**Supplementary Table 1.** List of the molecular descriptors used from PowerMV.

|  |  |  |
| --- | --- | --- |
| Pharmacophore  Fingerprint | Weighted Burden Number | Property |
| NEG\_01\_NEG- NEG\_07\_NEG  NEG\_03\_POS-NEG\_07\_POS  NEG\_01\_HBD-NEG\_07\_HBD  NEG\_03\_HBA-NEG\_07\_HBA  NEG\_02\_ARC-NEG\_07\_ARC  NEG\_02\_HYP-NEG\_07\_HYP  POS\_03\_POS-POS\_07\_POS  POS\_02\_HBD-POS\_07\_HBD  POS\_03\_HBA-POS\_07\_HBA  POS\_02\_ARC-POS\_07\_ARC  POS\_02\_HYP-POS\_07\_HYP  HBD\_03\_HBD-HBD\_07\_HBD  HBD\_03\_HBA-HBD\_07\_HBA  HBD\_02\_ARC-HBD\_07\_ARC  HBD\_02\_HYP-HBD\_07\_HYP  HBA\_03\_HBA-HBA\_07\_HBA  HBA\_03\_ARC-HBA\_07\_ARC  HBA\_02\_HYP-HBA\_07\_HYP  ARC\_01\_ARC-ARC\_07\_ARC  ARC\_02\_HYP-ARC\_07\_HYP  HYP\_01\_HYP-HYP\_07\_HYP | WBN\_GC\_L\_0.25, WBN\_GC\_H\_0.25,  WBN\_GC\_L\_0.50, WBN\_GC\_H\_0.50,  WBN\_GC\_L\_0.75, WBN\_GC\_H\_0.75,  WBN\_GC\_L\_1.00, WBN\_GC\_H\_1.00,  WBN\_EN\_L\_0.25, WBN\_EN\_H\_0.25,  WBN\_EN\_L\_0. 50, WBN\_EN\_H\_0. 50,  WBN\_EN\_L\_0.75, WBN\_EN\_H\_0.75,  WBN\_EN\_L\_1.00, WBN\_EN\_H\_1.00,  WBN\_LP\_L\_0.25, WBN\_ LP \_H\_0.25,  WBN\_ LP \_L\_0. 50, WBN\_ LP \_H\_0. 50,  WBN\_ LP \_L\_0.75, WBN\_ LP \_H\_0.75,  WBN\_ LP \_L\_1.00, WBN\_ LP \_H\_1.00 | XLogP, PSA, NumRot,  NumHBA, NumHBD, MW,  BBB, BadGroup |