

Supplementary Materials

Structure-Based Virtual Screening and *De Novo* Design of PIM1 Inhibitors with Anticancer Activity from Natural Products

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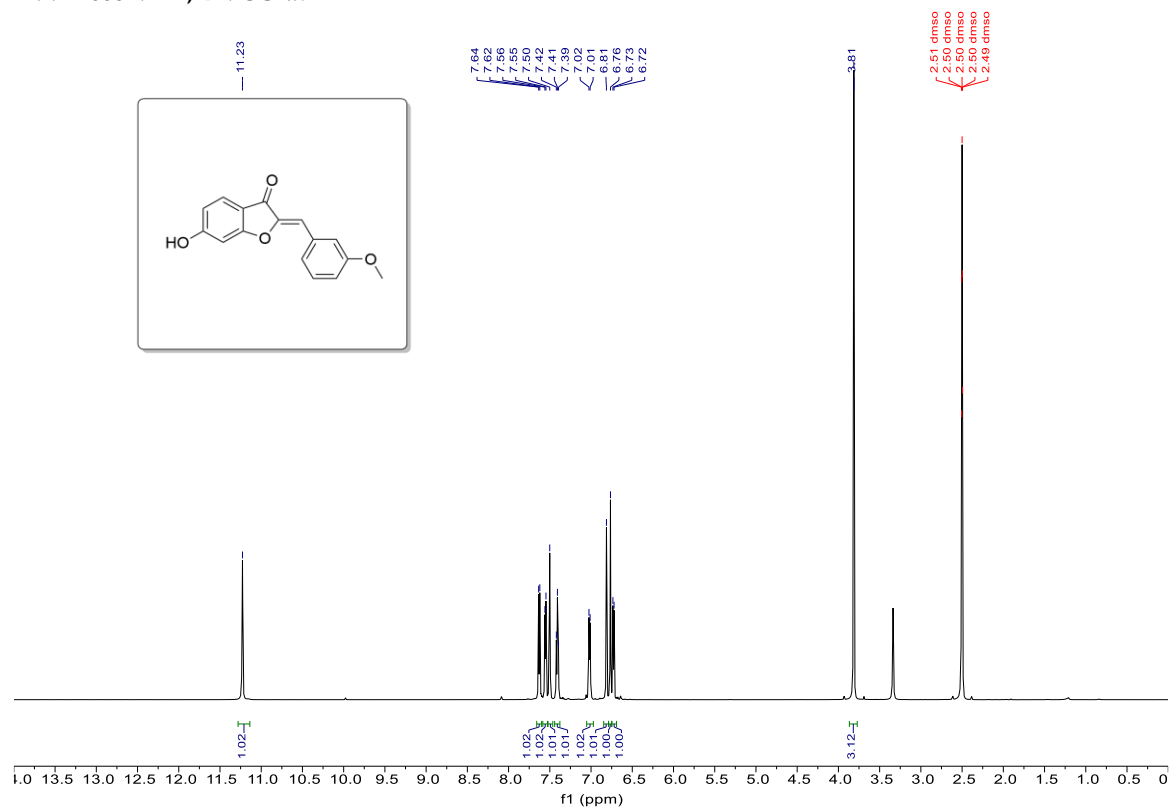
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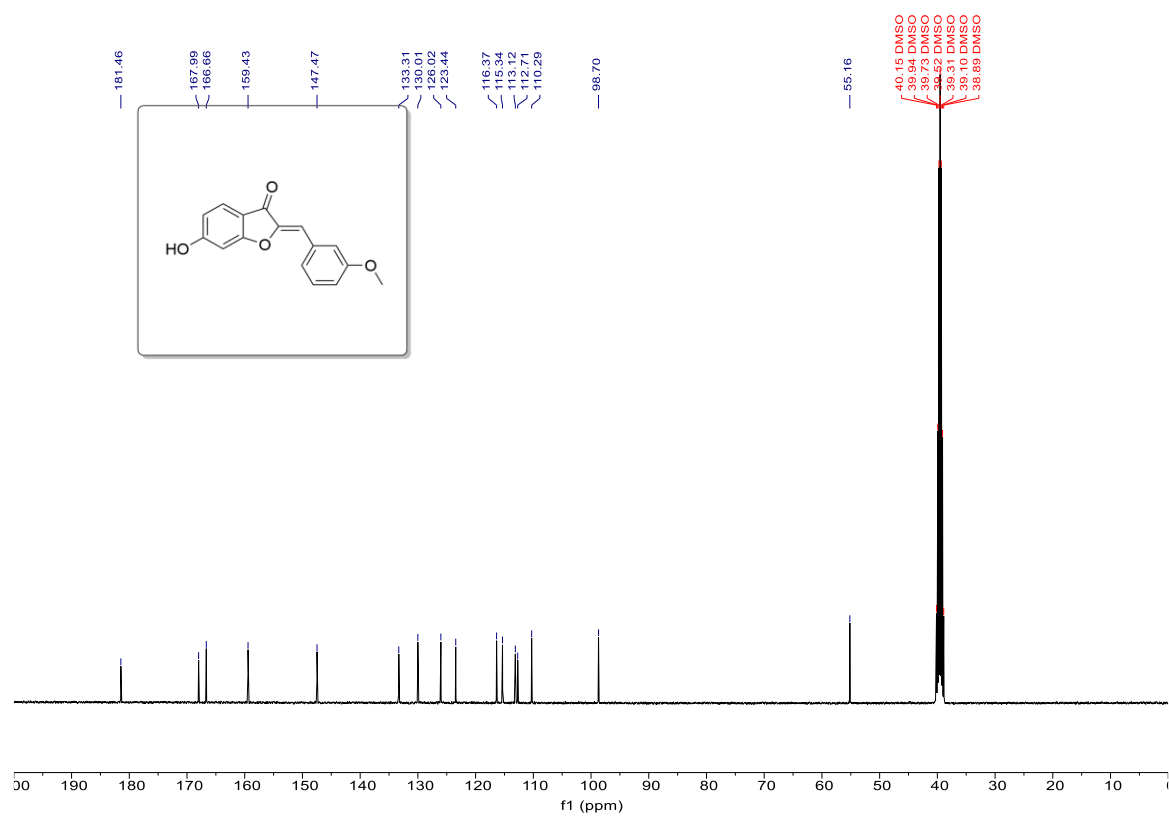
Figure S1. Spectral copies of ¹H- and ¹³C- NMR data for compounds **5**, **10**, **13**, **15**, and **16**.

(Z)-6-Hydroxy-2-(3-methoxybenzylidene)benzofuran-3(2H)-one (5)

¹H NMR 600 MHz, DMSO-*d*₆

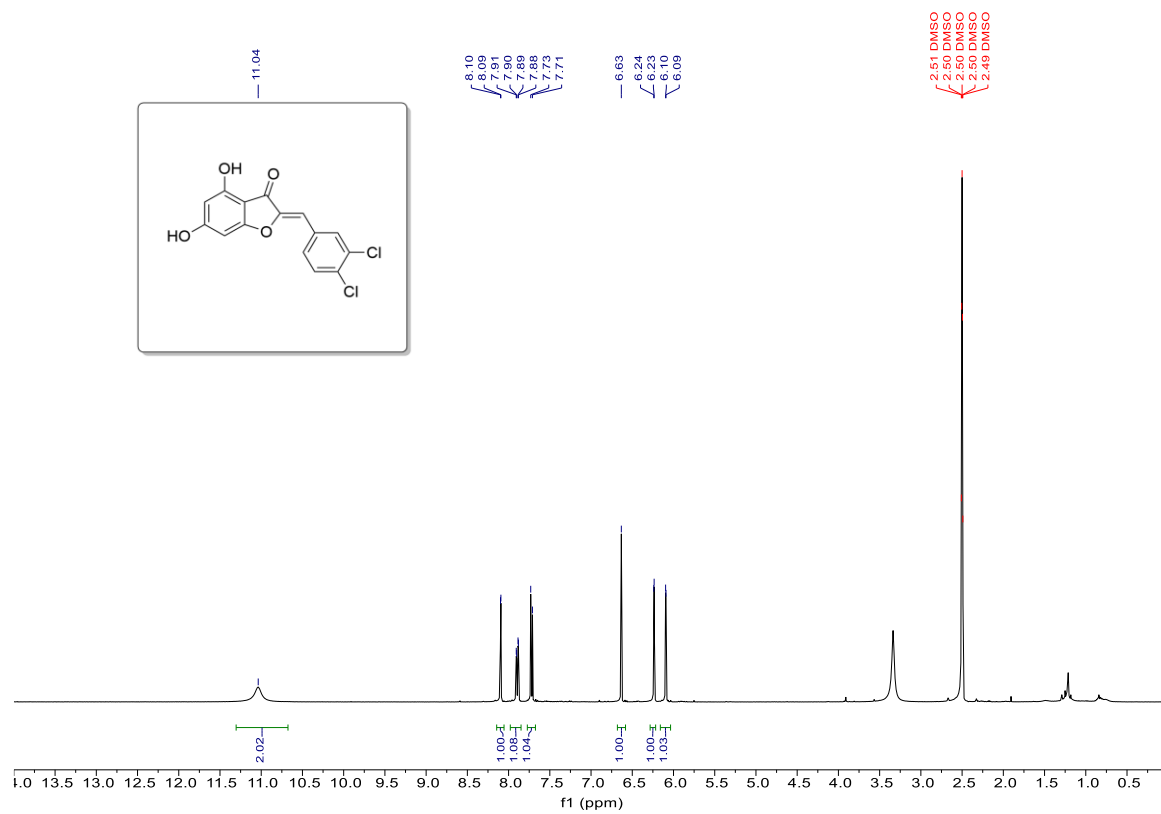


¹³C NMR 100 MHz, DMSO-*d*₆

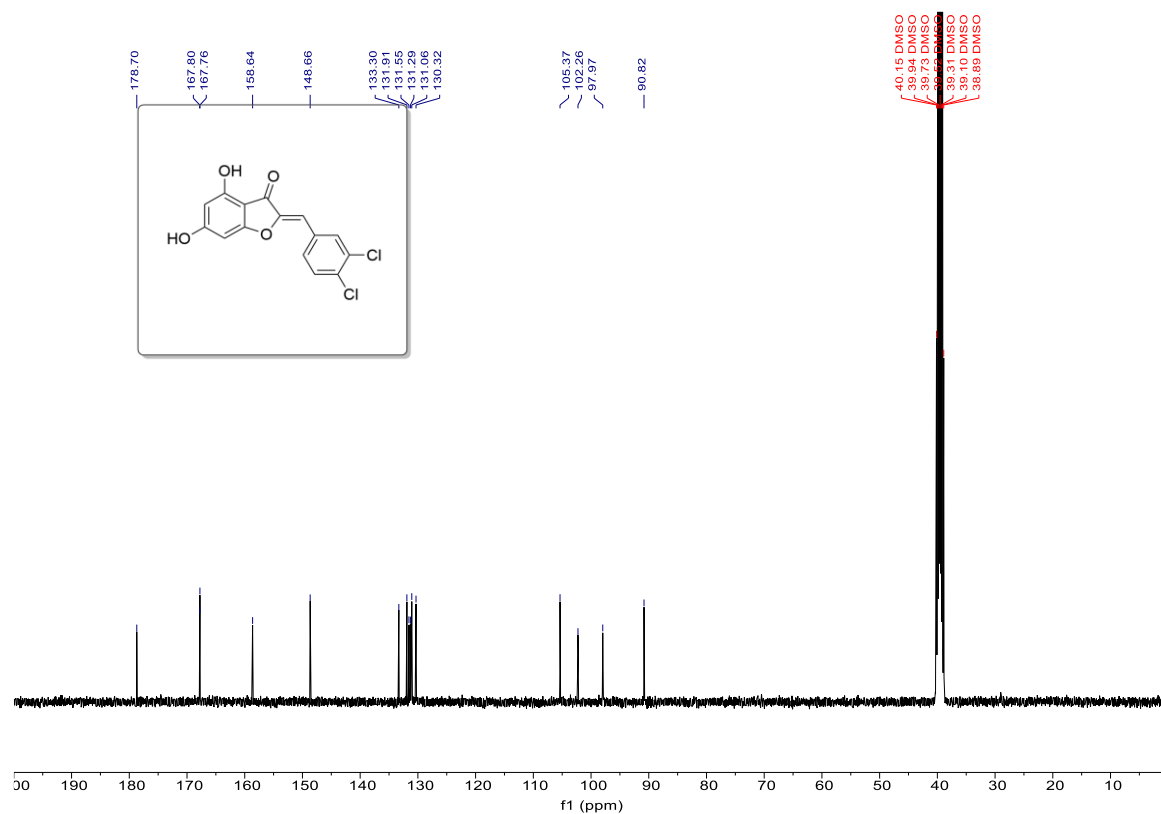


(Z)-2-(3,4-Dichlorobenzylidene)-4,6-dihydroxybenzofuran-3(2H)-one (10)

¹H NMR 400 MHz, DMSO-*d*₆

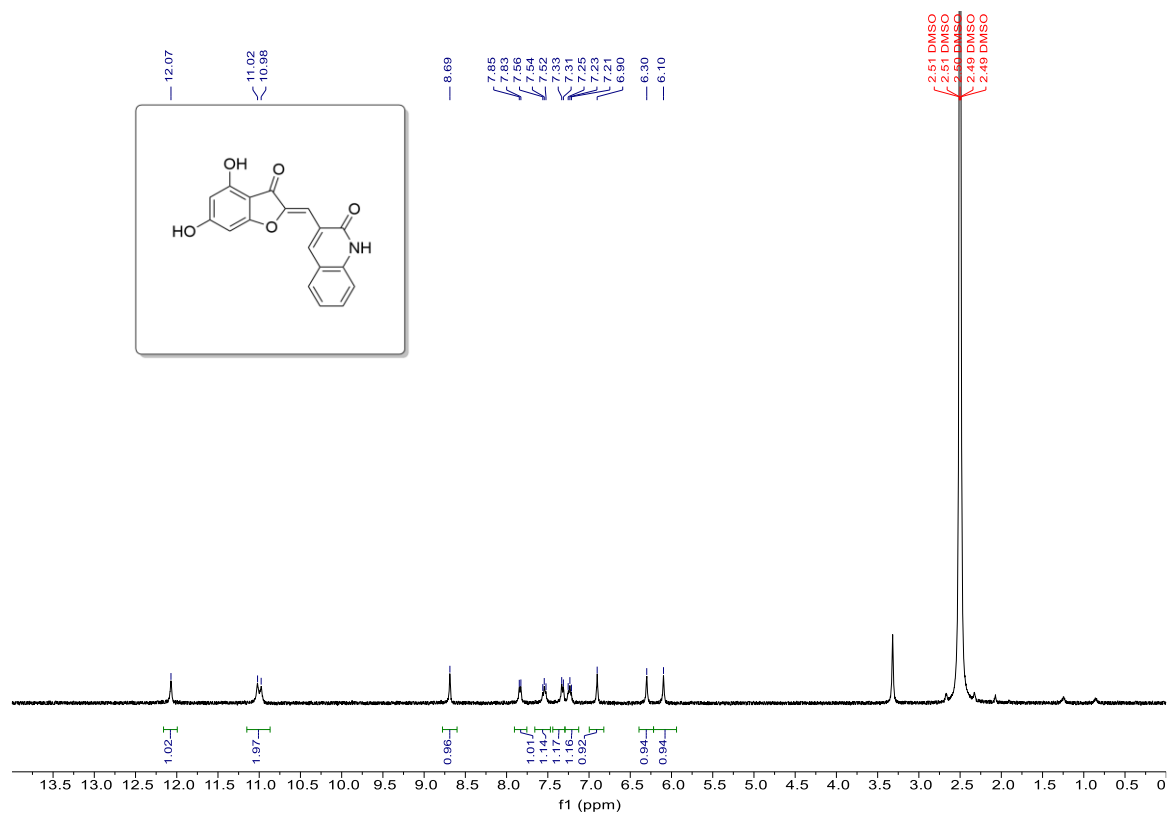


¹³C NMR 100 MHz, DMSO-*d*₆

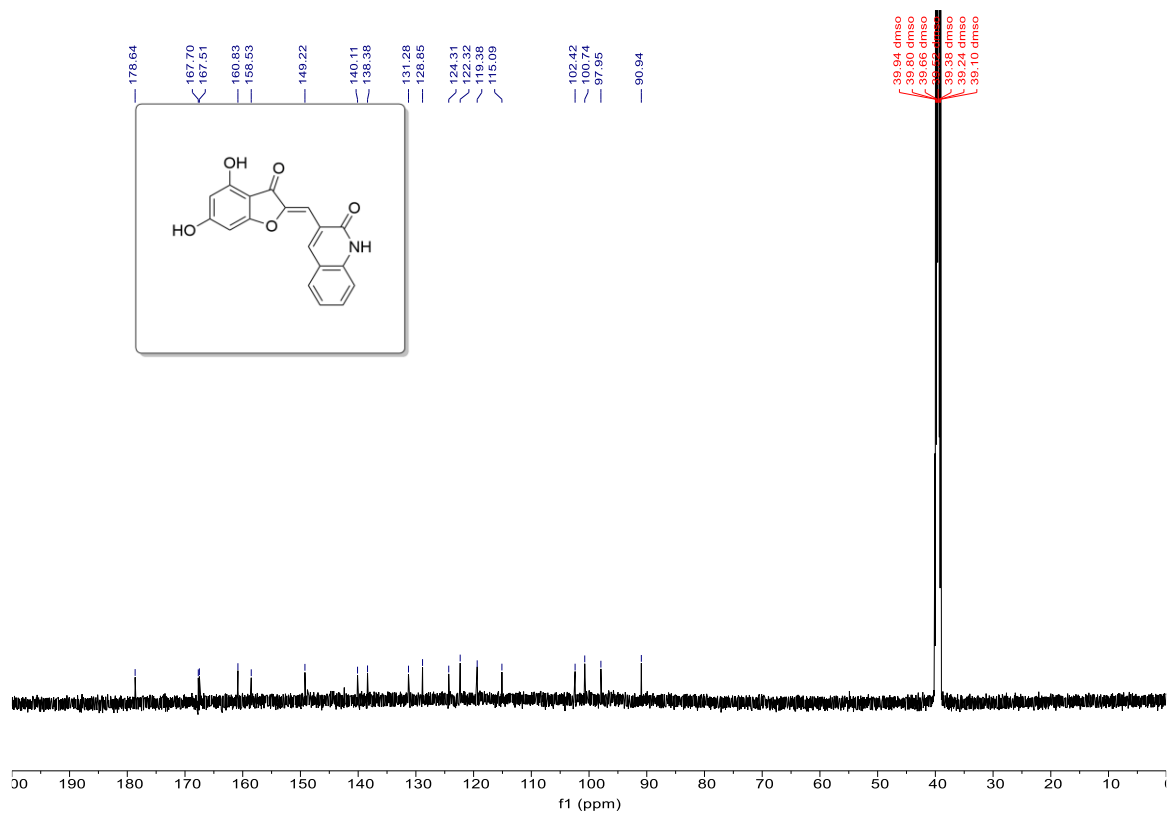


(Z)-3-((4,6-Dihydroxy-3-oxobenzofuran-2(3H)-ylidene)methyl)quinolin-2(1H)-one (13)

¹H NMR 400 MHz, DMSO-*d*₆

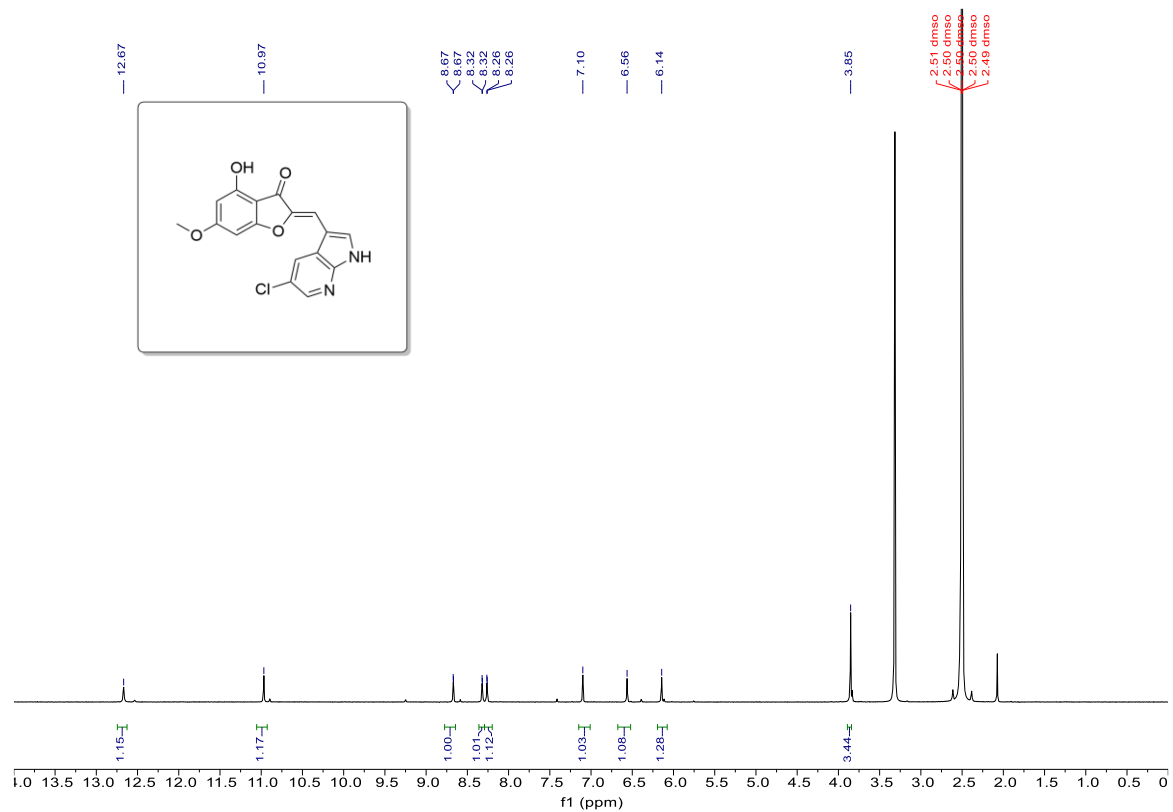


¹³C NMR 150 MHz, DMSO-*d*₆

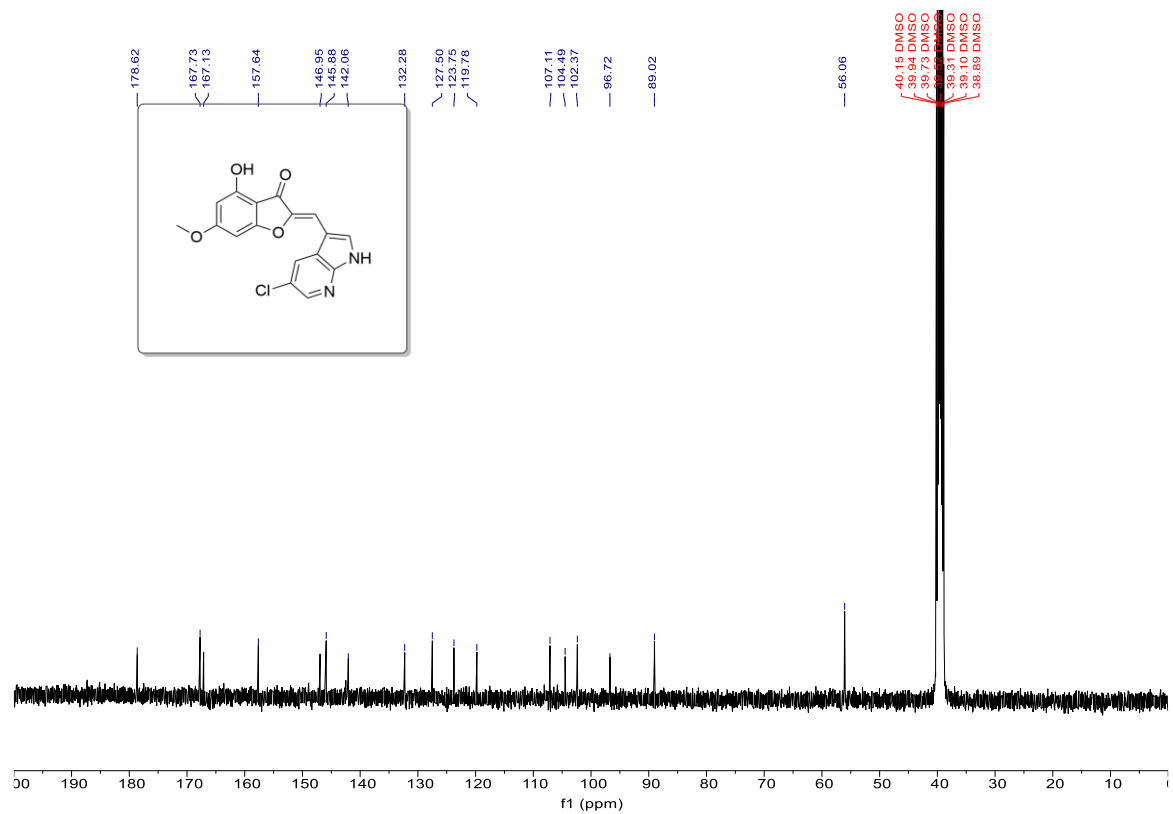


(Z)-2-((5-Chloro-1H-pyrrolo[2,3-b]pyridin-3-yl)methylene)-4-hydroxy-6-methoxybenzofuran-3(2H)-one (15)

^1H NMR 600 MHz, $\text{DMSO-}d_6$



^{13}C NMR 100 MHz, $\text{DMSO-}d_6$



(Z)-2-((2-Chloro-7H-pyrrolo[2,3-d]pyrimidin-5-yl)methylene)-4,6-dihydroxybenzofuran-3(2H)-one (16)

¹H NMR 600 MHz, DMSO-*d*₆

