# Fw: Article Review Request | BMS-MC-2019-78

From: Rajesh (rkht_2008@rediffmail.com)

To: sandeo24@yahoo.co.in

Date: Thursday, 1 August, 2019, 11:57 am IST

From: Nimra Amin <admin@bentham.manuscriptpoint.com>
Sent: Wed, 29 May 2019 22:41:11
To: rkht_2008@rediffmail.com
Subject: Article Review Request | BMS-MC-2019-78

Reference#: BMS-MC-2019-78

Submission Title: theoretical Study of interactions energies between residues of the active site of Hsp90 and the geldanamycin analogues using Quantum Mechanics/Molecular Mechanics (QM/MM) methods.

Dear Dr. Rajesh H. Tale,

Your name has been recommended as a potential reviewer for this submission which has been submitted for publication in Medicinal Chemistry. If you are interested to carry out this review, then please follow the instructions given below. We would appreciate if you could kindly complete this review within the next 2 weeks.

The submitted abstract is also inserted below, for your convenience. We are also sending you the link ( ) of the Instructions for Authors, from where you can get guidance about the scope of the journal and any other related matters to facilitate your review.

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**Abstract:**
(Hsp90) 90KDa heat shock proteins are molecular chaperone involved in process of cellular oncogenesis, hence its marked importance as a therapeutic target. An inhibitor of Hsp90 chaperone activity is the geldanamycin, a thready compound that has the power to bind to the binding of ATP in the N-terminal of Hsp90 domain site, however this reported in clinical trials hepatotoxic damage, which I pitting to its disuse. On the other hand, taking advantage that the geldanamycin joins successfully Hsp90, efforts have focused on the search for similar that they have the same or better effect and both exhibited lower effects than its predecessor, as it has been the case with the similar 17-AAG and 17-DMAG. In order to know the chemical factors influencing the growth or decay of the biological activity of such compounds have been evaluated different computational techniques such as docking and 3DQSAR, however it has not been considered in a quantitative way what happens within the active site represented in terms of interaction energy, as it has been evaluated in this work. To evaluate interaction energies found that the Lys58 is essential for the union of the analogs to the active site of Hsp90, and that the activity of these will depend on if these have on the C-11 position of the macrocycle a group of small and at the same time attractor of electrons, as it is reflected with the series C-11 hydroxy and methoxy C-11. Theses outcomes were supported with Quantum Similarity and reactivity indices using the Density Funtional Theory in order to understand the non-covalent stabilization in the active site for theses compounds.

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Best regards,

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