Supporting Information

Substituted 5,5'-diphenyl-2-thioxo-imidazolidin-4-one as CB_1 cannabinoid receptor ligands: synthesis and pharmacological evaluation.

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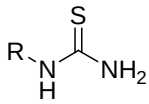
General procedure for the synthesis of benzil derivatives (X=Cl, Br, I): Briefly, suitably substituted benzaldehyde derivatives (0.27 mole) and sodium cyanide (0.08 mole) were refluxed in ethanol (65 mL) and water (50 mL) for 3 hours. After cooling, the resulting oil was extracted with chloroform. Following removal of the solvent under reduced pressure, the resulting benzoin was oxidized by heating with nitric acid. Upon completion of the oxidation, the solution was poured into water and the precipitate crystallized.

4,4'-dichlorobenzil: (CAS number: 3457-46-3) Spectral data in accordance to the literature[i]. Yield after crystallization: 54%

4,4'-dibromobenzil: (CAS number: 35578-47-3) Spectral data in accordance to the literature[23]. Yield after crystallization: 48%

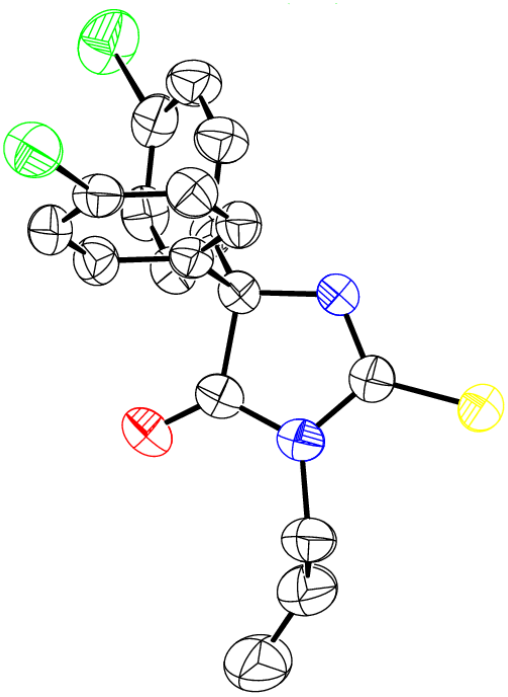
4,4'-diiodobenzil: (CAS number: 65699-84-5) Spectral data in accordance to the literature[37]. Yield after crystallization: 45%

Alkylthiourea derivatives (2a-2l) synthesized, characteristic infrared peaks (KBr, ν in cm^{-1})



Compound	R=	IR spectra
2a	$-C_2H_5$	1436.1, 1569.3, 3280.2, 3350.8
2b	- *i*-C_3H_7	1434.2, 1575.4, 3260.4, 3341.2
2c	- *n*-C_4H_9	1437.9, 1562.9, 3277.4, 3351.7
2d	- *i*-C_4H_9	1435.2, 1593.4, 3242.4, 3399.7
2e	$-C_7H_{15}$	1442.8, 1566.6, 3286.2, 3392.9
2f	$-C_8H_{17}$	1431.5, 1567.0, 3227.3, 3398.9
2g	$-C_6H_{11}$	1442.5, 1561.4, 3270.3, 3334.6
2h	$-(CH_2)_3-OCH_3$	1451.2, 1566.7, 3243.5, 3396.4
2i	$-CH_2-CH=CH_2$	1443.1, 1562.9, 3275.5, 3339.2
2j	$-CH_2-C_6H_5$	1451.8, 1552.6, 3246.7, 3394.2
2k	$-(CH_2)_2-C_6H_5$	1431.7, 1560.0, 3246.5, 3386.2
2l	Furan-2-yl-methyl	1437.8, 1545.9, 3279.1, 3398.3

Crystal structure of compound 28.



ORTEP diagram (50% probability) of 3-allyl-5,5'-bis-(4-bromo-phenyl)-2-thioxo-imidazolidin-4-one (**28**).

X-ray analysis:

Suitable crystals of compound **28** obtained by crystallization from ethanol were mounted with a quartz fibre on a goniometer head of a CAD4 Nonius diffractometer. After determination of the cell parameter using 25 well-centered reflections, complete diffraction data sets were collected. The structures were solved using direct methods and refined by full matrix least squares on F2 using the program Shelxl97[ii]. All non-hydrogen atoms were treated anisotropically while a riding model was applied for the hydrogens. Analytical correction for absorption was introduced.

Colourless plate, monoclinic, $P2_1/c$, a= 12.189(2) Å, b=10.6980(10) Å , c=16.737(4) Å, α= 90°, β=123.608(15)°, γ=90°, V=1817.7(6) $Å^3$, Z = 4, μ = 6.788 mm^{-1}, D_x = 1.704 g/cm^3, λ (Cu Kα) = 1.54478 Å, F(000) = 920, T = 293 K, 3734 unique reflections (R_{int} =

0.017), 217 refined parameters, R_1 = 0.0389 for 3734 $F_o>4\sigma(F_o)$, R_1 = 0.0572 for all data (3883) and wR_2 = 0.1106, GOF = S = 1.02, $\Delta_{\rho min}$ = -0.6 e/ Å^3, $\Delta_{\rho max}$ = 0.82 e/ Å^3.

Crystal data tables contents:

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Table S1 - Crystal Data and Details of the Structure Determination for: **28**

Crystal Data			
Formula	C18 H14 Br2 N2 O S		
Formula Weight	466.19		
Crystal System	Monoclinic		
Space group	P21/c (No. 14)		
a, b, c [Angstrom]	12.189(2)	10.6980(10)	16.737(4)
alpha, beta, gamma [deg]	90	123.608(15)	90
V [Ang**3]	1817.7(6)		
Z	4		
D(calc) [g/cm**3]	1.704		
Mu(CuKa) [/mm]	6.788		
F(000)	920		
Crystal Size [mm]	0.02 x 0.11 x 0.30		

Data Collection

Temperature (K)	293
Radiation [Angstrom]	CuKa 1.54178
Theta Min-Max [Deg]	4.4, 74.8
Dataset	-14: 15 ; 0: 13 ; -14: 20
Tot., Uniq. Data, R(int)	3883, 3734, 0.017
Observed data [I > 2.0 sigma(I)]	2925

Refinement

Nref, Npar	3734, 217
R, wR2, S	0.0389, 0.1106, 1.02

w = 1/[\s^2^(Fo^2^)+(0.0580P)^2^+1.1860P] where P=(Fo^2^+2Fc^2^)/3

Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.60, 0.82

Table S2 - Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms for: **28**

Atom	x	y	z	U(eq) [Ang^2]
Br1	0.22842(5)	0.29234(4)	0.57088(4)	0.0824(2)
Br2	0.50515(4)	0.97972(5)	0.33500(3)	0.0717(2)
S1	-0.19329(9)	1.04630(9)	0.36566(7)	0.0553(3)
O1	-0.1052(2)	0.7344(2)	0.18819(17)	0.0568(8)
N1	-0.1660(2)	0.8892(3)	0.25150(19)	0.0481(8)
N2	0.0000(2)	0.8881(2)	0.40228(18)	0.0444(8)
C1	0.1631(4)	0.4486(3)	0.5073(3)	0.0541(11)
C2	0.0470(4)	0.4522(3)	0.4192(3)	0.0553(11)
C3	0.0040(3)	0.5649(3)	0.3701(2)	0.0495(10)
C4	0.0775(3)	0.6723(3)	0.4092(2)	0.0435(9)
C5	0.1936(4)	0.6658(4)	0.4996(3)	0.0571(11)
C6	0.2368(4)	0.5548(4)	0.5491(3)	0.0609(12)
C7	0.0406(3)	0.7986(3)	0.3578(2)	0.0426(9)
C8	-0.0848(3)	0.7979(3)	0.2544(2)	0.0458(9)

C9	-0.1169(3)	0.9397(3)	0.3410(2)	0.0451(10)
C10	0.1543(3)	0.8483(3)	0.3524(2)	0.0423(9)
C11	0.2172(3)	0.9594(3)	0.3945(2)	0.0486(10)
C12	0.3217(3)	0.9996(3)	0.3892(3)	0.0550(11)
C13	0.3601(3)	0.9282(3)	0.3406(2)	0.0510(10)
C14	0.2973(3)	0.8188(4)	0.2969(3)	0.0541(11)
C15	0.1946(3)	0.7784(3)	0.3027(3)	0.0517(11)
C16	-0.2883(3)	0.9297(4)	0.1624(3)	0.0609(12)
C17	-0.3991(4)	0.8452(5)	0.1292(3)	0.0763(16)
C18	-0.4760(5)	0.8086(5)	0.0402(4)	0.104(2)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S3 - Hydrogen Atom Positions and Isotropic Displacement Parameters for: **28**

Atom	x	y	z	U(iso) [Ang^2]
H2	0.04720	0.90600	0.46240	0.0530
H2A	-0.00270	0.37990	0.39240	0.0660
H3	-0.07510	0.56810	0.31030	0.0590
H5	0.24310	0.73790	0.52730	0.0690
H6	0.31450	0.55150	0.60980	0.0730
H11	0.18980	1.00770	0.42660	0.0580
H12	0.36490	1.07410	0.41820	0.0660
H14	0.32370	0.77210	0.26360	0.0650
H15	0.15180	0.70400	0.27310	0.0620
H16A	-0.31220	1.01170	0.17270	0.0730
H16B	-0.27140	0.93780	0.11230	0.0730
H17	-0.41600	0.81590	0.17370	0.0910
H18A	-0.46120	0.83670	-0.00560	0.1250
H18B	-0.54560	0.75450	0.02270	0.1250

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Table S4 - (An)isotropic Displacement Parameters for: **28**

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Br1	0.1043(4)	0.0663(3)	0.0944(4)	0.0342(2)	0.0661(3)	0.0252(2)
Br2	0.0567(2)	0.0965(3)	0.0680(3)	-0.0029(2)	0.0383(2)	-0.0131(2)
S1	0.0532(4)	0.0621(5)	0.0521(5)	0.0035(4)	0.0300(4)	0.0121(4)
O1	0.0622(14)	0.0600(14)	0.0425(13)	-0.0091(11)	0.0255(11)	-0.0075(12)
N1	0.0437(13)	0.0525(15)	0.0403(14)	-0.0012(12)	0.0184(11)	0.0000(12)
N2	0.0434(13)	0.0509(15)	0.0355(13)	-0.0029(11)	0.0198(11)	0.0032(11)
C1	0.068(2)	0.0495(18)	0.061(2)	0.0171(16)	0.0458(19)	0.0142(16)
C2	0.068(2)	0.0461(18)	0.061(2)	-0.0006(16)	0.0415(19)	-0.0026(16)
C3	0.0530(18)	0.0513(18)	0.0449(18)	-0.0023(14)	0.0276(15)	-0.0020(14)
C4	0.0483(16)	0.0462(16)	0.0405(16)	0.0005(13)	0.0274(14)	0.0025(13)
C5	0.0580(19)	0.0550(19)	0.048(2)	0.0037(16)	0.0229(16)	0.0000(16)
C6	0.061(2)	0.066(2)	0.048(2)	0.0121(18)	0.0253(17)	0.0080(18)
C7	0.0434(15)	0.0449(16)	0.0380(16)	-0.0037(13)	0.0216(13)	-0.0010(13)
C8	0.0475(16)	0.0449(16)	0.0419(17)	0.0008(14)	0.0229(14)	-0.0047(13)
C9	0.0473(16)	0.0444(16)	0.0477(18)	0.0023(14)	0.0288(14)	-0.0023(13)
C10	0.0423(15)	0.0454(16)	0.0365(15)	0.0035(13)	0.0201(13)	0.0028(13)
C11	0.0506(17)	0.0455(17)	0.0483(18)	-0.0022(14)	0.0265(15)	0.0005(14)
C12	0.0538(18)	0.0524(19)	0.057(2)	-0.0046(16)	0.0296(16)	-0.0092(15)
C13	0.0436(16)	0.061(2)	0.0443(18)	0.0063(16)	0.0218(14)	0.0002(15)
C14	0.0537(18)	0.062(2)	0.053(2)	-0.0031(17)	0.0335(16)	0.0028(16)
C15	0.0532(18)	0.0495(18)	0.052(2)	-0.0071(15)	0.0289(16)	-0.0025(15)
C16	0.054(2)	0.067(2)	0.048(2)	0.0046(18)	0.0196(16)	0.0055(17)
C17	0.056(2)	0.086(3)	0.073(3)	-0.002(2)	0.027(2)	0.002(2)
C18	0.066(3)	0.105(4)	0.099(4)	-0.029(3)	0.019(3)	-0.002(3)

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The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for
Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and
h(i) are the Reflection Indices.

Table S5 - Bond Distances (Angstrom) for: **28**

Br1	-C1	1.903(4)	C10	-C15	1.395(5)
Br2	-C13	1.903(4)	C11	-C12	1.393(6)
S1	-C9	1.662(4)	C12	-C13	1.373(5)
O1	-C8	1.203(4)	C13	-C14	1.368(5)
N1	-C8	1.372(5)	C14	-C15	1.378(6)
N1	-C9	1.379(4)	C16	-C17	1.456(7)
N1	-C16	1.474(5)	C17	-C18	1.306(7)
N2	-C7	1.457(4)	C2	-H2A	0.9304
N2	-C9	1.330(4)	C3	-H3	0.9296
N2	-H2	0.8598	C5	-H5	0.9297
C1	-C2	1.367(6)	C6	-H6	0.9302
C1	-C6	1.375(6)	C11	-H11	0.9305
C2	-C3	1.388(5)	C12	-H12	0.9301
C3	-C4	1.379(5)	C14	-H14	0.9286
C4	-C7	1.530(4)	C15	-H15	0.9300
C4	-C5	1.388(5)	C16	-H16A	0.9694
C5	-C6	1.375(6)	C16	-H16B	0.9717
C7	-C10	1.533(6)	C17	-H17	0.9302
C7	-C8	1.550(4)	C18	-H18A	0.9293
C10	-C11	1.378(5)	C18	-H18B	0.9303

Table S6 - Bond Angles (Degrees) for: **28**

C8	-N1	-C9	111.7(3)	C7	-C10	-C15	118.5(3)
C8	-N1	-C16	123.4(3)	C7	-C10	-C11	122.3(3)
C9	-N1	-C16	124.9(3)	C11	-C10	-C15	119.2(4)
C7	-N2	-C9	113.6(3)	C10	-C11	-C12	120.2(3)
C7	-N2	-H2	123.21	C11	-C12	-C13	119.3(3)
C9	-N2	-H2	123.18	C12	-C13	-C14	121.3(4)

C2	-C1	-C6	121.4(3)	Br2	-C13	-C12	119.9(3)
Br1	-C1	-C2	119.4(3)	Br2	-C13	-C14	118.8(3)
Br1	-C1	-C6	119.2(3)	C13	-C14	-C15	119.5(4)
C1	-C2	-C3	119.3(3)	C10	-C15	-C14	120.5(3)
C2	-C3	-C4	120.6(3)	N1	-C16	-C17	114.1(4)
C5	-C4	-C7	117.5(3)	C16	-C17	-C18	123.4(5)
C3	-C4	-C7	123.9(3)	C1	-C2	-H2A	120.38
C3	-C4	-C5	118.6(3)	C3	-C2	-H2A	120.33
C4	-C5	-C6	121.3(4)	C2	-C3	-H3	119.74
C1	-C6	-C5	118.8(4)	C4	-C3	-H3	119.63
N2	-C7	-C8	99.8(3)	C4	-C5	-H5	119.39
N2	-C7	-C4	111.7(3)	C6	-C5	-H5	119.32
C4	-C7	-C10	110.2(3)	C1	-C6	-H6	120.51
C8	-C7	-C10	107.5(3)	C5	-C6	-H6	120.64
N2	-C7	-C10	112.1(3)	C10	-C11	-H11	119.89
C4	-C7	-C8	115.1(3)	C12	-C11	-H11	119.90
N1	-C8	-C7	106.4(3)	C11	-C12	-H12	120.32
O1	-C8	-N1	126.3(3)	C13	-C12	-H12	120.37
O1	-C8	-C7	127.2(3)	C13	-C14	-H14	120.27
N1	-C9	-N2	108.1(3)	C15	-C14	-H14	120.25
S1	-C9	-N2	127.0(2)	C10	-C15	-H15	119.85
S1	-C9	-N1	124.9(3)	C14	-C15	-H15	119.64
N1	-C16	-H16A	108.74	C16	-C17	-H17	118.26
N1	-C16	-H16B	108.69	C18	-C17	-H17	118.36
C17	-C16	-H16A	108.86	C17	-C18	-H18A	119.96
C17	-C16	-H16B	108.72	C17	-C18	-H18B	119.96
H16A	-C16	-H16B	107.51	H18A	-C18	-H18B	120.07

Table S7 - Torsion Angles (Degrees) for: **28**

C9	-N1	-C8	-O1	176.7(4)
C9	-N1	-C8	-C7	-6.4(4)
C16	-N1	-C8	-O1	-5.0(6)
C16	-N1	-C8	-C7	171.9(3)
C8	-N1	-C9	-S1	-176.2(3)
C8	-N1	-C9	-N2	3.7(4)
C16	-N1	-C9	-S1	5.6(5)
C16	-N1	-C9	-N2	-174.5(3)
C8	-N1	-C16	-C17	78.3(5)
C9	-N1	-C16	-C17	-103.7(5)
C9	-N2	-C7	-C4	-126.6(3)
C9	-N2	-C7	-C8	-4.5(4)
C9	-N2	-C7	-C10	109.1(3)
C7	-N2	-C9	-S1	-179.2(3)
C7	-N2	-C9	-N1	1.0(4)
Br1	-C1	-C6	-C5	175.4(4)
C2	-C1	-C6	-C5	-1.7(8)
Br1	-C1	-C2	-C3	-175.7(4)
C6	-C1	-C2	-C3	1.3(8)
C1	-C2	-C3	-C4	0.3(7)
C2	-C3	-C4	-C5	-1.6(6)
C2	-C3	-C4	-C7	176.9(4)
C3	-C4	-C5	-C6	1.2(7)
C7	-C4	-C5	-C6	-177.3(4)
C3	-C4	-C7	-N2	110.4(4)
C3	-C4	-C7	-C8	-2.5(5)
C3	-C4	-C7	-C10	-124.3(4)
C5	-C4	-C7	-N2	-71.2(5)

Table S7 - Torsion Angles (Degrees) for: **28** (continued)

C5	-C4	-C7	-C8	175.9(4)
C5	-C4	-C7	-C10	54.1(4)
C4	-C5	-C6	-C1	0.4(8)
C4	-C7	-C8	-O1	-57.1(5)
C4	-C7	-C8	-N1	126.0(3)
C10	-C7	-C8	-O1	66.1(4)
C10	-C7	-C8	-N1	-110.7(3)
N2	-C7	-C10	-C11	6.3(4)
N2	-C7	-C10	-C15	-173.5(3)
N2	-C7	-C8	-N1	6.3(3)
N2	-C7	-C8	-O1	-176.9(4)
C4	-C7	-C10	-C15	61.4(4)
C8	-C7	-C10	-C11	115.0(3)
C8	-C7	-C10	-C15	-64.8(4)
C4	-C7	-C10	-C11	-118.8(3)
C15	-C10	-C11	-C12	-1.5(5)
C7	-C10	-C15	-C14	-179.3(3)
C7	-C10	-C11	-C12	178.8(3)
C11	-C10	-C15	-C14	1.0(5)
C10	-C11	-C12	-C13	0.8(5)
C11	-C12	-C13	-C14	0.4(5)
C11	-C12	-C13	-Br2	-178.6(3)
Br2	-C13	-C14	-C15	178.1(3)
C12	-C13	-C14	-C15	-0.9(6)
C13	-C14	-C15	-C10	0.2(6)
N1	-C16	-C17	-C18	-133.7(5)

Table S8 - Contact Distances(Angstrom) for: **28**

Br1	.C9_a	3.522(4)	C2	.O1_g	3.252(5)
Br2	.S1_b	3.4919(16)	C2	.C1_a	3.562(8)
Br2	.H6_c	3.1658	C3	.O1	3.137(4)
S1	.Br2_d	3.4919(16)	C5	.C15	3.515(6)
S1	.C14_e	3.700(4)	C8	.C2_e	3.586(6)
S1	.N2_f	3.316(3)	C9	.Br1_a	3.522(4)
S1	.H16A	2.7361	C11	.O1_e	3.216(4)
S1	.H14_e	3.0390	C12	.O1_e	3.342(5)
S1	.H15_e	3.1298	C14	.S1_g	3.700(4)
S1	.H2_f	2.4576	C15	.C5	3.515(6)
S1	.H5_f	3.1799	C15	.O1	3.081(5)
O1	.C3	3.137(4)	C17	.O1	3.361(6)
O1	.C15	3.081(5)	C1	.H16B_g	2.9476
O1	.C17	3.361(6)	C2	.H16B_g	3.0626
O1	.C2_e	3.252(5)	C4	.H15	2.8996
O1	.C11_g	3.216(4)	C5	.H2	2.9909
O1	.C12_g	3.342(5)	C8	.H15	2.9026
O1	.H3	2.5781	C8	.H3	2.6097
O1	.H15	2.6477	C10	.H5	2.7619
O1	.H16B	2.7575	C11	.H2	2.9186
O1	.H2A_e	2.8171	C11	.H3_e	3.0870
O1	.H11_g	2.9057	C15	.H2A_e	2.9762
N1	.N2	2.193(4)	C17	.H12_g	3.0953
N2	.N1	2.193(4)	C18	.H12_g	2.7511
N2	.S1_f	3.316(3)	H2	.C5	2.9909
N2	.H11	2.4723	H2	.C11	2.9186
C1	.C2_a	3.562(8)	H2	.H11	2.3910
C2	.C8_g	3.586(6)	H2	.S1_f	2.4576

Table S8 - Contact Distances(Angstrom) for: **28** (continued)

H2A	.O1_g	2.8171	H12	.C18_e	2.7511
H2A	.C15_g	2.9762	H14	.S1_g	3.0390
H3	.O1	2.5781	H15	.O1	2.6477
H3	.C8	2.6097	H15	.C4	2.8996
H3	.C11_g	3.0870	H15	.C8	2.9026
H5	.C10	2.7619	H15	.S1_g	3.1298
H5	.S1_f	3.1799	H16A	.S1	2.7361
H6	.Br2_h	3.1658	H16B	.O1	2.7575
H11	.N2	2.4723	H16B	.H18A	2.3156
H11	.H2	2.3910	H16B	.C1_e	2.9476
H11	.O1_e	2.9057	H16B	.C2_e	3.0626
H12	.C17_e	3.0953	H18A	.H16B	2.3156

Table S9 - Hydrogen Bonds (Angstrom, Deg) for: **28**

N2 -- H2 .. S1	0.8600	2.4600	3.316(3)	177.00	3_576
C3 -- H3 .. O1	0.9300	2.5800	3.137(4)	119.00	.
C11 -- H11 .. N2	0.9300	2.4700	2.827(5)	103.00	.
C16 -- H16A .. S1	0.9700	2.7400	3.180(4)	109.00	.

Translation of Symmetry Code to Equiv.Pos

a =[3566.00] = -x,1-y,1-z
b =[1655.00] = 1+x,y,z
c =[4564.00] = x,3/2-y,-1/2+z
d =[1455.00] = -1+x,y,z
e =[2555.00] = -x,1/2+y,1/2-z
f =[3576.00] = -x,2-y,1-z
g =[2545.00] = -x,-1/2+y,1/2-z
h =[4565.00] = x,3/2-y,1/2+z

Appendix : Characteristic infrared peaks and elemental analysis data of compounds 3 to 36

3-Ethyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (3). IR (KBr, cm^{-1}) ν 3261 (NH), 1716 (C=O), 1584 (-CS-), 1496 (C=C), 1447 (C=S). Calc. for $C_{17}H_{16}N_2OS$: C, 68.89; H, 5.44; N, 9.45; O, 5.40; S, 10.82 %. Found : C, 68.65; H, 5.22; N, 9.39%.

3-Isopropyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (4). IR (KBr, cm^{-1}) ν 3171 (NH), 1764 (C=O), 1584 (-CS-), 1507 (C=C), 1447 (C=S). Calc. for $C_{18}H_{18}N_2OS$: C, 69.95; H, 5.84; N, 9.02; O, 5.15; S, 10.32 %. Found: C, 69.65; H, 5.64; N, 9.11%.

3-Butyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (5). IR (KBr, cm^{-1}) ν 3179 (NH), 1743 (C=O), 1584 (-CS-), 1505 (C=C), 1448 (C=S). Calc. for $C_{19}H_{20}N_2OS$: C, 70.34; H, 6.21; N, 8.63; O, 4.93; S, 9.88 %. Found: C, 70.37; H, 6.07; N, 8.56 %.

3-Isobutyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (6). IR (KBr, cm^{-1}) ν 3319 (NH), 1716 (C=O), 1585 (-CS-), 1495 (C=C), 1447 (C=S). Calc. for $C_{19}H_{20}N_2OS$: C, 70.34; H, 6.21; N, 8.63; O, 4.93; S, 9.88 %. Found: C, 70.24; H, 6.00; N, 8.55 %.

3-Heptyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (7). IR (KBr, cm^{-1}) ν 3185 (NH), 1751 (C=O), 1585 (-CS-), 1512 (C=C), 1446 (C=S). Calc. for $C_{22}H_{26}N_2OS$: C, 72.09; H, 7.15; N, 7.64; O, 4.37; S, 8.75 %. Found: C, 72.01; H, 6.92; N, 7.66 %.

3-Octyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (8). IR (KBr, cm^{-1}) ν 3183 (NH), 1750 (C=O), 1584 (-CS-), 1508 (C=C), 1446 (C=S). Calc. for $C_{23}H_{28}N_2OS$: C, 72.59; H, 7.42; N, 7.36; O, 4.30; S, 8.43 %. Found: C, 72.49; H, 7.19; N, 7.38 %.

3-Cyclohexyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (9). IR (KBr, cm^{-1}) ν 3156 (NH), 1754 (C=O), 1583 (-CS-), 1512 (C=C), 1445 (C=S). Calc. for $C_{21}H_{22}N_2OS$: C, 71.97; H, 6.33; N, 7.99; O, 4.56; S, 9.15 %. Found: C, 71.90; H, 6.09; N, 8.01 %.

3-(3-Methoxy-propyl)-5,5-diphenyl-2-thioxo-imidazolidin-4-one (10). IR (KBr, cm^{-1}) ν 3176 (NH), 1744 (C=O), 1583 (-CS-), 1500 (C=C), 1445 (C=S). Calc. for $C_{19}H_{20}N_2O_2S$: C, 67.03; H, 5.92; N, 8.23; O, 9.40; S, 9.42 %. Found: C, 66.99; H, 5.71; N, 8.28 %.

3-(3-Hydroxy-propyl)-5,5-diphenyl-2-thioxo-imidazolidin-4-one (11). IR (KBr, cm^{-1}) ν 3413 (O-H), 3160 (NH), 1717 (C=O), 1584 (-CS-), 1488 (C=C), 1447 (C=S). Calc. for $C_{18}H_{18}N_2O_2S$: C, 66.23; H, 5.56; N, 8.58; O, 9.80; S, 9.82 %. Found: C, 66.04; H, 5.25; N, 8.31 %.

3-Allyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (12). IR (KBr, cm^{-1}) ν 3201 (NH), 1750 (C=O), 1584 (-CS-), 1494 (C=C), 1435 (C=S). Calc. for $C_{18}H1_6N_2OS$: C, 70.10; H, 5.23; N, 9.08; O, 5.19; S, 10.04 %. Found: C, 70.11; H, 4.97; N, 9.04 %.

3-Benzyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (13). IR (KBr, cm^{-1}) ν 3315 (NH), 1722 (C=O), 1585 (-CS-), 1484 (C=C), 1443 (C=S). Calc. for $C_{22}H_{18}N_2OS$: C, 73.71; H, 5.06; N, 7.82; O, 4.46; S, 8.94 %. Found: C, 73.64; H, 4.84; N, 7.73 %.

3-Phenethyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (14). IR (KBr, cm^{-1}) ν 3169 (NH), 1750 (C=O), 1584 (-CS-), 1509 (C=C), 1446 (C=S). Calc. for $C_{23}H_{20}N_2OS$: C, 74.16; H, 5.41; N, 7.52; O, 4.30; S, 8.61 %. Found: C, 74.41; H, 5.43; N, 7.53 %.

3-Furanylmethyl-5,5-diphenyl-2-thioxo-imidazolidin-4-one (15). IR (KBr, cm^{-1}) ν 3320 (NH), 1728 (C=O), 1584 (-CS-), 1487 (C=C), 1443 (C=S). Calc. for $C_{20}H_{16}N_2OS$: C, 68.94; H, 4.44; N, 7.99; O, 9.18; S, 9.20 %. Found: C, 69.04; H, 4.44; N, 7.99 %.

5,5-Bis-(4-chloro-phenyl)-3-isobutyl-2-thioxo-imidazolidin-4-one (16). IR (KBr, cm^{-1}) ν 3160 (NH), 1749 (C=O), 1592 (-CS-), 1507 (C=C), 1435 (C=S). Calc. for $C_{19}H_{18}Cl_2N_2OS$: C, 58.02; H, 4.61; Cl, 18.03; N, 7.12; O, 4.07; S, 8.15 %. Found: C, 57.95; H, 4.41; N, 7.04 %.

5,5-Bis-(4-chloro-phenyl)-3-heptyl-2-thioxo-imidazolidin-4-one (17). IR (KBr, cm^{-1}) ν 3151 (NH), 1747 (C=O), 1589 (-CS-), 1504 (C=C), 1435 (C=S). Calc. for

$C_{19}H_{18}Cl_2N_2OS.1/3H_2O$: C, 59.86; H, 5.63; Cl, 16.06; N, 6.35; O, 4.83; S, 7.26 %. Found: C, 59.95; H, 5.40; N, 6.16 %.

5,5-Bis-(4-chloro-phenyl)-3-octyl-2-thioxo-imidazolidin-4-one (18). IR (KBr, cm^{-1}) ν 3159 (NH), 1751 (C=O), 1591 (-CS-), 1491 (C=C), 1437 (C=S). Calc. for $C_{23}H_{26}Cl_2N_2OS$: C, 61.46; H, 5.83; Cl, 15.78; N, 6.23; O, 3.56; S, 7.13 %. Found: C, 61.44; H, 5.59; N, 6.13 %.

3-Benzyl-5,5-bis-(4-chloro-phenyl)-2-thioxo-imidazolidin-4-one (19). IR (KBr, cm^{-1}) ν 3153 (NH), 1750 (C=O), 1592 (-CS-), 1507 (C=C), 1424 (C=S). Calc. for $C_{22}H_{16}Cl_2N_2OS$: C, 61.83; H, 3.77; Cl, 16.59; N, 6.56; O, 3.74; S, 7.50 %. Found: C, 61.73; H, 3.58; N, 6.48 %.

5,5-Bis-(4-chloro-phenyl)-3-phenethyl-2-thioxo-imidazolidin-4-one (20). IR (KBr, cm^{-1}) ν 3172 (NH), 1758 (C=O), 1591 (-CS-), 1503 (C=C), 1434 (C=S). Calc. for $C_{23}H_{18}Cl_2N_2OS$: C, 62.59; H, 4.11; Cl, 16.06; N, 6.35; O, 3.62; S, 7.26 %. Found: C, 62.47; H, 4.00; N, 6.25 %.

5,5-Bis-(4-bromo-phenyl)-3-ethyl-2-thioxo-imidazolidin-4-one (21). IR (KBr, cm^{-1}) ν 3147 (NH), 1747 (C=O), 1584 (-CS-), 1505 (C=C), 1439 (C=S). Calc. for $C_{17}H_{14}Br_2N_2OS$: C, 45.23 H, 3.11; Br, 35.19; N, 6.17; O, 3.52; S, 7.06 %. Found: C, 45.23; H, 2.89; N, 6.04 %.

5,5-Bis-(4-bromo-phenyl)-3-isopropyl-2-thioxo-imidazolidin-4-one (22). IR (KBr, cm^{-1}) ν 3257 (NH), 1746 (C=O), 1586 (-CS-), 1472 (C=C), 1396 (C=S). Calc. for $C_{18}H_{16}Br_2N_2OS$: C, 46.17 H, 3.44; Br, 34.13; N, 5.98; O, 3.42; S, 6.85 %. Found: C, 46.20; H, 3.20; N, 5.90 %.

5,5-Bis-(4-bromo-phenyl)-3-butyl-2-thioxo-imidazolidin-4-one (23). IR (KBr, cm^{-1}) ν 3152 (NH), 1749 (C=O), 1584 (-CS-), 1511 (C=C), 1437 (C=S). Calc. for $C_{19}H_{18}Br_2N_2OS$: C, 47.32 H, 3.76; Br, 33.14; N, 5.81; O, 3.32; S, 6.65 %. Found: C, 47.29; H, 3.48; N, 5.79 %.

5,5-Bis-(4-bromo-phenyl)-3-isobutyl-2-thioxo-imidazolidin-4-one (24). IR (KBr, cm^{-1}) ν 3189 (NH), 1753 (C=O), 1587 (-CS-), 1508 (C=C), 1439 (C=S). Calc. for $C_{19}H_{18}Br_2N_2OS$: C, 47.32 H, 3.76; Br, 33.14; N, 5.81; O, 3.32; S, 6.65 %. Found: C, 47.36; H, 3.47; N, 5.78 %.

5,5-Bis-(4-bromo-phenyl)-3-heptyl-2-thioxo-imidazolidin-4-one (25). IR (KBr, cm^{-1}) ν 3151 (NH), 1746 (C=O), 1584 (-CS-), 1505 (C=C), 1435 (C=S). Calc. for $C_{22}H_{24}Br_2N_2OS$: C, 50.40; H, 4.61; Br, 30.48; N, 5.34; O, 3.05; S, 6.12 %. Found: C, 50.48; H, 4.37; N, 5.21 %.

5,5-Bis-(4-bromo-phenyl)-3-octyl-2-thioxo-imidazolidin-4-one (26). IR (KBr, cm^{-1}) ν 3152 (NH), 1745 (C=O), 1583 (-CS-), 1505 (C=C), 1435 (C=S). Calc. for $C_{23}H_{26}Br_2N_2OS$: C, 51.32; H, 4.87; Br, 29.68; N, 5.20; O, 2.97; S, 5.96 %. Found: C, 51.17; H, 4.62; N, 5.16 %.

5,5-Bis-(4-bromo-phenyl)-3-cyclohexyl-2-thioxo-imidazolidin-4-one (27). IR (KBr, cm^{-1}) ν 3154 (NH), 1749 (C=O), 1584 (-CS-), 1514 (C=C), 1451 (C=S). Calc. for $C_{21}H_{20}Br_2N_2OS$: C, 49.63; H, 3.97; Br, 31.44; N, 5.51; O, 3.15; S, 6.31 %. Found: C, 49.56; H, 3.73; N, 5.39 %.

3-Allyl-5,5-bis-(4-bromo-phenyl)-2-thioxo-imidazolidin-4-one (28). IR (KBr, cm^{-1}) ν 3146 (NH), 1757 (C=O), 1584 (-CS-), 1505 (C=C), 1427 (C=S). Calc. for $C_{18}H_{14}Br_2N_2OS$: C, 46.38; H, 3.03; Br, 34.28; N, 6.01; O, 3.43; S, 6.88 %. Found: C, 46.41; H, 2.87; N, 5.90 %.

3-Benzyl-5,5'-bis-(4-bromo-phenyl)-2-thioxo-imidazolidin-4-one (29). IR (KBr, cm^{-1}) ν 3153 (NH), 1750 (C=O), 1585 (-CS-), 1508 (C=C), 1424 (C=S).

5,5-Bis-(4-bromo-phenyl)-3-phenethyl-2-thioxo-imidazolidin-4-one (30). IR (KBr, cm^{-1}) ν 3177 (NH), 1759 (C=O), 1585 (-CS-), 1499 (C=C), 1435 (C=S). Calc. for $C_{23}H_{18}Br_2N_2OS$: C, 52.09; H, 3.42; Br, 30.14; N, 5.28; O, 3.02; S, 6.04 %. Found: C, 52.07; H, 3.13; N, 5.24 %.

3-Butyl-5,5-bis-(4-iodo-phenyl)-2-thioxo-imidazolidin-4-one (31). IR (KBr, cm^{-1}) ν 3153 (NH), 1759 (C=O), 1582 (-CS-), 1508 (C=C), 1433 (C=S). Calc. for $C_{19}H_{18}I_2N_2OS$: C, 39.60 H, 3.15; I, 44.05; N, 4.86; O, 2.78; S, 5.56 %. Found: C, 39.91; H, 2.85; N, 5.14 %.

3-Allyl-5,5-bis-(4-iodo-phenyl)-2-thioxo-imidazolidin-4-one (32). IR (KBr, cm^{-1}) ν 3150 (NH), 1758 (C=O), 1580 (-CS-), 1510 (C=C), 1427 (C=S). Calc. for $C_{18}H_{14}I_2N_2OS$: C, 38.59; H, 2.52; I, 45.31; N, 5.00; O, 2.86; S, 5.72 %. Found: C, 38.88; H, 2.31; N, 5.34%.

5,5'-Bis-(4-bromophenyl)-3-butyl-imidazolidine-2,4-dione (33). IR (KBr, cm^{-1}) ν 3217 (N-H), 2954 (C-H), 1768 (C=O), 1713 (C=O), 1488 (C=C). Calc. for: $C_{19}H_{18}Br_2N_2O_2$: C, 48.95; H, 3.89; Br, 34.28; N, 6.01; O, 6.86%. Found: C, 48.65; H, 3.81; N, 5.93%.

3-Benzyl-5,5'-bis-(4-bromophenyl)-imidazolidine-2,4-dione (34). IR (KBr, cm^{-1}) ν 3218 (NH), 1770 (C=O), 1708 (C=O), 1489 (C=C). Calc. for $C_{22}H_{16}Br_2N_2O_2$: C, 52.83; H, 3.22; Br, 31.95; N, 5.60; O, 6.40 %. Found: C, 52.72; H, 3.10; N, 5.57 %.

3-Butyl-5,5-bis-(4-iodo-phenyl)-imidazolidine-2,4-dione (35). IR (KBr, cm^{-1}) ν 3210 (NH), 1775 (C=O), 1700 (C=O), 1495 (C=C). Calc. for: $C_{19}H_{18}I_2N_2O_2$: C, 40.74; H, 3.24; I, 45.31; N, 5.00; O, 5.71%. Found: C, 40.96; H, 2.92; N, 5.33%.

3-Allyl-5,5-bis-(4-iodo-phenyl)-imidazolidine-2,4-dione (36). IR (KBr, cm^{-1}) ν 3212 (NH), 1778 (C=O), 1704 (C=O), 1498 (C=C). Calc. for: $C_{18}H_{14}I_2N_2O_2$: C, 39.73; H, 2.59; I, 46.64; N, 5.15; O, 5.88%. Found: C, 39.73; H, 2.31; N, 5.31%.

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