Article

Supplementary data

The Maxi-K (BK) Channel Antagonist Penitrem A as A Novel Breast Cancer Targeted Therapeutic

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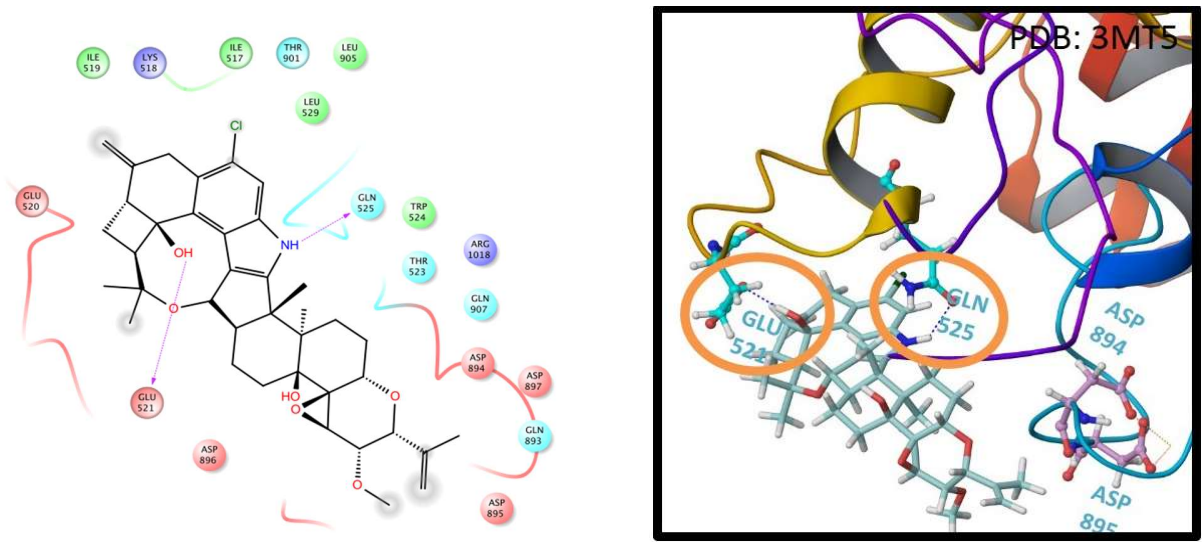
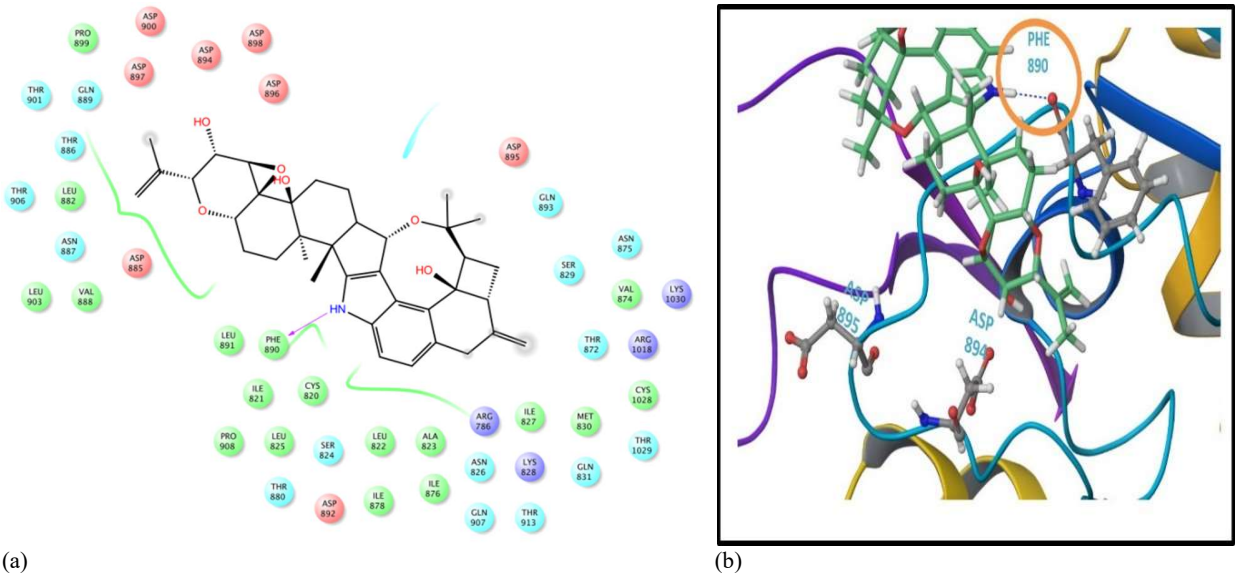


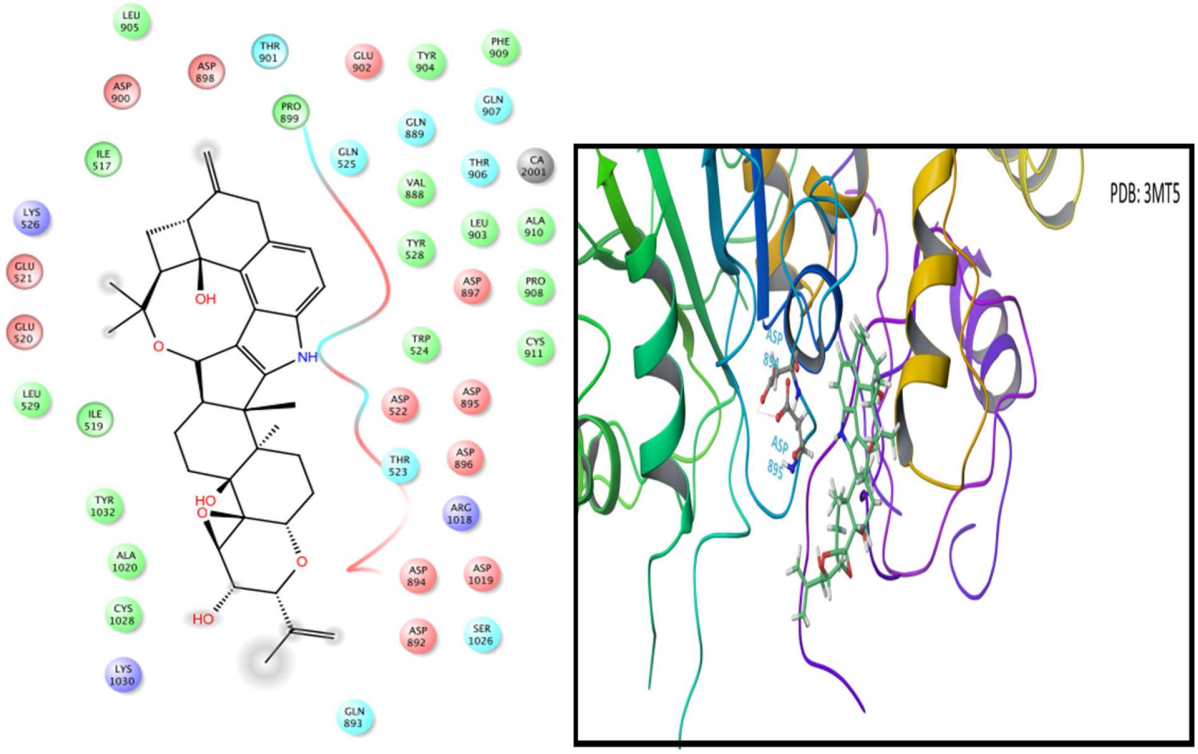
(a) (b)

Figure S1. The 2D binding mode and interactions of **3** at the calcium bowel of the BK channel PDB crystal structure 3MT5. Its C-15 tertiary hydroxyl group contributed hydrogen bonding donor interaction with GLU521 while its NH-1 showed hydrogen bonding donor interaction with GLN525. (b) The overlay of the 3D structure of **3** at the calcium bowel of the BK channel PDB crystal structure 3MT5.



(a) (b)

Figure S2. (a) The 2D binding mode and interactions of **2** at the calcium bowel of the BK channel PDB crystal structure 3NAF. Penitrem E showed only one interaction, its NH-1 contributed hydrogen bonding donor interaction with PHE890. (b) The overlay of 3D structure of **2** at the calcium bowel of the BK channel PDB crystal structure 3NAF.



(a) (b)

Figure S3: No interaction of **2** at the calcium bowel of the PDB: 3MT5 crystal structure of the BK channel.