

## Supplementary Information

### Supplementary Information 1

The SMILES and respective Log BCF values of each compound of the dataset; The descriptors of the PLS based QSPR model; The descriptors of the PLS based q-RASPR model; PPDB screened output file obtained from PRI tool; Excluded compounds from the original dataset; List of descriptors involved during entire modelling procedure.

### Supplementary Information 2

Chemical diversity plot of training and test sets (**Fig. S1**). Different PLS plots (**Figs: S2-S4**) of the developed PLS-based q-RASPR models for Log BCF endpoint. Ranking of the compounds of PPDB based on their bioaccumulative potential (**Fig. S5**). Detailed list of RASPR descriptors and their definition in **Table S1**. Twenty most and least bioaccumulative screened pesticides from the Pesticide Properties DataBase (PPDB) in **Table S2**.