Proprietary modeling platforms to support regulatory interactions: A vendor's perspective

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Why Are We Here Today?

- "The primary concern that prevents a regulatory agency from incorporating predictions generated from proprietary modeling platforms into their decision-making processes is the lack of open access to the platforms and underlying models and databases"
  - **NOT TRUE!**
- "Regulators, academics, or members of the general public may not be able to replicate the model predictions, or to evaluate the predictive capability of the model within a desired chemical space"
  - **NOT TRUE!**
- "Is access to all modeling platforms (source code) and databases used to generate model outputs required to verify the output?"
  - **NO!**
- "Is evaluation of a model by the platform developer sufficient to provide confidence in the outputs of a model?"
  - **YES!**

Proprietary Modeling Platforms – The Reality…

- Proprietary modeling platforms are:
  - **Driving the vast majority of internal R&D activities** at companies
    - >200 global customers for Simulations Plus; 100s more outsource modeling projects
  - **Integrated into 100s of university courses (for free)** to teach and train students
  - **Implementing significant (and consistent) innovation** driven through collaborations between commercial software vendors, companies, and government/academic groups
    - Examples include funded consortiums through IMI, Cosmetics Europe, and the FDA
  - **Accessed by trained regulatory scientists globally** to efficiently support filings/applications

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- MYTH: 'Data' is hidden
  - ✓ **FACT: Software is fully documented and referenced**
    - ✓ **Product manual is an open book – ALL equations & references available for review**
  - ✓ **FACT: ALL model variables (data) can be viewed/modified/saved in various formats (e.g., Access databases, Excel spreadsheets, ASCII text files)**
- MYTH: Not available for everyone
  - ✓ **FACT: Free teaching licenses available**
  - ✓ **FACT: Discounted (or free, if allowed) licenses for regulatory agencies**
- MYTH: We don't know what it is doing
  - ✓ **FACT: 1000s of peer-reviewed journal articles, scientific posters, and conference presentations showcase predictability for different applications**

Suitability for Regulatory Support

- **Code/version/quality control**
  - ✓ Strict SOPs when implementing 'Voice-of-Customer' selected functionality
  - ✓ Feature/bug reports logged and assigned to different teams
  - ✓ New versions and patches released annually
- **'Real world' implementation & compliance considerations**
  - ✓ Consistent system validation procedures (to ensure compliance)
  - ✓ Access privilege definitions (administrator, user, reviewer)
  - ✓ Global support staff to address technical questions and train users
- **Platform qualification provides 'reproducibility confidence' to regulators**
  - ✓ 1000s of peer-reviewed journal articles, scientific posters, and conference presentations showcase predictability for different applications
  - ✓ No need for computer scientists on staff to review logic code, variable definitions, etc.

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Are we creating problems that don't exist?
Let's work together to find logical solutions!