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Supporting information for article:

ss-NMR and single-crystal X-ray diffraction in the elucidation of a new polymorph of bischalcone (1*E*,4*E*)-1,5-bis(4-fluorophenyl)penta-1,4-dien-3-one

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Figure S1. 1H NMR spectra (500 MHz, CDCl3) δ (ppm) for the compounds **1**: 7.70 (d, 2H; J 15.87; H7 and H7'), 7.61 (m, 4H; H2, H6, H2' and H6'), 7.11 (t, 4H; J 8.70; H3, H5, H3' and H5'), 6.99 (d, 2H; J 15.87; H8 and H8'). **2**: 7.68 (d, 2H; J 15.87; H7 and H7'), 7.54 (m, 4H; H2, H6, H2' and H6'), 7.39 (m, 4H; H3, H5, H3' and H5'), 7.03 (d, 2H; J 15.87; H8 and H8'). **3**: 7.66 (d, 2H; J 15.87; H7 and H7'), 7.55 (m, 4 H; H2, H6, H2' and H6'), 7.47 (m, 4H; H3, H5, H3' and H5'), 7.04 (d, 2H; J 15.87; H8 and H8'). The superscript (') in hydrogen labels refers to the other atoms of molecule, related by two-fold axis symmetry and hidden in the figure for clarity.

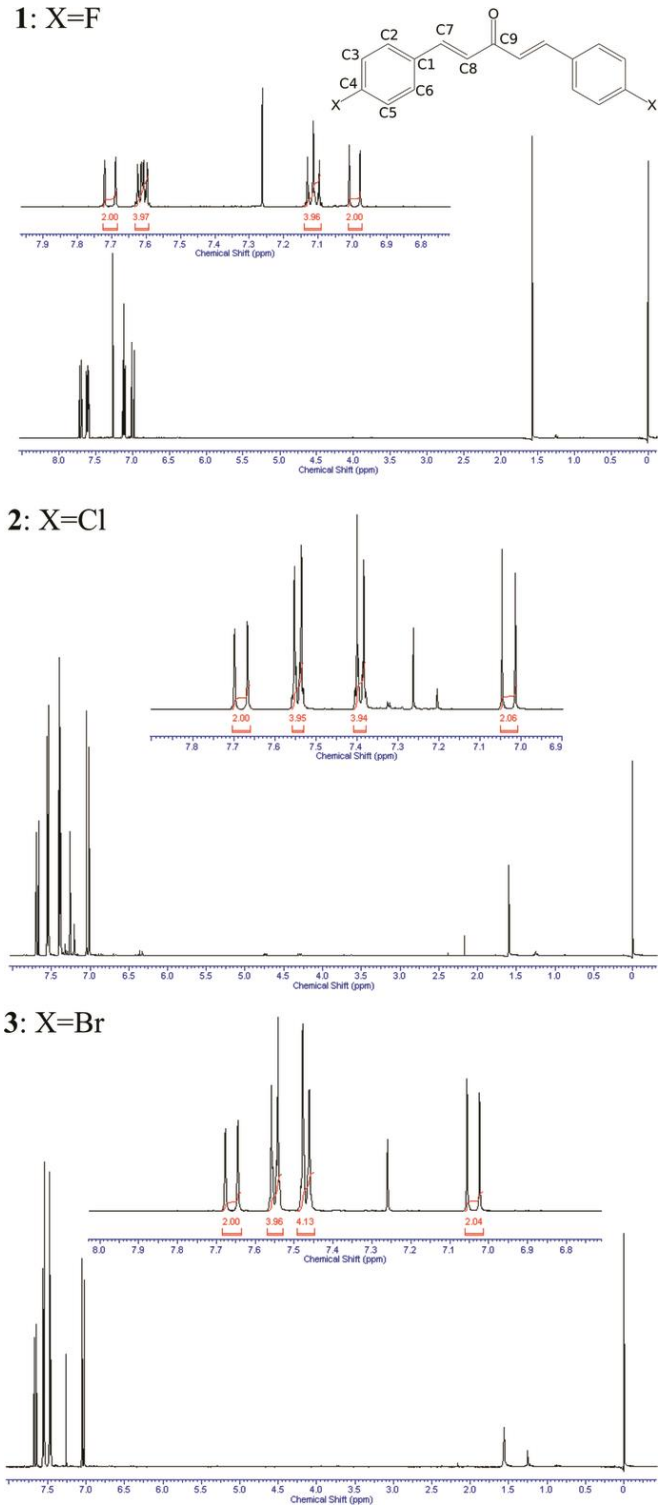

Figure S2. 13C NMR spectra (125 MHz, CDCl3) δ (ppm) for the compounds **1**: 188.46 (C9), 165.10 (C4 and C4'), 142.09 (C7 and C7'), 131.06 (C2, C6, C2' and C6'), 130.26 (C1 and C1'), 125,15 (C8 and C8'), 116.27 (C3, C5, C3' and C5'). **2**: 188.34 (C9), 142.06 (C7 and C7'), 136.54 (C1 and C1'), 133.25 (C4 and C4'), 129.56 (C2, C6, C2' and C6'), 129.31 (C3, C5, C3' and C5'), 125.75 (C8 and C8'). **3**: 188.33 (C9), 142.19 (C7 and C7'), 133.67 (C1 and C1'), 132.28 (C3, C5, C3' and C5'), 129.76 (C2, C6, C2' and C6'), 125.83 (C4, C8, C4' and C8'). The superscript (') in carbon labels refers to the other atoms of molecule, related by two-fold axis symmetry and hidden in the figure for clarity.

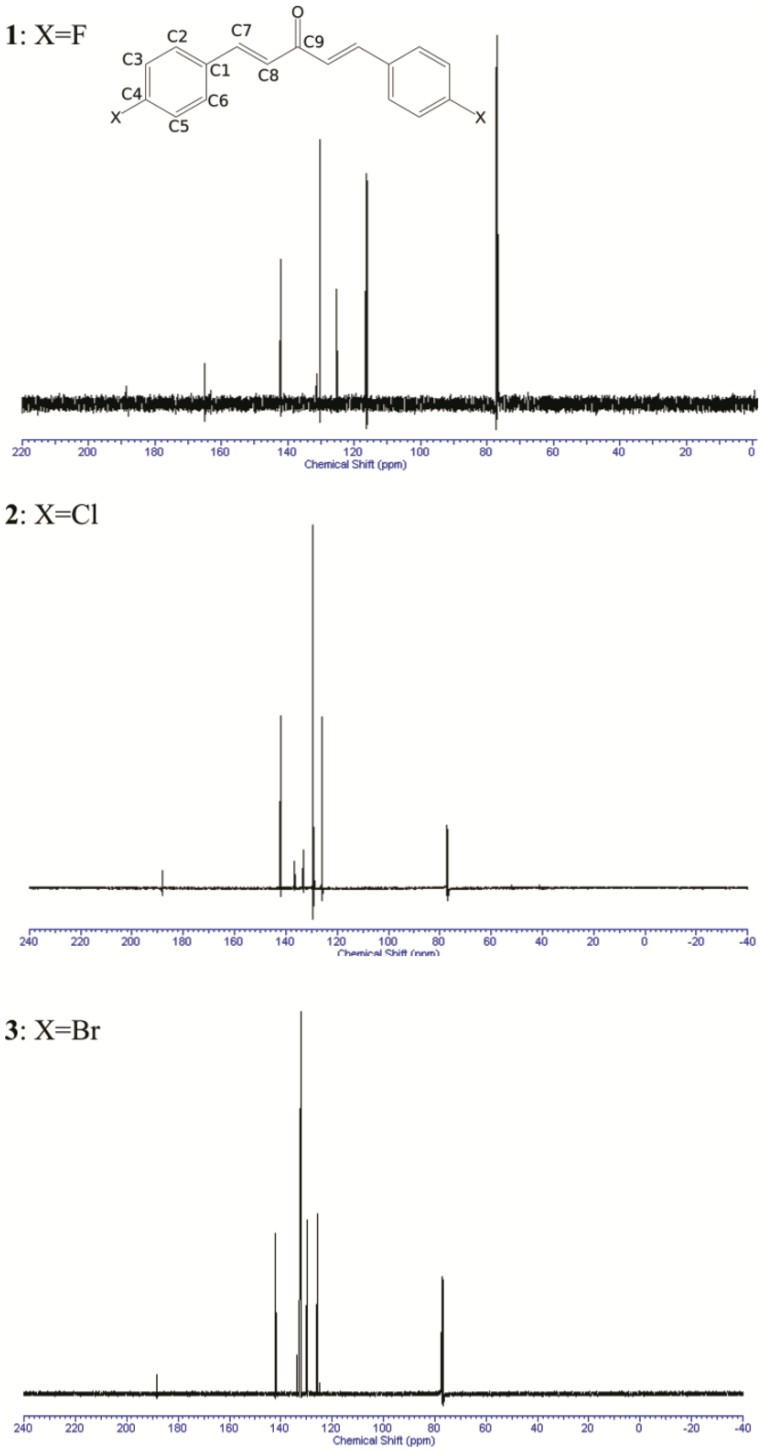

Figure S3. ESI(+)-orbitrap mass spectrum of compounds **1**-**3**. The *m/z* observed correspond to a bischalcone with a further hydrogen (proton) from the formic acid ([M+H]+). The found (and expected) *m/z* for [M+H]+ were 271.0953 (271.2813), 303.0384 (303.2222) and 392.9414 (393.0925) for **1**, **2** and **3**, respectively.

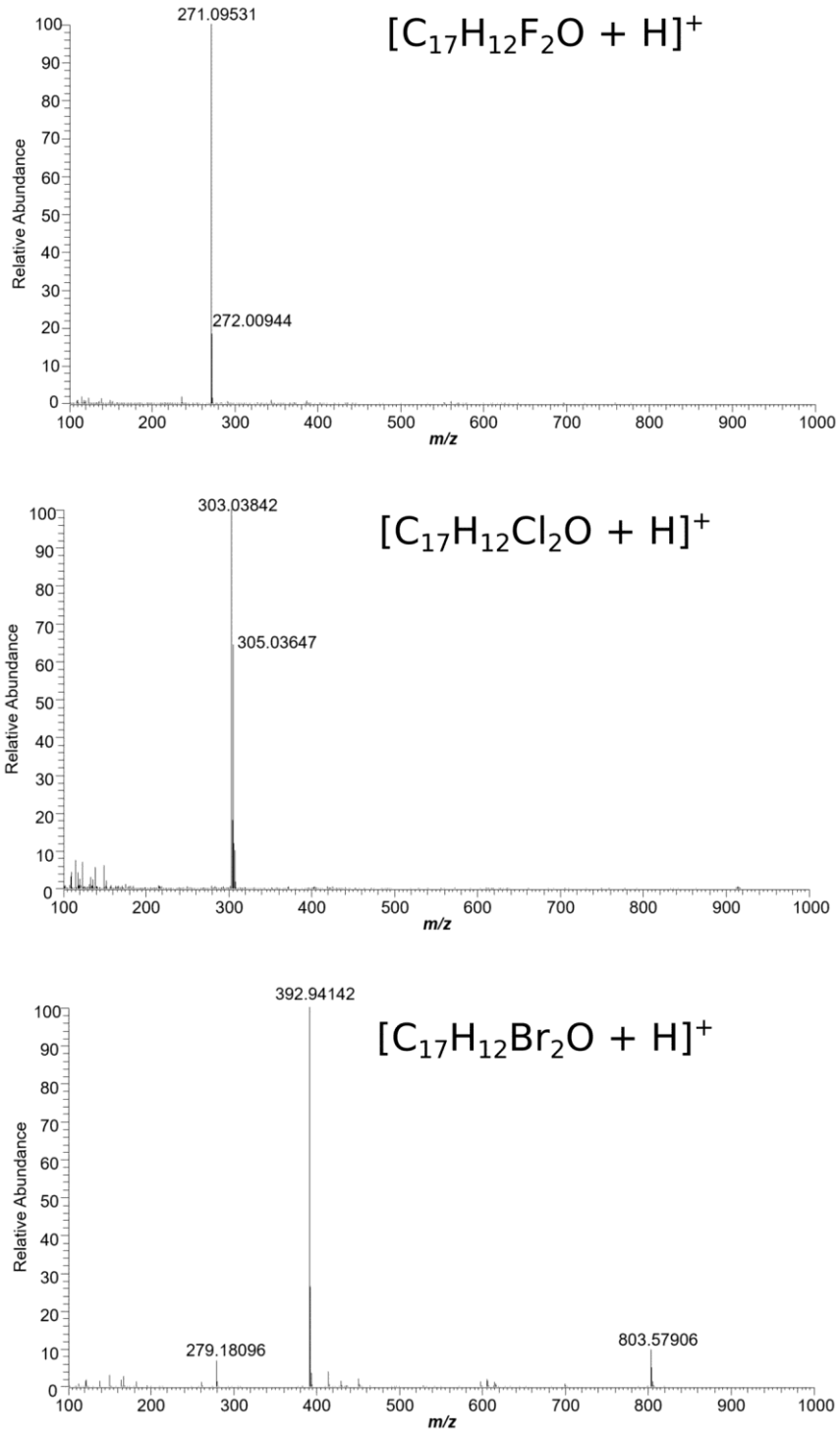

Figure S4. Infrared spectra of the compounds **1** (black), **2** (red) and **3** (blue). Assignments of vibrational modes (KBr, cm-1): 3051 [ν(O–H)], 1654 [ν(C=O)], 1594 [ν(C=C)], 1414 [ν(C=C)Ar], 1010 [in plane δ(C–H)Ar], 822 [out of plane δ(C–H)Ar], 519 [ν(C–F)] for **1**; 3050 [ν(O–H)], 1648 [ν(C=O)], 1589 [ν(C=C)], 1489 [ν(C=C)Ar], 1088 [in plane δ(C–H)Ar], 984 [out of plane δ(C–H)Ar], 489 [ν(C–Cl)] for **2**; 3051 [ν(O–H)], 1650 [ν(C=O)], 1592 [ν(C=C)], 1402 [ν(C=C)Ar], 1009 [in plane δ(C-H)Ar], 823 [out of plane δ(C–H)Ar], 488 [ν(C–Br)] for **3**.

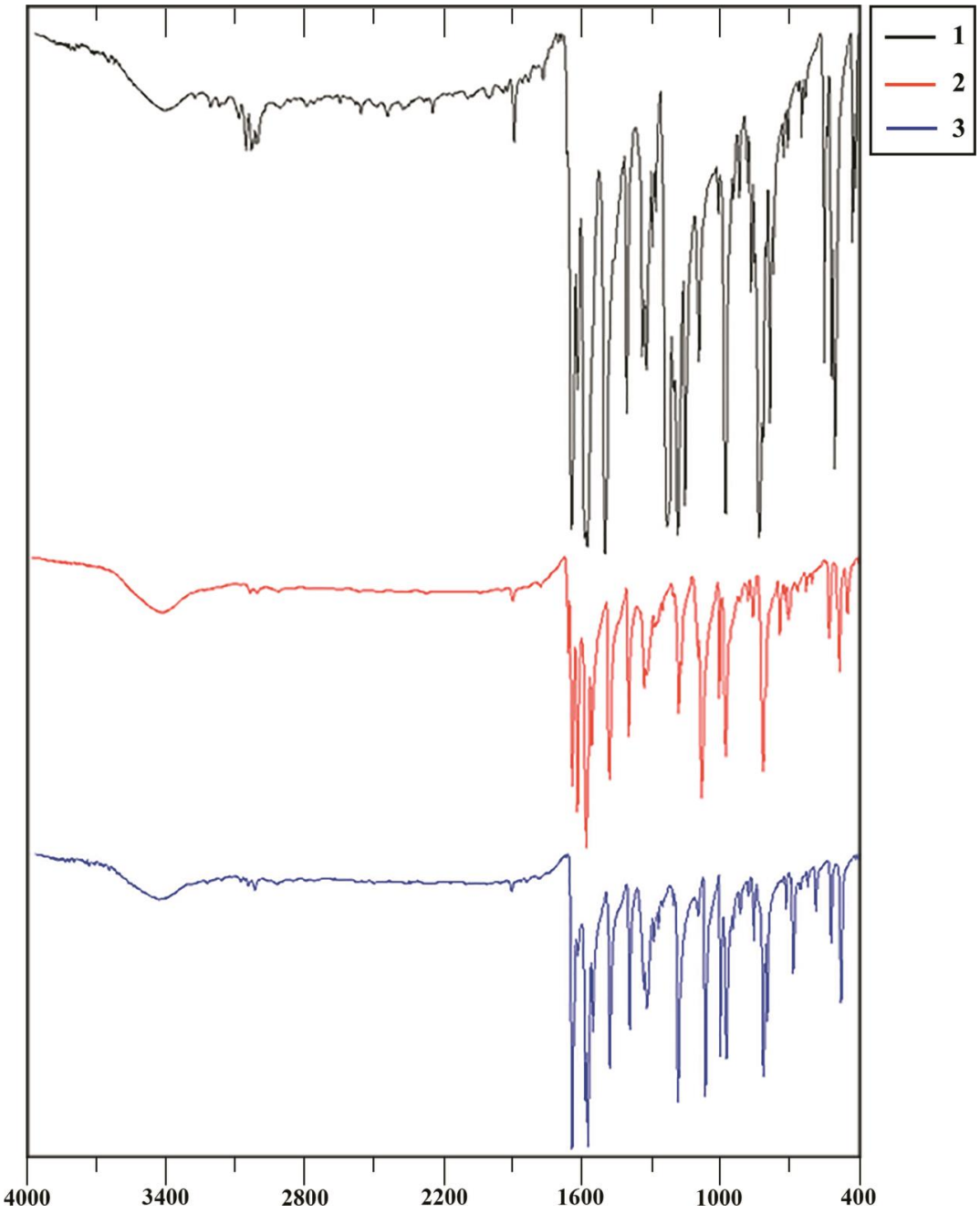

Figure S5. Full 13C ss-NMR spectrum of our polymorph of **1**.

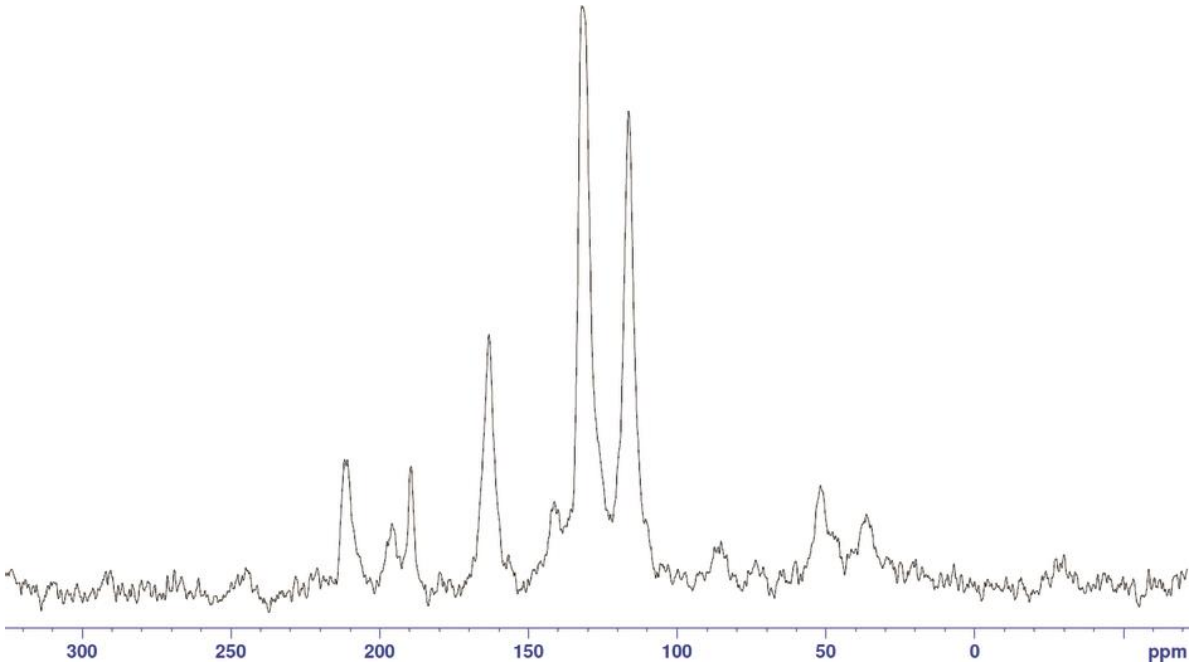

Table S1. Hydrogen-bond geometry (Å, °) for the literature polymorph of **1** (Butcher *et al*., 2007).

D – H · · · A	D – H	H· · ·A	D· · · A	D – H · · · A
C3AA – H3AA · · · F2CA	0.95	2.56	3.415 (4)	150
C3BA – H3BA · · · F2A^{iii}	0.95	2.66	3.319 (3)	127
C14A – H14A · · · F1B	0.95	2.66	3.342 (3)	129
C14C – H14C · · · F1A^{iii}	0.95	2.56	3.382 (3)	145

Symmetry code: (iii) x, -1+y, z