

**Szerves Kémiai Intézet 2016-ben megjelent publikációi**  
(Frissítve:2017. április 11.)

1. Ábrányi-Balogh P , Jablonkai E , Henyecz R , Milen M , Keglevich G  
Theoretical calculations on the mechanism of the T3P®-promoted esterification and amidation of phosphinic acids  
*CURRENT ORGANIC CHEMISTRY* 20:(10) pp. 1135-1142. (2016)  
Link(ek): [\\$ DOI](#), [WoS](#), [Scopus](#)
2. Ábrányi-Balogh P , Földesi T , Grün A , Volk B , Keglevich G , Milen M  
Synthetic study on the T3P®-promoted one-pot preparation of 1-substituted-3,4-dihydro-β-carbolines by the reaction of tryptamine with carboxylic acids  
*TETRAHEDRON LETTERS* 57:(18) pp. 1953-1957. (2016)  
Link(ek): [\\$ DOI](#), [WoS](#), [Scopus](#)
3. Abranyi-Balogh Peter , Volk Balazs , Keglevich Gyorgy , Milen Matyas  
Computational study on the synthesis of 1-phenyl-3,4-dihydro-β-carboline: T3P-promoted one-pot formation from tryptamine vs. POCl<sub>3</sub>-mediated ring closure of Nb-benzoyltryptamine. The first DFT investigation of the Bischler-Napieralski reaction  
*COMPUTATIONAL AND THEORETICAL CHEMISTRY* 1097: pp. 48-60. (2016)  
Link(ek): [\\$ DOI](#), [WoS](#), [Scopus](#)
4. Ádám Madarász , Zsolt Dósa , Szilárd Varga , Tibor Soós , Antal Csámpai , Imre Pápai  
Thiourea Derivatives as Bronsted Acid Organocatalysts  
*ACS CATALYSIS* 6: pp. 4379-4387. (2016)  
Link(ek): [REAL](#), [\\$ DOI](#), [WoS](#), [Scopus](#), [Egyéb URL](#)
5. Andrić Filip , Bajusz Dávid , Rácz Anita , Šegan Sandra , Héberger Károly  
Multivariate assessment of lipophilicity scales—computational and reversed phase thin-layer chromatographic indices  
*JOURNAL OF PHARMACEUTICAL AND BIOMEDICAL ANALYSIS* 127: pp. 81-93. (2016)  
Link(ek): [REAL](#), [DOI](#), [WoS](#)
6. Aradi Klára , Bombicz Petra , Novák Zoltán  
Modular Copper-Catalyzed Synthesis of Chromeno[4,3-b]quinolines with the Utilization of Diaryliodonium Salts  
*JOURNAL OF ORGANIC CHEMISTRY* 81:(3) pp. 920-931. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#), [Scopus](#), [Egyéb URL](#)
7. Bagi P , Karaghiosoff K , Czugler M , Hessz D , Kállay M , Kubinyi M , Szilvási T , Pongrácz P , Kollár L , Timári I , Kövér KE , Drahos L , Fogassy E , Keglevich G  
Synthesis, Characterization, and Application of Platinum(II) Complexes Incorporating Racemic and Optically Active 4-Chloro-5-Methyl-1-Phenyl-1,2,3,6-Tetrahydrophosphinine Ligand  
*HETEROATOM CHEMISTRY* 27:(2) pp. 91-101. (2016)  
Link(ek): [REAL](#), [\\$ DOI](#), [WoS](#), [Scopus](#), [SciFinder](#)
8. Bajusz D , Ferenczy GG , Keseru GM  
Discovery of Subtype Selective Janus Kinase (JAK) Inhibitors by Structure-Based Virtual Screening  
*JOURNAL OF CHEMICAL INFORMATION AND MODELING* 56:(1) pp. 234-247. (2016)  
Link(ek): [DOI](#), [WoS](#), [Scopus](#)
9. Bajusz Dávid , Ferenczy György G , Keserű György M  
Ensemble docking-based virtual screening yields novel spirocyclic JAK1 inhibitors  
*JOURNAL OF MOLECULAR GRAPHICS AND MODELLING* 70: pp. 275-283. (2016)  
Link(ek): [DOI](#)
10. Bako I , Mayer I  
On Dipole Moments and Hydrogen Bond Identification in Water Clusters  
*JOURNAL OF PHYSICAL CHEMISTRY A* 120:(25) pp. 4408-4417. (2016)  
Link(ek): [REAL](#), [\\$ DOI](#), [WoS](#)
11. Bako Imre , Mayer Istvan  
Hierarchy of the Collective Effects in Water Clusters  
*JOURNAL OF PHYSICAL CHEMISTRY A* 120:(4) pp. 631-638. (2016)  
Link(ek): [REAL](#), [PubMed](#), [DOI](#), [WoS](#)

12. Bártai-Konczos A , Veres Z , Szabó M , Ioja E , László G , Török G , Homolya L , Jemnitz K  
Comparative study of CYP2B1/2 induction and the transport of bilirubin and taurocholate in rat hepatocyte-mono- and hepatocyte-Kupffer cell co-cultures  
*JOURNAL OF PHARMACOLOGICAL AND TOXICOLOGICAL METHODS* 82: pp. 1-8. (2016)  
Link(ek):  [REAL](#), [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)
13. Bazso FL , Ozohanics O , Schlosser G , Ludanyi K , Vekey K , Drahos L  
Quantitative Comparison of Tandem Mass Spectra Obtained on Various Instruments  
*JOURNAL OF THE AMERICAN SOCIETY FOR MASS SPECTROMETRY* 27:(8) pp. 1357-1365. (2016)  
Link(ek):  [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)
14. Bence Hégyely , Péter R Nagy , György G Ferenczy , Mihály Kállay  
Exact density functional and wave function embedding schemes based on orbital localization  
*JOURNAL OF CHEMICAL PHYSICS* 145:(6) Paper 064107. (2016)  
Link(ek):  [REAL](#), [DOI](#), [WoS](#), [Scopus](#)
15. Benedek A , Horvath A , Hirmondo R , Ozohanics O , Bekesi A , Modos K , Revesz A , Vekey K , Nagy GN , Vertessy BG  
Potential steps in the evolution of a fused trimeric all-beta dUTPase involve a catalytically competent fused dimeric intermediate.  
*FEBS JOURNAL* 283:(18) pp. 3268-3286. (2016)  
Link(ek):  [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)
16. Berkes Barbara , Ozsváth Kristóf , Molnár Laura , Gáti Tamás , Holczbauer Tamás , Kardos György , Soós Tibor  
Expedient and Diastereodivergent Assembly of Terpenoid Decalin Subunits having Quaternary Stereocenters through Organocatalytic Robinson Annulation of Nazarov Reagent  
*CHEMISTRY-A EUROPEAN JOURNAL* 22:(50) pp. 18101-18106. (2016)  
Link(ek):  [REAL](#), [DOI](#)
17. Bihari T , Babinszki B , Gonda Z , Kovacs S , Novak Z , Stirling A  
Understanding and Exploitation of Neighboring Heteroatom Effect for the Mild N-arylation of Heterocycles with Diaryliodonium Salts under Aqueous Conditions: A Theoretical and Experimental Mechanistic Study.  
*JOURNAL OF ORGANIC CHEMISTRY* 81:(13) pp. 5417-5422. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)
18. Bombicz Petra  
Gyógyszeralapanyagok krisztallográfiai vizsgáló módszerei: -  
*GYÓGYSZERÉSZET* 60:(3) pp. 133-139. (2016)
19. Chernichenko K , Lindqvist M , Kotai B , Nieger M , Sorochkina K , Papai I , Repo T  
Metal-Free sp<sup>2</sup>-C-H Borylation as a Common Reactivity Pattern of Frustrated 2-Aminophenylboranes  
*JOURNAL OF THE AMERICAN CHEMICAL SOCIETY* 138:(14) pp. 4860-4868. (2016)  
Link(ek):  [DOI](#), [PubMed](#), [WoS](#)
20. Claraz Aurélie , Sahoo Gokarneswar , Berta Dénes , Madarász Ádám , Pápai Imre , Pihko Petri M  
A Catalyst Designed for the Enantioselective Construction of Methyl- and Alkyl-Substituted Tertiary Stereocenters  
*ANGEWANDTE CHEMIE-INTERNATIONAL EDITION* 55:(2) pp. 669-673. (2016)  
Link(ek):  [DOI](#), [PubMed](#), [Egyéb URL](#)
21. Csaba Jobbágy , Péter Baranyai , Gábor Marsi , Barbara Rácz , Liang Li , Panče Naumov , Andrea Deák  
Novel gold(I) diphosphine-based dimers with aurophilicity triggered multistimuli light-emitting properties  
*JOURNAL OF MATERIALS CHEMISTRY C* 4: pp. 10253-10264. (2016)  
Link(ek):  [REAL](#), [DOI](#)
22. Csimbók Ervin , Takács Daniella , Balog József A. , Egyed Orsolya , May-Nagy Nóra V. , Keserű György Miklós  
The first synthesis of isoxazolo[3,4-c]pyridine-7-ones  
*TETRAHEDRON LETTERS* 57:(39) pp. 4401-4404. (2016)  
Link(ek):  [REAL](#), [DOI](#)
23. Demeter O , Fodor E A , Kállay M , Mező G , Németh K , Szabó P T , Kele P  
A Double-Clicking Bis-Azide Fluorogenic Dye for Bioorthogonal Self-Labeling Peptide Tags  
*CHEMISTRY-A EUROPEAN JOURNAL* 22: pp. 6382-6388. (2016)  
Link(ek):  [REAL](#), [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)

24. Éles János , Bozó Éva , Hornok Katalin , Szentirmay Éva , Beke Gyula , Borza István , Vágó István , Huszár József , Bényei Gyula , Domány György , Keserű György Miklós , Greiner István  
Bradykinin B1 receptor antagonist molekula kutatása fájdalom kezelésére  
*MAGYAR KÉMIAI FOLYÓIRAT - KÉMIAI KÖZLEMÉNYEK* 122:(2-4) pp. 154-161. (2016)  
Link(ek): [REAL-J](#)
25. Eördögh Ádám , Steinmeyer Jeannine , Peewasan Krisawan , Schepers Ute , Wagenknecht Hans-Achim , Kele Péter  
Polarity sensitive bioorthogonally applicable far-red emitting labels for postsynthetic nucleic acid labeling by copper-catalyzed and copper-free cycloaddition  
*BIOCONJUGATE CHEMISTRY* 27:(2) pp. 457-464. (2016)  
Link(ek): [REAL](#), [DOI](#), [PubMed](#), [WoS](#)
26. Faigl F , Erdélyi Zs , Holzbauer T , Mátravölgyi B  
Highly efficient stereoconservative syntheses of new, bifunctional atropisomeric organocatalysts  
*ARKIVOC* (3) pp. 242-261. (2016)  
Link(ek): [DOI](#), [REAL](#), [WoS](#), [Scopus](#)
27. Faigl F , Deák Sz , Mucsi Z , Hergert T , Balázs L , Boros S , Balázs B , Holzbauer T , Nyerges M , Mátravölgyi B  
A novel and convenient method for the preparation of 5-(diphenylmethylene)-1H-pyrrol-2(5H)-ones; synthesis and mechanistic study  
*TETRAHEDRON* 72:(35) pp. 5444-5455. (2016)  
Link(ek): [REAL](#), [DOI](#), [WoS](#), [Scopus](#)
28. Fazakas Á , Szelényi Z , Szénási G , Nyíró G , Szabó PM , Patócs A , Tegze N , Fekete BC , Molvarec A , Nagy B , Jakus J , Örsi F , Karádi I , Vereckei A  
Genetic predisposition in patients with hypertension and normal ejection fraction to oxidative stress  
*JOURNAL OF THE AMERICAN SOCIETY OF HYPERTENSION* 10:(2) pp. 124-132. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#), [Scopus](#) .
29. Ferenczy György G , Keserű György M  
On the enthalpic preference of fragment binding  
*MEDCHEMCOMM* 7:(2) pp. 332-337. (2016)  
Link(ek): [DOI](#), [Egyéb URL](#)
30. Ferenczy György G , Keserű György M  
Ligand Efficiency Metrics and their Use in Fragment Optimizations  
In: Daniel A Erlanson , Wolfgang Jahnke (szerk.)  
Fragment-based Drug Discovery Lessons and Outlook . Weinheim: Wiley-VCH Verlag GmbH & Co. KGaA, 2016. pp. 75-98.  
(ISBN:9783527683604)  
Link(ek): [DOI](#), [Egyéb URL](#) ;
31. Györfly Balázs A , Gulyássy Péter , Gellén Barbara , Völgyi Katalin , Madarasi Dóra , Kis Viktor , Ozohanics Olivér , Papp Ildikó , Kovács Péter , Lubec Gert , Dobolyi Árpád , Kardos József , Drahos László , Juhász Gábor , Kékesi Katalin A  
Widespread alterations in the synaptic proteome of the adolescent cerebral cortex following prenatal immune activation in rats  
*BRAIN BEHAVIOR AND IMMUNITY* 56: pp. 289-309. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)
32. Gyula Tamás Gál , Nóra Veronika May , Petra Bombicz  
Crystal structure of levomepromazine maleate  
*ACTA CRYSTALLOGRAPHICA SECTION E: CRYSTALLOGRAPHIC COMMUNICATIONS* E72: pp. 612-615. (2016)  
Link(ek): [DOI](#)
33. Horvath G , Bencsura A , Simon A , Tochtrop GP , DeKoster GT , Covey DF , Cistola DP , Toke O  
Structural determinants of ligand binding in the ternary complex of human ileal bile acid binding protein with glycocholate and glycochenodeoxycholate obtained from solution NMR.  
*FEBS JOURNAL* 283:(3) pp. 541-555. (2016)  
Link(ek): [REAL](#), [DOI](#), [PubMed](#)
34. Iashin V , Chernichenko K , Papai I , Repo T  
Atom-Efficient Synthesis of Alkynylfluoroborates Using BF<sub>3</sub>-Based Frustrated Lewis Pairs  
*ANGEWANDTE CHEMIE-INTERNATIONAL EDITION* 55:(45) pp. 14146-14150. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#)

35. Inbal Tuvi-Arad , András Stirling  
The Distortive Nature of Temperature – A Symmetry Analysis  
*ISRAEL JOURNAL OF CHEMISTRY* 56: pp. 1067-1075. (2016)  
Link(ek): [DOI](#)
36. János Galambos , György Domány , Katalin Nógrádi , Gábor Wágner , György M Keserű , Amrita Bobok , Sándor Kolok , Mónika L Mikó-Bakk , Mónika Vastag , Katalin Sághy , János Kóti , Zoltán Szakács , Zoltán Béni , Krisztina Gál , Zsolt Szombathelyi , István Greiner  
4-Aryl-3-arylsulfonyl-quinolines as negative allosteric modulators of metabotropic GluR5 receptors: From HTS hit to development candidate  
*BIOORGANIC & MEDICINAL CHEMISTRY LETTERS* 26:(4) pp. 1249-1252. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#)
37. Jeney A , Hujber Z , Szoboszlai N , Fullár A , Oláh J , Pap É , Márk Á , Kriston C , Kralovánszky J , Kovalszky I , Vékey K , Sebestyén A  
Characterisation of bioenergetic pathways and related regulators by multiple assays in human tumour cells  
*CANCER CELL INTERNATIONAL* 16:(1) Paper 4. (2016)  
Link(ek): [DOI](#), [SE Repozitórium](#), [PubMed](#), [WoS](#), [Scopus](#)
38. Jobbagy C , Baranyai P , Szabo P , Holczbauer T , Racz B , Li L , Naumov P , Deak A  
Unexpected formation of a fused double cycle trinuclear gold(i) complex supported by ortho-phenyl metallated aryl-diphosphine ligands and strong aurophilic interactions.  
*DALTON TRANSACTIONS* 45:(31) pp. 12569-12575. (2016)  
Link(ek): [REAL](#), [DOI](#), [PubMed](#)
39. Kardos J , Szabo Z , Heja L  
Framing Neuro-Glia Coupling in Antiepileptic Drug Design.  
*JOURNAL OF MEDICINAL CHEMISTRY* 59:(3) pp. 777-787. (2016)  
Link(ek): [REAL](#), [DOI](#), [PubMed](#)
40. Kelemen AA , Kiss R , Ferenczy GG , Kovacs L , Flachner B , Lorincz Z , Keseru GM  
Structure-Based Consensus Scoring Scheme for Selecting Class A Aminergic GPCR Fragments  
*JOURNAL OF CHEMICAL INFORMATION AND MODELING* 56:(2) pp. 412-422. (2016)  
Link(ek): [REAL](#), [PubMed](#), [DOI](#), [WoS](#), [Scopus](#)
41. Kelemen AA , Szabo BP , Kovacs P , Keseru GM  
The first synthesis of furo[2,3-c]pyridazin-4(1H)-one derivatives  
*TETRAHEDRON LETTERS* 57:(1) pp. 64-66. (2016)  
Link(ek): [DOI](#), [WoS](#)
42. Keseru GM , Erlanson DA , Ferenczy GG , Hann MM , Murray CW , Pickett SD  
Design Principles for Fragment Libraries: Maximizing the Value of Learnings from Pharma Fragment-Based Drug Discovery (FBDD) Programs for Use in Academia  
*JOURNAL OF MEDICINAL CHEMISTRY* 59:(18) pp. 8189-8206. (2016)  
Link(ek): [REAL](#), [PubMed](#), [DOI](#), [WoS](#)
43. Kirischuk S , Heja L , Kardos J , Billups B  
Astrocyte sodium signaling and the regulation of neurotransmission  
*GLIA* 64:(10) pp. 1655-1666. (2016)  
Link(ek): [REAL](#), [DOI](#), [PubMed](#), [WoS](#)
44. Kiss Róbert , Bajusz Dávid , Baskin Rebekah , Tóth Katalin , Monostory Katalin , Sayeski Peter P , Keserű György M  
Identification of 8-Hydroxyquinoline Derivatives Active Against Somatic V658F Mutant JAK1-Dependent Cells  
*ARCHIV DER PHARMAZIE* 349:(12) pp. 925-933. (2016)  
Link(ek): [DOI](#), [Scopus](#)
45. Kiss Róbert , Keserű György Miklós  
Structure-based discovery and binding site analysis of histamine receptor ligands  
*EXPERT OPINION ON DRUG DISCOVERY* 11:(12) pp. 1165-1185. (2016)  
Link(ek): [REAL](#), [DOI](#)
46. Knorr G , Kozma E , Herner A , Lemke EA , Kele P  
New Red-Emitting Tetrazine-Phenoxazine Fluorogenic Labels for Live-Cell Intracellular Bioorthogonal Labeling Schemes  
*CHEMISTRY-A EUROPEAN JOURNAL* 22:(26) pp. 8972-8979. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)

47. Kovács K , He SJ , Mile V , Földes T , Pápai I , Takács E , Wojnárovits L  
Ionizing radiation induced degradation of monuron in dilute aqueous solution  
*RADIATION PHYSICS AND CHEMISTRY: THE JOURNAL FOR RADIATION PHYSICS RADIATION CHEMISTRY AND RADIATION PROCESSING* 124: pp. 191-197. (2016)  
Link(ek):  [Teljes dokumentum](#), [DOI](#), [WoS](#), [Scopus](#)
48. Kozma E , Nikić I , Varga B R , Aramburu I V , Kang J H , Fackler O T , Lemke E A , Kele P  
Hydrophilic trans-Cyclooctenylated Non-Canonical Amino Acids for Fast Intracellular Protein Labeling  
*CHEMBIOCHEM* 17:(16) pp. 1518-1524. (2016)  
Link(ek):  [REAL](#), [DOI](#), [PubMed](#), [WoS](#)
49. Krisztina Nikowitz , Attila Domján , Klára Pintye-Hódi , Géza Regdon jr  
Multivariate calibration of the degree of crystallinity in intact pellets by X-ray powder diffraction  
*INTERNATIONAL JOURNAL OF PHARMACEUTICS* 502: pp. 107-116. (2016)  
Link(ek): [DOI](#), [WoS](#), [Scopus](#)
50. Livia Naszályi Nagy , András Polyák , Judith Mihály , Ágnes Szécsényi , Imola Csilla Szigyártó , Zsuzsanna Czégény , Emma Jakab , Péter Németh , Balázs Magda , Pál T Szabó , Zsuzsanna Veres , Katalin Jemnitz , Imre Bertóti , Róbert Péter Jóba , György Trencsényi , Lajos Balogh , Attila Bóta  
Silica@zirconia@poly(malic acid) nanoparticle: a promising nanocarrier for theranostic applications  
*JOURNAL OF MATERIALS CHEMISTRY B* 4:(25) pp. 4420-4429. (2016)  
Link(ek):  [REAL](#), [DOI](#), [WoS](#)
51. Ma X , Lubin H , Ioja E , Kekesi O , Simon A , Apati A , Orban TI , Heja L , Kardos J , Marko IE  
Straightforward and effective synthesis of gamma-aminobutyric acid transporter subtype 2-selective acyl-substituted azaspiro[4.5]decanes.  
*BIOORGANIC & MEDICINAL CHEMISTRY LETTERS* 26:(2) pp. 417-423. (2016)  
Link(ek):  [REAL](#), [DOI](#), [PubMed](#)
52. Madarász Ádám , Berta Dénes , Paton Robert S  
Development of a True Transition State Force Field from Quantum Mechanical Calculations  
*JOURNAL OF CHEMICAL THEORY AND COMPUTATION* 12: pp. 1833-1844. (2016)  
Link(ek):  [DOI](#), [Egyéb URL](#)
53. Marta Z , Bobaly B , Fekete J , Magda B , Imre T , Meszaros KV , Szabo PT  
Pushing quantitation limits in micro UHPLC-MS/MS analysis of steroid hormones by sample dilution using high volume injection.  
*JOURNAL OF PHARMACEUTICAL AND BIOMEDICAL ANALYSIS* 129: pp. 135-141. (2016)  
Link(ek): [DOI](#), [PubMed](#), [Scopus](#)
54. Martonfalvi Z , Bianco P , Ferenczy G , Naftz K , Kellermayer M  
Dynamics of Transitions through the Molten-Globule State Enhance Contractility of Titin  
*BIOPHYSICAL JOURNAL* 110:(31) pp. 301A-302A. (2016)  
60th Annual Meeting of the Biophysical-Society. Los Angeles,  
Link(ek): [WoS](#)
55. May Nóra Veronika , Gál Gyula Tamás , Rapi Zsolt , Bakó Péter  
Crystal structure of diethyl 3-(3-chlorophenyl)- 2,2-dicyanocyclopropane-1,1-dicarboxylate  
*ACTA CRYSTALLOGRAPHICA SECTION E: CRYSTALLOGRAPHIC COMMUNICATIONS* E72: pp. 253-256. (2016)  
Link(ek):  [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)
56. May Nóra Veronika , Gál Gyula Tamás , Rapi Zsolt , Bakó Péter  
Crystal structure of diethyl 2-acetoxy-2-[3-(4-nitrophenyl)- 3-oxo-1-phenylpropyl]malonate  
*ACTA CRYSTALLOGRAPHICA SECTION E: CRYSTALLOGRAPHIC COMMUNICATIONS* E72: pp. 257-260. (2016)  
Link(ek):  [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)
57. Mayer I  
Restoring rotational invariance of Lowdin populations  
*STRUCTURAL CHEMISTRY* 27:(1) pp. 51-55. (2016)  
Link(ek):  [REAL](#), [DOI](#), [WoS](#)
58. Mayer István  
Bond Orders and Energy Components: Extracting Chemical Information from Molecular Wave Functions  
Boca Raton; London; New York; Singapore: CRC Press, 2016. 229 p.  
(ISBN:9781420090116)

59. Mercedesz Törincsi , Melinda Nagy , Tamás Bihari , András Stirling , Pál Kolonits , Lajos Novak  
Rearrangements of Cycloalkenyl Aryl Ethers  
*MOLECULES* 21:(4) pp. 503-515. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)
60. Merkel M , Arndt S , Ploschik D , Cserép G B , Wenge U , Kele P , Wagenknecht H-A  
Scope and limitations of typical copper-free bioorthogonal reactions with DNA: Reactive 2'-deoxyuridine triphosphates for postsynthetic labeling  
*JOURNAL OF ORGANIC CHEMISTRY* 81:(17) pp. 7527-7538. (2016)  
Link(ek): [REAL](#), [DOI](#), [PubMed](#), [WoS](#)
61. Milen Mátyás , Ábrányi-Balogh Péter , Volk Balázs  
β-Karbolinvázis vegyületek szintézise  
*MAGYAR KÉMIAI FOLYÓIRAT - KÉMIAI KÖZLEMÉNYEK* 122:(2-4) pp. 172-178. (2016)  
Link(ek): [REAL-J](#)
62. Miskolczy Z , Biczók L , Jablonkai I  
The origin of the dual fluorescence of protonated ellipticine in water  
*CHEMICAL PHYSICS LETTERS* 644: pp. 292-295. (2016)  
Link(ek): [REAL](#), [DOI](#), [WoS](#), [Scopus](#)
63. Miskolczy Z , Biczók L , Jablonkai I  
Multiple inclusion complex formation of protonated ellipticine with cucurbit[8]uril: thermodynamics and fluorescence properties  
*SUPRAMOLECULAR CHEMISTRY* 28:(9-10) pp. 842-848. (2016)  
Link(ek): [REAL](#), [DOI](#), [WoS](#), [Scopus](#)
64. Nagy GN , Suardiaz R , Lopata A , Ozohanics O , Vékey K , Brooks BR , Leveles I , Tóth J , Vértessy BG , Rosta E  
Structural Characterization of Arginine Fingers: Identification of an Arginine Finger for the Pyrophosphatase dUTPases  
*JOURNAL OF THE AMERICAN CHEMICAL SOCIETY* 138:(45) pp. 15035-15045. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)
65. Navratil M , Tykvarit J , Schimer J , Pachel P , Navratil V , Rokob TA , Hlouchova K , Rulisek L , Konvalinka J  
Comparison of human glutamate carboxypeptidases II and III reveals their divergent substrate specificities  
*FEBS JOURNAL* 283:(13) pp. 2528-2545. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#)
66. Nóra V. May , Zsolt Szentendrei , Gyula T. Gál , Valerio di Marco  
STRUCTURE DETERMINATION OF COPPER(II)-HYDROXYPIRIDINECARBOXYLIC ACID DERIVATIVES IN SOLID AND SOLUTION PHASES  
In: Hungarian Chemical Society  
13th European Biological Inorganic Chemistry Conference . Konferencia helye, ideje: Budapest , Magyarország , 2016.08.26 - 2016.09.01. Budapest: Magyar Kémikusok Egyesülete (MKE), 2016. p. P224. 1 p.  
(ISBN:9789639970670)
67. Olivér Éliás , Katalin Nógrádi , György Domány , Zoltán Szakács , János Kóti , Csaba Szántay Jr , Ákos Tarcsay , György M Keszér , Anikó Gere , Béla Kiss , Dalma Kurkó , Sándor Kolok , Zsolt Némethy , Zoltán Kapui , Éva Hellinger , Mónika Vastag , Katalin Sággy , Rita Kedves , István Gyertyán  
The influence of 5-HT<sub>2A</sub> activity on a 5-HT<sub>2C</sub> specific in vivo assay used for early identification of multiple acting SERT and 5-HT<sub>2C</sub> receptor ligands  
*BIOORGANIC & MEDICINAL CHEMISTRY LETTERS* 26:(3) pp. 914-920. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#)
68. Pape VFS , Tóth S , Füredi A , Szebényi K , Lovrics A , Szabó P , Wiese M , Szakács G  
Design, synthesis and biological evaluation of thiosemicarbazones, hydrazinobenzothiazoles and arylhydrazones as anticancer agents with a potential to overcome multidrug resistance  
*EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY* 117: pp. 335-354. (2016)  
Link(ek): [REAL](#), [PubMed](#), [DOI](#), [Scopus](#)
69. Péter Keglevich , Péter Ábrányi-Balogh , Áron Szigetvári , Csaba Szántay Jr , Csaba Szántay , László Hazai  
Studies on the mechanism of quaternization of the catharanthine part of vinblastine and vincristine  
*TETRAHEDRON LETTERS* 57: pp. 1672-1677. (2016)  
Link(ek): [DOI](#), [WoS](#), [Scopus](#)

70. Petra Bombicz  
X-ray crystallography  
*CRYSTALLOGRAPHY REVIEW* 22:(1) pp. 79-81. (2016)  
Link(ek): [DOI](#);
71. Pócsfalvi G , Stanly C , Fiume I , Schlosser G , Turiák L , Vékey K  
A proteomic insight into plant-derived nanovesicles  
In: 10th Central and Eastern European Proteomic Conference . Konferencia helye, ideje: Budapest , Magyarország , 2016.10.11 -2016.10.14. Budapest: p. 154.
72. Prokai A , Csohany R , Sziksz E , Pap D , Balicza-Himer L , Boros S , Magda B , Vannay A , Kis-Petik K , Fekete A , Peti-Peterdi J , Szabo AJ  
Calcineurin-Inhibition Results in Upregulation of Local Renin and Subsequent Vascular Endothelial Growth Factor Production in Renal Collecting Ducts.  
*TRANSPLANTATION* 100:(2) pp. 325-333. (2016)  
Link(ek): [SE Repozitórium](#), [DOI](#), [PubMed](#), [WoS](#), [Scopus](#) .
73. Quast R B , Ballion B , Stech M , Sonnabend A , Varga B R , Wüstenhagen D A , Kele P , Schiller S M , Kubick S  
Cell-free synthesis of functional human epidermal growth factor receptor: Investigation of ligandindependent dimerization in Sf21 microsomal membranes using noncanonical amino acids  
*SCIENTIFIC REPORTS* 6: p. 34048. (2016)  
Link(ek): [DOI](#), [REAL](#)
74. Rábai M , Nagy NV , May Z , László C , Szentmihályi K  
Characterization of paramagnetic iron(III) and manganese(II) content of some medical herbs by electron paramagnetic resonance (EPR) spectroscopy  
*Jökull Journal* 66:(2) pp. 295-305. (2016)  
Link(ek): [REAL](#)
75. Rác A , Bajusz D , Fodor M , Héberger K  
Comparison of classification methods with "n-class" receiver operating characteristic curves: A case study of energy drinks  
*CHEMOMETRICS AND INTELLIGENT LABORATORY SYSTEMS* 151: pp. 34-43. (2016)  
Link(ek): [REAL](#), [DOI](#), [WoS](#), [Scopus](#)
76. Rapi Zsolt , Ozohanics Oliver , Tóth Gábor , Bakó Péter , Höfler Lajos , Nemcsok Tamás , Kánya Nándor , Keglevich György  
Syntheses and complexing ability of  $\alpha$ -d-gluco- and  $\alpha$ -d-xylofuranoside-based lariat ethers  
*JOURNAL OF INCLUSION PHENOMENA AND MACROCYCLIC CHEMISTRY* 85:(1) pp. 19-32. (2016)  
Link(ek): [DOI](#), [WoS](#), [Scopus](#), [Egyéb URL](#)
77. Rokob TA  
Pathways for Arene Oxidation in Non-Heme Diiron Enzymes: Lessons from Computational Studies on Benzoyl Coenzyme A Epoxidase  
*JOURNAL OF THE AMERICAN CHEMICAL SOCIETY* 138:(44) pp. 14623-14638. (2016)  
Link(ek): [DOI](#), [REAL](#), [WoS](#)
78. Rokob TA , Chalupsky J , Bim D , Andrikopoulos PC , Srnc M , Rulisek L  
Mono- and binuclear non-heme iron chemistry from a theoretical perspective  
*JOURNAL OF BIOLOGICAL INORGANIC CHEMISTRY* 21:(5-6) pp. 619-644. (2016)  
Link(ek): [DOI](#), [PubMed](#), [REAL](#), [WoS](#)
79. Sajó Ráchel , Tőke Orsolya , Hajdú István , Jankovics Hajnalka , Micsonai András , Dobó József , Kardos József , Vonderviszt Ferenc  
Structural plasticity of the Salmonella FliS flagellar export chaperone  
*FEBS LETTERS* 590:(8) pp. 1103-1113. (2016)  
Link(ek): [REAL](#), [DOI](#), [PubMed](#), [WoS](#), [Scopus](#), [Egyéb URL](#)
80. Sodar BW , Kittel A , Palocz K , Vukman KV , Osteikoetxea X , Szabo-Taylor K , Nemeth A , Sperlagh B , Baranyai T , Giricz Z , Wiener Z , Turiak L , Drahos L , Pallinger E , Vekey K , Ferdinandy P , Falus A , Buzas EI  
Low-density lipoprotein mimics blood plasma-derived exosomes and microvesicles during isolation and detection  
*SCIENTIFIC REPORTS* 6: Paper 24316. 12 p. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)

81. Söveges B , Imre T , Szende T , Póti Á L , Cserép G B , Hegedűs T , Kele P , Németh K  
Systematic study of protein labeling by fluorogenic probes using cysteine targeting vinyl sulfone-cyclooctyne tags  
*ORGANIC & BIOMOLECULAR CHEMISTRY* 14:(25) pp. 6071-6078. (2016)  
Link(ek):  [REAL](#), [DOI](#), [PubMed](#), [WoS](#)
82. Stirling A , Rozgonyi T , Krack M , Bernasconi M  
Prebiotic NH<sub>3</sub> Formation: Insights from Simulations  
*INORGANIC CHEMISTRY* 55:(4) pp. 1934-1939. (2016)  
Link(ek):  [DOI](#), [WoS](#)
83. Szakács Z , Bojtár M , Drahos L , Hessz D , Kállay M , Vidóczy T , Bitter I , Kubinyi M  
The kinetics and mechanism of photooxygenation of 4'-diethylamino-3-hydroxyflavone  
*PHOTOCHEMICAL & PHOTOBIOLOGICAL SCIENCES* 15:(2) pp. 219-227. (2016)  
Link(ek):  [DOI](#),  [REAL](#), [PubMed](#), [WoS](#), [Scopus](#)
84. Szorcsik A , Matyuska F , Benyei A , Nagy N V , Szilagyi R K , Gajda T  
A novel 1,3,5-triaminocyclohexane-based tripodal ligand forms a unique tetra(pyrazolate)-bridged tricopper(II) core: solution equilibrium, structure and catecholase activity  
*DALTON TRANSACTIONS* 45: pp. 14998-15012. (2016)  
Link(ek):  [REAL](#), [DOI](#), [WoS](#)
85. Tamas Holczbauer , Attila Domján , Csaba Fodor  
Crystal structure of diaquatris(1-ethyl-1H-imidazole-jN3 )(sulfato-jO)nickel(II)  
*ACTA CRYSTALLOGRAPHICA SECTION E: CRYSTALLOGRAPHIC COMMUNICATIONS* E72: pp. 374-377. (2016)  
Link(ek):  [DOI](#), [REAL](#), [WoS](#), [Scopus](#)
86. Toke O , Vonderviszt F  
Amphipathic helical ordering of the flagellar secretion signal of Salmonella flagellin.  
*BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS* 476:(4) pp. 641-647. (2016)  
Link(ek):  [REAL](#),  [DOI](#), [PubMed](#), [WoS](#), [Scopus](#)
87. Tóth Eszter , Vékey Károly , Ozohanics Oliver , Jekő Anita , Dominczyk Iwona , Widlak Piotr , Drahos László  
Changes of protein glycosylation in the course of radiotherapy  
*JOURNAL OF PHARMACEUTICAL AND BIOMEDICAL ANALYSIS* 118: pp. 380-386. (2016)  
Link(ek): [DOI](#), [Scopus](#)
88. Varga M , Berkesi O , Darula Z , May NV , Palagyi A  
Structural characterization of allomelanin from black oat  
*PHYTOCHEMISTRY* 130: pp. 313-320. (2016)  
Link(ek):  [REAL](#), [DOI](#), [PubMed](#), [WoS](#)
89. Zhivonitko VV , Sorochkina K , Chernichenko K , Kotai B , Foldes T , Papai I , Telkki VV , Repo T , Koptug I  
Nuclear spin hyperpolarization with ansa-aminoboranes: a metal-free perspective for parahydrogen-induced polarization  
*PHYSICAL CHEMISTRY CHEMICAL PHYSICS* 18:(40) pp. 27784-27795. (2016)  
Link(ek): [DOI](#), [PubMed](#), [WoS](#)
90. Zsolt Rapi , Alajos Grün , György Keglevich , András Stirling , Péter Bakó  
Synthesis of a-D-galactose-based azacrown ethers and their application as enantioselective catalysts in Michael reactions  
*NEW JOURNAL OF CHEMISTRY* 40:(9) pp. 7856-7865. (2016)  
Link(ek):  [DOI](#), [WoS](#), [Scopus](#)