Electronic Supplementary Information

Comprehensive Theoretical Insights on Spectroscopic Characterization, Solvent Effect (Polar and Nonpolar) in Electronic behavior, Topological Insights, and Molecular Docking Prediction of Taurolidine

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Supplementary Figures

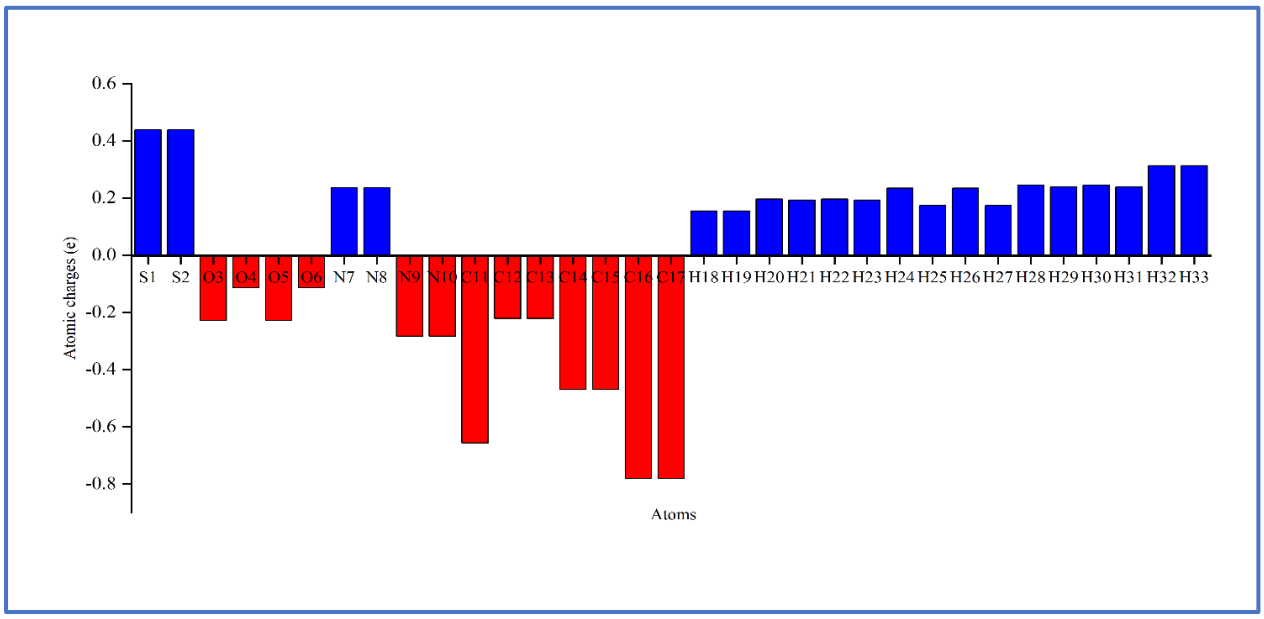
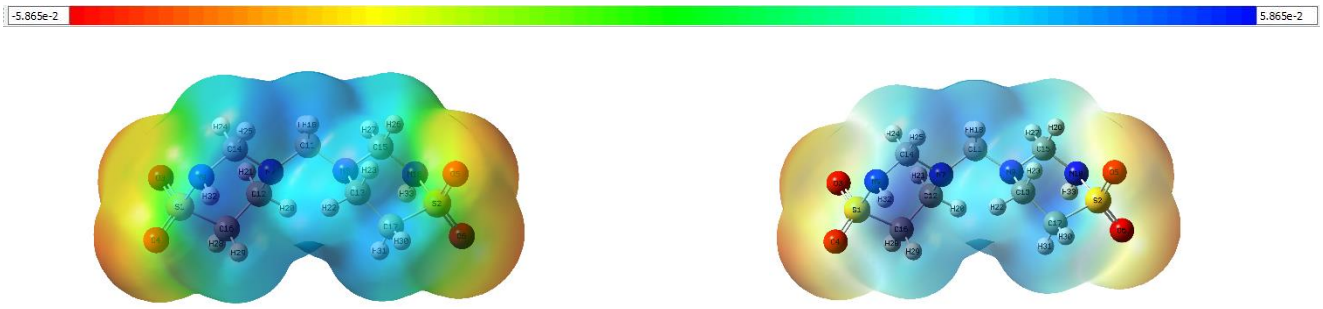
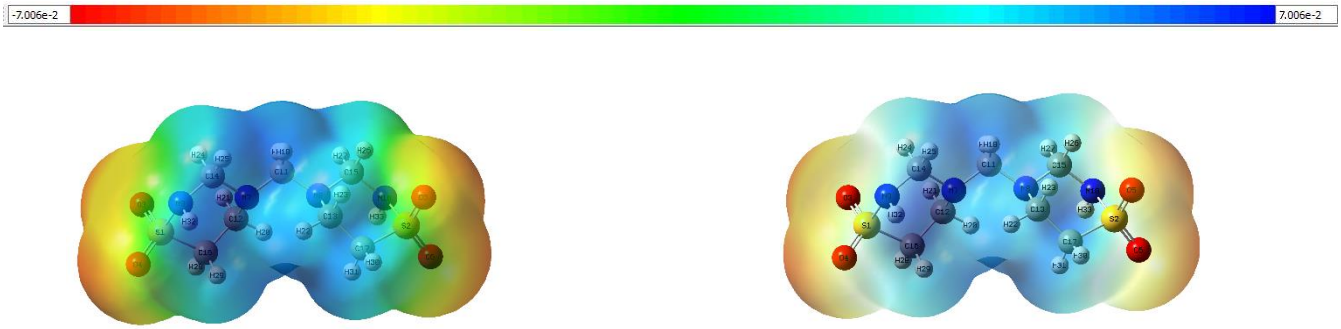


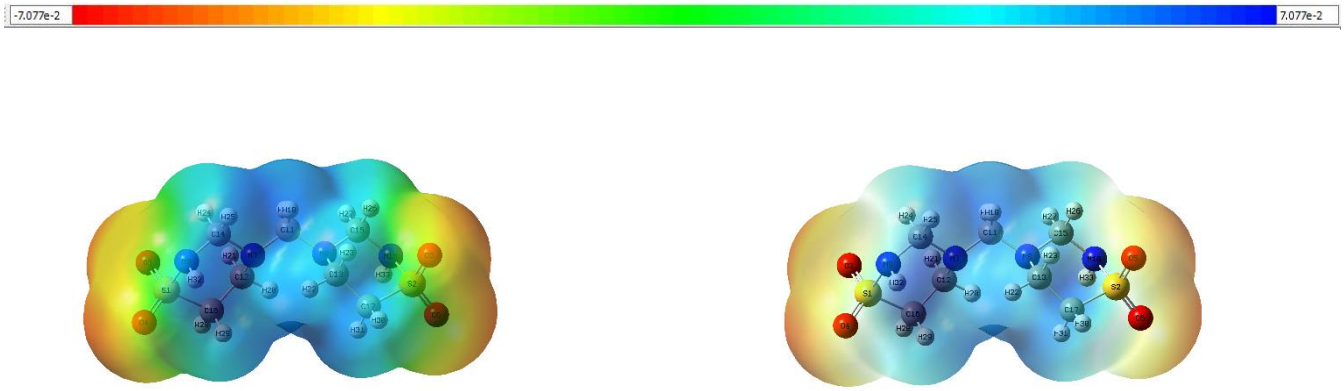
Fig. S1. Mulliken charge distribution of taurolidine



Gas



Ethanol



Water

Fig. S2(a). electrostatic potential surfaces of taurolidine in the gas phase and polar solvents

Chloroform

Toluene

Fig. S2(b). electrostatic potential surfaces of taurolidine in the nonpolar solvents

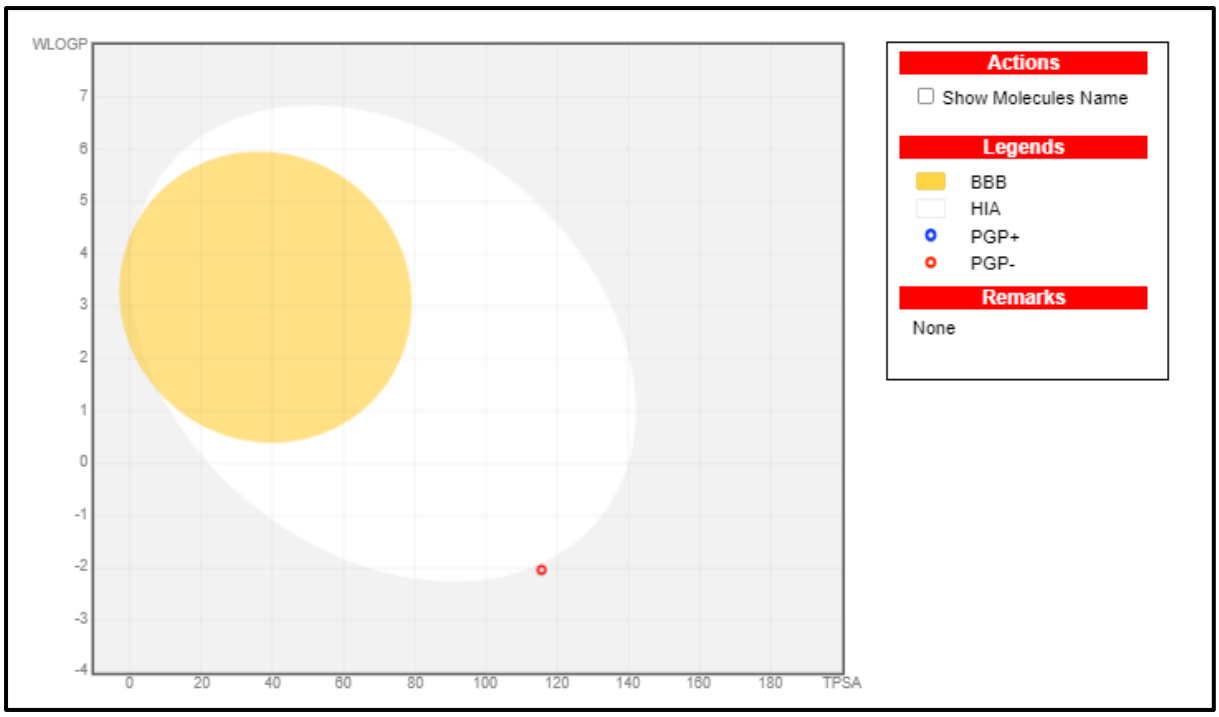


Fig. S3(a). Boiled egg diagram of taurolidine

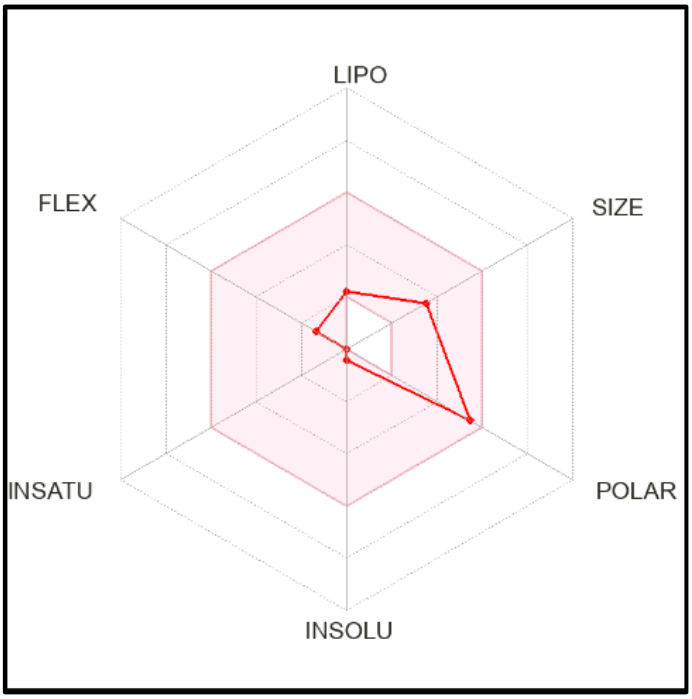


Fig. S3(b). Bioavailability radar of taurolidine

Supplementary tables

Table S1: The ADME prediction of taurolidine

Parameters	**2TFBZ**	**Parameters**	**2TFBZ**
Formula	$C_7H_{16}N_4O_4S_2$	CYP1A2 inhibitor	No
Molecular weight	284.36 g/mol	CYP2C19 inhibitor	No
Number of heavy atoms	17	CYP2C9 inhibitor	No
Number of aromatic heavy atoms	0	CYP2D6 inhibitor	No
Fraction Csp^3	1.0	CYP3A4 inhibitor	No
Number of rotatable bonds	2	LogKp (skin permeation)	-9.21 cm/s
Number of hydrogen bond acceptors	8	**Drug-likeness**	
Number of hydrogen bond donors	2	Lipinski	0
Molear refrectivity	76.52	Ghose	1
TPSA	115.58 $Å^2$	Veber	Yes
Lipophilicity		**Medicinal Chemistry**	
$LogP_{o/w}$	0.36	PAINS	0
Water solubility		Brenk	0
Log	-0.43	**Leadlikeness**	Yes
Solubility	1.05xE+02 mg/ml	**Synthetic Accessibility**	3.39
Absorption		**Bioavailability Score**	0.55
GI	Low		
Distribution			
BBB permeation	No		
P-gp substrate	No		