Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for "The effect of fluorination on the surface structure of truxenones"

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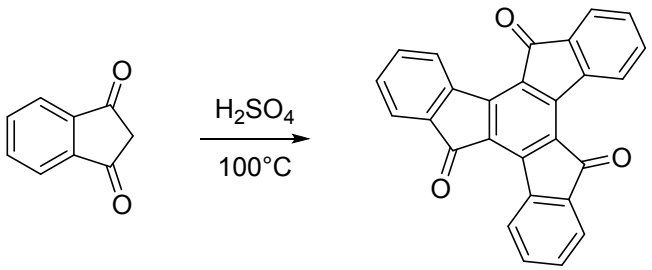
S1 – Synthesis and NMR analysis of truxenone

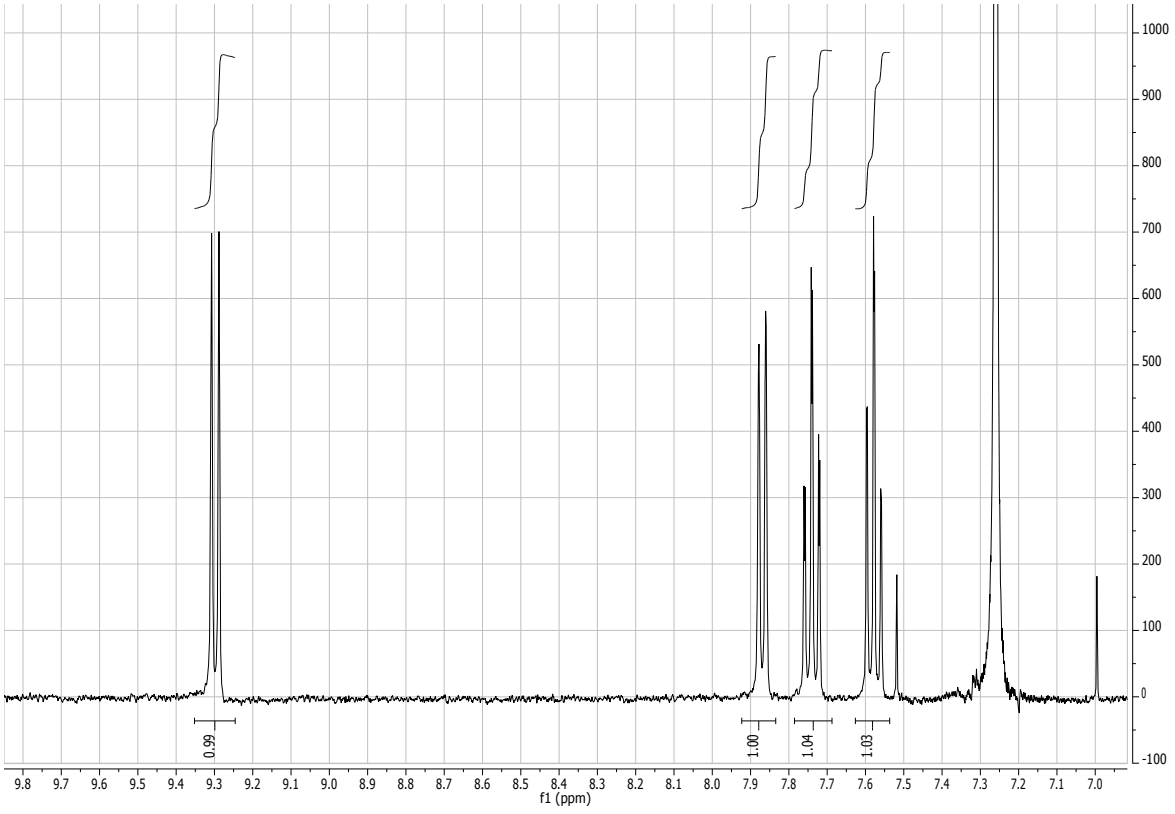


1

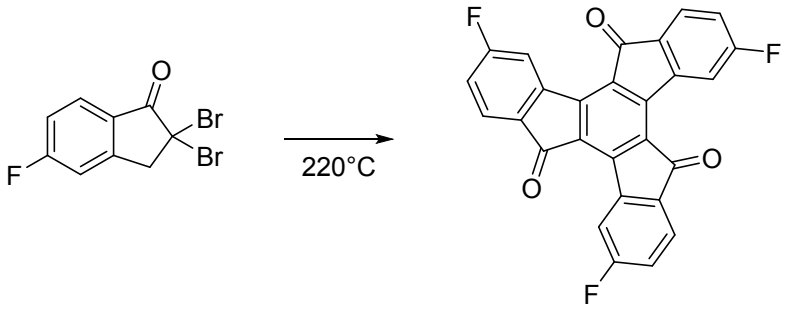
Truxenone (1)

1,3-Indanedione (20.00g, 137 mmol) was added portion-wise to concentrated sulphuric acid (200 ml) under stirring. The reaction mixture was heated to 100°C for 3 hours and subsequently poured onto ice (1L). The crude product was isolated by filtration and washed with copious amounts of water and acetone. The title compound was obtained as a yellow solid (13.81 g, 35.9 mmol, 79% yield) after trituration with dichloromethane.

1H NMR (400 MHz, chloroform-d, 293 K) δ 9.30 (dt, J = 7.7, 1.0 Hz, 1H), 7.90 – 7.83 (dt, J = 7.4, 1.0 Hz, 1H), 7.74 (td, J = 7.7, 1.0 Hz, 1H), 7.58 (td, J = 7.4, 1.0 Hz, 1H).



S2 – Synthesis and NMR analysis of 4,9,14-trifluorotruxenone

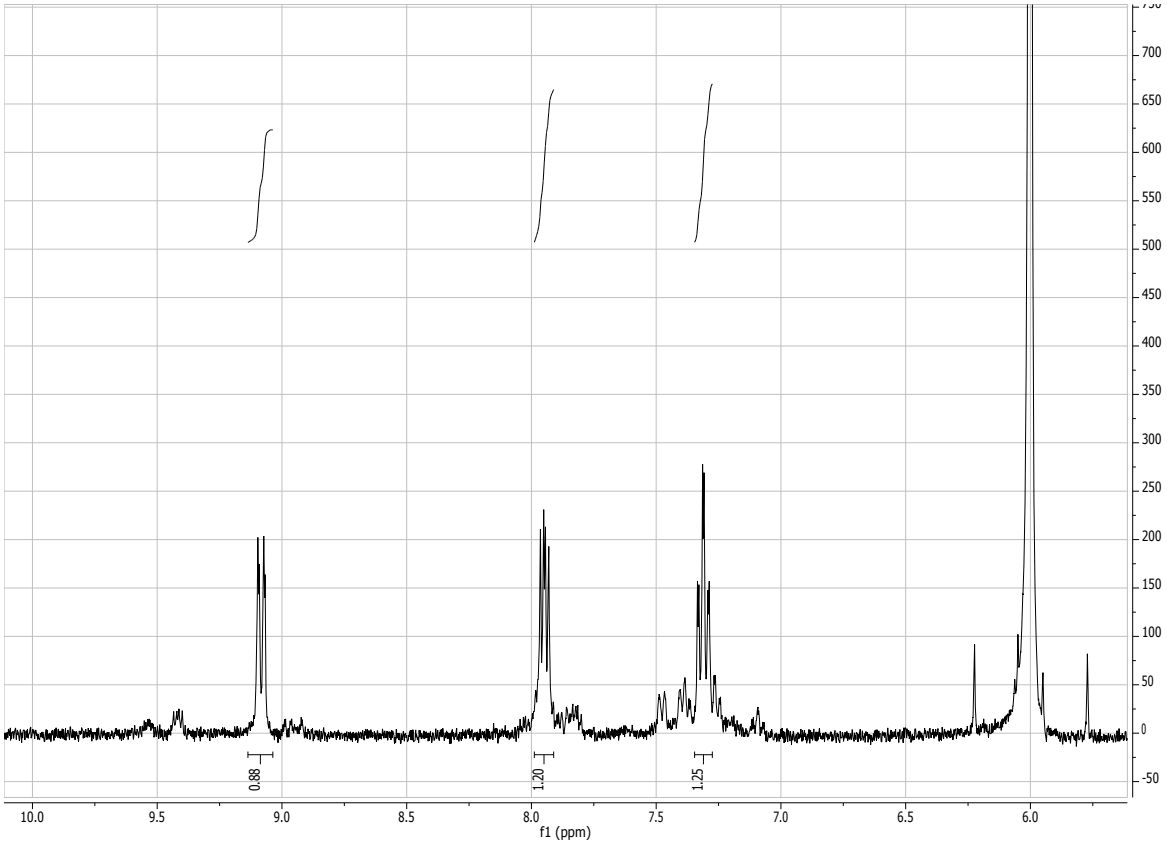


2

4,9,14-Trifluorotruxenone (2)

2,2-Dibromo-5-fluoroindan-1-one (1.40 g, 4.55 mmol) was placed in a round-bottom flask and under argon flow heated to 220°C with stirring for 1 hour. The crude product was washed with chloroform and dichloromethane to afford the title compound as a yellow solid (172 mg, 0.392 mmol, 26% yield).

1H NMR (400 MHz, 1,1,2,2-tetrachloroethane-d2, 393 K) δ 9.08 (dd, J = 9.5, 2.2 Hz, 1H), 7.95 (dd, J = 8.2, 5.3 Hz, 1H), 7.31 (td, J = 8.2, 2.2 Hz, 1H).



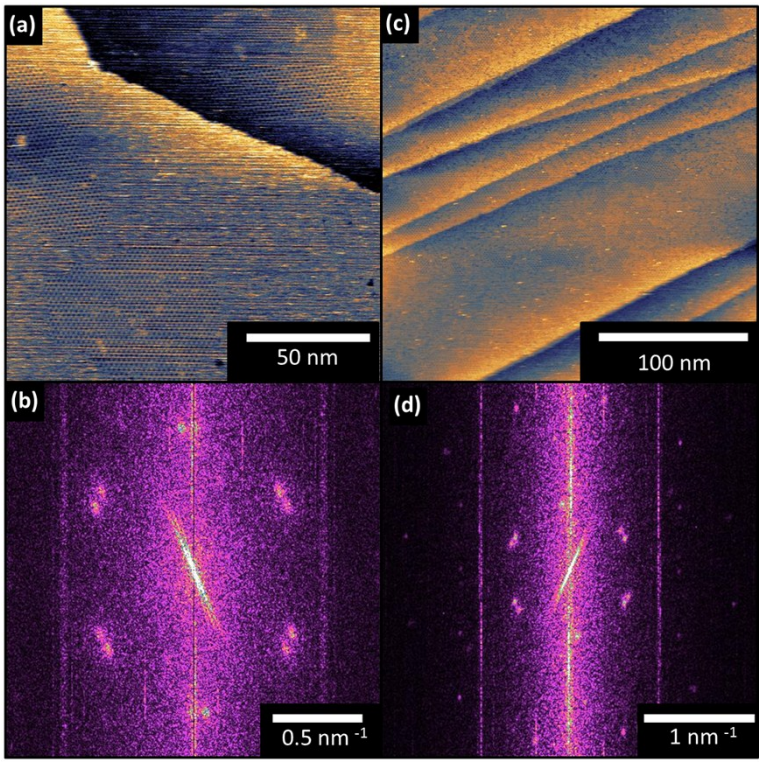


Figure S3 - STM images of F_3-truxenone / Cu (111) with corresponding 2D-FFT images at (a) high (V_S = −2 V, I_T = 65 pA) / (b) and lower (c) (V_S = −1.5 V, I_T = 125 pA) / (d) magnification.