Electronic Supplementary Material (ESI) for RSC Advances.

Ring-Opening Cyclization of Activated Spiroaziridine Oxindoles with Heteroarenes: A Facile Synthetic Approach to Spiroxindole Fused Pyrroloindolines

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Contents

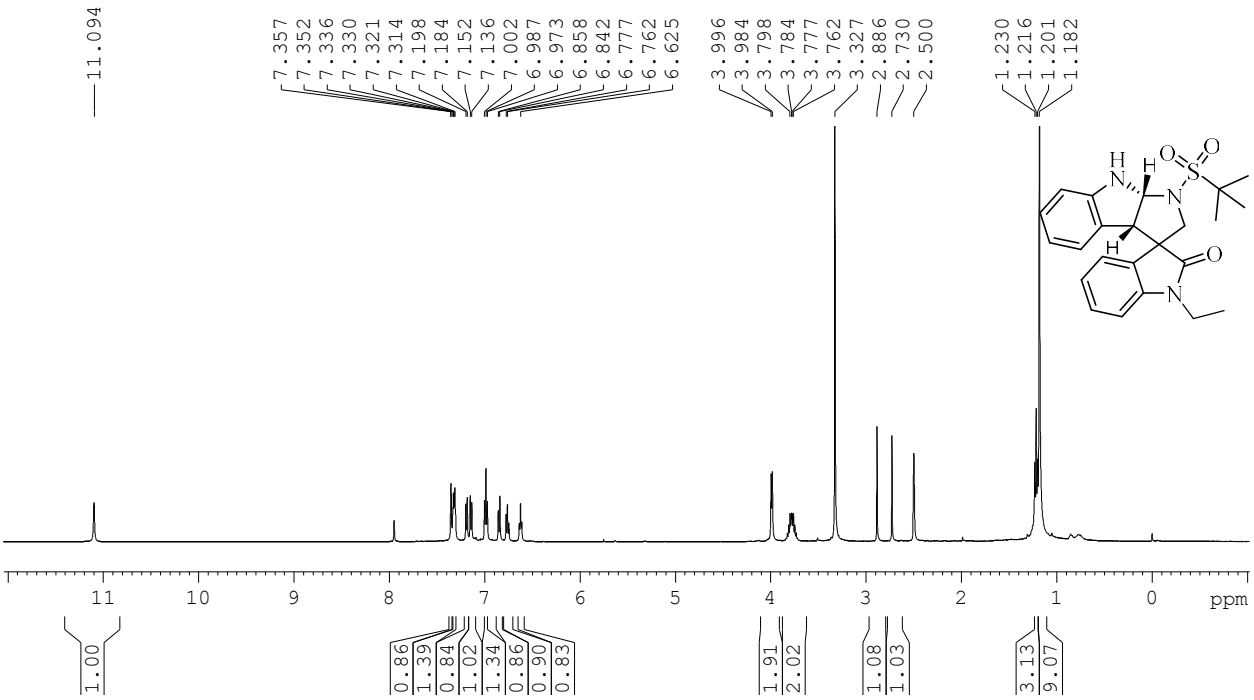
X-ray Crystallography: X-ray data for the compound KA7788 was collected at room temperature on a Bruker D8 QUEST instrument with an IμS Mo microsource (λ = 0.7107 A) and a PHOTON-100 detector. The raw data frames were reduced and corrected for absorption effects using the Bruker Apex 3 software suite programs.[1]The structure was solved using intrinsic phasing method[2] and further refined with the SHELXL[2] program and expanded using Fourier techniques. Anisotropic displacement parameters were included for all non-hydrogen atoms. All C bound H atoms were positioned geometrically and treated as riding on their parent C atoms [C-H = 0.93-0.97 Å, and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H or $1.2U_{eq}(C)$ for other H atoms]. The crystal was found to be twinned. The structure was refined using the hklf 5 routine with all reflections, resulting in a BASF value of 0.095 (2).

Crystal structure determination of [KA778_TWIN]

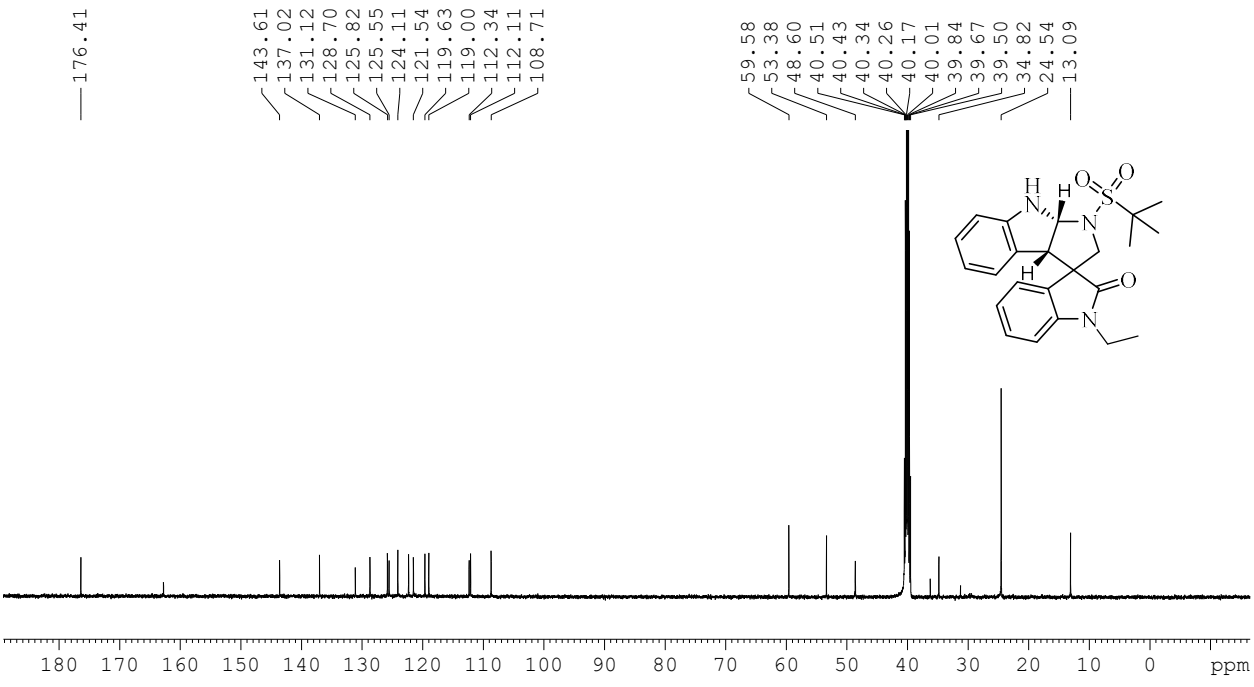
Crystal Data for $C_{24}H_{28}N_3O_3ClS$ (*M* =474.00 g/mol): tetragonal, space group $P4_3$ (no. 78), *a* = 7.53409(9) Å, *c* = 42.4001(5) Å, *V* = 2406.74(6) $Å^3$, *Z* = 4, *T* = 294.15 K, μ(MoKα) = 0.276 mm^{-1}, *Dcalc* = 1.308 g/cm^3, 18924 reflections measured (5.408° ≤ 2Θ ≤ 52.498°), 18924 unique (R_{sigma} = 0.1111) which were used in all calculations. The final R_1 was 0.0689 (I >2σ(I)) and wR_2 was 0.1363 (all data). CCDC 1970416 contains supplementary Crystallographic data for the structure. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0) 1223 336 033; email: deposit@ccdc.cam.ac.uk].

References:

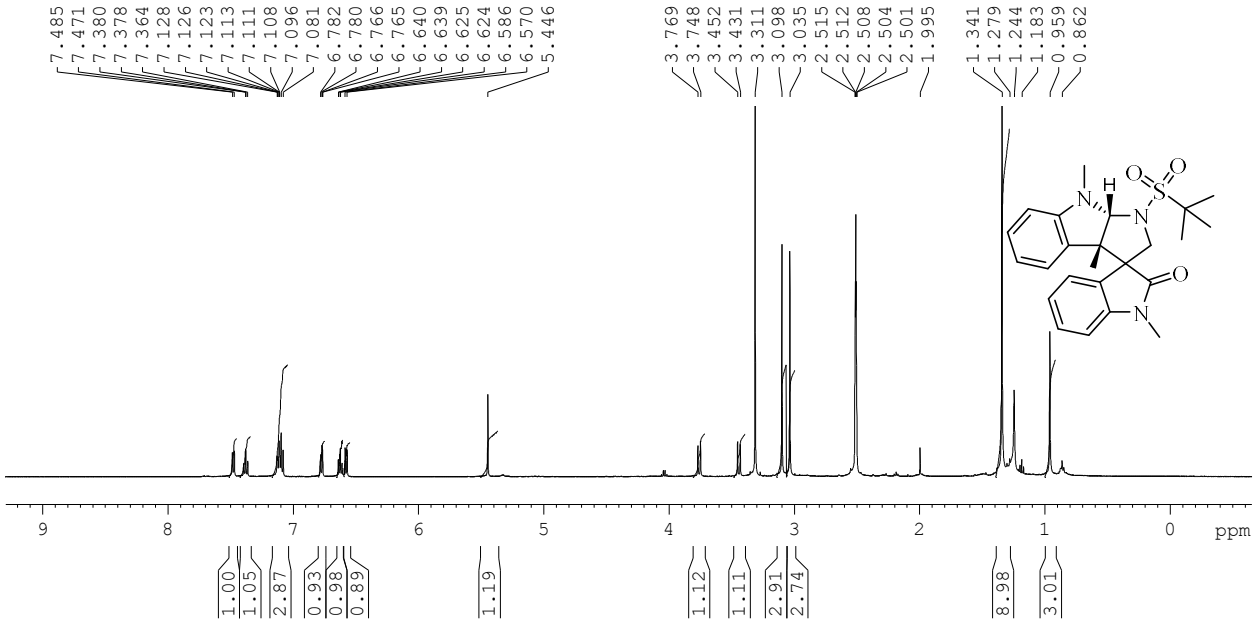
1. Bruker (2016). APEX3, SAINT and SADABS. Bruker AXS, Inc., Madison, Wisconsin, USA.
2. Sheldrick G. M. (2015**)** ActaCrystallogr C71: 3-8.



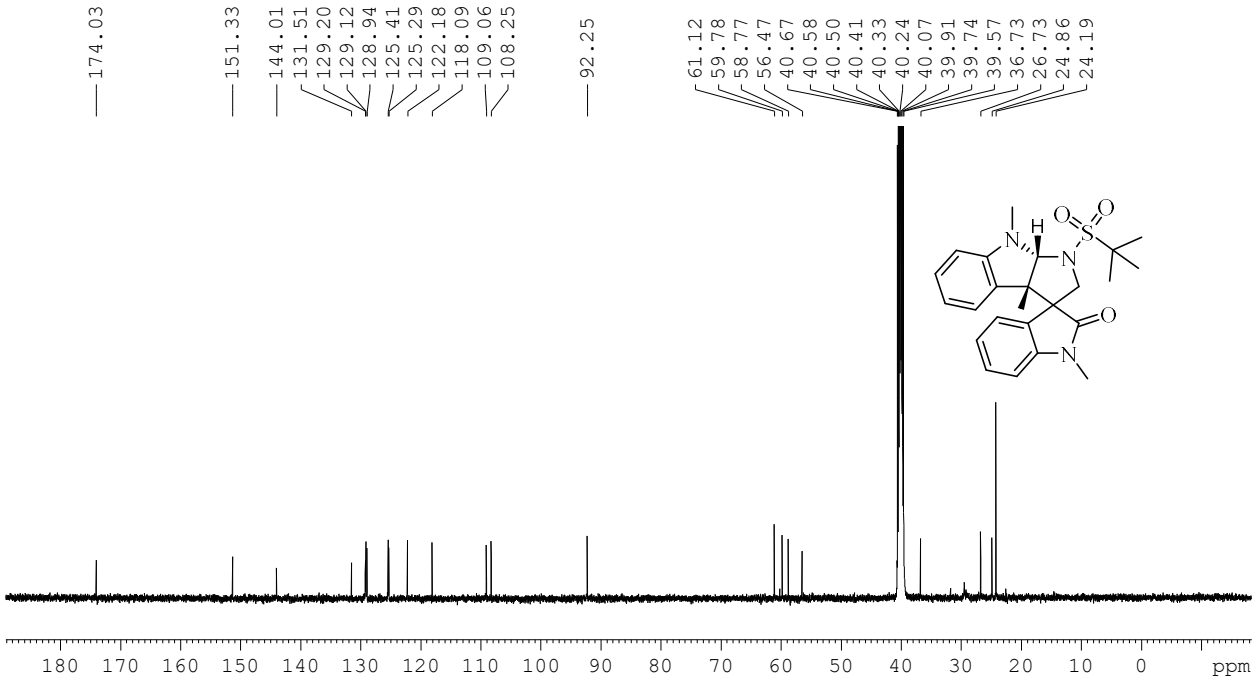
^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound 3a



^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound 3a



^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound 3b



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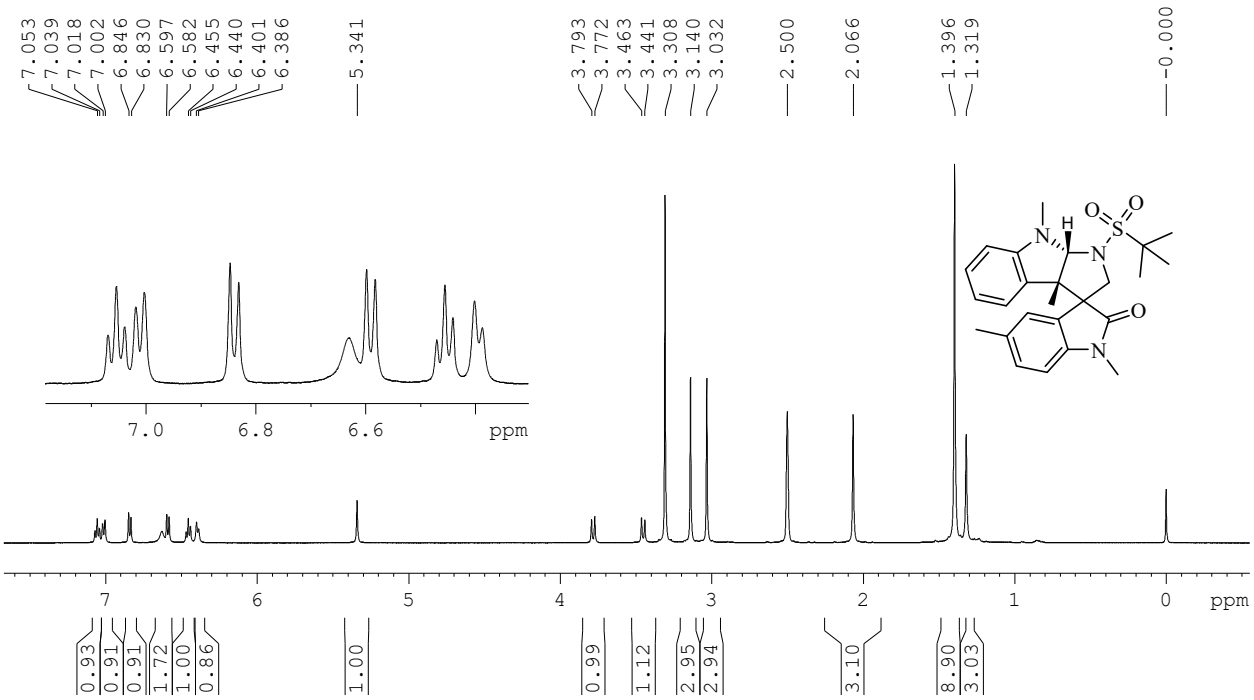
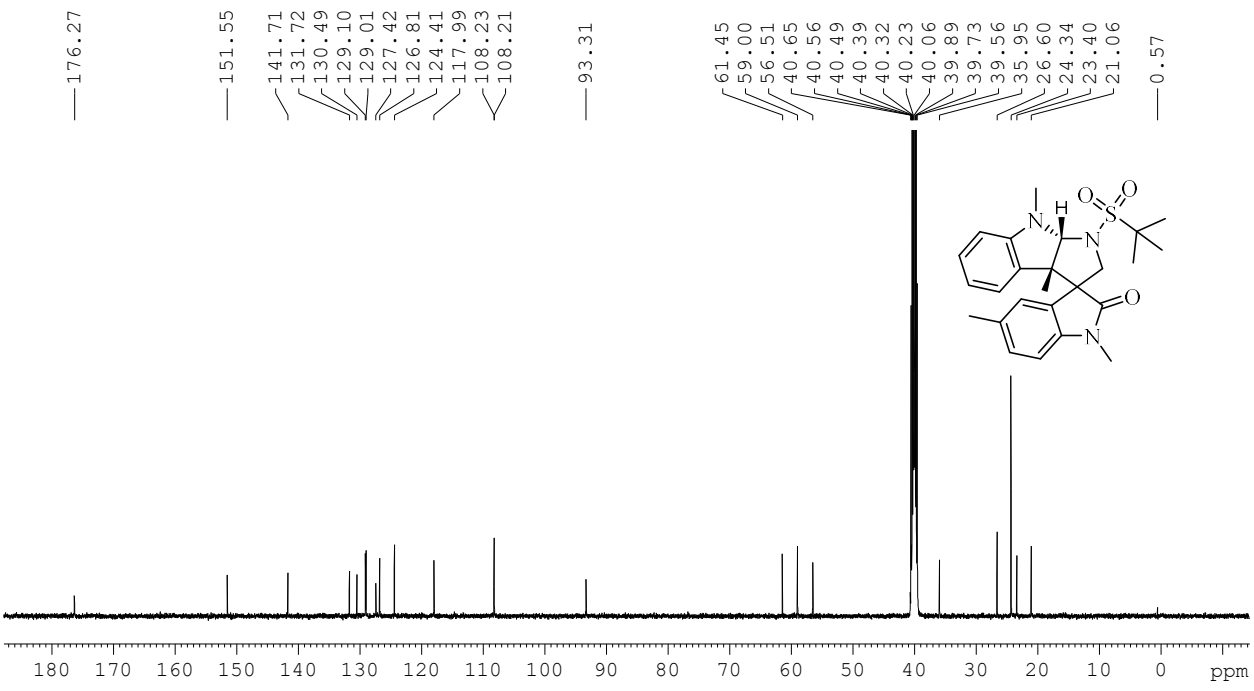


^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound 3c



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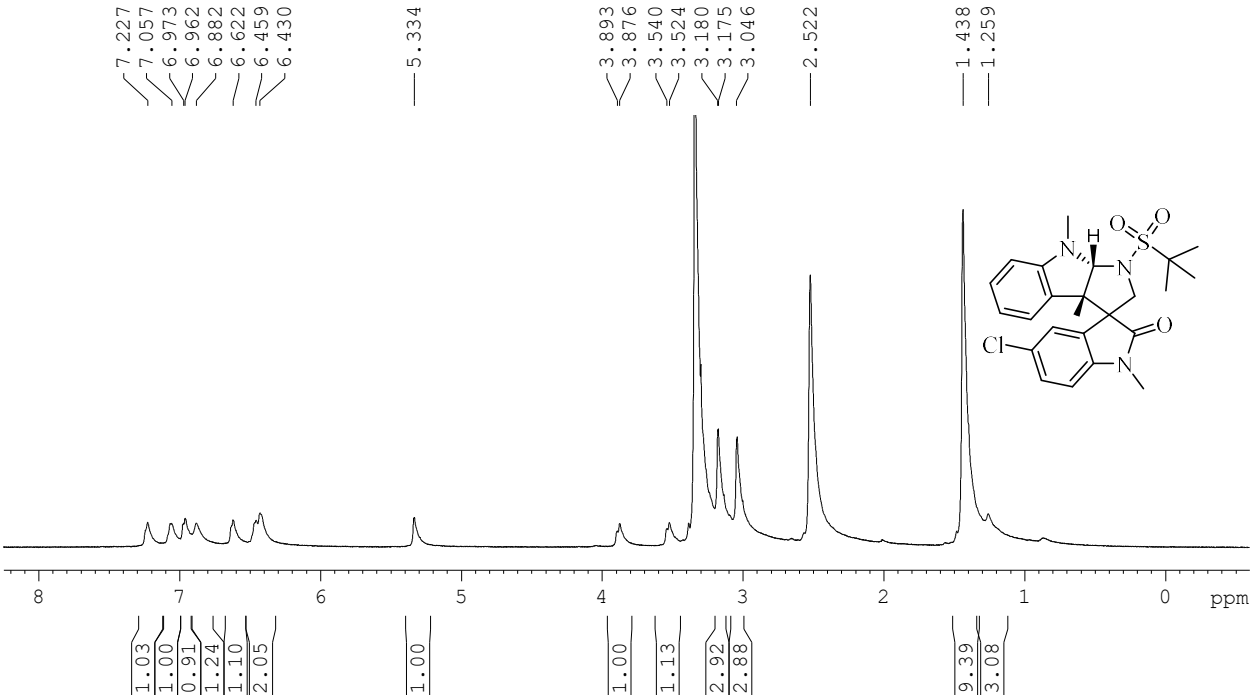

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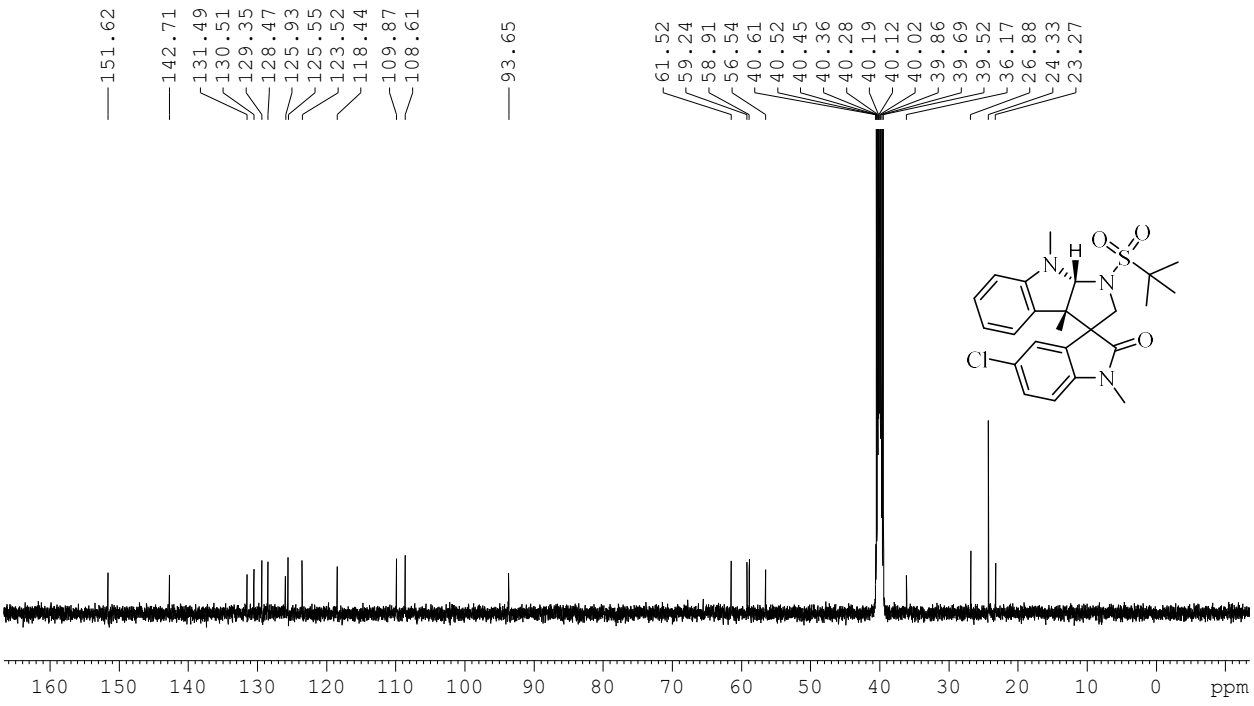

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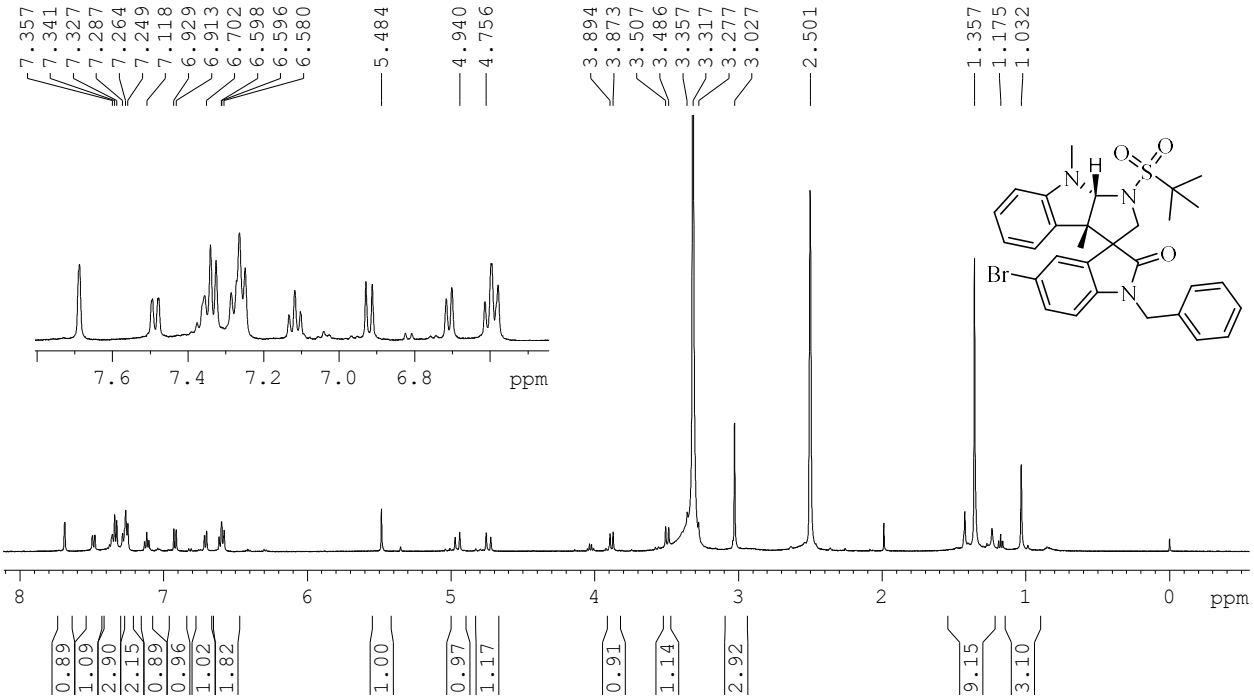

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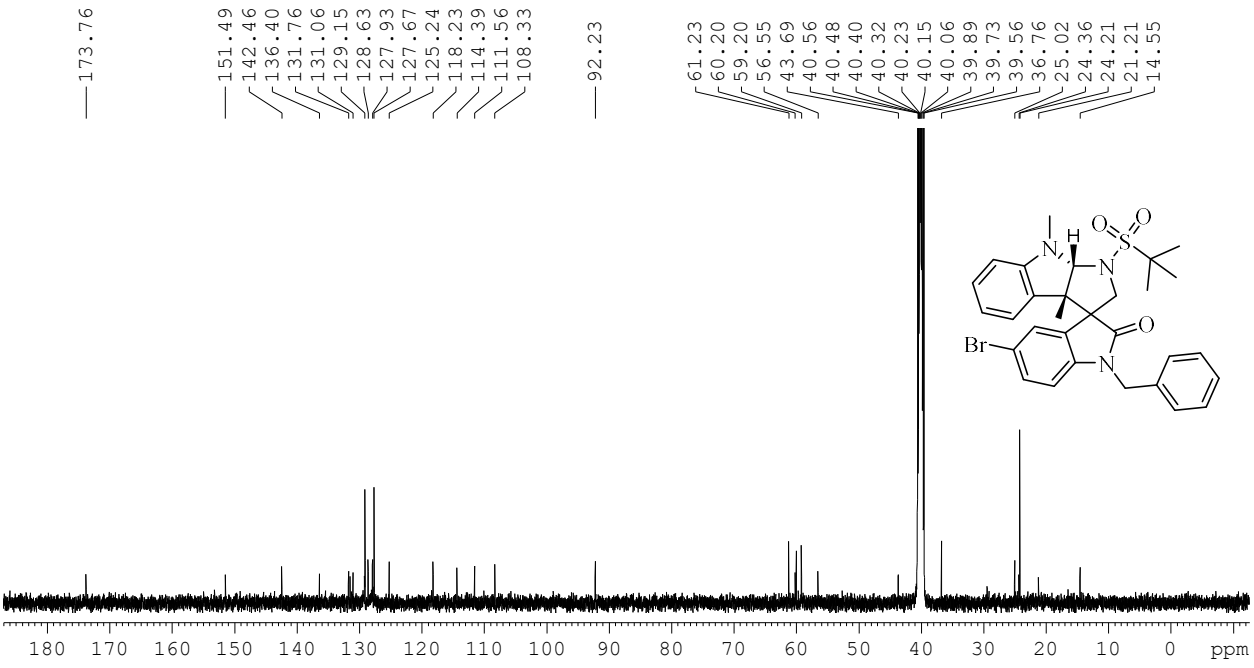
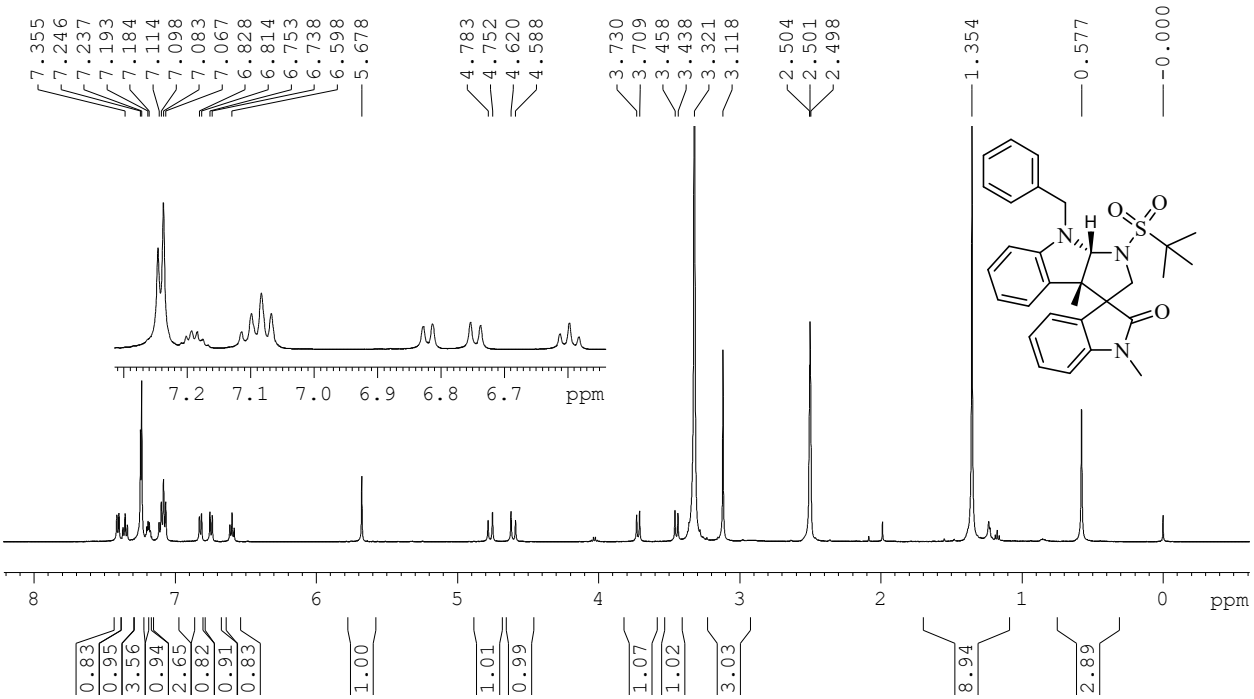


^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound 3e



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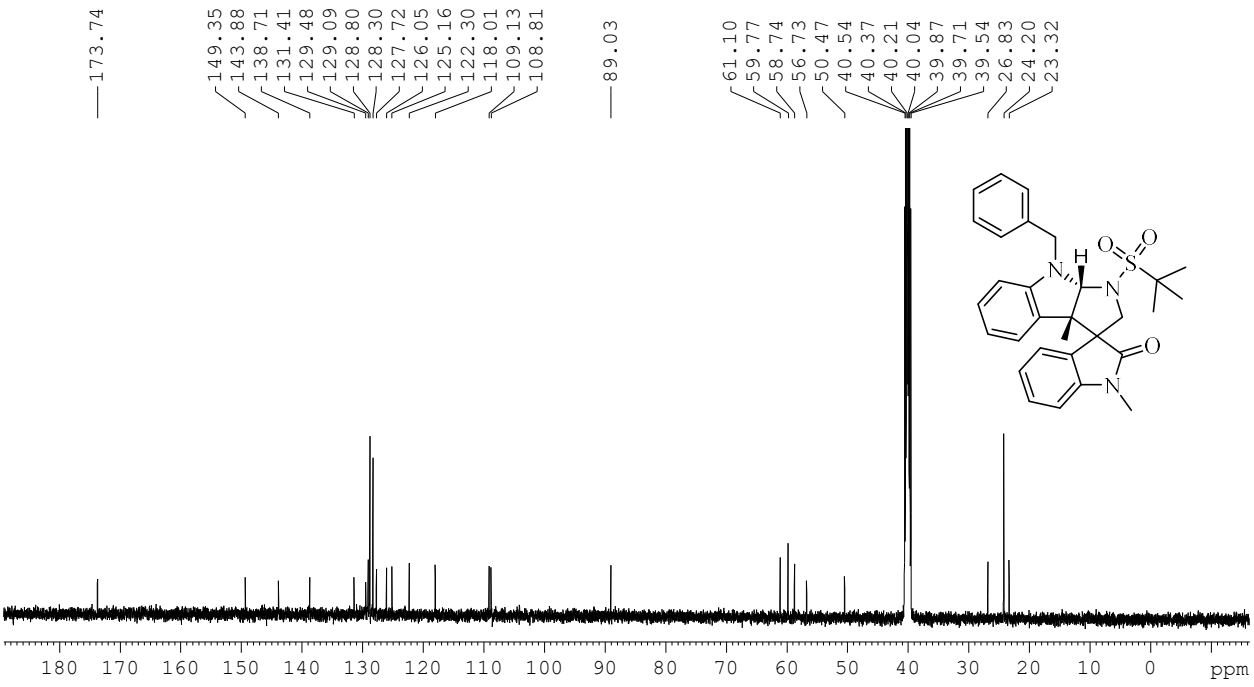

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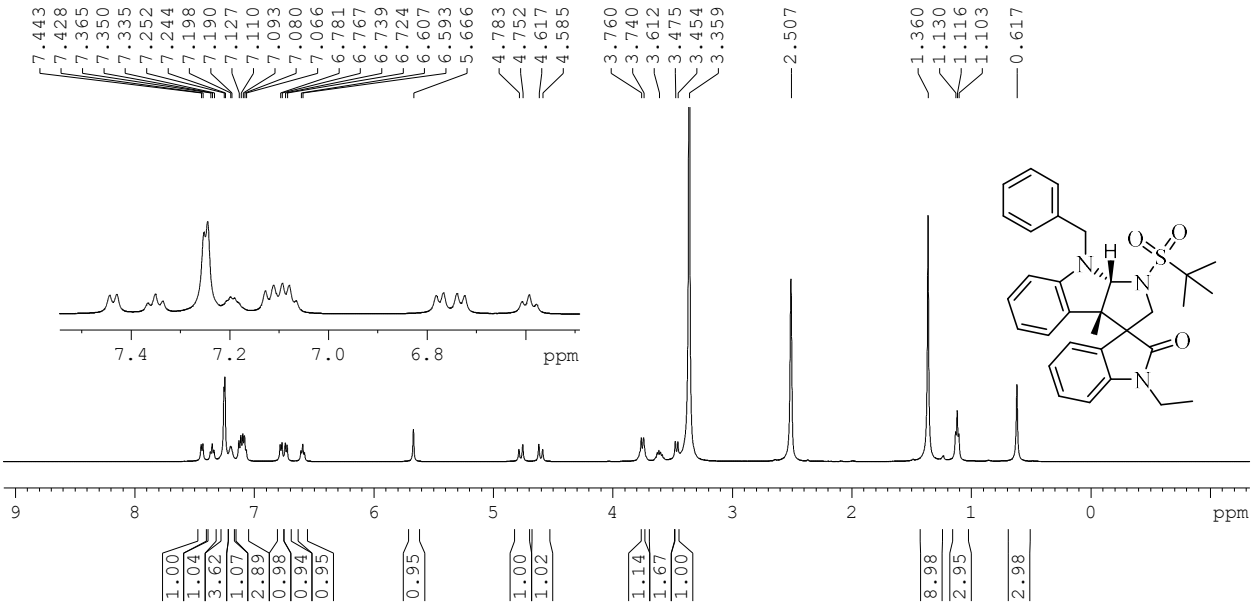

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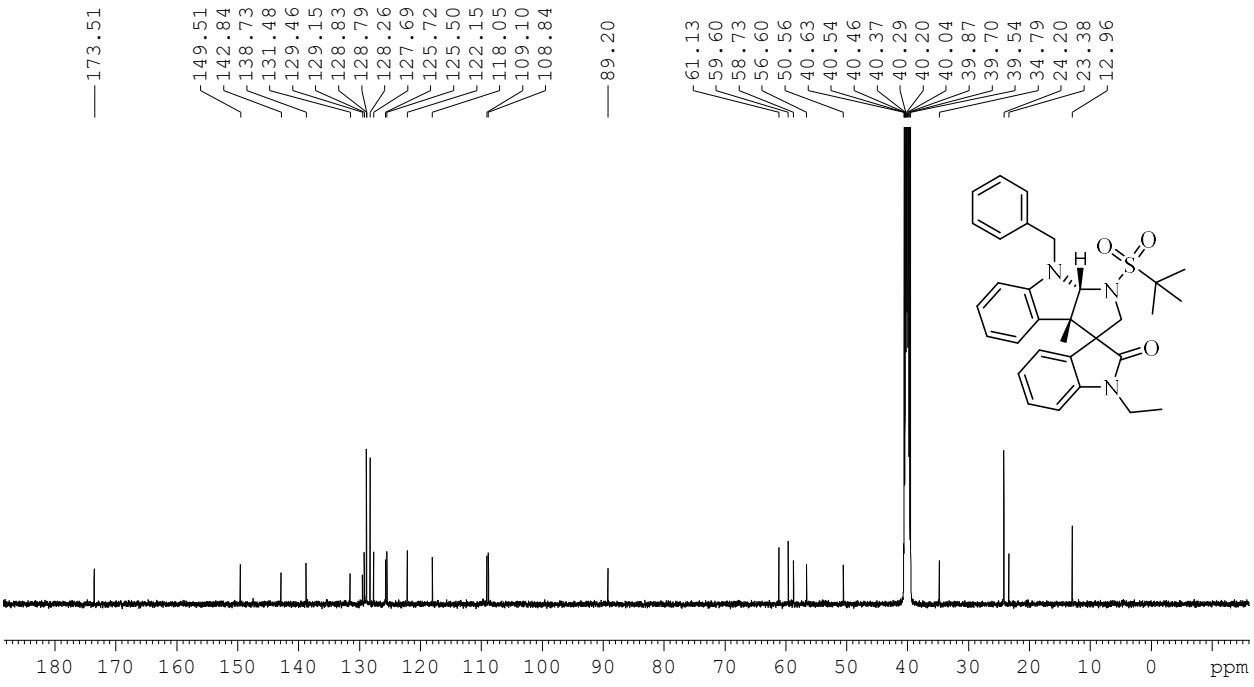

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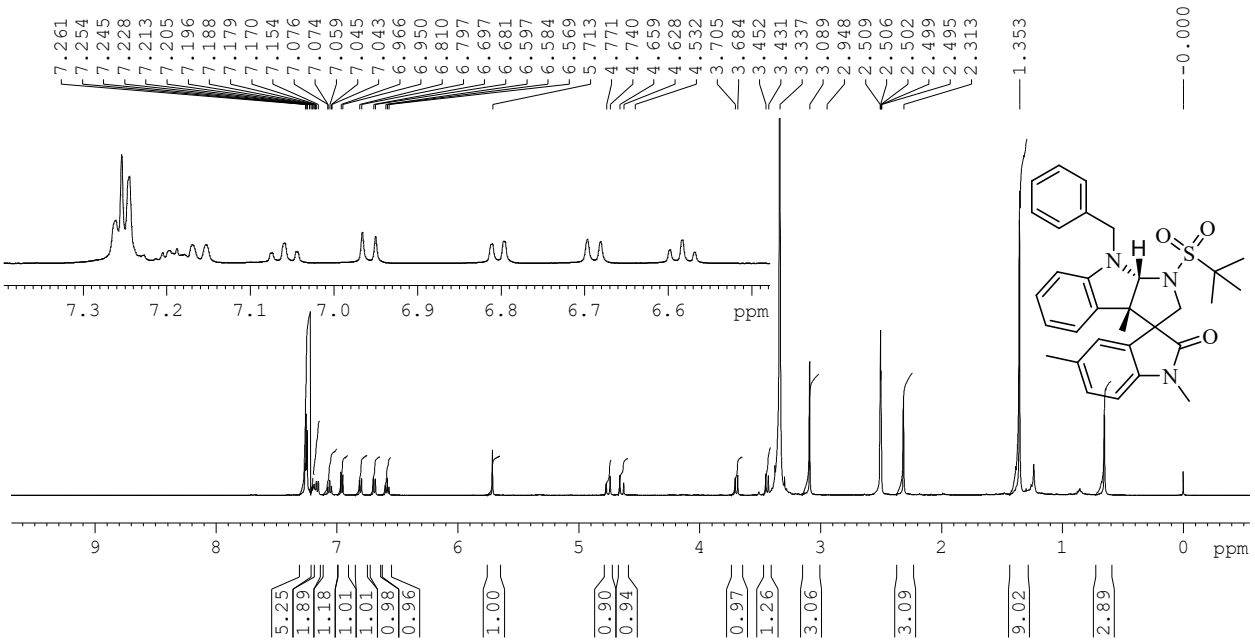

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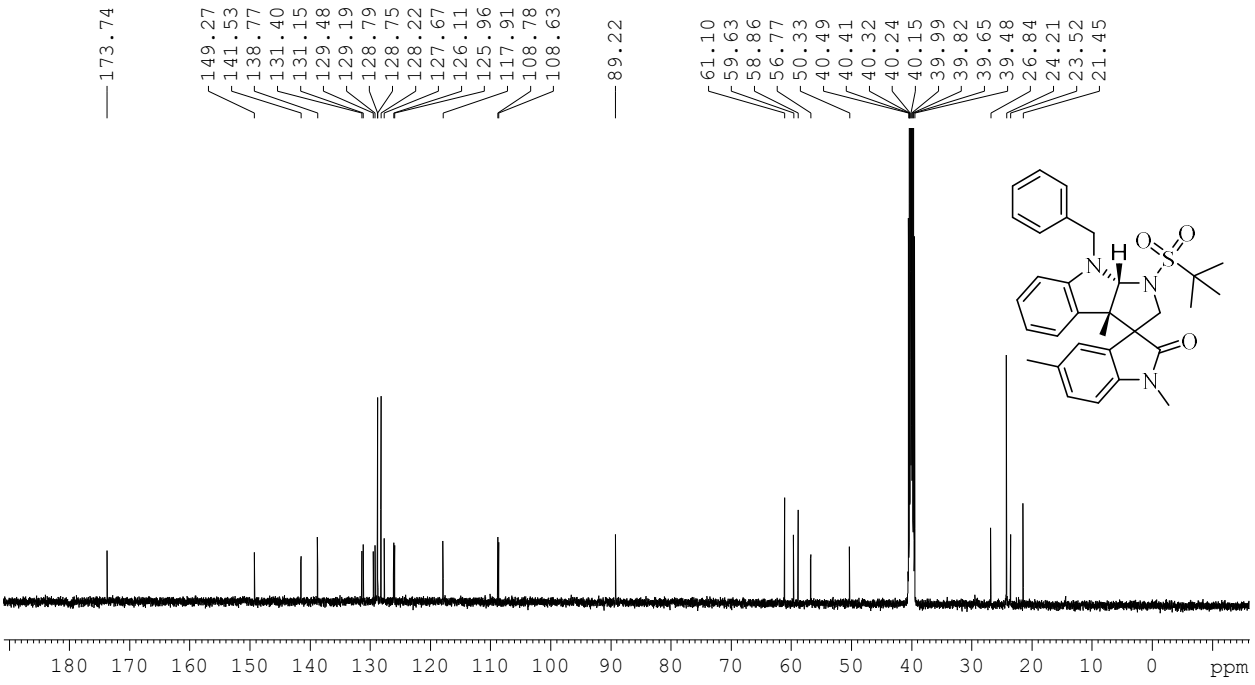
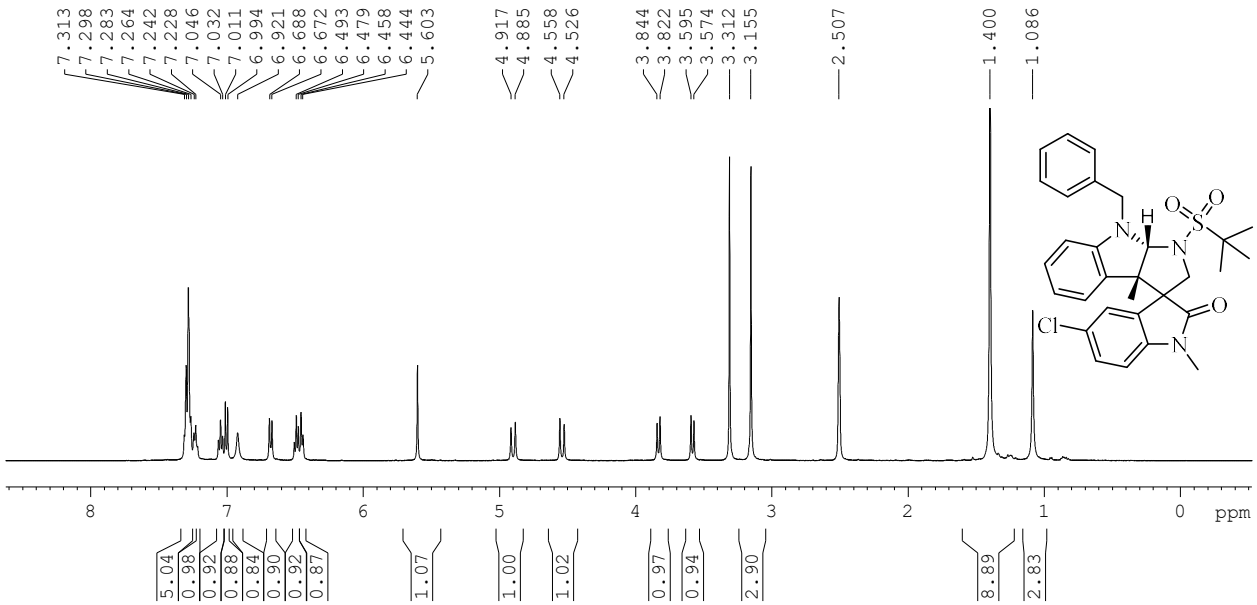


^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound 3h



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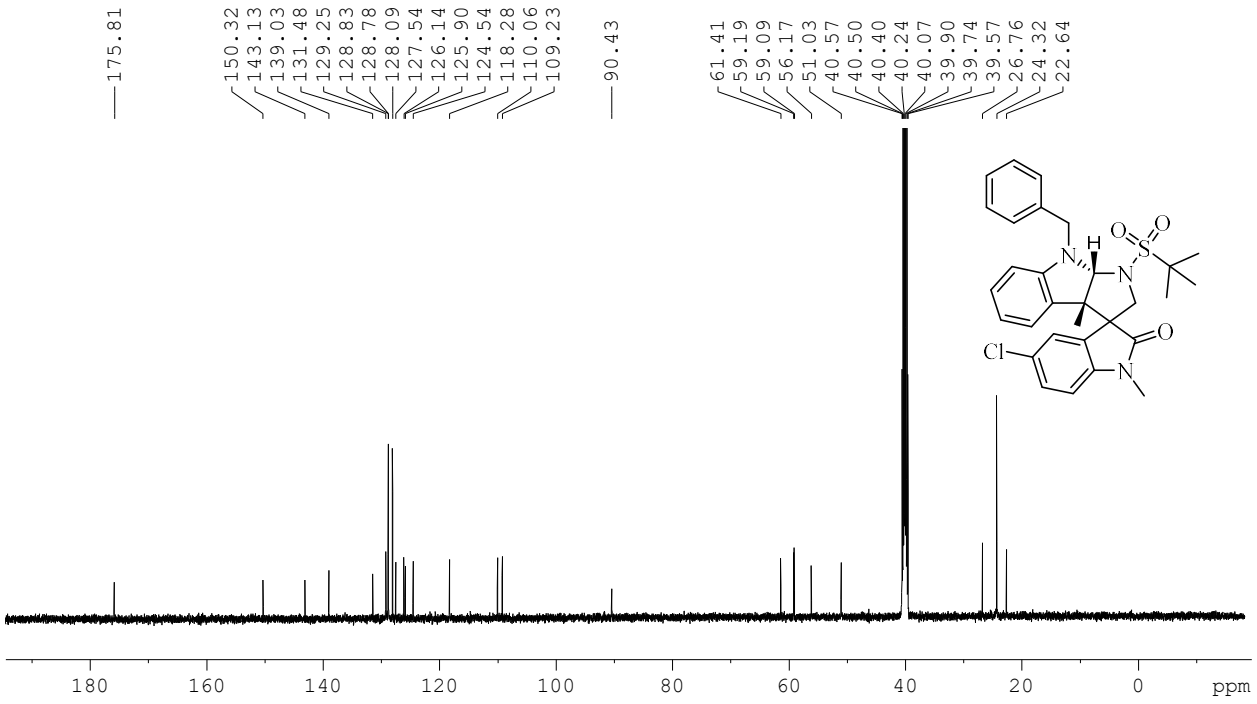

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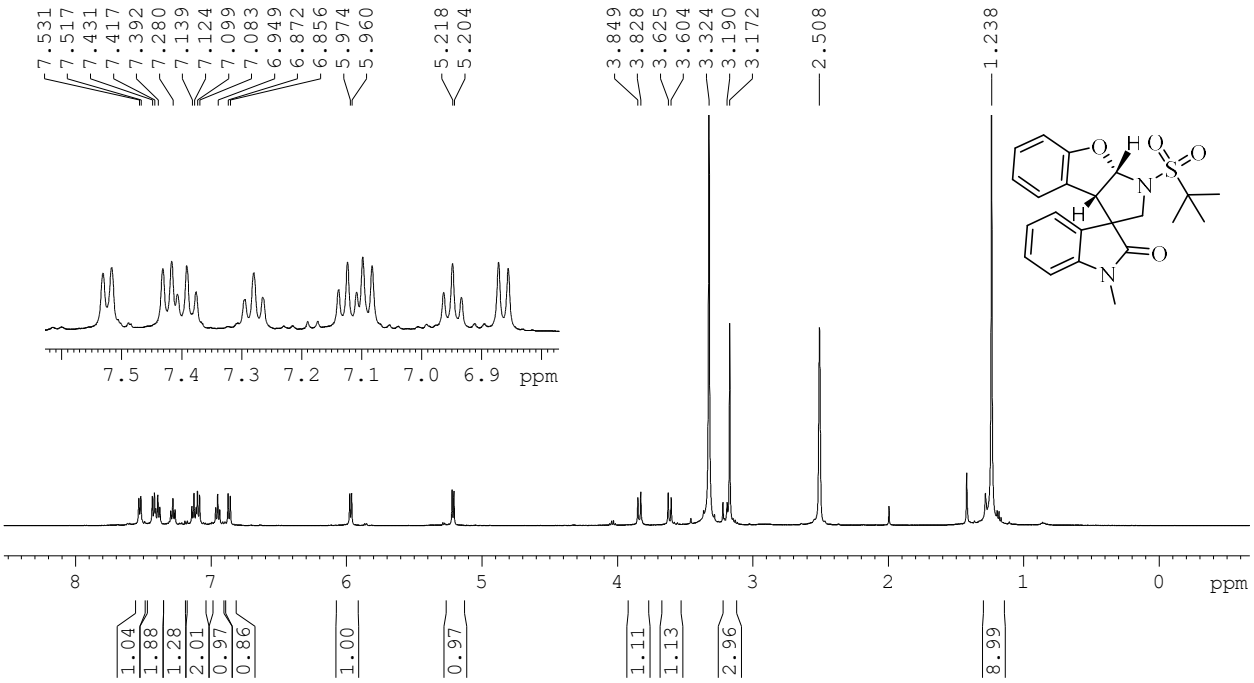
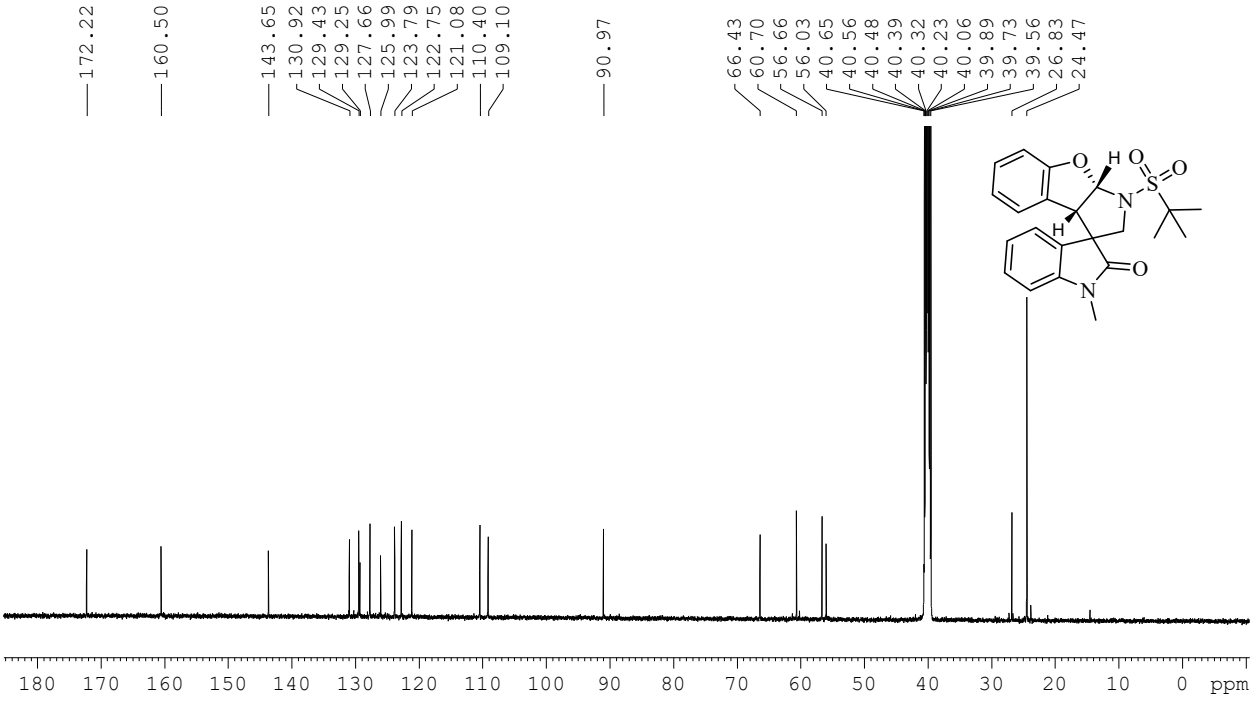


^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound 5a



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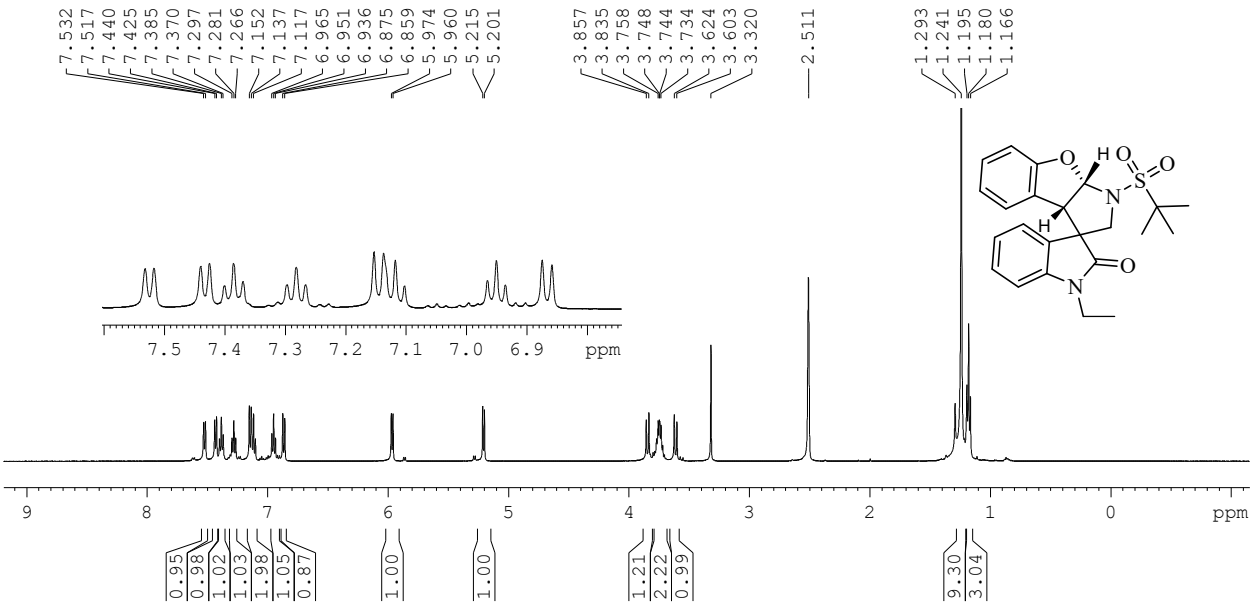

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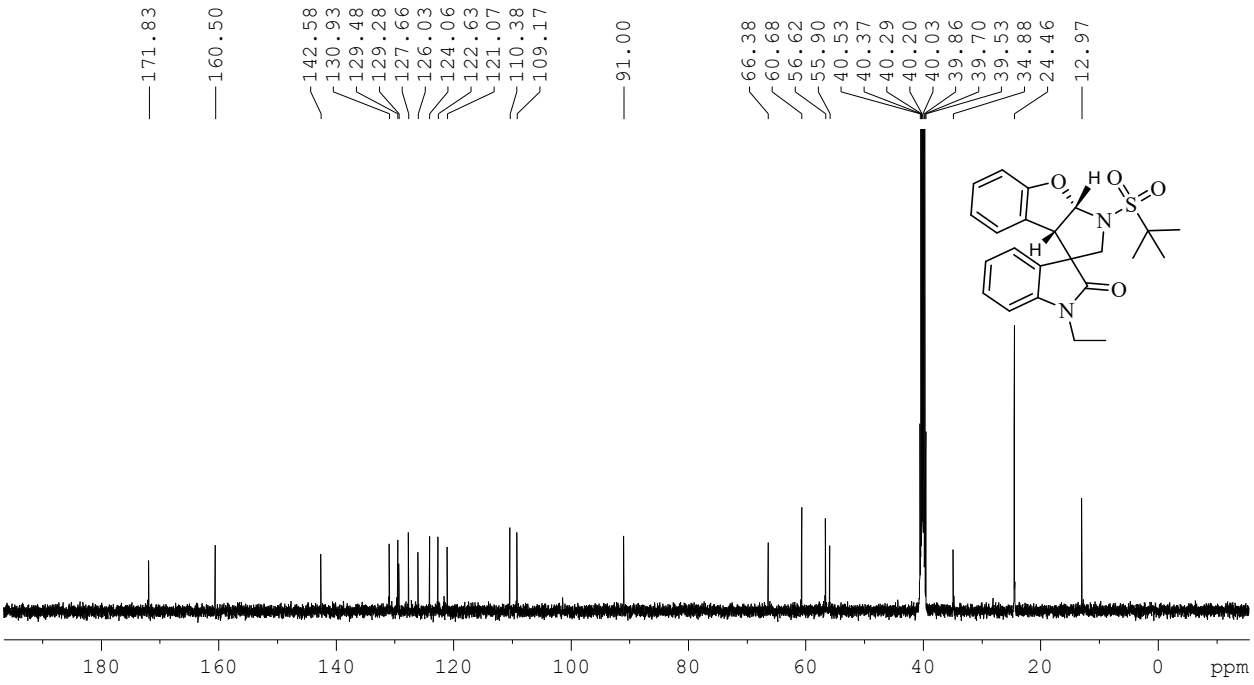

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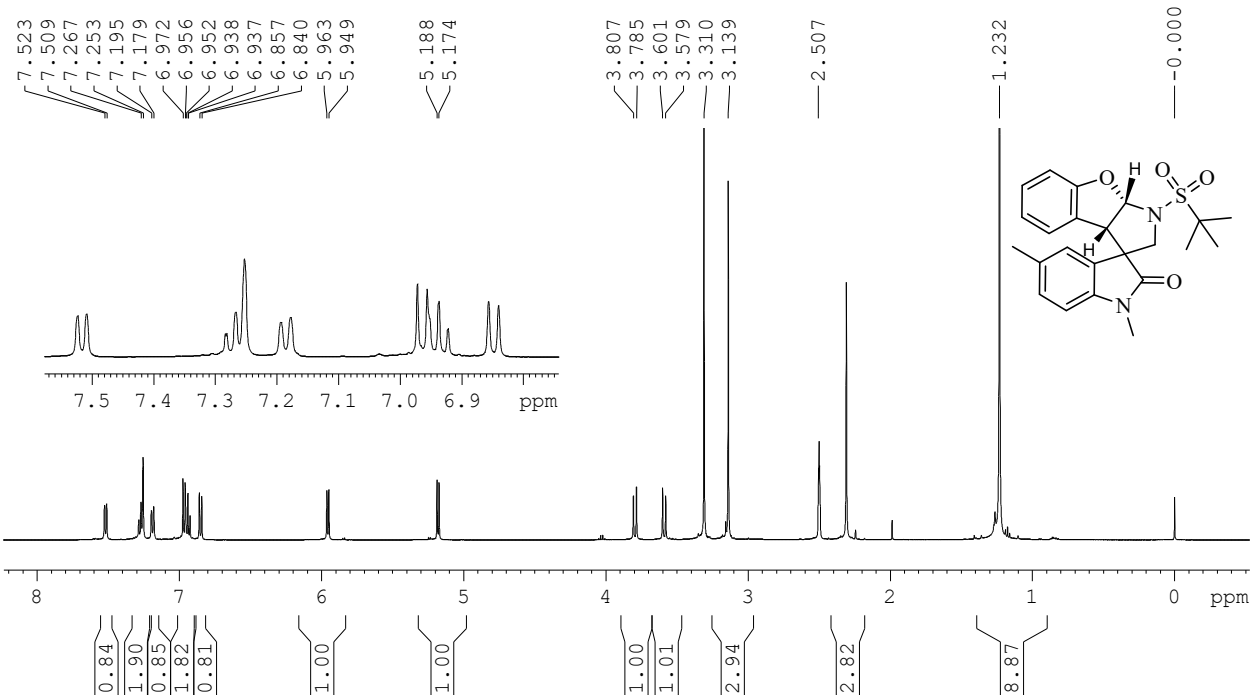

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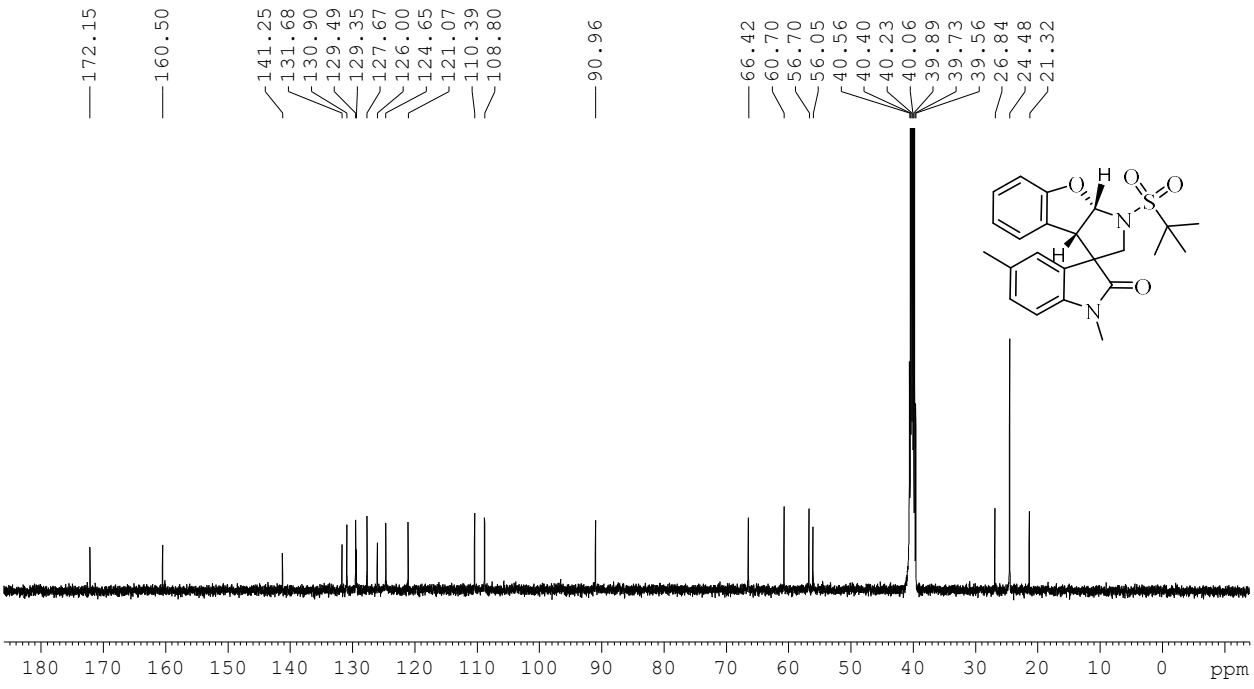

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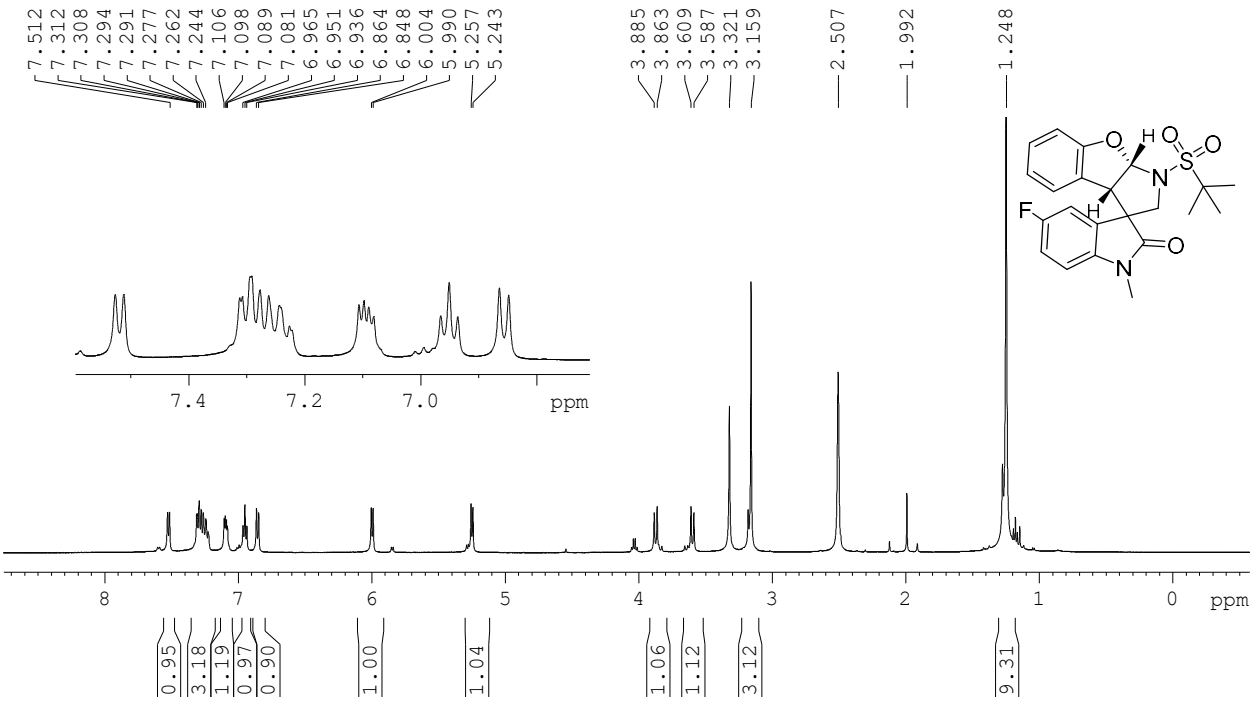

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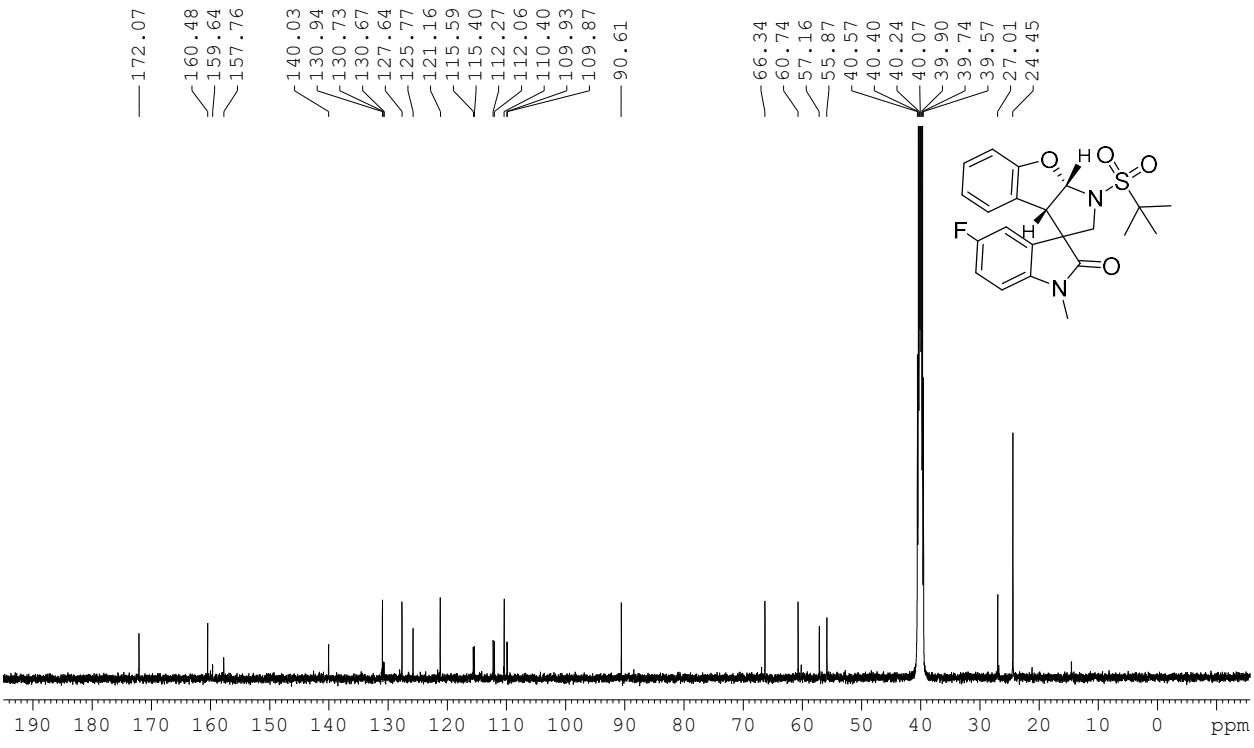

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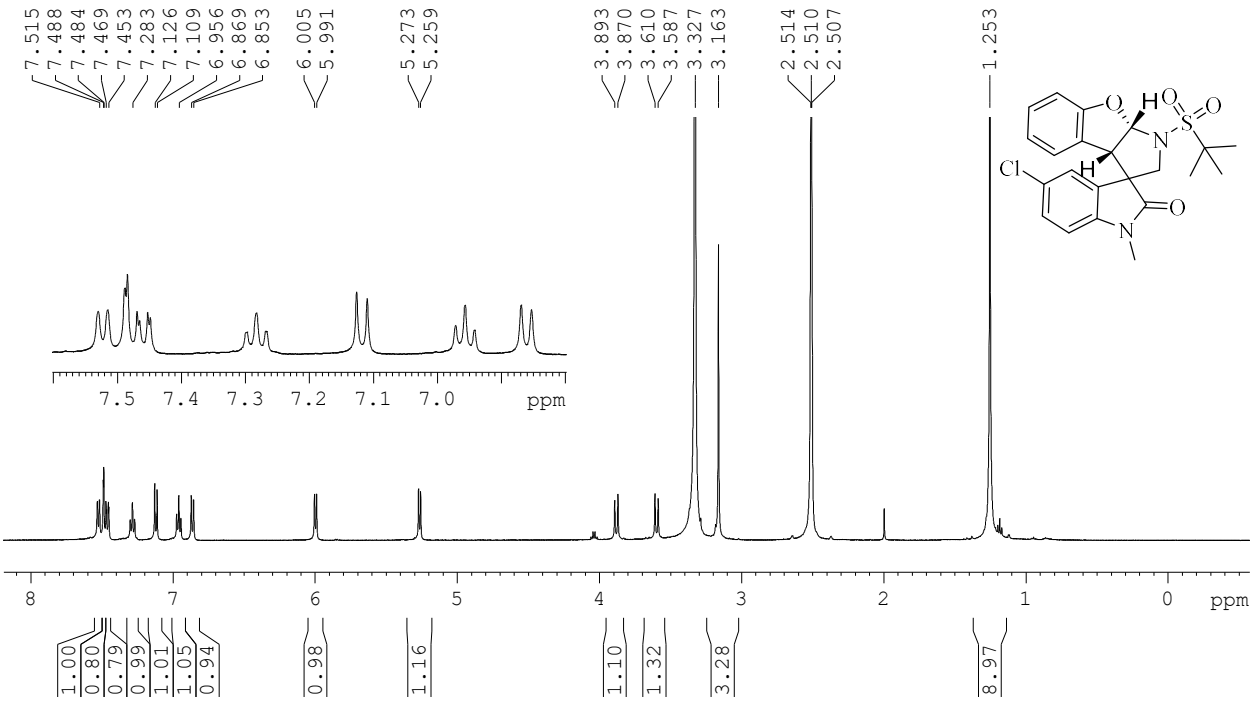

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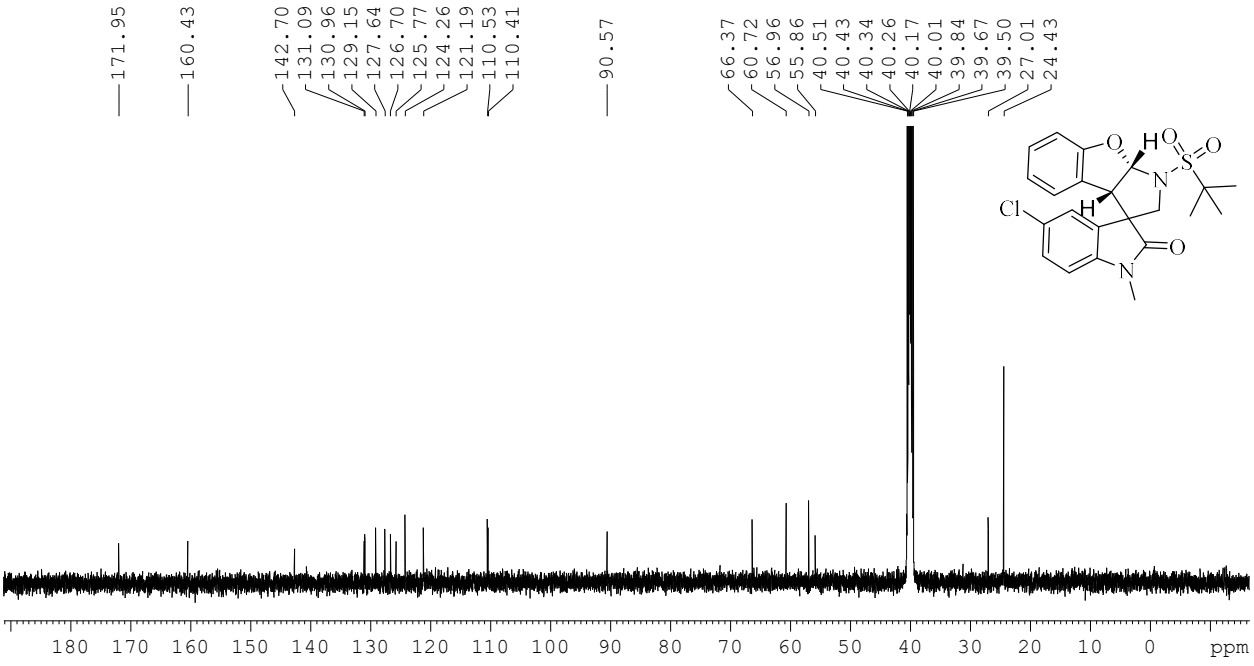

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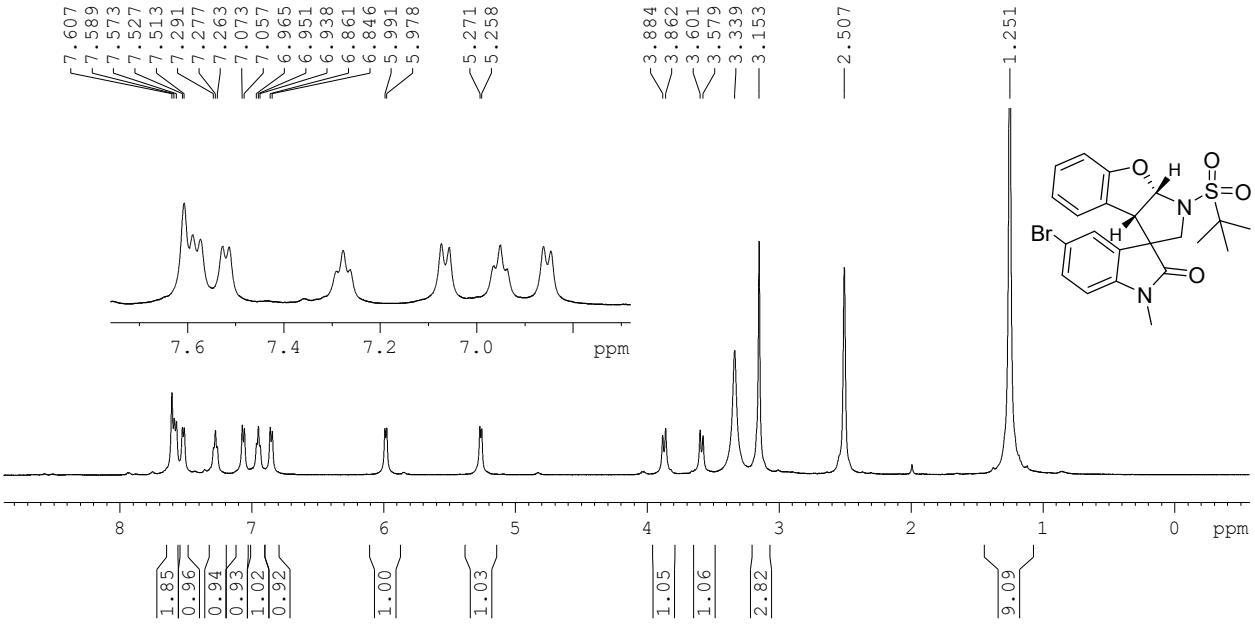

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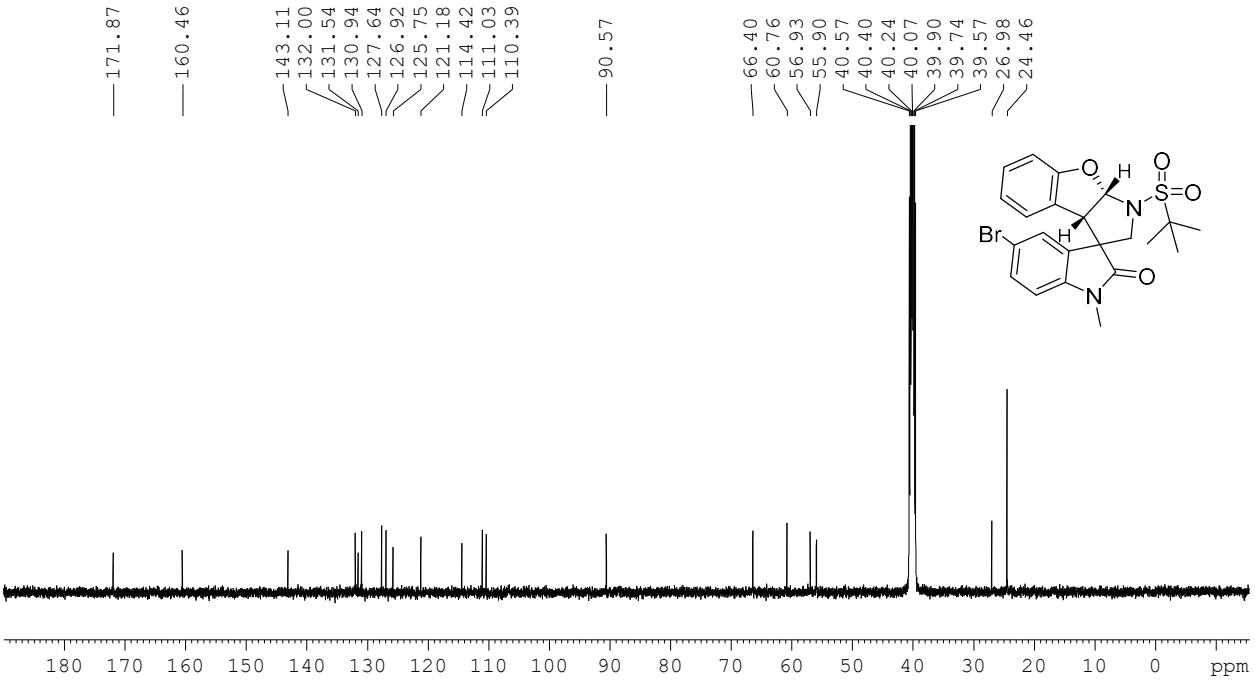

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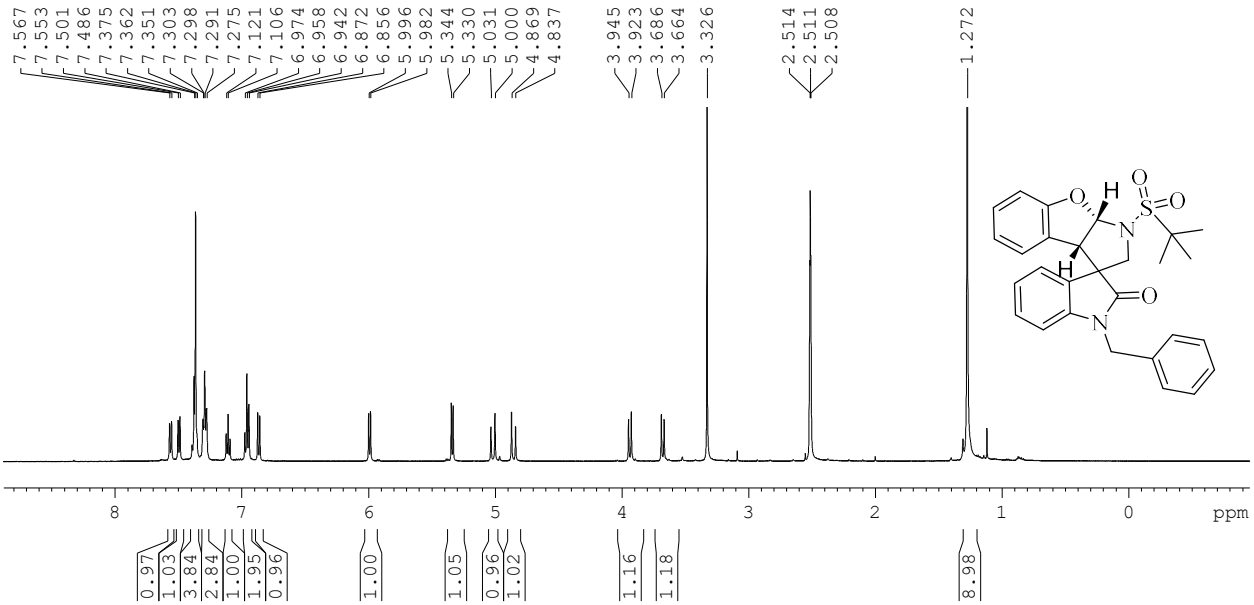

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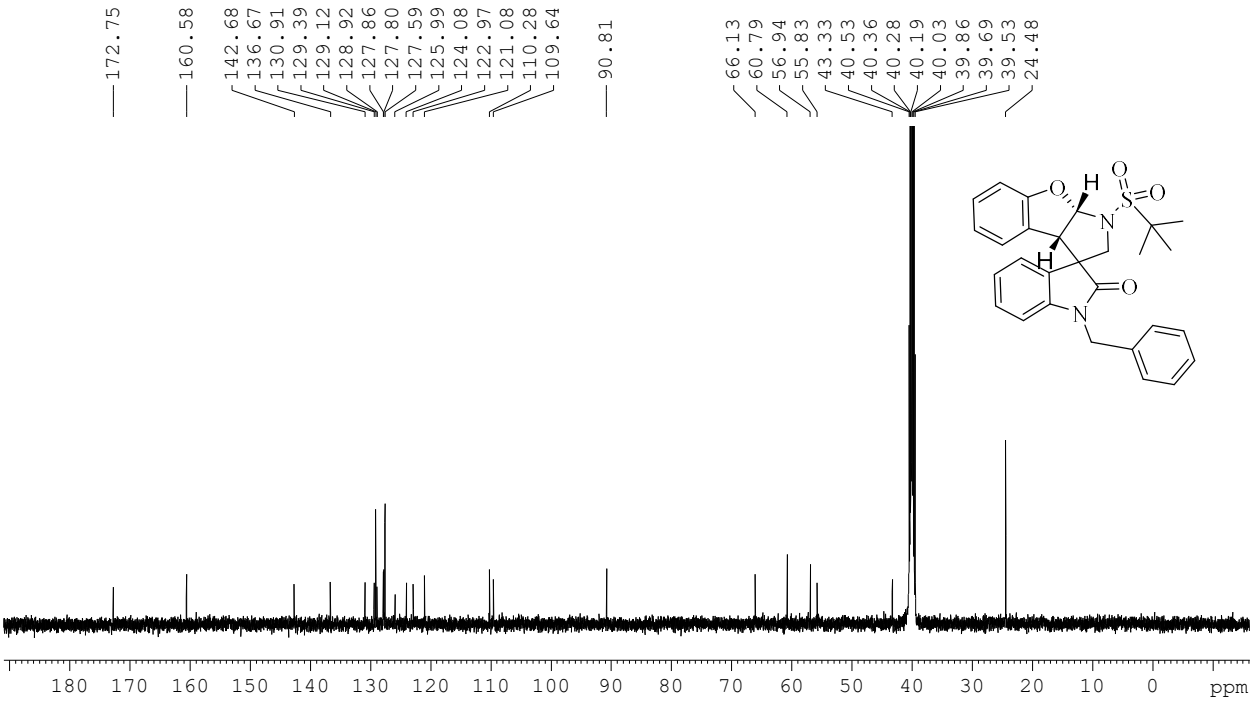

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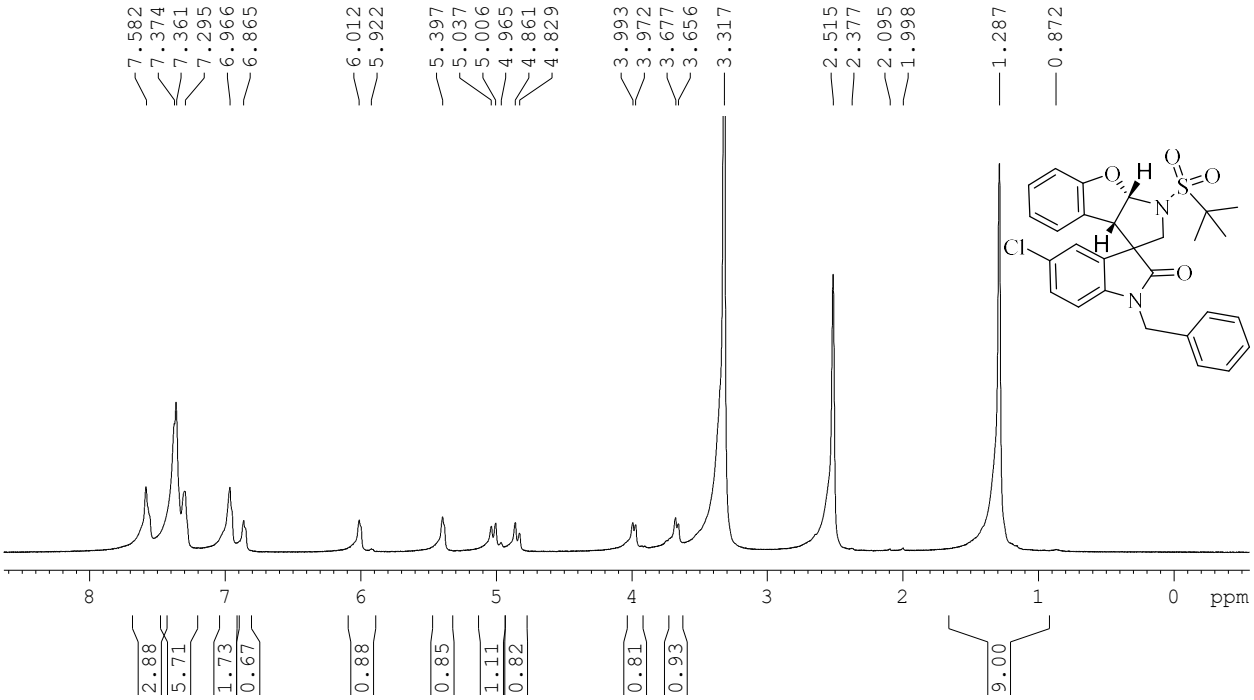

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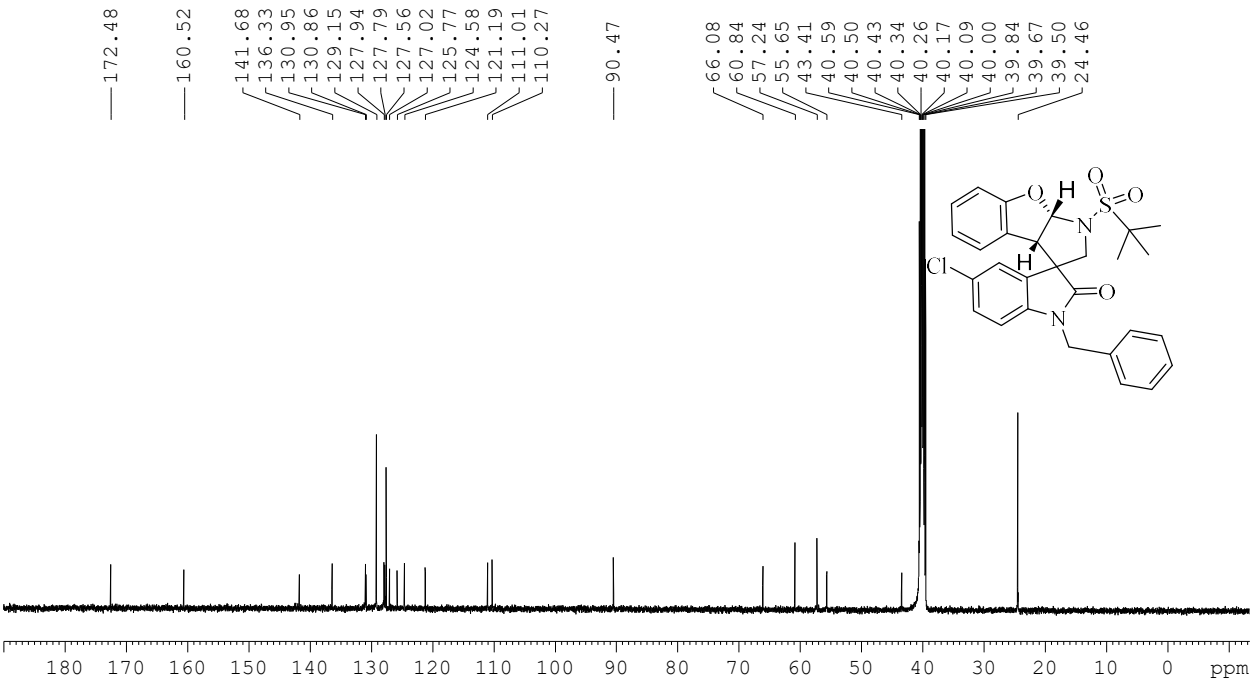

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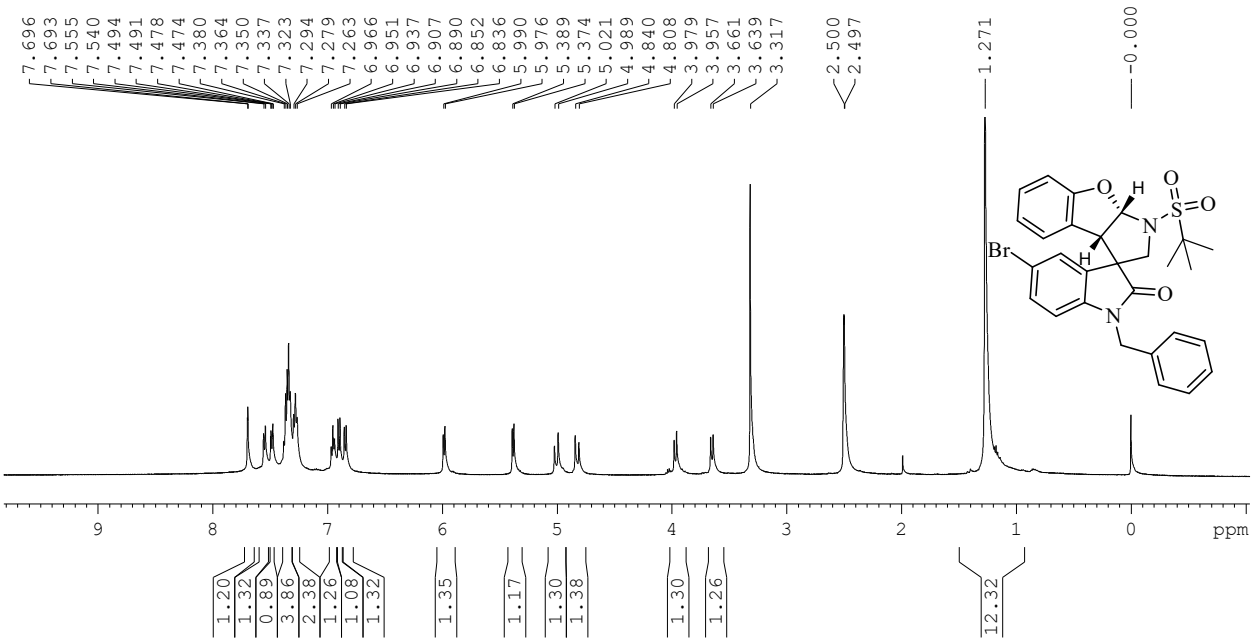

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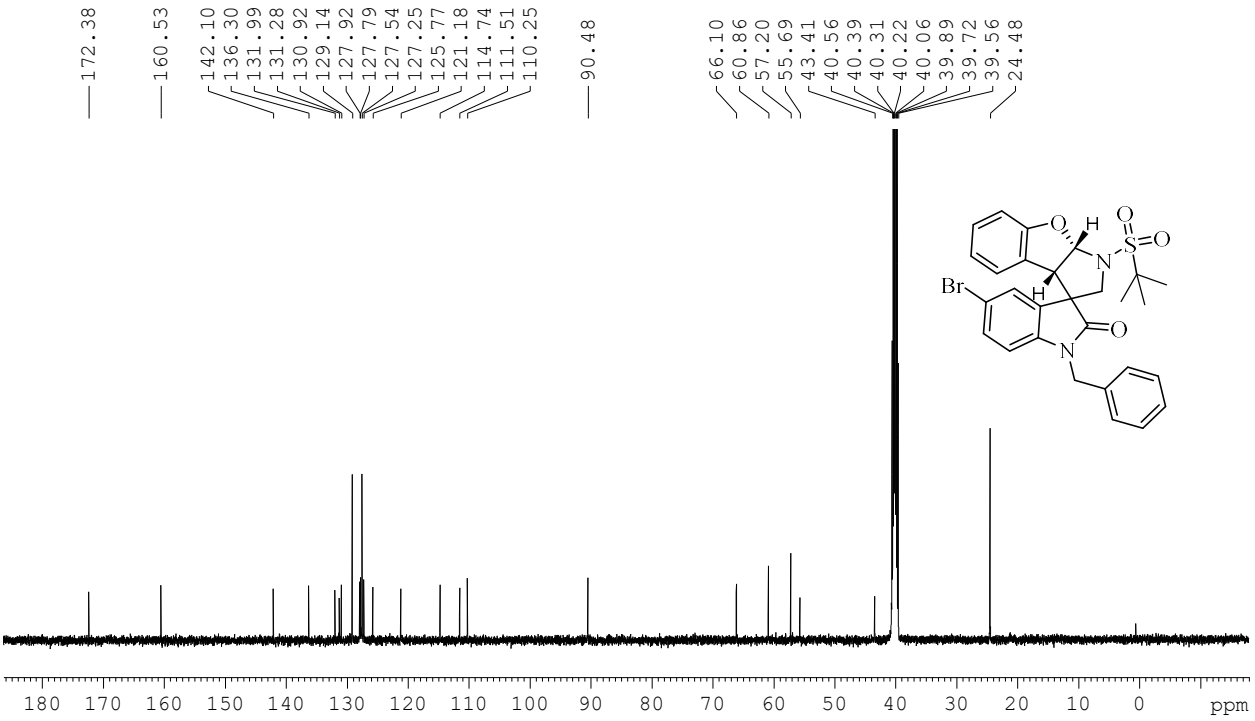

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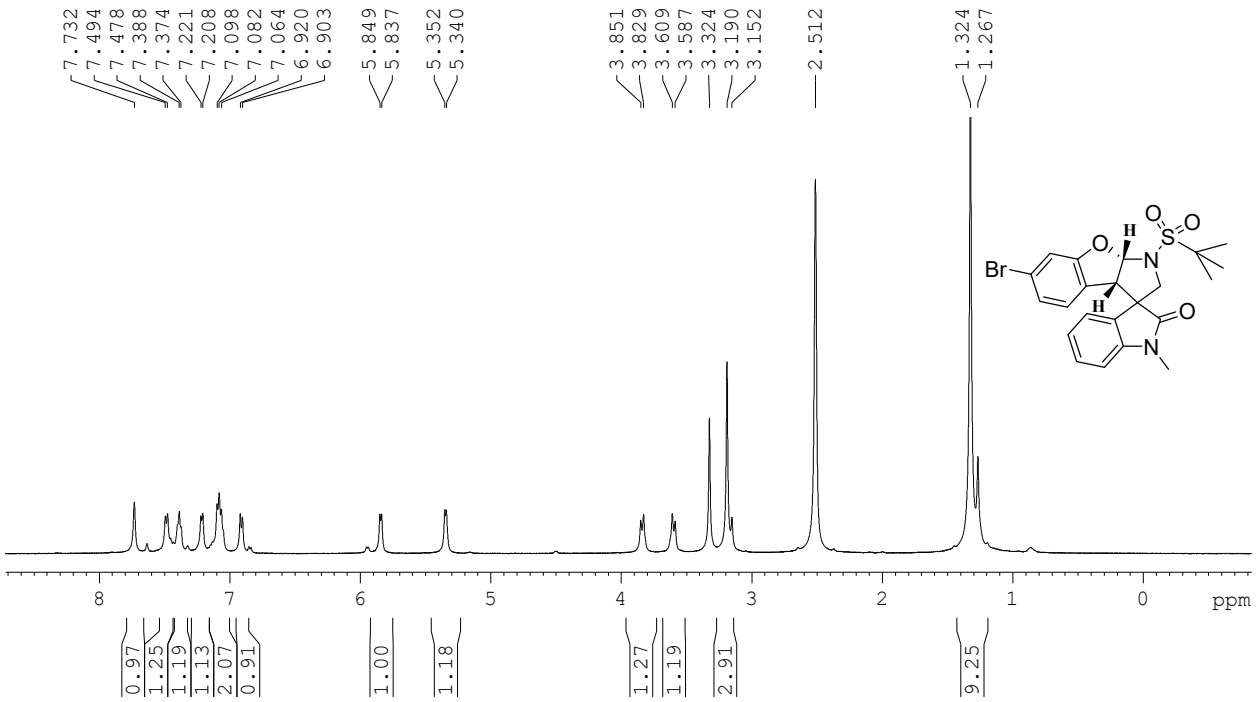

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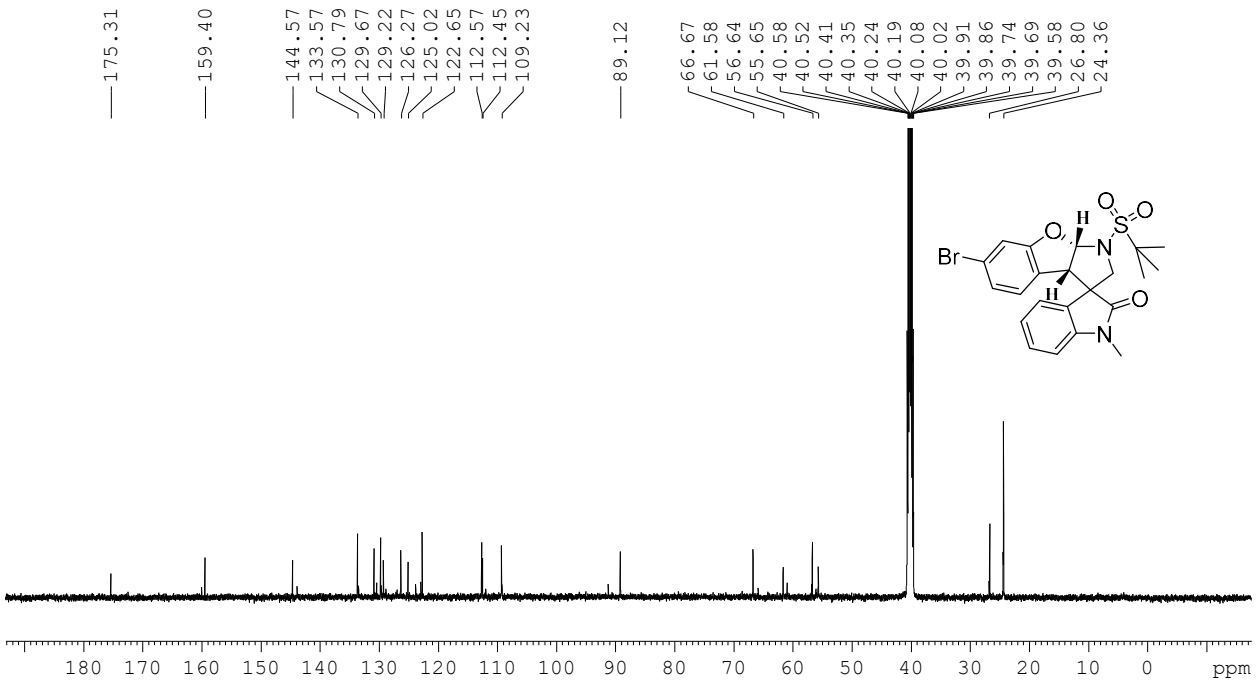

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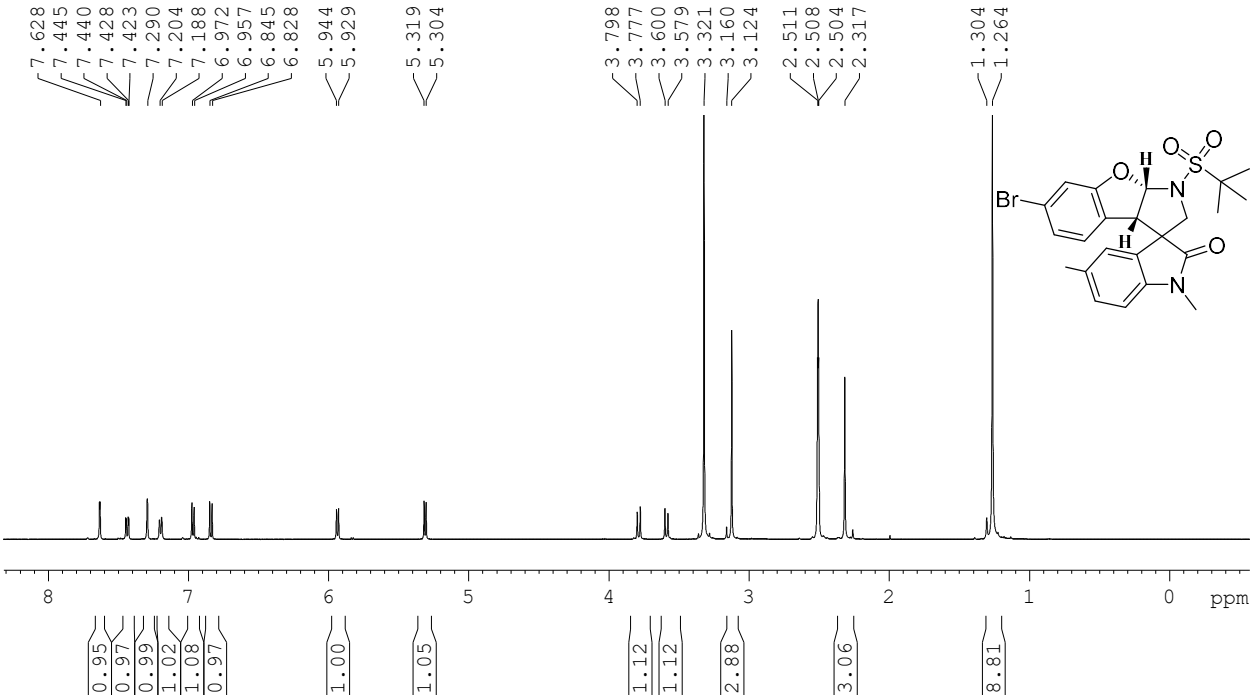

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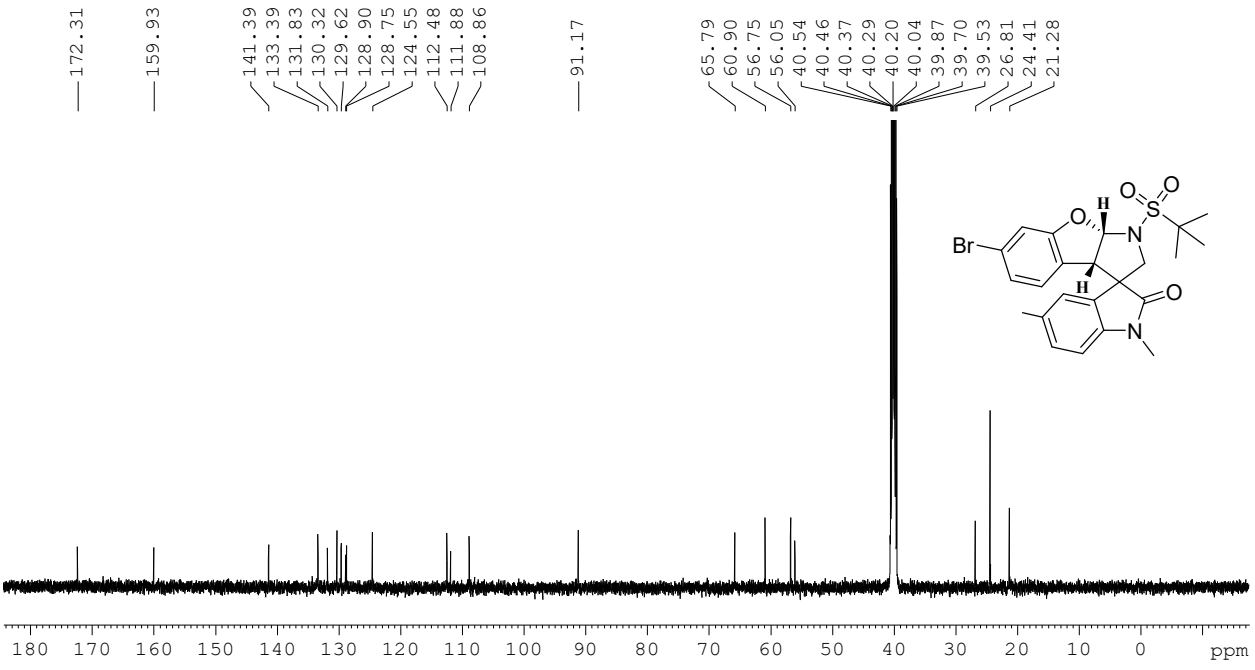

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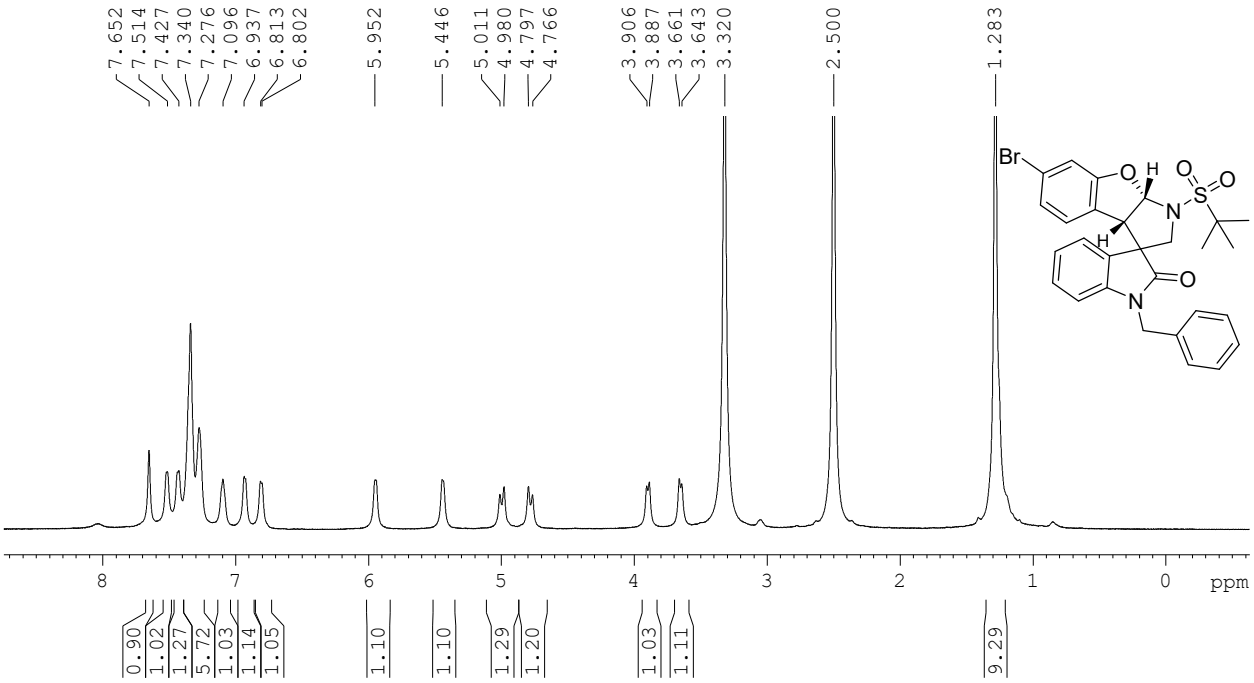

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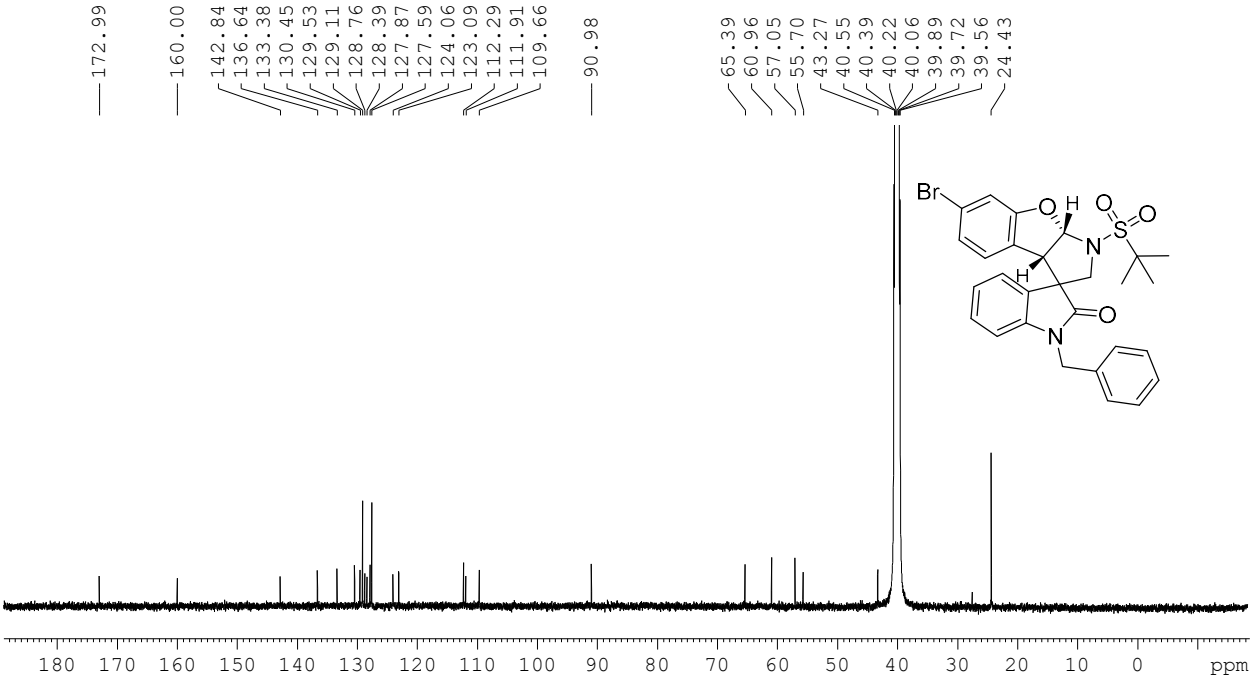

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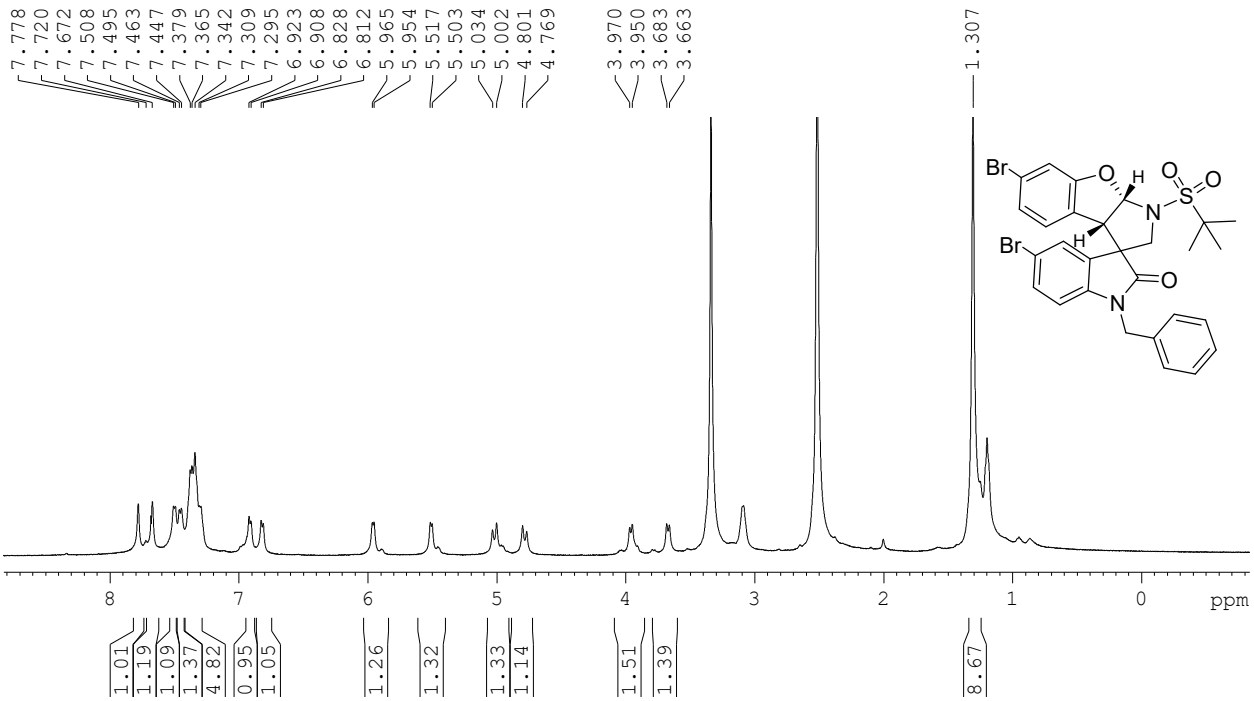

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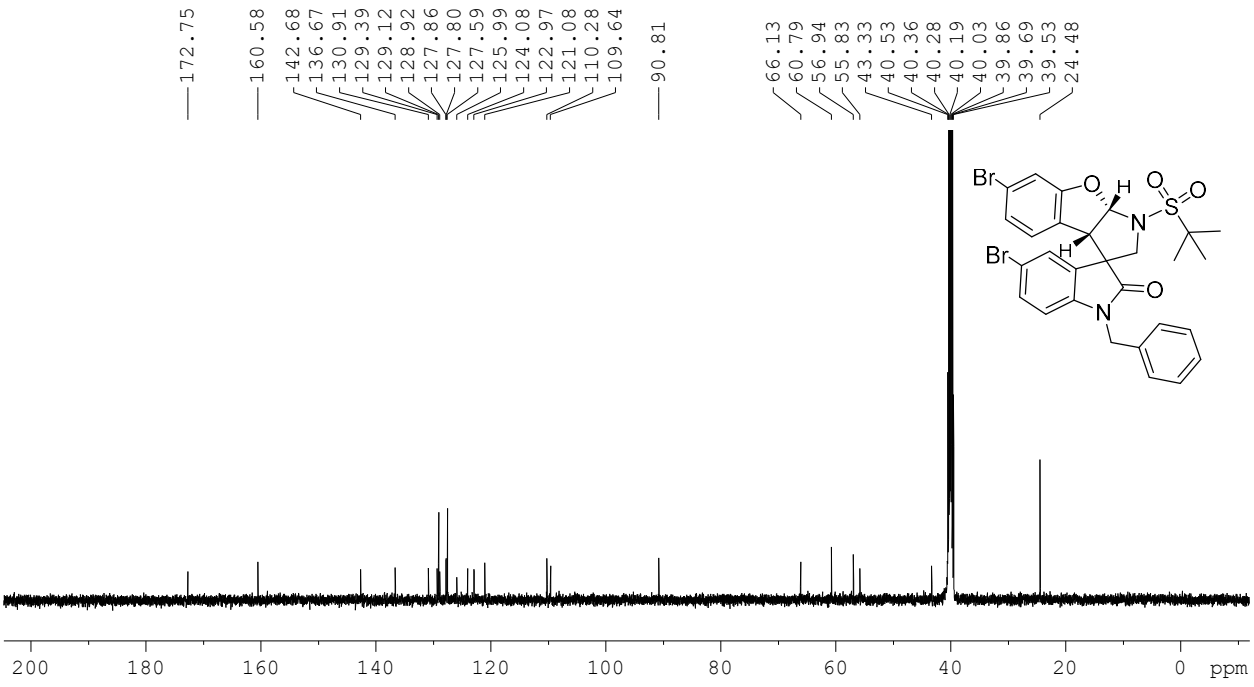

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