IMP

AI in Analytical Chemistry

Smarter Data, Faster Decisions

Industry Intelligence White Paper

Analytical Science | AI & ML | Method Development | Data Integrity

IMP InterMediaPartners GmbH

www.intermediapartners.de

B2B INDUSTRY INTELLIGENCE | IMP INTERMEDIAPARTNERS

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Executive Summary

> ***Analytical chemistry generates the most data-dense workflows in pharmaceutical development — yet most of that data has never been systematically mined. AI is not changing what analysts measure. It is changing what can be learned from measurements already being taken.***
>
> — IMP Industry Intelligence

Analytical chemistry sits at the foundation of pharmaceutical development and quality assurance — yet it has been among the last scientific disciplines to benefit from artificial intelligence. The reasons are structural: analytical data is high-dimensional, highly instrument-specific, and embedded in regulatory frameworks that reward reproducibility over innovation. These factors have slowed AI adoption while simultaneously making it more valuable.

This white paper maps where AI is genuinely transforming analytical workflows, where adoption remains in the pilot phase, and what the barriers to broader deployment look like in practice. It addresses the full spectrum of analytical science — from method development and spectral interpretation to stability data analysis, impurity profiling, and real-time release testing. It also examines the significant communication gap between analytical technology vendors and the scientific audiences they are trying to reach.

50%
reduction in method development time with AI-assisted DoE

3×
more impurities identified through AI-assisted spectral deconvolution

<15%
of pharma labs have deployed AI in routine analytical workflows

Sources: indicative internal estimate

1. AI-assisted spectral interpretation and chromatographic data analysis are the most mature applications, with demonstrated value across multiple instrument platforms and data types.
2. Method development acceleration through AI-driven design of experiments represents the highest near-term value opportunity for most analytical laboratories.
3. Regulatory frameworks for AI-assisted analytical decisions remain under development — ICH and FDA guidance is evolving, and proactive engagement is essential.
4. Analytical instrument vendors are communicating AI capabilities in terms that do not map to how analytical scientists evaluate new tools — creating a significant trust gap.

02

The Analytical Challenge in Modern Drug Development

Modern pharmaceutical development places unprecedented demands on analytical science. As drug molecules have grown more complex — biologics, oligonucleotides, ADCs, cell and gene therapies — the analytical challenges have scaled non-linearly. The data volumes, structural complexity, and regulatory expectations associated with characterising these molecules strain the capacity of analytical laboratories operating with traditional methods.

The Data Volume Problem

A single biologics development programme can generate millions of analytical data points — mass spectra, chromatograms, NMR spectra, stability data, dissolution profiles — before a molecule reaches Phase I. The analytical scientists responsible for interpreting this data face an increasingly impossible task using manual methods.

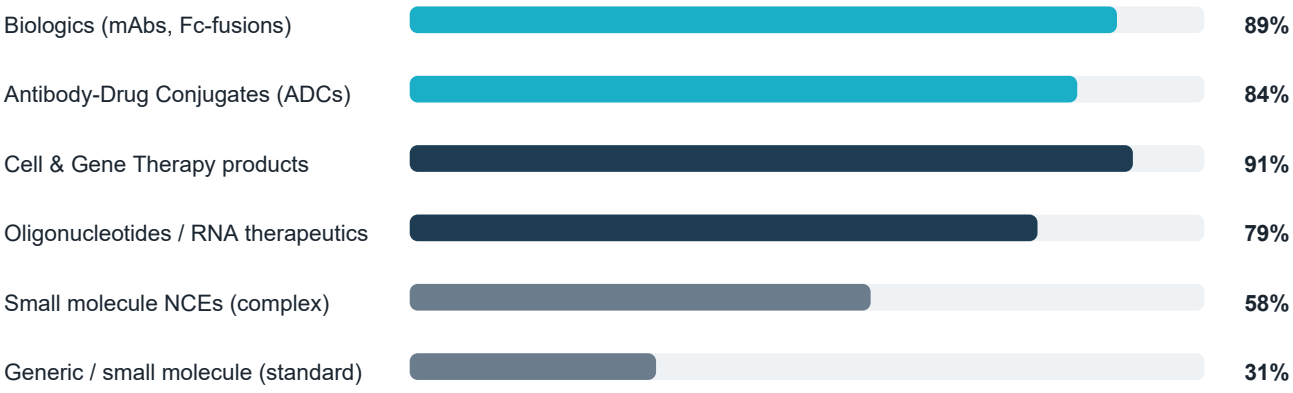
High-resolution mass spectrometry alone can generate gigabytes of data per day. Traditional data review workflows — expert review of individual spectra — cannot scale to meet the demands of modern development timelines.

The Complexity Escalation

The structural complexity of new molecular entities — and the corresponding complexity of their impurity profiles — has outpaced the capacity of traditional analytical methods to provide timely characterisation. Biologics require monitoring of dozens of critical quality attributes (CQAs). ADCs require simultaneous characterisation of antibody, linker, and payload components.

The question is no longer whether analytical science needs AI tools. It is which applications are mature enough to deploy, and which require further development before they can meet the regulatory bar.

Analytical Workload Growth by Modality



Analytical complexity index relative to 2015 baseline — indicative estimates from industry surveys

03

AI Technology Landscape for Analytical Science

The AI tools available for analytical chemistry span from embedded instrument software to standalone data science platforms and cloud-based analysis services. Navigating this landscape requires clarity about which problems each tool category is designed to solve.

AI Application	Core Capability	Maturity	Typical Use Case
Chromatographic data analysis	Peak detection, integration, deconvolution	★★★★★	Routine QC, impurity profiling
Spectral interpretation (MS)	Structure elucidation, library matching	★★★★■	Unknown impurity ID
NMR data processing	Automated assignment, quantification	★★★■■	Mixture analysis, metabolomics
Method development DoE	Condition optimisation, robustness design	★★★★■	HPLC, dissolution method dev.
Stability data modelling	Degradation kinetics, shelf-life prediction	★★★■■	ICH stability studies
Multi-attribute monitoring	Simultaneous CQA tracking (biologics)	★★★■■	Biologic characterisation
Real-time release testing	Process analytics, PAT integration	★★■■■	Manufacturing QC
Image analysis (microscopy)	Particle sizing, morphology, cell analysis	★★★★■	Formulation QC, cell therapy

★ = Deployment maturity (★★★★★ = widely deployed · ★★■■■ = emerging)

Embedded vs. Standalone AI

A critical distinction shapes how organisations approach AI in analytical workflows. Embedded AI — built into instrument software from vendors such as Waters, Agilent, Bruker, and Thermo Fisher — is more immediately deployable but less flexible. Standalone AI platforms — including Dotmatics, Signals, and emerging dedicated solutions — offer greater analytical depth but require more significant integration investment. Most organisations will need a combination of both, coordinated through a laboratory informatics architecture that allows data to flow between systems.

04

Where AI Delivers Value in Analytical Workflows

AI value in analytical chemistry is concentrated in the intersection of high data volume, pattern recognition requirements, and the need for consistent, auditable decision-making. The applications below represent the clearest evidence of real-world impact.

AI-Assisted Method Development

AI-driven design of experiments for HPLC method development represents the most immediately accessible and broadly applicable value opportunity. Machine learning models trained on historical method development data can predict optimal gradient conditions, column chemistry, and mobile phase composition with sufficient accuracy to reduce screening laboratory experiments by 60–80%. The ROI is rapid and measurable — typically realised within the first three to five method development projects following implementation.

Spectral Deconvolution and Unknown Impurity Identification

High-resolution mass spectrometry generates complex spectral data that challenges even experienced analysts when multiple impurities are present at trace levels. AI-powered deconvolution algorithms can identify co-eluting components and propose structural assignments with a speed and sensitivity that manual interpretation cannot approach. For ADC and biologic characterisation, where the impurity space is particularly complex, this capability has direct impact on development timelines and regulatory submission quality.

Automated Chromatographic Data Review

Integration of chromatographic peaks — determining where a peak begins and ends, and accurately calculating its area — is a deceptively complex analytical challenge that is routinely performed thousands of times per week in quality control laboratories. AI-assisted peak integration reduces manual review burden by 40–70% in validated implementations while improving consistency and creating a complete audit trail. The regulatory implications of AI-assisted integration are well-defined, making this one of the most regulatorily straightforward AI applications in analytical science.

Stability Data Analysis and Shelf-Life Prediction

ICH stability studies generate extensive longitudinal datasets that are traditionally analysed through linear regression models that often fail to capture degradation kinetics accurately. Machine learning approaches to stability modelling can incorporate non-linear degradation pathways, environmental interactions, and formulation variables to produce more accurate shelf-life predictions — with direct impact on development efficiency and regulatory submission quality.

05

Data Integrity, Validation and Regulatory Considerations

The regulatory dimension of AI in analytical chemistry is more developed than in most other areas of pharmaceutical AI — and more complex. Data integrity requirements, method validation frameworks, and the need for human oversight of AI-generated analytical decisions create a regulatory landscape that must be navigated carefully.

> ***The question regulators ask is not whether the AI performed correctly in the validation study. It is whether you can demonstrate that it will perform correctly on every sample you have not yet tested — and whether your scientists understand the boundaries of that assurance.***
>
> — Regulatory Affairs Director, global analytical CRO

01 Method Validation for AI-Assisted Procedures

ICH Q2(R2) provides the framework for analytical method validation. The core validation parameters — accuracy, precision, specificity, linearity, range and robustness — apply equally to AI-assisted analytical workflows.

Additional considerations arise when AI components influence analytical decisions. These include ensuring that model performance remains within its validated operating domain and that mechanisms must exist to detect model drift or performance degradation. Regulatory discussions increasingly reference the FDA's AI/ML-Based Software as a Medical Device (SaMD) Action Plan, which emphasises lifecycle monitoring, real-world performance evaluation and good machine learning practice for AI-enabled systems.

02 Audit Trail and Human Oversight Requirements

Data integrity regulations (FDA 21 CFR Part 11, EU GMP Annex 11) require complete, accurate, and attributable audit trails. AI-assisted analytical decisions must be traceable — the algorithm version, the model parameters, and the data inputs must all be captured. Human oversight requirements vary by application and risk level, but the principle of 'human in the loop' for final release decisions remains a regulatory expectation in most contexts.

03 Model Lifecycle Management

AI models used in regulated analytical workflows require formal lifecycle management — including version control, change management procedures, and periodic performance review. The concept of model drift — gradual degradation in model performance as the distribution of input data shifts over time — is particularly relevant for models trained on historical analytical data that may not represent the full scope of future samples.

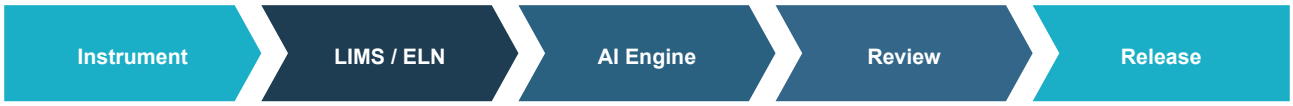
04 Transfer and Implementation Qualification

When AI-assisted analytical methods are transferred between laboratories, sites, or analytical platforms, the transfer process must address both the method itself and the AI component. Standard method transfer protocols require adaptation to include AI model performance verification, and the equivalence criteria must be defined in terms that capture AI-specific performance parameters.

06

Integration into Analytical Laboratory Operations

Integrating AI into analytical laboratory operations requires navigating a complex ecosystem of instruments, informatics systems, and regulatory requirements. The organisations achieving the most successful implementations share a consistent approach: they treat informatics architecture as the foundation, not as an afterthought.



Integration Layer	AI Requirement	Key Consideration	Readiness
Instrument software	Embedded AI, direct data capture	Vendor lock-in risk	High
LIMS connectivity	Structured data transfer, metadata	API availability varies	Medium
ELN integration	Context linking, method versioning	Data model alignment	Medium
Standalone AI platform	Data normalisation, model management	Validation scope increases	Medium
Regulatory submission	Audit trail, method documentation	Reviewer acceptance varies	Low–Med

The Analyst's Changing Role

The deployment of AI in analytical workflows fundamentally changes what analytical scientists spend their time on — and requires explicit investment in role redefinition and training. Routine data review tasks that occupied 40–60% of analytical scientist time in traditional workflows are substantially automated. The capacity this creates is valuable only if it is redirected towards higher-order analytical challenges: method strategy, interpretation of complex results, regulatory science, and the development and validation of the AI tools themselves. Organisations that invest in this transition consistently extract more value from AI investment than those that treat automation as headcount reduction.

07

Industry Signals: Early Adopters and Emerging Practice

Large Pharma — Systematic Platform Deployment

The leading pharmaceutical companies have moved beyond pilot programmes to systematic AI deployment in analytical workflows — particularly for high-volume QC testing and biologics characterisation. Investment is concentrated in LIMS-integrated AI platforms that can process standardised analytical data formats at scale. The organisations achieving the most impact are those that have standardised data capture across sites before deploying AI, rather than attempting to retrofit AI onto fragmented data environments.

Analytical CROs — Capability as Differentiator

Analytical contract research organisations are investing in AI capability as a competitive differentiator in an increasingly commoditised market. AI-assisted method development, accelerated stability analysis, and high-throughput impurity characterisation allow analytical CROs to offer faster turnaround and higher analytical depth — at price points that are competitive with larger organisations that have not yet invested in AI infrastructure.

Instrument Vendors — AI-Native Platforms

Major analytical instrument vendors — Waters, Agilent, Bruker, Thermo Fisher Scientific — are competing aggressively on the AI capability of their data processing software. The transition from traditional data processing algorithms to machine learning-based interpretation is accelerating, driven by customer demand for automated workflows that reduce manual review burden while maintaining regulatory compliance.

Regulators — Evolving Guidance

Regulatory agencies are actively developing frameworks for AI-assisted analytical decisions. FDA's Digital Health Centre of Excellence has issued preliminary guidance on AI/ML in laboratory software. ICH is reviewing Q2(R2) in the context of AI applications. Organisations engaging proactively with regulatory agencies on AI validation strategies are shaping emerging guidance in ways that will benefit early movers.

08

Strategic Questions for Analytical Science Leaders

Effective AI integration in analytical science requires decisions that go beyond technology selection. These strategic questions address the dimensions most frequently underweighted in analytical AI planning.

Q1

What is the state of your analytical data architecture?

AI tools for analytical science are only as valuable as the data they can access. Is your analytical data structured, standardised, and accessible in formats that AI platforms can consume? Organisations that have invested in LIMS standardisation and data governance before AI deployment consistently achieve better outcomes.

Q2

Which applications offer the clearest regulatory pathway?

Not all AI applications in analytical science carry equal regulatory risk. AI-assisted peak integration and method development optimisation have clearer regulatory frameworks than AI-assisted release decisions. Have you mapped the regulatory pathway for each application before investment?

Q3

What is your validation strategy for AI-assisted methods?

Validation of AI-assisted analytical methods requires adaptation of standard ICH Q2 frameworks. Do you have internal expertise to develop AI-specific validation protocols, or do you need external regulatory science support? How will you address model lifecycle management requirements?

Q4

How will you manage the embedded vs. standalone AI decision?

Each analytical application involves a choice between embedded AI (from instrument vendors) and standalone AI platforms. Have you mapped the tradeoffs — deployment speed, flexibility, validation scope, and long-term vendor dependency — across your portfolio of AI applications?

Q5

What does the analyst role look like after AI deployment?

AI will substantially change how analytical scientists spend their time. Have you defined what higher-value activities will be pursued with the capacity AI creates? Investment in role redefinition and skills development alongside AI deployment determines whether capacity gains translate into scientific or business value.

09

The Communication Gap in Analytical Technology Marketing

Analytical technology vendors face a distinctive communication challenge: their primary customers — analytical scientists — are among the most technically sophisticated and evaluatively rigorous audiences in the pharmaceutical industry. They are deeply sceptical of marketing claims that are not supported by reproducible experimental evidence.

> ***Tell me what the algorithm got wrong, and I will trust what it gets right. Vendors who only show me the success cases are telling me they do not understand how analytical science works.***
>
> — Principal Analytical Scientist, top-20 pharmaceutical company

What Vendors Communicate	What Analytical Scientists Evaluate	The Gap
AI accuracy claims	Performance on edge cases and failures	Curated benchmarks
Software feature lists	Regulatory validation pathway	Compliance left unaddressed
Algorithm sophistication	Interpretability and auditability	Black box problem
Integration claims	Specific LIMS/ELN connectivity	Abstract assurances
Customer references	Peer-reviewed validation data	Testimonials vs. evidence

The Content-as-Trust Framework

IMP InterMediaPartners has developed a practical framework for organisations navigating this challenge: a structured three-phase approach moving from awareness to authority to qualified lead generation. In Phase 1, content establishes market presence and signals domain expertise. In Phase 2, deeper formats — briefings, roundtables, expert series — build trust with specific audience segments. In Phase 3, targeted activation converts established trust into measurable commercial engagement.

Strategic Resource Allocation: Investment vs. Expenditure

Implementation of the Content-as-Trust Framework should be viewed as a strategic capital investment in long-term market authority rather than a cyclical marketing expense. The required budget scale is fundamentally driven by two variables: the technical complexity of the underlying solution and the current maturity of the organization's data infrastructure.

While initial pilot phases focus on establishing core technical credibility, full-scale deployment scales proportionally with the breadth of the target audience and the depth of required expert engagement. Organizations typically find that the initial investment is rapidly offset by shortened sales cycles, higher-qualified lead generation, and the reduction of "knowledge-gap" friction in technical procurement.

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Implications for B2B Communication Strategy

Analytical technology vendors that build credibility with their target audience share a consistent approach: they communicate the way scientists think. Evidence first. Limitations acknowledged. Validation pathways addressed. Peer-reviewed publications cited. This is not a communication style choice — it is a prerequisite for engagement with a scientifically sophisticated audience.

Peer-Reviewed Application Studies ★★★★★	Publications in journals such as the Journal of Pharmaceutical and Biomedical Analysis, Analytical Chemistry, c&en and LCGC demonstrate AI capability in the format that analytical scientists trust above all others. Even where full journal publication is not feasible, preprint publication on ChemRxiv or bioRxiv provides credibility that marketing materials cannot achieve.
Method Development Case Studies with Raw Data ★★★★★	Detailed accounts of AI-assisted method development — including the data, the algorithm parameters, the validation approach, and the outcome compared to traditional methods. Analytical scientists evaluate the methodology, not the conclusion. Showing the work is what builds trust.
Regulatory Science White Papers ★★★★■	Analysis of evolving regulatory frameworks for AI in analytical chemistry — ICH guidance, FDA thinking, EMA position papers — positions a vendor as a partner in navigating regulatory complexity rather than a product supplier. Regulatory science content reaches the QA and regulatory affairs stakeholders who are often the most influential voices in AI adoption decisions.
Validation Protocol Templates and Guidance ★★★★■	Practical tools that help analytical laboratories validate AI-assisted methods — protocol templates, IQ/OQ/PQ guidance, audit trail requirements documentation — directly address the implementation barrier that most commonly delays AI adoption decisions.
Scientific Symposia and User Communities ★★★■■	Peer-to-peer scientific events where analytical scientists share experiences with AI tools — independently, without vendor framing — build the kind of trust that cannot be manufactured through marketing. Vendors that invest in creating these spaces, and then step back, consistently develop stronger scientific credibility than those that dominate the content.

★ = Deployment maturity (★★★★★ = widely deployed · ★★■■■ = emerging)

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Outlook and Recommendations

AI in analytical chemistry is at an earlier stage of adoption than AI in process chemistry or synthesis — but the trajectory is clear. The analytical data volumes generated by modern pharmaceutical development are already beyond the capacity of manual review, and the pressure will only intensify as biologics, cell and gene therapies, and other complex modalities grow as a proportion of development pipelines.

The regulatory frameworks that have historically slowed AI adoption in analytical science are beginning to mature. Organisations that build AI capability now — including the validation expertise, the data infrastructure, and the regulatory science knowledge — will be positioned to move faster as frameworks solidify.

For Analytical Science Leaders

- → Prioritise analytical data standardisation and LIMS infrastructure before AI platform selection.
- → Build internal regulatory science capability for AI method validation — do not leave this to vendors.
- → Start with high-volume, lower-risk applications — chromatographic data review, method development DoE — before tackling complex release decision AI.
- → Define what analytical scientists will do with the capacity AI creates before deploying it.

For Analytical Technology Vendors

- → Lead with peer-reviewed evidence, not performance claims — your target audience evaluates evidence, not marketing.
- → Address the regulatory validation pathway explicitly in all AI product communication.
- → Publish the failure cases alongside the success cases — analytical scientists trust vendors who acknowledge limitations.
- → Invest in regulatory science content that helps customers navigate the compliance landscape.

For B2B Marketing in Analytical Science

- → Audit all AI-related content against the evaluation criteria of analytical scientists, not procurement decision-makers.
- → Build content programmes around validation evidence, regulatory science, and peer-reviewed application data.
- → Invest in scientist-authored content — analyst credibility is not transferable from marketing departments.
- → Create independent scientific communities around AI in analytical chemistry — and let them speak for themselves.

About IMP InterMediaPartners

IMP InterMediaPartners GmbH specialises in B2B marketing and content strategy for complex industrial and technology markets — including pharmaceutical manufacturing, chemical R&D;, and laboratory technology.
We help organisations translate technical expertise into market authority through structured demand architecture, knowledge-transfer content, and precision media deployment.

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