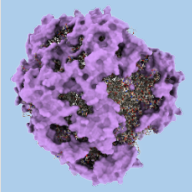


**EVONANO will reduce the simulation time to define a good nanoparticle design by using a complex deep learning approach**

### Solvent Accessible Surface Area (SASA)




- **87% decline** on average in 300 ns
- **Steady-state SASA denotes efficacy** of the drug design

**SASA**

### Objectives

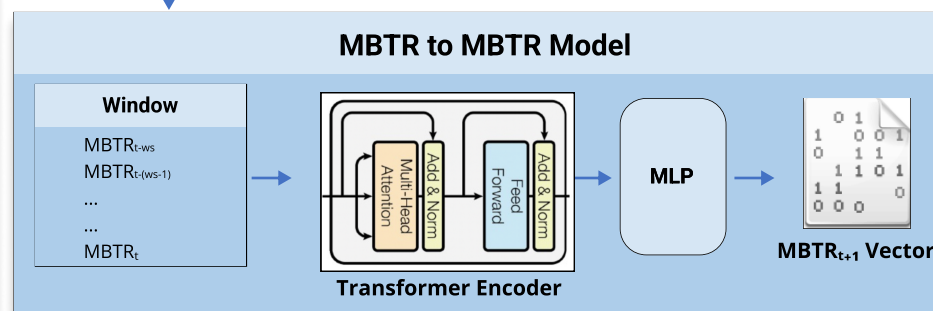
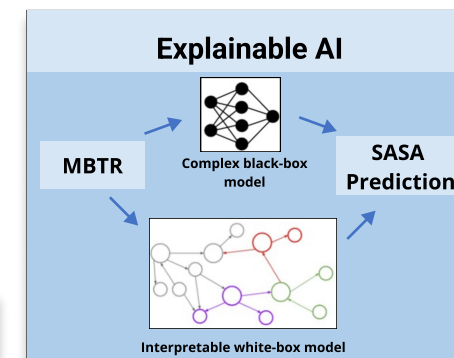
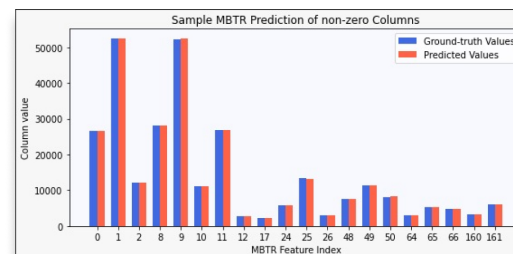
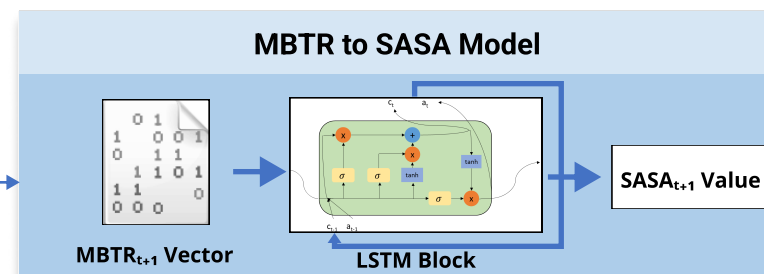
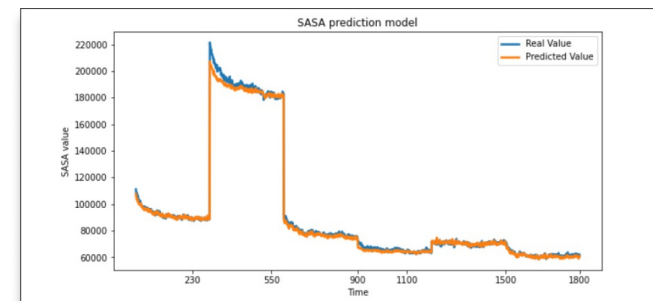
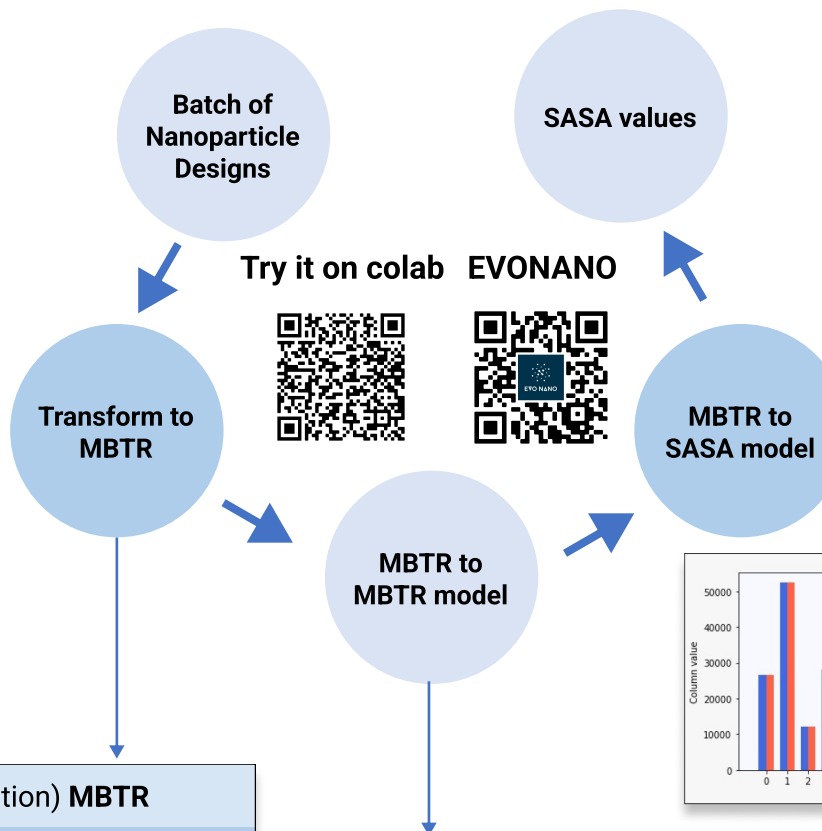
- Implement an approach to **reduce the simulation time** for a given design
- Provide **accurate prediction** of SASA value using neural networks
- **Explain the decision-making** process by the model

### (Many-body Tensor Representation) MBTR



**Atomic coordinates** → **Dscribe Library** → **MBTR Vector**

- MBTR descriptors are **robust** to nanoparticle **permutations, rotations**
- Used to **lower the dimensionality** of data significantly



### Challenges

- **Limited amount of data**
- Working with **Complex data**
- Dealing with **multivariate regression**