Supplementary material

In Silico and In Vitro Studies of 4-Hydroxycoumarin-Based Heterocyclic Enamines as Potential Anti-Tumor Agents

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Table S1. IC_{50} values of synthesized compounds (3a-i) by potato disc tumor assay.

Sample	IC_{50} (mg/mL) value	Sample	IC_{50} (mg/mL) value
3a	5±0.5	3f	27.7±3
3b	37.1±4	3g	1.12±0.2
3c	2.12±0.3	3h	1.70±0.3
3d	22.7±3	3i	29.6±4
3e	2.33±0.2	Vinblastine (Standard)	7.5±0.6

(A)

(B)
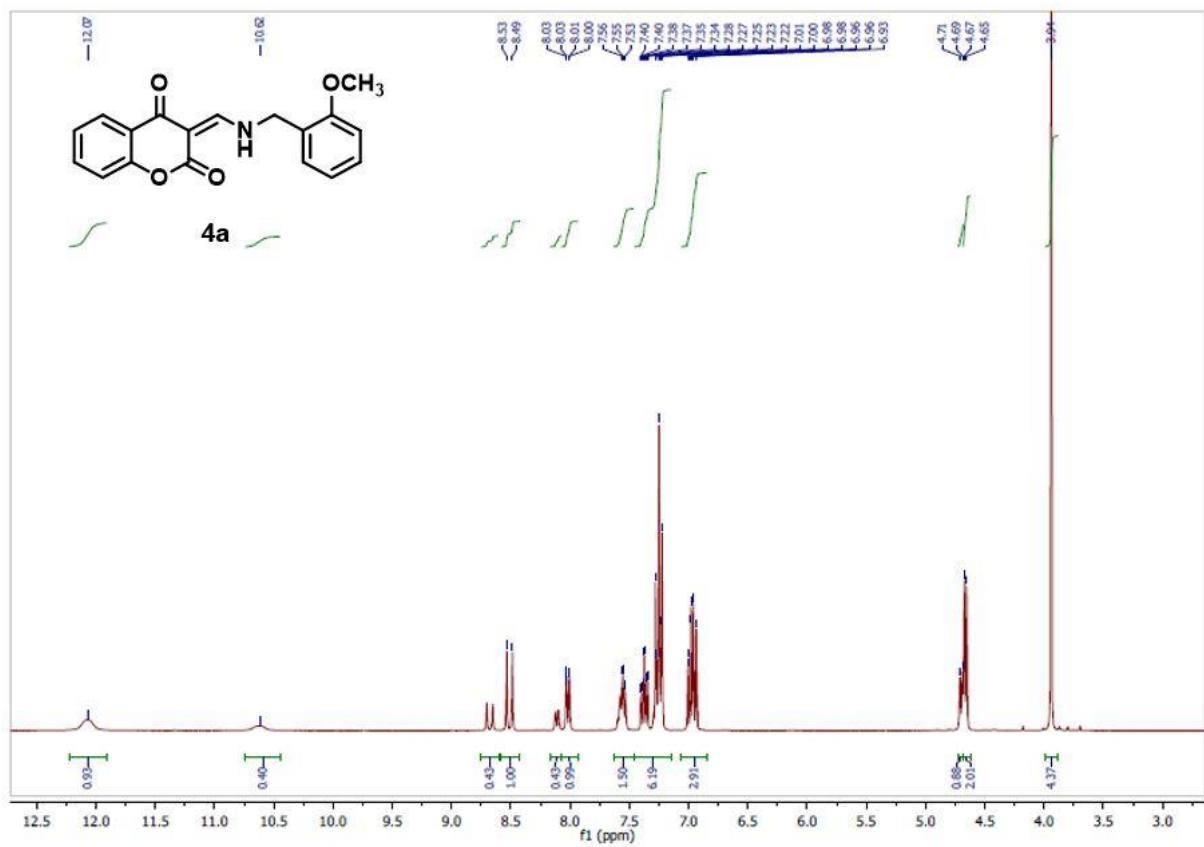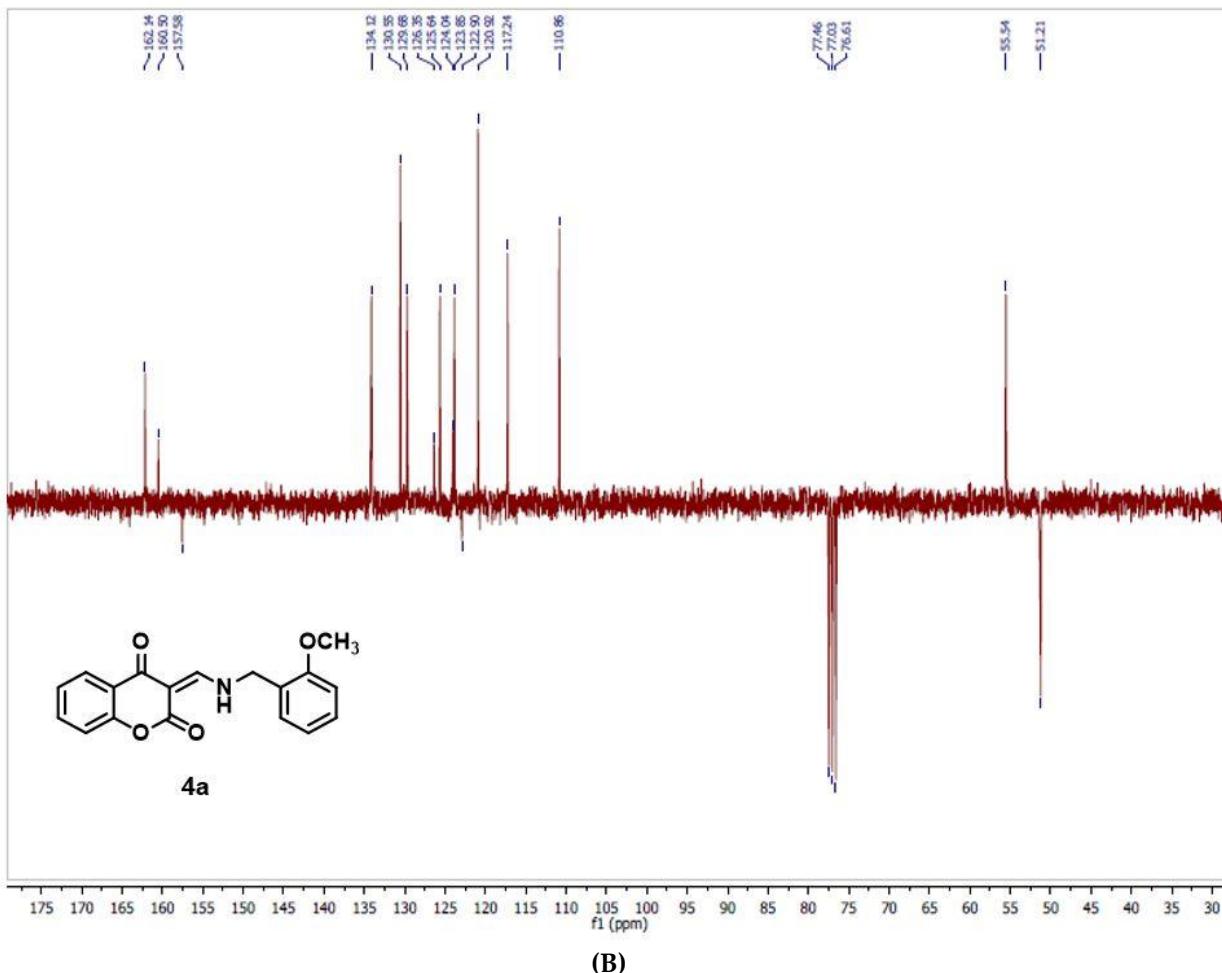
Figure S1. (**A**) ^{1}H-NMR spectrum of **4a.** (**B**) ^{13}C-NMR spectrum of **4a**.

(A)

(B)
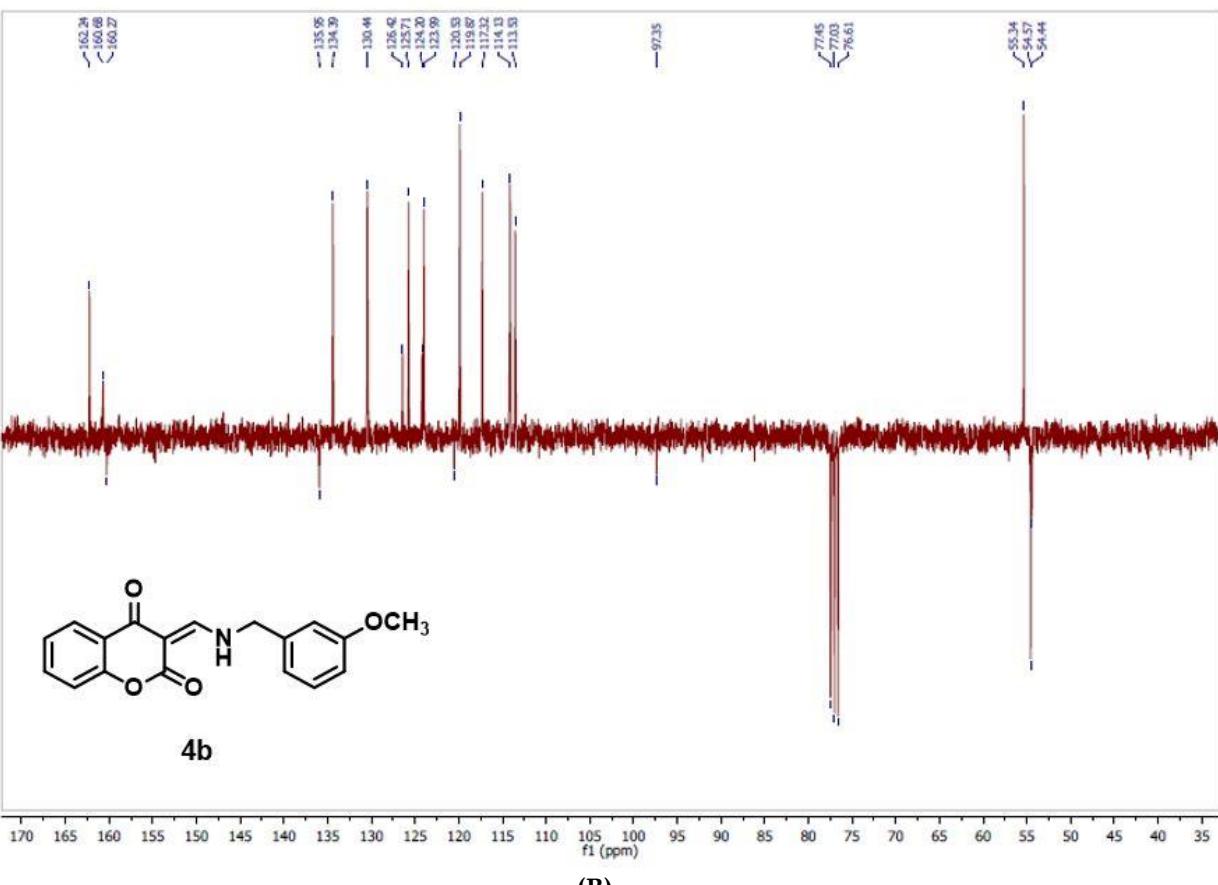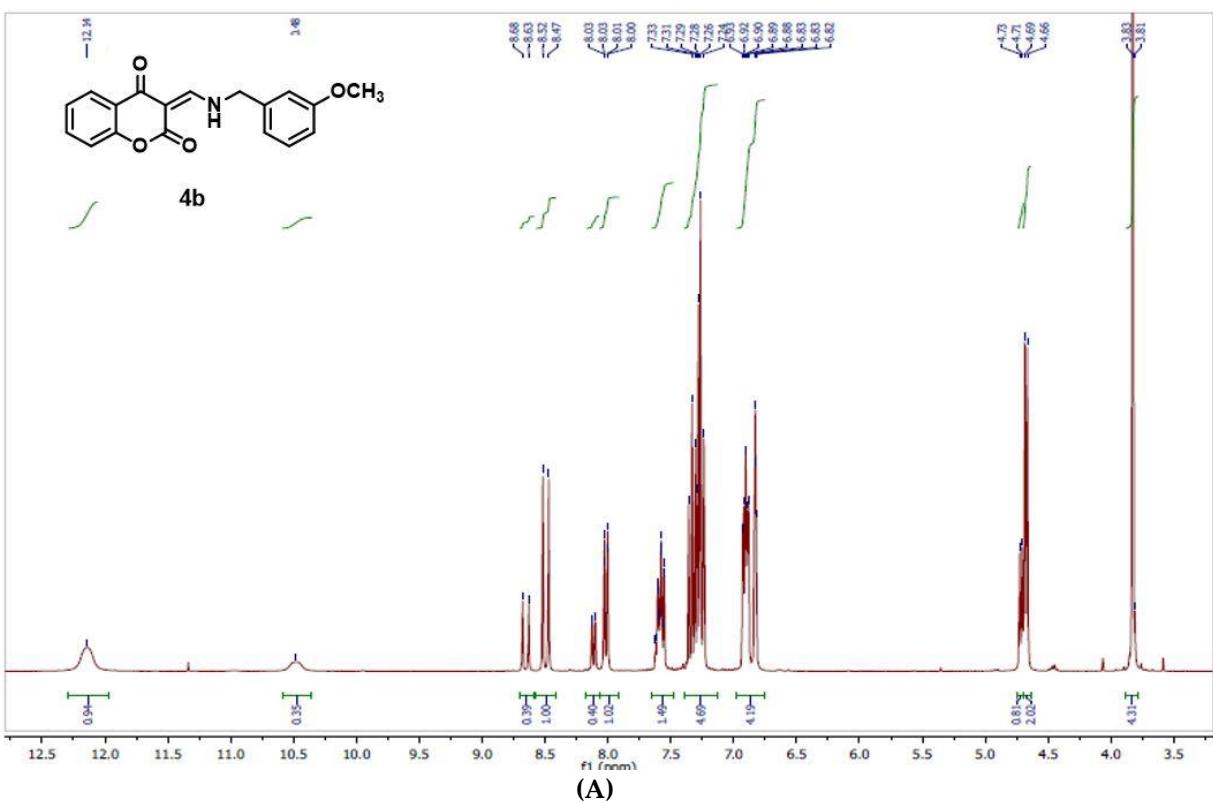
Figure S2. (**A**) ^{1}H-NMR spectrum of **4b.** (**B**) ^{13}C-NMR spectrum of **4b**.

(A)

(B)
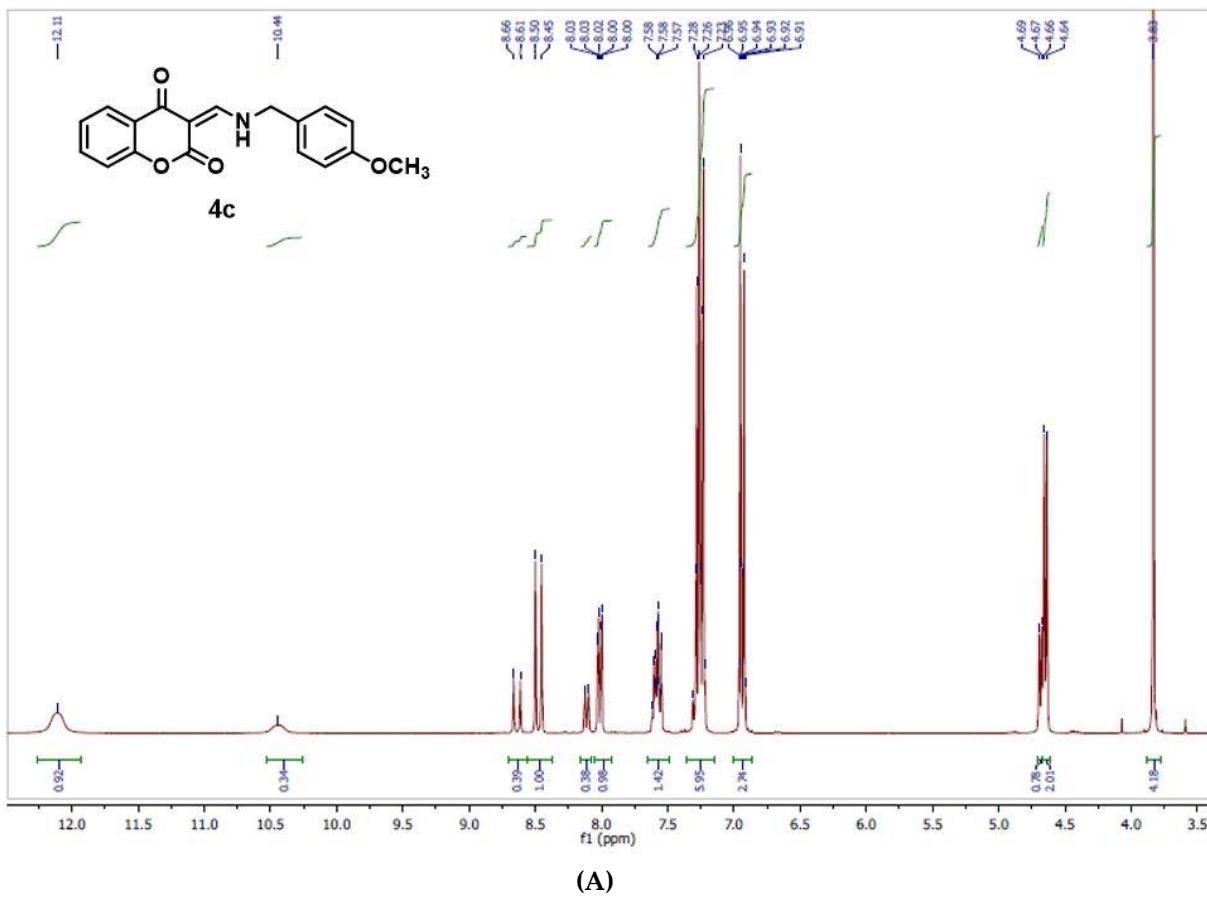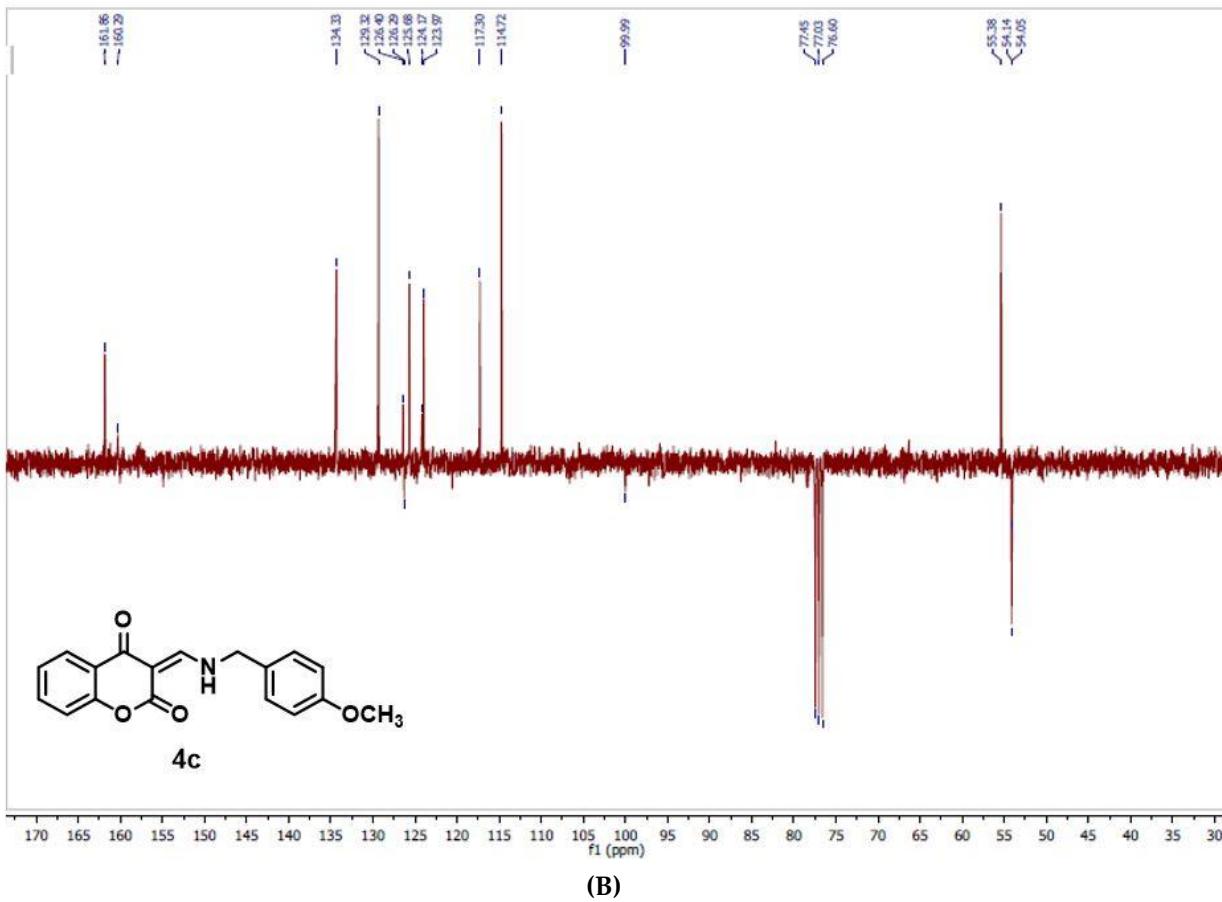
Figure S3. (**A**) ^{1}H-NMR spectrum of **4c**. (**B**) ^{13}C-NMR spectrum of **4c**.

(A)
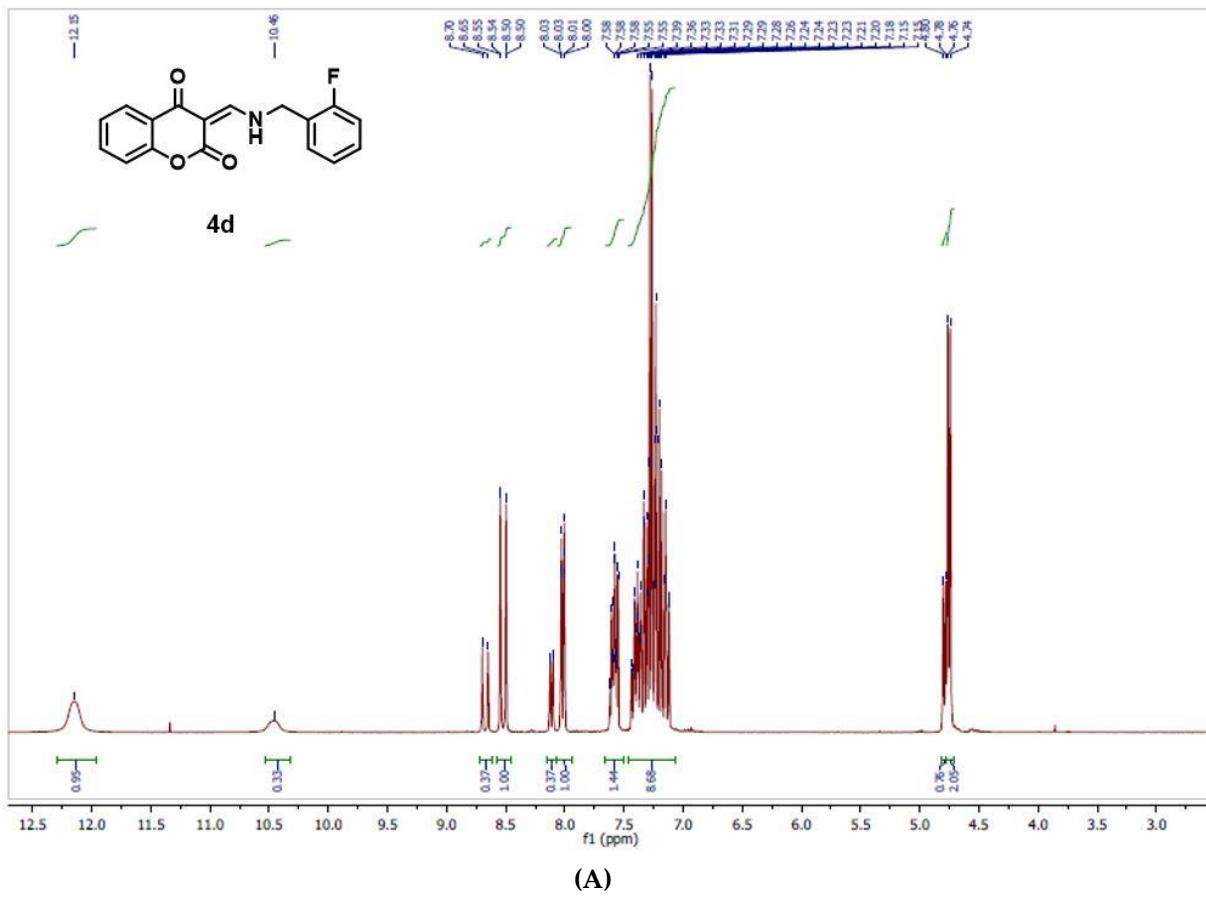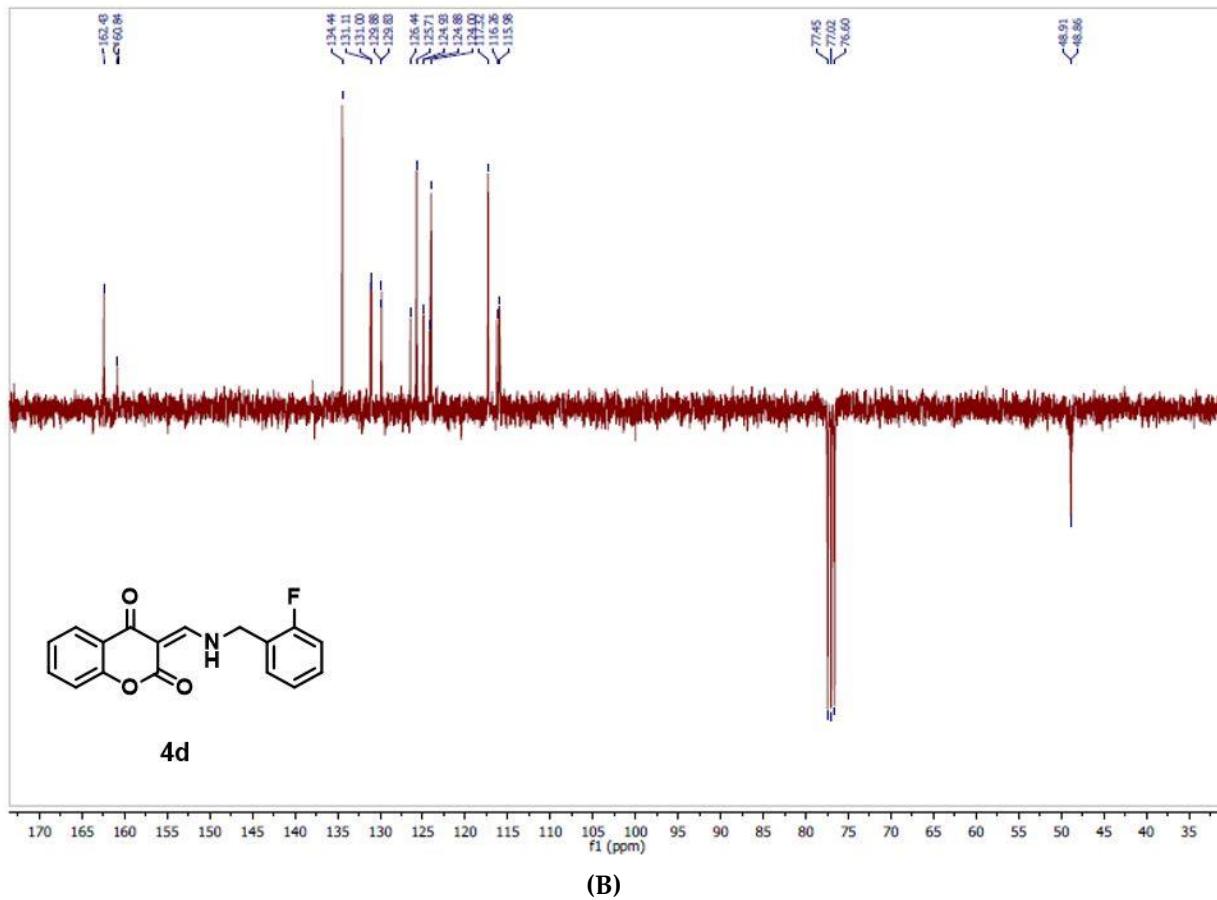
Figure S4. (**A**) ^{1}H-NMR spectrum of **4d.** (**B**) ^{13}C-NMR spectrum of **4d**.

(A)
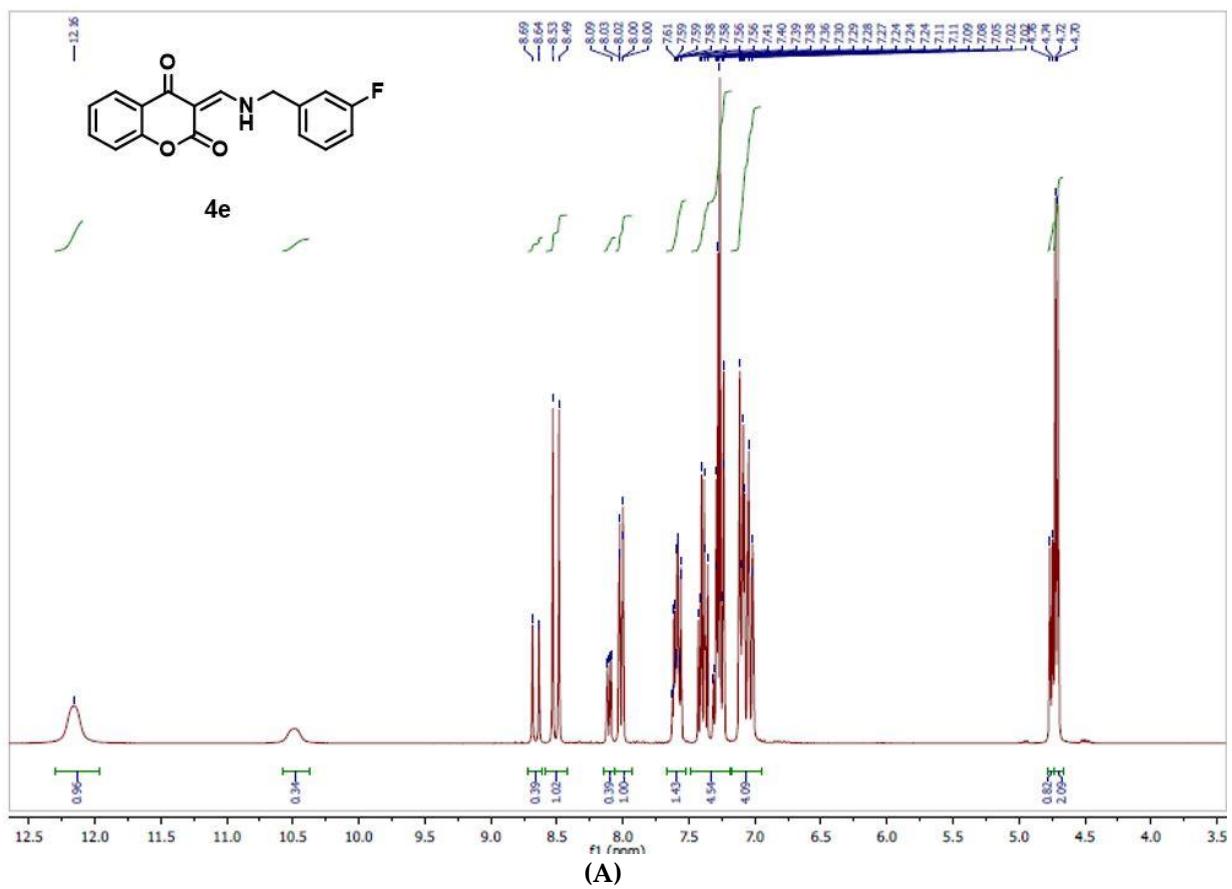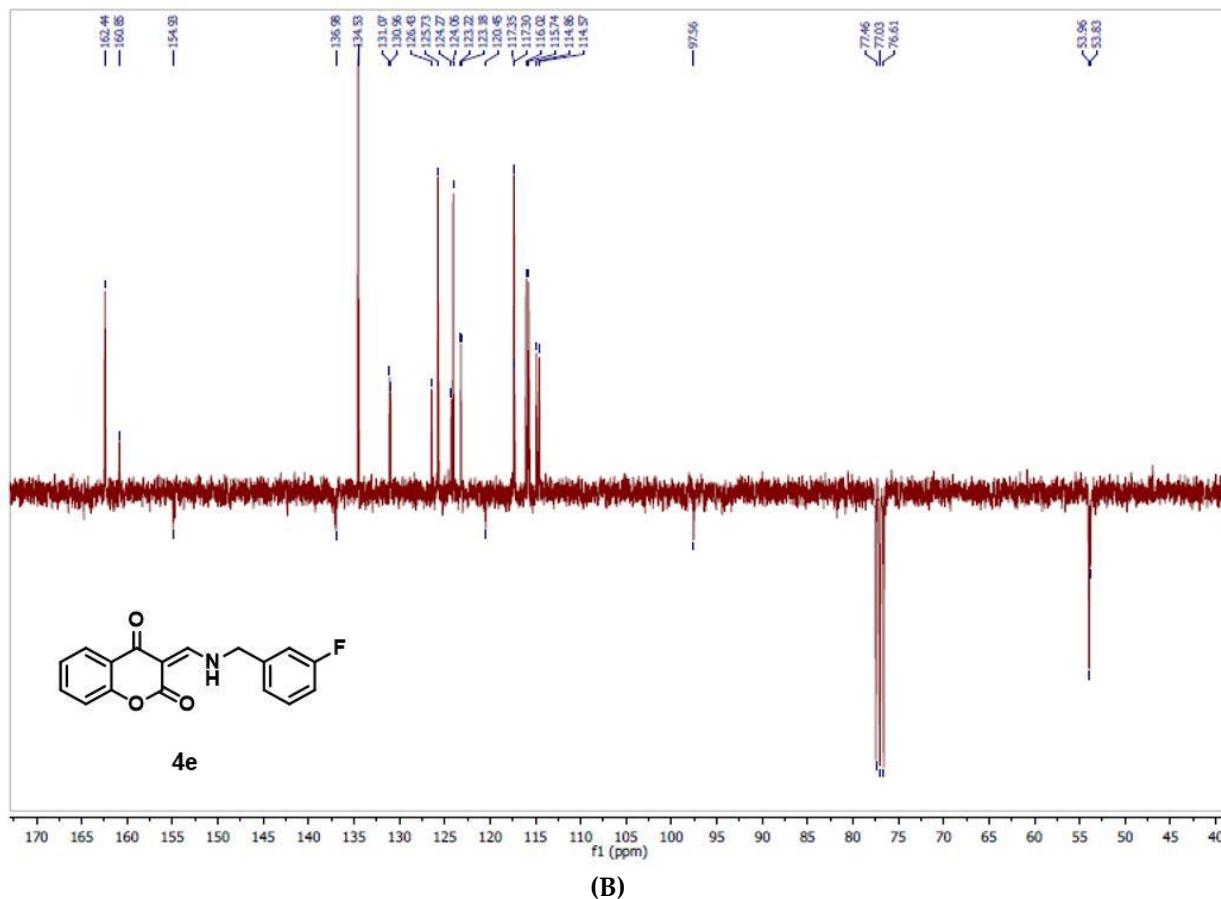
Figure S5. (**A**) ^{1}H-NMR spectrum of **4e.** (**B**) ^{13}C-NMR spectrum of **4e**.

(A)
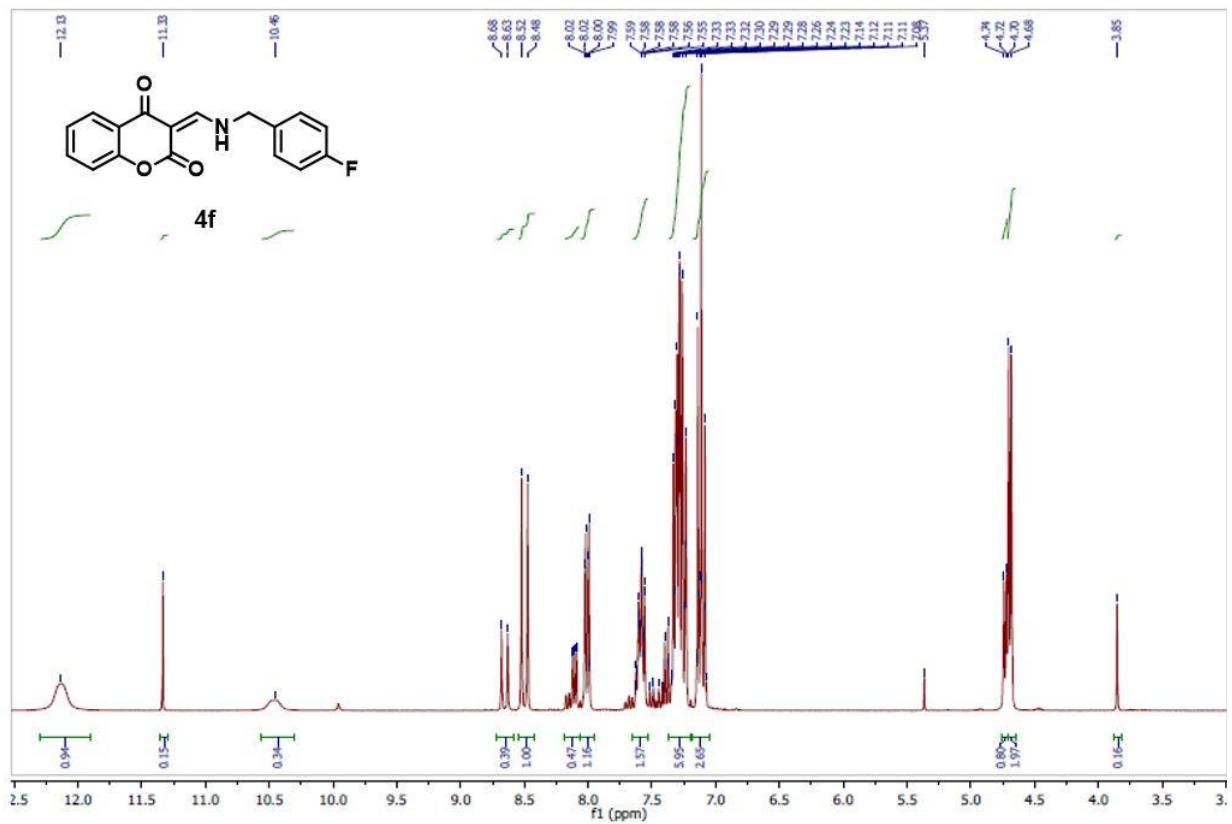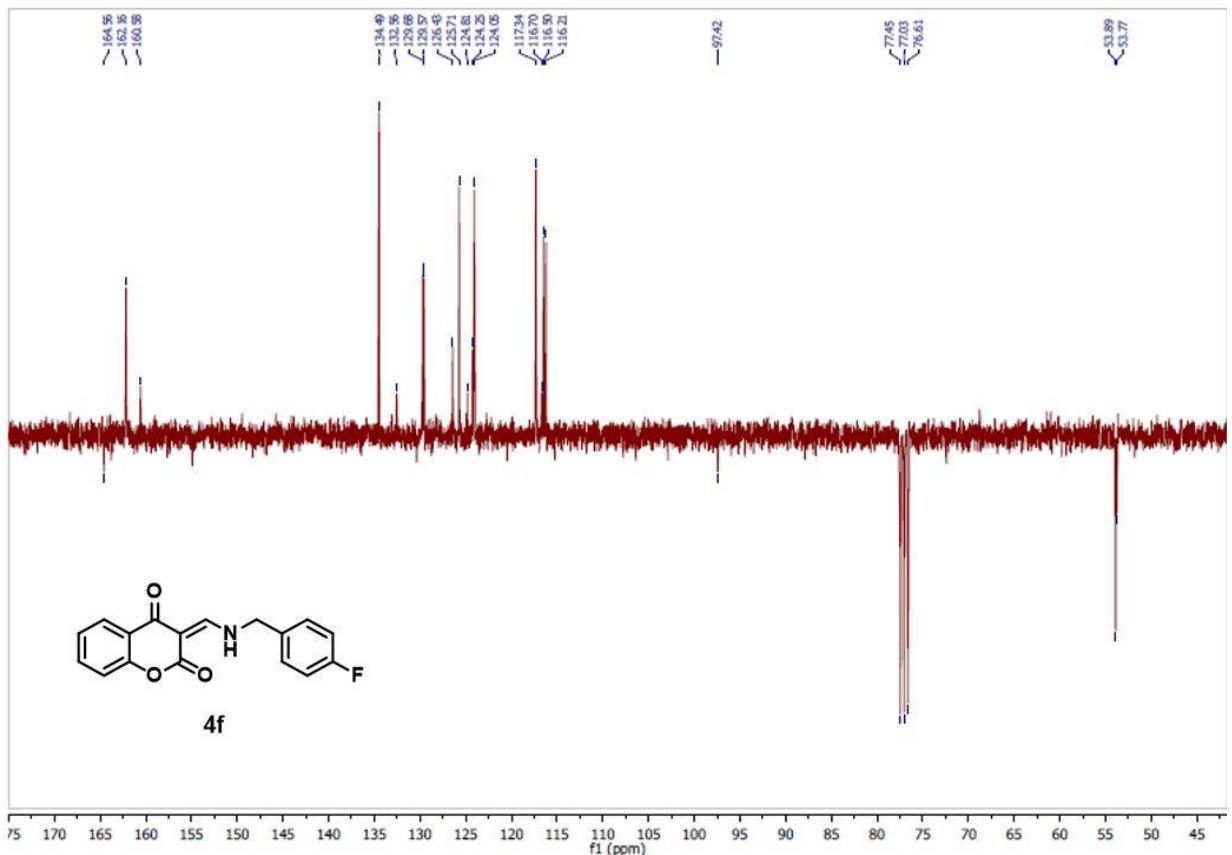
**Figure S6.** (A) ^{1}H-NMR spectrum of **4f**. (B) ^{13}C-NMR spectrum of **4f**.

(A)
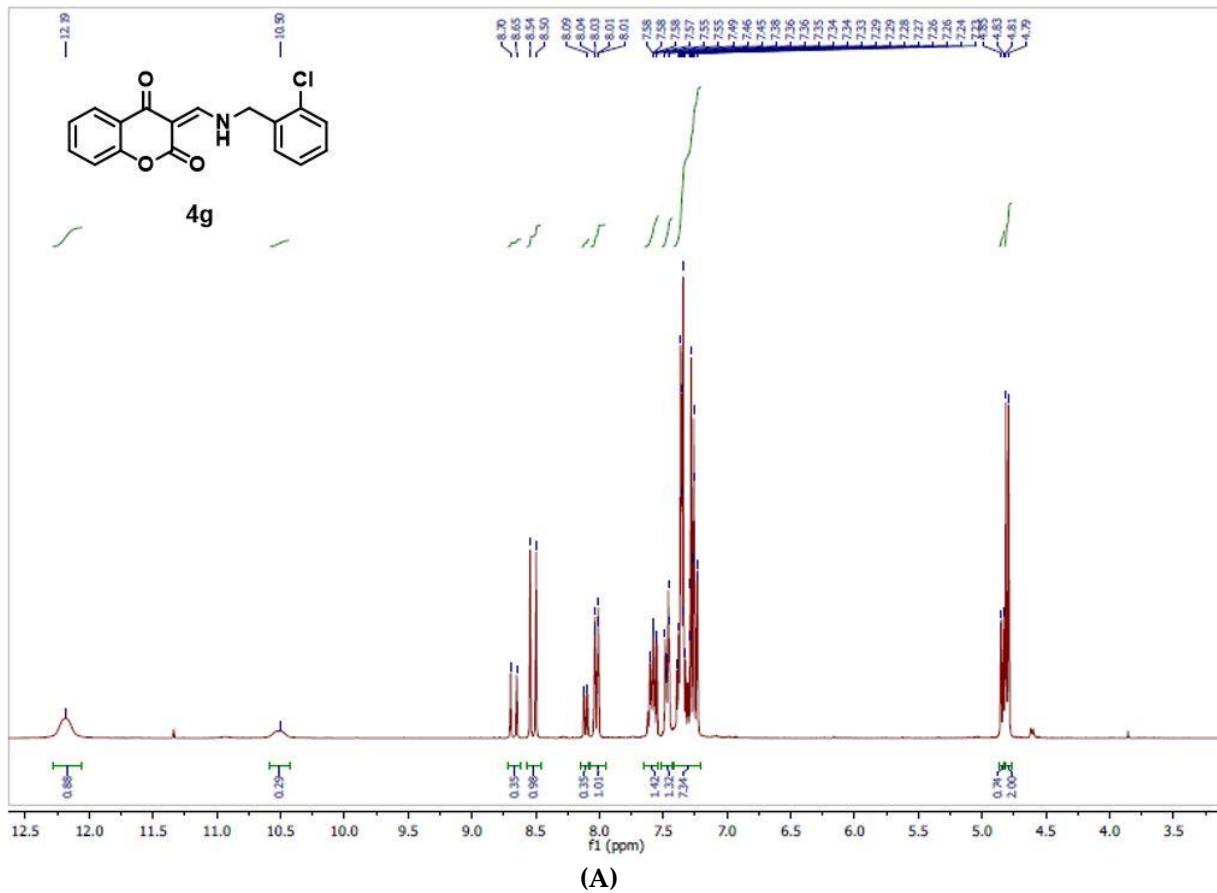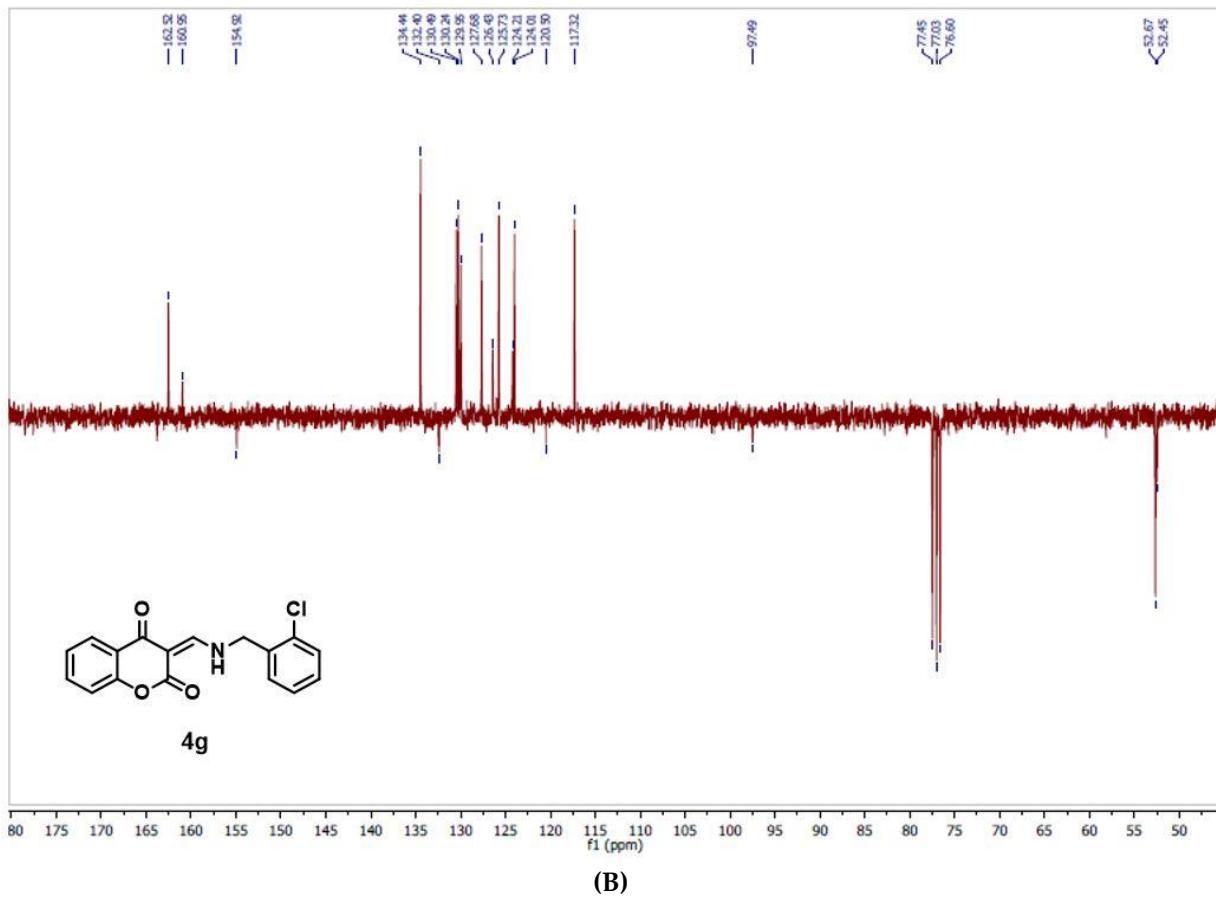
**Figure S7.** (**A**) ^{1}H-NMR spectrum of **4g**. (**B**) ^{13}C-NMR spectrum of **4g**.

(A)

4h

(B)
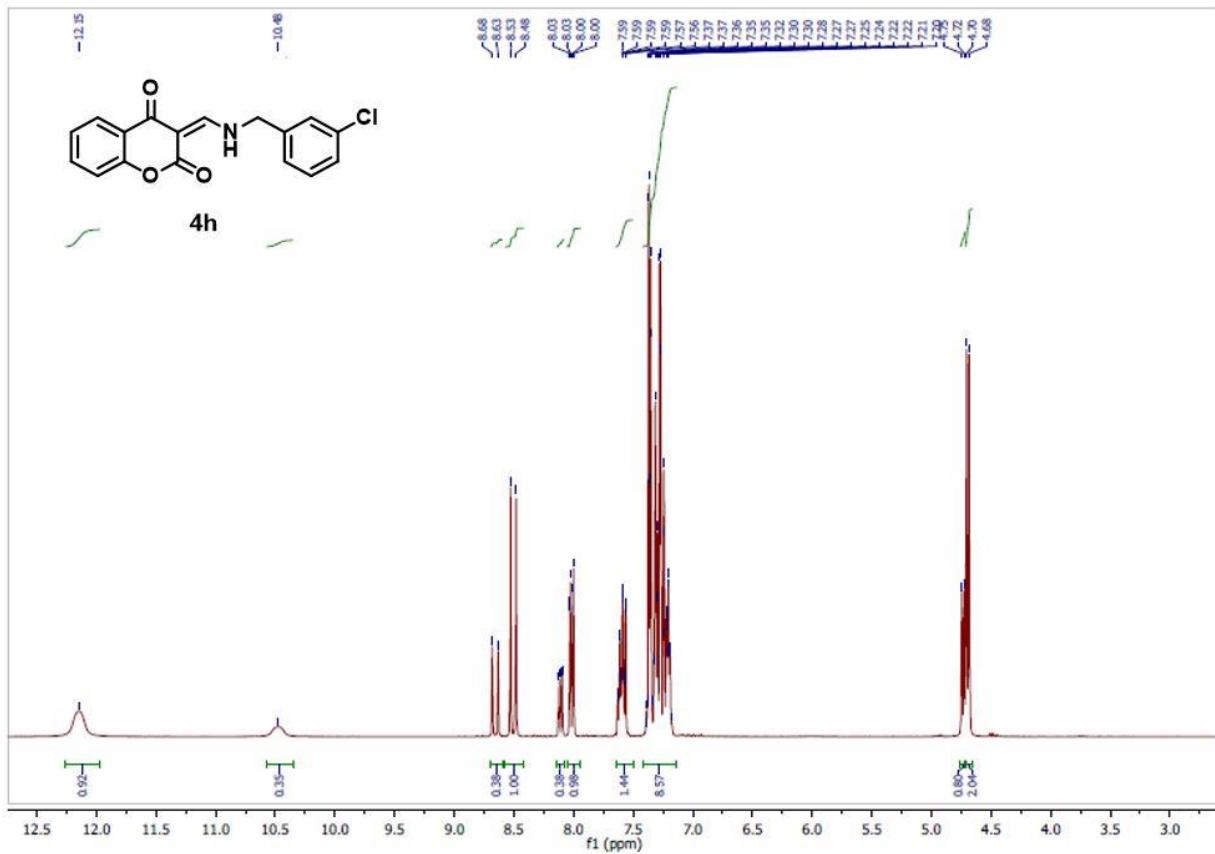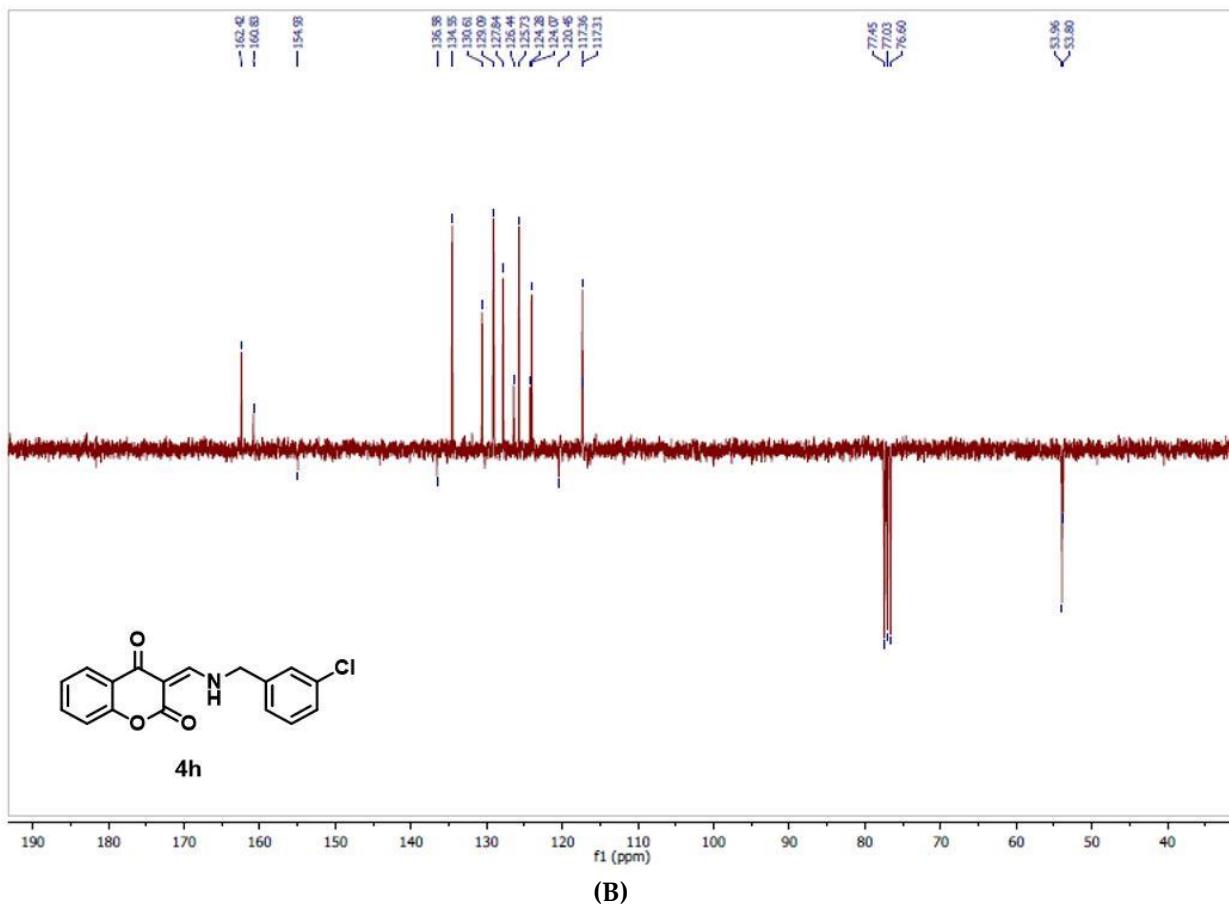
Figure S8. (**A**) ^{1}H-NMR spectrum of **4h**. (**B**) ^{13}C-NMR spectrum of **4h**.

(A)

(B)
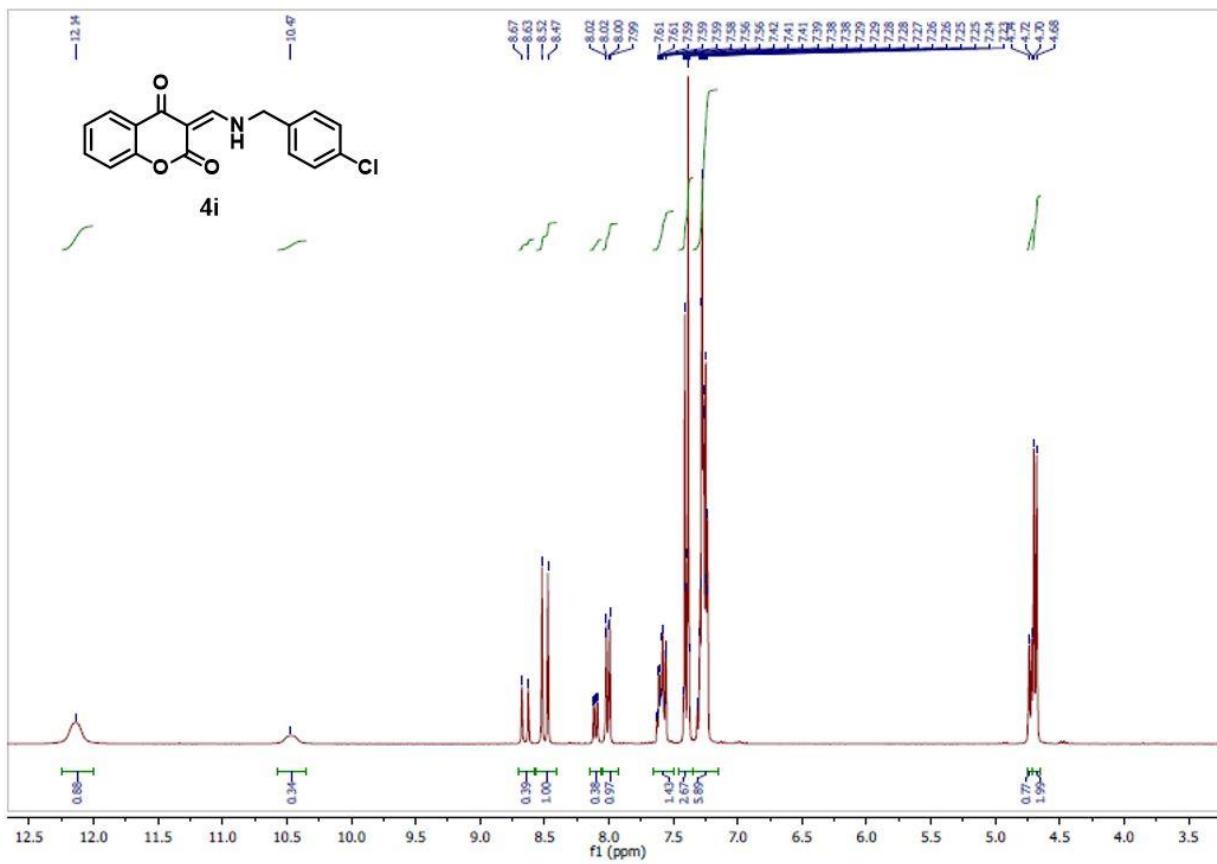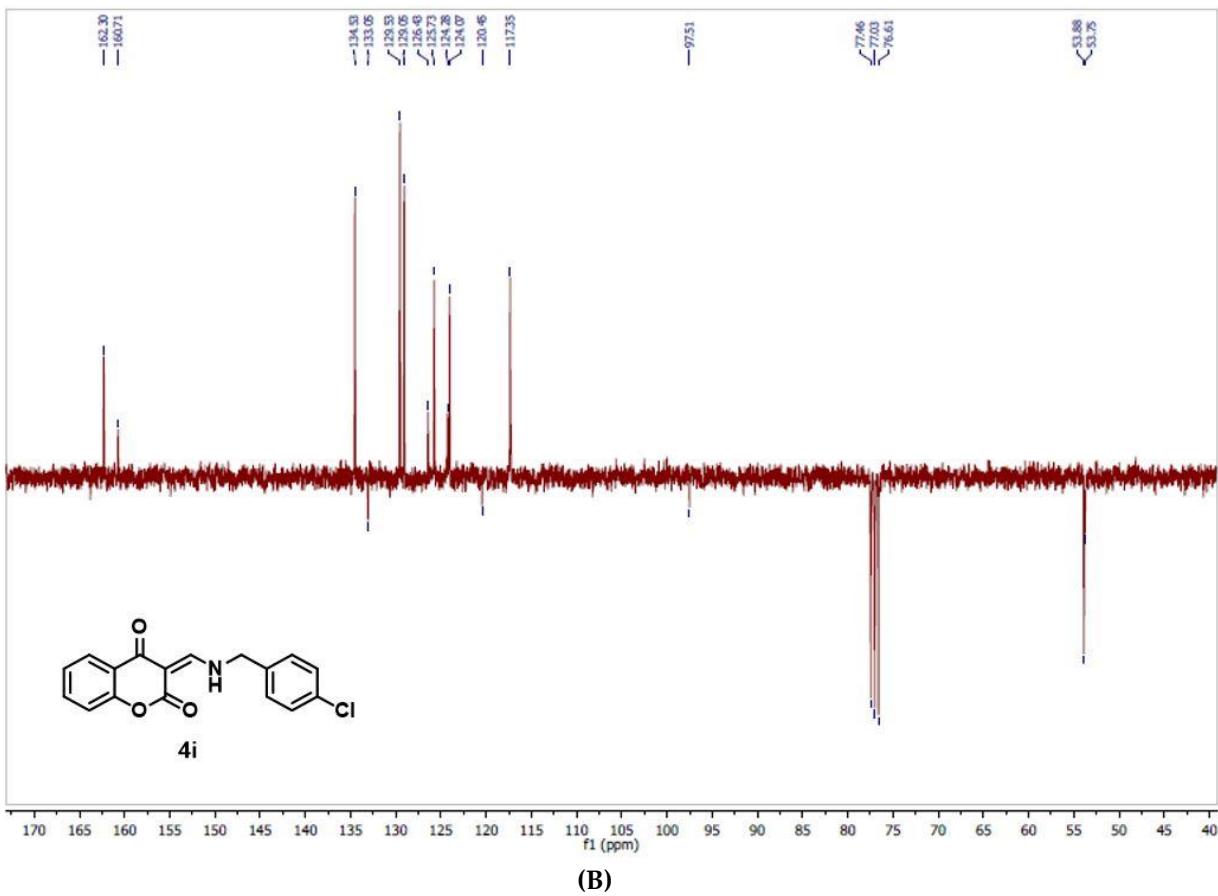
Figure S9. (**A**) ^{1}H-NMR spectrum of **4i**. (**B**) ^{13}C-NMR spectrum of **4i**.


(4a)

(4b)


(4c)

(4d)

(4e)

(4f)

(4g)

(4h) **Vinblastine**


(4i) **Native ligand (5XG) of CDK-8**
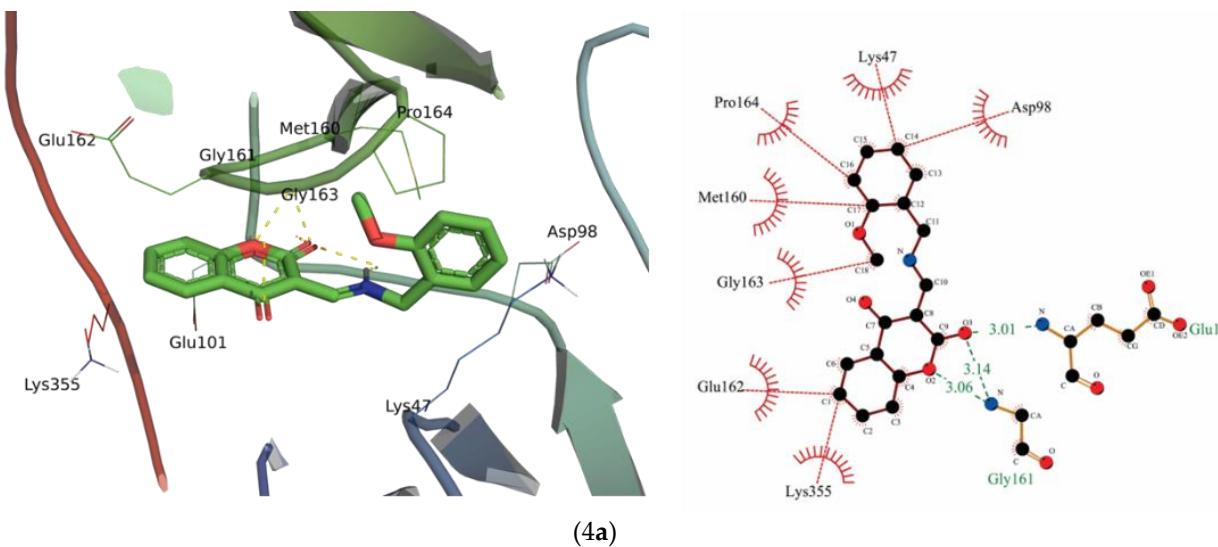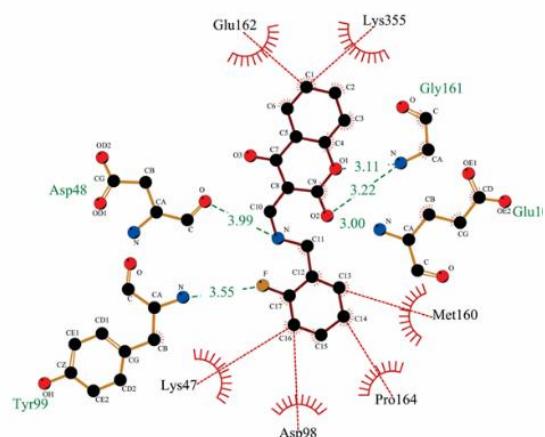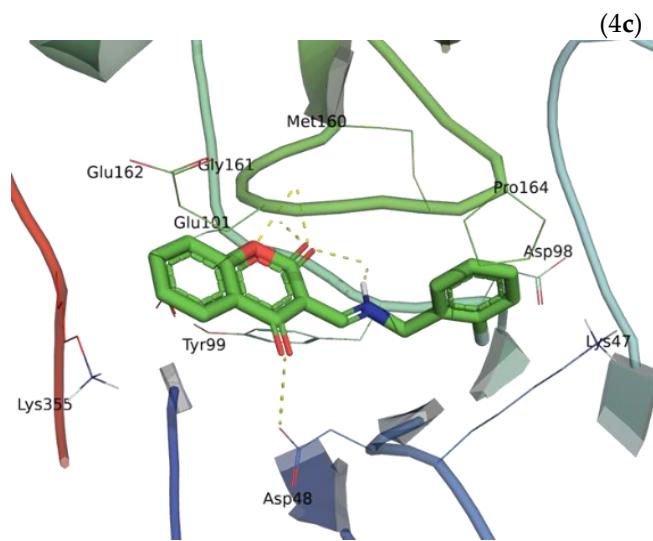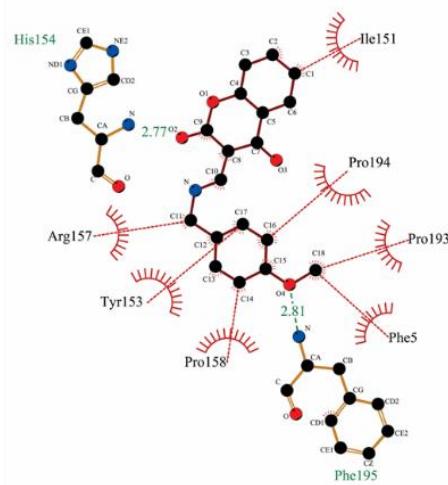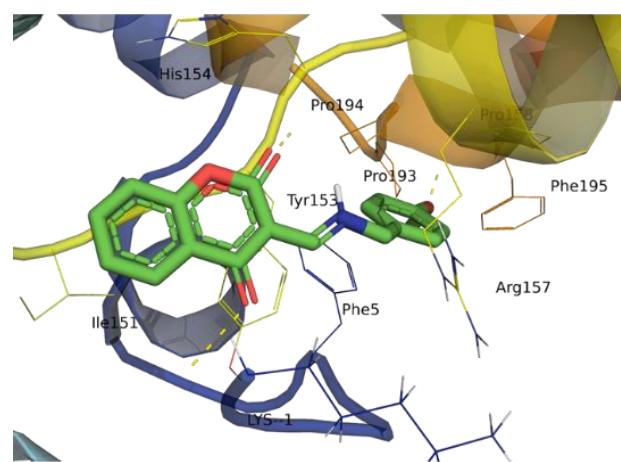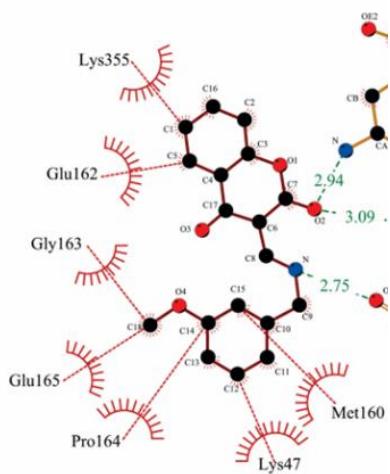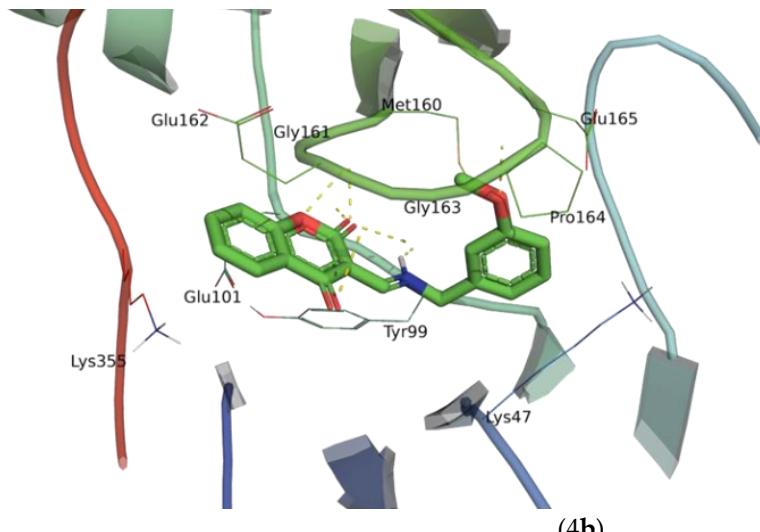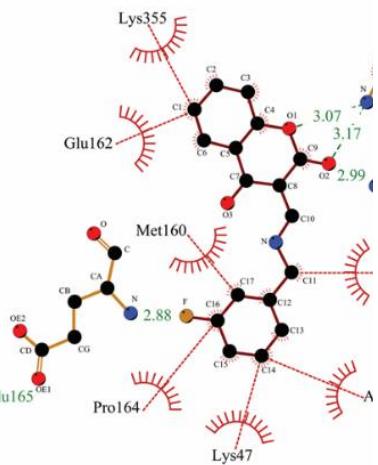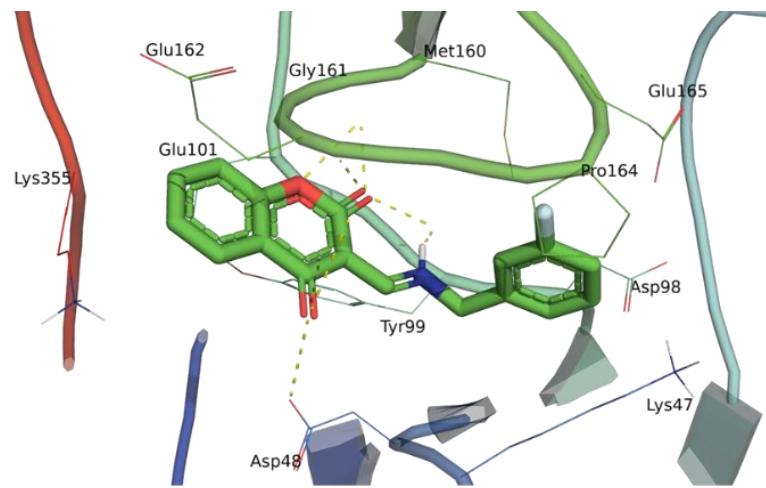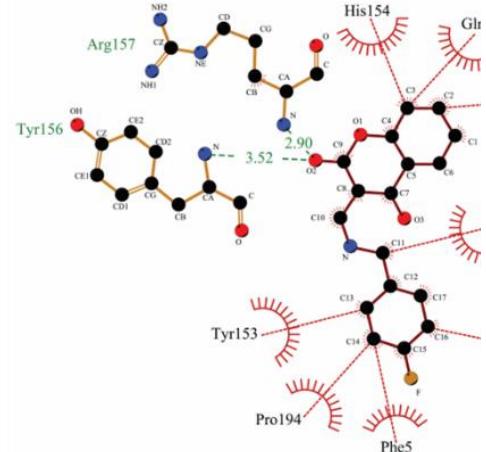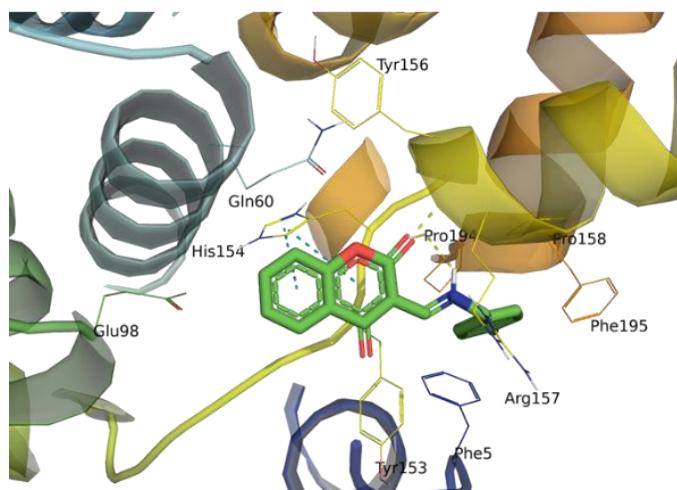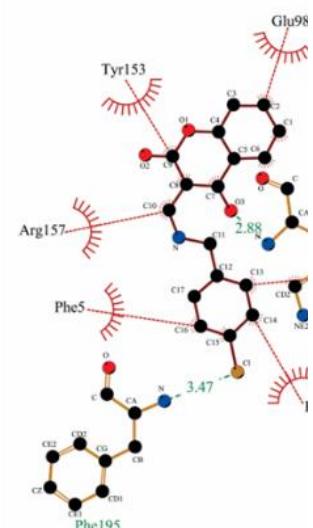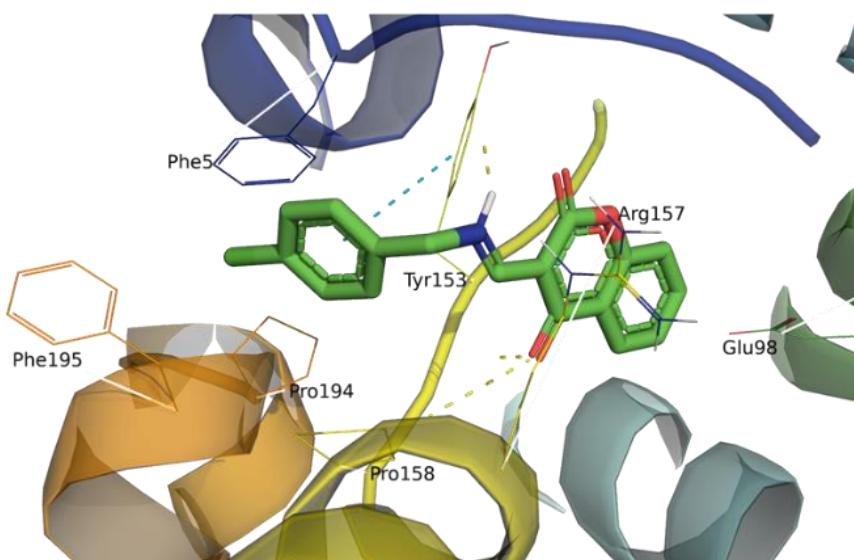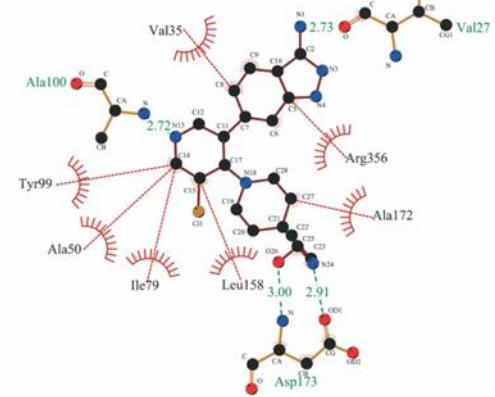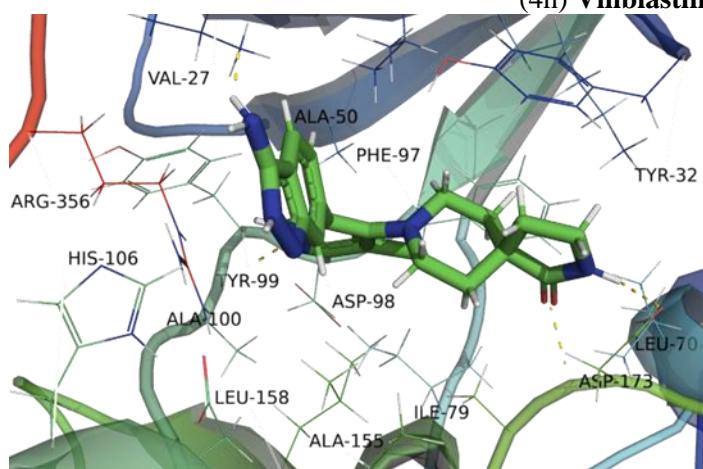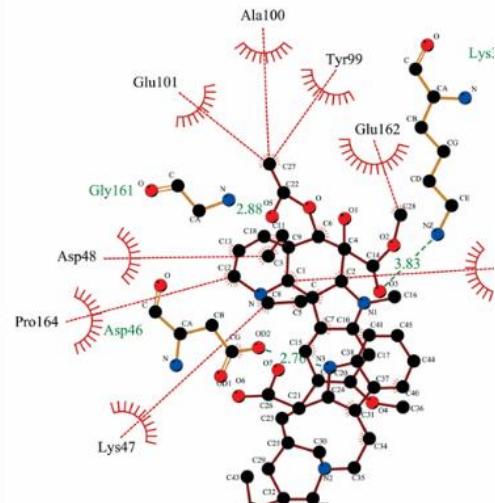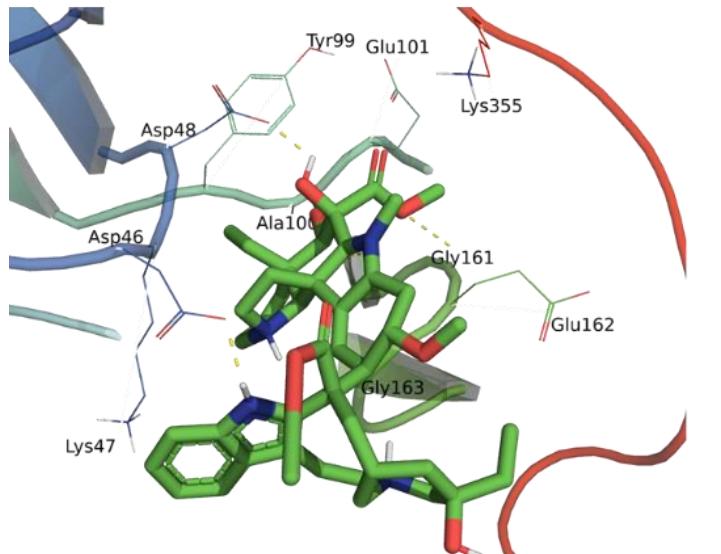
Figure S10. Docking Simulations of Compounds (4a-i, Vinblastine and native ligand) with CDK-8 protein.