**SUPPLEMENTARY DATA**

**Phenolic Acid – β-cyclodextrin Complexation Study to Mask Bitterness in Wheat Bran: A Machine-Learning-based QSAR Study**

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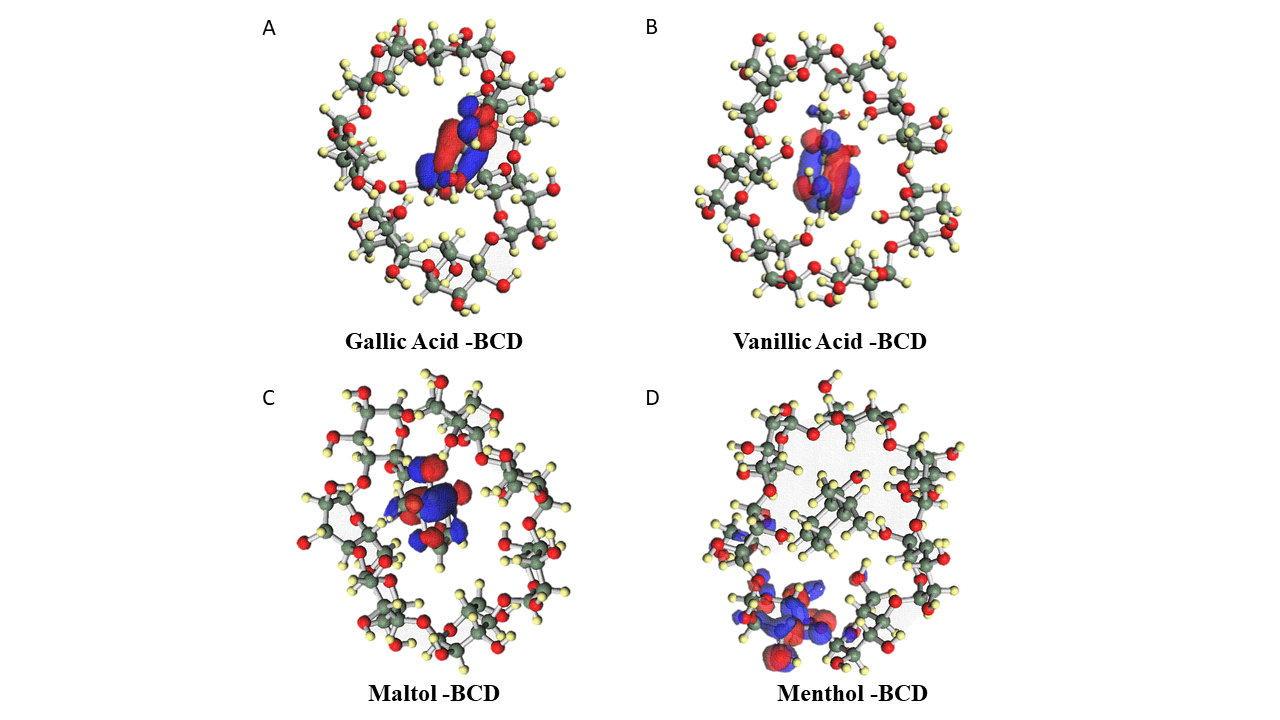
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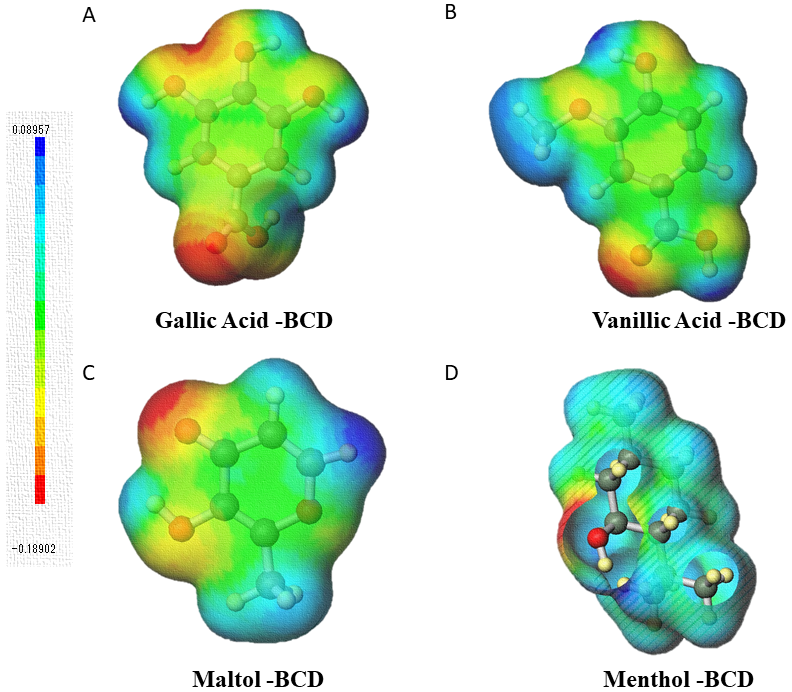
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**Fig S2.** Electrostatic potential graph showing the saturation patterns of polar and non-polar groups in molecules

**Figure S1**: Electronic orbitals of BCD-complexed molecules, showing the location of their HOMO-LUMO orbitals.



**Figure S2**: Electrostatic potential graph showing the saturation patterns of polar and non-polar groups in molecules