
References

1. Salama NN, Eddington ND, Fasano A. Tight junction modulation and its relationship to drug delivery. *Adv Drug Deliv Rev.* 58(1), 15–28 (2006).
2. Yun Y, Cho YW, Park K. Nanoparticles for oral delivery: Targeted nanoparticles with peptidic ligands for oral protein delivery. *Adv Drug Deliv Rev.* 65(6), 822–832 (2013).
3. Anselmo AC, Mitragotri S. An overview of clinical and commercial impact of drug delivery systems. *Journal of Controlled Release.* 190, 15–28 (2014).
4. Viswanathan P, Muralidaran Y, Ragavan G. Chapter 7 - Challenges in oral drug delivery: a nano-based strategy to overcome [Internet]. In: *Nanostructures for Oral Medicine.* Andronescu E, Grumezescu AM (Eds.), Elsevier, 173–201 (2017).
5. Boyd BJ, Bergström CAS, Vinarov Z, *et al.* Successful oral delivery of poorly water-soluble drugs both depends on the intraluminal behavior of drugs and of appropriate advanced drug delivery systems. *European Journal of Pharmaceutical Sciences.* 137, 104967 (2019).
6. Schittny A, Philipp-Bauer S, Detampel P, Huwyler J, Puchkov M. Mechanistic insights into effect of surfactants on oral bioavailability of amorphous solid dispersions. *Journal of Controlled Release* [Internet]. 320, 214–225 (2020).
7. Machado TC, Kuminek G, Cardoso SG, Rodríguez-Hornedo N. The role of pH and dose/solubility ratio on cocrystal dissolution, drug supersaturation and precipitation. *European Journal of Pharmaceutical Sciences.* 152, 105422 (2020).
8. Amidon GL, Lennernäs H, Shah VP, Crison JR. A Theoretical Basis for a Biopharmaceutic Drug Classification: The Correlation of in Vitro Drug Product Dissolution and in Vivo Bioavailability. *Pharm Res.* 12(3), 413–420 (1995).
9. Sun DD, Lee PI. Haste Makes Waste: The Interplay Between Dissolution and Precipitation of Supersaturating Formulations. *AAPS J.* 17(6), 1317–1326 (2015).
10. Wojnarowska Z, Grzybowska K, Hawelek L, *et al.* Molecular Dynamics, Physical Stability and Solubility Advantage from Amorphous Indapamide Drug. *Mol Pharm.* 10(10), 3612–3627 (2013).
11. Zhang J, Guo M, Luo M, Cai T. Advances in the development of amorphous solid dispersions: The role of polymeric carriers. *Asian J Pharm Sci.* 18(4), 100834 (2023).
12. Butreddy A. Hydroxypropyl methylcellulose acetate succinate as an exceptional polymer for amorphous solid dispersion formulations: A review from bench to clinic. *European Journal of Pharmaceutics and Biopharmaceutics.* 177, 289–307 (2022).

13. Han J, Tang M, Yang Y, *et al.* Amorphous solid dispersions: Stability mechanism, design strategy and key production technique of hot melt extrusion. *Int J Pharm.* 646, 123490 (2023).
14. <https://www.accessdata.fda.gov/scripts/cder/daf/index.cfm>.
15. CHMP. Viekirax (ombitasvir / paritaprevir / ritonavir) What is Viekirax and what is it used for?. Available from: www.ema.europa.eu/contact.
16. Laitinen R, Löbmann K, Strachan CJ, Grohgan H, Rades T. Emerging trends in the stabilization of amorphous drugs. *Int J Pharm.* 453(1), 65–79 (2013).
17. Dengale SJ, Grohgan H, Rades T, Löbmann K. Recent advances in co-amorphous drug formulations. *Adv Drug Deliv Rev* [Internet]. 100, 116–125 (2016).
18. Tan DK, Davis DA, Miller DA, Williams RO, Nokhodchi A. Innovations in Thermal Processing: Hot-Melt Extrusion and KinetiSol® Dispersing. *AAPS PharmSciTech.* 21(8) (2020).
19. Baird JA, Van Eerdenbrugh B, Taylor LS. A Classification System to Assess the Crystallization Tendency of Organic Molecules from Undercooled Melts. *J Pharm Sci.* 99(9), 3787–3806 (2010).
20. Graeser KA, Patterson JE, Zeitler JA, Gordon KC, Rades T. Correlating thermodynamic and kinetic parameters with amorphous stability. *European Journal of Pharmaceutical Sciences.* 37(3–4), 492–498 (2009).
21. Mahlin D, Bergström CAS. Early drug development predictions of glass-forming ability and physical stability of drugs. *European Journal of Pharmaceutical Sciences.* 49(2), 323–332 (2013).
22. Paudel A, Worku ZA, Meeus J, Guns S, Van den Mooter G. Manufacturing of solid dispersions of poorly water soluble drugs by spray drying: Formulation and process considerations. *Int J Pharm.* 453(1), 253–284 (2013).
23. Van Eerdenbrugh B, Baird JA, Taylor LS. Crystallization Tendency of Active Pharmaceutical Ingredients Following Rapid Solvent Evaporation—Classification and Comparison with Crystallization Tendency from Under cooled Melts. *J Pharm Sci.* 99(9), 3826–3838 (2010).
24. Van den Mooter G. The use of amorphous solid dispersions: A formulation strategy to overcome poor solubility and dissolution rate. *Drug Discov Today Technol.* 9(2), e79–e85 (2012).
25. Baghel S, Cathcart H, O’Reilly NJ. Polymeric Amorphous Solid Dispersions: A Review of Amorphization, Crystallization, Stabilization, Solid-State Characterization, and Aqueous Solubilization of Biopharmaceutical Classification System Class II Drugs. *J Pharm Sci.* 105(9), 2527–2544 (2016).
26. Rams-Baron M, Wojnarowska Z, Grzybowska K, *et al.* Toward a Better Understanding of the Physical Stability of Amorphous Anti-Inflammatory

- Agents: The Roles of Molecular Mobility and Molecular Interaction Patterns. *Mol Pharm.* 12(10), 3628–3638 (2015).
27. Hancock BC, Shamblin SL, Zografi G. Molecular mobility of amorphous pharmaceutical solids below their glass transition temperatures. *Pharm Res.* 12(6), 799–806 (1995).
 28. Kauzmann Walter. The Nature of the Glassy State and the Behavior of Liquids at Low Temperatures. *Chem Rev.* 43(2), 219–256 (1948).
 29. Kissi EO, Grohganz H, Löbmann K, Ruggiero MT, Zeitler JA, Rades T. Glass-Transition Temperature of the β -Relaxation as the Major Predictive Parameter for Recrystallization of Neat Amorphous Drugs. *J Phys Chem B.* 122(10), 2803–2808 (2018).
 30. Gordon M, Taylor JS. Ideal Copolymers and the Second-Order Transitions of Synthetic Rubbers. I. Noncrystalline Copolymers. *Rubber Chemistry and Technology.* 26(2), 323–335 (1953).
 31. Wu JX, Yang M, Berg F van den, Pajander J, Rades T, Rantanen J. Influence of solvent evaporation rate and formulation factors on solid dispersion physical stability. *European Journal of Pharmaceutical Sciences.* 44(5), 610–620 (2011).
 32. Hilton JE, Summers MP. The effect of wetting agents on the dissolution of indomethacin solid dispersion systems. *Int J Pharm.* 31(1–2), 157–164 (1986).
 33. Bookwala M, Wildfong PLD. The Implications of Drug-Polymer Interactions on the Physical Stability of Amorphous Solid Dispersions. *Pharm Res.* (2023).
 34. Geneidi ASH, Ali AA, Salama RB. Solid Dispersions of Nitrofurantoin, Ethotoin, and Coumarin with Polyethylene Glycol 6000 and Their Coprecipitates with Povidone 25,000. *J Pharm Sci.* 67(1), 114–116 (1978).
 35. Doherty C, York P. Fresemide crystal forms; solid state and physicochemical analyses. *Int J Pharm.* 47(1–3), 141–155 (1988).
 36. Yoshioka M, Hancock BC, Zografi G. Inhibition of indomethacin crystallization in poly(vinylpyrrolidone) coprecipitates. *J Pharm Sci.* 84(8), 983–986 (1995).
 37. Taylor LS, Zografi G. Spectroscopic Characterization of Interactions Between PVP and Indomethacin in Amorphous Molecular Dispersions. *Pharm Res.* 14(12), 1691–1698 (1997).
 38. Wegiel LA, Zhao Y, Mauer LJ, Edgar KJ, Taylor LS. Curcumin amorphous solid dispersions: the influence of intra and intermolecular bonding on physical stability. *Pharm Dev Technol.* 19(8), 976–986 (2014).
 39. Trasi NS, Baird JA, Kestur US, Taylor LS. Factors Influencing Crystal Growth Rates from Undercooled Liquids of Pharmaceutical Compounds. *J Phys Chem B.* 118(33), 9974–9982 (2014).

40. Chen H, Pui Y, Liu C, *et al.* Moisture-Induced Amorphous Phase Separation of Amorphous Solid Dispersions: Molecular Mechanism, Microstructure, and Its Impact on Dissolution Performance. *J Pharm Sci.* 107(1), 317–326 (2018).
41. Amponsah-Efah KK, Mistry P, Eisenhart R, Suryanarayanan R. The Influence of the Strength of Drug–Polymer Interactions on the Dissolution of Amorphous Solid Dispersions. *Mol Pharm.* 18(1), 174–186 (2021).
42. Song Y, Yang X, Chen X, Nie H, Byrn S, Lubach JW. Investigation of Drug–Excipient Interactions in Lapatinib Amorphous Solid Dispersions Using Solid-State NMR Spectroscopy. *Mol Pharm.* 12(3), 857–866 (2015).
43. Sarode AL, Sandhu H, Shah N, Malick W, Zia H. Hot Melt Extrusion for Amorphous Solid Dispersions: Temperature and Moisture Activated Drug–Polymer Interactions for Enhanced Stability. *Mol Pharm.* 10(10), 3665–3675 (2013).
44. Sarode AL, Sandhu H, Shah N, Malick W, Zia H. Hot melt extrusion (HME) for amorphous solid dispersions: Predictive tools for processing and impact of drug–polymer interactions on supersaturation. *European Journal of Pharmaceutical Sciences.* 48(3), 371–384 (2013).
45. Chen Y, Wang S, Wang S, *et al.* Initial Drug Dissolution from Amorphous Solid Dispersions Controlled by Polymer Dissolution and Drug-Polymer Interaction. *Pharm Res.* 33(10), 2445–2458 (2016).
46. Chen Y, Liu C, Chen Z, *et al.* Drug–Polymer–Water Interaction and Its Implication for the Dissolution Performance of Amorphous Solid Dispersions. *Mol Pharm.* 12(2), 576–589 (2015).
47. Sarabu S, Kallakunta VR, Bandari S, *et al.* Hypromellose acetate succinate based amorphous solid dispersions via hot melt extrusion: Effect of drug physicochemical properties. *Carbohydr Polym.* 233, 115828 (2020).
48. Pui Y, Chen Y, Chen H, *et al.* Maintaining Supersaturation of Nimodipine by PVP with or without the Presence of Sodium Lauryl Sulfate and Sodium Taurocholate. *Mol Pharm.* 15(7), 2754–2763 (2018).
49. Khougaz K, Clas S. Crystallization Inhibition in Solid Dispersions of MK-0591 and Poly(vinylpyrrolidone) Polymers. *J Pharm Sci* [Internet]. 89(10), 1325–1334 (2000).
50. Que C, Qi Q, Zemlyanov DY, *et al.* Evidence for Halogen Bonding in Amorphous Solid Dispersions. *Cryst Growth Des.* 20(5), 3224–3235 (2020).
51. Marsac PJ, Li T, Taylor LS. Estimation of Drug–Polymer Miscibility and Solubility in Amorphous Solid Dispersions Using Experimentally Determined Interaction Parameters. *Pharm Res.* 26(1), 139–151 (2009).
52. NetworkGels_Lecture8.

53. Knopp MM, Tajber L, Tian Y, *et al.* Comparative Study of Different Methods for the Prediction of Drug–Polymer Solubility. *Mol Pharm.* 12(9), 3408–3419 (2015).
54. Qian F, Huang J, Hussain MA. Drug–Polymer Solubility and Miscibility: Stability Consideration and Practical Challenges in Amorphous Solid Dispersion Development. *J Pharm Sci.* 99(7), 2941–2947 (2010).
55. Laitinen R, Priemel PA, Surwase S, *et al.* Theoretical Considerations in Developing Amorphous Solid Dispersions. 35–90 (2014).
56. Prasad D, Chauhan H, Atef E. Amorphous Stabilization and Dissolution Enhancement of Amorphous Ternary Solid Dispersions: Combination of Polymers Showing Drug–Polymer Interaction for Synergistic Effects. *J Pharm Sci.* 103(11), 3511–3523 (2014).
57. Mura P, Moyano JR, González-Rodríguez ML, Rabasco-Alvaréz AM, Cirri M, Maestrelli F. Characterization and Dissolution Properties of Ketoprofen in Binary and Ternary Solid Dispersions with Polyethylene Glycol and Surfactants. *Drug Dev Ind Pharm.* 31(4–5), 425–434 (2005).
58. Démuth B, Nagy ZK, Balogh A, *et al.* Downstream processing of polymer-based amorphous solid dispersions to generate tablet formulations. *Int J Pharm.* 486(1–2), 268–286 (2015).
59. Zhu L, Wong L, Yu L. Surface-Enhanced Crystallization of Amorphous Nifedipine. *Mol Pharm.* 5(6), 921–926 (2008).
60. Caron V, Tajber L, Corrigan OI, Healy AM. A Comparison of Spray Drying and Milling in the Production of Amorphous Dispersions of Sulfathiazole/Polyvinylpyrrolidone and Sulfadimidine/Polyvinylpyrrolidone. *Mol Pharm.* 8(2), 532–542 (2011).
61. Ayenew Z, Paudel A, Van den Mooter G. Can compression induce demixing in amorphous solid dispersions? A case study of naproxen–PVP K25. *European Journal of Pharmaceutics and Biopharmaceutics.* 81(1), 207–213 (2012).
62. Li W, Buckton G. Using DVS-NIR to assess the water sorption behaviour and stability of a griseofulvin/PVP K30 solid dispersion. *Int J Pharm.* 495(2), 999–1004 (2015).
63. Wlodarski K, Sawicki W, Kozyra A, Tajber L. Physical stability of solid dispersions with respect to thermodynamic solubility of tadalafil in PVP-VA. *European Journal of Pharmaceutics and Biopharmaceutics.* 96, 237–246 (2015).
64. Lehmkemper K, Kyeremateng SO, Bartels M, Degenhardt M, Sadowski G. Physical stability of API/polymer-blend amorphous solid dispersions. *European Journal of Pharmaceutics and Biopharmaceutics.* 124, 147–157 (2018).
65. Tian Y, Jones DS, Andrews GP. An Investigation into the Role of Polymeric Carriers on Crystal Growth within Amorphous Solid Dispersion Systems. *Mol Pharm.* 12(4), 1180–1192 (2015).

66. Yang Z, Nollenberger K, Albers J, Craig D, Qi S. Molecular Indicators of Surface and Bulk Instability of Hot Melt Extruded Amorphous Solid Dispersions. *Pharm Res.* 32(4), 1210–1228 (2015).
67. Breitenbach J. Melt extrusion: from process to drug delivery technology. *European Journal of Pharmaceutics and Biopharmaceutics.* 54(2), 107–117 (2002).
68. Janssens S, Van den Mooter G. Review: physical chemistry of solid dispersions. *Journal of Pharmacy and Pharmacology.* 61(12), 1571–1586 (2009).
69. Marsac PJ, Shamblin SL, Taylor LS. Theoretical and Practical Approaches for Prediction of Drug–Polymer Miscibility and Solubility. *Pharm Res.* 23(10), 2417–2426 (2006).
70. Kyeremateng SO, Pudlas M, Woehrlé GH. A Fast and Reliable Empirical Approach for Estimating Solubility of Crystalline Drugs in Polymers for Hot Melt Extrusion Formulations. *J Pharm Sci.* 103(9), 2847–2858 (2014).
71. Anuprabha Meena TPSSGATMS. Investigation of thermal and viscoelastic properties of polymers relevant to hot melt extrusion - II: Cellulosic polymers. *J. Excipients and Food Chem.*, 46–55 (2014).
72. Tapan Parikh SSGAMATMS. Investigation of thermal and viscoelastic properties of polymers relevant to hot melt extrusion, III: polymethacrylates and polymethacrylic acid based polymers. *J. Excipients and Food Chem*, 56–64 (2104).
73. Gupta SS, Solanki N, Serajuddin ATM. Investigation of Thermal and Viscoelastic Properties of Polymers Relevant to Hot Melt Extrusion, IV: Affinisol™ HPMC HME Polymers. *AAPS PharmSciTech.* 17(1), 148–157 (2016).
74. Vasconcelos T, Marques S, das Neves J, Sarmiento B. Amorphous solid dispersions: Rational selection of a manufacturing process. *Adv Drug Deliv Rev.* 100, 85–101 (2016).
75. Desai J, Alexander K, Riga A. Characterization of polymeric dispersions of dimenhydrinate in ethyl cellulose for controlled release. *Int J Pharm.* 308(1), 115–123 (2006).
76. Shanbhag A, Rabel S, Nauka E, *et al.* Method for screening of solid dispersion formulations of low-solubility compounds—Miniaturization and automation of solvent casting and dissolution testing. *Int J Pharm.* 351(1), 209–218 (2008).
77. Engers D, Teng J, Jimenez-Novoa J, *et al.* A Solid-State Approach to Enable Early Development Compounds: Selection and Animal Bioavailability Studies of an Itraconazole Amorphous Solid Dispersion. *J Pharm Sci.* 99(9), 3901–3922 (2010).

78. Yoshihashi Y, Iijima H, Yonemochi E, Terada K. Estimation of physical stability of amorphous solid dispersion using differential scanning calorimetry. *J Therm Anal Calorim.* 85(3), 689–692 (2006).
79. Singh A, Van den Mooter G. Spray drying formulation of amorphous solid dispersions. *Adv Drug Deliv Rev.* 100, 27–50 (2016).
80. Cal K, Sollohub K. Spray Drying Technique. I: Hardware and Process Parameters. *J Pharm Sci.* 99(2), 575–586 (2010).
81. Dobry DE, Settell DM, Baumann JM, Ray RJ, Graham LJ, Beyerinck RA. A Model-Based Methodology for Spray-Drying Process Development. *J Pharm Innov.* 4(3), 133–142 (2009).
82. Xie T, Taylor LS. Dissolution Performance of High Drug Loading Celecoxib Amorphous Solid Dispersions Formulated with Polymer Combinations. *Pharm Res.* 33(3), 739–750 (2016).
83. Censi R, Gigliobianco MR, Dubbini A, Malaj L, Di Martino P. New Nanometric Solid Dispersions of Glibenclamide in Neusilin® UFL2. *AAPS PharmSciTech.* 17(5), 1204–1212 (2016).
84. Purohit HS, Taylor LS. Miscibility of Itraconazole–Hydroxypropyl Methylcellulose Blends: Insights with High Resolution Analytical Methodologies. *Mol Pharm.* 12(12), 4542–4553 (2015).
85. Keratichevanun S, Yoshihashi Y, Sutanthavibul N, Terada K, Chatchawalsaisin J. An Investigation of Nifedipine Miscibility in Solid Dispersions Using Raman Spectroscopy. *Pharm Res.* 32(7), 2458–2473 (2015).
86. Milne M, Liebenberg W, Aucamp M. The Stabilization of Amorphous Zopiclone in an Amorphous Solid Dispersion. *AAPS PharmSciTech.* 16(5), 1190–1202 (2015).
87. Fong SYK, Ibisogly A, Bauer-Brandl A. Solubility enhancement of BCS Class II drug by solid phospholipid dispersions: Spray drying versus freeze-drying. *Int J Pharm.* 496(2), 382–391 (2015).
88. van Drooge DJ, Hinrichs WLJ, Visser MR, Frijlink HW. Characterization of the molecular distribution of drugs in glassy solid dispersions at the nano-meter scale, using differential scanning calorimetry and gravimetric water vapour sorption techniques. *Int J Pharm.* 310(1), 220–229 (2006).
89. Lim SM, Pang ZW, Tan HY, Shaikh M, Adinarayana G, Garg S. Enhancement of docetaxel solubility using binary and ternary solid dispersion systems. *Drug Dev Ind Pharm.* 41(11), 1847–1855 (2015).
90. Wlodarski K, Sawicki W, Haber K, *et al.* Physicochemical properties of tadalafil solid dispersions – Impact of polymer on the apparent solubility and dissolution rate of tadalafil. *European Journal of Pharmaceutics and Biopharmaceutics.* 94, 106–115 (2015).

91. van Drooge DJ, Braeckmans K, Hinrichs WLJ, Remaut K, De Smedt SC, Frijlink HW. Characterization of the Mode of Incorporation of Lipophilic Compounds in Solid Dispersions at the Nanoscale Using Fluorescence Resonance Energy Transfer (FRET). *Macromol Rapid Commun.* 27(14), 1149–1155 (2006).
92. Kanwate BW, Ballari R V, Kudre TG. Influence of spray-drying, freeze-drying and vacuum-drying on physicochemical and functional properties of gelatin from *Labeo rohita* swim bladder. *Int J Biol Macromol.* 121, 135–141 (2019).
93. Huang S, Williams RO. Effects of the Preparation Process on the Properties of Amorphous Solid Dispersions. *AAPS PharmSciTech.* 19(5), 1971–1984 (2018).
94. Valkama E, Haluska O, Lehto V-P, Korhonen O, Pajula K. Production and stability of amorphous solid dispersions produced by a Freeze-drying method from DMSO. *Int J Pharm.* 606, 120902 (2021).
95. Srinarong P, de Waard H, Frijlink HW, Hinrichs WLJ. Improved dissolution behavior of lipophilic drugs by solid dispersions: the production process as starting point for formulation considerations. *Expert Opin Drug Deliv.* 8(9), 1121–1140 (2011).
96. Pasquali I, Bettini R, Giordano F. Supercritical fluid technologies: An innovative approach for manipulating the solid-state of pharmaceuticals. *Adv Drug Deliv Rev.* 60(3), 399–410 (2008).
97. Tabbakhian M, Hasanzadeh F, Tavakoli N, Jamshidian Z. Dissolution enhancement of glibenclamide by solid dispersion: solvent evaporation versus a supercritical fluid-based solvent-antisolvent technique.
98. Yin X, Daintree LS, Ding S, *et al.* Itraconazole solid dispersion prepared by a supercritical fluid technique: preparation, in vitro characterization, and bioavailability in beagle dogs. *Drug Des Devel Ther.* 9, 2801–2810 (2015).
99. Liu X, Lu M, Guo Z, Huang L, Feng X, Wu C. Improving the Chemical Stability of Amorphous Solid Dispersion with Cocrystal Technique by Hot Melt Extrusion. *Pharm Res.* 29(3), 806–817 (2012).
100. Wan F, Bohr A, Maltesen MJ, *et al.* Critical Solvent Properties Affecting the Particle Formation Process and Characteristics of Celecoxib-Loaded PLGA Microparticles via Spray-Drying. *Pharm Res.* 30(4), 1065–1076 (2013).
101. Bohr A, Yang M, Baldursdóttir S, *et al.* Particle formation and characteristics of Celecoxib-loaded poly(lactic-co-glycolic acid) microparticles prepared in different solvents using electrospraying. *Polymer (Guildf).* 53(15), 3220–3229 (2012).
102. D. Craig MR. Thermal Analysis of Pharmaceuticals.
103. S. Gaisford VKPH. Principles of Thermal Analysis and Calorimetry. Royal society of chemistry.

104. Danley RL. New heat flux DSC measurement technique. *Thermochim Acta*. 395(1), 201–208 (2002).
105. Ma X, Williams RO. Characterization of amorphous solid dispersions: An update. *J Drug Deliv Sci Technol*. 50, 113–124 (2019).
106. P.K. Gallagher MEBRK. Handbook of Thermal Analysis and Calorimetry. (1998).
107. Baird JA, Taylor LS. Evaluation of amorphous solid dispersion properties using thermal analysis techniques. *Adv Drug Deliv Rev*. 64(5), 396–421 (2012).
108. Mahieu A, Willart J-F, Dudognon E, Danède F, Descamps M. A New Protocol to Determine the Solubility of Drugs into Polymer Matrixes. *Mol Pharm*. 10(2), 560–566 (2013).
109. Askin S, Zhao M, Gonçalves AD, Gaisford S, Craig DQM. The Development of Quasi-isothermal Calorimetry for the Measurement of Drug–Polymer Miscibility and Crystallization Kinetics: Olanzapine-Loaded PLGA Microparticles. *Mol Pharm*. 15(8), 3332–3342 (2018).
110. Guigo N, Sbirrazzuoli N. Chapter 10 - Thermal Analysis of Biobased Polymers and Composites. In: *Handbook of Thermal Analysis and Calorimetry*. Vyazovkin S, Koga N, Schick C (Eds.), Elsevier Science B.V., 399–429 (2018).
111. Pokharkar VB, Mandpe LP, Padamwar MN, Ambike AA, Mahadik KR, Paradkar A. Development, characterization and stabilization of amorphous form of a low Tg drug. *Powder Technol*. 167(1), 20–25 (2006).
112. Puri V, Dantuluri AK, Bansal AK. Barrier Coated Drug Layered Particles for Enhanced Performance of Amorphous Solid Dispersion Dosage Form. *J Pharm Sci*. 101(1), 342–353 (2012).
113. Dalsania S, Sharma J, Munjal B, Bansal AK. Impact of Drug-Polymer Miscibility on Enthalpy Relaxation of Irbesartan Amorphous Solid Dispersions. *Pharm Res*. 35(2), 29 (2018).
114. Kaushal AM, Bansal AK. Thermodynamic behavior of glassy state of structurally related compounds. *European Journal of Pharmaceutics and Biopharmaceutics*. 69(3), 1067–1076 (2008).
115. Blaabjerg LI, Lindenberg E, Löbmann K, Grohganz H, Rades T. Glass Forming Ability of Amorphous Drugs Investigated by Continuous Cooling and Isothermal Transformation. *Mol Pharm*. 13(9), 3318–3325 (2016).
116. Guo Y, Shalaev E, Smith S. Physical stability of pharmaceutical formulations: solid-state characterization of amorphous dispersions. *TrAC Trends in Analytical Chemistry*. 49, 137–144 (2013).
117. Descamps M, Dudognon E, Willart J-F. The Amorphous State In: *Polymorphism in the Pharmaceutical Industry*, 189–239 (2018).

118. Thakral S, Terban MW, Thakral NK, Suryanarayanan R. Recent advances in the characterization of amorphous pharmaceuticals by X-ray diffractometry. *Adv Drug Deliv Rev.* 100, 183–193 (2016).
119. Blaabjerg LI, Bulduk B, Lindenberg E, Löbmann K, Rades T, Grohganz H. Influence of Glass Forming Ability on the Physical Stability of Supersaturated Amorphous Solid Dispersions. *J Pharm Sci.* 108(8), 2561–2569 (2019).
120. Liu X, Zhou L, Zhang F. Reactive Melt Extrusion To Improve the Dissolution Performance and Physical Stability of Naproxen Amorphous Solid Dispersions. *Mol Pharm.* 14(3), 658–673 (2017).
121. Beneš M, Pekárek T, Beránek J, *et al.* Methods for the preparation of amorphous solid dispersions – A comparative study. *J Drug Deliv Sci Technol.* 38, 125–134 (2017).
122. Li N, Gilpin CJ, Taylor LS. Understanding the Impact of Water on the Miscibility and Microstructure of Amorphous Solid Dispersions: An AFM–LCR and TEM–EDX Study. *Mol Pharm.* 14(5), 1691–1705 (2017).
123. Moseson DE, Mugheirbi NA, Stewart AA, Taylor LS. Nanometer-Scale Residual Crystals in a Hot Melt Extruded Amorphous Solid Dispersion: Characterization by Transmission Electron Microscopy. *Cryst Growth Des.* 18(12), 7633–7640 (2018).
124. S'ari M, Blade H, Cosgrove S, *et al.* Characterization of Amorphous Solid Dispersions and Identification of Low Levels of Crystallinity by Transmission Electron Microscopy. *Mol Pharm.* 18(5), 1905–1919 (2021).
125. Zhao P, Hu G, Chen H, *et al.* Revealing the roles of polymers in supersaturation stabilization from the perspective of crystallization behaviors: A case of nimodipine. *Int J Pharm.* 616, 121538 (2022).
126. Liu X, Feng X, Williams RO, Zhang F. Characterization of amorphous solid dispersions. *J Pharm Investig.* 48(1), 19–41 (2018).
127. Saboo S, Taylor LS. Water-induced phase separation of miconazole-poly (vinylpyrrolidone-co-vinyl acetate) amorphous solid dispersions: Insights with confocal fluorescence microscopy. *Int J Pharm.* 529(1), 654–666 (2017).
128. de Araujo GLB, Benmore CJ, Byrn SR. Local Structure of Ion Pair Interaction in Lapatinib Amorphous Dispersions characterized by Synchrotron X-Ray diffraction and Pair Distribution Function Analysis. *Sci Rep.* 7(1), 46367 (2017).
129. Sahoo A, Kumar NSK, Suryanarayanan R. Crosslinking: An avenue to develop stable amorphous solid dispersion with high drug loading and tailored physical stability. *Journal of Controlled Release.* 311–312, 212–224 (2019).
130. Tres F, Treacher K, Booth J, *et al.* Real time Raman imaging to understand dissolution performance of amorphous solid dispersions. *Journal of Controlled Release.* 188, 53–60 (2014).

131. Fini A, Cavallari C, Ospitali F. Raman and thermal analysis of indomethacin/PVP solid dispersion enteric microparticles. *European Journal of Pharmaceutics and Biopharmaceutics*. 70(1), 409–420 (2008).
132. Kapourani A, Valkanioti V, Kontogiannopoulos KN, Barmapalexis P. Determination of the physical state of a drug in amorphous solid dispersions using artificial neural networks and ATR-FTIR spectroscopy. *Int J Pharm X*. 2, 100064 (2020).
133. Yuan X, Sperger D, Munson EJ. Investigating Miscibility and Molecular Mobility of Nifedipine-PVP Amorphous Solid Dispersions Using Solid-State NMR Spectroscopy. *Mol Pharm*. 11(1), 329–337 (2014).
134. Lu X, Huang C, Lowinger MB, *et al*. Molecular Interactions in Posaconazole Amorphous Solid Dispersions from Two-Dimensional Solid-State NMR Spectroscopy. *Mol Pharm*. 16(6), 2579–2589 (2019).
135. Yuan X, Xiang T-X, Anderson BD, Munson EJ. Hydrogen Bonding Interactions in Amorphous Indomethacin and Its Amorphous Solid Dispersions with Poly(vinylpyrrolidone) and Poly(vinylpyrrolidone-co-vinyl acetate) Studied Using ¹³C Solid-State NMR. *Mol Pharm*. 12(12), 4518–4528 (2015).
136. Nie H, Su Y, Zhang M, *et al*. Solid-State Spectroscopic Investigation of Molecular Interactions between Clofazimine and Hypromellose Phthalate in Amorphous Solid Dispersions. *Mol Pharm*. 13(11), 3964–3975 (2016).
137. Song Y, Zemlyanov D, Chen X, *et al*. Acid–Base Interactions of Polystyrene Sulfonic Acid in Amorphous Solid Dispersions Using a Combined UV/FTIR/XPS/ssNMR Study. *Mol Pharm*. 13(2), 483–492 (2016).
138. Lubach JW, Hau J. Solid-State NMR Investigation of Drug–Excipient Interactions and Phase Behavior in Indomethacin-Eudragit E Amorphous Solid Dispersions. *Pharm Res*. 35(3), 65 (2018).
139. Lipinski CA, Lombardo F, Dominy BW, Feeney PJ. Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings. *Adv Drug Deliv Rev*. 23(1), 3–25 (1997).
140. McNeil SE. Nanotechnology for the biologist. *J Leukoc Biol* [Internet]. 78(3), 585–594 (2005).
141. Wegiel LA, Mauer LJ, Edgar KJ, Taylor LS. Mid-infrared spectroscopy as a polymer selection tool for formulating amorphous solid dispersions. *Journal of Pharmacy and Pharmacology*. 66(2), 244–255 (2014).
142. Liu H, Taylor LS, Edgar KJ. The role of polymers in oral bioavailability enhancement; a review. *Polymer (Guildf)*. 77, 399–415 (2015).
143. Robles H. Vinyl Acetate. In: *Encyclopedia of Toxicology*, Elsevier, 929–931 (2014).

144. Weuts I, Kempen D, Decorte A, *et al.* Phase behaviour analysis of solid dispersions of loperamide and two structurally related compounds with the polymers PVP-K30 and PVP-VA64. *European Journal of Pharmaceutical Sciences*. 22(5), 375–385 (2004).
145. Weuts I, Kempen D, Decorte A, *et al.* Physical stability of the amorphous state of loperamide and two fragment molecules in solid dispersions with the polymers PVP-K30 and PVP-VA64. *European Journal of Pharmaceutical Sciences*. 25(2), 313–320 (2005).
146. Sarpal K, Delaney S, Zhang GGZ, Munson EJ. Phase Behavior of Amorphous Solid Dispersions of Felodipine: Homogeneity and Drug–Polymer Interactions. *Mol Pharm*. 16(12), 4836–4851 (2019).
147. Kestur US, Taylor LS. Role of polymer chemistry in influencing crystal growth rates from amorphous felodipine. *CrystEngComm*. 12(8), 2390 (2010).
148. Sun Y, Tao J, Zhang GGZ, Yu L. Solubilities of Crystalline Drugs in Polymers: An Improved Analytical Method and Comparison of Solubilities of Indomethacin and Nifedipine in PVP, PVP/VA, and PVAc. *J Pharm Sci*. 99(9), 4023–4031 (2010).
149. American Pharmacists Association. Handbook of pharmaceutical excipients. .
150. Ghosh I, Snyder J, Vippagunta R, *et al.* Comparison of HPMC based polymers performance as carriers for manufacture of solid dispersions using the melt extruder. *Int J Pharm*. 419(1), 12–19 (2011).
151. Lu X, Li M, Huang C, *et al.* Atomic-Level Drug Substance and Polymer Interaction in Posaconazole Amorphous Solid Dispersion from Solid-State NMR. *Mol Pharm*. 17(7), 2585–2598 (2020).
152. Konno H, Taylor LS. Ability of Different Polymers to Inhibit the Crystallization of Amorphous Felodipine in the Presence of Moisture. *Pharm Res*. 25(4), 969–978 (2008).
153. Xie T, Taylor LS. Improved Release of Celecoxib from High Drug Loading Amorphous Solid Dispersions Formulated with Polyacrylic Acid and Cellulose Derivatives. *Mol Pharm*. 13(3), 873–884 (2016).
154. Gui Y, McCann EC, Yao X, Li Y, Jones KJ, Yu L. Amorphous Drug–Polymer Salt with High Stability under Tropical Conditions and Fast Dissolution: The Case of Clofazimine and Poly(acrylic acid). *Mol Pharm*. 18(3), 1364–1372 (2021).
155. Kapourani A, Andriotis EG, Chachlioutaki K, *et al.* High-Drug-Loading Amorphous Solid Dispersions via In Situ Thermal Cross-Linking: Unraveling the Mechanisms of Stabilization. *Mol Pharm*. 18(12), 4393–4414 (2021).
156. Solutions P. AFFINISOL™ HPMC HME For Hot Melt Extrusion.

157. Altamimi MA, Neau SH. A study to identify the contribution of Soluplus® component homopolymers to the solubilization of nifedipine and sulfamethoxazole using the melting point depression method. *Powder Technol.* 338, 576–585 (2018).
158. Doble A. The pharmacology and mechanism of action of riluzole. *Neurology.* 47(6_suppl_4) (1996).
159. Grossman RG, Fehlings MG, Frankowski RF, *et al.* A Prospective, Multicenter, Phase I Matched-Comparison Group Trial of Safety, Pharmacokinetics, and Preliminary Efficacy of Riluzole in Patients with Traumatic Spinal Cord Injury. *J Neurotrauma.* 31(3), 239–255 (2014).
160. Bryson HM, Fulton B, Benfield P. Riluzole. *Drugs.* 52(4), 549–563 (1996).
161. Fda. RILUTEK® (riluzole) Tablets Rx only. .
162. CHMP. 7 Westferry Circus • Canary Wharf • London E14 4HB • United Kingdom Riluzole Zentiva [Internet]. Available from: www.ema.europa.eu.
163. <https://www.drugs.com/availability/generic-rilutek.html>. Accessed on 24 Dec 2023.
164. Deepika D, Sharma RP, Schuhmacher M, Kumar V. An integrative translational framework for chemical induced neurotoxicity – a systematic review. *Crit Rev Toxicol.* 50(5), 424–438 (2020).
165. Schrödinger Release 2019-4: MacroModel, Schrödinger; LLC: New York, NY, USA, 2019.
166. Schrödinger Release 2019-4: Desmond Molecular Dynamics System, D. E. Shaw Research, New York, NY, 2019. Maestro-Desmond Interoperability Tools, Schrödinger, New York, NY, 2019.
167. Terao, K. (2014). Poly(acrylic acid) (PAA). In: Kobayashi, S., Müllen, K. (eds) *Encyclopedia of Polymeric Nanomaterials*. Springer, Berlin, Heidelberg.
168. <https://coatings.specialchem.com/product/r-ashland-plasdone-s-630-copovidone>, accessed on 16th January 2023.
169. https://www.ashland.com/file_source/Ashland/Industries/Pharmaceutical/Links/PC-12624.6_AquaSolve_HPMCAS_Physical_Chemical_Properties, accessed on 16th January 2023. .
170. Schrödinger Release 2019-4: Glide, Schrödinger, LLC, New York, NY, 2019. .
171. Gaussian 09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, *et al.* Inc., Wallingford CT, 2010.
172. Stewart JJP. Application of the PM6 method to modeling the solid state. *J Mol Model.* 14(6), 499–535 (2008).
173. Hill JG. Gaussian basis sets for molecular applications. *Int J Quantum Chem.* 113(1), 21–34 (2013).

174. Vreven T, Byun KS, Komáromi I, *et al.* Combining Quantum Mechanics Methods with Molecular Mechanics Methods in ONIOM. *J Chem Theory Comput.* 2(3), 815–826 (2006).
175. Tomasi J, Mennucci B, Cancès E. The IEF version of the PCM solvation method: an overview of a new method addressed to study molecular solutes at the QM ab initio level. *Journal of Molecular Structure: THEOCHEM.* 464(1–3), 211–226 (1999).
176. Bharti K, Mittal P, Mishra B. Formulation and characterization of fast dissolving oral films containing buspirone hydrochloride nanoparticles using design of experiment. *J Drug Deliv Sci Technol.* 49, 420–432 (2019).
177. Saxena D, Maiti P. Utilization of ABS from plastic waste through single-step reactive extrusion of LDPE/ABS blends of improved properties. *Polymer (Guildf).* 221, 123626 (2021).
178. Vikas, Viswanadh MK, Mehata AK, *et al.* Bioadhesive chitosan nanoparticles: Dual targeting and pharmacokinetic aspects for advanced lung cancer treatment. *Carbohydr Polym.* 274, 118617 (2021).
179. Lapuk SE, Zubaidullina LS, Ziganshin MA, Mukhametzyanov TA, Schick C, Gerasimov AV. Kinetic stability of amorphous solid dispersions with high content of the drug: A fast scanning calorimetry investigation. *Int J Pharm.* 562, 113–123 (2019).
180. CHIENG N, AALTONEN J, SAVILLE D, RADES T. Physical characterization and stability of amorphous indomethacin and ranitidine hydrochloride binary systems prepared by mechanical activation. *European Journal of Pharmaceutics and Biopharmaceutics.* 71(1), 47–54 (2009).
181. Wang B, Wang D, Zhao S, *et al.* Evaluate the ability of PVP to inhibit crystallization of amorphous solid dispersions by density functional theory and experimental verify. *European Journal of Pharmaceutical Sciences.* 96, 45–52 (2017).
182. Walden DM, Bunday Y, Jagarapu A, Antontsev V, Chakravarty K, Varshney J. Molecular Simulation and Statistical Learning Methods toward Predicting Drug–Polymer Amorphous Solid Dispersion Miscibility, Stability, and Formulation Design. *Molecules.* 26(1), 182 (2021).
183. Yang G, Park S-J. Deformation of Single Crystals, Polycrystalline Materials, and Thin Films: A Review. *Materials.* 12(12), 2003 (2019).
184. Kissi EO, Kasten G, Löbmann K, Rades T, Grohganz H. The Role of Glass Transition Temperatures in Coamorphous Drug–Amino Acid Formulations. *Mol Pharm.* 15(9), 4247–4256 (2018).
185. Forster A, Hempenstall J, Tucker I, Rades T. Selection of excipients for melt extrusion with two poorly water-soluble drugs by solubility parameter calculation and thermal analysis. *Int J Pharm.* 226(1–2), 147–161 (2001).

186. Chan C-K, Chu I-M. Effect of hydrogen bonding on the glass transition behavior of poly(acrylic acid)/silica hybrid materials prepared by sol–gel process. *Polymer (Guildf)*. 42(14), 6089–6093 (2001).
187. Al-Obaidi H, Buckton G. Evaluation of Griseofulvin Binary and Ternary Solid Dispersions with HPMCAS. *AAPS PharmSciTech*. 10(4), 1172 (2009).
188. Mistry P, Mohapatra S, Gopinath T, Vogt FG, Suryanarayanan R. Role of the Strength of Drug–Polymer Interactions on the Molecular Mobility and Crystallization Inhibition in Ketoconazole Solid Dispersions. *Mol Pharm*. 12(9), 3339–3350 (2015).
189. Pugliese A, Toresco M, McNamara D, *et al.* Drug–Polymer Interactions in Acetaminophen/Hydroxypropylmethylcellulose Acetyl Succinate Amorphous Solid Dispersions Revealed by Multidimensional Multinuclear Solid-State NMR Spectroscopy. *Mol Pharm*. 18(9), 3519–3531 (2021).
190. Miyoshi T, Takegoshi K, Hikichi K. High-resolution solid state ¹³C n.m.r. study of the interpolymer interaction, morphology and chain dynamics of the poly(acrylic acid)/poly(ethylene oxide) complex. *Polymer (Guildf)*. 38(10), 2315–2320 (1997).
191. Mahamid J, Sharir A, Addadi L, Weiner S. Amorphous calcium phosphate is a major component of the forming fin bones of zebrafish: Indications for an amorphous precursor phase. *Proceedings of the National Academy of Sciences*. 105(35), 12748–12753 (2008).
192. Mondal PK, T A, Rao V, Chopra D. Crystal structure analysis of the biologically active drug molecule riluzole and riluzolium chloride. *Acta Crystallogr E Crystallogr Commun*. 75(8), 1084–1089 (2019).
193. Potter CB, Davis MT, Albadarin AB, Walker GM. Investigation of the Dependence of the Flory–Huggins Interaction Parameter on Temperature and Composition in a Drug–Polymer System. *Mol Pharm*. 15(11), 5327–5335 (2018).
194. Meng F, Dave V, Chauhan H. Qualitative and quantitative methods to determine miscibility in amorphous drug–polymer systems. *European Journal of Pharmaceutical Sciences*. 77, 106–111 (2015).
195. Baghel S, Cathcart H, O’Reilly NJ. Theoretical and experimental investigation of drug-polymer interaction and miscibility and its impact on drug supersaturation in aqueous medium. *European Journal of Pharmaceutics and Biopharmaceutics*. 107, 16–31 (2016).
196. Rim PB, Runt JP. Melting point depression in crystalline/compatible polymer blends. *Macromolecules*. 17(8), 1520–1526 (1984).
197. Newman A, Zografi G. Commentary: Considerations in the Measurement of Glass Transition Temperatures of Pharmaceutical Amorphous Solids. *AAPS PharmSciTech*. 21(1), 26 (2020).

198. Puri V, Dantuluri AK, Kumar M, Karar N, Bansal AK. Wettability and surface chemistry of crystalline and amorphous forms of a poorly water soluble drug. *European Journal of Pharmaceutical Sciences*. 40(2), 84–93 (2010).
199. Hörter D, Dressman JB. Influence of physicochemical properties on dissolution of drugs in the gastrointestinal tract IPII of original article: S0169-409X(96)00487-5. The article was originally published in *Advanced Drug Delivery Reviews* 25 (1997) 3–14.1. *Adv Drug Deliv Rev*. 46(1–3), 75–87 (2001).
200. Sander JRG, Bučar D, Henry RF, Zhang GGZ, MacGillivray LR. Pharmaceutical Nano-Cocrystals: Sonochemical Synthesis by Solvent Selection and Use of a Surfactant. *Angewandte Chemie International Edition*. 49(40), 7284–7288 (2010).
201. Varghese S, Ghoroi C. Improving the wetting and dissolution of ibuprofen using solventless co-milling. *Int J Pharm*. 533(1), 145–155 (2017).
202. Song K, Lee J, Choi S-O, Kim J. Interaction of Surface Energy Components between Solid and Liquid on Wettability, and Its Application to Textile Anti-Wetting Finish. *Polymers (Basel)*. 11(3), 498 (2019).
203. Costa P, Sousa Lobo JM. Modeling and comparison of dissolution profiles. *European Journal of Pharmaceutical Sciences*. 13(2), 123–133 (2001).
204. Berry MR, Likar MD. Statistical assessment of dissolution and drug release profile similarity using a model-dependent approach. *J Pharm Biomed Anal*. 45(2), 194–200 (2007).
205. Kozbial A, Li Z, Conaway C, *et al.* Study on the Surface Energy of Graphene by Contact Angle Measurements. *Langmuir*. 30(28), 8598–8606 (2014).
206. Owens DK, Wendt RC. Estimation of the surface free energy of polymers. *J Appl Polym Sci*. 13(8), 1741–1747 (1969).
207. Yang B, Wei C, Qian F, Li S. Surface Wettability Modulated by Surfactant and Its Effects on the Drug Release and Absorption of Fenofibrate Solid Dispersions. *AAPS PharmSciTech*. 20(6), 234 (2019).
208. Kaelble DH. Dispersion-Polar Surface Tension Properties of Organic Solids. *J Adhes*. 2(2), 66–81 (1970).
209. Jasani MS, Kale DP, Singh IP, Bansal AK. Influence of Drug–Polymer Interactions on Dissolution of Thermodynamically Highly Unstable Cocrystal. *Mol Pharm*. 16(1), 151–164 (2019).
210. Baghel S, Cathcart H, O’Reilly NJ. Understanding the generation and maintenance of supersaturation during the dissolution of amorphous solid dispersions using modulated DSC and ¹H NMR. *Int J Pharm*. 536(1), 414–425 (2018).

211. Ueda K, Higashi K, Moribe K. Unusual Correlation between the Apparent Amorphous Solubility of a Drug and Solubilizer Concentration Revealed by NMR Analysis. *Mol Pharm.* 19(9), 3336–3349 (2022).
212. Abraham RJ, Mobli M. An NMR, IR and theoretical investigation of ^1H Chemical Shifts and hydrogen bonding in phenols. *Magnetic Resonance in Chemistry.* 45(10), 865–877 (2007).
213. Ahuja N, Katare OP, Singh B. Studies on dissolution enhancement and mathematical modeling of drug release of a poorly water-soluble drug using water-soluble carriers. *European Journal of Pharmaceutics and Biopharmaceutics.* 65(1), 26–38 (2007).
214. Abu-Diak OA, Jones DS, Andrews GP. An Investigation into the Dissolution Properties of Celecoxib Melt Extrudates: Understanding the Role of Polymer Type and Concentration in Stabilizing Supersaturated Drug Concentrations. *Mol Pharm.* 8(4), 1362–1371 (2011).
215. Saboo S, Mugheirbi NA, Zemlyanov DY, Kestur US, Taylor LS. Congruent release of drug and polymer: A “sweet spot” in the dissolution of amorphous solid dispersions. *Journal of Controlled Release.* 298, 68–82 (2019).
216. Bharti K, Deepika D, Kumar M, *et al.* Development and Evaluation of Amorphous Solid Dispersion of Riluzole with PBPK Model to Simulate the Pharmacokinetic Profile. *AAPS PharmSciTech.* 24(8), 219 (2023).
217. Kumar D, Thipparaboina R, Modi SR, Bansal AK, Shastri NR. Effect of surfactant concentration on nifedipine crystal habit and its related pharmaceutical properties. *J Cryst Growth.* 422, 44–51 (2015).
218. Li J, Fan N, Wang X, *et al.* Interfacial interaction track of amorphous solid dispersions established by water-soluble polymer and indometacin. *European Journal of Pharmaceutical Sciences.* 106, 244–253 (2017).
219. Mercury2022_3_UserGuide.
220. Abouhakim H, Nilsson Lill SO, Quayle MJ, Norberg ST, Hassanpour A, Pask CM. The crystal structure, morphology and mechanical properties of diaquabis(omeprazole)magnesium dihydrate. *Acta Crystallogr B Struct Sci Cryst Eng Mater.* 76(2), 275–284 (2020).
221. Chen H, Yang W, Chen H, *et al.* Surface modification of Mitoxantrone-loaded PLGA nanospheres with chitosan. *Colloids Surf B Biointerfaces.* 73(2), 212–218 (2009).
222. X_ray_Photoelectron_Spectroscopy.
223. Yang Y, Si Z, Cai D, *et al.* High-hydrophobic CF₃ groups within PTFPMS membrane for enhancing the furfural pervaporation performance. *Sep Purif Technol.* 235, 116144 (2020).

-
224. Jeffries B, Wang Z, Graton J, *et al.* Reducing the Lipophilicity of Perfluoroalkyl Groups by $\text{CF}_2-\text{F}/\text{CF}_2-\text{Me}$ or CF_3/CH_3 Exchange. *J Med Chem.* 61(23), 10602–10618 (2018).
225. Robalo JR, Huhmann S, Kokschi B, Vila Verde A. The Multiple Origins of the Hydrophobicity of Fluorinated Apolar Amino Acids. *Chem.* 3(5), 881–897 (2017).
226. Muller N. When Is a Trifluoromethyl Group More Lipophilic than a Methyl Group? Partition Coefficients and Selected Chemical Shifts of Aliphatic Alcohols and Trifluoroalcohols. *J Pharm Sci.* 75(10), 987–991 (1986).
227. Bharti K, Dubey G, Kumar M, *et al.* A multifaceted approach for grading of polymers for the development of stable amorphous solid dispersion of Riluzole. *J Drug Deliv Sci Technol.*, 105158 (2023).
228. Speed DE. Environmental aspects of planarization processes. In: *Advances in Chemical Mechanical Planarization (CMP)*, Elsevier, 257–320 (2022).
229. Gupta P, Bansal AK, Thilagavathi R, Chakraborti AK. Differential molecular interactions between the crystalline and the amorphous phases of celecoxib. *Journal of Pharmacy and Pharmacology.* 57(10), 1271–1278 (2010).
230. Gupta P, Chawla G, Bansal AK. Physical Stability and Solubility Advantage from Amorphous Celecoxib: The Role of Thermodynamic Quantities and Molecular Mobility. *Mol Pharm.* 1(6), 406–413 (2004).
231. Dash RP, Babu RJ, Srinivas NR. Two Decades-Long Journey from Riluzole to Edaravone: Revisiting the Clinical Pharmacokinetics of the Only Two Amyotrophic Lateral Sclerosis Therapeutics. *Clin Pharmacokinet.* 57(11), 1385–1398 (2018).
232. Lacomblez L, Bensimon G, Leigh P, *et al.* Long-term safety of riluzole in amyotrophic lateral sclerosis. *Amyotrophic Lateral Sclerosis and Other Motor Neuron Disorders.* 3(1), 23–29 (2002).
233. Dharmadasa T, Kiernan MC. Riluzole, disease stage and survival in ALS. *Lancet Neurol.* 17(5), 385–386 (2018).
234. Bensimon G, Doble A. The tolerability of riluzole in the treatment of patients with amyotrophic lateral sclerosis. *Expert Opin Drug Saf.* 3(6), 525–534 (2004).
235. Brouwers J, Brewster ME, Augustijns P. Supersaturating Drug Delivery Systems: The Answer to Solubility-Limited Oral Bioavailability? *J Pharm Sci.* 98(8), 2549–2572 (2009).
236. Tsai Y-M, Chien C-F, Lin L-C, Tsai T-H. Curcumin and its nano-formulation: The kinetics of tissue distribution and blood–brain barrier penetration. *Int J Pharm.* 416(1), 331–338 (2011).
-

237. Ravi PR, Vats R, and Reddy K.U. Validation of a Simple, Rapid and Sensitive LC Method for Quantification of Riluzole in Rat Plasma and its Pharmacokinetic Application. *J Bioanal Biomed.* s6 (2012).
238. Rohatgi A. WebPlotDigitizer (Version 3.9) [Computer software]. 2015. Available from: <https://automeris.io/WebPlotDigitizer>.
239. Liboux A Le, Lefebvre P, Roux Y Le, *et al.* Single- and Multiple-Dose Pharmacokinetics of Riluzole in White Subjects. *The Journal of Clinical Pharmacology.* 37(9), 820–827 (1997).
240. Chandu BR, Nama S, Kanala K, Challa BR, Shaik RP, Khagga M. Quantitative estimation of riluzole in human plasma by LC-ESI-MS/MS and its application to a bioequivalence study. *Anal Bioanal Chem.* 398(3), 1367–1374 (2010).
241. Longo DM, Shoda LKM, Howell BA, Coric V, Berman RM, Qureshi IA. Assessing Effects of BHV-0223 40 mg Zydis Sublingual Formulation and Riluzole 50 mg Oral Tablet on Liver Function Test Parameters Utilizing DILIsym. *Toxicological Sciences.* 175(2), 292–300 (2020).
242. Rodgers T, Rowland M. Physiologically based pharmacokinetic modelling 2: Predicting the tissue distribution of acids, very weak bases, neutrals and zwitterions. *J Pharm Sci.* 95(6), 1238–1257 (2006).
243. Utsey K, Gastonguay MS, Russell S, Freling R, Riggs MM, Elmokadem A. Quantification of the Impact of Partition Coefficient Prediction Methods on Physiologically Based Pharmacokinetic Model Output Using a Standardized Tissue Composition. *Drug Metabolism and Disposition.* 48(10), 903–916 (2020).
244. Wishart DS. DrugBank: a comprehensive resource for in silico drug discovery and exploration. *Nucleic Acids Res.* 34(90001), D668–D672 (2006).
245. Hu Z, Lu J, Zhao Y. A physiologically based pharmacokinetic model of alvespimycin in mice and extrapolation to rats and humans. *Br J Pharmacol.* 171(11), 2778–2789 (2014).
246. Campbell JL, Andersen ME, Hinderliter PM, *et al.* PBPK Model for Atrazine and Its Chlorotriazine Metabolites in Rat and Human. *Toxicological Sciences.* 150(2), 441–453 (2016).
247. Stevens AJ, Campbell JL, Travis KZ, *et al.* Paraquat pharmacokinetics in primates and extrapolation to humans. *Toxicol Appl Pharmacol.* 417, 115463 (2021).
248. Brown RP, Delp MD, Lindstedt SL, Rhomberg LR, Beliles RP. Physiological Parameter Values for Physiologically Based Pharmacokinetic Models. *Toxicol Ind Health.* 13(4), 407–484 (1997).
249. Emond C, Raymer JH, Studabaker WB, Garner CE, Birnbaum LS. A physiologically based pharmacokinetic model for developmental exposure to BDE-47 in rats. *Toxicol Appl Pharmacol.* 242(3), 290–298 (2010).

-
250. Sharma RP, Kumar V, Schuhmacher M, Kolodkin A, Westerhoff H V. Development and evaluation of a harmonized whole body physiologically based pharmacokinetic (PBPK) model for flutamide in rats and its extrapolation to humans. *Environ Res.* 182, 108948 (2020).
 251. Loccisano AE, Campbell JL, Andersen ME, Clewell HJ. Evaluation and prediction of pharmacokinetics of PFOA and PFOS in the monkey and human using a PBPK model. *Regulatory Toxicology and Pharmacology.* 59(1), 157–175 (2011).
 252. Shah DK, Betts AM. Towards a platform PBPK model to characterize the plasma and tissue disposition of monoclonal antibodies in preclinical species and human. *J Pharmacokinet Pharmacodyn.* 39(1), 67–86 (2012).
 253. Davies B, Morris T. Physiological Parameters in Laboratory Animals and Humans. *Pharm Res.* 10(7), 1093–1095 (1993).
 254. Milane A, Tortolano L, Fernandez C, Bensimon G, Meininger V, Farinotti R. Brain and Plasma Riluzole Pharmacokinetics: Effect of Minocycline Combination. *Journal of Pharmacy & Pharmaceutical Sciences.* 12(2), 209 (2009).
 255. U. S. Environmental Protection Agency, 2006.
 256. Deepika D, Kumar V. The Role of “Physiologically Based Pharmacokinetic Model (PBPK)” New Approach Methodology (NAM) in Pharmaceuticals and Environmental Chemical Risk Assessment. *Int J Environ Res Public Health.* 20(4), 3473 (2023).
 257. Ganeshpurkar A, Singh R, Tripathi P, *et al.* Effect of sulfonamide derivatives of *phenylglycine* on scopolamine-induced amnesia in rats. *Ibrain.* 9(1), 13–31 (2023).
 258. Bithu BS, Reddy NR, Prasad SK, Sairam K, Hemalatha S. *Prosopis cineraria* : A potential nootropic agent. *Pharm Biol.* 50(10), 1241–1247 (2012).
 259. Patel RJ, Patel AA, Patel HP. Stabilized amorphous state of riluzole by immersion-rotavapor method with synthesized mesoporous SBA-15 carrier to augment in-vitro dissolution. *J Drug Deliv Sci Technol.* 61, 102270 (2021).
 260. Marsac PJ, Rumondor ACF, Nivens DE, Kestur US, Stanciu L, Taylor LS. Effect of temperature and moisture on the miscibility of amorphous dispersions of felodipine and poly(vinyl pyrrolidone). *J Pharm Sci.* 99(1), 169–185 (2010).
 261. Narasimham L, Barhate VD. Physico-chemical characterization of some beta blockers and anti-diabetic drugs - potentiometric and spectrophotometric pKa determination in different co-solvents. *European Journal of Chemistry.* 2(1), 36–46 (2011).
 262. Fehlings MG, Wilson JR, Frankowski RF, *et al.* Riluzole for the treatment of acute traumatic spinal cord injury: rationale for and design of the NACTN Phase I clinical trial. *J Neurosurg Spine.* 17(Suppl1), 151–156 (2012).
-

263. Mah PT, Peltonen L, Novakovic D, Rades T, Strachan CJ, Laaksonen T. The effect of surfactants on the dissolution behavior of amorphous formulations. *European Journal of Pharmaceutics and Biopharmaceutics*. 103, 13–22 (2016).
264. Correa-Soto CE, Gao Y, Indulkar AS, Zhang GGZ, Taylor LS. Role of surfactants in improving release from higher drug loading amorphous solid dispersions. *Int J Pharm*. 625, 122120 (2022).
265. Indulkar AS, Lou X, Zhang GGZ, Taylor LS. Insights into the Dissolution Mechanism of Ritonavir–Copovidone Amorphous Solid Dispersions: Importance of Congruent Release for Enhanced Performance. *Mol Pharm*. 16(3), 1327–1339 (2019).
266. Yang R, Zhang GGZ, Zemlyanov DY, Purohit HS, Taylor LS. Release Mechanisms of Amorphous Solid Dispersions: Role of Drug-Polymer Phase Separation and Morphology. *J Pharm Sci*. 112(1), 304–317 (2023).
267. Remy A-J, Camu W, Ramos J, Blanc P, Larrey D. Acute hepatitis after riluzole administration. *J Hepatol*. 30(3), 527–530 (1999).

List of Publications

Publications from the research work

1. K. Bharti, G. Dubey, M. Kumar, A. Jha, M. Upadhyay, P. S. Mali, A. Kumar, P.V. Bharatam, and B. Mishra. "A multifaceted approach for grading of polymers for the development of stable amorphous solid dispersion of Riluzole." *Journal of Drug Delivery Science and Technology* 90 (2023): 105158. doi: 10.1016/j.jddst.2023.105158
2. K. Bharti, D. Deepika, M. Kumar, A. Jha, M. Manjit, Akhilesh, V. Tiwari, V. Kumar, and B. Mishra. "Development and Evaluation of Amorphous Solid Dispersion of Riluzole with PBPK Model to Simulate the Pharmacokinetic Profile." *AAPS PharmSciTech* 24, no. 8 (2023): 219. doi: 10.1208/s12249-023-02680-y
3. K. Bharti, A. Jha, M. Kumar, M. Manjit, A.P. Satpute. "Impact of Surface Properties on the Supersaturation of Drug in Dissolution Media: A case study of Riluzole" (Under preparation)
4. K. Bharti, C. Sahu, and B. Mishra. "Evaluation of functionality of two cyclodextrin polymers for the preparation of inclusion complex of quercetin based on its wetting properties" (Under preparation)

Other publications

- 1 M. Kumar, A. Jha , K. Bharti, P. Kumbhar, V. Dhapte-Pawar, and B. Mishra. "Lipid-coated Nanocrystals of Paclitaxel as Dry Powder for Inhalation: Characterization, In-Vitro Performance, and Pharmacokinetic Assessment." *Colloids and Surfaces B: Biointerfaces*, (2024) p.113865. doi: 10.1016/j.colsurfb.2024.113865
- 2 M. Manjit, M. Kumar, K. Kumar, D.R. Madhukiran , A. Jha, K. Bharti, Z. Rain, P. Prakash, and B. Mishra. "Fabrication of dual drug-loaded polycaprolactone–gelatin composite nanofibers for full thickness diabetic wound healing." *Therapeutic Delivery* 0 (2023): 5-21. doi: 10.4155/tde-2023-0083
- 3 M. Manjit, K. Kumar, M. Kumara, A. Jha, K. Bharti, P. Tiwari, R. Tilak, V. Singh, B. Koch, and B. Mishra "Fabrication of gelatin coated polycaprolactone nanofiber scaffolds co-loaded with luliconazole and naringenin for treatment of Candida infected diabetic wounds." *Int. J. Bio. Macromol.* (2024) p. 129621 doi: 10.1016/j.ijbiomac.2024.129621
- 4 M. Manjit, M. Kumar, A. Jha, K. Bharti, K. Kumar, P. Tiwari, R. Tilak, V. Singh, B. Koch, and B. Mishra. "Formulation and characterization of polyvinyl alcohol/chitosan composite nanofiber co-loaded with silver nanoparticle & luliconazole encapsulated poly lactic-co-glycolic acid nanoparticle for treatment of diabetic foot ulcer." *Int. J. Bio. Macromol.* (2024): p. 128978 doi: 10.1016/j.ijbiomac.2023.128978
- 5 M.i Upadhyay, R.V. Hosur, A. Jha, K. Bharti, P.S. Mali, A.K Jha, B. Mishra and A. Kumar "Myricetin encapsulated chitosan nanoformulation for management of type 2 diabetes: Preparation, optimization, characterization and in vivo activity." *Biomater. Adv.* (2023), 153. doi: 10.1016/j.bioadv.2023.213542

- 6 P. Kesharwani, D. Deepika, K. Bharti, A. Jain, S. Sharma, B. Mishra, and V. Kumar, "Pharmacotherapeutic and Computational Approaches for Biopharmaceutical Considerations towards Drug Development and Delivery against COVID-19", *Lett. Appl. NanoBioScience*. (2023), 12 (4), 128 doi: 10.33263/LIANBS124.128
- 7 M. Kumar, A. Jha, K. Bharti, G. Parmar and B. Mishra "Advances in lipid-based pulmonary nanomedicine for the management of inflammatory lung disorders". *Nanomedicine*. 2022, 17, 913-934 doi: 10.2217/nmm-2021-0389
- 8 M. Das, M. Kumar, A. Jha, Madhukiran DR, K. Bharti, S. Mondal, and B. Mishra "A Review on Screening Models for Potential Therapeutic Candidates and Targets Against SARS-CoV-2." *J Pharmacol Tox Met*. 2021, 22, 1-23 doi: 10.2174/1389450121666201228122845
- 9 K. Sarkar, M. Kumar, A. Jha, K. Bharti, M. Das, and B. Mishra "Nanocarriers for tuberculosis therapy: Design of safe and effective drug delivery strategies to overcome the therapeutic challenges". *J. Drug Deliv. Sci. Technol.* (2021): 102850 doi: 10.1016/j.jddst.2021.102850
- 10 N. Komanna, K. Bharti, D.B. Surekha, S. Thokala, and B. Mishra. "Formulation, Characterization and Optimization of Self Emulsifying Drug Delivery System of Losartan Potassium." *J. Drug Deliv. Sci. Technol.* 2020, 60, 102026 doi: 10.1016/j.jddst.2020.102026
- 11 K. Bharti, P. Mittal, and B. Mishra. "Formulation and Characterization of Fast Dissolving Oral Films containing Buspirone Hydrochloride Nanoparticles using Design of Experiment." *J. Drug Deliv. Sci. Technol.* (2018), 49, 420-432 doi: 10.1016/j.jddst.2018.12.013

Book Chapters

1. K. Bharti, and B. Mishra, "Biopharmaceutical and Pharmacokinetic Considerations". *Controlled and Novel Drug Delivery*. CBS Publishers and Distributors, (2023), 1-33.
2. K. Bharti, A. Jha, M. Kumar, and B. Mishra "Functionalization of natural gums: A scientific tools to improve their properties and applications". *Natural Gums: Extraction, Properties, And Applications*, Elsevier. doi: 10.1016/B978-0-323-99468-2.00003-6
3. K. Bharti, and B. Mishra. "pH-Responsive Biomaterials in Drug Delivery." *Functional Biomaterials: Drug Delivery and Biomedical Applications*. Singapore: Springer Singapore, (2022), 37-74. doi: 10.1007/978-981-16-7152-4_2
4. K. Bharti, M. Kumar, A. Jha and, B. Mishra. "Nanobubbles to aid drug delivery." *Systems of Nanovesicular Drug Delivery*. Academic Press, 2022. 323-336. doi: 10.1016/B978-0-323-91864-0.00019-X
5. M. Kumar, A. Jha, K. Bharti, and B. Mishra, "Nanovesicles for hepatic-targeted drug delivery", *Applications of Nanovesicular Drug Delivery*, (2022), 201-217. doi: 10.1016/B978-0-323-91865-7.00015-8
6. A. Jha, M. Kumar, K. Bharti, and B. Mishra. "Glycosomes: a new tool for effective drug delivery." *Systems of Nanovesicular Drug Delivery*. Academic Press, (2022). 277-291. doi: 10.1016/B978-0-323-91864-0.00010-3

7. A. Jha, M. Kumar, K. Bharti, M. Manjit, and B. Mishra. "Biopolymer-based tumor microenvironment-responsive nanomedicine for targeted cancer therapy." *Nanomedicine 0* (2024). doi: 10.2217/nnm-2023-0302

8 M. Kumar, A. Jha, K. Bharti, M. Manjit, and B. Mishra. "Polysaccharide-based antimicrobial hydrogels as wound dressing materials." *Polysaccharides-Based Hydrogels* (2024), 405-428. doi: 10.1016/B978-0-323-99341-8.00010-7