

## Supplementary information

---

### Development of novel and green NiFe<sub>2</sub>O<sub>4</sub>/geopolymer nanocatalyst based on bentonite for synthesis of imidazole heterocycles by ultrasonic irradiations

Zoleikha Hajizadeh, Fateme Radinekiyan,<sup>1</sup> Reza Eivazzadeh-keihan, Ali Maleki\*

*Catalysts and Organic Synthesis Research Laboratory, Department of Chemistry, Iran*

*University of Science and Technology, Tehran 16846-13114, Iran*

\*Corresponding author. E-mail: [maleki@iust.ac.ir](mailto:maleki@iust.ac.ir)

<sup>1</sup>Co-first author

---

#### Table of contents

---

<i>Entry</i>	<i>Subject</i>	<i>Page</i>
1	Table 1. Physical properties of geopolymer and NiFe <sub>2</sub> O <sub>4</sub> /geopolymer samples from BET analysis	S2
2	Table 2. Optimization of different parameters for model reaction	S3
3	Fig. S1. Reusability of nanocatalyst in the synthesis of <b>4a</b>	S4
4	Fig. S2. FT-IR spectrums of recycled nanocatalyst	S5
5	Fig. S3. EDX analysis of recycled nanocatalyst	S6
6	Fig. S4. FT-IR spectrum of the product ( <b>4a</b> )	S7
7	Fig. S5. <sup>1</sup> H NMR of the product ( <b>4a</b> )	S8
8	Fig. S6. <sup>13</sup> C NMR of the product ( <b>4a</b> )	S9
9	Fig. S7. FT-IR spectrum of the product ( <b>4i</b> )	S10
10	Fig. S8. <sup>1</sup> H NMR of the product ( <b>4i</b> )	S11
11	Fig. S9. <sup>13</sup> C NMR of the product ( <b>4i</b> )	S12

---

**Table 1.** Physical properties of geopolymer and NiFe<sub>2</sub>O<sub>4</sub>/geopolymer samples from BET analysis.

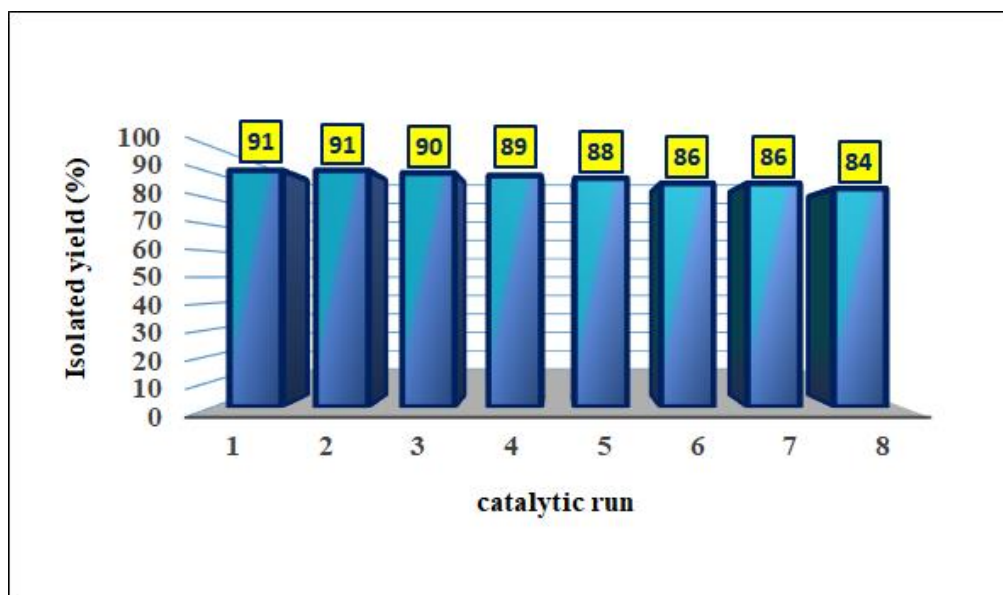
Physical Properties	Geopolymer Sample	NiFe <sub>2</sub> O <sub>4</sub> /geopolymer
Surface area (m <sup>2</sup> /g)	1.13	0.30
Pore size (nm)	14.28	19.82
The total pore volume of pores (cm <sup>3</sup> /g)	0.004	0.069

**Table 2.** Optimization of different parameters for model reaction.<sup>a</sup>

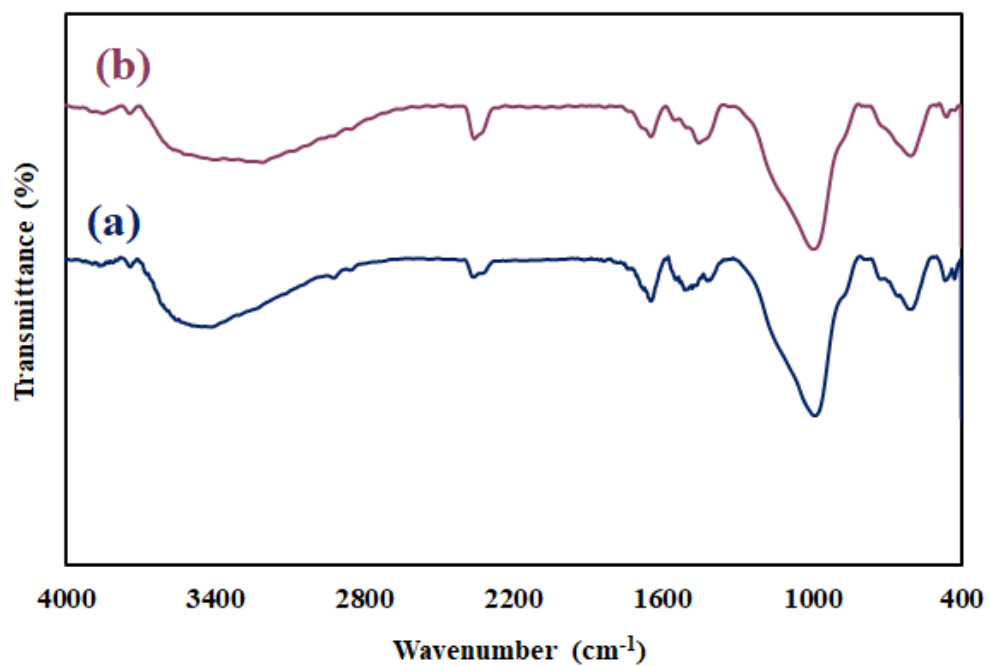
Entry	Solvent	Catalyst (g)	Condition/Temperature (°C)	Time (min)	Yield <sup>b</sup> (%)
1	EtOH	Nanocomposite (0.03)	r.t. / 27	277	75
2	EtOH	Nanocomposite (0.03)	Reflux / 90	155	89
3	Free-solvent	Nanocomposite (0.03)	Ultrasonic bath / 80	18	trace
4	H <sub>2</sub> O	Nanocomposite (0.03)	Ultrasonic bath / 80	18	No reaction
5	EtOH	Nanocomposite (0.03)	Ultrasonic bath / 80	18	91
6	MeOH	Nanocomposite (0.03)	Ultrasonic bath / 80	18	76
7	CH <sub>2</sub> Cl <sub>2</sub>	Nanocomposite (0.03)	Ultrasonic bath / 80	18	84
8	CH <sub>3</sub> CN	Nanocomposite (0.03)	Ultrasonic bath / 80	18	69
9	Toluene	Nanocomposite (0.03)	Ultrasonic bath / 80	18	trace
10	EtOH	-	Ultrasonic bath / 80	30	trace
11	EtOH	Bentonite (0.03)	Ultrasonic bath / 80	25	No reaction
12	EtOH	NiFe <sub>2</sub> O <sub>4</sub> (0.03)	Ultrasonic bath / 80	25	38
13	EtOH	Geopolymer (0.03)	Ultrasonic bath / 80	25	20
14	EtOH	Nanocomposite (0.01)	Ultrasonic bath / 80	18	65
15	EtOH	Nanocomposite (0.02)	Ultrasonic bath / 80	18	71
16	EtOH	Nanocomposite (0.04)	Ultrasonic bath / 80	18	89
17	EtOH	Nanocomposite (0.05)	Ultrasonic bath / 80	18	90

<sup>a</sup>The reaction condition: benzil (0.8 mmol), benzaldehyde (0.8 mmol), ammonium acetate (2.0 mmol), Ethanol (7 mL) ultrasonic irradiations.

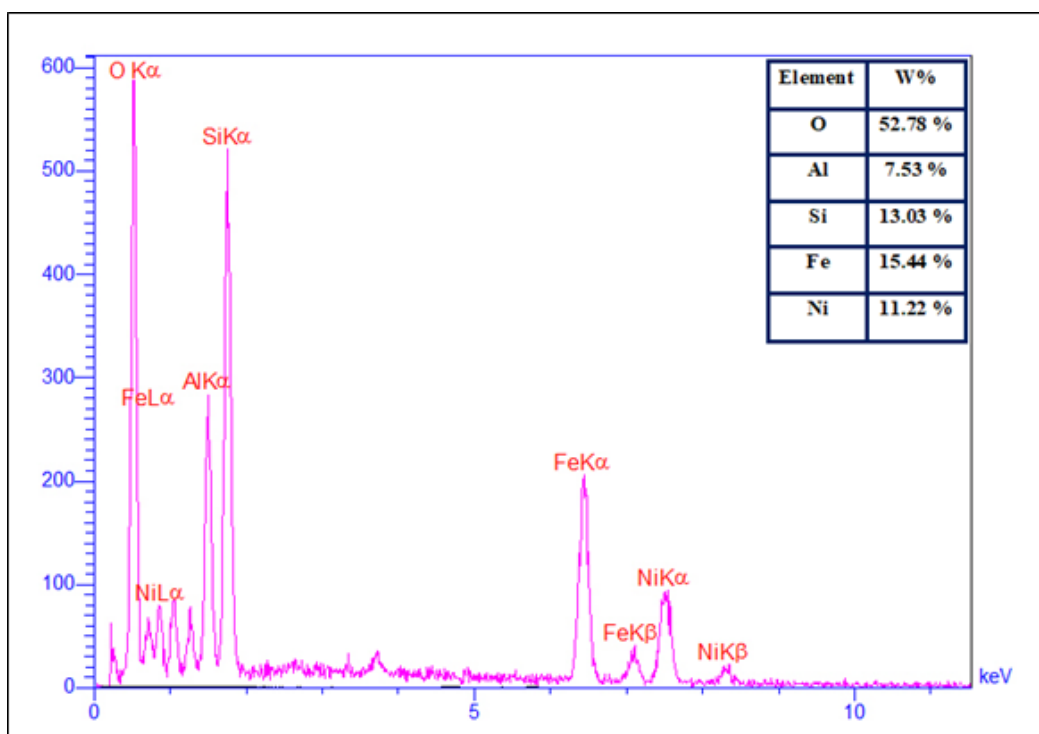
<sup>b</sup> Isolated yield.



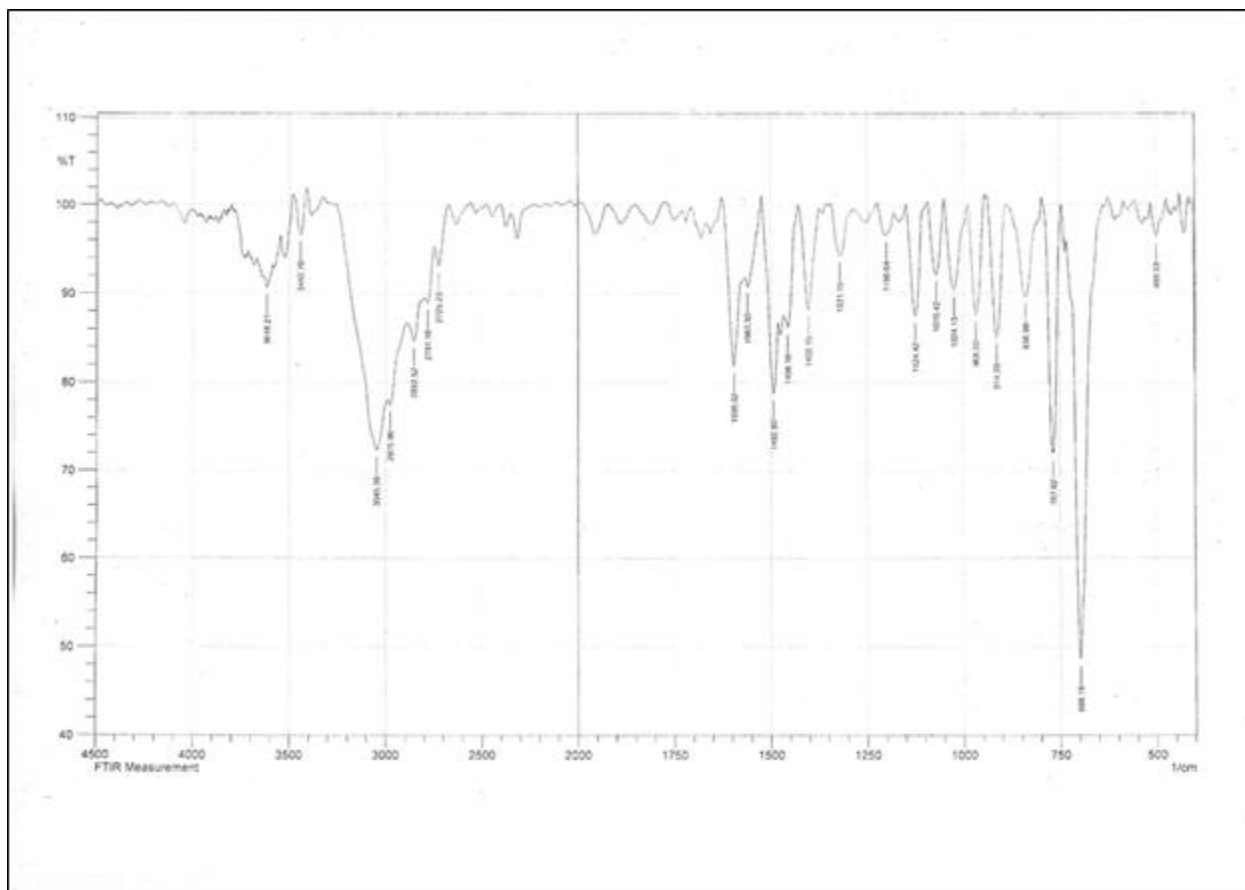
**Fig. S1.** The Reusability of NiFe<sub>2</sub>O<sub>4</sub>/geopolymer nanocatalyst in the synthesis of **4a**.



**Fig. S2.** FT-IR spectra of (a) NiFe<sub>2</sub>O<sub>4</sub>/geopolymer nanocomposite, (b) recycled nanocatalyst.



**Fig. S3.** The EDX analysis of recycled  $\text{NiFe}_2\text{O}_4$ /geopolymer nanocomposite.



**Fig. S4.** The FT-IR spectrum of the product (**4a**).

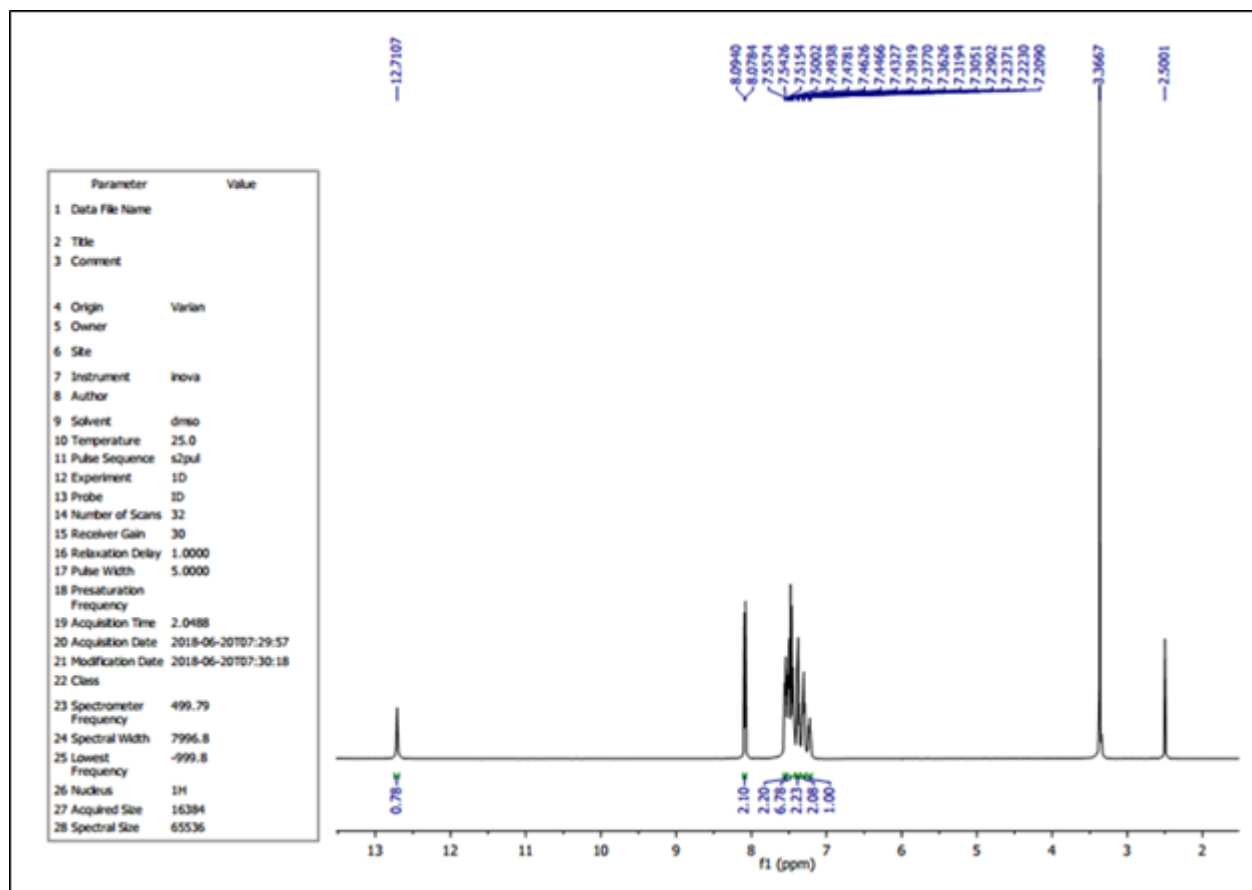
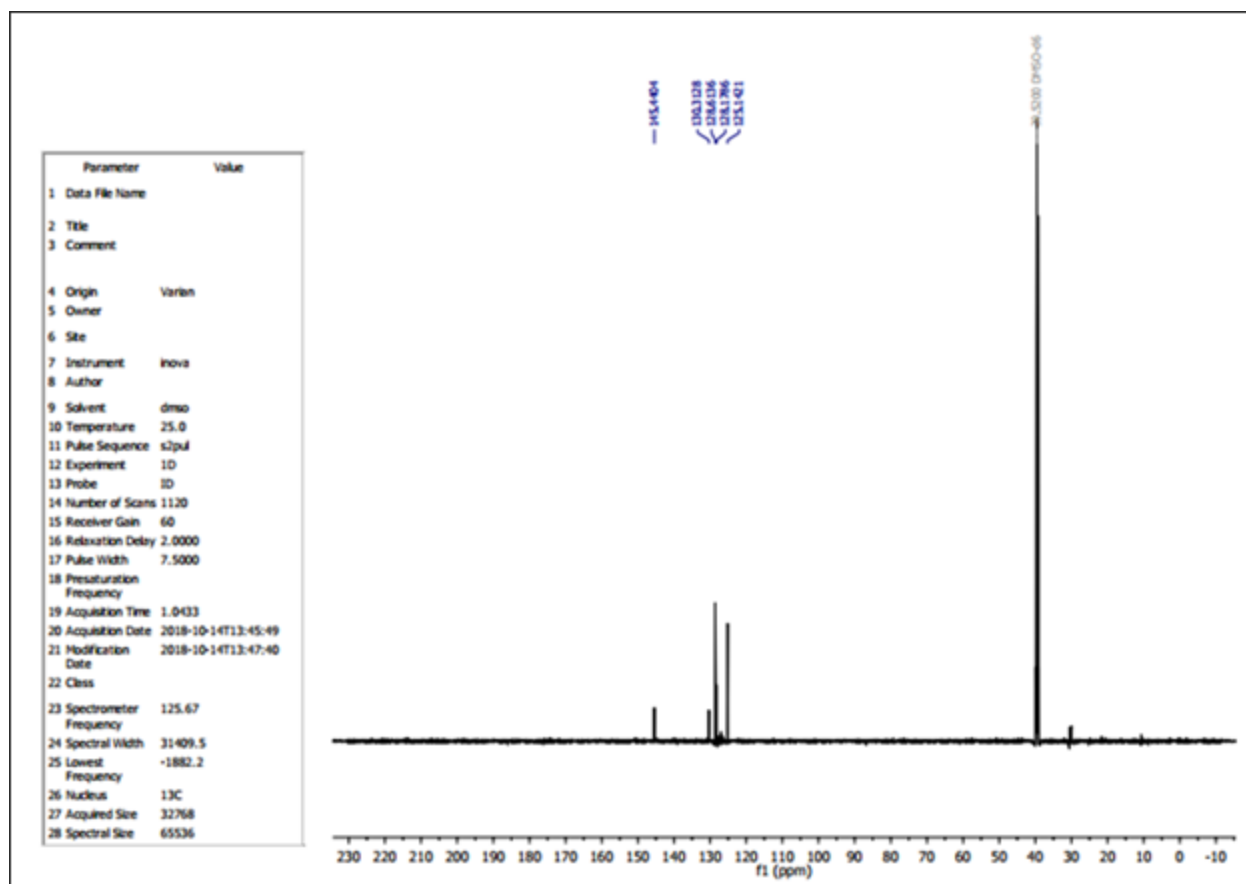
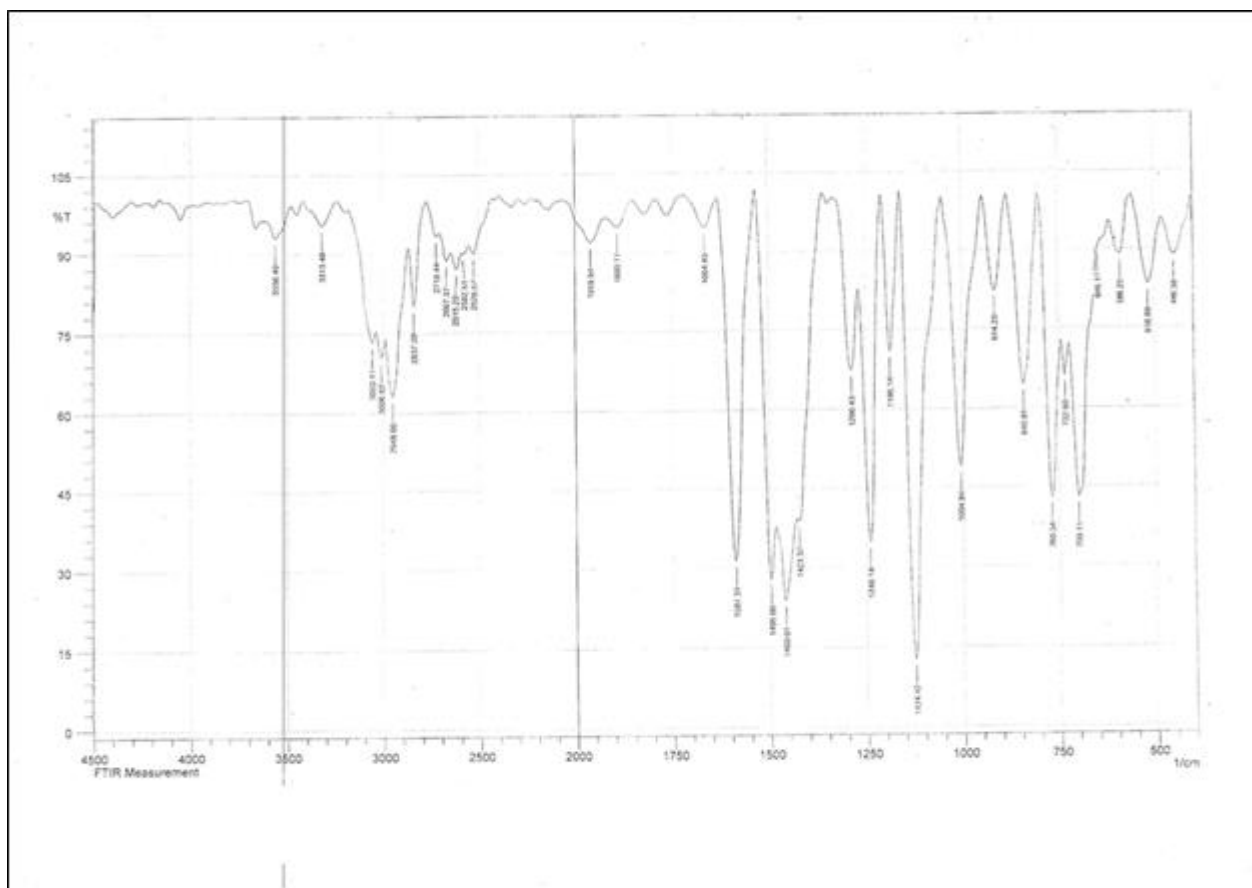


Fig. S5. The  $^1\text{H}$  NMR of the product (**4a**).

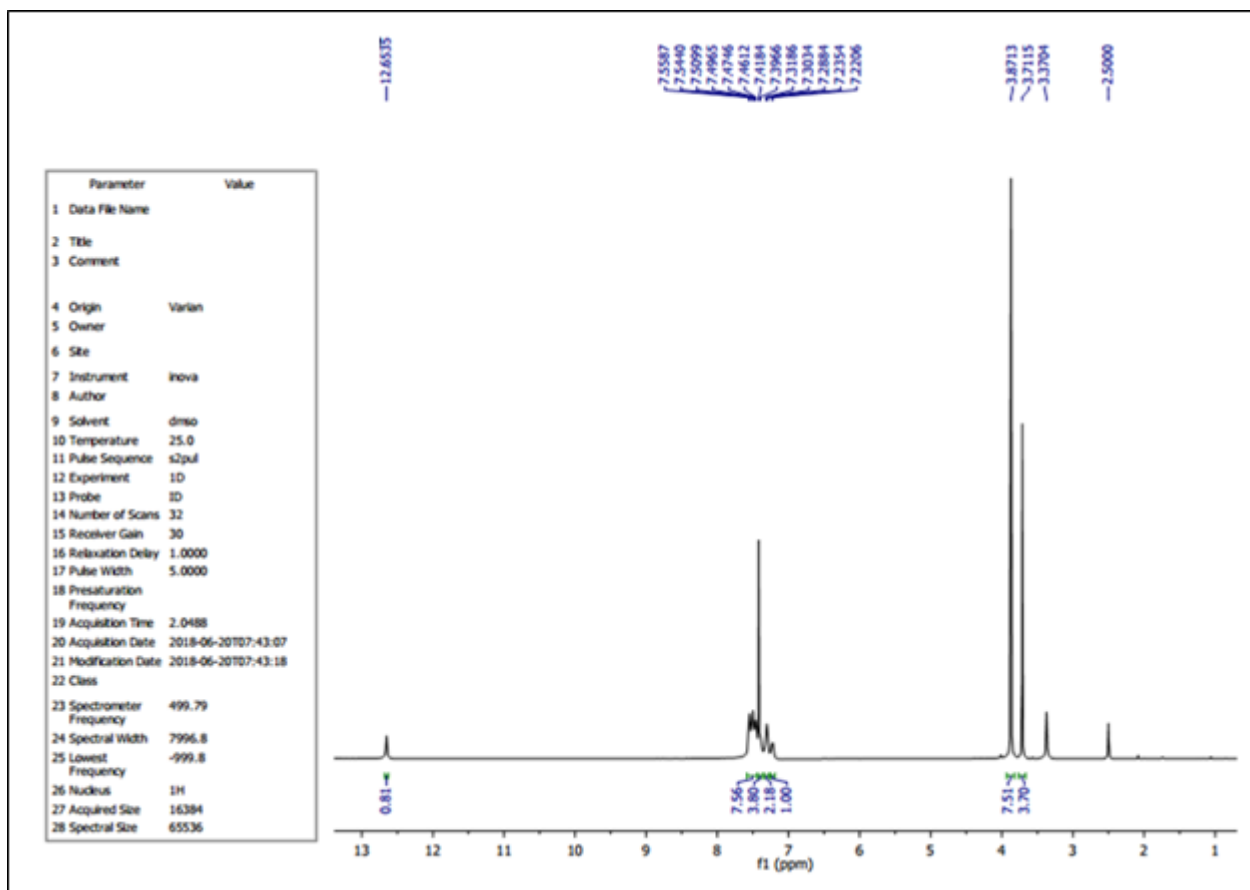




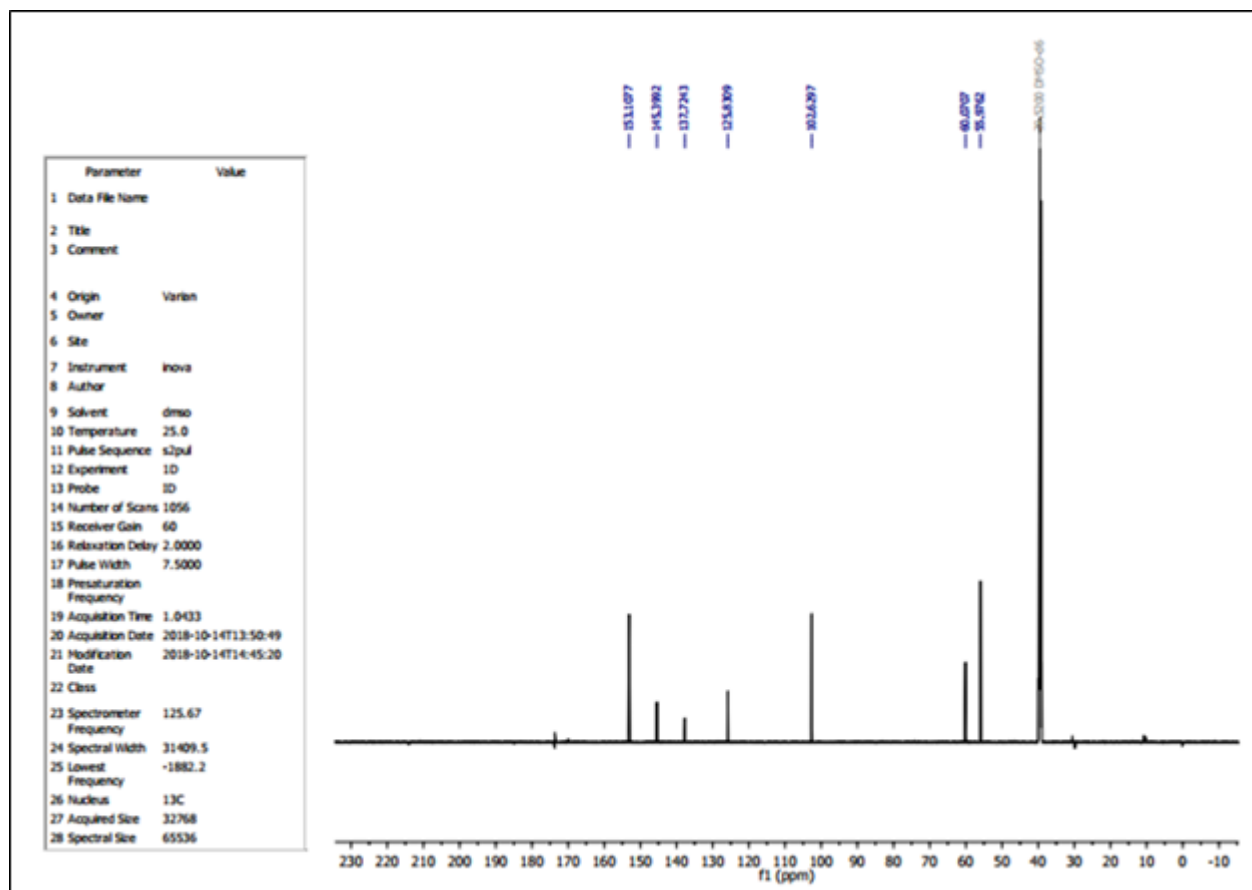
**Fig. S6.** The <sup>13</sup>C NMR of the product (**4a**).



**Fig. S7.** The FT-IR spectrum of the product (**4i**).



**Fig. S8.** The <sup>1</sup>H NMR of the product (**4i**).



**Fig. S9.** The <sup>13</sup>C NMR of the product (**4i**).