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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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molbank@mdpi.com
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland
Tel: +41 61 683 77 34
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Basel, September 2019

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5-(4-Bromophenyl)-7-(2,4-dimethoxyphenyl)-4,7-dihydrotetrazolo[1,5-*a*]pyrimidine (/1422-8599/2018/4/M1037)

by **Kautsar Ul Haq (https://sciprofiles.com/profile/author/MThkb3dPRkl1M3FFWDZ2TWdvVi9kZWZkNE82NVBUUEJoMm1Od0FXNy9MWT0=)** ,
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Hery Suwito (https://sciprofiles.com/profile/87893)
Molbank **2018**, *2018*(4), M1037; **https://doi.org/10.3390/M1037 (https://doi.org/10.3390/M1037)** - 17 Dec 2018
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Abstract A derivative of dihydrotetrazolopyrimidine 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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Open Access Short Note (/1422-8599/2018/4/M1036/pdf)

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

by **R. Alan Aitken (https://sciprofiles.com/profile/359182)** ,
Alexandra M. Z. Slawin (https://sciprofiles.com/profile/author/WjBjRmpTUjdNUUlBMWI0WXREMFpqTW1vdWVrMjQyTVJHNlFnZDZuVnVQST0=) and
Pei-pei Yeh (https://sciprofiles.com/profile/author/NU02VitNM0tWYWZMR011a1NFVEt6My8wV0RXTFVGTmk3NDE1a0JjelV6Yz0=)
Molbank **2018**, *2018*(4), M1036; **https://doi.org/10.3390/M1036 (https://doi.org/10.3390/M1036)** - 13 Dec 2018
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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)**
(This article belongs to the Section **Structure Determination (/journal/molbank/sections/structure_determination_molbank)**)

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Open Access Short Note (/1422-8599/2018/4/M1035/pdf)

1-(2-Hydroxyethyl)imidazolidine-2-thione (/1422-8599/2018/4/M1035)

by **See Mun Lee (https://sciprofiles.com/profile/832864)** ,
Ainnul Hamidah Syahadah Azizan (https://sciprofiles.com/profile/author/Y1liYVh4Qk5tMkJVT0Z4b0hRQWlWM0ZtRGpOREMzbVc4WkRxRjByWFAwMD0=)
and
Edward R. T. Tiekink (https://sciprofiles.com/profile/348831)
Molbank **2018**, *2018*(4), M1035; **https://doi.org/10.3390/M1035 (https://doi.org/10.3390/M1035)** - 03 Dec 2018
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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, ^{1}H, ^{13}C{^{1}H}, and 2D (COSY, NOESY, HSQC, and **[...] Read more.**
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Open Access Short Note (/1422-8599/2018/4/M1034/pdf)

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)** ,
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Amany S. Hegazy (https://sciprofiles.com/profile/author/S3QxZjV3MEptTEpkNC9CTjAzaHA5cXVUUnNKREpLQWtQTi8rRlA4RE1hQD0=)

M. Kariuki (https://sciprofiles.com/profile/author/NzNFalIPc1o3M1pWZEFxMC93RFFqRUt0S3lkaERORkhlTkhMTGVqTnJhdz0=) and
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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Open Access Communication (/1422-8599/2018/4/M1033/pdf)

Ureido Derivatives of Neoabietic Acid (/1422-8599/2018/4/M1033)

by Xinyu Gao (https://sciprofiles.com/profile/author/emNHeG1GMUR4OVhjSkVTak1vZzc4dDArdlBmRTAyRG8yVE9lSUptUDlFND0=) ,
Niping Feng (https://sciprofiles.com/profile/author/T3NlZGh2MlUzOGYrWjlxWWR1ZEF5Y0k0aXRaTFlqN21ad0pEQnlmWUdEUT0=) ,
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Jianguo Cao (https://sciprofiles.com/profile/562622) and
Guozheng Huang (https://sciprofiles.com/profile/author/d28xODZtMVBmYkgwZ2Zvc0ZGenNyckRjZWhzUXV5QWVNUUNQMVNpZlhQYz0=)

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 ^{1}H-NMR, ^{13}C-NMR and HRMS spectral analysis. **Full article (/1422-8599/2018/4/M1033)**

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Open Access Communication (/1422-8599/2018/4/M1032/pdf)

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) and
Laurent Guyard (https://sciprofiles.com/profile/author/RXQ1ZU9hNmRGZ1E1RnJsL01SSmUyMlFlT3V2bWNScVRkZStGTzV2RFFQTT0=)

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 ^{1}H and ^{13}C-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)

by Stanimir Manolov (https://sciprofiles.com/profile/170124) , Iliyan Ivanov (https://sciprofiles.com/profile/39867) and
Yulian Voynikov (https://sciprofiles.com/profile/author/QUVGM0ZuVWl0UlNTOElwVkZLMUdmZVZZc241VExBdUxtQzBhTlBkdjJxWT0=)

Molbank **2018**, *2018*(4), M1031; https://doi.org/10.3390/M1031 (https://doi.org/10.3390/M1031) - 22 Nov 2018
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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) (^{1}H-NMR and ^{13}C-NMR), UV, IR, and mass spectral data. **Full article (/1422-8599/2018/4/M1031)**

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Open Access Short Note (/1422-8599/2018/4/M1030/pdf)

N-[4-(1-Methyl-1*H*-imidazol-2-yl)-2,4′-bipyridin-2′-yl]benzene-1,4-diamine (/1422-8599/2018/4/M1030)

by Dhafer S. Zinad (https://sciprofiles.com/profile/634257) , Dunya L. AL-Duhaidahaw (https://sciprofiles.com/profile/386683) ,
Ahmed Al-Amiery (https://sciprofiles.com/profile/7303) and Abdul Amir H. Kadhum (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
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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 (SNAr) reaction that afforded the target compound. The synthesized compound was characterized **[...] Read more.**

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Open Access Short Note (/1422-8599/2018/4/M1029/pdf)

Ethyl 4-(2-fluorophenyl)-6-methyl-2-thioxo-1-(*p*-tolyl)-1,2,3,4-tetrahydropyrimidine-5-carboxylate (/1422-8599/2018/4/M1029)

by Itamar Luís Gonçalves (https://sciprofiles.com/profile/164423) ,
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Solange Cristina Garcia (https://sciprofiles.com/profile/19180) and Vera Lucia Eifler-Lima (https://sciprofiles.com/profile/25331)
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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Open Access Short Note (/1422-8599/2018/4/M1028/pdf)

[*O*-Isopropyl-*N*-(4-nitrophenyl)thiocarbamato-*κS*]-(tri-4-tolylphosphine-*κP*)gold(I) (/1422-8599/2018/4/M1028)

by Chien Ing Yeo (https://sciprofiles.com/profile/424298) and Edward R. T. Tiekink (https://sciprofiles.com/profile/348831)
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, $(4\text{-tolyl})_3PAu[SC(O\text{-}i\text{-}Pr)=NC_6H_4NO_2\text{-}4]$ (**1**) are described. Spectroscopy exhibited the expected features confirming the formation of the compound. The molecular structure of **[...] Read more.**
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Open Access Short Note (/1422-8599/2018/4/M1027/pdf)

(*E*)-3-[3-(4-Morpholinophenyl)acryloyl]-2*H*-chromen-2-one (/1422-8599/2018/4/M1027)

by Hery Suwito (https://sciprofiles.com/profile/87893) ,
Helda Dwi Hardiyanti (https://sciprofiles.com/profile/author/d28xQlRBUzBEOEhyWHk4MW1DSXJvT2pMczYwalJsZ1BRUy9xSDlLa1A4UT0=) ,
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,
Alfinda Novi Kristanti (https://sciprofiles.com/profile/325866) and
Miratul Khasanah (https://sciprofiles.com/profile/author/SGFBdEtLVG1sbmtEVXlDSy9ROUtaNTZ5ZEpkYnJUSjkwTkZVb0dDUWw0Zz0=)
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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Open Access Feature Paper Short Note (/1422-8599/2018/4/M1026/pdf)

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

by Duc Hoàng Lande (https://sciprofiles.com/profile/author/eGVWazZ5UGZYVUE4ZmpFNEcycXVkbUNrU3U5bEJYSU8rdFEvR3hnd1N3WT0=) ,
Conrad Kunick (https://sciprofiles.com/profile/15702) and Johann Grünefeld (https://sciprofiles.com/profile/516725)
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)**
(This article belongs to the Section **Organic Synthesis (/journal/molbank/sections/organic_synthesis_molbank)**)

Open Access Short Note (/1422-8599/2018/4/M1025/pdf)

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

by William Henderson (https://sciprofiles.com/profile/author/dXJTME1YcGV5Rm9RNjlLYzVYOHZ0UkdDRVRleUpqRXZmSDZ6TjB1YndjND0=) ,
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Edward R. T. Tiekink (https://sciprofiles.com/profile/348831)
Molbank **2018**, *2018*(4), M1025; https://doi.org/10.3390/M1025 (https://doi.org/10.3390/M1025) - 12 Oct 2018
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Abstract The tris(2-cyanoethyl)phosphine (tcep) complex $[RuCl_2\{P(CH_2CH_2CN)_3\}(\eta^6\text{-}p\text{-cymene})]$ (*p*-cymene = $p\text{-}CH_3C_6H_4{}^iPr$) was synthesised by the bridge-splitting reaction of the chlorido-dimer $[RuCl_2($ **[...] Read more.**
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Purine-Furan and Purine-Thiophene Conjugates (/1422-8599/2018/4/M1024)

by Zigfrīds Kapilinskis (https://sciprofiles.com/profile/527002) , Irina Novosjolova (https://sciprofiles.com/profile/515967) and
Māris Turks (https://sciprofiles.com/profile/300615)

Mc **18**, *2018*(4), M1024; **https://doi.org/10.3390/M1024 (https://doi.org/10.3390/M1024)** - 08 Oct 2018
Vie 41

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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Open Access Communication (/1422-8599/2018/4/M1023/pdf)

1-Methyl-3-{4-[(4-(2-oxo-2,3-dihydro-1*H*-benzimidazol-1-yl)piperidin-1-yl)benzyl]}-2-phenylindole (/1422-8599/2018/4/M1023)

by **Jean Guillon (https://sciprofiles.com/profile/355905)** ,
Solène Savrimoutou (https://sciprofiles.com/profile/author/NnRwWGhQNy9ueS9mdnRhbFA1M3plZEFhMUZZRXZlRzJXd2pKdnl4dTdKWGMzRU5ZK3k3aG1Kb
Sandra Rubio (https://sciprofiles.com/profile/author/aHBtKzNuZ21SK0Y5d0h2ekZFcFhueWZySTJqdDZwRzlwa0ZlV0pDY3VPOD0=) and
Vanessa Desplat (https://sciprofiles.com/profile/author/UGdSZ1plbE1Yd0MxR0hxd2x3Y2k5UUdJeXlsZGlPd0kwcjdnWEVQWFk4RT0=)
Molbank **2018**, *2018*(4), M1023; **https://doi.org/10.3390/M1023 (https://doi.org/10.3390/M1023)** - 04 Oct 2018
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Abstract The 1-methyl-3-{4-[(4-(2-oxo-2,3-dihydro-1*H*-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, ^{1}H-NMR, ^{13}C-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 (/1422-8599/2018/4/M1022)

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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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Antonya Todorova (https://sciprofiles.com/profile/author/MHJOUUplc21JcWxmNWFlSWx3Yzc2UT09) ,
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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 ^{1}H-NMR, ^{13}C-NMR, IR, MS, and elemental analysis. **Full article (/1422-8599/2018/4/M1021)**
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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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E-Mail () **Website (http://ch-www.st-and.ac.uk/staff/raa/group)**
School of Chemistry, University of St Andrews North Haugh, St Andrews Fife, KY16 9ST, UK
Tel. (01334) 463865; Fax: (01334) 463865

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

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E-Mail () **Website (https://www.kingston.ac.uk/staff/profile/professor-fawaz-aldabbagh-462/)**
Department of Pharmacy, School of Life Sciences, Pharmacy & Chemistry, Kingston University, Penrhyn Road, Kingston upon Thames, KT1 2EE, UK

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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

Dr. Jose Berna

E-Mail () **Website (http://webs.um.es/ppberna/miwiki/doku.php)**
Department of Organic Chemistry, Faculty of Chemistry, University of Murcia, 30100 Murcia, Spain

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

Prof. Dr. Fang-Rong Chang

E-Mail () **Website (http://nphs.kmu.edu.tw/index.php/en-GB/faculty)**
Graduate Institute of Natural Products, College of Pharmacy, Kaohsiung Medical University, No. 100, Shih-Chuan 1st Road, Kaohsiung, 80708, Taiwan

Interests: natural products chemistry; medicinal chemistry; transgenic plant (arabidopsis) reportor assay; epigenetic modulation for microbial secondary metabolites; functional food; ethnopharmacology

Prof. Dr. Gregory K. Friestad

E-Mail () **Website (https://chem.uiowa.edu/people/gregory-k-friestad)**

De of Chemistry, University of Iowa, Iowa City, IA 52242 USA
Tel 35-1364; Fax: +1 319 335 1270
Interests: asymmetric synthesis methodology; free radical reactions; organometallic reagents; natural product synthesis; asymmetric catalysis

Prof. Dr. Bartolo Gabriele
E-Mail () Website1 (http://www.unical.it/portale/strutture/dipartimenti_240/ctc/didattica/homedid/docenti/ordinari/gabriele/) Website2 (https://www2.scopus.com/authid/detail.uri?authorId=7003277013)
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 (Cosenza), Italy
Tel. +390984492815; Fax: +390984492044
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; extraction, characterization, and evaluation of the biological activity of bioactive principles from natural matrices
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E-Mail () Website (http://ucy.ac.cy/dir/en/component/comprofiler/userprofile/koutenti)
Department of Chemistry, University of Cyprus, P. O. Box 20537, 1678 Nicosia, Cyprus
Tel. 0035722892783
Interests: heterocyclic chemistry; sulfur-nitrogen heterocycles; synthetic methods; azaacenes; zwitterionic acenes; stable organic radicals; biologically active heterocycles; isothiazoles; 1,2,3-dithiazoles; 1,2,6-thiadiazines;1,2,4-benzotriazines
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E-Mail () Website (https://www.tu-braunschweig.de/pharmchem/forschung/kunick)
Institut für Medizinische und Pharmazeutische Chemie, Technische Universität Braunschweig, Beethovenstraße 55, 38106 Braunschweig, Germany
Interests: medicinal chemistry; pharmaceutical chemistry; synthesis of heterocycles; protein kinase inhibitors

Dr. Raffaella Mancuso
E-Mail ()
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: 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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E-Mail () **Website (http://gr.xjtu.edu.cn/web/mengge)**
Chemistry Department, Fudan University, Shanghai 200433, China
Fax: +86 029 82655424
Interests: medicinal heterocyclic chemistry; indoles; indazoles; pyridines; thiazoles; thiadiazoles; pyrroles; computer aided drug design; molecular probe

Prof. Dr. Hideto Miyabe
E-Mail () **Website (http://www2.huhs.ac.jp/~h070012h/)**
School of Pharmacy, Hyogo 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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Prof. Dr. Luke R. Odell
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Organic Pharmaceutical Chemistry, Department of Medicinal Chemistry, BMC, Uppsala University, Box 574, SE-751 23 Uppsala, Sweden
Tel. +4618-471 4297
Interests: heterocyclic chemistry; multicomponent reactions; catalysis; medicinal chemistry; synthetic methodology
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Prof. Dr. Thierry Ollevier
E-Mail () **Website (http://www.chm.ulaval.ca/tollevier)**

De of Chemistry, Pavillon Alexandre-Vachon, 1045, Avenue de la Médecine, Université Laval, Québec, G1V 0A (/)
Tel. +1 418 656 5034; Fax: +1 418 656 7916
Interests: synthetic methodology; asymmetric catalysis; Lewis acids

Dr. Luc Patiny

E-Mail () **Website (http://cheminformatics.epfl.ch)**

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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Department of Chemical Sciences, Università degli Studi di Napoli Federico II, Via Cintia 21, 80126 Napoli, Italy
Interests: organic and medicinal chemistry; organic synthesis; catalytic oxidative processes; marine natural products; nucleosides chemistry
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E-Mail () **Website (http://zioc.ru/institute/laboratories/laboratory-of-polysulphur-nitrogen-heterocycles-n31?lang=en)**

1. N. D. Zelinsky Institute of Organic Chemistry Russian Academy of Sciences, 47 Leninsky Prospekt, 119991 Moscow, Russia
2. Nanotechnology Education and Research Center, South Ural State University, 454080 Chelyabinsk, Russia
Tel. +7-499-1355327
Interests: heterocyclic chemistry; sulfur-nitrogen heterocycles; selenium heterocycles; synthetic methods; biologically active compounds; organic sensitizers for DSSCs and OLEDs; sulfur monochloride
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Dr. Bernd Schneider

E-Mail () **Website (http://www.ice.mpg.de)**

Max Planck Institute for Chemical Ecology, Hans-Knöll-Str. 8, Beutenberg Campus, 07745 Jena, Germany
Interests: natural products chemistry; chemical ecology; plant natural products; NMR of small molecules

Prof. Dr. Jonathan W. Steed

E-Mail () **Website (http://www.dur.ac.uk/jon.steed)**

De of Chemistry, Durham University, University Science Laboratories, South Road, Durham DH1 3LE, UK
Fa +1 384 4737
Interests: supramolecular chemistry; gels; molecular materials and the molecular solid state; pharmaceutical solid forms; platinum group transition metal chemistry

Prof. Dr. Ping-Jyun Sung

E-Mail () **Website (http://marine-natural-product-sung.weebly.com/235263951123460200272534520154.html)**

1. National Museum of Marine Biology and Aquarium, Pingtung 944, Taiwan
2. Graduate Institute of Marine Biology, National Dong Hwa Univesity, Pingtung 944, Taiwan
3. Department of Marine Biotechnology and Resources, National Sun Yat-sen University, Kaohsiung 804, Taiwan
4. Chinese Medicine Research and Development Center, China Medical University Hospital, Taichung 404, Taiwan
5. Graduate Institute of Natural Products, Kaohsiung Medical University, Kaohsiung 807, Taiwan

Tel. 886-8-8825037; Fax: 886-8-8825087
Interests: marine natural products; marine chemical ecology; bioactive substances from cultured marine invertebrates
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E-Mail () **Website1 (https://www1.gifu-u.ac.jp/~kassei1/)** **Website2 (https://www1.gifu-u.ac.jp/~kassei1/)**

Center for Highly Advanced Integration of Nano and Life Sciences (G- CHAIN), Gifu University, 1-1 Yanagido, Gifu, Gifu 501-1193, Japan
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Prof. Dr. Kristof Van Hecke

E-Mail () **Website (https://www.xstruct.ugent.be)**

Universiteit Gent, Ghent, Belgium
Tel. +32(0)9264 48 70
Interests: structures; X-ray diffraction; bioinorganic chemistry; metal complexes; coordination chemistry
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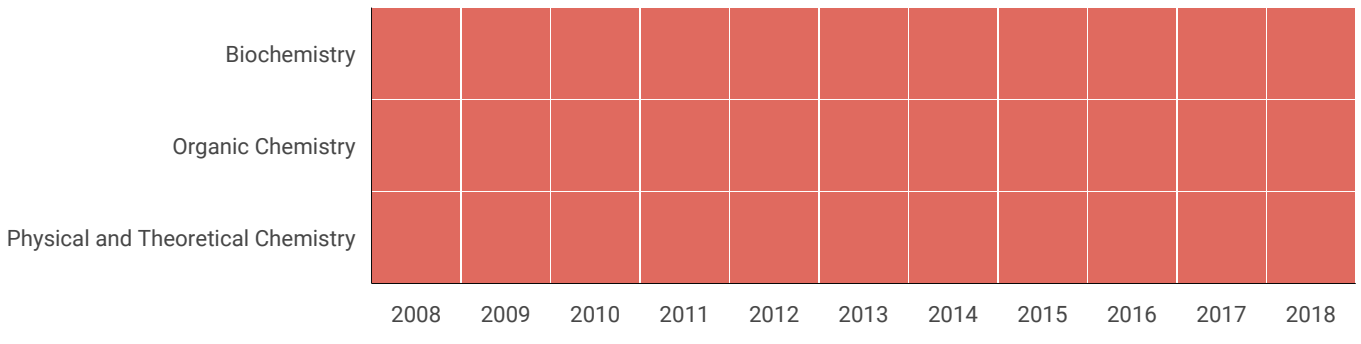

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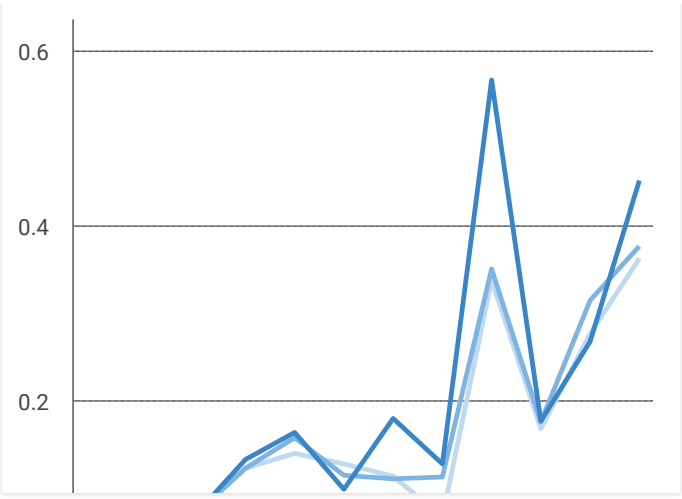

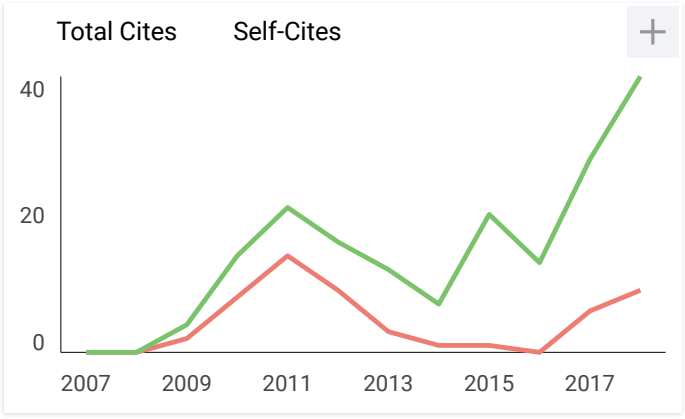

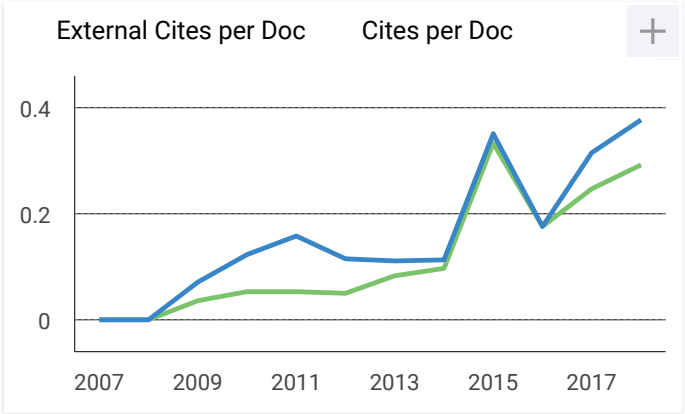

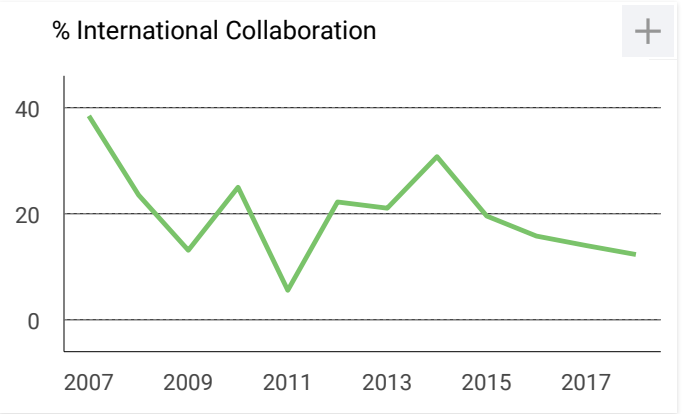

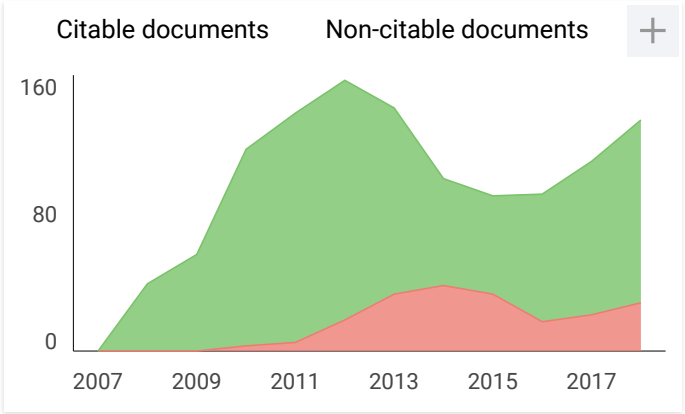

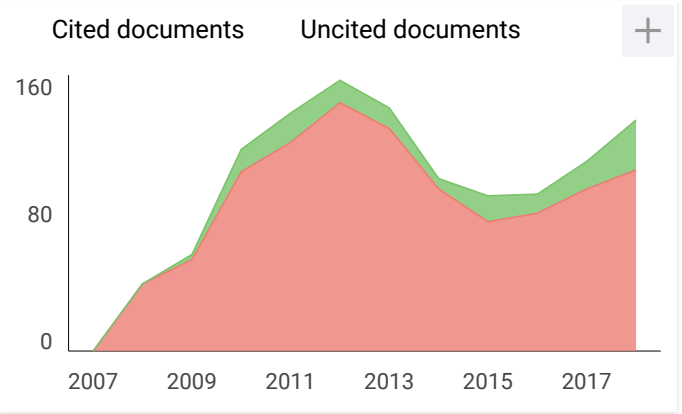

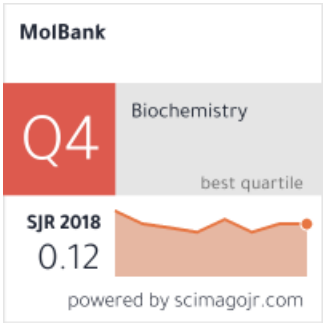

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Short Note

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

Hery Suwito *, Helda Dwi Hardiyanti, Kautsar Ul Haq, Alfinda Novi Kristanti and Miratul Khasanah

Department of Chemistry, Faculty of Science and Technology, Airlangga University, Surabaya 60115, Indonesia; hyuga.helda@gmail.com (H.D.H.); Kautsar.ul.haq-2016@fst.unair.ac.id (K.U.H.); alfinda-n-k@fst.unair.ac.id (A.N.K.); miratul-k@fst.unair.ac.id (M.K.)

* Correspondence: herys08032002@yahoo.com or hery-s@fst.unair.ac.id; Tel.: +62-31-5922-427

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

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 title compound was established using spectroscopic data FTIR, HRESI-MS, ^{1}H- and ^{13}C-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 Dicussion

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.

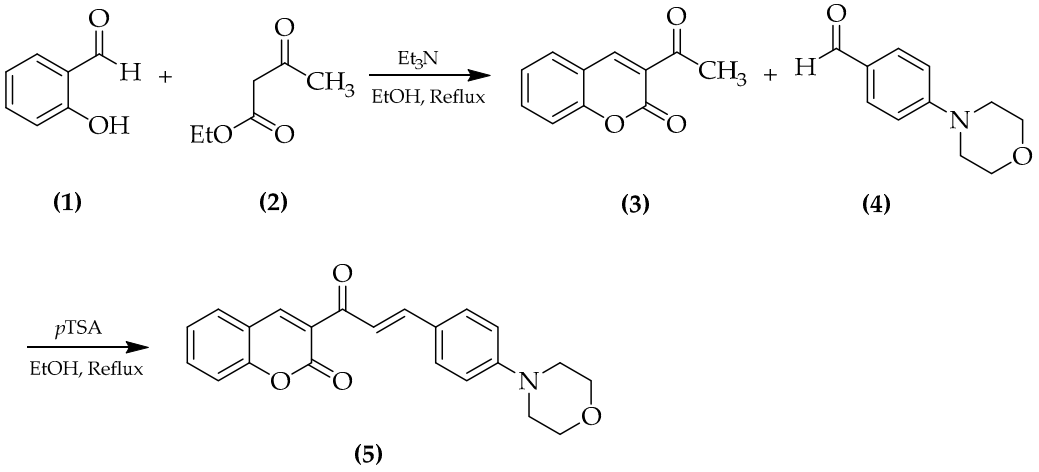


Figure 1. Synthesis pathway of the target molecule.

(*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). ^{1}H-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).

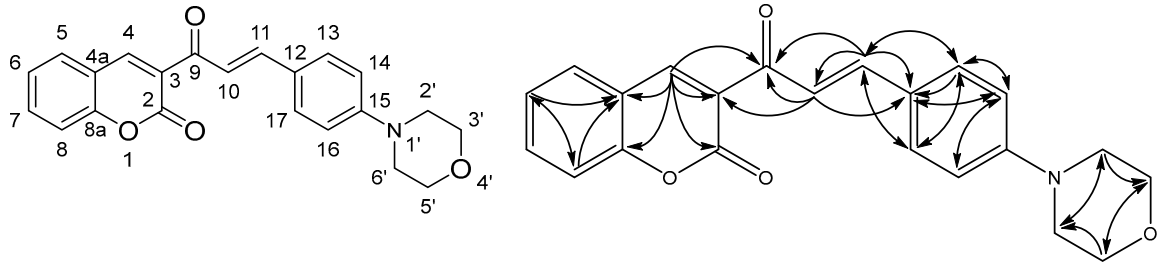
This paper discusses only the title compound **5** because compound **3** is already known. The spectroscopy data of compound **3** are presented in Supplementary Materials (Figures S1–S4). The HRMS spectrum of the title compound showed a positive molecular ion of $[M + Na]^+$ at m/z = 384.1215, suitable 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 ^{1}H-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 $CDCl_3$.

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′



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

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 IC_{50} of 0.90 μM for breast cancer cells line T47D and of 2.32 μM 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 GF_{254} (0.25 mm) employing different solvents. The TLC spot was detected using UV light (λ = 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 (^{1}H-, and ^{13}C-APT)

was recorded on a JEOL JNM-ECS400 spectrometer (at 400 and 100 MHz) (JEOL Ltd., Tokyo, Japan) with $CDCl_3$ 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% CO_2. 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 IC_{50} 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, ^{1}H-NMR, ^{13}C-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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