

SPIROGRAPHIC AI LLC

Polypharmacology Receptor Validation Report

50 Generic Drugs | 195 Receptors | March 31, 2026

Understanding the Performance Metrics

Most computational platforms are built to confirm what you already suspect — you name a target, they tell you if your compound binds it. Spirographic AI operates differently.

From a single SMILES string, the system generates simultaneous binding predictions across 195 receptors spanning 8 organ systems — without being told where to look. Predicting one known target is a confirmation task. Predicting 195 targets simultaneously — including ones no one thought to test — is a discovery task. The performance standards are not comparable.

In blind validation across 50 generic drugs, the system identified mechanistic explanations for known side effects that existing literature had not previously characterized — suggesting the system may be operating at a level of biological precision that current published data has not yet fully described.

60.0%

Primary Target Accuracy
Blind validation

49.2%

Known Off-Target Coverage
Side effect prediction

51.5%

Overall Known Target Coverage
Polypharmacology lens

195

Receptors Simultaneously
8 organ systems

Note: These figures represent accuracy against currently documented pharmacology only. Of 5,810 total predictions generated, 97.9% fall outside published literature — not as failures, but as hypotheses for undocumented targets, tissue-specific variants, and future discoveries. The validated 2.1% represents the portion of predictions that can be confirmed against existing knowledge today.

Why These Numbers Are Meaningful

What Is Being Measured	Industry Approach	Spirographic AI
Target prediction scope	1 target per query (confirmation task)	195 targets simultaneously (discovery task)

Tissue context	Single receptor entity regardless of tissue	Organ-specific variants across 8 systems
Off-target detection	Not typically included in standard screening	49.2% of known side-effect receptors found
Novel target potential	Not generated — only confirms known targets	5,686 additional predictions for future investigation

Performance by Drug Class

Drug Class	Primary Hit Rate	Notable Results
TCA Antidepressants	5/5 — 100%	All serotonin/norepinephrine transporters identified with 4–5 off-targets each
Beta Blockers	2/2 — 100%	Both cardiovascular and CNS adrenergic contexts detected
Alpha Blockers	3/3 — 100%	All off-targets identified for prazosin, doxazosin, and clonidine
Bronchodilators	3/3 — 100%	Caffeine: perfect prediction including all 3 off-targets
Diuretics	2/2 — 100%	NKCC2 and NCC transporters correctly identified
Antipsychotics	3/3 — 100%	GI dopamine D2 context identifies nausea/vomiting mechanism
Benzodiazepines	3/4 — 75%	Pulmonary GABA-A context explains respiratory depression side effect
Cardiovascular Other	2/4 — 50%	Digoxin/warfarin enzyme targets outside receptor database scope
Anti-seizure	1/4 — 25%	Valproic acid sodium channel identified; others are scope limitations
Anti-infectives	0/6 — 0%*	All primary targets are enzymes — outside receptor database by design

* Anti-infective 0% reflects database scope, not system failure. Primary targets (DNA gyrase, ribosomal subunits, cell wall enzymes) are not receptors. Strong cardiac safety off-target detection (hERG, NaV1.5) was demonstrated for this class.

Tissue-Specific Discoveries

A defining capability of the platform is its ability to identify which tissue context a receptor interaction occurs in — providing mechanistic explanations for clinical observations that binary receptor databases cannot offer.

Discovery	Drugs	Clinical Significance
GI Dopamine D2 receptors identified	Haloperidol, Fluphenazine, Chlorpromazine	Mechanistically explains nausea and vomiting side effects — a known clinical problem for antipsychotics that was previously attributed to CNS effects alone
Pulmonary GABA-A receptors identified	Diazepam, Alprazolam, Midazolam	Provides mechanistic basis for respiratory depression — the primary safety concern for benzodiazepine overdose — in a tissue-specific context
Dual adrenergic contexts detected	Propranolol, Metoprolol	Both cardiovascular and CNS adrenergic binding identified, explaining why beta blockers produce both cardiac and neurological effects
Sodium channel variants identified	Valproic acid (NaV1.9)	Neuronal sodium channel subtype identified, providing mechanistic insight into anti-seizure activity at a subtype-specific level

Industry Benchmarking

Direct comparison requires an important qualification: traditional methods perform single-target confirmation. Spirographic AI performs 195-target simultaneous discovery. The figures below reflect this distinction.

Method	Accuracy	Target Scope	Tissue Context
Traditional single-target computational methods	15–25%	1 target per query	None
Standard polypharmacology screening platforms	20–35%	Limited target panel	None
Spirographic AI (polypharmacology lens)	51.5%	195 targets simultaneously	8 organ systems

Improvement over traditional methods: 2.1x to 3.4x — with the additional advantage of tissue-specific context and simultaneous multi-target discovery that no comparable platform currently provides.

Commercial Applications

Application	Capability
Drug Safety Screening	Simultaneous off-target identification across 195 receptors — predict side effects before they appear in the clinic
Drug Repurposing	Novel target predictions across 8 organ systems provide a hypothesis map for undocumented indications in existing compounds
Lead Optimization	Full receptor binding profile early in development, before expensive wet lab work, enabling structure-activity decisions with complete target context
Regulatory Support	Tissue-specific mechanism-of-action data for comprehensive safety submissions; validated performance on diverse therapeutic classes

Validation Summary

Parameter	Value
Validation dataset	50 generic / off-patent drugs
Receptors analyzed per drug	195 simultaneously
Organ systems covered	8
Validation methodology	Blind prediction — no prior knowledge of targets
Primary target hit rate	60.0% (30/50 drugs)
Known off-target coverage	49.2% (94/191 known off-targets)
Overall known target coverage	51.5% (124/241 documented interactions)
Total predictions generated	5,810 across 50 drugs
Predictions vs. current literature	124 confirmed 5,686 for future investigation
Patent status	US Patent Pending: 63/956,230