

Furthermore, assessing the economic viability of the GPU-based approach, including long-term operational costs and energy efficiency, could ensure its sustainability. Standardising protocols for simulation workflows would help maintain consistency and reproducibility, which are critical for scientific and industrial adoption. Finally, fostering multidisciplinary collaboration with experts in pharmacology, bioinformatics, and hardware engineering could enhance the methodology's robustness and broaden its applicability. By addressing these areas, this CUDA-based approach could further solidify its role as a transformative tool in *in silico* drug discovery, reducing reliance on animal testing and accelerating the pace of research.

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