Heavy hydrocarbon mixture property prediction using machine learning

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bp

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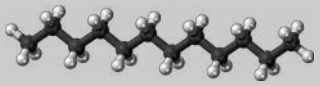
Black box neural network

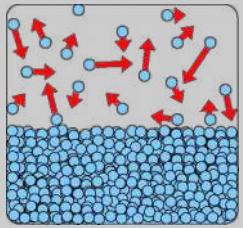
Molecule



Neural network

Viscosity

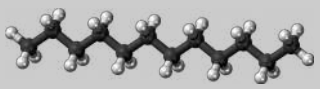
Volatility



Flash point

Training the network

Molecule



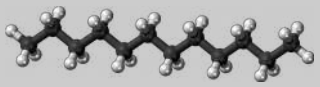
Viscosity

Volatility

Flash point

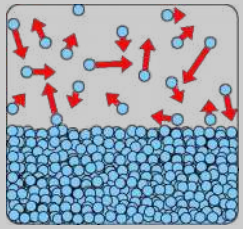
Using the network

Molecule



Viscosity

Volatility



Flash point

Neural network capabilities

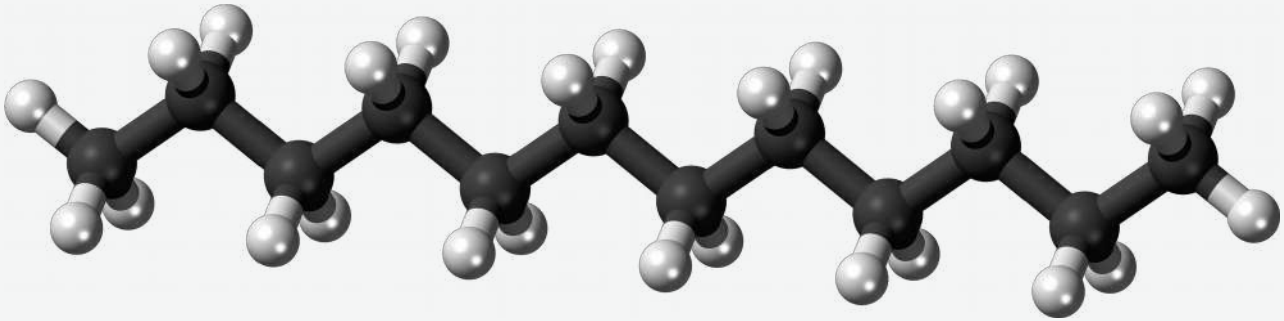
Deep learning on high-value fragmented data

Exploit underlying noise in data

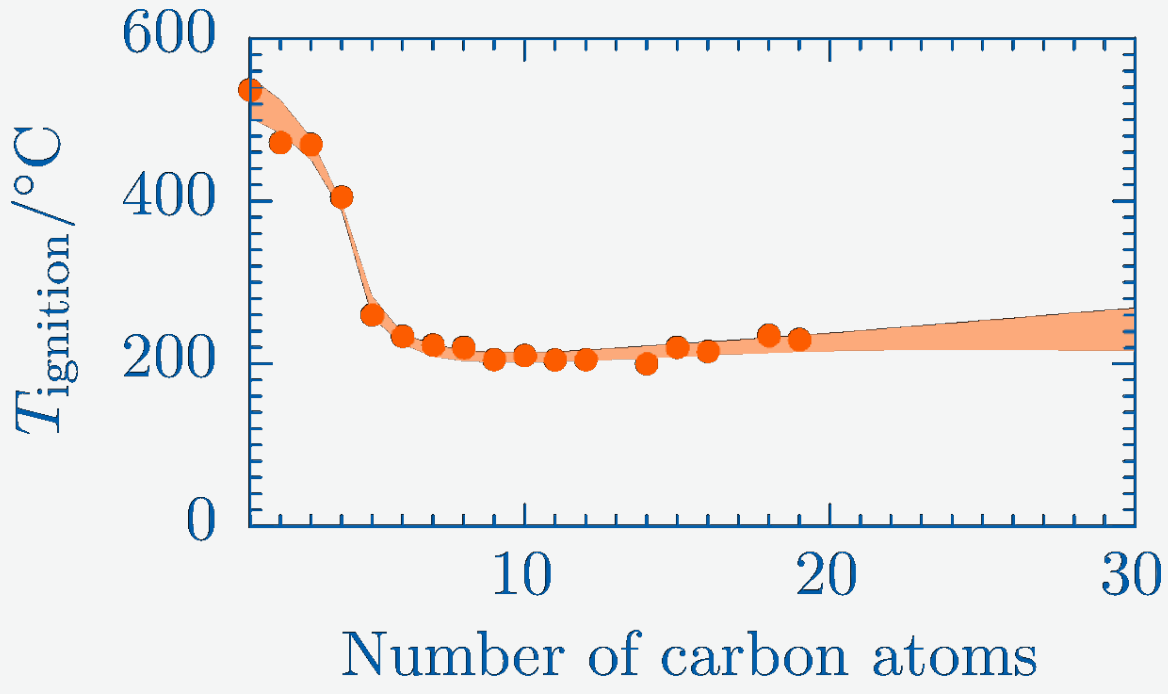
Merge experiments and simulations into a holistic lubricant design tool

Experimentally proven materials and drugs design with 7 companies, founded start-up intellegens

Straight chain alkanes



Preliminary results



Outlook

Apply deep learning to high-value data

Characterize mixtures of branched alkanes

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