Chemistry of Heterocyclic Compounds **2020**, 56 (8), 1103–1107

3-Amino-4-(1-amino-2-cyanovinyl)furazans: synthesis and cyclization

Kirill V. Strizhenko[1], Leonid S. Vasil'ev[1], Kyrill Yu. Suponitsky[1], Aleksei B. Sheremetev[1]*

[1] *N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, 47 Leninsky Ave., Moscow 119991, Russia; e-mail: sab@ioc.ac.ru*

SUPPLEMENTARY INFORMATION

X-ray diffraction study of compound **7** was carried out using SMART APEX2 CCD diffractometer (λ(Mo-Kα)=0.71073 Å, graphite monochromator, *ω*-scans) at 100K. Collected data were processed by the SAINT and SADABS programs incorporated into the APEX2 program package.[1] The structures were solved by the direct methods and refined by the full-matrix least-squares procedure against F^2 in anisotropic approximation. The refinement was carried out with the SHELXTL program.[2]

Crystallographic data for compound **7**: $C_6H_5N_7O$ are monoclinic, space group *Cc*: *a* = 3.5688(10) Å, *b* = 13.272(4) Å, *c* = 16.134(5) Å, β = 91.014(4)°, *V* = 764.1(4) Å^3, *Z* = 4, *M* = 191.17, d_{cryst} = 1.662 g·cm^{-3}. wR^2 = 0.0947 calculated on F^2_{hkl} for all 2002 independent reflections with 2θ < 58.0°, (GOF = 1.139, R = 0.0387 calculated on F_{hkl} for 1817 reflections with I > 2σ(I)). Crystallographic data (excluding structure factors) for the structure have been deposited at the Cambridge Crystallographic Data Centre (CCDC) as supplementary publication No. CCDC **2001287**. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

Quantum chemical calculations were carried out at M052X/6-311G(df,pd) level of approximation using the Gaussian program.[3] Theoretical electron density was analyzed in terms of "Atoms in molecules" theory[4] using the AIMAll program.[5]

Molecule 7 contains many active proton-donor and proton-acceptor centers thereby forming 3-D H-bonded network in the crystal (Figure S1).

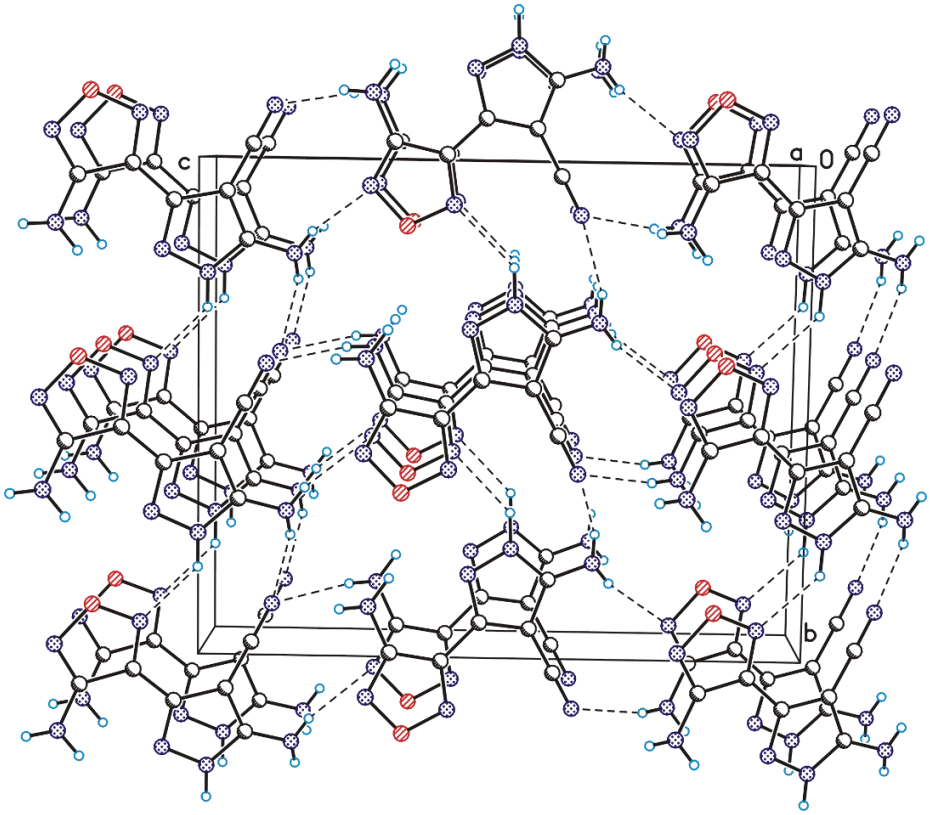

Figure S1. Crystal packing fragment of compound **7**. 3-D H-bonded network.

References

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2. G. M. Sheldrick, *Acta Crystallogr*., **2015**, *C71*, 3-8.

3. Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Kudin, K. N., Jr.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, Revision E.01, Gaussian, Inc.: Wallingford, 2004.

4. Bader, R.F.W. *Atoms in Molecules. A Quantum Theory*, Clarendon Press, Oxford, 1990.

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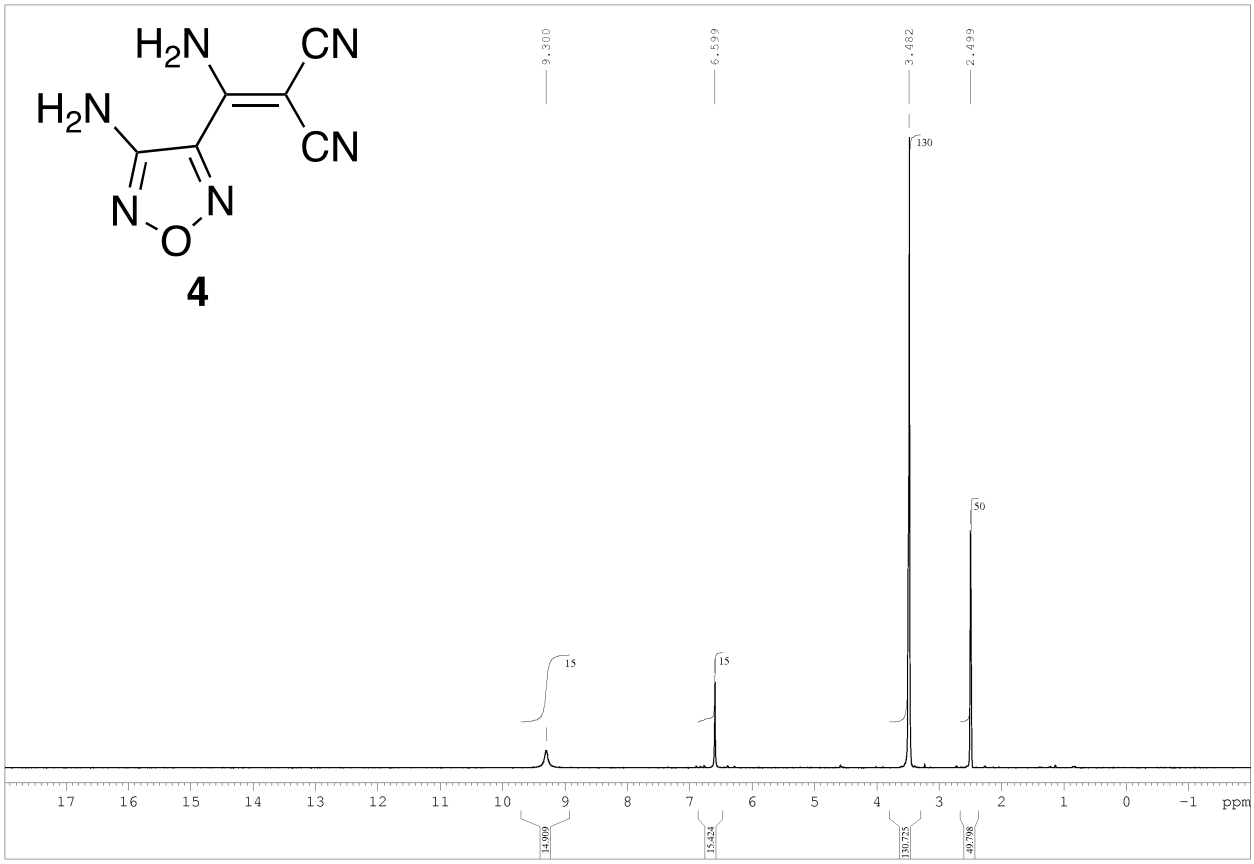
NMR spectra for compounds **4-10**

^{1}H NMR



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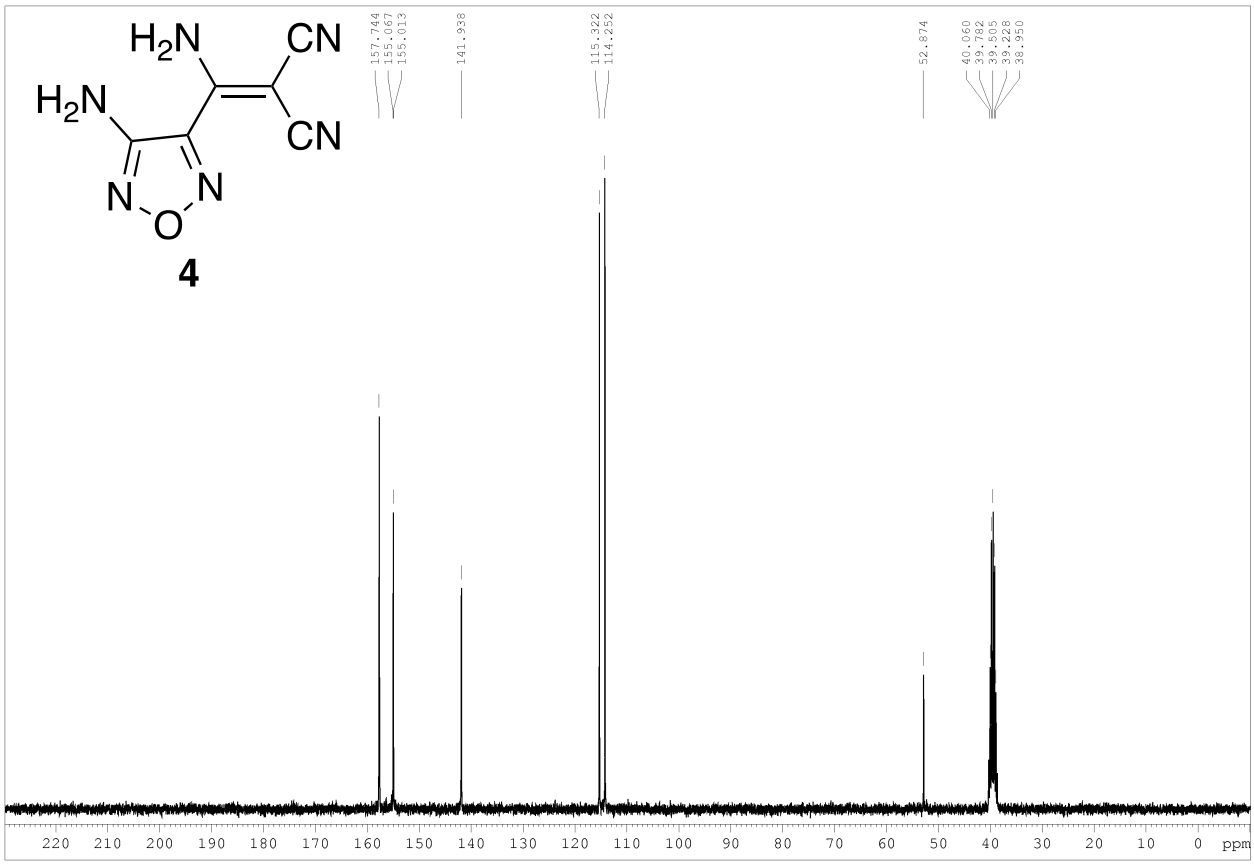

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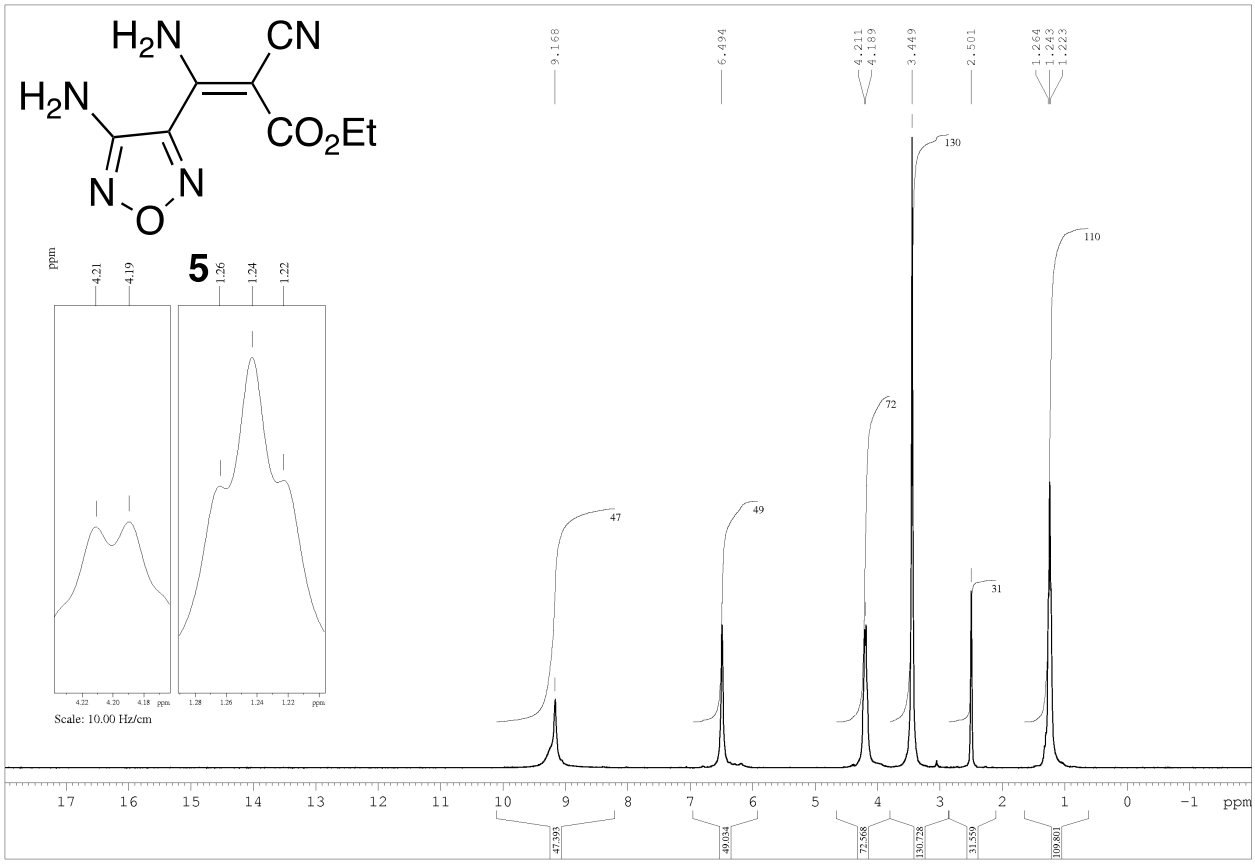

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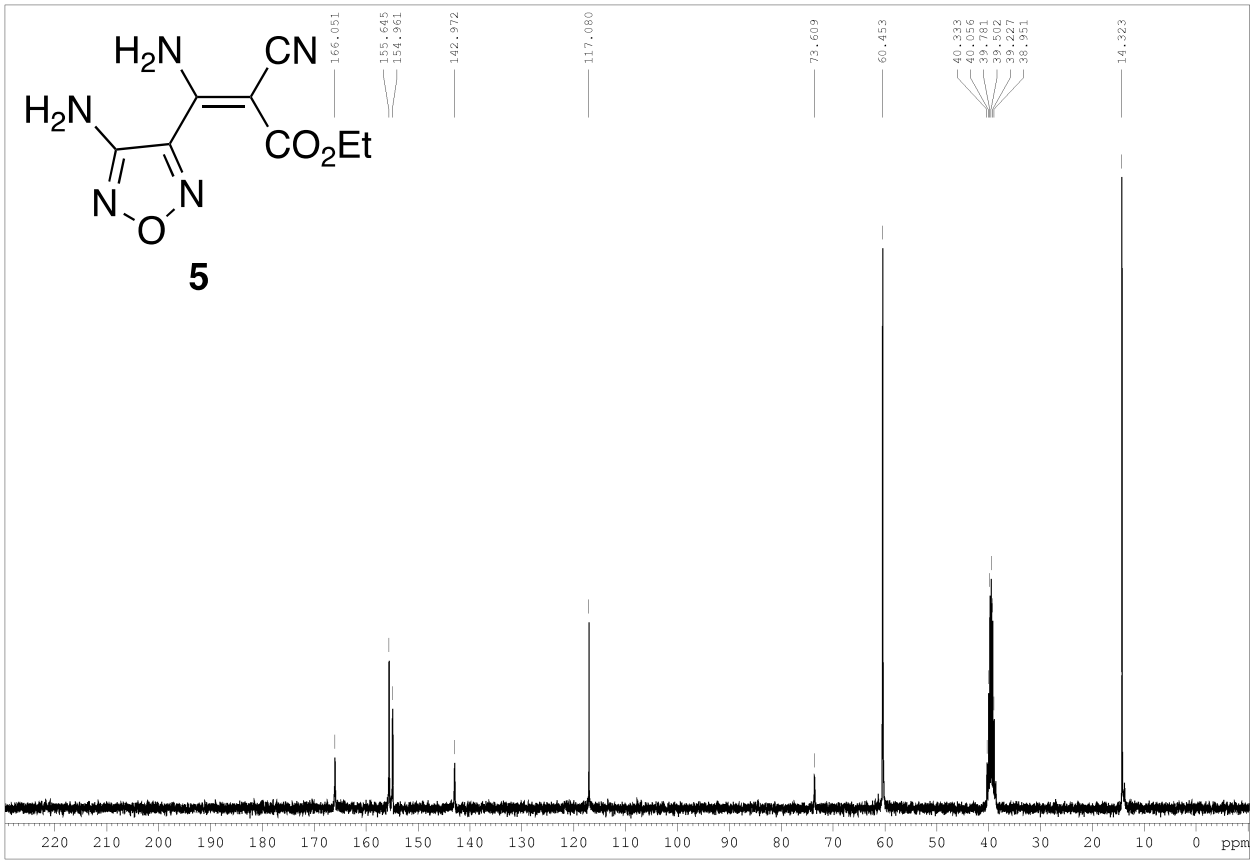

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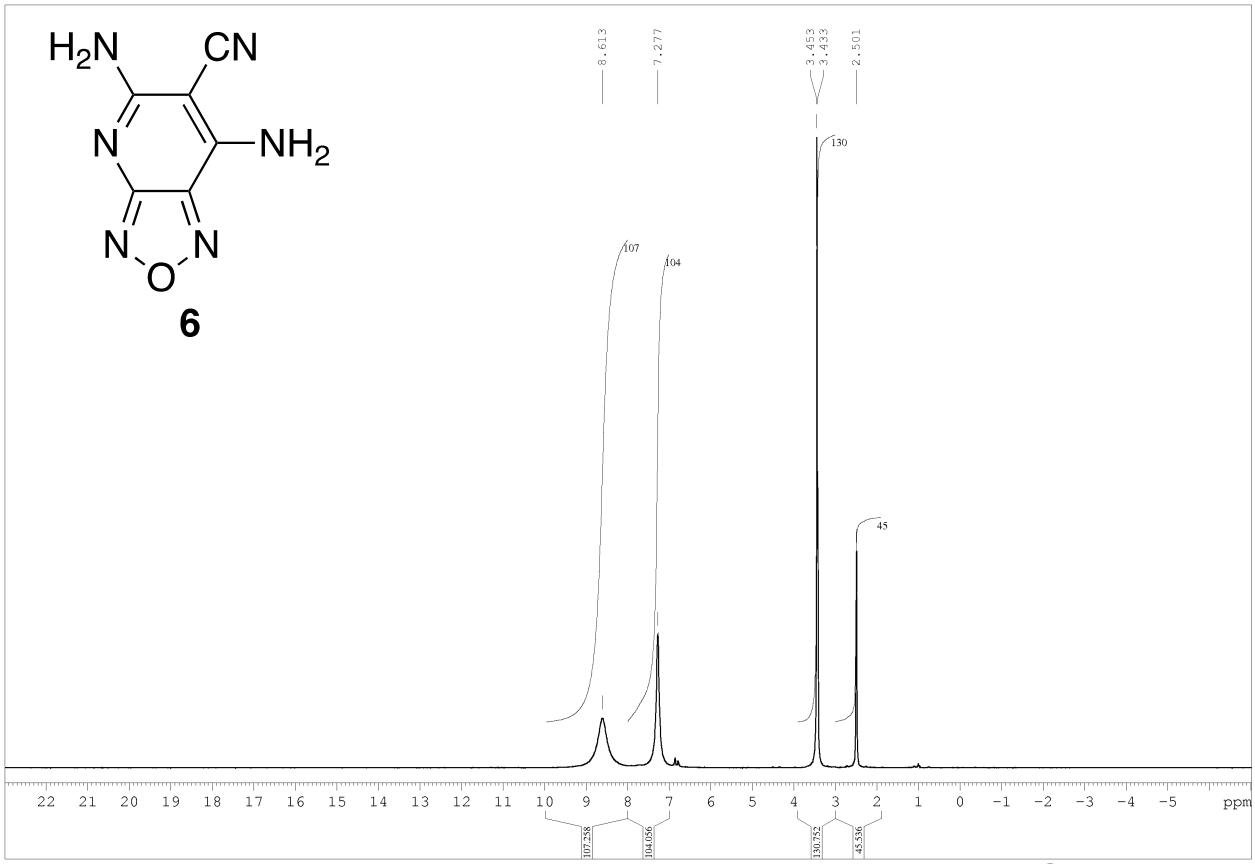

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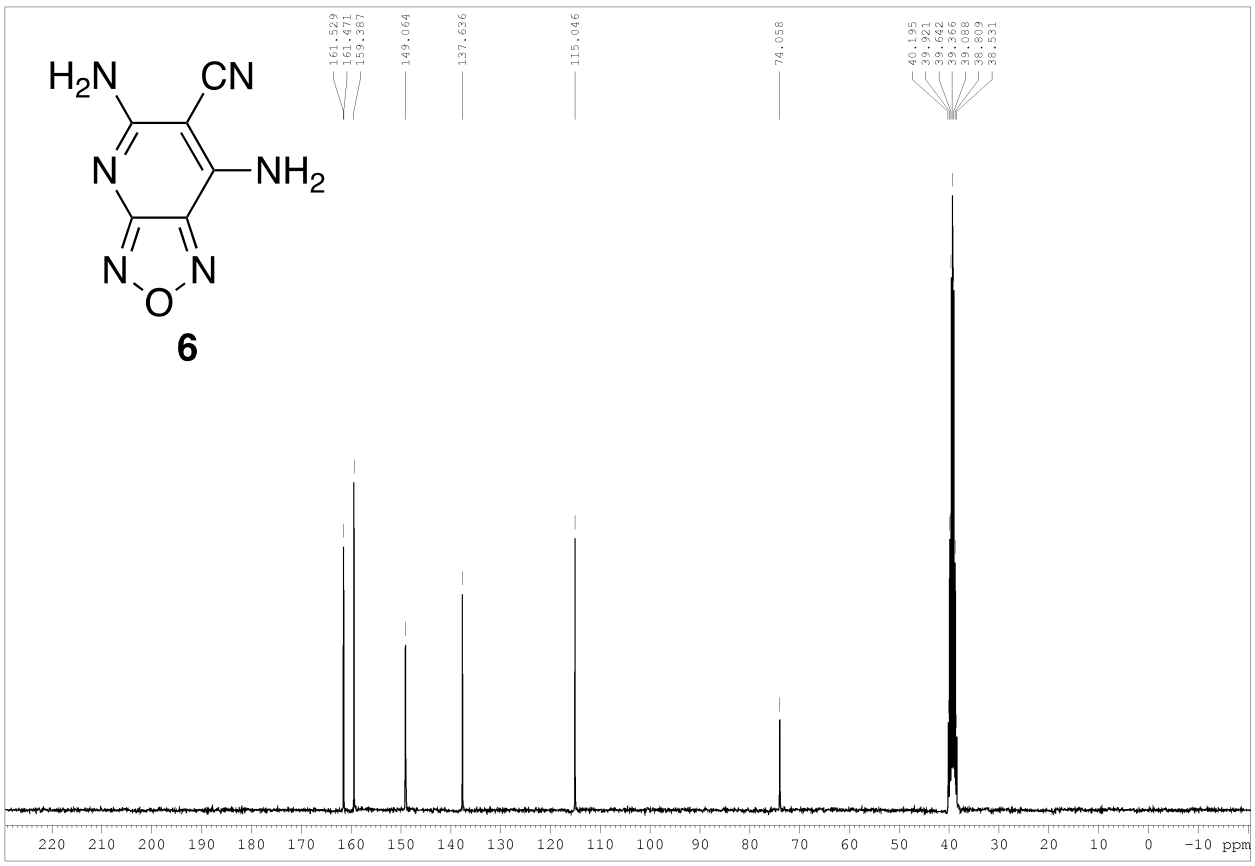

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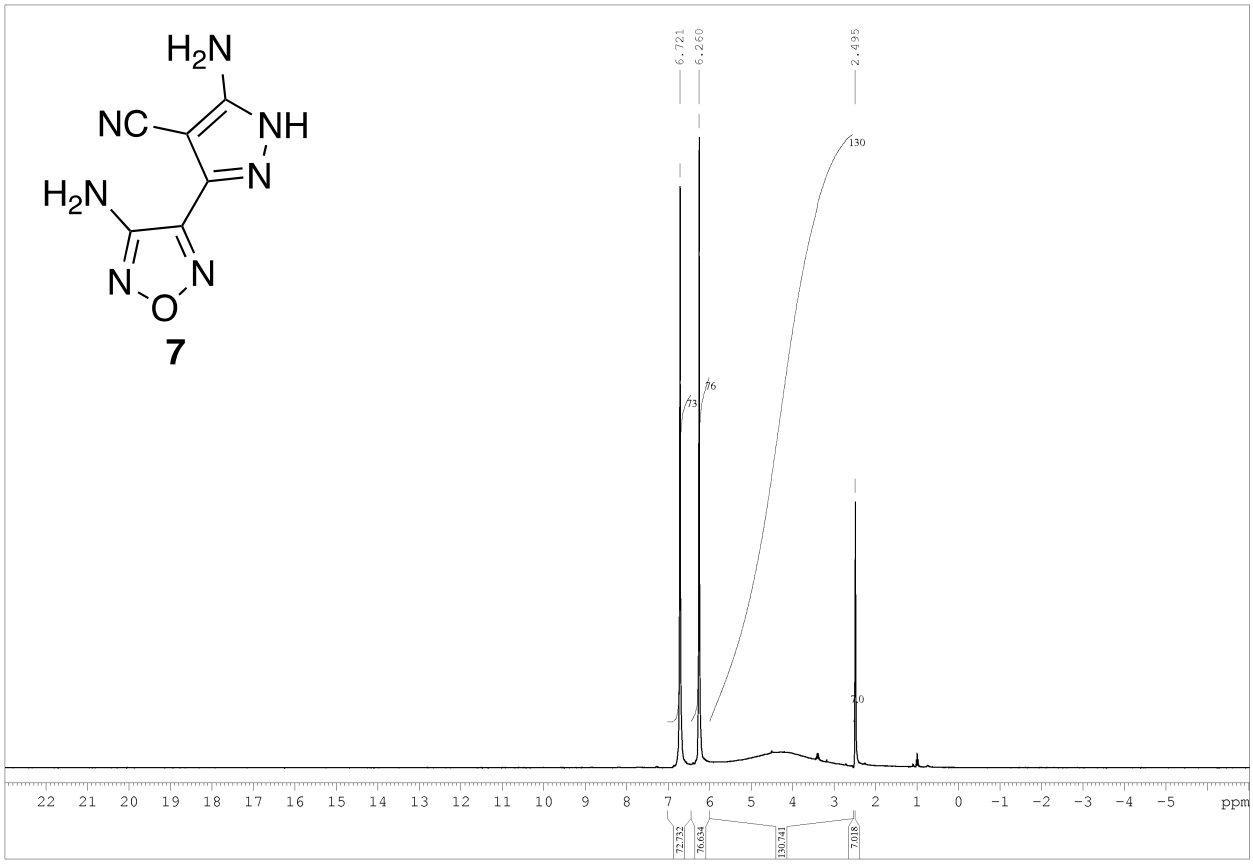

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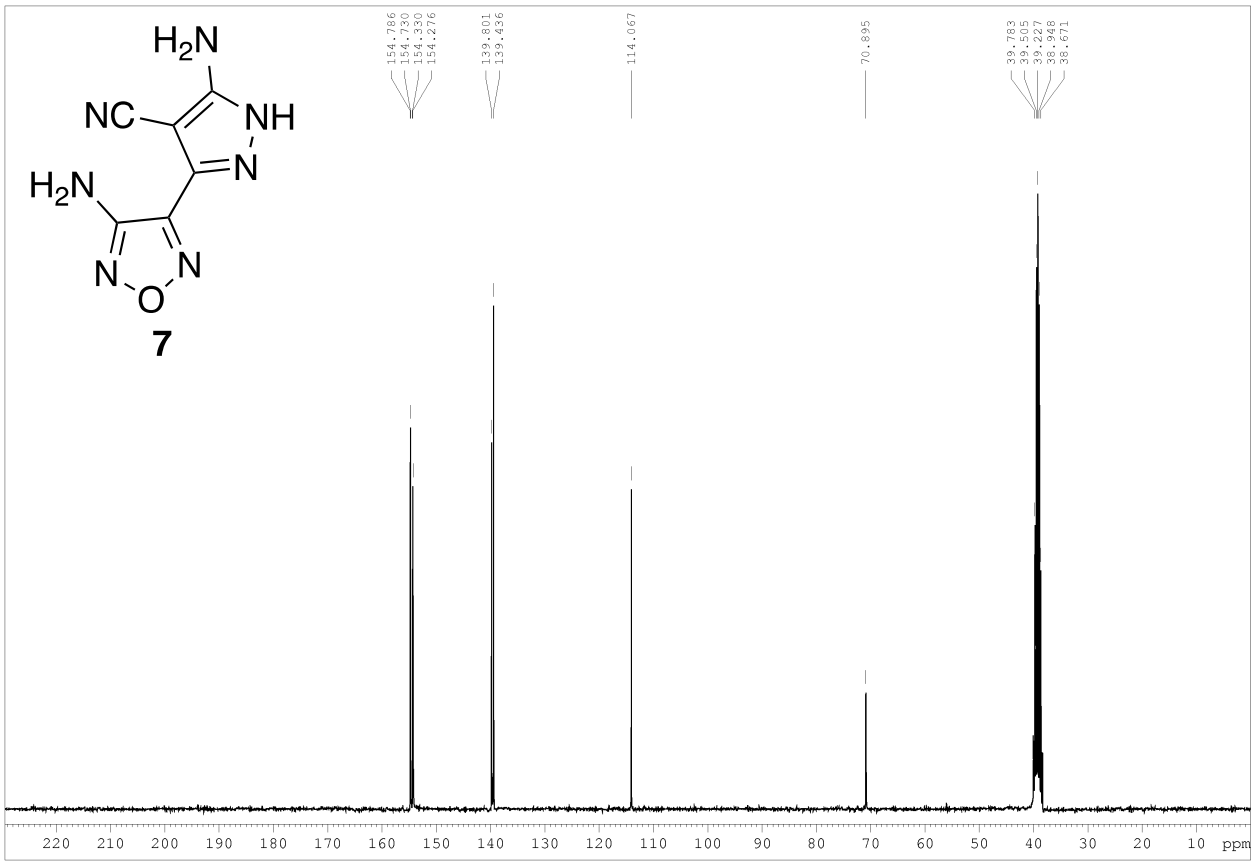

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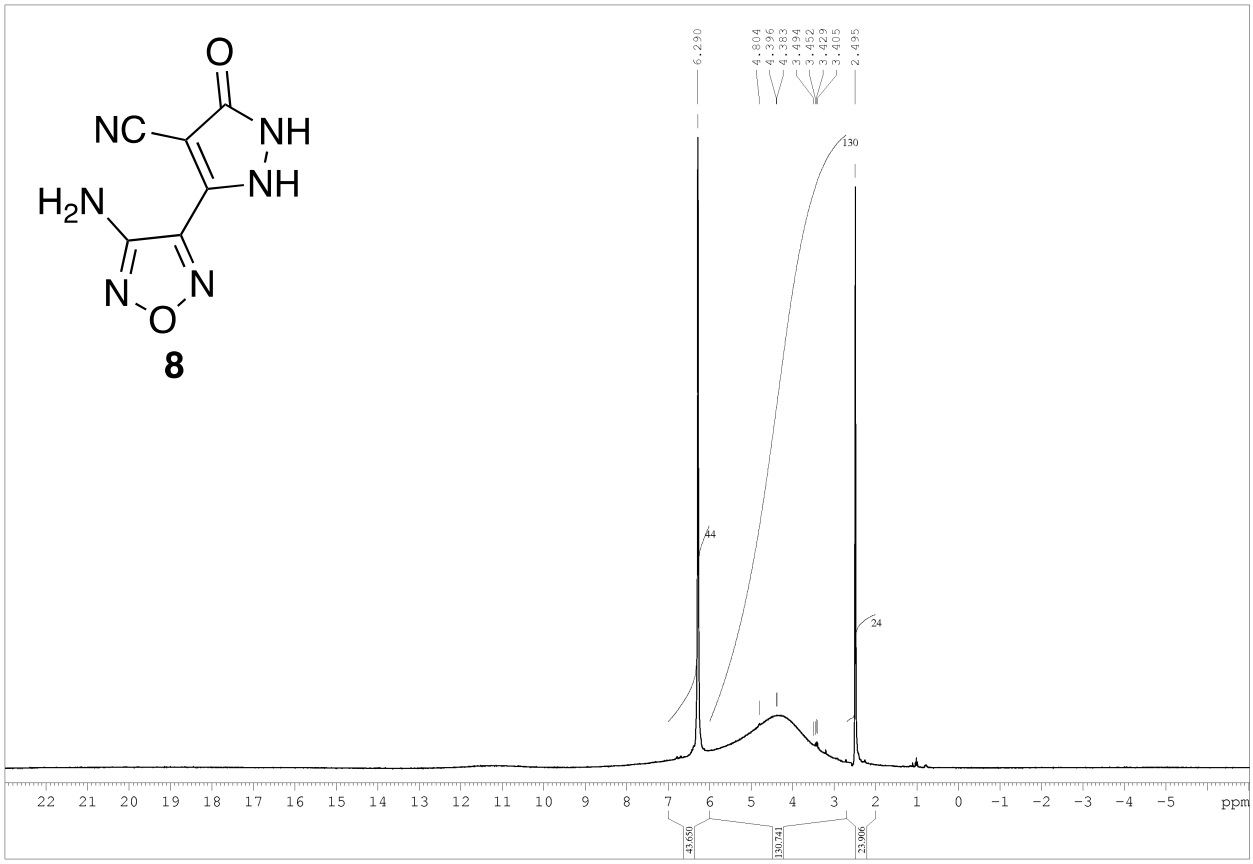

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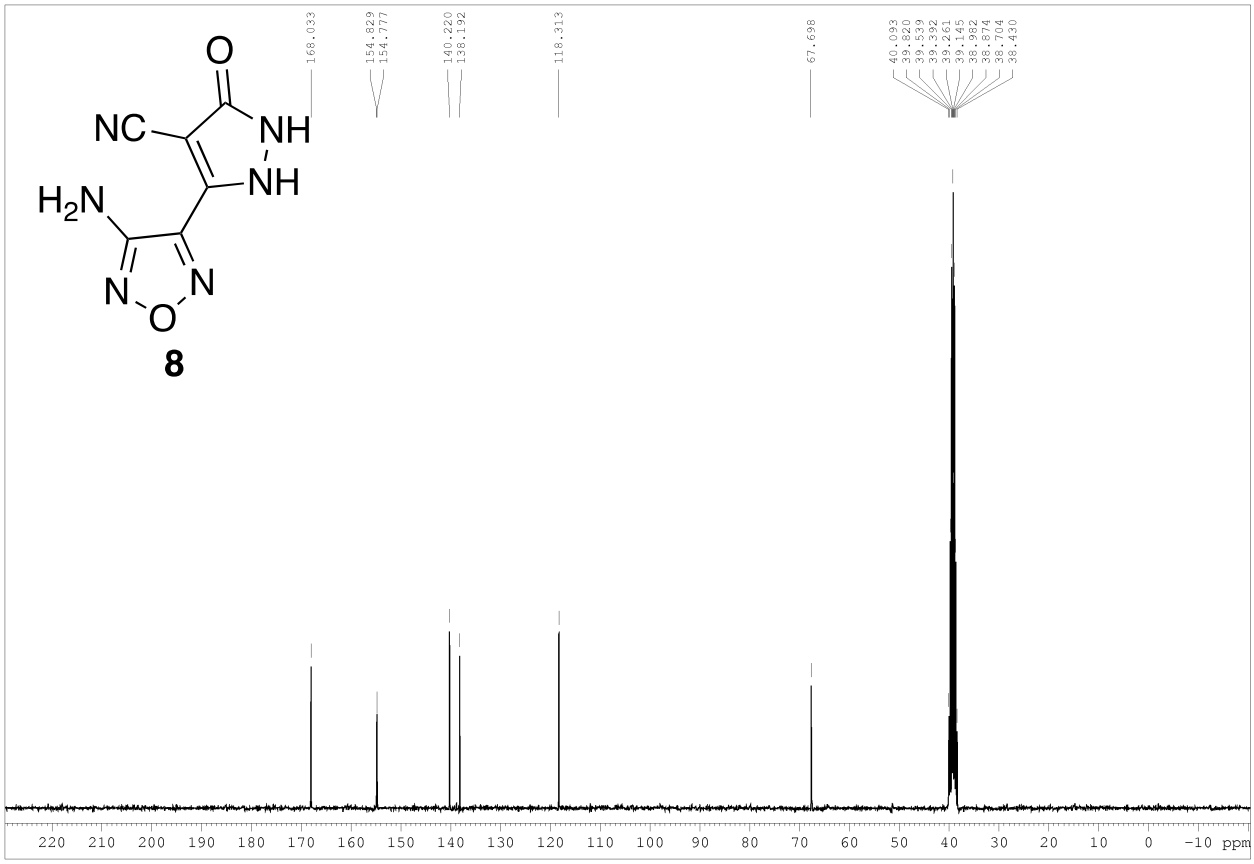

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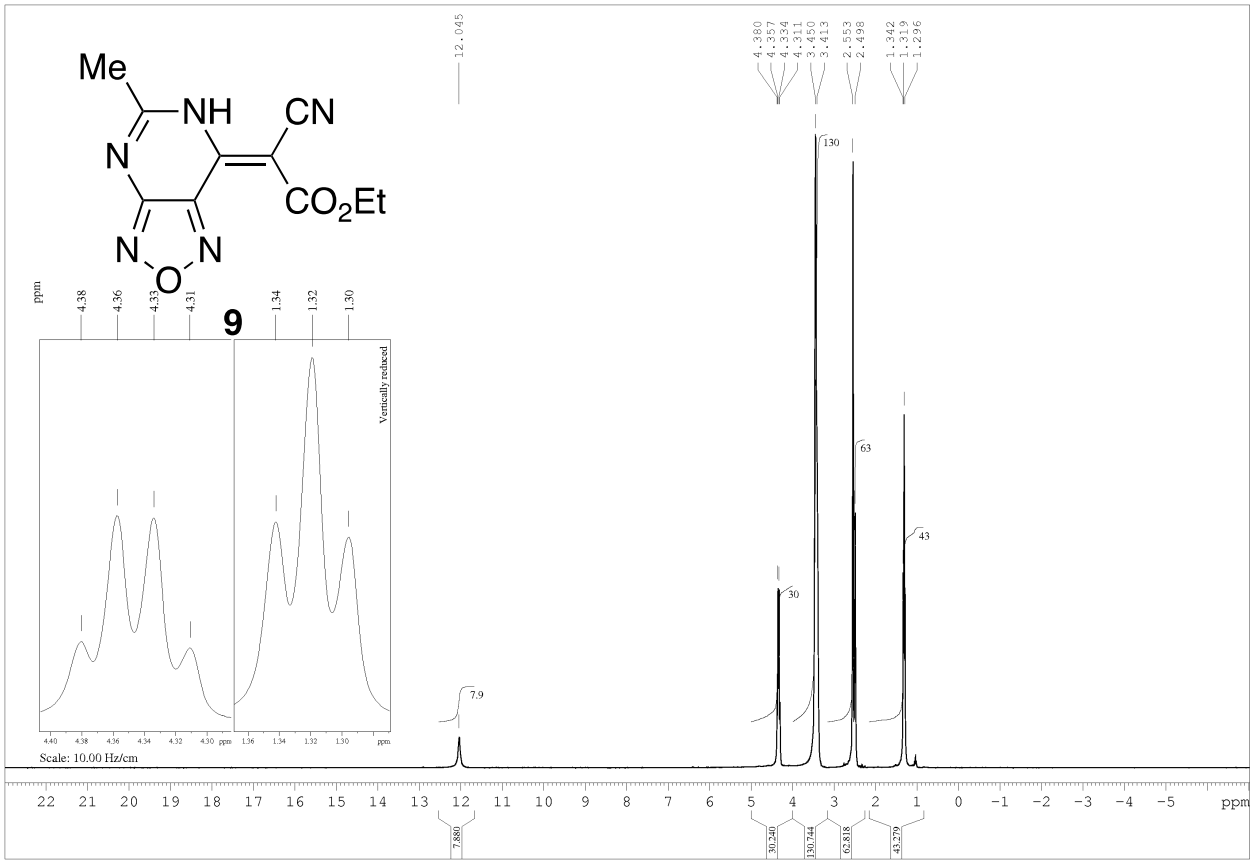

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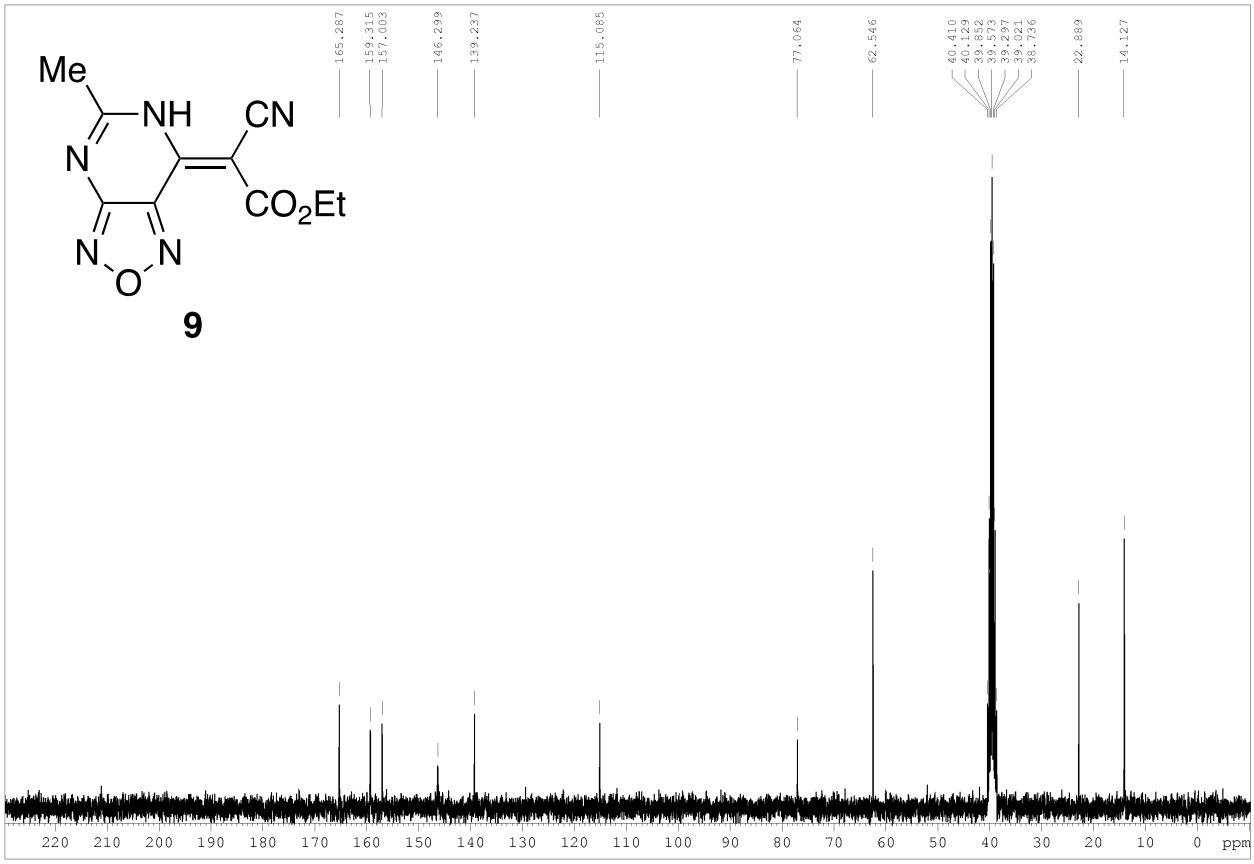

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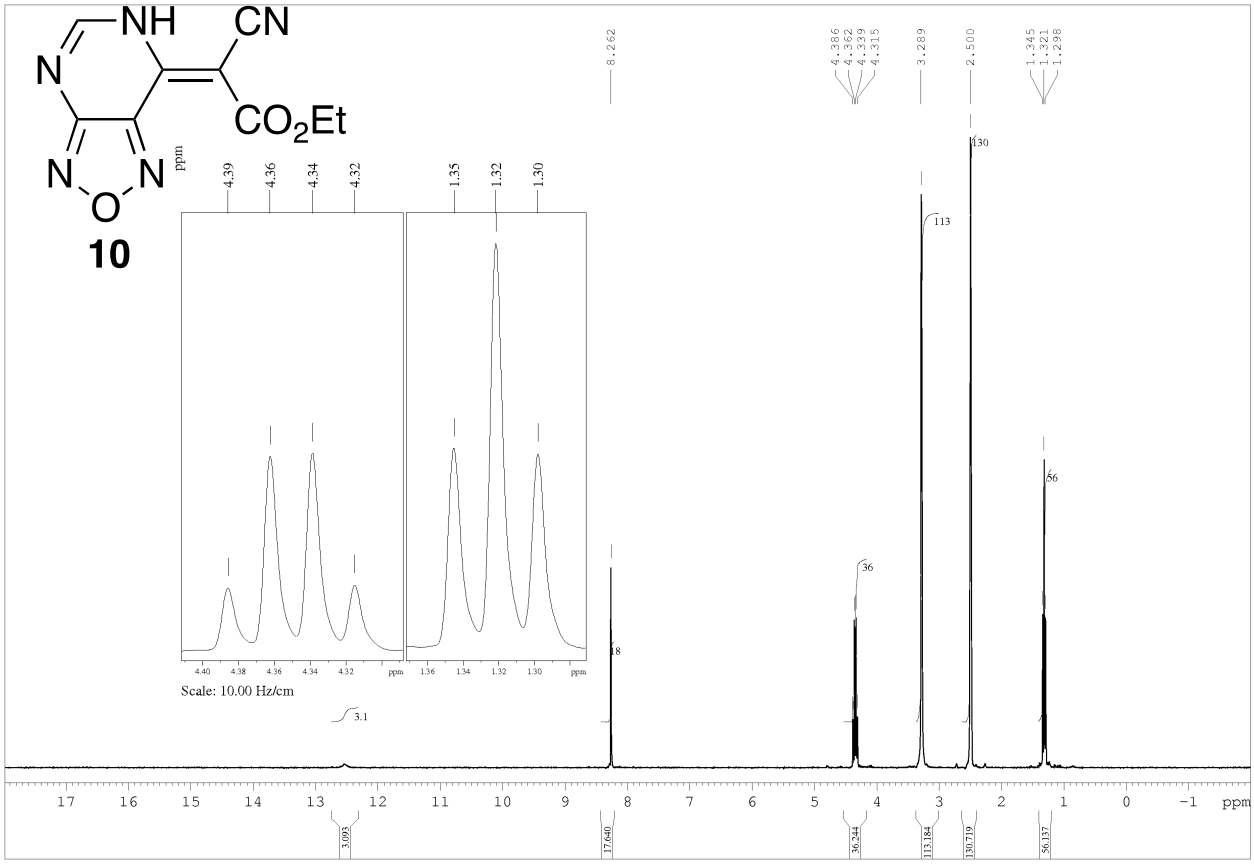

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