

Supporting Information

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(4-Nitrobenzo[*b*]furan-2-yl)(3,4,5-trimethoxyphenyl)methanone (7a). The residue was recrystallized with petroleum ether to give **7a** as a yellow solid, (336 mg, 94%), $R_f=0.35$ (PE/EtOAc 7/3), mp 153-155 °C. $^1\text{H-NMR}$ (CDCl_3) δ : 3.96 (s, 3H), 3.99 (s, 6H), 7.36 (s, 2H), 7.66 (t, $J=8.4$ Hz, 1H), 8.02 (d, $J=8.4$ Hz, 1H), 8.18 (s, 1H), 8.34 (d, $J=8.4$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta=$ 56.4, 56.6, 61.2, 107.4, 107.6, 114.8, 119.2, 120.9, 122.5, 127.4, 127.6, 131.4, 142.1, 143.3, 153.3, 154.4, 156.4, 182.7 ppm. MS (ESI): $[\text{M}+1]^+=358.2$.

(5-Nitrobenzo[*b*]furan-2-yl)(3,4,5-trimethoxyphenyl)methanone (7b). The residue was recrystallized with petroleum ether to give **7b** as an orange solid, (318 mg, 89%), $R_f=0.34$ (PE/EtOAc 8/2), mp 190-191 °C. $^1\text{H-NMR}$ (CDCl_3) δ : 3.96 (s, 6H), 3.98 (s, 3H), 7.34 (s, 2H), 7.66 (s, 1H), 7.75 (d, $J=9.2$ Hz, 1H), 8.41 (dd, $J=8.8$ and 2.0 Hz, 1H), 8.71 (d, $J=2.0$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta=$ 56.2, 56.4, 61.3, 107.2, 107.4, 114.8, 119.0, 120.9, 122.4, 127.3, 127.4, 131.3, 142.0, 143.1, 153.3, 154.3, 156.3, 182.6 ppm. MS (ESI): $[\text{M}+1]^+=358.4$.

(3-Methyl-5-nitrobenzo[*b*]furan-2-yl)(3,4,5-trimethoxyphenyl)methanone (7c). The residue was recrystallized with petroleum ether to give **7c** as a yellow solid, (204 mg, 55%), $R_f=0.38$ (PE/EtOAc 7/3), mp 200-202 °C. $^1\text{H-NMR}$ (CDCl_3) δ : 2.68 (s, 3H), 3.92 (s, 3H), 3.94 (s, 6H), 7.38 (s, 2H), 7.62 (d, $J=9.0$ Hz, 1H), 8.39 (dd, $J=9.0$ and 2.2 Hz, 1H), 8.67 (d, $J=2.0$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta=$ 41.1, 56.3, 56.5, 61.2, 107.3, 107.5, 114.7, 119.0, 120.8, 122.4, 127.3, 127.5, 131.3, 142.1, 143.2, 153.2, 154.4, 156.3, 182.8 ppm. MS (ESI): $[\text{M}+1]^+=372.4$.

(6-Nitrobenzo[*b*]furan-2-yl)(3,4,5-trimethoxyphenyl)methanone (7d). The residue was recrystallized with petroleum ether to give **7d** as a brown solid, (186 mg, 52%), $R_f=0.38$ (PE/EtOAc 7/3), mp 175-177 °C. $^1\text{H-NMR}$ (CDCl_3) δ : 3.96 (s, 3H), 3.98 (s, 6H), 7.39 (s, 2H), 7.63 (s, 1H), 7.86 (d, $J=8.8$ Hz, 1H), 8.34 (d, $J=8.8$ Hz, 1H), 8.54 (s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta=$ 56.3, 56.5, 61.3, 107.4, 107.5, 114.7, 119.1, 120.8, 122.4, 127.3, 127.4, 131.4, 142.2, 143.3, 153.4, 154.5, 156.5, 182.7 ppm. MS (ESI): $[\text{M}+1]^+=358.1$.

(7-Nitrobenzo[*b*]furan-2-yl)(3,4,5-trimethoxyphenyl)methanone (7e). The residue was recrystallized with petroleum ether to give **7e** as a brown solid, (339 mg, 95%), $R_f=0.35$ (PE/EtOAc 7/3), mp 155-157 °C. $^1\text{H-NMR}$ (CDCl_3) δ : 3.99 (s, 3H), 4.04 (s, 6H), 7.25 (s, 1H), 7.55 (d, $J=8.0$ Hz, 1H), 7.86 (s, 2H), 8.10 (d, $J=8.4$ Hz, 1H), 8.39 (d, $J=8.4$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta=$ 56.2, 56.4, 61.4, 107.3, 107.7, 114.5, 119.2, 120.8, 122.4, 127.3, 127.5, 131.3, 142.0, 143.2, 153.2, 154.3, 156.3, 182.7 ppm. MS (ESI): $[\text{M}+1]^+=358.2$.

(5-Methoxy-3-methyl-7-nitrobenzo[*b*]furan-2-yl)(3,4,5-trimethoxyphenyl)methanone (7f). The residue, purified by crystallization with petroleum ether, furnished **7f** as a brown solid, (353 mg, 88%), $R_f=0.34$ (PE/EtOAc 1/1), mp 82-84 °C. $^1\text{H-NMR}$ (CDCl_3) δ : 2.71 (s, 3H), 3.88 (s, 6H), 3.92 (s, 3H), 3.96 (s, 3H), 7.48 (s, 1H), 7.82 (s, 2H), 7.94 (s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta=$ 10.1, 56.2, 56.5, 56.9, 61.3, 104.1, 104.4, 107.2, 107.6, 110.4, 110.7, 127.6, 130.2, 131.6, 142.2, 145.0, 145.8, 153.0, 153.4, 183.3 ppm. MS (ESI): $[\text{M}+1]^+=402.6$.

(6-Methoxy-5-nitrobenzo[*b*]furan-2-yl)(3,4,5-trimethoxyphenyl)methanone (7g). The residue, purified by crystallization with diethyl ether, furnished **7g** as a brown solid, (263 mg, 68%), $R_f=0.35$ (PE/EtOAc 1/1), mp 172-173 °C. $^1\text{H-NMR}$ (CDCl_3) δ : 3.95 (s, 6H), 3.97 (s, 3H), 4.04 (s, 3H), 7.27 (s, 2H), 7.28 (s, 1H), 7.33 (d, $J=2.0$ Hz, 1H), 7.26 (s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta=$ 56.3, 56.5, 56.8, 61.1, 107.2, 107.6, 108.8, 109.0, 109.7, 109.8, 121.3, 123.9, 128.3, 133.2, 144.2, 147.0, 148.3, 152.9, 184.3 ppm. MS (ESI): $[\text{M}+1]^+=388.6$.

(6-Methoxy-3-methyl-5-nitrobenzo[*b*]furan-2-yl)(3,4,5-trimethoxyphenyl)methanone (7h). The residue, purified by crystallization with petroleum ether, furnished **7h** as a yellow solid, (361 mg, 90%), $R_f=0.38$ (PE/EtOAc 7/3), mp 146-148 °C. $^1\text{H-NMR}$ (CDCl_3) δ : 2.61 (s, 3H), 3.94 (s, 6H), 3.97 (s, 3H), 4.03 (s, 3H), 7.17 (s, 1H), 7.34 (s, 2H), 8.22 (s, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta=$ 10.4, 56.1, 56.4, 56.8, 61.0, 107.1, 107.3, 108.8, 109.0, 109.2, 110.0, 123.8, 128.4, 133.2, 144.4, 147.0, 148.3, 152.7, 152.9, 184.3 ppm. MS (ESI): $[\text{M}+1]^+=402.4$.

(7-Methoxy-5-nitrobenzo[*b*]furan-2-yl)(3,4,5-trimethoxyphenyl)methanone (7i). The residue, purified by crystallization with petroleum ether, furnished **7i** as a yellow solid, (317 mg, 82%), $R_f=0.36$ (PE/EtOAc 1/1), mp 182-184 °C. $^1\text{H-NMR}$ (CDCl_3) δ : 3.94 (s, 6H), 3.96 (s, 3H), 3.98 (s, 3H), 7.44 (s, 2H), 7.68 (s, 1H), 7.85 (d, $J=2.0$ Hz, 1H), 8.32 (d, $J=2.0$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta= 56.2, 56.4, 56.7, 61.1, 107.1, 107.5, 108.7, 109.0, 109.6, 109.9, 121.2, 123.8, 128.2, 133.2, 144.3, 147.0, 148.2, 152.8, 184.4$ ppm. MS (ESI): $[\text{M}+1]^+=388.3$.

(7-Methoxy-3-methyl-5-nitrobenzo[*b*]furan-2-yl)(3,4,5-trimethoxyphenyl)methanone (7j). The residue, purified by crystallization with diethyl ether, furnished **7j** as a yellow solid, (273 mg, 68%), $R_f=0.34$ (PE/EtOAc 8/2), mp 76-78 °C. $^1\text{H-NMR}$ (CDCl_3) δ : 2.69 (s, 3H), 3.95 (s, 6H), 3.97 (s, 3H), 4.10 (s, 3H), 7.51 (s, 2H), 7.84 (d, $J=1.0$ Hz, 1H), 8.28 (d, $J=1.0$ Hz, 1H); $^{13}\text{C NMR}$ (100 MHz, CDCl_3): $\delta= 10.2, 56.1, 56.3, 56.7, 61.1, 104.1, 104.3, 107.5, 107.7, 110.4, 110.6, 127.5, 130.1, 131.8, 142.4, 145.2, 146.0, 153.0, 153.2, 183.4$ ppm. MS (ESI): $[\text{M}+1]^+=402.0$.

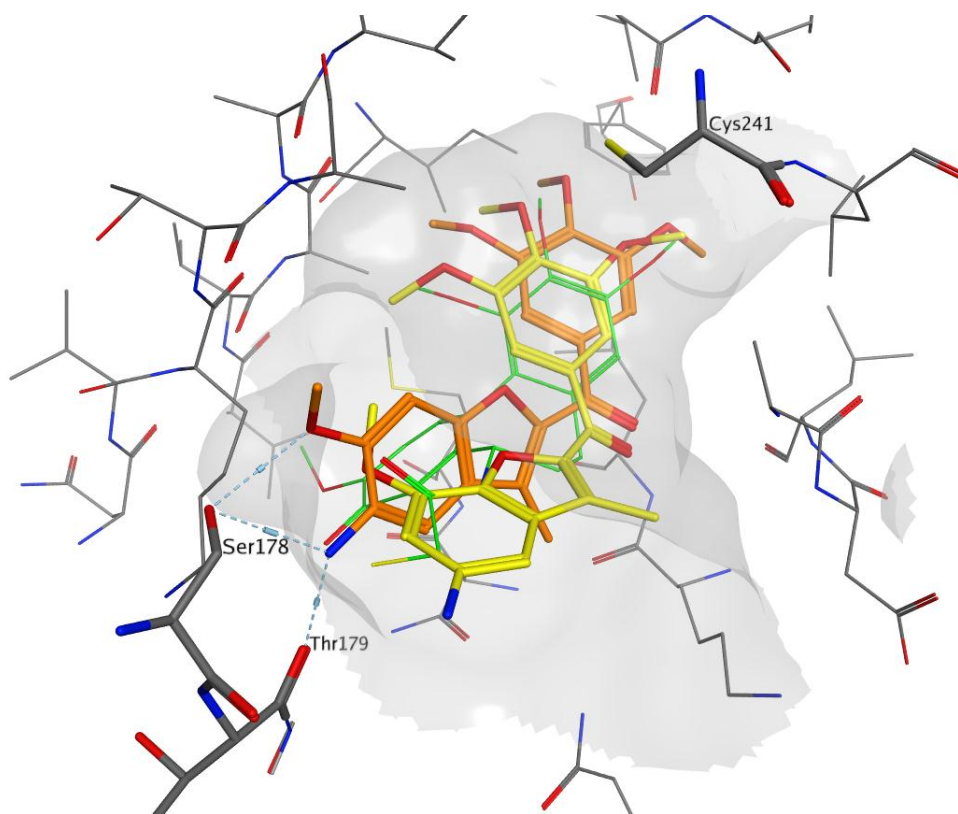


Figure S1. Docked pose of **3h** (orange) and **3j** (yellow) overlapped with DAMA-colchicine (green) in the colchicine-site of tubulin.