

## Supplementary Data:

# New Insights into the Structural Requirements of Isatin-derived Pro-apoptotic Agents against Acute Myeloid Leukemia

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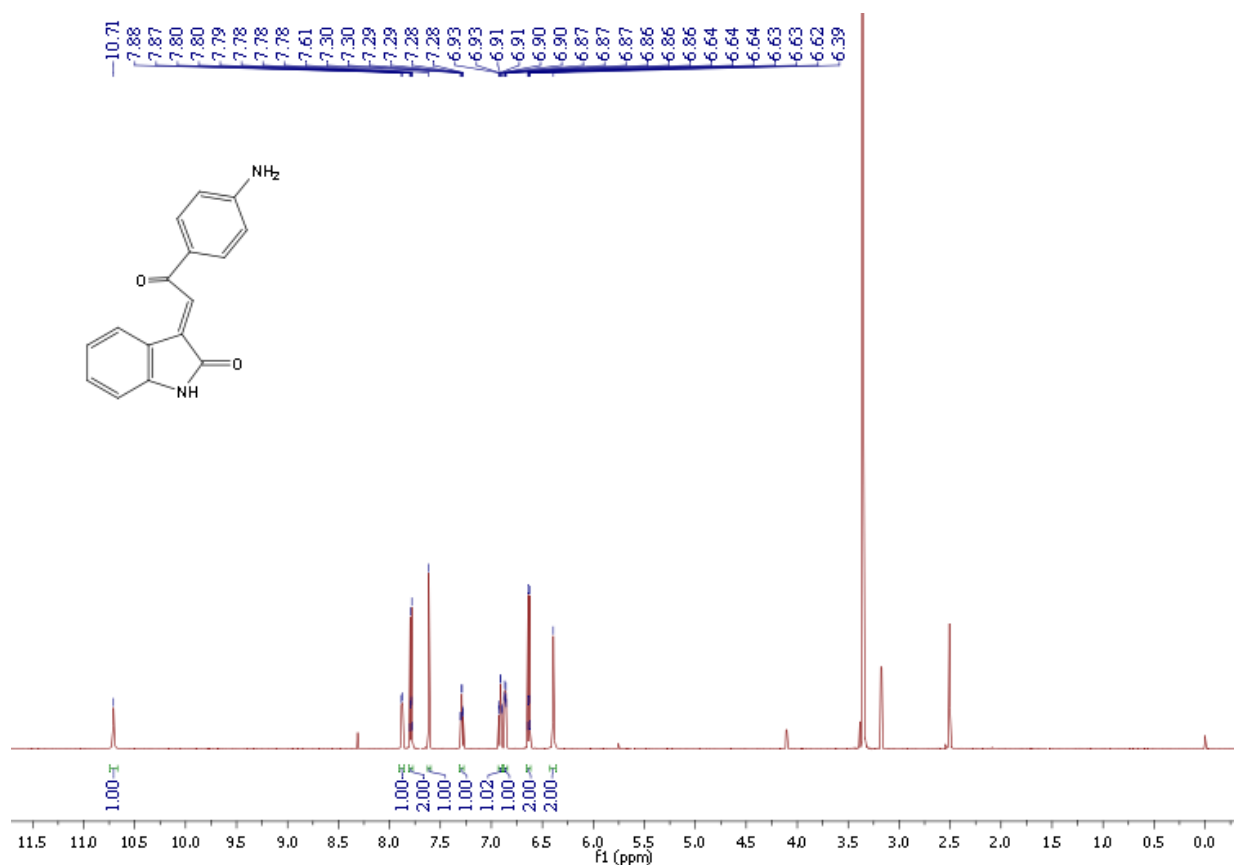


Figure S1: <sup>1</sup>H-NMR spectrum of compound 3 (600 MHz, DMSO/*d*<sub>6</sub>)

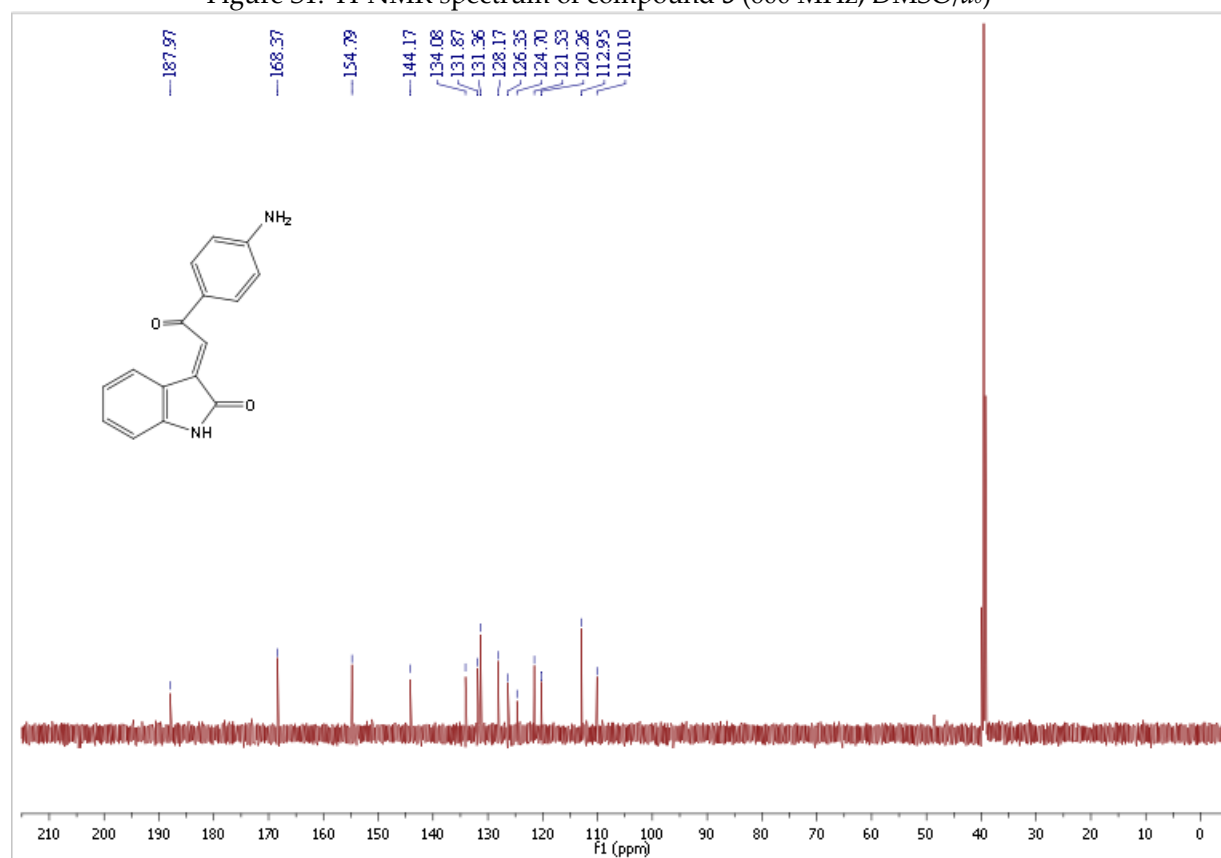


Figure S2: <sup>13</sup>C-NMR spectrum of compound 3 (150 MHz, DMSO/*d*<sub>6</sub>)

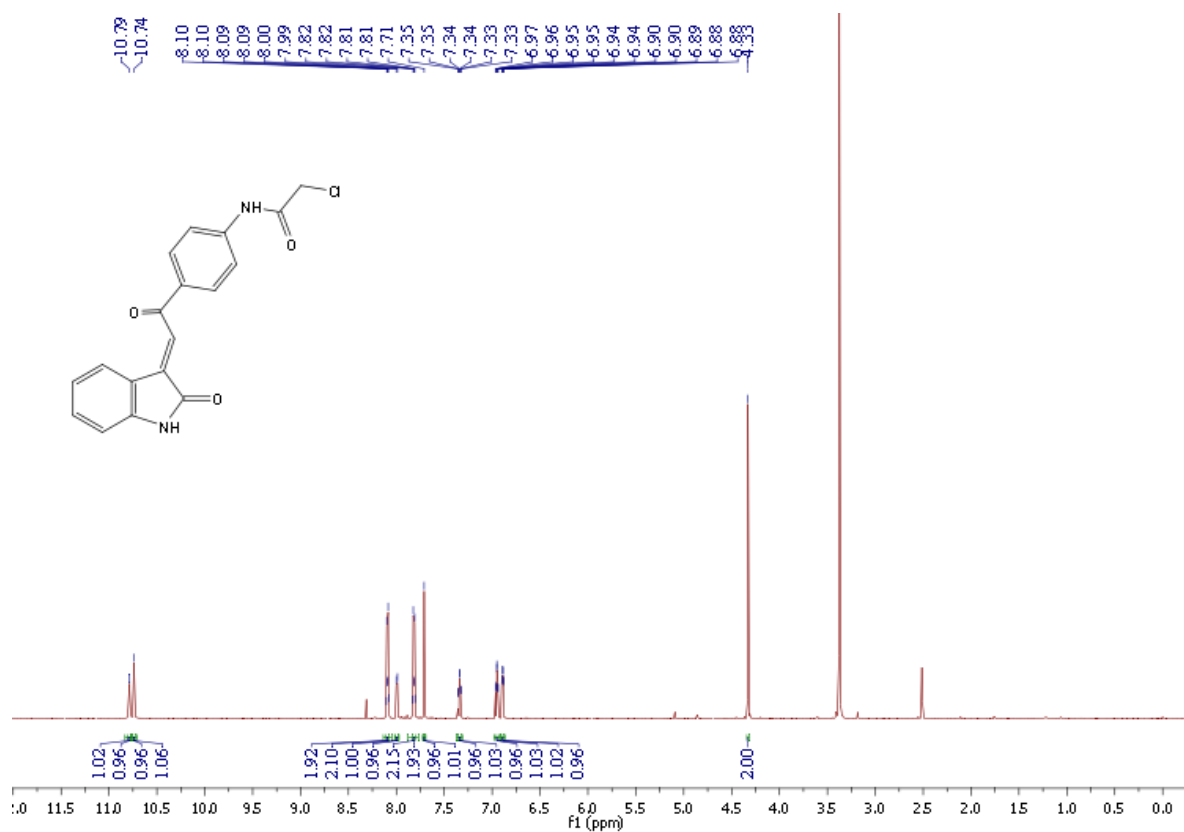


Figure S3: <sup>1</sup>H-NMR spectrum of compound 4 (600 MHz, DMSO/*d*<sub>6</sub>)

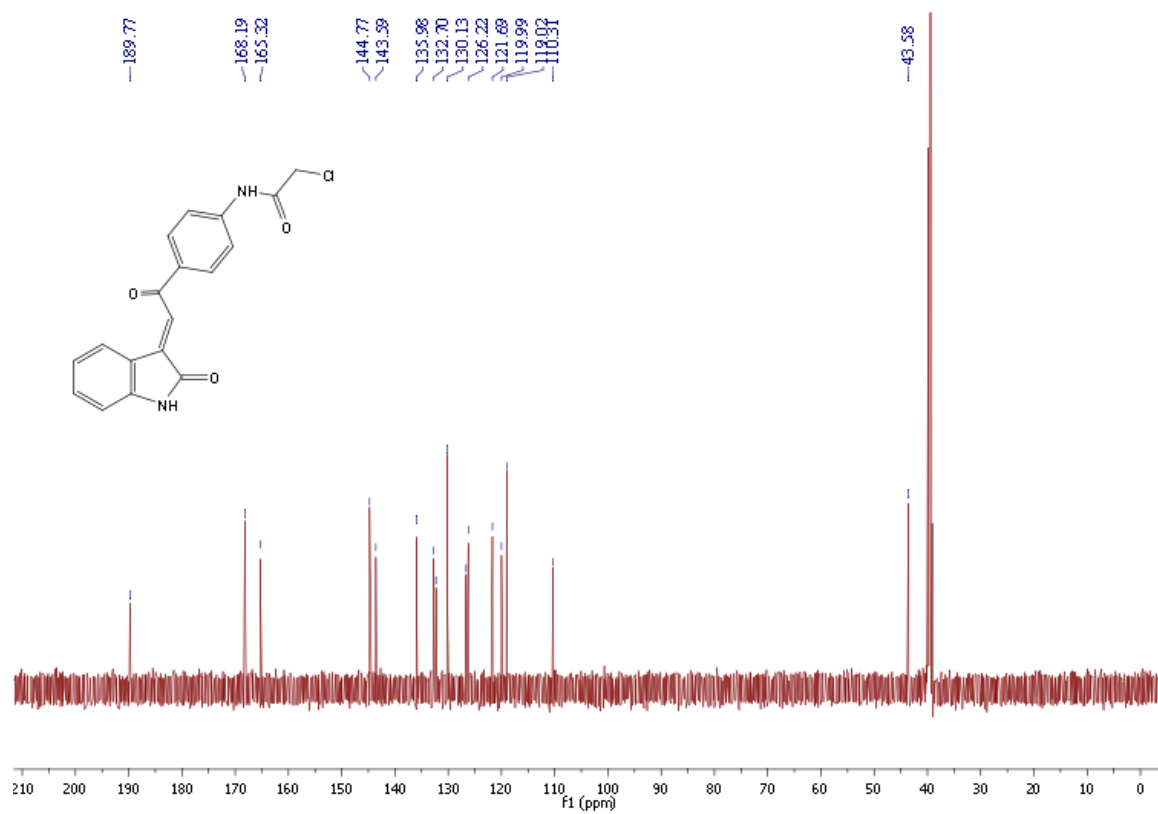


Figure S4: <sup>13</sup>C-NMR spectrum of compound 4 (150 MHz, DMSO/*d*<sub>6</sub>)

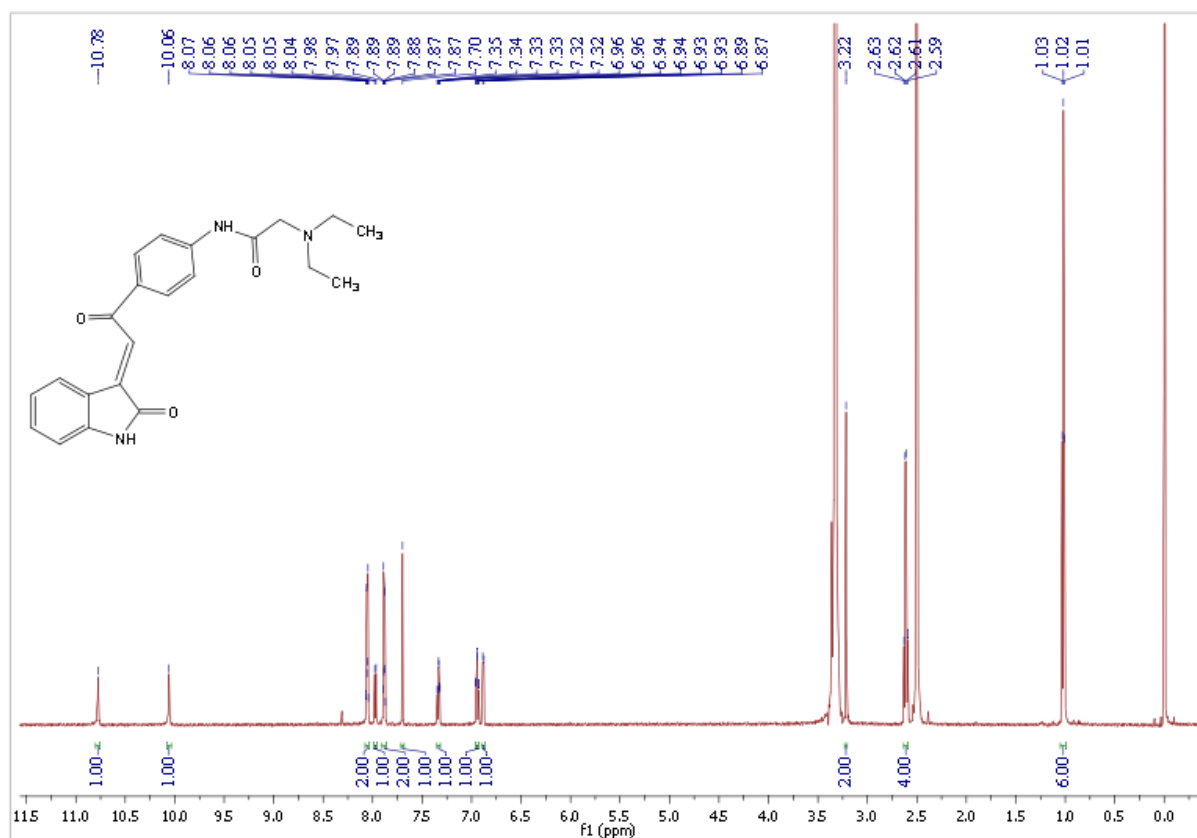


Figure S5: <sup>1</sup>H-NMR spectrum of compound 5a (600 MHz, DMSO/*d*<sub>6</sub>)

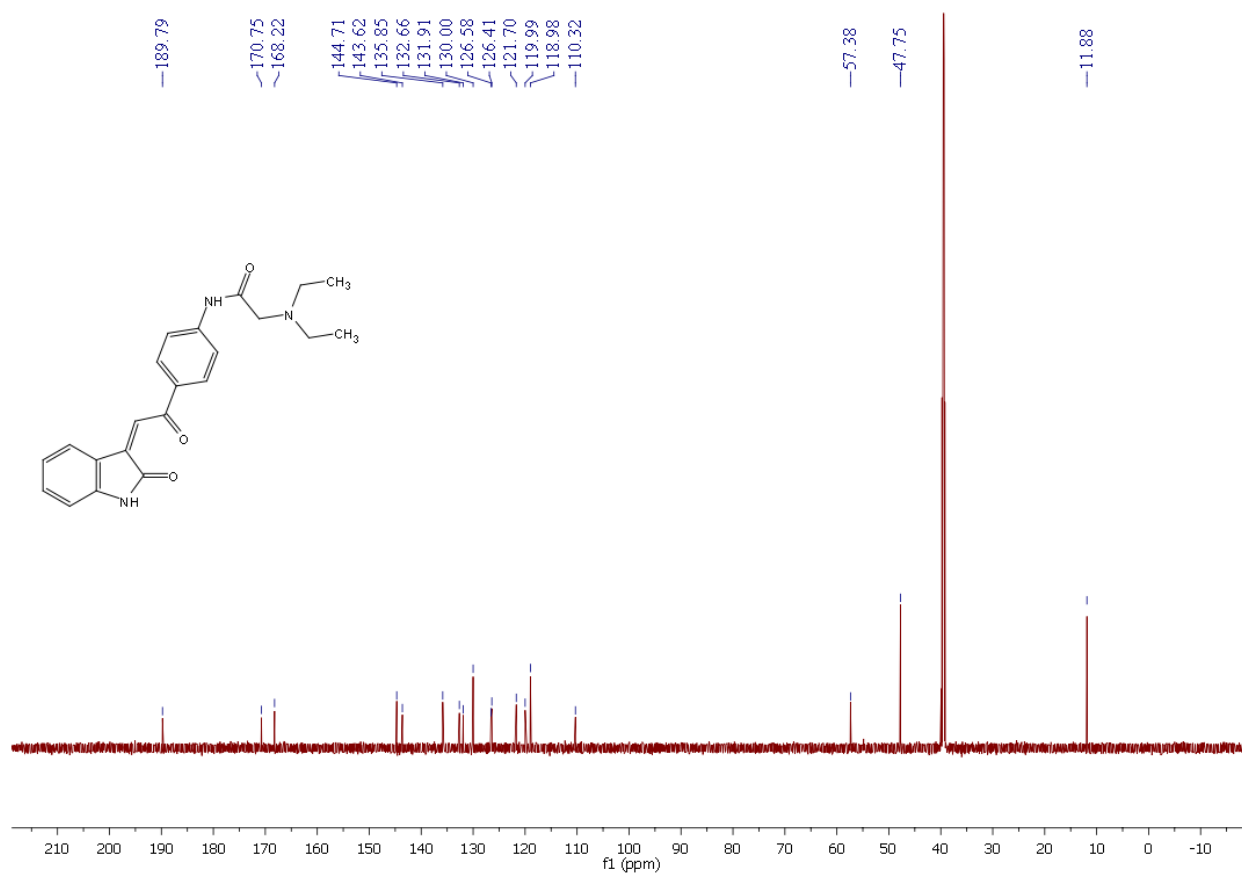


Figure S6: <sup>13</sup>C-NMR spectrum of compound 5a (150 MHz, DMSO/*d*<sub>6</sub>)

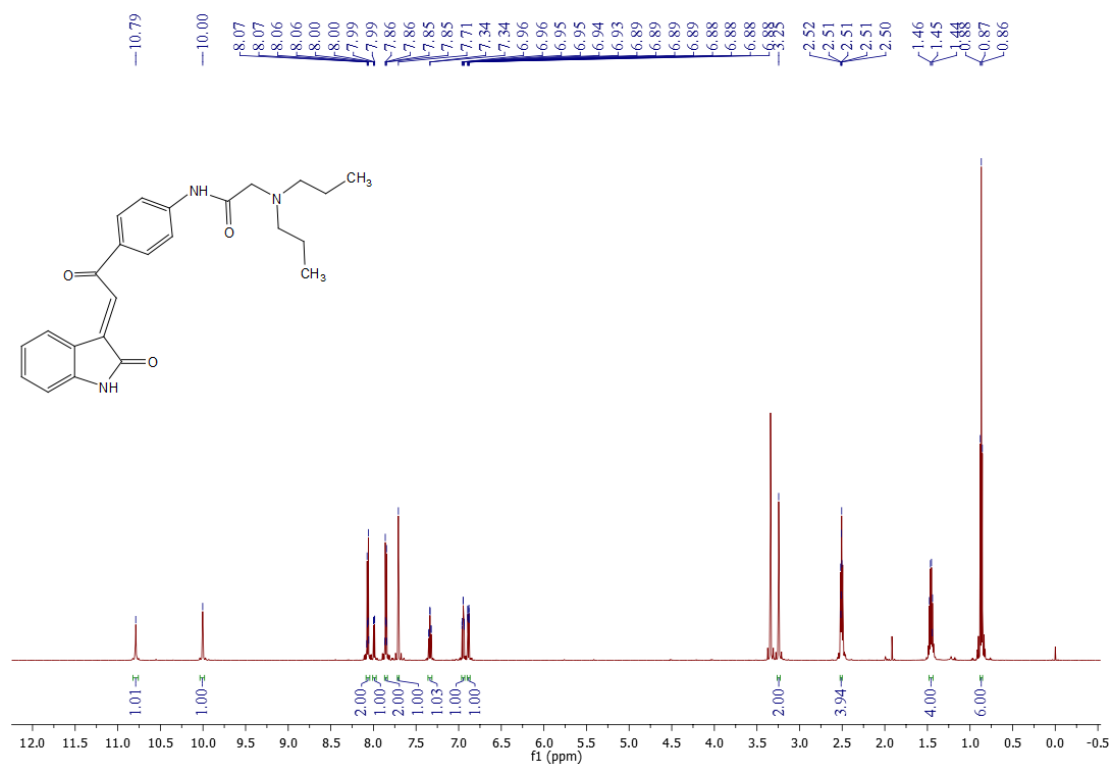


Figure S7: <sup>1</sup>H-NMR spectrum of compound **5b** (600 MHz, DMSO/*d*<sub>6</sub>)

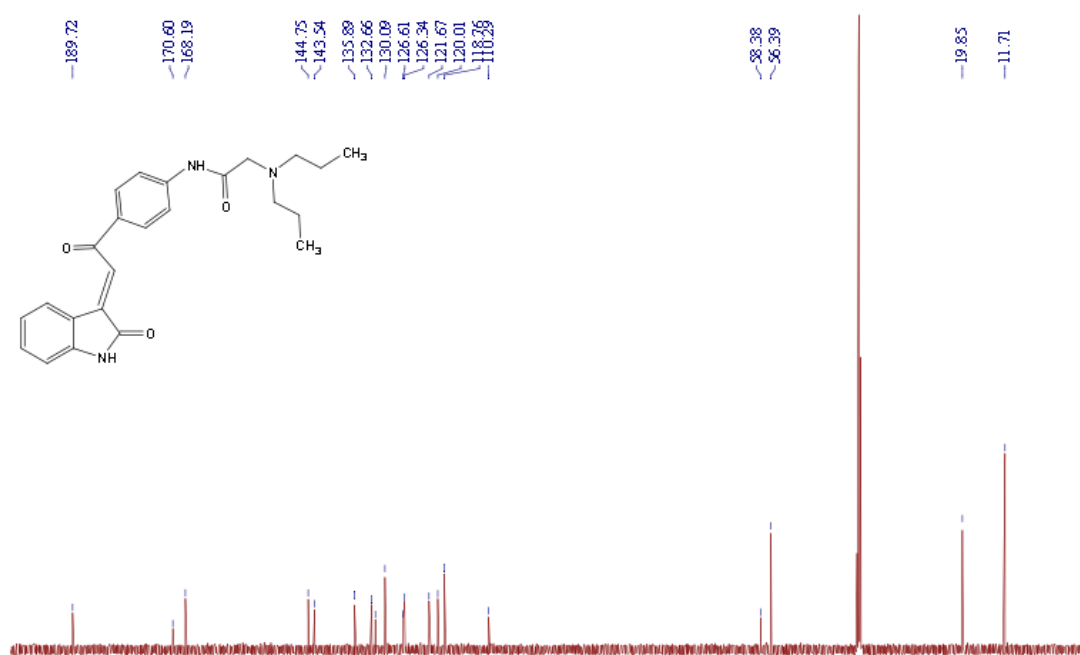


Figure S8: <sup>13</sup>C-NMR spectrum of compound **5b** (150 MHz, DMSO/*d*<sub>6</sub>)

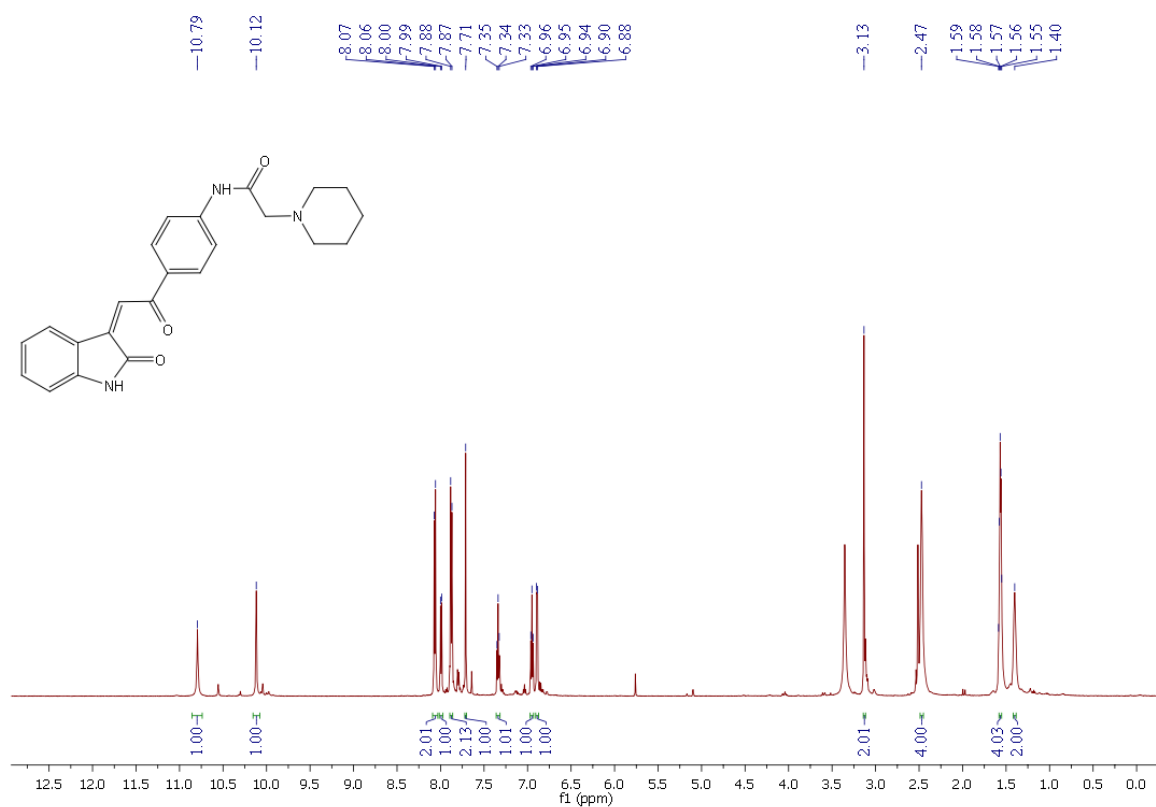


Figure S9: <sup>1</sup>H-NMR spectrum of compound 5c (600 MHz, DMSO/*d*<sub>6</sub>)

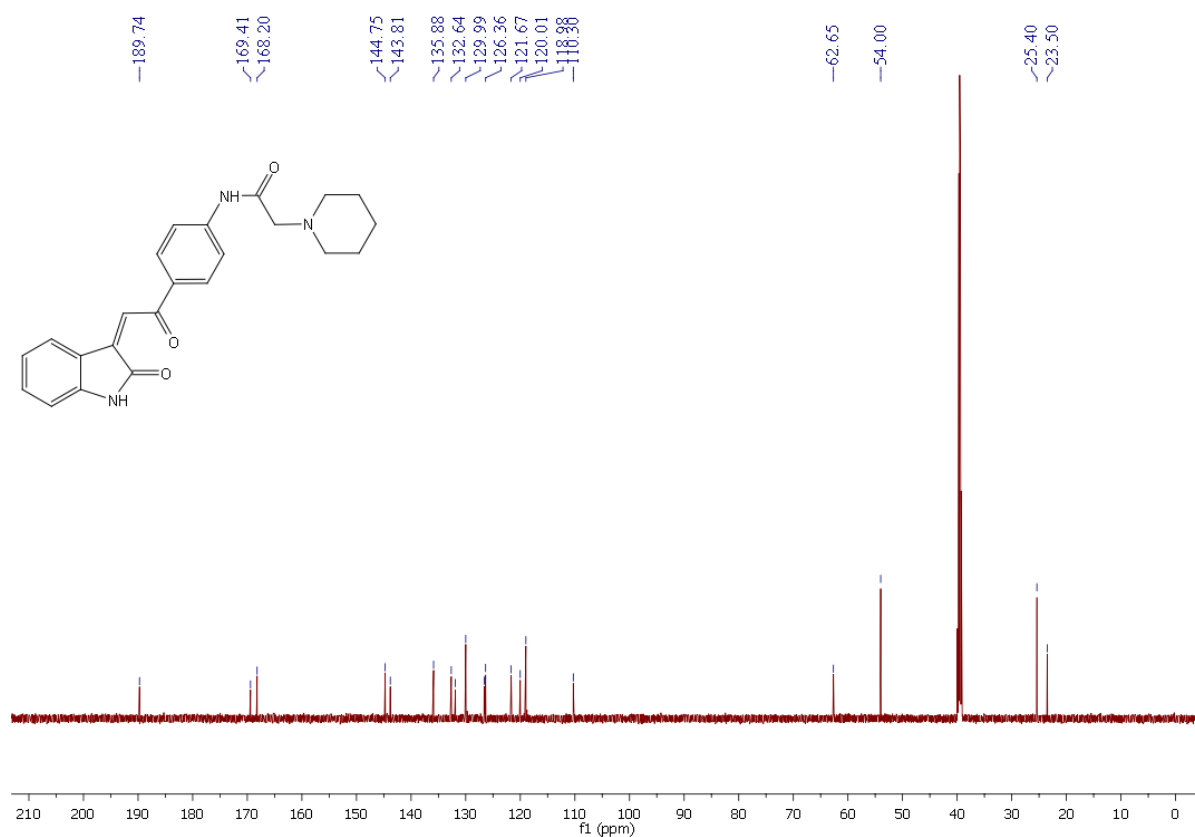


Figure S10: <sup>13</sup>C-NMR spectrum of compound 5c (150 MHz, DMSO/*d*<sub>6</sub>)

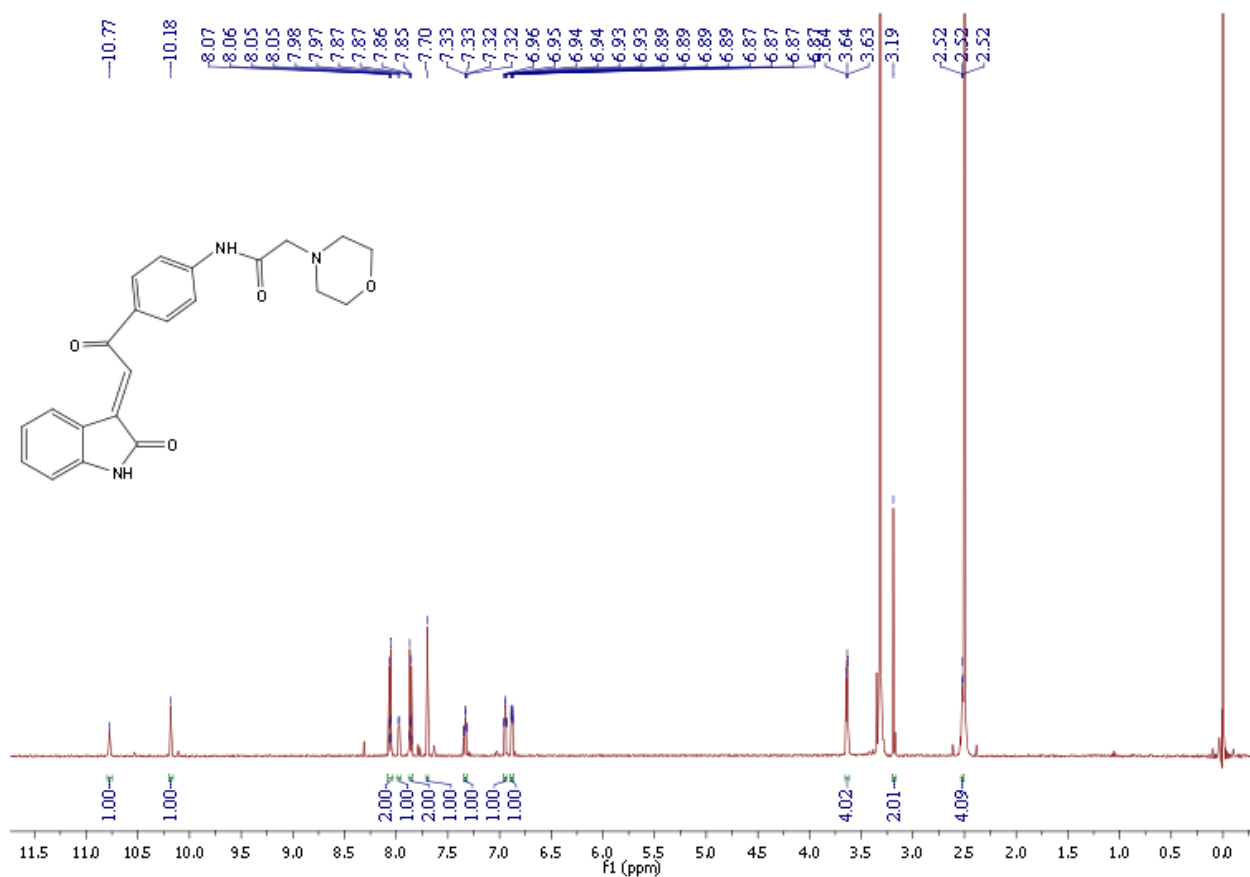


Figure S11: <sup>1</sup>H-NMR spectrum of compound 5d (600 MHz, DMSO/*d*<sub>6</sub>)

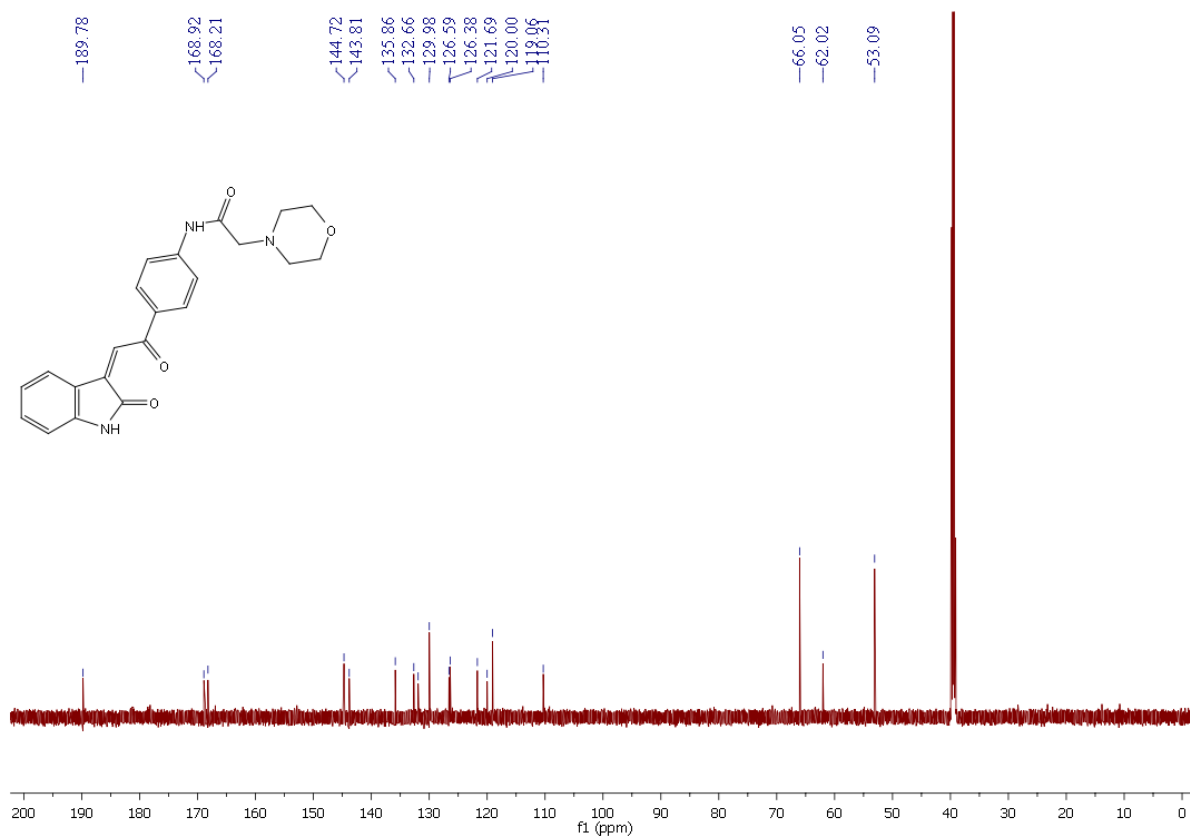


Figure S12: <sup>13</sup>C-NMR spectrum of compound 5d (150 MHz, DMSO/*d*<sub>6</sub>)

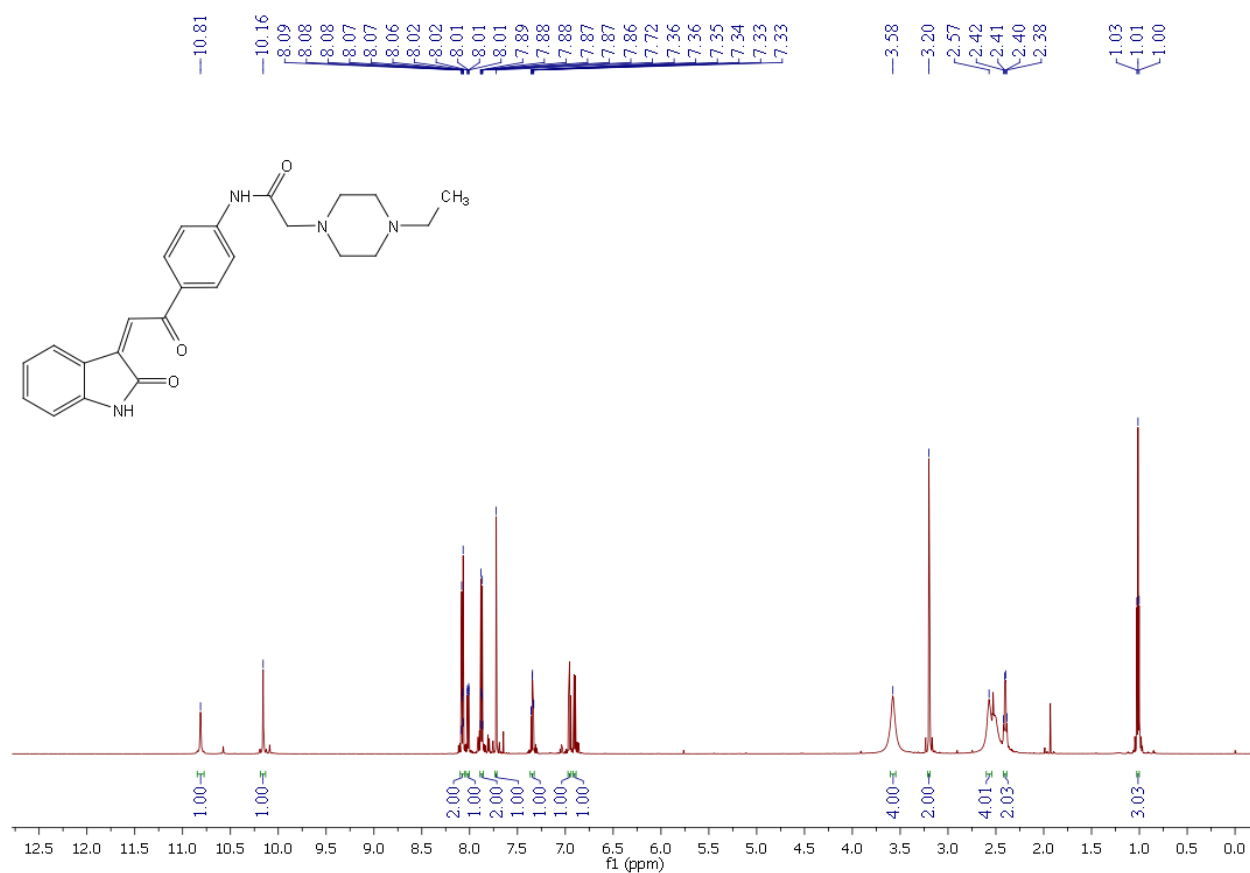


Figure S13: <sup>1</sup>H-NMR spectrum of compound 5e (600 MHz, DMSO/*d*<sub>6</sub>)

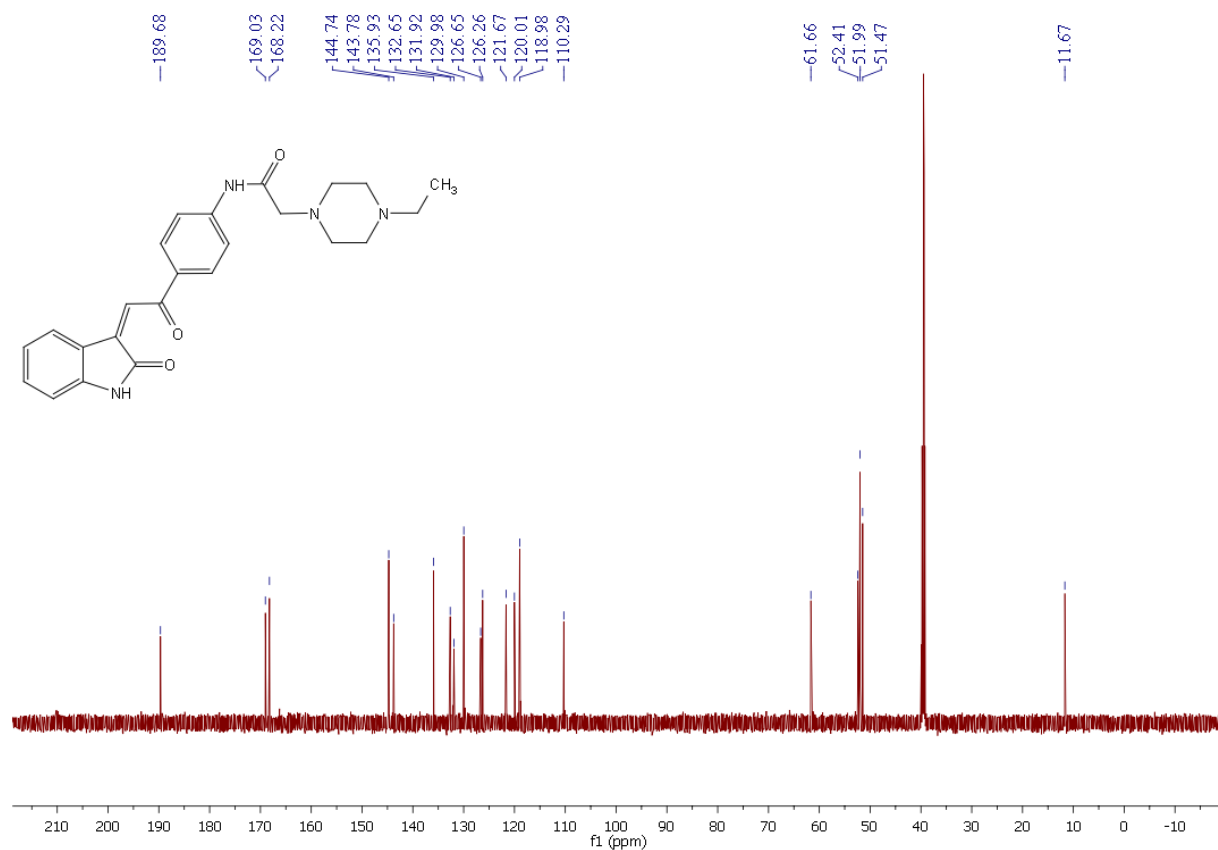


Figure S14: <sup>13</sup>C-NMR spectrum of compound 5d (150 MHz, DMSO/*d*<sub>6</sub>)



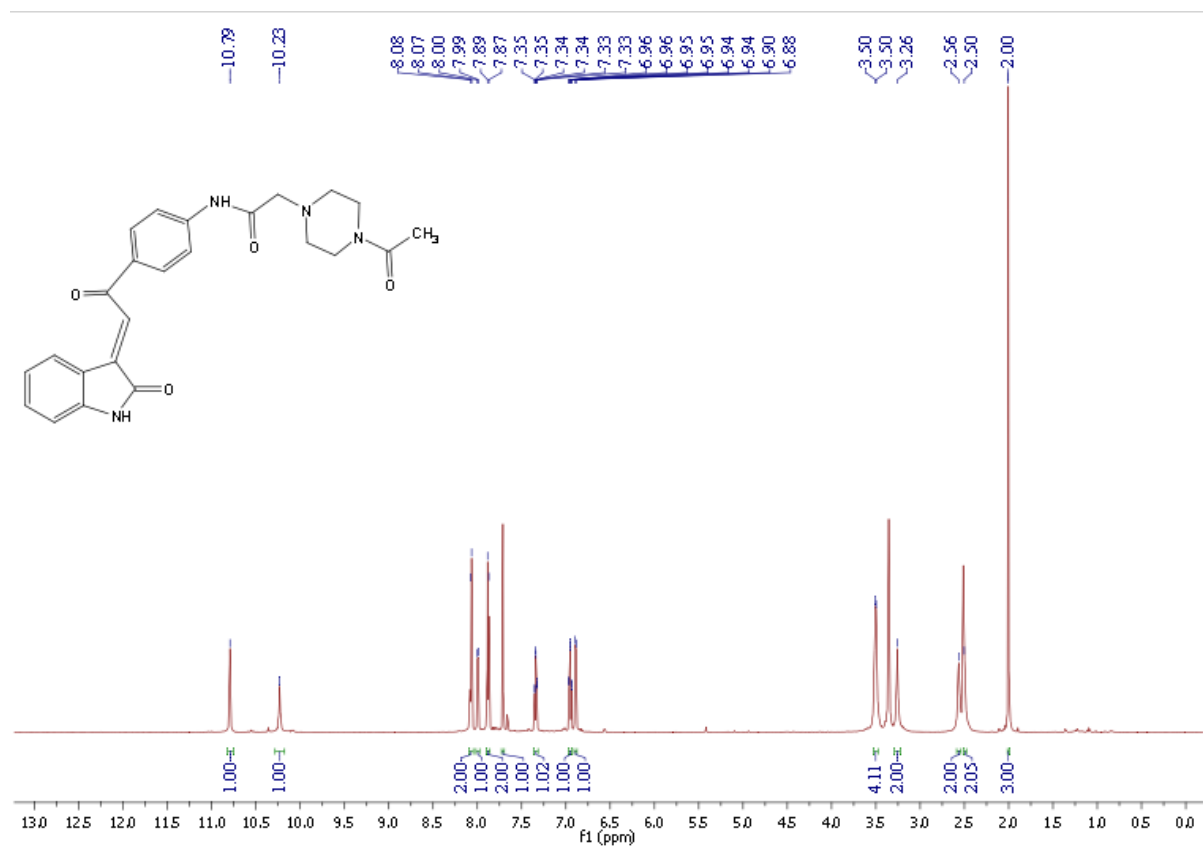


Figure S15: <sup>1</sup>H-NMR spectrum of compound 5f (600 MHz, DMSO/*d*<sub>6</sub>)

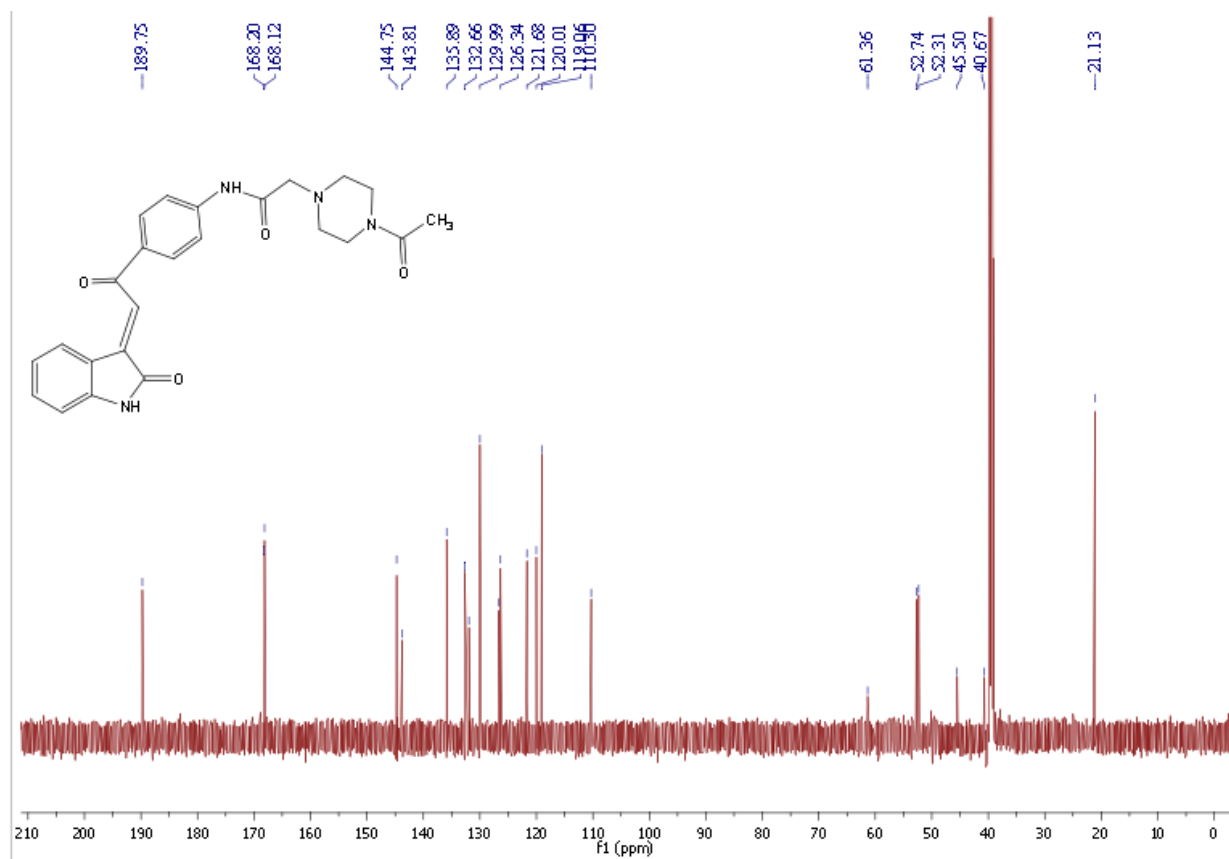


Figure S16: <sup>13</sup>C-NMR spectrum of compound 5f (150 MHz, DMSO/*d*<sub>6</sub>)

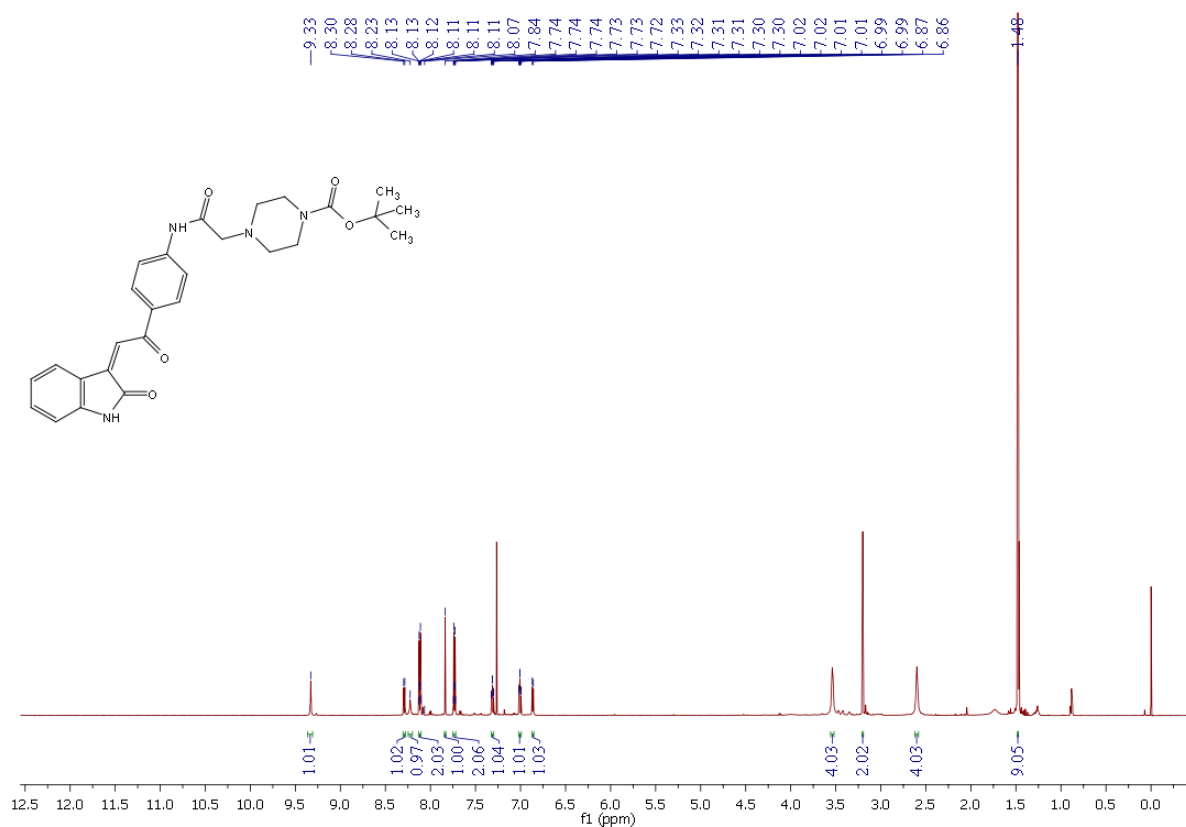


Figure S17: <sup>1</sup>H-NMR spectrum of compound **5g** (600 MHz, CDCl<sub>3</sub>)

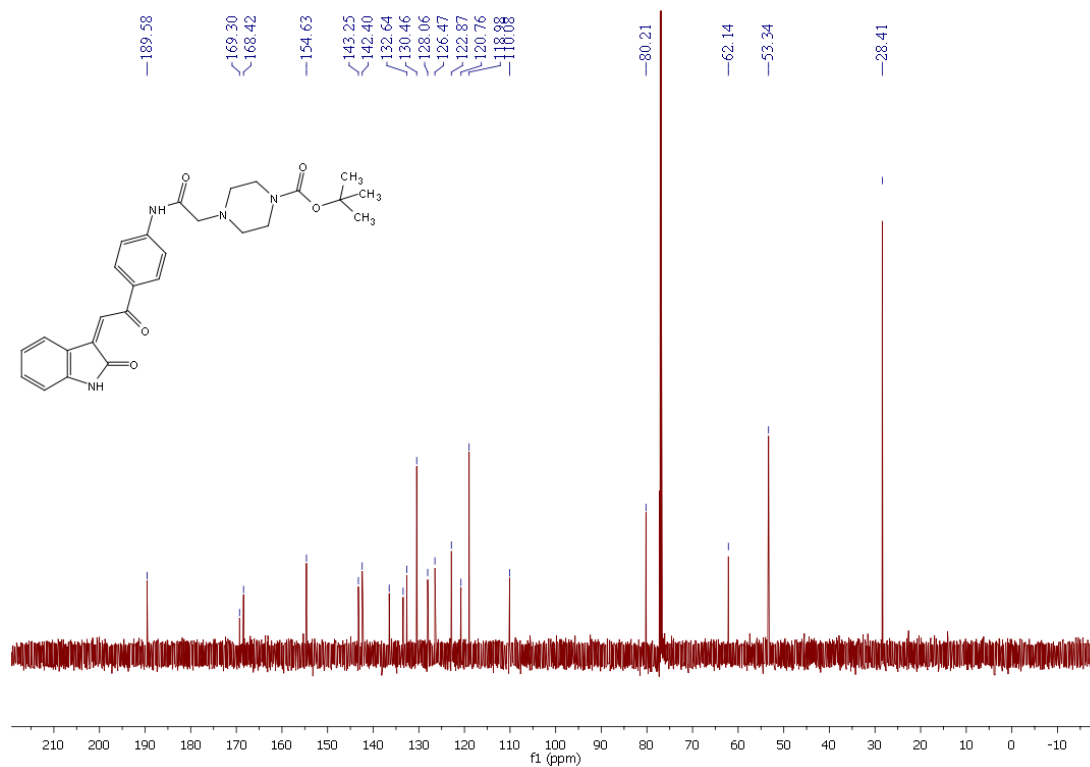


Figure S18: <sup>13</sup>C-NMR spectrum of compound **5g** (150 MHz, CDCl<sub>3</sub>)

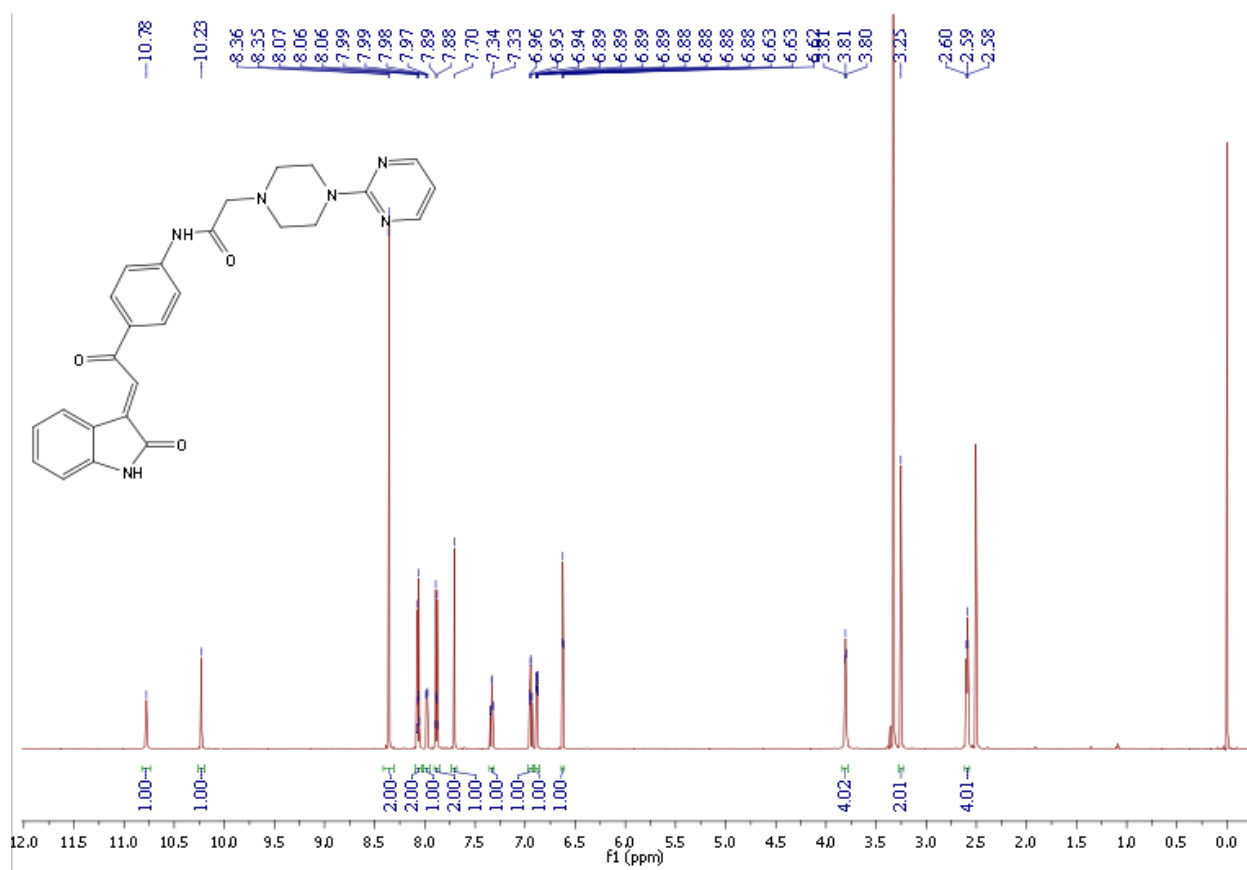


Figure S19: <sup>1</sup>H-NMR spectrum of compound **5h** (600 MHz, DMSO/*d*<sub>6</sub>)

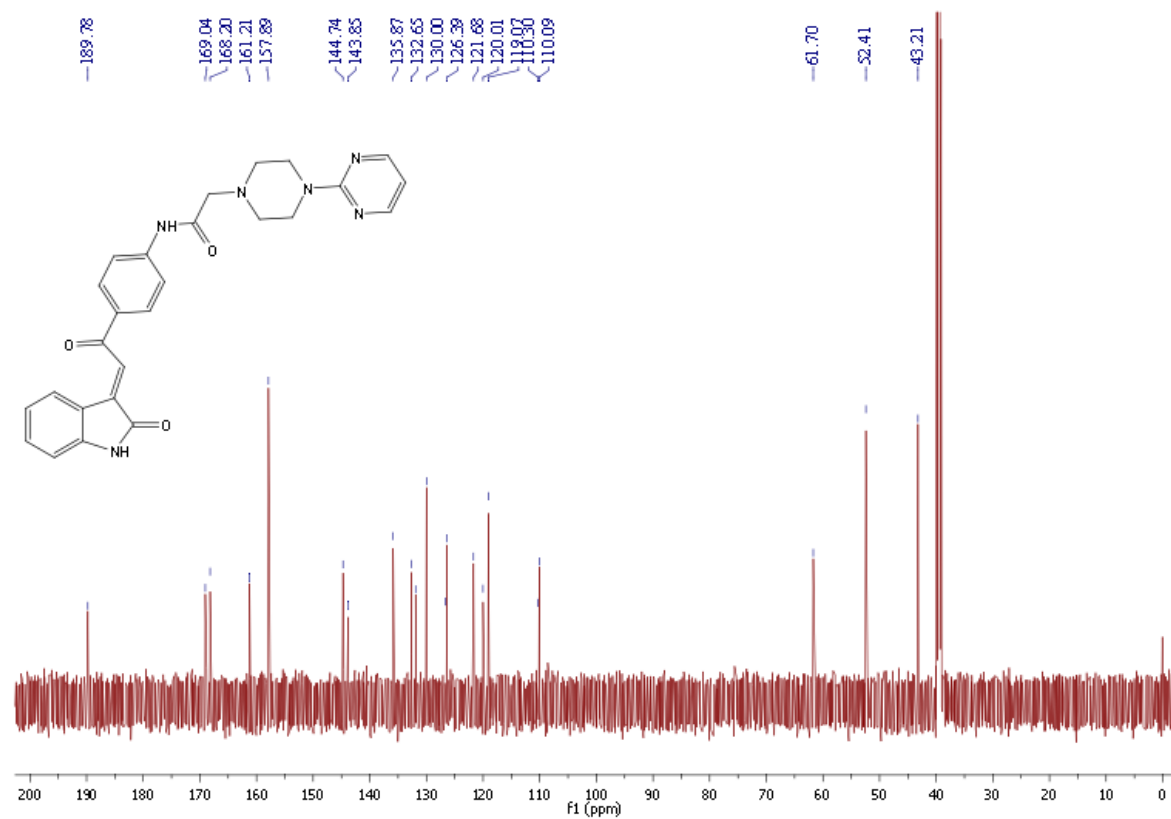


Figure S20: <sup>13</sup>C-NMR spectrum of compound **5h** (150 MHz, DMSO/*d*<sub>6</sub>)

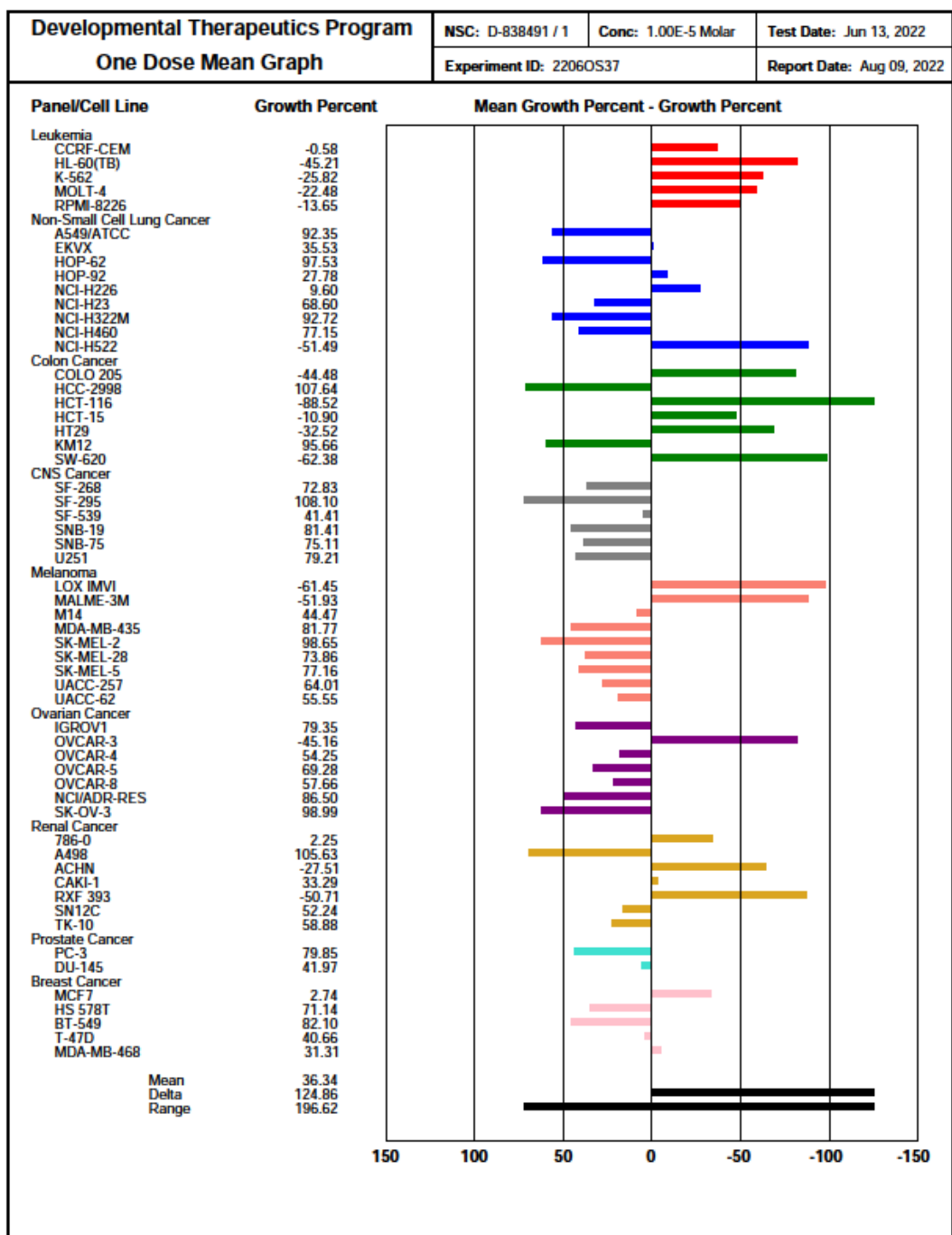


Figure S21. NCI SRB assay mean graph of compound **5a** at 10  $\mu$ M concentration.

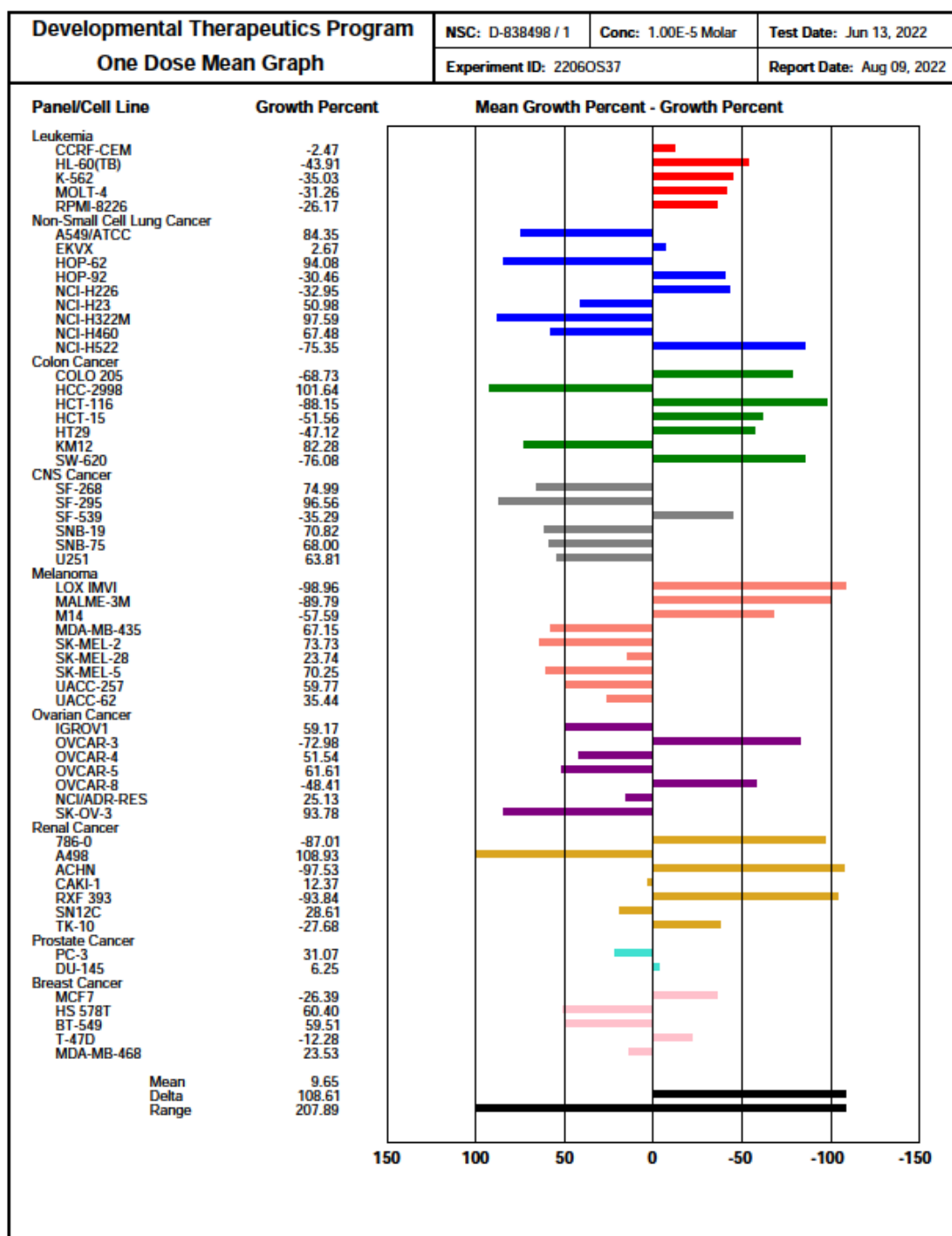


Figure S22. NCI SRB assay mean graph of compound **5b** at 10  $\mu$ M concentration.

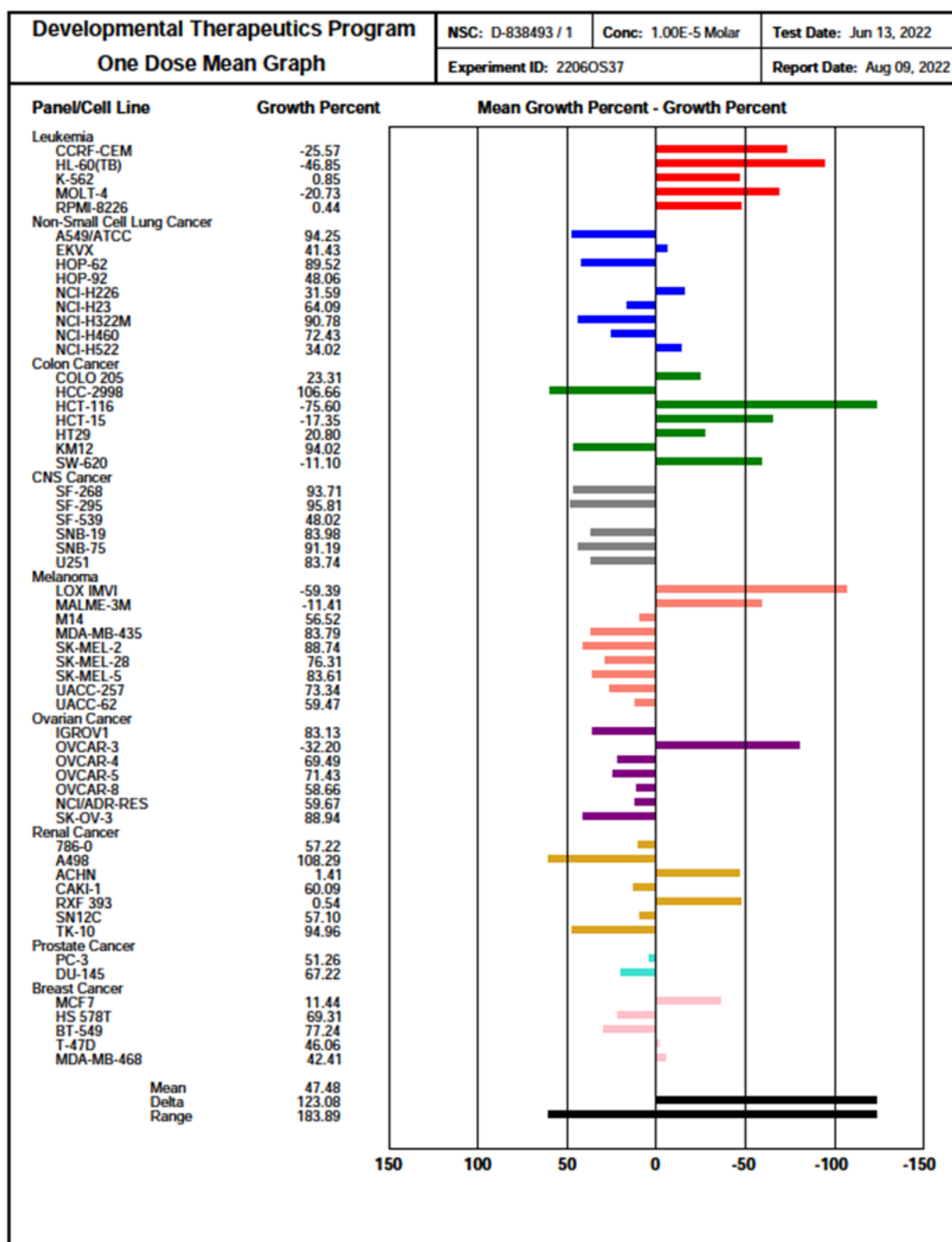


Figure S23. NCI SRB assay mean graph of compound 5c at 10  $\mu$ M concentration.

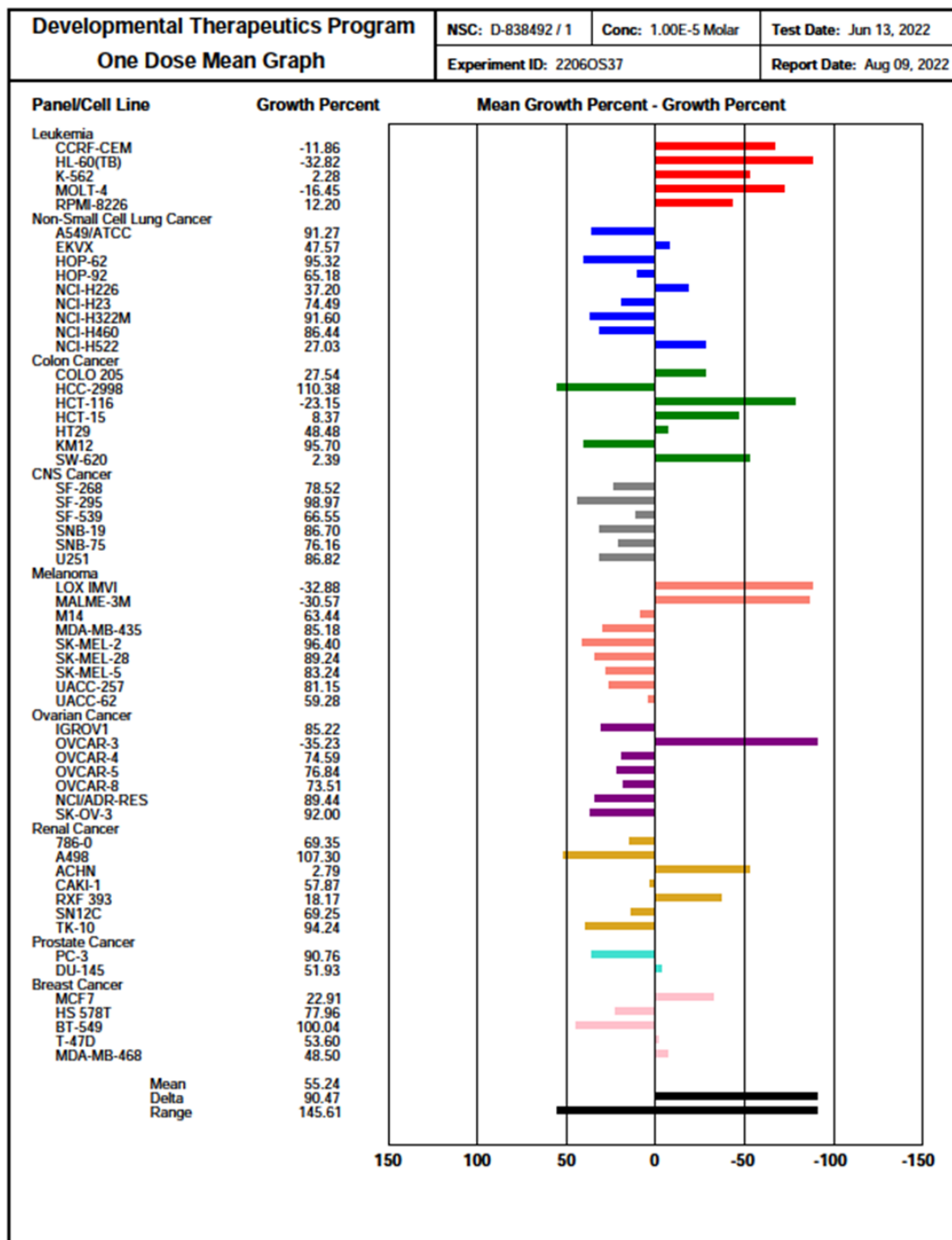


Figure S24. NCI SRB assay mean graph of compound 5d at 10 μM concentration.

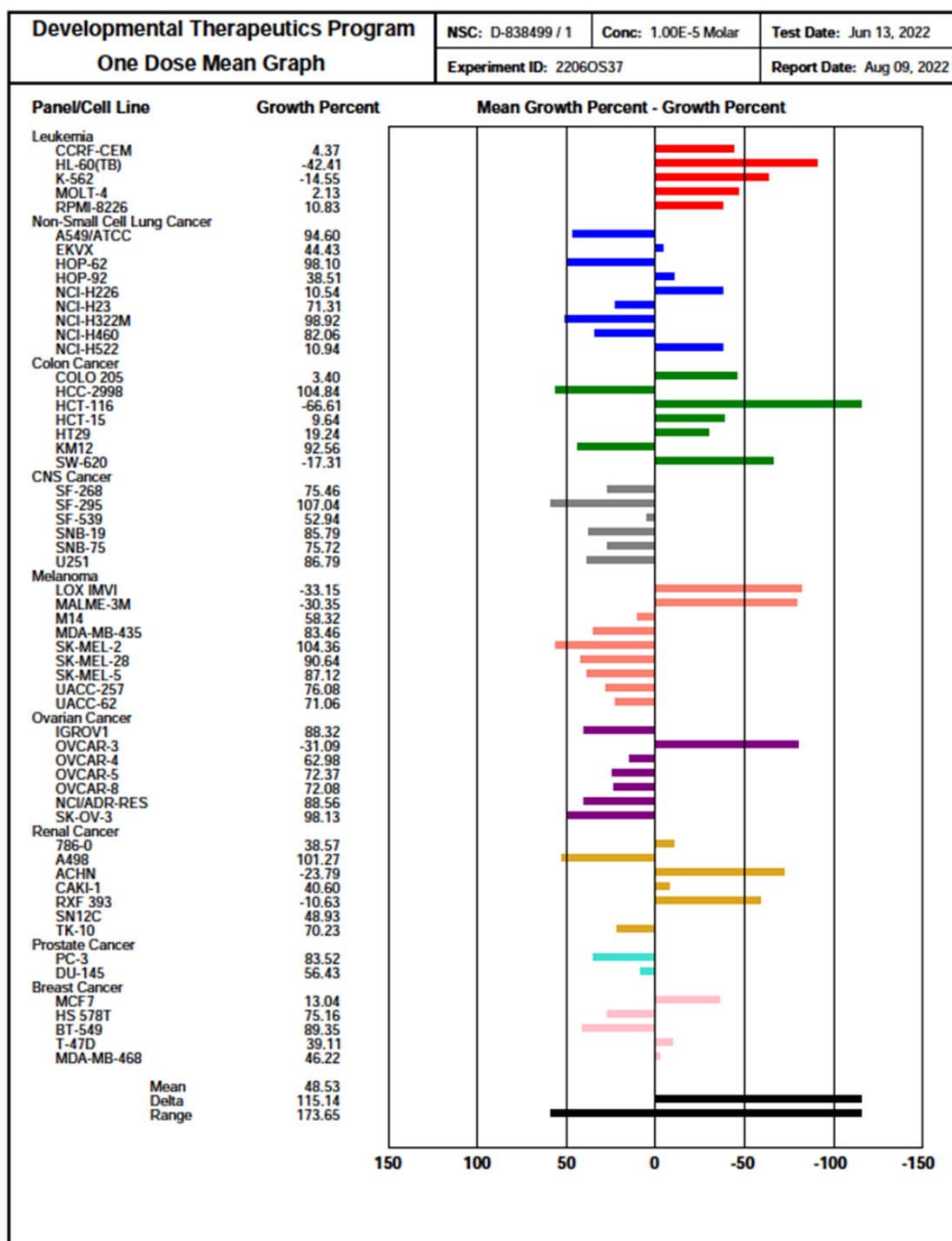


Figure S25. NCI SRB assay mean graph of compound **5e** at 10  $\mu$ M concentration.



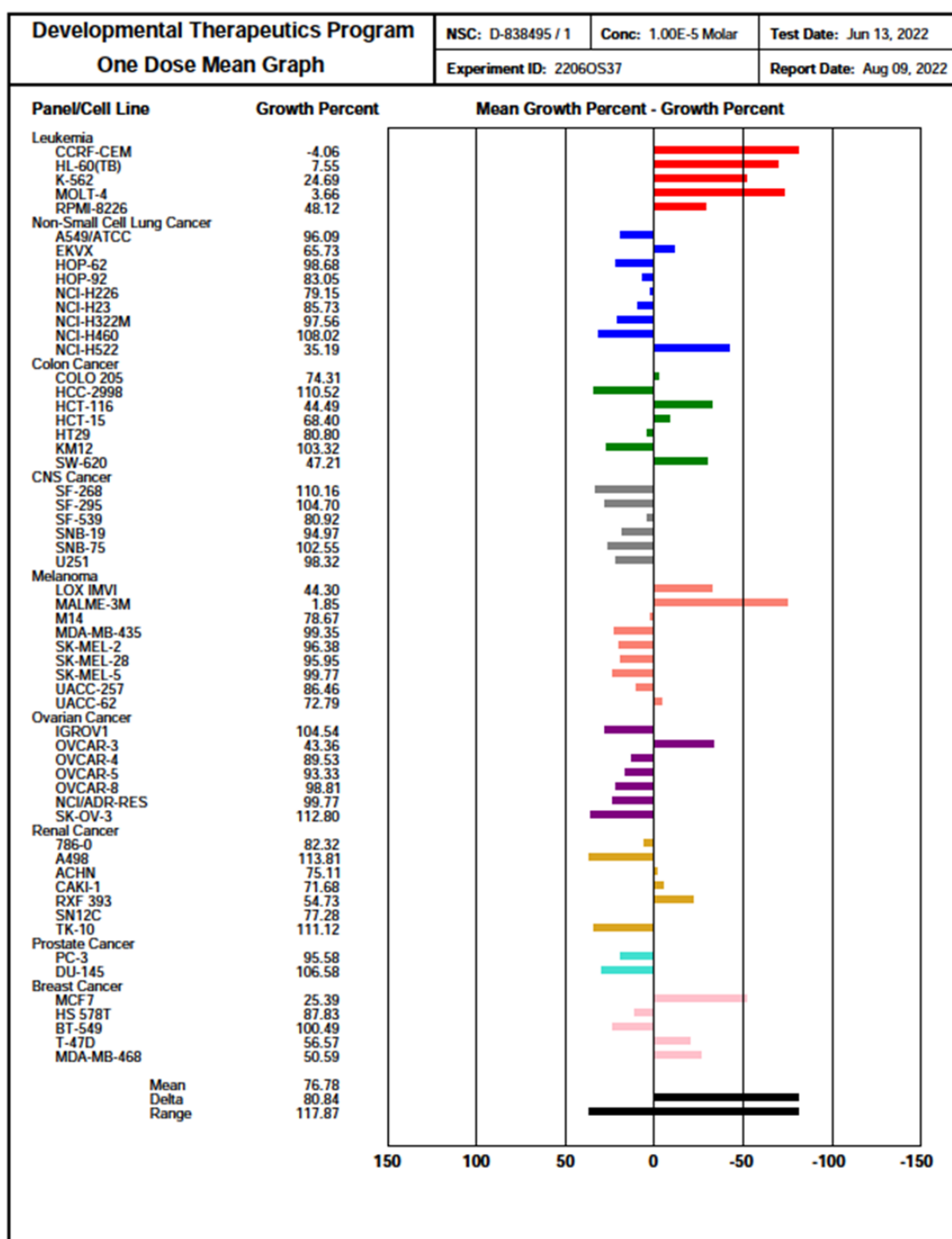


Figure S26. NCI SRB assay mean graph of compound 5f at 10  $\mu$ M concentration.

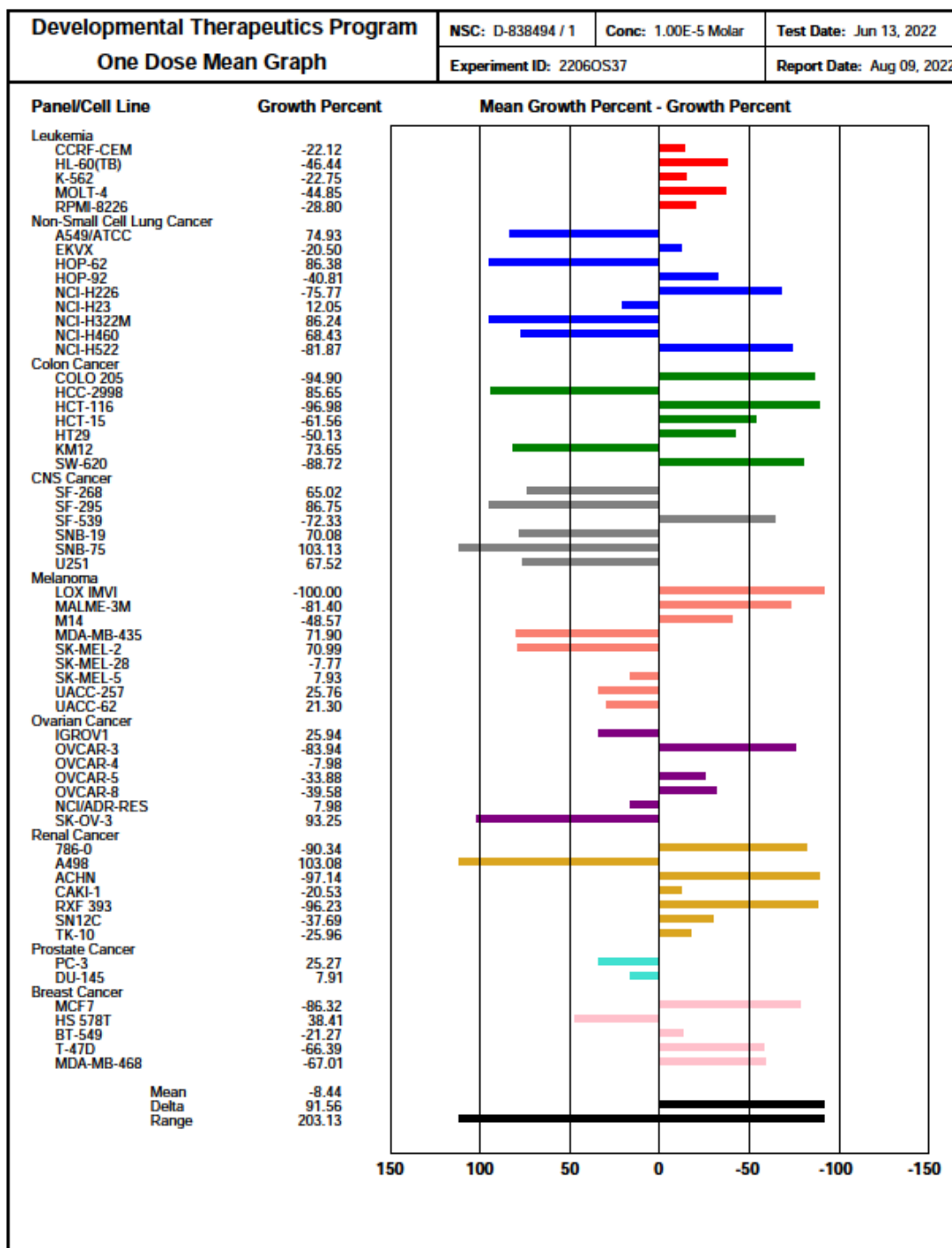


Figure S27. NCI SRB assay mean graph of compound **5g** at 10  $\mu$ M concentration.

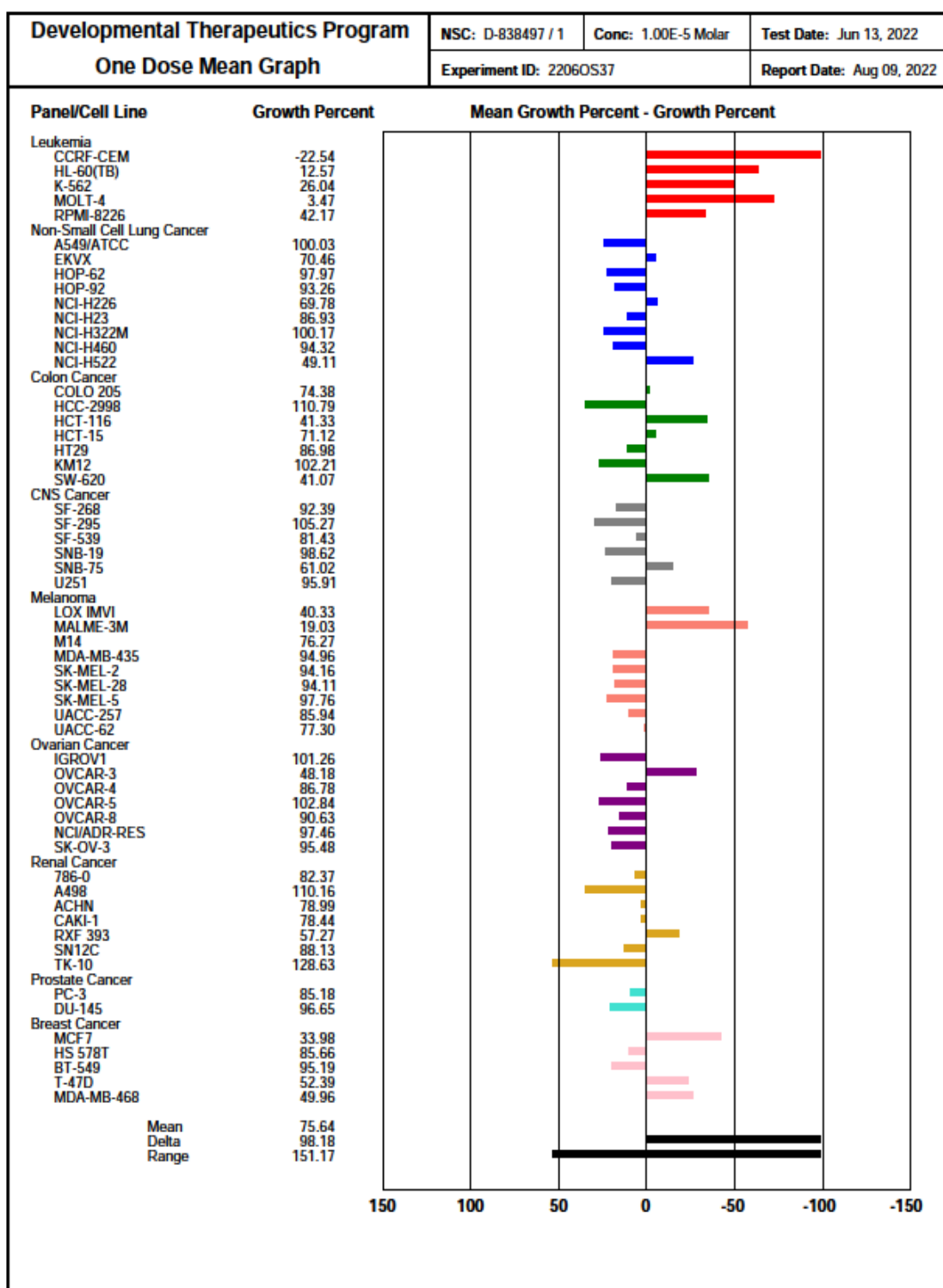


Figure S28. NCI SRB assay mean graph of compound **5h** at 10  $\mu$ M concentration.