

Supplementay Table 3: The overlapping genes for compound targets and NSCLC-related targets

Number	Protein name	Gene name
1	Progesterone receptor	PGR
2	Prostaglandin G/H synthase 1	PTGS1
3	Prostaglandin G/H synthase 2	PTGS2
4	Heat shock protein HSP 90	HSP90AA1
5	Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit, gamma isoform	PIK3CG
6	mRNA of PKA Catalytic Subunit C-alpha	PRKACA
7	Beta-2 adrenergic receptor	ADRB2
8	Apoptosis regulator Bcl-2	BCL2
9	Apoptosis regulator BAX	BAX
10	Caspase-9	CASP9
11	Transcription factor AP-1	JUN
12	Caspase-3	CASP3
13	Caspase-8	CASP8
14	Protein kinase C alpha type	PRKCA
15	Transforming growth factor beta-1	TGFB1
16	Microtubule-associated protein 2	MAP2
17	Androgen receptor	AR
18	Cytochrome P450 17A1	CYP17A1
19	Estrogen receptor	ESR1
20	Aromatase	CYP19A1
21	Estrogen receptor beta	ESR2
22	Glucocorticoid receptor	NR3C1
23	M-phase inducer phosphatase 2	CDC25B
24	Acetylcholinesterase	ACHE
25	Bone morphogenetic protein 2	BMP2
26	Proto-oncogene serine/threonine-protein kinase Pim-1	PIM1
27	Serum albumin	ALB
28	Estradiol 17-beta-dehydrogenase 1	HSD17B1
29	Caspase-7	CASP7
30	Mitogen-activated protein kinase 1	MAPK1
31	Collagenase 3	MMP13
32	Prothrombin	F2
33	Vascular endothelial growth factor receptor 2	KDR
34	Peroxisome proliferator-activated receptor gamma	PPARG
35	Cell division protein kinase 2	CDK2
36	Mitogen-activated protein kinase 14	MAPK14
37	Mitogen-activated protein kinase 8	MAPK8
38	Nitric oxide synthase, endothelial	NOS3
39	Epidermal growth factor receptor	EGFR
40	ADAM 17	ADAM17
41	Annexin A5	ANXA5
42	Proto-oncogene tyrosine-protein kinase Src	SRC

43 3-phosphoinositide-dependent protein kinase 1	PDPK1
44 Tyrosine-protein phosphatase non-receptor type 11	PTPN11
45 Liver carboxylesterase 1	CES1
46 Serine/threonine-protein kinase Chk1	CHEK1
47 TGF-beta receptor type-1	TGFBR1
48 Integrin alpha-L	ITGAL
49 Arachidonate 5-lipoxygenase	ALOX5
50 Phospholipase A2, membrane associated	PLA2G2A
51 Histone deacetylase 4	HDAC4
52 Cocaine esterase	CES2
53 Toll-like receptor 9	TLR9
54 Histone deacetylase 2	HDAC2
55 Macrophage migration inhibitory factor	MIF
56 Retinoic acid receptor beta	RARB
57 Aryl hydrocarbon receptor	AHR
58 Glutathione S-transferase P	GSTP1
59 Ephrin type-B receptor 4	EPHB4
60 Mitogen-activated protein kinase 10	MAPK10
61 Cholinesterase	BCHE
62 Cyclin-A2	CCNA2
63 B-Raf proto-oncogene serine/threonine-protein kinase	BRAF
64 Insulin-like growth factor 1 receptor	IGF1R
65 Proto-oncogene tyrosine-protein kinase LCK	LCK
66 Retinoic acid receptor RXR-alpha	RXRA
67 NAD(P)H dehydrogenase [quinone] 1	NQO1
68 Thymidylate synthase	TYMS
69 Cathepsin B	CTSB
70 Prostaglandin E2 receptor EP4 subtype	PTGER4
71 Tyrosine-protein phosphatase non-receptor type 22	PTPN22
72 Stromelysin-1	MMP3
73 Oxysterols receptor LXR-beta	NR1H2
74 Dipeptidyl peptidase IV	DPP4
75 Tyrosine-protein phosphatase non-receptor type 1	PTPN1
76 DNA (cytosine-5)-methyltransferase 1	DNMT1
77 Heat shock cognate 71 kDa protein	HSPA8
78 Nitric oxide synthase, inducible	NOS2
79 DNA topoisomerase II	TOP2A
80 Transcription factor p65	RELA
81 Inhibitor of nuclear factor kappa-B kinase subunit beta	IKBKB
82 RAC-alpha serine/threonine-protein kinase	AKT1
83 Tumor necrosis factor	TNF
84 Interstitial collagenase	MMP1
85 Signal transducer and activator of transcription 1-alpha/beta	STAT1
86 Cell division control protein 2 homolog	CDK1
87 Heme oxygenase 1	HMOX1
88 Cytochrome P450 3A4	CYP3A4

89 Cytochrome P450 1A2	CYP1A2
90 Cytochrome P450 1A1	CYP1A1
91 Intercellular adhesion molecule 1	ICAM1
92 E-selectin	SELE
93 Nuclear receptor subfamily 1 group I member 2	NR1I2
94 Cytochrome P450 1B1	CYP1B1
95 Insulin receptor	INSR
96 Glutathione S-transferase Mu 1	GSTM1
97 NADPH oxidase 4	NOX4
98 Tyrosine-protein kinase receptor FLT3	FLT3
99 Multidrug resistance-associated protein 1	ABCC1
100 P-glycoprotein 1	ABCB1
101 ATP-binding cassette sub-family G member 2	ABCG2
102 Tyrosine-protein kinase SYK	SYK
103 Glycogen synthase kinase-3 beta	GSK3B
104 Matrix metalloproteinase 9	MMP9
105 Matrix metalloproteinase 2	MMP2
106 Cyclin-dependent kinase 5	CDK5
107 cyclin B1	CCNB1
108 Death-associated protein kinase 1	DAPK1
109 Receptor-type tyrosine-protein phosphatase C	PTPRC
110 1	MCL1
111 Telomerase reverse transcriptase	TERT
112 Carbonic anhydrase 9	CA9
113 Tubulin alpha-1A chain	TUBA1A
114 Hepatocyte nuclear factor 4-alpha	HNF4A
115 Ras-related C3 botulinum toxin substrate 1	RAC1
116 Cytochrome P450 2C9	CYP2C9
117 Protein kinase C epsilon type	PRKCE
118 Amyloid beta A4 protein	APP
119 Cell division protein kinase 6	CDK6
120 Dihydrofolate reductase	DHFR
121 Serine/threonine-protein kinase 6	AURKA
122 Vascular endothelial growth factor A	VEGFA
123 Estrogen receptor	CCND1
124 Bcl-2-like protein 1	BCL2L1
125 Cyclin-dependent kinase inhibitor 1	CDKN1A
126 Interleukin-10	IL10
127 Retinoblastoma-associated protein	RB1
128 Cell division protein kinase 4	CDK4
129 Interleukin-6	IL6
130 Cellular tumor antigen p53	TP53
131 NF-kappa-B inhibitor alpha	NFKBIA
132 DNA topoisomerase 1	TOP1
133 E3 ubiquitin-protein ligase Mdm2	MDM2
134 Proliferating cell nuclear antigen	PCNA

135	Receptor tyrosine-protein kinase erbB-2	ERBB2
136	Baculoviral IAP repeat-containing protein 5	BIRC5
137	Interleukin-2	IL2
138	Interferon gamma	IFNG
139	Interleukin-4	IL4
140	CD40 ligand	CD40LG
141	Hepatocyte growth factor receptor	MET
142	Poly [ADP-ribose] polymerase 1	PARP1
143	Macrophage metalloelastase	MMP12
144	Cathepsin D	CTSD
145	Proto-oncogene c-Fos	FOS
146	Urokinase-type plasminogen activator	PLAU
147	Pro-epidermal growth factor	EGF
148	Cyclin-dependent kinase inhibitor 2A, isoforms 1/2/3	CDKN2A
149	NADPH--cytochrome P450 reductase	POR
150	Ornithine decarboxylase	ODC1
151	RAF proto-oncogene serine/threonine-protein kinase	RAF1
152	Superoxide dismutase [Cu-Zn]	SOD1
153	Hypoxia-inducible factor 1-alpha	HIF1A
154	78 kDa glucose-regulated protein	HSPA5
155	Caveolin-1	CAV1
156	Myc proto-oncogene protein	MYC
157	Tissue factor	F3
158	Gap junction alpha-1 protein	GJA1
159	Interleukin-1 beta	IL1B
160	C-C motif chemokine 2	CCL2
161	Interleukin-8	CXCL8
162	Protein kinase C beta type	PRKCB
163	Heat shock protein beta-1	HSPB1
164	Thrombomodulin	THBD
165	Plasminogen activator inhibitor 1	SERPINE1
166	Collagen alpha-1(I) chain	COL1A1
167	Phosphatidylinositol-3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN	PTEN
168	Interleukin-1 alpha	IL1A
169	Myeloperoxidase	MPO
170	Nuclear factor erythroid 2-related factor 2	NFE2L2
171	Serine/threonine-protein kinase Chk2	CHEK2
172	Heat shock factor protein 1	HSF1
173	C-reactive protein	CRP
174	C-X-C motif chemokine 10	CXCL10
175	Inhibitor of nuclear factor kappa-B kinase subunit alpha	CHUK
176	Osteopontin	SPP1
177	Runt-related transcription factor 2	RUNX2
178	Ras association domain-containing protein 1	RASSF1
179	Transcription factor E2F1	E2F1

180	Transcription factor E2F2	E2F2
181	Insulin-like growth factor-binding protein 3	IGFBP3
182	Insulin-like growth factor II	IGF2
183	Interferon regulatory factor 1	IRF1
184	Receptor tyrosine-protein kinase erbB-3	ERBB3
185	Ras GTPase-activating protein 1	RASA1
186	Serine/threonine-protein kinase Aurora-B	AURKB
187	PI3-kinase p85-alpha subunit	PIK3R1
188	Focal adhesion kinase 1	PTK2
189	Serine/threonine-protein kinase PLK1	PLK1
190	Casein kinase II subunit alpha	CSNK2A1
191	C-X-C chemokine receptor type 1	CXCR1
192	ALK tyrosine kinase receptor	ALK
193	Tyrosine-protein kinase receptor UFO	AXL
194	Microtubule-associated protein tau	MAPT
195	Myosin light chain kinase, smooth muscle	MYLK
196	DNA-(apurinic or apyrimidinic site) lyase	APEX1
197	Basic fibroblast growth factor receptor 1	FGFR1
198	Bone morphogenetic protein 7	BMP7
199	S-methyl-5-thioadenosine phosphorylase	MTAP
200	Retinoic acid receptor RXR-beta	RXRB
201	Retinoic acid receptor alpha	RARA
202	Receptor tyrosine-protein kinase erbB-4	ERBB4
203	Fatty acid-binding protein, adipocyte	FABP4
204	Smoothed homolog	SMO
205	Neuronal acetylcholine receptor subunit alpha-4	CHRNA4
206	P-selectin	SELP
207	SPARC	SPARC
208	C-X-C chemokine receptor type 2	CXCR2
209	Dual specificity mitogen-activated protein kinase kinase 1	MAP2K1
210	Thrombopoietin receptor	MPL
211	TGF-beta receptor type-2	TGFBR2
212	Heparin-binding growth factor 1	FGF1
213	Thymidine phosphorylase	TYMP
214	Angiotensin-converting enzyme	ACE
215	Caspase-1	CASP1
216	Dual specificity mitogen-activated protein kinase kinase 4	MAP2K4
217	Proto-oncogene tyrosine-protein kinase receptor Ret	RET
218	Superoxide dismutase [Mn], mitochondrial	SOD2
219	Fibroblast growth factor receptor 2	FGFR2
220	Endothelin-1 receptor	EDNRA
221	Plasminogen	PLG
222	Fatty acid synthase	FASN
223	Catalase	CAT
224	Cytosolic phospholipase A2	PLA2G4A
225	Canalicular multispecific organic anion transporter 1	ABCC2

226 Serine/threonine-protein kinase mTOR	MTOR
227 Catenin alpha-1	CTNNA1
228 Non-receptor tyrosine-protein kinase TYK2	TYK2
229 Cytochrome c	CYCS
