SUPPLEMENTARY INFORMATION

A novel reaction of 2-phenacyl mercaptoimidazole with acetic anhydride: Formation of an imidazothiazole with loss of a phenyl group

SHASHIPRABHA^{*a\$}, NAGARAJAN K^{a,#*}, SAJESH P THOMAS^b, SURESH P
NAYAK^c, SUNDARRAJA RAO K^a, SHRIDHARA K^a and GURU ROW T N^b

^aAlkem laboratories Ltd, R&D centre, Bangalore 560 058, India.

^bSolid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore
560012, India.

^cDepartment of Chemistry, Mangalore University, Mangalore, India.

E-mail address: shashi-sudha@sdmcujire.in; dknb69@yahoo.com

#Present Address: #1, 1st Floor, House No. 007. Serene Urbana, Ozone
Urbana, Southegowdanahalli, Bangalore 562 110, India

Figure 1: ^1H NMR spectrum of 1-(3-methylimidazo[2,1-*b*][1,3]thiazol-2-yl)ethanonehydrobromide (14)

Figure 2: Expanded ^1H NMR spectrum of 1-(3-methylimidazo[2,1-*b*][1,3]thiazol-2-yl)ethanonehydrobromide(14)

Figure 3: ^{13}C NMR spectrum of 1-(3-methylimidazo[2,1-*b*][1,3]thiazol-2-yl)ethanone hydrobromide (14)

Figure 4. Expanded ^{13}C NMR spectrum of 1-(3-methylimidazo[2,1-*b*][1,3]thiazol-2-yl)ethanonehydrobromide (14)

Figure 5. DEPT spectrum of 1-(3-methylimidazo[2,1-*b*][1,3]thiazol-2-yl)ethanonehydrobromide (14)

Figure 6. Mass spectrum of 1-(3-methylimidazo[2,1-*b*][1,3]thiazol-2-yl)ethanonehydrobromide (14)

Figure 7. IR spectrum of 1-(3-methylimidazo[2,1-*b*][1,3]thiazol-2-yl)ethanonehydrobromide(14)

Figure 8. ¹H NMR spectrum of 2-(1H-imidazol-2-ylsulfanyl)-1-phenylethanonehydrobromide (12)

Figure 9. Expanded ^1H NMR spectrum of 2-(1H-imidazol-2-ylsulfanyl)-1-phenylethanone (12)

Figure 10. Mass spectrum of 2-(1*H*-imidazol-2-ylsulfanyl)-1-phenylethanonehydrobromide (12)

Figure 11. ^1H NMR spectrum of 1,1'-(2-thioxo-1*H*-imidazole-1,3(2*H*)-diyl)diethanone (16)

Figure 12. Mass spectrum of 1,1'-(2-thioxo-1*H*-imidazole-1,3(2*H*)-diyl)diethanone (16)

Figure 13. ¹H NMR spectrum of 2-(1*H*-benzimidazol-2-ylsulfany)-1-phenylethanone hydrobromide (17)

Figure 14. Expanded ¹H NMR spectrum of 2-(1*H*-benzimidazol-2-ylsulfanyl)-1-phenylethanone hydrobromide (17)

Figure 15. Mass spectrum of 2-(1H-benzimidazol-2-ylsulfanyl)-1-phenylethanone hydrobromide (17)

Figure 16. ^1H NMR spectrum 1-(3-methyl[1,3]thiazolo[3,2-*a*]benzimidazol-2-yl)ethanone (18)

Figure 17. Mass spectrum of 1-(3-methyl[1,3]thiazolo[3,2-*a*]benzimidazol-2-yl)ethanone (18)