Società Italiana di Tossicologia (SITOX)

Training Workshop on:

***In Silico* Methods in Hazard Identification**

25 January 2019 at the Università degli Studi di Milano,

Dipartimento DISFeB, Via G. Balzaretti 9, Aula A

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| 9.30am | Registration |  |
| 10.00am | Welcome and Introduction to the Training Course   * Housekeeping | Prof Corrado Galli |
| 10.10am | Introduction to *In Silico* Toxicology   * + Moving from 20th to 21st Century Toxicology   + From Chemistry Computational Methods | Mark Cronin |
| 10.40am | Introduction to *In Silico* Toxicology Case Studies   * + *In silico* assessment of the hazard of skin sensitisation potential of two fragrance molecules | Mark Cronin |
| 11.00am | Molecular Similarity (for Hazard Assessment)   * + “Find that Person” – Class Exercise | Chihae Yang |
| 11.15am | Break |  |
| 11.30 | Structure-Activity Relationships and Structural Alerts for Hazard Identification   * + 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   * 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 | *In Silico* Toxicology: Future Aspirations and Opportunities   * + Keeping up with the regulations   Sum up | Mark Cronin, Corrado Galli |
| 16.00 | Close |  |