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SUPPLEMENTARY MATERIAL TO

A survey on the characterization and biological activity of isatin derivatives

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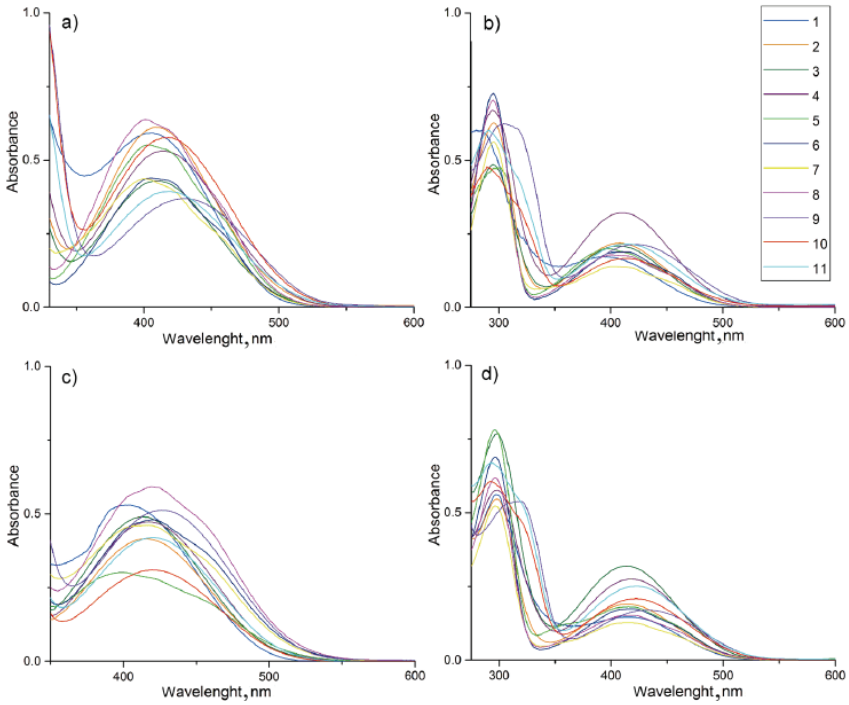

Fig. S-1. UV–Vis absorption spectra of compounds 1–11 (names and structures in the main text) in a) Acetone, b) AcN, c) BzOH and d) DMF.[1]

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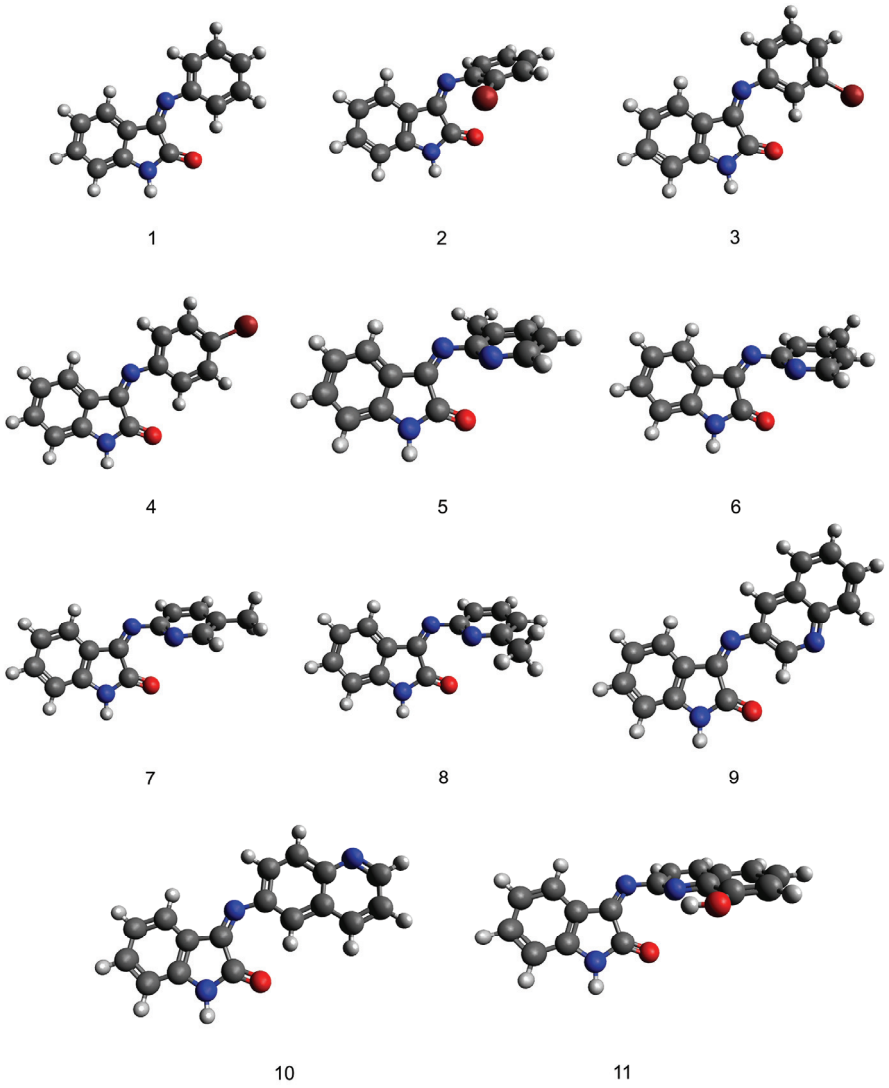

Fig. S-2. Optimized geometry of the investigated compounds.[1]

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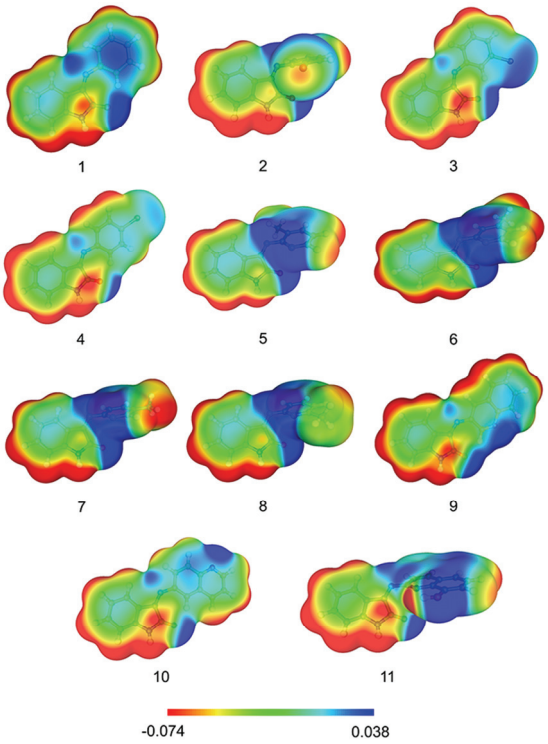

Fig. S-3. MEP potential of investigated compounds.[1]

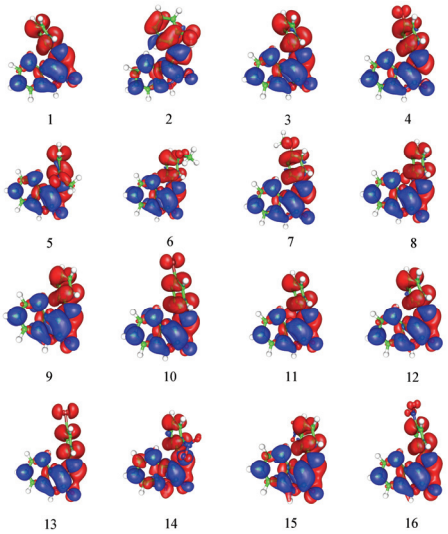

Fig. S-4a. ICT processes from ground state (red) to excited state (blue) of compounds **1-16** for *E* isomers.[2] (Published with the permission of Elsevier)

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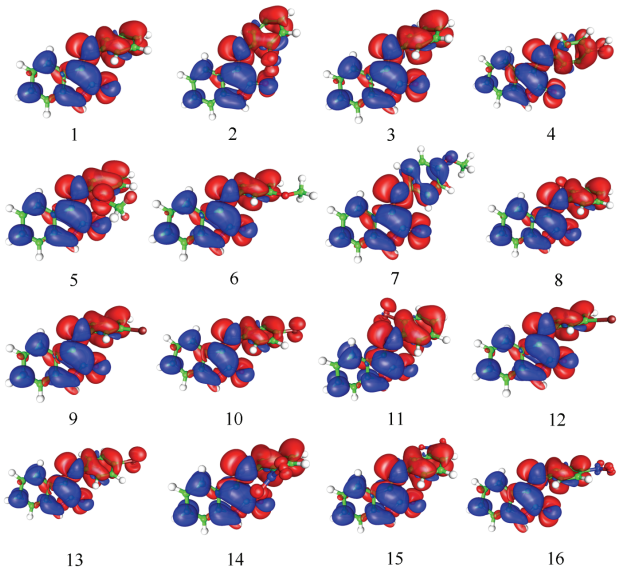

Fig. S-4b. ICT processes from ground state (red) to excited state (blue) of compounds **1**–**16** for Z isomers.[2] (Published with the permission of Elsevier)

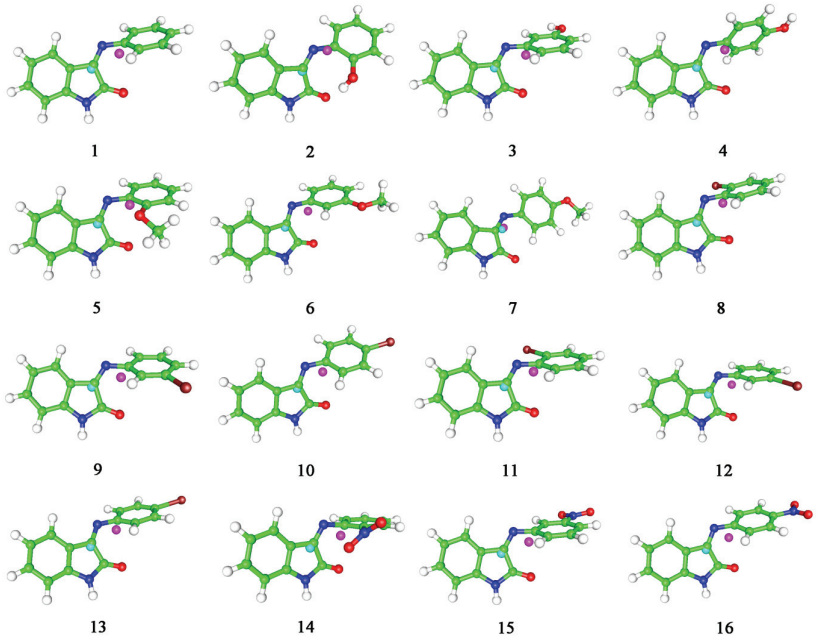

Fig. S-5. ICT in compounds **1**–**16** for *Z* isomers. Positions of barycenters for charge loss (cyan circle) and charge gain (violet circle) upon transition.[2] (Published with the permission of Elsevier)

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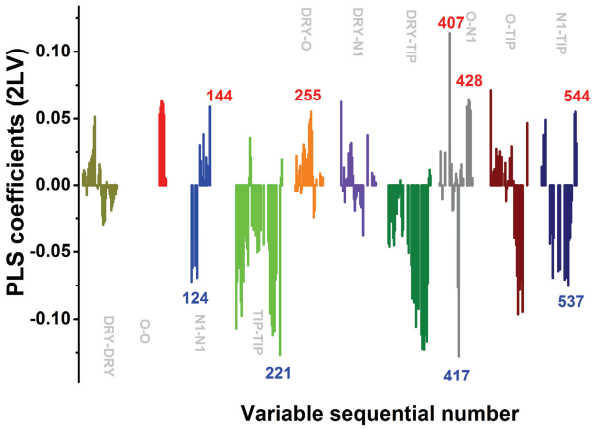

Fig. S-6. PLS coefficients plot.[2] (Published with the permission of Elsevier)

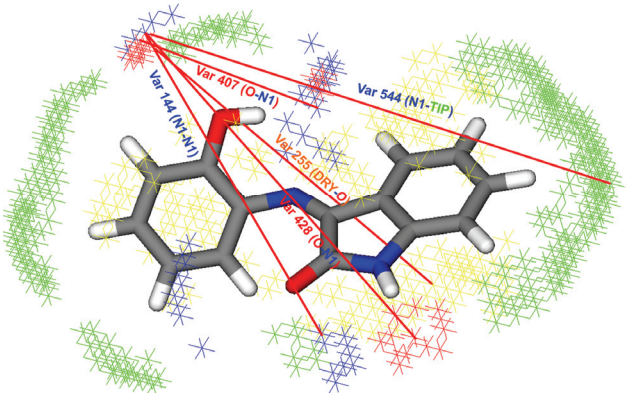

Fig. S-7. Compound **4.2** as a model for more potent compounds.[2] (Published with the permission of Elsevier)

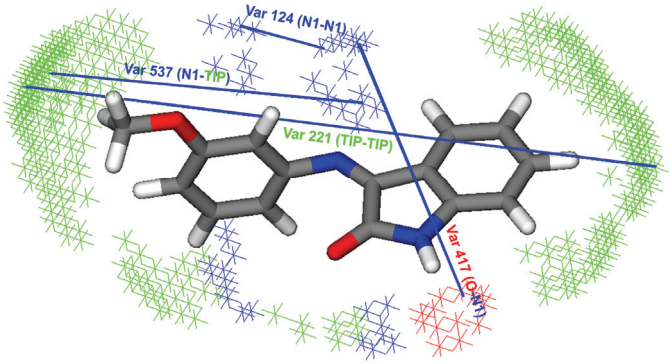

Fig. S-8. Compound **4.2** as a model for less potent compounds.[2] (Published with the permission of Elsevier)

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1. D. R. Brkić, A. R. Božić, V. D. Nikolić, A. D. Marinković, H. Elshaflu, J. B. Nikolić, S. Ž. Drmanić, *J. Serb. Chem. Soc.* **81** (2016) 979 (https://doi.org/10.2298/JSC160119049B)
2. D. R. Brkić, A. R. Božić, A. D. Marinković, M. K. Milčić, N. Ž. Prlainović , F.H. Assaleh , I. N. Cvijetić , J. B. Nikolić, S. Ž. Drmanić, *Spectrochim. Acta, A* **196** (2018) 16 (https://doi.org/10.1016/j.saa.2018.01.080).

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