

Additional file 11. List of PDB70 template structures used by the ColabFold algorithm for modeling of individual protein complex chains.*

5HT7R			
PDB ID	Protein Name	Orgaism	Ligand
2R4R	Beta-2 adrenergic receptor	<i>Homo sapiens</i>	None
4AMJ	Beta-1 adrenergic receptor	<i>Meleagris gallopavo</i>	Carvedilol (agonist)
4IAQ	5-Hydroxytryptamine Receptor 1B	<i>Homo sapiens</i>	Dihydroergotamine
4IAR	5-Hydroxytryptamine Receptor 1B	<i>Homo sapiens</i>	Ergotamine
6H7L	Beta-1 adrenergic receptor	<i>Meleagris gallopavo</i>	Dobutamine (agonist)
6IBL	Beta-1 adrenergic receptor	<i>Meleagris gallopavo</i>	Formoterol (agonist)
6KR8	Beta-2 adrenergic receptor	<i>Homo sapiens</i>	None
7BVQ	Beta-1 adrenergic receptor	<i>Homo sapiens</i>	Carazolol
7CKW	D(1A) dopamine receptor	<i>Homo sapiens</i>	Fenoldopam
7CKY	D(1A) dopamine receptor	<i>Homo sapiens</i>	PW0464
7DH5	Beta-3 adrenergic receptor	<i>Canis lupus familiaris</i>	Mirabegron
7E2X	5-Hydroxytryptamine Receptor 1A	<i>Homo sapiens</i>	None
7E32	5-Hydroxytryptamine Receptor 1D	<i>Homo sapiens</i>	Serotonin
7E33	5-Hydroxytryptamine Receptor 1E	<i>Homo sapiens</i>	Serotonin
7EXD	5-Hydroxytryptamine Receptor 1F	<i>Homo sapiens</i>	Lasmiditan
7EZM	Cholecystokinin A receptor	<i>Homo sapiens</i>	None
7JOZ	D(1A) dopamine receptor	<i>Homo sapiens</i>	Non-catechol agonist
7JVP	D(1A) dopamine receptor	<i>Homo sapiens</i>	SKF-83959
CDK5			
1OB3	PfPK5	<i>Plasmodium falciparum</i>	None
1UA2	CDK7	<i>Homo sapiens</i>	ATP
1UNL	CDK5/p25	<i>Homo sapiens</i>	R-Roscovitine
1V0B	PfPK5 (T198A mutant)	<i>Plasmodium falciparum</i>	None
1V0O	PfPK5	<i>Plasmodium falciparum</i>	Indirubin-5-sulphonate
3GBZ	CMGC CDK	<i>Giardia lamblia ATCC 50803</i>	None
3GC0	CMGC CDK	<i>Giardia lamblia ATCC 50803</i>	AMP
3NIZ	CDK CGD5_2510	<i>Cryptosporidium parvum</i>	ADP
3QHR	pCDK2/CyclinA	<i>Homo sapiens, Mus musculus</i>	ADP
4AU8	CDK5	<i>Homo sapiens</i>	Compound 4a
4KRC	CDK PHO85	<i>Saccharomyces cerevisiae S288C</i>	ATP-γ-S

4KRD	CDK PHO85/Pcl10	Saccharomyces cerevisiae S288C	None
4YC3	CDK1/CyclinB1/CKS2	<i>Homo sapiens</i>	None
5G6V	CDK16	<i>Homo sapiens</i>	Inhibitor
6GU2	CDK1/CyclinB/CKS2	<i>Homo sapiens</i>	Flavopiridol
6O9L	CDK7	<i>Homo sapiens</i>	None
6Q4G	CDK2	<i>Homo sapiens</i>	FragLite37
6Q4K	CDK2	<i>Homo sapiens</i>	FragLite38
6XBZ	CDK7	<i>Homo sapiens</i>	AGS
7B5Q	CDK7	<i>Homo sapiens</i>	ICEC0942

Gas

PDB ID	Protein Name	Organism	Ligand
1CIP	Guanine nucleotide-binding protein G(i) subunit alpha-1	<i>Rattus norvegicus</i>	GNP
1SHZ	Guanine nucleotide-binding protein G(i) subunit alpha-1	<i>Rattus norvegicus</i>	GDP
1TAD	Guanine nucleotide-binding protein G(t) subunit alpha-1	<i>Bos taurus</i>	GDP
1TAG	Guanine nucleotide-binding protein G(t) subunit alpha-1	<i>Bos taurus</i>	GDP
1TND	Guanine nucleotide-binding protein G(t) subunit alpha-1	<i>Bos taurus</i>	GSP
1ZCA	Guanine nucleotide-binding protein subunit alpha-12	<i>Mus musculus</i>	GDP
1ZCB	Guanine nucleotide-binding protein subunit alpha-13	<i>Mus musculus</i>	GDP
3CX8	Guanine nucleotide-binding protein subunit alpha-13	<i>Mus musculus</i>	GDP
4EKC	Guanine nucleotide-binding protein G(q) subunit alpha	<i>Mus musculus</i>	GDP
4EKD	Guanine nucleotide-binding protein G(q) subunit alpha	<i>Mus musculus</i>	GDP
4N0D	Guanine nucleotide-binding protein G(i) subunit alpha-1	<i>Rattus norvegicus</i>	GNP
5DO9	Guanine nucleotide-binding protein G(q) subunit alpha	<i>Mus musculus</i>	GDP
6AU6	Guanine nucleotide-binding protein G(s) subunit alpha isoforms short	<i>Homo sapiens</i>	GDP
6CMO	Guanine nucleotide-binding protein G(i) subunit alpha-1	<i>Homo sapiens</i>	None
6NE6	G-protein alpha subunit Galpha7	<i>Naegleria fowleri</i>	None

7BPH	Guanine nucleotide-binding protein G(s) subunit alpha isoforms short	<i>Homo sapiens</i>	GNP
7FIG	Engineered guanine nucleotide-binding protein G(s) subunit alpha	<i>Bos taurus</i>	None
7RKF	Guanine nucleotide-binding protein subunit alpha-11	<i>Homo sapiens</i>	GDP
7SQ2	Guanine nucleotide-binding protein G(q) subunit alpha	<i>Mus musculus</i>	GDP

*The templates chosen to model the 5-HT7R in *h5HT7/CDK5*, *m5HT7/CDK5* and *5HT7/Gas* were the same in all 3 individual cases. Same for *hCDK5* and *mCDK5* – the templates chosen by ColabFold algorithm were the same.