

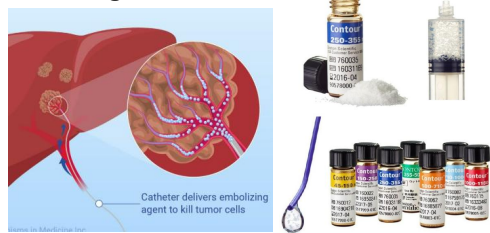
Controlled Release of Gemcitabine with Partially Molecular Imprinted Microspheres for Cancer Therapy

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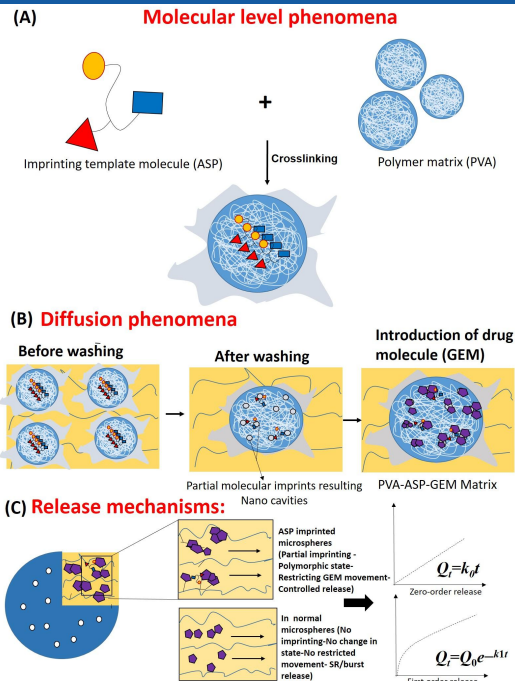
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BACKGROUND

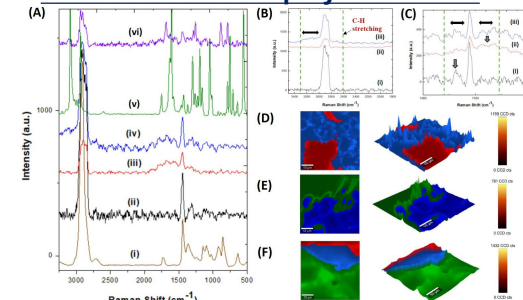
- Used for localized drug delivery and tumor embolization
- Block tumor blood supply, leading to shrinkage or cell death



PROPOSED MECHANISM

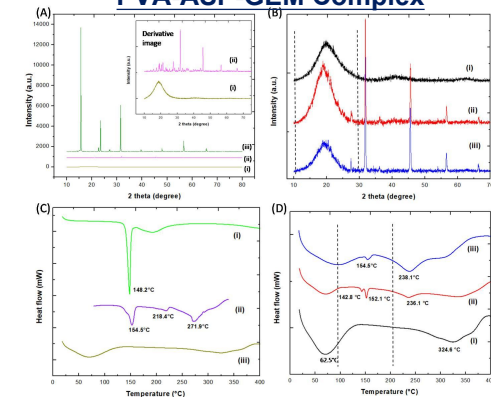


(1) Correlating Structural and Chemical Information of PMI polymer blends



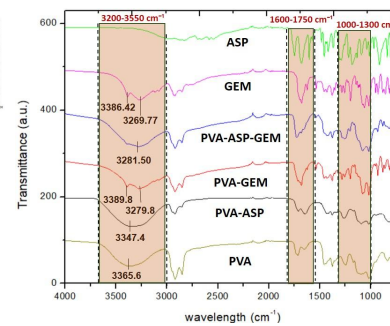
C-H stretch shift and CH₂ bend confirm PVA-ASP-GEM interactions and altered crystallinity.

(2) Structural & Thermal Modifications in PVA-ASP-GEM Complex

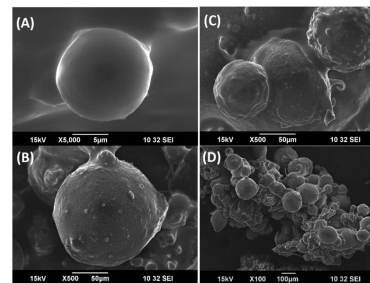


XRD shows reduced amorphous nature and GEM peaks (27–75°); ASP peaks absent after washing. Peak shifts indicate polymorphic transitions. DSC: new peak at 154.5 °C and broad peak at 238.1 °C confirm enhanced thermal stability. Results align with TGA

(3) Polymorphic Transitions & Molecular Interactions



(4) Morphological Differences in Microspheres



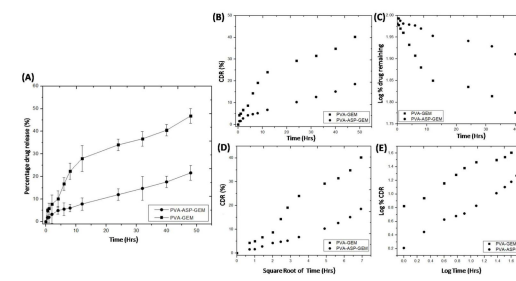
(A&C) PVA microspheres: smooth, uniform, single-phase. (B&D) PVA-ASP-GEM: rough, porous, aggregated, confirming ASP-GEM imprinting and complexation

(5) Controlled Drug Release in PMI-Based Microspheres

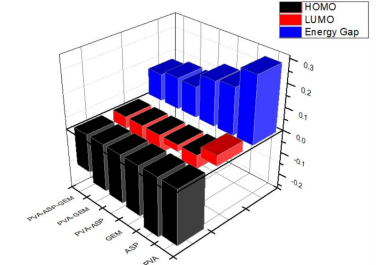
PMI microspheres: superior. PVA-ASP-GEM: zero-order, 21.6% GEM in 48 h. PVA-GEM: faster, 46.85% with burst release

RESULTS

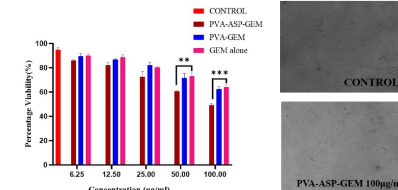
Zero-order release kinetics



PVA-ASP-GEM had a lower energy gap, indicating enhanced stability



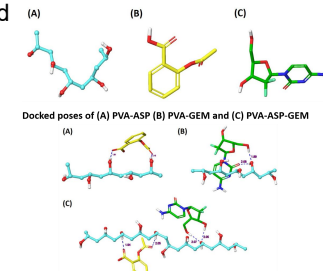
(6) In-vitro Cytotoxicity Assay



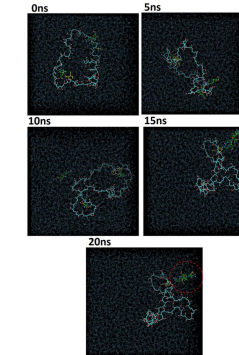
PVA-ASP-GEM microspheres significantly enhanced gemcitabine's efficacy against cancer cells compared to non-imprinted formulation

(7) Theoretical and quantum insights using computational study

Geometry-optimized structures of (A) PVA, (B) ASP, and (C) GEM using DFT method



Molecular dynamics (MD)



Hydrogen bonding between ASP and GEM forms stable complexes, delaying GEM release via stable cavities

CONCLUSION

This study shows that aspirin (ASP)-based partial molecular imprinting (PMI) in PVA microspheres stabilizes gemcitabine (GEM), enabling controlled release through chemical and structural modifications, supported by experimental and computational evidence

Thrivikraman Sreejith, Vr V, Kamalasanan K, Thankappan Presanna A. Quantum Insights into Partially Molecular Imprinted Microspheres for Anticancer Therapeutics: Experimental and Theoretical Studies. **ACS Biomater Sci Eng.** 2024 Nov 11;10(11):7005-7017.