New Thioureides of the 2-phenetylbenzoic Acid with Potential Antimicrobial Activity. III

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We report here a continuation of our research on the synthesis and characterization of some new thioureides of the 2-phenethylbenzoic acid. These new compounds were synthesized by the addition of various primary aromatic amines to the 2-phenethylbenzoyl isothiocyanate. We established the necessary reaction conditions in order to obtain the best yields and high purity compounds. The ^{1}H-NMR, ^{13}C- NMR and IR spectra and the elemental analysis confirmed the chemical structure and the purity of the new compounds.

Keywords: Thioureides, thiourea derivatives, 2-phenethylbenzoic acid derivatives

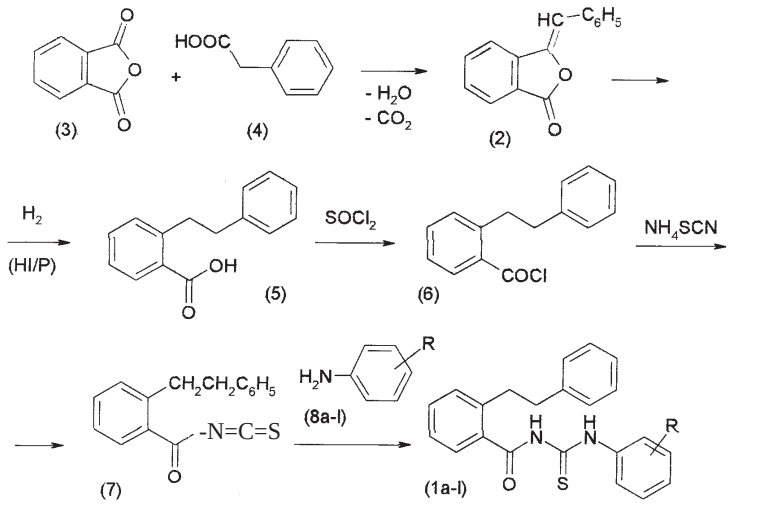
The specialized literature [1-3] mentions many compounds with a thioureide moiety as having antimicrobial activity as well as other therapeutical properties (diuretic, antidiabetic, tuberculostatic, sedative, antidepressant). In this paper we present the continuation of our research concerning the thioureides class [4-11], focusing on the 2-phenethylbenzoic acid thioureides, in order to extend the number of compounds with potential antimicrobial activity.

Experimental part

The new thioureides (1a-l) were obtained by a four stages process. According to [12] 3-benzylidenephtalide (2) was obtained by the condensation of the phthalic anhydride (3) with phenylacetic acid (4) followed by decarboxylation. The reduction of 3-benzylidenephtalide with hydroiodic acid and red phosphorous by the method presented by [13] leads to 2-phenethylbenzoic acid (5), transformed afterwards in the corresponding acid chloride (6) by heating it with thionyl chloride. By condensation of the 2-phenethylbenzoyl chloride with ammonium thiocyanate in anhydrous acetone we obtained 2-phenethylbenzoyl isothiocyanate (7). This is consequentially used without separation from the reaction medium. The new compounds were synthesized by the addition of various primary aromatic amines (8a-l) to the aforementioned isothiocyanate (fig.1).

General synthesis method for the new thioureides of the 2-phenethylbenzoic acid (1a-l)

In a round-bottom flask equipped with a reflux condenser 2.45 g (0.01 mol) of 2-phenethylbenzoyl chloride are dissolved in 15 mL of anhydrous acetone, adding subsequently 0.76 g (0.01 mol) of ammonium thiocyanate in advance dried by heating at 100°C. The reaction mixture is heated to reflux for one hour. After cooling at room temperature 0.01 mol of the corresponding aromatic amine (8a-l) are added and the mixture is refluxed for another hour. The desired products are separated by pourring the mixture in 500 mL of ice and water and subsequent filtration. The obtained thioureides are purified by recristalization from isopropanol.



1a, 8a : R= 2-OCH_3 1d, 8d : R= 2-OC_2H_5 1g, 8g : R= 2-NO_2 1j, 8j : R= 2-CH_3, 5-NO_2
1b, 8b : R= 3-OCH_3 1e, 8e : R= 3-OC_2H_5 1h, 8h : R= 3-NO_2 1k, 8k : R= 3-NO_2, 4-CH_3
1c, 8c : R= 4-OCH_3 1f, 8f : R= 4-OC_2H_5 1i, 8i : R= 4-NO_2 1l, 8l : R= 2-OC_2H_5, 5-NO_2

Fig. 1. The synthesis of the new thioureides

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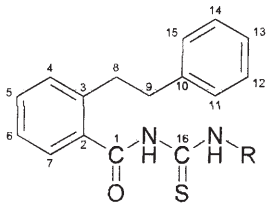


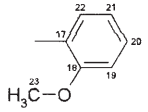
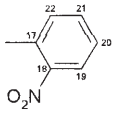
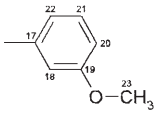
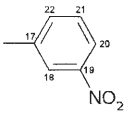
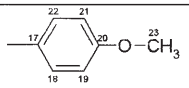
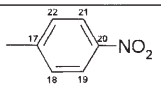
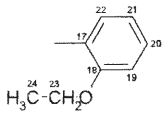
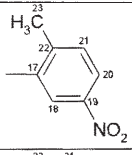
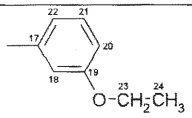
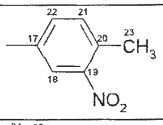
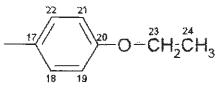
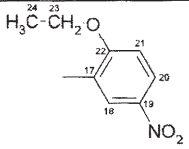
Compound	R	Compound	R
1a		1g	
1b		1h	
1c		1i	
1d		1j	
1e		1k	
1f		1l	

Table 1
THE NOTATIONS USED FOR THE CHEMICAL SHIFTS ASSIGNMENT

Analytic tests

The melting points were recorded with an Electrothermal 9100 apparatus and are uncorrected. The elemental analysis was performed on a Perkin Elmer CHNS/O Series II 2400 Analyser and the IR spectra were performed using a Brucker Vertex 70 apparatus. The ^{1}H-NMR spectra were obtained at 300 MHz and the ^{13}C-NMR spectra were recorded at 75.076 MHz using a Varian Gemini 300 BB apparatus. We used DMSO-d6 as solvent and tetramethylsilane as internal standard. For the protons chemical shifts assignment we used the notations mentioned in the table 1.

Results and discussions

We obtained other twelve new thioureides of the 2-phenethylbenzoic acid. The elemental analysis and the IR and NMR spectroscopy confirmed the molecular structures of the new compounds and their purity. The obtained thioureides will be further investigated to determinate their antimicrobial activity.

N-(2-Phenetyl-benzoyl)-N'-(2-methoxyphenyl)-thiourea (1a)

White crystals, m.p. 97-98°C (isopropanol), yield 65%, $C_{23}H_{22}N_2OS$.

^{1}H-NMR(dmso-d6, δ ppm, J Hz): 12.96(bs, 1H, NH); 11.90(bs, 1H, NH); 8.64(d, 1H, H-22, 7.6); 7.53(dd, 1H, H-7, 1.3, 7.5); 7.46(td, 1H, H-13, 7.6, 1.4); 7.37÷7.16(m, 8H, H-arom); 7.14(dd, 1H, H-19, 1.4, 8.3); 7.01(td, 1H, H-21, 8.3, 1.4); 3.89(s, 3H, H-23); 3.03(m, 2H, H-8, syst. A_2B_2); 2.87(m, 2H, H-9, syst. A_2B_2).

^{13}C-NMR(dmso-d6, δ ppm): 177.80(C-16); 170.84(C-1); 150.53(C-18); 141.47(Cq); 139.89(Cq); 133.90(Cq); 126.98(Cq); 130.93(CH); 129.97(CH); 128.31(C-12-14); 128.29(C-11-15); 128.21(CH); 126.60(CH); 125.98(CH); 125.90(CH); 123.02(CH); 119.85(CH); 111.39(CH); 56.11(C-23); 37.38(C-8); 35.40(C-9).

FT-IR(ATR in solid, ν cm^{-1}): 3407w; 3308m; 3171w; 3055m; 3019m; 2966w; 1664m 1598m; 1527vs; 1486vs; 1456vs; 1344s; 1315m; 1287m; 1238s; 1175m; 1140vs; 1071w; 1024m; 946w; 859w; 748s; 698m; 671m; 640w; 607w; 558w; 524w; 435w.

Calculated: C 70.74; H 5.68; N 7.17; S 8.21, Experimental: C 71.00; H 5.81; N 7.03; S 8.09.

N-(2-Phenetyl-benzoyl)-N'-(3-methoxyphenyl)-thiourea (1b)

White crystals, m.p. 101-102°C (isopropanol), yield 70%, $C_{23}H_{22}N_2OS$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 12.40(bs, 2H, NH); 7.53(dd, 1H, H-7, 1.3, 7.5); 7.46(td, 1H, H-13, 7.6, 1.4); 7.37÷7.13(m, 10H, H-arom); 6.85(ddd, 1H, H-20, 1.0, 2.6, 8.2); 3.77(s, 3H, H-23); 3.03(m, 2H, H-8, syst. A_2B_2); 2.87(m, 2H, H-9, syst. A_2B_2).

^{13}C-NMR(dmso-d6, δ ppm): 178.68(C-16); 170.78(C-1); 159.37(C-18); 141.38(Cq); 139.88(Cq); 139.10(Cq); 134.02(Cq); 130.90(CH); 129.95(CH); 129.52(CH); 128.40(C-12-14); 128.30(C-11-15); 128.22(CH); 125.96(CH); 125.87(CH); 116.22(CH); 111.23(CH); 109.67(CH); 55.28(C-23); 37.18(C-8); 35.00(C-9).

FT-IR(ATR in solid, ν cm^{-1}): 3185m; 3024s; 2957m; 2932m; 2862w; 2835w; 1672m; 1600m; 1563s; 1526vs; 1487s; 1454s; 1346s; 1271vs; 1200w; 1155vs; 1067m;

1035m; 986w; 954w; 893w; 851w; 805w; 770m; 740s; 717m; 690m; 675m; 643w; 588w; 543w; 511w; 478w; 451w.

Calculated: C 70.74; H 5.68; N 7.17; S 8.21, Experimental: C 70.89; H 5.69; N 7.09; S 8.29.

N-(2-Phenetyl-benzoyl)-N'-(4-methoxyphenyl)-thiourea (1c)

White crystals, m.p. 121-122°C (isopropanol), yield 72%, $C_{23}H_{22}N_2OS$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 12.40(bs, 2H, NH); 7.58(d, 2H, H-18-22, 9.0); 7.53(dd, 1H, H-7, 1.3, 7.5); 7.46(td, 1H, H-13, 7.6, 1.4); 7.32(t, 2H, H-12-14, 7.6); 7.30÷7.14(m, 5H, H-arom); 6.98(d, 2H H-19-21, 9.0); 3.77(s, 3H, H-23); 3.03(m, 2H, H-8, syst. A_2B_2); 2.87(m, 2H, H-9, syst. A_2B_2).

^{13}C-NMR(dmso-d6, δ ppm): 179.09(C-16); 170.76(C-1); 157.39(C-18); 141.41(Cq); 139.83(Cq); 134.18(Cq); 130.95(Cq); 130.81(CH); 129.94(CH); 128.38(CH); 128.36(C-12-14); 128.31(C-11-15); 128.18(CH); 125.96(CH); 125.86(C-18-22); 113.84(C-19-21); 55.34(C-23); 37.20(C-8); 35.04(C-9).

FT-IR(ATR in solid, ν cm^{-1}): 3145m; 3020m; 2953m; 2929m; 2867m; 2834w; 1674s; 1590w; 1509vs; 1452s; 1329w; 1297m; 1240s; 1157vs; 1112m; 1061m; 1032m; 949w; 861w; 838w; 797w; 754m; 693m; 656w; 607w; 557w; 520w; 430w.

Calculated: C 70.74; H 5.68; N 7.17; S 8.21, Experimental: C 70.71; H 5.54; N 7.26; S 8.38.

N-(2-Phenetyl-benzoyl)-N'-(2-ethoxyphenyl)-thiourea (1d)

White crystals, m.p. 129-130°C (isopropanol), yield 68%, $C_{24}H_{24}N_2OS$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 13.18(s, 1H, NH); 11.78(s, 1H, NH); 8.81(d, 1H, H-22, 8.0); 7.53(dd, 1H, H-7, 1.3, 7.5); 7.46(t, 1H, H-13, 7.5); 7.33(t, 2H, H-12-14, 7.5); 7.36÷7.14(m, 8H, H-arom); 7.12(d, 1H, H-19, 8.2); 7.00(t, 1H, H-21, 7.7); 4.15(q, 2H, H-23, 7.0); 3.03(m, 2H, H-8, syst. A_2B_2); 2.87(m, 2H, H-9, syst. A_2B_2); 1.36(t, 3H, H-24, 7.0).

^{13}C-NMR(dmso-d6, δ ppm): 177.27(C-16); 170.64(C-1); 149.45(C-18); 141.34(Cq); 139.86(Cq); 133.78(Cq); 127.36(Cq); 130.88(CH); 129.97(CH); 128.21(C-12-14, C-11-15); 128.21(CH); 128.16(CH); 126.27(CH); 125.90(CH); 125.82(CH); 122.06(CH); 119.75(CH); 112.29(CH); 64.42(C-23); 37.29(C-8); 35.14(C-9); 14.47(C-24)

FT-IR(ATR in solid, ν cm^{-1}): 3421m; 3240w; 3159w; 3117w; 3022m; 2987m; 2943m; 1681m; 1598m; 1547vs; 1511vs; 1485vs; 1449vs; 1346s; 1311s; 1284s; 1223s; 1147s; 1114s; 1034s; 952m; 741s; 698m; 674m; 627m; 602m; 560w; 533w; 503w; 461w; 432w.

Calculated: C 71.26; H 5.98; N 6.92; S 7.93, Experimental: C 71.02; H 6.14; N 7.06; S 8.06.

N-(2-Phenetyl-benzoyl)-N'-(3-ethoxyphenyl)-thiourea (1e)

White crystals, m.p. 102-103°C (isopropanol), yield 63%, $C_{24}H_{24}N_2OS$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 12.40(s, 1H, NH); 11.80(s, 1H, NH); 4.04(q, 2H, H-23, 6.9); 3.03(m, 2H, H-8, syst. A_2B_2); 2.87(m, 2H, H-9, syst. A_2B_2); 1.34(t, 3H, H-24, 6.9).

^{13}C-NMR(dmso-d6, δ ppm): 178.27(C-16); 170.56(C-1); 141.27(C-18); 139.77(Cq); 139.74(Cq); 133.78(Cq); 127.36(Cq); 130.88(CH); 129.97(CH); 128.21(C-12-14, C-11-15); 128.21(CH); 128.16(CH); 126.27(CH); 125.90(CH); 125.82(CH); 122.06(CH); 119.75(CH); 110.01(CH); 63.16(C-23); 37.07(C-8); 34.86(C-9); 14.55 (C-24).

FT-IR(ATR in solid, ν cm^{-1}): 3399m; 3215w; 3029w; 2928w; 2201m; 1669m; 1597m; 1557vs; 1503vs; 1447vs; 1394s; 1340s; 1272s; 1238s; 1142s; 1114s; 1042s; 919m; 863s; 761m; 700m; 674m; 638m; 601w; 563w; 520w; 475w; 442w.

Calculated: C 71.26; H 5.98; N 6.92; S 7.93, Experimental: C 71.21; H 6.14; N 7.11; S 7.88.

N-(2-Phenetyl-benzoyl)-N'-(4-ethoxyphenyl)-thiourea (1f)

White crystals, m.p. 127-128°C (isopropanol), yield 66%, $C_{24}H_{24}N_2OS$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 12.34(s, 1H, NH); 11.73(s, 1H, NH); 7.57(d, 2H, H-18-22, 9.0); 7.53(dd, 1H, H-7, 1.3, 7.5); 7.46(t, 1H, H-13, 7.5); 7.32(t, 2H, H-12-14, 7.5); 7.28÷7.14(m, 5H, H-arom); 6.97(d, 2H H-19-21, 9.0); 4.04(q, 2H, H-23, 6.9); 3.03(m, 2H, H-8, syst. A_2B_2); 2.87(m, 2H, H-9, syst. A_2B_2); 1.34(t, 3H, H-24, 6.9)

^{13}C-NMR(dmso-d6, δ ppm): 178.91(C-16); 170.60(C-1); 156.69(C-18); 141.31(Cq); 139.77(Cq); 133.93(Cq); 130.65(Cq); 130.80(CH); 129.87(CH); 128.28(C-12-14); 128.23(C-11-15); 128.09(CH); 125.89(CH); 125.84(C-18-22); 125.79(CH); 114.27(C-19-21); 63.24(C-23); 37.12(C-8); 34.94(C-9); 14.59(C-24).

FT-IR(ATR in solid, ν cm^{-1}): 3401m; 3125w; 3040w; 2979m; 2928m; 2869w; 1669m; 1596m; 1555s; 1502vs; 1393w; 1339m; 1237m; 1173w; 1142s; 1113m; 1041m; 918w; 827w; 762m; 702w; 672w; 633m; 600w; 560w; 521m; 473w; 442w.

Calculated: C 71.26; H 5.98; N 6.92; S 7.93, Experimental: C 71.03; H 5.93; N 7.08; S 7.85.

N-(2-Phenetyl-benzoyl)-N'-(2-nitrophenyl)-thiourea (1g)

White crystals, m.p. 124-125°C (isopropanol), yield 59%, $C_{22}H_{19}N_3O_3S$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 12.10(vbs, 2H, NH); 8.13(dd, 1H, H-19, 1.5, 8.2); 7.99(dd, 1H, H-22, 1.2, 8.2); 7.81(td, 1H, H-21, 8.2, 1.5); 7.58(dd, 1H, H-7, 1.4, 7.5); 7.56(td, 1H, H-20, 8.2, 1.2); 7.48(td, 1H, H-13, 1.5, 7.4); 7.38÷7.15(m, 7H, H-arom); 3.04(m, 2H, H-8, syst. A_2B_2); 2.88(m, 2H, H-9, syst. A_2B_2).

^{13}C-NMR(dmso-d6, δ ppm): 180.58(C-16); 170.53(C-1); 144.01(C-18); 141.30(Cq); 139.90(Cq); 133.89(Cq); 130.95(Cq); 133.72(C-21); 130.95(C-13); 130.00(CH); 129.87(C-22); 128.32(C-11-15); 128.21(CH); 128.12(CH); 127.72(CH); 125.88(CH); 125.83(CH); 124.83(CH); 37.12(C-8); 34.94(C-9).

FT-IR(ATR in solid, ν cm^{-1}): 3168m; 3055m; 3021m; 1680m; 1606w; 1579w; 1497vs; 1463vs; 1342s; 1310m; 1275m; 1243s; 1149s; 1057m; 952m; 859w; 785w; 732m; 693m; 658w; 610w; 563w; 523w; 455w.

Calculated: C 64.85; H 5.19; N 10.19; S 7.87, Experimental: C 64.98; H 5.03; N 10.38; S 7.85.

N-(2-Phenetyl-benzoyl)-N'-(3-nitrophenyl)-thiourea (1h)

White crystals, m.p. 114-115°C (isopropanol), yield 69%, $C_{22}H_{19}N_3O_3S$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 12.60(s, 1H, NH); 11.94(s, 1H, NH); 8.76(t, 1H, H-18, 1.0); 8.10(ddd, 1H, H-20, 1.0, 2.3, 8.2); 8.03(ddd, 1H, H-22, 1.0, 2.3, 8.2); 7.68(t, 1H, H-21, 8.2); 7.51(dd, 1H, H-7, 1.2, 8.2); 7.44(td, 1H, H-13, 1.5, 7.6); 7.31(t, 2H, H-12-14, 7.6); 7.31÷7.12(m, 5H, H-arom); 3.02(m, 2H, H-8, syst. A_2B_2); 2.86(m, 2H, H-9, syst. A_2B_2).

^{13}C-NMR(dmso-d6, δ ppm): 179.85(C-16); 170.47(C-1); 147.53(C-19); 141.36(Cq); 140.02(Cq); 139.20(Cq); 133.74(Cq); 131.24(CH); 131.06(CH); 130.00(CH); 128.37(C-11-15); 128.30(C-12-14); 128.28(CH); 125.97(CH); 125.89(CH); 120.90(CH); 119.17(CH); 104.34(CH); 37.18(C-8); 34.93(C-9).

FT-IR(ATR in solid, ν cm^{-1}): 3385m; 3103w; 3015m; 2914w; 2858w; 1675m; 1600m; 1557s; 1518vs; 1496vs;

1341s; 1313s; 1250m; 1139s; 1082m; 910w; 885w; 808w; 757m; 700w; 672m; 644w; 609w; 563w; 523w; 451w.

Calculated: C 64.85; H 5.19; N 10.19; S 7.87, Experimental: C 65.03; H 5.27; N 10.25; S 7.99.

N-(2-Phenetyl-benzoyl)-N'-(4-nitrophenyl)-thiourea (1i)

White crystals, m.p. 145-146°C (isopropanol), yield 51%, $C_{22}H_{19}N_3O_3S$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 12.10(bs, 2H, NH); 8.29(d, 2H, H-19-21, 9.1); 8.10(d, 2H, H-18-22, 9.1); 7.54(d, 1H, H-7, 7.5); 7.46(t, 1H, H-13, 7.5); 7.33(t, 2H, H-12-14, 7.4); 7.31÷7.13(m, 5H, H-arom); 3.04(m, 2H, H-8, syst. A_2B_2); 2.89(m, 2H, H-9, syst. A_2B_2).

^{13}C-NMR(dmso-d6, δ ppm): 178.96(C-16); 170.50(C-1); 144.04(C-20); 141.27(Cq); 139.98(Cq); 133.72(Cq); 133.69(Cq); 130.97(CH); 129.93(CH); 128.30(C-18-22); 128.28(C-11-15); 128.21(C-12-14); 125.87(CH); 125.79(CH); 124.23(C-19-21); 123.92(CH); 37.08(C-8); 34.81(C-9).

FT-IR(ATR in solid, ν cm^{-1}): 3176m; 3167w; 3025m; 2930m; 2856w; 1687m; 1608w; 1596w; 1564m; 1509vs; 1456m; 1315s; 1257s; 1164s; 1109m; 1060w; 1026w; 966w; 948w; 866w; 849m; 785w; 753m; 736m; 694m; 651w; 609w; 588w; 525w; 486w.

Calculated: C 64.85; H 5.19; N 10.19; S 7.87, Experimental: C 64.73; H 5.17; N 10.47; S 7.69.

N-(2-Phenetyl-benzoyl)-N'-(2-methyl-5-nitrophenyl)-thiourea (1j)

White crystals, m.p. 133-134°C (isopropanol), yield 58%, $C_{23}H_{21}N_3O_3S$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 12.10(bs, 2H, NH); 8.65(d, 1H, H-18, 1.3); 8.09(dd, 1H, H-20, 1.3, 8.4); 7.61(d, 1H, H-21, 8.4); 7.55(dd, 1H, H-7, 1.2, 8.1); 7.46(td, 1H, H-13, 1.5, 7.6); 7.38÷7.14(m, 7H, H-arom); 3.04(m, 2H, H-8, syst. A_2B_2); 2.88(m, 2H, H-9, syst. A_2B_2); 2.40(s, 3H, H-23).

^{13}C-NMR(dmso-d6, δ ppm): 180.01(C-16); 170.74(C-1); 145.61(C-19); 141.81(Cq); 141.43(Cq); 139.92(Cq); 134.32(Cq); 133.91(Cq); 131.51(CH); 130.98(CH); 130.02(CH); 128.33(C-11-15, C-12-14); 128.19(CH); 125.99(CH); 125.91(CH); 121.33(CH); 121.23(CH); 37.38(C-8); 35.26(C-9); 17.89(C-23).

FT-IR(ATR in solid, ν cm^{-1}): 3243w; 3111w; 3083w; 3015w; 2868w; 1675m; 1601w; 1515vs; 1451m; 1337w; 1265m; 1249m; 1193m; 1154m; 1127w; 1083w; 1062w; 1031w; 896w; 855w; 833w; 802w; 761m; 739m; 698m; 661w; 611w; 565w; 528w; 477w; 443w.

Calculated: C 65.85; H 5.05; N 10.02; S 7.64, Experimental: C 65.57; H 5.37; N 10.04; S 7.60.

N-(2-Phenetyl-benzoyl)-N'-(4-methyl-3-nitrophenyl)-thiourea (1k)

White crystals, m.p. 150-151°C (isopropanol), yield 58%, $C_{23}H_{21}N_3O_3S$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 12.10(vbs, 2H, NH); 8.52(d, 1H, H-18, 1.2); 7.86(dd, 1H, H-21, 1.3, 8.2); 7.55÷7.51(m, 2H, H-7, H-22); 7.45(td, 1H, H-13, 1.5, 7.6); 7.36÷7.14(m, 7H, H-arom); 3.04(m, 2H, H-8, syst. A_2B_2); 2.88(m, 2H, H-9, syst. A_2B_2); 2.53(s, 3H, H-23).

^{13}C-NMR(dmso-d6, δ ppm): 179.46(C-16); 170.54(C-1); 148.27(C-19); 141.81(Cq); 141.37(Cq); 139.98(Cq); 137.04(Cq); 133.89(Cq); 130.53(Cq); 132.87(CH); 130.98(CH); 129.99(CH); 129.47(CH); 128.37(C-11-15); 128.28(C-12-14); 128.27(CH); 125.97(CH); 125.87(CH); 120.09(CH); 37.17(C-8); 34.93(C-9); 19.31(C-23).

FT-IR(ATR in solid, ν cm^{-1}): 3134s; 3084m; 3059m; 3021m; 1669s; 1600w; 1577w; 1526vs; 1488vs; 1449s; 1377m; 1337s; 1254m; 1197w; 1147s; 1066m; 1029w; 985w; 900w; 857w; 831w; 802w; 777w; 744m; 696m; 659m; 625w; 565w; 518w; 470w; 445w; 423w.

Calculated: C 65.85; H 5.05; N 10.02; S 7.64, Experimental: C 65.97; H 5.01; N 9.94; S 7.80.

N-(2-Phenetyl-benzoyl)-N'-(2-ethoxy-5-nitrophenyl)-thiourea (1l)

White crystals, m.p. 153-154°C (isopropanol), yield 67%, $C_{24}H_{23}N_3O_4S$.

^{1}H-NMR(dmso-d6, δ ppm, *J* Hz): 12.10(vbs, 2H, NH); 9.96(d, 1H, H-18, 2.8); 8.13(dd, 1H, H-20, 2.8, 9.1); 7.55(dd, 1H, H-7, 1.4, 7.6); 7.46(td, 1H, H-13, 1.5, 7.6); 7.37÷7.12(m, 8H, H-arom); 4.30(q, 2H, H-23, 7.0); 3.04(m, 2H, H-8, syst. A_2B_2); 2.88(m, 2H, H-9, syst. A_2B_2); 1.41(t, 3H, H-24, 7.0).

^{13}C-NMR(dmso-d6, δ ppm): 177.88(C-16); 171.20(C-1); 150.37(C-22); 141.41(Cq); 140.11(Cq); 139.62(Cq); 133.89(Cq); 127.79(Cq); 131.03(CH); 130.08(CH); 128.40(CH); 128.28(C-12-14, C-11-15); 125.96(CH); 125.87(CH); 121.98(CH); 116.17(CH); 111.82(CH); 65.72(C-23); 37.35(C-8); 35.15(C-9); 14.26(C-24).

FT-IR(ATR in solid, ν cm^{-1}): 3263w; 3098w; 3022w; 2982m; 2960w; 2936w; 2864w; 1682m; 1615w; 1595w; 1559s; 1516vs; 1489s; 1469m; 1453w; 1395m; 1357vs; 1340s; 1319s; 1268s; 1245s; 1223s; 1178w; 1155m; 1133m; 1109m; 1083w; 1060m; 1036m; 929w; 901w; 857w; 814m; 762m; 742m; 694s; 639w; 619w; 569w; 526w; 456w.

Calculated: C 64.13; H 5.16; N 9.35; S 7.13, Experimental: C 64.34; H 5.01; N 9.34; S 7.02.

Conclusions

Continuing our research in the antimicrobial substances field we synthesized twelve new compounds, thioureides of the 2-phenethylbenzoic acid. The chemical structure of the synthesized compounds have been confirmed by elemental analysis, IR and NMR spectroscopy. The obtained thioureides will be further investigated to determinate their antimicrobial activity.

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