**Hírlevél**

**MTA Szénhidrát, Nukleinsav és Antibiotikumkémiai Munkabizottság**

**2018. január**

1. **A munkabizottsági ülés időpontja:**

**2018. május 23.-25. (szerda-péntek)**

**Meghívott előadók:**

**Jitka Moravcova (Prága, VSCHT)**

**Carlo Unverzagt (Universität Bayreuth)**

1. A Munkabizottság nagy szeretettel gratulál **Szente Lajos** Professzor Úrnak a **Gábor Dénes-Díjhoz**, melyet december 14-én adtak át a Parlamentben munkássága elismeréseként.
2. Gratulálunk **Vágvölgyiné Tóth Mariettának** és **Lázár Lászlónak** a habilitált doktori fokozat megszerzéséhez.
3. **A Munkabizottság tagjainak eredményei, megjelent közleményei** (a teljesség igénye nélkül)**:**

**Boosting the NMR assignment of carbohydrates with clean in-phase correlation experiments**

**Tamás Gyöngyösi, István Timári, Jens Haller, Martin R.M. Koos, Burkhard Luy and Katalin E. Kövér**

**ChemPlusChem, 2018, DOI: 10.1002/cplu.201700452**

Abstract

We report novel CLIP-COSY based homo- and heteronuclear correlation experiments for the rapid, semi-automated NMR assignment of small-to-medium-sized molecules. The homonuclear CLIP-COSY and corresponding relayed experiments employ the perfect-echo based mixing sequence for in-phase coherence transfer between directly and/or indirectly coupled proton spins. The combined analysis of the resulting CLIP-COSY and relayed spectra allows to easily track down layer by layer the proton-proton connectivity network. In larger molecular structures the narrow chemical shift range of protons may, however, compromise the efficacy of the homonuclear correlation based assignment strategy. To overcome this inherent limitation, we have devised an HSQC-variant of the CLIP-COSY experiment that takes advantage of the larger chemical shift range of the heteronucleus. We demonstrate that combined treatment of HSQC-CLIP-COSY(-relayed) and standard HSQC spectra facilitates simultaneous and semi-automatic assignment of 1H and 13C resonances of medium-sized molecules, such as pentasaccharides. Besides, the recently introduced PSYCHE broadband homonuclear decoupling scheme has been also implemented into the devised homo- and heteronuclear CLIP-COSY based experiments, resulting in fully decoupled high resolution pure-shift correlation spectra.

**Gita Jančaříková, Mihály Herczeg, Eva Fujdiarová, Josef Houser, Katalin E. Kövér, Anikó Borbás, Michaela Wimmerová and Magdolna Csávás**

**Synthesis of -L-fucopyranoside-presenting glycoclusters and investigation of their interaction with Photorhabdus asymbiotica lectin (PHL)**

**Chemistry - A European Journal, 2018, Doi: 10.1002/chem.201705853**

Abstract: *Photorhabdus asymbiotica* is gram-negative bioluminescent bacteria that is not only as effective an insect pathogen as other members of the genus, but also a bacterium that causes serious diseases in humans. The recently identified bangle lectin PHL from *P. asymbiotica* verifiably modulates an immune response of humans and insects, which supports the idea that the lectin might play an important role in the host-pathogen interaction. Dimeric PHL contains up to seven l-fucose specific binding sites per monomer, and in order to target multiple binding sites of PHL, α-L-fucoside-containing di-, tri- and tetravalent glycoclusters were synthesized. Methyl gallate and pentaerythritol were chosen as multivalent scaffolds, and the fucoclusters were built from the above-mentioned cores by coupling with different oligoethylene bridges and propargyl α-l-fucosides using 1,3-dipolar azide-alkyne cycloaddition. The interaction between fucoside derivates and PHL was investigated by several biophysical and biological methods, ITC and SPR measurements, hemagglutination inhibition assay and an investigation of bacterial aggregation properties were carried out. Moreover, details of the interaction between PHL and propargyl α-L-fucoside as a monomer unit were revealed using X-ray crystallography. Besides this, the interaction with multivalent compounds was studied by NMR techniques. The newly synthesized multivalent fucoclusters proved to be up to several orders of magnitude better ligands than the natural ligand, L-fucose.

**Carotenoid glycoside isolated and identified from cyanobacterium Cylindrospermopsis raciborskii**

**Veronika Nagy, Attila Agócs, József Deli, Gergely Gulyás-Fekete, Tünde-Zita Illyés, Tibor Kurtán, Erika Turcsi, Szabolcs Béni, Miklós Dékány, Andreas Ballot, Gábor Vasas**

**Journal of Food Composition and Analysis 2018, 65, 6-10.**

Abstract

The freshwater cyanobacterium *Cylindrospermopsis raciborskii* was investigated for carotenoid composition. Besides β-carotene, echinenone and canthaxanthin an unknown carotenoid was found to be the main component. This compound was isolated and subsequently acetylated for structural elucidation. The acetyl derivative was fully characterized by UV-Vis, NMR and HRMS techniques. The detailed 1H and 13C NMR chemical shift assignment of the unknown carotenoid supported the unequivocal identification of 2-hydroxy-(3R,2’S)-myxol 2’-α-L-fucoside.

**Characterization of Cladosporols from the Marine Algal-Derived Endophytic Fungus Cladosporium cladosporioides EN-399 and Configurational Revision of the Previously Reported Cladosporol Derivatives**

**Hong-Lei Li, Xiao-Ming Li, Attila Mándi, Sándor Antus, Xin Li, Peng Zhang, Yang Liu, Tibor Kurtán, Bin-Gui Wang**

**J. Org. Chem. 2017, 82, 9946-9954.**

Abstract: Four new cladosporol derivatives, cladosporols F−I (1−4), the known cladosporol C (5), and its new epimer, cladosporol J (6), were isolated and identified from the marine algal-derived endophytic fungus *Cladosporium cladosporioides* EN-399. Their structures were determined by detailed interpretation of NMR and MS data, and the absolute configurations were established on the basis of TDDFT-ECD and OR calculations. The configurational assignment of cladosporols F (1) and G (2) showed that the previously reported absolute configuration of cladosporol A and all the related cladosporols need to be revised from (4’R) to (4’S). Compounds 1−6 showed antibacterial activity against Escherichia coli, Micrococcus luteus, and Vibrio harveyi with MIC values ranging from 4 to 128 μg/mL. Compound 3 showed significant cytotoxicity against A549, Huh7, and LM3 cell lines with IC50 values of 5.0, 1.0, and 4.1 μM, respectively, and compound 5 showed activity against H446 cell line with IC50 value of 4.0 μM.

**Dynamic Kinetic Resolution of Ethyl 1,2,3,4-Tetrahydro-β-carboline-1-carboxylate: Use of Different Hydrolases for Stereocomplementary Processes**

**Rita Megyesi, Attila Mándi, Tibor Kurtán, Enikő Forró, Ferenc Fülöp**

**Eur. J. Org. Chem. 2017, 4713-4718.**

Abstract: Both enantiomers of 1,2,3,4-tetrahydro-β-carboline-1-carboxylic acid have been prepared by dynamic kinetic resolution of the corresponding ethyl ester (±)-1. CAL-B-catalysed hydrolysis of (±)-1·HCl in NH4OAc buffer (pH 8.0, 30 °C) provided amino acid (R)-2·HCl with 98 % ee and 90 % yield in 20 min. The hydrolysis with Alcalase in borate buffer (pH 8.0, 30 °C) showed S selectivity and the product (S)-2·HCl was obtained with 60 % ee and 66 % yield in 45 h. The absolute configuration of (S)-2 was determined by TDDFT electronic circular dichroism and optical rotation calculations.

*A havi rendszerességű hírlevélben megjelentetni kívánt anyagot kérjük minden hónap utolsó napjáig elküldeni a* *csavas.magdolna@science.unideb.hu* *email címre.*

 ***Eredményekben és sikerekben gazdag új évet kívánok!***

Üdvözlettel: Csávás Magdolna

 a munkabizottság titkára

2018. január 18.