**Table S1.** GBM: List of physio-chemical properties and predicted toxicology and ADME for top 20 ligands. Toxicology and ADME predictions are probabilities in the range [0,1]\*.



\*Listed are NSC-626388, NSC-652525, NSC-634724, NSC-641172, NSC-9858, NSC-660032, NSC-39310, NSC-606174, NSC-690391, NSC-326757, NSC-613799, NSC-369395, NSC-603071, NSC-603073, NSC-673596, NSC-94600, NSC-10460, NSC-96641, NSC-652524, and NSC-688500. Receptor binding energies, promiscuity, genotoxicity, skin sensitivity, and aquatic toxicity from SMARTS hits not listed.

**Table S2.** Melanoma: List of physio-chemical properties and predicted toxicology and ADME for top 20 ligands. Toxicology and ADME predictions are probabilities in the range [0,1]\*.



\*Listed are NSC-713198, NSC-667933, NSC-679749, NSC-707982, NSC-745321, NSC-714363, NSC-643416, NSC-380856, NSC-649750, NSC-27034, NSC-656160, NSC-690040, NSC-672425, NSC-750908, NSC-643735, NSC-677959, NSC-194618, NSC-656159, NSC-658142, and NSC-656204. Receptor binding energies, promiscuity, genotoxicity, skin sensitivity, and aquatic toxicity from SMARTS hits not listed.

**Table S3.** Ovarian: List of physio-chemical properties and predicted toxicology and ADME for top 20 ligands. Toxicology and ADME predictions are probabilities in the range [0,1]\*.



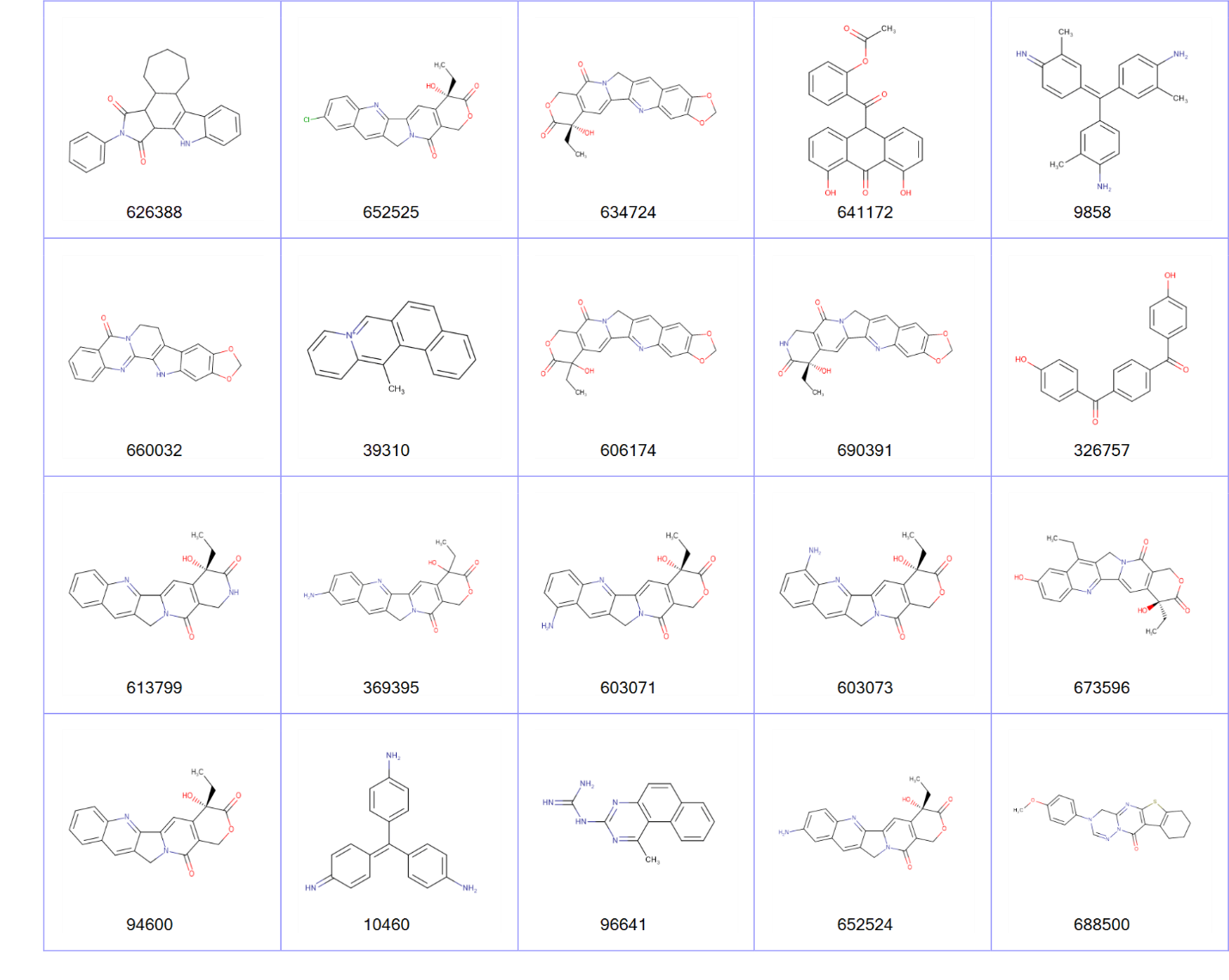
\*Listed are NSC-690273, NSC-720028, NSC-720447, NSC-720702, NSC-753018, NSC-722392, NSC-634398, NSC-690678, NSC-675223, NSC-656204, NSC-621457, NSC-726393, NSC-692229, NSC-257450, NSC-116536, NSC-70811, NSC-117192, NSC-753598, NSC-72881, and NSC-5332. Receptor binding energies, promiscuity, genotoxicity, skin sensitivity, and aquatic toxicity from SMARTS hits not listed.

**Table S4.** Renal papillary: List of physio-chemical properties and predicted toxicology and ADME for top 20 ligands. Toxicology and ADME predictions are probabilities in the range [0,1]\*.



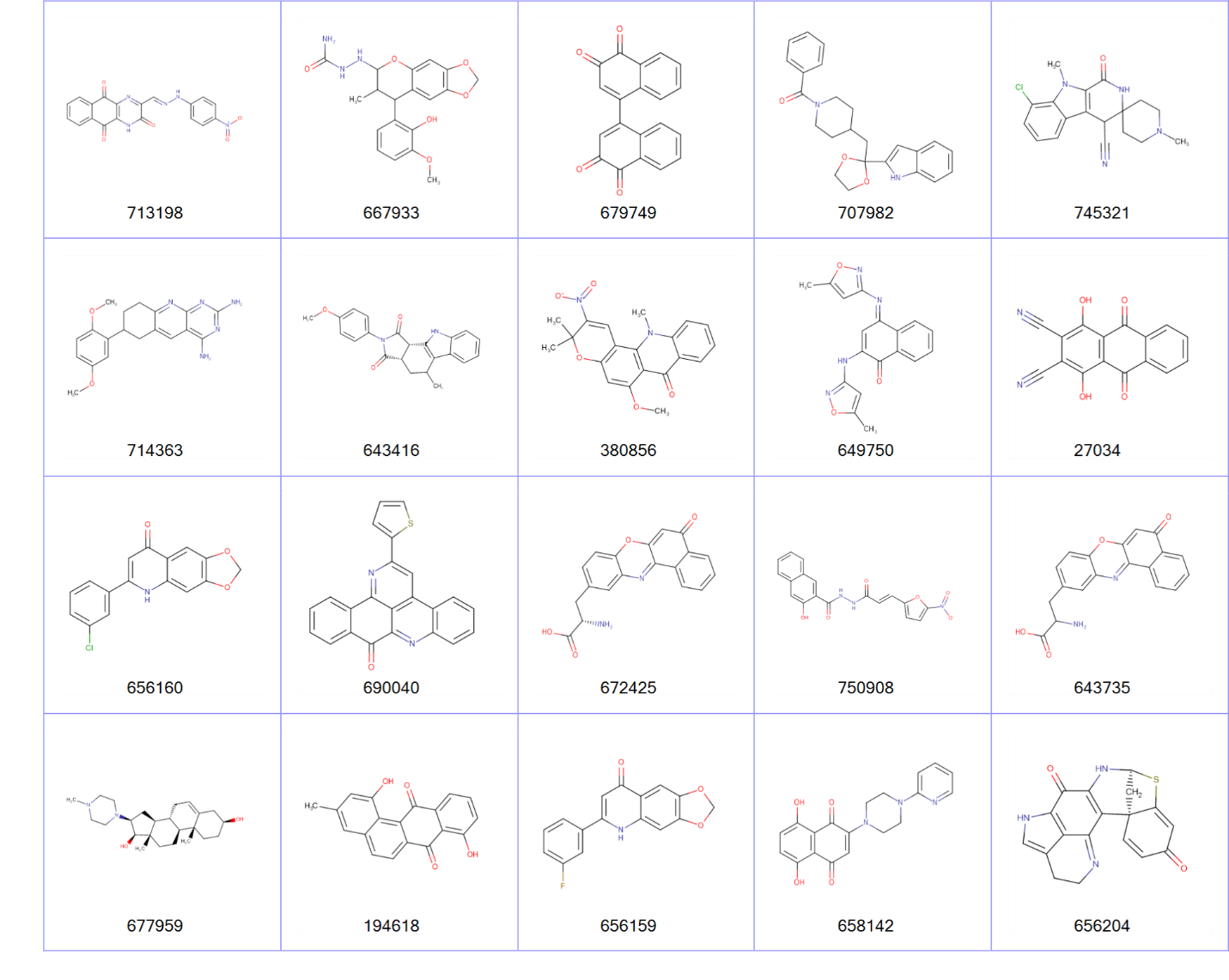
\*Listed are NSC-606174, NSC-668836, NSC-696921, NSC-682298, NSC-766292, NSC-249910, NSC-766871, NSC-702015, NSC-682571, NSC-726184, NSC-683608, NSC-756420, NSC-751644, NSC-757177, NSC-407807, NSC-726364, NSC-756350, NSC-772545, NSC-626735, and NSC-729037. Receptor binding energies, promiscuity, genotoxicity, skin sensitivity, and aquatic toxicity from SMARTS hits not listed.

**Figure S1.** 2D structures of top 20 drug-like ligands for GBM.\*

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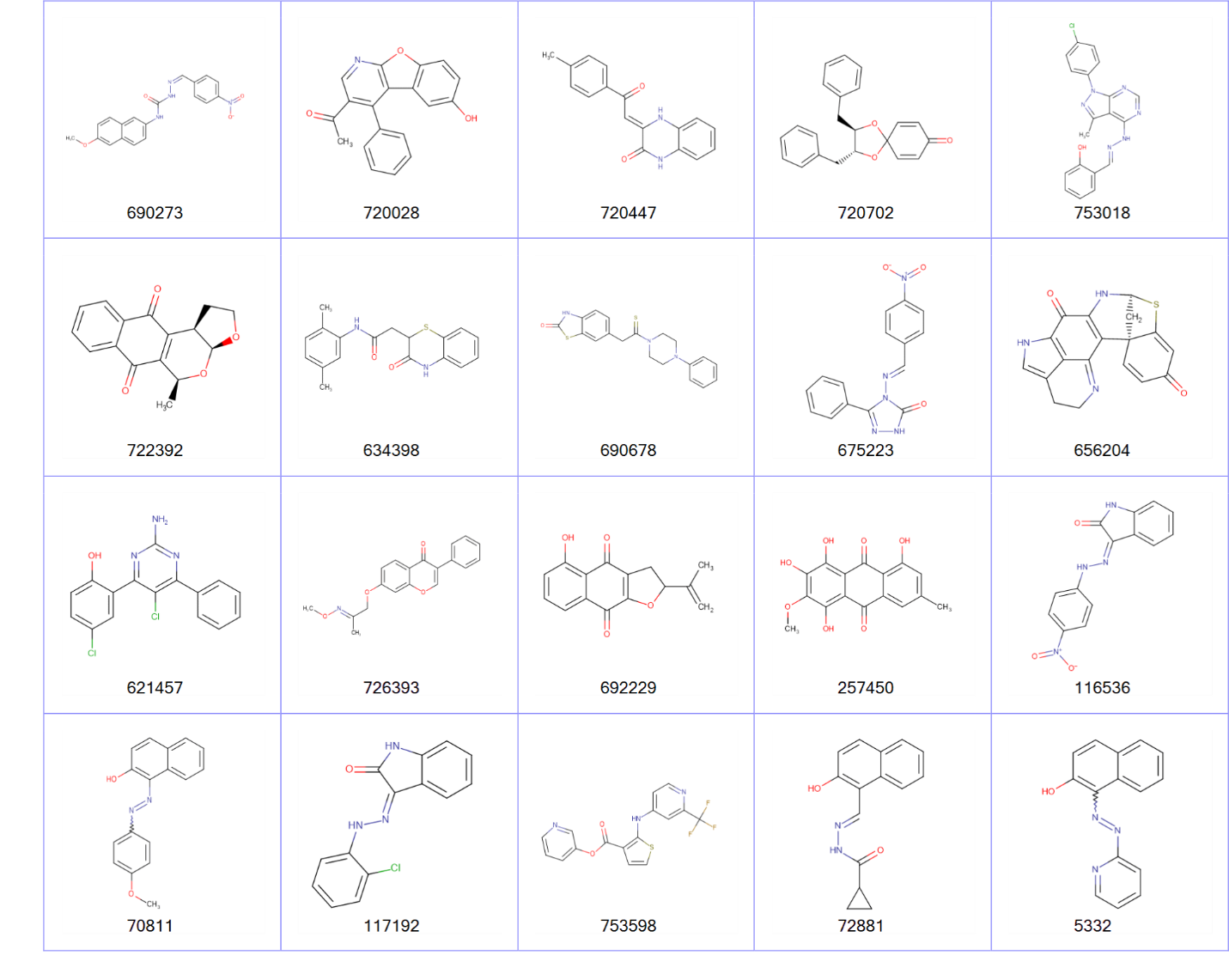
\*Listed are NSC-626388, NSC-652525, NSC-634724, NSC-641172, NSC-9858, NSC-660032, NSC-39310, NSC-606174, NSC-690391, NSC-326757, NSC-613799, NSC-369395, NSC-603071, NSC-603073, NSC-673596, NSC-94600, NSC-10460, NSC-96641, NSC-652524, and NSC-688500.

**Figure S2.** 2D structures of top 20 drug-like ligands for melanoma.\*

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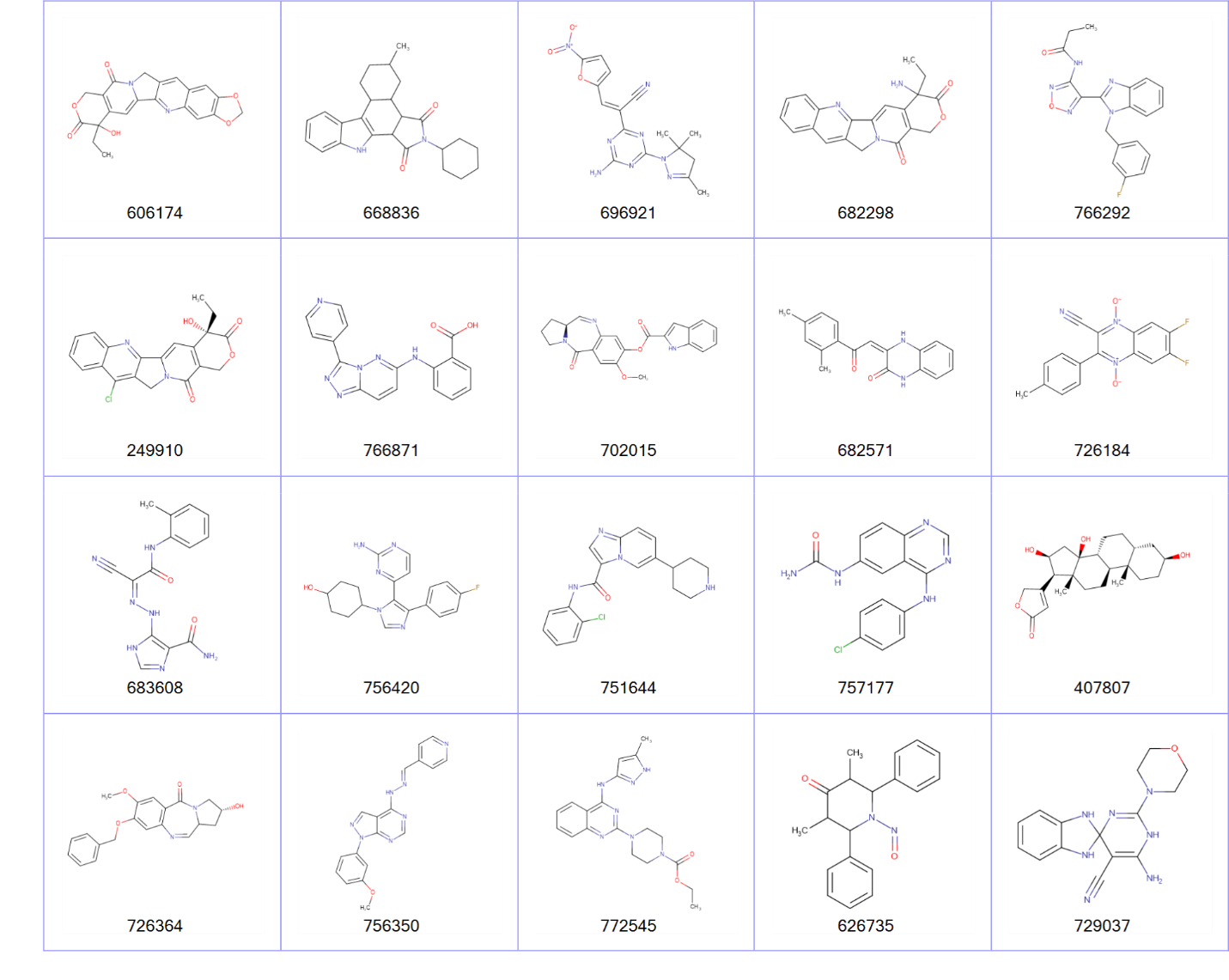
\*Listed are NSC-713198, NSC-667933, NSC-679749, NSC-707982, NSC-745321, NSC-714363, NSC-643416, NSC-380856, NSC-649750, NSC-27034, NSC-656160, NSC-690040, NSC-672425, NSC-750908, NSC-643735, NSC-677959, NSC-194618, NSC-656159, NSC-658142, and NSC-656204.

**Figure S3.** 2D structures of top 20 drug-like ligands for ovarian cancer.\*

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\*Listed are NSC-690273, NSC-720028, NSC-720447, NSC-720702, NSC-753018, NSC-722392, NSC-634398, NSC-690678, NSC-675223, NSC-656204, NSC-621457, NSC-726393, NSC-692229, NSC-257450, NSC-116536, NSC-70811, NSC-117192, NSC-753598, NSC-72881, and NSC-5332.

**Figure S4.** 2D structures of top 20 drug-like ligands for renal papillary cancer.\*

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\*Listed are NSC-606174, NSC-668836, NSC-696921, NSC-682298, NSC-766292, NSC-249910, NSC-766871, NSC-702015, NSC-682571, NSC-726184, NSC-683608, NSC-756420, NSC-751644, NSC-757177, NSC-407807, NSC-726364, NSC-756350, NSC-772545, NSC-626735, and NSC-729037.