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Gefitinib hydrochloride anti-cancer drug solubility in supercritical carbon dioxide: Thermodynamic modeling

Oxycodone hydrochloride (OXH), is a potent opioid derived from natural sources and partially synthesized, which is commonly prescribed in the medical field for managing moderate to severe pain. OXH, a colourless and odorless crystalline substance, is obtained from the opium alkaloid known as thebaine. It's worth noting that OXH displays minimal solubility in alcohol, with a low octanol-water partition coefficient of 0.7. The meticulous mechanism underlying the effects of OXH is not yet fully comprehended within academic circles. OXH and its active metabolites, including nor oxycodone, oxymorphone, and noroxymorphone, exhibit opioid agonist properties in the academic context. Supercritical fluids (SCFs) can dissolve substances similar to liquids and exhibit transport properties like gases, including high porosity and low stickiness. SCFs are distinguished by surpassing the critical temperature (Tc) and pressure (Pc), enabling them to manifest properties of liquids and gases.

The solubility of OXH in supercritical carbon dioxide (SC-CO2) was investigated at temperature (308 to 338 K) and pressure (120 to 270 bar). The solubility ranged from 0.007 to 0.109 g/L, corresponding to mole fractions ranging from 0.051×10-5 to 0.699×10-5. Three different model groups were used to analyze the experimental data. The first group comprised seven semi-empirical models, with three to six adjustable parameters. These models include Sparks, Sodeifian 1 and 2, Bian, Jouyban, Gordillo and Jafari-Nejad. The second group employed two state equations, namely the Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK) with van der Waals mixing rule. The average absolute relative deviation percentage (AARD%) was 9.73 and 10.63 for PR and SRK, respectively. The third group utilized four machine learning algorithms including DNN, RF, MLP and DTs with the respective R2 values 0.992, 0.980, 0.964 and 0.961, respectively. All of the models exhibited satisfactory agreement with the experimental data. Finally, the enthalpies of vaporization (79.71 kJ/mol) and solvation (-19.25 kJ/mol) were calculated.

Keywords: Gefitinib hydrochloride; Sodeifian model; Solubility; sPC-SAFT.

Biography

Gholamhossein Sodeifian born in 1971 and graduated in chemical engineering (MS) from University of Tehran, in 1997 and received his doctorate (PhD), in polymer Engineering from Tarbiat Modares University, Tehran, in 2002. After that, he has worked till now as a chemical engineering professor, at University of Kashan, and teaches many courses such as advanced mass transfer, supercritical fluid technology, optimization and modeling, advanced rheology of non-Newtonian fluids and polymer melts, mechanical and physical properties of polymers, experimental design, and especial methods in separation processes and drug delivery in pharmaceutical systems. His researches focused on extraction of essential and seed oils, solubility measurement of solid drugs, micro and nano-particle formation of pharmaceutical materials in supercritical carbon dioxide (SC-CO2), and other new techniques. He has developed for the first time in the world a new and efficient technique for nanoparticle formation, i.e., US-RESOLV. He has published more than 98 ISI scientific papers with five inventions and nine books in Persian language. Also, his named in the world's top 2% of scientists list in 2020, 2021, 2022 and 2023.

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