

# Draft Programme HRSMC Course Applied machine learning for chemistry 2026

April 8-May 1, 2026, UvA Science Park/UL/RUG/TUE

<b><u>Wednesday April 8</u></b>	<b><u>UvA Science Park – room H0.08</u></b>
10.00 - 12.00	Programming in Python by Prof. dr. Luuk Visscher
<i>Coffee break</i>	
12.15 - 13.15	Programming in Python by Prof. dr. Luuk Visscher
<b><u>Thursday April 9- Tuesday April 14</u></b>	Self-study Python
<b><u>Wednesday April 15</u></b>	<b><u>UvA Science Park – room H0.08</u></b>
10.00 - 12.00	Introduction to Machine Learning by Prof. dr. ir. Bernd Ensing
<i>Lunch break</i>	
13.00 - 15.00	Practical Part
<b><u>Thursday April 16</u></b>	<b><u>UvA Science Park – room A1.16</u></b>
10.00 - 12.00	Bayesian optimization for cost-effective molecular predictions by Dr. Alberto Pérez de Alba Ortíz
<i>Lunch break</i>	
12.45 - 14.45	Practical Part by Eline Kempkes
<b><u>Friday April 17</u></b>	<b><u>UvA Science Park – room H0.08</u></b>
10.00 - 12.00	Introduction to graph neural networks and generative AI by Prof. dr. ir. Bernd Ensing
<i>Lunch break</i>	
13.00 - 15.00	Practical Part
<b><u>Thursday April 23</u></b>	<b><u>RUG Feringa Building – room 5616.0125</u></b>
10.00 - 12.00	Hyperparameter optimisation by Dr. Robert Pollice
<i>Lunch break</i>	
13.00 - 14.00	Hyperparameter optimisation by Dr. Robert Pollice
14.00 - 17.00	Computer Practical
<b><u>Friday April 24</u></b>	<b><u>TU/e Ceres Building – room ICMS 0.31 (ground floor)</u></b>
10.00 - 12.00	Introduction to chemical language modelling by Dr. Francesca Grisoni
<i>Lunch break</i>	
13.00 - 15.00	hands-on practice
<b><u>Friday May 1</u></b>	<b><u>Leiden University Gorlaeus Building – room GM4.13</u></b>
10.00 - 12.00 (11.00 coffee break, Atrium)	AlphaFold Meets De Novo Drug Design - Structural Protein Information in Multitarget Molecular Generative Models by Prof. dr. Gerard van Westen
<i>Lunch break</i>	
13.00 - 17.00 (14.00 coffee break, Atrium)	Practical part
17.15-18.30	Drinks, Fusie (Gorlaeus Building, Ground Floor)