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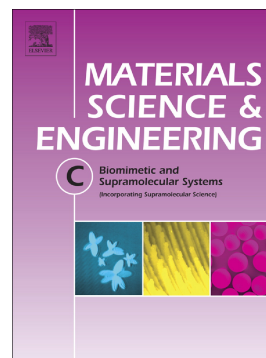
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PII: S0928-4931(17)33853-5  
DOI: doi:[10.1016/j.msec.2018.09.031](https://doi.org/10.1016/j.msec.2018.09.031)  
Reference: MSC 8894  
To appear in: *Materials Science & Engineering C*  
Received date: 29 September 2017  
Revised date: 28 July 2018  
Accepted date: 10 September 2018

Please cite this article as: A.R. Firooz, M. Movahedi, H. Sabzyan , A new selective optode for the determination of iron(III) based on the immobilization of morin on triacetylcellulose: A combined experimental and computational study. Msc (2018), doi:[10.1016/j.msec.2018.09.031](https://doi.org/10.1016/j.msec.2018.09.031)

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**A new selective optode for the determination of iron(III) based on the immobilization of morin on triacetylcellulose; A combined experimental and computational study**

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**Abstract**

Accurate and fast measurement of the iron ion in biological, pharmaceutical and medical samples is of great applied importance. In this work, a novel optical sensor (optode) for the Fe(III) ion is fabricated based on the immobilization of morin (2',3,4',5,7-pentahydroxyflavone) on a triacetylcellulose membrane. Chemical binding of the Fe(III) ion with the immobilized morin is monitored spectrophotometrically at 334 nm. The prepared optode shows excellent response over a wide range of concentrations from  $1.06 \times 10^{-10}$  to  $4.73 \times 10^{-5}$  M with a detection limit of  $4.23 \times 10^{-11}$  M Fe(III). Effects of the factors determining sensitivity of the optode are studied and optimized. The prepared optical sensor shows good selectivity toward the Fe(III) ion in the presence of a number of other metal ions. The developed sensor is applied successfully and satisfactorily for the determination of iron in three pharmaceutical, one plasma and two serum samples. In addition, concentration of the Fe(III) ion in two tap water samples are measured using standard addition method. Density functional theory (TD) B3LYP/6-311++G\*\* method is used to investigate structure and binding characteristics, and calculate the UV-Vis spectrum of the Fe(III)-morin complex.

**Keywords:** Fe(III) ion; Morin; Optode; Triacetylcellulose; iron(III) optical sensor; Serum iron; DFT

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