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The X-ray crystal structure of *Z*-**3**

The structure of *Z*-**3**was found to contain a small isolated residual electron density peak of ca. 0.6 eÅ^{-3} situated adjacent to a centre of symmetry (it is ca. 1.3 Å away from its symmetry related counterpart) and about 3 Å away from the O(25) oxygen atom. (By contrast, the next nine largest residual electron density peaks are all clustered around the main molecule.) Being a lone peak and at a plausible hydrogen bonding distance from an oxygen atom, this peak was assigned as the oxygen of a water molecule [O(40)], and by comparison of its thermal parameter with those of the main molecule its occupancy was estimated as being ca. 10%. The hydrogen atoms associated with this water molecule were not located.

Crystal data for *Z*-**3**: $C_{25}H_{25}NO_4S_2 \cdot 0.10H_2O$, M = 469.38, triclinic, $P\bar{1}$ (no. 2), a = 9.1743(3), b = 9.9834(4), c = 13.0708(4) Å, α = 79.253(3), β = 76.645(3), γ = 86.290(3)°, V = 1144.06(7) Å^3, Z = 2, D_c = 1.363 g cm^{-3}, μ(Mo-Kα) = 0.266 mm^{-1}, T = 173 K, pale yellow platy needles, Oxford Diffraction Xcalibur 3 diffractometer; 5098 independent measured reflections (R_{int} = 0.0160), F^2 refinement, R_1(obs) = 0.0392, wR_2(all) = 0.1024, 3652 independent observed absorption-corrected reflections [$|F_o| > 4\sigma(|F_o|)$, $2\theta_{max}$ = 58°], 295 parameters. CCDC 775144.

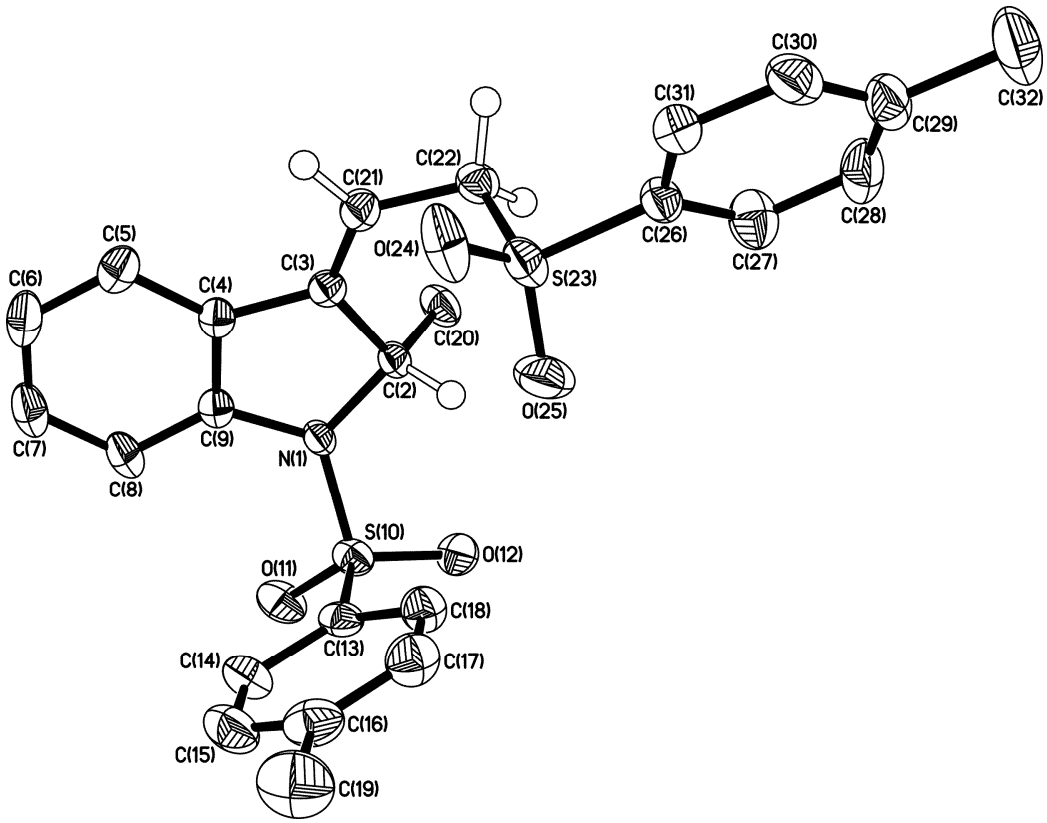

Fig. S1 The molecular structure of *Z*-**3** (50% probability ellipsoids).

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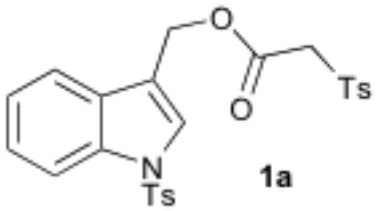

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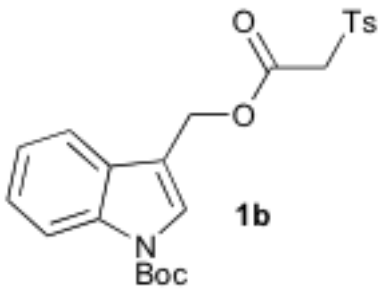

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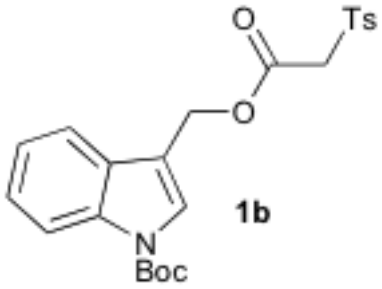

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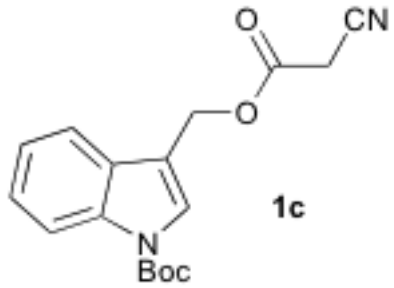

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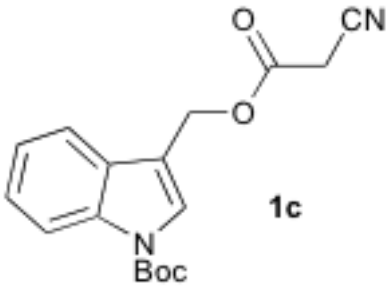

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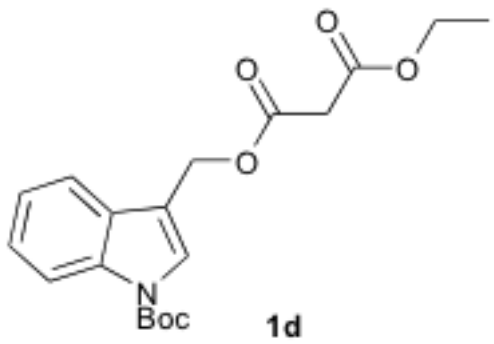

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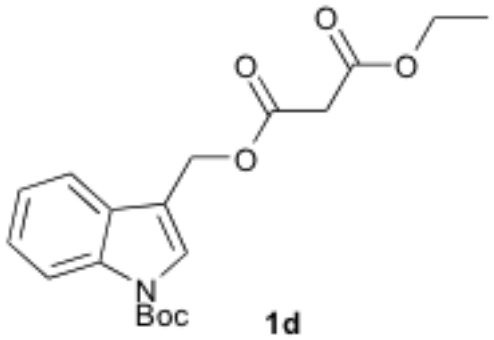

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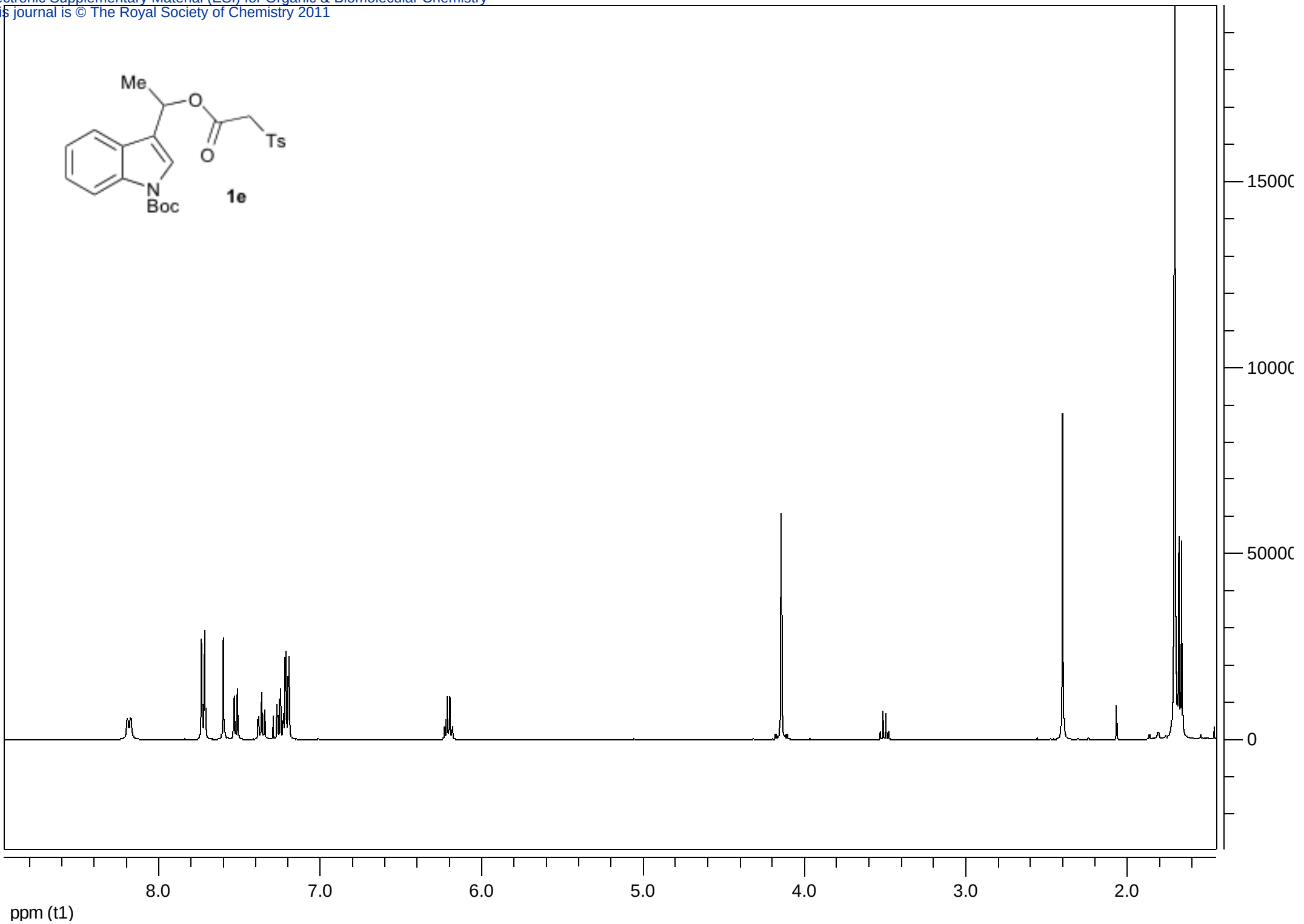

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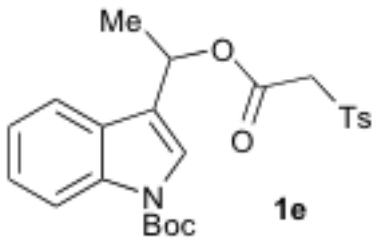

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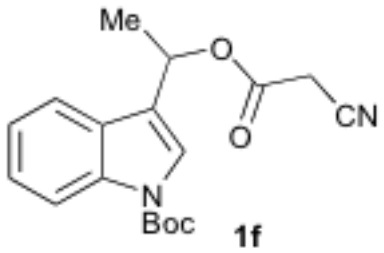

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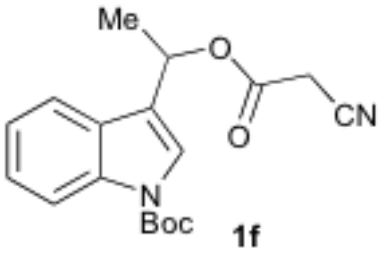

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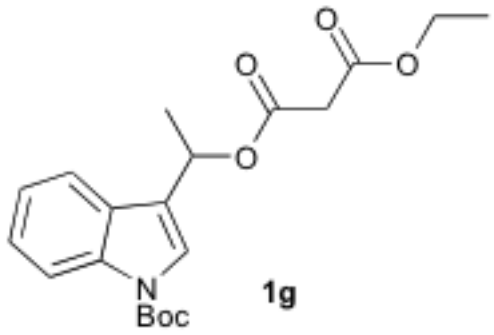

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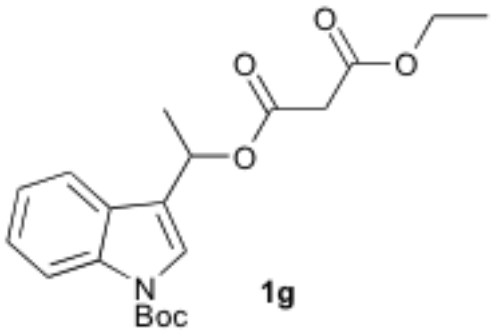

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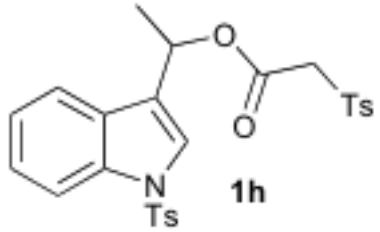

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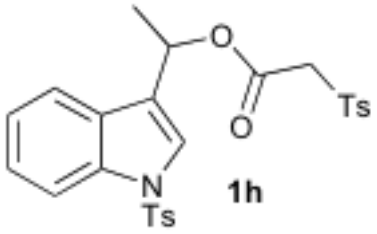

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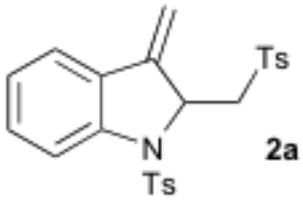

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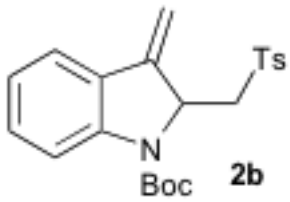

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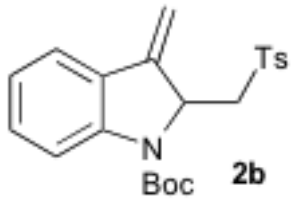

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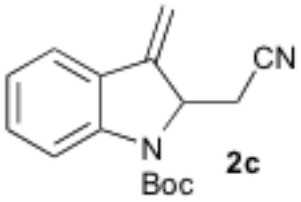

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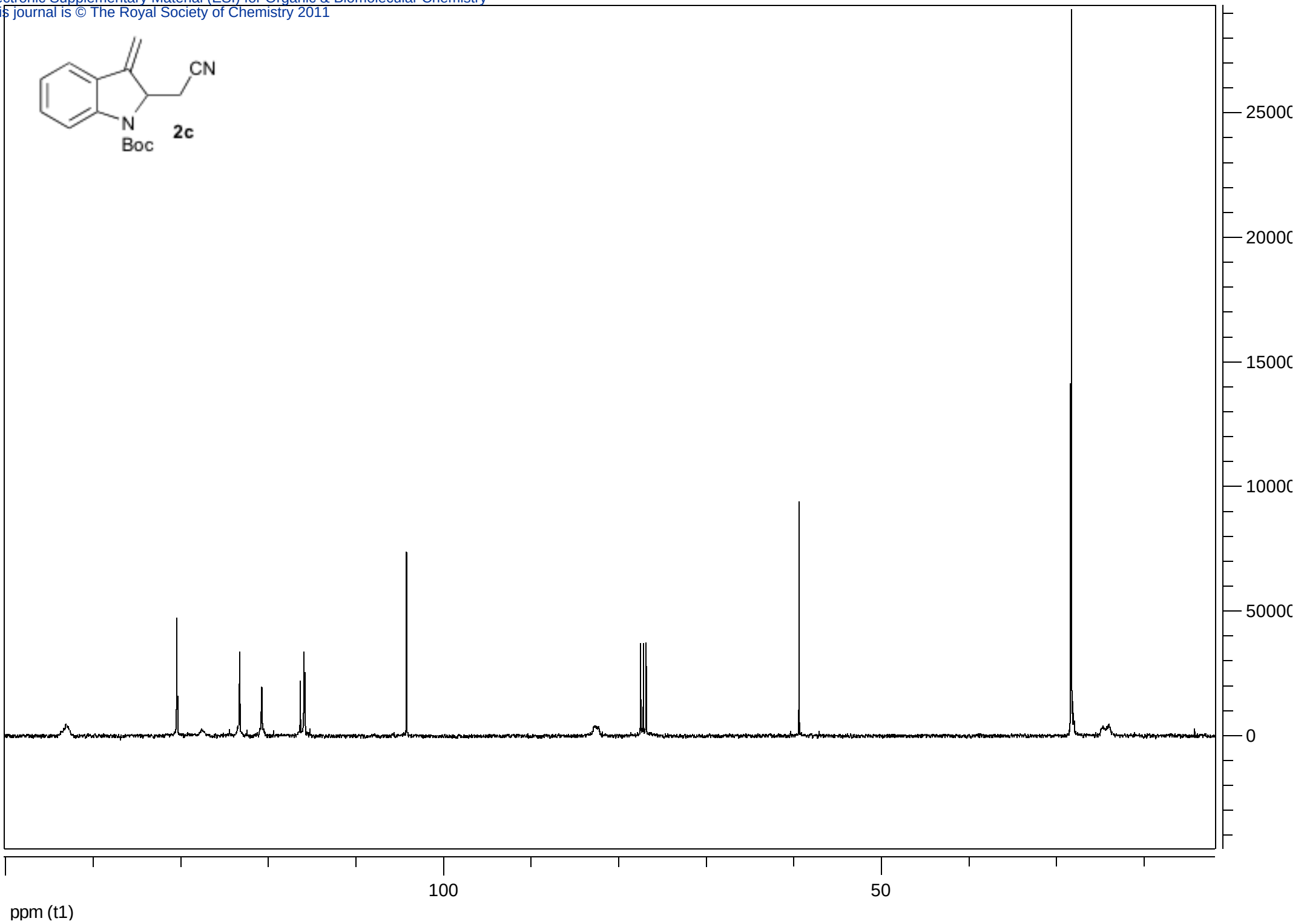

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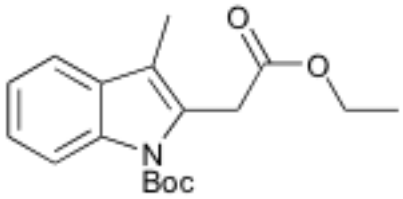

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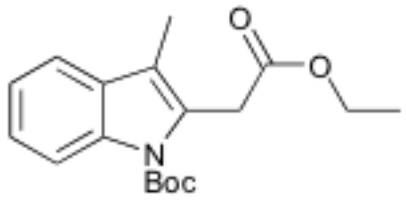

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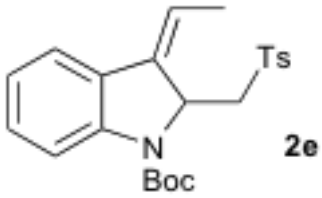

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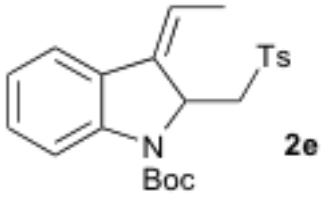

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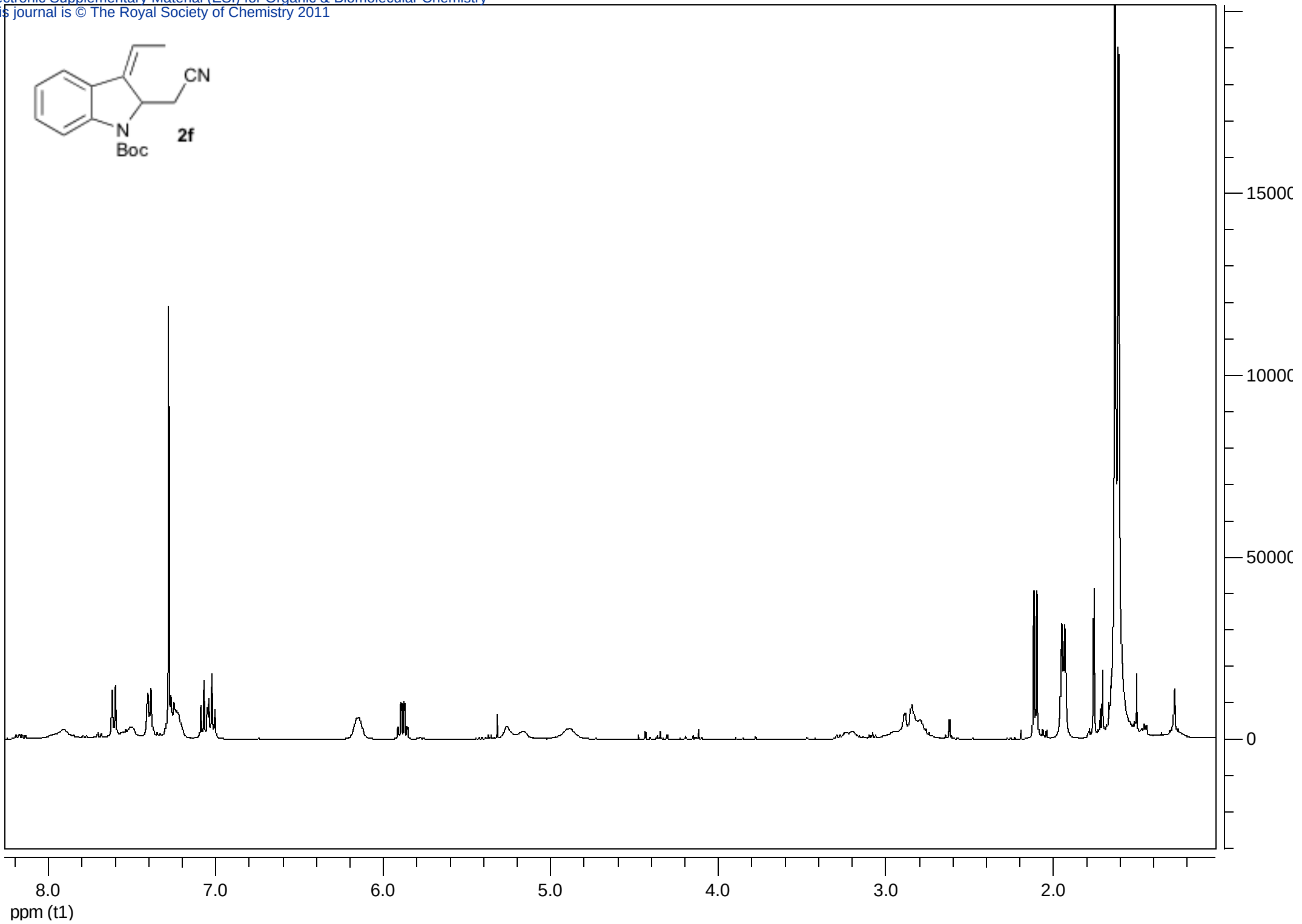

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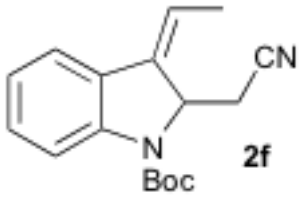

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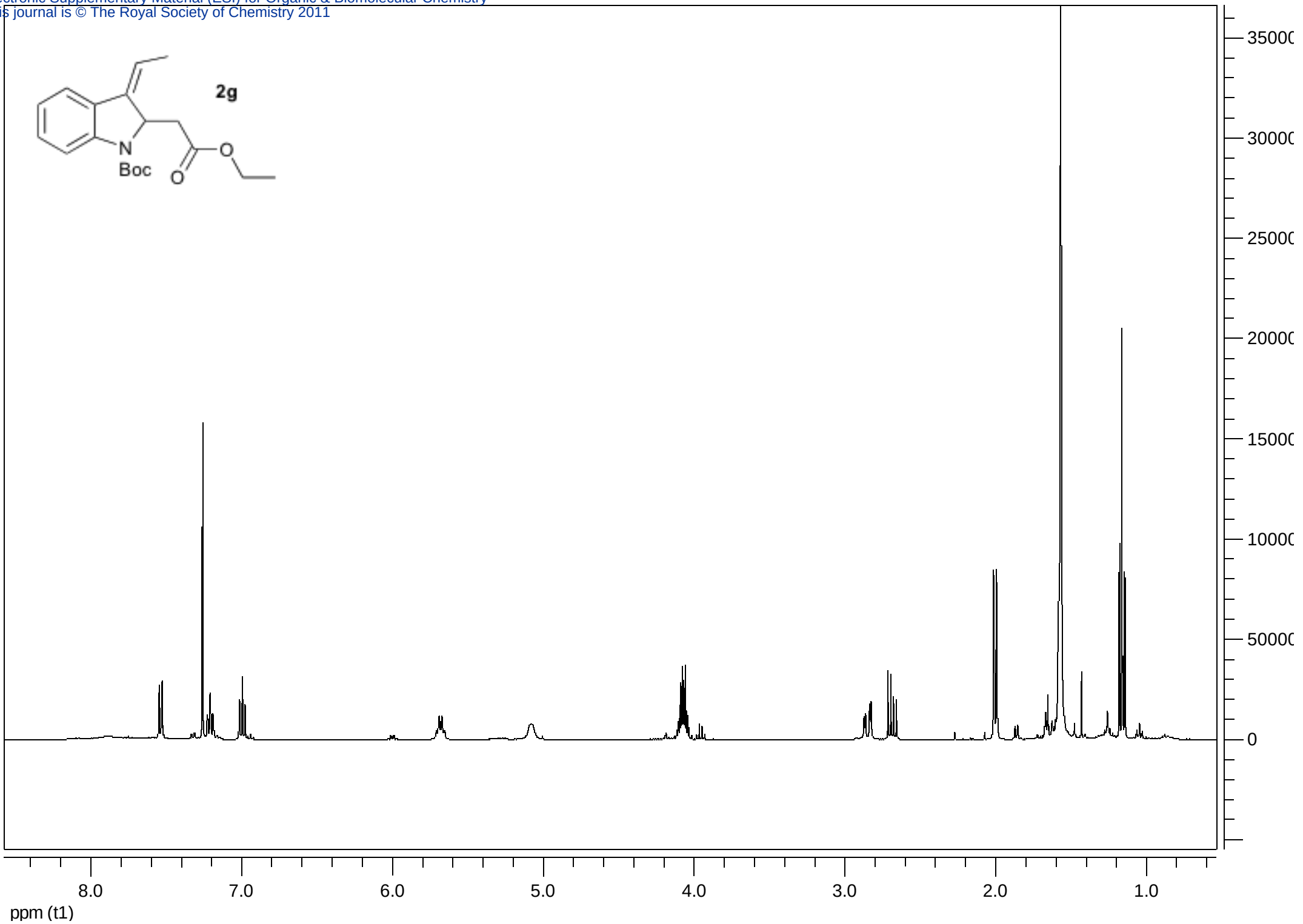

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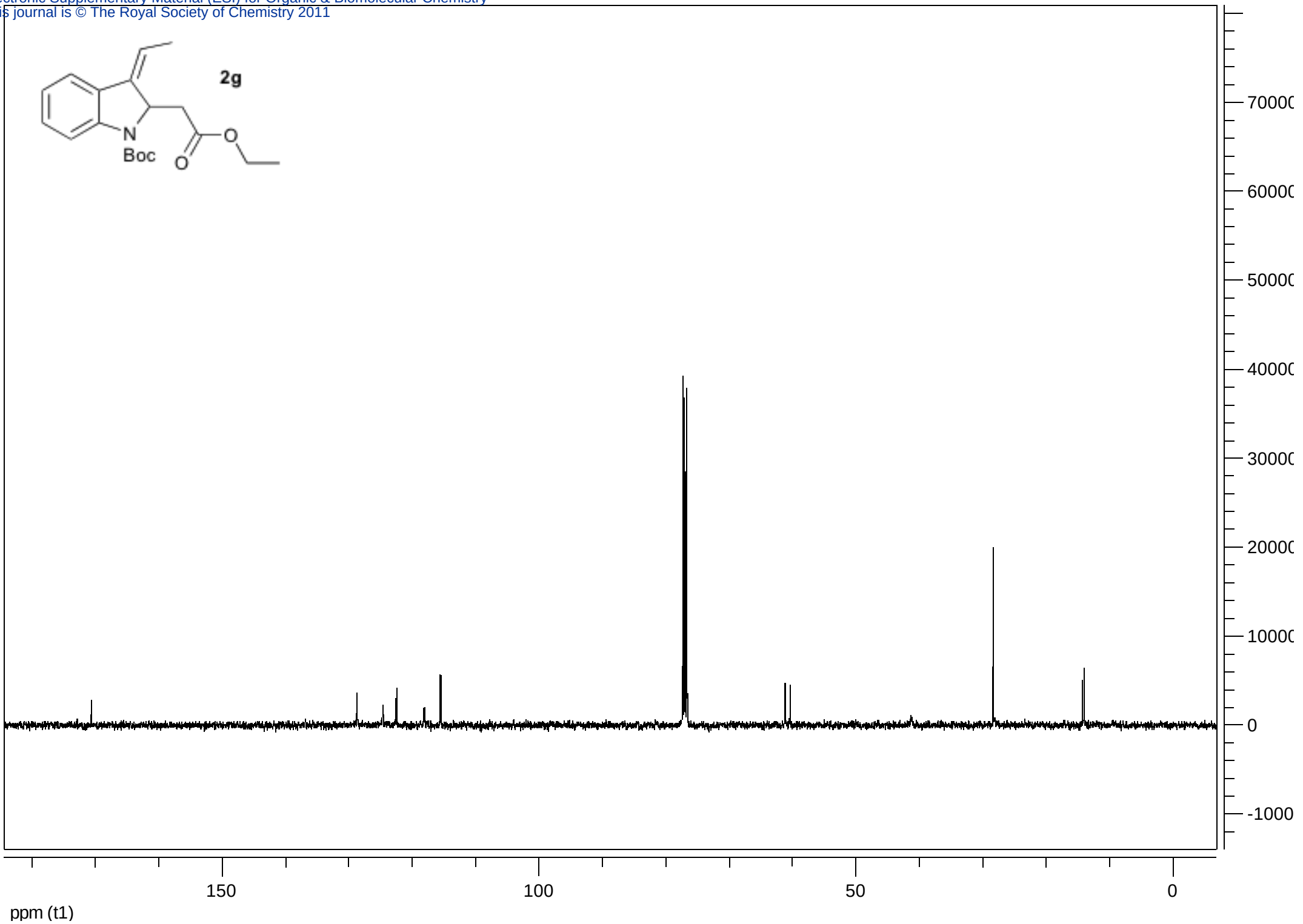

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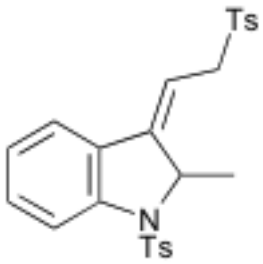

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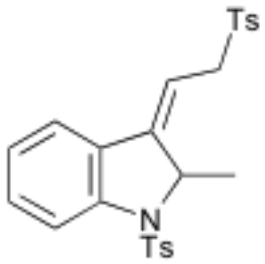

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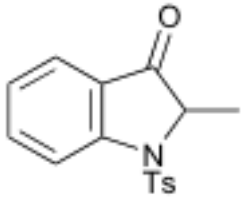

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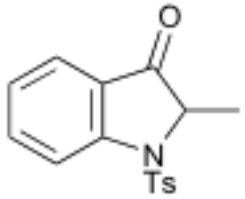

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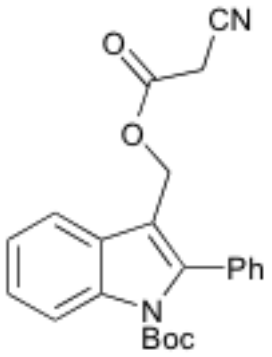

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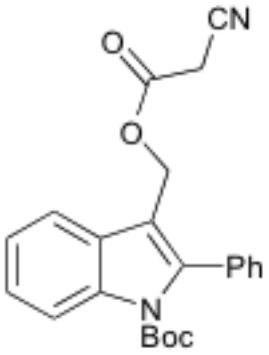

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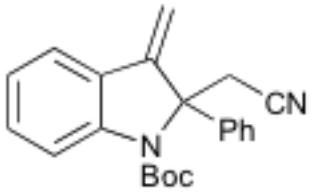

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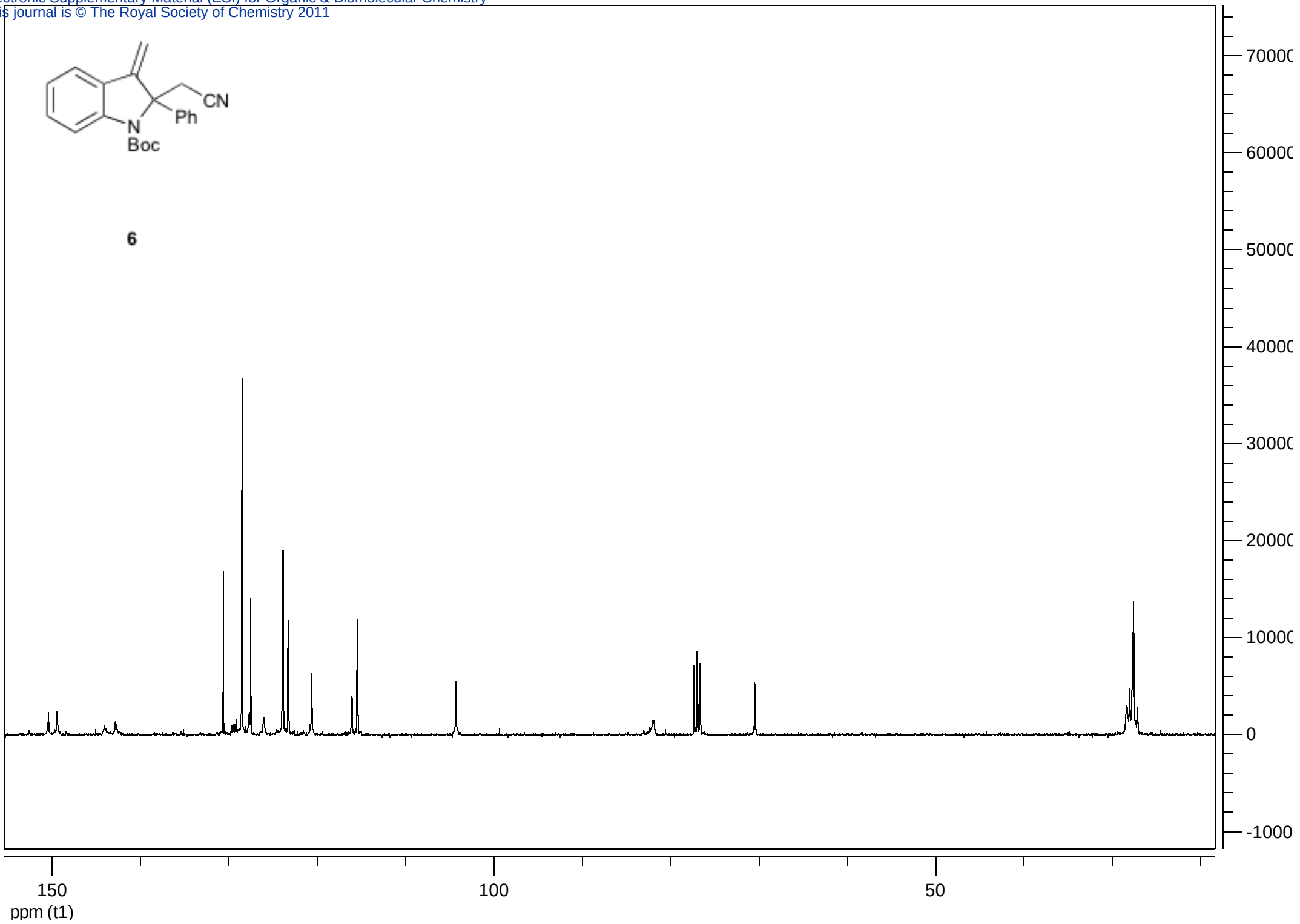

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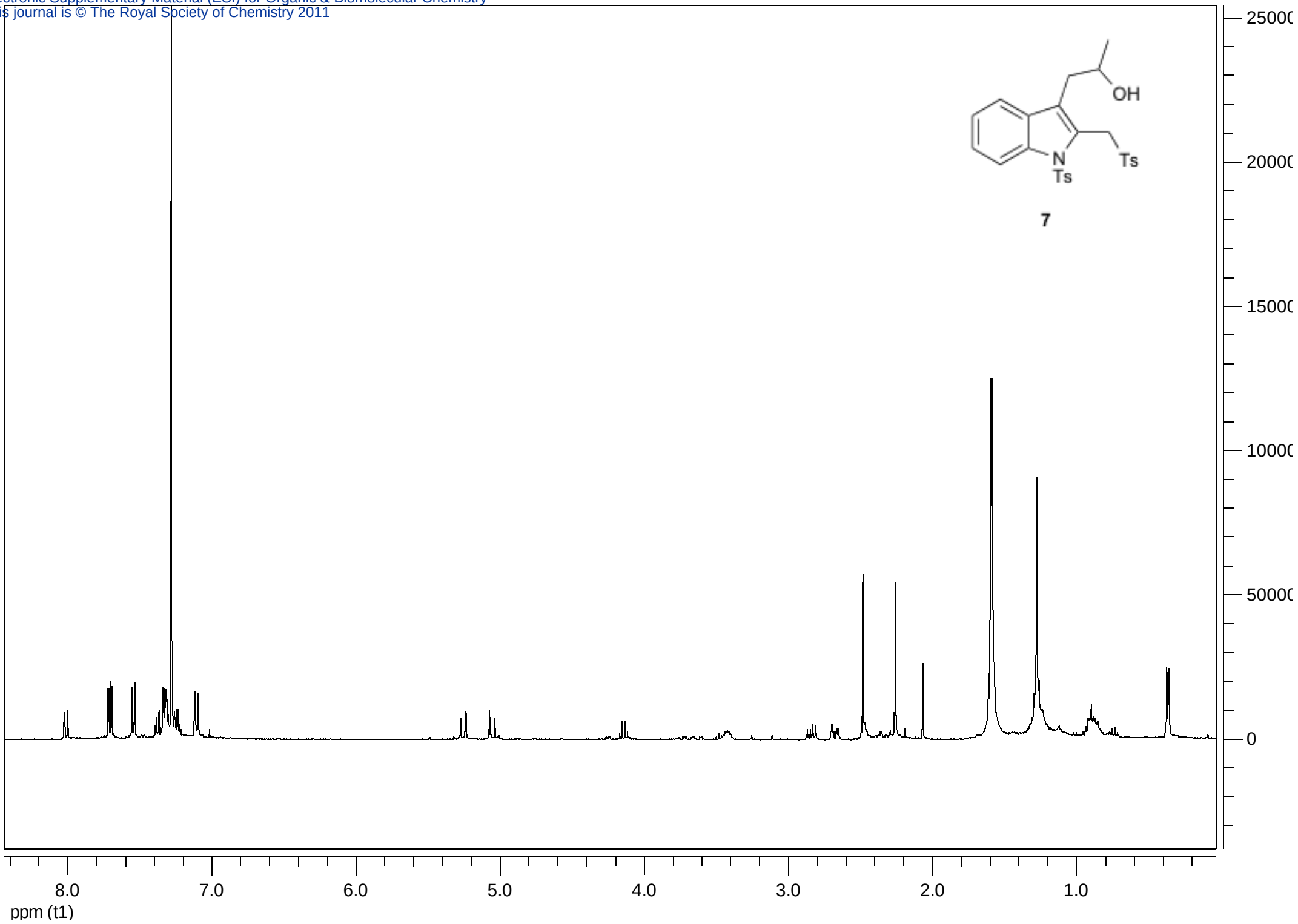

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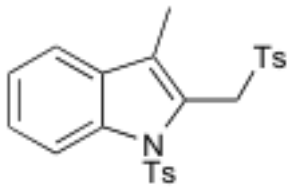

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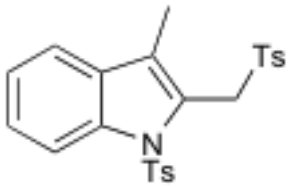

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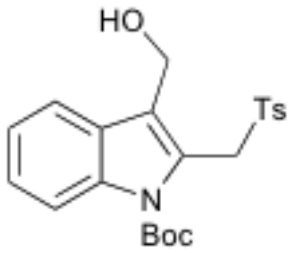

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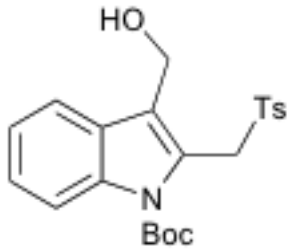

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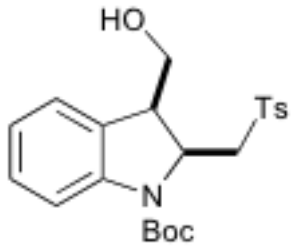

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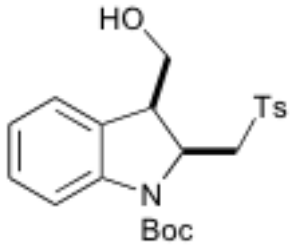

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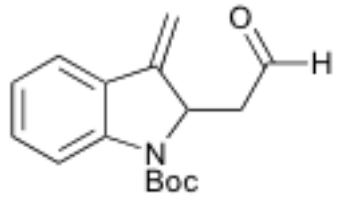

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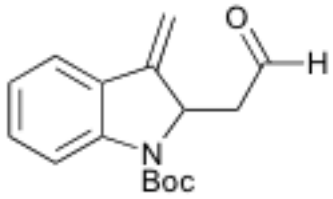

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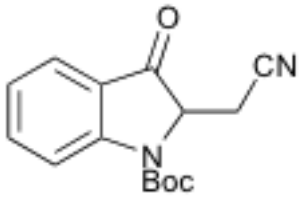

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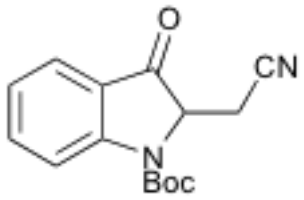

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