# The emergence of the multi-target cell membrane chromatography intelligent screening workstation as an internationally original achievement

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The Multi-Target Cell Membrane Chromatography Intelligent Screening Workstation (MCMC-ISW) represents an innovative "many-to-many" bionic 2D chromatographic system, which ingeniously integrates "multi-target synchronous recognition" with "intelligent screening" (Figure 1A). In its first dimension, the instrument employs multi-target cell membrane chromatography models to isolate active constituents from complex Traditional Chinese Medicine (TCM) preparations via specific receptor-ligand interactions. Subsequently, the second dimension, seamlessly coupled through column-switching technology with reversed-phase high-performance liquid chromatography (RP-HPLC), facilitates the online separation and identification of these active compounds. A dedicated database and intelligent analysis system then perform real-time integration and interpretation of the two-dimensional data, thereby elucidating the material basis of TCM efficacy and its underlying "multi-target, multi-pathway" mechanisms of action (Figure 1B). Furthermore, through its fully autonomous, integrated design, the MCMC-ISW has overcome critical technical challenges, including parallel multi-target

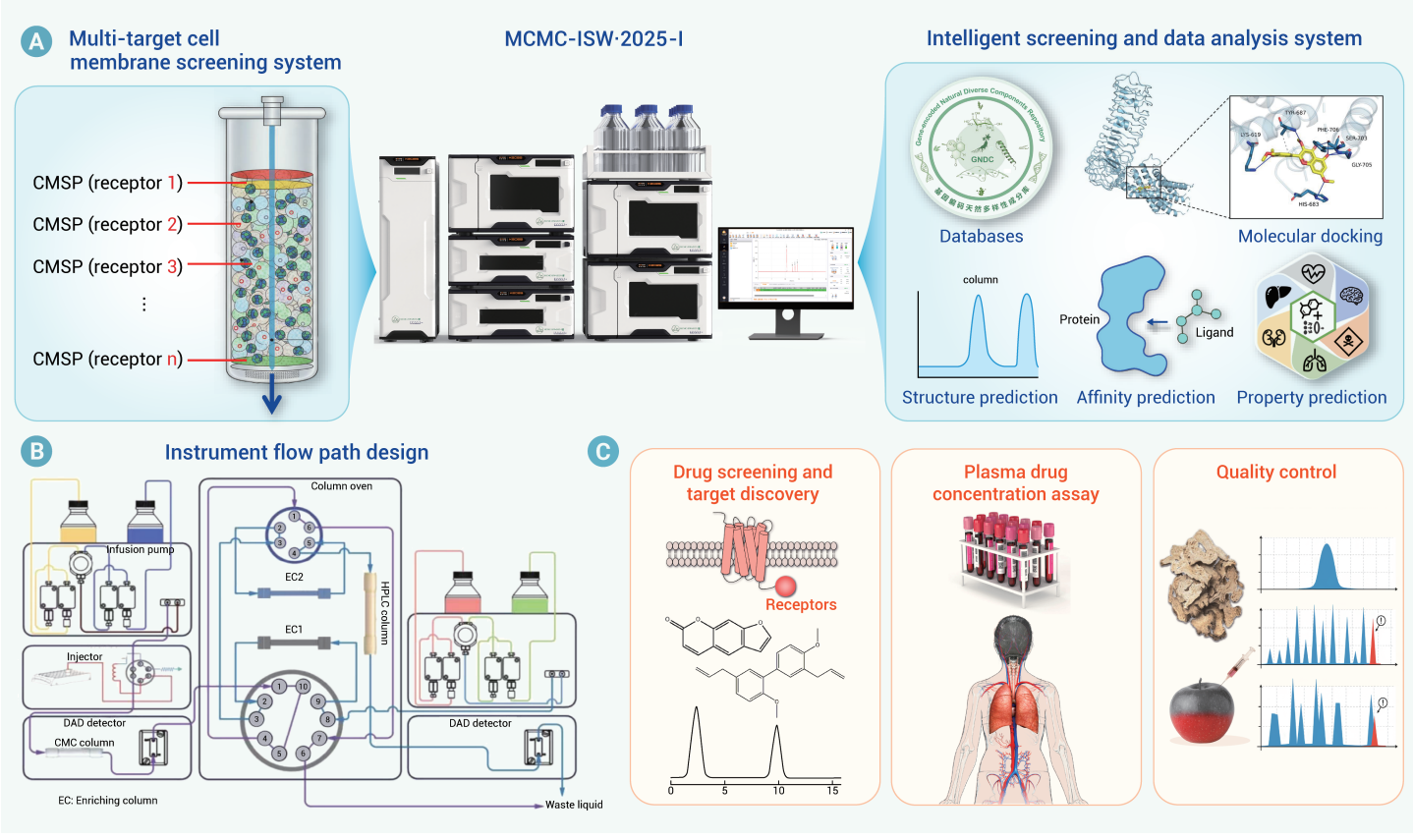


**Figure 1. Core systems and applications of the MCMC-ISW** (A) The two primary functional modules. (B) Fluidic path design of the system. (C) Diverse application scenarios.

screening and intelligent data deconvolution, thereby breaking through the technical bottlenecks associated with the efficient immobilization of bionic membranes and high-throughput screening.

Collectively, this instrument provides a pioneering "Chinese Solution" for deciphering the traditional "black box" of TCM, ultimately paving the way for a new, intelligent era in complex system research. It is poised to serve as a robust and sophisticated technological platform that will profoundly advance TCM modernization, innovative drug discovery, and quality control.

On October 16, 2025, the Sichuan Association for Science and Technology Enterprise Innovation Service Center convened an expert panel to evaluate the scientific and technological achievements of the "MCMC-ISW" project. This groundbreaking instrument was jointly developed by Chengdu University of Traditional Chinese Medicine, Xi'an Jiaotong University, and Hanon Advanced Technology Group Co., Ltd.

Presided over by Academician Liu Liang, the appraisal proceedings involved a meticulous review of the technical documentation, a comprehen-

sive presentation from the project team, and a live demonstration of the instrument. Following thorough deliberations, the expert panel unanimously affirmed that the MCMC-ISW is an internationally original innovation that fills a critical global void in its field. The panel further concluded that the instrument exhibits advanced and reliable overall performance, coupled with user-friendly operation, thereby representing a landmark scientific and technological achievement of major significance.

The instrument features two major innovations. Firstly, it establishes a novel, integrated research paradigm for TCM that seamlessly merges "biological target recognition" with "intelligent information processing." By deeply integrating a sophisticated hardware screening platform with an intelligent software analytics system, it systematically addresses the fundamental questions of "which components are effective and through what mechanisms," thereby providing a pivotal tool for deciphering TCM's scientific basis.[1,2] Secondly, it achieves full-chain autonomy and intelligent integration, from core components to the entire system. The project overcame key technological hurdles, such as high-precision multi-channel coordination and intelligent system integration, successfully transforming a laboratory prototype into an advanced, stable, and commercially viable end-product, thus bridging the critical gap from proprietary technology to mature instrumentation.[3]

The intelligent analysis module of MCMC-ISW primarily comprises three components: 1) A comprehensive TCM component database GNDC, containing over 234 million naturally diverse bioactive substances—including 2.32 million specialized metabolites, 229.77 million peptide sequences, 260,000 carbohydrates, and sRNAs—integrated with structural information, biological activities, and ADMET properties. This enables systematic molecular-level characterization of TCM constituents. 2) A target structure library covering multiple protein types such as GPCR receptors, supplemented by structural prediction tools like AlphaFold3, provides the structural basis for molecular recognition. Leveraging these data and structural resources, a high-throughput molecular docking platform was developed. Using AutoDock Vina, it systematically docks more than 38,000 natural small molecules with GPCR receptors, generating binding energies and conformational data to form a computational chemistry-based lead candidate set. 3) The Graph-Sequence Fusion Framework for Drug-Target Affinity (GSF-DTA) prediction model further refines this process by extracting and cross-integrating features from both graph structures and sequence information. It enables high-precision prediction and ranking of drug–target affinity, facilitating intelligent and fine-grained screening of the massive docking results. This culminates in the selection of candidate molecules with the highest potential binding activity, establishing a complete computational analysis pipeline from high-throughput preliminary screening to accurate prediction.

The MCMC-ISW system has undergone rigorous validation, with its performance metrics robustly demonstrating its reliability and precision. It exhibits high sensitivity with a detection limit of 1 ng/mL, alongside exceptional stability and precision, as evidenced by a relative standard deviation (RSD) not exceeding 3% during analysis. These definitive data collectively ensure the accuracy and repeatability of screening results, providing strong support for the platform's technical credibility.

Its utility is broad and substantiated by numerous case studies. In TCM modernization, it systematically identifies multi-target active ingredients from complex formulae; for instance, discovering salvianolic acid C from *Salvia miltiorrhiza* to inhibit EGFR and FGFR4, and hesperidin from Citrus aurantium to block SARS-CoV-2.[4,5] In drug safety, it detects allergenic components in TCM injections, enabling early risk. Furthermore, its application extends to precision medicine, screening for immune checkpoint inhibitors and central nervous system drugs, thereby offering a highly efficient, integrated solution for life science research (Figure 1C).

The MCMC-ISW system developed in this study demonstrates significant advantages in the field of drug screening, offering several breakthroughs compared to traditional Surface Plasmon Resonance (SPR) or Bio-Layer Interferometry (BLI) technologies. Unlike SPR/BLI, which requires immobilizing targets on chips, an approach often limited to single targets, moderate throughput, potential loss of native target conformation, and high costs, the MCMC-ISW utilizes the cell membrane as the stationary phase. This strategy better preserves the native activity and conformation of target proteins, providing interaction information more reflective of physiological conditions. It enables a paradigm shift from "target-driven" to "ligand-driven" screening, allowing direct discovery of active components from complex systems such as TCM extracts and herbal formulations. The system supports simultaneous high-throughput screening of multiple targets (≥3), with core consumables being self-preparable. The chromatographic columns maintain efficacy for >7 days, and the cost per screening cycle is significantly lower than that of SPR/BLI.

The successful development of the "MCMC-ISW 2025-I" marks the official entry of chromatography-based TCM complex system research into an intelligent "multi-component, multi-target" analysis era. More importantly, this achievement signifies a major leap from original theory to autonomous, high-end scientific instrumentation, thereby strongly aligning with national strategic priorities for advancing TCM modernization and achieving self-reliance in sophisticated scientific instruments.

Research team behind the MCMC-ISW system has overcome a series of technical bottlenecks to advance the integration of chromatography and artificial intelligence in natural medicine analysis. To address limited stability of cell membrane stationary phases, the team systematically evaluated strategies such as TCT covalent coupling and Flag-tag antibody immobilization, and developed a specialized protective solution that significantly enhanced phase activity and operational lifetime. When dealing with complex sample matrices typical of TCM, the system successfully combined the separation power of 2D chromatography with AI-powered knowledge graph cross-validation. This integration enabled precise identification of active compounds by effectively filtering out nonspecific bindings. In response to AI models' dependency on high-quality data and computational resources, the researchers implemented continuous multi-source data integration and adopted a modular architecture supporting both local and cloud deployment. They also launched the publicly accessible GNDC database (https://cbcb.cdutcm.edu.cn/gndc/), substantially improving system transparency and credibility.

Looking ahead, the instrument platform is set to incorporate column array configurations and organoid-mimetic chromatography columns. To tackle reproducibility challenges in multi-target column preparation—traced largely to manual processes—the team is now pursuing full automation in column packing to enable standardized, batch production.

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## AUTHOR CONTRIBUTIONS

All authors contributed to the manuscript and approved the final version.

## DECLARATION OF INTERESTS

The authors declare no competing interests.