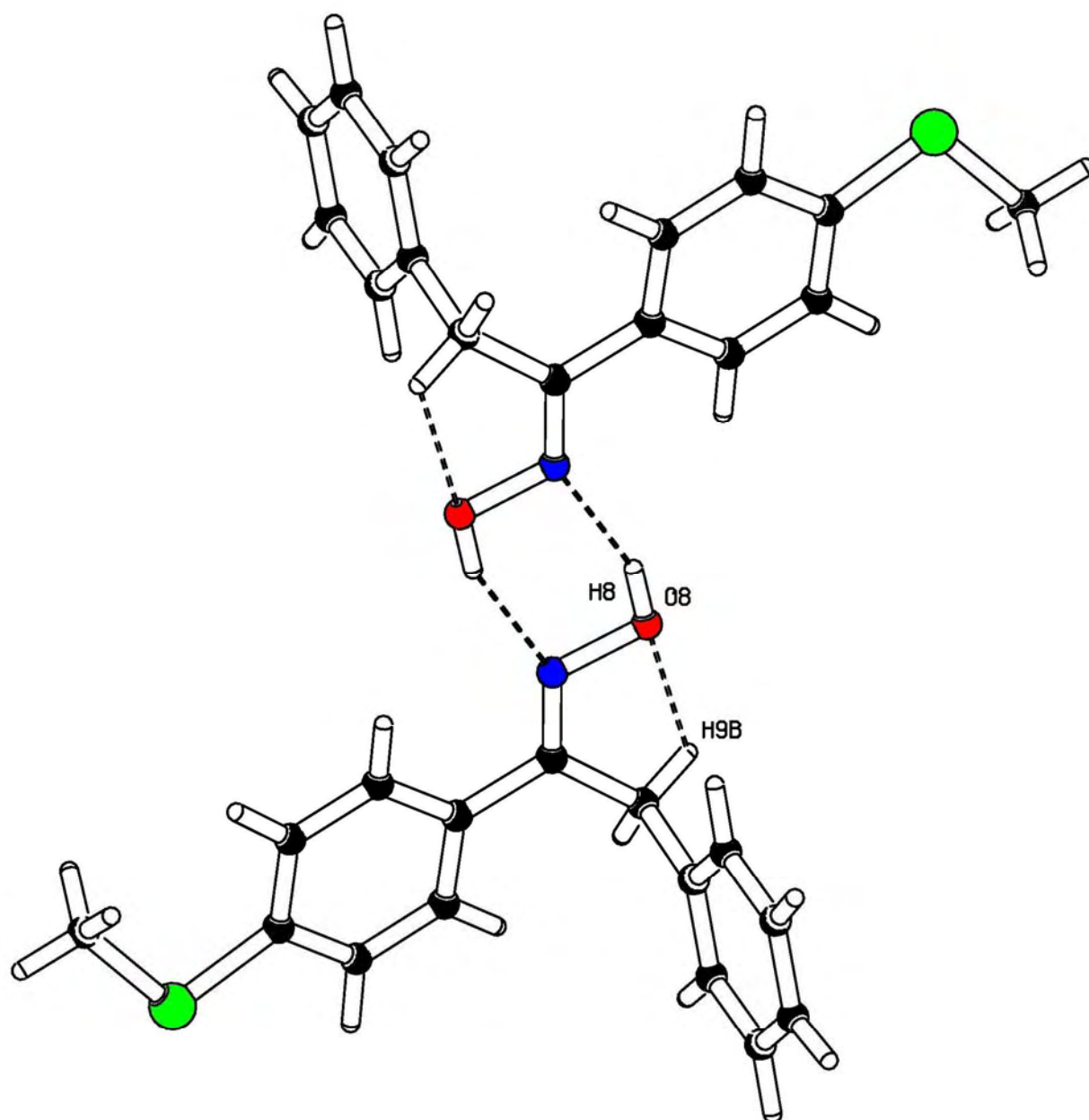
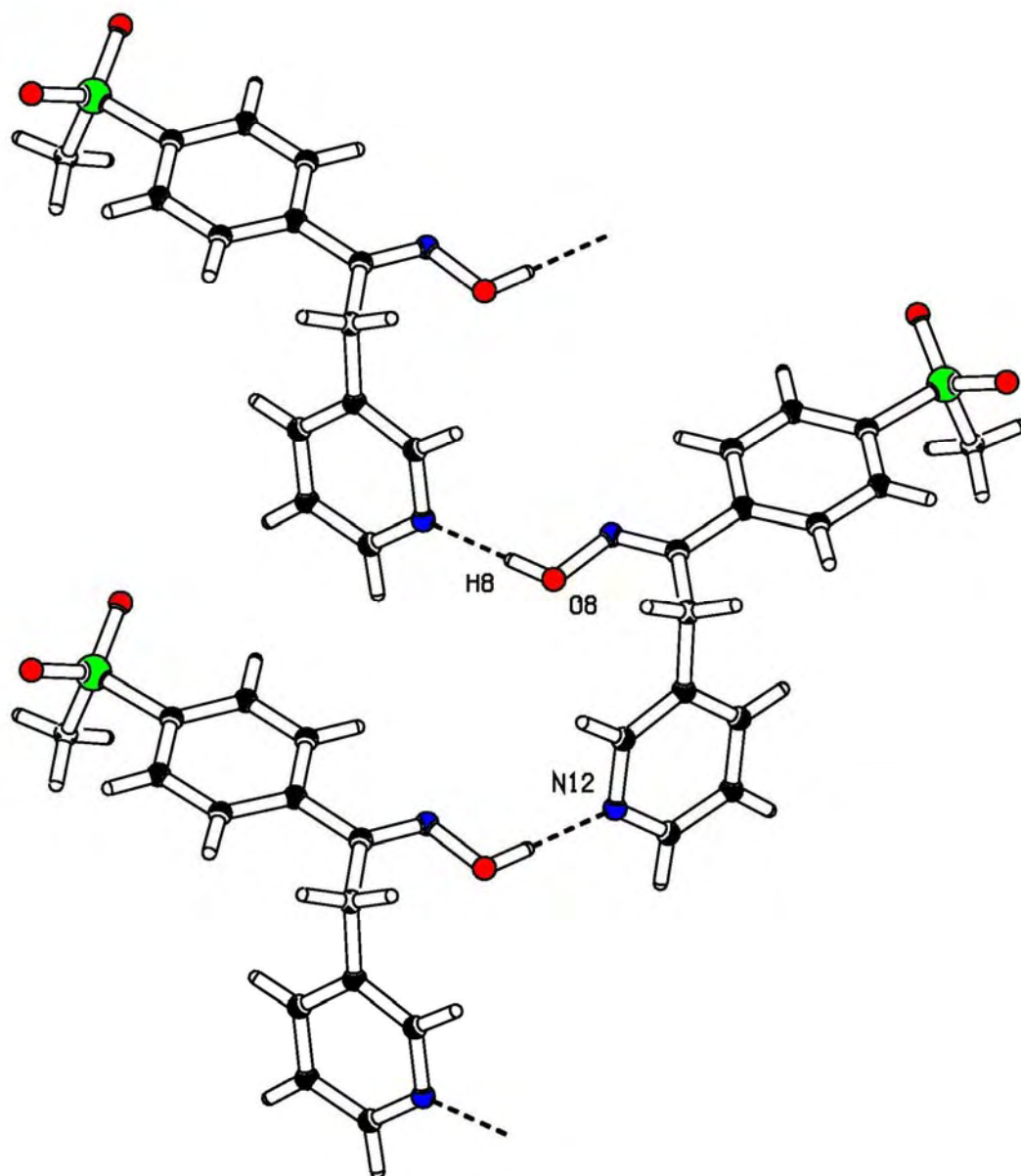


Supplementary Material for 1,2-Diaryl(3-pyridyl)ethanone Oximes. Intermolecular Hydrogen Bonding Networks Revealed by X-ray Diffraction, by Ermitas Alcalde *, Neus Mesquida *, Carmen Alvarez-Rúa , Rosa Cuberes , Jordi Frigola and Santiago García-Granda , *Molecules*, **2008**, *13*, 301-318 (<http://www.mdpi.org/molecules/papers/13020301.pdf>)

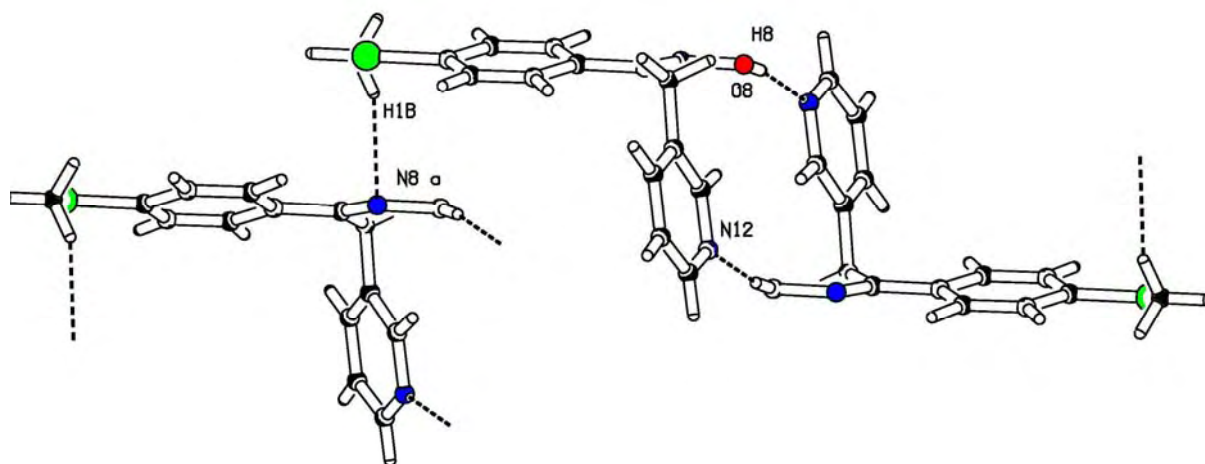
12 pages



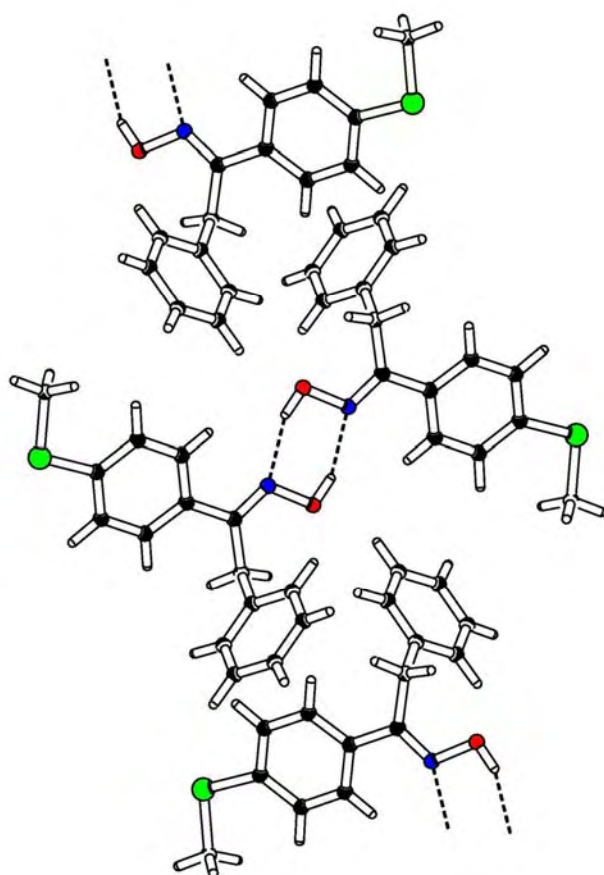
Oxime 6



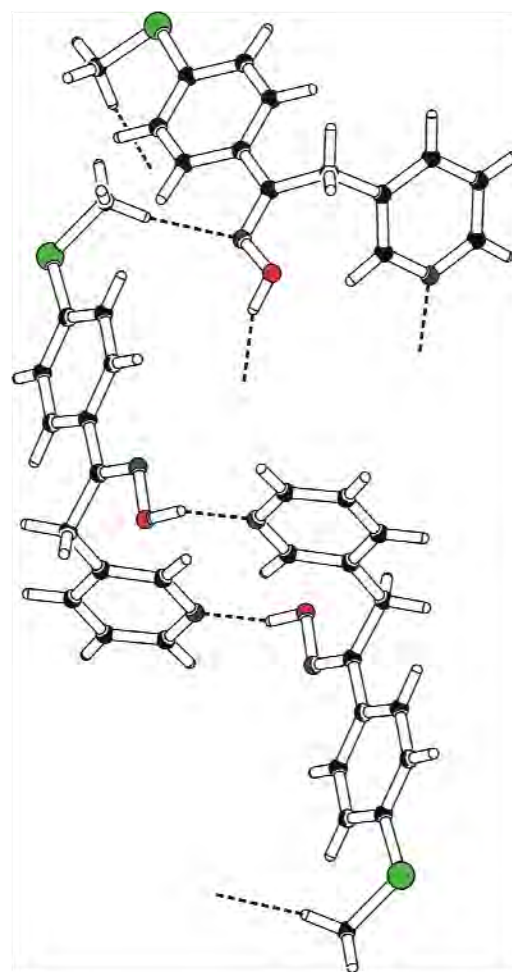
Oxime 7



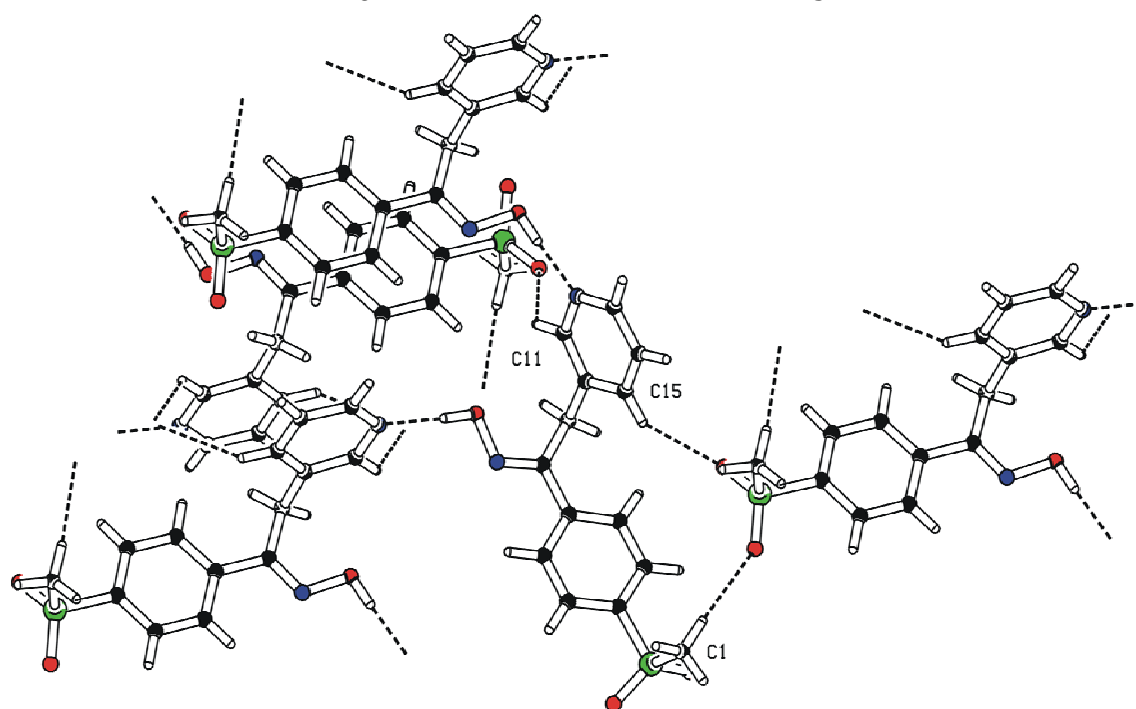
Oxime 9



6

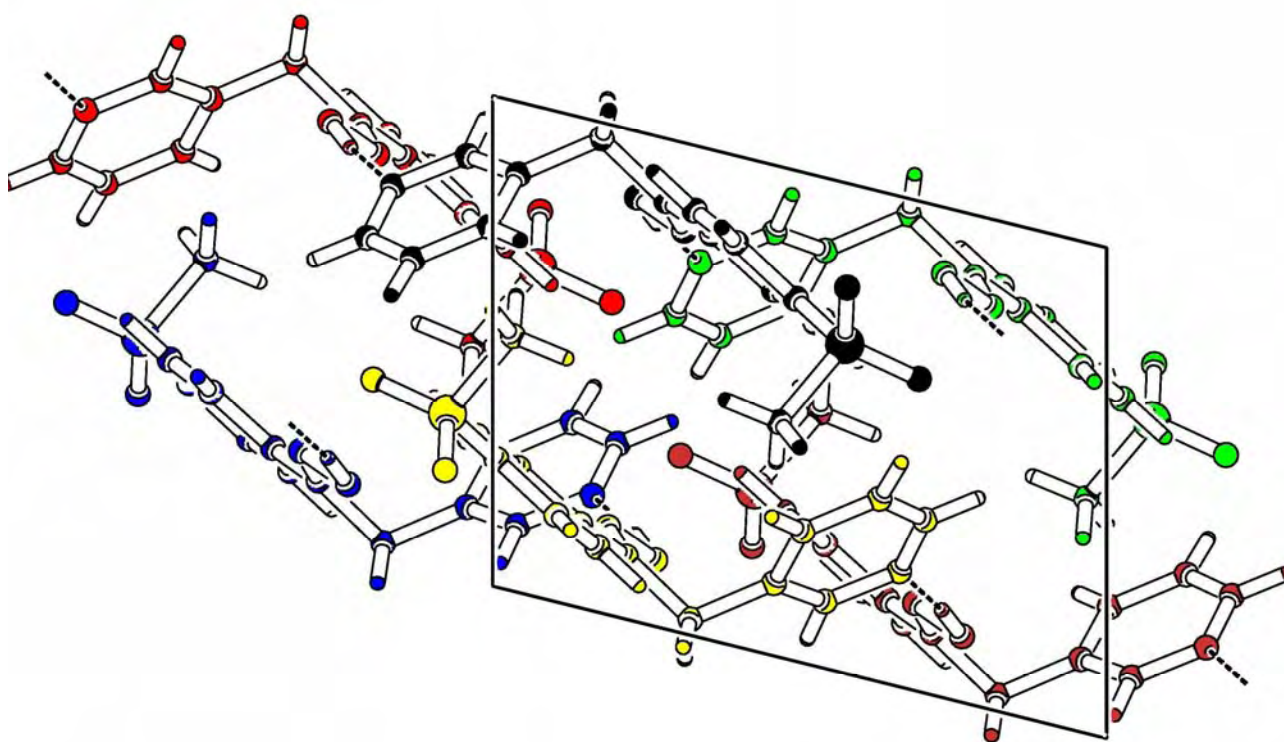


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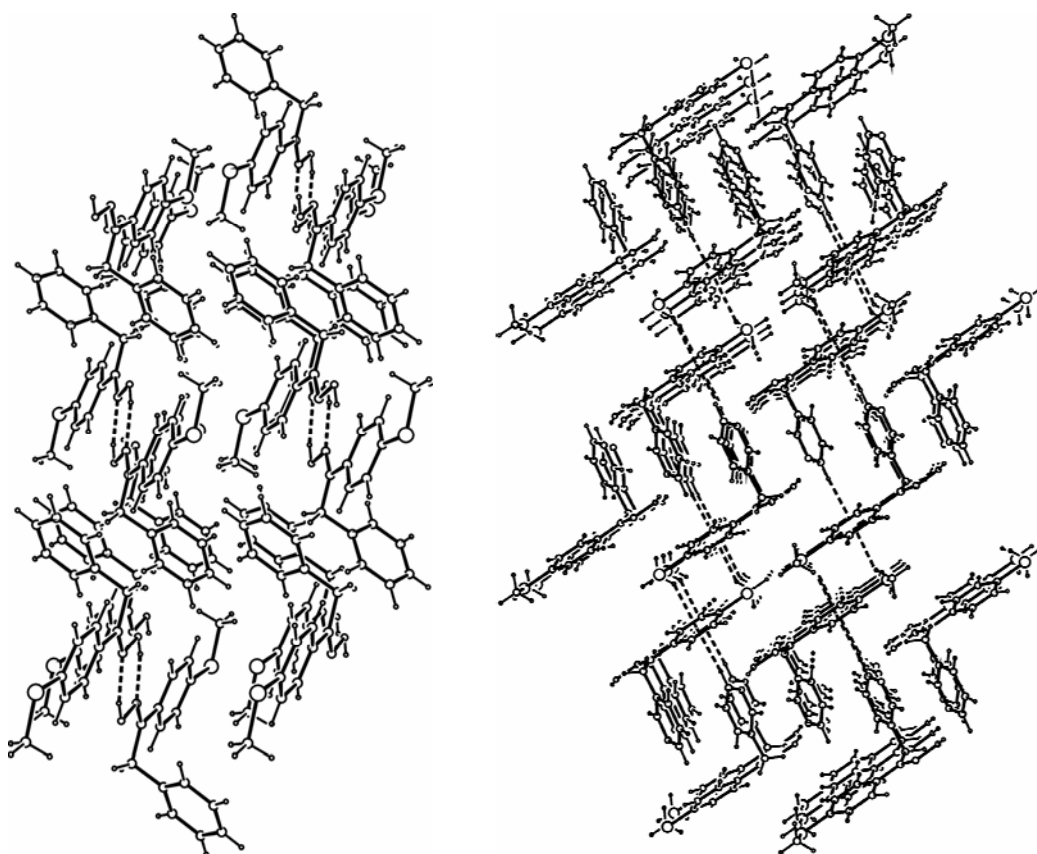


7

Crystal structure of 6, 7 and 9 viewed down the crystallographic *a* axis.

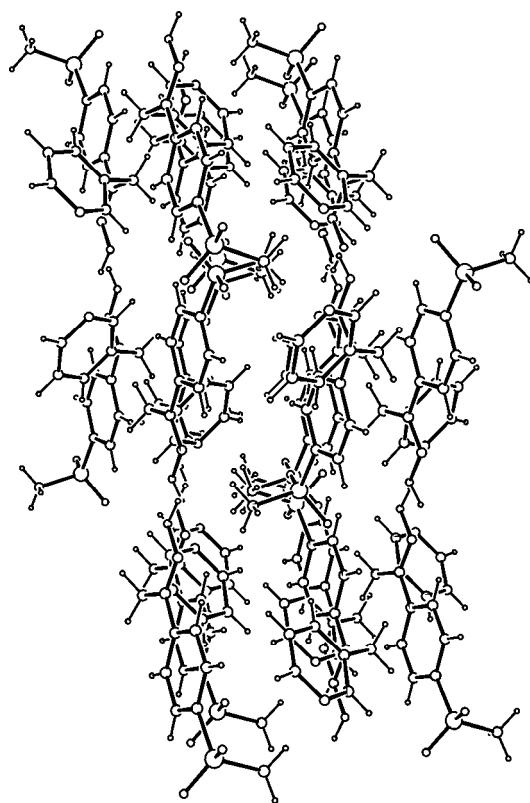


Crystal structure of oxime 7 viewed down the crystallographic *b* axis.



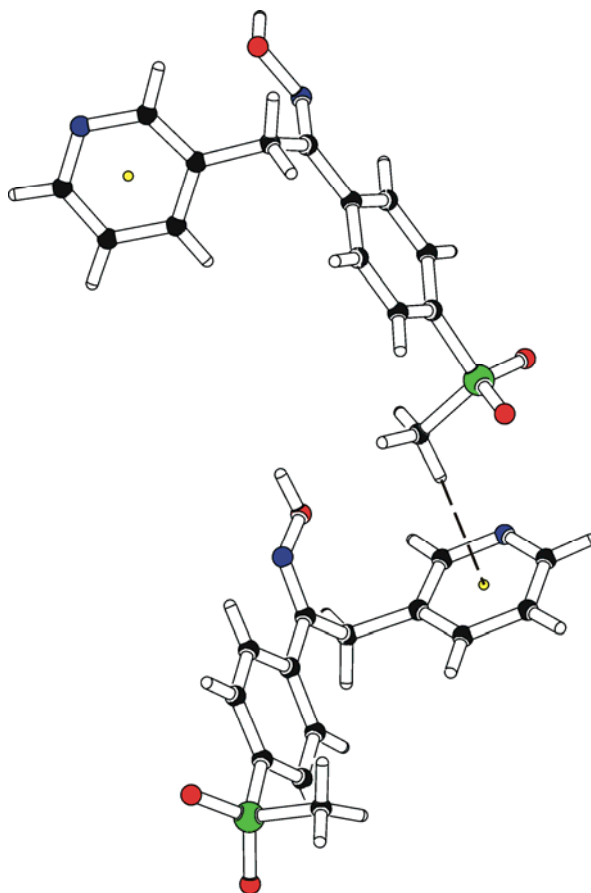
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9

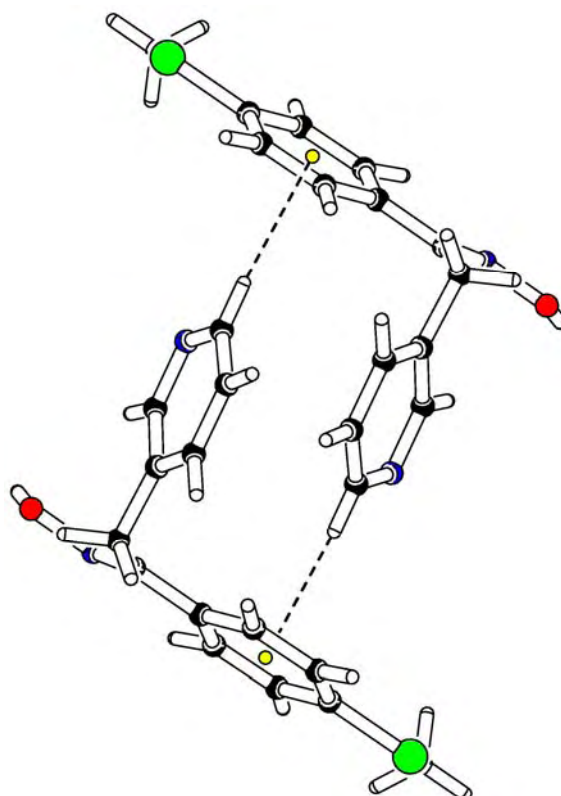


7

Perspective view of crystal packing of oximes 6, 7 and 9.



CH/π Hydrogen bonds: Oxime 7.



CH/π Hydrogen bonds: Oxime 9.

1,2-DIARYL(3-PYRIDIL)ETHANONES AND DERIVATIVES

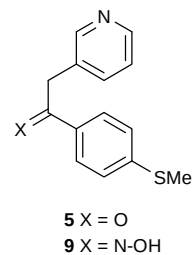
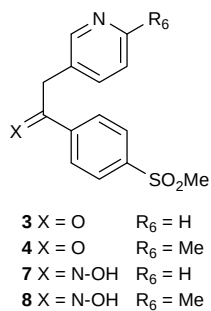
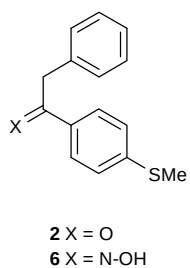
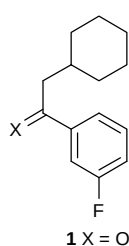
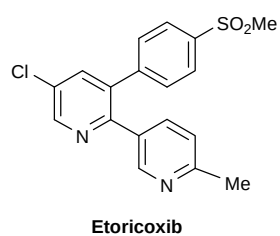
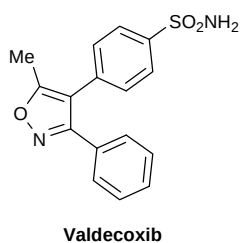
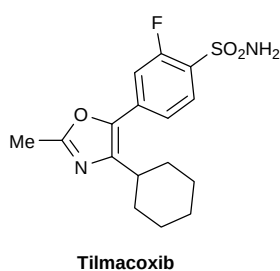
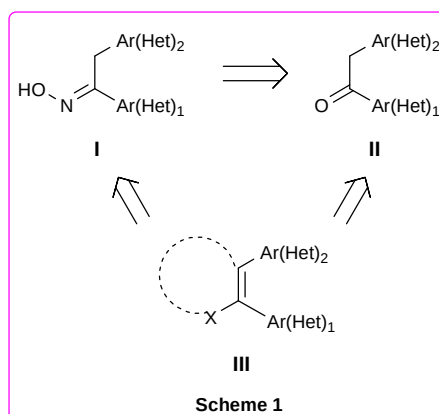
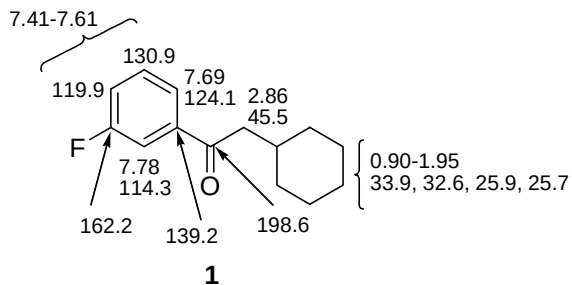


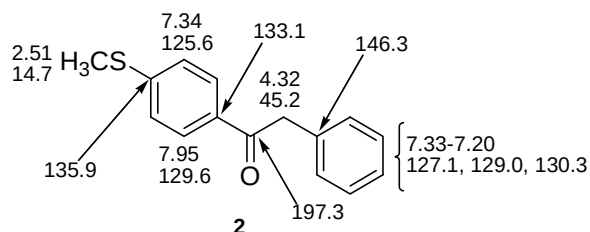
Figure 1

¹H NMR AND ¹³C NMR ASSIGNMENTS OF ETHANONES 1-5**• 2-Cyclohexyl-1-(3-fluorophenyl)ethanone (1)**

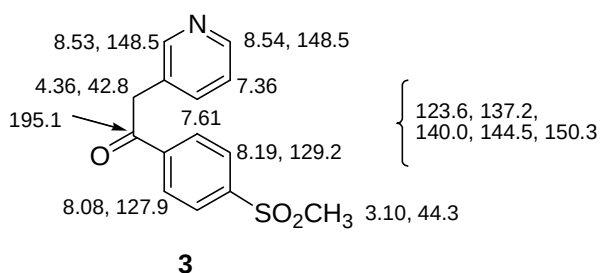
¹H NMR (DMSO-d₆, 200 MHz)
¹³C NMR (DMSO-d₆, 50.3 MHz)

**• 1-[4-(Methylthio)phenyl]-2-phenylethanone (2)**

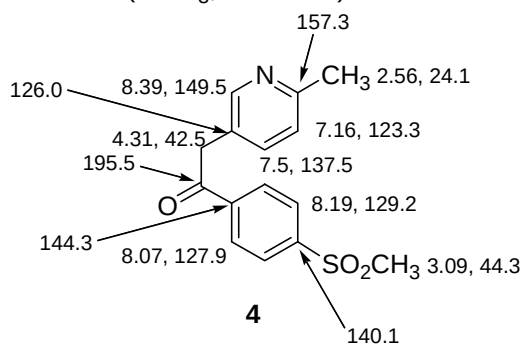
¹H NMR (DMSO-d₆, 300 MHz)
¹³C NMR (DMSO-d₆, 75.4 MHz)
 HMQC

**• 1-[4-(Methylsulfonyl)phenyl]-2-pyridin-3-ylethanone (3)**

¹H NMR (CDCl₃, 300 MHz)
¹³C NMR (CDCl₃, 75.4 MHz)

**• 2-(6-Methylpyridin-3-yl)-1-[4-(methylsulfonyl)phenyl]ethanone (4)**

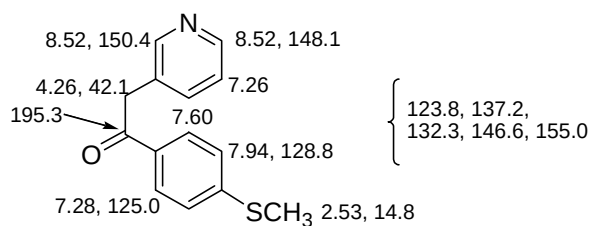
¹H NMR (CDCl₃, 200 MHz)
¹³C NMR (CDCl₃, 50.3 MHz)



• **1-[4-(Methylthio)phenyl]-2-pyridin-3-ylethanone (5)**

^1H NMR (CDCl_3 , 200 MHz)

^{13}C NMR (CDCl_3 , 50.3 MHz)



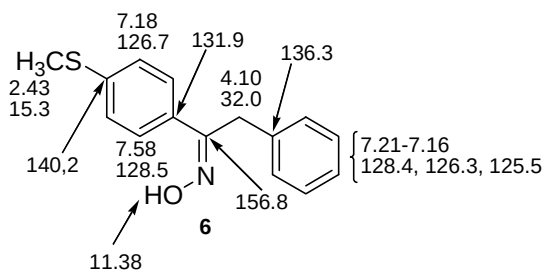
5

^1H NMR AND ^{13}C NMR ASSIGNMENTS OF KETOXIMES 6,7 AND 9

• **1-[4-(Methylthio)phenyl]-2-phenylethanone oxime (6)**

^1H NMR ($\text{DMSO}-d_6$, 200 MHz)

^{13}C NMR (CDCl_3 , 75.4 MHz)

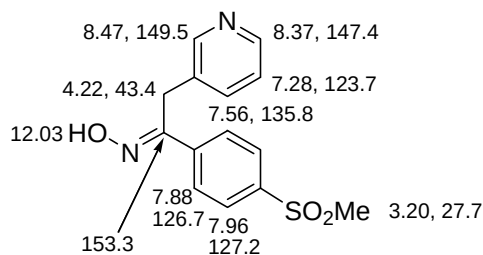


6

• **1-[4-(Methylsulfonyl)phenyl]-2-pyridin-3-ylethanone oxime (7)**

^1H NMR (400 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (50.3 MHz, $\text{DMSO}-d_6$)



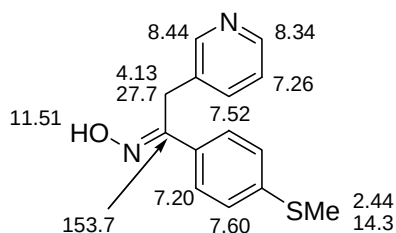
Quaternary aromatic C: 140.7, 140.0 and 132.5

7

• **1-[4-(Methylthio)phenyl]-2-pyridin-3-ylethanone oxime (9)**

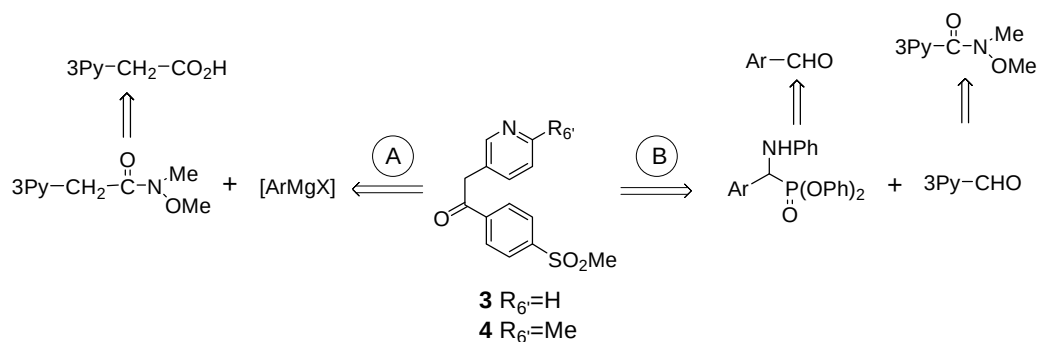
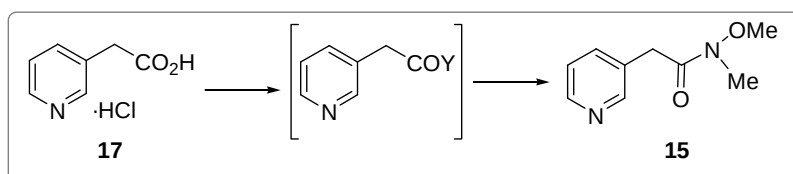
^1H NMR (200 MHz, $\text{DMSO}-d_6$)

^{13}C NMR (75.4 MHz, $\text{DMSO}-d_6$)

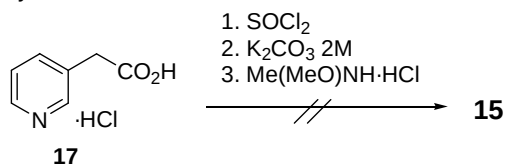


9

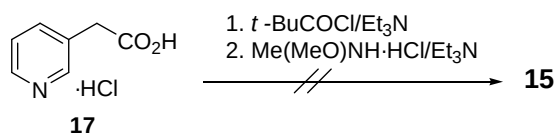
SYNTHESIS OF 1-ARYL-2-(3-PYRIDYL)ETHANONES 3-5

METHOD A: Synthesis of *N*-methoxy-*N*-methyl-2-pyridin-3-ylacetamide (15)

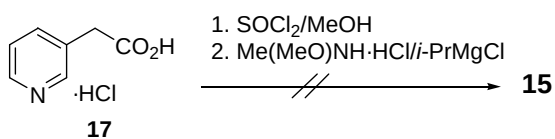
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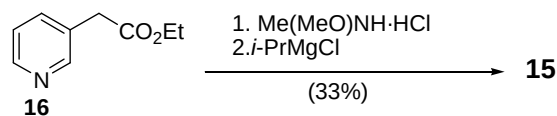
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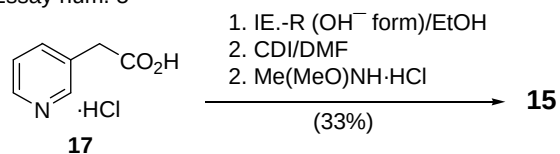
• Essay num. 3



• Essay num. 4



• Essay num. 5



• Essay num. 6

