

Publications – Prof. Dr. Pierre Koch (*as Corresponding Author)

Research articles, reviews:

2022

76. Müller, C., Gleixner, J., Tahk, M.-J., Kopanchuk, S., Laasfeld, T., Weinhart, M., Schollmeyer, D. Betschart, M. U., Lüdeke, S., **Koch, P.**, Rinken, A., Keller, M. Structure-based design of high-affinity fluorescent probes for the neuropeptide Y Y1 receptor. *J. Med. Chem.*, 2022, 65, 4832-4853.
75. Andreev, S., Pantsar, T., Tesch, R., Kahlke, N., El-Gokha, A., Ansideri, F., Grätz, L., Romasco, J., Sita, G., Geibel, C., Lämmerhofer, M., Tarozzi, A., Knapp, S., Laufer, S. A., **Koch, P.*** Addressing a Trapped High-Energy Water: Design and Synthesis of Highly Potent Pyrimidoindole-based Glycogen Synthase Kinase-3 β inhibitors. *J. Med. Chem.* 2022, 65, 1283-1301.
74. Tormählen, N. W., Martorelli, M., Kuhn, A., Maier, F., Guezguez, J., Burnet, M., Albrecht, W., Laufer, S. A., **Koch, P.*** Design and Synthesis of Highly Selective Brain Penetrant p38 α Mitogen-Activated Protein Kinase Inhibitors. *J. Med. Chem.* 2022, 65, 1225-1242.
73. Andreev, S., Plank, N., Schollmeyer, D., **Koch, P.*** (S)-3-(3-((7-Ethynyl-9H-pyrimido[4,5-*b*]indol-4-yl)amino)piperidin-1-yl)propanenitrile. *Molbank* 2022, 2022, M1437.
72. Boskovic, M., Andreev, S., Schollmeyer, D., **Koch, P.*** 12*H*-Dibenzo[*d,g*][1,2,3]trisenocin-12-ol. *Molbank* 2022, 2022, M1418.

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71. Schade, N., **Koch, P.**, Ansideri, F., Krystof, V., Hilgeroth, A. Evaluation of Novel Substituted Europyridines as Inhibitors of Protein Kinases Related to Tau Pathology in Alzheimer's Disease. *Med. Chem. (Sharjah, United Arab Emirates)* 2021, 17, 844-855.
70. Reynders, M. Chaikwad, A., Berger, B.-T., Bauer, K., **Koch, P.**, Laufer, S., Knapp, S., Trauner, D. Controlling the Covalent Reactivity of a Kinase Inhibitor with Light. *Angew. Chem. Int. Ed.* 2021, 60, 20178-20183.
69. Eitel, M., Zinad, D., Schollmeyer, D., Gross, H., **Koch, P.*** Selective Mono-de-O-acetylation of the Per-O-acetylated Brasilicardin Carbohydrate Side Chain. *Carbohydrate Res.* 2021, 504, 108312.
68. Andreev, S., Schollmeyer, D., **Koch, P.*** 1-(3-((7-Fluoro-9*H*-pyrimido[4,5-*b*]indol-4-yl)(methyl) amino)piperidin-1-yl)propan-1-one. *IUCr data* 6, x210159.
67. Botas, A., Eitel, M., Schwarz, P. N., Buchmann, A., Costales, P., Núñez, L. E., Cortés, J., Morís, F., Krawiec, M., Wolański, M., Gust, B., Rodriguez, M., Fischer, W.-N., Jandeleit, B., Zakrzewska-Cerwińska, J., Wohlleben, W., Stegmann, E., **Koch, P.*** Méndez, C., Gross, H. Genetic engineering in combination with semisynthesis leads to a new route for gram-scale production of the immunosuppressive natural product brasilicardin A. *Angew. Chem. Int. Ed.* 2021, 60, 13536-13541.
66. Wolański, M., Krawiec, M., Schwarz, P.N., Stegmann, E., Wohlleben, W., Buchmann, A., Gross, H., Eitel, M., **Koch, P.**, Botas, A., Méndez, C., Núñez, L.E., Morís, F., Cortés, J., Zakrzewska-Cerwińska, J. LysRNT: A novel regulator involved in the biosynthesis of the immunosuppressant brasilicardin. *Eng. Life Sci.* 2021, 21, 4-18.

2020

65. Majer, T., Schollmeyer, D., **Koch, P.**, Gross, H. (2*S*,3'*S*,3*a*'*R*,5'*R*,7*a*'*R*)-5'-((*E*)-5-(Furan-3-yl)-2-methylpent-1-en-1-yl)-3-hydroxy-3',4,7'-trimethyl-1',2',3',3*a*',5',7*a*'-hexahydro-5*H*-spiro[furan-2,4'-inden]-5-one. *IUCr data* 2020, 5, x201578.

64. Andreev, S., Pantsar, T., El-Gokha, A., Ansideri, F., Kudolo, M., Anton, D. B., Sita, G., Romasco, J., Geibel, C., Lämmerhofer, M., Goettert, M. I., Tarozzi, A., Laufer, S. A., **Koch, P.*** Discovery and Evaluation of Enantiopure 9*H*-pyrimido[4,5-*b*]indoles as Nanomolar GSK-3 β Inhibitors with Improved Metabolic Stability. *Int. J. Mol. Sci.* 2020, 21, 7823.
63. **Koch, P.*** Inhibitors of cJun N-terminal kinase 3. In: Laufer, S. (eds) Proteinkinase Inhibitors. *Topics in Med. Chem.* 2020, vol. 36. Springer, Cham. https://doi.org/10.1007/7355_2020_98 (Buchkapitel)

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62. Heider, F., Pantsar, T., Kudolo, M., Ansideri, F., De Simone, A., Pruccoli, L., Schneider, T., Goettert, M. I., Tarozzi, A., Andrisano, V., Laufer, S. A., **Koch, P.*** Pyridinylimidazoles as GSK3 β inhibitors: the impact of tautomerism on compound activity via water networks. *ACS Med. Chem. Lett.* 2019, 10, 1407–1414.
61. Andreev, S., Pantsar, T., Ansideri, F., Kudolo, M., Forster, M., Schollmeyer, D., Laufer, S. A., **Koch, P.*** Design, Synthesis and Biological Evaluation of 7-Chloro-9*H*-pyrimido[4,5-*b*]indole-based Glycogen synthase kinase-3 β inhibitors. *Molecules* 2019, 24, 2331.
60. Heider, F., Ansideri, F., Tesch, R., Pantsar, T., Haun, U., Döring, E., Kudolo, M., Poso, A., Albrecht, W., Laufer, S. A., **Koch, P.*** Pyridinylimidazoles as dual Glycogen Synthase Kinase 3 β /p38 α Mitogen-activated Protein Kinase Inhibitors. *Eur. J. Med. Chem.* 2019, 175, 309-329.
59. Elgokha, A., Ansideri, F., Andreev, S., Schollmeyer, D., Laufer, S. A., **Koch, P.*** N¹-{4-[2-(Methylthio)-1*H*-imidazol-5-yl]pyridin-2-yl}benzene-1,4-diamine. *Molbank* 2019, 2019, M1048.

2018

58. Ernst, C., Heidrich, J., Sessler, C., Sindlinger, J., Schwarzer, D., **Koch, P.**, Boeckler, F. M. Switching Between Bicyclic and Linear Peptides-The Sulfhydryl-Specific Linker TPSMB Enables Reversible Cyclization of Peptides. *Frontiers Chem.* 2018, 6, 484.
57. Ernst, C., Sindlinger, J., Schwarzer, D., **Koch, P.**, Boeckler, F. M. The Symmetric Tetravalent Sulfhydryl-Specific Linker NATBA Facilitates a Combinatorial “Tool Kit” Strategy for Phage Display-Based Selection of Functionalized Bicyclic Peptides. *ACS Omega* 2018, 3, 13261-12368.
56. Eitel, M., Schollmeyer, D., Gross, H, **Koch, P.*** (2*S*, 3*S*)-2-Azaniumyl-4-[(1*S*, 4*aS*, 4*bS*, 6*S*, 7*S*, 8*aS*, 10*aS*)-6,7-dihydroxy-2,4*b*,8,8,10*a*-pentamethyl-1,4,4*a*,4*b*,5,6,7,8,8*a*,9,10,10*a*-dodecahydrophenanthren-1-yl]-3-methoxybutanoate–methanol–water (1/1/1). *IUCrData* 2018, 3, x181194.
55. Ansideri, F., Macedo, J. T., Eitel, M., El-Gokha, A., Zinad, D. S., Scarpellini, C., Kudolo, M., Schollmeyer, D., Boeckler, F. M., Blaum, B. S., Laufer, S. A., **Koch, P.*** Structural Optimization of a Pyridinylimidazole Scaffold: Shifting the Selectivity from p38 α Mitogen-Activated Protein Kinase to c-Jun N-terminal Kinase 3. *ACS Omega* 2018, 3, 7809-7831.
54. **Koch, P.**, Brunschweiger, A., Namisvajan, V., Ullrich, S., Maurca, A., Lazzaretto, B., Küppers, P., Hinz, S., Hockemeyer, J., Wiese, M., Heer, J., Alcaro, S., Kiec-Kononowicz, K., Müller, C. E. Probing substituents in the 1- and 3-position: Tetrahydropyrazino-annelated water-soluble xanthine derivatives as multi-target drugs with potent adenosine receptor antagonistic activity. *Frontiers Chem.* 2018, 6, 206.
53. Chaikuad, A., **Koch, P.**, Laufer, S. A., Knapp, S. Das Cysteinom der Proteinkinasen als Zielstruktur in der Arzneistoffentwicklung. *Angew. Chem.* 2018, 130, 4456-4470. (Review)
Chaikuad, A., **Koch, P.**, Laufer, S. A., Knapp, S. The Cysteinome of Protein Kinases as a Target in Drug Development. *Angew. Chem. Int. Ed.* 2018, 57, 4372-4385. (Review)
52. Ansideri, F., Andreev, S., Kuhn, A., Albrecht, W., Laufer, S. A., **Koch, P.*** A Diverse and Versatile Regiospecific Synthesis of Tetrasubstituted Alkylsulfanylimidazoles p38 α Mitogen-Activated Protein Kinase Inhibitors. *Molecules* 2018, 23, 221.

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51. Koch, P.,* Ansideri, F. 2-Alkylsulfanyl-4(5)-aryl-5(4)-heteroarylimidazoles: an Overview on Synthetic Strategies and Biological Activity. *Arch. Pharm.*, 2017, 350, e1700258. (Review)
50. Heider, F., Haun, U., Döring, E., Kudolo, M., Sessler, C., Albrecht, W., Laufer, S., Koch, P.* From 2-alkylsulfanylimidazoles to 2-alkylimidazoles: An approach towards metabolically more stable p38 α MAP kinase inhibitors. *Molecules* 2017, 22, 1729.
49. Eitel, M., Schollmeyer, D., Koch, P.* (E)-(1-Pyridin-4-yl)-propran-1-one O-tosyl oxime. *IUCrData* 2017, 2, x171602.
48. Steudel, F. A, Mohr, C. J., Steegen, B., Nguyen, H. Y., Barnert, A., Steinle, M., Berr-Hammer, S., Koch, P., Lo, W.-Y., Schroth, W., Hoppe, R., Brauch, H., Ruth, P., Huber, S. M., Lukowski, R. SK4 channels modulate Ca²⁺-signalling and cell cycle progression in murine breast cancer. *Mol. Oncol.* 2017, 11, 1172-1188.
47. Ansideri, F., Dammann, M., Boeckler, F. M., Koch, P.* Fluorescence polarization-based competition binding assay for c-Jun N-terminal kinases 1 and 2. *Anal. Biochem.* 2017, 532, 26-28.
46. Muth, F., El-Gokha, A., Ansideri, F., Eitel, M., Döring, E. Sievers-Engler, A., Lange, A., Boeckler, F. M., Lämmerhofer, M., Koch, P.,* Laufer, S. A. Tri- and Tetrasubstituted Pyridinylimidazoles as Covalent Inhibitors of c-Jun N-Terminal Kinase 3. *J. Med. Chem.* 2017, 60, 594-607.

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43. Ansideri, F., Lange, A., El-Gokha A., Boeckler, F. M., Koch, P.* Fluorescence polarization-based assay for detecting compounds binding to inactive JNK3 and p38 α MAP Kinase. *Anal. Biochem.* 2016, 503, 28-40.
42. Ansideri, F., Schollmeyer, D., Koch, P.* 1-(3',6'-Dihydroxy-3-oxo-3H-spiro[isobenzofuran-1,9'-xanthen]-5-yl)-3-[4-({4-[1-(4-fluorophenyl)-1H-imidazol-5-yl]pyridin-2-yl}amino)phenyl]thiourea methanol monosolvate. *IUCrData* 2016, 1, x1608040.
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40. Eitel, M., Schollmeyer, D., Koch, P.* (E)-(1-Pyridin-4-yl)-propran-1-one oxime. *IUCrData* 2016, 1, x160803.

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39. Lange, A., Günther, M., Buettner, F. M., Zimmermann, M. O., Heidrich, J., Hennig, S., Zahn, S., Schall, C., Sievers-Engler, A., Ansideri, F., Koch, P., Laemmerhofer, M., Stehle, T., Laufer, S. A., Boeckler, F. M. Targeting the Gatekeeper MET146 of c-Jun N-terminal kinase 3 (JNK3) Induces a Bivalent Halogen / Chalcogen Bond. *J. Am. Chem. Soc.* 2015, 137, 14640-14652.
38. Jung, M. E., Chamberlain, B. T., Koch, P., Niazi, K. R. Synthesis and Biological Activity of a Brasilicardin A Analogue Featuring a Simplified Core. *Org. Lett.* 2015, 17, 3608-3611.
37. Elgokha, A., Laufer, S. A., Koch, P.* An optimized and versatile synthesis to pyridinylimidazole-type p38 α mitogen activated protein kinase inhibitors. *Org. Biomol. Chem.* 2015, 13, 10699-10704.
36. Gehringer, M., Muth, F., Koch, P., Laufer, S. A. c-Jun N-terminal kinase inhibitors: a patent review (2010 - 2014). *Expert Opin. Ther. Pat.* 2015, 25, 849-872. (Review)

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32. Brunschweiler, A., **Koch, P.**, Schlenk, M., Pineda, F., Küppers, P., Hinz, S., Köse, M., Ullrich, S., Hockemeyer, J., Wiese, M., Heer, J., Müller, C. E. 8-Benzyltetrahydropyrazino[2,1-f]purinediones: Water-Soluble Tricyclic Xanthine Derivatives as Multitarget Drugs for Neurodegenerative Diseases. *ChemMedChem* 2014, 9, 1704-1724.

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2013

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Patents:

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