| Title/Authors |  
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| **1** | **Structural Studies of Site Specific Mutants of p22HBP**  
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| **2** | **Studying the Metabolic Profiling of Potential Probiotic or Synbiotic Cheeses by NMR Spectroscopy**  
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| **3** | **Metabonomics of Pregnancy: An NMR Study of Maternal Urine**  
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<td><strong>Structure Determination of Some Oxygen and Nitrogen Heterocyclic Compounds by NMR</strong>&lt;br&gt;Raquel S. G. R. Seixas, Catia I. C. Esteves, Cristela M. Brito, Stéphanie B. Leal, Diana C. G. A. Pinto, Clementina M. M. Santos,&lt;br&gt;Ana M. L. Seca, Artur M. S. Silva, José A. S. Cavaleiro&lt;br&gt;1 Department of Chemistry &amp; QOPNA, University of Aveiro, 3810-193 Aveiro, Portugal&lt;br&gt;2 DCTD, University of Azores, 9501-801 Ponta Delgada, Açores&lt;br&gt;3 Department of Vegetal Production and Technology, School of Agriculture, Campus de Santa Apolónia, 5301-855 Bragança, Portugal</td>
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<td><strong>NMR Characterization of Novel Flavone-Nitrogen Heterocycle Conjugates</strong>&lt;br&gt;Regina M. S. Sousa, Diana C. G. A. Pinto, Artur M. S. Silva, Maria A. F. Faustino, Vanda Vaz Serra, Maria G. P. M. S. Neves, José A. S. Cavaleiro&lt;br&gt;1 Department of Chemistry &amp; QOPNA, University of Aveiro, 3810-193 Aveiro, Portugal</td>
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<td><strong>NMR Crystallography of Amoxicillin Trihydrate</strong>&lt;br&gt;S. M. Santos, J. Rocha, L. Mafra&lt;br&gt;1 Department of Chemistry, CICECO, University of Aveiro, 3810-193 Aveiro, Portugal</td>
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<td><strong>Solid-state NMR Techniques and Computational Methods Combined for the Assignment of Glutathione</strong>&lt;br&gt;Mariana Sardo, Renée Siegel, Sérgio M. Santos, João Rocha, José Richard B. Gomes and Luis Mafra&lt;br&gt;1 Department of Chemistry, CICECO, University of Aveiro, 3810-193 Aveiro, Portugal</td>
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<td><strong>Study of the Propylsulphonic Acid-functionalized PMO by High-resolution 1H Solid-State NMR Spectroscopy</strong>&lt;br&gt;R. Siegel, E. Domingues, R. De Sousa, F. Jérôme, C. M. Morais, N. Bion, P. Ferreira, L. Mafra&lt;br&gt;1 Department of Chemistry, CICECO, University of Aveiro, 3810-193 Aveiro, Portugal&lt;br&gt;2 Department of Ceramics and Glass Engineering, CICECO, University of Aveiro, 3810-193 Aveiro, Portugal&lt;br&gt;3 Laboratoire de Catalyse en Chimie Organique, University of Poitiers, 4 rue Michel Brunet, BP633 86022 Poitiers Cedex, France</td>
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**Structure determination of some oxygen and nitrogen heterocyclic compounds by NMR**

Raquel S. G. R. Seixas, Cáitia I. C. Esteves, Cristela M. Brito, Stéphanie B. Leal, Diana G. G. A. Pinto, Ania M. L. Seca, Artur M. S. Silva, José A. S. Cavaleiro

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**Introduction**

Oxygen heterocyclic compounds are widely distributed in Nature, being chromone and xanthone derivatives some examples. For instance, the xanthone ring system is a structural motif prevalent in higher plants such as those of Guttiferae and Gentianaceae families. Both natural and synthetic derivatives often endowed with interesting pharmacological properties, such as anti-inflammatory, anti-tumour and antioxidant activities. Chromones and chromone derivatives play an important role in the normal human diet, due to their significant anti-inflammatory, anti-cancer and antioxidant activities.

Nitrogen heterocyclic compounds are also widely distributed in Nature, being 4-quinolones a large group that can be found, mainly, in plants of the Rutaceae family. However, a great number of the well-known derivates are of synthetic origin and have been designed to be used as drugs, mainly for the treatment of tuberculosis.

In view of these important properties, we have dedicated our investigation in the establishment of new synthetic methods for these types of compounds and also for the assessment of their biological properties. Naturally, we devote special attention to the structural characterization, mainly by NMR experiments, not only to confirm the product structure but also to unequivocally establish their stereochemistry.

The aim of this communication is to report some of our studies on the structural characterization of heterocyclic compounds by NMR spectroscopy.

**Oxygen heterocyclic compounds**

**Scheme 1**

**Figure 1**

**Figure 2**

**Figure 3**

(9) Seixas, R. S. G. R.; Silva, A. M. S.; Alkorta, I.; Elguero, J. Monatsh. Chem. 2011, 142, 446.

**Nitrogen heterocyclic compounds**

**Scheme 2**

**Figure 4**

**Figure 5**

**Figure 6**

(9) Seixas, R. S. G. R.; Silva, A. M. S.; Alkorta, I.; Elguero, J. Monatsh. Chem. 2011, 142, 446.