Table S1 Molecular docking between ligand and receptor from an LRl predicted by LRI-CNbDF on Dataset 1

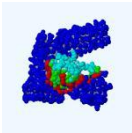
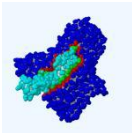
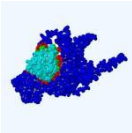
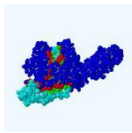
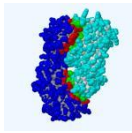
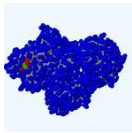
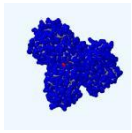
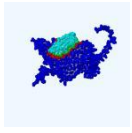
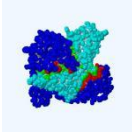
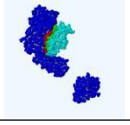
LRI(Gene Names)	Molecular docking	Binding Enegy (kcal/mol)	Hydrogen bonds	Interface area
CCL1-ADRA2A		-36.2	2.86	1741.8
CD70-CNR1		-19.3	3.71	1698.2
LYZ-CNR1		-35.8	2.90	2329.1
NDP-ADRA2A		-33.8	2.88	2628.4
TFPI-CNR1		-19.4	2.65	1741.9
THBS1-CNR1		-16.8	3.36	556.2
VWF-CNR1		-16.8	3.10	556.2
PDCD1LG2-CX3CR1		-25.3	2.72	1805.1
PRL-ADRA2A		-32.1	2.88	2731.3
WNT3-ADRA2A		-22.0	2.60	1167.3

Table S2 Molecular docking between ligand and receptor from an LRI predicted by LRI-CNbDF on Dataset 2

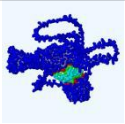
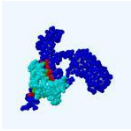
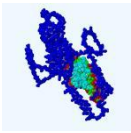
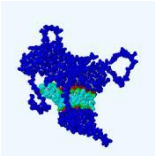
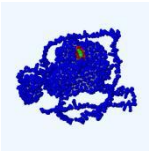
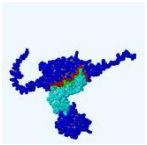
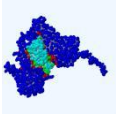
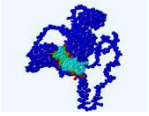
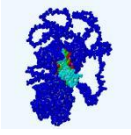
LRI(Gene Names)	Molecular docking	Binding Enegy (kcal/mol)	Hydrogen bonds	Interface area
Agrn-Fzd6		-37.5	3.52	2274.2
Bmp8b-Bmpr1b		-18.2	3.70	1074.5
Csf3-Acvr2b		-18.6	3.62	1294.4
Il5-Fzd6		-61.8	3.31	4442.4
Il33-Fzd6		-46.7	2.95	2965.5
Ptgs2-Fzd6		-17.4	2.73	547.1
Rspo2-Ackr4		-17.1	3.57	1123.3
Rspo2-Ccr1		-27.5	2.76	2446.6
Rspo2-Fzd6		-26.6	2.58	2306.7
Rspo2-Ptch1		-26.7	2.58	2496.0

Table S3 Molecular docking between ligand and receptor from an LRI predicted by LRI-CNbDF on Dataset 3

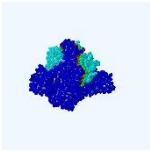
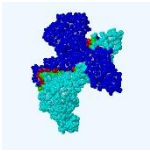
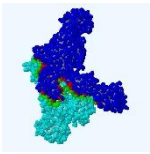
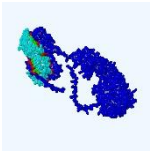
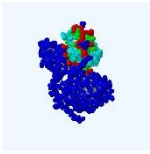
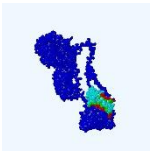
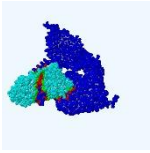
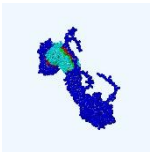
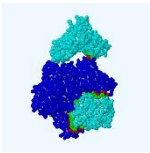
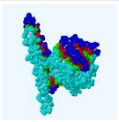
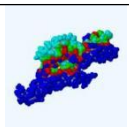
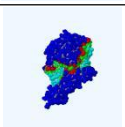
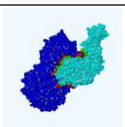
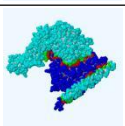
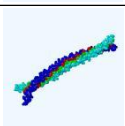
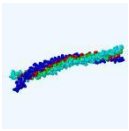
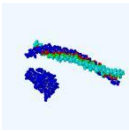
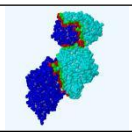
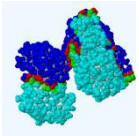
LRI(Gene Names)	Molecular docking	Binding Enegy (kcal/mol)	Hydrogen bonds	Interface area
Bmp10-Itgb1		-55.7	3.73	3742.3
Cdh1-Itgb1		-49.4	3.75	3546.0
Cntn2-Itgb1		-46.9	2.82	3723.2
Col2a1-Itga5		-39.2	3.04	2675.4
Fgf20-Fgfr2		-21.7	3.12	1404.8
Gnai2-Bmpr1b		-8.2	2.94	705.6
Hspg2-Itga5		-26.9	2.74	1678.6
Lama1-Itga5		-16.4	2.99	1941.1
Lama1-Itgav		-17.2	2.99	1732.7
Selplg-Itgb1		-47.4	3.76	3720.3

Table S4 Molecular docking between ligand and receptor from an LRI predicted by LRI-CNbDF on Dataset 4

LRI(Gene Names)	Molecular docking	Binding Enegy (kcal/mol)	Hydrogen bonds	Interface area
APOC-CTSD		-47.3	2.84	4251.6
FN1-BSG		-29.0	3.15	2169.1
FN1-PRDX4		-24.9	2.92	3067.2
ITGA5-COL4A5		-31.4	2.16	1991.7
ITGA5-CTSD		-42.2	3.7	2555.7
KRT1-AP2M1		-55.2	2.69	2467.0
KRT1-COL4A5		-55.2	2.69	2464.8
KRT1-PRDX4		-55	2.69	2454.4
TFRC-PRDX4		-56.7	3.36	5016.1
LGALS1-PRDX4		-26.1	2.92	3075.0

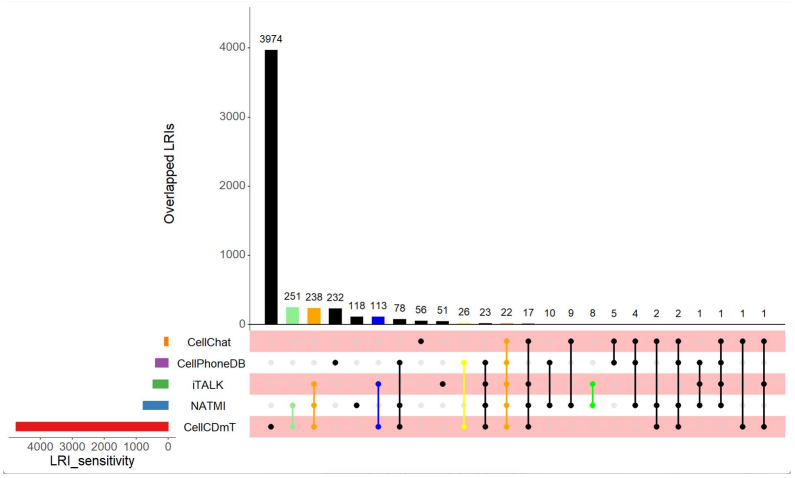


Figure S1. UpsetR map of Melanoma

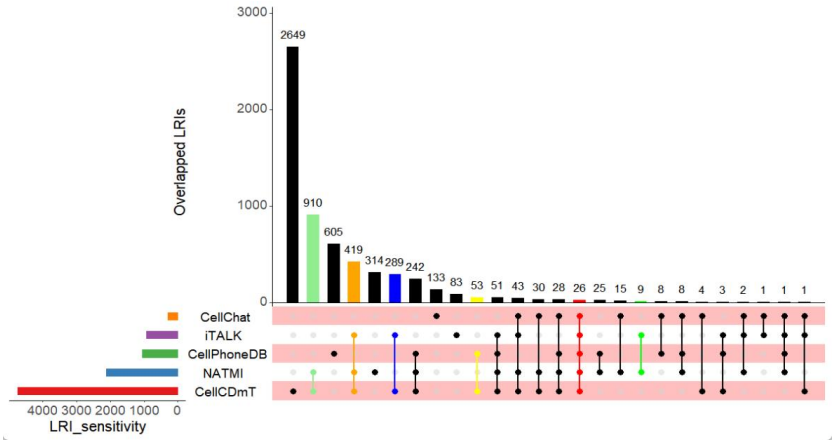


Figure S2. UpsetR map of HNSCC

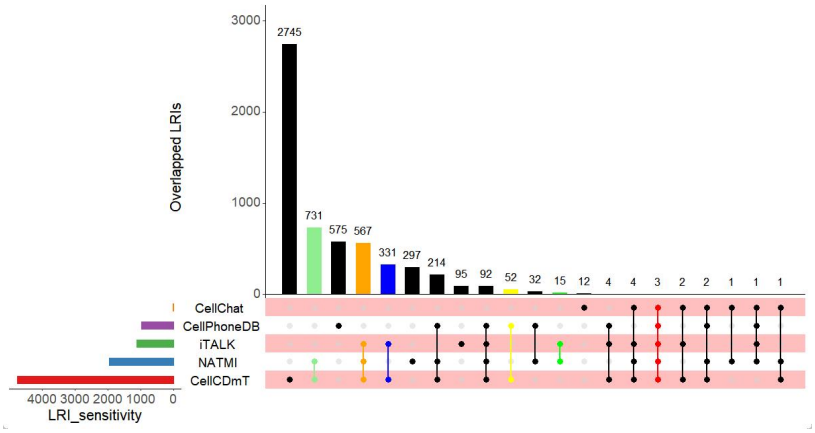


Figure S3. UpsetR map of CRC