



SOCIETÀ ITALIANA DI
TOSSICOLOGIA

Società Italiana di Tossicologia (SITOX) Training Workshop on: *In Silico* Methods in Hazard Identification



25 January 2019 at the Università Degli Studi di Milano

9.30am	Registration	
10.00am	Welcome and Introduction to the Training Course <ul style="list-style-type: none">• Housekeeping	Prof Corrado Galli
10.10am	Introduction to <i>In Silico</i> Toxicology <ul style="list-style-type: none">○ Moving from 20th to 21st Century Toxicology○ From Chemistry Computational Methods	Mark Cronin
10.40am	Introduction to <i>In Silico</i> Toxicology Case Studies <ul style="list-style-type: none">○ <i>In silico</i> assessment of the hazard of skin sensitisation potential of two fragrance molecules	Mark Cronin
11.00am	Molecular Similarity (for Hazard Assessment) <ul style="list-style-type: none">○ “Find that Person” – Class Exercise	Chihae Yang
11.15am	Break	
11.30	Structure-Activity Relationships and Structural Alerts for Hazard Identification <ul style="list-style-type: none">○ Demonstration of ChemTunes Quantitative Structure-Activity Relationships (QSARs)	Mark Cronin, Chihae Yang
12.30	Lunch	
13.30	Read-Across for Hazard Identification Weight of Evidence	Mark Cronin, Chihae Yang
14.15	The VEGA Software – Predicting Toxicity <ul style="list-style-type: none">• Demonstration	Emilio Benfenati
14.45	Break	
15.00	3D Proteome-Wide Scale Screening to Predict Toxic Effects by the Innovative SPILLO-PBSS Software	Alessandro Di Domizio
15.45	<i>In Silico</i> Toxicology: Future Aspirations and Opportunities <ul style="list-style-type: none">○ Keeping up with the regulations Sum up	Mark Cronin, Corrado Galli
16.00	Close	