

## SUPPLEMENTARY MATERIAL

### Insights on chalcone analogues with potential as antioxidant additive for diesel-biodiesel blends

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**Figure S1.** Angles between aromatic ring planes. BCH (a)  $\delta_1 = 6.75$  (Ring 1 and 2),  $\delta_2 = 13.03$  (Ring 2 and 3), NCH (b)  $\delta_3 = 9.24$  (Ring 1 and 2),  $\delta_4 = 6.62$  (Ring 2 and 3) and  $\delta_5 = 21.83$  (Ring 1 and 3)

**Table S1.** The experimental (X-ray) geometric parameters of BCH and NCH: bond lengths (Å).

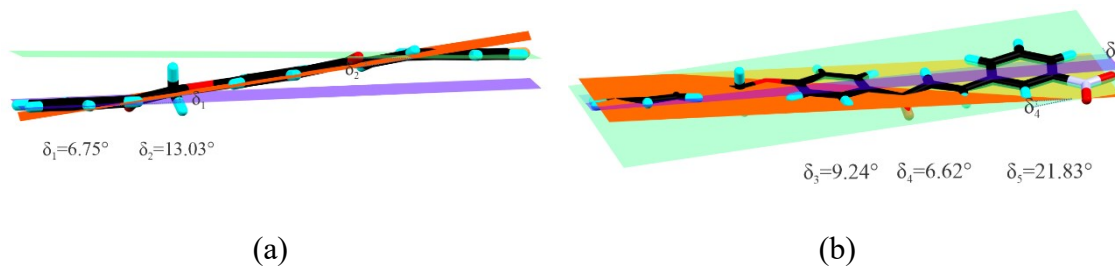
	BCH	NCH		BCH	NCH
Br1-C21	1.8985	-	C14-H14	0.9500	0.9500
O2-C9	1.3624	1.3708	C10-H10	0.9500	0.9499
O2-C8	1.4204	1.4221	C10-C11	1.3836	1.3845
O1-C7	1.2129	1.2136	C11-H11	0.9500	0.9500
O3-C15	1.2281	1.2273	C1-H1	0.9500	0.9500
C6-C7	1.4958	1.4895	C1-C2	1.3853	1.3836
C6-C1	1.3939	1.3960	C23-H23	0.9500	0.9500
C6-C5	1.3959	1.3933	C23-C22	1.3836	1.3833
C9-C14	1.3959	1.3942	C5-H5	0.9500	0.9500
C9-C10	1.3972	1.3931	C5-C4	1.3859	1.3903
C12-C13	1.4048	1.3998	C20-H20	0.9500	-
C12-C15	1.4859	1.4865	C20-C19	1.3854	1.3823
C12-C11	1.3956	1.3949	C8-H8A	0.9900	0.9900
C18-C17	1.4629	1.4620	C8-H8B	0.9900	0.9899
C18-C23	1.4020	1.4005	C19-H19	0.9500	0.9499
C18-C19	1.3962	1.3963	C4-H4	0.9500	0.9499
C16-H16	0.9500	0.9500	C4-C3	1.3823	1.3802
C16-C17	1.3290	1.3343	C22-H22	0.9500	0.9500
C16-C15	1.4831	1.4821	C2-H2	0.9500	0.9500
C13-H13	0.9500	0.9499	C2-C3	1.3957	1.3899
C13-C14	1.3799	1.3812	C3-H3	0.9500	0.9500
C7-C8	1.5161	1.5172	C21-H21	-	0.9500
C21-C20	1.3823	1.3805	O4-N1	-	1.2273
C21-C22	1.3821	1.3900	O5-N1	-	1.2242
C17-H17	0.9500	0.9500	N1-C20	-	1.4707

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**Table S2.** The experimental (X-ray) geometric parameters of BCH and NCH: bond angle (°).

	BCH	NCH		BCH	NCH
C9–O2–C8	117.04	117.12	H8A–C8–H8B	108.42	108.37
C7–C6–C1	118.19	118.21	C18–C19–C20	121.73	119.22
C7–C6–C5	122.50	122.31	C18–C19–H19	119.13	120.38
C1–C6–C5	119.31	119.48	C20–C19–H19	119.13	120.40
O2–C9–C14	115.51	115.37	C5–C4–H4	119.64	119.73
O2–C9–C10	124.63	124.42	C5–C4–C3	120.72	120.53
C14–C9–C10	119.86	120.20	H4–C4–C3	119.64	119.75
C13–C12–C15	123.70	123.75	C21–C22–C23	119.38	120.49
C13–C12–C11	118.07	118.24	C21–C22–H22	120.31	119.75
C15–C12–C11	118.20	117.87	C23–C22–H22	120.31	119.76
C17–C18–C23	122.33	123.09	C1–C2–H2	120.14	120.00
C17–C18–C19	119.49	118.73	C1–C2–C3	119.72	120.00
C23–C18–C19	118.18	118.16	H2–C2–C3	120.14	120.00
H16–C16–C17	119.61	119.87	C4–C3–C2	119.75	119.92
H16–C16–C15	119.61	119.87	C4–C3–H3	120.12	120.03
C17–C16–C15	120.79	120.26	C2–C3–H3	120.12	120.04
C12–C13–H13	119.69	119.77	C20–C21–H21	-	121.19
C12–C13–C14	120.61	120.46	C22–C21–H21	-	121.19
H13–C13–C14	119.69	119.76	N1–C20–C19	-	117.77
O1–C7–C6	121.58	121.96	N1–C20–C21		119.13
O1–C7–C8	121.72	121.39	O4–N1–O5	-	123.58
C6–C7–C8	116.69	116.64	O4–N1–C20	-	118.45
Br1–C21–C20	119.36	-	O5–N1–C20	-	117.96
Br1–C21–C22	118.94	-	C6–C1–H1	119.69	119.86
C20–C21–C22	121.69	117.62	C6–C1–C2	120.62	120.30
C18–C17–C16	127.01	127.13	H1–C1–C2	119.69	119.85
C18–C17–H17	116.50	116.43	C18–C23–H23	119.68	119.30
C16–C17–H17	116.49	116.43	C18–C23–C22	120.65	121.40
O3–C15–C12	120.52	120.69	H23–C23–C22	119.68	119.30
O3–C15–C16	120.77	120.69	C6–C5–H5	120.07	120.13
C12–C15–C16	118.71	118.61	C6–C5–C4	119.87	119.75
C9–C14–C13	120.40	120.26	H5–C5–C4	120.07	120.12
C9–C14–H14	119.80	119.87	C21–C20–H20	120.82	-
C13–C14–H14	119.80	119.87	C21–C20–C19	118.36	123.09
C9–C10–H10	120.46	120.64	H20–C20–C19	120.82	-
C9–C10–C11	119.09	118.73	O2–C8–C7	108.09	108.40
H10–C10–C11	120.46	120.63	O2–C8–H8A	110.08	110.02
C12–C11–C10	121.95	121.99	O2–C8–H8B	110.08	110.02
C12–C11–H11	119.02	119.01	C7–C8–H8A	110.08	110.01
C10–C11–H11	119.02	119.01	C7–C8–H8B	110.08	110.02



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