

Supporting Information

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Bioassay-Guided Isolation of Topoisomerase I Poison from *Paphiopedilum callosum* (Rchb.f.) Stein

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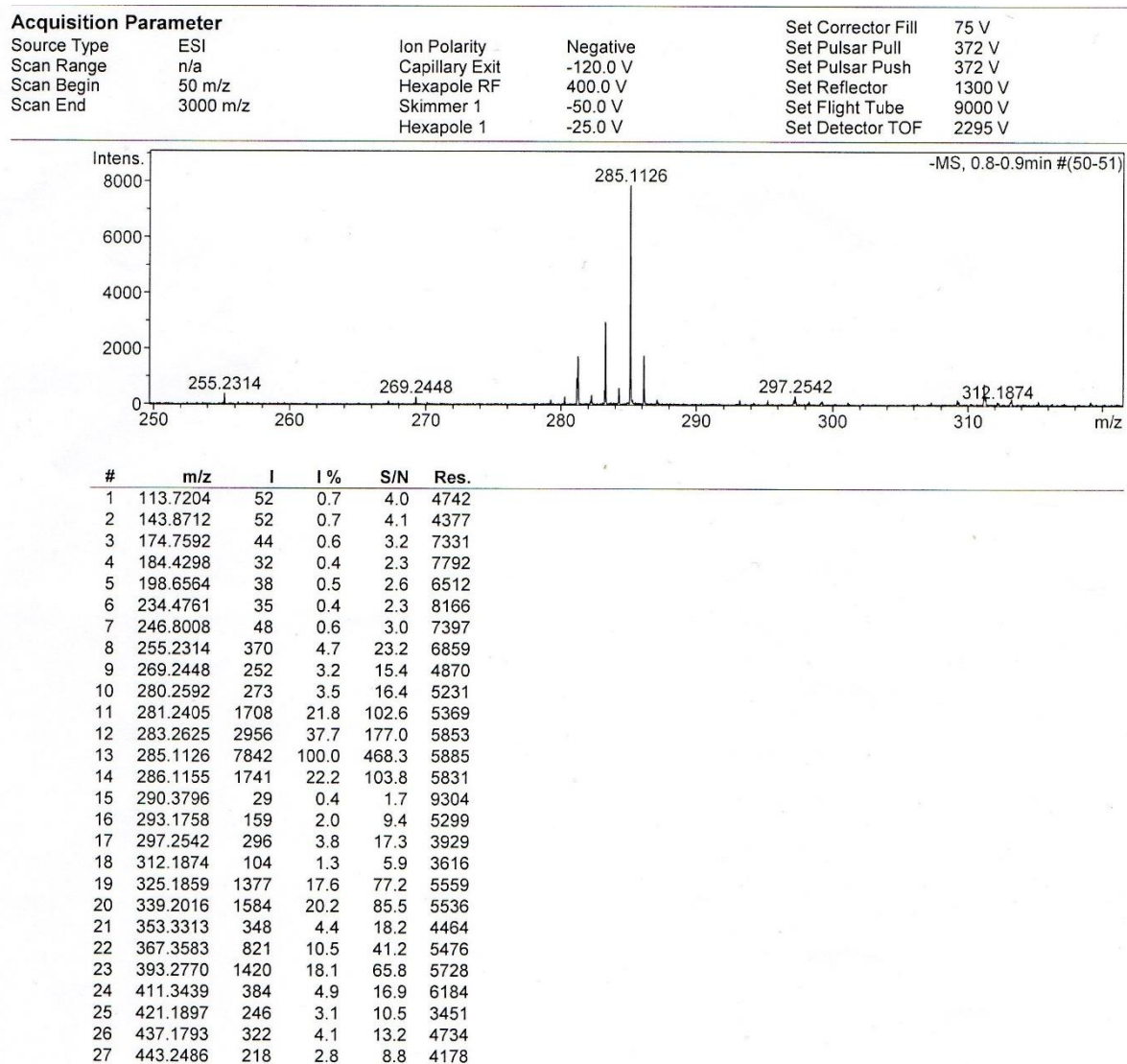


Figure S1: ESI-MS spectrum of compound **1**

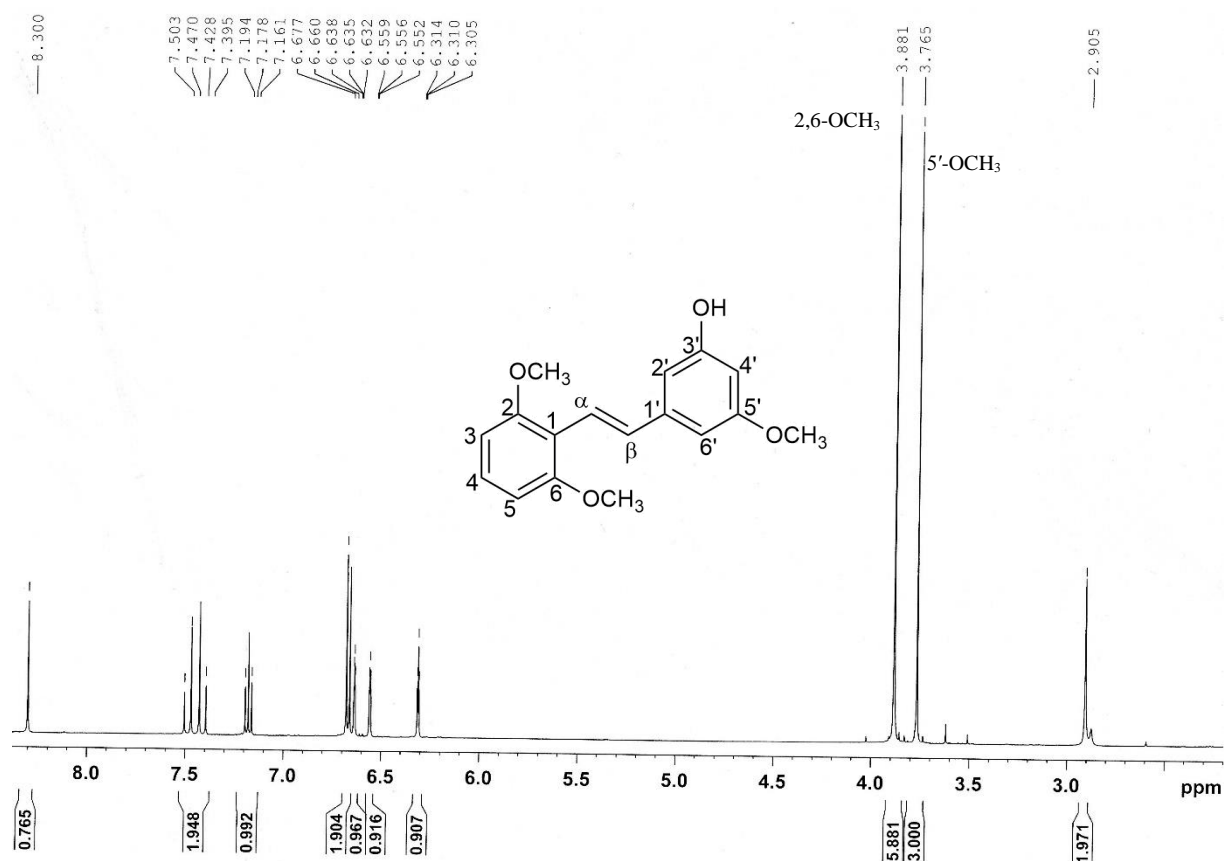


Figure S2: ¹H-NMR (500 MHz, Acetone-*d*₆) spectrum of compound **1**

3'-hydroxy-2,6,5'-trimethoxystilbene: yellowish brown semisolid. ¹H-NMR (Acetone-*d*₆, 500 MHz), δ : 3.77 (1H, s, OCH₃-5'), 3.88 (2H, s, OCH₃-2 /6), 6.31 (1H, t, H-4'), 6.56 (1H, t, H-6'), 6.64 (1H, t, H-2'), 6.67 (2H, d, H-3/5), 7.18 (1H, t, H-4), 7.41 (1H, d, H- α), 7.49 (1H, d, H- β), 8.30 (1H, s, OH-3'). ¹³C-NMR (Acetone-*d*₆, 125 MHz), δ : 55.4 (OCH₃-5'), 56.1 (OCH₃-2 /6), 101.2 (C-4'), 104.5 (C-6'), 104.9 (C-3/5), 106.2 (C-2'), 115.1 (C-1), 120.8 (C- α), 129.3 (C-4), 132.9 (C- β), 142.4 (C-1'), 159.5 (C-3'), 159.6 (C-2/6), 162.1 (C-5'). ESIMS: m/z = 285.1126 [M]⁻ for formula C₁₇H₁₈O₄.

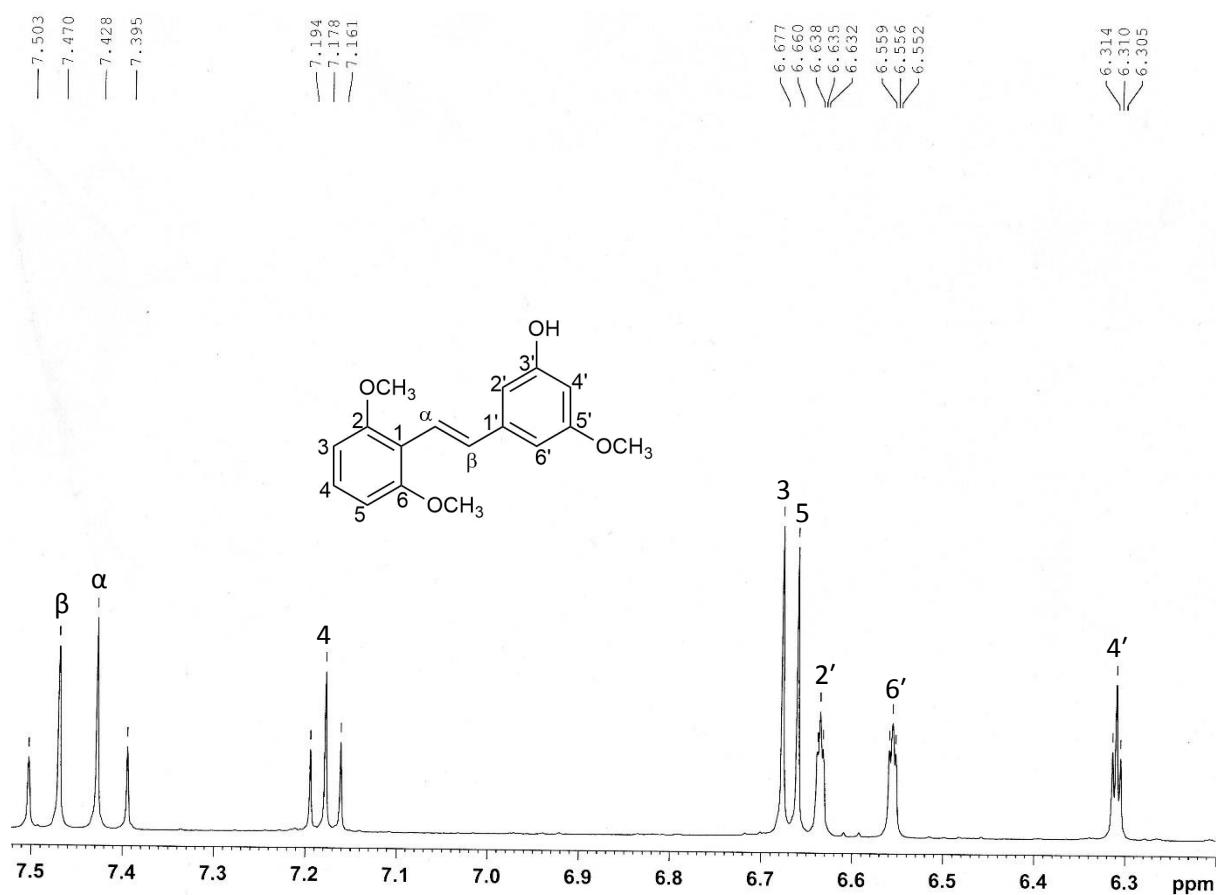


Figure S3: ^1H -NMR (500 MHz, Acetone- d_6) spectrum of compound **1** (from 6.3-7.5)

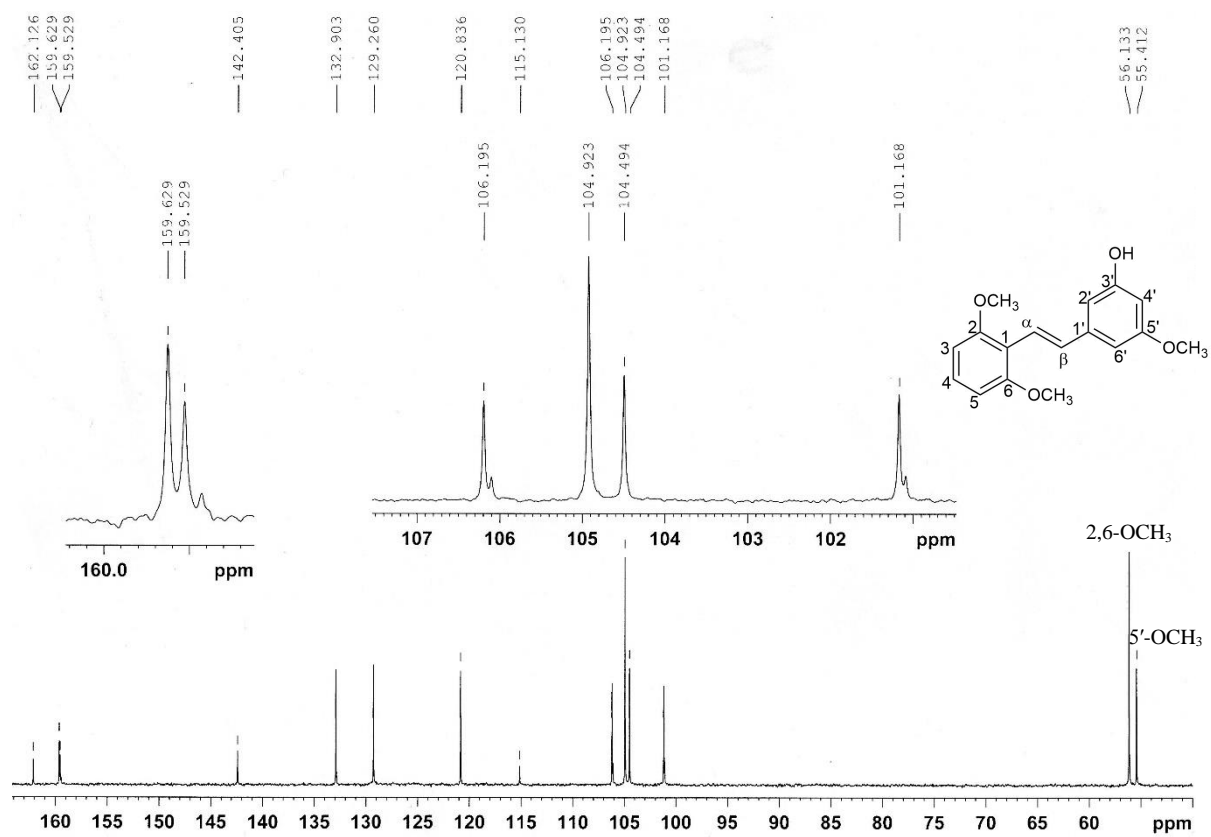


Figure S4: ^{13}C -NMR (125 MHz, Acetone- d_6) spectrum of compound **1**

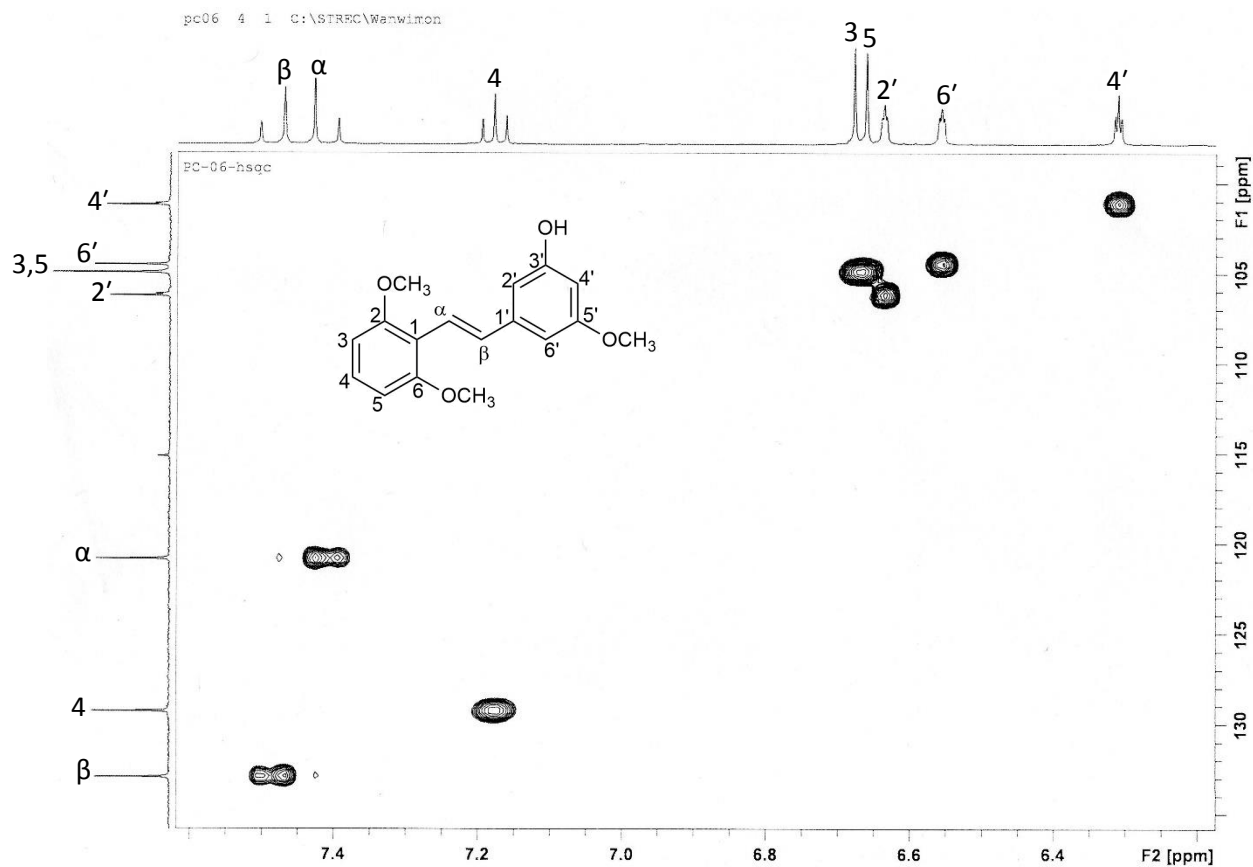


Figure S5: HSQC (500 MHz) spectrum of compound **1**

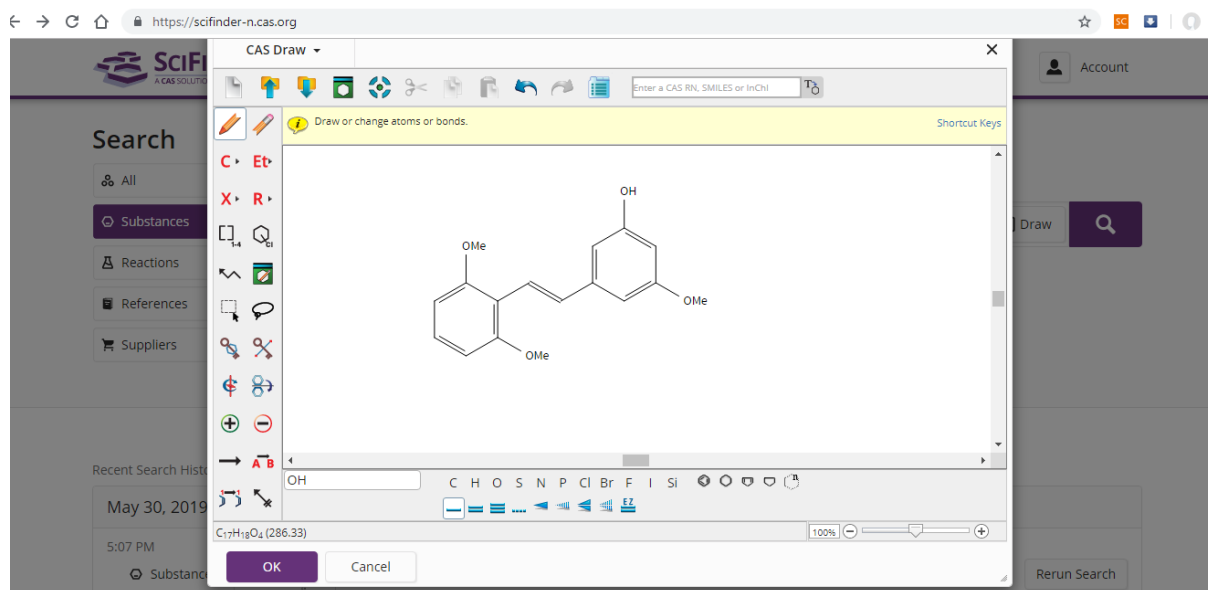


Figure S6: New compound search report of SciFinder

The top screenshot shows a successful search result for a substance. The header includes the SciFinder logo and a search bar with the text "Substances" and "Enter a query...". Below the header, there are tabs for "Structure Match", "As Drawn (0)", and "Substructure (4)". The main content area displays the title "Substances (4)" and a list of results with identifiers: 1445898-18-9, 1445896-86-5, and 1445897-49-3. The bottom screenshot shows a search result with no matches. The header is identical, but the main content area displays "Substances (0)" and a message: "We couldn't find any results. Please update your search query and try again."