Journal of the Serbian Chemical Society
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J. Serb. Chem. Soc. 84 (5) S114–S121 (2019)
Supplementary material

SUPPLEMENTARY MATERIAL TO

Anti-inflammatory activity of synthetic and natural glucoraphanin

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J. Serb. Chem. Soc. 84 (5) (2019) 445–453

*1-Thio-α-D-glucopyranoze 2,3,4,5-tetraacetate 1-[(1Z)-*N*-hydroxy-5-(methylsulfinyl)pentanimidate] (**2a**)*. Yield: 189 mg, 40 %; m.p.: 104–105 °C; IR (NaCl, cm^{-1}): 3286 (OH), 2924, 2850, 1751 (C=O), 1599 (C=N), 1376, 1226, 1043; ^{1}H-NMR (300 MHz, 300 K, $CDCl_3$, δ / ppm): 10.29 (1H, *s*, OH), 6.10 (1H, *d*, $J_{1,2}$ = 6.0 Hz, H1), 5.35 (1H, *t*, $J_{2,3} = J_{3,4}$ = 9.9 Hz, H3), 5.04–4.95 (2H, *m*, H2 & H4), 4.36-4.31 (1H, *m*, H5), 4.22 (1H, *dd*, $J_{5,6b}$ = 4.2 Hz & $J_{6a,6b}$ = 12.6 Hz, H6b), 4.05 (1H, *dd*, $J_{5,6a}$ = 1.2 Hz & $J_{6a,6b}$ = 12.6 Hz, H6a), 2.79-2.59 (2H, *m*, $SOCH_2$), 2.58–2.49 (5H, *m*, CH_3SO & CH_2C=N), 2.00, 1.97, 1.96 & 1.95 (4×s, 12H, 4×CH_3**3**COO), 1.76–1.68 (4H, *m*, $SOCH_2C\mathbf{H}_2C\mathbf{H}_2$); ^{13}C-NMR (75 MHz, 300 K, $CDCl_3$, δ / ppm): 170.1, 169.7, 169.4, 169.2 (4×CH_3*C*OO), 148.3 (C=N), 79.2 (C-1), 70.0 (C-5), 69.7 (C-3), 68.1 (C-2), 67.8 (C-4), 61.1 (C-6), 53.4 (C-2'), 37.8 (CH_3SO), 31.4 (C-5′), 25.7 (C-4′), 21.5 (C-3′), 20.6, 20.3 (2), 20.2 (4×**C**H_3COO); HRMS (ESI) (*m*/*z*) calcd. for $C_{20}H_{31}NaO_{11}NS_2$ $[M+Na]^+$: 548.1236. Found: 548.1227; R_f (90 % DCM/MeOH): 0.26; $[\alpha]_D^{20}$ (DCM, *c*: 0.38 g/mol): +148.8.

*Potassium salt of 1-thio-α-D-glucopyranoze 2,3,4,5-tetraacetate 1-[(1Z)-5--(methylsulfinyl)pentanimidate] (**3a**)*. Yield: 74 mg, 50 %; m.p.: 152–154 °C (dec.); IR (KBr, cm^{-1}): 2970, 2871, 1741 (C=O), 1600 (C=N), 1250, 1224, 1061; ^{1}H-NMR (300 MHz, 300 K, CD_3OD, δ / ppm): 6.22 (1H, *d*, $J_{1,2}$ = 5.7 Hz, H1), 5.34 (1H, *t*, $J_{2,3} = J_{3,4}$ = 9.9 Hz, H3), 5.16–5.07 (2H, *m*, H2 & H4), 4.40–4.34

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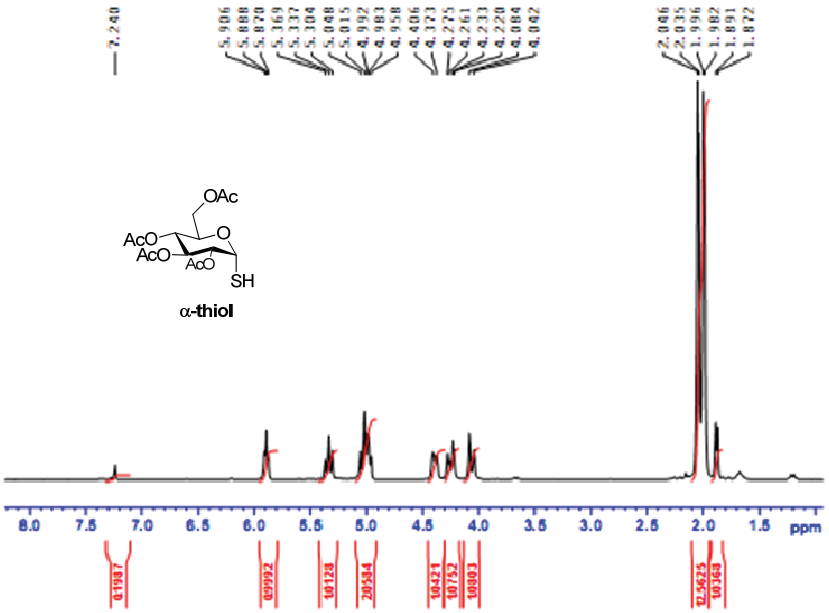
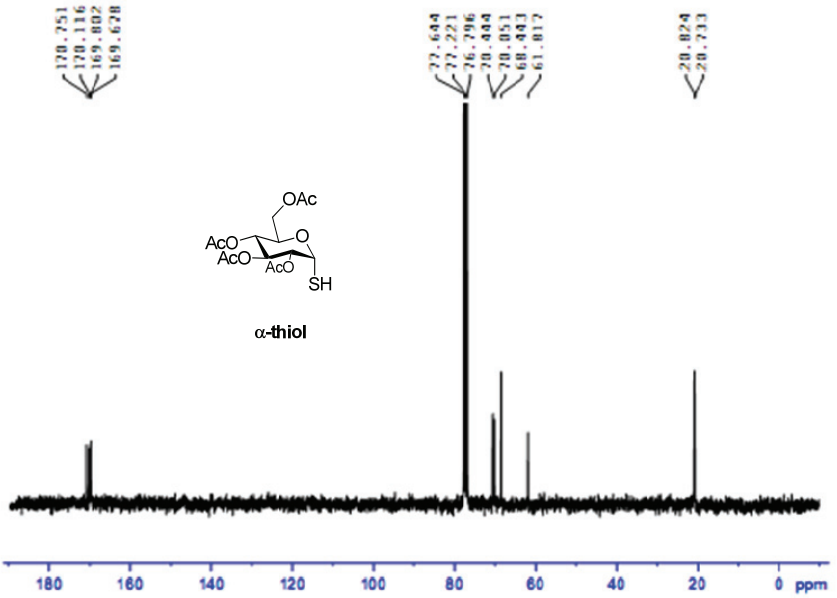
(1H, *m*, H5), 4.27 (1H, *dd*, $J_{5,6b}$ = 4.5 Hz & $J_{6a,6b}$ = 12.6 Hz, H6b), 4.13 (1H, *dd*, $J_{5,6a}$ = 2.1 Hz & $J_{6a,6b}$ = 12.6 Hz, H6a), 2.87–2.73 (2H, *m*, $SOCH_2$), 2.63–2.61 (5H, *m*, CH_3SO & $CH_2C{=}N$), 2.04, 2.02, 2.01 & 1.99 (12H, 4×*s*, 4×CH_3COO), 1.89–1.78 (4H, *m*, $SOCH_2C\mathbf{H}_2C\mathbf{H}_2$); ^{13}C-NMR (75 MHz, 300 K $CDCl_3$, δ / ppm): 170.5, 169.6, 169.5, 169.2 (4×CH_3COO), 156.1 (C=N), 78.7 (C-1), 69.7 (C-5 & C-3), 68.6 (C-2), 67.7 (C-4), 61.1 (C-6), 52.6 (C-5′), 36.3 (CH_3SO), 30.9 (C-2′), 25.2 (C-4′), 21.0 (C-3′), 18.9 (2), 18.7 (2) (4×$\mathbf{C}H_3COO$); HRMS (ESI) (*m*/*z*) calcd. for $C_{20}H_{30}O_{14}NS_3$ $[M–K]^-$: 604.0834. Found: 604.0841; R_f (20 % MeOH/DCM): 0.17; $[\alpha]_D^{25}$ (MeOH, *c*: 0.23 g/mol): +134.7.

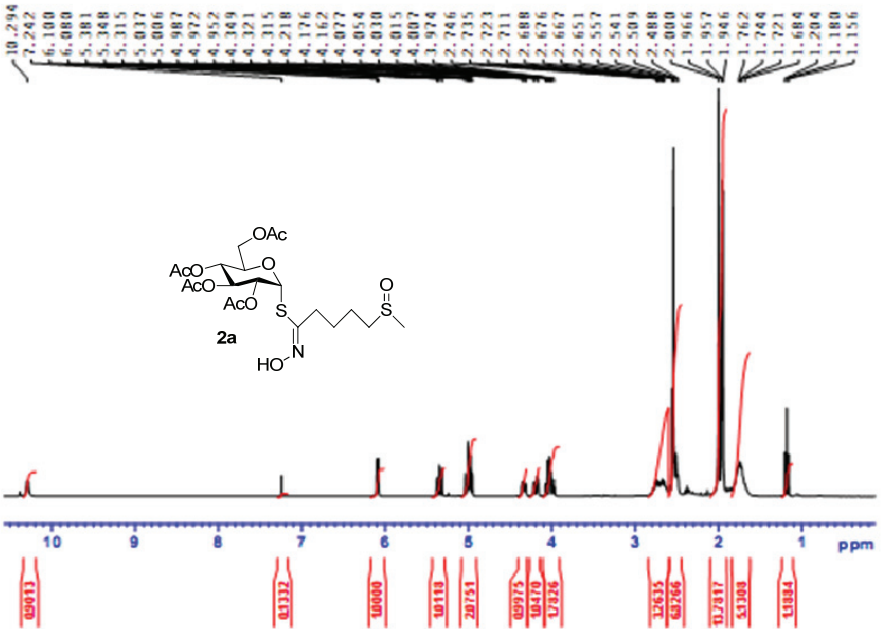
α-Thiol *^{1}H-NMR spectrum*



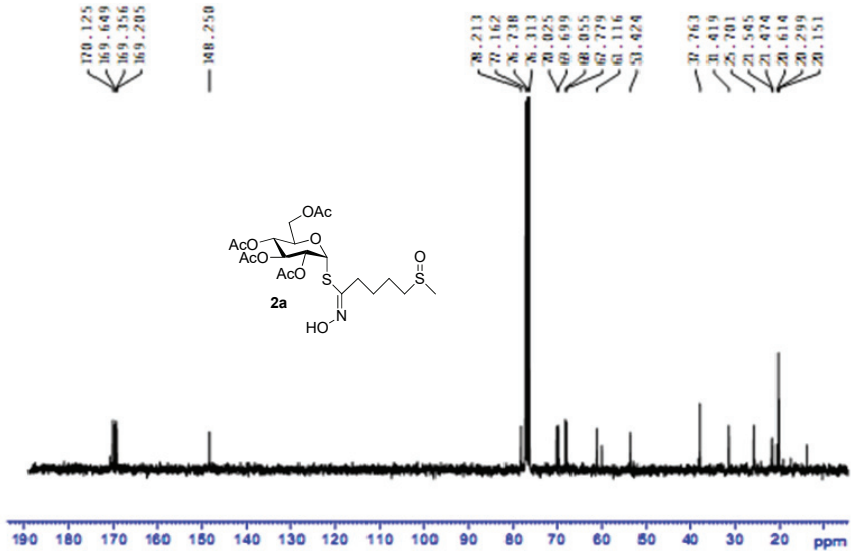
α-*Thiol* ^{13}*C-NMR spectrum*



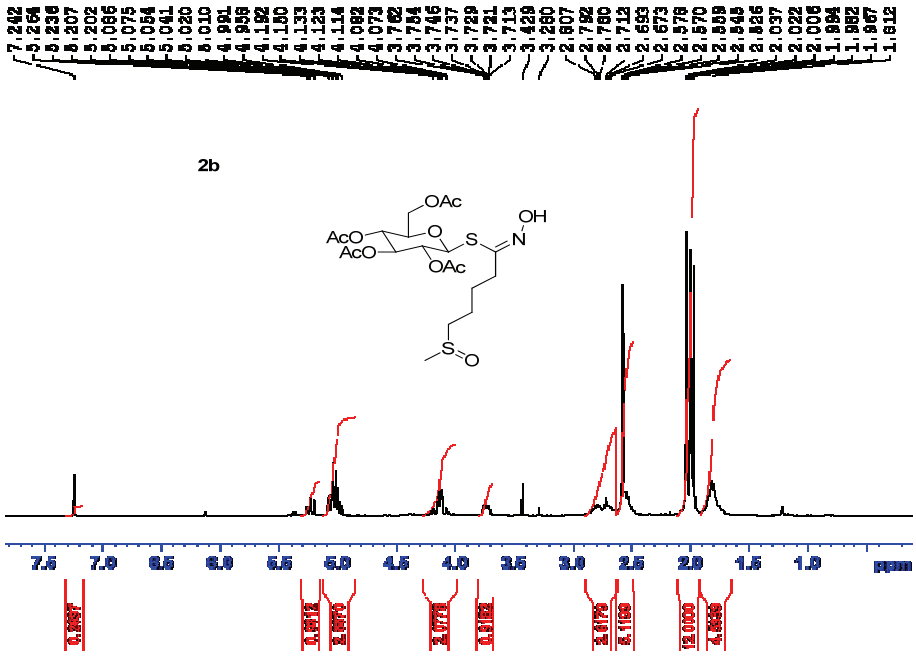
Compound ***2a*** ^{1}*H-NMR spectrum*



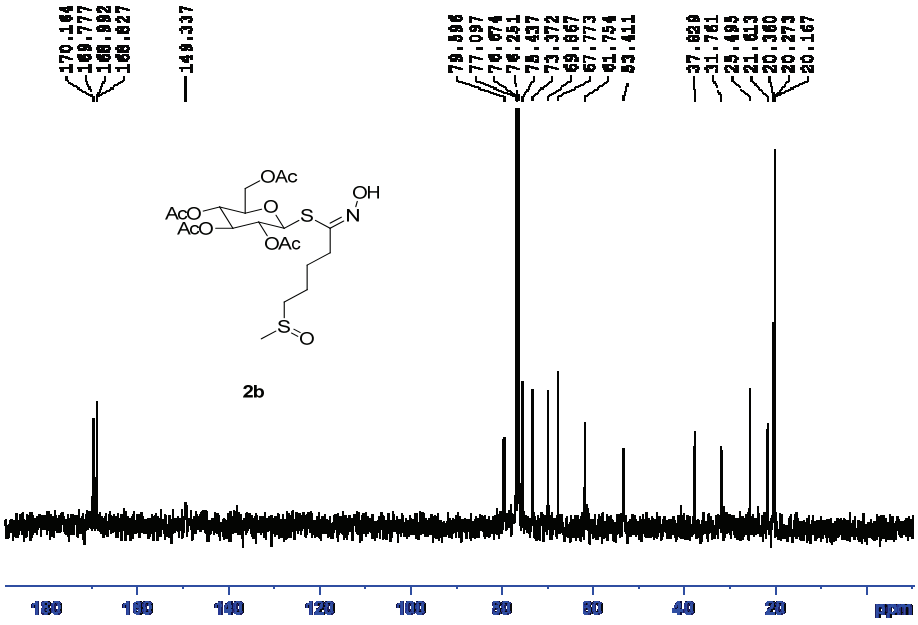
*Compound **2a** ^{13}C-NMR spectrum*



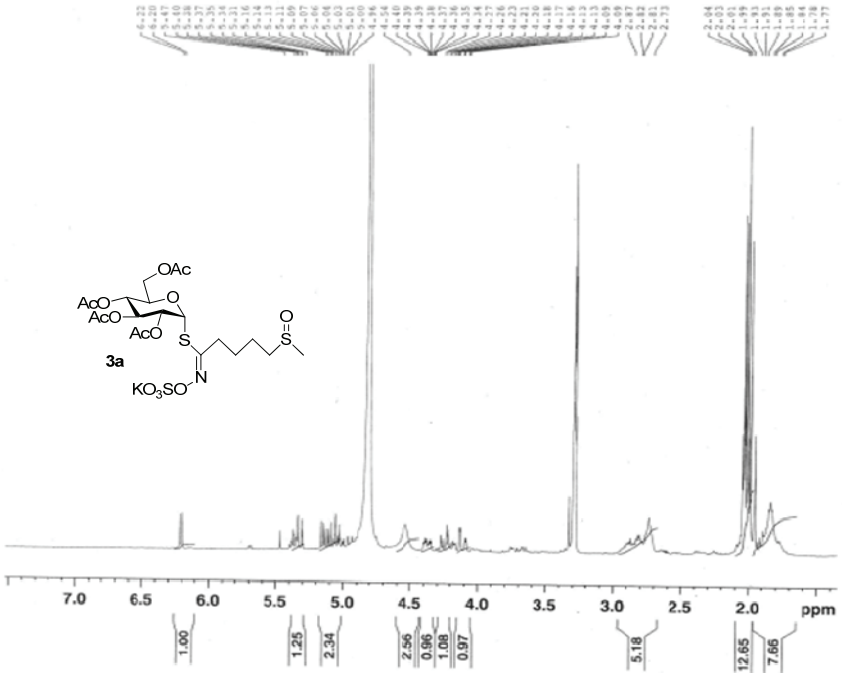
*Compound **2b** ^{1}H-NMR spectrum*



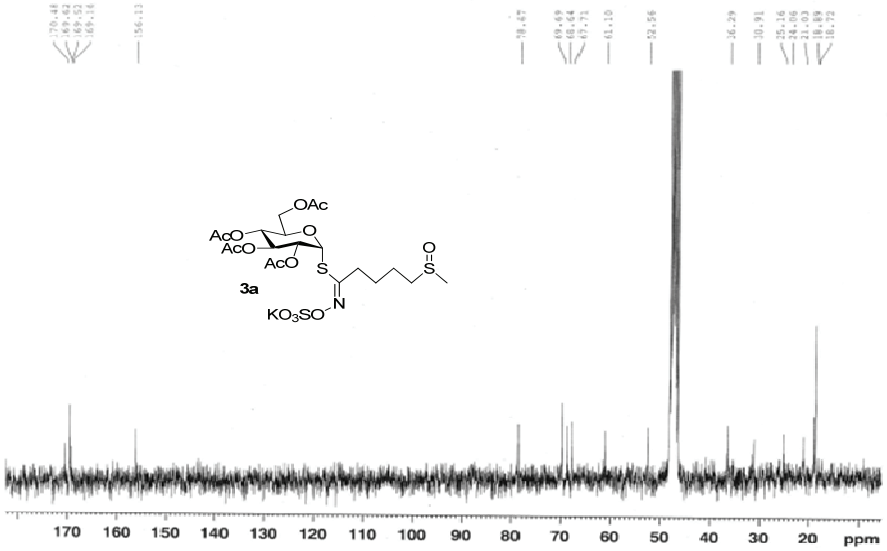
*Compound **2b** ^{13}C-NMR spectrum*



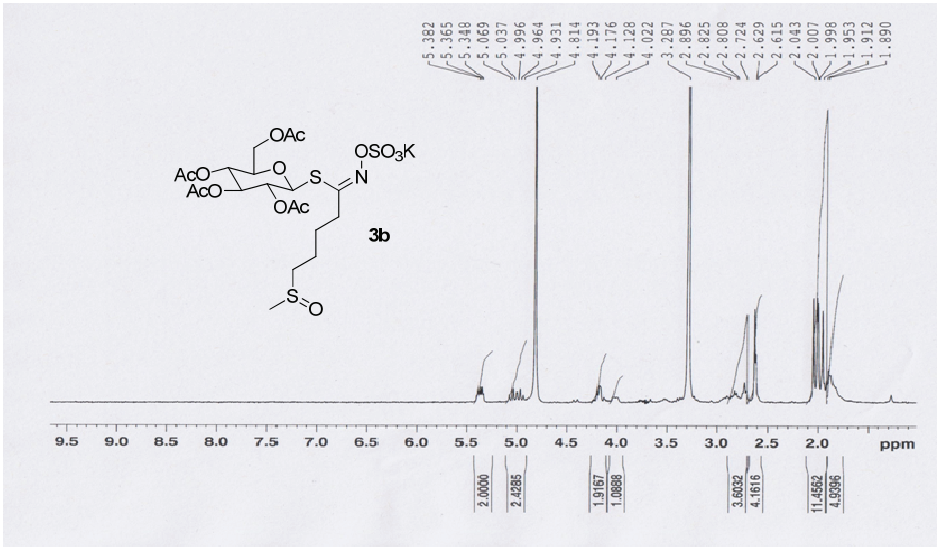
*Compound **3a** ^{1}H-NMR spectrum*



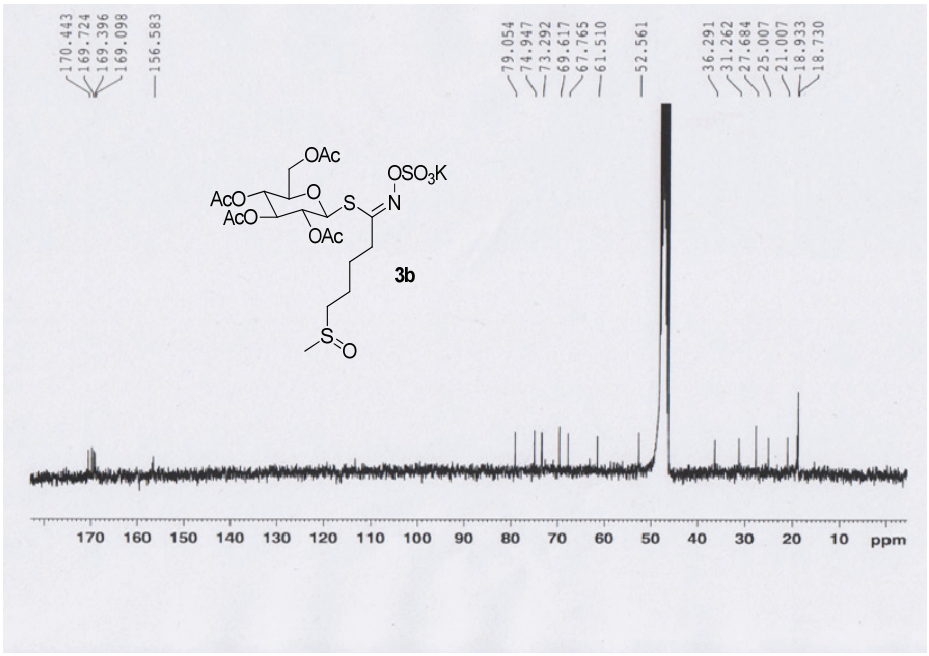
*Compound **3a** ^{13}C-NMR spectrum*



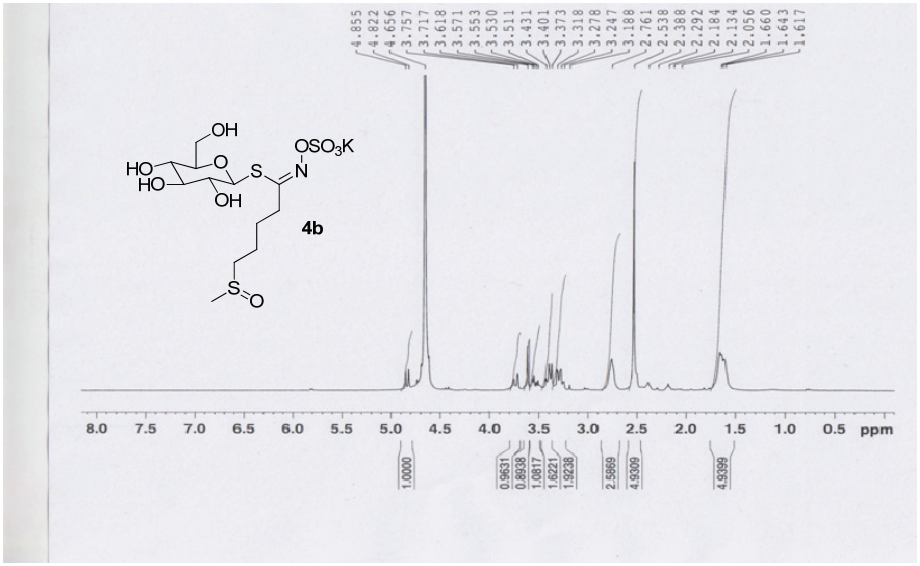
*Compound **3b** [1]H-NMR spectrum*



*Compound **3b** [13]C-NMR spectrum*



*Compound **4b** ^{1}H-NMR spectrum*



*Compound **4b** ^{13}C-NMR spectrum*