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A NEW HETEROCYCLIC COMPOUND FROM THE REACTION OF 9-METHYL-4,7-DIOXODODECANOIC ACID WITH HYDRAZINE

Chayanika Padumadasa[1*], G.M. Kamal B. Gunaherath[2], Ranga S. Jayakody[1] and Amila M. Abeysekera[1]

[1]Department of Chemistry, University of Sri Jayewardenepura, Sri Lanka
[2]Department of Chemistry, Open University of Sri Lanka, Sri Lanka
[*]chayanikapadumadasa@yahoo.com

Nitrogen containing heterocyclic compounds find many applications in the pharmaceutical industry. Here, we report the synthesis and characterization of a new N-heterocyclic compound by the reaction of 9-methyl-4,7-dioxododecanoic acid **(1)** and hydrazine **(2)** in aqueous ethanol. To the best of our knowledge the reported compound 1,9-diaza-5,9-didehydro-8-(2-methylpropyl)-bicylo[3.3.1]nonan-2-one **(3)** contains a previously unreported ring system. The structure of the compound was assigned on the basis of its GS-MS, ^{13}C, ^{1}H, COSY, HSQC, HMBC NMR and IR spectra. Reaction of 9-methyl-4,7-dioxododecanoic with hydrazine is shown in Figure 1.

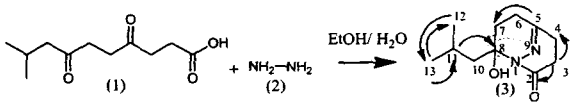

Figure 1: Reaction of 9-methyl-4,7-dioxododecanoic acid and hydrazine

The GC-MS showed a single peak on the chromatogram with a base peak at m/z 19 which corresponds to $[M-H_2O]^+$ ion. The ^{13}C NMR showed 11 signals indicating that all 1 carbons of the starting compound were incorporated in the product. Atoms C11 and C12 gave ris to two separate signals at δ 22.60 and δ 21.95. This assignment is supported by the presence of tw doublets centered at δ 0.895 and δ 0.865 which integrate for 3 H each in the ^{1}H NMR spectra. Th nonequivalence of the methyl groups arises due to the isobutyl group being attached to th asymmetric carbon C8 which occurred at δ 83.05. The observed chemical shift of the methylen carbon of the isobutyl group δ 46.38 was within the calculated range. The carbonyl carbon C2 wa seen at δ 170.55 and the carbon double bonded to N C3 at δ 159.65. The two CH2-CH2 fragment fell into two isolated ABXY systems and their respective protons gave rise to separate signals du to being incorporated into a conformationally rigid system with restricted free rotation. These signals were in the range of δ 1.5 – δ 2.8. Computational studies were carried out to assess th stability of the molecule. First the molecule was built using a molecular modeling softwa package and optimized using PM6semi-empirical level of theory. The optimized structure w used as the input for conformational analysis. Conformational analysis was carried out wi MMFF994s classical force field (FF) in the gas phase. The study showed that 3 is a stab molecule and has as its most stable conformation that shown in Figure 2.

Figure 2: Most stable conformer of
1,9-diaza-5,9-didehydro-8-(2-methylpropyl)-bicylo[3.3.1]nonan-2-one