

Supporting Information

Tailoring the structure, pH sensitivity and catalytic performance in Suzuki-Miyaura cross-couplings of Ln/Pd MOFs based on the 1,1'-di(*p*-carboxybenzyl)-2,2'-diimidazole linker

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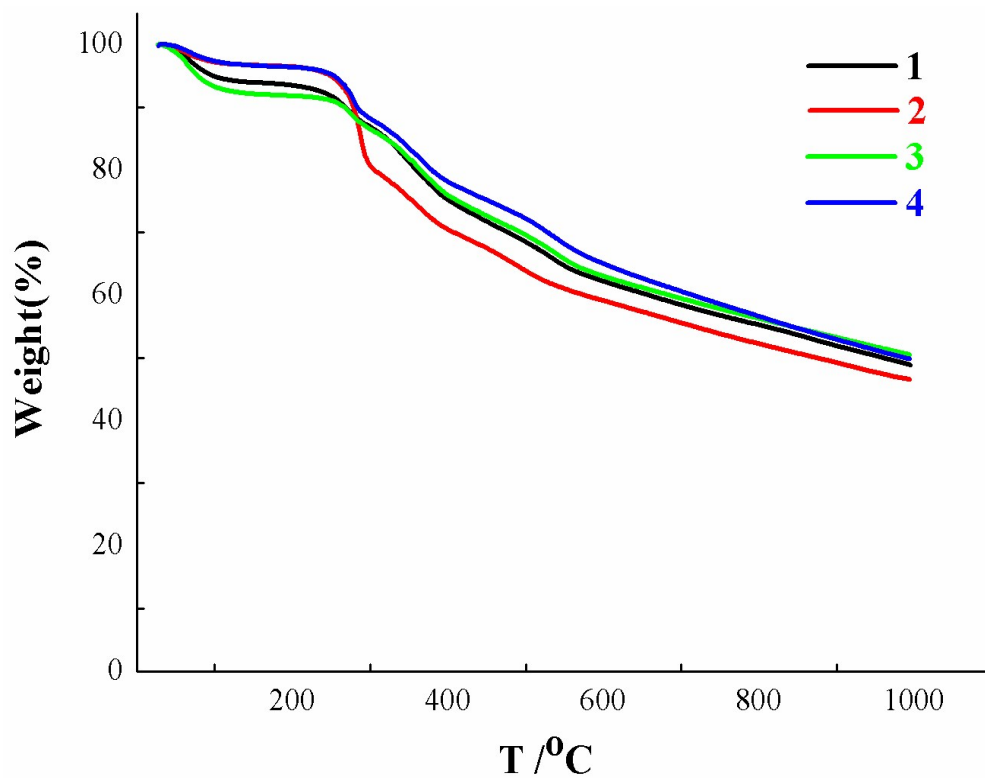


Fig. S1 TGA plots for different samples

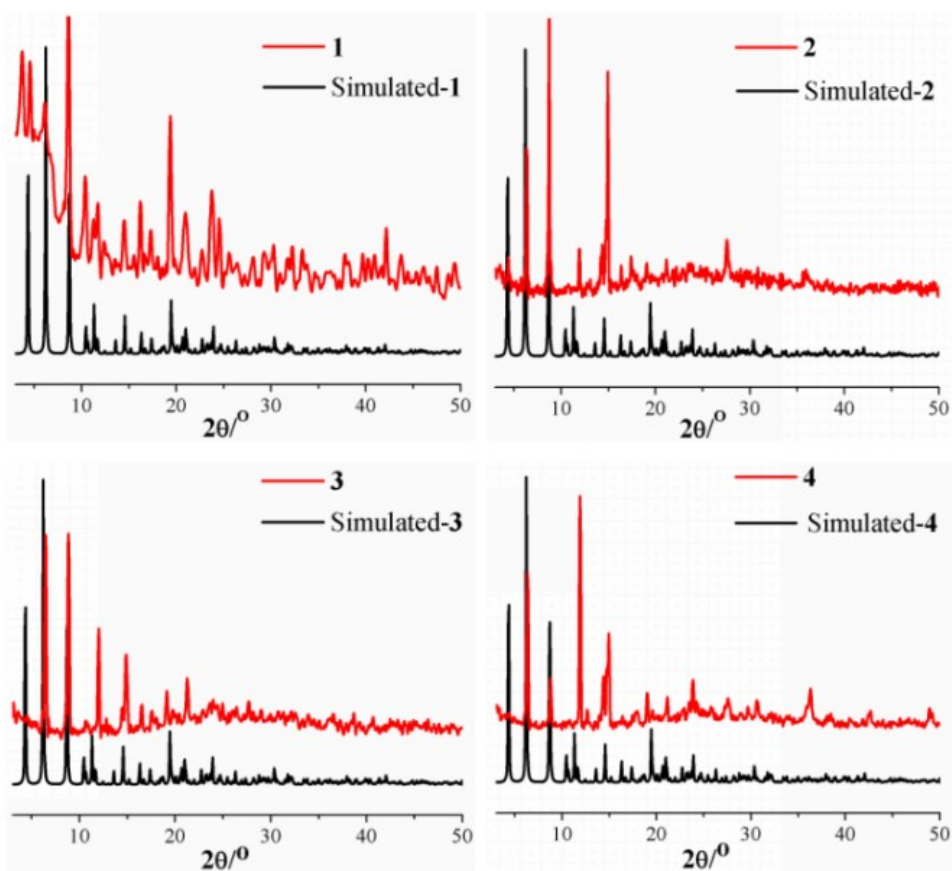


Fig. S2 X-ray powder diffraction patterns of 1-4

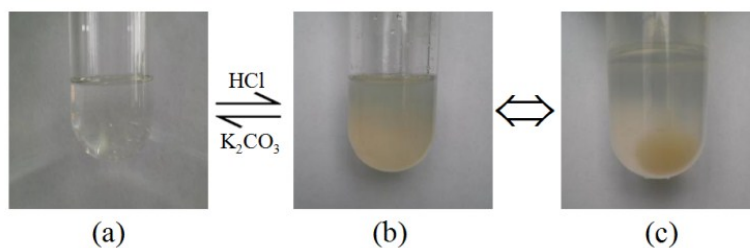


Fig. S3 (a) Complex **1** (0.4% mmol), K_2CO_3 (2.0 mmol) in H_2O (6.0 mL); (b) acidified with diluted HCl (2.0 mol L^{-1}) to $pH = 4$; (c) the mixture (b) after centrifugation.

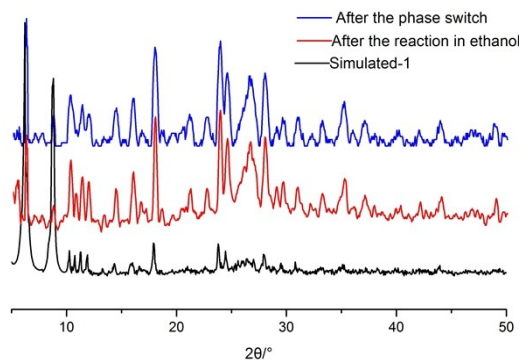


Fig. S4 X-ray powder diffraction patterns of **1**. Simulated (black); recovered after reaction in ethanol (red); precipitate [Fig. S3(c)] recovered from water after phase switch with acid (blue).

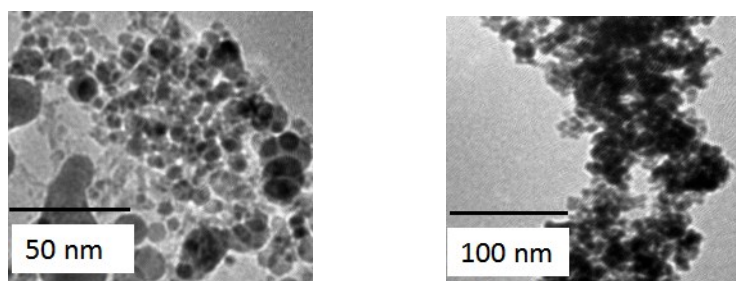


Fig. S5 TEM images of catalyst **1** after the reaction in water-ethanol (left) and water (right).

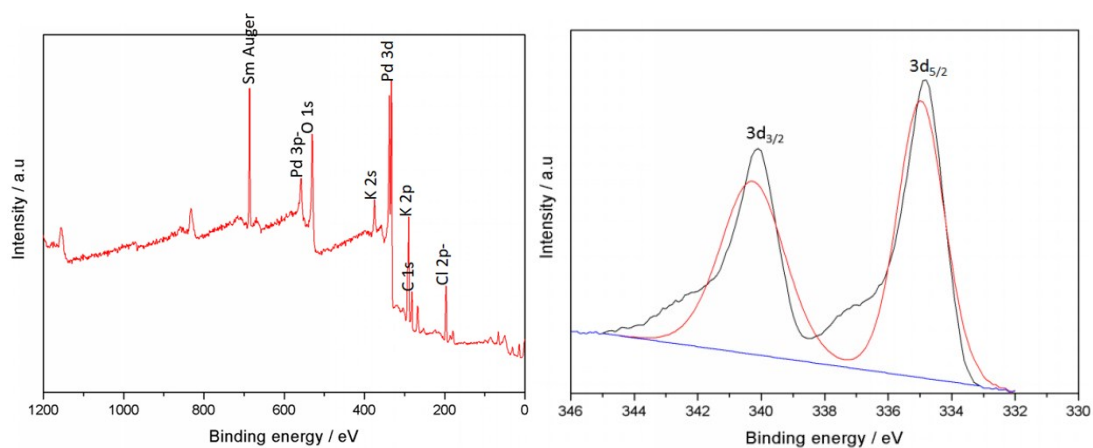


Fig. S6 XPS spectra of catalyst **1** after the reaction in water

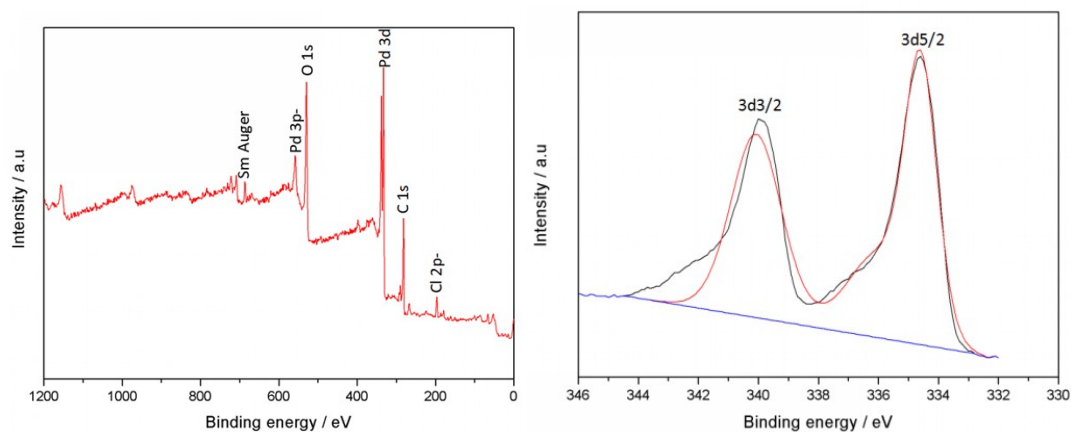


Fig. S7 XPS spectra of catalyst **1** after the reaction in water-ethanol

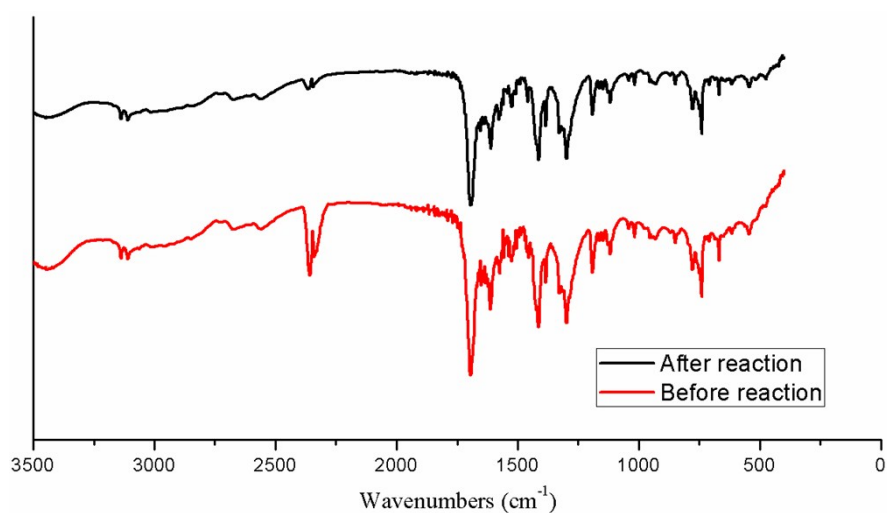


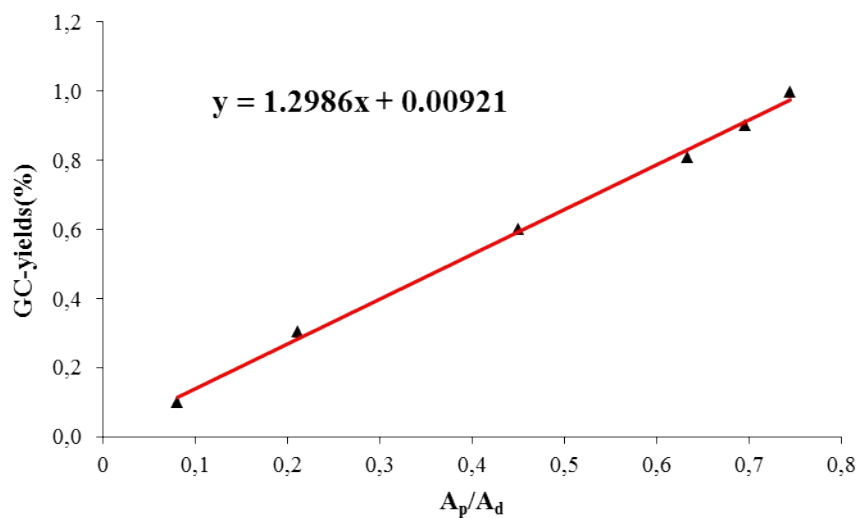
Fig. S8 IR spectra of **1**, before and after the cross-coupling reaction in ethanol

GC-yield Standard Curve

The response peak area ratios of the product and internal standard, n-hexadecane (A_p/A_d) were obtained from Agilent 7890A GC spectrometer. All the GC-yields were calculated by the formula of curve fitting.

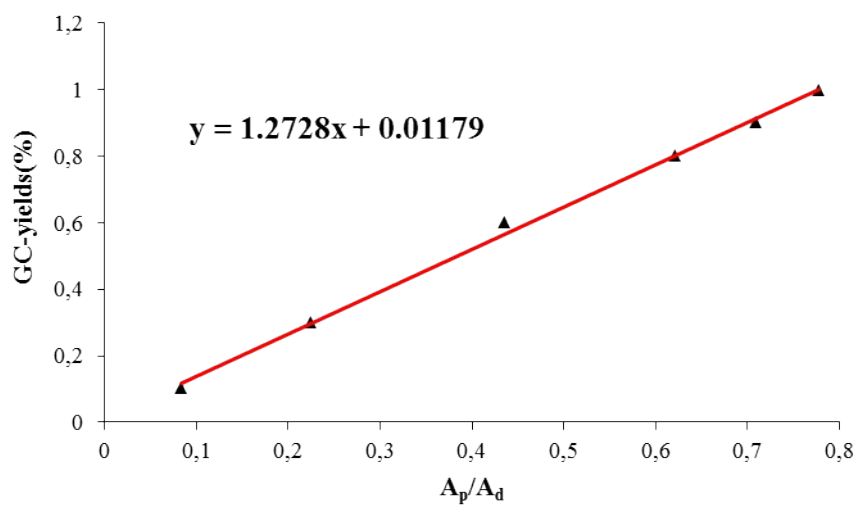
GC-Yield Standard Curve of biphenyl

A_p/A_d	0.0806	0.2106	0.4497	0.6333	0.6953	0.7448
Yields	0.1	0.30	0.60	0.81	0.90	1.00



GC-Yield Standard Curve of 4-Phenyltoluene

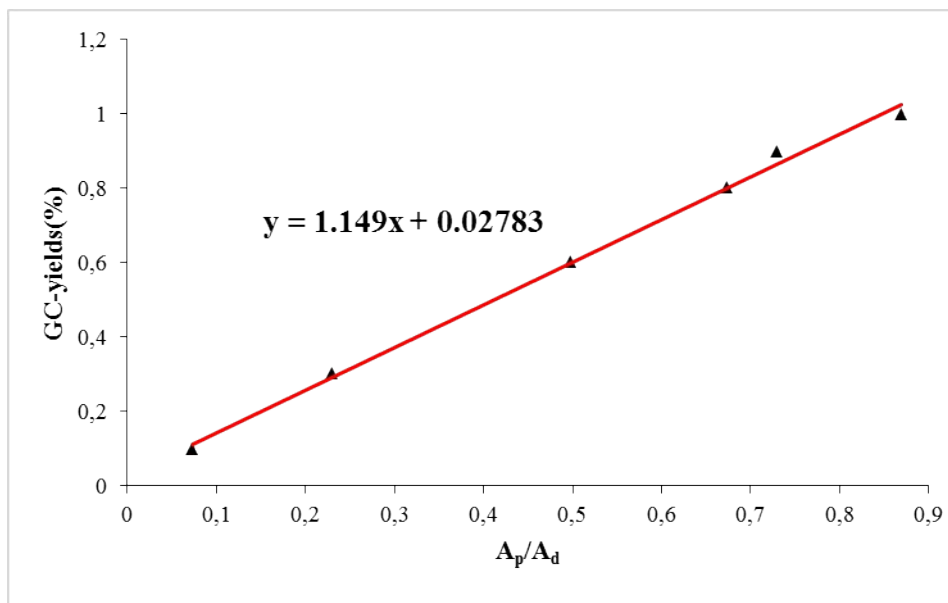
A_p/A_d	0.0833	0.2243	0.4362	0.6207	0.7095	0.7776
Yields	0.1	0.30	0.60	0.80	0.90	1.00



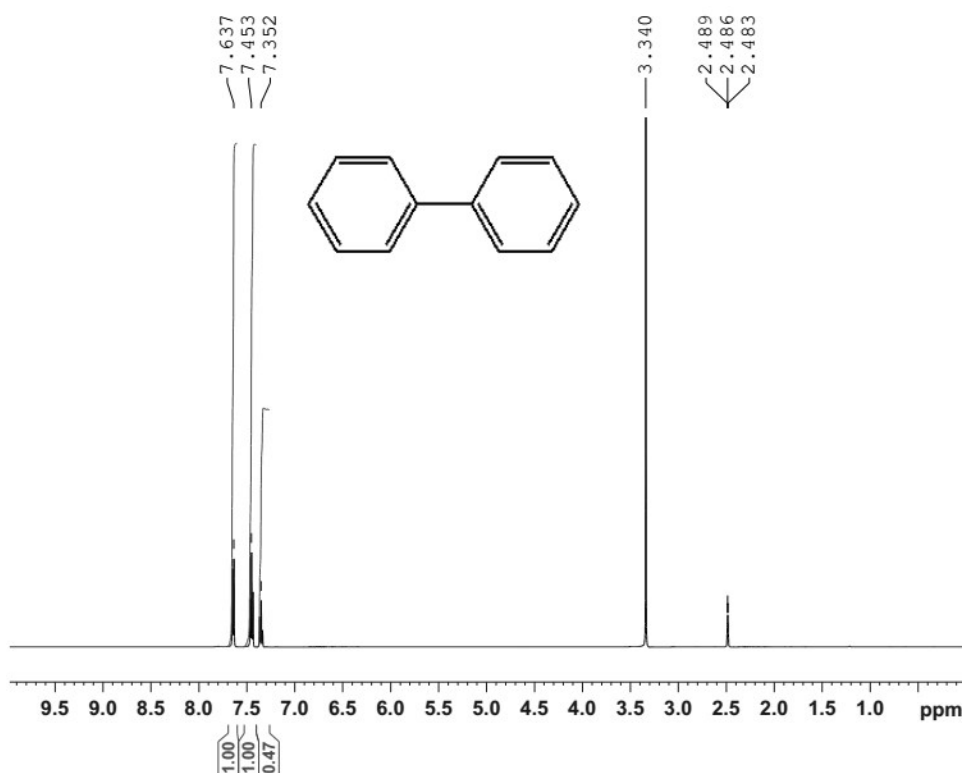
GC-Yield Standard Curve of 4-Phenylacetophenone

A_p/A_d	0.0730	0.2305	0.4982	0.6735	0.7293	0.8697
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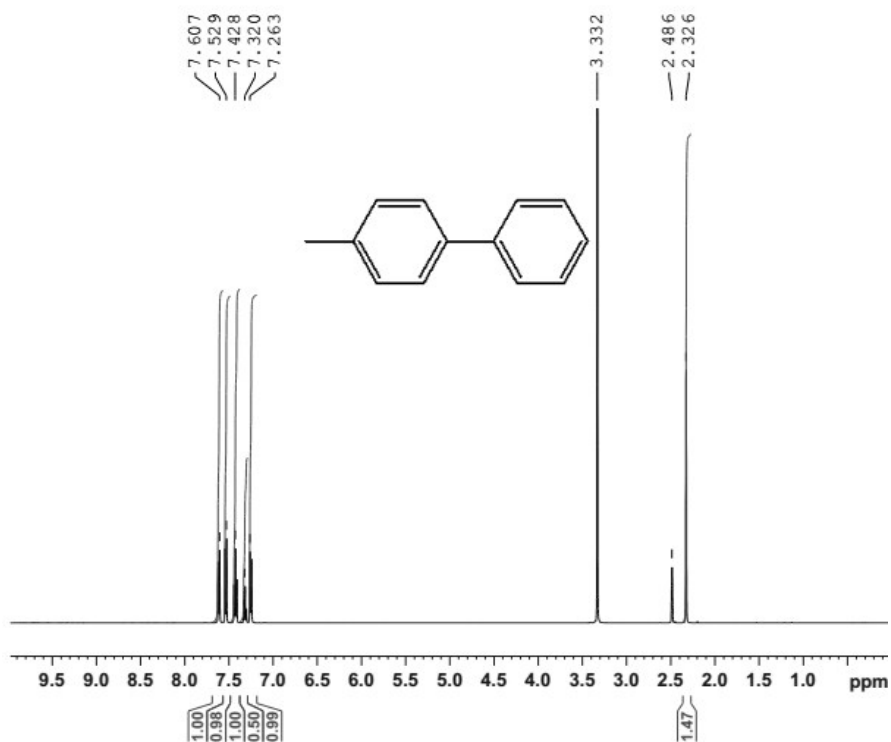
Yields	0.1	0.30	0.60	0.80	0.90	1.00
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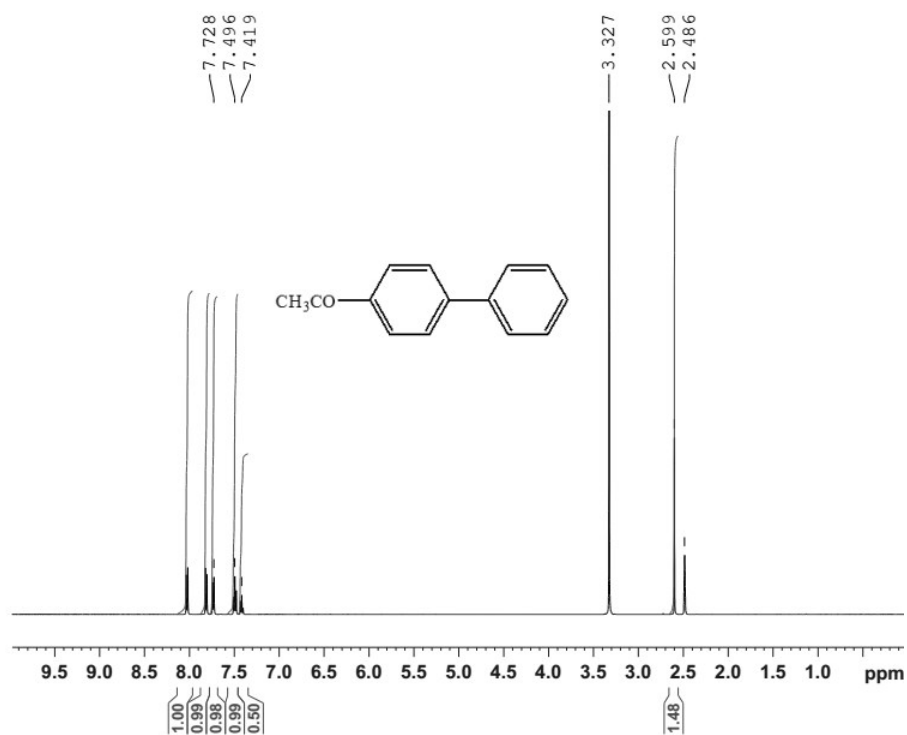
¹H NMR Spectra of products



Biphenyl: ¹H NMR (500 MHz, DMSO-*d*₆): $\delta = 7.35$ (*t*, 2H), 7.45(*t*, 4H), 7.64 (*d*, 4H).



4-Methyl-1,1'-biphenyl: ^1H NMR (500 MHz, $\text{DMSO-}d_6$): $\delta = 2.33$ (s, 3H), 7.26 (d, 2H), 7.32 (t, 1H), 7.43 (t, 2H), 7.53 (d, 2H), 7.61 (d, 2H).



4-Acetyl-1,1'-biphenyl: ^1H NMR (500 MHz, $\text{DMSO-}d_6$): $\delta = 2.60$ (s, 3H), 7.42 (t, 2H), 7.50 (t, 2H), 7.73 (d, 2H), 7.82 (d, 2H), 8.03 (d, 2H)