



***Chemistry Conference for Young Scientists
Blankenberge, Belgium***

F E B R U A R Y 1 9 - 2 1

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Dorottya Horváth - Budapest University of Technology and Economics - OMC-P-10

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Tamara Teski - Budapest University of Technology and Economics - OMC-P-2C

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Boriss Štrumfs - Latvian Institute of Organic Synthesis - OMC-P-2E

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Telli Fatma - Ege University - OMC-P-2H

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Kevin Bevernaege - Ghent University - OMC-P-2I

Tandem Functionalization of Dienes as a Rapid Entry Into N-Heterocyclic Scaffolds

Frederick Degroote - Ghent University - OMC-P-2J

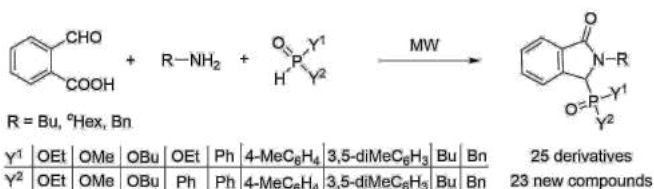
Novel Cyclopentannulations: Investigating The Synthetic Utility of Sulfur-Mediated (3+2) Cycloadditions

Synthesis of isoindolinone phosphonates and isoindolinone phosphine oxides

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Isoindoline derivatives are important compounds among nitrogen heterocycles. They were proved to be useful in a wide range of applications in the field of medicinal chemistry. During my research work, our aim was to synthesize (3-oxo-2,3-dihydro-1*H*-isoindol-1-yl)phosphonates and -phosphine oxides by the Kabachnik—Fields reaction and cyclization of 2-formylbenzoic acid, primary amines and various phosphorus reagents (dialkyl phosphites, ethyl phenyl-*H*-phosphinate and secondary phosphine oxides). According to the principles of “green chemistry”, the condensations were carried out under microwave (MW) irradiation, in the absence of any catalyst, and — as far as possible — without any solvent. At first, the reaction of 2-formylbenzoic acid, butyl amine and diethyl phosphite was studied. The transformation was optimized by changing the molar ratio of the starting materials, the temperature and the reaction time. Applying the optimal conditions, the condensation was extended to different amines and various >P(O)H reagents. Altogether 25 derivatives were prepared, from which 23 compounds are new compounds. The reactions were followed by gas chromatography (GC) and ³¹P NMR spectroscopy. The products synthesized were isolated by column chromatography, and were characterized by ³¹P, ¹H and ¹³C NMR spectroscopy, as well as by high resolution mass spectrometry (HRMS). Finally, the deoxygenation of one of the isoindolinone phosphine oxides, and the utilization of the so obtained phosphine as ligand in platinum complex was also investigated.



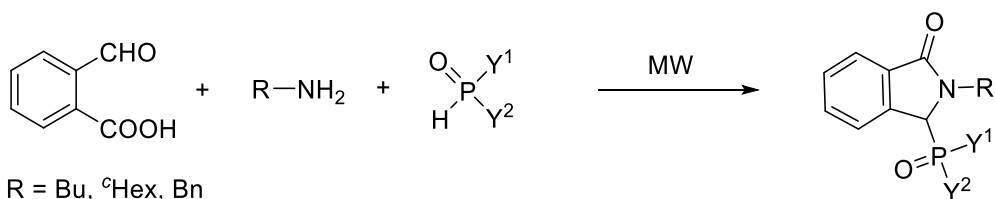
Fordítás

Izoindolinon-foszfónátok és izoindolinon-foszfín-oxidok szintézisének tanulmányozása

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A nitrogén tartalmú heterociklusok fontos képviselői az izoindolin-származékok, melyek sokrétű biológiai aktivitással rendelkezhetnek a gyógyszeripar területén. Kutatómunkám során célul tűztük ki (3-oxo-2,3-dihidro-1*H*-izoindol-1-il)foszfónátok és -foszfín-oxidok előállítását a 2-formilbenzoesav, primer aminok és különféle foszfor-reagensek (dialkil-foszfitek, etil-fenil-*H*-foszfínát vagy szekunder foszfín-oxidok) Kabachnik–Fields-reakcióját követő intramolekuláris gyűrűzárásával. A környezetbarát szemléletmódnak megfelelően, a kondenzációkat mikrohullámú (MW) besugárzás hatására, katalizátor és – lehetőség szerint – oldószer nélkül kívántuk megvalósítani.



R = Bu, ^cHex, Bn

Y ¹	OEt	OMe	OBu	OEt	Ph	4-MeC ₆ H ₄	3,5-diMeC ₆ H ₃	Bu	Bn	25 származék
Y ²	OEt	OMe	OBu	Ph	Ph	4-MeC ₆ H ₄	3,5-diMeC ₆ H ₃	Bu	Bn	23 új vegyület

Első lépésben a 2-formilbenzoesav, butilamin és dietil-foszfít modellreakciót tanulmányoztuk. A reakció paramétereinek (a reagensek mólaránya, a hőmérséklet, illetve a reakcióidő) változtatásával kerestük az optimális körülményeket. Az optimalizálást követően a kondenzációt további aminokra és >P(O)H reagensekre terjesztettük ki. Munkám során összesen 25 származékot szintetizáltunk, melyek közül 23 új vegyület. A reakciókat gázkromatográfiás (GC) mérésekkel, illetve ³¹P NMR spektroszkópiával követtük. A termékeket oszlopkromatográfia segítségével tisztítottuk, szerkezetüket ³¹P, ¹H és ¹³C NMR spektroszkópiával, illetve nagyfelbontású tömegspektrometriás (HRMS) vizsgálatokkal igazoltuk.

Tanulmányoztuk továbbá egy izoindolinon-foszfín-oxid deoxigénezését, majd a kapott foszfint platina-komplex szintézisében foszfor-lingandumként hasznosítottuk.