Visualizing Deep Neural Networks

David Koes

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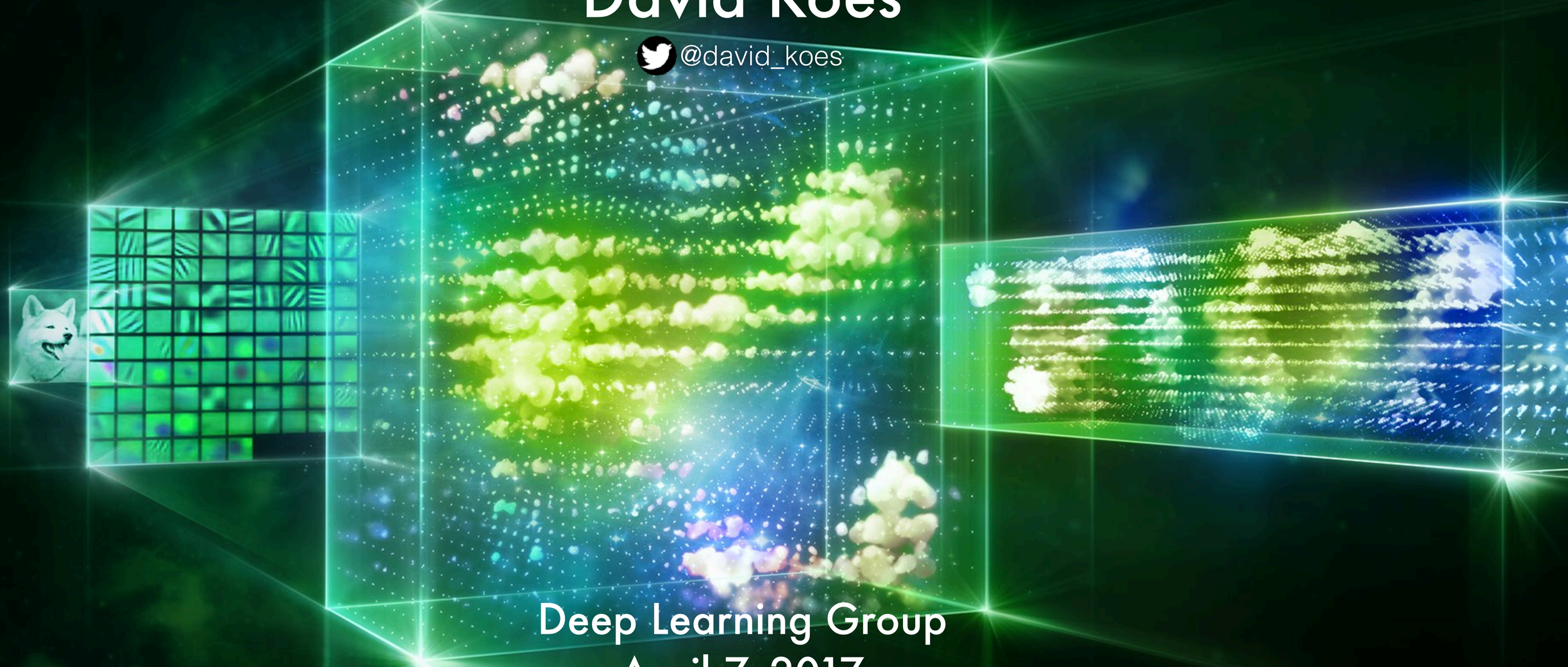

Deep Learning Group

April 7, 2017

Evaluating the visualization of what a Deep Neural Network has learned

Wojciech Samek† *Member, IEEE,* Alexander Binder†, Grégoire Montavon, Sebastian Bach, and Klaus-Robert Müller, *Member, IEEE,*

https://arxiv.org/pdf/1509.06321.pdf

Visualizing and Understanding Convolutional Networks

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https://arxiv.org/abs/1311.2901

On Pixel-Wise Explanations for Non-Linear Classifier Decisions by Layer-Wise Relevance Propagation

Sebastian Bach, Alexander Binder, Grégoire Montavon, Frederick Klauschen, Klaus-Robert Müller, Wojciech Samek

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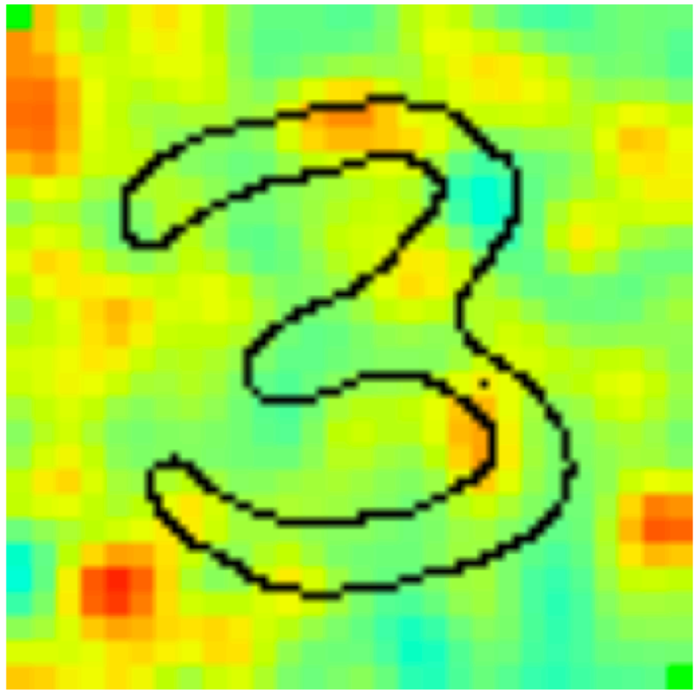
Heatmaps

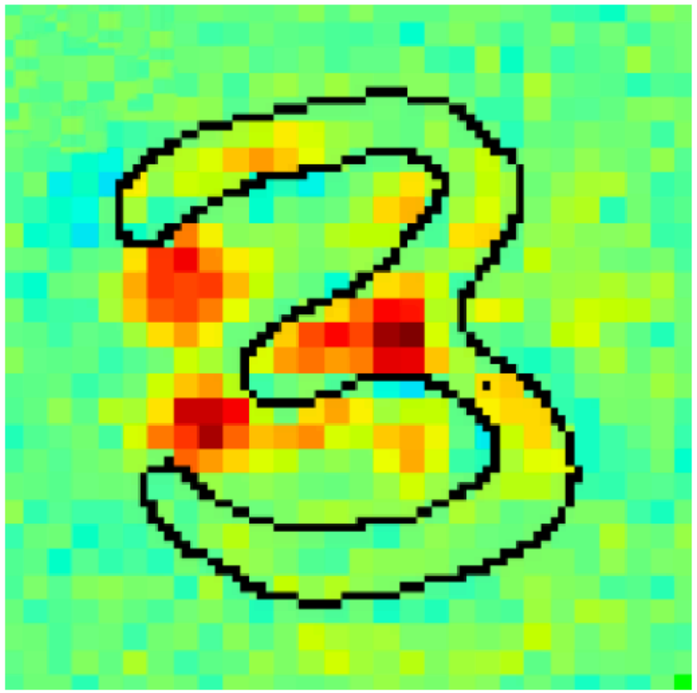
Map the neural network decision onto the input

Random

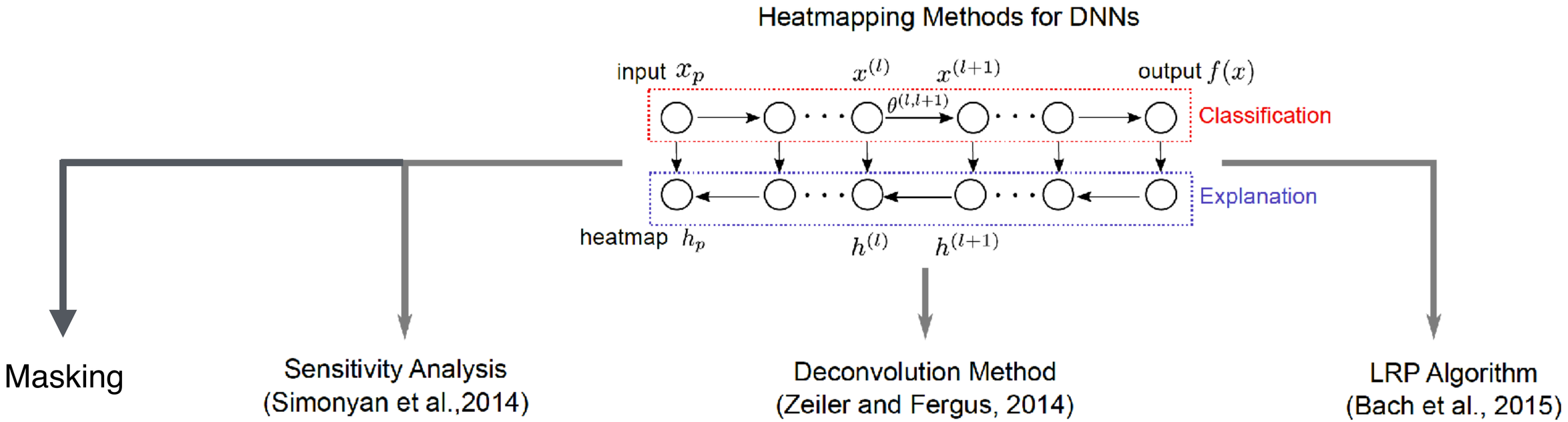


Segmentation

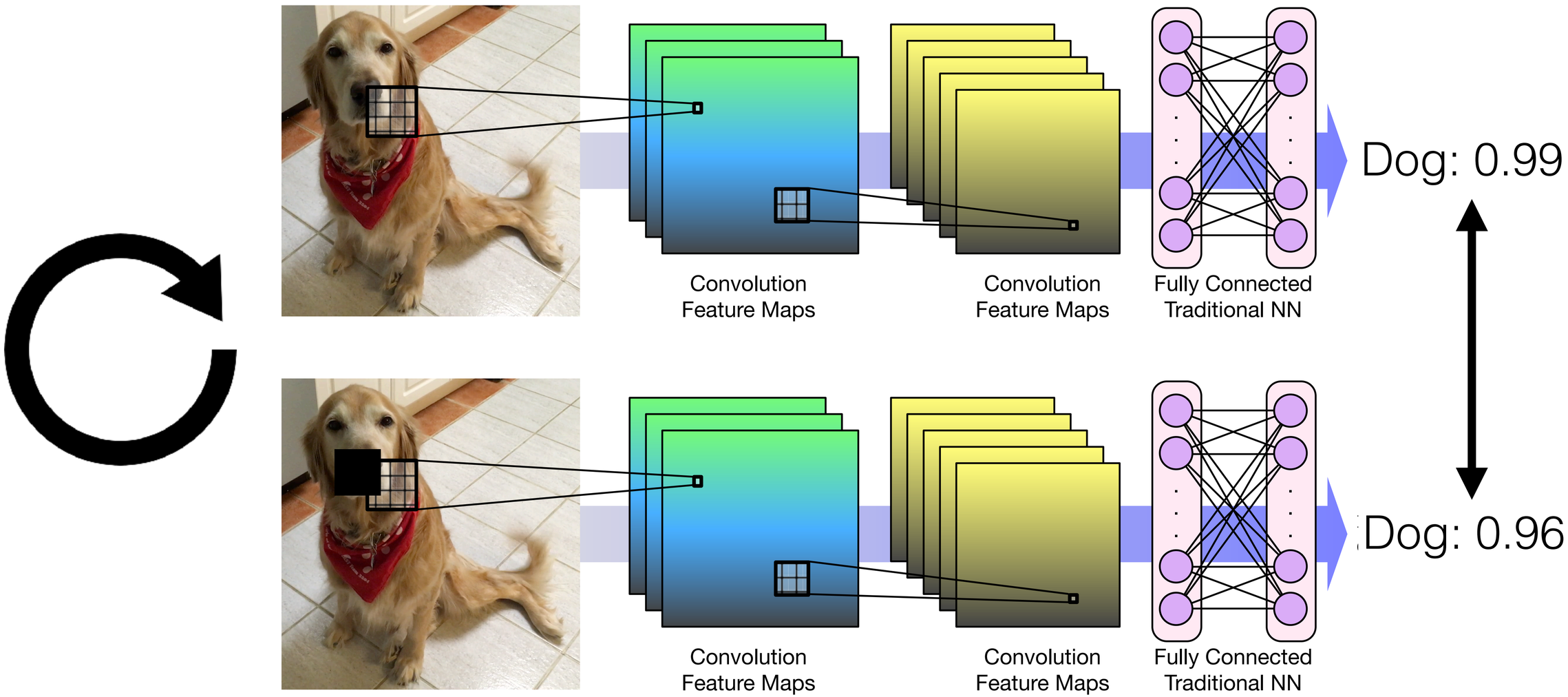
Relevance



Heatmapping DNNs



Masking


Convolution
Feature Maps
Convolution
Feature Maps
Fully Connected
Traditional NN
Dog: 0.99
Convolution
Feature Maps
Convolution
Feature Maps
Fully Connected
Traditional NN
Dog: 0.96

Sensitivity Analysis

Propagation

Chain rule for computing derivatives:

$$\nabla^{(l)} = \frac{\partial x^{(l+1)}}{\partial x^{(l)}} \nabla^{(l+1)}$$

Heatmap

local sensitivity (what makes a bird more/less a bird).

Relation to $f(x)$

$$h_p = \left|\left| \frac{\partial}{\partial x_p} f(x) \right|\right|_\infty$$

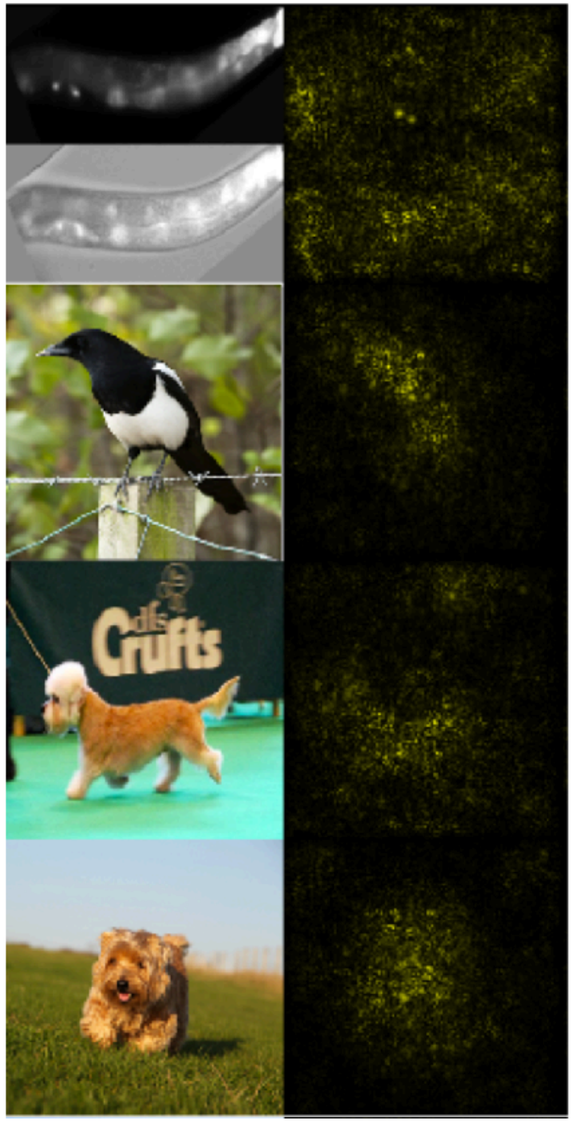
Applicable

any network with continuous locally differentiable neurons.

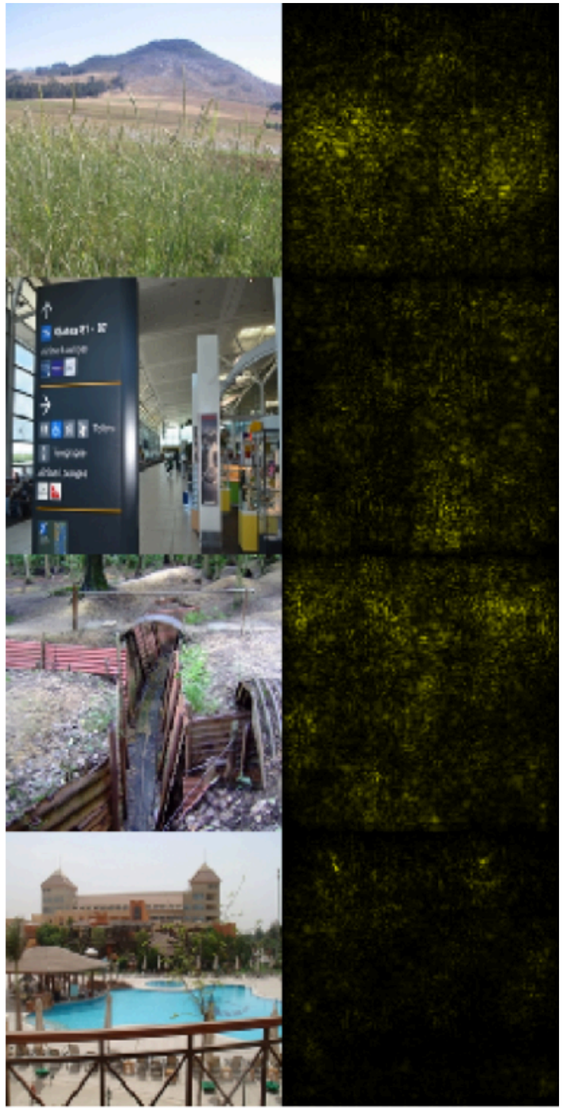
Drawbacks

(i) heatmap does not *fully* explain the image classification.

ILSVRC2012

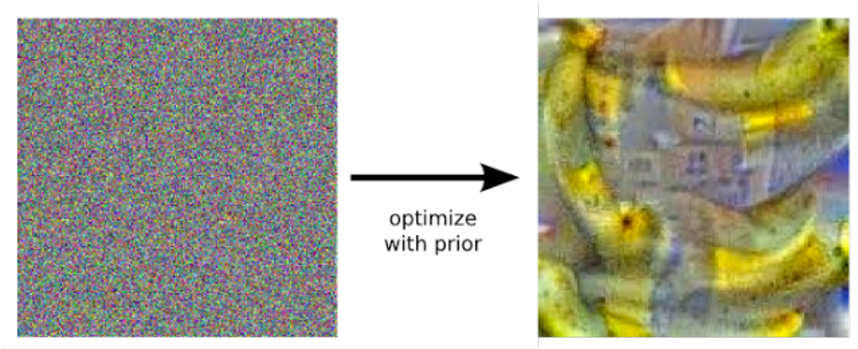


MIT Places



Sensitivity Analysis - Deep Dreams

https://research.googleblog.com/2015/06/inceptionism-going-deeper-into-neural.html



Sensitivity Analysis - Deep Dreams

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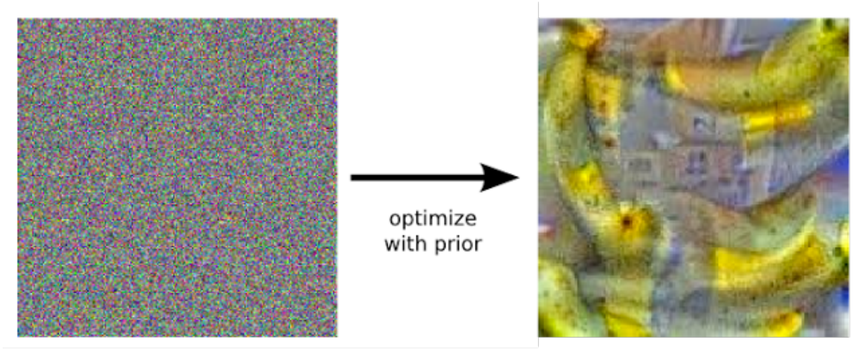
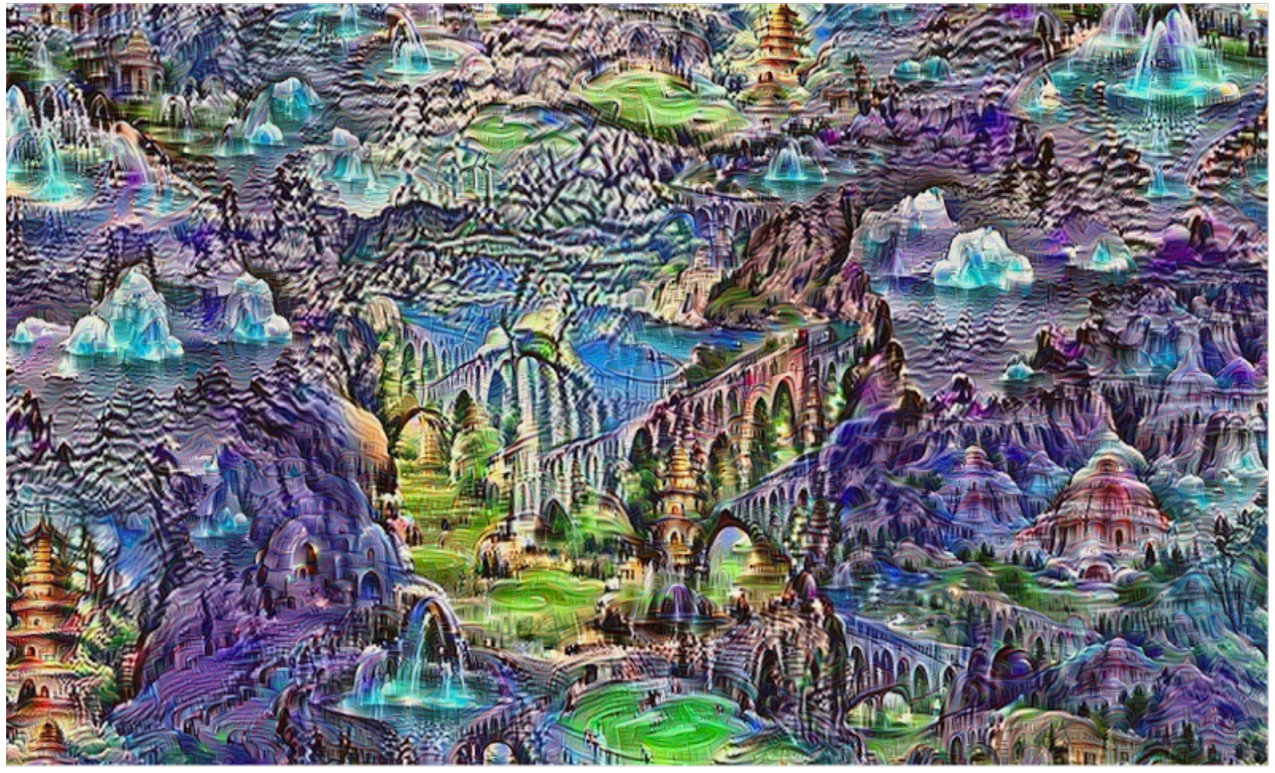
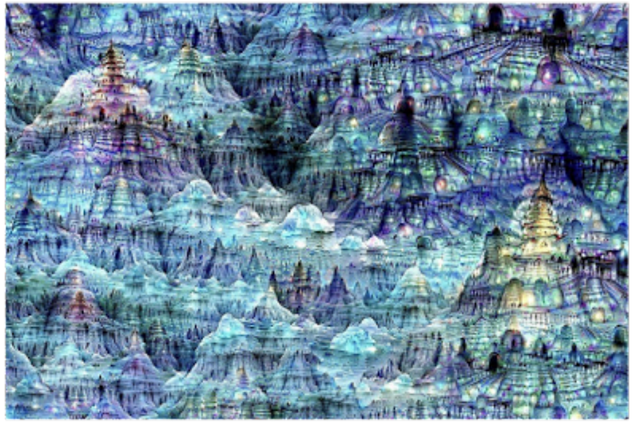
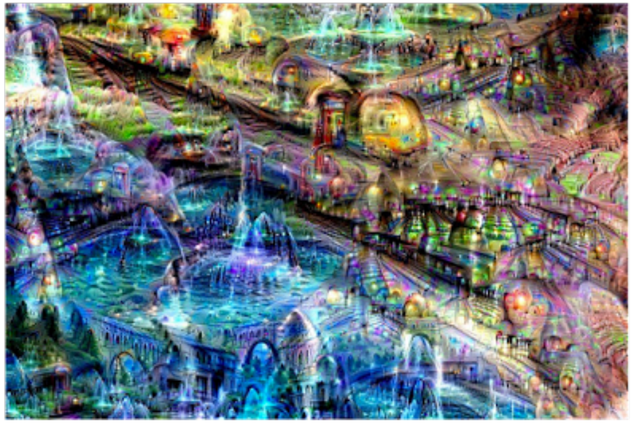
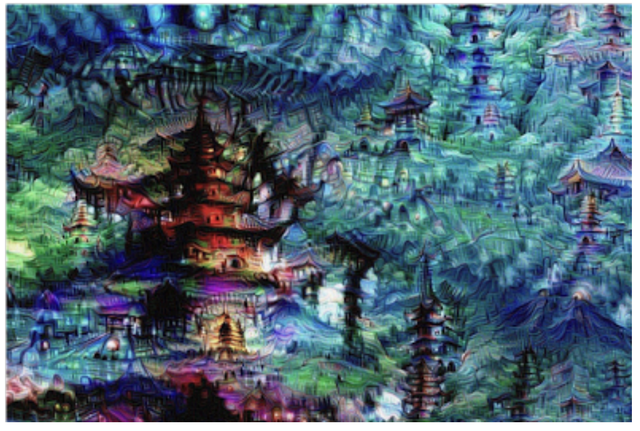




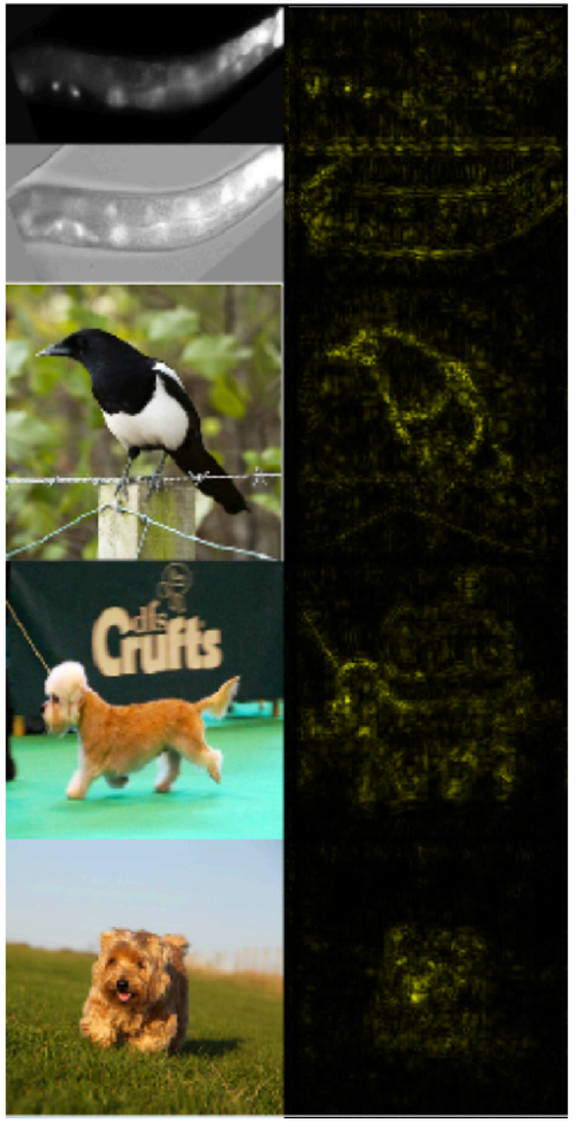





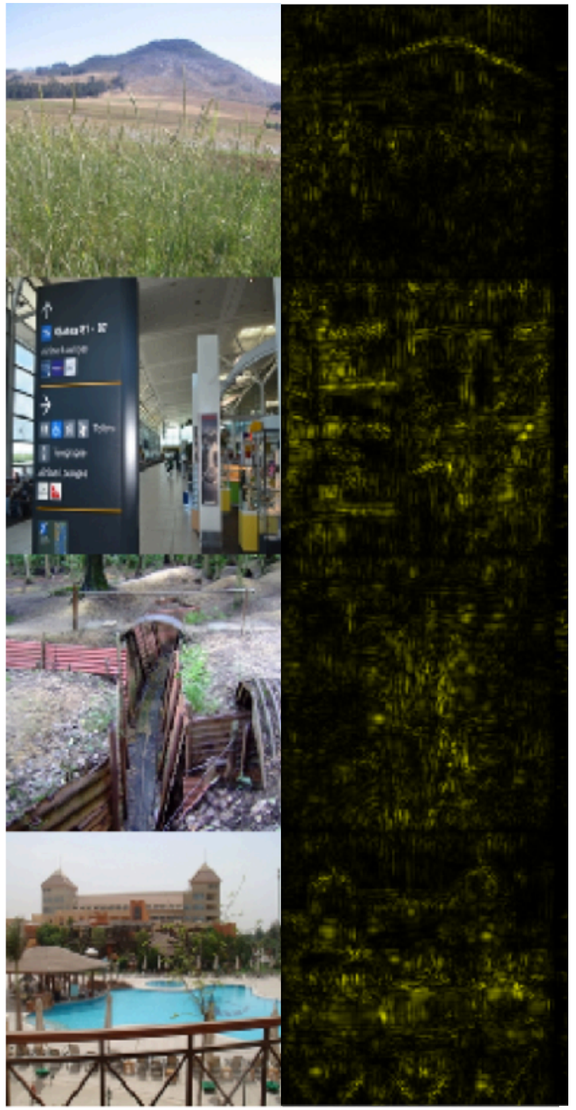
Deconvolution

Propagation	Backward mapping function: $h^{(l)} = m_{\text{dec}}(h^{(l+1)}; \theta^{(l,l+1)})$
Heatmap	matching input pattern for the classifed object in the image.
Relation to $f(x)$	not specified
Applicable	convolutional network with max-pooling and rectified linear units.
Drawbacks	(i) no direct correspondence between heatmap scores and contribution of pixels to the classification. (ii) image-specific information only from max-pooling layers.

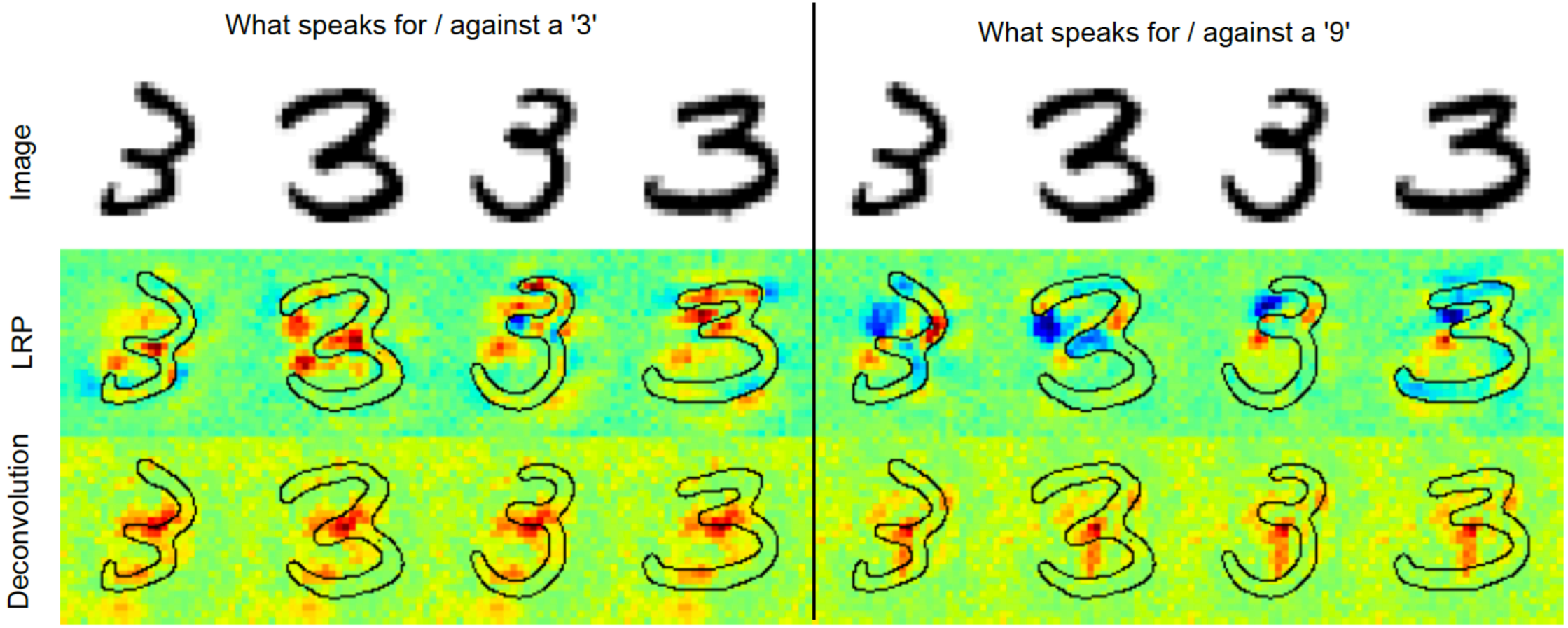
ILSVRC2012



MIT Places



Deconvolution



Layer-wise Relevance Propagation

Propagation

Backward mapping function
+ conservation principles:

$$h^{(l)} = m_{\text{lrp}}\left(h^{(l+1)}; x^{(l)}, \theta^{(l,l+1)}\right)$$

$$\sum_i h_i^{(l)} = \sum_j h_j^{(l+1)}$$

Heatmap

explanatory input pattern that indicates evidence for and against a bird.

Relation to $f(x)$

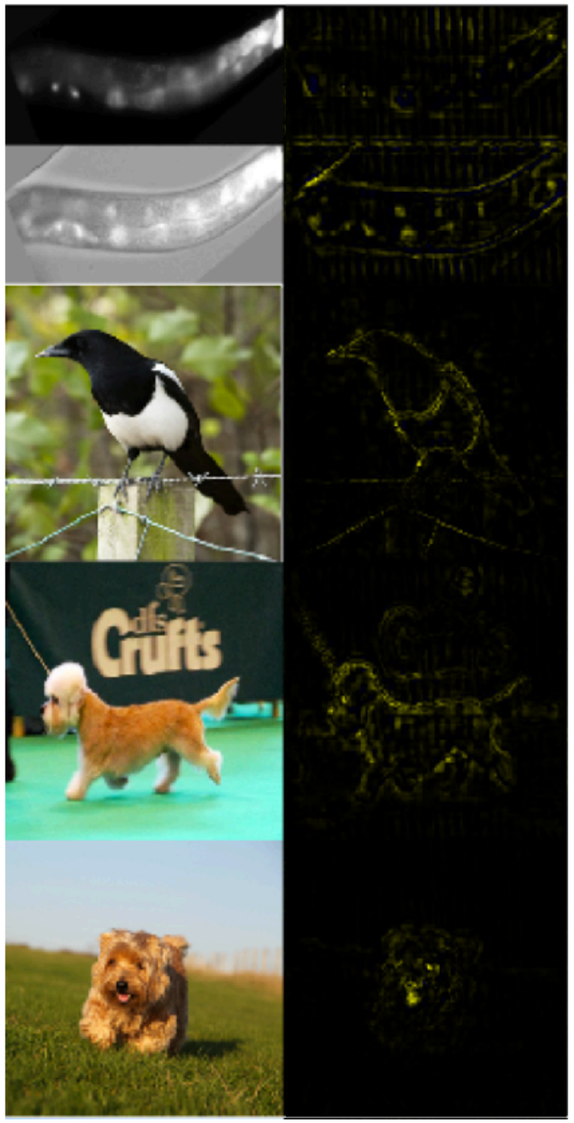
$$f(x) = \sum_p h_p$$

Applicable

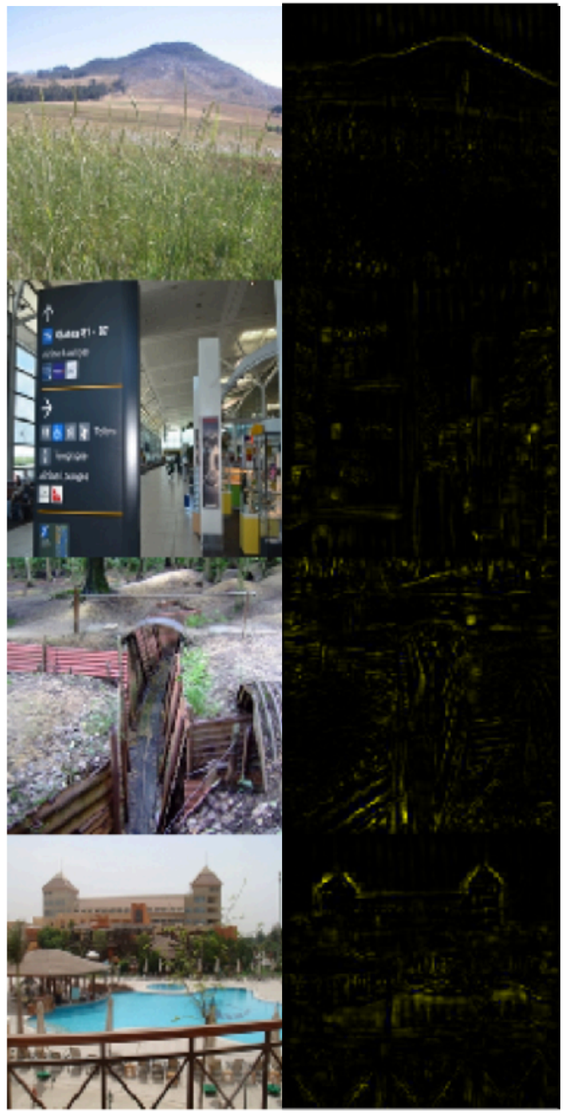
any network with monotonous activations
(even non-continuous units)

Drawbacks

ILSVRC2012



MIT Places



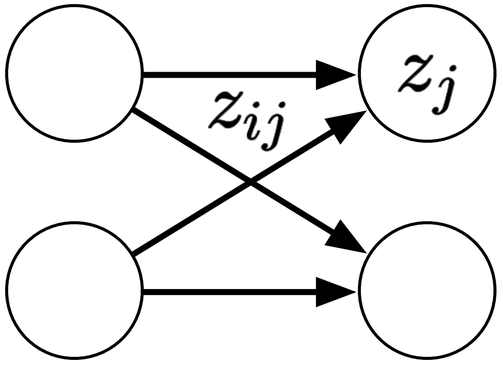
LRP

$$f(x) = \ldots = \sum_{d \in l+1} R_d^{(l+1)} = \sum_{d \in l} R_d^{(l)} = \ldots = \sum_{d} R_d^{(1)}$$

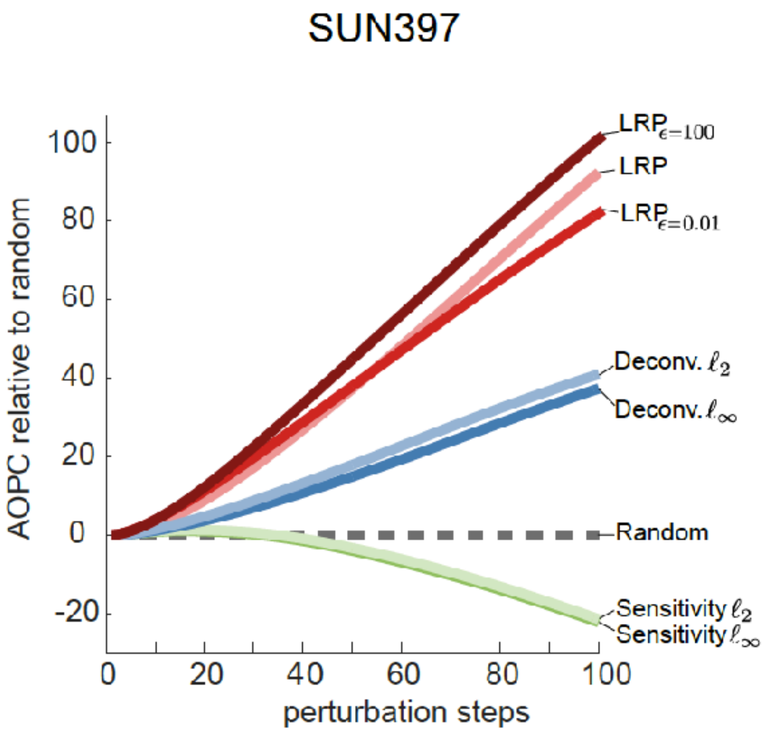
$$R_i^{(l)} = \sum_j \frac{z_{ij}}{\sum_{i'} z_{i'j} + \epsilon \, \mathrm{sign}(\sum_{i'} z_{i'j})} R_j^{(l+1)} \quad \textit{or} \quad R_i^{(l)} = \sum_j \left(\alpha \cdot \frac{z_{ij}^+}{\sum_{i'} z_{i'j}^+} + \beta \cdot \frac{z_{ij}^-}{\sum_{i'} z_{i'j}^-} \right) R_j^{(l+1)}$$

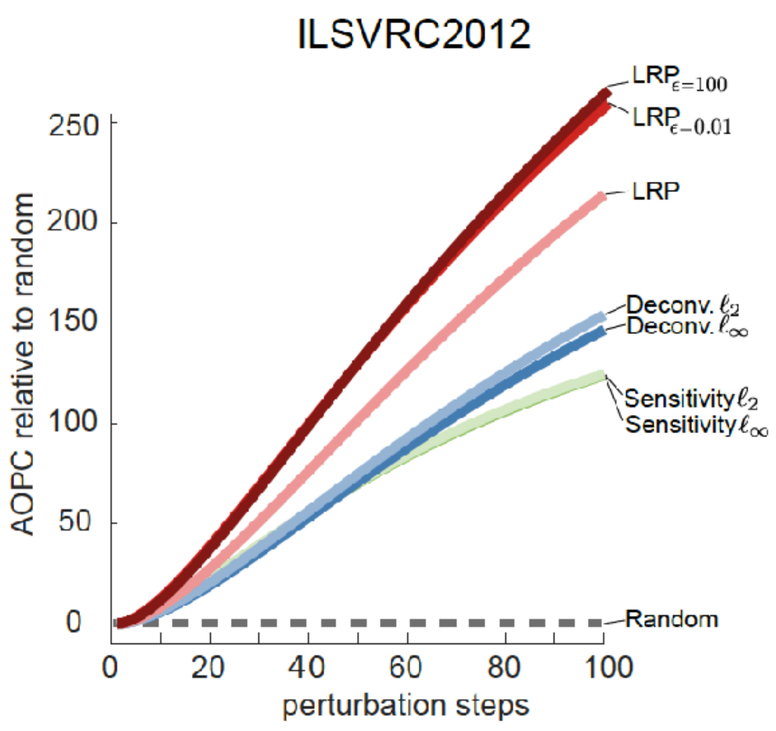
$$a_j^{(l+1)} = \sigma\left(\sum_i z_{ij} + b_j^{(l+1)} \right)$$

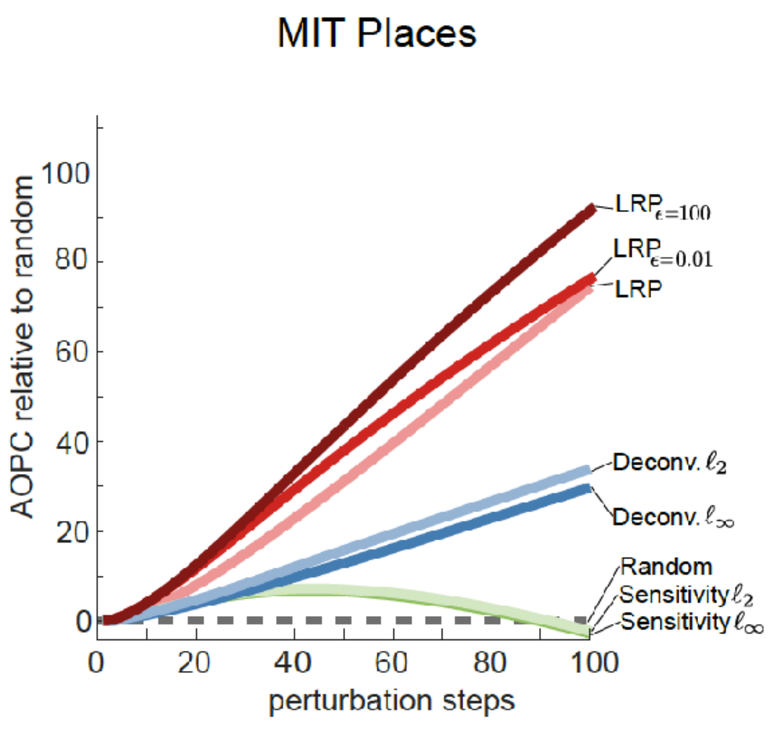
$$\text{with} \quad z_{ij} = a_i^{(l)} w_{ij}^{(l,l+1)}$$



Evaluating

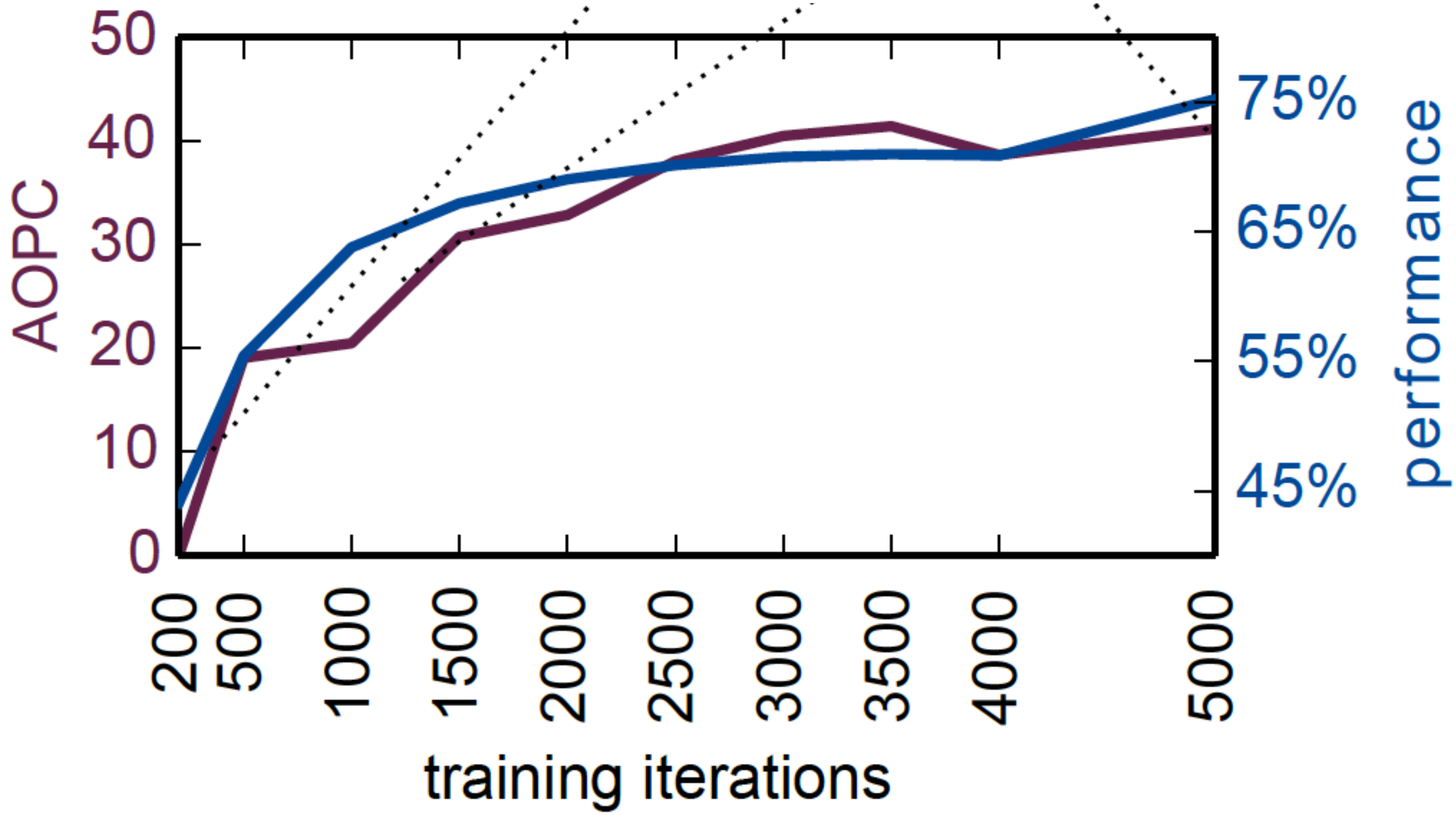




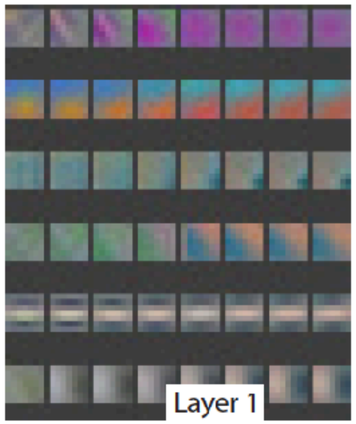


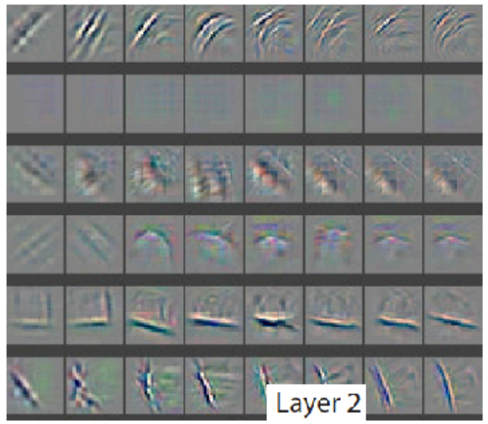
$$\text{AOPC} = \frac{1}{L+1}\left\langle \sum_{k=0}^{L} f(\boldsymbol{x}^{(0)}_{\text{MoRF}}) - f(\boldsymbol{x}^{(k)}_{\text{MoRF}}) \right\rangle_{p(\boldsymbol{x})}$$

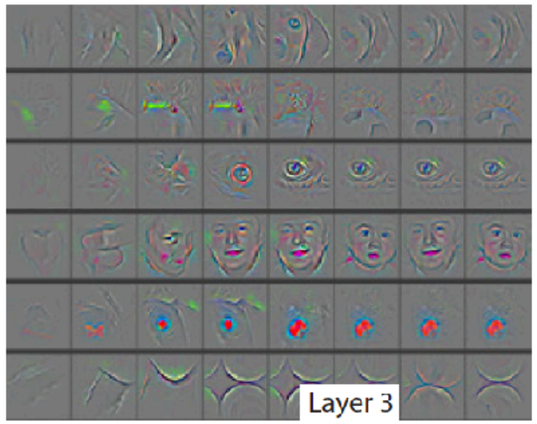
An interesting result?

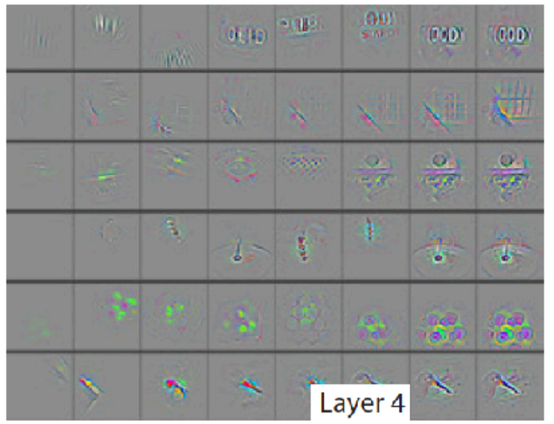


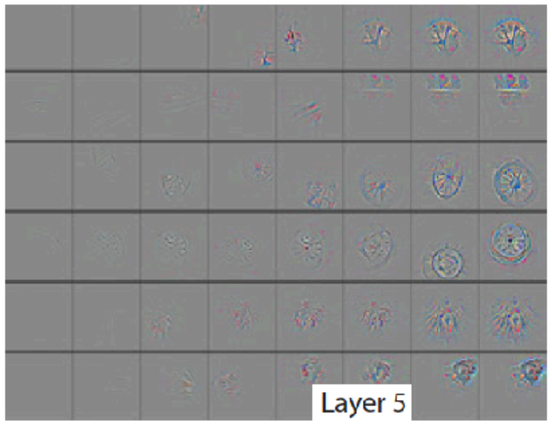
Beyond the output layer

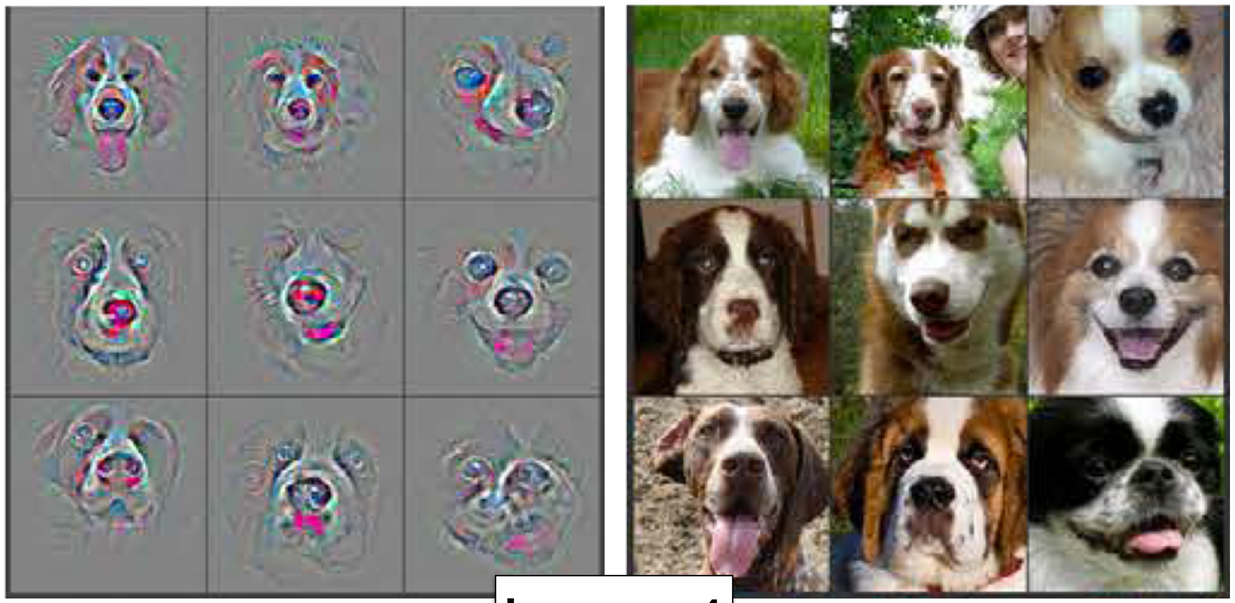










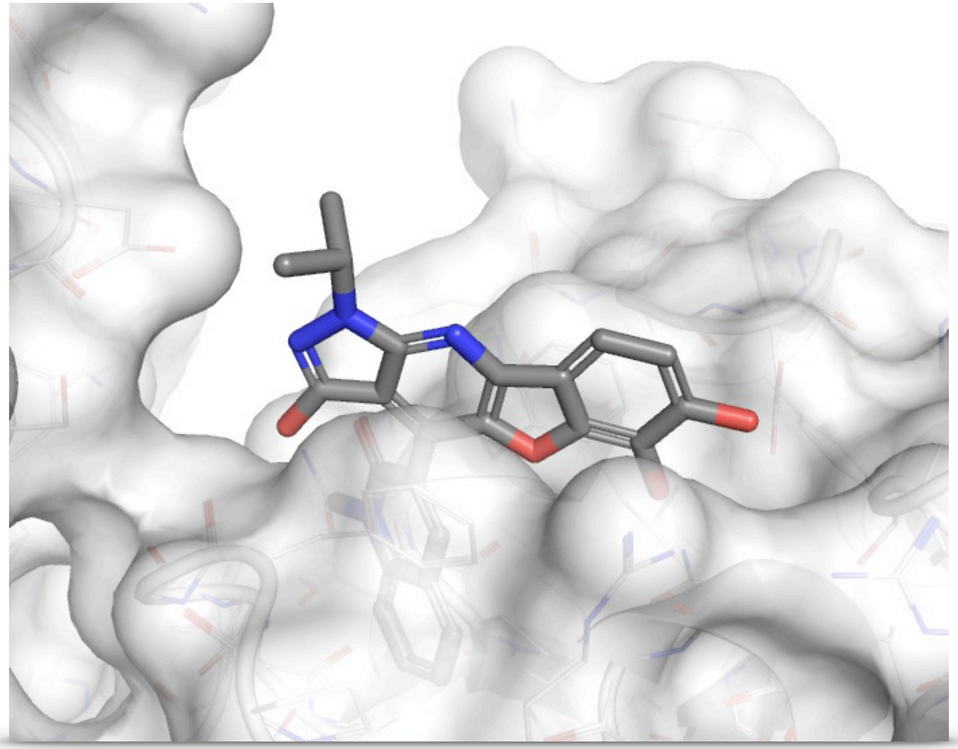


Layer 4

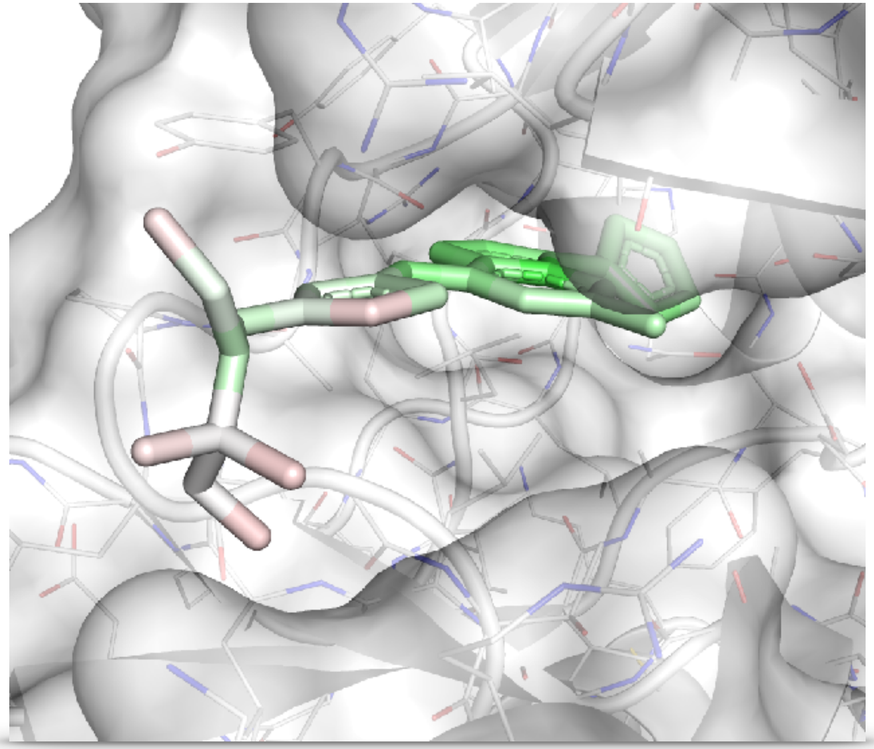
From the deconvolution paper

Structure Based Drug Design

Virtual Screening



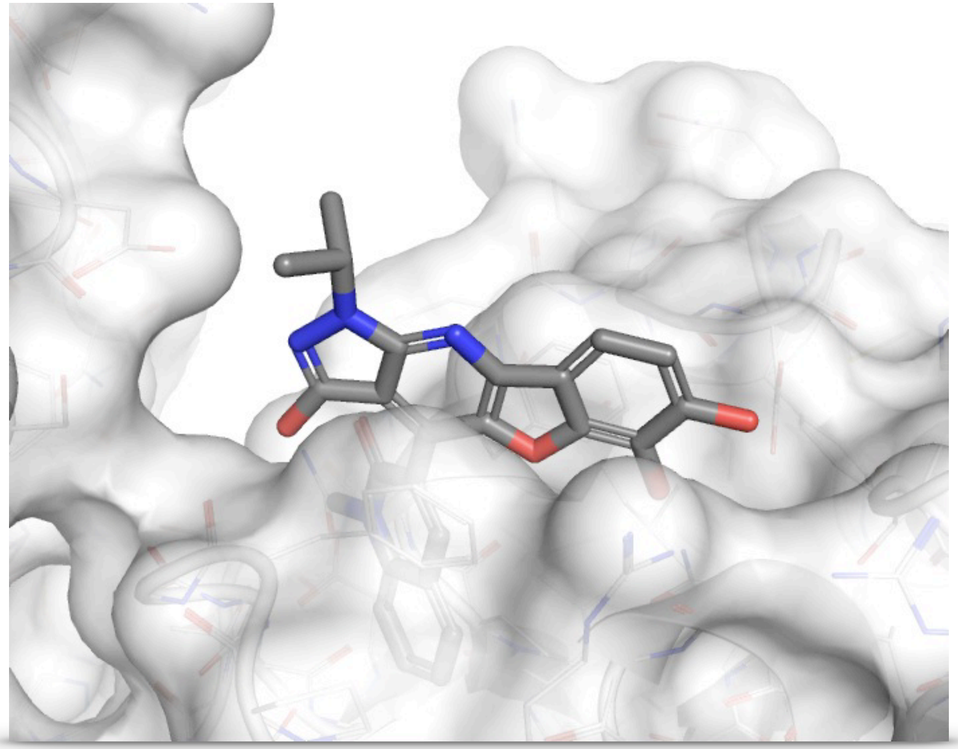
Lead Optimization



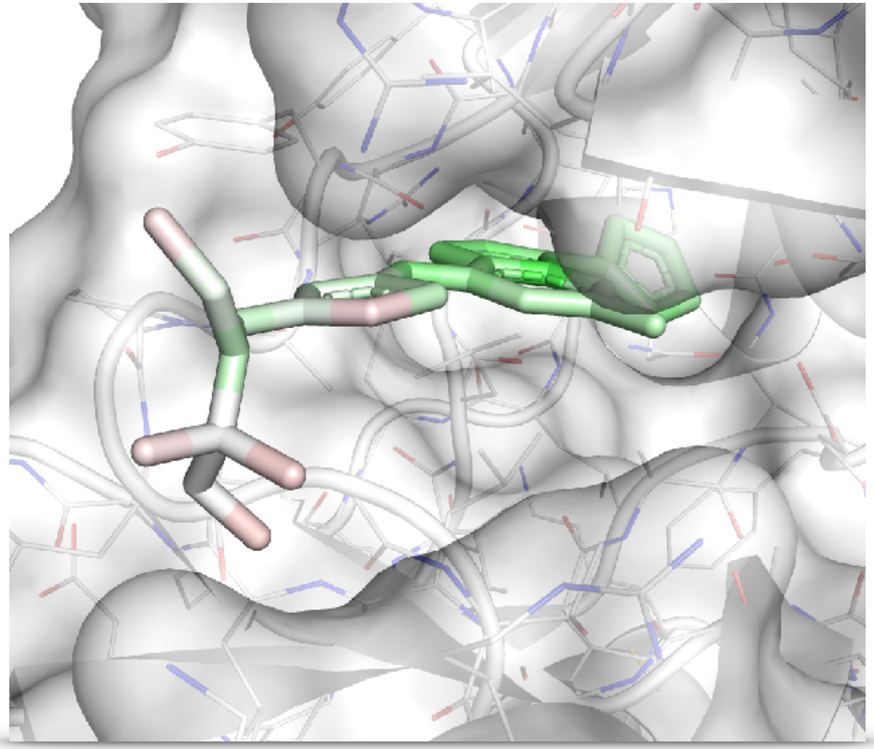
Pose Prediction → Binding Discrimination → Affinity Prediction

Structure Based Drug Design

Virtual Screening

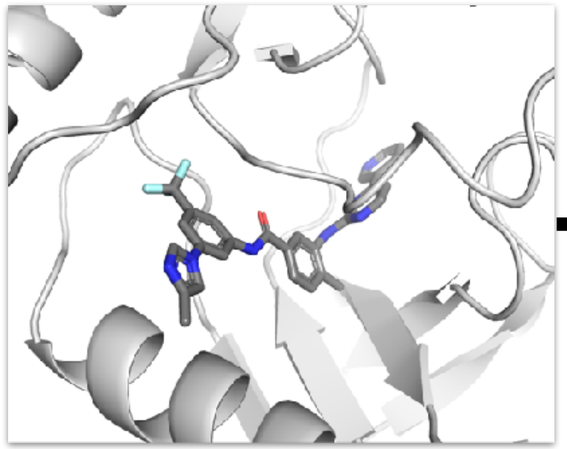


Lead Optimization



Pose Prediction → Binding Discrimination → Affinity Prediction

CNNs for Protein-Ligand Scoring



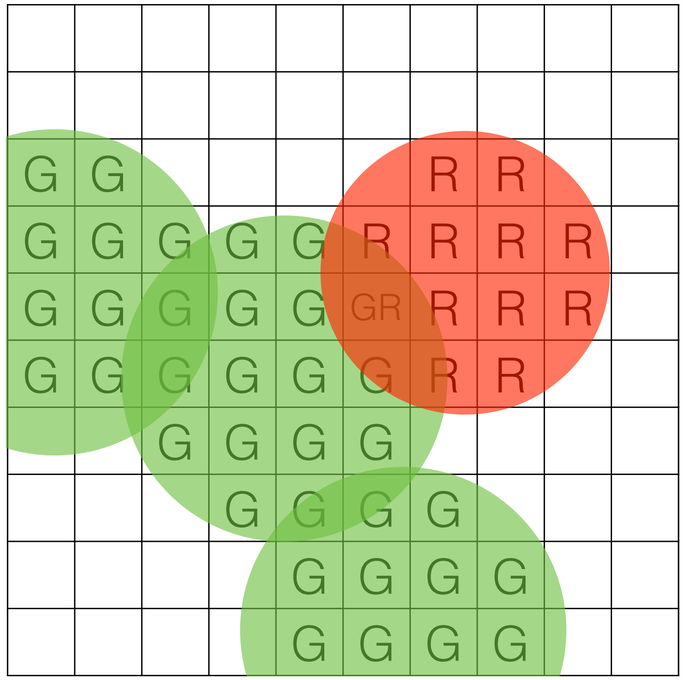
CNN

Pose Prediction

Binding Discrimination

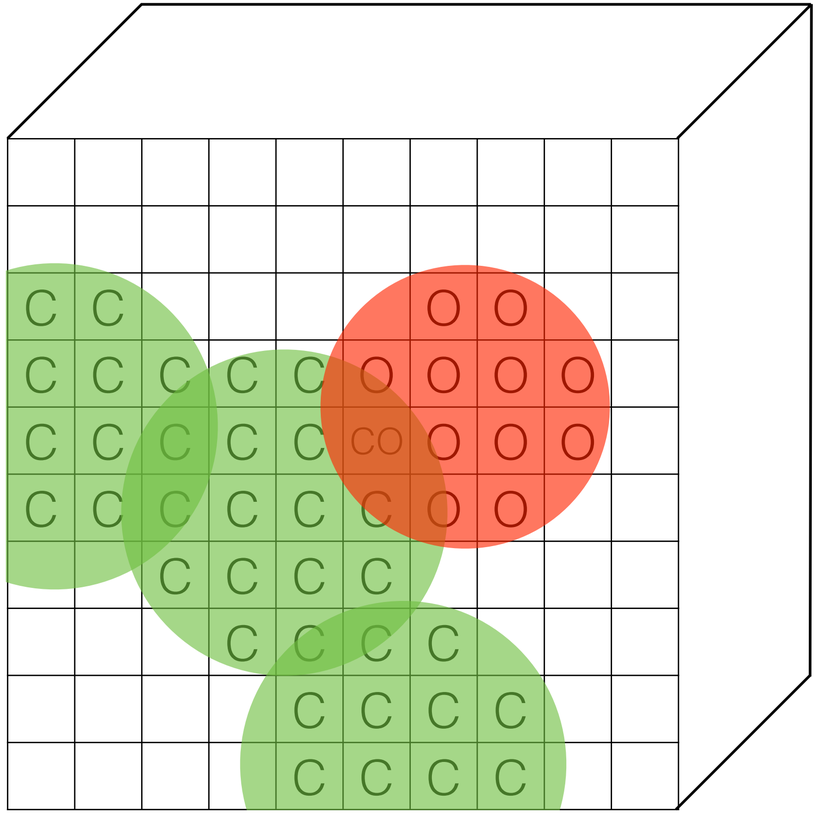
Affinity Prediction

Protein-Ligand Representation



(R,G,B) pixel

Protein-Ligand Representation



(R,G,B) pixel →

(Carbon, Nitrogen, Oxygen,…) **voxel**

The only parameters for this representation are the choice of **grid resolution**, **atom density**, and **atom types**.

Training Data

Pose Prediction

337 protein-ligand complexes

- curated for electron density
- diverse targets
- <10μM affinity
- **generate poses** with Vina
  - 745 <2Å RMSD (actives)
  - 3251 >4Å RMSD (decoys)

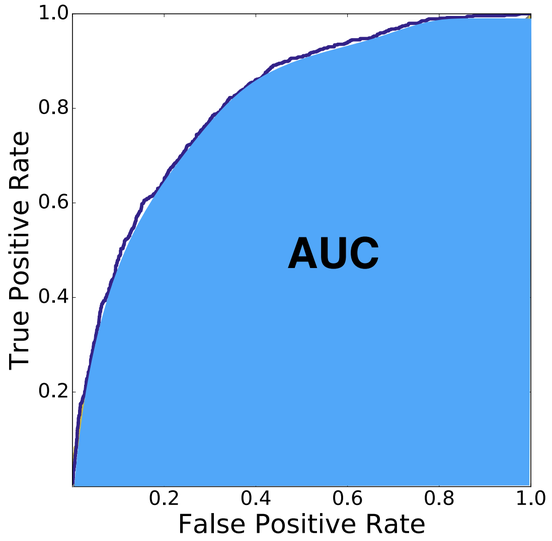
4056 protein-ligand complexes

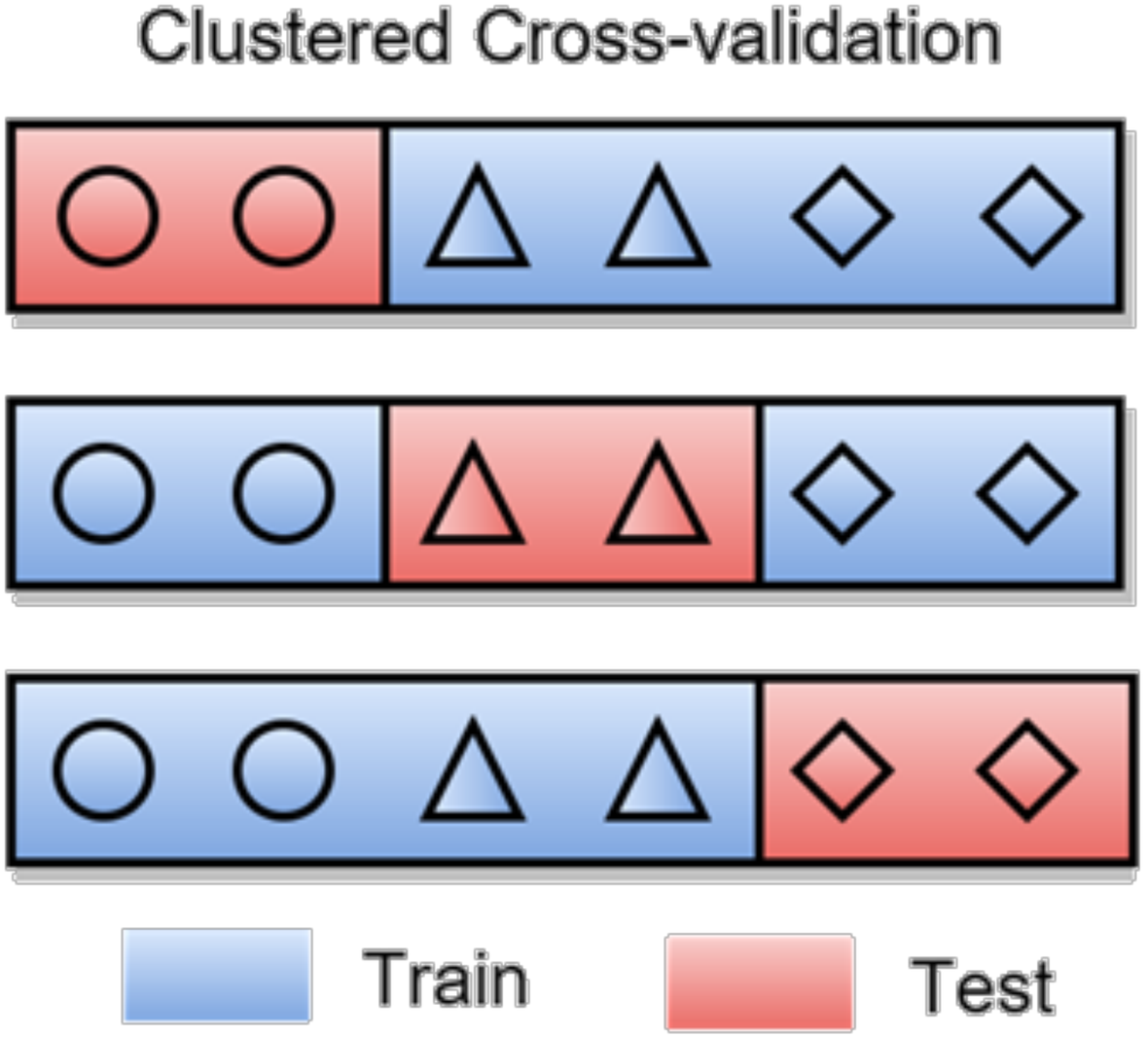
- diverse targets
- wide range of affinities
- **generate poses** with AutoDock Vina
- include minimized crystal pose
  - 8,688 <2Å RMSD (actives)
  - 76,743 >4Å RMSD (decoys)

Model Evaluation

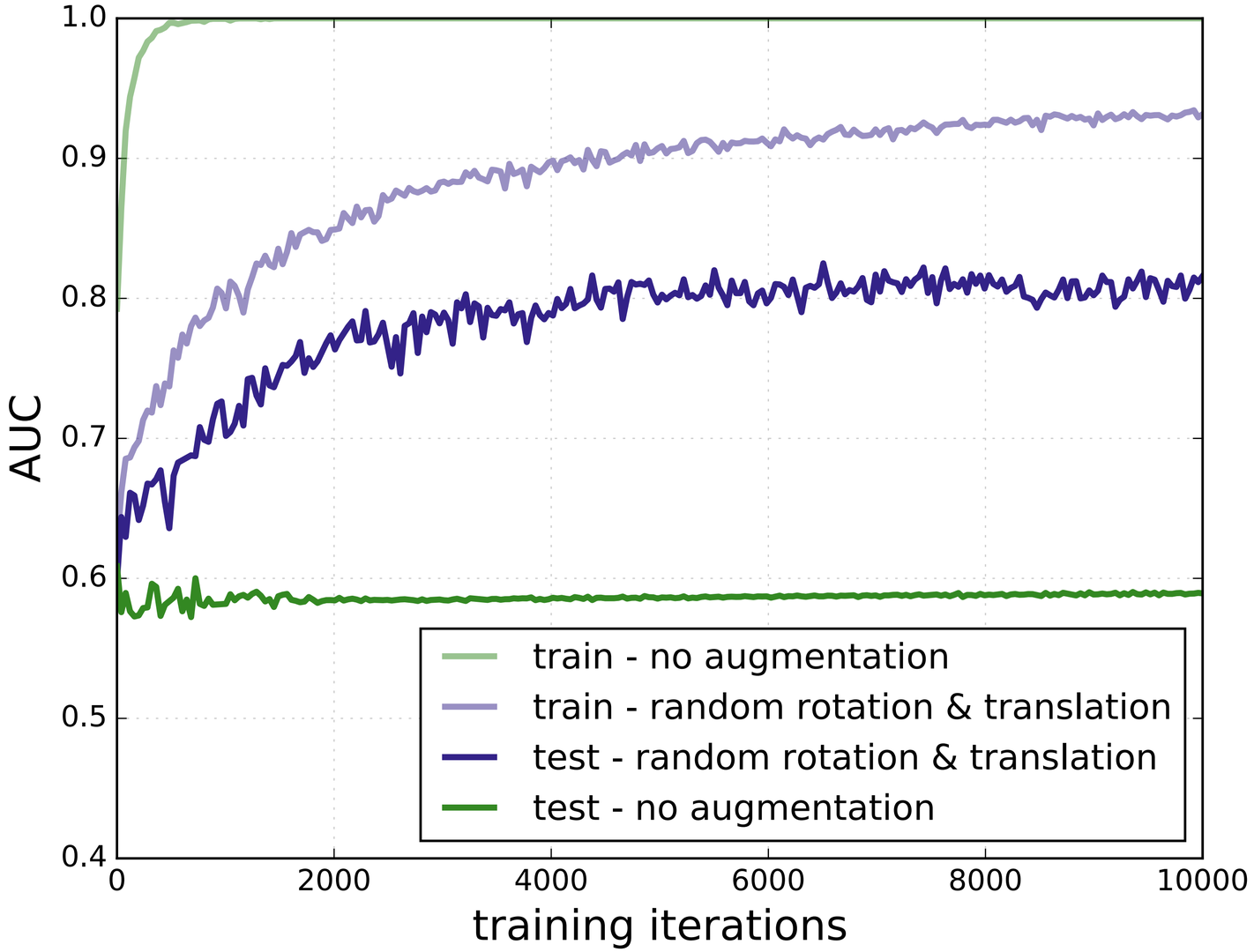
CSAR: >90% similar targets kept in same fold

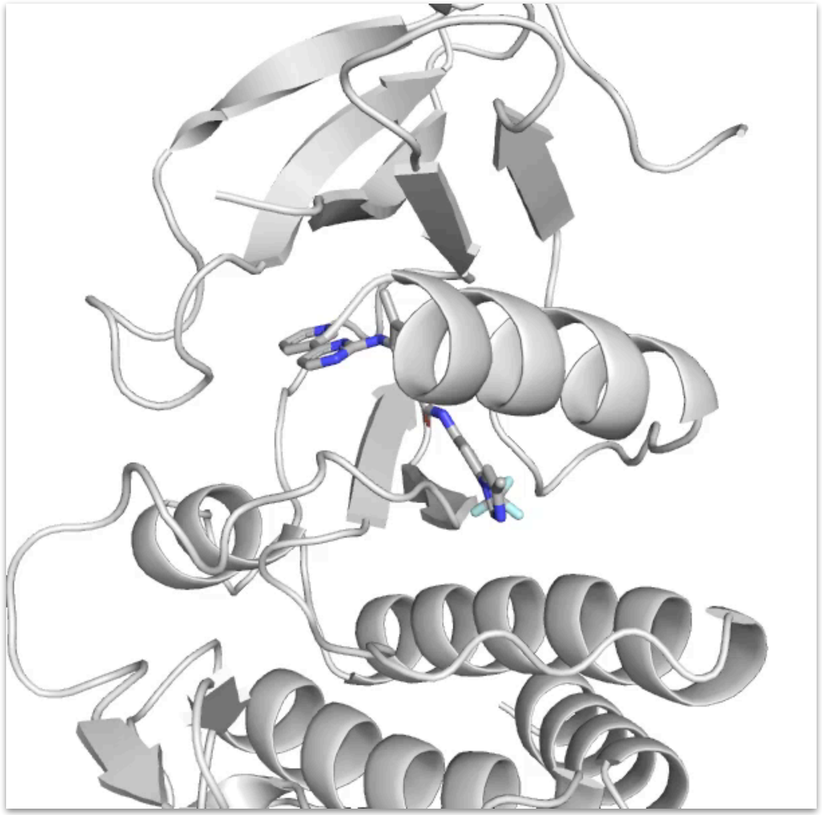
DUD-E & PDBbind: >80% similar targets kept in same fold



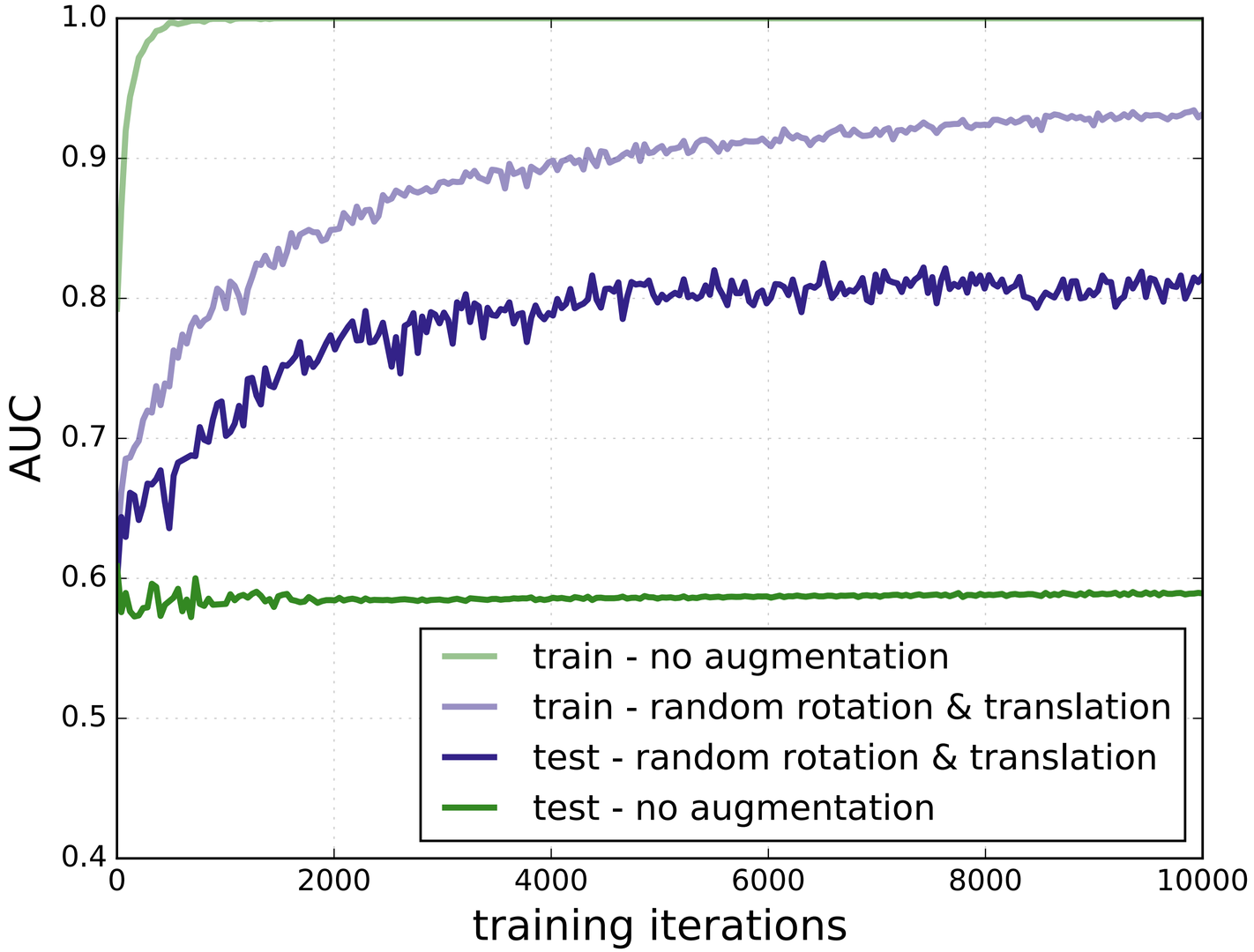


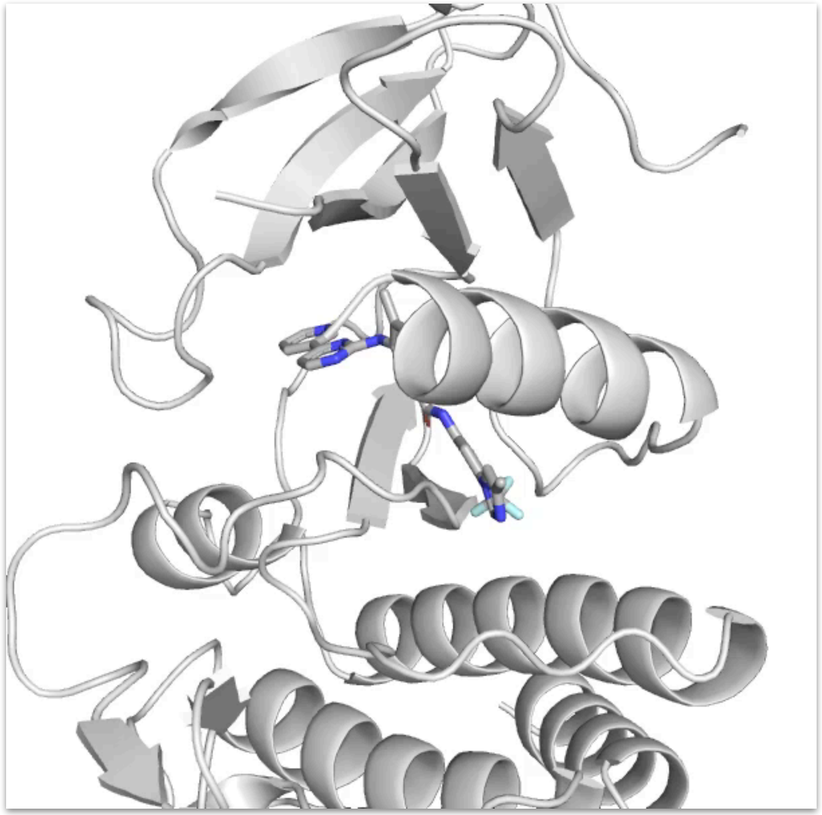
Data Augmentation



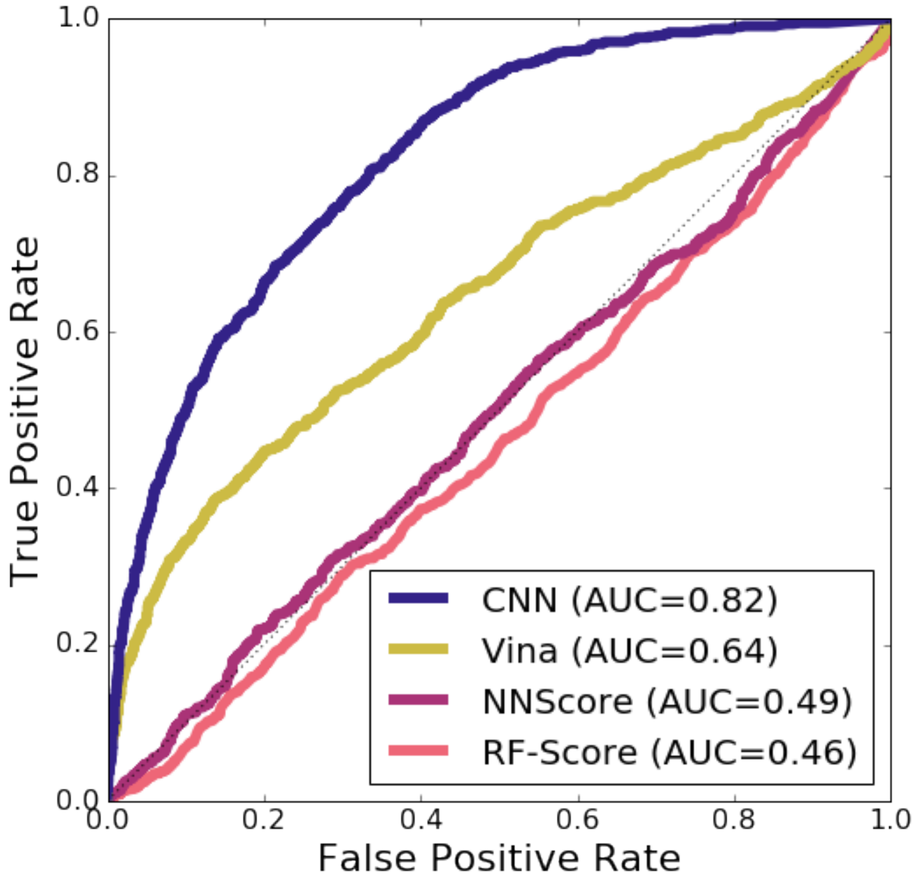


Data Augmentation

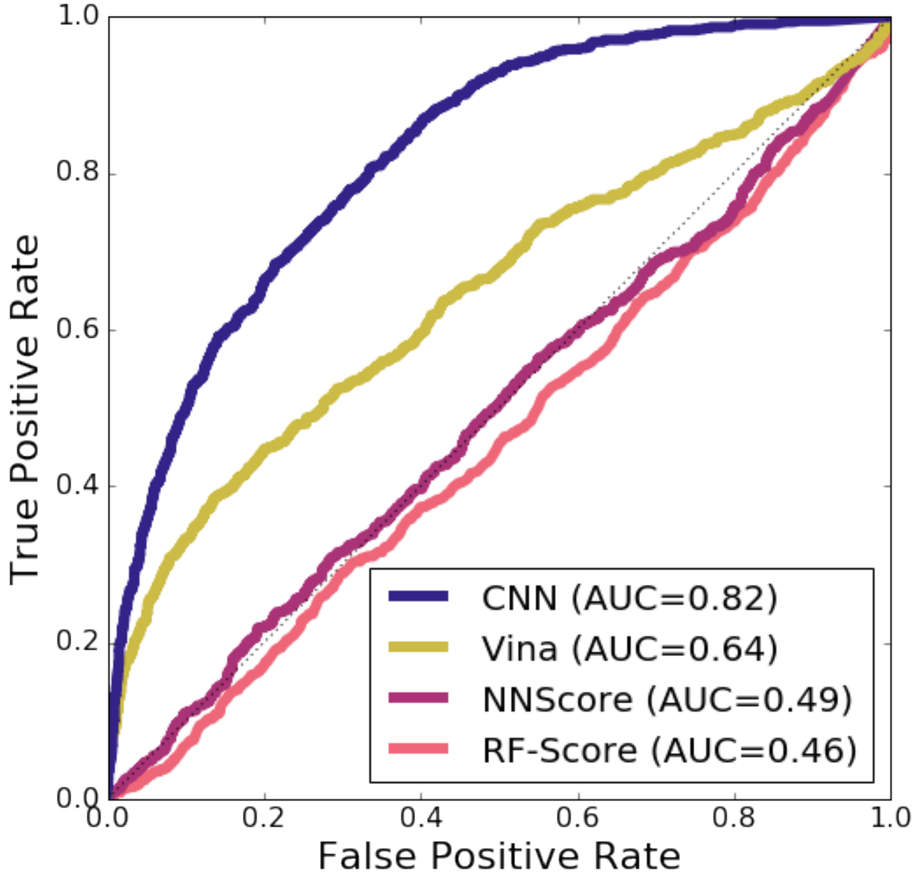




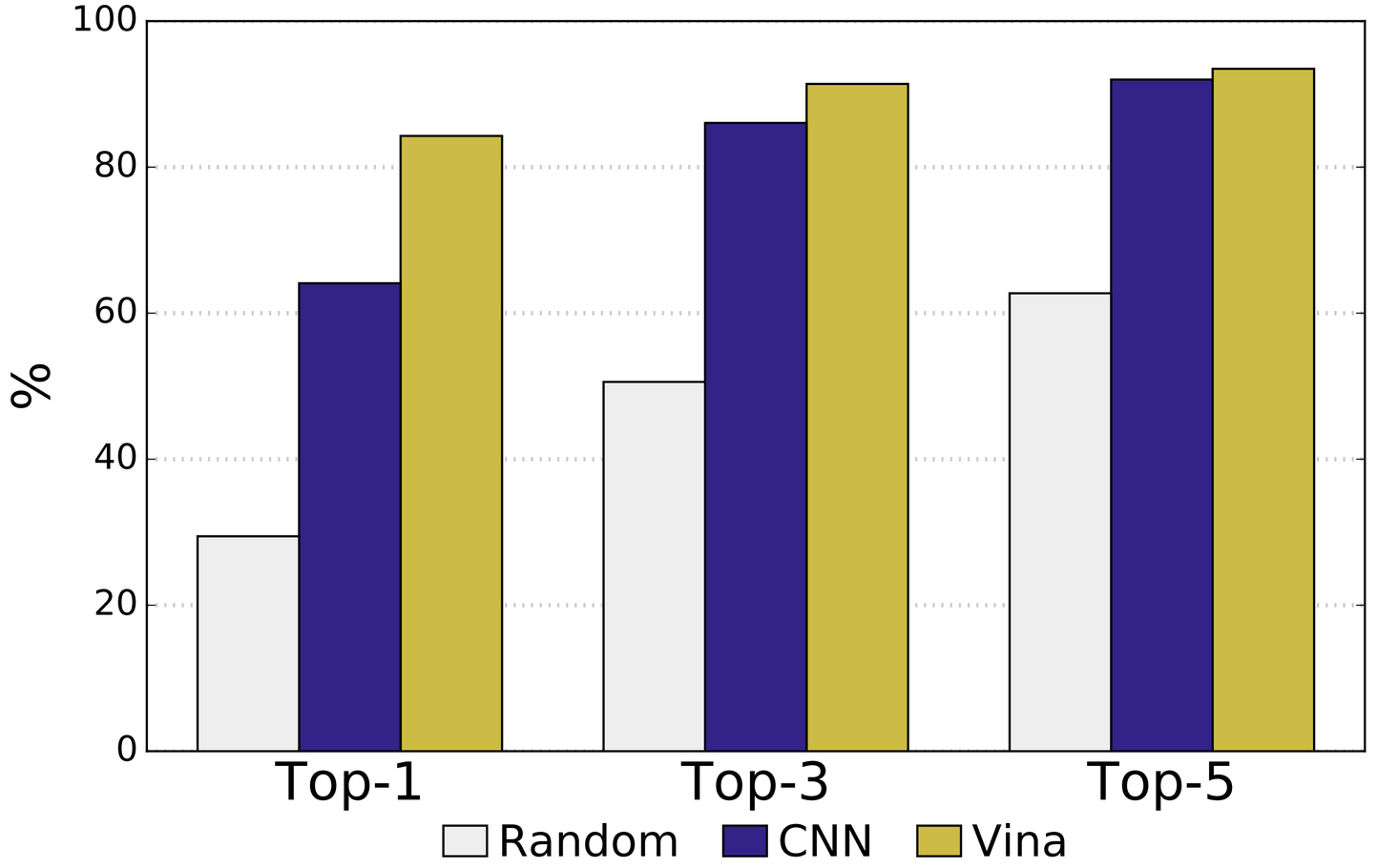
Pose Prediction (CSAR)



Pose Prediction (CSAR)

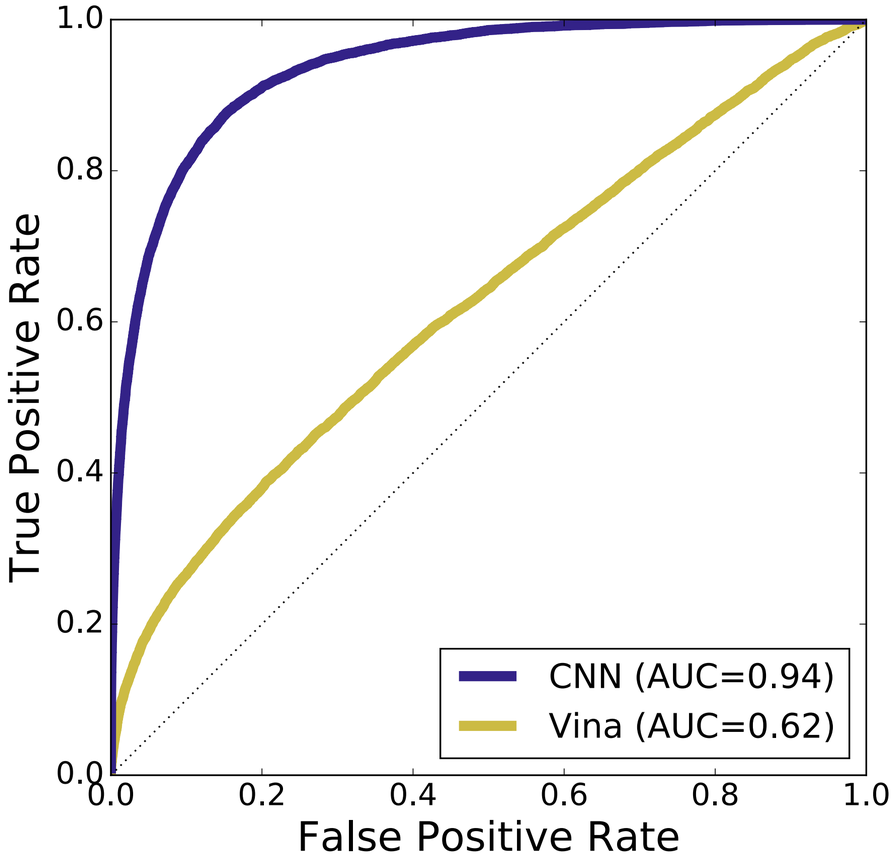


inter-target ranking

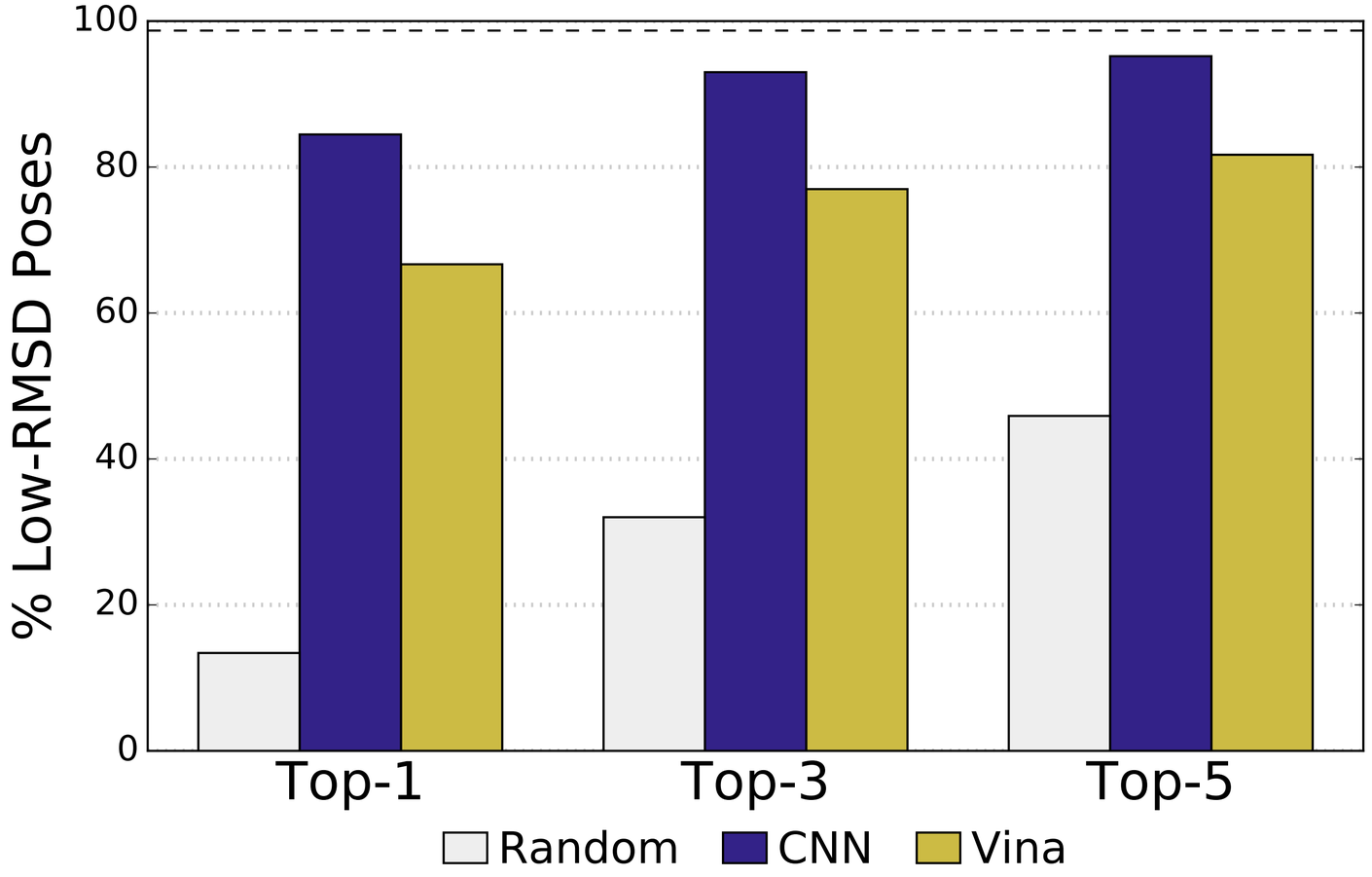


intra-target ranking

Pose Prediction (PDBbind)

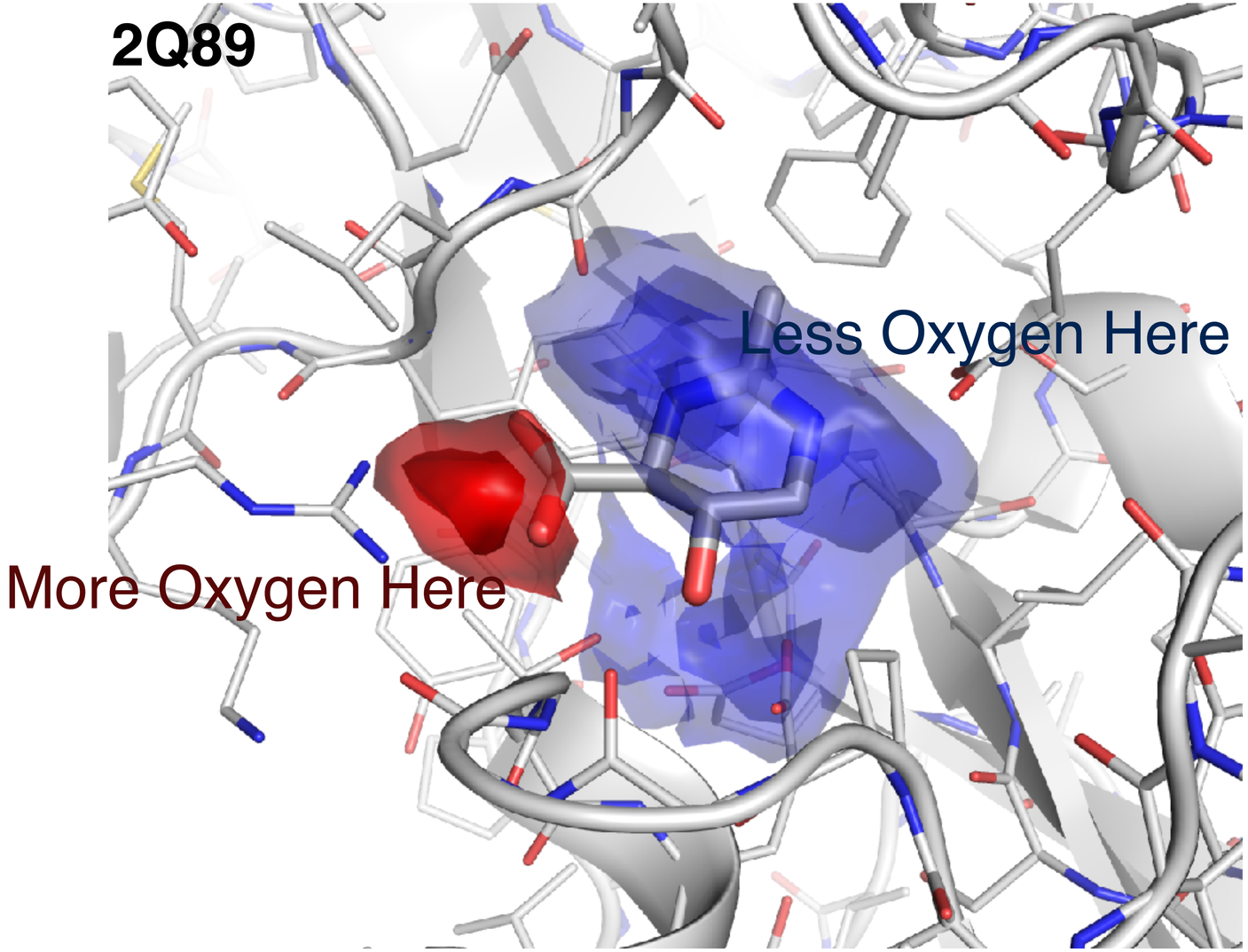


inter-target ranking



intra-target ranking

Beyond Scoring



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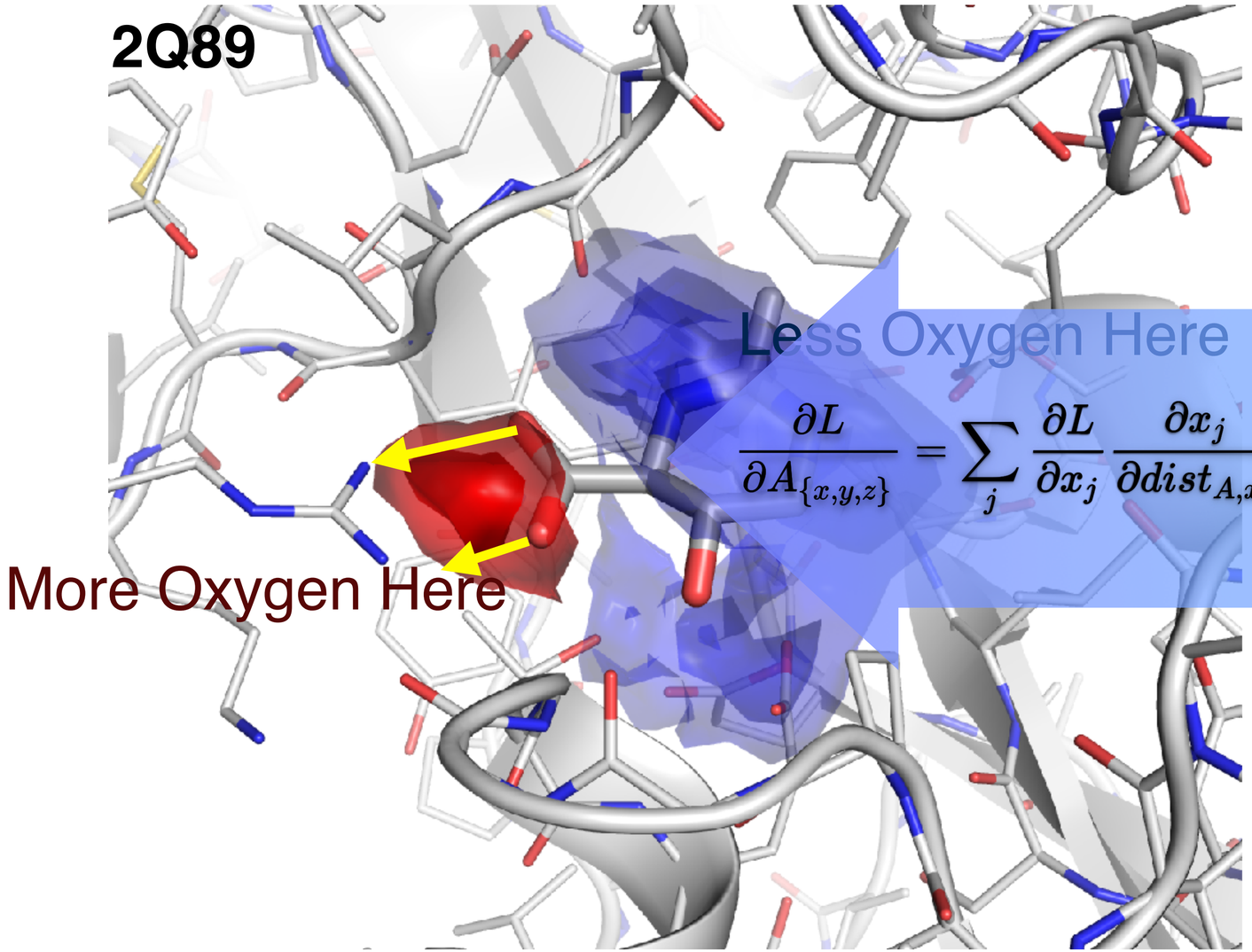
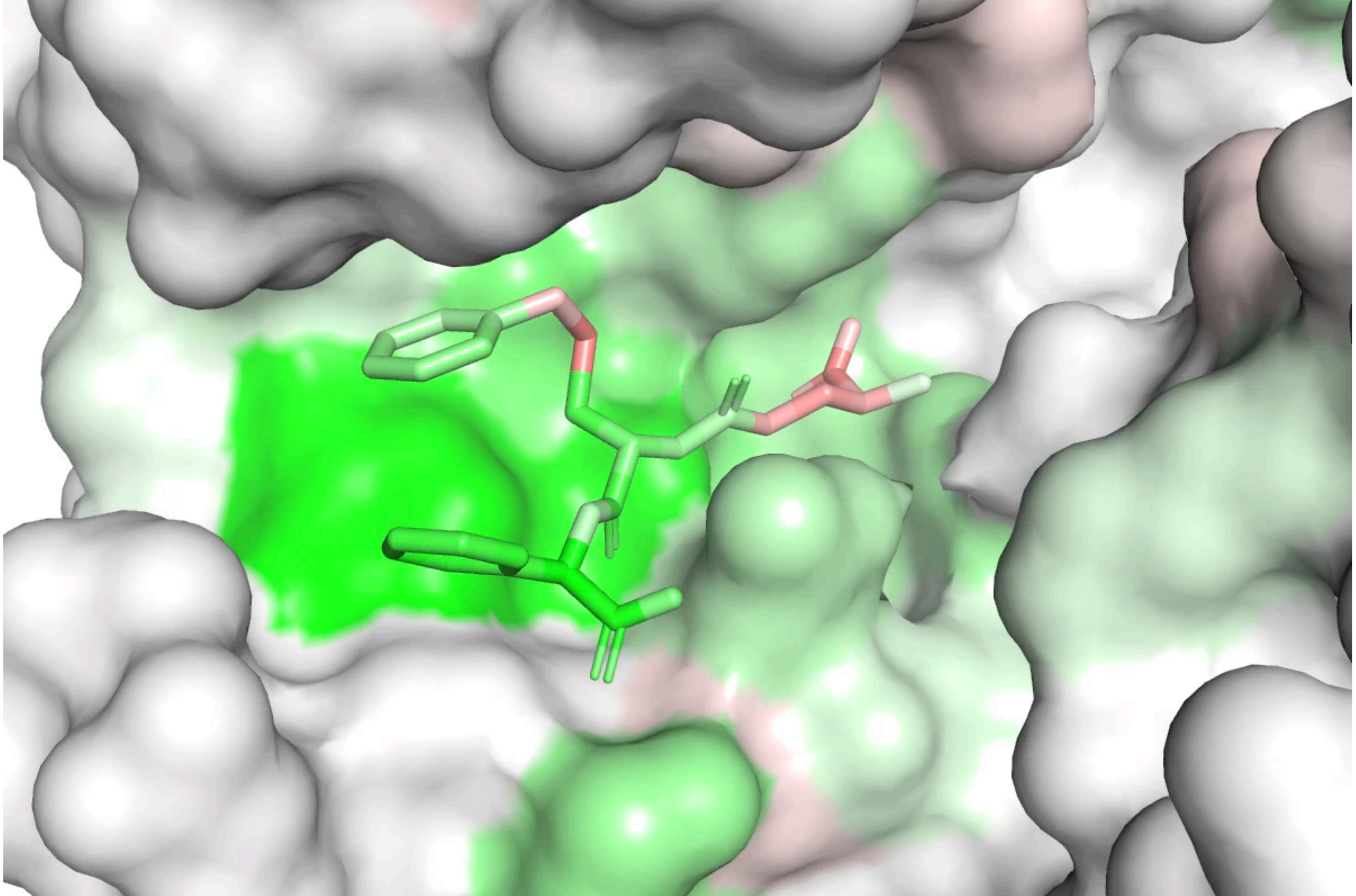
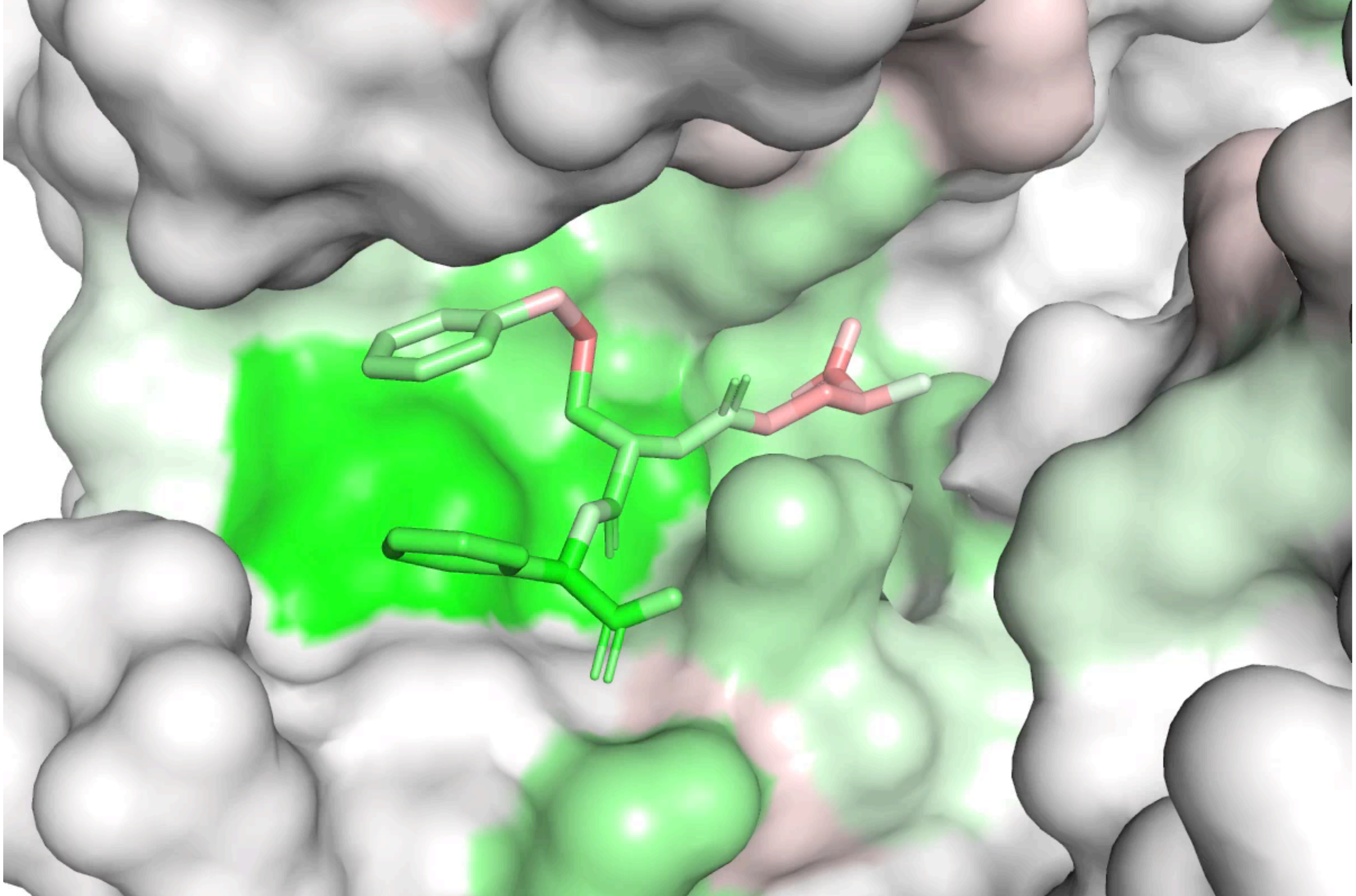
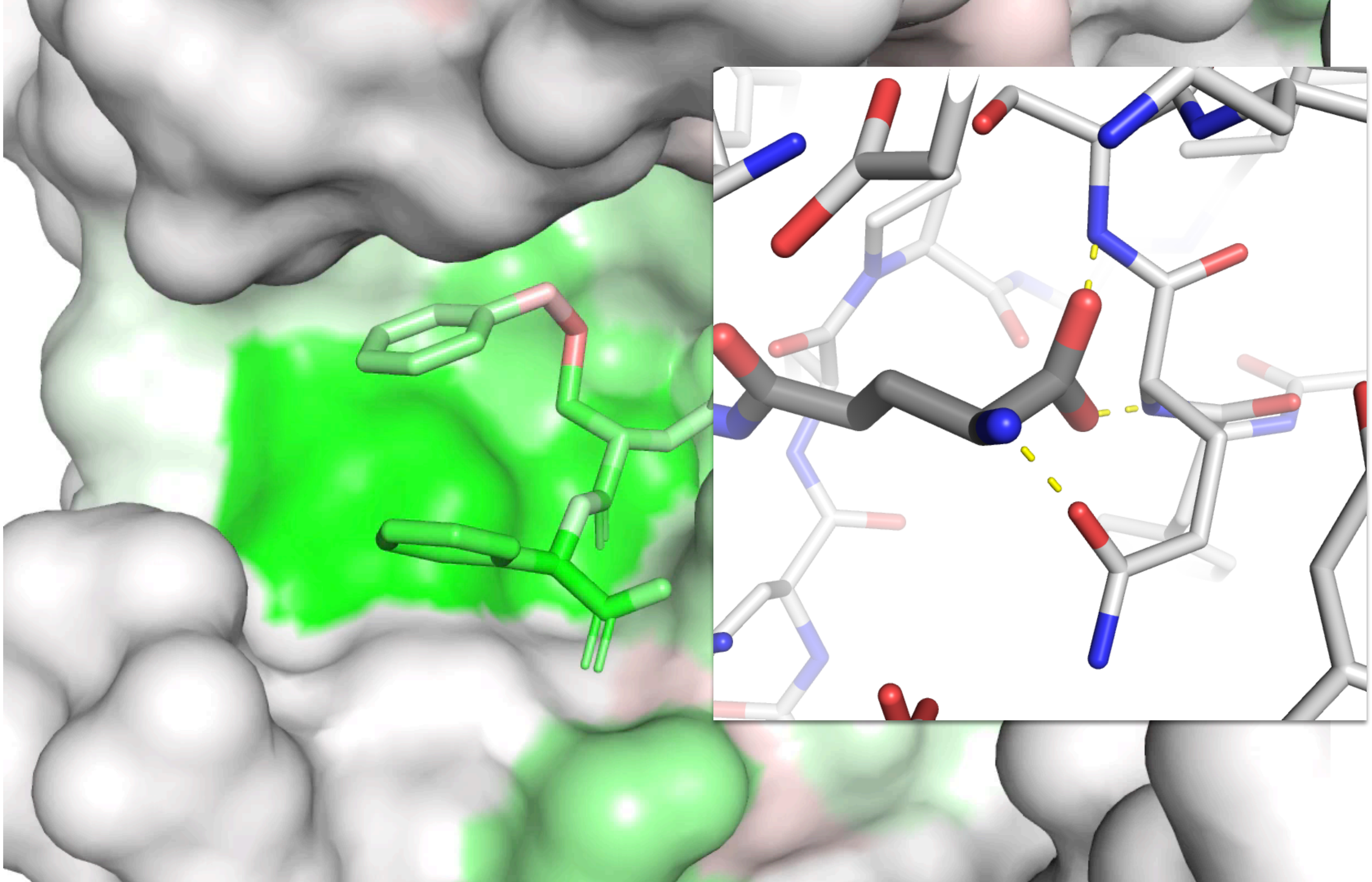
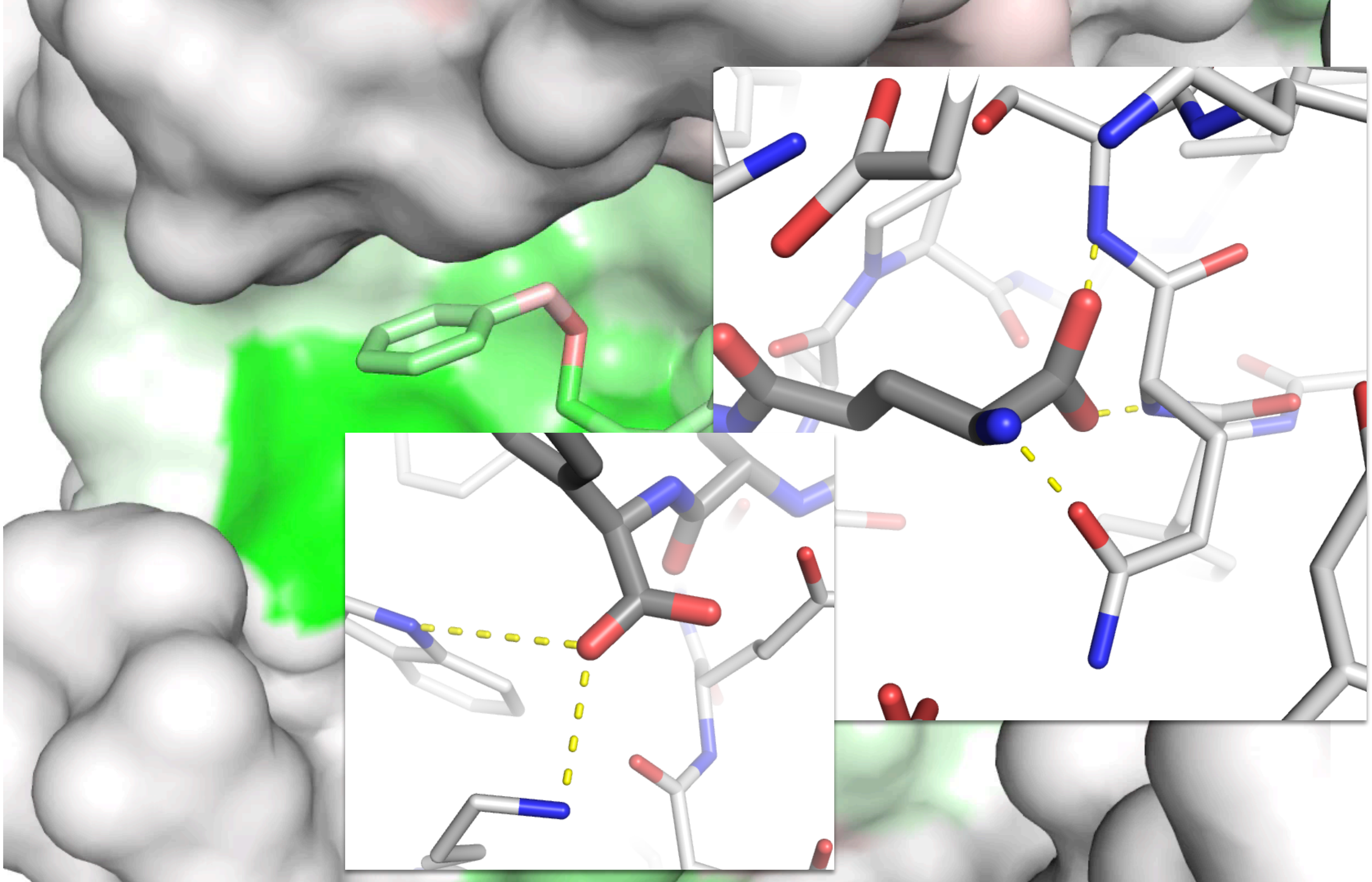


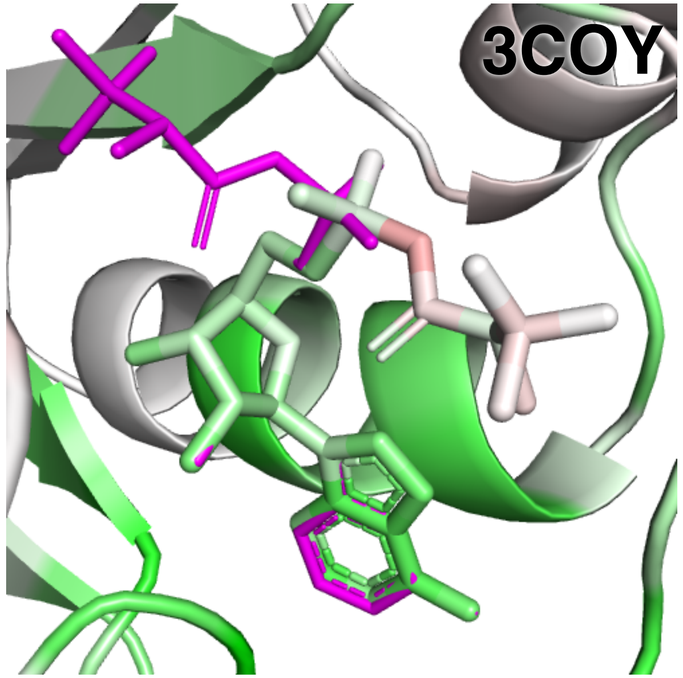


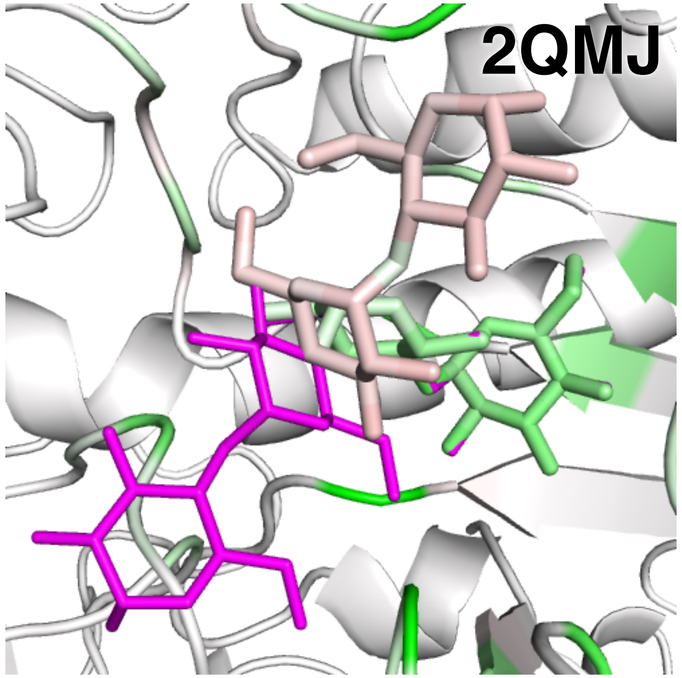


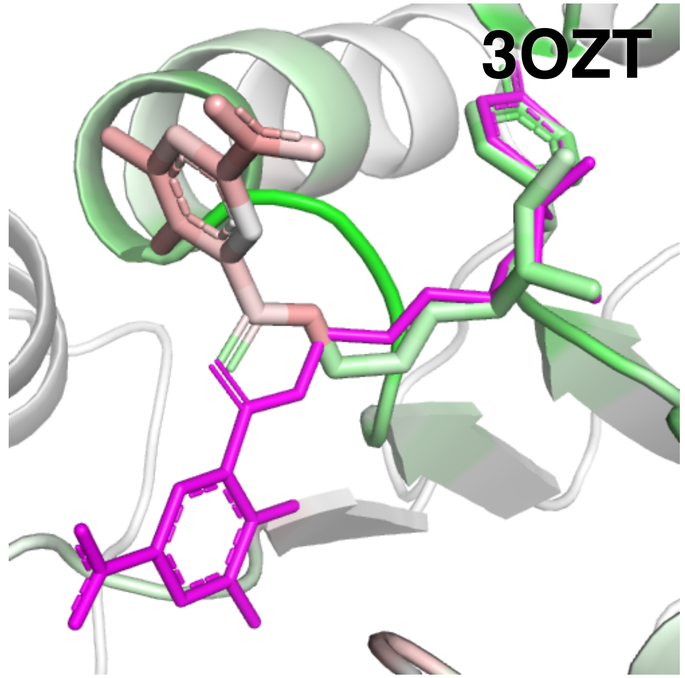




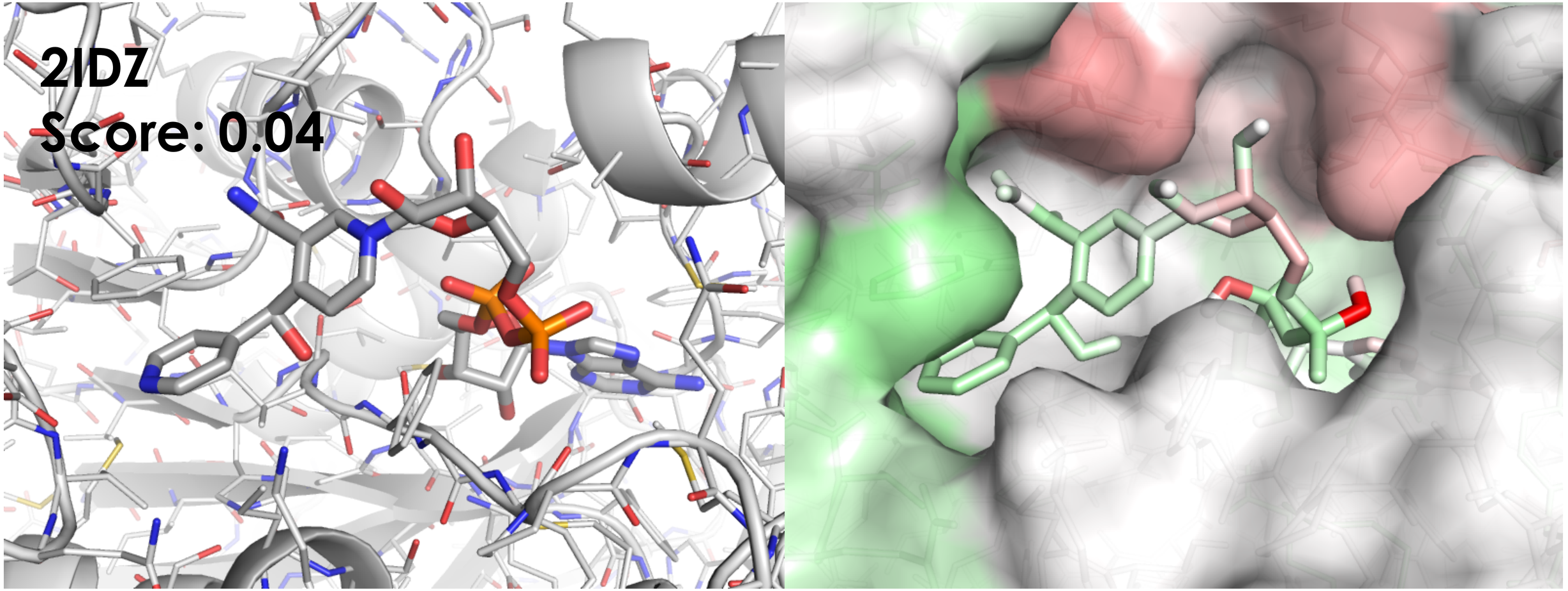
Visual Examples







Partially Aligned Poses
Masking



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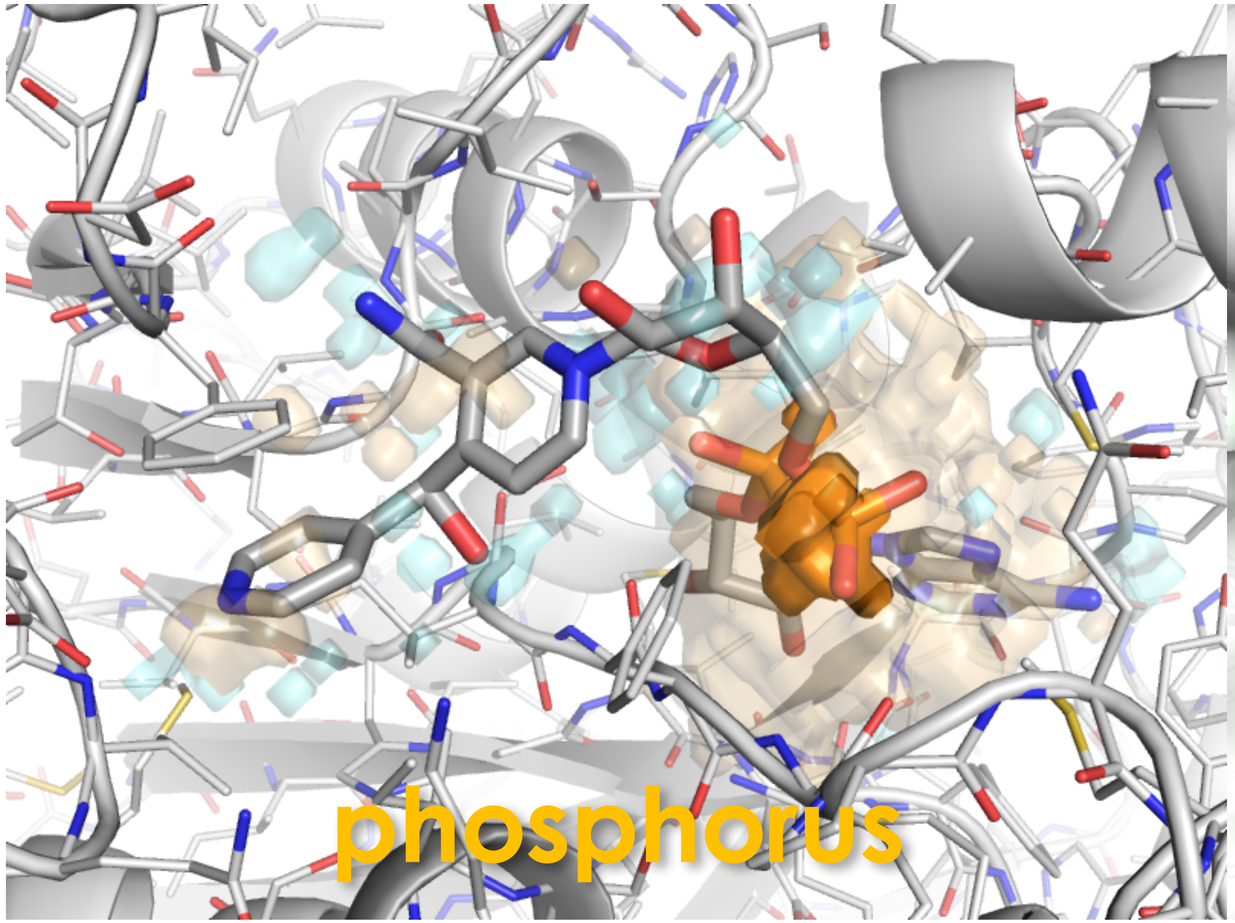
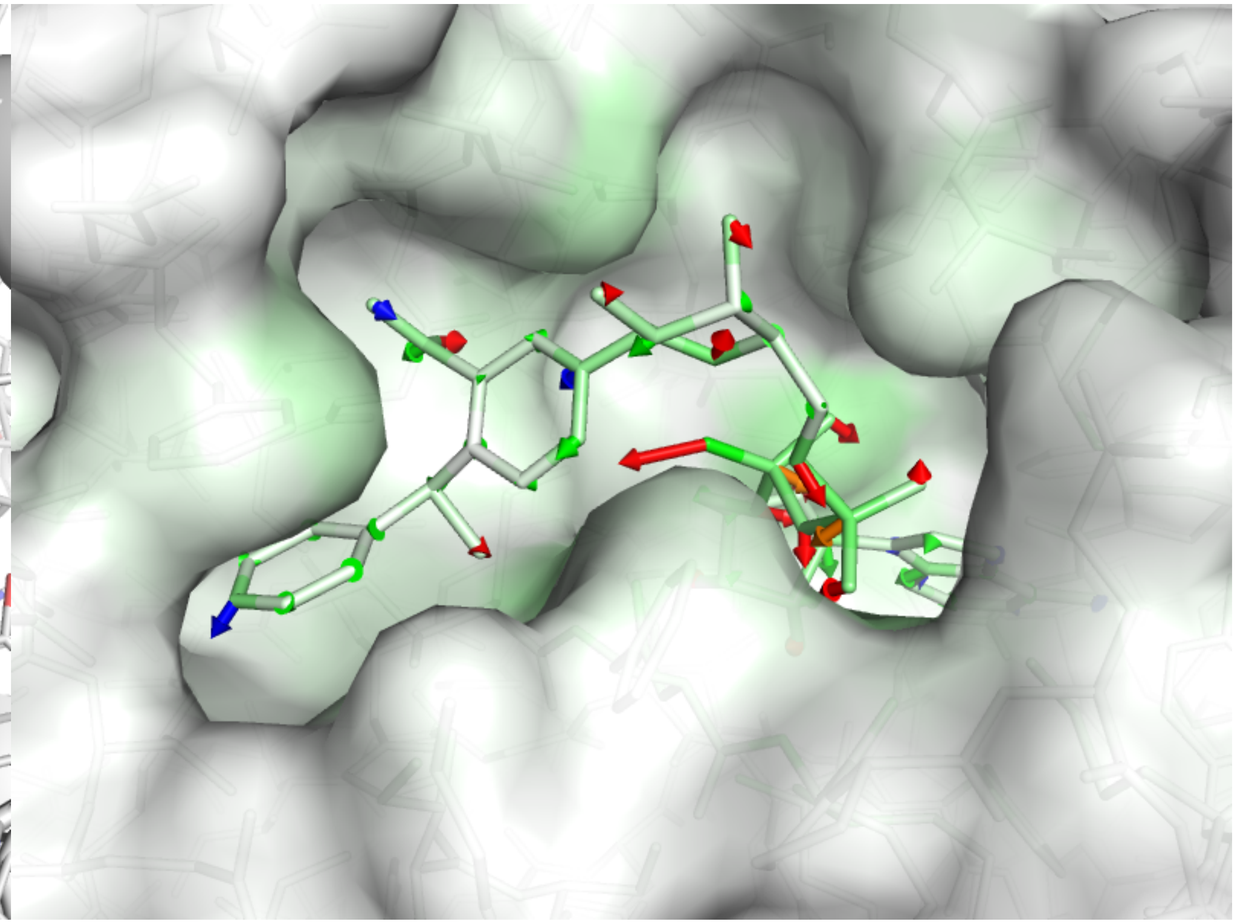
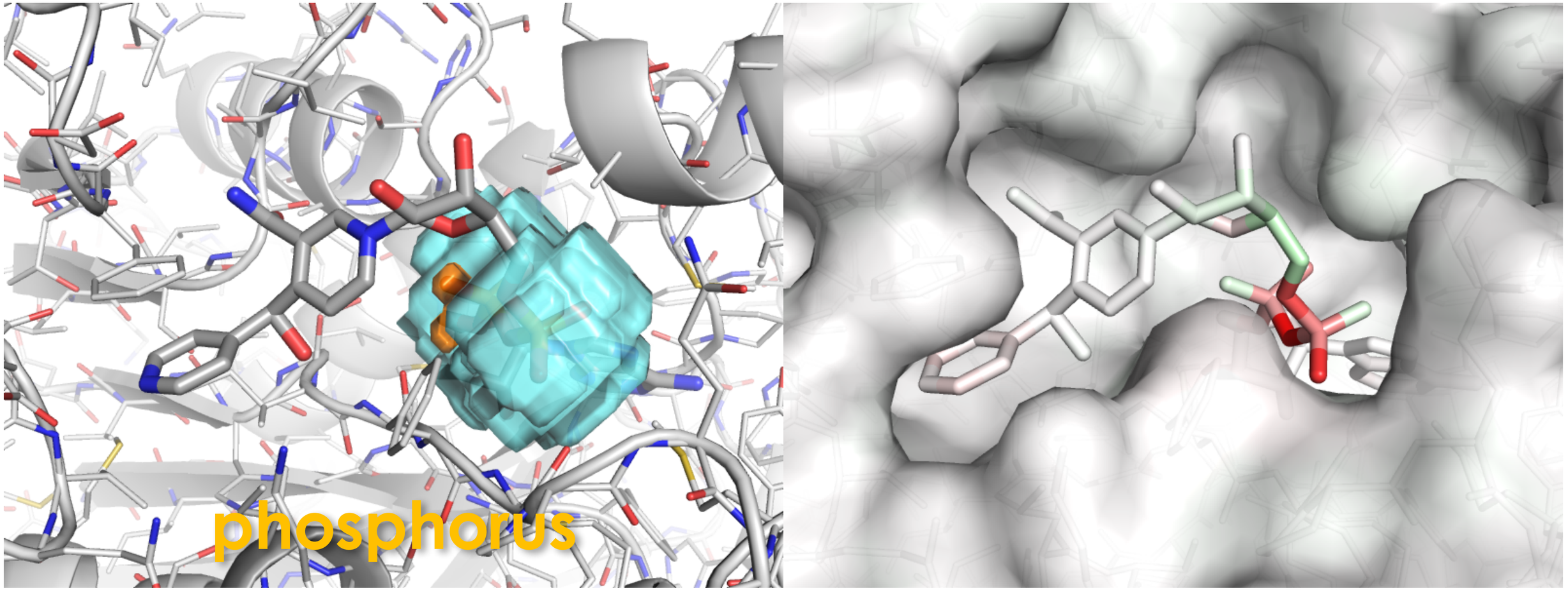
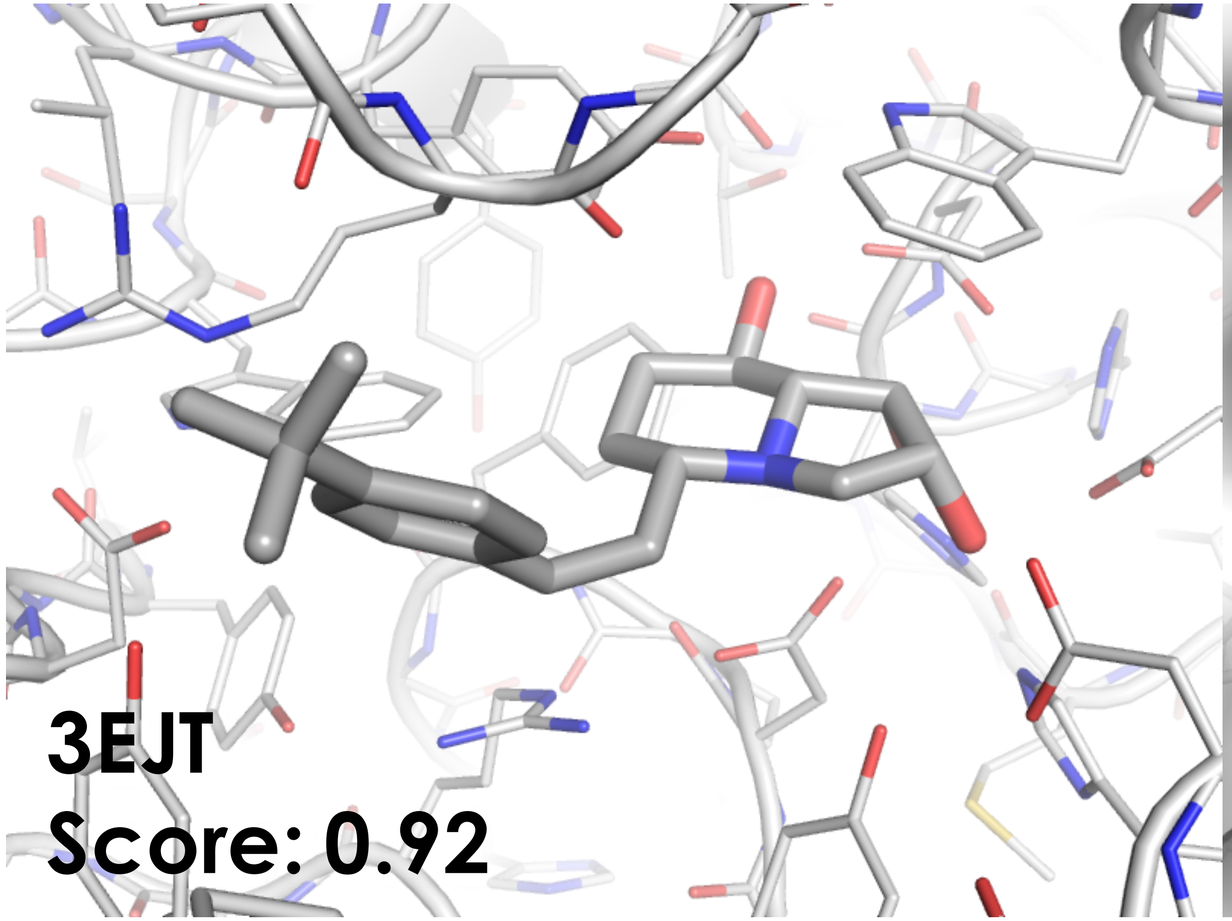


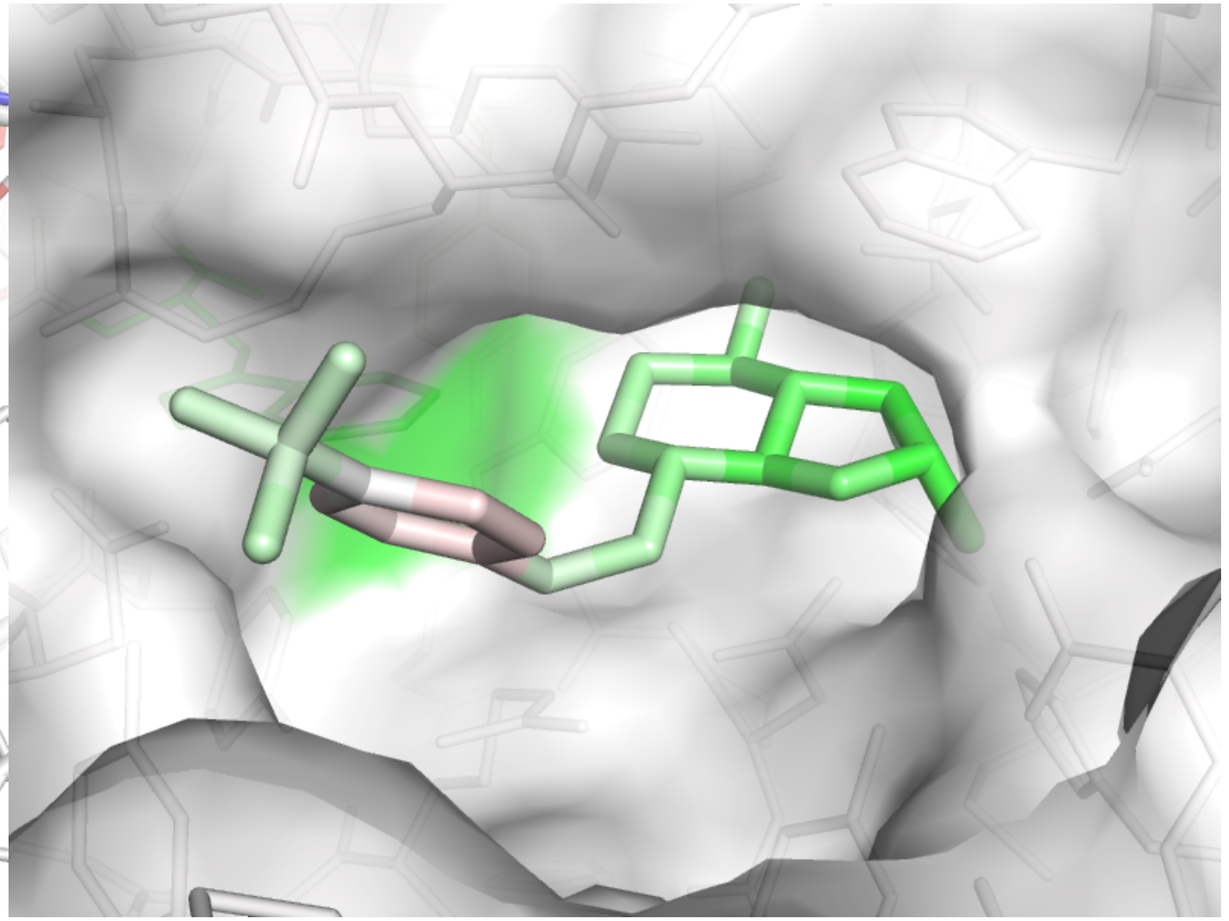


Gradients



Relevance





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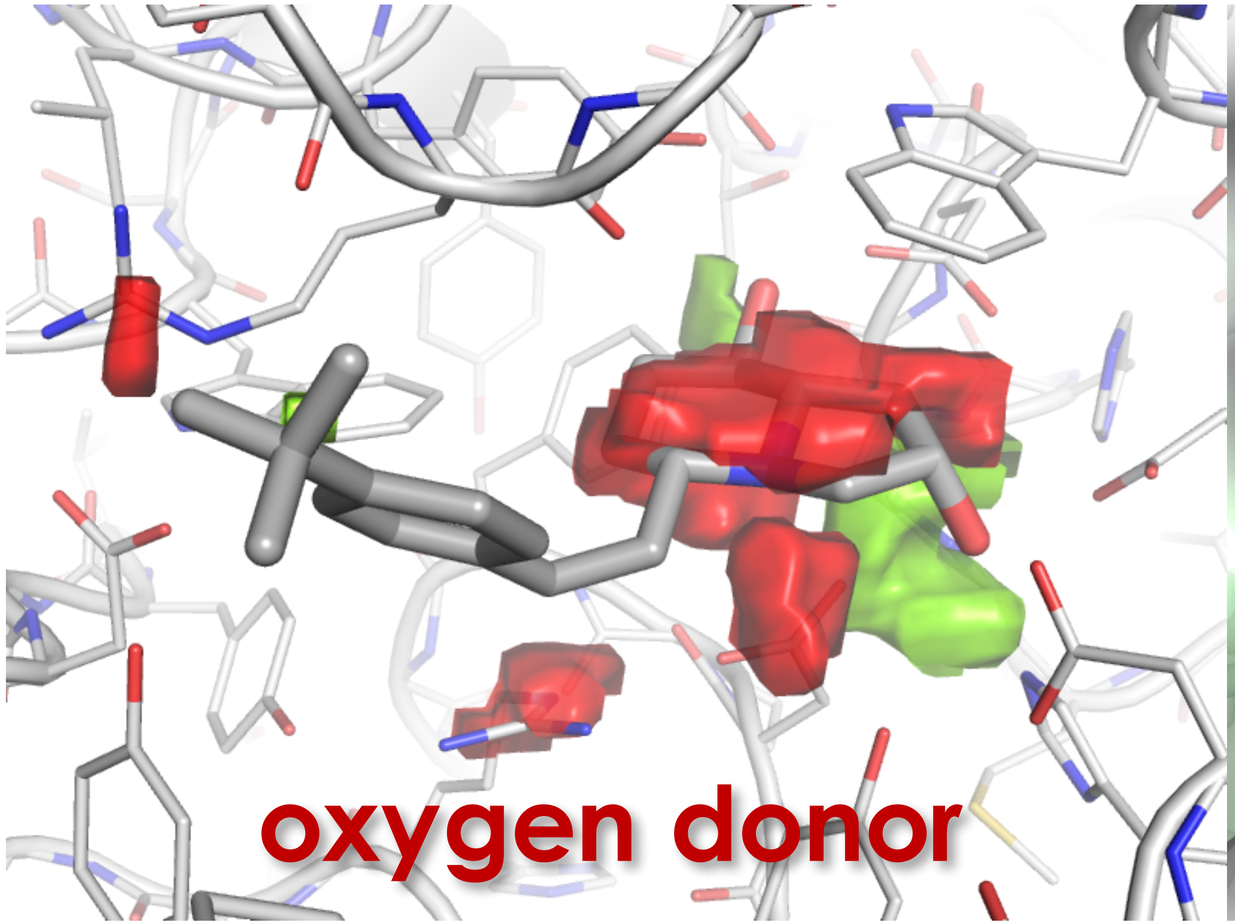
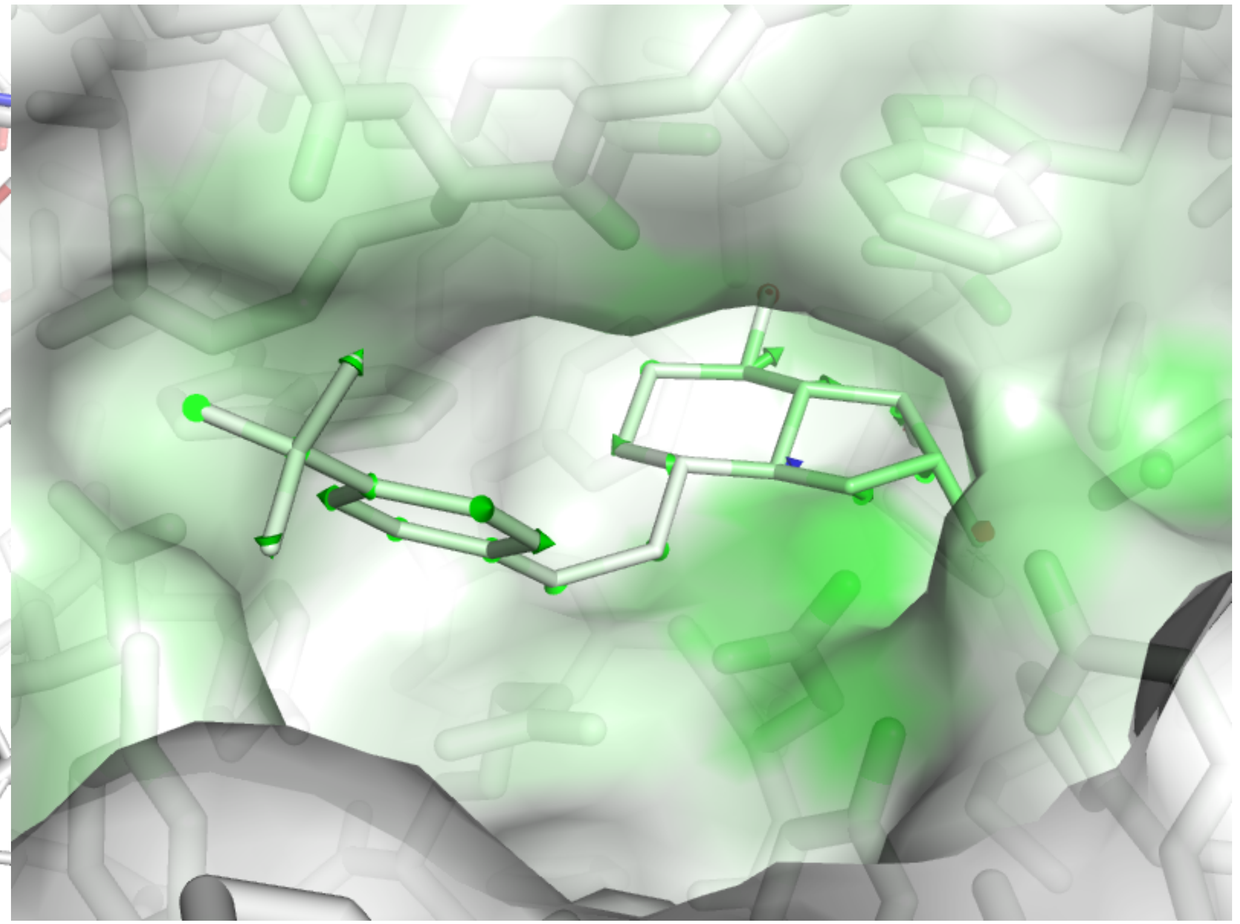
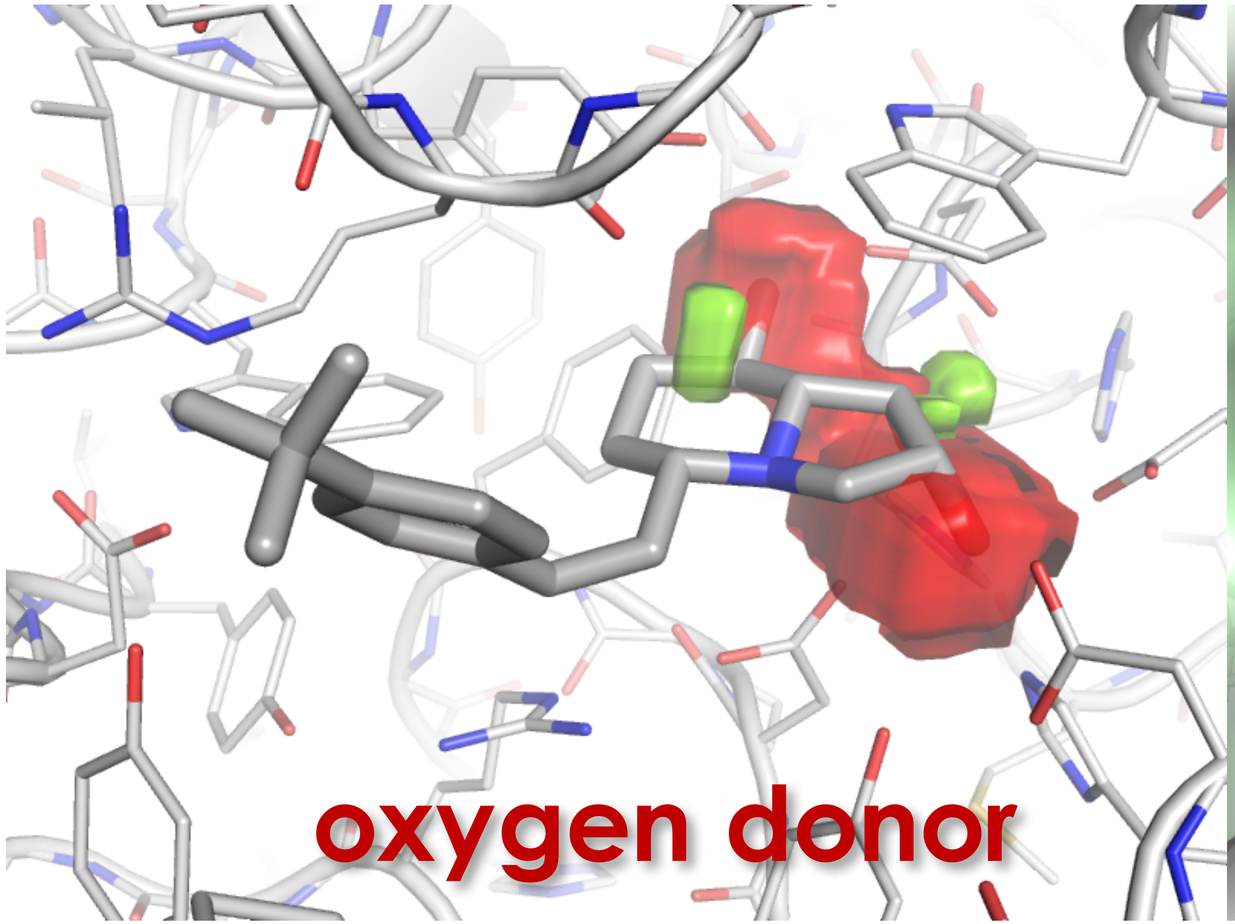
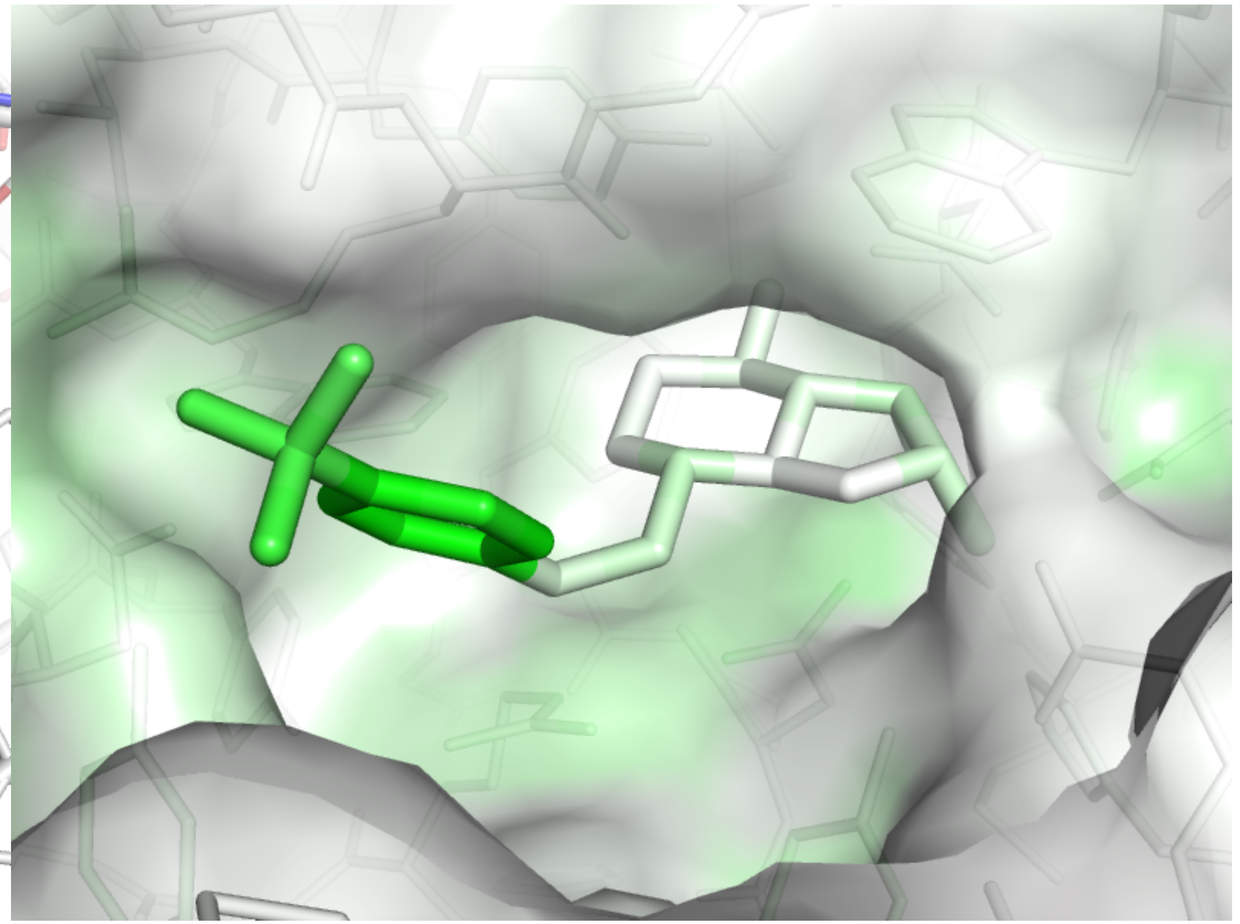




Gradients





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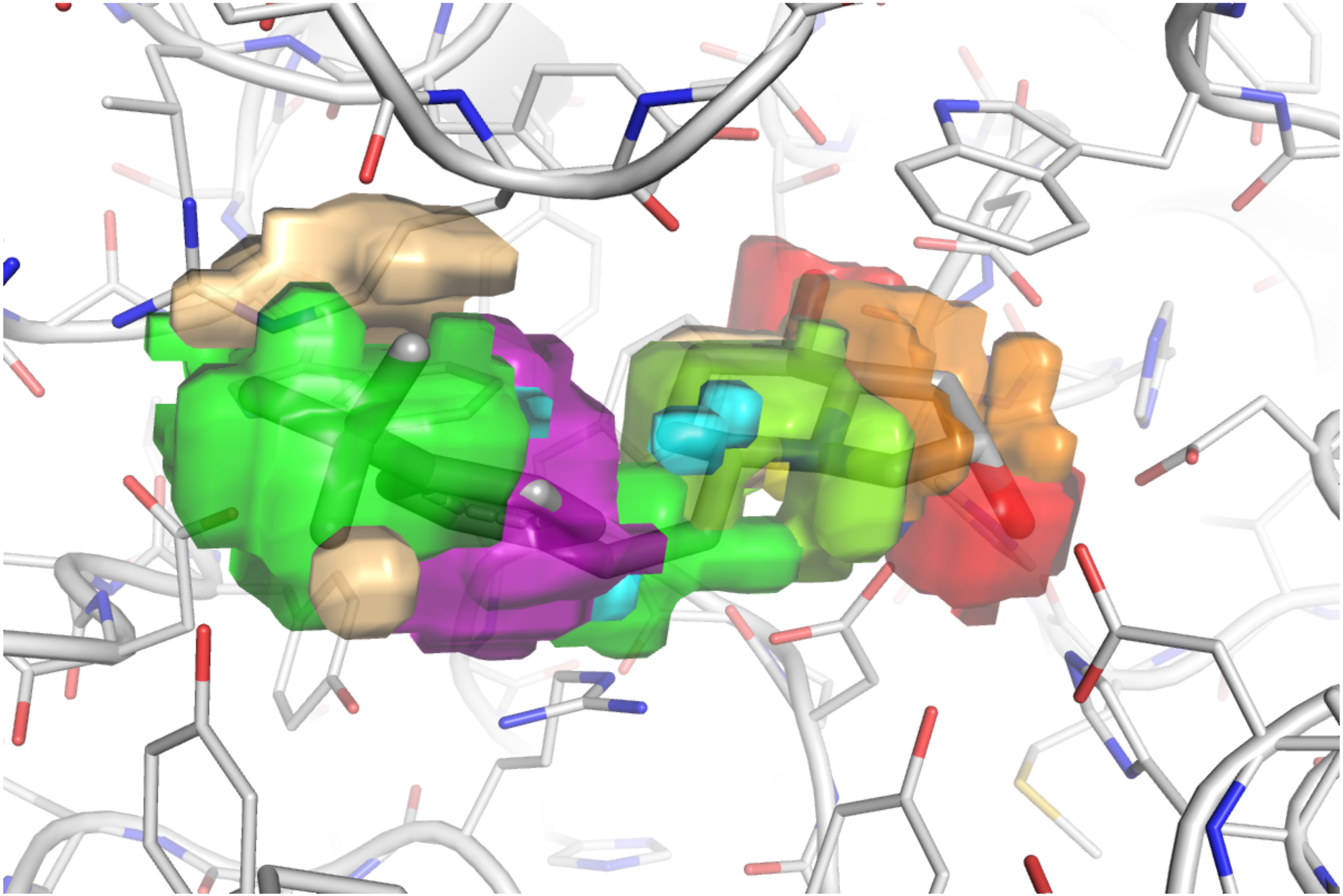
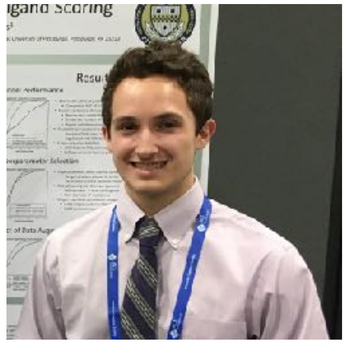
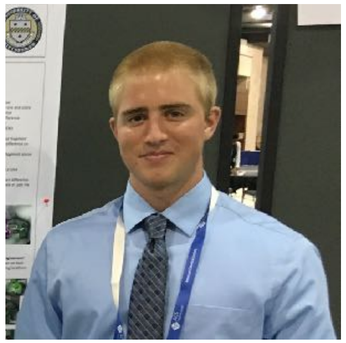


Acknowledgements

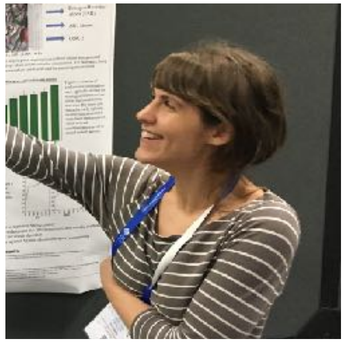


Matt Ragoza



Josh Hochuli

Elisa Idrobo



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