

2-Methyl-11-nitro-5,6-dihydro-2*H*-2,6-methano-1,3,5-benzoxadiazocin-4(3*H*)-one: synthesis, crystal structure and tautomerism in dipolar aprotic solvents

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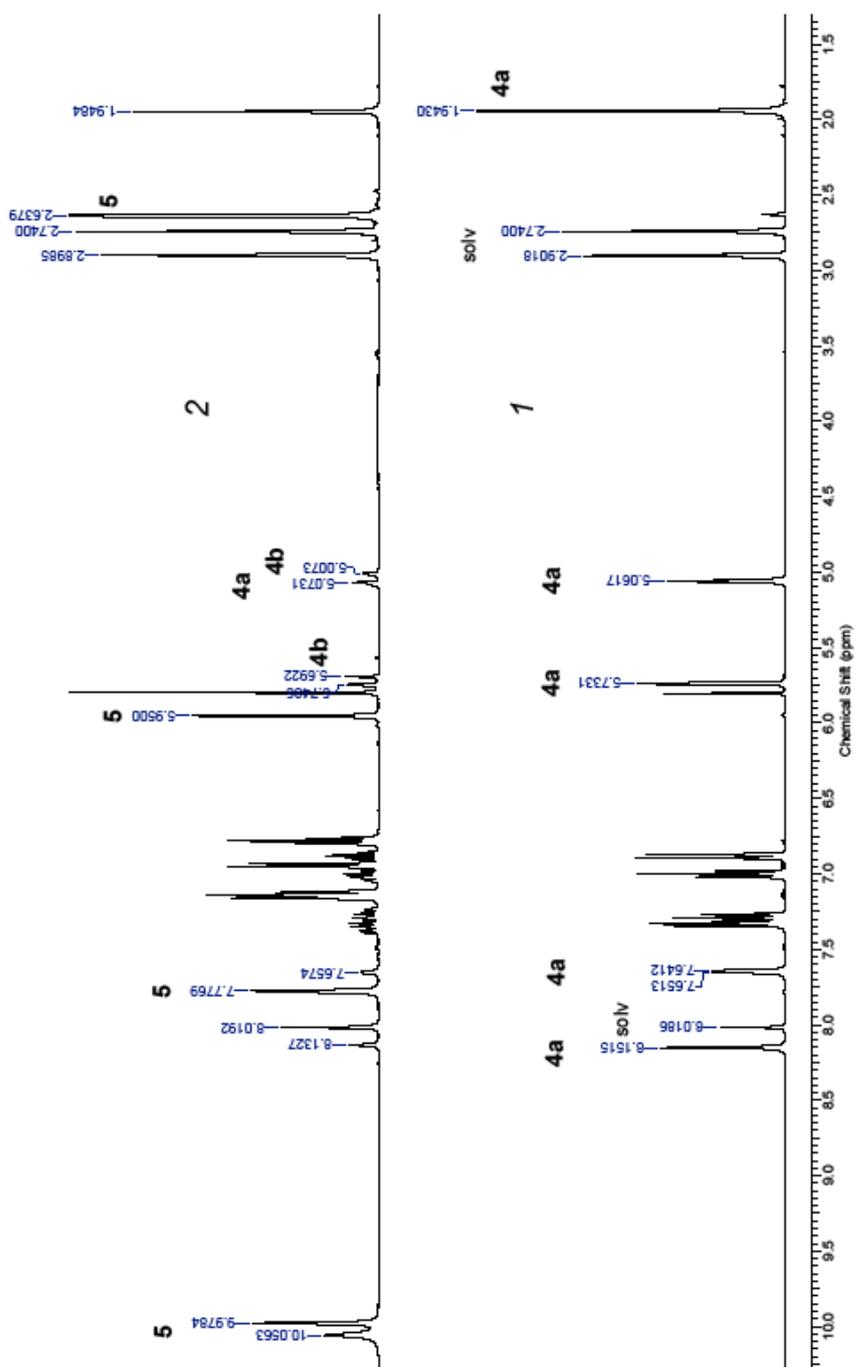


Figure S1 ^1H NMR spectra of compound **4a** in $\text{DMF-}d_7$, *1* – 20 min after dissolving, *2* – 96 h after dissolving.

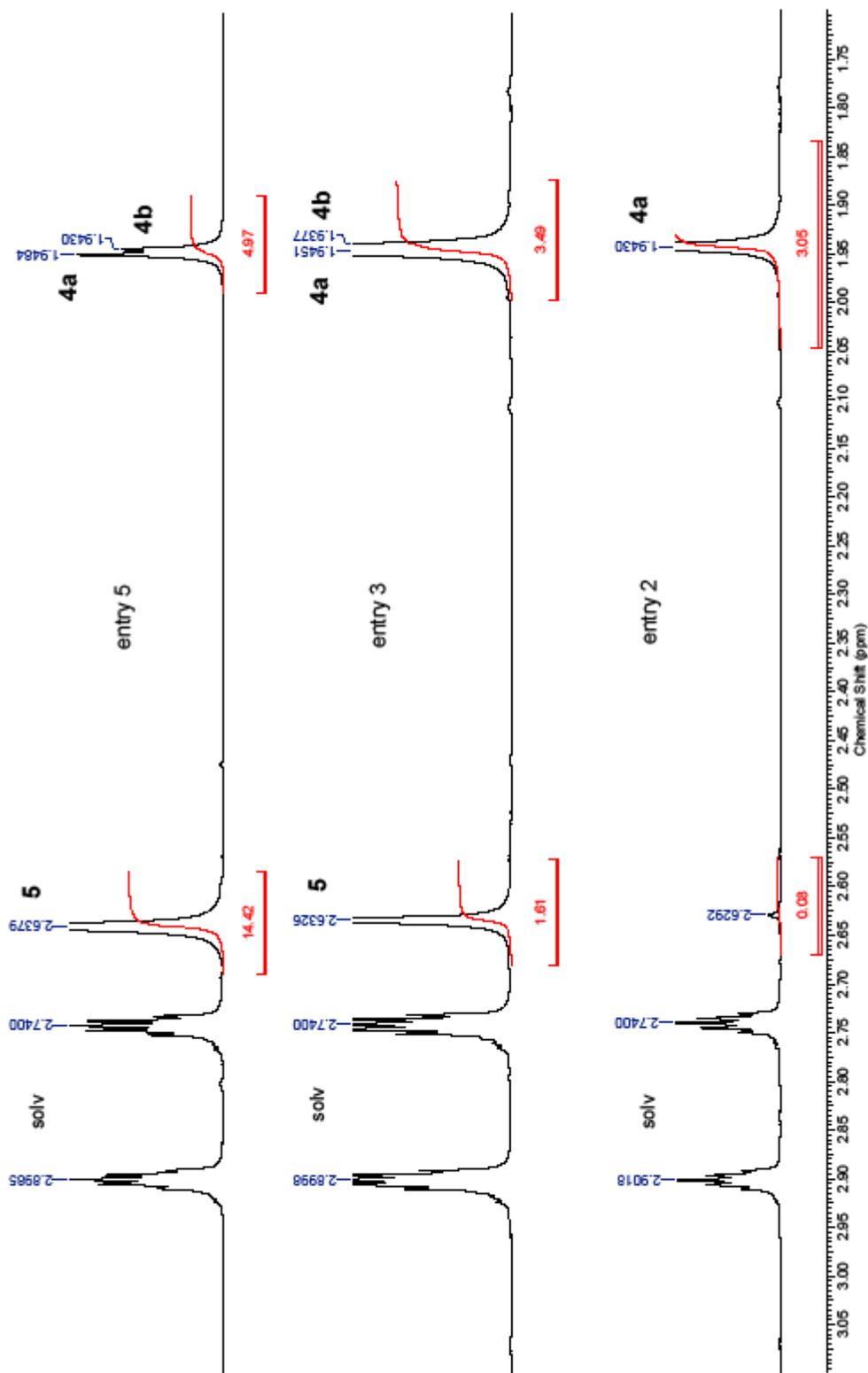


Figure S2 ^1H NMR spectra of compound **4a** in $\text{DMF-}d_7$, (range 1.7 – 3.1 ppm), entry 2 – 20 min after dissolving, entry 3 – 4 h after dissolving, entry 5 – 96 h after dissolving.

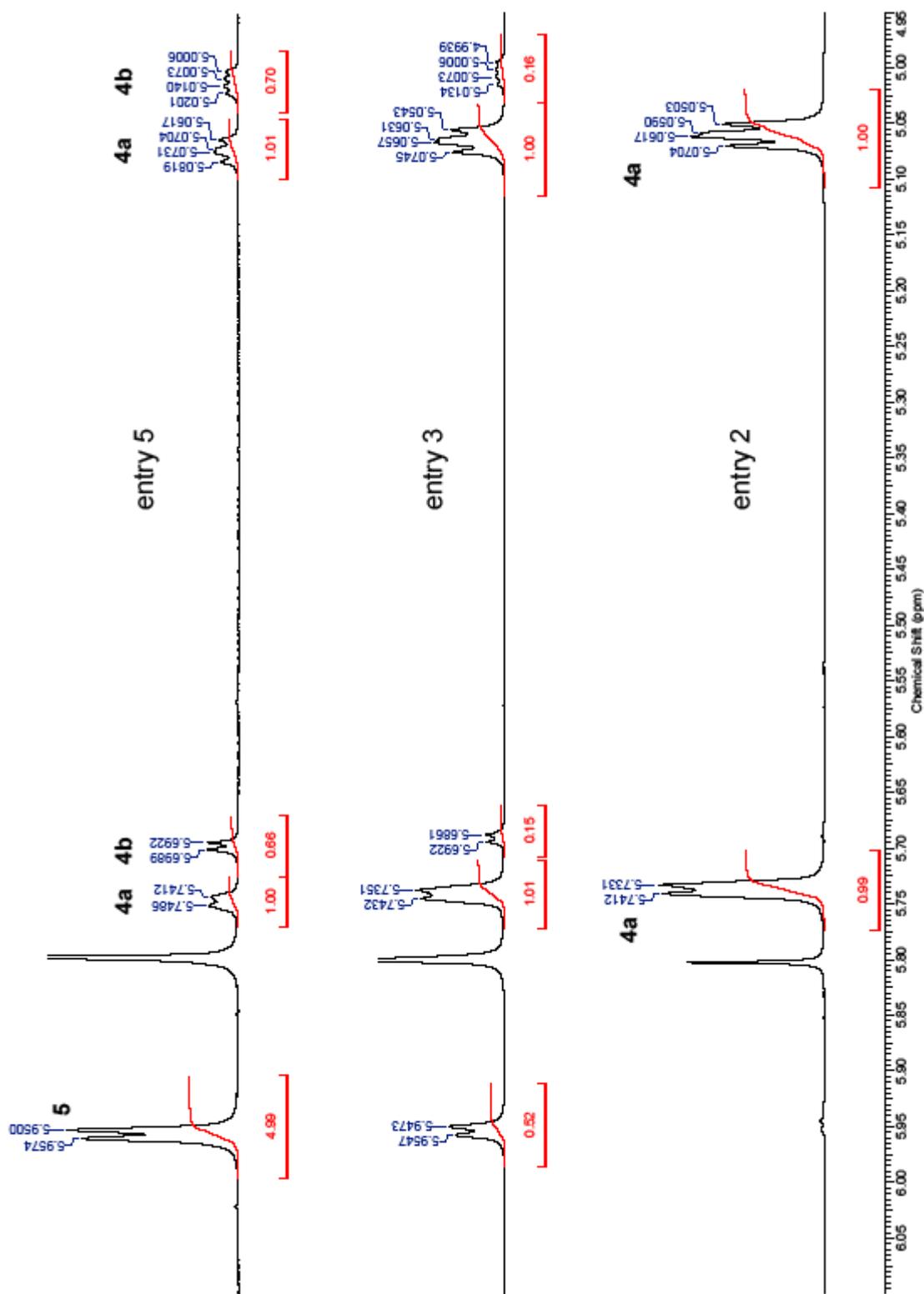


Figure S3 ^1H NMR spectra of the compound **4a** in $\text{DMF-}d_7$, (range 5.0 – 6.1 ppm), entry 2 – 20 min after dissolving, entry 3 – 4 h after dissolving, entry 5 – 96 h after dissolving.

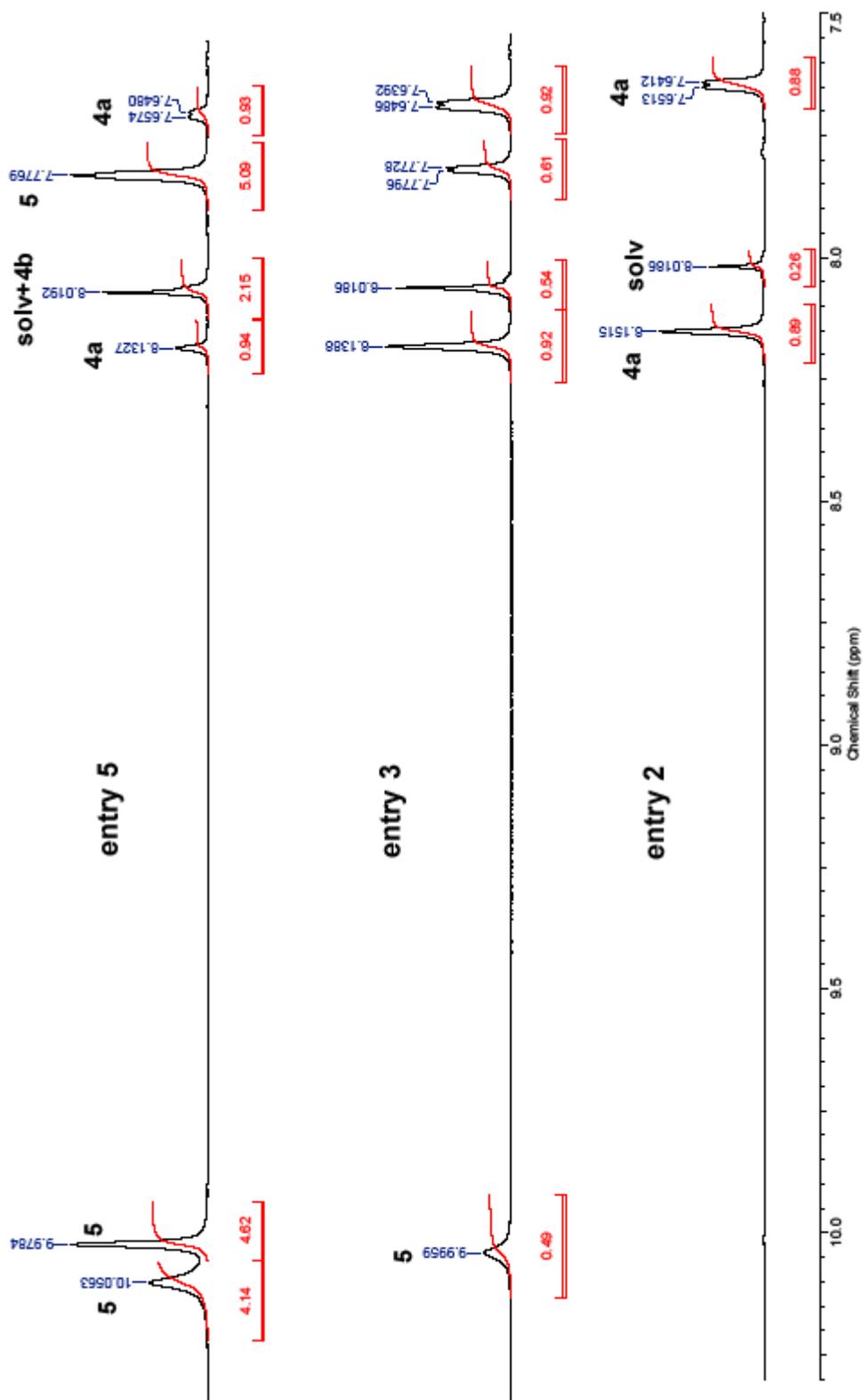


Figure S4 ^1H NMR spectra of the compound **4a** in $\text{DMF-}d_7$, (range 7.5 – 10.3 ppm), entry 2 – 20 min after dissolving, entry 3 – 4 h after dissolving, entry 5 – 96 h after dissolving.

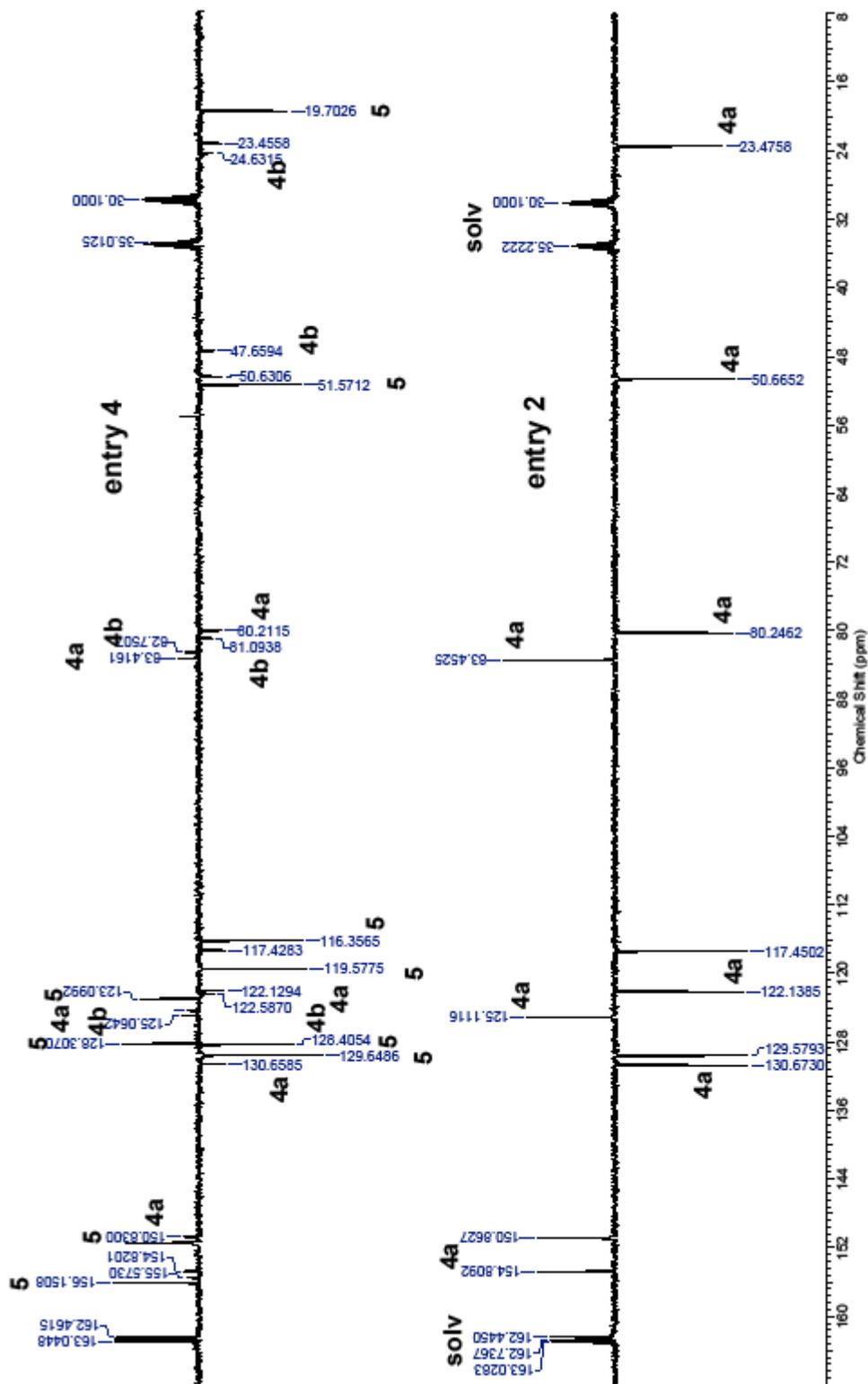


Figure S5 ^{13}C NMR spectra of the compound **4a** in $\text{DMF-}d_7$, entry 2 – 20 min after dissolving, entry 4 – 24 h after dissolving.

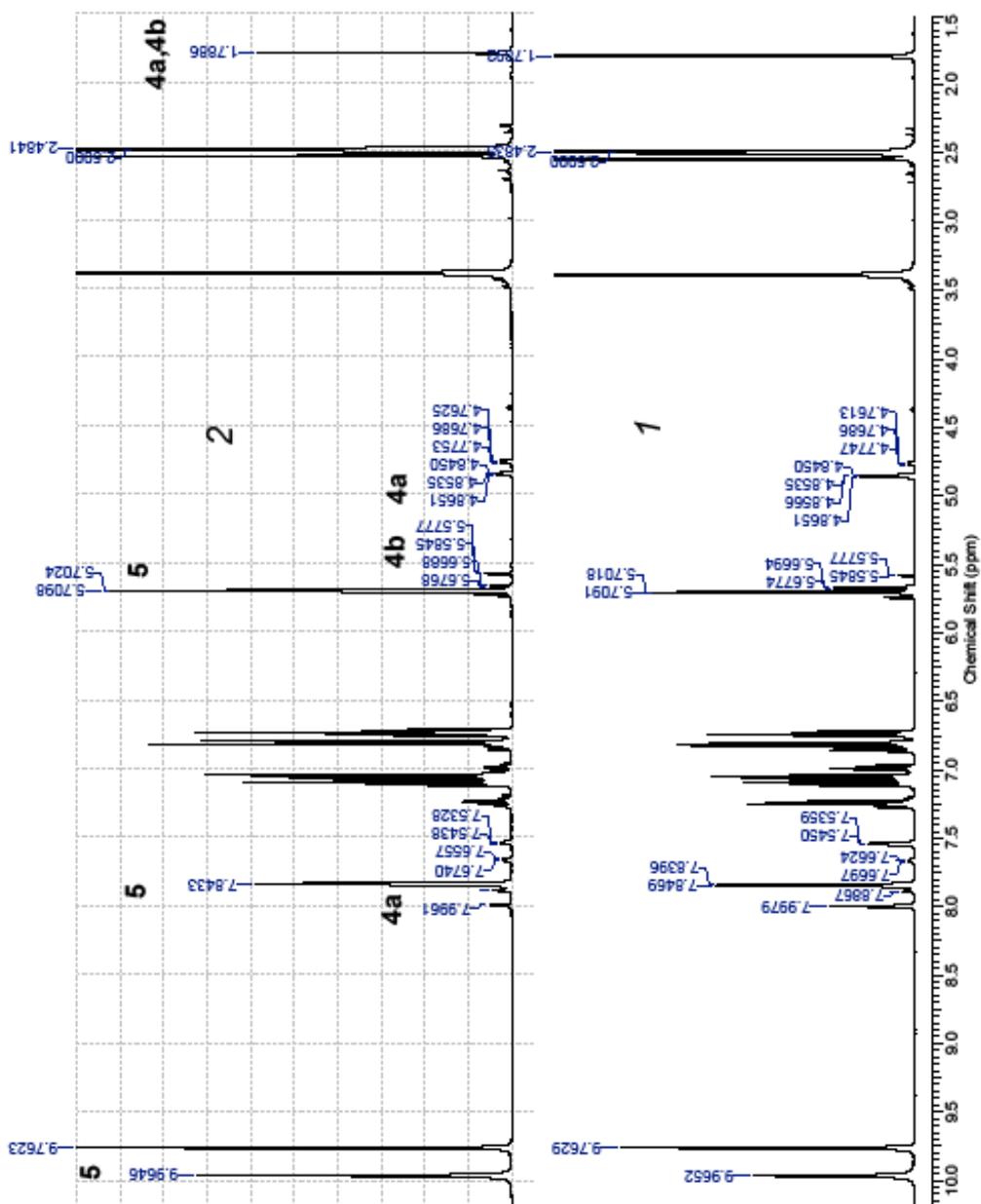


Figure S6 ^1H NMR spectra of the compound **4a** in $\text{DMSO-}d_6$, 1 – 15 min after dissolving, 2 – 24 h after dissolving.

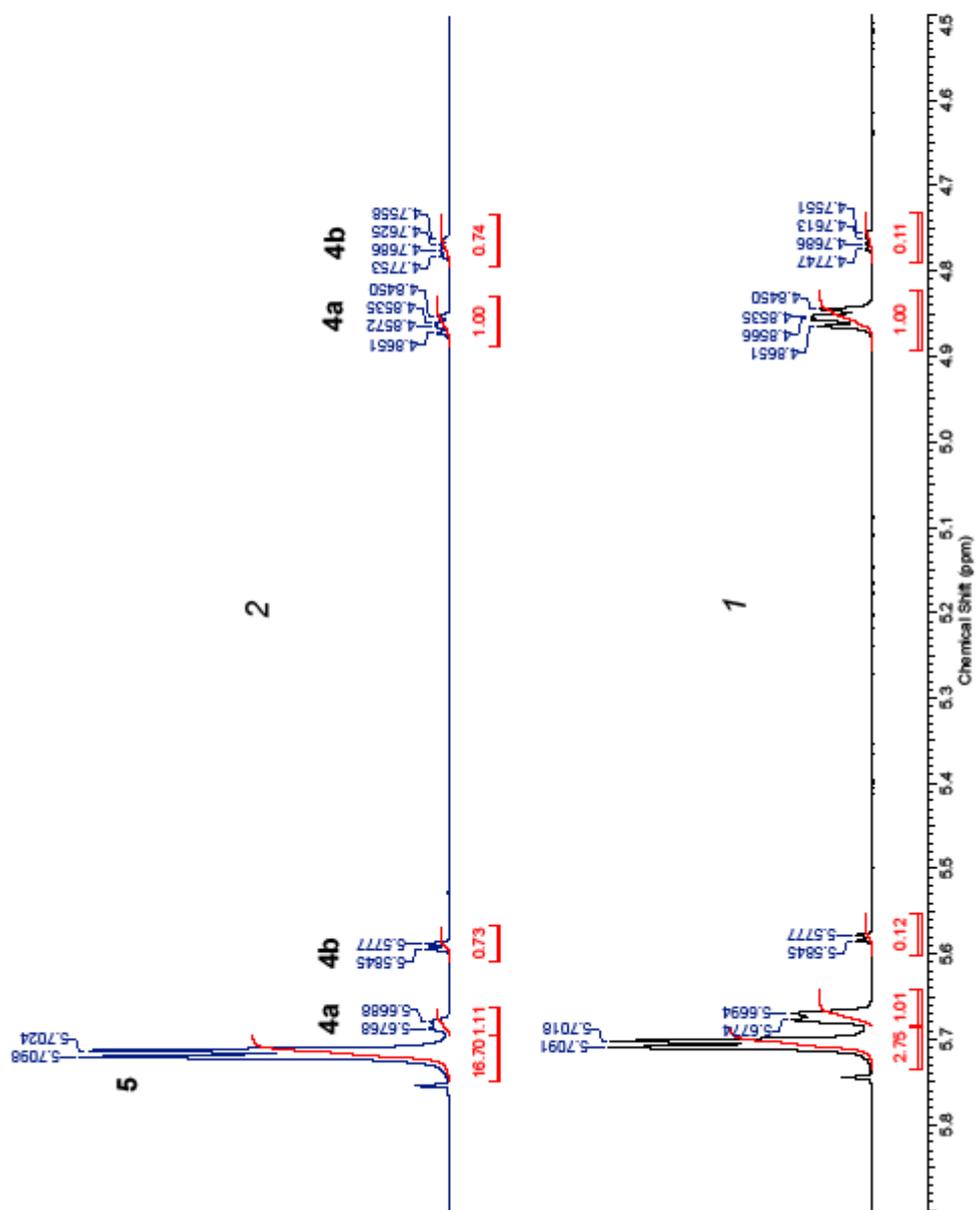


Figure S7 ^1H NMR spectra of the compound **4a** in $\text{DMSO-}d_6$, (range 4.5 – 5.9 ppm), 1 – 15 min after dissolving, 2 – 24 h after dissolving.

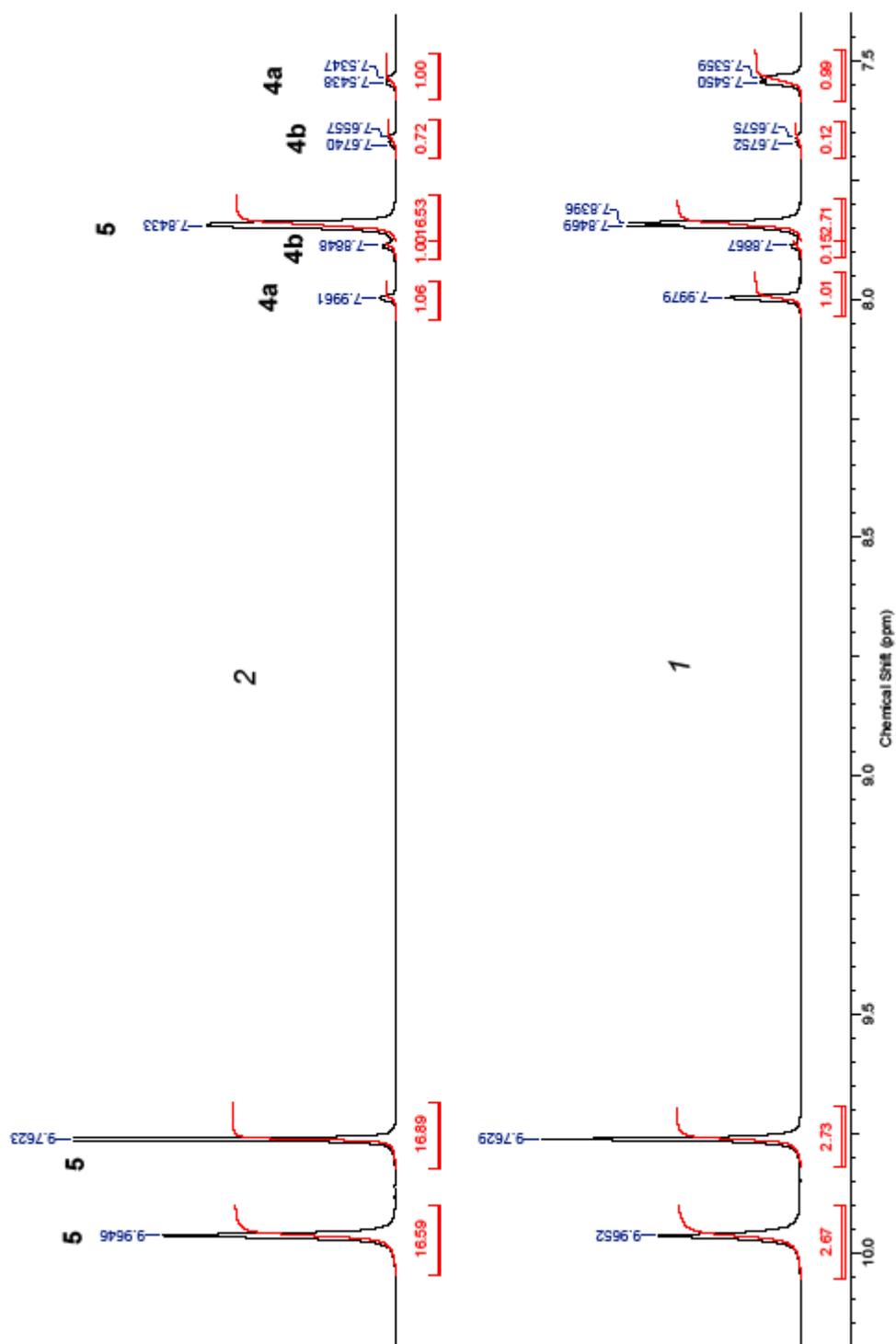


Figure S8 ^1H NMR spectra of the compound **4a** in $\text{DMSO-}d_6$, (range 7.4 – 10.3 ppm), *1* – 15 min after dissolving, *2* – 24 h after dissolving.

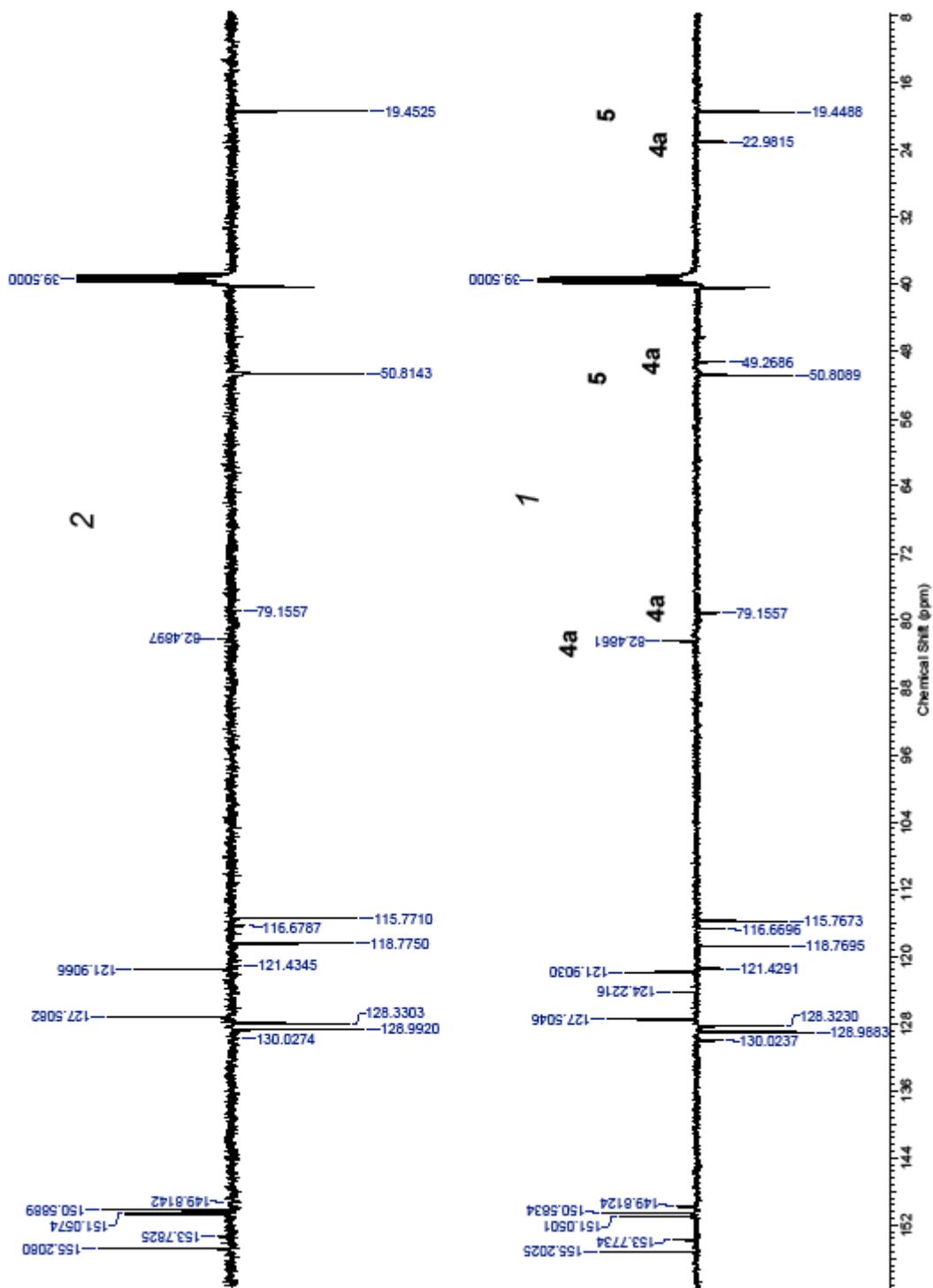


Figure S9 ^{13}C NMR spectra of the compound **4a** in $\text{DMSO-}d_6$, 1 – 15 min after dissolving, 2 – 24 h after dissolving.