

**Design of a structural framework with potential use to develop balanced
multifunctional agents against Alzheimer's disease**

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(Ling-Yi Kong);*

Table S1. Permeability (P_e 10^{-6} cm s $^{-1}$) in the PAMPA-BBB Assay of 9 Commercial Drugs Used in the Experiment Validation.

Compd	Bibl. ^a	Exp. ^b
Testosterone	17	10.50 ± 0.57
Piroxicam	2.5	1.72 ± 0.03
Desipramine	12	8.94 ± 0.46
Verapamil	16	13.36 ± 0.85
Lomefloxacin	1.1	0.32 ± 0.01
Corticosterone	5.1	1.09 ± 0.12
Progesterone	9.3	8.33 ± 0.25
Dopamine	0.2	0.83 ± 0.74
Hydrocortisone	1.9	1.14 ± 0.03

^aTaken from Ref. 1. ^bData are the mean ± SD of three independent experiments.

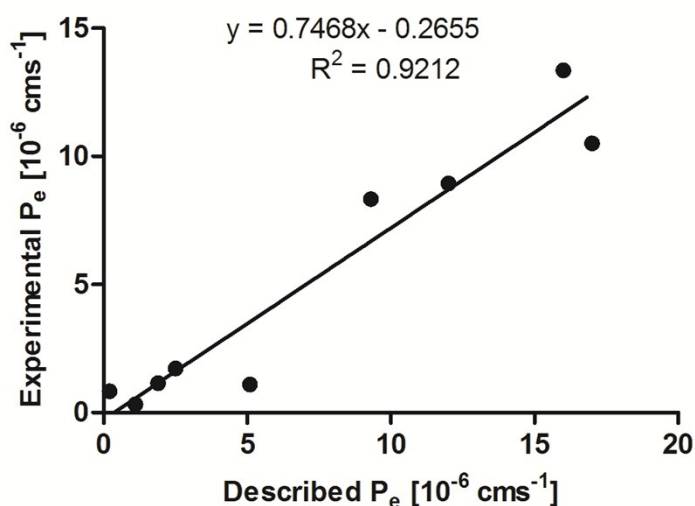


Fig. S1. Linear correlation between experimental and reported permeability of commercial drugs using the PAMPA-BBB assay.

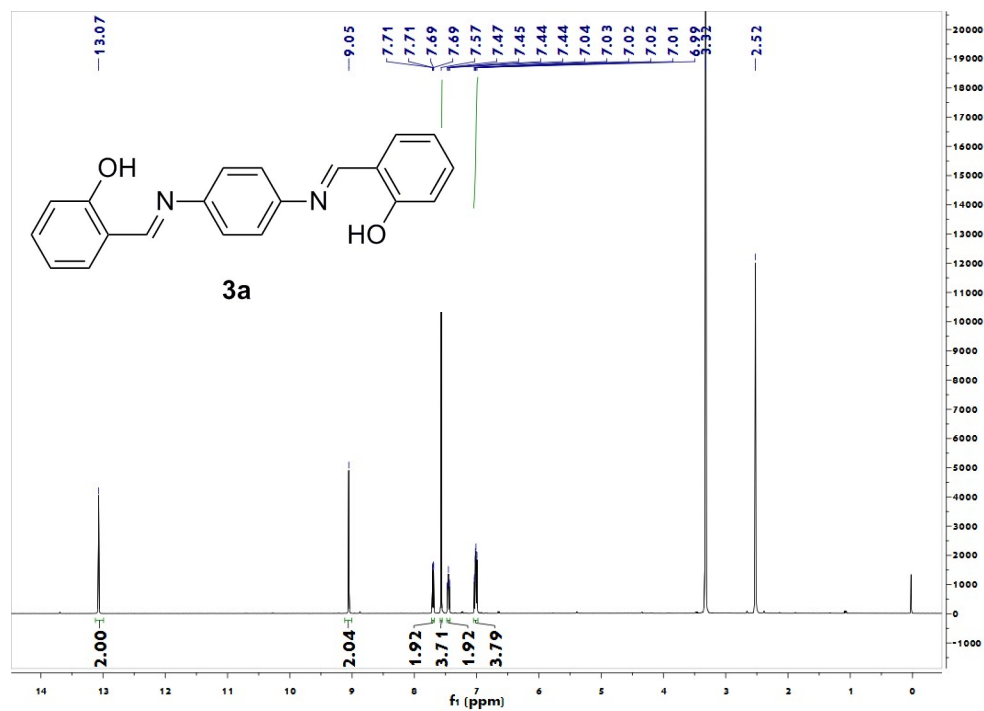
References

- [1] L. Di, E. H. Kerns, K. Fan, O. J. McConnell and G. T. Carter, *Eur. J. Med. Chem.* 2003, **38**, 223-232.

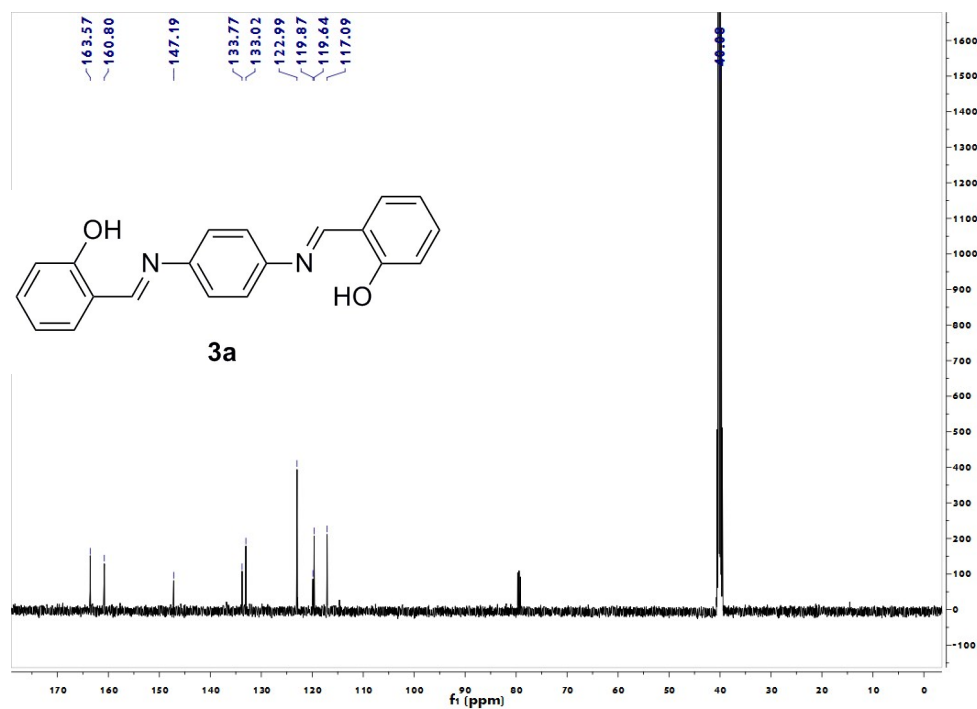
Contents

The representative ^1H NMR, ^{13}C NMR spectra, IR spectra and HRMS spectra of compounds.

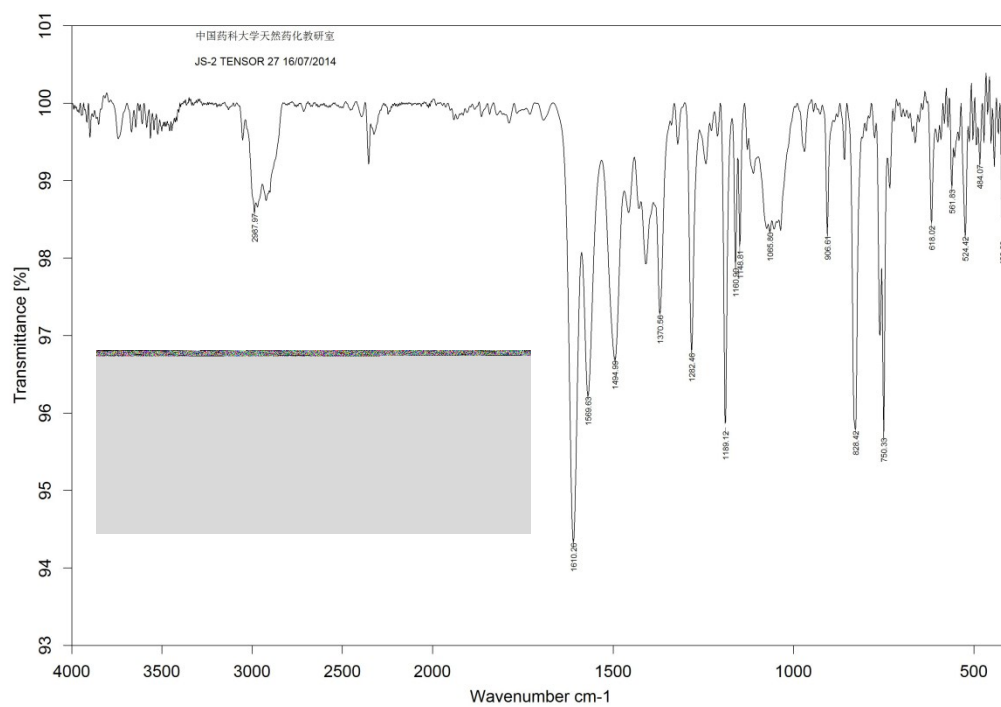
^1H NMR of compound **3a** in DMSO



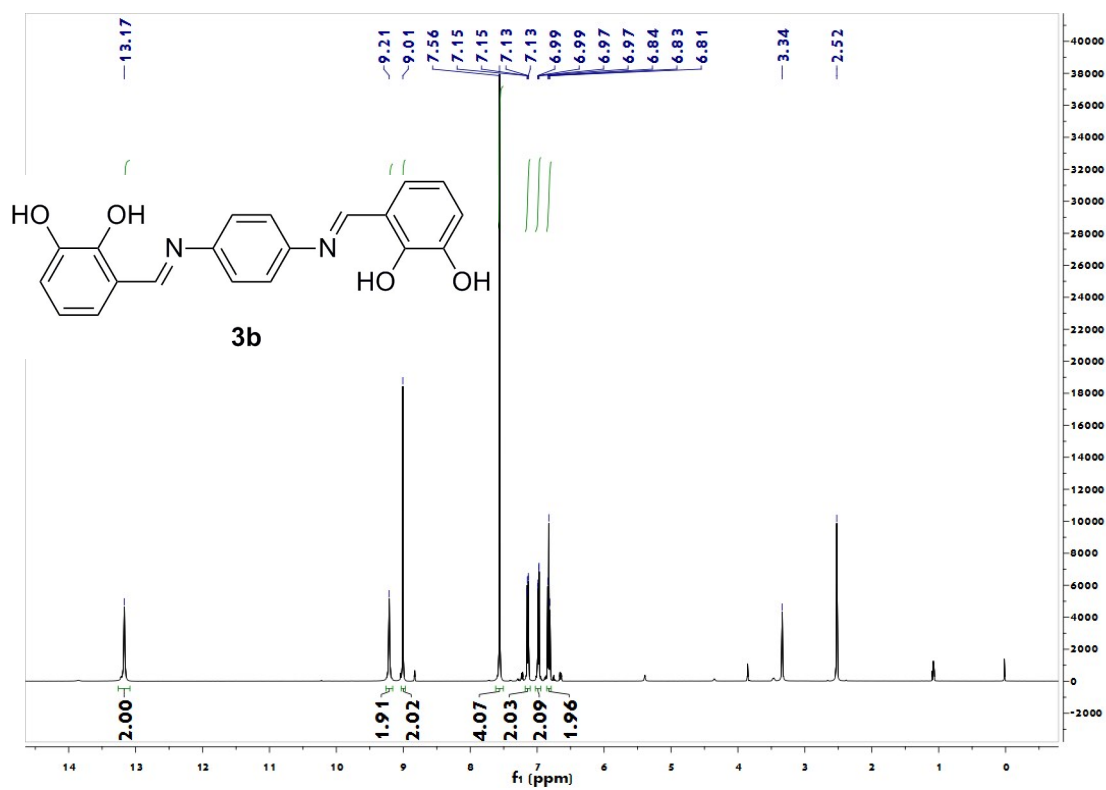
^{13}C NMR of compound **3a** in DMSO



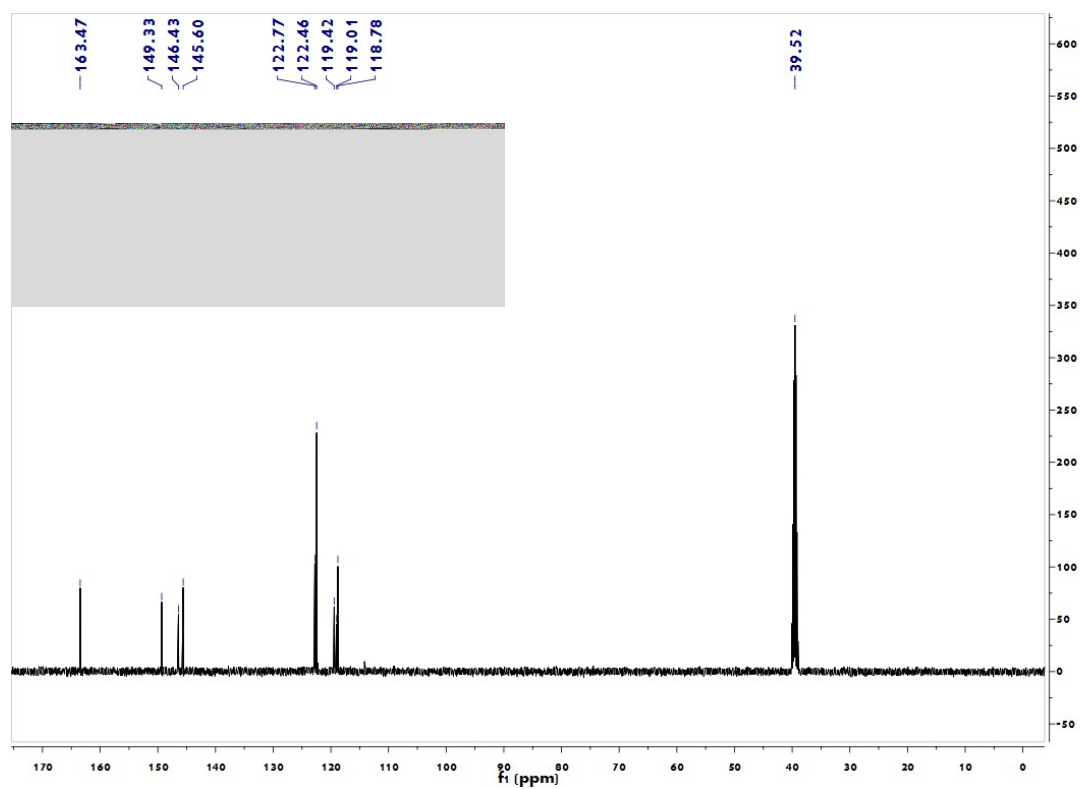
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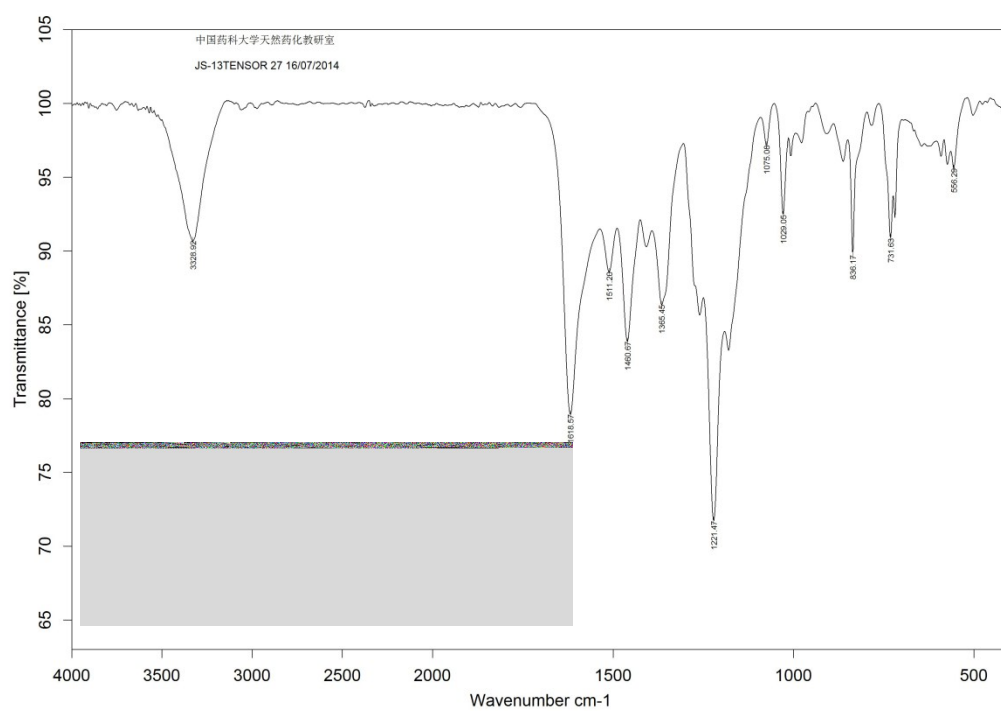
¹H NMR of compound **3b** in DMSO



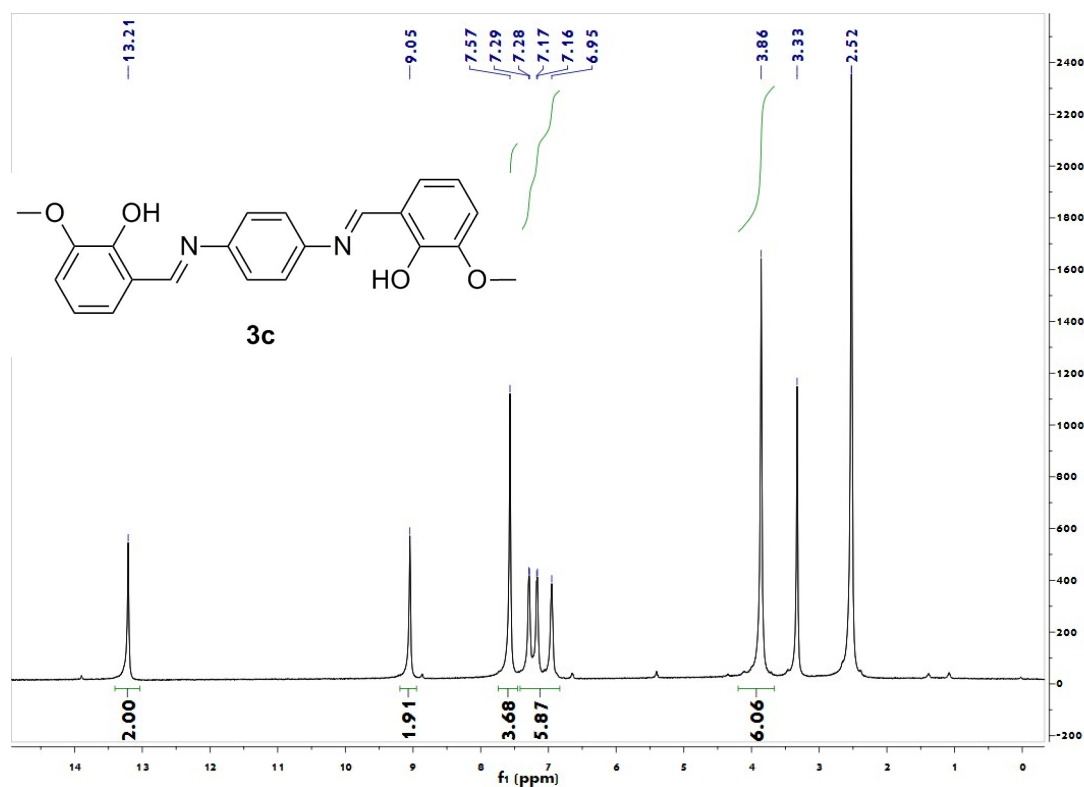
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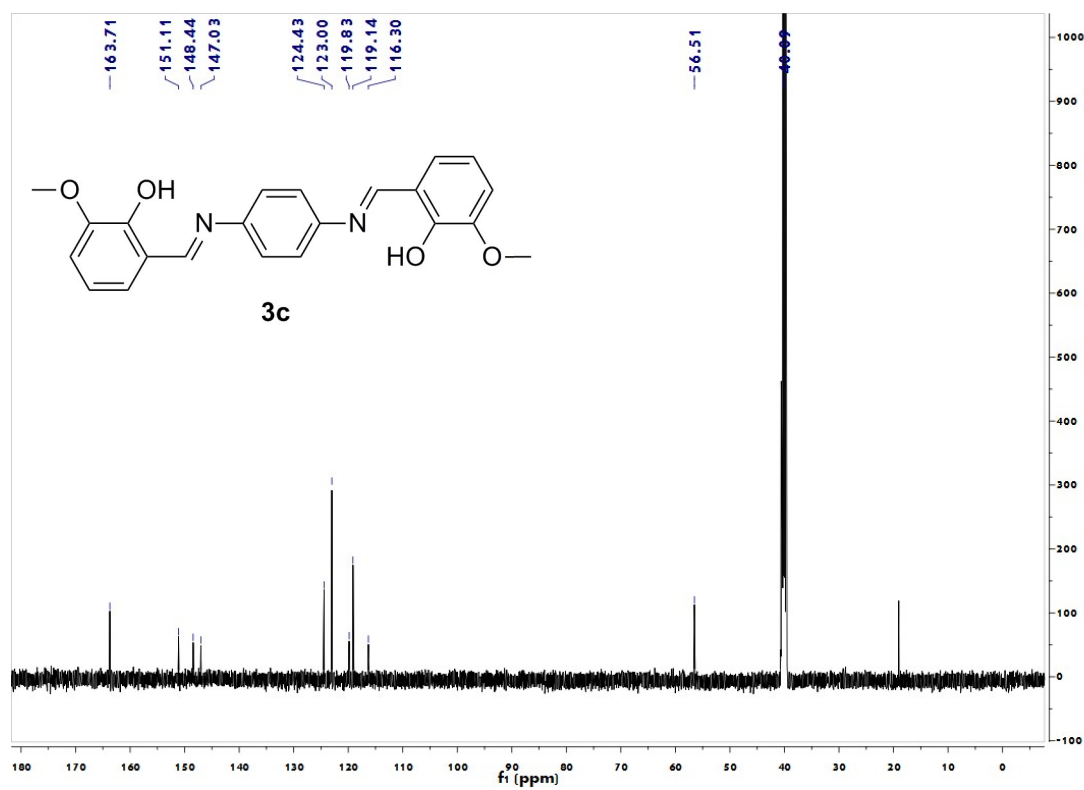
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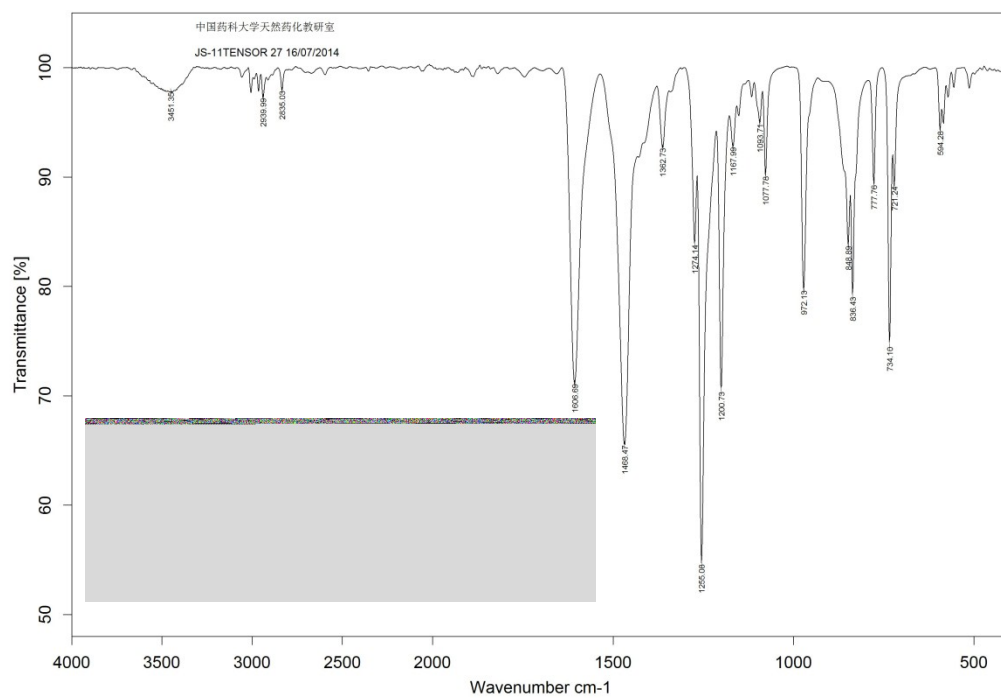
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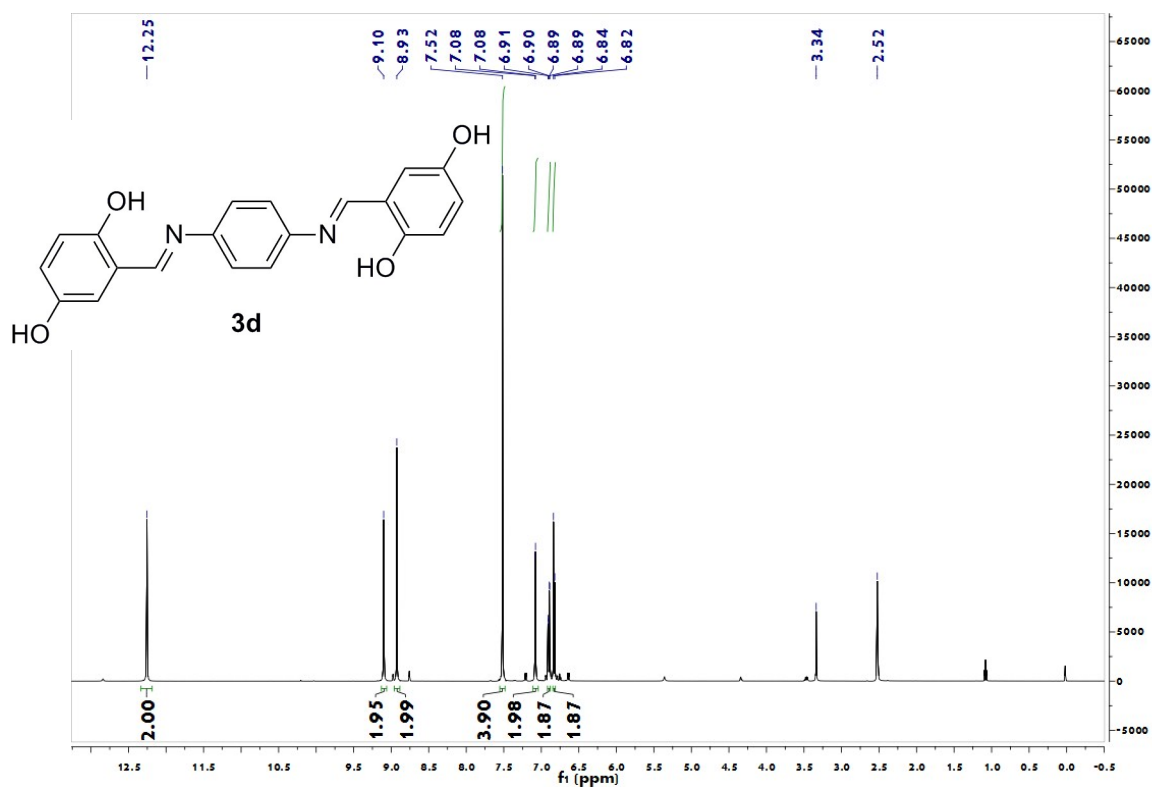
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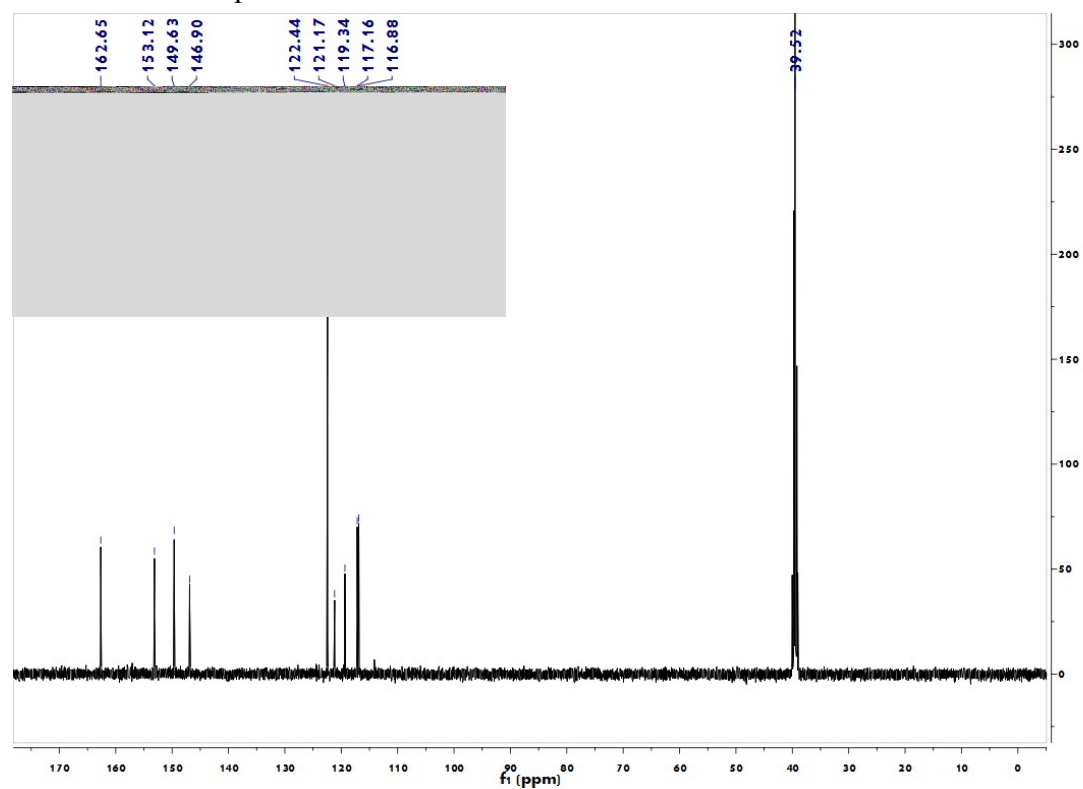
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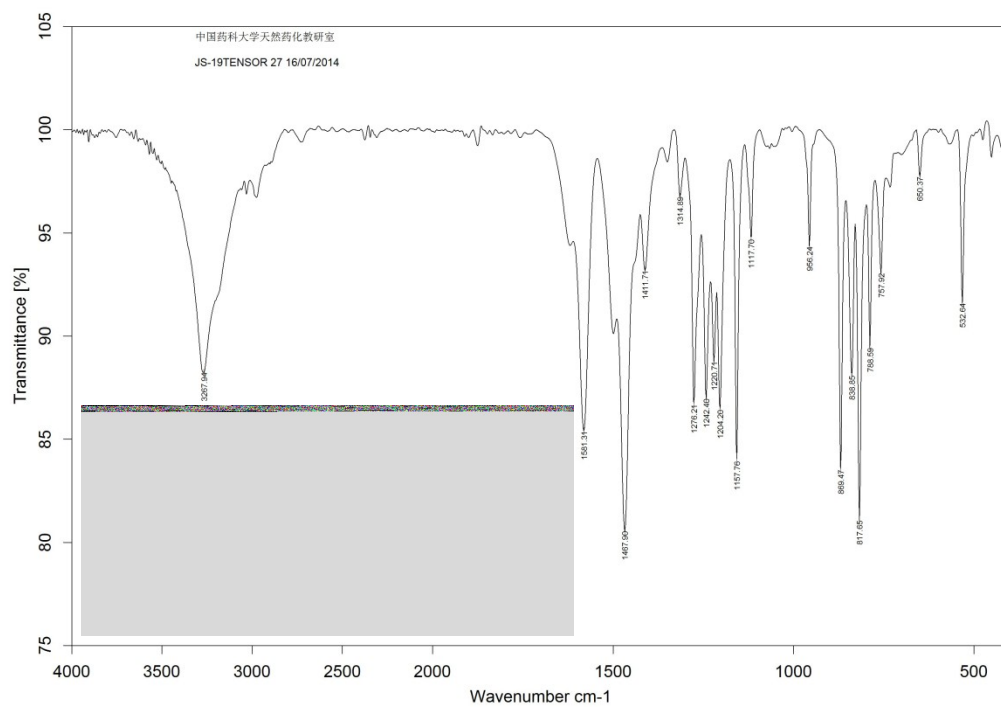
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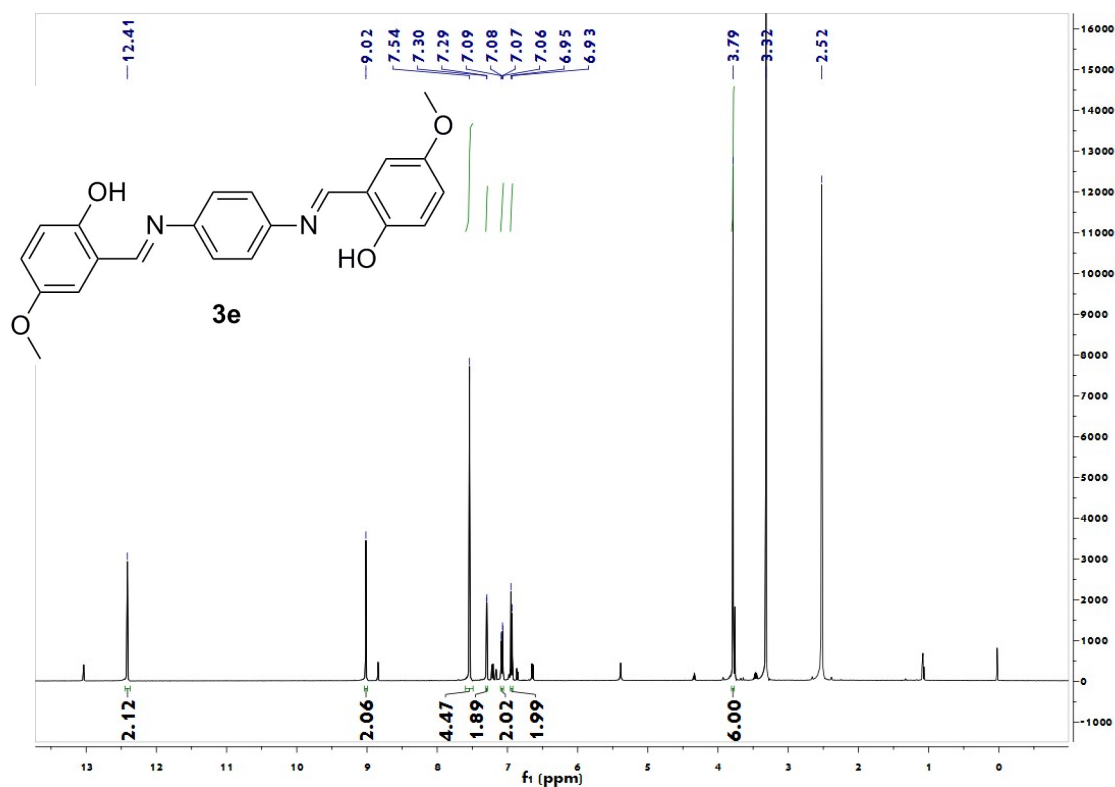
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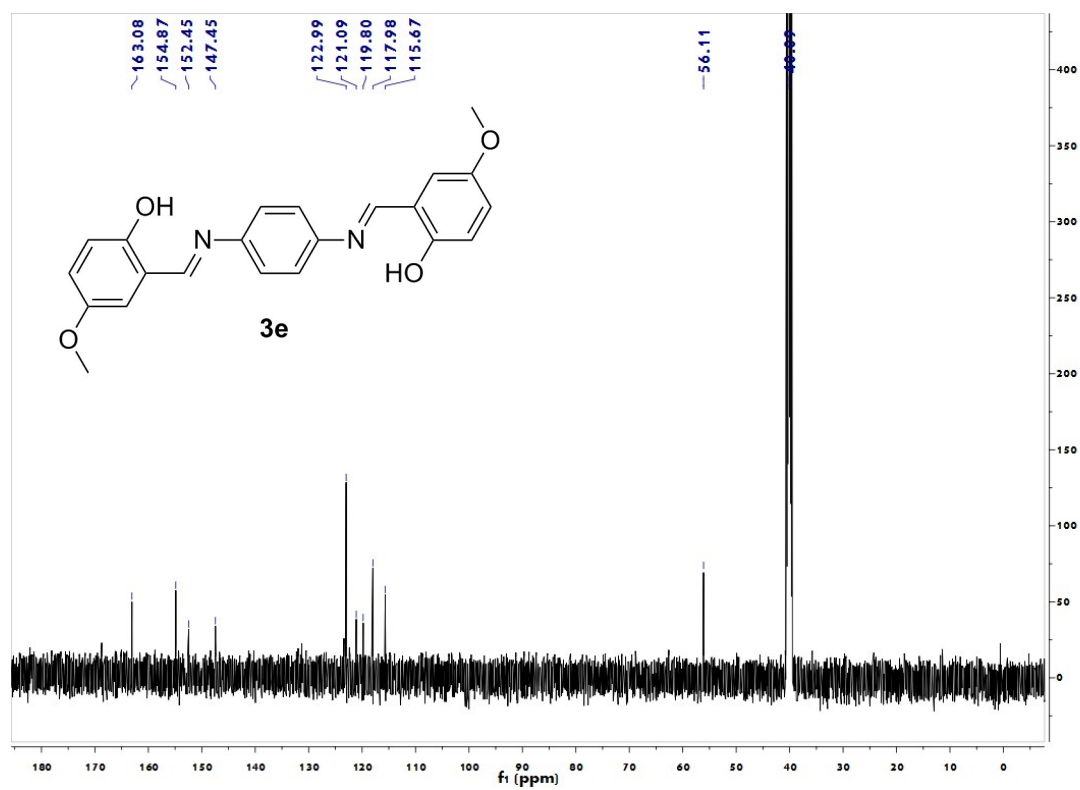
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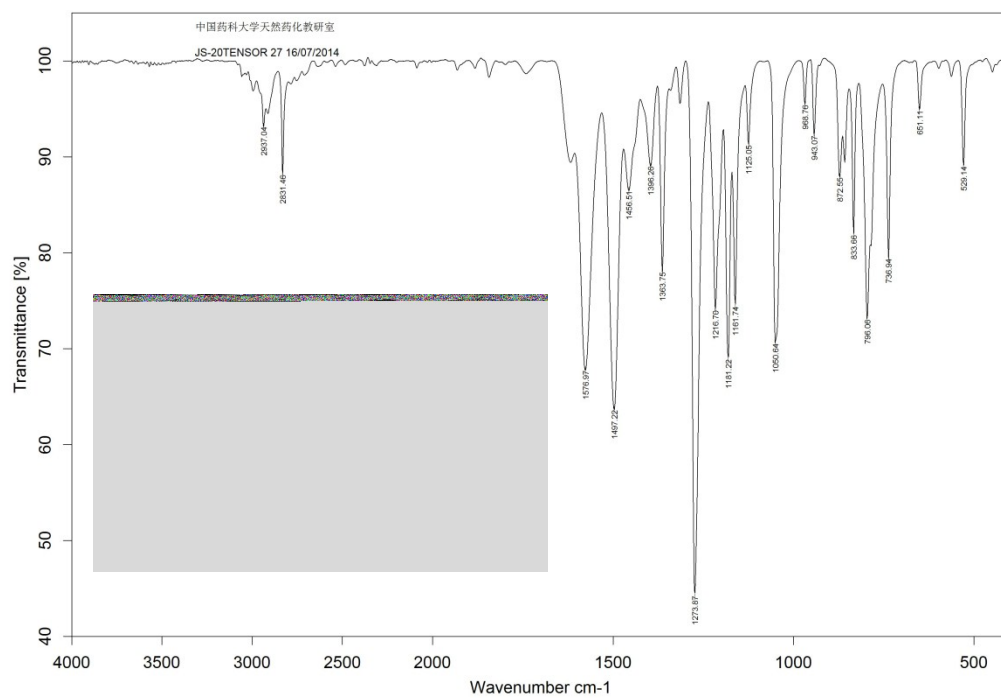
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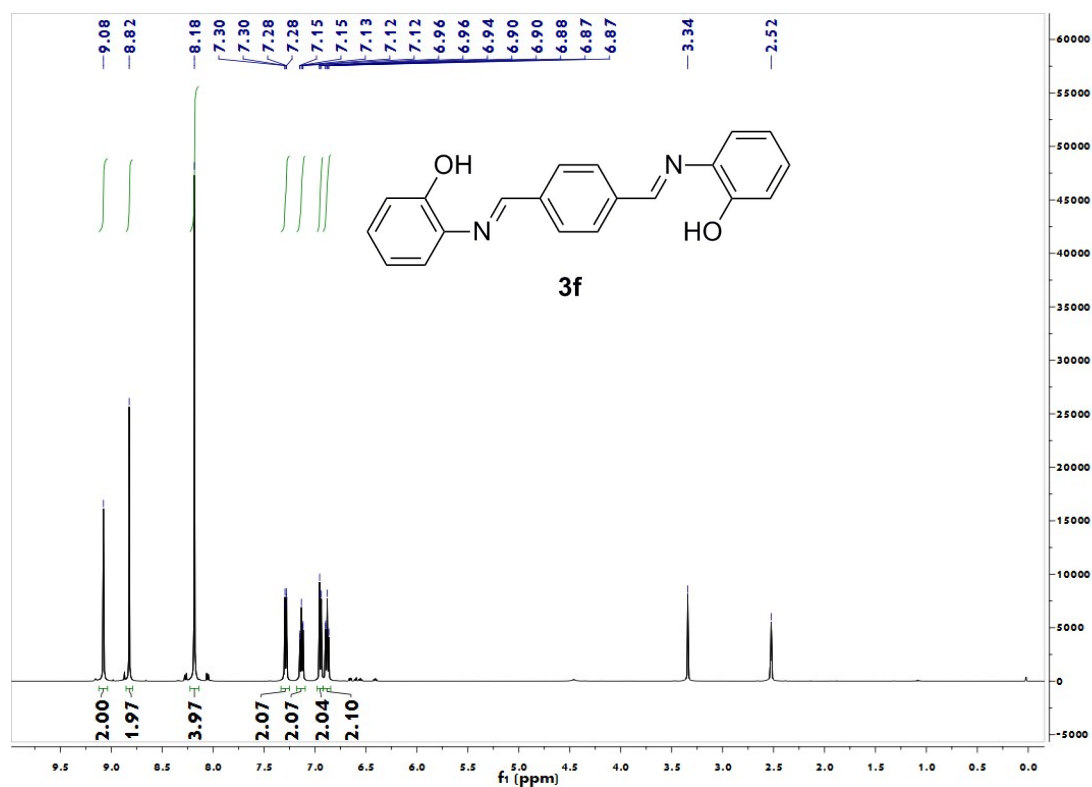
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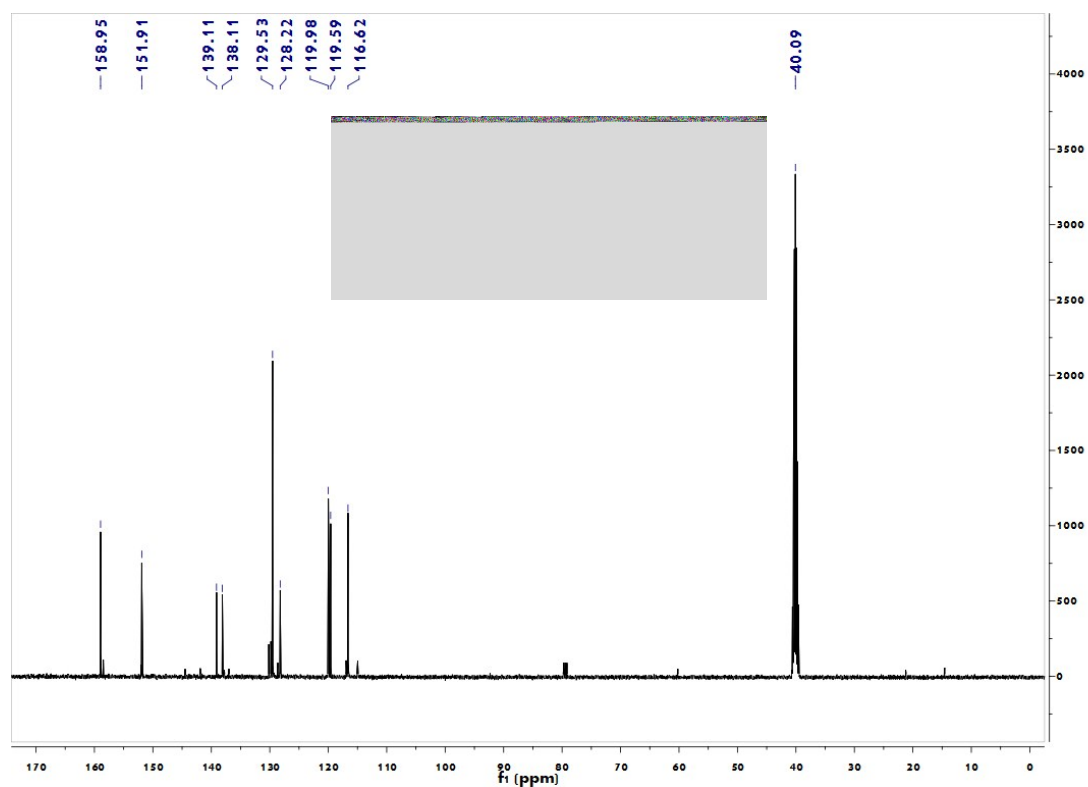
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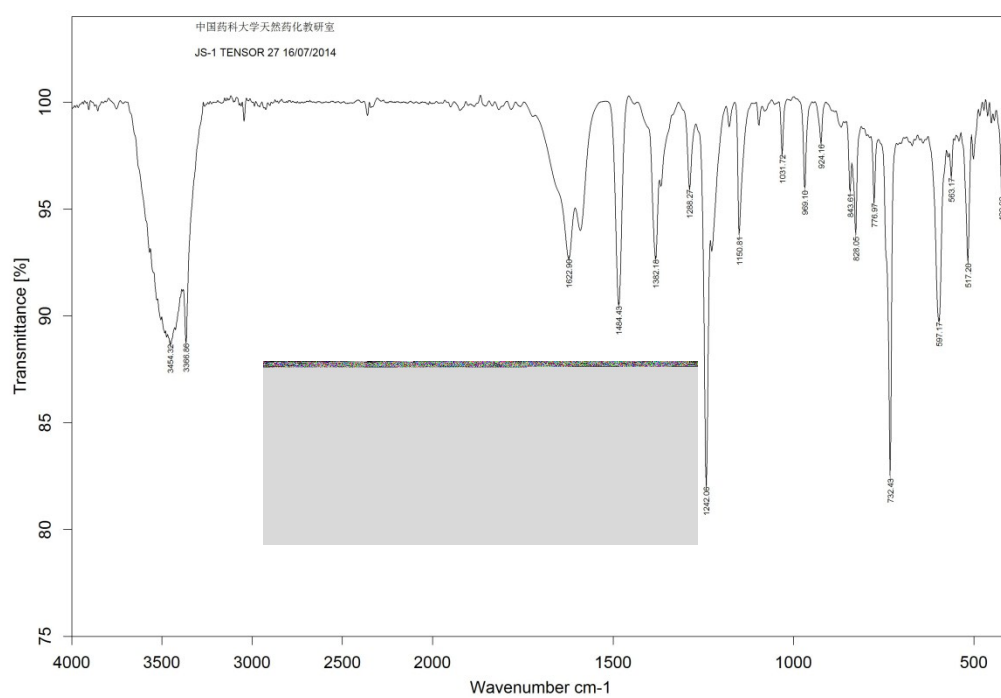
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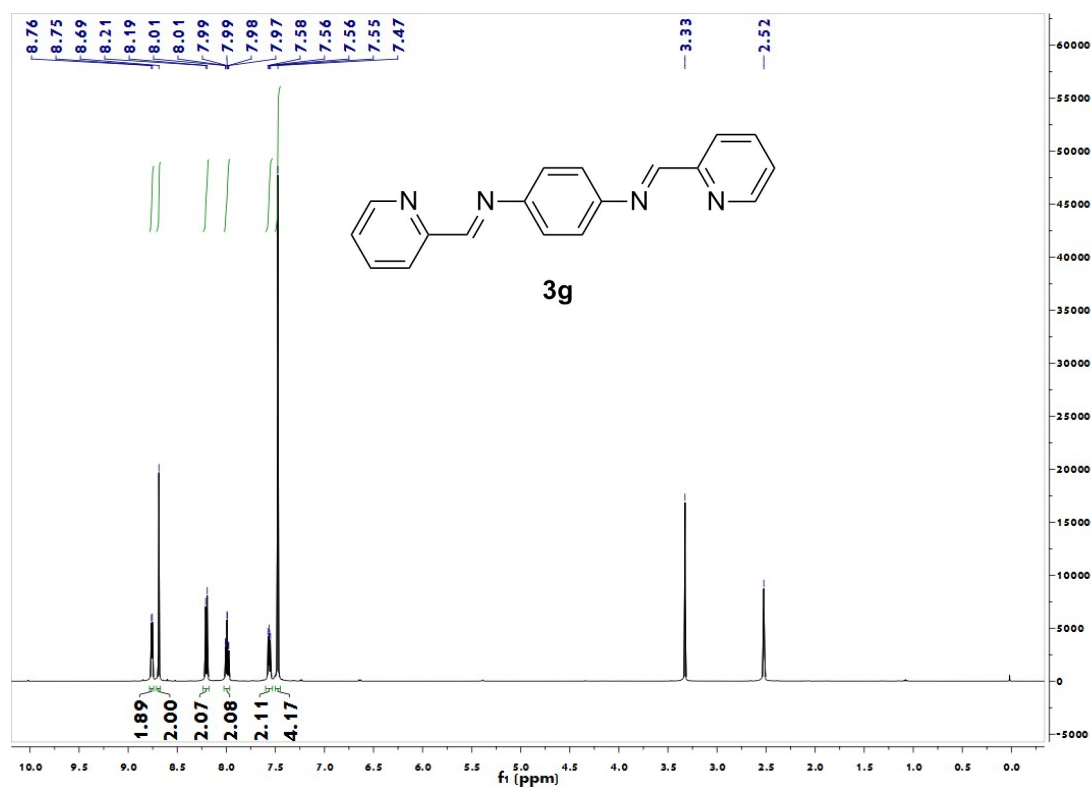
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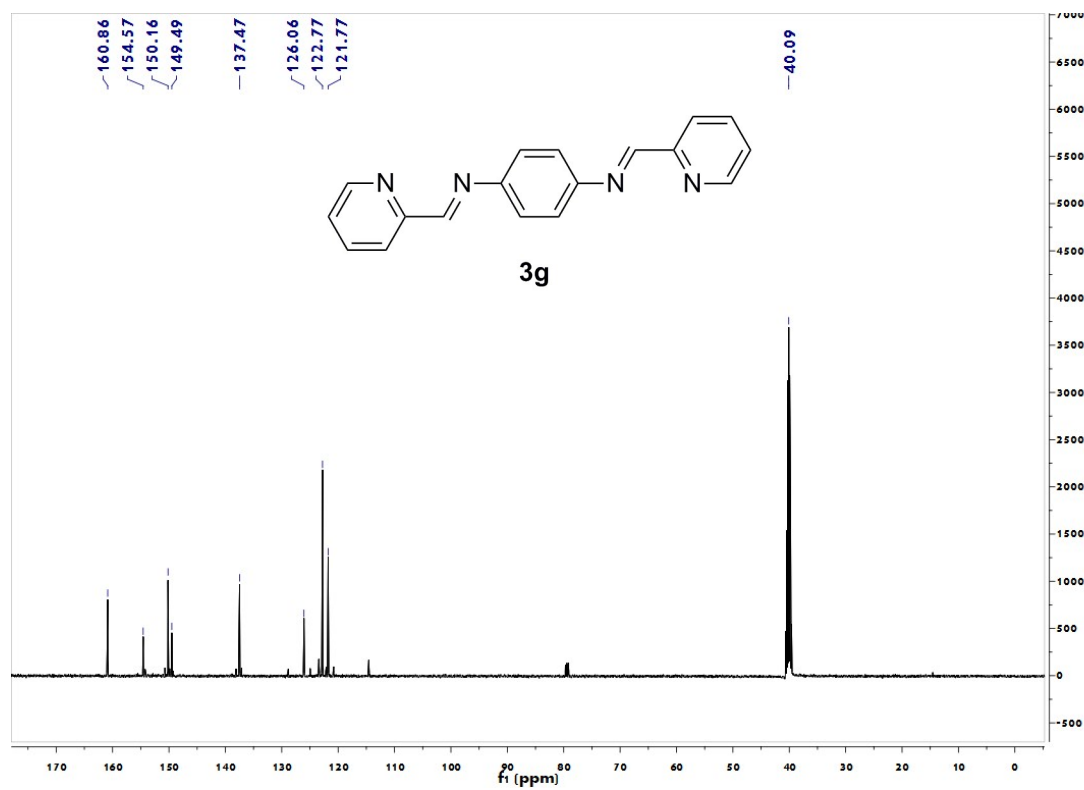
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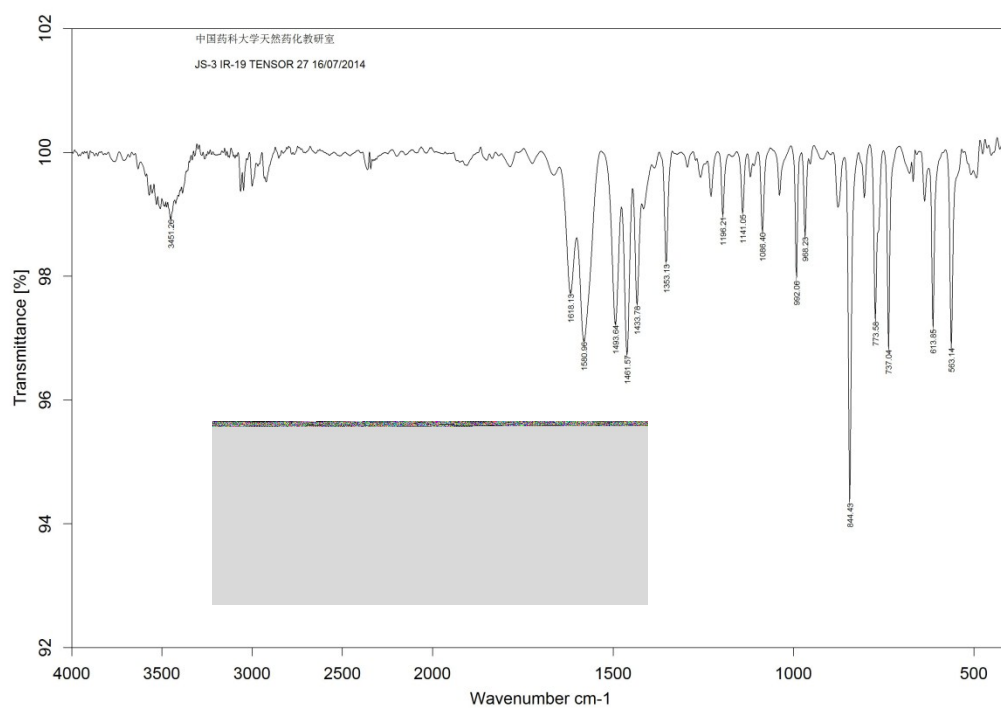
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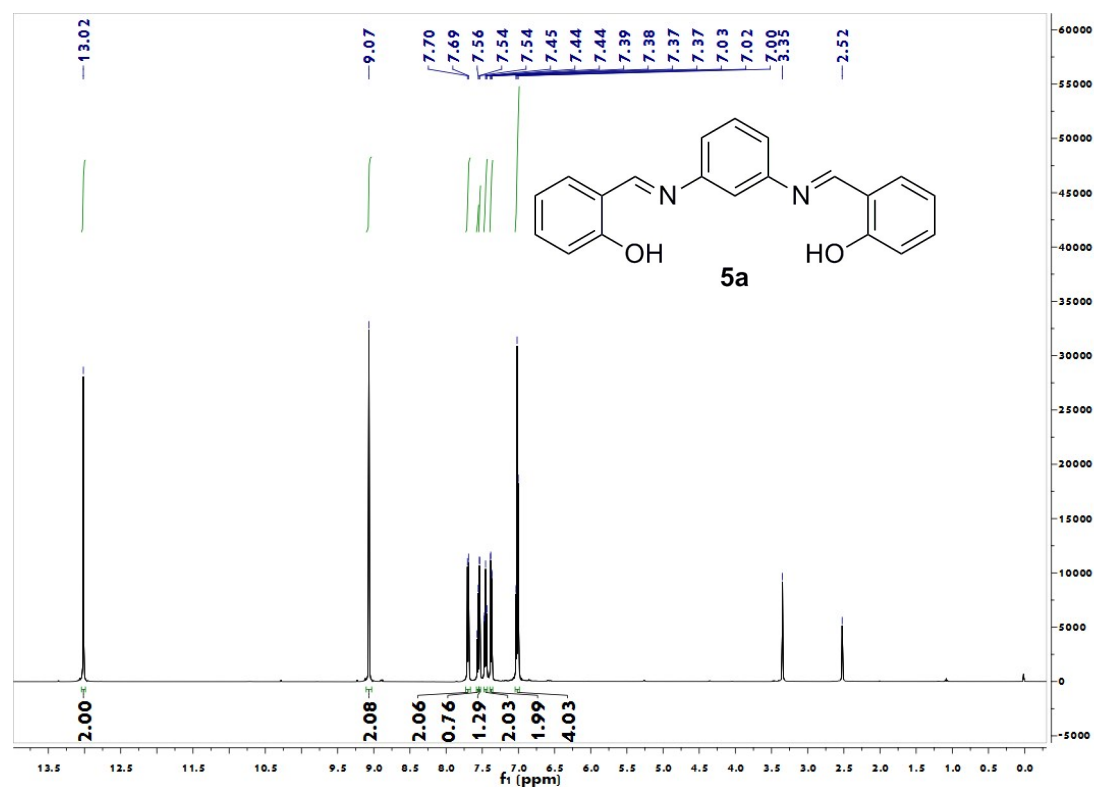
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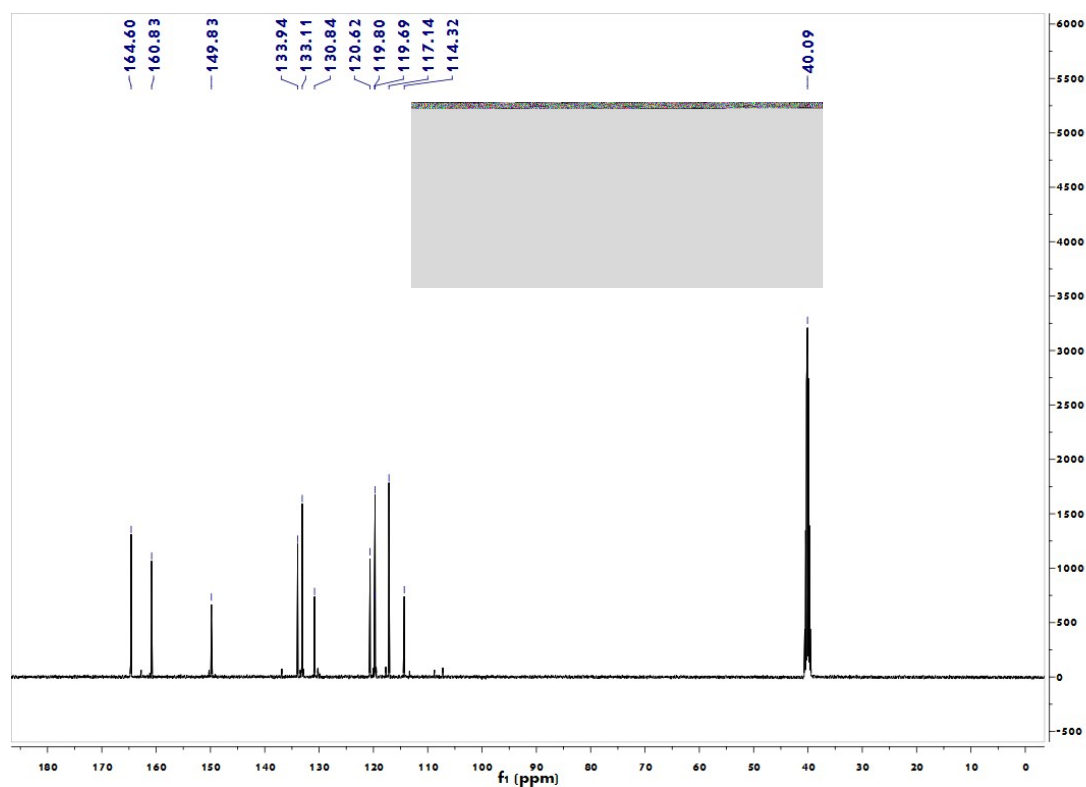
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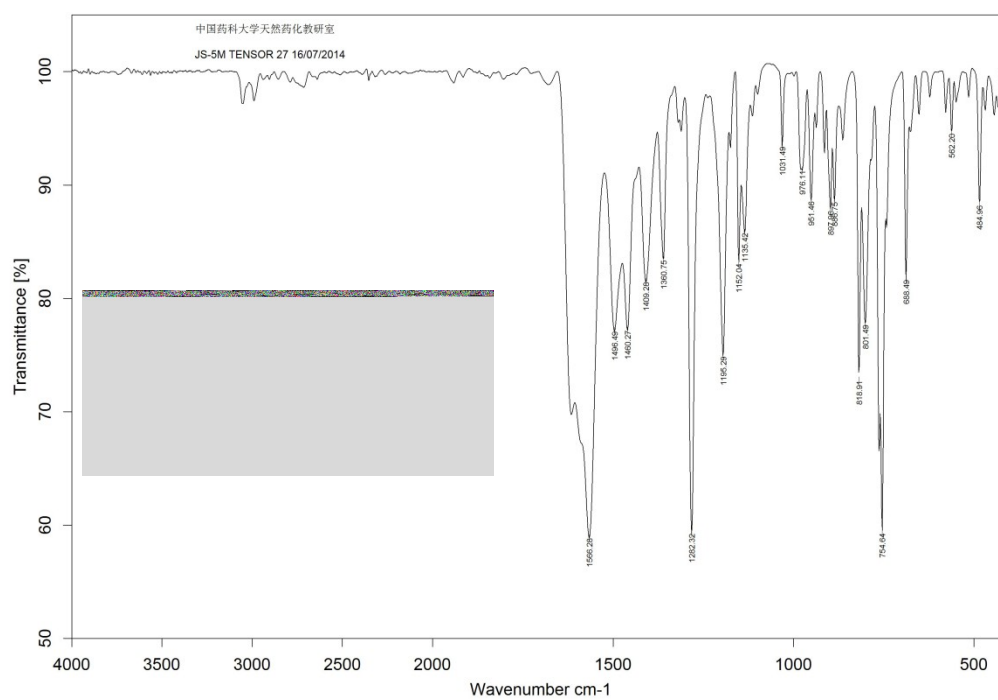
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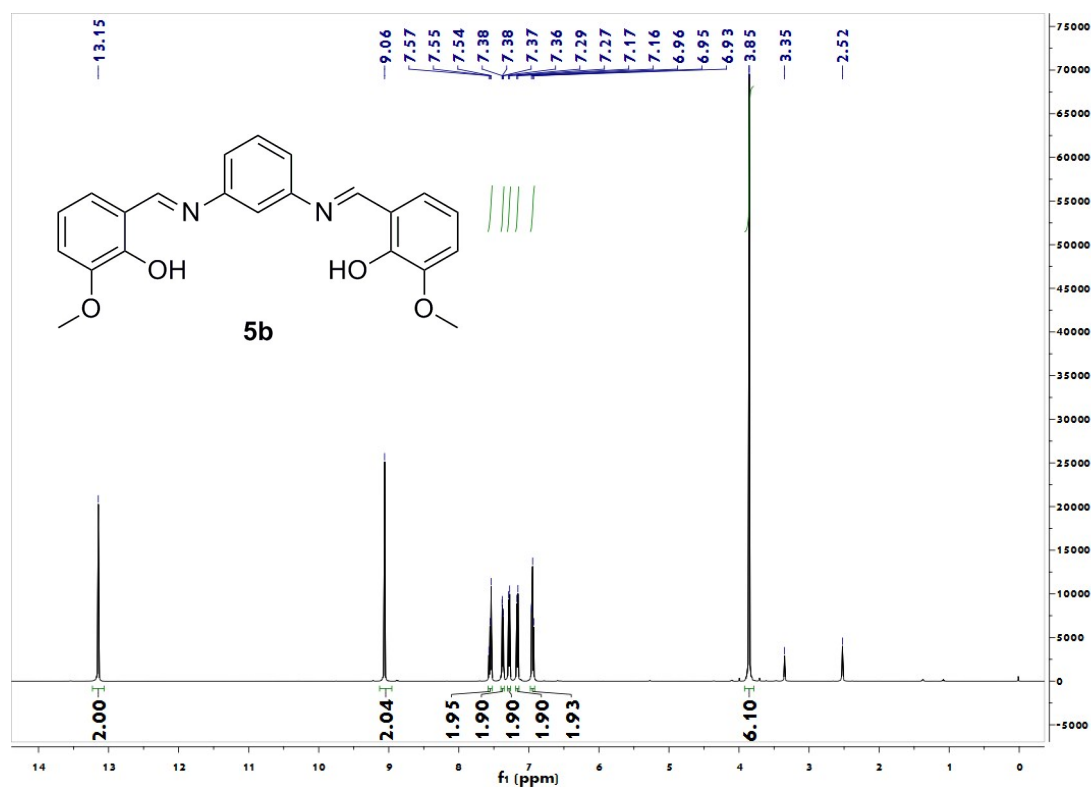
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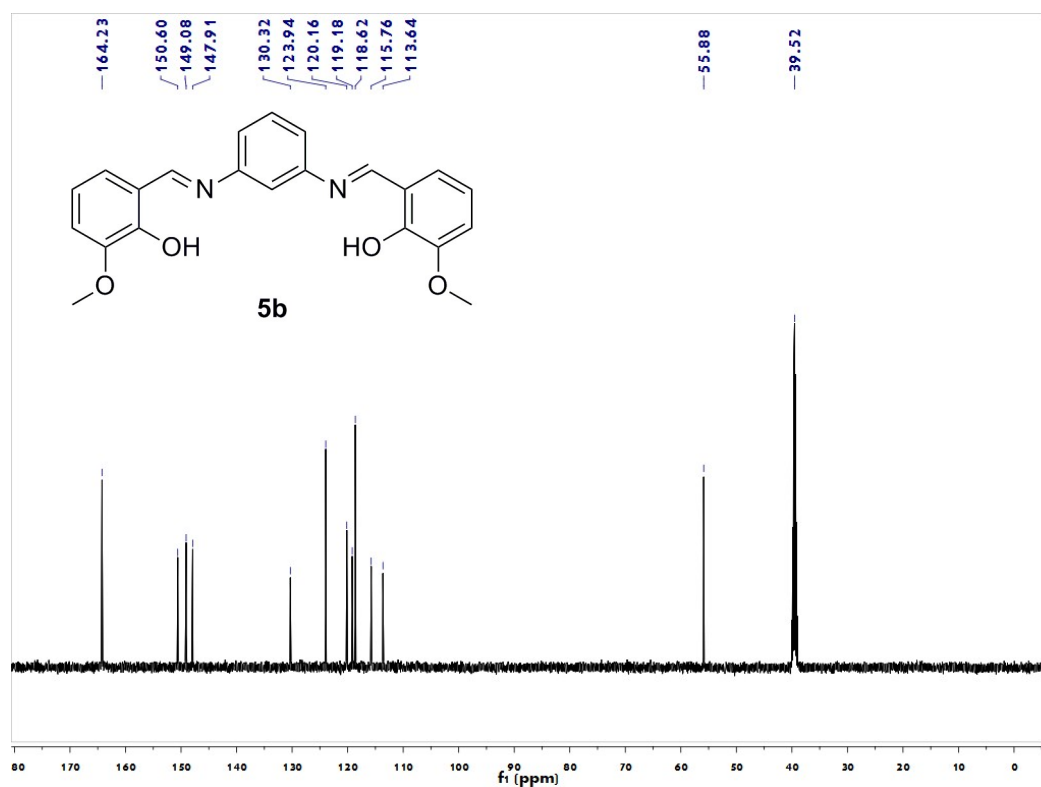
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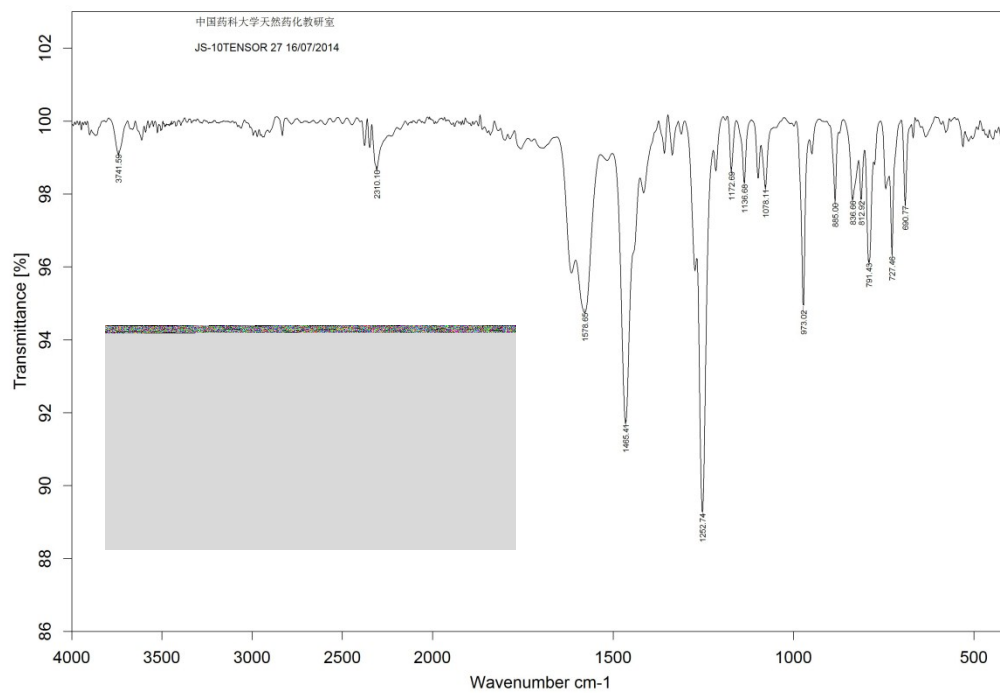
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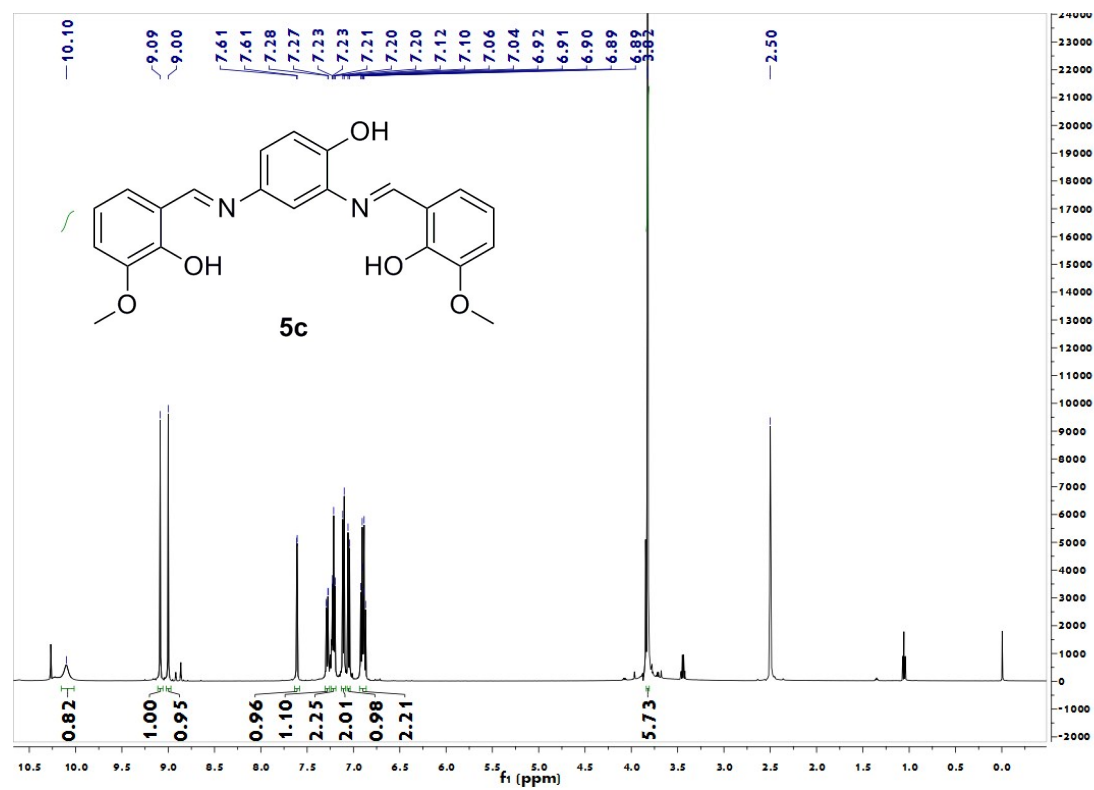
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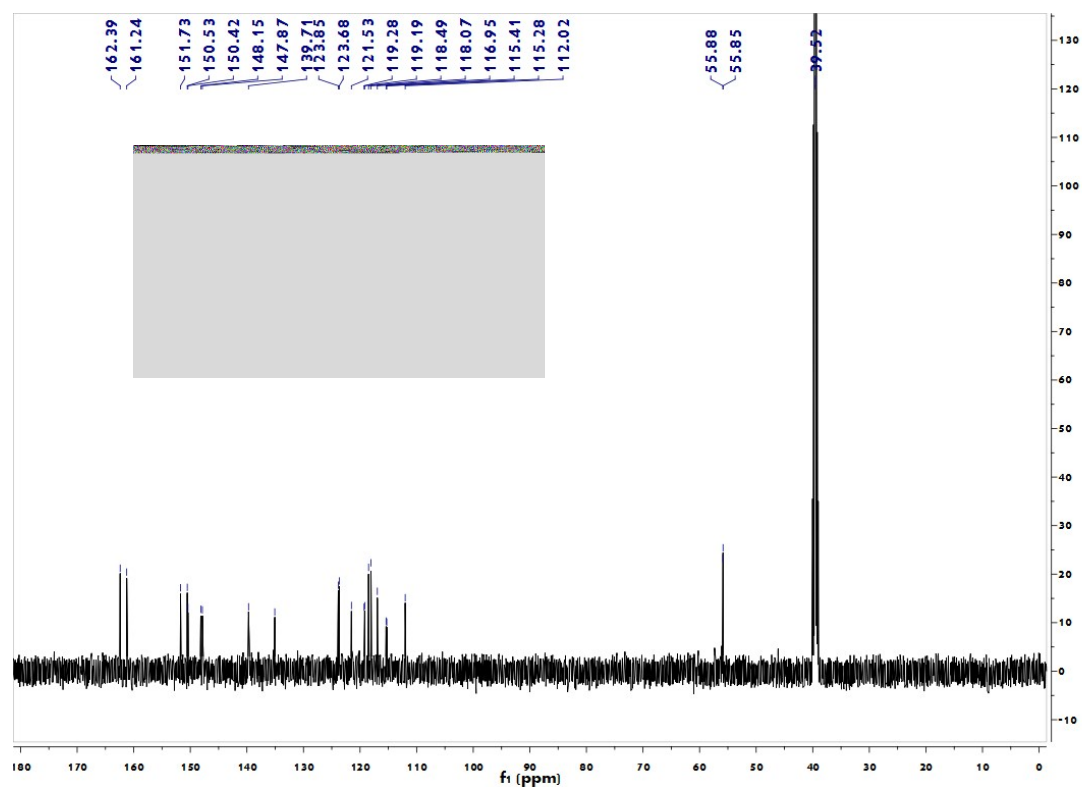
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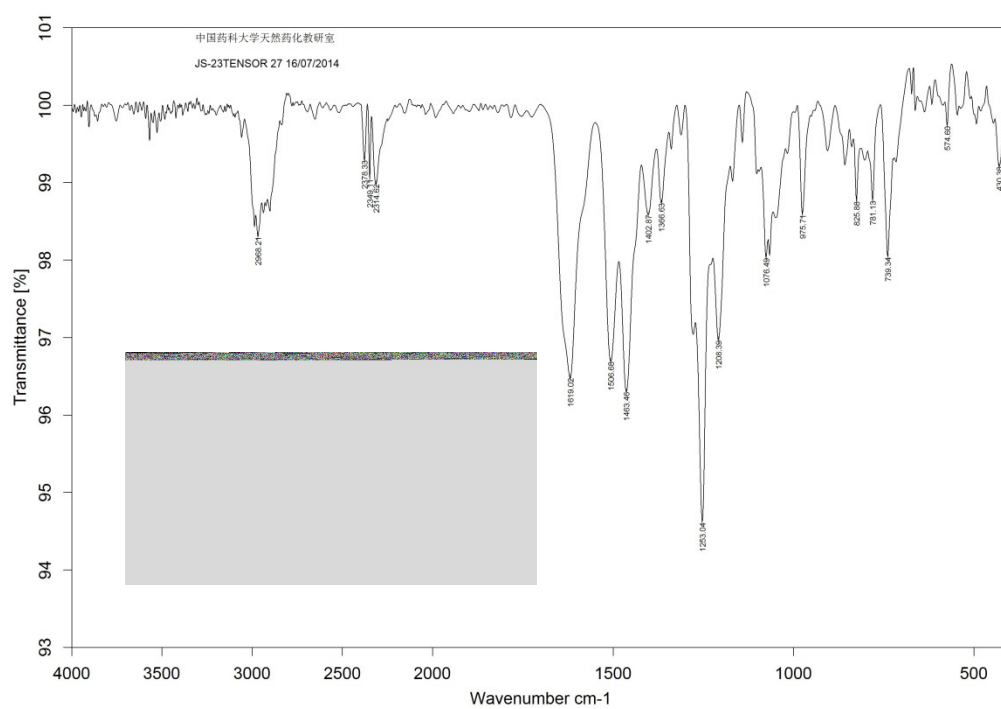
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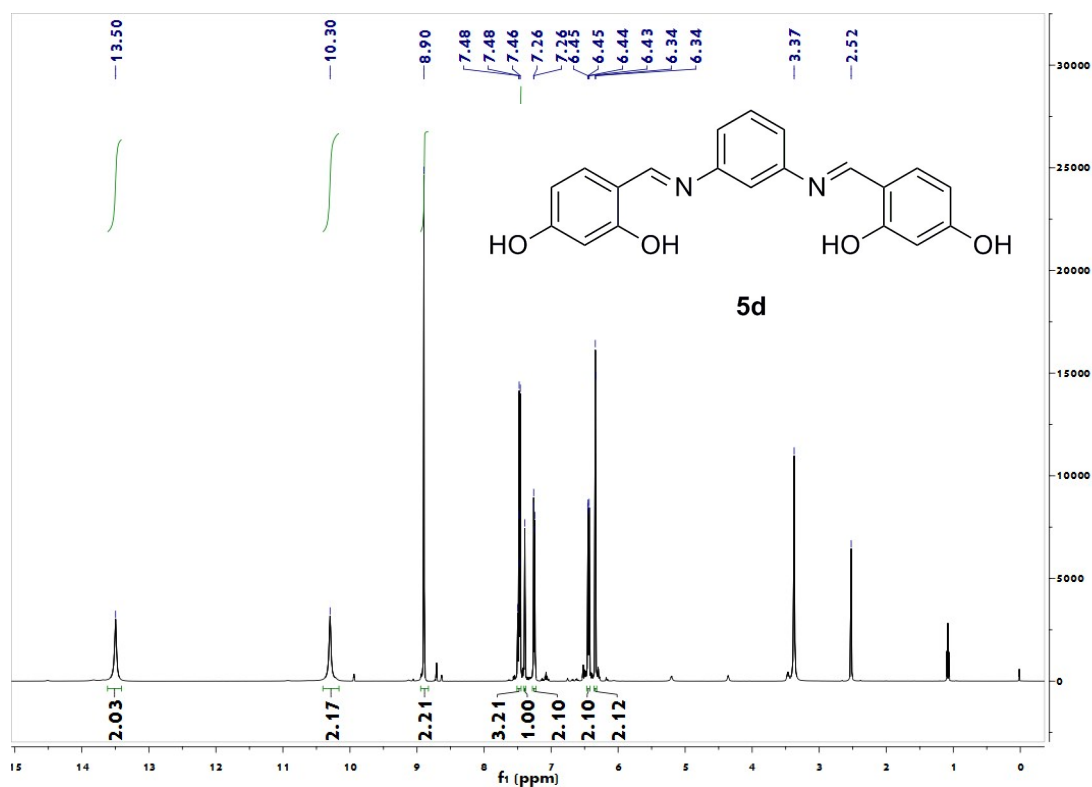
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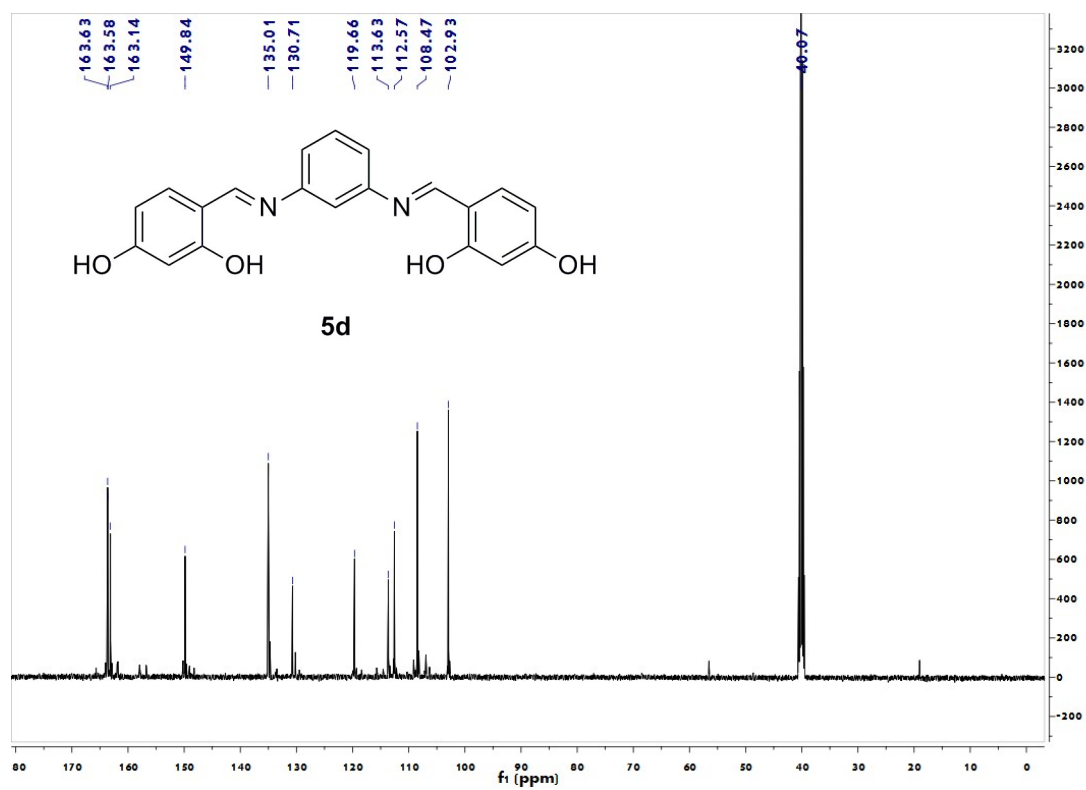
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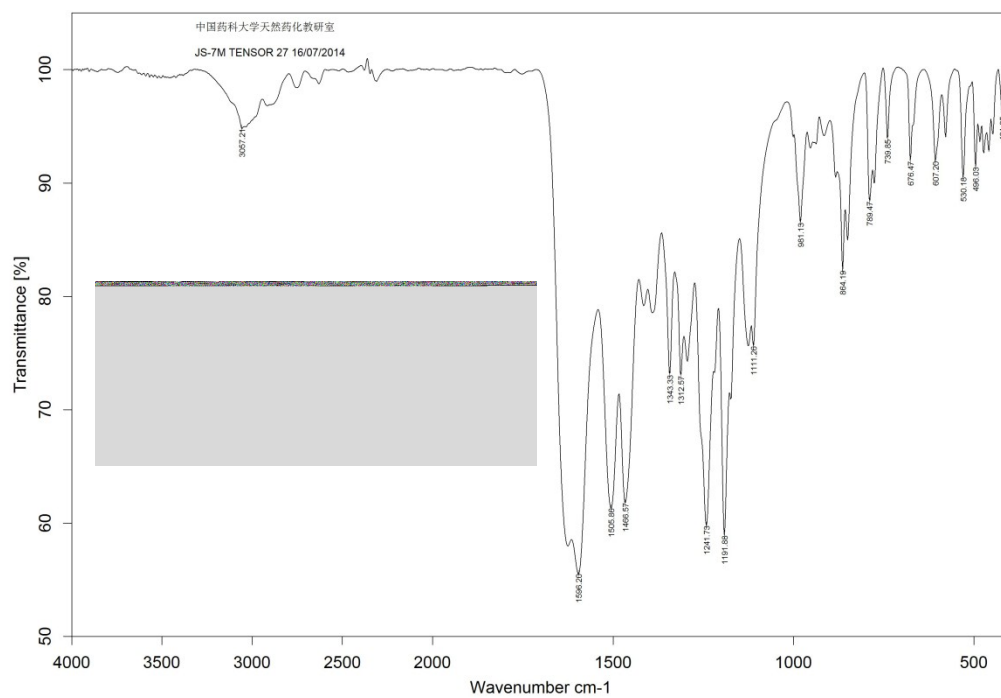
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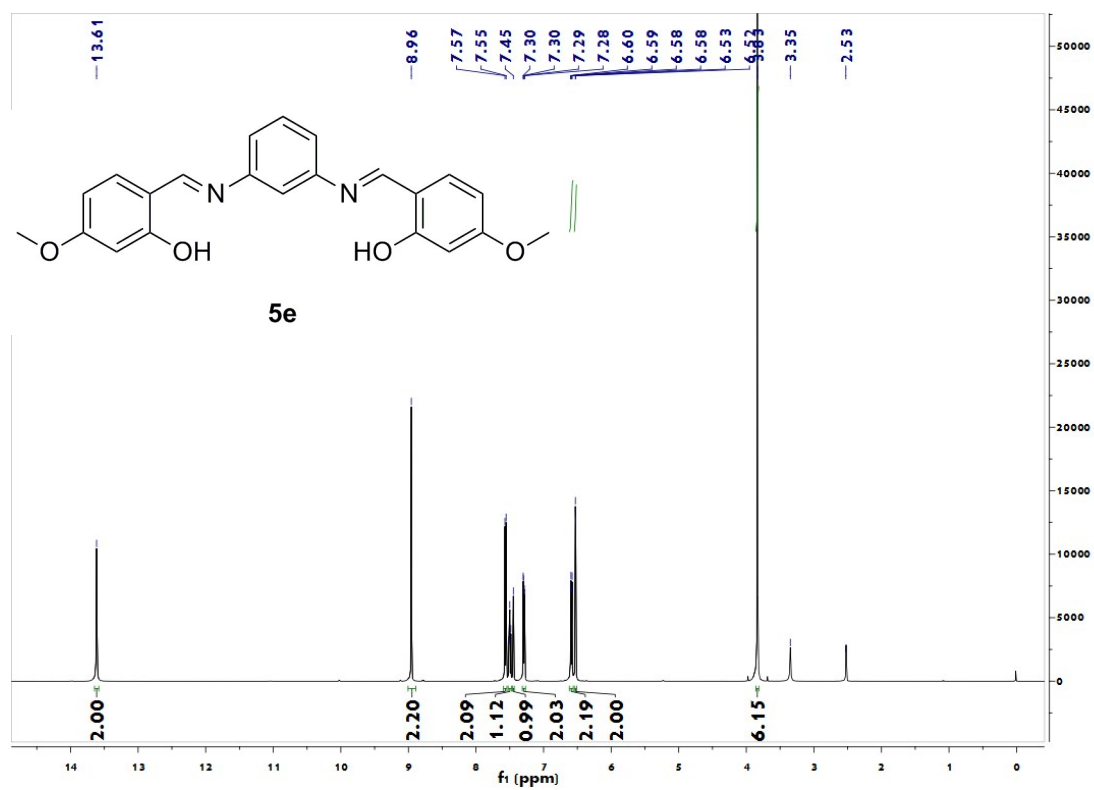
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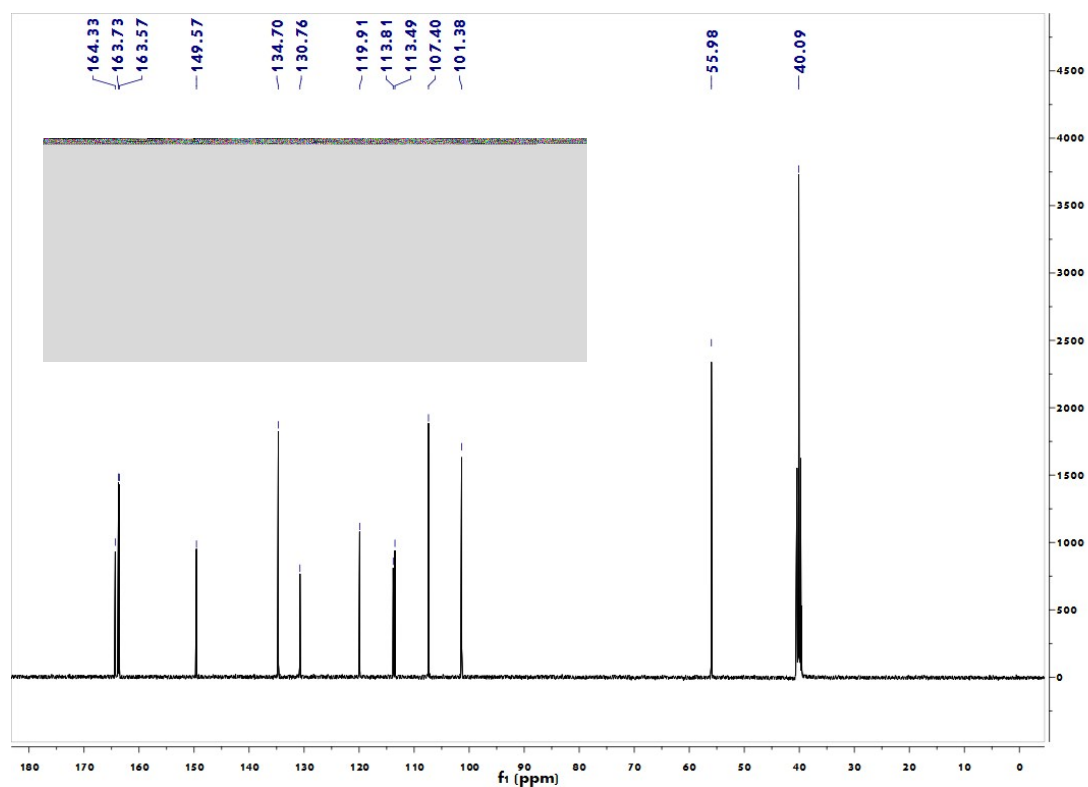
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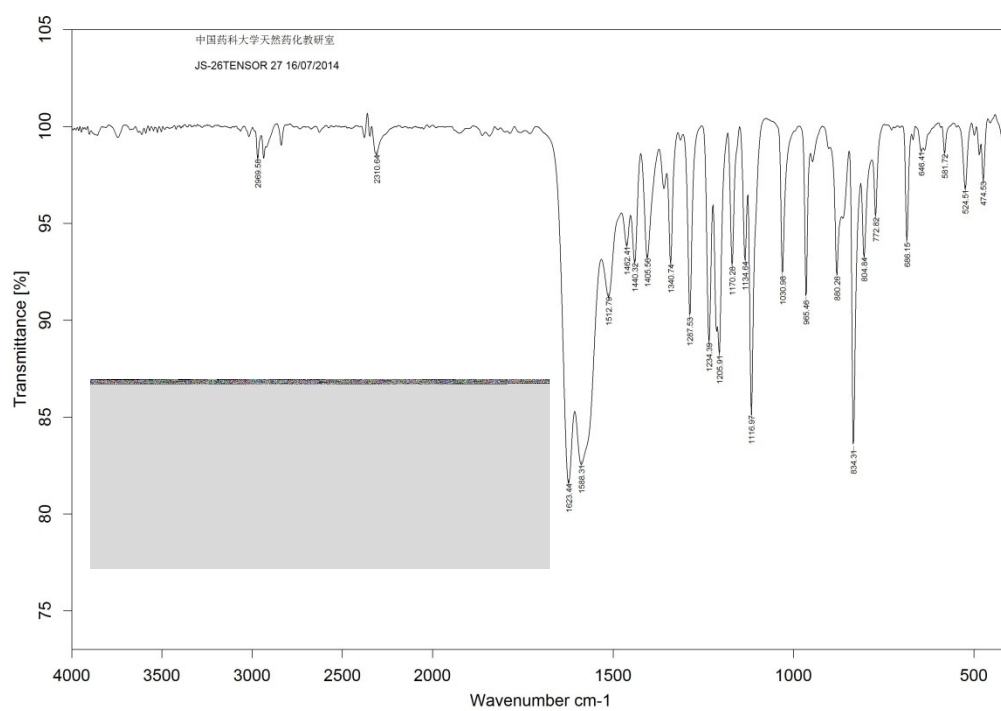
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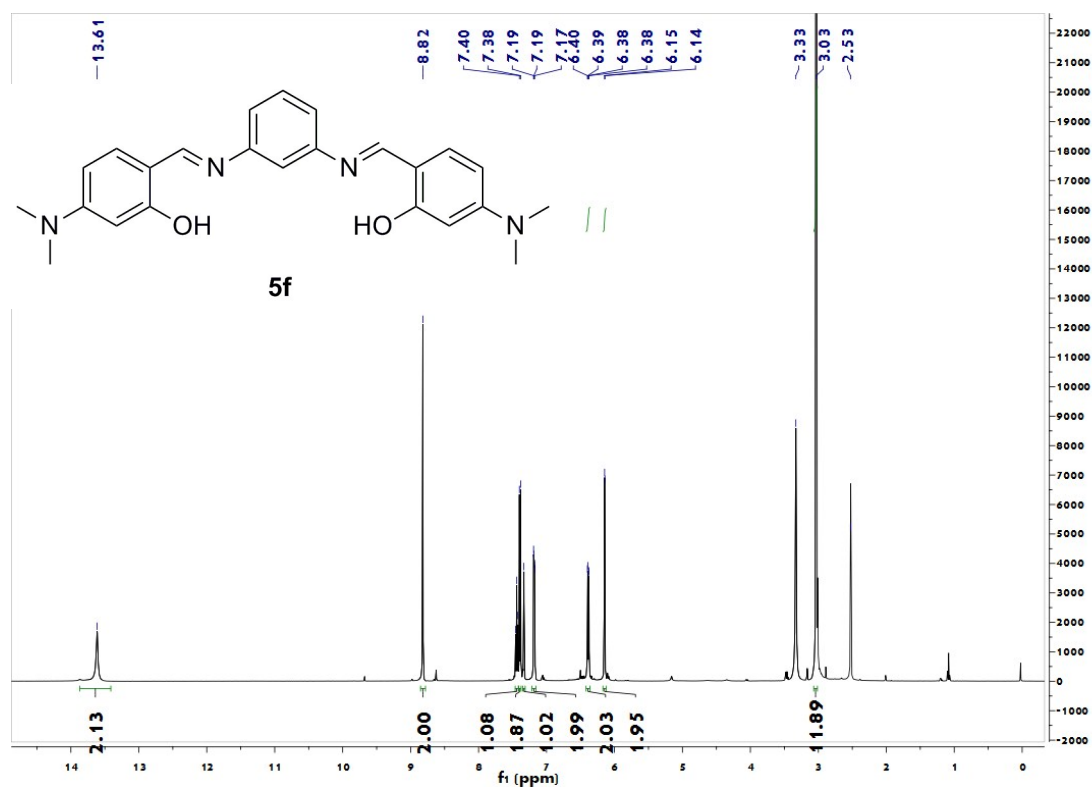
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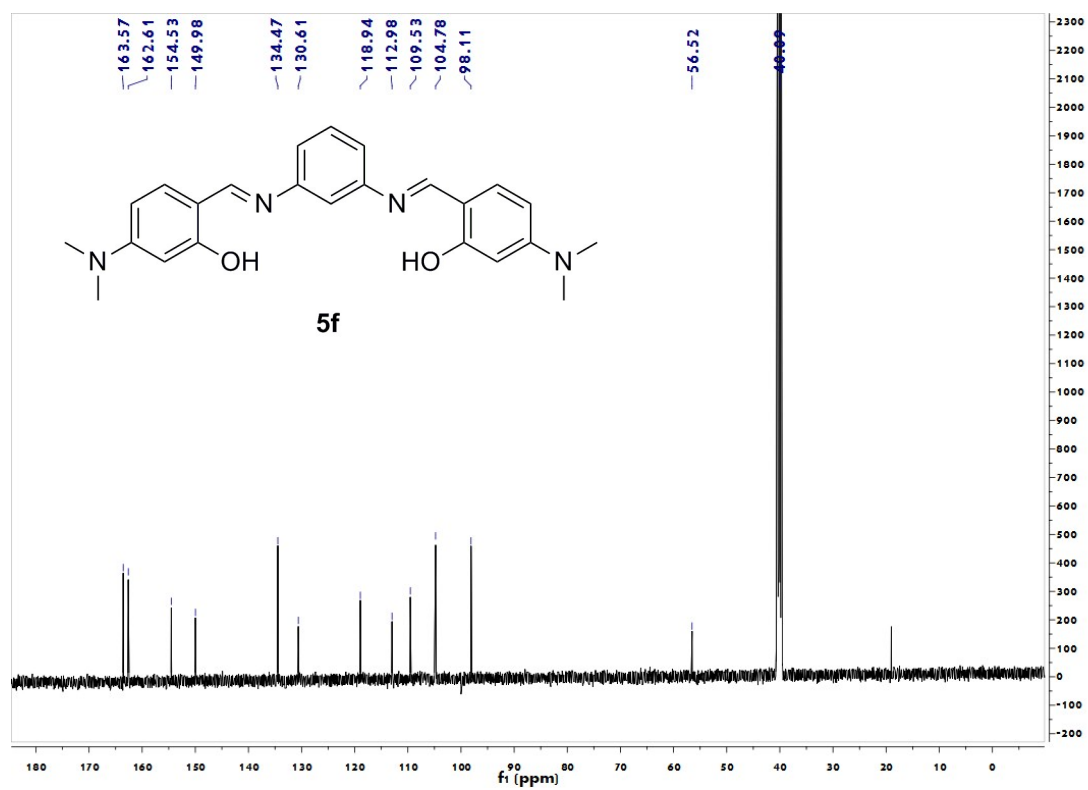
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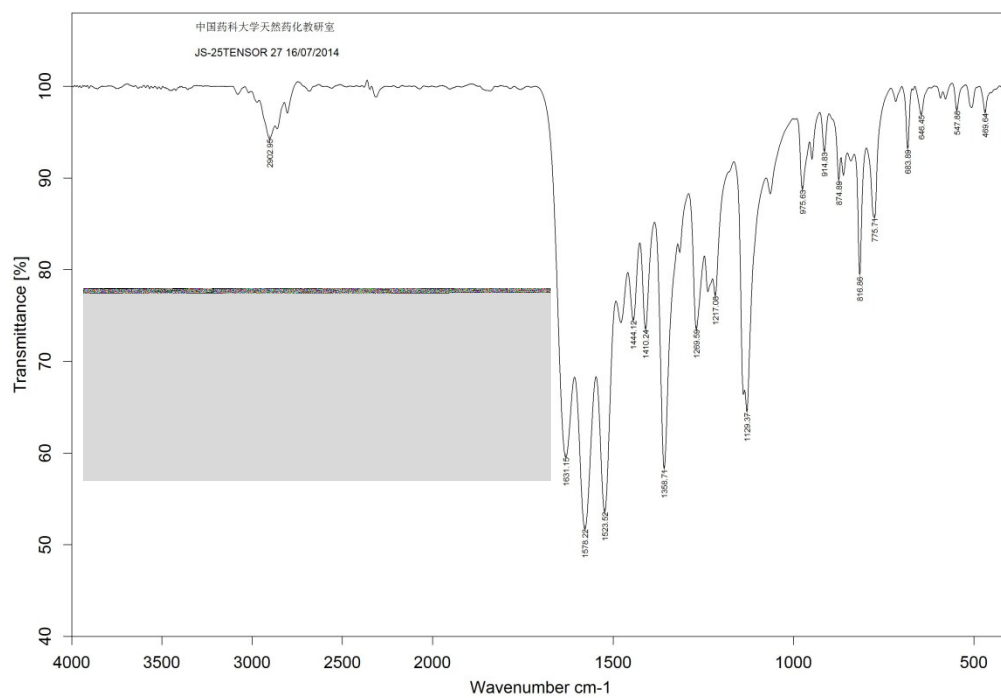
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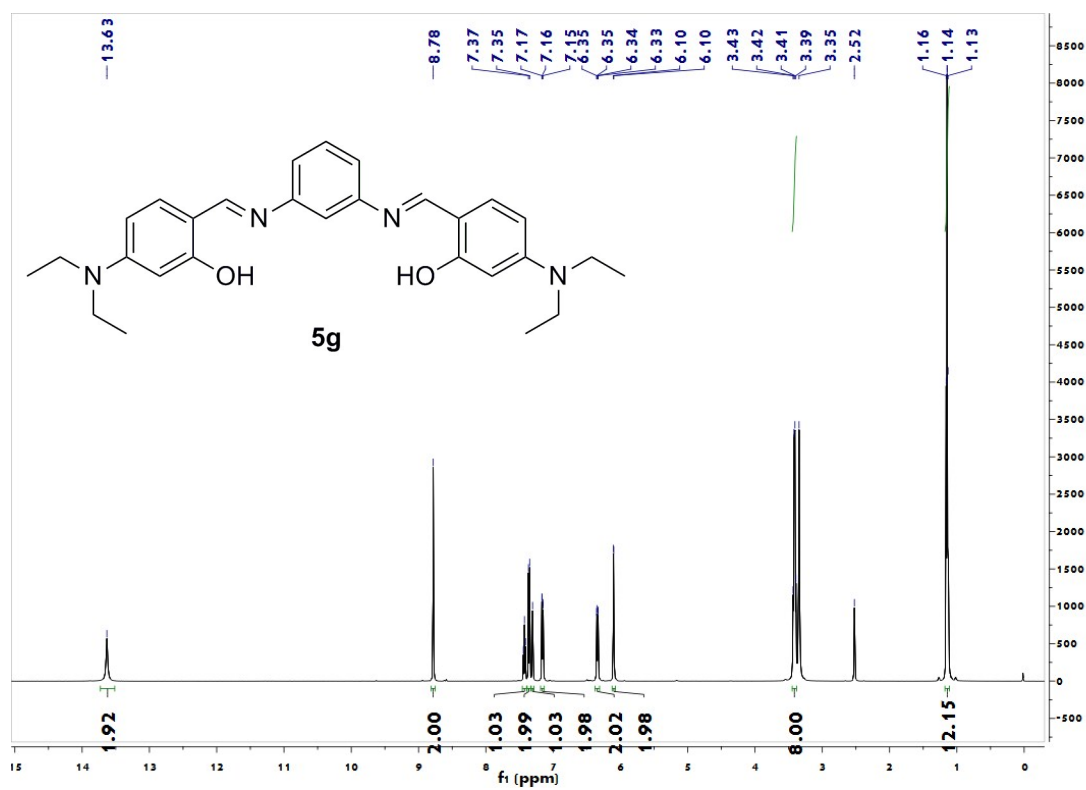
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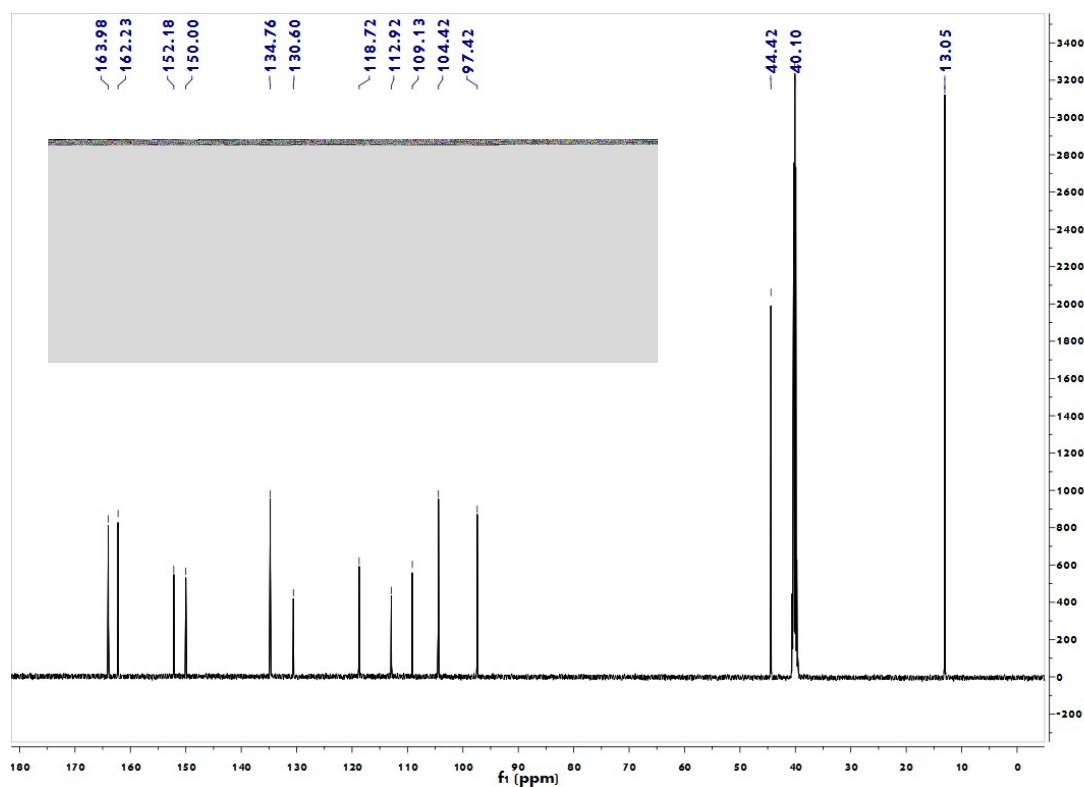
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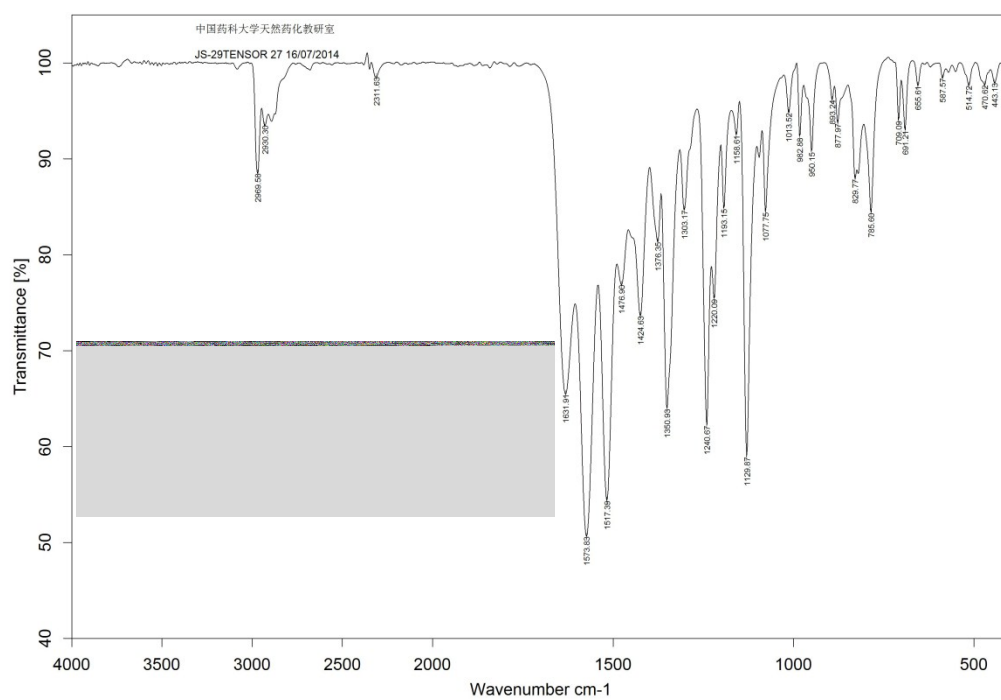
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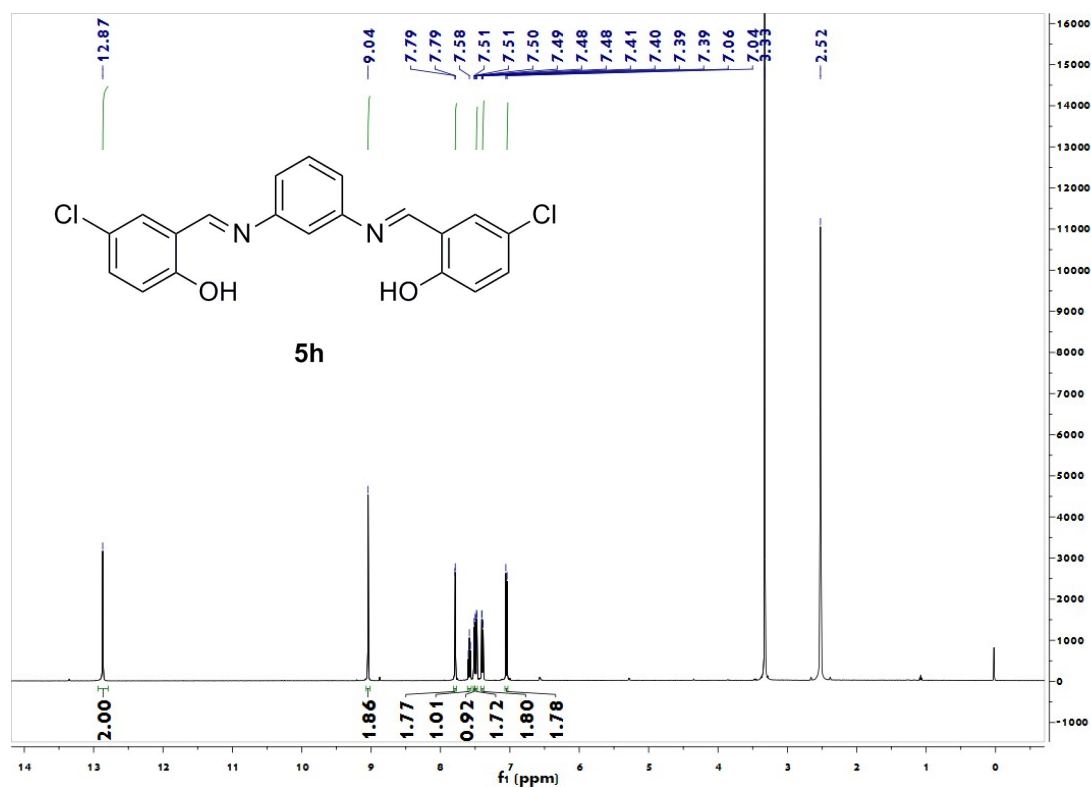
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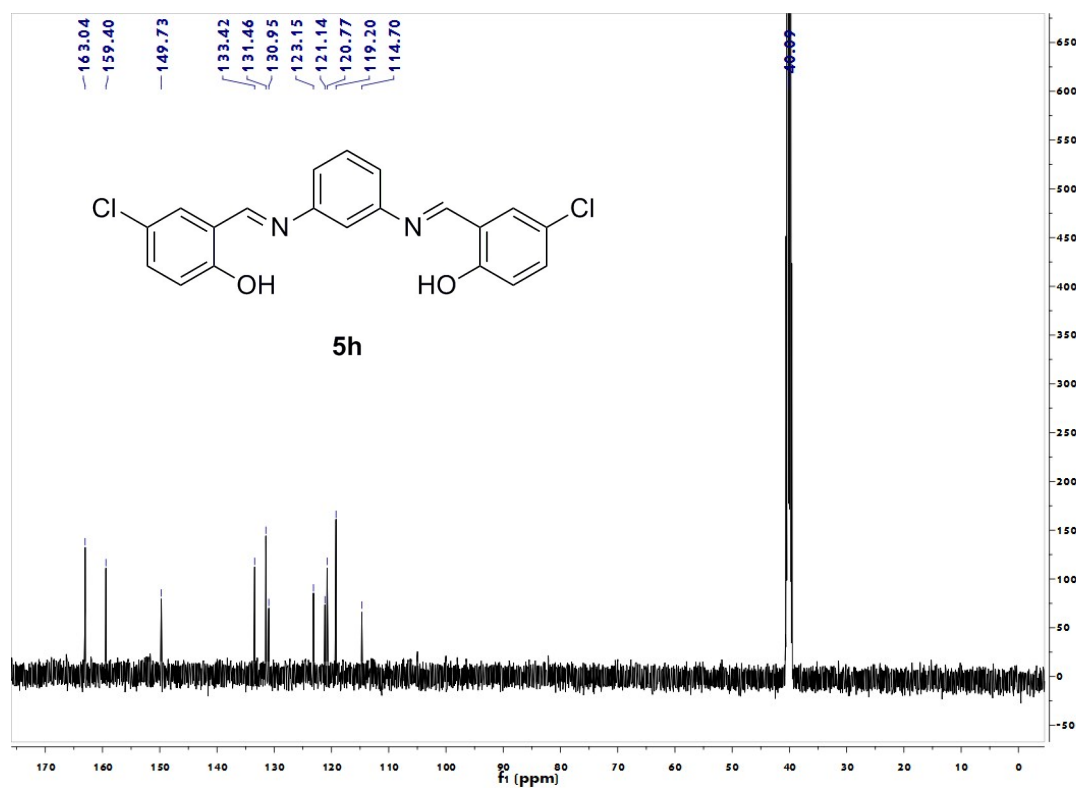
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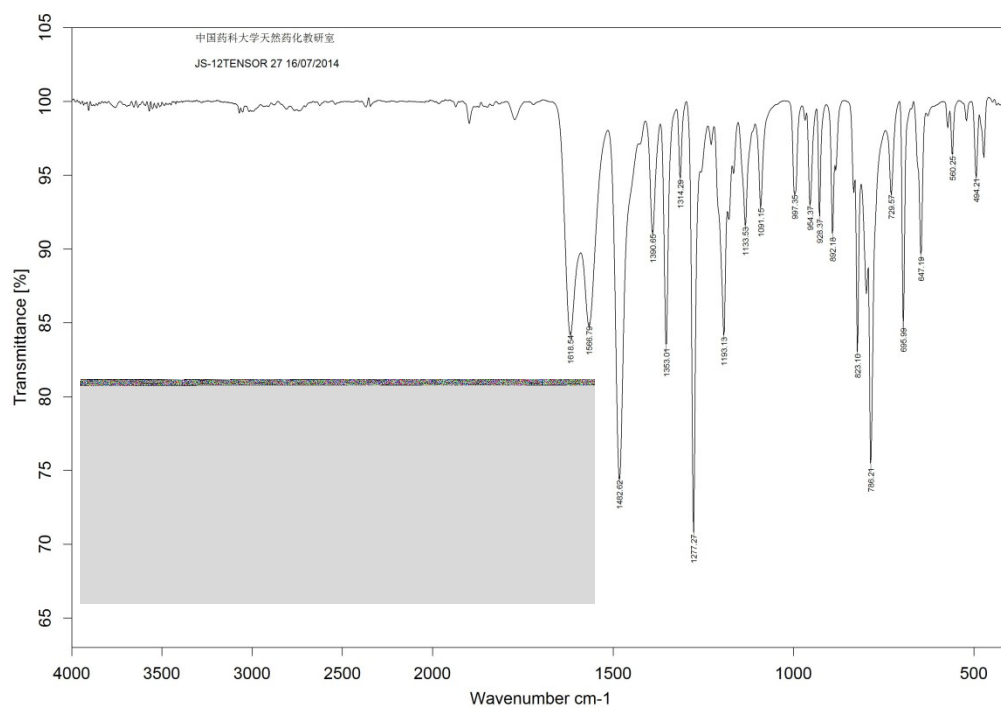
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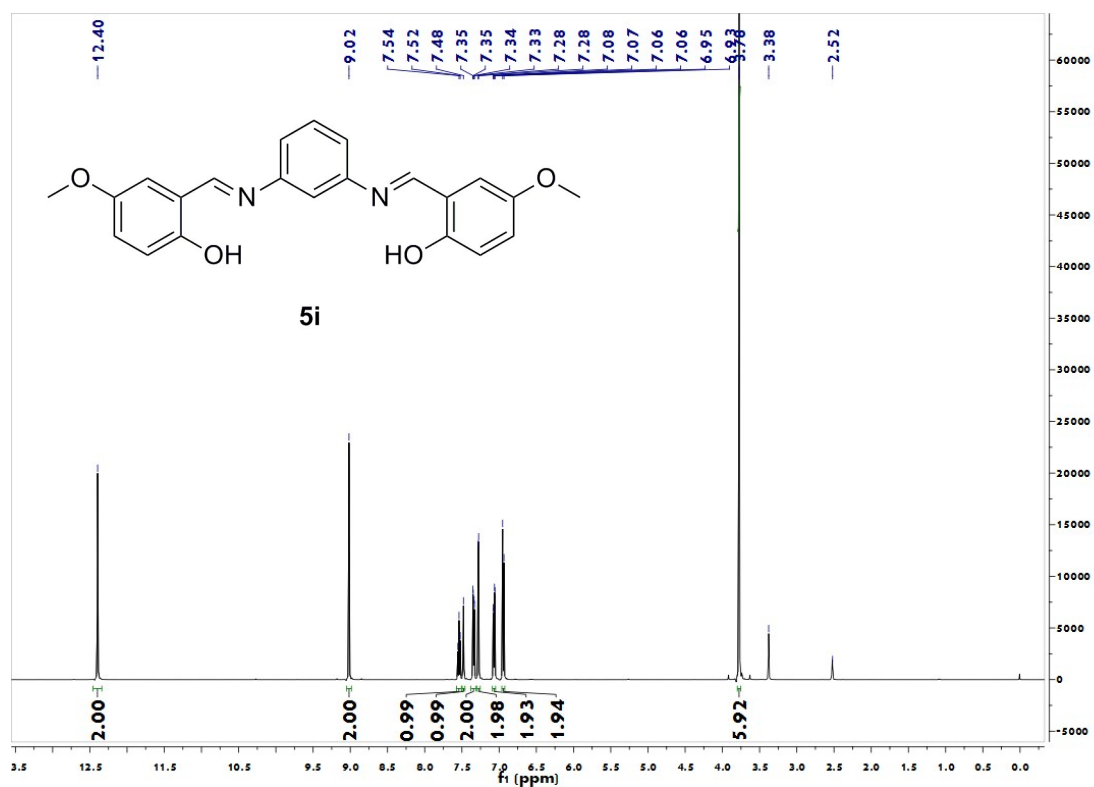
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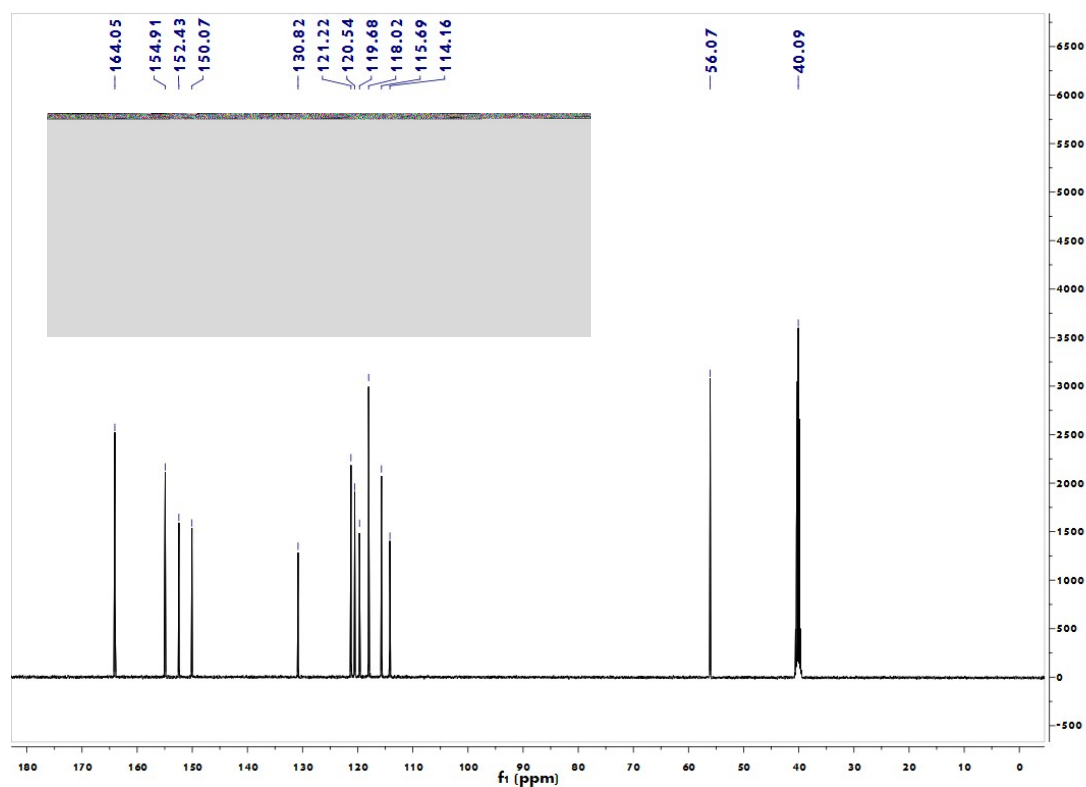
IR of compound **5h**



¹H NMR of compound **5i** in DMSO



^{13}C NMR of compound **5i** in DMSO



IR of compound **5i**

