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Supplementary Data

Investigation of Fe_3O_4@boehmite NPs as efficient and magnetically recoverable nanocatalyst in the homoselective synthesis of tetrazoles

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Abstract:

Magnetic boehmite nanoparticles (Fe_3O_4@boehmite NPs) were synthesized from a hybrid of boehmite and Fe_3O_4 nanoparticles. At first, boehmite nanoparticles (aluminum oxide hydroxide) were prepared *via* a simple procedure in water using commercially available materials such as sodium hydroxide and aluminum nitrate. Then, these nanoparticles were magnetized using Fe_3O_4 NPs in a basic solution of $FeCl_2.4H_2O$ and $FeCl_3.6H_2O$. Fe_3O_4@boehmite NPs have advantages of both boehmite nanoparticles and Fe_3O_4 magnetic materials. Magnetic boehmite nanoparticles have been characterized by various techniques such as TEM, SEM, EDS, WDX, ICP, FT-IR, Raman, XRD and VSM. SEM and TEM images confirmed that particles size are less than 50 nm in diameter with a cubic orthorhombic structure. Then, Fe_3O_4@boehmite NPs were applied as a homoselective, highly efficient, cheep, biocompatibility, heterogeneous and magnetically recoverable nanocatalyst in the synthesis of 5-substituted 1H-tetrazole derivatives. Fe_3O_4@boehmite NPs can be recycled for several runs in the synthesis of tetrazoles. Also, all tetrazoles were isolated in high yields, which reveals high activity of Fe_3O_4@boehmite NPs in the synthesis of tetrazole derivatives. Fe_3O_4@boehmite NPs shows a good homoselectivity in synthesis of 5-substituted 1H-tetrazole derivatives.

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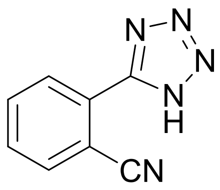
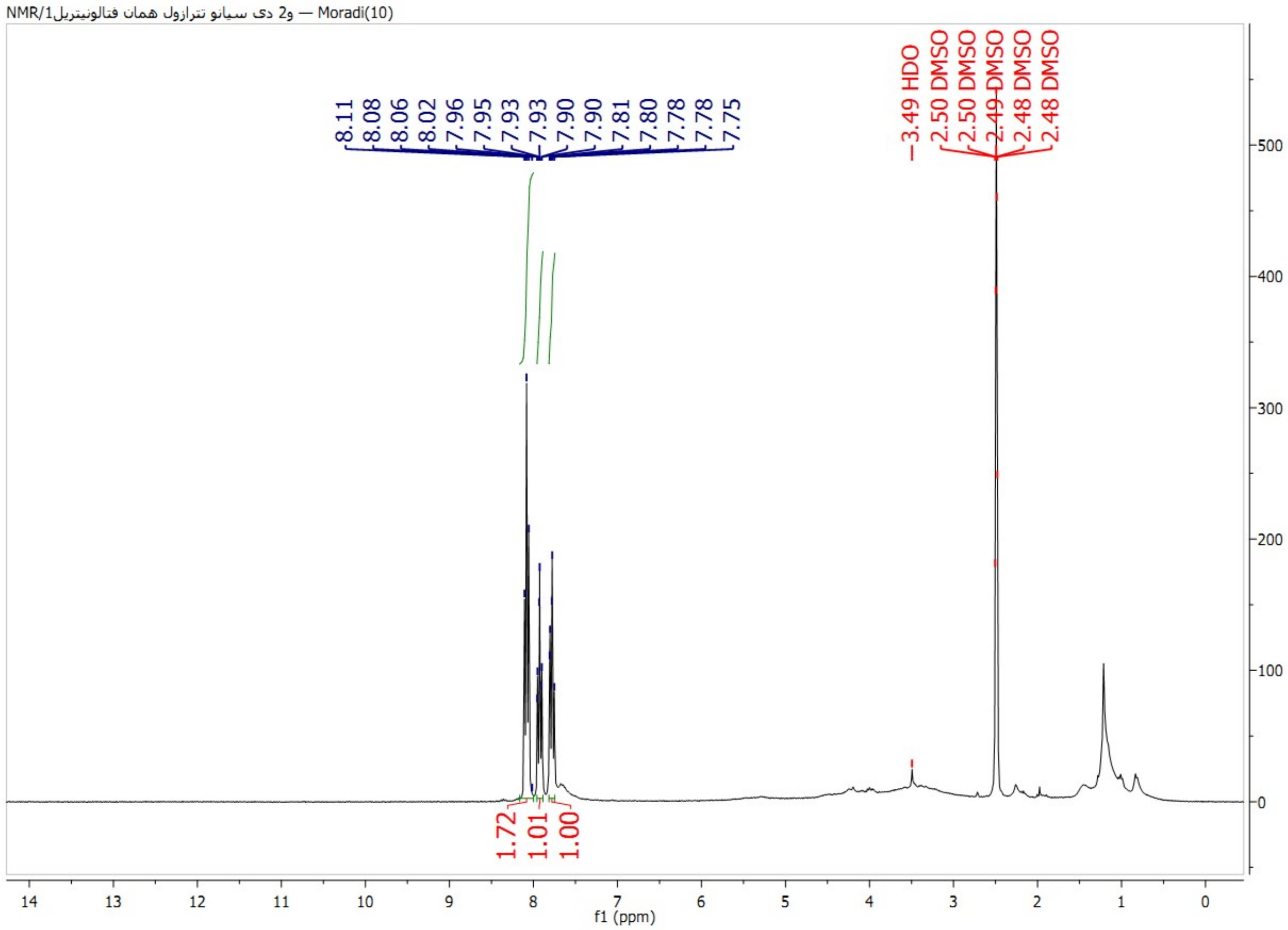
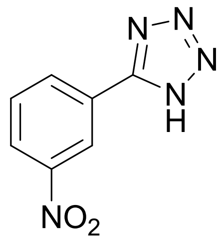
[1]H NMR spectral data



2-(1H-tetrazol-5-yl)benzonitrile

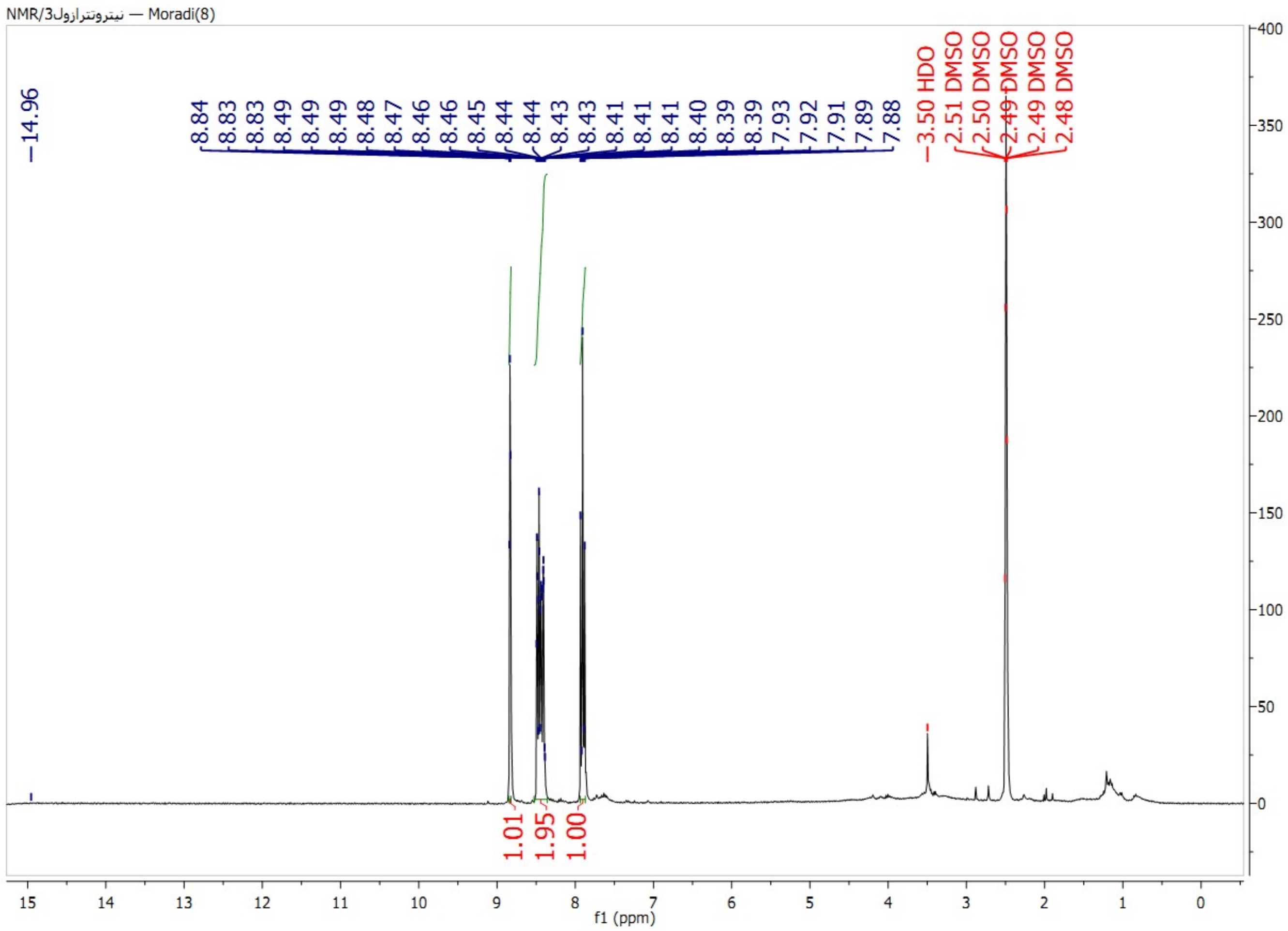
^{1}H NMR (400 MHz, $CDCl_3$): δ_H= 8.11-8.06 (t, *J*= 8 Hz, 2H), 7.96-7.90 (t, *J*= 12 Hz, 1H), 7.81-7.75 (t, *J*= 20 Hz, 1H)ppm.

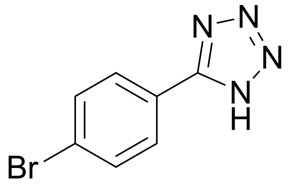




5-(3-nitrophenyl)-1H-tetrazole

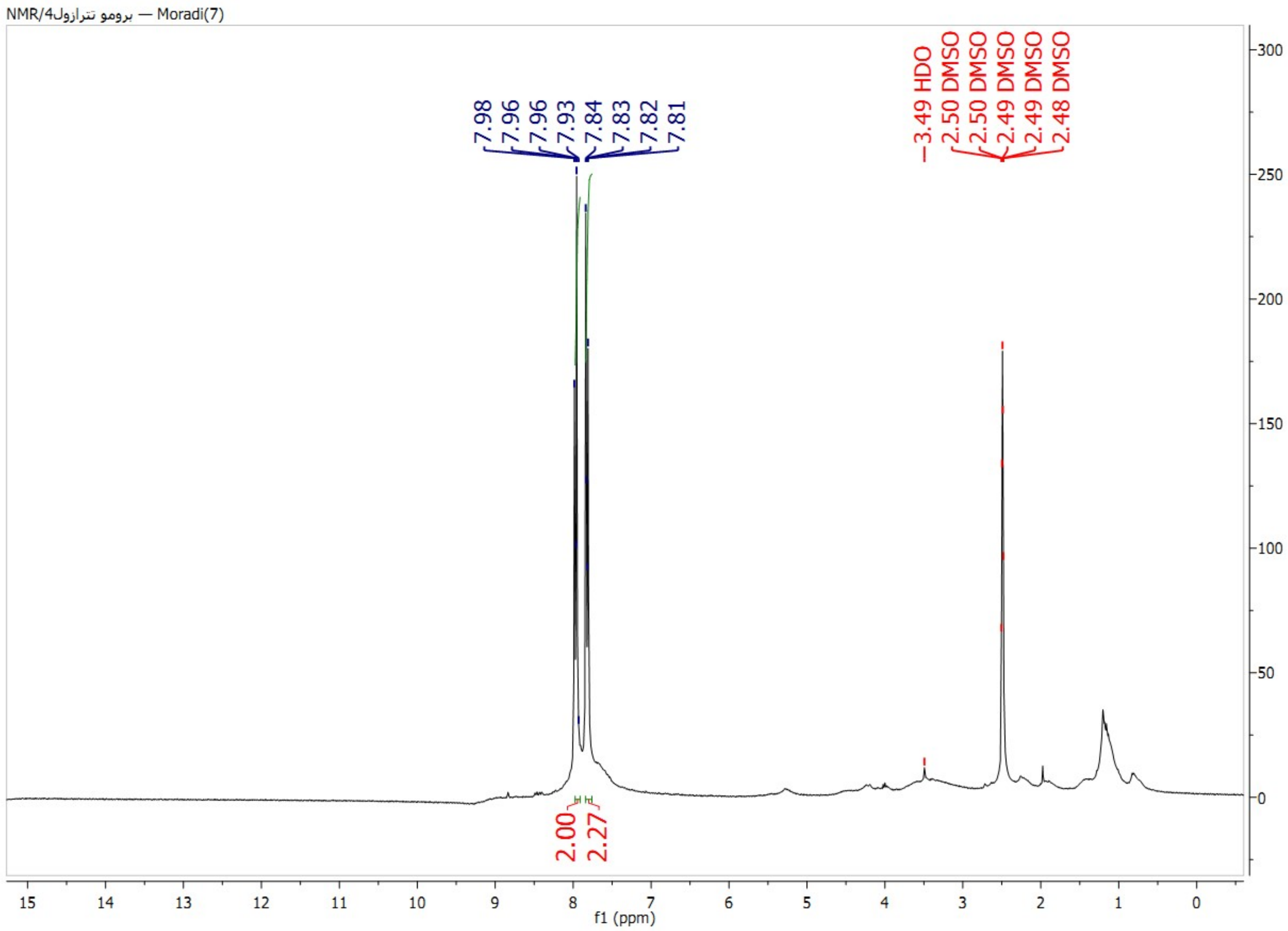
^{1}H NMR (400 MHz, $CDCl_3$): δ_H= 14.96 (br, 1H), 8.84-8.83 (t, *J*= 4 Hz, 1H), 8.49-8.39 (m, 2H), 7.93-7.88 (t, *J*= 8 Hz, 1H) ppm.

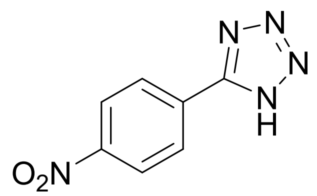




5-(4-bromophenyl)-1H-tetrazole

[1]H NMR (400 MHz, $CDCl_3$): δ_H= 7.98-7.96 (d, *J*= 8 Hz, 2H), 7.84-7.82 (d, *J*= 8 Hz, 2H) ppm.





5-(4-nitrophenyl)-1H-tetrazole

^{1}H NMR (400 MHz, $CDCl_3$): δ_H= 14.76 (br, 1H), 8.45-8.41 (d, *J*= 12 Hz, 2H), 8.30-8.27 (d, *J*= 12 Hz, 2H) ppm.