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SUPPLEMENTARY MATERIAL TO

Synthesis, structural characterization and myo activity of 4-naphthylhexahydroquinoline derivatives containing different ester groups

MİYASE GÖZDE GÜNDÜZ[1]*, EMİNE ALBAYRAK[1], FATMA İŞLİ[2], GÖKÇE SEVİM ÖZTÜRK FİNCAN[3], ŞENİZ YILDIRIM[4], RAHİME ŞİMŞEK[1], CİHAT ŞAFAK[1], YUSUF SARIOĞLU[3], SEMA ÖZTÜRK YIDIRIM[5] and RAY J. BUTCHER[6]

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[1]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Hacettepe University, Ankara 06100, Turkey, [2]Department of Rational Drug Use and Drug Supply Management, Turkish Medicines and Medical Devices Agency, Ankara 06520, Turkey, [3]Department of Pharmacology, Faculty of Medicine, Gazi University, Ankara 06500, Turkey, [4]Department of Pharmacology, Faculty of Medicine, Kırıkkale University, Kırıkkale 71450, Turkey, [5]Department of Physics, Faculty of Sciences, Erciyes University, Kayseri 38039, Turkey and [6]Department of Chemistry, Howard University, Washington DC 20059, USA

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CHARACTERIZATION OF THE SYNTHESIZED COMPOUNDS

*Methyl 2,6,6-trimethyl-4-(1-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**1**).* Yield: 76 %; m.p.: 223–225 °C; Anal. calcd. for $C_{24}H_{25}NO_3$: C, 76.77; H, 6.71; N, 3.73 %. Found: C, 76.72; H, 6.75; N, 3.75 %; IR (cm^{-1}): 3313 (N–H), 1703 (C=O, ester), 1647 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.75 (3H, *s*, 6-CH_3), 0.95 (3H, *s*, 6-CH_3), 1.62–1.76 (2H, *m*, H-7), 2.27 (3H, *s*, 2-CH_3), 2.51–2.57 (2H, *m*, H-8), 3.30 (3H, *s*, $COOCH_3$), 5.61 (1H, *s*, H-4), 7.29–8.66 (7H, *m*, Ar-H), 9.17 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 18.1 (2-CH_3), 22.9 (6-CH_3), 24.1 (C-8), 24.9 (6-CH_3), 31.4 (C-7), 38.8 (C-6), 40.0 (C-4), 50.3 ($COOCH_3$), 104.8 (C-3), 110.7 (C-4a), 122.4, 125.0, 125.8, 126.0, 126.2, 126.5, 127.6, 129.7, 136.2, 142.2 (naphthyl carbons), 144.0 (C-2), 149.3 (C-8a), 167.4 (**C**$OOCH_3$), 199.5 (C-5); ESI-MS (*m*/*z*): 399.18 $[M+1+Na]^+$, 398.18 $[M+Na]^+$ (100 %).

*Ethyl 2,6,6-trimethyl-4-(1-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**2**).* Yield: 80 %; m.p.: 210–212 °C; Anal. calcd. for $C_{25}H_{27}NO_3$: C, 77.09; H, 6.99; N, 3.60 %. Found: C, 77.05; H, 6.95; N, 3.62 %; IR (cm^{-1}):

* Corresponding author. E-mail: miyasegunduz@yahoo.com
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3291 (N–H), 1694 (C=O, ester), 1642 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.74 (3H, *s*, 6-CH_3), 0.85 (3H, *t*, J = 7.2 Hz, $CH_2C\mathbf{H}_3$), 0.96 (3H, *s*, 6-CH_3), 1.61-1.76 (2H, *m*, H-7), 2.28 (3H, *s*, 2-CH_3), 2.50–2.56 (2H, *m*, H-8), 3.74 (2H, *m*, J = 7.2 Hz, $C\mathbf{H}_2CH_3$), 5.60 (1H, *s*, H-4), 7.31–8.69 (7H, *m*, Ar-H), 9.14 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 13.8 ($COOCH_2\mathbf{C}H_3$), 18.1 (2-CH_3), 23.0 (6-CH_3), 24.1 (C-8), 24.9 (6-CH_3), 31.4 (C-7), 34.0 (C-6), 40.0 (C-4), 58.8 ($COO\mathbf{C}H_2CH_3$), 105.1 (C-3), 110.8 (C-4a), 124.8, 125.0, 125.80, 125.83, 126.1, 127.5, 130.3, 132.6, 135.2, 143.9 (naphthyl carbons), 147.0 (C-2), 149.2 (C-8a), 167.0 ($\mathbf{C}OOCH_2CH_3$), 199.5 (C-5); ESI-MS (*m*/*z*): 413.22 $[M+1+Na]^+$, 412.22 $[M+Na]^+$ (100 %).

*Isopropyl 2,6,6-trimethyl-4-(1-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**3**)*. Yield: 73 %; m.p.: 211–213 °C; Anal. calcd. for $C_{26}H_{29}NO_3$: C, 77.39; H, 7.24; N, 3.47 %. Found: C, 77.34; H, 7.26; N, 3.45 %; IR (cm^{-1}): 3293 (N–H), 1691 (C=O, ester), 1637 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.74 (3H, *s*, 6-CH_3), 0.96 (3H, *s*, 6-CH_3), 1.04 (3H, *d*, J = 6.0 Hz, $CH(C\mathbf{H}_3)_2$), 1.18 (3H, *d*, J = 6.0 Hz, $CH(C\mathbf{H}_3)_2$), 1.60–1.74 (2H, *m*, H-7), 2.29 (3H, *s*, 2-CH_3), 2.49–2.55 (2H, *m*, H-8), 4.62 (1H, *m*, $C\mathbf{H}(CH_3)_2$), 5.57 (1H, *s*, H-4), 7.31–8.72 (7H, *m*, Ar-H), 9.11 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 18.1 (2-CH_3), 20.8 ($CH(\mathbf{C}H_3)_2$), 21.5 ($CH(\mathbf{C}H_3)_2$), 23.0 (6-CH_3), 24.1 (C-8), 24.9 (6-CH_3), 31.5 (C-7), 34.0 (C-6), 40.0 (C-4), 65.7 ($\mathbf{C}H(CH_3)_2$), 105.6 (C-3), 110.7 (C-4a), 124.7, 125.0, 125.7, 126.0, 126.2, 126.3, 127.5, 130.4, 132.5, 143.7 (naphthyl carbons), 147.1 (C-2), 149.2 (C-8a), 166.4 ($\mathbf{C}OOCH(CH_3)_2$), 199.5 (C-5); ESI-MS (*m*/*z*): 427.22 $[M+1+Na]^+$, 426.22 $[M+Na]^+$ (100 %).

*Isobutyl 2,6,6-trimethyl-4-(1-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**4**)*. Yield: 72 %; m.p.: 170–172 °C; Anal. calcd. for $C_{27}H_{31}NO_3$: C, 77.67; H, 7.48; N, 3.35 %. Found: C, 77.71; H, 7.45; N, 3.34 %; IR (cm^{-1}): 3299 (N–H), 1697 (C=O, ester), 1646 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.50 (3H, *d*, J = 6.8 Hz, $CH(C\mathbf{H}_3)_2$), 0.63 (3H, *d*, J = 6.8 Hz, $CH(C\mathbf{H}_3)_2$), 0.74 (3H, *s*, 6-CH_3), 0.96 (3H, *s*, 6-CH_3), 1.47–1.59 (1H, *m*, $C\mathbf{H}(CH_3)_2$), 1.59–1.75 (2H, *m*, H-7), 2.31 (3H, *s*, 2-CH_3), 2.49–2.55 (2H, *m*, H-8), 3.46–3.56 (2H, *m*, $C\mathbf{H}_2CH(CH_3)_2$), 5.61 (1H, *s*, H-4), 7.31–8.73 (7H, *m*, Ar-H), 9.17 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 18.2 (2-CH_3), 19.0 ($CH(\mathbf{C}H_3)_2$), 22.5 (6-CH_3), 24.0 (C-8), 25.3 (6-CH_3), 27.8 ($\mathbf{C}H(CH_3)_2$), 34.3 (C-7), 36.7 (C-6), 39.9 (C-4), 69.7 ($COO\mathbf{C}H_2$), 102.6 (C-3), 108.9 (C-4a), 125.1, 125.8, 126.5, 127.1, 127.3, 127.8, 131.5, 132.8, 135.4, 138.7, 145.1 (naphthyl carbons), 145.9 (C-2), 150.0 (C-8a), 166.2 ($\mathbf{C}OOCH_2$), 199.8 (C-5); ESI-MS (*m*/*z*): 441.24 $[M+1+Na]^+$, 440.24 $[M+Na]^+$ (100 %).

tert-*Butyl 2,6,6-trimethyl-4-(1-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**5**)*. Yield: 83 %; m.p.: 243–245 °C; Anal. calcd. for $C_{27}H_{31}NO_3$: C, 77.67; H, 7.48; N, 3.35 %. Found: C, 77.65; H, 7.51; N, 3.32 %;

IR (cm^{-1}): 3212 (N–H), 1698 (C=O, ester), 1655 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.75 (3H, *s*, 6-CH_3), 0.96 (3H, *s*, 6-CH_3), 1.10 (9H, *s*, $C(CH_3)_3$), 1.59–1.74 (2H, *m*, H-7), 2.22 (3H, *s*, 2-CH_3), 2.49–2.54 (2H, *m*, 8-H), 5.55 (1H, *s*, H-4), 7.29–8.72 (7H, *m*, Ar-H), 9.03 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 18.0 (2-CH_3), 23.0 (6-CH_3), 24.1 (C-8), 25.0 (6-CH_3), 27.7 (COOC(**C**$H_3)_3$), 32.0 (C-7), 33.9 (C-6), 40.0 (C-4), 78.8 (**C**OOC$(CH_3)_3$), 107.0 (C-3), 110.2 (C-4a), 124.8, 125.0, 125.8, 126.0, 126.1, 126.2, 127.5, 130.3, 132.7, 142.0 (naphthyl carbons), 146.4 (C-2), 149.5 (C-8a), 166.7 (**C**OOC$(CH_3)_3$), 199.4 (C-5); ESI-MS (*m/z*): 441.30 $[M+1+Na]^+$, 440.29 $[M+Na]^+$ (100 %).

*2-Methoxyethyl 2,6,6-trimethyl-4-(1-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**6**).* Yield: 78 %; m.p:. 197–199 °C; Anal. calcd. for $C_{26}H_{29}NO_4$: C, 74.44; H, 6.97; N, 3.34 %. Found: C, 74.42; H, 7.01; N, 3.33 %; IR (cm^{-1}): 3299 (N–H), 1696 (C=O, ester), 1660 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.74 (3H, *s*, 6-CH_3), 0.96 (3H, *s*, 6-CH_3), 1.61–2.56 (4H, *m*, H-7,8), 2.29 (3H, *s*, 2-CH_3), 3.11 (3H, *s*, OCH_3), 3.21 (2H, *m*, COOC**H**$_2$), 3.84 (2H, *m*, CH_2C**H**$_2OCH_3$), 5.60 (1H, *s*, H-4), 7.31–8.70 (7H, *m*, Ar-H), 9.18 (1H, *s*, N–H); ^{13}C-NMR (100 Hz, DMSO-d_6, δ / ppm): 18.2 (2-CH_3), 23.0 (6-CH_3), 24.1 (C-8), 24.9 (6-CH_3), 31.4 (C-7), 33.9 (C-6), 40.0 (C-4), 57.8 (CH_2CH_2O**C**H_3), 62.0 (COO**C**H_2), 69.5 (CH_2**C**H_2OCH_3), 104.8 (C-3), 110.8 (C-4a), 124.9, 125.0, 125.7, 125.8, 126.1, 126.2, 127.5, 130.3, 132.7, 144.3 (naphthyl carbons), 146.8 (C-2), 149.2 (C-8a), 166.9 (**C**OOCH_2), 199.5 (C-5); ESI-MS (*m/z*): 443.22 $[M+1+Na]^+$, 442.21 $[M+Na]^+$ (100 %).

*2-(Methacryloyloxy)ethyl 2,6,6-trimethyl-4-(1-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**7**).* Yield: 75 %; m.p.: 155–157 °C; Anal. calcd. for $C_{29}H_{31}NO_5$: C, 73.55; H, 6.60; N, 2.96 %. Found: C, 73.50; H, 6.57; N, 2.95 %; IR (cm^{-1}): 3291 (N–H), 1703 (C=O, ester), 1655 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.73 (3H, *s*, 6-CH_3), 0.95 (3H, *s*, 6-CH_3), 1.62–1.72 (2H, *m*, H-7), 1.79 (3H, *s*, C(C**H**$_3$)=CH_2), 2.29 (3H, *s*, 2-CH_3), 2.49–2.56 (2H, *m*, H-8), 3.92–4.04 (4H, *m*, OC**H**$_2$C**H**$_2$O), 4.99 (1H, *s*, H-4), 5.59–5.88 (2H, *m*, C(CH_3)=C**H**$_2$), 7.31–8.68 (7H, *m*, Ar-H), 9.20 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 18.4 (2-CH_3), 18.7 (C(**C**H_3)=CH_2), 22.8 (6-CH_3), 24.2 (C-8), 25.0 (6-CH_3), 34.1 (C-7), 36.3 (C-6), 40.1 (C-4), 61.2 (OCH_2**C**H_2O), 62.9 (O**C**H_2CH_2O), 102.6 (C-3), 109.1 (C-4a), 125.1, 125.7 (naphthyl carbons), 126.6 (C(CH_3)=**C**H_2), 127.2, 127.4, 127.5, 131.5, 132.7, 133.8, 134.7 (naphthyl carbons), 135.2 (**C**(CH_3)=CH_2), 145.1 (naphthyl carbon), 145.5 (C-2), 149.6 (C-8a), 166.0 (**C**OOCH_2CH_2), 167.1 (**C**O(CH_3)=CH_2), 199.5 (C-5); ESI-MS (*m/z*): 497.27 $[M+1+Na]^+$, 496.27 $[M+Na]^+$ (100 %).

*Benzyl 2,6,6-trimethyl-4-(1-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**8**).* Yield: 78 %; m.p.: 167–169 °C; Anal. calcd. for $C_{30}H_{29}NO_3$: C, 79.80; H, 6.47; N, 3.10 %. Found: C, 79.83; H, 6.45; N, 3.09 %; IR (cm^{-1}):

3324 (N–H), 1710 (C=O, ester), 1648 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.74 (3H, *s*, 6-CH_3), 0.95 (3H, *s*, 6-CH_3), 1.60–2.56 (4H, *m*, H-7,8), 2.30 (3H, *s*, 2-CH_3), 4.73, 4.87 (2H, AB system, J_{AB} = 12.4 Hz, COOC**H**$_2$C$_6$H$_5$), 5.63 (1H, *s*, H-4), 6.91–8.63 (12H, *m*, Ar-H), 9.21 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm) 18.3 (2-CH_3), 23.0 (6-CH_3), 24.1 (C-8), 24.9 (6-CH_3), 31.4 (C-7), 33.9 (C-6), 40.0 (C-4), 64.5 (COO**C**H$_2$C$_6$H$_5$), 104.7 (C-3), 110.9 (C-4a), 124.9, 125.0, 125.6, 125.7, 126.1, 126.2, 126.4, 127.5, 127.6, 128.1, 130.3, 132.7, 135.3, 136.4, 137.2, 144.7 (naphthyl and phenyl carbons), 146.7 (C-2), 149.2 (C-8a), 166.7 (**C**OOCH$_2$C$_6$H$_5$), 199.5 (C-5); ESI-MS (*m*/*z*): 475.27 $[M+1+Na]^+$, 474.27 $[M+Na]^+$ (100 %).

*Methyl 2,6,6-trimethyl-4-(2-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**9**)*. Yield: 87 %; m.p.: 259–261 °C; Anal. Calcd. for $C_{24}H_{25}NO_3$: C, 76.77; H, 6.71; N, 3.73 %. Found: C, 76.69; H, 6.70; N, 3.75 %; IR (cm^{-1}): 3280 (N–H), 1702 (C=O, ester), 1645 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.87 (3H, *s*, 6-CH_3), 0.99 (3H, *s*, 6-CH_3), 1.57–1.75 (2H, *m*, H-7), 2.32 (3H, *s*, 2-CH_3), 2.50–2.55 (2H, *m*, H-8), 3.53 (3H, *s*, OCH_3), 5.06 (1H, *s*, H-4), 7.36–7.82 (7H, *m*, Ar-H), 9.19 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 18.3 (2-CH_3), 22.8 (6-CH_3), 24.1 (C-8), 25.1 (6-CH_3), 34.0 (C-7), 35.9 (C-6), 40.0 (C-4), 50.6 (COO**C**H$_3$), 102.5 (C-3), 109.0 (C-4a), 124.8, 125.1, 125.7, 126.5, 127.2, 127.4,127.6, 131.5, 132.8, 145.0 (naphthyl carbons), 145.4 (C-2), 149.8 (C-8a), 167.4 (**C**OOCH$_3$), 199.5 (C-5); ESI-MS (*m*/*z*): 398.20 $[M+Na]^+$ (100 %).

*Ethyl 2,6,6-trimethyl-4-(2-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**10**)*. Yield: 80 %; m.p.: 244–246 °C; Anal. calcd. for $C_{25}H_{27}NO_3$: C, 77.09; H, 6.99; N, 3.60 %. Found: C, 77.06; H, 6.95; N, 3.59 %; IR (cm^{-1}): 3289 (N–H), 1695 (C=O, ester), 1666 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.86 (3H, *s*, 6-CH_3), 0.99 (3H, *s*, 6-CH_3), 1.13 (3H, *t*, J = 7.08 Hz, CH_2CH_3), 1.68–1.77 (2H, *m*, H-7), 2.31 (3H, *s*, 2-CH_3), 2.50–2.55 (2H, *m*, H-8), 3.98 (2H, *q*, J = 7.08 Hz, C**H**$_2$CH$_3$), 5.04 (1H, *s*, H-4), 7.36–7.81 (7H, *m*, Ar-H), 9.14 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 14.1 (COOCH$_2$**C**H$_3$), 18.3 (2-CH_3), 22.9 (6-CH_3), 24.1 (C-8), 25.0 (6-CH_3), 34.1 (C-7), 36.2 (C-6), 40.0 (C-4), 59.0 (COO**C**H$_2$CH$_3$), 102.9 (C-3), 108.9 (C-4a), 125.1, 125.15, 125.7, 126.6, 127.2, 127.3, 127.6, 131.5, 132.7, 145.0 (naphthyl carbons), 145.1 (C-2), 149.8 (C-8a), 166.9 (**C**OOCH$_2$CH$_3$), 199.5 (C-5); ESI-MS (*m*/*z*): 413.21 $[M+1+Na]^+$, 412.21 $[M+Na]^+$ (100 %).

*Isopropyl 2,6,6-trimethyl-4-(2-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**11**)*. Yield: 76 %; m.p.: 258–260 °C; Anal. calcd. for $C_{26}H_{29}NO_3$: C, 77.39; H, 7.24; N, 3.47 %. Found: C, 77.35; H, 7.22; N, 3.44 %; IR (cm^{-1}): 3283 (N–H), 1702 (C=O, ester), 1665 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.86 (3H, *s*, 6-CH_3), 0.99 (3H, *s*, 6-CH_3), 1.02 (3H, *d*, J = 6.2 Hz, CH(C**H**$_3$)$_2$), 1.19 (3H, *d*, J = 6.2 Hz, CH(C**H**$_3$)$_2$), 1.60–1.75 (2H, *m*,

H-7), 2.29 (3H, *s*, 2-CH_3), 2.50–2.56 (2H, *m*, H-8), 4.78–4.81 (1H, *m*, C**H**(CH_3)$_2$), 5.01 (1H, *s*, H-4), 7.36–7.80 (7H, *m*, Ar-H), 9.10 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 18.2 (2-CH_3), 21.5 (CH(**C**H_3)$_2$), 21.8 (CH(**C**H_3)$_2$), 22.9 (6-CH_3), 24.1 (C-8), 25.0 (6-CH_3), 34.1 (C-7), 36.4 (C-6), 40.0 (C-4), 66.0 (**C**H(CH_3)$_2$), 103.3 (C-3), 108.9 (C-4a), 125.0, 125.3, 125.7, 126.7, 127.23, 127.29, 127.5, 131.5, 132.6, 144.7 (naphthyl carbons), 145.2 (C-2), 149.9 (C-8a), 166.4 (**C**OOCH(CH_3)$_2$), 199.4 (C-5); ESI-MS (*m*/*z*): 427.22 $[M+1+Na]^+$, 426.22 $[M+Na]^+$ (100 %).

*Isobutyl 2,6,6-trimethyl-4-(2-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**12**).* Yield: 73 %; m.p.; 291–293 °C; Anal. calcd. for $C_{27}H_{31}NO_3$: C, 77.67; H, 7.48; N, 3.35 %. Found: C, 77.70; H, 7.45; N, 3.32 %; IR (cm^{-1}): 3288 (N–H), 1696 (C=O, ester), 1663 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.77 (3H, *d*, *J* = 6.8 Hz, CH(C**H**$_3$)$_2$), 0.79 (3H, *d*, *J* = 6.8 Hz, CH(C**H**$_3$)$_2$), 0.85 (3H, *s*, 6-CH_3), 0.99 (3H, *s*, 6-CH_3),1.63–1.74 (1H, *m*, C**H**(CH_3)$_2$), 1.76–1.83 (2H, *m*, H-7), 2.34 (3H, *s*, 2-CH_3), 2.49–2.53 (2H, *m*, H-8), 3.67–3.75 (2H, *m*, OC**H**$_2$CH(CH_3)$_2$), 5.06 (1H, *s*, H-4), 7.37–7.79 (7H, *m*, Ar-H), 9.17 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 18.4 (2-CH_3), 18.9 (CH(**C**H_3)$_2$), 22.9 (6-CH_3), 24.1 (C-8), 25.1 (6-CH_3), 27.2, (**C**H(CH_3)$_2$) 34.0 (C-7), 36.2 (C-6), 40.0 (C-4), 69.2 (COO**C**H_2), 102.6 (C-3), 109.1 (C-4a), 125.1, 125.7, 126.6, 127.2, 127.4, 127.5, 131.5, 132.7, 135.2, 138.5, 145.1, 145.5, 149.6 (naphthyl carbons), 166.9 (**C**OOCH_2), 199.5 (C-5); ESI-MS (*m*/*z*): 441.24 $[M+1+Na]^+$, 440.23 $[M+Na]^+$ (100 %).

tert-*Butyl 2,6,6-trimethyl-4-(2-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**13**).* Yield: 79 %; m.p.: 267–269 °C; Anal. calcd. for $C_{27}H_{31}NO_3$: C, 77.67; H, 7.48; N, 3.35 %. Found: C, 77.70; H, 7.50; N, 3.33 %; IR (cm^{-1}): 3283 (N–H), 1703 (C=O, ester), 1663 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.85 (3H, *s*, 6-CH_3), 0.99 (3H, *s*, 6-CH_3), 1.31 (9H, *s*, C(C**H**$_3$)$_3$), 1.51–1.74 (2H, *m*, H-7), 2.26 (3H, *s*, 2-CH_3), 2.48–2.55 (2H, *m*, H-8), 4.96 (1H, *s*, H-4), 7.36–7.80 (7H, *m*, Ar-H), 9.02 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm):18.2 (2-CH_3), 23.2 (6-CH_3), 24.1 (C-8), 25.1 (6-CH_3), 27.8 (COOC(**C**H_3)$_3$), 34.1 (C-7), 36.7 (C-6), 40.0 (C-4), 78.7 (**C**OOC(CH_3)$_3$), 102.1 (C-3), 108.7 (C-4a), 125.0, 125.2, 125.7, 126.7, 127.2, 127.5, 127.9, 128.2, 131.5, 132.7 (naphthyl carbons), 143.8 (C-2), 145.3 (C-8a), 166.4 (**C**OOC(CH_3)$_3$), 199.3 (C-5); ESI-MS (*m*/*z*): 441.27 $[M+1+Na]^+$, 440.26 $[M+Na]^+$ (100 %).

*2-Methoxyethyl 2,6,6-trimethyl-4-(2-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**14**).* Yield: 85 %; m.p.: 176–178 °C; Anal. calcd. for $C_{26}H_{29}NO_4$: C, 74.44; H, 6.97; N, 3.34 %. Found C, 74.38; H, 6.94; N, 3.37 %; IR (cm^{-1}): 3296 (N–H), 1692 (C=O, ester), 1667 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.87 (3H, *s*, 6-CH_3), 0.99 (3H, *s*, 6-CH_3), 1.71–2.57 (4H, *m*, H-7,8), 2.30 (3H, *s*, 2-CH_3), 3.24 (3H, *s*, OC**H**3), 3.49 (2H, *m*,

COOC**H**$_2$), 4.06 (2H, *m*, CH$_2$C**H**$_2$O), 5.04 (1H, *s*, H-4), 7.37–7.80 (7H, *m*, Ar-H), 9.17 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm):18.3 (2-CH$_3$), 22.9 (6-CH$_3$), 24.1 (C-8), 25.0 (6-CH$_3$), 34.1 (C-7), 36.2 (C-6), 40.1 (C-4), 57.9 (CH$_2$CH$_2$O**C**H$_3$), 62.2 (COO**C**H$_2$), 69.9 (CH$_2$**C**H$_2$OCH$_3$), 102.8 (C-3), 108.9 (C-4a), 125.0, 125.1, 125.6, 126.6, 127.2, 127.3, 127.6, 131.6, 132.7, 145.1 (naphthyl carbons), 145.3 (C-2), 149.9 (C-8a), 166.8 (**C**OOCH$_2$), 199.5 (C-5); ESI-MS (*m*/*z*): 443.24 [M+1+Na]$^+$, 442.24 [M+Na]$^+$ (100 %).

*2-(Methacryloyloxy)ethyl 2,6,6-trimethyl-4-(2-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**15**).* Yield: 77 %; m.p.: 156–158 °C; Anal. calcd. for C$_{29}$H$_{31}$NO$_5$: C, 73.55; H, 6.60; N, 2.96 %. Found: C, 73.59; H, 6.62; N, 2.96 %; IR (cm^{-1}): 3191 (N–H), 1714 (C=O, ester), 1667 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.82 (3H, *s*, 6-CH$_3$), 0.95 (3H, *s*, 6-CH$_3$), 1.63–1.72 (2H, *m*, H-7), 1.75 (3H, *s*, C(CH$_2$)C**H**$_3$), 2.27 (3H, *s*, 2-CH$_3$), 2.45–2.51 (2H, *m*, H-8), 4.11–4.25 (4H, *m*, OC**H$_2$**C**H$_2$**O), 4.99 (1H, *s*, H-4), 5.54–5.88 (2H, *m*, C(CH$_3$)=C**H**$_2$), 7.31–7.74 (7H, *m*, Ar-H), 9.16 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 18.3 (2-CH$_3$), 18.8 (C(**C**H$_3$)=CH$_2$), 23.4 (6-CH$_3$), 24.6 (C-8), 25.5 (6-CH$_3$), 34.6 (C-7), 36.6 (C-6), 40.6 (C-4), 61.4 (OCH$_2$**C**H$_2$O), 63.1 (O**C**H$_2$CH$_2$O), 102.9 (C-3), 109.7 (C-4a), 125.51, 125.56, 126.1 (naphthyl carbons), 126.4 (C(CH$_3$)=**C**H$_2$), 127.0, 127.6, 127.8, 128.0, 132.1, 133.2 (naphthyl carbons), 135.9 (**C**(CH$_3$)=CH$_2$), 145.6 (naphthyl carbon), 146.3 (C-2), 150.1 (C-8a), 166.8 (**C**OOCH$_2$CH$_2$), 167.1 (**C**O(CH$_3$)=CH$_2$), 200.0 (C-5); ESI-MS (*m*/z): 497.10 [M+1+Na]$^+$, 496.10 [M+Na]$^+$ (100 %).

*Benzyl 2,6,6-trimethyl-4-(2-naphthyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate (**16**).* Yield: 70 %; m.p.: 173–175 °C; Anal. calcd. for C$_{30}$H$_{29}$NO$_3$: C, 79.80; H, 6.47; N, 3.10 %. Found: C, 79.78; H, 6.49; N, 3.09 %; IR (cm^{-1}): 3308 (N–H), 1698 (C=O, ester), 1651 (C=O, ketone); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 0.85 (3H, *s*, 6-CH$_3$), 0.98 (3H, *s*, 6-CH$_3$), 1.68–2.55 (4H, *m*, H-7,8), 2.33 (3H, *s*, 2-CH$_3$), 4.97, 5.05 (2H, AB system, J_{AB} = 13.2 Hz, COOC**H**$_2$C$_6$H$_5$), 5.06 (1H, *s*, H-4), 7.16–7.80 (7H, *m*, Ar-H), 7.16–7.80 (5H, *m*, C$_6$**H**$_5$), 9.21 (1H, *s*, N–H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 18.8 (2-CH$_3$), 23.4 (6-CH$_3$), 24.6 (C-8), 25.5 (6-CH$_3$), 34.5 (C-7), 36.7 (C-6), 40.6 (C-4), 65.2 (COO**C**H$_2$C$_6$H$_5$), 102.9 (C-3), 109.6 (C-4a), 125.6, 125.7, 126.1, 127.1, 127.7, 127.9, 128.11, 128.15, 128.2, 128.6, 132.1, 133.2, 135.1, 136.9, 137.1, 145.5 (naphthyl and phenyl carbons), 146.4 (C-2), 150.2 (C-8a), 167.1 (**C**OOCH$_2$C$_6$H$_5$), 200.0 (C-5); ESI-MS (*m*/*z*): 475.25 [M+1+Na]$^+$, 474.24 [M+Na]$^+$ (100 %).

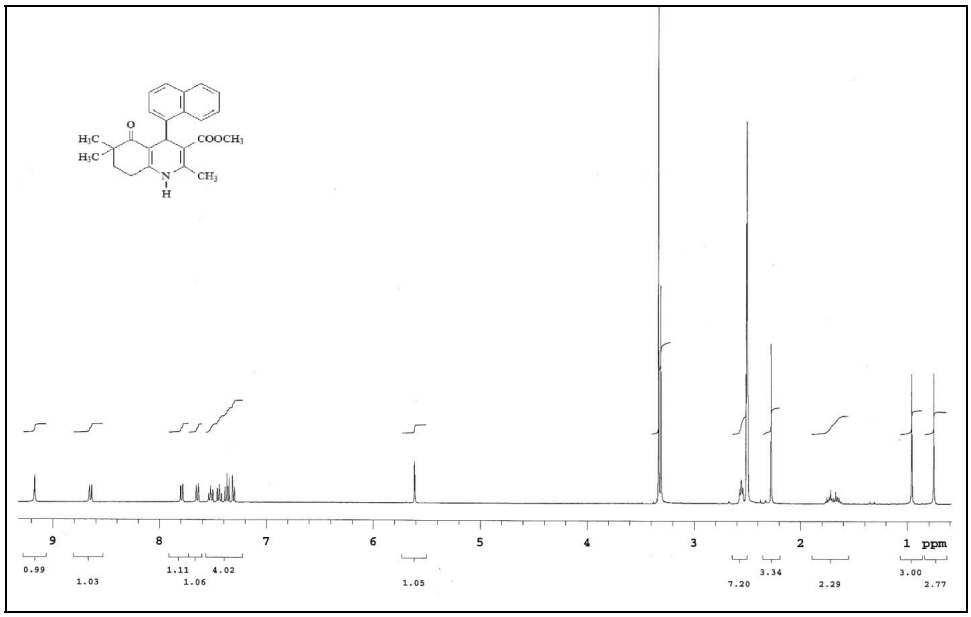


Fig. S-1. ^{1}H-NMR spectrum of compound **1**.

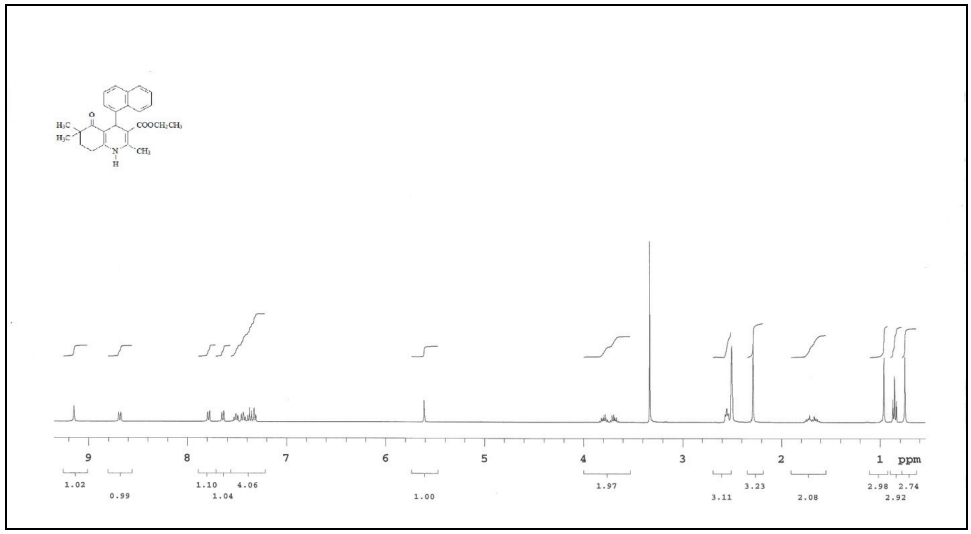


Fig. S-2. ^{1}H-NMR spectrum of compound **2**.

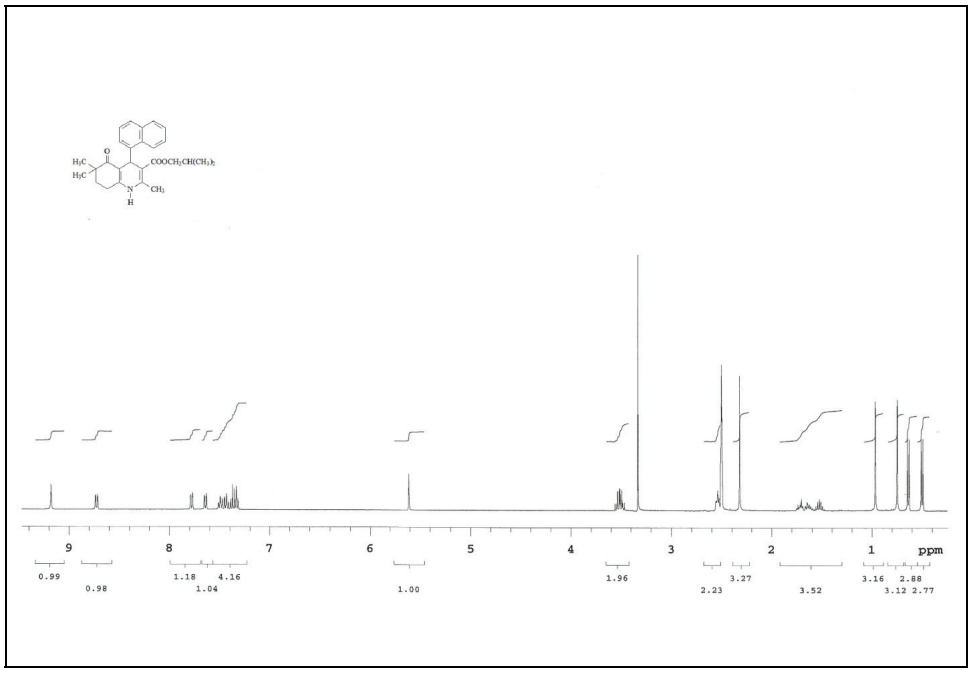


Fig. S-3. ^{1}H-NMR spectrum of compound **4**.

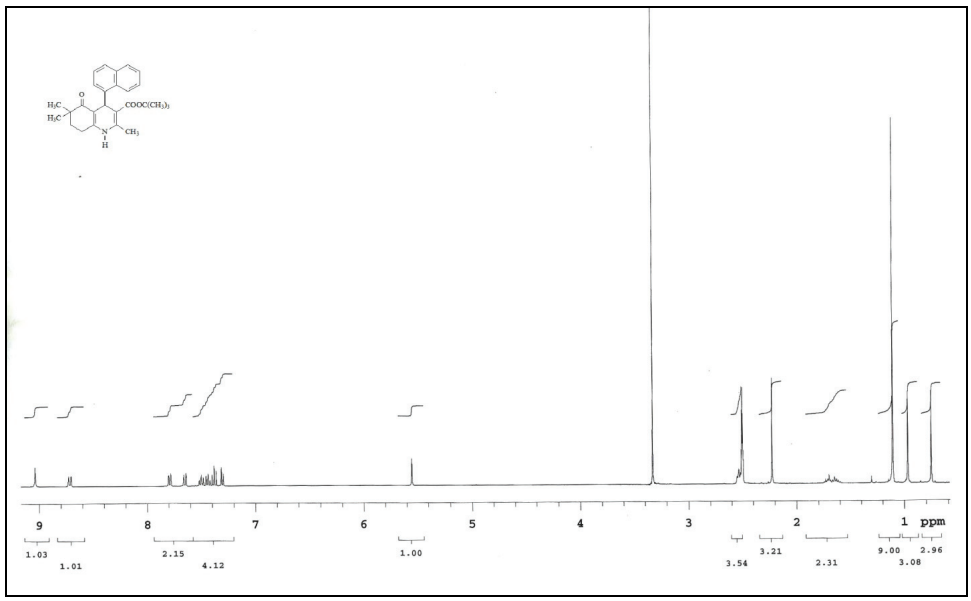


Fig. S-4. ^{1}H-NMR spectrum of compound **5**.

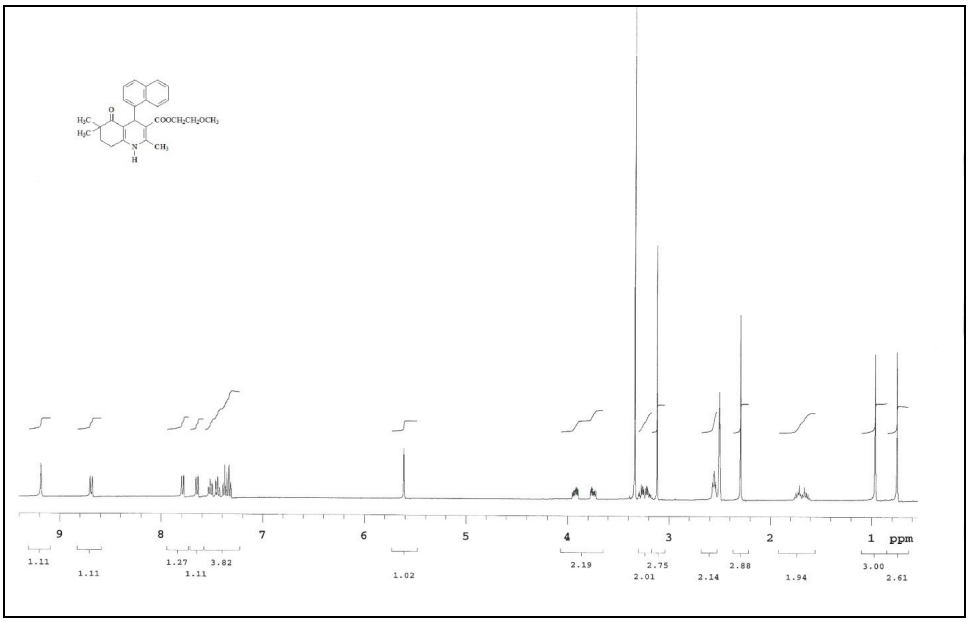


Fig. S-5. ^{1}H-NMR spectrum of compound **6**.

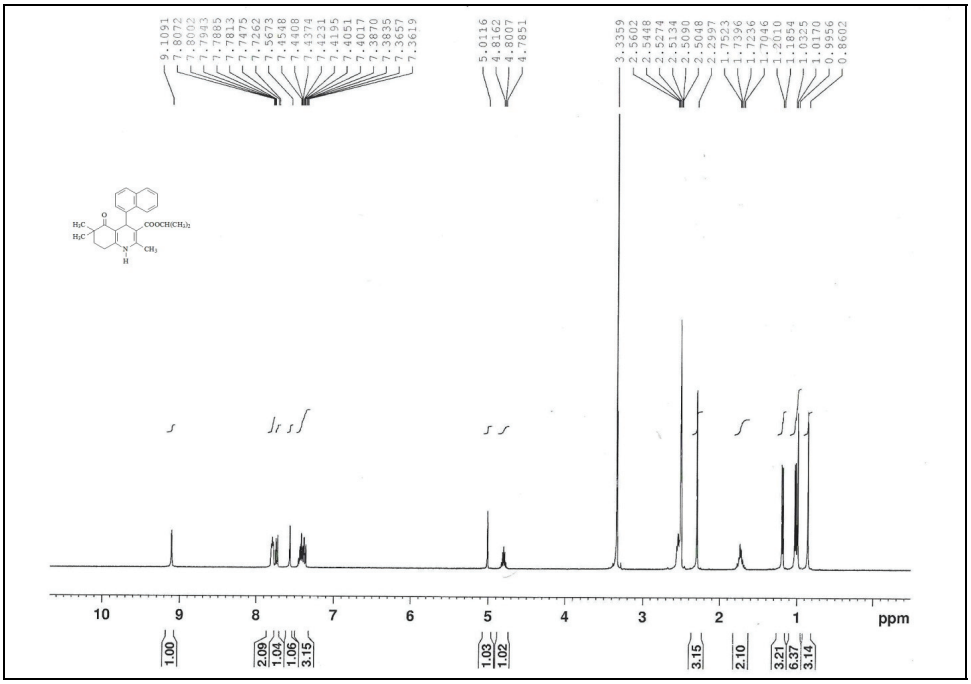


Fig. S-6. ^{1}H-NMR spectrum of compound **11**.

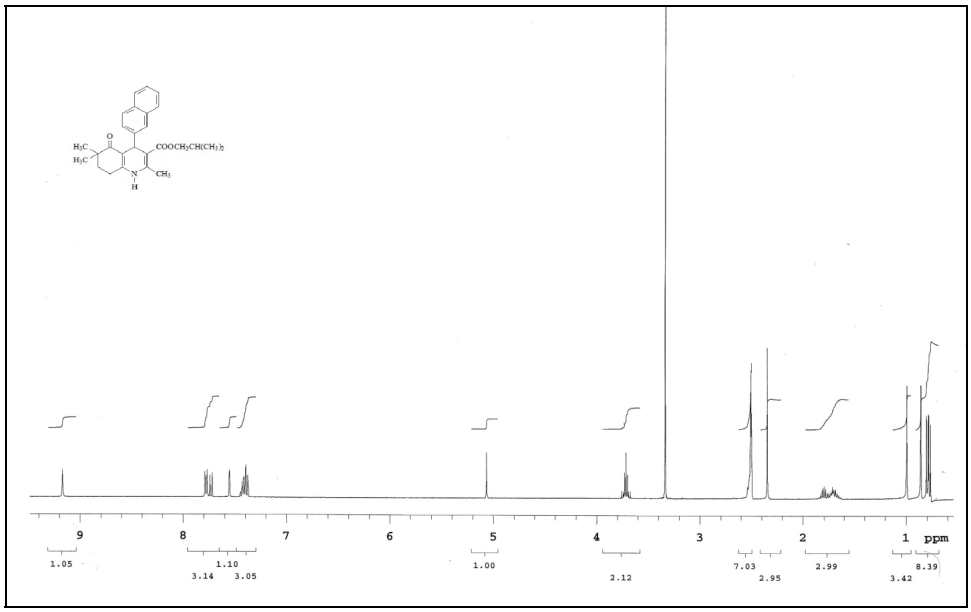


Fig. S-7. ^{1}H-NMR spectrum of compound **12**.

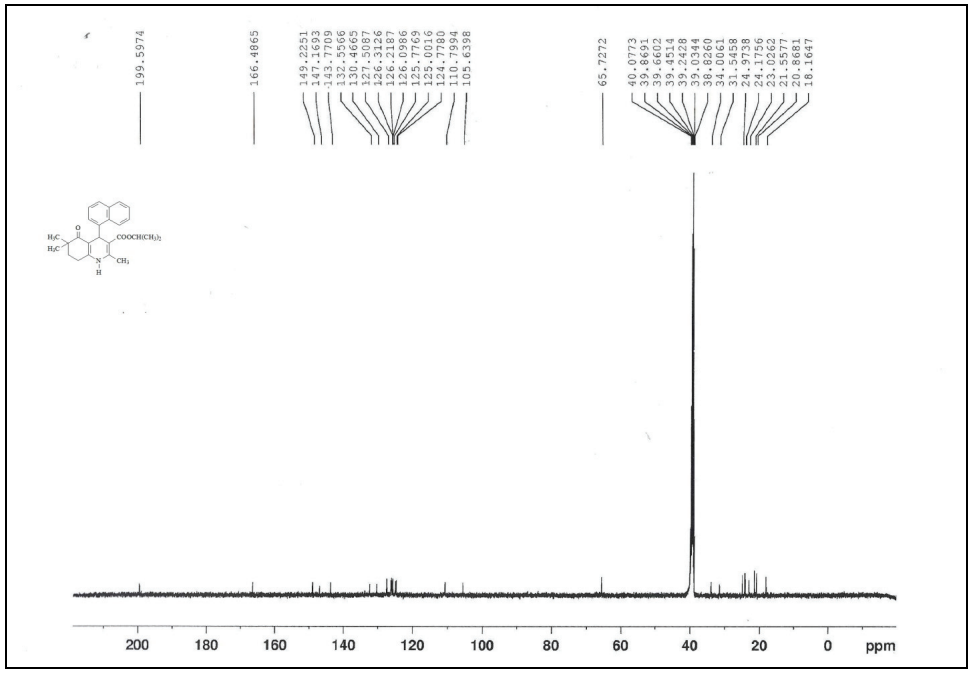


Fig. S-8. ^{13}C-NMR spectrum of compound **3**.

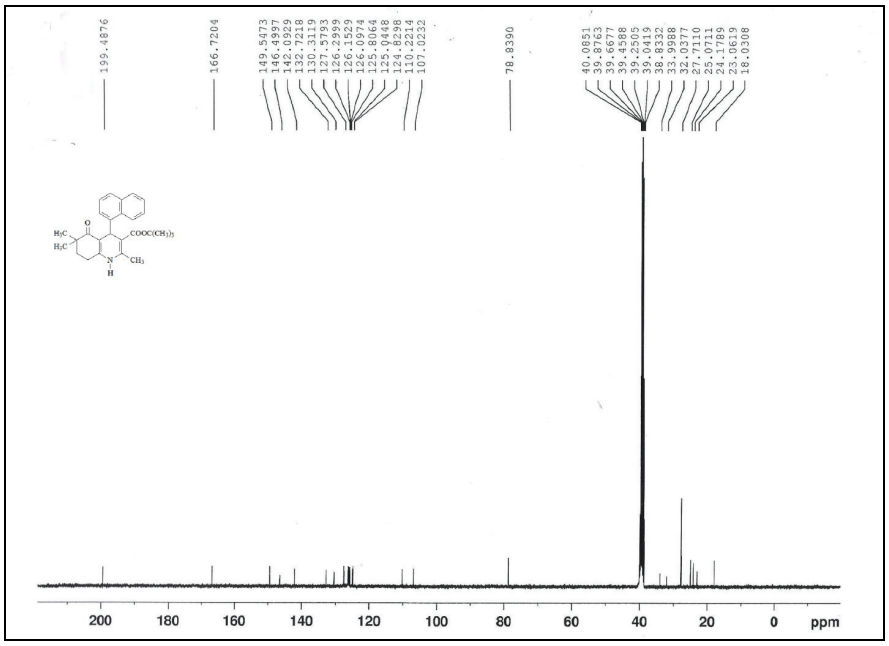


Fig. S-9. ^{13}C-NMR spectrum of compound **5**.

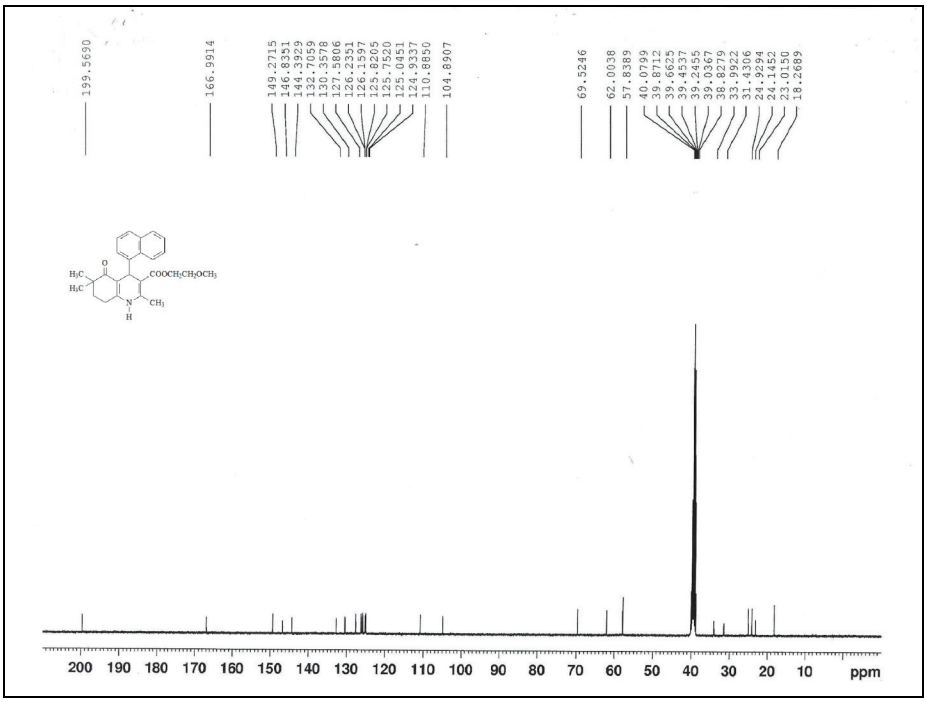


Fig. S-10. ^{13}C-NMR spectrum of compound **6**.

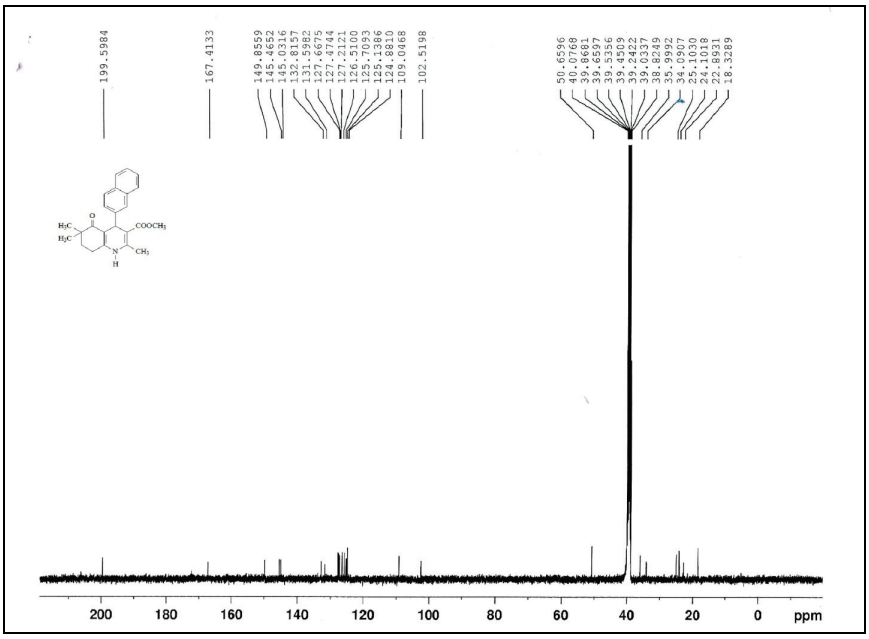


Fig. S-11. ^{13}C-NMR spectrum of compound **9**.

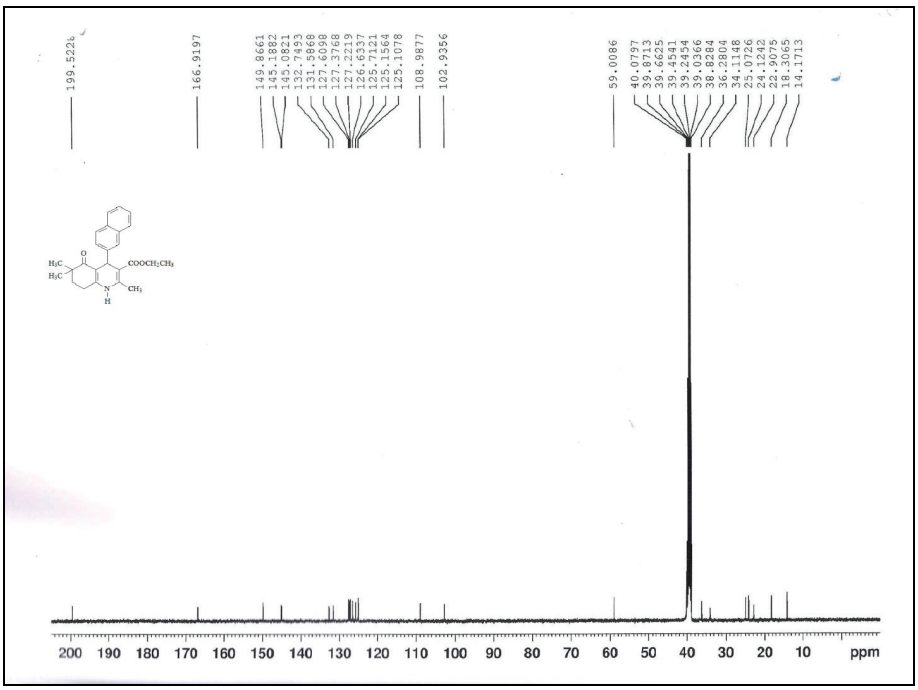


Fig. S-12. ^{13}C-NMR spectrum of compound **10**.

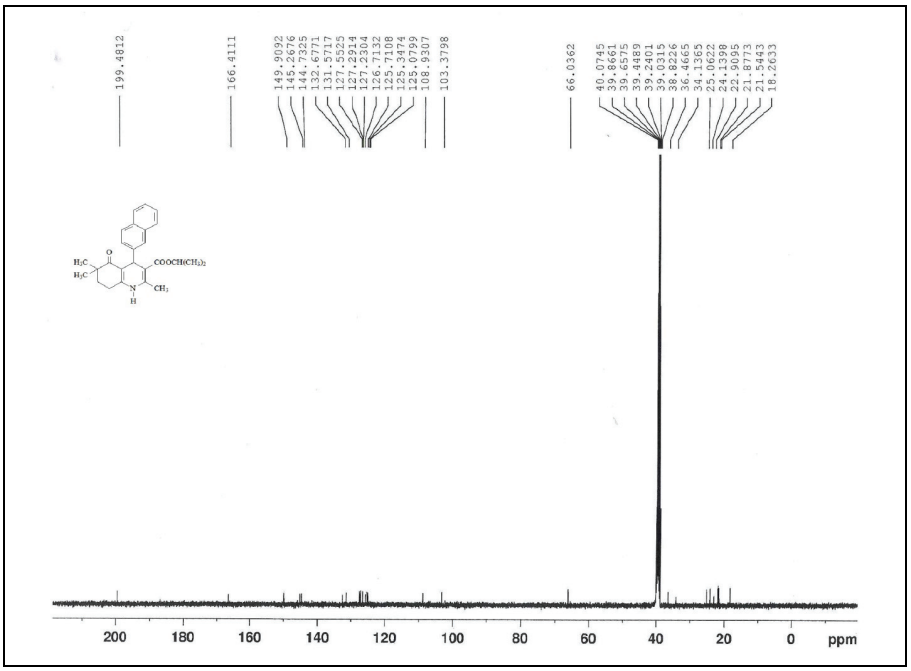


Fig. S-13. ^{13}C-NMR spectrum of compound **11**.

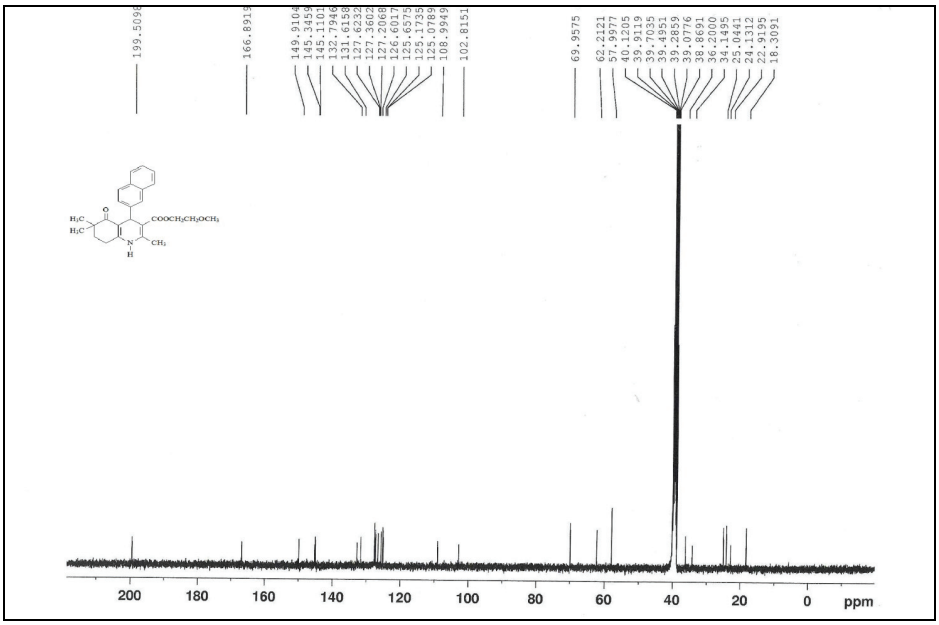


Fig. S-14. ^{13}C-NMR spectrum of compound **14**.

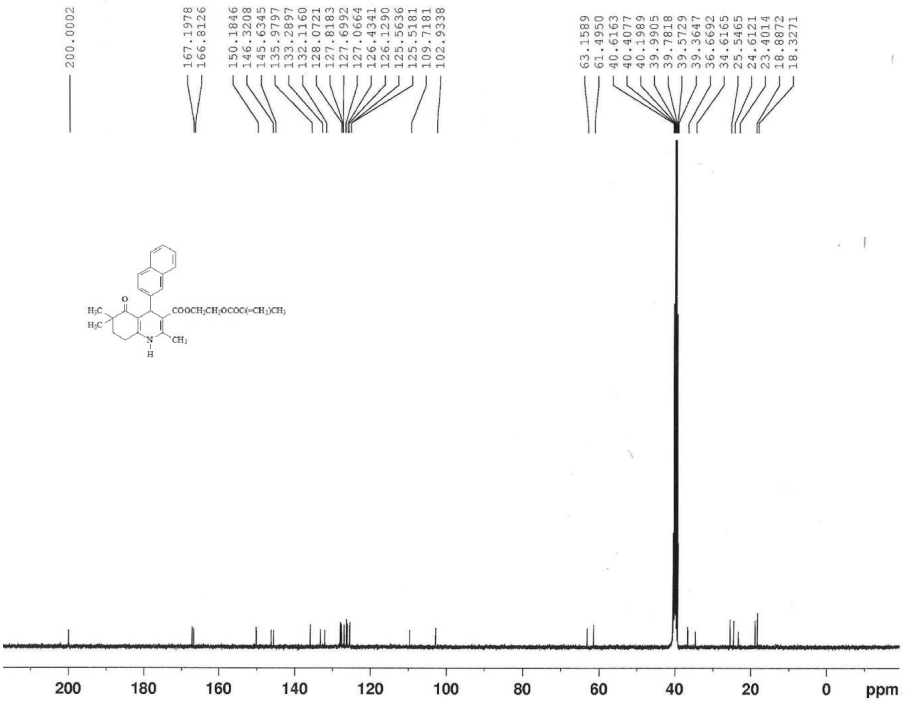


Fig. S-15. ^{13}C-NMR spectrum of compound **15**.

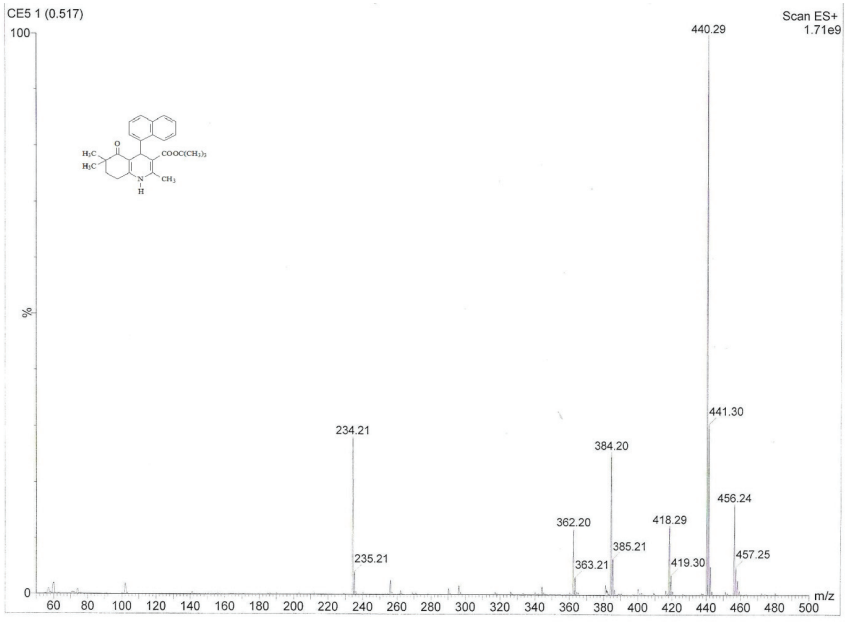


Fig. S-16. Mass spectrum of compound **5**.

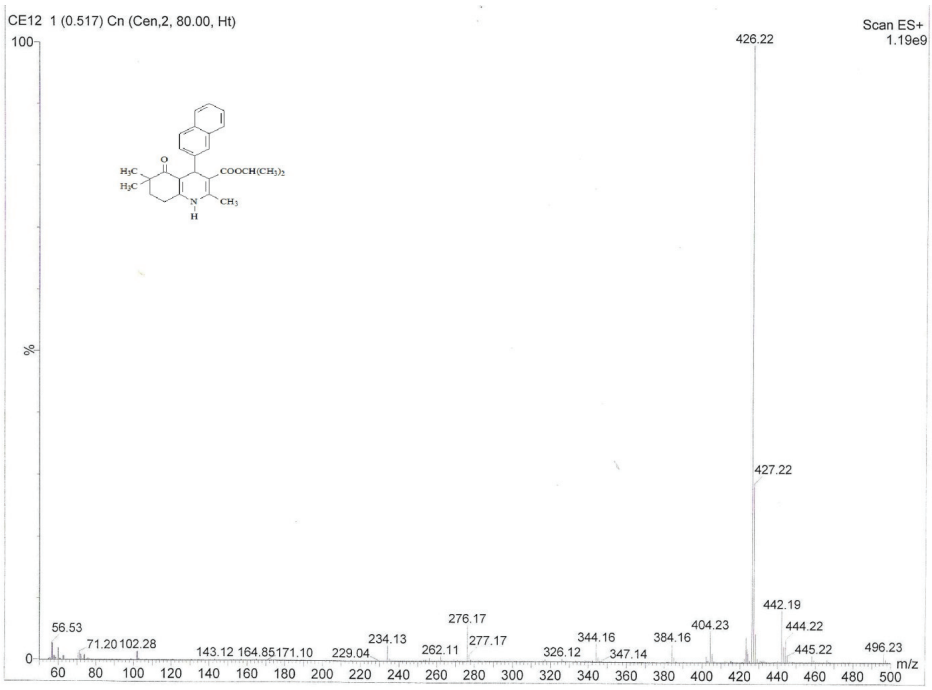


Fig. S-17. Mass spectrum of compound **11**.

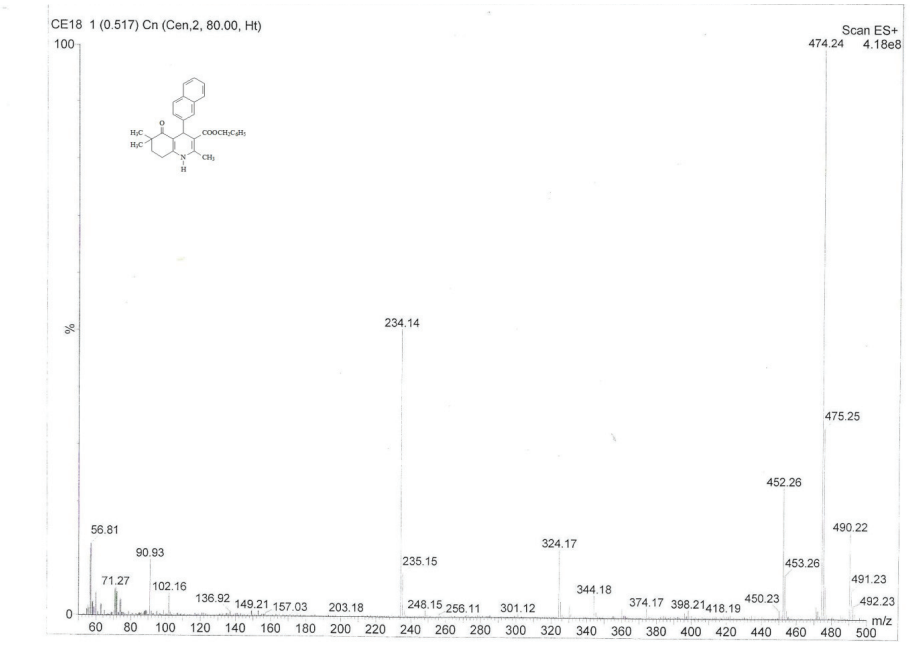


Fig. S-18. Mass spectrum of compound **16**.

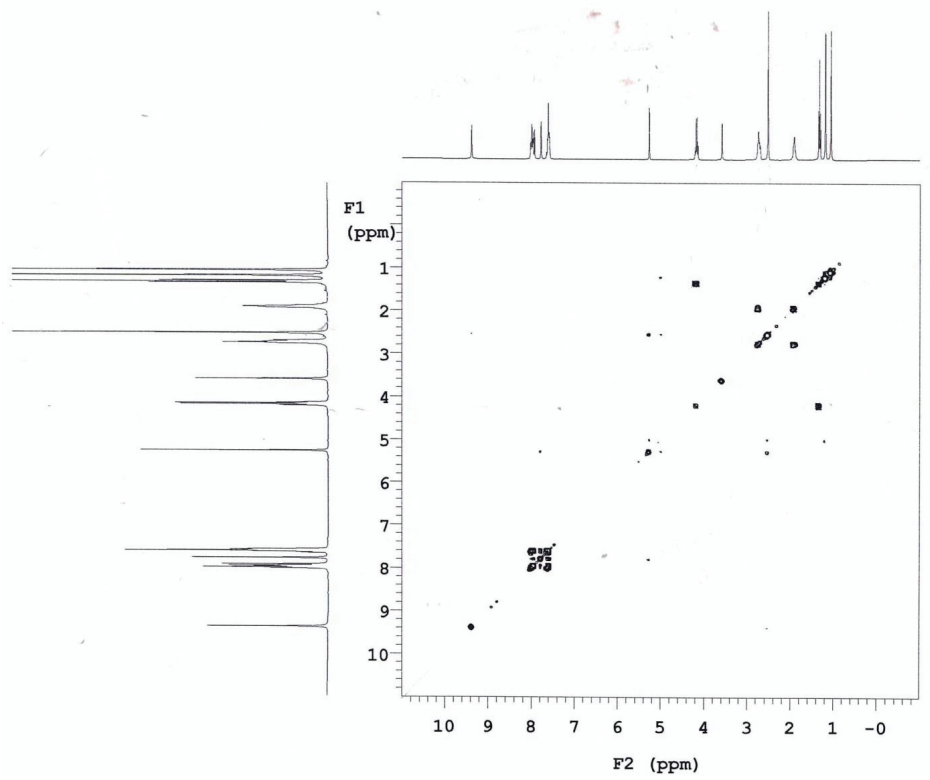


Fig. S-18. COSY spectrum of compound **2**.

TABLE S-I. Structural data of the synthesized compounds

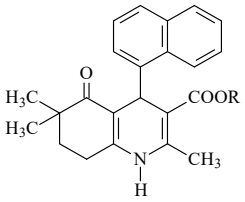
Compound	R	Melting point, °C	Empirical formula	Formula weight
				
1	CH_3	223–225	$C_{24}H_{25}NO_3$	375.47
2	C_2H_5	210–212	$C_{25}H_{27}NO_3$	389.49
3	$CH(CH_3)_2$	211–213	$C_{26}H_{29}NO_3$	403.52
4	$CH_2CH(CH_3)_2$	170–172	$C_{27}H_{31}NO_3$	417.55
5	$C(CH_3)_3$	243–245	$C_{27}H_{31}NO_3$	417.55
6	$CH_2CH_2OCH_3$	197–199	$C_{26}H_{29}NO_4$	419.52
7	$CH_2CH_2OCOC(=CH_2)CH_3$	155–157	$C_{29}H_{31}NO_5$	473.57
8	$CH_2C_6H_5$	167–169	$C_{30}H_{29}NO_3$	451.57

TABLE S-I. Continued

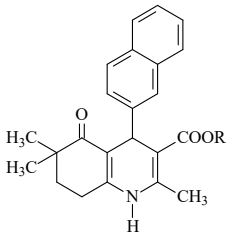
Compound	R	Melting point, °C	Empirical formula	Formula weight
				
9	CH_3	259–261	$C_{24}H_{25}NO_3$	375.47
10	C_2H_5	244–246	$C_{25}H_{27}NO_3$	389.49
11	$CH(CH_3)_2$	258–260	$C_{26}H_{29}NO_3$	403.52
12	$CH_2CH(CH_3)_2$	291–293	$C_{27}H_{31}NO_3$	417.55
13	$C(CH_3)_3$	267–269	$C_{27}H_{31}NO_3$	417.55
14	$CH_2CH_2OCH_3$	176–178	$C_{26}H_{29}NO_4$	419.52
15	$CH_2CH_2OCOC(=CH_2)CH_3$	156–158	$C_{29}H_{31}NO_5$	473.57
16	$CH_2C_6H_5$	173–175	$C_{30}H_{29}NO_3$	451.57

TABLE S-II. Crystal data and details of the structure determination of compound **10**

Formula	$C_{25}H_{27}NO_3$
Molecular weight	389.48
Crystal system	Orthorhombic
Space group	*Pbca*
a, *b*, *c* / Å	10.5179 (2), 12.1144 (3), 33.6297 (8)
α, β, γ / °	90, 90, 90
Volume, Å^3	4285.03 (18)
Z	8
D / g cm^{-3} (calculated)	1.207
F000	1664
Linear absorption coefficient, mm^{-1}	0.63
Absorption correction type	Multi-scan
Crystal size, mm^3	0.50×0.35×0.30
Diffractions radiation type	CuK_α
λ / Å	1.54184
Monochromator	Graphite
Diffractions measurement device type	Xcalibur, Ruby, Gemini
Diffractions measurement device	ω Scans
Total reflection number	15413
Independent reflection number	4374
Collected reflection for $I > 2\sigma(I)$	3821
R_{int}	0.029
h, *k*, *l* ranges	–12→12, –13→14, –38→41
θ_{min}, θ_{max} range, °	–4.96, 75.64
Solution	Direct methods, SHELXS-97, SHELXL-97, SHELXTL

TABLE S-II. Continued

Least squares refine weighting details	$w = 1/(\sigma^2(Fo^2) + (0.0764P)2 + 1.7455P)$, where $P = (Fo^2 + 2F_c^2)/3$
Number of variable	270
R	0.0479
wR	0.1326
$S(F^2)$	1.043
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e / Å^3)	0.39, –0.23

TABLE S-III. Selected bond lengths (Å) and bond and torsion angles (°)

O1—C5	1.2319 (19)	O3—C21	1.450 (2)
O2—C20	1.216 (2)	N1—C1	1.3642 (19)
O3—C20	1.3441 (18)	N1—C9	1.3905 (19)
C20—O3—C21	116.23 (13)	C11—C10—C7	121.60 (13)
C1—N1—C9	122.72 (13)	C19—C10—C7	119.49 (13)
N1—C1—C2	116.62 (13)	C10—C11—C12	121.39 (14)
O1—C5—C6	121.45 (13)	C15—C16—C17	120.98 (18)
O1—C5—C4	119.16 (13)	O2—C20—O3	122.15 (14)
C8—C9—N1	119.09 (13)	O2—C20—C8	123.13 (13)
C8—C9—C23	128.34 (14)	O3—C20—C8	114.71 (13)
N1—C9—C23	112.55 (13)	O3—C21—C22	107.31 (16)
C11—C10—C19	118.83 (14)		
N1—C1—C2—C3	155.38 (13)	C1—N1—C9—C8	−12.6 (2)
C1—C2—C3—C4	48.82 (17)	C1—N1—C9—C23	165.63 (14)
C3—C4—C5—O1	−151.82 (14)	C21—O3—C20—O2	−4.3 (2)
C25—C4—C5—O1	87.90 (17)	C21—O3—C20—C8	175.61 (16)
N1—C1—C6—C5	−177.12 (13)	C9—C8—C20—O2	−169.51 (15)
N1—C1—C6—C7	6.2 (2)	C7—C8—C20—O2	11.6 (2)
O1—C5—C6—C1	176.76 (14)	C9—C8—C20—O3	10.6 (2)
O1—C5—C6—C7	−6.5 (2)	C7—C8—C20—O3	−168.32 (13)
C20—C8—C9—N1	170.78 (13)	C20—O3—C21—C22	−173.42 (18)
C7—C8—C9—N1	−10.4 (2)		

TABLE S-IV. Hydrogen-bond geometry (Å, °); Symmetry code: (*i*) –*x*+3/2, *y*+1/2, *z*

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O2	0.98	2.45	2.8122(17)	101.6
N1—H1N···O1^i	0.83(2)	1.99(2)	2.8150(17)	171.6(19)
C23—H23B···O1^i	0.96	2.52	3.346(2)	143.7

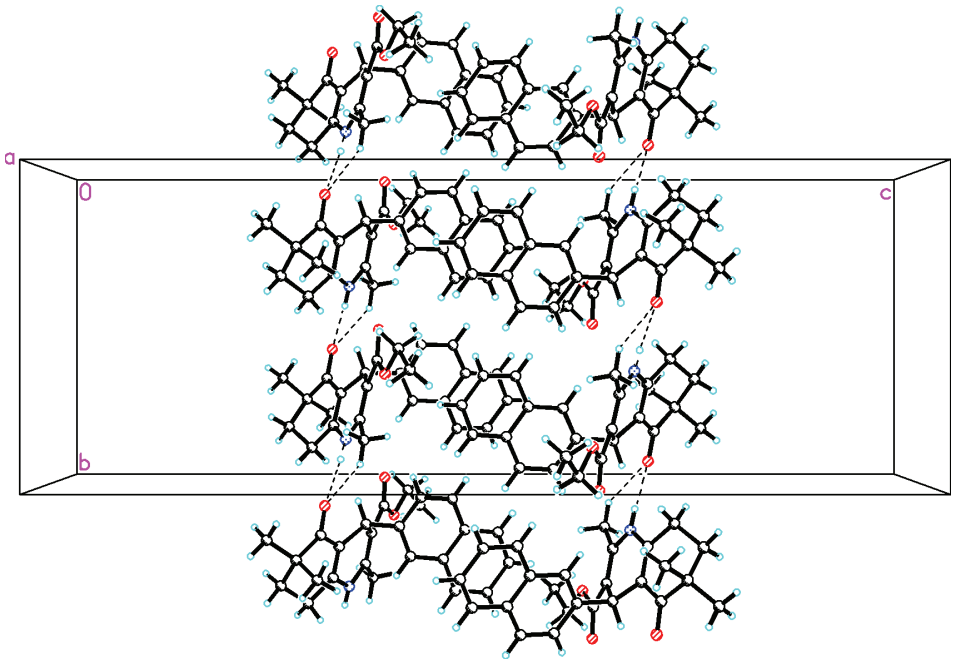


Fig. S-19. The packing and hydrogen bonding of compound **10** in the unit cell, viewed along the a axis. Hydrogen bonds are shown as dashed lines.