Preface

Quantitative structure–activity/property relationship (QSAR/QSPR) modelling has
been used in medicinal chemistry and computational toxicology for a long time. It
offers an in silico tool for the development of predictive models towards various
activity and property endpoints of a series of chemicals using the response data that
have been determined through experiments and molecular structure information
derived computationally or sometimes from experiments. Once developed and
validated, such models may be used for prediction of the response endpoint(s) for
new and untested chemicals and also for obtaining a mechanistic interpretation
of the structure–activity/property relationships. Although these techniques have
been successful in many lead optimization and risk assessment problems, their use
was previously limited to specific groups of researchers in the chemical sciences.
With the easy availability of QSAR-related software tools, QSAR/QSPR modelling
is now being exercised by a wider class of researchers; however, some of the users
might not have proper background theoretical knowledge in the area. It is desired
that QSAR/QSPR users should not depend solely on the available software for
model development; instead, they should have a basic working knowledge of the
theoretical aspects and principles of QSAR/QSPR modelling so that they can
develop statistically valid and predictive models which can be meaningfully
interpreted.

QSAR/QSPR of the present day is different from what it was during the initial
days of its evolution in the form of “Classical QSAR”. With the introduction of
newer (and higher dimensional) descriptors, the use of sophisticated chemometric
tools and rigorous validation strategies and integration with other ligand and
structure-based approaches, QSAR/QSPR of the present day is a recognized sci-
entific discipline. QSAR/QSPR is also finding newer applications in diverse fields
such as modelling properties/toxicities of nanomaterials, ionic liquids, chemical
mixtures, cosmetics, etc., making this an area of potential interest.
In this brief, we aim at introducing the fundamental concepts of QSAR/QSPR modelling in a nutshell to students of Chemical Sciences. The basic concepts seeded into the mind of the students would be a primer for the development of their further knowledge in the area through practical modelling exercises and/or additional readings.

Kolkata
December 2014

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A Primer on QSAR/QSPR Modeling
Fundamental Concepts
Roy, K.; Kar, S.; Das, R.N.
2015, X, 121 p. 47 illus., Softcover
ISBN: 978-3-319-17280-4