

Title: Synthesis and biological evaluation of 1-(2-(adamantan-1-yl)-1H-indol-5-yl)-3-substituted urea/thiourea derivatives as potential anticancer agents

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Supporting Information

Figure S1. The ¹H-NMR Spectra of compound **7s** and its identification

Figure S2. The ¹³C-NMR Spectra of compound **7s** and its identification

Spectra data of compounds **7a~7m**, **7o~7r**, **7t~7v**, **7x~7y** and **9b~9o**

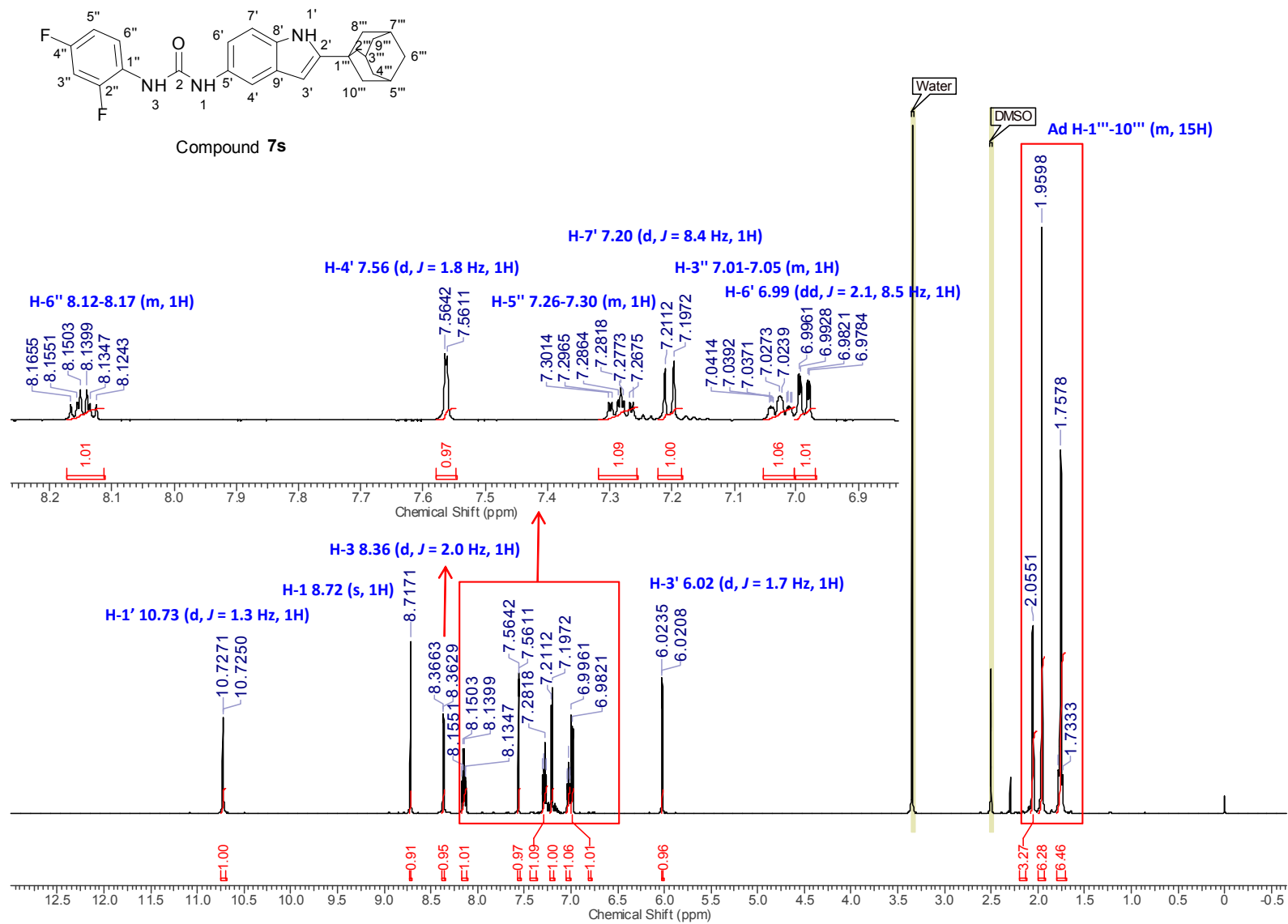


Figure S1. The $^1\text{H-NMR}$ Spectra of compound **7s** and its identification

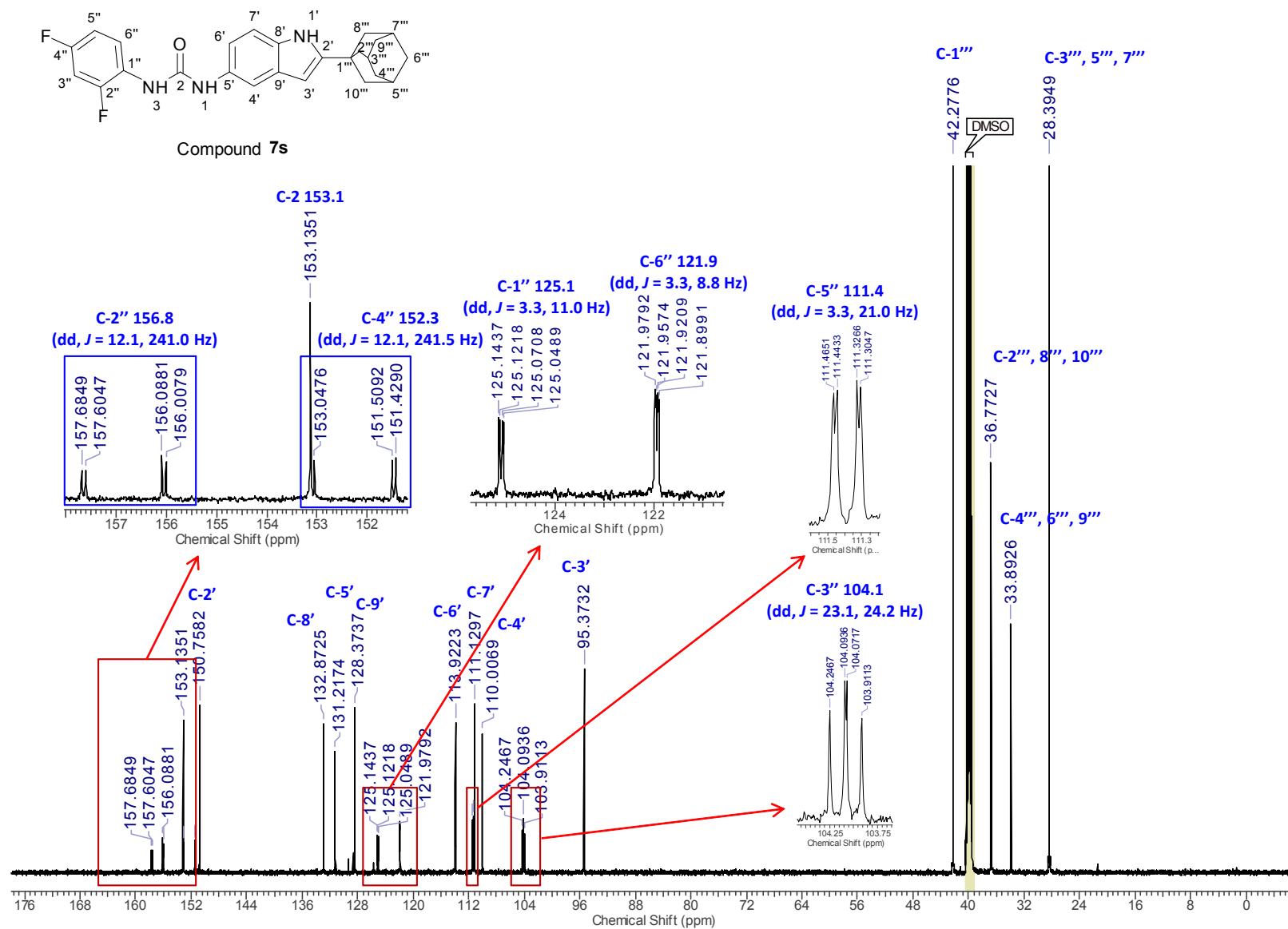


Figure S2. The ^{13}C -NMR Spectra of compound 7s and its identification

1-tert-butyl-3-(2-adamantine-1H-indol-5-yl)urea (7a): White solid; yield: 88.6%; mp: 247-248 °C; HPLC purity: 98.54% ($t_R = 18.25$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.60 (s, 1H, NH-1'), 7.87 (s, 1H, C=ONH-1), 7.45 (d, $J = 1.3$ Hz, 1H, Ar-H), 7.11 (d, $J = 8.4$ Hz, 1H, Ar-H), 6.88 (dd, $J = 1.8, 8.4$ Hz, 1H, Ar-H), 5.96 (d, $J = 1.6$ Hz, 1H, H-3'), 5.79 (s, 1H, C=ONH-3), 2.03-2.08 (m, 3H, Ad-H), 1.93-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H), 1.30 (s, 9H, $(\text{CH}_3)_3\text{C}$); ^{13}C NMR (150 MHz, DMSO- d_6): δ 155.5 (C=O), 150.4 (C-2'), 132.6 (Ar-C), 132.2 (Ar-C), 129.4 (Ar-C), 113.5 (Ar-CH), 110.9 (Ar-CH), 109.0 (Ar-CH), 95.2 (C-3'), 49.7 ($(\text{CH}_3)_3\text{C}$), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 29.7 (s, 3C, $(\text{CH}_3)_3\text{C}$), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{23}\text{H}_{32}\text{N}_3\text{O}^+$, 366.2540, found 366.2534; $[\text{M}+\text{Na}]^+$ calculated for $\text{C}_{23}\text{H}_{31}\text{N}_3\text{ONa}^+$, 388.2359, found 388.2351.

1-cyclobutyl-3-(2-adamantine-1H-indol-5-yl)urea (7b): White solid; yield: 86.6%; mp: 234-235 °C; HPLC purity: 92.8% ($t_R = 16.80$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.63 (d, $J = 1.1$ Hz, 1H, NH-1'), 7.95 (s, 1H, C=ONH-1), 7.45 (d, $J = 1.8$ Hz, 1H, Ar-H), 7.13 (d, $J = 8.4$ Hz, 1H, Ar-H), 6.92 (dd, $J = 1.9, 8.5$ Hz, 1H, Ar-H), 6.20 (d, $J = 8.3$ Hz, 1H, H-3'), 5.97 (d, $J = 1.5$ Hz, 1H, C=ONH-3), 4.10-4.19 (m, 1H, cyclobutyl-H), 2.16-2.23 (m, 2H, cyclobutyl-H), 2.03-2.08 (m, 3H, Ad-H), 1.92-1.98 (m, 6H, Ad-H), 1.79-1.87 (m, 2H, cyclobutyl-H), 1.72-1.79 (m, 6H, Ad-H), 1.54-1.65 (m, 2H, cyclobutyl-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 155.3 (C=O), 150.3 (C-2'), 132.5 (Ar-C), 132.2 (Ar-C), 128.3 (Ar-C), 114.0 (Ar-CH), 110.9 (Ar-CH), 109.7 (Ar-CH), 95.2 (C-3'), 44.7 (cyclobutyl-C), 42.1 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 31.8 (s, 2C, cyclobutyl-C), 28.4 (s, 3C, Ad-C), 14.8 (cyclobutyl-C); ESI-HRMS (+): m/z $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{23}\text{H}_{30}\text{N}_3\text{O}^+$, 364.2383, found 364.2377; $[\text{M}+\text{Na}]^+$ calculated for $\text{C}_{23}\text{H}_{29}\text{N}_3\text{ONa}^+$, 386.2203, found 386.2196.

1-butyl-3-(2-adamantine-1H-indol-5-yl)urea (7c): White solid; yield: 94.2%; mp: 237-239 °C; HPLC purity: 96.3% ($t_R = 24.80$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.62 (d, $J = 1.1$ Hz, 1H, NH-1'), 7.99 (s, 1H, C=ONH-1), 7.45 (d, $J = 1.8$ Hz, 1H, Ar-H), 7.12 (d, $J = 8.6$ Hz, 1H, Ar-H), 6.91 (dd, $J = 2.0, 8.6$ Hz, 1H, Ar-H), 5.96 (d, $J = 1.5$ Hz, 1H, H-3'), 5.90 (t, $J = 5.7$ Hz, 1H, C=ONH-3), 3.04-3.09 (m, 2H, butyl-H), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H), 1.37-1.43 (m, 2H, butyl-H), 1.27-1.35 (m, 2H, butyl-H), 0.89 (t, $J = 7.3$ Hz, 3H, butyl-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 156.3 (C=O), 150.4 (C-2'), 132.5 (Ar-C), 132.4 (Ar-C), 128.4 (Ar-C), 113.9 (Ar-CH), 110.9 (Ar-CH), 109.5 (Ar-CH), 95.2 (C-3'), 42.3 (Ad-C), 39.2 (butyl-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 32.5 (butyl-C), 28.4 (s, 3C, Ad-C), 20.0 (butyl-C), 14.2 (butyl-C); ESI-HRMS (+): m/z $[\text{M}+\text{H}]^+$ calculated for $\text{C}_{23}\text{H}_{32}\text{N}_3\text{O}^+$, 366.2541, found 366.2537; $[\text{M}+\text{Na}]^+$ calculated for $\text{C}_{23}\text{H}_{31}\text{N}_3\text{ONa}^+$, 388.2359, found 388.2354.

1-octyl-3-(2-adamantine-1H-indol-5-yl)urea (7d): White solid; yield: 95.6%; mp: 232-234 °C; HPLC purity: 96.9% ($t_R = 25.00$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.63 (d, $J = 1.1$ Hz, 1H, NH-1'), 8.01 (s, 1H, C=ONH-1), 7.46 (d, $J = 1.8$ Hz, 1H, Ar-H), 7.13 (d, $J = 8.6$ Hz, 1H, Ar-H), 6.92 (dd, $J = 2.0, 8.6$ Hz, 1H, Ar-H), 5.97 (d, $J = 1.5$ Hz, 1H, H-3'), 5.92 (t, $J = 5.6$ Hz, 1H, C=ONH-3), 3.06 (q, $J = 6.8$ Hz, 2H, octyl-H), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H), 1.38-1.45 (m, 2H, octyl-H), 1.20-1.32 (m, 10H, octyl-H), 0.84-0.89 (m, 3H, octyl-H); ^{13}C NMR (150

MHz, DMSO- d_6): δ 156.3 (C=O), 150.4 (C-2'), 132.5 (Ar-C), 132.4 (Ar-C), 128.4 (Ar-C), 113.9 (Ar-CH), 110.9 (Ar-CH), 109.6 (Ar-CH), 95.2 (C-3'), 42.3 (Ad-C), 39.6 (octyl-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 31.7 (octyl-C), 30.4 (octyl-C), 29.3 (octyl-C), 29.2 (octyl-C), 28.4 (s, 3C, Ad-C), 26.9 (octyl-H), 22.6 (octyl-H), 14.4 (octyl-H); ESI-HRMS (+): m/z [M+H]⁺ calculated for C₂₇H₄₀N₃O⁺, 422.3166, found 422.3163; [M+Na]⁺ calculated for C₂₇H₃₉N₃ONa⁺, 444.2985, found 444.2982.

1-cyclooctyl-3-(2-adamantine-1H-indol-5-yl)urea (7e): White solid; yield: 85.8%; mp: 214-215 °C; HPLC purity: 98.85% (t_R = 17.65 min); ¹H NMR (600 MHz, DMSO- d_6): δ 10.60 (d, J = 1.1 Hz, 1H, NH-1'), 7.91 (s, 1H, C=ONH-1), 7.45 (d, J = 1.7 Hz, 1H, Ar-H), 7.12 (d, J = 8.4 Hz, 1H, Ar-H), 6.90 (dd, J = 2.0, 8.6 Hz, 1H, Ar-H), 5.95 (d, J = 1.7 Hz, 1H, H-3'), 5.89 (d, J = 7.8 Hz, 1H, C=ONH-3), 3.67-3.73 (m, 1H, cyclooctyl-H), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 8H, Ad-6H and cyclooctyl-2H), 1.43-1.67 (m, 12H, cyclooctyl-H); ¹³C NMR (150 MHz, DMSO- d_6): δ 155.4 (C=O), 150.4 (C-2'), 132.6 (Ar-C), 132.3 (Ar-C), 128.4 (Ar-C), 113.6 (Ar-CH), 110.9 (Ar-CH), 109.2 (Ar-CH), 95.2 (C-3'), 49.1 (cyclooctyl-C), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 32.4 (s, 2C, cyclooctyl-C), 28.4 (s, 3C, Ad-C), 27.5 (s, 2C, cyclooctyl-C), 25.4 (cyclooctyl-C), 23.6 (s, 2C, cyclooctyl-C); ESI-HRMS (+): m/z [M+H]⁺ calculated for C₂₇H₃₈N₃O⁺ 420.3009, found 420.3004; [M+Na]⁺ calculated for C₂₇H₃₇N₃ONa⁺ 442.2829, found 442.2823.

1-(2-adamantine-1H-indol-5-yl)-3-phenethylurea (7f): White solid; yield: 90.3%; mp: 256-257 °C; HPLC purity: 97.6% (t_R = 18.74 min); ¹H NMR (600 MHz, DMSO- d_6): δ 10.63 (d, J = 1.3 Hz, 1H, NH-1'), 8.09 (s, 1H, C=ONH-1), 7.46 (d, J = 1.8 Hz, 1H, Ar-H), 7.29-7.33 (m, 2H, Ar-H), 7.24 (d, J = 7.0 Hz, 2H, Ar-H), 7.19-7.22 (m, 1H, Ar-H), 7.13 (d, J = 8.4 Hz, 1H, Ar-H), 6.91 (dd, J = 2.0, 8.6 Hz, 1H, Ar-H), 5.97 (d, J = 1.7 Hz, 1H, H-3'), 5.91 (t, J = 5.7 Hz, 1H, C=ONH-3), 3.30-3.34 (m, 2H, C=ONH-CH₂), 2.74 (t, J = 7.2 Hz, 2H, Ph-CH₂), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.71-1.79 (m, 6H, Ad-H); ¹³C NMR (150 MHz, DMSO- d_6): δ 156.2 (C=O), 150.4 (C-2'), 140.2 (Ar-C), 132.45 (Ar-C), 132.37 (Ar-C), 129.2 (s, 2C, C-3'',5''), 128.8 (s, 2C, C-2'',6''), 128.4 (Ar-C), 126.5 (Ar-CH), 114.0 (Ar-CH), 110.9 (Ar-CH), 109.6 (Ar-CH), 95.2 (C-3'), 42.3 (Ad-C), 41.2 (C=ONH-CH₂), 36.8 (s, 3C, Ad-C), 36.5 (Ph-CH₂), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z [M+H]⁺ calculated for C₂₇H₃₂N₃O⁺, 414.2540, found 414.2693; [M+Na]⁺ calculated for C₂₇H₃₁N₃ONa⁺, 436.2359, found 436.2355.

1-(2-adamantine-1H-indol-5-yl)-3-(3-phenylpropyl)urea (7g): White solid; yield: 90.4%; mp: 266-267 °C; HPLC purity: 97.6% (t_R = 18.13 min); ¹H NMR (600 MHz, DMSO- d_6): δ 10.64 (br s, 1H, NH-1), 8.06 (br s, 1H, C=ONH-1), 7.48 (s, 1H, Ar-H), 7.26-7.31 (m, 2H, Ar-H), 7.22 (d, J = 7.0 Hz, 2H, Ar-H), 7.13-7.20 (m, 2H, Ar-H), 6.95 (d, J = 8.1 Hz, 1H, Ar-H), 6.00-6.04 (m, 1H, H-3'), 5.98 (br s, 1H, C=ONH-3), 3.07-3.13 (m, 2H, C=ONH-CH₂), 2.57-2.65 (m, 2H, Ph-CH₂), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.71-1.79 (m, 8H, Ad-6H and Ph-CH₂CH₂); ¹³C NMR (150 MHz, DMSO- d_6): δ 156.4 (C=O), 150.4 (C-2'), 142.2 (Ar-C), 132.5 (Ar-C), 132.4 (Ar-C), 128.7 (s, 4C, C-2'',3'',5'',6''), 128.4 (Ar-C), 126.2 (Ar-CH), 114.0 (Ar-CH), 110.9 (Ar-CH), 109.7 (Ar-CH), 95.2 (C-3'), 42.3 (Ad-C), 39.2 (C=ONH-CH₂), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 33.0 (Ph-CH₂), 32.2 (Ph-CH₂CH₂), 28.4 (s,

3C, Ad-C); ESI-HRMS (+): m/z $[M+H]^+$ calculated for $C_{28}H_{34}N_3O^+$, 428.2696, found 428.2692; $[M+Na]^+$ calculated for $C_{28}H_{33}N_3ONa^+$, 450.2516, found 450.2511.

1-(2-adamantine-1H-indol-5-yl)-3-(4-phenylbutyl)urea (7h): White solid; yield: 87.9%; mp: 239-240 °C; HPLC purity: 95.5% (t_R = 21.24 min); 1H NMR (600 MHz, DMSO- d_6): δ 10.62(s, 1H, NH-1), 7.99 (s, 1H, C=ONH-1), 7.45 (s, 1H, Ar-H), 7.24-7.29 (m, 2H, Ar-H), 7.20 (d, J = 7.5 Hz, 2H, Ar-H), 7.11-7.18 (m, 2H, Ar-H), 6.92 (d, J = 8.6 Hz, 1H, Ar-H), 5.96 (s, 1H, H-3'), 5.92 (t, J = 5.6 Hz, 1H, C=ONH-3), 3.10 (q, J = 6.4 Hz, 2H, C=ONH- CH_2), 2.56-2.62 (t, J = 7.6 Hz, 2H, Ph- CH_2), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.71-1.79 (m, 6H, Ad-H), 1.55-1.62 (m, 2H, Ph- CH_2CH_2), 1.40-1.47 (m, 2H, Ph- $CH_2CH_2CH_2$); ^{13}C NMR (150 MHz, DMSO- d_6): δ 156.3 (C=O), 150.4 (C-2'), 142.7 (Ar-C), 132.45 (Ar-C), 132.43 (Ar-C), 128.8 (s, 2C, C-3'',5''), 128.7 (s, 2C, C-2'',6''), 128.4 (Ar-C), 126.1 (Ar-CH), 114.0 (Ar-CH), 110.9 (Ar-CH), 109.6 (Ar-CH), 95.2 (C-3'), 42.3 (Ad-C), 39.4 (C=ONH- CH_2), 36.8 (s, 3C, Ad-C), 35.4 (Ph- CH_2), 33.9 (s, 3C, Ad-C), 30.1 (Ph- $CH_2CH_2CH_2$), 28.9 (Ph- CH_2CH_2), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z $[M+H]^+$ calculated for $C_{29}H_{36}N_3O^+$, 442.2853, found 442.2847; $[M+Na]^+$ calculated for $C_{29}H_{35}N_3ONa^+$, 464.2672, found 464.2668.

1-(2-adamantine-1H-indol-5-yl)-3-(naphthalen-2-ylmethyl) urea (7i): White solid; yield: 87.6%; mp: 234-235 °C; HPLC purity: 94.6% (t_R = 18.90 min); 1H NMR (600 MHz, DMSO- d_6): δ 10.67 (d, J = 1.3 Hz, 1H, NH-1), 8.13-8.19 (m, 2H), 7.96 (d, J = 7.7 Hz, 1H, Ar-H), 7.86 (d, J = 7.9 Hz, 1H, Ar-H), 7.47-7.61 (m, 5H, Ar-H), 7.17 (d, J = 8.4 Hz, 1H, Ar-H), 6.96 (dd, J = 2.0, 8.6 Hz, 1H, Ar-H), 6.46 (t, J = 5.7 Hz, 1H, C=ONH-3), 5.99 (d, J = 1.7 Hz, 1H, H-3'), 4.78 (d, J = 5.7 Hz, 2H, C=ONH- CH_2), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H); ^{13}C NMR (150MHz, DMSO- d_6): δ 156.2 (C=O), 150.5 (C-2'), 136.3 (Ar-C), 133.8 (Ar-C), 132.5 (Ar-C), 132.3 (Ar-C), 131.4 (Ar-C), 129.0 (Ar-C), 128.4 (Ar-C), 127.9 (Ar-CH), 126.7 (Ar-CH), 126.3 (Ar-CH), 126.0 (Ar-CH), 125.8 (Ar-CH), 124.0 (Ar-CH), 114.0 (Ar-CH), 111.0 (Ar-CH), 109.7 (Ar-CH), 95.2 (C-3'), 42.3 (Ad-C), 41.3 (C=ONH- CH_2), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z $[M+H]^+$ calculated for $C_{30}H_{32}N_3O^+$, 450.2540, found 450.2535; $[M+Na]^+$ calculated for $C_{30}H_{31}N_3ONa^+$, 472.2359, found 472.2355.

1-(2-adamantine-1H-indol-5-yl)-3-(3-morpholinopropyl) urea (7j): White solid; yield: 89.6%; mp: 202.5-204.5 °C; HPLC purity: 95.2% (t_R = 18.67 min); 1H NMR (600 MHz, DMSO- d_6): δ 10.63 (d, J = 1.3 Hz, 1H, NH-1), 8.24 (s, 1H, C=ONH-1), 7.47 (d, J = 1.8 Hz, 1H, Ar-H), 7.14 (d, J = 8.6 Hz, 1H, Ar-H), 6.93 (dd, J = 2.0, 8.6 Hz, 1H, Ar-H), 5.97 (d, J = 1.7 Hz, 1H, H-3'), 5.90 (t, J = 5.4 Hz, 1H, C=ONH-3), 3.56-3.62 (m, 4H, morpholinyl-H), 3.20 (q, J = 6.2 Hz, 2H, C=ONH- CH_2), 2.34-2.44 (m, 6H), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 156.3 (C=O), 150.4 (C-2'), 132.44 (Ar-C), 132.43 (Ar-C), 128.4 (Ar-C), 113.9 (Ar-CH), 110.9 (Ar-CH), 109.6 (Ar-CH), 95.2 (C-3'), 66.7 (s, 2C, morpholinyl-C), 58.5 (s, 2C, morpholinyl-C), 53.7 (N- CH_2), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 36.5 (C=ONH- CH_2), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z $[M+H]^+$ calculated for $C_{25}H_{35}N_4O_2^+$, 423.2755, found 423.2750; $[M+Na]^+$ calculated for $C_{25}H_{34}N_4O_2Na^+$, 445.2574, found 445.2569.

1-(2-adamantine-1H-indol-5-yl)-3-o-tolylurea (7k): White solid; yield: 92.5%; mp: 262-263 °C; HPLC purity: 96.6% ($t_R = 19.56$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.71 (s, 1H, NH-1), 8.72 (s, 1H, C=ONH-1), 7.91 (d, $J = 7.9$ Hz, 1H, C=ONH-3), 7.77 (s, 1H, Ar-H), 7.59 (d, $J = 1.7$ Hz, 1H, Ar-H), 7.21 (d, $J = 8.4$ Hz, 1H, Ar-H), 7.12-7.18 (m, 2H, Ar-H), 7.02 (dd, $J = 2.0, 8.6$ Hz, 1H, Ar-H), 6.91 (t, $J = 7.4$ Hz, 1H, Ar-H), 6.03 (d, $J = 1.7$ Hz, 1H, H-3'), 2.25 (s, 3H, Ph- CH_3), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H); ^{13}C -NMR (150 MHz, DMSO- d_6): δ 153.5 (C=O), 150.6 (C-2'), 138.4 (Ar-C), 132.7 (Ar-C), 131.7 (Ar-C), 130.6 (Ar-C), 128.4 (Ar-C), 127.3 (Ar-CH), 126.6 (Ar-CH), 122.5 (Ar-CH), 121.0 (Ar-CH), 113.9 (Ar-CH), 111.1 (Ar-CH), 109.8 (Ar-CH), 95.4 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C), 18.4 (Ph- CH_3); ESI-HRMS (+): m/z [M+H] $^+$ calculated for $\text{C}_{26}\text{H}_{30}\text{N}_3\text{O}^+$, 400.2383, found 400.2380; [M+Na] $^+$ calculated for $\text{C}_{26}\text{H}_{29}\text{N}_3\text{ONa}^+$, 422.2203, found 422.2198.

1-(2-adamantine-1H-indol-5-yl)-3-p-tolylurea (7l): White solid; yield: 89.5%; mp: 317-319 °C; HPLC purity: 98.36% ($t_R = 19.80$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.69 (s, 1H, NH-1), 8.38 (s, 1H, C=ONH-1), 8.27 (s, 1H, C=ONH-3), 7.54 (d, $J = 1.7$ Hz, 1H, Ar-H), 7.33 (d, $J = 8.4$ Hz, 2H, Ar-H), 7.18 (d, $J = 8.6$ Hz, 1H, Ar-H), 7.06 (d, $J = 8.1$ Hz, 2H, Ar-H), 6.98 (dd, $J = 1.9, 8.5$ Hz, 1H, Ar-H), 6.01 (d, $J = 1.7$ Hz, 1H, H-3'), 2.23 (s, 3H, Ph- CH_3), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 153.5 (C=O), 150.6 (C-2'), 138.1 (Ar-C), 132.7 (Ar-C), 131.6 (Ar-C), 130.6 (Ar-C), 129.6 (s, 2C, C-3'', 5''), 128.4 (Ar-C), 118.5 (s, 2C, C-2'', 6''), 114.1 (Ar-CH), 111.0 (Ar-CH), 110.0 (Ar-CH), 95.3 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C), 20.8 (Ph- CH_3); ESI-HRMS (+): m/z [M+H] $^+$ calculated for $\text{C}_{26}\text{H}_{30}\text{N}_3\text{O}^+$, 400.2383, found 400.2382; [M+Na] $^+$ calculated for $\text{C}_{26}\text{H}_{29}\text{N}_3\text{ONa}^+$, 422.2203, found 422.2201.

1-(4-methoxyphenyl)-3-(2-adamantine-1H-indol-5-yl)urea (7m): White solid; yield: 92.0%; mp: 315-318 °C; HPLC purity: 96.6% ($t_R = 17.69$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.68 (s, 1H, NH-1), 8.30 (s, 1H, C=ONH-1), 8.22 (s, 1H, C=ONH-3), 7.53 (d, $J = 1.7$ Hz, 1H, Ar-H), 7.33-7.36 (m, 2H, Ar-H), 7.18 (d, $J = 8.6$ Hz, 1H, Ar-H), 6.98 (dd, $J = 1.9, 8.5$ Hz, 1H, Ar-H), 6.83-6.87 (m, 2H, Ar-H), 6.00 (d, $J = 1.7$ Hz, 1H, H-3'), 3.71 (s, 3H, OCH_3), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 154.6 (C-4''), 153.7 (C=O), 150.6 (C-2'), 133.8 (Ar-C), 132.7 (Ar-C), 131.7 (Ar-C), 128.4 (Ar-C), 120.2 (s, 2C, C-2'', 6''), 114.4 (s, 2C, C-3'', 5''), 114.1 (Ar-CH), 111.0 (Ar-CH), 110.0 (Ar-CH), 95.3 (C-3'), 55.6 (Ph- OCH_3), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z [M+H] $^+$ calculated for $\text{C}_{26}\text{H}_{30}\text{N}_3\text{O}_2^+$, 416.2333, found 416.2329; [M+Na] $^+$ calculated for $\text{C}_{26}\text{H}_{29}\text{N}_3\text{O}_2\text{Na}^+$, 438.2152, found 438.2148.

1-(2,4-dimethylphenyl)-3-(2-adamantine-1H-indol-5-yl)urea (7o): White solid; yield: 89.5%; mp: 271-273 °C; HPLC purity: 96.9% ($t_R = 19.60$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.69 (s, 1H, NH-1), 8.31 (s, 1H, C=ONH-1), 8.26 (s, 1H, C=ONH-3), 7.54 (d, $J = 1.7$ Hz, 1H, Ar-H), 7.23 (d, $J = 1.5$ Hz, 1H, Ar-H), 7.18 (d, $J = 8.4$ Hz, 1H, Ar-H), 7.16 (dd, $J = 2.0, 8.3$ Hz, 1H, Ar-H), 7.00 (d, $J = 8.3$ Hz, 1H, Ar-H), 6.98 (dd, $J = 2.0, 8.6$ Hz, 1H, Ar-H), 6.00 (d, $J = 1.5$ Hz, 1H, H-3'), 2.18 (s, 3H, Ph- CH_3), 2.15 (s, 3H, Ph- CH_3), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H);

¹³C NMR (150 MHz, DMSO-*d*₆): δ 153.5 (C=O), 150.6 (C-2'), 138.3 (Ar-C), 136.7 (Ar-C), 132.7 (Ar-C), 131.6 (Ar-C), 130.1 (Ar-CH), 129.4 (Ar-C), 128.4 (Ar-C), 119.8 (Ar-CH), 116.0 (Ar-CH), 114.0 (Ar-CH), 111.0 (Ar-CH), 110.0 (Ar-CH), 95.3 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C), 20.1 (Ph-CH₃), 19.1 (Ph-CH₃); ESI-HRMS (+): *m/z* [M+H]⁺ calculated for C₂₇H₃₂N₃O⁺, 414.2540, found 414.2541; [M+Na]⁺ calculated for C₂₇H₃₁N₃ONa⁺, 436.2359, found 436.2359.

1-(5-methoxy-2-methylphenyl)-3-(2-adamantine-1H-indol-5-yl)urea (7p): Purple solid; yield: 89.6%; mp: 285-287 °C; HPLC purity: 95.9% (*t*_R = 15.60 min); ¹H NMR (600 MHz, DMSO-*d*₆): δ 10.68 (s, 1H, NH-1), 8.51 (s, 1H, C=ONH-1), 7.62 (s, 1H, C=ONH-3), 7.59 (d, *J* = 8.8 Hz, 1H, Ar-H), 7.54 (d, *J* = 1.3 Hz, 1H, Ar-H), 7.18 (d, *J* = 8.4 Hz, 1H, Ar-H), 6.99 (dd, *J* = 8.6, 1.8 Hz, 1H, Ar-H), 6.77 (d, *J* = 2.8 Hz, 1H, Ar-H), 6.71 (dd, *J* = 8.8, 2.9 Hz, 1H, Ar-H), 6.00 (d, *J* = 1.5 Hz, 1H, H-3'), 3.71 (s, 3H, Ph-OCH₃), 2.22 (s, 3H, Ph-CH₃), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H); ¹³C NMR (150 MHz, DMSO-*d*₆): δ 155.4 (C-4''), 154.0 (C=O), 150.6 (C-2'), 132.6 (Ar-C), 132.0 (Ar-C), 131.3 (Ar-CH), 130.7 (Ar-C), 128.4 (Ar-C), 124.0 (Ar-C), 115.9 (Ar-CH), 113.9 (Ar-CH), 111.6 (Ar-CH), 111.0 (Ar-CH), 109.7 (Ar-CH), 95.3 (C-3'), 55.6 (Ph-OCH₃), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C), 18.6 (Ph-CH₃); ESI-HRMS (+): *m/z* [M+H]⁺ calculated for C₂₇H₃₂N₃O₂⁺, 430.2489, found 430.2490; [M+Na]⁺ calculated for C₂₇H₃₁N₃O₂Na⁺, 452.2308, found 452.2308.

1-(4-fluoro-2-methylphenyl)-3-(2-adamantine-1H-indol-5-yl)urea (7q): White solid; yield: 91.2%; mp: 270-271 °C; HPLC purity: 97.9% (*t*_R = 19.10 min); ¹H NMR (600 MHz, DMSO-*d*₆): δ 10.71 (s, 1H, NH-1), 8.65 (s, 1H, C=ONH-1), 7.82 (dd, *J* = 5.7, 9.0 Hz, 1H, Ar-H), 7.78 (s, 1H, C=ONH-3), 7.57 (d, *J* = 1.7 Hz, 1H, Ar-H), 7.20 (d, *J* = 8.6 Hz, 1H, Ar-H), 7.04 (dd, *J* = 2.8, 9.6 Hz, 1H, Ar-H), 7.01 (dd, *J* = 1.9, 8.5 Hz, 1H, Ar-H), 6.97 (dt, *J* = 3.0, 8.7 Hz, 1H, Ar-H), 6.02 (d, *J* = 1.7 Hz, 1H, H-3'), 2.26 (s, 3H, Ph-CH₃), 2.03-2.08 (m, 3H, Ad-H), 1.92-1.98 (m, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H); ¹³C NMR (150 MHz, DMSO-*d*₆): δ 158.0 (d, *J* = 237.7 Hz, Ar-CF), 153.7 (C=O), 150.7 (C-2'), 134.6 (d, *J* = 2.2 Hz, C-1''), 132.7 (Ar-C), 131.7 (Ar-C), 130.7 (d, *J* = 7.7 Hz, C-2''), 128.4 (Ar-C), 123.2 (d, *J* = 8.8 Hz, C-6''), 116.8 (d, *J* = 22.1 Hz, C-3''), 114.0 (Ar-CH), 112.8 (d, *J* = 22.1 Hz, C-5''), 111.1 (Ar-CH), 109.9 (Ar-CH), 95.3 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C), 18.3 (Ph-CH₃); ESI-HRMS (+): *m/z* [M+H]⁺ calculated for C₂₆H₂₉FN₃O⁺, 418.2289, found 418.2290, [M+Na]⁺ calculated for C₂₆H₂₈FN₃ONa⁺, 440.2109, found 440.2107.

1-(4-bromo-2-methylphenyl)-3-(2-adamantine-1H-indol-5-yl)urea (7r): White solid; yield: 89.6%; mp: 278-279 °C; HPLC purity: 96.1% (*t*_R = 22.10 min); ¹H NMR (600 MHz, DMSO-*d*₆): δ 10.71 (d, *J* = 1.3 Hz, 1H, NH-1), 8.78 (s, 1H, C=ONH-1), 7.93 (d, *J* = 8.8 Hz, 1H, Ar-H), 7.84 (s, 1H, C=ONH-1), 7.57 (d, *J* = 1.8 Hz, 1H, Ar-H), 7.37 (d, *J* = 2.0 Hz, 1H, Ar-H), 7.30 (dd, *J* = 2.4, 8.6 Hz, 1H, Ar-H), 7.20 (d, *J* = 8.4 Hz, 1H, Ar-H), 7.00 (dd, *J* = 2.0, 8.6 Hz, 1H, Ar-H), 6.02 (d, *J* = 1.7 Hz, 1H, H-3'), 2.24 (s, 3H, Ph-CH₃), 2.02-2.08 (m, 3H, Ad-H), 1.93-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H); ¹³C NMR (150 MHz, DMSO-*d*₆): δ 153.3 (C=O), 150.7 (C-2'), 138.0 (Ar-C), 132.81 (Ar-CH), 132.80 (Ar-C), 131.5 (Ar-C), 129.7 (Ar-CH), 129.2 (Ar-CH), 128.4 (Ar-C), 122.3 (Ar-CH), 113.9 (Ar-

CH), 113.8 (C-Br), 111.1 (Ar-CH), 109.9 (Ar-CH), 95.4 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C), 18.1 (Ph-CH₃); ESI-HRMS (+): m/z [M+H]⁺ calculated for C₂₆H₂₉BrN₃O⁺, 478.1489, found 478.1485; [M+Na]⁺ calculated for C₂₆H₂₈BrN₃ONa⁺, 500.1308, found 500.1305.

1-(2-fluoro-6-methylphenyl)-3-(1H-indol-2-adamantine-5-yl)urea (7t): White solid; yield: 91.2%; mp: 280-281 °C; HPLC purity: 96.3% (t_R = 18.25 min); ¹H NMR (600 MHz, DMSO-d₆): δ 10.70 (br s, 1H, NH-1), 8.47 (s, 1H, C=ONH-1), 7.73 (s, 1H, C=ONH-3), 7.53 (s, 1H, Ar-H), 7.16-7.21 (m, 2H, Ar-H), 7.07 (d, J = 8.1 Hz, 2H, Ar-H), 7.01 (dd, J = 1.7, 8.7 Hz, 1H, Ar-H), 6.01 (s, 1H, H-3'), 2.27 (s, 3H, Ph-CH₃), 2.03-2.08 (m, 3H, Ad-H), 1.93-1.97 (m, 6H, Ad-H), 1.73-1.80 (m, 6H, Ad-H); ¹³C NMR (150 MHz, DMSO-d₆): δ 158.3 (d, J = 244.3 Hz, Ar-CF), 153.8 (C=O), 150.6 (C-2'), 138.2 (Ar-C), 132.7 (Ar-C), 131.8 (Ar-C), 128.4 (Ar-C), 126.8 (d, J = 8.8 Hz, C-4''), 126.1 (d, J = 3.3 Hz, C-5''), 125.4 (d, J = 13.2 Hz, C-6''), 114.1 (Ar-CH), 113.4 (d, J = 20.9 Hz, C-3''), 111.0 (Ar-CH), 110.0 (Ar-CH), 95.3 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C), 18.3 (Ph-CH₃); ESI-HRMS (+): m/z [M+H]⁺ calculated for C₂₆H₂₉FN₃O⁺, 418.2289, found 418.2287; [M+Na]⁺ calculated for C₂₆H₂₈FN₃ONa⁺, 440.2109, found 440.2103.

1-(4-bromo-2-fluorophenyl)-3-(1H-indol-2-adamantine-5-yl)urea (7u): Pale yellow solid; yield: 87.7%; mp: 210-212 °C; HPLC purity: 98.6% (t_R = 13.68 min); ¹H NMR (600MHz, DMSO-d₆): δ 10.75 (d, J = 1.5 Hz, 1H, NH-1), 8.86 (s, 1H, C=ONH-1), 8.62 (d, J = 2.8 Hz, 1H, C=ONH-3), 8.48 (dd, J = 2.5, 7.2 Hz, 1H, Ar-H), 7.59 (d, J = 1.8 Hz, 1H, Ar-H), 7.20-7.24 (m, 2H, Ar-H), 7.11-7.15 (m, 1H, Ar-H), 6.99 (dd, J = 2.1, 8.5 Hz, 1H, Ar-H), 6.03 (d, J = 1.7 Hz, 1H, H-3'), 2.03-2.08 (m, Ad-H), 1.93-1.98 (m, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H); ¹³C NMR (150 MHz, DMSO-d₆): δ 152.7 (C=O), 151.9 (d, J = 241.0 Hz, Ar-CF), 150.8 (C-2'), 133.0 (Ar-C), 130.9 (Ar-C), 130.3 (d, J = 12.1 Hz, C-1''), 128.4 (Ar-C), 124.3 (d, J = 7.7 Hz, C-4''), 122.3 (Ar-CH), 117.2 (d, J = 20.9 Hz, C-3''), 116.7 (d, J = 3.3 Hz, C-5''), 113.9 (Ar-CH), 111.2 (Ar-CH), 110.1 (Ar-CH), 95.4 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z [M+H]⁺ calculated for C₂₅H₂₆BrFN₃O⁺, 482.1238, found 482.1242; [M+Na]⁺ calculated for C₂₅H₂₅BrFN₃ONa⁺, 504.1057, found 504.1058.

1-(2-fluoro-4-iodophenyl)-3-(1H-indol-2-adamantine-5-yl)urea (7v): White solid; yield: 87.3%; mp: 278-281 °C; HPLC purity: 97.2% (t_R = 14.90 min); ¹H NMR (600 MHz, DMSO-d₆): δ 10.74 (d, J = 1.1 Hz, 1H, NH-1), 8.80 (s, 1H, C=ONH-1), 8.50 (d, J = 2.6 Hz, 1H, C=ONH-3), 8.05 (t, J = 8.6 Hz, 1H, Ar-H), 7.62 (dd, J = 1.8, 10.6 Hz, 1H, Ar-H), 7.57 (d, J = 1.8 Hz, 1H, Ar-H), 7.48 (d, J = 8.6 Hz, 1H, Ar-H), 7.20 (d, J = 8.6 Hz, 1H, Ar-H), 6.99 (dd, J = 2.0, 8.6 Hz, 1H, Ar-H), 6.03 (d, J = 1.7 Hz, 1H, H-3'), 2.03-2.08 (m, 3H, Ad-H), 1.93-1.98 (m, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H); ¹³C NMR (150 MHz, DMSO-d₆): δ 152.8 (C=O), 152.0 (d, J = 245.4 Hz, Ar-CF), 150.8 (C-2'), 133.8 (d, J = 3.3 Hz, C-5''), 132.9 (Ar-C), 131.0 (Ar-C), 128.7 (d, J = 9.9 Hz, C-1''), 128.4 (Ar-C), 123.8 (d, J = 9.9 Hz, C-3''), 122.2 (Ar-C), 113.9 (Ar-CH), 111.2 (Ar-CH), 110.0 (Ar-CH), 95.4 (C-3'), 83.2 (d, J = 7.7 Hz, C-4''), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z [M+H]⁺ calculated for C₂₅H₂₆FIN₃O⁺, 530.1099, found 530.1102; [M+Na]⁺ calculated for C₂₅H₂₅FIN₃ONa⁺, 552.0919, found 552.0920.

1-(2-adamantine-1H-indol-5-yl)-3-(pyridin-3-yl)urea (7x): Pale yellow solid; yield: 85.6%; mp: 250-252 °C; HPLC purity: 99.16% ($t_R = 20.67$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.74 (s, 1H, NH-1), 8.71 (s, 1H, C=ONH-1), 8.60 (d, $J = 2.4$ Hz, 1H, C=ONH-3), 8.47 (s, 1H, Py-H), 8.16 (d, $J = 1.2, 4.7$ Hz, 1H, Py-H), 7.93-7.97 (m, 1H, Py-H), 7.55 (d, $J = 1.5$ Hz, 1H, Ar-H), 7.29 (dd, $J = 4.6, 8.3$ Hz, 1H, Py-H), 7.21 (d, $J = 8.4$ Hz, 1H, Ar-H), 7.01 (dd, $J = 2.0, 8.6$ Hz, 1H, Ar-H), 6.03 (s, 1H, H-3'), 2.03-2.08 (m, 3H, Ad-H), 1.94-1.97 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 153.5 (C=O), 150.8 (C-2'), 142.9 (Py-C), 140.3 (Py-C), 137.4 (Py-C), 133.0 (Ar-C), 131.1 (Ar-C), 128.4 (Ar-C), 125.3 (Py-C), 124.0 (Py-C), 114.3 (Ar-CH), 111.1 (Ar-CH), 110.5 (Ar-CH), 94.9 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z [M+H] $^+$ calculated for $\text{C}_{24}\text{H}_{27}\text{N}_4\text{O}^+$, 387.2179, found 387.2174; [M+Na] $^+$ calculated for $\text{C}_{24}\text{H}_{26}\text{N}_4\text{ONa}^+$, 409.1999, found 409.1994.

1-(2-adamantine-1H-indol-5-yl)-3-(pyrimidin-2-yl)urea (7y): Pale yellow solid; yield: 85.3%; mp: 207-210 °C; HPLC purity: 90.5% ($t_R = 19.78$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.76 (s, 1H, NH-1), 8.92 (s, 1H, C=ONH-1), 8.87 (s, 1H, C=ONH-3), 8.77-8.81 (m, 1H), 8.10 (s, 1H), 7.56 (s, 1H, Ar-H), 7.23 (d, $J = 8.6$ Hz, 1H, Ar-H), 7.03 (dd, $J = 1.9, 8.5$ Hz, 1H, Ar-H), 6.04 (d, $J = 1.5$ Hz, 1H, H-3'), 2.03-2.08 (m, 3H, Ad-H), 1.93-1.98 (m, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 153.2 (C=O), 151.9 (pyrimidinyl-C), 150.8 (C-2'), 146.6 (s, 2C, pyrimidinyl-C), 141.9 (pyrimidinyl-C), 133.1 (Ar-C), 130.8 (Ar-C), 128.4 (Ar-C), 114.5 (Ar-CH), 111.1 (Ar-CH), 110.8 (Ar-CH), 95.4 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z [M+H] $^+$ calculated for $\text{C}_{23}\text{H}_{26}\text{N}_5\text{O}^+$, 388.2132, found 388.2129; [M+Na] $^+$ calculated for $\text{C}_{23}\text{H}_{25}\text{N}_5\text{ONa}^+$, 410.1951, found 410.1951.

1-cyclobutyl-3-(2-adamantane-1H-indol-5-yl)thiourea (9b): White solid; yield: 85.6%; mp: 280-281 °C; HPLC purity: 97.6% ($t_R = 16.50$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.91 (br s, 1H, NH-1), 9.36 (br s, 1H, C=SNH-1), 8.12 (br s, 1H, C=SNH-3), 7.33 (s, 1H, Ar-H), 7.25 (d, $J = 8.4$ Hz, 1H, Ar-H), 6.87 (dd, $J = 1.7, 8.4$ Hz, 1H, Ar-H), 6.07 (d, $J = 1.5$, 1H, H-3'), 4.60-4.77 (m, 1H, cyclobutyl-H), 2.16-2.24 (m, 2H, cyclobutyl-H), 2.03-2.08 (m, 3H, Ad-H), 1.94-1.99 (m, 6H, Ad-H), 1.85-1.93 (m, 2H, cyclobutyl-H), 1.72-1.81 (m, 6H, Ad-H), 1.56-1.63 (m, 2H, cyclobutyl-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 180.1 (C=S), 151.0 (C-2'), 134.4 (Ar-C), 129.4 (Ar-C), 128.7 (Ar-C), 128.3 (Ar-CH), 125.8 (Ar-CH), 111.2 (Ar-CH), 95.7 (C-3'), 45.0 (cyclobutyl-C), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 31.8 (cyclobutyl-C), 30.6 (cyclobutyl-C), 28.4 (s, 3C, Ad-C), 27.6 (cyclobutyl-C); ESI-HRMS (+): m/z [M+H] $^+$ calculated for $\text{C}_{23}\text{H}_{30}\text{N}_3\text{S}^+$, 380.2155, found 380.2153; [M+Na] $^+$ calculated for $\text{C}_{23}\text{H}_{29}\text{N}_3\text{SNa}^+$, 402.1974, found 402.1973.

1-butyl-3-(2-adamantane-1H-indol-5-yl)thiourea (9c): White solid; yield: 91.8%; mp: 238-240 °C; HPLC purity: 97.3% ($t_R = 22.35$ min); ^1H NMR (600 MHz, DMSO- d_6): δ 10.91 (br s, 1H, NH-1), 9.25 (br s, 1H, C=SNH-1), 7.26-7.32 (m, 2H), 7.10-7.20 (m, 1H, Ar-H), 6.83 (d, $J = 8.4$ Hz, 1H, Ar-H), 6.08 (d, $J = 1.7$ Hz, 1H, H-3'), 3.41-3.47 (m, 2H, butyl-H), 2.04-2.09 (m, 3H, Ad-H), 1.94-1.98 (m, 6H, Ad-H), 1.72-1.81 (m, 6H, Ad-H), 1.48 (quin, $J = 7.3$ Hz, 2H, butyl-H), 1.27 (sxt, $J = 7.3$ Hz, 2H, butyl-H), 0.89 (t, $J = 7.3$ Hz, 3H, butyl-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 181.0 (C=S), 151.1 (C-

2'), 134.6 (Ar-C), 128.7 (Ar-C), 128.4 (Ar-C), 119.0 (Ar-CH), 116.8 (Ar-CH), 111.5 (Ar-CH), 95.8 (C-3'), 44.2 (butyl-C), 42.2 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 31.4 (butyl-C), 28.4 (s, 3C, Ad-C), 20.0 (butyl-C), 14.2 (butyl-C); ESI-HRMS (+): m/z $[M+H]^+$ calculated for $C_{23}H_{32}N_3S^+$, 382.2311, found 382.2309; $[M+Na]^+$ calculated for $C_{23}H_{31}N_3SNa^+$, 404.2131, found 404.2129.

1-hexyl-3-(2-adamantane-1H-indol-5-yl)thiourea (9d): White solid; yield: 91.3%; mp: 208-210 °C; HPLC purity: 98.3% (t_R = 22.67 min); 1H NMR (600 MHz, DMSO- d_6): δ 10.91 (br s, 1H, NH-1), 9.25 (br s, 1H, C=SNH-1), 7.23-7.33 (m, 2H), 7.11-7.21 (m, 1H, Ar-H), 6.83 (d, J = 8.4 Hz, 1H, Ar-H), 6.08 (d, J = 1.7 Hz, 1H, H-3'), 3.40-3.46 (m, 2H, hexyl-H), 2.04-2.09 (m, 3H, Ad-H), 1.94-1.98 (m, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H), 1.45-1.52 (m, 2H, hexyl-H), 1.22-1.32 (m, 6H, hexyl-H), 0.87 (t, J = 7.0 Hz, 3H, hexyl-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 181.0 (C=S), 151.1 (C-2'), 134.6 (Ar-C), 129.4 (Ar-C), 128.4 (Ar-C), 119.1 (Ar-CH), 116.8 (Ar-CH), 111.5 (Ar-CH), 95.8 (C-3'), 44.5 (hexyl-C), 42.2 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 31.7 (hexyl-C), 29.1 (hexyl-C), 28.4 (s, 3C, Ad-C), 26.5 (hexyl-C), 22.5 (hexyl-C), 14.4 (hexyl-C); ESI-HRMS (+): m/z $[M+H]^+$ calculated for $C_{25}H_{36}N_3S^+$, 410.2624, found 410.2621; $[M+Na]^+$ calculated for $C_{25}H_{35}N_3SNa^+$, 432.2444, found 432.2443.

1-cycloheptyl-3-(2-adamantane-1H-indol-5-yl)thiourea (9e): White solid; yield: 89.4%; mp: 289-291 °C; HPLC purity: 97.3% (t_R = 18.90 min); 1H NMR (600 MHz, DMSO- d_6): δ 10.89 (s, 1H, NH-1), 9.18 (s, 1H, C=SNH-1), 7.32 (d, J = 1.3 Hz, 1H, Ar-H), 7.25 (d, J = 8.4 Hz, 1H, Ar-H), 6.98 (br s, H, C=SNH-3), 6.86 (dd, J = 1.9, 8.5 Hz, 1H, Ar-H), 6.07 (d, J = 1.7 Hz, 1H, H-3'), 4.35-4.45 (m, 1H, cycloheptyl-H), 2.04-2.09 (m, 3H, Ad-H), 1.94-1.98 (m, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H), 1.43-1.66 (m, 12H, cycloheptyl-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 179.8 (C=S), 151.0 (C-2'), 134.4 (Ar-C), 130.1 (Ar-C), 128.4 (Ar-C), 118.8 (Ar-CH), 116.3 (Ar-CH), 111.3 (Ar-CH), 95.7 (C-3'), 53.9 (cycloheptyl-C), 42.2 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 32.1 (s, 2C, cycloheptyl-C), 28.4 (s, 3C, Ad-C), 27.2 (s, 2C, cycloheptyl-C), 23.9 (s, 2C, cycloheptyl-C); ESI-HRMS (+): m/z $[M+H]^+$ calculated for $C_{26}H_{36}N_3S^+$, 422.2624, found 422.2622; $[M+Na]^+$ calculated for $C_{26}H_{35}N_3SNa^+$, 444.2444, found 444.2446.

1-(2-adamantane-1H-indol-5-yl)-3-phenethylthiourea (9f): White solid; yield: 87.6%; mp: 243-245 °C; HPLC purity: 97.3% (t_R = 18.97 min); 1H NMR (600 MHz, DMSO- d_6): δ 10.91 (br s, 1H, NH-1), 9.37 (br s, 1H, C=SNH-1), 7.26-7.30 (m, 2H, C=SNH-3 and Ar-H), 7.25 (d, J = 8.3 Hz, 1H, Ar-H), 7.20 (d, J = 7.3 Hz, 4H, Ar-H), 6.77 (d, J = 8.3 Hz, 1H, Ar-H), 6.06 (s, 1H, H-3'), 3.60-3.70 (m, 2H, C=SNH- CH_2), 2.82 (t, J = 7.4 Hz, 2H, Ph- CH_2), 2.03-2.08 (m, 3H, Ad-H), 1.93-1.98 (m, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 180.9 (C=S), 151.1 (C-2'), 139.9 (Ar-CH), 134.6 (Ar-C), 129.1 (s, 2C, C-3'',5''), 128.8 (s, 2C, C-2'',6''), 128.5 (Ar-C), 126.5 (Ar-CH), 119.0 (Ar-CH), 116.9 (Ar-CH), 111.5 (Ar-CH), 95.8 (C-3'), 46.0 (C=SNH- CH_2), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 35.2 (Ph- CH_2), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z calculated for $C_{27}H_{32}N_3S^+$, 430.2311, found 430.2310; $[M+Na]^+$ calculated for $C_{27}H_{31}N_3SNa^+$, 452.2131, found 452.2132.

1-(2-adamantane-1H-indol-5-yl)-3-(3-phenylpropyl)thiourea (9g): White solid; yield: 89.4%; mp: 210-212 °C; HPLC purity: 95.9% (t_R = 19.65 min); 1H NMR (600 MHz, DMSO- d_6): δ 10.92 (br s, 1H, NH-1), 9.31 (br s, 1H, C=SNH-1), 7.25-7.32 (m, 5H), 7.15-7.22 (m, 3H, Ar-H), 6.85 (dd, J = 1.5, 8.4 Hz, 1H, Ar-H), 6.09 (d, J = 1.5 Hz, 1H, H-3'), 3.44-3.50 (m, 2H, C=SNH- CH_2), 2.57 (t, J = 7.7 Hz, 2H, Ph- CH_2), 2.03-2.08 (m, 3H, Ad-H), 1.93-1.98 (m, 6H, Ad-H), 1.80-1.84 (m, 2H, Ph- CH_2CH_2), 1.73-1.80 (m, 6H, Ad-H); ^{13}C NMR (150MHz, DMSO- d_6): δ 181.1 (C=S), 151.1 (C-2'), 142.2 (Ar-CH),

134.6 (Ar-C), 128.9 (Ar-C), 128.73 (s, 2C, C-3'',5''), 128.68 (s, 2C, C-2'',6''), 128.4 (Ar-C), 126.2 (Ar-CH), 119.1 (Ar-CH), 116.8 (Ar-CH), 111.5 (Ar-CH), 95.8 (C-3'), 44.2 (C=SNH-CH₂), 42.2 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 33.1 (Ph-CH₂), 31.0 (Ph-CH₂CH₂), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): *m/z* calculated for C₂₈H₃₄N₃S⁺, 444.2468, found 444.2464; [M+Na]⁺ calculated for C₂₈H₃₃N₃SNa⁺, 466.2287, found 466.2288.

1-(2-adamantane-1H-indol-5-yl)-3-(2-morpholinoethyl)thiourea (9h): White solid; yield: 87.6%; mp: 235-237 °C; HPLC purity: 94.6% (*t_R* = 19.09 min); ¹H NMR (600MHz, DMSO-d₆): δ 10.96 (br s, 1H, NH-1), 9.50 (br s, 1H, C=SNH-1), 7.27-7.35 (m, 2H, Ar-H), 7.19 (br s, 1H, C=SNH-3), 6.85 (d, *J* = 8.3 Hz, 1H, Ar-H), 6.08 (s, 1H, H-3'), 3.50-3.55 (m, 2H), 3.45-3.49 (m, 4H), 2.32-2.45 (m, 6H), 2.04-2.09 (m, 3H, Ad-H), 1.93-1.98 (m, 6H, Ad-H), 1.72-1.82 (m, 6H, Ad-H); ¹³C NMR (150 MHz, DMSO-d₆): δ 180.7 (C=S), 151.3 (C-2'), 134.6 (Ar-C), 129.6 (Ar-C), 128.5 (Ar-C), 118.8 (Ar-CH), 116.5 (Ar-CH), 111.6 (Ar-CH), 95.7 (C-3'), 66.6 (s, 2C, morpholinyl-C), 55.2 (N-CH₂), 53.4 (s, 2C, morpholinyl-C), 42.2 (Ad-C), 36.8 (s, 3C, Ad-C), 35.9 (C=SNH-CH₂), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): *m/z* [M+H]⁺ calculated for C₂₅H₃₅N₄OS⁺, 439.2526, found 439.2525; [M+Na]⁺ calculated for C₂₅H₃₄N₄OSNa⁺, 461.2346, found 461.2345.

1-(2-adamantane-1H-indol-5-yl)-3-(naphthalen-1ylmethyl)thiourea (9i): White solid; yield: 88.6%; mp: 238-241 °C; HPLC purity: 94.5% (*t_R* = 19.24 min); ¹H NMR (600 MHz, DMSO-d₆): δ 10.90 (s, 1H, NH-1), 9.49 (br s, 1H, C=SNH-1), 8.13 (d, *J* = 8.3 Hz, 1H, Ar-H), 7.94 (d, *J* = 7.7 Hz, 1H, Ar-H), 7.83 (d, *J* = 8.1 Hz, 1H, Ar-H), 7.68 (br s, 1H, C=SNH-3), 7.53-7.59 (m, 2H, Ar-H), 7.46-7.50 (m, 1H, Ar-H), 7.43-7.46 (m, 1H Ar-H), 7.36 (s, 1H, Ar-H), 7.26 (d, *J* = 8.4 Hz, 1H, Ar-H), 6.90 (dd, *J* = 1.6, 8.5 Hz, 1H, Ar-H), 6.06 (d, *J* = 1.7 Hz, 1H, H-3'), 5.18 (d, *J* = 5.3 Hz, 2H, CH₂), 2.02-2.07 (m, 3H, Ad-H), 1.92-1.97 (m, 6H, Ad-H), 1.70-1.80 (m, 6H, Ad-H); ¹³C NMR (150 MHz, DMSO-d₆): δ 181.6 (C=S), 151.0 (C-2'), 134.5 (Ar-C), 134.4 (Ar-C), 133.3 (Ar-C), 129.4 (Ar-C), 128.7 (Ar-C), 128.2 (Ar-C), 125.8 (Ar-CH), 119.3 (Ar-CH), 119.2 (Ar-CH), 117.0 (Ar-CH), 116.7 (Ar-CH), 116.6 (Ar-CH), 111.9 (Ar-CH), 111.1 (Ar-CH), 110.9 (Ar-CH), 110.0 (Ar-CH), 95.7 (C-3'), 55.9 (C=SNH-CH₂), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): *m/z* [M+H]⁺ calculated for C₃₀H₃₂N₃S⁺, 466.2311, found 466.2310; [M+Na]⁺ calculated for C₃₀H₃₁N₃SNa⁺, 488.2131, found 488.2133.

1-(2-adamantane-1H-indol-5-yl)-3-(2-(pyridin-2-yl)ethyl)thiourea (9j): White solid; yield: 88.3%; mp: 224-227 °C; HPLC purity: 94.6% (*t_R* = 16.90 min); ¹H NMR (600 MHz, DMSO-d₆): δ 10.94 (br s, 1H, NH-1), 9.40 (br s, 1H, C=SNH-1), 8.33 (br s, 1H, C=SNH-3), 7.66-7.74 (m, 1H, Py-H), 7.36-7.44 (m, 1H, Py-H), 7.23-7.28 (m, 2H), 7.16-7.22 (m, 2H), 6.77 (d, *J* = 8.1 Hz, 1H, Ar-H), 6.07 (s, 1H, H-3'), 3.75-3.86 (m, 2H, Py-CH₂CH₂), 2.98 (t, *J* = 6.7 Hz, 2H, Py-CH₂CH₂), 2.04-2.09 (m, 3H, Ad-H), 1.93-1.99 (br s, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H); ¹³C NMR (150 MHz, DMSO-d₆): δ 180.8 (C=S), 159.8 (Py-C), 151.2 (C-2'), 149.3 (Py-C), 137.0 (Py-C), 134.6 (Ar-C), 129.4 (Ar-C), 128.5 (Ar-C), 123.7 (Py-C), 121.9 (Py-C), 119.0 (Ar-CH), 116.8 (Ar-CH), 111.5 (Ar-C), 95.8 (C-3'), 44.2 (Py-CH₂CH₂), 42.2 (Ad-C), 37.3 (Py-CH₂CH₂), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C);

ESI-HRMS (+): m/z $[M+H]^+$ calculated for $C_{26}H_{31}N_4S^+$, 431.2264, found 431.2264; $[M+Na]^+$ calculated for $C_{26}H_{30}N_4SNa^+$, 453.2083, found 453.2083.

1-(2-adamantane-1H-indol-5-yl)-3-(2-(thiophen-2-yl)ethyl)thiourea (9k): White solid; yield: 90.6%; mp: 234-235 °C; HPLC purity: 95.6% (t_R = 17.90 min); 1H NMR (600 MHz, DMSO- d_6): δ 10.93 (s, 1H, NH-1), 9.43 (br s, 1H, C=SNH-1), 7.34 (dd, J = 1.0, 5.0 Hz, 1H, thienyl-H), 7.29 (br s, 1H, C=SNH-3), 7.26 (d, J = 8.4, 1H, Ar-H), 7.21-7.24 (m, 1H, Ar-H), 6.96 (dd, J = 3.4, 5.0 Hz, 1H, thienyl-H), 6.87 (d, J = 2.6 Hz, 1H, thienyl-H), 6.80 (dd, J = 1.1, 8.4 Hz, 1H, Ar-H), 6.08 (d, J = 1.5 Hz, 1H, H-3'), 3.69 (q, J = 6.8 Hz, 2H, thienyl- CH_2CH_2), 3.06 (t, J = 7.2 Hz, 2H, thienyl- CH_2CH_2), 2.04-2.09 (m, 3H, Ad-H), 1.93-1.99 (m, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 181.0 (C=S), 151.2 (C-2'), 142.0 (thienyl-C), 134.6 (Ar-C), 129.4 (Ar-C), 128.5 (Ar-C), 127.4 (thienyl-C), 125.6 (thienyl-C), 124.4 (thienyl-C), 119.0 (Ar-CH), 116.8 (Ar-CH), 111.5 (Ar-CH), 95.8 (C-3'), 46.0 (thienyl- CH_2CH_2), 42.2 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 29.4 (thienyl- CH_2CH_2), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z $[M+H]^+$ calculated for $C_{25}H_{30}N_3S_2^+$, 436.1876, found 436.1874; $[M+Na]^+$ calculated for $C_{25}H_{29}N_3S_2Na^+$, 458.1695 found 458.1694.

1-(2,4-dimethylphenyl)-3-(2-adamantane-1H-indol-5-yl)thiourea (9l): White solid; yield: 88.6%; mp: 242-243 °C; HPLC purity: 95.6% (t_R = 20.12 min); 1H NMR (600 MHz, DMSO- d_6): δ 10.88 (br s, 1H, NH-1), 9.42 (br s, 1H, C=SNH-1), 8.77 (br s, 1H, C=SNH-3), 7.40 (s, 1H, Ar-H), 7.26 (d, J = 8.4 Hz, 1H, Ar-H), 7.10 (d, J = 7.9 Hz, 1H, Ar-H), 7.01 (s, 1H, Ar-H), 6.92-6.98 (m, 2H, Ar-H), 6.08 (s, 1H, H-3'), 2.25 (s, 3H, Ph- CH_3), 2.19 (s, 3H, Ph- CH_3), 2.03-2.08 (m, 3H, Ad-H), 1.92-1.98 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 181.2 (C=S), 151.0 (C-2'), 135.8 (Ar-C), 135.1 (Ar-C), 134.6 (Ar-C), 131.2 (Ar-C), 129.4 (Ar-C), 128.7 (Ar-CH), 128.6 (Ar-C), 128.3 (Ar-CH), 126.9 (Ar-CH), 119.2 (Ar-CH), 116.9 (Ar-CH), 111.2 (Ar-CH), 95.8 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C), 21.0 (Ph- CH_3), 18.3 (Ph- CH_3); ESI-HRMS (+): m/z $[M+H]^+$ calculated for $C_{27}H_{32}N_3S^+$, 430.2311, found 430.2310; $[M+Na]^+$ calculated for $C_{27}H_{31}N_3SNa^+$, 452.2131, found 452.2134.

1-(3,4-dimethoxyphenyl)-3-(1H-indol-2-adamantine-5-yl) thiourea (9m): White solid; yield: 87.6%; mp: 287-289 °C; HPLC purity: 95.1% (t_R = 16.78 min); 1H -NMR (600 MHz, DMSO- d_6): δ 10.70 (s, 1H, NH-1), 8.35 (s, 1H, C=SNH-1), 8.24 (s, 1H, C=SNH-3), 7.55 (d, J = 1.5 Hz, 1H, Ar-H), 7.24 (s, 1H, Ar-H), 7.19 (d, J = 8.6 Hz, 1H, Ar-H), 6.99 (dd, J = 1.9, 8.5 Hz, 1H, Ar-H), 6.86 (s, 2H, Ar-H), 6.02 (d, J = 1.6 Hz, 1H, H-3'), 3.75 (s, 3H, OCH_3), 3.71 (s, 3H, OCH_3), 2.03-2.08 (m, 3H, Ad-H), 1.92-1.98 (m, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 180.9 (C=S), 150.6 (C-2'), 149.3 (Ar-C), 144.2 (Ar-C), 134.4 (Ar-C), 132.7 (Ar-C), 131.6 (Ar-C), 128.4 (Ar-C), 114.1 (Ar-CH), 113.1 (Ar-CH), 110.8 (Ar-CH), 110.3 (Ar-CH), 110.0 (Ar-CH), 104.2 (Ar-CH), 95.4 (C-3'), 56.4 (OCH_3), 55.8 (OCH_3), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); HRMS(+): m/z $[M+H]^+$ calculated for $C_{27}H_{32}N_3O_2S^+$, 462.2210, found 462.223; $[M+Na]^+$ calculated for $C_{27}H_{31}N_3O_2SNa^+$, 484.2029, found 484.2027.

1-(4-cyanophenyl)-3-(2-adamantane-1H-indol-5-yl)thiourea thiourea (9n): White solid; yield: 84.2%; mp: 245-247 °C; HPLC purity: 95.6% ($t_R = 17.90$ min); ^1H NMR (600MHz, DMSO- d_6): δ 10.75 (s, 1H, NH-1), 9.07 (s, 1H, C=SNH-1), 8.54 (s, 1H, C=SNH-3), 7.68-7.73 (m, 2H, Ar-H), 7.64 (d, $J = 8.8$ Hz, 2H, Ar-H), 7.56 (s, 1H, Ar-H), 7.22 (d, $J = 8.6$ Hz, 1H, Ar-H), 7.02 (dd, $J = 1.8, 8.6$ Hz, 1H, Ar-H), 6.03 (d, $J = 1.5$ Hz, 1H, H-3'), 2.02-2.08 (m, 3H, Ad-H), 1.92-1.98 (m, 6H, Ad-H), 1.72-1.80 (m, 6H, Ad-H); ^{13}C NMR (150 MHz, DMSO- d_6): δ 181.2 (C=S), 150.8 (C-2'), 145.2 (Ar-C), 133.7 (Ar-C), 133.1 (Ar-C), 130.8 (Ar-C), 128.3 (Ar-C), 119.9 (Ar-CH), 118.2 (Ar-CH), 114.3 (Ar-CH), 111.1 (Ar-CH), 110.6 (Ar-CH), 95.4 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C); ESI-HRMS (+): m/z [M+H] $^+$ calculated for $\text{C}_{26}\text{H}_{27}\text{N}_4\text{S}^+$, 427.1951, found 427.1950; [M+Na] $^+$ calculated for $\text{C}_{26}\text{H}_{26}\text{N}_4\text{SNa}^+$, 449.1770, found 449.1771.

1-(4-chloro-2-methylphenyl)-3-(1H-indol-2-adamantine-5-yl)thiourea (9o): White solid; yield: 85.6%; mp: 280-282 °C; HPLC purity: 97.1% ($t_R = 17.90$ min); ^1H -NMR (600 MHz, DMSO- d_6): δ 10.82 (d, $J = 1.3$ Hz, 1H, NH-1), 8.74 (s, 1H, C=SNH-1), 7.95 (d, $J = 8.6$ Hz, 1H, Ar-H), 7.85 (s, 1H, C=SNH-3), 7.58 (d, $J = 2.0$ Hz, 1H, Ar-H), 7.24 (d, $J = 2.4$ Hz, 1H, Ar-H), 7.21 (d, $J = 8.4$ Hz, 1H, Ar-H), 7.18 (dd, $J = 2.4, 8.7$ Hz, 1H, Ar-H), 7.01 (dd, $J = 2.0, 8.4$ Hz, 1H, Ar-H), 6.02 (d, $J = 1.7$ Hz, 1H, H-3'), 2.25 (s, 3H, Ph- CH_3), 2.02-2.08 (m, 3H, Ad-H), 1.92-1.98 (m, 6H, Ad-H), 1.72-1.79 (m, 6H, Ad-H). ^{13}C -NMR (150 MHz, DMSO- d_6): δ 181.1 (C=S), 150.7 (C-2'), 137.5 (Ar-C), 132.8 (Ar-C), 131.5 (Ar-C), 130.0 (Ar-C), 129.5 (Ar-CH), 128.4 (Ar-C), 126.3 (Ar-C), 125.9 (Ar-CH), 122.1 (Ar-CH), 114.0 (Ar-CH), 111.1 (Ar-CH), 110.0 (Ar-CH), 95.4 (C-3'), 42.3 (Ad-C), 36.8 (s, 3C, Ad-C), 33.9 (s, 3C, Ad-C), 28.4 (s, 3C, Ad-C), 18.1 (Ph- CH_3). ESI-HRMS (+): m/z [M+H] $^+$ calculated $\text{C}_{26}\text{H}_{29}\text{ClN}_3\text{S}^+$, 450.1765, found 450.1766; [M+Na] $^+$ calculated for $\text{C}_{26}\text{H}_{28}\text{ClN}_3\text{SNa}^+$, 472.1585, found 472.1587.