Mathematical Biology and Bioinformatics
2023. V. 18. № 1. P. s1–s7

Additional material to the article
Nambigari N. Mathematical Biology and Bioinformatics. 2023. V. 18. № 1. P. 72–88
doi: 10.17537/2023.18.72

SUPPLEMENTARY FIGURES S1–S3 AND TABLE S1

Fig. S1. Compatibility of PDGF-C protein model (3D) with its own amino acid sequence (1D) using Verify3D.

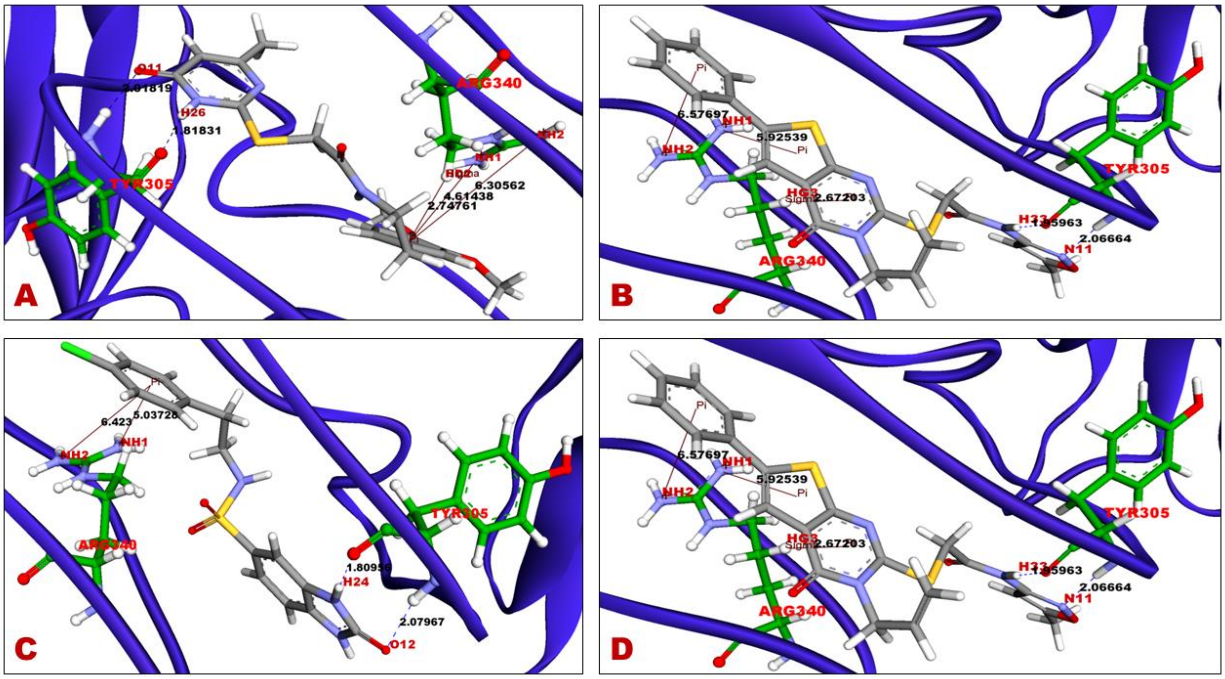


Fig. S2. Binding poses of ligands with PDGF-C protein. Schematic representation of poses of the ligands (A-D) (shown in grey colour sticks), bound to the PDGFC protein amino acid residues (shown in green color ball and sticks), forming H-bonds, π-π and π-cation interactions are represented in blue dotted and brown lines respectively.

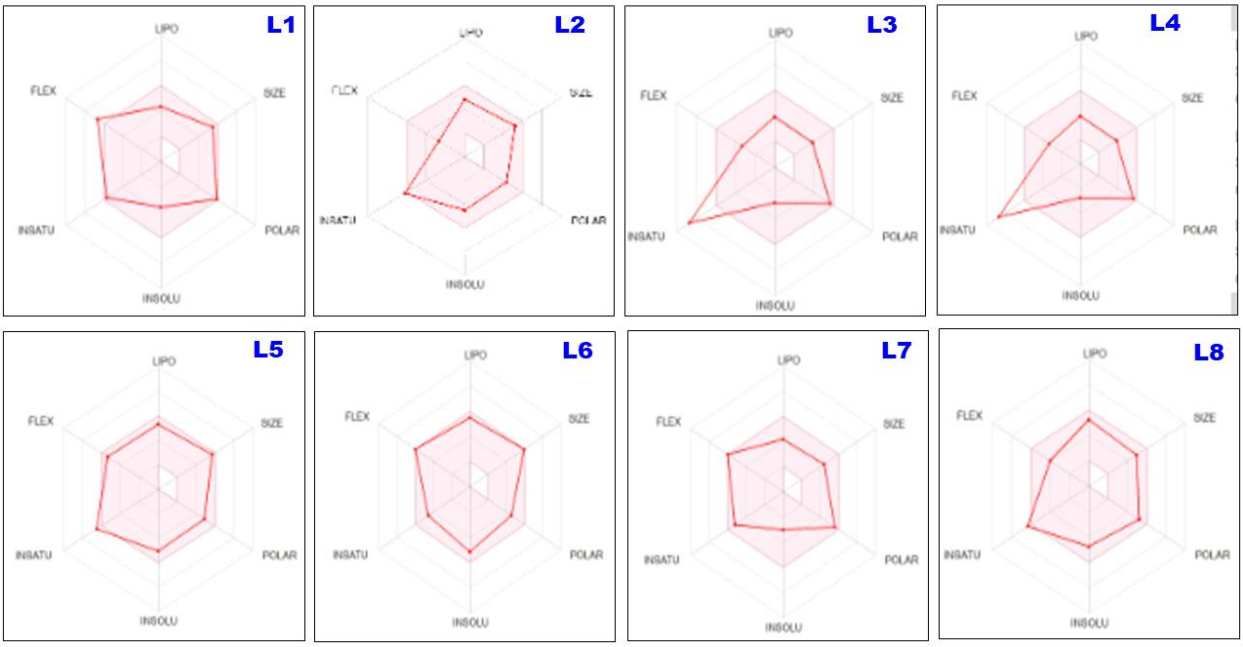
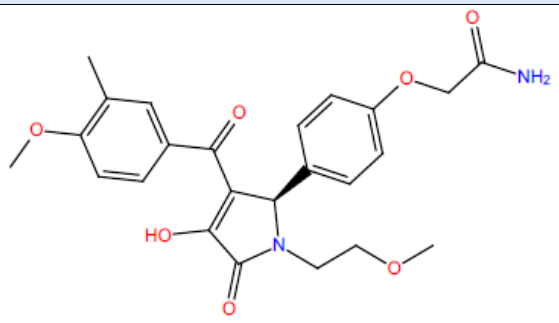
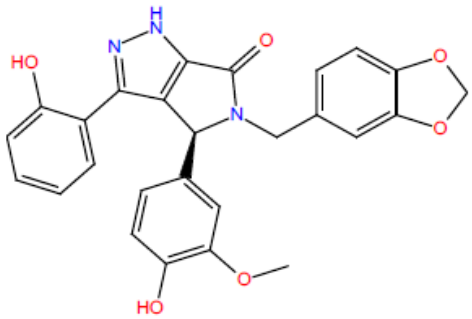
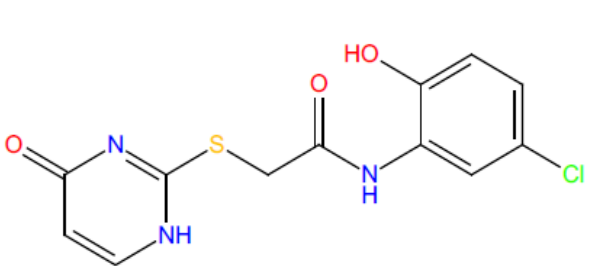
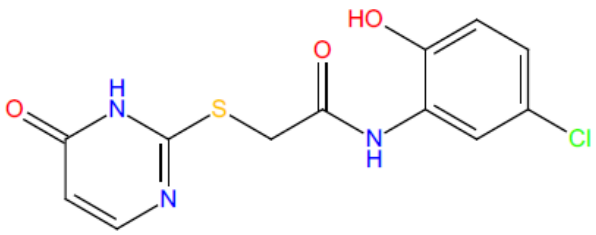
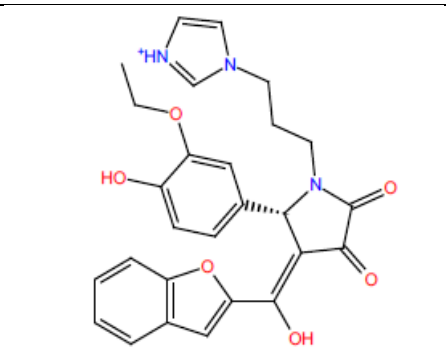
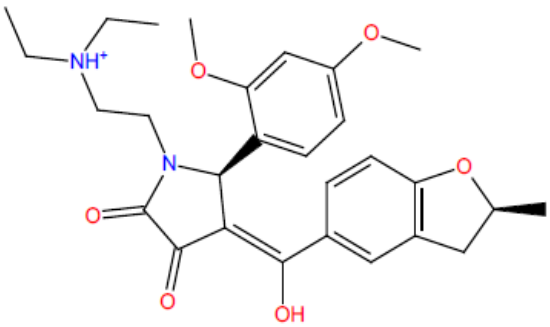
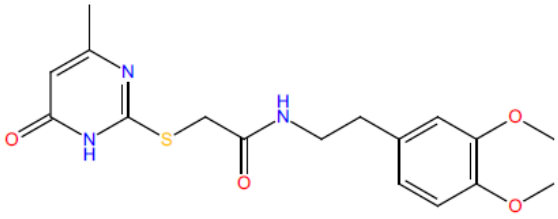
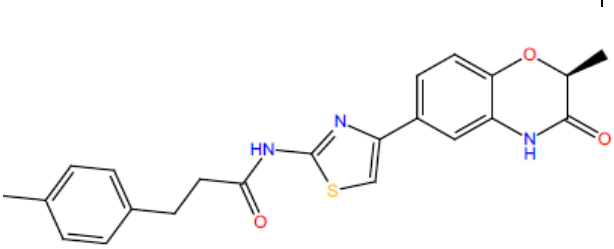
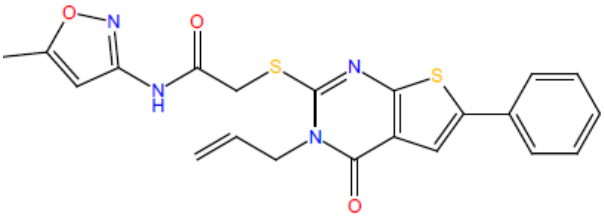
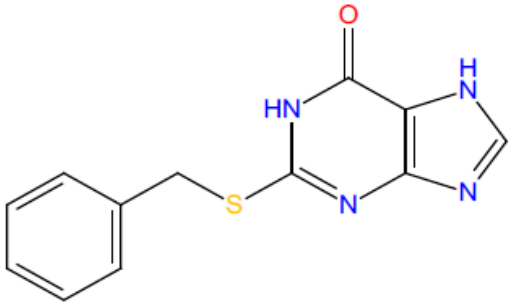
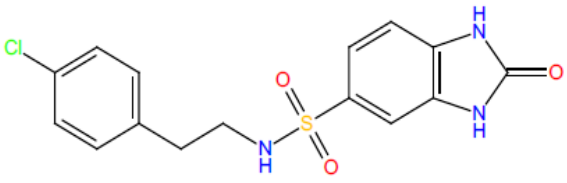


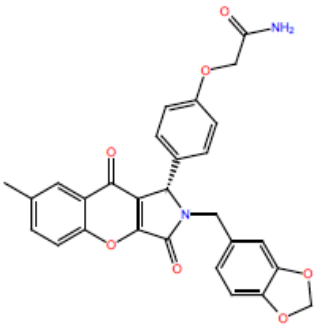
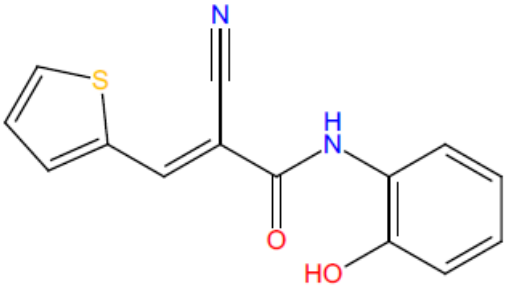
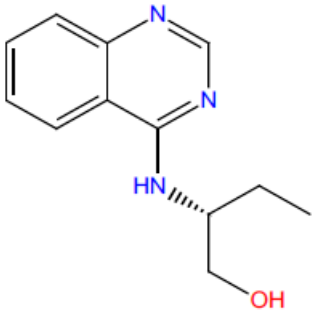
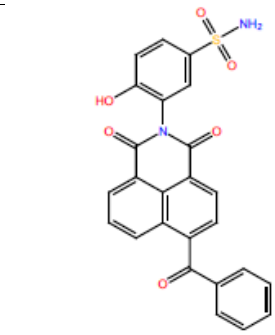
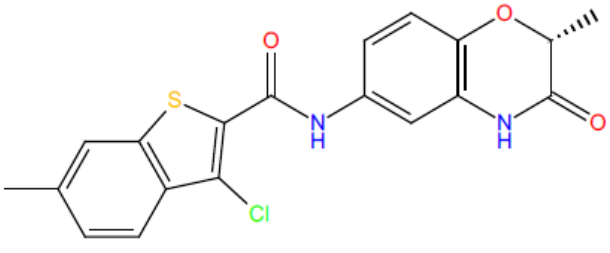
Fig. S3. Bioavailability radar plots. The bioavailability plot considers six physicochemical properties: lipophilicity, size, polarity, solubility, flexibility, and saturation.

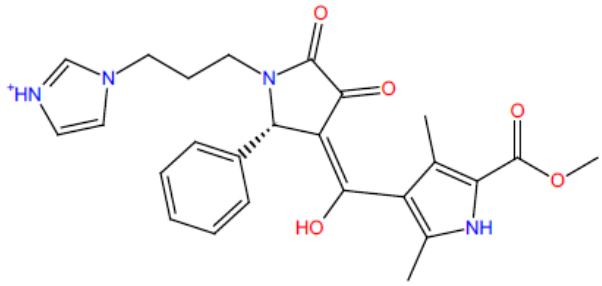
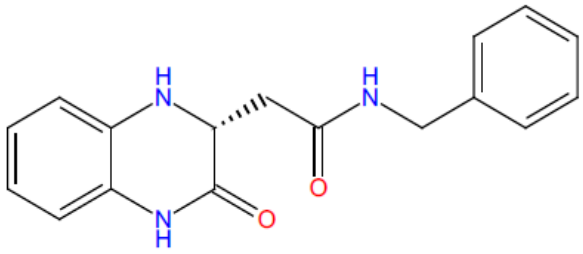
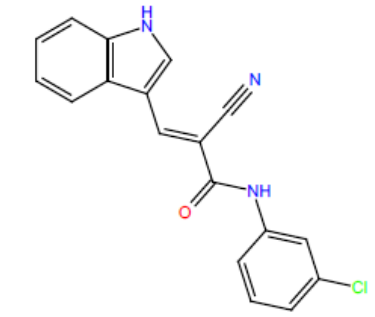
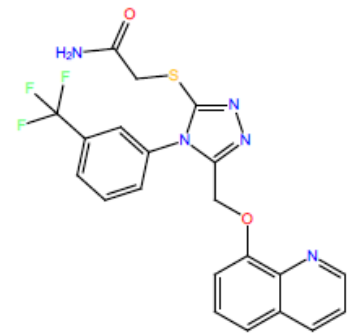
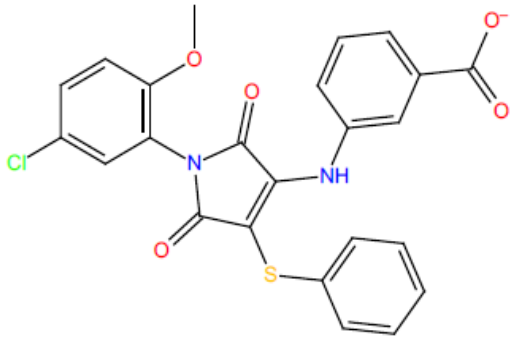
Table S1. Binding interactions of ligand molecules with PDGF-C protein*

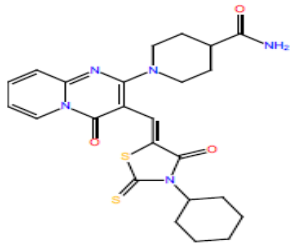
S.No/Id	Structure	Glide Score	Glide Energy	Hydrogen bond interactions
Ligand-82		–10.96	–57.54	ASN292:HD21 – :UNK:O29 LEU309:H – :UNK:O17 SER323:H – :UNK:O17 UNK:H37 – :LEU309:O UNK:H45 – :HIS321:O
Ligand-67		–10.56	–54.69	ASN292:HD21 – :UNK:O15 LYS322:HZ1 – :UNK:O30 LEU311:H – :UNK:O17 GLY341:H – :UNK:O29 THR343:H – :UNK:O30 UNK:H49 – :THR343:O

S.No/Id	Structure	Glide Score	Glide Energy	Hydrogen bond interactions
Ligand-134		–10.54	–57.67	TYR202:H – :UNK:O20 ARG253:H – :UNK:N1 UNK:H23 – :THR251:O UNK:H30 – :VAL227:O
Ligand-133		–10.28	–57.90	TYR202:H – :UNK:O20 ARG253:H – :UNK:N4 ALA285:H – UNK:O13 UNK:H23 – :THR251:O UNK:H30 – :VAL277:O
Ligand-85		–10.12	–55.18	LEU311:H – :UNK:O29 SER323:H – :UNK:O17 UNK:H43 – :SER342:OG
Ligand-86		–10.04	–55.13	LEU309:H – :UNK:O11 LEU311:H – :UNK:O28 SER323:H – :UNK:O17 UNK:H46 – :SER342:OG
Ligand-132		–10.01	–45.65	ASN292:HD21 – :UNK:O19 ASN292:HD21 – :UNK:O20 TYR305:H – :UNK:O11 UNK:H26 – :TYR305:O

S.No/Id	Structure	Glide Score	Glide Energy	Hydrogen bond interactions
Ligand-161		–10.00	–48.68	TYR305:H – :UNK:O16 UNK:H30 – :TYR305: O
Ligand-210		–9.99	–54.45	LYS304:H – :UNK:O14 TYR305:H – :UNK:N11 GLY341:H – :UNK:O18 UNK:H33 – :TYR305:O
Ligand-159		–9.71	–40.64	ARG253:H – :UNK:N1 ALA285: H – :UNK:O11
Ligand-186		–9.65	–40.19	LYS304:H – :UNK:O12 TYR305:H – :UNK: O12 UNK:H24 – :TYR305:O UNK:H27 – :GLU307:OE1

S.No/Id	Structure	Glide Score	Glide Energy	Hydrogen bond interactions
Ligand-91		–9.39	–59.70	GLY345:H – :UNK:O24 UNK:H52 – :LEU311:O
Ligand-18		–9.37	–47.57	UNK:H21 – :THR251:O UNK:H25 – :ILE200:O
Ligand-160		–9.27	–37.83	UNK: H17 – :THR251 : O UNK: H21 – :ILE200 : O TYR202:H – :UNK:N3
Ligand-17		–9.26	–56.64	SER323: H – :UNK: O17 UNK: H38 – :ASN290: O UNK: H44 – :HIS321: O
Ligand-95		–9.22	–44.41	LYS304:H – :UNK:O19 TYR305:H – :UNK:O19 UNK:H28 – :TYR305: O

S.No/Id	Structure	Glide Score	Glide Energy	Hydrogen bond interactions
Ligand-190		–9.19	–53.97	LEU311:H – :UNK: O16 THR343:H – :UNK: O21 GLY345: H – :UNK: O20 UNK: H61 – :GLU307: OE1
Ligand-204		–9.18	–45.52	UNK: H23 – :CYS280: O UNK: H24 – :CYS250: O UNK: H28 – :VAL277: O
Ligand-106		–9.08	–45.09	UNK: H27 – :THR251: O ALA285:H – :UNK: Cl16
Ligand-183		–9.08	–54.67	ASN292:HD21 – :UNK:N14 UNK: H38 – :ASN290: O UNK:H39 – :ASN292:OD1
Ligand-127		–9.07	–54.14	ASN292:HD21 – :UNK:O17 ARG340:HH11 – :UNK:O49 THR343:H – :UNK:O12 UNK:H33 – :GLY341:O

S.No/Id	Structure	Glide Score	Glide Energy	Hydrogen bond interactions
Ligand-127		–9.01	–57.11	ASN292:HD21 – :UNK:O17 LEU311:H – :UNK:O24 UNK: H51 – :THR343: O

*docked ligands obtained from virtual screening workflow showing hydrogen bonding and π–π interactions. Amino acids represented as 3-letter code