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In silico Prioritization of some Tetrazole Chalcones for Anticonvulsant Activity

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Abstract: *In silico* predictions of molecules have quenched the thirst of drug discovery as it provides insight for the prioritization of the molecules for *in vivo* or *in vitro* pharmacological evaluations. Molecules for series **PTC_{1-7}** and **$CPTC_{1-7}$** were subjected for *in silico* biological activity predictions, partition coefficient predictions (pLog P) and ADME predictions using PASS server, mol-inspiration software and PreADMET software respectively. This gave biological activity score (BAS), ADME predictions and LogP predictions (pLog P) for anticonvulsant activity. The standard Log P required for anticonvulsant activities being +2.00, molecules were also prioritized based on this pLogP criteria. In the protocol for BAS prediction, clinically used anticonvulsant agents were included and similarly followed for Log P predictions. The protocol was thus validated by comparing the correlation between pLog P and BAS. Molecules were also prioritized using the above protocol. The BAS score for selected the first five prioritized molecules was in the range of 0.30-0.61, Memantine showed a BAS of 0.93, which was used as standard in the prioritization protocol. The molecules $CPTC_3$ showed a BAS of 0.61 as compared with Memantine with BAS of 0.93. **PTC_3, PTC_2, PTC_1,$CPTC_2$, $CPTC_3$, & $CPTC_4$** can serve is an *in silico* lead and outcome of *in silico* virtual screening for BAS predictions with ADME property & pLog P prioritization. Thus molecules were prioritized for anticonvulsant activity.

Keywords: chalcones, In silico, BAS,PASS.

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