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
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Interests: organoelement chemistry; sulfur-nitrogen compounds; heterocycles; amidines; heteroamidines; free-radicals; electrochemistry; supramolecular chemistry; structural methods; crystallography; electron paramagnetic resonance spectroscopy



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Interests: free radical organic and polymer chemistry; heterocyclic and medicinal chemistry

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Interests: organic synthesis; methodology and spectroscopic analysis; heterocyclic chemistry; natural products; asymmetric synthesis; nitrogenated compounds of pharmaceutical interest; multicomponent reactions



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Interests: synthesis; synthetic use of flash vacuum pyrolysis; heterocyclic chemistry; reactive intermediates; organophosphorus; organosulfur; heavier main group chemistry

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Website (<https://community.dur.ac.uk/i.r.baxendale/index.php>)

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Department of Chemistry, Durham University, University Science Laboratories, South Road, Durham DH1 3LE, UK

Interests: organic synthesis and methodology; automation; chemical reactors; flow chemistry; enabling technologies; immobilised reagents and scavengers; heterocyclic chemistry



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Department of Organic Chemistry, Faculty of Chemistry, University of Murcia, 30100 Murcia, Spain

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Interests: self-assembly; mechanically interlocked molecules (rotaxanes and catenanes); hydrogen bond; template synthesis; molecular recognition; supramolecular chemistry



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Website (<https://www.researchgate.net/profile/Stefano-Derrico>)

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Department of Pharmacy, University of Naples Federico II, Via Domenico Montesano 49, 80131 Naples, Italy

Interests: solid-phase synthesis; chemistry of nucleosides; nucleotides and oligonucleotides; L-sugars; platinum complexes

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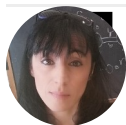
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Laboratory of Industrial and Synthetic Organic Chemistry (LISOC), Department of Chemistry and Chemical Technologies, University of Calabria, Via Pietro Bucci, 12/C, 87036 Arcavacata di Rende, CS, Italy

Interests: new syntheses of high value added molecules through catalytic assembly of simple units; innovative syntheses of heterocyclic molecules of pharmaceutical; agrochemical; or applicative interest; carbonylation chemistry; use of non-conventional solvents in organic synthesis; synthesis and semi-synthesis of bioactive compounds of pharmaceutical or agrochemical interest; synthesis of new materials for advanced applications;

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Interests: innovative syntheses of high-value molecules through catalytic process; new syntheses of heterocyclic compounds of pharmaceutical interest; carbonylation catalyzed chemistry; application of unconventional solvents in advanced organic synthesis; synthesis of novel materials for advanced applications

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Website (<https://chemistry.fudan.edu.cn/chemen/a3/58/c22420a238424/page.htm>)

Editorial Board Member

Chemistry Department, Fudan University, Shanghai 200433, China

Interests: medicinal heterocyclic chemistry; indoles; indazoles; pyridines; thiazoles; thiadiazoles; pyrroles; computer aided drug design; molecular probe



Prof. Dr. Hideto Miyabe (<https://sciprofiles.com/profile/64700>)

Website (<http://www2.huhs.ac.jp/~h070012h/>)

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School of Pharmacy, Hyogo Medical University of Health Sciences, 1-3-6 Minatojima, Chuo-ku, Kobe 650-8530, Japan

Interests: organic synthesis and methodology; radical reactions; organocatalysis; asymmetric catalysis; photochemistry; aryne chemistry

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Website (<https://katalog.uu.se/profile/?id=N6-1023>)

Editorial Board Member

Organic Pharmaceutical Chemistry, Department of Medicinal Chemistry, BMC, Uppsala University, Box 574, SE-751 23 Uppsala, Sweden

Interests: heterocyclic chemistry; multicomponent reactions; catalysis; medicinal chemistry; synthetic methodology

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Website (<http://cheminformatics.epfl.ch>)

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Director of Chemical Information, Institute of Chemical Sciences and Engineering (ISIC), Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Interests: chemoinformatics; chemical information; infrastructure for chemical research; online processing and data mining

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Dr. Vincenzo Piccialli (<https://sciprofiles.com/profile/9313>)

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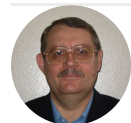
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Department of Chemical Sciences, University of Naples Federico II, Via Cinthia 4, 80126 Naples, Italy

Interests: organic and medicinal chemistry; organic synthesis; catalytic oxidative processes; marine natural products; [inorganic chemistry](#)  [cookies](#)  

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[Website \(http://zioc.ru/institute/laboratories/laboratory-of-polysulphur-nitrogen-heterocycles-n31?lang=en\)](http://zioc.ru/institute/laboratories/laboratory-of-polysulphur-nitrogen-heterocycles-n31?lang=en)

Editorial Board Member

N. D. Zelinsky Institute of Organic Chemistry Russian Academy of Sciences, 47 Leninsky Prospekt, 119991 Moscow, Russia

Interests: heterocyclic chemistry; sulfur-nitrogen heterocycles; selenium heterocycles; synthetic methods; biologically active compounds; organic sensitizers for DSSCs and OLEDs; 1,2,3-dithiazoles; 1,2,5-thiadiazoles; 1,2,5-oxadiazoles; disulfur dichloride

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National Museum of Marine Biology and Aquarium, Pingtung 944401, Taiwan

Interests: marine natural products; marine chemical ecology; bioactive substances from cultured marine invertebrates

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[Prof. Dr. Fang-Rong Chang \(https://sciprofiles.com/profile/45469\)](https://sciprofiles.com/profile/45469)

[Website \(https://orcid.org/0000-0003-2549-4193\)](https://orcid.org/0000-0003-2549-4193)

Section Board Member

Graduate Institute of Natural Products, College of Pharmacy, Kaohsiung Medical University, Kaohsiung, Taiwan

Interests: natural product chemistry on fungi; plants; and marine organisms; comparative mass spectrometry-based metabolomics strategies for the investigation of natural products secondary metabolites; functional and healthy food; new drugs development

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[Website \(https://chemistry.uconn.edu/person/nicholas-leadbeater/\)](https://chemistry.uconn.edu/person/nicholas-leadbeater/)

Section Board Member

Department of Chemistry, University of Connecticut, 55 North Eagleville Road, Storrs, CT 06269-3060, USA

Interests: methodology for organic synthesis; green chemistry; photocatalysis; electrochemistry; computational chemistry; reaction monitoring; chemical education



[Prof. Dr. Kristof Van Hecke \(https://sciprofiles.com/profile/279509\)](https://sciprofiles.com/profile/279509)

[Website \(https://www.xstruct.ugent.be\)](https://www.xstruct.ugent.be)

Section Board Member

Department of Chemistry, Ghent University, Krijgslaan 281, Building S3, 9000 Ghent, Belgium

Interests: structures; X-ray diffraction; bioinorganic chemistry; metal complexes; coordination chemistry

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
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


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


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Abstract A derivative of dihydropyrimidopyrimidine has been successfully synthesized through a cyclocondensation reaction between a chalcone derivative with 5-aminotetrazole. The molecular structure of the title compound was established based on Fourier transform infrared spectra (FTIR), high-resolution mass spectrometry (HRMS), 1D and 2D nuclear magnetic [...] [Read more](#).

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Tetrahydro-1,4-thiazine-3,5-dione (/1422-8599/2018/4/M1036)

by  [R. Alan Aitken \(https://sciprofiles.com/profile/359182\)](https://sciprofiles.com/profile/359182),

 [Alexandra M. Z. Slawin \(https://sciprofiles.com/profile/author/WjBjRmpTUjdNUUIBMWI0WXREMFpqTW1vdWVrMjQyTVJHNIFnZDZuVnVQST0=\)](https://sciprofiles.com/profile/author/WjBjRmpTUjdNUUIBMWI0WXREMFpqTW1vdWVrMjQyTVJHNIFnZDZuVnVQST0=) and

 [Pei-pei Yeh \(https://sciprofiles.com/profile/author/NU02VitNM0tWYWZMR011a1NFVEt6My8wV0RXTFVGtmk3NDE1a0JjeIV6Yz0=\)](https://sciprofiles.com/profile/author/NU02VitNM0tWYWZMR011a1NFVEt6My8wV0RXTFVGtmk3NDE1a0JjeIV6Yz0=)

Molbank **2018**, *2018*(4), M1036; <https://doi.org/10.3390/M1036> (<https://doi.org/10.3390/M1036>) - 13 Dec 2018

Cited by 3 (</1422-8599/2018/4/M1036#metrics>) | Viewed by 1526

Abstract The X-ray structure of the title compound contains eight molecules in the unit cell which form the basis of a herringbone arrangement of hydrogen bonded ribbons. [Full article \(/1422-8599/2018/4/M1036\)](#)

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[\(1422-8599/2018/4/M1035/pdf?version=1543831718\)](#)

[1-\(2-Hydroxyethyl\)imidazolidine-2-thione \(/1422-8599/2018/4/M1035\)](#)

by [See Mun Lee \(https://sciprofiles.com/profile/1437196\)](#),

[Ainnul Hamidah Syhadah Azizan \(https://sciprofiles.com/profile/author/Y1liYVh4Qk5tMkJVT0Z4b0hRQWIWM0ZtRGpOREMzbVc4WkRxRjByWFAwMD0=\)](#) and

[Edward R. T. Tiekink \(https://sciprofiles.com/profile/483242\)](#)

Molbank **2018**, *2018*(4), M1035; <https://doi.org/10.3390/M1035> (<https://doi.org/10.3390/M1035>) - 03 Dec 2018

Cited by 3 ([/1422-8599/2018/4/M1035#metrics](#)) | Viewed by 1788

Abstract 1-(2-Hydroxyethyl)imidazolidine-2-thione (**1**) was obtained as a product from an in situ reaction between *N*-(2-hydroxyethyl)ethylenediamine, carbon disulfide, potassium hydroxide, and di(4-fluorobenzyl)tin dichloride. Compound **1** was characterized by IR, UV, ¹H, ¹³C{¹H}, and 2D (COSY, NOESY, HSQC, and [...]) [Read more](#).

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[Synthesis and Structure Elucidation of *N*'-\(4-Methoxybenzylidene\)-5-methyl-1-phenyl-1*H*-1,2,3-triazole-4-carbohydrazide \(/1422-8599/2018/4/M1034\)](#)

by [Mohammad Hayal Alotaibi \(https://sciprofiles.com/profile/423214\)](#),

[Hanan A. Mohamed \(https://sciprofiles.com/profile/author/UXdUZm5KNzdKcmInUVhGbk9MdVRJMnVabXVVTmJ2cVRUQ2VEUGFSdnhxYz0=\)](#),

[Bakr F. Abdel-Wahab \(https://sciprofiles.com/profile/author/WG1ERHpqL3R5MDQ4MmpoRXA1Zm0rUHcwMFBFBW9CVFJmYU11QXh5VWZzd0=\)](#),

[Amany S. Hegazy \(https://sciprofiles.com/profile/author/S3QxZjV3MEptTEpkNC9CTjAzaHA5cXVUUnNKREpLQWtQTi8rRIA4RE1hOD0=\)](#),

[Benson M. Kariuki \(https://sciprofiles.com/profile/1708300\)](#) and [Gamal A. El-Hiti \(https://sciprofiles.com/profile/113754\)](#)

Molbank **2018**, *2018*(4), M1034; <https://doi.org/10.3390/M1034> (<https://doi.org/10.3390/M1034>) - 02 Dec 2018

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Abstract *N*'-(4-Methoxybenzylidene)-5-methyl-1-phenyl-1*H*-1,2,3-triazole-4-carbohydrazide (**3**) was synthesized in a yield of 88% from an acid-catalyzed reaction of 5-methyl-1-phenyl-1*H*-1,2,3-triazole-4-carbohydrazide and 4-methoxybenzaldehyde in ethanol under reflux for 2.5 h. The structure of **3** was confirmed by the data obtained from [...]) [Read more](#).

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[Ureido Derivatives of Neoabietic Acid \(1422-8599/2018/4/M1033\)](#)

by  [Xinyu Gao](https://sciprofiles.com/profile/author/emNHeG1GMUR4OVhjSkVTak1vZzc4dDArdIBmRTAyRG8yVE9ISuptUDIFND0=) (<https://sciprofiles.com/profile/author/emNHeG1GMUR4OVhjSkVTak1vZzc4dDArdIBmRTAyRG8yVE9ISuptUDIFND0=>),
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Molbank **2018**, *2018*(4), M1033; <https://doi.org/10.3390/M1033> (<https://doi.org/10.3390/M1033>) - 29 Nov 2018

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Abstract A series of ureido derivatives of neoabietic acid were synthesized by application of Curtius rearrangement reaction to neoabietic acid and amines. Structure characterization of these compounds was done by ¹H-NMR, ¹³C-NMR and HRMS spectral analysis. **Full article (1422-8599/2018/4/M1033)**

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[4'-\(5-Methylfuran-2-yl\)-2,2':6',2"-terpyridine: A New Ligand Obtained from a Biomass-Derived Aldehyde with Potential Application in Metal-Catalyzed Reactions \(1422-8599/2018/4/M1032\)](#)

by  [Jérôme Husson](https://sciprofiles.com/profile/160544) (<https://sciprofiles.com/profile/160544>) and
 [Laurent Guyard](https://sciprofiles.com/profile/author/RXQ1ZU9hNmRGZ1E1RnJsL01SSmUyMIFIT3V2bWNScVRkZStGTzV2RFFQTT0=) (<https://sciprofiles.com/profile/author/RXQ1ZU9hNmRGZ1E1RnJsL01SSmUyMIFIT3V2bWNScVRkZStGTzV2RFFQTT0=>)

Molbank **2018**, *2018*(4), M1032; <https://doi.org/10.3390/M1032> (<https://doi.org/10.3390/M1032>) - 24 Nov 2018







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Abstract The new ligand 4'-(5-methylfuran-2-yl)-2,2':6',2"-terpyridine (**1**) was prepared in one step from 2-acetylpyridine and 5-methylfurfural. The latter is an aldehyde that can be readily obtained from biomass. The new terpyridine molecule was characterized by ¹H and ¹³C-NMR spectroscopy as well [...] **Read more.**

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**[N-\[2-\(1*H*-Indol-3-yl\)ethyl\]-2-\(4-isobutylphenyl\)propanamide \(/1422-8599/2018/4/M1031\)](https://pub.mdpi-res.com/molbank/2018/4/M1031)**by  [Stanimir Manolov \(https://sciprofiles.com/profile/1355336\)](https://sciprofiles.com/profile/1355336),  [Iliyan Ivanov \(https://sciprofiles.com/profile/39867\)](https://sciprofiles.com/profile/39867) and [Yulian Voinikov \(https://sciprofiles.com/profile/author/QUVGM0ZuVWI0UINTOEIwVkJZLMUdmZVZc241VExBdUxtQzBhTIBkdjJxWT0=\)](https://sciprofiles.com/profile/author/QUVGM0ZuVWI0UINTOEIwVkJZLMUdmZVZc241VExBdUxtQzBhTIBkdjJxWT0=)  [\(toggle desktop layout cookie\)](#)  *Molbank* **2018**, *2018*(4), M1031; <https://doi.org/10.3390/M1031> (<https://doi.org/10.3390/M1031>) - 22 Nov 2018**Cited by 1** ([/1422-8599/2018/4/M1031#metrics](https://pub.mdpi-res.com/molbank/2018/4/M1031#metrics)) | Viewed by 1983

Abstract The compound in the title was prepared by reaction between tryptamine and ibuprofen using *N,N'*-dicyclohexylcarbodiimide as a “dehydrating” reagent. The structure of the newly synthesized compound was determined by nuclear magnetic resonance (NMR) (¹H-NMR and ¹³C-NMR), UV, IR, and mass spectral data. **Full article** ([/1422-8599/2018/4/M1031](https://pub.mdpi-res.com/molbank/2018/4/M1031))

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[N-\[4-\(1-Methyl-1*H*-imidazol-2-yl\)-2,4'-bipyridin-2'-yl\]benzene-1,4-diamine \(/1422-8599/2018/4/M1030\)](https://pub.mdpi-res.com/molbank/2018/4/M1030)by  [Dhafer S. Zinad \(https://sciprofiles.com/profile/634257\)](https://sciprofiles.com/profile/634257),  [Dunya L. AL-Duhaidahaw \(https://sciprofiles.com/profile/386683\)](https://sciprofiles.com/profile/386683), [Ahmed Al-Amiery \(https://sciprofiles.com/profile/7303\)](https://sciprofiles.com/profile/7303) and  [Abdul Amir H. Kadhum \(https://sciprofiles.com/profile/188855\)](https://sciprofiles.com/profile/188855)*Molbank* **2018**, *2018*(4), M1030; <https://doi.org/10.3390/M1030> (<https://doi.org/10.3390/M1030>) - 16 Nov 2018**Cited by 2** ([/1422-8599/2018/4/M1030#metrics](https://pub.mdpi-res.com/molbank/2018/4/M1030#metrics)) | Viewed by 1675

Abstract *N*-[4-(1-Methyl-1*H*-imidazol-2-yl)-2,4'-bipyridin-2'-yl]benzene-1,4-diamine was synthesized with a good yield by the reaction of 2'-chloro-4-(1-methyl-1*H*-imidazol-2-yl)-2,4'-bipyridine with 4-phenylenediamine. The functionalization of the pyridine was accomplished by a nucleophilic aromatic substitution (S_NAr) reaction that afforded the target compound. The synthesized compound was characterized [...] **Read more.**

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

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[Ethyl 4-\(2-fluorophenyl\)-6-methyl-2-thioxo-1-\(*p*-tolyl\)-1,2,3,4-tetrahydropyrimidine-5-carboxylate \(/1422-8599/2018/4/M1029\)](https://pub.mdpi-res.com/molbank/2018/4/M1029)by  [Itamar Luís Gonçalves \(https://sciprofiles.com/profile/164423\)](https://sciprofiles.com/profile/164423), [Luciano Porto Kagami \(https://sciprofiles.com/profile/author/NXVIVnJxeEhWZGFhN3hnWktYVWoyR2d2RCtSWFh0UtlwM1kzNEJ5c1c2bz0=\)](https://sciprofiles.com/profile/author/NXVIVnJxeEhWZGFhN3hnWktYVWoyR2d2RCtSWFh0UtlwM1kzNEJ5c1c2bz0=), [Gustavo Machado das Neves \(https://sciprofiles.com/profile/author/Wnk1UnZoV1RpMmRQRfo5Z200dEJ4OXR0bDJ2OTB4ald6ejgvQIRpaEhnTT0=\)](https://sciprofiles.com/profile/author/Wnk1UnZoV1RpMmRQRfo5Z200dEJ4OXR0bDJ2OTB4ald6ejgvQIRpaEhnTT0=), [Liliana Rockenbach \(https://sciprofiles.com/profile/1854204\)](https://sciprofiles.com/profile/1854204), [Leonardo Davi \(https://sciprofiles.com/profile/author/WWpFRWZvY3J3d3FUWDhuVHNMYVdSa0NEZzMvbzVkcGJuTi9WREIBd3JsYz0=\)](https://sciprofiles.com/profile/author/WWpFRWZvY3J3d3FUWDhuVHNMYVdSa0NEZzMvbzVkcGJuTi9WREIBd3JsYz0=)

 [Alceu Felipe Soares](https://sciprofiles.com/profile/author/SW1qdzhBYjk3cHczQ0s1cEY4QzliTWg0bW54bHdsMEpNMkdOSVFPcHpaWT0=) (<https://sciprofiles.com/profile/author/SW1qdzhBYjk3cHczQ0s1cEY4QzliTWg0bW54bHdsMEpNMkdOSVFPcHpaWT0=>),
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Molbank **2018**, *2018*(4), M1029; <https://doi.org/10.3390/M1029> (<https://doi.org/10.3390/M1029>) - 13 Nov 2018

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Abstract The Biginelli reaction is a highly versatile reaction that leads to dihydropyrimidinones/thiones. This scaffold is reported as being a privileged structure due to its ability to interact with biological targets. Synthesis of ethyl 4-(2-fluorophenyl)-6-methyl-2-thioxo-1-(*p*-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate was achieved through the Biginelli reaction using [...] [Read more](#).

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[*O*-Isopropyl-*N*-(4-nitrophenyl)thiocarbamato- κ S]-(tri-4-tolylphosphine- κ P)gold(I) ([/1422-8599/2018/4/M1028](https://doi.org/10.3390/2018/4/M1028))

by [Chien Ing Yeo](https://sciprofiles.com/profile/424298) (<https://sciprofiles.com/profile/424298>) and [Edward R. T. Tiekink](https://sciprofiles.com/profile/483242) (<https://sciprofiles.com/profile/483242>)

Molbank **2018**, *2018*(4), M1028; <https://doi.org/10.3390/M1028> (<https://doi.org/10.3390/M1028>) - 05 Nov 2018

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Abstract The synthesis, spectroscopic characterization and X-ray crystal structure of the title compound, (4-tolyl)₃PAu[SC(O-*i*-Pr)=NC₆H₄NO₂-4] (1) are described. Spectroscopy exhibited the expected features confirming the formation of the compound. The molecular structure of [...] [Read more](#).

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  [/1422-8599/2018/4/M1027/pdf?version=1540825443](https://doi.org/10.3390/2018/4/M1027/pdf?version=1540825443) 

(*E*)-3-[3-(4-Morpholinophenyl)acryloyl]-2*H*-chromen-2-one ([/1422-8599/2018/4/M1027](https://doi.org/10.3390/2018/4/M1027))

by [Hery Suwito](https://sciprofiles.com/profile/87893) (<https://sciprofiles.com/profile/87893>),

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Molbank **2018**, *2018*(4), M1027; <https://doi.org/10.3390/M1027> (<https://doi.org/10.3390/M1027>) - 29 Oct 2018

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Abstract A new compound (*E*)-3-[3-(4-morpholinophenyl)acryloyl]-2*H*-chromen-2-one, a coumarin based chalcone derivative, has been successfully synthesized employing a molecular hybridization method through the reaction between 3-acetylcoumarin and 4-morpholinobenzaldehyde using a Claisen–Schmidt reaction using *p*TSA as a catalyst. The structure of the [...] [Read more.](#)

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[2,3,4-Trioxo-1-\(1*H*-pyrrolo\[2,3-*b*\]pyridin-7-ium-7-yl\)-cyclobutan-1-ide \(/1422-8599/2018/4/M1026\)](#)

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Molbank **2018**, *2018*(4), M1026; <https://doi.org/10.3390/M1026> (<https://doi.org/10.3390/M1026>) - 12 Oct 2018

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Abstract 2,3,4-Trioxo-1-(1*H*-pyrrolo[2,3-*b*]pyridin-7-ium-7-yl)-cyclobutan-1-ide was obtained by reaction of squaric acid with 7-azaindole in acetic anhydride. [Full article \(/1422-8599/2018/4/M1026\)](#)

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[Dichlorido\(\$\eta^6\$ -*p*-cymene\)\[tris\(2-cyanoethyl\)phosphine\]ruthenium\(II\) \(/1422-8599/2018/4/M1025\)](#)

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Abstract The tris(2-cyanoethyl)phosphine (tcep) complex [RuCl₂{P(CH₂CH₂CN)₃}(η^6 -*p*-cymene)] (*p*-cymene = *p*-CH₃C₆H₄ⁱPr) was synthesised by the bridge-splitting reaction of the chlorido-dimer [RuCl₂([...] [Read more.](#)

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Abstract Furyl and thienyl moieties were introduced into a purine structure to elevate its fluorescence properties, while a trityl group was used to increase the amorphous properties of the purine compounds. The title compounds were prepared by a sequence involving a Mitsunobu, a S [...]. [Read more.](#)
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[1-Methyl-3-{4-\[\(4-\(2-oxo-2,3-dihydro-1H-benzimidazol-1-yl\)piperidin-1-yl\)benzyl\]}-2-phenylindole \(\(1422-8599/2018/4/M1023\)\)](https://pub.mdpi-res.com/molbank/molbank-2018-M1023/article_deploy/html/images/molbank-2018-M1023-ag-550.jpg?1570545288)

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Abstract The 1-methyl-3-{4-[(4-(2-oxo-2,3-dihydro-1H-benzimidazol-1-yl)piperidin-1-yl)benzyl]}-2-phenylindole compound has been successfully synthesized via a multistep pathway starting from 2-phenylindole. Structure characterization of this new indole derivative was done by FTIR, ¹H-NMR, ¹³C-NMR, and HRMS spectral analysis. The title compound showed high cytotoxic potential against [...]. [Read more.](#)
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Synthesis of 4-(2*H*-[1,2,4]-Triazol-5-ylsulfanyl)-1,2-dihydropyrazol-3-one via Ring-Switching Hydrazinolysis of 5-Ethoxymethylidenethiazolo [3,2-*b*][1,2,4]triazol-6-one

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Abstract 4-(1*H*-[1,2,4]-Triazol-5-ylsulfanyl)-1,2-dihydropyrazol-3-one (**4**) was synthesized with a yield of 55% via ring-switching hydrazinolysis of 5-ethoxymethylidenethiazolo[3,2-*b*][1,2,4] triazol-6-one (**3**) in ethanol medium. The initial 1*H*-[1,2,4]-triazole-3-thiol (**1**) was modified via a two-step reaction: S-alkylation [...] [Read more](#).

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6-[1-Acetyl-5-(4-methoxyphenyl)-4,5-dihydro-1*H*-pyrazol-3-yl]-2(3*H*)-benzoxazolone (/1422-8599/2018/4/M1021)

by  [Yordanka Ivanova \(https://sciprofiles.com/profile/160318\)](https://sciprofiles.com/profile/160318),

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Molbank **2018**, *2018*(4), M1021; <https://doi.org/10.3390/M1021> (<https://doi.org/10.3390/M1021>) - 30 Sep 2018

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Abstract The title compound, 6-[1-acetyl-5-(4-methoxyphenyl)-4,5-dihydro-1*H*-pyrazol-3-yl]-2(3*H*)-benzoxazolone, was synthesized by condensation of 6-[3-(4-methoxyphenyl)-2-propenoyl]-2(3*H*)-benzoxazolone (**1**) and hydrazine hydrate in acetic acid in 84% yield. The structure of the target compound was confirmed using ¹H-NMR, ¹³C-NMR, IR, MS, and elemental analysis. [Full article \(/1422-8599/2018/4/M1021\)](#)

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Short Note

(E)-3-[3-(4-Morpholinophenyl)acryloyl]-2H-chromen-2-one

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Received: 23 September 2018; Accepted: 25 October 2018; Published: 29 October 2018



Abstract: A new compound (E)-3-[3-(4-morpholinophenyl)acryloyl]-2H-chromen-2-one, a coumarin based chalcone derivative, has been successfully synthesized employing a molecular hybridization method through the reaction between 3-acetylcoumarin and 4-morpholinobenzaldehyde using a Claisen–Schmidt reaction using *p*TSA as a catalyst. The structure of the title compound was established using spectroscopic data FTIR, HRESI-MS, ¹H- and ¹³C-NMR. The anticancer activity against breast cancer cells line T47D and cervix cancer cells line HeLa was determined using an MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assay.

Keywords: molecular hybridization; coumarin-chalcone; anticancer

1. Introduction

Combining different pharmacophoric moieties from different bioactive compounds to generate a new hybrid compound showing better affinity and efficacy, with fewer undesired side effects, than the parent compounds becomes a new concept in drug design and development, which is known as molecular hybridization [1]. An example of such hybridization is a compound constructed from coumarin and chalcones. Coumarins are secondary metabolites possessing a benzopyran ring that can also be found as synthetic products and are already known for their various pharmacological activities such as antimycobacterial [2], inhibitor of HIV-1 [3], inhibitor of platelet aggregation, and to smooth muscle contraction in vitro [4]. Meanwhile, chalcones (1,3-diaryl-2-propen-1-ones) belong to the group of flavonoids, which can be obtained from a plant origin and from synthesis. The bioactivities of chalcones are well known, such as cytotoxic agents against tumor cells [5], along with being antimalarial [6,7], antibacterial [8,9], and anticancer [10]. The pharmacological activities of coumarin–chalcone derivatives containing urea moiety as an anticancer agent has also been reported [11].

Based on this consideration, we designed a coumarin–chalcone hybrid compound containing morpholino-phenyl moiety and synthesized it successfully through a Claisen–Schmidt reaction. Furthermore, the prepared compound was evaluated in relation to its anticancer activity against breast cancer cell line T47D and cervix cancer cell line HeLa using an MTT assay.

2. Results and Discussion

The title compound **5** was prepared using a two-step reaction. The first step was the synthesis of 3-acetylcoumarin **3** from the reaction of 2-hydroxybenzaldehyde **1** with ethyl acetoacetate **2**. Compounds of the ketocoumarin type are usually synthesized from salicylaldehyde using a cyclic

secondary amine piperidine [12]. However, in our experiment, we used triethyl amine, a tertiary amine, as a catalyst.

Compound **3** was then reacted with 4-morpholinobenzaldehyde **4** to furnish the target molecule **5** employing a Claisen–Schmidt reaction. First, we conducted the synthesis of compound **5** using a solution of KOH 40% as a catalyst as is generally used for aldol condensation. However, we did not get the desired product. We assumed that KOH solution hydrolyzed the 3-acetylcoumarin. Then we decided to use *p*-toluenesulfonic acid (*p*TSA) as a catalyst, and the reaction proceeded to give the desired product. The reaction process is displayed in Figure 1.

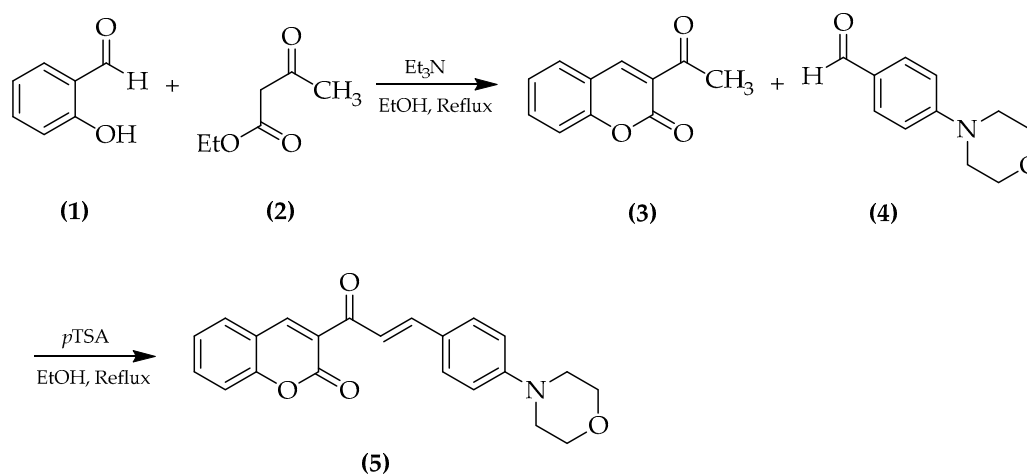


Figure 1. Synthesis pathway of the target molecule.

(*E*)-3-[3-(4-Morpholinophenyl)acryloyl]-2*H*-chromen-2-one: red needle crystal (0.88 g, 24%), R_f 0.58 (*n*-hexane:ethyl acetate 3:2), HRMS(ESI) $[M + Na]^+$ for $C_{22}H_{19}NO_4$ $m/z = 384.1212$ (calculated) and 384.1215 (observed); IR (DRS, KBr, cm^{-1}): 3094 (C–H aromatic), 2855 (C–H aliphatic), 1724 (C=O ketone), 1605 (C=C conjugated), 1572 (C=C aromatic), 1171 (C–O ether). 1H -NMR (400 MHz, $CDCl_3$) δ_H 8.57 (s, 1H), 7.85 (d, $J = 15.6$ Hz, 1H), 7.79 (d, $J = 15.6$ Hz, 1H), 7.66 (m, 2H), 7.61 (d, $J = 8.9$ Hz, 2H), 7.39 (d, $J = 8.3$ Hz, 1H), 7.34 (t, $J = 7.6$ Hz, 1H), 6.89 (d, $J = 8.9$ Hz, 2H), 3.86 (t, $J = 5.3$ Hz, 4H), 3.28 (t, $J = 5.3$ Hz, 4H). ^{13}C -NMR (101 MHz, $CDCl_3$) δ_C 186.3 (C), 159.6 (C), 155.3 (C), 153.0 (C), 147.8 (CH), 145.6 (CH), 134.1 (CH), 130.9 (CH), 130.1 (CH), 125.9 (C), 125.8 (C), 125.0 (CH), 120.6 (CH), 118.8 (C), 116.8 (CH), 114.6 (CH), 66.7 (CH_2), 48.0 (CH_2).

This paper discusses only the title compound **5** because compound **3** is already known. The spectroscopy data of compound **3** are presented in Supplementary Materials (Figures S1–S4). The HRMS spectrum of the title compound showed a positive molecular ion of $[M + Na]^+$ at $m/z = 384.1215$, suitable for a molecular formula of $C_{22}H_{19}NO_4$, which corresponded to 14 equivalent double bonds of (Supplementary Materials Figure S6). Analysis of the FTIR spectrum showed a stretching vibration band of a C–H aromatic bond at ν_{max} (cm^{-1}) 3094, and followed subsequently with a stretching vibration band of a C–H aliphatic bond at 2855, vibration band of ketone group at 1724, vibration band of conjugated alkene at 1605, vibration band of C–C aromatic bond at 1572, and stretching vibration band of C–O ether group at 1171 cm^{-1} (Supplementary Materials Figure S5).

From the 1H -NMR spectrum, the existence of a coumarin fragment substituted at position 3 was shown via four signals, those were three signals of aromatic protons at 7.66, 7.39, and 7.34 ppm and a signal of a conjugated olefinic proton at 8.57 ppm. The presence of a chalcone scaffold with *E* geometry was proved via two coupled ($J = 15.6$ Hz) olefinic proton signals at 7.85 and 7.79 ppm. Furthermore, a para disubstituted benzene fragment was shown via two coupled ($J = 8.9$ Hz) aromatic signals at 7.61 ppm and 6.89 ppm. The existence of a morpholine fragment was proved by two triplet signals at 3.86 and 3.28 ppm with the integration of four for each signal representing two symmetrical ethylene fragment (Supplementary Materials Figure S7a,b). The spectrum of ^{13}C -NMR

exhibited 18 signals indicating that the molecular structure consisted of 8 symmetrical carbon atoms (Supplementary Materials Figure S8), whereas the correlation of the proton atoms with carbon atoms were assigned using the 2-D NMR experiment of Heteronuclear Multiple Bond Correlation (HMBC) (Supplementary Materials Figure S10) and Heteronuclear Multiple-Quantum Correlation (HMQC) (Supplementary Materials Figure S9) as shown in Table 1 and Figure 2 below.

Table 1. NMR data of the title compound in CDCl₃.

No. Atom	δ_H (ppm) (mult, J Hz)	δ_C (ppm)	HMBC
2		159.6	
3		125.8	
4	8.57 (s, 1H)	147.8	C-2, C-3, C-4a, C-5, C-8a, C-9
4a		118.8	
5	7.66 (m, 2H) overlapped with H-7	130.1	
6	7.34 (t, J = 7.6 Hz, 1H)	125.0	C-4a, C-8
7	7.66 (m, 2H) overlapped with H-5	134.1	
8	7.39 (d, J = 8.3 Hz, 1H)	116.8	C-4a, C-6
8a		155.3	
9		186.3	
10	7.79 (d, J = 15.6 Hz, 1H)	120.6	C-3, C-9, C-12
11	7.85 (d, J = 15.6 Hz, 1H)	145.6	C-9, C-10, C-12, C-13, C-17
12		125.9	
13, 17	7.61 (d, J = 8.9 Hz, 2H)	130.9	C-11, C-13, C-14, C-15, C-16, C-17
14, 16	6.89 (d, J = 8.9 Hz, 2H)	114.6	C-12, C-13, C-14, C-16, C-17
2', 6'	3.86 (t, J = 5.3 Hz, 4H)	48.0	C-2', C-3', C-5', C-6'
3', 5'	3.28 (t, J = 5.3 Hz, 4H)	66.7	C-2', C-3', C-5', C-6'

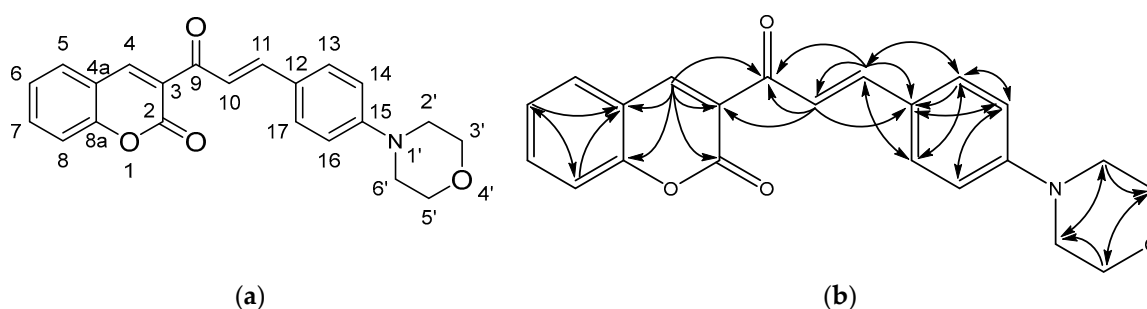


Figure 2. (a) Structure numbering, and (b) HMBC correlation of the title compound.

The anticancer activity of the prepared compound against cervix cancer cells line HeLa and breast cancer cells line T47D was determined using an MTT assay, and revealed an IC₅₀ of 0.90 μ M for breast cancer cells line T47D and of 2.32 μ M for cervix cancer cell HeLa, and it can be considered as not active as an anticancer compound (Supplementary Materials Table S1).

3. Materials and Methods

3.1. General

All reagents and solvents were provided from the commercial sources (E.Merck, Darmstadt, Germany or Sigma Aldrich, St. Louis, MO, USA) and used without prior purification. The reaction progress was monitored via a Thin Layer Chromatography (TLC) experiment using an aluminium silica gel plate GF₂₅₄ (0.25 mm) employing different solvents. The TLC spot was detected using UV light ($\lambda = 254$ nm). The FTIR spectrum was recorded on a IRTracer100 spectrometer (Shimadzu, Kyoto, Japan) using a diffuse reflectance method), whereas the mass spectrum was recorded on a HRESIMS QTOF micrOTOF-Q II Bruker Compass (Billerica, MA, USA). The NMR spectrum (¹H-, and ¹³C-APT)

was recorded on a JEOL JNM-ECS400 spectrometer (at 400 and 100 MHz) (JEOL Ltd., Tokyo, Japan) with CDCl₃ as the solvent and internal standard.

3.2. Synthesis of 3-Acetylcoumarin 3

The mixture of 0.65 g (5 mmol) ethyl acetoacetate, 0.61 g (5 mmol) salicylaldehyde, and three drops of triethylamine in 10 mL ethanol was refluxed in a round bottom flask for 8 h. The reaction progress was monitored via TLC and was stopped when it completed. The precipitate was filtered off and recrystallized using ethanol.

3.3. Synthesis of the Title Compound 5

The mixture of 3-acetylcoumarin 3 (0.1881 g; 1 mmol), 4-morpholinobenzaldehyde 4 (1.1911 g; 1 mmol), and *p*TSA (0.034 g; 0.2 mmol) in 10 mL ethanol was refluxed for 6 h. The reaction progress was monitored with TLC and stopped at completion. The precipitate was then filtered off and subjected to column chromatography for purification using *n*-hexane:ethyl acetate (3:2) as a mobile phase to furnish the pure title compound.

3.4. Evaluation of Anticancer Activity

The evaluation of the anticancer activity of the title compound was conducted using an MTT assay following the protocol of Tabata et al. [13]. The cancer cells were seeded in a 96-well plate at a density of 1×10^4 cells/well with a phenol red-free RPMI (Roswell Park Memorial Institute medium) 1640 medium (containing 10% FBS (fetal bovine serum)) and maintained for 24 h. Subsequently, the tested compound (various concentrations) was applied for 24 h. After addition of 0.5% MTT solution, the incubation was continued for a further 4 h at 37 °C/5% CO₂. The stop solution (0.04 N HCl in isopropanol) was added to the culture medium to each well. Then, the absorbance at 570 nm (peak) and 630 nm (bottom) was measured using an ELISA (Enzyme-Linked Immunosorbent Assay) reader. It was conducted in triplicate. Doxorubicin was used as a positive control. The value of IC₅₀ was determined using a probit analysis (SPSS 17, IBM Analytics, New York, NY, USA).

4. Conclusions

We have successfully synthesized a new compound (*E*)-3-[3-(4-morpholinophenyl)acryloyl]-2*H*-chromen-2-one through a Claisen–Schmidt reaction using a molecular hybridization method between 3-acetylcoumarin, 4-morpholinobenzaldehyde, and *p*TSA as a catalyst.

Supplementary Materials: The following are available online, FTIR, HRESI-MS, ¹H-NMR, ¹³C-NMR (APT) spectra, and anticancer evaluation of the title compound are reported in the Supplementary Materials as Figures S1–S10 and Table S1.

Author Contributions: H.S. brought the idea, managed the research, and wrote the paper. H.D.H. performed the synthesis, K.U.H. and A.N.K. analyzed the whole spectra, while M.K. conducted the anticancer test. All the authors have read the draft.

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Conflicts of Interest: The authors declare no conflict of interest.

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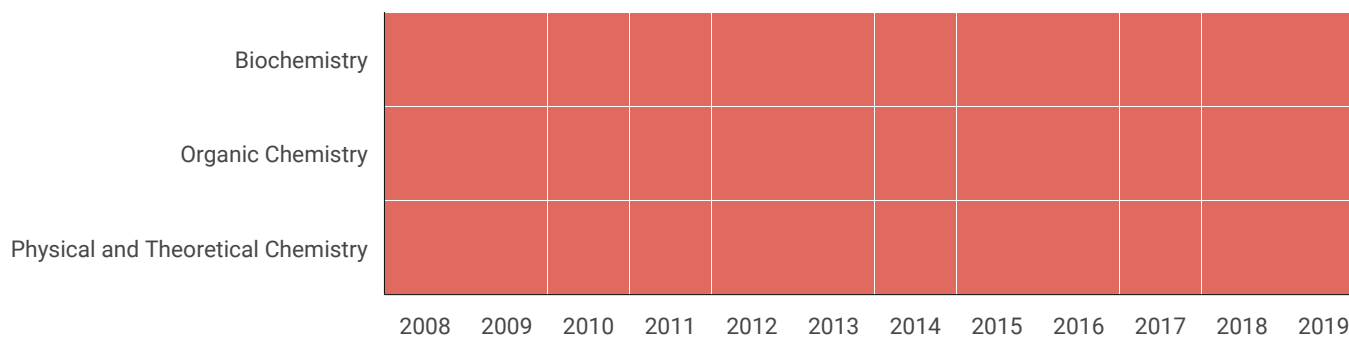
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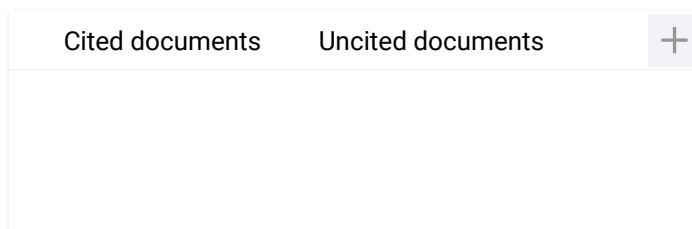
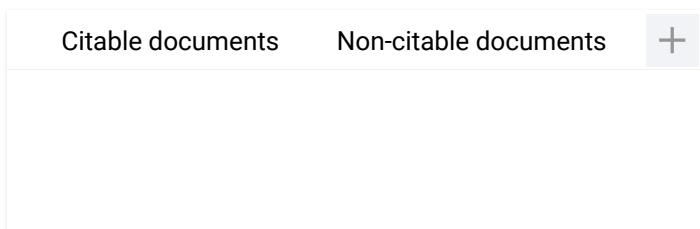
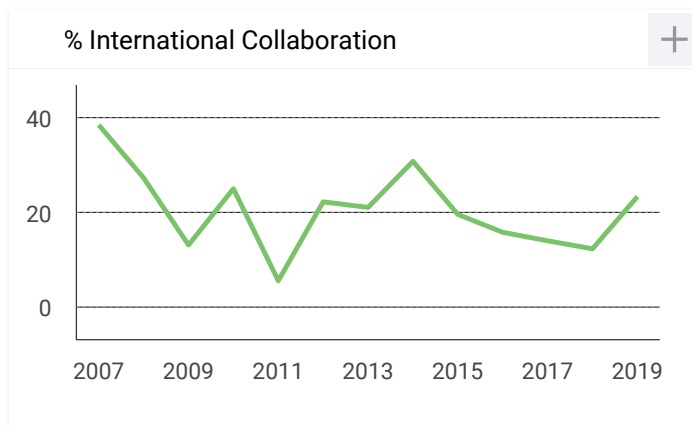
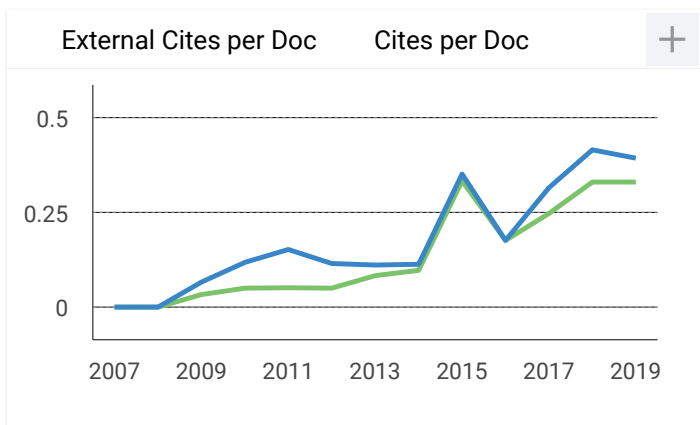
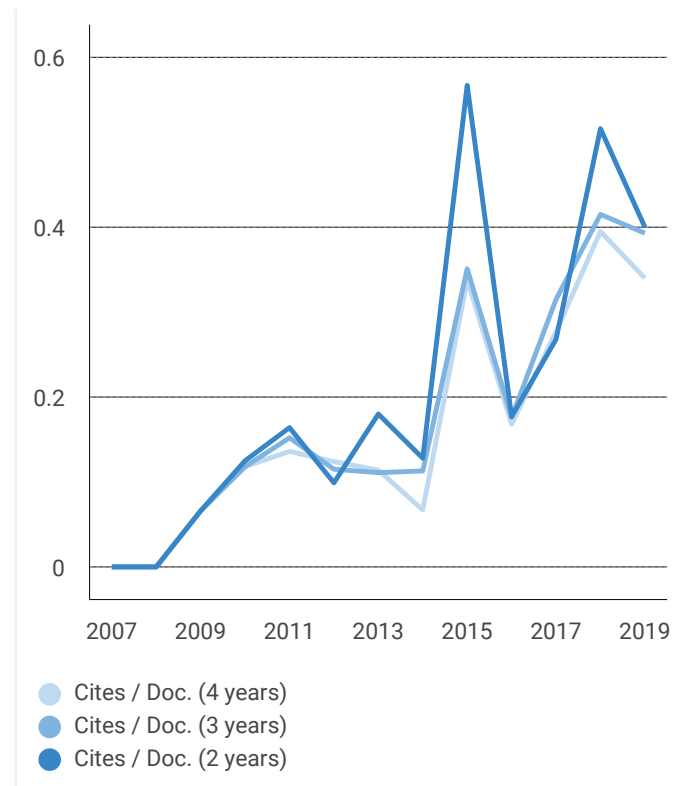
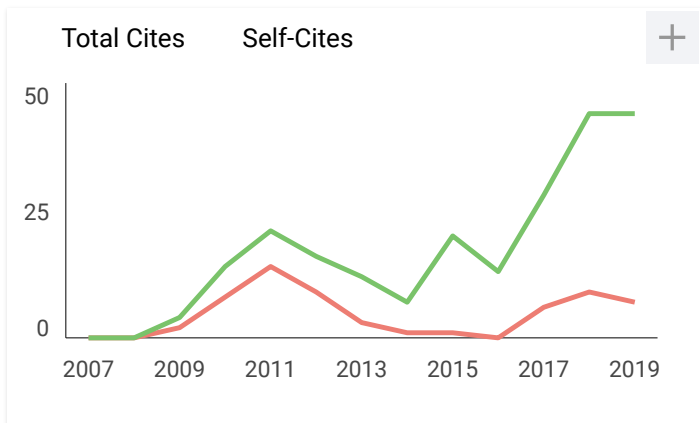
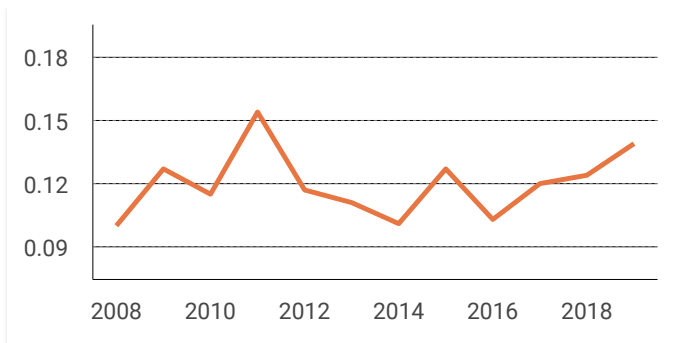


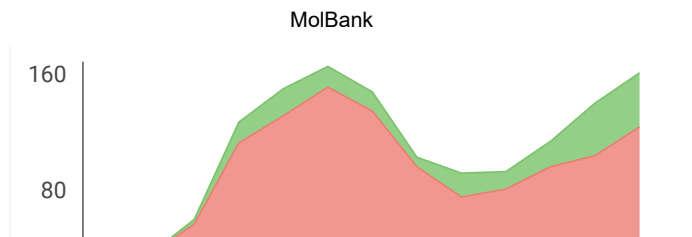
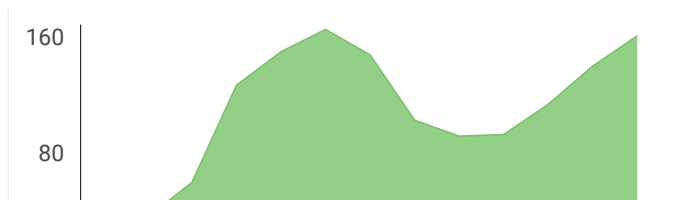
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