

Supplementary Material

3-Phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine

Alia D. Aouant and George Varvounis*

Section of Organic Chemistry and Biochemistry, Department of Chemistry
University of Ioannina, 451 10 Ioannina, Greece

*Correspondence: gvarvoun@uoi.gr

¹ H NMR spectrum of compound 2	S1
LRMS (ESI) spectrum of compound 2	S2
¹ H NMR spectrum of compound 5	S3
¹ H NMR spectrum of compound 5 expanded in the aromatic region	S4
¹³ C NMR spectrum of compound 5	S5.
DEPT-90 ¹³ C NMR spectrum of compound 5	S6
¹ H- ¹ H TOCSY NMR spectrum of compound 5	S7
¹ H- ¹ H NOESY NMR spectrum of compound 5	S8
¹ H- ¹³ C HSQC NMR spectrum of compound 5	S9
¹ H- ¹³ C HMBC NMR spectrum of compound 5	S10
¹ H and ¹³ C NMR chemical shift assignments of compound 5	S11
UV spectrum of compound 5	S12
IR spectrum of compound 5	S13
HRMS (ESI) spectrum of compound 5	S14

Figure S1: ^1H NMR (400 MHz) spectrum of (*E*)-1-[(2-phenylhydrazono)methyl]naphthalen-2-ol (**2**) in $\text{DMSO-}d_6$

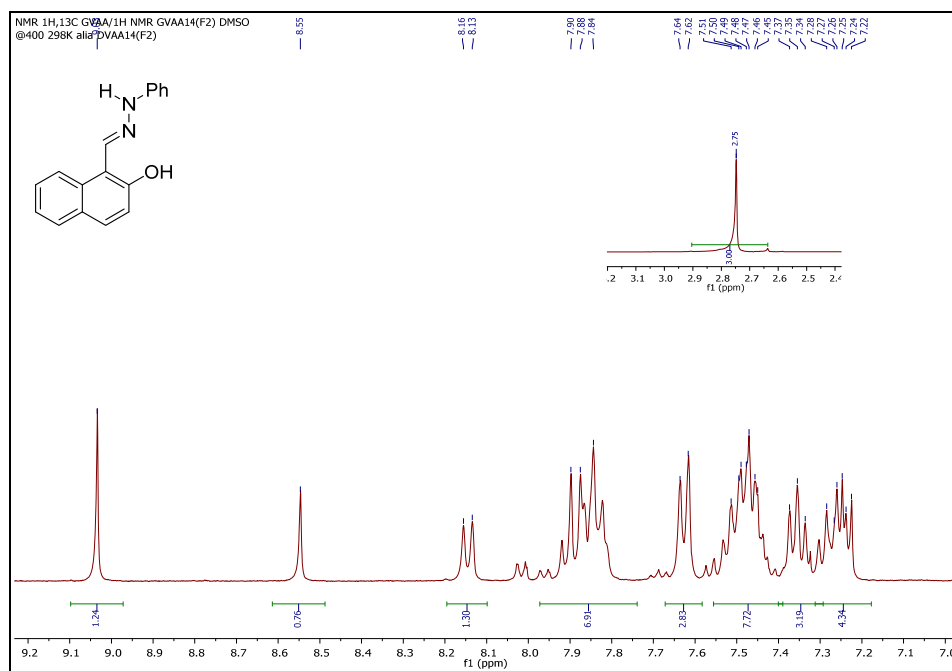


Figure S2. LRMS (ESI) spectrum of (*E*)-1-[(2-phenylhydrazono)methyl]naphthalen-2-ol (**2**) in MeOH containing 0.1% NH_4OH

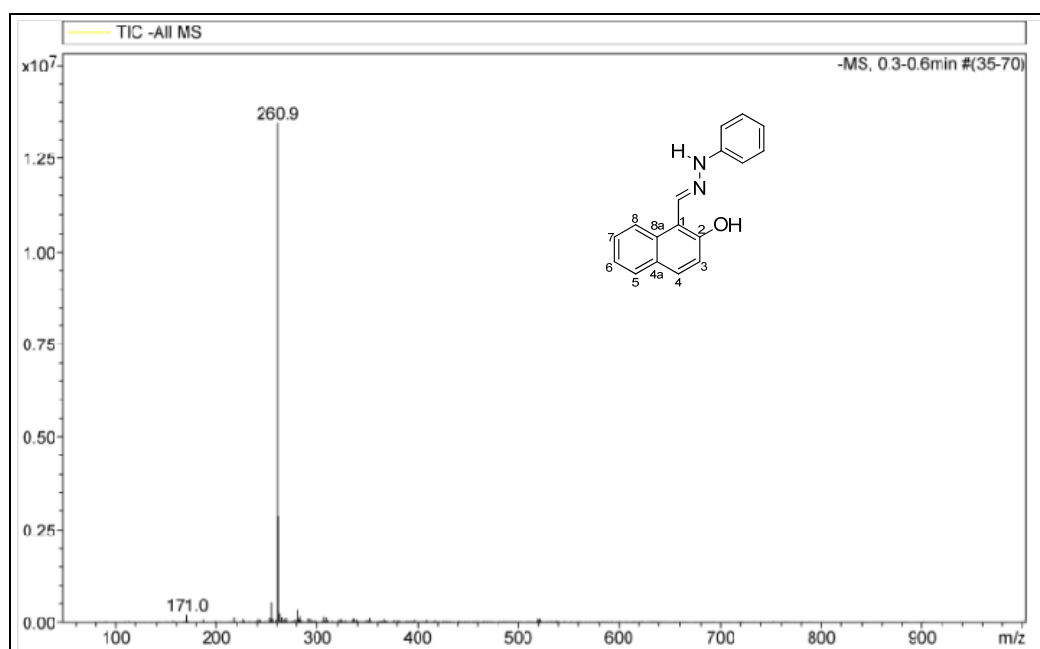


Figure S3. ^1H NMR (500 MHz) spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine (**5**) in $\text{DMSO-}d_6$

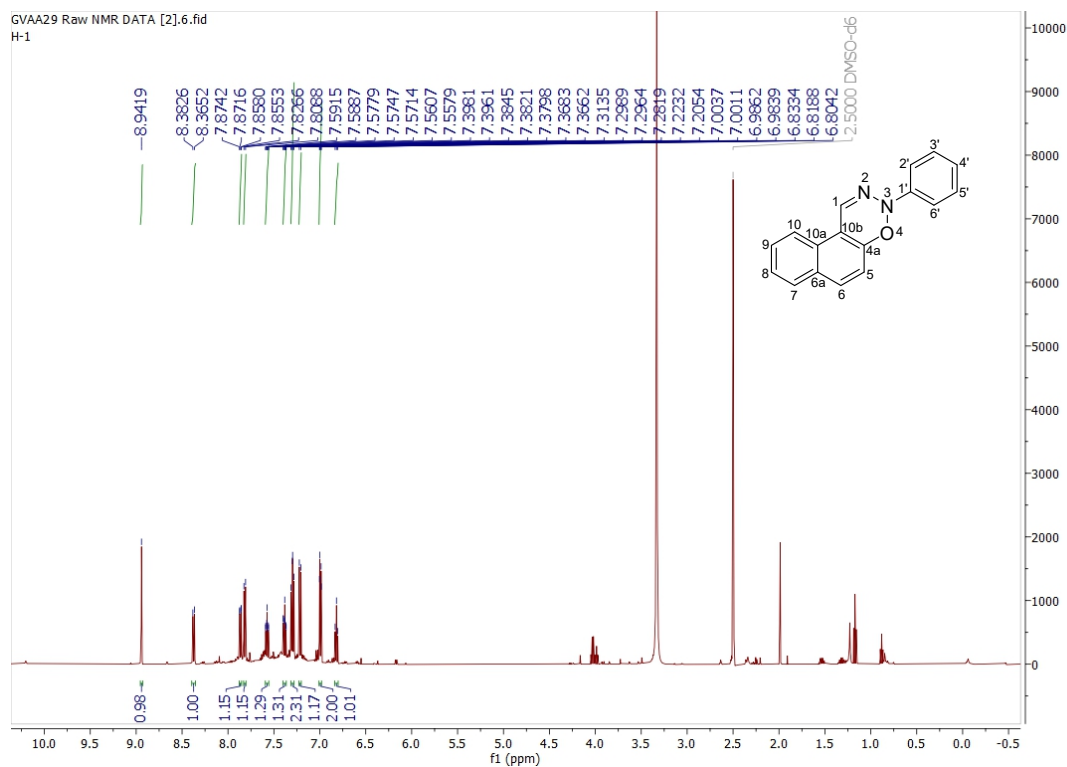


Figure S4. ^1H NMR (500 MHz) spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine (**5**) in $\text{DMSO-}d_6$ (expanded in the aromatic region)

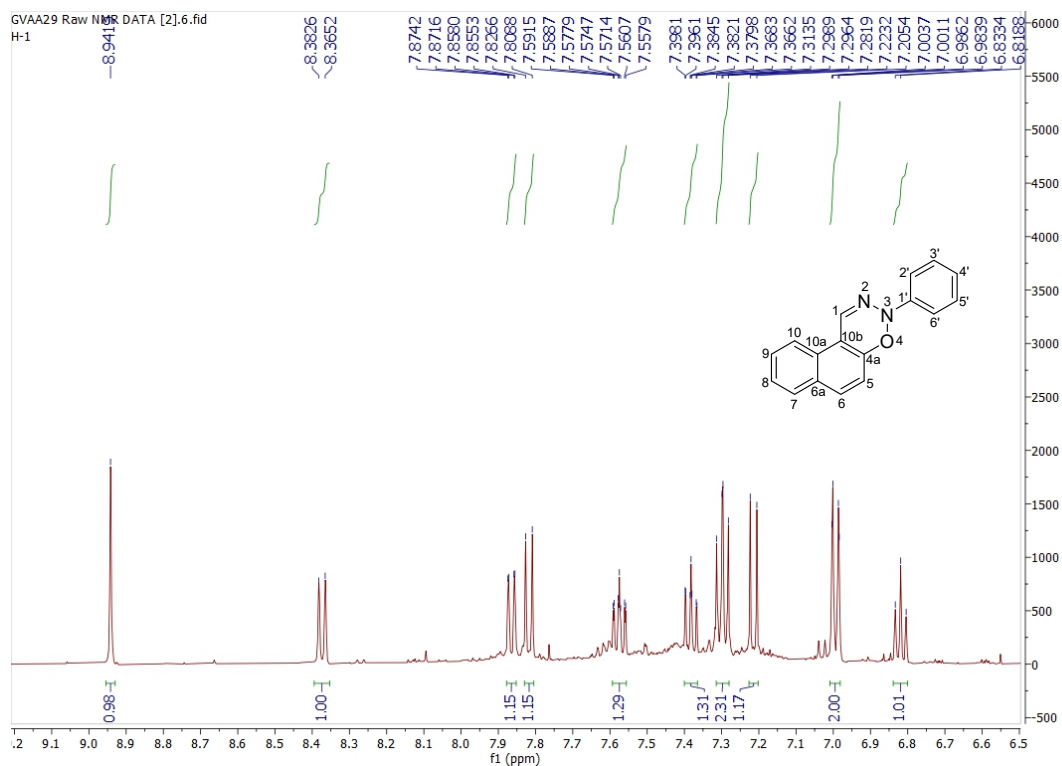


Figure S5. ^{13}C NMR (100.6 MHz) spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine (**5**) in $\text{DMSO-}d_6$

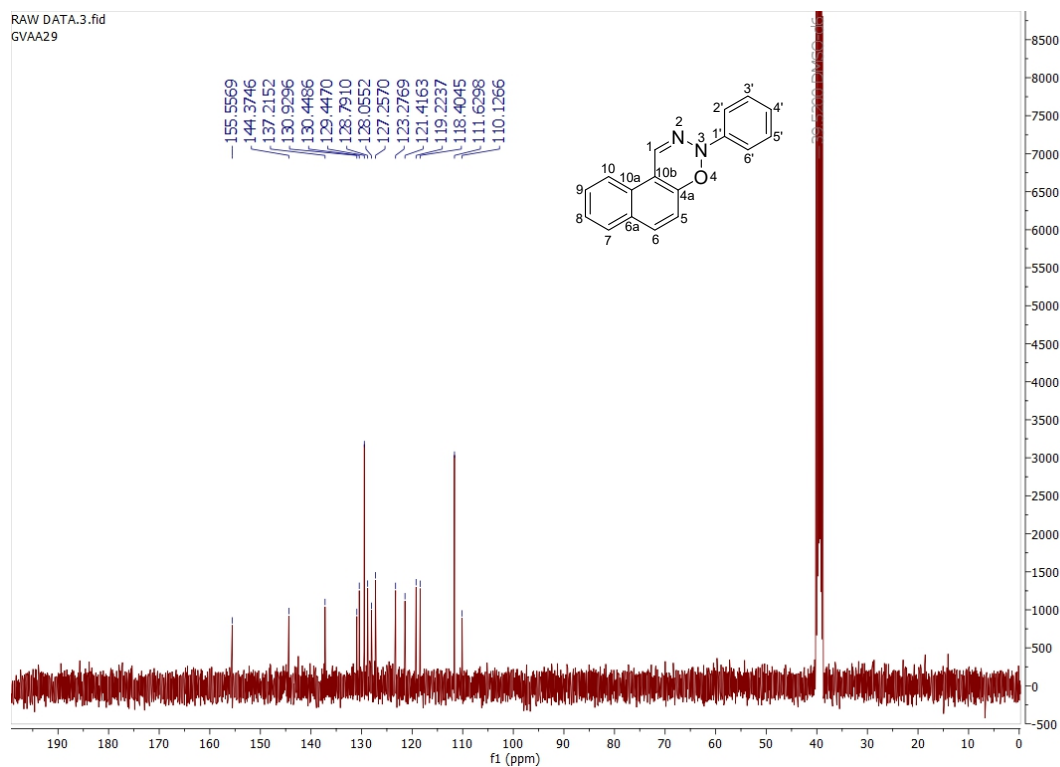


Figure S6. DEPT-90 NMR (100.6 MHz) spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine (**5**) in $\text{DMSO-}d_6$

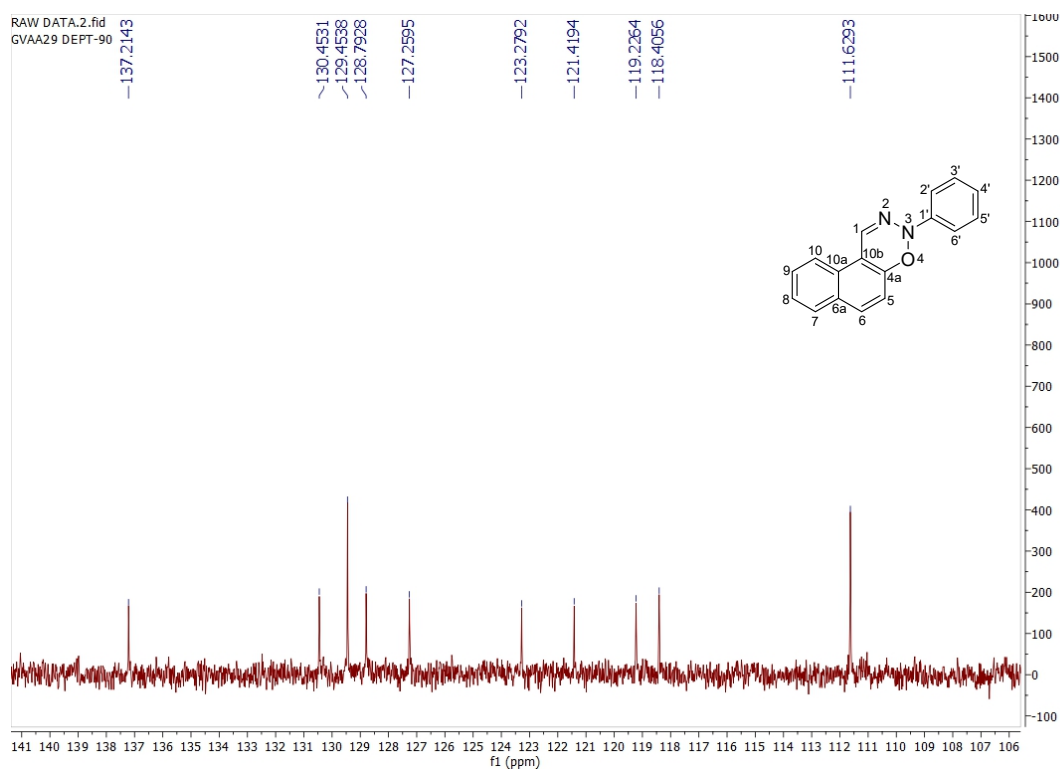


Figure S7. ^1H - ^1H TOCSY NMR (400 MHz) spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*]-[1,2,3]oxadiazine (**5**) in $\text{DMSO-}d_6$

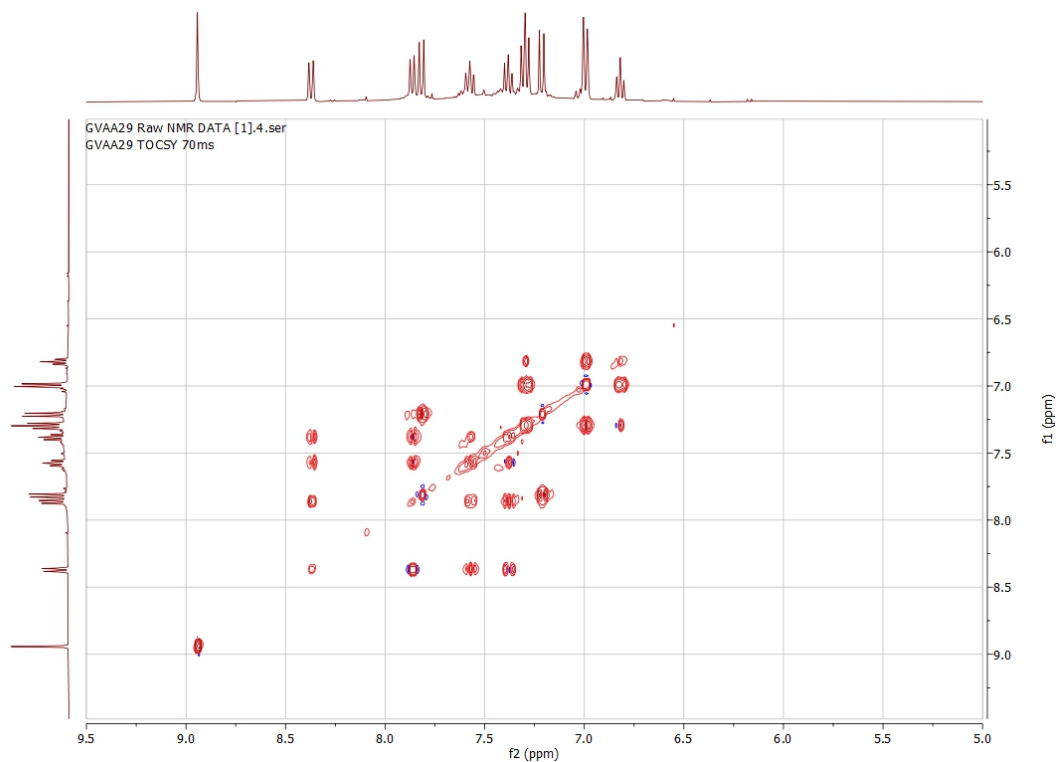


Figure S8. ^1H - ^1H NOESY NMR (400 MHz) spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*]-[1,2,3]oxadiazine (**5**) in $\text{DMSO-}d_6$

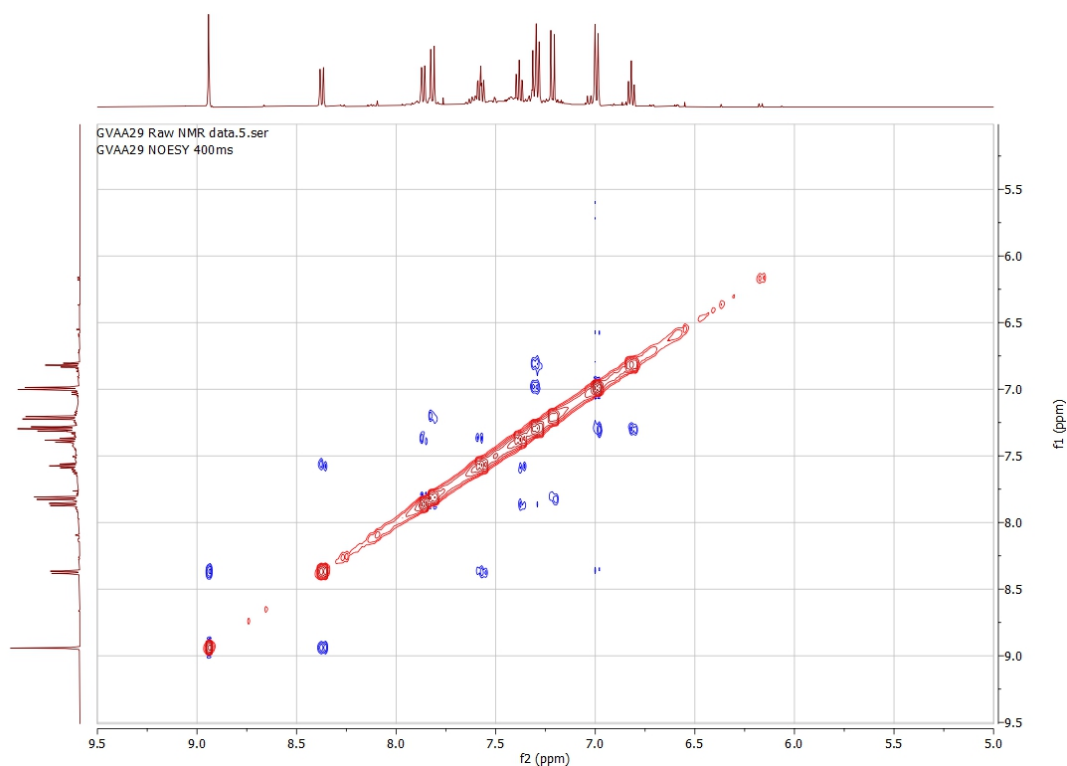


Figure S9. ^1H - ^{13}C HSQC NMR (500 MHz) spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine (**5**) in $\text{DMSO-}d_6$

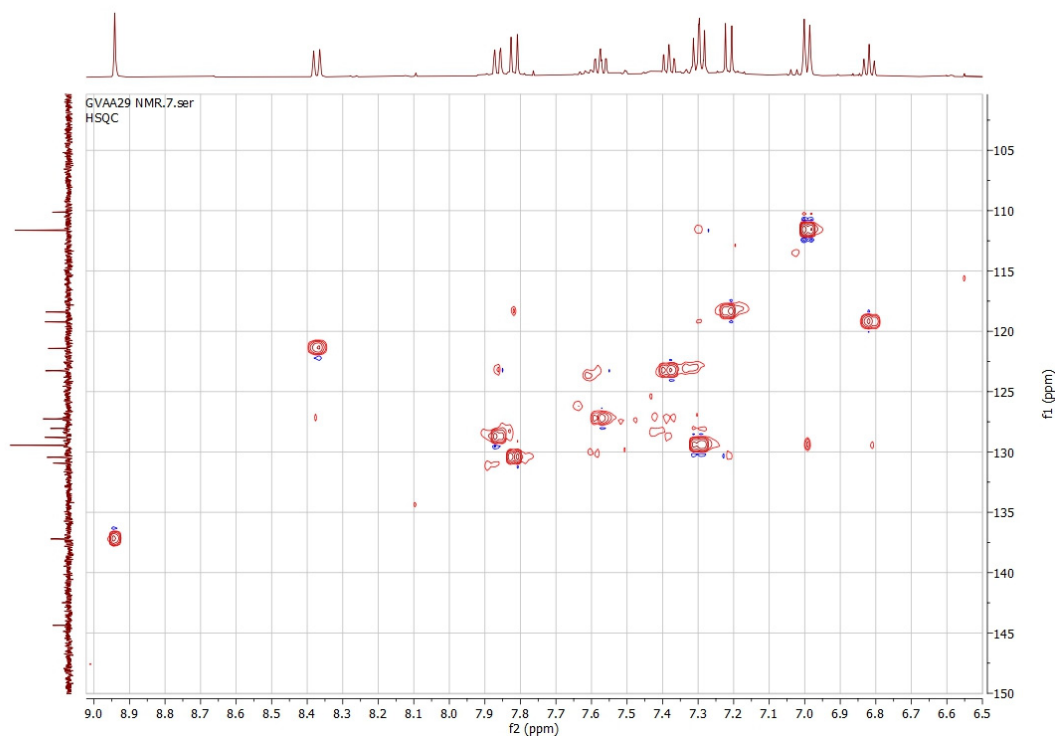


Figure S10. ^1H - ^{13}C HMBC NMR (500 MHz) spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine (**5**) in $\text{DMSO-}d_6$

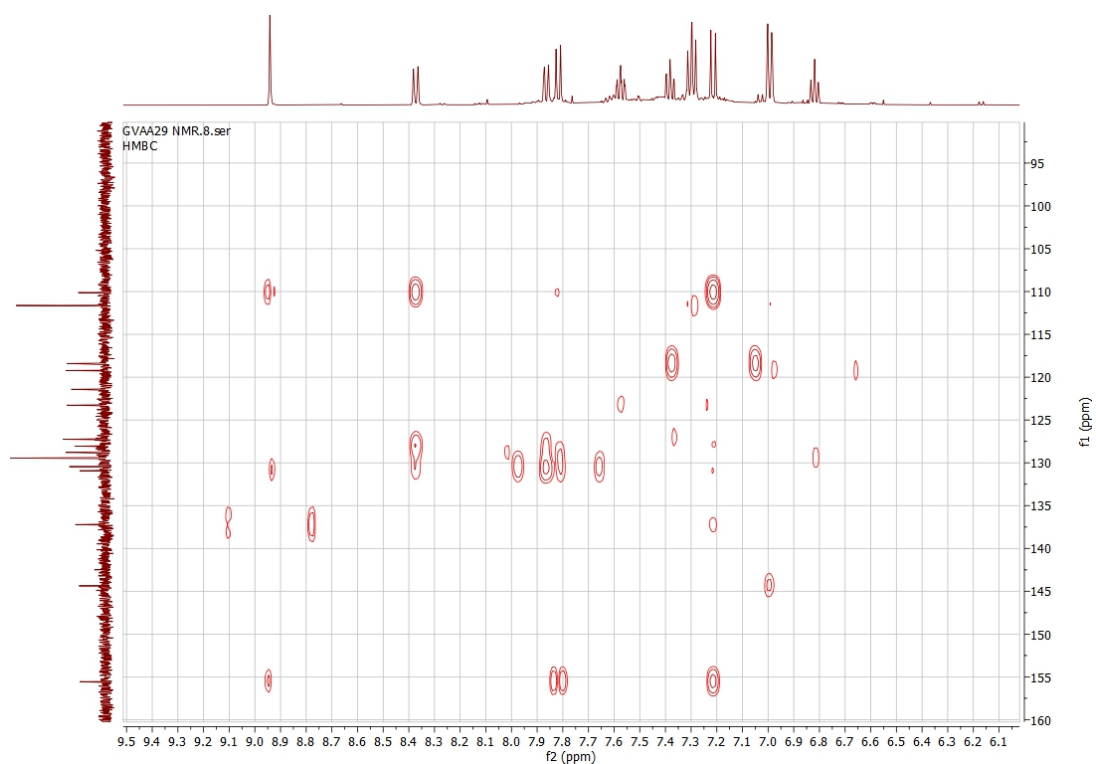


Figure S11. Complete ^1H and ^{13}C NMR chemical shift assignments (ppm) of 3-phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine (**5**).

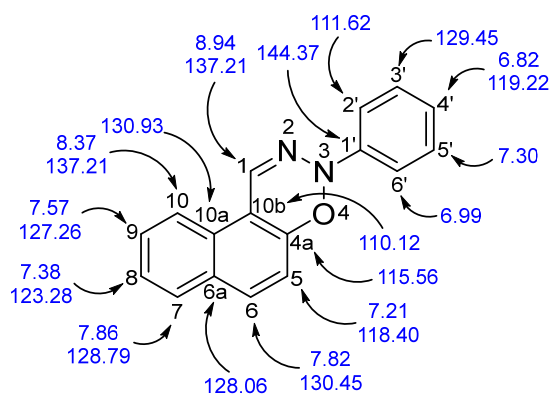


Figure S12. UV spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine (**5**) in MeCN

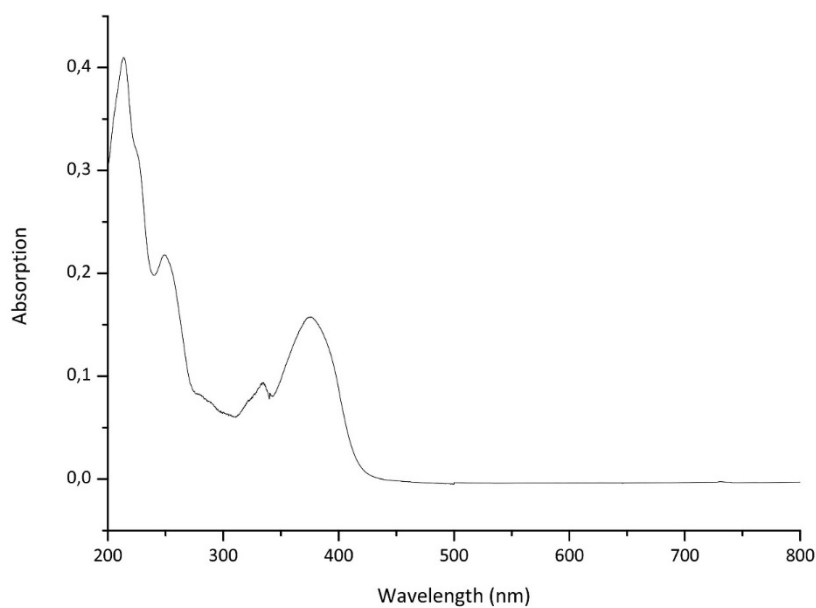


Figure S13. IR spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine (**5**) (solid state).

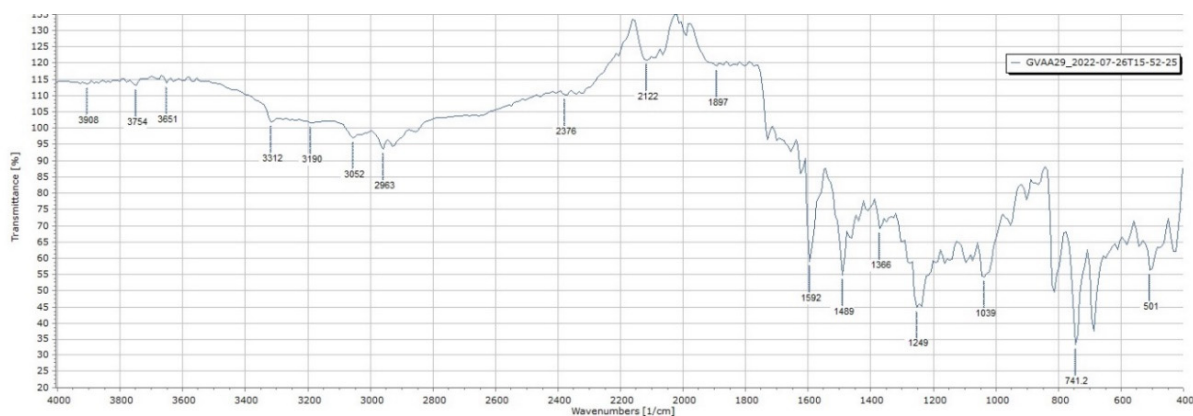


Figure S14. HRMS (ESI) spectrum of 3-phenyl-3*H*-naphtho[1,2-*e*][1,2,3]oxadiazine (**5**) in MeOH containing 0.1% HCOOH

