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Database issue

RadioPharm: the database of radiopharmaceuticals

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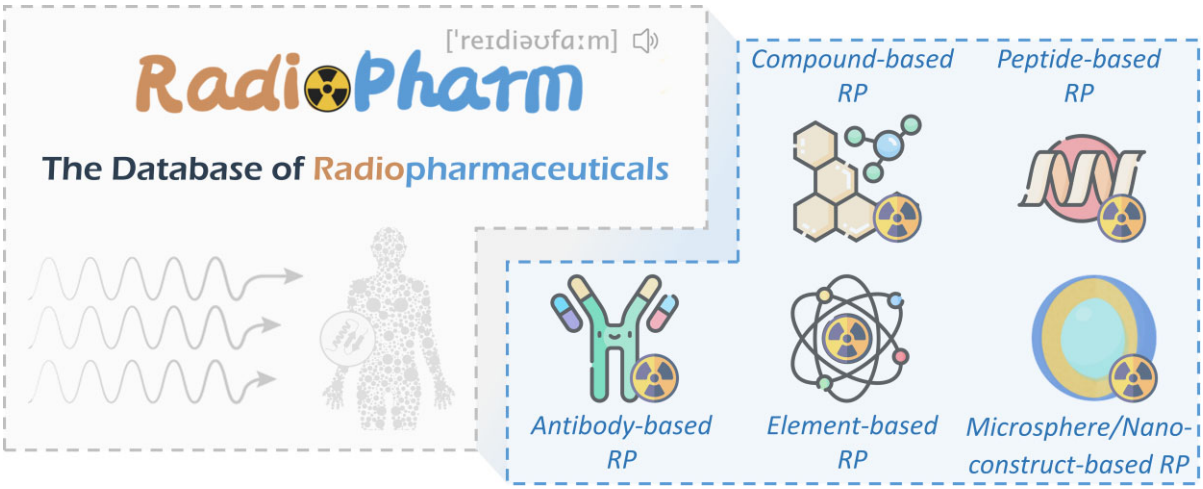
Abstract

Radiopharmaceuticals (RPs) have emerged as a promising group of therapeutic/diagnostic agents with tremendous pharmaceutical advantages and profitable market value. With the rapid advances in this direction, there is an increasing demand for a knowledge base providing RP-relevant data. However, no such database has been available yet. Herein, a database *RadioPharm* was therefore developed to depict the pharmaceutical data for 3141 RPs and the radioactive characteristics for the nuclide in each RP. Particularly, our *RadioPharm* is unique in (i) providing the largest number of RPs (including 68 approved, 575 in clinical trials, and 2498 investigative RPs) among the existing databases, (ii) offering the comprehensive radioactive characteristics for the radionuclide in each RP, and (iii) implementing a multidirectional approach for data retrieval (from diverse perspectives of RP, radionuclide, target, and indication). Because of the important role of all those accumulated data in radiopharmaceutical research, *RadioPharm* is expected to attract broad interest from research community, which is now fully accessible by all users at https://idrblab.org/radiopharm/.

Graphical abstract



Introduction

Radiopharmaceuticals (RPs) have emerged as a promising group of therapeutic/diagnostic agents that possess tremendous pharmaceutical advantages and considerable market value [1–4]. Over the recent decade, with the rapid advances in radionuclide production [5] and conjugate preparation

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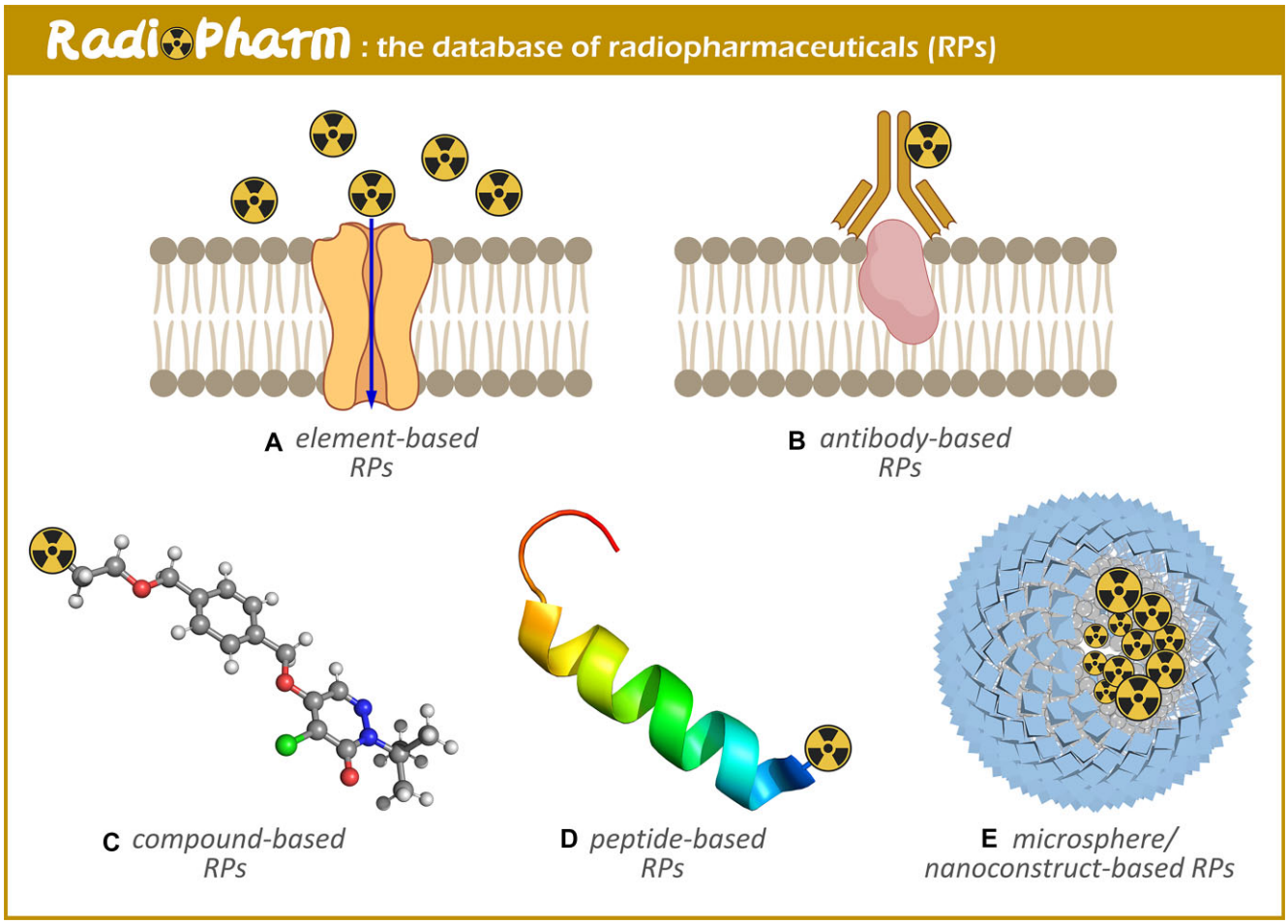

Figure 1. Schematic illustration of RPs in *RadioPharm* classified by five radiation delivery types. (**A**) Element-based RPs; (**B**) antibody-based RPs; (**C**) compound-based RPs; (**D**) peptide-based RPs; and (**E**) microsphere/nanoconstruct-based RPs.

technologies [6], RPs have made revolutionary progress in diverse classes of diseases (including oncology [7], nervous system disorders [8], circulatory system disease [9], inflammatory disease [10], etc.), resulting in a total of 68 agents being approved by the U.S. Food and Drug Administration. Taking Lutetium Lu 177 vipivotide tetraxetan (*Pluvicto*®, approved in 2022) as an example, its approval was granted for the treatment of prostate-specific membrane antigen-positive metastatic castration-resistant prostate cancer and achieved an annual sale of $1.3 billion in 2024, making *Pluvicto* a blockbuster drug [11]. Many pharmaceutical enterprises have thus been prompted to shift their research and development focus to RPs [12], and over 10 000 RP-related research articles have been published within the past three years [13–17].

As reported, pharmaceutical data on RPs (including chemical structures, mechanisms of action, pharmacokinetic properties, clinical status, drug-likeness, adverse effects, and personalized dosage recommendations) are essential for the development, optimization, and clinical evaluation of new RPs [18–20]. Furthermore, the radioactive characteristics of radionuclides in those RPs (such as physical half-life, energy of radiation, radiation ranges, linear energy transfer (LET) profiles, nuclide sources, decay modes, and cytotoxicity) are crucial for the production of RPs and the assurance of their pharmaceutical efficacies and dosimetry-dependent safeties [21–23]. In other words, with the booming application of AI in modern biomedical studies, it is highly demanded to accumulate both types of the above data for accelerating the discovery of next-generation RPs [24, 25].

Until now, several databases have been established to offer RP-related data, many of which remain active and freely accessible. Some of these, including PubChem [26], ChEMBL [27], and DrugMAP [28], offer RP information as part of a broader collection of chemical data. Some others focus on providing the personnel, equipment, and infrastructure of RPs in low- and middle-income countries (such as NUMDAB [29]) and describing the data of drug interactions and adverse reactions for some RPs (Datinrad [30], FPVD [31], etc.). However, no database is available for providing the detailed pharmaceutical data for RPs along with in-depth radioactive characteristics of the radionuclide in each RP. Due to the importance of these types of RP data, it is demanded to have an RP database that can serve as an indispensable complement to the existing ones offering RP-related data.

Herein, a database, entitled *RadioPharm*, was therefore developed to comprehensively detail the pharmaceutical data for 3141 RPs and the radioactive characteristics of the radionuclide in each RP. It is unique in (i) systematically portraying the largest number of RPs (including 68 approved, 575 in clinical trials, and 2498 investigative RPs) among available databases, (ii) featuring comprehensive characterization of the radioactive characteristics of the radionuclide in each RP, and (iii) implementing a multidirectional approach for information retrieval (from diverse perspectives of RP, radionuclide,

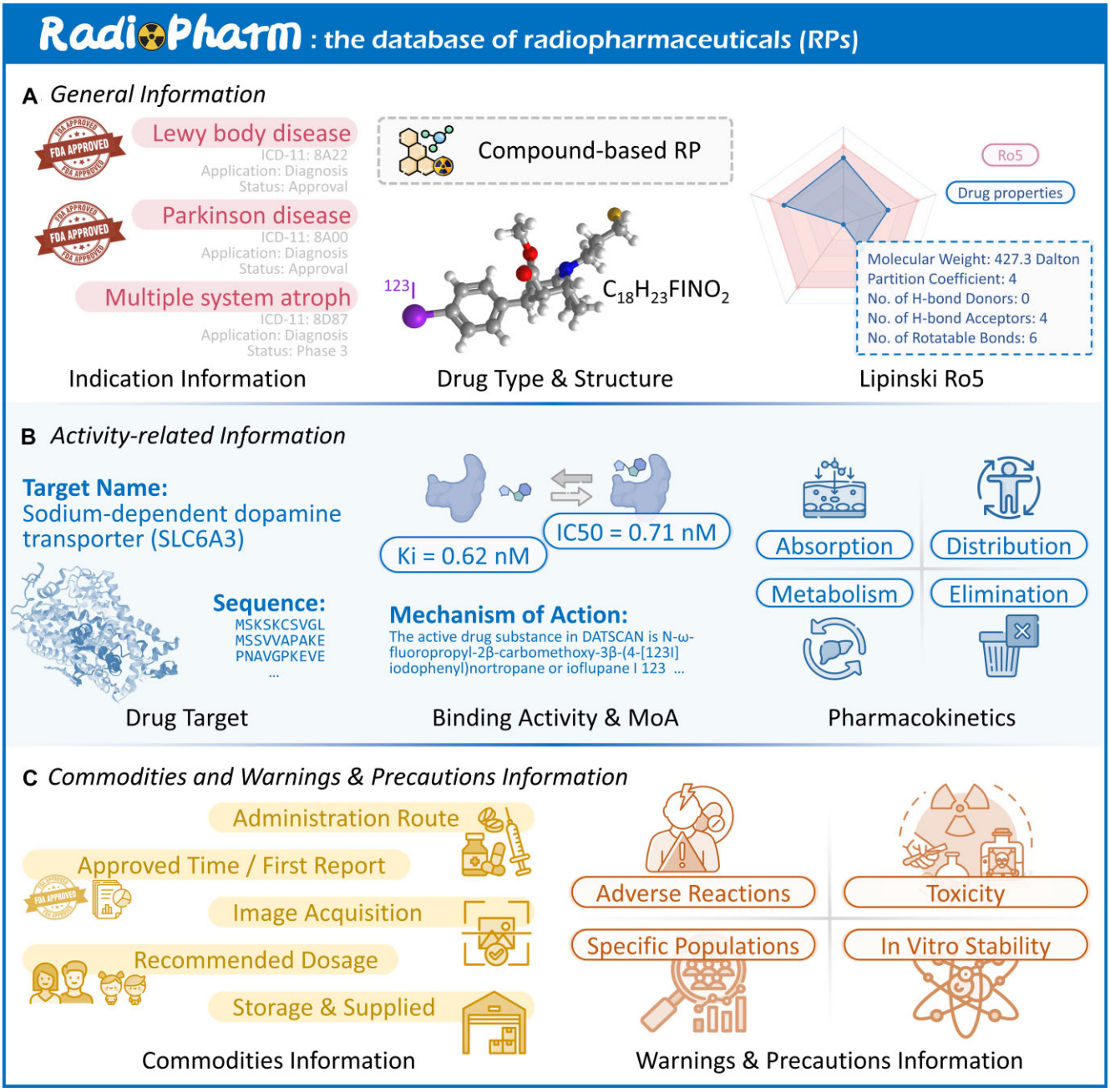

Figure 2. Schematic illustration of the information provided on a typical RP page of *RadioPharm*. (**A**) The general information of RP, such as RP name, drug type, disease indication, clinical status, chemical structure, physicochemical properties, and chemical descriptors. (**B**) The activity-related information of RP, such as RP's drug targets, biological half-life, pharmacokinetic characteristics, and mechanism of action. (**C**) The commodities, warnings, and precautions information of RP, such as administration route, recommended dosage, adverse drug reaction, and radiation risk.

target, and indication). Because of the significant role of all those accumulated data in radiopharmaceutical research, *RadioPharm* is expected to attract broad interest from the research community, which is now fully accessible by all users at https://idrblab.org/radiopharm/.

Factual content and data retrieval

Systematically collecting the data of RPS

Explicit data on RPs and their affiliated information were collected using the following procedure. *First*, the *pharmaceutical data* of RPs were identified by searching those keyword combinations of "radiopharmaceutical + pharmacokinetics," "radiopharmaceutical + mechanism of action," "radiopharmaceutical + radionuclide," "radiopharmaceutical + half-life," etc.Then, a total of 3141 RPs belonging to five radiation delivery types (as illustrated in Fig. 1; element- [32], compound- [33], peptide- [34], antibody- [35], and microsphere/nanoconstruct-based [36]) were compiled, which contained 68 approved, 575 in clinical trials, and 2498 investigative RPs of the detailed pharmaceutical data (including chemical structures, modes of action, pharmacokinetic properties, biological half-life, etc.). Third, those radioactive characteristics of radionuclides in the collected RPs were further gathered through a systematic literature review and on-

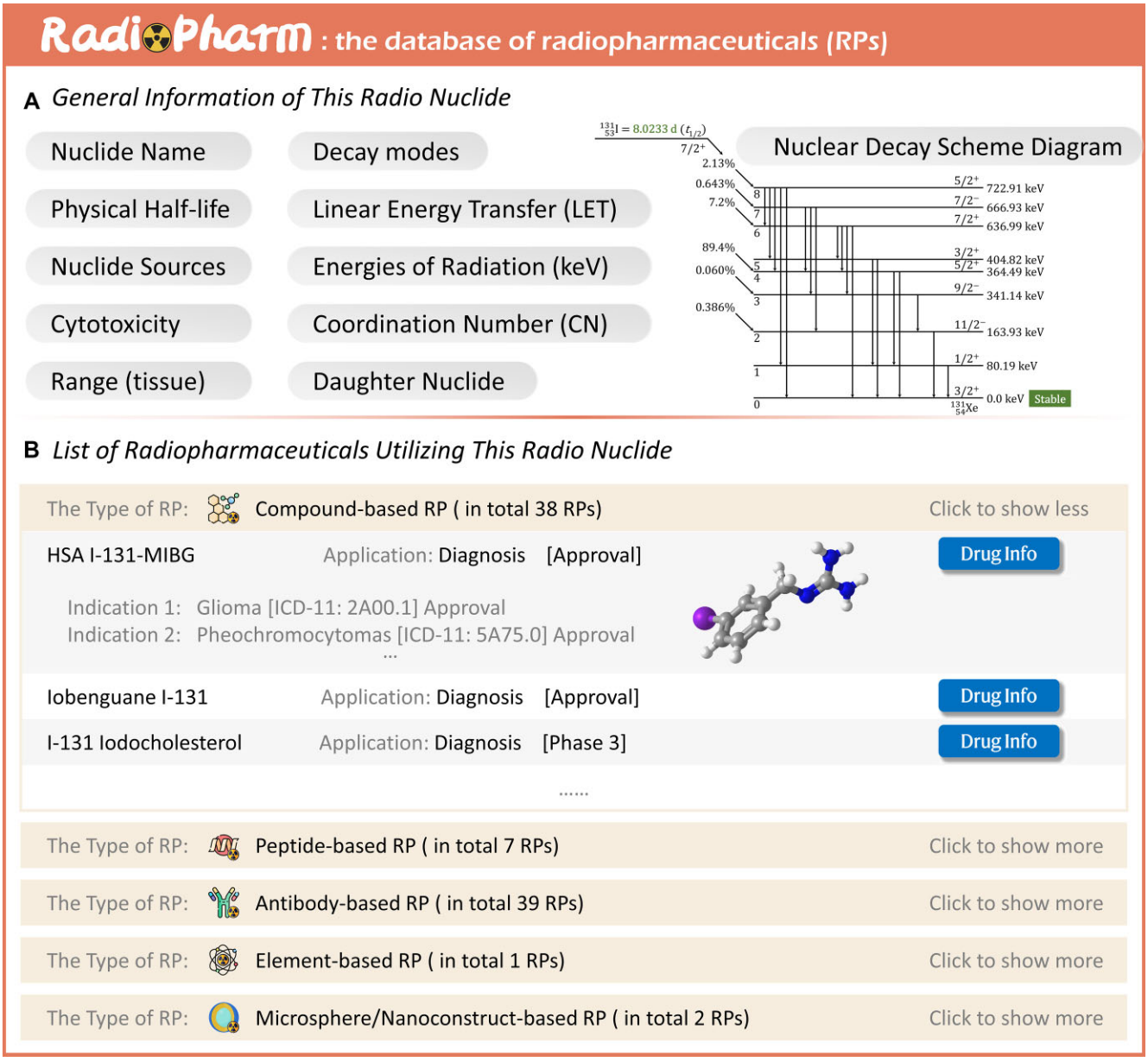

Figure 3. Schematic description of the information illustrated on a typical page for radionuclides in *RadioPharm*. (**A**) The general information of nuclide, such as nuclide name, physical half-life, decay mode, nuclide source, linear energy transfer, energy of radiation, radiation range, daughter nuclide, and nuclear decay scheme diagram. (**B**) A list of RPs utilizing this radionuclide that were ordered based on their radiation delivery type (element-based, antibody-based, compound-based, peptide-based, microsphere/nanoconstruct-based), application type (therapeutic, diagnostic), and clinical status. A user can link to specific drug by clicking the corresponding "Drug Info," making it convenient to quickly obtain the relevant RP corresponding to this nuclide.

line resources [37–39], bringing about a variety of characteristics for 73 radionuclides: physical half-life, energy of radiation, radiation ranges, LET profiles, decay modes, cytotoxicity, radionuclide sources, etc.Finally, various types of search engines (including the keyword-based, classification-based, structure-based, etc.) were developed and implemented in *RadioPharm*, with the data cross-linked to a variety of well-established databases, such as PubChem [40], UniProt [41], DrugBank [42], ChEMBL [43], TTD [44], NCBI Gene [45], DrugMAP [46], and others.

RPs of diverse radiation delivery types

The RPs of five radiation delivery types were collected for this study, including element-based, antibody-based, compound-based, peptide-based, and microsphere/nanoconstruct-based ones [47–49]. The element-based *RPs* include those composed of pure elements, such as ^{129}Xe [50], as well as compounds formed by a radionuclide with other elements through ionic bonds, such as $^{223}RaCl_2$ [51]. The compound-based *RPs* refer to those covalently combining the radionuclide with a compound, such as ^{18}F-fluorodeoxyglucose [52], as well as those covalently joining a metal ion with chelating agents, such as ^{99m}Tc sulfur colloid [53]. The peptide-based *RPs* indicate those structures in which radionuclides are linked to peptides as vectors via chelating agents, such as ^{177}Lu vipivotide tetraxetan [54], as well as those in which radionuclides are combined with proteins, such as ^{131}I human serum albumin [55]. The antibody-based *RPs* denote those in which a radionuclide is conjugated to an anti-

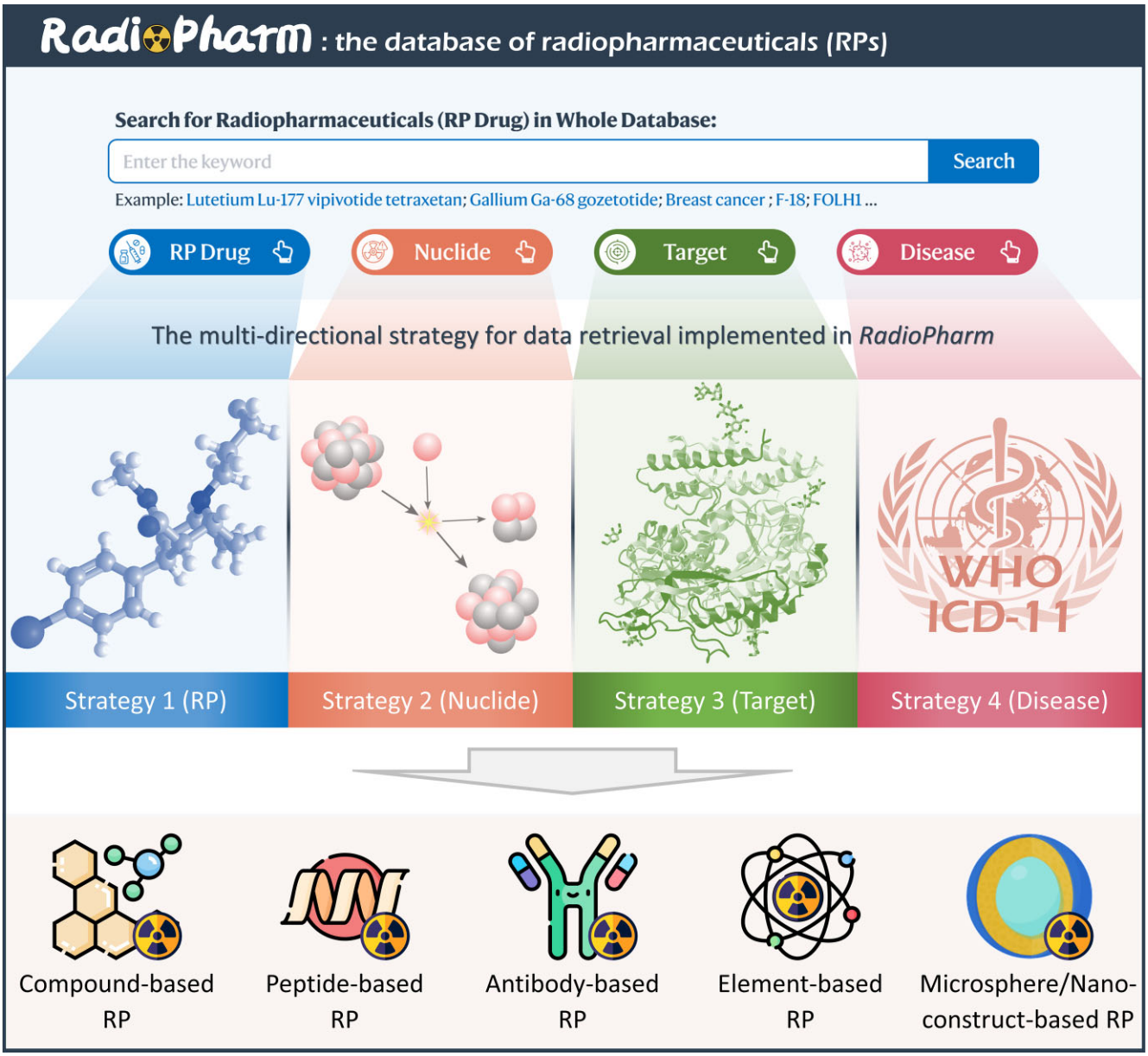

Figure 4. The multidirectional strategy for data retrieval implemented in *RadioPharm*. The data could be retrieved from four different perspectives (RP, nuclide, target, and disease), which could facilitate the retrievals of the pharmaceutical data for RPs and the radioactive characteristics of the radionuclide in each RP. Furthermore, this approach could also help to identify the sequential, structural, and physicochemical characteristics of RP-relevant targets and discover the therapeutic class, clinical status, and RP type for all collected disease indications.

body, and the targeting ability of antibody is used to deliver the radionuclide to the disease site, thereby exerting a targeted therapeutic or diagnostic effect, such as ^{68}Ga-PMD22 [56]. The microsphere/nanoconstruct-based *RPs* stand for those formulated through precise encapsulation or conjugation of radionuclides within microspheres and nanostructured carriers, such as ^{90}Y resin microspheres [57], ^{89}Zr-dextran nanoparticles [58], and ^{212}Pb-hydrogel nanoparticles [59].

As shown in Fig. 2, the pharmaceutical data for the 3141 RPs across five radiation delivery types were provided, including chemical structures, mechanisms of action, pharmacokinetic properties, clinical status, drug-likeness, adverse effects, personalized dosage recommendations, and so on. Such data were used by recent works to effectively potentiate RP therapy by avoiding excessively rapid tumor clearance [60], successfully design selective RPs of favorable brain uptake, dosimetric properties, and metabolic profiles [61], and efficiently identify radioprotective ligands by offsetting the binding of RPs to healthy organs [62]. On a typical RP page of *RadioPharm*, three categories of data were provided, which included the general information of RP (as shown in Fig. 2A), the activity-related information of RP (as shown in Fig. 2B), and the commodities, warnings, and precautions information of RP (as shown in Fig. 2C). These data were fully available to access, which were critical for the development, optimization, and clinical assessment of new RPs.

Radioactive characteristics of the radionuclides in all those RPs

As the core component of RPs, radionuclides involve considerations such as decay modes, physical half-lives, radiation energy and type, particle range, LET, etc. Such physical properties can directly influence the diagnostic/therapeutic applications of RPs [63–65]. For example, the decay mode determines the type and energy of the emitted particle, directly affecting the diagnostic or therapeutic use of the RP, and different decay types result in varying radiation levels, which are directly related to radiation protection design, patient dose burden, and dosimetry calculation [66]; the physical half-life is one of the key parameters in RP research, the duration of which needs to align with the *in vivo* distribution and metabolic processes of RPs to ensure that diagnosis/treatment is performed within the optimal time window [67]; the radiation energy and type are core parameters with alpha particles suitable for accurately killing small-range lesions and beta ones applicable for treating larger lesions [68]; and the LET affects the treatment range and tissue penetration depth, thereby guiding personalized RP selection and combination strategies [69]. All in all, the radioactive characteristics of the radionuclide are essential for ensuring the safety and efficacy of RPs, which were therefore systematically documented in our *RadioPharm* database.

Taking the nuclide ^{131}I as an example (as shown in Fig. 3A), the general information of this nuclide was systematically provided, such as radionuclide name, physical half-life, main decay mode, radionuclide source, LET, energy of radiation, cytotoxicity, radiation range, daughter nuclide, and nuclear decay scheme diagram. In other words, the radioactive characteristics of each radionuclide were provided qualitatively/quantitatively. Moreover, a list of RPs utilizing radionuclide ^{131}I was also described (as shown in Fig. 3B), which organized the corresponding RPs based on their radiation delivery type (such as element-based, antibody-based, compound-based, peptide-based, and microsphere/nanoconstruct-based ones), along with application type (therapeutic/diagnostic) and clinical status. Moreover, users can link to specific drugs by clicking the corresponding "Drug Info," making it convenient to quickly obtain the relevant RPs associated with this radionuclide.

Implementation of a multidirectional approach for data retrieval

In *RadioPharm*, a multidirectional approach for data retrieval was implemented. Users could perform a fuzzy search using specified keywords, such as "radiopharmaceuticals," "radionuclide," "target name," or "disease name" in the full-data search box on the webpage, while explicit searches from multiple perspectives could enable substantially enhanced data retrieval. As illustrated in Fig. 4, a multidirectional search from the perspectives of RP, radionuclide, target, and disease was realized. This approach could facilitate the retrieval of pharmaceutical data for RPs and the radioactive characteristics of the radionuclide in each RP. Furthermore, this approach could also help to identify the sequential, structural, and physicochemical characteristics of RP-related targets and discover the therapeutic class, clinical status, and RP type for all collected diseases. Moreover, to facilitate users' access and analysis of *RadioPharm* data, the collected raw data were carefully cleaned and then systematically standardized. These standardizations included (i) all the RPs, radionuclides, and targets being cross-linked to authoritative databases and (ii) all disease indications being standardized according to the latest International Classification of Diseases (ICD-11) that is officially released by the World Health Organization. Additionally, a user-friendly interface was created to enable convenient browsing and searching of data. All RP-relevant data could be viewed, accessed, and downloaded directly from the online *RadioPharm* without any login requirement.

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Conflict of interest

None declared.

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Data availability

All radiopharmaceuticals can be viewed, accessed, and downloaded from *RadioPharm*, which is freely accessible without any login requirement by all users at https://idrblab.org/radiopharm/.

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