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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**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 Table 1

<table>
<thead>
<tr>
<th>Disease</th>
<th>ICD-9 codes</th>
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<tbody>
<tr>
<td>Hypertension</td>
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<td>Migraine Pain</td>
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<td>Cancer</td>
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<tr>
<td>Prostate</td>
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<tr>
<td>Breast</td>
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<td>Lung and Bronchus</td>
<td>162.0, 162.2, 162.3, 162.4, 162.5, 162.8, 162.9</td>
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<td>Colon and Rectum</td>
<td>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, 203.0, 220.4, 235.2</td>
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<td>Urinary Bladder</td>
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<td>Melanoma of Skin</td>
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<td>Kidney and Renal Pelvis</td>
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<td>Oral Cavity and Pharynx</td>
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<td>Leukemia</td>
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<td>Pancreas</td>
<td>157</td>
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<tr>
<td>Corpus and Uterus, NOS</td>
<td>179, 182, 233.2</td>
</tr>
</tbody>
</table>
Fig. S1. Chemical structure of compounds that are selective to cancer targets
Supporting Information Figure 2

H460

Dihydroergotamine  Astemizole  Phosphofructokinase  Ergotamine D-tartrate

Losartan  Lapatinib  Dasatinib  Bexarotene

IC_{50}=67.4±1.0\mu M  IC_{50}=90±6.4\mu M  IC_{50}=0.0002±0.0007\mu M  IC_{50}=25.4±1.2\mu M

IC_{50}=31.5±0.8\mu M  IC_{50}=N/A  IC_{50}=N/A  IC_{50}=52.3±2.3\mu M
Supporting Information Figure 3

H1299

Dihydroergotamine

IC50=70.1±9.6(μM)

Ergotamine D-tartrate

IC50=25.2±2.9(μM)

Astemizole

IC50=12.5±0.7(μM)

Posophyllotoxin

IC50=0.003±0.632(μM)

Losartan

IC50=N/A

Dasatinib

IC50=6.3±10.4(μM)

Lapatinib

IC50=41.3±1.5(μM)

Bexarotene

IC50=43.9±2.1(μM)
Supporting Information Figure 4

A549

Dihydroergotamine

IC_{50}=42.8±2.2(μM)

Asterizole

IC_{50}=9.8±0.5(μM)

Posophyllotoxin

IC_{50}=6.0±0.9(μM)

Ergotamine D-tartrate

IC_{50}=13.5±1.1(μM)

Losartan

IC_{50}=62.8±7.3(μM)

Lapatinib

IC_{50}=97.2±10.0(μM)

Dasatinib

IC_{50}=6.09±0.04(μM)

Bexarotene

IC_{50}=57.8±3.9(μM)
Supporting Information Figure 5

W138
Dihydroergotamine
IC50=79.6 ± 24.1 (μM)

Astemizole
IC50=7.5 ± 1.6 (μM)

Pogophyllotoxin
IC50=N/A

Ergotamine
IC50=57.1 ± 4.5 (μM)

Losartan
IC50=8.5 ± 3.6 (μM)

Lepatinib
IC50=32.2 ± 1.1 (μM)

Pasalinib
IC50=6.7 ± 0.4 (μM)

Bezafibrate
IC50=75.7 ± 19.5 (μM)
Supporting Information Figure 6

Graph showing body weight changes over time for different treatment groups:
- Vehicle (n=10)
- Losartan 50mg (n=10)
- Montelukast 10mg (n=10)
- Astemizole 10mg (n=5)

Y-axis: Body Weight (grams)
X-axis: Time (days)