**Supplementary data**

**Insight into structural features of phenyltetrazole derivatives as ABCG2 inhibitors for the treatment of multidrug resistance in cancer**

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**Supplementary Fig. 1S** Predicted vs Observed *pIC50* plot of (A) training set, (B) test set compounds.

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| **Supplementary Fig. 2S** Structures of compounds showing importance of descriptor *nAtomLC* |

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| **Supplementary Fig. 3S** Structures of compounds showing importance of descriptor *minHBint5* |

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| **Supplementary Fig. 4S** Structures of compounds showing importance of descriptor *piPC10* |

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| **Supplementary Fig. 5S** Structures of compounds showing importance of descriptor *ATSC4i* |

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| **Supplementary Fig. 6S** Structures of compounds showing importance of descriptor *ATSC4c* |
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| **Supplementary Fig. 7S** The structures of compounds **03**, **04**, **05**, **19** |

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| **Supplementary Fig. 8S** The structures of compounds **63**, **64**, **65** |

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| **C:\Users\Bhagwati\Autodockvina\6eti\6_cpd_64_2d.png**  **Supplementary Fig. 9S** 2D diagram showing binding interactions of compound 64  C:\Users\Bhagwati\Autodockvina\6eti\1_cpd_27_2d.png  **Supplementary Fig. 10S** 2D diagram showing importance of –NO2  group in making H-bond with T435 residue (compound **27**) |

**Supplementary Table 1S. Y-randomization results for training set and test set for the 2D QSAR**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Test Set** | | **Training Set** | |
| **Model** | ***R*** | ***R2*** | ***R*** | ***R2*** |
| Original | 0.925943 | 0.857371 | 0.82565 | 0.681699 |
| Random 1 | 0.416494 | 0.173468 | 0.263293 | 0.069323 |
| Random 2 | 0.269648 | 0.07271 | 0.182641 | 0.033358 |
| Random 3 | 0.345275 | 0.119215 | 0.548226 | 0.300551 |
| Random 4 | 0.730119 | 0.533074 | 0.301087 | 0.090654 |
| Random 5 | 0.786094 | 0.617943 | 0.390734 | 0.152673 |
| Random 6 | 0.721348 | 0.520343 | 0.394003 | 0.155238 |
| Random 7 | 0.652865 | 0.426233 | 0.228911 | 0.0524 |
| Random 8 | 0.468805 | 0.219778 | 0.474681 | 0.225322 |
| Random 9 | 0.705497 | 0.497726 | 0.326127 | 0.106359 |
| Random 10 | 0.186474 | 0.034773 | 0.299583 | 0.08975 |
| Average *r* : | 0.528262 |  | 0.340929 |  |
| Average *r2* : | 0.321526 |  | 0.127563 |  |
| *cR2p* | 0.70415 |  | 0.620868 |  |