Supplementary data for the article:

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Supporting Information

Theoretical study of nitrodibenzofurans: a possible relationship between molecular properties and mutagenic activity

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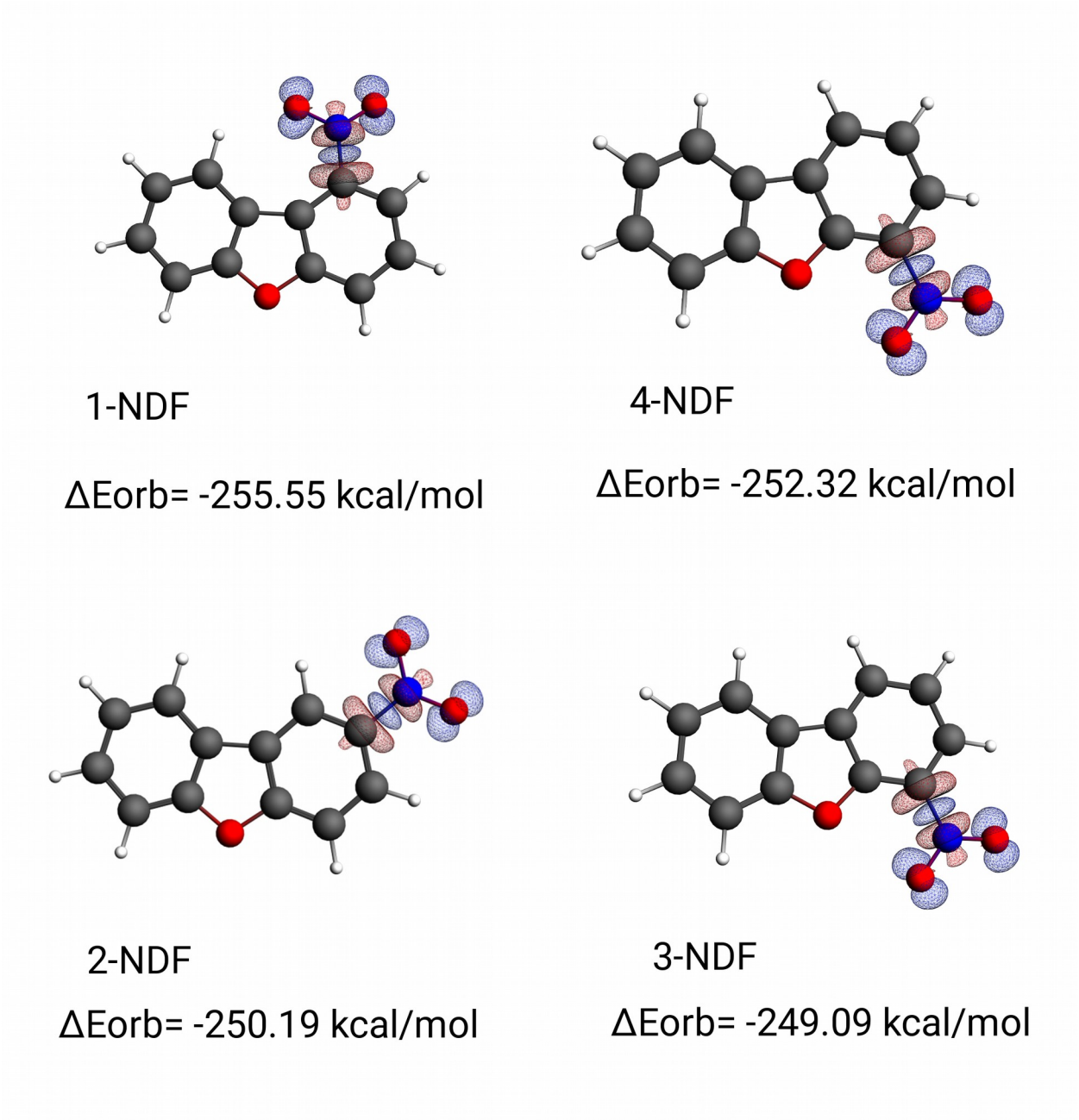

Fig. S1 The deformation density plots $\Delta\rho_1$ corresponding to most important Natural Orbital for Chemical Valence (NOCV) [1,2] pair of orbitals and orbital stabilization energies (ΔE_{orb}) for 1-NDF, 4-NDF, 2-NDF, and 3-NDF, respectively, obtained at the BP86(D)/TZ2P level of theory (the contour values: ±0.008 a.u). The results correspond to the dibenzofuran moiety-NO_2 fragmentation.The direction of the charge flow in the deformation density plot Δρ is from the red to the blue region.

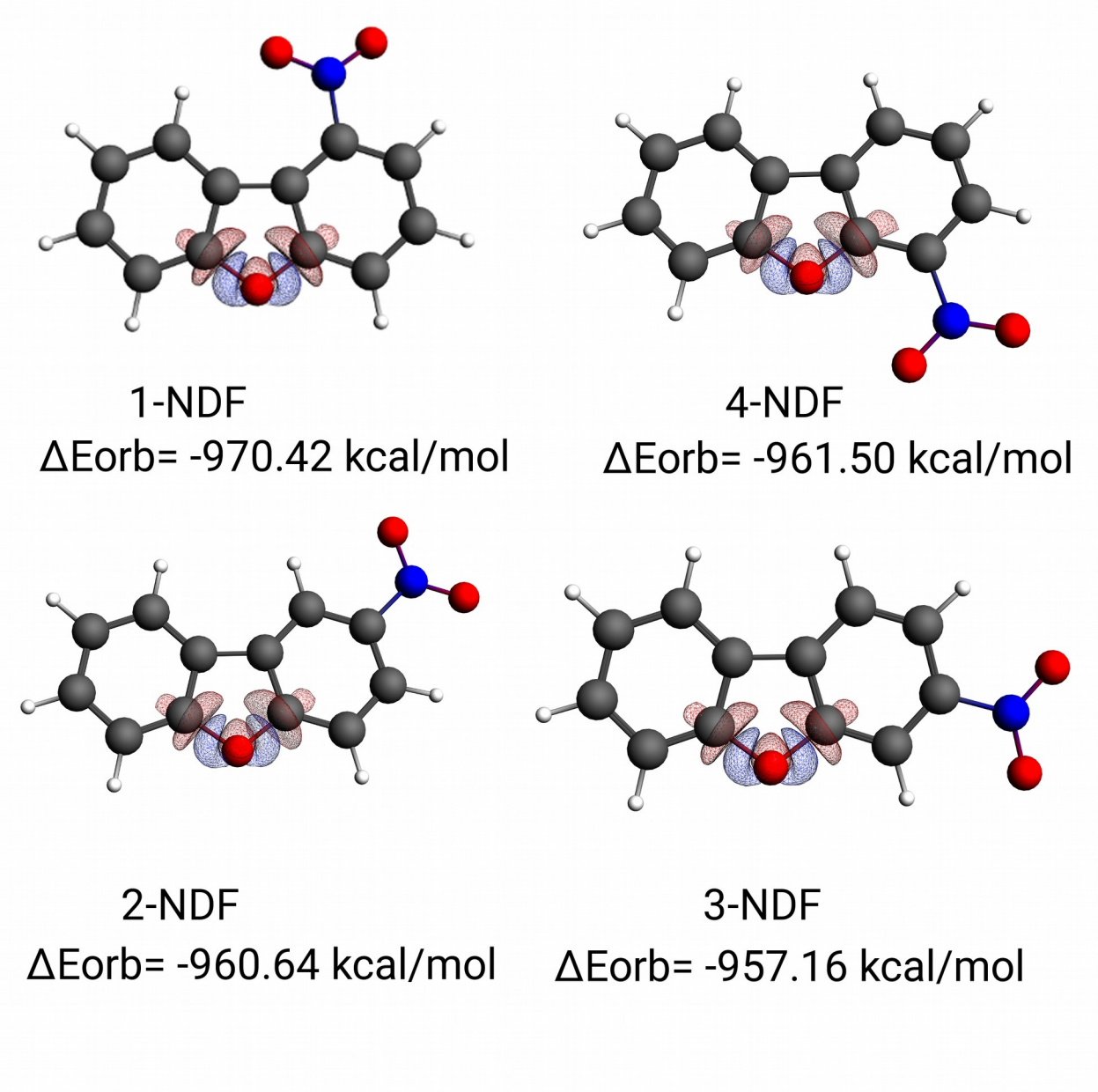

Fig. S2 The deformation density plots $\Delta\rho_1$ corresponding to most important Natural Orbital for Chemical Valence (NOCV)[1,2] pair of orbitals and orbital stabilization energies (ΔE_{orb}) for 1-NDF, 4-NDF, 2-NDF, and 3-NDF, respectively, obtained at the BP86(D)/TZ2P level of theory (the contour values: ±0.01 a.u). The results correspond to the central ring oxygen-rest of NDF moiety fragmentation. The direction of the charge flow in the deformation density plot $\Delta\rho$ is from the red to the blue region.

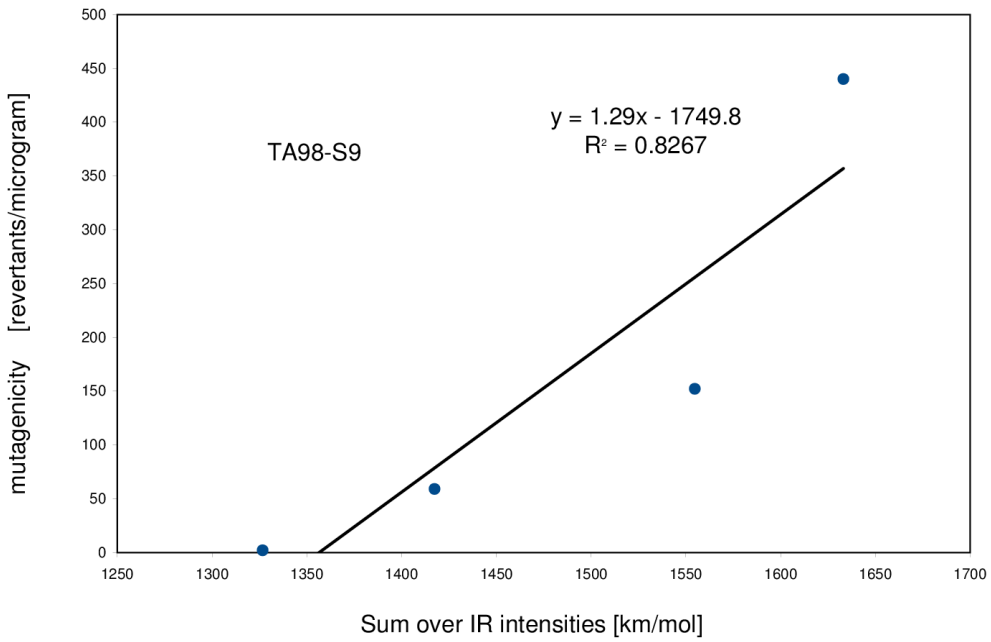

Fig. S3 The relationship between the ΣI_{IR} values of NDBFs calculated at the B3LYP/6-311+G(2df,p) level and the *Salmonella typhimurium* TA98 without S9 mix mutagenic activity [3].

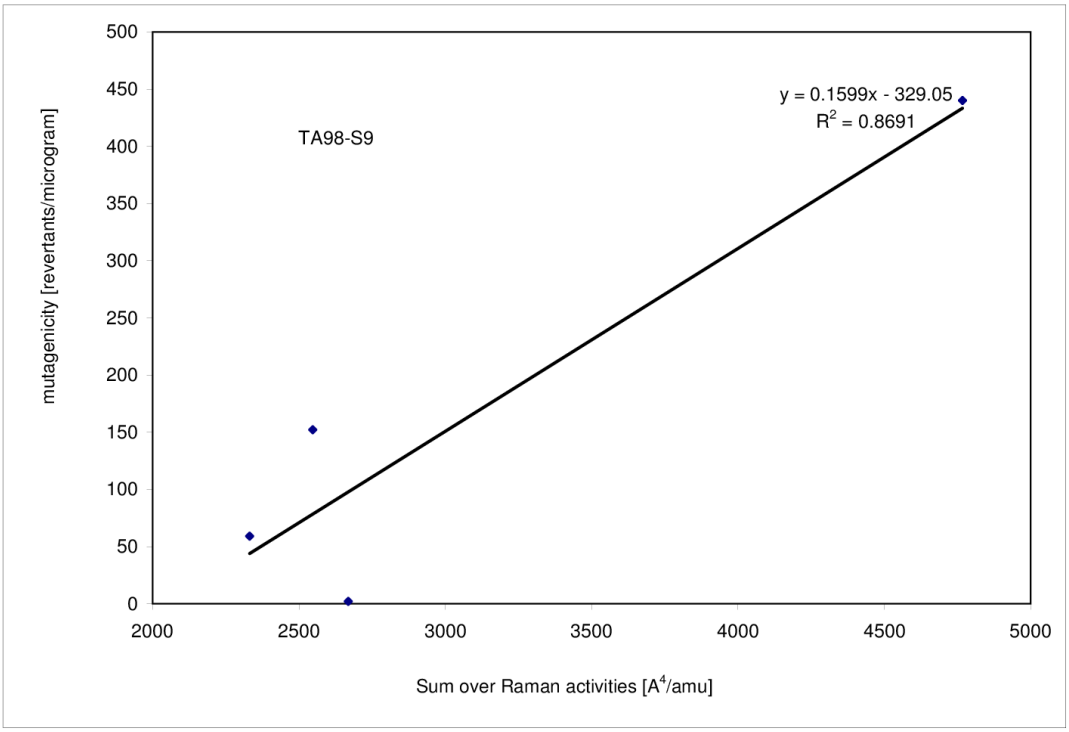

Fig. S4 The relationship between the ΣA_{Raman} values of NDF calculated at the B3LYP/6-311+G(2df,p) level and the *Salmonella typhimurium* TA98 without S9 mix mutagenic activity [3].

Literature

[1] M. Mitoraj, A. Michalak, J. Mol. Model. 13 (2007) 347-355.

[2] A. Michalak, M. Mitoraj, T. Ziegler J. Phys. Chem. A 112 (2008) 1933.

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