AI and Drug Discovery

Assignment # 1

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Task

Pick one type of cancer and identify 20 associated genes/proteins. For each gene/protein, determine whether an experimentally resolved 3D structure is available in the Protein Data Bank (PDB).

Instructions

- Do literature search to identify genes/proteins associated with the cancer.
- Or use biological databases such as GeneCards, UniProt, NCBI Gene, or the Human Protein Atlas to confirm gene/protein function and disease relevance.
- Search the Protein Data Bank (PDB) to check whether an experimental structure is available.
- If available, report at least one representative PDB ID. If not, write “No structure available”.
- Provide all the information into a table: gene symbol, protein name cancer type, PDB structure available (yes/no), PDB Id

Disease Name: Cholangiocarcinoma

Table of Related Genes/Proteins:

No.	Gene symbol	Protein name	Cancer type	PDB structure available (Yes/No)	PDB ID
1	**ABCA2 [3]**	ATP-binding cassette sub-family A member 2	Cholangiocarcinoma	No	—
2	**AKT1 [2]**	AKT serine/threonine kinase 1	Cholangiocarcinoma	Yes	7FCV
3	**ANXA4 [11]**	Annexin A4	Cholangiocarcinoma	Yes	9GA7
4	**ApoE [12]**	Apolipoprotein E	Cholangiocarcinoma	No	—
5	**ARID1A [1]**	AT-rich interactive domain-containing protein 1A	Cholangiocarcinoma	Yes	9A0K
6	**BAP1 [1]**	BRCA1 associated protein 1	Cholangiocarcinoma	Yes	7VPW
7	**CEACAM5 [7]**	CEA cell adhesion molecule 5	Cholangiocarcinoma	Yes	9U93
8	**FGFR2 [1]**	Fibroblast growth factor receptor 2	Cholangiocarcinoma	Yes	8STG
9	**IDH1 [1]**	Isocitrate dehydrogenase (NADP(+)) 1	Cholangiocarcinoma	Yes	8HB9

No.	Gene symbol	Protein name	Cancer type	PDB structure available (Yes/No)	PDB ID
10	**IDH2 [1]**	Isocitrate dehydrogenase (NADP(+)) 2	Cholangiocarcinoma	Yes	5I96
11	**KRAS [1]**	KRAS proto-oncogene, GTPase	Cholangiocarcinoma	Yes	6N65
12	**KRT7 [8]**	Keratin 7	Cholangiocarcinoma	No	—
13	**LAMTOR3 [10]**	Late endosomal/lysosomal adaptor, MAPK and MTOR activator 3	Cholangiocarcinoma	Yes	1VET
14	**MMP7 [4]**	Matrix metallopeptidase 7 (Matrilysin)	Cholangiocarcinoma	Yes	2DDY
15	**MUC1 [5]**	Mucin 1	Cholangiocarcinoma	Yes	8AXH
16	**MUC5B [5]**	Mucin 5B	Cholangiocarcinoma	Yes	8OER
17	**POSTN [9]**	Periostin	Cholangiocarcinoma	Yes	5WT7
18	**PTCH1 [1]**	Patched 1	Cholangiocarcinoma	Yes	6DMB
19	**SPP1 [6]**	Secreted phosphoprotein 1 (Osteopontin)	Cholangiocarcinoma	No	—

No.	Gene symbol	Protein name	Cancer type	PDB structure available (Yes/No)	PDB ID
20	**tp53 [1]**	Tumor protein p53	Cholangiocarcinoma	No	—

The genes/proteins were verified for involvement in cholangiocarcinoma using The Human Protein Atlas, and their 3D structures were searched in the RCSB Protein Data Bank (RCSB PDB).

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