Report on the literature review: uncertainty quantification for complex models

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Supplementary material: literature_review_sup1_summary.xlsx

Content:

1 Background and objective

Model-informed drug development (MIDD) plays a crucial role not only in drug development[1] but also in drug evaluation by regulatory agencies[2,3]. A key component of MIDD is the use of complex mechanistic models, such as Physiologically Based Pharmacokinetic (PBPK)[4] and Quantitative Systems Pharmacology (QSP)[5] models. Unlike statistical models, which are based on data, PBPK and QSP models are built on an understanding of physiology, drug characteristics, and pharmacology. These models are typically intricate, with numerous parameters derived from previous preclinical and clinical studies.

By leveraging prior knowledge of the system and the drugs being studied, PBPK and QSP models are often used for extrapolations. This includes determining the first-in-human dose based on preclinical data, predicting pharmacokinetic and pharmacodynamic (PKPD) profiles in special situations (such as drug-drug interactions) and special populations (such as pediatric patients), aiding in dose adjustment decisions, and optimizing clinical trial designs[6,7].

Despite the theoretical and predictive appeal of complex mechanistic models, their practical applications are hindered by several limitations. One major issue is the lack of specific information on mechanisms and physiological parameter values, especially from special populations during model building[8]. This gap, along with other weaknesses, reduces the credibility of these models.

For example, current approaches for PBPK and QSP models do not adequately assess uncertainty due to their complexity and the sources of set parameters. Most physiological parameters are fixed at average values from literature, without accounting for parameter uncertainty and variability. Drug-specific parameters, derived from observed data (in vitro, in vivo, and/or clinical), are also fixed without considering potential bias and uncertainty from experimental setups and *in vitro-in vivo* extrapolation (IVIVE)[4,8]. Furthermore, when parameters are estimated based on clinical data, the uncertainty of those parameters is usually not evaluated or reported.

Additionally, the adage "all models are wrong" applies here; no matter how complex, these models cannot fully represent biological systems, contributing further to model uncertainty. This impairs the predictability of complex models. Discrepancies between simulated data and observed data are typically described using concise metrics, such as the average (absolute) fold prediction error[9]. Models are sometimes validated by comparing the prediction error to an arbitrary value (e.g., 2-fold or 3-fold), which may not provide a clear understanding of the pharmacological significance of these differences. Moreover, fold-change metrics can oversimplify the diversity in a model's predictive performance and lack the sensitivity needed to detect variations among specific subgroups.

Although sensitivity analysis is regularly conducted, as suggested by regulatory agencies, to evaluate the robustness of PBPK models[10,11], the output is often fold-based uncertainty and/or graphs, focusing on a small portion of key and/or uncertain parameters. Validation data are not directly involved in sensitivity analyses. The above challenges create difficulties for regulators to assess a model's predictive capabilities and its applicability beyond the data used for its development. Further research is needed to develop better methods for characterizing and reporting uncertainty in a model's predictive performance.

In recent years, machine learning (ML) has garnered significant interest in drug discovery and development due to its ability to address several critical challenges in the field[12,13]. During the drug discovery stage, ML algorithms can identify new drug targets, predict potential adverse effects, and optimize drug candidates. In preclinical studies, ML can predict the pharmacokinetic (PK), pharmacodynamic (PD), and safety profiles of new drug candidates. Across different phases of clinical trials, ML approaches can enhance trial management and treatment decisions. For example, ML can predict dose-limiting toxicities[14] and improve dose-finding in phase I studies[15] making more efficient recruitment of trial participants and reducing the required sample size of the phase II studies[16], and build reliable disease progression models by combining ML and pharmacometrics approaches in phase III clinical trials[17].

Similar to mechanism-based models, uncertainty quantification is essential for advancing the reliability and robustness of ML models. However, a widely adopted framework for uncertainty quantification in machine learning is still lacking[18], underscoring the need for further research and development in this area.

Uncertainty quantification (UQ) provides a computational framework for quantifying uncertainties in both inputs and outputs, thereby facilitating predictions with quantified and reduced uncertainties[19]. Typically, UQ involves one or more mathematical models for a quantity of interest, with some uncertainty regarding the correct form of the model or models. These uncertainties are often treated probabilistically[20]. An appropriate UQ method is essential for regulatory decision making which may depend on type I error and power related to hypothesis tests or on confidence intervals / credible intervals related to parameter estimation or prediction. UQ becomes more important when using complicated analysis methods and/or complex models. For example, in previous work, members of our consortium (UU) have demonstrated that in some model-integrated methods based on population pharmacometric models, UQ methods based on information matrices showed inflated type I error, while type I error could be controlled with a more appropriate UQ method (sampling importance resampling)[21–23].

Another group in our consortium (UMG) contributed to the literature on another UQ method, namely Bayesian random-effects meta-analysis, in particular in the setting of a few studies[24]. Shrinkage estimation in these models can be applied to implement dynamic borrowing across different types of studies[25], regions[26] or dose regimens (combinations of doses and frequencies)[27]. More generally, Bayesian hierarchical models are a flexible framework for evidence synthesis, borrowing of information and prediction, as well as a powerful UQ method, especially for applications where variability and uncertainty arise from multiple sources. That is specifically of interest for this project, which focuses on complex mechanistic models, the parameters of which are from literature and data from multiple studies.

Other UQ methods are also of interest for application in complex models used in drug development and evaluation. These include Bayesian calibration[28], model discrepancy analysis[29], and surrogate modeling (e.g., based on polynomial chaos expansion)[30,31]. Various approaches of sensitivity analysis can also be further explored, separately or in combination: (1) probabilistic sensitivity analysis[32] assesses uncertainty by assuming input parameter uncertainty distributions, in contrast to the current practice in PBPK modeling, which often uses fixed values (i.e., deterministic sensitivity analysis). (2) Global sensitivity analysis[33,34] considers parametric correlations to provide a more comprehensive assessment of model sensitivity. An alternative approach involves using prior information, such as the frequentist prior, to link preclinical and clinical data through PBPK models. This method, employed by Mats Karlsson[35,36] (a member of our consortium), estimates model parameters while assessing uncertainty.

In summary, there is a significant lack of well-established and widely recognized methods for assessing the uncertainty of complex models in drug development and evaluation. Recent advancements in uncertainty quantification offer an opportunity to enhance the methodologies for evaluating and validating PBPK, QSP, and ML models, thereby increasing the credibility of these modeling tools for regulatory decision-making.

Against this backdrop, the present literature review seeks to provide a comprehensive overview of the current state of the art in uncertainty quantification for complex models applied in drug development and regulatory evaluation, including physiologically based pharmacokinetic models, quantitative systems pharmacology models, and machine learning approaches. Specifically, it summarizes existing knowledge on the properties, interpretability, and applicability of UQ methods within these contexts, thereby establishing a robust foundation for selecting candidate methods for further investigation in this project.

The twofold primary objectives of this review are:

1. To identify and characterize existing UQ methods used in PBPK, QSP, and ML models within the framework of regulatory decision-making in drug development.
2. To explore UQ methodologies from broader disciplines, including statistics, toxicology, engineering, and analytical chemistry, that may be adaptable to these complex modeling approaches.

2 Methods

2.1 Literature review search

We conducted the literature review in three main steps: searching in databases, screening abstracts, and extracting information from the full texts.

2.1.1 Searching in databases

We conducted a comprehensive literature search in three electronic databases to reduce the risk of missing relevant articles and to minimize the risk of bias in the results: PubMed was chosen to cover literature in biomedicine, health, and related fields such as life sciences,

behavioral sciences, chemical sciences, and bioengineering. MathSciNet was used to cover publications in mathematics and statistics. Scopus was selected as an interdisciplinary database, expanding the scope of the first two with a broad range of research topics. Based on the preliminary plan, we iteratively refined our search terms to balance the number of retrieved papers while ensuring sufficient coverage of UQ methods. As an adaptive design, the search approach was validated against four UQ-related papers referenced in the background of this report [28–30,32]. If the search results failed to capture most of these papers or yielded an excessive number of irrelevant ones, the terms were revised and the search was repeated iteratively.

The search strategy of Objective 1 was to combine two areas:

1. **Uncertainty quantification/analysis**: centered on the core term *"uncertainty"* and including specific methods such as Bayesian hierarchical meta-regression, Bayesian calibration, model discrepancy analysis, surrogate modeling, probabilistic sensitivity analysis, uncertainty propagation, interval analysis, fuzzy computations, and frequentist approaches.

2. **Complex models**:
    a. PBPK & QSP related models: physiologically based pharmacokinetic (PBPK) modeling, physiologically based biopharmaceutics modeling (PBBM), quantitative systems pharmacology (QSP), PBPK models used in toxicology, quantitative systems toxicology (QST)
    b. machine learning (ML) models

The two areas were combined using the logical operator **"AND"**. A fuzzy search strategy was applied to capture spelling variations. For example, the search term "uncertaint*" was used for capturing all the variations of "uncertainty". For ML models, given the large number of potential papers dealing with ML and the scope of the current project, the searching strategy was adjusted to focus on "drug development" to provide a reasonable number of papers for the next step.

To address Objective 2 (broadening the scope of the systematic review), we relaxed the constraint requiring the combination of the two categories with "AND" for the database that contained most methodological information, namely MathSciNet. Instead, specific method terms were treated in the same way as complex model terms in MathSciNet. This means that papers containing either specific methods (e.g., Bayesian calibration) or complex model terms were captured, enabling broader exploration of UQ methodology papers without substantially inflating the total number of retrieved records. This adjustment was appropriate given that MathSciNet primarily indexes mathematical and statistical publications, with comparitively fewer publications using the defined search terms. We applied the same strategy in Scopus, which increased the number of hits from 277 (See Table 3) to 859. Given this substantial increase, and considering time and resource limitations, we implemented the expanded search scope only in MathSciNet, as handling such a large number of papers was not feasible.

The finalized search terms are shown in 3.1 Literature review search.

2.1.2 Screening abstracts

The search results from the first step were imported into the review software **Rayyan** for screening. Records were screened according to predefined inclusion and exclusion criteria. The screening process was conducted independently by two reviewers, and any disagreements regarding the eligibility of a paper were resolved by a third reviewer, who made the final decision.

The predefined inclusion and exclusion criteria are listed as follows:

Table 1: Inclusion and Exclusion Criteria for Selection of publications

Inclusion Criteria	Exclusion Criteria
Research and methodological publications explicitly discussing UQ methods.	Publications are not aligned with the primary objective of evaluating UQ methods in modeling contexts.
Studies presenting case applications of UQ methods in PBPK, QSP, or ML models, including clinical trials, simulation studies, and modelling analyses.	Studies employing UQ methods solely for parameter estimation or sensitivity analysis without a focus on UQ methodology (e.g., local sensitivity analysis).
Publications involving alternative modeling frameworks where UQ methods may be potentially applicable to the current research scope.	Articles lacking full-text availability or access.

2.1.3 Extract information from full texts

The full-text extraction process began with the retrieval of full-text articles using **Zotero**. Publications without accessible full texts were excluded, and duplicates were removed. To support efficient data extraction within the constraints of time and resources, the AI-powered tool **Elicit** was employed. Designed for systematic reviews, **Elicit** automates labor-intensive research tasks such as summarizing papers, extracting data from full texts, and synthesizing findings. During extraction, it presents the retrieved information accompanied by explanations and highlights of the corresponding text from the source, which enables reviewers to efficiently verify the accuracy of the extraction. A set of ten representative papers was used to define and train the extraction instructions, which were subsequently applied across the entire collection of selected studies. The instructions for the columns of text extraction are listed in Appendix 1.

All extracted information was then manually verified to ensure accuracy. This was done by clicking on the hyperlinks supplied by **Elicit** to verify the extracted information. In cases where **Elicit** produced incorrect or incomplete outputs, the information was corrected based on the publications manually. Finally, the verified information was organized and summarized in a

spreadsheet to support further analysis. Through our manual verification, we found that **Elicit** offers notable advantages, particularly in saving time by automating the extraction process and reducing manual effort in verifying the accuracy of extraction (**Elicit** hyperlinks the extracted information to locations in the manuscripts where that information was found). It also shows strong accuracy in extracting some information from both full texts and tables, such as type of model, software used, software availability and so on. However, its accuracy is limited when categorizing content or summarizing information that is not explicitly stated in the text, for example, identifying the type of paper (application or method) or the stage of drug development was challenging for **Elicit**.
The search results were organized with the following 20 columns:

Table 2: Columns for Text Extraction

ID	Related to drug development: Yes/No
Title	Purpose of the model
Authors	Type of product
Source/Journal	Therapeutic area
Year	Stage of drug development
DOI/Full text link	Simulation for evaluating UQ methods: Yes/No
Inclusion: Yes/No, if no, put reason in comments	Software availability: Open source/Commercial/Open source+Commercial/No
Type of paper: Methodology/Application/Review	Code availability: Open source/Commercial platform with given parameters/upon request to the authors/No
Type of model: PBPK/QSP/ML/Others	Software used
UQ methods	Comments

2.2 Quantitative and qualitative analysis

Characteristics of articles and proposed methods were described by using descriptive analyses such as line charts and bar charts. The collected categorical variables were summarized by providing absolute and relative frequencies. To enable an overview of the uncertainty quantification methods, model names as they were proposed by the authors were classified into broader classes of models. The main characteristics of these suggested

categories are introduced, and examples for the categories were provided. All statistical analyses were performed in R (version 4.5.1).

3 Results

3.1 Literature review search

A comprehensive database search retrieved 764 distinct publications related to PBPK and QSP models as of July 3rd, 2025, and 75 publications related to ML models as of July 10th, 2025. The search captured three of the four pre-specified quality control (QC) papers. The remaining paper, *Good practices for quantitative bias analysis* [32], was not captured because the abstract contained only the term “uncertainty” and none of the other specific search terms listed in 2.1.1 Searching in the databases. We tested an expanded search scope by adding the term “bias analysis,” but this substantially increased the number of records (n=3254) that focused on bias more broadly and for fields with less relevance for the purpose of this review (such as epidemiologic research in general) rather than uncertainty quantification approaches suitable for mechanistic models. It is worth noting that it was not a strict requirement for the search to capture all QC papers, given the constraints of time and resources. Therefore, we kept the original search terms and incorporated this paper during the full-text extraction stage.

The finalized search terms and the corresponding stepwise results are summarized as follows:

Table 3: Final Search Terms for Literature Review on PBPK & QSP related models

Model type	Database	Search No.	Search terms	Results
PBPK & QSP related models	Scopus	1	TITLE-ABS-KEY (uncertaint* W/3 (quantif* OR propagat* OR bayesian OR frequentist OR stochastic OR "surrogate models" OR metamodels OR distribution* OR interval OR sensitivity OR discrepanc* OR fuzzy OR analysis))	269,705
		2	TITLE-ABS-KEY (pbpk OR pharmacokinetic* OR pharmacometric* OR "systems pharmacology" OR qsp OR “quantitative systems toxicology” OR qst OR “physiologically based biopharmaceutics” OR pbbm)	403,563
		3	#1 AND #2	277
	MathSciNet via EBSCOhost	1	TI uncertaint* OR AB uncertaint*	36,787
		2	PO "92C45" 92C45 (1991–now) Kinetics in biochemical problems (pharmacokinetics, enzyme kinetics, etc.)	1499
		3	TI pbpk OR“quantitative systems toxicology” OR qst OR pharmacokinetic* OR pharmacometric* OR "systems pharmacology" OR qsp OR "physiologically based biopharmaceutics" OR pbbm OR "bayesian calibration" OR "probabilistic sensitivity" OR "model discrepanc*" OR "surrogate based" OR AB pbpk OR pharmacodynamic* OR pharmacokinetic* OR pharmacometric* OR "systems pharmacology" OR qsp OR "physiologically based biopharmaceutics" OR pbbm OR "bayesian calibration" OR "probabilistic sensitivity" OR "model discrepanc*" OR "surrogate based" OR“quantitative systems toxicology” OR qst	954
		4	#2 OR #3	
		5	#1 AND #4	100
	PubMed	1	"Uncertainty"[Mesh]	
		2	"quantify uncertainty"[tiab:~3] OR "quantifying uncertainty"[tiab:~3] OR "quantification uncertainty"[tiab:~3] OR "propagation uncertainty"[tiab:~3] OR "bayesian uncertainty"[tiab:~3] OR "frequentist uncertainty"[tiab:~3] OR "stochastic uncertainty"[tiab:~3] OR "surrogate models uncertainty"[tiab:~3] OR "metamodels uncertainty"[tiab:~3] OR "distribution uncertainty"[tiab:~3] OR "interval uncertainty"[tiab:~3] OR "quantify uncertainties"[tiab:~3] OR "quantifying uncertainties"[tiab:~3] OR "quantification uncertainties"[tiab:~3] OR "propagation uncertainties"[tiab:~3] OR "bayesian uncertainties"[tiab:~3] OR "frequentist uncertainties"[tiab:~3] OR "stochastic uncertainties"[tiab:~3] OR "surrogate models uncertainties"[tiab:~3] OR "metamodels uncertainties"[tiab:~3] OR "distribution uncertainties"[tiab:~3] OR "interval	

			uncertainties"[tiab:~3] OR "discrepancy uncertainty"[tiab:~3] OR "fuzzy uncertainty"[tiab:~3] OR " sensitivity uncertainty"[tiab:~3] OR "discrepancy uncertainties"[tiab:~3] OR "fuzzy uncertainties"[tiab:~3] OR " sensitivity uncertainties"[tiab:~3] OR “uncertainty analysis” [tiab:~3] OR “uncertainties analysis” [tiab:~3]	
		3	#1 OR #2	
		4	"Pharmacokinetics"[Mesh] OR "pharmacokinetics" [Subheading] OR “Toxicology” [Mesh]	
		5	pbpk[tiab] OR pharmacokinetic*[tiab] OR pharmacometric*[tiab] OR "systems pharmacology"[tiab] OR qsp[tiab] OR “quantitative systems toxicology” [tiab] OR qst [tiab] OR “physiologically based biopharmaceutics” [tiab] OR pbbm[tiab]	
		6	#4 OR #5	
		7	#3 AND #6	534

Table 4: Final Search Terms for Literature Review on ML models

Model type	Database	Search No.	Search terms	Results
ML models	Scopus	1	TITLE-ABS-KEY (uncertaint* W/3 (learn* OR machine* OR deep* OR bayesian OR xgboost OR "random forest" OR predict* OR "model prediction" OR "neural network" OR "Gaussian process"))	41,683
		2	TITLE-ABS-KEY ("drug development”)	138,385
		3	#1 AND #2	73
	MathSciNet via EBSCOhost	1	pc:68T *68T: Artificial Intelligence	33,340
		2	ti:uncertaint* OR ab:uncertaint*	14,816
		3	#1 AND #2	362
		4	ti:(learn* OR machine* OR deep* OR bayesian OR xgboost OR "random forest" OR predict* OR	97,953

			"model prediction" OR "neural network" OR "Gaussian process")	
		5	#2 AND #4	1083
		6	#1 AND #2 AND #4	56
		7	ti:"drug development" OR ab:"drug development"	77
		8	#6 AND #7	1
	PubMed	1	"Uncertainty"[Mesh]	
		2	"machine learning"[tiab:~3] OR "deep learning"[tiab:~3] OR "bayesian regression"[tiab:~3] OR "xgboost regression"[tiab:~3] OR "random forest"[tiab:~3] OR "model prediction"[tiab:~3] OR "neural network"[tiab:~3] OR "Gaussian process"[tiab:~3]	344,394
		3	#1 AND #2	949
		4	"drug development"[tiab]	52,536
		5	#3 AND #4	2

Following the abstract screening stage, 481 publications (57.3%) were excluded due to irrelevance to the review objectives. After incorporating the remaining QC paper into the database, a total of 358 abstracts were subjected to full-text retrieval. Of these, 65 were excluded, resulting in 293 publications included in the final analysis (see PRISMA flow diagram **Figure 1**).

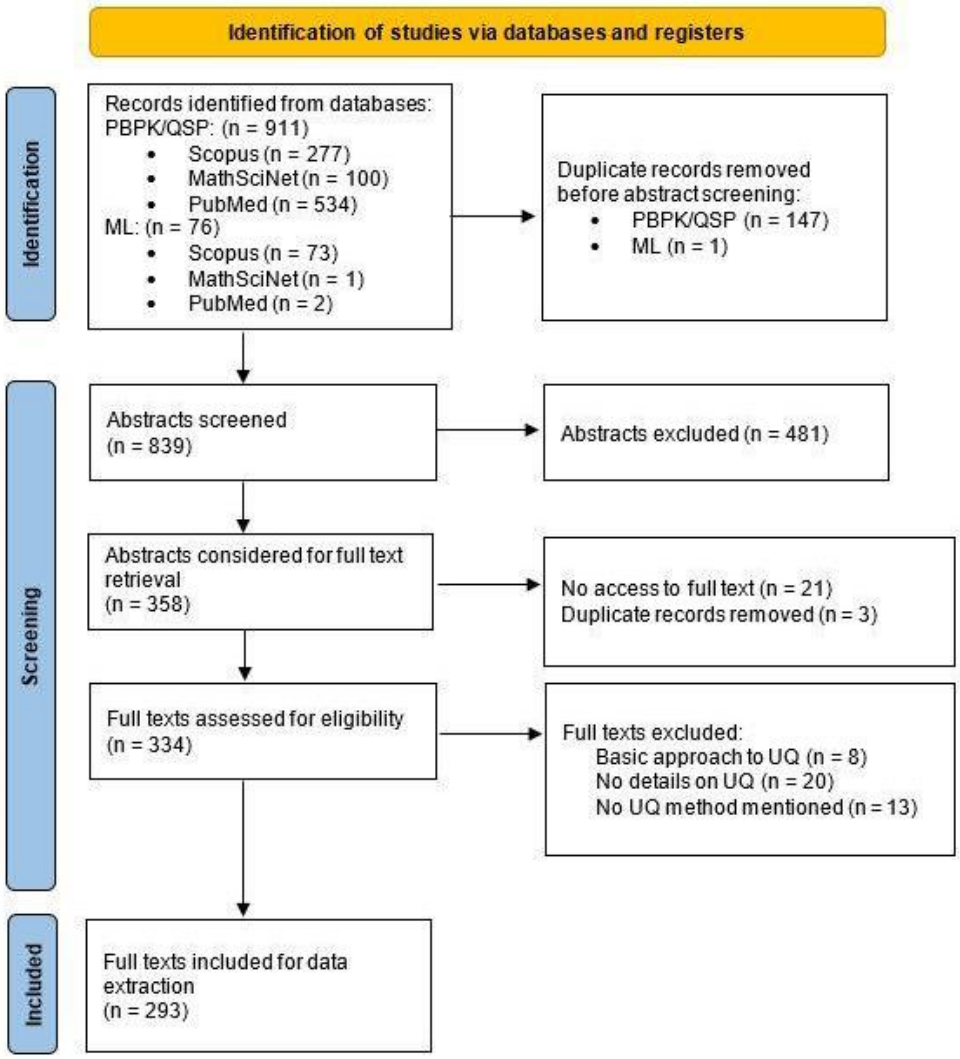

Figure 1: PRISMA 2020 flow diagram

The most frequent reasons for exclusion during the full-text review were: (i) the absence of any mention of UQ methods, (ii) insufficient methodological details regarding UQ approaches. Additional exclusions were made for articles focusing on topics outside the scope of this review and for studies describing well-established techniques for complex models, such as local sensitivity analysis, uncertainty factor analysis, and confidence interval approach.

3.2 Quantitative and qualitative analysis

A table with all extraction information is provided as **Supplementary material**.
75 % of the articles in our review were published in 2010 or later. Only 18 articles were published before 2000. **Figure 2** shows the publication years of included articles by type of paper. The number of publications is summarized and plotted with one datapoint for each 5-year period. The year 2025 is not included because the year is not yet over and it starts a new 5-year period that would be incomplete and thus misleading in the plot.

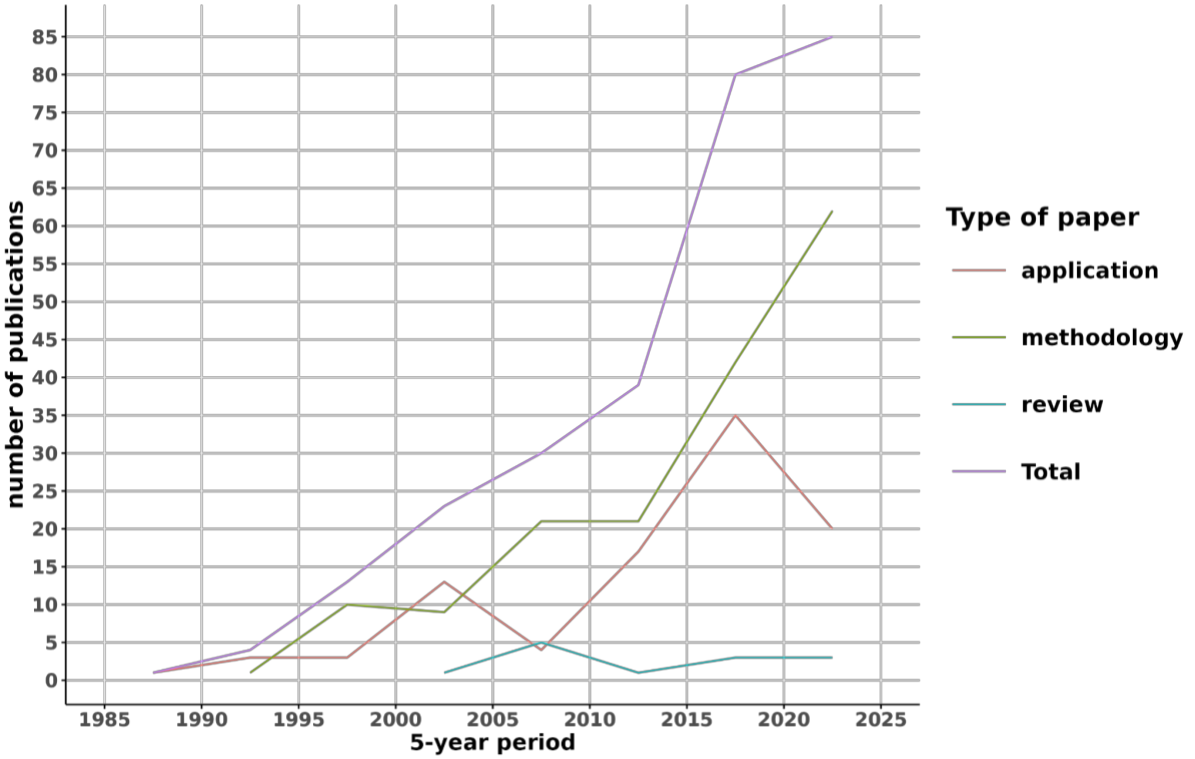

Figure 2: Time trend of the number of publications by type of paper

The largest proportion of included articles (53%, n=198) are methodological, 31% (n=103) are applications, and 4% (n=14) are reviews.

Figure 3 shows which types of complex models were addressed. Physiologically based pharmacokinetic models (PBPK) represented the largest group of complex models that were applied or investigated in the included articles (28%, n=95). Quantitative systems pharmacology (QSP) models were only explicitly studied in 3 articles. 11% of the articles addressed uncertainty quantification for machine learning models. The remaining articles (48%, n=159) are either purely theoretical without a focus on a specific complex model, categorized as “Others”. Figure 4 breaks down the models within the “Others” category. This category includes “less complex” pharmacological models (n=31), such as pharmacokinetic/pharmacodynamic (PK/PD) models. It also covers models related to the field of medicine (n=42), mathematical methods and theory (n = 42), environmental modeling and risk assessment (n=19), human risk and safety assessment (n= 17), engineering-related models (n = 5), and epidemiology models (n = 3).

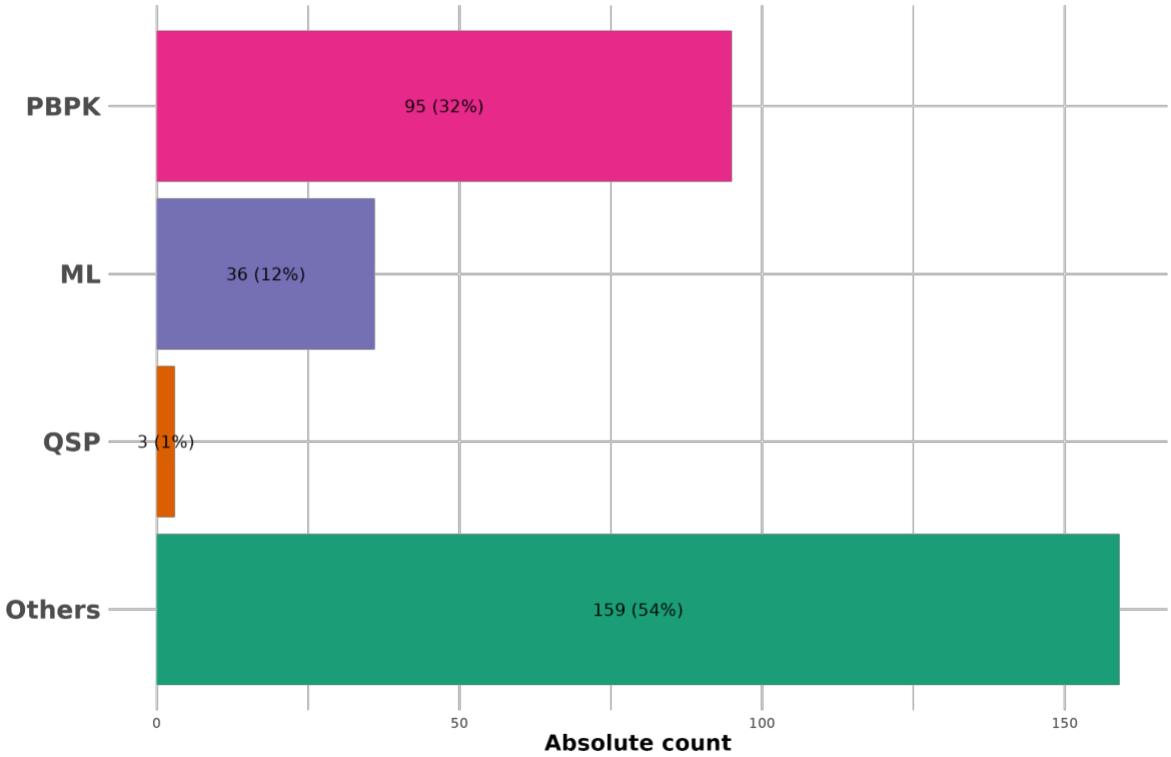

Figure 3: Absolute number of included articles by type of complex model

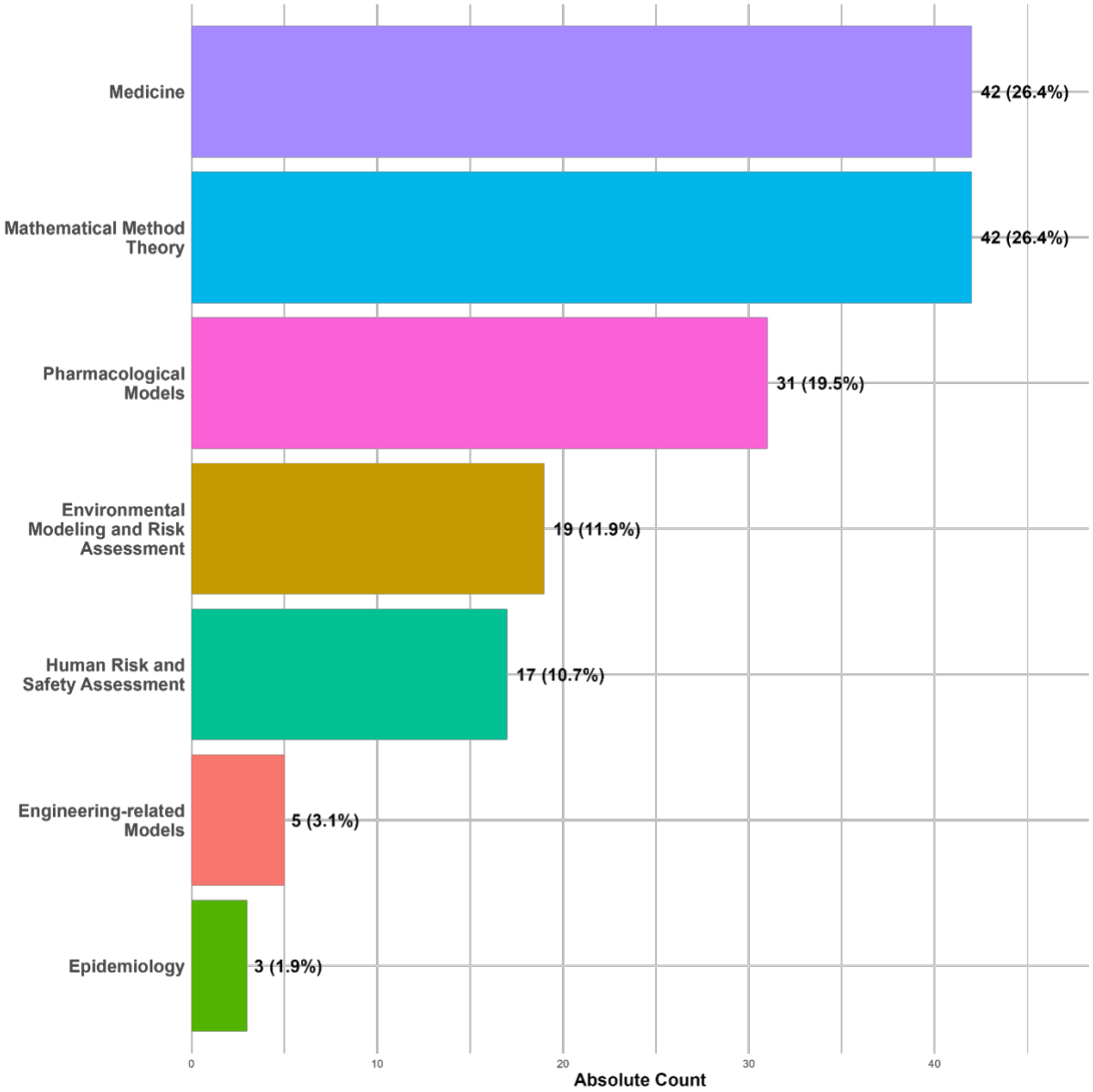

Figure 4: Absolute number of articles by type of models in the “Others” category (n=159)

In total, 129 articles conducted some simulation on uncertainty quantification methods which corresponds to 44% of articles. 36% of articles used and specified an open source software to implement uncertainty quantification methods, mostly R and Python. 22% (n=29) of articles used commercial platforms, e.g. Matlab, WinBUGS, @RISK (Palisade Corporation), NONNEM or Oracle Crystal Ball. A large proportion of articles did not specify the software that was used (41%, n=53). Code or scripts are available for only 25% (n=32) of articles with simulations. Most of those are open access (19%, n=24) (see **Figure 5**). Some articles provide code only upon request to the authors (n=6) or in the form of parameter information that can be used as inputs for commercial platforms (n=2). Examples for software used for specific uncertainty quantification methods can be found in the column “software used” in the extraction table that is provided as **Supplementary material** (filter by columns `UQ method - rough` or `UQ method - fine`).

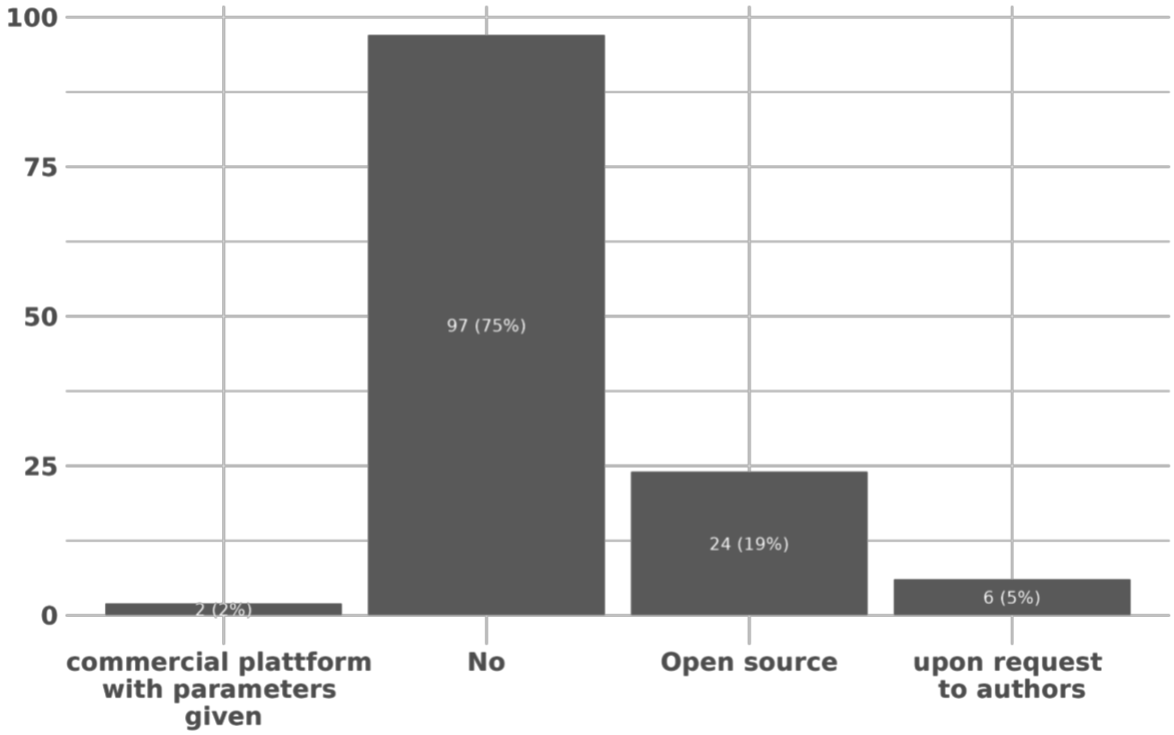

Figure 5: Absolute number of articles with a simulation study by type of code availability

About half of both methodological papers and applications were related to the development, repurposing or maintenance of a drug or vaccine for clinical use (see **Figure 6**). Drug development was defined to include drug discovery, chemistry and pharmacology, nonclinical safety testing, dose finding, manufacturing, clinical trials, and regulatory submissions. 73% of the applications related to drug development focused on a specific therapeutic area compared to 53% of methodological articles. Details and examples for therapeutic areas, types of products, stage of drug development and purpose of the pharmacokinetic model can be found by filtering the extraction table that is provided as **Supplementary material** (`Drug therapy development`=”Yes”).

Among the 14 reviews identified in the search, 8 focused on drug development. The most frequently mentioned UQ methods in these reviews were Bayesian approaches, particularly Bayesian hierarchical meta-regression and Bayesian Markov chain Monte Carlo (MCMC) analysis. Other methods noted included Monte Carlo simulation, uncertainty propagation, and fuzzy computations.

The remaining 6 reviews, which were outside the context of drug development, highlighted a more diverse set of UQ methods. These included Bayesian approaches such as Bayesian hierarchical meta-regression and Bayesian calibration, as well as parametric bootstrapping, Monte Carlo simulation, MCMC simulation, Gaussian process surrogate modeling, uncertainty propagation, uncertainty factors, sensitivity analysis, and likelihood-based methods.

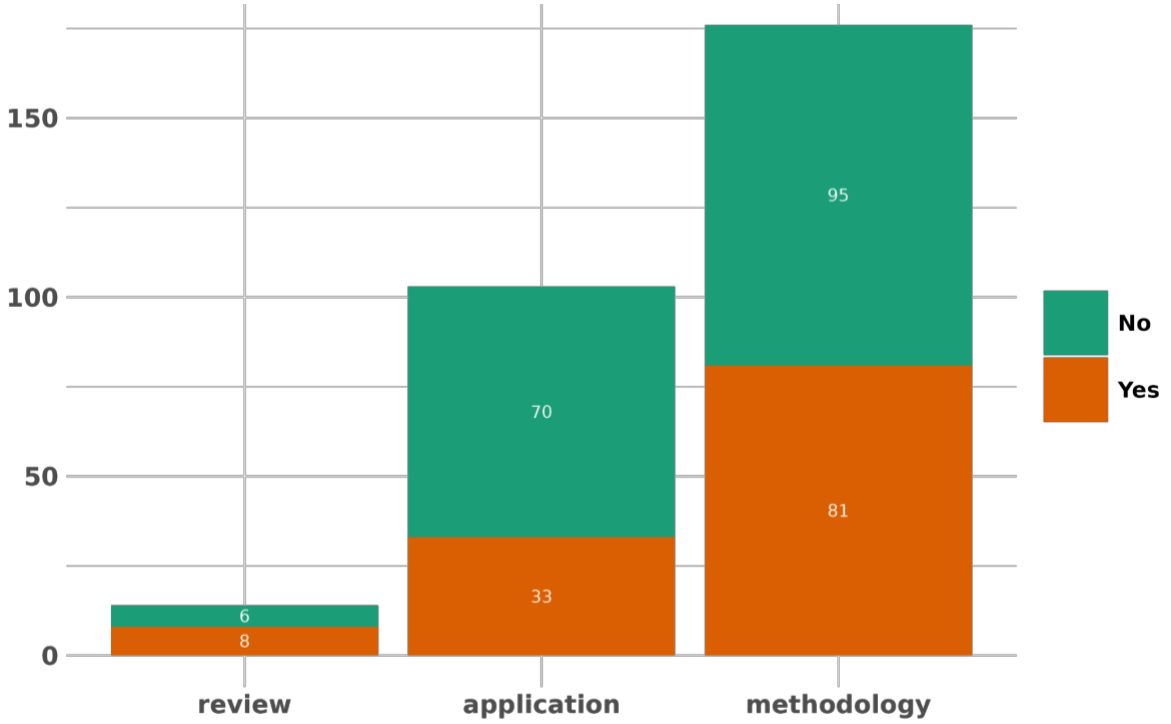

Figure 6: Absolute number of articles related to drug development by type of paper

3.3 Classification of uncertainty quantification methods

In the literature, there is currently no comprehensive summary and classification of all uncertainty quantification (UQ) methods, and as a result, the screening process began without the guidance of such a framework. During the screening, specific names of methods as well as more general keywords like sensitivity analysis and uncertainty propagation were extracted. Subsequently, these identified methods were organized into broader categories to provide a more structured analysis of the results. This classification resulted in six categories: Global Sensitivity Analysis, Uncertainty Propagation, Bayesian Methods, Basic Frequentist Approaches, Stochastic and Uncertain Differential Equations and other methods. Of these groups, the first four were further subdivided. A list of all included papers, along with the extracted keywords and methods related to uncertainty quantification can be found in the **Supplementary material**.

Global Sensitivity Analysis can be defined as “[...] the study of how the uncertainty in the outcome of a model can be distributed to different sources of uncertainty in the input model”[37]. It assesses the contribution of inputs to output variability and can identify non-linear interactions. Examples include the Morris method[39], Sobol indices[38], polynomial chaos expansion[41] and the Fourier Amplitude Sensitivity Test[40]. To address the varying degree of theoretical complexity in the approaches, three subcategories were introduced: simulation-based methods, e.g. Morris method, advanced analytical methods, e.g. polynomial chaos expansion[41] and other methods that were not detailed enough to be placed into one of the mentioned categories above. The degree of complexity lies on a continuous scale and can therefore only roughly be approximated by this categorization.

Uncertainty Propagation involves predicting how uncertainties in input variables propagate through models to affect outputs. While global sensitivity analysis and uncertainty propagation methods are closely connected, the former is more concerned with uncertainty in the input variables, whereas the latter focuses more on the outcome variables. Techniques in this category can further be divided into probabilistic and non-probabilistic approaches. Prominent examples for the latter are fuzzy computation and interval analysis[42]. Probabilistic approaches often require a simulation method e.g. Monte Carlo simulation[43] to assess the propagation of uncertainty either simply through the original model or in a more complex approach through a surrogate model[44], e.g. Kriging method[45]. Other probabilistic approaches that did not fit into the two categories "Basic simulation" or "Surrogate model" or were not detailed enough to classify, were grouped into a third subcategory for probabilistic approaches, resulting in four subcategories for uncertainty propagation in total.

Bayesian methods describe uncertainty in parameter estimates by incorporating prior knowledge along with the likelihood of observed data to update the probability distribution of the parameters. They encompass a wide variety of different methods and therefore are further subdivided into Bayesian hierarchical modelling, Bayesian calibration, and Bayesian machine learning methods e.g. using Monte Carlo dropout to assess the epistemic uncertainty of a neural network[46]. Again, a category was introduced for other Bayesian methods. Assessing the resulting posterior distribution relies mostly on simulation-based methods, e.g. Markov Chain Monte Carlo sampling[47].

Frequentist methods in the context of uncertainty quantification can range from basic techniques like standard errors to more complex techniques involving confidence intervals and hypothesis tests for model parameters. To further differentiate the methods in the context of uncertainty quantification three subgroups were introduced, likelihood-based methods, resampling and other frequentist methods. Likelihood-based methods help to characterize the uncertainty associated with model parameters through the likelihood function, e.g. log-likelihood profiling relying on the likelihood ratio test[48]. Resampling involves repeatedly drawing samples from a dataset to assess the stability and reliability of statistical estimates. Resampling techniques such as bootstrapping and the jackknife method allow for the estimation of parameter uncertainty without relying heavily on parametric models[49,50].

The methods in the category uncertain/stochastic differential equations (UDE/SDE) arise from replacing the model equations of a pharmacometric model, which are typically ordinary differential equations, with uncertain differential equations or stochastic differential equations. The use of UDEs and SDEs allows for direct modeling and assessment of noises on model parameters, e.g. measurement error, intra- or interindividual variability. While stochastic pharmacokinetic models are driven by the Brownian motion, uncertain pharmacokinetic models are driven by the Liu process[51], which was designed under the framework of uncertainty theory as a stationary independent increment process whose increments are normal uncertain variables rather than random variables[52].

Methods that could not be placed into one of the categories above based on the extracted information were combined in a separate group, later referred to as "Other". If a paper applies or compares multiple different methods, all the corresponding categories were assigned, resulting in an analysis of the absolute number of mentions per category rather than the proportional distribution. As illustrated in **Figure 7,** the Bayesian methods were used most

often followed by simulation-based techniques in global sensitivity analysis and uncertainty propagation. Methods that involve a more complex theoretical setup like uncertain differential equations or surrogate modeling are applied less frequently.

It is important to note that even for a specific method, the categories of this framework are not fully disjoint. The classification is also dependent on the thoroughness of the description of the uncertainty quantification within a paper, which can vary significantly and therefore can lead to ambiguities which result in a considerable use of the “Other” category.

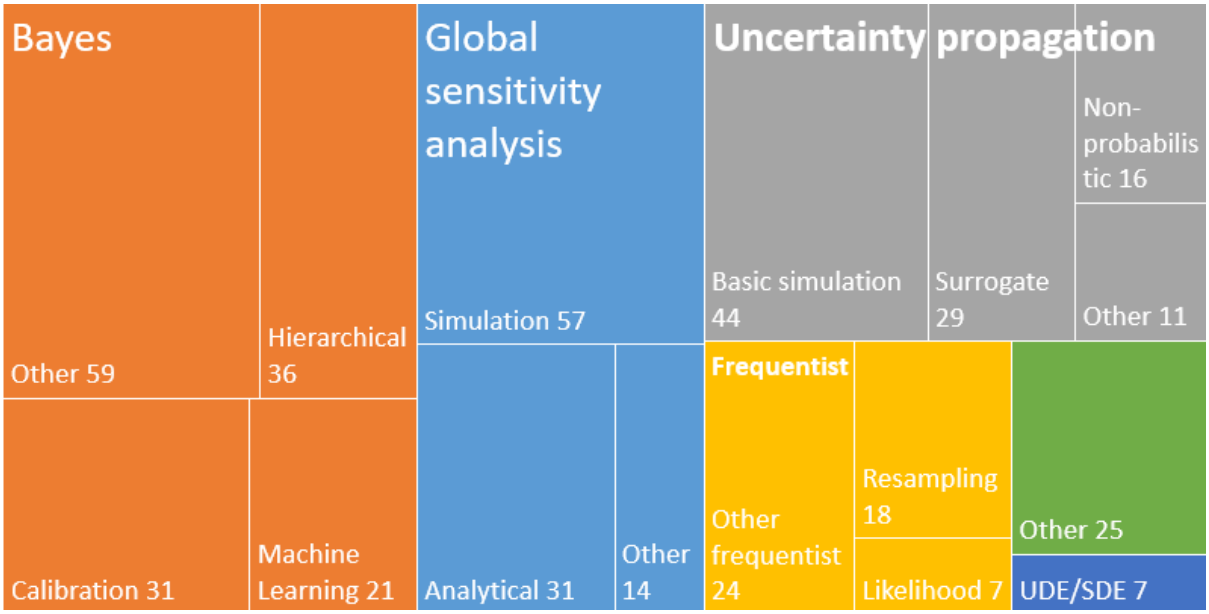

Figure 7: Classification of uncertainty quantification methods with absolute number of occurrences in all included articles

As illustrated in **Figure 8**, simulation-based global sensitivity analysis and uncertainty propagation were the most frequently applied or studied types of uncertainty quantification methods in current articles that apply to physiologically based pharmacokinetic models (PBPK) or quantitative systems pharmacology (QSP) models. Bayesian and frequentist methods were applied less often in this field than overall (compare **Figure 7**).

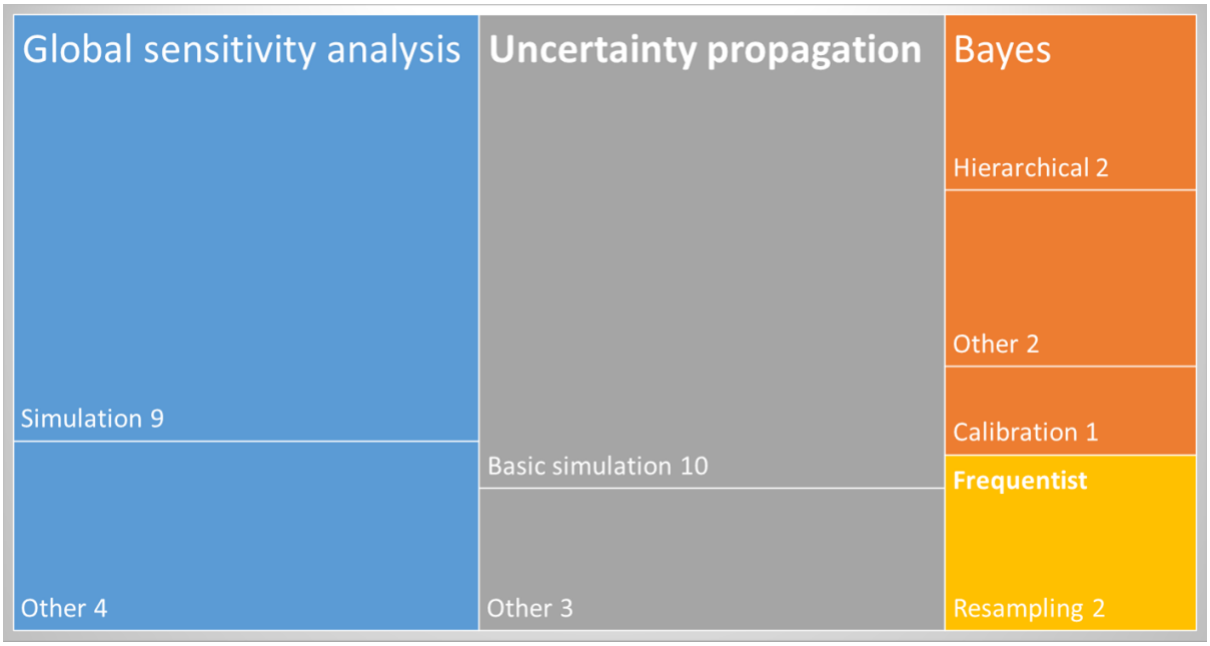

Figure 8: Uncertainty quantification methods applied or investigated in the context of PBPK or QSP models in the last 10 Years (since 2015)

3.4 List of highly relevant papers for further work

During the full text extraction, 19 papers were identified as highly relevant to the project aim. These papers covered both methodological developments and applications of advanced UQ techniques that could be considered for future simulation studies, such as Bayesian hierarchical modeling and global sensitivity analysis. It should be noted that the selection of specific UQ techniques for the coming simulation study will be addressed later and the purpose of this collection is solely to provide a broad reference base. The selected papers and their key contributions are summarized below:

1. A Bayesian population PBPK model for multiroute chloroform exposure[53].
   Applied Bayesian hierarchical modeling method to assess the UQ of a PBPK model.
2. A computational workflow for probabilistic quantitative in vitro to in vivo extrapolation[54].
   Employed global sensitivity analysis with the approximate Bayesian computation to evaluate the UQ of a PBPK model.
3. A framework for 2-stage global sensitivity analysis of GastroPlus™ compartmental models[55].
   Applied global sensitivity analysis to evaluate the UQ of a PBPK model.
4. A fuzzy physiologically based pharmacokinetic modeling framework to predict drug disposition in humans[56].
   Proposed a PBPK framework using fuzzy computations to assess UQ.
5. A generalized polynomial chaos-based method for efficient Bayesian calibration of uncertain computational models[57].
   Provided theoretical foundations for Bayesian calibration and polynomial chaos methods.
6. A Novel Method for Assessing Drug Degradation Product Safety Using Physiologically-Based Pharmacokinetic Models and Stochastic Risk Assessment[58].

Applied probabilistic sensitivity analysis to assess UQ of a PBPK model.

7. A sequential calibration and validation framework for model uncertainty quantification and reduction[59].
   Reviewed advanced UQ methods, including Bayesian calibration and Gaussian process surrogate modeling.
8. Analysis of PBPK models for risk characterization[60].
   Applied Bayesian hierarchical modeling method for UQ of a PBPK model.
9. Assessing drug distribution in tissues expressing P-glycoprotein using physiologically based pharmacokinetic modeling: identification of important model parameters through global sensitivity analysis[61].
   Identified key model parameters using global sensitivity analysis to evaluate UQ.
10. Bayesian calibration of computer models[62].
    Illustrated the Bayesian calibration methodology.
11. Bayesian calibration of multistate stochastic simulators[63].
    Focused on Bayesian calibration methods for large-scale models.
12. Bayesian calibration, validation, and uncertainty quantification of diffuse interface models of tumor growth[64].
    Discussed Bayesian calibration techniques and Bayesian inference methods.
13. Bayesian evaluation of a physiologically based pharmacokinetic (PBPK) model for perfluorooctane sulfonate (PFOS) to characterize the interspecies uncertainty between mice, rats, monkeys, and humans: Development and performance verification[65].
    Applied Bayesian hierarchical modeling method to assess the UQ of a PBPK model.
14. Bayesian methods for uncertainty factor application for derivation of reference values[66].
    Applied Bayesian approaches to UQ in a PBPK model.
15. Human Variability in Carboxylesterases and carboxylesterase-related Uncertainty Factors for Chemical Risk Assessment[67].
    Used Bayesian hierarchical modeling method to assess UQ of a PBPK model for chemical risk assessment.
16. Improving the estimation of parameter uncertainty distributions in nonlinear mixed effects models using sampling importance resampling[68].
    Introduced sampling importance resampling to improve UQ estimation.
17. Probabilistic framework for the estimation of the adult and child toxicokinetic intraspecies uncertainty [69].
    Discussed probabilistic sensitivity analysis and uncertainty propagation methods.
18. Uncertainty quantification and propagation in surrogate-based Bayesian inference[70].
    Focused on Bayesian approaches to surrogate modeling and UQ.
19. Using machine learning surrogate modeling for faster QSP VP cohort generation[71].
    Applied ML surrogate modeling for a QSP model.

4 Conclusion and discussion

This review shows a clear gap in the availability of well-established methods for UQ tailored to complex models in drug development and regulatory evaluation, as illustrated in **Figure 8**. Nonetheless, a diverse range of UQ techniques originating from disciplines such as mathematics and statistics, engineering, analytical chemistry, and toxicology holds substantial

potential for application in this context, as illustrated in **Figure 7**. Among these, global sensitivity analysis, uncertainty propagation, and Bayesian approaches emerged as the most frequently reported and widely applied methods.

The findings underscore the critical importance of adapting adequate UQ methodologies to improve the reliability and robustness of PBPK, QSP, and ML models. By identifying promising candidate methods from both within and outside drug development, this review lays the groundwork for targeted simulation studies. These next steps will provide a robust evidence base for selecting and refining UQ methods that can meaningfully enhance decision-making in drug development and evaluation.

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Appendix 1

The columns and the corresponding instructions that are used in full-text extraction step

Column	Instructions
Inclusion	Include or exclude the paper based on the following criteria: **Inclusion criteria:** - Research and methodological publications discussing uncertainty quantification (UQ) methods. - Publications, presenting case studies, where UQ methods for PBPK, QSP, and ML models have been applied (clinical trials, simulation study, and modeling). - Publications including other types of models that the UQ method may be potentially useful for our case **Exclusion criteria:** - Investigations/publications that are not relevant to the main objective: - Do not focus on UQ for modeling problems considered. - Case study using UQ methods for estimation, but not focusing on UQ. For example: Local sensitivity analysis…
Type of paper: Methodology/Application/Review	- Only one answer is allowed for each paper. If a paper includes elements of several different publication types, decide from context which one fits the main purpose of the paper best and use this as an answer. The main focus of the paper decide if the paper should be classified as methodology or application, or review. You can ignore single aspects of the paper that suggest a category that differs from the main focus of the paper. - Papers that focus on application, i.e., the purpose of the study is to understand, develop, design, etc, models regarding a specific product or drug should be categorized as "application". For example, some PBPK paper applies some existing UQ method to develop a good model for that application, but do not specifically evaluate the used UQ method in comparison to other models. - Classify papers as methodology if the main purpose and focus of the paper is to introduce or evaluate UQ methodology, such as adapting or extending a model framework. -Classify papers as "application" if the paper used an uncertainty method for estimation rather than focusing on the uncertainty method development or evaluation
UQ methods	Extract the statistical methods used for uncertainty estimation& qualification. E.g., Bayesian hierarchical meta-regression, Bayesian calibration, model discrepancy analysis, surrogate modeling, probabilistic sensitivity analysis, uncertainty propagation, interval analysis, fuzzy computations, frequentist.
Drug therapy development: Yes/No	- Check if the paper is related to the development, repurposing or maintenance of a drug or vaccine for clinical use. Drug development includes drug discovery, chemistry and pharmacology, nonclinical safety testing, dose finding, manufacturing, clinical trials, and regulatory submissions. - Also include papers that focus on existing drugs

Drug therapy development: Therapeutic area	Check if the paper is related to drug therapy or vaccine development. If yes, state the therapeutic area the drug is applied in and the corresponding ICD 11 code. If no: give precisely the answer: "not applicable".
Drug therapy development: Type of the product: small molecule, biologics, not applicable	Check if the paper is related to drug therapy or vaccine development. If yes, state the type of product. If no: give precisely the answer: "not applicable".
Drug therapy development: Stage of drug development	Check if the paper is related to drug therapy or vaccine development. If the paper is related to drug therapy or vaccine development and: - the stage is clearly stated in the paper, use that term and add "(stated)" or - the stage is not clearly stated but you can tell from context, state your best guess and add "(guess)" or - the stage is not mentioned and also not clear from context, state "not specified". If the paper is not related to drug therapy or vaccine development just state: "not applicable"
Drug therapy development: Purpose of the model	Check if the paper is related to drug therapy or vaccine development. If yes give the purpose of the used pharmacometric model. Examples are: dose finding, identification of subpopulations. If the paper is not related to drug therapy or vaccine development just state: "not applicable"
Simulation	Determine whether the paper uses a simulation study to evaluate uncertainty quantification methods. If the simulation is solely used for assessing model prediction, respond with "No"
Software availability	Is the software and skripts that were used to implement the uncertainty models described in the paper? The information is often given in the data availability statement. Use the following categories: open source, commercial platform, no. - Open source means that the code is publicly availiable for example scripts that are provided in the appendix and ready to use. The information which programming language or plattform was used is not sufficient. Skripts or code have to be provided or there should be instructions on how or where to access code that is freely availiable somewhere - commercial platform means a commercial platform is used which does not allow to easily reproduce the analyses. The information which programming language or plattform was used is not sufficient by itself. Instructions to access skripts or code or at least some parameter values or model equations used for specifying the model have to be given - no means the software to reproduce the results is not

	mentionned at all or there are no instructions on how to implement the model in the software (no instructions on skript or code availiability or configuration of model parameters or model equations) - only 1 of the 3 categories can be chosen
code availability	Were code or scripts, or model parameters, provided that allow reproduction of the UQ models? If no instructions are given in the paper on how to access code, scripts or how to reproduce the model using specified model parameters and equations then classify this as "no". "commercial platform with given parameters" means a commercial platform was used, and instructions to access scripts or code or at least some parameter values or model equations necessary to reproduce the model are given. Open source means that code/skript are contained in the paper or appendix, or instructions are given on how to freely access the code/scripts somewhere else, and the analyses can be reproduced using open source software. "Upon request to the authors" means that code or instructions for reproducibility are not directly available in the paper, but there is a specific statement in the paper offering readers to obtain code or scripts from the authors.
software used	Include the names of any software, packages, programming languages, etc., used in the study to estimate the uncertainty quantification model. Leave blank if no such software was used or mentioned.

Supplementary material:
literature_review_sup1_summary.xlsx

Bibliographic information and extracted information for all articles included in our systematic review.

Title	Authors	DOI	DOI link	Venue	Citation count	Year	Inclusion	Type of paper	Type of model	Uncertainty quantification methods	UQ method - rough	UQ method - fine	Drug therapy development	Drug therapy development: Therapeutic area	Drug therapy development: Type of the product	Drug therapy development: Stage of drug development	Drug therapy development: Purpose of the model	Simulation	Software availability	code availability	software used
"AI-MCMC" for the parametric analysis of the hormonal therapy of cancer	Fuzhang Wang, M Idrees, Ayesha Sohail	10.1016/j.chaos.2021.111618	https://doi.org/10.1016/j.chaos.2021.111618	Chaos, Solitons and Fractals	11	2021	Yes	methodology	Others	Sobol sensitivity analysis (global SA), Monte-Carlo estimation	Sensitivity analysis	SA - simulation	Yes	not applicable	not applicable	not applicable	The purpose of the model is to simulate and analyze the effects of chemotherapy and immunotherapy on tumor cells, focusing on pharmacokinetic-pharmacodynamic (PK-PD) effects and the effectiveness of different administration methods.	No	Commercial platform	No	MATLAB Simulink
Bayesian model calibration for block copolymer self-assembly: Likelihood-free inference and expected information gain computation via measure transport	Baptista, Ricardo, Cao, Lianghao, Chen, Joshua, Ghattas, Omar, Li, Fengyi, Marzouk, Youssef M., Oden, J. Tinsley	10.1016/j.jcp.2024.112844	https://doi.org/10.1016/j.jcp.2024.112844	Journal of Computational Physics	3	2024	Yes	methodology	Others	Bayesian calibration, likelihood-free inference (LFI), expected information gain (EIG), measure transport	Bayes, Other	Bayes - calibration	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to block copolymer self-assembly and lithography, not drug therapy or vaccine development)	Yes	Open source	Open source	- TransportMaps Python package - FEniCS library - hIPPylib python package - Python programming language
A Bayesian model calibration framework to evaluate brain tissue characterization experiments.	Teferra, Kirubel, Brewick, Patrick T.	10.1016/j.cma.2019.112604	https://doi.org/10.1016/j.cma.2019.112604	Computer Methods in Applied Mechanics and Engineering	19	2019	Yes	methodology	Others	Bayesian calibration, nested sampling algorithm, probabilistic sensitivity analysis	Sensitivity analysis, Bayes	SA - simulation, Bayes - calibration	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to mechanical properties of brain tissue and simulation-based applications, not drug therapy or vaccine development)	No	Open source	No	MultiNest
A trichloroethylene risk assessment using a Monte Carlo analysis of parameter uncertainty in conjunction with physiologically-based pharmacokinetic modeling.	Cronin WJ 4th, Oswald EJ, Shelley ML, Fisher JW, Flemming CD	10.1111/j.1539-6924.1995.tb00752.x	https://doi.org/10.1111/j.1539-6924.1995.tb00752.x	Risk analysis : an official publication of the Society for Risk Analysis	35	1995	Yes	methodology	PBPK	Monte Carlo simulation, sensitivity analysis	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	not applicable (the paper is related to risk assessment for trichloroethylene and not to drug therapy or vaccine development)	Yes	Commercial platform	Commercial platform with given parameters	PBPK SIM, developed by Clement International Corporation
Bayesian estimation of pharmacokinetic parameters for DCE-MRI with a robust treatment of enhancement onset time.	Orton MR, Collins DJ, Walker-Samuel S, d'Arcy JA, Hawkes DJ, Atkinson D, Leach MO	10.1088/0031-9155/52/9/005	https://doi.org/10.1088/0031-9155/52/9/005	Physics in medicine and biology	38	2007	Yes	methodology	Others	Bayesian methods, marginal posterior distribution	Bayes	Bayes - Other	Yes	Oncology; C00-D49	not applicable	clinical trials (guess)	The purpose of the pharmacometric model is to assist in clinical drug trials by providing physiological insights into tissue behavior, particularly through improved estimation of pharmacokinetic parameters and onset detection. This is relevant to drug therapy development in oncology.	Yes	Commercial platform	No	Matlab
A probabilistic approach for deriving acceptable human intake limits and human health risks from toxicological studies: general framework.	Slob W, Pieters MN	10.1023/b:rian.0000005924.18154.60	https://doi.org/10.1023/b:rian.0000005924.18154.60	Risk analysis : an official publication of the Society for Risk Analysis	212	1998	Yes	methodology	Others	Monte Carlo calculations, Bootstrap method, Probabilistic sensitivity analysis,	Sensitivity analysis, basic frequentist	SA - simulation, Freq - resampling, Freq - Other	Yes	not applicable	small molecule	not applicable	Not applicable (the paper is related to toxicological risk assessment rather than drug therapy or vaccine development)	Yes	No	No	Not mentioned
Application of physiologically based kinetic (PBK) modelling in the next generation risk assessment of dermally applied consumer products.	Moxon TE, Li H, Lee MY, Piechota P, Nicol B, Pickles J, Pendlington R, Sorrell I, Baltazar MT	10.1016/j.tiv.2019.104746	https://doi.org/10.1016/j.tiv.2019.104746	Toxicology in vitro : an international journal published in association with BIBRA	41	2020	Yes	methodology	PBPK	Monte Carlo simulations, local sensitivity analysis, coefficient of variation (CV) analysis	Sensitivity analysis, basic frequentist	SA - analytical	No	not applicable	not applicable	not applicable	not applicable (the paper is related to consumer product safety assessment, not drug therapy development)	Yes	Commercial platform	No	GastroPlus 9.6, GastroPlus PSA, Python (v3.7)
An assessment and quantitative uncertainty analysis of the health risks to workers exposed to chromium contaminated soils.	Paustenbach DJ, Meyer DM, Sheehan PJ, Lau V	10.1177/074823379100700304	https://doi.org/10.1177/074823379100700304	Toxicology and industrial health	60	1991	Yes	application	Others	Monte Carlo statistical simulation	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental health risk assessment, not drug therapy or vaccine development)	No	Commercial platform	Commercial platform with given parameters	@RISK (Palisade Corporation, 1989)
Analysis of uncertainty in theoretical methods of cardiac output measurement using the "Monte Carlo" technique.	Kennedy RR, Baker AB	10.1093/bja/71.3.403	https://doi.org/10.1093/bja/71.3.403	British journal of anaesthesia	8	1993	Yes	application	Others	Monte Carlo simulation	Uncertainty propagation	UP - prob - basic sim	Yes	anaesthesia	not applicable	not applicable	Not applicable (the paper is related to cardiac output measurement using anaesthetic agents)	No	No	No	Pascal, 'C', Macintosh Toolbox 'random' function
Bootstrap resampling: a powerful method of assessing confidence intervals for doses from experimental data	Iwi, G., Millard, R. K., Palmer, A. M., Preece, A. W., Saunders, M.	10.1088/0031-9155/44/4/021	https://doi.org/10.1088/0031-9155/44/4/021	Physics in Medicine & Biology	37	1999	Yes	methodology	Others	Bootstrap resampling	basic frequentist	Freq - resampling, Freq - Other	No	not applicable	not applicable	not applicable	not applicable (the paper is related to radiation dosimetry and not drug therapy or vaccine development)	No	No	No	Not metioned
Assessing parameter uncertainty in small-n pharmacometric analyses: value of the log-likelihood profiling-based sampling importance resampling (LLP-SIR) technique.	Broeker A, Wicha SG	10.1007/s10928-020-09682-4	https://doi.org/10.1007/s10928-020-09682-4	Journal of pharmacokinetics and pharmacodynamics	21	2020	Yes	methodology	Others	- Standard Error (SE) - Bootstrap (BS) - Log-likelihood Profiling (LLP) - Bayesian approaches (BAY) - Sampling Importance Resampling (SIR) - SE-SIR - BS-SIR - LLP-SIR	basic frequentist, Bayes	Bayes - Other, Freq - Other, Freq - likelihood, Freq - resampling	Yes	not applicable	not applicable	not specified	The purpose of the pharmacometric model is to assess parameter uncertainty in small datasets, which is crucial for drug development, particularly in understanding pharmacokinetics and dose finding.	Yes	Commercial platform	No	NONMEM 7.4.3, R 3.6.1, PsN 4.7.0, MCMC, NUTS
A probabilistic approach to obtaining limiting estimates of radionuclide concentration in biota	Higley KA, Domotor SL, Antonio EJ	10.1016/S0265-931X(02)00117-0	https://doi.org/10.1016/S0265-931X(02)00117-0	Journal of environmental radioactivity	24	2003	Yes	application	Others	- Stratified Monte-Carlo Latin Hypercube Sampling - Qualitative (local) sensitivity analysis	Uncertainty propagation, Sensitivity analysis	UP - prob - basic sim, SA - simulation	No	not applicable	not applicable	not applicable	not applicable	No	Commercial platform	No	CrystalBall TM software
Assessing drug distribution in tissues expressing P-glycoprotein using physiologically based pharmacokinetic modeling: identification of important model parameters through global sensitivity analysis.	Fenneteau F, Li J, Nekka F	10.1007/s10928-009-9134-8	https://doi.org/10.1007/s10928-009-9134-8	Journal of pharmacokinetics and pharmacodynamics	15	2009	Yes	methodology	PBPK	Monte-Carlo simulations, Partial Rank Correlation Coefficients (PRCC), Global Sensitivity Analysis (GSA)	Sensitivity analysis, basic frequentist	SA - simulation	Yes	not applicable	small molecule	early stages of drug discovery or preclinical development	The purpose of the pharmacometric model is to improve the understanding of drug distribution in tissues expressing P-glycoprotein (P-gp), which is crucial for drug therapy development by identifying important input parameters that affect model outcomes and reducing uncertainty in model predictions.	No	Commercial platform	No	Matlab (The Mathworks, Inc.) and the Statistic Matlab toolbox

A fuzzy physiologically based pharmacokinetic modeling framework to predict drug disposition in humans.	Seng KY, Vicini P, Nestorov IA	10.1109/IEMBS.2006.260879	https://doi.org/10.1109/IEMBS.2006.260879	Conference proceedings : ... Annual International Conference of the IEEE Engineering in Medicine and Biology Society. IEEE Engineering in Medicine and Biology Society. Annual Conference	1	2006	Yes	methodology	PBPK	Fuzzy computations, fuzzy arithmetic, sparse grid interpolation, vertex method	Uncertainty propagation	UP - non prob	Yes	Psychiatry and Neurology; 6A00-6A9Z	small molecule	Not specified	The purpose of the model is to inform drug selection during early drug discovery and to predict intravenous pharmacokinetic profiles in humans before in vivo experiments, aiding in clinical candidate selection.	No	Commercial platform	No	MATLAB 7.0
An empirical multivariate log-normal distribution representing uncertainty of biokinetic parameters for 137Cs.	Miller G, Melo D, Martz H, Bertelli L	10.1093/rpd/ncn131	https://doi.org/10.1093/rpd/ncn131	Radiation protection dosimetry	5	2008	Yes	methodology	Others	Bayesian analysis, importance sampling, multivariate log-normal distribution, stratified sampling, Latin Hypercube sampling	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	not applicable (the paper is related to radiation exposure and internal dosimetry, not drug therapy or vaccine development)	Yes	No	No	Los Alamos UF code
Bayesian analysis of a rat formaldehyde DNA-protein cross-link model.	Yang Y, Allen BC, Tan YM, Liao KH, Clewell HJ 3rd	10.1080/15287391003689234	https://doi.org/10.1080/15287391003689234	Journal of toxicology and environmental health. Part A	-	2010	Yes	application	Others	Bayesian hierarchical analysis using Markov chain Monte Carlo (MCMC) for uncertainty quantification	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	not applicable	Yes	No	No	MCSim, Bayesian Output Analysis (BOA) program
Analysis of PBPK models for risk characterization.	Bois FY	10.1111/j.1749-6632.1999.tb08093.x	https://doi.org/10.1111/j.1749-6632.1999.tb08093.x	Annals of the New York Academy of Sciences	47	1999	Yes	methodology	PBPK	- Bayesian framework for risk characterization - Hierarchical statistical modeling - Markov chain Monte Carlo (MCMC) simulations - Monte Carlo simulations	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable (the paper is about risk characterization using PBPK models, not directly about drug therapy development)	not applicable (the paper is related to risk characterization and toxicokinetics, not drug therapy or vaccine development)	No	No	No	MCSim program
Analytical expressions for combining population pharmacokinetic parameters from different studies.	Dokoumetzidis A, Aarons L	10.1080/10543400802071360	https://doi.org/10.1080/10543400802071360	Journal of biopharmaceutical statistics	7	2008	Yes	methodology	Others	Bayesian hierarchical approach using normal-inverse-gamma (NIG) and normal-inverse-Wishart (NIW) distributions for uncertainty quantification; application of Bayes' theorem for combining hyperparameters; use of WinBUGS for setting up informative priors and model fitting.	Bayes	Bayes - hierachical	Yes	Nervous system disorders; ICD-11 code not specified in the paper	small molecule	not specified (guess: preclinical or early clinical)	The purpose of the pharmacometric model is to assist in drug therapy development by providing a method for combining different analyses of population pharmacokinetic studies, which can be used for dose finding and understanding population variability.	No	Commercial platform	No	WinBUGS 1.4, Pharmaco plug-in, NONMEM
Analysis of the uncertainty in internal dose estimate resulting from biological stochastic variability of excretion.	Molokanov A, Blanchardon E	10.1093/rpd/ncl551	https://doi.org/10.1093/rpd/ncl551	Radiation protection dosimetry	1	2007	Yes	methodology	PBPK	Monte Carlo simulation technique, log-normal distribution assumption, standard deviation calculation	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	not applicable	Yes	No	No	Monte Carlo simulation technique (no specific software or programming language mentioned)
A continuous-time adaptive particle filter for estimations under measurement time uncertainties with an application to a plasma-leucine mixed effects model.	Krengel A, Hauth J, Taskinen MR, Adiels M, Jirstrand M	10.1186/1752-0509-7-8	https://doi.org/10.1186/1752-0509-7-8	BMC systems biology	8	2013	Yes	methodology	Others	- Sequential Monte Carlo (SMC) methods - Bayesian methods - Monte Carlo simulation - Adaptive stepsize choice	Bayes	Bayes - Other	Yes	Diabetes; E10-E14	not applicable	not applicable	identification of subpopulations	No	Commercial platform	No	Mathematica, R
Bayesian optimal designs for pharmacokinetic models: Sensitivity to uncertainty	Dokoumetzidis, A., Aarons, L.	10.1080/10543400701514007	https://doi.org/10.1080/10543400701514007	Journal of Biopharmaceutical Statistics	15	2007	Yes	methodology	Others	Bayesian optimal designs (ED and API criteria), Bayesian methods for incorporating prior uncertainty,	Bayes	Bayes - Other	Yes	not applicable (the paper is related to pharmacokinetics but does not specify a therapeutic area or a particular drug)	not applicable	not specified (the paper is related to drug therapy development, likely preclinical or early clinical stages, but the stage is not explicitly mentioned)	Optimization of experimental designs for pharmacokinetic studies	No	Commercial platform	Open source	MATLAB, MATLAB Optimization Toolbox
Bayesian evaluation of a physiologically-based pharmacokinetic (PBPK) model of long-term kinetics of metal nanoparticles in rats.	Sweeney LM, MacCalman L, Haber LT, Kuempel ED, Tran CL	10.1016/j.yrtph.2015.06.019	https://doi.org/10.1016/j.yrtph.2015.06.019	Regulatory toxicology and pharmacology : RTP	37	2015	Yes	application	PBPK	Bayesian calibration, Bayesian population analysis using Markov chain Monte Carlo (MCMC) simulation, probabilistic sensitivity analysis	Bayes, Sensitivity analysis	Bayes - calibration, UP - prob - basic sim	No	not applicable	not applicable	not specified (the paper is related to drug therapy development but does not explicitly state the stage)	not applicable (the paper is focused on toxicokinetic modeling of metal nanoparticles in rats, not drug therapy or vaccine development)	No	Commercial platform	Commercial platform with given parameters	- Matlab: Initial model development - MCSim (version 5.3.1): Model simulation - acslX (version 3.0.2.1): Monte Carlo analysis - Microsoft Excel: Data visualization and comparison
Assessing Toxicokinetic Uncertainty and Variability in Risk Prioritization.	Wambaugh JF, Wetmore BA, Ring CL, Nicolas CI, Pearce RG, Honda GS, Dinallo R, Angus D, Gilbert J, Sierra T, Badrinarayanan A, Snodgrass B, Brockman A, Strock C, Setzer RW, Thomas RS	10.1093/toxsci/kfz205	https://doi.org/10.1093/toxsci/kfz205	Toxicological sciences : an official journal of the Society of Toxicology	61	2019	Yes	methodology	Others	Bayesian methods, Monte Carlo simulation, Markov Chain Monte Carlo (MCMC), uncertainty propagation	Uncertainty propagation, Bayes	Bayes - Other, UP - prob - basic sim	No	not applicable	not applicable	not applicable	not applicable (the paper is related to chemical risk assessment and not drug therapy or vaccine development)	Yes	Open source	Upon request to the authors	- R version 3.5.1 - R package "httk" version 1.10 - JAGS software version 4.3 - R packages "runjags" and "rjags"
Bayesian model selection validates a biokinetic model for zirconium processing in humans.	Schmidl D, Hug S, Li WB, Greiter MB, Theis FJ	10.1186/1752-0509-6-95	https://doi.org/10.1186/1752-0509-6-95	BMC systems biology	24	2012	Yes	methodology	PBPK	Bayesian modeling approach, Bayes factors, simulated annealing, MCMC sampling	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable (the paper is related to radiation protection and biokinetic modeling, not drug therapy or vaccine development)	not applicable (the paper is related to radiation protection and biokinetic modeling, not drug therapy or vaccine development)	No	Commercial platform	Open source	MATLAB
A Novel Method for Assessing Drug Degradation Product Safety Using Physiologically-Based Pharmacokinetic Models and Stochastic Risk Assessment	Nguyen HQ, Stamatis SD, Kirsch LE	10.1002/jps.24452	https://doi.org/10.1002/jps.24452	Journal of Pharmaceutical Sciences	8	2015	Yes	methodology	PBPK	Monte Carlo (MC) sampling, probabilistic sensitivity analysis	Sensitivity analysis	SA - simulation	Yes	Pain management or analgesia; ICD 11 code: Not explicitly mentioned but potentially related to codes under "Pain" or "Neurological disorders"	small molecule	not specified (the paper is related to drug therapy development, likely in preclinical or early clinical stages, but the stage is not explicitly mentioned)	The purpose of the PBPK model is to estimate human safe exposure levels for drug degradation products by comparing human and rat exposure levels, focusing on target tissue exposure and leveraging physiological knowledge.	No	No	Upon request to the authors	R software with FME and deSolve packages

Bayesian networks for clinical decision support in lung cancer care.	Sesen MB, Nicholson AE, Banares-Alcantara R, Kadir T, Brady M	10.1371/journal.pone.0082349	https://doi.org/10.1371/journal.pone.0082349	PloS one	140	2013	Yes	application	ML	Bayesian Networks with directed acyclic graph and underlying joint probability distribution	Bayes	Bayes - ML	No	not applicable (the paper is about treatment selection and survival prediction in lung cancer care, not drug therapy development)	not applicable	not applicable	not applicable	No	Commercial platform	No	- MatLab BNT toolbox - WEKA 3 machine learning software - Java implementation of CaMML - PostgreSQL
Bayesian PBPK modeling using R/Stan/Torsten and Julia/SciML/Turing.Jl.	Elmokadem A, Zhang Y, Knab T, Jordie E, Gillespie WR	10.1002/psp4.12926	https://doi.org/10.1002/psp4.12926	CPT: pharmacometrics & systems pharmacology	9	2023	Yes	application	PBPK	Bayesian inference,Global sensitivity analysis, Markov Chain Monte Carlo (MCMC) methods, No U-Turn Sampler (NUTS), Gelman-Rubin statistic	Sensitivity analysis, Bayes	Bayes - Other, SA - simulation	Yes	Neurological disorders; LD50.0 (Fragile X syndrome)	small molecule	Phase I	not applicable (the paper focuses on methodology and tools for Bayesian PBPK modeling rather than a specific purpose like dose finding or subpopulation identification)	No	Open source	Open source	- R/Stan/Torsten - Julia/SciML/Turing.jl - cmdstanr - GlobalSensitivity.jl - MCMCChains.jl - StatsPlots.jl
An automated sampling importance resampling procedure for estimating parameter uncertainty.	Dosne AG, Bergstrand M, Karlsson MO	10.1007/s10928-017-9542-0	https://doi.org/10.1007/s10928-017-9542-0	Journal of pharmacokinetics and pharmacodynamics	116	2017	Yes	methodology	Others	- Sampling Importance Resampling (SIR) - Covariance matrix - Bootstrap - Stochastic simulations and estimations (SSE)	basic frequentist	Freq - resampling	Yes	not applicable	not applicable	Clinical trial phase (guess)	- Quantifying drug interactions - Calculating the power of a prospective trial - Proposing dose regimen adaptations - Designing efficient clinical trials	No	Commercial platform	Upon request to the authors	PsN, NONMEM 7.3, RStudio 0.98 with R 3.1.2
Bayesian methods for uncertainty factor application for derivation of reference values.	Simon TW, Zhu Y, Dourson ML, Beck NB	10.1016/j.yrtph.2016.05.018	https://doi.org/10.1016/j.yrtph.2016.05.018	Regulatory Toxicology and Pharmacology	21	2016	Yes	methodology	PBPK	Bayesian methods, Bayesian Markov Chain Monte Carlo methods	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental toxicity assessments, not drug therapy or vaccine development)	Yes	No	No	EPA's Benchmark Dose Software; specialized software for Monte Carlo simulation (not specified)
A Unified Probabilistic Framework for Dose-Response Assessment of Human Health Effects.	Chiu WA, Slob W	10.1289/ehp.1409385	https://doi.org/10.1289/ehp.1409385	Environmental health perspectives	75	2015	Yes	review	Others	- Bayesian analysis - Translating BMD confidence limits into distributions - Parametric bootstrapping - Monte Carlo (MC) simulation	Bayes, basic frequentist	Bayes - Other, Freq - resampling	No	not applicable	not applicable	not applicable	Not applicable (the paper is focused on chemical hazard assessment, not drug therapy or vaccine development)	Yes	Open source	Open source	PROAST software, R package (version 3.2.2)
A linear uncertain pharmacokinetic model driven by Liu process	Liu, Z., Yang, X.	10.1016/j.apm.2020.08.061	https://doi.org/10.1016/j.apm.2020.08.061	Applied Mathematical Modelling	37	2021	Yes	methodology	Others	Uncertain differential equation	UDE/SDE		Yes	not specified	not specified	optimization/refinement (guess)	The purpose of the model is to provide a more accurate representation of pharmacokinetics for drug therapy development, particularly for intravenous infusions of anticancer drugs. It helps in determining steady-state drug concentrations and comparing different drug formulations.	No	No	No	Not mentioned (no information on software used is included in the paper)
Analysis of cellular kinetic models suggest that physiologically based model parameters may be inherently, practically unidentifiable.	Brown LV, Coles MC, McConnell M, Ratushny AV, Gaffney EA	10.1007/s10928-022-09819-7	https://doi.org/10.1007/s10928-022-09819-7	Journal of pharmacokinetics and pharmacodynamics	2	2022	Yes	methodology	PBPK	Markov Chain Monte Carlo (MCMC), Bayesian methodologies, Adaptive Covariance Monte Carlo	Bayes	Bayes - Other	Yes	not specified	not applicable	Clinical trials (guess)	The purpose of the model is to calculate metrics such as total drug exposure in different patient populations, which is important for drug discovery and clinical trials.	No	No	Open source	SciPy, PINTS curve_fit or basinhopping
Are Non-animal Systemic Safety Assessments Protective? A Toolbox and Workflow.	Middleton AM, Reynolds J, Cable S, Baltazar MT, Li H, Bevan S, Carmichael PL, Dent MP, Hatherell S, Houghton J, Kukic P, Liddell M, Malcomber S, Nicol B, Park B, Patel H, Scott S, Sparham C, Walker P, White A	10.1093/toxsci/kfac068	https://doi.org/10.1093/toxsci/kfac068	Toxicological sciences : an official journal of the Society of Toxicology	40	2022	Yes	methodology	PBPK	Bayesian model (C max error distribution model), Monte Carlo Markov chain algorithms, Leave-one-exposure-out strategy for calibration	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	not applicable (the paper is focused on systemic safety assessments for consumer goods, not drug therapy development)	No	No	Open source	- Stan (probabilistic programming language) - Python 3.8 - PyStan v2.19 - NumPy v1.19 - SciPy v1.6 - pandas v1.2 - matplotlib v3.3
Biomarker-based calibration of retrospective exposure predictions of perfluorooctanoic acid	Shin, H.-M., Steenland, K., Ryan, P.B., Vieira, V.M., Bartell, S.M.	10.1021/es4053736	https://doi.org/10.1021/es4053736	Environmental Science and Technology	10	2014	Yes	methodology	Others	Bayesian calibration, sensitivity analysis	Sensitivity analysis, Bayes	SA - simulation, Bayes - calibration	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental exposure assessment, not drug therapy or vaccine development)	Yes	No	No	Not mentioned (no software or programming languages are explicitly mentioned as being used in the study)
A Stochastic Model Predictive Control Approach to Deal with Cancerous Tumor Growth	Hernández-Rivera, A., Velarde, P., Zafra-Cabeza, A., Maestre, J.M.	10.1109/CoDIT58514.2023.10284136	https://doi.org/10.1109/CoDIT58514.2023.10284136	9th 2023 International Conference on Control, Decision and Information Technologies, CoDIT 2023	1	2023	Yes	methodology	Others	Probabilistic constraints; Chance-constrained model predictive approach; Normal distribution functions for stochastic variables	Other		Yes	Oncology; C00-D49	small molecule	Preclinical (guess)	The purpose of the model is to optimize drug dosing to minimize side effects while reducing tumor size, which aligns with dose finding and optimization in drug therapy development.	Yes	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used for the study)
A novel Bayesian strategy for the identification of spatially varying material properties and model validation: an application to static elastography	Koutsourelakis, Phaedon-Stelios	10.1002/nme.4261	https://doi.org/10.1002/nme.4261	International Journal for Numerical Methods in Engineering	47	2012	Yes	methodology	Others	Bayesian techniques, model discrepancy analysis, MCMC sampling, Expectation-Maximization algorithm	Bayes, Sensitivity analysis	SA - analytical, Bayes - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to medical imaging and elastostatics, not drug therapy or vaccine development)	Yes	No	No	Not mentioned (the paper does not specify any software or programming languages used)
Bayesian evaluation of a physiologically based pharmacokinetic (PBPK) model for perfluorooctane sulfonate (PFOS) to characterize the interspecies uncertainty between mice, rats, monkeys, and humans: Development and performance verification	Chou, W.-C., Lin, Z.	10.1016/j.envint.2019.03.058	https://doi.org/10.1016/j.envint.2019.03.058	Environment International	72	2019	Yes	application	PBPK	Bayesian Hierarchical statistical analysis using Markov chain Monte Carlo (MCMC) simulation, Prior distributions for population variances and unknown error, Delayed Rejection Adaptive Metropolis (DRAM) sampling, sensitivity analysis	Bayes, Sensitivity analysis	Bayes - hierachical, SA - simulation	No	not applicable	not applicable	not applicable	not applicable (the paper is related to toxicokinetic modeling for risk assessment, not drug therapy or vaccine development)	No	Open source	Open source	- R language (version 3.5.2) - R package "mrgsolve" - R software package "FME"

Bayesian inference informed by parameter subset selection for a minimal PBPK brain model.	Dadashova K, Smith RC, Haider MA, Reich BJ	10.1098/rsta.2024.0219	https://doi.org/10.1098/rsta.2024.0219	Philosophical transactions. Series A, Mathematical, physical, and engineering sciences	1	2025	Yes	methodology	PBPK	Bayesian inference, Markov chain Monte Carlo (MCMC) techniques, Delayed Rejection Adaptive Metropolis (DRAM), Posterior Predictive Distribution (PPD), Credible intervals, Prediction intervals	Bayes	Bayes - Other	Yes	not specified	biologics	not specified (guess: preclinical or early clinical stage)	The purpose of the model is to refine the subset of identifiable parameters, quantify uncertainties, and enhance model predictions for antibody therapeutics in the brain.	No	Commercial platform	No	MATLAB, MCMC toolbox, ode15s
Application of Physiologically Based Pharmacokinetic/Pharmacodynamic Modeling in Cumulative Risk Assessment for N-Methyl Carbamate Insecticides	Zhang, X., Knaak, J.B., Tomero-Velez, R., Blancato, J.N., Dary, C.C.	10.1016/B978-0-12-374367-1.00073-2	https://doi.org/10.1016/B978-0-12-374367-1.00073-2	Hayes' Handbook of Pesticide Toxicology	3	2010	Yes	application	PBPK	- Traditional Monte Carlo approach - Bayesian Markov chain Monte Carlo analysis - Fuzzy simulation approach - Sensitivity analysis - Variability analysis - Bayesian analysis for parameter optimization	Sensitivity analysis, Bayes, Uncertainty propagation	UP - non prob, Bayes - Other, SA - simulation	No	not applicable	not applicable	not applicable	not applicable (the paper is related to pesticide exposure and risk assessment, not drug therapy or vaccine development)	No	No	No	Not mentioned
Bayesian pharmacokinetic modeling of dynamic contrast-enhanced magnetic resonance imaging: Validation and application	Mittermeier, A., Ertl-Wagner, B., Ricke, J., Dietrich, O., Ingrisch, M.	10.1088/1361-6560/ab3a5a	https://doi.org/10.1088/1361-6560/ab3a5a	Physics in Medicine and Biology	5	2019	Yes	application	Others	Bayesian probabilistic modeling (posterior probability distributions, posterior predictive checks) and bootstrapping	Bayes, basic frequentist	Bayes - Other, Freq - resampling	Yes	Breast cancer; C50	not specified	not specified	Assessment of treatment response	No	Open source	Open source	SciPy, Stan, scikit-learn
Bayesian Analytical Methods in Cardiovascular Clinical Trials: Why, When, and How	Heuts, S., Kawczynski, M.J., Sayed, A., Urbut, S.M., Albuquerque, A.M., Mandrola, J.M., Kaul, S., Harrell, F.E., Gabrio, A., Brophy, J.M.	10.1016/j.cjca.2024.11.002	https://doi.org/10.1016/j.cjca.2024.11.002	Canadian Journal of Cardiology	6	2025	Yes	review	Others	Bayesian hierarchical meta-regression	Bayes	Bayes - hierachical	Yes	Cardiovascular; I00-I99	small molecule	not specified (guess: Phase III or IV)	not applicable (the paper discusses Bayesian analysis in cardiovascular clinical trials but does not specify a pharmacometric model for drug therapy development)	No	Open source	Open source	R (cmdstanr, rstan, rstanarm, brms), Python (pystan, pymc), Julia (Turing.jl), JASP, SPSS, Stata, Matlab
Bayesian knowledge integration for an in vitro–in vivo correlation model	Erhardt, E.M., Ursino, M., Biewenga, J., Jacobs, T., Gasparini, M.	10.1002/bimj.201700263	https://doi.org/10.1002/bimj.201700263	Biometrical Journal	5	2019	Yes	methodology	Others	Bayesian hierarchical modeling	Bayes	Bayes - hierachical	Yes	not applicable (the paper does not specify the therapeutic area or provide an ICD 11 code)	small molecule	not specified (the paper discusses various stages but does not clearly state a specific stage)	The purpose of the pharmacometric model is to optimize the exposure of a compound during drug development, particularly for formulations with extended release or lag in absorption, and to serve as a surrogate for in vivo bioequivalence studies.	No	Open source	Open source	- R package nlme - R package nlmixr - Software package Stan - R package rstan
A Critical Assessment of Kriging Model Variants for High-Fidelity Uncertainty Quantification in Dynamics of composite Shells	Mukhopadhyay, T., Chakraborty, S., Dey, S., Adhikari, S., Chowdhury, R.	10.1007/s11831-016-9178-z	https://doi.org/10.1007/s11831-016-9178-z	Archives of Computational Methods in Engineering. State of the Art Reviews	149	2017	Yes	methodology	Others	- Surrogate modeling using Kriging variants (Ordinary Kriging, Universal Kriging based on pseudo-likelihood estimator, Blind Kriging, Co-Kriging, Universal Kriging based on marginal likelihood estimator) - Monte Carlo Simulation (MCS) - Stochastic Kriging for addressing noise in uncertainty propagation	Uncertainty propagation	UP - prob - surrogate	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to engineering and materials science, not drug therapy or vaccine development)	No	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used for the study)
Bayesian parameter identification for Turing systems on stationary and evolving domains.	Campillo-Funollet, Eduard, Venkataraman, Chandrasekhar, Madzvamuse, Anotida	10.1007/s11538-018-0518-z	https://doi.org/10.1007/s11538-018-0518-z	Bulletin of Mathematical Biology. A Journal Devoted to Research at the Interface of the Life and Mathematical Sciences	27	2019	Yes	methodology	Others	Bayesian framework, Markov chain Monte Carlo (MCMC) methods, parallel Metropolis-Hastings algorithm	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is not related to drug therapy or vaccine development)	No	No	Open source	Python, Scipy, multiprocessing module from Python Standard Library
Bayesian calibration of computer models.	Kennedy, Marc C., O'Hagan, Anthony	10.1111/1467-9868.00294	https://doi.org/10.1111/1467-9868.00294	Journal of the Royal Statistical Society. Series B. Statistical Methodology	3972	2001	Yes	methodology	Others	Bayesian calibration, Gaussian process modeling, model discrepancy analysis	Bayes, Sensitivity analysis	Bayes - calibration, SA - analytical	Yes	not applicable (the paper discusses pharmacokinetic modeling but does not specify a therapeutic area or ICD 11 code)	not specified	not specified	dose finding	No	No	No	Not mentioned (the paper does not specify any software used in the study)
Bayesian calibration and uncertainty analysis for computationally expensive models using optimization and radial basis function approximation.	Bliznyuk, Nikolay, Ruppert, David, Shoemaker, Christine, Regis, Rommel, Wild, Stefan, Mugunthan, Pradeep	10.1198/106186008X32068 1	https://doi.org/10.1198/106186008X32068 1	Journal of Computational and Graphical Statistics	119	2008	Yes	methodology	Others	Bayesian calibration, surrogate modeling (RBF interpolation)	Uncertainty propagation, Bayes	UP - prob - surrogate, Bayes - calibration	No	not applicable	not applicable	not applicable	not applicable	Yes	Open source	Open source	MATLAB
A generalized polynomial chaos-based method for efficient Bayesian calibration of uncertain computational models.	Tagade, Piyush M., Choi, Han-Lim	10.1080/17415977.2013.823411	https://doi.org/10.1080/17415977.2013.823411	Inverse Problems in Science and Engineering	17	2014	Yes	methodology	Others	Bayesian calibration, generalized Polynomial Chaos (gPC), Markov Chain Monte Carlo (MCMC), Karhunen-Loeve expansion	Bayes, Uncertainty propagation	Bayes - calibration, UP - prob - surrogate	No	not applicable	not applicable	not applicable	not applicable	No	No	No	Not mentioned
Bayesian calibration, validation, and uncertainty quantification of diffuse interface models of tumor growth.	Hawkins-Daarud, Andrea, Prudhomme, Serge, van der Zee, Kristoffer G., Oden, J. Tinsley	10.1007/s00285-012-0595-9	https://doi.org/10.1007/s00285-012-0595-9	Journal of Mathematical Biology	110	2013	Yes	methodology	Others	- Bayesian calibration - Bayesian inference methods	Bayes	Bayes - calibration	No	not applicable	not applicable	not applicable	not applicable (the paper is focused on tumor growth modeling and does not address drug therapy or vaccine development)	Yes	No	No	QUESO, DAKOTA
A deep-learning-based surrogate model for data assimilation in dynamic subsurface flow problems.	Tang, Meng, Liu, Yimin, Durlofsky, Louis J.	10.1016/j.jcp.2020.109456	https://doi.org/10.1016/j.jcp.2020.109456	Journal of Computational Physics	268	2020	Yes	methodology	Others	Surrogate modeling	Uncertainty propagation	UP - prob - surrogate	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to geological modeling and subsurface flow prediction, not drug therapy or vaccine development)	No	No	No	AD-GPRS, CNN-PCA, SGeMS
Bayesian calibration of multistate stochastic simulators.	Pratola, Mathew T., Chkrebtii, Oksana	-	https://www.jstor.org/stable/44841921	Statistica Sinica	7	2018	Yes	methodology	Others	- Bayesian calibration - Markov chain Monte Carlo (MCMC) algorithm - Emulation/surrogate modeling	Bayes, Uncertainty propagation	Bayes - calibration, UP - prob - surrogate	No	not applicable	not applicable	not applicable	not applicable	Yes	Open source	Open source	R (R Core Team (2012)), cmce package on CRAN
A dynamic evolution scheme for structures with interval uncertainties by using bidirectional sequential Kriging method.	Liu, Yisi, Wang, Xiaojun, Wang, Lei	10.1016/J.CMA.2019.01.041	https://doi.org/10.1016/J.CMA.2019.01.041	Computer Methods in Applied Mechanics and Engineering	35	2019	Yes	methodology	Others	- Bidirectional sequential Kriging (BSK) method - Interval finite element method (IFEM) - Collocation methods (CM) - Interval analysis	Uncertainty propagation	UP - prob - surrogate, UP - non prob	No	not applicable	not applicable	not applicable	not applicable (the paper is related to structural dynamics and not drug therapy or vaccine development)	Yes	No	No	Not mentioned (no specific software, packages, or programming languages are mentioned in the paper for estimating the uncertainty quantification model)

Bayesian inference and uncertainty quantification for medical image reconstruction with Poisson data.	Zhou, Qingping, Yu, Tengchao, Zhang, Xiaoqun, Li, Jinglai	arXiv:1903.02075	https://doi.org/10.48550/arXiv.1903.02075	SIAM Journal on Imaging Sciences	23	2020	Yes	methodology	Others	Bayesian inference	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to medical image reconstruction, not drug therapy or vaccine development)	No	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used)
Bayesian calibration, validation and uncertainty quantification for predictive modelling of tumour growth: a tutorial.	Collis, Joe, Connor, Anthony J., Paczkowski, Marcin, Kannan, Pavitra, Pitt-Francis, Joe, Byrne, Helen M., Hubbard, Matthew E.	10.1007/s11538-017-0258-5	https://doi.org/10.1007/s11538-017-0258-5	Bulletin of Mathematical Biology. A Journal Devoted to Research at the Interface of the Life and Mathematical Sciences	45	2017	Yes	methodology	Others	Bayesian calibration, Markov chain Monte Carlo (MCMC), robust Bayesian analysis	Bayes	Bayes - calibration	Yes	Cancer (2A00-2F9Z)	not applicable	not specified (the paper is related to drug therapy but does not specify a stage of development)	The purpose of the model is to guide patient therapy via prediction, potentially involving patient-specific predictions for therapy planning. This could include identifying optimal treatment strategies or predicting patient responses to therapy.	No	Commercial platform	Upon request to the authors	Matlab
A local hybrid surrogate-based finite element tearing interconnecting dual-primal method for nonsmooth random partial differential equations.	Eigel, Martin, Gruhlke, Robert	10.1002/nme.6571	https://doi.org/10.1002/nme.6571	International Journal for Numerical Methods in Engineering	4	2021	Yes	methodology	Others	Surrogate modeling, stochastic Galerkin method, multilevel Monte Carlo (MLMC)	Uncertainty propagation	UP - prob - surrogate	No	not applicable	not applicable	not applicable	not applicable	Yes	Open source	Open source	- ALEA python library - FEniCS - UMFPACK - Custom implementation for discrete random coordinate spaces
A sequential calibration and validation framework for model uncertainty quantification and reduction.	Jiang, Chen, Hu, Zhen, Liu, Yixuan, Mourelatos, Zissimos P., Gorsich, David, Jayakumar, Paramsothy	10.1016/j.cma.2020.113172	https://doi.org/10.1016/j.cma.2020.113172	Computer Methods in Applied Mechanics and Engineering	81	2020	Yes	review	Others	- Direct Bayesian Calibration (DBC) - Kennedy and O'Hagan (KOH) framework - Optimization-Based Calibration (OBC) - Sequential Calibration and Validation (SeCAV) framework - Gaussian Process (GP) surrogate modeling - Bayesian inference	Bayes, Uncertainty propagation	Bayes - calibration, UP - prob - surrogate	No	not applicable	not applicable	not applicable	not applicable	No	No	No	Not metioned
A machine learning-based probabilistic computational framework for uncertainty quantification of actuation of clustered tensegrity structures.	Ge, Yipeng, He, Zigang, Li, Shaofan, Zhang, Liang, Shi, Litao	-	-	Computational Mechanics	5	2023	Yes	application	Others	- Surrogate modeling - Monte Carlo simulation - Global Sensitivity Analysis (GSA)	Sensitivity analysis, Uncertainty propagation	UP - prob - surrogate, SA - simulation	No	not applicable	not applicable	not applicable (the paper is about tensegrity structures and their applications in engineering, not related to drug therapy or vaccine development)	Not applicable (the paper is related to mechanical engineering and robotics, not drug therapy or vaccine development)	No	No	No	Not metioned
Bayesian assessment of uncertainty in viscosity closure models for turbidity currents computations.	Zio, Souleymane, da Costa, Henrique F., Guerra, Gabriel M., Paraizo, Paulo L. B., Camata, Jose J., Elias, Renato N., Coutinho, Alvaro L. G. A., Rochinha, Fernando A.	10.1016/j.cma.2018.08.023	https://doi.org/10.1016/j.cma.2018.08.023	Computer Methods in Applied Mechanics and Engineering	7	2018	Yes	methodology	Others	- Bayesian framework - Hierarchical Bayesian calibration - Model discrepancy analysis - Marginalized Gaussian Approximation likelihood - Markov Chain Monte Carlo (MCMC) methods	Bayes, Sensitivity analysis, basic frequentist	Bayes - hierachical, SA - analytical, Freq - likelihood	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to geological phenomena and sediment transport, not drug therapy or vaccine development)	Yes	Commercial platform	No	- DAKOTA library - Residual Based Variational Multiscale Method (RBVMS) - Large Eddy Simulation (LES)
Bayesian calibration for large-scale fluid structure interaction problems under embedded/immersed boundary framework.	Cao, Shunxiang, Huang, Daniel Zhengyu	10.1002/nme.6916	https://doi.org/10.1002/nme.6916	International Journal for Numerical Methods in Engineering	12	2022	Yes	methodology	Others	Bayesian calibration, Kalman inversion (including unscented Kalman filter)	Bayes	Bayes - calibration	No	not applicable	not applicable	not applicable	Not applicable (the paper is not related to drug therapy or vaccine development)	Yes	Open source	Open source	AERO-Suite 2, Julia
A Surrogate-based Variance Reduction Approach to Multifidelity Uncertainty Quantification - with Applications in Automotive Systems.	Yang, Hang	dx.doi.org/10.7302/4635	https://dx.doi.org/10.7302/4635	ProQuest LLC, Ann Arbor, MI	1	2022	Yes	methodology	Others	- Monte Carlo (MC) method - Generalized Polynomial Chaos (gPC) - CVPC (multifidelity variance reduction method integrating gPC with MC) - Surrogate methods: response surface models, metamodels, emulators - Gaussian process models - Low-rank decomposition methods - Sparse grid interpolation methods - Reduced basis approximations - Neural networks - Variance-based global sensitivity analysis using total-effect Sobol' indices	Uncertainty propagation, Sensitivity analysis	UP - prob - surrogate, SA - simulation, SA - analytical	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to automotive systems and uncertainty quantification, not drug therapy or vaccine development)	Yes	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used in the study)
An efficient Bayesian uncertainty quantification approach with application to k-ω-γ transition modeling.	Zhang, Jincheng, Fu, Song	10.1016/j.compfluid.2017.11.007	https://doi.org/10.1016/j.compfluid.2017.11.007	Computers \& Fluids. An International Journal	31	2018	Yes	methodology	Others	Bayesian calibration, adaptive high-dimensional model representation (HDMR), stochastic collocation (SC) based on generalized polynomial chaos (gPC), Bayesian inference	Bayes, Uncertainty propagation	Bayes - calibration, UP - prob - surrogate	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to fluid dynamics and aerodynamics, not drug therapy or vaccine development)	Yes	No	No	- R package: MHadaptive - R package: GPC
A novel sensitivity analysis method for multi-input-multi-output structures considering non-probabilistic correlations.	Ouyang, Heng, Zhou, Hongbin, Wang, Haoyang, Duan, Shuyong, Han, Xu	10.1016/j.cma.2024.117285	https://doi.org/10.1016/j.cma.2024.117285	Computer Methods in Applied Mechanics and Engineering	1	2024	Yes	methodology	Others	- Non-probabilistic variance propagation equation - Dimensional normalization method - Vector projection method - Non-probabilistic sensitivity analysis	Uncertainty propagation, Sensitivity analysis	UP - non prob, SA - analytical	No	not applicable	not applicable	not applicable	not applicable	Yes	No	No	Monte Carlo Simulation (MCS)
Bayesian calibration of imperfect computer models using physics-informed priors.	Spitieris, Michail, Steinsland, Ingelin	10.48550/arXiv.2201.06463	http://dx.doi.org/10.48550/arXiv.2201.06463	Journal of Machine Learning Research (JMLR)	8	2023	Yes	methodology	Others	Bayesian calibration, model discrepancy analysis, Hamiltonian Monte Carlo sampling, physics-informed priors, Gaussian processes	Sensitivity analysis, Bayes	Bayes - calibration, SA - analytical	No	not applicable (the paper is related to cardiovascular modeling and not drug therapy or vaccine development)	not applicable	not applicable	not applicable	Yes	Open source	Open source	STAN (probabilistic programming language), Hamiltonian Monte Carlo (HMC) sampling, No U-Turn Sampler (NUTS)

An active machine learning approach for optimal design of magnesium alloys using Bayesian optimisation	Ghorbani, M., Boley, M., Nakashima, P.N.H., Birbilis, N.	10.1038/s41598-024-59100-9	https://doi.org/10.1038/s41598-024-59100-9	Scientific Reports	7	2024	Yes	application	ML	- Probabilistic Gaussian process regressor model - Bayesian optimisation - Acquisition function (upper confidence bound)	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	not applicable	No	Open source	Open source	- Web tool with graphical user interface (GUI) - GitHub - Google Collaboratory notebook
Bayesian meta-analytical methods to incorporate multiple surrogate endpoints in drug development process	Bujkiewicz, S., Thompson, J.R., Riley, R.D., Abrams, K.R.	10.1002/sim.6776	https://doi.org/10.1002/sim.6776	Statistics in Medicine	26	2016	Yes	methodology	Others	Bayesian multivariate meta-analysis, Markov chain Monte Carlo (MCMC) simulation, Bayesian credibility intervals, non-informative prior distributions	Bayes	Bayes - hierachical	Yes	Neurology; 8A40	not applicable	not specified (the paper is related to drug therapy development, likely in Phase II or III, but the stage is not explicitly mentioned)	The purpose of the model is to evaluate surrogate endpoints to predict clinical outcomes in drug therapy development, specifically to reduce uncertainty by including multiple surrogate endpoints.	Yes	Open source	Open source	WinBUGS, R, R2WinBUGS package, OpenBUGS, R2OpenBUGS
Bayesian synergistic metamodeling (BSM) for physical information infused data-driven metamodeling	Kuok, Sin-Chi, Yuen, Ka-Veng	10.1016/j.cma.2023.116680	https://doi.org/10.1016/j.cma.2023.116680	Computer Methods in Applied Mechanics and Engineering	5	2024	Yes	methodology	Others	Bayesian synergistic metamodeling (BSM)	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	Not applicable (the paper is not related to drug therapy or vaccine development)	Yes	No	No	Not mentioned
Blood–brain barrier penetration prediction enhanced by uncertainty estimation	Tong, X., Wang, D., Ding, X., Tan, X., Ren, Q., Chen, G., Rong, Y., Xu, T., Huang, J., Jiang, H., Zheng, M., Li, X.	10.1186/s13321-022-00619-2	https://doi.org/10.1186/s13321-022-00619-2	Journal of Cheminformatics	28	2022	Yes	methodology	ML	Entropy, MC-dropout, Multi-initial, FPsDist, LatentDist, Random method, modZ weighted average algorithm	Bayes	Bayes - ML	Yes	- Therapeutic area: Central Nervous System (CNS) diseases and metastatic brain tumors - ICD 11 code: 8A40 (Alzheimer's disease), 2C10 (Malignant neoplasm of brain)	small molecule	early-stage drug discovery (guess)	The purpose of the model is to enhance the early drug discovery process by rapidly exploring blood-brain barrier permeability (BBBp) in silico, facilitating high-throughput screening and lead optimization of BBBp molecules for CNS diseases and metastatic brain tumors.	No	Open source	Open source	- RDKit toolkit - Epik module of Maestro - scikit-learn (for RF and MLP) - TensorFlow or PyTorch (for GROVER and Attentive FP) - Python (for implementation of machine learning models and uncertainty estimation methods)
Assessing the Impact of Tissue Target Concentration Data on Uncertainty in In Vivo Target Coverage Predictions	Tiwari, A., Luo, H., Chen, X., Singh, P., Bhattacharya, I., Jasper, P., Tolsma, J.E., Jones, H.M., Zutshi, A., Abraham, A.K.	10.1002/psp4.12126	https://doi.org/10.1002/psp4.12126	CPT: Pharmacometrics and Systems Pharmacology	11	2016	Yes	methodology	Others	Global Sensitivity Analysis (GSA) using Partial Rank Correlation Coefficients (PRCCs) and Derivative-based Global Sensitivity Measure	Sensitivity analysis	SA - analytical	Yes	- Rheumatoid arthritis: M05-M06 - Crohn's disease: K50.0 - Psoriasis: L40.0	biologics	Preclinical (guess)	The purpose of the model is to predict target coverage, which is essential for drug therapy development by helping to establish appropriate doses and ensure efficacy.	Yes	Commercial platform	No	J2 Dynamic Modeling and Optimization Software (RES Group, 2016)
A Bayesian approach for determining the no effect concentration and hazardous concentration in ecotoxicology	David R Fox	10.1016/j.ecoenv.2009.09.012	https://doi.org/10.1016/j.ecoenv.2009.09.012	Ecotoxicology and Environmental Safety	70	2010	Yes	methodology	Others	Bayesian modeling, Markov chain Monte Carlo (MCMC) methods, Bayesian credibility intervals	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to ecotoxicology and environmental risk assessment, not drug therapy or vaccine development)	No	Open source	Open source	WinBUGS, BurtiOz
A Probabilistic Method for Species Sensitivity Distributions Taking into Account the Inherent Uncertainty and Variability of Effects to Estimate Environmental Risk	Fadri Gottschalky, Bernd Nowack	10.1002/ieam.1334	https://doi.org/10.1002/ieam.1334	Integrated Environmental Assessment and Management	60	2013	Yes	methodology	Others	Probabilistic sensitivity analysis, Monte Carlo simulations, frequentist statistical methods (95% confidence intervals)	Sensitivity analysis, basic frequentist	SA - simulation	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental risk assessment, not drug therapy or vaccine development)	No	No	No	R (R Development Core Team 2008)
A physiologically-based kinetic (PBK) model for work-related diisocyanate exposure: Relevance for the design and reporting of biomonitoring studies	B Scholten, J Westerhout, A Pronk, R Stierum, J Vlaanderen, R Vermeulen, K Jones, T Santonen, L Portengen, Shoji Nakayama	10.1016/j.envint.2023.107917	https://doi.org/10.1016/j.envint.2023.107917	Environment International	4	2023	Yes	methodology	PBPK	- Global sensitivity analysis using extended Fourier Amplitude Sensitivity Test (eFAST) - Monte-Carlo simulation	Sensitivity analysis	SA - analytical, SA - simulation	No	not applicable	not applicable	not applicable	not applicable (the paper is related to occupational exposure assessment and not drug therapy or vaccine development)	No	Commercial platform	No	MCSim (version 6.2), R package PKSensi (version 1.2.3)
A Multi-Modal Graph Neural Network Framework for Parkinson's Disease Therapeutic Discovery	Ömer Akgüller, Mehmet Ali Balcı, Gabriela Cioca	10.3390/ijms26094453	https://doi.org/10.3390/ijms26094453	International journal of molecular sciences	-	2025	Yes	application	ML	Monte Carlo dropout for epistemic uncertainty estimation; aleatoric uncertainty estimation through predictive mean and variance; scaling of uncertainty scores by a factor of 0.5.	Bayes	Bayes - ML	Yes	Neurology/Neurodegenerative diseases; G20	small molecule	preclinical (guess)	The purpose of the model is to identify and prioritize multi-target drug repurposing candidates for Parkinson's disease by predicting drugs that can target multiple critical proteins involved in PD pathogenesis, such as lysosomal dysfunction, mitochondrial impairment, synaptic disruption, and neuroinflammation.	No	No	No	Cytoscape (v3.4.0), clusterMaker2 plugin
A framework for 2-stage global sensitivity analysis of GastroPlus TM compartmental models	Megerle L Scherholz, James Forder, Ioannis P Androulakis	10.1007/s10928-018-9573-1	https://doi.org/10.1007/s10928-018-9573-1	Journal of Pharmacokinetics and Pharmacodynamics	18	2018	Yes	methodology	PBPK	Global sensitivity analysis, Morris method, Sobol's sensitivity analysis	Sensitivity analysis	SA - simulation	Yes	- Acetaminophen: Pain relief and fever reduction (no specific ICD 11 code mentioned) - Risperidone: Psychiatric disorders (ICD 11 code: 6A20 - Schizophrenia) - Atenolol: Cardiovascular diseases (ICD 11 code: I10 - Essential hypertension) - Furosemide: Cardiovascular diseases (ICD 11 code: I10 - Essential hypertension)	small molecule	not specified	The purpose of the model is to inform model structure and understand physiological mechanisms influencing pharmacokinetic responses, which is relevant to drug therapy development by analyzing how parameterization affects drug behavior.	No	Commercial platform	No	GastroPlus, AutoIt, MATLAB R2017a
A first-generation physiologically based pharmacokinetic (PBPK) model of alphatocopherol in human influenza vaccine adjuvant	Million A Tegenge, Robert J Mitkus	10.1016/j.yrtph.2015.02.005	https://doi.org/10.1016/j.yrtph.2015.02.005	Regulatory Toxicology and Pharmacology	17	2015	Yes	application	PBPK	Monte Carlo simulations with Latin hypercube sampling	Uncertainty propagation	UP - prob - basic sim	Yes	Infectious diseases; B34.9 (Influenza, unspecified)	biologics	not specified (guess: preclinical or early clinical stage)	The purpose of the model is to estimate the biodistribution of α-tocopherol in humans following a single dose of squalene-containing adjuvant, which informs regulatory risk-benefit analyses and explains immunodynamics.	No	Commercial platform	No	Vensim Professional ®

A Computational Workflow for Probabilistic Quantitative in Vitro to in Vivo Extrapolation	Nicole C Kleinstreuer, Zhichao Liu, George Loizou, Kevin Mcnally, Alex Hogg	10.3389/fphar.2018.00508	https://doi.org/10.3389/fphar.2018.00508	Frontiers in Pharmacology	24	2018	Yes	methodology	PBPK	- Global sensitivity analysis (GSA) - Approximate Bayesian Computation (ABC) - Markov Chain Monte Carlo (MCMC) simulation	Sensitivity analysis, Bayes	SA - simulation, Bayes - Other	Yes	not applicable	not applicable	not specified (the paper is related to drug therapy development, but the stage is not clearly stated or inferred from context)	not applicable (the paper is related to toxicological assessments rather than drug therapy or vaccine development)	Yes	Open source	No	- acslX TM software - R language - RStudio - deSolve package - Sensitivity package - reshape package - ggplot2 package - md2c package - PROAST version 65.0 - R version 3.4.1
A Combined Estimation and Multi-Parametric Model Predictive Control Approach for Intravenous Anaesthesia	Ioana Nascu, Romain S C Lambert, Efstratios N Pistikopoulos	10.1109/SMC.2014.6974295	https://doi.org/10.1109/SMC.2014.6974295	IEEE International Conference on Systems, Man and Cybernetics	7	2014	Yes	application	Others	Global sensitivity analysis, specifically Sobol's method of sensitivity indices, which is a variance-based approach using ANOVA decomposition.	Sensitivity analysis	SA - Other	Yes	Anaesthesia; ICD 11 code not explicitly mentioned but related to anaesthesia	small molecule	not specified (the paper is related to drug therapy but does not specify the stage of drug development)	The purpose of the pharmacometric model is to control the depth of anesthesia by estimating key pharmacokinetic and pharmacodynamic parameters and using these estimates in a model predictive control strategy.	Yes	No	No	Not mentioned (the paper does not specify any software or programming languages used)
A Bayesian population PBPK model for multiroute chloroform exposure	Yuching Yang, X U Xu, Panos G Georgopoulos	10.1038/jes.2009.29	https://doi.org/10.1038/jes.2009.29	Journal of Exposure Science and Environmental Epidemiology	41	2009	Yes	methodology	PBPK	Bayesian hierarchical modeling, Bayesian calibration, Markov chain Monte Carlo (MCMC) simulation	Bayes	Bayes - hierachical, Bayes - calibration	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to toxicological assessment of chloroform exposure, not drug therapy or vaccine development)	No	Commercial platform	No	Matlab (The Mathworks Inc, 2008)
Bridging across OECD 308 and 309 Data in Search of a Robust Biotransformation Indicator	Mark Honti, Stefan Hahn, Dieter Hennecke, Thomas Junker, Prasit Shrestha, Kathrin Fenner	-	-	Environmental Science and Technology	39	2016	Yes	application	Others	Bayesian calibration, Markov chain Monte Carlo sampling	Bayes	Bayes - calibration	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental science and chemical biotransformation, not drug therapy or vaccine development)	No	No	No	not mentionned
Calibration experimental design considering field response and model uncertainty	Zhen Hu, Dan Ao, Sankaran Mahadevan	-	-		44	2017	Yes	methodology	ML	- Bayesian calibration - Model discrepancy analysis - Surrogate modeling (Kriging) - Global sensitivity analysis (GSA) - Data compression techniques (low-rank data compression)	Bayes, Sensitivity analysis, Uncertainty propagation	Bayes - calibration, UP - prob - surrogate, SA - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is not related to drug therapy or vaccine development)	Yes	No	No	Abaqus for finite element simulations, MATLAB Kriging toolbox
Cerebral Glioma Grading Using Bayesian Network with Features Extracted from Multiple Modalities of Magnetic Resonance Imaging	Jisu Hu, Wenbo Wu, Bin Zhu, Huiting Wang, Renyuan Liu, Xin Zhang, Ming Li, Yongbo Yang, Jing Yan, Fengnan Niu, Chuanshuai Tian, Kun Wang, Haiping Yu, Weibo Chen, Suiren Wan, Yu Sun, Bing Zhang	-	-	PLoS ONE	23	2016	Yes	application	ML	Bayesian Network, K2 algorithm, maximum likelihood estimation, leave-one-out analysis, receiver operating characteristic (ROC) analysis, posterior probability computation	Bayes	Bayes - ML	No	not applicable	not applicable	not applicable	not applicable (the paper is related to diagnostic imaging and grading of gliomas, not drug therapy or vaccine development)	No	No	No	- K2 algorithm - JMP software - LCModel
Characterization and Management of Uncertainties in Toxicological Risk Assessment: Examples from the Opinions of the European Food Safety Authority	Alberto Mantovani	-	-	Methods in molecular biology	7	2018	Yes	review	Others	- Expert elicitation of probabilistic distributions - Uncertainty propagation in the form of Benchmark dose (BMD) approach with confidence intervals (95% confidence limits)	Uncertainty propagation	UP - Other	No	not applicable	not applicable	not applicable (the paper is about toxicological risk assessment of chemicals, not drug therapy or vaccine development)	Not applicable (the paper is related to toxicological risk assessment, not drug therapy or vaccine development)	No	No	No	Not mentioned (the paper does not specify any software used for uncertainty quantification)
Comparison of interval and Monte Carlo simulation for the prediction of postprandial glucose under uncertainty in type 1 diabetes mellitus	R Calm, M García-Jaramillo, J Bondia, M A Sainz, J Vehí	-	-	Comput. Methods Programs Biomed.	25	2011	Yes	methodology	Others	Monte Carlo simulation (MCS), Modal interval analysis (MIA)	Uncertainty propagation	UP - non prob	Yes	Endocrinology; E10	biologics	not specified (the paper is related to insulin therapy optimization but does not specify a stage of drug development)	The purpose of the model is to optimize insulin therapy by predicting glucose excursions under uncertainty, which can lead to safer and more robust insulin infusion algorithms.	Yes	Commercial platform	No	Borland C++ Builder (version 6.0), C/C++ programming language
Comparison of statistical and deterministic frameworks of uncertainty quantification.	Frenklach, Michael, Packard, Andrew, Garcia-Donato, Gonzalo, Paulo, Rui, Sacks, Jerome	-	-	SIAM/ASA Journal on Uncertainty Quantification	37	2016	Yes	methodology	Others	- Bound-to-bound data collaboration (B2B): deterministic approach using semidefinite programming algorithms - Bayesian calibration and prediction (BCP): statistical and Bayesian approach	Bayes, Other	Bayes - calibration	No	not applicable	not applicable	not applicable	not applicable (the paper is not related to drug therapy or vaccine development)	No	No	No	WinBUGS, R (MCMC algorithm)
Comparison of surrogate-based uncertainty quantification methods for computationally expensive simulators	N E Owen, P Challenor, P P Menon, S Bennani	-	-	SIAM/ASA J. Uncertain. Quantification	67	2018	Yes	methodology	Others	Polynomial chaos and Gaussian process emulation are the uncertainty quantification methods used in this paper. These are both surrogate-based methods used to approximate expensive simulators. Additionally, Monte Carlo simulation is mentioned as a conventional approach for tasks such as sensitivity analysis and calibration.	Uncertainty propagation, Sensitivity analysis	UP - prob - surrogate, SA - simulation	No	not applicable	not applicable	not applicable	Not applicable (the paper is not related to drug therapy or vaccine development)	Yes	Open source	No	R package DiceKriging
Computational algorithm for solving drug pharmacokinetic model under uncertainty with nonsingular kernel type Caputo-Fabrizio fractional derivative	Nesrine Harrouche, Shaher Momani, Shatha Hasan, Mohammed Al-Smadi	-	-		33	2021	Yes	methodology	Others	Fuzzy computations	Uncertainty propagation	UP - non prob	No	not applicable	not applicable	not specified	Understanding drug absorption and extraction rates under uncertainty, considering factors like bioavailability and physiological characteristics.	Yes	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used)
Computational Approaches for Developing Informative Prior Distributions for Bayesian Calibration of PBPK Models	Jimena L Davis, Rogelio Tomero-Velez, R Woodrow Setzer	-	-		4	2012	Yes	methodology	PBPK	Bayesian statistical methods, Bayesian calibration	Bayes	Bayes - calibration	No	not applicable (the paper does not specify a therapeutic area or ICD 11 code)	not applicable	not applicable	not applicable (the paper is related to risk assessments rather than drug therapy or vaccine development)	No	No	No	Not mentioned (the paper does not specify any software or programming languages used)
Confronting variability with uncertainty in the ecotoxicological impact assessment of down-the-drain products	Mélanie Douziech, Rik Oldenkamp, Rosalie Van Zelm, Henry King, A Jan Hendriks, Anne-Sophie Picheux, Mark A J Huijbregts, Olga-Ioanna Kalantzi	-	-	Environment International	18	2019	Yes	methodology	Others	Two-dimensional Monte Carlo (2D MC) simulation, Spearman correlation coefficients, Uncertainty and variability ratios (UR and VR)	basic frequentist		No	not applicable	not applicable	not applicable	Not applicable (the paper is related to ecotoxicological impact assessment of down-the-drain products, not drug therapy or vaccine development)	No	No	No	R
Considerations for Improving High to Low Dose Extrapolation for Regulatory Risk Assessment	Lauren Zeise	-	-		0	2007	Yes	review	PBPK	- Probability distributions - Hierarchical Bayesian approach	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	not applicable (the paper is related to environmental risk assessment, not drug therapy or vaccine development)	No	No	No	Not mentioned (the paper does not specify any software used for uncertainty quantification)
Constructing Time-Resolved Species Sensitivity Distributions Using a Hierarchical Toxico-Dynamic Model	Guillaume Kon, Kam King, Marie Laure Delignette-Muller, Ben J Kefford, Christophe Piscart, Sandrine Charles	-	-	Environmental Science and Technology	22	2015	Yes	application	Others	Bayesian hierarchical modeling, uncertainty propagation, shrinkage behavior	Uncertainty propagation, Bayes	Bayes - hierachical, UP - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental risk assessment, not drug therapy or vaccine development)	No	Open source	Open source	Stan via RStan

Dealing with Measurement Uncertainties as Nuisance Parameters in Bayesian Model Calibration \ast	Kellin Rumsey, \dagger\ddagger, Gabriel Huerta \ddagger, Justin Brown \ddagger, Lauren Hund \dagger	-	-	SIAM/ASA J. Uncertain. Quantification	7	2020	Yes	methodology	Others	Bayesian Model Calibration (BMC), model discrepancy analysis, moment penalization prior	Sensitivity analysis, Bayes	SA - analytical, Bayes - calibration	No	not applicable	not applicable	not applicable	not applicable	No	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used)
Deep Gaussian Processes for Calibration of Computer Models (with Discussion) *	Sébastien Marmin, Maurizio Filippone	-	-	Bayesian Analysis	13	2022	Yes	methodology	Others	Bayesian calibration, model discrepancy analysis, surrogate modeling, stochastic variational inference, deep Gaussian processes, Gaussian processes with random feature approximations	Sensitivity analysis, Uncertainty propagation, Bayes	SA - analytical, Bayes - calibration, UP - prob - surrogate	No	not applicable	not applicable	not applicable	Not applicable (the paper is not related to drug therapy or vaccine development)	Yes	No	Open source	not mentioned
Demonstration of the relationship between sensitivity and identifiability for inverse uncertainty quantification	Xu Wu, Koroush Shirvan, Tomasz Kozlowski	-	-	Journal of Computational Physics	30	2019	Yes	methodology	Others	- Bayesian calibration - Model discrepancy analysis - Surrogate modeling (Gaussian Process) - Full Bayesian Approach (FBA) - Modular Bayesian Approach (MBA) - Probabilistic sensitivity analysis (Sobol' indices) - Uncertainty propagation - Markov Chain Monte Carlo (MCMC) sampling	Bayes, Sensitivity analysis, Uncertainty propagation	Bayes - calibration, SA - analytical, UP - prob - surrogate, SA - simulation	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to nuclear engineering, not drug therapy or vaccine development)	No	No	No	not mentionned
Derivation of site-specific remediation goals by incorporating the bioaccessibility of polycyclic aromatic hydrocarbons with the probabilistic analysis method	Ruihuan Zhang, Dan Han, Lin Jiang*, Maosheng Zhong*, Jing Liang, Tianxiang Xia, Ying Zhao, D Aga	-	-	Journal of Hazardous Materials	20	2019	Yes	application	Others	Monte Carlo analysis (MCA)	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental remediation and risk assessment, not drug therapy or vaccine development)	Yes	Commercial platform	No	@RISK (7.5) software of Palisade
Development and specification of physiologically based pharmacokinetic models for use in risk assessment	Rebecca A Clewell, Harvey J Clewell	-	-	Regulatory toxicology and pharmacology : RTP	144	2007	Yes	review	PBPK	- Hierarchical Bayesian approaches - Markov chain Monte Carlo (MCMC) simulation - Sensitivity analysis - Monte Carlo techniques - Likelihood methods	Bayes, Sensitivity analysis, basic frequentist	Bayes - hierachical, SA - simulation, Freq - likelihood	No	not applicable	not applicable	not specified	not applicable (the paper is focused on risk assessment for environmental and occupational chemicals, not drug therapy or vaccine development)	No	No	No	not mentioned
Development of a Physiologically Based Pharmacokinetic Model for Inorganic Mercury Salts in Rodents and Humans and Its Application in the Derivation of Health-Based Toxicity Metrics	Yu-Sheng Lin, Nan-Hung Hsieh, Nagalakshmi Keshava, Wei-Chun Chou, Geoffrey C Peterson, Jeffrey Gift	-	-	Environmental Science and Technology	0	2025	Yes	application	PBPK	Bayesian hierarchical framework, Markov chain Monte Carlo (MCMC), variance-based global sensitivity analysis (GSA), probabilistic sensitivity analysis, lognormal distribution for residual errors	Bayes, Sensitivity analysis	Bayes - hierachical, SA - simulation	No	not applicable	not applicable	not applicable	not applicable (the paper is related to toxicokinetics and risk assessment, not drug therapy or vaccine development)	No	Open source	Open source	MCSim version 6.2
Development of a Physiologically Based Pharmacokinetic Model of Trichloroethylene and Its Metabolites for Use in Risk Assessment	Harvey J Clewell, P Robinan Gentry, Tammie R Covington, Jeffery M Gearhart2 the, K S Crump	-	-	Environmental Health Perspectives	153	2000	Yes	application	PBPK	Monte Carlo analysis, sensitivity analysis	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	not applicable	No	Commercial platform	No	PBPK_SIM (K.S. Crump Group, Ruston, LA)
Development of human dermal PBPK models for the bisphenols BPA, BPS, BPF, and BPAF with parallel-layered skin compartment: Basing on dermal administration studies in humans	Man Hu, Zhichun Zhang, Yining Zhang, Ming Zhan, Weidong Qu, Gengsheng He, Ying Zhou, Adrian Covaci	-	-	Science of the Total Environment	14	2023	Yes	application	PBPK	Monte Carlo simulation, probabilistic sensitivity analysis (using truncated normal distributions), uncertainty propagation (using uncertainty coefficients), Global Sensitivity Analysis (GSA)	Sensitivity analysis, Uncertainty propagation	SA - simulation, UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental chemical risk assessment, not drug therapy or vaccine development)	No	Open source	Open source	- DeSolve R software (for simulations) - "soboljansen" package of R (for global sensitivity analysis)
DIRECT MC CONVERSION OF ABSORBED DOSE TO GRAPHITE TO ABSORBED DOSE TO WATER FOR 60 Co RADIATION	J E Lye, D J Butler, R D Franich, P D Harty, C P Oliver, G Ramanathan, D V Webb, T Wright	-	-	-		2013	Yes	application	Others	Sensitivity analysis, Monte Carlo simulations, uncertainty propagation, and type B uncertainty estimation	Sensitivity analysis, Uncertainty propagation	UP - Other, SA - Other	No	not applicable	not applicable	not applicable	not applicable (the paper is related to radiation dosimetry and calibration, not drug therapy or vaccine development)	No	No	No	not mentioned
Dosimetric characterization of an 192 Ir brachytherapy source with the Monte Carlo code PENELOPE	Francisco Javier Casado, Salvador Garci `a-Pareja, Elena Cenizo, Beatriz Mateo, Coral Bodineau, Pedro Gala	-	-	-		2010	Yes	application	Others	- Statistical (type A) uncertainties: Monte Carlo simulations - Systematic (type B) uncertainties: Cell average effect, cross-section uncertainties - Uncertainty propagation: Intensity-weighted average for photon emission intensity - Frequentist approach: Use of coverage factor (k) for uncertainty weighting	Uncertainty propagation, basic frequentist	UP - Other	No	not applicable	not applicable	not applicable (the paper is related to radiation therapy and brachytherapy, not drug therapy or vaccine development)	Not applicable (the paper is related to radiation therapy and dosimetry, not drug therapy or vaccine development)	No	Commercial platform	No	PENELOPE code, PENGEOM subroutines package
Efficient calibration for high-dimensional computer model output using basis methods	James M Salter, Daniel B Williamson	-	-	International Journal for Uncertainty Quantification	7	2019	Yes	methodology	Others	- Emulation using statistical models (emulators) - History matching - Gaussian processes - Mahalanobis distance for implausibility measure - Basis methods for surrogate modeling	Uncertainty propagation	UP - prob - surrogate	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to climate modeling, not drug therapy or vaccine development)	Yes	No	No	not mentioned
Efficient DCE-MRI Parameter and Uncertainty Estimation Using a Neural Network	Yannick Bliesener, Jay Acharya, Krishna S Nayak	-	-	IEEE Transactions on Medical Imaging	16	2019	Yes	application	ML	Bayesian estimation using a neural network to approximate the joint posterior distribution of tracer-kinetic parameters with a non-informative uniform prior.	Bayes	Bayes - ML	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to monitoring brain tumor treatment response rather than drug therapy development)	No	No	No	Neural network architecture (custom-built)
Efficient Sensitivity/Uncertainty Analysis Using the Combined Stochastic Response Surface Method and Automated Differentiation: Application to Environmental and Biological Systems	S S Isukapalli, A Roy, P G Georgopoulos	-	-	Risk Analysis	110	2000	Yes	methodology	PBPK	- Stochastic Response Surface Method (SRSM) - Automatic Differentiation of FORTRAN (ADIFOR) - Polynomial Chaos Expansion (surrogate modeling) - Monte Carlo simulation - Latin Hypercube Sampling (LHS) - Probabilistic sensitivity analysis - Uncertainty propagation	Sensitivity analysis, Uncertainty propagation	SA - analytical, UP - prob - basic sim, UP - prob - surrogate	No	not applicable	not applicable	not applicable	not applicable (the paper is related to uncertainty analysis in environmental and biological systems rather than drug therapy development)	Yes	No	No	ADIFOR, FORTRAN, Maple
Estimation of pressure-particle velocity impedance measurement uncertainty using the Monte Carlo method	Eric Brandão, Rodolfo C C Flesch, Arcanjo Lenzi, Carlos A Flesch, Eric Branda	-	-	Journal of the Acoustical Society of America	14	2011	Yes	application	Others	Monte Carlo method (MCM)	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to acoustic impedance measurement, not drug therapy or vaccine development)	Yes	No	No	Not mentioned (the paper does not specify any software or programming languages used)
EVALUATING AND EXPRESSING THE PROPAGATION OF UNCERTAINTY IN CHEMICAL FATE AND BIOACCUMULATION MODELS	Matthew Macleod, Alison J Fraser, Don Mackay	-	-	Environmental Toxicology and Chemistry	230	2002	Yes	methodology	Others	First-order analytical sensitivity and uncertainty analysis, Monte Carlo analysis, graphical technique for uncertainty propagation, Taylor series expansion for uncertainty propagation, log-normal distributions for uncertainty description	Sensitivity analysis, Uncertainty propagation	UP - prob - surrogate, SA - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental chemical fate models, not drug therapy or vaccine development)	No	Commercial platform	Open source	Crystal Ball (for MCMC)
Evaluating parameter availability for physiologically based pharmacokinetic (PBPK) modeling of perfluorooctanoic acid (PFOA) in zebrafish †	Manoochehr Khazaee, Carla A Ng	-	-	Environmental Science: Processes & Impacts	22	2017	Yes	application	PBPK	Monte Carlo uncertainty and sensitivity analysis, partial rank correlation coefficient analysis	Sensitivity analysis, Uncertainty propagation	UP - Other, SA - Other	No	not applicable	not applicable	not applicable (the paper is about environmental contaminant modeling, not drug therapy or vaccine development)	not applicable (the paper is related to environmental contaminant modeling, not drug therapy or vaccine development)	No	No	No	Not mentioned (the paper does not specify any software used for the uncertainty quantification model)

Evaluating the impact of anatomical and physiological variability on human equivalent doses using PBPK models	Celia M Schacht, Annabel E Meade, Amanda S Bernstein, Bidya Prasad, Paul M Schlosser, Hien T Tran, Dustin F Kapraun	-	-	Toxicological Sciences	2	2025	Yes	application	PBPK	- Monte Carlo (MC) sampling	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to chemical risk assessment, not drug therapy or vaccine development)	No	Open source	Open source	- R version 3.6.0 - MCSim model specification language - C - R package "deSolve"
Evaluation of the Uncertainty in an Oral Reference Dose for Methylmercury Due to Interindividual Variability in Pharmacokinetics	Harvey J Clewell, J Jeffery, M Gearhart, P Robinan Gentry, Tammie R Covington, Cynthia B Vanlandingham, Kenny S Crump, Annette M Shipp'	-	-	Risk Analysis	143	1999	Yes	application	PBPK	Monte Carlo analysis, sensitivity analysis (analytical sensitivity coefficients and correlation analysis)	Sensitivity analysis	SA - analytical, SA - simulation	No	not applicable	not applicable	not applicable	not applicable (the paper is related to environmental health guidelines, not drug therapy or vaccine development)	No	No	No	Not mentioned (the paper does not specify any software or programming language used for the analysis)
Evaluation of uncertainty in input parameters to pharmacokinetic models and the resulting uncertainty in output	David Farrar, Bruce Allen, Kenny Crump, Annette Shipp	-	-	Toxicology Letters	80	1989	Yes	application	PBPK	Uncertainty propagation, Monte Carlo simulation using Latin-hypercube procedure, probabilistic sensitivity analysis	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	not applicable (the paper is related to risk assessment, not drug therapy or vaccine development)	No	No	No	Not mentioned
Exact Gradients Improve Parameter Estimation in Nonlinear Mixed Effects Models with Stochastic Dynamics	Helga Kristin Olafsdottir, Jacob Leander, Joachim Almquist, Mats Jirstrand	-	-	AAPS Journal	8	2018	Yes	methodology	Others	Extended Kalman Filter (EKF)	Other		No	not applicable (the paper is related to drug therapy development but does not specify a therapeutic area or provide an ICD 11 code)	not applicable	not applicable	not applicable	Yes	Commercial platform	Upon request to the authors	Mathematica 11, NONMEM
EXPERIENCING A PROBABILISTIC APPROACH TO CLARIFY AND DISCLOSE UNCERTAINTIES WHEN SETTING OCCUPATIONAL EXPOSURE LIMITS	David Vernez, Sandrine Fraize-Frontier, Raymond Vincent, Stéphane Binet, Christophe Rousselle	-	-	International Journal of Occupational Medicine and Environmental Health	1	2018	Yes	methodology	Others	Monte Carlo techniques, uncertainty propagation, probabilistic distribution assignment	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is about occupational exposure limits, not drug therapy or vaccine development)	No	No	No	R Statistical Software (version 3.2)
FAST DIMENSION-REDUCED CLIMATE MODEL CALIBRATION AND THE EFFECT OF DATA AGGREGATION 1	Won Chang, Murali Haran, Roman Olson, Klaus Keller	-	-	-		2014	Yes	application	Others	Bayesian reduced-dimensional calibration, Gaussian process-based approach, Metropolis-Hastings algorithm, model discrepancy analysis	Bayes, Sensitivity analysis	SA - analytical, Bayes - calibration	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to climate model calibration, not drug therapy or vaccine development)	No	No	No	R (PORT routine)
Forward and backward uncertainty quantification with active subspaces: Application to hypersonic flows around a cylinder	Andrea F Cortesi, Paul G Constantine, Thierry E Magin, Pietro M Congedo	-	-	Journal of Computational Physics	23	2019	Yes	application	Others	- Bayesian calibration - Surrogate modeling - active subspace - Monte Carlo (MC) sampling - Kernel density estimation	Uncertainty propagation, Bayes, Other	Bayes - calibration, UP - prob - surrogate	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to aerospace engineering and fluid dynamics, not drug therapy or vaccine development)	No	No	No	COSMIC code, Python SciKit Learn
Gaussian processes with built-in dimensionality reduction: Applications to high-dimensional uncertainty propagation	Rohit Tripathy, Ilias Bilionis, Marcial Gonzalez	-	-	Journal of Computational Physics	67	2016	Yes	methodology	ML	probabilistic version of active subspaces (Gaussian process regression with built-in dimensionality reduction)	Sensitivity analysis	SA - analytical	No	not applicable	not applicable	not applicable	Not applicable (the paper is not related to drug therapy or vaccine development)	No	Open source	Open source	Python, GPy module
Global uncertainty and sensitivity analysis of a food-web bioaccumulation model.	Stefano Ciavatta	-	-	-		2009	Yes	application	Others	- Morris method for preliminary screening - Monte Carlo simulations for exploring input-output relationships - State Dependent Regression (SDR) model for partitioning variance	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental risk assessment and not drug therapy or vaccine development)	No	Open source	No	SimLab, SS-ANOVA-R
Gradient and Uncertainty Enhanced Sequential Sampling for Global Fit	Sven Lämmle, Can Bogoclu, Kevin Cremanns, Dirk Roos	-	-	Computer Methods in Applied Mechanics and Engineering	5	2023	Yes	methodology	ML	global surrogate modelling: - Predictive posterior uncertainty - Variance estimation (heteroscedastic variance estimate) - Predicted standard deviation	Uncertainty propagation, basic frequentist	UP - prob - surrogate	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to engineering applications and does not discuss drug therapy or vaccine development)	No	Open source	Open source	- Python (programming language) - scikit-optimize (library) - scikit-learn (library) - scipy (library) - TensorFlow (backend for DGCN) - pygmo (package for evolutionary strategies)
Hierarchical deep compartment modeling: A workflow to leverage machine learning and Bayesian inference for hierarchical pharmacometric modeling	Ahmed Elmokadem |, Matthew Wiens, Timothy Knab |, Kiersten Utsey, Samuel P Callisto |, Daniel Kirouac, Ahmed Elmokadem	-	-	Clinical and Translational Science	1	2024	Yes	methodology	Others	Hierarchical deep compartment modeling with Bayesian inference, Markov Chain Monte Carlo (MCMC) techniques	Bayes	Bayes - ML	No	Not applicable (the paper does not specify the therapeutic area or the drug's application)	not applicable	not specified	not applicable	No	Open source	Open source	- Julia (programming language) - Flux.jl (package for neural network construction) - Turing.jl (package for Bayesian inference and MCMC) - ShapML.jl (package for Shapley values) - Optim.jl (package for optimization) - NLopt.jl (package for optimization)
Hierarchical modelling of species sensitivity distribution: development and application to the case of diatoms exposed to several herbicides	Guillaume Kon, Kam King, Floriane Larras, Sandrine Charles, Marie Laure Delignette-Muller	-	-	Ecotoxicology and Environmental Safety	21	2015	Yes	methodology	Others	Bayesian inference using Gibbs sampling via Markov Chain Monte Carlo (MCMC) simulation, uncertainty propagation, Bayesian hierarchical modeling	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental toxicology and ecological risk assessment, not drug therapy or vaccine development)	No	Open source	Open source	JAGS, R, R package rjags, R package dclone
Hierarchical stochastic metamodels based on moving least squares and polynomial chaos expansion Application to the multiobjective reliability-based optimization of space truss structures	Rajan Filomeno Coelho, Jérémy Lebon, Philippe Bouillard	-	-		42	2010	Yes	methodology	Others	hierarchical stochastic metamodels based on moving least squares and spectral decomposition (by polynomial chaos expansion)	Uncertainty propagation	UP - prob - surrogate	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to structural engineering and optimization, not drug therapy or vaccine development)	Yes	No	No	not mentioned
HUMAN EXPOSURE ASSESSMENT II: QUANTIFYING AND REDUCING THE UNCERTAINTIES	Gary K Whitmyre, Jeffrey H Driver, Michael E Ginev An, M E Ginevan, Silver Spring, Robert G Tardiff, Scott R Baker	-	-	Toxicology and industrial health	16	1992	Yes	methodology	PBPK	- Stochastic approaches - Monte Carlo simulations - Information analysis techniques - Bivariate analysis	Other		No	not applicable	not applicable	not applicable	Not applicable (the paper is related to human exposure assessment, not drug therapy or vaccine development)	No	No	No	Not mentioned
Human health risk assessment of pharmaceuticals in water: An uncertainty analysis for meprobamate, carbamazepine, and phenytoin	Arun Kumar, Irene Xagoraraki	-	-	Regulatory toxicology and pharmacology : RTP	96	2010	Yes	methodology	Others	Monte Carlo uncertainty analysis, first-order linear approximation for variance attribution analysis	Uncertainty propagation	UP - prob - surrogate, UP - prob - basic sim	No	not applicable	not applicable	not applicable	not applicable (the paper is related to risk assessment of pharmaceuticals in water, not drug therapy or vaccine development)	No	Commercial platform	No	Microsoft Excel

Can Population Modelling Principles be Used to Identify Key PBPK Parameters for Paediatric Clearance Predictions? An Innovative Application of Optimal Design Theory	Elisa A M Calvier, Thu Thuy Nguyen, Trevor N Johnson, Amin Rostami-Hodjegan, Dick Tibboel, Elke H J Krekels, Catherijne A J Knibbe	-	-	Pharmaceutical Research	8	2018	Yes	application	PBPK	Frequentist methods: Global sensitivity analysis, Uncertainty propagation using Monte Carlo methods (sampling from uniform distributions), Relative standard errors (rse), Relative root mean square error (rmse)	Sensitivity analysis, Uncertainty propagation, basic frequentist	SA - Other, UP - prob - basic sim	Yes	hepatic metabolism	small molecule	not specified (the paper is related to drug therapy development, but the specific stage is not cleafly stated)	dose finding, support paediatric clinical trial design	Yes	Open source	Open source	- PFIM program 4.0 (extended R program) for optimal design procedures - Simcyp software V15.R1 for PBPK simulations - NONMEM version 7.3 and Perl-speaks-NONMEM software package version 4.6.0 for stochastic simulations
cLRT-Mod: An efficient methodology for pharmacometric model-based analysis of longitudinal phase II dose finding studies under model uncertainty	Simon Buatois, Sebastian Ueckert, Nicolas Frey, Sylvie Retout, France Mentré	-	-	-		2021	Yes	methodology	Others	- Combined likelihood ratio test (cLRT) - Monte Carlo simulations - Coverage probability computation - Model averaging (MA) with AIC as information criterium and frequentist approach for weight calculation - Model selection (MS) with AIC as information criterium	Other, basic frequentist		Yes	Type 2 diabetes mellitus; ICD 11 code: 5A11	small molecule	Phase II (stated)	dose finding	Yes	Commercial platform	No	NONMEM7.4, PSN 4.4.8
Deep Supramolecular Language Processing for Co-Crystal Prediction	Rebecca Birolo, Rıza Özçelik, Andrea Aramini, Roberto Gobetto, Michele R Chierotti, Francesca Grisoni	-	-	Angewandte Chemie	1	2025	Yes	methodology	ML	- Majority voting , whereby the number of agreements in the predicted class per each molecular pair is used as a measure of confidence (the higher, the better) - Standard deviation-based estimation	Other		Yes	Musculoskeletal and connective tissue disorders; ICD 11 code: M00-M99	small molecule	not specified (guess: discovery/optimization)	The purpose of the DeepCocrystal model is to predict co-crystallization pairs to enhance pharmacokinetic properties of drugs, thereby accelerating drug development.	No	Open source	Open source	DeepCocrystal, Convolutional Neural Networks (CNNs)
Combining Model-Based Clinical Trial Simulation, Pharmacoeconomics, and Value of Information to Optimize Trial Design	Daniel Hill-Mcmanus, Dyfrig A Hughes	-	-	-		2021	Yes	methodology	PBPK	Monte Carlo simulation, uncertainty propagation, constant coefficient of variation model, variance-covariance matrix estimation	Uncertainty propagation, basic frequentist	UP - prob - basic sim	Yes	Gout; M10	small molecule	Phase III (stated)	The purpose of the pharmacometric model is to generate prior distributions for Bayesian decision-theoretic trial design, which involves simulating treatment effects under specific conditions such as dose-taking behavior and patient population characteristics, and to identify optimal sample sizes that maximize the expected return on investment (ROI) for the pharmaceutical company.	Yes	No	No	R version 3.5.1
Comparative Analysis of Chemical Descriptors by Machine Learning Reveals Atomistic Insights into Solute-Lipid Interactions Published as a part of the Molecular Pharmaceuticsvirtual special issue"Advances in Small and Large Molecule Pharmaceutics Research across Ireland"	Johann Justus, Andrea Lange, Jochem Anelli, Martin Alsenz, Patrick J Kuentz, Wiebke O'dwyer, Nicole Saal, Brendan T Wyttenbach, Griffin, Brendan T Griffin -, Lange -, Andrea Anelli -, Martin Kuentz, Patrick J O'dwyer -, Wiebke Saal, Nicole Wyttenbach	-	-	-		2024	Yes	application	QSP	Ensemble modeling with subsampling and standard deviation estimation; calibration and rescaling of predicted distributions	Other		Yes	not applicable (the paper is related to drug formulation development but does not specify a therapeutic area or ICD 11 code)	small molecule	Preclinical (guess)	prediction of dose loading in lipids	No	Open source	No	- Scikit-learn - Numpy
Complex Bayesian Modeling Workflows Encoding and Execution Made Easy With a Novel WinBUGS Plugin of the Drug Disease Model Resources Interoperability Framework	Cristiana Larizza, Elisa Borella, Lorenzo Pasotti, Paima Tartaglione, Mike Smith, Stuart Moodie, Paolo Magni	-	-	CPT: Pharmacometrics & Systems Pharmacology	3	2018	Yes	methodology	Others	Bayesian hierarchical modeling, Bayesian estimation, uncertainty propagation, stochastic simulations, Markov Chain Monte Carlo (MCMC) algorithms, informative and weakly informative priors	Bayes	Bayes - hierachical	Yes	e.g. Diabetes; ICD-11 code: 5A10	not applicable	not applicable (the paper is about modeling tools and not directly related to drug therapy or vaccine development)	not applicable (the paper focuses on improving pharmacometric modeling workflows rather than drug therapy or vaccine development)	No	Open source	Open source	DDMoRe Interoperability Framework (IOF) tools: estimation: - WinBUGS - NONMEM - Monolix diagnostics: - PsN - Xpose Simulation: - Simulx - Sim-Cyp optimization: - PopED - PFIM
Conformal prediction-based machine learning in Cheminformatics: Current applications and new challenges	Mario Astigarraga, Andrés Sánchez-Ruiz, Gonzalo Colmenarejo	-	-	Artificial Intelligence in the Life Sciences	1	2025	Yes	methodology	ML	Conformal Prediction (CP) Standard Deviation (SD) of residuals, Ensemble methods, Bootstrapping, Quantile regression, Monte Carlo dropout, Bayesian methods (mentionned as alternative methods)	Bayes, basic frequentist	Bayes - ML, Freq - resampling	Yes	not applicable	not applicable	not specified (the paper is related to drug therapy development, focusing on QSAR and molecular screening, but does not specify a particular stage)	not applicable (the paper is related to Cheminformatics and QSAR modeling, not directly to drug therapy development or vaccine development)	No	Open source	Open source	- Python modules: crepes (https://github.com/henrikbostrom/crepes), MAPIE (https://github.com/nilslacroix/MAPIE) and torchCP (https://github.com/ml-stat-Sustech/TorchCP) - R packages: conformal (https://github.com/isidroc/conformal, no longer maintained), conformalInference (https://github.com/ryantibs/conformal), AdaptiveConformal (https://github.com/herbps10/AdaptiveConformal), cfcausal (https://github.com/lihualei71/cfcausal) - Scala-CP (https://github.com/mcapuccini/scala-cp)
Conformalized Graph Learning for Molecular ADMET Property Prediction and Reliable Uncertainty Quantification	Peiyao Li, Lan Hua, Zhechao Ma, Wenbo Hu, Ye Liu, Jun Zhu	-	-	Journal of Chemical Information and Modeling	4	2024	Yes	methodology	ML	- Conformalized Fusion Regression (CFR) - Deep Ensemble (Ensemble) - Monte Carlo Dropout (Dropout) - Ensemble-based Conformal Prediction (CP) - Inductive Conformal Prediction (ICP) - Posthoc calibration using Isotonic Regression (IR) - Conformalized Quantile Regression (CQR) - Conformal Residual-based Regression (CRR)	Bayes, Other	Bayes - ML	Yes	not applicable (the paper is related to drug discovery and development but does not specify a particular therapeutic area or ICD 11 code)	not applicable	early-stage drug development (guess)	The purpose of the model is to enhance the efficiency and safety of early-stage drug development by providing accurate predictions and reliable uncertainty quantification for compound prioritization.	No	Open source	Open source	- Python - Chemprop framework - GitHub: https://github.com/peiyaoli/Conformal-ADMET-Prediction
DeepSIBA: chemical structure-based inference of biological alterations using deep learning †	C Fotis, N Meimetis, A Sardis, L G Alexopoulos	-	-	-		2020	Yes	methodology	ML	Deep ensembles with Gaussian mixture for uncertainty estimation, using coefficient of variation (CV) as a measure of predictive uncertainty.	Other		Yes	Cancer; C00-D49	small molecule	Early-stage drug discovery (guess)	The purpose of the model is to aid in the identification of compounds with desired biological effects, enhancing drug discovery by predicting efficacy and toxicity profiles.	No	Open source	Open source	Keras, TensorFlow, R

Development and evaluation of uncertainty quantifying machine learning models to predict piperacillin plasma concentrations in critically ill patients	Jame Verhaeghe, Sofie A M Dhaese, Thomas De Corte, David Vander Mijnsbrugge, Heleen Aardema, Jan G Zijlstra, Alain G Verstraete, Veronique Stove, Pieter Colin, Femke Ongenae, Jan J De Waele, Sofie Van Hoecke	-	-	BMC Medical Informatics and Decision Making	17	2022	Yes	application	ML	- Quantile Ensemble method - Gaussian processes - Absolute Distribution Coverage Error (ADCE) - Distribution Coverage Error (DCE)	Other		Yes	Infectious diseases; ICD 11 code: 1A00-1A9Z	small molecule	not specified (the paper is about optimizing existing drug therapy rather than new drug development)	The purpose of the model is to predict plasma concentrations of piperacillin to guide dosing regimen adaptations and ensure therapeutic drug concentrations are achieved, providing uncertainty quantification for clinical decision-making.	No	Open source	Open source	Python (version 3.8.5), NumPy (version 1.19.1), TensorFlow
Diazepam Pharamacokinetics from Preclinical to Phase I Using a Bayesian Population Physiologically Based Pharmacokinetic Model with Informative Prior Distributions in Winbugs	Ivelina Gueorguieva, Leon Aarons, Malcolm Rowland	-	-	Journal of Pharmacokinetics and Pharmacodynamics	32	2006	Yes	methodology	PBPK	Bayesian analysis with Markov Chain Monte Carlo (MCMC) simulations, use of informative and non-informative priors, convergence checks using trace plots and diagnostic tests like CODA, Raftery and Lewis criterion, and Heidelberger and Welch stationarity tests.	Bayes	Bayes - Other	Yes	e.g. Anxiety disorders; 6B0Z	small molecule	Phase I (guess)	The purpose of the model is to predict human pharmacokinetics based on preclinical data, which is essential for dose finding and understanding how drugs behave in the human body.	No	Commercial platform	No	WinBUGS
EANM guidance document: dosimetry for first-in-human studies and early phase clinical trials	Caroline Stokke, Silvano Gnesin, Johannes Tran-Gia, Francesco Cicone, Søren Holm, Marta Cremonesi, Joh Blakkisrud, Thomas Wendler, Nic Gillings, Ken Herrmann, Felix M Mottaghy, Jonathan Gear	-	-	European Journal of Nuclear Medicine and Molecular Imaging	18	2024	Yes	review	PBPK	- Goodness-of-fit for uncertainty estimation - Ordinary least squares (OLS) for fitting uncertainty - Generalized least squares (GLS) for propagating uncertainty - Uncertainty propagation using population distribution	Uncertainty propagation	UP - prob - basic sim, UP - Other	Yes	not applicable (the paper does not specify a particular therapeutic area or ICD 11 code)	small molecule, biologics	First-in-human and early phase clinical trials (guess)	The purpose of the model is dose finding and identification of the therapeutic window to optimize treatment regimens.	No	No	No	not mentioned
Effect of uncertainty about population parameters on pharmacodynamics-based prediction of clinical trial power B	Holger Kraiczi, Marianne Frise	-	-	Contemporary Clinical Trials	5	2005	Yes	methodology	Others	- Bayesian methods (full parametric modeling, independent normal and inverse Gamma distributions) - Variance-based sensitivity analysis - Reference to Sobol' sensitivity indices	Bayes, Sensitivity analysis	Bayes - Other, SA - Other	Yes	Cardiovascular diseases; I10-I15	small molecule	Phase II or Phase III (guess)	The purpose of the pharmacometric model is to predict the power of clinical trials by incorporating uncertainty about population parameters, which helps in distinguishing important from unimportant parameters for precise power predictions and resource allocation.	No	Commercial platform	No	S and S-Plus 6.0 for Windows
Empirical Quantification of Predictive Uncertainty Due to Model Discrepancy by Training with an Ensemble of Experimental Designs: An Application to Ion Channel Kinetics	Joseph G Shuttleworth, Chon Lok, Lei, Dominic G Whittaker, Monique J Windley, Adam P Hill, Simon P Preston, Gary R Mirams	-	-	Bulletin of Mathematical Biology	12	2023	Yes	methodology	Others	Model discrepancy analysis, Interval analysis	Sensitivity analysis, Uncertainty propagation	SA - analytical, UP - non prob	Yes	Cardiovascular diseases; ICD 11 code: 9A00-Z95	small molecule	not specified (the paper is related to drug safety assessment, but the specific stage of drug development is not mentioned)	Drug safety assessment: Testing whether the expected dynamics of I Kr under drug block are expected to cause problems.	No	Open source	Open source	- CMA-ES - PINTS interface
ENHANCING UNCERTAINTY QUANTIFICATION IN DRUG DISCOVERY WITH CENSORED REGRESSION LABELS	Emma Svensson, Hannah Rosa Friesacher, Susanne Winiwarter, Lewis Mervin, Adam Arany, Ola Engkvist	-	-	-		2024	Yes	methodology	ML	Censored labels combined with: - Ensemble-based methods/Bayesian learning (Monte-Carlo-Dropout, ensembles of neural networks, Bayes by Backprop) - Gaussian models (mean-variance estimation) without censored labels: - random forests - Evidential deep learning	Bayes	Bayes - ML	Yes	not applicable (the paper does not specify a therapeutic area or provide an ICD 11 code)	small molecule	early stages (guess)	drug discovery, deciding which experiments to pursue	Yes	Open source	Open source	- Scikit-learn - PyTorch - Python 3.11
Estimating the predictive quality of dose-response after model selection	Chuanpu Hu, Yingwen Dong	-	-	-		2007	Yes	methodology	Others	Data perturbation using Monte Carlo approximations for estimating standard errors and prediction errors; Frequentist approach	basic frequentist		Yes	not applicable (the paper is related to drug development but does not specify a therapeutic area or provide enough information to assign an ICD 11 code)	not applicable	Early clinical stage (guess)	dose finding (predicting the dose that achieves a target effect, finding MED or MTD)	Yes	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used in the study)
Estimation of species-and sex-specific PFAS pharmacokinetics in mice, rats, and non-human primates using a Bayesian hierarchical methodology	Todd J Zurlinden, Michael W Dzierlenga, Dustin F Kapraun, Caroline Ring, Amanda S Bernstein, Paul M Schlosser, Viktor Morozov, Lawrence Lash	-	-	Toxicology and Applied Pharmacology	1	2025	Yes	application	Others	Bayesian hierarchical meta-regression, Bayesian calibration, uncertainty propagation	Bayes	Bayes - hierachical, Bayes - calibration	Yes	not applicable	not applicable	early stages (guess)	understand how drugs behave in different species, extrapolation of pharmacokinetic data from animals to humans	No	Open source	Open source	- Webplot digitizer - Python v3.12 - PyMC v. 5.7.2 - Bambi - ArviZ v. 0.16.1 - Matplotlib v3.7.1
Evaluation of physiologically based pharmacokinetic models for use in risk assessment †	Weihsueh A Chiu, Hugh A Barton, Robert S Dewoskin, Paul Schlosser, Chad M Thompson, Babasaheb Sonawane, John C Lipscomb, Kannan Krishnan	-	-	Journal of Applied Toxicology	138	2007	Yes	review	PBPK	- Monte Carlo simulation - Bayesian MCMC analysis	Bayes	Bayes - Other	Yes	not applicable	not applicable	not applicable	Not applicable (the paper is focused on environmental risk assessment, not drug therapy or vaccine development)	No	No	No	Not mentionned
Finding sensitive parameters in internal dose calculations for radiopharmaceuticals commonly used in clinical nuclear medicine	Vladimir Spielmann, Wei Bo Li, Maria Zankl	-	-	Radiation and Environmental Biophysics	3	2018	Yes	methodology	Others	- Sampling-based regression method (partial rank correlation coefficients) - Variance-based method	Sensitivity analysis	SA - simulation	Yes	not applicable (the paper is focused on radiopharmaceuticals in nuclear medicine, not drug therapy development)	not applicable	clinical trial phase (guess)	radiopharmaceutical dosimetry	No	No	No	- Software tool modified from a code by Iman et al. (1985) - Computer program DoseU developed at the Helmholtz Zentrum München
Fuzzy Simulation of Pharmacokinetic Models: Case Study of Whole Body Physiologically Based Model of Diazepam	Ivelina I Gueorguieva, Ivan A Nestorov, Malcolm Rowland	-	-	Journal of Pharmacokinetics and Pharmacodynamics	43	2004	Yes	application	PBPK	Fuzzy simulations, Monte Carlo simulations, Fuzzy-probabilistic approach	Uncertainty propagation	UP - non prob	Yes	Anxiety disorders (6B00), Insomnia (7A00), Seizures (6A00), Muscle spasms (7B00)	small molecule	early-stage drug development (guess)	dose finding, identification of subpopulations	Yes	Commercial platform	No	MATLAB 6.1, lsqcurvefit function
Global sensitivity analysis in physiologically-based pharmacokinetic/ pharmacodynamic models of inhaled and opioids anesthetics and its application to generate virtual populations	Frank Sa, ´nchez Restrepo, Mauricio Alher, ´ndez Hema, Valdivieso, Mauricio Hema, ´ndez Valdivieso	-	-	-		2022	Yes	methodology	PBPK	Global sensitivity analysis (GSA) using the Sobol method for variance decomposition	Sensitivity analysis	SA - analytical	Yes	General anesthesia; ICD 11 code not explicitly mentioned but related to anesthesia	small molecule	not specified (guess: preclinical or early clinical stage)	The purpose of the model is to evaluate controller stability and performance in the context of patient variability, which is relevant to drug therapy development. It also aids in improving model performance and efficiency by identifying critical parameters affecting drug response.	No	Open source	Open source	- R version 4.0.3 - R package "deSolve" version 1.28 - R package "sensitivity" version 1.23.1 - R package "GenSA" version 1.1.7 - C language
Global sensitivity analysis of Open Systems Pharmacology Suite physiologically based pharmacokinetic models	Abdulkarim Najjar, ‖ Abdullah Hamadeh, Sophia Krause, Andreas Schepky, Andrea Edginton	-	-	CPT: Pharmacometrics & Systems Pharmacology	3	2024	Yes	methodology	PBPK	Probabilistic uncertainty analysis, Morris method, Sobol method, EFAST method, Frequentist approach using percentiles (2.5th, 50th, 97.5th) for uncertainty quantification	Sensitivity analysis, basic frequentist	SA - analytical	Yes	e.g. Itraconazole: Antifungal therapy (ICD 11 code: B35-B49) e.g. Midazolam: Sedation/Anesthesia (ICD 11 code: 6A00-6A9Z)	small molecule	not specified (guess: preclinical or clinical stage)	identification of input parameters that require optimization based on experimental data; evaluation of sensitivity of pharmacokinetic parameters and their ratios in drug-drug interaction studies	No	Open source	Open source	- Open Systems Pharmacology (OSP) Suite - OSP Global Sensitivity R package - R programming language

Global Sensitivity Analysis of the Rodgers and Rowland Model for Prediction of Tissue: Plasma Partitioning Coefficients: Assessment of the Key Physiological and Physicochemical Factors That Determine Small-Molecule Tissue Distribution	Estelle Yau, Andrés Olivares-Morales, Michael Gertz, Neil Parrott, Adam S Darwich, Leon Aarons, Kayode Ogungbenro	-	-	AAPS Journal	19	2020	Yes	methodology	PBPK	- Global sensitivity analysis (GSA) - Latin hypercube sampling (LHS) - Partial rank correlation coefficients (PRCC) - Monte Carlo sampling - Local sensitivity analysis (SA) - Bayesian approach for parameter estimation	Sensitivity analysis	SA - simulation	Yes	not applicable	small molecule	Drug discovery and early development stages (guess)	The purpose of the model is to aid in drug development by predicting tissue:unbound plasma partition coefficients (Kpus) and the volume of distribution at steady state (Vss), which are crucial for selecting the first dose in humans and dosing frequency. It also aims to reduce PBPK model dimensionality by identifying key parameters that influence drug distribution.	No	Open source	No	R v.3.4.2, RStudio v.1.0.153
Handling uncertainties in toxicity modelling using a fuzzy filter	S Kumary, M Kumarz, R Stollx, U Kragl	-	-	SAR and QSAR in environmental research (Print)	14	2007	Yes	methodology	Others	Fuzzy computations, Energy-gain bounding criterion	Uncertainty propagation	UP - non prob	Yes	not applicable	not applicable	not applicable (the paper is related to toxicity modeling, not directly to drug therapy or vaccine development)	Not applicable (the paper is focused on toxicity modeling for environmental and health risk assessment, not drug therapy or vaccine development)	No	Commercial platform	Commercial platform with given parameters	MATLAB 6.5
Hierarchical Stochastic Model in Bayesian Inference for Engineering Applications: Theoretical Implications and Efficient Approximation	Stephen Wu, Panagiotis Angelikopoulos, James L Beck, Petros Koumoutsakos	-	-	-		2018	Yes	methodology	Others	- Hierarchical Bayesian Models (HBMs)	Bayes	Bayes - hierachical	Yes	Cancer; C00-D49	biologics	Preclinical/Clinical (guess)	The purpose of the pharmacometric model is to refine predictions of drug behavior by accounting for uncertainties in model parameters and prediction errors, which is relevant to optimizing drug therapy.	Yes	No	No	BASIS (software for Bayesian inference)
How Sure Can We Be about ML Methods-Based Evaluation of Compound Activity: Incorporation of Information about Prediction Uncertainty Using Deep Learning Techniques	Igor Sieradzki, Damian Leśniak, Sabina Podlewska, Igor F Tsigelny, Bernard Maigret	-	-	Molecules	2	2020	Yes	methodology	ML	Dropout-based uncertainty estimation (using stochasticity introduced by dropout during inference to measure variance across multiple runs)	Bayes	Bayes - ML	Yes	e.g. Neurological disorders, Psychiatric disorders	small molecule	not specified (the paper is related to drug therapy development, but the specific stage is not clearly stated)	The purpose of the model is to aid in the selection and optimization of compounds during virtual screening experiments, which is a part of drug therapy development. It helps in identifying potentially active compounds by estimating prediction uncertainty.	No	Open source	No	DeepChem package
Human Variability in Carboxylesterases and carboxylesterase-related Uncertainty Factors for Chemical Risk Assessment	E Di Consiglio, K Darney, F M Buratti, L Turco, S Vichi, E Testai, L S Lautz, J L C M Dorne, Angela Mally	-	-	Toxicology Letters	18	2021	Yes	methodology	PBPK	Hierarchical Bayesian meta-analysis	Bayes	Bayes - hierachical	Yes	not applicable (the paper discusses drug metabolism but does not specify a single therapeutic area or provide an ICD 11 code)	small molecule	not specified	The purpose of the model is to improve the assessment of clinical outcomes for pharmaceuticals metabolized by CES and to support the design of prodrugs using information on CES-specific tissue distribution.	No	Open source	Open source	- R (version 3.5) - Jags (version 4.2.0) - EndNote (version X8)
Methods in Clinical Pharmacology Series Bridging the gap: a review of dose investigations in paediatric investigation plans	Lisa V Hampson, Ralf Herold, Martin Posch, Julia Saperia, Anne Whitehead	-	-	British Journal of Clinical Pharmacology	14	2014	Yes	review	PBPK	Bayesian methods	Bayes	Bayes - Other	Yes	not applicable	not applicable	Clinical trial phase (guess)	dose finding, identification of subpopulations, verification of extrapolation assumptions	No	No	No	R
SEE PROFILE	Catherine Enright Valeo, Michael G Madden, Niall Madden, John G Laffey, Catherine G Enright	-	-		0	2014	Yes	methodology	Others	Bayesian uncertainty quantification using Dynamic Bayesian Networks with Gaussian distributions for measurement error modeling and prediction of means and standard deviations.	Bayes	Bayes - ML	Yes	Endocrinology; 5A1	biologics	not specified (the paper is related to drug therapy but does not specify the stage of drug development)	The purpose of the model is to dynamically re-estimate model parameters for optimizing insulin therapy in critically ill patients, which aligns with dose finding and identification of subpopulations.	No	No	No	Not mentioned
Human variability in glutathione-S-transferase activities, tissue distribution and major polymorphic variants: Meta-analysis and implication for chemical risk assessment	Franca Maria Buratti, Keyvin Darney, Susanna Vichi, Laura Turco, Emma Di Consiglio, Leonie S Lautz, Camille Béchaux, Jean-Lou Christian, Michel Dorne, Emanuela Testai	-	-	Toxicology Letters	23	2020	Yes	application	Others	Bayesian meta-analysis, probabilistic distributions, uncertainty factors (UFs), coefficient of variation (CV)	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	not applicable (the paper is related to chemical risk assessment)	No	No	No	
Human variability in influx and efflux transporters in relation to uncertainty factors for chemical risk assessment.	Darney K, Turco L, Buratti FM, Di Consiglio E, Vichi S, Roudot AC, Béchaux C, Testai E, Dorne JLCM, Lautz LS	10.1016/j.fct.2020.111305	https://doi.org/10.1016/j.fct.2020.111305	Food and chemical toxicology : an international journal published for the British Industrial Biological Research Association	19	2020	Yes	methodology	PBPK	Bayesian hierarchical meta-regression, probabilistic sensitivity analysis, uncertainty propagation	Bayes, Sensitivity analysis, Uncertainty propagation	SA - Other, UP - Other, Bayes - hierachical	Yes	not applicable (the paper does not specify a particular therapeutic area or ICD 11 code)	small molecule	not specified (method would be used in risk assessment)	The purpose of the model is to quantify human variability in drug metabolism	No	Open source	Upon request to the authors	R (version 3.5), Jags (4.2.0), EndNote (X8)
Human variability in polymorphic CYP2D6 metabolism: Implications for the risk assessment of chemicals in food and emerging designer drugs	Darney, K., Lautz, L.S., Béchaux, C., Wiecek, W., Testai, E., Amzal, B., Dorne, J.L.C.M.	10.1016/j.envint.2021.106760	https://doi.org/10.1016/j.envint.2021.106760	Environment International	17	2021	Yes	methodology	PBPK	Bayesian hierarchical meta-regression, Bayesian calibration, MCMC simulations	Bayes	Bayes - hierachical, Bayes - calibration	Yes	not applicable (the paper does not focus on a specific therapeutic area)	small molecule	not specified (method would be used in risk assessment)	the paper is focused on understanding variability in drug metabolism	No	Open source	Open source	- R (version 3.5) - Jags (4.2.0) - Benchmark dose modeling tool of the European Food Safety Authority (EFSA) - EndNote (X8)
Identification of dynamical systems with structured uncertainty	John A Burns, Eugene M Cliff, Terry L Herdman	-	-		5	2018	Yes	methodology	Others	Bayesian methods for model discrepancy analysis, bounded-error parameter estimation (BEPE), bound-to-bound (B2B)	Bayes, Sensitivity analysis	Bayes - Other, SA - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is not related to drug therapy or vaccine development)	Yes	Commercial platform	No	MATLAB (specifically, the lsqnonlin routine)
Identifying Bayesian optimal experiments for uncertain biochemical pathway models	Natalie M Isenberg, Susan D Mertins, Byung-Jun Yoon, Kristofer G Reyes, Nathan M Urban	-	-	Scientific Reports	0	2023	Yes	methodology	Others	Bayesian optimal experimental design (BOED), Hamiltonian Monte Carlo (HMC), standard deviation computation, sigmoidal curve fitting	Bayes	Bayes - Other	Yes	e.g. Cancer; C00-D49	e.g. small molecule	Preclinical (guess)	mathematically describing cellular reaction networks that include drug mechanisms of action	Yes	Open source	Upon request to the authors	- Programming language: Julia - Probabilistic programming library: Turing.jl - Sampler: No U-Turn Sampler (NUTS) - ODE model evaluation library: DifferentialEquations.jl
Impact of Exposure Uncertainty on the Association between Perfluorooctanoate and Preeclampsia in the C8 Health Project Population	Scott M Bartell, Raghavendhran Avanasi, Hyeong-Moo Shin, Verónica M Vieira, David A Savitz	-	-	Environmental Health Perspectives	15	2016	Yes	application	Others	Monte Carlo simulations, probabilistic sensitivity analysis, law of total variance for uncertainty decomposition	Sensitivity analysis	SA - analytical, SA - simulation	No	not applicable	not applicable	not applicable	not applicable	No	Open source, Commercial platform	No	MATLAB, R
Improvements in Estimating Bioaccumulation Metrics in the Light of Toxicokinetic Models and Bayesian Inference	Aude Ratier, Christelle Lopes, Sandrine Charles	-	-	-		2022	Yes	application	Others	Bayesian inference, Bayesian framework, posterior probability distributions, quantiles (50%, 75%, 97.5%) for credible intervals	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental risk assessment and not to drug therapy or vaccine development)	No	Open source	Open source	- MOSAIC bioacc web service - R-package rbioacc on CRAN

Improving the estimation of parameter uncertainty distributions in nonlinear mixed effects models using sampling importance resampling	Anne-Gaë ¨lle Dosne, Martin Bergstrand, Kajsa Harling, Mats O Karlsson	-	-	-		2016	Yes	methodology	Others	- Sampling importance resampling (SIR) - Asymptotic covariance matrix - Bootstrap (parametric and nonparametric) - Log-likelihood profiling	basic frequentist	Freq - resampling, Freq - likelihood	Yes	- Moxonidine: Cardiovascular diseases (ICD 11 code: BA00-BA99) - Pefloxacin: Infectious diseases (ICD 11 code: 1A00-1A99) - Phenobarbital: Neurological disorders (ICD 11 code: 8A00-8A99)	small molecule	Phase II or Phase III (guess)	dose finding, optimizing dosing regimen	Yes	Commercial platform	No	NONMEM 7.2 and 7.3, PsN 3.5.9 and above, RStudio 0.98, R 3.1.2
Improving Uncertainty in Widmark equation calculations: Alcohol volume, Strength and Density	Peter D Maskell, R Alex Speers, Dawn L Maskell	-	-	Science & justice : journal of the Forensic Science Society	10	2017	Yes	application	Others	Monte Carlo Simulation, General Error Propagation (GEP)	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to forensic toxicology and improving Widmark equation calculations, not drug therapy or vaccine development)	Yes	Commercial platform	No	GUM Workbench EDU Software Version 2.4.1.384 (Metrodata GmbH)
IN-SILICO PREDICTION OF DRUG PROPERTIES IN MAN USING PRECLINICAL DATA AND COMPUTER-ASSISTED DRUG DEVELOPMENT	Roberto Gomeni, Christine Falcoz, Carla D'angeli, Alan Bye	-	-		6	2001	Yes	application	Others	Monte Carlo simulations, stochastic modeling, coefficient of variation for interindividual variability, sensitivity index for sensitivity analysis, probabilistic sensitivity analysis, uncertainty propagation	Sensitivity analysis, Uncertainty propagation	UP - Other, SA - Other	Yes	Central Nervous System (CNS) disorders; ICD 11 code not explicitly mentioned but likely related to F00-F99 codes	not specified	Phase I and Phase II (guess)	dose finding, identification of optimal in-vivo release characteristics	No	Commercial platform	No	- Trial Simulator - NON-MEM - SAS software
Incorporation of in vitro metabolism data and physiologically based pharmacokinetic modeling in a risk assessment for chloroprene	Harvey J Clewell, Jerry L Campbell, Cynthia Van Landingham, Allison Franzen, Miyoung Yoon, Darol E Dodd, Melvin E Andersen, P Robinan Gentry	-	-	Inhalation Toxicology	13	2019	Yes	application	PBPK	Monte Carlo uncertainty analysis, parameter sensitivity analysis using normalized sensitivity coefficients	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental health risk assessment, not drug therapy or vaccine development)	No	Open source	Upon request to the authors	- Advanced Continuous Simulation Language (ACSL) - R (open source programming language) - Crystal Ball Release 11.1.2.3.850
Influence of the uncertainty in the validation of PBPK models: A case-study for PFOS and PFOA	Francesc F Abrega, Martí Nadal, Marta Schuhmacher, L Domingo, Vikas Kumar	-	-	Regulatory toxicology and pharmacology : RTP	23	2016	Yes	application	PBPK	Uncertainty propagation using Latin Hypercube Sampling (LHS) and frequentist statistical validation using Student's t-test.	Uncertainty propagation	UP - prob - basic sim	No	not applicable (the paper is related to environmental health risk assessment rather than drug therapy development)	not applicable	not applicable (the paper is about environmental health risk assessment using PBPK models, not drug therapy development)	Not applicable (the paper is related to environmental pollutant modeling rather than drug therapy development)	No	No	No	Not mentioned (the paper does not specify any software used for the study)
INFLUENCES OF PARAMETER UNCERTAINTIES WITHIN THE ICRP-66 RESPIRATORY TRACT MODEL: A PARAMETER SENSITIVITY ANALYSIS	Thomas E Huston, Eduardo B Farfa ´n, Wesley Emmett Bolch	-	-	Health Physics	15	2003	Yes	application	Others	probabilistic sensitivity analysis, uncertainty propagation, global sensitivity analysis, Latin hypercube sampling, multivariate regression model	Sensitivity analysis, Uncertainty propagation	SA - simulation, UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper focuses on the effects of inhaled aerosols)	No	No	No	- LUDUC (Lung Dose Uncertainty Code) - Software developed by Iman et al. (1985) for calculating SRRCs and PRCCs
Insulin Minimal Model Indexes and Secretion: Proper Handling of Uncertainty by a Bayesian Approach	Paolo Magni, Giovanni Sparacino, Riccardo Bellazzi, Gianna Maria Toffolo, Claudio Cobelli	-	-	Annals of Biomedical Engineering	13	2004	Yes	methodology	Others	Bayesian methodology implemented by Markov chain Monte Carlo (MCMC)	Bayes	Bayes - Other	Yes	- Diabetes mellitus Typ 2; 5A11 - Diabetes mellitus Typ 1; 5A10	biologics	not specified	paper is focused on understanding insulin secretion and β-cell function	Yes	No	No	
Inter-ethnic differences in CYP3A4 metabolism: A Bayesian meta-analysis for the refinement of uncertainty factors in chemical risk assessment	Keyvin Darney, Emanuela Testai, Franca M Buratti, Emma Di Consiglio, Emma E J Kasteel, Nynke Kramer, Laura Turco, Susanna Vichi, Alain-Claude Roudot, Jean-Lou Dome, Camille Béchaux	-	-	Computational Toxicology	13	2019	Yes	application	Others	Bayesian hierarchical modeling	Bayes	Bayes - hierachical	Yes	not specified	not specified	not specified	chemical risk assessment)	No	Open source	No	JAGS software, R (version 3.5), EndNote (X8)
Interpretable Deep-Learning pK a Prediction for Small Molecule Drugs via Atomic Sensitivity Analysis	Joseph Decorte, Benjamin Brown, Rathmell Jeffrey, Jens Meiler	-	-	-		2024	Yes	application	ML	- Standard deviation (σ) as a measure of confidence - Brier score for evaluating classification model output - discrete distribution for each molecule in question	basic frequentist, Other		Yes	not specified	small molecule	hit-to-lead or lead optimization	The purpose of the model is to predict pK a values for small molecule drugs, generalize predictions to novel compounds, and optimize physicochemical liabilities through atomic sensitivity analysis, which aids in lead compound optimization and structure preparation for protein-ligand docking.	No	Open source	Open source	- C++ (programming language) - Biology and Chemistry Library (BCL) (software package) - Intel Xenon W-2295 CPU cores (hardware) - Nvidia RTX A5000 GPU (hardware) - Corina (software tool) - Molecular Operating Environment (MOE) (software tool)
Investigating the uncertainty of prediction accuracy for the application of physiologically based pharmacokinetic models to animal-free risk assessment of cosmetic ingredients	Shimpei Terasaka, Akane Hayashi, Yuko Nukada, Masayuki Yamane, Lesa Aylward	-	-	Regulatory toxicology and pharmacology : RTP	2	2022	Yes	methodology	PBPK	- Use of the 97.5th percentile of the logarithm of the fold error to calculate the modeling uncertainty factor (MUF). - Calculation of the absolute average fold error (AAFE) to assess prediction accuracy.	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	Not applicable (the paper is focused on animal-free risk assessment for cosmetic ingredients, not drug therapy or vaccine development)	Yes	Commercial platform	Commercial platform with given parameters	- ADMET Predictor version 9.5 - GastroPlus version 9.7 - Microsoft Excel - GraphPad Prism 7 - Open Babel
Investigation of the impact of pharmacokinetic variability and uncertainty on risks predicted with a pharmacokinetic model for chloroform	Bruce C Allen, Tammie R Covington, Harvey J Clewell	-	-	Toxicology	51	1996	Yes	application	PBPK	Monte Carlo simulation, normal distributions for interindividual variability and parameter uncertainty, sensitivity analysis, multistage model for dose-response fitting, probabilistic sensitivity analysis using correlated trivariate normals.	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to risk assessment of chloroform, not drug therapy or vaccine development)	No	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used for the uncertainty quantification model)
Lifetime PCB 153 bioaccumulation and pharmacokinetics in pilot whales: Bayesian population PBPK modeling and Markov chain Monte Carlo simulations	Liesbeth Weijs, Anthony C Roach, Raymond S H Yang, Robin Mcdougall, Michael Lyons, Conrad Housand, Detlef Tibax, Therese Manning, John Chapman, Katelyn Edge, Adrian Covaci, Ronny Blust	-	-	Chemosphere	14	2013	Yes	application	PBPK	Bayesian approach with Markov chain Monte Carlo (MCMC) simulations	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable (the paper is focused on environmental toxicology and not related to drug therapy or vaccine development)	not applicable (the paper is related to environmental toxicology and not drug therapy or vaccine development)	No	Commercial platform	Open source	acslX/Libero software (AEgis Technologies, Orlando, FL)
Linking fate model in freshwater and PBPK model to assess human internal dosimetry of B(a)P associated with drinking water	Philippe Ciffroy, T Tanaka, E Johansson, C Brochot	-	-	Environmental Geochemistry and Health	7	2011	Yes	application	PBPK	- Probability density functions (PDFs) for input parameters - Bayesian approach for updating generic PDFs with site-specific measurements - Monte Carlo method for uncertainty propagation - Regression methods for sensitivity analysis - Probabilistic sensitivity analysis - Uncertainty propagation through random sampling	Bayes, Sensitivity analysis, Uncertainty propagation	UP - prob - basic sim, Bayes - Other, SA - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is focused on environmental exposure and toxicokinetics, not drug therapy or vaccine development)	No	Commercial platform	Commercial platform with given parameters	Ecolego

Machine learning in drug development: Characterizing the effect of 30 drugs on the QT interval using Gaussian process regression, sensitivity analysis, and uncertainty quantification	Francisco Sahli Costabal, Kristen Matsuno, Jiang Yao, Paris Perdikaris, Ellen Kuhl	-	-	Computer Methods in Applied Mechanics and Engineering	86	2019	Yes	application	ML	- Hierarchical Bayesian model - Gaussian process regression - Latin hypercube design - Posterior variance	Bayes, Sensitivity analysis	Bayes - hierachical, SA - simulation	Yes	Cardiovascular diseases, specifically arrhythmias; I49.0 (Other specified arrhythmias)	small molecule	not specified (the paper is related to drug therapy development but does not explicitly state the stage of drug development)	The purpose of the model is to predict QT interval lengths and identify relevant ion channels for QT interval prolongation, supporting the design of safe and effective drugs by understanding their effects on the QT interval.	No	Open source, Commercial platform	No	Abaqus, SciPy, L-BFGS
Mapping 18 F-FDG Kinetics Together with Patient-Specific Bootstrap Assessment of Uncertainties: An Illustration with Data from a PET/CT Scanner with a Long Axial Field of View	Qi Wu, Fengyun Gu, Liam D O'suilleabhain, Hasan Sari, Song Xue, Kuangyu Shi, Axel Rominger, Finbarr O'sullivan	-	-	-		2024	Yes	application	Others	Image-based bootstrapping methodology, Log-linear modeling	basic frequentist	Freq - resampling	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to clinical decision-making in cancer treatment using PET biomarkers, not drug therapy or vaccine development)	No	No	No	
Markov Chain Monte Carlo Algorithm based metabolic flux distribution analysis on Corynebacterium glutamicum	Visakan Kadirkamanathan, Jing Yang, Stephen A Billings, Phillip C Wright, Jonathan Wren	-	-	Nature Biotechnology	1118	2006	Yes	methodology	Others	Markov Chain Monte Carlo (MCMC) approach, Truncated Gaussian multiplicative models	Other		No	not applicable	not applicable	not applicable	Not applicable (the paper is related to metabolic flux analysis and not to drug therapy or vaccine development)	Yes	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used for uncertainty quantification)
Mathematical and statistical model misspecifications in modelling immune response in renal transplant recipients	H T Banks, R A Everett, Shuhua Hu, Neha Murad, H T Tran	-	-		3	2018	Yes	application	Others	- Difference-based method - Iterative weighted least squares technique - Modified residual plots	Other		No	not applicable	not applicable	not applicable	not applicable (the paper is not related to drug therapy or vaccine development)	No	Commercial platform	No	MATLAB (specifically, the inbuilt MATLAB function fmincon)
Maximum Entropy Technique and Regularization Functional for Determining the Pharmacokinetic Parameters in DCE-MRI	Zahra Amini Farsani, Volker J Schmid, Zahra Amini Farsani	-	-	Journal of digital imaging	0	2022	Yes	methodology	Others	Bayesian inference, Maximum Entropy Technique (MET) with regularization functionals	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	not applicable (the paper is related to pharmacokinetic parameter estimation in DCE-MRI, not directly to drug therapy or vaccine development)	No	Commercial platform	Upon request to the authors	MATLAB, KernelDistribution, ksdensity, lasso, ridge, gmres
Measures of Uncertainty of Pharmacokinetic and Pharmacodynamic Parameter Estimates: A New Computerized Algorithm	Serge Guzy, C Anthony Hunt	-	-	-		1996	Yes	methodology	Others	- Variance-covariance matrix (VCM) - G&H algorithm (the new method, involves generating new hypothetical data sets and fitting them to the model to estimate parameter reliability)	basic frequentist		Yes	Pain management and anti-inflammatory treatment; ICD-11 code: M79.1 (Other specified soft tissue disorders) or M79.0 (Rheumatism, unspecified)	small molecule	not specified (guess: preclinical or early clinical stage)	The purpose of the pharmacometric model is to provide a more accurate and reliable measurement of pharmacokinetic parameters, which is crucial for understanding drug pharmacokinetics and optimizing dosing regimens in drug therapy development.	Yes	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used)
Michaelis-Menten pharmacokinetics based on uncertain differential equations	Zhe Liu, Rui Kang	-	-	-		2022	Yes	methodology	QSP	Uncertainty theory, theory of uncertain differential equations, Belief reliability theory, Generalized moment estimations, Expected value calculations, -region calculations	UDE/SDE		Yes	not applicable (the paper is related to pharmacokinetics but does not specify a therapeutic area or disease being treated)	not specified	not specified (guess: preclinical or early clinical stage)	The purpose of the model is to better represent dynamic noises in pharmacokinetics, which is crucial for understanding how drugs are metabolized and eliminated from the body. It is used to investigate pharmacokinetic indexes such as drug concentration, half-life, and area under the curve, which are important for drug therapy development.	No	No	No	Not mentioned (the paper does not specify any software or programming languages used)
Model selection for assessing the effects of doxorubicin on triple-negative breast cancer cell lines	Anna M Claudia, Resende, Ernesto A B F Lima, Regina C Almeida, Matthew T Mckenna, Thomas E Yankeelov, M Resende	-	-	Journal of Mathematical Biology	4	2022	Yes	application	Others	Bayesian calibration, Bayesian inference, multi-level Monte Carlo algorithm	Bayes	Bayes - calibration	Yes	Breast cancer; C50	small molecule	not specified	The purpose of the pharmacometric model is to evaluate treatment responses and identify the most accurate model for describing cell growth and response to doxorubicin, which can inform dose finding and understanding of how different cell lines respond to treatment.	No	Open source	Upon request to the authors	QUESO (Quantification of Uncertainty for Estimation, Simulation, and Optimization) library
Model-based process development for hydrophobic interaction chromatography by considering prediction uncertainty analysis	Yu-Xiang Yang, Shan-Jing Yao, Dong-Qiang Lin	-	-	Journal of Chromatography A	0	2025	Yes	application	Others	Bayesian inference with Markov Chain Monte Carlo (MCMC)	Bayes	Bayes - Other	Yes	not applicable (the paper is related to biopharmaceutical process development but does not specify a therapeutic area or ICD 11 code)	biologics	not specified (the paper is related to drug therapy development, but the specific stage is not clearly stated or inferred from context)	the paper is related to biopharmaceutical process development (hydrophobic interaction chromatography (HIC))	No	Open source, Commercial platform	No	- CADET (chromatography analysis and design toolkit) - emcee (Python library for Markov Chain Monte Carlo)
Model-Based Robust Filtering and Experimental Design for Stochastic Differential Equation Systems	Guang Zhao, Xiaoning Qian, Byung-Jun Yoon, Francis J Alexander, Edward R Dougherty	-	-	IEEE Transactions on Signal Processing	15	2020	Yes	methodology	Others	Bayesian uncertainty propagation, Mean Objective Cost of Uncertainty (MOCU), Intrinsically Bayesian Robust (IBR) filtering	Bayes	Bayes - Other	Yes	not specified	not specified	not specified	Estimation of drug concentration levels	Yes	No	No	Not mentioned (no specific software or programming languages are mentioned in the paper)
Modeling and Analysis of Individualized Pharmacokinetics and Pharmacodynamics for Volatile Anesthesia	Alexandra Krieger, Nicki Panoskaltsis, Athanasios Mantalaris, Michael C Georgiadis, Efstratios N Pistikopoulos	-	-	IEEE Transactions on Biomedical Engineering	35	2014	Yes	application	Others	local and global sensitivity analysis, Probabilistic sensitivity analysis using the Sobol method and high-dimensional model representation (HDMR) with GUI-HDMR software	Sensitivity analysis	SA - analytical	Yes	Anesthesia; ICD 11 code: 5A00.0Z (Anesthesia, unspecified)	small molecule	not specified	The purpose of the pharmacometric model is to optimize drug administration by identifying individual pharmacodynamic parameters for personalized health care and safe model predictive control.	No	Commercial platform	No	GUI-HDMR software, gPROMS
Modeling Macroinvertebrate Community Dynamics in Stream Mesocosms Contaminated with a Pesticide	Mira Kattwinkel, Peter Reichert, Johanna Rüegg, Matthias Liess, Nele Schuwirth	-	-	Environmental Science and Technology	23	2016	Yes	application	Others	Bayesian inference, Bayesian parameter inference, uncertainty propagation, interval analysis	Uncertainty propagation, Bayes	UP - non prob, Bayes - Other	No	not applicable	not applicable	not applicable	not applicable (the paper is related to ecotoxicology, not drug therapy or vaccine development)	No	No	No	R programming language (in parts)
Modelling and sensitivity analysis of urinary platinum excretion in anticancer chemotherapy for the recovery of platinum	Karel Folens, Séverine Thérèse, F C Mortier, Janis Baeten, Karen Couvreur, Robin Michelet, Krist V Gernaey, Thomas De Beer, Gijs Du Laing, Ingmar Nopens	-	-		3	2016	Yes	application	Others	Global Sensitivity Analysis (GSA), Generalised Likelihood Uncertainty Estimation (GLUE), Sobol sampling	Sensitivity analysis, basic frequentist	SA - simulation, Freq - likelihood	No	not applicable	not applicable	not applicable	not applicable (the paper is focused on environmental and economic aspects of platinum recovery rather than drug therapy development)	No	No	No	SigmaPlot 13
Modelling and simulation of variability and uncertainty in toxicokinetics and pharmacokinetics	Ivan Nestorov	-	-	Toxicology Letters	62	2001	Yes	review	PBPK	- Fuzzy computations - MC simulationsd	Uncertainty propagation	UP - non prob	Yes	e.g. Psychiatric disorders; 6B0Z	e.g. small molecule	Preclinical (guess)	e.g. study underlying processes and perform animal-to-human extrapolations	No	No	No	Not mentioned (no specific software or programming language is mentioned in the paper)

Modelling ecological and human exposure to POPs in Venice lagoon -Part II: Quantitative uncertainty and sensitivity analysis in coupled exposure models	Artur Radomyski, Elisa Giubilato, Philippe Ciffroy, Andrea Critto, Céline Brochot, Antonio Marcomini, D Barcelo	-	-	Science of the Total Environment	23	2016	Yes	application	PBPK	- Probabilistic distribution functions (PDFs) for parameter values - Monte Carlo sampling for probabilistic simulations - Morris screening method - Regression-based sensitivity analysis - Extended Fourier Amplitude Sensitivity Test (EFAST)	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	not applicable (the paper is related to environmental exposure modeling, not drug therapy or vaccine development)	No	Open source	No	MERLIN-Expo
Modelling of oscillatory cortisol response in horses using a Bayesian population approach for evaluation of dexamethasone suppression test protocols	Felix Held, Carl Ekstrand, Marija Cvijovic, Johan Gabrielsson, Mats Jirstrand	-	-	Journal of Pharmacokinetics and Pharmacodynamics	3	2019	Yes	application	Others	Bayesian hierarchical modeling, Non-linear mixed-effects (NLME) approach, Posterior predictive checks (PPCs), Bayesian inference using Stan, Credible intervals (CIs)	Bayes	Bayes - hierachical	Yes	Pituitary pars intermedia dysfunction (PPID)	small molecule	not specified (the paper is related to drug therapy but does not specify the stage of drug development)	Dose finding and optimization for dexamethasone suppression test protocols	No	Open source	No	Stan version 2.18.0, CmdStan, NUTS sampler, Hamiltonian Monte Carlo (HMC)
Modelling the exposure to chemicals for risk assessment: a comprehensive library of multimedia and PBPK models for integration, prediction, uncertainty and sensitivity analysisthe MERLIN-Expo tool	P Ciffroy, B Alfonso, A Altenpohl, Z Banjac, J Bierkens, C Brochot, A Critto, T De Wilde, G Fait, T Fierens, J Garratt, E Giubilato, E Grange, E Johansson, A Radomyski, K Reschwann, N Suciu, T Tanaka, A Tediosi, M Van Holderbeke, F Verdonck, D Barcelo	-	-	-		2016	Yes	methodology	PBPK	- Probability density functions (PDFs) for uncertain parameters - Morris approach (one-factor-at-a-time screening design) - Regression-based approaches - Variance-based methods (Sobol, FAST, EFAST) - Probabilistic simulation	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	Not applicable	No	Open source	No	MERLIN-Expo
Multi-view uncertainty deep forest: An innovative deep forest equipped with uncertainty estimation for drug-induced liver injury prediction	Qiong Tan, Yuqi Wen, Yong Xu, Kunhong Liu, Song He, Xiaochen Bo	-	-	Information Sciences	4	2024	Yes	methodology	ML	- Single Deterministic Methods - Bayesian Methods - Ensemble Methods - Test-Time Augmentation Methods - Opinion as an alternative to probability	Bayes, Other	Bayes - Other	Yes	Liver diseases; ICD 11 code: 1E40.0 (Drug-induced liver injury)	not specified	not specified (guess: preclinical or clinical trial phase)	The purpose of the model is to aid in the early identification of potential liver-related adverse effects associated with drug candidates, improving drug development efficiency and patient safety.	Yes	No	No	scikit-learn
Multispecies Machine Learning Predictions of In Vitro Intrinsic Clearance with Uncertainty Quantification Analyses	Raquel Rodríguez-Pérez, Markus Trunzer, Nadine Schneider, Bernard Faller, Grégori Gerebtzoff	-	-	Molecular Pharmaceutics	22	2022	Yes	application	ML	- Ensemble variance for epistemic uncertainty estimation - Aleatoric uncertainty: large-scale data variability analysis	Other		Yes	not specified	not specified	Lead optimization (guess)	The purpose of the model is to predict intrinsic clearance (CL int) for new compounds to facilitate early informed decisions for compound prioritization in drug development.	Yes	Open source	No	- PyTorch - chemprop (version 1.3.1) - RDKit (version 2019.03.3) - scikit-learn library - XGB (Extreme Gradient Boosting)
Nearest Neighbor Gaussian Process for Quantitative Structure-Activity Relationships	Anthony Difranzo, Robert P Sheridan, Andy Liaw, Matthew Tudor	-	-	Journal of Chemical Information and Modeling	8	2020	Yes	methodology	ML	- Gaussian Processes (GPs) for native uncertainty estimation - QSAR model	Other		Yes	not specified	not specified	Discovery (guess)	the paper is related to drug discovery	Yes	Open source	Open source	- Python (programming language) - scikit-learn (library) - LightGBM (library) - annoy (python package) - scikit-optimize (package)
Normalizing Flow-Based Distribution Estimation of Pharmacokinetic Parameters in Dynamic Contrast-Enhanced Magnetic Resonance Imaging	Ke Fang, Zejun Wang, Qi Xia, Yingchao Liu, Bao Wang, Zhaowei Cheng, Jian Cheng, Xinyu Jin, Ruiliang Bai, Lanjuan Li	-	-	IEEE Transactions on Biomedical Engineering	1	2024	Yes	methodology	ML	- normalizing flow model-based parameters distribution estimation neural network (FPDEN) - Normalizing flow models for posterior distribution estimation - Maximum likelihood estimation (MLE) loss - Standard deviation of marginal distributions for uncertainty estimation - Coefficient of variation (COV) for relative uncertainty	Other		No	not applicable	not applicable	not applicable	not applicable (the paper is focused on improving diagnostic accuracy in glioma grading, not on drug therapy or vaccine development)	Yes	Open source	Open source	PyTorch
On implementing Jeffreys' substitution likelihood for Bayesian inference concerning the medians of unknown distributions	Andrew P Grieve	-	-	Pharmaceutical statistics	1	2022	Yes	application	Others	Bayesian inference using Jeffreys' Substitution Likelihood (JSL), equal-tailed credible intervals, Highest Posterior Density (HPD) intervals, Bayes factors, tipping point analysis	Bayes	Bayes - Other	Yes	Infections; ICD 11 code: Not specified in the paper, but related to bacterial infections	small molecule	Clinical trials (guess)	Bioequivalence assessment: To determine whether two formulations of a drug have comparable blood levels by comparing the area under the plasma concentration time profile (AUC).	Yes	Open source	Upon request to the authors	R programming language (Bååth's R code for JSL)
On the computation of output bounds on parallel inputs pharmacokinetic models with parametric uncertainty	Diego De Pereda, Sergio Romero-Vivo, Jorge Bondia	-	-	Mathematical and computer modelling	5	2013	Yes	methodology	Others	- Monte Carlo methods - Region-based approaches - Interval analysis - Monotonicity analysis	Uncertainty propagation	UP - prob - basic sim	Yes	e.g. Endocrine disorders (5A80) - Diabetes mellitus	e.g. biologics	not specified (the paper is related to drug therapy but does not specify the stage of development)	Improving the accuracy of pharmacokinetic models for drug therapy development	Yes	Commercial platform	No	- Matlab - IntLab (toolbox for interval analysis) - VNODE-LP (package for interval analysis)
On the incorporation of chemical-specific information in risk assessment	Harvey J Clewell Iii, Melvin E Andersen, Bas J Blaauboer	-	-	Toxicology Letters	33	2008	Yes	review	PBPK	- Parameter sensitivity analysis - Monte Carlo uncertainty analysis - Hierarchical Bayesian analytical methods (Markov chain Monte Carlo analysis)	Sensitivity analysis, Bayes	Bayes - hierachical, SA - simulation	Yes	not specified	not specified	not specified	the paper is related to chemical risk assessment	No	No	No	- no software used
On the quantification of inter-test variability in ecotoxicity data with application to species sensitivity distributions	Peter S Craig, Graeme L Hickey, Robert Luttik, Dick De Zwart	-	-	-		2012	Yes	methodology	Others	Bayesian hierarchical modeling, Markov chain Monte Carlo (MCMC) sampling methods, Jeffreys prior for non-informative prior distribution	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to ecotoxicological hazard assessment and not to drug therapy or vaccine development)	Yes	Open source	Open source	R
On the uncertainties of photon mass energy-absorption coefficients and their ratios for radiation dosimetry	S Khandan, P Kashian, Rezaeian, Pedro Andreo, David T Burns, Francesc Salvat	-	-	Physics in Medicine and Biology	75	2012	Yes	application	Others	- Statistical methods for uncertainty estimation: Monte Carlo (MC) calculations for Type A uncertainties. - Methods for Type B uncertainties: Assuming a normal distribution and evaluating the standard deviation; using rectangular or triangular distributions; invoking the GUM concept of a coverage factor (k = 2) for 95% confidence limits. - Combination of Type A and Type B uncertainties in quadrature to obtain the combined standard uncertainty.	basic frequentist, Other		No	not applicable	not applicable	not applicable	Not applicable (the paper is related to radiation dosimetry, not drug therapy or vaccine development)	No	Commercial platform	Commercial platform with given parameters	- EGSnrc - PENELOPE
On the Use of Hierarchical Probabilistic Models for Characterizing and Managing Uncertainty in Risk/Safety Assessment	Ralph L Kodell, James J Chen	-	-	Risk Analysis	9	2007	Yes	methodology	Others	- Hierarchical probabilistic models - Bayesian hierarchical model - Monte Carlo simulation for uncertainty propagation	Bayes	Bayes - hierachical	Yes	not specified	not specified	not specified	risk/safety assessment	No	No	No	Monte Carlo simulation (no specific software mentioned)
Ontogeny equations with probability distributions for anthropomorphic measurements in preterm and term neonates and infants for use in a PBPK model ☆	Xiaoxia Yang, Huali Wu, Darshan Mehta, Mary C Sullivan, Jian Wang, Gilbert J Burckart, John A Troutman, Jeffrey W Fisher	-	-	Computational Toxicology	10	2019	Yes	application	PBPK	Monte Carlo simulations, probabilistic distributions (normal and log-normal), uncertainty propagation through simulation	Uncertainty propagation	UP - prob - basic sim	Yes	Antimicrobial therapy; ICD 11 code: Not explicitly provided in the paper, but potentially related to codes under "Infections" or "Antimicrobial resistance."	small molecule	not specified	The purpose of the pharmacometric model is to support the development of PBPK models for neonates, which is a critical step in drug therapy development, particularly for drugs like PIP and TAZ.	No	Open source	No	R, Excel, SigmaPlot
Optimal dose and uncertainty estimation for individualized drug administration using pharmacokinetic models ☆	Giuseppe Pesenti, Marco Foppoli, Davide Manca	-	-	Computers and Chemical Engineering	0	2021	Yes	application	PBPK	Monte Carlo analysis, uncertainty propagation, interval analysis, frequentist	Uncertainty propagation	UP - prob - basic sim	Yes	Oncology; 2A85.0	small molecule	not specified (the paper is related to optimizing dosing protocols for an existing drug, but the specific stage of drug development is not mentioned)	dose finding, identification of subpopulations	No	Commercial platform	No	MATLAB R2020b

Parameter estimation of fractional uncertain differential equations	Cheng Luo, Guo-Cheng Wu, Ting Jin	-	-	Soft Computing - A Fusion of Foundations, Methodologies and Applications	1	2024	Yes	methodology	Others	- uncertainty theory, uncertain differential equations - generalized moment estimation	UDE/SDE		Yes	not specified	not specified	not specified	The purpose of the model is to account for uncertainty in drug metabolism (e.g. Reaction rate in chemical kinetics) due to dynamic internal and external factors, improving understanding and prediction of drug pharmacokinetics under uncertain conditions.	Yes	No	No	Not mentioned (the paper explicitly states that no data or code was used)
PARAMETER ESTIMATION USING INTERVAL COMPUTATIONS *	Laurent Granvilliers, Jorge Cruz, Pedro Barahona	-	-	SIAM Journal on Scientific Computing	26	2004	Yes	methodology	Others	Interval analysis	Uncertainty propagation	UP - non prob	Yes	not specified	not specified	not specified	The purpose of the model is to predict drug concentrations in body fluids and calculate clinically useful parameters such as half-life, volume of distribution, clearance, and bioavailability, which are essential for dose finding and understanding pharmacokinetic properties.	No	No	No	RealPaver
PBK modelling of topical application and characterisation of the uncertainty of C max estimate: A case study approach	Hequn Li, Joe Reynolds, Ian Sorrell, David Sheffield, Ruth Pendlington, Richard Cubberley, Beate Nicol, Lawrence Lash	-	-	-		2022	Yes	methodology	PBPK	Bayesian statistical model, Hamiltonian Monte Carlo algorithm	Bayes	Bayes - Other	Yes	topically applied chemicals, e.g. analgesic	small molecule	pre-clinical (guess)	predicting kinetic profiles for topically administrated drugs	No	Open source, Commercial platform	No	- GastroPlus 9.8 - PyStan 2.19 - Python 3.8 - Matplotlib 3.3 - NumPy 1.19 - Pandas 1.2 - SciPy 1.6
Performance of recurrent neural networks with Monte Carlo dropout for predicting pharmacokinetic parameters from dynamic contrast-enhanced magnetic resonance imaging data	Kenya Murase, Atsushi Nakamoto, Noriyuki Tomiyama	-	-	-		2025	Yes	application	ML	Monte Carlo dropout (MCD)	Bayes	Bayes - ML	No	not applicable	not applicable	not applicable	not applicable (the paper is related to predicting pharmacokinetic parameters for medical treatment planning and prognosis prediction, not directly to drug therapy development)	Yes	Open source	No	- Python 3.10.12 - Keras 3.5.0 - Tensorflow 2.17.1 - DCENET (https://github.com/olivercham pion/DCENET) - pydcemri (https://github.com/welcheb/py dcemri/blob/master) - deep_ivim (https://github.com/sebbarb/d eep_ivim)
Pharmacokinetic model based on multifactor uncertain differential equation	Z Liu, Y Yang	-	-	Applied Mathematics and Computation	16	2020	Yes	methodology	Others	Uncertainty theory, theory of uncertain differential equations, α-paths, generalized moment estimations, confidence intervals	UDE/SDE, basic frequentist		Yes	not specified	not specified	not specified (the paper is related to drug therapy development, but the specific stage is not clearly stated)	optimization of biological experiments with drugs, design of new drugs, reassessment of old drugs, improvement of drug utilization	No	No	No	Not mentioned (no software or programming languages are mentioned in the paper)
Pharmacokinetics with intravenous infusion of two-compartment model based on Liu process	Zhe Liu, Rui Kang	-	-	Communications in Statistics - Theory and Methods	4	2023	Yes	methodology	Others	Uncertainty theory, theory of uncertain differential equations, Liu processes, generalized moment estimation, uncertain hypothesis test, linear uncertainty distribution L(0, 1), confidence intervals	UDE/SDE, basic frequentist		Yes	not specified	not specified	not specified	The purpose of the model is to provide essential pharmacokinetic parameters.	No	No	No	not specified
Physics-informed covariance kernel for model-form uncertainty quantification with application to turbulent flows	Jin-Long Wu, Carlos Michelén-Ströfer, Heng Xiao, Kevin T Crofton	-	-	Computers & Fluids	21	2019	Yes	methodology	Others	Gaussian processes, physics-informed covariance kernel, Bayesian inference, Karhunen-Loève (KL) modes, Ensemble Kalman inversion	Uncertainty propagation	UP - prob - surrogate	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to turbulence modeling and not drug therapy or vaccine development)	Yes	Open source	No	OpenFOAM, simpleFoam, SIMPLE algorithm
Physiologically based kinetic (PBK) modeling of propiconazole using a machine learning-enhanced read-across approach for interspecies extrapolation	Yaoxing Wu, Gabriel Sinclair, Raghavendhran Avanasi, Alison Pecquet, Shoji Nakayama	-	-	Environment International	3	2024	Yes	application	ML	Local sensitivity analysis, Monte Carlo simulations for uncertainty analysis	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	not applicable (the paper is related to agrochemical risk assessment, not drug therapy or vaccine development)	No	Open source	Open source	- RStudio v2023.06.1 + 524 - R package deSolve v1.40 - R package FME v1.3.6.3 - statsmodels 0.14.1 in Python IDLE 3.12.2 - WebPlotDigitizer v4.6
Physiologically Based Pharmacokinetic (PBPK) Modeling of the Bisphenols BPA, BPS, BPF, and BPAF with New Experimental Metabolic Parameters: Comparing the Pharmacokinetic Behavior of BPA with Its Substitutes	Cecile Karrer, Thomas Roiss, Natalie Von Goetz, Darja Gramec Skledar, Lucija Peterlin Mašι, Konrad Hungerbühler	-	-	Environmental Health Perspectives	84	2018	Yes	application	PBPK	2D Monte Carlo analysis, probabilistic sensitivity analysis, uncertainty propagation, trapezoidal distributions, truncated normal distributions, coefficients of variation (CV)	Sensitivity analysis, Uncertainty propagation	SA - Other, UP - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental chemical exposure and not drug therapy or vaccine development)	No	Open source	Open source	R, version 3.3.2
Population PBPK modeling using parametric and nonparametric methods of the Simcyp Simulator, and Bayesian samplers	Janak R Wedagedera |, Anthonia Afuape, | Siri, Kalyan Chirumamilla, Hiroshi Momiji |, Robert Leary |, Mike Dunlavey |, Richard Matthews, Khaled Abduljalil, Masoud Jamei |, Frederic Y Bois, Janak R Wedagedera	-	-	CPT: Pharmacometrics & Systems Pharmacology	14	2022	Yes	methodology	PBPK	- Frequentist methods: Quasi-random parametric expectation maximization (QRPEM) (UQ: confidence intervalls), Nonparametric adaptive grid estimation (NPAG) (UQ: none) - Bayesian methods: Metropolis-Hastings (MH), Hamiltonian Markov Chain Monte Carlo (HMCMC) (UQ: posterior distributions)	basic frequentist, Bayes	Bayes - Other	Yes	Respiratory diseases; CA40.0 (Asthma), CA40.1 (COPD)	small molecule	not specified	The purpose of the pharmacometric model is to aid in drug therapy development by testing parametric assumptions, improving simulations for clinical trials, and estimating population variability for drug-drug interactions, special populations, and bioequivalence assessments.	No	Open source, Commercial platform	No	- Simcyp version 20 - GNU MCSim - R package rstan - R
Predicting Drug-Induced Liver Injury with Bayesian Machine Learning	Dominic P Williams, Stanley E Lazic, Alison J Foster, Elizaveta Semenova, Paul Morgan	-	-	Chemical Research in Toxicology	76	2019	Yes	application	ML	Bayesian machine learning with data-driven prior distribution, Laplace distribution for β parameters, and propagation of uncertainty through predictions	Bayes	Bayes - ML	Yes	Liver diseases; ICD 11 code: K76.0 (Drug-induced liver injury)	not specified	not specified	The purpose of the model is to predict drug-induced liver injury (DILI) severity and uncertainty, guiding the selection of optimal drug candidates and informing further studies to mitigate potential risks during drug development.	No	Open source	Open source	- Stan (version 2.18) - RStan (version 2.18.2) - Python (PyMC3) - Julia (Turing)
Predicting in vitro assays related to liver function using probabilistic machine learning	Flavio M Morelli, Marian Raschke, Natalia Jungmann, Michaela Bairlein, Marina García De Lomana, Mathieu Vinken, A B S T R A C T	-	-	Toxicology	0	2025	Yes	methodology	ML	- Bayesian inference - Logistic regression with independent Gaussian priors - Logistic regression with a regularized horseshoe prior - Bayesian Additive Regression Trees (BART) - Gaussian Process with a Matérn Kernel (GP) - No-U-Turn-Sampler (NUTS) algorithm - Markov Chain Monte Carlo (MCMC) chains - Uncertainty propagation	Bayes	Bayes - ML	Yes	Liver function; K71.0 (Drug-induced liver injury)	not specified	Drug discovery (guess)	predicting in vitro assay outcomes related to liver function and DILI risk	Yes	Open source	Open source	- PyMC - PyMCBART - BlackJAX - No-U-Turn-Sampler (NUTS) - arViz - UMAP
Prediction of Multi-Pharmacokinetics Property in Multi-Species: Bayesian Neural Network Stacking Model with Uncertainty	Yuanyuan Zhang, Zhiyin Xie, Fu Xiao, Jie Yu, Zhehuan Fan, Shihui Sun, Jiangshan Shi, Zunyun Fu, Xutong Li, Dingyan Wang, Mingyue Zheng, Xiaomin Luo, Mingyue Zheng -, Xiaomin Luo -, Yuanyuan Zhang -	-	-	Molecular Pharmaceutics	0	2024	Yes	application	ML	Bayesian Neural Networks (BNN)	Bayes	Bayes - ML	Yes	not specified	not specified	drug discovery	The purpose of the PKStack model is to predict pharmacokinetic parameters for drug therapy development, specifically for optimizing and assessing PK properties before early phase clinical trials.	No	No	No	- scikit-learn 1.0.2 - lightgbm 3.3.5 - xgboost 1.6.2 - DeepChem 2.7.2 - SHAP

Predictive inference for best linear combination of biomarkers subject to limits of detection	Tahani Coolen-Maturi	-	-	Statistics in Medicine	10	2017	Yes	methodology	Others	Nonparametric Predictive Inference (NPI) using lower and upper probabilities to quantify uncertainty	Other		No	not applicable	not applicable	not applicable	Not applicable (the paper is related to diagnostic test accuracy, not drug therapy or vaccine development)	Yes	No	No	not specified
Probabilistic design space exploration and optimization via bayesian approach for a fluid bed drying process	Qingbo Meng, David Bogle, Vassilis M Charitopoulos, A B S T R A C T	-	-	European Journal of Pharmaceutical Sciences	0	2025	Yes	methodology	ML	Bayesian approach, surrogate modeling, joint normal uncertainty distribution, covariance matrix computation	Bayes, Uncertainty propagation	UP - prob - surrogate, Bayes - Other	Yes	not applicable (the paper is related to pharmaceutical manufacturing processes but does not specify a therapeutic area or drug)	guess: small molecule	pharmaceutical manufacturing process	Probabilistic design space exploration and optimization for a fluid bed drying process	Yes	No	No	gPROMS FormulatedProduct digital platform, MATLAB, Minitab (version 21)
Probabilistic Framework for the Estimation of the Adult and Child Toxicokinetic Intraspecies Uncertainty Factors	Michael Pelekis, Mark J Nicolich, Joseph S Gauthier	-	-	Risk Analysis	35	2003	Yes	methodology	Others	- Probability density functions (PDFs) for parameter description - Monte Carlo simulation for probabilistic analysis - Uncertainty propagation through repeated simulations - Probabilistic sensitivity analysis through repeated simulations	Sensitivity analysis, Uncertainty propagation	SA - simulation, UP - prob - basic sim	Yes	not specified	not specified	not applicable	the paper is related to toxicokinetics and risk assessment	Yes	Commercial platform	No	ACSL SIM, Version 11.8.4 (Aegis Technologies Group, Huntsville, AL)
Probabilistic Risk Assessment -The Keystone for the Future of Toxicology	Thomas Hartung, Alexandra Maertens, Emily Golden, Thomas H Luechtefeld, Sebastian Hoffmann, Katya Tsaioun	-	-	-		2022	Yes	review	Others	- Monte Carlo method - first-and second-order reliability method (FORM/SORM) - non-parametric and parametric bootstrap methods - maximum likelihood estimation - Bayesian networks - probabilistic physiology-based pharmacokinetic (PBPK) modeling - Bayesian approaches - value of information analysis	Uncertainty propagation, Bayes, basic frequentist	UP - Other, Bayes - ML, Bayes - Other, Freq - Other, Freq - resampling	Yes	not specified	not specified	not specified (the paper is related to drug therapy but does not specify a stage of drug development)	the paper is primarily about probabilistic risk assessment in toxicology	No	No	No	- no software used
Probabilistic Temporal Prediction of Continuous Disease Trajectories and Treatment Effects Using Neural SDEs	Joshua Durso-Finley, Berardino Barile, Jean-Pierre Falet, Douglas L Arnold, Nick Pawlowski, Tal Arbel	-	-	International Conference on Medical Image Computing and Computer-Assisted Intervention	2	2024	Yes	application	ML	Sampling-based variance estimation using Neural Stochastic Differential Equations (NSDEs) with Monte Carlo simulation (running NSDE multiple times with different Brownian noise samples)	UDE/SDE		Yes	particularly for diseases with long term, complex, heterogeneous evolutions and no cure, e.g. Neurological diseases; G35	e.g. small molecule, biologics	Phase III or Phase IV (guess)	identification of subpopulations, prediction of treatment effects	No	No	No	Not mentioned (the paper does not explicitly mention any specific software, packages, or programming languages used)
Propagation of Population PK and PD Information Using a Bayesian Approach: Dealing with Non-Exchangeability	Aristides Dokoumetzidis, Leon Aarons	-	-	Journal of Pharmacokinetics and Pharmacodynamics	4	2005	Yes	methodology	Others	Bayesian hierarchical modeling, Markov Chain Monte Carlo (MCMC) methods, parametric priors (normal, Wishart, Gamma distributions), quantile-quantile (Q-Q) plots, standard deviation of MCMC chains	Bayes	Bayes - hierachical	Yes	not applicable (the paper is related to drug therapy development but does not specify a therapeutic area)	small molecule	Early clinical trials (guess)	The purpose of the model is to implement a conservative prior in Bayesian analysis to deal with non-exchangeability between prior and test populations, and to assess the statistical power of detecting differences in drug potency, which is relevant to drug therapy development.	Yes	Open source	No	WinBUGS
QSAR modeling without descriptors using graph convolutional neural networks: the case of mutagenicity prediction	Chiakang Hung, Giuseppina Gini	-	-	Molecular diversity	24	2021	Yes	methodology	ML	Bayesian Graph Convolutional Neural Networks (GCNs), Aleatoric and Epistemic uncertainty estimation	Bayes	Bayes - ML	Yes	not specified	not applicable	Preclinical (guess)	mutagenicity prediction	No	Open source	Open source	Python, RDKit, TensorFlow
Quantifying and Communicating Uncertainty in Preclinical Human Dose-Prediction	M Sundqvist, A Lundahl, Någård, U Bredberg, P Gennemark	-	-	CPT: Pharmacometrics & Systems Pharmacology	11	2015	Yes	review	Others	Monte-Carlo simulation, probabilistic sensitivity analysis, log-normal distributions, fuzzy computations, interval analysis	Uncertainty propagation	UP - non prob, UP - prob - basic sim	Yes	Not mentioned (the paper does not specify the therapeutic area or provide an ICD 11 code)	not specified	Preclinical (guess)	dose finding, ranking lead-optimization compounds, informing design of early clinical trials	No	Commercial platform	No	Matlab
Quantifying Uncertainty Bounds in Anesthetic PKPD Models	Stéphane Bibian, Guy A Dumont, Mihai Huzmezan, Craig R Ries	-	-	Annual International Conference of the IEEE Engineering in Medicine and Biology Society	8	2004	Yes	methodology	Others	- Multiplicative unstructured uncertainty weighting function - Frequency domain analysis - Interval analysis (envelope method) - Uncertainty propagation	Uncertainty propagation	UP - non prob	Yes	Anesthesia; ICD 11 code: 6A00.0 (Anesthesia)	small molecule	not specified (the paper is related to optimizing drug delivery systems rather than developing new drugs)	The purpose of the model is to quantify uncertainty bounds in PKPD models to improve controller design for anesthetic drug delivery, aiming to reduce uncertainty and enhance stability and performance of closed-loop systems.	Yes	No	No	Not mentioned (no software or programming languages are mentioned in the paper)
Quantitative global sensitivity analysis of a biologically based dose-response pregnancy model for the thyroid endocrine system	Annie Lumen, Kevin Mcnally, Nysia George, Jeffrey W. Fisher, George D. Loizou	10.3389/fphar.2015.00107	-	Frontiers in Pharmacology	25	2015	Yes	methodology	PBPK	- Morris screening method - Gaussian Emulation process - Gaussian Process regression for surrogate modeling - Probabilistic sensitivity analysis (main and total effect sensitivity indices) - latin hypercube sampling design	Sensitivity analysis, Uncertainty propagation	UP - prob - surrogate, SA - simulation	No	no	not applicable	not applicable (the paper is about methodology and application of BBDR models, not drug therapy development)	not applicable (the paper is focused on environmental exposure and thyroid function, not drug therapy development)	Yes	Open source, Commercial platform	No	- Advanced Continuous Simulation Language (acslX) version 3.0 - DigitizeIT 1.5 - Gaussian Emulation Machine (GEM) software - Gaussian Process regression model - R scripts from appendix of McNally et. al. (2011) (just for Lowry plots)
Quantitative steady-state bounds in biomolecular circuits due to bounded multi-parametric perturbations.	Gunjan Chorasiya, Rudra Prakash, Shaunak Sen	10.1109/LCSYS.2023.3289569	-	IEEE Control Systems Letters	-	2023	Yes	methodology	Others	- Interval Analysis - Banach Contraction Theorem	Uncertainty propagation	UP - non prob	No	not applicable	not applicable	not applicable	Not applicable	No	No	No	n/a
Real-Time Personalised Pharmacokinetic-Pharmacodynamic Modelling in Propofol Anesthesia through Bayesian Inference	Nicolò Malagutti, Grace McGinness, Dilip A. Nithyanandam	10.1109/EMBC40787.2023.10339991	-	Proceedings of the Annual International Conference of the IEEE Engineering in Medicine and Biology Society, EMBS	2	2023	Yes	application	Others	Bayesian inference implemented through a particle filter algorithm	Bayes	Bayes - Other	Yes	Anesthesia; ICD 11 code not explicitly mentioned in the paper, but related to anesthesia	small molecule	not applicable (the paper is about optimizing drug therapy rather than developing a new drug or vaccine)	The purpose of the pharmacometric model is to refine a prior pharmacokinetic-pharmacodynamic model using Bayesian inference to estimate patient-specific parameters in real-time, aiming to improve the prediction of individual patients' responses to propofol for safe and effective anesthesia management.	Yes	No	No	Not mentioned (no specific software, packages, or programming languages are mentioned in the paper)
Reassessing benzene risks using internal doses and Monte-Carlo uncertainty analysis.	Louis Anthony Cox Jr.	10.1289/ehp.961041413	-	Environmental Health Perspectives	-	1996	Yes	methodology	PBPK	Bayesian Monte Carlo uncertainty analysis with maximum-entropy probabilities and Bayesian conditioning	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	not applicable	Yes	No	No	Not mentioned (the paper does not specify any software or programming languages used for the uncertainty quantification model)

Representing model discrepancy in bound-to-bound data collaboration.	Wenyu Li, Arun Hedge, James Oreluk, Andrew Packard, Michael Frenklach	10.1137/19M1270185	-	SIAM/ASA Journal on Uncertainty Quantification	4	2021	Yes	methodology	Others	- Bayesian inference - Bayesian calibration (for comparison) - Bayesian history matching (for comparison) - bound-to-bound data collaboration (B2BDC) - surrogate modeling - model discrepancy analysis	Bayes, Uncertainty propagation, Sensitivity analysis	UP - prob - surrogate, Bayes - Other, SA - analytical, Bayes - calibration	No	not applicable	not applicable	not applicable	not applicable	Yes	Open source, Commercial platform	Open source	- MATLAB - B2BDC toolbox - fmincon (MATLAB function) - SeDuMi (SDP solver) - CVX (modeling system for convex optimization) - fseminf (MATLAB function)
Revised assessment of cancer risk to dichloromethane: part I Bayesian PBPK and dose-response modeling in mice.	Dale J Marino, Harvey J Clewell, P Robinan Gentry, Tammie R Covington, C Eric Hack, Raymond M David, David A Morgott	10.1016/j.yrtph.2005.12.007	-	Regulatory toxicology and pharmacology : RTP	48	2006	Yes	application	PBPK	- Bayesian inference - Markov Chain Monte Carlo (MCMC) analysis - Bayesian hierarchical modeling - potential scale reduction for convergence monitoring - sequential calibration approach	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	not applicable (the paper is related to environmental health risk assessment, not drug therapy or vaccine development)	Yes	Open source, Commercial platform	No	- GNU MCSim - TOX_RISK (Version 5.3)
Risk-Based Environmental Remediation: Bayesian Monte Carlo Analysis and the Expected Value of Sample Information	M. E. Dakins, J. E. Toll, M. J. Small, K. P. Brand	10.1111/j.1539-6924.1996.tb01437.x	-	Risk analysis : an official publication of the Society for Risk Analysis	97	1996	Yes	methodology	Others	- Bayesian Monte Carlo analysis - Monte Carlo methods - Sensitivity analysis - Expected value of including uncertainty (EVIU)	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental remediation, not drug therapy or vaccine development)	Yes	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used in the study)
Separating uncertainty and physiological variability in human PBPK modelling: The example of 2-propanol and its metabolite acetone.	D. Huizer, R. Oldenkamp, A.M.J. Ragas, J.G.M. van Rooij, M.A.J. Huijbregts	10.1016/j.toxlet.2012.08.016	-	Toxicology Letters	18	2012	Yes	application	PBPK	- Bayesian techniques for defining parameter distributions - Nested Monte Carlo simulation to separate variability and uncertainty in predictions - Spearman rank correlation coefficients	Sensitivity analysis, Bayes	SA - simulation, Bayes - Other	No	not applicable	not applicable	not applicable (the paper is focused on PBPK modeling for chemical exposure, not drug therapy or vaccine development)	not applicable (the paper is related to toxicology and risk assessment, not drug therapy or vaccine development)	Yes	Open source, Commercial platform	No	- IndusChemFate (PBPK tool, freeware) - Microsoft Excel (for the IndusChemFate model) - Crystal Ball (Oracle, version 11) (for nested Monte Carlo simulation)
Simple Relations Between Administered and Internal Doses in Compartmental Flow Models	Louis Anthony Cox	10.1111/j.1539-6924.1995.tb00313.x	-	Risk Analysis	-	1995	Yes	methodology	PBPK	- AUC area under curve analysis	Other		No	not applicable	not applicable	not applicable	not applicable	No	No	No	n/a
Site-specific reference dose for methylmercury for fish-eating populations	Harvey J Clewell, Kenny S Crump, P Robinan Gentry, Annette M Shipp	10.1016/S0378-3820(99)00075-2	-	Fuel Processing Technology	-	2000	Yes	application	PBPK	- Benchmark dose approach - Monte Carlo uncertainty analysis - Hypercube method - PBPK modeling - Uncertainty factor application	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable	No	No	No	n/a
Sorafenib metabolism, transport, and enterohepatic recycling: physiologically based modeling and simulation in mice.	Andrea N Edginton, Eric I Zimmerman, Aksana Vasilyeva, Sharyn D Baker, John C Panetta	10.1007/s00280-016-3018-6	-	Cancer chemotherapy and pharmacology	-	2016	Yes	application	PBPK	- uncertainty propagation analysis - global sensitivity analysis using partial rank correlation coefficients (PRCC) - frequentist parameter estimation via weighted least squares - Latin hypercube sampling (LHS) for uncertainty analysis/propagation - partial rank correlation coefficients (PRCC)	Uncertainty propagation, Sensitivity analysis, basic frequentist	UP - prob - basic sim, SA - simulation	No	not applicable	not applicable	not applicable	not applicable (The purpose of the pharmacometric model is to evaluate the complex mechanisms of sorafenib metabolism and transport, guide future extrapolation to a human model, understand sorafenib-related efficacy and dose-limiting toxicities, identify factors contributing to high exposure variability, aid in individualizing sorafenib dosing by considering genetic variations, and optimize dosing when combined with genomic data.)	Yes	Commercial platform	No	- PK-Sim version 5.3.2 - MoBi Toolbox for MATLAB version 3.3.2 - MATLAB
Statistical analysis of a general adsorption kinetic model with randomness in its formulation. An application to real data.	Carlos Andreu-Vilarroig, Juan-Carlos Cortés, Ana Navarro-Quiles, Sorina-Madalina Sferle	10.46793/match.90-1.019A	https://doi.org/10.46793/match.90-1.019A	MATCH. Communications in Mathematical and in Computer Chemistry	2	2023	Yes	methodology	Others	- Random Least Mean Square (RLMS) method - Bayesian technique	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	Not applicable	Yes	Open source, Commercial platform	No	- Mathematica - RStudio - WinBUGS - R2Winbugs package - coda package
Statistical analysis of Clewell et al. PBPK model of trichloroethylene kinetics	Frederic Yves Bois	10.1289/ehp.00108s2307	-	Environmental Health Perspectives	63	2000	Yes	application	PBPK	- Bayesian hierarchical population statistical model - Markov chain Monte Carlo (MCMC): Gibbs sampling and - Metropolis-Hasting sampling - uncertainty propagation through posterior parameter distributions and geometric standard deviations (GSDs)	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	not applicable (the paper is focused on toxicology and risk assessment rather than drug therapy development)	Yes	No	Open source	GNU MCSim
Statistical Analysis of Fisher et al. PBPK Model of Trichloroethylene Kinetics	Frederic Yves Bois	10.1289/ehp.00108s2275	-	Environmental Health Perspectives	-	2000	Yes	application	PBPK	- Bayesian hierarchical population modeling - MCMC techniques for uncertainty propagation	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	not applicable	Yes	Open source	No	GNU MCSim
Statistical issues in toxicokinetic modeling: a Bayesian perspective	Pascale Bernillon, Frederic Y. Bois	10.1289/ehp.00108s5883	-	Environmental Health Perspectives	-	2000	Yes	methodology	PBPK	- Bayesian hierarchical statistical framework - Markov chain Monte Carlo (MCMC) methods - multilevel models of uncertainty/variability	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to chemical risk assessment, not drug therapy or vaccine development)	Yes	No	No	Not mentioned (the paper discusses methodological approaches but does not specify software or programming languages used)
Statistical uncertainty in hazardous terrestrial concentrations estimated with aquatic ecotoxicity data	Laura Golstejn, Rosalie Van Zelm, A Jan Hendriks, Mark A J Huijbregts	10.1016/j.chemosphere.2013.05.007	-	Chemosphere	13	2013	Yes	methodology	Others	- Monte Carlo simulations - Quantitative structure-activity relationship (QSAR) - Uncertainty propagation	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental risk assessment, not drug therapy or vaccine development)	Yes	Commercial platform	No	Crystal Ball (Oracle, Release 11.1.2.0.00) in Microsoft Excel
Stochastic response surface methods (SRSMs) for uncertainty propagation: application to environmental and biological systems.	S S Isukapalli, A Roy, P G Georgopoulos	10.1111/j.1539-6924.1998.tb01301.x	-	Risk analysis : an official publication of the Society for Risk Analysis	412	1998	Yes	methodology	PBPK	- Stochastic Response Surface Methods (SRSMs) - Monte Carlo methods (for comparison) - Latin Hypercube Sampling (for comparison)	Sensitivity analysis	SA - analytical, SA - simulation	No	not applicable	not applicable	not applicable (the paper is related to environmental and biological systems modeling, not drug therapy or vaccine development)	not applicable (the paper is related to toxicology and environmental health rather than drug therapy development)	Yes	Commercial platform	No	SimuSolv
Surrogate-based uncertainty and sensitivity analysis for bacterial invasion in multi-species biofilm modeling.	A Trucchia, M R Mattei, V Luongo, L Frunzo, M C Rochoux	-	-	Communications in Nonlinear Science and Numerical Simulation	5	2019	Yes	application	ML	- Surrogate modeling (training emulator) - Monte Carlo random sampling - Sobol' indices for global sensitivity analysis - Cross-validation error metric - Least-Angle Regression gPC-type expansion	Sensitivity analysis	SA - analytical, SA - simulation	No	not applicable	not applicable	not applicable	Not applicable (the paper is focused on biofilm modeling and does not address drug therapy or vaccine development)	Yes	Open source, Commercial platform	No	Matlab, OpenTURNS Python package, batman package

T-ALPHA: A Hierarchical Transformer-Based Deep Neural Network for Protein-Ligand Binding Affinity Prediction with Uncertainty-Aware Self-Learning for Protein-Specific Alignment	Kyro, G.W.; Smaldone, A.M.; Shee, Y.; Xu, C.; Batista, V.S.	10.1021/acs.jcim.4c02332	-		Journal of Chemical Information and Modeling	-		2025	Yes	methodology	ML	Monte Carlo dropout, Bayesian inference (approximated through Monte Carlo dropout), smoothed weighting scheme for precision-weighted loss	Bayes	Bayes - ML	Yes	TODO	TODO	hit identification and lead optimization	hit identification and lead optimization: predicting protein-ligand binding affinity	No	Open source	Open source	- T-ALPHA - Python - PyTorch (v2.4.1+cu121) - PyTorch Geometric (v2.6.0) - PyTorch Lightning - KeOps - SciPy
Tensor algorithms for advanced sensitivity metrics.	Ballester-Ripoll, Rafael; Paredes, Enrique G.; Pajarola, Renato	10.1137/17M1160252	-		SIAM/ASA Journal on Uncertainty Quantification			2018	Yes	methodology	ML	Surrogate modeling using the tensor train decomposition (TT) model, variance-based sensitivity analysis (SA), Sobol tensor train for variance components and sensitivity indices, computation of effective dimension, mean dimension, dimension distribution, and Shapley values.	Sensitivity analysis	SA - analytical	No	not applicable	not applicable	not applicable	not applicable	Yes	Open source	Open source	ttpy toolbox (Python library)
Testing the coherence between occupational exposure limits for inhalation and their biological limit values with a generalized PBPK-model: The case of 2-propanol and acetone	D. Huizer, M.A.J. Huijbregts, J.G.M. van Rooij, A.M.J. Ragas	10.1016/j.yrtph.2014.05.004	-		Regulatory toxicology and pharmacology : RTP	5		2014	Yes	application	PBPK	- Nested Monte Carlo simulation - modified Spearman rank correlation method	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to occupational exposure limits and biological limit values, not drug therapy or vaccine development)	Yes	Commercial platform	No	Crystal Ball software (Oracle, version 11)
The estimation and translation uncertainties in applying NOAEL to clinical dose escalation.	Chao Chen, Silvia Maria Lavezzi, David McDougall	10.1111/cts.13831	-		Clinical and Translational Science	0		2024	Yes	methodology	Others	- Probabilistic sensitivity analysis - Monte Carlo simulation - Statistical analysis of variability using percent coefficient of variation (CV%) - Probabilistic modeling using sigmoidal E max function	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	Not applicable	Yes	Open source	No	R version 4.1.1
The Impact of Cytochrome P450 2E1-Dependent Metabolic Variance on a Risk-Relevant Pharmacokinetic Outcome in Humans	John C Lipscomb, Linda K Teuschler, Jeff Swartout, Doug Popken, Tony Cox, Gregory L Kedderis	10.1111/j.0272-4332.2003.00397.x	-		Risk analysis : an official publication of the Society for Risk Analysis	-		2003	Yes	application	PBPK	- Monte Carlo simulation - Method of moments to combine distributions - Mixture distribution modeling - Goodness of fit testing - Uncertainty propagation through PBPK modeling - Probabilistic sensitivity analysis	Uncertainty propagation, Sensitivity analysis	SA - analytical, UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental health risk assessment rather than drug therapy or vaccine development)	Yes	Commercial platform	No	- SAS 8.0 Analyst routine - StatFit software - SimuSolv software - MATLAB software
The quantification of uncertainties in internal doses assessed from monitoring measurements.	G Etherington	10.1093/rpd/nci556	-		Radiation Protection Dosimetry	2		2007	Yes	methodology	PBPK	- Monte-Carlo simulations - novel method	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	not applicable (the paper is related to radiation exposure and internal dosimetry, not drug therapy or vaccine development)	Yes	No	No	MS Visual Basic 6.0, IMBA (Integrated Modules for Bioassay Analysis)
The use of Markov chain Monte Carlo uncertainty analysis to support a Public Health Goal for perchloroethylene	Tammie R Covington, P Robinan Gentry, Cynthia B Van Landingham, Melvin E Andersen, Janet E Kester, Harvey J Clewell	10.1016/j.yrtph.2006.06.008	-		Regulatory toxicology and pharmacology : RTP	-		2007	Yes	application	PBPK	- Bayesian hierarchical analysis - Markov chain Monte Carlo (MCMC) analysis - probabilistic sensitivity analysis	Bayes, Sensitivity analysis	Bayes - hierachical, SA - simulation	No	not applicable	not applicable	not applicable	not applicable (the paper is related to environmental health and risk assessment, not drug therapy or vaccine development)	Yes	Open source	No	MCSim
To be certain about the uncertainty: Bayesian statistics for 13C metabolic flux analysis.	Axel Theorell, Samuel Leweke, Wolfgang Wiechert, Katharina Nöh	10.1002/bit.26379	https://pubmed.ncbi.nlm.nih.gov/28695999/		Biotechnology and bioengineering	-		2017	Yes	methodology	Others	- Fisherian statistics - Profile Likelihoods - Parametric bootstrap	basic frequentist	Freq - likelihood, Freq - resampling	No	not applicable	not applicable	not applicable	not applicable	Yes	Open source	No	13CFLUX2, IPOPT
Transport and dynamics of toxic pollutants in the natural environment and their effect on human health: research gaps and challenge.	Andrew Hursthouse, George Kowalczyk	10.1007/s10653-008-9213-6	-		Environmental geochemistry and health	-		2009	Yes	review	PBPK	- Default safety factors for interspecies and intraspecies variability - Uncertainty factors - Chemical-specific uncertainty factors - Physiologically based pharmacokinetic (PBPK) modeling	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	not applicable (the paper is focused on environmental pollutants and their impact on human health, not drug therapy or vaccine development)	No	No	No	Not applicable
Trial Probability of Success for Testing 3-Way PK/PD Similarity With Multiple Endpoints	Rachid el Galta, Susanne Schmitt, Ramin Arani, Arne Ring	-	-			-		2025	Yes	methodology	Others	- Assurance method (expected power approach) - Monte Carlo simulations - Probabilistic sensitivity analysis	Sensitivity analysis	SA - simulation	Yes	not applicable	not applicable	not applicable (design methodology)	The purpose of the model is to demonstrate the similarity between a biosimilar candidate and two versions of the originator drug by establishing a three-way similarity in multiple coprimary endpoints, specifically focusing on pharmacokinetics (PK) and pharmacodynamics (PD) studies.	Yes	Open source	Upon request to the authors	R Shiny app, R programming language
Uncertain pharmacokinetic model based on uncertain differential equation	Z Liu, Y Yang	10.1016/j.amc.2021.126118	-		Applied Mathematics and Computation	-		2021	Yes	methodology	Others	- Method of moments - Confidence intervals - Uncertain differential equations - Derivation of uncertainty distributions and inverse uncertainty distributions	UDE/SDE		No	not applicable	not applicable	not applicable	not applicable	No	No	No	Not applicable
Uncertainties in doses from intakes of radionuclides assessed from monitoring measurements.	G Etherington, A Birchall, M Puncher, A Molokanov, E Blanchardon	10.1093/rpd/nci152	-		Radiation protection dosimetry	-		2006	Yes	methodology	PBPK	Monte Carlo simulations, Bayesian statistical methods	Bayes	Bayes - Other	No	not applicable (Therapeutic area: Thyroid disorders; ICD 11 code: CA73.0 (Thyroid cancer), 5A00.0 (Hyperthyroidism))	not applicable	not applicable (the paper is about internal dosimetry and radiation exposure, not drug therapy or vaccine development)	Not applicable (the paper is related to radiation exposure and dosimetry, not drug therapy or vaccine development)	Yes	No	No	Not mentioned (the paper does not specify the names of any software, packages, or programming languages used)
Uncertainty aggregation and reduction in structure-material performance prediction.	Hu, Zhen; Mahadevan, Sankaran; Ao, Dan	10.1007/s00466-017-1448-6	https://doi.org/10.1007/s00466-017-1448-6		Computational Mechanics	-		2018	Yes	methodology	Others	- Surrogate model - Kriging surrogate modeling method - Bayesian network approach for uncertainty quantification and aggregation - Bayesian updating for uncertainty reduction - Global sensitivity analysis (GSA) for identifying uncertainty contributions - Monte Carlo simulation (MCS) for forward propagation of uncertainties - Particle filter (PF) method for approximating posterior distributions - Model validation using Bayesian hypothesis testing (BHT) - Integration of Bayesian calibration with model validation	Uncertainty propagation, Bayes, Sensitivity analysis	Bayes - ML, Bayes - calibration, UP - prob - basic sim, SA - analytical, UP - prob - surrogate	No	not applicable	not applicable	not applicable	not applicable	Yes	No	No	
Uncertainty analysis in 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) cancer dose-response for three occupational cohorts.	Zhaomin Dong, Guanxiang Yuan, Jianying Hu	10.1016/j.envint.2015.12.010	-		Environment International	10		2016	Yes	application	PBPK	- Uncertainty propagation - probabilistic sensitivity analysis - Robustness analysis using noise	Sensitivity analysis, Uncertainty propagation	SA - Other, UP - Other	No	not applicable	not applicable	not applicable (the paper is related to risk assessment and management of TCDD exposure, not drug therapy or vaccine development)	not applicable (the paper is related to environmental health risk assessment, not drug therapy or vaccine development)	Yes	Open source	Open source	Not mentioned (the paper does not specify any software, packages, or programming languages used)

Uncertainty Analysis in Pharmacokinetics and Pharmacodynamics: Application to Naratriptan	Ivelina Gueorguieva, Ivan A Nestorov, Leon Aarons, Malcolm Rowland	10.1007/s11095-005-6629-x	-		Pharmaceutical Research	-		2005	Yes	application	PBPK	- Fuzzy sets theory - Global sensitivity analysis - Extended Fourier Amplitude Sensitivity Test (FAST) - Fuzzy simulations - Monte Carlo simulations	Sensitivity analysis, Uncertainty propagation	UP - non prob, SA - Other, SA - analytical	Yes	G43 (Migraine)	small molecule	clinical trial simulation	The purpose of the pharmacometric model is to predict pain relief in patients following naratriptan administration, incorporating parametric uncertainty and assessing interindividual variability to improve model predictiveness.	Yes	Commercial platform	No	- SimLab 1.1 - MATLAB 6 - Stanford Graphics 3.0c
Uncertainty analysis in the task of individual monitoring data.	A Molokanov, V Badjin, G Gasteva, E Antipin	10.1093/oxfordjournals.rpd.a006267	-		Radiation protection dosimetry	-		2003	Yes	methodology	Others	- Monte Carlo simulation technique - parameter uncertainty analysis	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to radiation exposure and internal dose assessment, not drug therapy or vaccine development)	Yes	No	No	Not mentioned (the paper does not specify the software used)
Uncertainty analysis of doses from ingestion of plutonium and americium.	M. Puncher, J. D. Harrison	10.1093/rpd/ncr032	-		Radiation protection dosimetry	-		2012	Yes	application	PBPK	- Parameter uncertainty analysis - Sensitivity analysis - Log-normal distributions for uncertainty quantification - Latin Hypercube sampling algorithm - Monte Carlo calculations for uncertainty propagation - Sensitivity coefficients for identifying important parameters	Sensitivity analysis, Uncertainty propagation	SA - simulation, UP - prob - basic sim	No	not applicable	not applicable	not applicable	not applicable	Yes	Commercial platform	No	IMBA Professional Plus, IMBA Uncertainty Plus, Weighted Likelihood Monte-Carlo sampling method
Uncertainty analysis of the nonideal competitive adsorption-donnan model: effects of dissolved organic matter variability on predicted metal speciation in soil solution.	J. E. Groenenberg, G. F. Koopmans, R. N. Comans	10.1021/es902615w	-		Environmental Science & Technology	-		2010	Yes	methodology	Others	- Monte Carlo simulations - Latin hypercube sampling	Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental science and not drug therapy or vaccine development)	Yes	No	No	- UNCSAM: for parameter sampling and statistical analysis of Monte Carlo simulations - ORCHESTRA: for speciation modeling including the NICA-Donnan model - MINTEQ database: for inorganic speciation and binding to LMWOA
Uncertainty analysis of the urinary excretion of plutonium.	A Luciani, H Doerfel, E Polig	10.1093/oxfordjournals.rpd.a006263	-		Radiation protection dosimetry	-		2003	Yes	application	PBPK	- Monte Carlo simulations with Latin hypercube sampling for uncertainty propagation - Variance comparison tests and mean comparison tests for uncertainty estimation - Geometric standard deviation (GSD) for representing spread of values - Frequentist statistical tests on logarithmic values - Sensitivity analysis (from prior work)	Uncertainty propagation, basic frequentist	UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to biokinetics of plutonium, not drug therapy or vaccine development)	Yes	No	No	Not mentioned (no specific software or programming languages are mentioned in the paper)
Uncertainty analysis of the weighted equivalent lung dose per unit exposure to radon progeny in the home.	J W Marsh, A Birchall, G Butterweck, M. D Dorrian, C Huet, X Ortega, A Reineking, G Tymen, Ch Schuler, A Vargas, G Vezzu, J Wendt	10.1093/oxfordjournals.rpd.a006092	-		Radiation protection dosimetry	-		2002	Yes	application	Others	- Monte Carlo simulation - Latin hypercube sampling - probabilistic sensitivity analysis - uncertainty propagation - scenario analysis over multiple distributions	Uncertainty propagation, Sensitivity analysis	SA - simulation, UP - prob - basic sim	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to radiation exposure and dosimetry, not drug therapy or vaccine development)	Yes	Commercial platform	No	RADEP (Radon Dose Evaluation Program)
Uncertainty and sensitivity analysis of biokinetic models for radiopharmaceuticals used in nuclear medicine.	W.B. Li, C. Hoeschen	10.1093/rpd/ncq064	-		Radiation Protection Dosimetry		19	2010	Yes	methodology	PBPK	- Latin hypercube sampling - Regression and partial correlation analysis - Standardized rank regression coefficient (SRRC) - Partial rank correlation coefficient (PRCC) - Uncertainty factor (UF)	Sensitivity analysis	SA - simulation	Yes	not applicable	not applicable	not applicable	the paper is related to radiopharmaceuticals in nuclear medicine	Yes	No	No	BIOKINDOS
Uncertainty and Sensitivity Analysis of Spatial Predictions of Heavy Metals in Wheat	D. J. Brus, M. J. W. Jansen	10.2134/jeq2004.0882	https://pubmed.ncbi.nlm.nih.gov/15724924/		Journal of Environmental Quality			2004	Yes	application	Others	- Sensitivity analysis - Monte Carlo simulations (implied by the use of simulated values) - Latin Hypercube Sampling (LHS) - Geostatistical methods (simple indicator kriging) - Uncertainty propagation	Sensitivity analysis, Uncertainty propagation	SA - simulation, UP - prob - basic sim	No	not applicable	not applicable	not applicable	not applicable	Yes	Commercial platform	No	GenStat: RSEARCH, USAGE 2.0
Uncertainty and variability in the exposure reconstruction of chemical incidents - the case of acrylonitrile.	D. Huizer, A.M.J. Ragas, R. Oldenkamp, J.G.M. van Rooij, M.A.J. Huijbregts	10.1016/j.toxlet.2014.07.019	-		Toxicology Letters	-		2014	Yes	application	PBPK	- Nested Monte Carlo simulations for uncertainty propagation - Spearman rank correlation coefficients for assessing variability and uncertainty influence - Parameter importance analyses for understanding uncertainty contributions	Uncertainty propagation, Sensitivity analysis	SA - simulation, UP - prob - basic sim	No	not applicable	not applicable	not applicable	not applicable	Yes	No	No	not mentioned
Uncertainty estimation in dynamic contrast-enhanced MRI.	Anders Garpebring, Patrik Brynolfsson, Jun Yu, Ronnie Wirestam, Adam Johansson, Thomas Asklund, Mikael Karlsson	10.1002/mrm.24328	-		Magnetic resonance in medicine	-		2013	Yes	methodology	Others	- Multivariate linear error propagation - Monte Carlo simulations - Covariance calculation	Uncertainty propagation	UP - prob - basic sim	Yes	Oncology (2A00-2F9Z)	imaging, measuring, diagnostic, dynamic contract-enhanced MRI (DCE-MRI)	not specified (the paper is related to drug therapy development but does not specify the stage)	The purpose of the model is to aid in the development and usage of antiangiogenic drugs by providing imaging biomarkers.	Yes	Commercial platform	No	Matlab 2010b
Uncertainty propagation for SPECT/CT-based renal dosimetry in (177)Lu peptide receptor radionuclide therapy.	Johan Gustafsson, Gustav Brolin, Maurice Cox, Michael Ljungberg, Lena JOhansson, Katarina Sjögreen Gleisner	10.1088/0031-9155/60/21/8329	-		Physics in medicine and biology	-		2015	Yes	application	PBPK	- Monte Carlo (MC) method - uncertainty propagation - bootstrapping	basic frequentist	Freq - resampling	Yes	Neuroendocrine tumors; ICD-11 code: 2C12.0 (Neuroendocrine tumour of uncertain behaviour of pancreas)	biologics, radionuclide therapy (RNT)	not specified (the paper does not explicitly mention the stage of drug development, but it implies clinical use)	not applicable (the paper is focused on dosimetry and uncertainty analysis in radionuclide therapy, not drug therapy development)	Yes	No	No	SIMIND MC program
Uncertainty quantification in the Henry problem using the multilevel Monte Carlo method.	Dmitry Logashenko, Alexander Litvinenko, Raul Tempone, Ekaterina Vasilyeva, Gabriel Wittum	10.1016/j.jcp.2024.112854	-		Journal of Computational Physics	-		2024	Yes	methodology	Others	- Multilevel Monte Carlo (MLMC) method - Monte Carlo (MC) sampling - Surrogate-based methods (generalized polynomial chaos approximation and stochastic Galerkin)	Uncertainty propagation	UP - prob - surrogate	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to hydrogeological modeling and not to drug therapy or vaccine development)	Yes	Open source	No	- ug4 simulation software toolbox - MPI for parallelization
Uncertainty Quantification Using Neural Networks for Molecular Property Prediction	Lior Hirschfeld, Kyle Swanson, Kevin Yang, Regina Barzilay, Connor W. Coley	10.1021/acs.jcim.0c00502	-		Journal of Chemical Information and Modeling	-		2020	Yes	methodology	ML	- Ensemble-based methods: Traditional Ensembling, Bootstrapping, Snapshot Ensembling, Monte Carlo Dropout Ensembling - Mean-Variance Estimation (MVE) - Distance-based methods: Tanimoto distance - Union-based methods: Gaussian Process (GP), Random Forest (RF) - Fingerprint-based methods: Gaussian Process (GP), Random Forest (RF)	Bayes, basic frequentist	Bayes - ML, Freq - resampling	No	not applicable (the paper is related to drug discovery but does not specify a particular therapeutic area or disease)	not applicable	not applicable	not applicable (the paper is related to drug discovery, not drug therapy development or vaccine development)	Yes	Open source	Open source	Chemprop, RDKit, GPy's SparseGPRegression, skleam's RandomForestRegressor
Uncertainty, variability, and sensitivity analysis in physiological pharmacokinetic models.	D Krewski	-	https://pubmed.ncbi.nlm.nih.gov/8580927/		Journal of biopharmaceutical statistics	-		1995	Yes	methodology	PBPK	Monte Carlo methods, Bootstrap procedure	basic frequentist	Freq - resampling	No	not applicable	not applicable	not specified	not applicable	Yes	No	No	SimuSolv
Use of a probabilistic PBPK/PD model to calculate Data Derived Extrapolation Factors for chlorpyrifos.	Torka S Poet, Charles Timchalk, Michael J Bartels, Jordan N Smith, Robin Mcdougal, Daland R Juberg, Paul S Price	10.1016/j.yrtph.2017.02.014	https://pubmed.ncbi.nlm.nih.gov/28238854/		Regulatory toxicology and pharmacology : RTP			2017	Yes	application	PBPK	- Sensitivity analysis - Monte Carlo analysis - Parametric bootstrap technique - Probabilistic sensitivity analysis	Sensitivity analysis, basic frequentist	SA - simulation, Freq - resampling	No	not applicable	not applicable	not applicable	not applicable (the paper is related to human health risk assessments for chemical exposure, not drug therapy or vaccine development)	Yes	Open source	Upon request to the authors	acslXv3.0.2.1, Physiological Parameters for PBPK Modeling software
Using Stochastic Differential Equations for PK/PD Model Development	Niels Rode Kristensen, Henrik Madsen, Steen Hvass Ingwersen	10.1007/s10928-005-2105-9	-		Journal of pharmacokinetics and pharmacodynamics	-		2005	Yes	methodology	PBPK	- Frequentist methods, including asymptotic Gaussianity (normality) for parameter estimation and marginal t-tests for significance testing - Significance as measure of model uncertainty	basic frequentist		Yes	not applicable (the paper is about model development for drug therapy methodology)	not applicable	not applicable	identification of appropriate model structure for PK/PD modeling	Yes	Open source, Commercial platform	No	- CTSM (version 2.3) - S-PLUS (version 6.1)

Validation of Bayesian modeling approach of uncertainty in organ doses using post-mortem measurements.	Maia Avtandilashvili, Martin Šefl, Joey Y Zhou, Sergey Y Tolmachev	10.1038/s41598-025-04799-3	-	Scientific reports	-		2025	Yes	application	PBPK	- Bayesian statistical approach - Latin hypercube sampling - sensitivity analysis	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	not applicable (the paper is related to radiation exposure and dose estimation, not drug therapy or vaccine development)	Yes	Open source, Commercial platform	No	- USTUR-iRAD (in-house code for radiation dosimetry) - Python 3.9 (programming language) - IMBA Professional Plus internal dosimetry software (for validation)
Variability and epistemic uncertainty in water ingestion rates and pharmacokinetic parameters, and impact on the association between perfluorooctanoate and preeclampsia in the C8 Health Project population.	Raghavendhran Avanasi, Hyeong-Moo Shin, Veronica M Vieira, Scott M Bartell	10.1016/j.envres.2016.01.011	-	Environmental Research		14	2016	Yes	application	PBPK	- Monte Carlo simulation - probabilistic sensitivity analysis	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	Not applicable	Yes	Open source, Commercial platform	No	MATLAB, R
Variability and uncertainty: interpretation and usage of pharmacometric simulations and intervals	Chuanpu Hu	10.1007/s10928-022-09817-9	-	Journal of pharmacokinetics and pharmacodynamics	-		2022	Yes	methodology	Others	- Variance-covariance matrix of parameter estimates - Bootstrap methods - Monte Carlo simulations - Interval analysis (e.g., confidence intervals)	basic frequentist	Freq - Other, Freq - resampling	No	not applicable (the paper is related to drug therapy development but does not specify a particular therapeutic area or ICD 11 code)	not applicable	not applicable	not applicable	No	No	No	Not applicable
Use of Probabilistic Expert Judgment in Uncertainty Analysis of Carcinogenic Potency	John S Evans, George M Gray, Robert L Sielken, Andrew E Smith, Ciriaco Valdez-Flores, John D Graham, Kenneth P Cantor, Jack Siemiatycki, Michael A Pereira, Byron E Butterworth, Richard H Reitz, Lorenz Rhomberg, U S Environmental, Dale Hattis, Thomas B Starr	-	-	Regulatory toxicology and pharmacology : RTP		103	1994	Yes	application	Others	Bayesian methods, bootstrap estimates of parameter uncertainty	Bayes, basic frequentist	Bayes - Other, Freq - resampling	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to carcinogenic risk assessment, not drug therapy or vaccine development)	No	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used in the study)
Surrogate-based sequential Bayesian experimental design using non-stationary Gaussian Processes	Piyush Pandita, Panagiotis Tsilifis, Nimish M Awalgaonkar, Ilias Bilionis, Jitesh Panchal	-	-			19	2021	Yes	methodology	Others	Bayesian hierarchical model	Bayes	Bayes - hierachical	No	not applicable	not applicable	not applicable	not applicable	No	Open source	Open source	- AdaptiveSDOE (open-source package) - Python (programming language) - Finite element simulator (software used for simulation)
The Yin-Yang of CYP3A4: a Bayesian meta-analysis to quantify inhibition and induction of CYP3A4 metabolism in humans and refine uncertainty factors for mixture risk assessment	Nadia Quignot, Witold Wiecek, Billy Amzal, Jean-Lou Dorne	-	-		-		2018	Yes	application	Others	Bayesian hierarchical meta-regression, Bayesian calibration,probabilistic uncertainty factors	Bayes	Bayes - hierachical, Bayes - calibration	Yes	not applicable (the paper is related to drug therapy development but does not specify a particular therapeutic area or disease)	small molecule	not specified (guess: preclinical or early clinical stage)	The purpose of the model is to integrate human variability in metabolism and toxicokinetics interactions to derive uncertainty factors for chemical risk assessment, which is relevant to drug therapy development.	No	Open source	No	- Markov Chain Monte Carlo software Stan - R (version 3.3) - R packages: tidyverse, broom, ggplot2
Uncertainty analysis in internal dose calculations for cerium considering the uncertainties of biokinetic parameters and S values	Vladimir Spielmann, Wei Bo Li, Maria Zankl, Juan Camilo, Ocampo Ramos, Nina Petoussi-Henss	-	-	Radiation and Environmental Biophysics		1	2020	Yes	application	Others	Uncertainty propagation, Latin hypercube sampling, frequentist methods (confidence intervals)	basic frequentist, Uncertainty propagation	UP - prob - basic sim	No	not applicable	not applicable	not applicable (the paper is related to radiation dosimetry and risk analysis, not drug therapy or vaccine development)	Not applicable (the paper is related to radiation dosimetry and risk analysis, not drug therapy or vaccine development)	No	No	No	- In house software package (for calculating S values) - EGSnrc (Monte Carlo radiation transport code) - UnDose (computer code written in C#)
Uncertainty quantification for the random HIV dynamical model driven by drug adherence	Dingding Yan, Mengqi He, Sanyi Tang	-	-	Journal of Theoretical Biology		0	2024	Yes	application	Others	- Adaptive generalized polynomial chaos (gPC) - Monte Carlo (MC) sampling - Global sensitivity analysis using the Sobol index	Sensitivity analysis	SA - analytical, SA - simulation	Yes	HIV infection; B20-B24	not applicable	not specified (the paper is related to optimizing existing drug therapies rather than developing new drugs)	The purpose of the model is to study the uncertainty quantification in HIV drug therapy, particularly how drug adherence affects treatment efficacy, and to design individual-based optimal antiretroviral strategies.	Yes	No	No	Not mentioned (the paper does not specify the names of any software, packages, or programming languages used in the study)
Uncertainty quantification and propagation in surrogate-based Bayesian inference	Philipp Reiser, Javier Enrique Aguilar, Anneli Guthke, Paul-Christian Bürkner, B Philipp Reiser	-	-	Statistics and computing		3	2025	Yes	methodology	Others	- Bayesian approach to surrogate modeling - Uncertainty propagation methods: - Point Estimate - Expected-Posterior (E-Post) - Expected-Likelihood (E-Lik) - Expected-Log-Likelihood (E-Log-Lik) - Simulation-based Calibration (SBC)	Bayes, basic frequentist	Bayes - Other, Freq - likelihood	No	not applicable	not applicable	not applicable	not applicable (the paper is not related to drug therapy or vaccine development)	Yes	Open source	Open source	Stan
Uncertainty Quantification for Computer Models With Spatial Output Using Calibration-Optimal Bases	James M Salter, Daniel B Williamson, John Scinocca, Viatcheslav Kharin	-	-	Journal of the American Statistical Association		60	2018	Yes	methodology	Others	- Bayesian calibration - History matching with iterative refocusing - Model discrepancy analysis - Surrogate modeling (through the use of emulators) - Optimal rotation algorithm for basis vectors	Bayes, Sensitivity analysis	Bayes - calibration, SA - analytical	No	not applicable	not applicable	not applicable	Not applicable (the paper is about climate model tuning and not related to drug therapy or vaccine development)	No	Open source	Open source	R programming language

Robust PBPK/PD-Based Model Predictive Control of Blood Glucose	Stephan Schaller, Jörg Lippert, Lukas Schaupp, Thomas R Pieber, Andreas Schuppert, Thomas Eissing	-	-	IEEE Transactions on Biomedical Engineering	29	2016	Yes	application	PBPK	Robustness analysis, parameter estimation, model calibration, simulation-based evaluation	Other		Yes	Endocrinology; ICD 11 code: 5A10	not applicable	not applicable (the paper is related to the development of a medical device/system for glucose control, not drug therapy or vaccine development)	The purpose of the PBPK/PD model is to predict blood glucose levels and adjust insulin doses for personalized treatment in type 1 diabetes mellitus patients, which is a form of drug therapy development related to insulin treatment.	No	Commercial platform	Commercial platform with given parameters	- PK-Sim 5.1 - MoBi 3.1 - MoBi Toolbox for MATLAB - MATLAB (including MATLAB GUIDE and optimization toolbox functions fmincon and fminbnd)
Uncertainty quantified discovery of chemical reaction systems via Bayesian scientific machine learning	Emily Nieves, Raj Dandekar, Chris Rackauckas, Pasquale Palumbo	-	-	bioRxiv	6	2024	Yes	methodology	ML	Bayesian inference analysis, Preconditioned Stochastic Gradient Langevin Descent (pSGLD) Bayesian framework,	Bayes	Bayes - Other	Yes	not applicable	not applicable	not applicable	the paper is related to QSP	Yes	Open source	Open source	- Julia programming language - Flux.jl (for LSTM modules) - GitHub (for data hosting)
EXPOSURE! EXPOSURE! SESSION UNCERTAINTY ANALYSIS OF THE ESTIMATED INGESTION RATES USED TO DERIVE THE METHYLMERCURY REFERENCE DOSE	Jeff Swartout, Glenn Rice	-	-	Drug and chemical toxicology (New York, N.Y. 1978)	35	2000	Yes	application	Others	Monte Carlo analysis, probabilistic sensitivity analysis	Sensitivity analysis	SA - simulation	No	not applicable	not applicable	not applicable	not applicable	No	Commercial platform	Upon request to the authors	- S-PLUS (version 3.2) - Crystal Ball (version 3.2) - Excel (version 5.0)
When Is a Model Good Enough? Deriving the Expected Value of Model Improvement via Specifying Internal Model Discrepancies *	Mark Strong, Jeremy E Oakley	-	-	SIAM/ASA J. Uncertain. Quantification	58	2014	Yes	methodology	Others	- Bayesian framework for structural uncertainty quantification - Internal discrepancy analysis - Probabilistic sensitivity analysis - Uncertainty propagation	Bayes, Sensitivity analysis	Bayes - Other, SA - analytical	Yes	HIV/AIDS, B20-B24	small molecule	not specified (guess: post-marketing or clinical use)	The purpose of the model is to predict costs and health outcomes (in life years) under two decision options, zidovudine monotherapy versus zidovudine plus lamivudine combination therapy, in people with HIV.	Yes	No	No	R
Relative robustness of NOEC and ECx against large uncertainties in data	Yoshinari Tanaka, Kensei Nakamura, Hiroyuki Yokomizo	-	-	PLoS ONE	15	2018	Yes	methodology	Others	- Uncertainty factors - Information-gap method - Bootstrapping - Jackknife resampling	basic frequentist	Freq - resampling	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental safety and chemical regulation, not drug therapy or vaccine development)	Yes	Open source	No	R, nls2 package
Uncertainty Quantification in Internal Dose Calculations for Seven Selected Radiopharmaceuticals	Vladimir Spielmann, Wei Bo Li, Maria Zankl, Uwe Oeh, Christoph Hoeschen	-	-	Journal of Nuclear Medicine	12	2015	Yes	application	PBPK	Uncertainty propagation, Latin hypercube sampling	Uncertainty propagation	UP - prob - basic sim	Yes	not applicable	not applicable	not applicable (the paper is about uncertainty analysis of existing radiopharmaceuticals, not drug therapy development)	not applicable (the paper is related to radiopharmaceuticals and nuclear medicine, not drug therapy or vaccine development)	No	No	No	DoseU (written in C#)
Validation of Bayesian Analysis of Compartmental Kinetic Models in Medical Imaging	Arkadiusz Sitek, Quanzheng Li, Georges El Fakhri, Nathaniel M Alpert	-	-	Physica medica (Testo stampato)	5	2017	Yes	methodology	PBPK	Bayesian analysis, Markov Chain Monte Carlo (MCMC) methods	Bayes	Bayes - Other	No	not applicable (the paper is related to diagnostic imaging using FDG, not drug therapy development)	not applicable	not applicable	not applicable	Yes	No	No	Not mentioned (the paper does not specify any software, packages, or programming languages used in the study)
Using the Stochastic Collocation Method for the Uncertainty Quantification of Drug Concentration Due to Depot Shape Variability	J Samuel Preston, Tolga Tasdizen, Christi M Terry, Alfred K Cheung, Robert M Kirby	-	-	IEEE Transactions on Biomedical Engineering	12	2009	Yes	methodology	Others	combination of component shape parameterization with the stochastic collocation method ("sampling" extension to generalized polynomial chaos)	Other		Yes	Vascular diseases; ICD 11 code: BA00-BA9Z	small molecule	preclinical (guess)	The purpose of the model is to study the effect of depot shape on drug concentration and delivery, which is part of analyzing the efficacy of a drug delivery method for limiting neointimal hyperplasia growth in hemodialysis patients.	Yes	No	No	not mentioned
Quantifying Uncertainty in Predictions of Hepatic Clearance	James A Rogers, Jayson Wilbur, Susan Cole, Paul W Bernhardt, Jaye Lynn Bupp, Morgan J Lennon, Nathan Langholtz, Christopher Paul Steiner	-	-		1	2011	Yes	methodology	Others	Bayesian modeling, Bayesian credible intervals, posterior predictive checks, Deviance information criterion (DIC) values	Bayes	Bayes - Other	Yes	not applicable (the paper is related to drug therapy development but does not specify the therapeutic area or ICD 11 code)	small molecule	Preclinical (guess)	The purpose of the model is to predict human pharmacokinetic parameters for drug therapy development, specifically for determining dosing regimens and assessing uncertainty in preclinical predictions.	No	No	No	WinBUGS software, version 1.4; R language
Reinforcement learning and Bayesian data assimilation for model-informed precision dosing in oncology	Corinna Maier, | Niklas Hartung, Charlotte Kloft, | Wilhelm Huisinga, Wilhelm Huisinga	-	-		1	2020	Yes	methodology	Others	Bayesian data assimilation (DA) using Bayes' formula and particle-based approximation of the posterior distribution	Bayes	Bayes - Other	Yes	Oncology; C34.0	small molecule	not specified (the paper is related to drug therapy development, but the specific stage is not clearly stated)	The purpose of the model is to improve the efficacy and safety of drug therapies by controlling neutropenia through model-informed precision dosing (MIPD) using Bayesian data assimilation (DA) and reinforcement learning (RL).	No	Open source	Open source	MATLAB
SF-Rx: A Multioutput Deep Neural Network-Based Framework Predicting Drug-Drug Interaction under Realistic Conditions for Safe Prescription	Daeun Kim, Jaehong Yu, Sang-Hun Bae, Jihyun Lee	-	-	Journal of Chemical Information and Modeling	0	2025	Yes	methodology	ML	- Gini impurity - Expected calibration error (ECE) - Monte Carlo dropout	Bayes	Bayes - ML	Yes	not applicable (the paper is related to drug therapy development but does not specify a particular therapeutic area or ICD 11 code)	small molecule	not specified (the paper is related to drug therapy development, but the specific stage is not clearly stated)	The purpose of the SF-Rx model is to predict drug-drug interactions (DDIs) by incorporating pharmacokinetic and pharmacodynamic features, aiming to improve patient safety and facilitate the development of effective combination therapies.	Yes	Open source	Open source	- LightGBM - PyTorch Lightning - Python-based libraries
Uncertainties on Lung Doses from Inhaled Plutonium	Matthew Puncher, Alan Birchall, Richard K Bull	-	-	Radiation Research	32	2011	Yes	application	Others	Bayesian methods, specifically Bayesian posterior probability distributions and the WeLMoS method (an extension of weighted likelihood Monte Carlo Sampling), are used for uncertainty quantification.	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	not applicable (the paper is related to radiation exposure and lung dose estimation, not drug therapy or vaccine development)	No	No	No	not mentioned

Using machine learning surrogate modeling for faster QSP VP cohort generation	Renée C Myers, Florian Augustin, | Jérémy Huard, Christina M Friedrich	-	-	CPT: Pharmacometrics & Systems Pharmacology	8	2023	Yes	methodology	QSP	Surrogate modeling	Uncertainty propagation	UP - prob - surrogate	Yes	Psoriasis; L40.0	not applicable	not specified (the paper is related to drug therapy development, but the stage is not explicitly mentioned)	The purpose of the model is to de-risk the development of novel therapies by creating a wide range of virtual patients to explore variability and uncertainty in clinical responses, and to anticipate outcomes ahead of clinical data. This includes identifying potential subpopulations and predicting trial outcomes.	Yes	Open source	Open source	- SimBiology (MATLAB, 2020) - Regression Learner App 11 - MATLAB scripts
Unorthodox parallelization for Bayesian quantum state estimation	Hanson H Nguyen, Kody J H Law, Joseph M Lukens	-	-	New Journal of Physics	0	2025	Yes	methodology	Others	Bayesian inference, Markov chain Monte Carlo (MCMC), preconditioned Crank-Nicholson Metropolis-Hastings algorithm, parallelization of independent MCMC chains, intrachain autocorrelation time diagnostics	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to quantum state tomography and Bayesian inference, not drug therapy or vaccine development)	Yes	Commercial platform	No	MATLAB, Qiskit Experiments 0.7.0 library
TERRESTRIAL WILDLIFE RISK ASSESSMENT FOR TCDD IN LAND-APPLIED PULP AND PAPER MILL SLUDGE	Ossi Meyn, Maurice Zeeman, Michael J Wise, Susan E Keane	-	-	-		1997	Yes	application	PBPK	Monte Carlo analysis	Other		No	not applicable	not applicable	not applicable	Not applicable (the paper is related to environmental risk assessment, not drug therapy or vaccine development)	Yes	Commercial platform	No	@RISK as an add-in to Lotus 1-2-3
UNCERTAINTIES IN INTERNAL DOSES CALCULATED FOR MAYAK WORKERS-A STUDY OF 63 CASES	G Miller, R Guilmette, L Bertelli, T Waters, S A Romanov, Y V Zaytseva	-	-	Radiation Protection Dosimetry	15	2008	Yes	methodology	PBPK	Bayesian methods, discrete empirical Bayes approximation, Poisson-lognormal uncertainty model, Monte Carlo simulations for intra-individual uncertainty	Bayes	Bayes - Other	No	not applicable	not applicable	not applicable	Not applicable (the paper is related to radiation exposure and dose calculation, not drug therapy or vaccine development)	No	Commercial platform	No	Los Alamos UF code