

Supplementary data

UV-Visible spectroscopy

The UV-visible spectral data of the both compounds in methanol solvent were recorded within 200-800 nm range. In the range of 200–350 nm in methanol, both compounds are experimental electronic spectra show wide absorption bands. Despite the system having lone electron pairs on the tertiary nitrogen atom, it is widely known that the $n \rightarrow p^*$ transition is absent from benzimidazole compounds¹⁻³. This wide band in the 250–350 range can therefore be attributed to $p \rightarrow p^*$ in the benzimidazole ring. The visible absorption bands for both compounds correspond to the electron transition between the HOMO and LUMO, according to calculations of molecular orbital geometry. According to molecular orbital analysis, p atomic orbitals make up the majority of frontier molecular orbitals. As a result, the $p \rightarrow p^*$ transitions are predominantly responsible for electronic transitions from the HOMO-2, HOMO-1, and HOMO to the LUMO⁴. As demonstrated in figure 3, the HOMO and LUMO orbitals are delocalized on the whole molecule, but the HOMO-1 and LUMO +1 electron clouds are delocalized on the cyclopentyl group and benzimidazole, respectively.

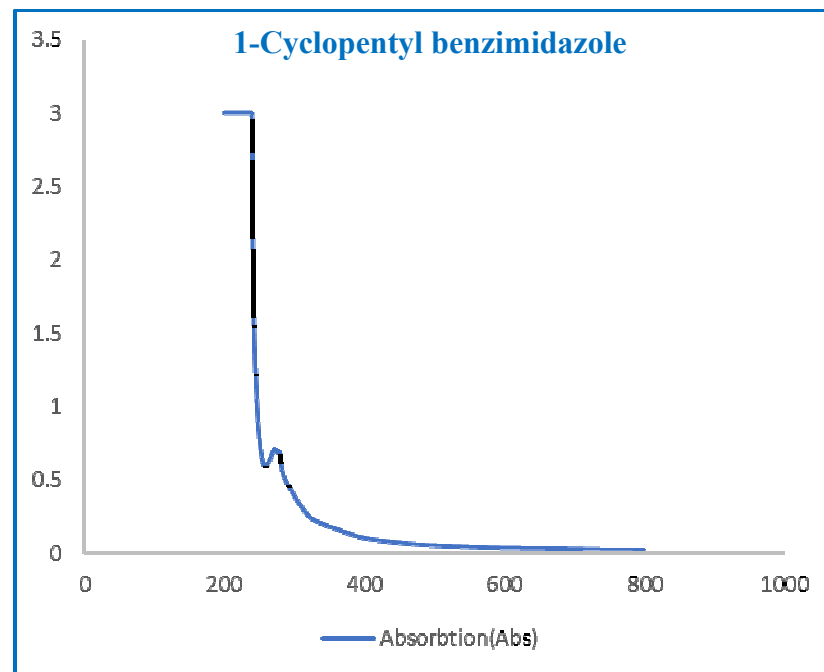
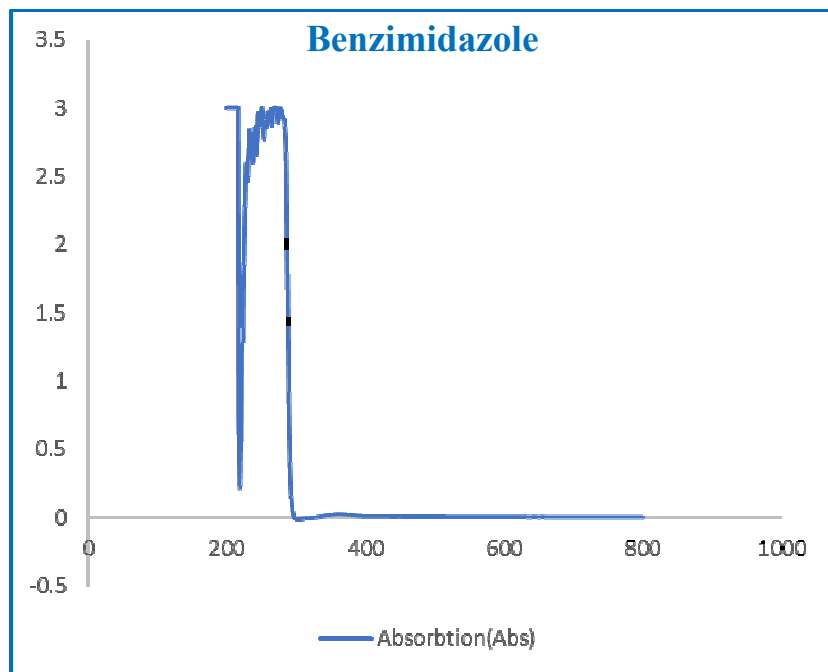


Fig. S1: Spectrum of UV-Visible Benzimidazole and Drug.

High Performance Liquid Chromatography (HPLC)

The duration of the compound passage through the column and onto the detector is indicated by the retention time. The compound may be moderately polar or not strongly maintained by the stationary phase of the column, as indicated by the retention time of 2.245 minutes, which indicates that it elutes comparatively early⁵⁻⁷. A single, distinct peak can be seen in this HPLC (High-Performance Liquid Chromatography) chromatogram at a retention duration of roughly 2.245 minutes. The chromatogram allows for the elaboration of the following points. The peak sharpness indicates a pure, well-resolved chemical, indicating that the sample that was fed into the HPLC most likely contained a single, dominating component. The peak maximum height of more than 500 indicates that there is a comparatively high concentration of the component in the sample. At 230 nm, a wavelength frequently employed to identify substances that absorb in the UV spectrum, the examination was carried out. In summary, the sample is single, sharp peak suggests that it is probably quite pure, with no notable contaminants found in the same range.

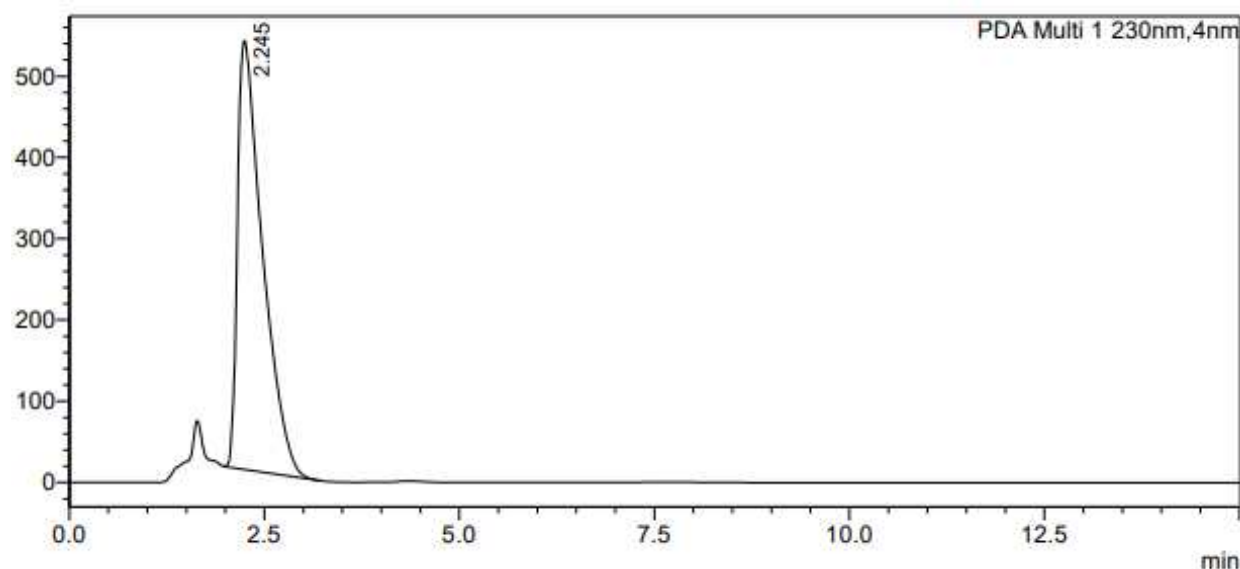


Fig. S2: Chromatogram of synthesized compound

References

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