ABSTRACT

Rheumatoid arthritis (RA), an autoimmune disorder, has been on increase in the whole world including Pakistan. In this disease the self-antigens are recognized by the, its own immune system causing damage to joints and associated cartilages. The drugs used to treat include anti-rheumatics and anti-inflammatory used in combinations also result in various side effects. Corticosteroids have also been used to treat the disease but are associated with severe side effects. and The Current work was performed to design the analogues of anti-rheumatics followed by their screening for their potential to act as a new lead compounds as drug candidate. Amongst the 5 anti-rheumatics, including azathioprine (Aza), leflunomide (Lef), sulfasalazine (Sul), methotrexate (Met), hydroxychloquine (hChlo) 61 derivatives were designed by adding/substituting different modifying groups utilizing Chemsketch and from these 61 only 15 derivatives showed potential to act as possible drug derivatives. Out of 15 only 4 derivatives/ analogues have been selected as the most potential drug candidate because of their high number of interaction and low energy value (most stable) and higher drug likeness score. Moreover, much higher drug likeness score of hChlo-1, Met-2, Met-3 and Lef 10 compared to the standard (original) molecule means have less side effects than those of the standard and expected to serve as alternative drug to treat RA with least or negligible side effects.