

## **MetaPath, an international database on pesticide metabolism.**

### **Background**

MetaPath is an international collaborative project, developed in member countries of the OECD. It offers the availability of a database for the metabolism of pesticides in animals, plants, and in the various compartments of the environment. Originally developed by the Chemical Laboratory of Mathematical Bourgas (Bulgaria) and the US EPA, the database is now also carried by a group of users (MetaPath Users Group, MUG), including several member countries, organizations or industrials over the world.

This database consists of metabolic pathways for each pesticides as well as all the information available for the assessment of their metabolism. It is associated with a search interface that allows a cross-sectional analysis of the occurrence of metabolites in different organisms and to detect metabolites common to several pesticides; it will also predict the metabolic profile of a new molecule.

MetaPath consists of two modules; the first is the base containing all metabolic profiles and different assessment tools and research. The second module is independent software called *MSS composer (Metabolism Study Summary composer)* that allows to format summaries of existing data on the metabolism for incorporation in the database. A third module will be developed, and will consist of a modeling tool for predicting the metabolic profiles depending on the chemical properties of the active substance and matrices investigated. All of these modules will be integrated into the Qsar Toolbox tool, available on the OECD portal.

The *MSS composer* integrates data from evaluation reports generated by the various members of the MUG, such as DAR (Draft Assessment Reports) in Europe or the DER (Data Evaluation Report) in the United States or directly from the studies for new active substances. It also allows generating specific study reports in a text format that are used by the authorities in each country for their own evaluation. The *MSS composer* aims to serve as a portal for the electronic submission of data by industry in the context of authorization applications from institutions.

To date the MetaPath database already contains more than six hundred summaries of studies relating to pesticides metabolism in rats and farm animals, plants and rotational crops. The metabolism of more than three hundred active substances is well referenced and has been analyzed through several case studies conducted by the US-EPA, PMRA and Anses. The database is currently populated by the MUG with the aim to cover exhaustively all active substances.

### **Relevance to CCPR:**

MetaPath aims to become a common tool, available in the OECD Toolbox, which can be used by all agencies in charge of assessing pesticide risk worldwide. It also aims to standardize the electronic submission of data on the metabolism of pesticides and to share the results of the evaluation of the data. It will facilitate the harmonization of the regulatory assessment over

the world, particularly in terms of residue definition and integration of new common metabolites from different active substances or different organisms. Common residue definition is a key point for codex MRL acceptance all over the world.

**Speaker :** Xavier Sarda (France) on behalf of the Metapath User Group.

The screenshot displays the 'Metabolic Pathways' software interface. The main window shows a metabolic pathway for Acetamidin (14C-N6-25) in laying hens. The pathway starts with Acetamidin and branches into several metabolites, with some highlighted in red and others in blue. The interface includes a search bar, a list of chemical descriptors on the left, and a detailed information panel on the right.

**Metabolic Pathways - Highlight treatment groups**

**Common fields:**  
Laying hens; female; in vivo; oral; 10 mg/kg diet; white leghorn hybrids

**Coloring and specific:**  
 [0] excreta  
 [0] egg white  
 [0] egg yolk  
 [0] liver  
 [0] muscle  
 [0] skin (+fat)

**Treatment group:**  
Laying hens, female, in vivo, egg white, oral, 10 mg/kg diet, single dose (radioisotoped); white leghorn hybrids

**Reference:**  
Bunl, R., BA. 7.202 (1997): 14C-N6-25 (Acetamidin): Absorption, Distribution, Metabolism and Excretion after Repeated Oral Administration to Laying Hens

**Subjects:**  
• Species - Laying hens  
• Gender - Female (5 subjects)  
• Weight - Between 1.7 - 2 kg (female)  
• Age - 8 months old  
• Strain - White leghorn hybrids  
• Source - Geflügelzucht/Rüegg, CH-8330 Pfäfers/Switzerland  
• Housing - Metabolism units allowing the collection of excreta and eggs  
• Diet - Powdered hen feed ad libitum  
• Water - Tap water ad libitum