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SUPPLEMENTARY MATERIAL TO

Synthesis of new derivatives of hydrazinecarbothioamides and 1,2,4-triazoles and evaluation of their antimicrobial activity

LAURA I. SOCEA[1]*, GABRIEL SARAMET[2], CONSTANTIN DRAGHICI[3], BOGDAN SOCEA[4], VLAD D. CONSTANTIN[4] and MANUELA A. RADU-POPESCU[5]

[1]Organic Chemistry Department, Faculty of Pharmacy, "Carol Davila" University of Medicine and Pharmacy, 6 Traian Vuia Street, 020956, Bucharest, Romania, [2]Pharmaceutical Technology Department, Faculty of Pharmacy, "Carol Davila" University of Medicine and Pharmacy, 6 Traian Vuia, 020956 Bucharest, Romania, [3]"C. D. Nenitzescu" Institute of Organic Chemistry, Romanian Academy, 202B Splaiul Independentei, 060023 Bucharest, Romania, [4]Faculty of General Medicine, "Carol Davila" University of Medicine and Pharmacy, St. Pantelimon Emergency Hospital, 340–342, Soseaua Pantelimon Street, 021623, Bucharest, Romania and [5]General and Pharmaceutical Microbiology Department, Faculty of Pharmacy, "Carol Davila" University of Medicine and Pharmacy, 6 Traian Vuia Street, 020956, Bucharest, Romania

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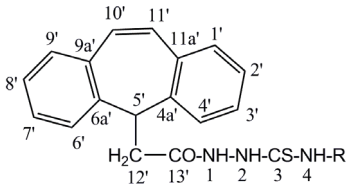
PHYSICAL, ANALYTICAL AND SPECTRAL DATA FOR THE SYNTHESIZED COMPOUNDS



Scheme S-1. Atom numbering of the general structure for **6**–**9**.

N-*(4-Chlorophenyl)-2-(5*H-*dibenzo[*a,d*][7]annulen-5-ylacetyl)hydrazinecarbothioamide (**6**).* Yield: 78.6 %; m.p.: 172–173 °C; Anal. calcd. for $C_{24}H_{20}ClN_3OS$ (FW: 433.95): C, 66.43; H, 4.65; N, 9.68 %. Found: C, 66.40; H, 4.66; N, 9.70 %; IR (KBr, cm^{-1}): 3321, 3147 (N–H stretching), 3065, 3017 (C–H stretching of aromatic ring), 2976, 2851 (CH_2 stretching), 1682 (C=O stretching), 1605, 1595, 1522, 1492, 1253 (C=S stretching), 765 (C–Cl); ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 9.80 (2H, *s*, NH), 9.68 (1H, *s*, NH), 7.50–7.20 (12H, *m*, Ar-H), 7.03 (2H, *s*, H10′, H11′), 4.66 (1H, *t*, J = 7.1 Hz, H5′) axial isomer, 3.76 (1H, *t*, J = 7.1 Hz, H5′) equatorial isomer, 2.62 (2H, *d*, J = 7.1 Hz, H12′)

* Corresponding author. E-mail: laurasocea@gmail.com

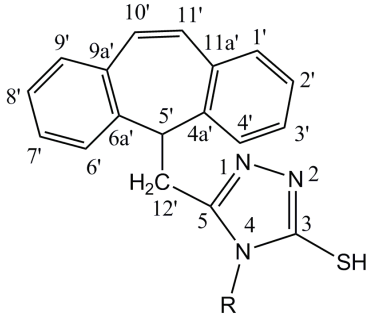
axial isomer; ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 180.78 (C=S), 170.08 (C=O), 140.05 (2C_q), 139.55 (C_q), 138.87 (C_q), 137.99 (C_q), 133.76 (C_q), 131.27 (C10′, C11′) equatorial isomer, 130.98 (CH), 130.81 (C10′, C11′) axial isomer, 129.63 (CH), 129.52 (CH), 128.76 (CH), 128.51 (CH) equatorial isomer, 127.97 (CH), 127.58 (CH) equatorial isomer, 126.51 (CH), 125.51 (CH) equatorial isomer, 48.60 (C5′), 34.61 (C12′) axial isomer, 33.21 (C12′) equatorial isomer; UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / L·mol^{-1}·cm^{-1}))): 206.2 (4.51), 224.7 (4.40), 279.3 (4.22).

N-*(4-Bromophenyl)-2-(5*H-*dibenzo[*a,d*][7]annulen-5-ylacetyl)hydrazinecarbothioamide (**7**)*. Yield: 83.1 %; m.p.: 197–198 °C; Anal. Calcd. for $C_{24}H_{20}BrN_3OS$ (FW: 478.40): C, 60.25; H, 4.21; N, 8.78 %. Found: C, 60.26; H, 4.22; 8.78 %; IR (KBr, cm^{-1}): 3342, 3340, 3141 (N–H stretching), 3052, 3019 (C–H stretching of aromatic ring), 2970, 2873 (CH_2 stretching), 1673 (C=O stretching), 1586, 1531, 1488, 1257 (C=S stretching), 621 (C–Br); ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 9.72 (2H, *s*, NH), 9.53 (1H, *s*, NH), 7.50 (2H, *d*, *J* = = 8.6 Hz, H-bromophenyl), 7.45–7.20 (10H, *m*, Ar-H), 7.03 (2H, *s*, H10′, H11′), 4.65 (1H, *t*, *J* = 7.3 Hz, H5′) axial isomer, 3.80 (2H, *d*, *J* = 7.1 Hz, H12′) equatorial isomer, 3.75 (1H, *t*, *J* = 7.3 Hz, H5′) equatorial isomer, 2.61 (2H, *d*, *J*=7.1 Hz, H12′) axial isomer; ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 180.73 (C=S), 170.03 (C=O), 140.05 (C_q), 139.55 (C_q), 138.43 (C_q), 133.74 (C_q), 131.27 (C10′, C11′) equatorial isomer, 130.89 (C10′, C11′) axial isomer, 130.87 (CH), 130.80 (CH), 129.62 (CH), 129.52 (CH), 128.51 (CH) equatorial isomer, 127.57 (CH), equatorial isomer, 126.50 (CH), 125.51 (CH) equatorial isomer, 122.55 (CH) equatorial isomer, 117.22 (C–Br), 48.57 (C5′), 34.59 (C12′) axial isomer, 33.19 (C12′) equatorial isomer; UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / L·mol^{-1}·cm^{-1}))): 204.4 (4.35), 226.4 (4.20), 281.9 (4.20).

*2-(5*H-*Dibenzo[*a,d*][7]annulen-5-ylacetyl)*-N-*(4-iodophenyl)hydrazinecarbothioamide (**8**)*. Yield: 69.5 %; m.p.: 194–195 °C; Anal. Calcd. for $C_{24}H_{20}IN_3OS$ (FW: 525.40): C, 54.86; H, 3.84; N, 8.00 %. Found: C, 54.88; H, 3.84; N, 8.02 %; IR (KBr, cm^{-1}): 3339, 3304, 3141 (N–H stretching), 3051, 3015 (C–H stretching of aromatic ring), 2969, 2874 (CH_2 stretching), 1674 (C=O stretching), 1582, 1530, 1510, 1486, 1258 (C=S stretching); 516 (C–I); ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 9.72 (2H, *s*, NH), 9.52 (H, *s*, NH), 7.66 (2H, *d*, *J* = 8.6 Hz, H-iodophenyl), 7.50–7.20 (10H, *m*, aromatic), 7.03 (2H, *s*, H10′, H11′), 4.65 (1H, *t*, *J* = 7.3 Hz, H5′) axial isomer, 3.75 (1H, *t*, *J* = 7.3 Hz, H5′) equatorial isomer, 2.60 (2H, *d*, *J* = 7.3 Hz, H12′); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 180.75 (C=S), 170.11 (C=O), 140.05 (C_q), 139.54 (C_q), 138.43 (C_q), 136.77 (C_q) 134.86 (C_q), 133.74 (C_q), 131.27 (C10′,C11′) equatorial isomer, 130.84 (C10′,C11′) axial isomer, 129.62 (CH), 129.52 (CH), 128.76 (CH), 128.54 (CH) equatorial isomer, 127.58 (CH) equatorial isomer, 126.50 (CH), 125.51 (CH) equatorial isomer, 122.95 (CH) equatorial isomer, 89.55

(C–I), 49.59 (C5′), 34.60 (C12′); UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / L·mol^{-1}·cm^{-1}))): 207.0 (4.54), 223.8 (4.46), 283.7 (4.30).

*2-(5*H*-Dibenzo[*a,d*][7]annulen-5-ylacetyl)-*N*-(2-phenylethyl)hydrazinecarbothioamide* (***9***). Yield: 74.6 %; m.p.: 183–185 °C; Anal. Calcd. for $C_{26}H_{25}N_3OS$ (FW: 427.56): C, 73.04; H, 5.89; N, 9.83 %. Found: C, 73.04; H, 5.87; N, 9.81 %; IR (KBr, cm^{-1}): 3359, 3304, 3232 (N–H stretching), 3062, 3023 (C–H stretching of aromatic ring), 2969, 2862 (CH_2 stretching), 1699 (C=O stretching), 1562, 1542, 1493, 1249 (C=S stretching); ^{1}H-NMR (300 MHz, DMSO-d_6, δ / ppm): 10.12 (H, *s*, NH) equatorial isomer, 9.52 (H, *s*, NH) axial isomer, 9.36 (H, *s*, NH) equatorial isomer, 9.15 (H, *s*, NH) axial isomer, 7.40––7.10 (13H, *m*, Ar-H), 7.02 (2H, *s*, H10′, H11′), 4.62 (1H, *t*, *J* = 7.1 Hz, H5′) axial isomer, 3.74 (1H, *t*, *J* = 7.1 Hz, H5′) equatorial isomer, 3.53 (2H, *m*, NH–CH_2), 2.72 (2H, *t*, *J* = 8.2 Hz, C**H**$_2$–C_6H_5), 2.55 (2H, *d*, *J* = 7.1 Hz, H12′); ^{13}C-NMR (75 MHz, DMSO-d_6, δ / ppm): 181.16 (C=S), 170.03 (C=O), 140.25 (C_q) equatorial isomer, 139.85 (C_q), 139.47 (C_q), 139.10 (C_q), 133.75 (C_q), 131.25 (C10′, C11′) equatorial isomer, 130.77 (C10′, C11′) axial isomer, 129.57 (CH), 129.52 (CH), 128.76 (CH), 128.63 (CH), 127.58 (CH), 127.60 (CH), 127.42 (CH), 126.53 (CH), 126.15 (CH), 125.52 (CH) equatorial isomer, 48.73 (C5′), 45.10 (CH_2–NH), 34.84 (**C**H_2–C_6H_5), 34.43 (C12′); UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / L·mol^{-1}·cm^{-1}))): 205.3 (4.50), 222.9 (4.46), 285.5 (4.04).



Scheme S-2. The general structure of **10–13** with atom numbering.

*4-(4-Chlorophenyl)-5-(5*H*-dibenzo[*a,d*][7]annulen-5-ylmethyl)-4*H*-1,2,4-triazole-3-thiol* (***10***). Yield: 78.6 %; m.p.: 177–179 °C; Anal. Calcd. for $C_{24}H_{18}ClN_3S$ (FW: 415.93): C, 69.30; H, 4.36; N, 10.10 %. Found: C, 69.28; H, 4.38; N, 10.10 %; IR (KBr, cm^{-1}): 3383 (N–H stretching), 3066, 3020 (C–H stretching of aromatic ring), 2929, 2845 (CH_2 stretching), 1566, 1495, 1458, 1231 (C=S stretching), 768 (C–Cl); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 11.90 (1H, *s*, SH), 7.43 (2H, *d*, *J* = 8.5 Hz, H-chlorophenyl), 7.35–7.10 (8H, *m*, Ar-H), 6.83 (2H, *s*, H10′, H11′), 6.77 (2H, *d*, *J* = 8.5 Hz, H-chlorophenyl), 4.41 (1H, *t*, *J* = 7.9 Hz, H5′), 2.98 (2H, *d*, *J* = 7.9 Hz, H12′); ^{13}C-NMR (75 MHz, $CDCl_3$,

δ / ppm): 167.97 (triazole-C3), 151.54 (triazole-C5), 138.48 ($2C_q$), 136.02 (C_q), 133.91 (C_q), 131.54 (C–Cl), 130.77 (C10′, C11′), 130.14 (CH), 129.92 (CH), 129.56 (CH), 129.28 (CH), 53.20 (C5′), 26.13 (C12′); UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / L·mol^{-1}·cm^{-1}))): 207.0 (4.53), 222.9 (4.47), 277.5 (4.21).

*4-(4-Bromophenyl)-5-(5*H*-dibenzo[*a,d*][7]annulen-5-ylmethyl)-4*H*-1,2,4-triazole-3-thiol (**11**)*. Yield: 90.0% m.p.: 133–135°C; Anal. Calcd. for $C_{24}H_{18}BrN_3S$ (FW: 460.38 g/mol): C, 62.61; H, 3.94; N, 9.13; Found: C, 62.61; H, 3.92; N, 9.16; IR (KBr, cm^{-1}): 33392 (N–H stretching), 3066, 3020 (C–H stretching of aromatic ring), 2930, 2845 (CH_2 stretching), 1561, 1491, 1435, 1231 (C=S stretching), 570 (C–Br); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 11.82 (1H, *s*, SH), 7.59 (2H, *d*, *J* = 8.3 Hz, H-bromophenyl), 7.30–7.05 (8H, *m*, Ar-H), 6.71 (2H, *d*, *J* = 8.3 Hz, H-bromophenyl), 6.62 (2H, *s*, H10′, H11′) 4.41 (1H, *t*, *J* = 7.9 Hz, H5′), 2.98 (2H, *d*, *J* = 7.9 Hz, H12′); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 168.00 (triazole-C3), 151.51 (triazole-C5), 138.47 (C_q), 133.91 (C_q), 132.06 (Cq), 130.78 (C10′, C11′), 130.15 (CH), 129.81 (CH), 129.56 (CH), 129.28 (CH), 124.11 (C–Cl), 53.21 (C5′), 26.13 (C12′); UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / L·mol^{-1}·cm^{-1}))): 202.6 (4.42), 222.3 (4.33), 283.7 (3.87).

*5-(5*H*-Dibenzo[*a,d*][7]annulen-5-ylmethyl)-4-(4-iodophenyl)-4*H*-1,2,4-triazole-3-thiol (**12**)*. Yield: 74.5 %; m.p.: 200–202 °C; Anal. Calcd. for $C_{24}H_{18}IN_3S$ (FW: 507.39): C, 56.81; H, 3.58; N, 8.26 %. Found: C, 56.81; H, 3.57; N, 8.28 %; IR (KBr, cm^{-1}): 3371 (N–H stretching), 3062, 3019 (C–H stretching of aromatic ring), 2928, 2840 (CH_2 stretching), 1578, 1563, 1491, 1459, 1228 (C=S stretching), 571 (C–I); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 11.58 (1H, *s*, SH), 7.75 (2H, *d*, *J* = 8.6 Hz, H-iodophenyl), 7.25–7.05 (8H, *m*, Ar-H), 6.59 (2H, *s*, H10′, H11′), 6.54 (2H, *d*, *J* = 8.6 Hz, H-iodophenyl), 4.35 (1H, *t*, *J* = 7.9 Hz, H5′), 2.93 (2H, *d*, *J* = 7.9 Hz, H12′); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 168.08 (triazole-C3), 151.50 (triazole-C5), 133.92 (C_q), 132.80 (C_q), 130.95 (CH), 130.80 (C10′, C11′), 130.47 (C_q), 130.18 (CH), 129.93 (CH), 129.62 (CH), 129.29 (CH), 95.77 (C–I), 53.20 (C5′), 26.16 (C12′); UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / L·mol^{-1}·cm^{-1}))): 206.2 (4.53), 229.1 (4.44), 278.4 (4.21).

*5-(5*H*-Dibenzo[*a,d*][7]annulen-5-ylmethyl)-4-(2-phenylethyl)-4*H*-1,2,4-triazole-3-thiol (**13**)*. Yield: 77.0 %; m.p.: 107–109 °C; Anal. Calcd. for $C_{26}H_{23}N_3S$ (FW: 409.54): C, 76.25; H, 5.66; N, 10.26 %. Found: C, 76.26; H, 5.65; N, 10.26 %; IR (KBr, cm^{-1}): 3401 (N–H stretching), 3064, 3025 (C–H stretching of aromatic ring), 2945, 2861 (CH_2 stretching), 1566, 1493, 1454, 1277 (C=S stretching); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 11.44 (1H, *s*, SH), 7.35–7.10 (11H, *m*, Ar-H), 7.06 (2H, *d*, *J* = 6.8 Hz, arom. H-phenylethyl), 6.99 (2H, *s*, H10′, H11′), 4.45 (1H, *t*, *J* = 7.5 Hz, H5′), 3.73 (2H, *t*, *J* = 7.0 Hz, CH_2–N4––triazole), 2.80 (2H, *t*, *J* = 7.0 Hz, CH_2-phenyl), 2.67 (2H, *d*, *J* = 7.5 Hz, H12′); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 166.57 (triazole-C3), 151.70 (triazole-C5),

138.48 (C_q), 137.80 (C_q), 131.11 (C10′, C11′), 130.10 (CH), 129.98 (CH), 129.86 (CH), 129.41 (CH), 127.34 (CH), 127.15 (CH), 52.81 (C5′), 45.21 (CH_2––N4-triazole), 34.12 (CH_2--phenyl), 26.13 (C12′); UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / L·mol^{-1}·cm^{-1}))): 207.0 (4.54), 225.6 (4.37), 256.4 (4.25), 287.2 (4.12).

*4-(4-Chlorophenyl)-3-(5*H*-dibenzo[*a,d*][7]annulen-5-ylmethyl)-5-(methylsulfanyl)- 4*H*-1,2,4-triazole (**14**)*. Yield: 69.1 %; m.p.: 81–83 °C; Anal. Calcd. for $C_{25}H_{20}ClN_3S$ (FW: 429.96): C, 69.84; H, 4.69; N, 9.77 %. Found: C, 69.82; H, 4.70; N, 9.77 %; IR (KBr, cm^{-1}): 3056, 3017 (aromatic C–H), 2983, 2928 (CH_2 + CH_3 stretching), 1493, 1448, 1432, 768 (C–Cl), 727 (C–S–C); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 7.36 (2H, *d*, *J* = 8.7 Hz, H-chlorophenyl), 7.30–7.05 (8H, *m*, Ar-H), 6.53 (2H, *s*, H10′, H11′), 6.51 (2H, *d*, *J* = 8.7 Hz, H-chlorophenyl), 4.62 (1H, *t*, *J* = 7.9 Hz, H5′), 3.09 (2H, *d*, *J* = 7.9 Hz, H12′), 2.57 (3H, *s*, CH_3–S); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 154.94 (triazole-C3), 151.43 (triazole-C5), 139.32 (C_q), 135.80 (C_q), 133.97 (C_q), 130.73 (C10′, C11′), 130.01 (CH), 129.95 (CH), 129.86 (CH), 129.15 (CH), 128.64 (CH), 126.94 (CH); 54.26 (C5′), 25.30 (C12′), 14.80 (CH_3–S); UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / L mol^{-1}·cm^{-1}))): 207.9 (4.53), 220.0 (4.48), 287.2 (4.11).

*4-(4-Bromophenyl)-3-(5*H*-dibenzo[*a,d*][7]annulen-5-ylmethyl)-5-(methylsulfanyl)- 4*H*-1,2,4-triazole (**15**)*. Yield: 66.2 %; m.p.: 128–130 °C; Anal. Calcd. for $C_{25}H_{20}BrN_3S$ (FW: 474.41): C, 63.29; H, 4.25; N, 8.86 %. Found: C, 63.28; H, 4.27; N, 8.85 %; IR (KBr, cm^{-1}): 3041, 3015 (aromatic C–H), 2970, 2926, 2854 (CH_2 + CH_3 stretching), 1509, 1489, 1455, 768 (C–S–C), 563 (C–Br); ^{1}H--NMR (300 MHz, $CDCl_3$, δ / ppm): 7.69 (2H, *d*, *J* = 8.8 Hz, H-bromophenyl) equatorial isomer, 7.52 (2H, *d*, *J* = 8.8 Hz, H-bromophenyl) equatorial isomer, 7.50 (2H, *d*, *J* = 8.8 Hz, H-bromophenyl) axial isomer, 7.32–7.12 (H, *m*, Ar-H), 6.96 (2H, *m*, Ar-H), 6.73 (2H, *s*, H10′, H11′) axial isomer, 6.54 (2H, *s*, H10′, H11′) equatorial isomer, 6.46 (2H, *d*, *J* = 8.8 Hz, H-bromophenyl) axial isomer, 4.62 (1H, *t*, *J* = 7.7 Hz, H5′) axial isomer, 4.08 (1H, *t*, *J* = 7.7 Hz, H5′) equatorial isomer, 3.65 (2H, *d*, *J* = 7.7 Hz, H12′) equatorial isomer, 3.06 (2H, *d*, *J* = 7.7 Hz, H12′) axial isomer, 2.62 (3H, *s*, CH_3–S), 2.57 (3H, *s*, CH_3–S); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 155.11 (triazole-C3), 154.54 (triazole-C5), 139.22 (C_q), 136.73 (C_q), 133.89 (C_q), 133.74 (CH), 132.80 (CH), 130.94 (C10′, C11′), 130.71 (CH), 130.65 (CH), 129.62 (CH), 129.14 (CH), 129.06 (CH), 128.81 (CH), 128.55 (CH), 128.07 (CH), 127.89 (CH), 126.56 (C_q), 123.71 (C_q), 54.19 (C5′) axial isomer, 52.34 (C5′) equatorial isomer, 27.35 (C12′) equatorial isomer, 25.21 (C12′) axial isomer, 14.88 (CH_3–S) equatorial isomer, 14.74 (CH_3–S) axial isomer; UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / L·mol^{-1}·cm^{-1}))): 207.9 (4.55), 222.9 (4.52), 287.2 (4.11).

*3-(5*H*-Dibenzo[*a,d*][7]annulen-5-ylmethyl)-4-(4-iodophenyl)-5-(methylsulfanyl)-4*H*-1,2,4-triazole (**16**)*. Yield: 69.3 %; m.p.: 99–101 °C; Anal. Calcd. for

$C_{25}H_{20}IN_3S$ (FW: 521.41): C, 57.59; H, 3.87; N, 8.06 %. Found: C, 57.57; H, 3.89; N, 8.05 %; IR (KBr, cm^{-1}): 3058, 3016 (aromatic C–H), 2927, 2852 (CH_2 + CH_3 stretching), 1489, 1447, 1431, 768 (C–S–C), 564 (C–I); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 7.71 (2H, *d*, *J* = 8.4 Hz, CH-iodophenyl), 7.35–7.10 (8H, *m*, Ar-H), 6.53 (2H, *s*, H10′, H11′), 6.31 (2H, *d*, 8.4, H-iodophenyl), 4.61 (1H, *t*, *J* = 7.7 Hz, H5′), 3.06 (2H, *d*, *J* = 7.7 Hz, H12′), 2.57 (3H, *s*, CH_3–S); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 154.82 (triazole-C3), 151.28 (triazole-C5), 139.21 (C_q), 138.85 (C_q), 133.90 (C_q), 132.50 (C_q), 130.69 (C10′, C11′), 129.24 (CH), 129.11 (CH), 128.96 (CH), 126.90 (CH); 95.24 (C–I), 54.21 (C5′), 25.18 (C12′), 14.79 (CH_3–S); UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / $L\cdot mol^{-1}$ cm^{-1}))): 207.0 (4.56), 229.1 (4.24), 289.0 (4.11).

*3-(5*H*-Dibenzo[*a,d*][7]annulen-5-ylmethyl)-5-(methylsulfanyl)-4-(2-phenyl-ethyl)-4*H*-1,2,4-triazole (**17**)*. Yield: 67.6 %; m.p.: 100–102 °C; Anal. Calcd. for $C_{27}H_{25}N_3S$ (FW: 423.57): C, 76.56; H, 5.97; N, 9.92 %. Found: C, 76.56; H, 5.95; N, 9.93 %; IR (KBr, cm^{-1}): 3061, 3021 (aromatic C–H), 2929, 2854 (CH_2 & CH_3 stretching), 1515, 1495, 1466, 768 (C–S–C); ^{1}H-NMR (300 MHz, $CDCl_3$, δ / ppm): 7.25–7.10 (11H, *m*, Ar-H), 6.91 (2H, *s*, H10′, H11′), 6.81 (2H, *dd*, *J* = 1.6 and 7.7 Hz, arom. H-phenylethyl), 4.60 (1H, *t*, *J* = 7.7 Hz, H5′), 3.36 (2H, *t*, *J* = 7.4 Hz, CH_2–N4-triazole), 2.80 (2H, *d*, *J* = 7.7 Hz, C12′), 2.50 (2H, *t*, *J* = 7.4 Hz C**H**$_2$–C_6H_5), 2.48 (3H, *s*, S–CH_3); ^{13}C-NMR (75 MHz, $CDCl_3$, δ / ppm): 154.58 (triazole-C3), 150.34 (triazole-C5), 139.60 (C_q), 136.77 (C_q), 133.92 (C_q), 131.12 (C10′, C11′), 130.30 (CH), 129.91 (CH), 129.31 (CH), 128.87 (CH); 128.77 (CH), 127.22 (CH), 53.80 (C5′), 44.49 (CH_2–N4-triazole), 36.02 (CH_2–C_6H_5), 25.82 (C12′), 15.62 (CH_3–S); UV–Vis (CH_3OH, 2.5×10^{-5} M, λ_{max} / nm (log (ε / $L\cdot mol^{-1}\cdot cm^{-1}$))): 207.0 (4.34), 230.0 (4.15), 292.5 (3.79).