

WinBinVec (Supplementary Figures and Tables)

Abdollahi et al.

Table 1: TCGA Whole Exome Sequencing dataset.

Number	Cancer Type	Population	Organ	Number	Cancer Type	Population	Organ
1	ACC	79	Adrenal Gland	18	LUSC	494	Lung
2	BLCA	406	Bladder	19	MESO	82	Pleura
3	BRCA	1038	Breast	20	OV	279	GYN
4	CESC	302	GYN	21	PAAD	175	Pancreatic
5	CHOL	36	Bile duct	22	PCPG	179	Adrenal Gland
6	COAD	427	CRC	23	PRAD	495	Male Rep. Sys.
7	DLBC	37	Bone marrow	24	READ	153	CRC
8	ESCA	163	Esophagus	25	SARC	253	Other
9	GBM	157	Brain	26	SKCM	468	Melanoma
10	HNSC	497	Head and Neck	27	STAD	379	Stomach
11	KICH	66	Kidney	28	TGCT	134	Male Rep. Sys.
12	KIRC	335	Kidney	29	THCA	491	Thyroid
13	KIRP	286	Kidney	30	THYM	118	Thymus
14	LAML	116	Bone marrow	31	UCEC	538	GYN
15	LGG	507	Brain	32	UCS	56	GYN
16	LIHC	369	Liver	33	UVM	80	Melanoma
17	LUAD	513	Lung				

Table 2: Number of available cell lines in each cancer type in MEDICI dataset.

Cancer Type	Cell Lines	Cancer Type	Cell Lines	Cancer Type	Cell Lines
Breast	11	Bone Marrow	4	Stomach	4
Brain	16	CRC	17	Lung	10
Male Reproductive System	3	Pancreatic	12	Liver	1
GYN	23	Melanoma	7	Kidney	2
Esophagus	8	Bladder	1	TOTAL	119

Table 3: All Protein-Protein Interactions Including their PDB, chains, and RefSeq Identifications.

PDB	RefSeq ID (First Partner Protein)	Chain	RefSeq ID (Second Partner Protein)	Chain
4FAO	NM_000020 (ACVRL1)	C	NM_001106 (ACVR2B)	E
4R3Z	NM_004757 (AIMP1)	A	NM_002887 (RARS)	B
4K71	NM_000477 (ALB)	A	NM_004107 (FCGRT)	B
4K71	NM_000477 (ALB)	A	NM_001136019 (FCGRT)	B
4N0U	NM_000477 (ALB)	D	NM_004048 (B2M)	B
5KHU	NM_013367 (ANAPC4)	I	NM_003903 (CDC16)	J
5KHU	NM_173473 (ANAPC16)	E	NM_001256 (CDC27)	F
2MSE	NM_000039 (APOA1)	A	NM_001654 (ARAF)	D
2MSE	NM_000039 (APOA1)	A	NM_001256197 (ARAF)	D
5YZ0	NM_130384 (ATRIP)	C	NM_001184 (ATR)	A
5GRQ	NM_000489 (ATRX)	C	NM_001141969 (DAXX)	A
5GRQ	NM_000489 (ATRX)	C	NM_001350 (DAXX)	A

4J2L	NM_000332 (ATXN1)	A	NM_015125 (CIC)	C
5ODT	NM_003600 (AURKA)	A	NM_006342 (TACCC3)	B
4RA0	NM_021913 (AXL)	C	NM_000820 (GAS6)	A
6QFM	NM_014417 (BBC3)	B	NM_021960 (MCL1)	A
5MQF	NM_005872 (BCAS2)	K	NM_002669 (PLRG1)	D
5MQF	NM_005872 (BCAS2)	K	NM_001253 (CDC5L)	L
1V11	NM_000709 (BCKDHA)	A	NM_000056 (BCKDHB)	B
2VPB	NM_004326 (BCL9)	B	NM_015617 (PYGO1)	A
2GL7	NM_004326 (BCL9)	C	NM_030756 (TCF7L2)	B
3R85	NM_138578 (BCL2L1)	A	NM_014320 (HEBP2)	E
4HNJ	NM_138578 (BCL2L1)	A	NM_014417 (BBC3)	C
6B7G	NM_017745 (BCOR)	B	NM_004529 (MLLT3)	A
4HPL	NM_017745 (BCOR)	A	NM_032673 (PCGF1)	B
5JH5	NM_021946 (BCORL1)	D	NM_032590 (KDM2B)	A
2KBW	NM_197966 (BID)	B	NM_021960 (MCL1)	A
6HPR	NM_001166 (BIRC2)	A	NM_181838 (UBE2D2)	C
3M0A	NM_001165 (BIRC3)	D	NM_021138 (TRAF2)	A
4AUQ	NM_139317 (BIRC7)	B	NM_021009 (UBC)	C
2QJ9	NM_004329 (BMPR1A)	D	NM_001200 (BMP2)	B
2H62	NM_004329 (BMPR1A)	C	NM_001106 (ACVR2B)	D
1JM7	NM_007294 (BRCA1)	A	NM_000465 (BARD1)	B
1N0W	NM_000059 (BRCA2)	B	NM_002875 (RAD51)	A
1N0W	NM_000059 (BRCA2)	B	NM_133487 (RAD51)	A
5KHU	NM_001211 (BUB1B)	Q	NM_002358 (MAD2L1)	T
5MQF	NM_003910 (BUD31)	Q	NM_016403 (CWC15)	R
1GZP	NM_004048 (B2M)	B	NM_001764 (CD1B)	A
1XZ0	NM_004048 (B2M)	B	NM_001763 (CD1A)	A
2X0G	NM_001743 (CALM2)	B	NM_004938 (DAPK1)	A
3H11	NM_001228 (CASP8)	B	NM_003879 (CFLAR)	A
1NW9	NM_032996 (CASP9)	B	NM_001167 (XIAP)	A
2W96	NM_053056 (CCND1)	A	NM_000075 (CDK4)	B
5L2W	NM_001238 (CCNE1)	B	NM_001798 (CDK2)	A
5KHU	NM_001256 (CDC27)	F	NM_004661 (CDC23)	C
1GRN	NM_001791 (CDC42)	A	NM_004308 (ARHGAP1)	B
4I5L	NM_001254 (CDC6)	B	NM_014225 (PPP2R1A)	A
3FF7	NM_004360 (CDH1)	A	NM_005810 (KLRG1)	C
1JSU	NM_004064 (CDKN1B)	C	NM_001798 (CDK2)	A
6ATH	NM_004064 (CDKN1B)	C	NM_001237 (CCNA2)	B
1BI7	NM_000077 (CDKN2A)	B	CDK6	A
4CXA	NM_016507 (CDK12)	A	NM_001099402 (CCNK)	B
1FQ1	NM_001798 (CDK2)	B	NM_005192 (CDKN3)	A
1FQ1	NM_001798 (CDK2)	B	NM_001330173 (CDKN3)	A
1JSU	NM_001798 (CDK2)	A	NM_001237 (CCNA2)	B
3G33	NM_000075 (CDK4)	A	NM_001760 (CCND3)	B
5FWK	NM_000075 (CDK4)	K	NM_007065 (CDC37)	E
1BI8	CDK6	A	NM_079421 (CDKN2D)	B
5IUS	NM_014143 (CD274)	C	NM_005018 (PDCD1)	A
1XWD	NM_000735 (CGA)	A	NM_000510 (FSHB)	B
4D10	NM_004236 (COPS2)	B	NM_016129 (COPS4)	D
4D10	NM_006837 (COPS5)	E	NM_006833 (COPS6)	F
4D10	NM_006710 (COPS8)	H	NM_001164095 (COPS7A)	G
4D10	NM_006710 (COPS8)	H	NM_001164093 (COPS7A)	G
4D10	NM_006710 (COPS8)	H	NM_016319 (COPS7A)	G
4D10	NM_006710 (COPS8)	H	NM_001164094 (COPS7A)	G
4WRL	NM_005211 (CSF1R)	A	NM_000757 (CSF1)	B
4DKD	NM_005211 (CSF1R)	C	NM_152456 (IL34)	A
1JWH	NM_001895 (CSNK2A1)	A	NM_001320 (CSNK2B)	C
1JDH	NM_001098210 (CTNNB1)	A	NM_030756 (TCF7L2)	B

3TX7	NM_001098210 (CTNNB1)	A	NM_205860 (NR5A2)	B
2GL7	NM_001098210 (CTNNB1)	A	NM_004326 (BCL9)	C
1T08	NM_001098210 (CTNNB1)	A	NM_020248 (CTNNBIP1)	B
1U6G	NM_003592 (CUL1)	A	NM_014248 (RBX1)	B
3TDU	NM_020640 (DCUN1D1)	A	NM_003592 (CUL1)	C
5ZAL	NM_001291628 (DICER1)	A	TARBP2	B
5ZAL	NM_177438 (DICER1)	A	TARBP2	B
5ZAL	NM_030621 (DICER1)	A	TARBP2	B
5ZAL	NM_001271282 (DICER1)	A	TARBP2	B
5YX2	NM_022552 (DNMT3A)	A	NM_013369 (DNMT3L)	B
5WB7	NM_005228 (EGFR)	A	NM_001432 (EREG)	E
3NJP	NM_005228 (EGFR)	A	EGF	C
1MOX	NM_005228 (EGFR)	A	NM_003236 (TGFA)	C
4ZJV	NM_005228 (EGFR)	A	NM_018948 (ERRFI1)	C
6CZW	NM_001430 (EPAS1)	A	NM_001668 (ARNT)	B
3MBW	NM_004431 (EPHA2)	A	NM_004428 (EFNA1)	B
4RIW	NM_001982 (ERBB3)	A	NM_005228 (EGFR)	B
3U7U	NM_001042599 (ERBB4)	A	NM_004495 (NRG1)	G
3U7U	NM_001042599 (ERBB4)	A	NM_013964 (NRG1)	G
5IVW	NM_000122 (ERCC3)	V	NM_000400 (ERCC2)	W
4A11	NM_000082 (ERCC8)	B	NM_001923 (DDB1)	A
5WUK	NM_004456 (EZH2)	B	NM_003797 (EED)	A
6C23	NM_004456 (EZH2)	K	NM_004973 (JARID2)	E
5V4B	NM_001257069 (FBXW7)	B	NM_170679 (SKP1)	A
5V4B	NM_033632 (FBXW7)	B	NM_170679 (SKP1)	A
5V4B	NM_001349798 (FBXW7)	B	NM_170679 (SKP1)	A
5W59	NM_023110 (FGFR1)	B	NM_002010 (FGF9)	A
1CVS	NM_023110 (FGFR1)	C	NM_002006 (FGF2)	A
1EVT	NM_023110 (FGFR1)	C	NM_000800 (FGF1)	A
2FDB	NM_000141 (FGFR2)	P	NM_006119 (FGF8)	M
2FDB	NM_000141 (FGFR2)	P	NM_033165 (FGF8)	M
4J23	NM_000141 (FGFR2)	A	NM_000800 (FGF1)	B
6NFJ	NM_005117 (FGF19)	C	NM_175737 (KLB)	A
1NUN	NM_000141 (FGFR2)	B	NM_004465 (FGF10)	A
1RY7	NM_000142 (FGFR3)	B	NM_000800 (FGF1)	A
1II4	NM_002006 (FGF2)	A	NM_000141 (FGFR2)	E
2MTP	NM_001110556 (FLNA)	A	NM_000419 (ITGA2B)	B
5T89	NM_002019 (FLT1)	X	NM_001025366 (VEGFA)	V
3QS7	FLT3	E	NM_001204503 (FLT3LG)	A
3QS7	FLT3	E	NM_001204502 (FLT3LG)	A
3QS7	FLT3	E	NM_001459 (FLT3LG)	A
4BSK	NM_002020 (FLT4)	A	NM_005429 (VEGFC)	C
4BSK	NM_182925 (FLT4)	A	NM_005429 (VEGFC)	C
4BSK	NM_001354989 (FLT4)	A	NM_005429 (VEGFC)	C
4YC7	NM_052905 (FMNL2)	B	NM_001791 (CDC42)	A
2OCF	NM_212476 (FN1)	D	NM_000125 (ESR1)	A
5DC0	NM_212476 (FN1)	A	NM_007313 (ABL1)	B
4LG0	NM_002015 (FOXO1)	A	NM_005238 (ETS1)	B
2AS5	NM_014491 (FOXP2)	F	NM_012340 (NFATC2)	N
3QRF	NM_014009 (FOXP3)	F	NM_012340 (NFATC2)	N
5OY4	NM_005479 (FRAT1)	X	GSK3B	A
1XWD	FSHR	C	NM_000510 (FSHB)	B
1X79	NM_013365 (GGA1)	A	NM_004703 (RABEP1)	B
1BP3	NM_000515 (GH1)	A	NM_000949 (PRLR)	B
1BP3	NM_000515 (GH1)	A	NM_001204317 (PRLR)	B
6NIY	NM_000516 (GNAS)	A	NM_002074 (GNB1)	B
6NIY	NM_001243774 (GNG2)	G	NM_001742 (CALCR)	R
6NIY	NM_001243773 (GNG2)	G	NM_001742 (CALCR)	R

6NIY	NM_053064 (GNG2)	G	NM_001742 (CALCR)	R
4D10	NM_212492 (GPS1)	A	NM_003653 (COPS3)	C
2L5G	NM_004489 (GPS2)	A	NM_006312 (NCOR2)	B
5H8F	NM_007327 (GRIN1)	B	NM_000833 (GRIN2A)	A
5H8F	NM_007327 (GRIN1)	B	NM_001134407 (GRIN2A)	A
3GTU	NM_000848 (GSTM2)	A	NM_000849 (GSTM3)	B
1WQ1	NM_176795 (HRAS)	R	NM_002890 (RASA1)	G
4K81	NM_176795 (HRAS)	B	NM_004490 (GRB14)	A
2C5L	NM_176795 (HRAS)	A	NM_016341 (PLCE1)	C
4URU	NM_176795 (HRAS)	R	NM_005633 (SOS1)	S
6AXG	NM_176795 (HRAS)	B	NM_170604 (RASGRP4)	A
1HE8	NM_176795 (HRAS)	B	NM_001282427 (PIK3CG)	A
1TOP	NM_002162 (ICAM3)	B	NM_002209 (ITGAL)	A
2L29	NM_000612 (IGF2)	B	NM_000876 (IGF2R)	A
5FUC	NM_000600 (IL6)	A	NM_000565 (IL6R)	C
1P9M	NM_002184 (IL6ST)	A	NM_000600 (IL6)	B
2KSO	NM_001567 (INPPL1)	B	NM_004431 (EPHA2)	A
3ZJY	NM_014652 (IPO13)	B	NM_001412 (EIF1AX)	C
3ZJY	NM_014652 (IPO13)	B	NM_006325 (RAN)	A
1ZOQ	NM_001571 (IRF3)	A	NM_004380 (CREBBP)	C
5IXD	NM_002227 (JAK1)	A	NM_170743 (IFNLR1)	B
6E2Q	NM_001322195 (JAK2)	A	NM_000121 (EPOR)	M
6E2Q	NM_001322194 (JAK2)	A	NM_000121 (EPOR)	M
6E2Q	NM_004972 (JAK2)	A	NM_000121 (EPOR)	M
6E2Q	NM_001322196 (JAK2)	A	NM_000121 (EPOR)	M
2X1X	NM_002253 (KDR)	R	NM_005429 (VEGFC)	E
5NLB	NM_012289 (KEAP1)	A	NM_003590 (CUL3)	B
2E9W	NM_000222 (KIT)	A	NM_003994 (KITLG)	C
5F6K	NM_170606 (KMT2C)	C	NM_004674 (ASH2L)	A
6EPP	NM_033360 (KRAS)	R	NM_005633 (SOS1)	S
5BRK	NM_004690 (LAT51)	B	NM_018221 (MOB1A)	A
4ZRI	NM_014572 (LAT52)	C	NM_000268 (NF2)	A
4KT1	NM_018490 (LGR4)	A	RSPO1	E
2HYI	NM_002370 (MAGOH)	A	NM_007359 (CASC3)	D
2HYI	NM_002370 (MAGOH)	A	NM_014740 (EIF4A3)	C
2HYI	NM_002370 (MAGOH)	A	NM_005105 (RBM8A)	B
4IZ7	NM_002745 (MAPK1)	C	NM_003768 (PEA15)	B
4IZ7	NM_138957 (MAPK1)	C	NM_003768 (PEA15)	B
6U2G	NM_002755 (MAP2K1)	A	NM_004333 (BRAF)	B
2Y4I	NM_002755 (MAP2K1)	C	NM_173598 (KSR2)	B
2KYL	NM_015112 (MAST2)	A	NM_000314 (PTEN)	B
1NLW	NM_197957 (MAX)	B	NM_002357 (MXD1)	A
3PK1	NM_021960 (MCL1)	A	NM_138763 (BAX)	B
5JA4	NM_004526 (MCM2)	C	NM_013432 (TONSL)	D
1YCR	MDM2	A	NM_000546 (TP53)	B
2VJE	MDM2	A	NM_002393 (MDM4)	B
2MPS	MDM2	A	NM_005427 (TP73)	B
3U88	NM_130802 (MEN1)	A	NM_005933 (KMT2A)	M
3U88	NM_000244 (MEN1)	A	NM_005933 (KMT2A)	M
3U88	NM_130801 (MEN1)	A	NM_005933 (KMT2A)	M
3U88	NM_130800 (MEN1)	A	NM_005933 (KMT2A)	M
3U88	NM_130804 (MEN1)	A	NM_005933 (KMT2A)	M
3U88	NM_130803 (MEN1)	A	NM_005933 (KMT2A)	M
1SHY	NM_000245 (MET)	B	NM_000601 (HGF)	A
2O8B	NM_000179 (MSH6)	B	NM_000251 (MSH2)	A
4QT8	NM_020998 (MST1)	C	NM_002447 (MST1R)	B
5WBU	MTOR	B	NM_022372 (MLST8)	D
5H64	MTOR	A	NM_020761 (RPTOR)	B

2FAP	MTOR	B	NM_000801 (FKBP1A)	A
2FAP	MTOR	B	NM_054014 (FKBP1A)	A
5WBH	MTOR	A	NM_003161 (RPS6KB1)	W
1NKP	NM_002467 (MYC)	A	NM_197957 (MAX)	B
3MOP	NM_002468 (MYD88)	A	NM_001570 (IRAK2)	K
5MV9	NM_000260 (MYO7A)	A	NM_005709 (USH1C)	B
6IGX	NM_022346 (NCAPG)	B	NM_015341 (NCAPH)	A
1H2T	NM_002486 (NCBP1)	C	NM_007362 (NCBP2)	Z
1WLP	NM_000265 (NCF1)	B	NM_000101 (CYBA)	A
1XT9	NM_006156 (NEDD8)	B	NM_145204 (SENP8)	A
1M4U	NM_005450 (NOG)	A	NM_001719 (BMP7)	L
2F8X	NM_017617 (NOTCH1)	K	NM_014757 (MAML1)	M
2F8X	NM_017617 (NOTCH1)	K	NM_015874 (RBPJ)	C
5L0R	NM_017617 (NOTCH1)	B	NM_152305 (POGLUT1)	A
6PY8	NM_017617 (NOTCH1)	F	NM_001004354 (NRARP)	B
1BND	NM_002527 (NTF3)	B	NM_170735 (BDNF)	A
1WWW	NM_002529 (NTRK1)	X	NM_002506 (NGF)	V
1JGN	NM_002568 (PABPC1)	A	NM_016480 (PAIP2)	B
1WMH	NM_016948 (PARD6A)	B	NM_002740 (PRKCI)	A
1B72	NM_002585 (PBX1)	B	NM_002144 (HOXB1)	A
3MJG	NM_002609 (PDGFRB)	X	NM_002608 (PDGFB)	A
1ZY8	NM_003477 (PDHX)	K	NM_000108 (DLD)	A
5IFE	NM_032758 (PHF5A)	D	NM_012433 (SF3B1)	C
6NCT	NM_006218 (PIK3CA)	A	NM_181504 (PIK3R1)	B
6PYU	NM_005026 (PIK3CD)	A	NM_181504 (PIK3R1)	B
5MQF	NM_002669 (PLRG1)	D	NM_014691 (AQR)	U
5VBN	NM_006231 (POLE)	B	NM_002692 (POLE2)	A
2PRG	NM_005037 (PPARG)	A	NM_147223 (NCOA1)	C
2IE3	NM_014225 (PPP2R1A)	A	NM_002715 (PPP2CA)	C
5MQF	PRPF8	A	NM_004247 (EFTUD2)	B
6DMY	NM_000264 (PTCH1)	A	NM_000193 (SHH)	B
4R3Z	NM_005051 (QARS)	C	NM_002887 (RARS)	B
2FJU	NM_018890 (RAC1)	A	NM_004573 (PLCB2)	B
2FJU	NM_018890 (RAC1)	A	NM_001284299 (PLCB2)	B
4YON	NM_018890 (RAC1)	B	NM_020820 (PREX1)	A
3B13	NM_018890 (RAC1)	B	NM_004946 (DOCK2)	A
3SUA	NM_018890 (RAC1)	A	NM_002673 (PLXNB1)	D
1E96	NM_018890 (RAC1)	A	NM_000433 (NCF2)	B
2YBF	NM_020165 (RAD18)	B	NM_003337 (UBE2B)	A
2MRE	NM_020165 (RAD18)	B	NM_021009 (UBC)	A
4PK7	NM_006265 (RAD21)	B	NM_006603 (STAG2)	A
1C1Y	NM_002880 (RAF1)	B	NM_002884 (RAP1A)	A
4G0N	NM_002880 (RAF1)	B	NM_176795 (HRAS)	A
5MQF	NM_018047 (RBM22)	P	NM_016652 (CRNL1)	O
2AZE	NM_000321 (RB1)	C	NM_007111 (TFDP1)	A
2AZE	NM_000321 (RB1)	C	NM_005225 (E2F1)	B
2LSP	NM_021975 (RELA)	A	NM_058243 (BRD4)	B
6GL7	NM_020975 (RET)	F	NM_001495 (GFRA2)	D
6GL7	NM_020975 (RET)	F	NM_004558 (NRTN)	B
3MV5	NM_005163 (AKT1)	A	GSK3B	C
1O6K	NM_001626 (AKT2)	A	GSK3B	C
3T5G	NM_005614 (RHEB)	A	NM_002601 (PDE6D)	B
1CXZ	NM_001664 (RHOA)	A	NM_002741 (PKN1)	B
1CXZ	NM_001664 (RHOA)	A	NM_213560 (PKN1)	B
6BC0	NM_001664 (RHOA)	F	NM_001177693 (ARHGEF28)	A
4XH9	NM_001664 (RHOA)	B	NM_005863 (NET1)	A
1OW3	NM_001664 (RHOA)	B	NM_004308 (ARHGAP1)	A
1X86	NM_001664 (RHOA)	B	NM_015313 (ARHGEF12)	A

4KNG	NM_017763 (RNF43)	E	NM_003667 (LGR5)	A
4JHP	NM_000328 (RPGR)	C	NM_002601 (PDE6D)	B
4KNG	RSPO1	M	NM_017763 (RNF43)	E
1H9D	NM_001001890 (RUNX1)	A	NM_001755 (CBFB)	B
3DZU	NM_002957 (RXRA)	A	NM_005037 (PPARG)	D
4ZO1	NM_002957 (RXRA)	B	NM_000461 (THR8B)	X
1TGZ	NM_021627 (SENP2)	A	NM_003352 (SUMO1)	B
5IFE	NM_012433 (SF3B1)	C	NM_012426 (SF3B3)	A
5IFE	NM_012433 (SF3B1)	C	NM_031287 (SF3B5)	B
5C4V	NM_005414 (SKIL)	B	NM_005359 (SMAD4)	A
1P22	NM_170679 (SKP1)	B	NM_033637 (BTRC)	A
5JH5	NM_170679 (SKP1)	B	NM_032673 (PCGF1)	C
1MR1	NM_005359 (SMAD4)	A	NM_003036 (SKI)	C
1U7V	NM_005359 (SMAD4)	B	NM_005901 (SMAD2)	A
1U7F	NM_005359 (SMAD4)	B	NM_005902 (SMAD3)	A
5GJK	NM_003073 (SMARCB1)	B	NM_003074 (SMARCC1)	A
6OT0	NM_005631 (SMO)	R	NM_002069 (GNAI1)	A
5MQF	NM_004814 (SNRNP40)	F	NM_015891 (CDC40)	E
5MQF	NM_003090 (SNRPA1)	W	NM_016059 (PPI1)	V
3NBY	NM_005701 (SNUPN)	B	NM_006325 (RAN)	C
5DIS	NM_005701 (SNUPN)	C	NM_003400 (XPO1)	A
5MQF	NM_012245 (SNW1)	C	NM_002669 (PLRG1)	D
1O4X	NM_003106 (SOX2)	B	NM_002697 (POU2F1)	A
1YC0	NM_003710 (SPINT1)	I	NM_001528 (HGFAC)	A
4EOZ	NM_003563 (SPOP)	A	NM_003590 (CUL3)	B
5HKY	NM_001318537 (SPRY2)	B	NM_005188 (CBL)	A
5HKY	NM_005842 (SPRY2)	B	NM_005188 (CBL)	A
5HKY	NM_001318538 (SPRY2)	B	NM_005188 (CBL)	A
5HKY	NM_001318536 (SPRY2)	B	NM_005188 (CBL)	A
3LBX	NM_003126 (SPTA1)	A	NM_001024858 (SPTB)	B
3LBX	NM_003126 (SPTA1)	A	NM_001355436 (SPTB)	B
5MQF	NM_016333 (SRRM2)	S	NM_020943 (CWC22)	T
2WTK	NM_000455 (STK11)	C	NM_001003787 (STRADA)	B
2WTK	NM_000455 (STK11)	C	NM_016289 (CAB39)	A
3AAD	NM_004606 (TAF1)	A	NM_014034 (ASF1A)	B
4Z6Y	NM_016495 (TBC1D7)	B	NM_000368 (TSC1)	C
6ERP	NM_003201 (TFAM)	C	NM_005035 (POLRMT)	A
3KFD	NM_003242 (TGFBR2)	E	TGFB1 (TGFB1)	A
5TX4	NM_003242 (TGFBR2)	A	NM_003238 (TGFB2)	B
2PJY	NM_003242 (TGFBR2)	B	NM_003239 (TGFB3)	A
3V96	NM_003254 (TIMP1)	A	NM_002425 (MMP10)	B
1CF4	NM_005781 (TNK2)	B	NM_001791 (CDC42)	A
1QBK	NM_002270 (TNPO1)	B	NM_006325 (RAN)	C
5YVG	NM_002270 (TNPO1)	A	NM_004960 (FUS)	X
2MEJ	NM_000546 (TP53)	B	NM_138578 (BCL2L1)	A
2LY4	NM_000546 (TP53)	B	NM_002128 (HMGB1)	A
2K8F	NM_000546 (TP53)	B	NM_001429 (EP300)	A
2RUK	NM_000546 (TP53)	A	NM_005316 (GTF2H1)	B
2B3G	NM_000546 (TP53)	B	NM_002945 (RPA1)	A
1YCS	NM_000546 (TP53)	A	NM_001031685 (TP53BP2)	B
1YCS	NM_000546 (TP53)	A	NM_005426 (TP53BP2)	B
6CO2	NM_005657 (TP53BP1)	C	NM_152395 (NUDT16)	A
1F3V	NM_021138 (TRAF2)	B	NM_001323552 (TRADD)	A
1F3V	NM_021138 (TRAF2)	B	NM_003789 (TRADD)	A
6I3V	NM_016399 (TRIAP1)	A	NM_013237 (PRELID1)	F
1Y8Q	NM_005499 (UBA2)	B	NM_005500 (SAE1)	A
1XD3	NM_021009 (UBC)	B	NM_006002 (UCHL3)	A
1FBV	UBE2L3	C	NM_005188 (CBL)	A

1Y8X	NM_003969 (UBE2M)	A	NM_198195 (UBA3)	B
4WQO	NM_000551 (VHL)	A	NM_003591 (CUL2)	D
6HR2	NM_000551 (VHL)	B	NM_003072 (SMARCA4)	A
1LM8	NM_000551 (VHL)	V	NM_005648 (ELOC)	C
1LM8	NM_000551 (VHL)	V	NM_007108 (ELOB)	B
1M10	NM_000552 (VWF)	A	NM_000173 (GP1BA)	B
6FBS	NM_018383 (WDR33)	B	NM_006693 (CPSF4)	C
6FBS	NM_018383 (WDR33)	B	NM_013291 (CPSF1)	A
5MQF	NM_020196 (XAB2)	M	NM_015484 (SYF2)	N
5DIS	NM_003400 (XPO1)	A	NM_006325 (RAN)	B
2L1L	NM_003400 (XPO1)	B	NM_006823 (PKIA)	A
6BX8	NM_002771 (PRSS3)	A	NM_006287 (TFPI)	E
6HAR	NM_002771 (PRSS3)	A	NM_000484 (APP)	E
5JBT	NM_002771 (PRSS3)	A	NM_001642 (APLP2)	X
4U30	NM_002771 (PRSS3)	A	NM_001633 (AMBP)	X
4U32	NM_002771 (PRSS3)	A	SPINT2	X
4NO0	LILRB1	D	NM_002339 (LSP1)	C
4NO0	LILRB1	D	NM_004048 (B2M)	B
2DYP	LILRB2	D	NM_004048 (B2M)	B
6MPP	NM_002116 (HLA-A)	A	NM_004048 (B2M)	C
3PTH	NM_002568 (PABPC1)	A	NM_015155 (LARP4B)	B
4LWZ	NM_001080467 (MYO5B)	B	NM_004663 (RAB11A)	A
2D07	NM_003211 (TDG)	A	NM_006937 (SUMO2)	B
1WYW	NM_003211 (TDG)	A	NM_003352 (SUMO1)	B
5B38	NM_013289 (KIR3DL1)	G	NM_004048 (B2M)	B
6S53	NM_003348 (UBE2N)	E	NM_021009 (UBC)	F
6HBY	NM_002124 (HLA-DRB1)	B	NM_019111 (HLA-DRA)	A
2AFF	NM_002417 (MKI67)	A	NM_032390 (NIFK)	B
5J28	NM_002417 (MKI67)	C	NM_002710 (PPP1CC)	A
1YA5	NM_133378 (TTN)	A	NM_003673 (TCAP)	T
3KNB	NM_133378 (TTN)	A	NM_015311 (OBSL1)	B
3E2U	NM_002956 (CLIP1)	E	NM_004082 (DCTN1)	A
5Y1Z	NM_183047 (ZMYND8)	C	NM_080881 (DBN1)	A
4NT6	NM_002117 (HLA-C)	A	NM_004048 (B2M)	B
2RVB	NM_004628 (XPC)	A	NM_005316 (GTF2H1)	B
3MMY	NM_016320 (NUP98)	B	NM_003610 (RAE1)	A
3MMY	NM_016320 (NUP98)	B	NM_001015885 (RAE1)	A
4DXR	NM_182961 (SYNE1)	B	NM_001199579 (SUN2)	A
6DAD	NM_000719 (CACNA1C)	C	NM_006888 (CALM1)	A
5NVN	NM_004095 (EIF4EBP1)	B	NM_004846 (EIF4E2)	A
2FYL	NM_002332 (LRP1)	B	NM_002337 (LRPAP1)	A
2YLE	NM_020066 (FMN2)	B	NM_020148 (SPIRE1)	A
5CLL	NM_006325 (RAN)	A	NM_006267 (RANBP2)	B
1Z5S	NM_006267 (RANBP2)	D	NM_002883 (RANGAP1)	C
3Q6S	NM_138484 (SGO1)	E	NM_006807 (CBX1)	A
5L3Q	NM_003139 (SRPRA)	B	NM_003136 (SRP54)	A
3N3K	NM_005154 (USP8)	A	NM_021009 (UBC)	B
2GWF	NM_005154 (USP8)	A	NM_005785 (RNF41)	B
3F7P	NM_000445 (PLEC)	A	ITGB4	C
4PJ1	NM_002156 (HSPD1)	A	NM_002157 (HSPE1)	O
6FYH	NM_031407 (HUWE1)	A	NM_018955 (UBB)	B
5C6H	NM_031407 (HUWE1)	B	NM_021960 (MCL1)	A
5OO6	NM_015908 (SRRT)	C	NM_007362 (NCBP2)	B
6IGM	NM_006662 (SRCAP)	H	NM_022496 (ACTR6)	G
5NVL	NM_001103146 (GIGYF2)	B	NM_004846 (EIF4E2)	A
3K6G	NM_005652 (TERF2)	D	NM_018975 (TERF2IP)	A
3VU7	NM_002912 (REV3L)	Z	NM_006341 (MAD2L2)	C
4GK0	NM_002912 (REV3L)	C	NM_016316 (REV1)	E

4YOC	NM_001379 (DNMT1)	A	NM_003470 (USP7)	C
5WVO	NM_001379 (DNMT1)	C	NM_001177413 (RPS27A)	A
5WVO	NM_001379 (DNMT1)	C	NM_001135592 (RPS27A)	A
5WVO	NM_001379 (DNMT1)	C	NM_002954 (RPS27A)	A
5YDR	NM_001379 (DNMT1)	B	NM_018955 (UBB)	A
4XC2	NM_152903 (KBTBD6)	E	NM_007278 (GABARAP)	A
4X86	NM_080703 (BAG6)	B	NM_014235 (UBL4A)	A
6AU8	NM_080703 (BAG6)	C	NM_015949 (GET4)	A
2N9P	NM_080703 (BAG6)	C	RNF126 (RNF126)	A
3FMP	NM_005085 (NUP214)	A	NM_007242 (DDX19B)	B
6OEL	NM_000206 (IL2RG)	C	NM_000418 (IL4R)	B
6OEL	NM_000206 (IL2RG)	C	NM_001257406 (IL4R)	B
5M5E	NM_000206 (IL2RG)	C	NM_000586 (IL2)	D
5M5E	NM_000206 (IL2RG)	C	NM_001346223 (IL2RB)	B
5M5E	NM_000206 (IL2RG)	C	NM_001346222 (IL2RB)	B
5M5E	NM_000206 (IL2RG)	C	NM_000878 (IL2RB)	B
4DHX	NM_003906 (MCM3AP)	A	NM_020189 (ENY2)	B
3DXC	NM_001164 (APBB1)	A	NM_000484 (APP)	B
2KRB	NM_003758 (EIF3J)	B	NM_001037283 (EIF3B)	A
2KRB	NM_003758 (EIF3J)	B	NM_003751 (EIF3B)	A
2KRB	NM_003758 (EIF3J)	B	NM_001362791 (EIF3B)	A
3QB4	NM_004329 (BMPR1A)	B	GDF5	A
6GR8	NM_003160 (AURKC)	A	NM_020238 (INCENP)	B
6OAU	NM_178172 (GPIHBP1)	C	NM_000237 (LPL)	A
6DFX	NM_002123 (HLA-DQB1)	B	NM_002122 (HLA-DQA1)	A
6Q2J	NM_207410 (GFRAL)	C	NM_020975 (RET)	E
6MUN	NM_013444 (UBQLN2)	B	NM_002810 (PSMD4)	A
6I2I	NM_006082 (TUBA1B)	A	NM_178014 (TUBB)	B
6J56	NM_004999 (MYO6)	A	NM_005488 (TOM1)	C
6NPY	NM_002759 (EIF2AK2)	B	NM_004895 (NLRP3)	A
6CSU	NM_014985 (CEP152)	B	NM_025180 (CEP63)	C
6S8S	NM_004397 (DDX6)	A	NM_025083 (EDC3)	B
6RRK	NM_005862 (STAG1)	B	NM_006265 (RAD21)	C
6QFI	NM_021960 (MCL1)	A	NM_001204108 (BCL2L11)	B
6QFI	NM_021960 (MCL1)	A	NM_138621 (BCL2L11)	B
6QFI	NM_021960 (MCL1)	A	NM_138622 (BCL2L11)	B
6QFI	NM_021960 (MCL1)	A	NM_138627 (BCL2L11)	B
6O81	NM_003907 (EIF2B5)	A	NM_014239 (EIF2B2)	C
6DCX	NM_006663 (PPP1R13L)	C	NM_002708 (PPP1CA)	A
6Q8I	NM_018225 (SMU1)	A	NM_006083 (IK)	C
6O5B	NM_138357 (MCU)	J	NM_033318 (SMDT1)	F
6IEH	MTREX	B	NM_017970 (NRDE2)	A
5ZLZ	NM_000602 (SERPINE1)	I	NM_000930 (PLAT)	E
6AJ4	NM_033407 (DOCK7)	A	NM_001791 (CDC42)	B
6GHM	NM_001031685 (TP53BP2)	C	NM_002708 (PPP1CA)	A
6GHM	NM_005426 (TP53BP2)	C	NM_002708 (PPP1CA)	A
6AGO	NM_018489 (ASH1L)	A	NM_006791 (MORF4L1)	C
6IXV	NM_004844 (SH3BP5)	A	NM_004663 (RAB11A)	E
6N89	NM_002265 (KPNB1)	A	NM_005318 (H1F0)	B
6FP6	NM_005125 (CCS)	B	NM_000454 (SOD1)	A
6IRA	NM_007327 (GRIN1)	A	NM_000833 (GRIN2A)	D
6IRA	NM_007327 (GRIN1)	A	NM_001134407 (GRIN2A)	D
6I3F	NM_000537 (REN)	B	NM_000029 (AGT)	A
6GU4	NM_031966 (CCNB1)	B	NM_001786 (CDK1)	A
5ZOJ	NM_005901 (SMAD2)	A	LEMD3	D
6EKK	NM_006861 (RAB35)	C	NM_024820 (DENND1A)	A
6A5Z	NM_005123 (NR1H4)	A	NM_002957 (RXRA)	D
6AGF	NM_000334 (SCN4A)	A	NM_001037 (SCN1B)	B

6E7C	NM_178012 (TUBB2B)	B	NM_006082 (TUBA1B)	A
6DV2	NM_000183 (HADHB)	A	NM_000182 (HADHA)	G
5ZMC	NM_002502 (NFKB2)	A	NM_005238 (ETS1)	B
5ZMC	NM_001261403 (NFKB2)	A	NM_005238 (ETS1)	B
5ZMC	NM_001288724 (NFKB2)	A	NM_005238 (ETS1)	B
6A69	NM_001682 (ATP2B1)	A	NM_012428 (NPTN)	B
6GZH	NM_001240 (CCNT1)	B	NM_001261 (CDK9)	A
5Y6L	NM_004990 (MARS)	A	NM_004446 (EPRS)	B
6A70	NM_000297 (PKD2)	A	NM_001009944 (PKD1)	B
6FZW	NM_000090 (COL3A1)	A	NM_002593 (PCOLCE)	D
5XV6	NM_014741 (ATG13)	A	NM_021934 (ATG101)	B
5Y31	NM_021723 (ADAM22)	A	NM_005097 (LGI1)	B

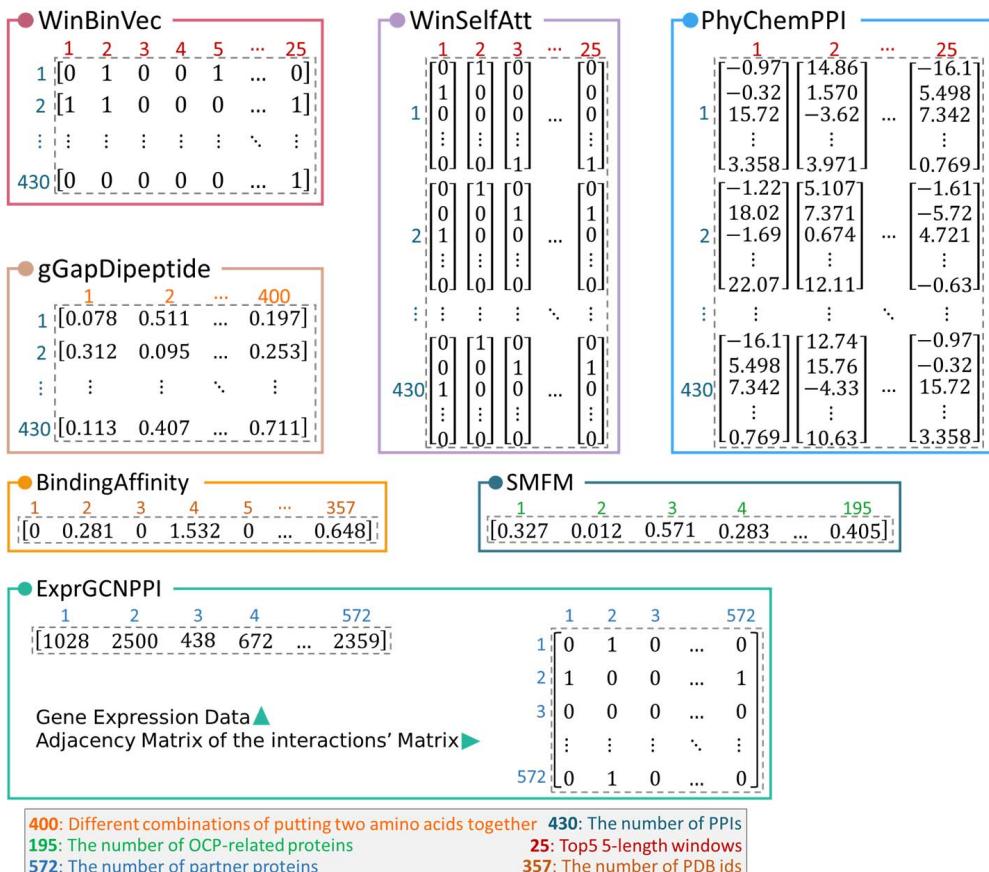


Figure 1: A representation of the input features extracted from one sample in various models.

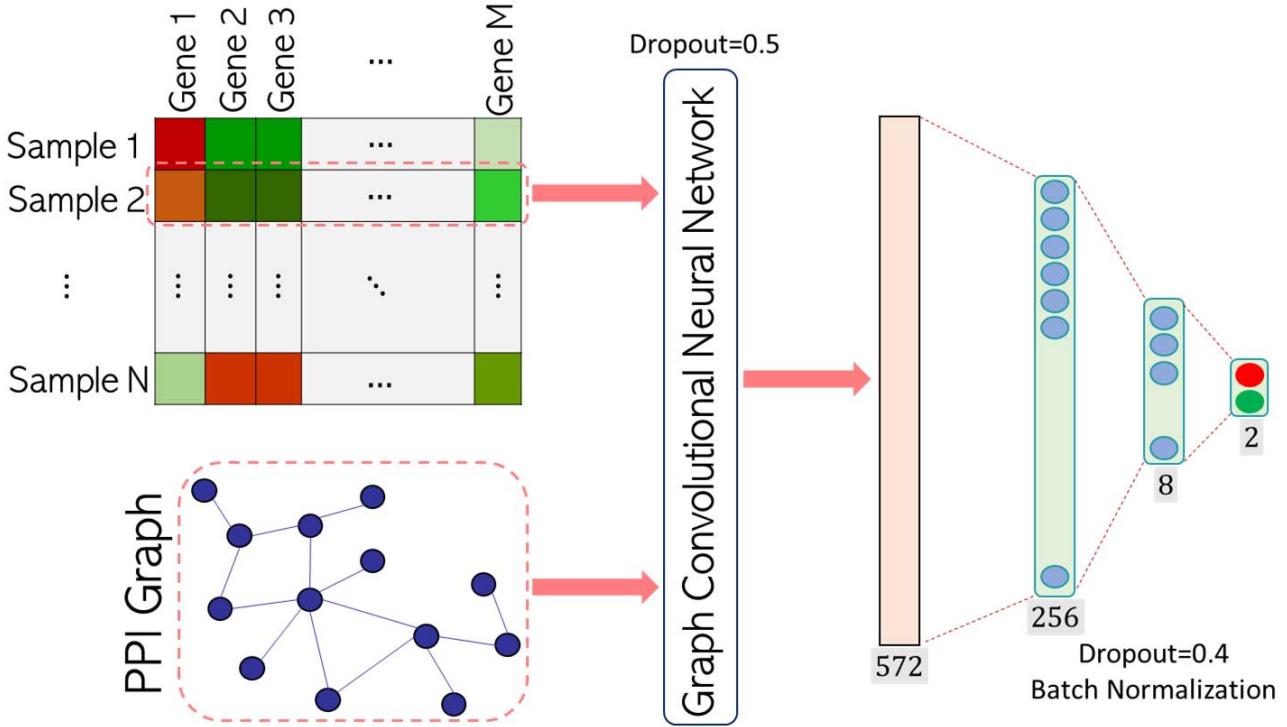


Figure 2: The ExprGCNPPPI architecture. This model accepts gene expression values of the partner proteins involved in the PPIs alongside with the network of interactions and pass through a graph convolutional neural network. Finally, the extracted features from previous stage are fed into fully connected layers. Here, the network of the interactions is represented by an adjacency matrix.

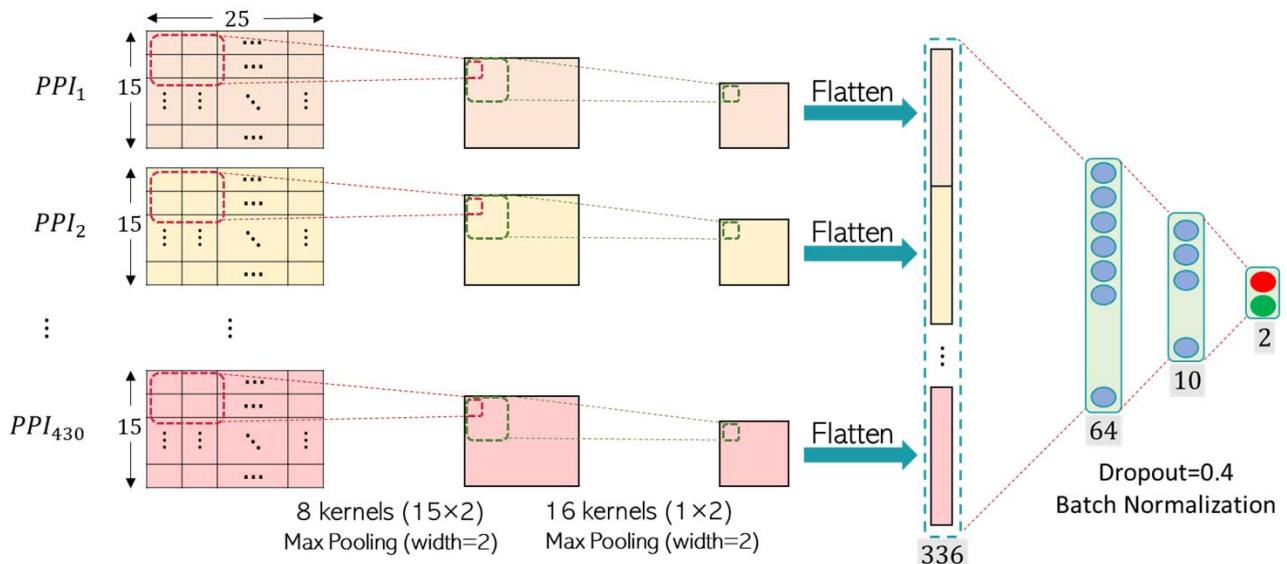


Figure 3: The PhyChemPPI architecture. The input features of this model consist of the biophysicochemical properties of the amino acids in the PPI sequences. The input features are passed through two convolutional layers. Finally, the results are flattened and fed into fully connected layers.

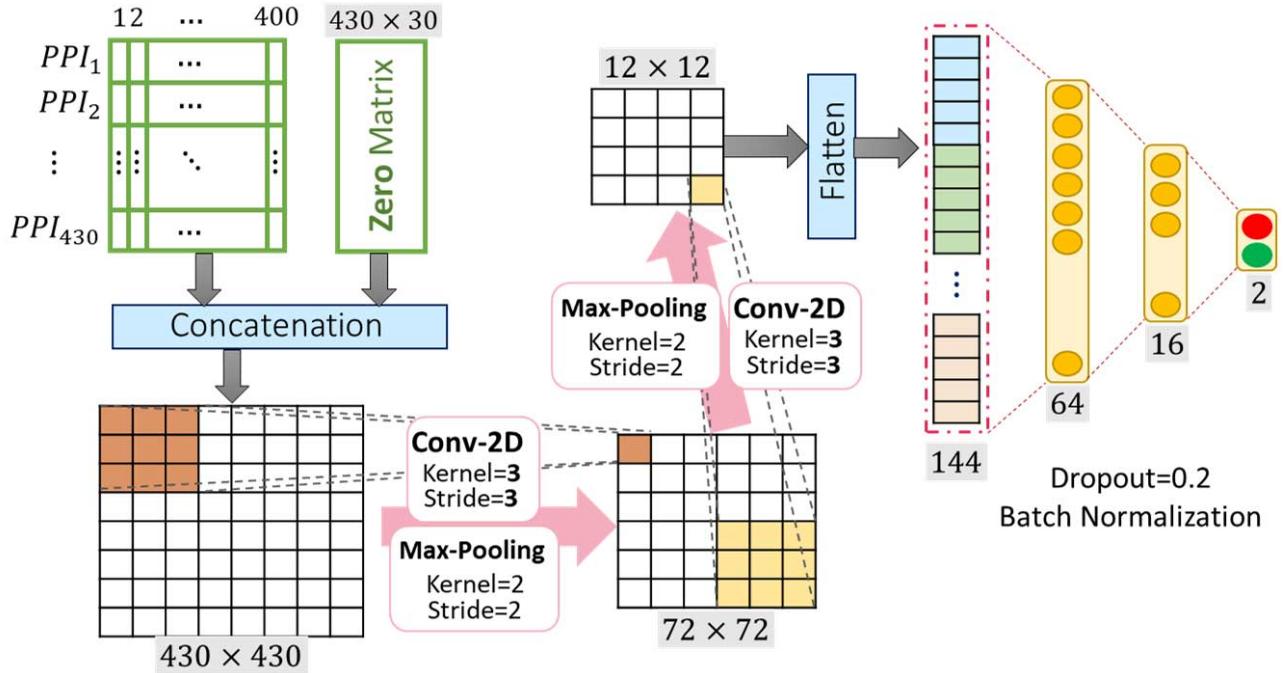


Figure 4: The gGapDipeptide architecture. The gGapDipeptide captures features from g-gap dipeptide that contains PPIs 400-dimensional vectors. The gGapDipeptide model consists of two main components: firstly, it passes the input features through convolutional layers. Then, the obtained features are passed through fully connected layers.

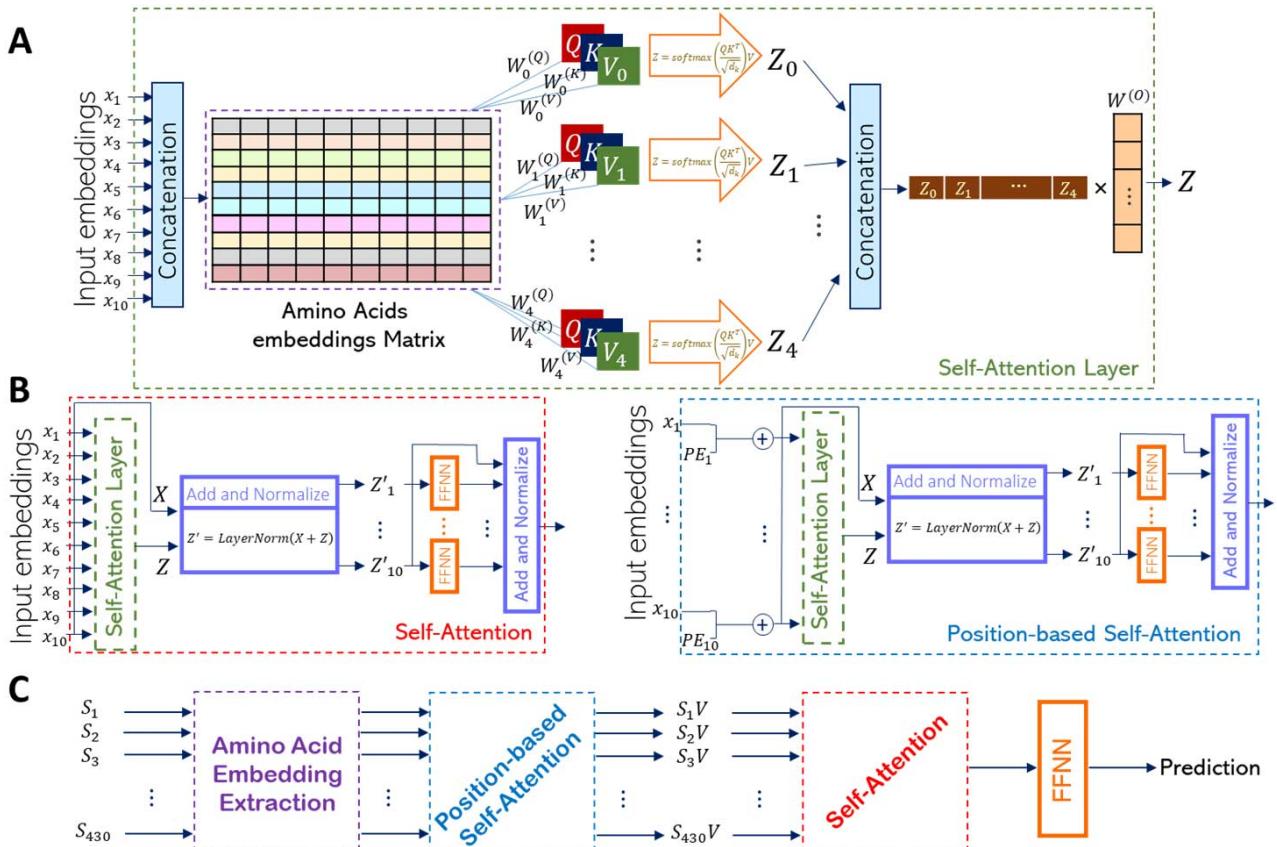


Figure 5: The WinSelfAtt architecture. (A) Self-Attention layer architecture. This layer utilizes five $\{Query, Key, Value\}$ triples. (B) Self-Attention and Position-based Self-Attention modules. (C) The WinSelfAtt model architecture consists of three modules: Position-based Self-Attention, Self-Attention, and prediction modules.

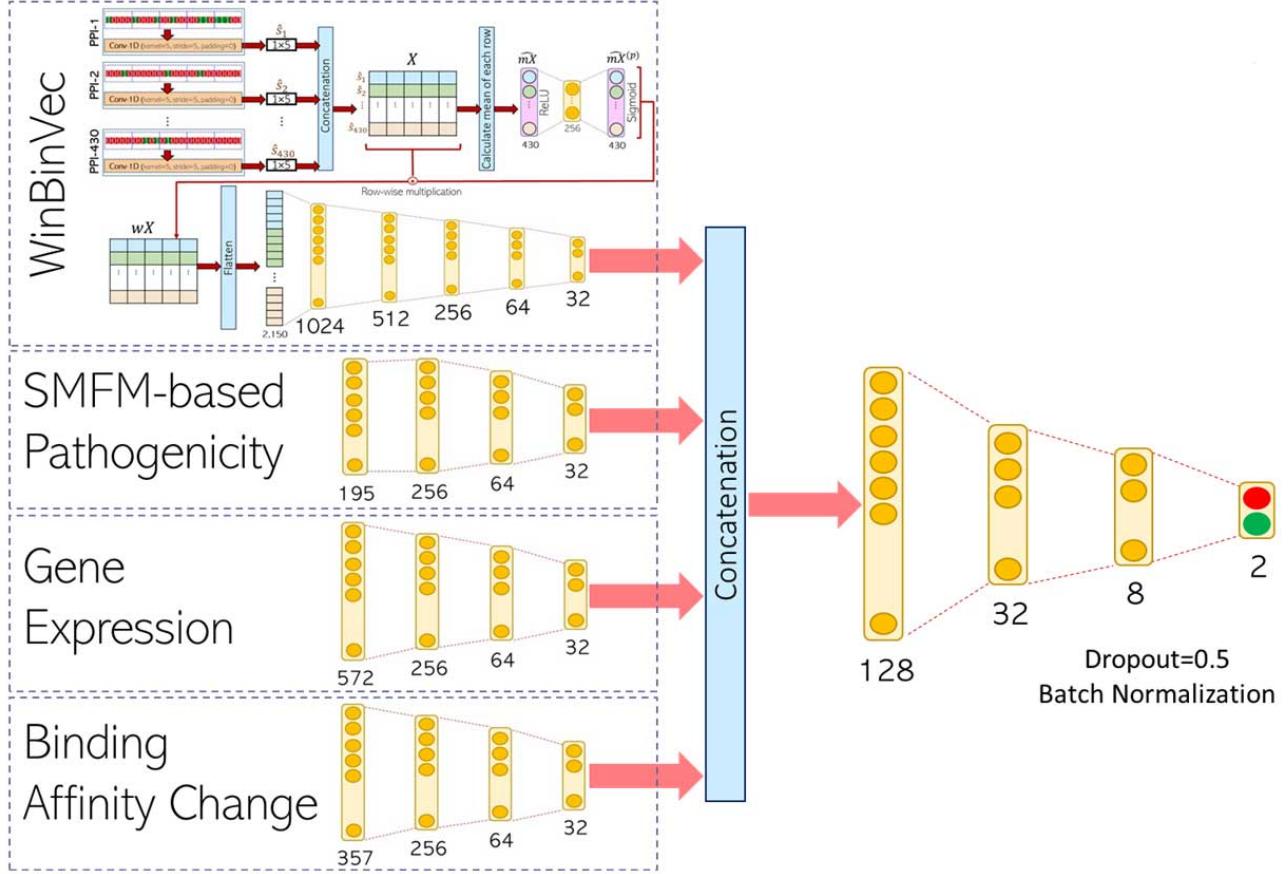


Figure 6: The FusionPPI architecture. This model employs four different types of input features that achieved better performance than the others. These input features consist of window-based binary vectors, pathogenicity scores of the OCP-reported proteins, gene expression values of the partner proteins in the PPIs, and binding affinity changes upon mutations.

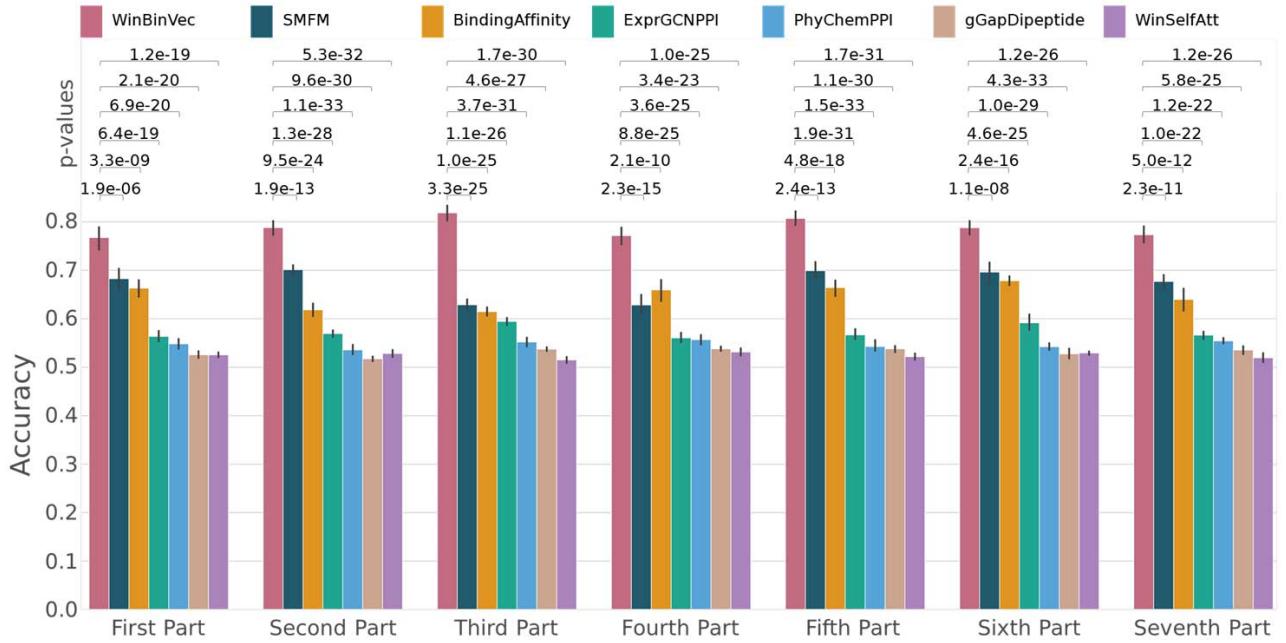


Figure 7: Metastasis Stage Prediction Accuracy using different models. The numbers above the bars represent the p-values. To obtain each dot in the figure, we performed 10-fold cross-validation with three repetitions.

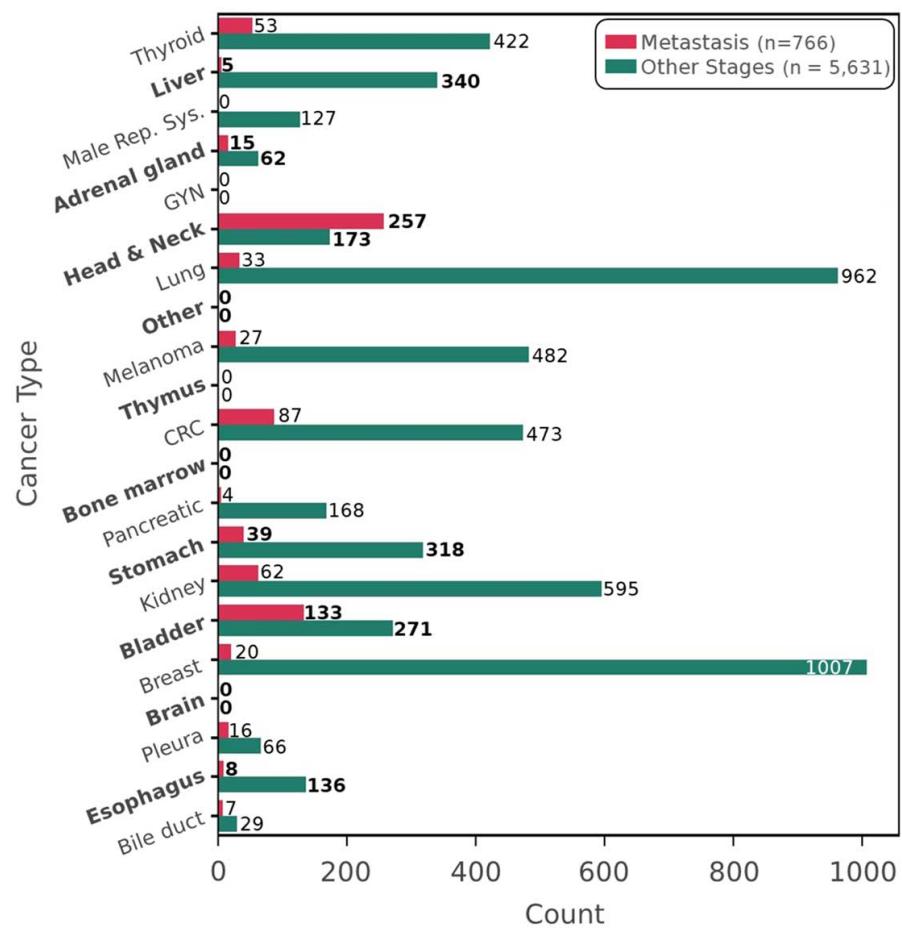


Figure 8: Metastasis stage and the other stages population in different cancer types. In total, there are 766 patients in the metastasis stage and 5 631 patients are in the other stages including stages 1, 2, and 3.

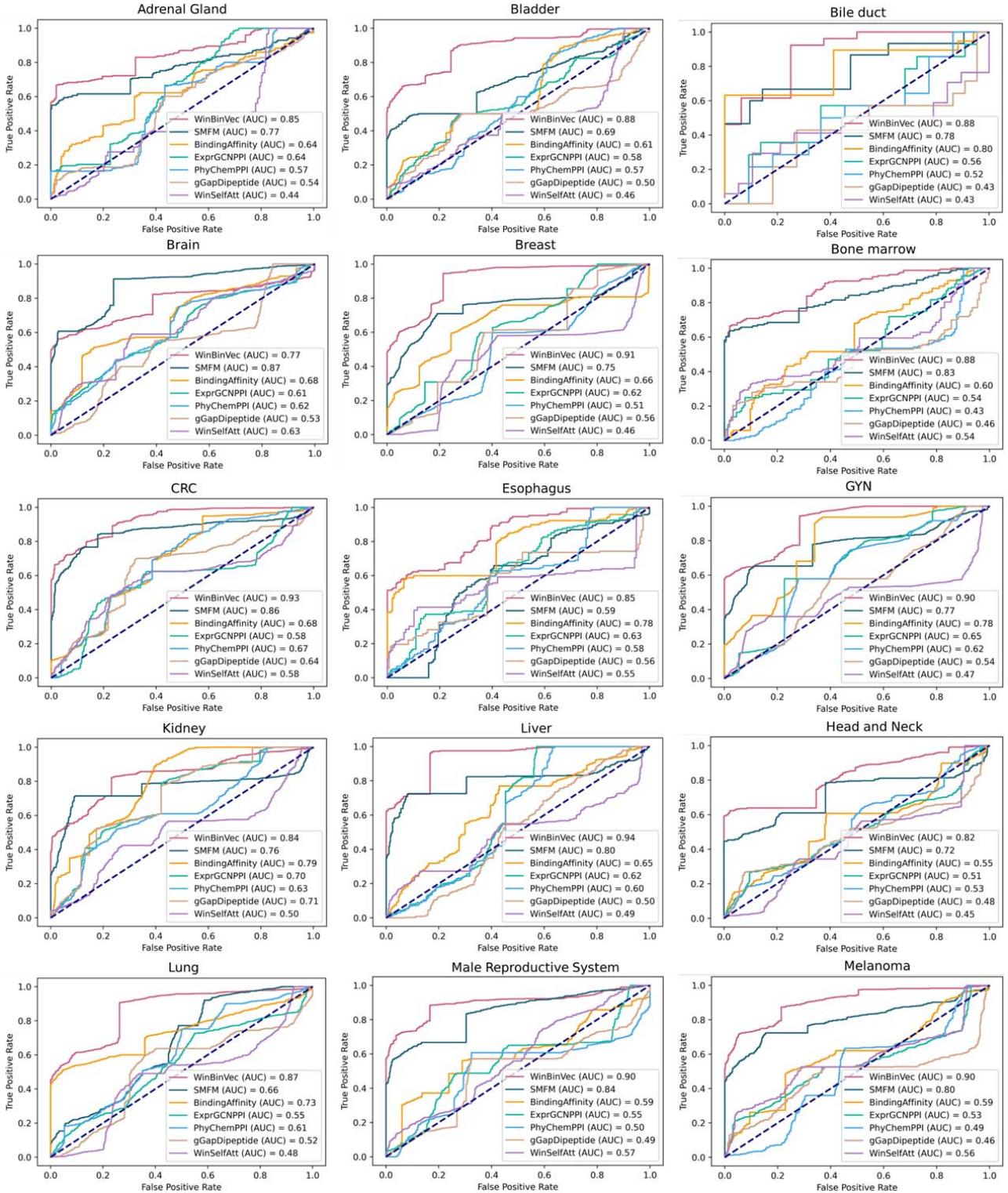


Figure 9: ROC plots and AUC values of the seven different deep learning models.

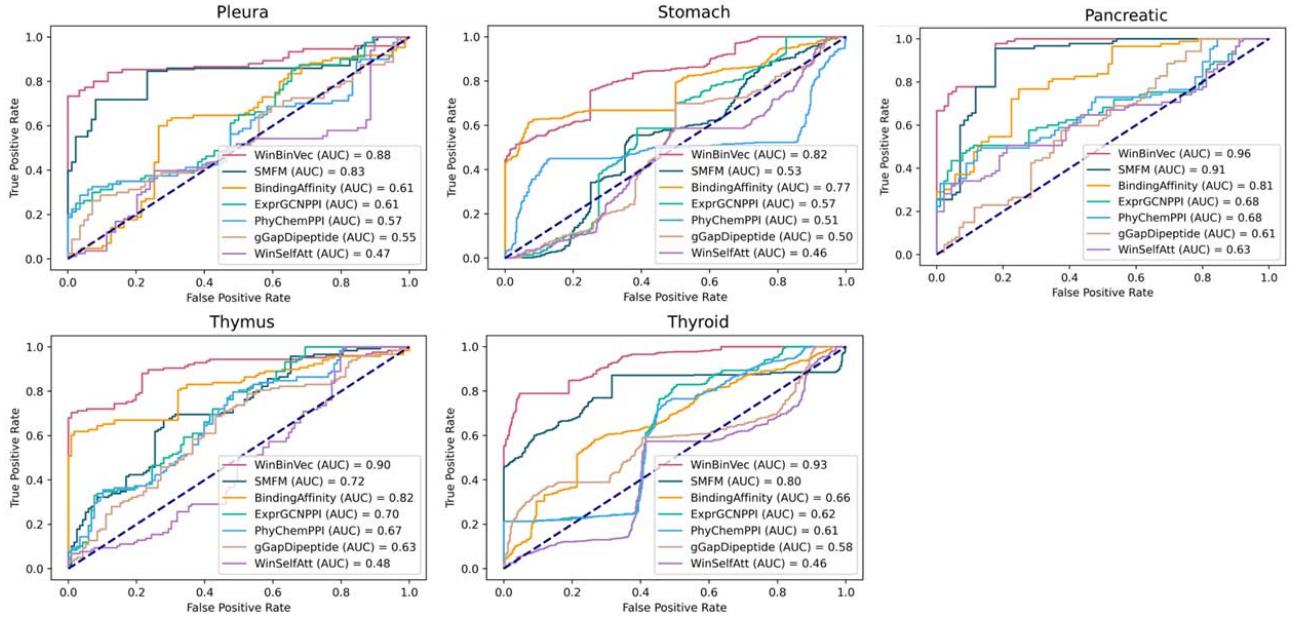


Figure 10: ROC plots and AUC values of the seven different deep learning models.

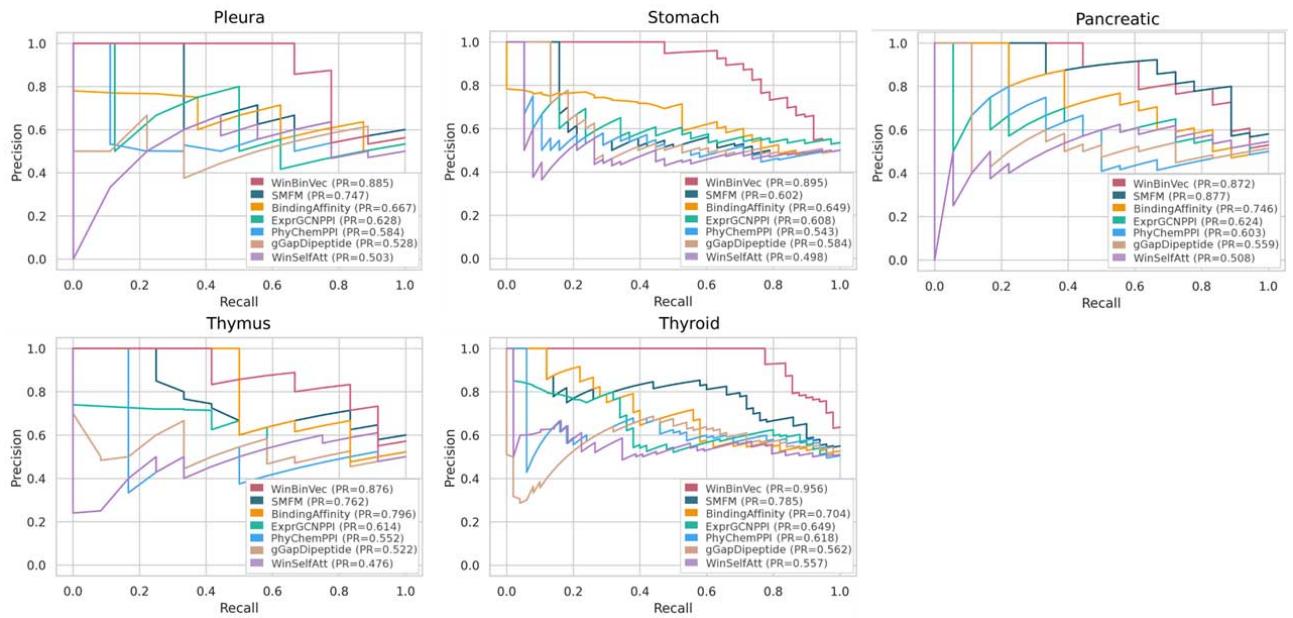


Figure 11: Precision-Recall curves and PR values of the seven different deep learning models.

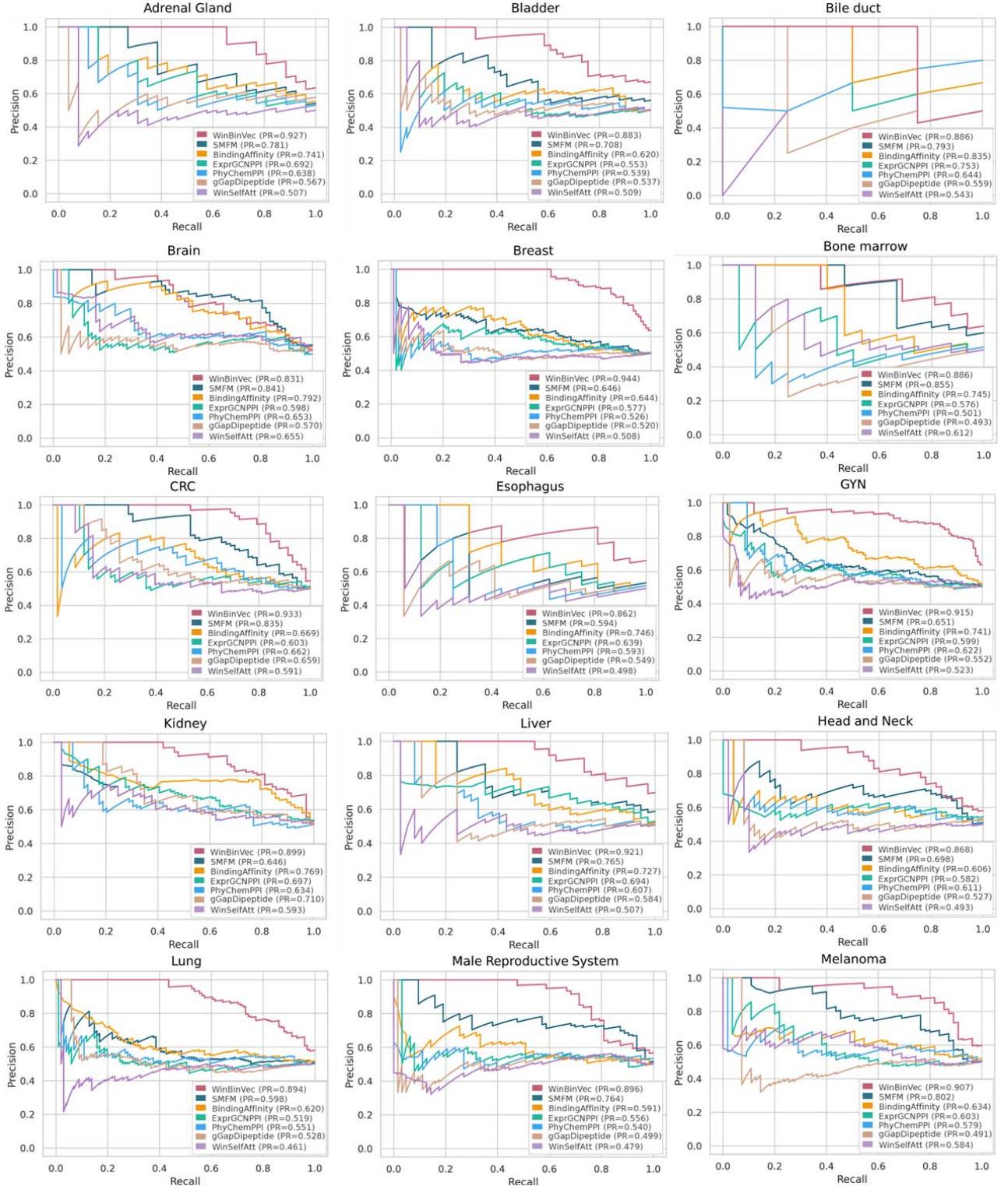


Figure 12: Precision-Recall curves and PRC values of the seven different deep learning models.

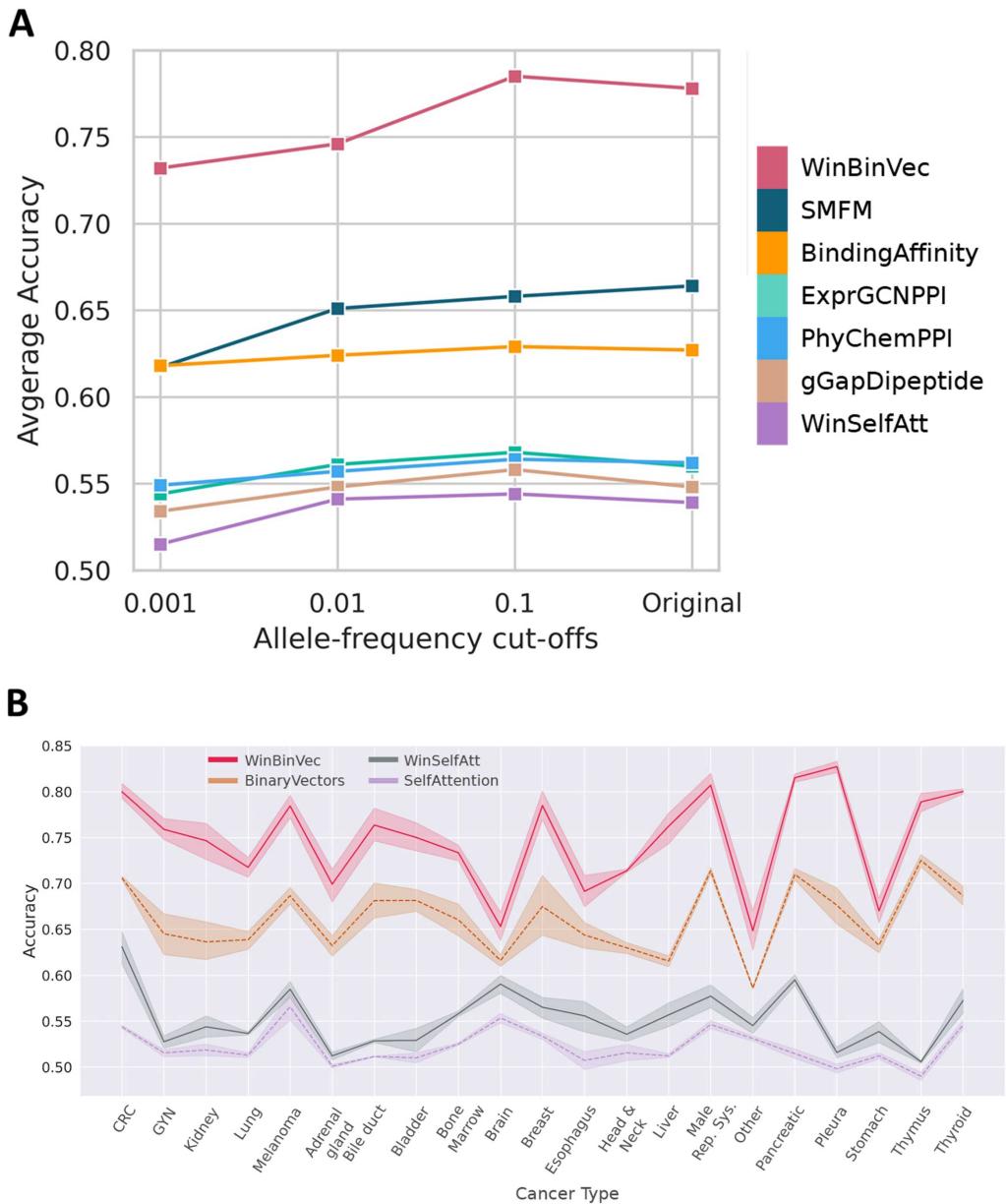


Figure 13: (A) The performance of the models using different allele Frequency cut-offs. (B) Comparing the performance of the WinBinVec and the WinSelfAtt models in two cases: 1) using selected windows as input features, 2) using whole PPI sequence as input feature.

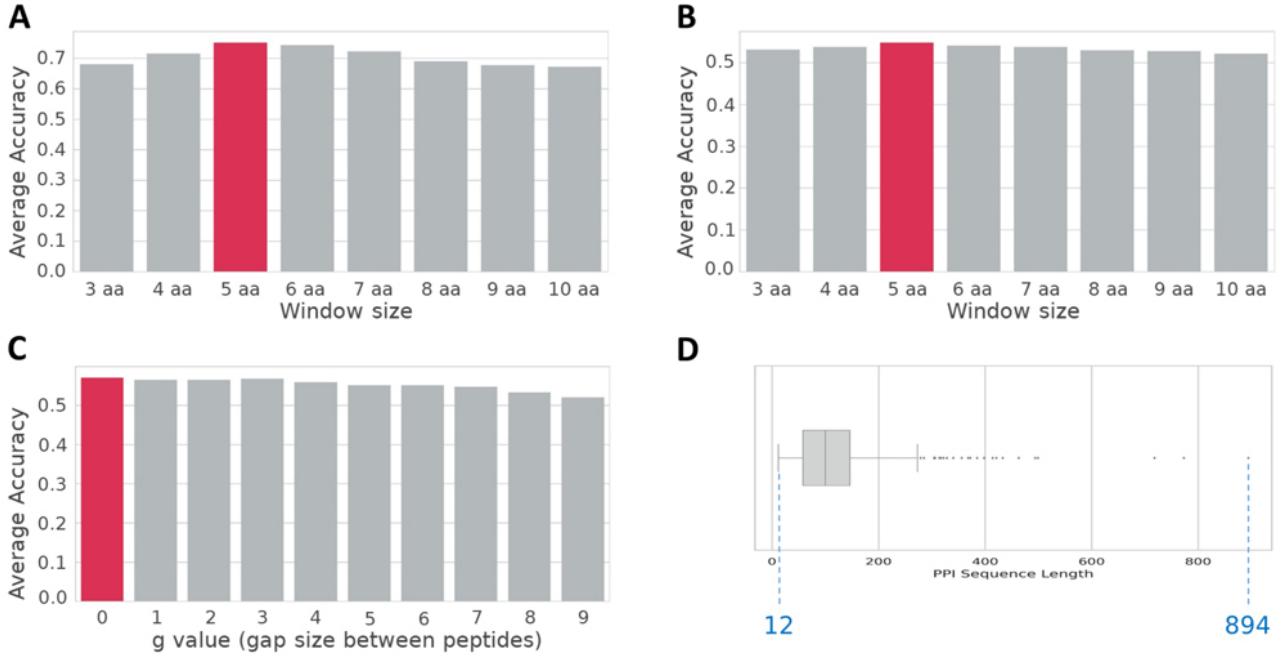


Figure 14: The averaged accuracy comparison of the models with different parameter's value. (A) Window size of 5 amino acids outperforms the others for the WinBinVec model, (B) window size of 5 amino acids outperforms the others for the WinSelfAtt model, and (C) in the gGapDipeptide model, $g = 0$, outperforms the other g values. (D) Protein-protein interactions' sequence length box plot.

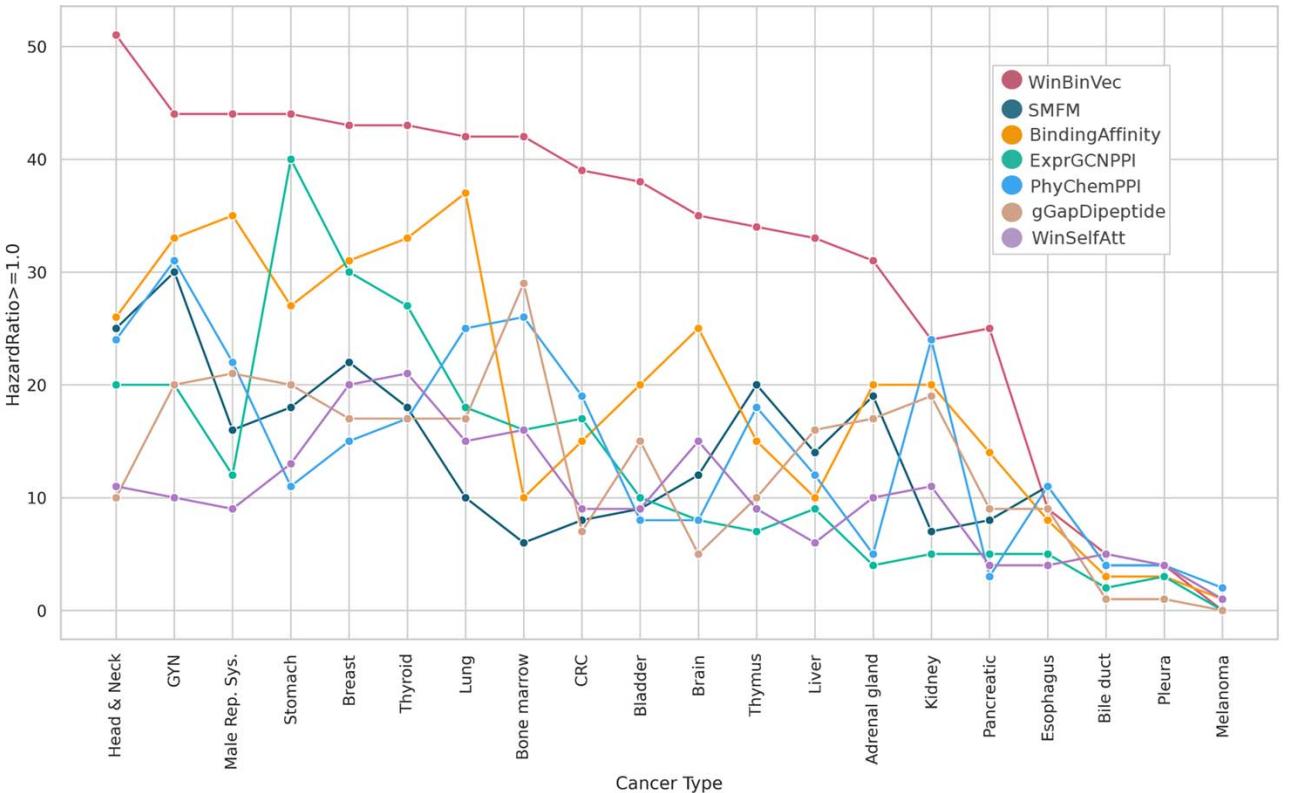


Figure 15: The number of essential PPIs (Top-100 PPIs) that are satisfied hazard ratio ≥ 1.0 with $pvalue \leq 0.05$ predicted by different models.

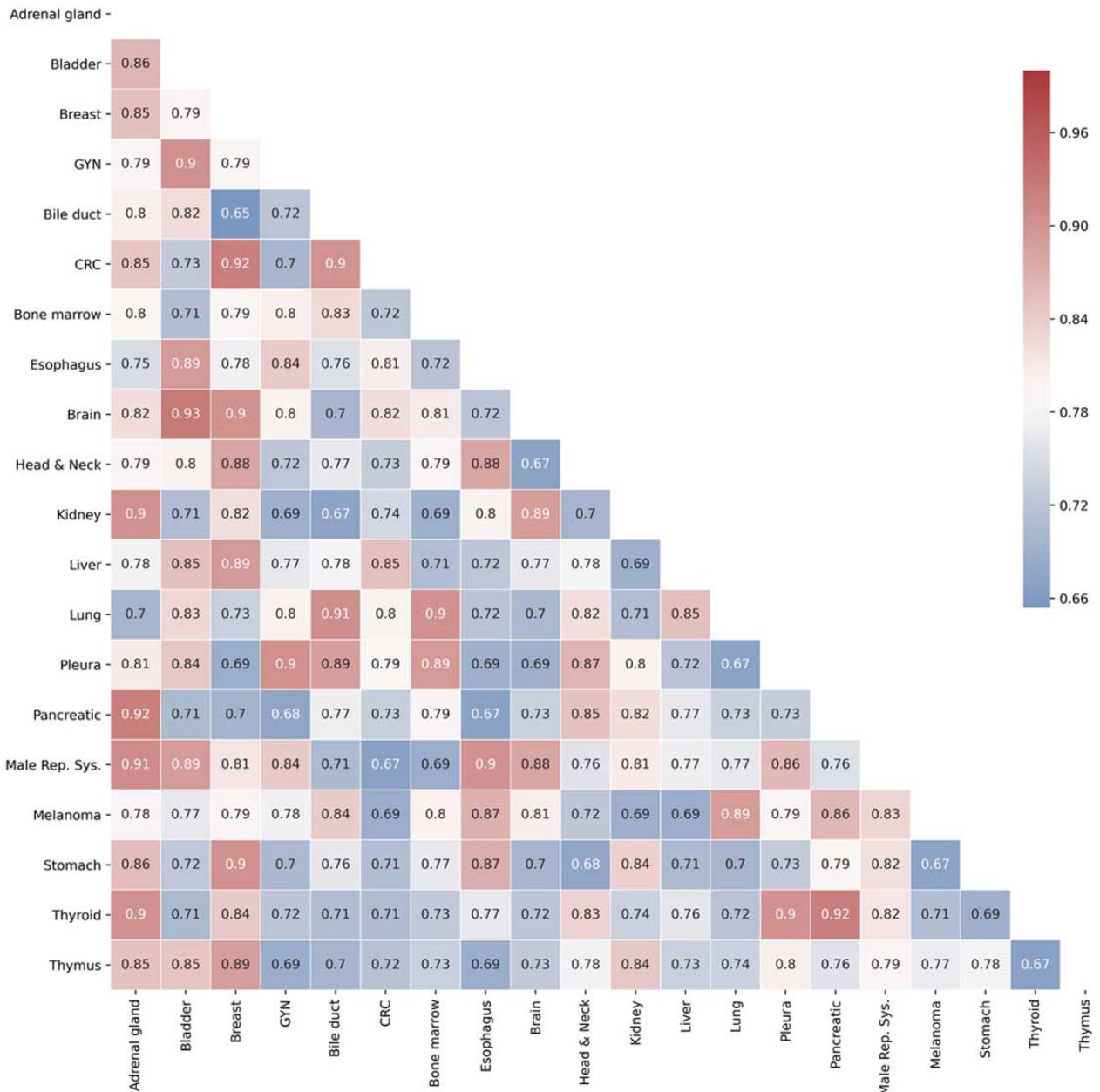
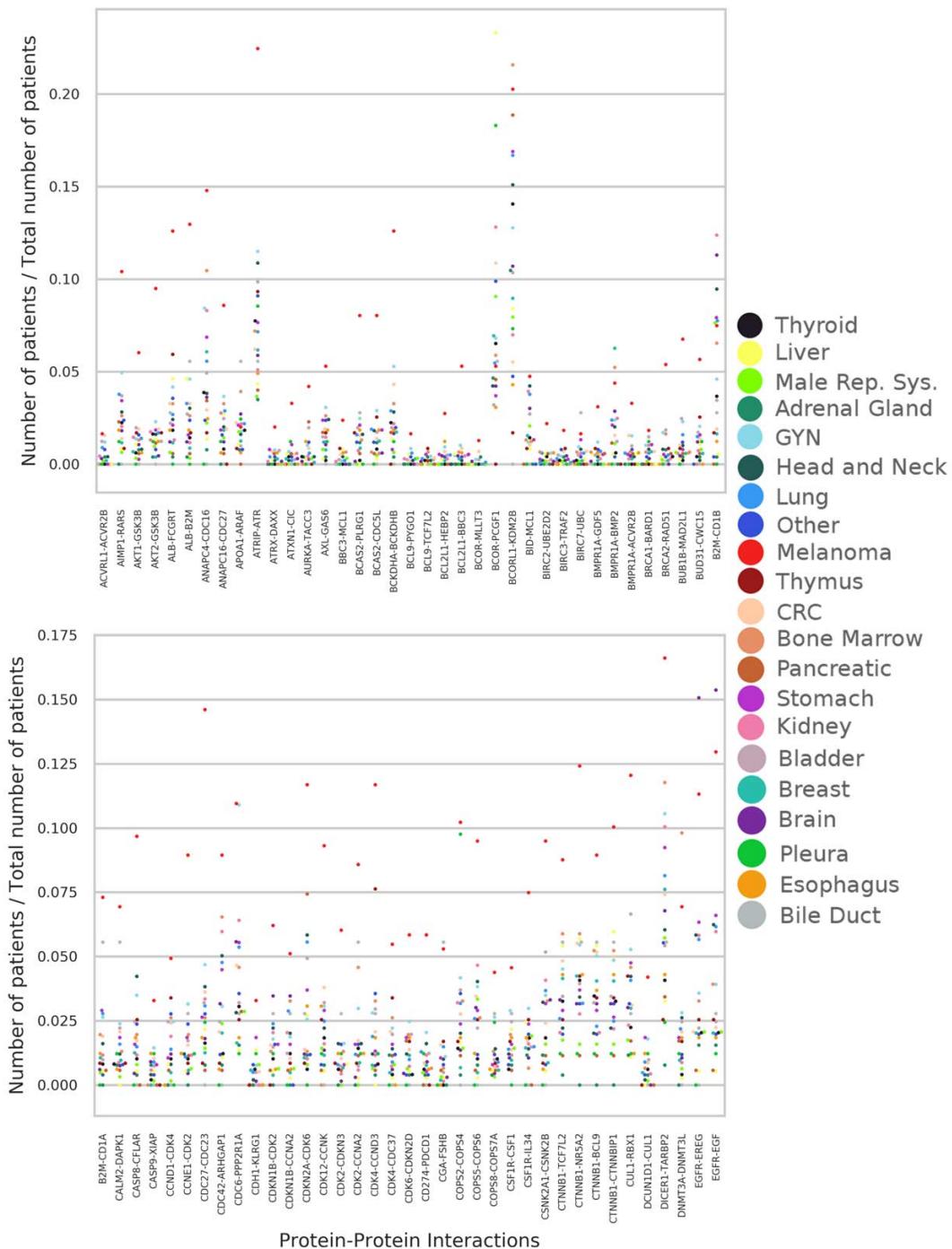


Figure 16: The mean accuracy of the WinBinVec model using one-vs-one classification.



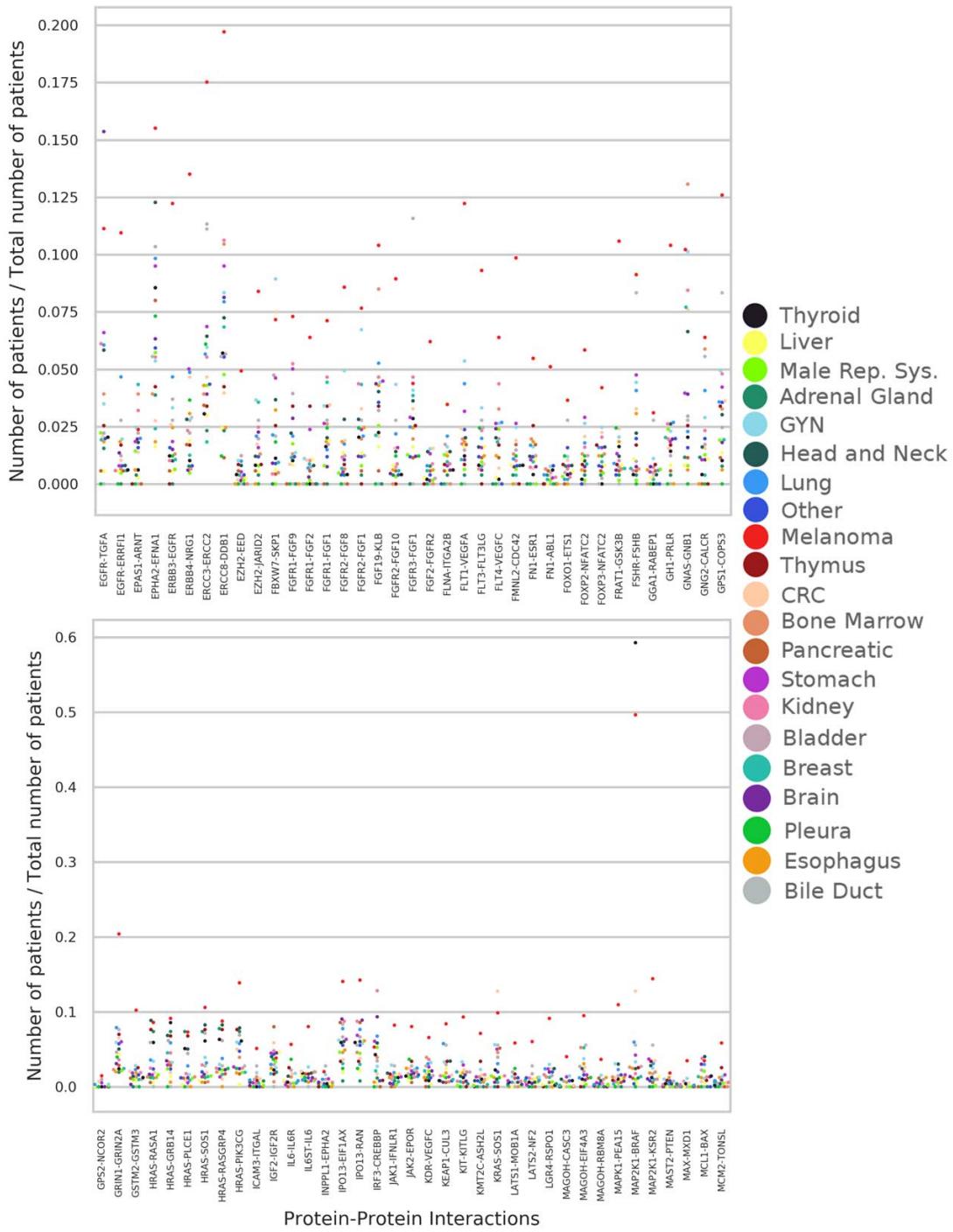


Figure 18: The mutation ratio of different PPIs in various cancer types.

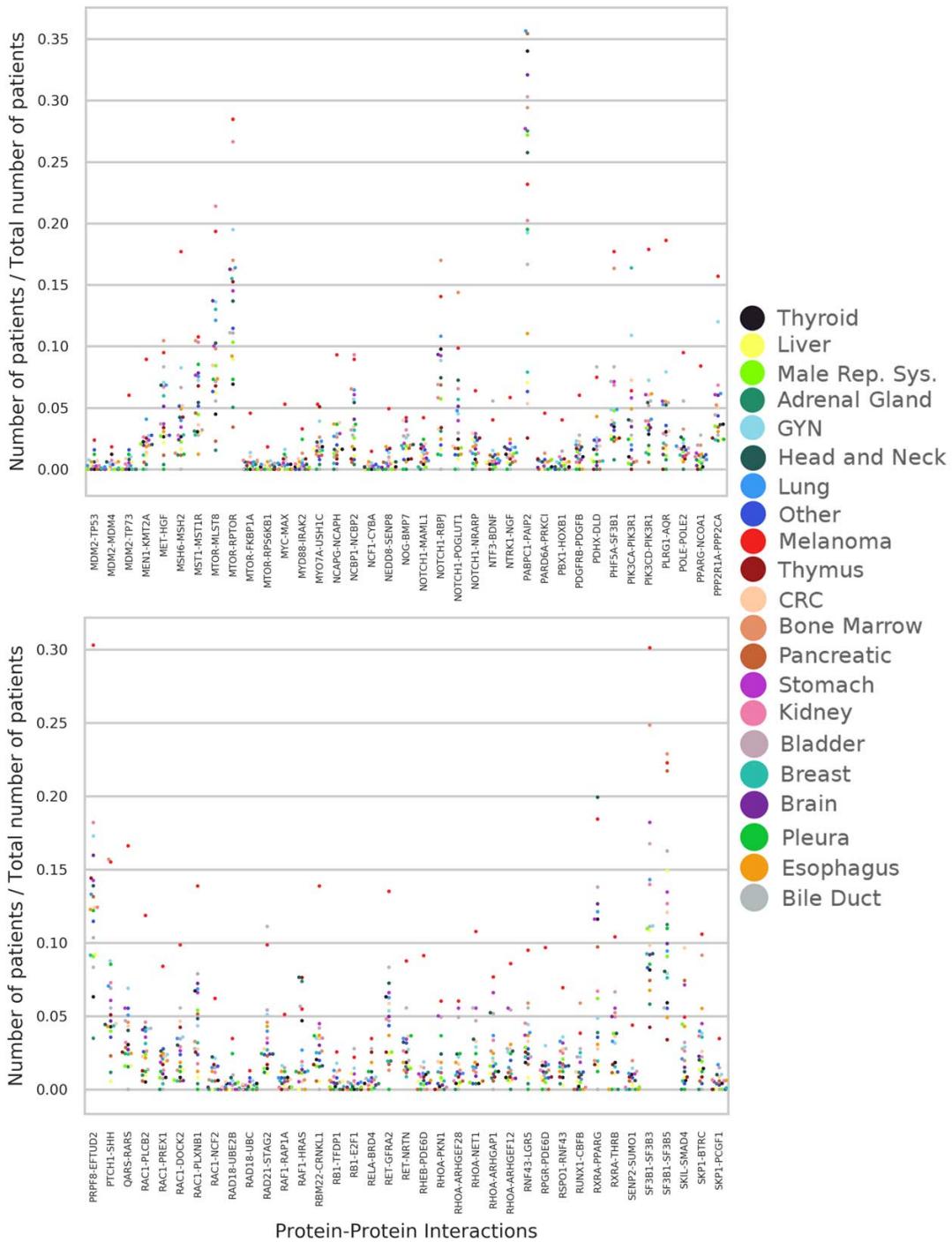


Figure 19: The mutation ratio of different PPIs in various cancer types.

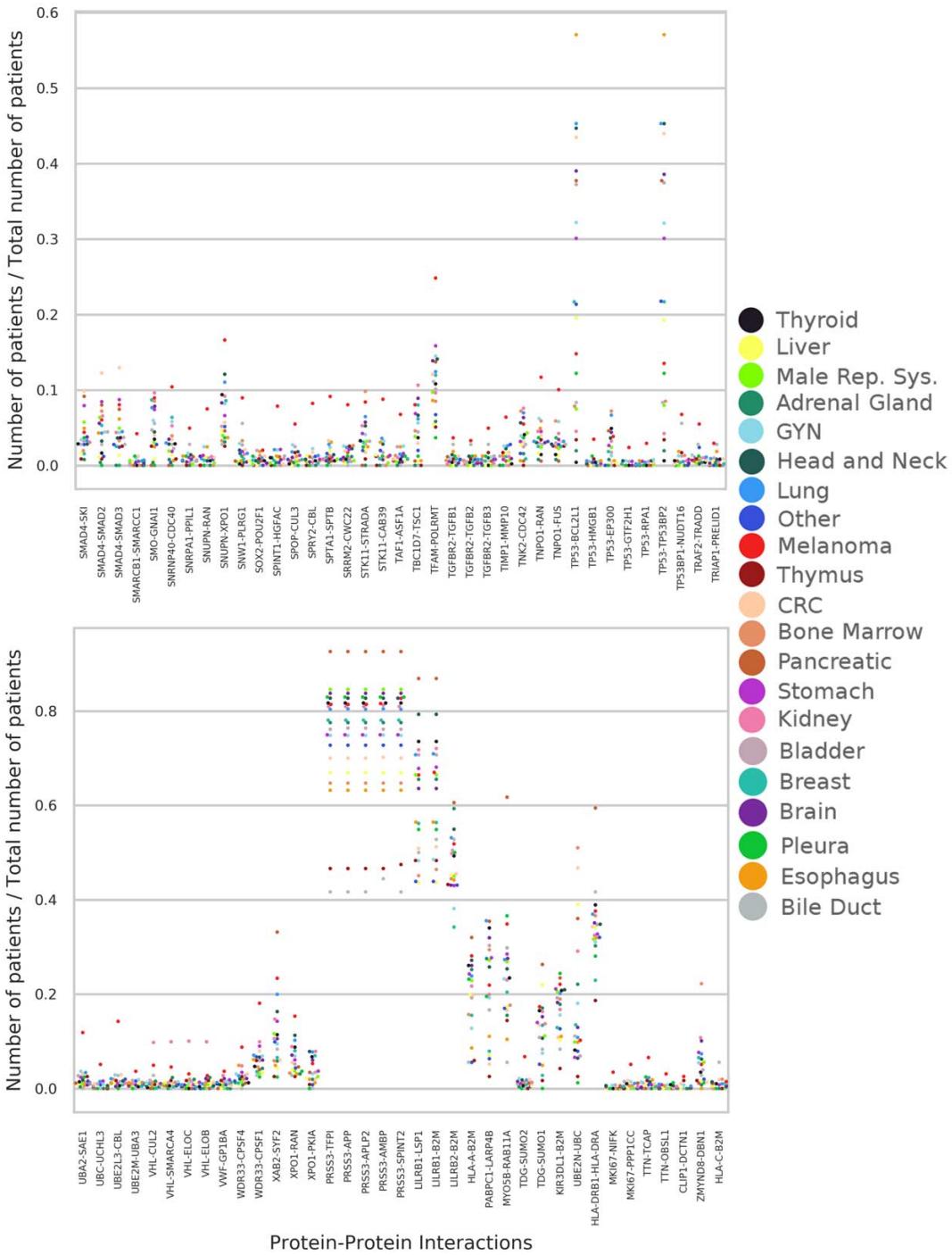


Figure 20: The mutation ratio of different PPIs in various cancer types.

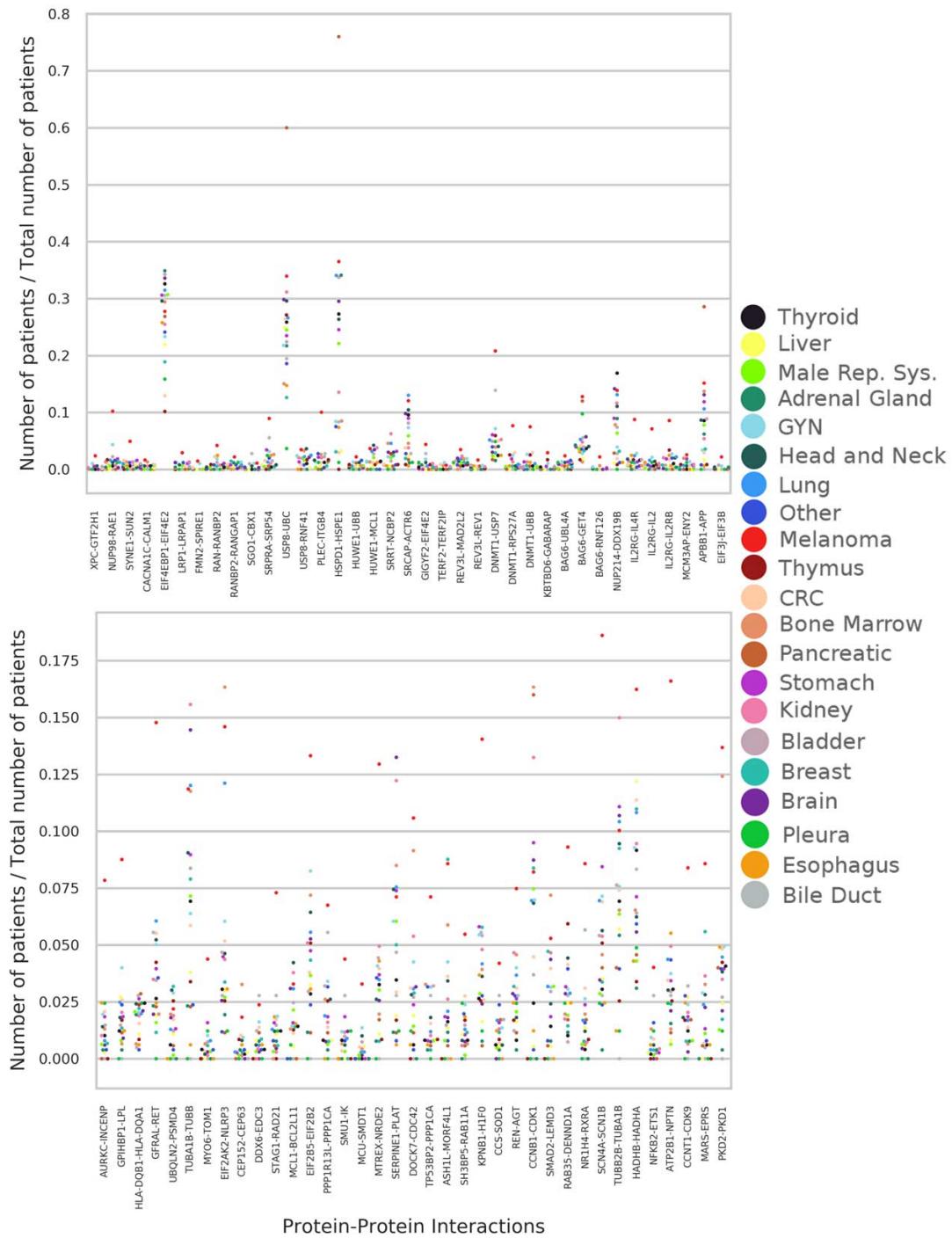


Figure 21: The mutation ratio of different PPIs in various cancer types.

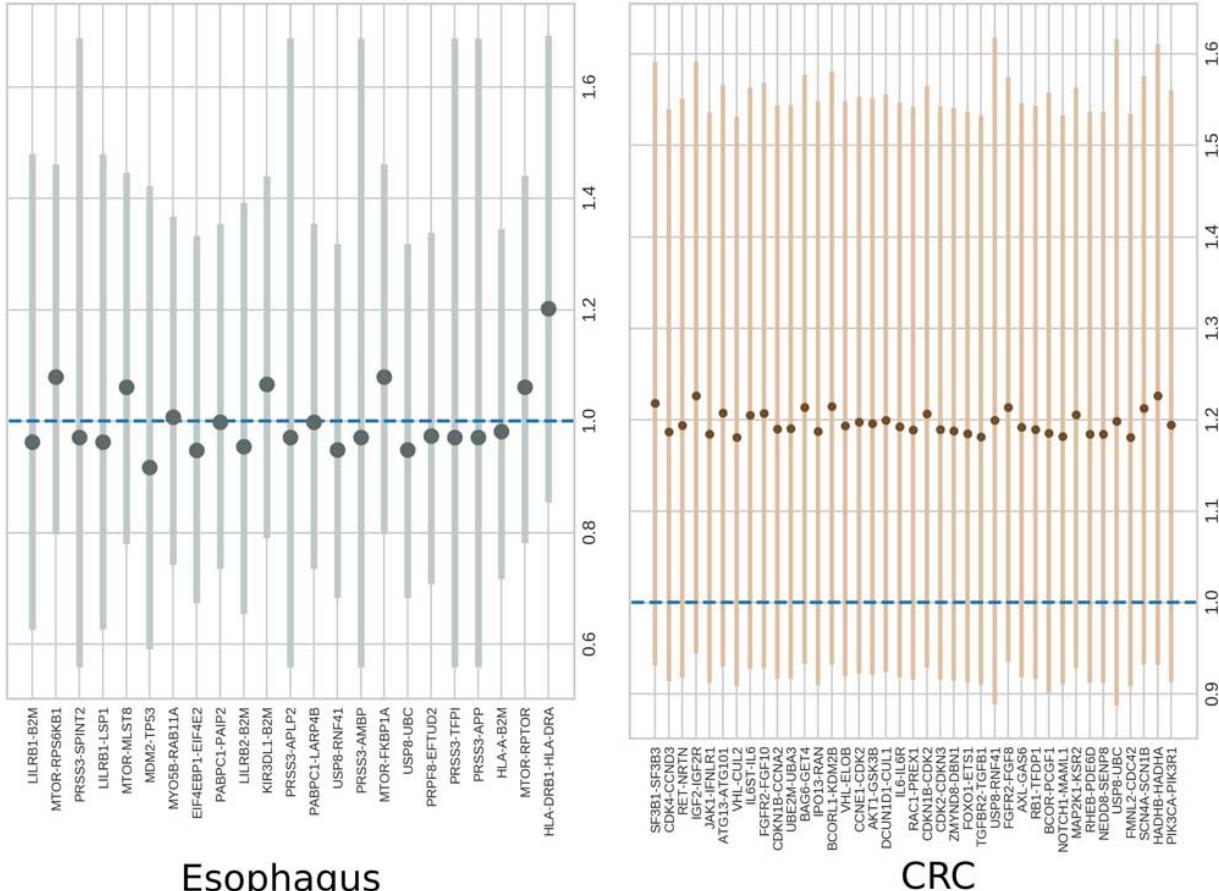
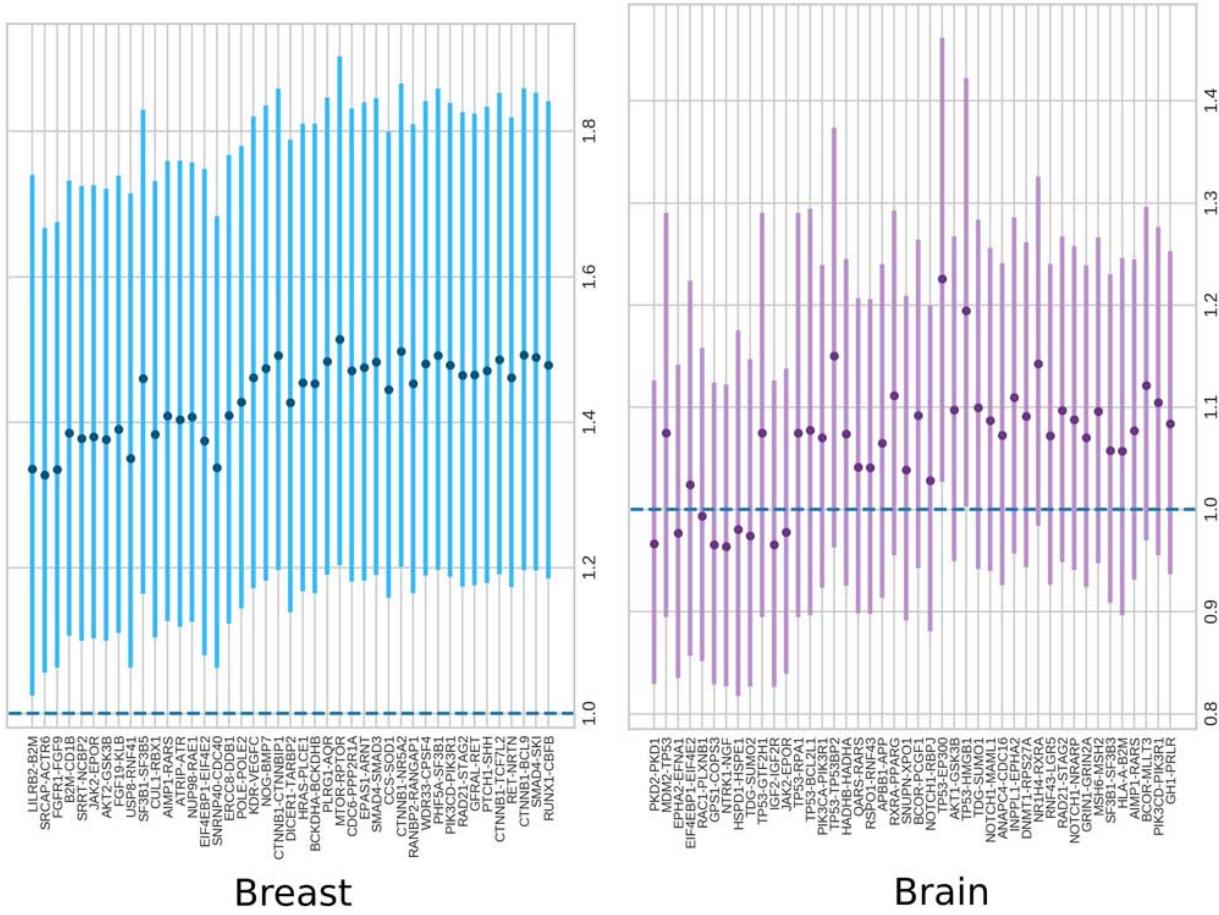


Figure 22: Breast, Brain, Esophagus, and CRC Essential PPIs' Cox Proportional Plots ($pvalue < 0.05$).

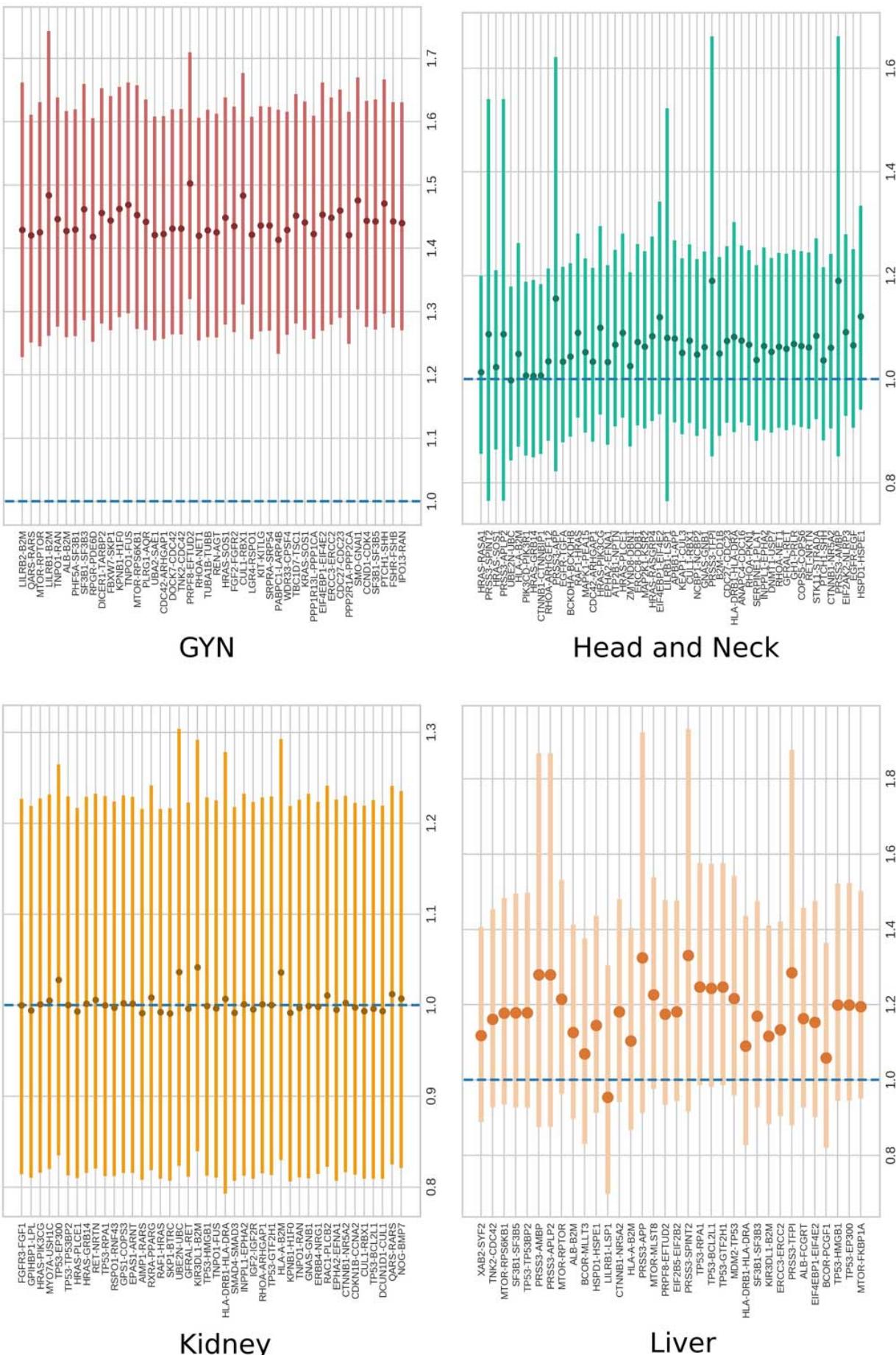


Figure 23: GYN, Head and Neck, Kidney, and Liver Essential PPIs' Cox Proportional Plots ($pvalue < 0.05$).

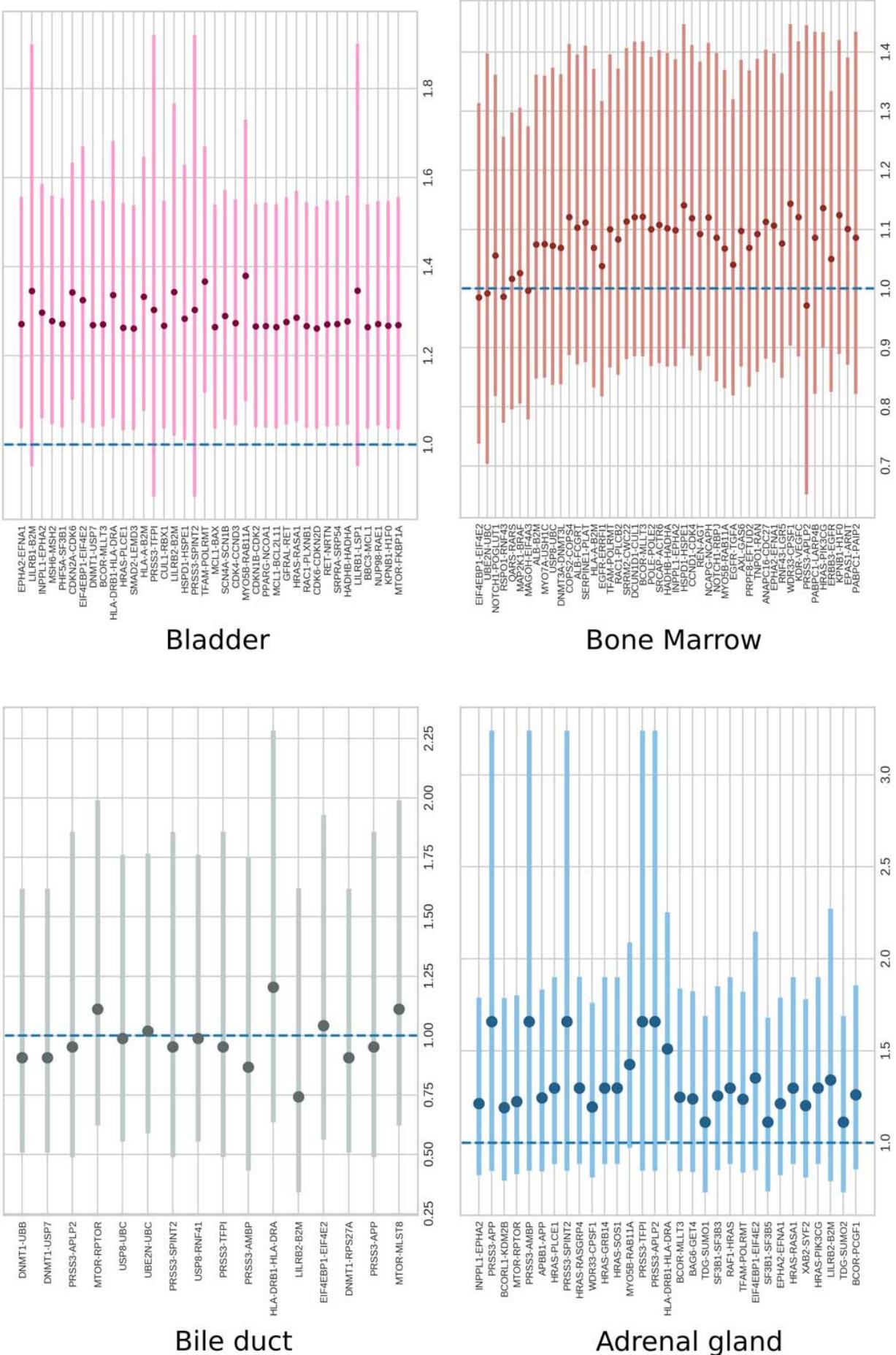
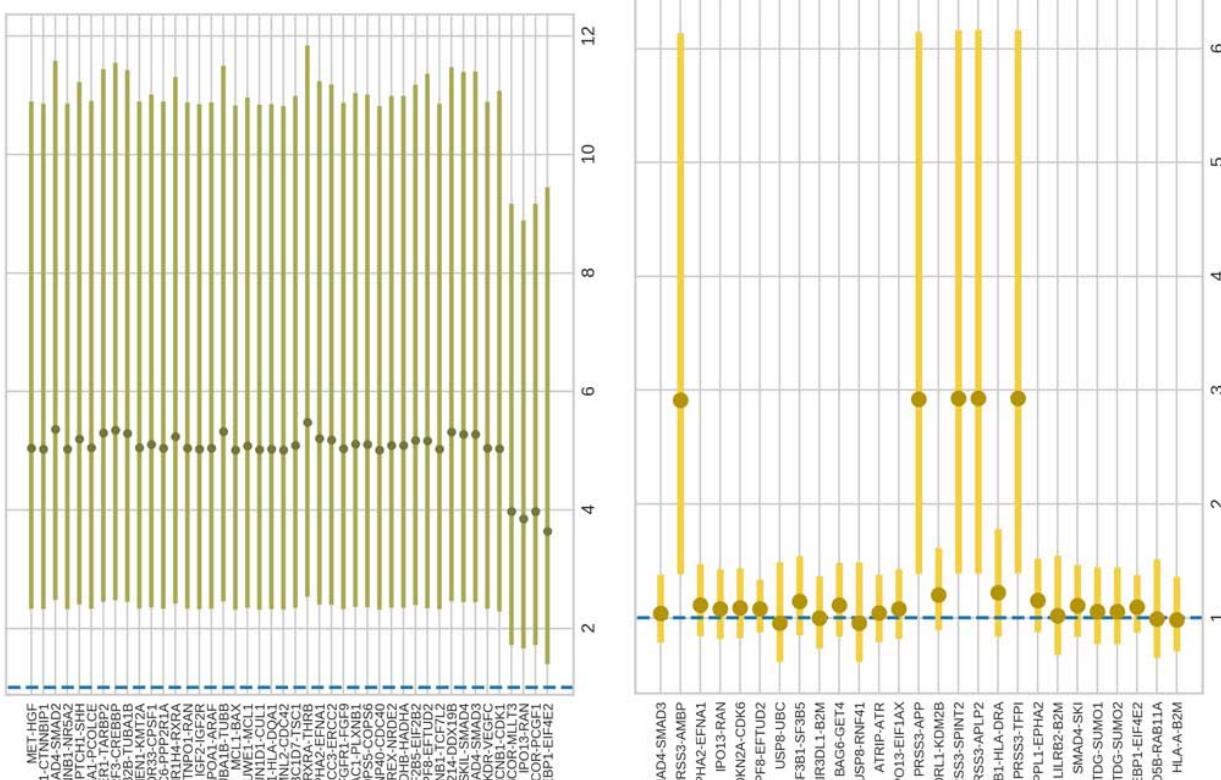
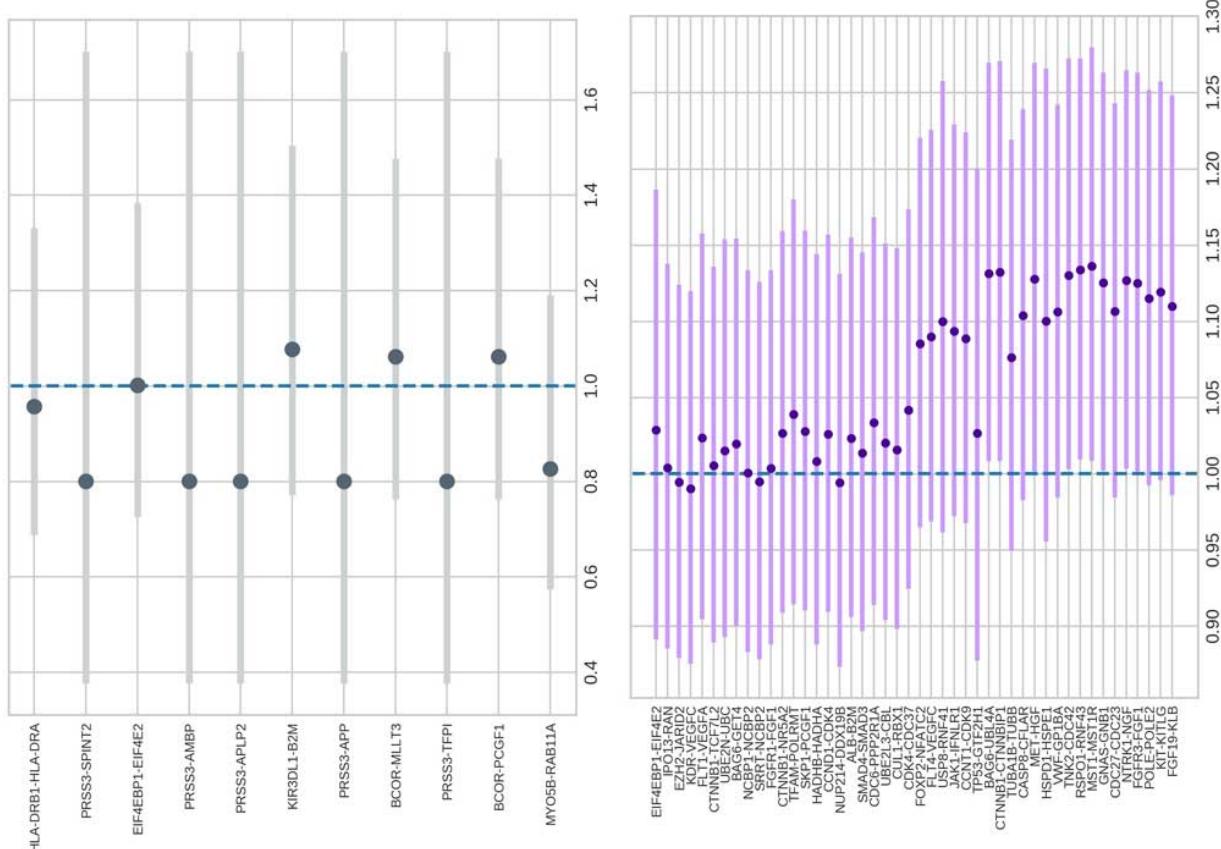


Figure 24: Bladder, Bone Marrow, Bile Duct, and Adrenal Gland Essential PPIs' Cox Proportional Plots ($pvalue < 0.05$).



Male Reproductive System

Pancreatic



Pleura

Lung

Figure 25: Male Reproductive System, Pancreatic, Pleura, and Lung Essential PPIs' Cox Proportional Plots ($pvalue < 0.05$).

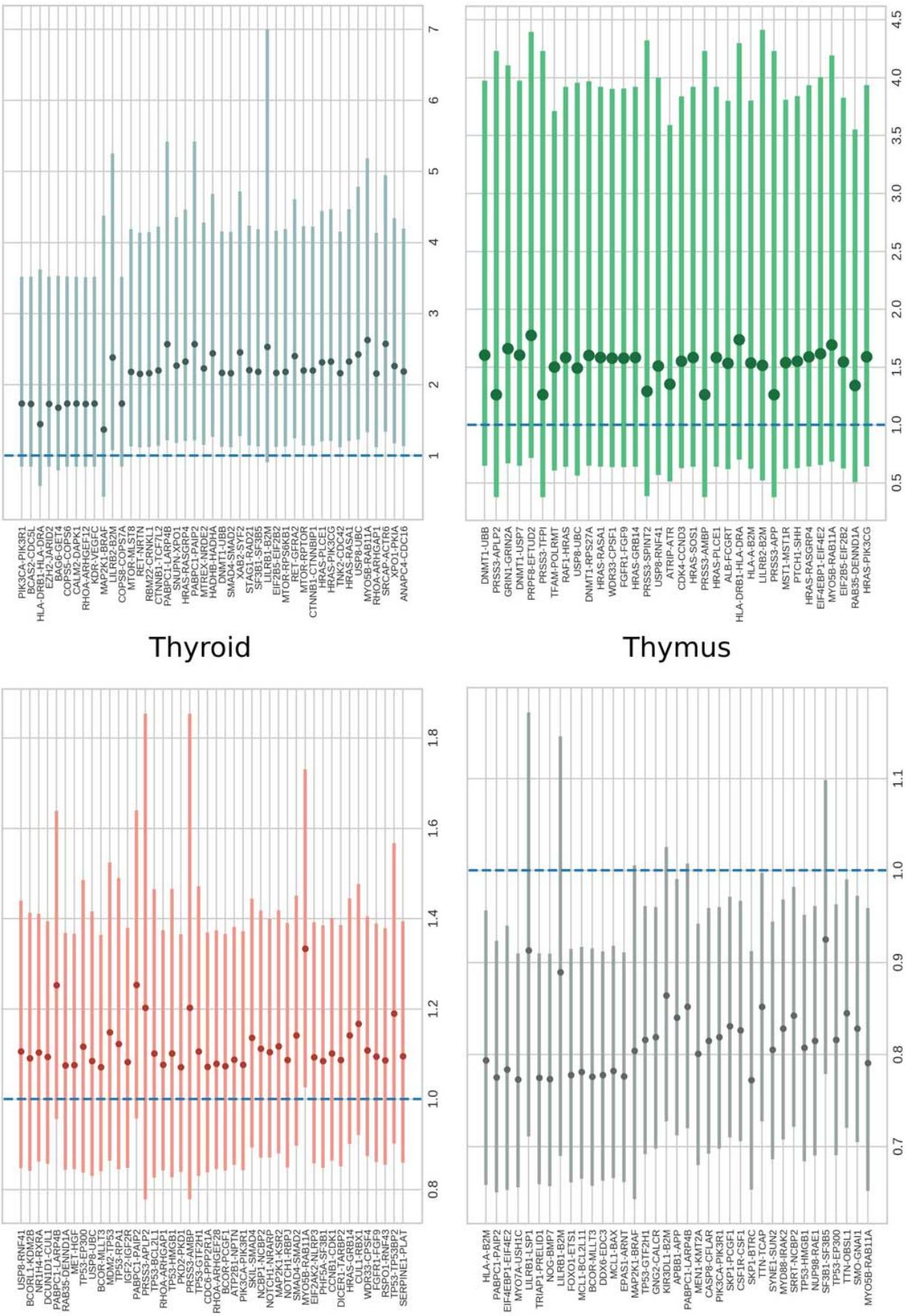


Figure 26: Thyroid, Thymus, Stomach, and Melanoma Essential PPIs' Cox Proportional Plots ($pvalue < 0.05$).

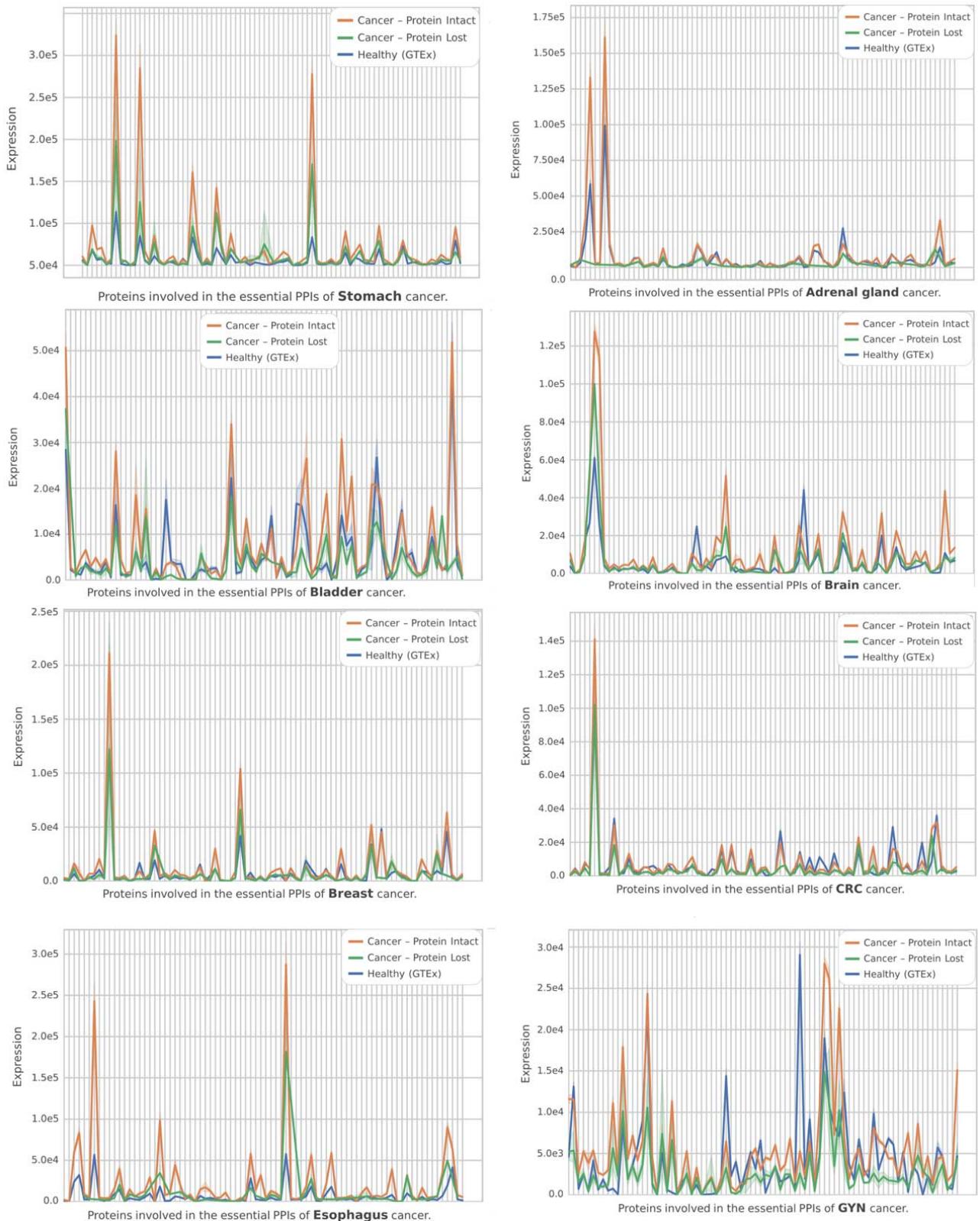


Figure 27: Gene Expressions in different cancer types. Each partner protein has three different expression levels in: normal tissues, tissues that the protein contains at least one mutation, tissues that the protein has no mutation.

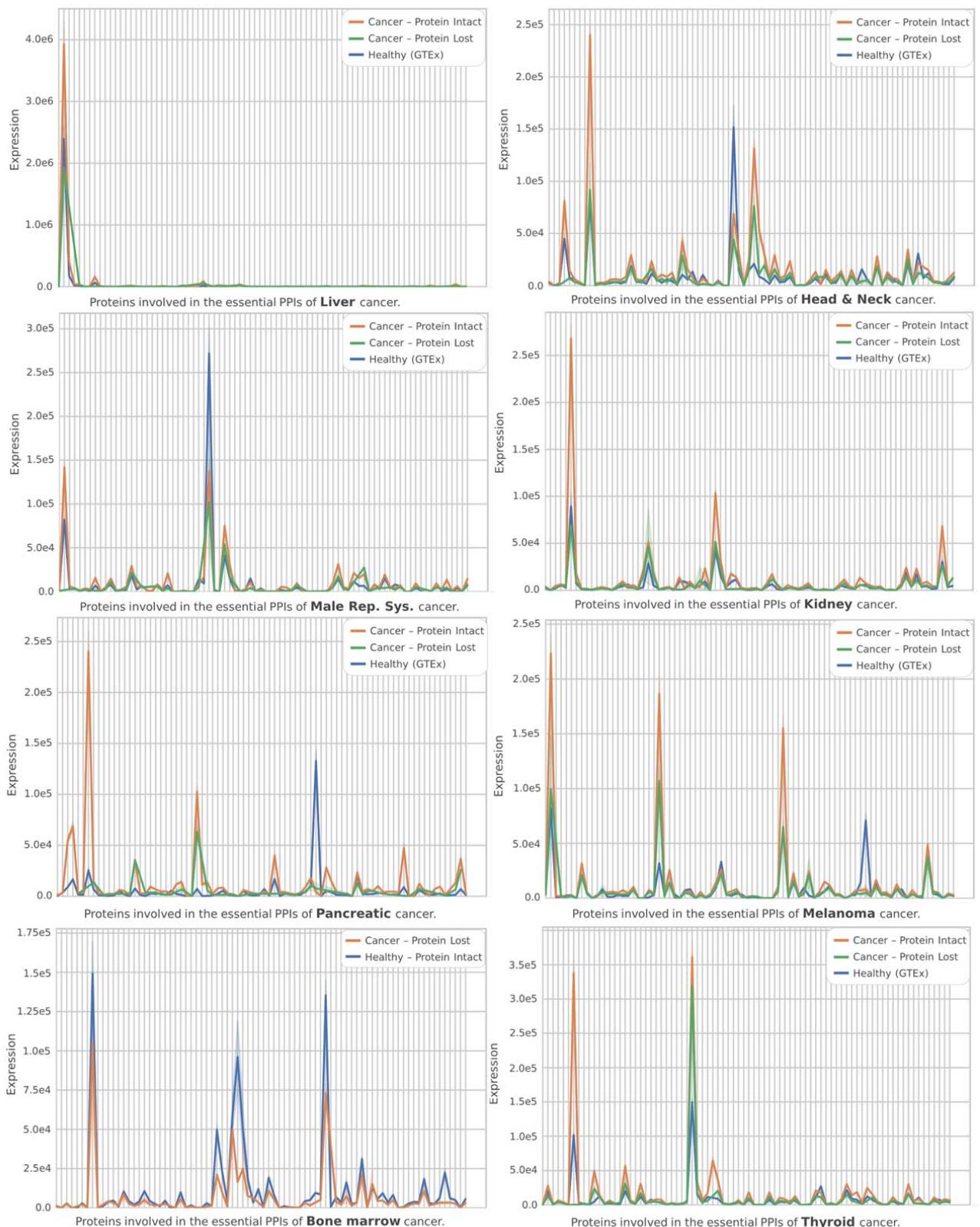


Figure 28: Gene Expressions in different cancer types. Each partner protein has three different expression levels in: normal tissues, tissues that the protein contains at least one mutation, tissues that the protein has no mutation.

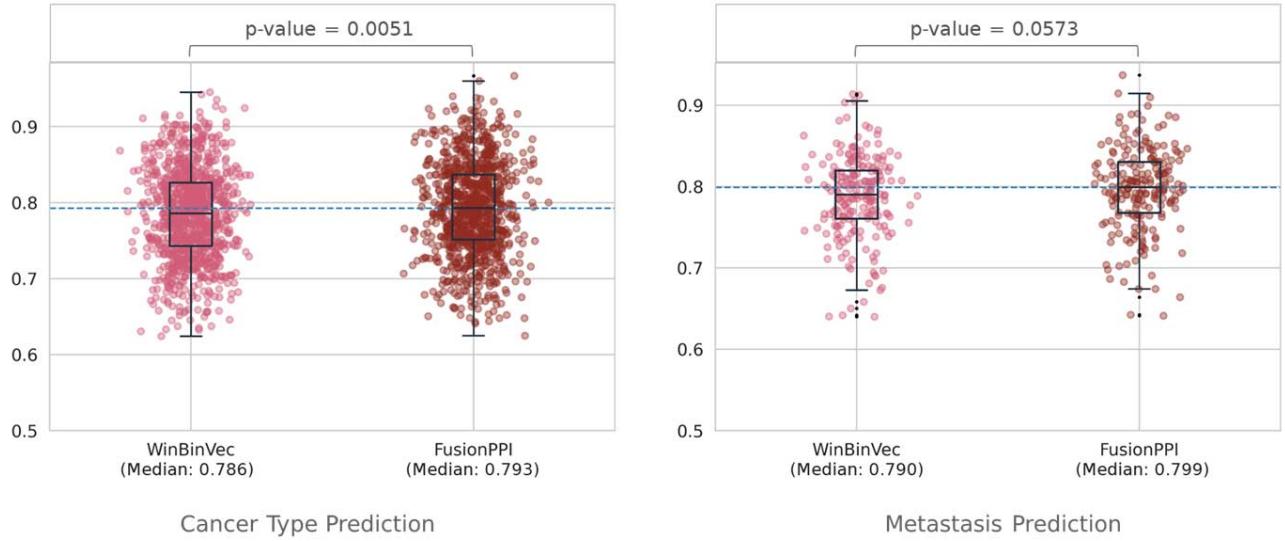


Figure 29: The comparison of the accuracy of the FusionPPI model with the WinBInVec model for predicting cancer types and metastasis. We used 10-fold cross-validation with five repetitions for each model.

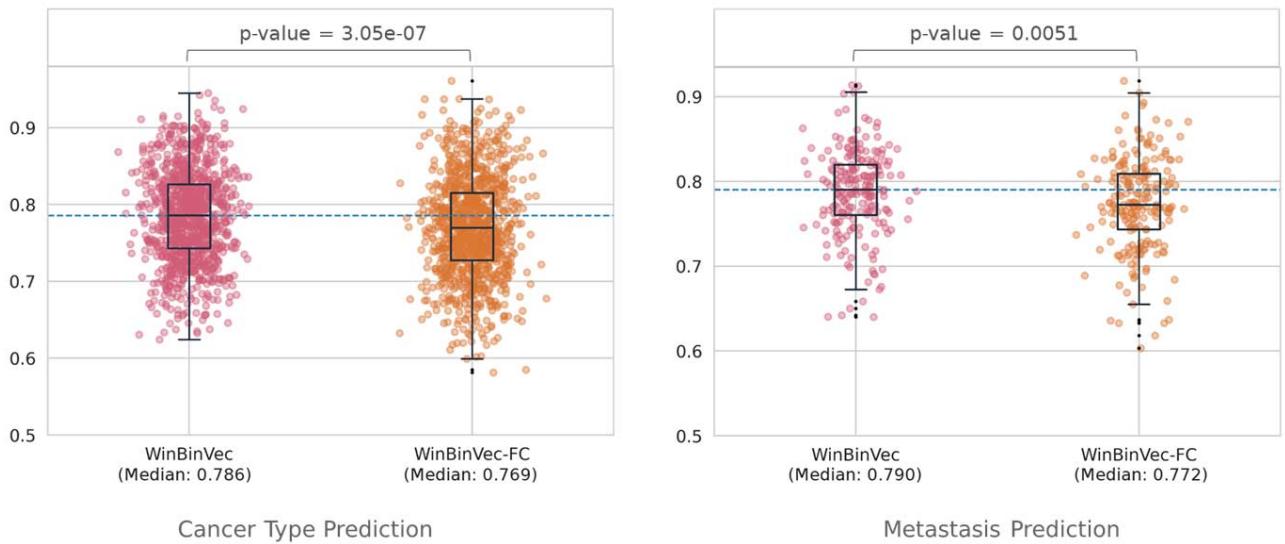


Figure 30: The comparison of the two versions of the WinBinVec model: The WinBinVec model that utilizes one-dimensional convolutional modules versus the WinBinVec model that utilizes fully connected layers instead. We used 10-fold cross-validation with five repetitions for each model