

## Polymer incarcerated Palladium catalyzed facile *in situ* carbonylation for the synthesis of aryl aldehydes and diaryl ketones using CO surrogates at ambient conditions

Tusar Kanto Dey<sup>a</sup>, Priyanka Basu<sup>a‡</sup>, Sk Riyajuddin<sup>b‡</sup>, Aniruddha Ghosh<sup>a‡</sup>, Kaushik Ghosh<sup>b</sup>, and Sk. Manirul Islam<sup>a\*</sup>

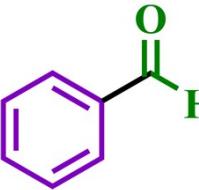
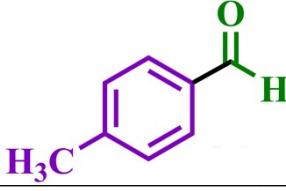
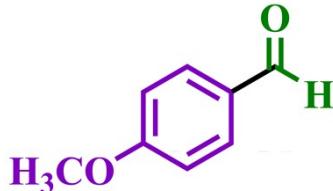
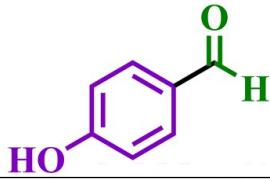
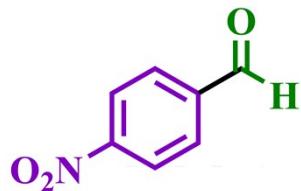
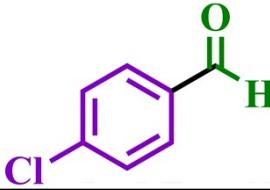
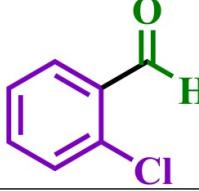
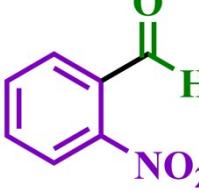
<sup>a</sup>Department of Chemistry, University of Kalyani, Kalyani, Nadia 741235, West Bengal, India

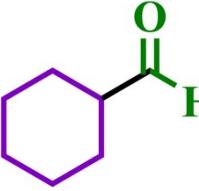
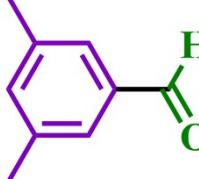
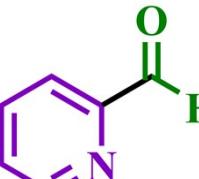
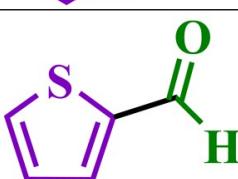
<sup>b</sup>Institute of Nano Science and Technology, Mohali, Punjab-160062, India

<sup>‡</sup>These authors contributed equally.

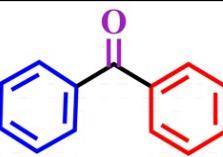
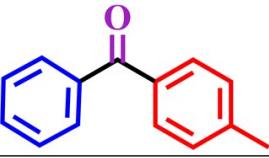
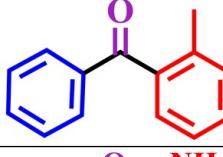
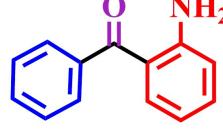
Serial no.	Contents	Pages
1.	<sup>1</sup> HNMR data of respective products for insitu carbonylative formylation of aryl iodides	S2-S3
2.	<sup>1</sup> HNMR data of respective products for insitu carbonylative S-M coupling reaction	S3-S4
3.	<sup>1</sup> HNMR copies of respective products for insitu carbonylative formylation of aryl iodides	S5-S11
4.	<sup>1</sup> HNMR copies of respective products for insitu carbonylative S-M coupling reaction	S12-S17
5.	FTIR spectra of respective products for insitu carbonylative formylation of aryl iodides	S17-S24
6.	FTIR spectra of respective products for insitu carbonylative S-M coupling reaction	S24-S29

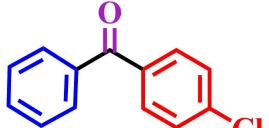
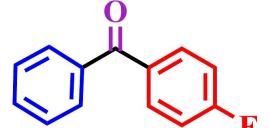
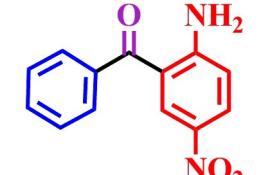
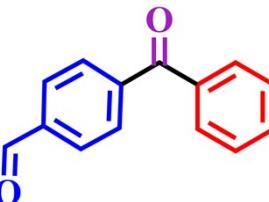
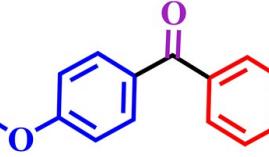
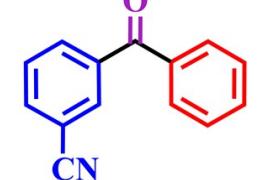
**1. *<sup>1</sup>HNMR data of insitu carbonylative products***

	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.445-7.539 (m, 2H), 7.582-7.644 (m, 1H), 7.865-7.886 (m, 2H), 10.008 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ2.441 (s, 3H), 7.322-7.342 (d, J=8 Hz, 2H), 7.769-7.789 (t, J=7.2 Hz, 2H), 9.965 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ3.892 (s, 3H), 6.991-7.018 (m, 2H), 7.825-7.853 (m, 2H), 9.887 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ6.373 (s, 1H), 6.948-6.990 (m, 2H), 7.791-7.840 (m, 2H), 9.865 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ8.004-8.026 (m, 2H), 8.325-8.346 (d, J=8.4 Hz, 2H), 10.128 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.529-7.550 (m, 2H), 7.828-7.860 (m, 2H), 10.005 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.276-7.367 (m, 2H), 7.423-7.465 (m, 1H), 7.815-7.839 (m, 1H), 10.386 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ6.967-7.029 (m, 2H), 7.495-7.557 (m, 2H), 9.878 (s, 1H), 11.026 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.766-7.845 (m, 2H), 7.968-7.991 (m, 1H), 8.135-8.158 (m, 1H), 10.448 (s, 1H) ppm.

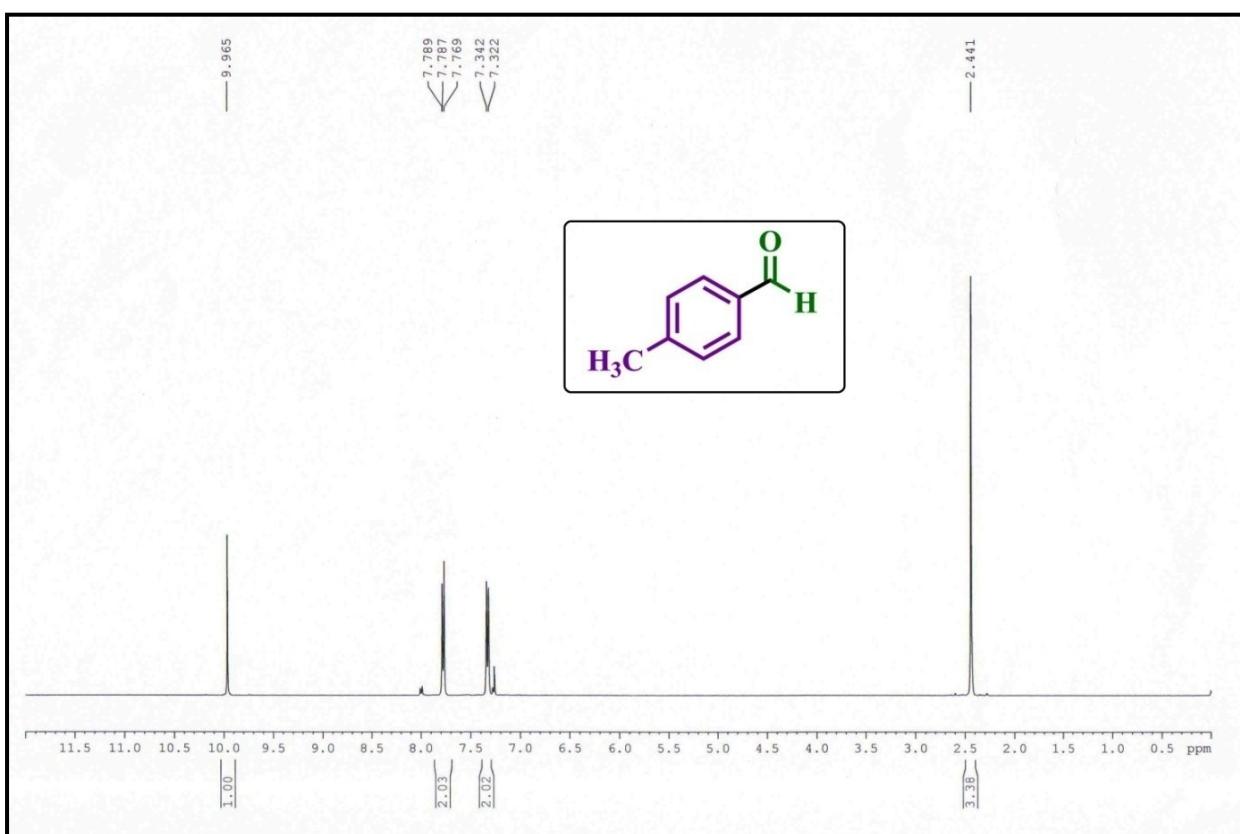
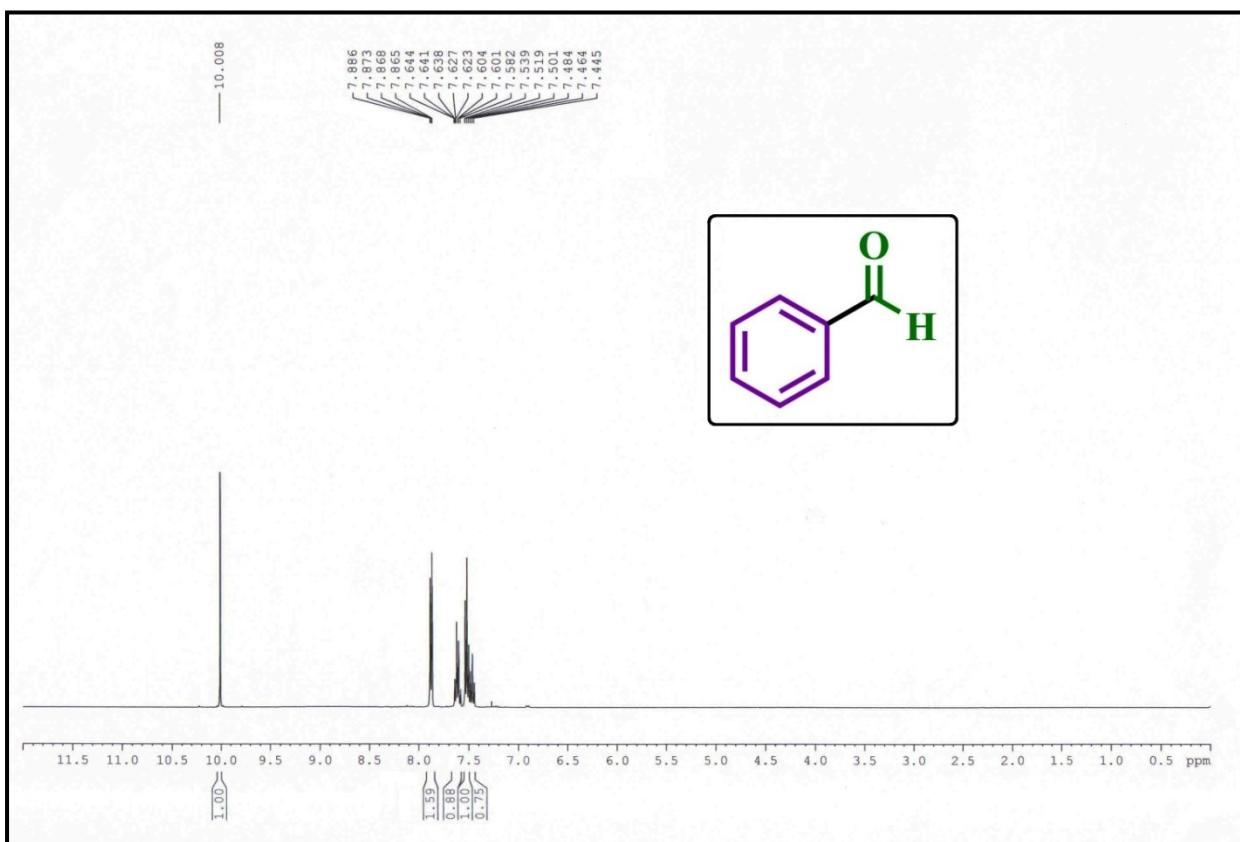
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ1.320-1.508 (m, 5H), 1.646-1.669 (t, J=5.6 Hz, 1H), 1.752-1.789 (m, 2H), 1.930-1.961 (t, J=10.4 Hz, 2H), 2.297-2.371 (m, 1H)
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ3.793 (s, 3H), 6.363-6.369 (d, J=2.4 Hz, 1H), 6.461-6.488 (m, 1H), 7.354-7.375 (d, J=8.4 Hz, 1H), 9.652 (s, 1H), 11.427 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ2.263 (s, 6H), 7.131 (s, 1H), 7.358 (s, 2H), 9.814 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.537-7.571 (m, 1H), 7.883-7.925 (m, 1H), 7.973-7.995 (m, 1H), 8.806-8.818 (d, J=4.8 Hz, 1H), 10.099 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.116-7.138 (t, J=4 Hz, 1H), 7.675-7.709 (m, 2H), 9.849 (s, 1H) ppm.

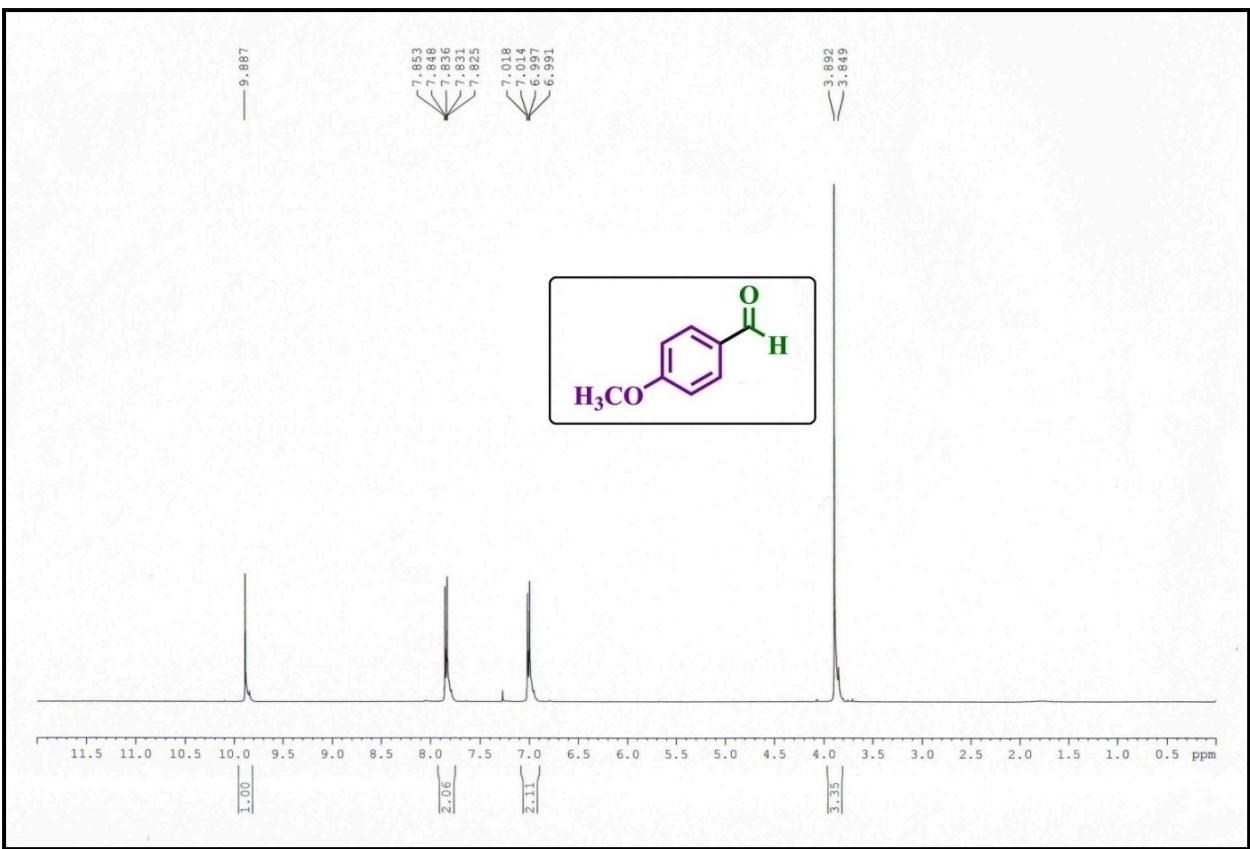
## 2. <sup>1</sup>HNMR data of diaryl ketone

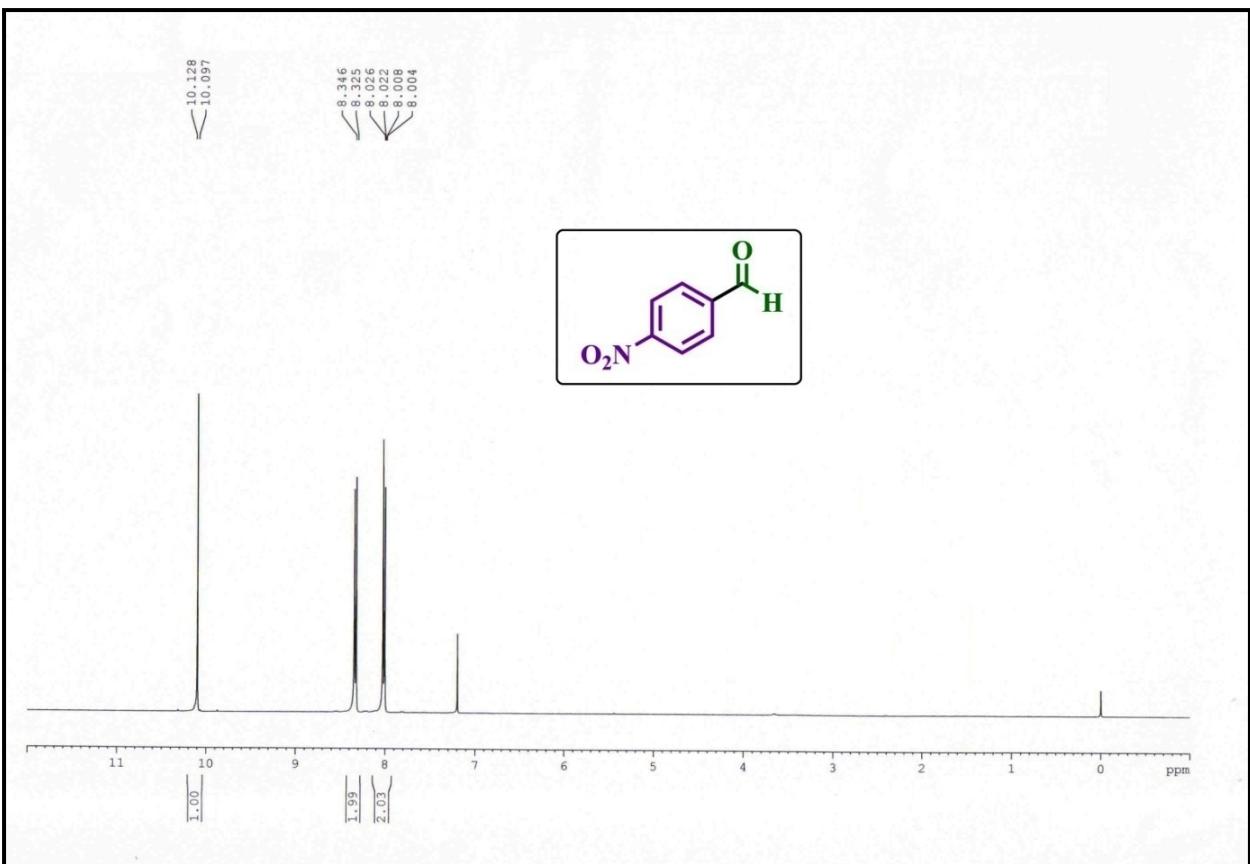
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.312-7.350 (m, 4H), 7.418-7.460 (m, 2H), 7.604-7.676 (m, 4H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ2.589 (s, 3H), 7.398-7.435 (t, J=7.2 Hz, 2H), 7.476-7.537 (m, 3H), 7.592-7.629 (m, 2H), 7.732-7.750 (d, J=7.2 Hz, 2H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ2.373 (s, 3H), 7.322-7.462 (m, 5H), 7.495-7.552 (m, 2H), 7.658-7.676 (d, J=7.2 Hz, 2H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ6.136 (s, 2H), 6.607-6.645 (m, 1H), 6.749-6.770 (d, J=8.4 Hz, 1H), 7.282-7.335 (m, 1H), 7.457-7.496 (m, 3H), 7.527-7.571 (m, 1H), 7.653-7.676 (m, 2H) ppm.

	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.368-7.432 (m, 4H), 7.507-7.544 (t, <i>J</i> =7.2 Hz, 1H), 7.663-7.705 (m, 4H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.023-7.073 (m, 2H), 7.356-7.394 (m, 1H), 7.462-7.502 (m, 3H), 7.648-7.671 (t, <i>J</i> =8 Hz, 2H), 7.711-7.753 (m, 2H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ6.765-6.788 (d, <i>J</i> =9.2 Hz, 1H), 6.935 (s, 2H), 7.520-7.555 (t, <i>J</i> =6.8 Hz, 2H), 7.610-7.678 (m, 3H), 8.171-8.193 (d, <i>J</i> =8.8 Hz, 1H), 8.500 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.279-7.746 (m, 8H), 7.878-7.941 (m, 1H), 10.016 (s, 1H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ5.103-5.115 (d, <i>J</i> =4.8 Hz, 2H), 7.016-7.064 (m, 2H), 7.303-7.356 (m, 2H), 7.385-7.404 (m, 4H), 7.416-7.564 (m, 6H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ3.775 (m, 3H), 6.663-6.693 (m, 2H), 7.396-7.432 (t, <i>J</i> =7.2 Hz, 2H), 7.535-7.566 (m, 3H), 7.730-7.749 (d, <i>J</i> =7.6 Hz, 2H) ppm.
	<sup>1</sup> HNMR (400 MHz, CDCl <sub>3</sub> ): δ7.489-7.699 (m, 4H), 7.771-7.889 (m, 3H), 8.037-8.060 (m, 2H) ppm.

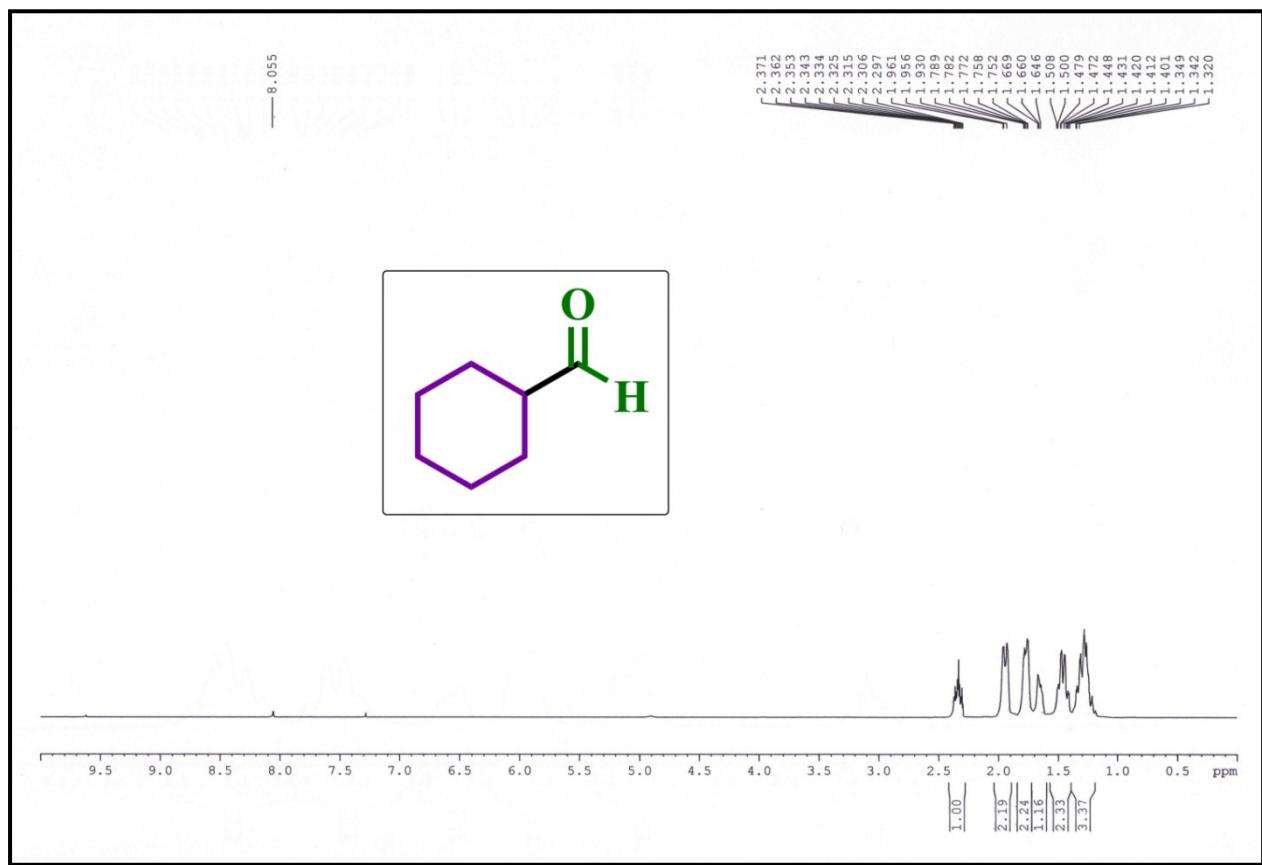
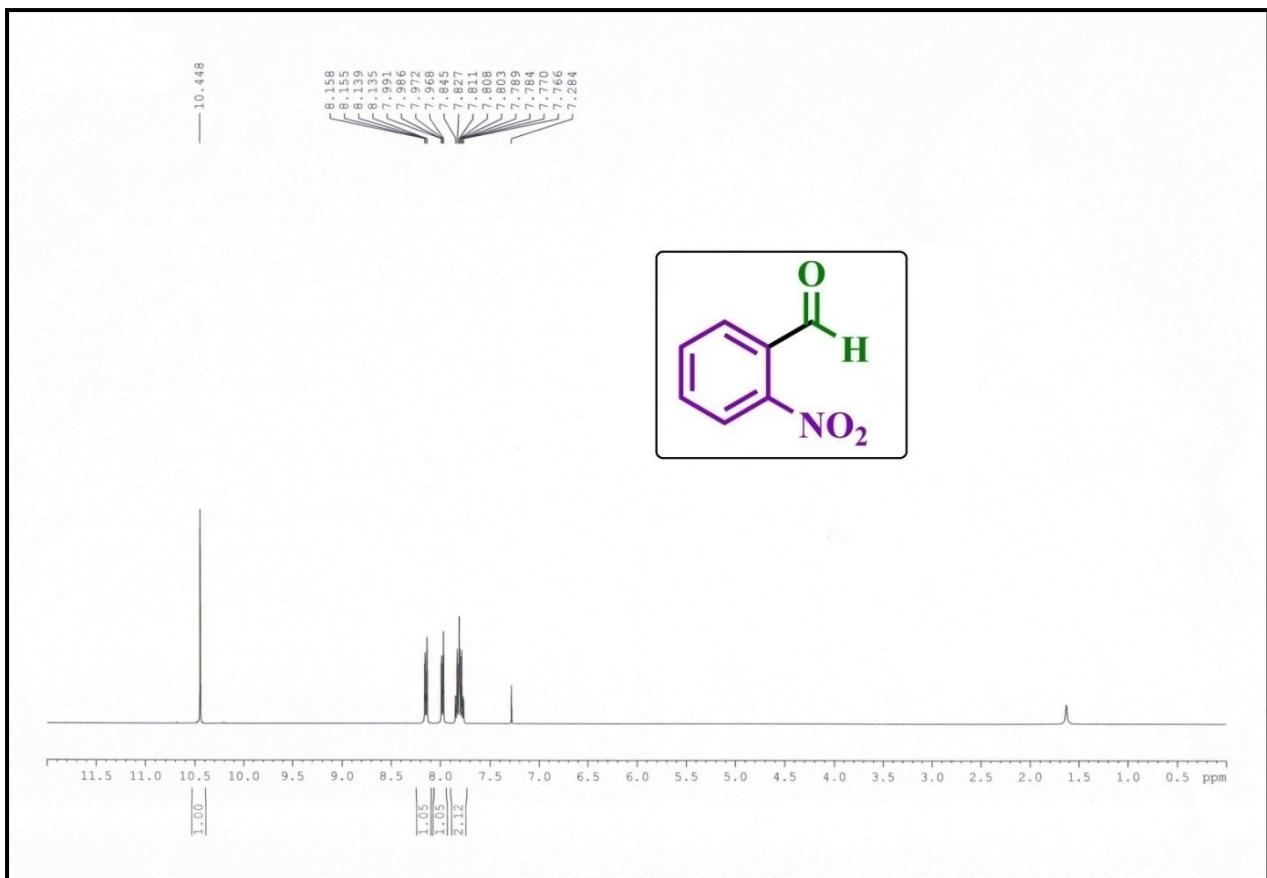
### 3. *<sup>1</sup>H NMR copies of insitu carbonylative products*

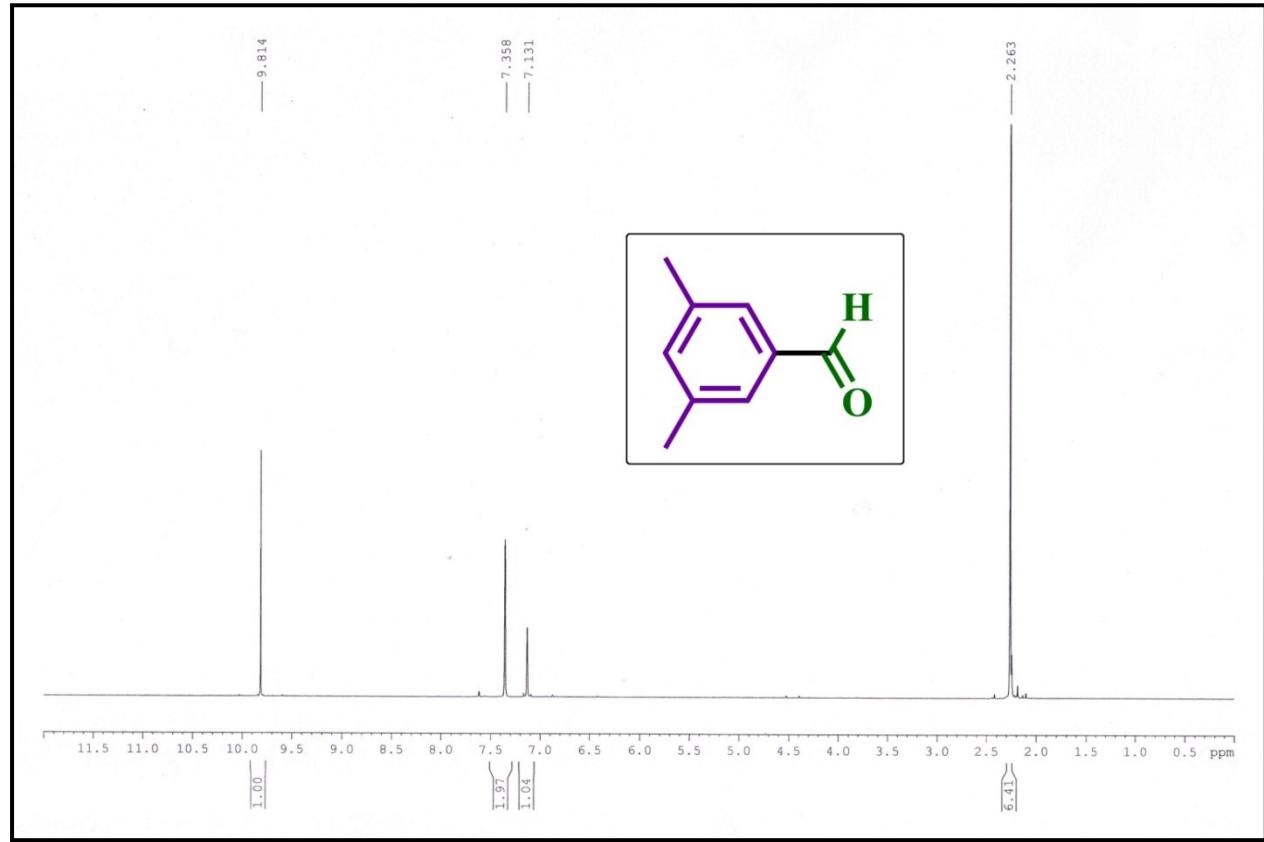
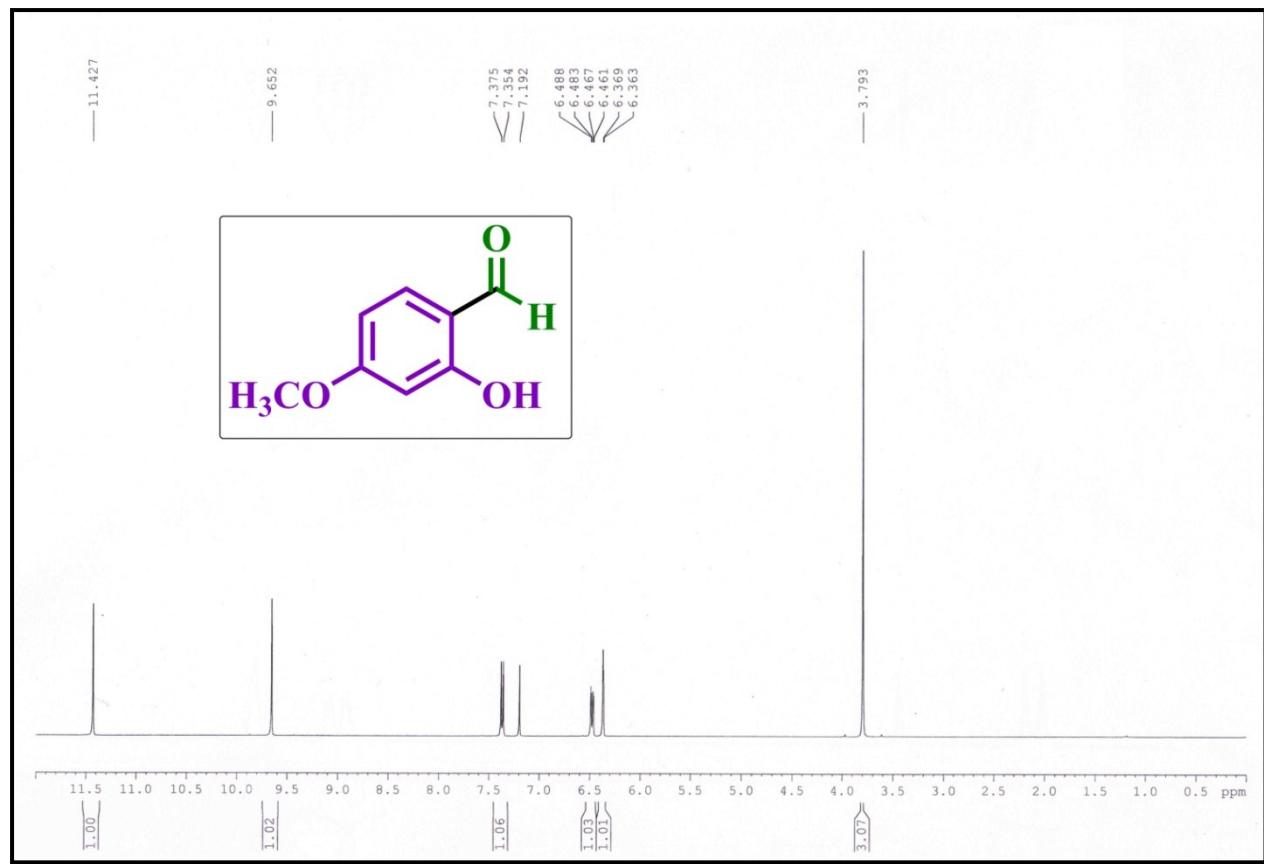


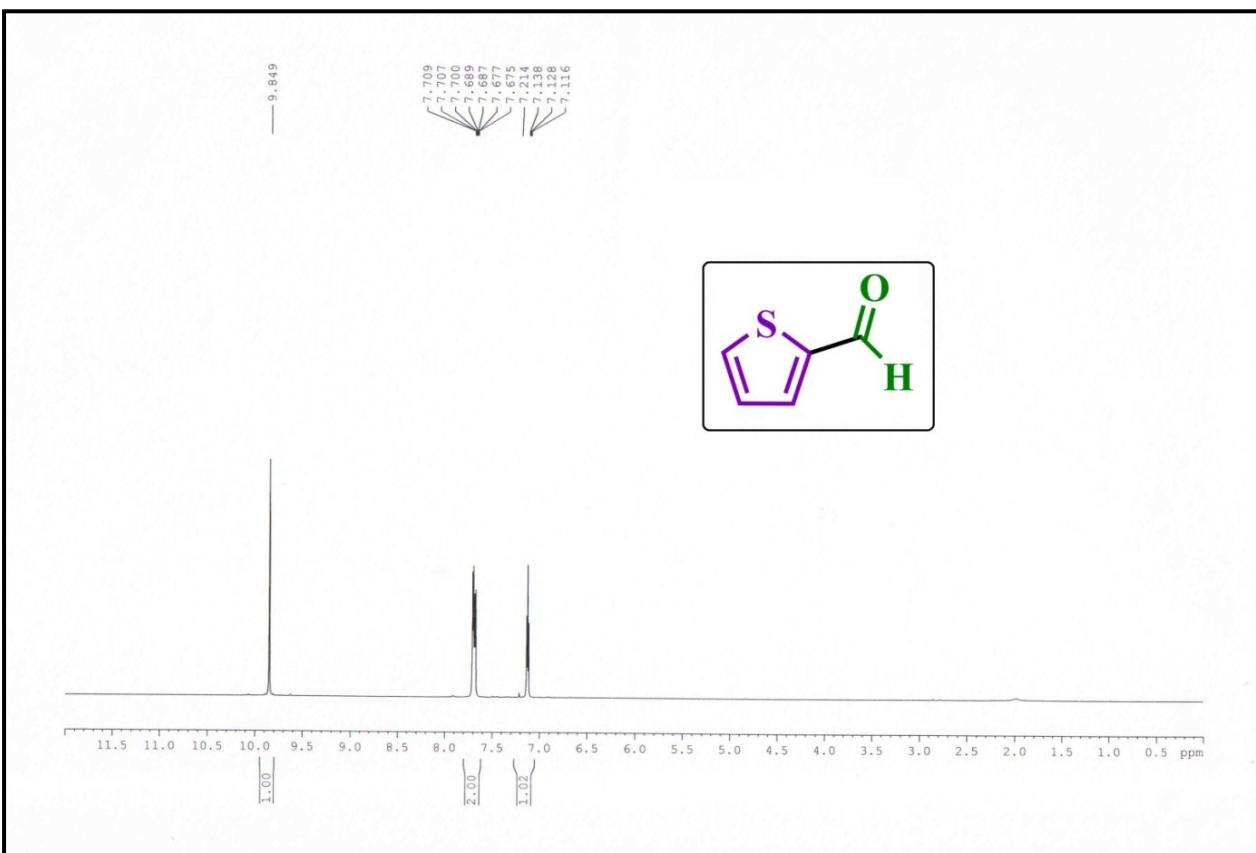
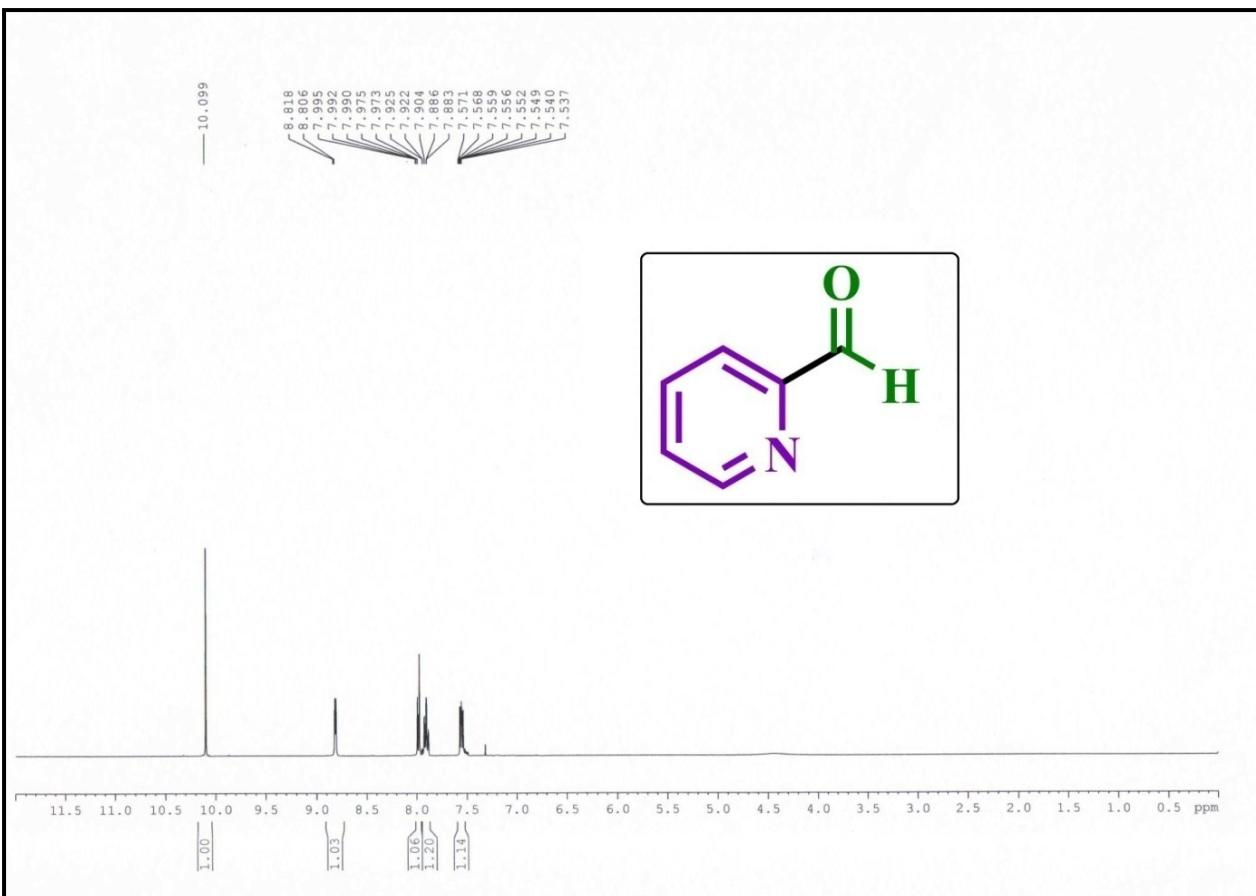




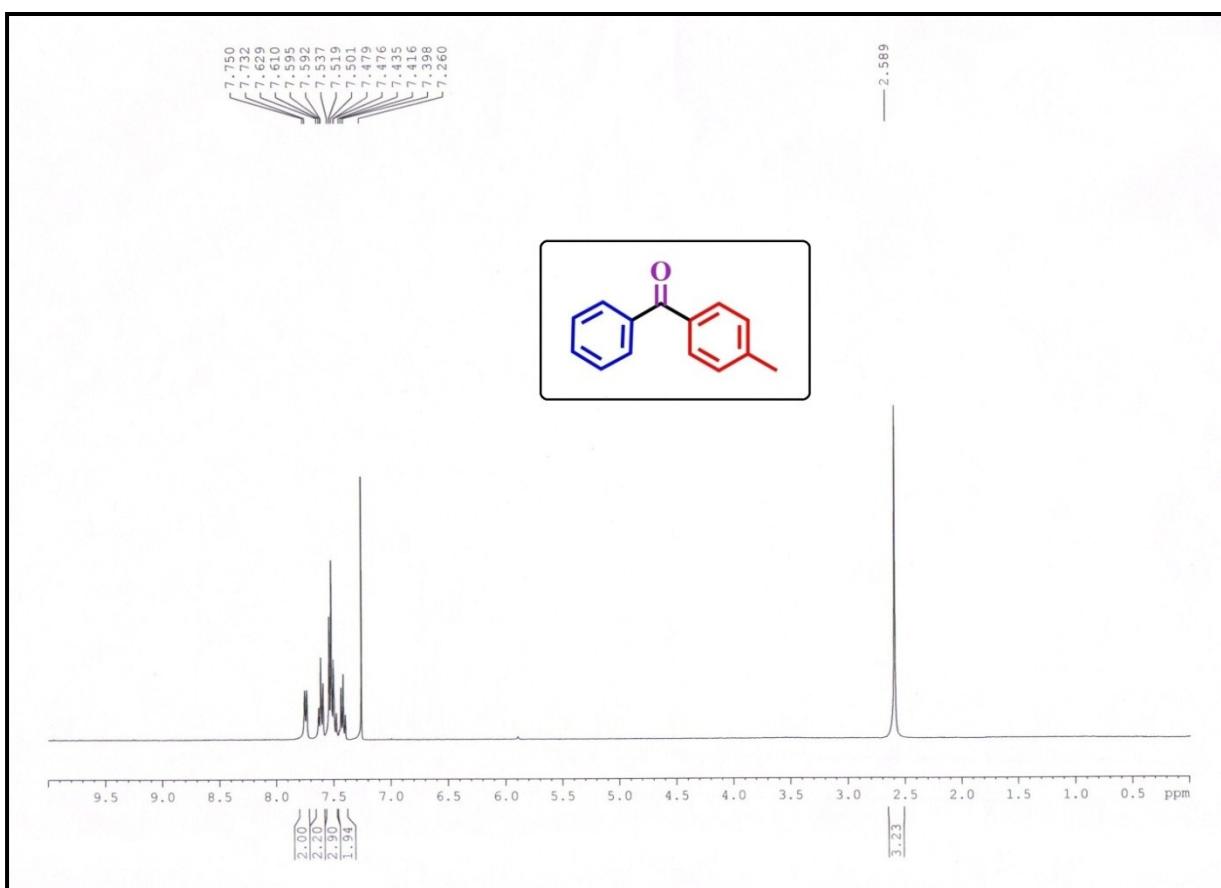
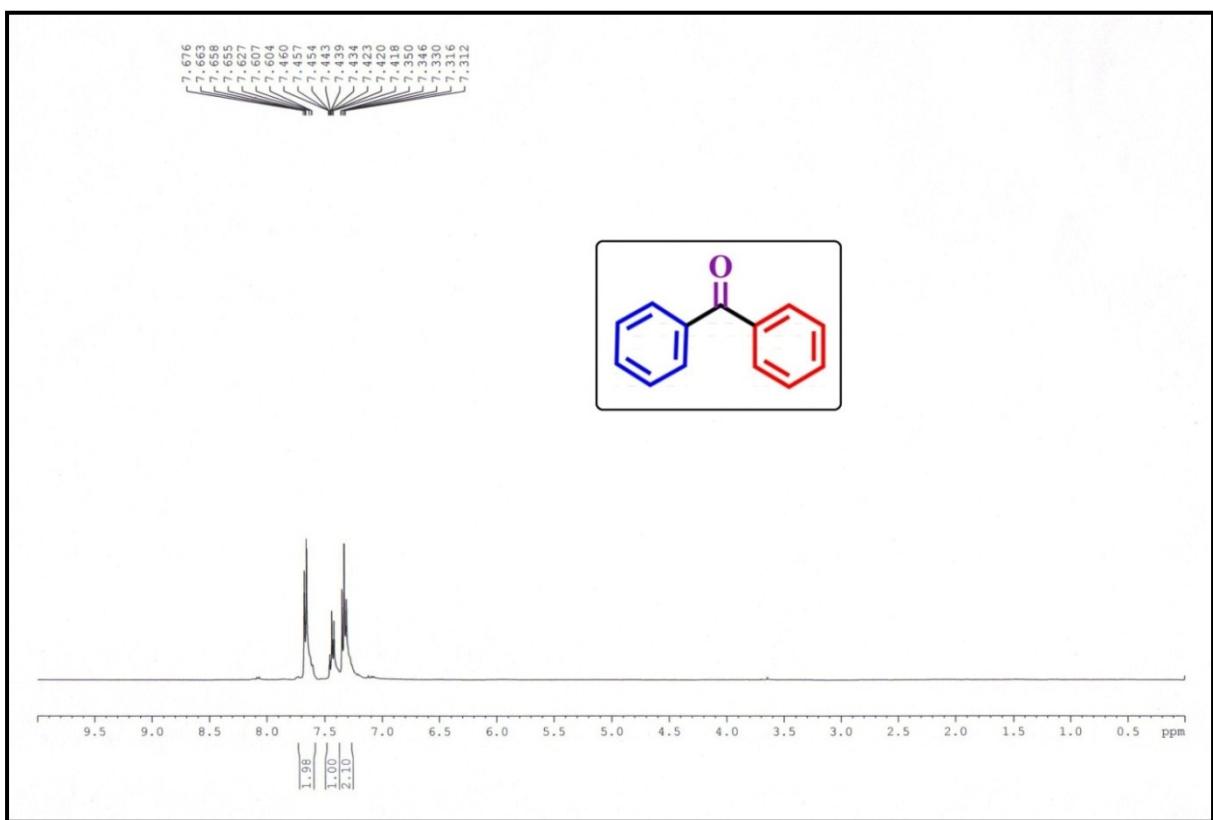


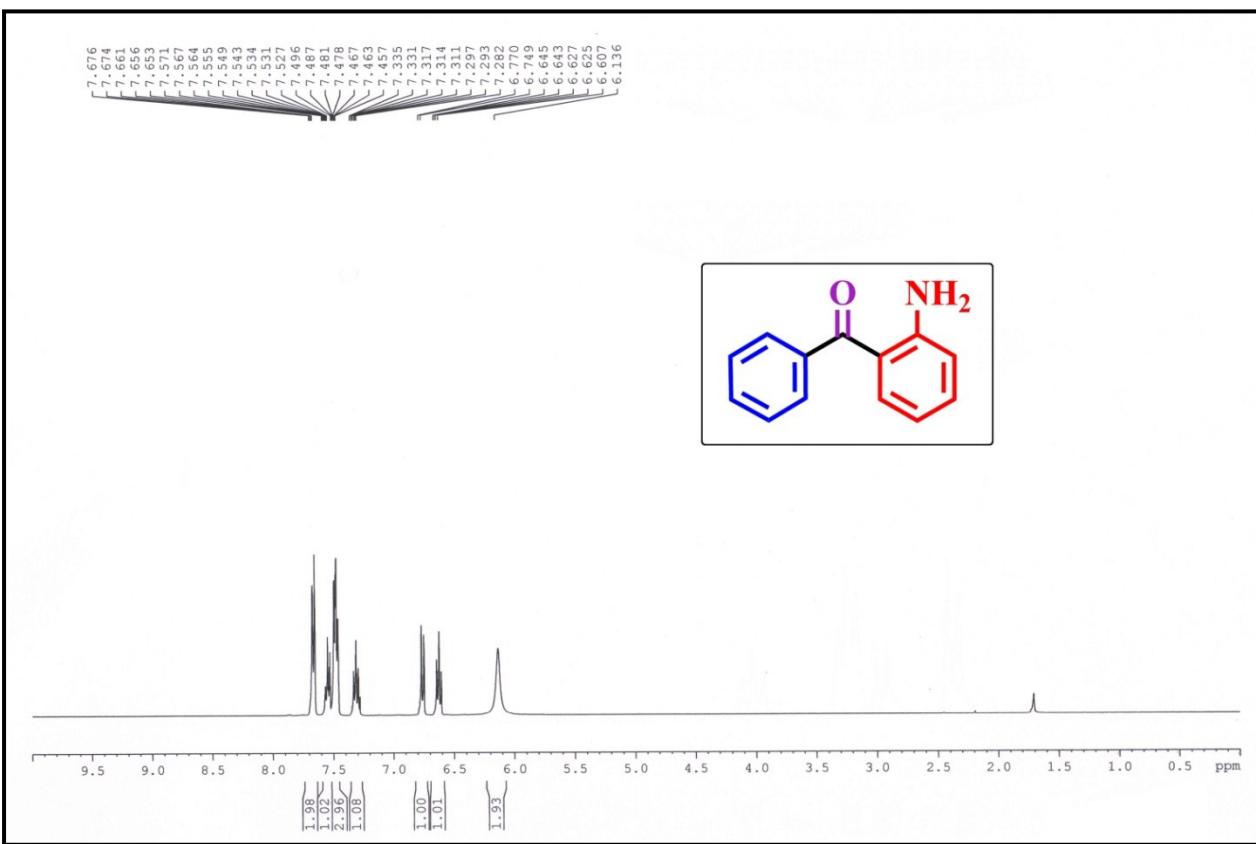
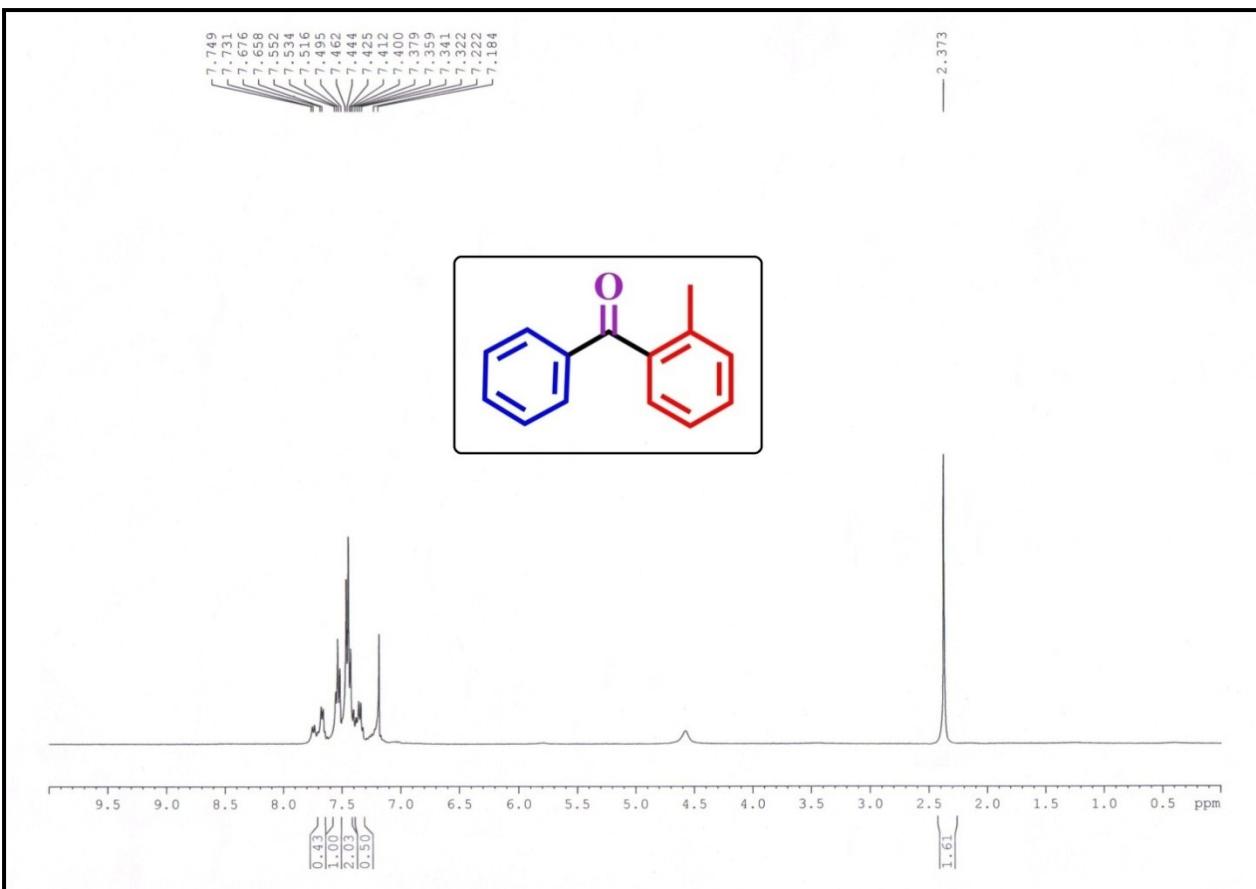


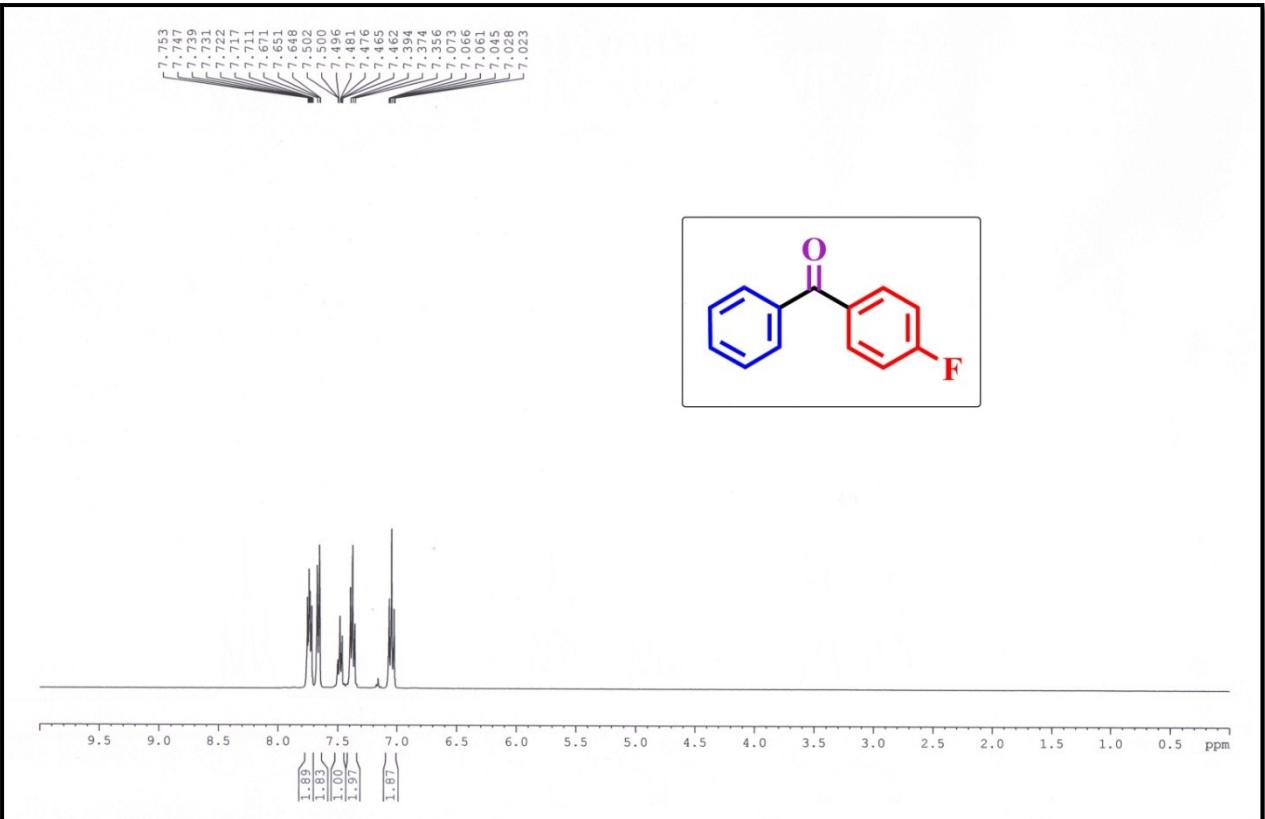
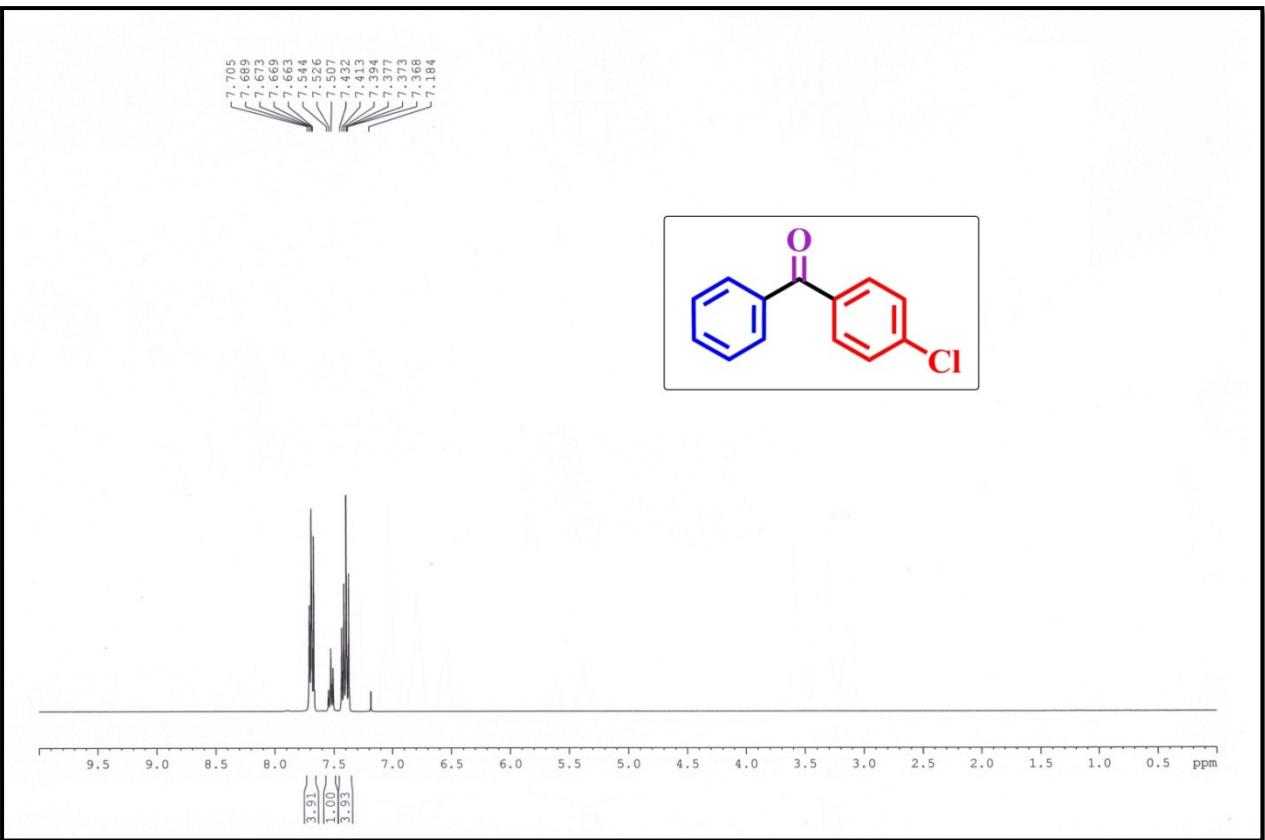


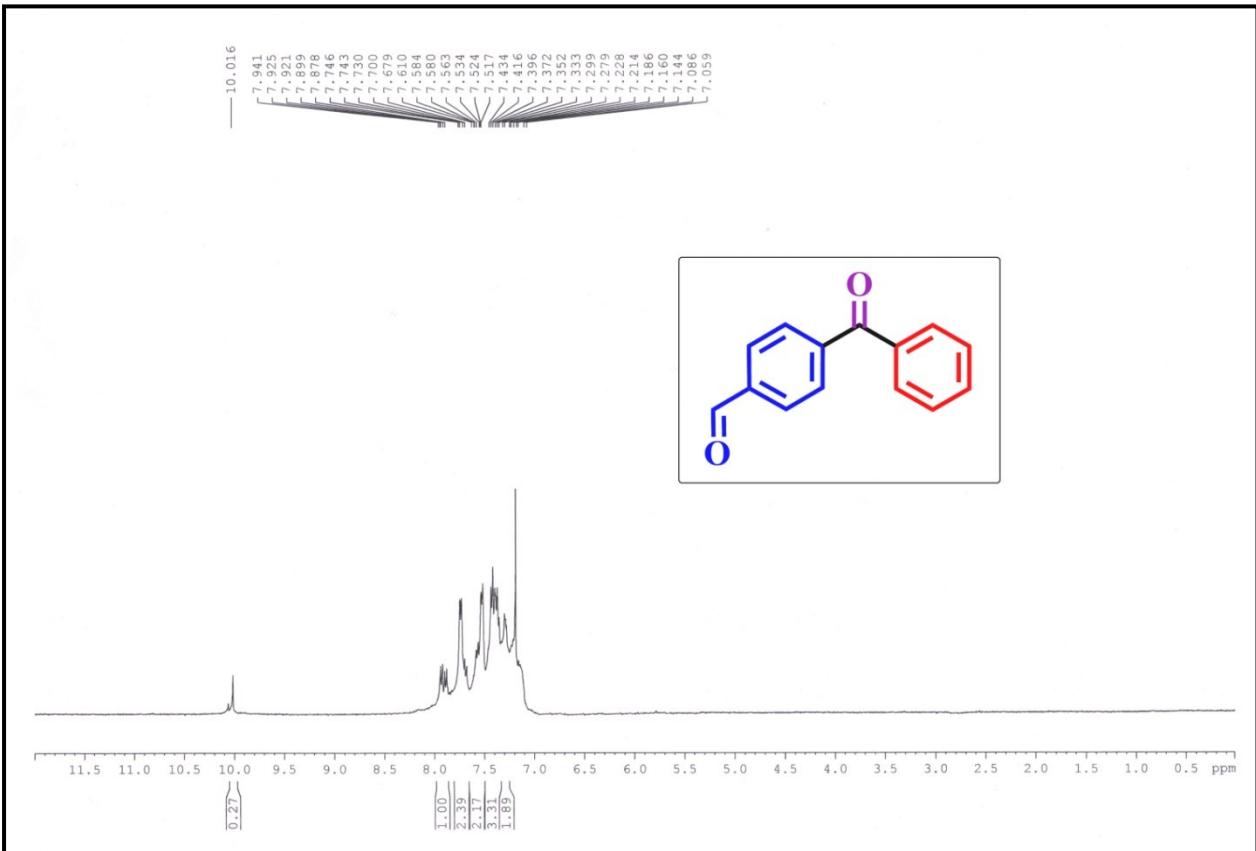
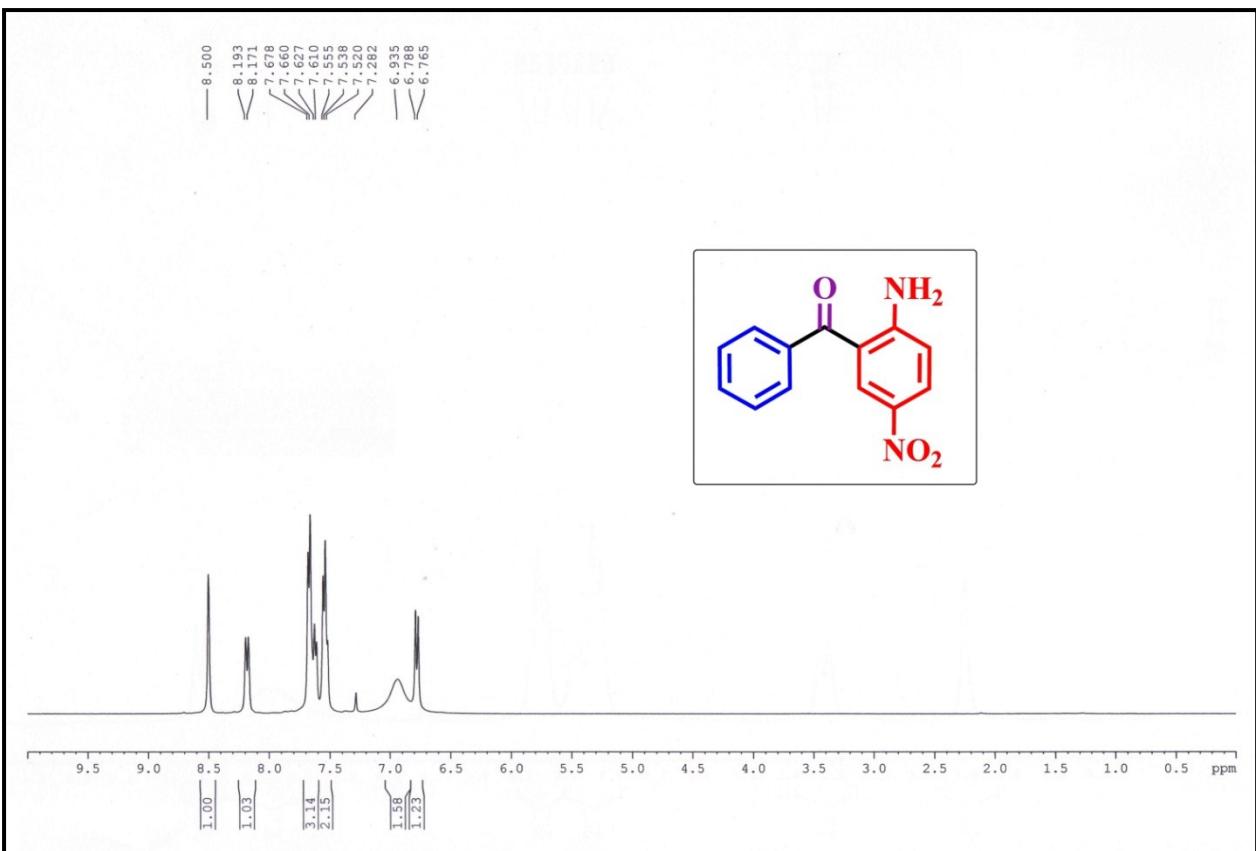


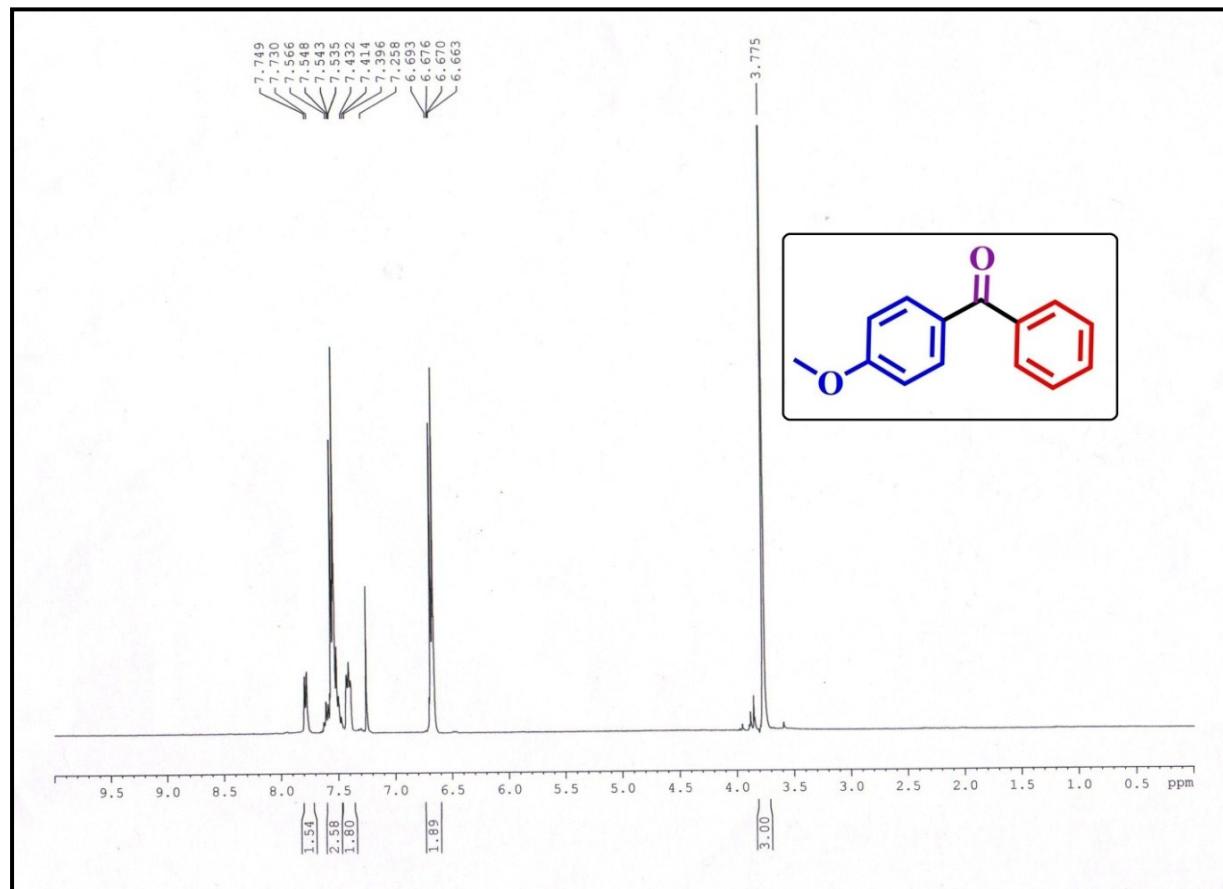
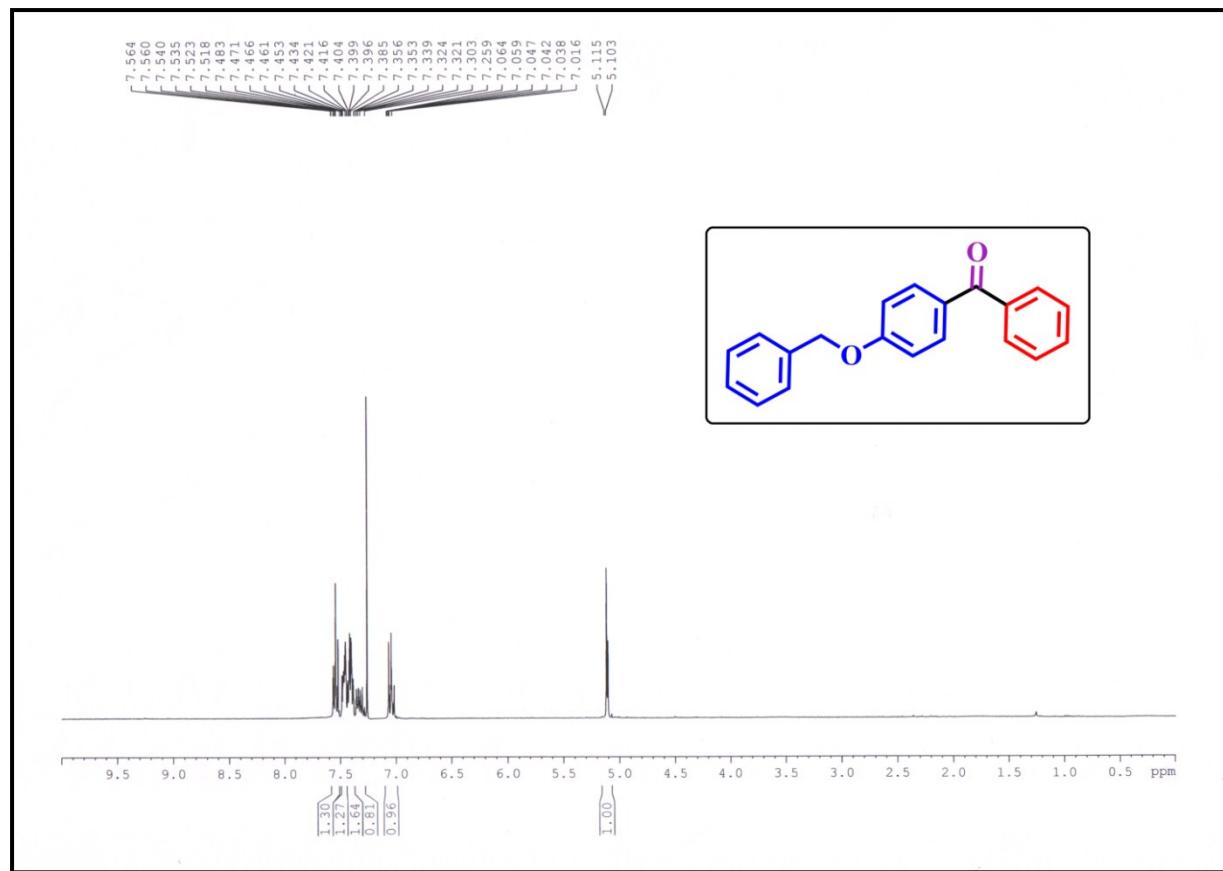
**4. *<sup>1</sup>H NMR copies of diaryl ketone***

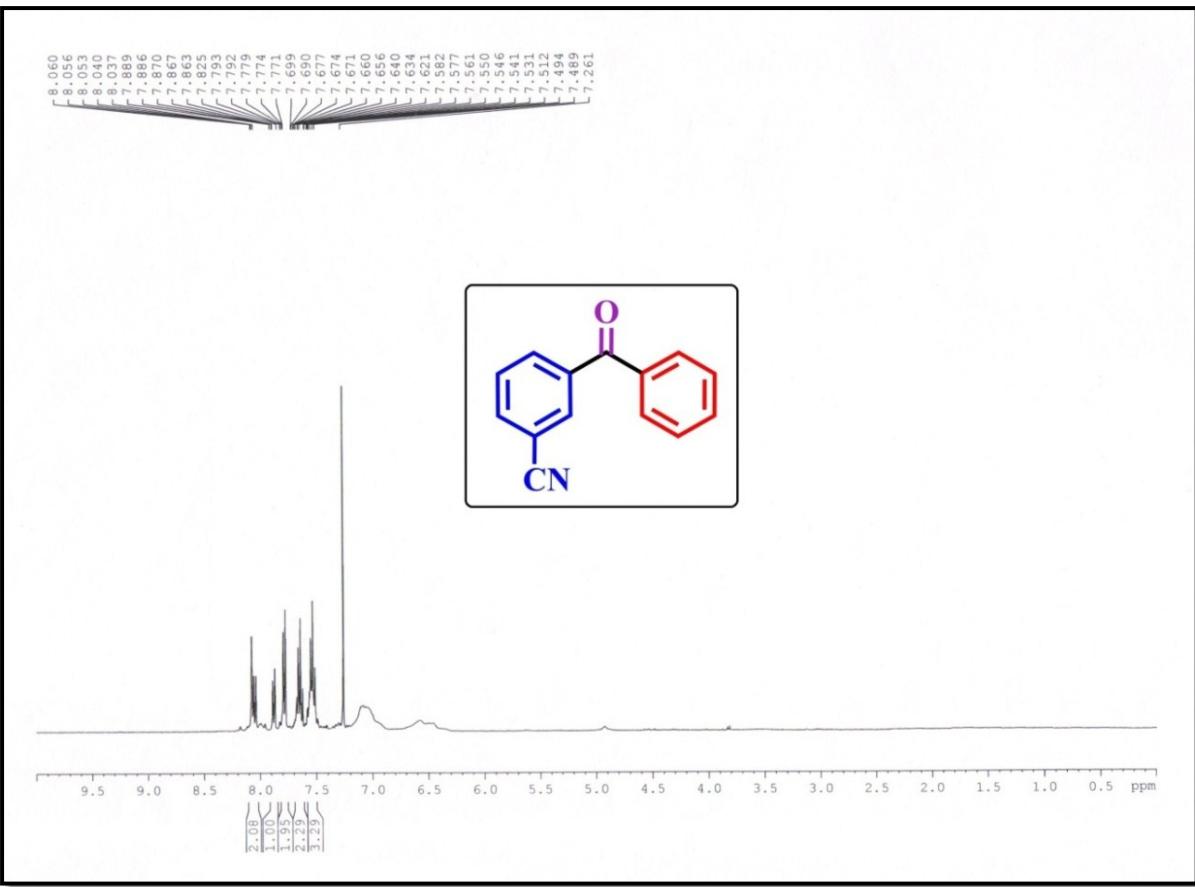




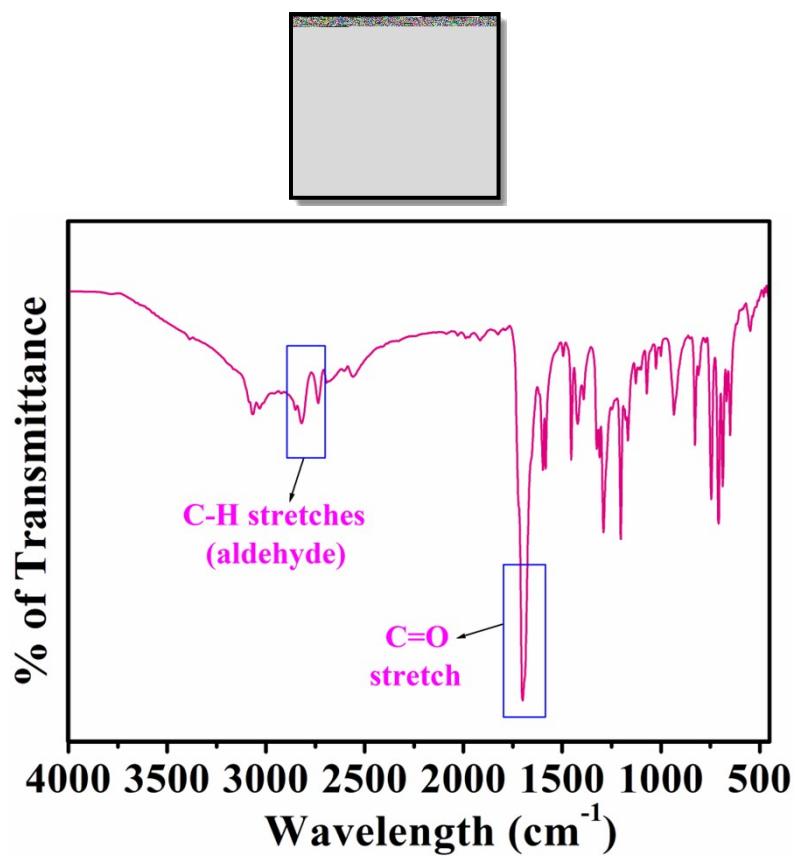


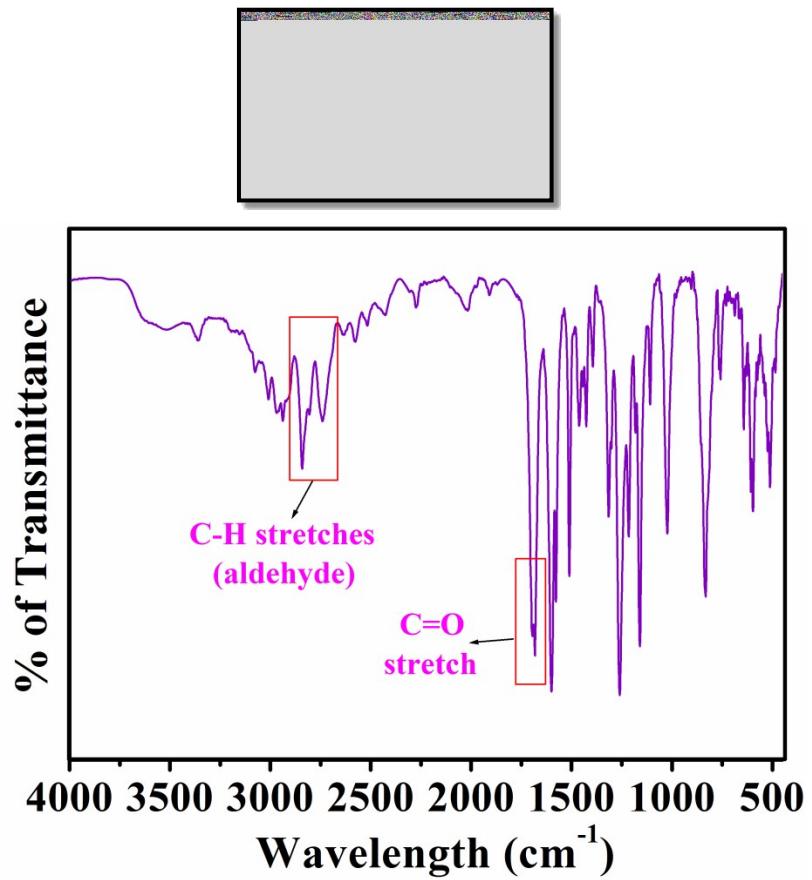
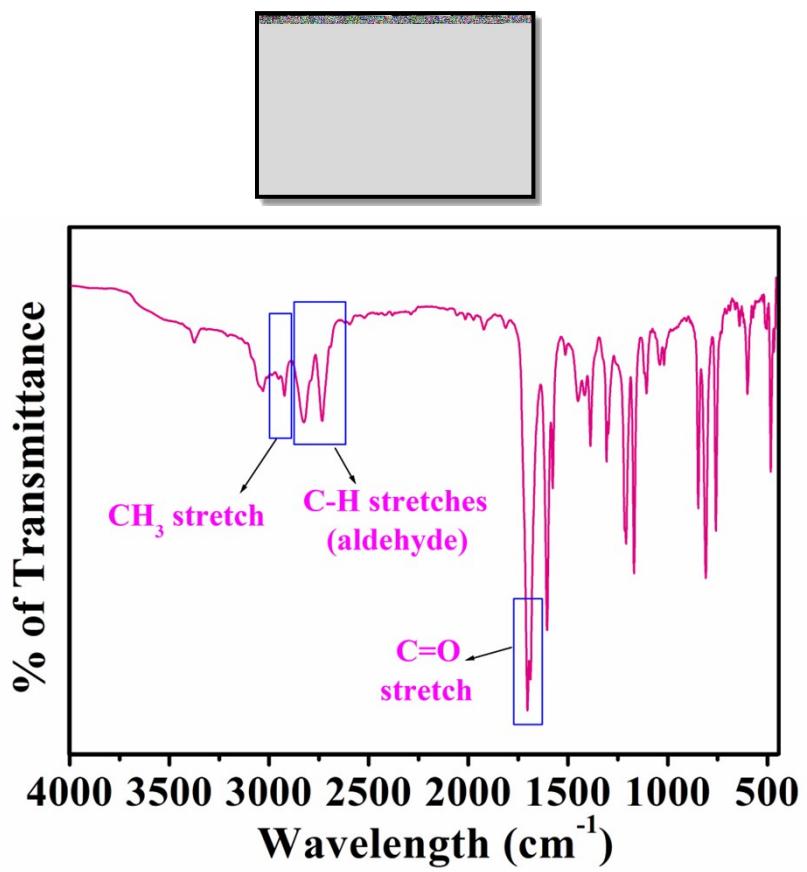


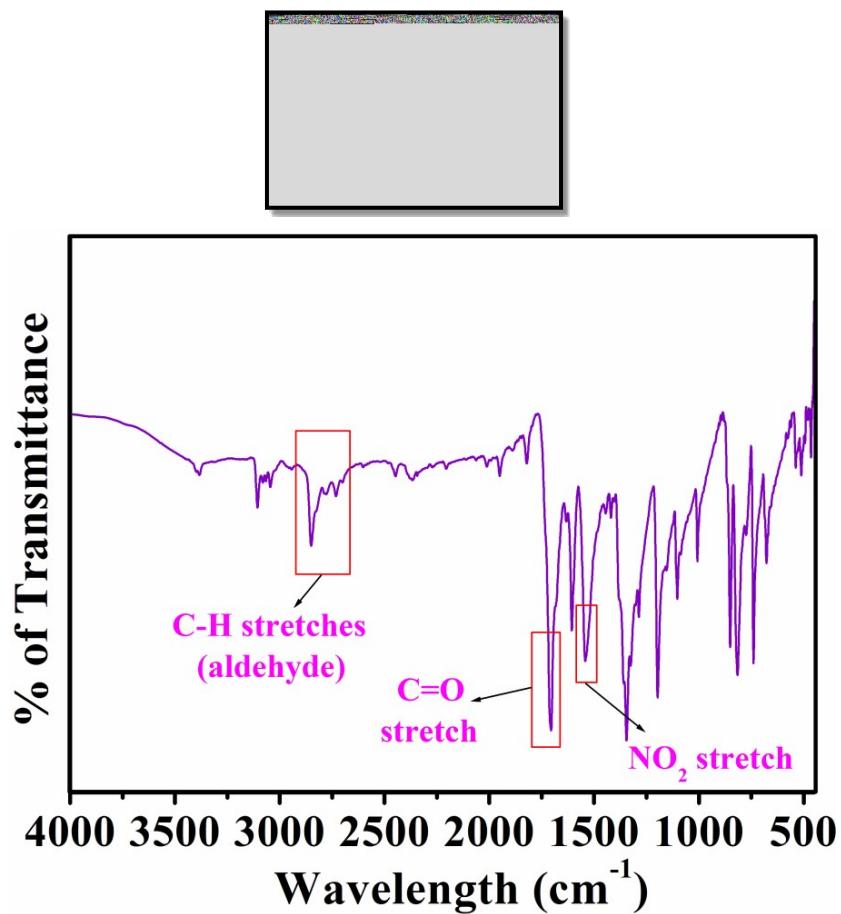
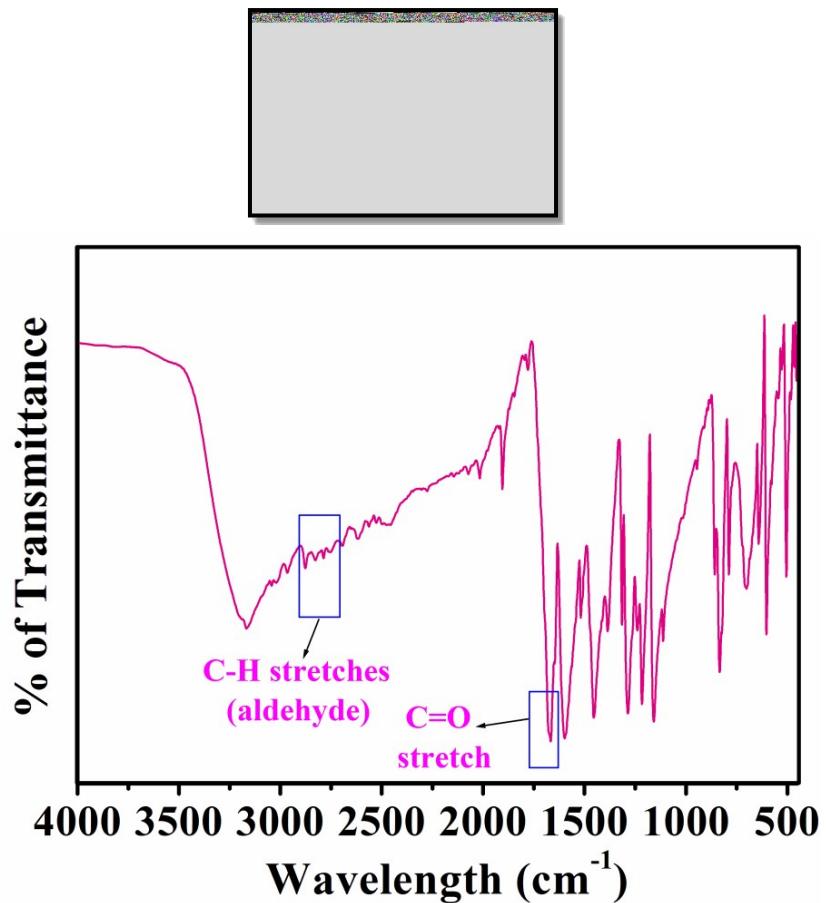


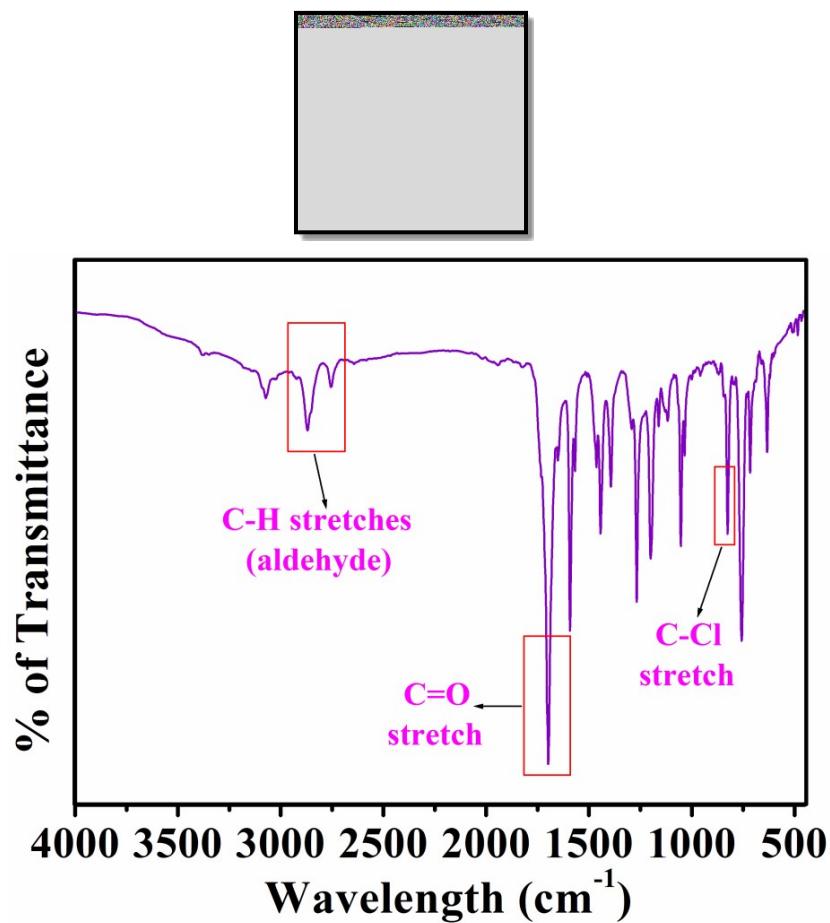
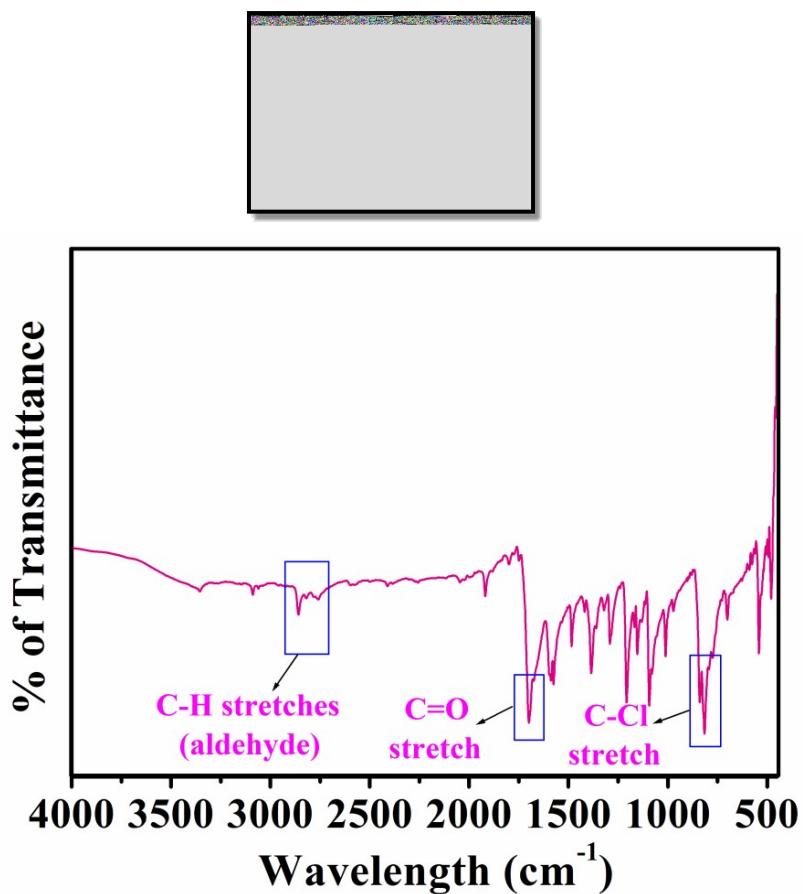


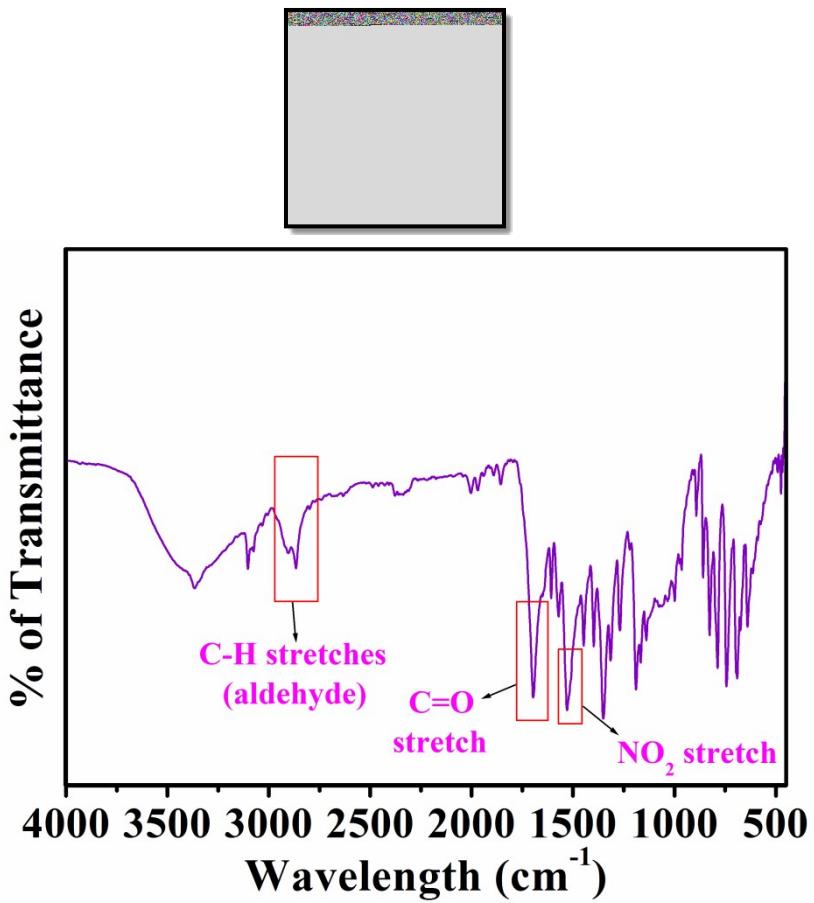
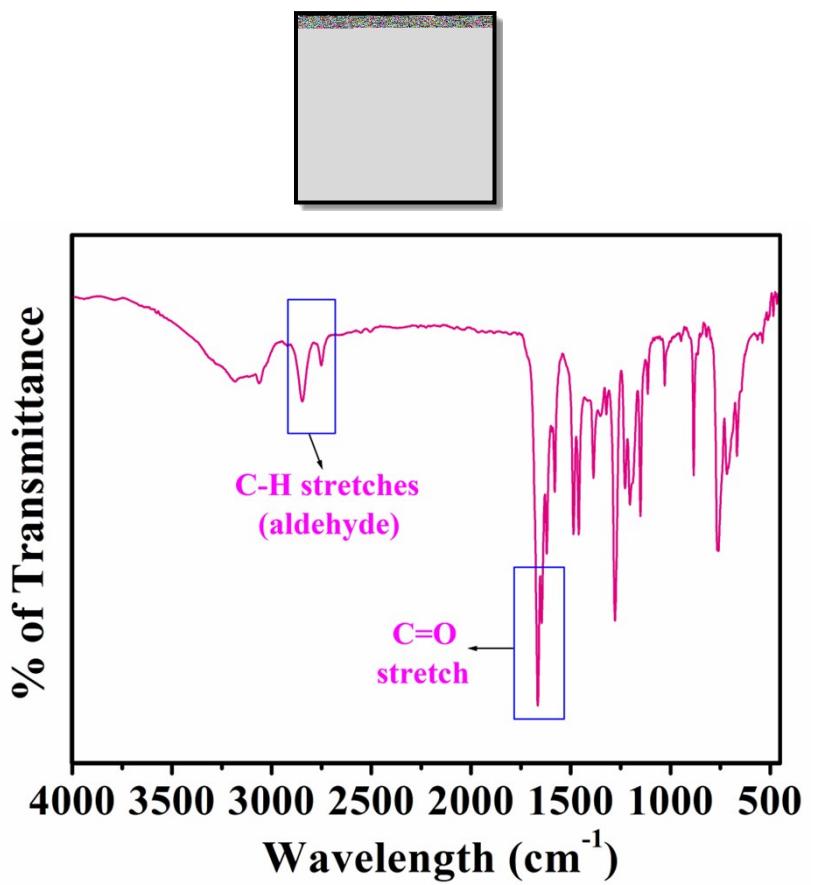
##### ***5. FTIR spectra of insitu carbonylative products***

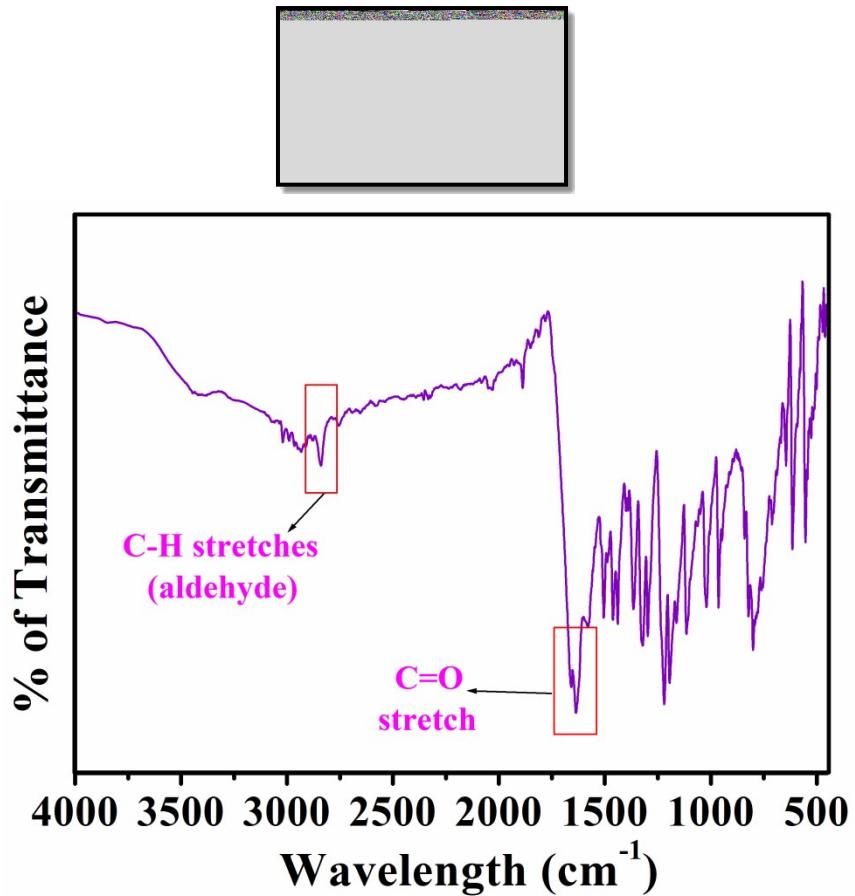
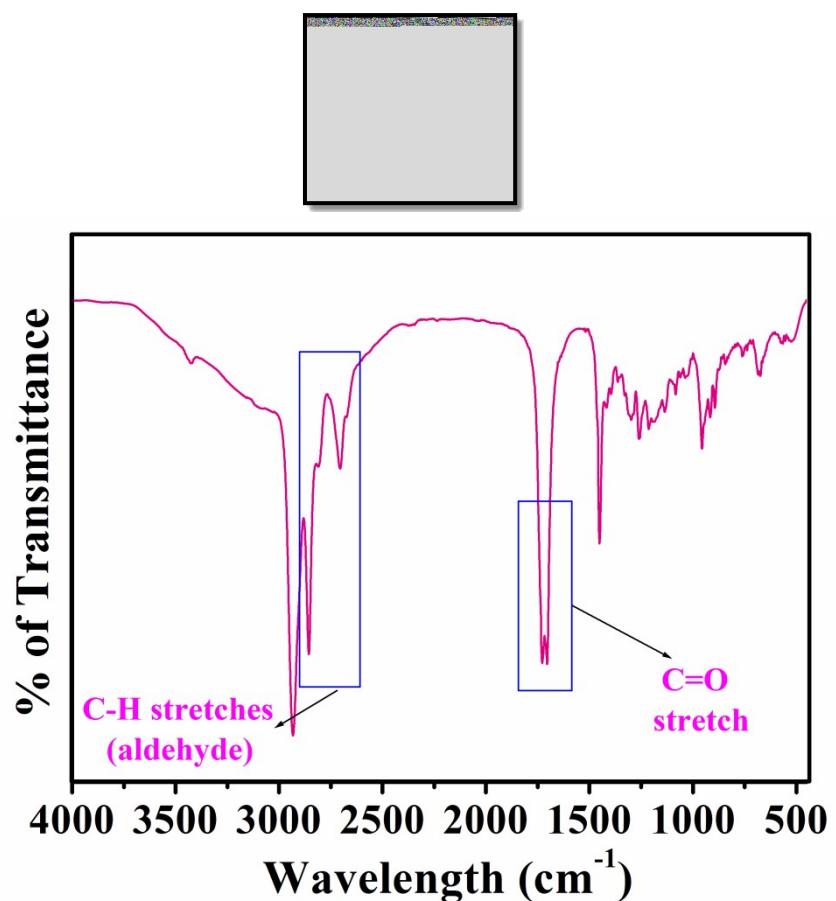


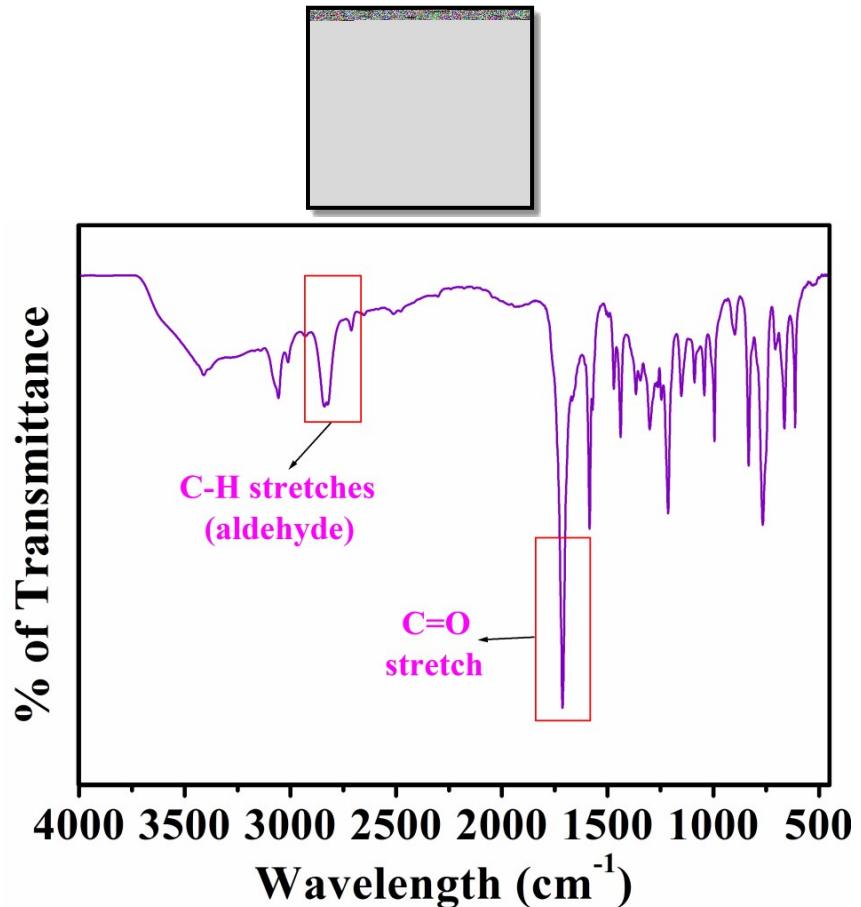
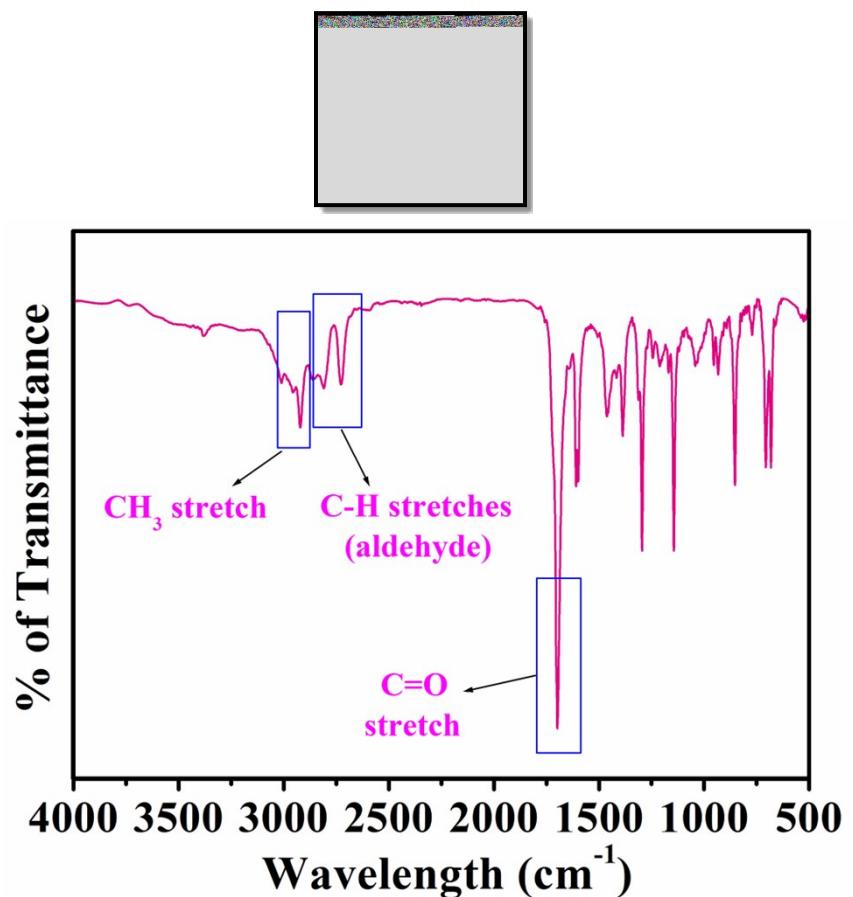


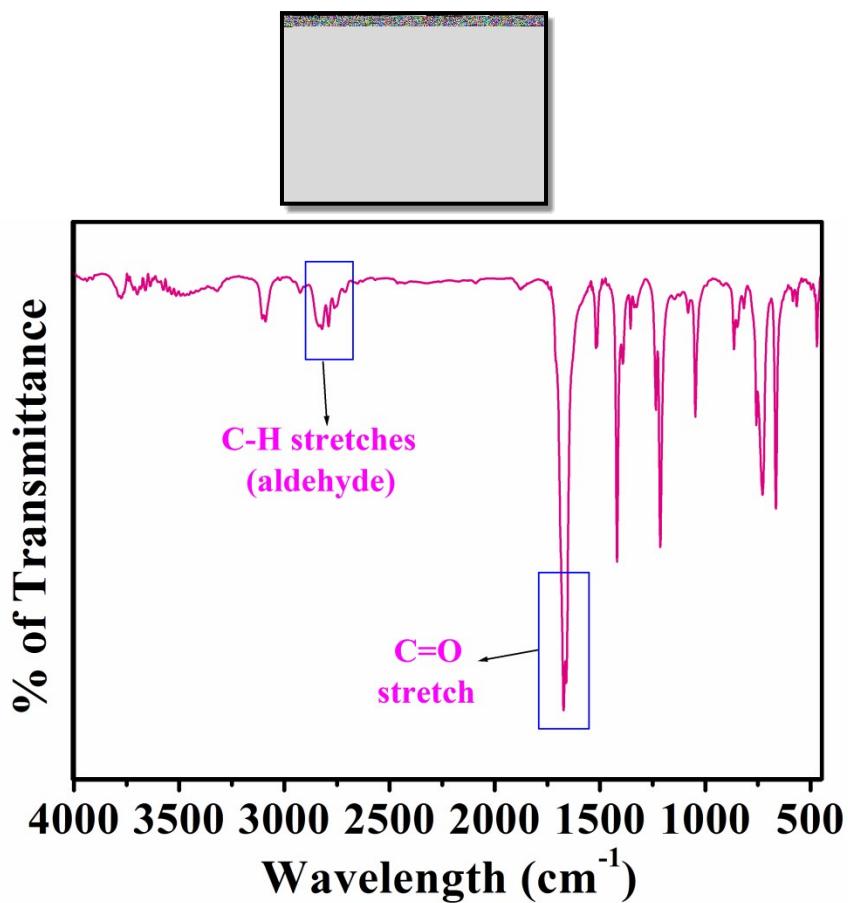












#### 6. FTIR spectra of diaryl ketone

