Supplementary Materials

Metal-free air oxidation in a convenient cascade approach for the access to Isoquinoline-1,3,4(2*H*)-triones

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Contents

Single crystals suitable for X-ray diffraction studies of compound **3a** were obtained by recrystallization from $CHCl_3$/hexane solution. The X-ray molecular structure is shown in Figure S1. Bond distances and angles are similar to those of analogous iso-quinoline-1,3,4-trione compounds (R. M. Ghalib, C. S. Chidan Kumar, R. Hashim, O. Sulaiman and H.-K. Fun Acta Cryst. E , **2015**, 71, o6-o7).

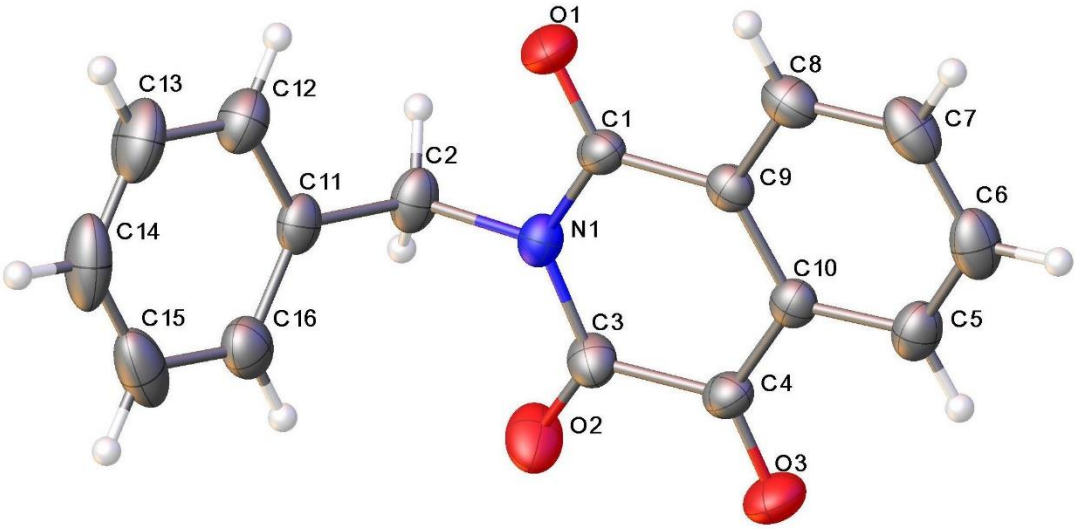


Figure 1. The X-ray molecular structure of compound **3a**.

X-ray crystallography

Colourless prismatic single crystals of compound **3a** suitable for X-ray diffraction analysis were obtained by $CHCl_3$/hexane solution.

A suitable crystal (0.44 mm × 0.35 mm × 0.27 mm)

was glued on a glass fiber and measured at room temperature at room temperature with a Bruker D8 QUEST diffractometer equipped with a PHOTON100 detector using Cu$K\alpha$ radiation (λ= 1.54178 Å). Indexing was performed using APEX3.[1] Data integration and reduction were performed using SAINT.[1] Absorption correction was performed by multi-scan method in SADABS.[1]

The structure was solved by Direct Methods using SIR2014[2] and refined by means of full matrix least-squares based on F^2 using the program SHELXL.[3] 18760 reflections were collected, resulting in 2328 independent reflections (R_{int} = 0.0199, R_{sigma} = 0.0123).

Non-hydrogen atoms were refined anisotropically, hydrogen atoms were positioned geometrically and included in structure factors calculations, but not refined. 181 refinable parameters were finally considered, final disagreement R indices (all data) are: R =0.0496,

wR_2 = 0.1249. The maximum and minimum residual densities were respectively 0.18/-0.20 eÅ^{-3}.

Crystal structures were drawn using OLEX2.[4]

Crystal data. Formula: $C_{16}H_{11}NO_3$, Formula weight: 265.26, Crystal system: monoclinic, Space group: $P2_1/n$, a = 13.148(2) Å , b = 7.3323(8) Å, c= 13.8239(12) Å, β107.179(9)° V= /Å1273.2(3) Å^3, Z= 4, ϱ_{calc}=1.384 g/cm^3, μ= 0.795mm^{-1}, F(000)=552.0

Supporting Information Available: Diffraction data in cif format of compounds **3a**

CCDC 1915668

References

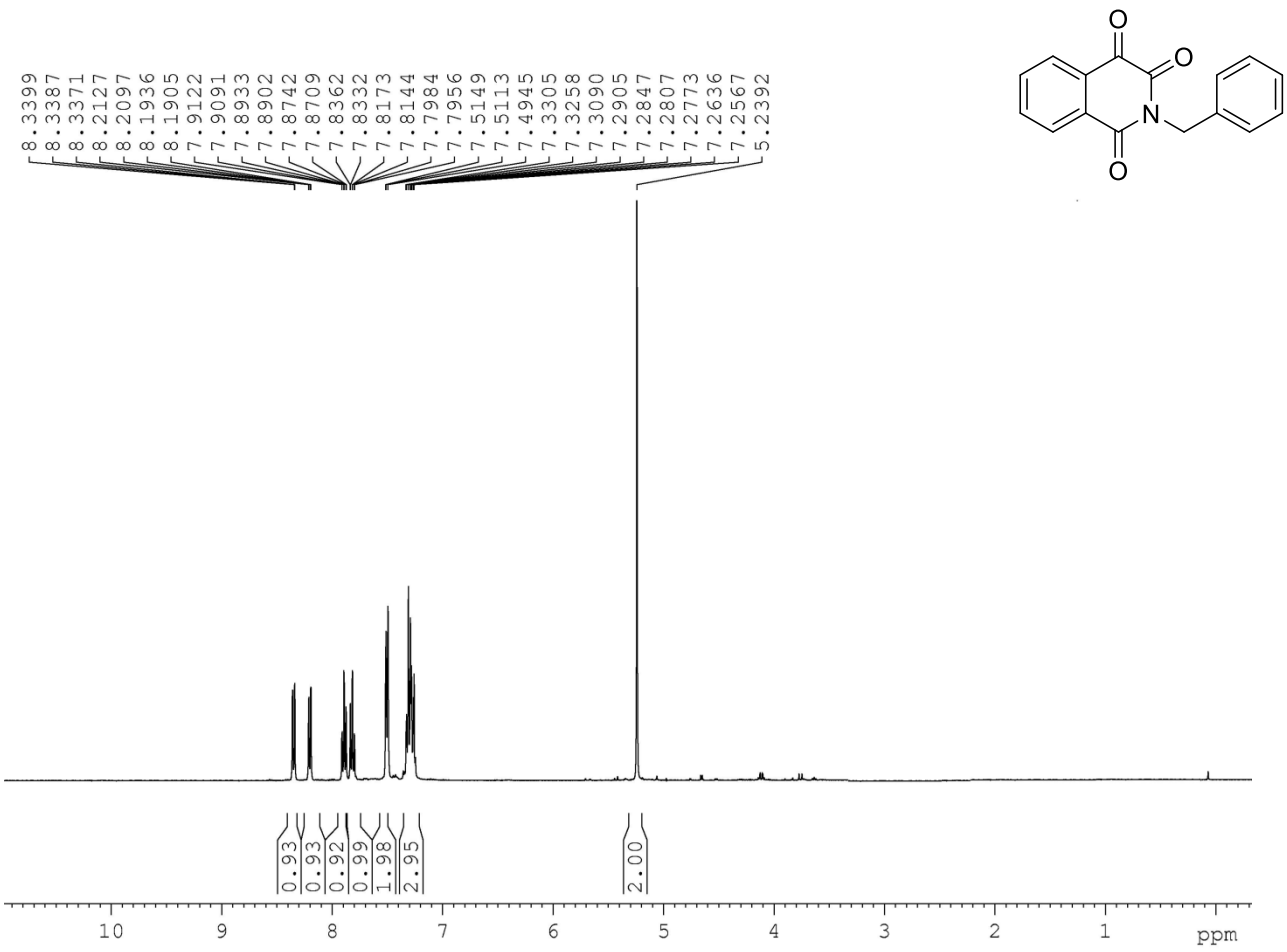
[1] CrystalClear, Crystal Structure Analysis Package, Rigaku-Molecular Structure Corp.

[2] APEX3, SAINT, SADABS. Bruker AXS Inc., Madison, Wisconsin, USA. Bruker AXS Inc., Madison, Wisconsin, USA, **2012**.

[3] Burla, M. C.; Caliandro, R.; Carrozzini, B.; Cascarano, G. L.; Cuocci, C.; Giacovazzo, C.; Mallamo, M.; Mazzone, A.; Polidori, G. Crystal structure determination and refinement via SIR2014. *J. Appl. Cryst.* **2015**, *48*, 306-309.

[4] Sheldrick, G. M. Crystal structure refinement with SHELXL. *Acta Cryst.* **2015**, *C71*, 3–8

[5] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Cryst.* **2009**, *42*, 339–341.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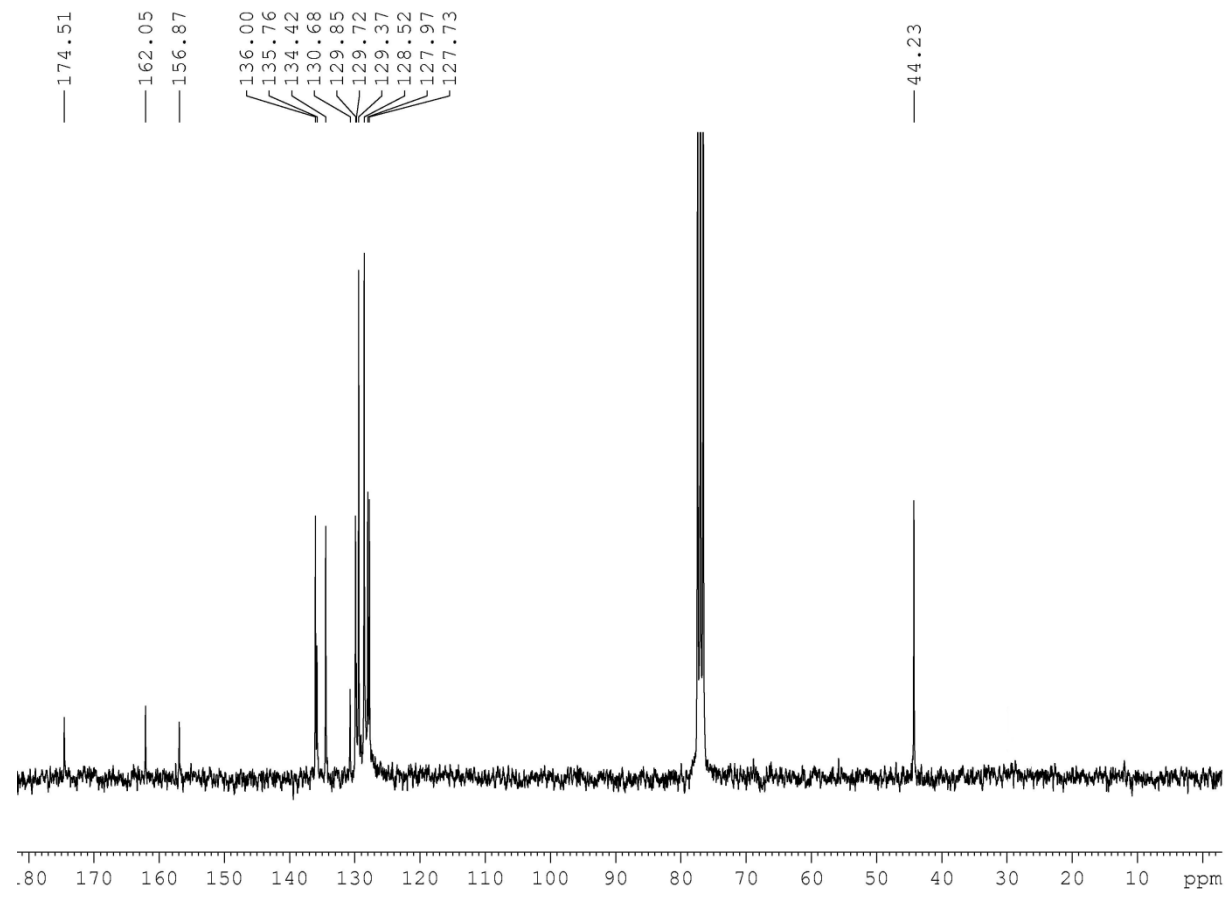
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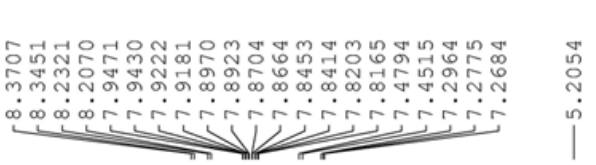
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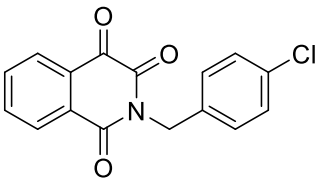
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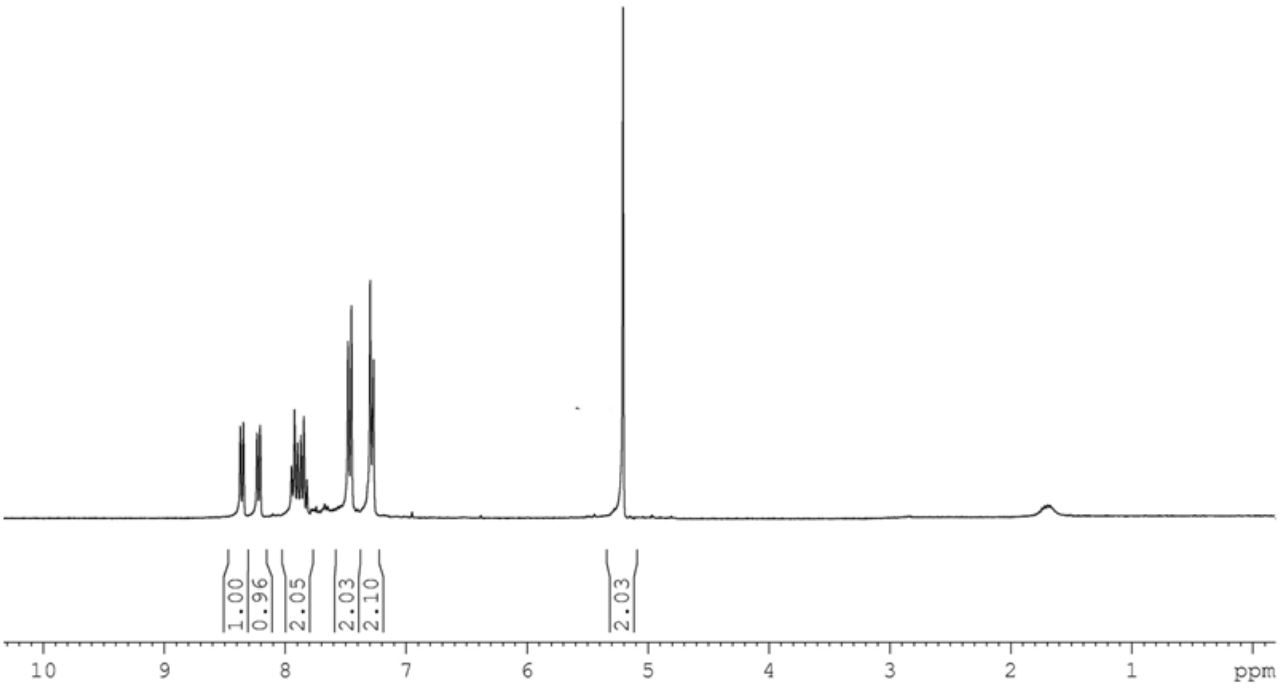
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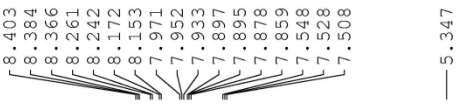
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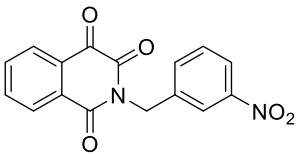
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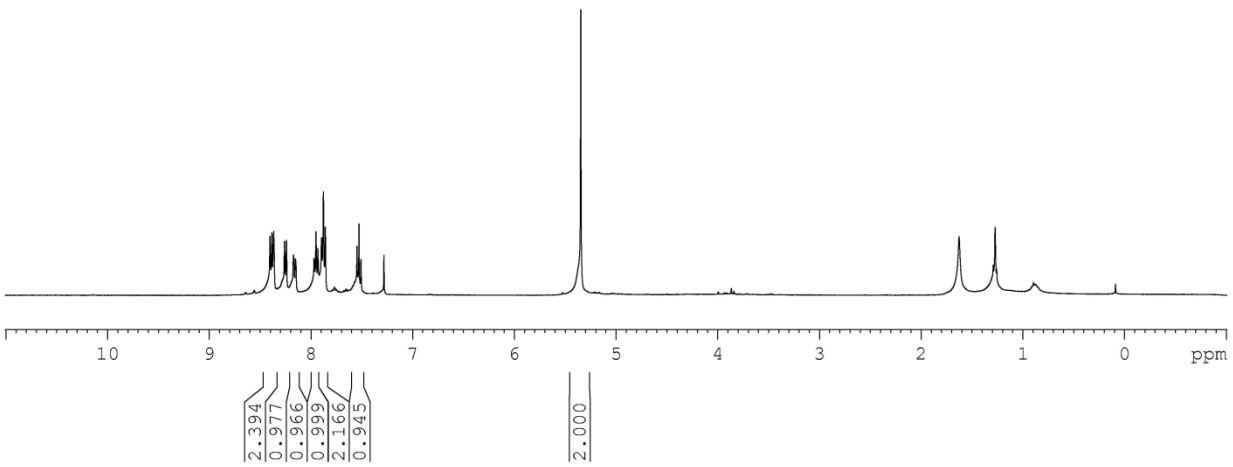
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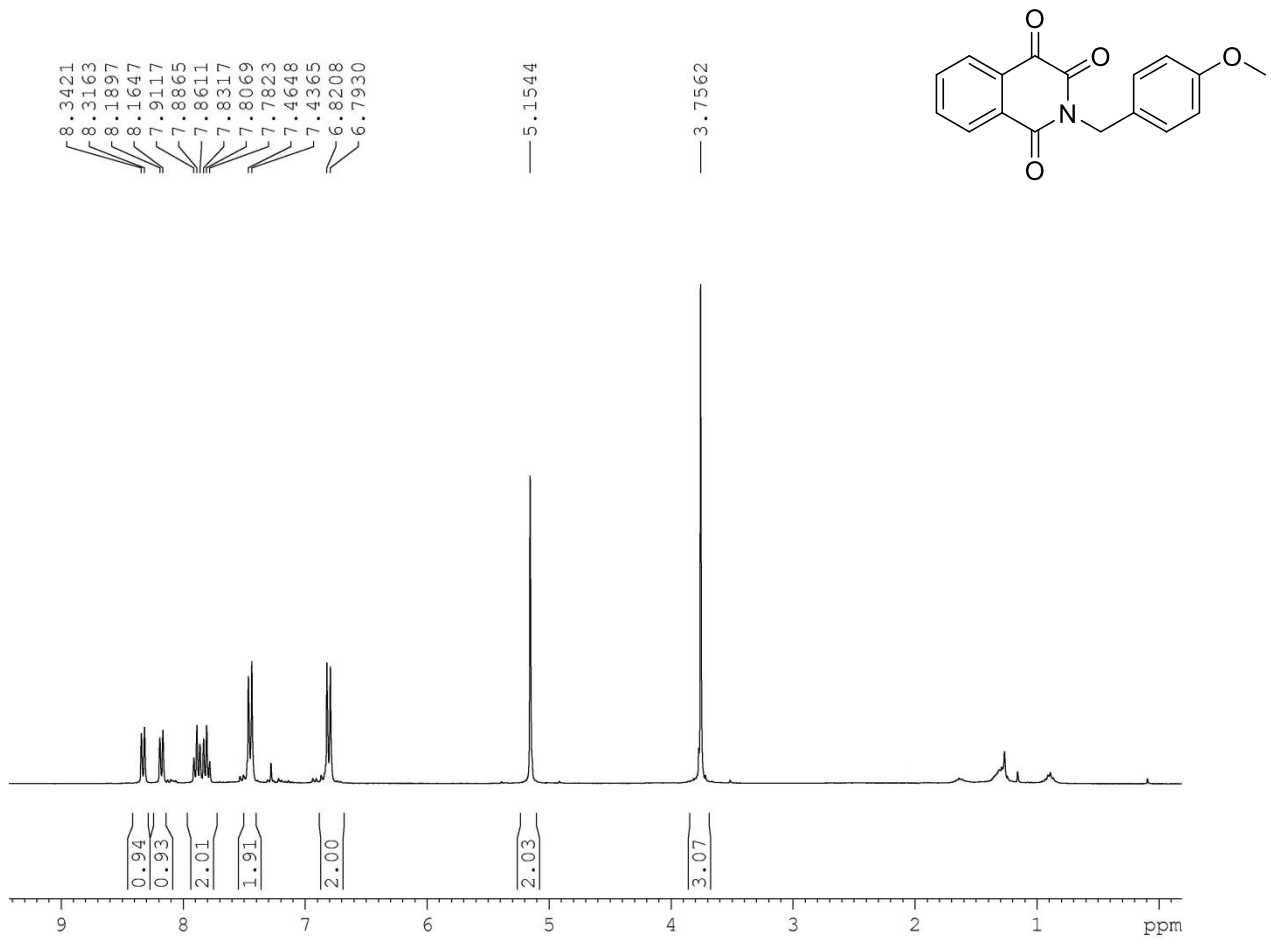
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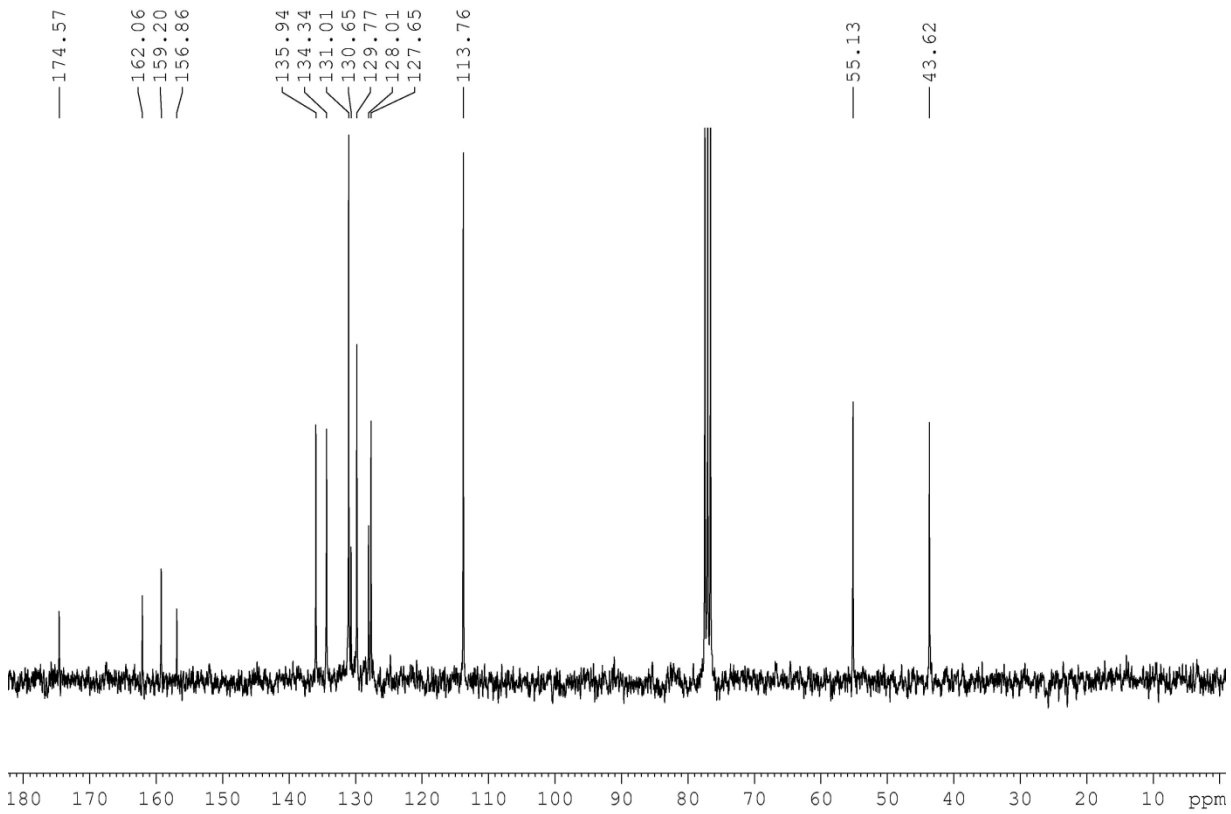
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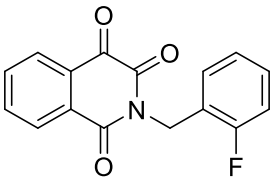
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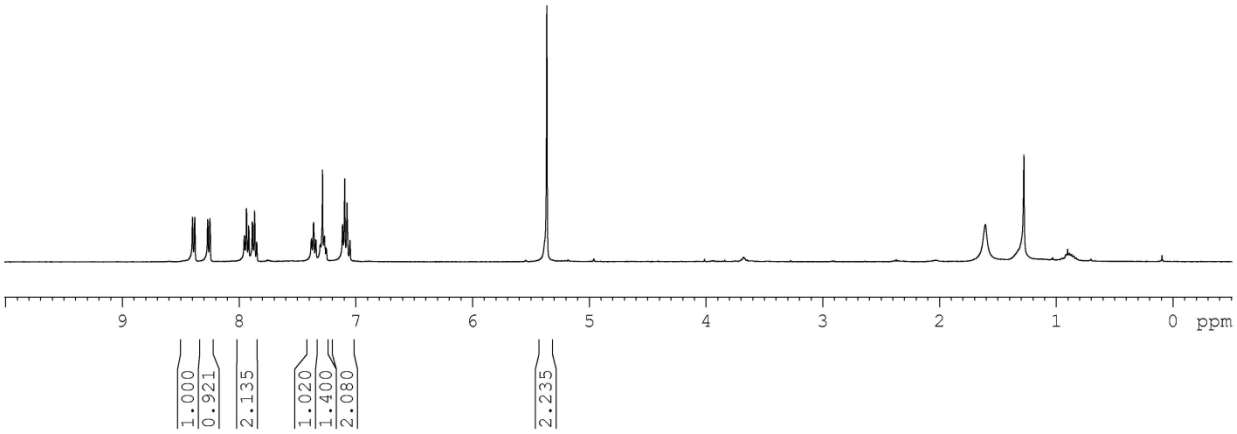
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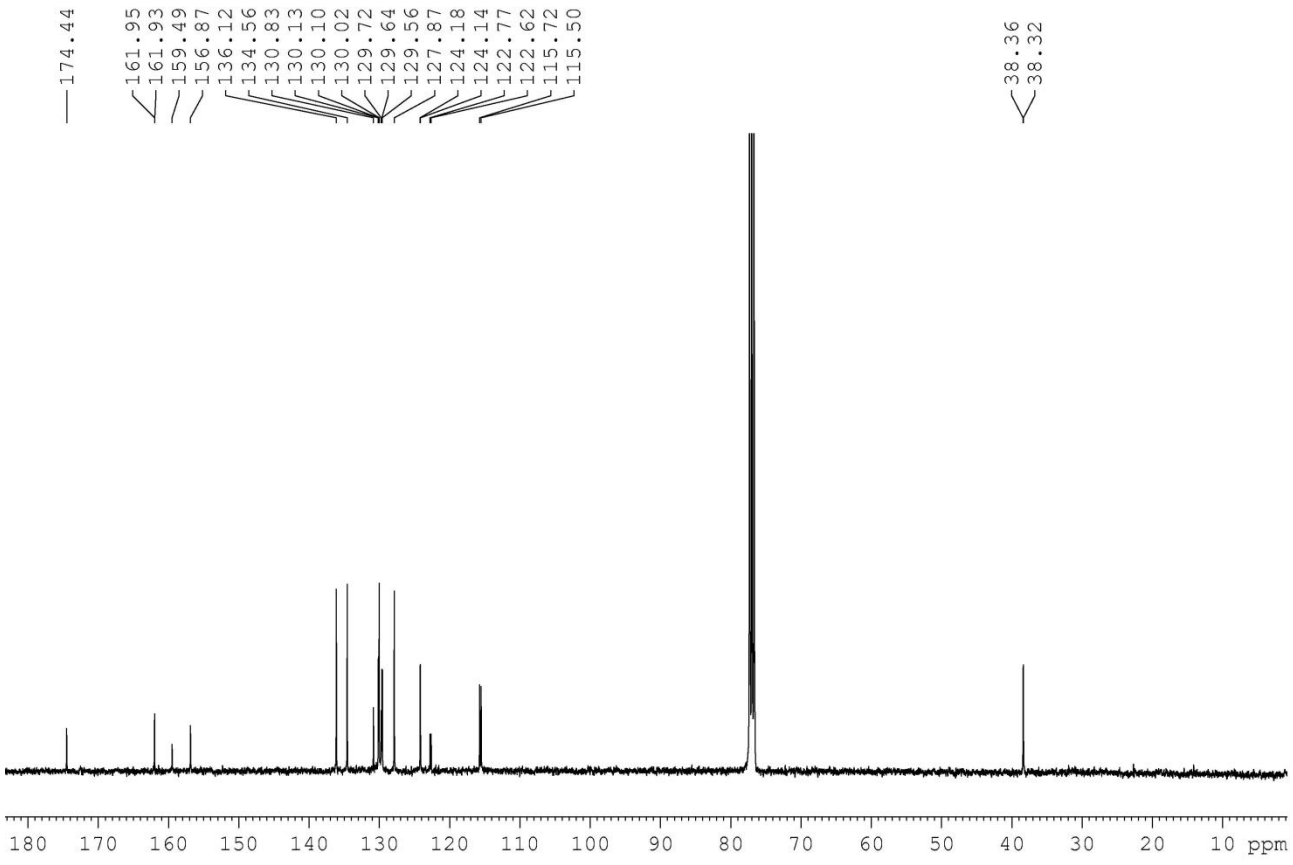
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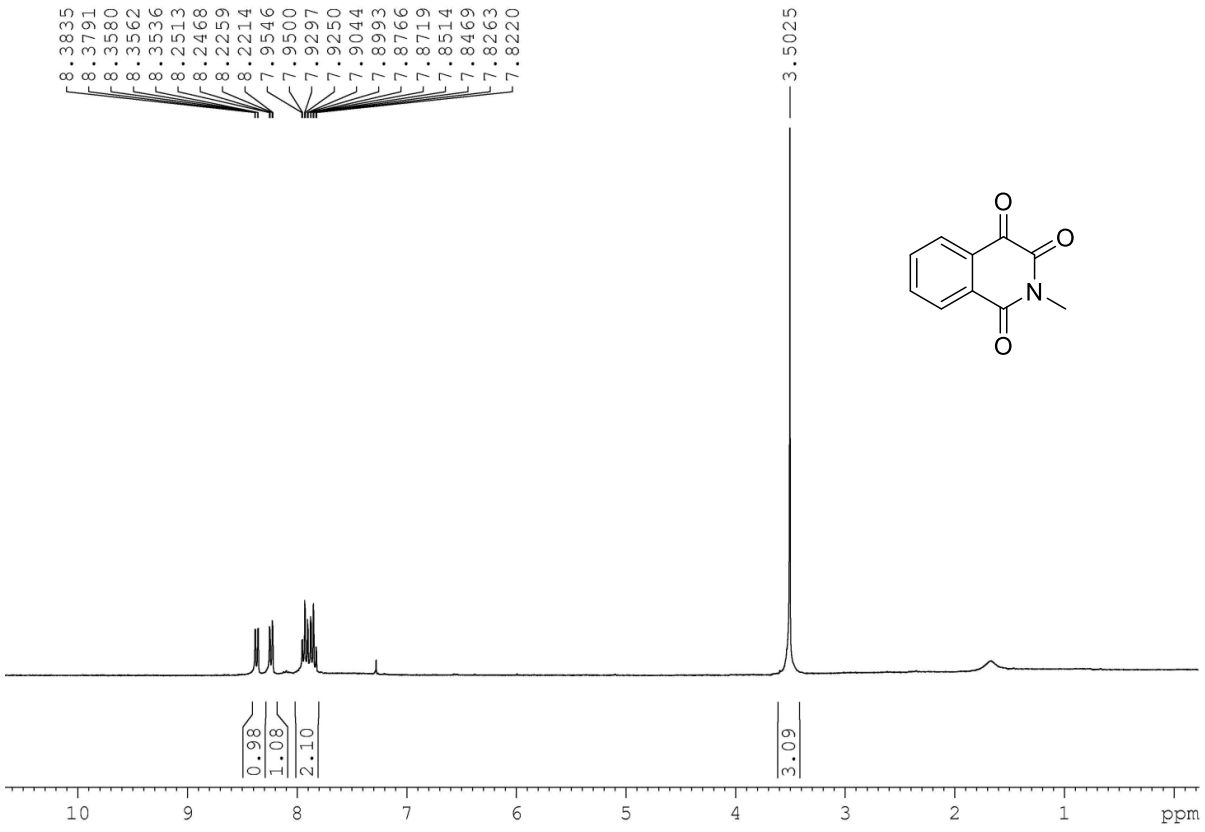
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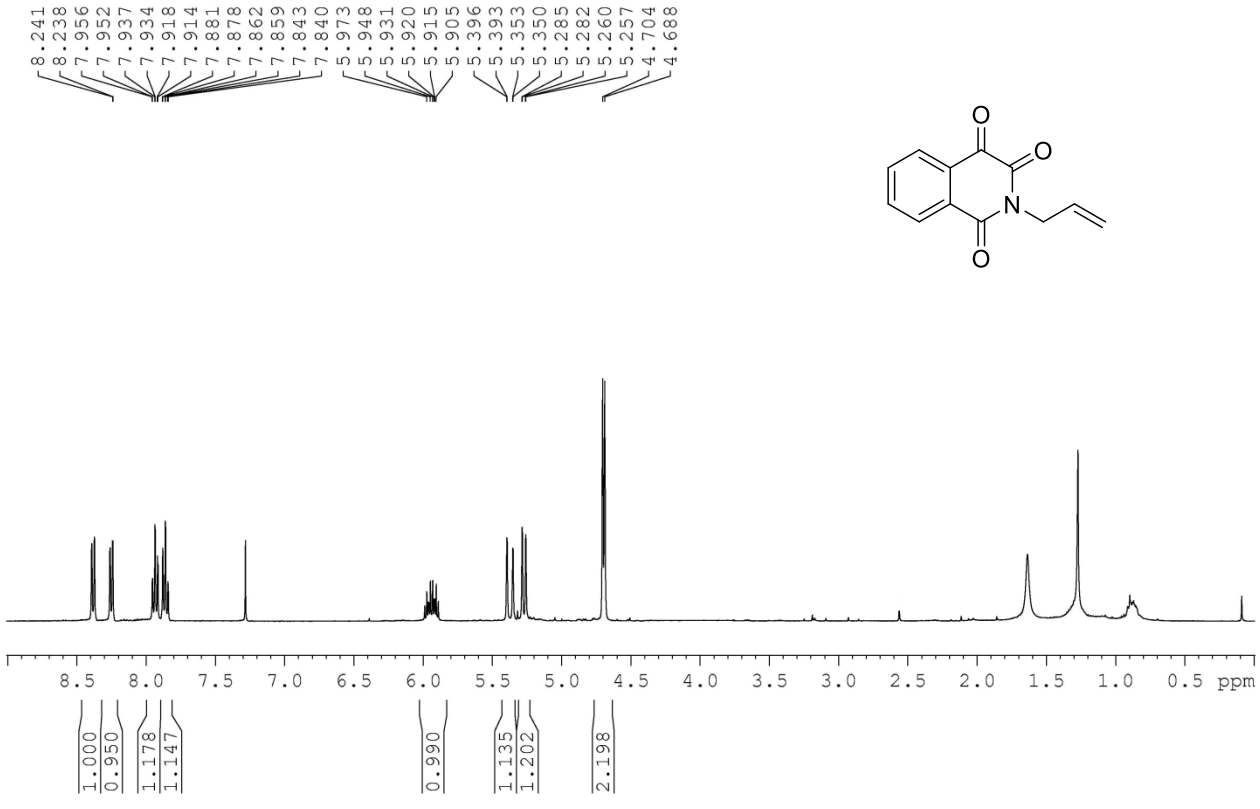
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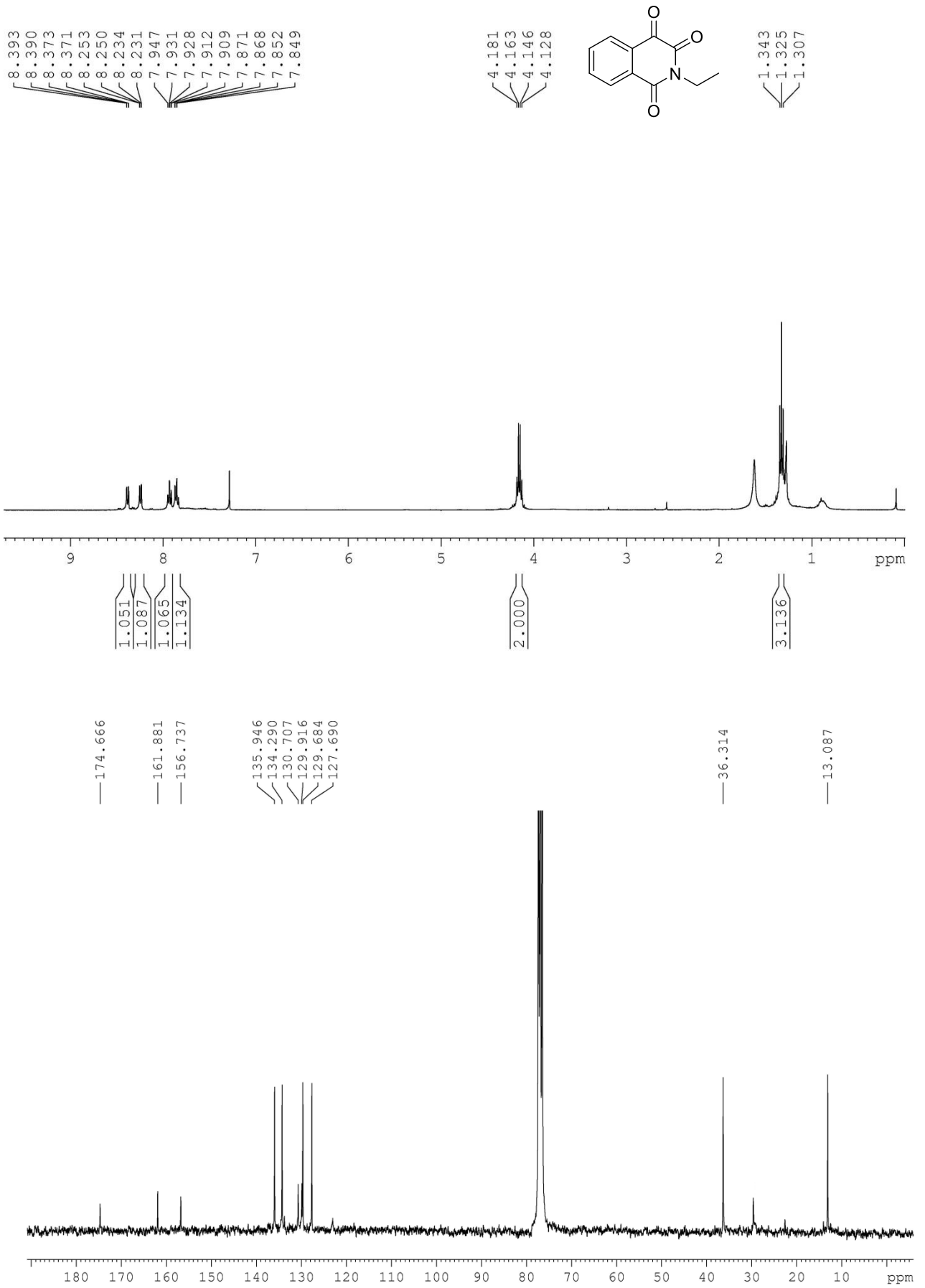
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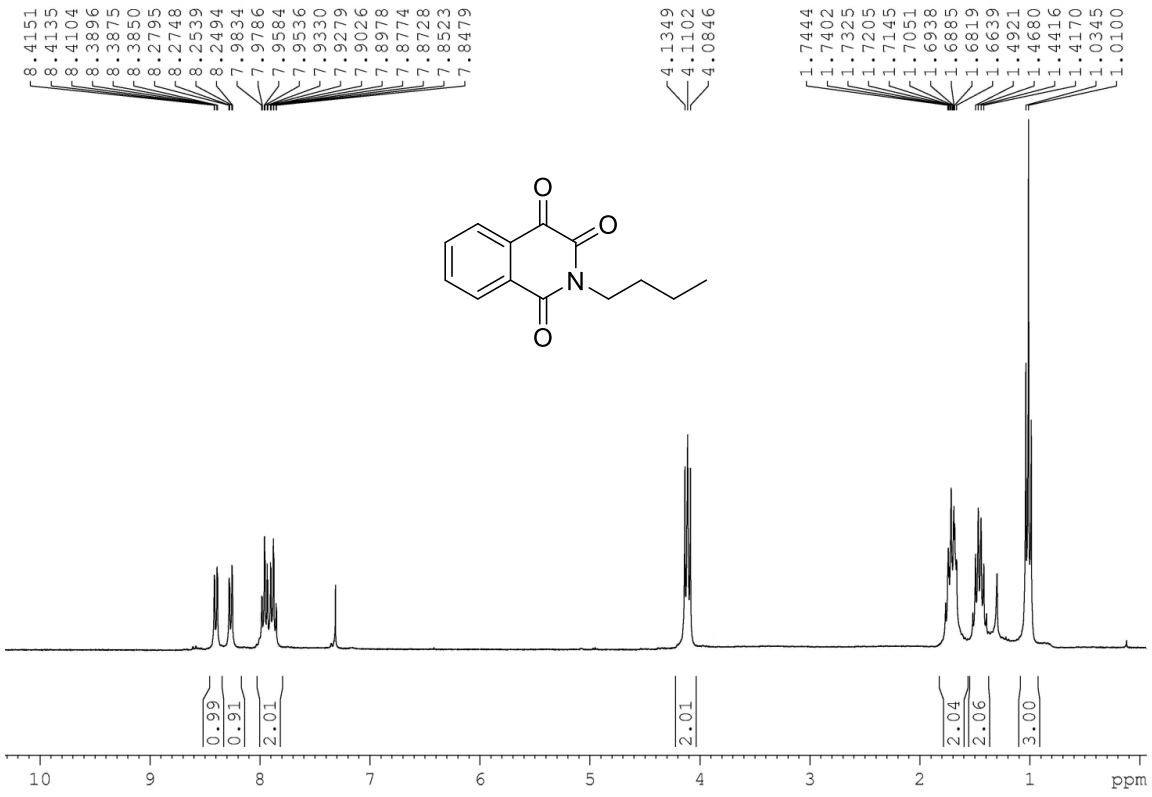
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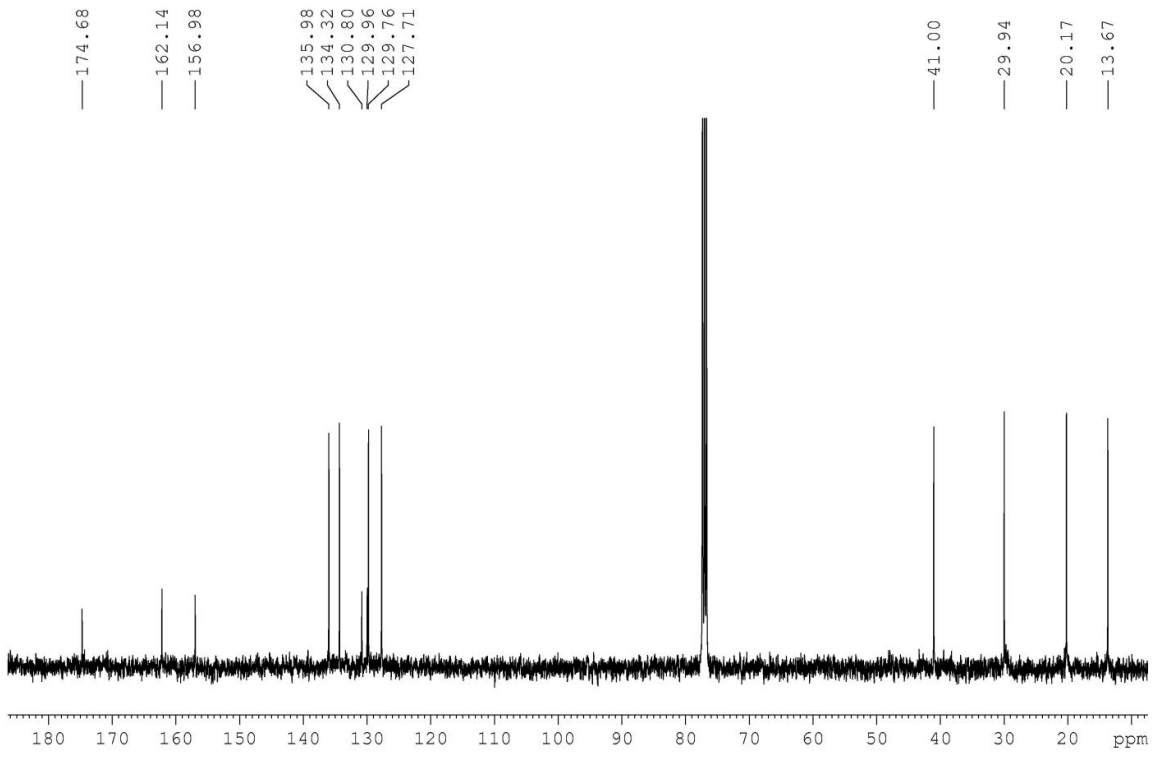
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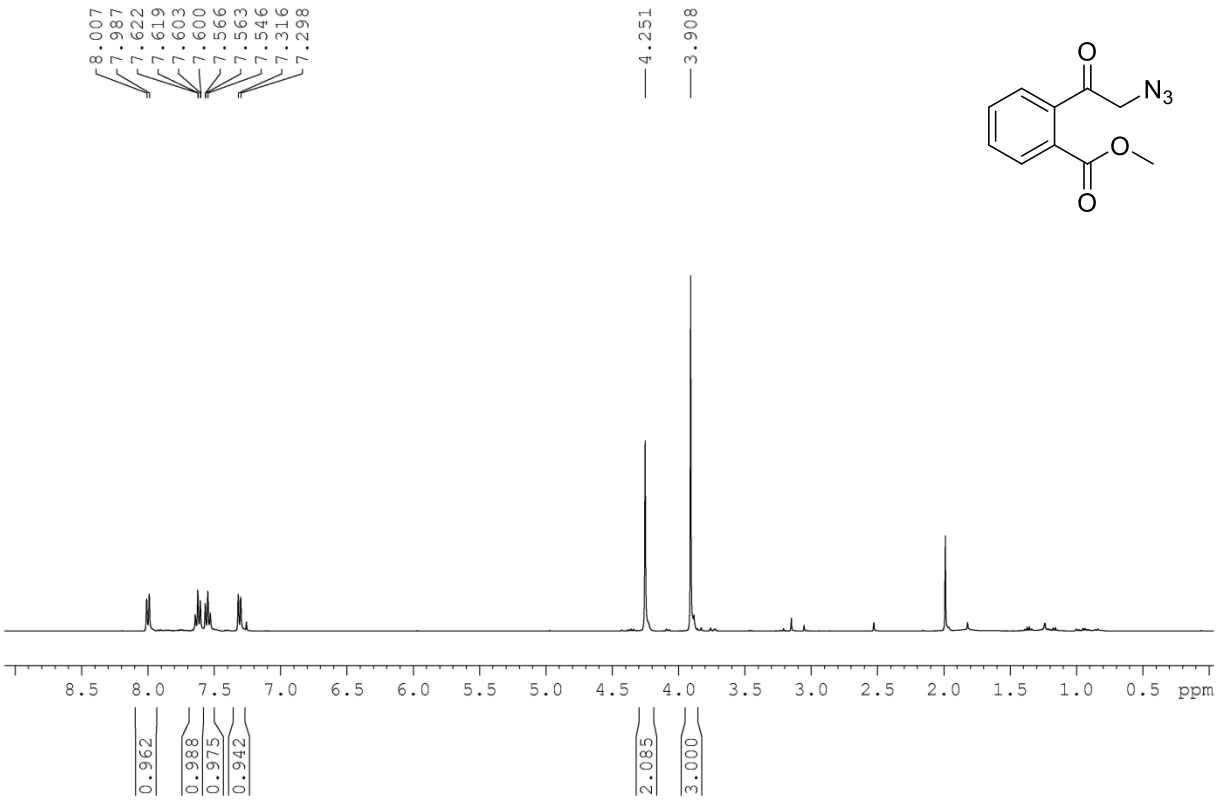
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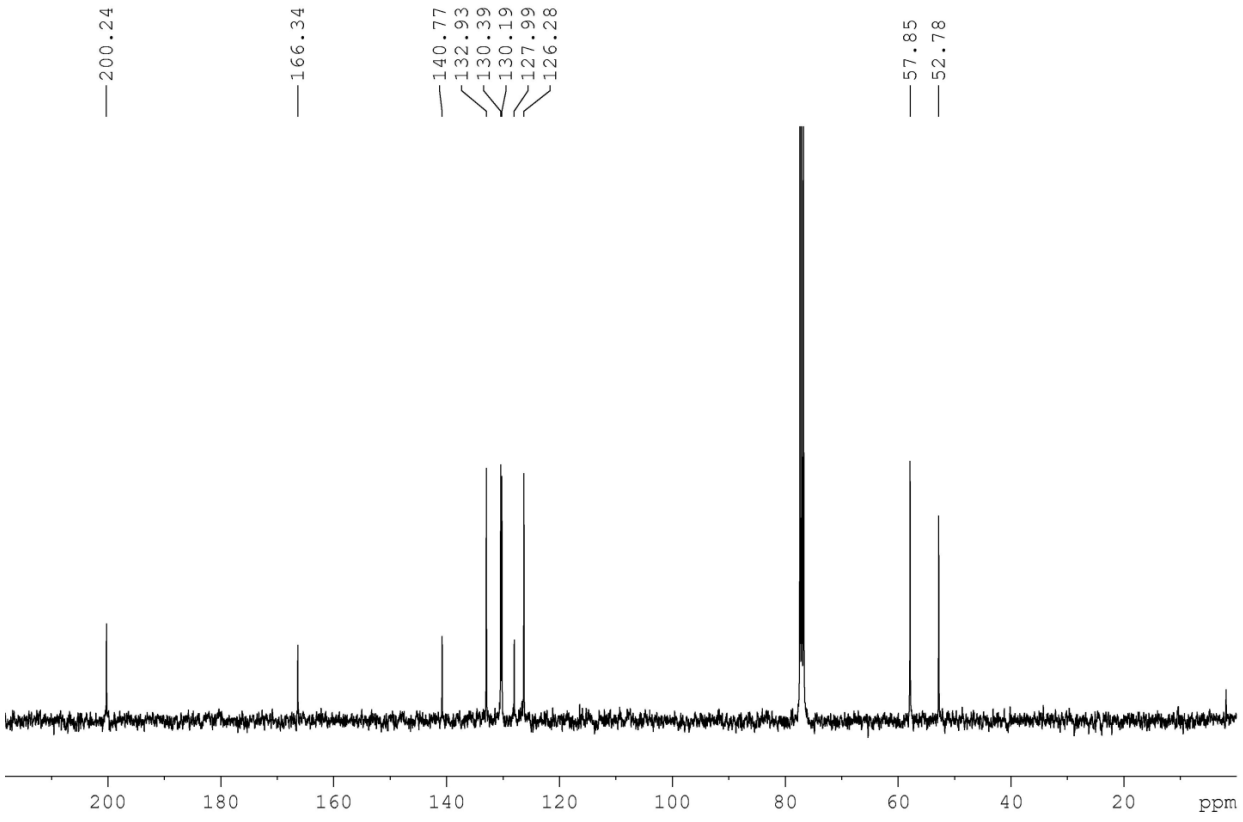
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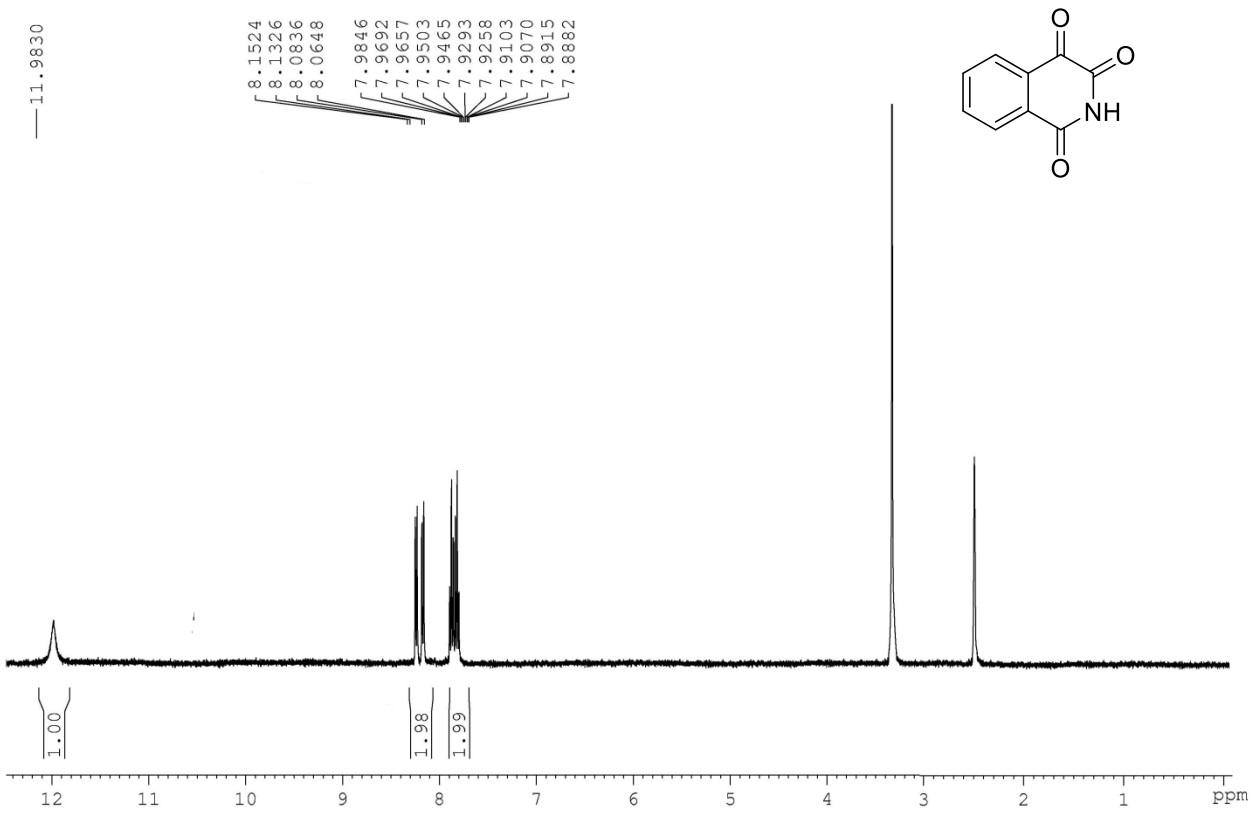
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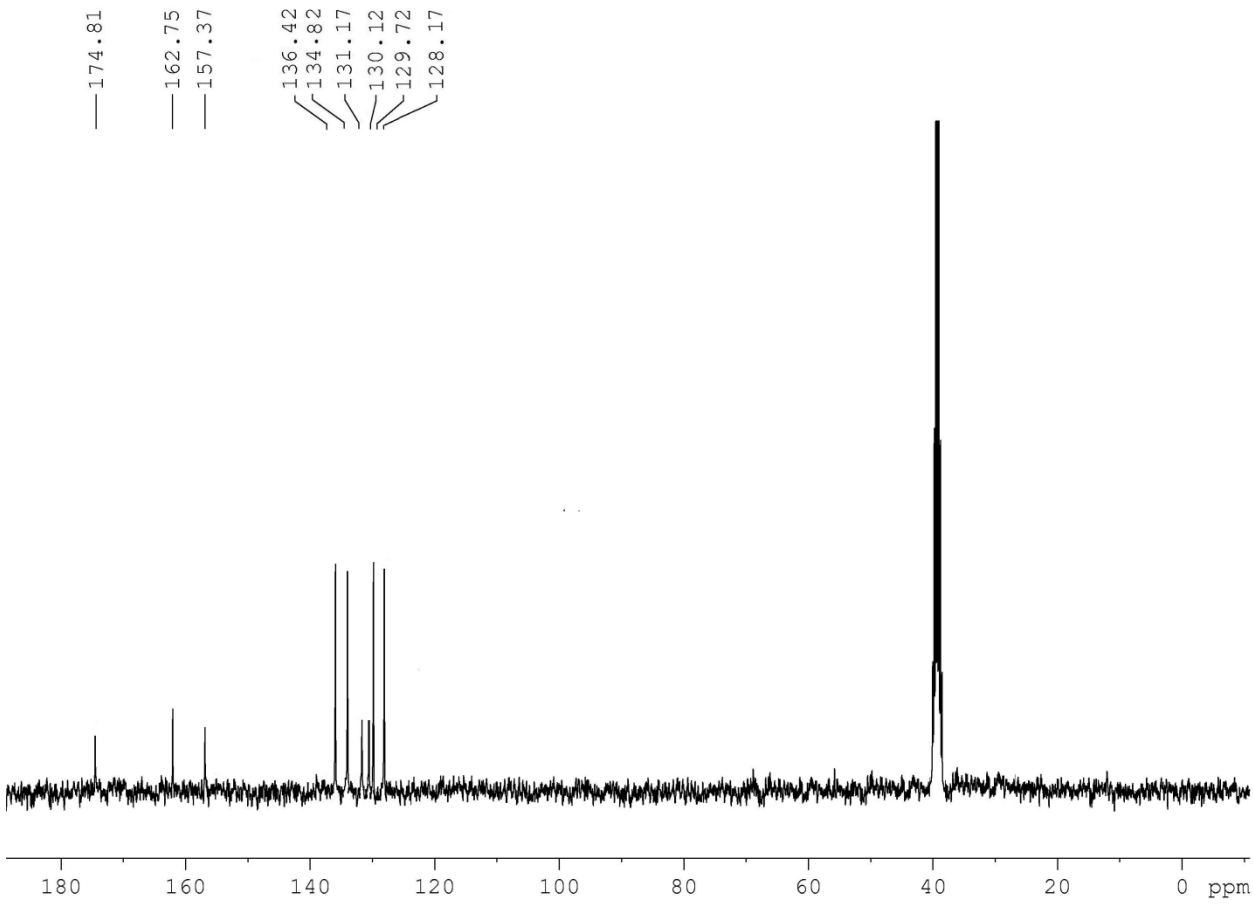
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