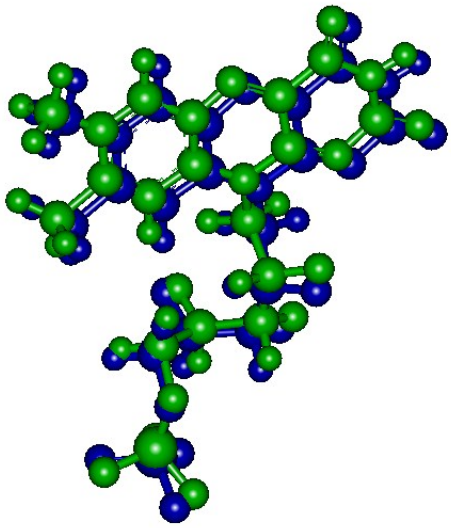
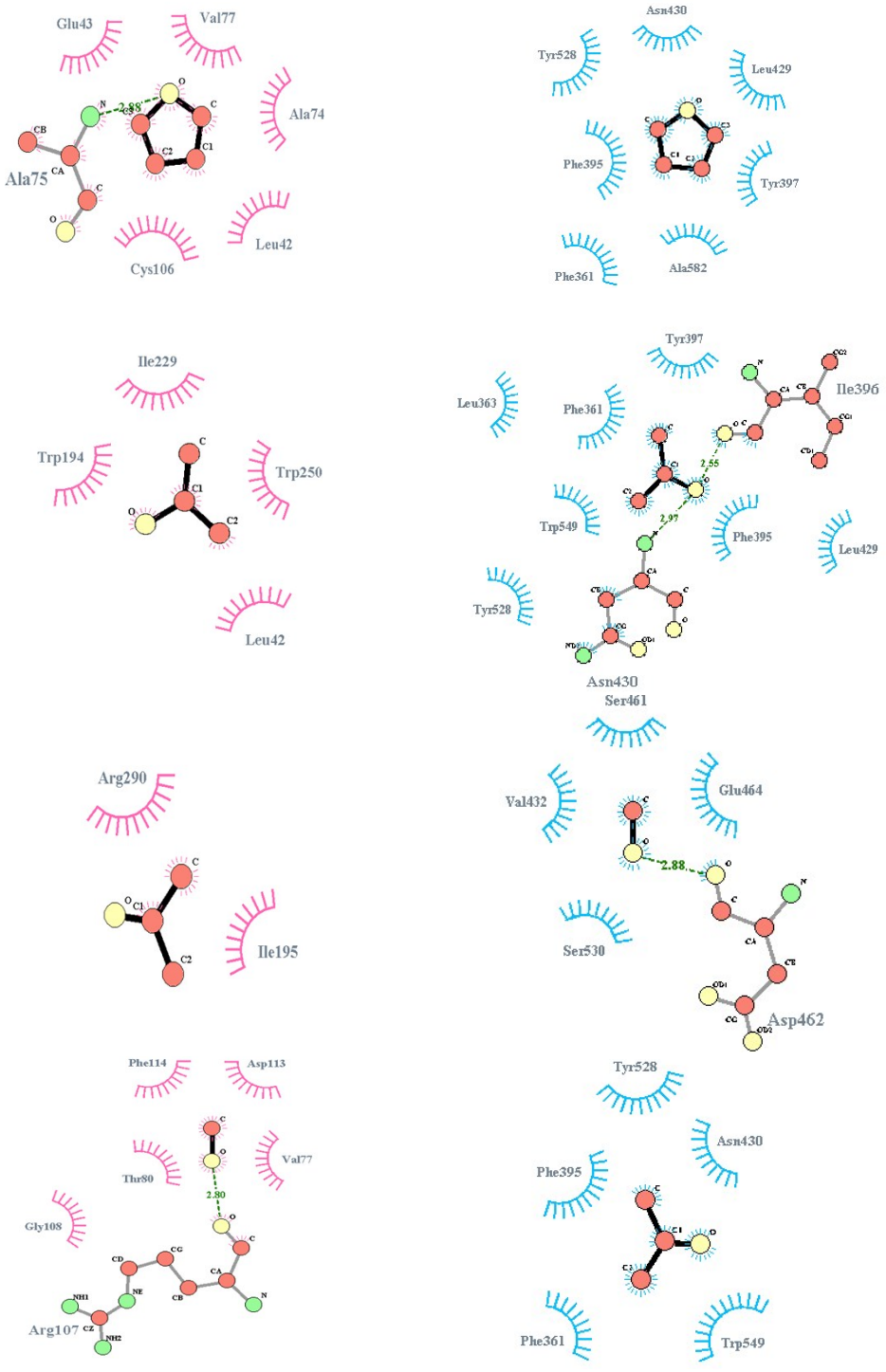
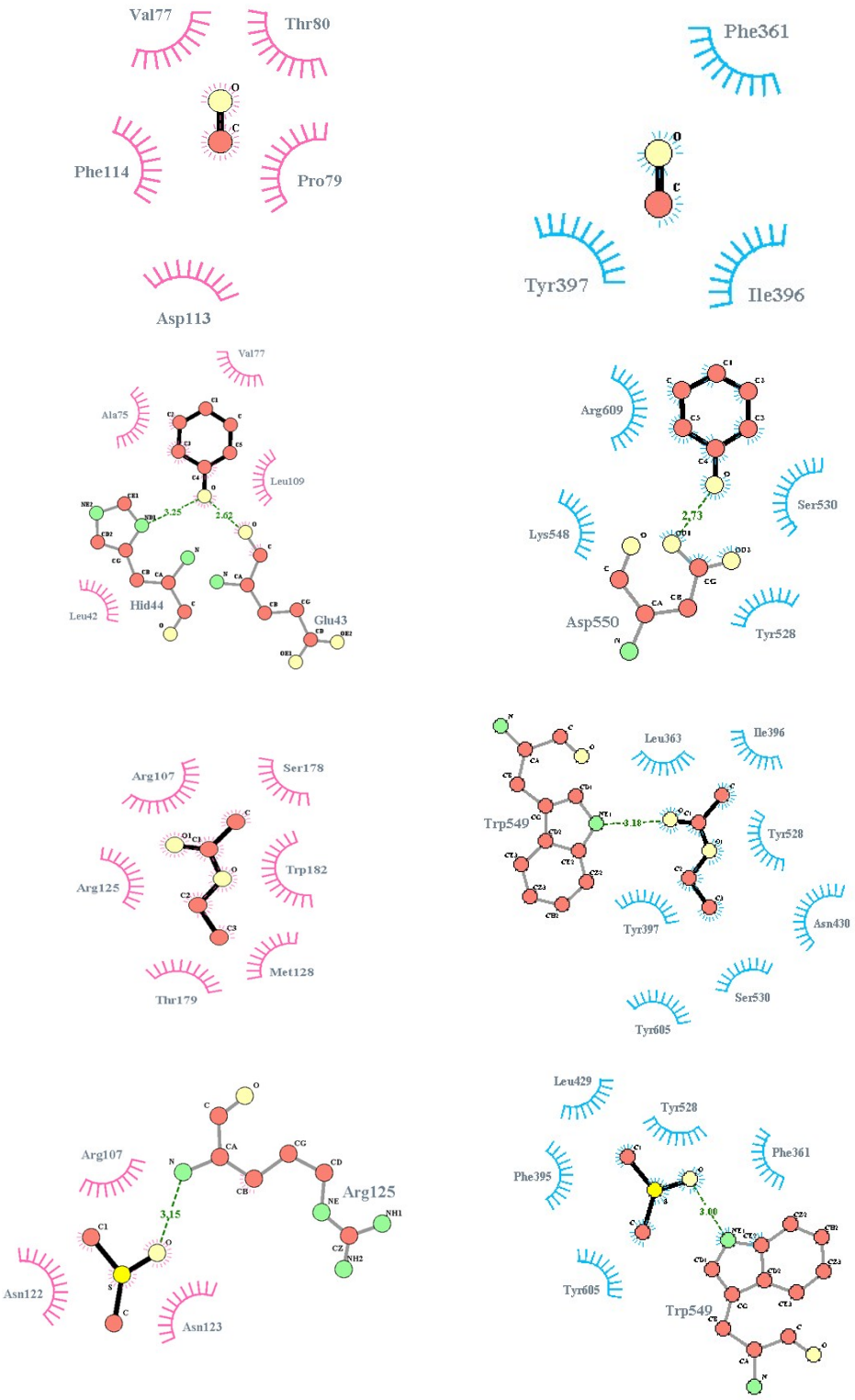


Fig. S1 The FMN overlay between the best Amber score conformation (green color) and original conformation (blue color).



a b

Fig. S2 (a) Hydrogen bond interaction patterns and hydrophobic contacts between four J-shaped organic solvents (THF, isopropanol, acetone, methanol from top to bottom) and the side chain and backbone of binding residues in Q67Lucα, where the hydrogen bond contact is expressed by green lines and hydrophobic contact groups are expressed by eyelash shaped curve. (b) Hydrogen bond interaction patterns and hydrophobic contacts between four J-shaped organic solvents and the side chain and backbone of binding residues in Q67Lucβ.



(a) (b)

Fig.S3 (a) Hydrogen bond interaction patterns and hydrophobic contacts between four S-shaped organic solvents (formaldehyde, phenol, EAC, DMSO from top to bottom) and the side chain and backbone of binding residues in Q67Lucα, where the hydrogen bond contact is expressed by green lines and hydrophobic contact groups are expressed by eyelash shaped curve. (b) Hydrogen bond interaction patterns and hydrophobic contacts between four S-shaped organic solvents and the side chain and backbone of binding residues in Q67Lucβ.

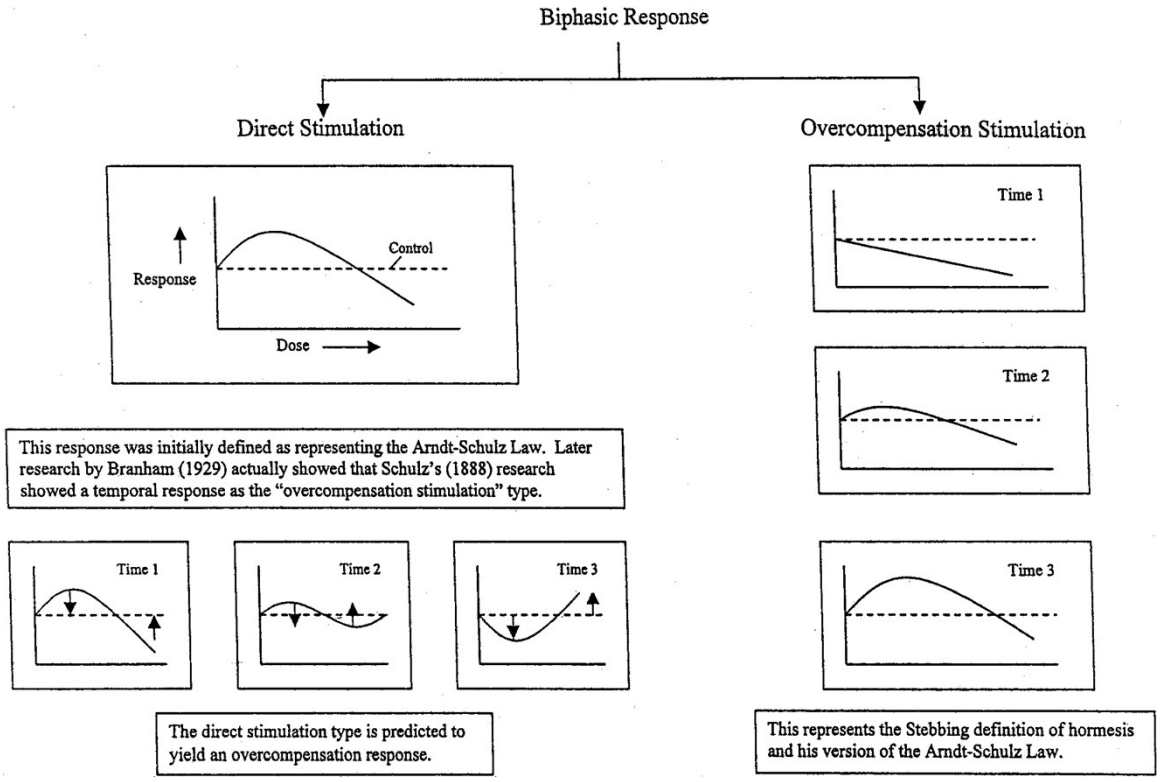


Fig. S4 Comparison of direct stimulation and overcompensation stimulation hormesis (from Calabrese and Baldwin[53])