

Electronic Supplementary Information

Computational study on the Structural and Spectroscopic Properties, Solvent Effects, Topological Insights, and Biological Activities of 2-[1-(2, 4-dichlorobenzyl)-1H-indazol-3-yl] Propan-2-ol as an Anticonvulsant Drug

J. Jenifer ^a, A. Ram Kumar ^b, S. Selvaraj ^{a,*}

^a Department of Physics, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences (SIMATS), Chennai, 602105, Tamil Nadu, India.

^b Department of Biotechnology, Saveetha School of Engineering, Saveetha Institute of Medical and Technical Sciences (SIMATS), Chennai, 602105, Tamil Nadu, India.

*Corresponding Author Email: sselvaphy@gmail.com

Received:16-12-2024; Revised:11-03-2025; Accepted: 22-03-2025; Published: 30-03-2025

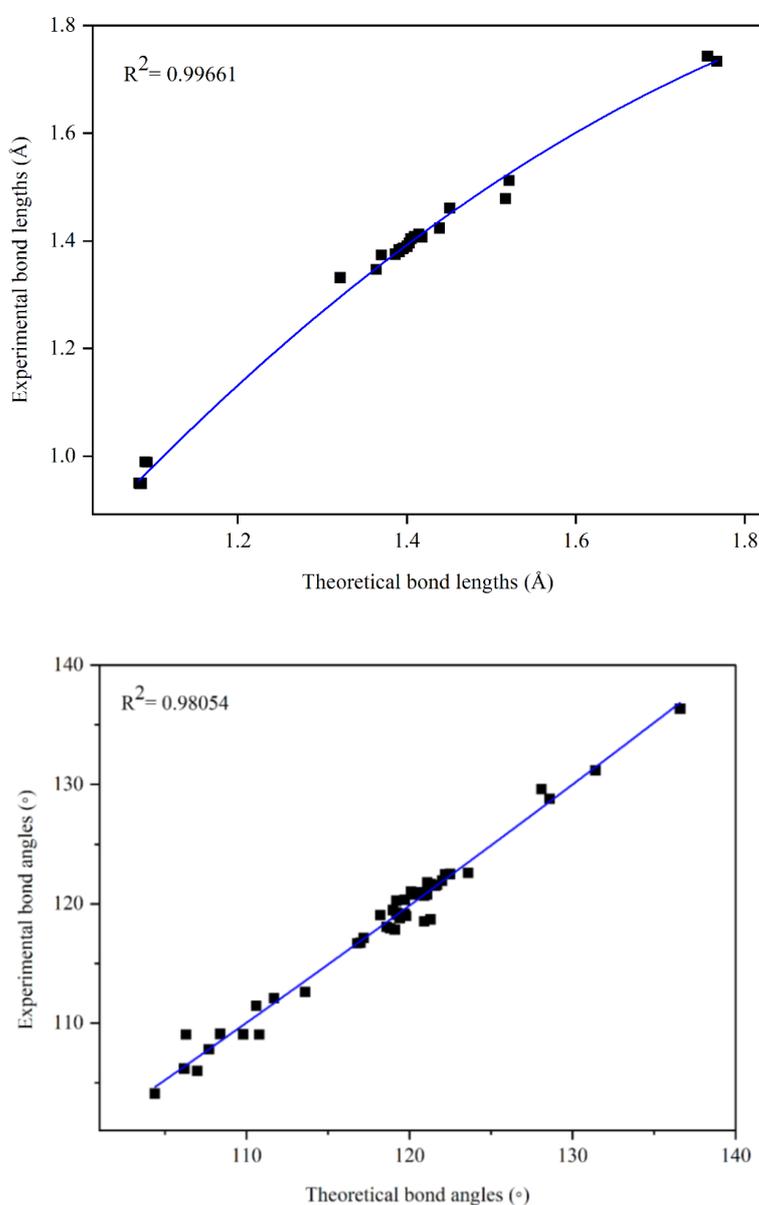
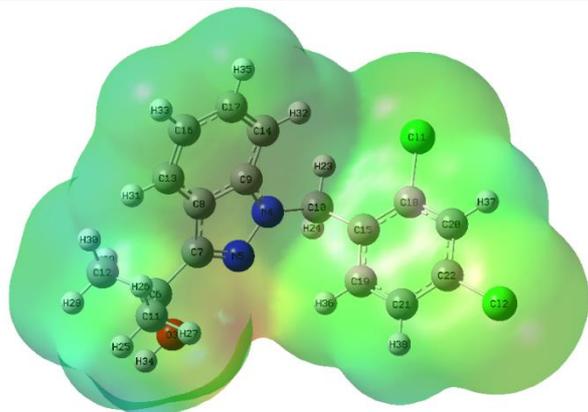
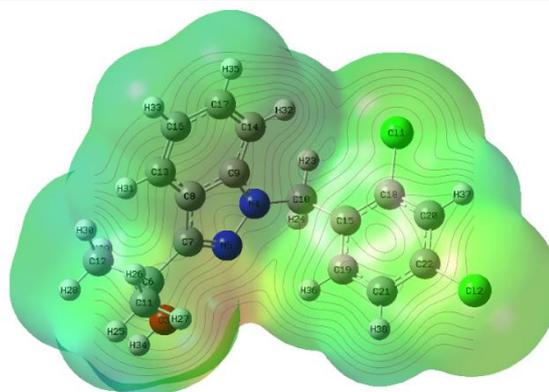


Fig. S1. Correlation graph for bond lengths and angles of DCBIP

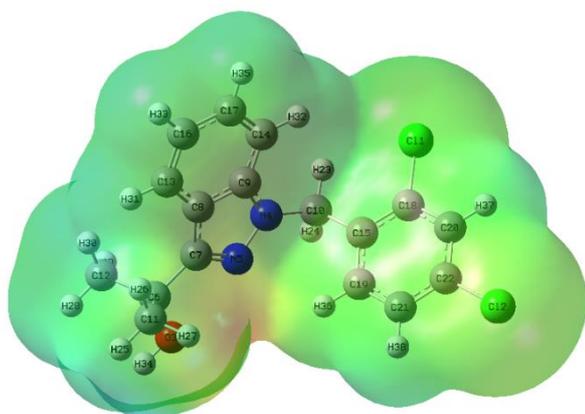
-7.844e-2  7.844e-2



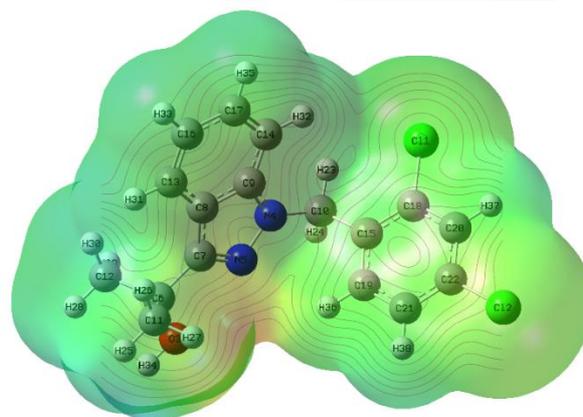
Acetone



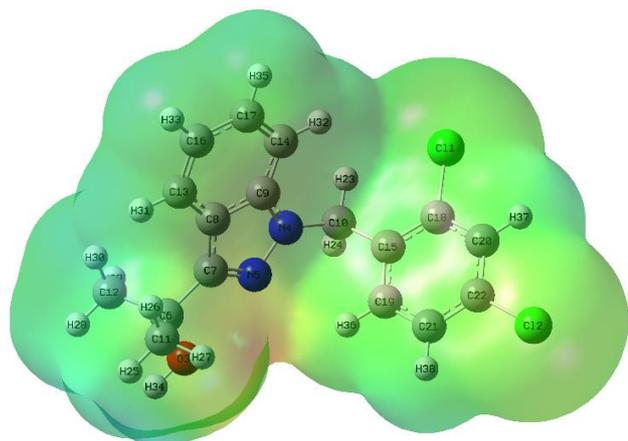
-7.885e-2  7.885e-2



Methanol



-7.929e-2  7.929e-2



Water

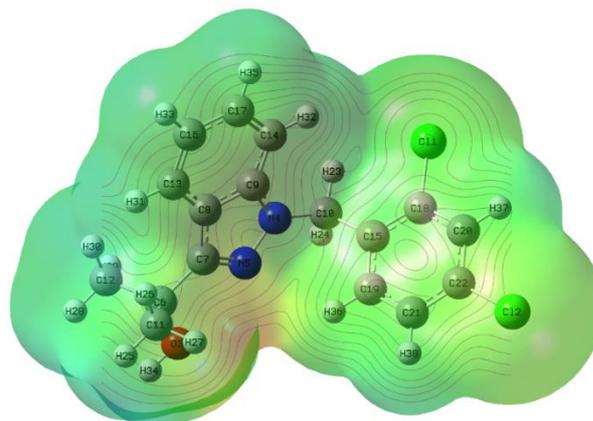
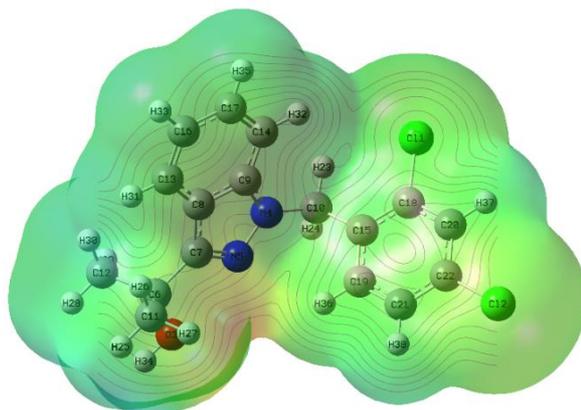
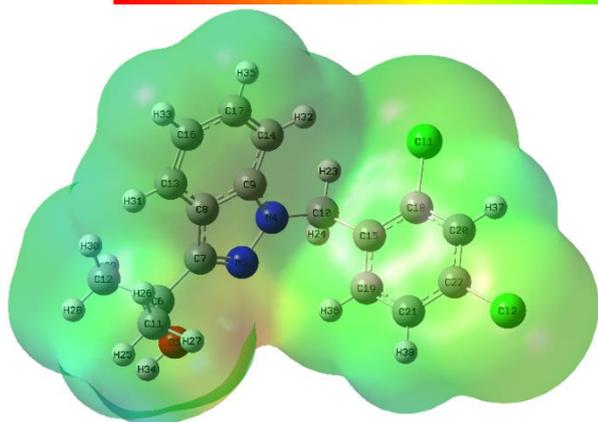


Fig. S2. Total electron density and the contour map with the MEP surface of DCBIP in polar solvents.

-7.540e-2



7.540e-2

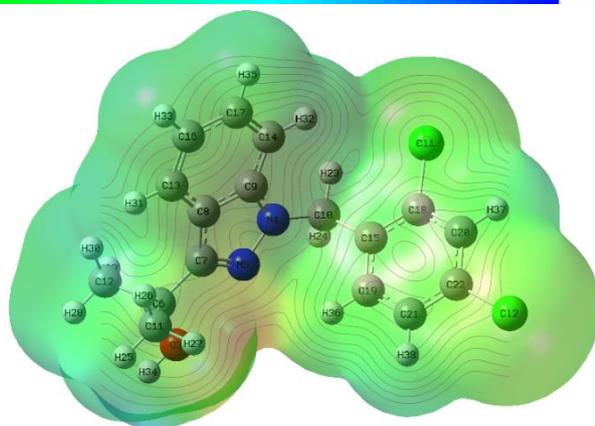
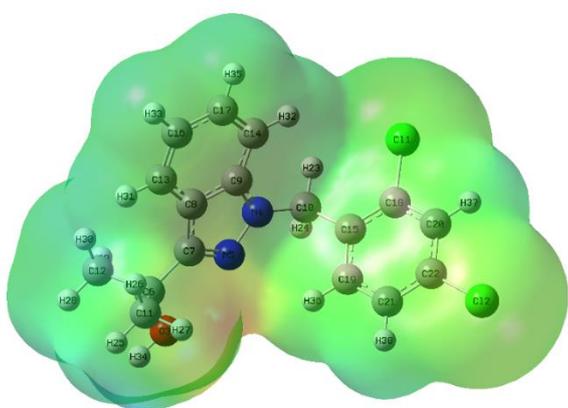


Chloroform

-7.207e-2



7.207e-2

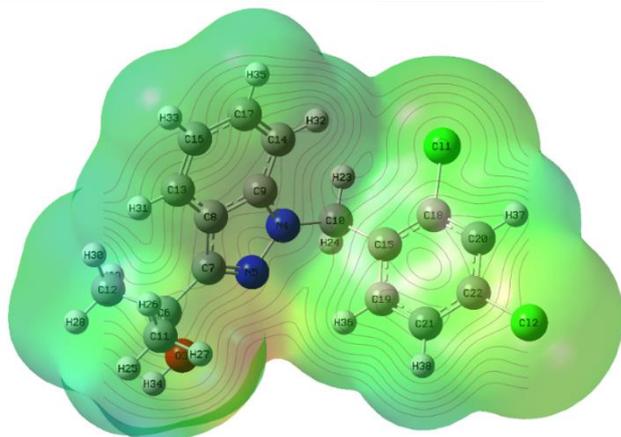
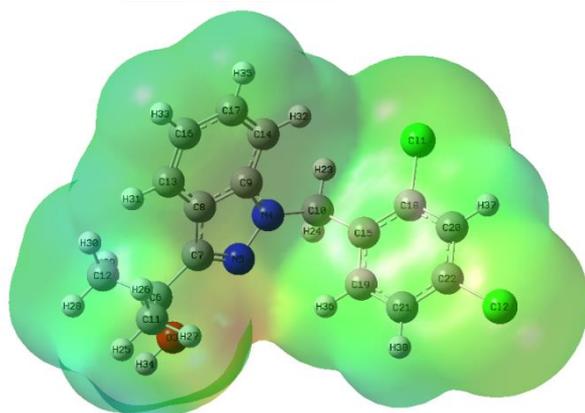


Cyclohexane

-7.279e-2



7.279e-2



Toluene

Fig. S3. Total electron density and the contour map with the MEP surface of DCBIP in non-polar solvents.

Table S1

Mulliken atomic charges of DCBIP.

Atoms	Atomic Charges	Atoms	Atomic Charges	Atoms	Atomic Charges
Cl ₁	-0.01328	C ₁₄	-0.08882	H ₂₇	0.122584
Cl ₂	-0.00929	C ₁₅	0.130959	H ₂₈	0.089348
O ₃	-0.54232	C ₁₆	-0.09607	H ₂₉	0.126239
N ₄	-0.40505	C ₁₇	-0.10644	H ₃₀	0.104753
N ₅	-0.34159	C ₁₈	-0.14893	H ₃₁	0.086595
C ₆	0.227317	C ₁₉	-0.10846	H ₃₂	0.102323
C ₇	0.270334	C ₂₀	-0.05014	H ₃₃	0.083672
C ₈	-0.00719	C ₂₁	-0.06733	H ₃₄	0.298967
C ₉	0.367637	C ₂₂	-0.09334	H ₃₅	0.089026
C ₁₀	-0.12338	H ₂₃	0.135231	H ₃₆	0.141521
C ₁₁	-0.31421	H ₂₄	0.156311	H ₃₇	0.131359
C ₁₂	-0.31601	H ₂₅	0.089693	H ₃₈	0.118373
C ₁₃	-0.14447	H ₂₆	0.104099	-	-

**Table
S2**
ADME

prediction of DCBIP.

Parameters	DCBIP
Formula	C ₁₇ H ₁₆ Cl ₂ N ₂ O
Molecular weight	335.23 g/mol
Number of heavy atoms	22
Fraction Csp ³	0.24
Number of rotatable bonds	3
Number of hydrogen bond acceptors	2
Number of hydrogen bond donors	1
Molar refractivity	91.13
TPSA (Topological polar surface area)	38.05 Å ²

Lipophilicity	
Log p _{o/w}	3.18

Water solubility	
Log S (ESOL)	-4.85
Solubility	1.43e ⁻⁰⁵ mg/mol

Absorbance	
GI	High

Distribution	
BBB permeation	Yes
P-gp substrate	No

Metabolism	
CYP1A2 inhibitor	Yes
CYP2C19 inhibitor	Yes
CYP2C9 inhibitor	Yes
CYP2D6 inhibitor	Yes
CYP3A4 inhibitor	No
LogKp (skin permeation)	-5.39 cm/s

Drug-likeness	
Lipinski	Yes, 0 Violation
Ghose	Yes
Veber	Yes

Medicinal Chemistry	
PAINS	0 alert
Brenk	0 alert

Lead likeness		No
Synthetic Accessibility		2.64
Bioavailability score		0.55
