

## SUPPLEMENTARY MATERIAL

### Dosimetry and Toxicity Studies of the Novel Sulfonamide Derivative of Sulforhodamine 101( $^{18}\text{F}$ ]SRF101) at a Preclinical Level

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#### MATERIALS AND METHODS

The percentage of injected activity, residence time and absorbed dose calculations were used as input for OLINDA/EXM V1.0 according to the procedure described in section 2.3. OLINDA/EXM V1.0 does not provide information regarding human intestine content mass; however, this data can be obtained from Cristy and Eckerman dosimetric models, which are based-on ICRP-23 [31] information.

In terms of effective dose, OLINDA/EXM V1.0 implements recommendations from ICRP-60 [32].

#### RESULTS

Table S1 shows the mass values from ICRP-23 used for mass scaling for both the dosimetric models and the S-factors for several organs available in OLINDA/EXM V1.0. Residence times used in OLINDA/EXM V1.0 are included in table S2. Absorbed and effective dose values for adult male and female dosimetric models from OLINDA/EXM V1.0 are listed in table S3.

#### DISCUSSION

In this case, several organs showed total absorbed dose values of the same order of magnitude, which is associated with the excretion path of the radiopharmaceutical. The mean effective dose was obtained from OLINDA/EXM V1.0 using the male and female dosimetric models from Cristy and Eckerman and using the tissue-weighting factors from ICRP-60 is 5.51  $\mu\text{Sv}/\text{MBq}$  and 7.43  $\mu\text{Sv}/\text{MBq}$ , respectively. These figures are comparable to other PET tracers using the same isotope.

For an administrated activity of 350 MBq, this would correspond to 1.93 mSv and 2.60 mSv for male and female dosimetric models implemented in OLINDA/EXM V1.0, respectively.

**Table S1. Mass values from ICRP-23 used for mass scaling for each organ in male/female dosimetric models and S-factors available in OLINDA/EXM V1.0.**

Organ	Male		Female	
	mass (g)	S-factor <sup>a</sup> (mGy/MBq-s)	mass (g)	S-factor <sup>a</sup> (mGy/MBq-s)
Brain	1400	4.62E-05	1200	5.28E-05
Heart	330	1.54E-04	240	2.00E-04
Kidneys	310	1.69E-04	275	1.83E-04
Lower Large Intestine Contents	135	1.63E-04 <sup>b</sup>	135	1.77E-04 <sup>b</sup>
Small Intestine Contents	400	5.48E-05 <sup>c</sup>	375	6.61E-05 <sup>c</sup>
Upper Large Intestine Contents	220	1.07E-04 <sup>d</sup>	210	1.21E-04 <sup>d</sup>
Liver	1800	3.40E-05	1400	4.46E-05
Lungs	1000	4.69E-05	800	5.93E-05
Spleen	180	2.82E-04	150	3.39E-04
Remainder	63056	1.28E-06	52127	1.60E-06
Whole body	68831	---	56912	---

<sup>a</sup>S-factor refers to self-irradiation.

<sup>b</sup>S-factor for lower large intestine wall considering lower large intestine content as a source.

<sup>c</sup>S-factor for small intestine wall considering small intestine content as a source.

<sup>d</sup>S-factor for upper large intestine wall considering upper large intestine content as a source.

**Table S2. Residence times (T) used for dosimetric estimations in OLINDA/EXM V1.0.**

Organ	T <sub>male</sub> (h)	T <sub>female</sub> (h)
Brain	2.37E-04	2.46E-04
Heart	9.67E-05	8.51E-05
Kidneys	4.84E-03	5.19E-03
Lower Large Intestine Contents	3.50E-02	4.26E-02
Small Intestine Content	1.04E-01	1.18E-01
Upper Large Intestine Contents	5.71E-02	6.62E-02
Liver	5.69E-02	5.35E-02
Lungs	2.25E-03	2.18E-03
Spleen	5.19E-05	5.23E-05
Remainder	6.75E-02	6.75E-02

**Table S3. Absorbed dose and effective dose results for adult male and female dosimetric models from OLINDA/EXM V1.0.**

Target Organ	Male		Female	
	Total (mGy/MBq)	Effective Dose (mSv/MBq)	Total (mGy/MBq)	Effective Dose (mSv/MBq)
Adrenals	1.44E-03	3.60E-06	1.89E-03	4.72E-06
Brain	1.19E-04	2.98E-07	1.53E-04	3.81E-07
Breasts	4.67E-04	2.34E-05	6.00E-04	3.00E-05
Gallbladder Wall	3.79E-03	---	5.16E-03	---
LLI Wall	2.29E-02	2.75E-03	3.04E-02	3.65E-03
Small Intestine	2.35E-02	5.87E-05	3.21E-02	8.04E-05
Stomach Wall	1.73E-03	2.08E-04	2.37E-03	2.84E-04
ULI Wall	2.65E-02	6.63E-04	3.49E-02	8.74E-04
Heart Wall	7.35E-04	---	9.72E-04	---
Kidneys	4.48E-03	1.12E-05	5.45E-03	1.36E-05
Liver	7.77E-03	3.88E-04	9.71E-03	4.86E-04
Lungs	9.29E-04	1.11E-04	1.20E-03	1.45E-04
Muscles	1.03E-03	2.56E-06	1.38E-03	3.45E-06
Ovaries	4.98E-03	9.96E-04	7.29E-03	1.46E-03
Pancreas	1.62E-03	4.05E-06	2.14E-03	5.35E-06
Red Marrow	1.39E-03	1.67E-04	1.83E-03	2.20E-04
Osteogenic Cells	9.89E-04	9.89E-06	1.35E-03	1.35E-05
Skin	5.23E-04	5.23E-06	6.84E-04	6.84E-06
Spleen	9.19E-04	2.30E-06	1.30E-03	3.25E-06
Testes	6.21E-04	0.00E+00	---	---
Thymus	4.88E-04	1.22E-06	6.34E-04	1.58E-06
Thyroid	3.72E-04	1.86E-05	4.47E-04	2.24E-05
Urinary Bladder Wall	1.60E-03	7.98E-05	2.18E-03	1.09E-04
Uterus	3.43E-03	8.58E-06	4.93E-03	1.23E-05
Total Body	1.53E-03	---	2.05E-03	---
Effective dose (mSv/MBq)	5.51E-03		7.43E-03	