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SUPPLEMENTARY MATERIAL TO

Synthesis of and theoretical research on some azine derivatives and investigation of their antimicrobial activities

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CONTENTS

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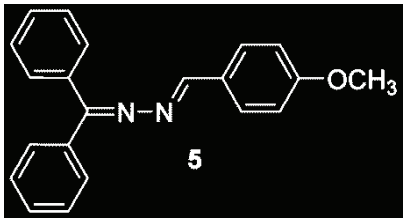
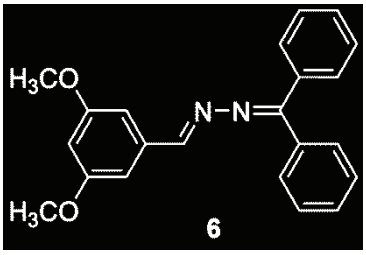
SPECTROSCOPIC DATA OF MAIN COMPOUNDS

*1-(diphenylmethylene)-2-(4-methoxybenzylidene)hydrazine (**5**)*



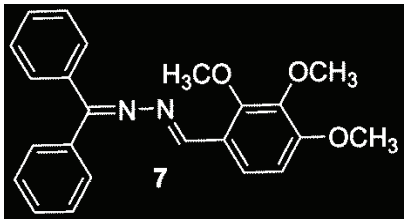
Yield: 97%, yellow solid, m.p. 95-96 °C. R_f: 0.66 (Ethyl acetate/P.Ether, 1:4)
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (s, 1H), 7.84-7.72 (m, 2H), 7.65 (d, *J* = 8.8 Hz, 2H), 7.56-7.35 (m, 8H), 6.93 (d, *J* = 8.8 Hz, 2H), 3.86 (s, 3H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.02, 161.86, 159.30, 138.51, 135.58, 130.49, 130.21, 130.13, 129.12, 128.88, 128.23, 127.53, 127.46, 114.16, 55.37.
FT-IR (cm^{-1}): 1605 (HC=N), 1567 (C=N), 1511, 1491, 1443, 1413, 1301, 1252.
Elemental Anal.Calcd. for $C_{21}H_{18}N_2O$ C, 80.23; H, 5.77; N, 8.91 Found C, 80.36; H, 5.42; N,8.93.

*1-(3,5-dimethoxybenzylidene)-2-(diphenylmethylene)hydrazine (**6**):*



Yield: 96%, yellow solid, m.p. 86-87 °C.
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 7.75 (dd, *J* = 8.2, 1.3 Hz, 2H), 7.53 – 7.33 (m, 8H), 6.85 (d, *J* = 2.3 Hz, 2H), 6.54 (t, *J* = 2.3 Hz, 1H), 3.79 (s, 6H).
^{13}C NMR (100 MHz, $CDCl_3$) δ 166.27, 160.86, 158.84, 138.23, 136.58, 135.29, 130.57, 130.32, 129.20, 129.06, 128.27, 127.47, 106.12, 103.42, 55.41.
FT-IR (cm^{-1}): 1590 (HC=N), 1456, 1425, 1356, 1297, 1202.
Elemental Anal.Calcd. for $C_{22}H_{20}N_2O_2$ C, 76.72; H, 5.85; N, 8.13; Found: C, 76.79; H, 5.78; N, 8.10.

1-(diphenylmethylene)-2-(2,3,4-trimethoxybenzylidene)hydrazine (7):



Yield: 97%, yellow solid, m.p. 70-72 °C.

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.51 (s, 1H), 7.82-7.71 (m, 2H), 7.49-7.35 (m, 8H), 6.94 (s, 2H), 3.91 (s, 3H), 3.84 (s, 6H, 2xOCH_3).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.18, 158.56, 153.40, 140.48, 138.24, 135.46, 130.61, 130.31, 130.17, 129.18, 129.01, 128.68, 128.29, 127.90, 127.44, 105.44, 60.94, 56.07 (2C).

FT-IR (cm^{-1}): 1574 (C=N), 1502 (C=C aromatic), 1461, 1414, 1359 (C-N), 1126.

Elemental Anal. Calcd. for $C_{23}H_{22}N_2O_3$ C, 73.78; H, 5.92; N, 7.48 Found: C, 73.34; H, 5.58; N, 7.76.

TABLE S-I. HOMO, LUMO, HOMO-LUMO gap and selected molecular properties of **5**, **6,** and **7**

		Energy (eV)		Energy gap (eV)	Ionization Potential (I) (eV)	Electron affinity (A) (eV)	Global Hardness (η) (eV)	Electronegativity (χ) (eV)	Chemical potential (μ) (eV)	Global Softness (σ) $(eV)^{-1}$	Global electrophilicity (ω) (eV)
	HOMO	-5.987	$\Delta E_{HOMO-LUMO}$	4.083	5.987	1.904	2.042	3.946	-3.946	0.245	3.813
	LUMO	-1.904									
5	HOMO-1	-6.088	$\Delta E_{(H-1)-(L+1)}$	5.131	6.088	0.956	2.566	3.522	-3.522	0.195	2.418
	LUMO+1	-0.956									
	HOMO	-5.922	$\Delta E_{HOMO-LUMO}$	4.058	5.922	1.864	2.029	3.893	-3.893	0.246	3.735
	LUMO	-1.864									
6	HOMO-1	-5.992	$\Delta E_{(H-1)-(L+1)}$	5.069	5.992	0.923	2.535	3.457	-3.457	0.197	2.358
	LUMO+1	-0.923									
	HOMO	-5.791	$\Delta E_{HOMO-LUMO}$	3.993	5.791	1.797	1.997	3.794	-3.794	0.250	3.604
	LUMO	-1.797									
7	HOMO-1	-5.791	$\Delta E_{(H-1)-(L+1)}$	4.902	5.791	0.888	2.451	3.339	-3.339	0.204	2.275
	LUMO+1	-0.888									

$I = -E_{HOMO}$, $A = -E_{LUMO}$, $\eta = ((I-A))/2$, $\chi = ((I+A))/2$, $\mu = (-(I+A))/2$, $\sigma = 1/2\eta$, $\omega = \mu^2/2\eta$

NMR SPECTRA OF MAIN COMPOUNDS

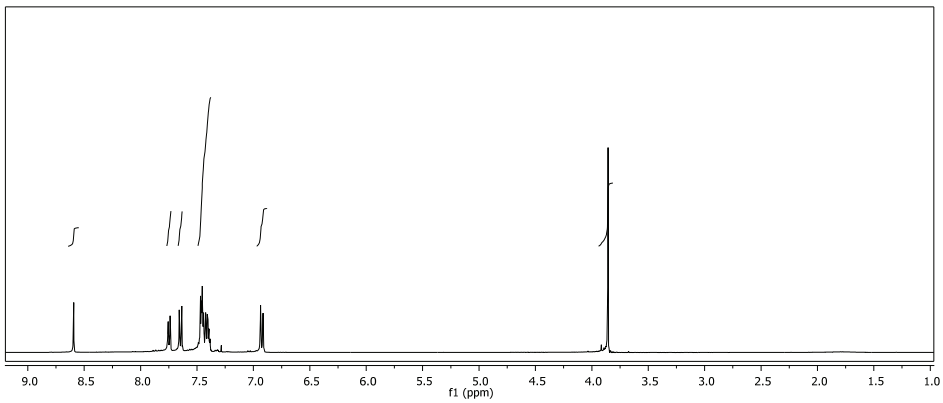


Figure S-1. ^{1}H NMR spectrum of 1-(diphenylmethylene)-2-(4-methoxybenzylidene)hydrazine (**5**) in $CDCl_3$

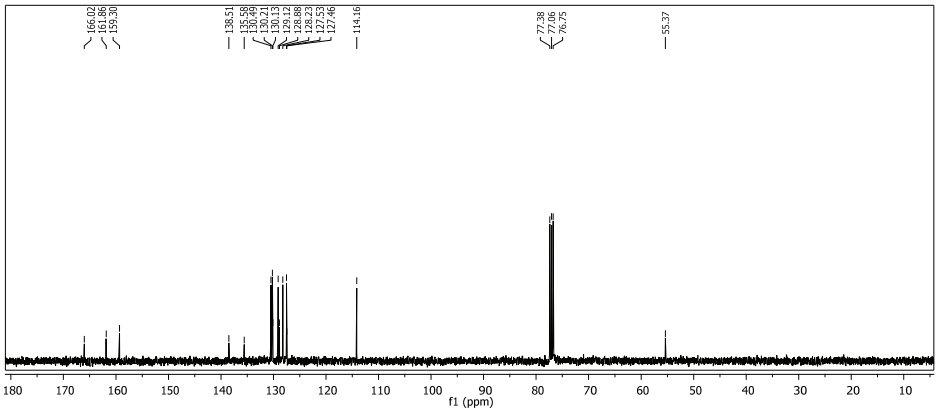


Figure S-2. ^{13}C NMR spectrum of 1-(diphenylmethylene)-2-(4-methoxybenzylidene)hydrazine (**5**) in $CDCl_3$

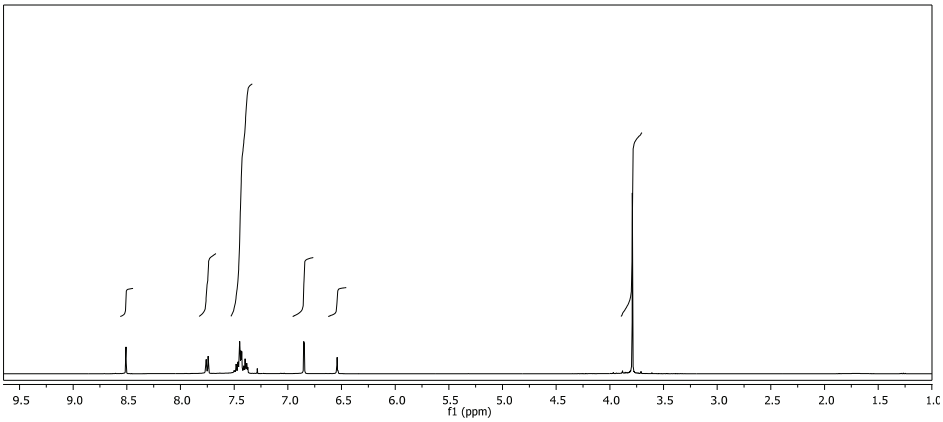


Figure S-3. ^{1}H NMR spectrum of 1-(3,5-dimethoxybenzylidene)-2-(diphenylmethylene)hydrazine (**6**) in $CDCl_3$

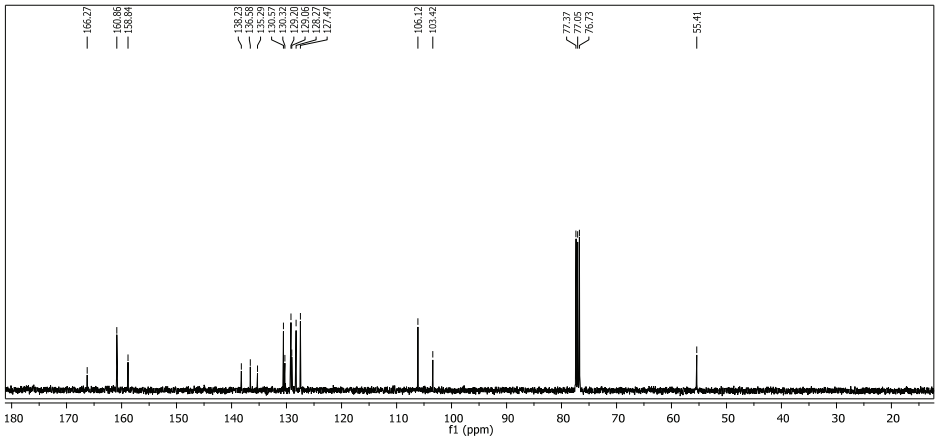


Figure S-4. ^{13}C NMR spectrum of 1-(3,5-dimethoxybenzylidene)-2-(diphenylmethylene)hydrazine (**6**) in $CDCl_3$

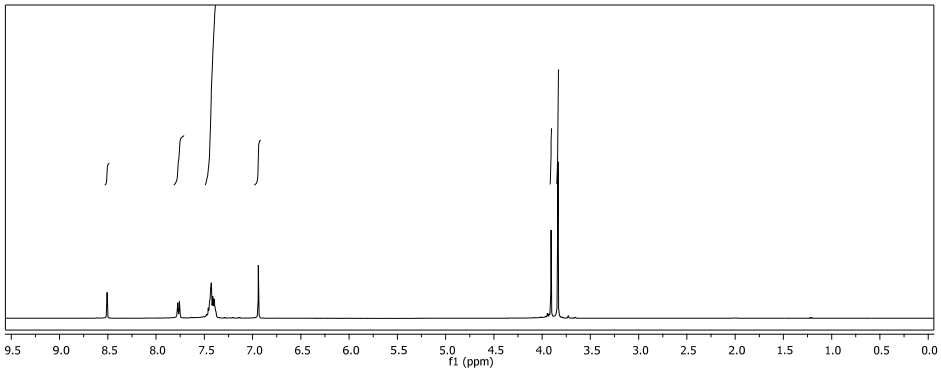


Figure S-5. ^{1}H NMR spectrum of 1-(diphenylmethylene)-2-(2,3,4-trimethoxybenzylidene)hydrazine (**7**) in $CDCl_3$

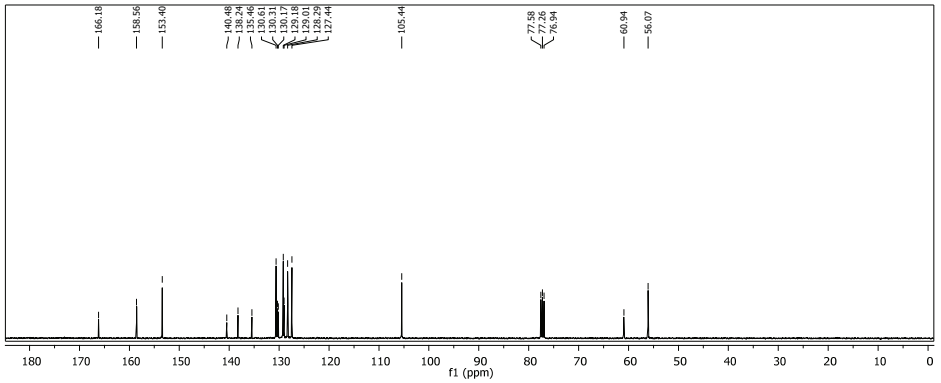


Figure S-6. ^{13}C NMR spectrum of 1-(diphenylmethylene)-2-(2,3,4-trimethoxybenzylidene)hydrazine (**7**) in $CDCl_3$