

Arylglyoxal oximes as putative C-nucleophiles in eliminative nucleophilic substitution process

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Experimental (general)

¹H NMR and ¹³C NMR spectra were recorded on a Bruker DRX-500 instrument at working frequencies 500.13 MHz for ¹H and 125.76 MHz for ¹³C. Chemical shifts were expressed in parts per million (ppm) and referenced to the appropriate NMR solvent peaks. Mass spectra were recorded on a Finnigan MAT/INCOS 50 mass spectrometer at 70 eV using direct probe injection. Elemental analysis was performed on an automated Perkin-Elmer 2400 CHN micro-analyzer.

Molecular and crystal structure of compound **3a**

The central [1,2,5]oxadiazolo[3,4-*b*]pyrazine bicycle of **3a** is almost planar (rms deviation is 0.036 Å). The (*para*-methoxyphenyl)ketovinyl substituent is practically coplanar to the central bicycle [the twist angle is 6.07(8)°], due to the presence of both the long chain of conjugated bonds and the intramolecular N4—H4...O9 hydrogen bond [N...O 2.600(3) Å, H...O 1.83(3) Å, ∠N—H...O 137(3)°]. The other *para*-methoxyphenyl substituent is rotated by 46.65(5)° relative to this bicycle due to steric reasons.

The bond lengths and angles in the [1,2,5]oxadiazolo[3,4-*b*]pyrazine bicycle of **3a** are very close to those found for similar compounds.¹⁻⁴

The crystal packing of **3a** is stabilized by weak C—H...O and C—H...N hydrogen bonds.

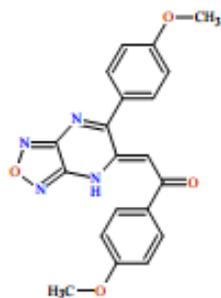
References

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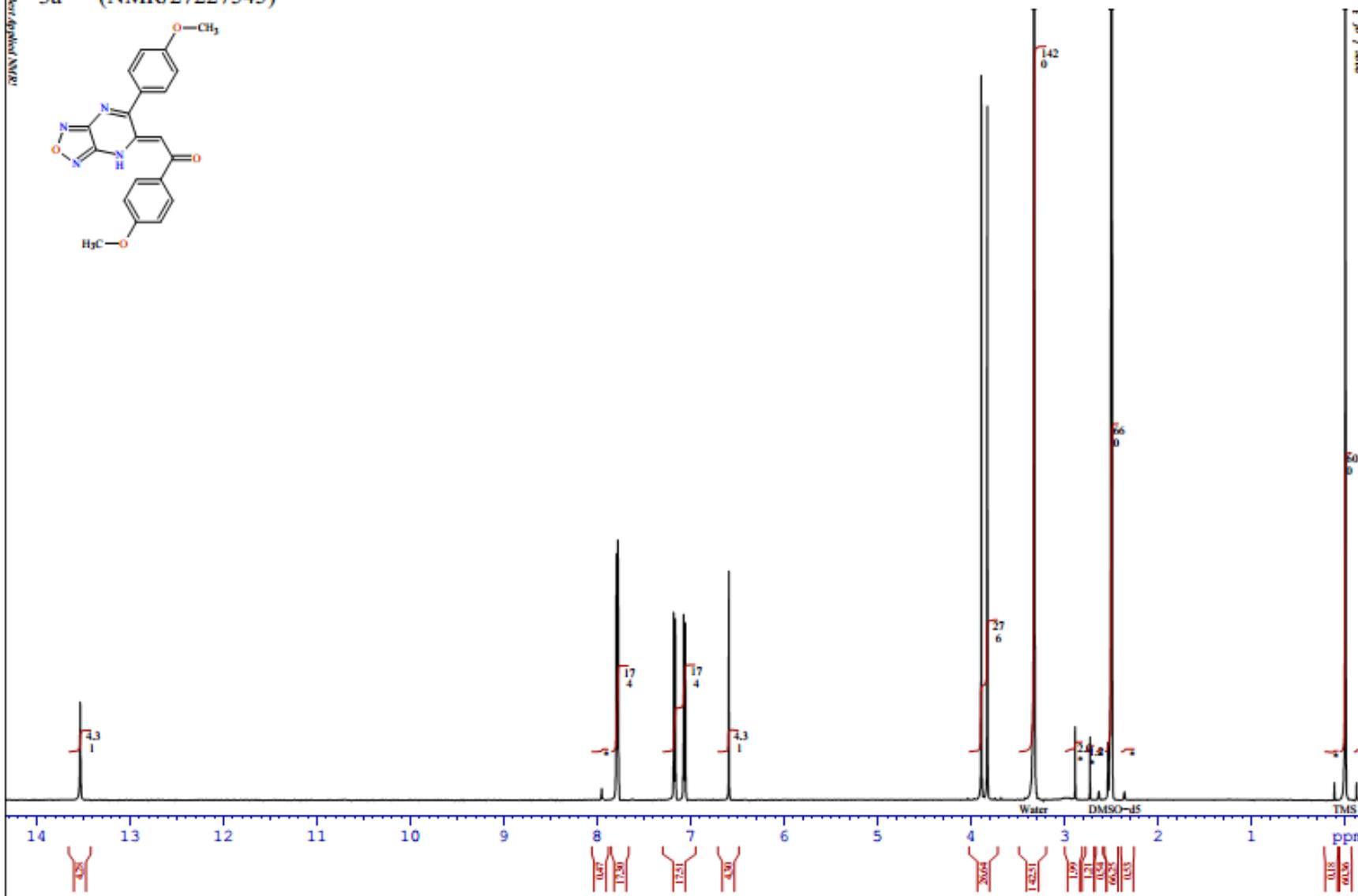
NMR spectra of compounds 3a and 3b

3a (NMR/27227545)

Found protons = 16 impurity* = 4.8 %

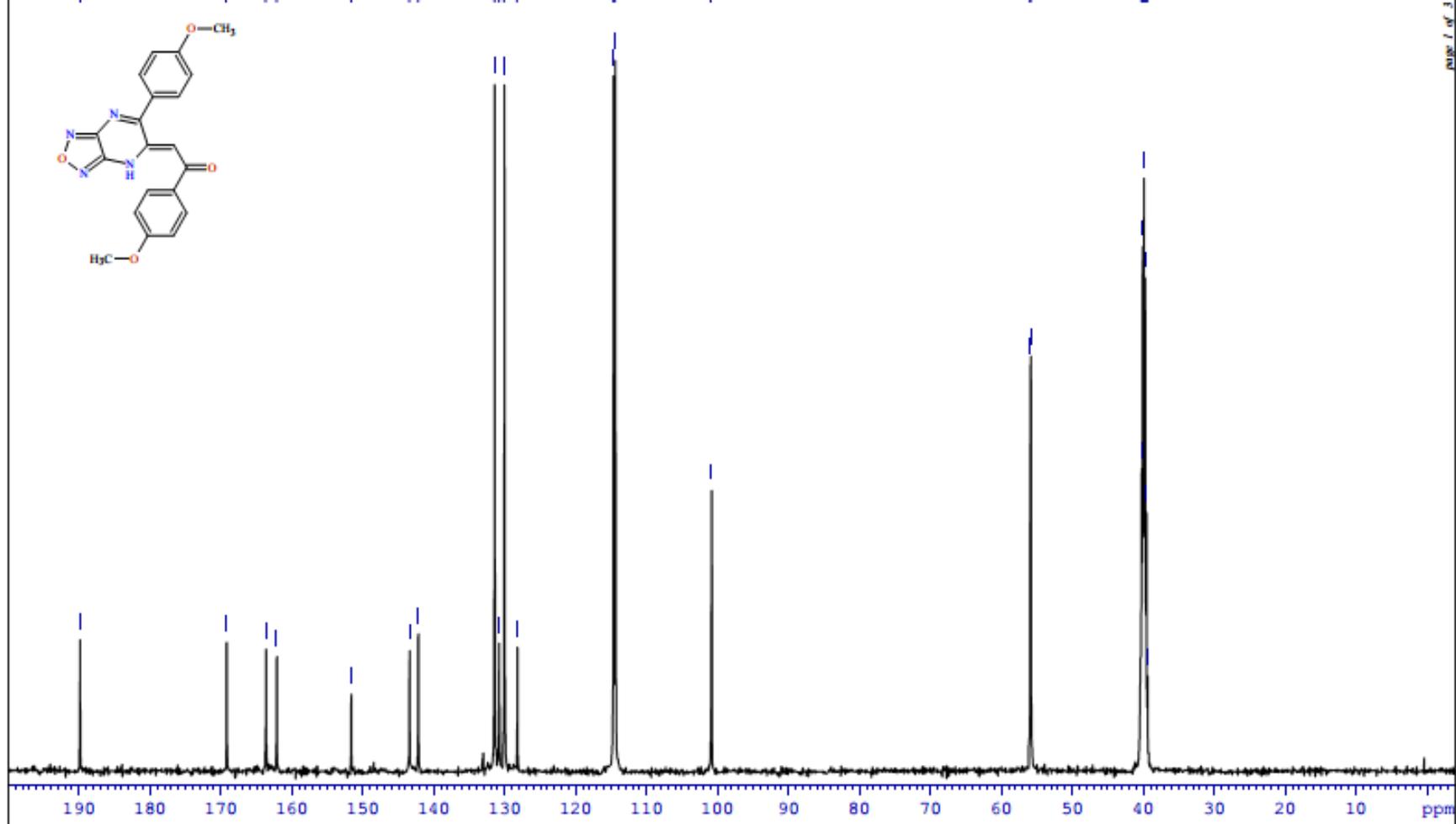
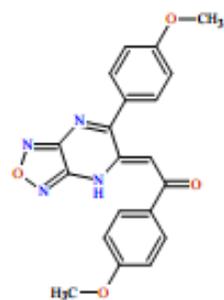


The Best of NMR



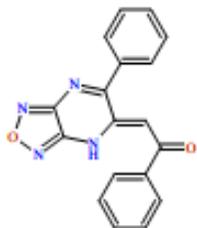
The Best of NMR

3a (NMR/27227716)



3b (NMR/27227048)

Found protons = 17 impurity* < 0.1 %



The Best of NMR

page 1 of 3

