Melinda: A Multimodal Dataset for Biomedical Experiment Method Classification

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Abstract

We introduce a new dataset, Melinda, for Multimodal biomedical experiment method classification. The dataset is collected in a fully automated distant supervision manner, where the labels are obtained from an existing curated database, and the actual contents are extracted from papers associated with each of the records in the database. We benchmark various state-of-the-art NLP and computer vision models, including unimodal models which only take either caption texts or images as inputs, and multimodal models. Extensive experiments and analysis show that multimodal models, despite outperforming unimodal ones, still need improvements especially on a less-supervised way of grounding visual concepts with languages, and better transferability to low-resource domains. We release our dataset and the benchmarks to facilitate future research in multimodal learning, especially to motivate targeted improvements for applications in scientific domains.

1 Introduction

Biocuration, the activity of manually organizing biological information, is a crucial yet human-effort-intensive process in biomedical research (ISB 2018). Organizing such knowledge in a structured way is very important for accelerating science since it facilitates downstream tasks such as scientific information retrieval (Craven, Kumlien et al. 1999; Mohan et al. 2018; Burns et al. 2018; Burns, Li, and Peng 2019), and question answering (Ben Abacha et al. 2019; Nguyen et al. 2019; He et al. 2020).

One such curation task is recognizing experiment methods, which identifies the underlying experimental protocols that result in the figures in research articles. It can be formulated as a multi-class classification task, which takes as inputs the figures and their captions, and outputs the corresponding experiment types that generate the figures, as illustrated in Figure 1.

The task is inherently multimodal as biocurators need to take both the figure and the caption into consideration to make their decisions (Demner-Fushman et al. 2012). While scientists can do the task with perfect accuracy, the requirements of manual labeling from experts hinder the scalability of the process. It is thus imperative to develop advanced language and computer vision multimodal tools to help accelerate the aforementioned scientific discovery process.

However, automatically identifying the experiment methods poses significant challenges for multimodal processing tools. One major challenge is how to ground the visual concepts to language. Most current visual-linguistics multimodal models (Li et al. 2019; Lu et al. 2019; Su et al. 2020; Chen et al. 2020) rely on a robust object detection module to identify predefined objects for grounding finer granularity of visual and linguistics concepts. However, as it requires extra efforts from experts, scientific images often lack ground truth object annotations, and the transfer of pretrained detection models suffers from significant domain shifts. As a result, this specific domain would appreciate multimodal mod-
els particularly with less-supervised grounding paradigms. In addition, it is expensive to collect annotations from domain experts; the lack of sizable benchmark datasets hinders the development of multimodal models tailored to the biomedical domain.

To spur research in this area, we introduce MELINDA, a dataset for multimodal biomedical experiment method classification that is created through a fully automated distantly supervised process (Mintz et al. 2009). Specifically, we leverage an existing biomedical database, IntAct (Orchard et al. 2013), to get the experiment method labels, and then properly extract the actual contents from papers pointed by the records in IntAct to pair with the obtained labels. MELINDA features 2,833 figures paired with their corresponding captions. We further segment captions into sub-sections referring to different sub-figures in the images, resulting in a total of 5,371 data records along with the labels of the experiment methods used to generate the sub-figures.

We benchmark several state-of-the-art models on the proposed experiment method classification task, including unimodal vision and language models and multimodal ones. Experiments suggest that multimodality is helpful for achieving better performances. However, the performances are still far from expert human-level, which suggests several area of improvements, including less reliance on object detection for grounding linguistic representations with visual sources, as well as finer-grained multimodal groundings.

Our work sheds light on future research in: (1) more generally applicable multimodal models, and (2) better transfer learning techniques in low resource domains such as scientific articles (Gururangan et al. 2020). We summarize our main contributions as follows:

- A multimodal dataset mapping compound figures and associated captions from biomedical research articles to the labels of experiment methodologies, to help spur the research on multimodal understanding for scientific articles.
- We conducted extensive experiments to benchmark and analyze various unimodal and multimodal models against the proposed dataset, suggesting several future directions for multimodal models in scientific domain.

2 The MELINDA Dataset

We introduce a new multimodal dataset, MELINDA, for biomedical experiment method classification. Each data instance is a unique tuple consisting of a figure, an associated sub-caption for the targeted sub-figure(s), and an experiment method label coming from the IntAct database. IntAct stores manually annotated labels for experiment method types, paired with their corresponding sub-figure identifiers and ids to the original paper featuring the figure, and structures them into an ontology. Each major category has different levels of granularity. This work mainly focuses on two major categories of experiments for identifying molecular interactions: participant identification (Par) and interaction detection (Int) methods\(^\text{4}\) each has two levels of granularity, coarse and fine (choice of the granularity depends on downstream applications). Samples of data and their labels are as exemplified in Figure 2 (more are in the appendix).

Each record in IntAct consists of the aforementioned expert curated information to a specific article in the Open Access PubMed Central\(^\text{5}\)(OA-PMC). According to the IntAct guideline, figure captions are sufficiently descriptive for justifying the underlying methods of the figures, and hence are properly extracted instead of including the body of text in the articles. The details of the dataset collection procedures and its statistics are described in the following sections.

2.1 Data Collection Pipeline

Our dataset is collected through three main procedures, as illustrated in Figure 2: (1) Obtain the experiment method labels and sub-figure identifiers from IntAct. (2) Localize the

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\(^\text{3}\)https://www.ebi.ac.uk/intact/

\(^\text{4}\)Molecular interaction experiments require two types of assay: participant detection methods identify the molecules involved in the interaction and the interaction detection methods identify the types of interactions occurring between the two molecules.

\(^\text{5}\)A publicly available subset of the PubMed collections: https://www.ncbi.nlm.nih.gov/pmc/tools/openftlist/
Figure 3: **Data collection pipeline**: Our collection pipeline is *distantly supervised* and fully automatable. It consists of three main steps: (1) Retrieve the PDF article in the OA-PMC set using the PubMed id from the IntAct database. (2) Extract the caption blocks using an in-house PDF interpreter, and localize the nearby corresponding figures. (3) Segment the caption blocks into sub-captions. Combining all three steps with the paired labels gives a single data record in our MELINDA dataset.

indicated figures and their captions in the pointed PDF articles. (3) Segment the captions into sub-captions so each can target a sub-figure of the figures obtained in step (2). As the overall procedure adopts a fully automated *distant supervision* approach, our dataset could be seamlessly expanded as additional articles being added to the OA-PMC set.

**Ground Truth IntAct Label Extraction.** By properly parsing and mapping the *PSI-MI2* 6 formatted IntAct records, each individually extracted instance can form a unique tuple of *(experiment-method-labels, sub-figure-id)*, where the *sub-figure-id* is a concatenation of the PubMed id of an article and the sub-figure identifier.

**Text and Image Extraction.** The OA-PMC paper ids are then used to search and download the indicated PDF articles. The textual and image contents are extracted using an in-house PDF interpreter, which leverages spatial indexing over each page to support content extractions. We extract contiguous word blocks across the articles, and the figure captions are localized by detecting the keywords ‘Fig’ or ‘Figure’. The corresponding figures are cropped out by searching for large rectangular regions with low text densities nearby the captions. Note that although the classification task concerns sub-figures, **we do not further segment a figure into sub-figures** as we expect the models to work with the capability of attending to the right sub-figures given the captions. Moreover, there are captions cross-referencing multiple sub-figures, and thus full figures should be preserved.

**Sub-Caption Segmentation.** Captions for compound figures are first tokenized into sentences followed by a text cleansing preprocessing, and then grouped into proper corresponding sub-captions through the following steps: (1) Descriptions before the first sentence containing sub-figure identifiers, e.g. ”(A)”, ”(A-C)”, are extracted as the *opening common* text. (2) The sentence containing a detected sub-figure identifier and all of its subsequent ones until the next sentence containing different identifier(s) is found, are extracted as the *main* sub-caption for that particular identifier. (3) Descriptions after the last sentence containing identifiers, are regarded as the *closing common* text, as researchers may put some summary texts at the end. Hence, a proper sub-caption is a concatenation of all of the above, which ensures no relevant contents of a sub-caption is overlooked. More details of our data collection pipeline can be found in the appendix and our released code repository.

### 2.2 Data Quality Assessment

Since our dataset is created by distant supervision from IntAct, for which if we perfectly pair the labels with corresponding figures and subcaptions, the *expert* human performances should remain ~100%. Therefore, the quality of the data instances rely on the quality of content extraction and pairing. In order to estimate the quality of the extracted contents, we randomly sample 100 instances for a manual inspection. With the corresponding original papers provided, we ask three non-domain-expert annotators to assess the quality mainly in terms of how good the image cropping is and how accurate the caption extractions are (the results were computed via majority vote). The inter-annotator agreement Fleiss’ Kappa for the following results are 0.804 for images and 0.676 for captions assessments.

Table [a] shows the inspection results of the extracted (and cropped) images on if they are missing any important regions, or containing any noises. Among the sampled images, 92% (*i.e.* 34+58) of the images are showing reasonably good quality, with 8% of them missing some details due to the cropping. The quality of the extracted (and segmented) sub-captions, as well as whether they match the associated sub-figure images, is summarized in Table [b]. Over 96% of

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6An XML format: http://psidev.info/mif

7The data collection pipeline and our benchmark models can be found at [https://github.com/PlusLabNLP/melinda](https://github.com/PlusLabNLP/melinda)
the sampled data can be regarded as good, while 4% of them have issues such as partial texts missing. It is worth noting that even in this proportion of data which misses some details, the majority parts of the captions (and the figures) are still properly preserved.

### 2.3 Dataset Details

#### General Statistics

There are in total 5,371 data instances in our dataset, generated from 1,497 OA-PMC articles, with 2,833 uniquely extracted images, as summarized in Table 2. The total unique label counts of each level in the original IntAct database and our collected dataset is summarized in Table 3. The charts can be examined jointly with Table 2 for better understandings.

#### Data Splits

We split the whole dataset into three subsets: train, validation, and test sets, with a ratio of 80% – 10% – 10%. In order to prevent models from exploiting certain patterns in the same research article to make predictions during the test time, we assure that no data records extracted from the same paper is split into different subsets, i.e., denote $id$ as the paper id from OA-PMC, $\{id | id \in \text{set}_1\} \cap \{id | id \in \text{set}_j\} = \emptyset, i, j \in \{\text{train}, \text{val}, \text{test}\}, i \neq j$. Additionally, we ensure that the labels are distributed evenly in the three sets according to the coarse participant method, as illustrated in Figure 6.

#### Benchmark Models

We benchmark several state-of-the-art vision, language and multimodal models against our dataset, that differ primarily by the modalities they encode. Specifically, we consider unimodal models which take either an image (image-only) or a caption (caption-only) as input, and multimodal models that take both. All the output layers for classification are multi-layer perceptrons (MLPs) followed by a softmax layer.
3.1 Unimodal Models

- **Image-Only**: We adopt a variant of convolutional neural networks, ResNet-101 (He et al., 2016), and initialize the networks with two sets of pretrained weights: (1) ImageNet classification task (Deng et al., 2009), and (2) backbone of Mask R-CNN on object detection task (He et al., 2017). We finetune the final three ResNet blocks (from a total of five), given the consistency of early level features across visual domains (more details in the appendix).

- **Caption-Only**: We mainly consider the two de-facto variants of language models: LSTM-based (Hochreiter and Schmidhuber, 1997), and transformer-based (Vaswani et al., 2017) models. Our LSTM models take input word embeddings from Bio-GloVe (300-d) (Burns, Li, and Schmidhuber, 2017). For transformer-based models, we consider two state-of-the-art pretrained masked language models (MLM): BERT (Devlin et al., 2019) trained on scientific corpora, dubbed SciBERT (Beltagy, Lo, and Cohan, 2019), and RoBERTa (Liu et al., 2019b).

We experiment caption-only models with and without the masked language finetuning on the caption sentences of our dataset, by constructing a corpus where each sentence is a caption from the train and validation sets. We use RoBERTa-large and uncased version of SciBERT to initialize the language models’ weights.

3.2 Multimodal Models

- **Naive Late Fusion (NLF)**: The images and captions are encoded by its best performing unimodal models – ResNet (ImageNet weights) and SciBERT respectively, which are then concatenated (late fusion) and fed into MLPs.

- **Stacked Attention Network (SAN)** (Yang et al., 2016): is a multi-step co-attention based framework that has demonstrated good performances on Visual Question Answering (VQA) benchmark (Antol et al., 2015). The image and caption encoders are same as in NLF.

- **ViL-BERT**: Vision-and-Language BERT (Lu et al., 2019), an extension of BERT model which learns a joint visual-and-linguistics representation through coattentional transformer layers on top of unimodal visual and textual streams. The model has two major proxy pretraining objectives: (1) textual and visual masked learning, where the visual stream requires the model to predict missing masked-out regions of input images (visual-MLM), and (2) image-text alignment prediction, which extends BERT’s next sentence prediction (NSP).

- **VL-BERT**: As the concurrent work to ViL-BERT, the visual-linguistics BERT model (Su et al., 2020) (VL-BERT) performs the multimodal co-attention in an early fusion manner with a single stream of transformer models. VL-BERT also adopts textual and visual masked learning pretraining objectives, while excluding the image-text multimodal alignment prediction.

The two multimodal BERT models are initialized with the SciBERT pretrained weights directly to their textual parts. For both ViL-BERT and VL-BERT, the visual-MLM leverages region of interests (ROIs) proposed by the object detection module, as well as the predicted class labels with high confidences. Due to significant domain shifts between the pretrained object detectors and our dataset, we experiment inclusion and exclusion of various of their proposed pretraining objectives (mainly concerning the visual masked prediction) when finetuning on our dataset.

3.3 Training Details.

The hyper-parameters for each model are manually tuned against our dataset, and the trained model checkpoints used to evaluate are selected by the best performing ones on the validation set. All models are trained independently for each method type. More details of the hyper-parameters and experimental setups can be found in the appendix.
4 Experiments and Analysis

Our experiments aim to: (1) Benchmark the performances of the baseline models described in the previous section, and (2) compare and analyze how and what these models learn.

**Quantitative Results.** Table 4 summarizes the model performances on the test set, including the majority baseline that selects the most frequent classes in different label types. All the models, after training on the train set, outperform the majority baseline by large margins, which indicates the sizable training set is effective in transferring knowledge learned from these pretrained models. The image-only models, despite not having indicators of which sub-figure to look at, still surpass the majority baseline, which we hypothesize that the models still learn the salience in the images to make the correct predictions. Both transformer-based caption-only models benefit from the masked language finetuning on the captions. Figure 7 shows a sampled side-by-side comparisons between unimodal models (left) and multimodal models (right) of label type $Int_{fine}$. It can be seen that the salience on the images clearly transition from being more dispersed to more detailed and finer-grained from unimodal to multimodal models. Likewise, multimodal models attend less on the common words such as from, and, of, and weight more on domain specific words. The image-only models, without the disambiguation from the captions, tend to focus more on spurious patterns as hinted in the first and second row. While the multimodal models exhibit diverged attentions in the images, it captures the keyword fluorescence that the unimodal language model fails to grasp. The third row of Figure 7 shows a failure case of multimodal models, where both unimodal models focused closer to the common objects seen in their original training datasets. Such hypothesis is also shown in the performance comparisons within the visual-linguistics multimodal models, where they tend to perform better without the visual-MLM objective. However, within VI-L-BERT, the multimodal alignment objective shown to be beneficial in most label types. In general, there are still huge gaps between model accuracies and expert human performances (>100% accuracy), especially for the fine-grained types.

**Visualizing What Models Learn.** We utilize Grad-CAM [Selvaraju et al. 2017] for visualizing the model salience on the images and SmoothGrad [Smilkov et al. 2017] on the captions. Figure 7 shows a sampled side-by-side comparisons between unimodal models (left) and multimodal models (right) of label type $Int_{fine}$. It can be seen that the salience on the images clearly transition from being more dispersed to more detailed and finer-grained from unimodal to multimodal models. Likewise, multimodal models attend less on the common words such as from, and, of, and weight more on domain specific words. The image-only models, without the disambiguation from the captions, tend to focus more on spurious patterns as hinted in the first and second row. While the multimodal models exhibit diverged attentions in the images, it captures the keyword fluorescence that the unimodal language model fails to grasp. The third row of Figure 7 shows a failure case of multimodal models, where both unimodal models focused closer to the ideal regions in their inputs (note the sub-figure identifier “(a)” in the caption), and hence make the correct predictions. We hypothesize that multimodal models may capture wrong information due to relatively stronger influences by the ROIs proposed by the inherited object detection module (refer to the overlaid yellow-colored ROIs).

| Modalities | Models | Variants | $Par_{coarse}$ | $Int_{coarse}$ | $Par_{fine}$ | $Int_{fine}$ |
|------------|--------|----------|----------------|----------------|--------------|--------------|
| —          | Majority Baseline | —        | 55.88          | 63.67          | 48.96        | 23.18        |
| Image-Only | ResNet-101 init. from ImageNet | —        | 63.84          | 70.24          | 50.87        | 28.50        |
| Caption-Only | LSTM w. BioGloVe | —        | 59.20          | 68.02          | 49.00        | 35.30        |
| | RoBERTa w/o MLM finetuning | —        | 74.60          | 86.00          | 60.00        | 64.70        |
| | w. MLM finetuning | —        | 75.40          | 88.60          | 63.00        | 67.10        |
| | SciBERT w/o MLM finetuning | —        | 76.60          | 87.60          | 62.10        | 65.70        |
| | w. MLM finetuning | —        | 77.70          | 87.00          | 64.90        | 67.10        |
| Multi-Modal | NLF w/o language part MLM finetuning | —        | 76.60          | 87.10          | 61.10        | 67.30        |
| | w. language part MLM finetuning | —        | 73.70          | 87.90          | 62.80        | 70.20        |
| | SAN w/o language part MLM finetuning | —        | 72.30          | 88.60          | 61.90        | 70.40        |
| | w. language part MLM finetuning | —        | 71.60          | 88.90          | 62.80        | 70.40        |
| | VI-L-BERT w/o MLM & NSP | —        | 78.20          | 90.64          | 66.26        | 72.15        |
| | w. MLM & NSP & visual-MLM | —        | 78.60          | 90.83          | 65.57        | 72.84        |
| | w. MLM & NSP | —        | 76.47          | 90.48          | 64.19        | 71.80        |
| | w. MLM & visual-MLM | —        | 77.90          | 89.76          | 65.82        | 74.02        |

Table 4: Model accuracies on the test set: the two label categories are denoted as $Par$, and $Int$ for participant and interaction method respectively. The label hierarchy is indicated as the subscript, e.g. $Par_{coarse}$ indicates coarse types of participant method. The best performances for each type of labels are bolded, and in all cases the two advanced multimodal models achieve the best performances. Particularly for the two multimodal models, the variants without the visual-MLM objectives perform the best.
5 Related Works

Multimodal Datasets. There are numerous datasets for multimodal machine learning in existence, including visual storytelling (Huang et al. 2016), visual-linguistics reasoning (Johnson et al. 2017; Hasan et al. 2019), Wang et al. 2019; Liu et al. 2020), and multimodal question answering (QA) (Antol et al. 2015; Tapaswi et al. 2016; Kembhavi et al. 2016; 2017; Lei et al. 2018; Yagioglu et al. 2018; Das et al. 2018; Zellers et al. 2019). As these works focus on more general domains, our work offers a dataset in the hope of motivating research in domains that often require expertise for labelling, such as biomedical.

Experiment Method Classification. The closest prior work (Burns, Li, and Peng 2019) has used the figure captions from OA-PMC set to perform similar experiment method classification task. In our MELINDA dataset, we put forth to extract the visual information in conjunctions with the caption texts, and collect a larger-scale dataset.

Automating Biocuration & Biomedical Tasks. Integrating computational approaches into the workflow of biocuration can be seen in many applications such as constructing genomics knowledge base (Baumgartner Jr et al. 2007), biomedical document classification (Cohen 2006; Shatkay, Chen, and Boststein 2007; Jiang et al. 2017; Simon et al. 2019), biomedical text mining (Dowell et al. 2009), and human-in-the-loop curation (Lee et al. 2018). Some prior works also adopt multimodal machine learning for general biomedical information extractions (Schlegl et al. 2015; Eickhoff et al. 2017; Zhang et al. 2017), as well as textual extraction (Burns, Dasigi, and Hovy 2017), medical image captioning (Shin et al. 2016), and automated diagnosis from medical images (Jing, Xie, and Xing 2018; Wang et al. 2018; Liu et al. 2019a).

Our work aims to further facilitate research in automating biocuration by providing a sizeable multimodal dataset, along with the data collection tool. We benchmark various unimodal and multimodal models with analysis on their strengths that suggest potential improvements.

6 Conclusions and Future Work

In this work, we introduce a new multimodal dataset, MELINDA, for biomedical experiment method classification. Our dataset comprises extracted image-caption pairs with the associated experiment method labels. As our data is collected in a fully automated distant supervision manner, the dataset is easily expandable.

We benchmark the proposed dataset against various baseline models, including state-of-the-art vision models, language models, and multimodal (visual-linguistics) models. The results show that despite multimodal models generally demonstrate superior performances, there are still huge rooms for improvements in the current visual-linguistics grounding paradigms, especially for domain specific data. Hence, we hope this work could motivate the future advancements in multimodal models, primarily on: 1) low resource domains and better transfer learning, 2) a less-supervised multimodal grounding method with less reliance on robust pretrained object detectors.
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A More on The MELINDA Dataset

A.1 All Label Types

The descriptions of the experiment method labels featured in our MELINDA dataset, across all levels of the two categories, can be referred to from the original IntAct database specifically for participant identification method types, and interaction detection method types. In our full release of the MELINDA dataset, we also include a .tsv file for the hierarchical mappings among the coarse and fine label types.

A.2 Details of Sub-Caption Segmentation

Segmentation In general, we try to segment the sub-captions as systematically as possible. There are compound sub-figure identifiers that can refer to multiple sub-figures at once, e.g. "(A,C)" or e.g. "(A-D)" will represent sub-figures "A" and "C", and sub-figures "A" to "D", respectively. In these cases, we will assign the sentences to each of these detected (or inferred, in the "(A-D)" case) sub-figure identifiers. The opening common is usually well-preserved, while the closing common may inevitably contain some information dedicated to the last mentioned identifier. In order to eliminate the risk of potential information loss caused by excluding the closing common texts, we compromise to this heuristic to include the last few sentences.

Preprocessing We also conduct preprocessing and text cleansing during the sub-caption segmentation. The extracted word blocks sometimes contain dashed words where the dash is inserted among a single word due to the line change in PDF articles. We replace these dashes by checking if the word with the dash removed exists in a common English dictionary. For those words that do not exist, we simply preserve the dash within the words. We also run spell checkers to ensure spellings for common English words are correct as much as possible.

A.3 More Exemplar Data Points

We provide more random sampled exemplar data for a more diverse visual preview of our dataset in Figure 8.

Expert Justifications of Requirements of Multimodality: As discussed in the third paragraph of the introduction in Section 1, different experiment methods can generate visually similar figures, while captions can disambiguate them. Oppositely, captions alone do not necessarily determine the visual presentation to be of specific types. Specifically, for the IntAct database used as distant supervision to construct our dataset, in the IntAct curation annotation manual page 5, the storage schema implies at the experiment level curators are required to look at the paper figures. And in page 9, the example term "From Fig 7..." indicates that curators are expected to interpret both the figures and captions for labelling. There are similar examples throughout the manual, which are verified by an expert in the biomedical field.

Sample Human Estimations: There are various cues that a human expert would likely to focus on when determining the experiment method labels. For example, for the label identification-by-antibody, the presence of specific bands in a blot diagram corresponding to the precise molecular weight of the named antibody in the captions, would be the

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1 https://www.ebi.ac.uk/ols/ontologies/mi
2 https://www.ebi.ac.uk/ols/ontologies/mi/terms?iri=http%3A%2F%2Fpurl.obolibrary.org%2Ffbo%2F00001&viewMode=All&siblings=false
3 https://www.ebi.ac.uk/ols/ontologies/mi/terms?iri=http%3A%2F%2Fpurl.obolibrary.org%2Ffbo%2F00002&viewMode=All&siblings=false
4 https://www.ebi.ac.uk/intact/site/doc/IntActCurationManual2016.pdf?conversationContext=1
Table 5: **Label Distributions**: of the raw IntAct records.

| Label                        | Count (%) |
|------------------------------|-----------|
| predetermined-participant    | 58.96     |
| identification-by-antibody   | 33.63     |
| nucleotide-sequence-identification | 4.56   |
| Identification-by-mass-spectrometry | 1.02    |
| unassigned                   | 0.61      |
| tag-visualisation             | 0.94      |
| protein-sequence-identification | 0.28    |

A.4 Label Distributions

As hinted by Figure 8, the label distribution in the original IntAct records is imbalanced, which very likely resemble the real world distribution of the experimental protocols being conducted. This could pose challenges and inspire interesting future directions in machine learning models on tackling these domain specific areas. Our non-processed raw data has the label distribution on the **PartCoarse** label type shown in Table 5 (The shown numbers are of label-count percentages). We would also like to point out that the finer-grained classes, such as **Int(Fine)** have a more even distribution. Since there are in total 85 classes for **Int(Fine)**, we hereby show the mean and the standard deviations of the label-count percentages, which are: mean/std = 1.18/3.50 as compared to 14.29/21.18 of 7 classes in **Part(Coarse)**. On the other hand, we also show in Table 5 the performances of the majority baselines (always predicting the majority class) are significantly worse than the best performing models, which implies proper training could potentially still yield good performances on the current data distributions. We do hope to expand our dataset to an even larger-scaled and possibly more balanced one when more publicly available articles are added to the OA-PMC set, particularly for the labels that are on the lower amount spectrum.

**B More Details on Experiments**

### B.1 Model & Training Details

All the benchmarked models are trained on a single Nvidia GeForce 2080Ti GPU[12] on a CentOS 7 operating system. The hyper-parameters for each model are manually tuned against our dataset, and the trained model checkpoints used to evaluate are selected by the best performing ones on the validation set. All the models are individually trained for each type of the labels.

The implementations of the transformer-based caption-only models are extended from the huggingface[13] code base, which are implemented in PyTorch[15]. The image-only models and their pretrained weights are borrowed from torchvision[14] and the official Mask-RCNN implementations from Facebook AI Research[16]. Note that we are just using the pretrained weights to initialize only the CNN part, i.e. we are not using the ROI pooled features, so in our image-only models, no region proposal network (RPN) is used. Implementations for both VL-BERT and ViL-BERT are adapted from the original author-released code repositories, which can be found in their papers.

**Visual-MLM** For the masked image ROI region classification or masked visual token modeling in VL-BERT and ViL-BERT, dubbed as visual-MLM in this paper, we use the authors’ original public repositories for obtaining the region labels in the proposed ROIs in the images. Since the two repositories both generally adopt detectron2 module from Facebook AI Research, the label space comes from the Visual Genome (Krishna et al. 2017) object categories, which has 1,600 total number of class labels, plus one indicating the background class.

**Hyper-parameters** For image-only models and caption-only models, it takes roughly 2-4 hours to train for the number of epochs specified in Table 6. For NLF and SAN models, it takes approximately 4 hours to train. For the two visual-linguistics models, it takes roughly 6-8 hours to train including the finetuning on experiment classification phases. Since some of the baseline models incorporate finetuning on our MELINDA corpus, we also list the hyperparameters such phase of training uses in Table 7. We also include the search bounds and number of trials in Table 8 all of our models adopt the same search bounds and the same ranges of trials.

For long captions in the dataset, we generally truncate it with maximum number of tokens (BPE or wordpiece tokens) = 128.

**Vision Models** As mentioned in Section 3 the benchmark models section, we only fine-tune the later layers in ResNet-101, due to the observations that the features in early CNN layers are generally shared across different visual domains (Yosinski et al. 2014). We also empirically verify that finetuning all the layers does not yield significant improvements.

**Validation Results** We also include the model performances on the validation set, where we select each of the best performing models to evaluate on the unseen test set. The comprehensive results can be found in Table 9.

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12[https://www.nvidia.com/en-us/geforce/graphics-cards/rtx-2080-ti/](https://www.nvidia.com/en-us/geforce/graphics-cards/rtx-2080-ti/)

13[https://github.com/huggingface/transformers](https://github.com/huggingface/transformers)

14[https://pytorch.org/](https://pytorch.org/)

15[https://github.com/pytorch/vision](https://github.com/pytorch/vision)

16[https://github.com/facebookresearch/detectron2](https://github.com/facebookresearch/detectron2)
Table 6: **Hyper-parameters used for each of our baseline models during finetuning phase on our MELINDA dataset:** For each label type (coarse and fine participant and interaction), we use the same set of hyperparameters. Initial LR denotes initial learning rate. All the models are trained with Adam optimizers. We include number of parameters of each model in the last column, denoted as # params.

| Modalities          | Models                        | Batch Size | Initial LR    | # Training Epochs | Gradient Accumulation Steps | # Params |
|---------------------|-------------------------------|------------|---------------|-------------------|-----------------------------|----------|
| Image-Only          | ResNet101 init. from ImageNet | 16         | $1 \times 10^{-5}$ | 20                | -                           | 44.5M    |
|                     | ResNet101 init. from MSCoCo   | 16         | $1 \times 10^{-5}$ | 20                | -                           | 44.5M    |
| Caption-Only        | LSTM w. BioGlove              | 4          | $2 \times 10^{-6}$ | 4                 | 1                           | 5.4M     |
|                     | RoBERTa-Large                 | 4          | $2 \times 10^{-6}$ | 4                 | 2                           | 355.4M   |
|                     | SciBERT-Base-Uncased          | 4          | $2 \times 10^{-6}$ | 4                 | 2                           | 109.9M   |
| Multi-Modal         | Naive Late Fusion (NLF)       | 4          | $2 \times 10^{-6}$ | 4                 | 2                           | 126.5M   |
|                     | Stacked Attention Network (SAN)| 4         | $2 \times 10^{-6}$ | 4                 | 2                           | 130.8M   |
|                     | VIL-BERT (w. MLM)             | 8          | $1 \times 10^{-5}$ | 20                | 1                           | 171.2M   |
|                     | VIL-BERT (w. MLM & NSP)       | 8          | $1 \times 10^{-5}$ | 20                | 1                           | 171.2M   |
|                     | VIL-BERT (w. MLM & NSP & visual-MLM) | 8       | $1 \times 10^{-5}$ | 20                | 1                           | 171.2M   |
|                     | VL-BERT (w. MLM)              | 4          | $7 \times 10^{-5}$ | 20                | 4                           | 155.6M   |
|                     | VL-BERT (w. MLM & visual-MLM) | 2          | $7 \times 10^{-5}$ | 20                | 4                           | 155.6M   |

Table 7: **Hyper-parameters used for language models with MELINDA corpus finetuning phase:** the hyperparameters for caption-only models are also adopted for the two non-transformer based multimodal models for their language part encoders. All the models are trained with Adam optimizers.

| Modalities          | Models                        | Batch Size | Initial LR    | # Training Epochs | Gradient Accumulation Steps |
|---------------------|-------------------------------|------------|---------------|-------------------|-----------------------------|
| Caption-Only        | RoBERTa-Large                 | 4          | $1 \times 10^{-5}$ | 50                | 1                           |
|                     | SciBERT-Base-Uncased          | 4          | $1 \times 10^{-5}$ | 50                | 1                           |
| Multi-Modal         | VIL-BERT (w. MLM)             | 8          | $5 \times 10^{-5}$ | 20                | 1                           |
|                     | VIL-BERT (w. MLM & NSP)       | 8          | $5 \times 10^{-5}$ | 20                | 1                           |
|                     | VIL-BERT (w. MLM & NSP & visual-MLM) | 8       | $5 \times 10^{-5}$ | 20                | 1                           |
|                     | VL-BERT (w. MLM)              | 4          | $7 \times 10^{-5}$ | 20                | 4                           |
|                     | VL-BERT (w. MLM & visual-MLM) | 2          | $7 \times 10^{-5}$ | 20                | 4                           |

B.2 More Attention Visualizations

As an extension to Figure [7] in the main paper, we provide additional visualization examples for a more in-depth look into what models have learned in Figure [9]. Similar trends are observed in both Figure [9] and Figure [7] and we also provide the proposed ROIs from the object detection module in the third row where the multimodal model fails in the coarse interaction label type.

Additionally, in order to further quantify how models attend differently with different modalities of inputs, we examine 20 randomly sampled data instances from the test set. We find that among which there were 13 times (65%) that the multimodal models attended on the correct sub-figures, while image-only models only had 9 times (45%). The difference between them is roughly the same as those results shown in Table 4 for the coarse-grained label types.

B.3 Top-30 attended tokens

For a more in-depth understanding of what models learn from different modalities, we are interested in an overview of distributional shifts of attended words across unimodal language models and the language streams in the multimodal models. For each caption in the test set, we obtain the top-20 attended tokens by applying SmoothGrad [Smilkov et al., 2017], and then aggregate the results of every captions in the test set as an overall top-attended-token-count histogram. The results for the two types of coarse-grained labels are visualized in Figure [10]. One can see that multimodal models (blue regions) tend to focus on more label-type-specific words, such as interaction in Figure [10].

Denote the frequency of a token $t_i$ in a dataset as $f_{t_i, set}$, the average relative changes of the top-$N$ attended tokens transitioning from participant to interaction label types is computed by: $rac{1}{N} \sum_{i=1}^{N} |f_{t_i, participant} - f_{t_i, interaction}|/f_{t_i, participant}$. Following this computation, the general trend of unimodal (language) models do not change much (the two red regions) by a 21.8% of relative changes, while it is shown that multimodal models are more susceptible to the salient decisive tokens that they exhibit relative changes by a larger margin of 33.4%.

Similarly, we also visualize the top-30 attended tokens for the two finer grained labels, as shown in Figure [11]. We find that, similar to the coarse labels, unimodal language models share similar distributional trends across the participant and interaction types, while multimodal models are more susceptible to label types. The computed quantitative relative
| Type            | Batch Size | Initial LR       | # Training Epochs | Gradient Accumulation Steps |
|-----------------|------------|------------------|-------------------|----------------------------|
| Bound (lower–upper) | 2–16       | $1 \times 10^{-4}$–$1 \times 10^{-6}$ | 3–50             | 1–4                        |
| Number of Trials | 2–4        | 2–3              | 2–4              | 1–2                        |

Table 8: **Search bounds**: for the hyperparameters of all the benchmarked models.

| Modalities | Models | Variants | Par\textsubscript{coarse} | Int\textsubscript{coarse} | Par\textsubscript{fine} | Int\textsubscript{fine} |
|------------|--------|----------|---------------------------|---------------------------|-----------------------|------------------------|
| —          | Majority Baseline | —       | 62.36                     | 63.02                     | 57.68                 | 22.04                  |
| Image-Only | ResNet-101   | init. from ImageNet | 68.52                     | 70.98                     | 58.56                 | 24.07                  |
|            |           | init. from MSCoCo | 64.73                     | 69.42                     | 56.02                 | 26.15                  |
| LSTMcaption-Only | LSTM w. BioGloVe | —       | 64.37                     | 66.82                     | 58.35                 | 33.41                  |
| Caption-Only | RoBERTa     | w/o MLM finetuning | 78.20                     | 81.50                     | 65.70                 | 60.36                  |
|            |           | w. MLM finetuning | 77.73                     | 83.74                     | 67.04                 | 61.47                  |
| SciBERT    | w/o MLM finetuning | 77.30     | 86.40                     | 62.10                     | 65.70                 |                        |
|            |           | w. MLM finetuning | 74.17                     | 86.19                     | 65.70                 | 58.13                  |
| Multi-Modal | NLF         | w/o language part MLM finetuning | 75.95                     | 86.90                     | 67.04                 | 58.80                  |
|            |           | w. language part MLM finetuning | 75.49                     | 87.08                     | 65.92                 | 61.02                  |
| SAN         | w/o language part MLM finetuning | 77.70     | 86.90                     | 67.48                     | 59.69                 |                        |
|            |           | w. language part MLM finetuning | 74.60                     | 87.50                     | 65.92                 | 59.47                  |
| ViL-BERT    | w. MLM     | —       | 72.83                     | 85.97                     | 65.92                 | 63.25                  |
|            | w. MLM & NSP | 75.28     | 86.86                     | 62.36                     | 63.03                 |                        |
|            | w. MLM & NSP & visual-MLM | 73.05     | 87.31                     | 61.69                     | 63.03                 |                        |
| VL-BERT     | w. MLM     | —       | 76.05                     | 87.52                     | 66.91                 | 67.48                  |
|            | w. MLM & visual-MLM | 75.49     | 87.19                     | 65.52                     | 66.86                 |                        |

Table 9: **Model accuracies on the validation set**: the two label categories are denoted as Par, and Int for participant and interaction method respectively. The label hierarchy is indicated as the subscript, e.g. Par\textsubscript{coarse} indicates coarse types of participant method. The best performances for each type of label are bolded. In most cases, multimodal models outperform the unimodal models except for the coarse participant type.

Changes between the two finer-grained sets, are 30.2% and 28.1% for the multimodal models and unimodal models respectively. For the fine-grained sets, the two relative changes are not differ by a large margin, which we hypothesize that the fine-grained sets are substantially harder for both multimodal and unimodal models to perform well.

### C Releases

The full dataset along with its documentation will be released in a timely manner. We will release the cleaned code repository which encompasses the majority of the codes used to generate the experimental results in this paper. The repository will also include codes for the VL-BERT model, adapted from the original publicly available repository, for exemplifying how we adapt the existing models to our dataset and setups. We will also release our *distantly supervised* data collection tool (all components of the three main steps in our data collection pipeline), with well documented guidelines of usages. We hope by sharing these tools, more interest could be gained into developing better multimodal models especially for traditionally low resource areas such as biomedical domains.
Figure 9: Saliency Comparisons on Int\textsubscript{coarse} (highest-lowest attention → red-blue for images and dark red-light yellow for captions): In each row: (a) independent unimodal models – ResNet-101 & SciBERT; (b) multimodal model – VL-BERT. From top to bottom the correctness of predictions between (unimodal, multimodal) is: (✓, ✓), (✓, ×), and (✓, ✓) for coarse interaction (left half) type, and the predictions for both unimodal models and multimodal models are all correct for the coarse participant (right half) label type. For coarse interaction label type, similar observations can be seen in Figure\textsuperscript{7} that unimodal models tend to have more dispersed attended regions, while multimodal models have more focused and finer-grained salience maps. We again show top confident ROIs in the failure case for multimodal model in the third row. Some of the ROIs are nearby or co-located with the highest attended regions, which can hypothetically cause the mis-focus and results in incorrect predictions. For coarse participant label type, the label space is smaller, and hence it may be easier for unimodal models to capture certain patterns to make correct predictions.
Figure 10: **Top-30 attended tokens across whole test set on coarse label types** (blue regions of VL-BERT, and red regions of SciBERT): For each caption, we compute the top-20 attended tokens using SmoothGrad, and then combine the top-attended token counts from all the captions in the test set for an overall most attended (top-30) tokens, with lemmatization applied. The token counts are normalized w.r.t the maximum values across the two models.

Figure 11: **Top-30 attended tokens across whole test set on fine label types** (blue regions of VL-BERT, and red regions of SciBERT). Similar to Figure 10 but on the fine-grained label types.