

## Supplementary Information

# Hydroxyurea, thiourea, and urea derivatives of coumarins: synthesis, characterization, molecular docking, DFT calculations, pharmacokinetics and anticancer potency

Anand Kumar Yadav<sup>a</sup>, Manoj Silwal<sup>b</sup>, Neeta Singh<sup>a</sup>, Achyut Adhikari<sup>a</sup> & Paras Nath Yadav<sup>\*a</sup>,

<sup>a</sup> Central Department of Chemistry, Tribhuvan University, Kathmandu, Nepal

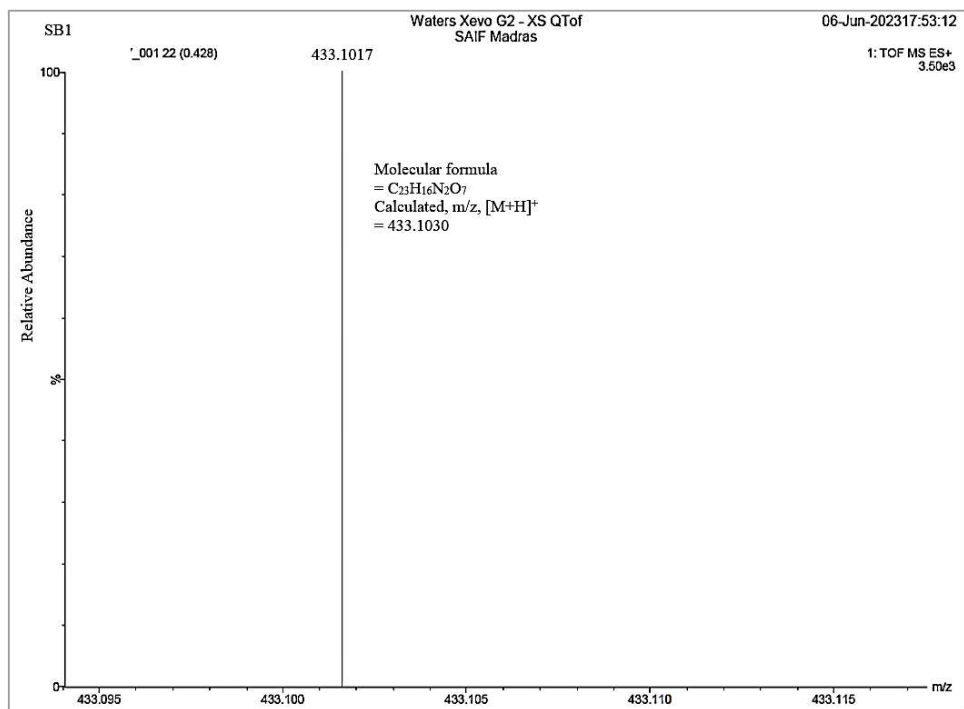
<sup>b</sup> New Horizon English Boarding Secondary School, Rupandehi, Butwal, Nepal

E-mail: pnyadav219@gmail.com, paras.yadav@tu.edu.np

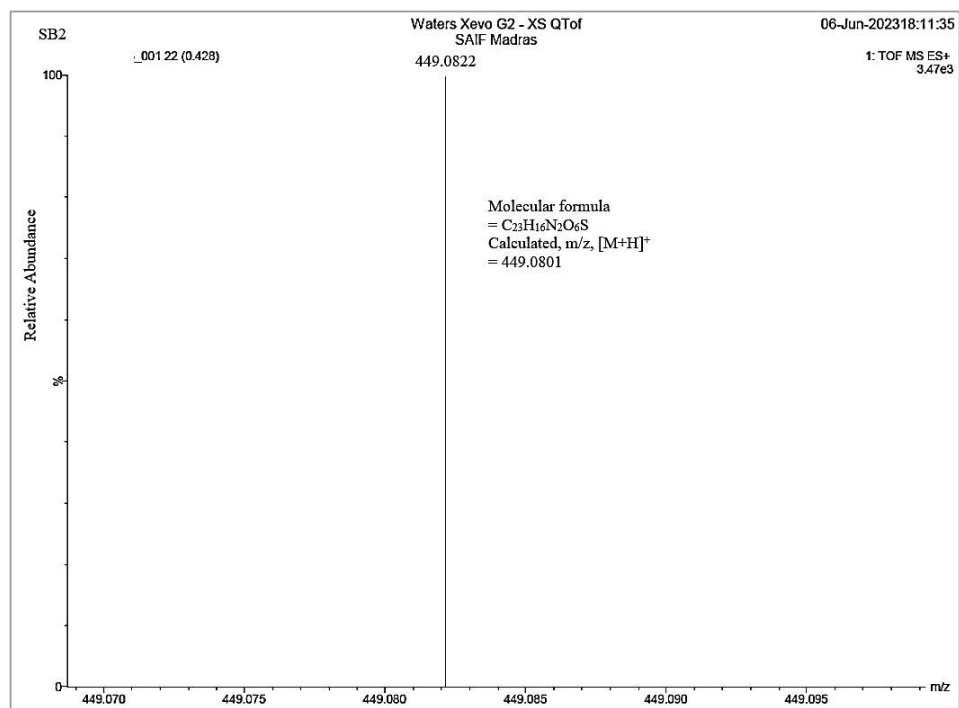
Received 15 December 2024; accepted (revised) 2 June 2025

### Table of contents

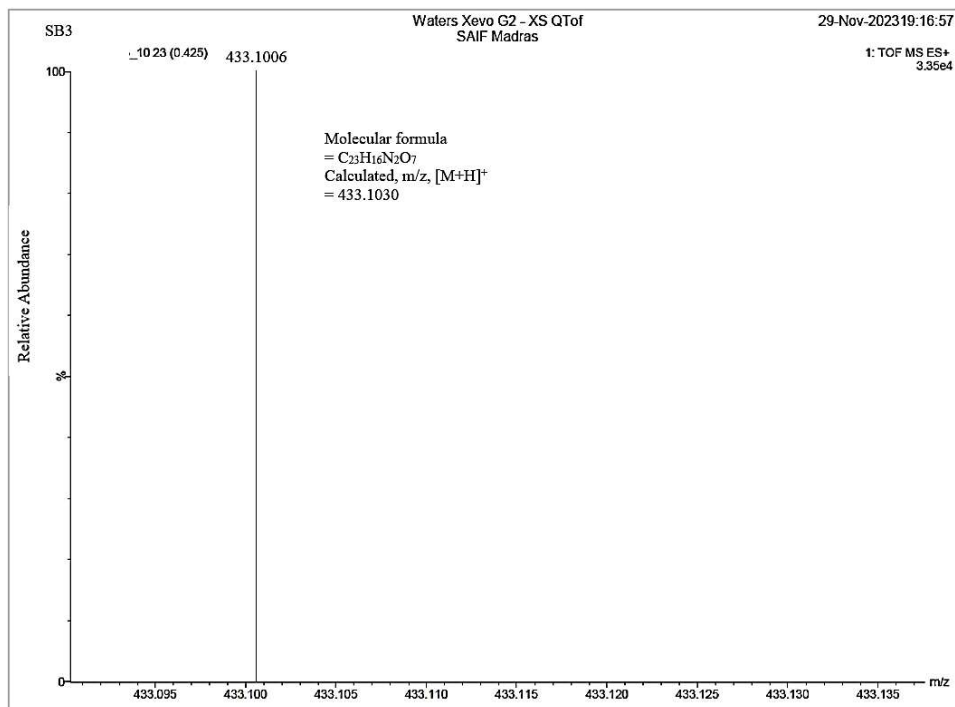
S. No.	Particulars	Pages
1	Table of contents	1
1	HRMS-ESI spectra of the compounds, S1-S7	2-5
2	<sup>1</sup> H NMR spectra of the compounds, S8-S14	5-8
3	C <sup>13</sup> NMR spectra of the compounds, S15-S21	9-12
4	FT-IR spectra of the compounds, S22-S28	12-15
5	UV-Vis. spectra of the compounds, S29-S35	16-17
6	2D and 3D plots, molecular docking, S36-S41	17-19



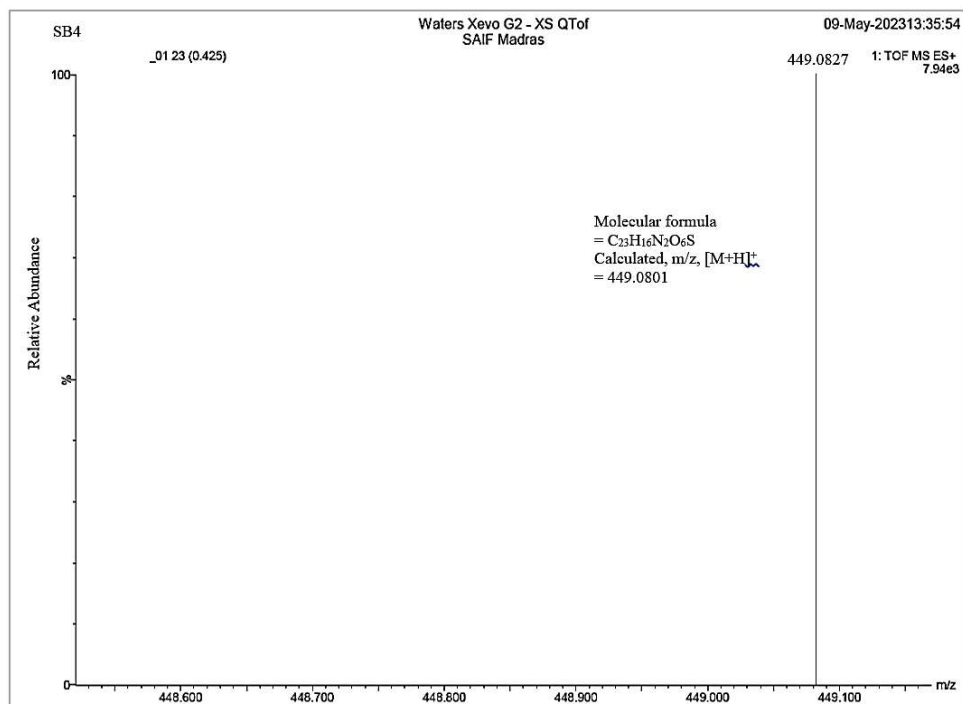
**Figure S1.** Esi-HRMS of 1,3-bis[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB1)



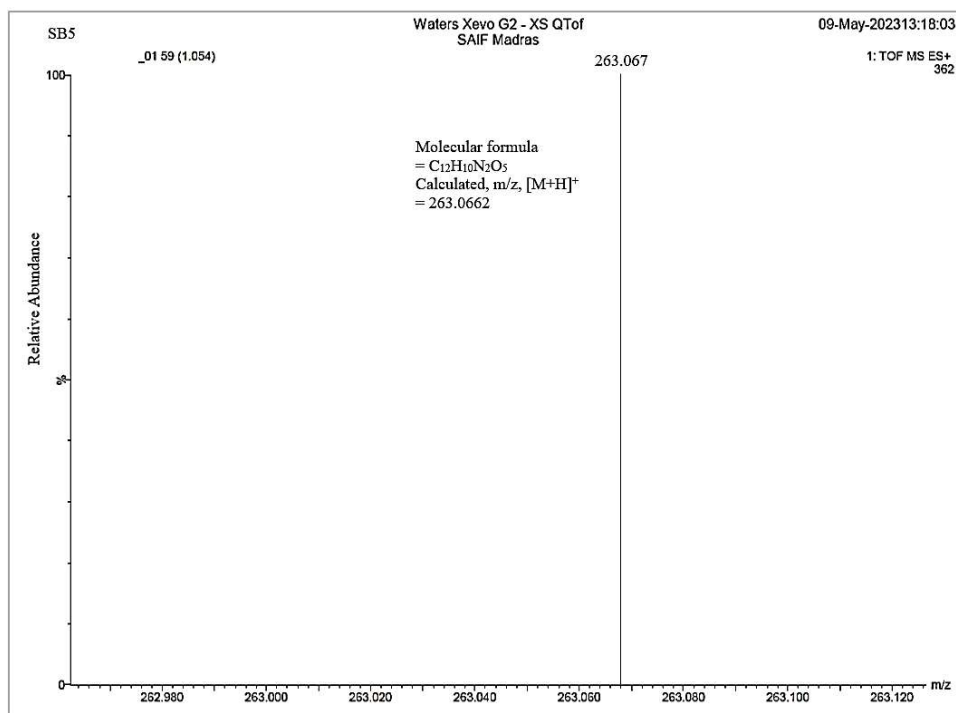
**Figure S2.** Esi-HRMS of 1,3-bis[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]thiourea (SB2)



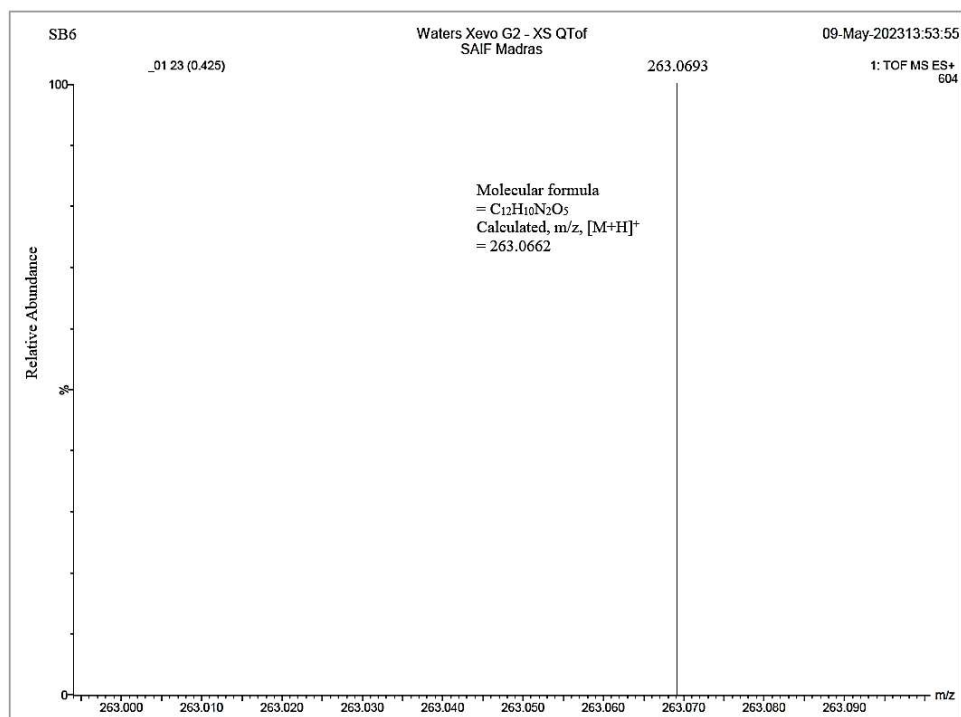
**Figure S3.** Esi-HRMS of 1,3-bis[(1*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB3)



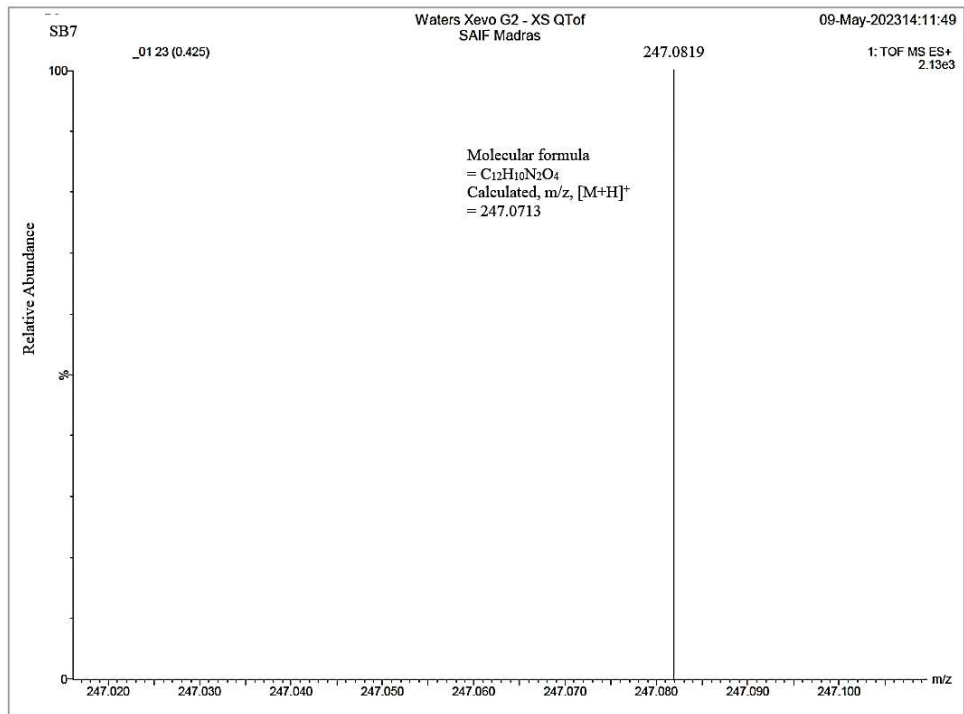
**Figure S4.** Esi-HRMS of 1,3-bis[(1*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]thiourea (SB4)



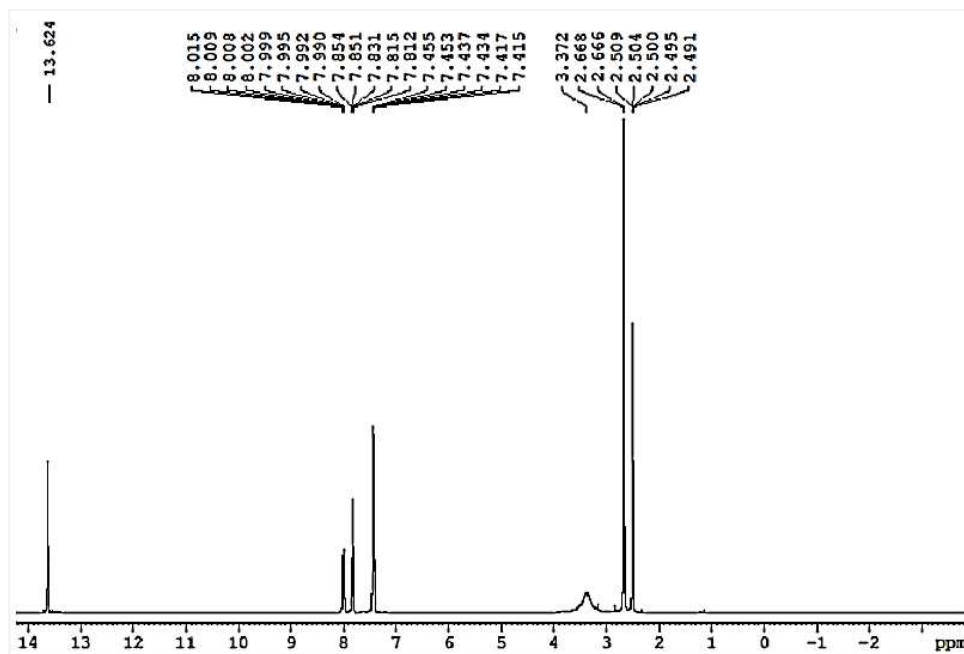
**Figure S5.** Esi-HRMS of 1-hydroxy-3-[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB5)



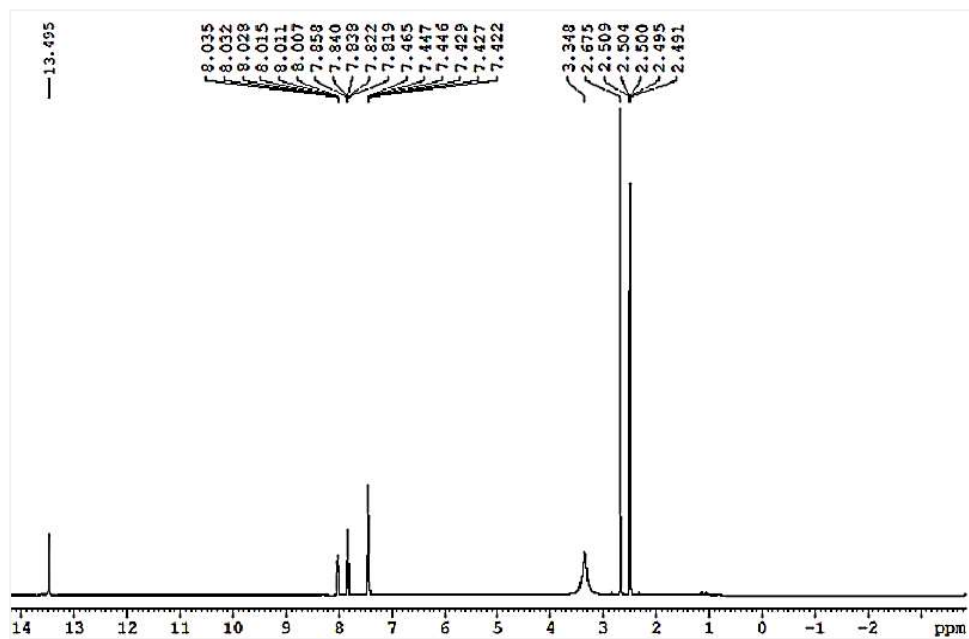
**Figure S6.** Esi-HRMS of 1-hydroxy-3-[(1*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB6)



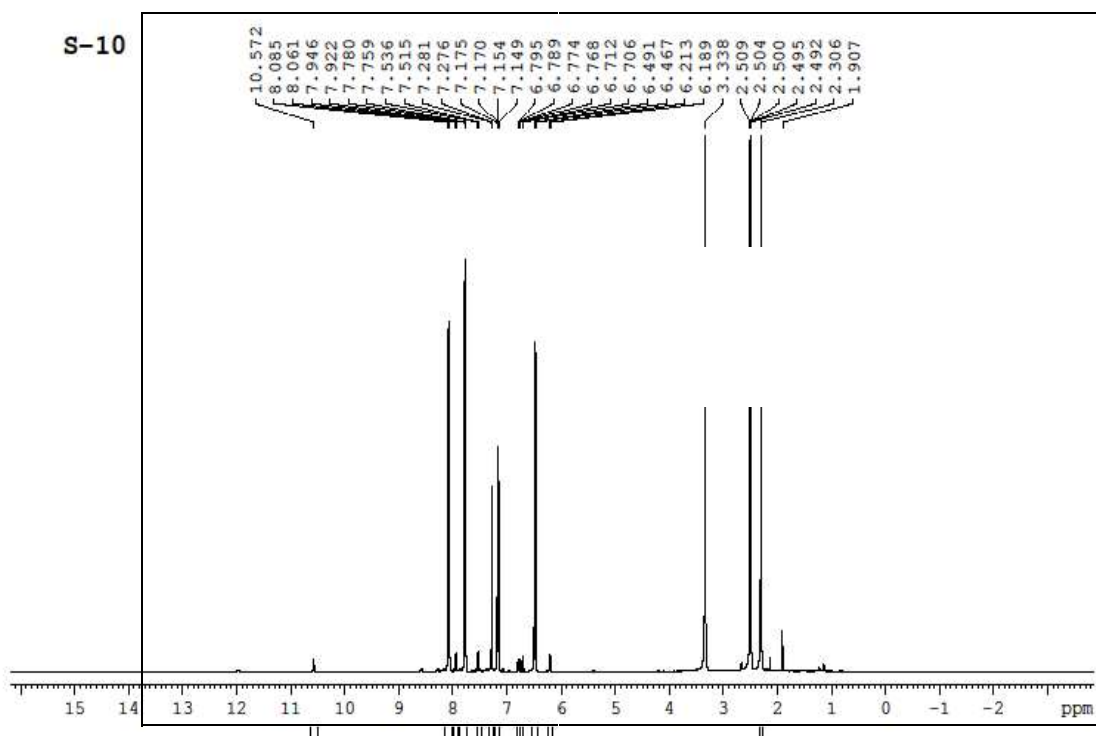
**Figure S7.** Esi-HRMS of 1-hydroxy-3-[(1*E*)-1-(2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB7)



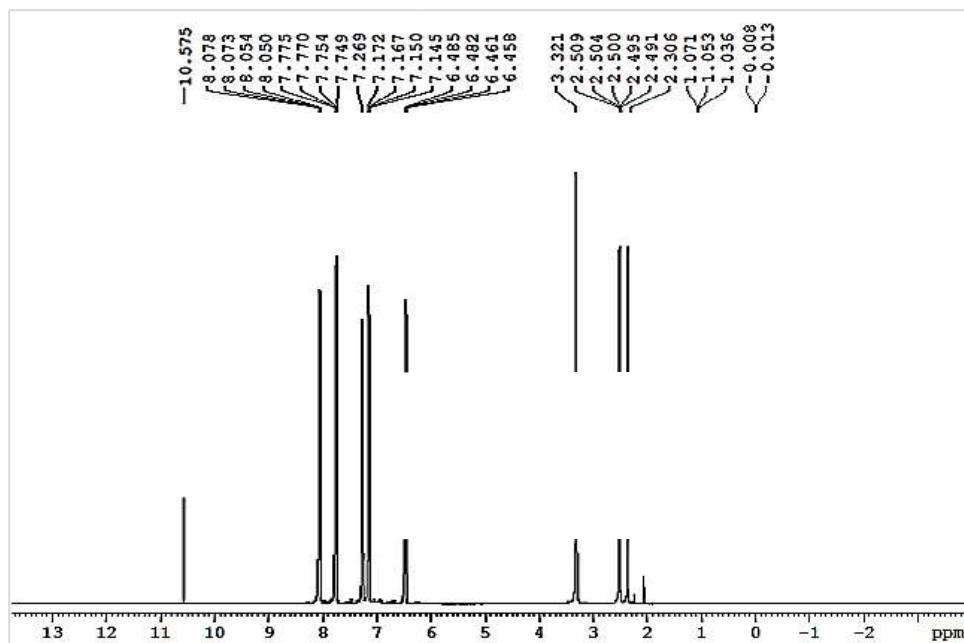
**Figure S8.** <sup>1</sup>H NMR of 1,3-bis[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB1)



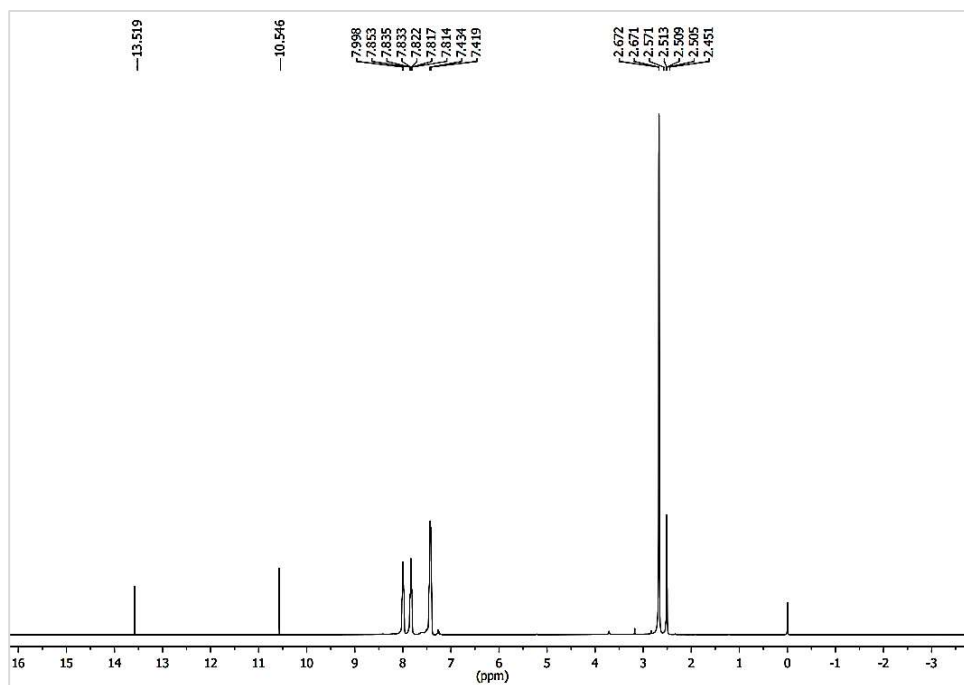
**Figure S9.**  $^1\text{H}$  NMR of 1,3-bis[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]thiourea (SB2)



**Figure S10.**  $^1\text{H}$  NMR of 1,3-bis[(1*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB3)

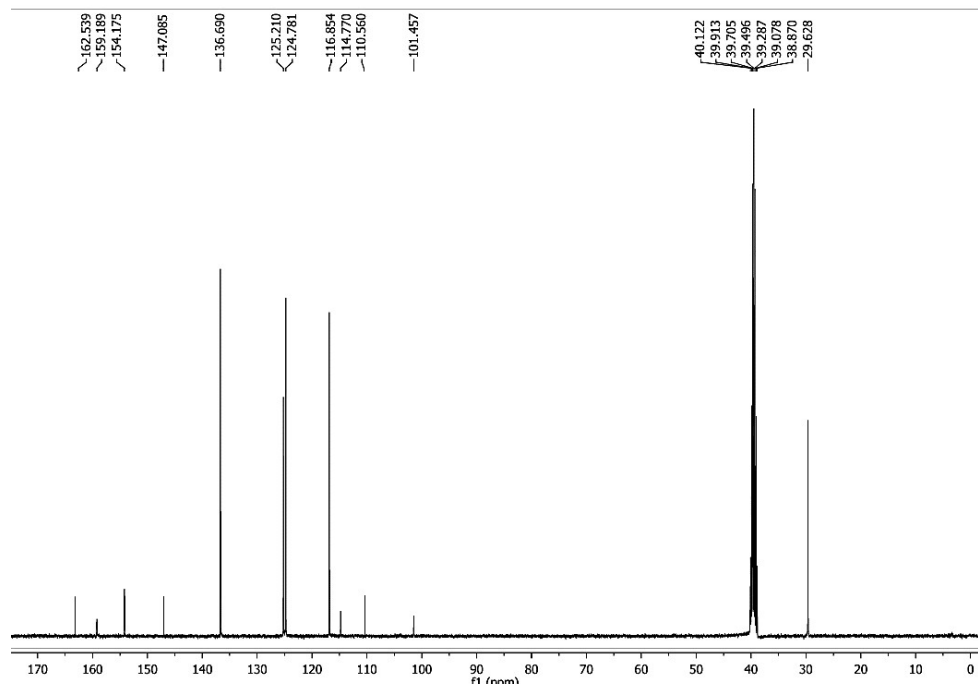


**Figure S11.**  $^1\text{H}$  NMR of 1,3-bis[(1*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]thiourea (SB4)

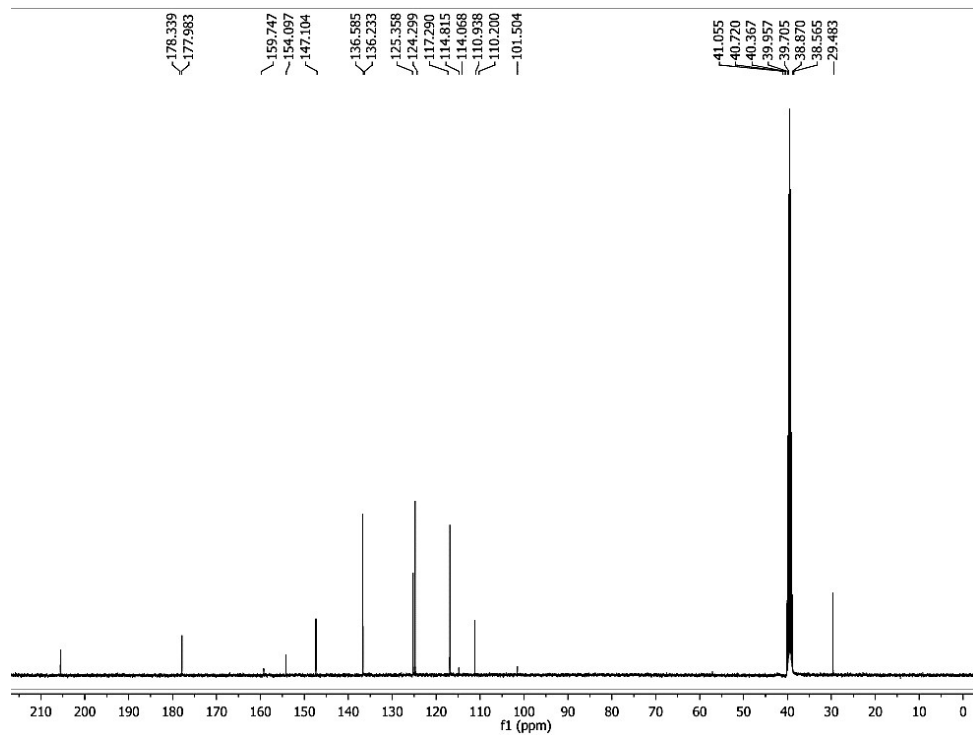


**Figure S12.**  $^1\text{H}$  NMR of 1-hydroxy-3-[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB5)



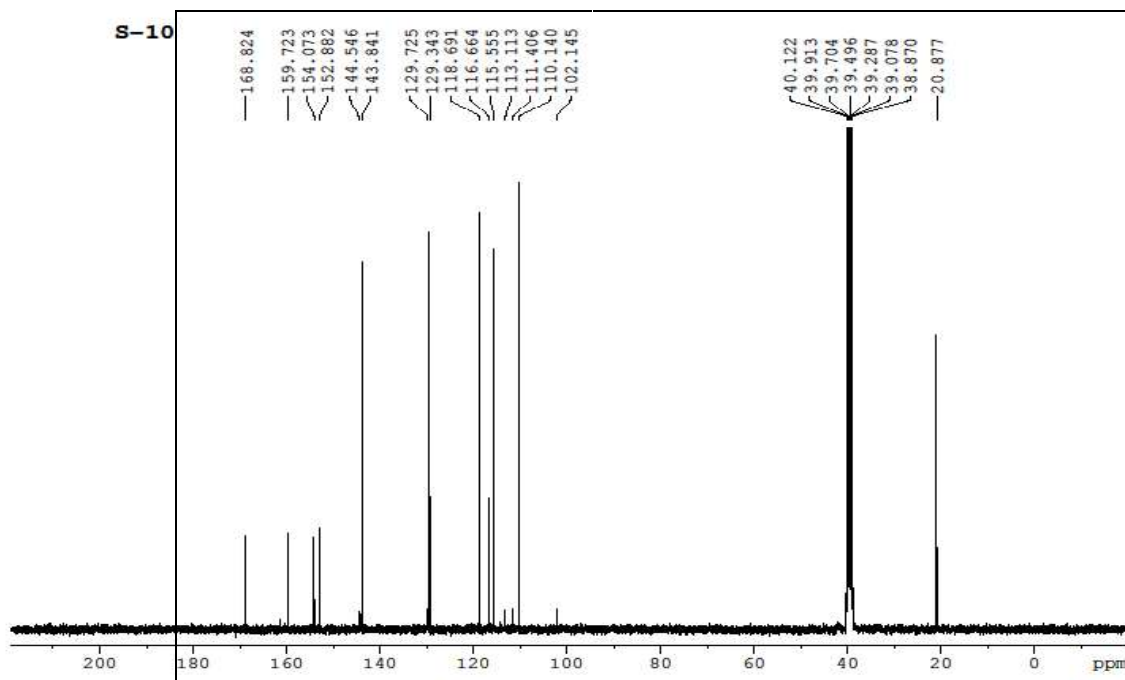


**Figure S15.**  $C^{13}$ -NMR of 1,3-bis[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB1)

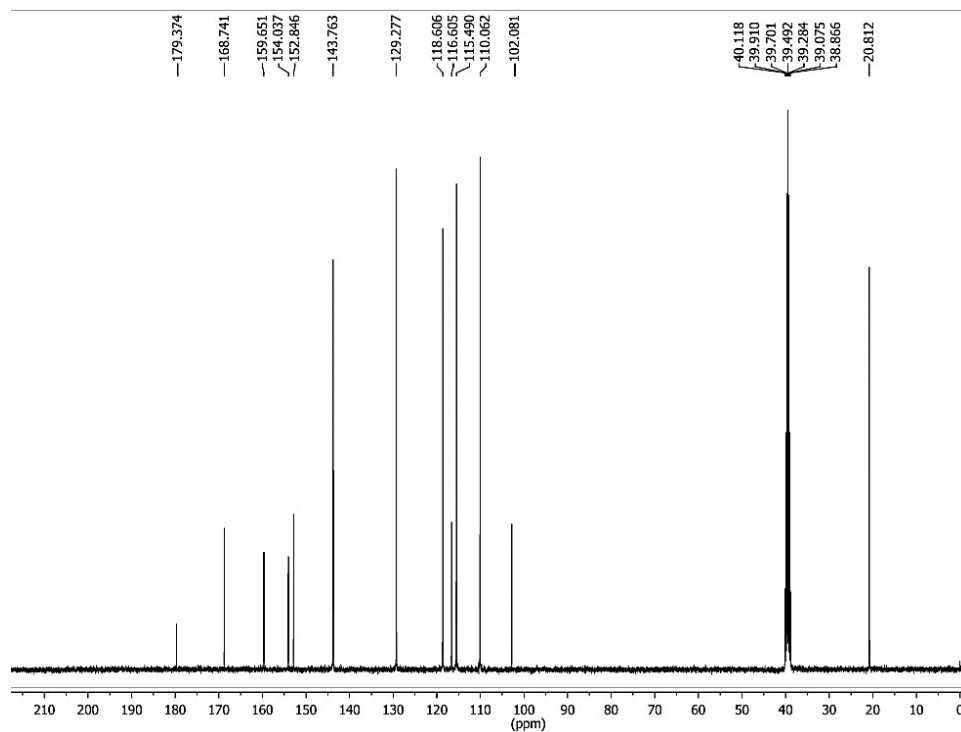


**Figure S16.**  $C^{13}$ -NMR of 1,3-bis[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]thiourea (SB2)

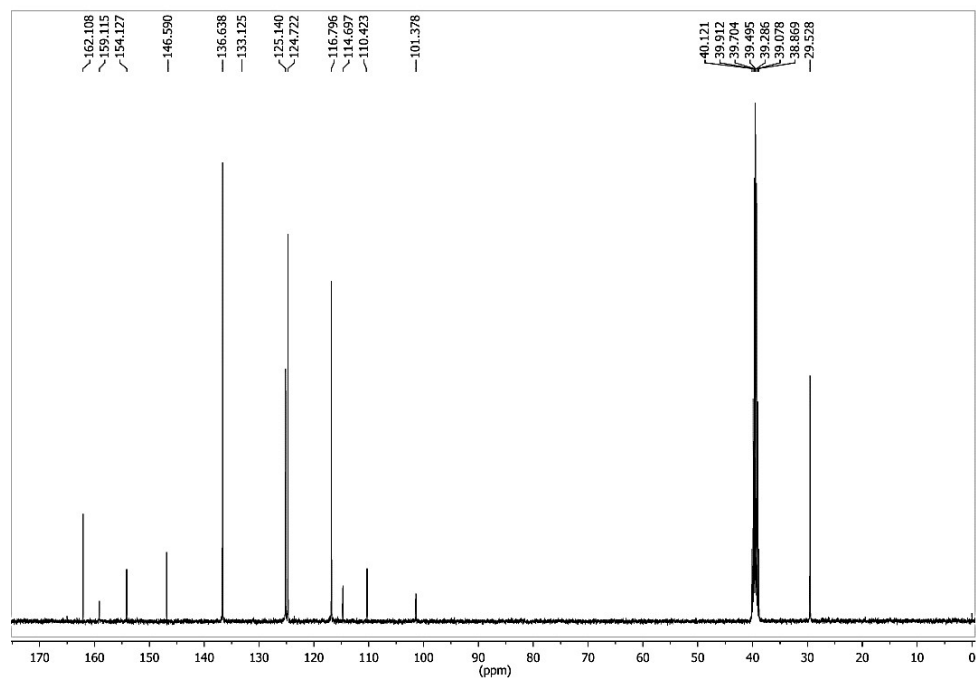
S-10



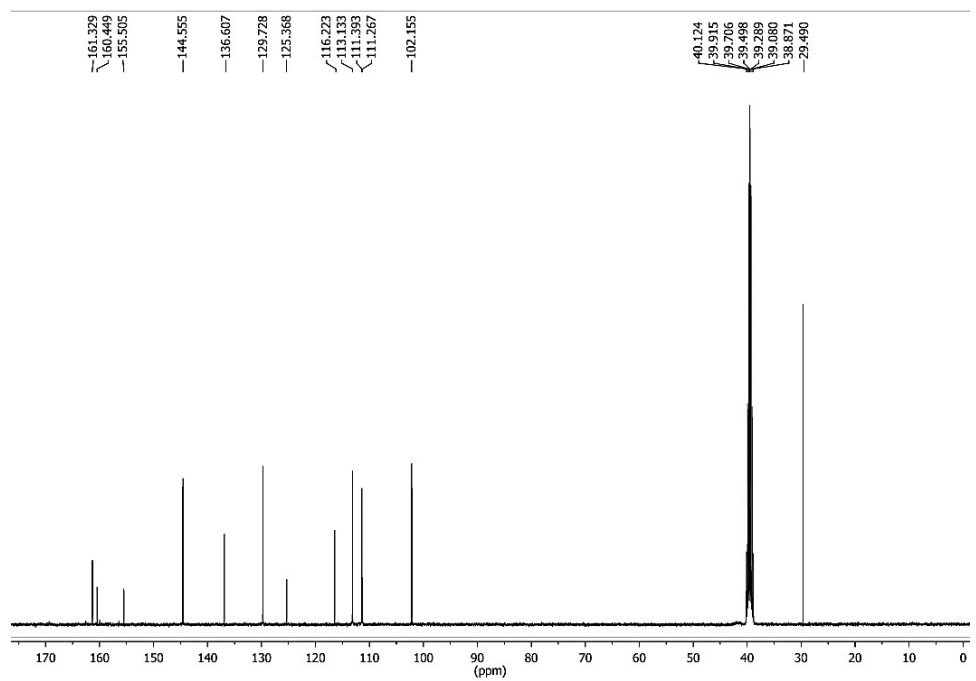
**Figure S17.**  $C^{13}$ -NMR of 1,3-bis[(*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB3)



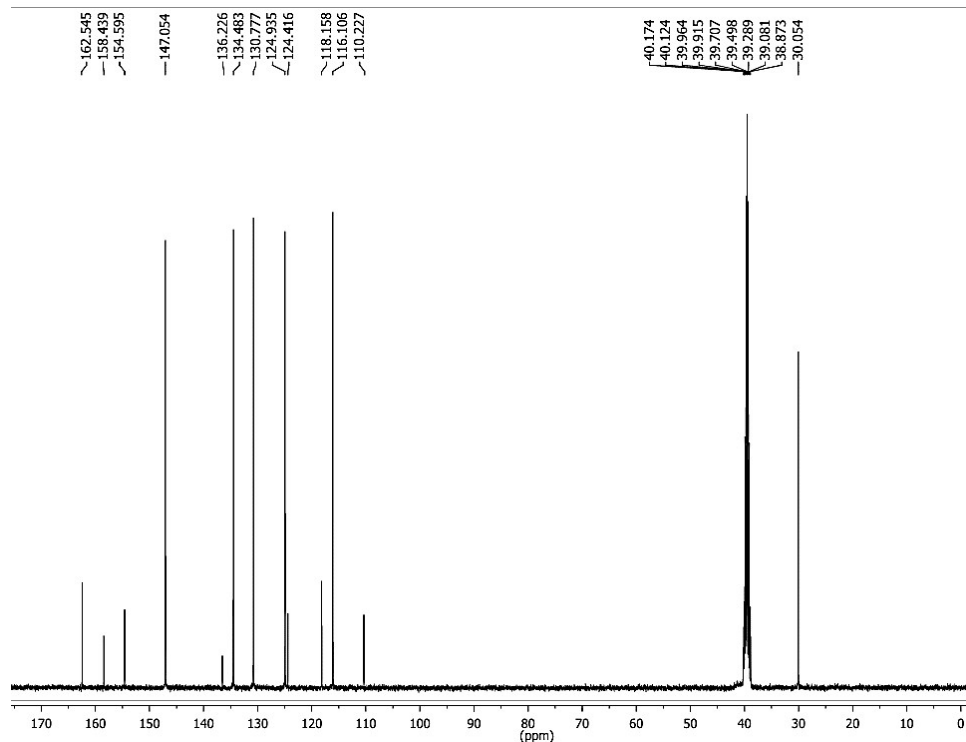
**Figure S18.**  $C^{13}$ -NMR of 1,3-bis[(*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]thiourea (SB4)



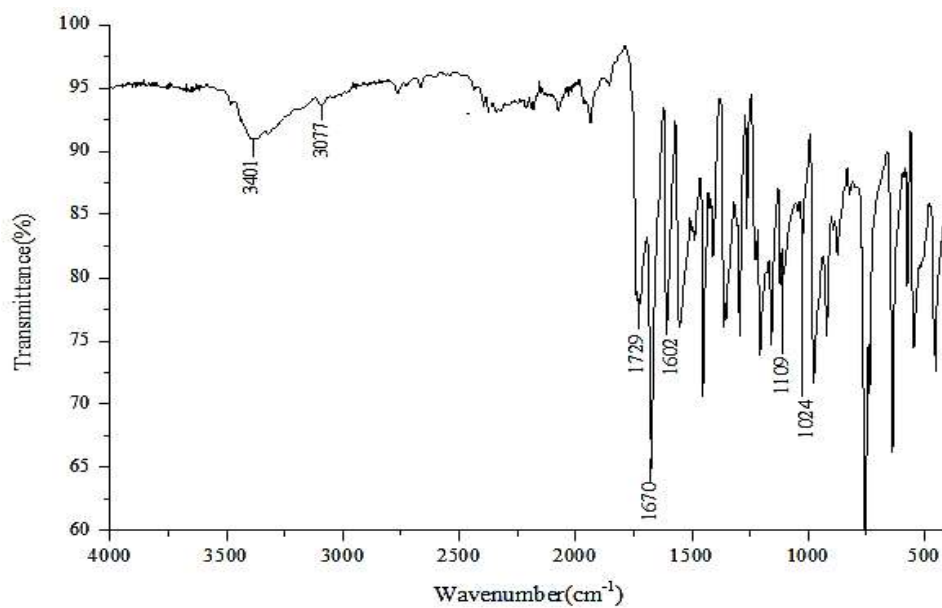
**Figure S19.**  $C^{13}$ -NMR of 1-hydroxy-3-[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB5)



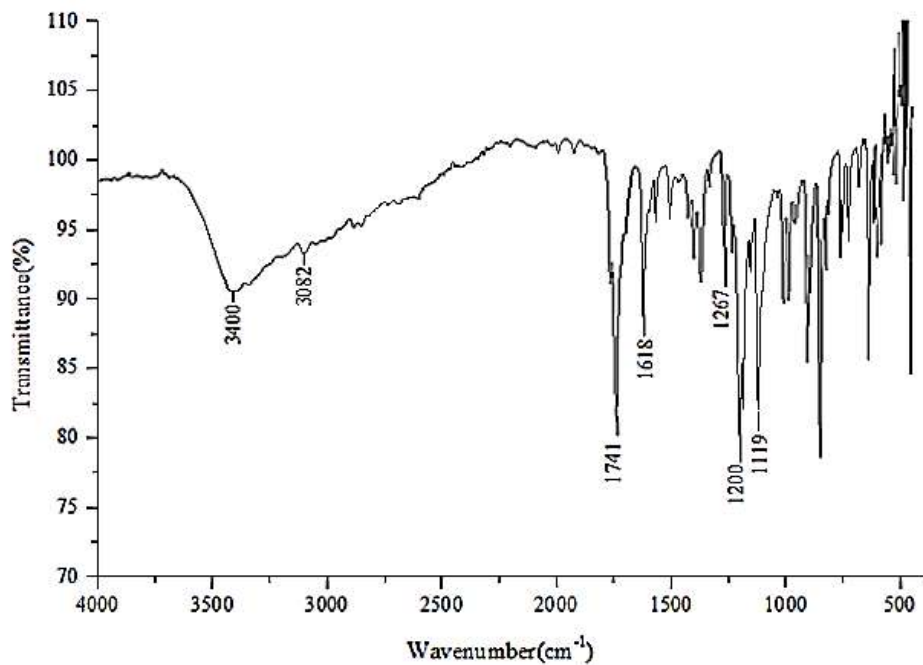
**Figure S20.**  $C^{13}$ -NMR of 1-hydroxy-3-[(1*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB6)



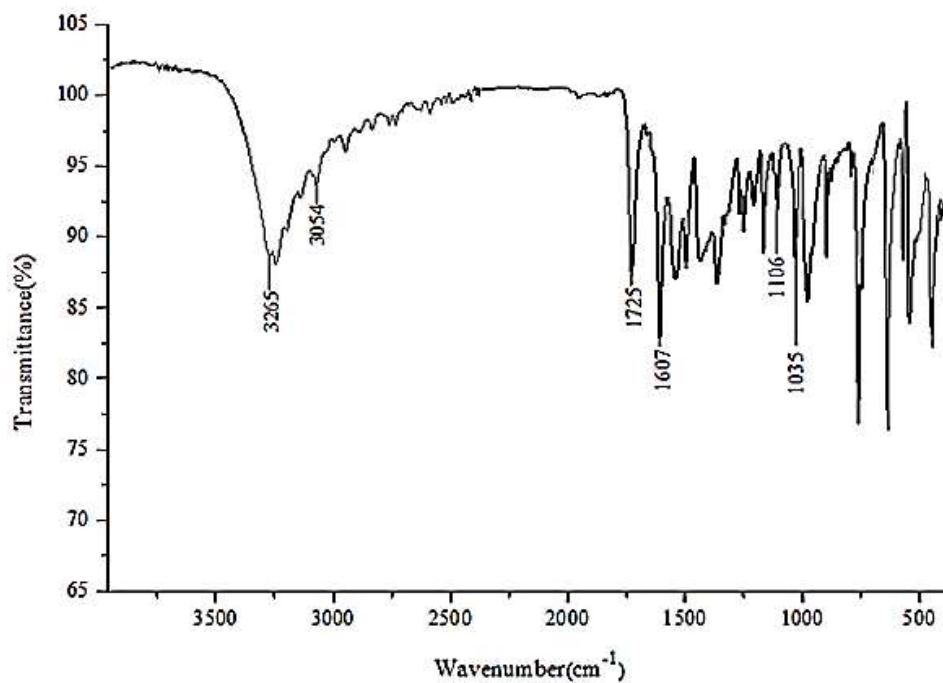
**Figure S21.**  $C^{13}$ -NMR of 1-hydroxy-3-[(1*E*)-1-(2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB7)



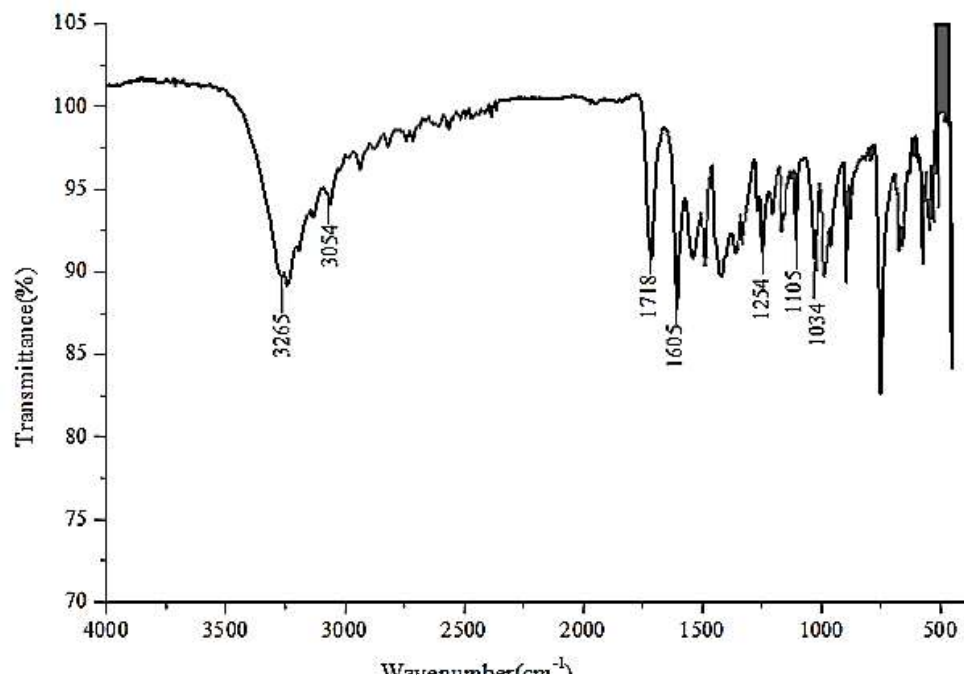
**Figure S22.** FT-IR of 1,3-bis[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB1)



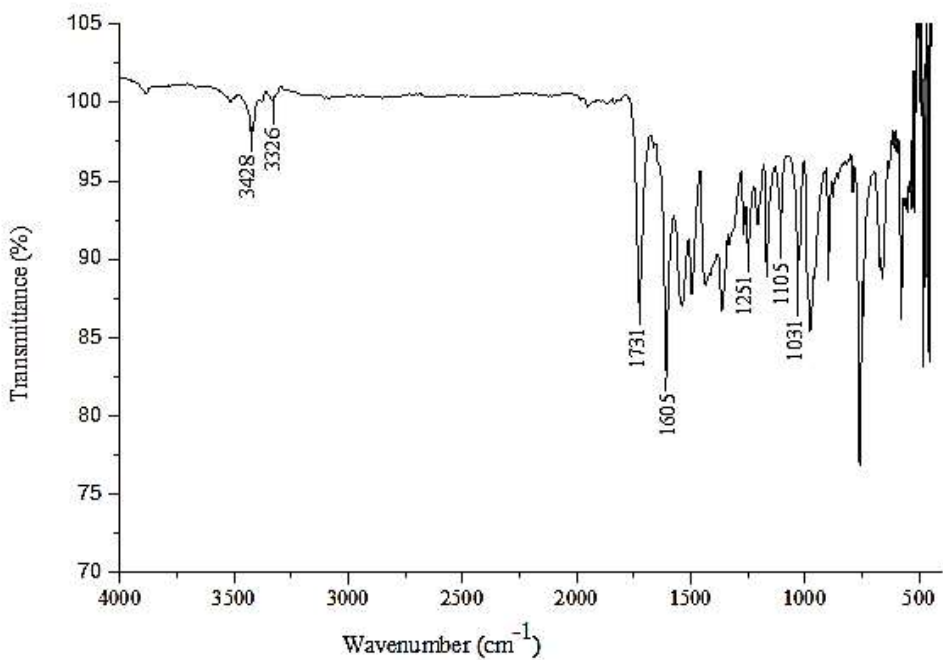
**Figure S23.** FT-IR of 1,3-bis[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]thiourea (SB2)



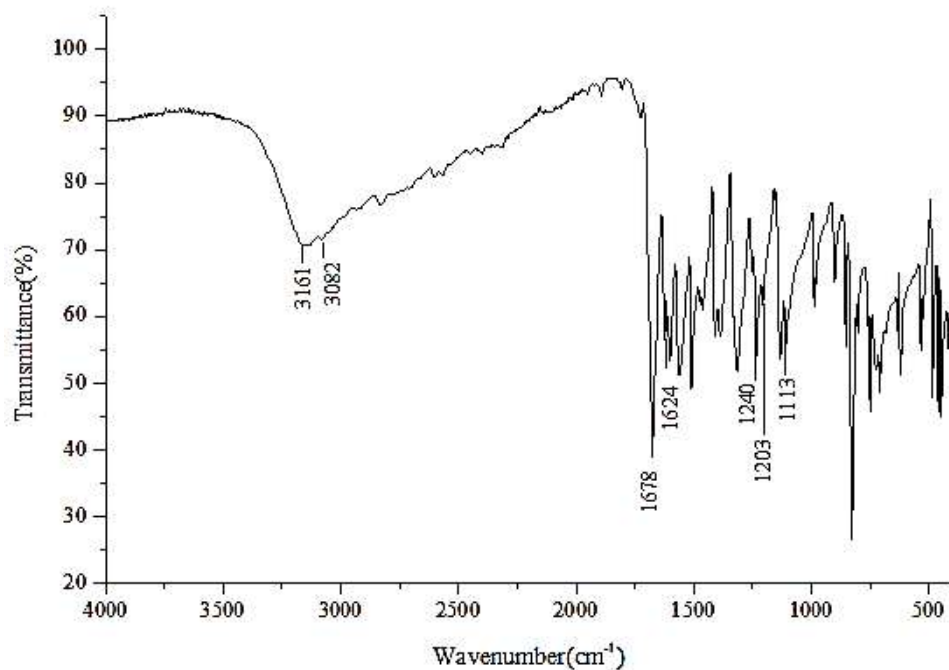
**Figure S24.** FT-IR of 1,3-bis[(1*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB3)



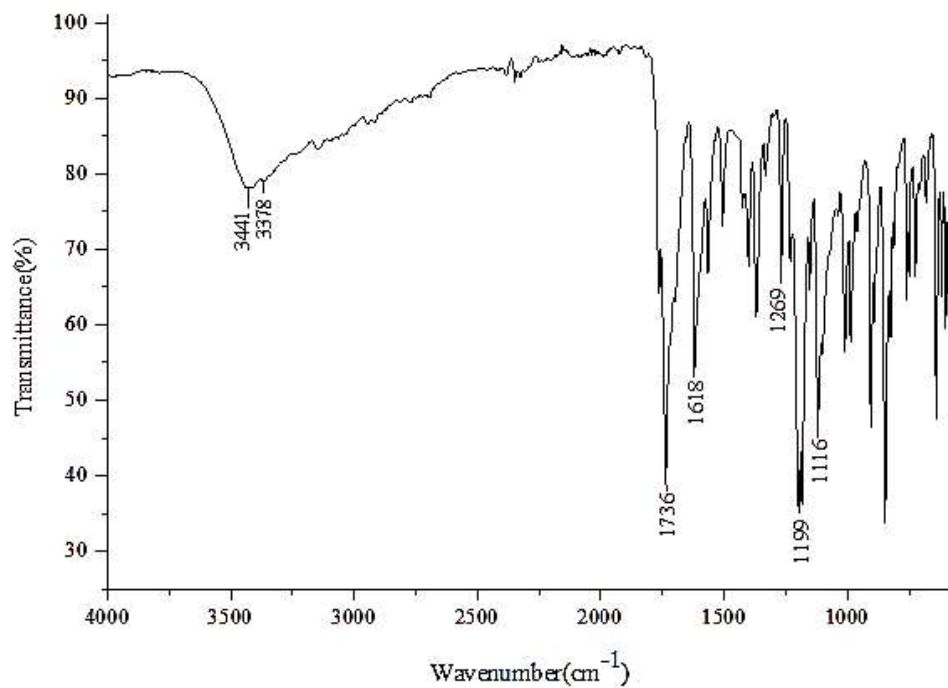
**Figure S25.** FT-IR of 1,3-bis[(E)-1-(7-hydroxy-2-oxo-2H-chromen-3-yl)ethylidene]thiourea (SB4)



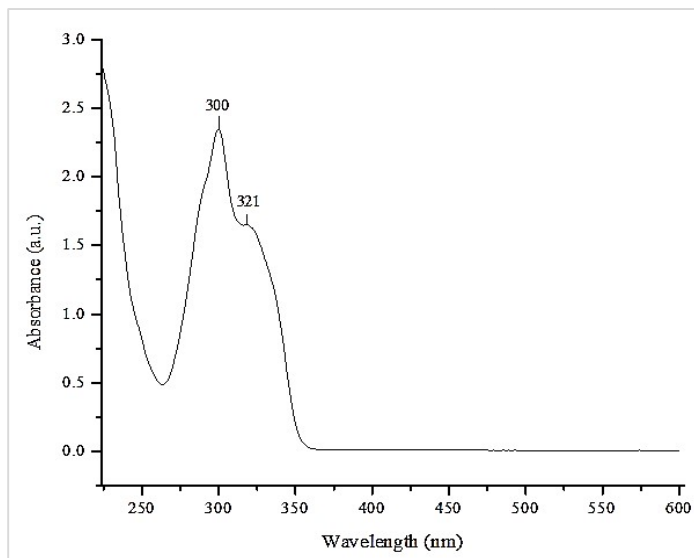
**Figure S26.** FT-IR of 1-hydroxy-3-[(E)-1-(4-hydroxy-2-oxo-2H-chromen-3-yl)ethylidene]urea (SB5)



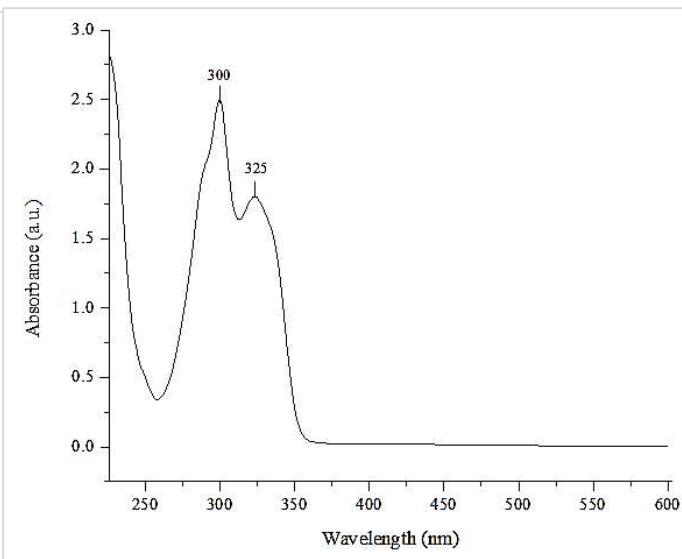
**Figure S27.** FT-IR of 1-hydroxy-3-[(1E)-1-(7-hydroxy-2-oxo-2H-chromen-3-yl)ethylidene]urea (SB6)



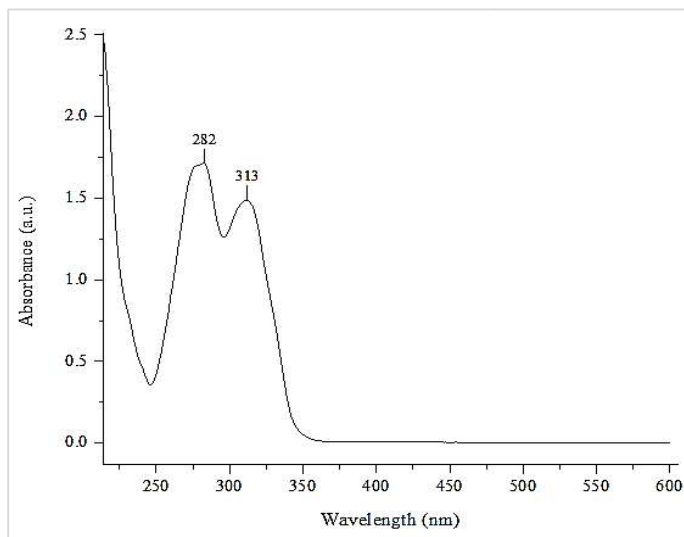
**Figure S28.** FT-IR of 1-hydroxy-3-[(1E)-1-(2-oxo-2H-chromen-3-yl)ethylidene]urea (SB7)



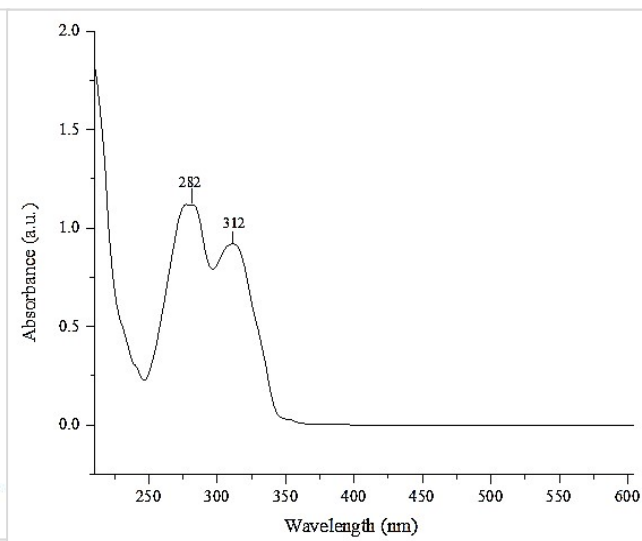
**Figure S29.** UV-Vis spectra of 1,3-bis[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB1)



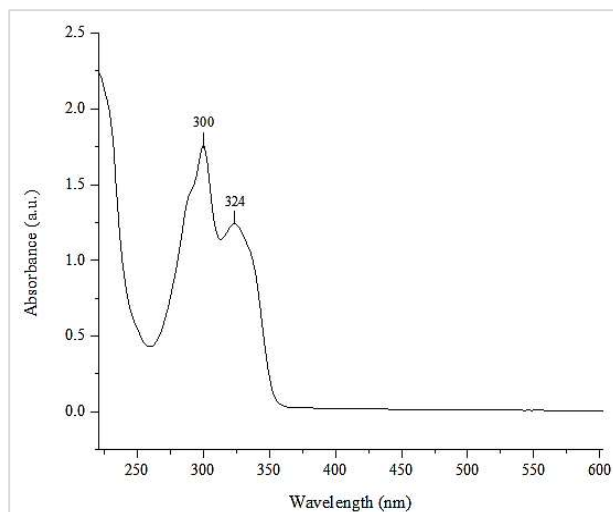
**Figure S30.** UV-Vis spectra of 1,3-bis[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]thiourea (SB2)



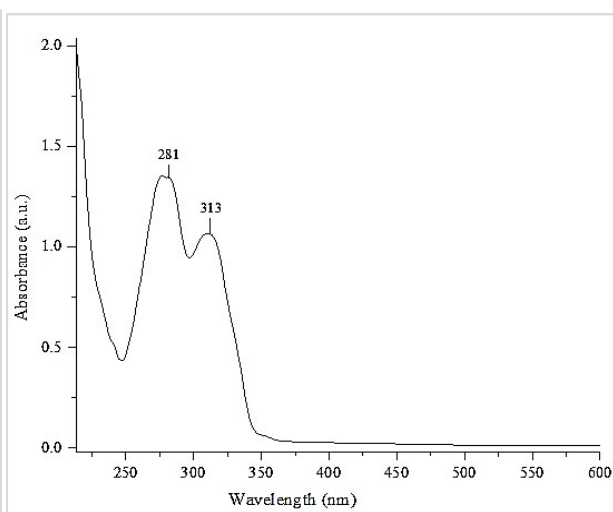
**Figure S31.** UV-Vis spectra of 1,3-bis[(1*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB3)



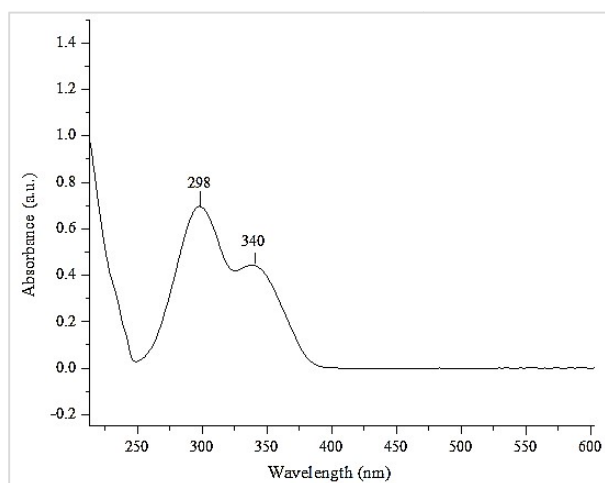
**Figure S32.** UV-Vis spectra of 1,3-bis[(1*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]thiourea (SB4)



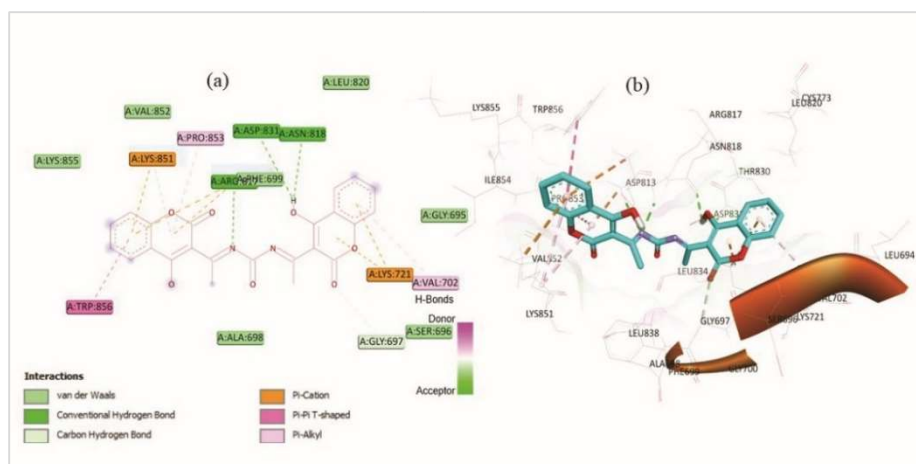
**Figure S33.** UV-Vis spectra of 1-hydroxy-3-[(1*E*)-1-(4-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB5)



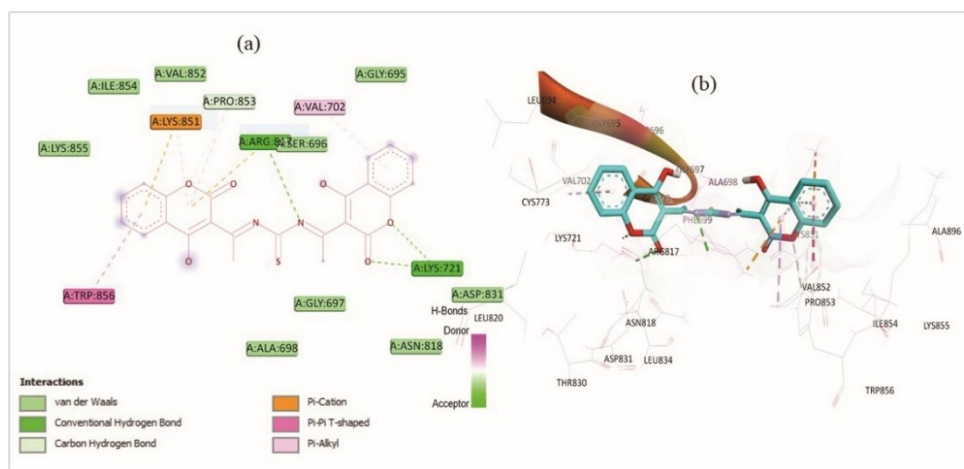
**Figure S34.** UV-Vis spectra of 1-hydroxy-3-[(1*E*)-1-(7-hydroxy-2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB6)



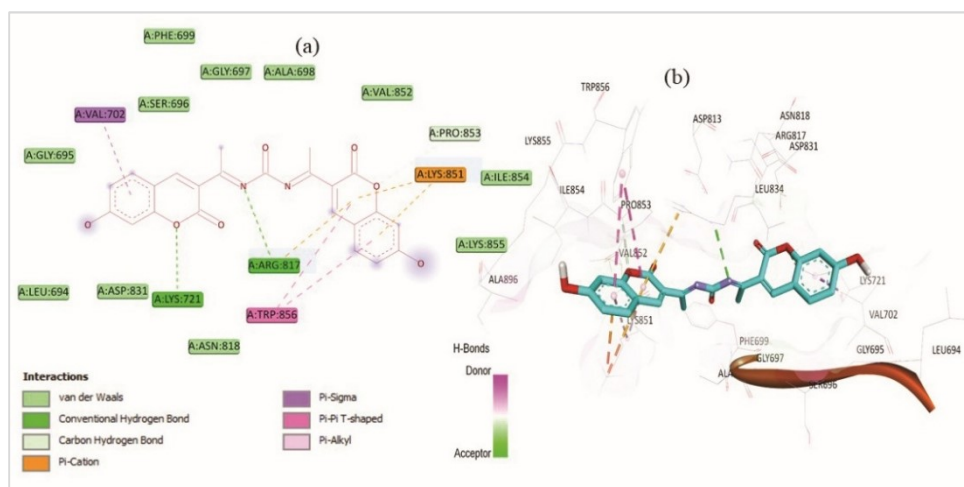
**Figure S35.** UV-Vis spectra of 1-hydroxy-3-[(1*E*)-1-(2-oxo-2*H*-chromen-3-yl)ethylidene]urea (SB7)



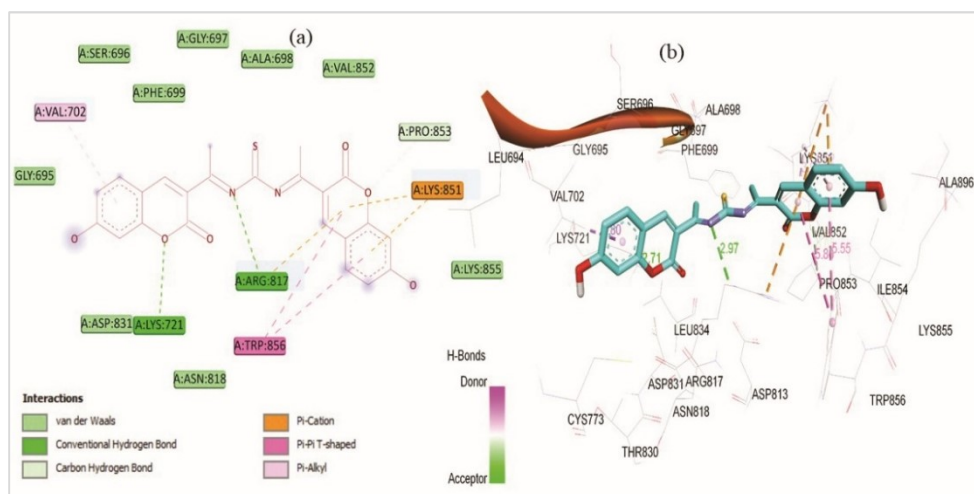
**Figure S36.** 2D, 3D plots with different types of interactions displaying best docked pose of 'SB1' with EGFR



**Figure S37.** 2D, 3D plots with different types of interactions displaying best docked pose of ‘SB2’ with EGFR



**Figure S38.** 2D, 3D plots with different types of interactions displaying best docked pose of ‘SB3’ with EGFR



**Figure S39.** 2D, 3D plots with different types of interactions displaying best docked pose of ‘SB4’ with EGFR

