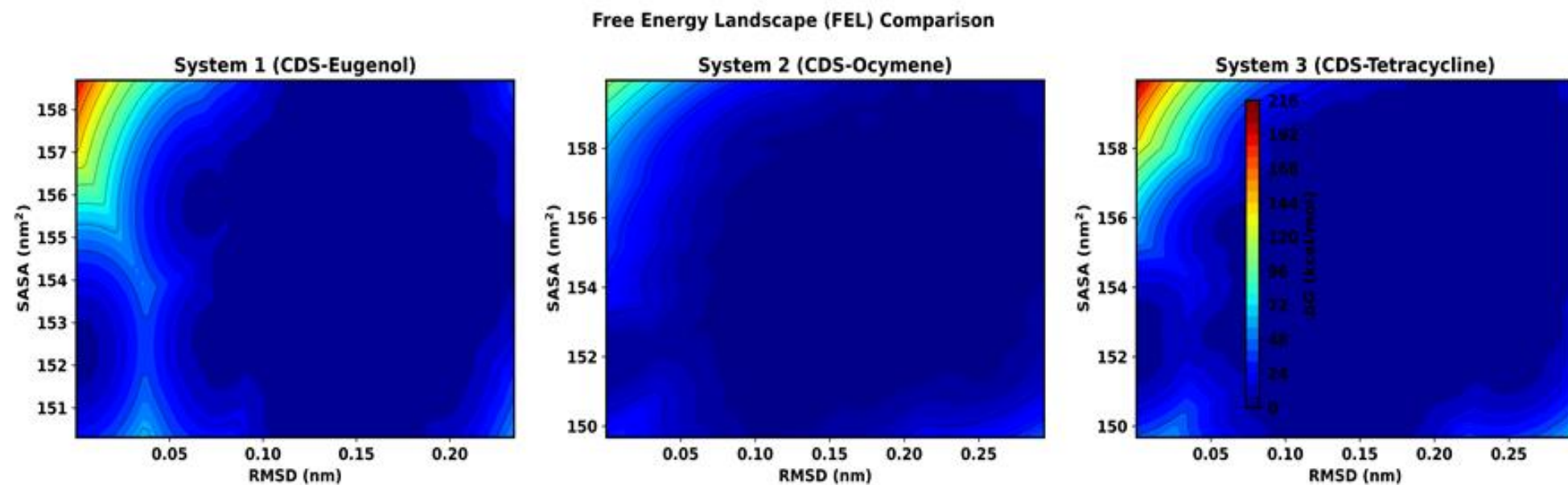
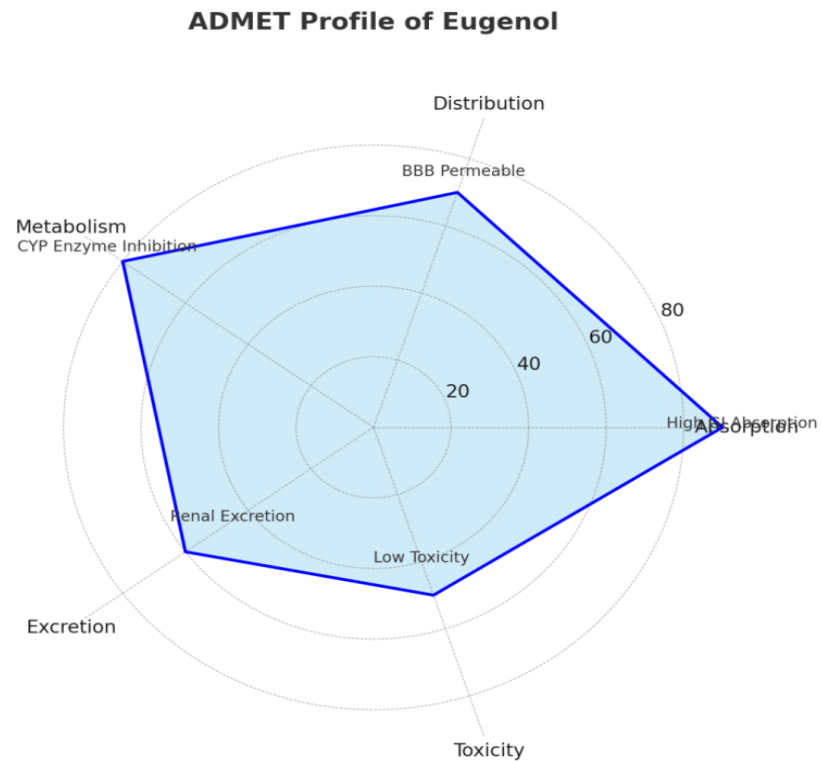


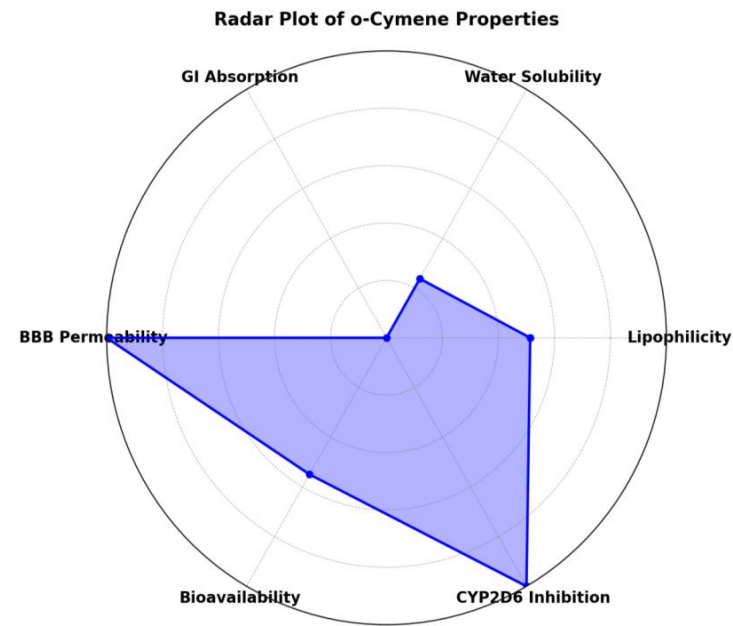


Supplementary Figure S1. Two-dimensional FEL (2D-FEL) of CDS in complex with Eugenol, o-Cymene, and Tetracycline, constructed using RMSD and SASA as reaction coordinates

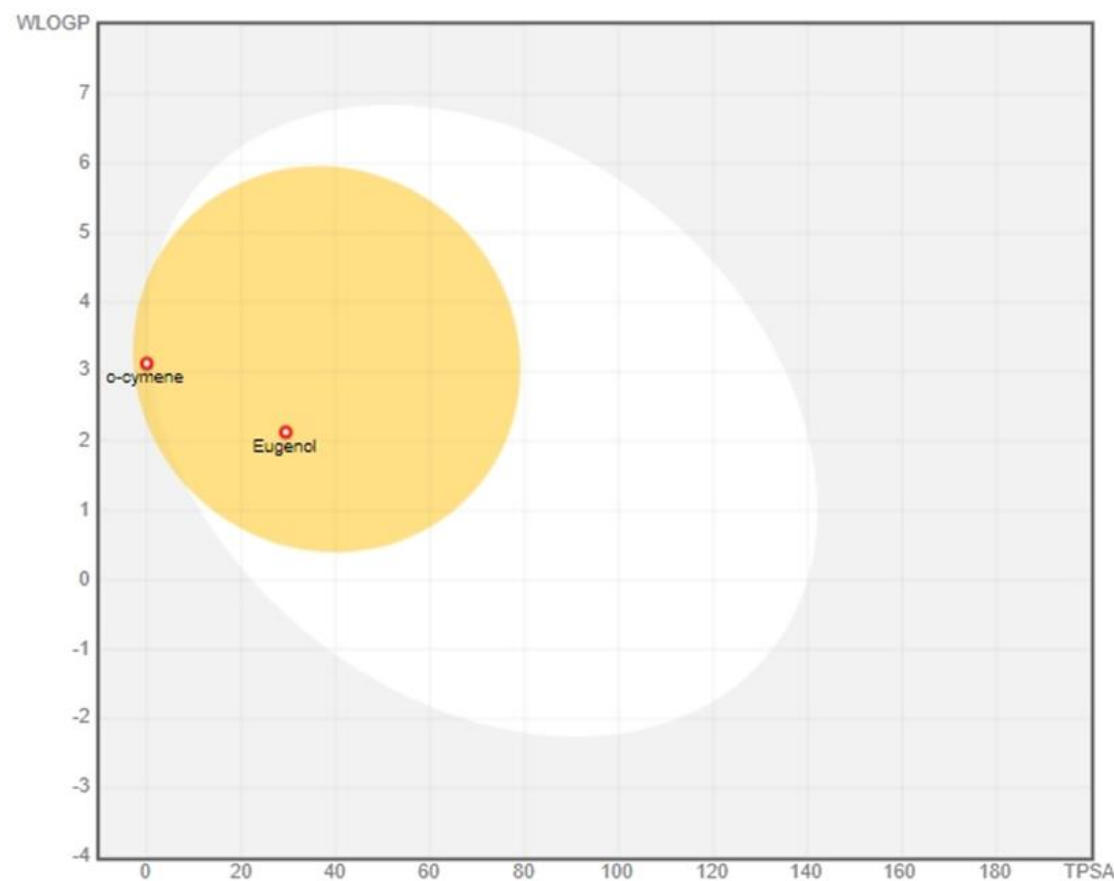
(a)



(b)



Supplementary Figure S2. Radar plot visualizing the ADMET profile of (a) eugenol and (b) o-Cymene highlighting key properties such as absorption, distribution, metabolism, excretion, and toxicity



Supplementary Figure S3. Boiled egg plot predicting GI absorption, blood-brain barrier permeation. The yellow region indicates the optimal area for blood-brain permeation, the white region represents GI absorption, and the red dots indicate that all compounds are not P-gp substrates.