# Deep Q-learning for the selection of optimal isocratic scouting runs in liquid chromatography

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**Gold statement**
- Machine learning for method development
- Reinforcement learning algorithm successfully selects scouting runs
- Application to the Neue-Kuss retention model

**Introduction**
Optimizing chromatographic conditions to obtain adequate separations for complex samples can still be a challenging task in chromatography. Retention modelling can help simplify this process. The main aim of this study was to develop a decision-making algorithm, based on reinforcement learning, that can automatically select suitable scouting runs to build such retention models.

**Body**
A suitable retention model is selected that can adequately predict the retention factor (k) of a compound as a function of the percentage of modifier in the mobile phase. To build this retention model, a reinforcement learning algorithm is trained to select adequate scouting runs for a large dataset of 10.000 simulated compounds, that mimic the retention behaviour of real compounds with a wide range in physicochemical properties. The algorithm is trained by rewarding it for picking scouting runs that result in adequate predictions of the retention factor, and punishing it when picking scouting runs that either lead to excessive analysis times, or have already been selected before. It is demonstrated that a reinforcement learning algorithm can be trained successfully to select a minimum number of scouting runs for real compounds, based on the characteristics of these compounds, and leading to retention models that can adequately predict the retention behaviour of these compounds over a wide range of mobile phase compositions.

**Conclusion**
The developed reinforcement learning algorithm selects scouting runs that result in retention models that perform equally well as retention models based on a large number (10) of scouting runs in only a fraction of the analysis time.