- In compound discovery, to select for further investigation those chemicals from among a set of candidates which are less or more likely to have toxic effects.

- Priorization of chemicals of environmental concern to permit the selection of those most in need of bioassay, inasmuch as the great majority of chemicals have not been, and never will be, tested.

- Investigation of detoxification by studying the effects of modifications of the structure on the toxic effect.

- Investigation of the toxic effects of putative metabolites.

- Identification of compounds for risk assessment.

- Assessment of mutagenicity and carcinogenicity indicators (Ashby and Tennant, 1988).

The SAR method can also be used to understand the potential toxic action of a novel compound, once the molecular structure has been determined. In theory, at least, it should be possible to compare the salient clinico-pathological findings, obtained from a thorough epidemiological study, with the GC/MS data and molecular configuration of the found compound, and to try to match the two sets of observations. There is, however, one severe limitation to the SAR method: current models cannot handle mixtures if there is any presupposition of interaction between compounds, i.e., synergism or antagonism, because very few data exist for such mixtures.