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The scope of *Molbank* is reflected by its three journal sections:

- Organic Synthesis
- Natural Products
- Structure Determination

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Table of Contents

Molbank, Volume 2018 (/1422-8599/2018), Issue 3 (September 2018)

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Open Access Short Note (/1422-8599/2018/3/M1020/pdf)

***O*-Methyl *m*-Tolylcarbamothioate (/1422-8599/2018/3/M1020)**

by Chien Ing Yeo (https://sciprofiles.com/profile/424298) and Edward R. T. Tiekink (https://sciprofiles.com/profile/348831)

Molbank **2018**, *2018*(3), M1020; https://doi.org/10.3390/M1020 (https://doi.org/10.3390/M1020) - 15 Sep 2018

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Abstract The synthesis, spectroscopic, and crystallographic characterisation of the title compound, *O*-methyl *m*-tolylcarbamothioate, MeOC(=S)N(H)(*m*-tolyl) (**1**), are described. The crystallographic study confirms the structure determined by spectroscopy and shows the presence of the thioamide tautomer, a *syn*-disposition of **[...] Read more.**

(This article belongs to the Section **Structure Determination (/journal/molbank/sections/structure_determination_molbank)**)

Open Access Short Note (/1422-8599/2018/3/M1019/pdf)

(*E*)-1-(2′,4′-Dimethyl)-(5-acetylthiazole)-(2,4″-difluorophenyl)-prop-2-en-1-one (/1422-8599/2018/3/M1019)

by Afzal Shaik (https://sciprofiles.com/profile/143503) , Mahamuda Sultana Shaik (https://sciprofiles.com/profile/517114) and Srinivasa Babu Puttagunta (https://sciprofiles.com/profile/author/bGJheUV3RDNsaXNXZndDZ3gvUkVLTmtrTENxSWMzQmNGM010aXFxRzJMYz0=)

Molbank **2018**, *2018*(3), M1019; https://doi.org/10.3390/M1019 (https://doi.org/10.3390/M1019) - 13 Sep 2018

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Abstract Thiazole and chalcone motifs are of research interest to medicinal chemists due to their array of synthetic and biological utility. Hence, in the present study we intended to prepare (*E*)-1-(2′,4′-dimethyl)-(5-acetylthiazole)-(2,4″-difluorophenyl)-prop-2-en-1-one (**3c**) containing both these scaffolds. The compound **3c** was **[...] Read more.**

(This article belongs to the collection **Molecules from Catalytic Processes (/journal/molbank/special_issues/molecules_catalytic)**)

Open Access Feature Paper Short Note (/1422-8599/2018/3/M1018/pdf)

5-Amino-3-(diethylamino)-5*H*-benzo[4,5]imidazo[1,2-*b*][1,2,4,6]thiatriazine 1,1-Dioxide (/1422-8599/2018/3/M1018)

by Victor Tran (https://sciprofiles.com/profile/author/SkpiYk4yS21xZHJwSjZxS2dUTXFDVTZabFV4Zm9tQVQrT1NkcUZMWFhKND0=) , Craig M. Forsyth (https://sciprofiles.com/profile/author/VGs1VmNiZ2x6dzQ1Rmk3OXM2MGh6eXM3V1N6SDV5WGJXU0ZsV01pdEtSaz0=) and Craig L. Francis (https://sciprofiles.com/profile/128512)

Molbank **2018**, *2018*(3), M1018; https://doi.org/10.3390/M1018 (https://doi.org/10.3390/M1018) - 11 Sep 2018

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Abstract In the quest for discovery of novel bioactive molecules, new heterocyclic ring systems provide templates for exploration of uncharted chemical space. Herein, we describe the synthesis of a new benzo[4,5]imidazo[1,2-*b*][1,2,4,6]thiatriazine derivative from readily available 1,2-diaminobenzimidazole and *N*,*N*-diethyl-*N* **[...] Read more.**

(This article belongs to the Special Issue **Heteroatom Rich Organic Heterocycles (/journal/molbank/special_issues/Heteroatom_Heterocycles)**)

Open Access Feature Paper Short Note (/1422-8599/2018/3/M1017/pdf)

(*S*)-4-Isopropyl-5,5-diphenyloxazolidin-2-one (/1422-8599/2018/3/M1017)

by Raffaella Mancuso (https://sciprofiles.com/profile/383577) , Rossana Miliè (https://sciprofiles.com/profile/author/cHgwMExjUkZqOHU4WTNsUHBQcmdlMXB3QlphR2cvdVhDK0pWQmV6cmRwMD0=) , Ida Ziccarelli (https://sciprofiles.com/profile/author/L3JPcThYVU9UYVNYTmZBUmNmanJtMXVBNDkxdi9RekxxSFNRaDBWTmhaMD0=) , Mariangela Novello (https://sciprofiles.com/profile/author/ZDdCazlCWUprOFVEM2t6Q2hMK3VzcDE5TTVMTEE1dzVGczVpUVYwN2VhZz0=) , Nicola Della Ca' (https://sciprofiles.com/profile/186460) and Bartolo Gabriele (https://sciprofiles.com/profile/54431)

Molbank **2018**, *2018*(3), M1017; https://doi.org/10.3390/M1017 (https://doi.org/10.3390/M1017) - 31 Aug 2018

Cited by 1 (/1422-8599/2018/3/M1017#citedby) | Viewed by 523

Abstract (*S*)-4-Isopropyl-5,5-diphenyloxazolidin-2-one has been synthesized for the first time by the enantiospecific oxidative carbonylation of commercially available (*S*)-2-amino-3-methyl-1,1-diphenylbutan-1-ol. The cyclocarbonylation reaction was carried out at 100 °C in 1,2-dimethoxyethane (DME) as the solvent for 15 h, under 20 atm of **[...] Read more.**

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Open Access Short Note (/1422-8599/2018/3/M1016/pdf)

(1F-Chloro-3-Methyl-2-oxo-2,5-dihydrofuran-3-yl)-3-phenyl-4-oxa-2,6-diazabicyclo[3.2.0]hept-2-en-7-one (/1422-8599/2018/3/M1016)

by **Jun Fu (https://sciprofiles.com/profile/291883)** , **Victor Pham (https://sciprofiles.com/profile/503321)** , **Matthew-Alexander Tippin (https://sciprofiles.com/profile/author/VFk4cisrQThtZ1ZxeUNUaCsvc2dkQnJURTdVZ3QvSGt1Tno3NTJMWVBYZz0=)** , **Liankun Song (https://sciprofiles.com/profile/author/c3VVa1JlaTk2eFZ3NmR0b0htM1RhWkpDLzF5Q0ZBaUVWQ1UvRzhqWEhabz0=)** , **Xiaolin Zi (https://sciprofiles.com/profile/238706)** , **En Zhang (https://sciprofiles.com/profile/298719)** and **Hong-Min Liu (https://sciprofiles.com/profile/92371)**

Molbank **2018**, *2018*(3), M1016; **https://doi.org/10.3390/M1016 (https://doi.org/10.3390/M1016)** - 30 Aug 2018

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Abstract Efficient large-scale and feasible industrial synthesis of the 1-oxacephem core structure from 6-aminopenicillanic acid (6-APA) has been reported for several decades. Via the industrial synthesis route, a byproduct (compound **9**) containing a butenolide unit was purified and characterized by NMR and HRMS **[...] Read more.**

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Open Access Feature Paper Short Note **(/1422-8599/2018/3/M1015/pdf)**

(3-Ammonio-2,2-dimethyl-propyl)carbamate Dihydrate (/1422-8599/2018/3/M1015)

by **Jaqueline Heimgert (https://sciprofiles.com/profile/author/b21LR241NTBlUVphL3pJd0ZWTE94SExOdTEvQ0EyNlVTcm9DdGFmSzdjamtFSmZlQnBBMUFDdjN** , **Dennis Neumann (https://sciprofiles.com/profile/author/Q1YraXdpS1ZKaUdOMzMzYWh1NnlXaXFRQ2plMGh6QTVhUUtFdkpyWktkQT0=)** and **Guido J. Reiss (https://sciprofiles.com/profile/43640)**

Molbank **2018**, *2018*(3), M1015; **https://doi.org/10.3390/M1015 (https://doi.org/10.3390/M1015)** - 29 Aug 2018

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Abstract (3-Ammonio-2,2-dimethylpropyl)carbamate dihydrate was synthesised. The title compound was characterised by single crystal X-ray diffraction and IR-/Raman-spectroscopy. It has been demonstrated that a mixture of dilute acetic acid and 2,2-dimethyl-1,3-diaminopropane is able to capture CO_2 spontaneously from the atmosphere. An intramolecular hydrogen bond **[...] Read more.**

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1-[5-(4-Tolyl)-1,3,4-oxadiazol-2-yl]methanamine (/1422-8599/2018/3/M1014)

by **Ganesh Shimoga (https://sciprofiles.com/profile/author/M2ZEa1RlVFRDZzcvQkRSTmxkZnpkRjBCM2pjQ2dUOHQ4K1lDRVZQc2hQRT0=)** , **Eun-Jae Shin (https://sciprofiles.com/profile/451838)** and **Sang-Youn Kim (https://sciprofiles.com/profile/289515)**

Molbank **2018**, *2018*(3), M1014; **https://doi.org/10.3390/M1014 (https://doi.org/10.3390/M1014)** - 24 Aug 2018

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Abstract 1-[5-(4-Tolyl)-1,3,4-oxadiazol-2-yl]methanamine (**3**) has been successfully synthesized by reacting *p*-toluic hydrazide (**1**) and glycine (**2**) via the polyphosphoric acid condensation route. The course of the reaction was found to be high yielding (87%) and the title compound **[...] Read more.**

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Open Access Short Note **(/1422-8599/2018/3/M1013/pdf)**

5-[3-(4-Bromophenyl)-1-(2,5-dimethoxyphenyl)-3-oxopropyl]-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-tri-one (/1422-8599/2018/3/M1013)

by **Hery Suwito (https://sciprofiles.com/profile/87893)** , **Ria Hesty Purnama Sari (https://sciprofiles.com/profile/author/RlllMmtwcFo0WFV2bUp1akdGSmpJY3M2ODBpZmlJZXZVVndoVGtJUDFBZz0=)** , **Kautsar Ul Haq (https://sciprofiles.com/profile/author/NnE3V1d1enBkanp0Z0F0ekxFcXgwei9MdkN3NHlVWmRKMFJhUk5SR283SDA4aUFPYVl1S1MrVzdVZHN** and **Alfinda Novi Kristanti (https://sciprofiles.com/profile/325866)**

Molbank **2018**, *2018*(3), M1013; **https://doi.org/10.3390/M1013 (https://doi.org/10.3390/M1013)** - 23 Aug 2018

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Abstract The title compound was prepared by a two-step reaction. The first step was the formation of a chalcone derivative using Claisen–Schmidt condensation, which was followed by the Michael addition of the formed chalcone with 1,3-dimethylbarbituric acid. The structure of the prepared compound was **[...] Read more.**

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Open Access Short Note **(/1422-8599/2018/3/M1012/pdf)**

***N*-(4-Bromophenyl)methoxycarbothioamide (/1422-8599/2018/3/M1012)**

by **Chien Ing Yeo (https://sciprofiles.com/profile/424298)** and **Edward R.T. Tiekink (https://sciprofiles.com/profile/348831)**

Molbank **2018**, *2018*(3), M1012; **https://doi.org/10.3390/M1012 (https://doi.org/10.3390/M1012)** - 17 Aug 2018

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Abstract The synthesis, spectroscopic and crystallographic characterisation of the title compound, *O*-methyl-*N*-4-bromophenyl thiocarbamate, MeOC(=S)N(H)PhBr-4 (**1**), are described. Spectroscopy confirmed the formation of the compound and the molecular structure was determined crystallographically. Two independent but chemically similar molecules comprise the **[...] Read more.**

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Open Access Short Note **(/1422-8599/2018/3/M1011/pdf)**

3-(3,5-Difluorophenyl)-1-phenyl-1*H*-pyrazole-4-carbaldehyde (/1422-8599/2018/3/M1011)

by **Naveen Kumar (https://sciprofiles.com/profile/author/eld4NlE1SkJEbVJlbzNFZ0ZuNU4ydmJWTmc5R1NGWXhiOUl6azJuZjZoST0=)** , **Swamy Sreenivasa (https://sciprofiles.com/profile/48879)** , **Vasantha Kumar (https://sciprofiles.com/profile/author/RHgzRGEuQWp3Y1JScURURnJpb2JiVWNXZkdBdDhZbXdFWFBZL1FKM21GQT0=)** and **Nadigar Revansiddappa Mohan (https://sciprofiles.com/profile/49669)**

Molbank **2018**, *2018*(3), M1011; **https://doi.org/10.3390/M1011 (https://doi.org/10.3390/M1011)** - 01 Aug 2018

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Ablsmeier–Haack reaction of (*E*)-1-[1-(3,5-difluorophenyl)ethylidene]-2-phenylhydrazine (**1**) using dimethyl formamide in excess of phosphorus oxychloride by cor[illegible]l method, resulted in the synthesis of the title compound 3-(3,5-difluorophenyl)-1-phenyl-1*H*-pyrazole-4- carbaldehyde (**2**) in good yield and high purity. Structure characterization **[...] Read more.**

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Open Access Communication **(/1422-8599/2018/3/M1010/pdf)**

Benzyl (*R*)-2-(Acetylthio)Propanoate: A Promising Sulfur Isoster of (*R*)-Lactic Acid and Ester Precursors (/1422-8599/2018/3/M1010)

by **Ryosuke Sasaki (https://sciprofiles.com/profile/author/N0FuTjhqRC9rak5QZVlWQTFHbVFBcmJaRnZ6OFFSTWszS3YwWWdiOUg0ST0=)** , **Momoyo Kawamoto (https://sciprofiles.com/profile/author/dDJJeHpoVFdJNTZldGR4TmtNSWFXREplcjRlRHpnNnV1YTc1dTBpZHJBZz0=)** and **Yoo Tanabe (https://sciprofiles.com/profile/122999)**

Molbank **2018**, *2018*(3), M1010; **https://doi.org/10.3390/M1010 (https://doi.org/10.3390/M1010)** - 29 Jul 2018

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Abstract In this paper, an accessible chiral pool synthesis of benzyl (*R*)-2-(acetylthio)propanoate (acetylthiolactate), which is less odorous than the methyl or ethyl analogue, was performed through a clean S_N2 displacement reaction using available AcSK with tris[2-(2-methoxyethoxy)]ethylamine (TDA-1), starting from commercially **[...] Read more.**

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Open Access Short Note **(/1422-8599/2018/3/M1009/pdf)**

2-{[(4-Hydroxy-3,5-dimethoxyphenyl)methylidene]hydrazinylidene}-4-oxo-1,3-thiazolidin-5-yl Acetic Acid (/1422-8599/2018/3/M1009)

by **Sangeetha Karanth (https://sciprofiles.com/profile/author/Ung4NnJmOUM3NG5NdTEzaTFBcitVbUd2WWpqcXY0QURuNzA5NFlMUUN2Zz0=)** , **Badiadka Narayana (https://sciprofiles.com/profile/author/K2xyb1RJNHgyRVNueHFTK1ZjZ2doWWxXVVpzMlJ2VFJjNll1bkF1SWhEMnVjZXVtNkJST3M2bWljUz** , **Sharath Chandra Kodandoor (https://sciprofiles.com/profile/author/amN3QnZWbE1pT0cyWi9CS1A0bDczR0ZNdWdsVk54QytjZEpRbEUvUTl0cz0=)** and **Balladka Kunhanna Sarojini (https://sciprofiles.com/profile/361925)**

Molbank **2018**, *2018*(3), M1009; **https://doi.org/10.3390/M1009 (https://doi.org/10.3390/M1009)** - 29 Jul 2018

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Abstract Thia-Michael addition of 2-[(4-hydroxy-3,5-dimethoxyphenyl)methylidene]hydrazine-1-carbothioamide (**1**) with maleic anhydride results in the formation of the title compound 2-{[(4-hydroxy-3,5-dimethoxyphenyl)methylidene]hydrazinylidene}-4-oxo-1,3-thiazolidin-5-yl acetic acid **2**. The precursor **1** is synthesized by the reaction of 4-hydroxy-3,5-dimethoxybenzaldehyde and thiosemicarbazide in the presence of glacial acetic acid as **[...] Read more.**

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Open Access Short Note **(/1422-8599/2018/3/M1008/pdf)**

***N*-[2-(1*H*-Indol-3-yl)-1-(5-thioxo-4,5-dihydro-1,3,4-oxadiazol-2-yl)ethyl]-4-methylbenzenesulfonamide (/1422-8599/2018/3/M1008)**

by **Nikil Purushotham (https://sciprofiles.com/profile/author/TDVYSzlwSnlyOFFCMWRxUkJ1OVo2QldBb2hhK2tqWm9NZjhWREpacm4wYz0=)** and **Boja Poojary (https://sciprofiles.com/profile/293824)**

Molbank **2018**, *2018*(3), M1008; **https://doi.org/10.3390/M1008 (https://doi.org/10.3390/M1008)** - 25 Jul 2018

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Abstract *N*-[1-Hydrazinyl-3-(1*H*-indol-3-yl)-1-oxopropan-2-yl]-4-methylbenzenesulfonamide (**1**) on cyclization with carbon disulfide in ethanolic potassium hydroxide affords *N*-[2-(1*H*-indol-3-yl)-1-(5-thioxo-4,5-dihydro-1,3,4-oxadiazol-2-yl)ethyl]-4-methylbenzenesulfonamide (**2**) in 84% yield. The structure of compound **2** was supported by mass spectrometry, FT-IR and ^{1}H- and ^{13} **[...] Read more.**

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Open Access Short Note **(/1422-8599/2018/3/M1007/pdf)**

5,7-Dihydroxy-3,6-Dimethoxy-3′,4′-Methylendioxyflavone (/1422-8599/2018/3/M1007)

by **Tjitjik Srie Tjahjandarie (https://sciprofiles.com/profile/159161)** , **Ratih Dewi Saputri (https://sciprofiles.com/profile/257183)** , **Ulfatun Hasanah (https://sciprofiles.com/profile/464659)** , **Fida Rachmadiarti (https://sciprofiles.com/profile/464660)** and **Mulyadi Tanjung (https://sciprofiles.com/profile/190848)**

Molbank **2018**, *2018*(3), M1007; **https://doi.org/10.3390/M1007 (https://doi.org/10.3390/M1007)** - 23 Jul 2018

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Abstract

A new flavonoid derivative, namely 5,7-dihydroxy-3,6-dimethoxy-3′,4′-methylenedioxyflavone (**1**), was isolated from the leaves of *Melicope glabra* (Blume) T.G. Hartley. The structure of **1** was elucidated based on their UV, IR, HRESIMS, and 1D and 2D NMR spectral data. **Full article (/1422-8599/2018/3/M1007)**

(This article belongs to the Section **Natural Products (/journal/molbank/sections/natural_products_molbank)**)

Open Access Feature Paper Short Note **(/1422-8599/2018/3/M1006/pdf)**

Quercetin-3-oleate (/1422-8599/2018/3/M1006)

by **Gabriele Carullo (https://sciprofiles.com/profile/465289)** and **Francesca Aiello (https://sciprofiles.com/profile/262799)**

Molbank **2018**, *2018*(3), M1006; **https://doi.org/10.3390/M1006 (https://doi.org/10.3390/M1006)** - 20 Jul 2018

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Abstract Polyphenols are well-known health promoting agents, but they have some limitations due to their spontaneous oxidation. This evidence has limited their use as drugs in recent years. In this field, several chemical modifications have been proposed to overcome these restrictions; among these, esterification **[...] Read more.**

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Open Access Short Note (/1422-8599/2018/3/M1005/pdf)

1-(4-Hexylbenzoyl)-3-methylthiourea (/1422-8599/2018/3/M1005)

by Ruswanto Ruswanto (https://sciprofiles.com/profile/332479) ,
Richa Mardianingrum (https://sciprofiles.com/profile/author/UHVRUWl0VVM5Qml0VCt6dDY0TDhaSkw2S0JPYmxObG5wbTFxaWtFdXoxWT0=) ,
Tresna Lestari (https://sciprofiles.com/profile/author/MENkQ3JzZUJXR2RMOThEdVJ4cmF1N2taajV3aXBMZCtpbHBuWWdJd0Q4VT0=) ,
Tita Nofianti (https://sciprofiles.com/profile/author/R0lxeFZFSmVHdUJNWGV2Ly8ycmhtUWpWTE83OHJML3JvNFdycVVjK1cyRT0=) and
Siswandono Siswandono (https://sciprofiles.com/profile/author/cy93RjRiRFhpUkJWUVFqemYvTFBnMUhTUjNSamkvKytDdWtPc0hiRWZyaz0=)
Molbank **2018**, *2018*(3), M1005; https://doi.org/10.3390/M1005 (https://doi.org/10.3390/M1005) - 09 Jul 2018
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Abstract The 1-(4-hexylbenzoyl)-3-methylthiourea compound has been successfully synthesized by reacting 4-hexylbenzoyl chloride and 1-methylthiourea via the reflux method using a triethylamine catalyst. The 1-(4-hexylbenzoyl)-3-methylthiourea compound was identified by UV-visible, FT-IR, $^{13}C/^{1}H$-NMR and Mass spectrophotometry. From the activity test on four cancer **[...] Read more.**
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Open Access Short Note (/1422-8599/2018/3/M1004/pdf)

5-Hydroxy-3-(4-hydroxyphenyl)-8,8-dimethyl-6-(3-methylbut-2-enyl)pyrano[2,3-h]chromen-4-one (/1422-8599/2018/3/M1004)

by Giovanni Ribaudo (https://sciprofiles.com/profile/828603) ,
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Giuseppe Zagotto (https://sciprofiles.com/profile/189634)
Molbank **2018**, *2018*(3), M1004; https://doi.org/10.3390/M1004 (https://doi.org/10.3390/M1004) - 09 Jul 2018
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Abstract Natural and semi-synthetic compounds are being studied as novel phosphodiesterase 5 (PDE5) inhibitors for the treatment of erectile dysfunction, pulmonary hypertension, and lower urinary symptoms. *Maclura pomifera* is a source of flavonoids, one of the main classes of molecules investigated for these purposes. **[...] Read more.**
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3,3′-(Diazene-1,2-diyl)bis[4-(nitroamino)-1,2,5-oxadiazole 2-oxide] (/1422-8599/2018/3/M1003)

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Molbank **2018**, *2018*(3), M1003; https://doi.org/10.3390/M1003 (https://doi.org/10.3390/M1003) - 05 Jul 2018
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Abstract The nitramino derivatives of furoxans are of specific interest as precursors for the preparation of high energy salts with nitrogen-rich cations. In this communication, the 3,3′-(diazene-1,2-diyl)bis[4-(nitroamino)-1,2,5-oxadiazole 2-oxide] was prepared via nitration of available 4,4′-diamino-3,3′-diazenofuroxan; the best yield of the target compound was achieved **[...] Read more.**
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Open Access Communication (/1422-8599/2018/3/M1002/pdf)

2-[2-Methyl-5-phenyl-1-(3,4,5-trimethoxyphenyl)-1*H*-pyrrol-3-yl]-2-oxo-*N*-(pyridin-4-yl) acetamide (/1422-8599/2018/3/M1002)

by Ebrahim Saeedian Moghadam (https://sciprofiles.com/profile/408844) and Mohsen Amini (https://sciprofiles.com/profile/390413)
Molbank **2018**, *2018*(3), 1002; https://doi.org/10.3390/M1002 (https://doi.org/10.3390/M1002) - 28 Jun 2018
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Abstract We synthesized 2-[2-methyl-5-phenyl-1-(3,4,5-trimethoxyphenyl)-1*H*-pyrrol-3-yl]-2-oxo-*N*-(pyridin-4-yl) acetamide **4** as a novel compound derived from the indibulin and combretastatin scaffolds, which are known anti-mitotic agents, using a multistep reaction. We tested its cytotoxic activity against three breast cancer cell lines, namely, MCF-7, T47-D, **[...] Read more.**
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(*E*)-3-[3-(2-Butoxyquinolin-3-yl)acryloyl]-2-hydroxy-4*H*-chromen-4-one (/1422-8599/2018/3/1001)

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Jairo Quiroga (https://sciprofiles.com/profile/68297) and Braulio Insuasty (https://sciprofiles.com/profile/46790)
Molbank **2018**, *2018*(3), 1001; https://doi.org/10.3390/M1001 (https://doi.org/10.3390/M1001) - 21 Jun 2018
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Abstract The coumarinyl-quinolinylchalcone hybrid (*E*)-3-[3-(2-butoxyquinolin-3-yl)acryloyl]-2-hydroxy-4*H*-chromen-4-one **3b** was prepared in good yield from a Claisen-Schmidt condensation reaction between 3-acetyl-4-hydroxy-2*H*-chromen-2-one **1** and 2-butoxyquinoline-3-carbaldehyde **2** in methanol at reflux and catalyzed by KOH pellets. The structure of the synthesized compound **3b [...] Read more.**
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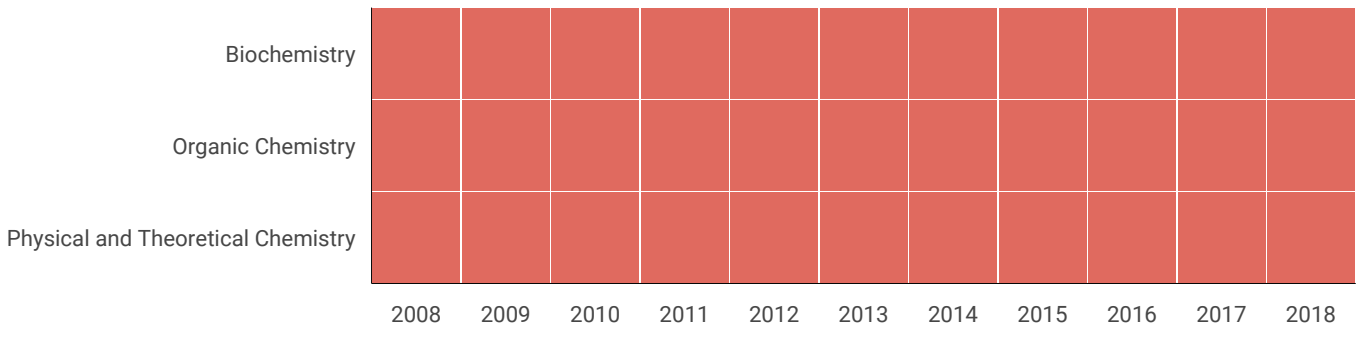

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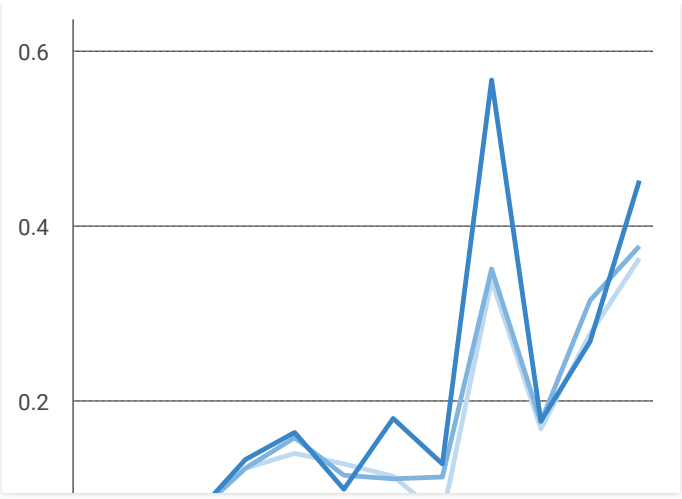

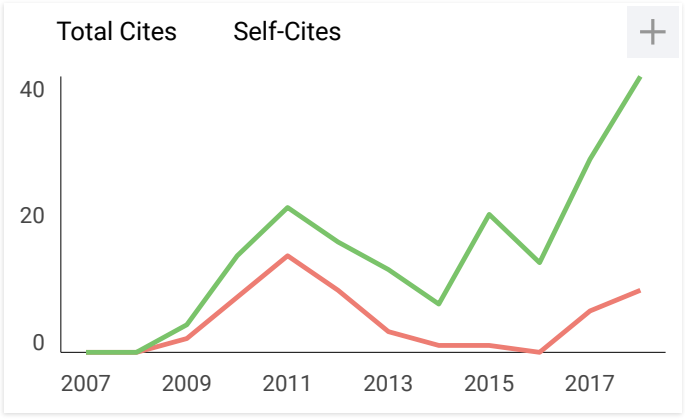

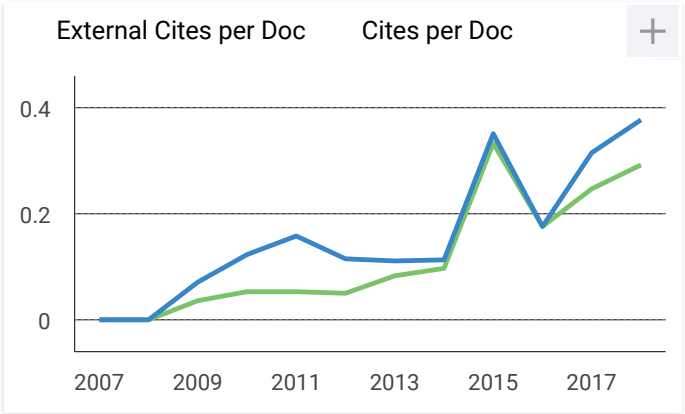

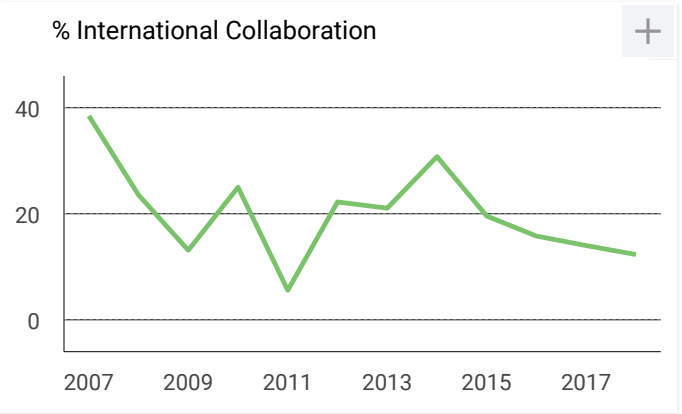

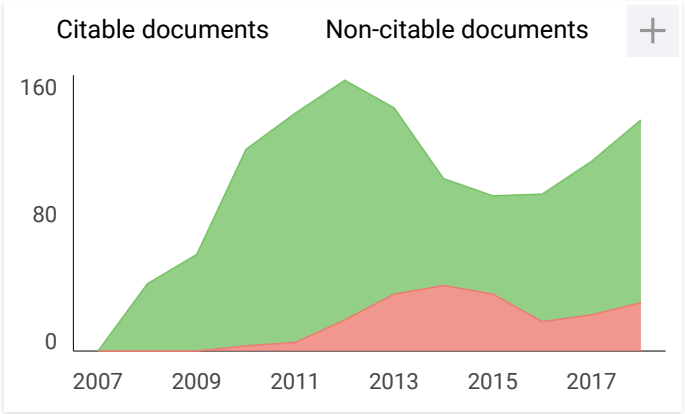

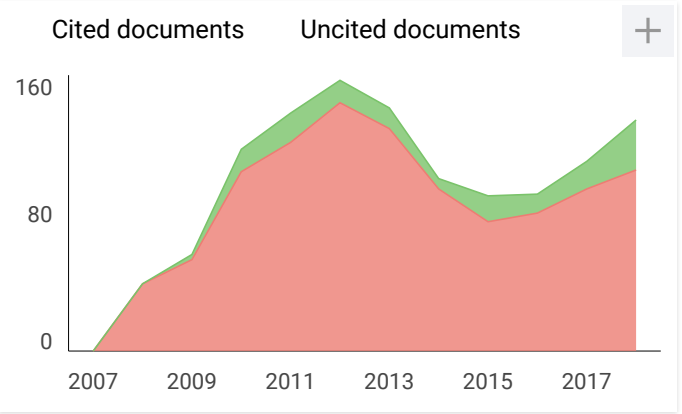

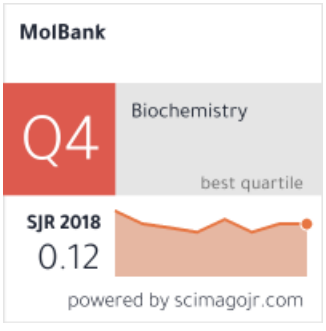

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5-[3-(4-Bromophenyl)-1-(2,5-dimethoxyphenyl)-3-oxopropyl]-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-tri-one

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Received: 2 August 2018; Accepted: 20 August 2018; Published: 23 August 2018

Abstract: The title compound was prepared by a two-step reaction. The first step was the formation of a chalcone derivative using Claisen–Schmidt condensation, which was followed by the Michael addition of the formed chalcone with 1,3-dimethylbarbituric acid. The structure of the prepared compound was established by spectral data: FTIR, HRESIMS, ^{1}H- and ^{13}C-NMR.

Keywords: chalcone derivative; 1,3-dimethylbarbituric acid; Michael addition

1. Introduction

Compounds possessing a dihydropyrimidine (DHPM) core attract the interest of researchers, either due to their wide spectrum bioactivities or from a synthesis point of view. The core of dihydropyrimidine can be constructed from a C–C–C and N–C–N scaffold, which may be formed by a Biginelli reaction [1] or cyclocondensation between an enone and urea or its analog. In general, preparation of a dihydropyrimidine derivative through cyclocondensation can be achieved by a reaction between chalcone as the source of the C–C–C unit and urea or its analog as the source of the N–C–N unit.

The molecular structure of dihydropyrimidine from a Biginelli product has a close resemblance to Hantsch 1,4-dihydropyridine, both being aza-analogues of nifedipine, which is well known as a calcium channel modulator [2]. Furthermore, DHPM derivatives are also known to exhibit antihypertensive [3], potassium channel antagonistic [4], antifilarial [5], anti-HIV [6,7], and antitumor [8] activities.

In continuing of our research, we intended to synthesize a 5,7-diphenyl-5,8-dihydropyrido [2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione (**3**) derivative through a Hantzsch cyclocondensation-type reaction constructed from a chalcone derivative (serving as the C–C–C unit) and 1,3-dimethylbarbituric acid (serving as the dioxopyrimidine unit) in the presence of ammonium chloride using triethylamine (TEA) acting as a Lewis base catalyst. Unfortunately, based on the spectroscopic evidence, the reaction stopped at the Michael addition process and did not proceed further to cyclocondensation. In this paper, we describe the synthesis and the characterization of the title compound.

2. Results

The title compound was synthesized in a two-step reaction. The synthesis was started by chalcone preparation employing Claisen–Schmidt condensation according to the procedure reported by Suwito et al., (2014) [9]. The next step was Michael addition between the chalcone with 1,3-dimethylbarbituric acid using TEA as a catalyst. The reaction process is displayed in Figure 1 below. In this article, we discuss only the preparation and structural characterization of compound **2** because compound **1** is already known. The title compound **2** was obtained as a white solid (171 mg; 34%).

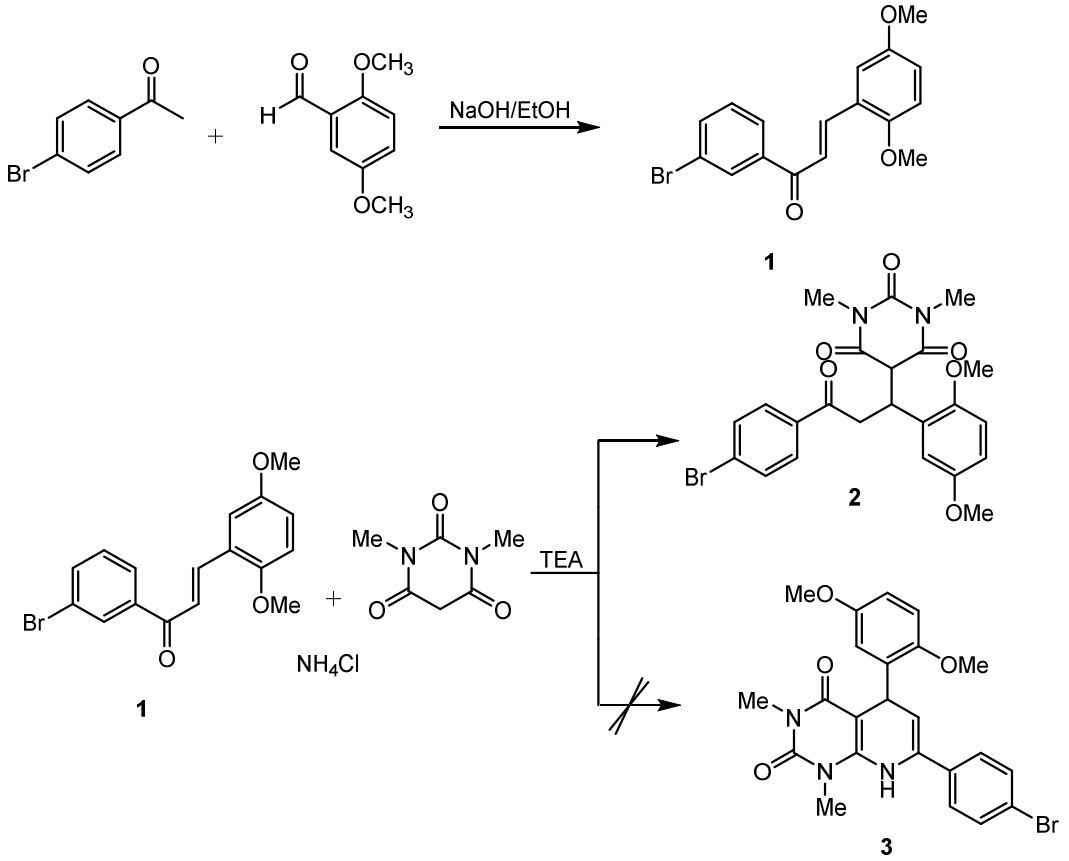


Figure 1. The reaction process for the synthesis of the title compound.

5-[3-(4-Bromophenyl)-1-(2,5-dimethoxyphenyl)-3-oxopropyl]-1,3-dimethyl-pyrimidine-2,4,6-trione: White solid (171.7 mg, 34%); Rf 0.512 ($CHCl_3$:ethyl acetate:*n*-hexane = 2:1:1); HRESIMS $[M - H]^-$ calculated for $C_{23}H_{22}N_2O_6Br$ 501.0661, found 501.0774; IR (DRS, KBr, cm^{-1}): 3080 (C–H aromatic), 2958 (m, CH aliphatic), 1745 (str, C=O ketone), 1618 (str, C=O amide), 1581.63 (str, C=C aromatic), 1203 (str, C–O–C ether), and 717 (C–Br); ^{1}H-NMR (400 MHz, DMSO-d_6) δ_H (ppm) 7.92 (d, J = 8.5 Hz, 2H), 7.75 (d, J = 8.4 Hz, 2H), 6.85 (d, J = 8.9 Hz, 1H), 6.77 (dd, J = 8.9 Hz, J = 2.9 Hz, 1H), 6.61 (d, J = 2.9 Hz, 1H), 4.43 (ddd, J = 8.3 Hz, J = 6.2 Hz, J = 4.4 Hz, 1H), 3.90 (dd, J = 18.3 Hz, J = 8.3 Hz, 1H), 3.79 (d, J = 4.4 Hz, 1H), 3.65 (s, 3H), 3.64 (s, 3H), 3.49 (dd, J = 18.3 Hz, J = 6.2 Hz, 1H), 2.93 (s, 3H), 2.92 (s, 3H); ^{13}C-NMR (101 MHz, DMSO-d_6) δ_C (ppm)197.8, 168.7, 168.3, 153.3, 151.9, 151.3, 136.1, 132.3, 130.5, 128.2, 127.9, 115.2, 113.3, 112.1, 56.3, 55.9, 53.2, 40.5, 37.1, 28.3, 28.2.

Two peaks of the molecular negative ion at m/z = 501.0774 and 503.0763 of the HRESIMS spectrum indicate that the prepared compound contains a bromine atom with the molecular formula $C_{23}H_{22}N_2O_6Br$ and possesses 13 degrees of unsaturation (Supplementary Materials, Figure S1). The analysis of IR spectra showed the existence of C–H aromatic, C–H aliphatic, C=O ketone, C=O amide, C=C aromatic, C_{alkyl}–O–C_{aryl} ether, and C–Br bonds which were indicated consecutively by peaks at ν_{max} (cm^{-1}) 3080, 2958, 1745, 1618, 1581, 1203, and 717, respectively (Supplementary Materials, Figure S2).

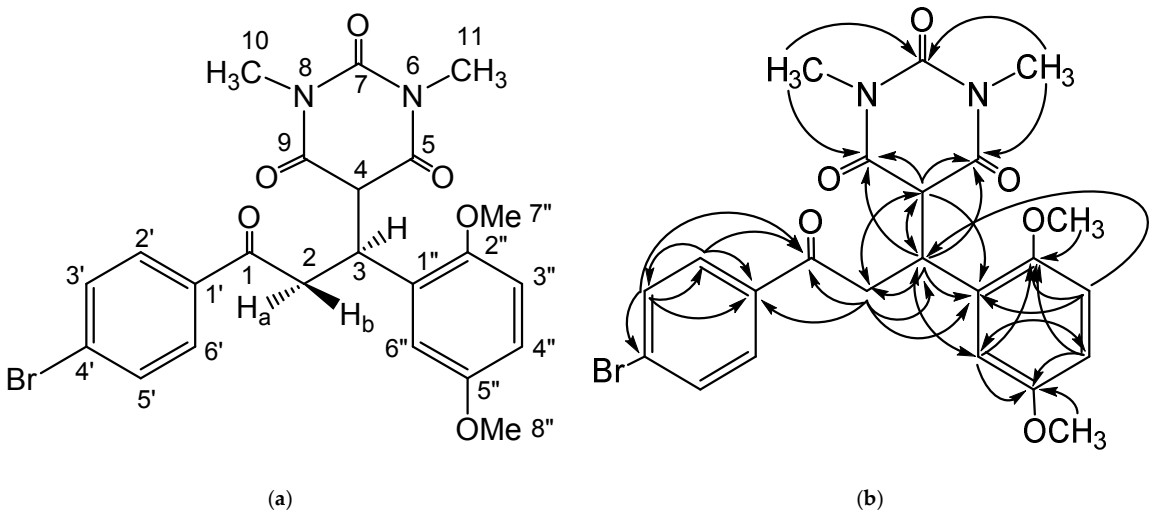
Spectroscopic data of ^{1}H-NMR (Table 1) showed an ABMX spin system which represented a –CH_2–CH–CH– fragment of the scaffold of the chalcone adduct with an active methylene. For this system, two signals at δ_H 3.90 (dd, 1H) and 3.49 ppm (dd, 1H) represented the existence of methylene diastereotopic fragment neighboring with a carbonyle group. Both signals showed a geminal coupling (J = 18.3 Hz). Protons appearing at δ_H 3.90 ppm (H_a) and 3.49 ppm (H_b) showed consecutively trans coupling (J = 8.3 Hz), and cis coupling (J = 6.2 Hz) with a proton at δ_H 4.43 ppm. The signal at

δ_H 4.43 ppm (ddd) represented a benzylic proton attached to a diastereotopic methylene, while the barbiturate fragment is exhibited by the existence of a vicinal coupling (J = 4.4 Hz) with a signal at δ_H 3.79 ppm. This signal represented a proton flanked by the two carbonyl groups of a barbiturate fragment. The existence of an aromatic ring was determined by five aromatic signals: two signals at δ_H 7.92 and 7.75 ppm appeared as a doublet with J = 8.5 Hz and integration of both. Both signals formed an AA'XX' spin system, which lead to the conclusion of a benzene fragment possessing two substituents at *para* position. While three other signals—appearing at δ_H 6.85 (d, J = 8.9 Hz, 1H), δ_H 6.77 (dd, J = 8.9 Hz, J = 2.9 Hz, 1H), and δ_H 6.61 (d, J = 2.9 Hz, 1H)—build an ABX spin system and represent a three substituted aromatic ring at position 1,2, and 4. Furthermore, the two signals at δ_H 3.65 ppm (s, 3H) and δ_H 3.64 (s, 3H) ppm indicated a methoxy proton attached at an aromatic ring, while the signals at δ_H 2.93 ppm (s, 3H) and δ_H 2.92 ppm (s, 3H) were signals of a methyl proton attached at the nitrogen atom of the barbiturate fragment (Supplementary Materials, Figure S3). The ^{13}C-NMR spectra (Table 1) showed 21 signals and represented all carbon atoms of the prepared compound (Supplementary Materials, Figure S4).

Table 1. NMR data of the target compound in DMSO-d_6.

No. Atom	δ_H (Mult, J Hz)	δ_C (ppm)	HMBC
1	-	197.9	
2	H_a = 3.90 (dd, 1H, J = 18.3 Hz, J = 8.3 Hz) H_b = 3.49 (dd, 1H, J = 18.3 Hz, J = 6.2 Hz)	40.5	C-1, C-3, C-4, C-1′, C-1″
3	4.43 (ddd, 1H, J = 8.3 Hz, J = 6.2 Hz, J = 4.4 Hz)	37.1	C-2, C-4, C-5, C-9, C-1″, C-6″
4	3.79 (d, 1H, J = 4.4 Hz)	53.2	C-2, C-3, C-5, C-9, C-1″
5	-	168.7	
6	-	-	
7	-	151.3	
8	-	-	
9	-	168.3	
10	2.93 (s, 3H)	28.21	C-9, C-7
11	2.92 (s, 3H)	28.31	C-5, C-7
1′	-	127.9	
2′, 6′	7.92 (d, 2H, J = 8.5 Hz)	132.3	C-1, C-1′, C-3′
3′, 5′	7.75 (d, 2H, J = 8.4 Hz)	130.5	C-1, C-1′, C-2′, C-4′
4′	-	136.1	
1″	-	128.3	
2″	-	153.4	
3″	6.85 (d, 1H, J = 8.9 Hz)	112.1	C-3, C-1″, C-2″
4″	6.77 (dd, 1H, J = 8.9 Hz, J = 2.9 Hz)	113.3	C-2″, C-5″, C-6″
5″	-	151.9	
6″	6.61 (d, 1H, J = 2.9 Hz)	115.2	C-3, C-2″, C-4″, C-5″
7″	3.64 (s, 3H)	56.3	C-2″
8″	3.65 (s, 3H)	55.9	C-5″

The scaffold of the Michael adduct was assigned by the HMBC experiment which showed a correlation of the proton at C-3 with some carbon atoms; the methylene carbon (δ_C 40.5 (C-2)), methyne carbon (δ_C 53.2 (C-4)), amide carbonyl of *N*,*N*′-dimethylbarbiturate ring (δ_C 168.3 (C-9)), and (δ_C 168.7 (C-5)). The existence of a methylene group at C-2 was proved by a correlation of a proton with carbonyl ketone (δ_C 197.9 (C-1)), C-3 (δ_C 37.1), and a long-range correlation of the C-2 proton with C-4 (δ_C 53.2) and C-1″ (δ_C 128.3). Additionally, the CH position of C-4 was assigned by the correlation of the C-4 proton with the amide carbonyl of the 1,3-dimethylpyrimidine ring (δ_C 168.3 (C-9)) and (δ_C 168.7 (C-5)), and the proton correlation with C-3 (δ_C 37.1) and C-2 (δ_C 40.5). The proton–carbon correlations of the HMBC experiment were suitable with the molecular structure of the prepared compound and are displayed in Figure 2 and Figure S5 (Supplementary Materials). Based on the structure elucidation, the prepared compound is a new compound.



(**a**) (**b**)

Figure 2. (**a**) Structure numbering, and (**b**) HMBC correlations of the prepared compound.

3. Materials and Methods

3.1. General

All reagents and solvents, purchased from E. Merck (Darmstadt, Germany) or Sigma Aldrich (St. Louis, MO, USA), were used without further purification. Reaction progress was monitored by thin-layer chromatography on silica gel GF254 aluminum sheets (0.25 mm) using various developing systems. Spots were detected under UV light (λ 254 nm). IR spectrum was recorded in KBr powder with the diffuse reflectance method on Fourier-transform Infrared spectrometer Shimadzu IRTracer100 (Kyoto, Japan). The mass spectrum was recorded on an High-resolution mass spectrometer, Waters LCT Premier XE (Santa Clara, CA, USA). NMR spectra (^{1}H-, ^{13}C-NMR, HMQC and HMBC) were recorded using the JEOL JNM-ECS400 (Tokyo, Japan) with $CDCl_3$ as a solvent and internal standard.

3.2. Synthesis of Chalcone Derivative

The synthesis of chalcone derivative was conducted following the procedure reported by Suwito et al. [9]. A mixture of 6 mmol 4′-bromoacetophenone, 6 mmol 2,5-dimetoxybenzaldehyde, and 30 mL ethanol was placed in a three neck round bottom flask (equipped with a reflux condenser, thermometer, and dropping funnel), stirred, and cooled under 10 °C. To the reaction mixture, 6 mL NaOH 40% solution was added dropwise and the temperature was kept under 10 °C, stirred for 1 h, and then stirred at room temperature for a further 5 h. The precipitate was filtered off and recrystallized using aqueous ethanol.

3.3. Synthesis of the Target Compound

A mixture of 1.2 mmol of 1,3-dimethylbarbituric acid, 1 mmol of chalcone derivative, 1 mmol of ammonium chloride, 100 µL TEA, and 5 mL methanol was placed in a round bottom flask, and refluxed at 80 °C for 7 h. The reaction mixture was then cooled at room temperature, and 10 mL water was added. The precipitate was then filtered off, washed with a cold aqueous ethanol solution, and recrystallized using aqueous ethanol.

4. Conclusions

In conclusion, we have successfully synthesized a new compound, that is 5-[3-(4-bromophenyl)-1-(2,5-dimethoxyphenyl)-3-oxopropyl]-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-tri-one through Michael addition from a chalcone derivative.

Supplementary Materials: The following are available online: the HRESIMS, FTIR, ^{1}H-NMR, ^{13}C-NMR, HMQC, HMBC spectra are reported in the Supplementary Materials as Figures S1–S6, respectively, and the structure refinement in Table S1.

Author Contributions: H.S. brought the idea, managed the research, and wrote the manuscript. R.H.P.S. performed the synthesis, K.U.H. performed the structure elucidation, while A.N.K corrected the manuscript. 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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