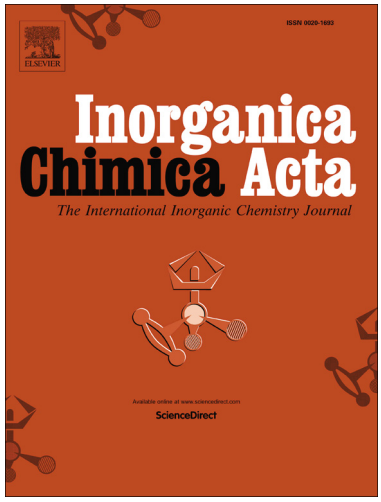

Research paper

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PII: S0020-1693(18)30498-5
DOI: https://doi.org/10.1016/j.ica.2018.06.004
Reference: ICA 18296

To appear in: *Inorganica Chimica Acta*

Received Date: 10 April 2018
Revised Date: 31 May 2018
Accepted Date: 3 June 2018

Please cite this article as: O.A. Varzatskii, A.V. Vologzhanina, V.V. Novikov, S.V. Vakarov, R.V. Oblap, Y.Z. Voloshin, Inhibition of DNA synthesis in the transcription system of Taq DNA polymerase by various iron and cobalt(II) tris-dioximate clathrochelates: *in vitro* study and X-ray structure of leader inhibitors, the carboxyl-terminated macrobicyclic complexes, *Inorganica Chimica Acta* (2018), doi: https://doi.org/10.1016/j.ica.2018.06.004

Inhibition of DNA synthesis in the transcription system of Taq DNA polymerase by various iron and cobalt(II) tris-dioximate clathrochelates: *in vitro* study and X-ray structure of leader inhibitors, the carboxyl-terminated macrobicyclic complexes†

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Abstract

A series of the iron and cobalt(II) mono- and bis-clathrochelates was *in vitro* tested in the transcription system of Taq DNA polymerase (DNAP), based on polymerase chain reaction. All these complexes were found to be micromolar transcription inhibitors, but only several clathrochelates with terminal biorelevant groups are inhibitors with IC_{50} in a low micromolar range from 5 to 40 μM. Highest *in vitro* inhibitory activity is observed for the iron(II) monoclathrochelates with two carboxyphenylsulfide substituents. Their monofunctionalized analog and *ortho*-, *meta*- or *para*-heterofunctionalized morpholine-containing complexes with the single carboxyphenylsulfide substituent showed a substantially less inhibitory activity. The former iron(II) monoclathrochelates are also more active inhibitors

† Other authors dedicate this paper to the memory of Prof. O. Varzatskii who suddenly passed away on 20 December 2017