Design, Synthesis, Physicochemical Properties, and Biological Activity of Thymidine Compounds Attached to 5,8-Quinolinedione Derivatives as Potent DT-Diaphorase Substrates

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Table S1. Interaction of selected hybrids with active site of NQO1 protein.

Ligand	H-bonding residues and length (Å)	π-interaction residues and length (Å)	Halogen interaction residues and length (Å)
6	TYR126 (3.39, 3.35) TYR128 (2.67) GLY193 (3.58)	TRP105 (4.71, 5.35) TYR128 (4.09, 5.21) PHE178 (5.88) HIS194 (4.71) FAD (3.65, 4.02, 4.11, 3.96, 5.21)	
7	TYR126 (3.29) TYR128 (2.71) GLY149 (3.48) GLY193 (3.54) FAD (2.43)	PRO66 (5.04) TRP105 (5.18, 4.57) TYR128 (4.70) PHE178 (5.39, 4.81) HIS194 (4.44) FAD (3.57, 4.07, 4.37, 3.90, 5.07)	
8	GLN66 (3.27) TYR128 (3.33) GLY193 (3.33)	TRP105 (4.66, 3.74) PHE106 (4.56) TYR128 (3.76, 4.62, 4.82) PHE178 (4.60, 4.07) HIS194 (4.41) FAD (4.05, 3.66, 4.80, 4.65, 4.64, 4.81)	GLY149 (3.13)

Figure S1. Spectra of 7-(3′-azido-3′-deoxythymidine)-6-chloro-5,8-quinolinedione **6**

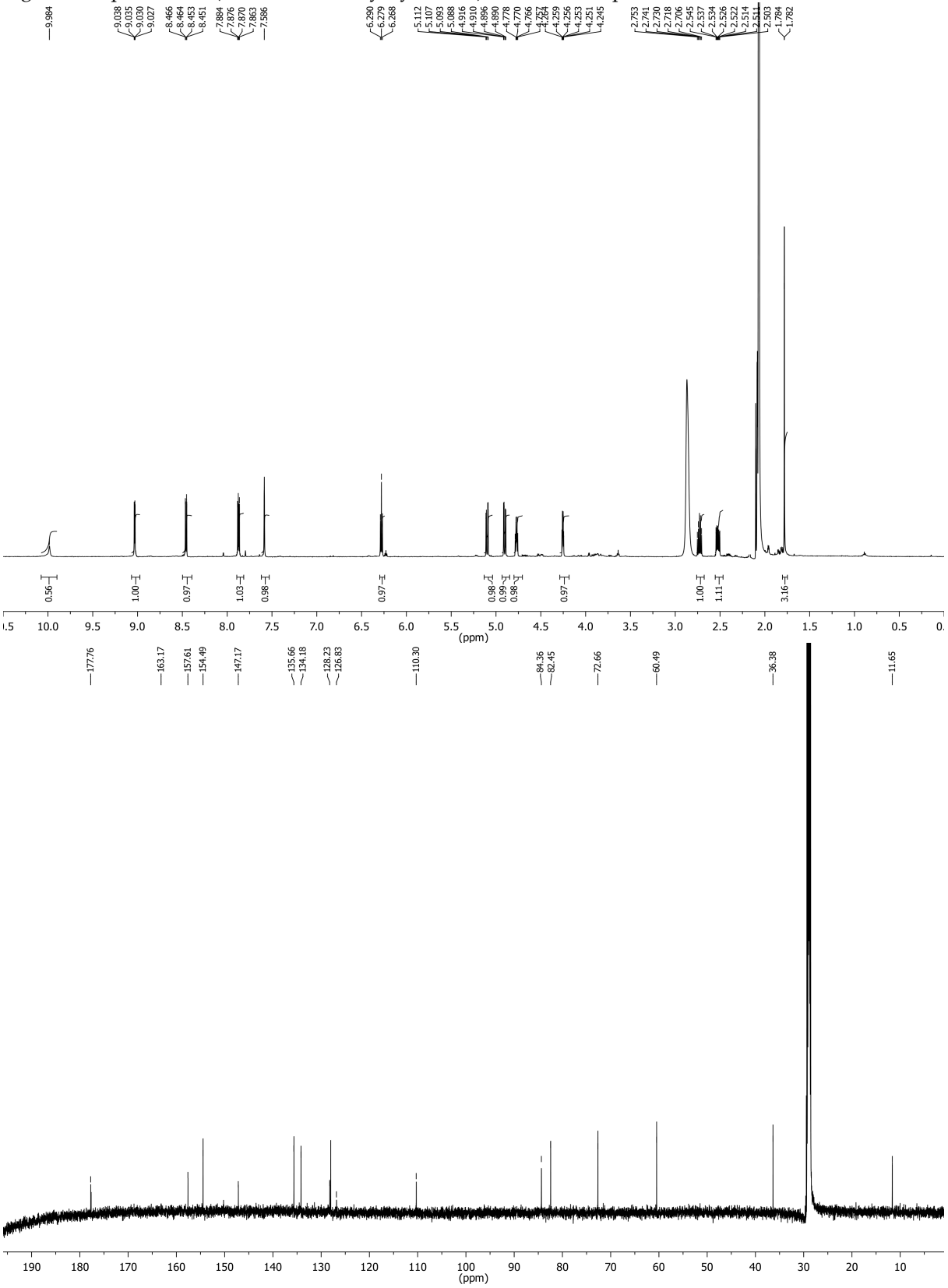


Figure S2. Spectra of 7-(3′-deoxythymidine)-6-chloro-5,8-quinolinedione **7**

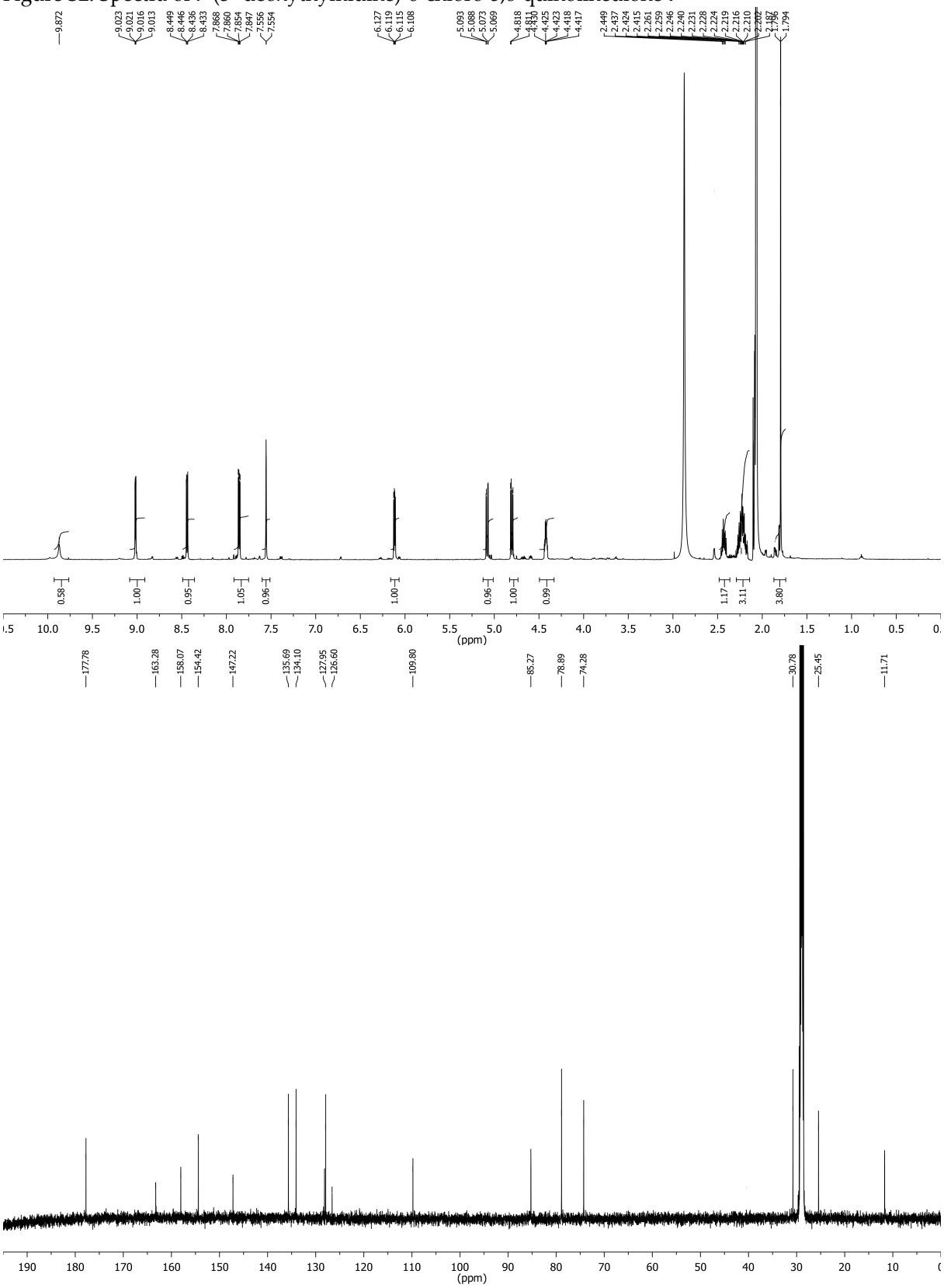
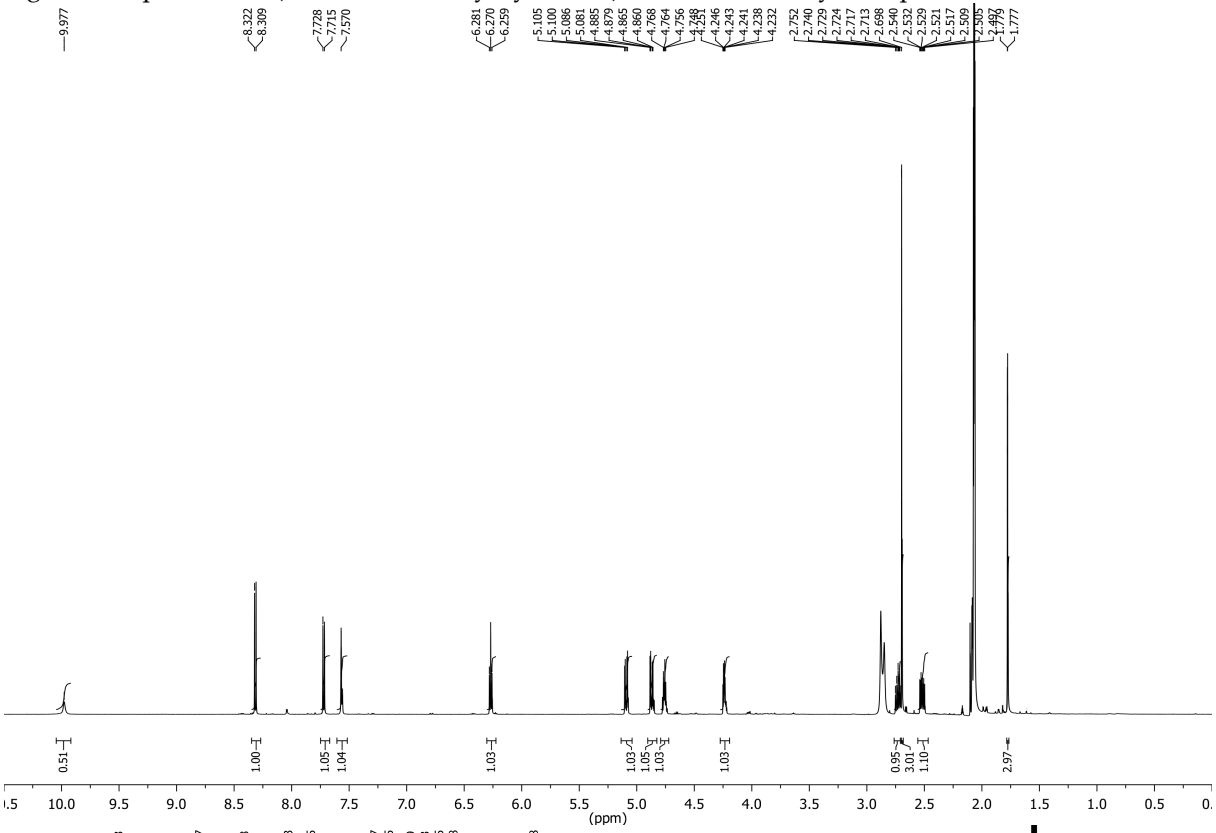


Figure S3. Spectra of 7-(3′-azido-3′-deoxythymidine)-6-chloro-2-methyl-5,8-quinolinedione **8**



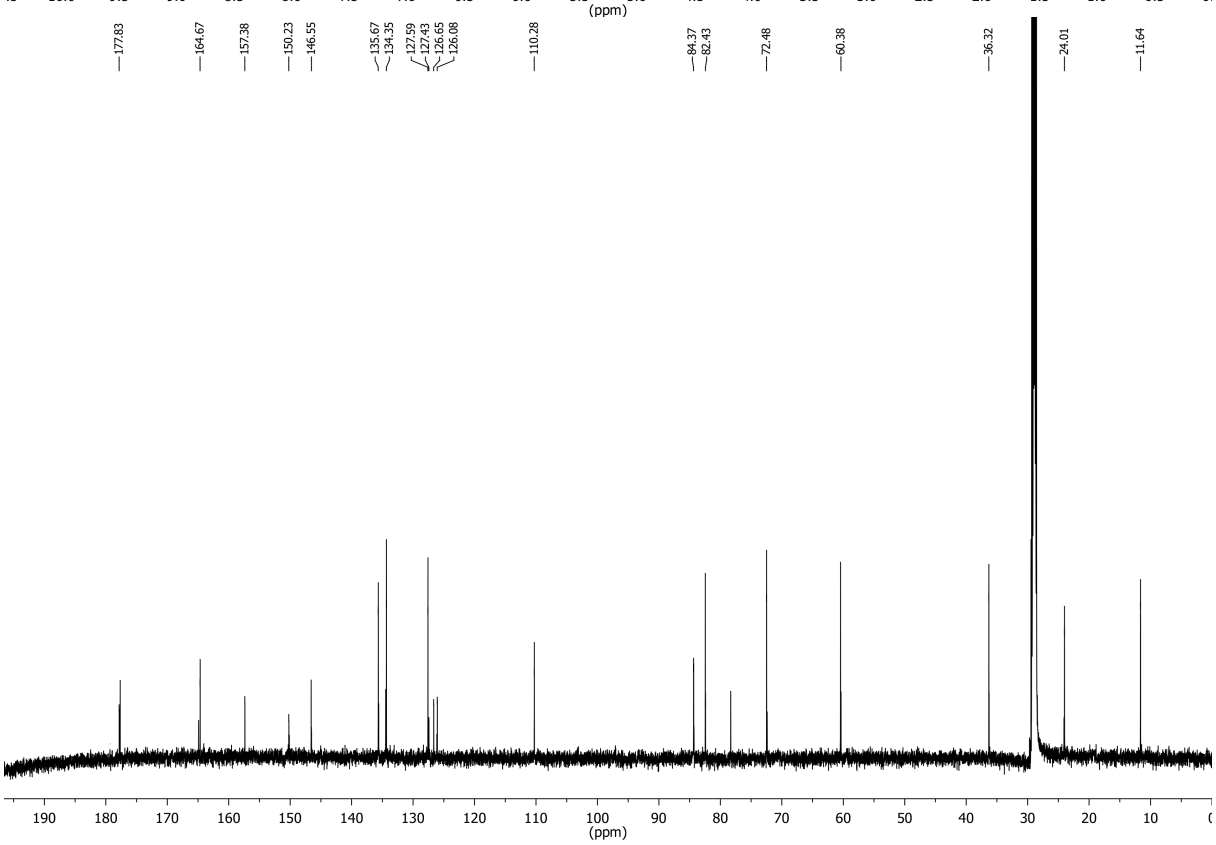
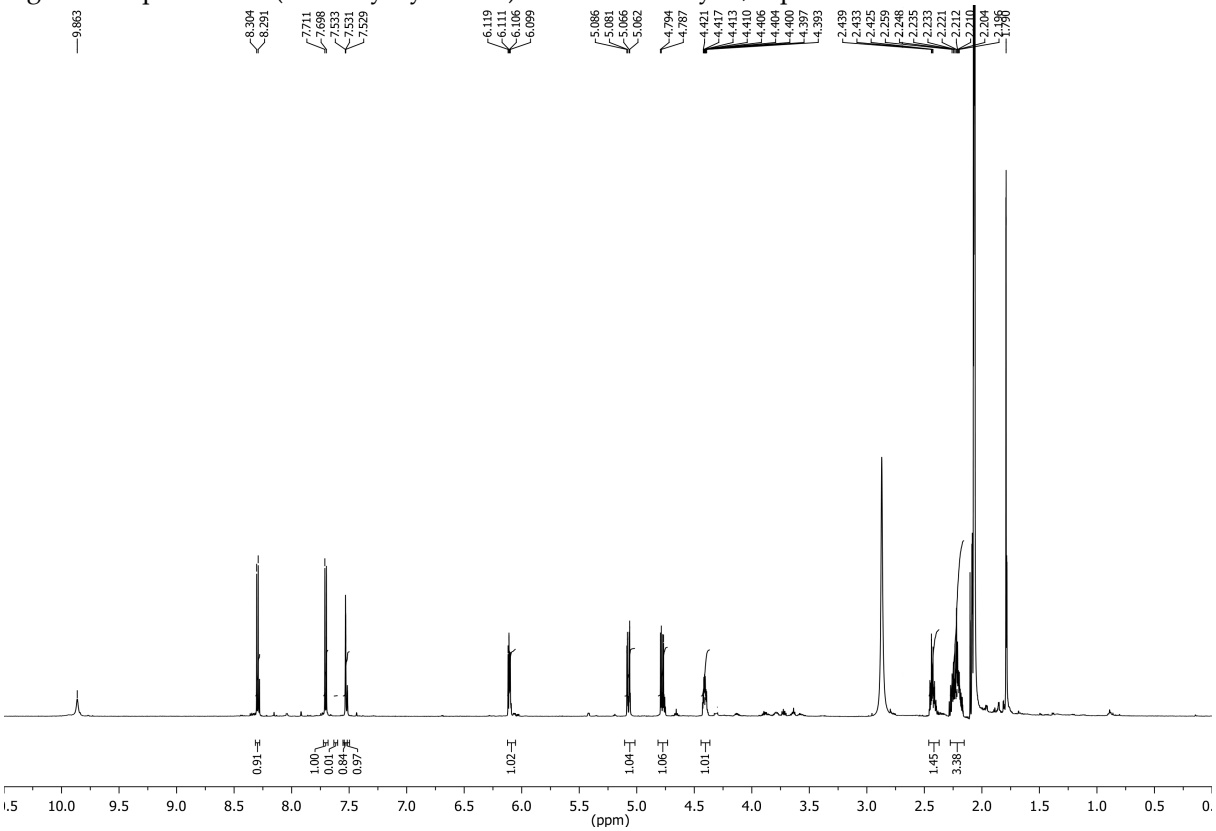


Figure S4. Spectra of 7-(3′-deoxythymidine)-6-chloro-2-metyl-5,8-quinolinedione **9**



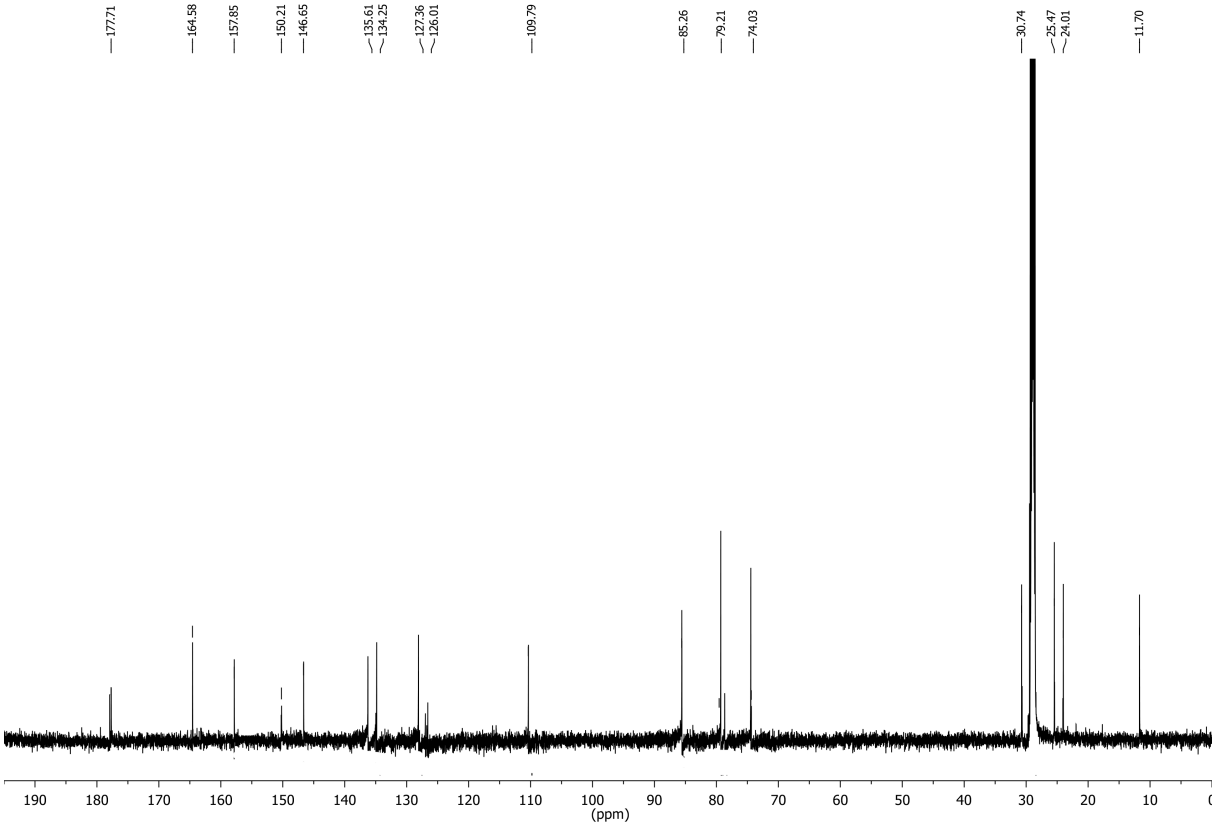
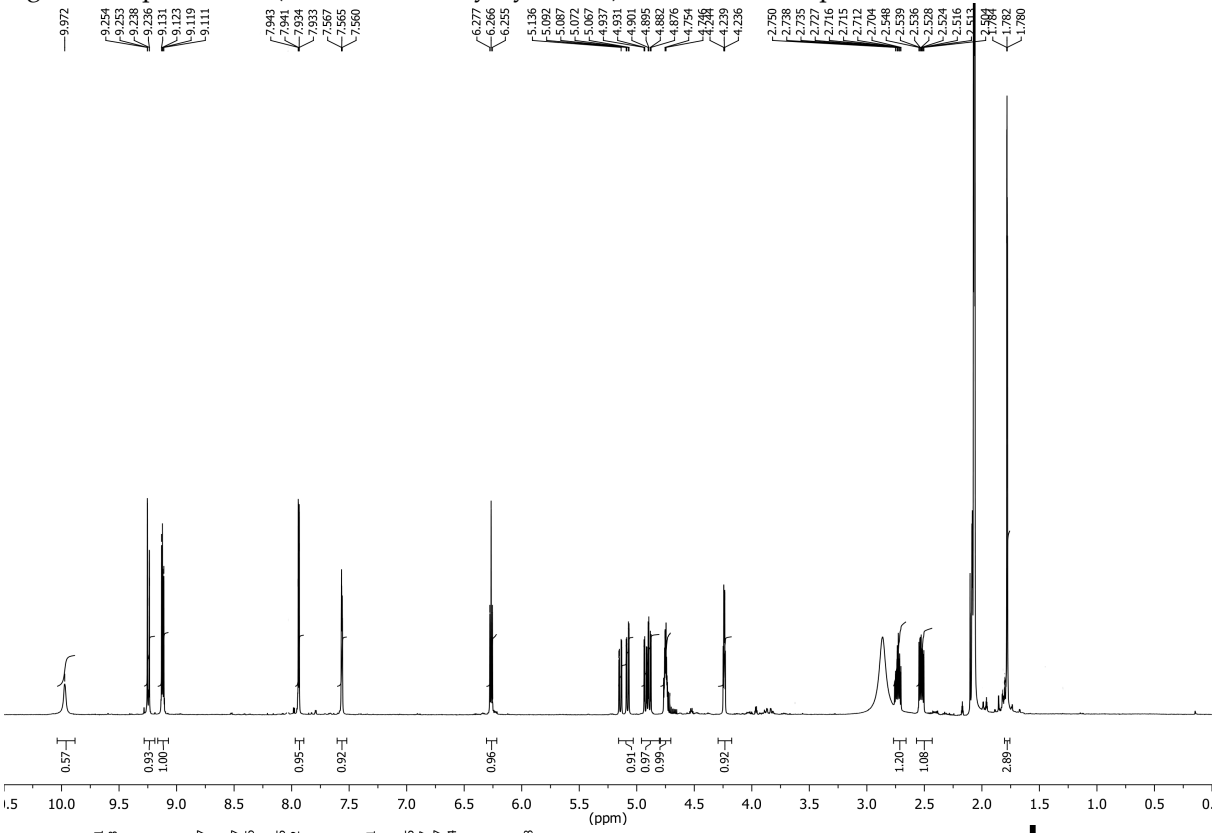
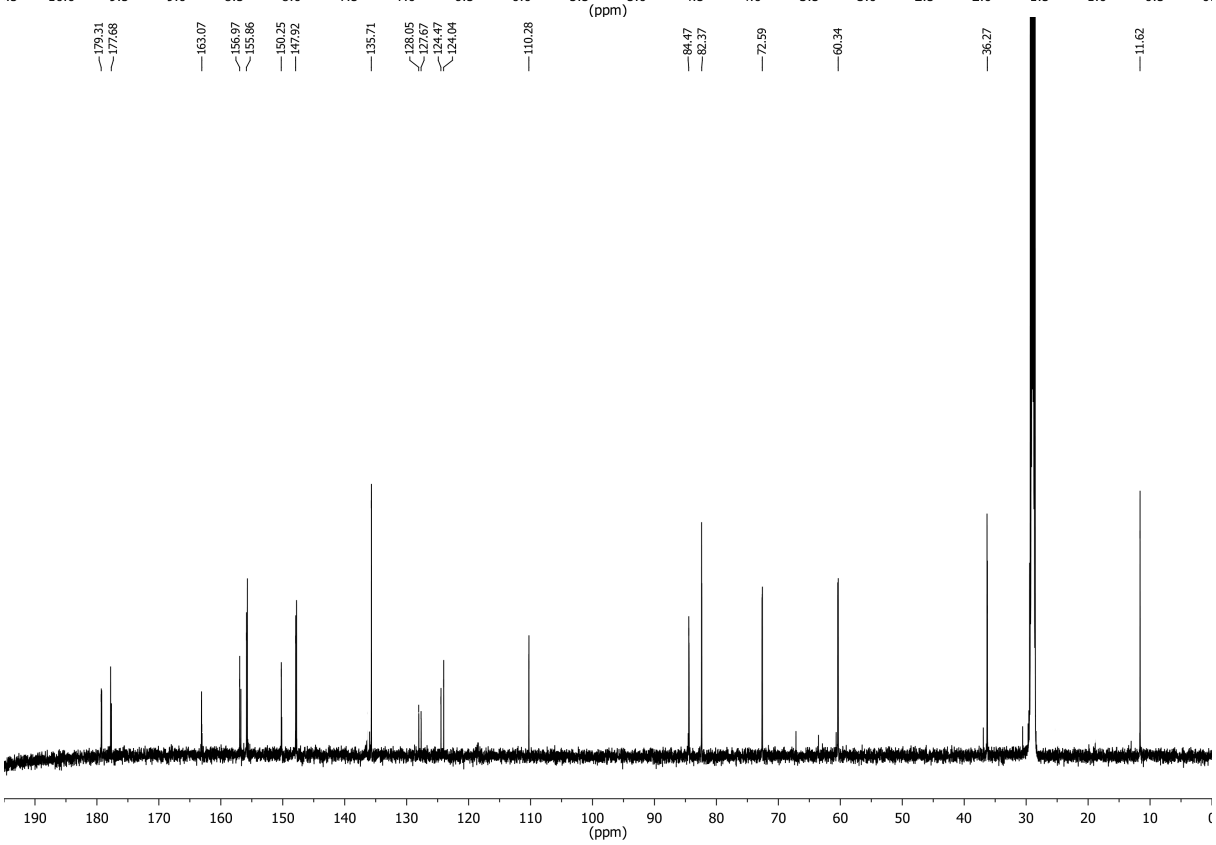


Figure S5. Spectra of 7-(3′-azido-3′-deoxythymidine)-6-chloro-5,8-isoquinolinedione **10**





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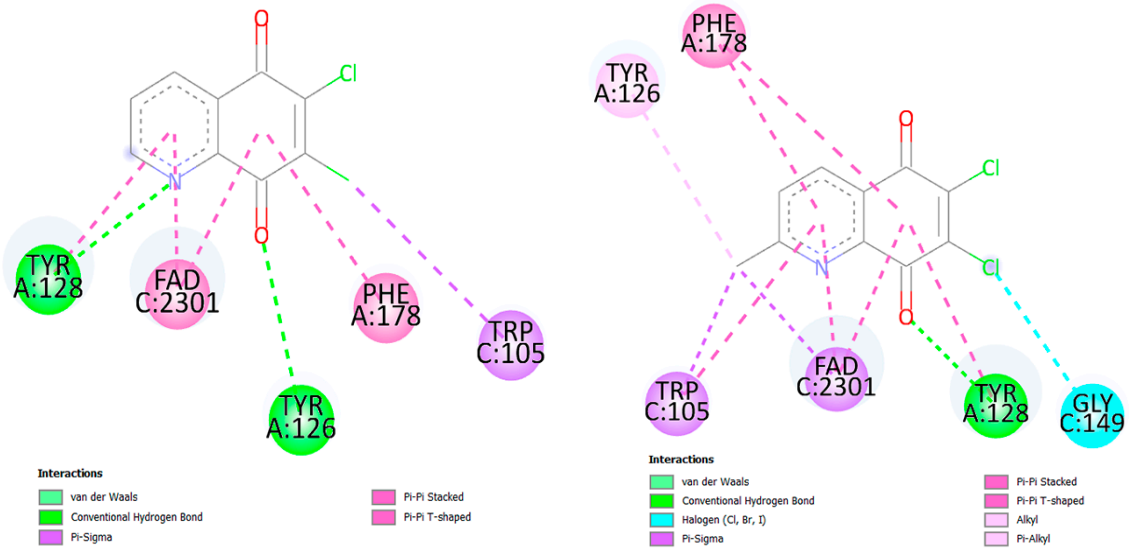

(**a**) (**b**)