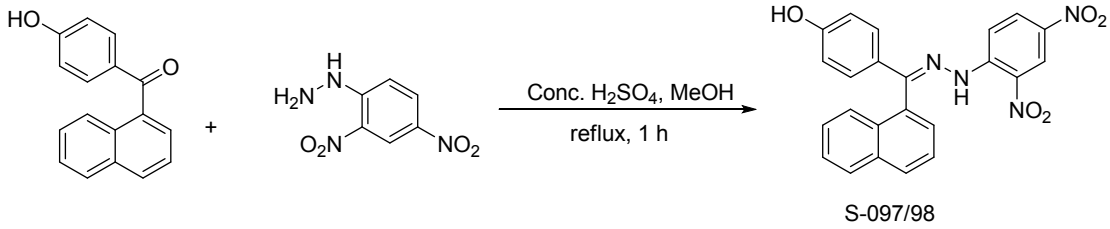
**Supplementary Information**

# Identification of a Novel Human DNA Ligase I Inhibitor that Promotes Cellular Apoptosis in DLD-1 cells: An *in silico* and *in vitro* Mechanistic Study




S-097/98

**Scheme 1:** Synthesis of S-097/98

## 1. Experimental procedure

In a round bottom flask, 1-napthyl-(4-hydroxyphenyl)ketone (2 mmole) was dissolved in methanol (10 ml). To the above solution, catalytic amount of conc. $H_2SO_4$ and an equimolar solution of 2,4-dinitrophenylhydrazine in methanol (10 ml) was added. The mixture was refluxed on a water bath for 1h, when a crystalline solid separated. The solution was cooled, the product was filtered and washed with methanol. It was recrystallized from excess of methanol as a brick red solid, yield 85%, mp 290-291$^0$C. Anal (%) Calcd. for $C_{23}H_{16}N_4O_5$; C, 64.48; H, 3.76; N, 13.08; found ;64.42; H, 3.74; N, 13.02; IR(KBR, $cm^{-1}$ ): 3389, 3019, 1646, 1385, 1216, 1069, 770, 669; $^1$H NMR (300 MHZ, DMSO-$d_6$), δ 10.72 (s, 1H), 10.06 (s, 1H), 8.71 (1H, s), 8.40-8.14 (4H, m), 7.78-7.49 (m, 7H), 6.82 (s, 2H); ESI-MS: (m/z); 428, found $[M+H]^+$ 429. [1]

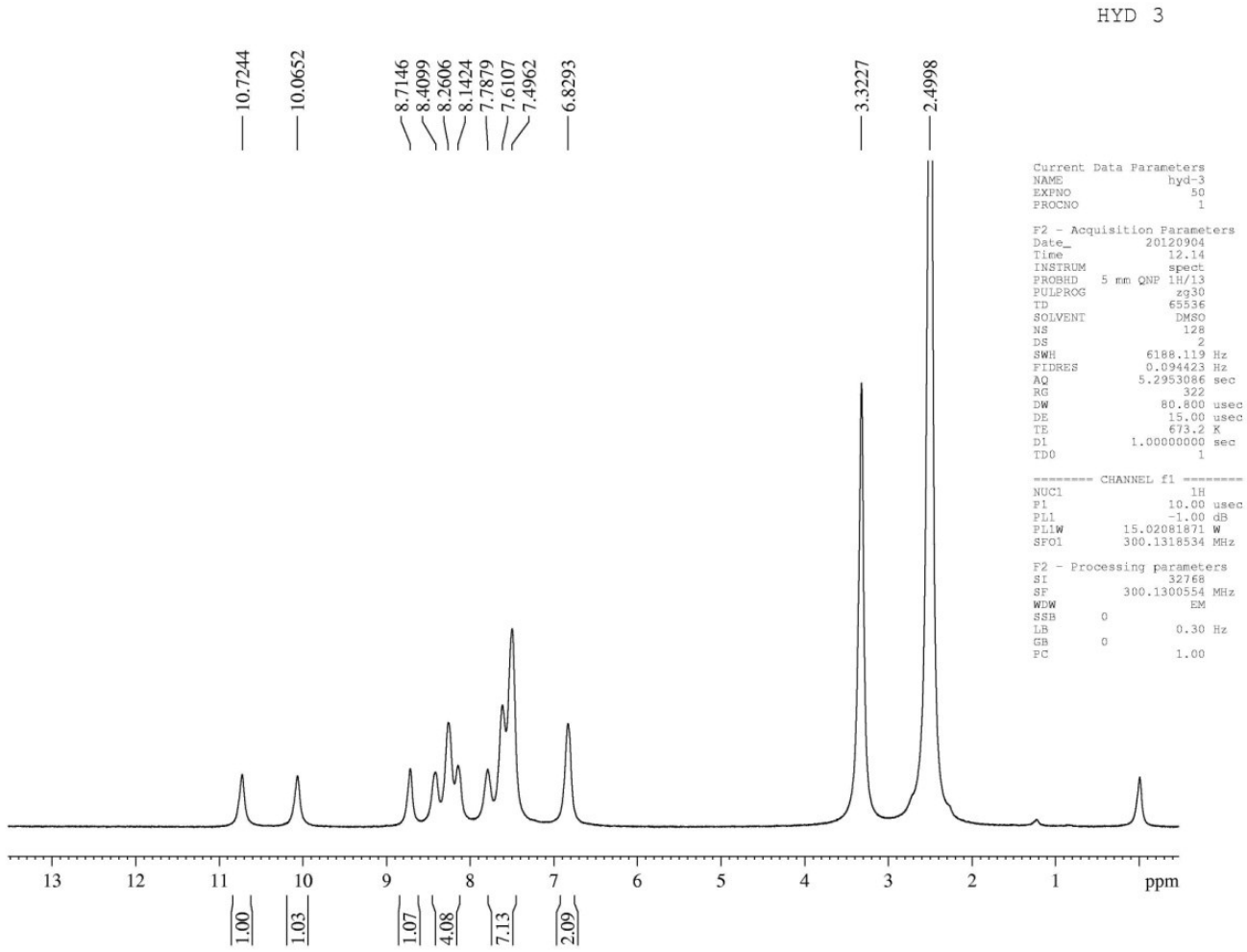



**Figure 1:** $^{1}$H NMR spectrum of compound S-097/98

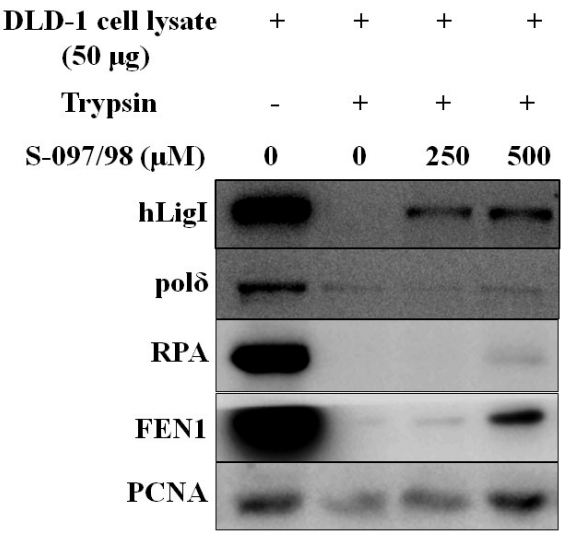



**Figure 2:** Western blot image of trypsin cleavage protection of different replication proteins in the presence of different concentrations of S-097/98. The image clearly shows that the compound provides maximum trypsin cleavage protection to hLigI as compared to other proteins like Polδ, RPA, FEN1 and PCNA. This indicates that hLigI is a major target for S-097/98.

**Reference**

1. J. Pandey, R. Pal, A. Diwedi, K. Hajela (2002) Synthesis of some new diaryl and triaryl hydrazone derivatives as possible estrogen receptor modulators. *Arzneim.-Forsh./Drug Res* 52: 39-44.