

#### **EVONANO:**

# **Evolvable Platform for Programmable** Nanoparticle-based Cancer Therapies









SASA<sub>t+1</sub> Value

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

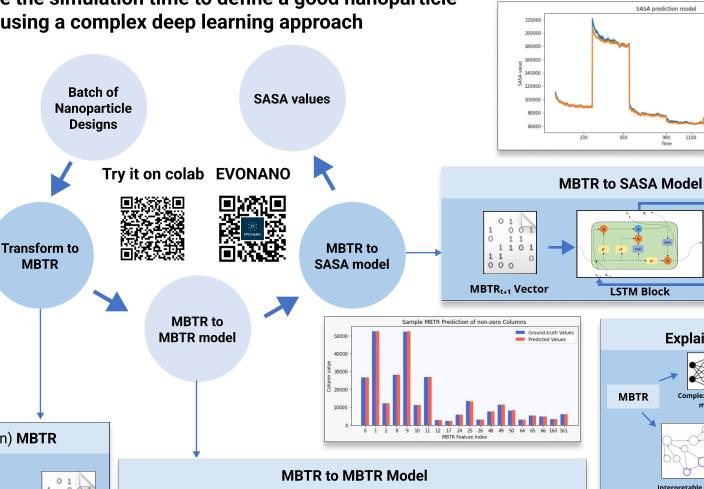
Window

MBTR<sub>t-ws</sub> MBTR<sub>t-(ws-1)</sub>

MBTR<sub>t</sub>

### Solvent Accessible Surface Area (SASA) 87% decline on average in 300 ns Steady-state SASA denotes efficacy of the drug design SASA Transform to **MBTR 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 1 1 0 1 **Atomic coordinates DScribe Library MBTR Vector** · MBTR descriptors are robust to nanoparticle permutations, rotations

Used to lower the dimensionality of data significantly



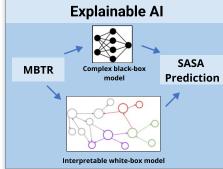
**Transformer Encoder** 

MLP

1 1 0 1

MBTR<sub>t+1</sub> Vector

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#### **Challenges**

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