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

|  |  |  |
| --- | --- | --- |
| Pharmacophore Fingerprint | Weighted Burden Number | Property |
| NEG\_01\_NEG- NEG\_07\_NEGNEG\_03\_POS-NEG\_07\_POSNEG\_01\_HBD-NEG\_07\_HBDNEG\_03\_HBA-NEG\_07\_HBANEG\_02\_ARC-NEG\_07\_ARCNEG\_02\_HYP-NEG\_07\_HYPPOS\_03\_POS-POS\_07\_POSPOS\_02\_HBD-POS\_07\_HBDPOS\_03\_HBA-POS\_07\_HBAPOS\_02\_ARC-POS\_07\_ARCPOS\_02\_HYP-POS\_07\_HYPHBD\_03\_HBD-HBD\_07\_HBDHBD\_03\_HBA-HBD\_07\_HBAHBD\_02\_ARC-HBD\_07\_ARCHBD\_02\_HYP-HBD\_07\_HYPHBA\_03\_HBA-HBA\_07\_HBAHBA\_03\_ARC-HBA\_07\_ARCHBA\_02\_HYP-HBA\_07\_HYPARC\_01\_ARC-ARC\_07\_ARCARC\_02\_HYP-ARC\_07\_HYPHYP\_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 |