Article

Hydrazones Derived from Methyl 4-Phenylpicolinimidate: Differences in Structure and Antimicrobial Activity

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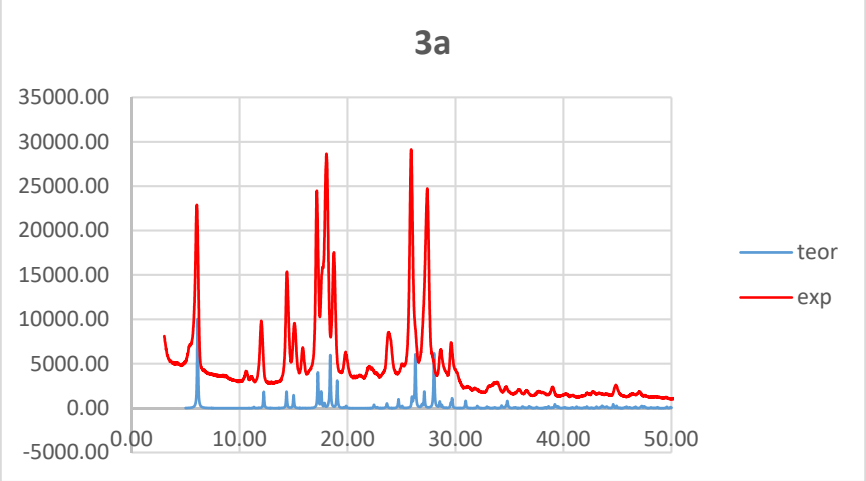
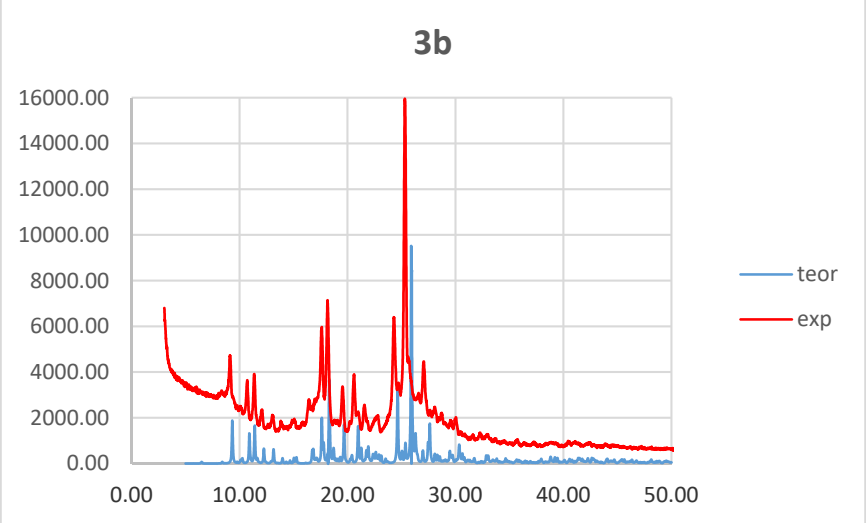
Supplementary Materials





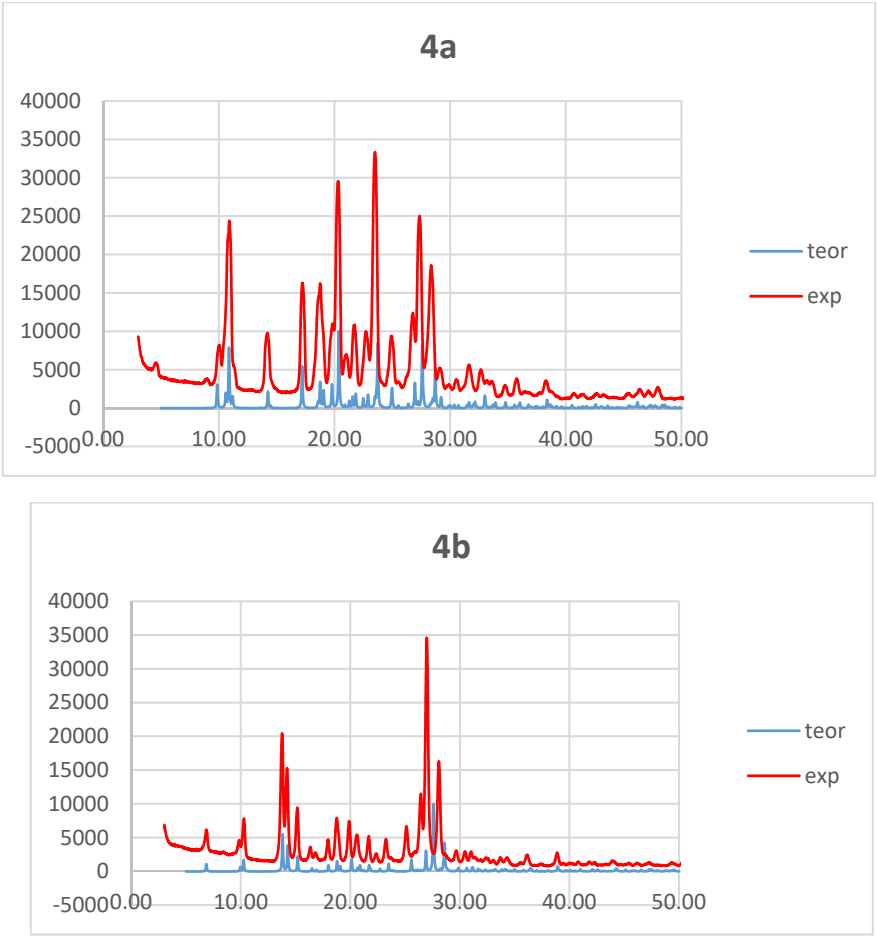


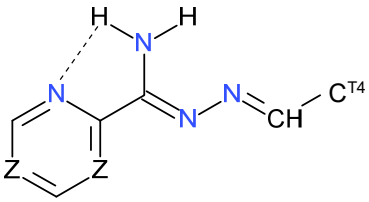
Figure S1. Powder diffraction patterns for the studied compounds- experimental and theoretical calculated for single crystal structure.

Table S1. Selected bonds lengths (Å) in the studied structures and the mean values found in similar compounds within Cambridge Structural Database [54]. CSD quests for molecular fragments are shown in Scheme A1. "X" denoted -NH_2 in **3a,b** and =O in **4a,b**, respectively.

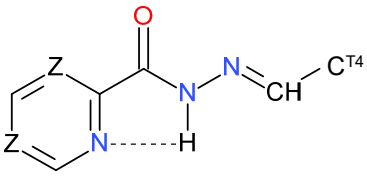
Crystal Structure(s)	C1-C	C1-N2	N2-N3	N3-C4	C4-C41	C4-X4(N,O)
3a	1.440(3)	1.285(2)	1.390(2)	1.311(2)	1.491(2)	1.342(2)
3b	1.453(3) 1.452(3) 1.448(4) 1.441(4)	1.290(3) 1.292(3) 1.280(5) 1.293(4)	1.390(3) 1.392(3) 1.397(3) 1.391(3)	1.312(3) 1.304(3) 1.298(4) 1.313(3)	1.489(3) 1.496(3) 1.485(4) 1.482(4)	1.333(3) 1.335(3) 1.344(5) 1.343(4)
Mean for **3a,b**	**1.447(5)**	**1.288(3)**	**1.391(3)**	**1.310(5)**	**1.489(4)**	**1.339(3)**
Mean (CSD)	**1.464(4)**	**1.279(5)**	**1.402(4)**	**1.306(6)**	**1.489(3)**	**1.341(4)**
4a	1.445(2)	1.280(2)	1.368(2)	1.361(2)	1.502(2)	1.222(1)
4b	1.447(2)	1.282(2)	1.369(2)	1.355(2)	1.504(2)	1.226(2)
Mean for **4a,b**	**1.446(2)**	**1.281(2)**	**1.369(2)**	**1.358(2)**	**1.503(2)**	**1.224(2)**
Mean (CSD)	**1.459(8)**	**1.278(5)**	**1.375(5)**	**1.349(6)**	**1.500(5)**	**1.224(5)**

Table S2. Selected torsion angles and dihedral angles (phy/phe) between planes defined by the pyridine and phenyl rings (°).

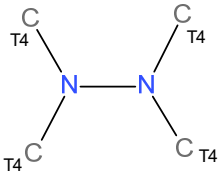
Crystal structure	C-C1-N2-N3	C1-N2-N3-C4	N2-N3-C4-C41	N3-C4-C41-N42	pyr/phe
3a	-179.8(1)	-178.3(1)	178.9(1)	-179.8(1)	28.5(2)
3b	-1.2(4) 0.3(3) 2.8(4) 0.1(4)	-178.9(2) -175.3(2) -169.5(3) -177.4(2)	-177.2(2) -179.4(2) -175.3(2) -177.9(2)	170.3(2) -172.7(2) -177.2(3) 176.8(2)	24.8(2) 31.8(3) 31.9(3) 13.8(2)
4a	179.1(1)	-173.3(1)	179.2(1)	1.2(2)	37.5(2)
4b	-178.4(1)	-173.8(1)	177.1(1)	6.7(2)	28.6(2)



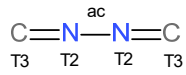
3a,3b, Z-CH or N
Found - 5 structures,
6 independent molecules



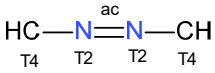
4a,4b, Z-CH or N
Found - 39 structures,
49 independent molecules



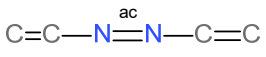
Found - 3 structures with N-N bond lenghsof about 1.50Å[Refcode: AZBNOW, RETHAZ, SOFQOT]



Found - 536 structures,
619 independent molecules
1.403(9) mean N-N
1.208(8) mean N=C



Found - 7 structures,
7 independent molecules
1.234(5) mean N=N



Found - 3 structures,
4 independent molecules
1.283(9) mean N=N
1.382(9) mean N-C

Scheme S1. CSD quests for similar molecular fragments. Tn refer to number (n) of atoms bonded.