Supporting information for

A novel NIR fluorescent probe for double-site and ratiometric detection of SO_2 derivatives and its application

Jianming Zhu[a], Fengyun Qin[a], Di Zhang[b*], Jun Tang[a], Wenya Liu[a], Wenbo Cao[c,*], Yong Ye[a,c]

[a] *Phosphorus Chemical Engineering Research Center of Henan Province, the College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou 450052, China.*
[b] *Institute of Agricultural Quality Standards and Testing Technology, Henan Academy of Agricultural Sciences, Zhengzhou 450002, China.*
[c] *School of Basic Medical Science, Zhengzhou University, Zhengzhou 450001, China*

[*] *Corresponding author; Email:* pandy811@163.com *(Di Zhang);* yeyong@zzu.edu.cn *(Yong Ye)*

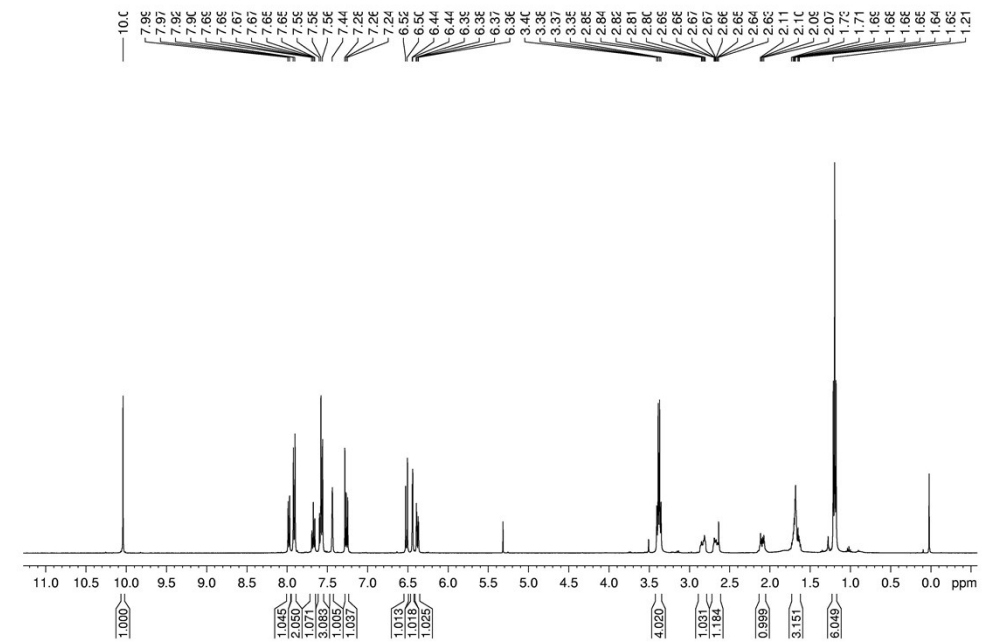


Fig. S1 ^{1}H NMR chart of probe **Q5** ($CDCl_3$, 400 MHz).

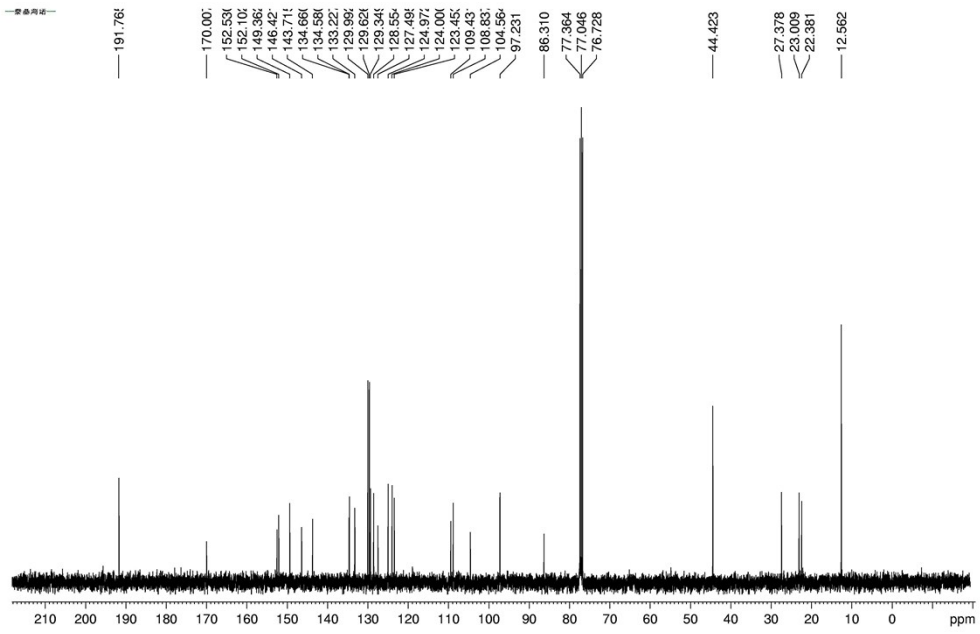


Fig. S2 ^{13}C NMR chart of probe **Q5** ($CDCl_3$, 100 MHz)

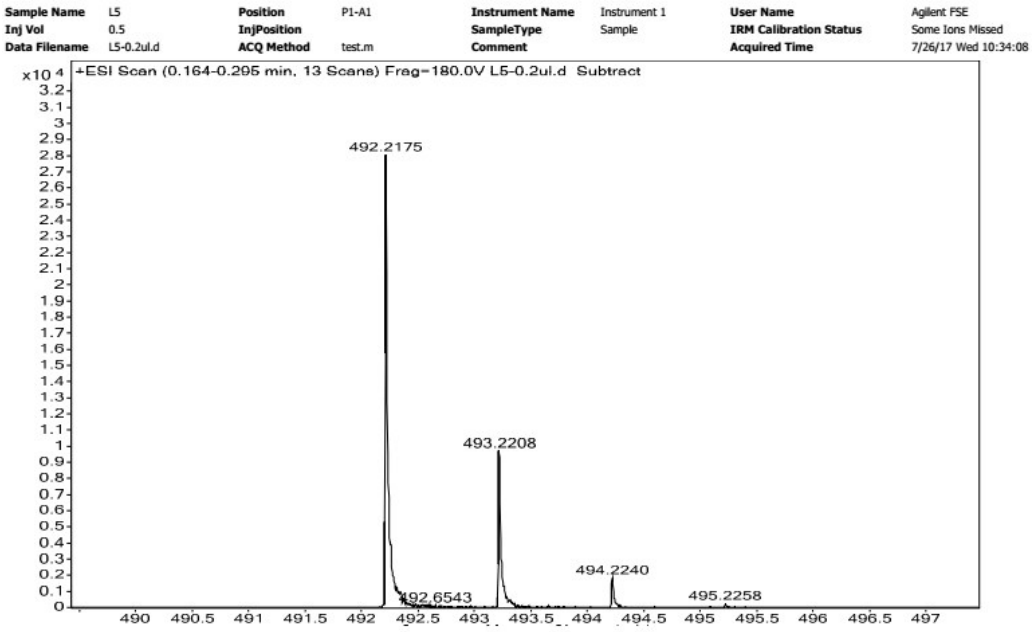


Fig. S3 ESI-HRMS spectrum of probe **Q5**.

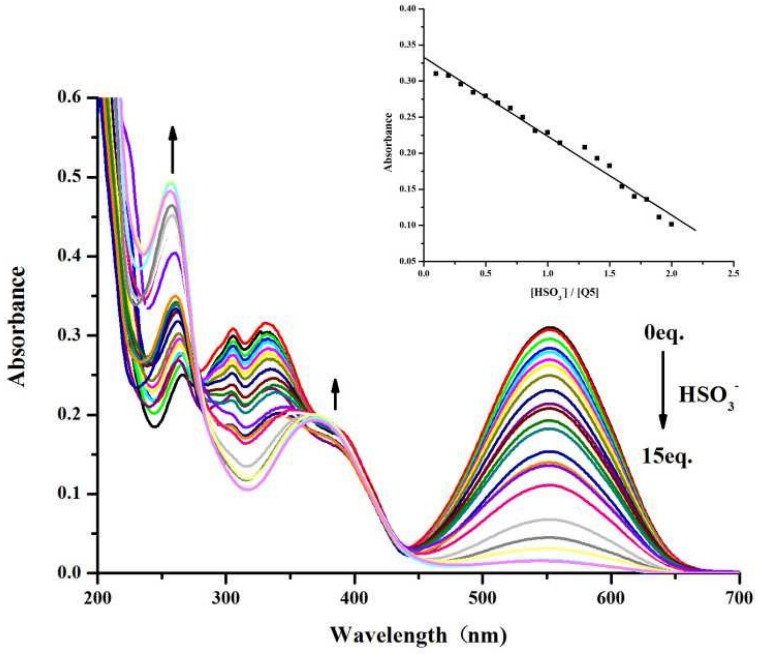


Fig. S4. Absorption spectra of **Q5** (10 μM) with gradual addition of various amounts of HSO_3^- (0-15 eq.) in MeOH/PBS buffer (3/7, v/v, 10 mM, pH = 7.40) solution. Inset shows linear relationship between the UV peak of the probe at 550 nm and HSO_3^- concentration.

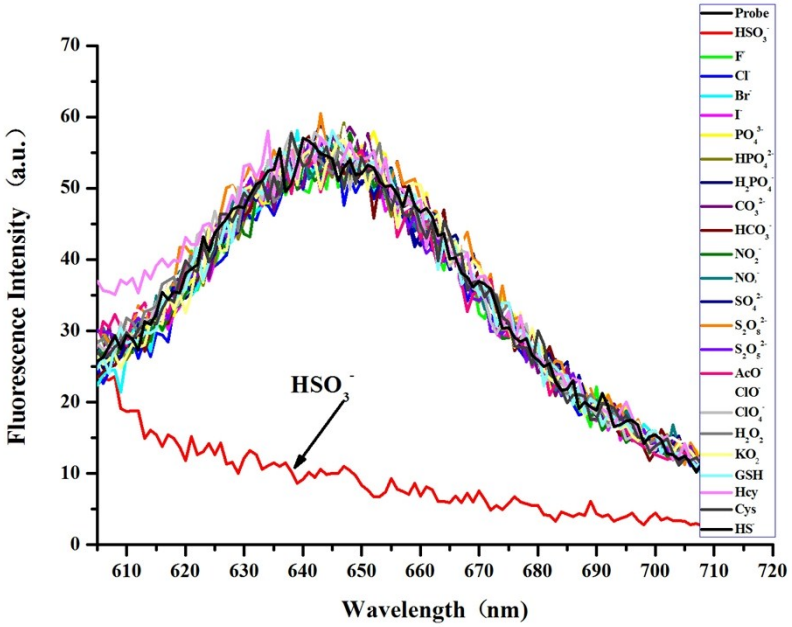
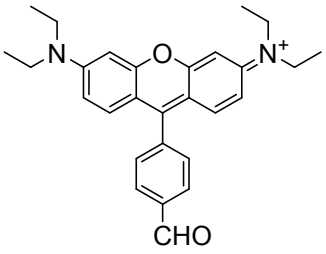
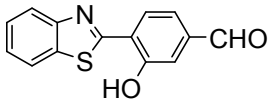
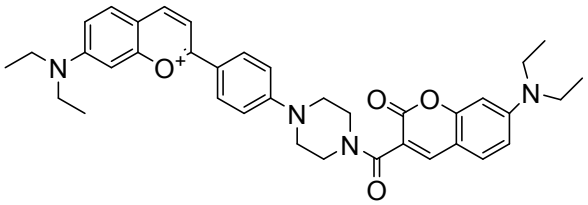
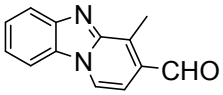
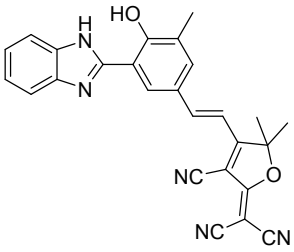
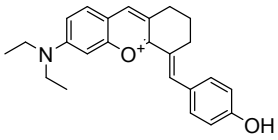
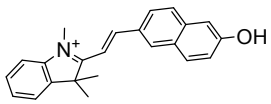
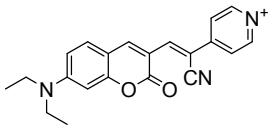
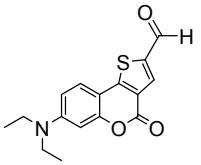
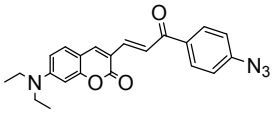
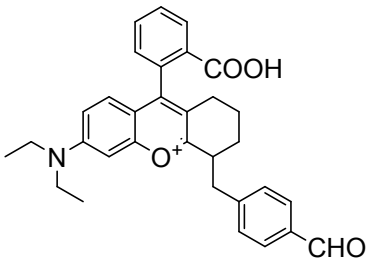


Fig. S5 Fluorescence intensity of probe **Q5** (10 μM) in the presence of 10 equiv different analytes in MeOH/PBS buffer (3/7, v/v, 10 mM, pH = 7.40) solution. (λ_{ex} = 580 nm).

Table S1 Reported fluorescent probes for the detection of HSO_3^-.

Ref	Probe structures	λex /λem	LOD (M)	Double-site
1		520 nm/ 580 nm	7× 10^{-8}	NO
2		377 nm/ 563 nm	3.3× 10^{-7}	NO
3		450nm/ 483 nm/633nm	1.7× 10^{-8}	NO
4		350nm/ 428/ 508nm	7× 10^{-7}	NO

5		400nm/ 483 nm	8.2× 10^{-7}	NO
6		570nm/ 650nm	1.2× 10^{-7}	NO
7		405nm/ 550nm	8.5× 10^{-7}	NO
8		550nm/ 630 nm	2.8× 10^{-6}	NO
9		385 nm/ 475 nm	2.3× 10^{-7}	NO
10		410 nm/ 460/ 590 nm	1.0× 10^{-7}	NO
Our Work		410 nm/ 485/ 650 nm	8.9× 10^{-8}	YES

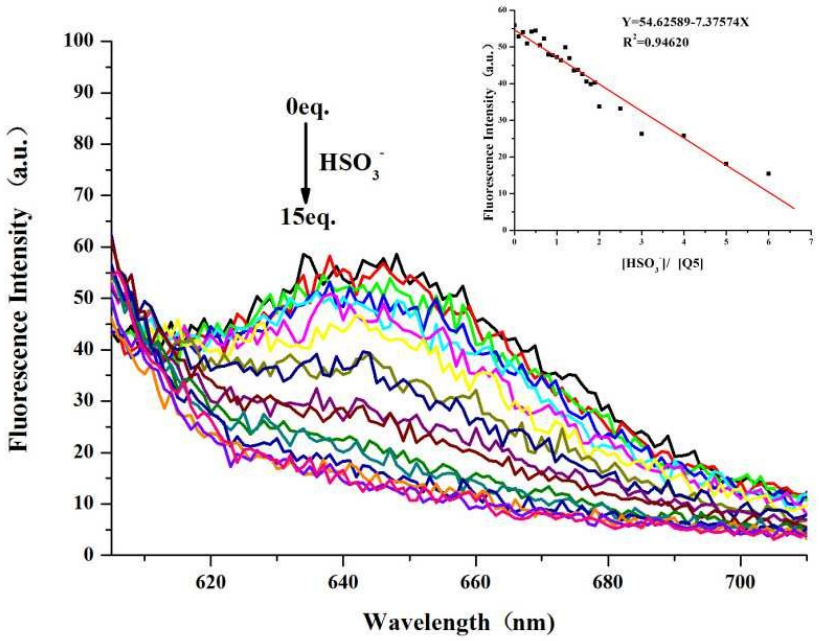


Fig. S6 Fluorescence emission spectra of compound **Q5** (10 μM) in the presence of different concentrations of HSO_3^- (0-15 equiv) in MeOH/PBS buffer (3/7, v/v, 10 mM, pH = 7.40) solution. Inset shows the linear responses with HSO_3^- concentrations (λ_{ex} = 580 nm).

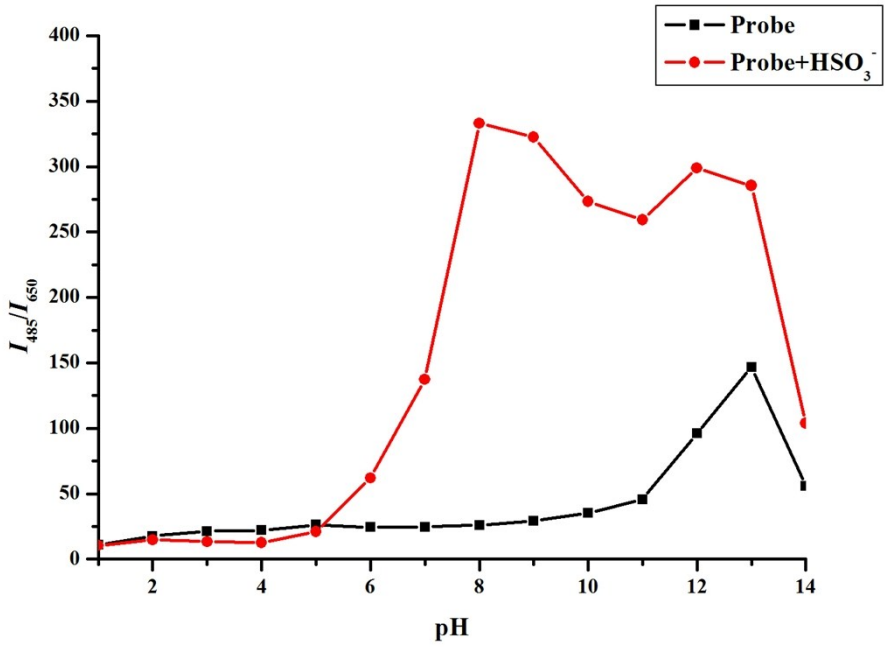


Fig. S7 The ratiometric fluorescence responses (F_{485}/F_{650}) of free **Q5** (10 μM) and in the presence of 10 eq. HSO_3^- in MeOH/PBS buffer (3/7, v/v, 10 mM) solution with different pH conditions (λ_{ex} = 410 nm, slit = 10 nm).

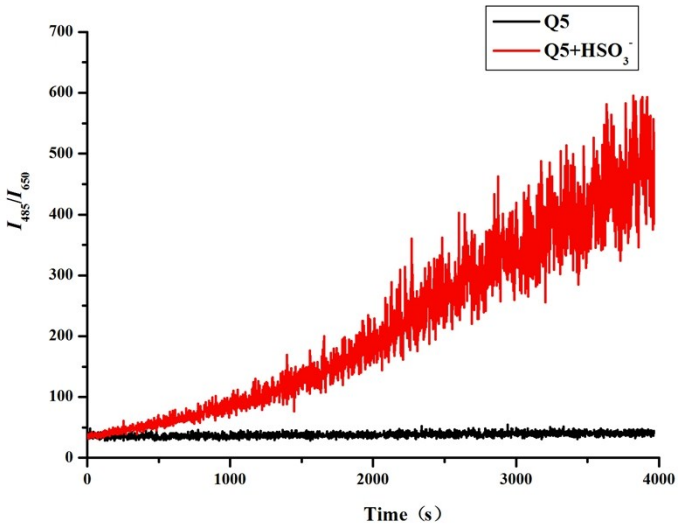


Fig. S8 Kinetics of fluorescence responses (F_{485}/F_{650}) of free **Q5** (10 μM) and after the addition of HSO_3^- (100 μM) in PBS (pH = 7.40, 10 mM, containing 30% MeOH). (λ_{ex} = 410 nm, slit = 10 nm).

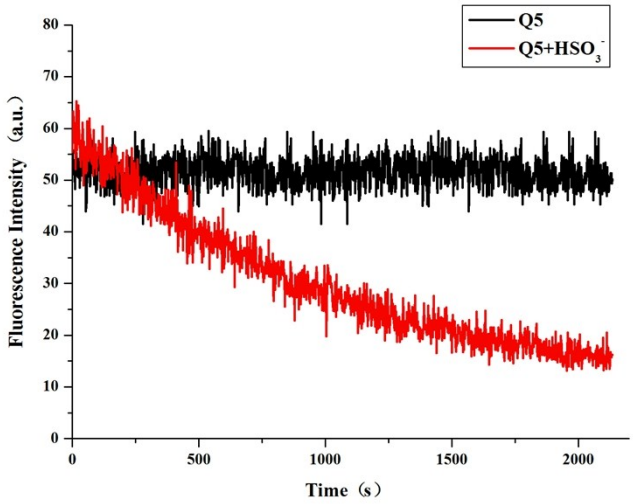


Fig. S9 Kinetics of the fluorescence responses (F_{650}) of **Q5** (10 μM) after the addition of HSO_3^- (100 μM) in PBS (pH = 7.40, 10 mM, containing 30% MeOH). (λ_{ex} = 580 nm, slit = 10 nm).

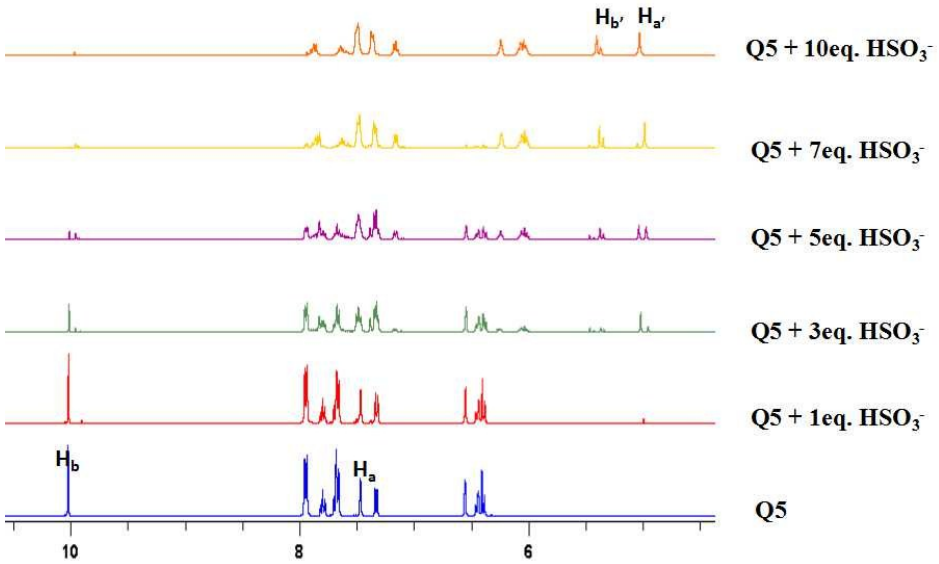


Fig. S10 The stack ^{1}H NMR spectrum of the mixture of probe **Q5** with different concentrations of HSO_3^- (0-10 equiv) in DMSO-d6.

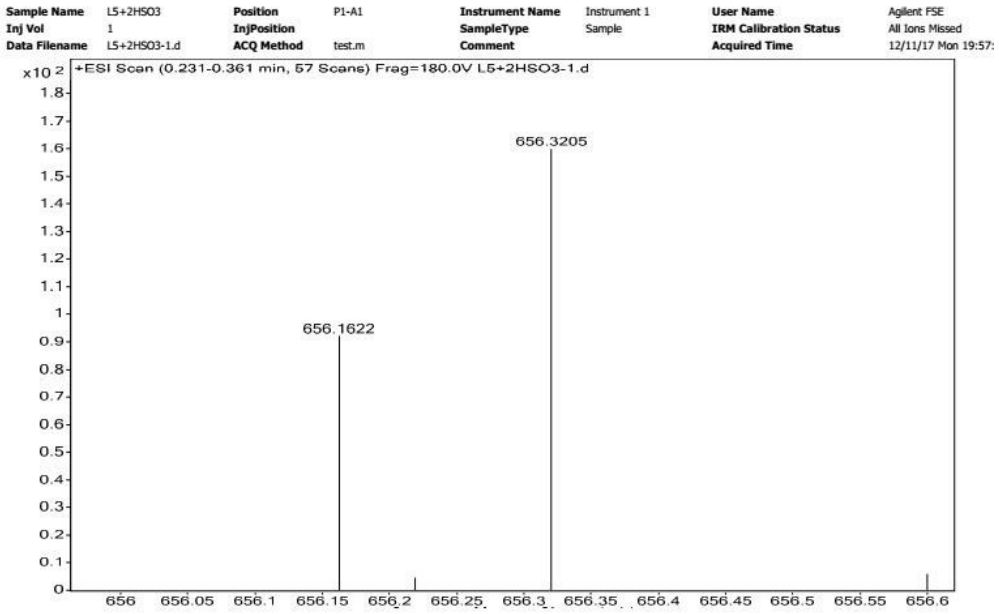


Fig. S11 ESI-HRMS spectrum of **Q5´**.

Reference

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