

ADME Hero™ Sample Report

AI-Generated Predictions of Key ADME Endpoints



NEZU
Biotech GmbH





Dear Client,

Imagine you are developing new anti-inflammatory drugs. After your screening, you identified promising molecules.

In this sample report (PDFs + table), you will find an analysis of dozens of ADME endpoints of those promising molecules. We compare their profiles to 1700+ commercialized drugs. We also compare them specifically to 63 anti-inflammatories and anti-rheumatic drugs.

These results give you a comprehensive overview of where your candidate molecules stand, compared to those of similar indication.

These are predictions made by our AI models. They were trained on high-quality, manually curated data.

Notice that some endpoints have multiple copies. For example, the CYP1A2 inhibitor has CYP1A2_A and CYP1A2_B. These are different models, trained on different molecules, assessed with different laboratory assays, and by different teams. This is analogous to second opinion about a given molecule.

We genuinely hope these results advance your drug development - on Earth and beyond.

Your friends at Nezu Biotech GmbH, Heidelberg, Germany.

You have the vision. We can help make it reality.

Click here to book a demo. Tell us about your molecules.

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Column	Description
Maximum Daily Dose	Human maximum recommended daily dose (MRDD) is the upper clinical dose at which a drug's therapeutic benefit remains acceptable before additional efficacy is lost or undesirable pharmacological and toxic effects begin to outweigh benefit. MRDD is important in drug discovery because it reflects human tolerance, pharmacological potency, systemic exposure, ADME behavior, and adverse-effect liability, and it can support estimation of safe starting doses for first-in-human trials or effect thresholds for non-pharmaceutical chemicals. High MRDD values mean a compound can generally be administered at a relatively higher dose before reaching the clinically limiting boundary, indicating lower relative potency or toxicity concern. Low MRDD values mean clinically relevant pharmacological or adverse effects occur at relatively lower doses, so concern for high potency, limited tolerance, toxicity risk, or a narrow safety margin is greater.
hERG Blocker	hERG inhibition describes the ability of a compound to block the hERG cardiac potassium channel, which carries the rapid delayed rectifier potassium current needed for normal cardiac repolarization. Blocking this channel can delay the heart's electrical reset, prolong the QT interval, and increase the risk of torsades de pointes, serious arrhythmias, or broader cardiac safety liabilities. Higher predicted values mean the compound is more likely to inhibit hERG channel activity and may have greater hERG-related cardiotoxicity. Lower predicted hERG inhibition means the compound is less likely to block hERG, so it is less likely to cause delayed cardiac repolarization, QT prolongation, or hERG-mediated arrhythmia risk.
AMES Mutagenicity	Ames mutagenicity describes whether a compound can induce genetic mutations in the bacterial reverse-mutation Ames assay, usually reflecting DNA damage caused directly or after metabolic activation. Here, higher predicted values may indicate greater risk of genotoxicity, DNA-adduct formation, carcinogenic potential, safety-related development failure, or human and environmental chemical hazard. Lower predicted Ames mutagenicity values mean the compound is less likely to cause mutation in the Ames assay, so it is more likely to be associated with lower genotoxicity concern, reduced DNA-damage liability, lower carcinogenicity warning, or better early safety profile.

Human Hepatotox	Human hepatotoxicity describes the potential of a compound to cause liver injury in humans, which may impair hepatic metabolism, detoxification, bile handling, and other essential liver functions. Hepatotoxic compounds can cause elevated liver enzymes, cellular injury, impaired liver function, clinically significant drug-induced liver injury, or broader liver safety liabilities. Higher predicted values mean the compound is more likely to be associated with human hepatotoxicity and may have greater liver toxicity risk. Lower predicted H-HT means the compound is less likely to cause human liver injury, so it is less likely to produce hepatocellular damage, impaired liver function, clinically relevant hepatotoxicity, or liver-related safety risk.
DILI A	Drug-induced liver injury (DILI) is clinically important because it has been a major cause of safety-related drug withdrawals, and severe human DILI is difficult to detect experimentally: it may not appear clearly in animal studies, may not be dose-related, and can occur rarely in patients. Here, higher predicted values mean the compound is more likely to be DILI-positive, which may indicate increased risk of clinically relevant liver injury, safety-related development failure, or post-marketing toxicity concern. Lower predicted DILI values mean the compound is less likely to be associated with drug-induced liver injury, so it is less likely to cause liver toxicity, hepatotoxic safety signals, development-stage safety failure.
Lethal Dose 50 Rats	LD50 describes the acute oral toxicity of a compound in rats, measured as the dose that causes death in 50% of exposed animals after oral administration; this corresponds to whole-organism systemic toxicity following gastrointestinal absorption, distribution, metabolism, and toxic effects on essential organs or physiological functions. Here, higher predicted values indicate greater acute toxicity, a lower dose needed to kill 50% of exposed rats, and increased concern for severe systemic toxicity or lethal poisoning. Lower values mean the compound is less acutely toxic to rats, and a higher oral dose is required to cause 50% mortality.
Rat Oral Acute Tox	Rat acute oral toxicity is important because it describes the ability of a compound to cause severe harmful effects or death after a single or short-term oral exposure, commonly summarized using the median lethal dose required to kill 50% of exposed rats. Here, higher predicted values mean the compound is more likely to be

	classified as toxic after oral administration, which indicate a lower lethal dose, greater systemic toxicity, increased risk of severe poisoning, and greater concern for acute oral exposure. Lower predicted rat acute oral toxicity values mean the compound is less likely to belong to the acutely toxic class under the defined classification threshold, so it is more likely to be associated with a higher lethal dose, lower risk of severe acute poisoning, reduced systemic toxicity after short-term oral exposure, or lower concern for this specific toxicity endpoint.
Androgen Receptor Activity	Androgen receptor (AR) activity is important because the androgen receptor controls androgen-dependent gene expression involved in reproductive development, sexual differentiation, fertility, muscle biology, and endocrine homeostasis. Here, higher predicted values mean the compound is more likely to perturb androgen-receptor signaling, which may indicate androgenic or anti-androgenic activity, disruption of hormone-responsive transcription, reproductive or developmental effects, and increased endocrine-disruption concern. Lower predicted androgen receptor activity values mean the compound is less likely to perturb AR signaling, so it is more likely to be associated with limited androgen-receptor engagement, lower risk of androgenic or anti-androgenic effects, reduced reproductive or developmental disruption, or lower concern for AR-mediated endocrine toxicity.
Androgen Receptor Ligand Binding Domain Activity	Androgen receptor ligand-binding-domain (AR-LBD) activity is important because direct interaction with the receptor's ligand-binding domain can alter androgen-receptor activation and interfere with androgen-dependent transcriptional programs. Here, higher predicted values mean the compound is more likely to bind to or perturb the AR ligand-binding domain, which may indicate direct androgen-receptor engagement, potential agonist or antagonist behavior, disruption of androgen signaling, and increased endocrine or reproductive toxicity concern. Lower predicted AR-LBD activity values mean the compound is less likely to interact with the androgen receptor ligand-binding domain, so it is more likely to be associated with weak or absent direct AR binding, lower probability of receptor-mediated androgenic or anti-androgenic activity, reduced endocrine disruption, or lower AR-LBD-related hazard.
Estrogen Receptor Activity	Estrogen receptor (ER) activity is important because estrogen receptors regulate hormone-responsive gene expression involved in reproduction, development, bone

	maintenance, cardiovascular physiology, and the function of many estrogen-sensitive tissues. Here, higher predicted values mean the compound is more likely to perturb estrogen-receptor signaling, which may indicate estrogenic or anti-estrogenic activity, altered hormone-responsive transcription, reproductive or developmental effects, and increased endocrine-disruption concern. Lower predicted estrogen receptor activity values mean the compound is less likely to perturb ER signaling, so it is more likely to be associated with limited estrogen-receptor engagement, lower risk of estrogenic or anti-estrogenic effects, reduced disruption of estrogen-dependent physiology, or lower concern for ER-mediated endocrine toxicity.
Estrogen Receptor Ligand Binding Domain	Estrogen receptor ligand-binding-domain (ER-LBD) activity is important because direct interaction with the receptor's ligand-binding domain can alter estrogen-receptor activation and interfere with estrogen-dependent transcriptional signaling. Here, higher predicted values mean the compound is more likely to bind to or perturb the ER ligand-binding domain, which may indicate direct estrogen-receptor engagement, potential agonist or antagonist behavior, disruption of estrogen signaling, and increased endocrine or reproductive toxicity concern. Lower predicted ER-LBD activity values mean the compound is less likely to interact with the estrogen receptor ligand-binding domain, so it is more likely to be associated with weak or absent direct ER binding, lower probability of estrogenic or anti-estrogenic activity, reduced endocrine disruption, or lower ER-LBD-related hazard.
Aromatase Activity	Aromatase activity is important because aromatase converts androgens into estrogens and is therefore essential for maintaining normal estrogen synthesis, reproductive function, sexual development, bone physiology, and endocrine balance. Here, higher predicted values mean the compound is more likely to inhibit or otherwise perturb aromatase activity, which may indicate reduced estrogen biosynthesis, altered androgen-to-estrogen balance, reproductive or developmental toxicity, and increased endocrine-disruption concern. Lower predicted aromatase activity values mean the compound is less likely to interfere with aromatase, so it is more likely to be associated with preserved estrogen synthesis, limited disruption of sex-hormone balance, lower risk of reproductive or developmental effects, or reduced

	aromatase-mediated endocrine hazard.
Aryl Hydrocarbon Receptor Activity	Aryl hydrocarbon receptor (AhR) activity is important because AhR is a ligand-activated transcription factor that regulates xenobiotic-response genes and can mediate chemical effects on metabolism, development, immune function, and carcinogenic signaling. Here, higher predicted values mean the compound is more likely to activate the AhR pathway, which may indicate stronger xenobiotic-receptor engagement, induction of AhR-regulated gene expression, altered chemical metabolism, and increased potential for AhR-mediated toxicological effects. Lower predicted AhR activity values mean the compound is less likely to activate the AhR pathway, so it is more likely to be associated with limited AhR engagement, reduced induction of AhR-responsive genes, lower risk of AhR-mediated endocrine or developmental disruption, or lower concern for this specific toxicity mechanism.
PPARG Activity	Peroxisome proliferator-activated receptor gamma (PPAR γ) activity is important because PPAR γ regulates adipocyte differentiation, lipid storage, glucose metabolism, insulin sensitivity, and inflammatory responses. Here, higher predicted values mean the compound is more likely to activate or perturb PPAR γ signaling, which may indicate altered adipogenesis, lipid or glucose homeostasis, metabolic endocrine disruption, and increased concern for obesogenic or other PPAR γ -mediated effects. Lower predicted PPAR γ activity values mean the compound is less likely to perturb PPAR γ signaling, so it is more likely to be associated with limited effects on adipocyte differentiation, lipid storage, glucose regulation, metabolic homeostasis, or PPAR γ -mediated toxicity.
Antioxidant Response Activity	Antioxidant response element (ARE) activity is important because ARE signaling, commonly regulated through the NRF2 pathway, is activated in response to oxidative or electrophilic stress and controls the expression of antioxidant and detoxification genes. Here, higher predicted values mean the compound is more likely to activate the ARE stress-response pathway, which may indicate oxidative or electrophilic cellular stress, increased demand for antioxidant defenses, induction of detoxification responses, and greater concern for chemically induced redox disturbance. Lower predicted ARE activity values mean the compound is less likely to activate the ARE pathway, so it is more likely to be

	associated with limited oxidative or electrophilic stress, reduced induction of antioxidant-response genes, lower disruption of cellular redox balance, or lower concern for this specific stress mechanism.
Are Nfr2 Luc Assay	Are-Nfr2 luciferase assay describes whether a compound activates keratinocytes through an antioxidant/electrophile response pathway, measured in an in vitro human keratinocyte-derived reporter cell line carrying a luciferase reporter; this corresponds to the keratinocyte activation key event in the skin-sensitization adverse outcome pathway. Here, higher predicted values mean the compound is more likely to increase the risk of electrophile-response activation, keratinocyte stress signaling, inflammatory skin response, or skin-sensitization hazard. Lower predicted values mean the compound is less likely to be associated with keratinocyte activation, so it is less likely to cause antioxidant-response-element induction, epidermal stress signaling, sensitization-related cellular activation, or dermal safety concern.
Mitochondrial Membrane Potential Disruption	Mitochondrial membrane-potential disruption is important because the mitochondrial electrochemical gradient is required for ATP production, oxidative phosphorylation, metabolite transport, and normal cellular survival. Here, higher predicted values mean the compound is more likely to disrupt mitochondrial membrane potential, which may indicate mitochondrial dysfunction, impaired energy production, increased oxidative stress, initiation of cell-death pathways, and greater concern for mitochondrial toxicity. Lower predicted mitochondrial membrane-potential activity values mean the compound is less likely to disrupt the mitochondrial gradient, so it is more likely to be associated with preserved mitochondrial function, maintained ATP production, lower risk of oxidative or apoptotic injury, or reduced mitochondrial toxicity concern.
Heat Shock Activity	Heat-shock response element activity is important because the heat-shock pathway protects cells from protein damage by inducing molecular chaperones in response to protein unfolding, misfolding, aggregation, or other disturbances of protein homeostasis. Here, higher predicted values mean the compound is more likely to activate the HSE pathway, which may indicate proteotoxic stress, disruption of protein folding or stability, increased chaperone demand, and greater concern for cellular damage caused by impaired proteostasis. Lower predicted

	HSE activity values mean the compound is less likely to activate the heat-shock response, so it is more likely to be associated with limited protein misfolding, reduced proteotoxic stress, preserved protein homeostasis, or lower concern for HSE-mediated cellular injury.
ATAD5 DNA Damage Activity	ATAD5 DNA-damage-response activity is important because ATAD5 participates in DNA replication, genome maintenance, and repair-associated processes, and its reporter activation can signal DNA damage or replication stress. Here, higher predicted values mean the compound is more likely to activate the ATAD5-associated stress response, which may indicate genotoxic damage, impaired DNA replication, genome instability, and increased concern for mutation, carcinogenicity, or other DNA-damage-related effects. Lower predicted ATAD5 activity values mean the compound is less likely to activate this DNA-damage-response pathway, so it is more likely to be associated with limited replication stress, reduced genotoxic signaling, lower risk of genome instability, or lower concern for ATAD5-associated DNA damage.
p53 Stress Response	p53 stress-response activity is important because p53 is a central tumor-suppressor pathway activated by DNA damage and other severe cellular stresses, leading to cell-cycle arrest, DNA repair, senescence, or apoptosis. Here, higher predicted values mean the compound is more likely to activate the p53 pathway, which may indicate DNA damage, genotoxic or cellular stress, impaired genome integrity, and increased concern for cytotoxic, mutagenic, or carcinogenic mechanisms. Lower predicted p53 activity values mean the compound is less likely to activate the p53 response, so it is more likely to be associated with limited DNA-damage signaling, lower cellular stress, reduced induction of cell-cycle arrest or apoptosis, or lower concern for p53-mediated toxicity.
Tetrahymena pyriformis Growth Inhibitor	IGC50 describes the growth-inhibitory toxicity of a compound to the freshwater ciliate Tetrahymena pyriformis, measured as the concentration that reduces organism growth by 50% relative to an untreated control; this corresponds to whole-cell toxic effects such as impaired metabolism, membrane function, energy production, nutrient uptake, or cell division. Here, higher predicted values indicate stronger toxicity, a lower concentration needed to inhibit 50% of Tetrahymena pyriformis growth, and increased concern for cellular dysfunction or aquatic environmental hazard. Lower values mean the compound is less growth-inhibitory to

	Tetrahymena pyriformis, and a higher concentration is required to reduce growth by 50%.
Daphnia magna Acute Tox	LC50DM describes the acute aquatic toxicity of a compound to Daphnia magna, measured as the concentration of a chemical in water that causes 50% mortality after 48 hours; this corresponds to whole-organism toxic effects following aquatic exposure, including uptake, internal distribution, and disruption of essential physiological functions. Here, higher predicted values indicate greater acute toxicity, a lower concentration needed to kill 50% of exposed Daphnia magna, and increased concern for freshwater invertebrate mortality or environmental hazard. Lower values mean the compound is less acutely toxic to Daphnia magna, and a higher concentration is required to cause 50% mortality.
Pimephales promelas Acute Tox	LC50FM describes the acute aquatic toxicity of a compound to fathead minnows (Pimephales promelas), measured as the concentration of a chemical in water that causes 50% mortality after 96 hours; this corresponds to whole-organism toxic effects following uptake through the gills, skin, or digestive tract and disruption of essential physiological systems. Here, higher predicted values indicate greater acute toxicity, a lower concentration needed to kill 50% of exposed fathead minnows, and increased concern for fish mortality or environmental hazard. Lower values mean the compound is less acutely toxic to fathead minnows, and a higher concentration is required to cause 50% mortality.
Direct Peptide Reactivity Assay	Direct peptide reactivity assay (DPRA) describes whether a compound can react chemically with proteins, modeled by depletion of synthetic cysteine- and lysine-containing peptides; this corresponds to the molecular initiating event of skin sensitization, where electrophilic or reactive chemicals covalently bind skin proteins and form antigenic hapten-protein complexes. Here, higher predicted values mean the compound is more likely to be DPRA-positive, which may indicate increased risk of peptide/protein reactivity, hapten formation, skin-sensitization initiation, or allergic contact dermatitis concern. Lower predicted DPRA values mean the compound is less likely to be associated with peptide reactivity, so it is less likely to cause covalent skin-protein binding, haptenation-driven immune activation, molecular initiating events for sensitization, or early dermal toxicity safety signals.
Human Cell Line	Human cell line activation test (h-CLAT) describes

Activation	whether a compound activates dendritic-cell-like immune responses in vitro, measured in THP-1 cells by flow-cytometric detection of CD86 and CD54 upregulation after chemical exposure; this corresponds to dendritic-cell activation, maturation, and mobilization in the skin-sensitization adverse outcome pathway. Here, higher predicted values indicate increased risk of dendritic-cell activation, antigen-presentation readiness, T-cell-mediated allergic sensitization, or human skin allergy concern. Lower predicted h-CLAT values mean the compound is less likely to be associated with dendritic-cell activation, less likely to cause CD86/CD54 upregulation, sensitization-related immune-cell activation, and allergic contact dermatitis hazard.
Local Lymph Node Assay	Local lymph node assay (LLNA) describes whether a compound causes skin sensitization in mice by measuring lymph node cell proliferation after topical exposure. Here, higher predicted values mean the compound is more likely to increase the risk of immune activation, animal sensitization hazard, or regulatory concern for allergic contact dermatitis. Lower predicted LLNA values mean the compound is less likely to be associated with mouse skin sensitization, so it is less likely to cause lymph-node proliferative immune responses, animal sensitization signals, dermal allergy hazard.
Human Patch Test	Human patch tests (HRIPT/HMT) describe whether a compound causes skin sensitization in humans, usually measured by human repeat insult patch tests or human maximization tests, where controlled skin exposure is used to determine whether the compound can produce allergic contact sensitization. Here, higher predicted values mean the compound is more likely to cause skin sensitization in humans. This may indicate increased risk of allergic contact dermatitis, cosmetic or topical-product safety concern, or human cutaneous immune toxicity. Lower predicted human patch-test values mean the compound is less likely to be associated with human skin sensitization, so it is less likely to cause allergic contact dermatitis, human sensitization hazard, topical safety signals, or development-stage dermal safety failure.



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