

1 **Arylsulfonamide chalcones as alternatives for fuel additives: joint venture**
2 **antioxidant activity and machine learning protocols**

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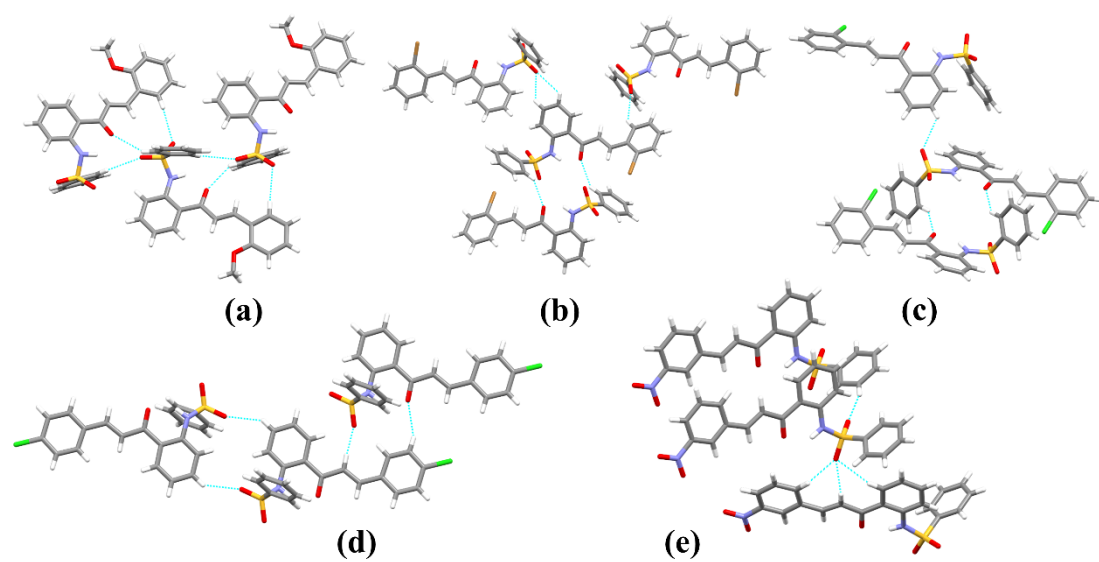
19 **1. Supplementary information**

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21 **Table S1.** Crystallographic data and refinement from Chal01 to Chal05 structures.

Parameters		Chal01	Chal02	Chal03	Chal04	Chal05
Chemical formula		C ₂₂ H ₁₉ O ₄ NS	C ₂₁ H ₁₆ O ₃ NSBr	C ₂₁ H ₁₆ O ₃ NSCl	C ₂₁ H ₁₆ O ₃ NSCl	C ₂₁ H ₁₆ O ₅ N ₂ S
Formula weight (g/mol)		393.44	442.34	397.86	397.86	408.42
Crystal system		monoclinic	monoclinic	monoclinic	triclinic	monoclinic
Space group		P2 ₁ /n	P2 ₁ /n	P2 ₁ /c	P $\bar{1}$	P2 ₁ /c
Z, Z'		4, 1	4, 1	4, 1	2, 1	4, 1
Unit cell parameters	a (Å)	11.670(12)	13.804(12)	13.795(7)	8.413(4)	14.014(16)
	b (Å)	12.555(13)	7.546(7)	7.584(4)	9.806(5)	7.656(9)
	c (Å)	13.331(14)	18.902(15)	20.272(9)	13.121(7)	18.38(2)
	α (°)	90	90	90	73.23(2)	90
	β (°)	101.004(3)	104.055(3)	62.896(3)	85.049(2)	101.242(4)
γ (°)		90	90	90	69.892(2)	90
Volume Cell (Å ³)		1917.6(3)	1910.2(3)	1888.07(17)	973.22(9)	1934.4(4)
Calculated density (g/cm ³)		1.363	1.5380	1.400	1.358	1.402
Goodness-of-fit		1.119	1.0514	1.040	1.022	1.047
Final R indices [I>2 σ (I)]	R ₁	0.0504	0.0314	0.0384	0.0444	0.0528
	wR ₂	0.1212	0.0730	0.1004	0.1089	0.1066
R indices (all data)	R ₁	0.0712	0.0410	0.0447	0.0646	0.0857
	wR ₂	0.1389	0.0778	0.1057	0.1211	0.1193

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24 **Figure S1.** Main interactions of the arylsulfonamide chalcones: Chal01 (a), Chal02 (b), Chal03
25 (c), Chal04 (d) and Chal05 (e).

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