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OpenDose: Open-Access Resource for Nuclear Medicine Dosimetry

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Radiopharmaceutical dosimetry depends on the localization in space and time of radioactive sources and requires the estimation of the amount of energy emitted by the sources deposited within targets. In particular, when computing resources are not accessible, this task can be performed using precomputed tables of specific absorbed fractions (SAFs) or S values based on dosimetric models. The aim of the OpenDose collaboration is to generate and make freely available a range of dosimetric data and tools. **Methods:** OpenDose brings together resources and expertise from 18 international teams to produce and compare traceable dosimetric data using 6 of the most popular Monte Carlo codes in radiation transport (EGSnrc/EGS++, FLUKA, GATE, Geant4, MCNP/MCNPX, and PENELOPE). SAFs are uploaded, together with their associated statistical uncertainties, in a relational database. S values are then calculated from monoenergetic SAFs on the basis of the radioisotope decay data presented in International Commission on Radiological Protection Publication 107. **Results:** The OpenDose collaboration produced SAFs for all source region and target combinations of the 2 International Commission on Radiological Protection Publication 110 adult reference models. SAFs computed from the different Monte Carlo codes were in good agreement at all energies, with SDs below individual statistical uncertainties. Calculated S values were in good agreement with OLINDA/EXM 2.0 (commercial) and IDAC-Dose 2.1 (free) software. A dedicated website (www.opendose.org) has been developed to provide easy and open access to all data. **Conclusion:** The OpenDose website allows the display and downloading of SAFs and the corresponding S values for 1,252 radionuclides. The OpenDose collaboration, open to new research teams, will extend data production

to other dosimetric models and implement new free features, such as online dosimetric tools and patient-specific absorbed dose calculation software, together with educational resources.

Key Words: nuclear medicine; dosimetry; open-access database; Monte Carlo methods

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The necessity of dosimetry in nuclear medicine is increasing with the remarkable development of targeted radionuclide therapy (1).

Absorbed doses in nuclear medicine are usually calculated using the MIRD formalism (2), with the following time-independent formulation:

$$D_{(Target, T_D)} = \sum_{Source} \tilde{A}_{(Source, T_D)} \times S_{(Target \leftarrow Source)}, \quad \text{Eq. 1}$$

where $D_{(Target, T_D)}$ is the mean absorbed dose (Gy) delivered to target tissue, $\tilde{A}_{(Source, T_D)}$ is the total number of nuclear transformations in the source (Bq·s), $S_{(Target \leftarrow Source)}$ is the mean absorbed dose to a given target per nuclear disintegration in the source (S value; Gy·Bq⁻¹·s⁻¹), and T_D is the dose integration period after administration of the radioactive material. S values are obtained from reference human models and used for model-based dosimetry or adjusted to the geometry of a specific patient (3). The calculation of S values (Eq. 2) requires a clear definition of the geometry of the model and isotope decay characteristics:

$$S_{(Target \leftarrow Source)} = \sum_i E_i Y_i \Phi_{i(Target \leftarrow Source, E_i)}, \quad \text{Eq. 2}$$

where $\Phi_{i(Target \leftarrow Source, E_i)}$ is the specific absorbed fraction (SAF; kg⁻¹) for radiation type i and E_i and Y_i are the energy (J) and yield (Bq⁻¹·s⁻¹), respectively, of radiation type i .

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Historically, SAFs and S values were computed from mathematic models and were the basis for International Commission on Radiological Protection (ICRP) reports for radiopharmaceutical dosimetry (4). Since the publication of ICRP Publication 103 (5), the ICRP recommends using voxel-based models, such as those presented in ICRP Report 110 (ICRP 110) (6). This is a logical evolution that accounts for the increasing availability of a refined description of human geometry. In addition, recent developments proposed polygonal mesh models (7), which can overcome voxel-based model limitations in the description of thin structures such as organ walls.

For decades, the reference S values for mathematic models were included in MIRDOSE and then in OLINDA/EXM (<http://www.doseinfo-radar.com>). They were easily accessible, and most dosimetric results presented to the Food and Drug Administration or European Medicines Agency for approval of a new radiopharmaceutical were obtained using these codes. OLINDA/EXM 1.0 is no longer available, and OLINDA/EXM 2.0 is part of Hermes Medical Solutions (<http://vueinnovations.com/olinda>). Moreover, SAFs and S values are no longer available on the Radiation Dose Assessment Resource website (<http://www.doseinfo-radar.com/>).

Recently, ICRP Report 133 (ICRP 133) (8) presented SAFs for 79 sources and 43 targets of the ICRP 110 computational models. On the basis of this dataset, Andersson et al. (9) proposed IDAC-Dose 2.1 desktop software for performing absorbed dose calculations.

SAFs are generated through intensive Monte Carlo simulations requiring substantial computational power. As a consequence, there is a delay between the publication of a model and its corresponding SAFs on the order of years. This delay might be amplified in coming years as the number of models and their level of complexity increase (10).

The OpenDose project is based on the idea that a collaborative approach enables this challenge to be addressed by offering a responsive network of shared dosimetric resources and expertise from several teams involved in radiopharmaceutical dosimetry. This approach allows the production and comparison of data with different codes, increasing the robustness of the results. The OpenDose collaboration strives to produce and disseminate dosimetric data that are traceable and reproducible and include associated uncertainties (11).

MATERIALS AND METHODS

Collaboration

The first meeting of the collaboration was held at the European Association of Nuclear Medicine Congress in Barcelona, Spain, in 2016. At this meeting, the structure of the OpenDose collaboration and its scientific priorities were defined and a collaboration agreement in which the teams committed to generate freely accessible dosimetric data that meet the FAIR Guiding Principles was drafted (12).

OpenDose currently includes 18 research teams at 30 institutes and has a steering committee composed of 1 representative per team. The collaboration organizes annual meetings to present results and discuss future actions.

Framework

A common framework (Fig. 1) has been defined to harmonize the different Monte Carlo codes and different units and formats used by the teams. Within this framework, each team is responsible for its own Monte Carlo simulations but uses the same input models and delivers the data in a common output format. Therefore, each collaboration member can independently contribute to data generation. The data produced are then collected and centralized in a database along with the models and radioisotope decay data. A dedicated website allows access to the database, displays SAFs, allows the calculation of S values, and allows downloading of the results.

Here we describe the details of the OpenDose framework.

Models and Radioisotope Decay Data

The first models considered within the collaboration were those defined in ICRP 110 (6). These voxel-based models represent the average anatomy of male and female subjects. The adult female is described by $299 \times 137 \times 348$ voxels for a size of $1.775 \times 1.775 \times 4.84$ mm, corresponding to a height of 1.63 m and a mass of 60 kg. The adult male is described by $254 \times 127 \times 222$ voxels for a size of $2.137 \times 2.137 \times 8.0$ mm, corresponding to a height of 1.76 m and a mass of 73 kg.

These models comprise 141 segmented regions (~20,000 target ← source combinations) and 53 different media. Because uncertainties from different regions cannot be summed after simulation, as deposited energies in adjacent regions are likely to be correlated, 31 compound regions were added to regroup parts of an organ (e.g., the kidneys are composed of regions 89–94). These additional 31 compound regions are the same as the target compound regions and “Total body except organ contents” defined in Tables D.1 and C.1 of ICRP 110, respectively (6).

The radioisotope decay data of ICRP Publication 107 (13) were considered for S value calculation. The ICRP Publication 107 provides electronic data for 1,252 radioisotopes.

Monte Carlo Simulations and Specific Absorbed Fractions

The variety of research teams offers a broad experience over 6 of the most widely used Monte Carlo codes in radiopharmaceutical dosimetry: EGSnrc/EGS++ (14), FLUKA (15), GATE (16), Geant4 (17), MCNP/MCNPX (18), and PENELOPE (19). These codes come from different research fields and implement different approaches to simulate radiation transport in matter, effectively offering the independent production of data. This approach allows verification of the production pipeline and increases the robustness of data.

Monte Carlo simulations estimate energy deposition in the models as a function of source location, particle type, and energy. Source location can be any region of the selected model from which particles are emitted isotropically. Monte Carlo simulations were performed for monoenergetic photons and electrons. A list of 91 energies ranging from 5 keV to 10 MeV was defined on the basis of the logarithmic energy distribution of β-emitters in ICRP Publication 107 (13). Physics models, the use of variance reduction techniques, and any other parameters are the choice of each team. However, to ensure the traceability and reproducibility of data, each team must keep track of all simulation parameters and files. At least 10^8 primary particles are recommended as a trade-off between good statistics and computation time. Statistical uncertainties are estimated for all quantities (energy deposited, absorbed dose) during the run time of the simulations using the history-by-history method (20). Each simulation provides absorbed doses and uncertainties at the individual voxel level (as binary matrices) as well as for target regions (as ASCII files).

From the simulated absorbed dose to a target, the SAF is calculated by dividing the absorbed dose by the initial energy (J) of the particles and by the number of simulated particles. Each team records the SAFs (and corresponding uncertainties) in a specific comma-separated values format with a specific naming convention to ease integration into the database.

Database

SAFs are stored in a relational Structured Query Language database as a function of parameters such as model (name, version), source and target (name, volume, mass), particle type, energy, and number of simulated particles. In addition to these parameters, data provenance (contact name, date) is stored to ensure traceability. The radioisotope decay data are also stored in the database to enable the calculation of S values.

S Value Calculation

A Python script was developed to calculate S values from SAFs, for any radioisotope, using Equation 2. First, SAFs are extracted from the

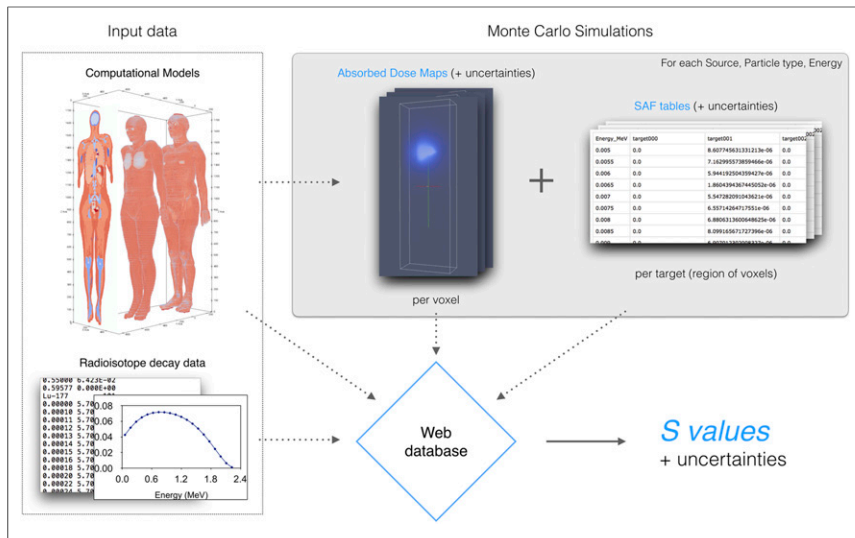


FIGURE 1. OpenDose framework. SAFs produced by Monte Carlo simulations are stored in database along with input data. Web application allows calculation, display, and downloading of SAFs and S values.

database and averaged over all Monte Carlo codes, increasing the robustness of the calculation. Then, SAFs are linearly interpolated to the energy of each radiation type of the radioisotope considered and multiplied by the corresponding yield ($\text{Bq}^{-1}\cdot\text{s}^{-1}$) and energy (J). For β -emission spectra, SAFs are integrated over energy bins. α -particles and α -recoil nuclei are considered to deposit their energy locally. Finally, all emission contributions are summed to obtain the S value for a selected model, source, target, and radioisotope. The S value is also calculated per particle type (photon, electron, alpha-particle) to provide more insight into the S value composition.

At each step of the calculation, the uncertainty of the S value is computed as

$$u(S_{(Target \leftarrow Source)})^2 = \sum_i (E_i Y_i u(\Phi_{i(Target \leftarrow Source, E_i)}))^2, \quad \text{Eq. 3}$$

where E_i and Y_i are the energy (J) and yield ($\text{Bq}^{-1}\cdot\text{s}^{-1}$), respectively, of radiation type i (for a given isotope) and $u(\Phi_{i(Target \leftarrow Source, E_i)})$ is the SAF statistical uncertainty (kg^{-1}) for radiation type i .

The computation is performed on demand to use the most up-to-date data (SAFs and nuclear data). No S values are stored in the database.

Website

A dedicated website was developed to provide access to all OpenDose data. A website has the advantages of being easily accessible on every device (without any installation) and being easy to keep up to date.

Verification of Produced Data

To assess the variability of results among the different Monte Carlo codes, comparisons were performed using 1 model for a restricted number of sources and energies. SAFs were computed by all teams for the ICRP 110 adult female model using the Liver and Blood Vessels Trunk as sources and monoenergetic photons and electrons of 0.05, 0.1, 0.2, 0.5, 1, 2, and 5 MeV. The Liver was chosen for its relevance in radiopharmaceutical dosimetry and its compact shape, whereas the Blood Vessels Trunk was chosen to test a more spatially complex source.

The SAFs for the source Liver were compared with the data published in ICRP 133 (8).

For the calculation of S values from the SAFs (Eq. 2), the database must contain at least 1 value for each model, source, target, and energy

combination. To meet this requirement, simulations were run with a reduced number of 10^7 particles with Geant4 10.5 to reach a complete dataset. S values for a source located in the Liver of the female model, 6 targets, and 3 radioisotopes commonly used in nuclear medicine (^{131}I , ^{177}Lu , and ^{90}Y) were compared with IDAC-Dose 2.1 (9) and OLINDA/EXM 2.0 (21).

RESULTS

Current Production Status

Producing a complete dataset for 1 model (e.g., the ICRP 110 adult female) requires approximately 30,000 simulations, representing approximately 750,000 CPU hours of computation. By sharing the workload and the computing resources of the teams (<https://www.ziemowit.hpc.polsl.pl/en>, <https://cc.in2p3.fr/en>, <https://www.calmip.univ-toulouse.fr>, and <https://nci.org.au>), the collaboration can produce data for a model

in a few months. Some developments to take advantage of large grid infrastructures have also been made (22).

As of October 2019, the database held 11,177,347 entries, representing data spread over 2 models, 141 sources, 172 targets, 2 particle types (photons and electrons), and 91 energies produced with 9 different Monte Carlo code versions.

Verification of Produced Data

For photons, SAFs from all of the teams are in good agreement at all energies for both sources. For example, SAFs have relative SDs ranging from 0.67% at 5 keV to 0.23% at 5 MeV for Liver \leftarrow Blood Vessels Trunk and from 0.69% at 5 keV to 0.16% at 5 MeV for Spleen \leftarrow Liver. For electrons, SAFs have higher statistical fluctuations, especially at low energy and for targets at large distances from the source. In particular, statistical uncertainties of SAFs for Brain \leftarrow Liver are close to 100% at less than 200 keV. As a consequence, the SAF SDs between the different Monte Carlo codes can reach 65.34% for Brain \leftarrow Liver and electrons of 100 keV and as low as 1.56% at 5 MeV. These high relative differences correspond to negligible absolute differences. For the target Spleen, which is closer to the Liver, the relative SDs range from 22.86% at 5 keV to 2.0% at 5 MeV.

SAFs from this preliminary assessment were also compared with data published in ICRP 133 (8). The overall agreement between OpenDose and ICRP 133 values was good, with mean relative differences of 1.65% for photons and 8.2% for electrons of greater than 200 keV. However, some large differences were noted for low-energy electrons, with a maximum relative difference of +120% for Thyroid \leftarrow Liver at 100 keV. This large difference likely was due to high statistical fluctuations in the data. Unfortunately, no information on the SAF uncertainties is given in ICRP 133. ICRP 133 values for Brain \leftarrow Liver at energies of less than 200 keV are equal to 0.0, which may indicate a lower statistical power of the ICRP 133 simulations than of the OpenDose data. These mean relative differences did not include Liver \leftarrow Liver SAF values, for which a systematic difference of 22% was found. This finding is explained by the modification of some target masses in ICRP 133 (Tables A.1 and A.2 from (8)) to add blood content; the original 1.400 kg for the Liver in the ICRP 110 adult female model was changed to 1.810 kg.

SAF values from a selection of different Monte Carlo codes are available in Supplemental Tables 1–8 (supplemental materials are available at <http://jnm.snmjournals.org>), along with SAFs from ICRP 133 for comparison. The “OpenDose mean” gives the mean and SD of all available Monte Carlo code values.

S values are available for the 2 models, 141 sources, 172 targets, and 1,252 radioisotopes considered so far within the OpenDose collaboration. Table 1 shows S values obtained for the adult female model and the comparison with IDAC-Dose 2.1 (9) and OLINDA/EXM 2.0 (21). In general, good agreement was found. In particular, OpenDose and IDAC-Dose 2.1 values were very close, as expected, as they use the same input model (ICRP 110), whereas OLINDA/EXM 2.0 values are calculated for a nonuniform rational basis spline adult female model based on ICRP Publication 89 (23). A systematic difference from IDAC-Dose 2.1 for Liver ← Liver can be explained by the mass adjustment made in the ICRP 133 SAF calculation.

Website

The OpenDose website is online at www.opendose.org. It provides information on the project, allows access to the SAF database, and allows calculation of the S values for 1,252 radionuclides. Results are displayed with interactive plots and can be downloaded in a comma-separated values format. Figure 2 shows the SAF section of the website, with results from all of the Monte Carlo codes. The available data should be used for research purposes only, and the website content is licensed under a Creative Commons Attribution-ShareAlike 4.0 International license.

DISCUSSION

The generation of dosimetric data represents a computing challenge because of the resources and time required to perform simulations. The idea of a collaborative framework designed for this purpose required a preliminary verification of the precision of the dosimetric estimations of the different Monte Carlo codes used within the community.

The comparison exercise proposed to members of the collaboration demonstrated that SAFs produced with different Monte Carlo codes exhibit low dispersion and are in good agreement with published ICRP 133 data. The uncertainties of the SAFs or the S values estimated by OpenDose are a good indicator of the limitations of the values themselves. For example, data for electrons of low energy show statistical limitations for targets far from the source. This information is not present in any other published SAF data. Calculated S values also show good agreement with IDAC-Dose 2.1, which uses the same model and radioisotope decay scheme. OpenDose and IDAC-Dose 2.1 S values differ only for some sources because ICRP integrated organ mass adjustments. OpenDose provides data corresponding to the models used in the Monte Carlo simulations, without any mass adjustments, to avoid any calculation approximation or radiation transport simplifications and to maintain a strict framework for data traceability and reproducibility.

The decay data presented in ICRP Publication 107 do not include corresponding standard uncertainties, so the reported standard uncertainty of the S value (Eq. 3) is purely statistical. For many common radionuclides used in nuclear medicine, the uncertainties in the decay data can be the dominant source of the uncertainty of the S value and should be included in any uncertainty estimation (24). In the future, nuclear data with reported standard uncertainties will be used in OpenDose (25).

During the last meeting (October 2019), the steering committee decided to include, as part of the OpenDose collaboration products, 2 open-source software products currently under development. The first

TABLE 1
OpenDose S Values Compared with IDAC-Dose 2.1 and OLINDA/EXM 2.0 for ¹³¹I, ¹⁷⁷Lu, and ⁹⁰Y in Liver of ICRP 110 Female Model

Target	¹³¹ I			¹⁷⁷ Lu			⁹⁰ Y		
	OpenDose	IDAC-Dose 2.1	OLINDA/EXM 2.0	OpenDose	IDAC-Dose 2.1	OLINDA/EXM 2.0	OpenDose	IDAC-Dose 2.1	OLINDA/EXM 2.0
Brain	1.492e-8 ± 9.5e-11	1.46e-8	1.47e-8	8.423e-10 ± 4.6e-12	8.44e-10	8.10e-10	1.084e-10 ± 2.6e-12	1.08e-10	4.27e-11
Gallbladder wall	6.355e-6 ± 1.2e-8	6.33e-6	2.43e-6	1.100e-6 ± 2.8e-9	1.09e-6	2.52e-7	2.228e-5 ± 2.5e-8	2.20e-5	5.16e-8
Liver	2.842e-5 ± 4.7e-9	2.20e-5	2.89e-5	1.753e-5 ± 1.3e-9	1.36e-5	1.76e-5	1.015e-4 ± 7.7e-9	7.83e-5	1.03e-4
Pancreas	2.165e-6 ± 2.9e-9	2.18e-6	2.15e-6	2.255e-7 ± 5.0e-10	2.27e-7	2.34e-7	4.518e-7 ± 1.3e-9	4.61e-7	1.54e-6
Spleen	7.654e-7 ± 1.7e-9	7.69e-7	4.12e-7	7.655e-8 ± 2.3e-10	7.69e-8	3.81e-8	7.824e-9 ± 5.3e-11	7.94e-9	2.35e-9
Thyroid	1.443e-7 ± 4.5e-10	1.44e-7	1.74e-7	1.282e-8 ± 9.9e-11	1.29e-8	1.61e-8	1.287e-9 ± 2.8e-11	1.43e-9	4.86e-10

Values are mean ± SD.

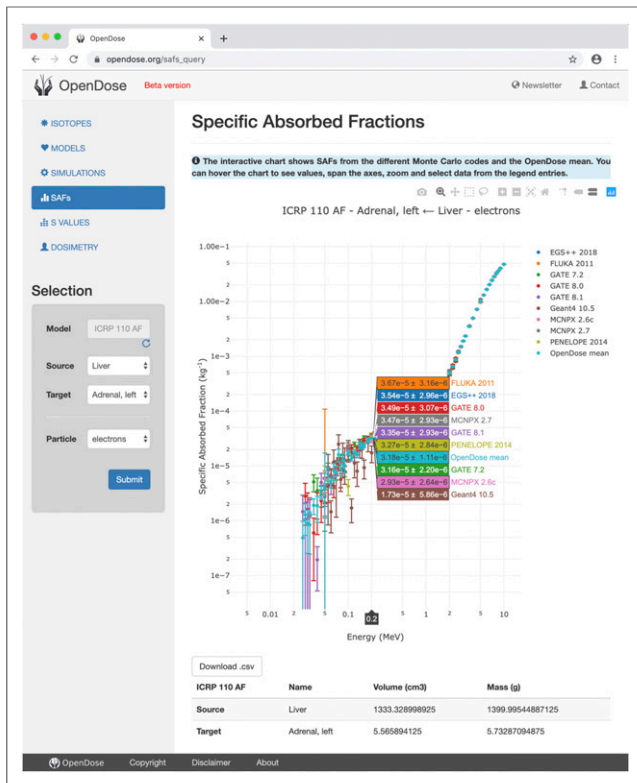


FIGURE 2. SAF section of OpenDose website allows display and downloading of data from all Monte Carlo codes.

implements model-based dosimetry and will be integrated in a future section of the website, whereas the second implements patient-specific dosimetry in a 3DSlicer (<https://www.slicer.org>) extension and will be available for downloading.

The future vision of OpenDose is to make the website a global resource for internal dosimetry, including dosimetric data, software, and education.

CONCLUSION

The aim of the OpenDose project is to establish a long-term international collaboration to generate an open-access database for nuclear medicine dosimetry. The collaboration includes 18 teams with expertise in radiopharmaceutical dosimetry, Monte Carlo methods, and high-performance computing. The initial task set for all partners to produce a set of simulations for a specific model allowed the definition of a common computational framework and the establishment of a unified format for results. OpenDose has now produced SAFs and uncertainties for the 2 ICRP 110 adult models, covering all source and target combinations, 2 particle types (photons and electrons), and 91 energies. Data production will continue and extend to other computational models.

The dedicated website is online at www.opendose.org. It allows easy access to the SAF database and the calculation of S values for 1,252 radionuclides. S values generated for the models considered so far are close to those already available in the literature. A new website section for performing model-based dosimetry calculations is under development.

The collaboration is open to new research teams willing to participate in any OpenDose-related activity, from the production of dosimetric data to the development of the website and dosimetry tools.

DISCLOSURE

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KEY POINTS

QUESTION: Can the practice of dosimetry in nuclear medicine be facilitated?

PERTINENT FINDINGS: The OpenDose collaboration brings together the resources and expertise of many research teams involved in radiopharmaceutical dosimetry. The www.opendose.org website provides a global repository for internal dosimetry, including data, software, and education material.

IMPLICATIONS FOR PATIENT CARE: The OpenDose project will help the practice of internal dosimetry by providing open-access resources.

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