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Supplementary Information

Synthesis and Mechanism of Formation of Oxadeazaflavines by Microwave Thermal Cyclization of *ortho*-Halobenzylidene Barbiturates

J. Daniel Figueroa-Villar,[a] and Sandra C. G. de Oliveira***

Grupo de Química Medicinal, Departamento de Química, Instituto Militar de Engenharia, Praça General Tibúrcio 80, Praia Vermelha, 22290-270 Rio de Janeiro-RJ, Brazil

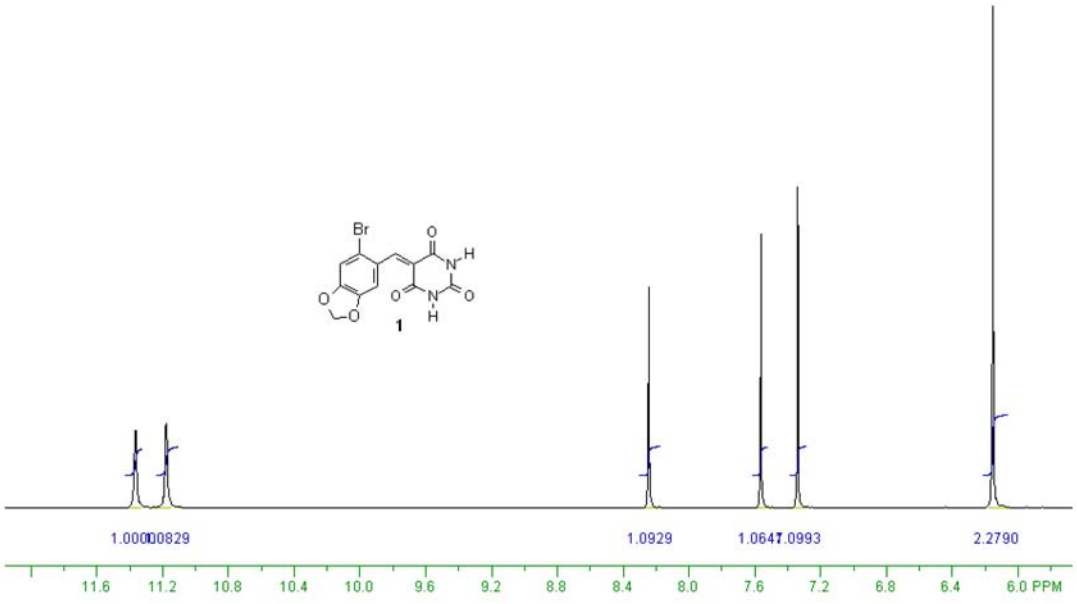

Figure S1. ^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of 6-bromopiperonylidene barbiturate (**1**).

*e-mail: figueroa@ime.eb.br

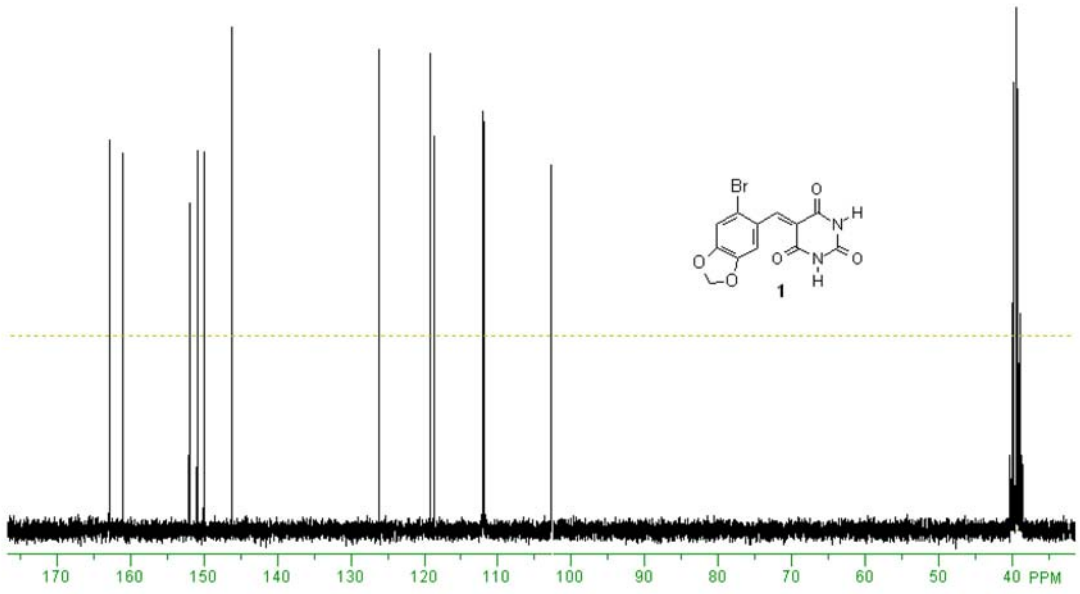

Figure S2. ^{13}C NMR spectrum (DMSO-d_6, 75 MHz) of 6-bromopiperonylidene barbiturate (**1**).

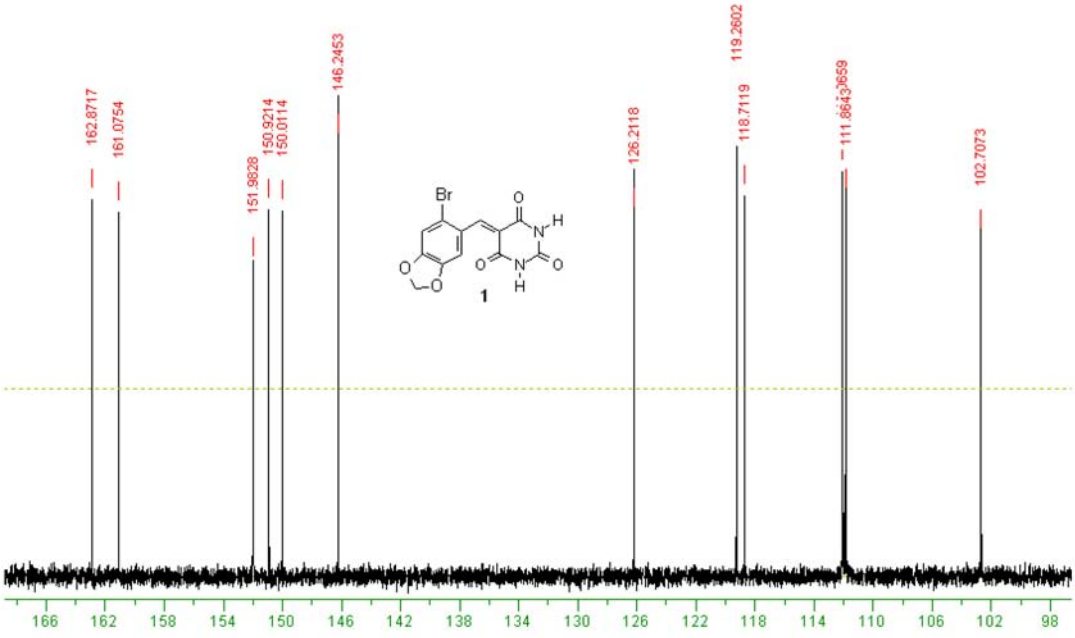

Figure S3. Expanded ^{13}C NMR spectrum of 6-bromopiperonylidene barbiturate (**1**).

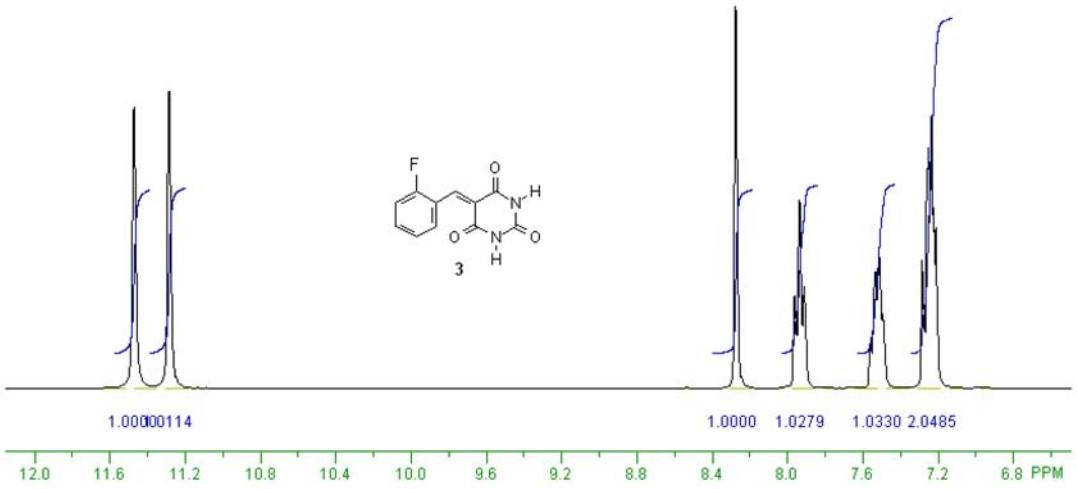

Figure S4. [1]H NMR spectrum (DMSO-d_6, 300 MHz) of *ortho*-fluorobenzylidene barbiturate (**3**).

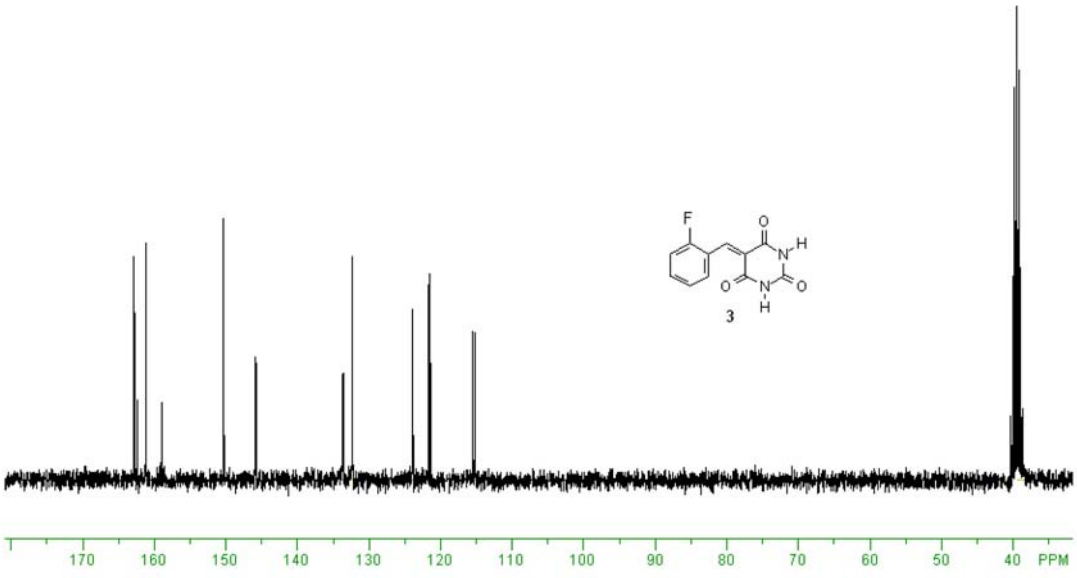

Figure S5. [13]C NMR spectrum (DMSO-d_6, 300 MHz) of *ortho*-fluorobenzylidene barbiturate (**3**).

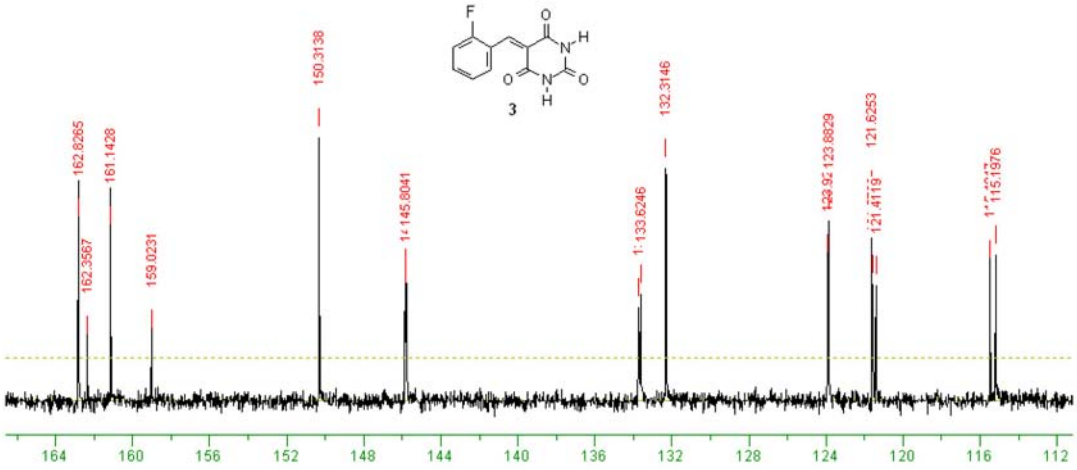

Figure S6. Expanded ^{13}C NMR spectrum of *ortho*-fluorobenzylidene barbiturate (**3**).

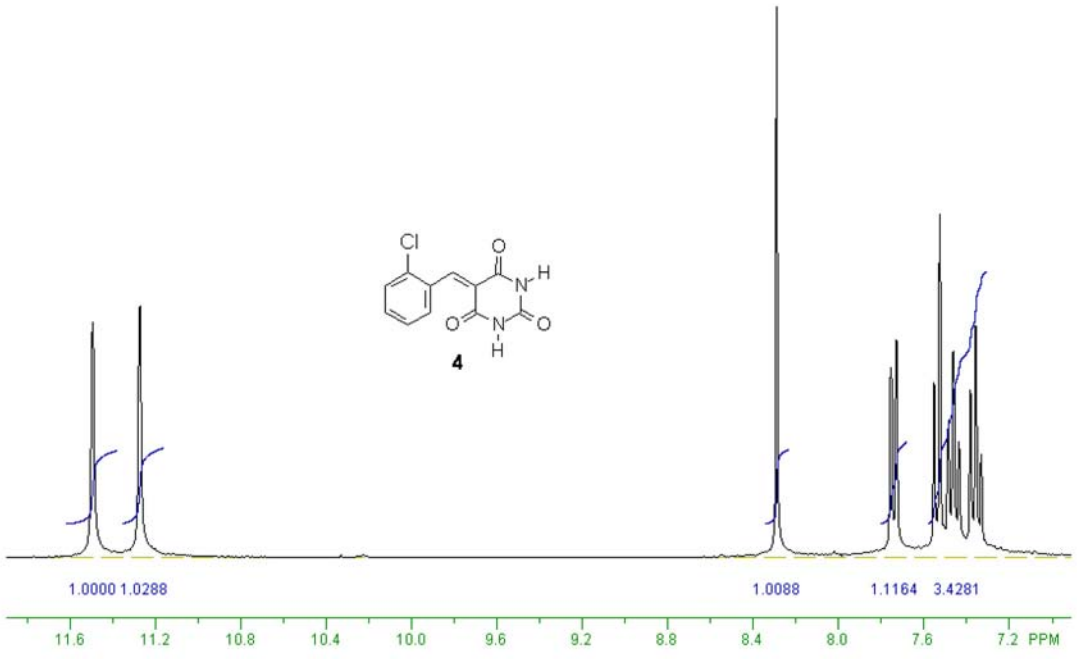

Figure S7. ^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of *ortho*-chlorobenzylidene barbiturate (**4**).

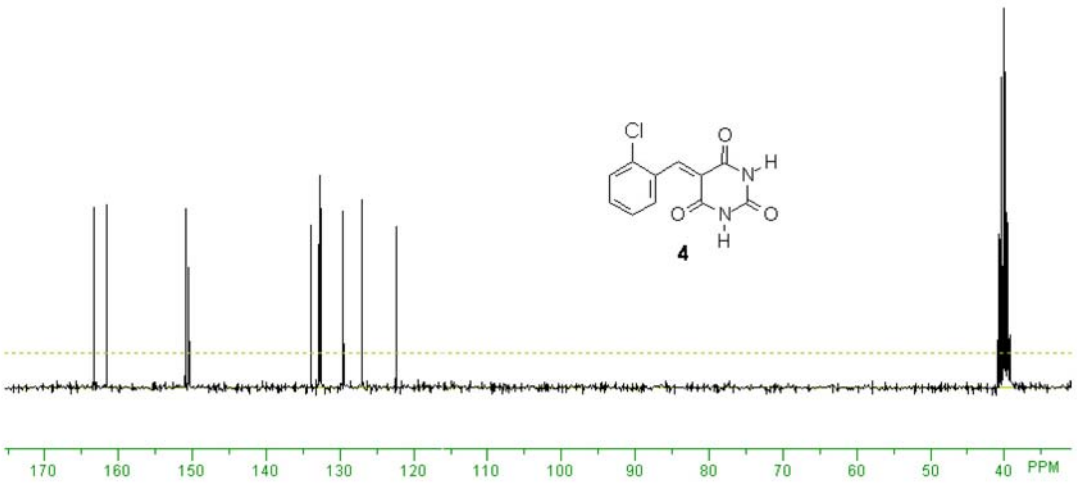

Figure S8. ^{13}C NMR spectrum (DMSO-d_6, 300 MHz) of *ortho*-chlorobenzylidene barbiturate (**4**).

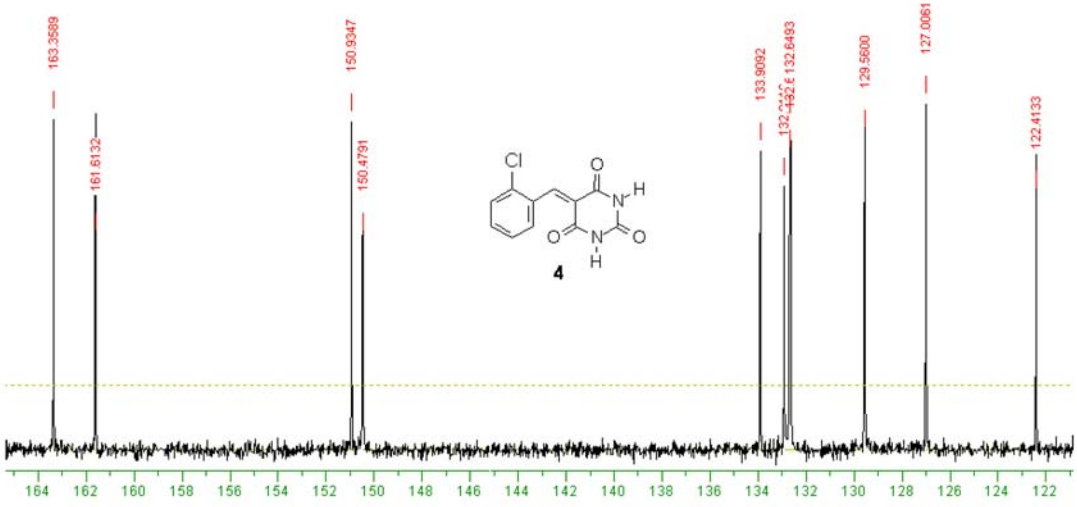

Figure S9. Expanded ^{13}C NMR spectrum of *ortho*-chlorobenzylidene barbiturate (**4**).

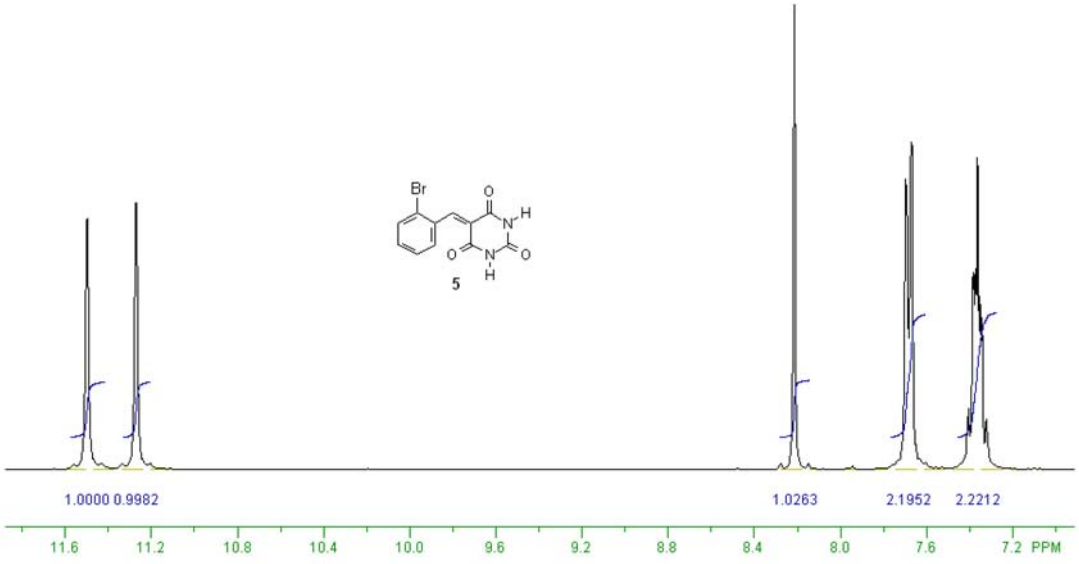

Figure S10. ^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of *ortho*-fluorobenzylidene barbiturate (**5**).

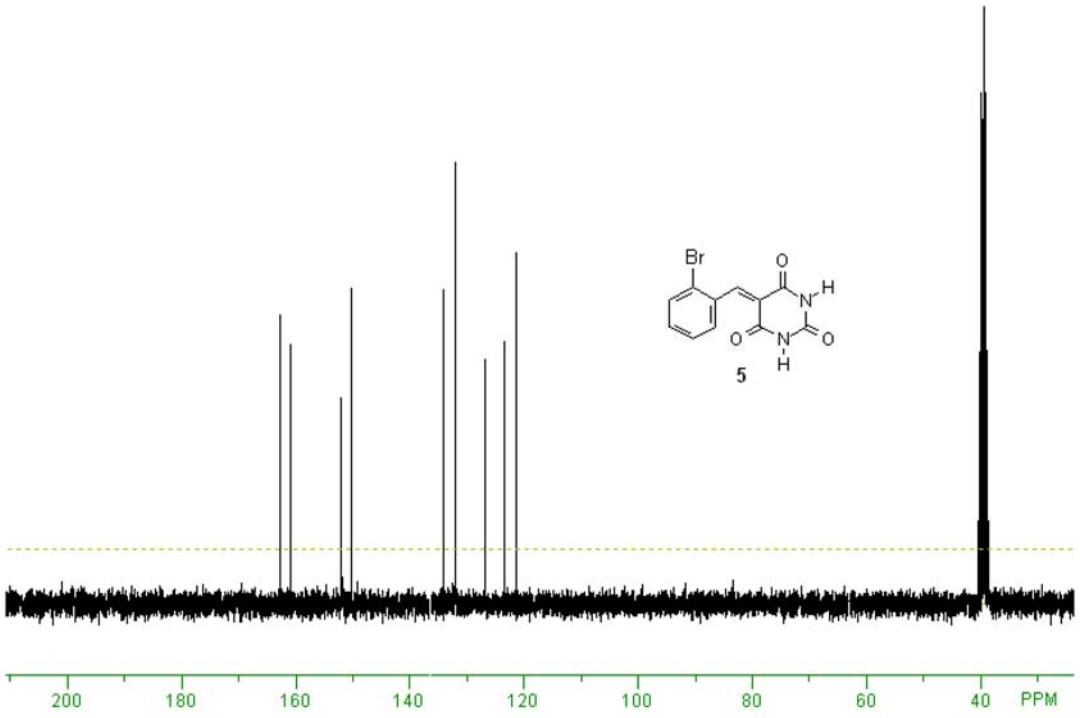

Figure S11. ^{13}C NMR spectrum (DMSO-d_6, 300 MHz) of *ortho*-fluorobenzylidene barbiturate (**5**).

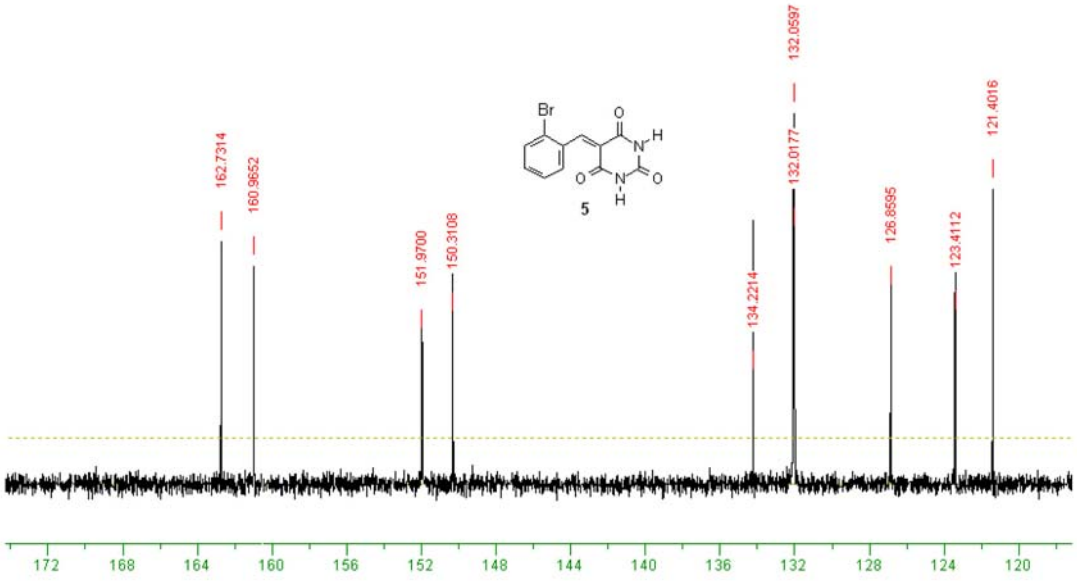

Figure S12. Expanded ^{13}C NMR spectrum of *ortho*-fluorobenzylidene barbiturate (**5**).

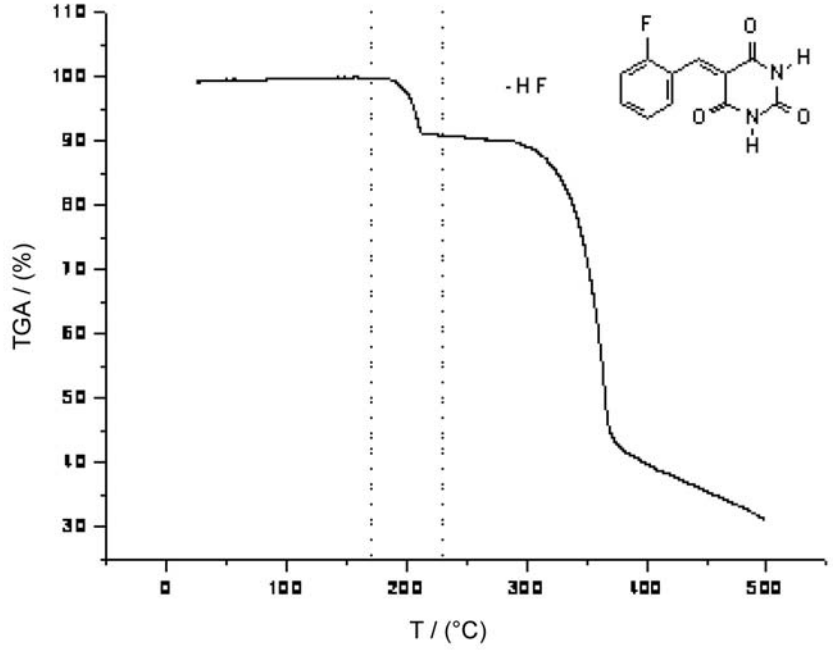

Figure S13. Thermogravimetric analysis (TGA) graphic of *ortho*-fluorobenzylidene barbiturate (**3**).

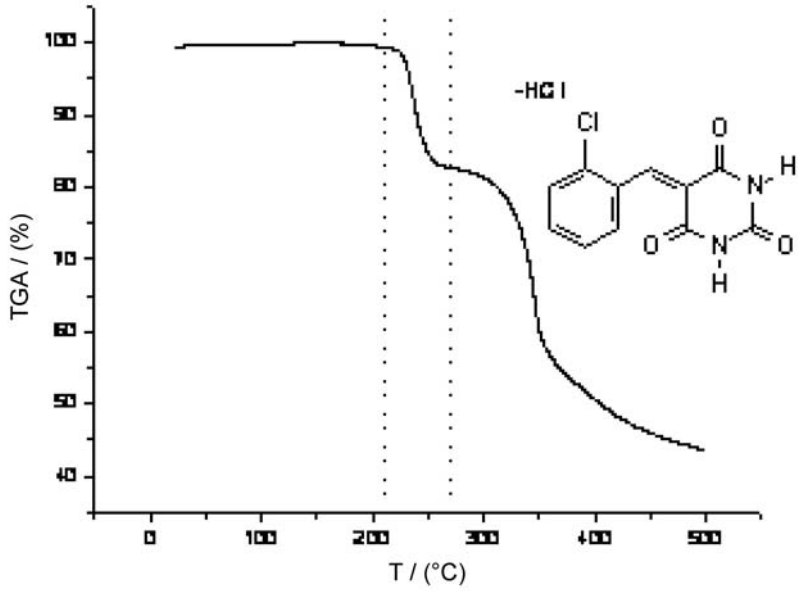

Figure S14. Thermogravimetric analysis (TGA) graphic of *ortho*-chlorobenzylidene barbiturate (**4**).

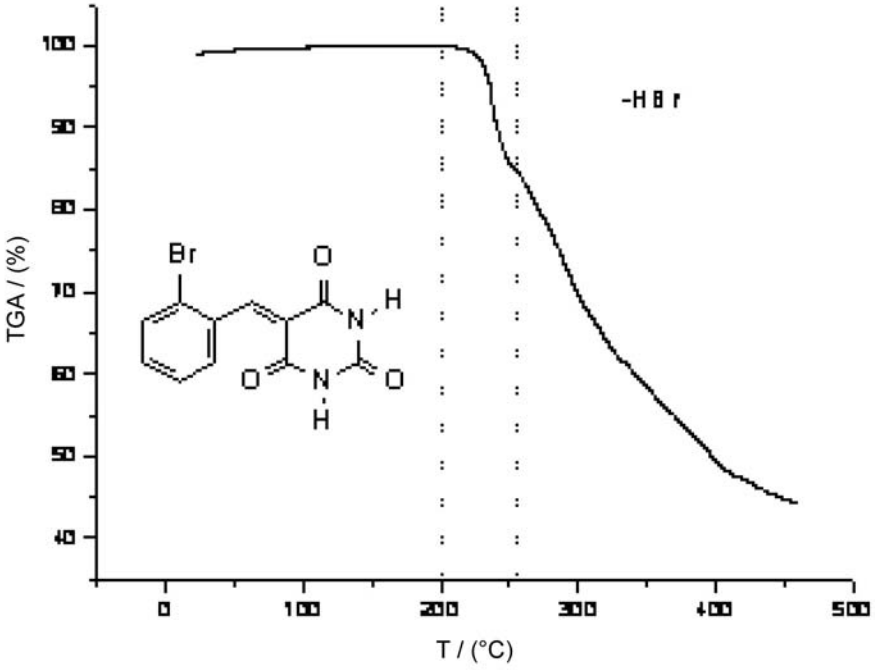

Figure S15. Thermogravimetric analysis (TGA) graphic of *ortho*-bromobenzylidene barbiturate (**5**).

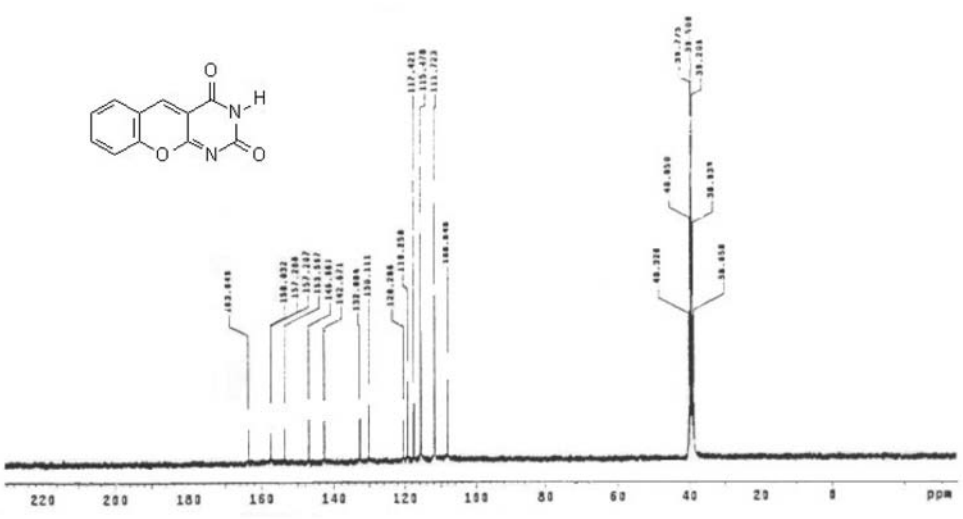

Figure S16. ^{13}C NMR spectrum (DMSO-d_6, 75 MHz) of 2H-chromeno[2,3-d]pyrimidine-2,4(3H)-dione (oxadeazaflavine).

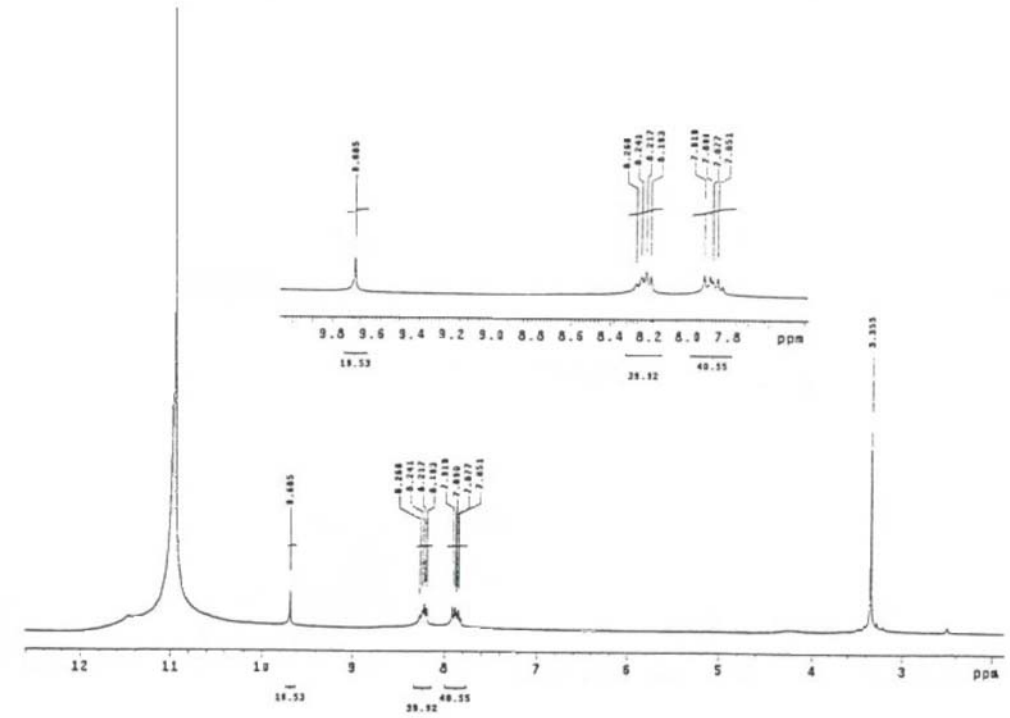

Figure S17. ^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of 2H-chromeno[2,3-d]pyrimidine-2,4(3H)-dione (oxadeazaflavine).

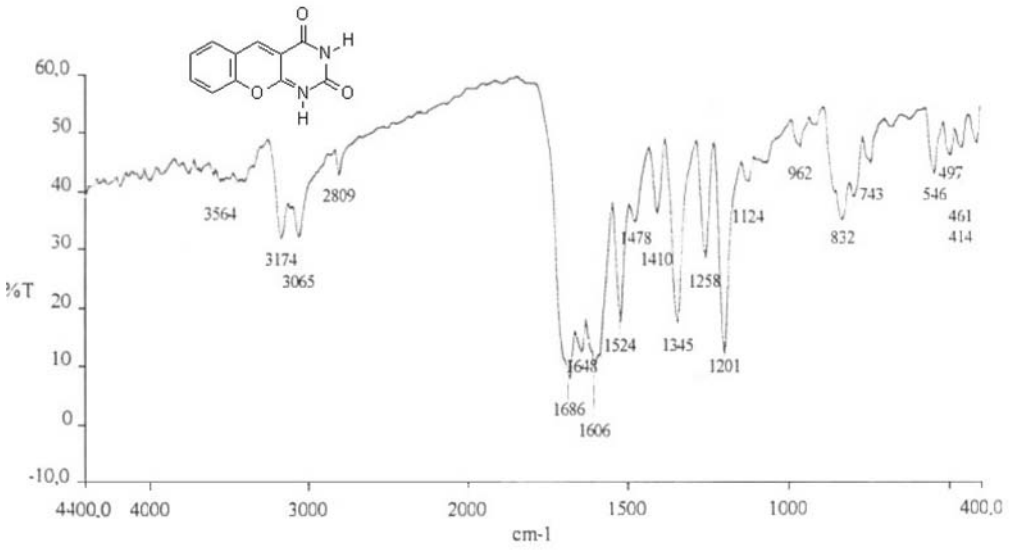

Figure S18. IR spectrum of 2H-chromeno[2,3-d]pyrimidine-2,4(3H)-dione (oxadeazaflavine).

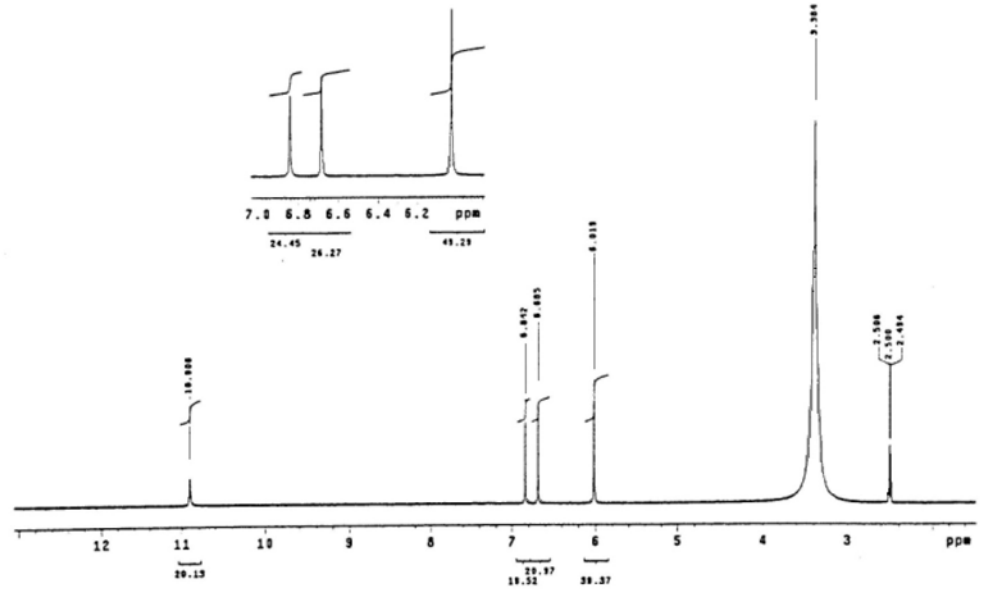

Figure S19. ^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of 2H-[1,3]dioxolo[4',5':6,7]chromeno[2,3-d]pyrimidine-2,4(3H)-dione (**2**).

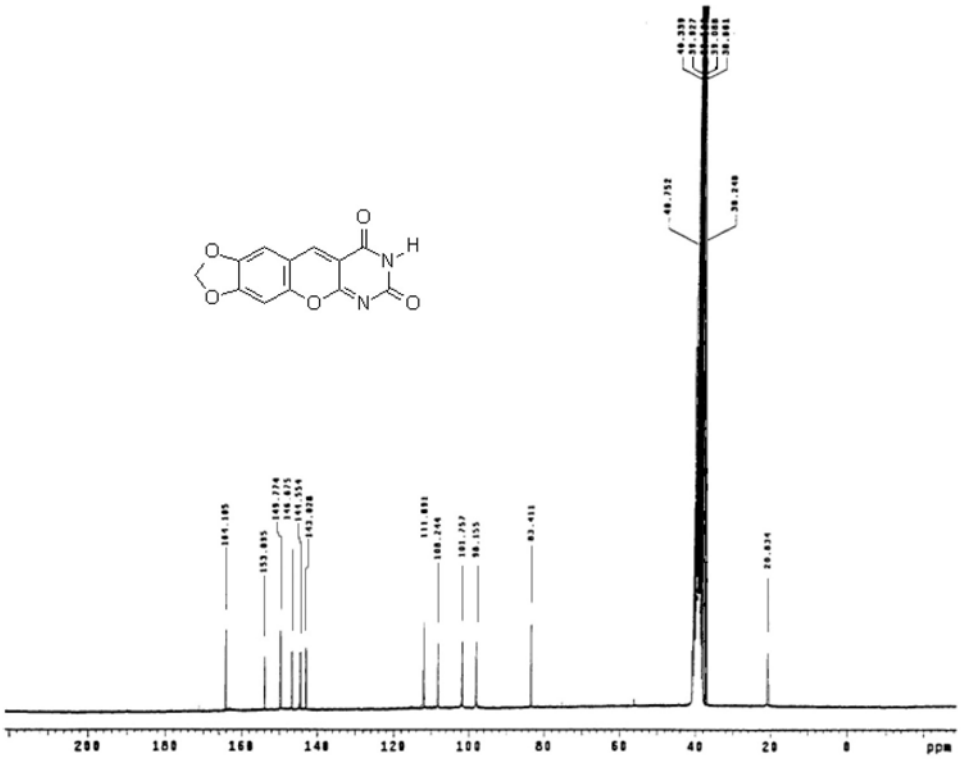

Figure S20. ^{1}H NMR spectrum (DMSO-d_6, 300 MHz) of 2H-[1,3]dioxolo[4',5':6,7]chromeno[2,3-d]pyrimidine-2,4(3H)-dione (**2**).

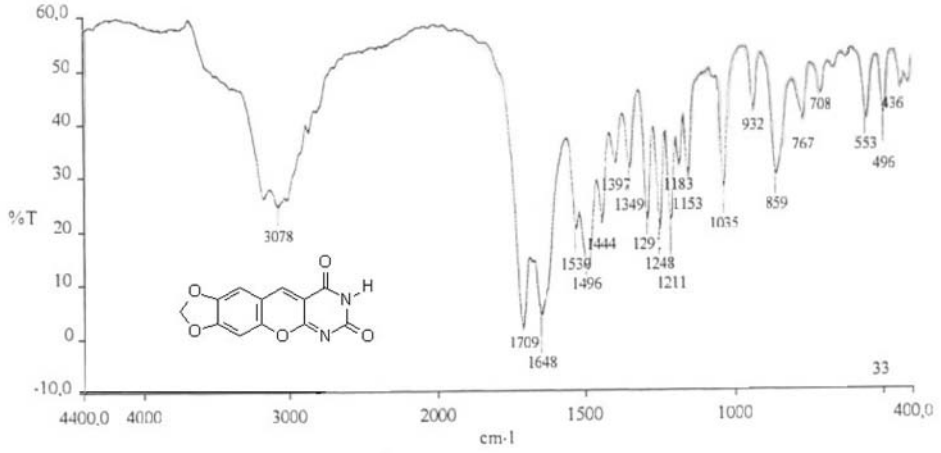

Figure S21. IR spectrum of 2H-[1,3]dioxolo[4',5':6,7]chromeno[2,3-d]pyrimidine-2,4(3H)-dione (**2**).