

1 SUPPLEMENTARY MATERIAL TO

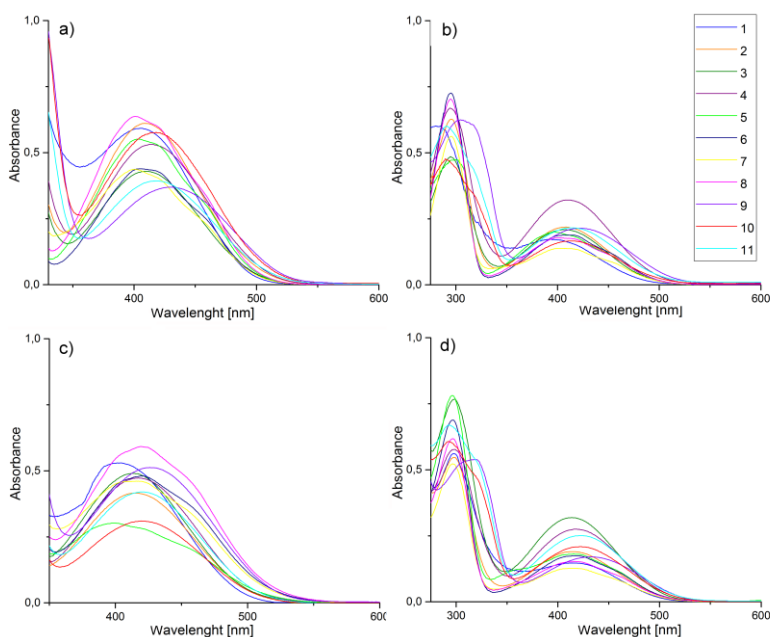
2 **A survey on the characterization and biological activity of isatin derivatives**

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16 Figure S1. UV-Vis absorption spectra of compounds 1–11 in a) Acetone, b) AcN, c) BzOH and d) DMF

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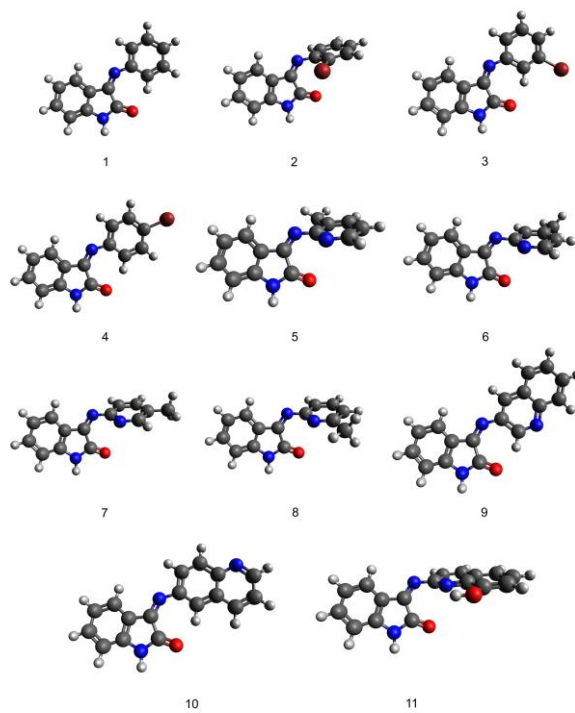


Figure S2. Optimized geometry of the investigated compounds

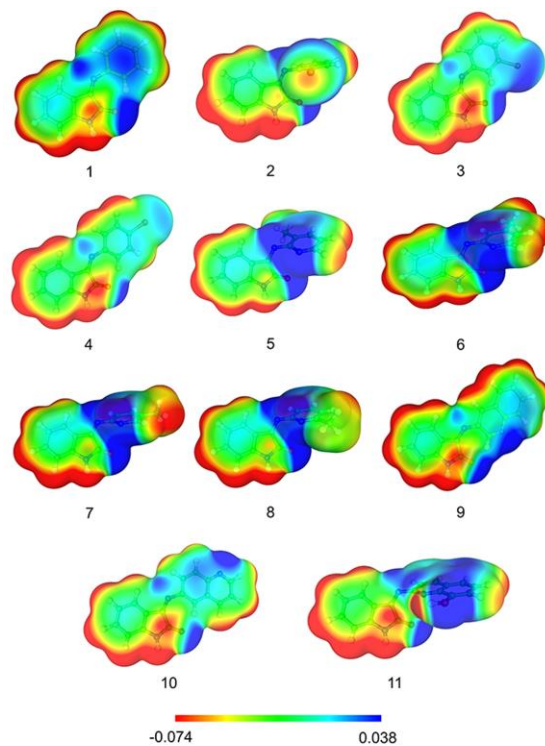
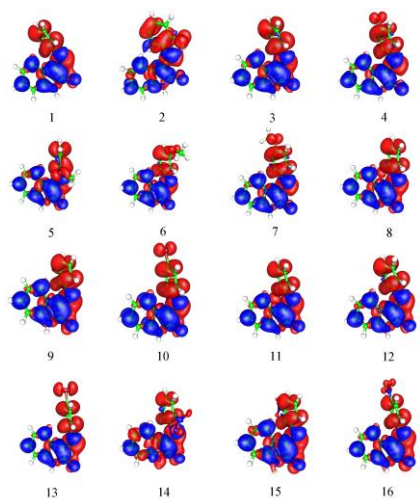


Figure S3. MEP potential of investigated compounds

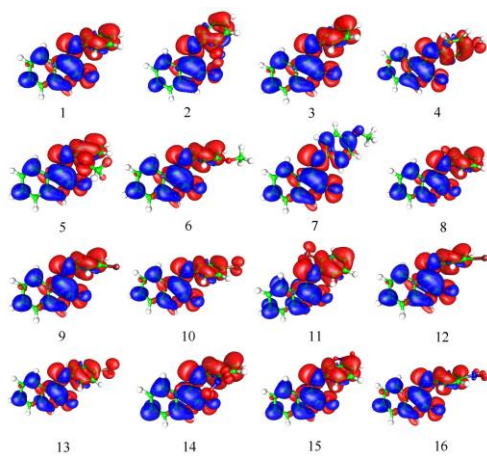
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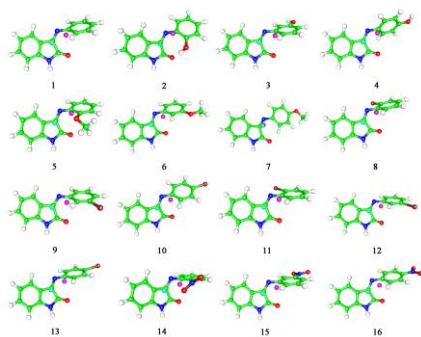
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Figure S4a. ICT processes from ground state (red) to excited state (blue) of compounds **1-16** for *E* isomers.



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Figure S4b. ICT processes from ground state (red) to excited state (blue) of compounds **1-16** for *Z* isomers



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Figure S5. ICT in compounds **1-16** for *Z* isomers. Positions of barycenters for charge loss (cyan circle) and charge gain (violet circle) upon transition

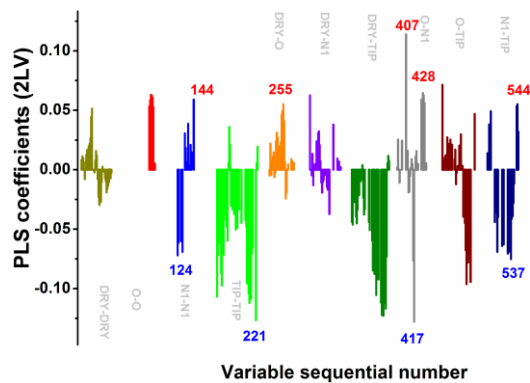


Figure S6. PLS coefficients plot

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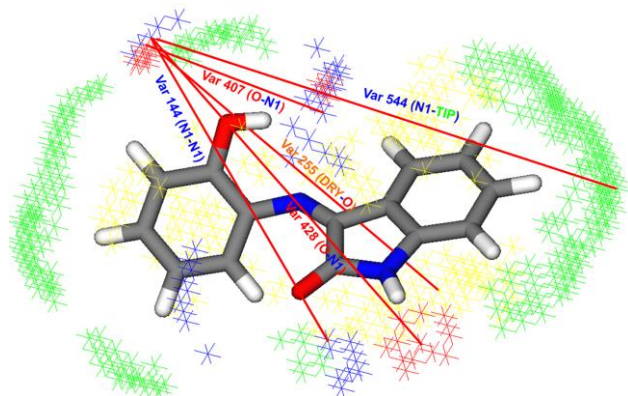


Figure S7. Compound 2 as a model for more potent compounds

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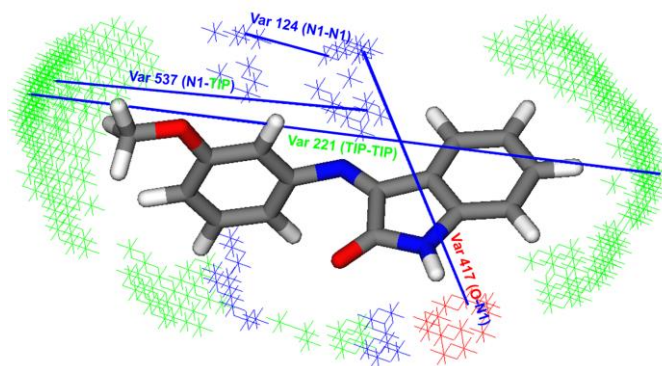


Figure S8. Compound 2 as a model for less potent compounds

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