## **Supplementary Information**

## Synthesis, Characterization and Evaluation of *in vitro* Antitumor Activities of Novel Chalcone-Quinolinone Hybrid Compounds

Giulio D. C. d'Oliveira,<sup>a</sup> Andrea F. Moura,<sup>b</sup> Manoel O. de Moraes,<sup>b</sup> Caridad Noda Perez<sup>a</sup> and Luciano M. Lião<sup>\*,a</sup>

<sup>a</sup>Instituto de Química, Universidade Feredal de Goiás, Campus Samambaia, 74690-900 Goiânia-GO, Brazil

<sup>b</sup>Núcleo de Pesquisas e Desenvolvimento de Medicamentos, Universidade Federal do Ceará, 60430-275 Fortaleza-CE, Brazil

General information

The degree of purity for compounds 16, 22, 31, 32, 33, 34 and 35, in which considerable amounts of solvent were in evidence, was calculated on the dry basis, i.e., disregarding the peaks of the solvents. In these compounds, the calculated solvent content was: 16, 9.5% diethyl ether and 1.7% dichloromethane; 22, 1.1% dichloromethane; 31, 16.0% dichloromethane and 2.1% diethyl ether; 32, 3.5% dichloromethane and 7.6% diethyl ether; 33, 3.3% dichloromethane and 10.3% diethyl ether; 34, 2.0% dichloromethane; 35, 11.2% dichloromethane. The calculation took into account the molecular weight and the contribution of all the hydrogens attributed to the compounds and to the solvents, by using the program TopSpin® 3.5.

<sup>\*</sup>e-mail: lucianoliao@ufg.br





Figure S2.  ${}^{13}C{}^{1}H$  NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 1.



Figure S3. High resolution mass spectrum of compound 1.



Figure S4. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 2.



Figure S5. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 2.



Figure S6. HSQC correlation map of compound 2.



Figure S7. HMBC correlation map of compound 2.



Figure S8. High resolution mass spectrum of compound 2.



Figure S9. Infrared spectrum (ATR) of compound 2.



Figure S10. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 3.



Figure S11. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 3.



Figure S12. High resolution mass spectrum of compound 3.



Figure S13. Infrared spectrum (ATR) of compound 3.



Figure S14. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 4.



Figure S15. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 4.



Figure S16. High resolution mass spectrum of compound 4.



Figure S17. Infrared spectrum (ATR) of compound 4.



Figure S18.  $^{1}$ H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 5.



**Figure S19.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound **5**.



Figure S20. High resolution mass spectrum of compound 5.



Figure S21. Infrared spectrum (ATR) of compound 5.



Figure S22. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 6.



Figure S23. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 6.



Figure S24. High resolution mass spectrum of compound 6.



Figure S25. Infrared spectrum (ATR) of compound 6.



Figure S26. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 7.



**Figure S27.** <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 7.



Figure S28. High resolution mass spectrum of compound 7.



Figure S29. Infrared spectrum (ATR) of compound 7.



Figure S30. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 8.



Figure S31. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 8.



Figure S32. High resolution mass spectrum of compound 8.



Figure S33. Infrared spectrum (ATR) of compound 8.



Figure S34. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 9.



Figure S35. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 9.



Figure S36. High resolution mass spectrum of compound 9.



Figure S37. Infrared spectrum (ATR) of compound 9.



Figure S38. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 10.





Figure S40. NOE differential spectrum of compound 10.



Figure S41. COSY correlation map of compound 10.



Figure S42. HSQC correlation map of compound 10.



Figure S43. HMBC correlation map of compound 10.



Figure S44. High resolution mass spectrum of compound 10.



Figure S45. Infrared spectrum (ATR) of compound 10.



Figure S46. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 11.



Figure S47. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 11.



Figure S48. NOE differential spectrum of compound 11.



Figure S49. High resolution mass spectrum of compound 11.



Figure S50. Infrared spectrum (ATR) of compound 11.



Figure S51. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 12.



Figure S52. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 12.



Figure S53. NOE differential spectrum of compound 12.



Figure S54. High resolution mass spectrum of compound 12.



Figure S55. Infrared spectrum (ATR) of compound 12.



Figure S56. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 13.



Figure S57. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 13.



Figure S58. NOE differential spectrum of compound 13.



Figure S59. High resolution mass spectrum of compound 13.



Figure S60. Infrared spectrum (ATR) of compound 13.



Figure S61. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 14.



Figure S62. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 14.



Figure S63. NOE differential spectrum of compound 14.



Figure S64. High resolution mass spectrum of compound 14.



Figure S65. Infrared spectrum (ATR) of compound 14.



Figure S66. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 15.



Figure S67. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 15.



Figure S68. NOE differential spectrum of compound 15.



Figure S69. High resolution mass spectrum of compound 15.



Figure S70. Infrared spectrum (ATR) of compound 15.



Figure S71. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 16.



Figure S72. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 16.



Figure S73. NOE differential spectrum of compound 16.



Figure S74. High resolution mass spectrum of compound 16.



Figure S75. Infrared spectrum (ATR) of compound 16.



Figure S76. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 17.


Figure S77. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 17.



Figure S78. NOE differential spectrum of compound 17.



Figure S79. High resolution mass spectrum of compound 17.



Figure S80. Infrared spectrum (ATR) of compound 17.



Figure S81. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 18.



Figure S82. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 18.



Figure S83. NOE differential spectrum of compound 18.



Figure S84. High resolution mass spectrum of compound 18.



Figure S85. Infrared spectrum (ATR) of compound 18.



Figure S86. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 19.



Figure S87. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 19.



Figure S88. NOE differential spectrum of compound 19.



Figure S89. High resolution mass spectrum of compound 19.



Figure S90. Infrared spectrum (ATR) of compound 19.



Figure S91. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 20.



Figure S92. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 20.



Figure S93. NOE differential spectrum of compound 20.



Figure S94. High resolution mass spectrum of compound 20.



Figure S95. Infrared spectrum (ATR) of compound 20.



Figure S96. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 21.



Figure S97. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 21.



Figure S98. NOE differential spectrum of compound 21.



Figure S99. High resolution mass spectrum of compound 21.



Figure S100. Infrared spectrum (ATR) of compound 21.



Figure S101. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 22.



Figure S102. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 22.



Figure S103. NOE differential spectrum of compound 22.



Figure S104. High resolution mass spectrum of compound 22.



Figure S105. Infrared spectrum (ATR) of compound 22.



Figure S106. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 23.



Figure S107. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 23.



Figure S108. NOE differential spectrum of compound 23.



Figure S109. High resolution mass spectrum of compound 23.



Figure S110. Infrared spectrum (ATR) of compound 23.



Figure S111. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 24.



Figure S112. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 24.



Figure S113. NOE differential spectrum of compound 24.



Figure S114. High resolution mass spectrum of compound 24.



Figure S115. Infrared spectrum (ATR) of compound 24.



Figure S116. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 25.



Figure S117. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 25.



Figure S118. NOE differential spectrum of compound 25.



Figure S119. High resolution mass spectrum of compound 25.



Figure S120. Infrared spectrum (ATR) of compound 25.



Figure S121. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 26.



Figure S122. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 26.



Figure S123. NOE differential spectrum of compound 26.



Figure S124. High resolution mass spectrum of compound 26.



Figure S125. Infrared spectrum (ATR) of compound 26.



Figure S126. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 27.



Figure S127. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 27.



Figure S128. NOE differential spectrum of compound 27.



Figure S129. High resolution mass spectrum of compound 27.



Figure S130. Infrared spectrum (ATR) of compound 27.



Figure S131. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 28.



Figure S132. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 28.



Figure S133. NOE differential spectrum of compound 28.



Figure S134. High resolution mass spectrum of compound 28.



Figure S135. Infrared spectrum (ATR) of compound 28.



Figure S136. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 29.



Figure S137. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 29.



Figure S138. NOE differential spectrum of compound 29.



Figure S139. High resolution mass spectrum of compound 29.



Figure S140. Infrared spectrum (ATR) of compound 29.



Figure S141. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 30.



Figure S142. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 30.



Figure S143. NOE differential spectrum of compound 30.



Figure S144. High resolution mass spectrum of compound 30.



Figure S145. Infrared spectrum (ATR) of compound 30.



Figure S146. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 31.



Figure S147. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 31.



Figure S148. NOE differential spectrum of compound 31.



Figure S149. High resolution mass spectrum of compound 31.



Figure S150. Infrared spectrum (ATR) of compound 31.



Figure S151. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 32.



Figure S152. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 32.



Figure S153. NOE differential spectrum of compound 32.



Figure S154. High resolution mass spectrum of compound 32.



Figure S155. Infrared spectrum (ATR) of compound 32.



Figure S156. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 33.



Figure S157. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 33.



Figure S158. NOE differential spectrum of compound 33.



Figure S159. High resolution mass spectrum of compound 33.



Figure S160. Infrared spectrum (ATR) of compound 33.



Figure S161. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 34.



Figure S162. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 34.



Figure S163. NOE differential spectrum of compound 34.



Figure S164. High resolution mass spectrum of compound 34.



Figure S165. Infrared spectrum (ATR) of compound 34.



Figure S166. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 35.


Figure S167. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 35.



Figure S168. NOE differential spectrum of compound 35.



Figure S169. High resolution mass spectrum of compound 35.



Figure S170. Infrared spectrum (ATR) of compound 35.



Figure S171. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 36.



Figure S172. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 36.



Figure S173. NOE differential spectrum of compound 36.



Figure S174. High resolution mass spectrum of compound 36.



Figure S175. Infrared spectrum (ATR) of compound 36.



Figure S176. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 37.



Figure S177. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 37.



Figure S178. NOE differential spectrum of compound 37.



Figure S179. High resolution mass spectrum of compound 37.



Figure S180. Infrared spectrum (ATR) of compound 37.



Figure S181. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 38.



Figure S182. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 38.



Figure S183. NOE differential spectrum of compound 38.



Figure S184. High resolution mass spectrum of compound 38.



Figure S185. Infrared spectrum (ATR) of compound 38.



Figure S186. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 39.



Figure S187. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 39.



Figure S188. NOE differential spectrum of compound 39.



Figure S189. High resolution mass spectrum of compound 39.



Figure S190. Infrared spectrum (ATR) of compound 39.



Figure S191. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 40.



Figure S192. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 40.



Figure S193. NOE differential spectrum of compound 40.



Figure S194. High resolution mass spectrum of compound 40.



Figure S195. Infrared spectrum (ATR) of compound 40.



Figure S196. <sup>1</sup>H NMR spectrum (500 MHz, CDCl<sub>3</sub>) of compound 41.



Figure S197. <sup>13</sup>C{<sup>1</sup>H} NMR spectrum (126 MHz, CDCl<sub>3</sub>) of compound 41.



Figure S198. NOE differential spectrum of compound 41.



Figure S199. High resolution mass spectrum of compound 41.



Figure S200. Infrared spectrum (ATR) of compound 41.

| Hadassa         | $\delta^{1}$ H (mult., J in Hz, H) |                       |                           |                           |  |
|-----------------|------------------------------------|-----------------------|---------------------------|---------------------------|--|
| Hydrogen        | 14                                 | 15                    | 16                        | 17                        |  |
| Н3              | 7.70 (dd, 0.98, 8.13,              | 7.71 (dd, 0.98,       | 7.70 (dd, 0.90, 8.15,     | 7.71 (dd, 1.05, 8.20, 1H) |  |
|                 | 1H)                                | 8.18, 1H)             | 1H)                       |                           |  |
| H4              | 7.54-7.59 (m, 4H)                  | 7.57 (ddd, 1.66,      | 7.54 (ddd, 1.73, 7.30,    | 7.54 (ddd, 1.66, 7.36,    |  |
|                 |                                    | 7.36, 8.16, 1H)       | 8.20, 1H)                 | 8.19, 1H)                 |  |
| H5              | 7.28-7.34 (m, 3H)                  | 7.28-7.34 (m, 5H)     | 7.27-7.31 (m, 3H)         | 7.27-7.32 (m, 3H)         |  |
| H6              | 7.92 (dd, 1.73, 7.83,              | 7.90 (dd, 1.63,       | 7.88 (dd, 1.63, 7.83,     | 7.89 (dd, 1.65, 7.80, 1H) |  |
|                 | 1H)                                | 7.83, 1H)             | 1H)                       |                           |  |
| H9              | 7.54-7.59 (m, 4H)                  | 7.59 (s, 1H)          | 7.50 (s, 1H)              | 7.52 (s, 1H)              |  |
| H10             | 6.48 (d, 0.75, 1H)                 | 6.53 (d, 0.75, 1H)    | 6.55 (d, 0.60, 1H)        | 6.56 (d, 0.60, 1H)        |  |
| H12/H16         | _                                  | 7.28-7.34 (m, 5H)     | 7.03-7.06 (m, 2H)         | 7.10-7.13 (m, 4H)         |  |
| H13/H15         | _                                  | 8.25-8.28 (m, 2H)     | 7.53-7.56 (m, 2H)         | 7.37-7.40 (m, 2H)         |  |
| H12             | 8.04 (t, 1.95, 1H)                 | _                     | _                         | _                         |  |
| H14             | 8.28 (ddd, 0.88, 2.25,             | _                     | _                         | _                         |  |
|                 | 8.23, 1H)                          |                       |                           |                           |  |
| H15             | 7.54-7.59 (m, 4H)                  | _                     | _                         | _                         |  |
| H16             | 7.40-7.42 (m, 1H)                  | -                     | _                         | -                         |  |
| H18/H22         | 7.28-7.34 (m, 3H)                  | 7.28-7.34 (m, 5H)     | 7.27-7.31 (m, 3H)         | 7.27-7.32 (m, 3H)         |  |
| H19/H21         | 6.79-6.82 (m, 2H)                  | 6.78-6.81 (m, 2H)     | 6.76-6.79 (m, 2H)         | 6.77-6.80 (m, 2H)         |  |
| H24/H28         | 7.09-7.12 (m, 2H)                  | 7.10-7.12 (m, 2H)     | 7.10-7.13 (m, 2H)         | 7.10-7.13 (m, 4H)         |  |
| H25/H27         | 7.24-7.27 (m, 2H)                  | 7.22-7.26 (m, 2H)     | 7.19-7.23 (m, 2H)         | 7.19-7.23 (m, 2H)         |  |
| H26             | 7.54-7.59 (m, 4H)                  | 7.53 (tt, 1.23, 7.49, | 7.49 (tt, 1.20, 7.46, 1H) | 7.49 (tt, 1.25, 7.45, 1H) |  |
|                 |                                    | 1H)                   |                           |                           |  |
| CH <sub>2</sub> | 3.96 (q, 7.02, 2H)                 | 3.96 (q, 7.02, 2H)    | 3.95 (q, 7.00, 2H)        | 3.95 (q, 7.00, 2H)        |  |
| CH <sub>3</sub> | 1.37 (t, 6.98, 3H)                 | 1.37 (t, 7.00, 3H)    | 1.36 (t, 7.00, 3H)        | 1.36 (t, 7.00, 3H)        |  |

Table S1. <sup>1</sup>H NMR spectral data assignments for the compounds 14 to 17 in CDCl<sub>3</sub>. Structures were presented in Scheme 2

| Undrogon        | $\delta^{1}$ H (mult., J in Hz, H) |                       |                       |                              |  |
|-----------------|------------------------------------|-----------------------|-----------------------|------------------------------|--|
| nyurogen        | 18                                 | 19                    | 20                    | 21                           |  |
| H3              | 7.71 (d, 8.10, 1H)                 | 7.71 (dd, 0.95,       | 7.71 (dd, 0.85, 8.20, | 7.71 (dd, 0.80, 8.15, 1H)    |  |
|                 |                                    | 8.25, 1H)             | 1H)                   |                              |  |
| H4              | 7.54-7.58 (m, 3H)                  | 7.57 (ddd, 1.65,      | 7.53-7.57 (m, 3H)     | 7.55 (ddd, 1.65, 7.38, 8.18, |  |
|                 |                                    | 7.43, 8.13, 1H)       |                       | 1H)                          |  |
| H5              | 7.30-7.34 (m, 3H)                  | 7.29-7.34 (m, 5H)     | 7.29 (dt, 1.07, 7.50, | 7.28-7.33 (m, 3H)            |  |
|                 |                                    |                       | 1H)                   |                              |  |
| H6              | 7.93 (dd, 1.50, 7.80,              | 7.91 (dd, 1.65,       | 7.89 (dd, 1.63, 7.78, | 7.89 (dd, 1.58, 7.83, 1H)    |  |
|                 | 1H)                                | 7.85, 1H)             | 1H)                   |                              |  |
| H9              | 7.59 (s, 1H)                       | 7.60 (s, 1H)          | 7.51 (s, 1H)          | 7.53 (s, 1H)                 |  |
| H10             | 6.50 (s, 1H)                       | 6.54 (s, 1H)          | 6.56 (s, 1H)          | 6.57 (s, 1H)                 |  |
| H12/H16         | -                                  | 7.29-7.34 (m, 5H)     | 7.03-7.06 (m, 2H)     | 7.10-7.13 (m, 4H)            |  |
| H13/H15         | -                                  | 8.25-8.28 (m, 2H)     | 7.53-7.57 (m, 3H)     | 7.37-7.40 (m, 2H)            |  |
| H12             | 8.04 (t, 1.98, 1H)                 | _                     | _                     | -                            |  |
| H14             | 8.28 (dd, 1.88, 8.23,              | _                     | _                     | -                            |  |
|                 | 1H)                                |                       |                       |                              |  |
| H15             | 7.54-7.58 (m, 3H)                  | _                     | _                     | _                            |  |
| H16             | 7.42 (d, 7.70, 1H)                 | _                     | _                     | _                            |  |
| H18/H22         | 7.30-7.34 (m, 3H)                  | 7.29-7.34 (m, 5H)     | 7.30-7.33 (m, 2H)     | 7.28-7.33 (m, 3H)            |  |
| H19/H21         | 6.81-6.84 (m, 2H)                  | 6.80-6.83 (m, 2H)     | 6.78-6.81 (m, 2H)     | 6.78-6.81 (m, 2H)            |  |
| H24/H28         | 7.11-7.13 (m, 2H)                  | 7.10-7.13 (m, 2H)     | 7.10-7.13 (m, 2H)     | 7.10-7.13 (m, 4H)            |  |
| H25/H27         | 7.24-7.29 (m, 2H)                  | 7.22-7.26 (m, 2H)     | 7.19-7.23 (m, 2H)     | 7.19-7.23 (m, 2H)            |  |
| H26             | 7.54-7.58 (m, 3H)                  | 7.53 (tt, 1.17, 7.46, | 7.48-7.51 (m, 1H)     | 7.49 (tt, 1.23, 7.48, 1H)    |  |
|                 |                                    | 1H)                   |                       |                              |  |
| CH <sub>3</sub> | 3.75 (s, 3H)                       | 3.77 (s, 3H)          | 3.74 (s, 3H)          | 3.74 (s, 3H)                 |  |

Table S2. <sup>1</sup>H NMR spectral data assignments for the compounds 18 to 21 in CDCl<sub>3</sub>. Structures were presented in Scheme 2

| Hydrogan  | $\delta^{1}$ H (mult., J in Hz, H) |                       |                       |                                  |  |
|-----------|------------------------------------|-----------------------|-----------------------|----------------------------------|--|
| nyulogeli | 22                                 | 23                    | 24                    | 25                               |  |
| Н3        | 7.70 (dd, 0.83, 8.18,              | 7.71 (dd, 1.00,       | 7.71 (dd, 0.80,       | 7.71 (dd, 0.93, 8.18, 1H)        |  |
|           | 1H)                                | 8.20, 1H)             | 8.20, 1H)             |                                  |  |
| H4        | 7.55-7.61 (m, 3H)                  | 7.59 (ddd, 1.68,      | 7.54-7.58 (m, 3H)     | 7.56 (ddd, 1.68, 7.35, 8.18, 1H) |  |
|           |                                    | 7.35, 8.18, 1H)       |                       |                                  |  |
| H5        | 7.32-7.37 (m, 3H)                  | 7.33-7.36 (m, 3H)     | 7.31 (dt, 1.13,       | 7.31 (ddd, 1.14, 7.36, 7.79, 1H) |  |
|           |                                    |                       | 7.59, 1H)             |                                  |  |
| H6        | 7.91 (dd, 1.55, 7.80,              | 7.90 (dd, 1.60,       | 7.88 (dd, 1.58,       | 7.88 (dd, 1.60, 7.80, 1H)        |  |
|           | 1H)                                | 7.75, 1H)             | 7.78, 1H)             |                                  |  |
| H9        | 7.62 (s, 1H)                       | 7.63 (s, 1H)          | 7.53 (s, 1H)          | 7.56 (s, 1H)                     |  |
| H10       | 6.49 (s, 1H)                       | 6.55 (s, 1H)          | 6.57 (s, 1H)          | 6.58 (s, 1H)                     |  |
| H12/H16   | _                                  | 7.29-7.32 (m, 2H)     | 7.00-7.03 (m, 2H)     | 7.07-7.10 (m, 2H)                |  |
| H13/H15   | _                                  | 8.27-8.29 (m, 2H)     | 7.54-7.58 (m, 3H)     | 7.38-7.41 (m, 2H)                |  |
| H12       | 8.02 (t, 1.93, 1H)                 | -                     | —                     | _                                |  |
| H14       | 8.30 (dd, 2.18, 8.28,              | _                     | _                     | -                                |  |
|           | 1H)                                |                       |                       |                                  |  |
| H15       | 7.55-7.61 (m, 3H)                  | _                     | _                     | -                                |  |
| H16       | 7.36-7.39 (m, 1H)                  | _                     | _                     | -                                |  |
| H18/H22   | 7.32-7.37 (m, 3H)                  | 7.33-7.36 (m, 3H)     | 7.34-7.37 (m, 2H)     | 7.34-7.37 (m, 2H)                |  |
| H19/H21   | 7.24-7.30 (m, 4H)                  | 7.27-7.29 (m, 2H)     | 7.24-7.27 (m, 2H)     | 7.24-7.27 (m, 2H)                |  |
| H24/H28   | 7.09-7.11 (m, 2H)                  | 7.09-7.12 (m, 2H)     | 7.10-7.12 (m, 2H)     | 7.10-7.12 (m, 2H)                |  |
| H25/H27   | 7.24-7.30 (m, 4H)                  | 7.22-7.26 (m, 2H)     | 7.19-7.23 (m, 2H)     | 7.19-7.23 (m, 2H)                |  |
| H26       | 7.55-7.61 (m, 3H)                  | 7.54 (tt, 1.25, 7.50, | 7.50 (tt, 1.21, 7.48, | 7.50 (tt, 1.60, 7.80, 1H)        |  |
|           |                                    | 1H)                   | 1H)                   |                                  |  |

Table S3. <sup>1</sup>H NMR spectral data assignments for the compounds 22 to 25 in CDCl<sub>3</sub>. Structures were presented in Scheme 2

| Undrogon  | $\delta^{1}$ H (mult., J in Hz, H) |                       |                       |                           |  |
|-----------|------------------------------------|-----------------------|-----------------------|---------------------------|--|
| nyulogeli | 26                                 | 27                    | 28                    | 29                        |  |
| Н3        | 7.70 (dd, 1.03, 8.18,              | 7.72 (dd, 0.73,       | 7.71 (dd, 0.95,       | 7.71 (dd, 0.78, 8.18, 1H) |  |
|           | 1H)                                | 8.08, 1H)             | 8.20, 1H)             |                           |  |
| H4        | 7.55-7.61 (m, 3H)                  | 7.59 (ddd, 1.66,      | 7.54-7.58 (m, 3H)     | 7.54-7.58 (m, 1H)         |  |
|           |                                    | 7.36, 8.14, 1H)       |                       |                           |  |
| H5        | 7.34 (ddd, 1.11, 7.41,             | 7.33 (dd, 1.08,       | 7.31 (ddd, 1.09,      | 7.31 (dt, 1.10, 7.55, 1H) |  |
|           | 7.74, 1H)                          | 7.59, 1H)             | 7.44, 7.74, 1H)       |                           |  |
| H6        | 7.91 (dd, 1.62, 7.83,              | 7.90 (dd, 1.55,       | 7.88 (dd, 1.55,       | 7.88 (dd, 1.60, 7.80, 1H) |  |
|           | 1H)                                | 7.85, 1H)             | 7.80, 1H)             |                           |  |
| H9        | 7.62 (s, 1H)                       | 7.64 (s, 1H)          | 7.53 (s, 1H)          | 7.56 (s, 1H)              |  |
| H10       | 6.47 (s, 1H)                       | 6.53 (s, 1H)          | 6.55 (s, 1H)          | 6.56 (s, 1H)              |  |
| H12/H16   | _                                  | 7.28-7.32 (m, 4H)     | 7.00-7.03 (m, 2H)     | 7.07-7.10 (m, 2H)         |  |
| H13/H15   | _                                  | 8.27-8.30 (m, 2H)     | 7.54-7.58 (m, 3H)     | 7.38-7.43 (m, 4H)         |  |
| H12       | 8.03 (t, 1.32, 1H)                 | _                     | _                     | _                         |  |
| H14       | 8.30 (ddd, 0.84, 2.21,             | _                     | _                     | -                         |  |
|           | 8.24, 1H)                          |                       |                       |                           |  |
| H15       | 7.55-7.61 (m, 3H)                  | _                     | _                     | -                         |  |
| H16       | 7.36-7.38 (m, 1H)                  | _                     | _                     | -                         |  |
| H18/H22   | 7.28-7.30 (m, 2H)                  | 7.28-7.32 (m, 4H)     | 7.27-7.30 (m, 2H)     | 7.28-7.31 (m, 2H)         |  |
| H19/H21   | 7.43-7.45 (m, 2H)                  | 7.43-7.46 (m, 2H)     | 7.40-7.43 (m, 2H)     | 7.38-7.43 (m, 4H)         |  |
| H24/H28   | 7.08-7.11 (m, 2H)                  | 7.10-7.12 (m, 2H)     | 7.10-7.12 (m, 2H)     | 7.10-7.12 (m, 2H)         |  |
| H25/H27   | 7.24-7.28 (m, 2H)                  | 7.23-7.27 (m, 2H)     | 7.19-7.23 (m, 2H)     | 7.19-7.23 (m, 2H)         |  |
| H26       | 7.55-7.61 (m, 3H)                  | 7.54 (tt, 1.16, 7.45, | 7.50 (tt, 1.23, 7.48, | 7.50 (tt, 1.25, 7.46, 1H) |  |
|           |                                    | 1H)                   | 1H)                   |                           |  |

Table S4. <sup>1</sup>H NMR spectral data assignments for the compounds 26 to 29 in CDCl<sub>3</sub>. Structures were presented in Scheme 2

| TT 1            | $\delta^{1}$ H (mult., J in Hz, H) |                       |                       |                           |  |
|-----------------|------------------------------------|-----------------------|-----------------------|---------------------------|--|
| Hydrogen        | 30                                 | 31                    | 32                    | 33                        |  |
| H3              | 7.50-7.54 (m, 3H)                  | 7.51-7.56 (m, 3H)     | 7.46-7.55 (m, 5H)     | 7.54 (dd, 1.13, 8.13, 1H) |  |
| H4              | 7.50-7.54 (m, 3H)                  | 7.51-7.56 (m, 3H)     | 7.46-7.55 (m, 5H)     | 7.49 (ddd, 1.59, 7.21,    |  |
|                 |                                    |                       |                       | 8.14, 1H)                 |  |
| H5              | 7.36 (ddd, 2.50, 5.95,             | 7.36 (ddd, 2.11,      | 7.32 (dt, 1.20, 7.48, | 7.32 (ddd, 1.29, 7.26,    |  |
|                 | 7.80, 1H)                          | 6.29, 7.81, 1H)       | 1H)                   | 7.71, 1H)                 |  |
| H6              | 7.96-7.98 (m, 1H)                  | 7.96 (dd, 1.35, 7.90, | 7.93 (dd, 1.58, 7.83, | 7.93 (dd, 1.53, 7.78, 1H) |  |
|                 |                                    | 1H)                   | 1H)                   |                           |  |
| H9              | 7.54 (s, 1H)                       | 7.54 (s, 1H)          | 7.46 (s, 1H)          | 7.48 (s, 1H)              |  |
| H10             | 6.89 (s, 1H)                       | 6.87 (s, 1H)          | 6.91 (s, 1H)          | 6.92 (s, 1H)              |  |
| H12/H16         | _                                  | 7.28-7.31 (m, 2H)     | 7.01-7.04 (m, 2H)     | 7.08-7.11 (m, 2H)         |  |
| H13/H15         | _                                  | 8.23-8.26 (m, 2H)     | 7.46-7.55 (m, 5H)     | 7.35-7.37 (m, 2H)         |  |
| H12             | 7.93 (t, 2.10, 1H)                 | _                     | _                     | -                         |  |
| H14             | 8.25 (ddd, 1.09, 2.21,             | _                     | _                     | _                         |  |
|                 | 8.19, 1H)                          |                       |                       |                           |  |
| H15             | 7.58 (t, 7.93, 1H)                 | _                     | _                     | _                         |  |
| H16             | 7.47-7.50 (m, 1H)                  | _                     | _                     | -                         |  |
| H19             | 6.99 (dd, 0.85, 8.35,              | 6.96 (dd, 0.80, 8.35, | 6.93 (dd, 0.70, 8.20, | 6.93 (dd, 0.95, 8.35, 1H) |  |
|                 | 1H)                                | 1H)                   | 1H)                   |                           |  |
| H20             | 7.24-7.30 (m, 3H)                  | 7.24-7.28 (m, 3H)     | 7.20-7.25 (m, 3H)     | 7.20-7.25 (m, 3H)         |  |
| H21             | 6.71 (dt, 1.08, 7.49,              | 6.73 (dt, 0.97, 7.51, | 6.69 (dt, 0.93, 7.51, | 6.69 (dt, 1.10, 7.54, 1H) |  |
|                 | 1H)                                | 1H)                   | 1H)                   |                           |  |
| H22             | 6.81 (dd, 1.60, 7.70,              | 6.84 (dd, 1.60, 7.70, | 6.82 (dd, 1.50, 7.60, | 6.83 (dd, 1.55, 7.70, 1H) |  |
|                 | 1H)                                | 1H)                   | 1H)                   |                           |  |
| H24/H28         | 7.13-7.16 (m, 2H)                  | 7.13-7.15 (m, 2H)     | 7.13-7.16 (m, 2H)     | 7.13-7.15 (m, 2H)         |  |
| H25/H27         | 7.24-7.30 (m, 3H)                  | 7.24-7.28 (m, 3H)     | 7.20-7.25 (m, 3H)     | 7.20-7.25 (m, 3H)         |  |
| H26             | 7.50-7.54 (m, 3H)                  | 7.51-7.56 (m, 3H)     | 7.46-7.55 (m, 5H)     | 7.48 (tt, 1.28, 7.43, 1H) |  |
| CH <sub>3</sub> | 3.92 (s, 3H)                       | 3.92 (s, 3H)          | 3.93 (s, 3H)          | 3.93 (s, 3H)              |  |

Table S5. <sup>1</sup>H NMR spectral data assignments for the compounds 30 to 33 in CDCl<sub>3</sub>. Structures were presented in Scheme 2

| II lassa | $\delta^{1}$ H (mult., J in Hz, H) |                    |                           |                              |  |
|----------|------------------------------------|--------------------|---------------------------|------------------------------|--|
| Hydrogen | 34                                 | 35                 | 36                        | 37                           |  |
| H3       | 7.75 (dd, 0.95, 8.20,              | 7.77 (dd, 0.73,    | 7.76 (dd, 0.75, 8.20,     | 7.76 (dd, 0.63, 8.18, 1H)    |  |
|          | 1H)                                | 8.18, 1H)          | 1H)                       |                              |  |
| H4       | 7.60 (ddd, 1.65,                   | 7.61 (ddd, 1.69,   | 7.58 (ddd, 1.66, 7.39,    | 7.57 (ddd, 1.66, 7.41,       |  |
|          | 7.47, 8.18, 1H)                    | 7.34, 8.16, 1H)    | 8.14, 1H)                 | 8.11, 1H)                    |  |
| H5       | 7.35 (ddd, 1.09,                   | 7.33-7.37 (m, 3H)  | 7.33 (dt, 1.08, 7.59, 1H) | 7.32 (dt, 1.05, 7.59, 1H)    |  |
|          | 7.41, 7.79, 1H)                    |                    |                           |                              |  |
| H6       | 7.93 (dd, 1.58, 7.83,              | 7.91 (dd, 1.43,    | 7.89 (dd, 1.50, 7.80,     | 7.89 (dd, 1.60, 7.85, 1H)    |  |
|          | 1H)                                | 7.73, 1H)          | 1H)                       |                              |  |
| H9       | 7.72 (s, 1H)                       | 7.73 (s, 1H)       | 7.63 (s, 1H)              | 7.65 (s, 1H)                 |  |
| H10      | 6.63 (s, 1H)                       | 6.69 (s, 1H)       | 6.71 (s, 1H)              | 6.72 (s, 1H)                 |  |
| H12/H16  | _                                  | 7.33-7.37 (m, 3H)  | 7.02-7.06 (m, 2H)         | 7.10-7.13 (m, 2H)            |  |
| H13/H15  | -                                  | 8.29-8.32 (m, 2H)  | 7.57-7.60 (m, 2H)         | 7.41-7.43 (m, 2H)            |  |
| H12      | 8.03 (t, 1.98, 1H)                 | _                  | _                         | _                            |  |
| H14      | 8.31 (ddd, 0.85,                   | _                  | _                         | _                            |  |
|          | 2.20, 8.25, 1H)                    |                    |                           |                              |  |
| H15      | 7.62 (t, 7.98, 1H)                 | _                  | _                         | -                            |  |
| H16      | 7.40-7.43 (m, 1H)                  | _                  | _                         | _                            |  |
| H18      | 8.21 (t, 2.48, 1H)                 | 8.22 (t, 2.55, 1H) | 8.24 (t, 2.35, 1H)        | 8.24 (t, 2.53, 1H)           |  |
| H20      | 8.16 (dddd, 0.70,                  | 8.15-8.17 (m, 1H)  | 8.12-8.15 (m, 1H)         | 8.11-8.14 (m, 1H)            |  |
|          | 1.05, 2.23, 8.20, 1H)              |                    |                           |                              |  |
| H21      | 7.55 (t, 7.95, 1H)                 | 7.54-7.59 (m, 2H)  | 7.50-7.55 (m, 2H)         | 7.49-7.54 (m, 2H)            |  |
| H22      | 7.84 (tdd, 0.94, 1.89,             | 7.83 (tdd, 0.96,   | 7.81 (tdd, 0.96, 1.91,    | 7.81 (tdd, 0.95, 1.90, 7.85, |  |
|          | 7.79, 1H)                          | 1.93, 7.80, 1H)    | 7.84, 1H)                 | 1H)                          |  |
| H24/H28  | 7.13-7.16 (m, 2H)                  | 7.12-7.15 (m, 2H)  | 7.12-7.15 (m, 2H)         | 7.13-7.16 (m, 2H)            |  |
| H25/H27  | 7.27-7.30 (m, 2H)                  | 7.25-7.29 (m, 2H)  | 7.22-7.26 (m, 2H)         | 7.21-7.25 (m, 2H)            |  |
| H26      | 7.57-7.60 (m, 1H)                  | 7.54-7.59 (m, 2H)  | 7.50-7.55 (m, 2H)         | 7.49-7.54 (m, 2H)            |  |

Table S6. <sup>1</sup>H NMR spectral data assignments for the compounds 34 to 37 in CDCl<sub>3</sub>. Structures were presented in Scheme 2

|          | $\delta^{1}$ H (mult., J in Hz, H) |                   |                           |                           |  |
|----------|------------------------------------|-------------------|---------------------------|---------------------------|--|
| Hydrogen | 38                                 | 39                | 40                        | 41                        |  |
| Н3       | 7.51 (ddd, 0.45,                   | 7.51 (ddd, 0.55,  | 7.49-7.53 (m, 3H)         | 7.49-7.53 (m, 3H)         |  |
|          | 1.50, 8.05, 1H)                    | 1.53, 8.08, 1H)   |                           |                           |  |
| H4       | 7.53-7.58 (m, 2H)                  | 7.52-7.56 (m, 2H) | 7.49-7.53 (m, 3H)         | 7.49-7.53 (m, 3H)         |  |
| H5       | 7.38 (ddd, 1.51,                   | 7.37 (ddd, 1.51,  | 7.34 (ddd, 3.55, 5.05,    | 7.34 (ddd, 3.35, 5.23,    |  |
|          | 7.06, 7.76, 1H)                    | 7.06, 7.74, 1H)   | 7.75, 1H)                 | 7.75, 1H)                 |  |
| H6       | 7.91 (ddd, 0.50,                   | 7.90 (ddd, 0.51,  | 7.86-7.89 (m, 1H)         | 7.86-7.89 (m, 1H)         |  |
|          | 1.58, 7.78, 1H)                    | 1.59, 7.76, 1H)   |                           |                           |  |
| H9       | 7.66 (s, 1H)                       | 7.66 (s, 1H)      | 7.56 (s, 1H)              | 7.59 (s, 1H)              |  |
| H10      | 6.86 (s, 1H)                       | 6.90 (s, 1H)      | 6.91 (s, 1H)              | 6.91 (s, 1H)              |  |
| H12/H16  | _                                  | 7.31-7.34 (m, 2H) | 7.03-7.06 (m, 2H)         | 7.09-7.13 (m, 5H)         |  |
| H13/H15  | _                                  | 8.28-8.31 (m, 2H) | 7.56-7.59 (m, 2H)         | 7.40-7.43 (m, 2H)         |  |
| H12      | 7.99 (t, 1.98, 1H)                 | _                 | _                         | _                         |  |
| H14      | 8.29 (ddd, 0.90,                   | _                 | _                         | _                         |  |
|          | 2.20, 8.23, 1H)                    |                   |                           |                           |  |
| H15      | 7.63 (t, 7.98, 2H)                 | _                 | _                         | _                         |  |
| H16      | 7.44 (tdd, 0.85,                   | _                 | _                         | _                         |  |
|          | 1.70, 7.70, 1H)                    |                   |                           |                           |  |
| H19      | 7.74 (dd, 1.28,                    | 7.72 (dd, 1.33,   | 7.70 (dd, 1.23, 7.98,     | 7.70 (dd, 1.38, 7.98, 1H) |  |
|          | 7.98, 1H)                          | 7.98, 1H)         | 1H)                       |                           |  |
| H20      | 7.14 (ddd, 1.60,                   | 7.14 (dt, 1.63,   | 7.09-7.13 (m, 3H)         | 7.09-7.13 (m, 5H)         |  |
|          | 7.43, 7.83, 1H)                    | 7.73, 1H)         |                           |                           |  |
| H21      | 7.01 (dt, 1.32,                    | 7.01 (dt, 1.30,   | 6.98 (dt, 1.23, 7.61, 1H) | 6.98 (dt, 1.48, 7.60, 1H) |  |
|          | 7.63, 1H)                          | 7.60, 1H)         |                           |                           |  |
| H22      | 6.74 (dd, 1.53,                    | 6.74 (dd, 1.58,   | 6.74 (dd, 1.48, 7.83,     | 6.75 (dd, 1.75, 7.85, 1H) |  |
|          | 7.83, 1H)                          | 7.88, 1H)         | 1H)                       |                           |  |
| H24/H28  | 7.11-7.14 (m, 2H)                  | 7.11-7.14 (m, 2H) | 7.09-7.13 (m, 3H)         | 7.09-7.13 (m, 5H)         |  |
| H25/H27  | 7.27-7.31 (m, 2H)                  | 7.25-7.29 (m, 2H) | 7.22-7.26 (m, 2H)         | 7.22-7.26 (m, 2H)         |  |
| H26      | 7.53-7.58 (m, 2H)                  | 7.52-7.56 (m, 2H) | 7.49-7.53 (m, 3H)         | 7.49-7.53 (m, 3H)         |  |

Table S7. <sup>1</sup>H NMR spectral data assignments for the compounds 38 to 41 in CDCl<sub>3</sub>. Structures were presented in Scheme 2

| Undrogon | $\delta^{1}$ H (mult., J in Hz, H) |                           |                           |                           |  |
|----------|------------------------------------|---------------------------|---------------------------|---------------------------|--|
| nyurogen | 42                                 | 43                        | 44                        | 45                        |  |
| H3       | 7.51-7.58 (m, 4H)                  | 7.51-7.57 (m, 4H)         | 7.48-7.54 (m, 4H)         | 7.49-7.54 (m, 4H)         |  |
| H4       | 7.51-7.58 (m, 4H)                  | 7.51-7.57 (m, 4H)         | 7.48-7.54 (m, 4H)         | 7.49-7.54 (m, 4H)         |  |
| H5       | 7.38 (ddd, 1.76,                   | 7.37 (ddd, 1.91, 6.66,    | 7.35 (ddd, 2.60, 5.98,    | 7.35 (ddd, 2.46, 6.09,    |  |
|          | 6.76, 7.76, 1H)                    | 7.74, 1H)                 | 7.75, 1H)                 | 7.76, 1H)                 |  |
| H6       | 7.93 (dd, 1.40,                    | 7.92 (ddd, 0.55, 1.50,    | 7.88-7.91 (m, 1H)         | 7.89-7.91 (m, 1H)         |  |
|          | 7.70, 1H)                          | 7.78, 1H)                 |                           |                           |  |
| H9       | 7.64 (s, 1H)                       | 7.65 (s, 1H)              | 7.55 (s, 1H)              | 7.57 (s, 1H)              |  |
| H10      | 6.91 (s, 1H)                       | 6.94 (s, 1H)              | 6.95 (s, 1H)              | 6.96 (s, 1H)              |  |
| H12/H16  | _                                  | 7.26-7.32 (m, 4H)         | 7.01-7.04 (m, 2H)         | 7.08-7.11 (m, 2H)         |  |
| H13/H15  | _                                  | 8.27-8.30 (m, 2H)         | 7.56-7.58 (m, 2H)         | 7.40-7.43 (m, 2H)         |  |
| H12      | 7.97 (t, 2.00, 1H)                 | _                         | _                         | _                         |  |
| H14      | 8.29 (ddd, 0.94,                   | _                         | _                         | _                         |  |
|          | 2.19, 8.14, 1H)                    |                           |                           |                           |  |
| H15      | 7.63 (t, 8.08, 1H)                 | _                         | _                         | _                         |  |
| H16      | 7.42 (tdd, 0.85,                   | _                         | _                         | _                         |  |
|          | 1.70, 7.70, 1H)                    |                           |                           |                           |  |
| H19      | 7.51-7.58 (m, 4H)                  | 7.51-7.57 (m, 4H)         | 7.48-7.54 (m, 4H)         | 7.49-7.54 (m, 4H)         |  |
| H20      | 7.24 (dt, 1.52, 7.75,              | 7.23 (ddd, 1.59, 7.49,    | 7.20 (dt, 1.55, 7.73, 1H) | 7.20 (ddd, 1.51, 7.44,    |  |
|          | 1H)                                | 7.96, 1H)                 |                           | 7.96, 1H)                 |  |
| H21      | 6.98 (dt, 1.40, 7.65,              | 6.98 (td, 1.28, 7.64, 1H) | 6.94 (dt, 1.32, 7.61, 1H) | 6.95 (dt, 1.30, 7.58, 1H) |  |
|          | 1H)                                |                           |                           |                           |  |
| H22      | 6.76 (dd, 1.68,                    | 6.76 (dd, 1.55, 7.85, 1H) | 6.76 (dd, 1.58, 7.83, 1H) | 6.76 (dd, 1.35, 7.75, 1H) |  |
|          | 7.83, 1H)                          |                           |                           |                           |  |
| H24/H28  | 7.12-7.14 (m, 2H)                  | 7.12-7.14 (m, 2H)         | 7.10-7.13 (m, 2H)         | 7.11-7.13 (m, 2H)         |  |
| H25/H27  | 7.28-7.32 (m, 2H)                  | 7.26-7.32 (m, 4H)         | 7.23-7.26 (m, 2H)         | 7.23-7.26 (m, 2H)         |  |
| H26      | 7.51-7.58 (m, 4H)                  | 7.51-7.57 (m, 4H)         | 7.48-7.54 (m, 4H)         | 7.49-7.54 (m, 4H)         |  |

Table S8. <sup>1</sup>H NMR spectral data assignments for the compounds 42 to 45 in CDCl<sub>3</sub>. Structures were presented in Scheme 2

| <u> </u> |               | Compound |        |        |
|----------|---------------|----------|--------|--------|
| Carbon   | 14            | 15       | 16     | 17     |
| C7       | 182.36        | 182.33   | 182.72 | 182.71 |
| C9       | 136.66        | 136.66   | 138.62 | 138.57 |
| C10      | 59.55         | 59.53    | 59.60  | 59.59  |
| C12/C16  | 125.17/134.48 | 130.60   | 131.50 | 131.33 |
|          | 18            | 19       | 20     | 21     |
| C7       | 182.35        | 182.31   | 182.69 | 182.70 |
| C9       | 136.72        | 136.70   | 138.67 | 138.62 |
| C10      | 59.53         | 59.51    | 59.57  | 59.56  |
| C12/C16  | 125.16/134.48 | 130.59   | 131.49 | 131.33 |
|          | 22            | 23       | 24     | 25     |
| C7       | 181.97        | 181.94   | 182.32 | 182.32 |
| C9       | 137.35        | 137.34   | 139.28 | 139.22 |
| C10      | 59.38         | 59.36    | 59.45  | 59.44  |
| C12/C16  | 125.11/134.26 | 130.50   | 131.38 | 131.23 |
|          | 26            | 27       | 28     | 29     |
| C7       | 181.95        | 181.92   | 182.30 | 182.30 |
| C9       | 137.39        | 137.39   | 139.32 | 139.27 |
| C10      | 59.43         | 59.40    | 59.50  | 59.50  |
| C12/C16  | 125.13/134.23 | 130.49   | 131.37 | 131.23 |
|          | 30            | 31       | 32     | 33     |
| C7       | 182.56        | 182.60   | 182.98 | 182.99 |
| C9       | 135.45        | 135.59   | 137.57 | 137.54 |
| C10      | 56.09         | 56.32    | 56.44  | 56.43  |
| C12/C16  | 124.44/135.81 | 130.67   | 131.60 | 131.42 |
|          | 34            | 35       | 36     | 37     |
| C7       | 181.36        | 181.36   | 181.73 | 181.73 |
| C9       | 138.17        | 138.24   | 140.15 | 140.09 |
| C10      | 59.31         | 59.23    | 59.35  | 59.34  |
| C12/C16  | 124.85/133.87 | 130.43   | 131.30 | 131.16 |
|          | 38            | 39       | 40     | 41     |
| C7       | 182.19        | 182.20   | 182.58 | 182.58 |
| C9       | 137.13        | 137.13   | 139.11 | 139.06 |
| C10      | 60.75         | 60.67    | 60.86  | 60.86  |
| C12/C16  | 124.66/134.92 | 130.46   | 131.40 | 131.25 |
|          | 42            | 43       | 44     | 45     |
| C7       | 182.17        | 182.19   | 182.57 | 182.58 |
| C9       | 137.06        | 137.09   | 139.06 | 139.02 |
| C10      | 58.56         | 58.51    | 58.73  | 58.73  |
| C12/C16  | 124.62/134.82 | 130.43   | 131.37 | 131.22 |

Table S9. <sup>13</sup>C NMR spectral data assignments of C7, C9, C10, C12 and C16 for the compounds 14 to 45 in CDCl<sub>3</sub>. Structures were presented in Scheme 2