The process commenced with the reaction between indole acetic acid and hydrazine, yielding the hydrazide.Nevertheless, this computer–aided drug design tool is crucial in the optimization of lead or ligands, thereby impro ving the process of drug design and development while unveiling the novel molecular pathways.Follo– wing this, the intermediate underwent a displacement reaction with various hydrazine derivatives and aromatic amino reagents, yielding the final indolyl triazoles (IT1–8).The purity of the synthesized compounds was confirmed using TL.C, employing a mobile phase consisting of ethyl acetate, n–hexane and methanol.Thus, PASS predicted promising pharmaco logical potential for the synthesized indolyl triazole compounds (IT1–8) particularly in antitubercular and anticancer contexts.Mass spectra analysis additionally con firmed the successful synthesis by verifying the existence of expected fragments of the molecular ion peak (M^{l}).It is significant that the 20 molecular structure determines the prediction of activity spectra for compounds; hence, the accuracy of the computation is not certain to be 100% regarding bioactivity.Subsequently, the hydrazide underwent a reaction with CS2 under basic conditions, leading to the form– ation of an indolyl oxadiazole thiol intermediate.Moreover, unique peaks were detected in both IR and NMR spectra, indicating their structural integrity conclusively.Table–1 displays the PASS profiles, derived from a large training dataset containing 60,000 bioactive compounds with 4,500 unique mechanisms and activities.At first, it was anticipated that all the substances would show anti–tuberculosis and anti–mycobacterial effects with Pa values near 0.5 and none of the compounds com were proj– ected to have antibacterial abilities.This sequential process facilitated displacement and cyclization reactions, ultimately resulting in the generation of the intermediate.Figt shows the anticipated bioactivity scores for all the synthesized compounds using Molinspiration.These results highlight the possibilty of swing compounds IT1 and 172 as GIR Hepatah and enryone tsahitors.The likelihood of specific activities is indicated by the calculated probabilities (Pa and Pi).However, the experimental results disagreed with these predictions, revealing significant antibacterial effects.It also facilitates the identifica tion of potential new leads through high–.throughput screening of compound series