## **Supporting Information**

## Synthesis, Biological and Computational Studies of Flavonoid Acetamide Derivatives

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Figure S1: <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): 3S1.



Figure S2: <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): 4S1.

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Figure S3: <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): 5S1.



Figure S4: <sup>1</sup>H NMR (400 MHz, D<sub>2</sub>O): 4S2.



Figure S5: <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): 3S3



Figure S6: <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): 4S3





Figure S8: FTIR spectrum of 3S3



Figure S9: FTIR spectrum of 4S3



Figure S10: FTIR spectrum of 5S3.

	Frequency(cm <sup>-1</sup> )		
Assignments	3\$3	4\$3	5\$3
Amide N-H	3423	3409	3379
Stretch			
Amide N-H	3312	3310	3314
Stretch			
Alkenyl C-H	3176	3186	3184
Stretch			
Alkyl C-H Stretch	2922	2915	2925
(C=O) Ketone	1665	1686	1690
(C=O) Amide	1592	1597	1591

Table S1: Assignments of FTIR bands for 3S3, 4S3, and 5S3 derivatives.



Figure 11: Decay curve for the reaction between DPPH and 3S0. Decrease in absorbance, at 517 nm of DPPH in methanol in the presence of various concentrations of 3S0 (1.0 -50  $\mu$ M)



Figure S12: Decay curve for the reaction between DPPH and 4S0. Decrease in absorbance, at 517 nm of DPPH in methanol in the presence of various concentrations of 4S0 (1.0 -50  $\mu$ M)



Figure S13: Decay curve for the reaction between DPPH and 5S0. Decrease in absorbance, at 517 nm of DPPH in methanol in the presence of various concentrations of 5S0 (1.0 -50  $\mu$ M)



Figure S14: Decay curve for the reaction between DPPH and 1S3. Decrease in absorbance, at 517 nm of DPPH in methanol in the presence of various concentrations of 1S3 (10 -115  $\mu$ M)



Figure S15: Decay curve for the reaction between DPPH and 3S3. Decrease in absorbance, at 517 nm of DPPH in methanol in the presence of various concentrations of 3S3 (15 -100  $\mu$ M)





Figure S16: Decay curve for the reaction between DPPH and 4S3. Decrease in absorbance, at 517 nm of DPPH in methanol in the presence of various concentrations of 4S3 ( $5.0 -100 \mu M$ )

Figure S17: Decay curve for the reaction between DPPH and 5S3. Decrease in absorbance, at 517 nm of DPPH in methanol in the presence of various concentrations of 5S3 (5.0-105  $\mu$ M)