

SUPPLEMENTARY INFORMATION

Discovery and Biological Characterization of 1-(1*H*-indol-3-yl)-9*H*-pyrido[3,4-*b*]indole as an Aryl Hydrocarbon Receptor Activator Generated by Photoactivation of Tryptophan by Sunlight

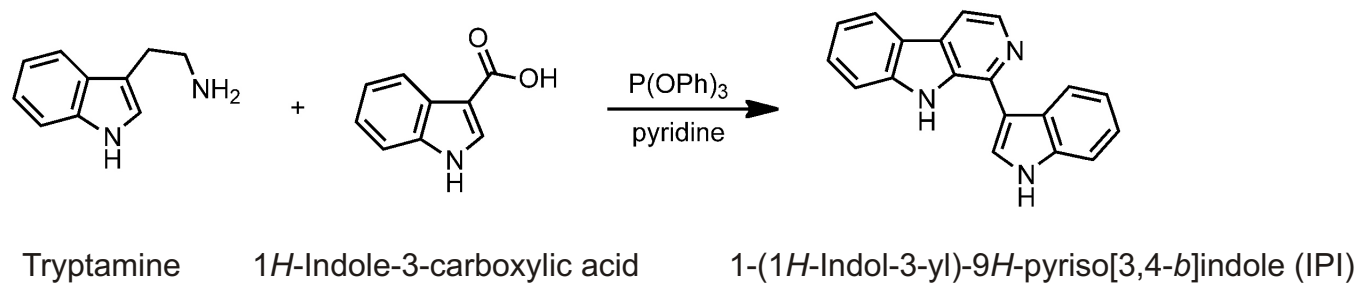
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Supplementary Figure 1. Synthesis of IPI

Supplementary Figure 2. ¹H NMR for synthesized IPI.

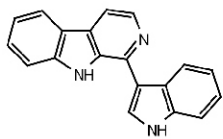
Supplementary Figure 3. ¹³C NMR for synthesized IPI.

Supplementary Figure 4. Detection of IPI in culture media

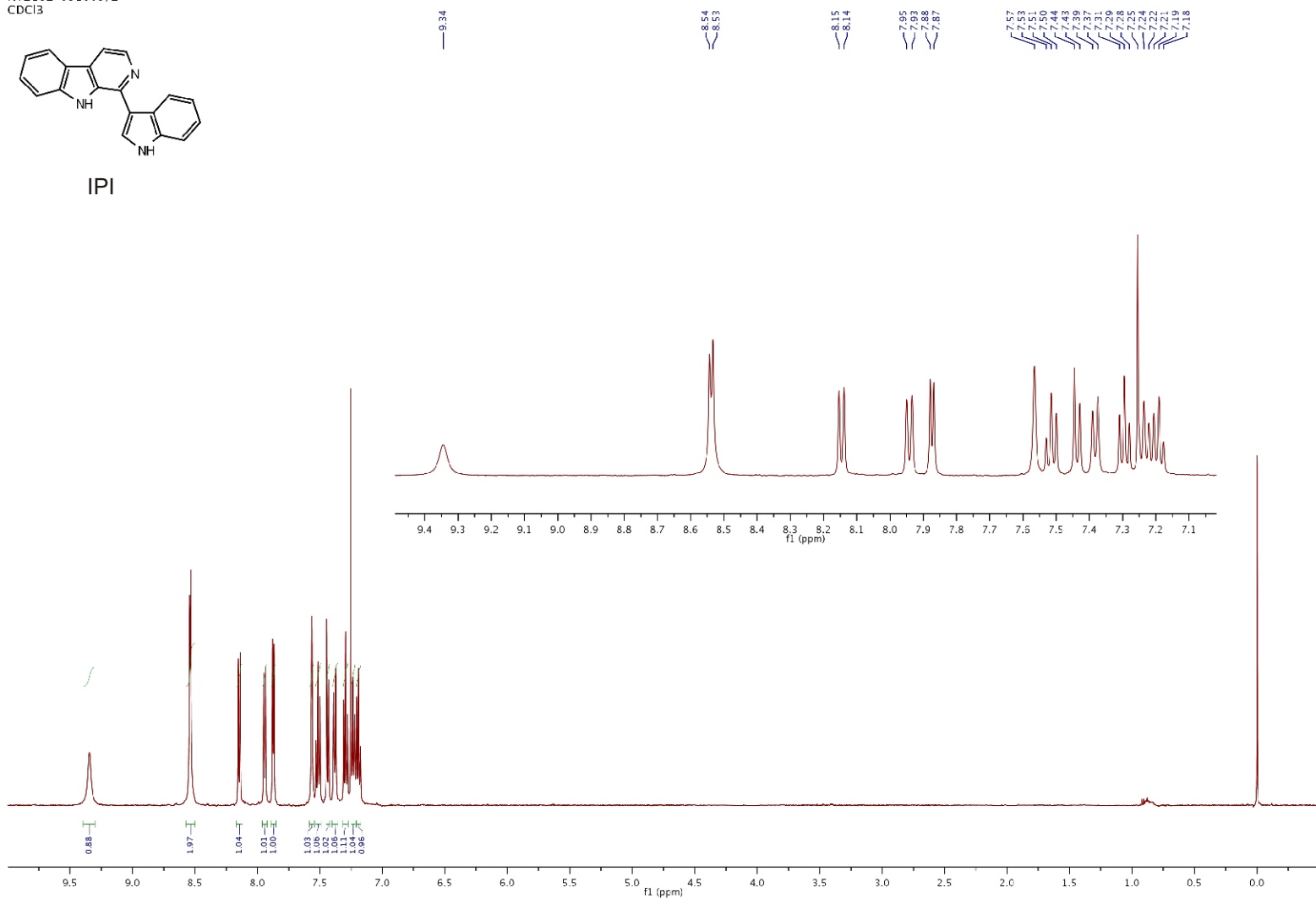


Supplementary Figure 1. The novel single step procedure used to synthesize IPI as described in *Results* (section 3.3).

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CDCl₃

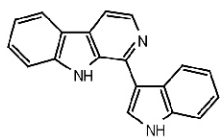


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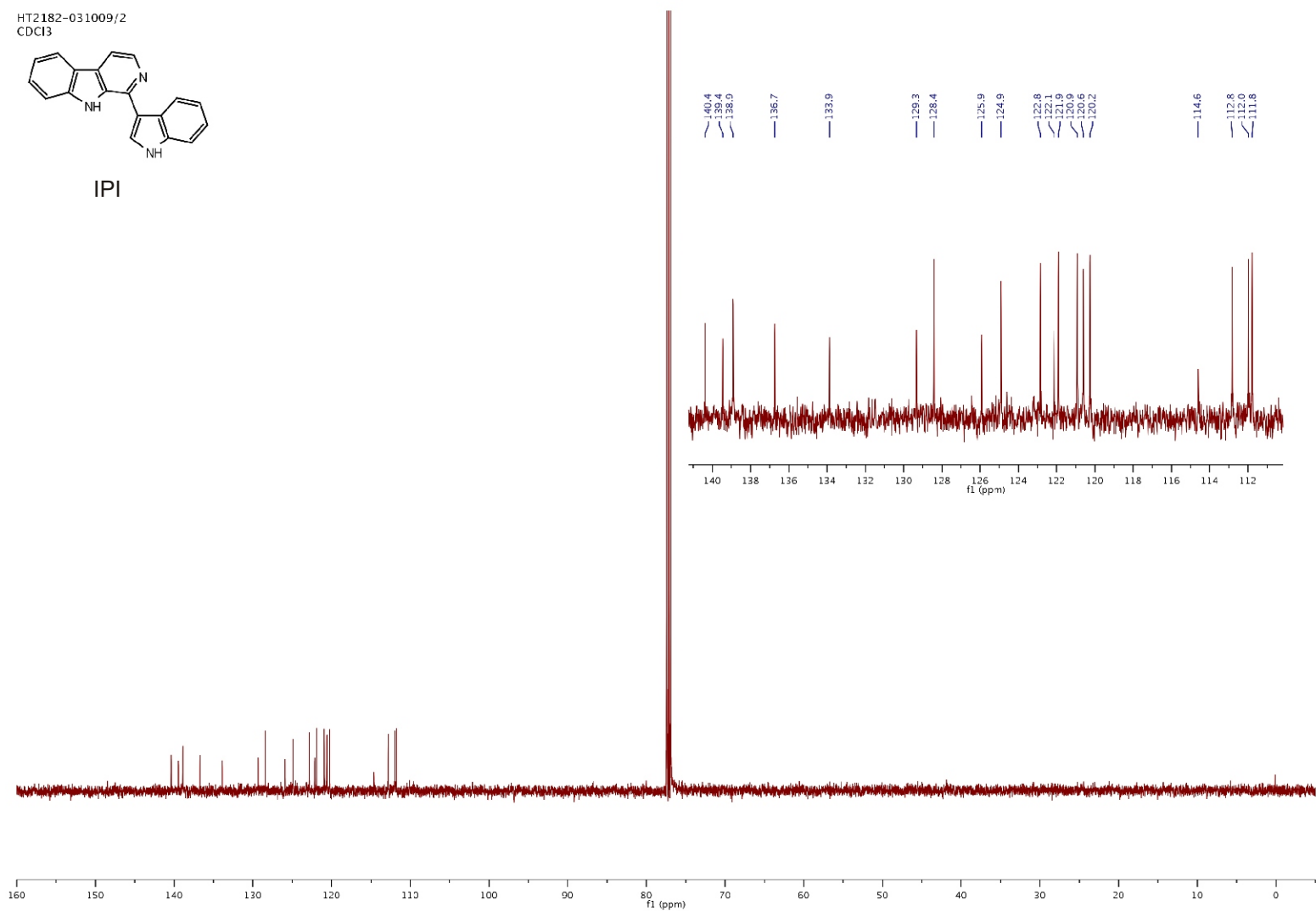


Supplementary Figure 2. ¹H NMR for synthesized IPI in CDCl₃, δ = 9.34 (brs, 1H), 8.58–8.50 (m, 1H), 8.15 (d, *J*=7.9, 1H), 7.94 (d, *J*=7.8, 1H), 7.87 (d, *J*=5.3, 1H), 7.57 (s, 1H), 7.51 (dd, *J*=7.4, 8.1, 1H), 7.44 (d, *J*=8.1, 1H), 7.38 (d, *J*=8.0, 1H), 7.29 (dd, *J*=7.4, 7.8, 1H), 7.24 (dd, *J*=7.5, 7.9, 1H), 7.19 (dd, *J*=7.5, 8.0, 1H).

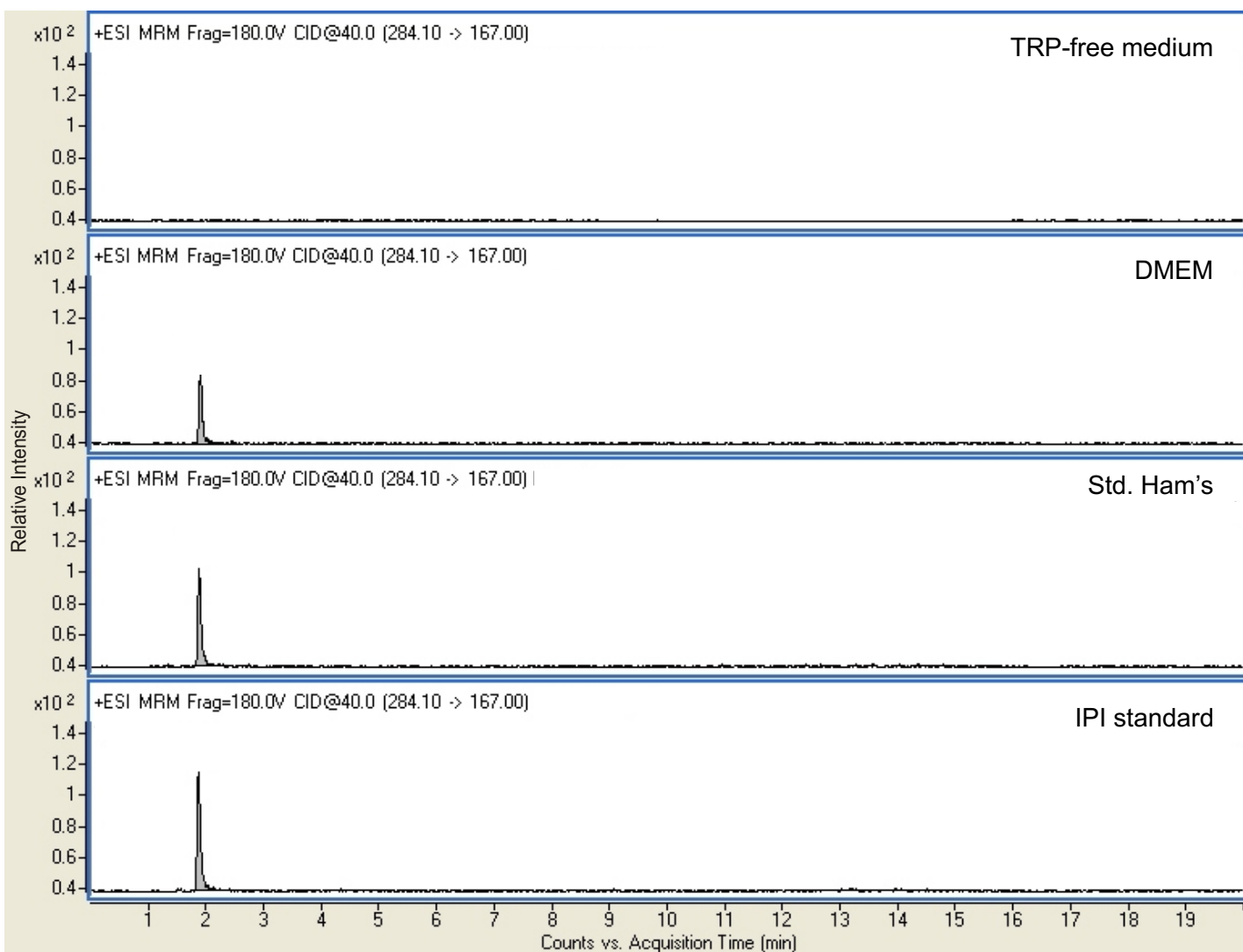
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Supplementary Figure 3. ¹³C NMR for synthesized IPI in CDCl₃, δ 140.4, 139.4, 138.9, 136.7, 133.9, 129.3, 128.4, 125.9, 124.9, 122.8, 122.1, 121.9, 120.9, 120.6, 120.2, 114.6, 112.8, 112.0, 111.8.



Supplementary Figure 4. Representative MRM traces for detection of IPI (transition m/z 284 → 167), in TRP-free medium, DMEM, Std. Ham's and IPI reference (0.41 nM in TRP-free medium), 20 μ l of medium injected for each, showing that IPI is present in culture media with routine handling under ambient light.