Supporting information

One-Pot Synthesis, Pharmacological Evaluation, docking study, and DFT calculations for selected imidazolidine-2,4-diones

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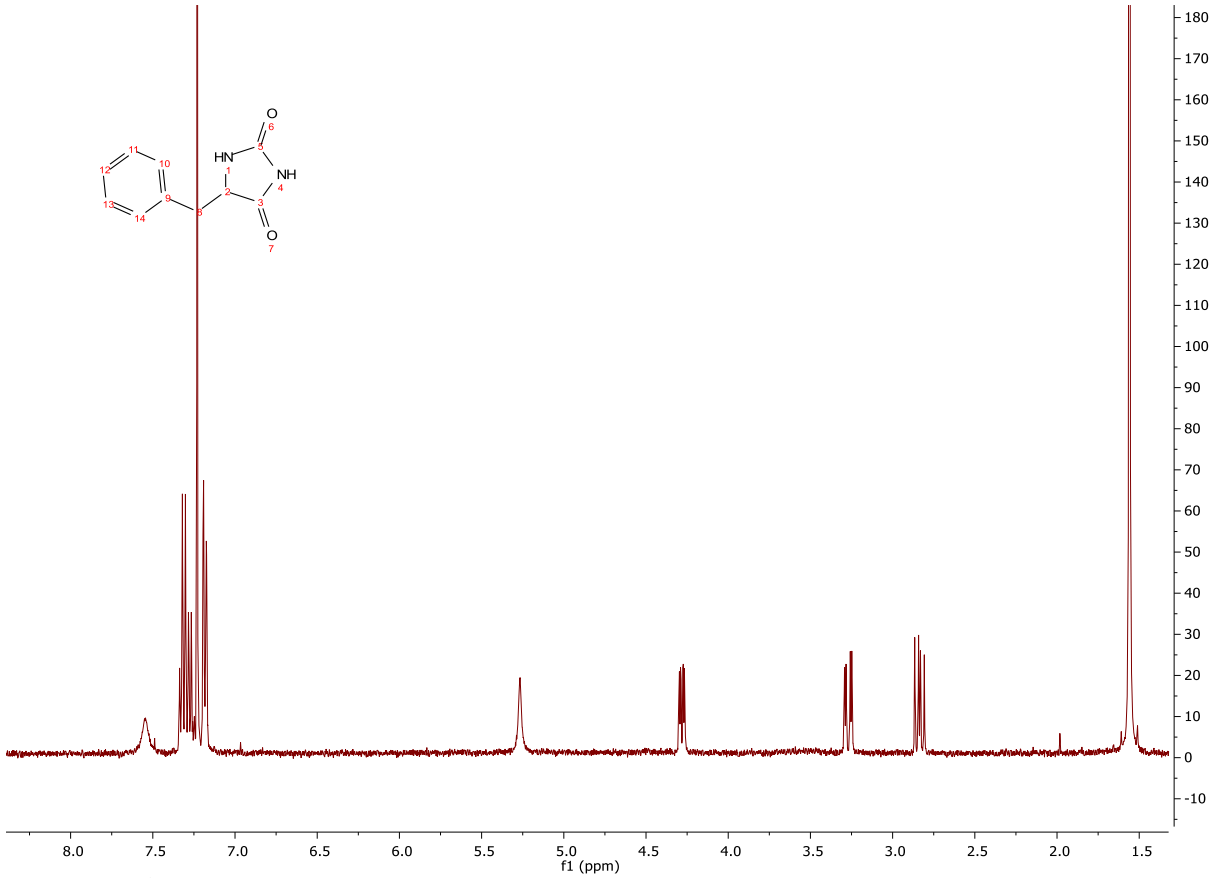


Figure S1: ^{1}H-NMR spectrum of **1**

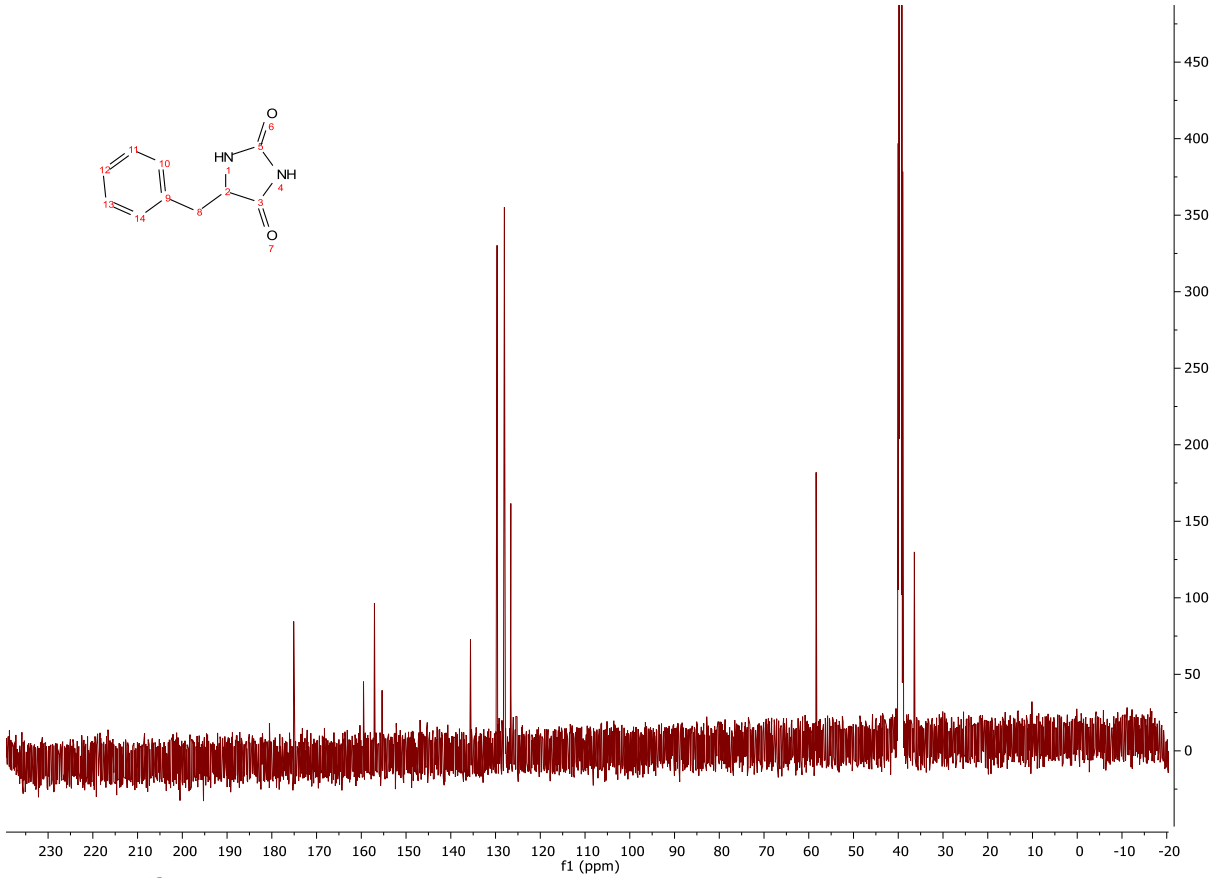


Figure S2: ^{13}C -NMR spectrum of **1**

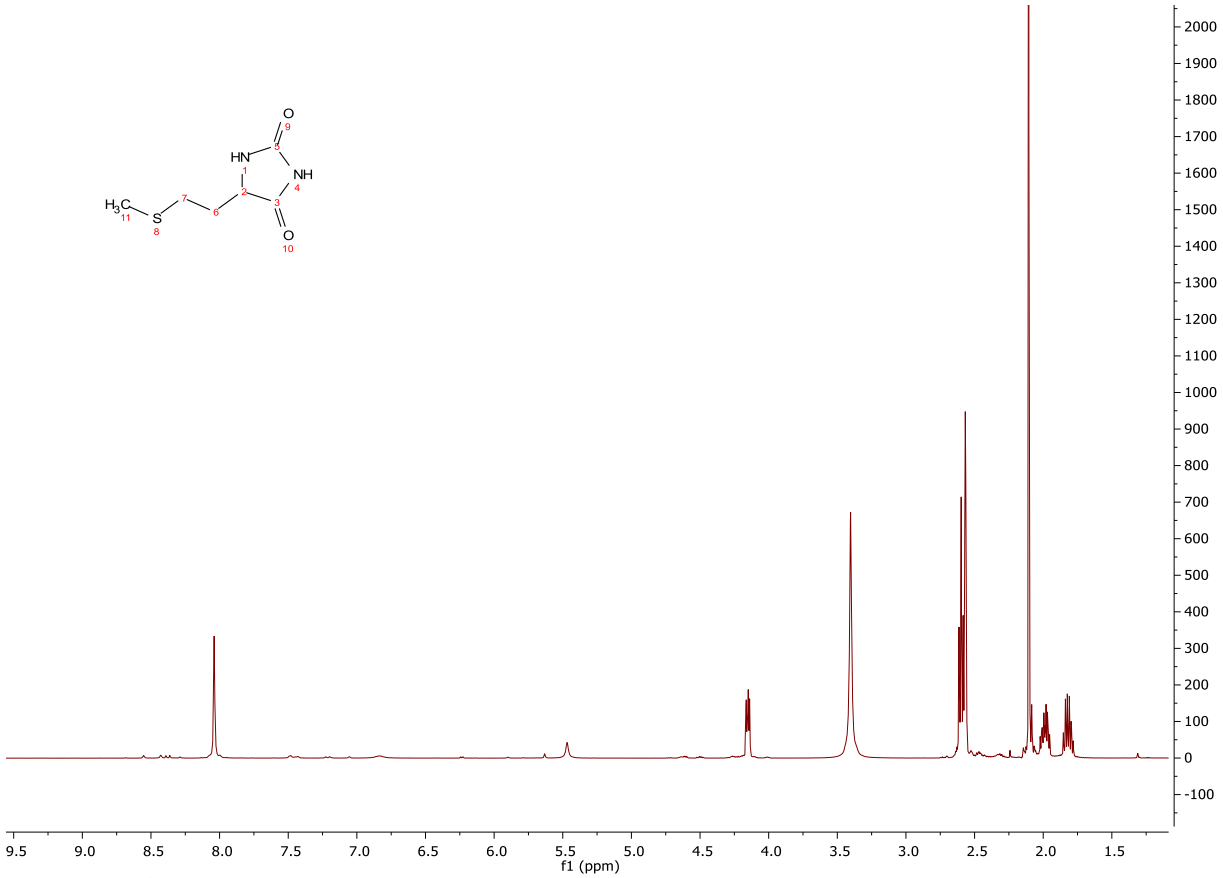


Figure S3: ^{1}H- NMR spectrum of **2**

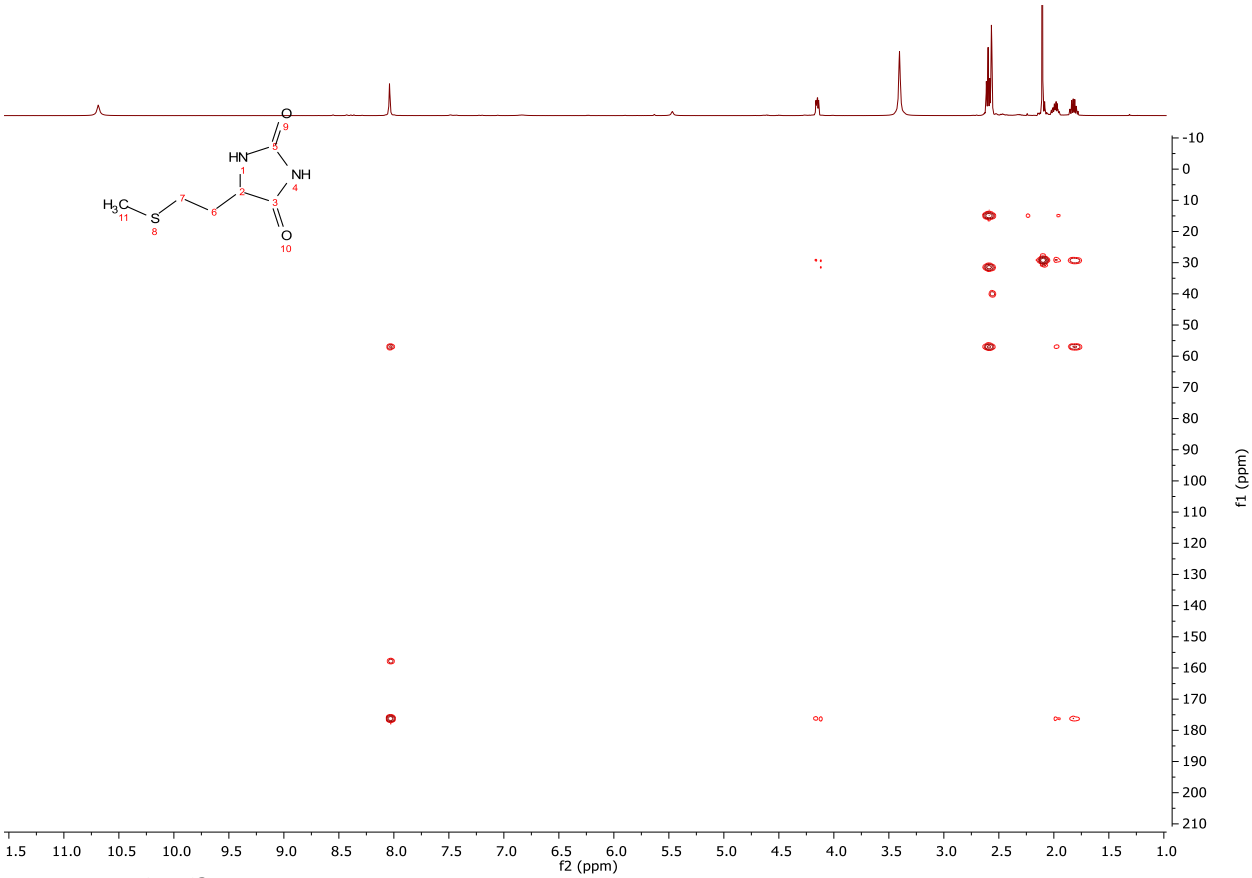


Figure S4: ^{1}H-^{13}C HMQC spectrum of natural abundance

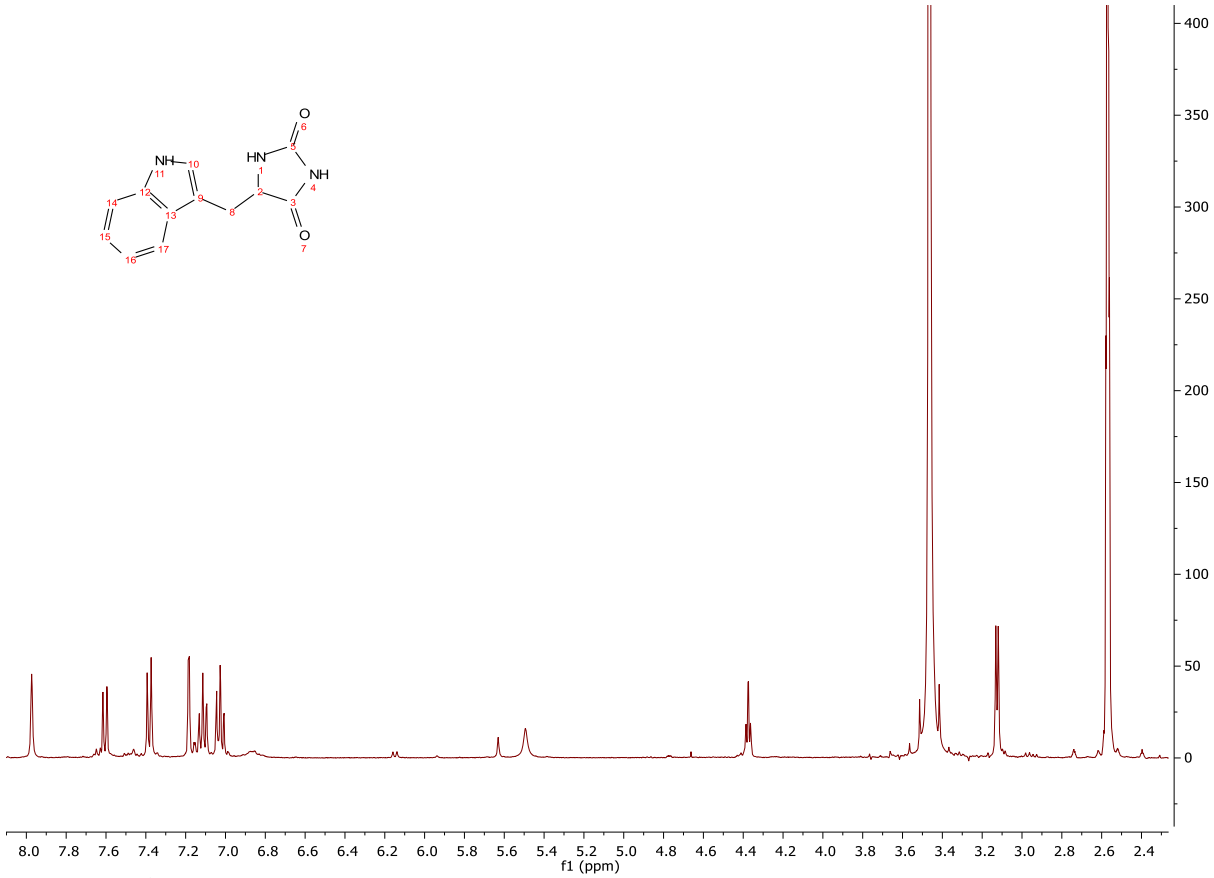


Figure S5: ^{1}H-NMR spectrum of **3**

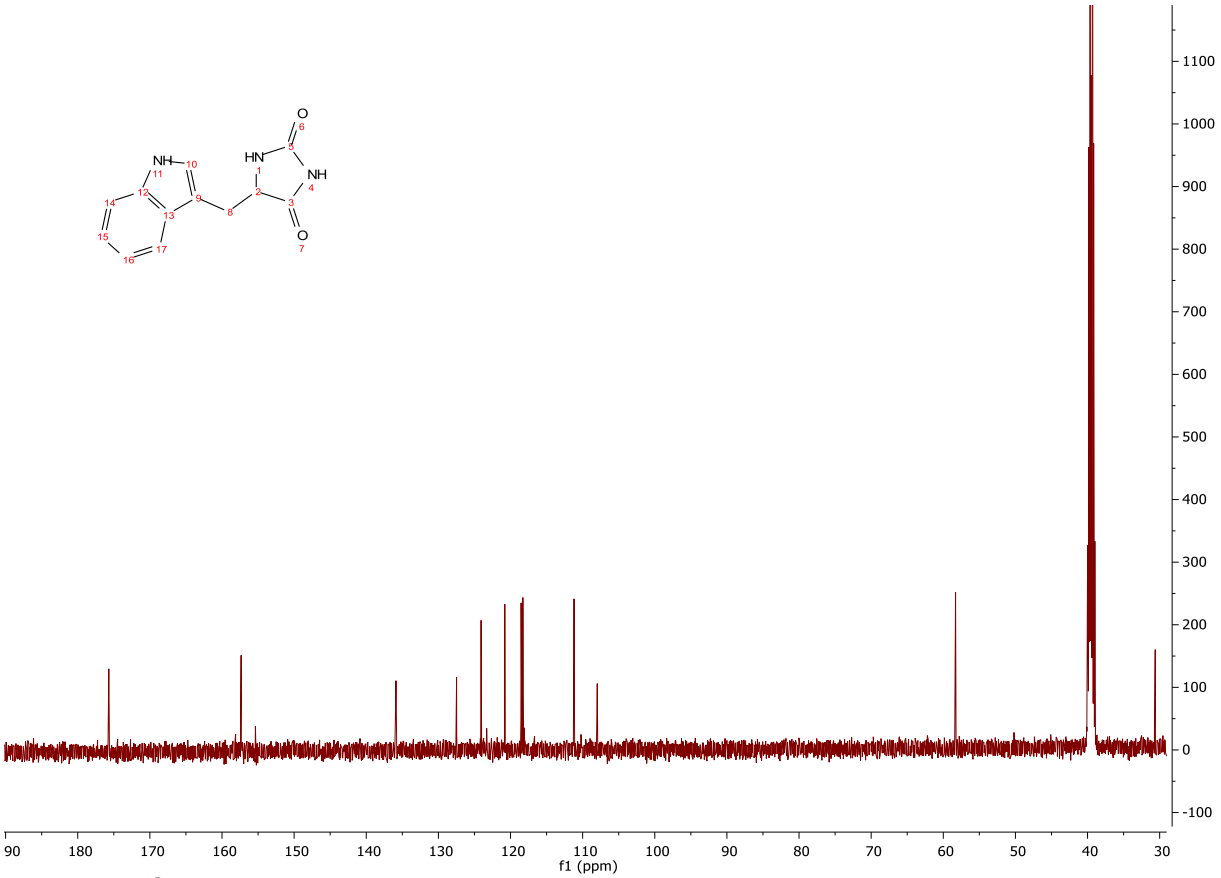


Figure S6: ^{13}C-NMR spectrum of **3**

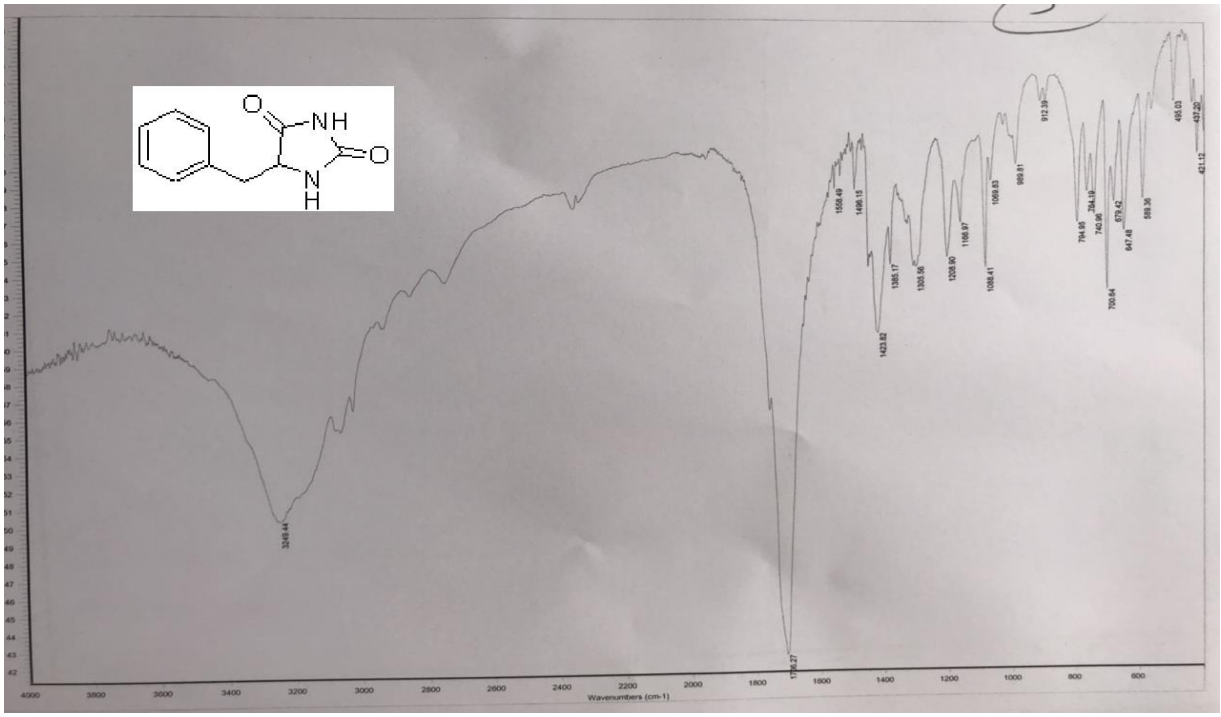


Figure S7: IR spectrum of **1**

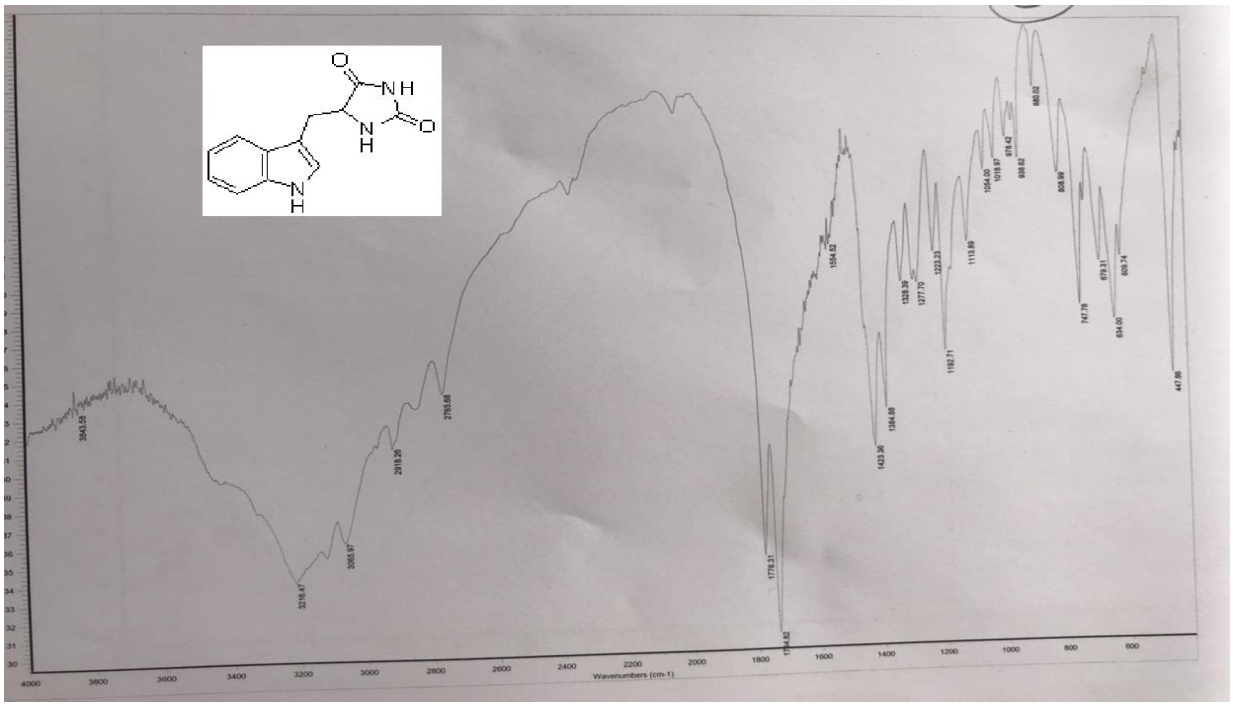
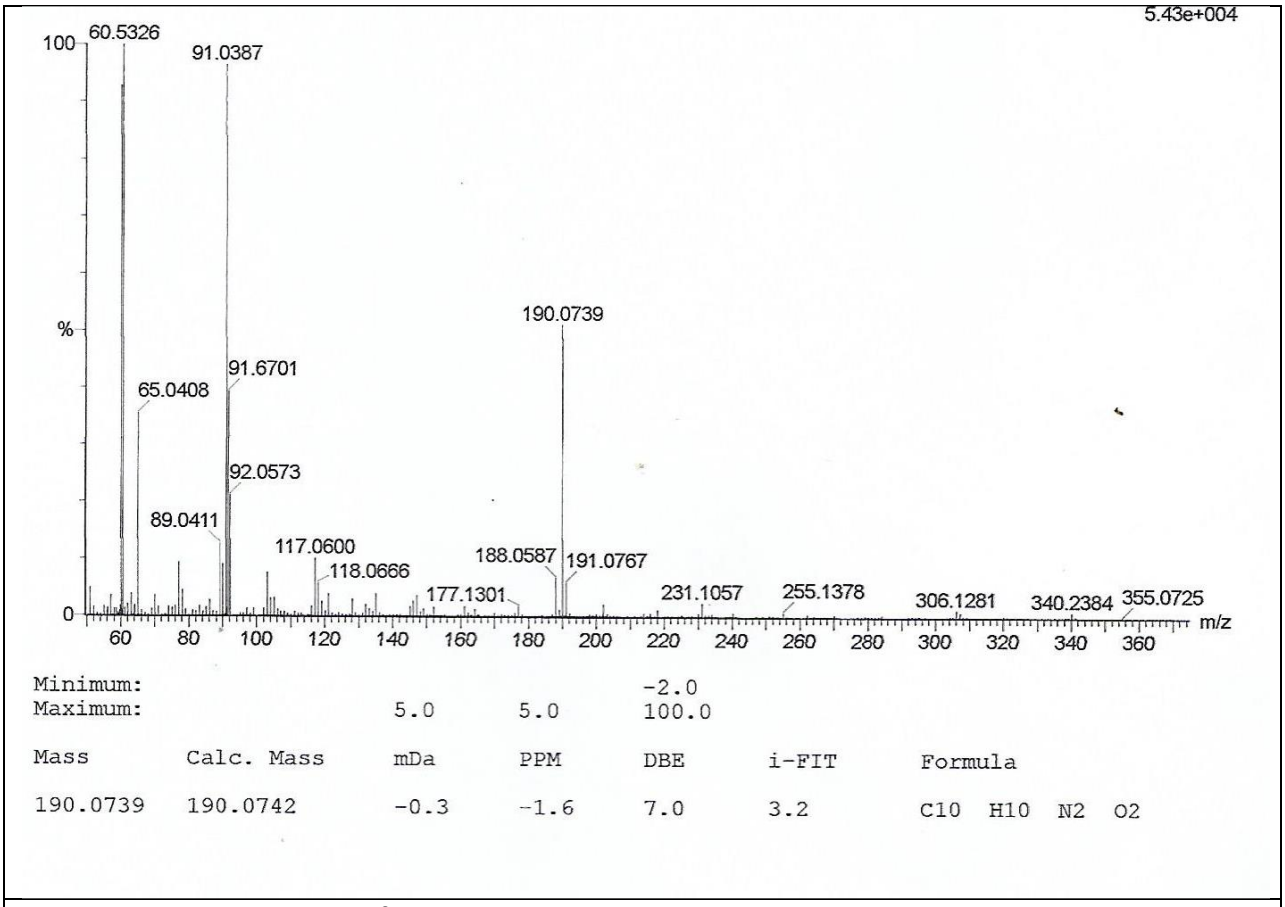
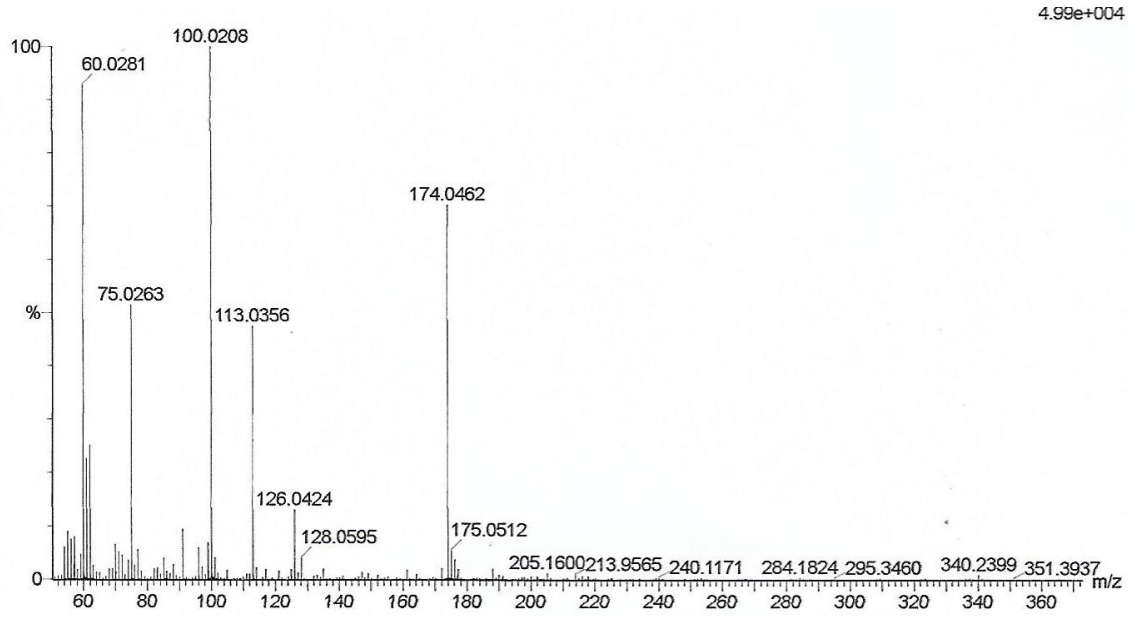


Figure S8: IR spectrum of **3**



Minimum:				-2.0		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
190.0739	190.0742	-0.3	-1.6	7.0	3.2	C10 H10 N2 O2

Figure S9: Mass spectrum of **1**



Minimum:				-2.0		
Maximum:		5.0	5.0	100.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
174.0462	174.0463	-0.1	-0.6	3.0	12.6	C6 H10 N2 O2 S

Figure S10: Mass spectrum of **2**

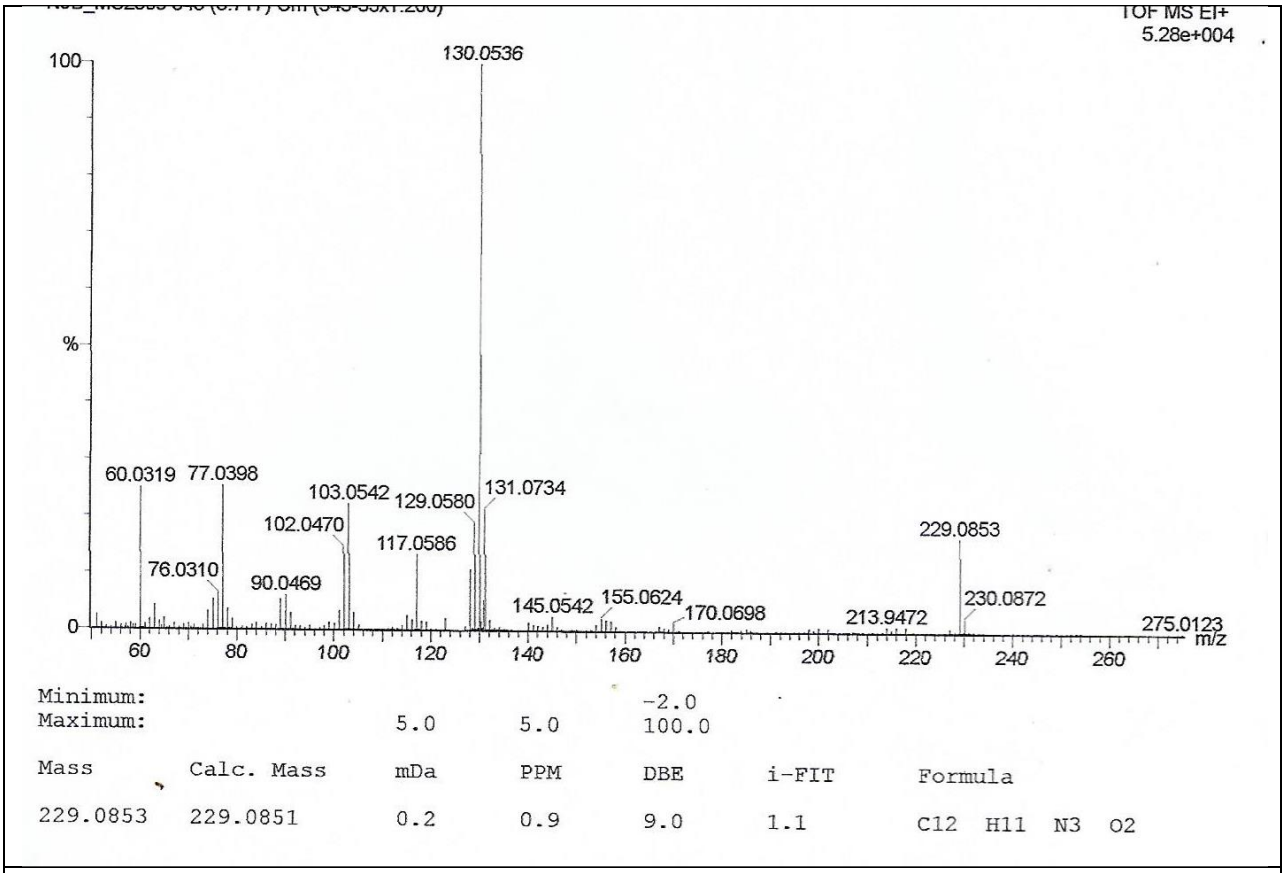
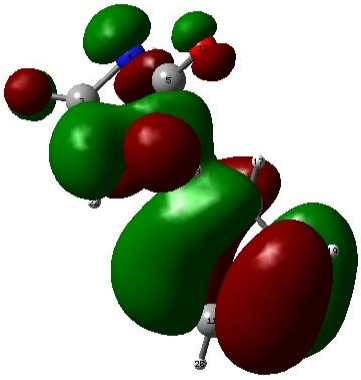


Figure S11: Mass spectrum of **3**

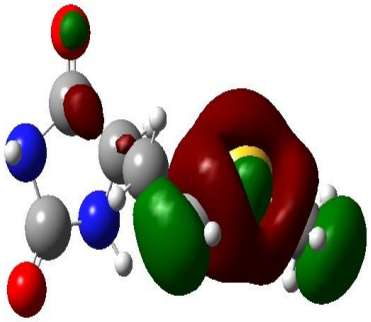
Table S1: Energy profile (in A.U) calculated at B3LYP with the 6-311þG(d,p) (R=H)		
Tautomeric form	Energy/ A.U	Dipole moment/ Debye
A	-375.2796	6.4897
B	-375.2377	7.2309
C	-375.2298	6.6671
D	-375.2730	5.6567
E	-374.7677	2.9735

Table S2: Relative E(Thermal), Zero-point vibration energy, Enthalpy, and heat capacity of **1**	
Sum of electronic and zero-point Energies	-646.703729/ A.U -
Zero-point vibrational energy	120.81299 (Kcal/Mol)
Sum of electronic and thermal Enthalpies=	-646.691471/A.U
E(Thermal)	127.912 (Kcal/Mol)
Constant volume molar heat capacity (CV)	43.630 Cal/Mol-Kelvin

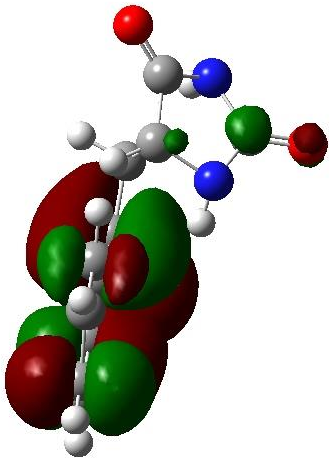
A



B



C



FigureS12: the frontier molecular orbitals HOMO and LUMO of compounds A) **1**, B) **2**, and C) **3**.