

## In this issue

### Enrichment of potent GSK-3 $\beta$ inhibitors

Glycogen synthase kinase-3 $\beta$  (GSK-3 $\beta$ ) is a unique multifunctional serine/threonine kinase that is inactivated by phosphorylation. GSK-3 $\beta$  has been linked to a diverse array of diseases like muscle hypertrophy, cancer, bipolar mood disorder, schizophrenia and diabetes. In addition, there is considerable interest in the clinical role of GSK-3 $\beta$  inhibitors with some compounds moving into the clinical phase of drug discovery time space.

P. K. Gadakar *et al.* report (page 1100) molecular docking experiments, in the active site of the X-ray crystal structures and induced fit models of GSK-3 $\beta$ . Using the docking score as the ranking metric, and by seeding the known GSK-3 $\beta$  inhibitors in a decoy set of World Drug



Index compounds enrichment was computed. They report that extra precision (XP) docking of compounds into the ensemble of protein structures either from X-ray data or induced fit models and ranking them by docking score leads to the best retrieval of actives in the top 5% and 10% of the database with significant enrichment. The study emphasizes the significance of induced fit models in such enrichment studies when experimental data are limited and it also clearly demonstrates that the XP docking leads to greater enrichment of the actives seeded amongst decoys. This methodology helps in prioritiz-

ing the compounds for screening to develop novel GSK3 $\beta$  modulators as early hits for drug discovery.

### Ethogram of courtship and mating behaviour of a lizard

Basic aspects of ethological studies are to decipher the meaning of animal's action and its origin. A prerequisite for deciphering the behavioural processes is to prepare an ethogram vis-à-vis a systematic chart of action patterns for a given behavioural repertoire such as courtship, mating, oviposition, aggression, mate selection and so on. Construction of an ethogram demands careful observations and recording of behaviour of the focal animals continuously for long period of time. This is followed by grouping of behavioural patterns in a coherent fashion leading to meaning of the behaviour.

Behavioural studies on Indian lizards are scanty. B. N. Pandav *et al.* (page 1164) present the ethogram of courtship and mating behaviour in



the garden lizard, *Calotes versicolor* (Agamidae) in captivity. They report 25 distinctive postures/gestures, orientation and simple movements exhibited by *C. versicolor* that are grouped into 14 functional categories. The functional categories are distinguished into three distinct phases of courtship and mating behaviour. The stereotypic pattern of ethogram related to courtship and mating behaviour described for *C. versicolor*

provides base line to undertake comparative studies on courtship and mating behaviour in other Indian agamids. Such studies are also helpful in elucidating the process of sexual selection, if any, in these lizards.

### Scotch broom

The montane grasslands of the Nilgiris, a complex ecosystem well known for its high diversity and endemism, is threatened by the expansion of introduced exotic woody plants. The problem is further aggravated due to a long period of inactivity by the management, possibly because the threat was poorly perceived and/or the deleterious consequences of the invasion were not highlighted well enough by the scientific community. M. P. Srinivasan *et al.* (page 1108) describe an effort to understand the threat posed by Scotch broom, one of the woody plant species introduced in the region as an ornamental during the colonial period. The population attributes of Scotch broom are quantified to determine if the population is indeed expanding and further plant community data is collated in invaded and uninvaded grasslands to examine the extent to which the invasion has modified the flora of the invaded grasslands. The data suggest that the current population trends of Scotch broom are a reason for concern, and though the decline in native species may seem less dramatic, the obvious changes in species composition as a result of invasion may push the ecosystem to a novel functional state. This work is a forerunner to a series of other experiments and surveys that are underway in the grasslands of the Nilgiris to gain a mechanistic understanding of the invasion process and also other aspects relating to community assembly and ecosystem functioning in these unique grasslands.