International Journal of Rehabilitation and Disability Studies
Vol 1 Issue 2 (2025)
Pages (13 - 24)

Available at
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Next-Generation AI in Neuro-development Multi-Omics Applications from Diagnosis to Care

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ARTICLE HISTORY

Received: 25 September 2025.
Accepted: 16 November 2025.
Published: 30 December 2025.

PEER REVIEW STATEMENT:

This article underwent double-blind peer review by 3 independent reviewers.

HOW TO CITE

Alshamsi, M., & Alhammadi, N. (2025). Next-Generation AI in Neuro-development Multi-Omics Applications from Diagnosis to Care. *International Journal of Rehabilitation & Disability Studies*, **1**(2), 13-24.
https://doi.org/10.54878/yrp30g15

ABSTRACT

Neurodevelopmental disorders (NDDs), including autism spectrum disorder (ASD), attention-deficit/hyperactivity disorder (ADHD), intellectual disability (ID), and rare genetic syndromes, affect millions of children worldwide and impose a significant global health burden. Current diagnosis relies primarily on behavioral assessments, which are subjective, delayed, and poorly suited to capture comorbidities. Biological testing remains limited, leading to diagnostic delays of years in ASD, ADHD, and rare syndromes. Advances in multi-omics like genomics, transcriptomics, proteomics, metabolomics, and epigenomics, together with artificial intelligence (AI) provide a transformative path toward precision medicine in NDDs. Genomic studies highlight the role of copy number variants and polygenic risk scores in risk stratification, while transcriptomic and proteomic analyses reveal synaptic and neuroinflammatory pathways relevant to pathogenesis. Metabolomic profiling of biofluids identifies mitochondrial and microbiome-linked biomarkers, and epigenomics offers an environment-responsive regulatory layer. AI enables integration of these high-dimensional datasets, overcoming the "curse of dimensionality" through deep embedding, graph learning, and multimodal fusion. Case studies demonstrate promising accuracies in early prediction of ASD and ADHD from placental transcriptomics, DNA methylation, and newborn metabolomics, with reported AUCs approaching 1.00. Beyond diagnosis, AI-driven multi-omics supports stratified interventions, from metabolic modulation to pathway-specific pharmacology and neuromodulation, while adaptive monitoring systems linking omics to electronic health records and wearable biosensors enable continuous, individualized care. However, small cohorts, limited replication, high costs, and ethical issues around privacy, equity, and algorithmic bias remain critical barriers. Future progress is contingent on the independent validation of existing models, a shift toward explainable AI (XAI) to elucidate biological mechanisms, and the adoption of privacy-preserving federated learning platforms to enhance data diversity and model robustness. Future directions demand longitudinal biobanking, federated learning, XAI frameworks, and cross-disciplinary collaboration to ensure robust translation. Integrating AI with multi-omics holds unprecedented potential to reshape neurodevelopmental care from diagnosis to lifelong management.

Keywords: *Neurodevelopmental Disorders (NDDs), Multi-Omics Integration, Artificial Intelligence (AI), Precision Medicine, Biomarker Discovery*

Introduction

Neurodevelopmental disorders (NDDs), notably autism spectrum disorder (ASD), attention-deficit/hyperactivity disorder (ADHD), intellectual disability (ID) and rare genetic syndromes affect a substantial portion of children worldwide. Recent estimates place ASD at roughly 0.4 % globally with higher rates in high-income countries (up to 0.7 %) .[1] In the United States, about 1 in 31 eight-year-olds (3.2 %) have ASD .[2] ADHD shows even greater reach: global childhood prevalence is around 6-8 %,[3] while recent U.S. estimates report that 11.4 % of children age 3-17 have ever been diagnosed. [4] Intellectual disability affects roughly 2-3 % of the general population. [3] Co-occurrence is common: ADHD traits appear in 25 %-32 % of individuals with autism and ID co-exists in 30 %-40 % .[3]

Diagnosis remains challenging. Clinical assessments rely heavily on behavioral observation, which varies by context, age and evaluator expertise. Biological tests are absent. These constraints delay personalized care and hinder early intervention. Against this backdrop, next-generation AI integrated with multi-omics data while including genomics, transcriptomics, proteomics, metabolomics and epigenomics offers a new frontier. This convergence promises improved early diagnosis, precise subtyping of disorders and tailored long-term management. AI-driven multi-omics integration holds transformative potential for early diagnosis, precision medicine and long-term care in neurodevelopmental health.

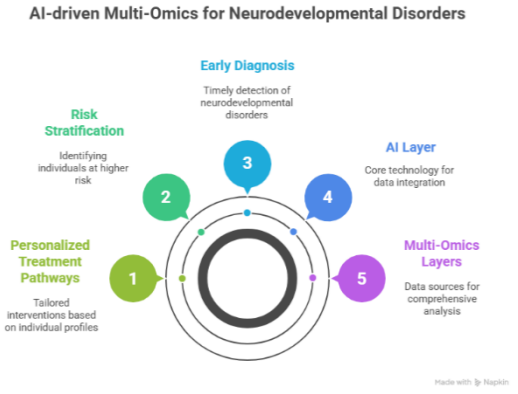


Figure 1: AI + Multi-Omics Framework for NDD

Landscape of Neurodevelopmental Disorders

Neurodevelopmental disorders impose a substantial global strain. In 2021, among children aged 0-14, autism spectrum disorder (ASD) affected roughly 857 per 100,000 individuals (0.86 %) and ADHD about 1,662 per 100,000 (1.66 %) figures derived from the Global Burden of Disease (GBD) study while corresponding burdens in disability-adjusted life years (DALYs) reached over 3.3 million for ASD and around 410,000 for ADHD in that group.[5] Broadly, the global prevalence of ASD stood at over 61 million individuals in 2021 approximately one in 127 people with an age-standardized rate of 788 per 100,000 and 11.5 million DALYs.[6]

ASD accounted for a leading cause of non-fatal health burden among those under 20 with DALY rates particularly high in high-income regions, up to 204 per 100,000. [7] ADHD prevalence across the lifespan in 2019 ranged between 0.83 % and 1.49 %, contributing about 0.8 % of global mental disorder DALYs.[8] Regionally, prevalence of ASD varies notably from just 0.02 % in China to over 3 % in Sweden while showing methodological and diagnostic differences.[9]

Current diagnosis depends on clinical observation, standardized behavioral assessments and in select cases genetic screening for rare syndromes. Yet these approaches introduce subjectivity, long delays and inconsistent results. For example, the average age at ASD diagnosis is approximately five years (around 60 months), often following years of concern. [10] In Scotland, patients may endure over four years for diagnostic confirmation.[11] In England, nearly 2.5 million individuals likely have ADHD, yet only a third hold formal diagnoses and waiting lists exceed half a million people.[12]

Further delays occur when conditions overlap. Children with both ADHD and autism may receive ASD diagnoses 1.5 to 2.6 years later than peers without ADHD.[13] People with rare genetic disorders bearing neuropsychiatric symptoms face mean diagnostic delays of over nine years, even as testing methods improved over decades.[14] These gaps late diagnosis, heterogeneous presentations, comorbidity and limited access

block early intervention, derail personalized care and stall therapeutic progress. The shortcomings reveal urgent need for precision in neurodevelopmental disorders diagnosis, early detection autism ADHD and recognition of limitations of current care.

Multi-Omics Approaches in Neurodevelopment

Genomics

Rare mutations such as copy number variants (CNVs) and polygenic risk scores (PRS) both contribute to neurodevelopmental disorders. In families affected by autism or ADHD, rare CNVs and PRS together explain roughly 10 % of variance in comorbid conditions, while PRS alone accounts for as little as 2 % in ADHD and 4 % in autism. [15] Recent methods like GenomicSEM help disentangle overlapping genetic risk between ADHD and ASD, improving PRS specificity and discriminatory power for diagnostic use. [16] However, PRS remains limited: its predictive accuracy is modest and in one cohort the highest ADHD-PRS decile conferred just a 4.4-fold increased relative risk. [17]

Transcriptomics

Altered gene expression in neural pathways is increasingly recognized in NDDs. Transcriptomic profiling often combined with neuroimaging has revealed ASD-related gene network modules that align with brain regions relevant to functional abnormalities, reinforcing the potential of imaging-transcriptomics for early biomarker discovery. [18]

Proteomics

Proteomic studies of synaptic structures in ASD uncover reduced expression of postsynaptic proteins including AMPA and NMDA receptor components (e.g., DLG4, Shank1-3), CAMK2α, neuroligins and neurexins implicating disrupted synaptic maturation in cognitive deficits [19] Broader proteomic-metabolomic analyses find dysregulation in mitochondrial bioenergetics (e.g., NDUV1), immune/inflammatory proteins (e.g., MBP), lipid metabolism (e.g., APOB-100) and synaptic function markers (e.g., SYT1) in ASD patients. [20]

Metabolomics

Biofluid metabolomic profiling reveals altered metabolites in ASD linked to fatty-acid metabolism (decanoyl-L-carnitine), oxidative stress (glutathione), mitochondrial dysfunction (arginine), energy metabolism (succinic acid), neurotransmitters (GABA) and microbiome interplay (tryptophan). [20] Integrated urine-based proteomic and metabolomic studies further identify neuroinflammation-related changes: 77 differential proteins and 277 metabolites with pathways such as leukocyte migration, antigen presentation and immune signaling enriched in ASD samples. [21]

Epigenomics

While neurodevelopmental epigenomic data remain sparse, integrating epigenomic data such as DNA methylation offers critical insight. It captures environment-responsive gene regulation layers and is a cornerstone of systems medicine approaches.[22]

Advantages of Omics Integration

Combining these omics yields a systems-medicine view. Multi-omics integration supported by network biology, deep learning, Bayesian networks, graph-based models, tools like mixOmics and joint pathway analyses facilitates detection of regulatory hierarchies and multi-modal biomarkers that single-omics cannot (Placeholder1)provide. [23] This strategy enhances diagnostic accuracy, clarifies mechanistic pathways and may guide therapeutic targeting. Genomics in autism, proteomics biomarkers ADHD and multi-omics integration neuroscience are advancing beyond descriptive data to actionable biology but only by embracing interconnected omics layers can we start to capture the full complexity of neurodevelopmental disorders.

Next-Generation AI and Data Integration

Artificial intelligence methods spanning classic machine learning, deep learning and graph neural networks are advancing the capacity to harness complex multi-omics in neurodevelopment. The burden of high-dimensional omics data, marked by thousands of features from small sample sets, poses a serious big-data challenge known as the

"curse of dimensionality." Techniques like deep embedding (as in frameworks such as OmiEmbed) reduce dimensionality and improve downstream task performance, from phenotype profiling to multi-omics integration or survival prediction.[24]

AI enables fusion across omics layers. A prime example comes from a large birth cohort study integrating placental transcriptomics and metabolomics to explore the placenta-brain axis. Using a multi-omics machine learning workflow, researchers achieved remarkably accurate classification of neurodevelopmental symptoms: 99.7 % for autism, 99.0 % for ADHD and 95.7 % for intellectual disability. [25] Such results illustrate potential of AI multi-omics integration to identify early biomarkers from biological fluid data, forging a route toward molecular diagnosis. In genomics and epigenomics, several studies show promise. One used deep learning models on placental CpG methylation data to predict autism in newborns with perfect accuracy (AUC = 1.00), implicating neuronal development pathways such as synapse formation and neurogenesis. [26] Another study applied explainable AI to gene-expression datasets from GEO, identifying hundreds of differentially expressed genes and potential ASD biomarkers such as HOXB3, SEMA4D and MID2. [27] However, a critical future need is to move beyond predictive accuracy alone. Research must prioritize explainable AI (XAI) approaches that demystify model decisions, linking predictions to specific, interpretable biological mechanisms. These examples reflect value of XAI and deep learning neurodevelopment strategies that combine disparate omics layers.

Developments in graph-based AI also offer promise. One multi-modal, multi-kernel graph-learning framework (MMKGL) encoded modalities such as imaging into learned graph embeddings. Applied to autism prediction, this method outperformed conventional models and spotlighted specific brain regions tied to pathology. [28] Most case studies currently focus on autism; direct examples for ADHD using proteomic or metabolomic data remain scarce. Yet machine learning classifiers have shown value for instance, peripheral blood mRNA models in toddlers achieved AUC of 0.88 using selected immune-related genes.[29] AI methods from machine learning through deep learning to graph neural networks offer powerful tools to manage the complexity of multi-omics data and fuse layers. Case studies demonstrate potential for early autism risk prediction via combined genomic/epigenomic markers and symptom classification using transcriptomic/metabolomic placental data. This emerging work signals a shift toward precision psychiatry, but it must be tempered small cohorts, lack of replication and overfitting risk demand continued rigor and independent validation.

Applications in Early Diagnosis

Early detection stands as a pivotal aim in neurodevelopmental care. AI-enabled models that fuse omics, imaging and behavioral inputs are reshaping the field of AI early diagnosis autism. One study applied deep learning to placental DNA methylation patterns. Using just five CpG sites, it predicted autism with perfect accuracy (AUC = 1.00, 100 % sensitivity and specificity).[30] Similarly, analysis of newborn leukocyte methylation achieved AUC = 1.00 with sensitivity at 97.5 % and specificity at 100 %, leveraging six CpG-based markers .[30] In newborn screening settings, integrating multi-omics newborn screening shows promise. Untargeted metabolomic profiling of dried blood spots identified biochemical markers in neonates who later developed autism, laying groundwork for molecular surveillance at birth .[31] Broader philosophical reviews affirm the potential to expand newborn screening programs through omics integration, though challenges remain in implementation cost, acceptability and scalability.[32] Real-world medical records also feed AI-based risk assessments. A machine learning model trained on electronic health records from over 780,000 children achieved an AUC of 0.86 in predicting ASD using early life data birth metrics, developmental milestones and familial variables. High-risk groups showed a 4.3-fold higher ASD incidence. [33] Another approach applied EHR-based Cox models to data collected before age one. By 360 days, the sensitivity reached nearly 60 % at 81 % specificity and performance improved when paired with caregiver surveys.[34]

Imaging and behavioral fusion also advance early detection. A digital phenotyping app using behavioral stimuli, computer vision and machine learning achieved AUC = 0.90 with 88 % sensitivity and 81 % specificity in identifying autism among toddlers.[35] Reviewer interpretations of AI-powered neuroimaging, including fMRI, EEG, and DTI, report accuracies ranging from 85 % to 99 % and highlight developmental windows (9-12 months) as critical for early biomarker extraction.[36] Case identification of specific syndromes such as Fragile X or Rett through AI-omics remains limited. Yet, early genetic or epigenetic biomarker detection in newborns suggests potential pathways for early identification of such conditions, especially with targeted omics panels integrated into newborn screening. Predictive models neurodevelopment that combines omics, clinical records and imaging hold remarkable promise for identifying autism risk before symptoms emerge. These approaches could extend into newborn screening frameworks. Still, limitations overfitting, cohort bias, scalability and the need for external validation across diverse populations must be addressed to ensure clinical translation.

Precision Medicine and Tailored Interventions

Precision medicine offers a path to overcome the limitations of one-size-fits-all care in neurodevelopmental disorders by stratifying patients on the basis of omics-derived biomarkers. Genomic and epigenomic profiles have begun to distinguish subgroups of autism spectrum disorder (ASD) and attention-deficit/hyperactivity disorder (ADHD) with distinct biological underpinnings. For instance, polygenic risk scores and methylation signatures linked to synaptic plasticity or dopaminergic signaling have been proposed as stratification tools, enabling clinicians to move beyond symptom-based categorization. This approach aligns with the growing demand for personalized treatment in multi-omics neurodevelopment research.[37]

Tailored interventions are advancing across multiple domains. Nutritional strategies informed by metabolomic data, such as correction of amino acid imbalances or modulation of gut-brain metabolites, are being investigated as adjunctive therapies in ASD. Pharmacological precision is emerging through identification of pathway-specific drug targets; for example, inhibitors of mTOR signaling in Fragile X syndrome or modulators of glutamatergic transmission in Rett syndrome. Neuromodulation approaches, including transcranial magnetic stimulation and closed-loop neurofeedback, may be personalized through biomarkers indicating cortical excitability profiles. Such interventions hold promise for reshaping developmental trajectories rather than simply alleviating symptoms.[38] Artificial intelligence has accelerated these developments by refining AI drug discovery in neurodevelopment. Deep learning platforms trained on proteomic and metabolomic data are capable of identifying candidate molecules that target synaptic function or metabolic dysregulation. Virtual screening combined with molecular dynamics further narrows therapeutic candidates, shortening the drug discovery pipeline. AI-driven trial design enables biomarker-guided stratification, improving power to detect treatment effects in heterogeneous populations while reducing attrition rates.[39]

Despite these advances, challenges remain. Most biomarkers lack replication across large cohorts and ethical considerations arise around stratification in pediatric populations. Clinical implementation is hindered by the high cost of multi-omics sequencing and the limited accessibility of computational infrastructure in routine care. Nonetheless, precision medicine in ASD and ADHD is progressing toward a systems-level framework in which omics signatures guide individualized therapies. The integration of AI and network biology provides a feasible path to overcome current diagnostic and therapeutic bottlenecks, moving neurodevelopmental care toward targeted, evidence-based personalization.[40]

AI in Long-Term Care and Monitoring

Long-term management of neurodevelopmental disorders such as autism spectrum disorder (ASD) and attention-deficit/hyperactivity disorder (ADHD) requires sustained, individualized

monitoring that extends well beyond initial diagnosis. The integration of multi-omics data with wearable biosensors, electronic health records (EHRs) and digital phenotyping provides an unprecedented opportunity to build dynamic care models. Wearable devices can capture continuous physiological data such as heart rate variability, sleep architecture and movement patterns, while digital platforms monitor social interactions, speech and attention through passive sensing. When combined with genomic and metabolomic information, these data streams create a multidimensional profile of patient trajectories.[41]

Artificial intelligence systems are increasingly being deployed to analyze these high-dimensional datasets, allowing for AI neurodevelopment care monitoring that surpasses traditional clinical follow-up. Machine learning models can identify subtle deviations in developmental progress, predicting therapy response or risk of regression months before such changes become clinically observable. Importantly, AI tools enable outcome quantification across diverse treatment modalities, from pharmacological interventions to behavioral therapies, thereby addressing the long-standing challenge of objectively measuring effectiveness in heterogeneous populations.[42]

One of the most promising applications is the development of adaptive interventions. AI platforms can update individualized care plans in real time, recommending therapy intensification, nutritional modification or neuromodulation adjustments based on continuously collected data. Such adaptivity is crucial in pediatric populations where developmental trajectories are highly dynamic. Integration of omics-informed risk stratification into EHR-linked monitoring systems may help prioritize high-need patients and optimize resource allocation.[43] Nevertheless, implementation barriers persist. Data interoperability across platforms remains limited, privacy concerns are magnified in pediatric care and disparities in access to digital health infrastructure risk widening inequities. Despite these obstacles, the convergence of digital health autism management, long-term ADHD AI monitoring and multi-omics integration positions AI as a transformative tool in sustaining individualized neurodevelopmental care throughout the lifespan.[40]

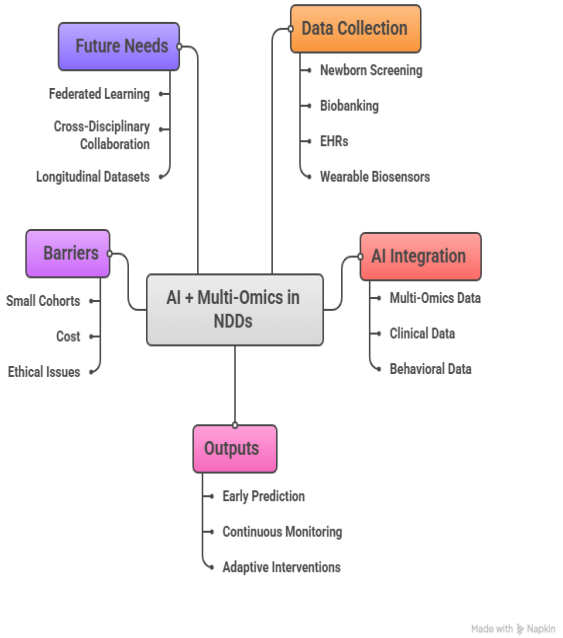
Ethical, Legal and Social Implications

The application of AI and multi-omics in neurodevelopmental disorders raises profound ethical, legal and social questions. Central among these is data privacy and security. Multi-omics datasets, when integrated with electronic health records, imaging and digital phenotyping, create highly identifiable patient profiles. Breaches of such information could expose not only medical vulnerabilities but also sensitive behavioral traits, making multi-omics privacy in neurodevelopment a critical safeguard for familiesEncryption, the use of federated learning platforms to enable analysis without centralizing sensitive data, and differential privacy are being explored, yet their effectiveness in pediatric research and long-term monitoring is still uncertain.44 Equity in access and algorithmic bias present additional concerns. AI models trained on predominantly Western, high-income population datasets may fail to generalize across diverse genetic and social groups, perpetuating disparities in autism or ADHD diagnosis. Without deliberate inclusion of underrepresented populations, predictive models risk reinforcing structural inequities in healthcare.45 Strategies to mitigate this, such as the secure integration of globally diverse datasets via federated learning, are essential to ensure model robustness and fairness.[45]

From a family and societal perspective, predictive diagnostics carry psychosocial implications. Early identification of autism spectrum disorder or fragile X variants may empower parents to seek intervention, but it also raises anxiety, stigma and potential misuse of information by insurers or educational institutions. The ethical challenges of AI autism diagnosis extend beyond accuracy, demanding attention to how families interpret and act on probabilistic risk information.[46] Regulatory frameworks have struggled to keep pace. While agencies such as the FDA and EMA are developing pathways for adaptive AI in healthcare, there is no consensus on standards for pediatric applications where predictive tools intersect with

long-term care. Policymakers must balance innovation with oversight, ensuring transparency, explainability and accountability in algorithmic decisions. Addressing AI ethics in healthcare requires multi-stakeholder collaboration, integrating technical safeguards with social dialogue. Without such measures, the promise of AI-driven neurodevelopmental care risks being undermined by ethical fragility.[47]

AI and Multi-Omics in Neurodevelopmental Disorders



Future Directions and Research Gaps

Despite rapid progress, significant challenges remain before AI-driven multi-omics integration can be fully realized in neurodevelopmental disorders (NDDs). A pressing technical frontier lies in the implementation of federated learning and decentralized AI, which allow multi-center data sharing without compromising privacy. The explicit adoption of such platforms is crucial to securely combine data across institutions, mitigating statistical bias and ensuring model robustness across global populations. Current research in NDDs is limited by fragmented datasets, often confined to single institutions or narrowly defined cohorts. Federated models could enable large-scale training across international sites, mitigating bias and enhancing generalizability while maintaining strict data governance.[25]

Another gap is the scarcity of longitudinal multi-omics datasets. Most existing studies are cross-sectional, capturing only a static snapshot of genetic, transcriptomic or metabolic profiles. Neurodevelopment, however, unfolds dynamically across childhood and adolescence. Without time-series data, it is difficult to model trajectories of risk, resilience and therapeutic response. There is a critical need for the establishment of longitudinal biobanks to track omics profiles over time. Establishing long-term, population-based biobanks will be essential for predictive accuracy and for the independent validation of predictive models.[48] Future progress also hinges on cross-disciplinary collaboration. Neuroscientists, bioinformaticians and clinicians must work alongside ethicists and data scientists to bridge technical discoveries with clinical translation. Current pipelines too often stall at proof-of-concept failing to deliver tools that can be deployed in pediatric clinics or community settings. Translating laboratory findings into actionable interventions remains a central bottleneck.[49] Finally, a forward-looking agenda requires attention to scalability, regulatory harmonization and equitable access. A key priority must be a paradigm shift in AI development from a sole focus on predictive accuracy to a mandatory demonstration of explainability (XAI), elucidating the biological why behind predictions. Without deliberate strategies, the future of AI in neurodevelopment risks advancing innovation for a select few, rather than addressing global needs. By identifying multi-omics research gaps and fostering AI neuroscience innovation, the field can move from theoretical promise to transformative clinical reality.[50]

Conclusion

The integration of AI and multi-omics is reshaping the landscape of neurodevelopmental disorders (NDDs) and it is offering unprecedented opportunities for earlier diagnosis, more precise stratification and continuous care across the lifespan. Genomic, transcriptomic, proteomic,

metabolomic and epigenomic insights when linked with behavioral and digital health data, provide a systems-level view that surpasses conventional diagnostic approaches. AI methods capable of handling such complexity are driving a shift toward multi-omics personalized medicine where interventions can be tailored to the unique biological and developmental profiles of each patient.

The promise extends beyond detection to lifelong AI neurodevelopment care. Adaptive monitoring platforms, integrating omics with wearable sensors and electronic health records, allow dynamic adjustments in therapy while creating feedback-driven care models that evolve alongside the individual. Such innovations, however, demand rigorous independent validation, equitable deployment and strong ethical governance to prevent bias, safeguard privacy and ensure societal trust. The field now faces a decisive juncture: without cross-disciplinary collaboration and clinical translation, progress risks remaining confined to academic silos. The path forward requires a commitment to explainable AI (XAI), federated learning for diverse data integration, and longitudinal biobanking to validate models over time. Future of AI in healthcare lies not only in technical capability but in the willingness to integrate neuroscience, bioinformatics, clinical medicine and regulatory oversight. With these foundations, AI-driven multi-omics can move from conceptual potential to transformative practice in neurodevelopmental care.

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