Electronic Supplementary Material (ESI) for Nanoscale.

Enabling Autonomous Scanning Probe Microscopy Imaging of Single Molecules with Deep Learning

- Supplementary Information -

Javier Sotres[1,2,*], Hannah Boyd[1,2], Juan F. Gonzalez-Martinez[1,2]

[1] Department of Biomedical Science, Faculty of Health and Society, Malmö University, 20506 Malmö, Sweden

[2] Biofilms-Research Center for Biointerfaces, Malmö University, 20506 Malmö, Sweden

[*] Corresponding author. E-mail: javier.sotres@mau.se

S1. Image augmentation for training Siamese networks

For training the Siamese network with triplet loss, the mined triplets were augmented before feeding them to the network. Augmentations included gentle (in order to be as close as possible to variations in topography expected to e.g., lateral drift, in real SPM experiments) zooming (up to ±20%), rotation (up to 10º) and shearing (up to 0.5º) of the images. Examples of mined triplets are provided in Fig. S1a along with augmented triplets in Fig. S1b.

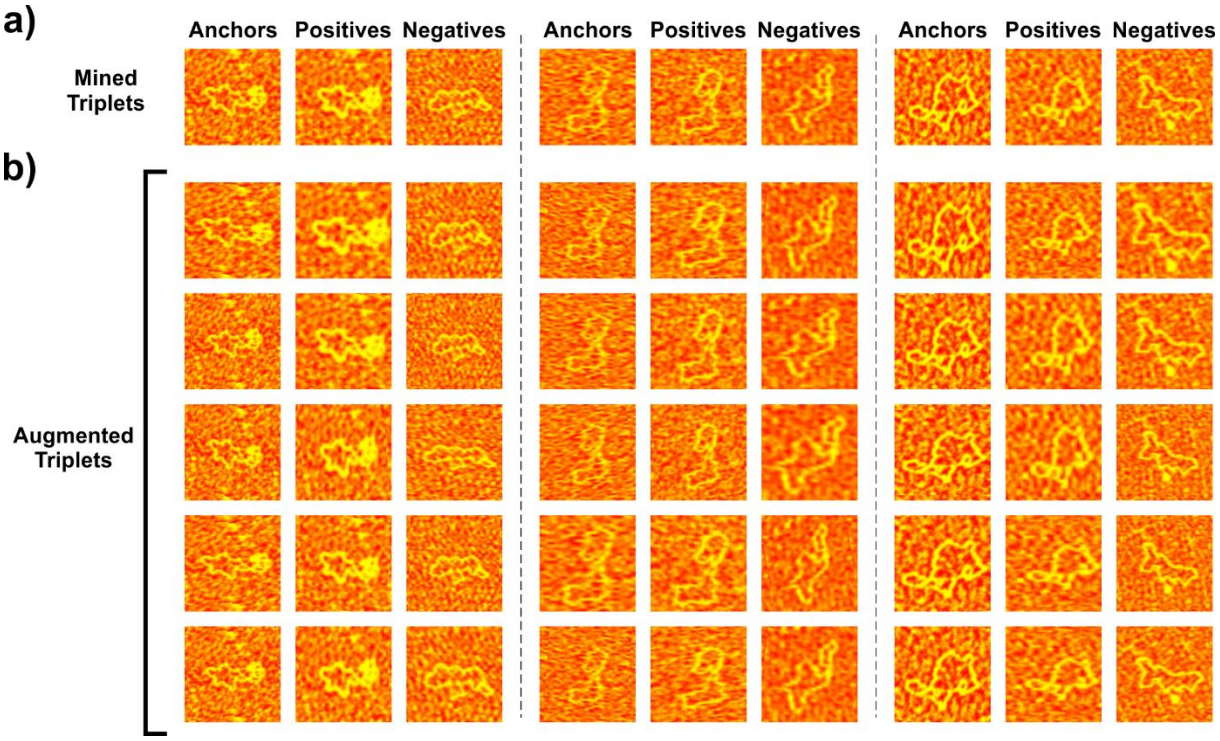

Figure S1. a) Examples of triplets mined from the dataset used to train our Siamese network. **b)** Triplets from a) after augmentation.