Supporting Informations

It is "Thiazoidene-2-imine" and not Imidazole-2-thione as the Reaction Product of 1-Benzoyl-3-phenylthiourea with Br_2/ Enolizable Ketone

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General information:

All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60-120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F_{254} (0.25mm). NMR spectra were recorded in $CDCl_3$ or DMSO-d_6 with tetra methyl silane as the internal standard for ^{1}H NMR (400 MHz) $CDCl_3$ or DMSO-d_6 solvent as the internal standard for ^{13}C NMR (100 MHz). Melting points were recorded on Buchi B-545 melting point apparatus and are uncorrected. IR spectra were recorded in KBr or neat on a Nicolet Impact 410 spectrophotometer.

Crystallographic Description:

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoKα radiation (λ = 0.71073 Å) at 298 K. Cell parameters were retrieved using SMART software and refined with SAINT on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS. The structure was solved by direct methods implemented in SHELX-9716 program and refined by full-matrix least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. All the colorless crystals were isolated in rectangular shape from absolute ethanol at room temperature

Procedure for the preparation of 1-benzoyl-3-phenyl-4-methyl-thiazolidene-2-imine (1a) using EDPBT.

1-Benzoyl-3-phenyl-thiourea (1 mmol) in acetone (5 mL) and triethylamine (1 mmol) was taken in a 50 mL three-necked flask. Maintaining the nitrogen atmosphere the reaction flask was fitted with rubber septums. Separetely in a 25 mL round bottom flask containing acetone (5 mL), 1,1'-(ethane-1,2-diyl)dipyridinium bistribromide (EDPBT) (0.5 mmol) was added and stirred for 10 minutes which was then added to above reactio

in dropwise under the atmosphere of nitrogen. After complition of the reaction (1 hrs) the precipitated 1,1'-(ethane-1,2-diyl)dipyridinium dibromide (EDPDB was filtered. The filtrate was concentrated and purified over a silicagel column using ethylacetete / hexane as eluent to yield 1-benzoyl-3-phenyl-4-methyl-thiazol**idene**-2-imine (**1a**).

Spectral data

1-Benzoyl-3-phenyl-4-methyl-thiazolidene-2-imine (1a):

Yield 74 %, mp 156-157^{o}C, IR (KBr): υ 3851, 3736, 3650, 1598, 1564, 1491, 1458, 1364, 1342, 1275, 1171, 1066, 1017, 903 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.08 (s, 3H, CH_3) 6.39 (s, 1H), 7.31 (m, 5H), 7.54 (m, 3H), 8.01 (m, 2H). Elemantal Anal. Calcd for $C_{17}H_{14}N_2OS$: C, 69.36; H, 4.79; N 9.52, S, 10.89. Found C, 69.47; H, 4.81; N 9.47, S, 10.78.

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1-Benzoyl-3,4-diphenyl-thiazolidene-2-imine (1b):

Yield 77 %, IR (KBr): υ 3105, 3064, 2927, 1598, 1559, 1566, 1492, 1466, 1450, 1435, 1337, 1279, 1200, 1166, 1024, 899, 713 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.70 (s, 1H), 7.12 (d, 2H, *J* = 8.4 Hz), 7.23 (m, 6H), 7.33 (t, 2H, *J* = 7.6 Hz), 7.39 (d, 3H, *J* = 7.0 Hz), 8.10 (d, 2H, *J* = 8.4 Hz), ^{13}CNMR (100 MHz, $CDCl_3$): δ 107.6, 128.1, 128.5, 128.6, 128.9, 129.0, 129.4, 130.7, 131.6, 136.8, 137.7, 139.2, 170.0, 174.7.

1-Benzoyl (4-hydroxy-3,4-diphenyl-thiazolidine)-2-imine (1d):

Yield 74 %, IR (KBr): υ 3222, 3064, 2927, 1595, 1562, 1474, 1392, 1324, 1210, 1017, 999, 790, 697 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.53 (d, 1H, *J* = 12.4 Hz), 3.72 (d, 1H, *J* = 12.4 Hz),7.20 (m, 10H), 7.40 (m, 1H), 7.49 (d, 2H, *J* = 7.6 Hz), 7.61 (s,1H), 7.85 (d, 2H, *J* = 7.0 Hz).^{13}CNMR (100 MHz, $CDCl_3$): δ 43.8, 93.4, 126.3, 126.7, 127.7, 127.8, 128.3, 128.9, 131.7, 136.1, 138.5, 141.1, 171.8, 175.2.

1-(3-Bromobenzoyl)-3-phenyl-4-methyl-thiazolidene-2-imine (2a):

Yield 80 %, IR (KBr): υ 3064, 2923, 1596, 1557, 1496, 1459, 1450, 1337, 1255, 1127, 1033, 907, 739 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.06 (s, 3H), 6.40 (s 1H), 7.17 (t, 1H, *J* = 8.0 Hz), 7.32 (d, 2H, *J* = 7.6 Hz), 7.54 (m, 4H), 7.93 (d, 1H, *J* = 6.8 Hz), 8.15

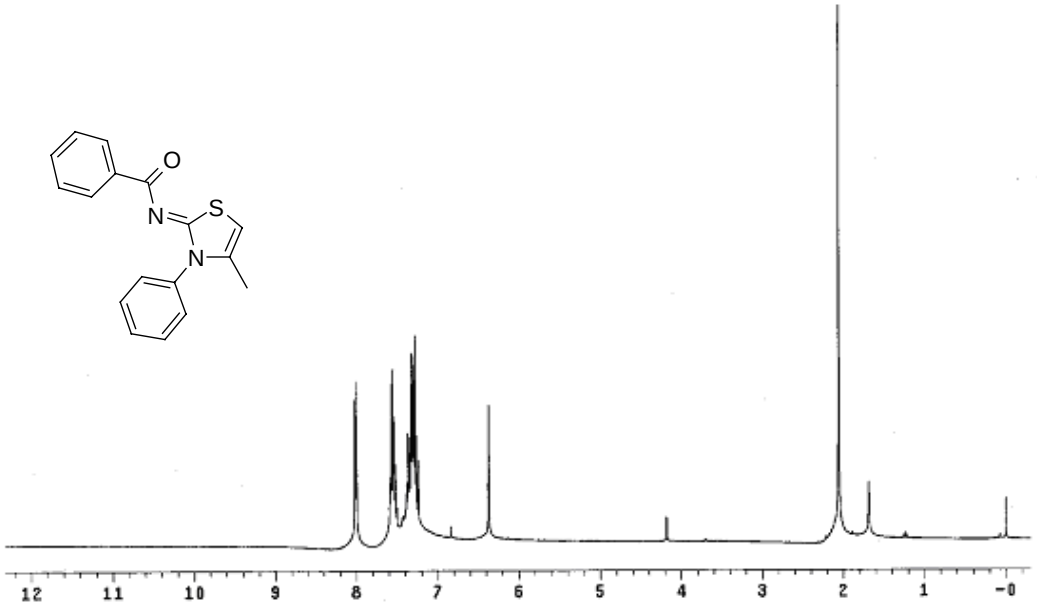
(s, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 15.2, 104.9, 122.2, 127.9, 128.1, 128.5, 129.6, 129.7, 132.5, 134.2, 134.7, 137.3, 139.1, 170.3, 172.9.

1-(3-Bromobenzoyl)-3,4-diphenyl-thiazolidene-2-imine (2b):

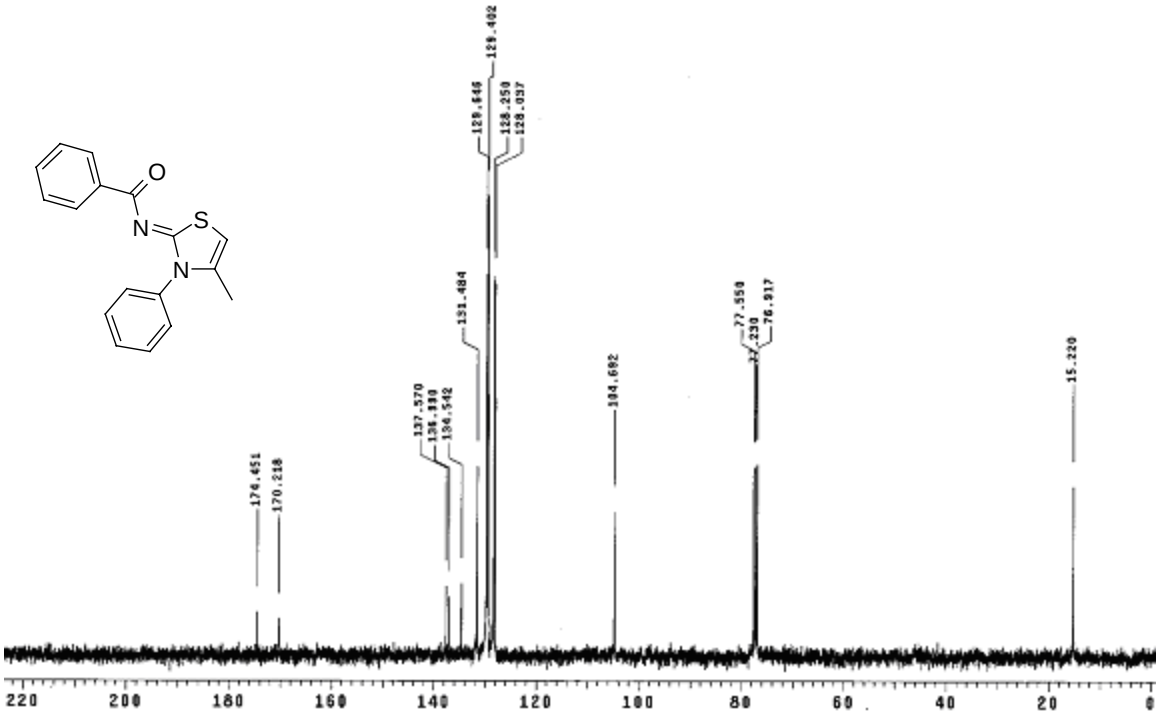
Yield 82 %, IR (KBr): υ 3058, 1599, 1559, 1438, 1337, 1280, 1193, 1066, 930, 746 cm^{-1}. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.74 (s, 1H), 7.13 (d, 2H, 7.2 Hz), 7.24 (m, 7H), 7.42 (d, 2H, *J* = 6.8 Hz), 7.53 (d, 1H, *J* = 8 Hz), 8.01 (d, 1H, *J* = 7.6 Hz), 8.23 (1H, s). ^{13}C NMR (100 MHz, $CDCl_3$): δ: 107.8, 122.3, 128.0, 128.6, 128.8, 129.0, 129.1, 129.7, 130.5, 132.6, 134.4, 137.6, 139.0, 139.4, 170.1, 173.2.

SPECTRA

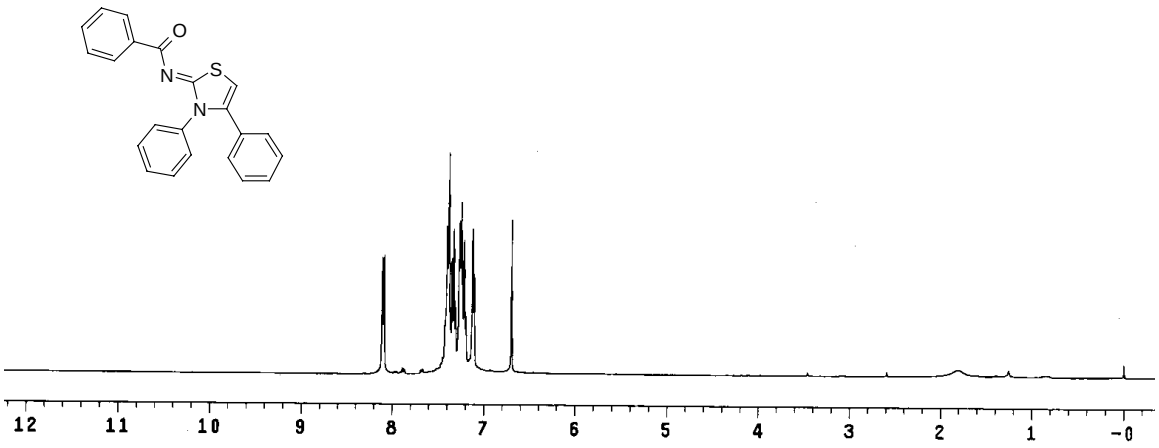
1-Benzoyl-3-phenyl-4-methyl-thiazolidene-2-imine (1a): ^{1}H NMR (400 MHz, $CDCl_3$):



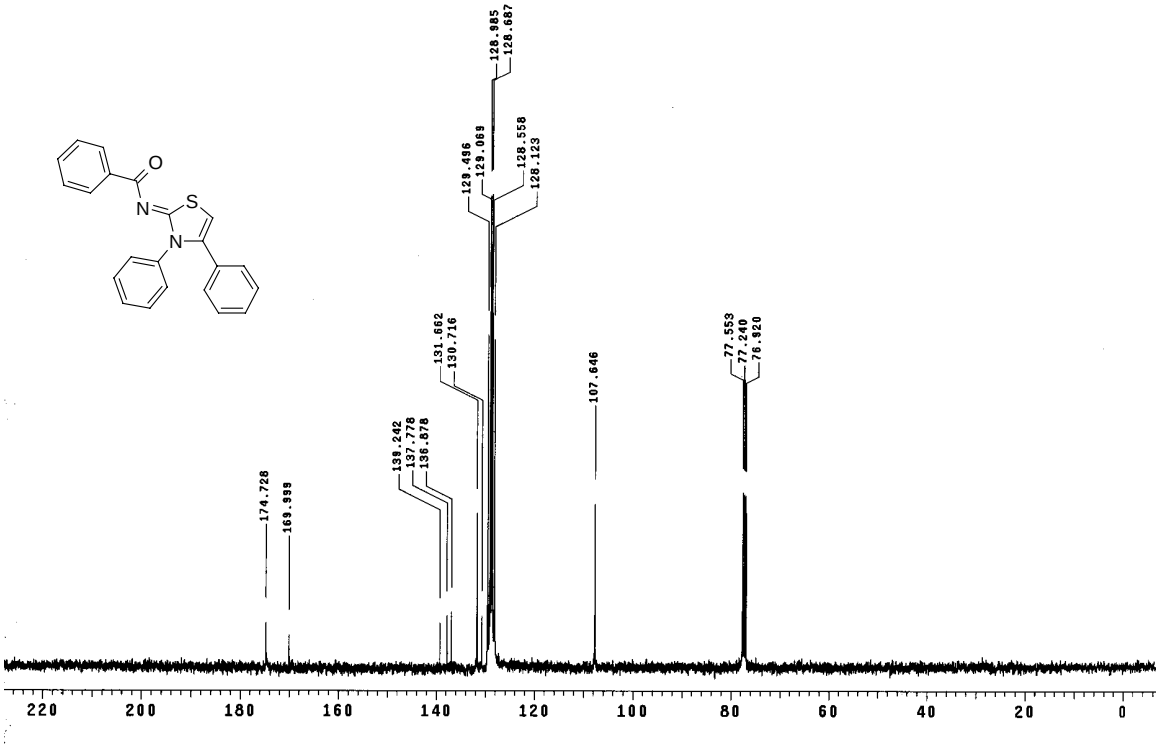
1-Benzoyl-3-phenyl-4-methyl-thiazolidene-2-imine (1a): ^{13}C NMR (100 MHz, $CDCl_3$):



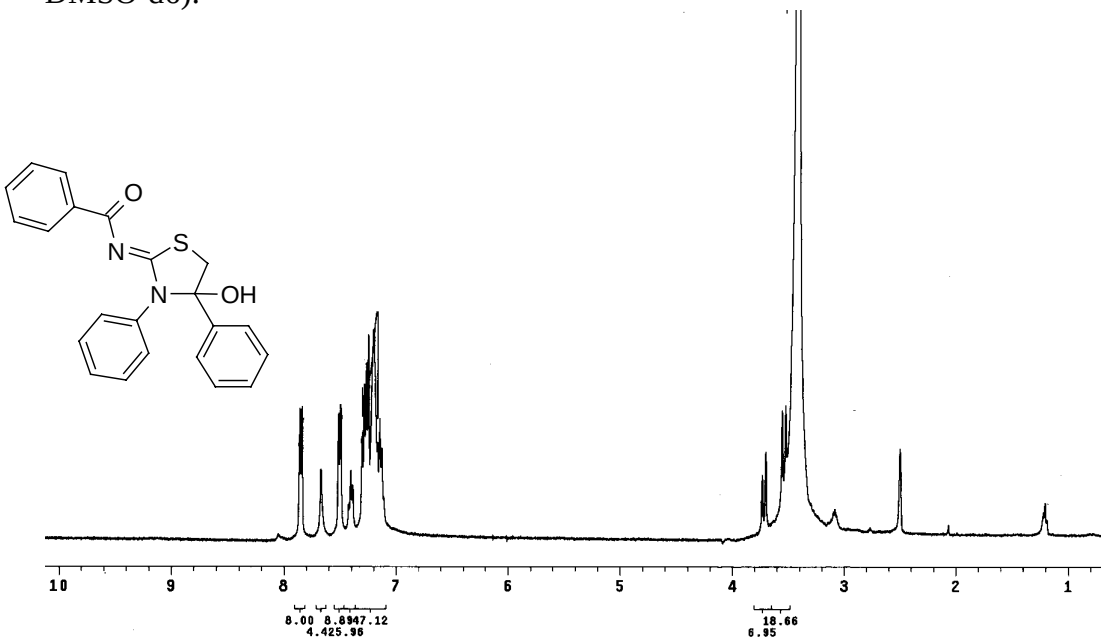
1-Benzoyl-3,4-diphenyl-thiazolidene-2-imine (1b): ^{1}H NMR (400 MHz, $CDCl_3$):



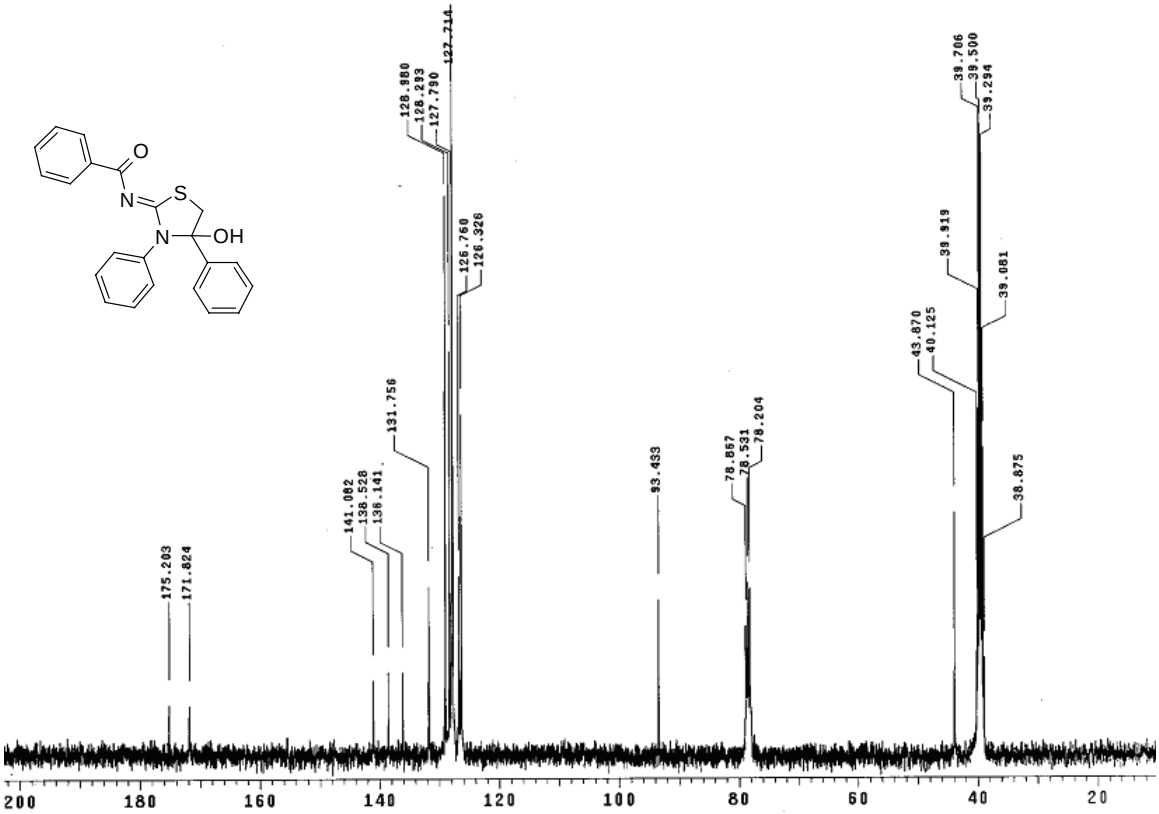
1-Benzoyl-(3,4-diphenyl-thiazolidene-2-imine (1b): ^{13}C NMR (100 MHz, $CDCl_3$):



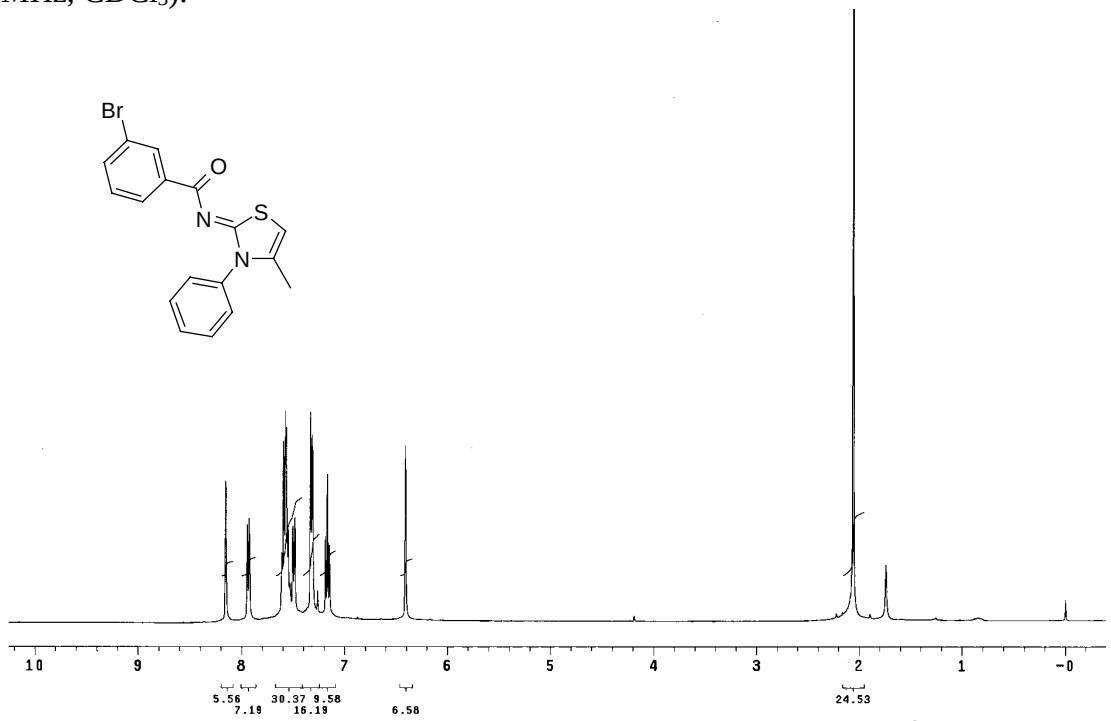
1-Benzoyl (4-hydroxy-3,4-diphenyl-thiazolidine)-2-imine (1d): ^{1}H NMR (400 MHz, DMSO-d6):



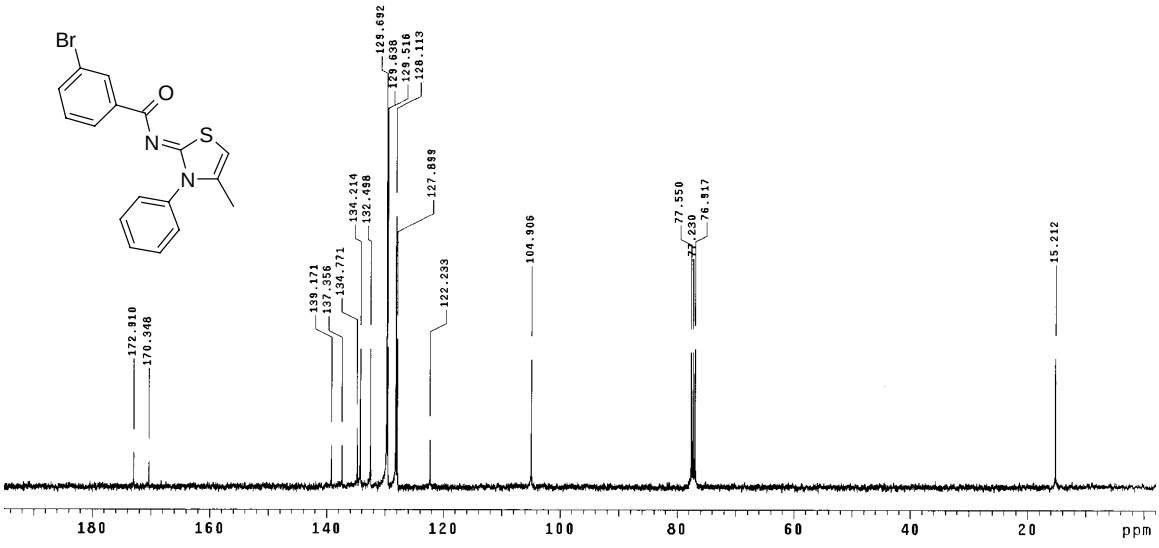
1-Benzoyl (4-hydroxy-3,4-diphenyl-thiazolidine)-2-imine (1d): ^{13}C NMR (100 MHz, DMSO-d6):



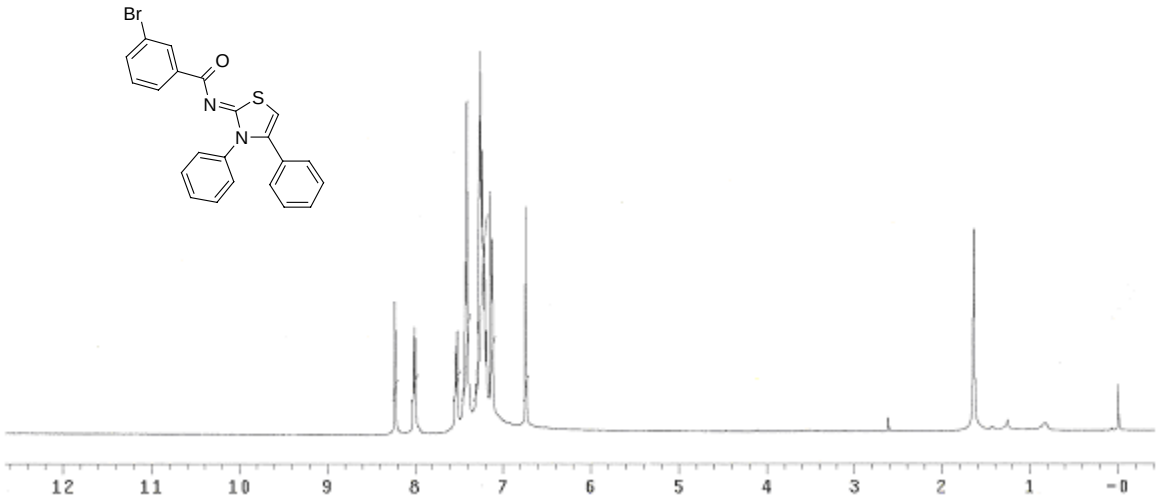
1-(3-Bromobenzoyl)-3-phenyl-4-methyl-thiazolidene-2-imine (2a): ^{1}H NMR (400 MHz, $CDCl_3$):



1-(3-Bromobenzoyl)-3-phenyl-4-methyl-thiazolidene-2-imine (2a) ^{13}C NMR (100 MHz, $CDCl_3$):



1-(3-Bromobenzoyl)-3,4-diphenyl-thiazolidene-2-imine (2b). ^{1}H NMR (400 MHz, $CDCl_3$):



1-(3-Bromobenzoyl)-3,4-diphenyl-thiazolidene-2-imine (2b). ^{13}C NMR (100 MHz, $CDCl_3$):