

## **Supplementary Information**

**for**

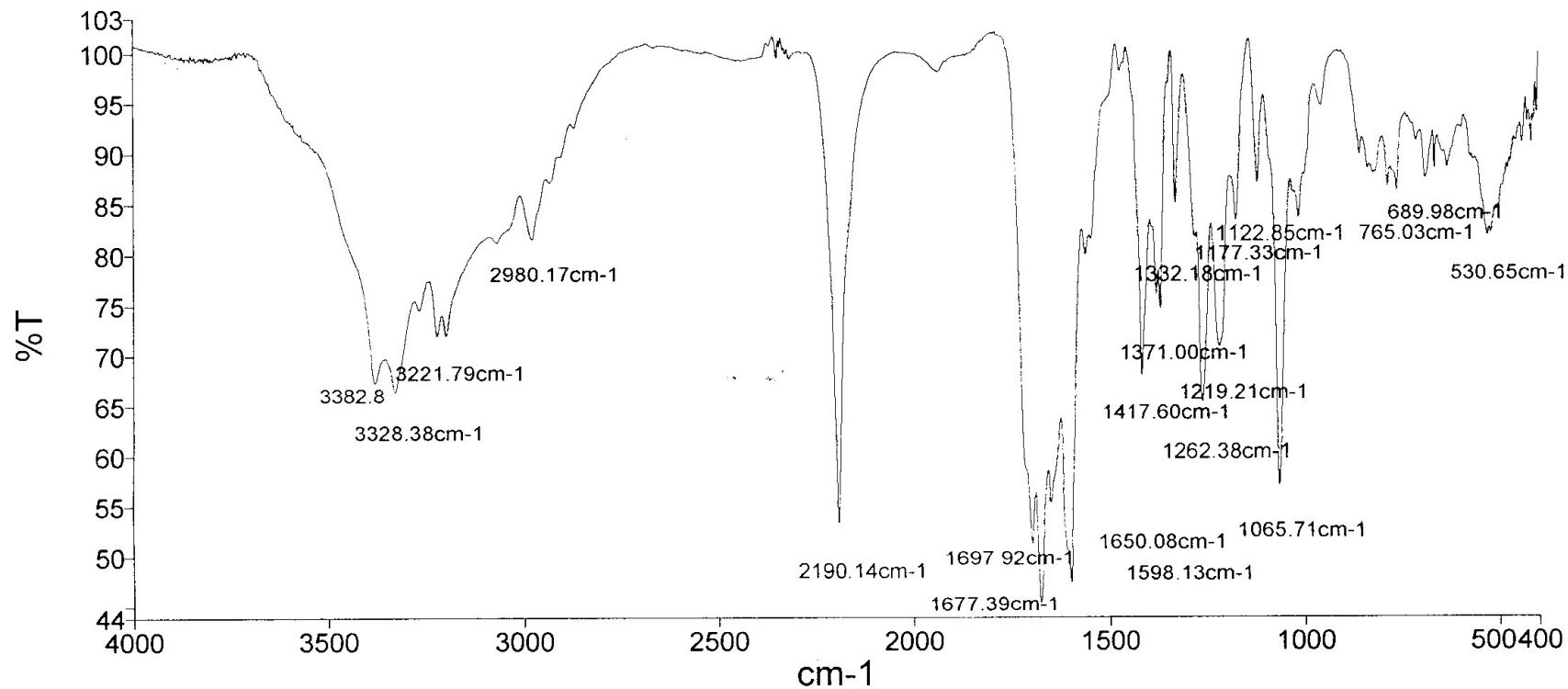
# **Synthesis of pyrazole derivatives in the presence of dioxomolybdenum complex supported on silica-coated magnetite nanoparticles as an efficient and easily recyclable catalyst**

Jamshid Rakhshah, Sadegh Salehzadeh\*, Ehsan Gowdini, Farahnaz Maleki, Saeed Baghery and Mohammad Ali Zolfigol

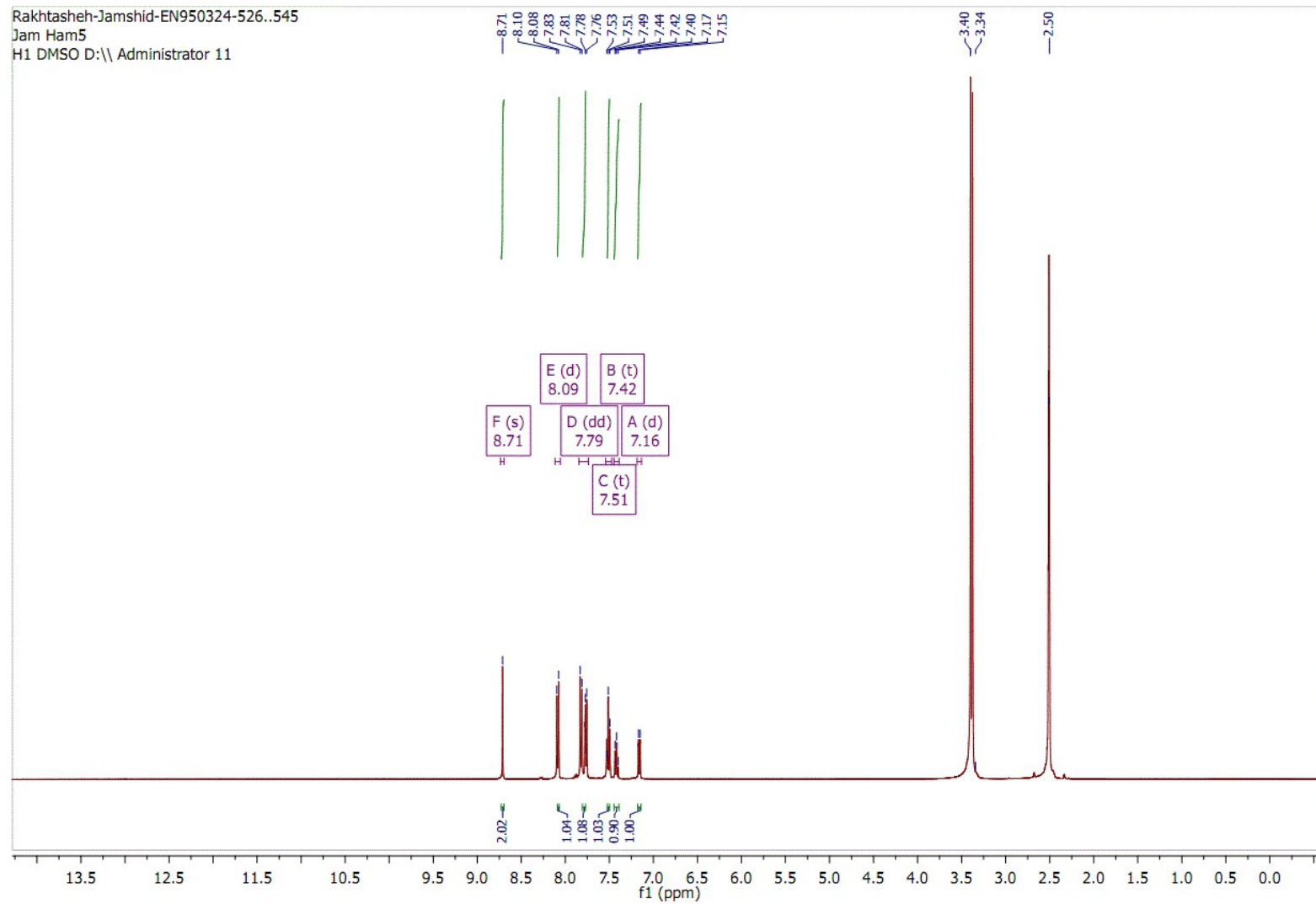
Faculty of Chemistry, Bu-Ali Sina University, Hamedan 6517838683, Iran

Analyst  
Date

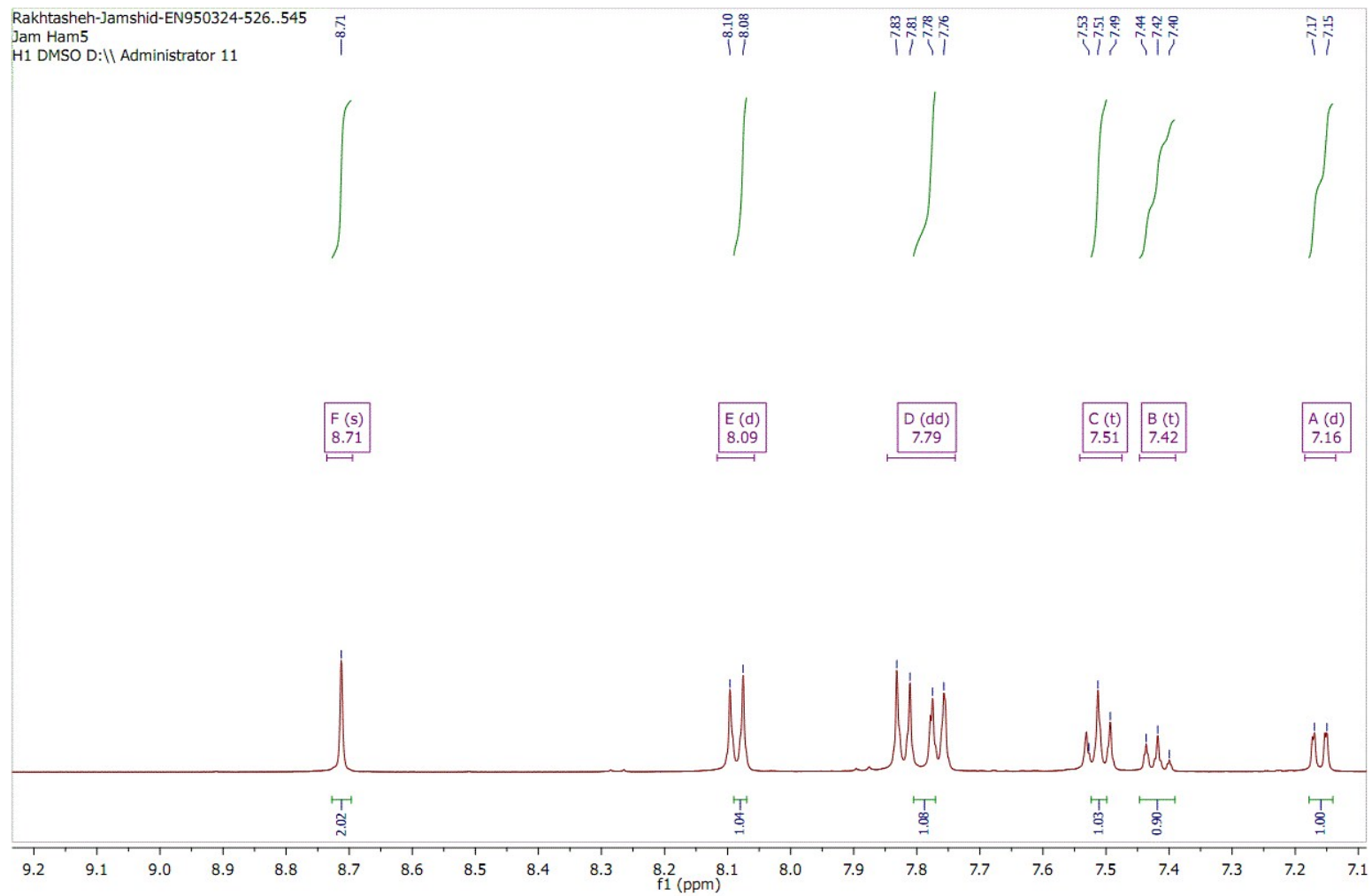
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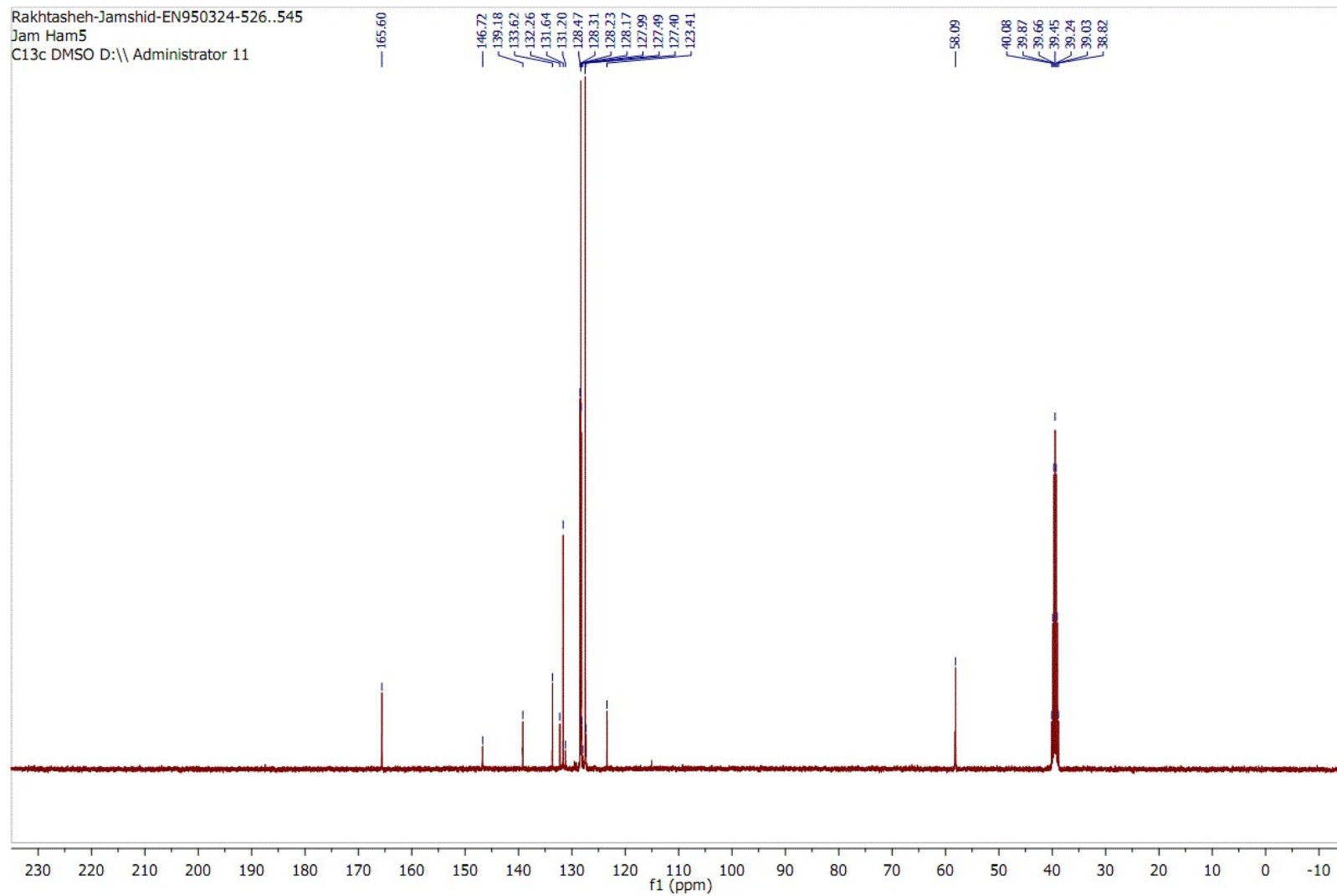
**Fig S1.** The IR of 5-amino-3-(perfluorophenyl)-1-phenyl-1H-pyrazole-4-carbonitrile (Table 3, entry 5)



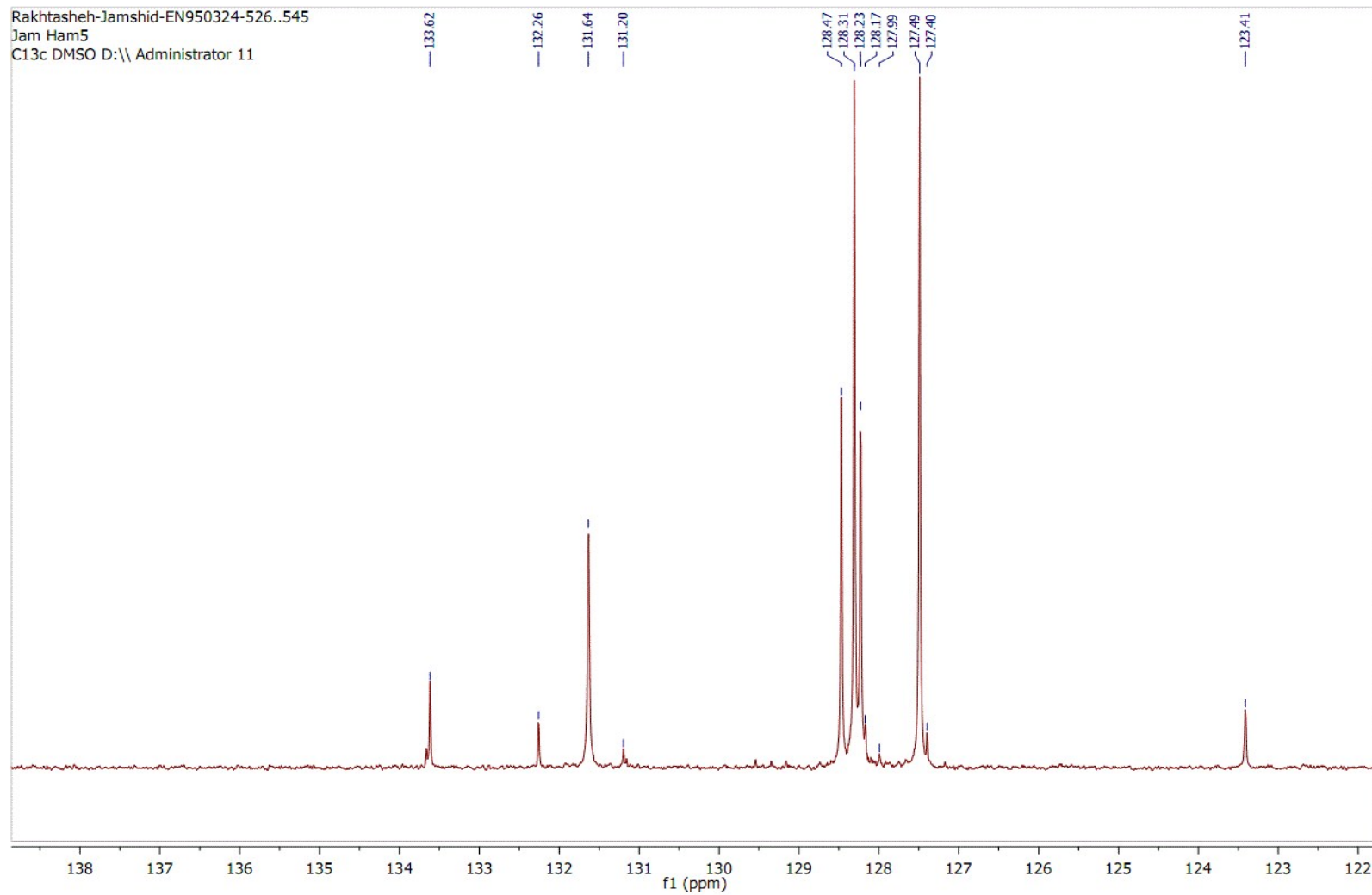
**Fig S2.** The  $^1\text{H}$  NMR of 5-amino-3-(perfluorophenyl)-1-phenyl-1H-pyrazole-4-carbonitrile (Table 3, entry 5)



**Fig S3.** The expanded  $^1\text{H}$  NMR of 5-amino-3-(perfluorophenyl)-1-phenyl-1H-pyrazole-4-carbonitrile (Table 3, entry 5)

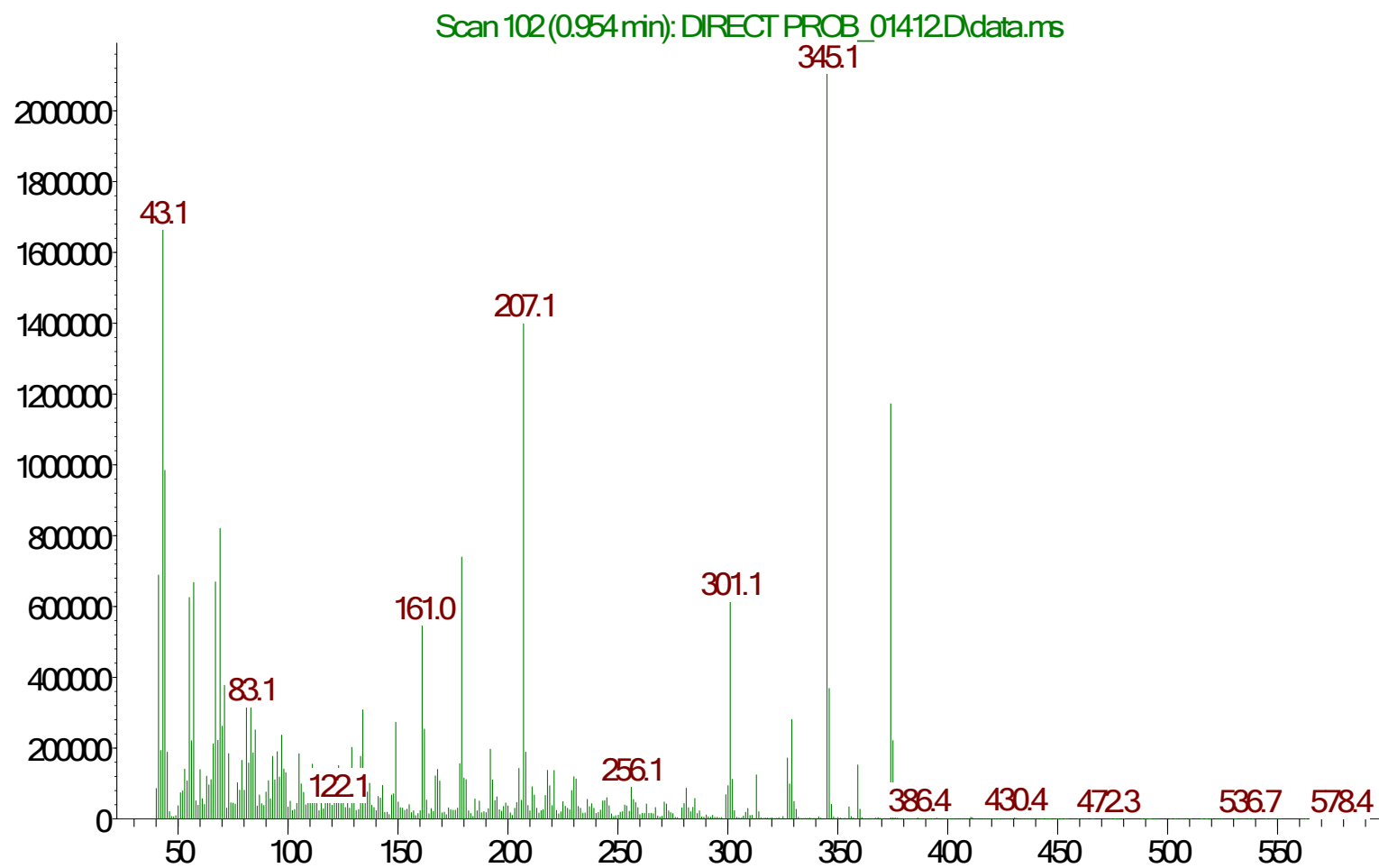


**Fig S4.** The  $^{13}\text{C}$  NMR of 5-amino-3-(perfluorophenyl)-1-phenyl-1H-pyrazole-4-carbonitrile (Table 3, entry 5)



**Fig S5.** The expanded  $^{13}\text{C}$  NMR of 5-amino-3-(perfluorophenyl)-1-phenyl-1H-pyrazole-4-carbonitrile (Table 3, entry 5)

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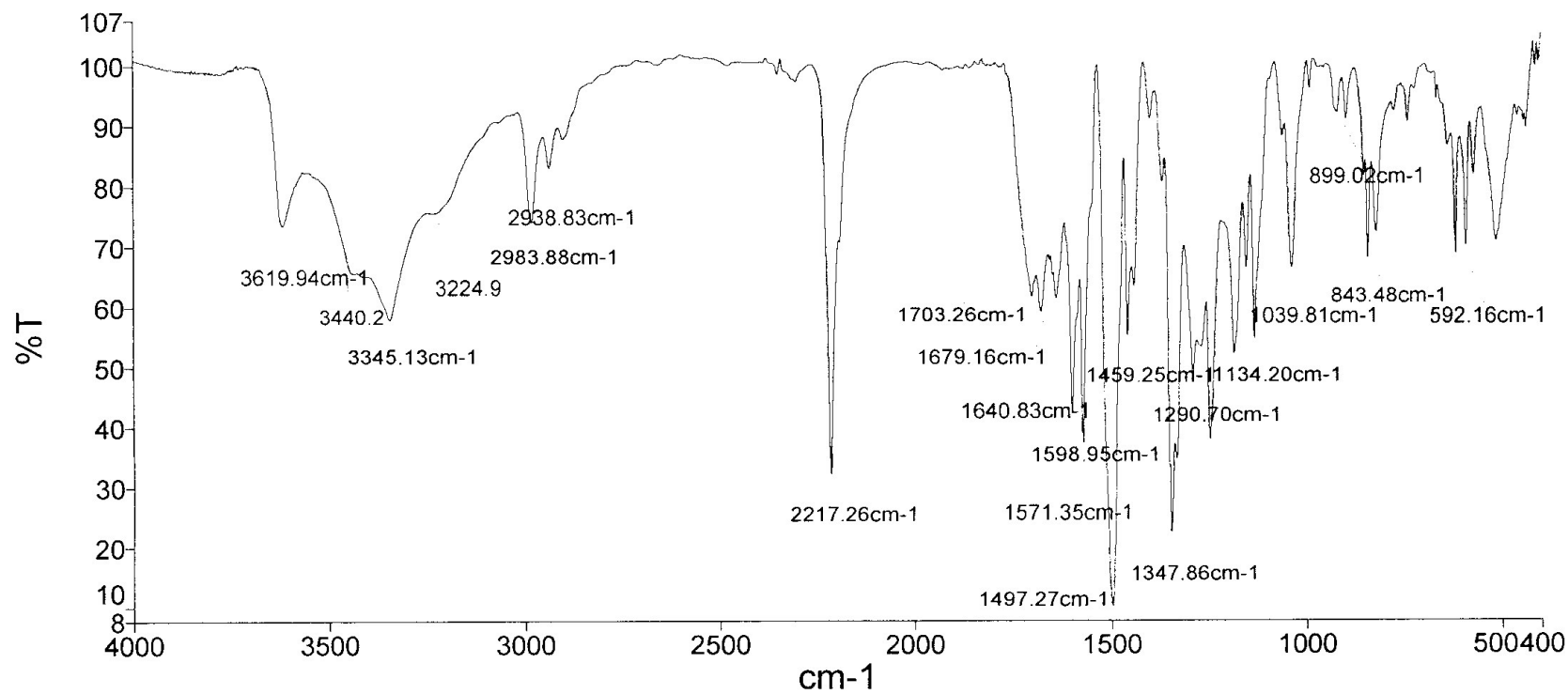


m/z→

**Fig S6.** The Mass spectrea of 5-amino-3-(perfluorophenyl)-1-phenyl-1H-pyrazole-4-carbonitrile (Table 3, entry 5)

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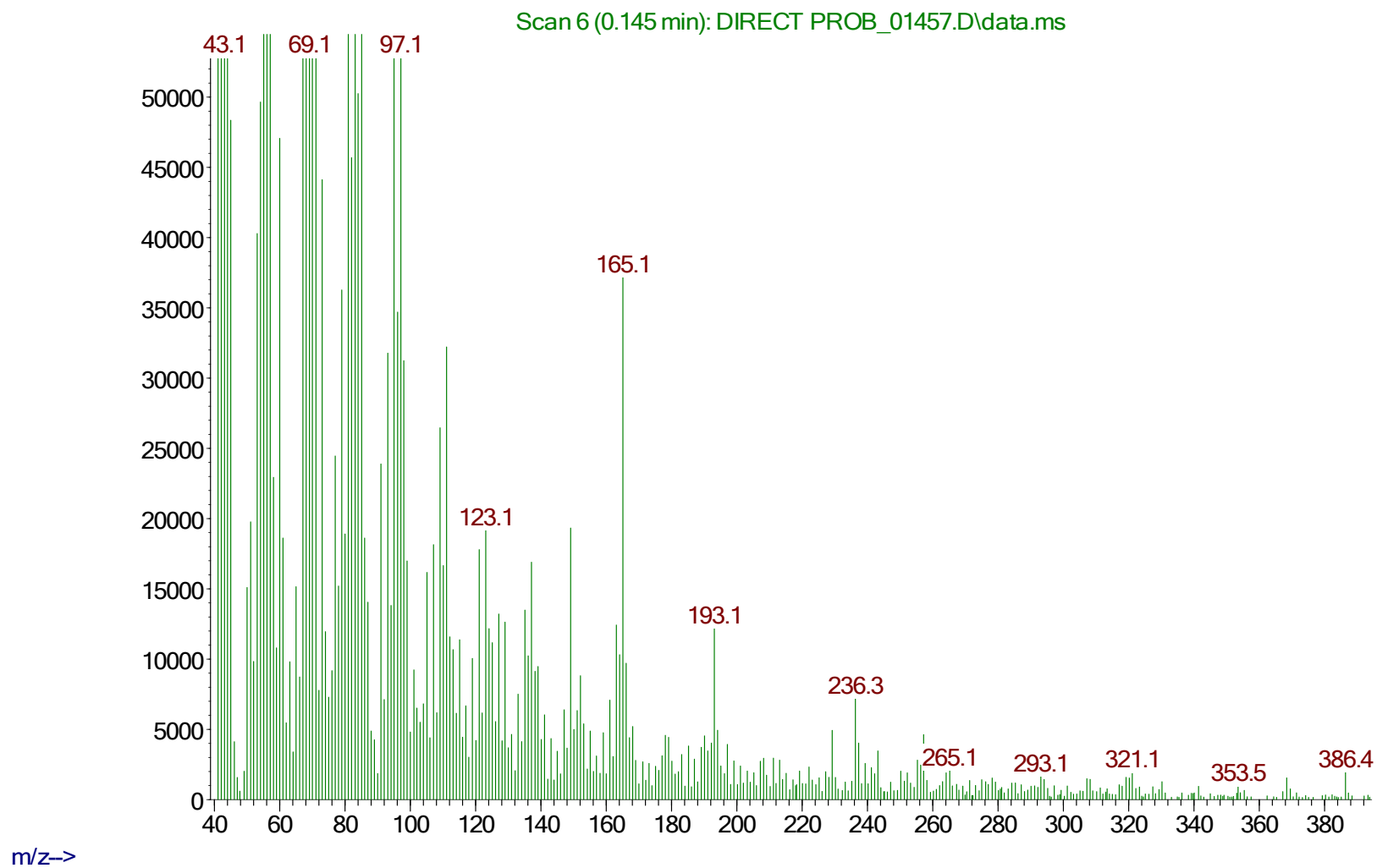
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**Fig S7.** The IR of 5-amino-1-phenyl-3-(ferrocene-yl)-1H-pyrazole-4-carbonitrile (Table 3, entry 6)



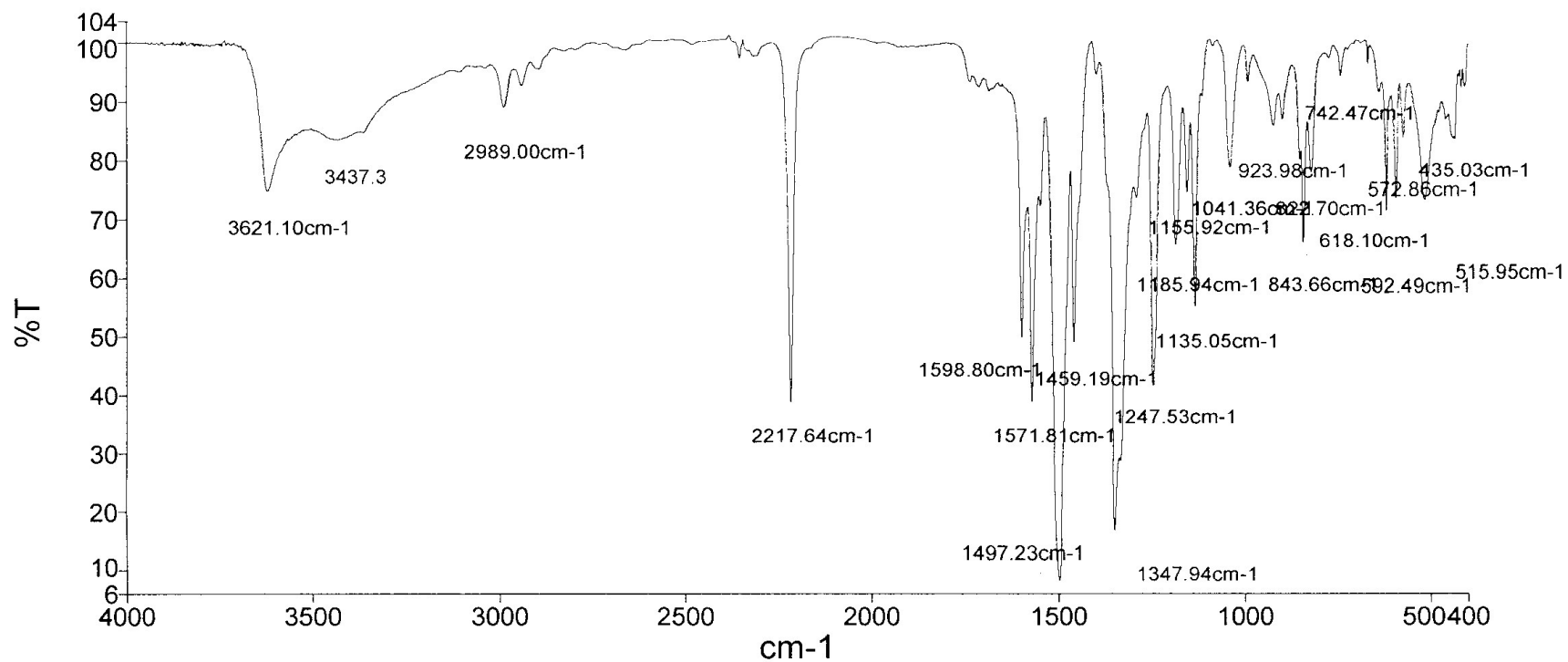
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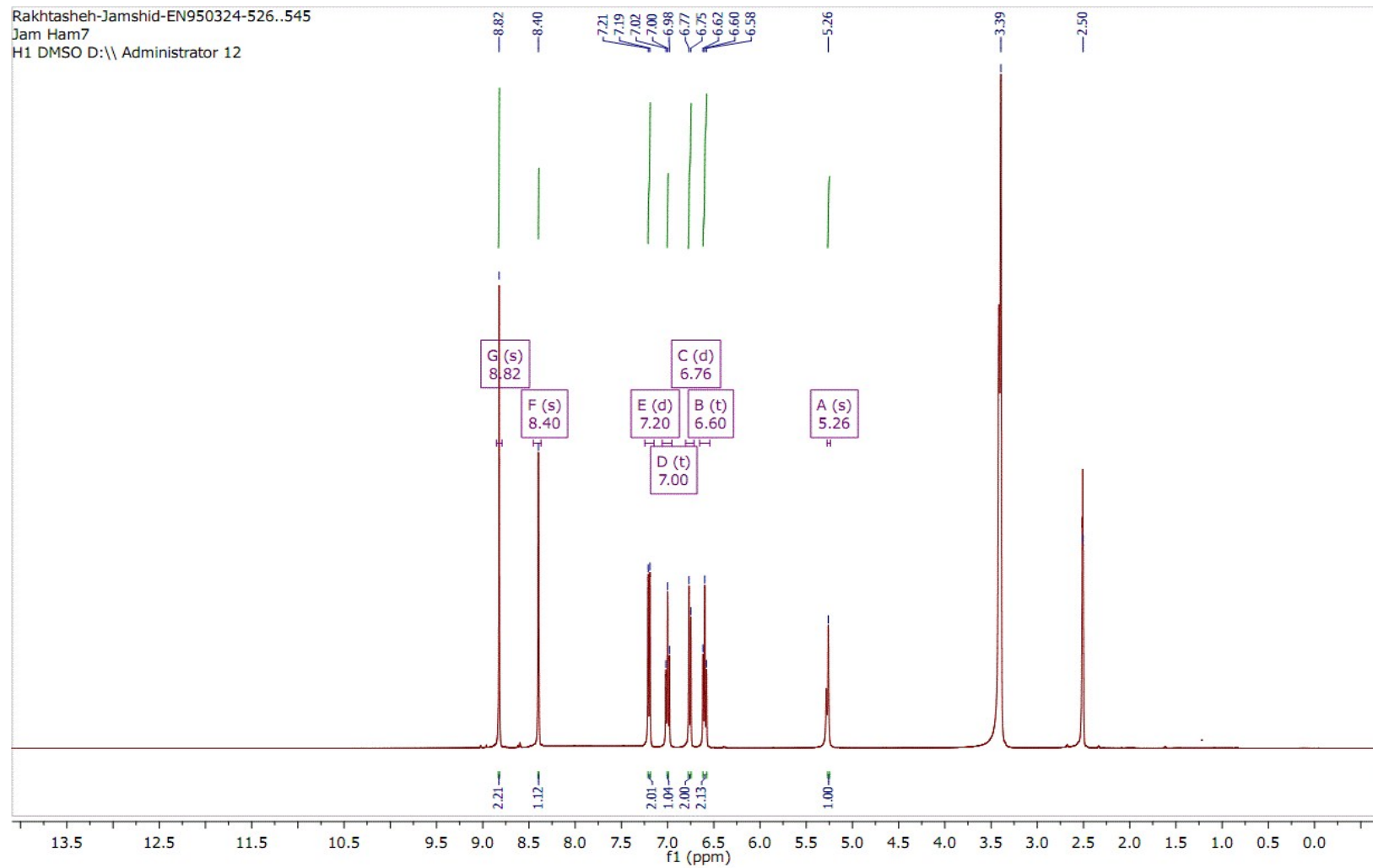
**Fig S8.** The Mass spectrea of 5-amino-1-phenyl-3-(ferrocene-yl)-1H-pyrazole-4-carbonitrile (Table 3, entry 6)

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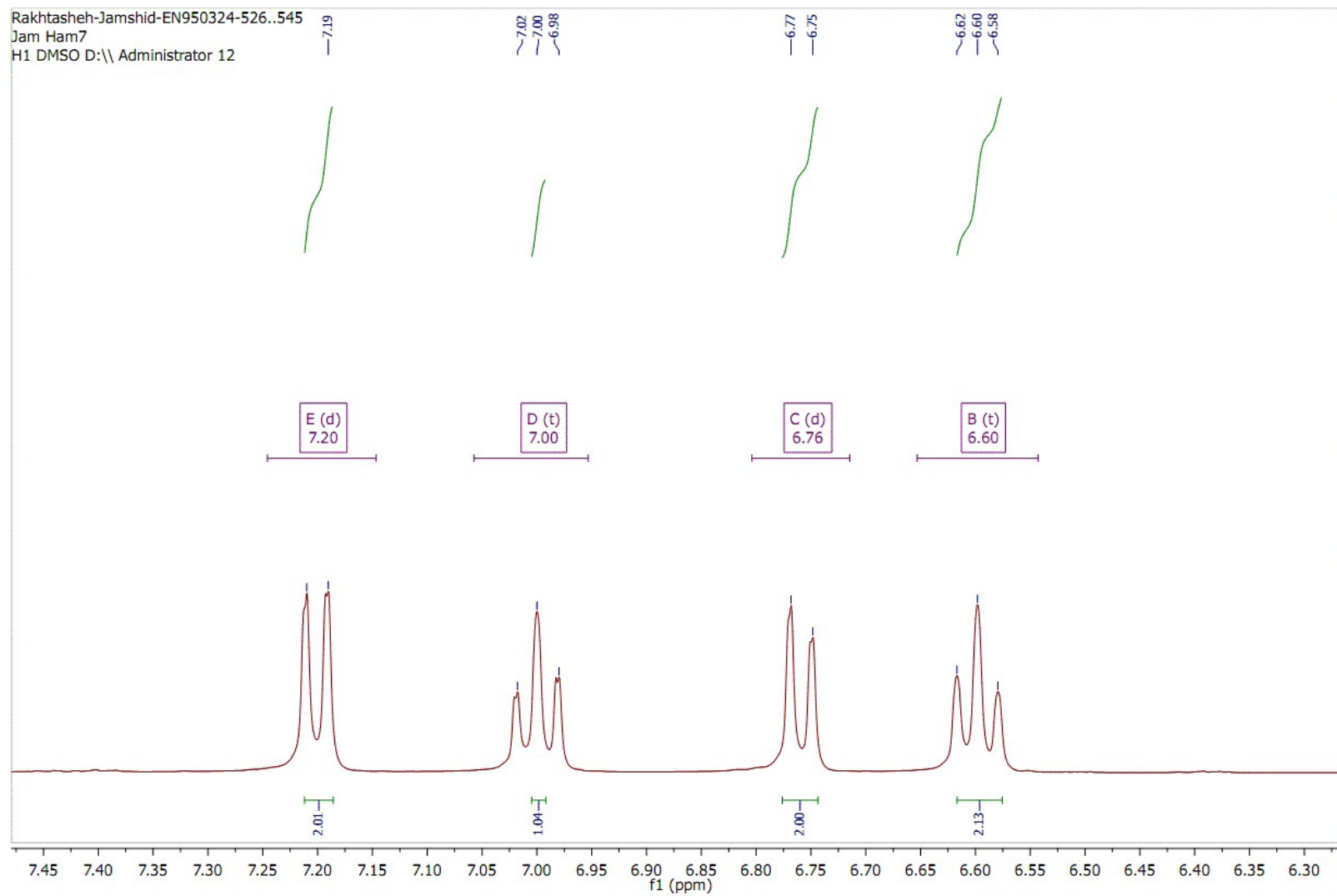
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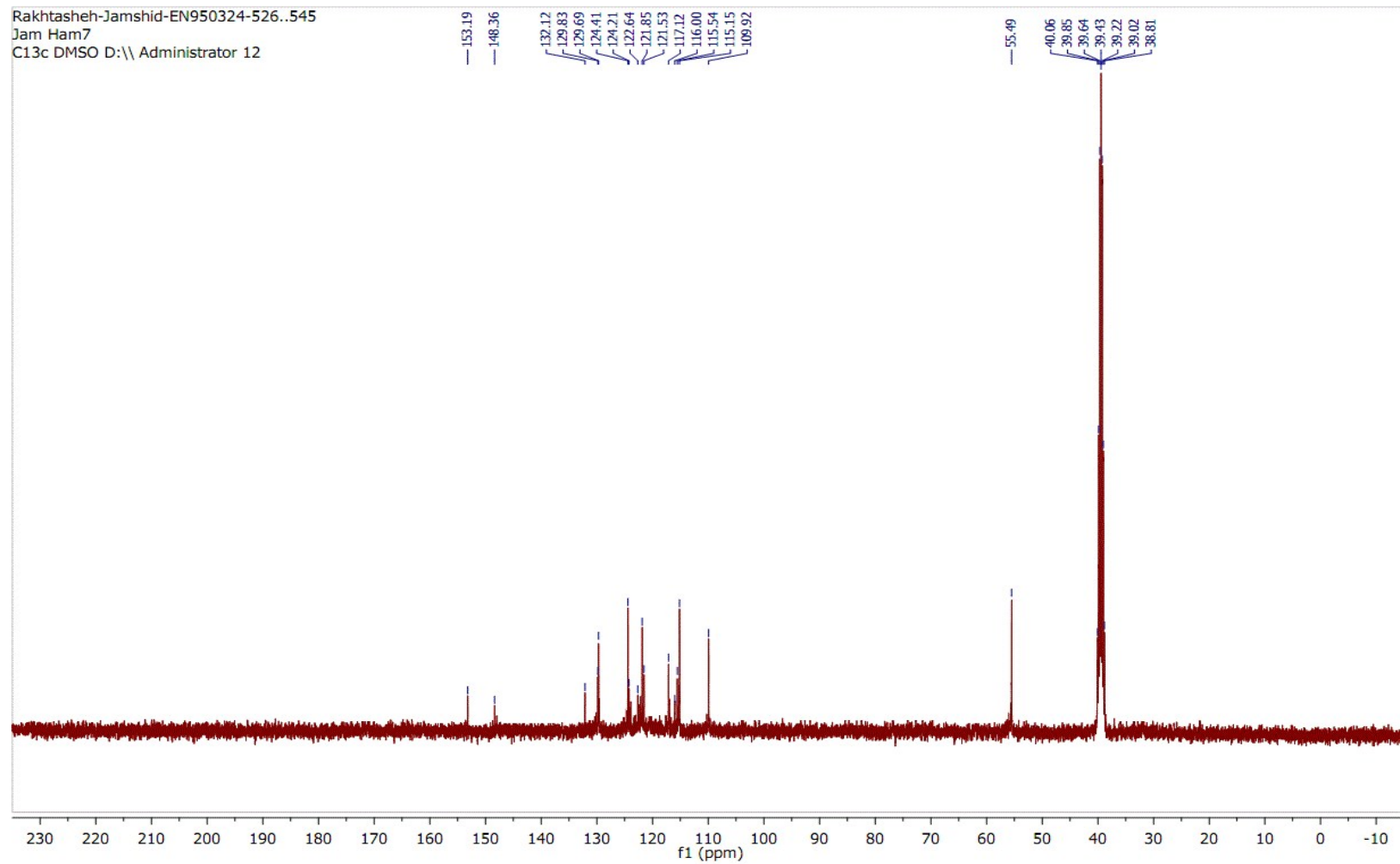
**Fig S9.** The IR of 5-amino-3-(5-fluoro-2-hydroxyphenyl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 7)



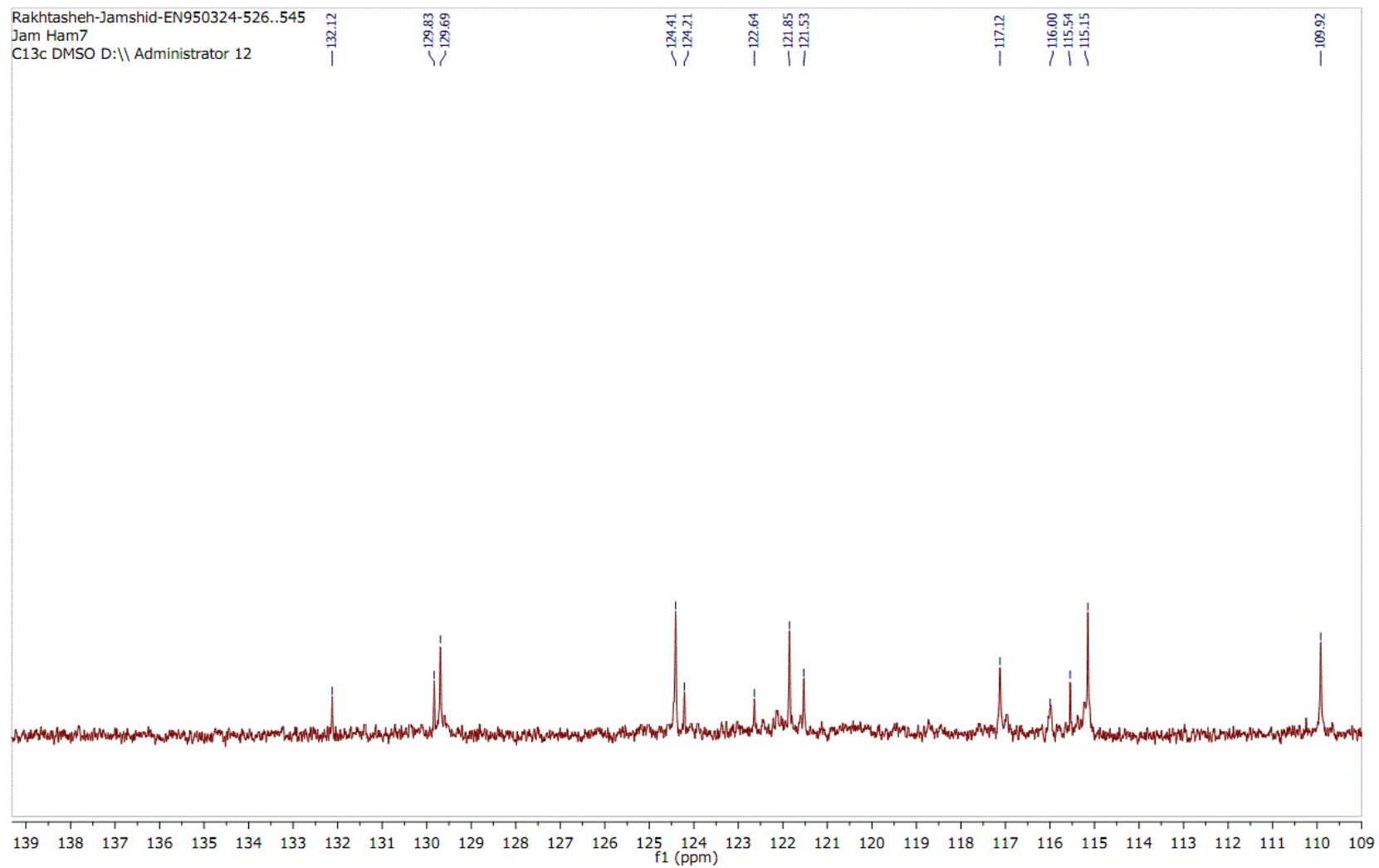
**Fig S10.** The  $^1\text{H}$  NMR of 5-amino-3-(5-fluoro-2-hydroxyphenyl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 7)



**Fig S11.** The expand  $^1\text{H}$  NMR of 5-amino-3-(5-fluoro-2-hydroxyphenyl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 7)

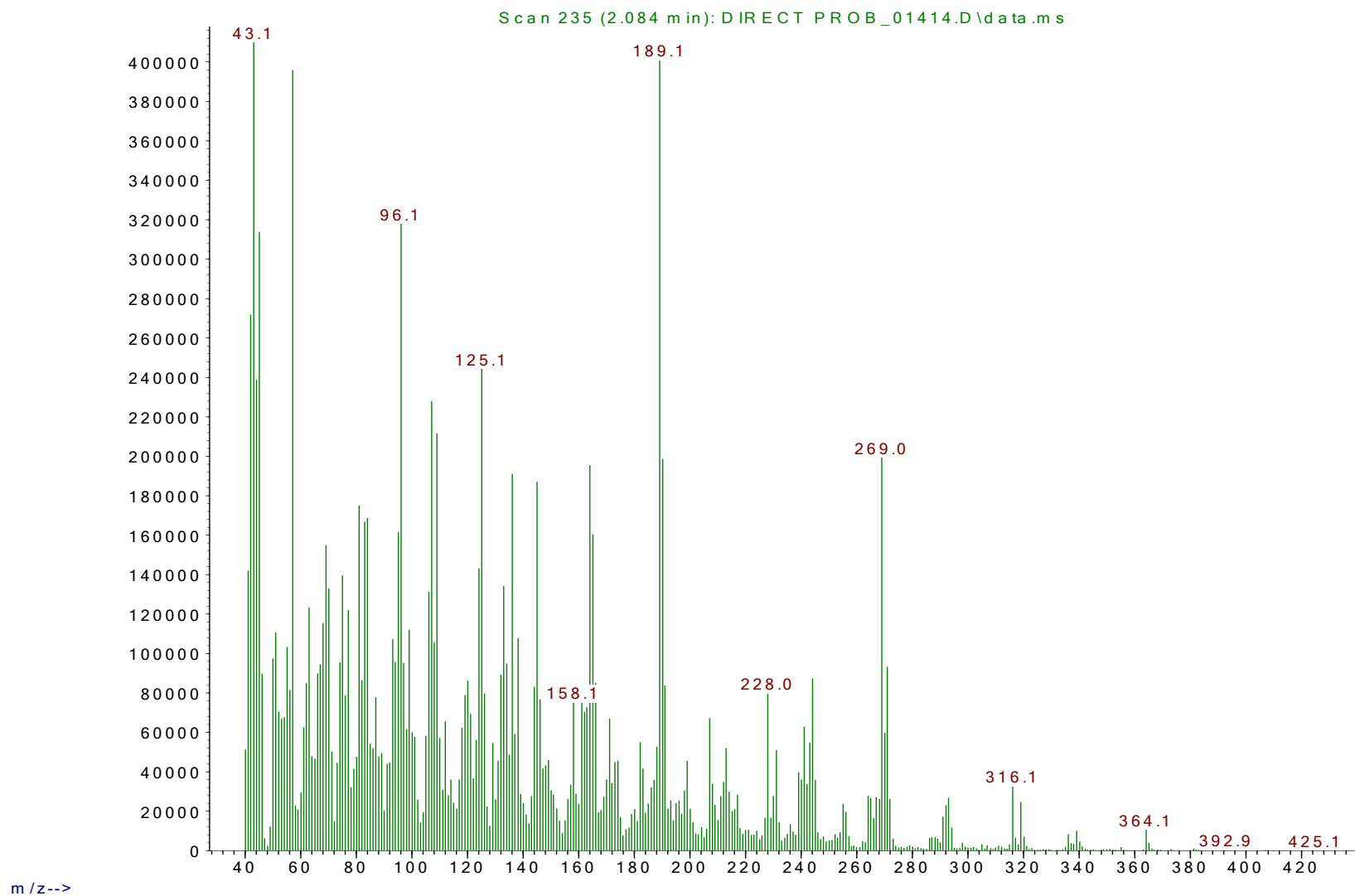


**Fig S12.** The  $^{13}\text{C}$  NMR of 5-amino-3-(5-fluoro-2-hydroxyphenyl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 7)



**Fig S13.** The expanded  $^{13}\text{C}$  NMR of 5-amino-3-(5-fluoro-2-hydroxyphenyl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 7)

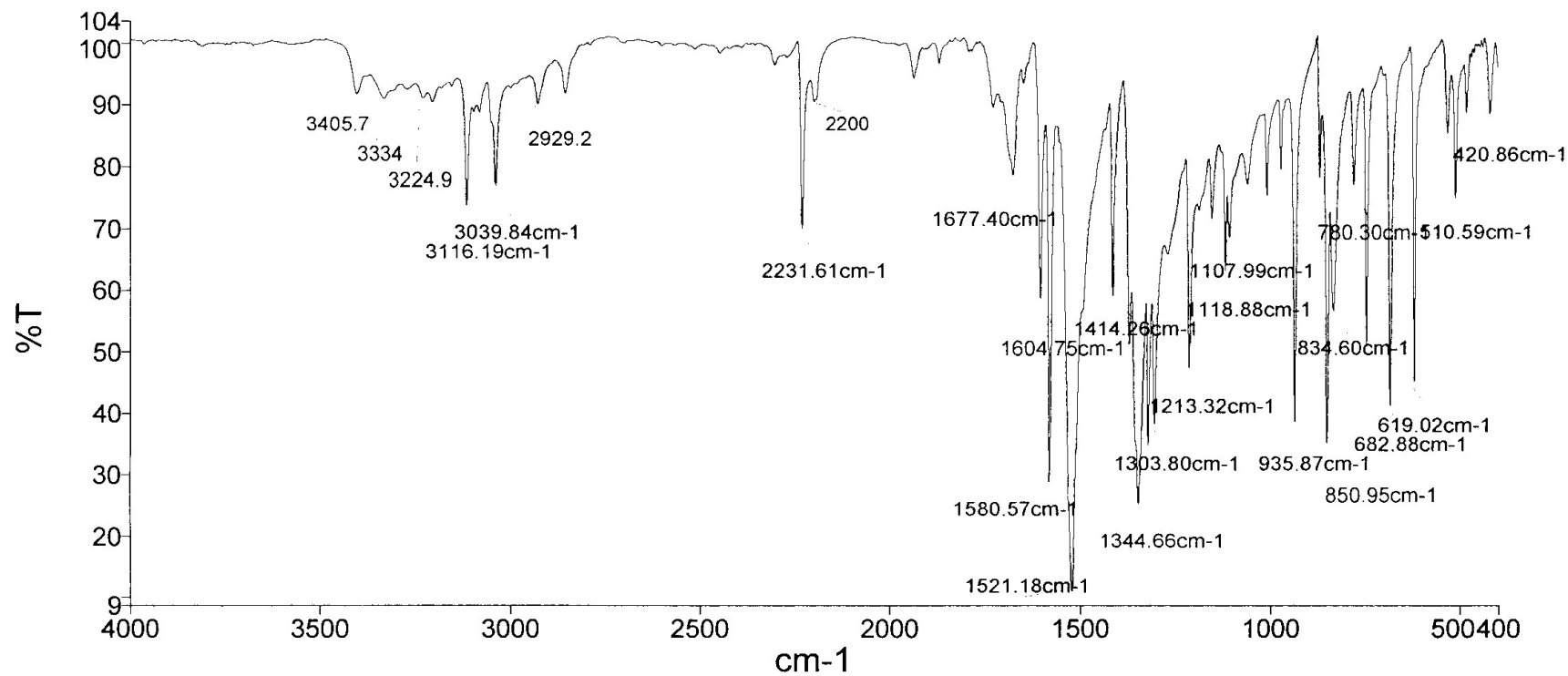
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**Fig S14.** The Mass spectra of 5-amino-3-(5-fluoro-2-hydroxyphenyl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 7)

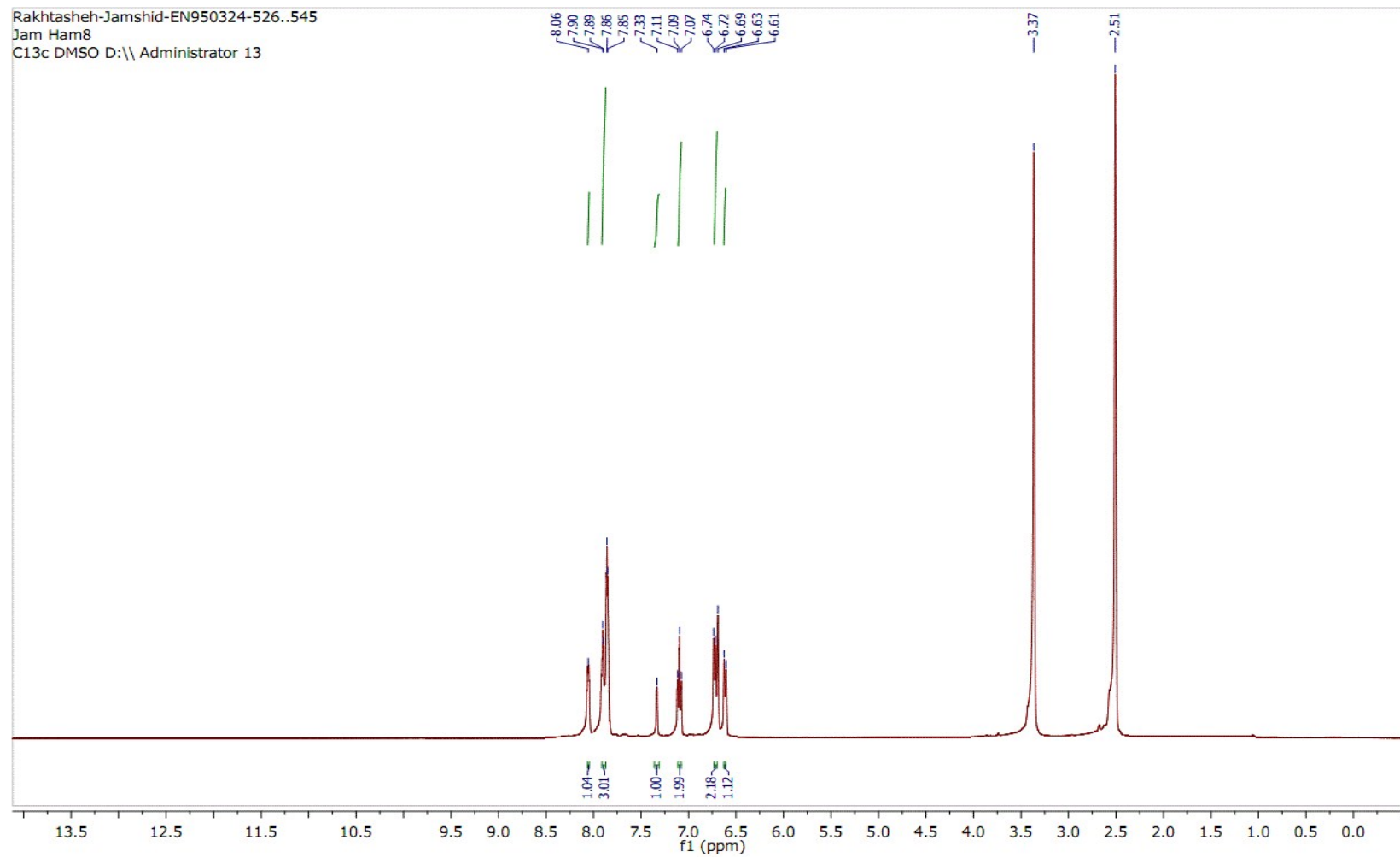
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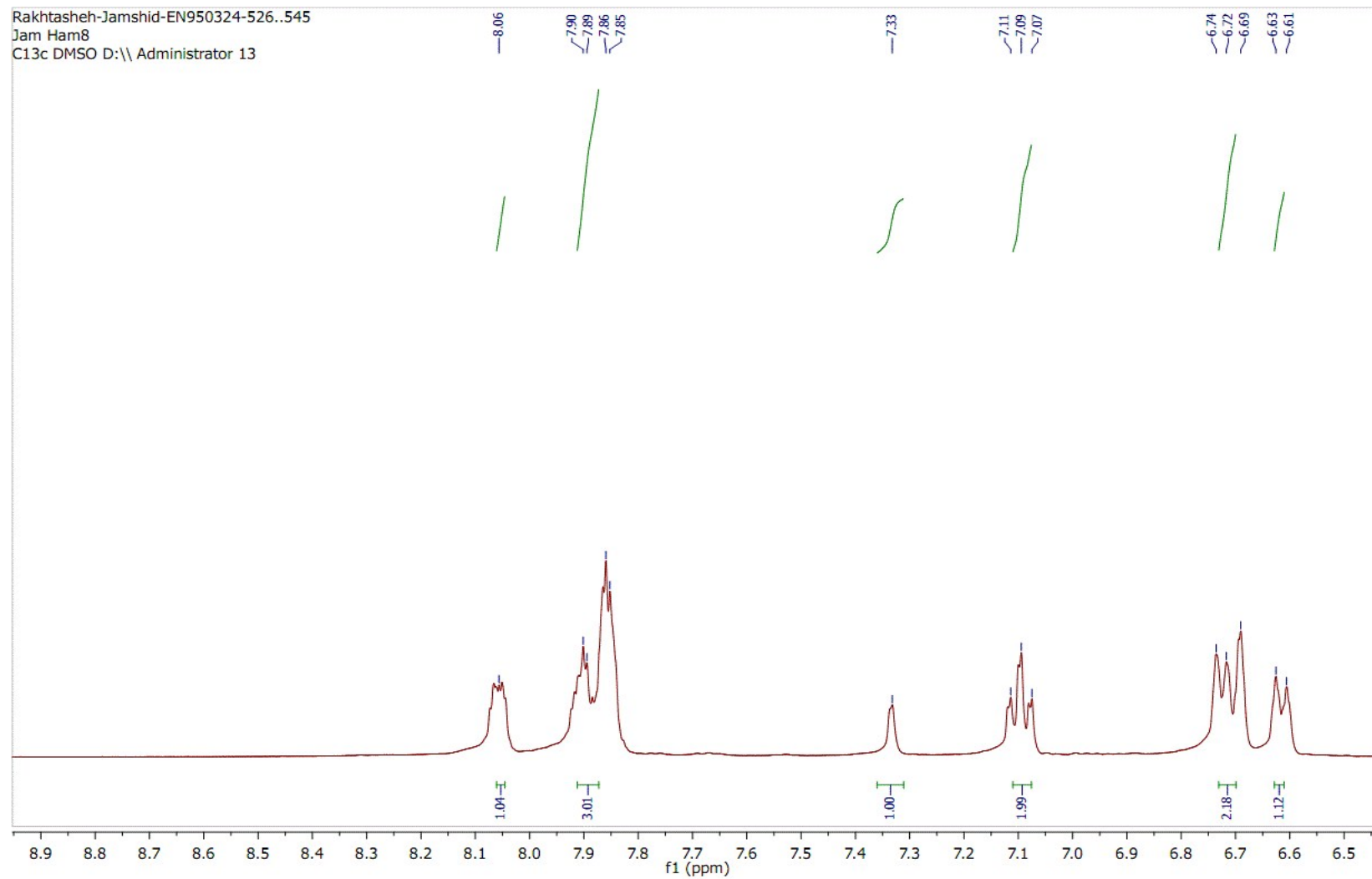


**Fig S15.** The IR of 5-amino-1-phenyl-3-(1H-pyrrol-2-yl)-1H-pyrazole-4-carbonitrile: (Table 3, entry 8)

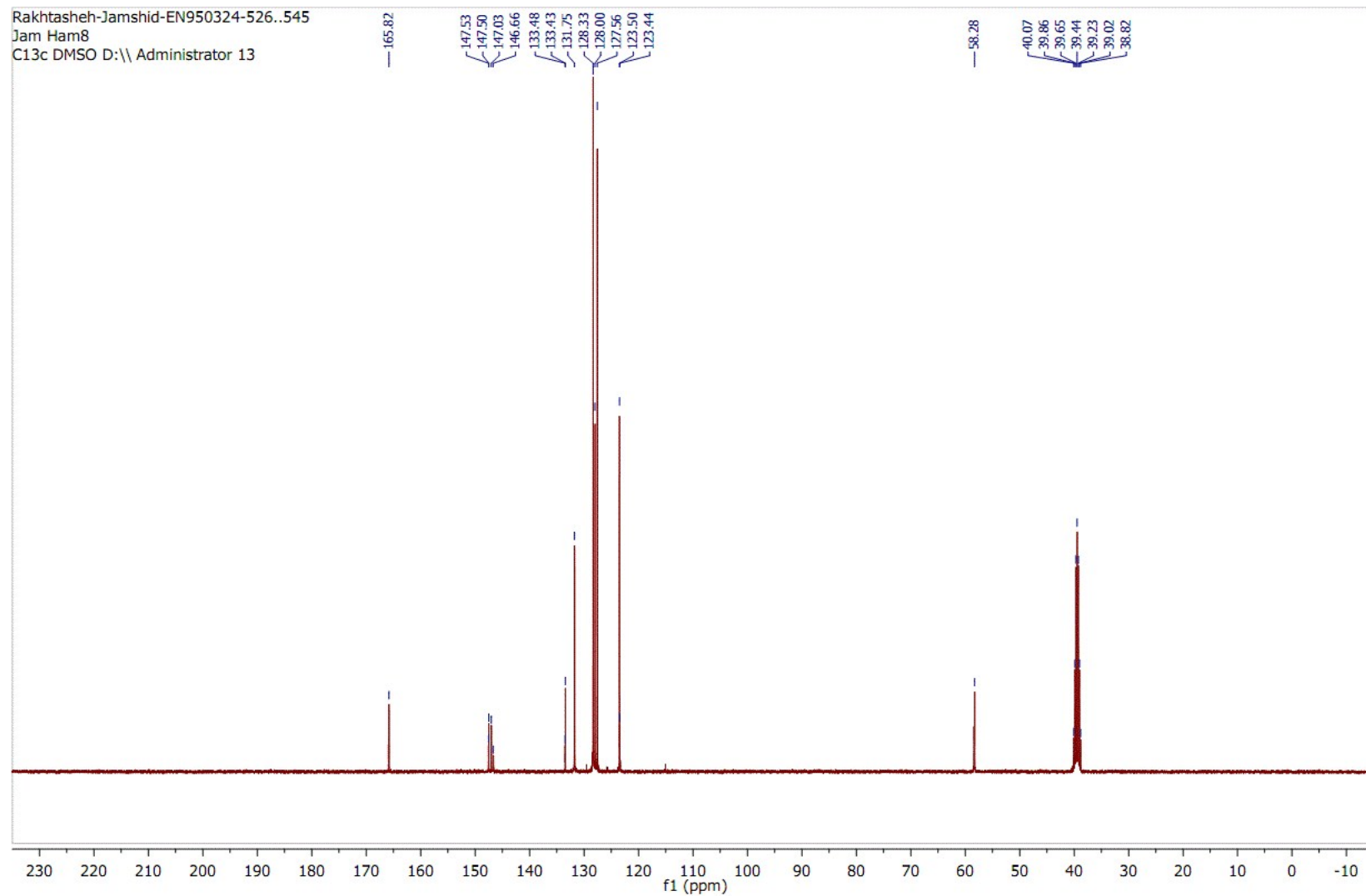




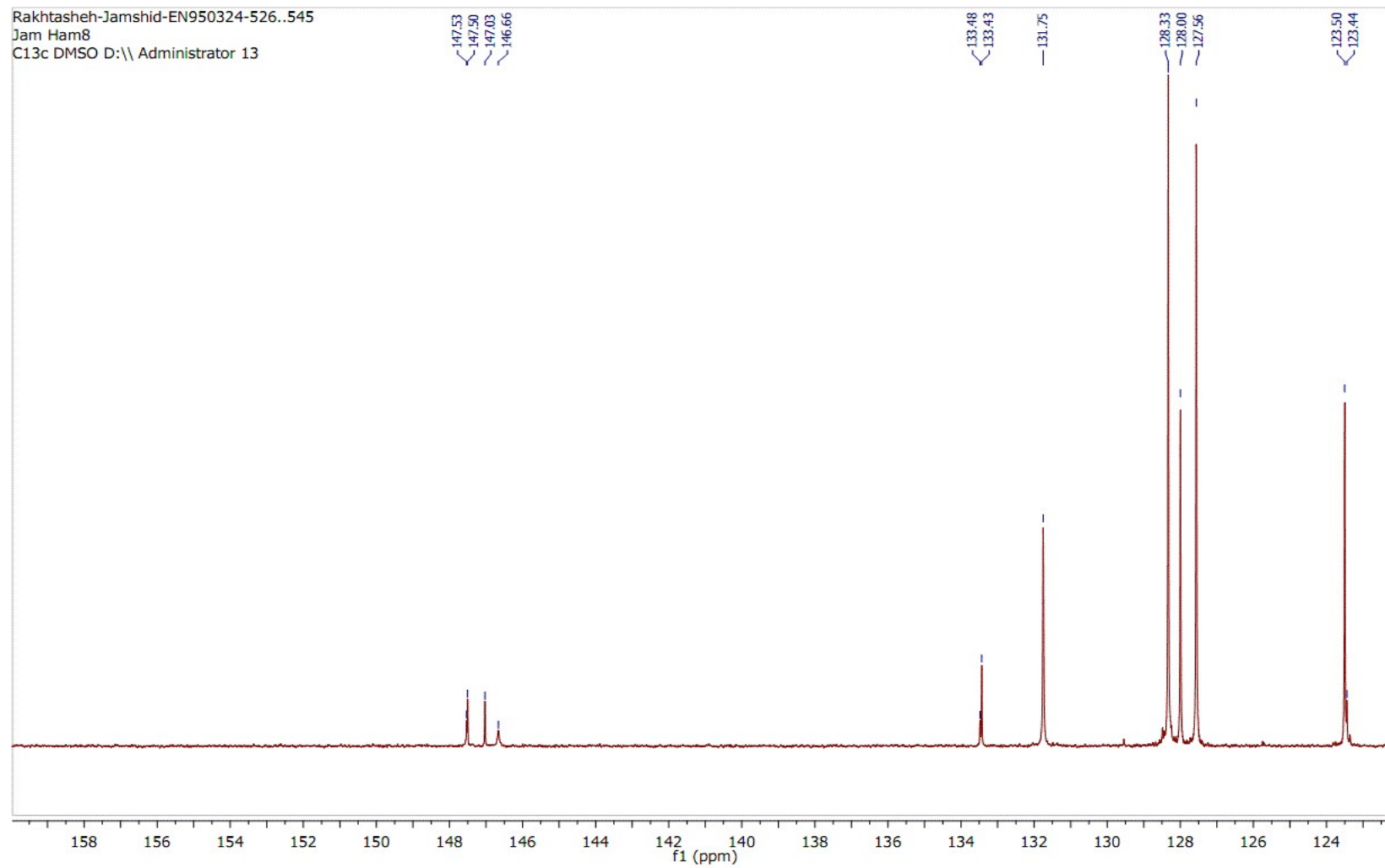
**Fig S16.** The  $^1\text{H}$  NMR of 5-amino-1-phenyl-3-(1H-pyrrol-2-yl)-1H-pyrazole-4-carbonitrile: (Table 3, entry 8)



**Fig S17.** The expanded  $^1\text{H}$  NMR of 5-amino-1-phenyl-3-(1H-pyrrol-2-yl)-1H-pyrazole-4-carbonitrile: (Table 3, entry 8)

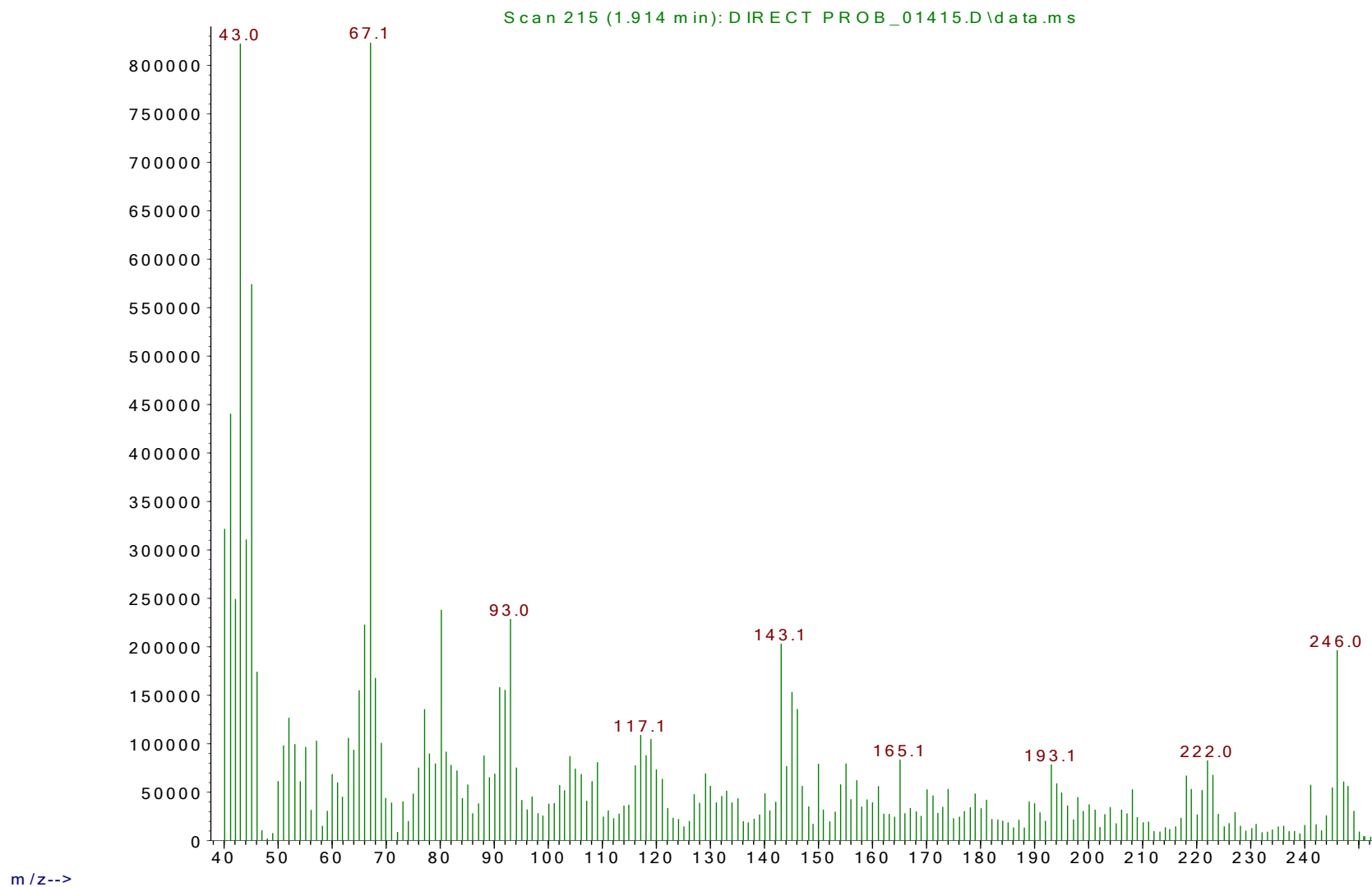


**Fig S18.** The  $^{13}\text{C}$  NMR of 5-amino-1-phenyl-3-(1H-pyrrol-2-yl)-1H-pyrazole-4-carbonitrile: (Table 3, entry 8)



**Fig S19.** The expanded  $^{13}\text{C}$  NMR of 5-amino-1-phenyl-3-(1H-pyrrol-2-yl)-1H-pyrazole-4-carbonitrile: (Table 3, entry 8)

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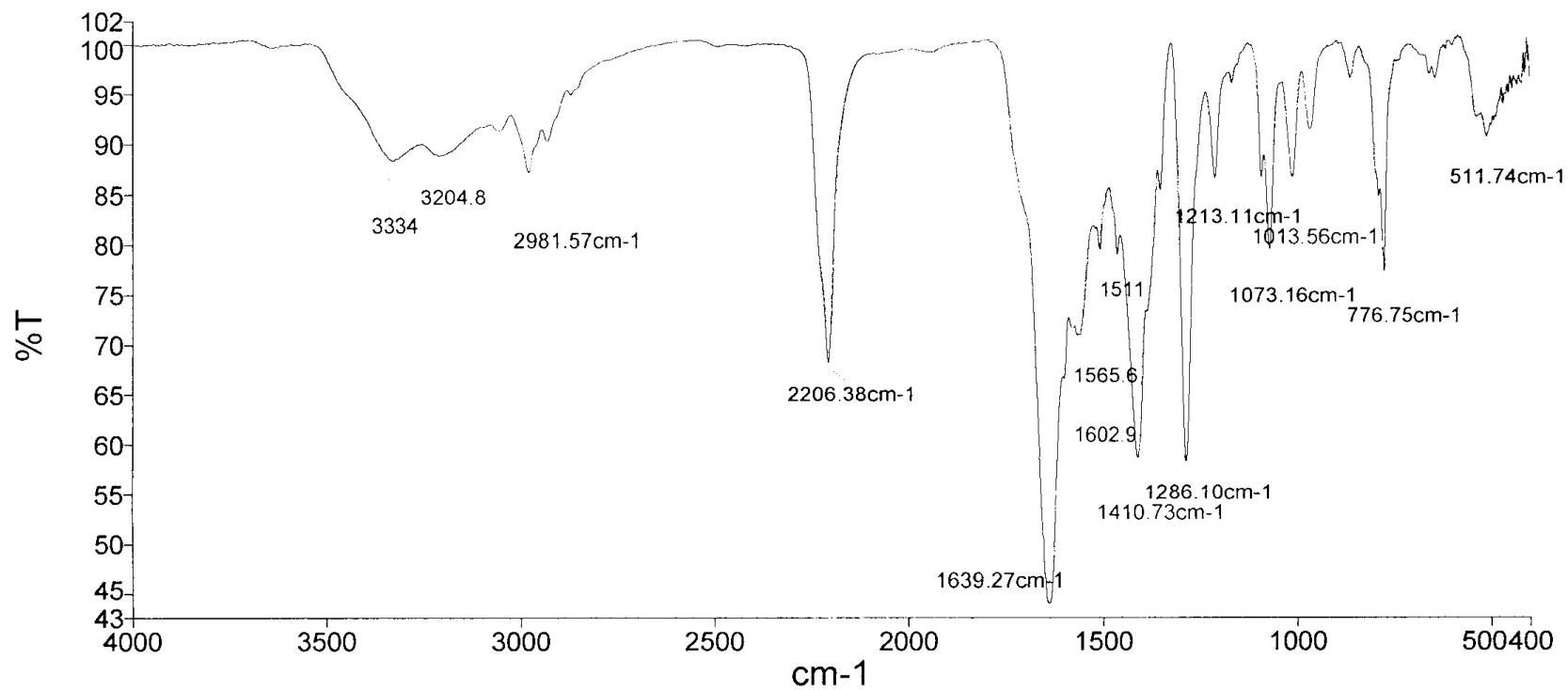
**Fig S20.** The Mass spectra of 5-amino-1-phenyl-3-(1H-pyrrol-2-yl)-1H-pyrazole-4-carbonitrile: (Table 3, entry 8)

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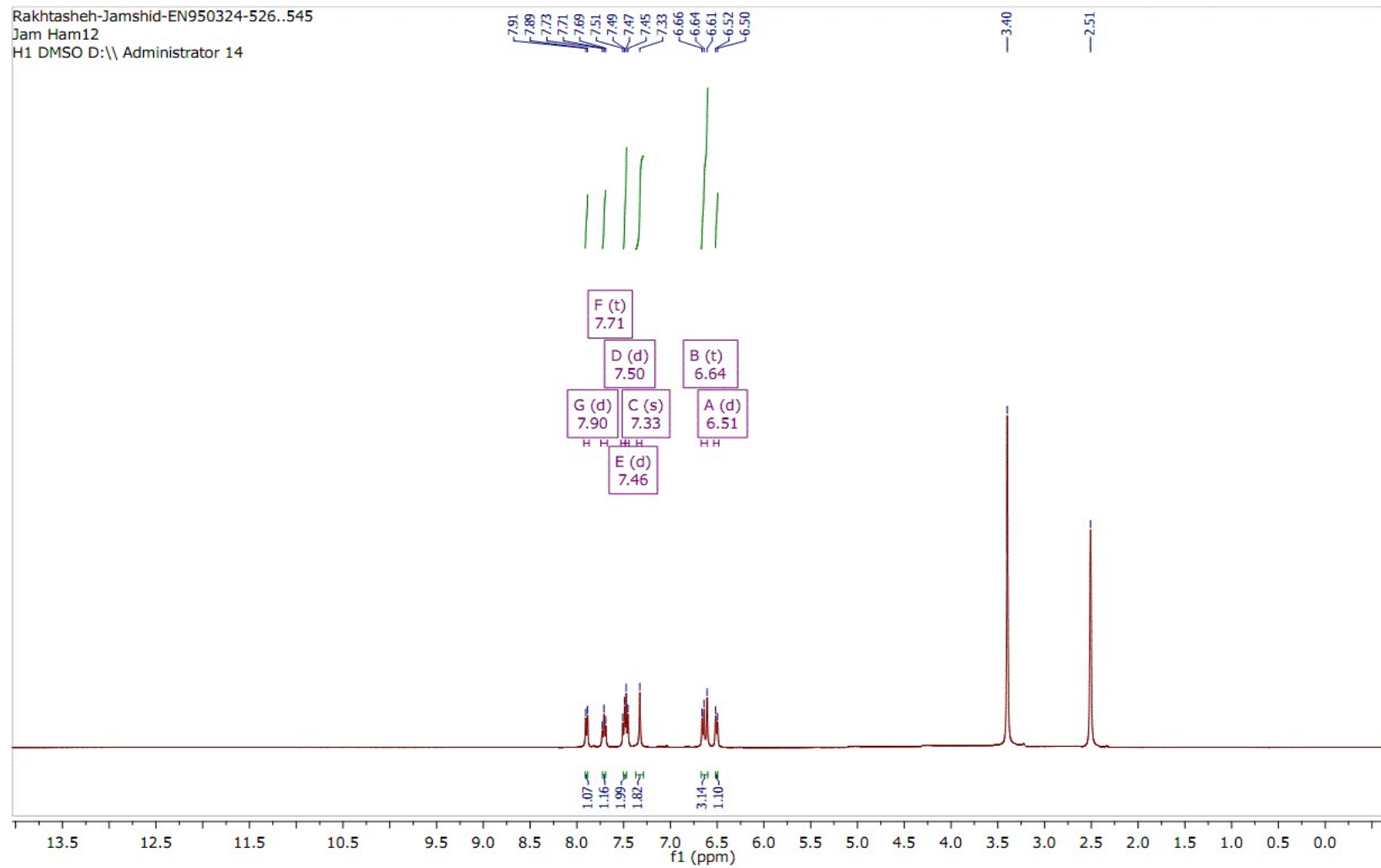
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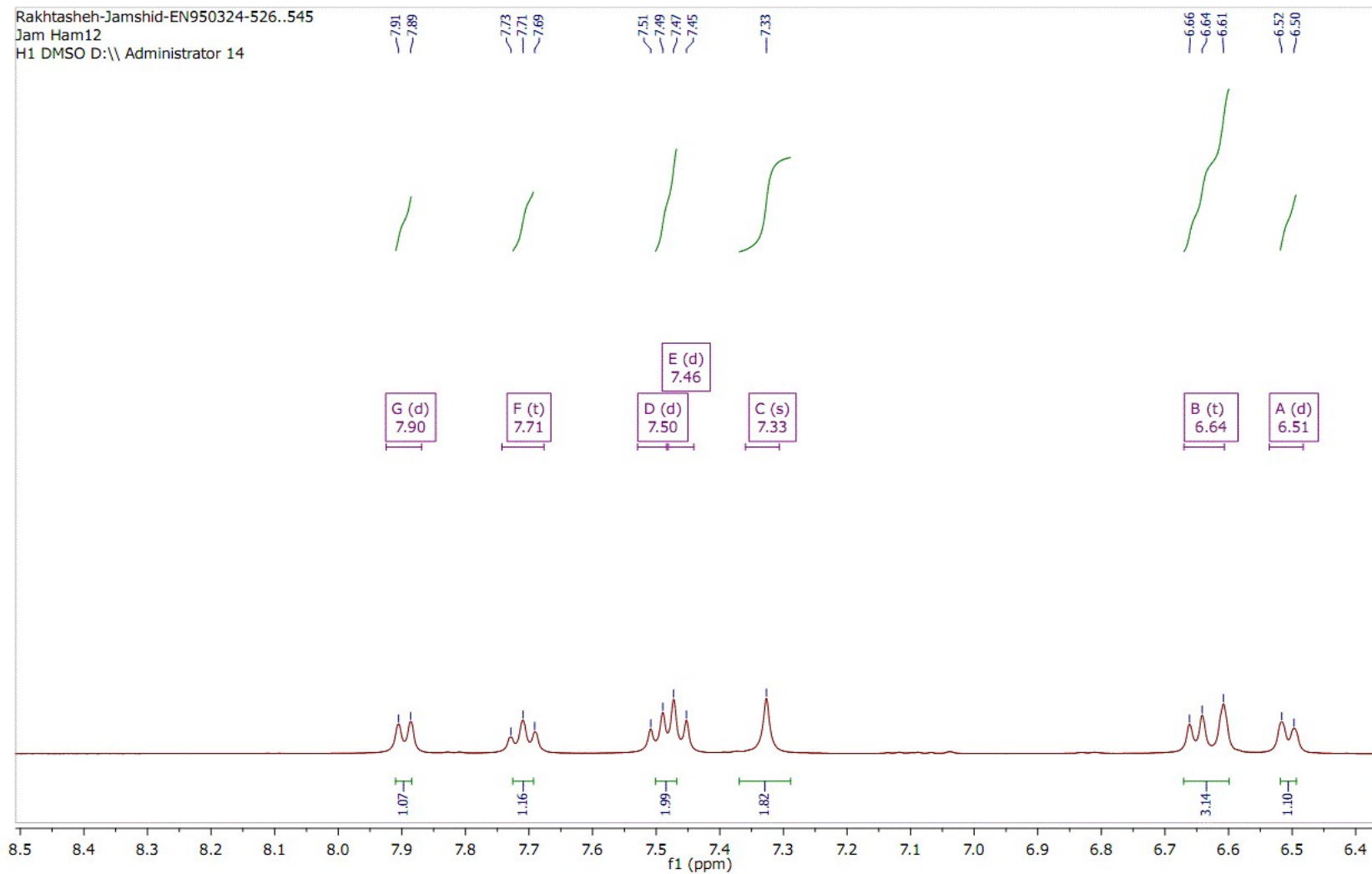
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**Fig S21.** The IR of 5-amino-3-(furan-2-yl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 12)

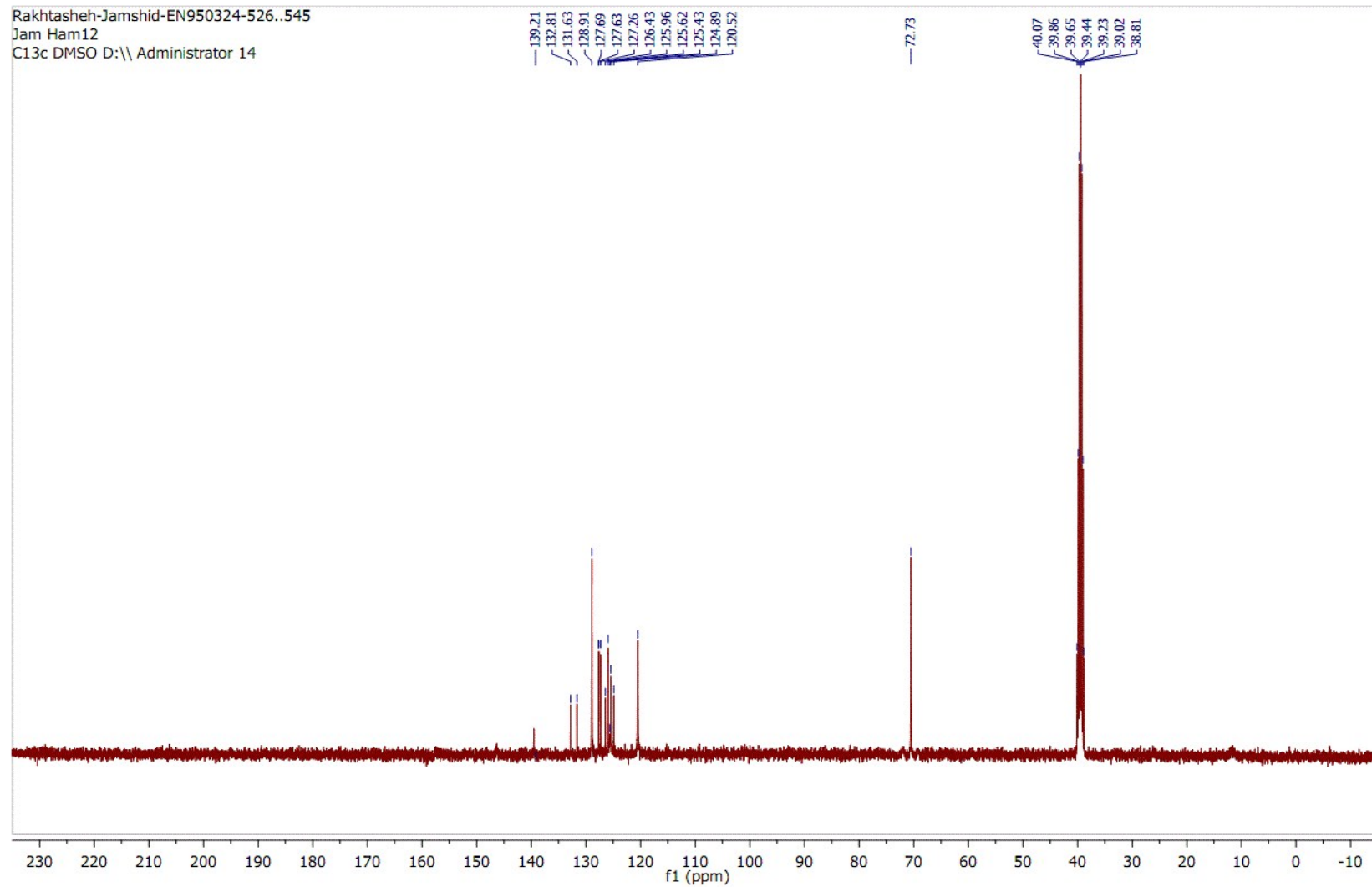


**Fig S22.** The  $^1\text{H}$  NMR of 5-amino-3-(furan-2-yl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 12)

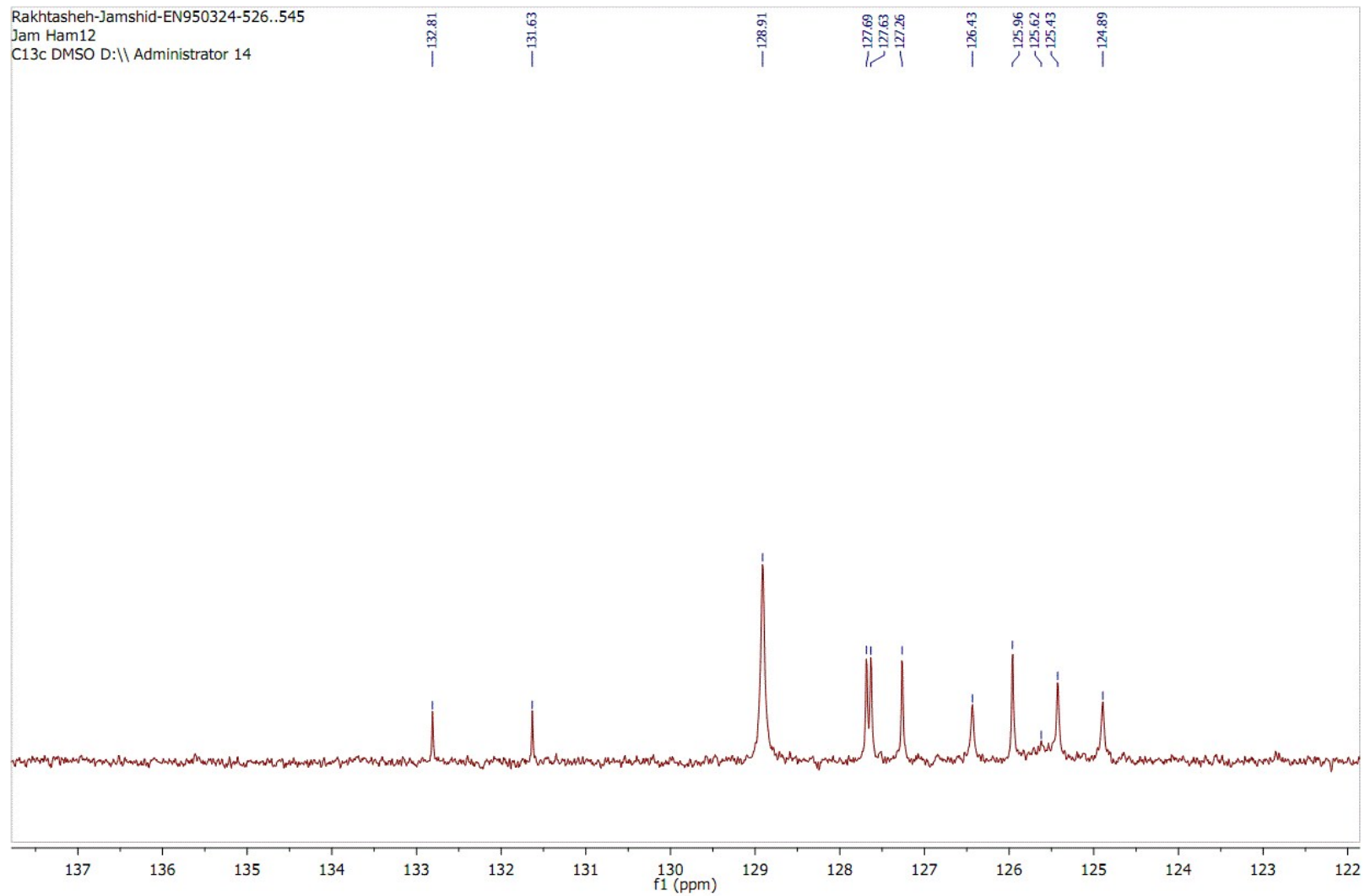


**Fig S23.** The expanded  $^1\text{H}$  NMR of 5-amino-3-(furan-2-yl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 12)



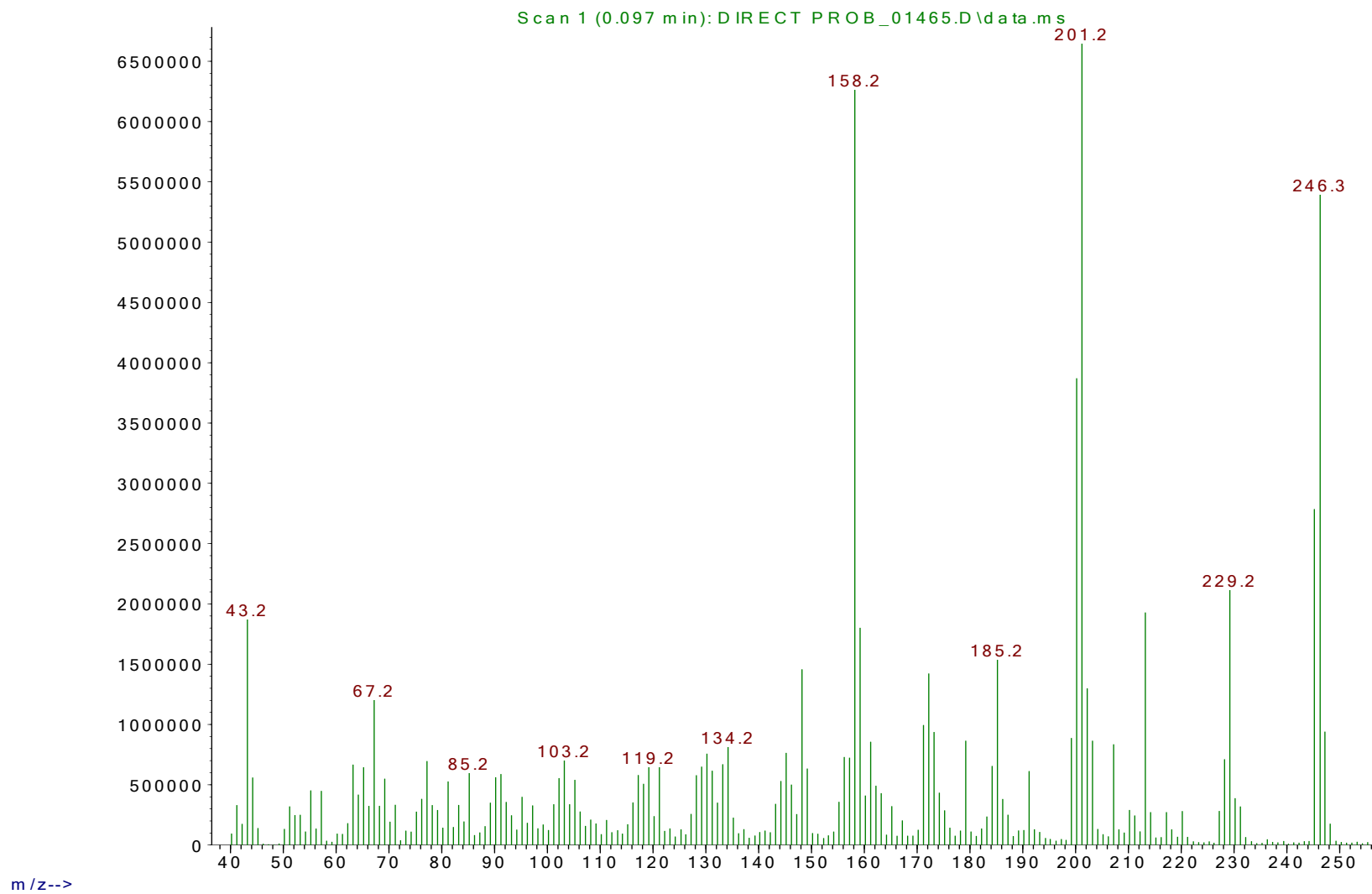


**Fig S24.** The  $^{13}\text{C}$  NMR of 5-amino-3-(furan-2-yl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 12)



**Fig S25.** The expanded  $^{13}\text{C}$  NMR of 5-amino-3-(furan-2-yl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 12)

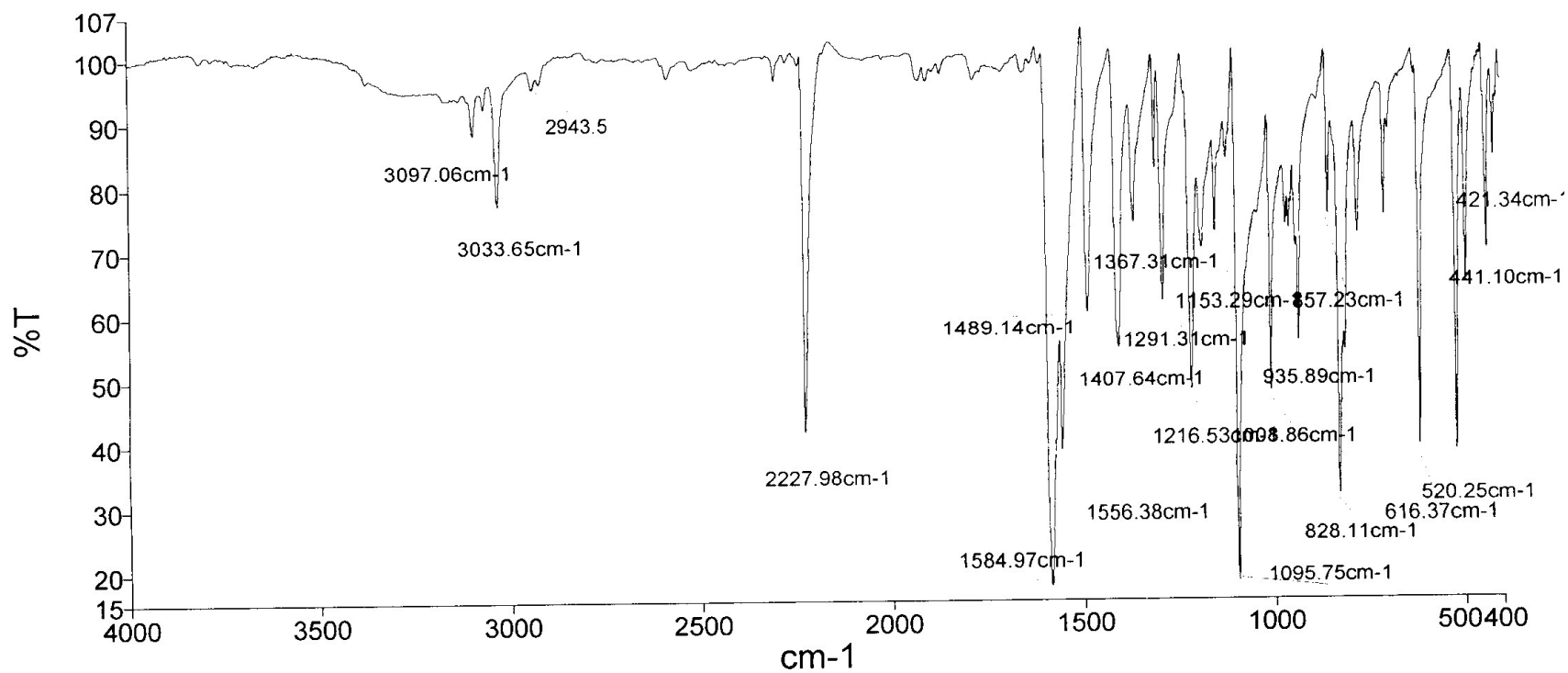
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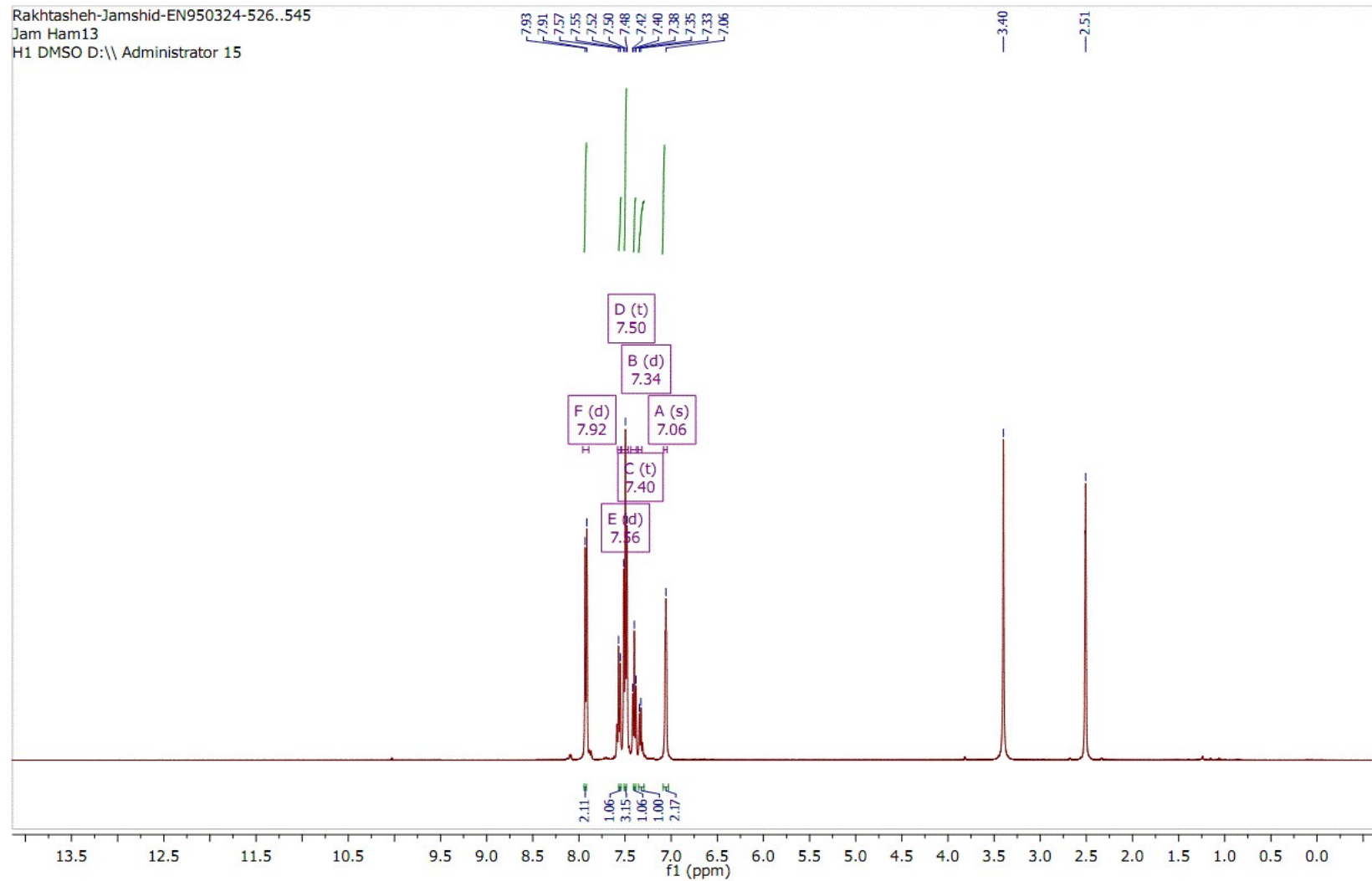
**Fig S26.** The Mass spectra of 5-amino-3-(furan-2-yl)-1-phenyl-1H-pyrazole-4-carbonitrile: (Table 3, entry 12)

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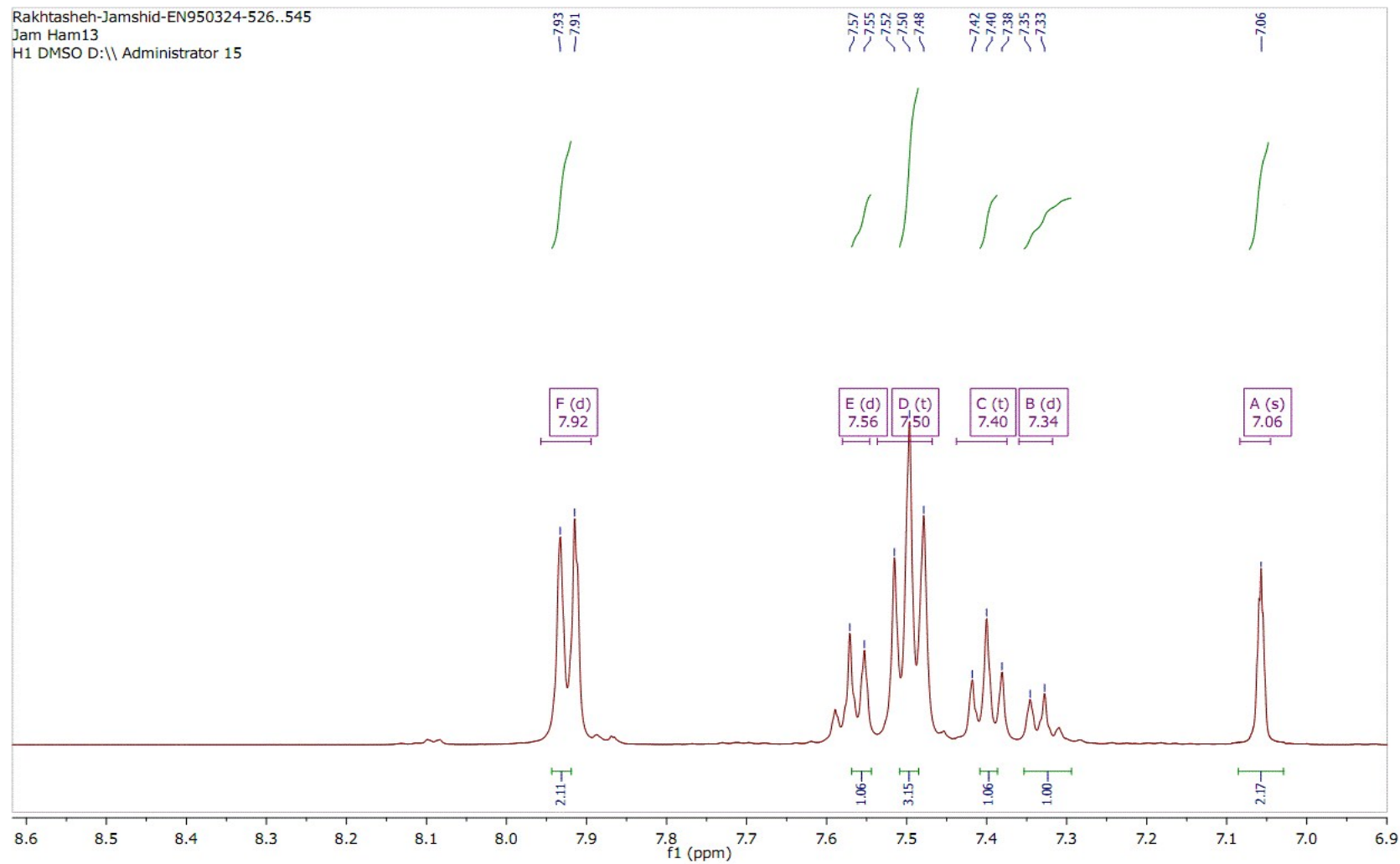
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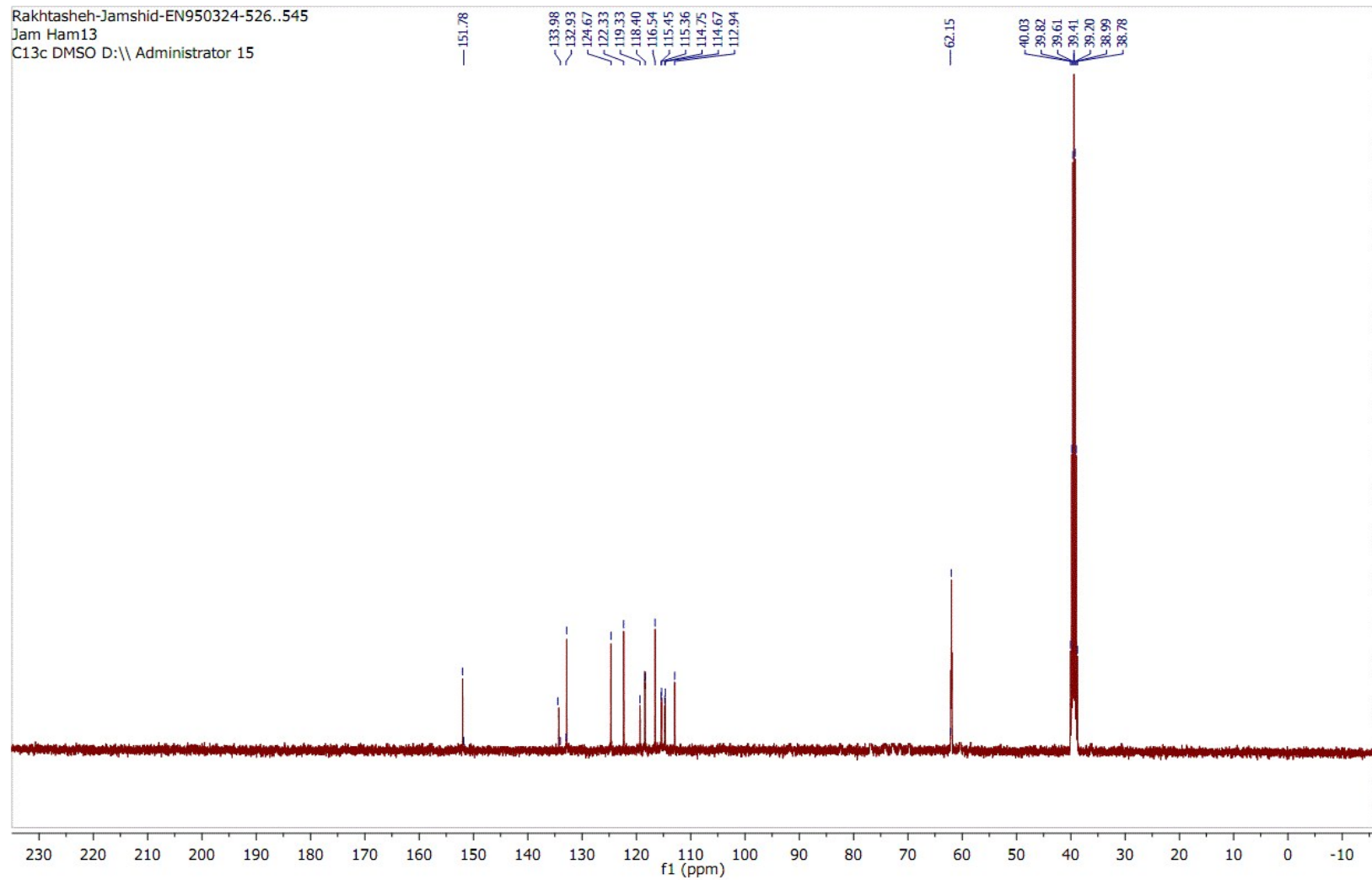
*Fig S27. The IR of 5-amino-1-phenyl-3-(thiophen-2-yl)-1H-pyrazole-4-carbonitrile: (Table 3, entry 13)*



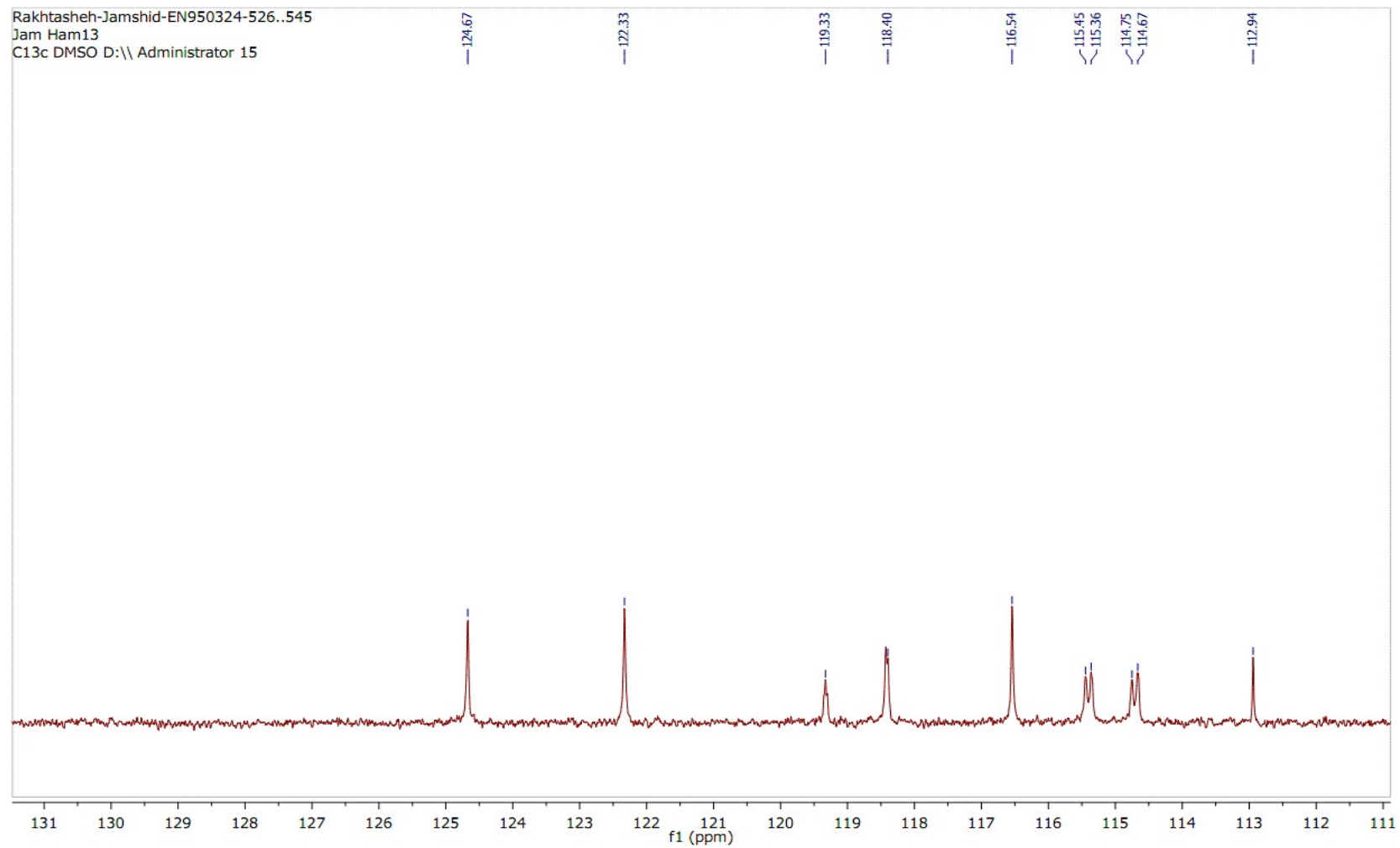
**Fig S28.** The  $^1\text{H}$  NMR of 5-amino-1-phenyl-3-(thiophen-2-yl)-1H-pyrazole-4-carbonitrile : ( Table 3, entry 13)



**Fig S29.** The expanded  $^1\text{H}$  NMR of 5-amino-1-phenyl-3-(thiophen-2-yl)-1H-pyrazole-4-carbonitrile : ( Table 3, entry 13)



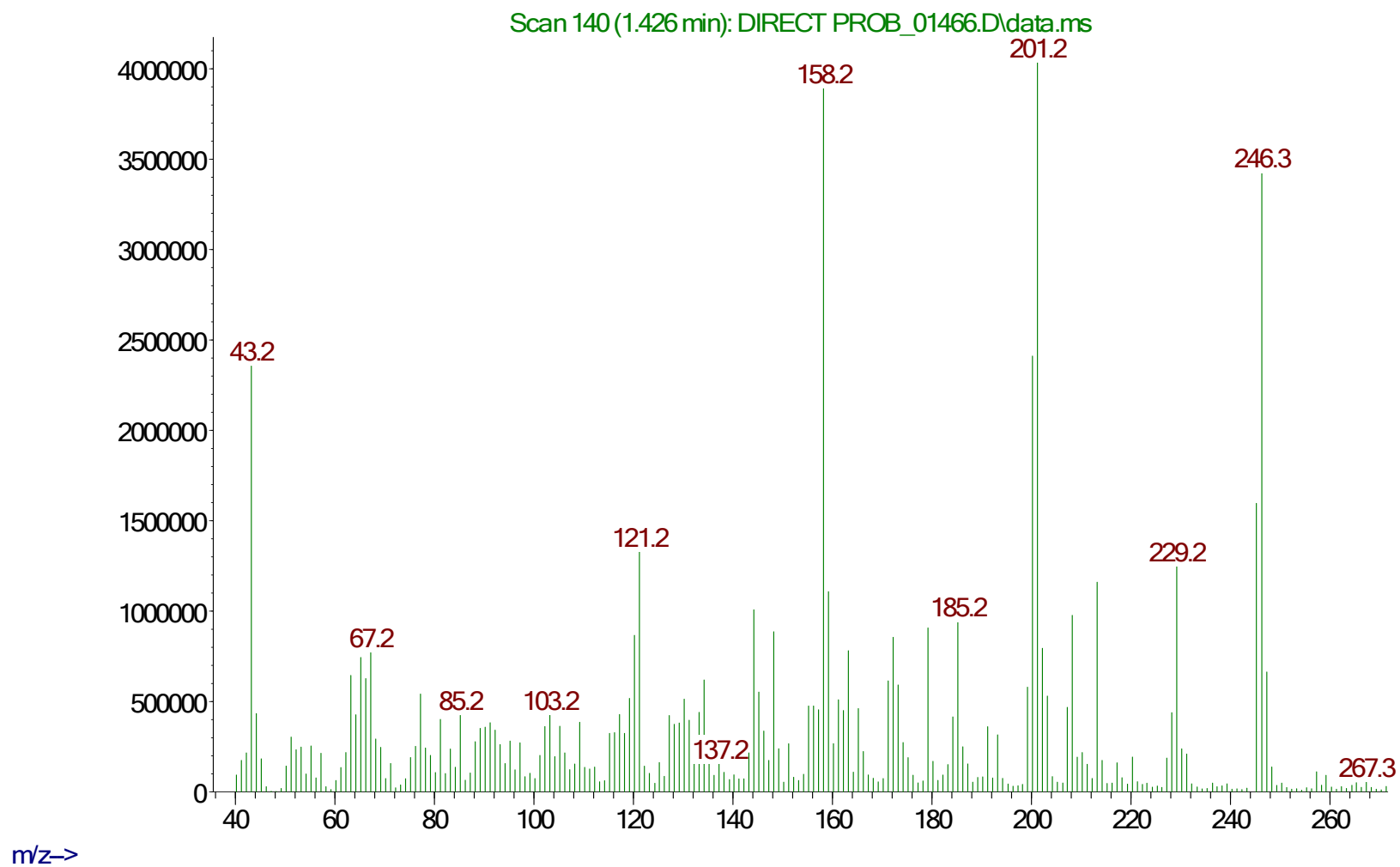
**Fig S30.** The  $^{13}\text{C}$  NMR of 5-amino-1-phenyl-3-(thiophen-2-yl)-1H-pyrazole-4-carbonitrile : ( Table 3, entry 13)



**Fig S31.** The expanded  $^{13}\text{C}$  NMR of 5-amino-1-phenyl-3-(thiophen-2-yl)-1H-pyrazole-4-carbonitrile : ( Table 3, entry 13)

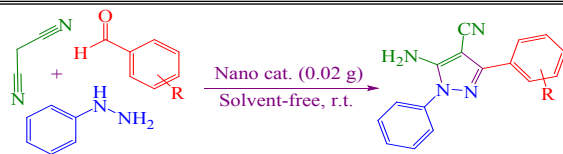


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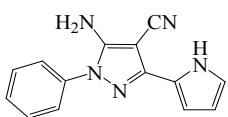
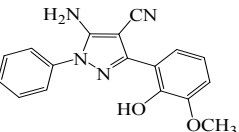
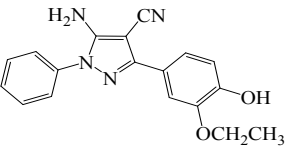
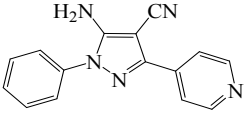
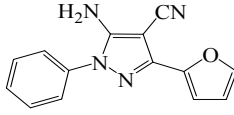
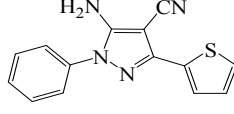
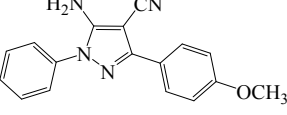
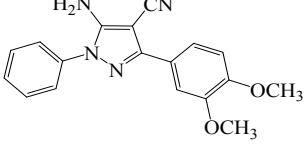
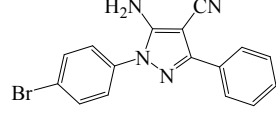


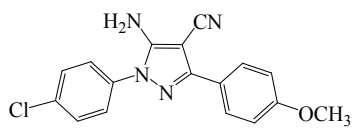
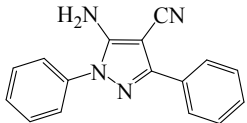
**Fig S32.** The Mass spectra of 5-amino-1-phenyl-3-(thiophen-2-yl)-1H-pyrazole-4-carbonitrile :( Table 3, entry 13)

**Table 3.** The three-component synthesis of 5-amino-pyrazole-4-carbonitrile derivatives in the presence of 0.02 g of nano catalyst.<sup>a</sup>

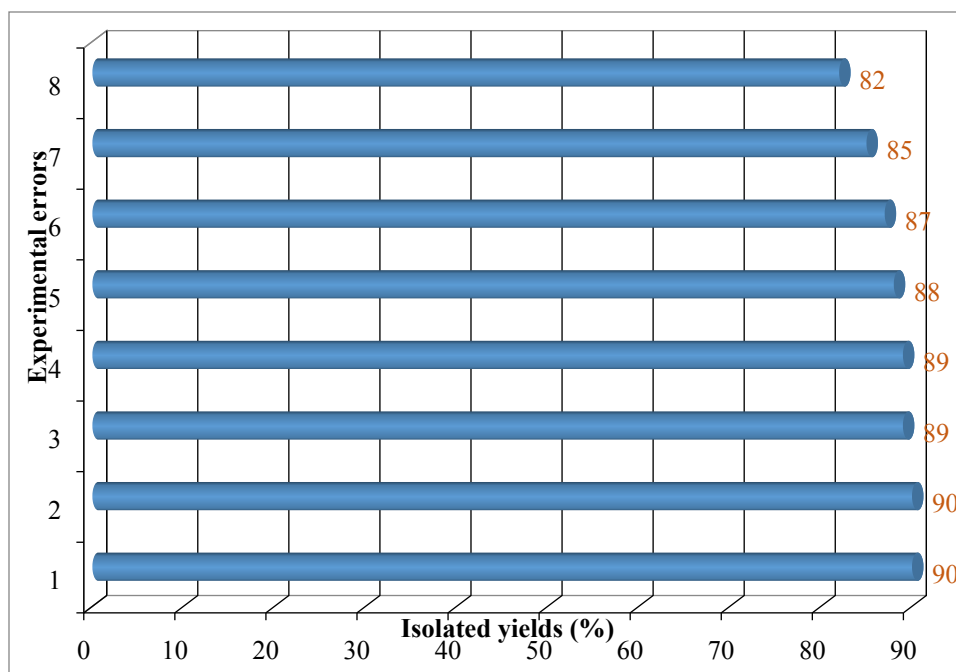


Entry	Product	Time (min)	Yield <sup>b</sup> (%)	M.p (°C) [Lit.] <sup>Ref.</sup>
1		10	95	175-177 (Yellow) <sup>30</sup>
2		15	93	221-223 (White) <sup>30</sup>
3		15	92	163-165 (Yellow) <sup>30</sup>
4		25	88	235-237 (Orange) <sup>30</sup>
5		10	94	158-160 (Orange)
6		25	88	>300 (Violet)
7		20	90	161-163 (Brown)

8		25	88	260-262 (Brown)
9		20	89	284-286 (Orange) <sup>30</sup>
10		20	90	225-227 (Orange) <sup>30</sup>
11		25	89	218-220 (Brown) <sup>43</sup>
12		25	87	168-170 (Brown)
13		25	87	163-165 (Brown)
14		20	90	112-114 (Red) <sup>43</sup>
15		20	90	125-127 (Orange) <sup>43</sup>
16		30	85	180-182 (Brown) <sup>45</sup>

17		25	85	210-212 (Orange)45
18		25	88	158-160 (Brown)44

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**Fig S33.** Reusability of  $Fe_3O_4@Si@MoO_2$  as a heterogeneous catalyst in 20 minutes.