Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting information

Chemoselective synthesis of *m*-teraryls through ring transformation of 2*H*-pyran-2-ones by 2-(1-arylethylidene) malononitriles

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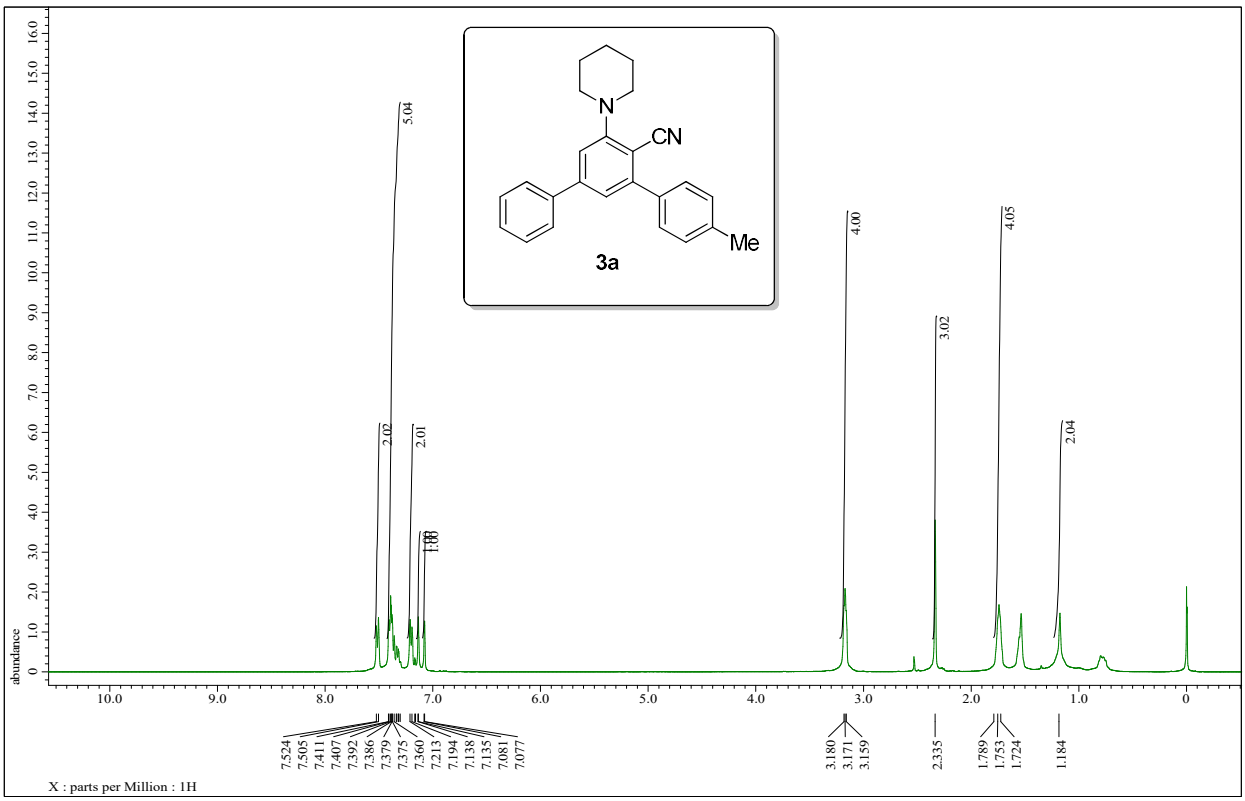
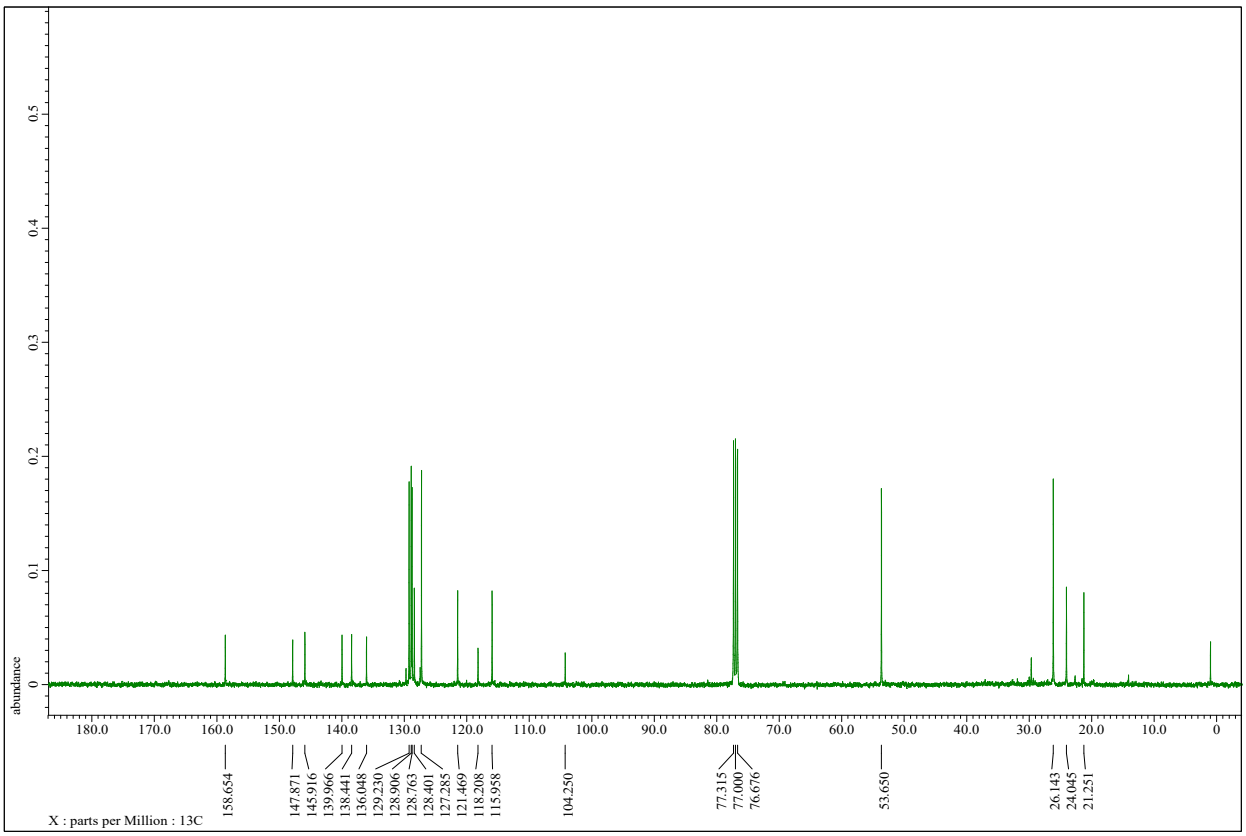
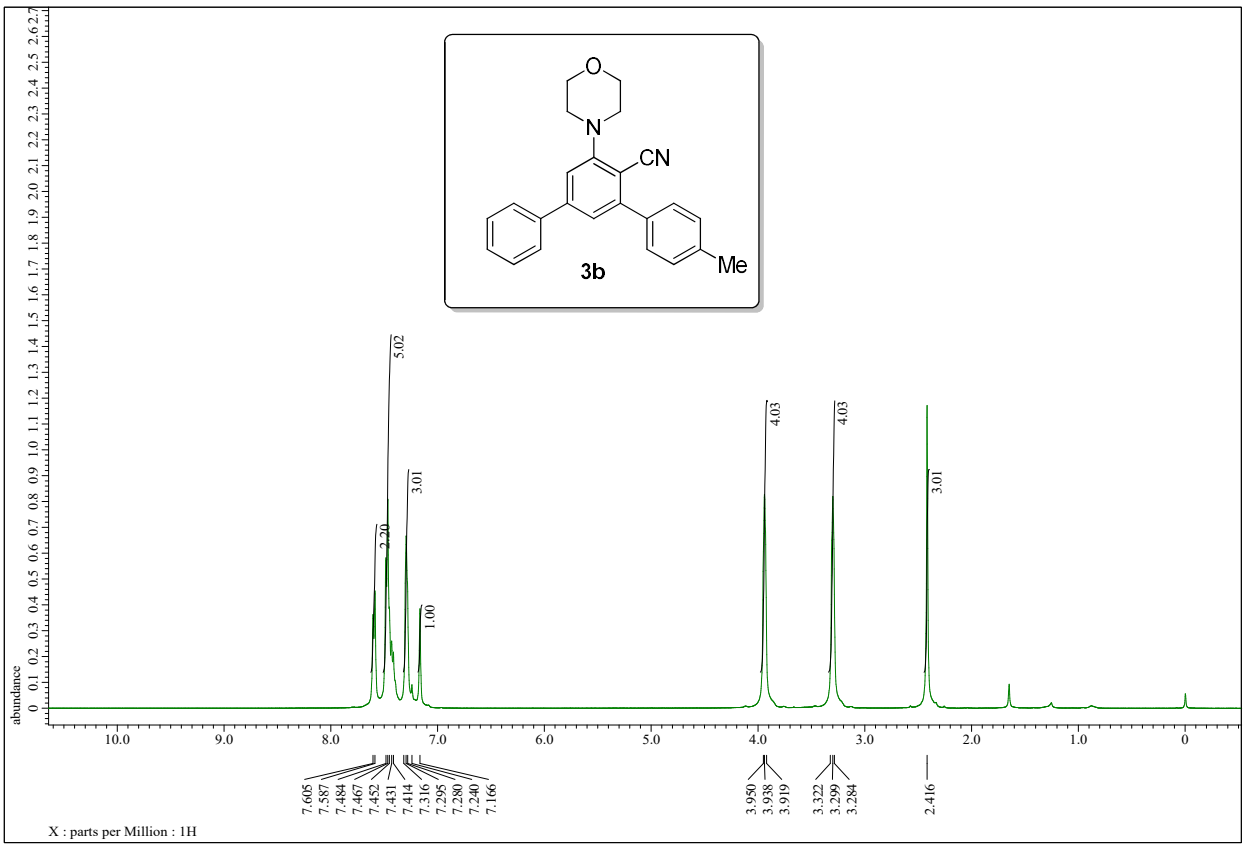
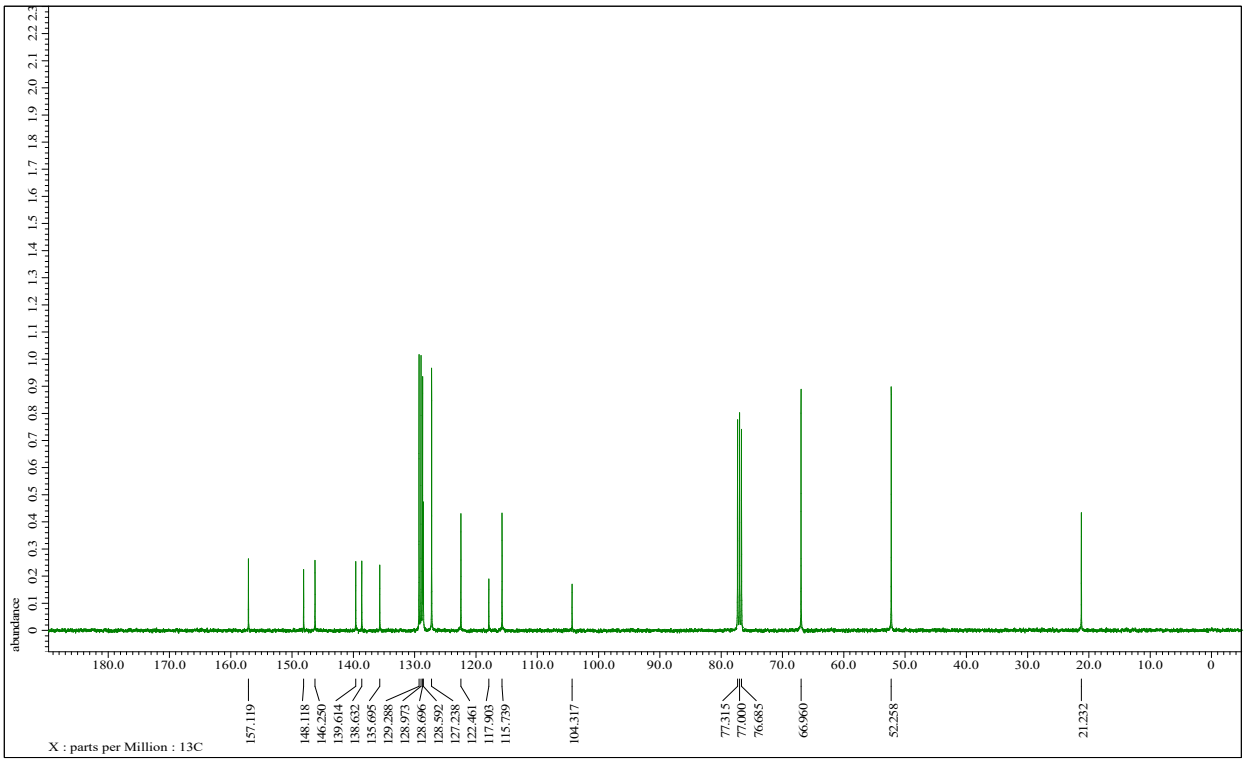
Crystal Data for 3i: Crystal data for C_{25} H_{23} Br N_2: A white crystal (0.240 x 0.200 x 0.200 mm^3) was mounted on a capillary tube for indexing and intensity data collection at 298K on an Oxford Xcalibur Sapphire3 CCD single-crystal diffractometer (MoKα radiation, λ = 0.71073 Å). Routine Lorentz and polarization corrections were applied, and an absorption correction was performed using the ABSCALE 3 program [CrysAlis Pro software system, Version 171.34; Oxford Diffraction Ltd., Oxford, U.K., 2011]. Patterson methods were used to locate the heavy metal atoms (SHELXS-86), and the remaining atoms were located from successive Fourier maps (SHELXL-97). All the non-hydrogen atoms were refined anisotropically; hydrogen atoms were located at calculated position using a riding model. All hydrogen atoms were calculated after each cycle of refinement using a riding model, with C−H = 0.93 Å + Uiso(H) = 1.2Ueq(C) for aromatic H atoms, and with C−H = 0.97 Å + Uiso(H) = 1.2Ueq(C) for methylene H atoms. Crystal data (CCDC No. 1869248): C_{25} H_{23} Br N_2; Mr = 431.35, crystal system: monoclinic; space group P 21/c, a = 13.2298(3) Å, b = 10.1625(3) Å, c = 15.5329 (5) Å, α = 90, β = 98.015 (2), γ = 90, V = 2067.97 (10), Z = 4, ρcalcd = 1.386 Mg/m^3 g cm-3, μ = 2.000 mm-1, F(000) = 888.0, R1 = 0.0421 (3031) and wR2 = 0.1059 for I>2σ(I) and 226 parameters, R1 = 0.0545 and wR2 = 0.1131, gof = 0.904 for all data.





^{1}H NMR and ^{13} C NMR 4''-methyl-5'-(piperidin-1-yl)-[1,1':3',1''-terphenyl]-4'-carbonitrile





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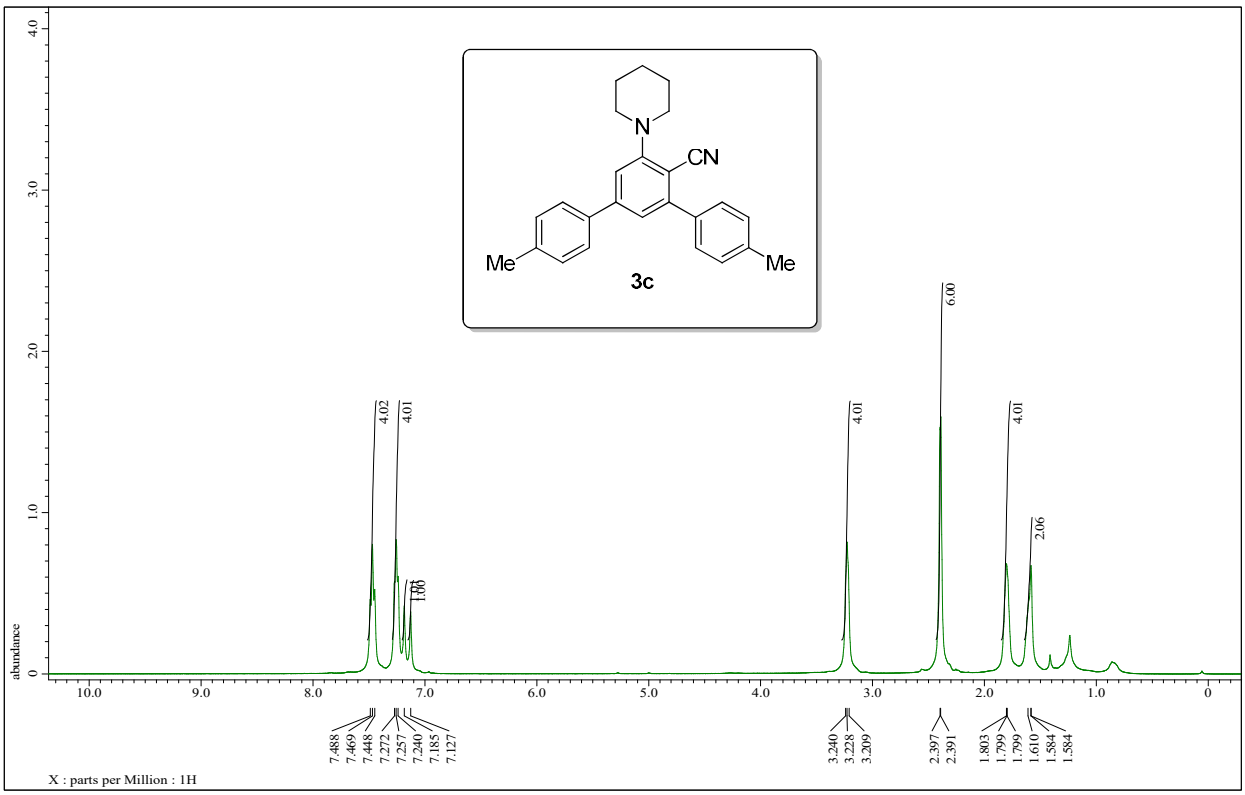

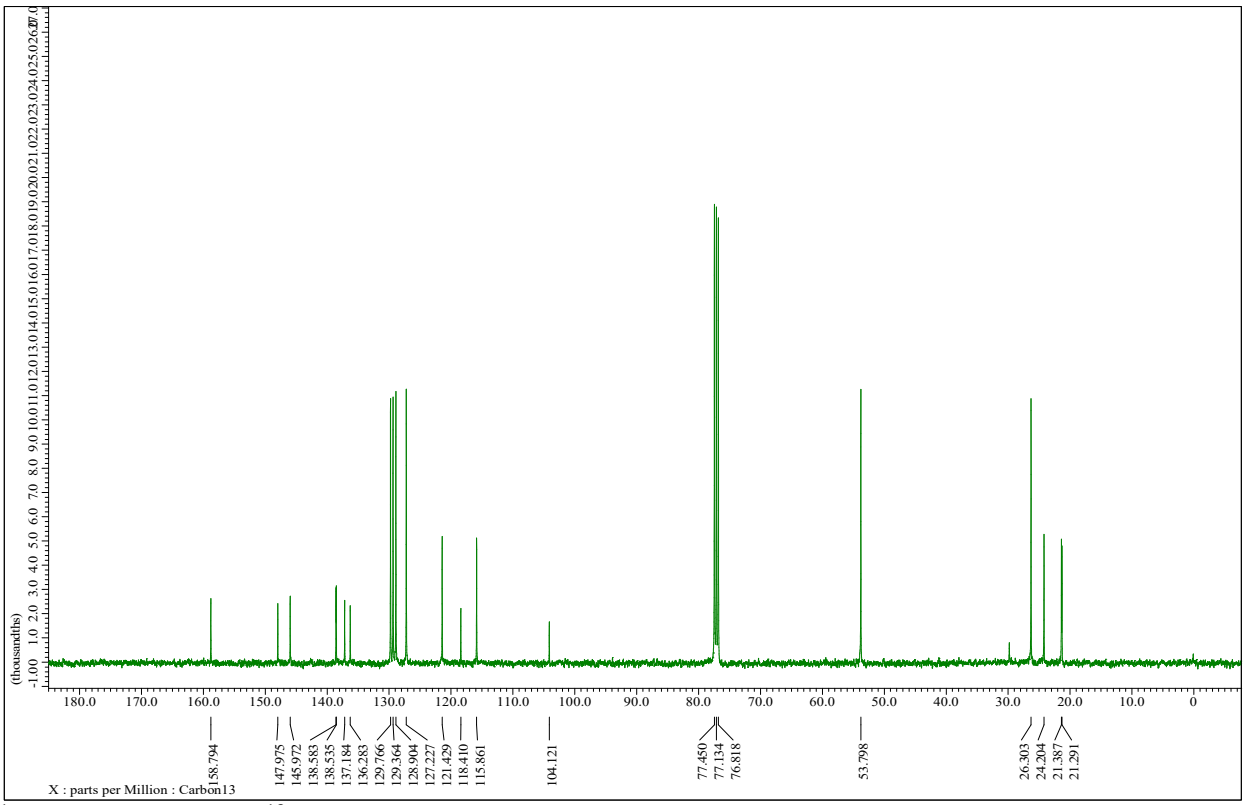

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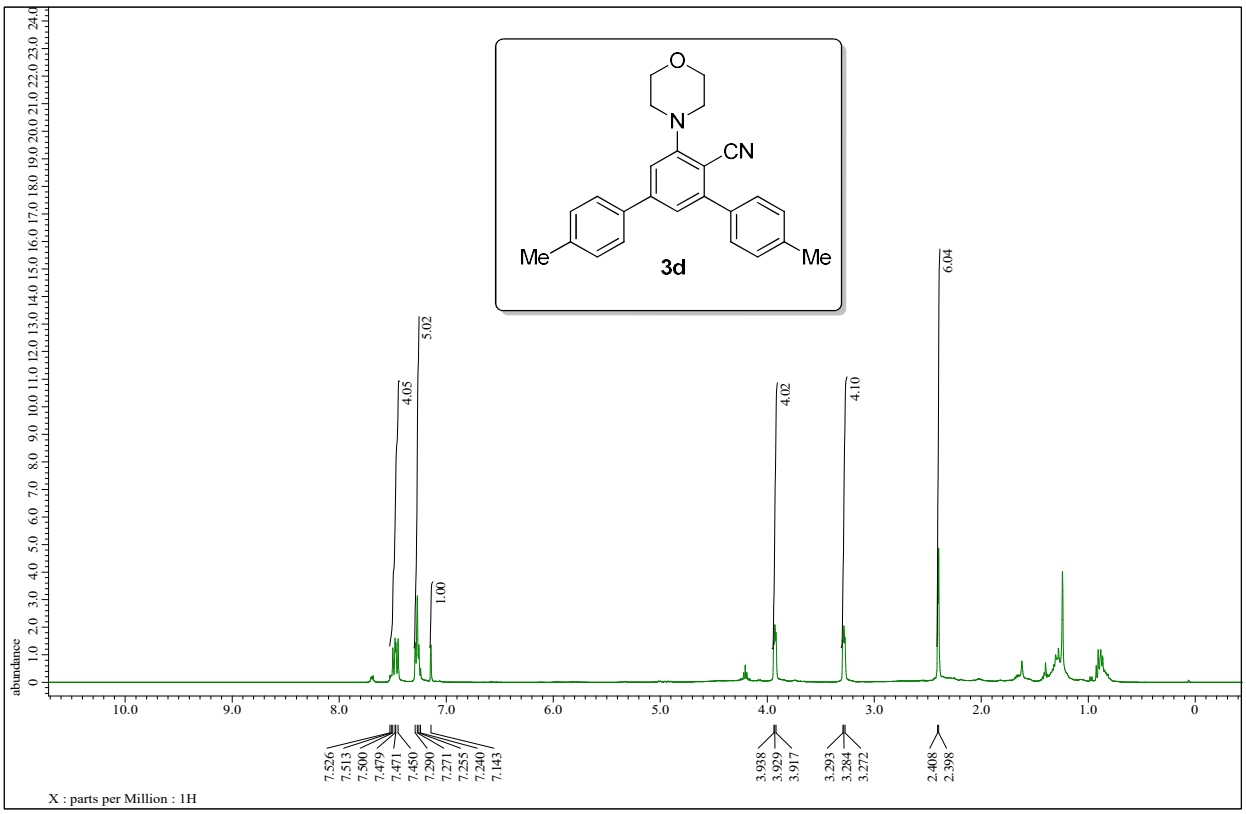

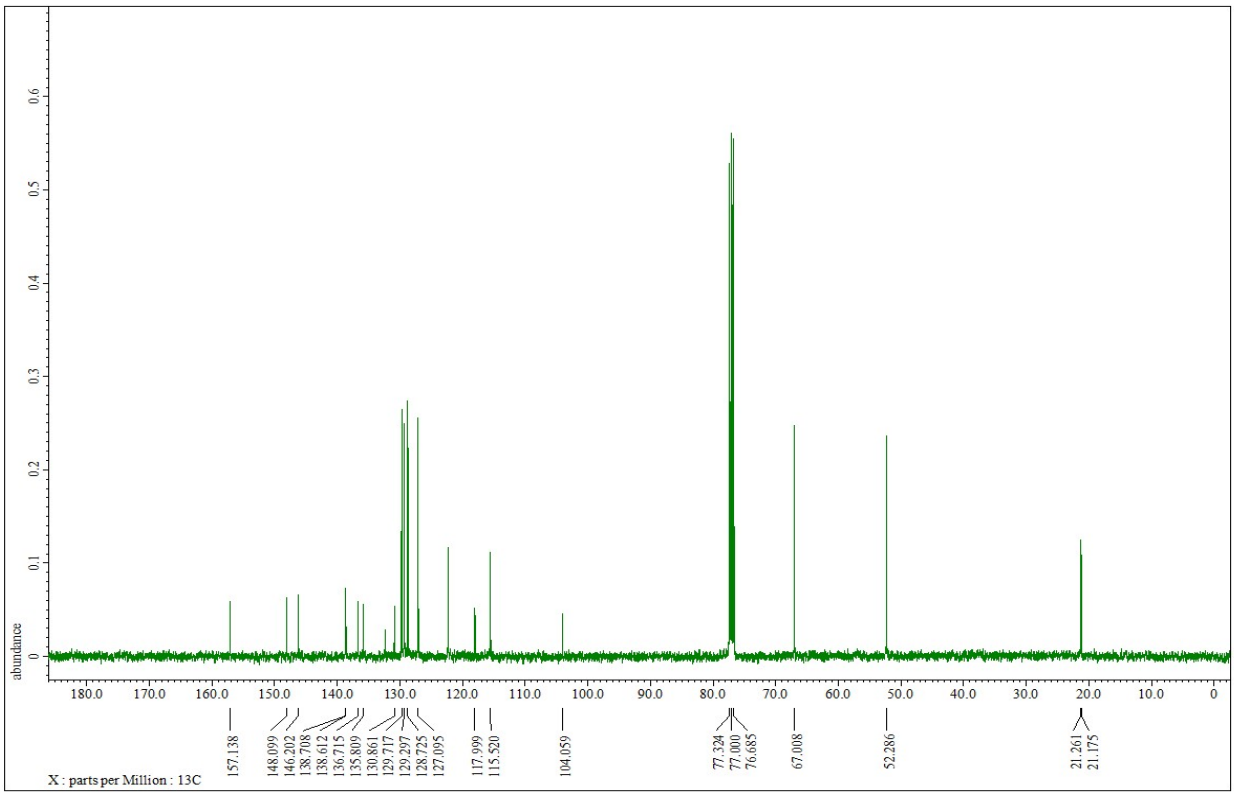

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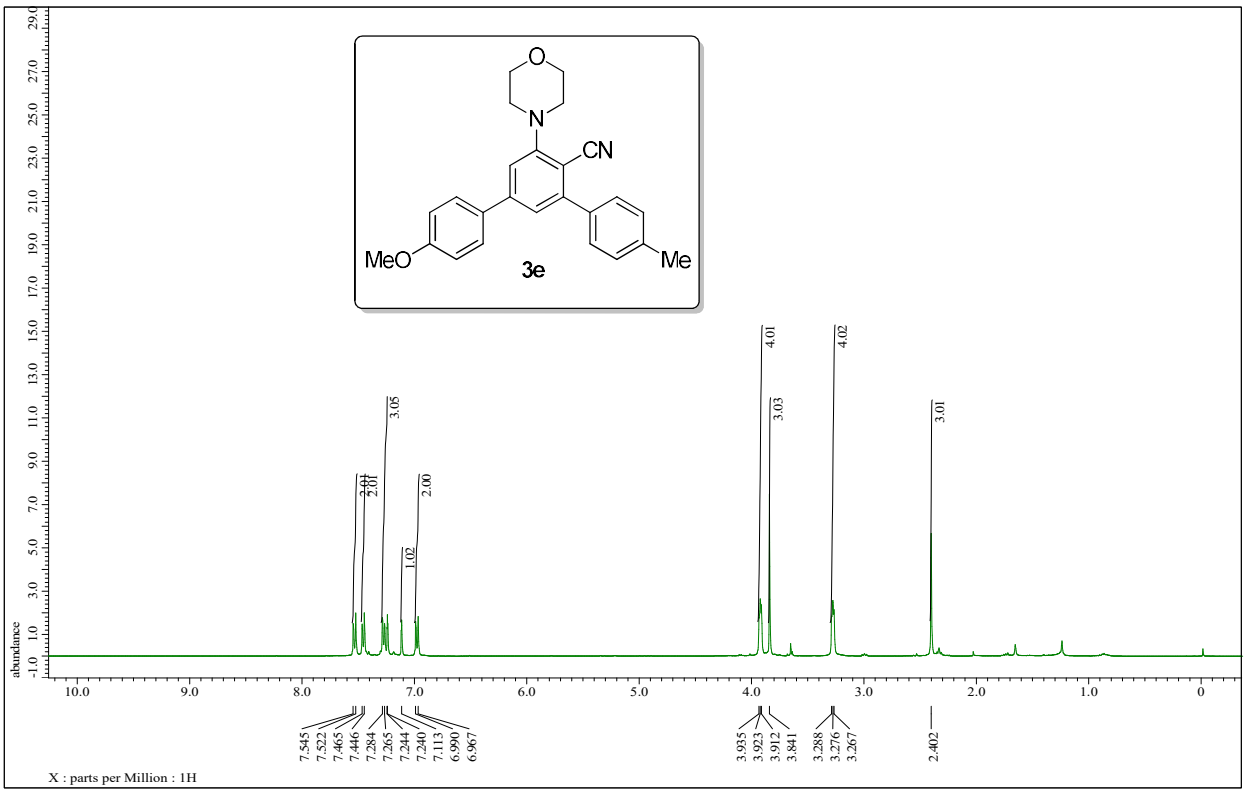

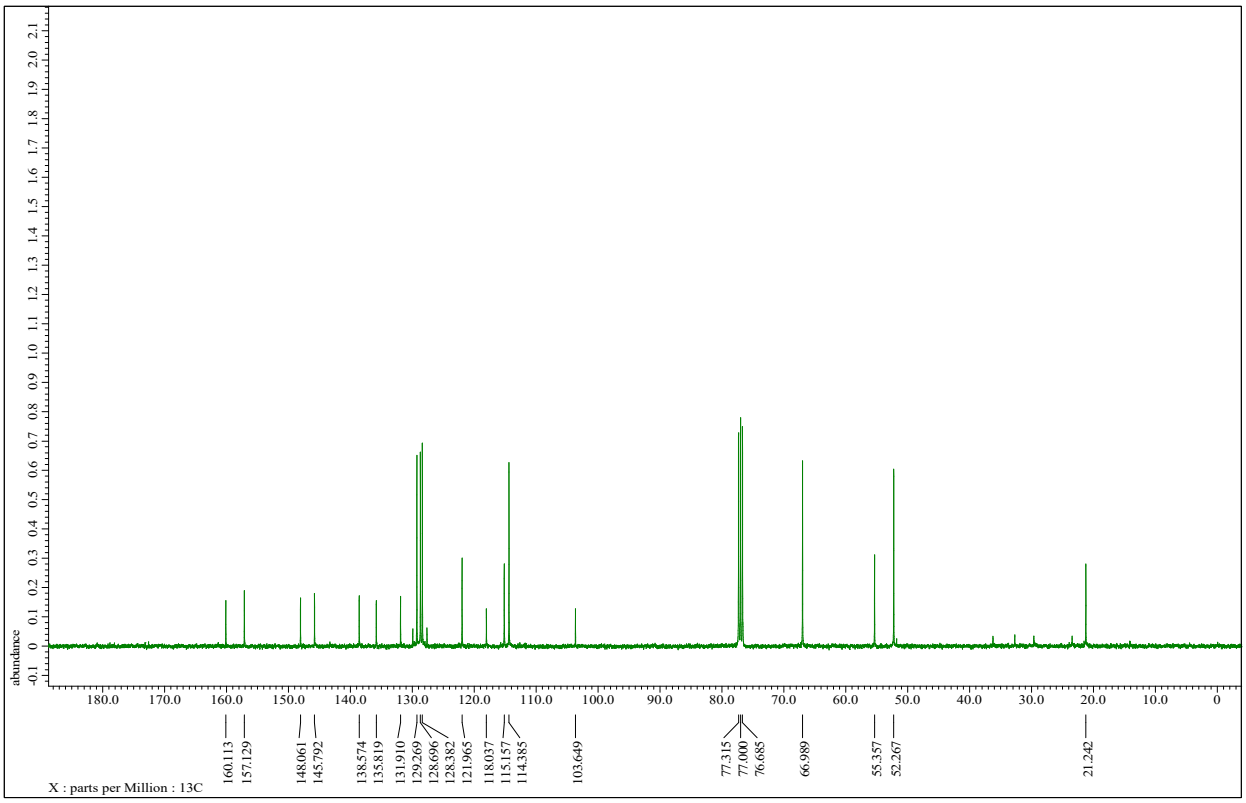

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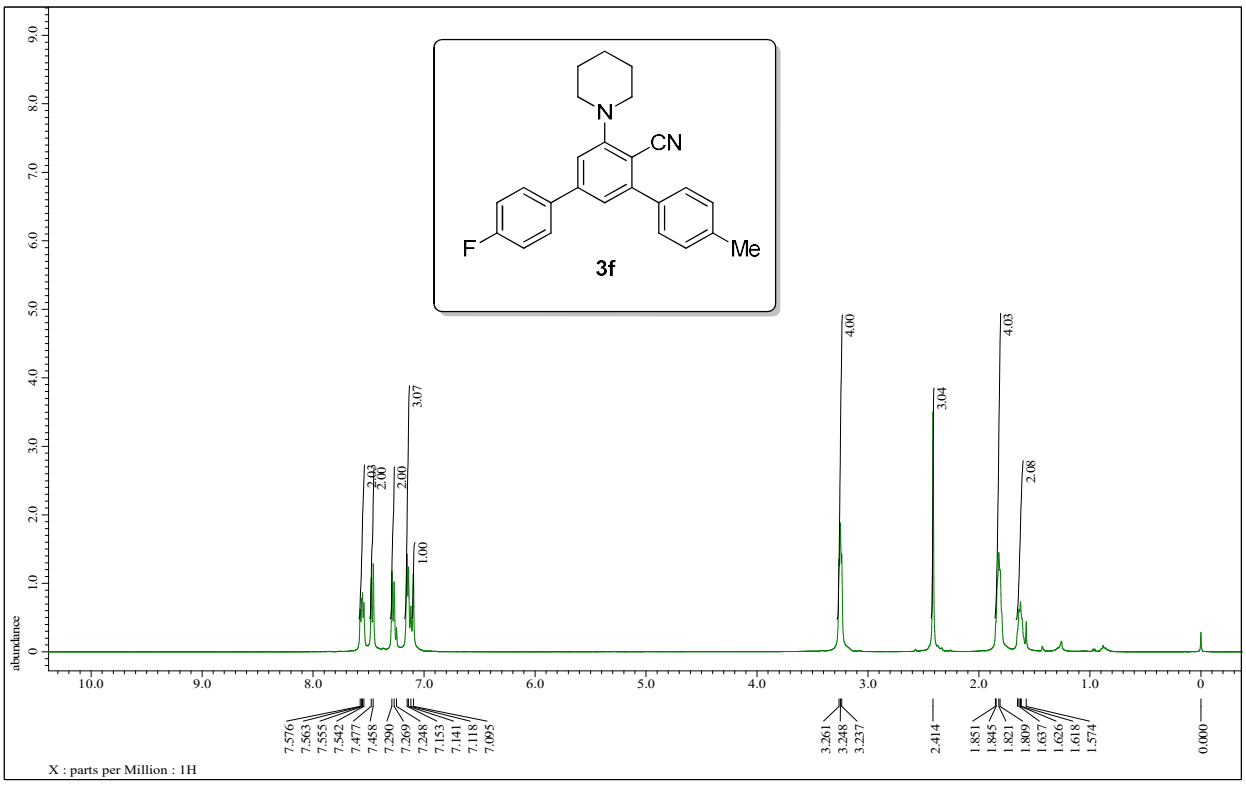

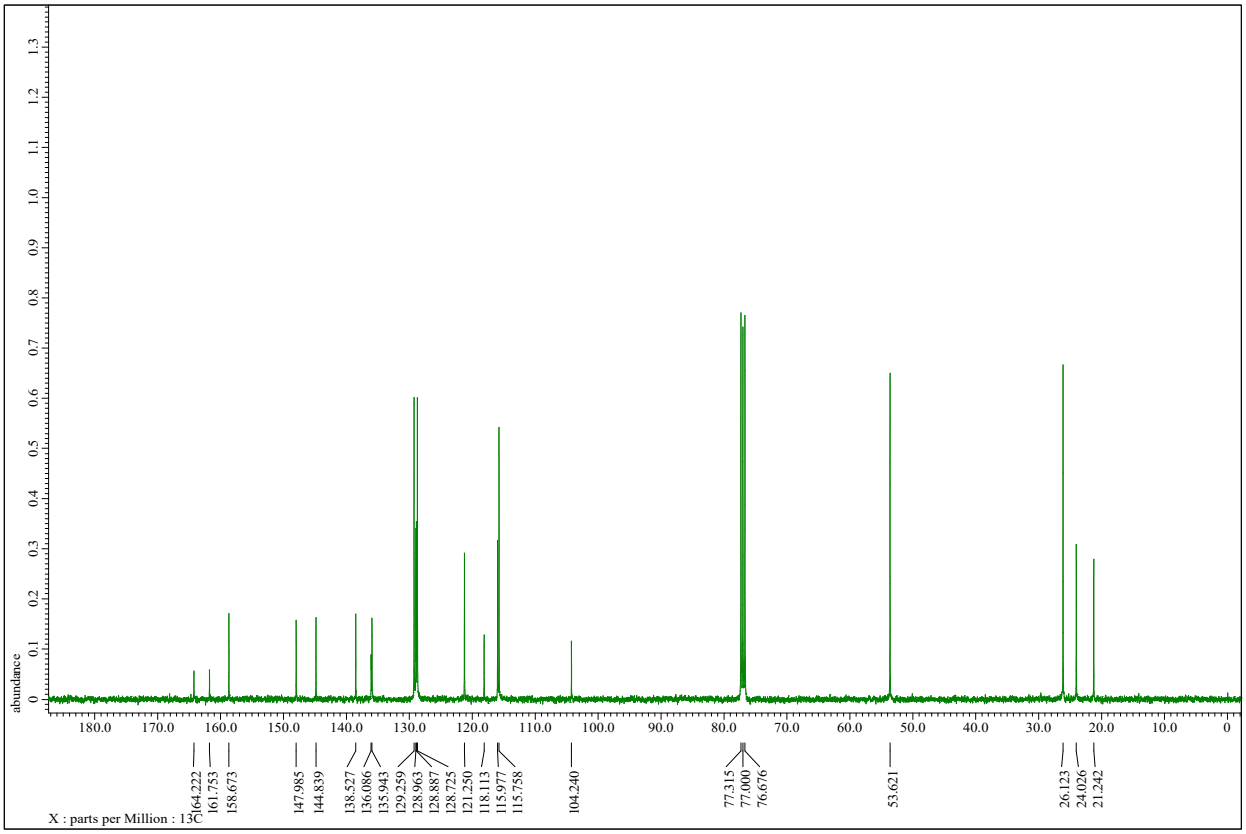

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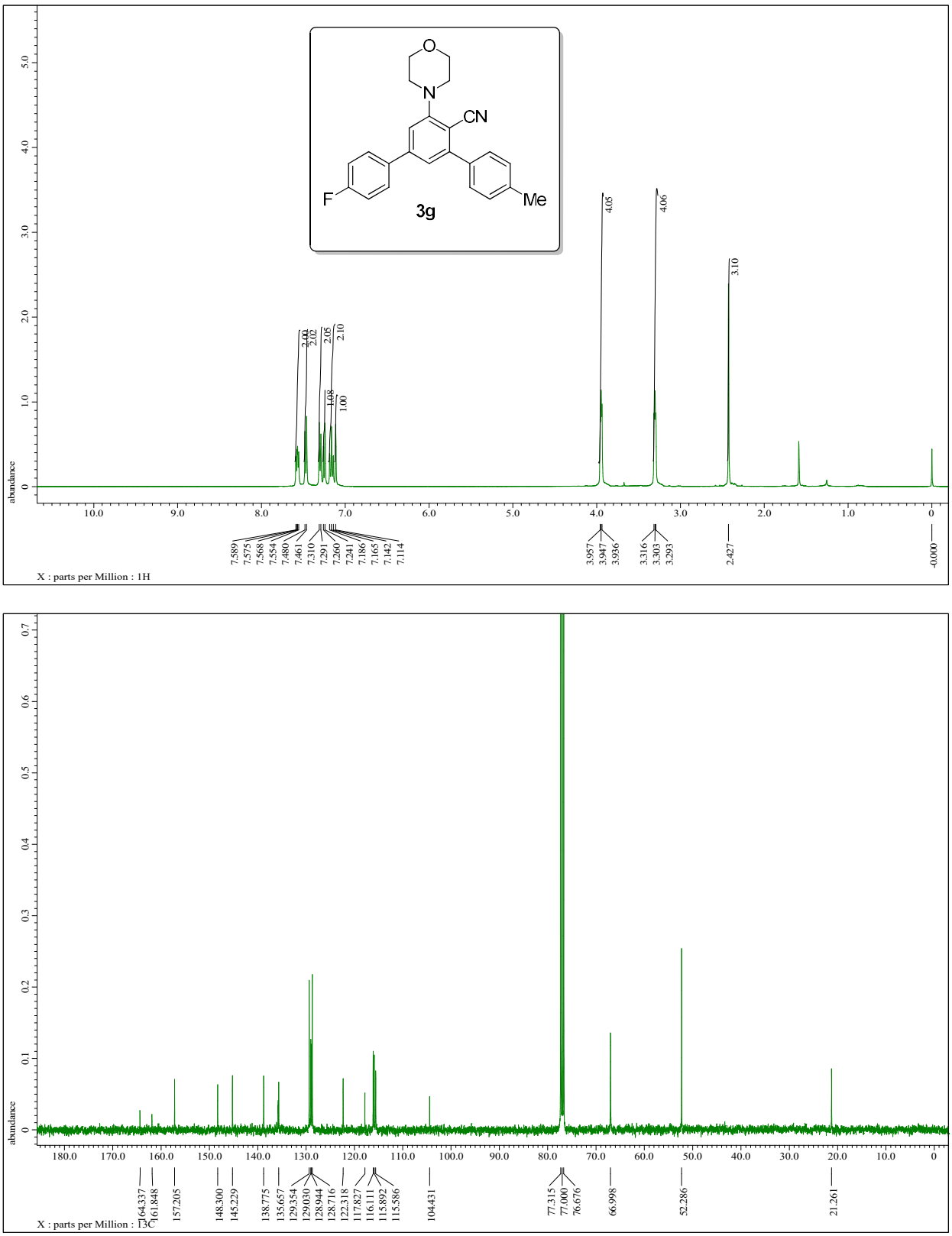

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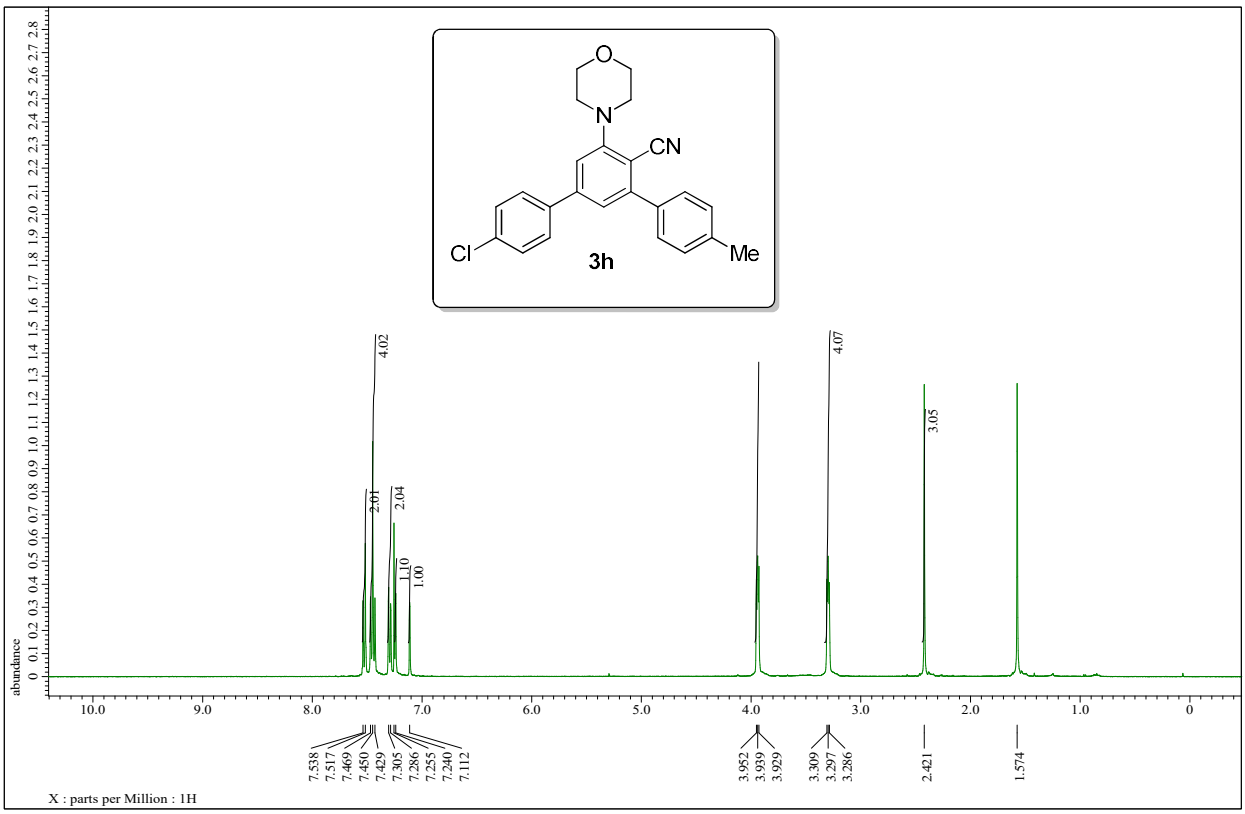

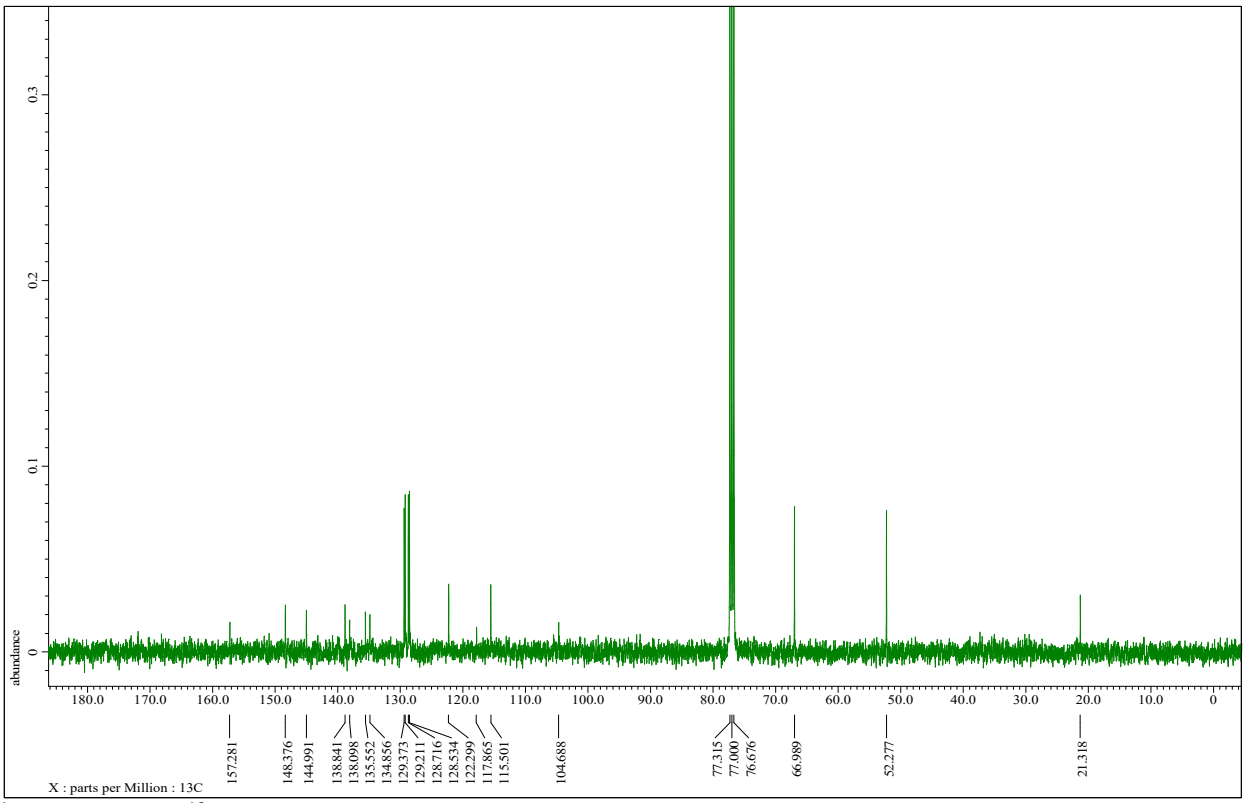

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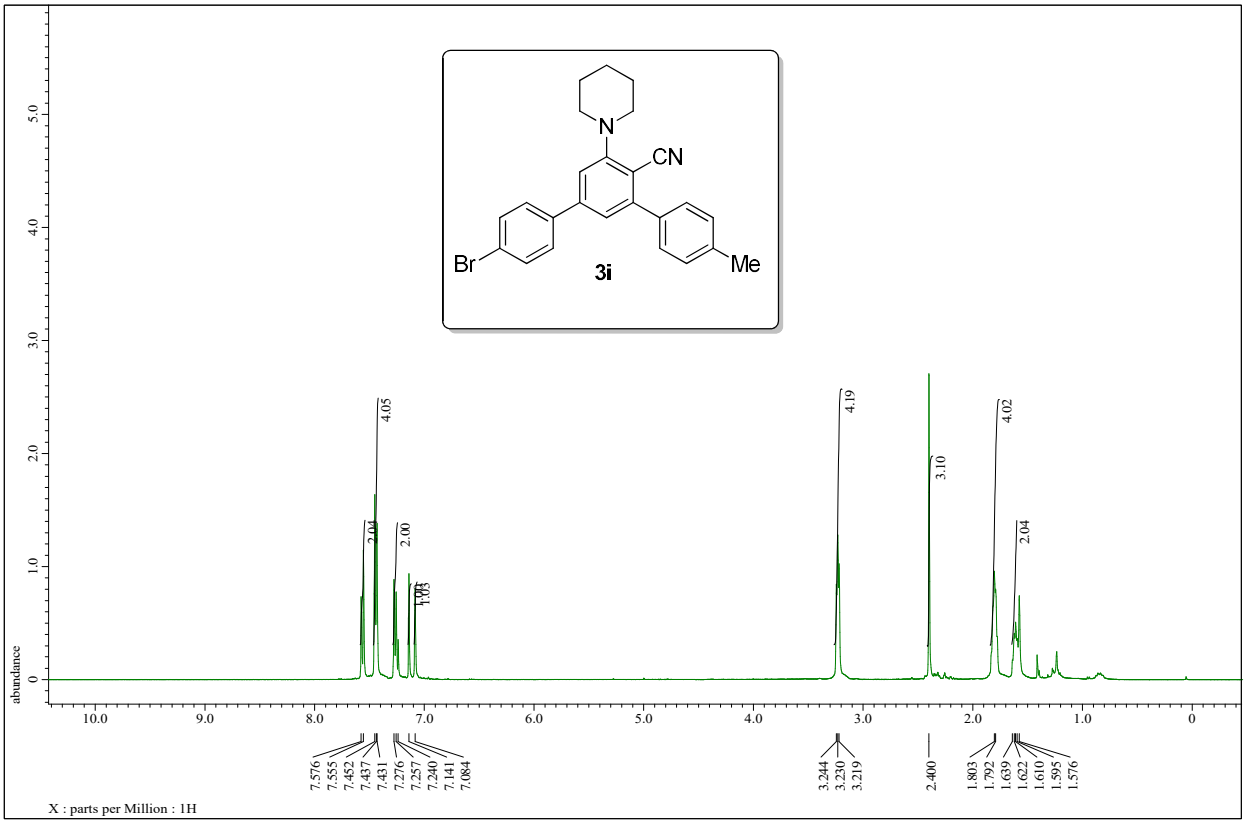

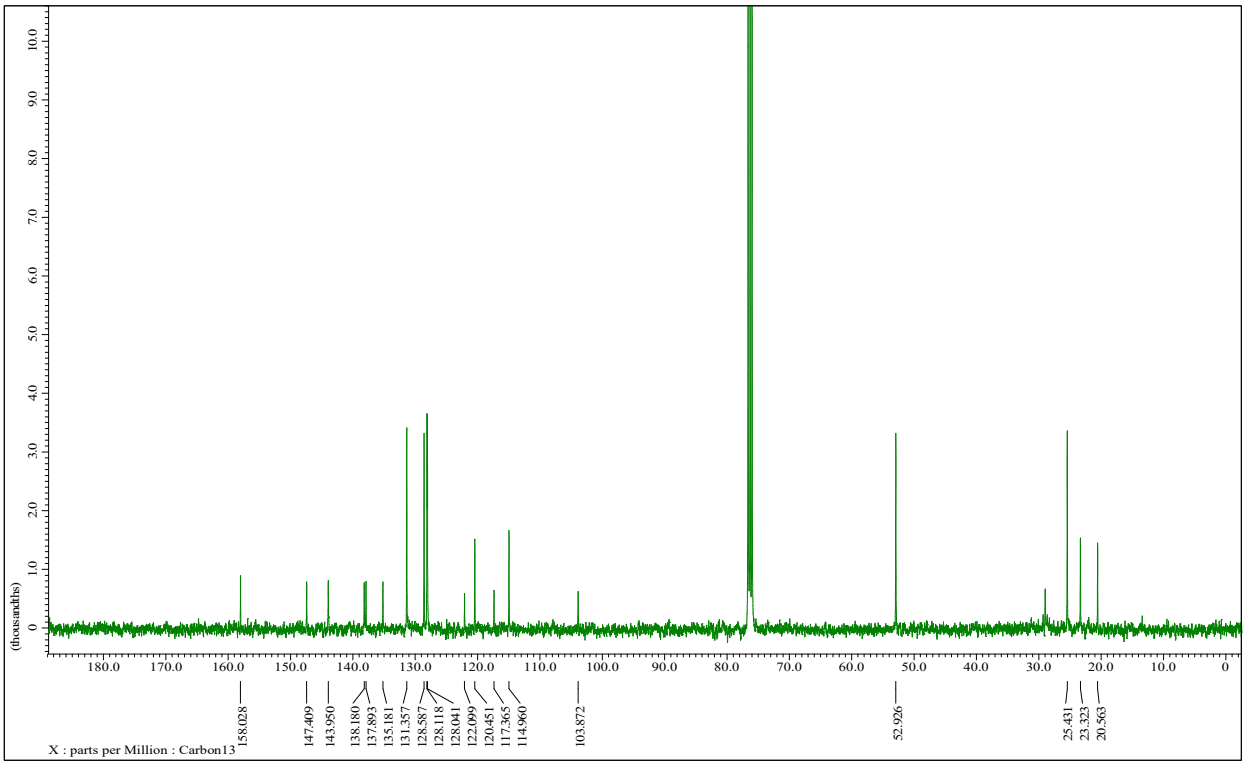

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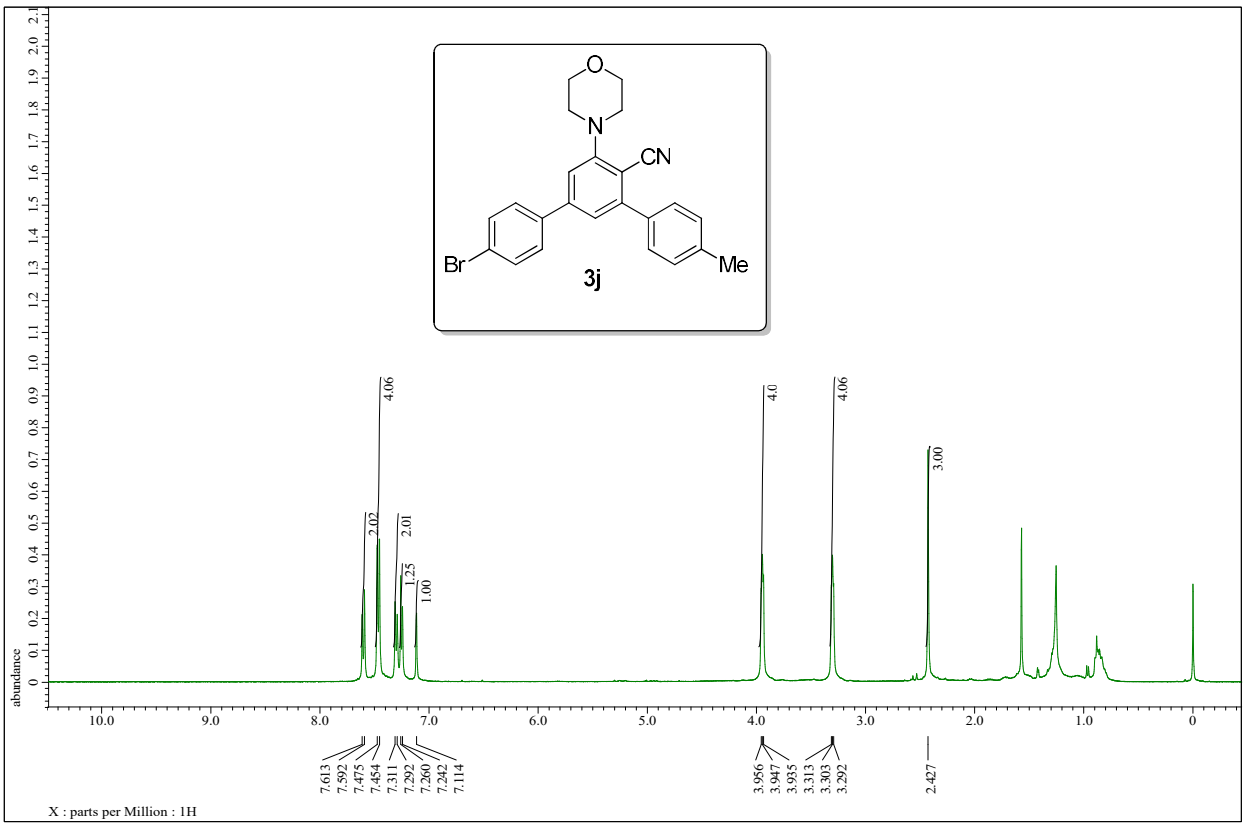

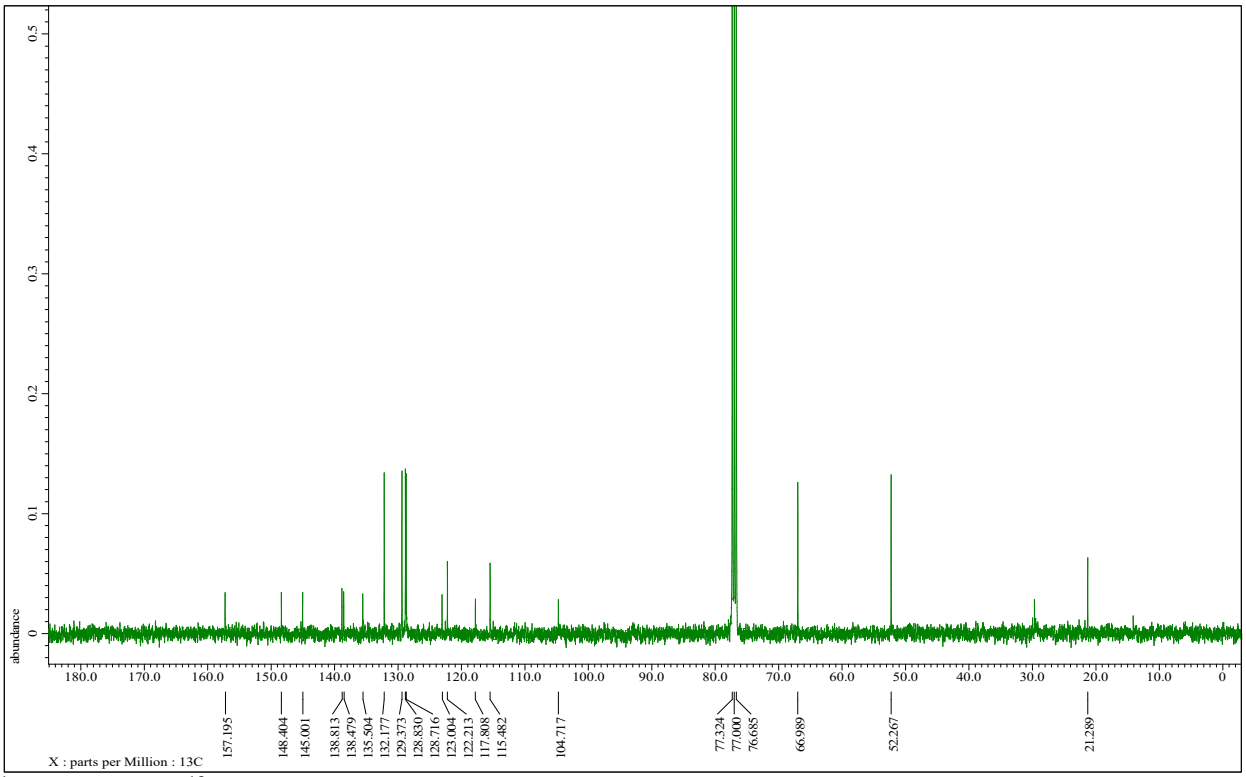

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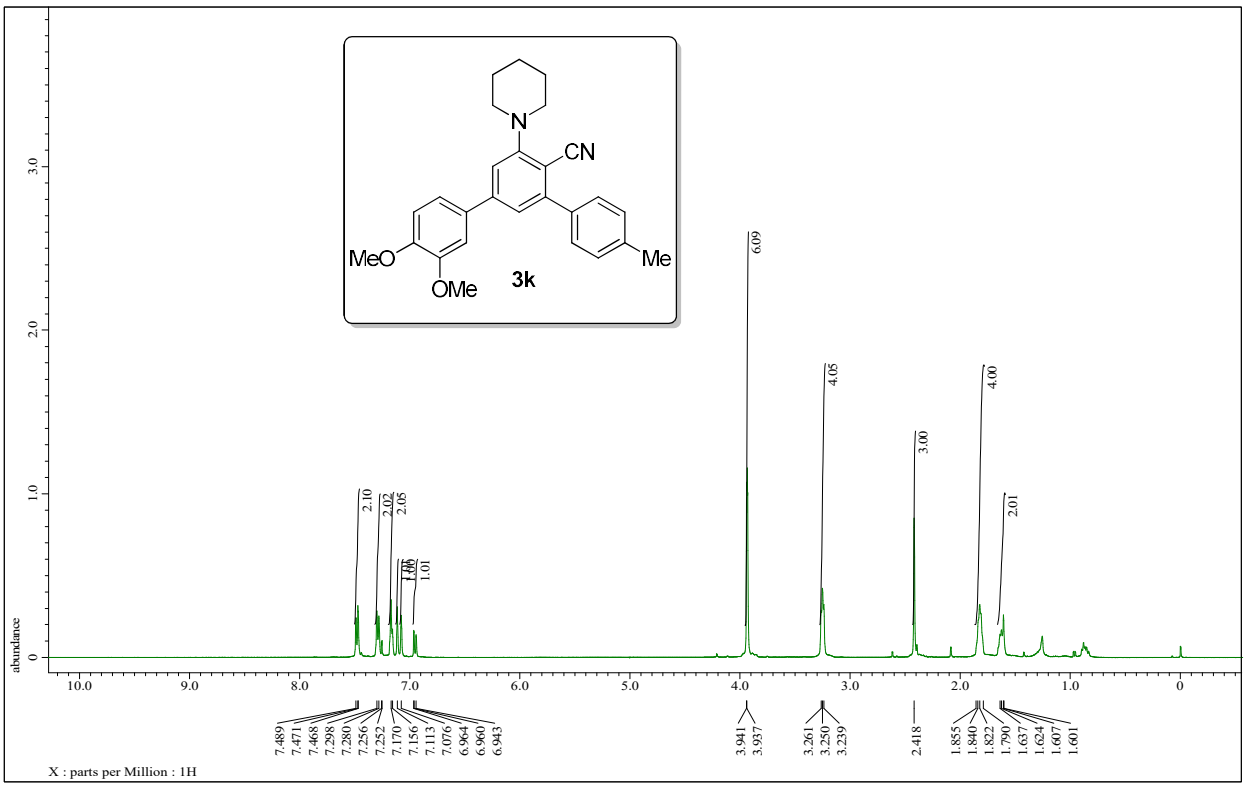

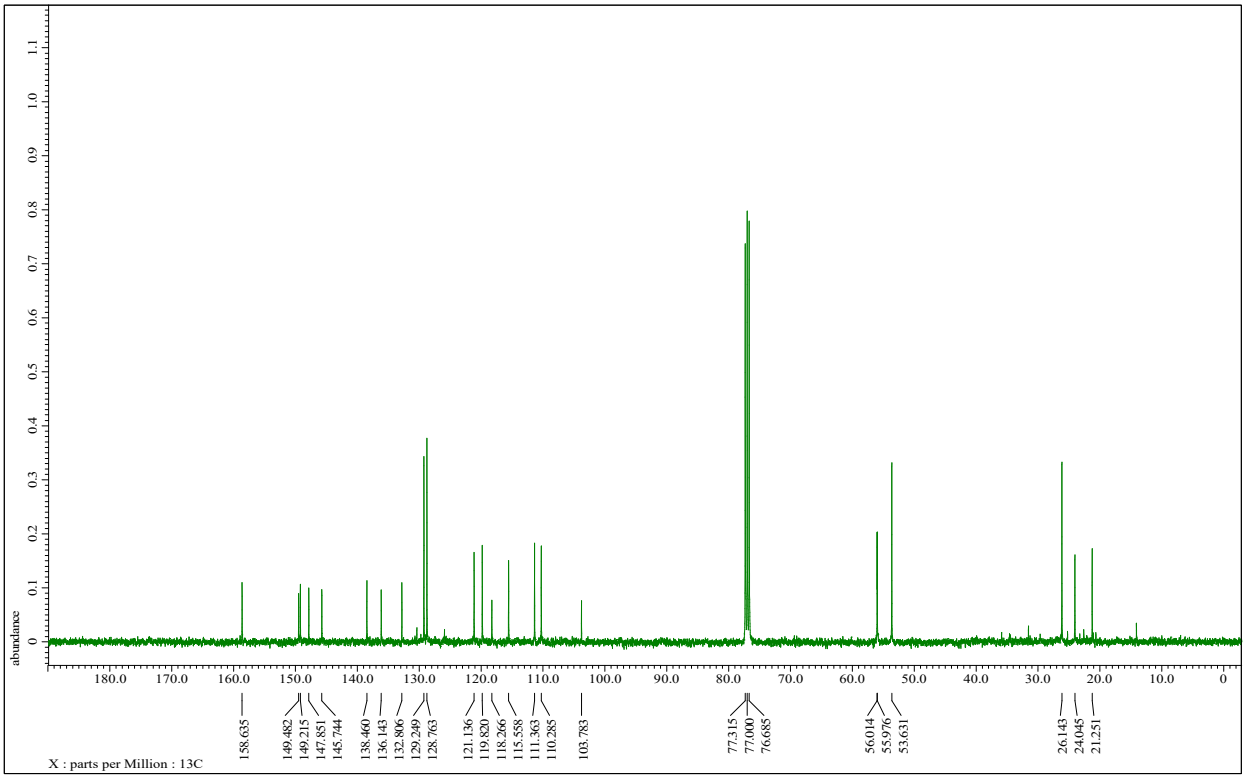

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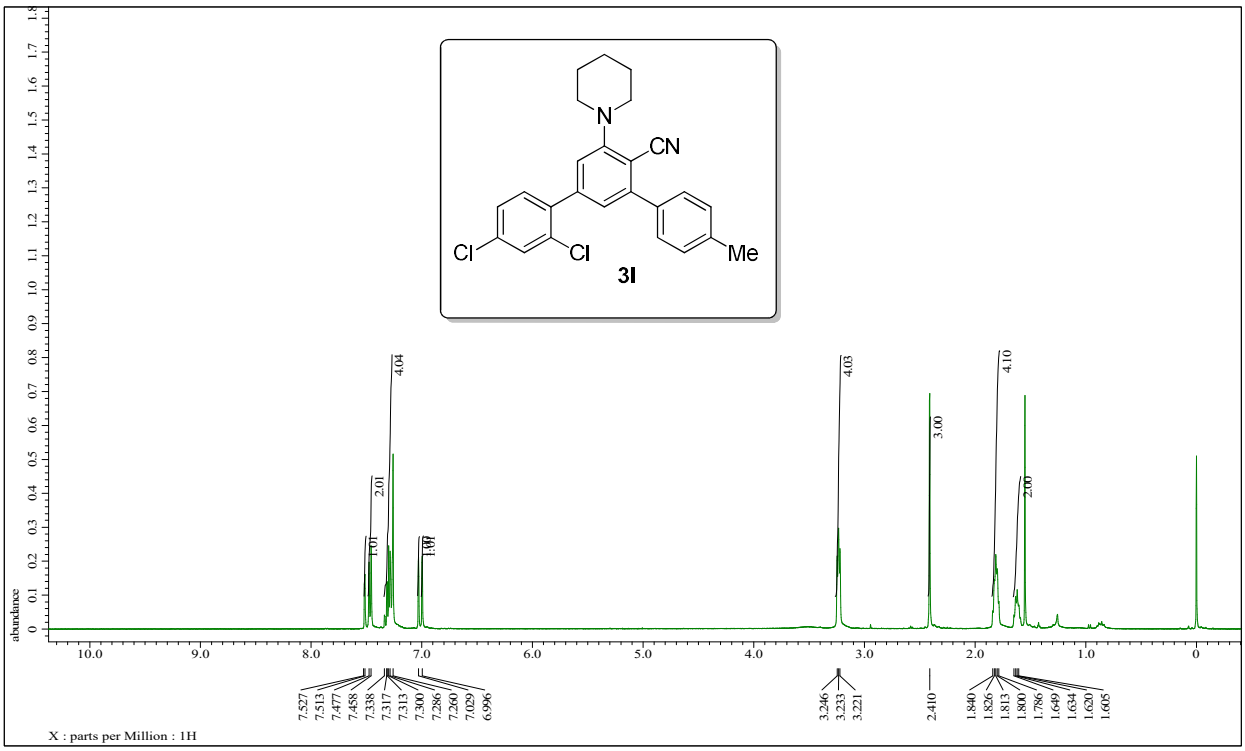

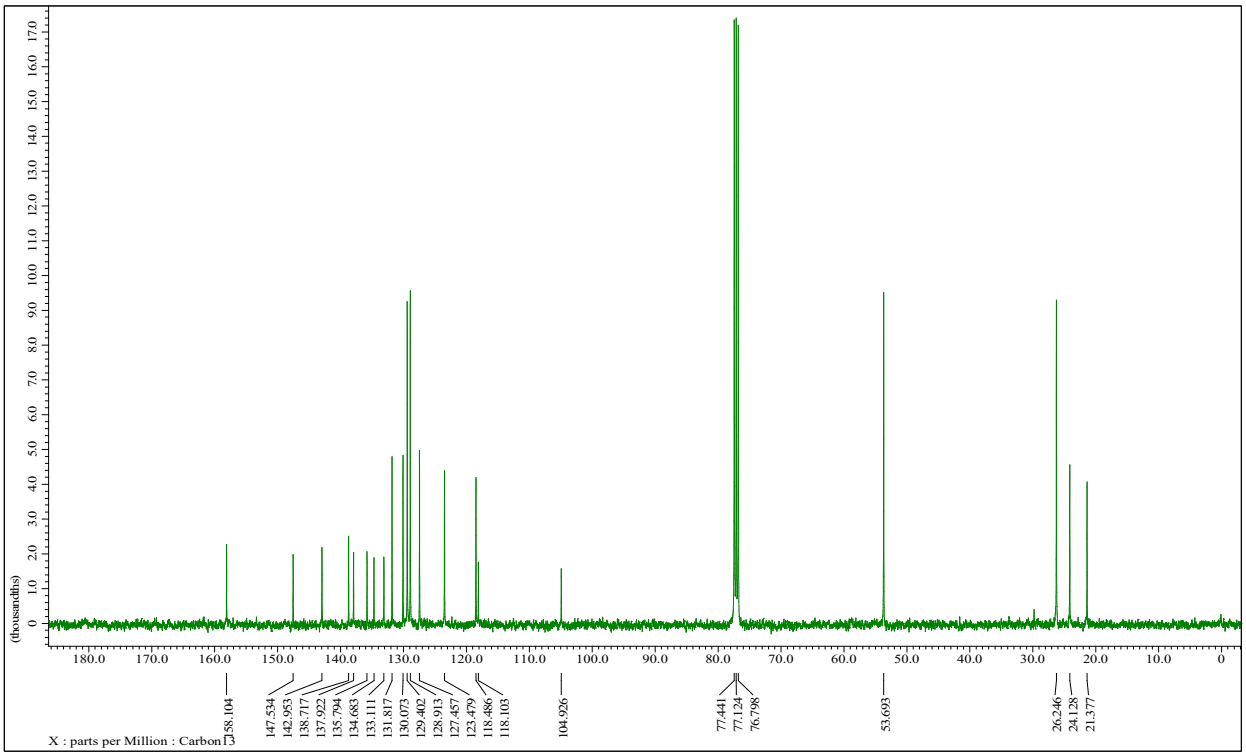

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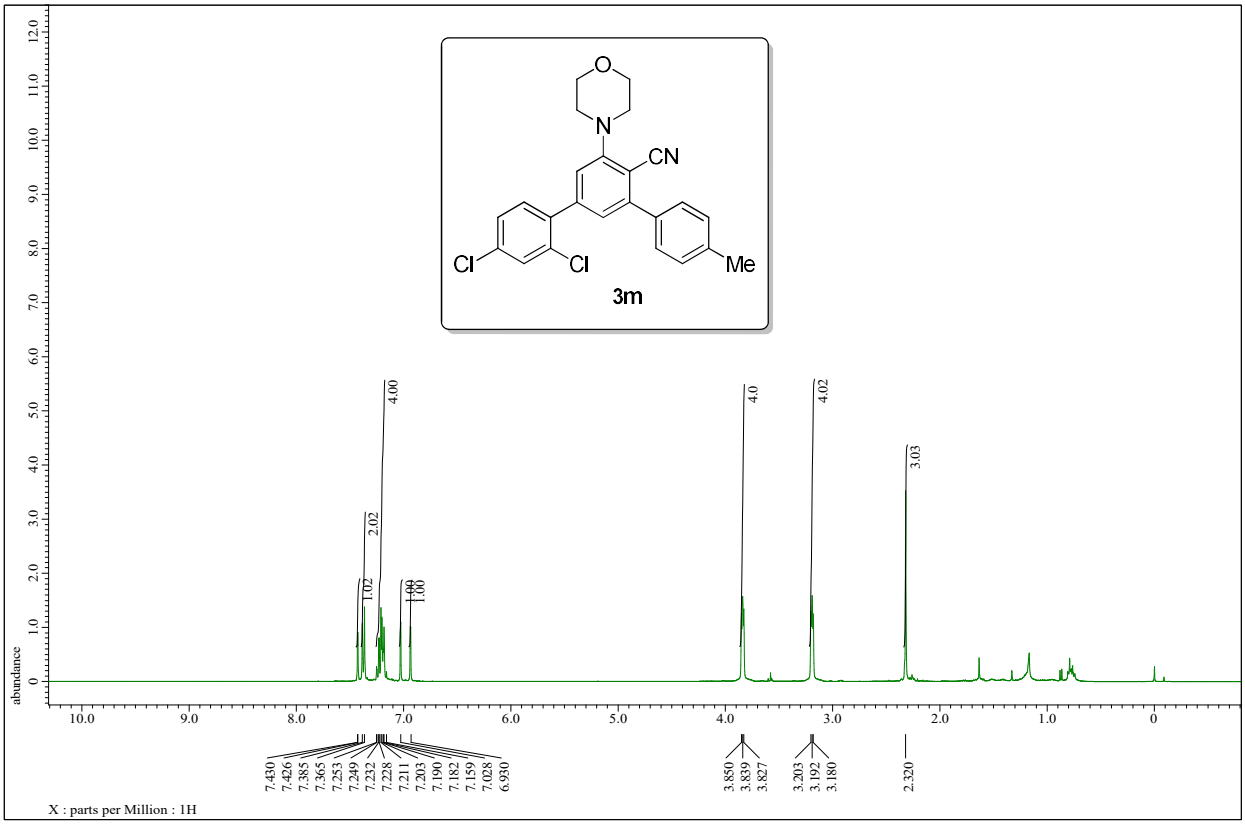

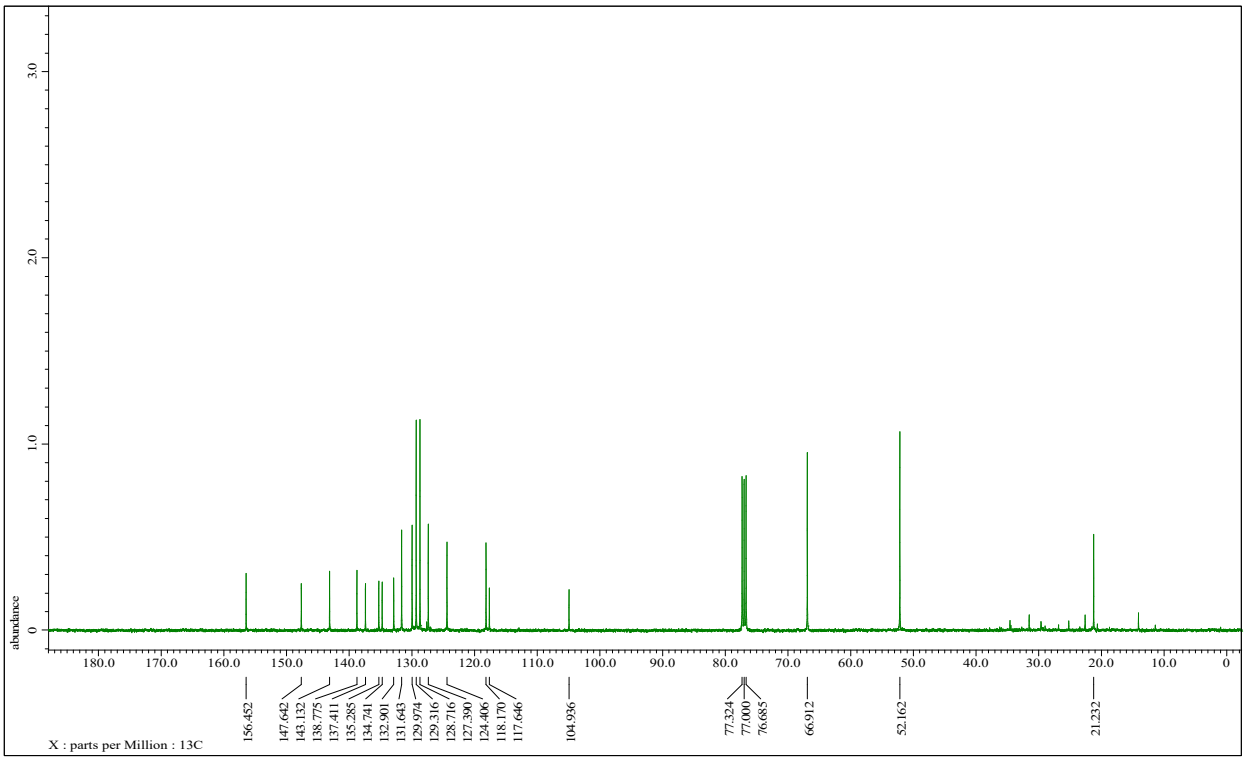

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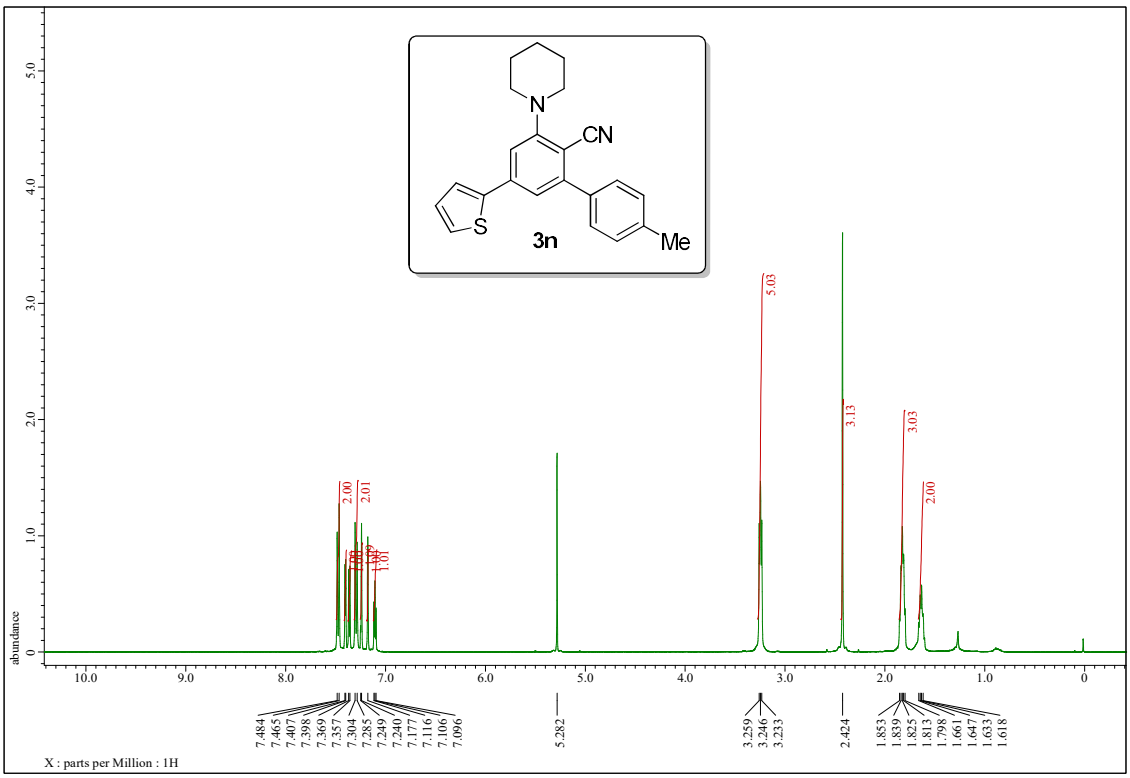
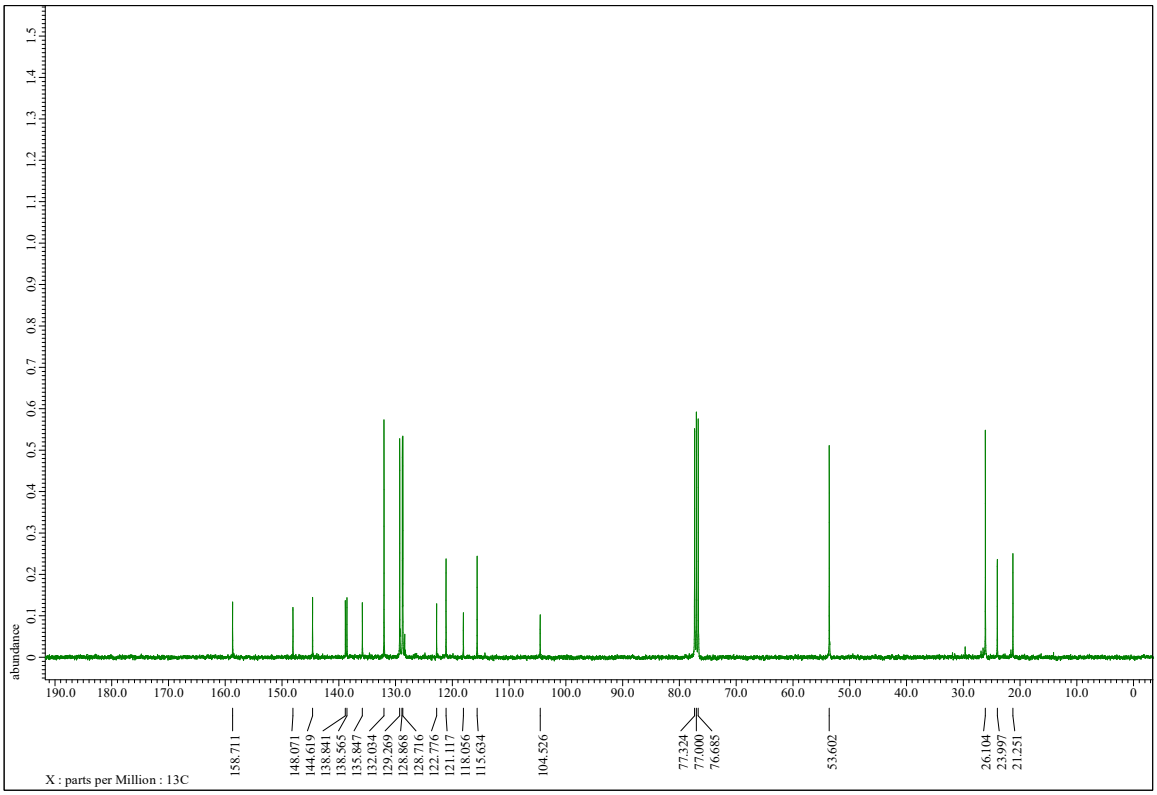
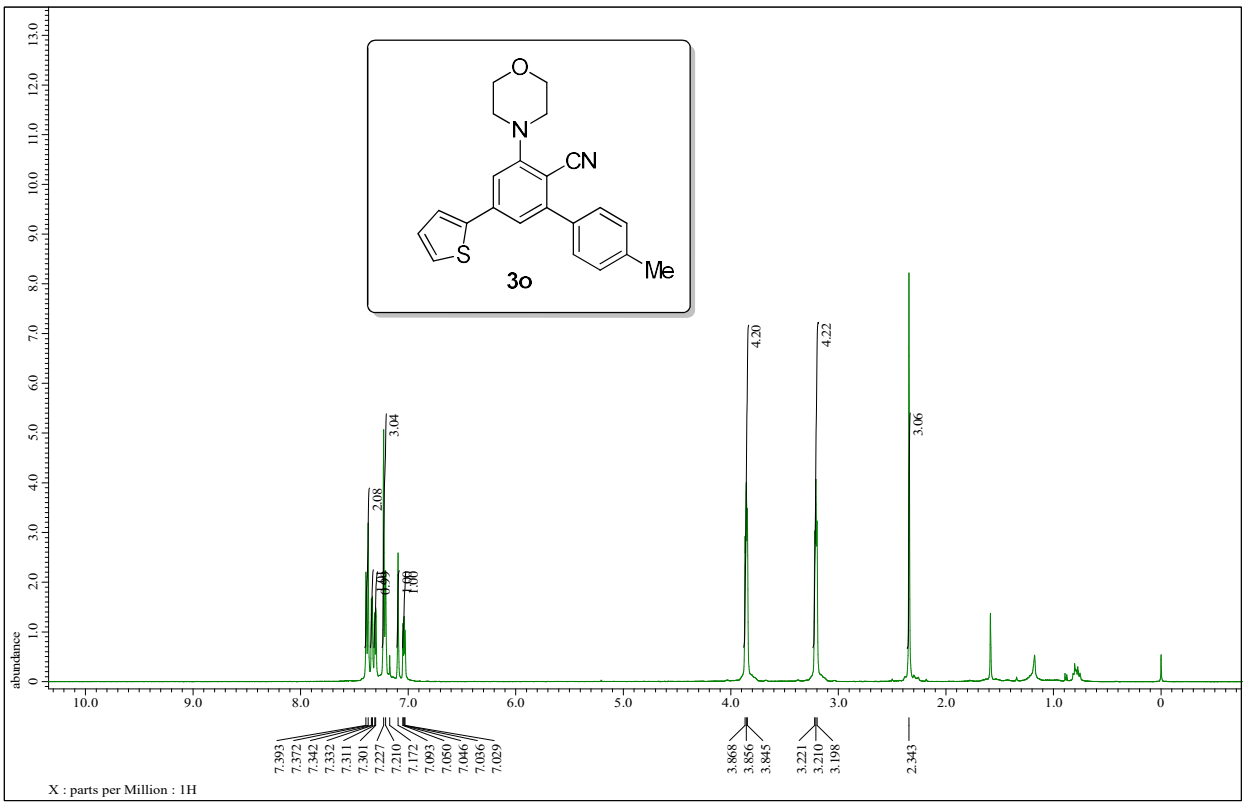
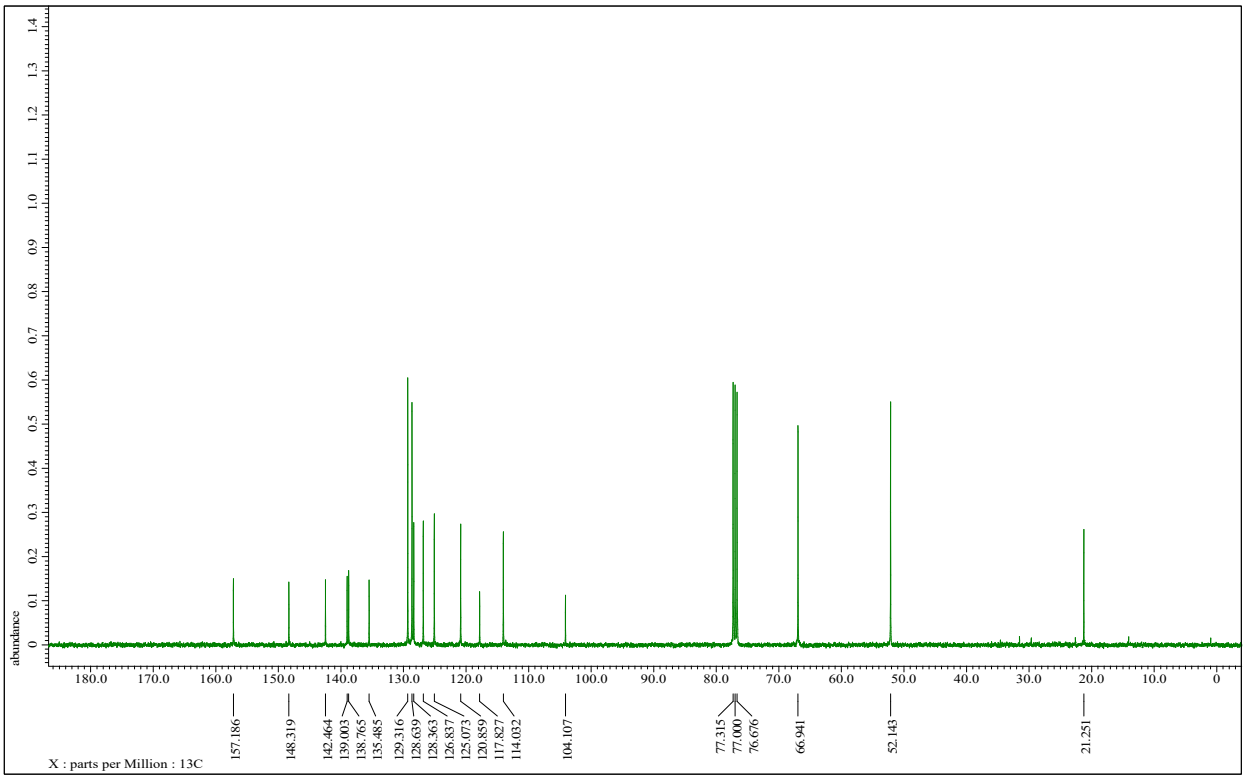




^{1}H NMR and ^{13}C NMR 4'-methyl-3-(piperidin-1-yl)-5-(thiophen-2-yl)-[1,1'-biphenyl]-2-carbonitrile





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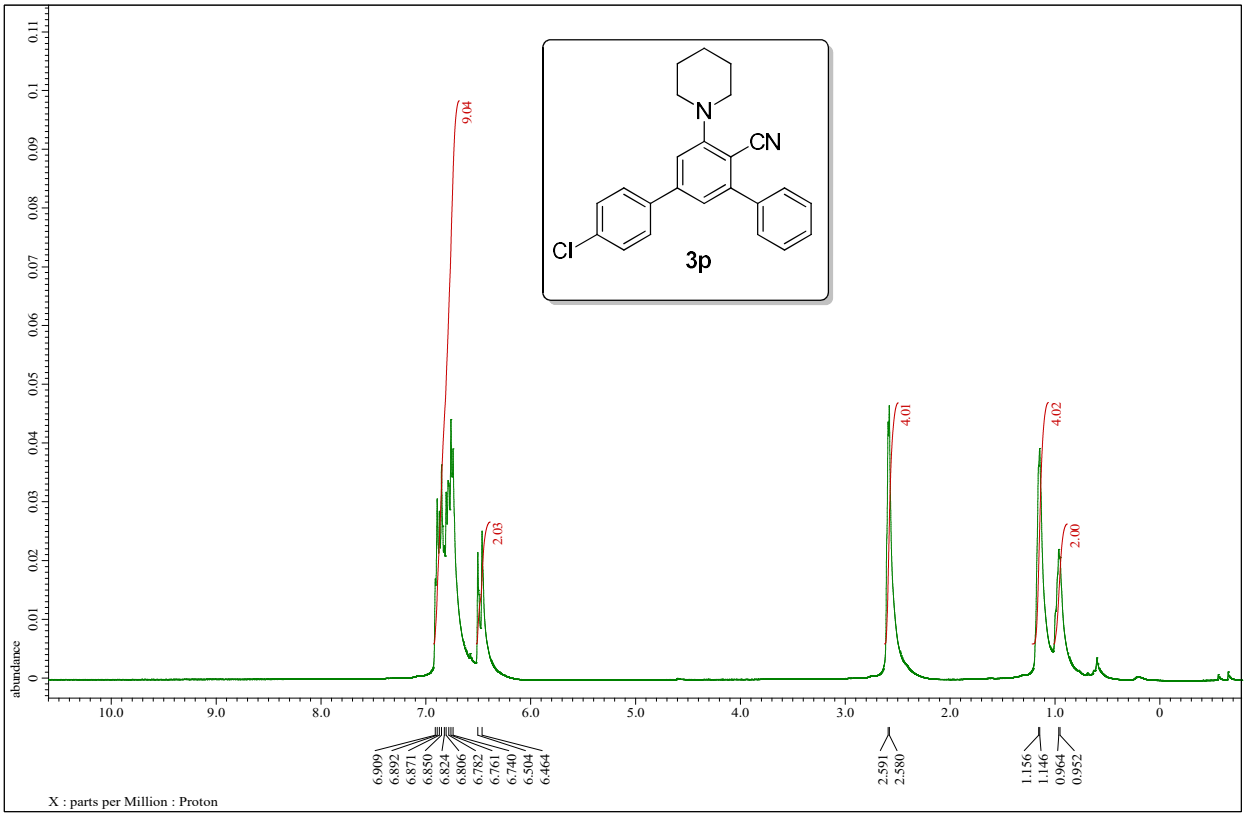

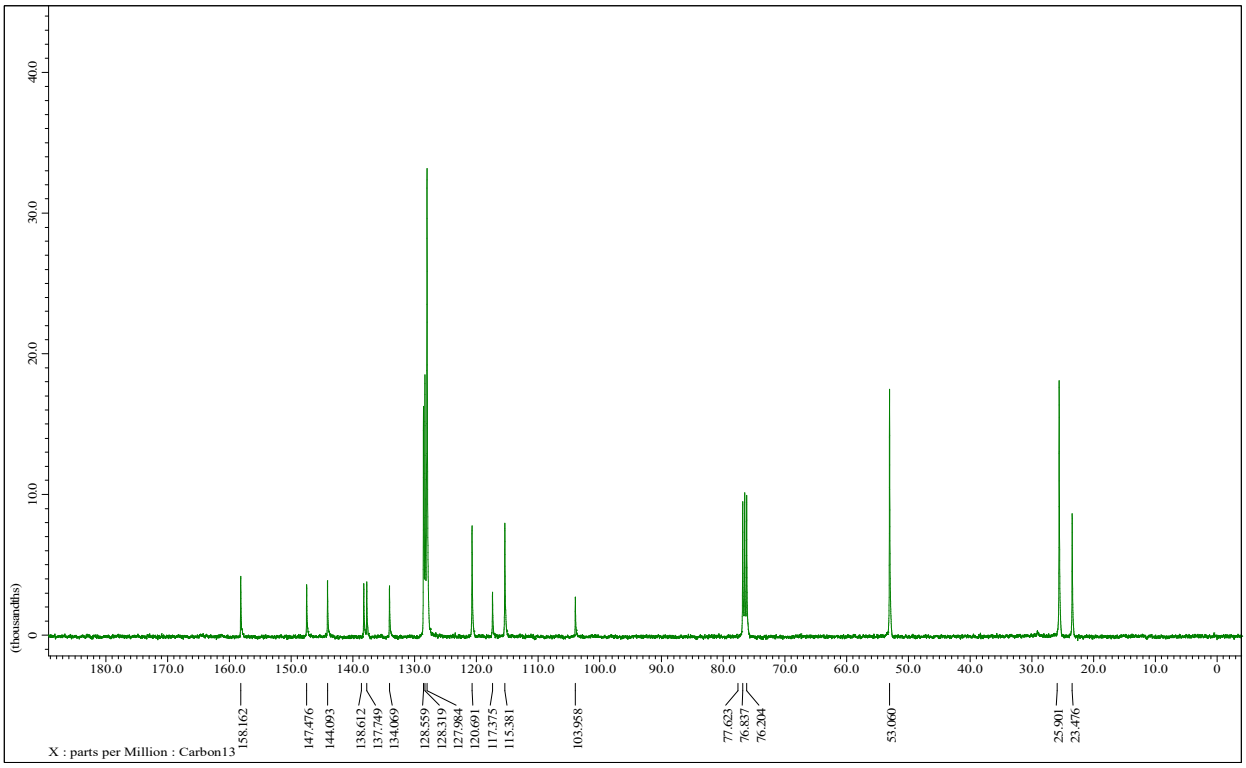

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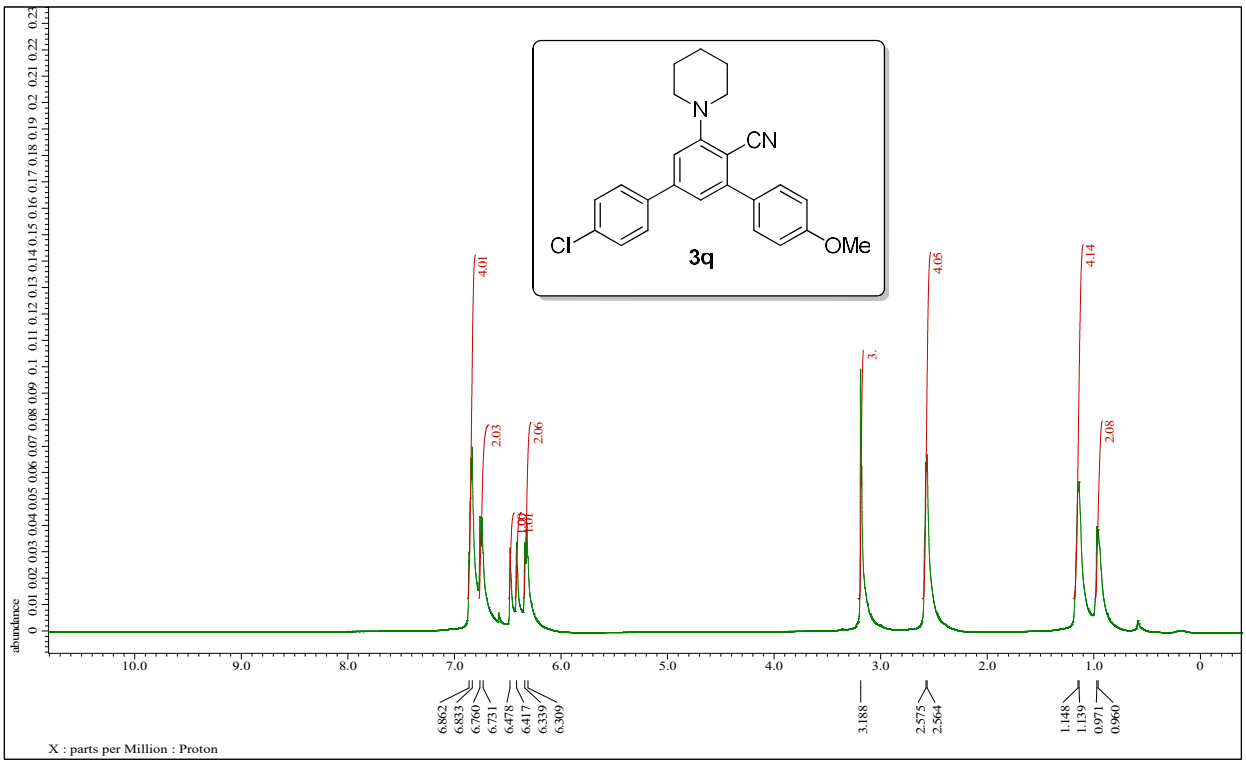

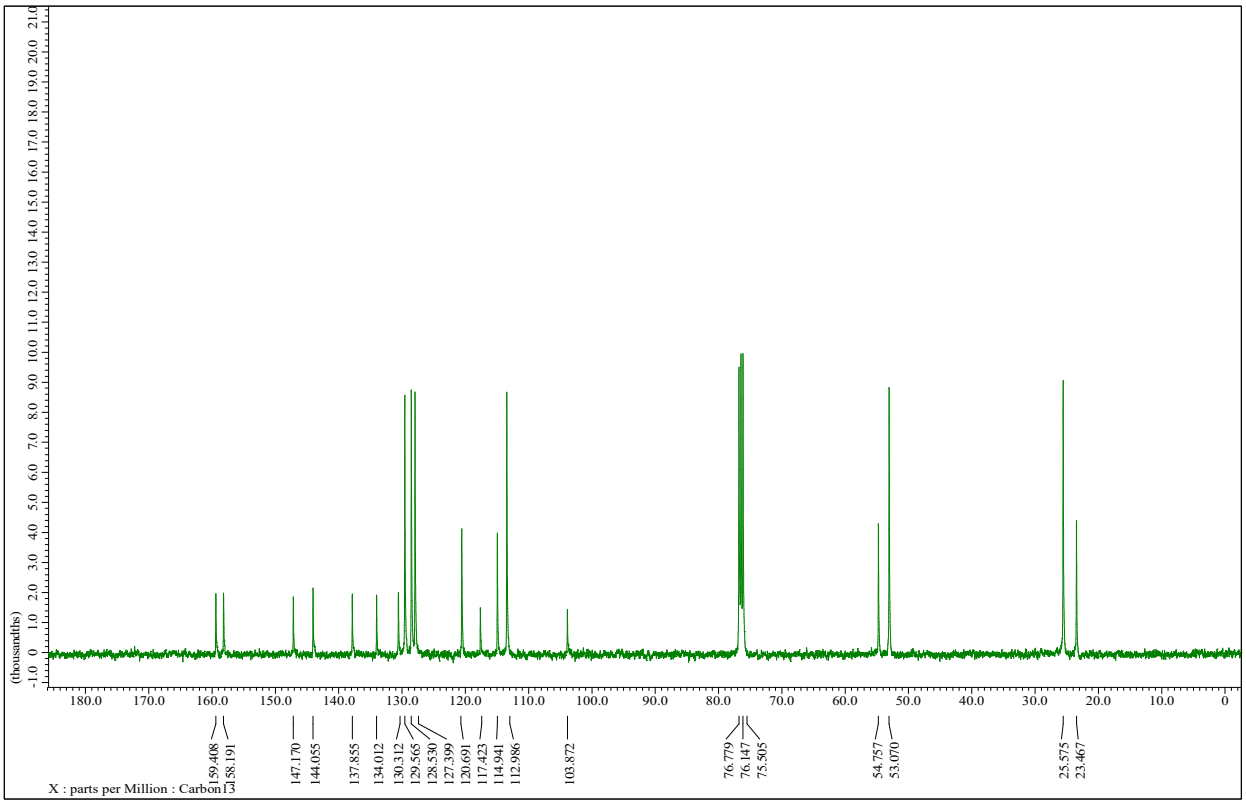

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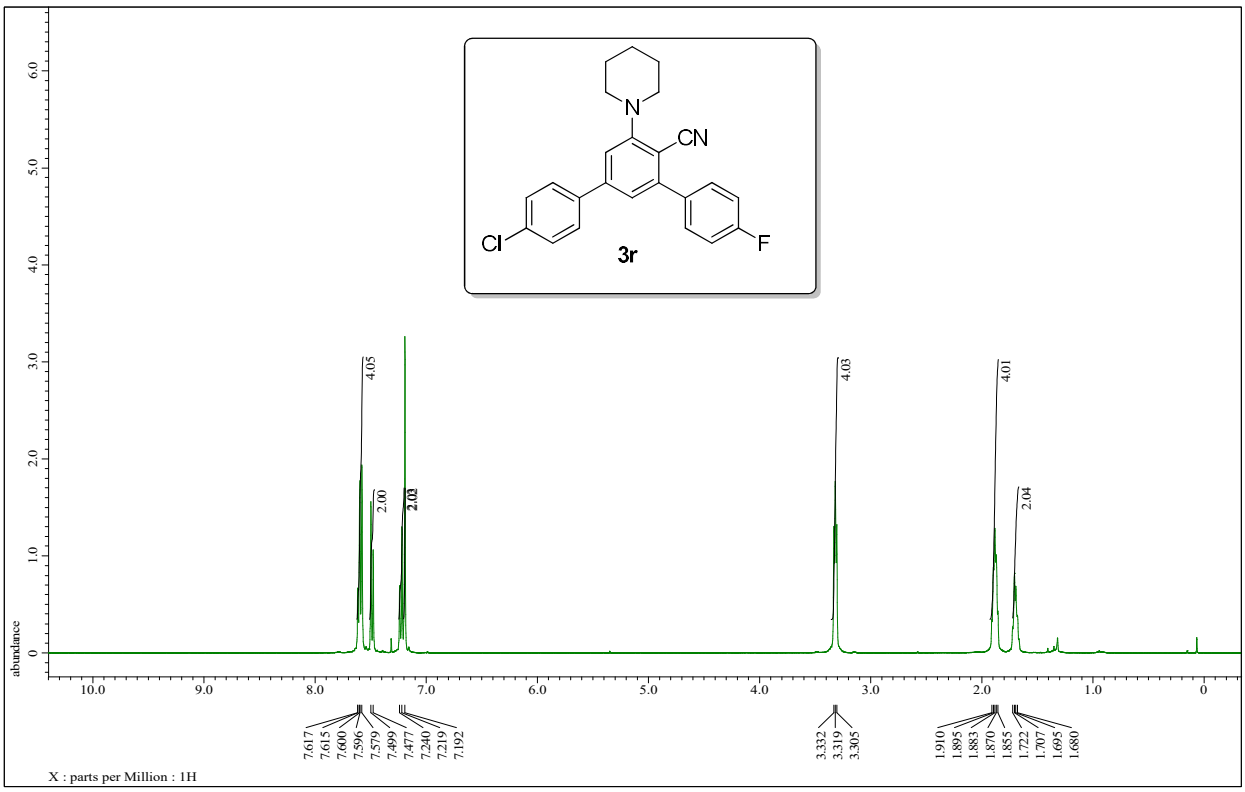

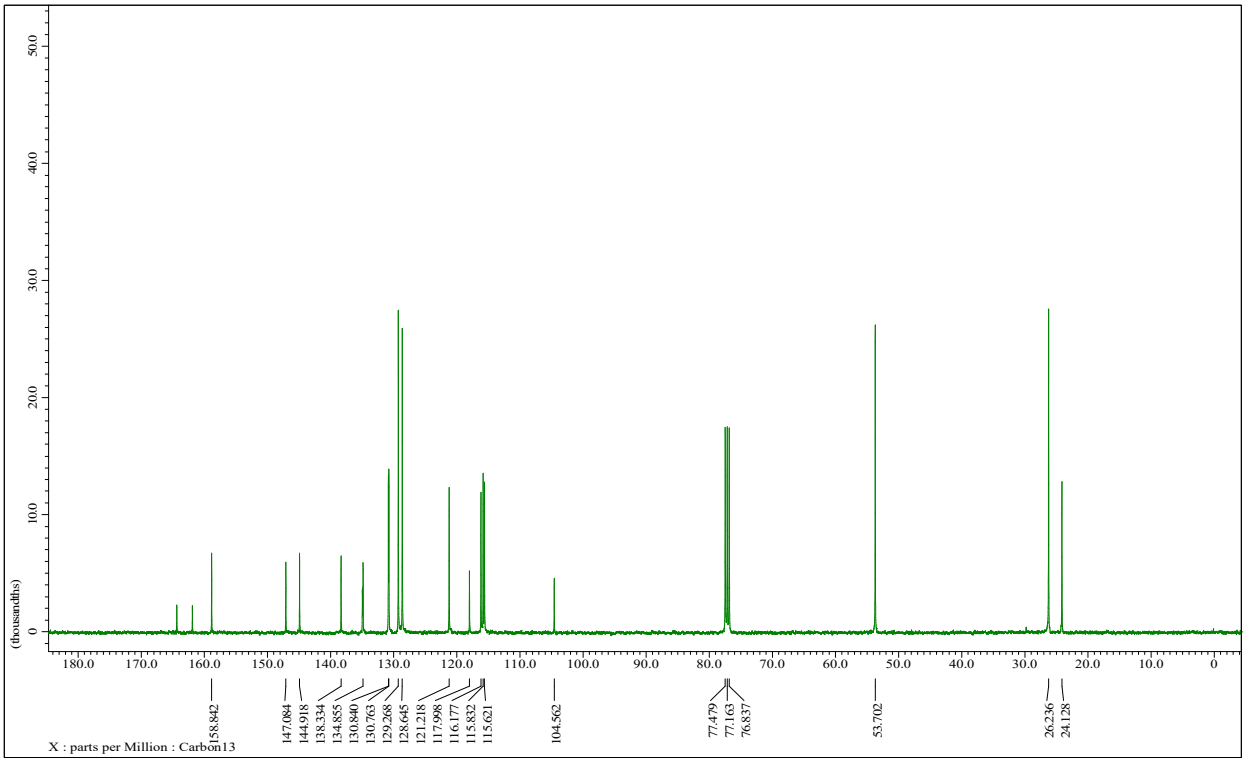

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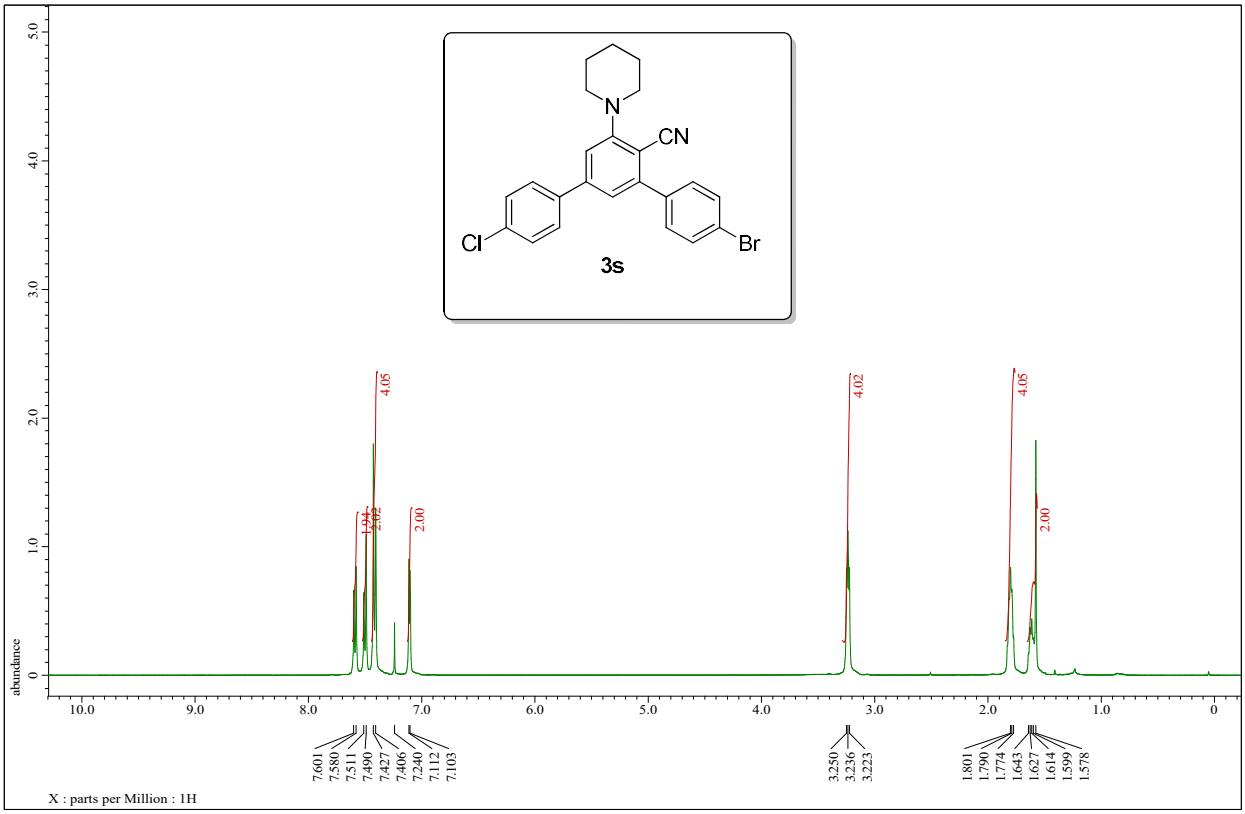

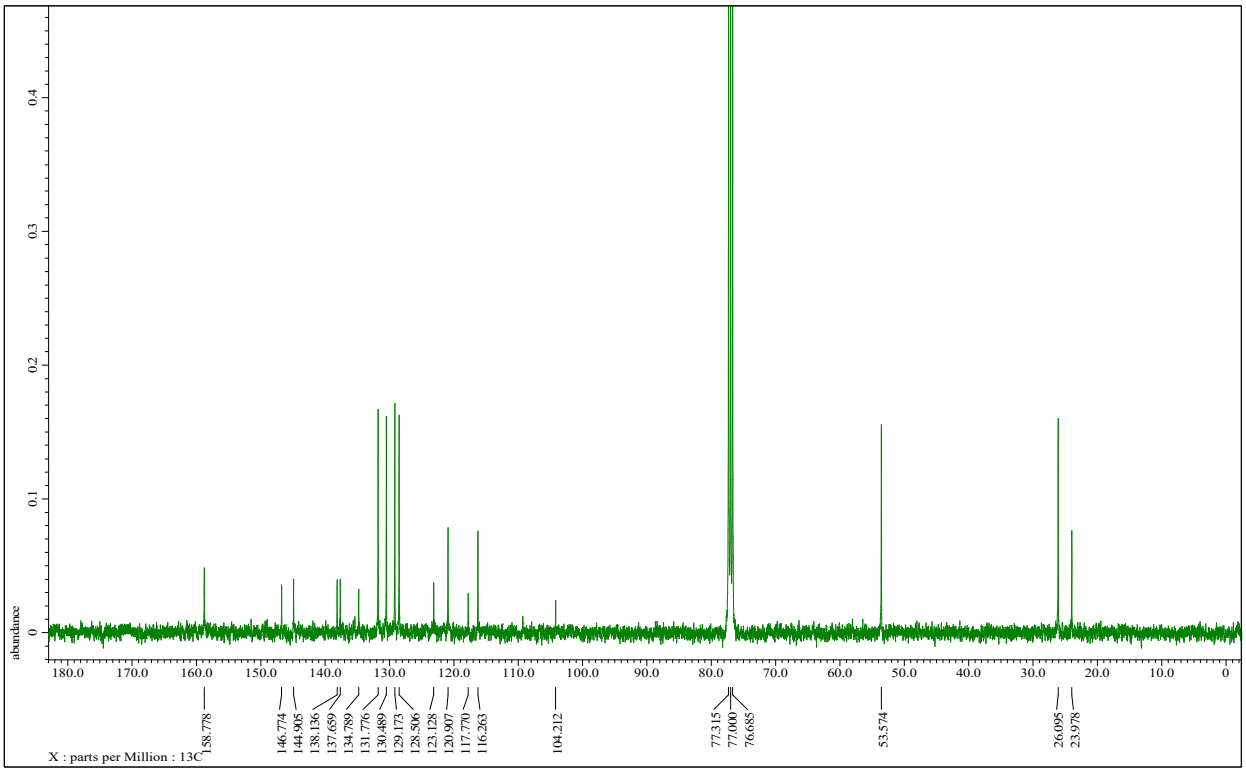

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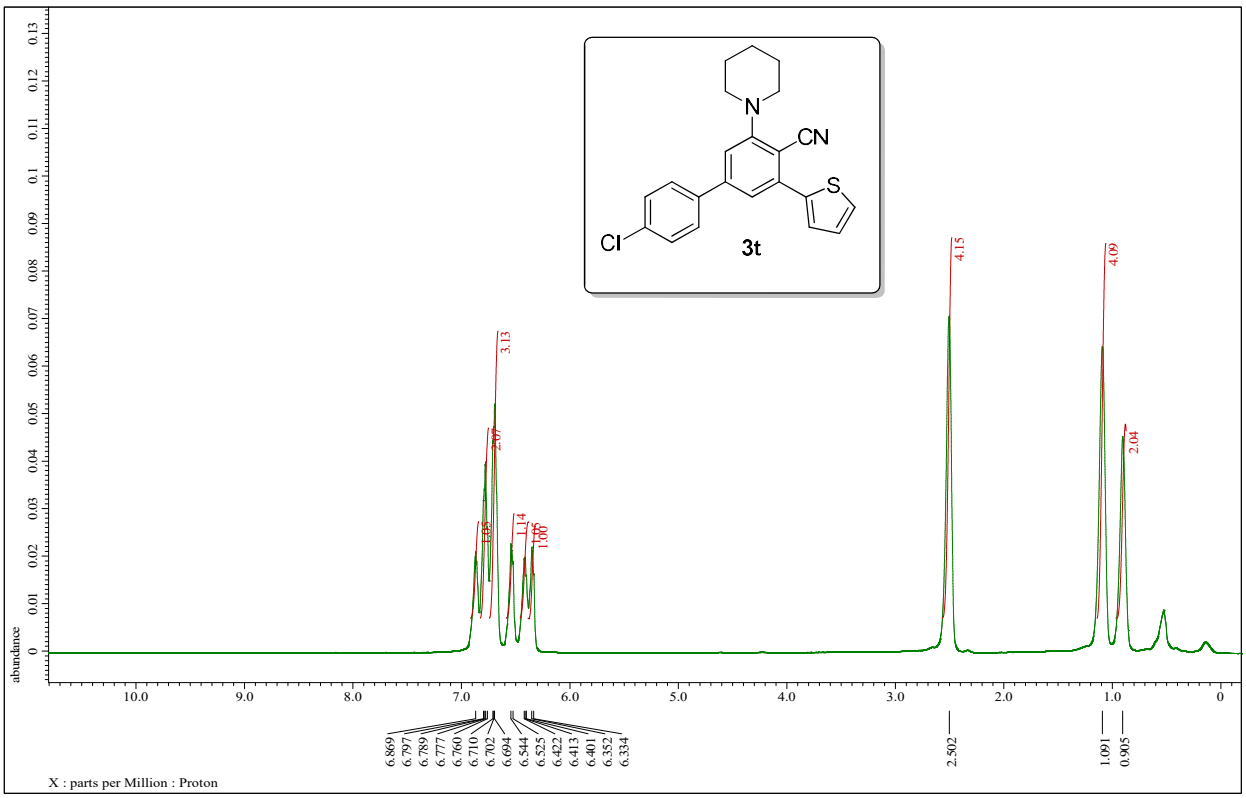
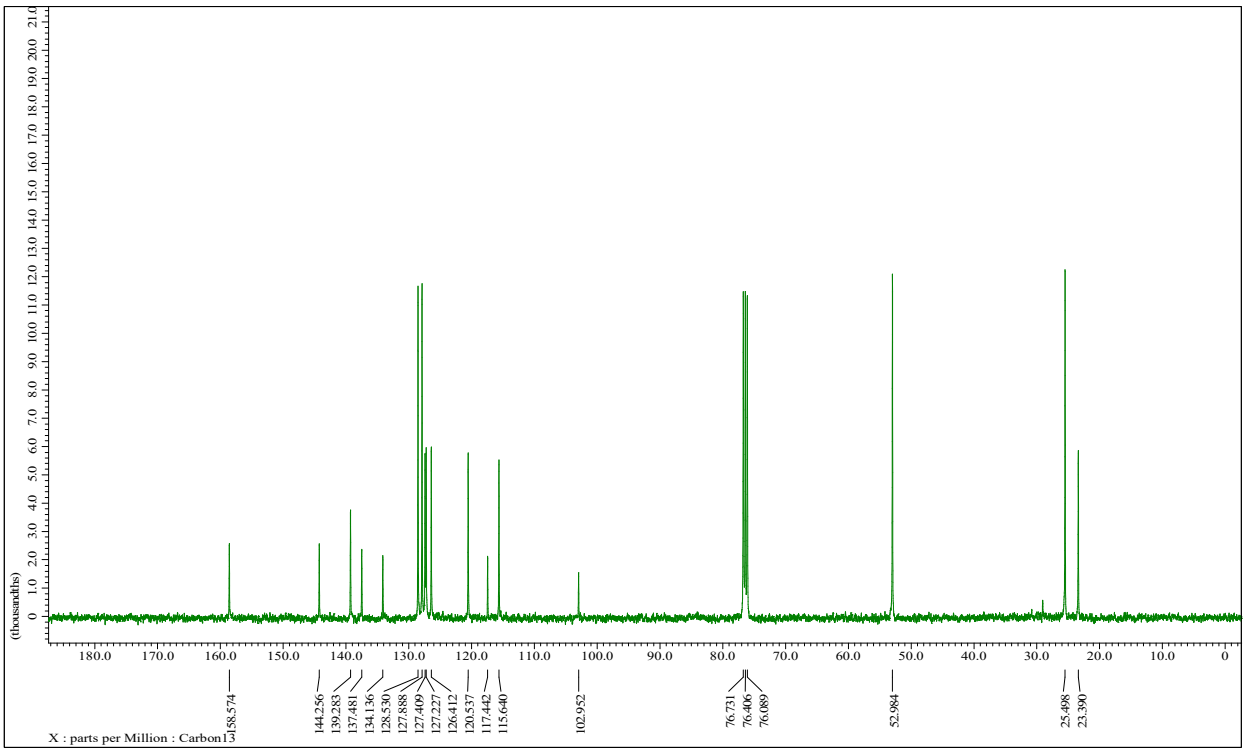
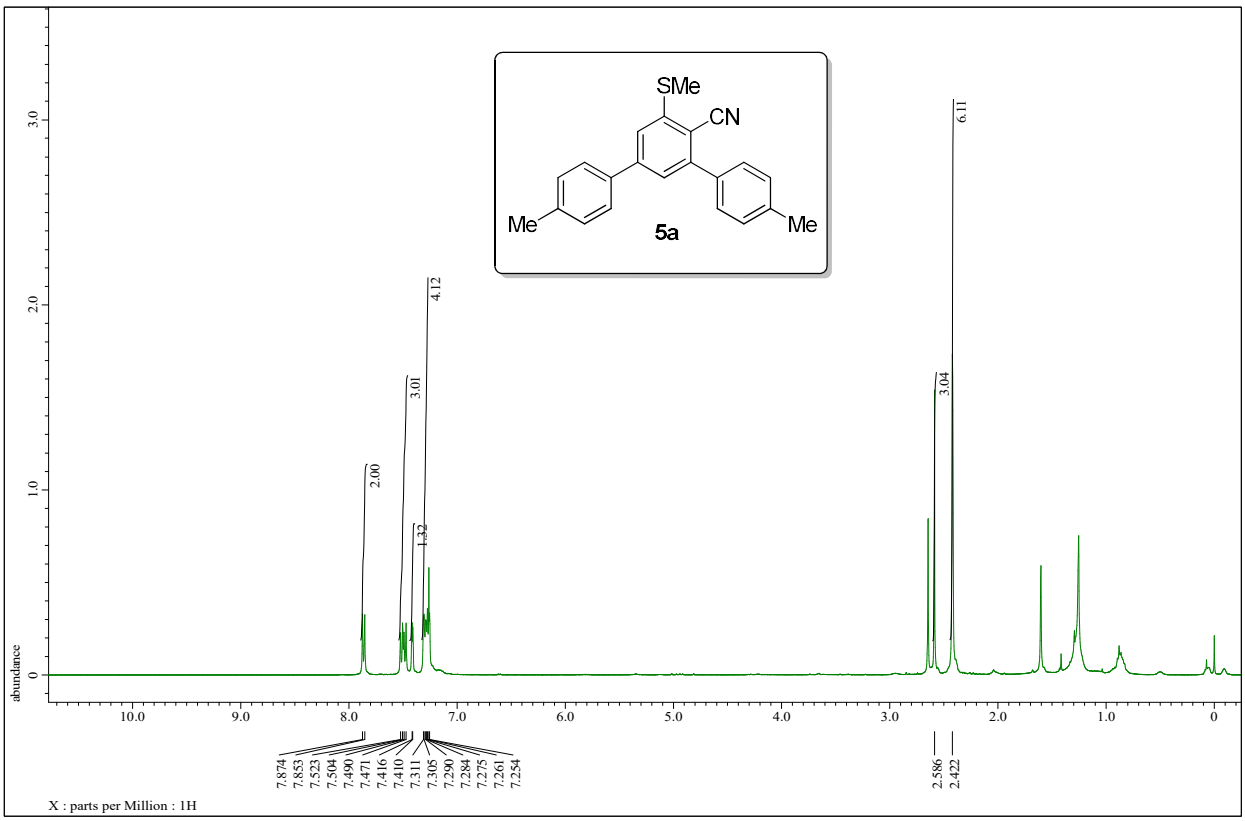
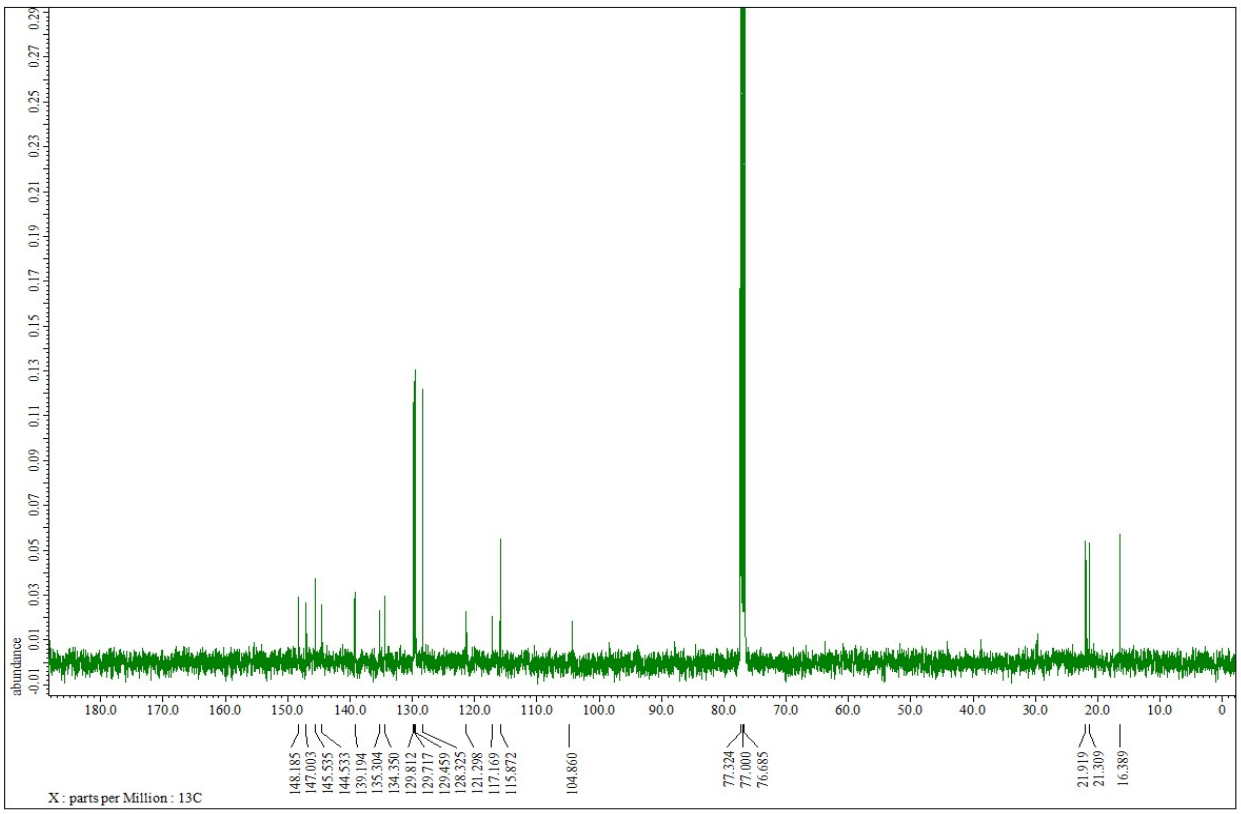




^{1}H NMR and ^{13}C NMR 4'-chloro-3-(piperidin-1-yl)-5-(thiophen-2-yl)-[1,1'-biphenyl]-4-carbonitrile





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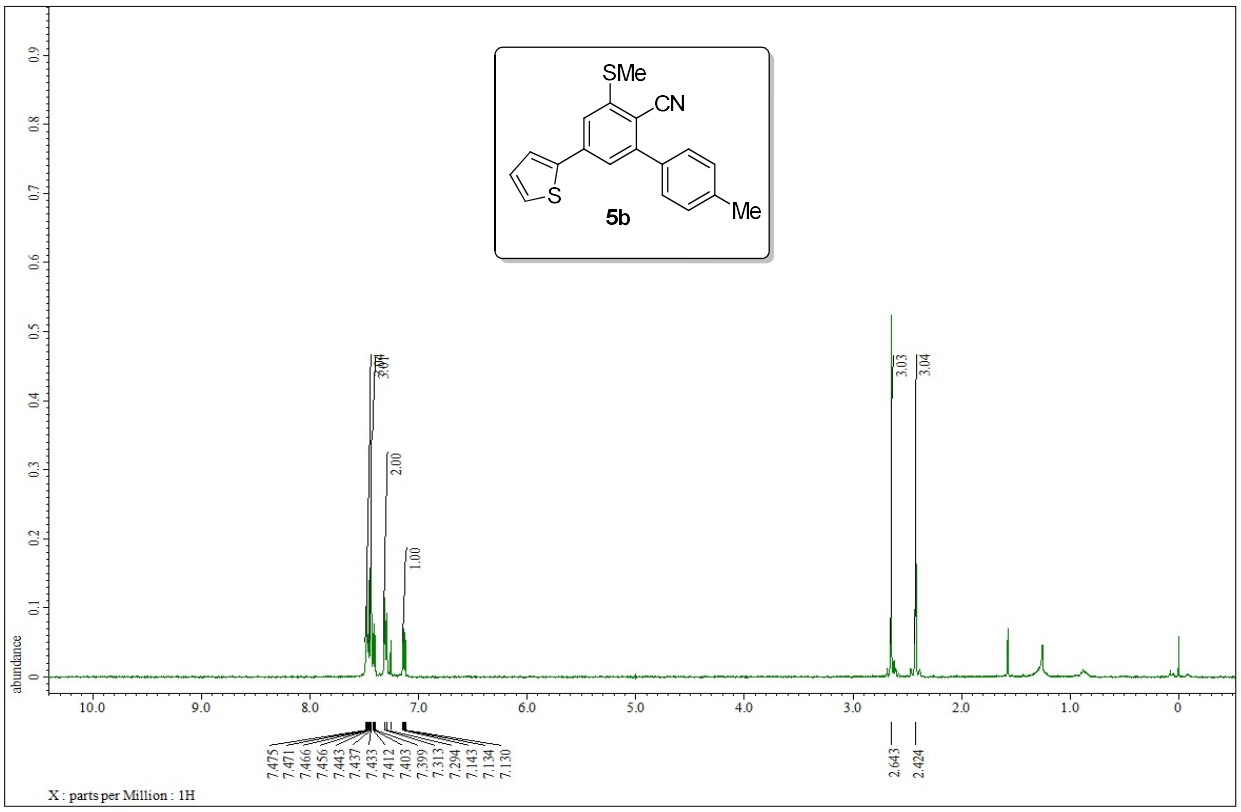

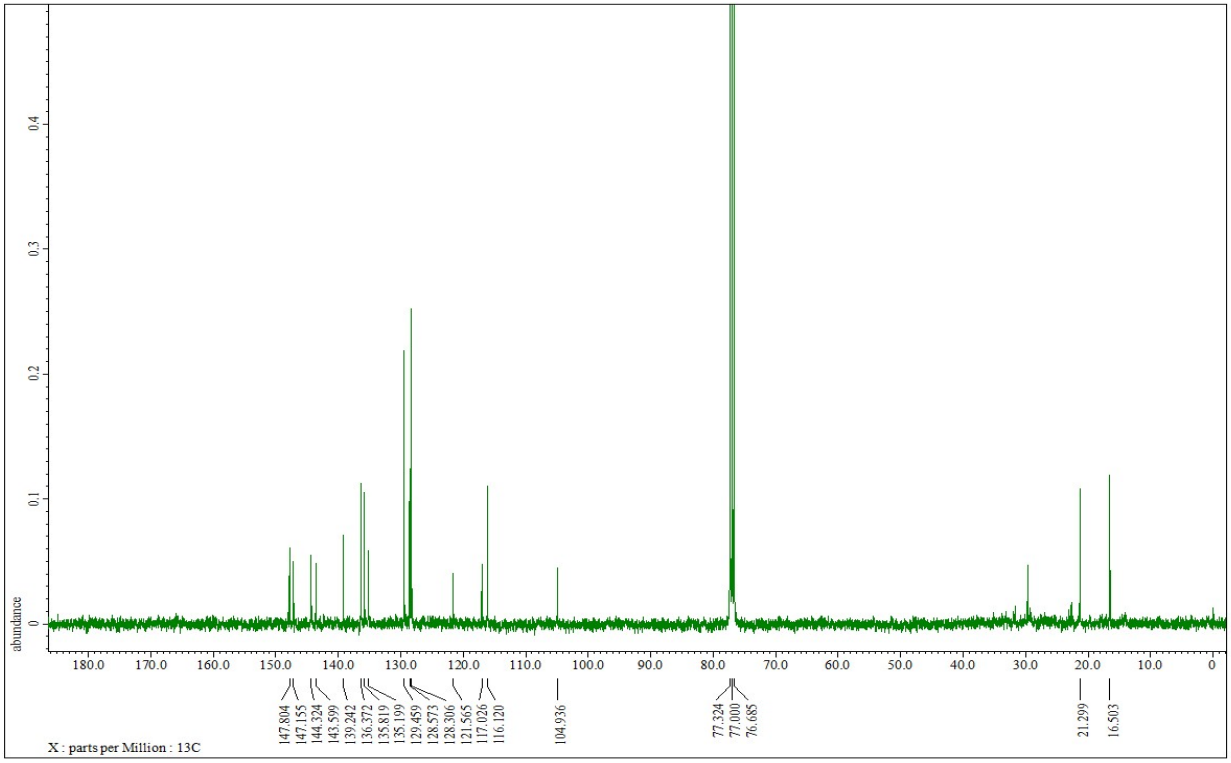

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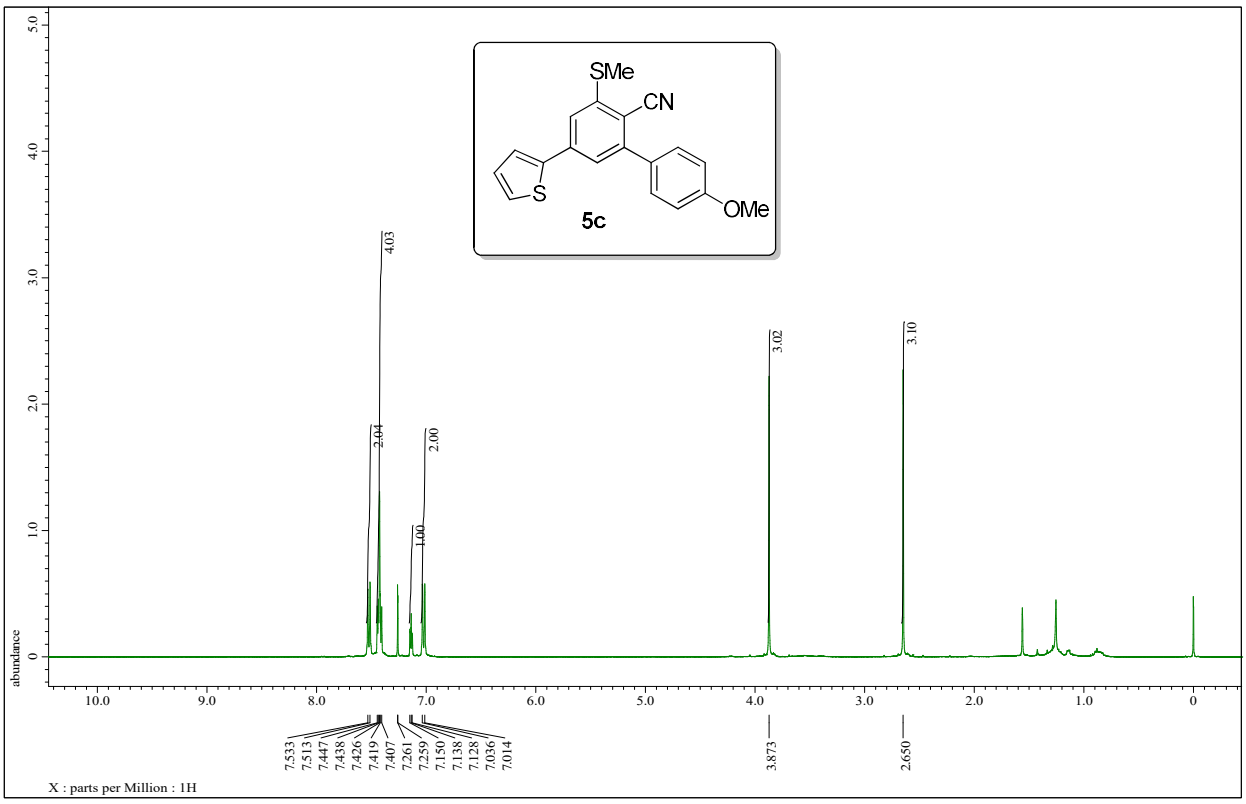

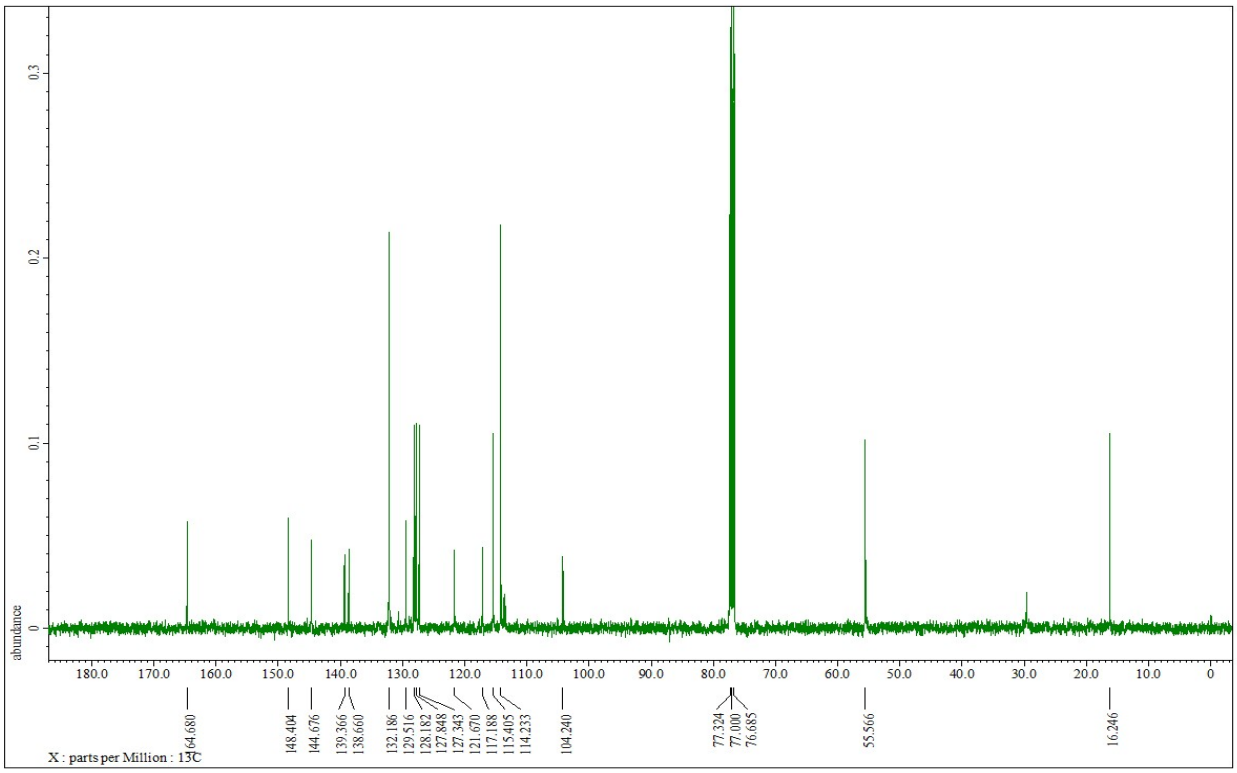

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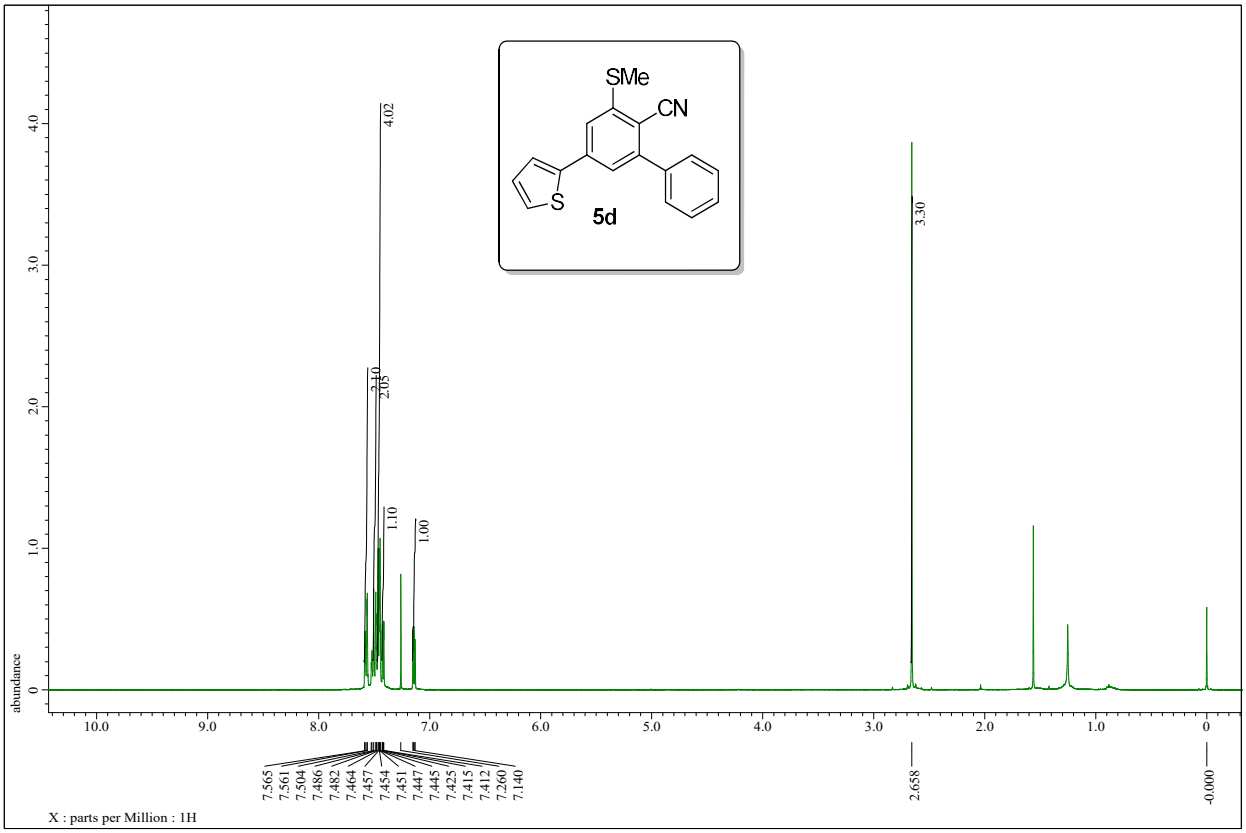

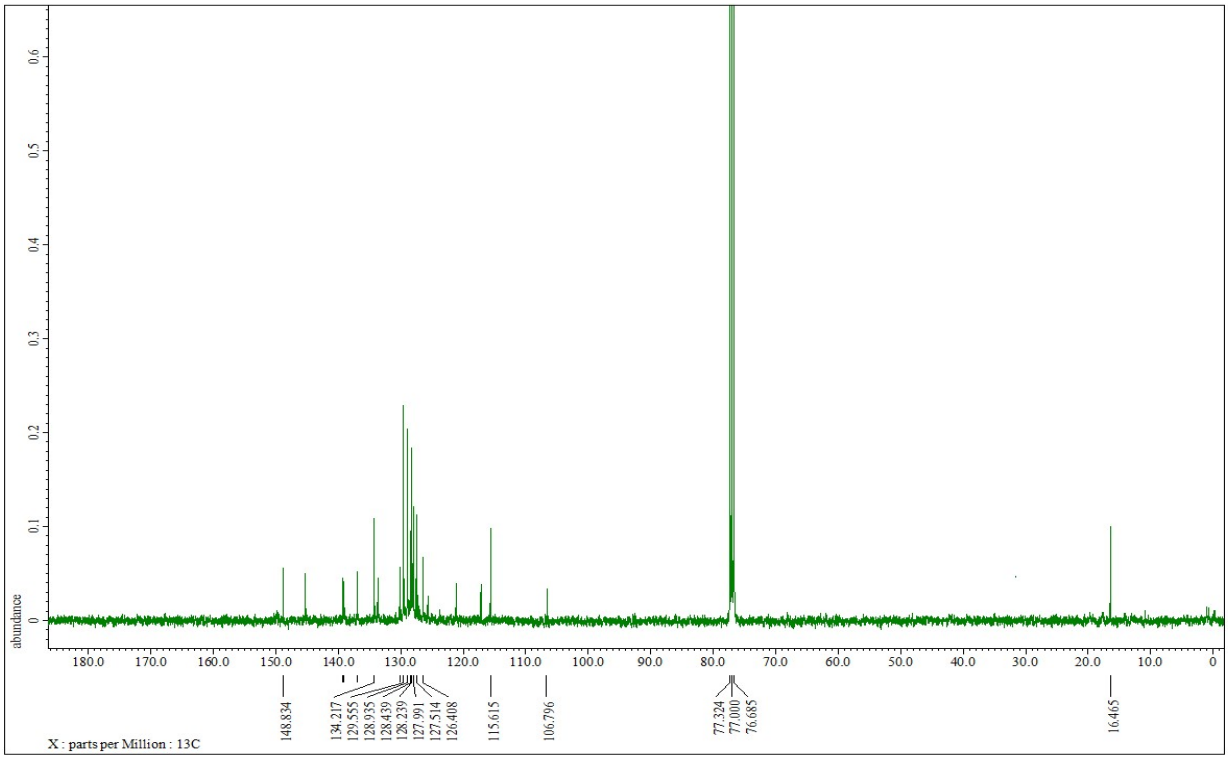

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