

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

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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

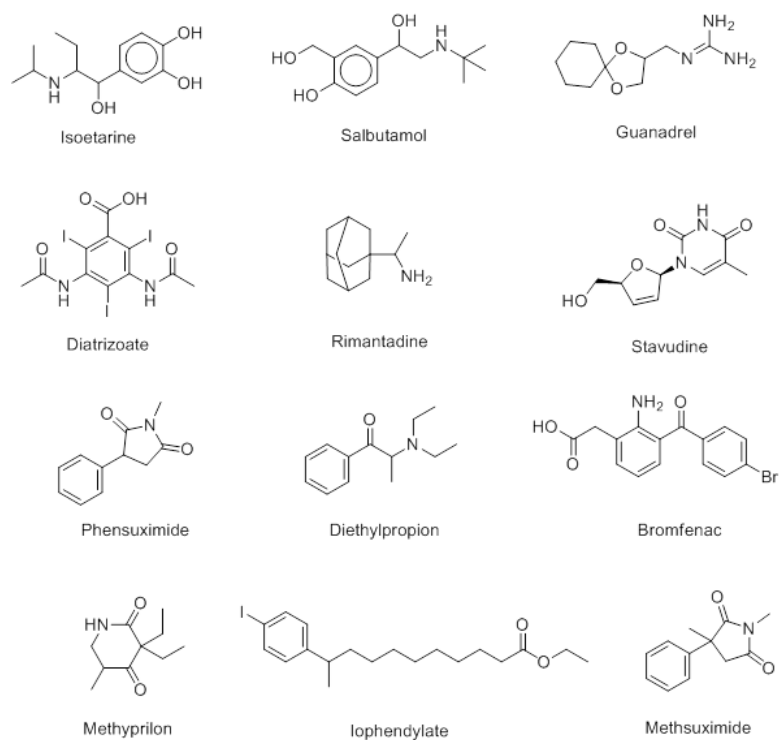
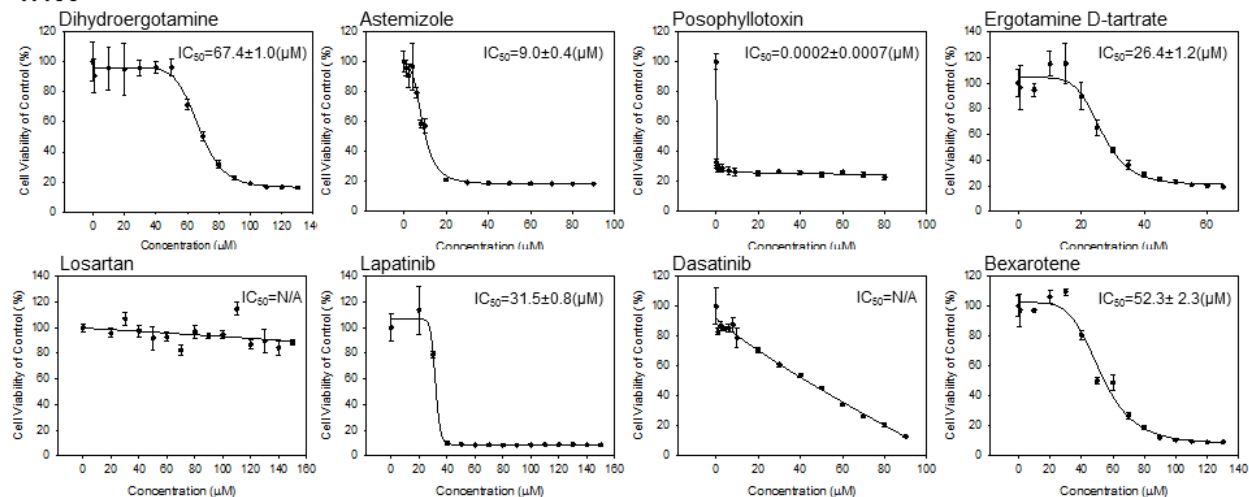


Fig. S1. Chemical structure of compounds that are selective to cancer targets

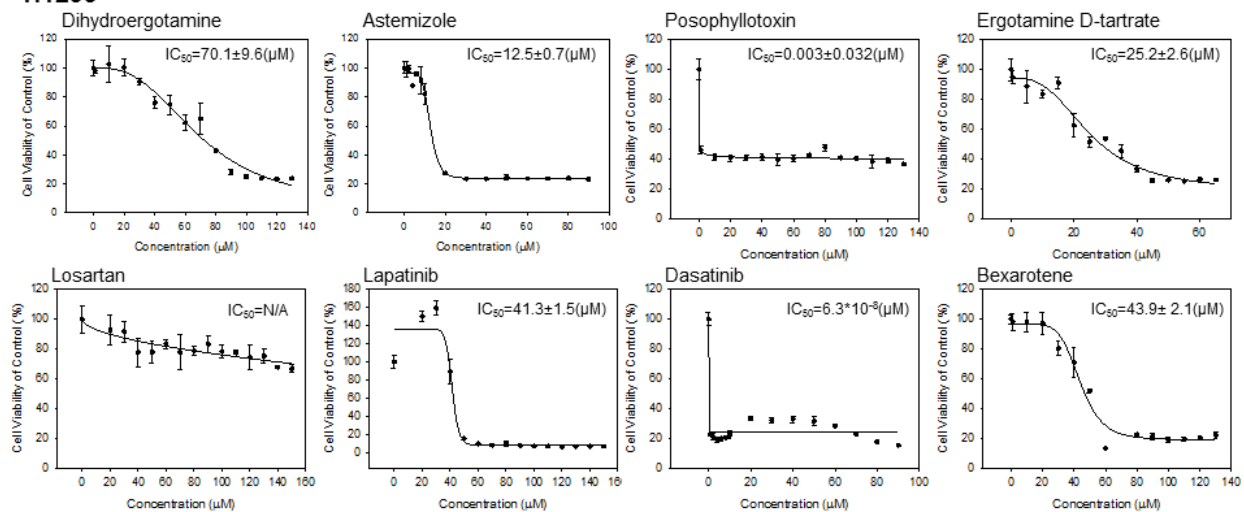
## Supporting Information Figure 2

### H460



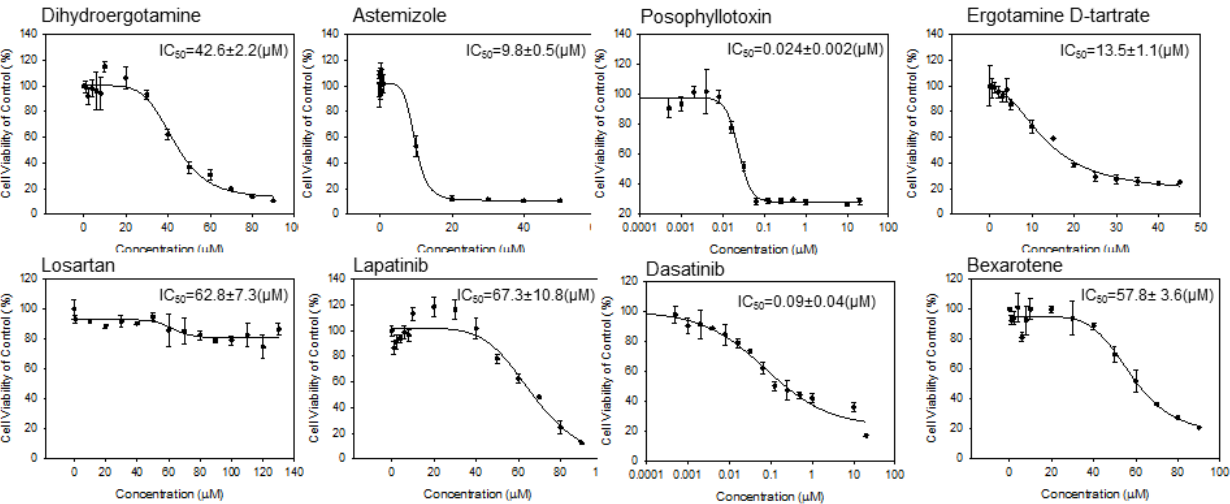
### Supporting Information Figure 3

#### H1299



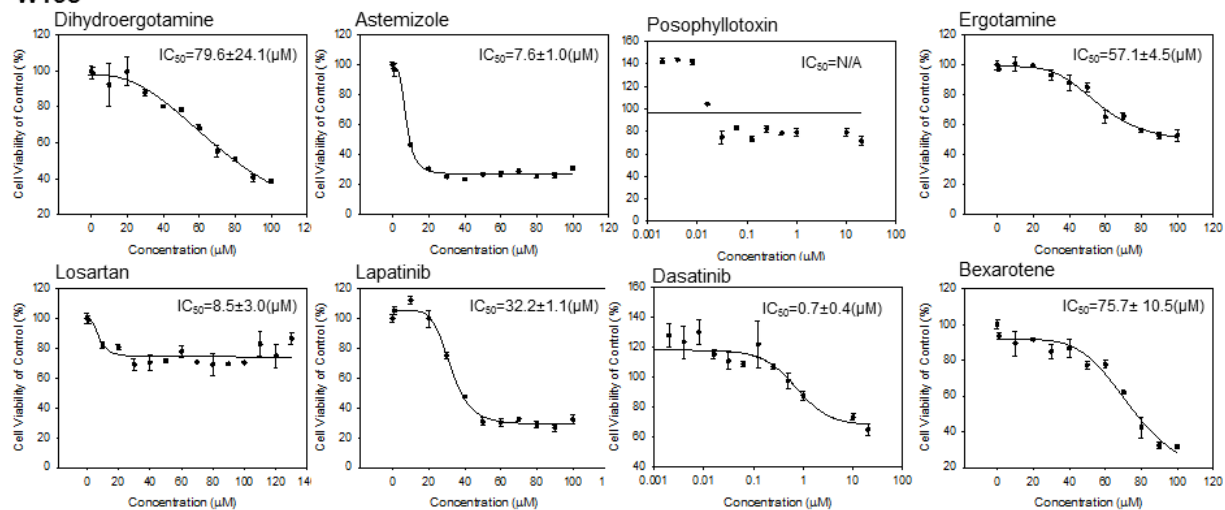
Supporting Information Figure 4

A549



## Supporting Information Figure 5

### W138



Supporting Information Figure 6

