

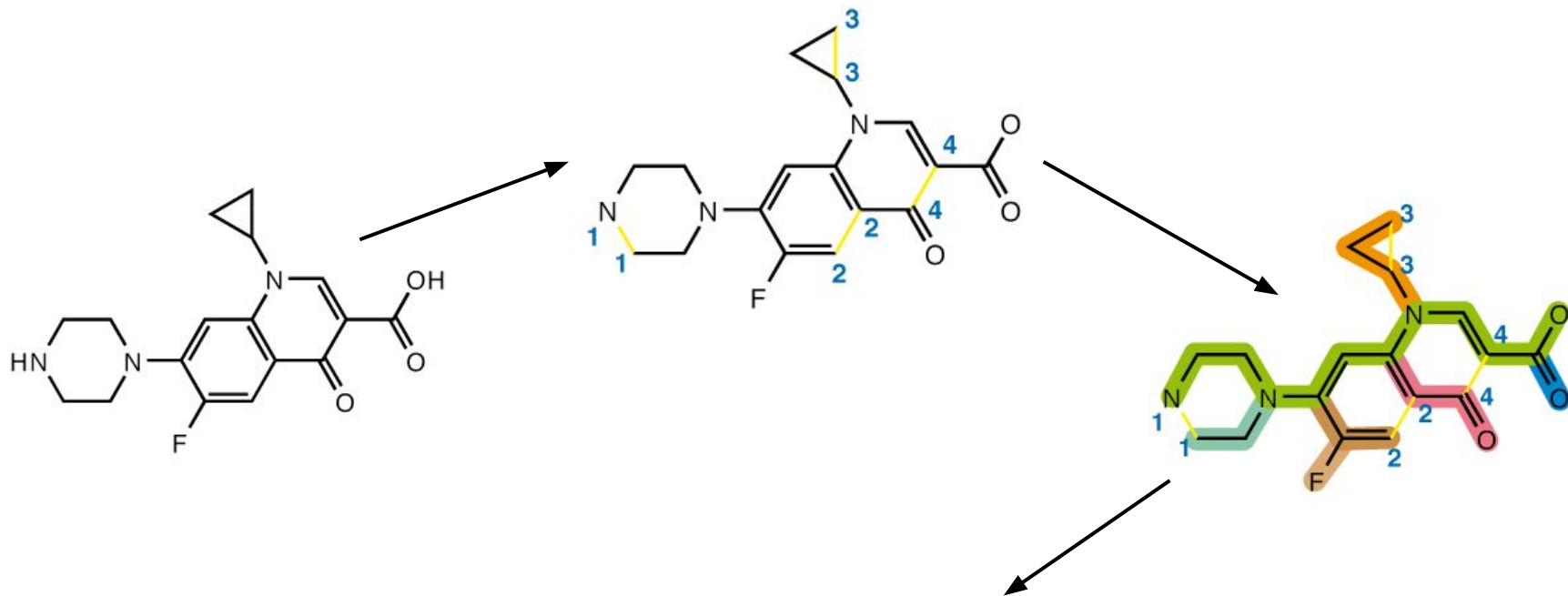
# Compound Scanner

Eugenij Ivankin

Vitaly Mahonin

Timolai Andreevich

Problem: a complex process to do by hand



```
N1CCN(CC1)C(C(F)=C2)=CC(=C2C4=O)N(C3CC3)C=C4C(=O)O
```

## Tech stack



TensorFlow

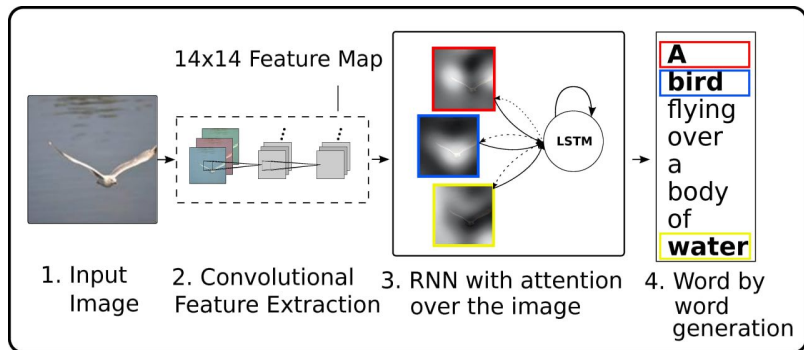


PyTorch

# Roadmap

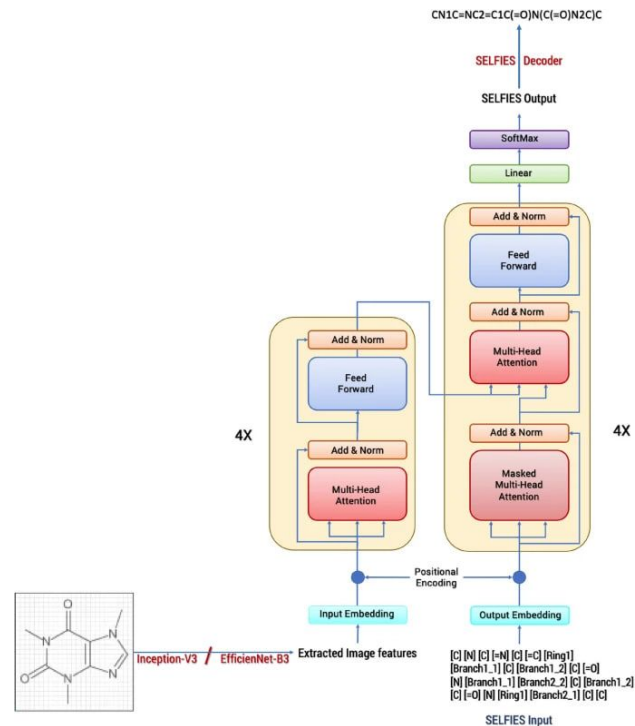
- + Predicting SMILES from the image
- + Draw formula from prediction for verification
- + Conversion to InChI
- + Conversion to IUPAC name (still using external api)
- Meaningful error messages
- Put model to the application to make it standalone
- Allow to modify the predicted compound

# Implementation: Comparing Neural Net Architectures



## CNN + LSTM with attention

Image source: <https://arxiv.org/pdf/1502.03044.pdf>



## CNN + Transformer with attention

Image source: <https://doi.org/10.1186/s13321-021-00538-8>



## App Release

[https://github.com/Senopiece/compound\\_scanner/releases/tag/v1.0.0](https://github.com/Senopiece/compound_scanner/releases/tag/v1.0.0)

# Acknowledgements

Thanks to our chemistry student friends & authors of DECIMER