

# Current Status of Methods for Defining the Applicability Domain of (Quantitative) Structure–Activity Relationships

## The Report and Recommendations of ECVAM Workshop 52<sup>1,2</sup>

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## Preface

This is the 52nd report of a series of workshops organised by the European Centre for the Validation of Alternative Methods (ECVAM). The main objective of ECVAM, as defined in 1993 by its Scientific Advisory Committee, is to promote the scientific and regulatory acceptance of alternative methods which are of importance to the biosciences, and that *reduce, refine or replace* the use of laboratory animals.

The ECVAM workshop on the quantitative structure-activity relationship applicability domain was held at ECVAM on 29 September–1 October 2004, under the chairmanship of Andrew Worth. The workshop was attended by experts from academia, industry, international organisations and regulatory authorities. The aim of the

workshop was to review the state of the art of methods for identifying the domain of applicability of structure-activity relationships (SARs) and quantitative structure-activity relationships (QSARs), collectively referred to as (Q)SARs. The report is intended to provide a source of input to the development of an OECD Guidance Document on (Q)SAR Validation. The report also makes recommendations for further research needed to understand and apply the concept of the (Q)SAR applicability domain (AD).

## Introduction

(Q)SARs are theoretical models that can be used to predict the physicochemical, biological and environmental properties of chemicals.

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<sup>1</sup>ECVAM — *The European Centre for the Validation of Alternative Methods.* <sup>2</sup>*This document represents the agreed report of the participants as individual scientists.*