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# Supplementary Information for New Journal of Chemistry

# Synthesis of New Mixed-Bistriarylmethanes and Novel 3,4-Dihydropyrimidin-2(1H)-ones

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#### 1. General Considerations

All materials were obtained from commercial sources and were used as received. The progress of the reactions was monitored by TLC analysis using polyester sheets pre-coated with silica gel-60 and fluorescent indicator (F-252),

commercially available from Merck company. Melting points were determined by Stuart SMP2 apparatus and are uncorrected. FT-IR spectra were recorded as KBr pellets using a Nicolet-Impact 400D spectrophotometer. <sup>1</sup>H, <sup>13</sup>C, APT, and GCOSY spectra were acquired on a Varian UNITYInova 500 MHz spectrometer.

#### 2. Methods

# 2.1. Preparation of silica-supported sulfuric acid

Sulfuric acid immobilized on silica gel (SiO<sub>2</sub>-H<sub>2</sub>SO<sub>4</sub>) was prepared according to literature.<sup>41</sup> Silica gel (10 g, 200-300 mesh) was dispersed in dry Et<sub>2</sub>O (100 mL). Under slow stirring, concentrated H<sub>2</sub>SO<sub>4</sub> (3.2 mL, 98%) was added dropwise to the resulting mixture over 10 minutes, and stirring continued at rt for a further 10 min. After removal of the volatiles, the resulting solid powder was dried overnight at 60 °C.

# 2.2. General procedure for the synthesis of formylated-triarylmethanes under grinding conditions (Table 2, 6a-h)

In an open mortar, a mixture of arene **4** (2.3 mmol), the corresponding dialdehyde **5** (1 mmol), and  $SiO_2-H_2SO_4$  (300 mg) was ground together using a pestle at room temperature for appropriate time (Table 2), and left to harden for about 2 hours. The progress of the reaction was monitored by TLC (*n*-hexane/EtOAc 10:4). Then, the resultant mixture was transferred into a flask and washed twice with ethanol (2 × 5 mL), and catalyst was separated by simple filtration. The crude product was purified by recrystallization from EtOH or flash column chromatography on silica gel, to provide product **6**.

# 2.3. General procedure for the synthesis of mixed-bistriarylmethanes under grinding conditions (Scheme 5, 13a-h)

A mixture of formylated-triarylmethane **6** (1 mmol), arene **4** (2.3 mmol), and  $SiO_2-H_2SO_4$  (300 mg) was ground in a mortar with a pestle at room temperature for allotted time, and left to harden for about 2 hours. The progress of the reaction was monitored by TLC (eluent: petroleum ether/EtOAc 1:1). Then, the resultant mixture was transferred into a flask and washed twice with CHCl<sub>3</sub> (2 × 5 mL), and catalyst was separated by simple filtration. The solvent was evaporated and the residue purified by recrystallization from EtOH or by flash column chromatography on silica gel; elution with 1:1 petroleum ether/EtOAc or 10:2 petroleum ether/MeOH, to obtain Pure mixed-bistriarylmethane **13.** 

# 2.4. General Procedure for the synthesis of 3,4-dihydropyrimidin-2(1H)-(thi)one-triarylmethane hybrid derivatives (Table 3, 17a-j).

A 25 mL round-bottom flask equipped with a magnetic stir bar was charged with formylated-triarylmethane **5** (1 mmol), ethylacetoacetate **15** (1.1 mmol), urea **16a** (1.5 mmol), and  $SiO_2-H_2SO_4$  (100 mg). The resulting mixture was stirred at 95 °C, for required time. The reaction progress was checked by TLC (*n*-Hexan/EtOAc 3:1 as eluent). Upon completion, EtOH (2 × 5 mL) was added to the reaction mixture and catalyst was filtered off. The volatiles of resulting organic solution was evaporated and the residue was washed twice by water (2 × 10 mL). The crude product was purified from EtOH, by flash column chromatography on silica gel; elution with 1:1 *n*-Hexan/EtOAc, to obtain pure product **17**.

# 3. Spectroscopic data

#### 3.1. Formylated-Triarylmethanes (6a-h), and compound 6i

4-(bis(3,4-dimethoxyphenyl)methyl)benzaldehyde (6a) 2h-j, 3r



White solid. Yield 91%. mp 128-129 °C. FT- IR (KBr):  $\tilde{v}$  2999, 2929, 1602, 1516, 1465, 1344, 1267, 1138, 1026, 858, 794, 756 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 9.99 (1H, s, C<u>H</u>O), 7.81 (2H, d, *J* = 8.2 Hz, 3,5-H 4-formylphenyl), 7.30 (2H, d, *J* = 8.2 Hz, 2,6-H 4-formylphenyl), 6.81 (2H, d, *J* = 8.3 Hz, 5-H vreatryl), 6.65 (2H, d, *J* = 2.0 Hz, 2-H veratryl), 6.59 (2H, dd, *J* = 8.3 Hz, *J* = 2 Hz, 6-H veratryl), 5.51 (1H, s, Ar<sub>3</sub>C<u>H</u>), 3.87 (6H, s, OMe), 3.77 (6H, s, OMe) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 191.83, 151.61, 149.04, 147.89, 135.58, 134.82, 129.97, 129.77, 121.45, 112.79, 111.14, 56.10, 55.90 ppm.

3-(bis(3,4-dimethoxyphenyl)methyl)benzaldehyde(6b) 3r



White solid. Yield 87%. mp 93-94 °C. FT- IR (KBr):  $\tilde{v}$  2997, 2933, 2829, 1697, 1588, 1512, 1461, 1357, 1242, 1137, 1020, 859, 813, 748, 756 cm<sup>-1</sup>. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>):  $\delta$  9.87 (1H, s, CHO), 7.67 (1H, d, *J* = 7.4 Hz, 4-H 3-formylphenyl), 7.56 (1H, s, 2-H 3-formylphenyl), 7.38 (1H, t, *J* = 7.5 Hz, 5-H 3-formylphenyl), 7.31 (1H, d, *J* = 7.4 Hz, 6-H 3-formylphenyl), 6.72 (2H, d, *J* = 8.3 Hz, 5-H vreatryl), 6.57 (2H, d, *J* = 2.0 Hz, 2-H veratryl), 6.52 (2H, dd, *J* = 8.3 Hz, *J* = 2.0 Hz, 6-H veratryl), 5.44 (1H, s, Ar<sub>3</sub>CH), 3.78 (6H, s, OMe), 3.68 (6H, s, OMe) ppm. <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>):  $\delta$  192.42, 148.94, 147.57, 145.66, 135.39, 130.51, 129.00, 127.78, 121.38, 112.63, 110.99, 55.87, 55.86, 55.64 ppm.

4-(bis (2-methoxy-5-methyl phenyl) methyl) benzaldehyde (6c)



White solid. Yield: 96%. mp 144-146 °C. FT- IR (KBr):  $\tilde{v}$  2939, 2833, 1700, 1602, 1573, 1497, 1463, 1386, 1241, 1109, 1034, 808 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  = 9.97 (s, 1H, C<u>H</u>O), 7.76 (d, *J* = 8.0 Hz, 2H, H<sub>e</sub>), 7.22 (d, *J* = 7.8 Hz, 2H, H<sub>f</sub>), 7.03 (d, *J* = 7.3 Hz, 2H, H<sub>c</sub>), 6.79 (d, *J* = 8.1 Hz, 2H, H<sub>b</sub>), 6.59 (s, 2H, H<sub>d</sub>), 6.20 (s, 1H, H<sub>a</sub>), 3.66 (s, 6H, OMe), 2.20 (s, 6H, Me) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  192.2, 155.2 (× 2), 134.3, 131.2, 131.0, 129.8, 129.5, 129.4, 128.0, 111.90, 55.8, 43.6, 20.7 ppm.

3-(bis (2-methoxy-5-methyl phenyl) methyl) benzaldehyde (6d)



White solid. Yield: 91%. mp 93-95 °C. FT- IR (KBr):  $\tilde{v}$  2999, 2922, 2834, 2727, 1699, 1609, 1583, 1497, 1383, 1241, 1110, 1034, 809 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  9.94 (s, 1H, C<u>H</u>O), 7.72 (d, *J* = 7.5 Hz, 1H, H<sub>f</sub>), 7.58 (s, 1H, H<sub>e</sub>), 7.40 (t, *J* = 7.6 Hz, 1H, H<sub>g</sub>), 7.35 (d, *J* = 7.6 Hz, 1H, H<sub>h</sub>), 7.03 (d, *J* = 7.1 Hz, 2H, H<sub>c</sub>), 6.79 (d, *J* = 8.2 Hz, 2H, H<sub>b</sub>), 6.59 (s, 2H, H<sub>d</sub>), 6.23 (s, 1H, H<sub>a</sub>), 3.67 (s, 6H, OMe), 2.21 (s, 6H, Me), ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  192.81, 155.17, 145.66, 136.26, 135.44, 131.36, 130.99, 130.69, 129.33, 128.52, 127.92, 126.87, 110.97, 55.86, 43.08, 20.76 ppm.

4-(bis(5-chloro-2-methoxyphenyl)methyl)benzaldehyde (6e)



White solid. Yield: 93%. mp 162-164 °C; FT- IR (KBr):  $\tilde{v}$  3013, 2960, 2903, 1835, 1700, 1605, 1485, 1244, 1212, 1122, 1028, 812, 766 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  9.99 (s, 1H, C<u>H</u>O), 7.80 (d, *J* = 8.0 Hz, 2H, H<sub>e</sub>), 7.19-7.22 (m, 4H, H<sub>c</sub> and H<sub>b</sub>), 6.81 (d, *J* = 8.7 Hz, 2H, H<sub>f</sub>), 6.70 (d, *J* = 2.6 Hz, 2H, H<sub>d</sub>), 6.12 (s, 1H, H<sub>a</sub>), 3.68 (s, 6H, OMe) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  191.94, 155.69, 149.80, 134.84, 132.48, 129.77, 129.72, 129.60, 127.83, 125.44, 112.05, 58.44, 55.87, 43.79 ppm.

4-(bis(5-bromo-2-methoxyphenyl)methyl)benzaldehyde (6f)



White solid. Yield: 89%. mp 117-119 °C. FT- IR (KBr):  $\tilde{v}$  3011, 2960, 2836, 1700, 1605, 1485, 1461, 1246, 1115, 1028, 810, 759 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 9.99 (s, 1H, C<u>H</u>O), 7.79 (d, *J* = 8.2 Hz, 2H, H<sub>e</sub>), 7.35 (dd, *J*<sub>I</sub> = 8.7 Hz, *J*<sub>2</sub> = 2.5 Hz, 2H, H<sub>c</sub>), 7.20 (d, *J* = 8.1 Hz, 2H, H<sub>f</sub>), 6.83 (d, *J* = 2.6 Hz, 2H, H<sub>b</sub>), 6.76 (d, *J* = 8.7 Hz, 2H, H<sub>d</sub>), 6.10 (s, 1H, H<sub>a</sub>), 3.67 (s, 6H, OMe) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 191.92, 156.20, 149.70, 134.85, 132.95, 132.39, 130.88, 129.77, 129.73, 112.86, 112.61, 58.43, 55.81, 43.80 ppm.

4-(bis(4-methoxy phenyl)methyl)benzaldehyde (6g)



Oily. Yield: 83%, FT-IR (KBr):  $\tilde{v}$  2933, 2834, 2735, 1699, 1606, 1510, 1464 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  9.99 (s, 1H, C<u>H</u>O), 7.81 (dd,  $J_1$  = 8.2 Hz,  $J_2$  = 1.6 Hz, 2H, H<sub>b</sub>), 7.29 (dd,  $J_1$  = 8.2 Hz,  $J_2$  = 1.6 Hz, 2H, H<sub>a</sub>), 7.02 (dd,  $J_1$  = 8.5 Hz,  $J_2$  = 1.6 Hz, 4H, H<sub>c</sub>), 6.85 (dd,  $J_1$  = 8.6 Hz,  $J_2$  = 1.6 Hz, 4H, H<sub>d</sub>), 5.53 (s, 1H, Ar<sub>3</sub>C<u>H</u>), 3.80 (s, 6H, OMe) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  191.95, 158.25, 151.93, 135.26, 130.24, 129.96, 129.80, 113.87, 55.35, 55.25 ppm.

4-(bis(3,4-dimethylphenyl)methyl)benzaldehyde (6h)



Oily. Yield 67%. FT- IR (KBr):  $\tilde{v}$  3011, 2921, 2856, 2732, 1701, 1604, 1574, 1502, 1452, 1212, 1168, 789, 757 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  10.02 (s, 1H, C<u>H</u>O), 7.84 (d, *J* = 8.0 Hz, 2H, H<sub>f</sub>), 7.36 (d, *J* = 8.0 Hz, 2H, H<sub>e</sub>), 7.12 (d, *J* = 7.6, 2H, H<sub>d</sub>), 6.97 (s, 2H, H<sub>b</sub>), 6.88 (d, *J* = 7.5 Hz, 2H, H<sub>c</sub>), 5.54 (s, 1H, H<sub>a</sub>), 2.30 (s, 6H, Me<sub>b</sub>), 2.26 (s, 6H, Me<sub>b</sub>) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  151.89, 140.56, 136.65, 134.84, 134.68, 130.10, 129.76, 129.75, 126.74, 56.41, 19.88, 19.38 ppm.

4-(bis(5-bromothiophen-2-yl)methyl)benzaldehyde (6i)



Oily. Yield 87%. FT- IR (KBr):  $\tilde{v}$  1699, 1604, 1436, 1210, 964, 913, 745, 512 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 10.01 (s, 1H, CHO), 7.87 (d, *J* = 8.3 Hz, 2H, H<sub>b</sub>), 7.45 (d, *J* = 8.2 Hz, 2H, H<sub>a</sub>), 6.92 (d, *J* = 3.8 Hz, 2H, H<sub>e</sub>), 6.59 (dd, *J*<sub>1</sub> = 3.8 Hz, *J*<sub>2</sub> = 1.1 Hz, 2H, H<sub>d</sub>), 5.74 (s, 1H, H<sub>c</sub>) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 191.44, 148.50, 146.70, 135.74, 130.16, 129.63, 128.93, 126.89, 124.06, 112.13, 74.86 ppm.

4-(bis(4-hydroxyphenyl)methyl)benzaldehyde (6j)



Oily. Yield 53%. FT- IR (KBr):  $\tilde{v}$  3367, 2926, 1694, 1601, 1510, 1217, 772 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  9.94 (s, 1H, CHO), 9.33 (sb, 2H, OH), 7.81 (d, *J* = 8.3 Hz, 2H, H<sub>b</sub>), 7.28 (d, *J* = 8.2 Hz, 2H, H<sub>a</sub>), 6.87 (d, *J* = 8.6 Hz, 4H, H<sub>c</sub>), 6.68 (d, *J* = 8.6 Hz, 4H, H<sub>d</sub>), 5.47 (s, 1H, Ar<sub>3</sub>CH) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  193.03, 156.23, 152.67, 134.72, 134.12, 130.32, 130.06, 129.96, 115.61, 54.87 ppm.

4-(bis(5-(tert-butyl)-2-hydroxyphenyl)methyl)benzaldehyde (6k)



White solid. Yield: 68%. mp 191-193 °C. FT- IR (KBr):  $\tilde{v}$  3537, 3375, 2959, 1682, 1601, 1509, 1461, 1419, 1392, 1272, 1215, 1123, 1089, 818 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 9.96 (s, 1H, CHO), 7.80 (d, *J* = 8.3 Hz, 2H, H*b*), 7.34 (d, *J* = 8.2 Hz, 2H, H<sub>a</sub>), 7.16 (dd, *J*<sub>1</sub> = 8.4 Hz, *J*<sub>2</sub> = 2.5 Hz, 2H, H<sub>d</sub>), 6.98 (d, *J* = 2.4 Hz, 2H, H<sub>e</sub>), 6.76 (d, *J* = 8.4 Hz, 2H, H<sub>c</sub>), 6.09 (s, 1H, Ar<sub>3</sub>CH), 5.74 (sb, 2H, OH), 1.19 (s, 18H, *tert*-Butyl) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 192.50, 150.97, 150.33, 143.87, 134.55, 129.83, 129.79, 127.78, 127.34, 124.85, 115.67, 44.49, 34.12, 31.40 ppm.

4-(14H-dibenzo[a,j]xanthen-14-yl)benzaldehyde (6l) 42,43



White solid. Yield: 93%. mp 253-254 °C. FT- IR (KBr):  $\tilde{v}$  3065, 2921, 2859, 2771, 1690, 1593, 1519, 1238, 827 cm<sup>-1</sup>. 1H NMR (500 MHz, DMSO-d<sub>6</sub>): δ 9.75 (s, 1H, CHO), 8.67 (d, *J* = 8.6 Hz, 2H), 7.92-7.98 (m, 4H), 7.86 (d, *J* = 8.2 Hz, 2H), 7.68 (d, *J* = 8.4,

2H), 7.6-7.65 (m, 2H), 7.57 (d, *J* = 8.9 Hz, 2H), 7.43-7.48 (m, 2H), 6.84 (s, 1H, Ar<sub>2</sub>C<u>H</u>) ppm. <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>): δ 192.64, 152.33, 148.45, 134.87, 131.26, 131.09, 130.18, 129.86, 129.11, 129.09, 127.54, 125.10, 123.70, 118.16, 116.95, 37.15 ppm.

#### 3.2. Adduct 12, mixed-bistriarylmethanes (13a-i), and product 14

1,3-bis(bis(2-methoxy-5-methylphenyl)methyl)benzene (12)



White Solid. Yield 21%. mp 216-218 °C. FT- IR (KBr):  $\tilde{v}$  3017, 2954, 2933, 2134, 1589, 1512, 1463, 1262, 1245, 1140, 1027, 755 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.11 (t, *J* = 7.6 Hz, 1H, H<sub>g</sub>), 6.96 (dd, *J*<sub>1</sub> = 8.2 Hz, *J*<sub>2</sub> = 2.2 Hz, 4H, Hc), 6.84 (dd, *J*<sub>1</sub> = 7.6 Hz, *J*<sub>2</sub> = 1.8 Hz, 2H, H<sub>f</sub>), 6.81 (s, 1H, H<sub>e</sub>), 6.73 (d, *J* = 8.2 Hz, 4H, H<sub>d</sub>), 6.54 (d, *J* = 2.2 Hz, 4H, H<sub>b</sub>), 6.04 (s, 2H, H<sub>a</sub>), 3.60 (s, 12H, OMe × 4), 2.17 (s, 12H, Me × 4) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  155.26, 143.44, 132.82, 130.78, 130.68, 129.01, 127.33, 127.25, 126.70, 111.01, 55.99, 43.29, 20.78 ppm.

4,4'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13a)



White solid. Yield 95%. mp 91-93 °C. FT- IR (KBr):  $\tilde{v}$  3028, 2933, 2834, 1606, 1500, 1462, 1414, 1242, 1183, 1139, 1108, 807, 638 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  6.99 (d, *J* = 8.2 Hz, 2H), 6.96 (dd, *J*<sub>1</sub> = 8.3 Hz, *J*<sub>2</sub> = 1.8 Hz, 4H), 6.89 (d, *J* = 8.2 Hz, 2H), 6.82 (t, *J* = 7.7 Hz, 4H), 6.69 (d, *J* = 1.7 Hz, 2H), 6.57 (dd, *J*<sub>1</sub> = 8.3 Hz, *J*<sub>2</sub> = 1.8 Hz, 4H), 6.53 (d, *J* = 1.7 Hz, 2H), 6.05 (s, 1H, Ar<sub>3</sub>CH), 5.40 (s, 1H, Ar<sub>3</sub>CH), 3.69 (s, 6H, OMe), 3.61 (s, 6H, OMe), 3.58 (s, 6H, OMe), 2.08 (s, 6H, Me) ppm. <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  155.18, 148.94, 147.66, 142.16, 141.83, 137.21, 132.13, 130.44, 129.22, 129.01, 128.78, 128.08, 121.46, 113.48, 112.14, 111.64, 56.07, 55.92, 55.79, 55.08, 42.38, 20.84 ppm.

4,4'-((3-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13b)



White solid. Yield 91%. mp 83-85 °C. FT- IR (KBr):  $\tilde{v}$  3031, 2934, 2833, 1604, 1512, 1624, 1414, 1242, 1183, 1139, 1029, 810, 750 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.16 (t, *J* = 7.9 Hz, 1H), 6.97 (dd, *J*<sub>1</sub> = 8.8 Hz, *J*<sub>2</sub> = 2.3 Hz, 2H), 6.86-6.94 (m, 3H), 7.75 (d, *J* = 8.2 Hz, 2H), 7.73 (d, *J* = 8.2 Hz, 2H), 6.60 (d, *J* = 2.1 Hz, 2H), 6.55-6.58 (m, 4H), 6.07 (s, 6H, Ar<sub>3</sub>CH), 5.37 (s, 6H, Ar<sub>3</sub>CH), 3.86 (s, 6H, OMe), 3.70 (s, 6H, OMe), 3.62 (s, 6H, OMe), 2.17 (s, 6H, Me) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 155.22, 148.62,

147.29, 143.90, 143.61, 137.06, 132.49, 130.68, 130.56, 129.04, 127.75, 127.40, 127.32, 126.61, 121.36, 112.75, 110.94, 110.75, 55.93, 55.85, 55.71, 43.19, 20.73 ppm.

4,4'-((4-(bis(5-chloro-2-methoxyphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13c)



White Solid. Yield 97%. mp 140-142 °C. FT- IR (KBr):  $\tilde{v}$  3018, 2955, 2834, 1512, 1461, 1439, 1243, 1159, 1121, 1026, 809, 645 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.16 (dd,  $J_1$  = 8.7 Hz,  $J_2$  = 2.6 Hz, 2H), 7.03 (d, J = 8.1 Hz, 2H), 6.82 (d, J = 8.2 Hz, 2H), 6.79 (t, J = 7.6 Hz, 4H), 6.73 (d, J = 2.6 Hz, 2H), 6.6-6.7 (m, 4H), 6.06 (s, 1H, Ar<sub>3</sub>CH), 5.44 (s, 1H, Ar<sub>3</sub>CH), 3.86 (s, 6H, OMe), 3.77 (s, 6H, OMe), 3.68 (s, 6H, OMe) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 155.76, 148.72, 147.42, 142.30, 139.90, 136.87, 133.94, 129.61, 129.18, 129.08, 127.30, 125.25, 121.39, 112.76, 112.03, 110.91, 55.94, 55.87, 55.80, 55.49, 42.96 ppm.

4,4'-((4-(bis(5-bromo-2-methoxyphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13d)



White solid. Yield 93%. mp 107-110 °C. FT- IR (KBr):  $\tilde{v}$  3029, 2933, 2832, 1589, 1511, 1460, 1245, 1185, 1138, 1029, 804, 621 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.96 (d, *J* = 8.1 Hz, 2H), 7.31 (dd, *J*<sub>1</sub> = 8.6 Hz, *J*<sub>2</sub> = 2.3 Hz, 2H), 7.03 (d, *J* = 8.1 Hz, 2H), 6.86 (d, *J* = 2.3 Hz, 2H), 6.79 (d, *J* = 8.5 Hz, 2H), 6.73 (d, *J* = 8.7 Hz, 2H), 6.6-6.7 (m, 6H), 6.05 (s, 1H, Ar<sub>3</sub>CH), 5.44 (s, 1H, Ar<sub>3</sub>CH), 3.86 (s, 6H, OMe), 3.77 (s, 6H, OMe), 3.67 (s, 6H, OMe) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 156.24, 148.72, 147.42, 142.32, 139.82, 136.87, 134.39, 132.41, 130.33, 129.19, 129.08, 121.39, 112.72, 112.57, 110.91, 55.87, 55.84, 55.49, 55.94 ppm.

2,2'-((4-(bis(4-methoxyphenyl)methyl)phenyl)methylene)bis(1-methoxy-4-methylbenzene) (13e)



White Solid. Yield 91%. mp 120-122 °C. FT- IR (KBr):  $\tilde{v}$  3024, 2933, 2832, 1608, 1508, 1461, 1289, 1242, 1030, 806 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  = 7.05 (dd,  $J_1$  = 5.2 Hz,  $J_2$  = 2.5 Hz, 4H), 6.95-7.02 (m, 6H), 6.80-6.16 (m, 4H), 6.77 (d, J = 8.2 Hz, 2H), 6.65 (d, J = 2.4 Hz, 2H), 6.16 (s, 1H, Ar<sub>3</sub>CH), 5.43 (s, 1H, Ar<sub>3</sub>CH), 3.79 (s, 6H. OMe), 3.68 (s, 6H, OMe), 2.21 (s, 6H, Me) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  157.89, 155.29, 141.82, 141.58, 136.84, 132.65, 130.76, 130.28, 129.21, 129.16, 128.77, 127.44, 113.55, 111.09, 56.05, 55.22, 54.85, 42.60, 20.79 ppm.

2,2'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(4-chloro-1-methoxybenzene) (13f)



White solid. Yield 88%. mp 175-188 °C. FT- IR (KBr):  $\tilde{v}$  3021, 2939, 2834, 1610, 1498, 1428, 1242, 1121, 907, 806, 645 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>): δ 7.16 (dd,  $J_1$  = 8.7 Hz,  $J_2$  = 2.7 Hz, 2H), 6.9-7.1 (m, 4H), 6.91 (d, J = 8.2 Hz, 2H), 6.78 (d, J = 8.5 Hz, 4H), 6.72 (d, J = 2.7 Hz, 2H), 6.61 (d, J = 2.0 Hz, 2H), 6.13 (s, 1H, Ar<sub>3</sub>CH), 6.03 (s, 1H, Ar<sub>3</sub>CH), 3.67 (s, 6H, OMe), 3.66 (s, 6H, OMe), 2.21 (s, 6H, Me) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>): δ 155.78, 155.27, 142.24, 139.15, 134.24, 132.59, 130.77, 129.74, 129.22, 129.20, 128.73, 127.46, 127.17, 125.26, 112.05, 111.11, 56.03, 55.49, 43.12, 42.87, 20.77 ppm.

4,4'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(2-bromothiophene) (13g)



White solid. Yield 93%. mp 101-103 °C. FT- IR (KBr):  $\tilde{v}$  3012, 2922, 2832, 1699, 1607, 1497, 1460, 1242, 1108, 1034, 964, 803, 722 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.14 (d, *J* = 8.3 Hz, 2H, H<sub>d</sub>), 7.03 (d, *J* = 8.2 Hz, 2H, H<sub>e</sub>), 7.00 (dd, *J*<sub>1</sub> = 8.1 Hz, *J*<sub>2</sub> = 2.4 Hz, 2H, H<sub>b</sub>), 6.88 (d, *J* = 3.8 Hz, 2H, H<sub>g</sub>), 6.77 (d, *J* = 8.2 Hz, 2H, H<sub>c</sub>), 6.61 (d, *J* = 2.3 Hz, 2H, H<sub>a</sub>), 6.57 (dd, *J*<sub>1</sub> = 3.8 Hz, *J*<sub>2</sub> = 1.1 Hz, 2H, H<sub>f</sub>), 6.15 (s, 1H, H<sub>i</sub>), 5.63 (s, 1H, H<sub>h</sub>), 3.67 (s, 6H, OMe), 2.21 (s, 6H, Me) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  154.89, 148.66, 143.79, 139.10, 132.22, 130.72, 129.63, 129.35, 129.23, 127.72, 127.58, 126.34, 111.39, 111.05, 56.00, 47.61, 42.75, 20.76 ppm.

2-((4-(bis(5-bromothiophen-2-yl)methyl)phenyl)(5-(tert-butyl)-2-methoxyphenyl)methyl)-4-(tert-butyl)phenol (13h)



Brown Solid. Yield 89%. mp 114-116 °C. FT- IR (KBr):  $\tilde{v}$  3395, 2960, 1607, 1505, 1416, 1268, 1214, 965, 758 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  722 (d, *J* = 8.3 Hz, 2H, Hd), 7.13-7.18 (m, 6H), 6.90 (d, *J* = 2.4 Hz, 2H), 6.89 (d, *J* = 3.75 Hz, 2H, H<sub>a</sub>), 6.76 (d, *J* = 8.4 Hz, 2H, H<sub>c</sub>), 6.58 (dd, *J*<sub>1</sub> = 3.75 Hz, *J*<sub>2</sub> = 0.8 Hz, 2H, H<sub>b</sub>), 5.92 (s, 1H, H<sub>f</sub>), 5.66 (s, 1H, H<sub>e</sub>), 4.97 (sb, 2H, OH), 1.19 (s, 18H, *tert*-Butyl) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  151.05, 148.30, 143.77, 141.42, 140.43, 129.56, 129.40, 128.31, 127.94, 127.28, 126.43, 124.81, 115.68, 111.55, 47.54, 44.51, 34.14, 31.40 ppm.

14-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-14H-dibenzo[a,j]xanthene (14)



White solid. Yield 96%. mp 263-265 °C. FT- IR (KBr):  $\tilde{v}$  3425, 2918, 1590, 1469, 1485, 1432, 1238, 1059, 1033, 801, 740 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  8.60 (d, *J* = 8.6 Hz, 2H), 7.85-7.95 (m, 4H), 7.55-7.62 (m, 2H), 7.51 (d, *J* = 8.9 Hz, 2H), 7.40-7.50 (m, 4H), 6.87 (dd, *J*<sub>1</sub> = 8.2 Hz, *J*<sub>2</sub> = 2.2 Hz, 2H), 6.66-6.74 (m, 4H), 6.64 (s, 1H, Ar<sub>2</sub>CH), 6.28 (d, *J* = 2.3 Hz, 2H), 5.83 (s, 1H, (naphthyl)<sub>2</sub>CH), 3.44 (s, 6H, OMe), 1.94 (s, 6H, Me) ppm. <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  154.98, 148.39, 143.33, 141.80, 131.83, 131.38, 131.08, 130.34, 129.41, 129.29, 129.01, 128.66, 128.02, 127.98, 127.24, 124.90, 123.84, 118.07, 117.75, 116.65, 56.05, 41.95, 36.75, 20.73 ppm.

#### 3.3. 3,4-dihydropyrimidin-2(1H)-(thi)ones (17a-j)

Ethyl 4-(4-(bis(3,4-dimethoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (17a)



White solid. Yield 94%. mp 221-223 °C. FT-IR (KBr):  $\tilde{v}$  3230, 3108, 3017, 1935, 2835, 1701, 1644, 1511, 1462, 1262, 1225, 1139, 1091, 1027, 768 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  = 8.47 (bs, 1H, NH<sub>h</sub>), 7.22 (d, *J* = 8.1 Hz, 2H, H<sub>e</sub>), 7.04 (d, *J* = 8.0 Hz, 2H, H<sub>f</sub>), 6.77 (d, *J* = 8.2 Hz, 2H, H<sub>c</sub>), 6.64 (d, *J* = 2.1 Hz, 2H, H<sub>d</sub>), 6.56 (dd, *J*<sub>1</sub> = 8.2 Hz, *J*<sub>2</sub> = 2 Hz, 2H, H<sub>b</sub>), 5.76 (bs, 1H, NH<sub>g</sub>), 5.40 (s, 1H, H<sub>a</sub>), 5.37 (d, *J* = 2.8 Hz, 1H, H<sub>j</sub>), 4.00-4.15 (m, 2H, diastrotopic-H<sub>i</sub> and H<sub>i</sub>), 3.85 (s, 6H, OMe<sub>n</sub>), 3.76 (s, 6H, OMe<sub>m</sub>), 2.33 (s, 3H, Me<sub>k</sub>), 1.14 (t, *J* = 7.2 Hz, 3H, Me<sub>L</sub>) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  165.64, 153.49, 148.75, 147.49, 146.39, 144.09, 141.69, 136.50, 136.48, 129.56, 126.51, 121.35, 112.70, 110.83, 101.27, 59.93, 55.84, 55.82, 55.80, 55.59, 55.37, 18.57, 14.17 ppm.

Ethyl 4-(3-(bis(3,4-dimethoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (17b)



White solid. Yield 83%. mp 107-109 °C. FT-IR (KBr):  $\tilde{v}$  3230, 3103, 3017, 2935, 2835, 1701, 1644, 1512, 1462, 1223, 1139, 1092, 1072, 771 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.44 (s, 1H, NH<sub>j</sub>), 7.22 (t, *J* = 7.6 Hz, 1H, H<sub>g</sub>), 7.17 (d, *J* = 7.6 Hz, 1H, H<sub>h</sub>), 7.04 (d, *J* = 2.2 Hz, 1H, H<sub>e</sub>), 7.00 (d, *J* = 7.6 Hz, 1H, H<sub>f</sub>), 6.75 (d, *J* = 8.4 Hz, 2H, H<sub>c</sub>), 6.64 (t, *J* = 2.4 Hz, 2H, H<sub>d</sub>), 6.54 (dd, *J*<sub>1</sub> = 8.3 Hz, *J*<sub>2</sub> = 1.5 Hz, 2H, H<sub>b</sub>), 5.86 (s, 1H, H<sub>a</sub>), 5.40 (b, 1H, NH<sub>i</sub>), 5.31 (d, *J* = 2.9 Hz, 1H, H<sub>p</sub>), 3.90-4.03 (m, 2H, diastrotopic H<sub>k</sub> and H<sub>k</sub>), 3.84 (s, 6H, OMe<sub>o</sub>), 3.74 (s, 6H, OMe<sub>n</sub>), 2.29 (s, 3H, Me<sub>m</sub>), 1.04 (t, *J* = 7.1 Hz, 3H, Me<sub>L</sub>) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  165.50, 153.41, 148.78, 147.52, 146.42, 144.64, 143.77, 136.54, 136.47, 128.79, 127.66, 124.33, 121.39, 121.31, 112.28, 110.90, 101.15, 59.81, 55.83, 55.74, 55.60, 18.38, 14.04 ppm.

Ethyl 4- (4-(bis(2- methoxy-5- methyl phenyl)methyl)phenyl)-6- methyl-2-oxo-1,2,3,4- tetrahydropyrimidine-5-carboxylate (17c)



White solid. Yield 96%. mp 205-207 °C. FT-IR (KBr):  $\tilde{v}$  3388, 3238, 3122, 2926, 1705, 1642, 1498, 1463, 1385, 1368, 1241, 1153, 1093, 1034, 807 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.23 (s, 1H, NH<sub>j</sub>), 7.16 (d, *J* = 7.9 Hz, 2H, H<sub>f</sub>), 6.99 (d, *J* = 2.5 Hz, 2H, H<sub>d</sub>), 6.97 (d, *J* = 2.9 Hz, 2H, H<sub>c</sub>), 6.75 (d, *J* = 8.2 Hz, 2H, H<sub>g</sub>), 6.58 (s, 2H, H<sub>e</sub>), 6.13 (s, 1H, H<sub>a</sub>), 5.53 (b, 1H, NH<sub>i</sub>), 5.35 (d, *J* = 2.7 Hz, 1H, H<sub>h</sub>), 3.97- 4.12 (m, 2H, diatrotopic-H<sub>m</sub> and H<sub>m</sub>), 3.65 (s (× 2), 6H, OMe), 2.34 (s, 3H, Me<sub>k</sub>), 2.19 (s, 6H, Me<sub>b</sub>), 1.10 (t, *J* = 7.1 Hz, 3H, Me<sub>L</sub>) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  165.66, 155.19, 153.10, 146.15, 143.88, 140.92, 132.32, 132.19, 130.68, 130.64, 129.59, 129.16, 127.53, 126.25, 110.94, 101.44, 59.77, 55.95, 55.70, 42.68, 20.75, 18.51, 14.11 ppm.

Ethyl 4-(4-(bis(5-chloro-2-methoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (17e)



White solid. Yield 95%. mp 144-146 °C. FT-IR (KBr):  $\tilde{v}$  3303, 3119, 2937, 2836, 1703, 1642, 1485, 1460, 1243, 1091, 812 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.04 (s, 1H, NH<sub>h</sub>), 7.20 (d, *J* = 8.1 Hz, 2H, H<sub>e</sub>), 7.17 (d, *J*<sub>1</sub> = 8.7 Hz, *J*<sub>2</sub> = 2.7 Hz, 2H, H<sub>c</sub>), 6.97 (d, *J* = 8.0 Hz, 2H, H<sub>f</sub>), 6.78 (d, *J* = 8.7 Hz, 2H, H<sub>d</sub>), 6.69 (d, *J* = 2.7 Hz, 2H, H<sub>b</sub>), 5.54 (bs, 1H, NH<sub>g</sub>), 5.37 (d, *J* = 2.7 Hz, 1H, H<sub>i</sub>), 3.97-4.2 (m (× 2), 2H, distrotopic-H<sub>j</sub> and H<sub>j'</sub>), 3.67 (s, 6H, OMe), 2.35 (s, 3H, Me<sub>k</sub>), 1.11 (t, *J* = 7.1 Hz, 3H, Me<sub>L</sub>) ppm. <sup>13</sup>C NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  165.64, 155.70, 153.39, 146.47, 141.81, 141.71, 133.66, 133.57, 129.60, 129.55, 129.45, 127.38, 126.64, 125.27, 111.96, 101.12, 59.88, 55.90, 55.53, 43.04, 18.48, 14.16 ppm.

Ethyl 4-(4-(bis(5-bromo-2-methoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (17f)



White solid. Yield 94%. mp 161-163 °C. FT-IR (KBr):  $\tilde{v}$  3404, 3117, 2936, 2836, 1702, 1647, 1484, 1396, 1369, 1243, 1114, 1089, 809 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.21 (bs, 1H, NH<sub>h</sub>), 7.31 (dd,  $J_1$  = 8.7 Hz,  $J_2$  = 2.5 Hz, 2H, H<sub>c</sub>), 7.21 (d, J = 8.2 Hz, 2H, H<sub>e</sub>), 6.96 (d, J = 8.0 Hz, 2H, H<sub>f</sub>), 6.80 (d, J = 2.6 Hz, 2H, H<sub>b</sub>), 6.73 (d, J = 8.7 Hz, 2H, H<sub>d</sub>), 6.02 (s, 1H, H<sub>a</sub>), 5.58 (bs, 1H, NH<sub>g</sub>), 5.37 (d, J = 2.7 Hz, 1H, H<sub>i</sub>), 3.96-4.16 (m (×2), 2H, diastrotopic-H<sub>j</sub> and H<sub>j</sub>'), 3.67 (s, 6H, OMe), 2.36 (s, 3H, Me<sub>k</sub>), 1.11 (t, J = 7.1 Hz, 3H, Me<sub>L</sub>) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  165.60, 156.19, 153.19, 146.37, 141.78, 141.66, 134.10, 133.98, 132.37, 132.31, 130.42, 129.47, 126.65, 112.72, 112.48, 101.15, 59.90, 55.85, 55.60, 43.01, 18.53, 14.23 ppm.

Ethyl 4-(4-(bis(3,4-dimethylphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (17g)



White solid. Yield 93%. mp 216-218 °C. FT-IR (KBr):  $\tilde{v}$  3235, 3109, 2971, 1709, 1681, 1655, 1453, 1231, 1089, 808 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, DMSO-d<sub>6</sub>):  $\delta$  9.16 (bs, 1H, NH<sub>h</sub>), 7.13 (d, *J* = 8.2 Hz, 2H, H<sub>e</sub>), 7.00-7.04 (m, 4H, H<sub>c</sub> and H<sub>f</sub>), 6.86 (bs, 2H, H<sub>d</sub>), 6.74 (dd, *J*<sub>1</sub> = 7.7 Hz, *J*<sub>2</sub> = 2 Hz, 2H, H<sub>b</sub>), 5.40 (bs, 1H, NH<sub>g</sub>), 5.36 (s, 1H, H<sub>a</sub>), 5.09 (d, *J* = 3.3 Hz, 1H, H<sub>j</sub>), 3.90-4.01 (m, 2H, diastrotopic-H<sub>i</sub> and H<sub>f</sub>), 2.21 (s, 3H, Me<sub>k</sub>), 2.15 (s, 6H, Me<sub>n</sub>), 2.12 (s, 6H, Me<sub>m</sub>), 1.05 (t, *J* = 7.1 Hz, Me<sub>L</sub>) ppm. <sup>13</sup>C NMR (125 MHz, DMSO-d<sub>6</sub>):  $\delta$  165.78, 152.58, 143.73, 143.09, 141.83, 141.77, 136.30, 134.27, 130.56, 129.75, 129.41, 126.71, 126.62, 99.73, 59.58, 54.40, 54.16, 19.92, 19.36, 18.22, 14.51 ppm.

Ethyl 4-(4-(bis(3,4-dimethoxyphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (17h)



White solid. Yield 91%. mp 173-175 °C. FT-IR (KBr).  $\tilde{v}$  3307, 3178, 2934, 2833, 1662, 156, 1511, 1461, 1415, 1246, 1183, 1138, 1026, 754 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.89 (s, 1H, NH<sub>h</sub>), 7.22 (bs, 1H, NH<sub>g</sub>), 7.20 (d, *J* = 7.9 Hz, 2H, H<sub>c</sub>), 6.64 (d, *J* = 2.1 Hz, 2H, H<sub>d</sub>), 6.56 (dd, *J*<sub>1</sub> = 8.3 Hz, *J*<sub>2</sub> = 2.1 Hz, 2H, H<sub>b</sub>), 5.40 (bs, 1H, H<sub>a</sub>), 4.04-4.14 (m, *J* = 2.9 Hz, H<sub>j</sub>), 3.86 (s, 6H, OMe<sub>n</sub>), 3.77 (s, 6H, OMe<sub>m</sub>), 2.36 (s, 3H, Me<sub>k</sub>), 1.15 (t, *J* = 7.1 Hz, 3H, Me<sub>L</sub>) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  174.54, 165.21, 148.81, 147.57, 144.65, 142.68, 140.33, 136.37, 129.74, 126.70, 121.38, 112.77, 110.94, 102.92, 60.34, 55.90, 55.86, 55.61, 18.26, 14.10 ppm.

Ethyl 4-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (17i)



White solid. Yield 92%. mp 203-205 °C. FT-IR (KBr):  $\tilde{v}$  3187, 2982, 2834, 1694, 1609, 1566, 1462, 1242, 1182, 1107, 1034, 755 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  8.52 (s, 1H, NH<sub>i</sub>), 7.15 (bs, 1H, NH<sub>h</sub>), 7.01 (d, *J* = 8.0 Hz, 2H, H<sub>d</sub>), 6.99 (dd, *J*<sub>1</sub> = 8.2 Hz, *J*<sub>2</sub> = 2.2 Hz, 2H, H<sub>c</sub>), 6.76 (d, *J* = 8.2 Hz, 2H, H<sub>f</sub>), 6.60 (d, *J* = 2.2 Hz, H<sub>b</sub>), 6.14 (s, 1H, H<sub>a</sub>), 5.35 (d, *J*, 2.9 Hz, 1H, H<sub>g</sub>), 3.98-4.16 (m, 2H, diastrotopic-H<sub>j</sub> and H<sub>j</sub>), 3.66 (s, 6H, OMe), 2.36 (s, 3H, Me<sub>k</sub>), 2.20 (s, 6H, Me<sub>m</sub>), 1.11 (t, *J* = 7.1 Hz, Me<sub>L</sub>) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  174.06, 165.32, 155.16, 144.40, 142.80, 139.69, 132.14, 132.05, 130.70, 130.68, 129.75, 129.18, 127.62, 126.55, 110.94, 110.92, 102.88, 60.19, 56.08, 55.96, 55.94, 42.68, 20.97, 18.02, 14.08 ppm.

Ethyl 1-allyl-4-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5carboxylate (17j)



White solid. Yield 54%. mp 161-163 °C. FT- IR (KBr):  $\tilde{v}$  3194, 2941, 1834, 1702, 1627, 1498, 1461, 1417, 1365, 1287, 1243, 1155, 1110, 1036, 756 cm<sup>-1</sup>. <sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>):  $\delta$  7.47 (bd, J = 3.7 Hz, NH<sub>h</sub>), 7.12 (d, J = 8.0 Hz, 2H, H<sub>e</sub>), 6.97-7.04 (m, 4H, H<sub>c</sub> and H<sub>d</sub>), 6.76 (d, J = 8.2 Hz, 2H, H<sub>f</sub>), 6.57 (d, J = 2.1 Hz, H<sub>b</sub>), 6.14 (s, 1H, H<sub>a</sub>), 5.81-5.92 (m, 1H, H<sub>j</sub>), 5.37 (d, J = 3.3 Hz, 1H, H<sub>g</sub>), 5.29 (d, J = 18.9 Hz, 1H, H<sub>L</sub>), 5.15 (d, J = 10.5 Hz, 1H, H<sub>i</sub>), 5.04 (d, J = 15.3 Hz, 1H, H<sub>i</sub>), 4.76 (d, J = 16.5 Hz, 1H, H<sub>k</sub>), 4.05-4.20 (m, 2H, diastrotopic-H<sub>m</sub> and H<sub>m'</sub>), 3.66 (s, 6H, OMe), 2.53 (s, 3H, Me<sub>n</sub>), 2.20 (s, 6H, Me<sub>p</sub>), 1.16 (t, J = 7.2 Hz, Me<sub>o</sub>) ppm. <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>):  $\delta$  178.83, 165.76, 155.18, 145.75, 144.25, 139.06, 133.40, 132.12, 132.07, 130.68, 129.71, 129.15, 127.60, 126.07, 116.64, 110.89, 108.15, 60.53, 55.94, 55.93, 53.96, 50.85, 42.65, 20.78, 16.35, 14.09 ppm.

#### 4. NMR Spectra

#### 4.1. Formylated-triarylmethanes



<sup>1</sup>H NMR spectrum of 4-(bis (2-methoxy-5-methyl phenyl) methyl) benzaldehyde (6c)



<sup>13</sup>C NMR spectrum of 4-(bis (2-methoxy-5-methyl phenyl) methyl) benzaldehyde (6c)



<sup>1</sup>H NMR spectrum of 3-(bis (2-methoxy-5-methyl phenyl) methyl) benzaldehyde (6d)



<sup>&</sup>lt;sup>13</sup>C NMR spectrum of 3-(bis (2-methoxy-5-methyl phenyl) methyl) benzaldehyde (6d)



<sup>1</sup>H NMR spectrum of 4-(bis(5-chloro-2-methoxyphenyl)methyl)benzaldehyde (6e)





<sup>1</sup>H NMR spectrum of 4-(bis(5-bromo-2-methoxyphenyl)methyl)benzaldehyde (6f)



<sup>13</sup>C NMR spectrum of 4-(bis(5-bromo-2-methoxyphenyl)methyl)benzaldehyde (6f)



<sup>1</sup>H NMR spectrum of 4-(bis(4-methoxy phenyl)methyl)benzaldehyde (6g)



Expanded <sup>1</sup>H NMR spectrum of 4-(bis(4-methoxy phenyl)methyl)benzaldehyde (6g)



<sup>13</sup>C NMR spectrum of 4-(bis(4-methoxy phenyl)methyl)benzaldehyde (6g)



<sup>1</sup>H NMR spectrum of 4-(bis(3,4-dimethylphenyl)methyl)benzaldehyde (6h)



<sup>13</sup>C NMR spectrum of 4-(bis(3,4-dimethylphenyl)methyl)benzaldehyde (6h)



<sup>1</sup>H NMR spectrum of 4-(bis(5-bromothiophen-2-yl)methyl)benzaldehyde (6i)



<sup>1</sup>H NMR spectrum of 4-(bis(5-bromothiophen-2-yl)methyl)benzaldehyde (6i)



<sup>1</sup>H NMR spectrum of 4-(bis(4-hydroxyphenyl)methyl)benzaldehyde (6j)



<sup>13</sup>C NMR spectrum of 4-(bis(4-hydroxyphenyl)methyl)benzaldehyde (6j)



<sup>13</sup>C NMR spectrum of 4-(bis(5-(tert-butyl)-2-hydroxyphenyl)methyl)benzaldehyde (6k)



3.75 8.60 8.55 8.60 8.55 8.50 8.45 8.40 8.35 8.30 8.25 8.20 8.15 8.10 8.05 8.00 7.95 7.90 7.85 7.80 7.75 7.70 7.65 7.60 7.55 7.50 7.45 7.40 f1 (ppm)

Expanded <sup>1</sup>H NMR spectrum of 4-(14H-dibenzo[a,j]xanthen-14-yl)benzaldehyde (6l)



<sup>13</sup>C NMR spectrum of 4-(14H-dibenzo[a,j]xanthen-14-yl)benzaldehyde (6l)

# 4.2. Adduct 12, mixed-bistriarylmethanes, and product 14





<sup>1</sup>H NMR spectrum of 1,3-bis(bis(2-methoxy-5-methylphenyl)methyl)benzene (12)





<sup>13</sup>C NMR spectrum of 1,3-bis(bis(2-methoxy-5-methylphenyl)methyl)benzene (12)



<sup>1</sup>H NMR spectrum of 4,4'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13a)



<sup>13</sup>C NMR spectrum of 4,4'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13a)



<sup>1</sup>H NMR spectrum of 4,4'-((3-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13b)



Expanded <sup>1</sup>H NMR spectrum of 4,4'-((3-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(1,2dimethoxybenzene) (**13b**)



<sup>13</sup>C NMR spectrum of 4,4'-((3-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13b)



Expanded <sup>13</sup>C NMR spectrum of 4,4'-((3-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (**13b**)



1H NMR spectrum of 4,4'-((4-(bis(5-chloro-2-methoxyphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13c)



dimethoxybenzene) (13c)



<sup>13</sup>C NMR spectrum of 4,4'-((4-(bis(5-chloro-2-methoxyphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (**13c**)



<sup>1</sup>H NMR spectrum of 4,4'-((4-(bis(5-bromo-2-methoxyphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13d)



<sup>13</sup>C NMR spectrum of 4,4'-((4-(bis(5-bromo-2-methoxyphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (13d)



Expanded <sup>13</sup>C NMR spectrum of 4,4'-((4-(bis(5-bromo-2-methoxyphenyl)methyl)phenyl)methylene)bis(1,2-dimethoxybenzene) (**13d**)



<sup>1</sup>H NMR spectrum of 2,2'-((4-(bis(4-methoxyphenyl)methyl)phenyl)methylene)bis(1-methoxy-4-methylbenzene) (**13e**)



Expanded <sup>1</sup>H NMR spectrum of 2,2'-((4-(bis(4-methoxyphenyl)methyl)phenyl)methylene)bis(1-methoxy-4-methylbenzene) (**13e**)



<sup>13</sup>C NMR spectrum of 2,2'-((4-(bis(4-methoxyphenyl)methyl)phenyl)methylene)bis(1-methoxy-4-methylbenzene) (13e)



Expanded <sup>13</sup>C NMR spectrum of 2,2'-((4-(bis(4-methoxyphenyl)methyl)phenyl)methylene)bis(1-methoxy-4-methylbenzene) (**13e**)



<sup>1</sup>H NMR spectrum of 2,2'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(4-chloro-1-methoxybenzene) (13f)



Expanded <sup>1</sup>H NMR spectrum of 2,2'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(4-chloro-1-methoxybenzene) (**13f**)



<sup>13</sup>C NMR spectrum of 2,2'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(4-chloro-1-methoxybenzene) (13f)



Expanded <sup>13</sup>C NMR spectrum of 2,2'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(4-chloro-1-methoxybenzene) (**13f**)



<sup>1</sup>H NMR spectrum of 4,4'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(2-bromothiophene) (13g)



Expanded <sup>1</sup>H NMR spectrum of 4,4'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(2-bromothiophene) (**13**g)



<sup>13</sup>C NMR spectrum of 4,4'-((4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)methylene)bis(2-bromothiophene) (13g)



<sup>1</sup>H NMR spectrum of 2,2'-((4-(bis(5-bromothiophen-2-yl)methyl)phenyl)methylene)bis(4-(tert-butyl)phenol) (13h)



<sup>13</sup>C NMR spectrum of 2,2'-((4-(bis(5-bromothiophen-2-yl)methyl)phenyl)methylene)bis(4-(tert-butyl)phenol) (13h)



<sup>&</sup>lt;sup>1</sup>H NMR spectrum of 14-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-14H-dibenzo[a,j]xanthene (14)





Expanded <sup>1</sup>H NMR spectrum of 14-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-14H-dibenzo[a,j]xanthene (14)

<sup>13</sup>C NMR spectrum of 14-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-14H-dibenzo[a,j]xanthene (14)

# 4.3. 3,4-dihydropyrimidin-2(1H)-(thi)ones



<sup>1</sup>H NMR spectrum of ethyl 4-(4-(bis(3,4-dimethoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5carboxylate (**17a**)



tetrahydropyrimidine-5-carboxylate (17a)



cdc13 55,70153 55,2165 55,2165 55,2165 55,2165 55,2165 55,2165 4,0026 4,00076 4,00076 4,00076 4,00076 3,30508 3,30508 3,30508 3,30507 3,3050 8.4478 7.2385 7.2385 7.2385 7.2333 2081 1889 1849 1698 9639 9754 .7827 7663 7495 7323 6395 6395 5.8634 0416 0373 0062 0062 9911 9456 -3.7410 3835 ~4.0149 ~3.9933 -3.9789 -3.9649 -3.9508 -39367 -39292 -39224 -39149 -3.9007 4.0008 -4.0291 4.0076 -2.2850 -1.05440402 1.0261 2.89 1.06 1.04 1.02 f1 (ppm) 2.30 2.25 f1 (ppm) 6.03 -8 2.35 3.85 5 3.80 f1 (ppm) 3.75 ĥ 3.98 3.96 f1 (ppm) 4.00 3.94 3.92 3.90 4.04 4.02 1.157 1.18 2.12 2.12 2.55 7 5.16 1.01-1.95 6.03 6.03 3.04-2.89-1.03-0.96 6 f1 (ppm) 3 1 13 12 11 10 9 8 5 4 2 0 -1 7

<sup>1</sup>H NMR spectrum of ethyl 4-(3-(bis(3,4-dimethoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5carboxylate (**17b**)



3.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8 5.7 5.6 5.5 5.4 5.3 f1 (ppm)

Expanded <sup>1</sup>H NMR spectrum of ethyl 4-(3-(bis(3,4-dimethoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-

tetrahydropyrimidine-5-carboxylate (17b)



<sup>13</sup>C NMR spectrum of ethyl 4-(3-(bis(3,4-dimethoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5carboxylate (**17b**)



<sup>1</sup>H NMR spectrum of ethyl 4- (4-(bis(2- methoxy-5- methyl phenyl)methyl)phenyl)-6- methyl-2-oxo-1,2,3,4- tetrahydropyrimidine-5-carboxylate (**17c**)



Expanded <sup>1</sup>H NMR spectrum of ethyl 4- (4-(bis(2- methoxy-5- methyl phenyl)methyl)phenyl)-6- methyl-2-oxo-1,2,3,4- tetrahydropyrimidine-5-carboxylate (**17c**)



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<sup>1</sup>H NMR spectrum of ethyl 4-(4-(bis(5-chloro-2-methoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4tetrahydropyrimidine-5-carboxylate (**17e**)



Expanded <sup>1</sup>H NMR spectrum of ethyl 4-(4-(bis(5-chloro-2-methoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**17e**)



tetrahydropyrimidine-5-carboxylate (**17e**)



<sup>1</sup>H NMR spectrum of ethyl 4-(4-(bis(5-bromo-2-methoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4tetrahydropyrimidine-5-carboxylate (**17f**)



Expanded <sup>1</sup>H NMR spectrum of ethyl 4-(4-(bis(5-bromo-2-methoxyphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**17f**)



tetrahydropyrimidine-5-carboxylate (17f)



<sup>1</sup>H NMR spectrum of ethyl 4-(4-(bis(3,4-dimethylphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4-tetrahydropyrimidine-5carboxylate (**17g**)



Expanded <sup>1</sup>H NMR spectrum of ethyl 4-(4-(bis(3,4-dimethylphenyl)methyl)phenyl)-6-methyl-2-oxo-1,2,3,4tetrahydropyrimidine-5-carboxylate (**17g**)



carboxylate (17g)



<sup>1</sup>H NMR spectrum of ethyl 4-(4-(bis(3,4-dimethoxyphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**17h**)



Expanded <sup>1</sup>H NMR of ethyl 4-(4-(bis(3,4-dimethoxyphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**17h**)





<sup>1</sup>H NMR spectrum of ethyl 4-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**17**i)



Expanded <sup>1</sup>H NMR spectrum of ethyl 4-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**17i**)



tetrahydropyrimidine-5-carboxylate (17i)



APT spectrum of ethyl 4-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4tetrahydropyrimidine-5-carboxylate (**17i**)



<sup>1</sup>H NMR spectrum of ethyl 1-allyl-4-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**17**j)



Expanded <sup>1</sup>H NMR spectrum of ethyl 1-allyl-4-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4tetrahydropyrimidine-5-carboxylate (**17**j)



<sup>1</sup>H-<sup>1</sup>H COSY spectrum of ethyl 1-allyl-4-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**17**j)



<sup>1</sup>H-<sup>1</sup>H COSY spectrum of ethyl 1-allyl-4-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**17**j)



<sup>1</sup>H-<sup>1</sup>H COSY spectrum of ethyl 1-allyl-4-(4-(bis(2-methoxy-5-methylphenyl)methyl)phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (**17**j)



tetrahydropyrimidine-5-carboxylate (17j)

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