Supplementary Materials for:

A Nucleotide-Copper (II) Complex Possessing Monooxygenase-Like Catalytic Function

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Table 1. Materials and regents

Materials	Abbreviation	CAS	Company
Adenosine monophosphate	AMP	4578-31-8	Aladdin
Cytidine monophosphate	CMP	6757-06-8	
Guanosine monophosphate	GMP	5550-12-9	
Uridine monophosphate	UMP	2287-36-8	
Adenosine	---	58-61-7	
Cytidine	---	65-46-3	
Guanosine	---	118-00-3	
Uridine	---	58-96-8	
Adenosine diphosphate	ADP	16178-48-6	
Cytidine diphosphate	CDP	34393-59-4	
Guanosine diphosphate	GDP	7415-69-2	
Uridine diphosphate	UDP	21931-53-3	
Adenosine triphosphate	ATP	987-65-5	
Cytidine triphosphate	CTP	36051-68-0	
Guanosine triphosphate	GTP	56001-37-7	
Uridine triphosphate	UTP	108321-53-5	
Tyramine hydrochloride	---	60-19-5	
L-Tyrosine hydrochloride	---	16870-43-2	
Pyrene	---	129-00-0	
Copper sulfate pentahydrate	CuSO4·5H2O	7758-99-8	
Hydrogen peroxide	H_2O_2	7722-84-1	
Tyrosinase from mushroom	Tyrosinase	9002-10-2	
AAAAAAAAAAAAAAAAAAAA	poly A20	---	Hippobio

CCCCCCCCCCCCCCCCCCCC	poly C20	---
GGGGGGGGGGGGGGGGGGGG	poly G20	---
TTTTTTTTTTTTTTTTTTTT	poly T20	---

Water was deionized using a Milli-Q system (≥18.25 MΩ·cm–1).

Figure S1 UV-vis spectra of tyramine oxidation reaction catalysed by Cu^{2+} and nucleotides. $[Cu^{2+}]$ = 0.1 mM, [nucleotides] = 10 mM, [tyramine] = 1 mM, $[H_2O_2]$ = 5 mM, in water (pH=8.0).

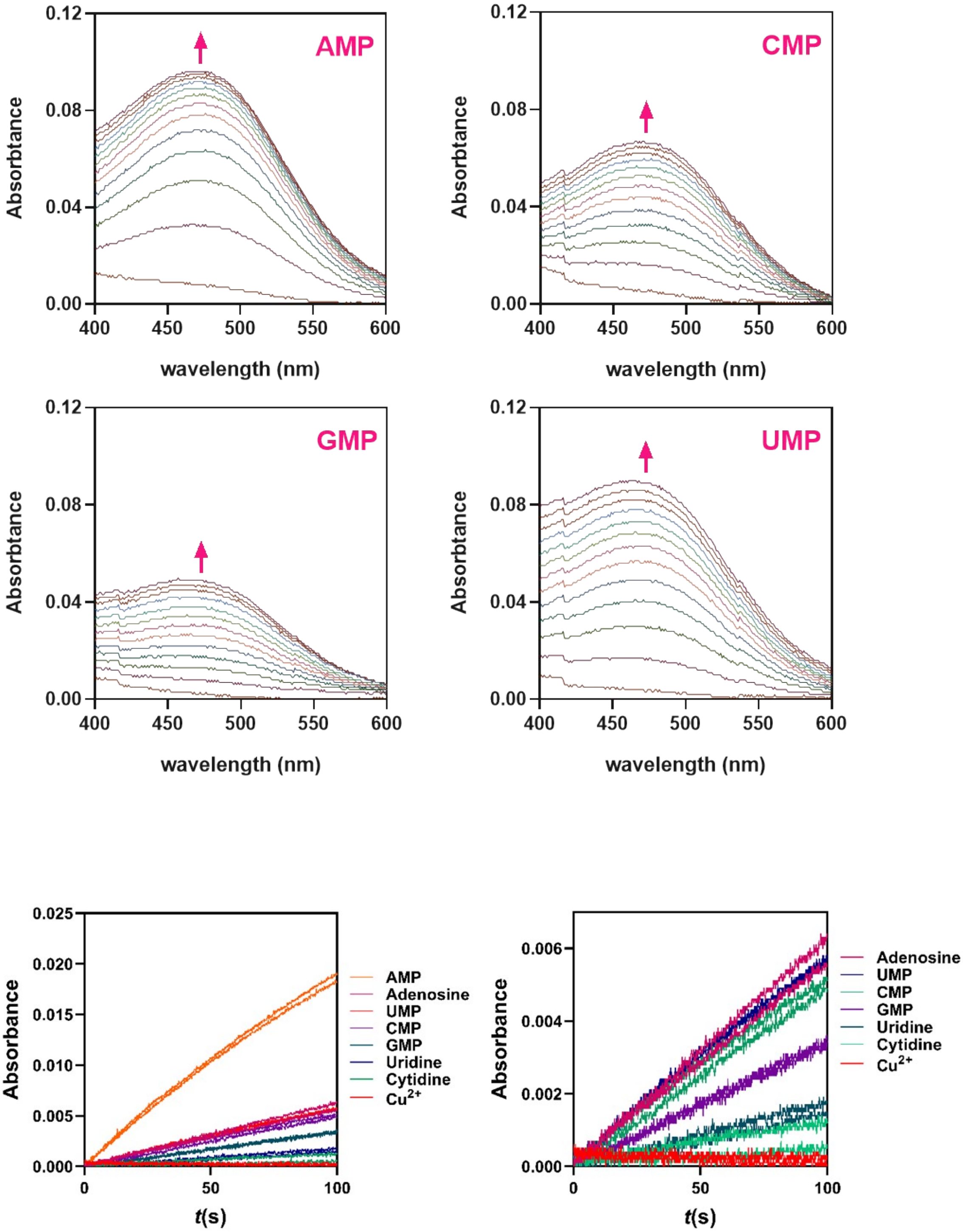
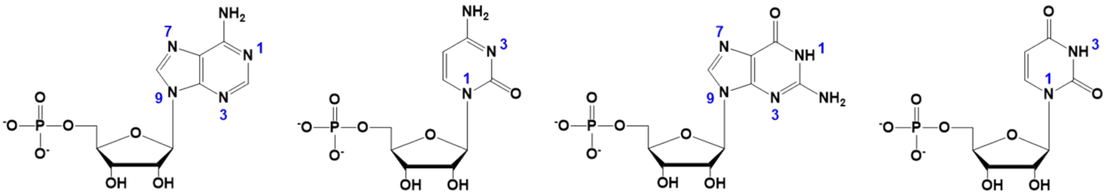


Figure S2 Structure of nucleoside monophosphate.



Adenosine monophosphate *Cytodine monophosphate* *Guanosine monophosphate* *Uridine monophosphate*

Figure S3 Ligands' concentration effect on velocity of tyramine's oxidation reaction catalysed by Cu^{2+} and A/C/G/UMP. Cu^{2+} (0.1 mM), H_2O_2 (5mM), tyramine (1mM). The data are presented as the mean ± s.d., with the error bars representing the s.d. and N= 3.

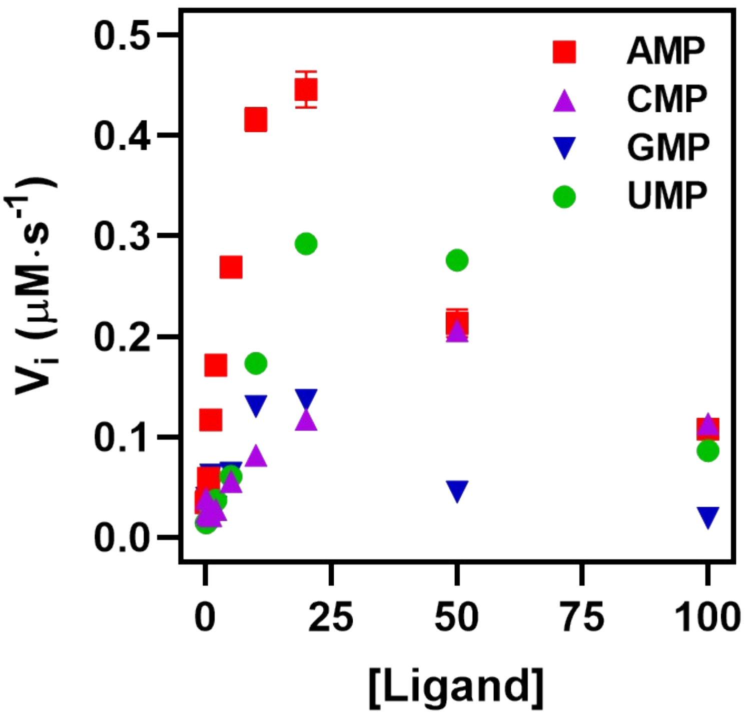


Figure S4 KCl effect on tyramine's oxidation reaction catalysed by Cu^{2+} and AMP. AMP (20 mM), Cu^{2+} (50 μM), H_2O_2 (5 mM), tyramine (1 mM). The data are presented as the mean ± s.d., with the error bars representing the s.d. and N= 3.

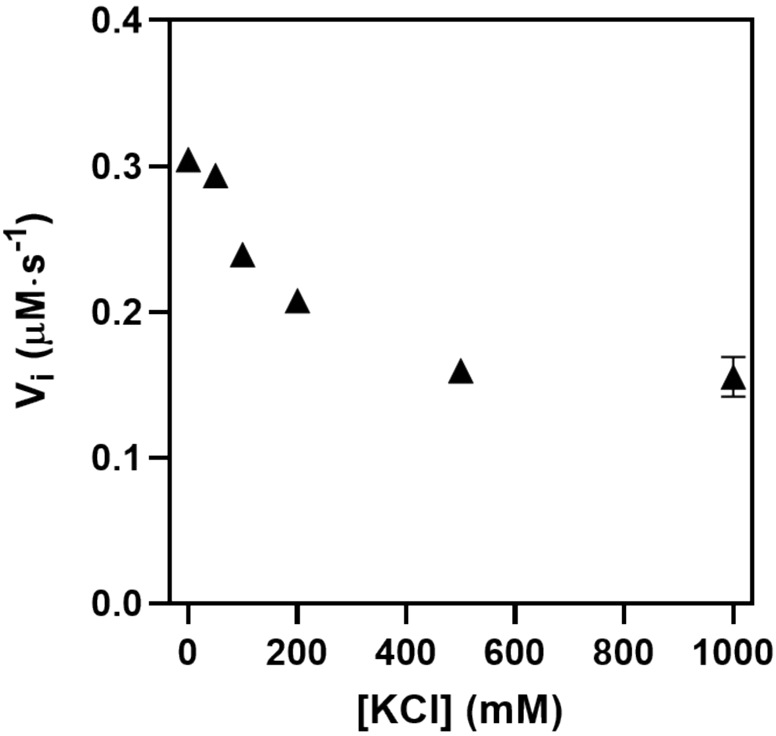


Figure S5 6 K CW-EPR of Cu^{2+}/AMP and Cu^{2+}/AMP/H_2O_2/tyramine. CuSO4 (500 μM), AMP (10 mM), H_2O_2 (1 mM), tyramine (1 mM), mwFreq (9.74GHz).

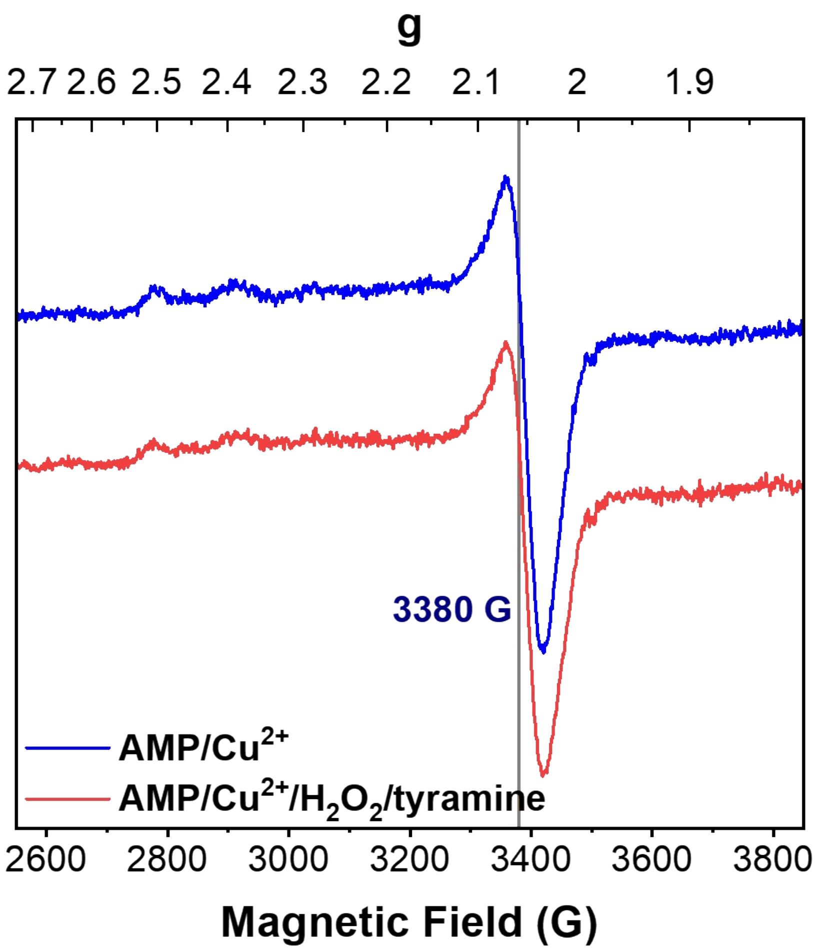


Figure S6 (A) Methanol concentration effect on the catalytic tyramine oxidation reaction. (B) EPR measurement of the system of Cu^{2+}/ CMP/ H_2O_2. 60% MeOH, 100 mM DMPO, 20 mM CMP, 100 μM Cu^{2+}, 100 μM H_2O_2. The data are presented as the mean ± s.d., with the error bars representing the s.d. and N= 3.

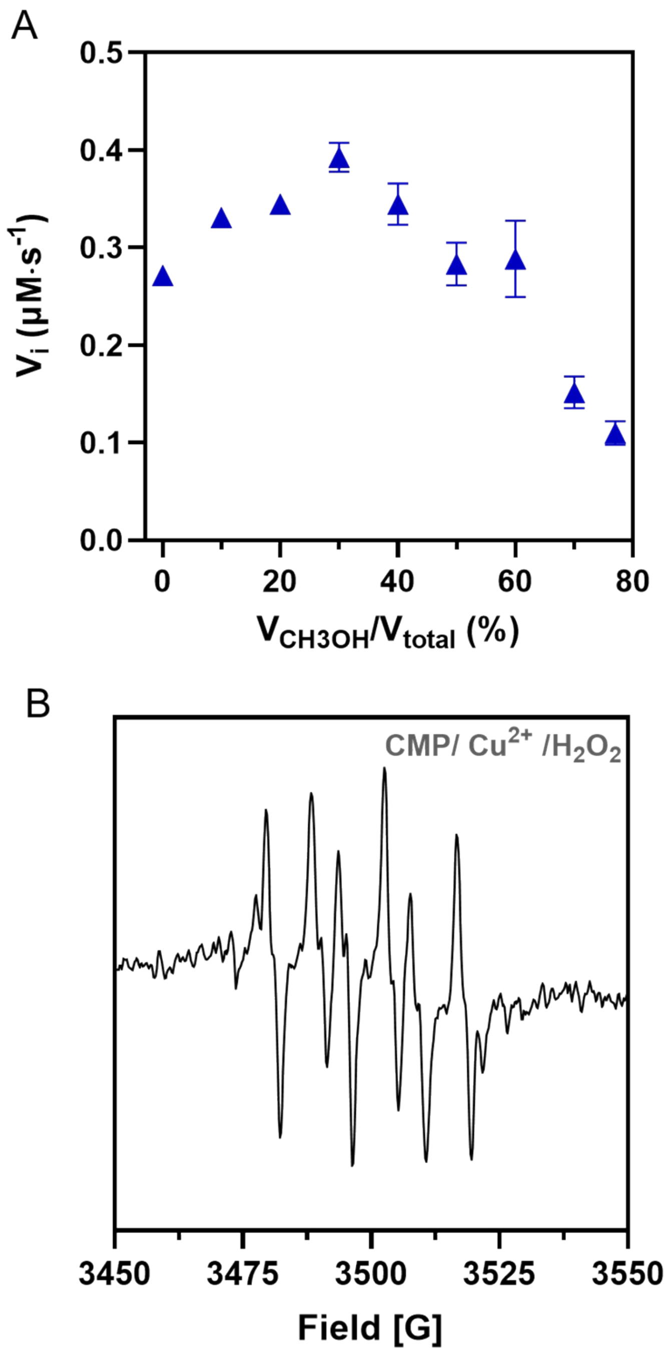


Figure S7 EPR measurement of the system of Cu^{2+}/ GMP/ H_2O_2. 60% MeOH, 100 mM DMPO, 20 mM GMP, 100 μM Cu^{2+}, 100 μM H_2O_2.

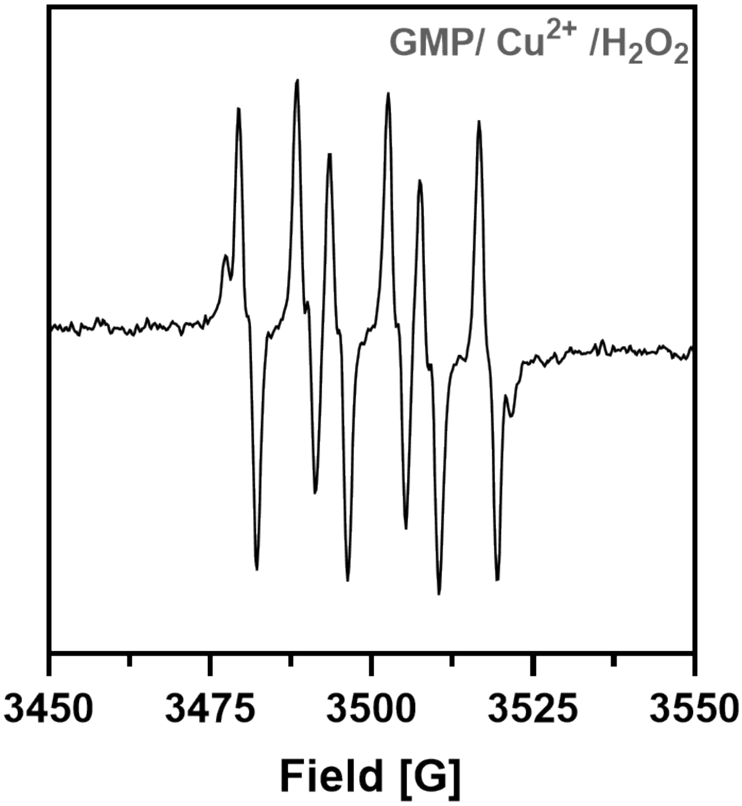


Figure S8 EPR measurement of the system of Cu^{2+}/ UMP/ H_2O_2. 60% MeOH, 100 mM DMPO, 20 mM UMP, 100 μM Cu^{2+}, 100 μM H_2O_2.

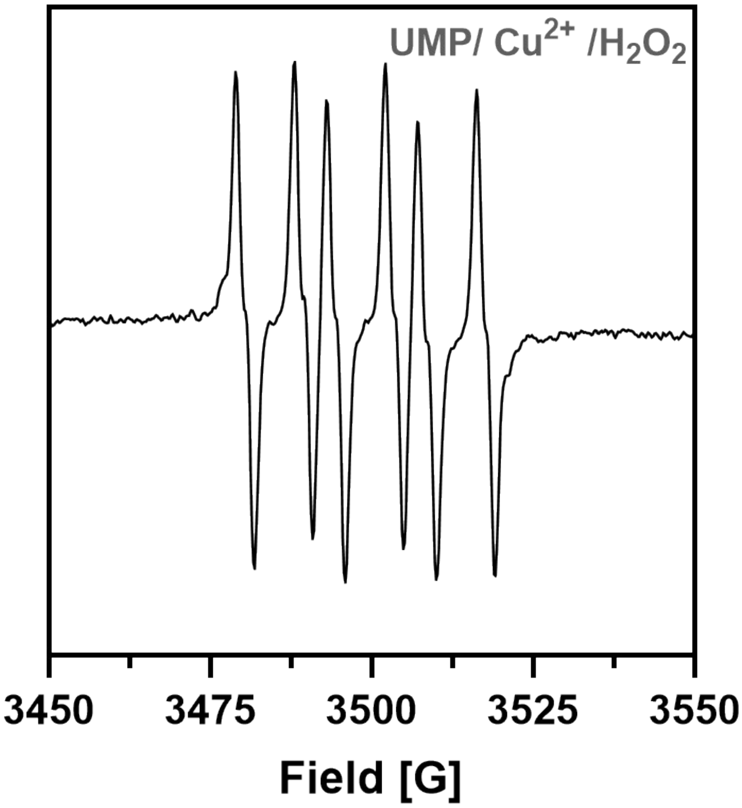


Figure S9 Free radical quenchereffect on tyramine's oxidation reaction catalysed by Cu^{2+}/ AMP. Cu^{2+} (0.1mM), AMP (20 mM), H_2O_2 (5 mM), tyramine (1 mM). TBA stands for tert-butanol, while SOD stands for superoxidase dismutase. The data are presented as the mean ± s.d., with the error bars representing the s.d. and N= 3.

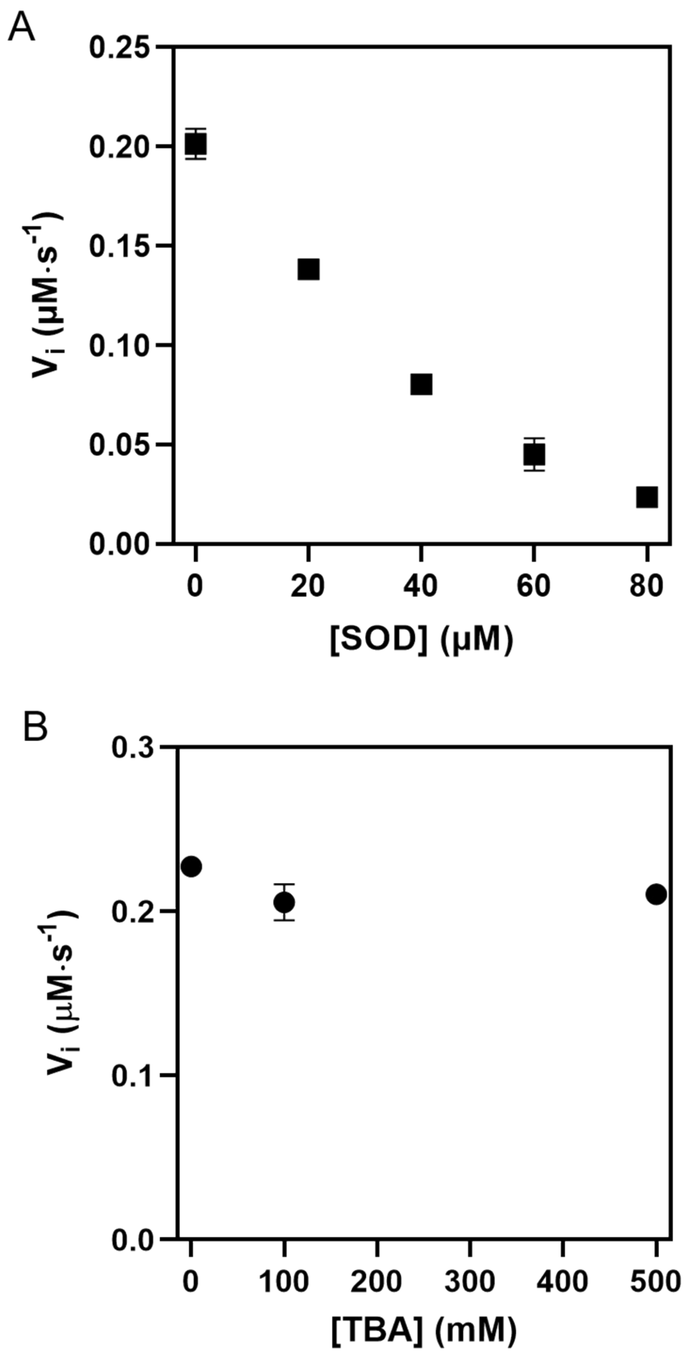


Figure S10 Density functional theory model of the ternary complex intermediate of nucleotides/ Cu^{2+}/tyramine/ H_2O_2, and the Isosurface map of IRI analyse, revealing both chemical bonds and weak interactions. IRI=1.2.

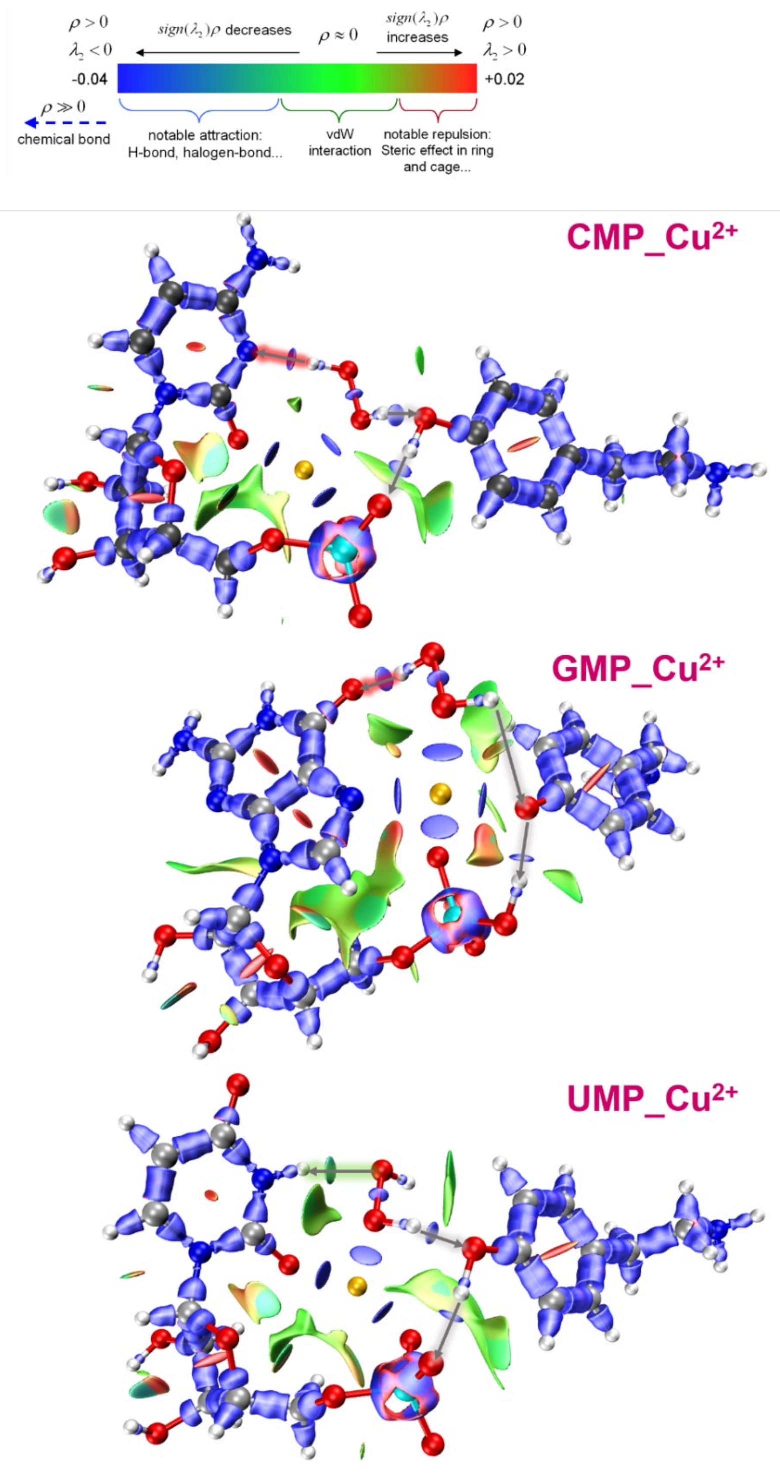


Figure S11 Free energy during the formation of HO_2• radical suggested by DFT calculations. Free energies and enthalpies were calculated at 298 K. The inserted figures were structure optimization and spin density computation during the formation of HO_2• radical suggested by DFT calculations.

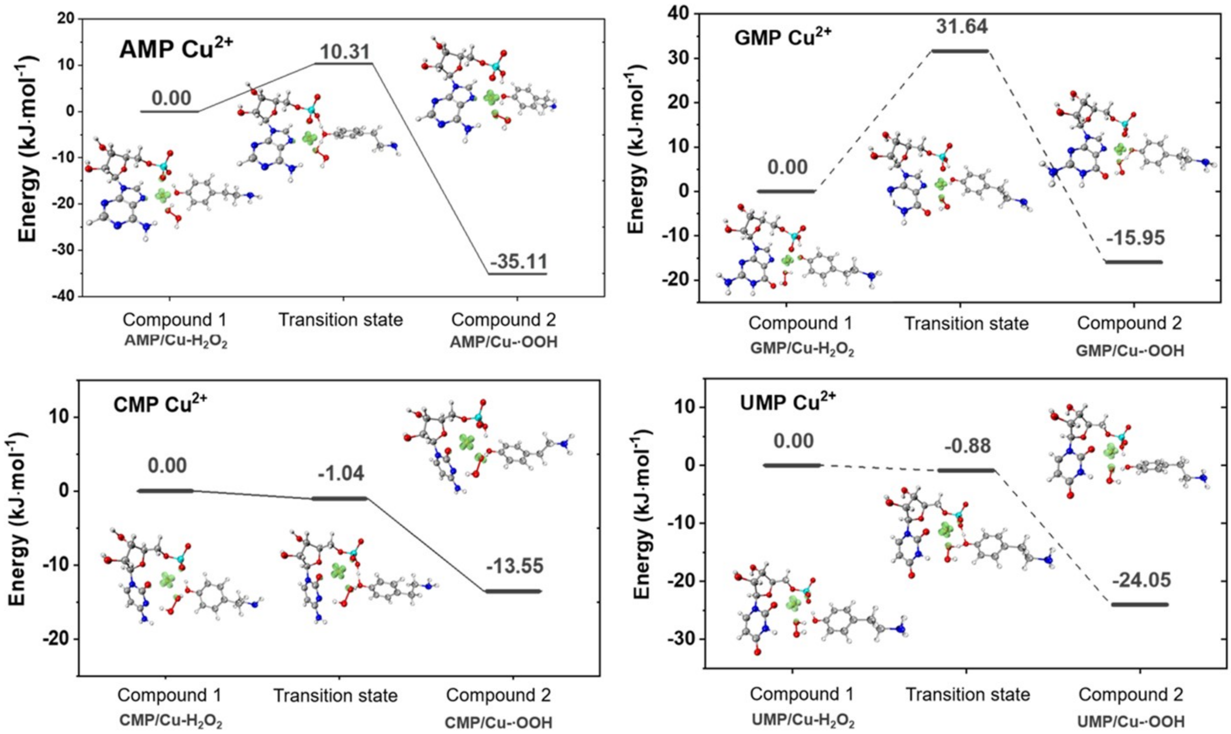


Figure S12 Active energy measurements of A/C/G/UMP and copper's catalytic reaction. [nucleotide] = 20 mM, [Cu^{2+}] = 50μM, H_2O_2 (1 mM), tyramine (1 mM).

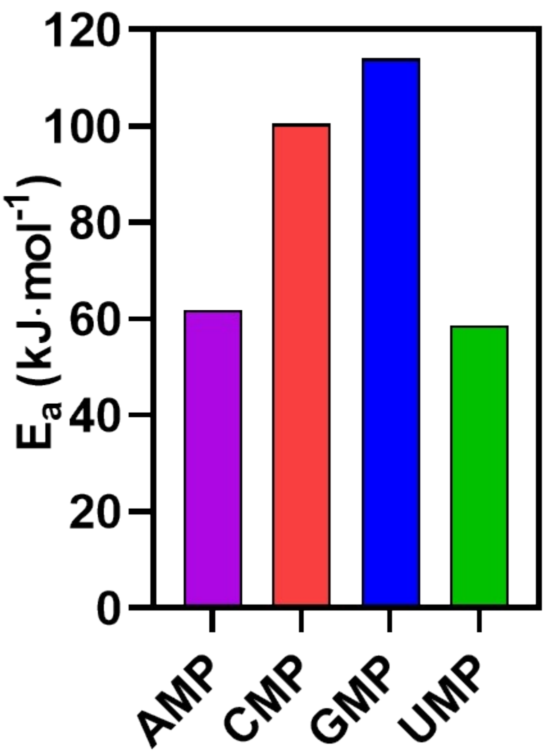


Figure S13 Deaeration effect on tyramine's oxidation reaction catalysed by Cu^{2+} and AMP. AMP (20 mM), Cu^{2+} (50 µM), H_2O_2 (5 mM), tyramine (1 mM). Insert was the initial reaction rate. The data were presented as the mean ± s.d., with the error bars representing the s.d. and N= 3.

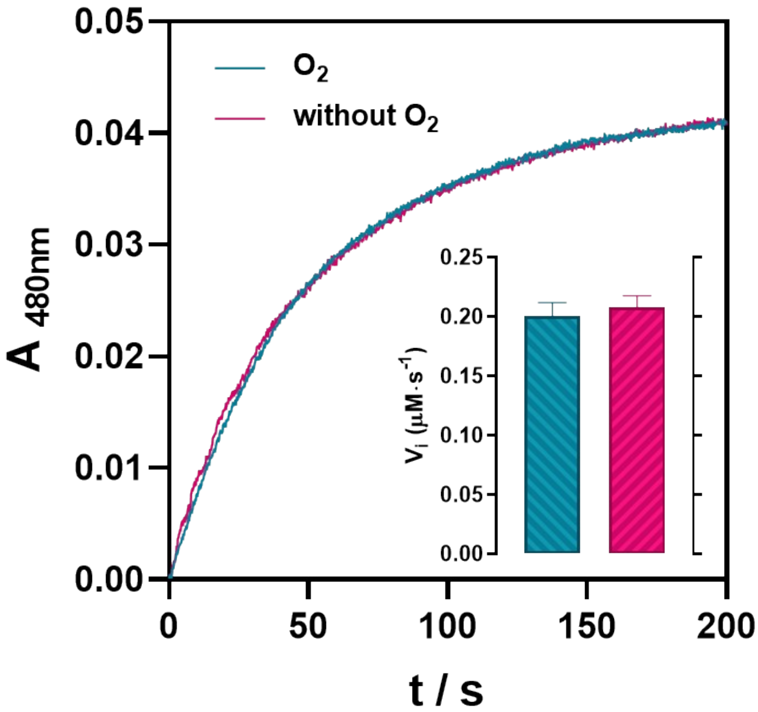


Figure S14 Proposal hydroxyl radical intermediate route.

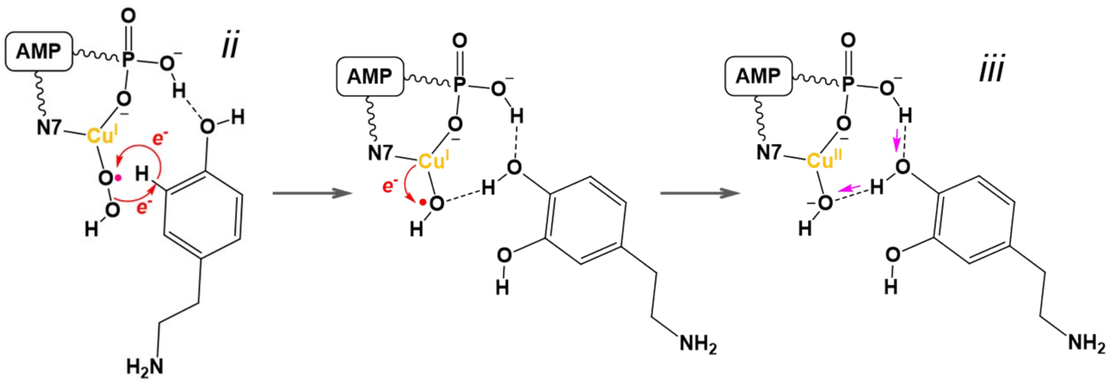


Figure S15 Comparison of DNA's and nucleotide's catalytic reactivity with Cu^{2+}. Cu^{2+} (50 Mm), H_2O_2 (5 mM), tyrosine (1 mM), nucleobase in nucleotides and ssDNA (20 mM). The data are presented as the mean ± s.d., with the error bars representing the s.d. and N= 3.

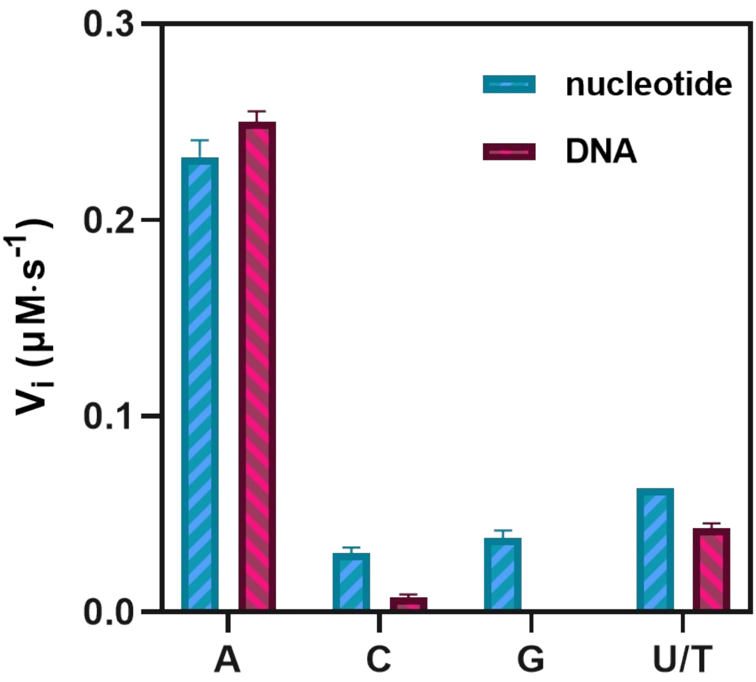


Figure S16 AMP concentration effect on the catalytic oxidation of tyramine. Cu^{2+} (50 μM), H_2O_2 (5 mM), tyramine (1 mM). The data are presented as the mean ± s.d., with the error bars representing the s.d. and N= 3.

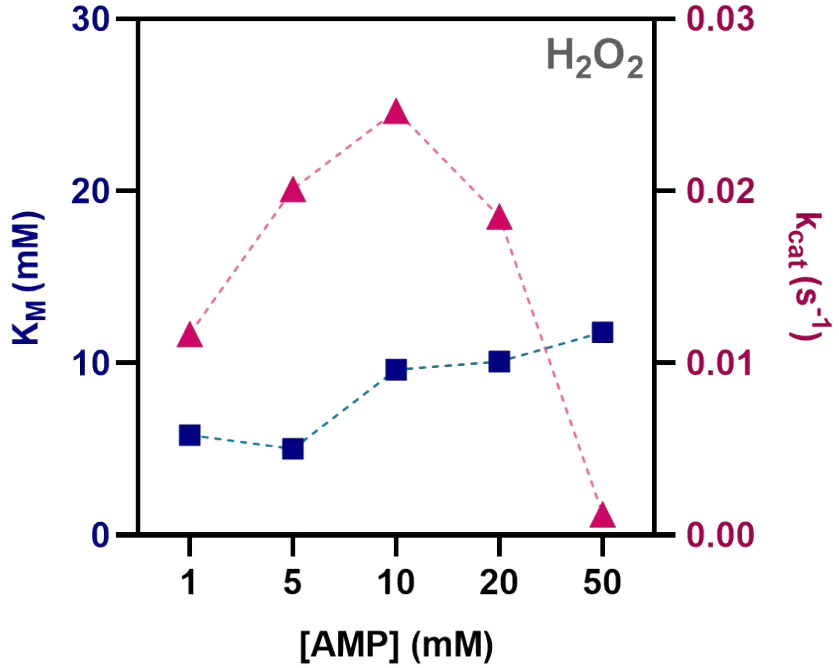


Figure S17 Oxidation of o-tert-butylphenol (A), dopamine (B) and tyrosine (C) catalysed by AMP/Cu^{2+}. AMP (2 mM), Cu^{2+} (100 μM), H_2O_2 (5 mM), tyrosine (1 mM), time interval (5 min).

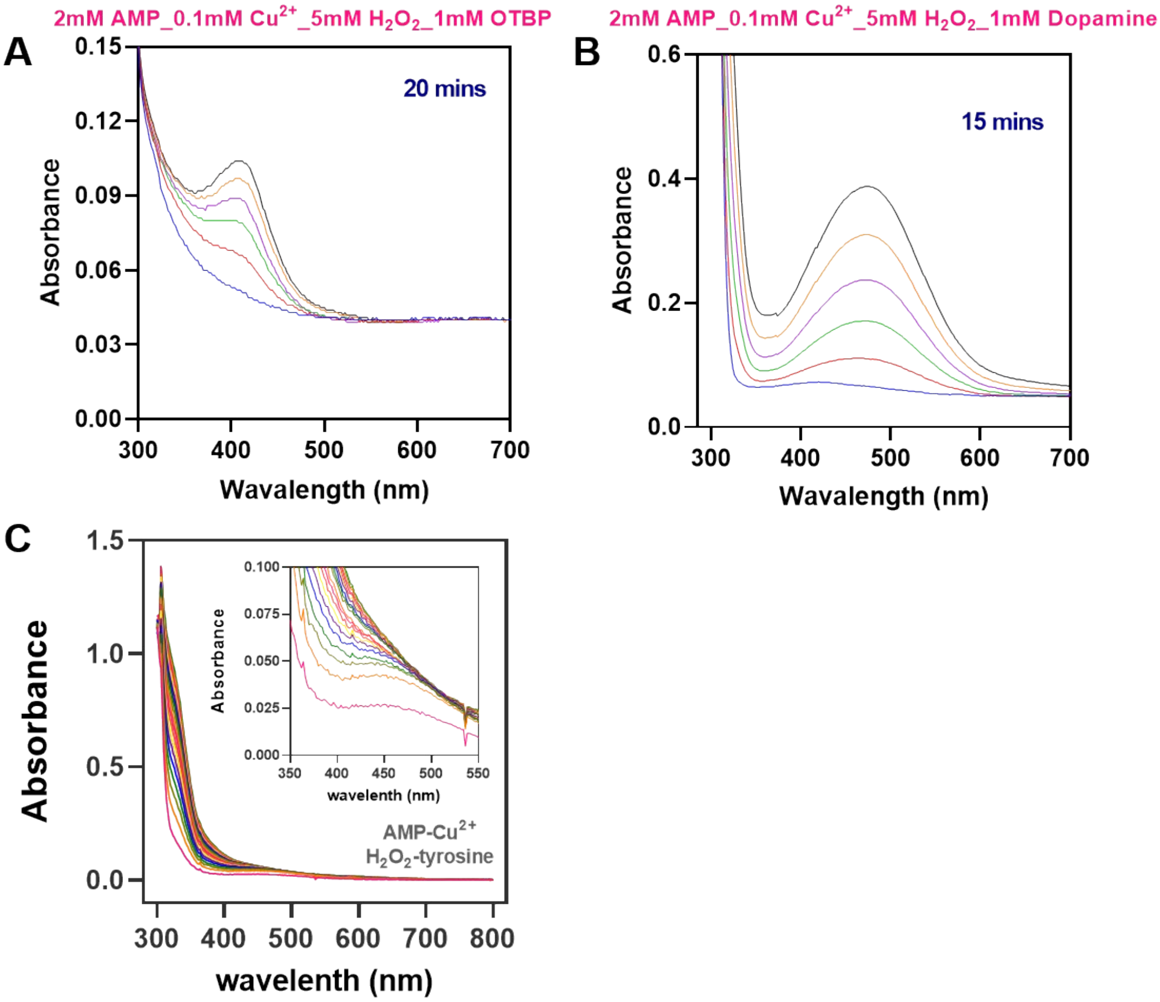


Figure S18 Temperature effect on oxidation of tyramine catalysed by AMP/Cu^{2+}, polyA20/Cu^{2+} and tyrosinase. AMP (20 mM), A20 (1 μM), Cu^{2+} (50 μM), H_2O_2 (1 mM), tyrosinase (10 μM), tyramine (1 mM). The data are presented as the mean ± s.d., with the error bars representing the s.d. and N = 3.

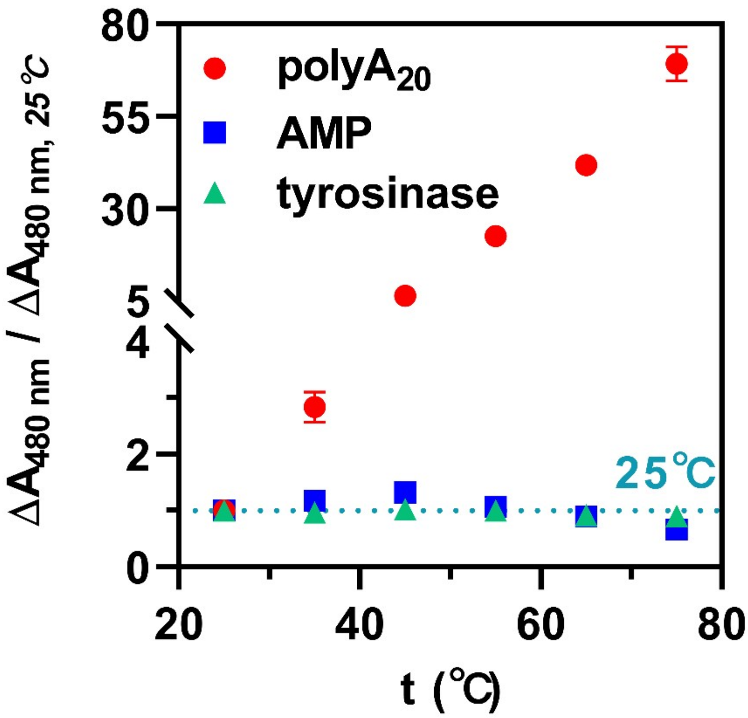


Figure S19 Temperature effect on oxidation of tyramine catalysed by AMP/Cu^{2+}, GMP/Cu2. polyG20 (1 μM), GMP (20 mM), Cu^{2+} (50 μM), H_2O_2 (1 mM), tyramine (1 mM). The data are presented as the mean ± s.d., with the error bars representing the s.d. and N = 3.

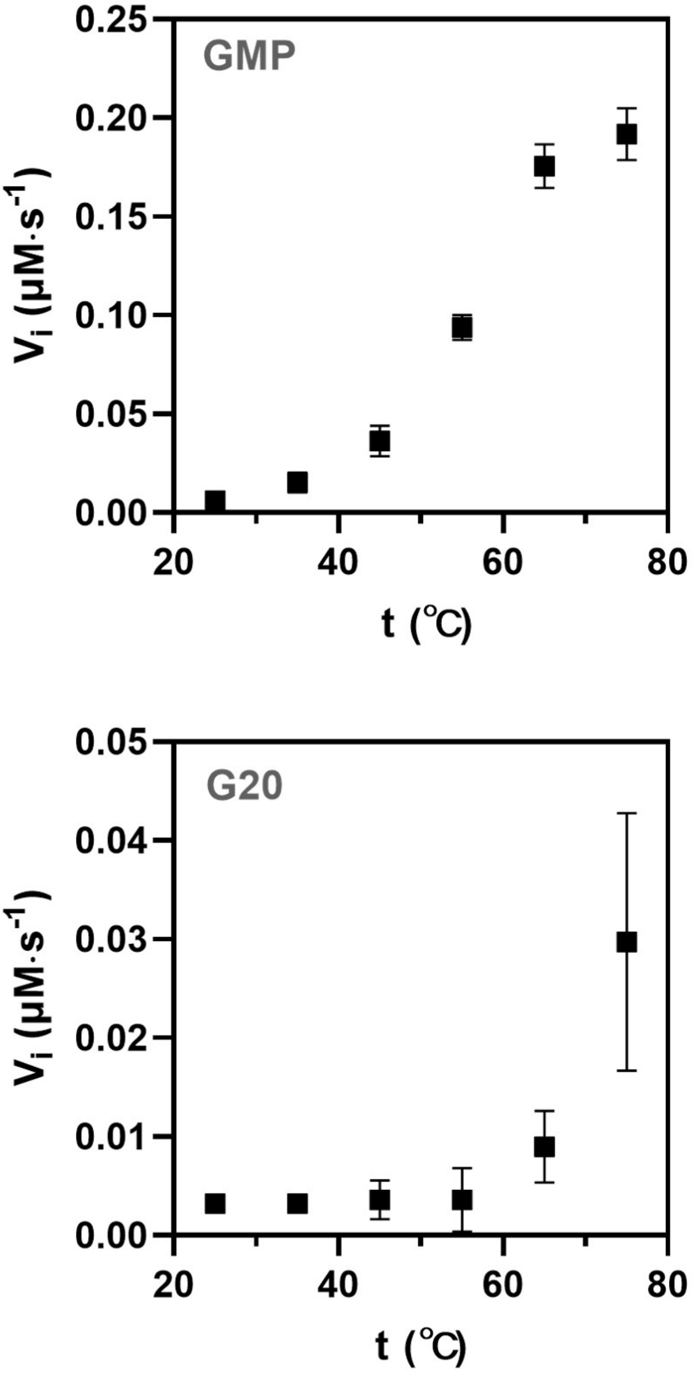


Figure S20 Oxidation of tyramine catalysed by Cu^{2+} and AMP/Cu^{2+} at different temperatures. [AMP] = 20 mM, [Cu^{2+}] = 50 μM, [tyramine] = 1 mM, [H_2O_2] = 1 mM.