

Title: Protein PKA and Cu (I) Binding

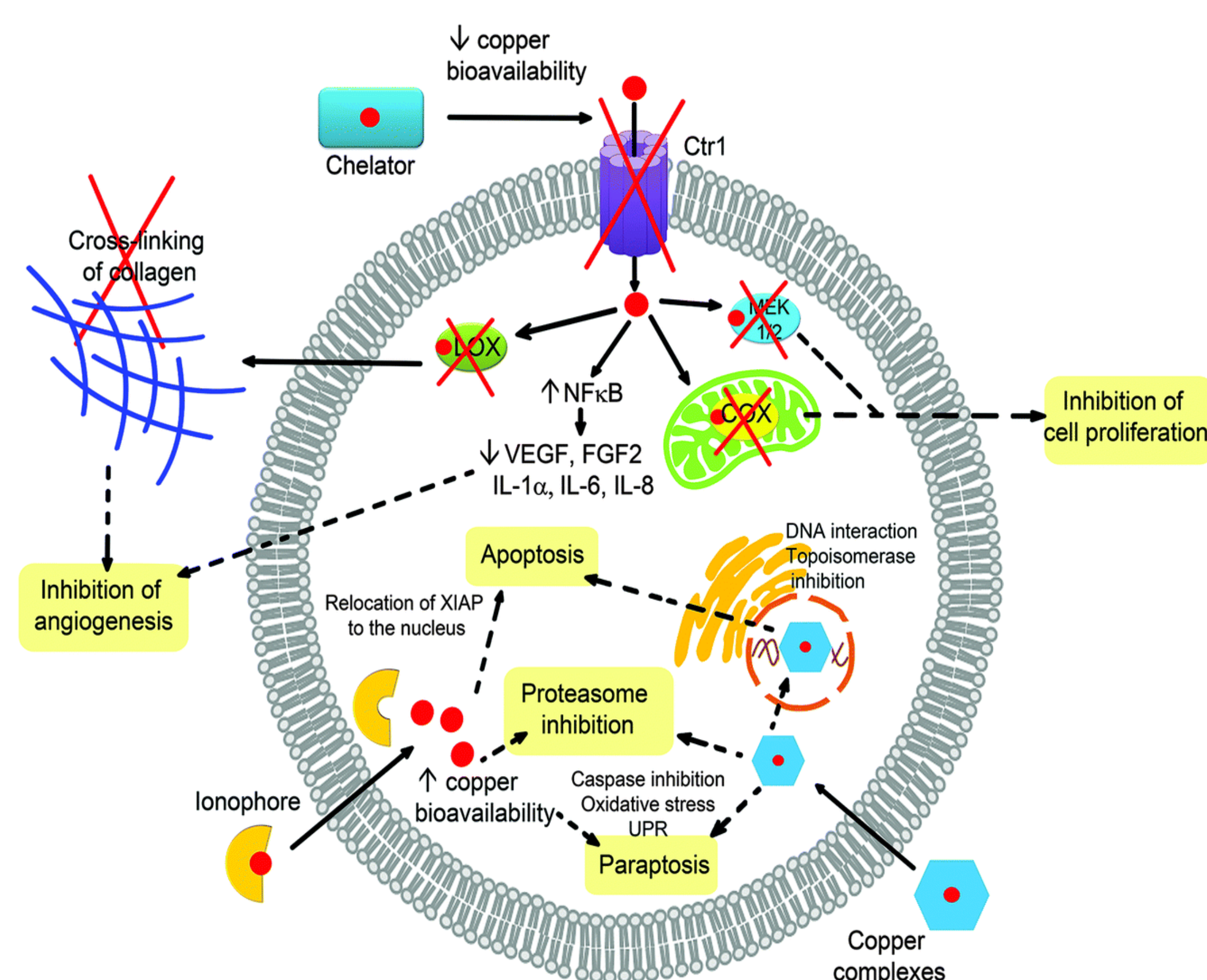


PRESENTER:
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BACKGROUND: Metal binding PKA's are vital to the structure and function of various proteins. By analyzing PKA values, (through PKA 17), of different amino acids that make up proteins, one can determine the strength of binding and apply these values to other areas of science.

METHODS

1. Assembled a table of Zn (II) binding affinities.
2. Download PDB files of the proteins being analyzed.
3. Identify the residue in question and trim up the PDB files.
4. Run the trimmed files through PKA 17.
5. Tabulate the final PKA values.



RESULTS

- I was able to amass a large Zn (II) binding affinity table that will be helpful for all scientists and researchers.
- Cys and Tyr PKA's were tabulated and determined that there is validity to PKA 17 and using these calculations for further applications.

Cu (I) Binding could be useful in Cancer Research, specifically the cis-Platin Treatment.

CYS	PDB ID	Residue #	Experimental pKa	Final pKa	Unsigned Error	Average Unsigned Error
	1HIC	C39	3.76	3.79	0.03	1.121
	3TRX	C32	6.3	6.61	0.31	1.121
	1JAE	C115	8.3	8.96	0.66	1.121
	1LIN	C147	8.86	8.21	0.65	1.121
	19D	C12	6.4	6.72	0.32	1.121
	1A23	C30	3.5	4.63	1.13	1.121
	1A23	C33	9.5	8.64	0.86	1.121
	1XDB	C32	7.1	7.7	0.6	1.121
	1XDB	C35	9.9	9.9	0	1.121
	1I7K	C102	10.9	9.38	1.52	1.121
	1JAS	C88	10.2	8.69	1.51	1.121
	1JBB	C87	11.1	8.23	2.87	1.121
	1GSS	C45	4.2	6.23	2.03	1.121
	3BPB	C249	8.9	8.43	0.47	1.121
	1MEK	C36	4.5	5.53	1.03	1.121
	1KCT	C232	6.86	6.3	0.56	1.121
	1CTE	C29	3.6	2.73	0.87	1.121
	1CPJ	C29	3.6	4.25	0.65	1.121
	1THE	C29	3.6	3.18	0.42	1.121
	1QLP	C232	6.86	8.35	1.49	1.121
	4MA9	C46	5.94	7.21	1.27	1.121
	4MA9	C165	8.64	10.58	1.94	1.121
	1P5F	C106	5.4	5.73	0.33	1.121
	10E	C283	5.6	4.99	0.61	1.121
	2L90	C72	8.2	6.24	1.96	1.121
	1EH6	C145	5.3	7.42	2.12	1.121
	1PPN	C25	3.32	2.25	1.07	1.121
	2HNP	C215	5.57	5.8	0.23	1.121
	1PPO	C25	2.88	2.43	0.45	1.121
	1M8B	C56	2.27	4.74	2.47	1.121
	1M8C	C56	2.27	2.52	0.25	1.121
	1DMU	C56	2.5	4.7	2.2	1.121
	2DVO	C56	2.23	4.28	2.05	1.121
	1B4Q	C22	3.6	5.73	2.13	1.121
	2H19	C74	8.48	7.7	0.78	1.121
	2H1A	C77	8.33	9.56	1.23	1.121
	2H1B	C77	7.4	8.92	1.52	1.121
	3C71	C74	7.2	6.18	1.02	1.121
	4IP1	C461	10.5	7.82	2.68	1.121
	2FWF	C461	9.3	7.89	1.41	1.121
	1D73	C40	7.2	6.03	1.17	1.121
	3C29	C106	6.4	4.41	1.99	1.121
	3CY6	C106	5.7	5.78	0.08	1.121
	3C2A	C106	6.1	5.73	0.37	1.121

TYR	PDB ID	Residue Number	Expt. PKA	Final PKA	Unsigned Error	Average Unsigned Error
	1BEG	12	>11.5	11.27	0.23	0.496
	1BEG	33	>12.0	11.25	0.76	0.496
	1BEG	47	>12.0	11.83	0.18	0.496
	1BEG	85	10.35	10.67	0.32	0.496
	1BEG	87	>12.0	11.28	0.73	0.496
	1BEO	33	>12.0	12.18	0.17	0.496
	1BEO	47	>12.0	12.56	0.55	0.496
	1BEO	87	>12.0	11.41	0.6	0.496
	1BEO	12	>11.5	11.06	0.44	0.496
	1BEO	85	10.35	11.19	0.84	0.496
	1BF4	8	>9.3	11.34	2.03	0.496
	1BF4	34	>10.0	10.21	0.79	0.496
	1C8C	8	>9.3	10.1	0.79	0.496
	1C8C	34	>10.0	10.37	0.36	0.496
	1RGG	30	11.3	10.97	0.33	0.496
	1RGG	49	10.6	11.16	0.56	0.496
	1PGB	33	>11	10.46	0.54	0.496
	2DVO	11	10.16	10.73	0.57	0.496
	2DVO	20	11.07	10.57	0.5	0.496
	2DVO	31	>12.5	11.24	1.27	0.496
	4PTI	10	10.4	10.74	0.34	0.496
	4PTI	21	11.1	11.8	0.7	0.496
	4PTI	23	11.7	11.64	0.06	0.496
	4PTI	35	11.1	10.85	0.25	0.496
	1RGG	86	>11.5	11.85	0.34	0.496
	1RGG	52	>11.5	11.08	0.43	0.496
	1RGG	55	>11.5	11.49	0.02	0.496
	1RGG	80	>11.5	11.41	0.1	0.496
	1RGG	81	>11.5	11.41	0.1	0.496
	2MB5	103	10.3	10.21	0.09	0.496
	2MB5	151	10.5	10.27	0.23	0.496
	1PGA	3	>11	11.73	0.72	0.496
	1PGA	45	>12	11.33	0.68	0.496
	1PGA	33	>11	10.55	0.45	0.496
	1PGB	3	>11	11.7	0.69	0.496
	1PGB	45	>12	10.61	1.4	0.496
	2LZT	20	10.3	10.49	0.19	0.496
	2LZT	23	9.8	10.44	0.6	0.496
	2LZT	53	12.1	11.61	0.49	0.496
	1MBC	103	10.3	10.65	0.35	0.496
	1MBC	151	10.5	10.44	0.06	0.496
	2ZTA	17	9.82	10.24	0.42	0.496
	1ANS	7	9.7	10.23	0.53	0.496
	1ANS	18	10.1	9.6	0.5	0.496
	1HRC	67	11	10.37	0.63	0.496

Protein	kd is	Source	Method	Notes
Human serum albumin (5IJF)	55nM	Protein	Experimental	"Parameters Influencing Zinc in Experimental Systems in Vivo and in Vitro"
Metallothionein (4MT2)	-1.6nM	Protein	Experimental	"Parameters Influencing Zinc in Experimental Systems in Vivo and in Vitro"
Calprotectin (5HLV)	25 pMolar	Protein	Experimental	"Parameters Influencing Zinc in Experimental Systems in Vivo and in Vitro"

ADDED INFO:

- PKA 17 considers assumptions in its calculations.
- This project could have been done with other amino acids; we however chose Cys and Tyr.

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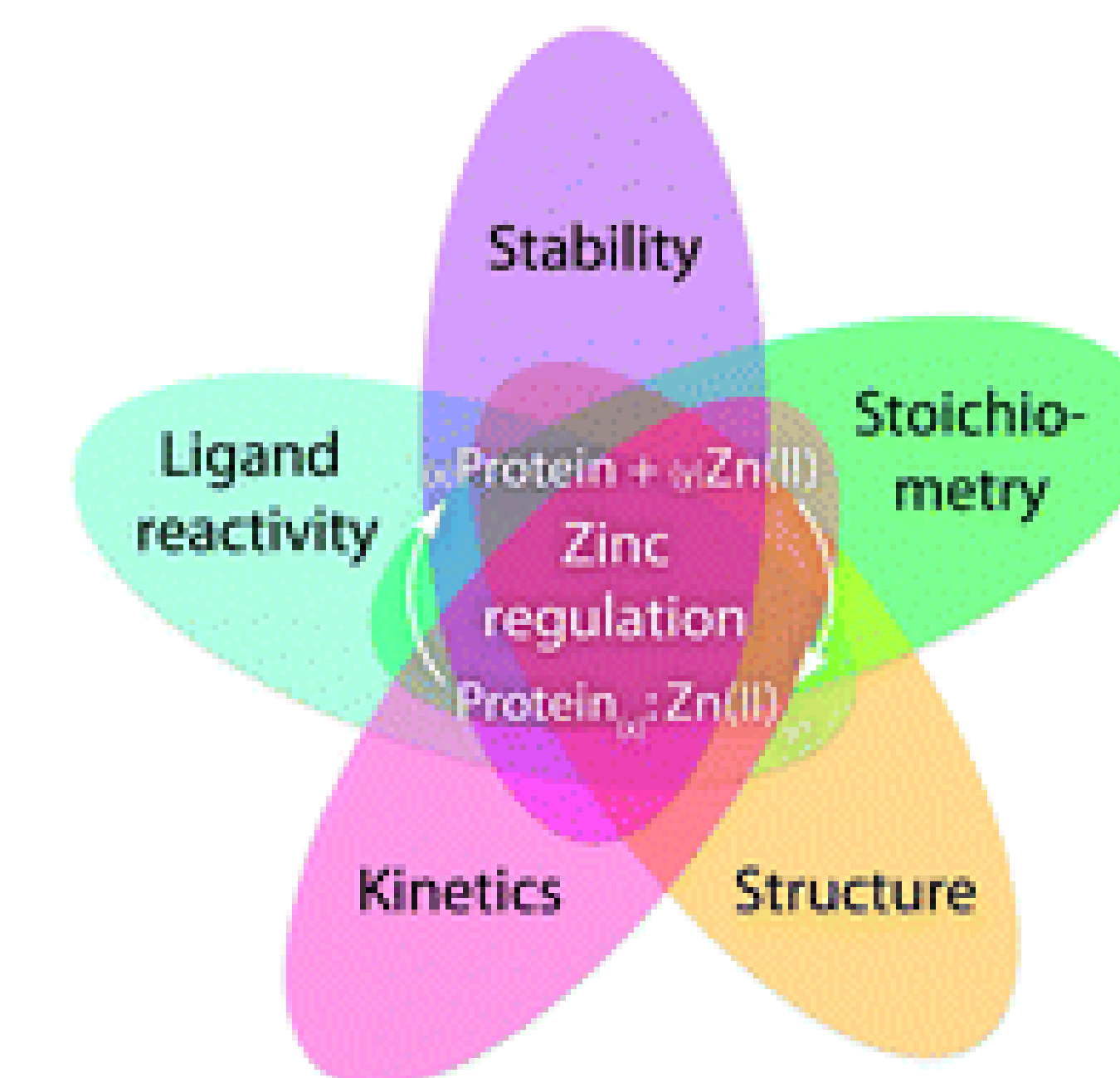
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