SUPPORTING INFORMATION

Design of potent fluoro-substituted chalcones as antimicrobial agents

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(E)-3-(4-fluorophenyl)-1-(2,4,6-trimethoxyphenyl)prop-2-en-1-one (11);

To a solution of 2,4,6-trimethoxyacetophenon (1) (1g, 4.75 mmol) in MeOH (20 mL) 4-F benzaldehyde (7) (0.6mL 7.6 mmol) and 50% KOH solution (10 mL) was added sequentially and stirred for 15 h at room temperature. After 15 h solvent was evaporated. 2M HCl solution (15 mL) was added and crude product was extracted with DCM (3x20 mL). The combined extracts were dried over Na₂SO₄. The solvent was removed in vacuo and the remaining residue purified via column chromatography over silica gel using gradient elution with EtOAc and Hexanes to yield compound 11, as a yellow solid (80% yield). Rf (EtOAc/Hexanes 30:70) = 0.27; MP = 122-123°C; IR (KBr, cm⁻¹) vmax 3502, 2941, 2841, 1651, 1599; Anal. calcd for C₁₈H₁₈O₄: C, 68.35; H, 5.42; Found: C, 68.16; H, 5.38

¹H NMR (400 MHz, CDCl₃) δ 7.52–7.48 (m, 2H), 7.32 (d, 1H, B part of AB system, J = 16 Hz.), 7.07–7.01 (m, 2H), 6.87 (d, 1H, A part of AB system, J = 16 Hz.), 6.15 (s, 2H), 3.84 (s, 3H), 3.76 (s, 6H).

¹³C NMR (100 MHz, CDCl₃) δ 194.1, 164.0 (d, C-20, J_CF=249.8 Hz), 162.7, 159.1, 142.8, 131.5, 130.4 (d, C-18, J_CF=8.4 Hz), 129.0, 116.1 (d, C-19, J_CF=21.7 Hz), 111.9, 90.9, 56.1, 55.7.

¹H NMR spectrum of compound 11.
$^{13}$C NMR spectrum of compound 11.