

ANTI-OXIDANT

TCU

College of Science & Engineering



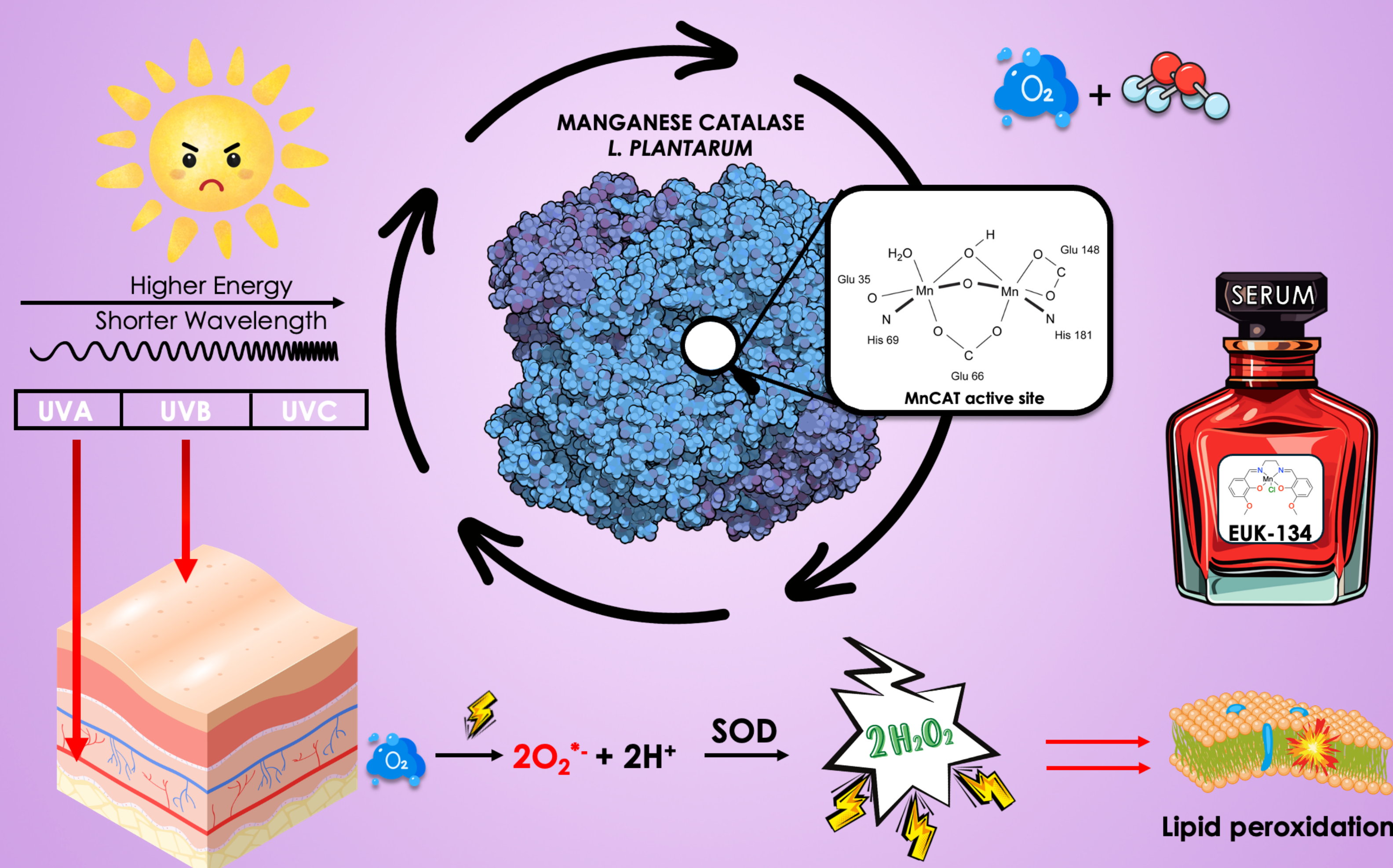
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CATALASE LIGAND MIMICS

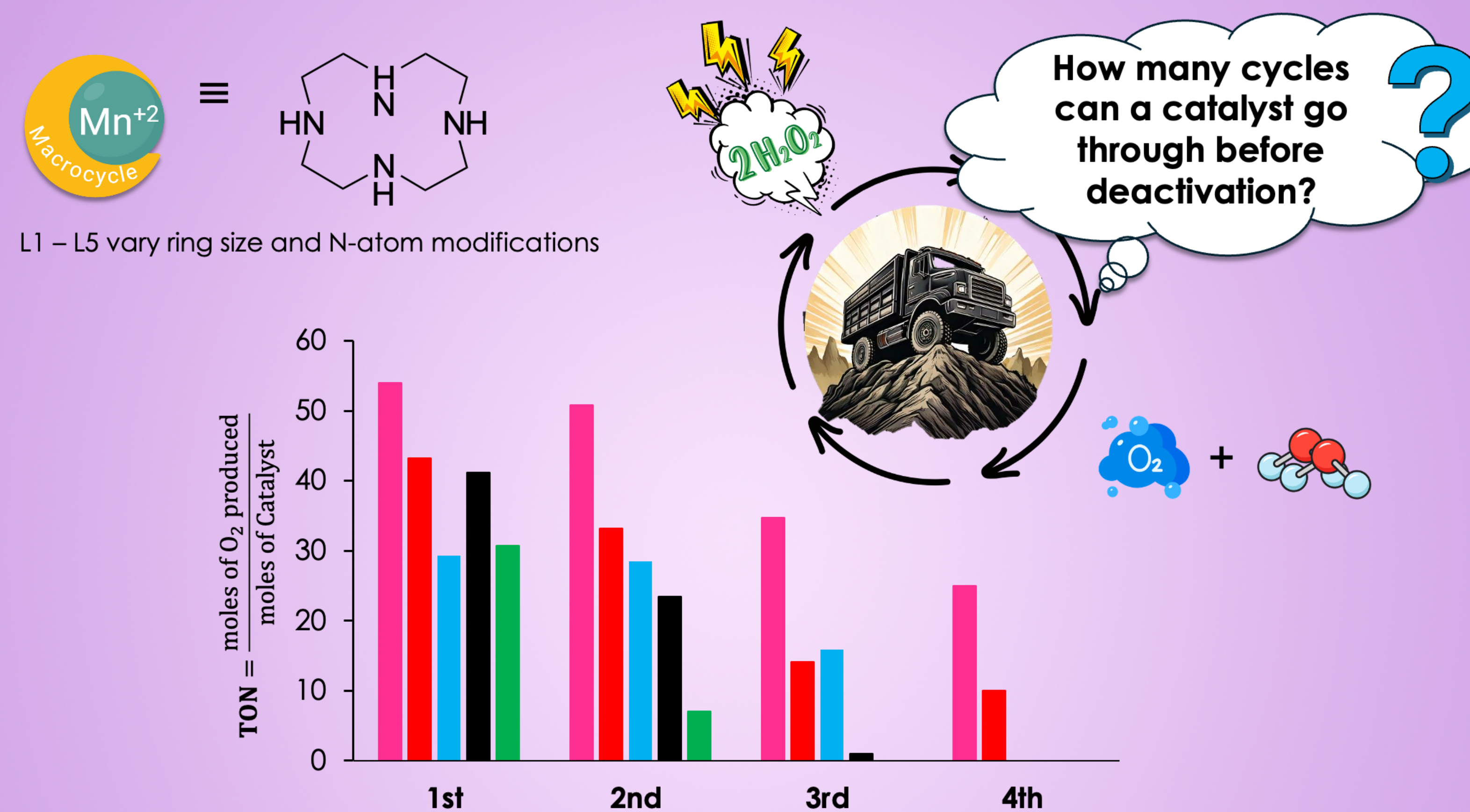
Background



Explore small molecules that mimic Nature's antioxidant mechanisms to protect against ROS damage to the skin



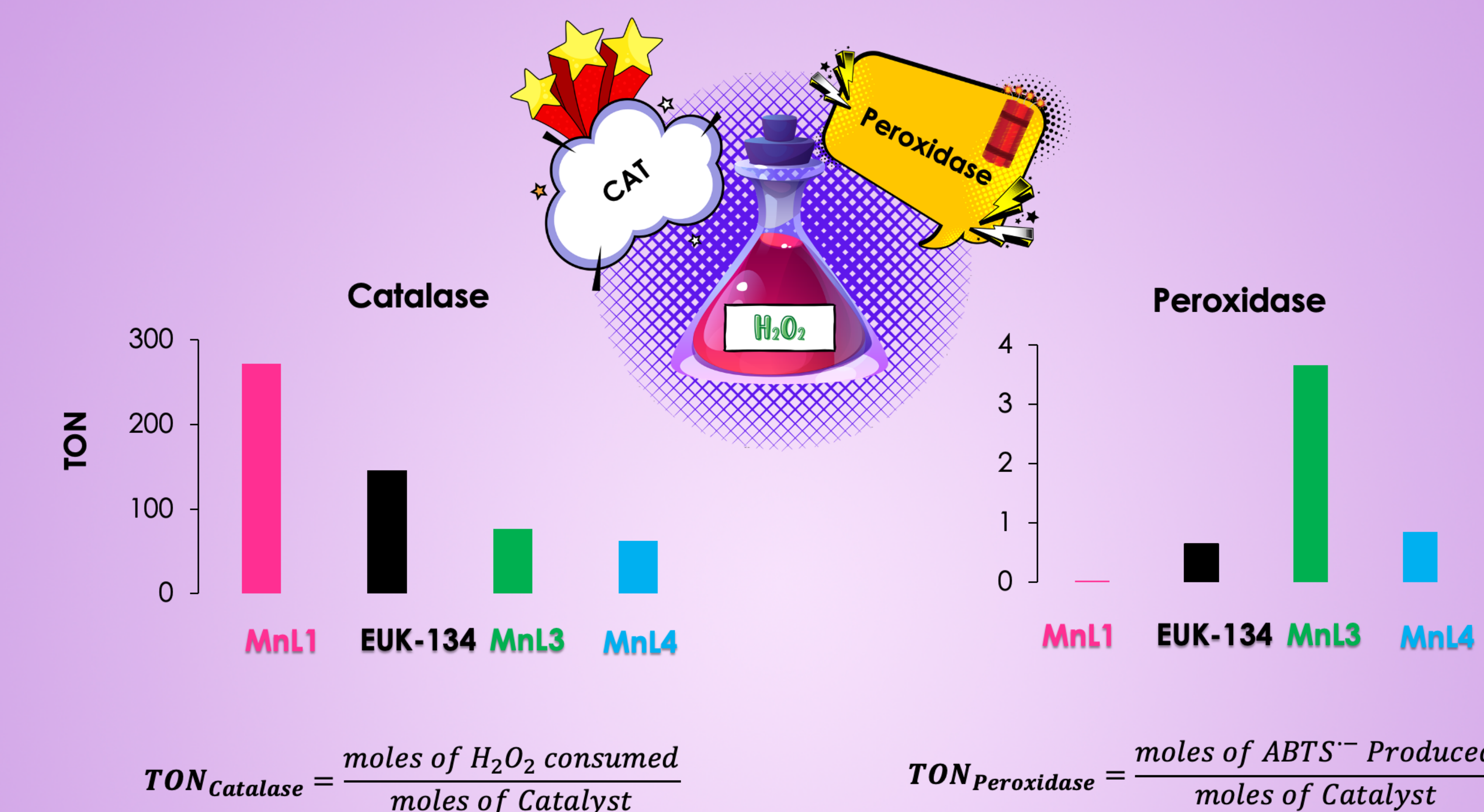
Robustness



	1st aliquot		2nd aliquot		3rd aliquot		4th aliquot		Total Time
	TON	TOF (s ⁻¹)	TON	TOF (s ⁻¹)	TON	TOF (s ⁻¹)	4th eq	TOF (s ⁻¹)	
EUK-134	41.24	0.2	24.06	0.06	1	0.01	-	-	7 min
MnL1	54.05	0.09	50.86	0.09	34.69	0.07	24.94	0.04	33 min
MnL2	45.23	0.01	33.19	0.01	14.13	0.01	10.05	0.01	4 hr
MnL3	30.7	0.06	7.01	0.06	-	-	-	-	1 hr
MnL4	29.34	0.06	28.5	0.05	-	-	-	-	1 hr

* Studies conducted at 1.5mM=MnL#, 150mM=H₂O₂

Selectivity



$$TON_{catalase} = \frac{\text{moles of } H_2O_2 \text{ consumed}}{\text{moles of Catalyst}}$$

$$TON_{peroxidase} = \frac{\text{moles of } ABTS^{\cdot-} \text{ Produced}}{\text{moles of Catalyst}}$$

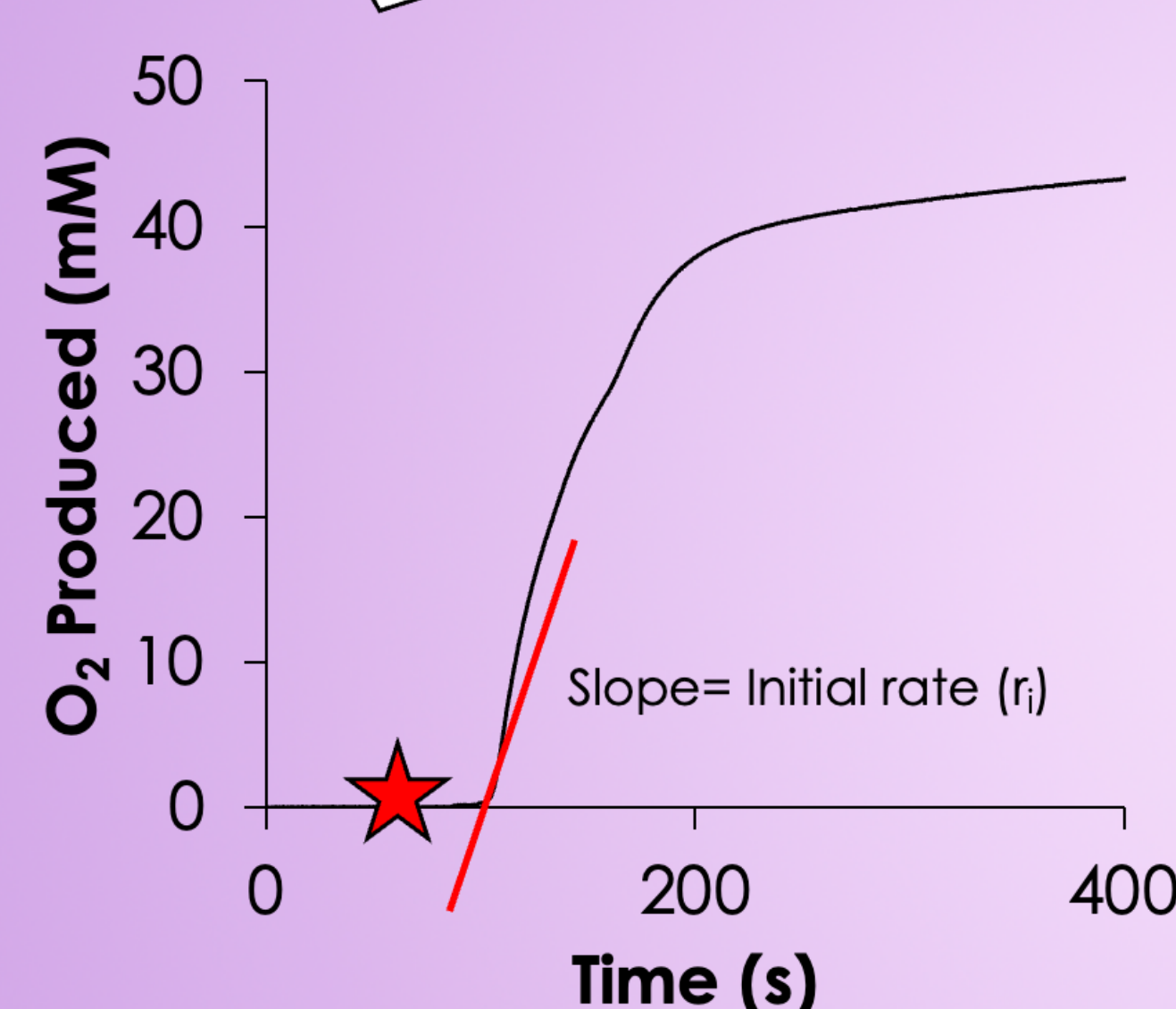
	Catalase (C)		Peroxidase (P)		Selectivity (C _{TON} /P _{TON})
	TON	TOF (s ⁻¹)	TON	TOF (s ⁻¹)	
MnL1	271.73	2.26E-01	0.02	3.20E-06	7.07E+04
EUK-134	145.41	2.02E-02	0.64	8.94E-05	2.26E+02
MnL3	76.37	6.36E-02	3.66	5.09E-04	1.25E+02
MnL4	62.1	9.00E-03	0.85	1.35E-04	6.66E+01

* Selectivity results conducted by Grant Elam from Oklahoma State University

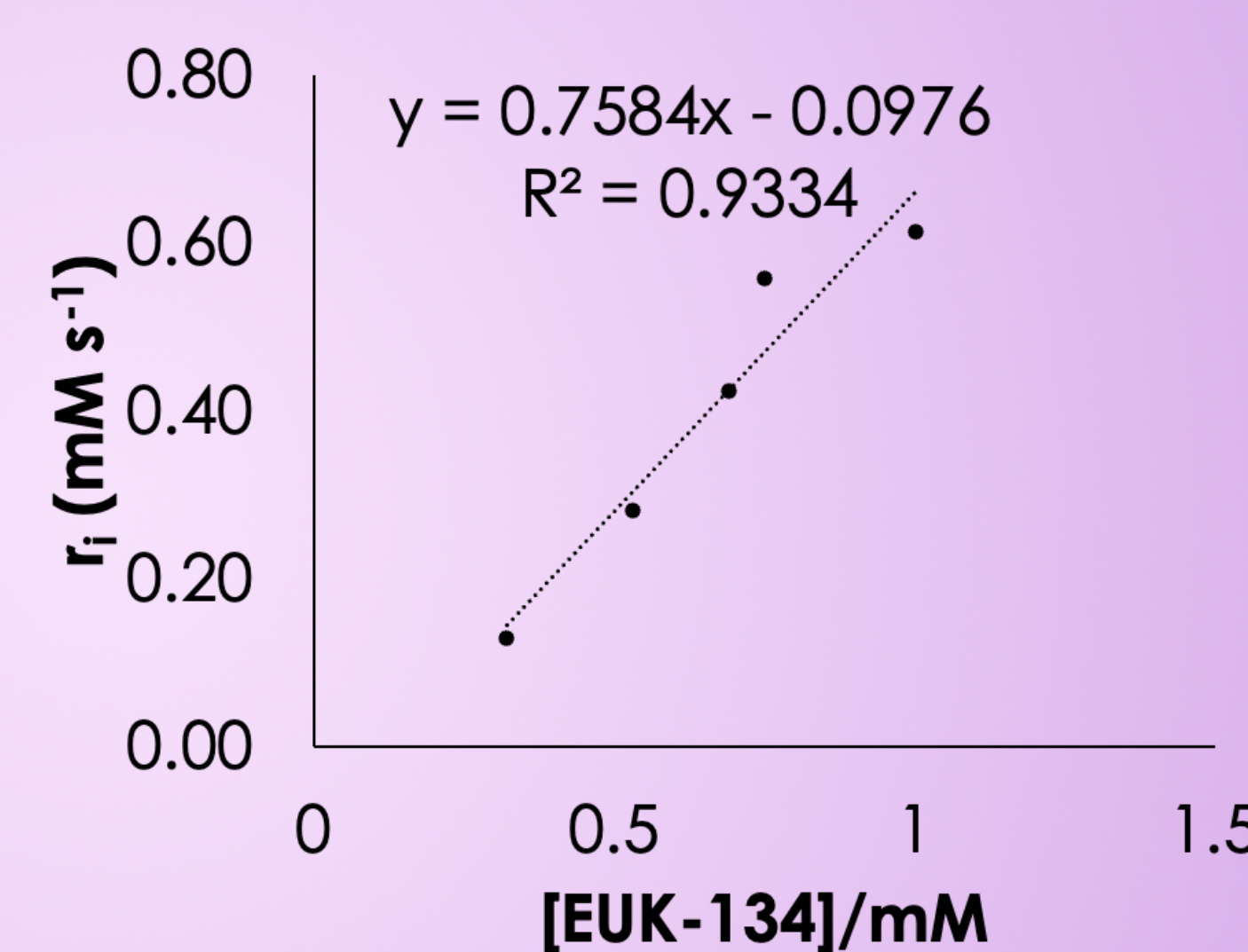
Rate



How do new MnCAT mimics compare to the current active ingredient (EUK-134) in anti-aging serums?



$$Rate = k[Catalyst]^n [Substrate]^m$$

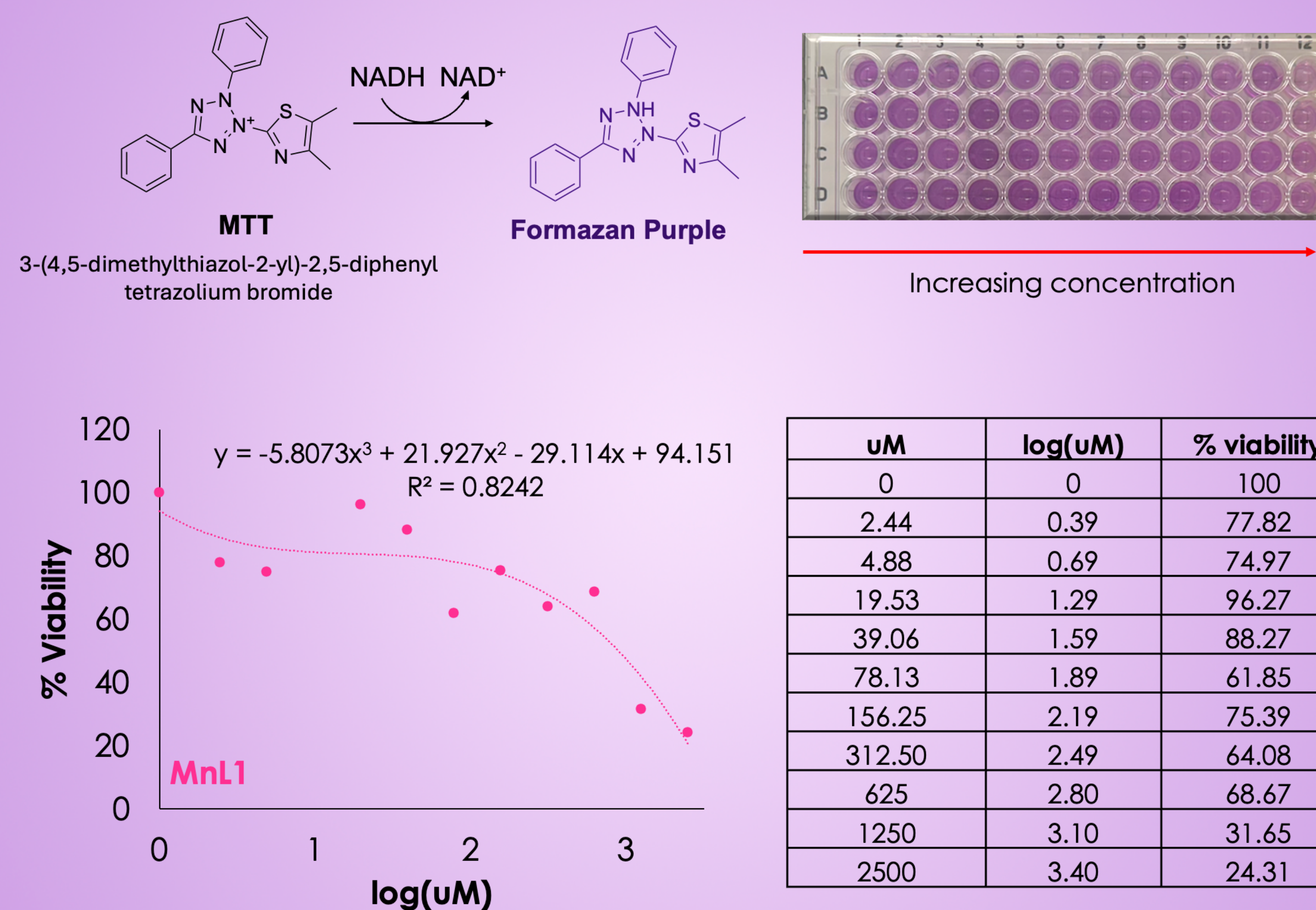


	k (M ⁻¹ s ⁻¹)
EUK-134	6.10
MnL1	2.10
MnL2	0.095
MnL3	3.68
MnL4	2.00

[EUK-134]	rate (mmol s ⁻¹)
0.32	0.13
0.53	0.28
0.69	0.42
0.75	0.56
1.00	0.61

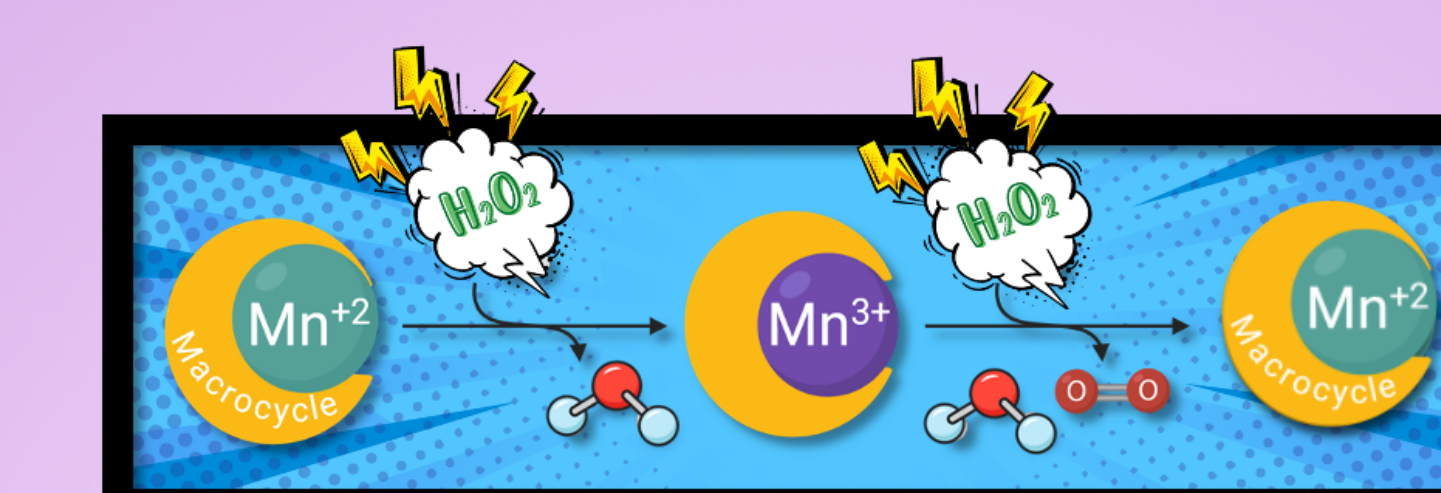
* Studies conducted under pseudo 1st order conditions

Cytotoxicity



* Studies conducted with Sarah Dunn

Conclusion & Credits



Structural variations impact the chemical environment, stability and reactivity of the MnL complexes. To assess whether these properties affect catalytic performance, a range of characteristics were evaluated relevant to catalase disproportionation:

- Robustness
- Selectivity
- Rate
- Cytotoxicity

Credits:
Grant Elam and Professor Tim Hubin, Southwest Oklahoma State University
Professor Ben Sherman and Giri Akkaraju
TCU Department of Chemistry & Biochemistry

