in water-rich regions in all binary mixtures, $G_{2,s}$ is higher than $G_{1,s}$. This result indicates that moxidectin has a more affinity for solvation by water with respect to alcohols in water-rich regions.

Table 2. Kirkwood-Buff functions D, Q, $G_{2,s}$ and $G_{1,s}$ in ethanol (1) + water (2) mixture at 298.15 K.

x_1	D (kJ·mol^{-1})	Q (kJ·mol^{-1})	$G_{1,s}$ (cm^3·mol^{-1})	$G_{2,s}$ (cm^3·mol^{-1})
0.00	-336.84	2.48	-2969	-516
0.05	-118.90	2.22	-1434	-660
0.10	-60.13	2.04	-994	-676
0.15	-36.20	1.91	-805	-672
0.20	-24.15	1.81	-705	-664
0.25	-17.25	1.73	-647	-655
0.30	-12.94	1.66	-611	-648
0.35	-10.06	1.58	-587	-643
0.40	-8.05	1.49	-570	-640
0.45	-6.58	1.39	-559	-639
0.50	-5.48	1.27	-551	-640
0.55	-4.64	1.15	-545	-644
0.60	-3.97	1.04	-540	-649
0.65	-3.44	0.94	-536	-654
0.70	-3.01	0.87	-531	-656
0.75	-2.66	0.86	-527	-650
0.80	-2.36	0.92	-523	-635
0.85	-2.11	1.08	-519	-612
0.90	-1.90	1.37	-517	-588
0.95	-1.72	1.82	-515	-567
1.00	-1.56	2.48	-514	-551

Table 3. Kirkwood-Buff functions D, Q, $G_{2,s}$, and $G_{1,s}$ in isopropanol (1) + water (2) mixture at 298.15 K.

x_1	D (kJ·mol^{-1})	Q (kJ·mol^{-1})	$G_{1,s}$ (cm^3·mol^{-1})	$G_{2,s}$ (cm^3·mol^{-1})
0.00	-230.71	2.48	-2196	-516
0.05	-94.26	2.40	-1187	-654
0.10	-50.91	2.26	-878	-677
0.15	-31.80	2.07	-746	-684
0.20	-21.74	1.85	-680	-689
0.25	-15.79	1.61	-643	-699
0.30	-11.99	1.36	-621	-715
0.35	-9.41	1.11	-608	-739
0.40	-7.58	0.88	-602	-776
0.45	-6.24	0.68	-600	-831
0.50	-5.23	0.51	-600	-906
0.55	-4.44	0.38	-601	-998
0.60	-3.82	0.32	-595	-1069
0.65	-3.32	0.31	-577	-1050
0.70	-2.91	0.37	-554	-938
0.75	-2.57	0.50	-535	-807
0.80	-2.29	0.72	-525	-709

0.85	-2.06	1.02	-519	-645
0.90	-1.85	1.41	-516	-604
0.95	-1.68	1.90	-515	-578
1.00	-1.53	2.48	-514	-561

Table 4. Kirkwood-Buff functions D, Q, $G_{2,S}$, and $G_{1,S}$ in ethylene glycol (1) + water (2) mixture at 298.15 K.

x_1	D (kJ·mol^{-1})	Q (kJ·mol^{-1})	$G_{1,S}$ (cm^3.mol^{-1})	$G_{2,S}$ (cm^3.mol^{-1})
0.00	-169.10	2.48	-1747	-516
0.05	-81.44	2.56	-1062	-602
0.10	-47.28	2.61	-811	-615
0.15	-30.69	2.63	-695	-612
0.20	-21.46	2.63	-633	-606
0.25	-15.81	2.63	-597	-599
0.30	-12.12	2.63	-574	-593
0.35	-9.58	2.63	-558	-587
0.40	-7.76	2.63	-548	-582
0.45	-6.41	2.64	-540	-577
0.50	-5.38	2.66	-534	-572
0.55	-4.58	2.69	-530	-568
0.60	-3.95	2.72	-526	-565
0.65	-3.44	2.76	-524	-561
0.70	-3.02	2.79	-522	-559
0.75	-2.67	2.82	-520	-556
0.80	-2.38	2.82	-519	-554
0.85	-2.13	2.80	-518	-552
0.90	-1.93	2.75	-517	-552
0.95	-1.75	2.64	-517	-551
1.00	-1.59	2.48	-516	-552

The extent of preferential solvation of moxidectin by alcohol $\delta x_{1,s}$ was determined as a function of mole fraction of alcohol in aqueous binary mixtures, and plotted against mole fraction of organic solvent in **Figure 2**. $\delta x_{1,s}$ was negative at $0.00 \leq x_1 < 0.15$ for isopropanol (1) + water (2), at $0.00 \leq x_1 < 0.20$ for ethanol (1) + water (2), and ethylene glycol (1) + water, at $0.00 \leq x_1 < 0.30$ for methanol (1) + water (2) mixtures. Therefore, moxidectin was preferentially solvated by water in water-rich regions in all binary aqueous mixtures studied here. The reason for this observation may be because of the enhancement effect of alcohols on the structuring of the hydrogen bonding water network around the solute [30].
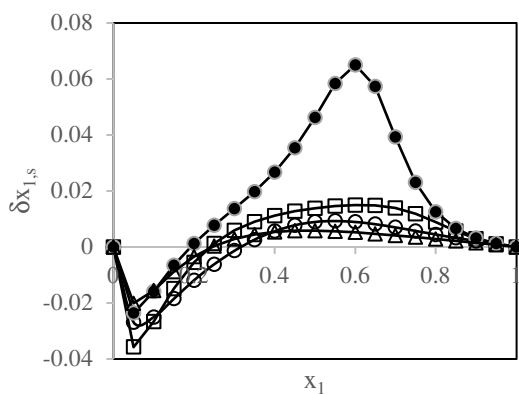

Figure 2. Preferential solvation of moxidectin by organic solvent as a mole fraction of methanol (○), ethanol (□), isopropanol (●), and ethylene glycol (Δ).

In water-rich region, the order of preferential solvation by water in mixtures is as ethanol (1) + water (2) > methanol (1) + water (2) > isopropanol (1) + water (2) > ethylene glycol (1) + water (2). Marcus showed that water molecules become more structured in presence of organic solvents such as alcohols. However, the enhancement effect was the least for ethylene glycol [31]. Furthermore, moxidectin can interact with water as a Lewis base by its oxygen atoms. Water is more acidic than alcohols and thus is more favorable to making such hydrogen bonding interactions with moxidectin. The $\delta x_{1,s}$ was positive for all binary mixtures beyond water-rich regions up to pure alcohol. This result reveals that moxidectin was solvated more selective by methanol, ethanol, isopropanol, and ethylene glycol rather than by water in these regions. Maximum value for preferential solvation was observed at x_1=0.55 for methanol (1) + water (2), at x_1=0.60 for ethanol (1) + water (2) and isopropanol (1) + water (2), and at x_1=0.45 for ethylene glycol (1) + water (2) mixtures. The reason for preferential solvation by alcohols may be related to the strong network structure of water. Cavity formation in water is a much more energy-consuming step in the solvation of moxidectin with respect to alcohols. In addition, all alcohols methanol, ethanol, isopropanol, and ethylene glycol are more basic than water, and thus can make more favorable interactions with acidic hydroxyl sites on moxidectin. It seems that moxidectin prefers to make such hydrogen bonding interactions with alcohols that with water in aqueous binary mixtures studied. The order of preferential solvation by alcohol, $\delta x_{1,s}$, in these regions is as isopropanol (1) + water (2) > ethanol (1) + water (2) > methanol (1) + water (2) > ethylene glycol (1) + water (2). This observation is in good agreement with the order of hydrogen bond acceptor capacity of solvents described by the Kamlet-Taft hydrogen bond acceptor parameter as $\beta = 0.84$ for isopropanol > $\beta = 0.75$ for ethanol > $\beta = 0.66$ for methanol > $\beta = 0.52$ for ethylene glycol > $\beta = 0.47$ for water [32]. It confirms that the hydrogen bonding interactions in which moxidectin acts as Lewis acid are mainly responsible for preferential solvation in these regions.

4. Conclusion

In this work, the approach of Inverse Kirkwood-Buff Integrals was successfully used for the analysis of experimental data of moxidectin in binary mixtures of water with methanol, ethanol, isopropanol, and ethylene glycol. Gibbs free energy of transfer of moxidectin from water to the mixture was calculated and used with other thermodynamic properties of mixture for computation of local mole fraction of solvents around moxidectin and extent of preferential solvation. Kirkwood-Buff integral functions and preferential solvation parameter indicate that moxidectin was solvated more by water in the water-rich region, and by alcohols in other remaining compositions up to pure organic solvent.

Authors' contributions

All authors contributed to data analysis, drafting and revising of the paper and agreed to be responsible for all the aspects of this work.

Declaration of competing interest

The authors declare no competing interest.

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Data availability

Data will be made available on request.

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