Exploring a Structural Protein-Drug Interactome for Drug Design and Repurposing: Genome–Wide Docking, Network Analysis, Patient Records Mining, Cellular and *In Vivo* Studies in Lung Cancer

Xiaodong Peng[3,8], Fang Wang [1], Liwei Li,[1,3] Khuchtumur Bum-Erdene,[1,3] Bo Wang[1, 14] Tony Sinn,[10,11] Karen Pollok,[10,11] George Sandusky,[13] Lang Li,[12] Nasser Hanna,[14] John Turchi,[14] Shadia I. Jalal,[14] and Samy Meroueh[1,3,7,9,11]

[1]Department of Biochemistry and Molecular Biology, [2]Department of Pharmacology and Toxicology, [3]Center for Computational Biology and Bioinformatics, [4]Stark Neuroscience Research Institute, [5]Indiana University Cancer Center, [6]Department of Medicine, [7]Medical Neuroscience Program, [8]Regenstrief Institute, Inc., [9]Department of Medical and Molecular Genetics, [10]Herman B Wells Center for Pediatric Research, [11]In vivo Therapeutics Core, [12]Department of Biostatistics, Indiana University School of Medicine, [13]Department of Pathology and Laboratory Medicine, [14]Department of Medicine, Indianapolis, IN 46202, [15]Department of Chemistry and Chemical Biology, Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, Indiana, 46202.

E-mail: smeroueh@iupui.edu

RECEIVED DATE (to be automatically inserted after your manuscript is accepted if required according to the journal that you are submitting your paper to)

TITLE RUNNING HEAD

Genome-wide docking of approved drugs for drug design and repurposing

Supporting Information

Supporting Information Table 1

Disease		ICD-9 codes
Hypertension		401, 402, 403, 404, 405
Migraine Pain		346
Cancer	Prostate	185, 233.4
	Breast	174, 233.0
	Lung and Bronchus	162.0, 162.2, 162.3, 162.4, 162.5, 162.8, 162,9
	Colon and Rectum	153.0, 153.1, 153.2, 153.3, 153.4, 153.6, 153.7, 153.8, 153.9, 154.0, 154.1, 154.8, 197.5, 230.3, 230.4, 235.2
	Urinary Bladder	188.1, 188.2, 188.3, 188.4, 188.5, 188.6, 188.7, 188.8, 188.9, 233.7
	Melanoma of Skin	172
	Non-Hodgkin Lymphoma	200.0, 200.1, 200.2, 200.3, 200.4, 200.5, 200.6, 200.7, 202.0, 202.1, 202.2, 202.7
	Kidney and Renal Pelvis	189.0, 189.1
	Oral Cavity and Pharynx	141, 142, 143, 144, 145, 146, 147, 148, 149, 230.0
	Leukimas	204, 205, 206, 207, 208
	Pancreas	157
	Corpus and Uterus, NOS	179, 182, 233.2

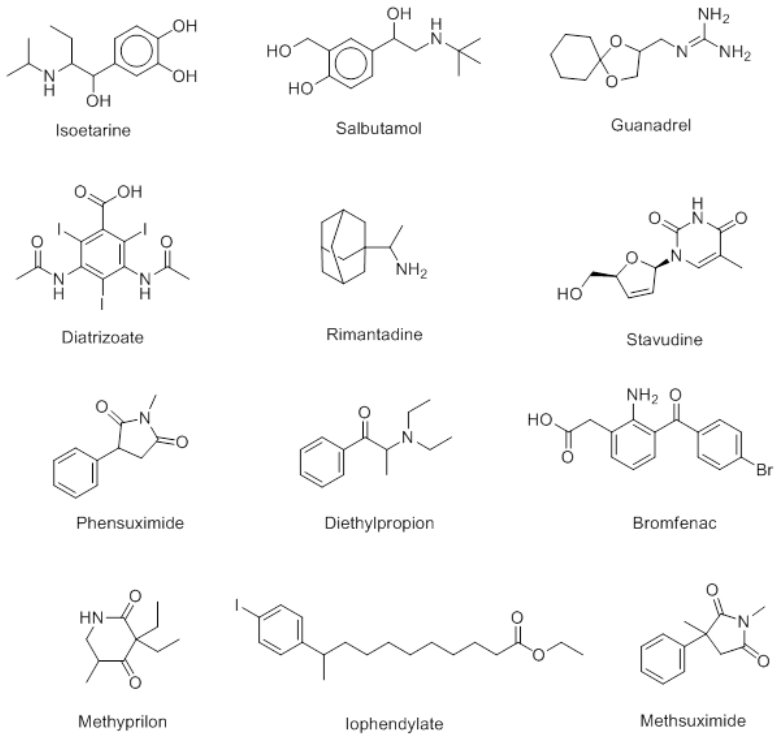
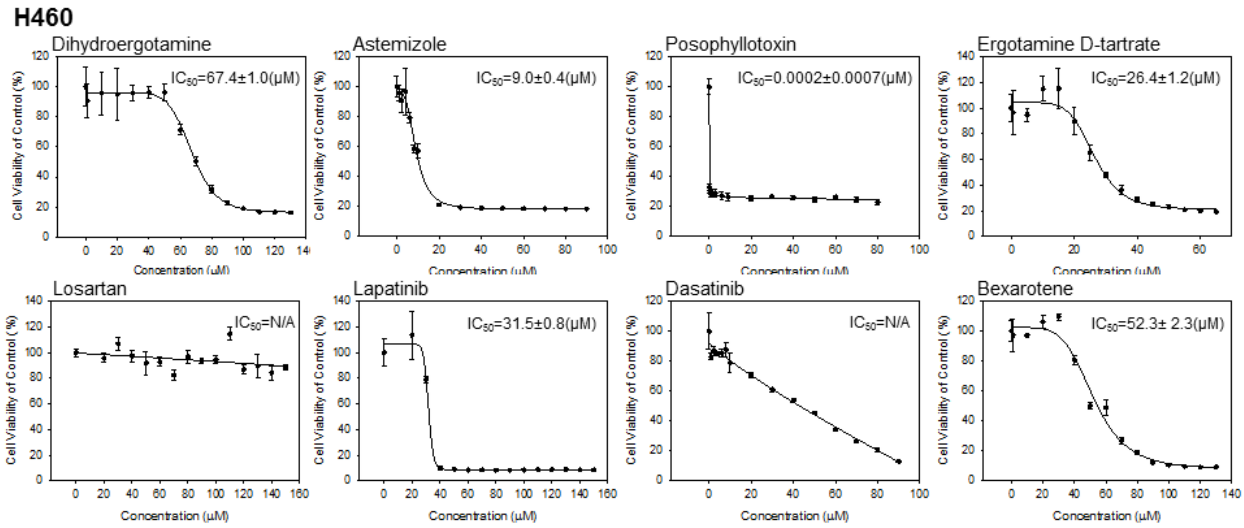
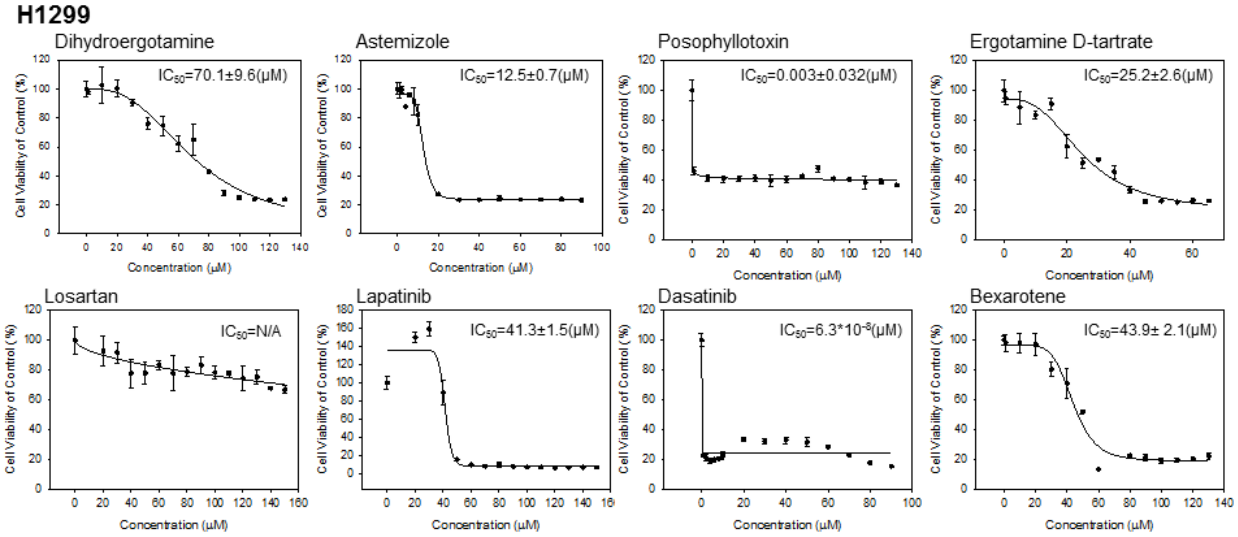


Fig. S1. Chemical structure of compounds that are selective to cancer targets

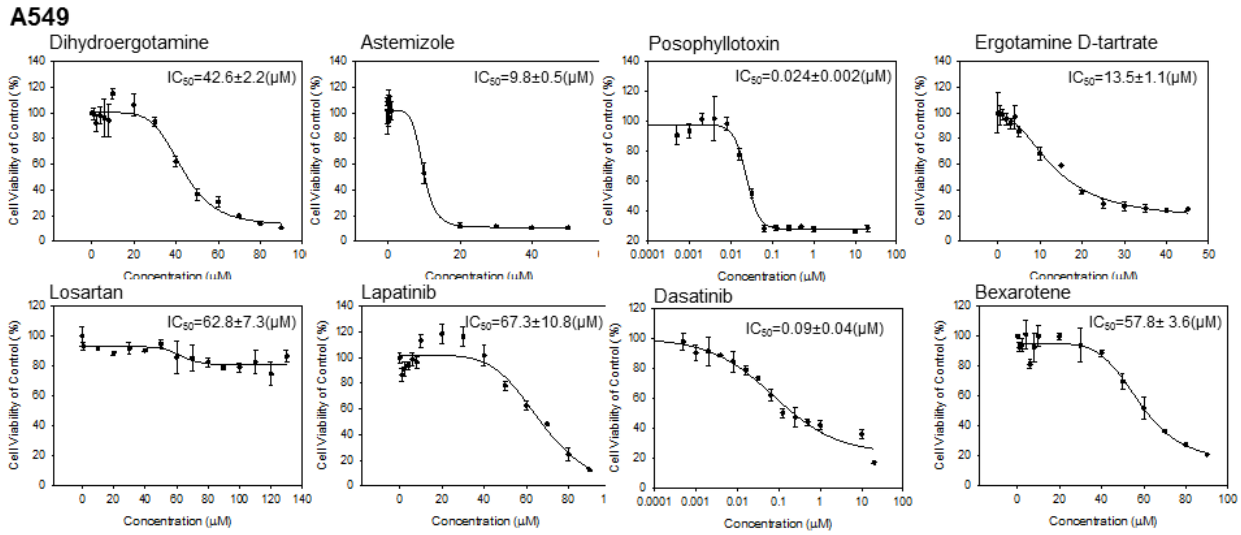
Supporting Information Figure 2



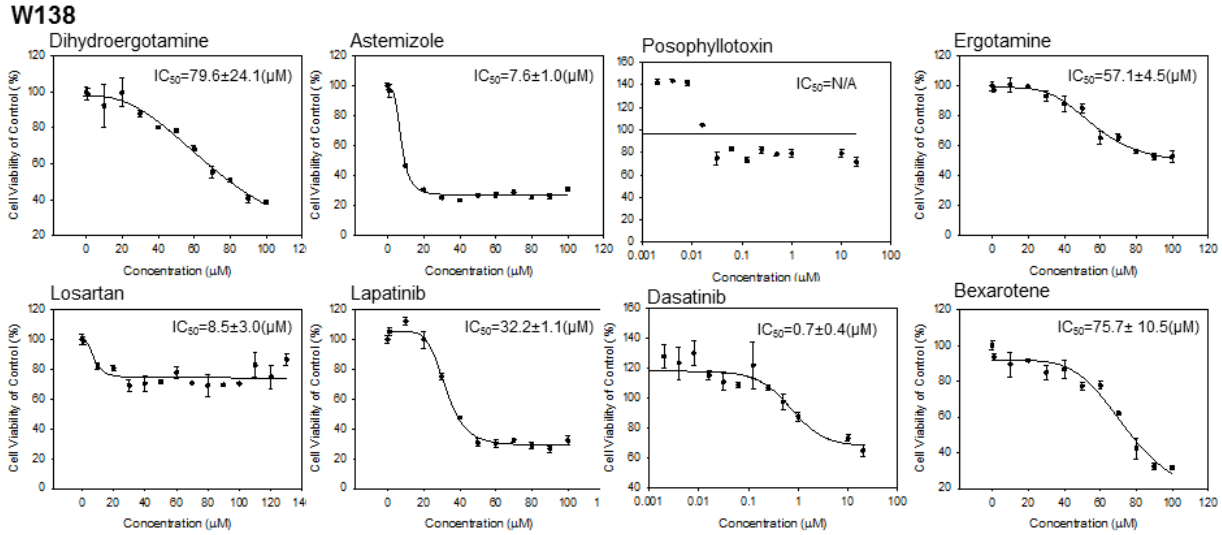
Supporting Information Figure 3



Supporting Information Figure 4



Supporting Information Figure 5



Supporting Information Figure 6