

Acute Oral Systemic Toxicity Modeling – End User Applications

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Since 1902

- Subsidiaries in 71 countries
- Sales in nearly
 200 countries
- >90,000 employees
- 200+ factories
- Sales: >**\$30B**
- R&D investment: \$~2B
- 55,000+ products
- 100,000+ patents



Five Business Groups





Toxicology at 3M

Toxicology group resides in the Medical Department

• Corporate staff group reporting through Research and Development

Approximately 25 individuals

• Includes division support toxicologists and the Strategic Toxicology Laboratory (STL)

Centralized resource for toxicology

• Coordinates all global toxicity testing and human health risk assessments





Computational Toxicology Program Development



Product development and regulatory applications

- Screening estimates
- Internal hazard profiling
- GHS classifications
- Chemical registrations (REACH, etc.)
- Supporting information for regulatory submittals and risk assessments

Approaches		
Applicability domain knowledge is critica		
Most useful on chemistries with low toxicity potential		
Add internal data for model building		

GHS categories – more confidence in ranges than a single value

Ability to see analogs used to produce the estimate is very useful

Successes	Challenges
Weight of evidence approach to increases reliability	Regulatory acceptance for submittals
Minimize reliance on any one tool or approach	Applicability domain issues – no estimates for unique chemistries or unfounded estimates produced
Greatly reduced animal testing on low toxicity chemistries	Limited utility for polymers, inorganic constituents
Experience has helped establish the most useful approaches	Decision making when estimates don't align



Important Considerations for Software

Ease of use and expertise required

Applicability domain knowledge is critical

Cost and availability – free is best!!

Ability to see analogs used to produce the estimate

Regulator usage and acceptance

Ability to add internal historical data for model building

Thank you