**Table S4. Docking molecular from compounds on the E-monomer (C-Terminal Harpin):** The best affinities calculated from molecular docking analysis on the E monomer (C-terminal Hairpin).

| Docking molecular from compounds on the E-monomer (C-Terminal Harpin). | | |
|---|---|---|
| Drug | Affinity (kcal/mol) | Amino acids |
| Irinotecan | -8.2 | Phe20, Phe23, Leu27, Leu73, Leu74, Val47, Val58, Ile46, Val49, Leu51, Tyr57, Ser55, Tyr59 |
| Nilotinib | -8.2 | Ser55, Tyr57, Tyr59, Leu74, Val75, Leu51, Val58, Val62, Arg69, Pro71, Val70 |
| Avodart | -8.1 | Val47, Leu27, Ile46, Leu51, Val70, Try57, Val58, Val49, Val75, Leu74, Pro71 |
| Fexofenadine | -8.0 | Val58, Val62, Val70, Try59, Val75, Tyr57, Ser55, Leu51, Leu65, Arg61, Ser67, Arg69, Pro71, Asp72 |
| Ternadin | -8.0 | Tyr57, Ser55, Val58, Leu51, Tyr59, Val75, Val62, Leu65, Ser67, Arg61, Ser68, Arg69, Val70, Asp72 |
| Lumacaftor | -7.9 | Ser55, Leu51, Val62, Ser68, Arg69, Tyr57, Pro71, Val75, Leu74, Val70, Val58 |
| Amaryl | -7.8 | Ser55, Tyr57, Val58, Val70, Pro71, Leu74, Val75, Val49, Leu27, Val47, Ile46, Ser50, Leu51 |
| Saquinavir | -7.7 | Val70, Arg61, Pro71, Tyr57, Leu74, Leu51, Phe56, Val52, Ser55, Tyr59, Val75, Val58 |
| Naldemidine | -7.7 | Lys63, Leu65, Arg69, Ser67, Ser68, Val70, Arg61, Leu74, Val62, Try59, Val58, Val75 |