Journal of the Serbian Chemical Society
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J. Serb. Chem. Soc. 85 (9) S415–S425 (2020) *Supplementary material*

SUPPLEMENTARY MATERIAL TO

A computational study of the chemical reactivity of isoxaflutole herbicide and its active metabolite using global and local descriptors

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J. Serb. Chem. Soc. 85 (9) (2020) 1163–1174

TABLE S-I. Global reactivity parameters, for isoxaflutole and diketonitrile (values between parentheses), evaluated at the X/6-311++G(2d,2p) (where X = B3LYP, M06, M06L and ωB97XD) level of theory and in the gas phase, employing the Koopmans' approximation

Level	I / eV	A / eV	μ / eV	η / eV	χ / eV	ω / eV	ω^+ / eV	ω^- / eV
B3LYP	7.42	2.52	–4.97	4.90	4.97	2.52	1.43	3.91
	(8.04)	(2.38)	(–5.21)	(5.66)	(5.21)	(2.39)	(1.27)	(3.87)
M06	7.72	2.27	–4.99	5.45	4.99	2.28	1.21	3.70
	(8.39)	(2.13)	(–5.26)	(6.26)	(5.26)	(2.21)	(1.09)	(3.72)
M06L	6.65	2.95	–4.80	3.70	4.80	3.12	2.03	4.43
	(6.98)	(2.73)	(–4.86)	(4.26)	(4.86)	(2.77)	(1.69)	(4.11)
ωB97XD	9.35	0.51	–4.93	8.85	4.93	1.37	0.42	2.88
	(10.16)	(0.45)	(–5.30)	(9.71)	(5.30)	(1.45)	(0.43)	(3.08)

TABLE S-II. Global reactivity parameters, for isoxaflutole and diketonitrile (values between parentheses), evaluated at the X/6-311++G(2d,2p) (where X = B3LYP, M06, M06L and ωB97XD) level of theory and in the aqueous phase, employing the Koopmans' approximation

Level	I / eV	A / eV	μ / eV	η / eV	χ / eV	ω / eV	ω^+ / eV	ω^- / eV
B3LYP	–7.32	–2.42	–4.87	–4.9	–4.87	–2.42	–1.36	–3.79
	(–7.92	(–2.16	(–5.04)	(–5.76)	(–5.04)	(–2.2)	(–1.12)	(–3.64)
M06	–7.65	–2.18	–4.91	–5.47	–4.91	–2.21	–1.15	–3.61
	–8.29	–2	(–5.14)	–6.29	–5.14	–2.1	–1.01	–3.58
M06L	–6.59	–2.92	–4.75	–3.67	–4.75	–3.08	–2	–4.38
	–6.89	–2.58	(–4.73)	–4.32	–4.73	–2.6	–1.55	–3.91
ωB97XD	–9.3	–0.43	–4.86	–8.87	–4.86	–1.33	–0.39	–2.83
	–10.06	–0.25	(–5.15)	–9.81	–5.15	–1.35	–0.37	–2.95

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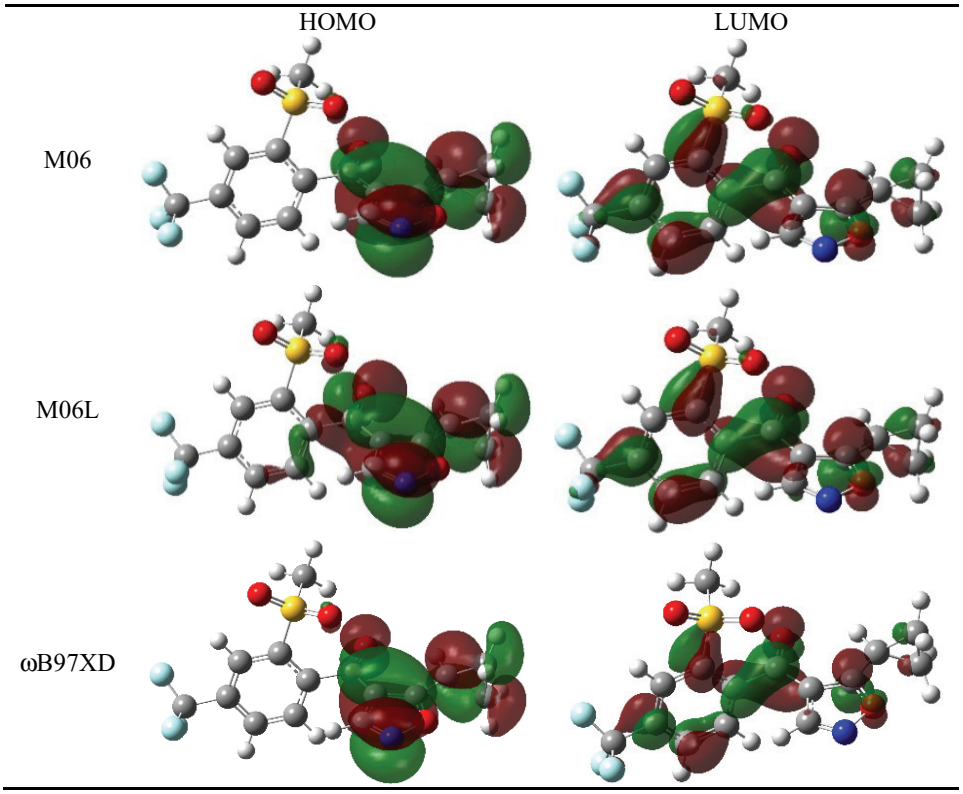

Fig. S-1. HOMO and LUMO's distributions on ISOX obtained at the X/6-311++G(2d,2p) (where X= M06, M06L and ωB97XD) level of theory employing the PCM solvation model. In all cases the isosurfaces were obtained at 0.08 e u.a.$^{-3}$.

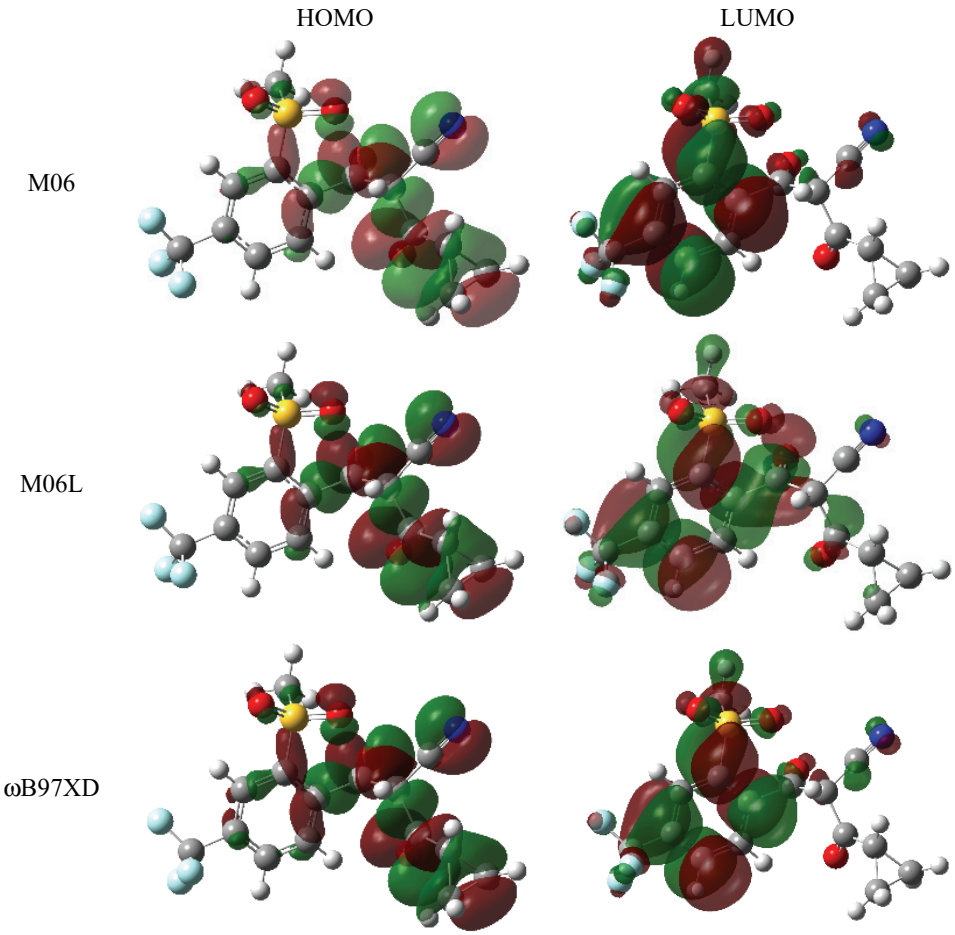

Fig. S-2. HOMO and LUMO's distributions on DKN obtained at the X/6-311++G(2d,2p) (where X= M06, M06L and ωB97XD) level of theory employing the PCM solvation model. In all cases the isosurfaces were obtained at e u.a.$^{-3}$.

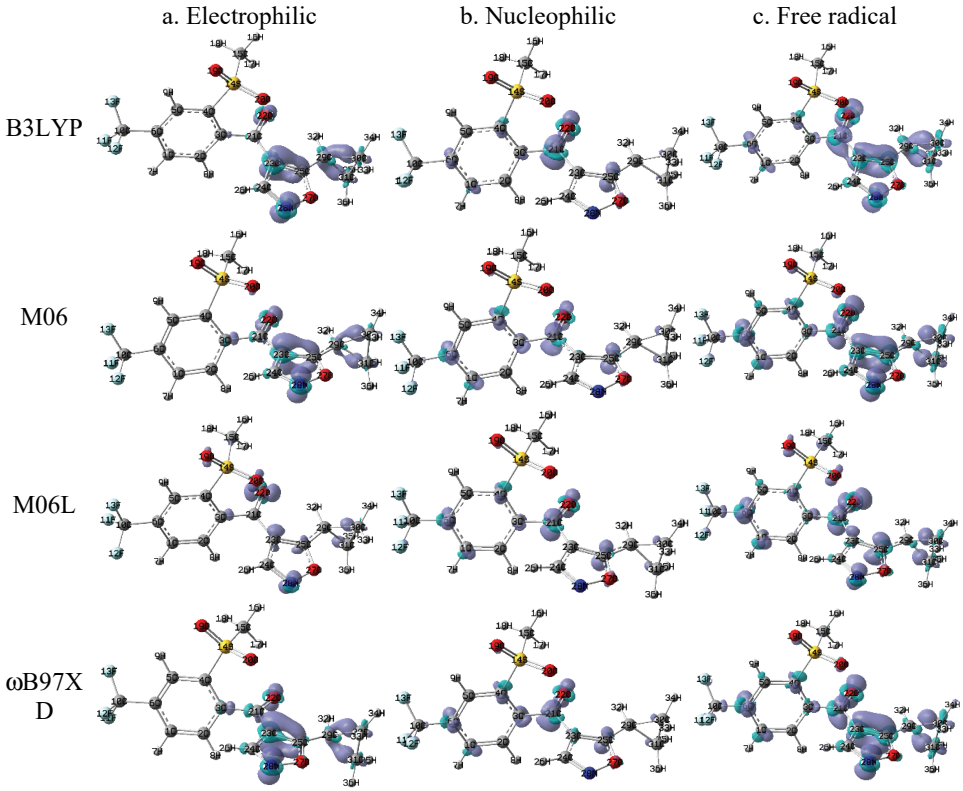

Fig. S-3. Isosurfaces of the Fukui functions for ISOX according to equations (10), (11) and (12) at the X/6-311++G(2d,2p) (where X= M06, M06L and ωB97XD) level of theory in the gas phase. In the case of (a) electrophilic, b) nucleophilic and c) free radical attacks. In all cases the isosurfaces were obtained at 0.007 e u.a.$^{-3}$.

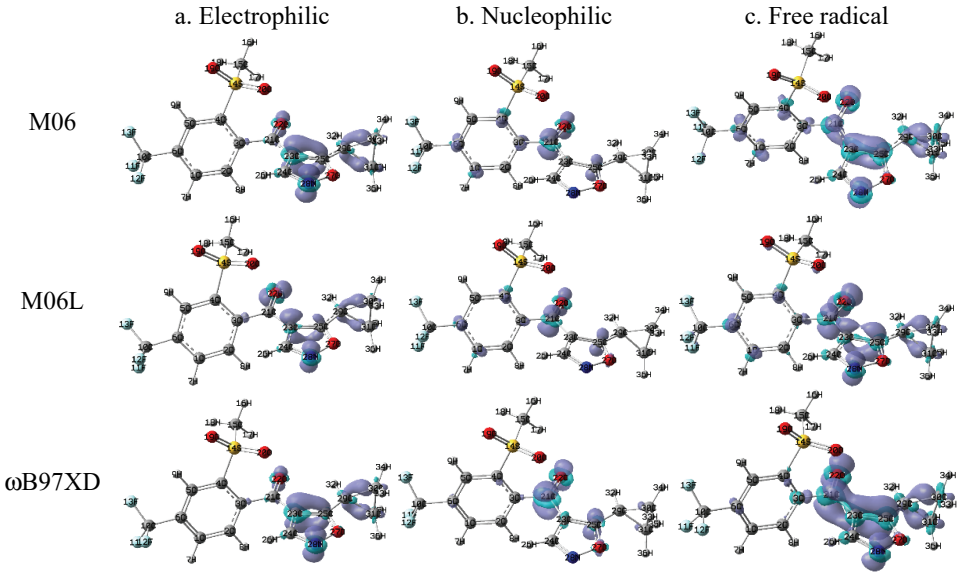

Fig. S-4. Isosurfaces of the Fukui functions for ISOX according to Eqs. (10)–(12) at the X/6-311++G(2d,2p) (where X = M06, M06L and ωB97XD) level of theory, in the aqueous phase, employing the PCM solvation model. In the case of: a) electrophilic, b) nucleophilic and c) free radical attacks. In all cases the isosurfaces were obtained at 0.007 e u.a.$^{-3}$.

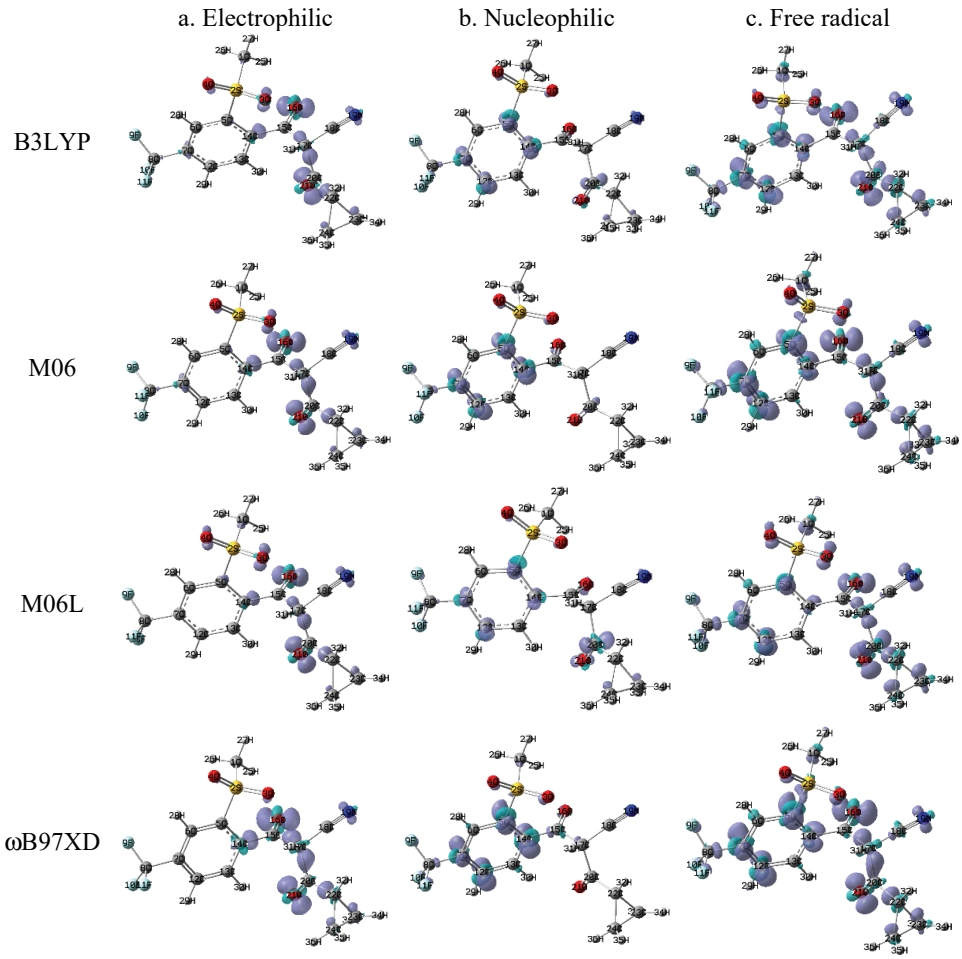

Fig. S-5. Isosurfaces of the Fukui functions for DKN according to Eqs. (10)–(12) at the X/6-311++G(2d,2p) (where X = M06, M06L and ωB97XD) level of theory in the gas phase. In the case of: a) electrophilic, b) nucleophilic and c) free radical attacks. In all cases the isosurfaces were obtained at 0.007 e u.a.$^{-3}$.

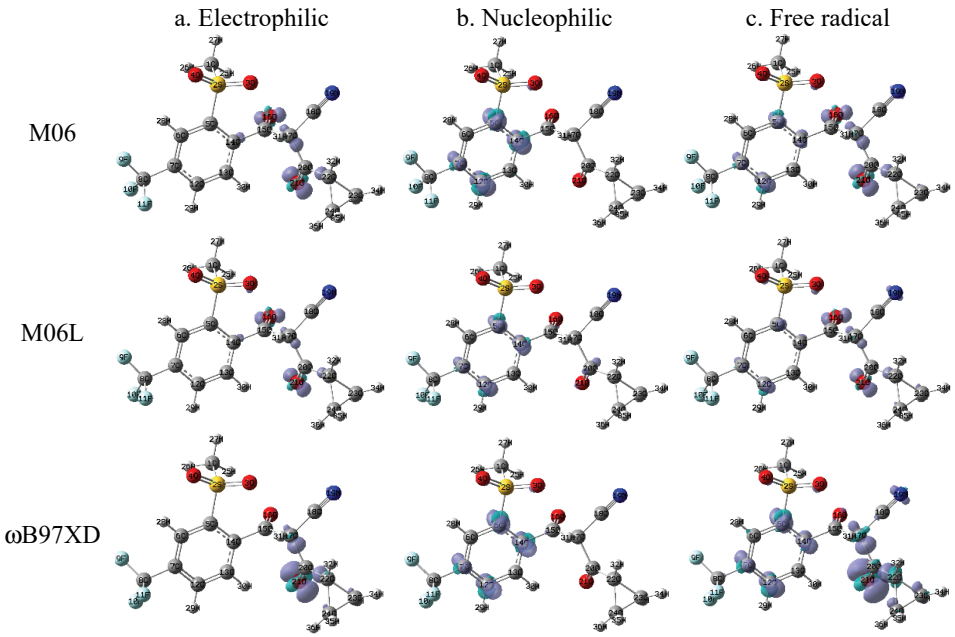

Fig. S-6. Isosurfaces of the Fukui functions for DKN according to Eqs. (10)–(12) at the X/6-311++G(2d,2p) (where X = M06, M06L and ωB97XD) level of theory, in the aqueous phase, employing the PCM solvation model. In the case of: a) electrophilic, b) nucleophilic and c) free radical attacks. In all cases the isosurfaces were obtained at 0.007 e u.a.$^{-3}$.

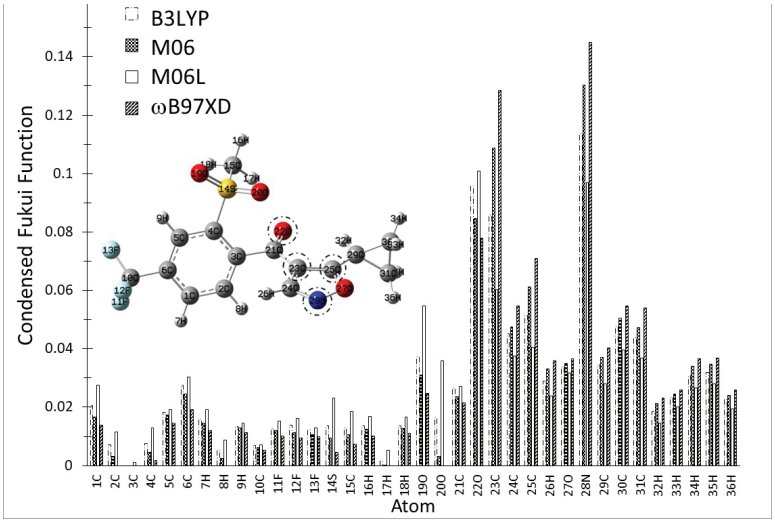

Fig. S-7. Condensed Fukui function values for electrophilic attacks on ISOX at the X/6-311++G (2d,2p) (where X = B3LYP, M06, M06L and ωB97XD) level of theory, in the gas phase employing Hirshfeld population and Eqs. (13)–(15), broken circles show the more reactive zones in each molecule.

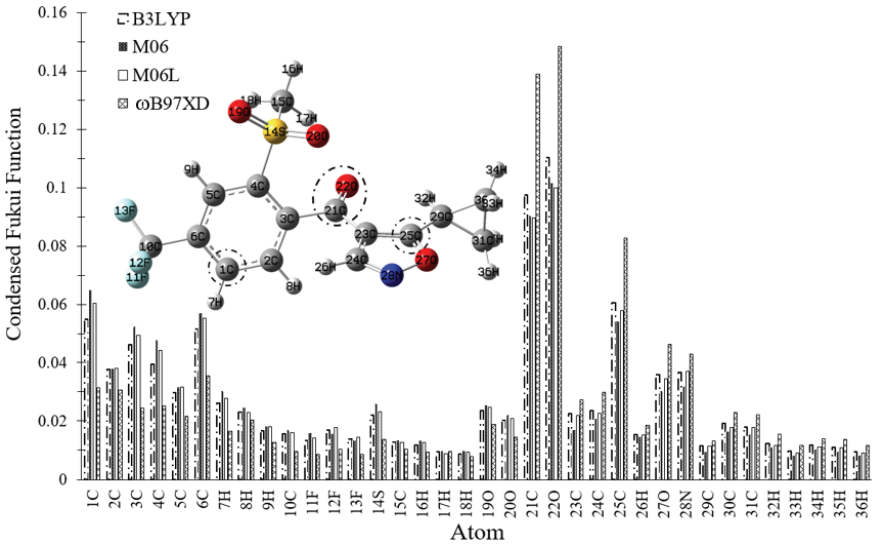

Fig. S-8. Condensed Fukui function values for nucleophilic attacks on ISOX at the X/6-311++G (2d,2p) (where X = B3LYP, M06, M06L and ωB97XD) level of theory, in the aqueous phase employing Hirshfeld population and Eqs. (13)–(15), broken circles show the more reactive zones in each molecule.

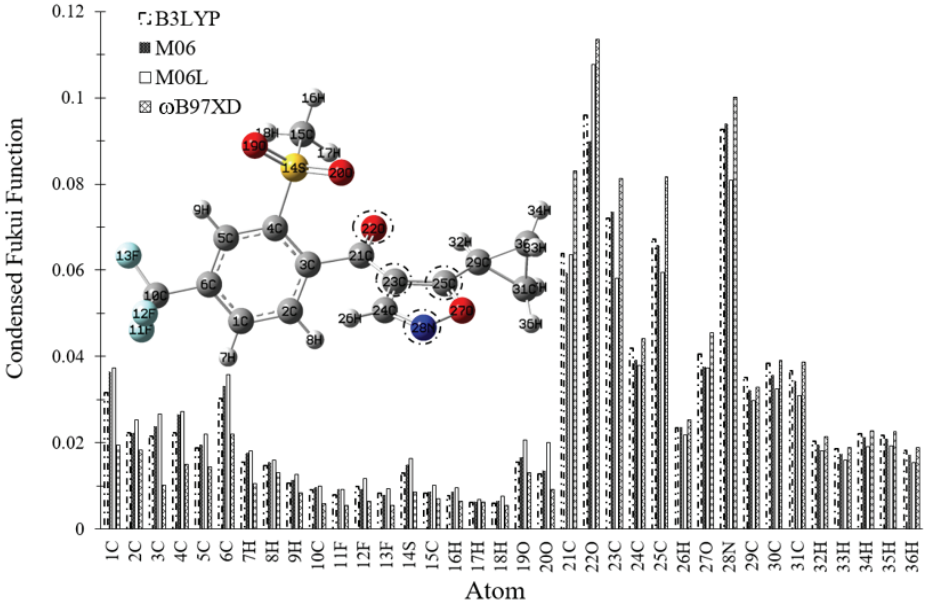

Fig. S-9. Condensed Fukui function values for free radical attacks on ISOX at the X/6-311++G (2d,2p) (where X = B3LYP, M06, M06L and ωB97XD) level of theory, in the aqueous phase employing Hirshfeld population and Eqs. (13)–(15), broken circles show the more reactive zones in each molecule.

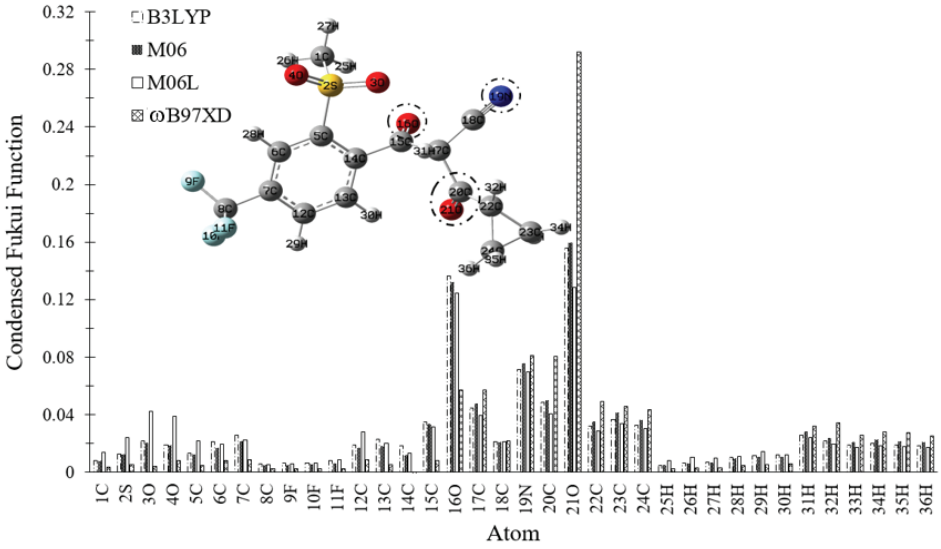

Fig. S-10. Condensed Fukui function values for electrophilic attacks on DKN at the X/6-311++G (2d,2p) (where X = B3LYP, M06, M06L and ωB97XD) level of theory, in the aqueous phase employing Hirshfeld population and Eqs. (13)–(15), broken circles show the more reactive zones in each molecule

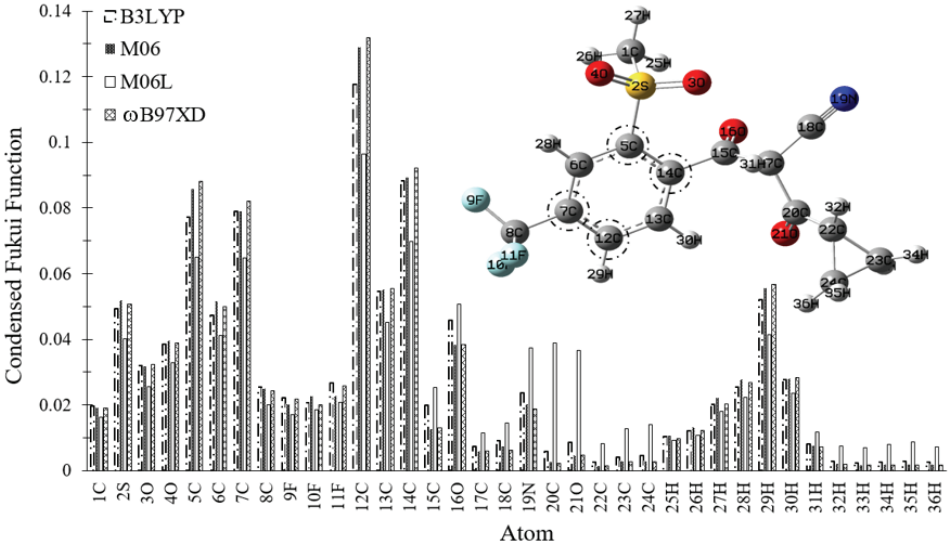

Fig. S-11. Condensed Fukui function values for nucleophilic attacks on DKN at the X/6-311++G (2d,2p) (where X=B3LYP, M06, M06L and ωB97XD) level of theory, in the aqueous phase employing Hirshfeld population and Eqs. (13)–(15), broken circles show the more reactive zones in each molecule.

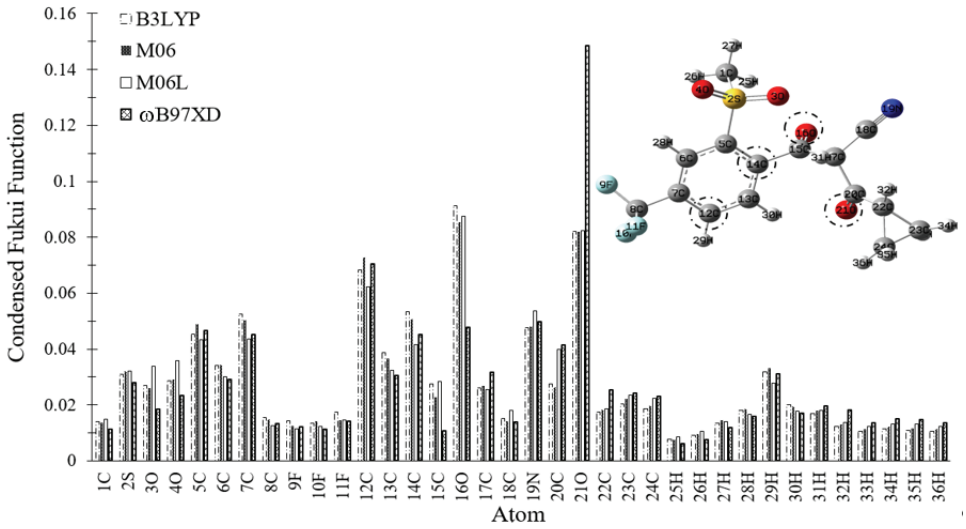

Fig. S-12. Condensed Fukui function values for free radical attacks on DKN at the X/6-311++G (2d,2p) (where X=B3LYP, M06, M06L and ωB97XD) level of theory, in the aqueous phase employing Hirshfeld population and Eqs. (13)–(15), broken circles show the more reactive zones in each molecule.

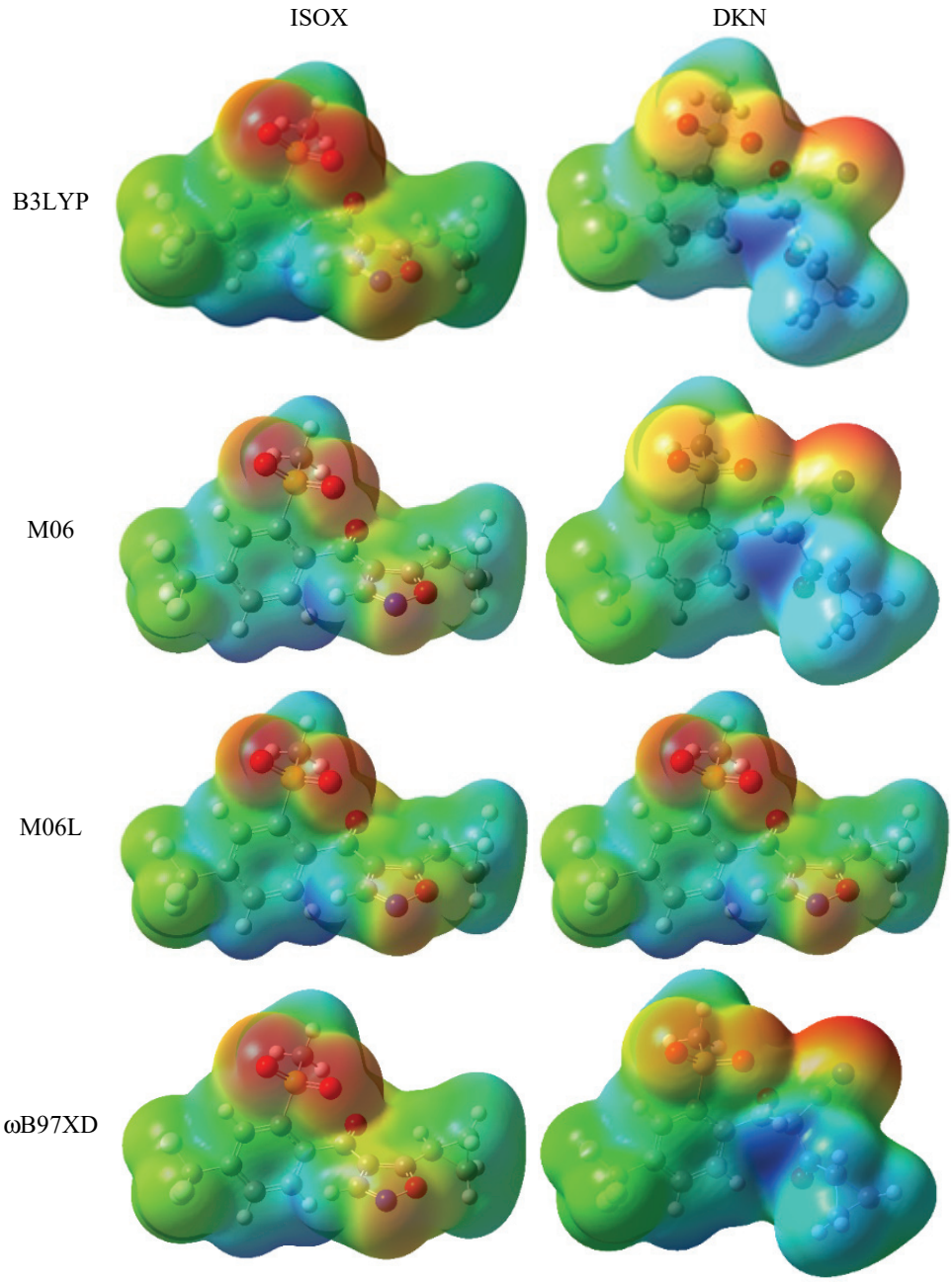

Fig. S-13. Mapping of the electrostatic potentials evaluated at the X/6-311++G(2d,2p) (where X = B3LYP, M06, M06L and ωB97XD) level of theory, in the aqueous phase, employing the PCM solvation model, onto a density isosurface (value =0.002 e u.a.$^{-3}$) for ISOX and DKN.