SUPPLEMENTARY MATERIAL

Conformational Study, Synthesis, and Characterization of Chalcones Using 4-Hydroxy-3-methoxybenzaldehyde

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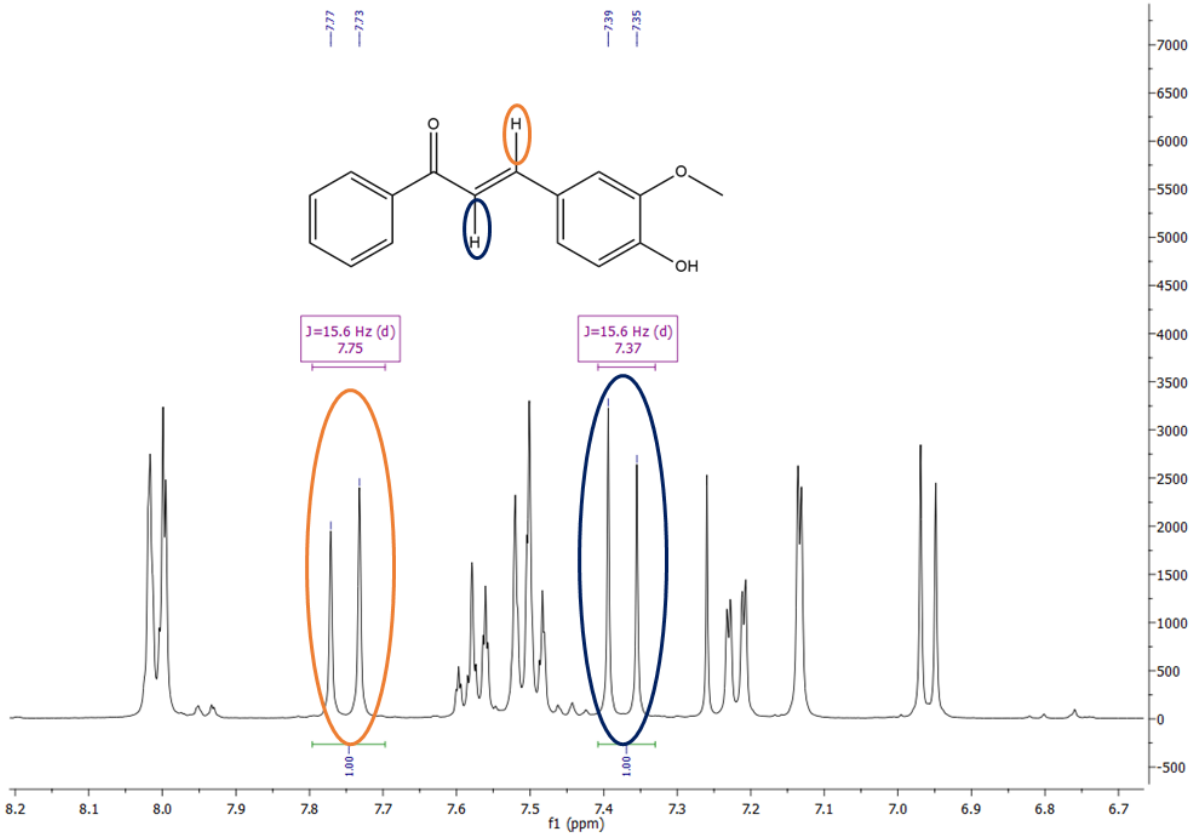

Figure S1: ^{1}H NMR spectrum of Chal 1 with approximation in the aromatic and vinylic region.

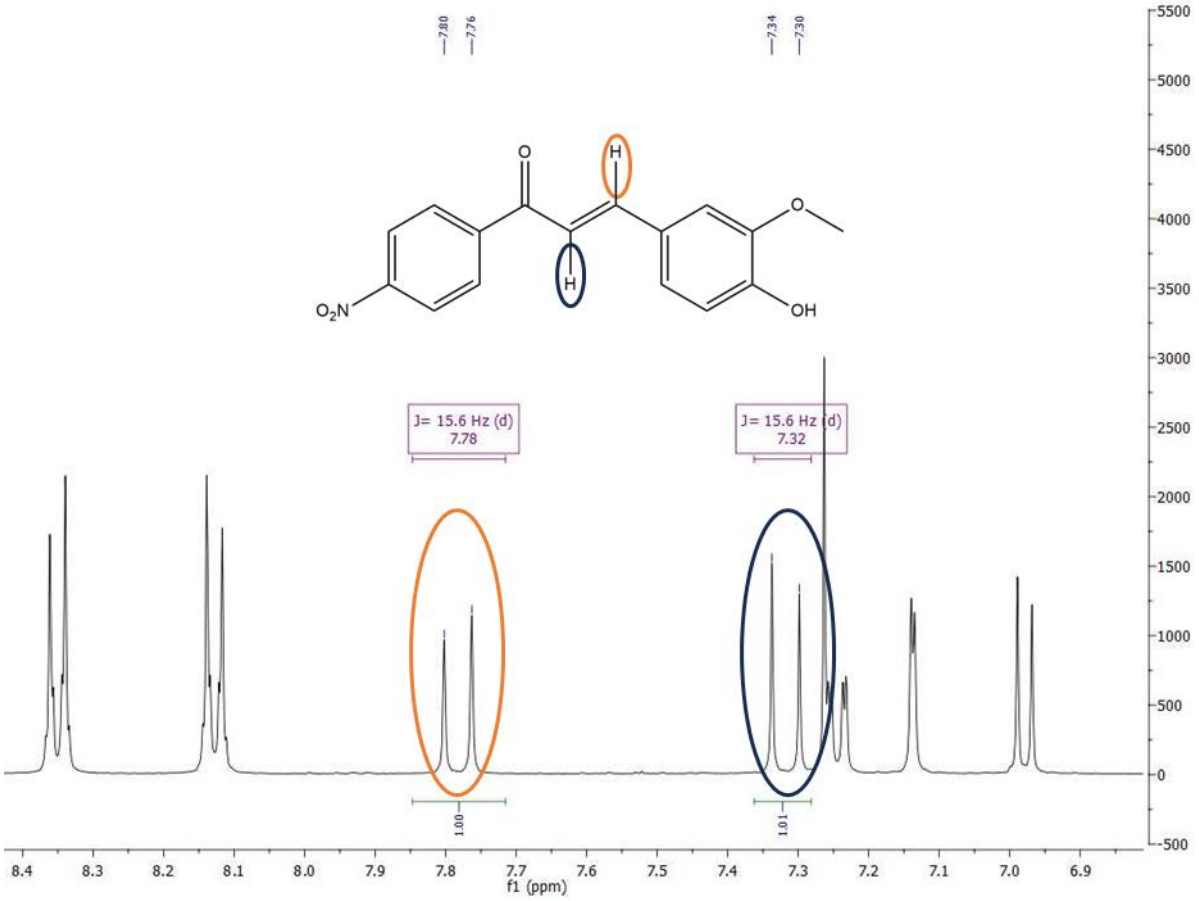

Figure S2: ^{1}H NMR spectrum of Chal 2 with approximation in the aromatic and vinylic region.

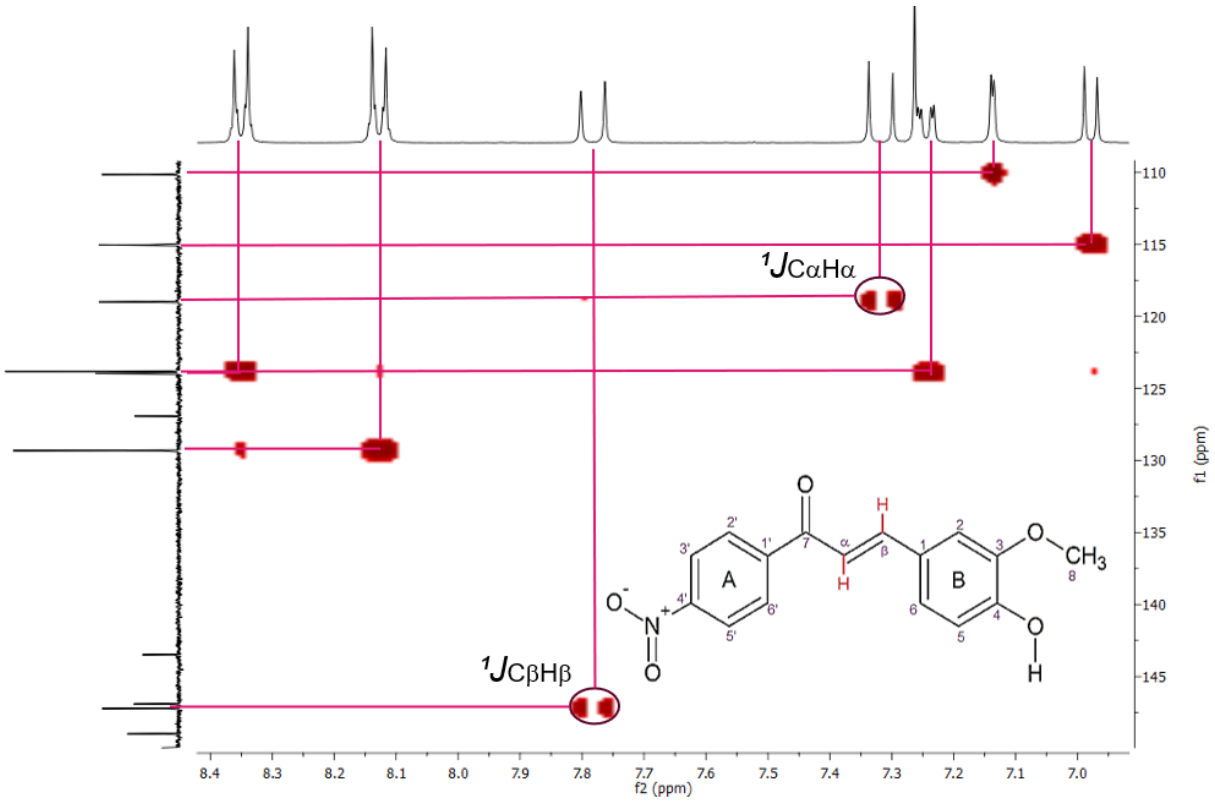

Figure S3: Two-dimensional HSQC NMR spectrum of Chal 2..

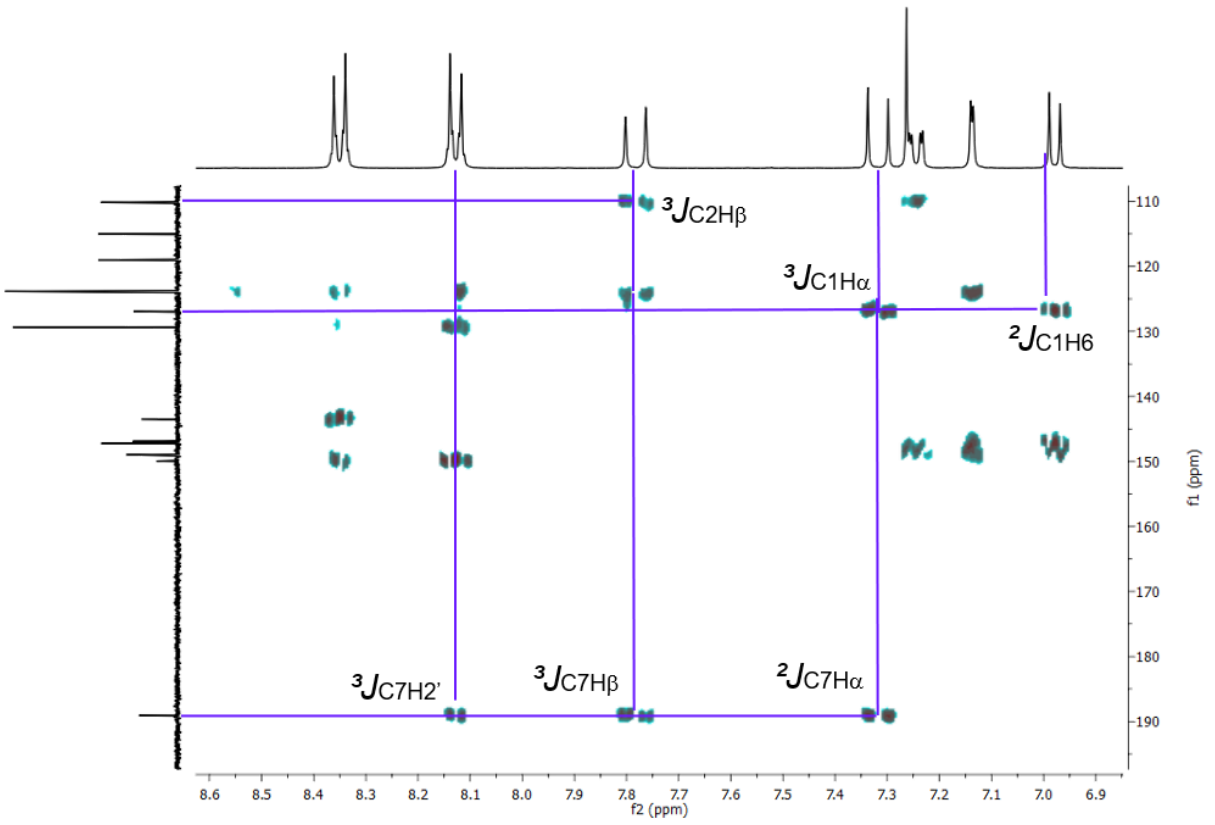

Figure S4: Two-dimensional HMBC NMR spectrum of Chal 2.

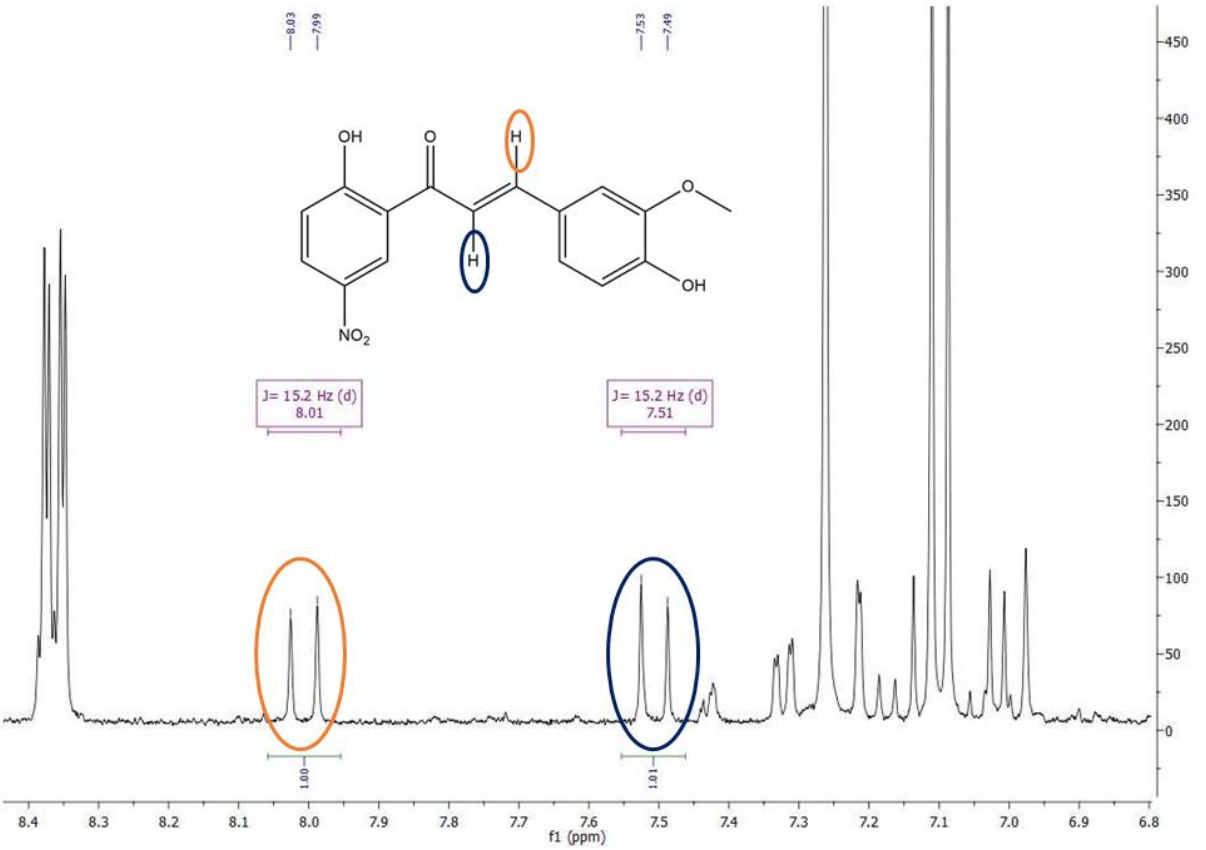

Figure S5: ^{1}H NMR spectrum of Chal 3 with approximation in the aromatic and vinylic region.

COMPOUND		ΔE	ANGLE		
		(kcal/mol)	*a*	*b*	*c*
CHAL 1	*s-trans*	1.61	153.42	167.57	146.99
	s-cis	0.89	7.26	179.91	162.29
	s-trans'	0.89	154.79	6.07	145.77
	s-cis	0.05	156.81	6.60	177.93
CHAL 2	*s-cis'*	0.00	158.15	7.34	2.85
	s-trans	0.45	36.71	158.40	177.91
	s-trans'	1.24	35.86	156.06	10.63
CHAL 3	*s-cis*	0.22	0.07	179.95	179.74
	s-cis'	0.00	0.02	0.01	179.99
	s-cis"	2.87	146.96	170.24	161.12
	s-trans	9.53	14.86	179.75	37.77

Table S1: Relative energies in kcal/mol and dihedral angles of the conformers of Chal 1, Chal 2, and Chal 3.