The following tables give an overview over the categories collected in the spreadsheet for the flr2mmcif script (https://github.com/Fluorescence-Tools/flr2mmcif)

Table 1: Information collected in the spreadsheet for flr2mmcif. The information is collected in different tabs of the spreadsheet. IDs in the tabs are used to refer to entries in other tabs.

	Excel Tabs for collecting information		
1.	**Citation** (Title, Authors, Journal, Year, DOI, ...)		
2.	**Entity**: Entities in the system		
	2.1.	Type of entity (polymer, non-polymer, water)	
	2.2.	Number of copies of the entity in the entity assembly	
	2.3.	Source of the entity	
	2.4.	If a polymer, give type and sequence. If not a polymer, give the chemical component ID (http://www.wwpdb.org/data/ccd), name, and formula	
3.	**Dataset** - Multiple datasets can be added to dataset groups		
	3.1.	Type of data (ihm_dataset_list, e.g. NMR data, SAS data, ...)	
		3.2.1.	Data deposited in a database? If so, where?
		3.2.2.	If not deposited in a database, deposited in a repository (e.g. Zenodo): DOI and URL
4.	**External files** - files within the datasets defined previously (file format, content of the file)		
5.	**Software** - software used e.g. for analyses or modeling (Name, classification, description, location where to find the software, e.g. URL)		
6.	**Instance** (AsymUnit)		
	6.1.	Details on the instance (entity, chain ID, sequence ID for start and end of the instance)	
	6.2.	Model representation	
		6.2.1.	How was the object modeled (atomistic, sphere, gaussian, ...)?
		6.2.2.	Was the object rigid or flexible?
		6.2.3.	How was the starting model obtained (experimental, ab initio, integrative, comparative model)? Chain ID of the starting model and sequence offset.
		6.2.4.	Corresponding dataset and external files
7.	If a **comparative model** (from homology modeling) was used, details can be given (asym ID and sequence IDs for model and template, sequence identity)		
8.	**Modeling protocol** (steps of the modeling protocol, number of models at the beginning and the end of the step, was the modeling multi-scale, multi-state, ordered, ensemble?)		
9.	**Modeling post process** - Post-processing steps after the modeling, e.g. clustering.		
10.	**Multi-state modeling** - if multiple states were modeled, information on the states (names, population fractions, type of states (e.g. structural conformations) can be given. States can be grouped. Models can be assigned to the states.		
11.	**Multi-state scheme** - e.g. kinetic schemes - described by connectivities between states		
	11.1.	Connectivity between states (start state, end state)	
	11.2.	Quantifying the exchange between states within the multi-state scheme	
		11.2.1.	Relaxation time either for the entire scheme or assigned to a specific connectivity between states (relaxation time, unit, amplitude)
		11.2.2.	Kinetic rate for a specific connectivity between states (transition rate constant, equilibrium constant)
12.	**Models** - Information about the models to be deposited (corresponding state, representative of an ensemble, modeling protocol, ...). Models can be grouped.		
13.	**Ensemble Info** - Information if an ensemble of models is deposited (how many models are in the ensemble? How many models are deposited, ...)		
14.	**Reference measurements** - Reference measurements for fluorescence lifetime experiments. Similar information to the FLR information (Table 2)		
15.	**FLR** - Fluorescence-specific information (see Table 2)		
16.	**FLR FPS MPP group** - Information for modeling in the FPS software when using the mean probe position approach. This is not recommended, but possible to use.		
17.	**FLR FPS global parameters** - Global parameters used in the FPS software		
18.	**FLR FRET Model distances** - Distances between probes for different probe pairs for each deposited model. From this, distance deviation w.r.t. the input value can be calculated.		
19.	**FLR FRET Model quality** - The quality of the deposited models based on the FRET data. Often given as χ^2 value.		

Table 2: Information categories of fluorescence expeirments from flrCIF collected in the spreadsheet for flr2mmcif (Tab "FLR"). Depending on the category, additional details are collected.

Collected information (FLR tab)		
Experiment and sample		
1.	**Instrument specification.** Components (lasers, optical elements, detectors, ...) and beam path: Free textual description of the parts	
2.	**Instrument settings. E**xcitation wavelengths, laser power, observation volume, spectral detection ranges, ...: Free textual description	
3.	**Experimental conditions** (e.g. temperature, buffers, ...): Free textual description	
4.	**Fluorescent probes on the sample**	
	4.1.	How many fluorescent probes were used?
	4.2.	Probe type. Which fluorescent probes were used?
	4.3.	Attachment of the probe. Extrinsic or intrinsic probe (e.g. tryptophan)?
	4.4	For extrinsic probe: How was the probe attached?
	4.5.	Chemical information on the probes (SMILES, INCHI code, etc.)
	4.6.	Location. Where were the probes attached? (entity, residue, atom)
	4.7.	Nature of residues. Were the residues to which the probes were attached modified or mutated? If so, details can be provided?
	4.8.	Specificity of labeling. Was the labeling ambiguous?
5.	**Förster radius** for FRET experiments	
6.	Additional information (raw and metadata). For each of the results of a measurement for a sample, additional information such as corresponding **datasets** or **external files** can be provided.	
Analysis workflow		
7.	**Analysis.** What kind of analysis was performed?	
	7.1.	Intensity-based analysis: The report of several correction parameters is required. The ones currently implemented in flrCIF follow the definitions from Hellenkamp et al. (2018) [1].
	7.2.	Lifetime-based analysis: Information about reference measurements (e.g. Donor- or Acceptor-only measurements) should be provided as well as the employed fit model.
8.	**FRET distance restraints.** List of FRET-based distance restraints that were used in the structural modeling approach together with corresponding errors.	
	8.1.	Assignment. In case of multiple states, the same FRET pair could yield multiple distances
Fluorescence-specific information on modeling procedure		
9.	**Dye simulation type.** FRET efficiency-derived inter-dye distances are inter-probe distances, which are not easily converted to distances on the biomolecule. One approach to tackle this issue is the use of accessible volume calculations, where the label is implicitly described using the length of the linker, the width of the linker, and the size of the probe radius [2]. Other approaches might include additional information into these accessible volumes [3, 4]. At the moment, flrCIF contains a description of the used Accessible Volume (AV) parameters, if the FPS (FRET positioning and screening) program [2, 5] is used. Note: The definitions for the FPS software were made exemplarily due to familiarity with the software. flrCIF can however be easily extended to support parameters for other software as well.	

References

1. Hellenkamp, B., et al., *Precision and accuracy of single-molecule FRET measurements-a multi-laboratory benchmark study.* Nature Methods, 2018. **15**(9): p. 669-676.
2. Kalinin, S., et al., *A toolkit and benchmark study for FRET-restrained high-precision structural modeling.* Nature Methods, 2012. **9**(12): p. 1218-1225.
3. Dimura, M., et al., *Quantitative FRET studies and integrative modeling unravel the structure and dynamics of biomolecular systems.* Current Opinion in Structural Biology, 2016. **40**: p. 163-185.
4. Lerner, E., et al., *FRET-based dynamic structural biology: Challenges, perspectives and an appeal for open-science practices.* eLife, 2021. **10**: p. e60416.
5. Dimura, M., et al., *Automated and optimally FRET-assisted structural modeling.* Nature Communications, 2020. **11**(1): p. 5394.