

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

Research articles, reviews:

2025

84. Wydra, V. R., Plank, N., Zwirner, S., Selig, R., Rasch, A., Masberg, B., Lämmerhofer, M., Zender, L., Koch, P., Albrecht, W., Laufer, S. A. "Ligand First" Approach toward Selective, Covalent JNK2/3 Inhibitors. *J. Med. Chem.* 2025, asap. <https://pubs.acs.org/doi/10.1021/acs.jmedchem.5c00884>
83. Schettler, F., Gattor, A. **Koch, P.**, Keller, M. Characterization of [³H]Propionylated Human Peptide YY – a New Probe for Neuropeptide Y Y₂ Receptor Binding Studies. *ACS Pharmacol. Transl. Sci.*, ASAP, 2025, 8, 785-799.

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82. Martorelli, M., Dengler, M., Laux, J., Fischer, T., Vaiceliunaite, A., Hahn, U., Cruces, S. Pokoj, C., de Oliveira de Cunha, L., Wohlbold, L., **Koch, P.**, Laufer, S., Burnet, M., Maier, F. A Defined Diet Combined with Sonicated Inoculum Provides a High Incidence, Moderate Severity Form of Experimental Autoimmune Encephalomyelitis (EAE). *ACS Pharmacol. Transl. Sci.*, 2024, 7, 3827-3845.
81. **Koch, P.**, Schollmeyer, D. 1-[(2-Chlorophenyl)diphenylmethyl]-1*H*-pyrazole. *IUCr data* 2024, 8, x241152.
80. Scheuerer, S., Motlova, L., Schäker-Hübner, L., Sellmer, A., Feller, F., Ertl, F. J., **Koch, P.**, Hansen, F. K., Barinka, C., Mahboobi, S. Biological and structural investigation of tetrahydro-β-carboline-based selective HDAC6 inhibitors with improved stability. *Eur. J. Med. Chem.* 2024, 276, 116676.
79. Ganser, K., Stansky, N., Abed, T., Quintanilla-Martinez, L., Gonzalez-Menendez, I., Naumann, U., **Koch, P.**, Krueger, M., Ruth, P., Huber, S. M., Eckert, F. K_{Ca} channel targeting impairs DNA repair and invasiveness of patient-derived glioblastoma stem cells in culture and orthotopic mouse xenografts which only in part is predictable by K_{Ca} expression levels. *Int. J. Cancer.* 2024, 155, 1886-1901.

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78. Stansky, N., Ganser, K., Quintanilla-Martinez, L., Gonzalez-Menendez, I., Naumann, U., Eckert, F. **Koch, P.**, Huber, S. M., Ruth, P. Efficacy of combined tumor irradiation and K_{Ca}3.1-targeting with TRAM-34 in a syngeneic glioma mouse model. *Sci. Rep.* 2023, 13, 202604.
77. Hoffelner, B. S., Andreev, S., Plank, N., **Koch, P.*** Photocaging of Pyridinylimidazole-Based Covalent JNK3 Inhibitors Affords Spatiotemporal Control of the Binding Affinity in Live Cells. *Pharmaceuticals* 2023, 16, 246.

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-3β 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 p38α 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.

2021

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. Chaikuad, 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-Czerwińska, 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-3β 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) Protein Kinase Inhibitors. *Topics in Med. Chem.* 2020, vol. 36. Springer, Cham. https://doi.org/10.1007/7355_2020_98.

2019

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 GSK3β 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-3β 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 3β/p38α 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.*** (2S, 3S)-2-Azaniumyl-4-[(1S, 4aS, 4bS, 6S, 7S, 8aS, 10aS)-6,7-dihydroxy-2,4b,8,8,10a-pentamethyl-1,4,4a,4b,5,6,7,8,8a,9,10,10a-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.**, Brunschweiler, 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 Cysteine 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.

2017

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)-propan-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.

2016

45. Buchmann, A., Eitel M., **Koch, P.**, Schwarz, P. N., Stegmann, E., Wohlleben, W., Wolański, M., Krawiec, M., Zakrzewska-Czerwińska, J., Méndez, C., Botas, A., Núñez, L. E., Morís, F., Cortés, J., Gross, H. High-Quality Draft Genome Sequence of the Actinobacterium *Nocardia terpenica* IFM

0406, Producer of the Immunosuppressant Brasilicardins, Using Illumina and PacBio Technologies. *Genome Announc.* 2016, 4, e01391-16.

44. Brunschweiler, A., **Koch, P.**, Schlenk, M., Rafehi, M., Radjainia, H., Küppers, P., Hinz, H., Pineda, F., Wiese, M., Hockemeyer, J., Heer, J., Denonne, F., Müller, C. E. 8-Substituted 1,3-dimethyltetrahydropyrazino[2,1-*f*]purinediones: Water-soluble adenosine receptor antagonists and monoamine oxidase B inhibitors. *Bioorg. Med. Chem.* 2016, 24, 5462-5480.
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-3*H*-spiro[isobenzofuran-1,9'-xanthen]-5-yl)-3-[4-({4-[1-(4-fluorophenyl)-1*H*-imidazol-5-yl]pyridin-2-yl}amino)phenyl]thiourea methanol monosolvate. *IUCrData* 2016, 1, x1608040.
41. El-Gokha A., Schollmeyer, D., **Koch, P.*** 4-Methyl-*N*-(4-methylpyridin-2-yl)-*N*-(3,4,5,6-tetrahydro-2*H*-pyran-4-yl)pyridin-2-amine. *IUCrData* 2016, 1, x160804.
40. Eitel, M., Schollmeyer, D., **Koch, P.*** (*E*)-(1-Pyridin-4-yl)-propan-1-one oxime. *IUCrData* 2016, 1, x160803.

2015

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.
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35. Muth, F., Günther, M., Bauer, S. M., Döring, E., Fischer, S., Maier, J., Drückes, P., Köppler, J., Trappe, J., Rothbauer, U., **Koch, P.**, Laufer, S. A. Tetra-Substituted Pyridinylimidazoles As Dual Inhibitors of p38 α Mitogen-Activated Protein Kinase and c-Jun N-Terminal Kinase 3 for Potential Treatment of Neurodegenerative Diseases. *J. Med. Chem.* 2015, 58, 443-456.
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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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2012

30. Abu Thaher, B., Arnsmann, M., Totzke, F., Ehlert, J. E., Kubbutat, M. H. G., Schachtele, C., Zimmermann, M. O., **Koch, P.**, Boeckler, F. M., Laufer, S. Tri- and Tetrasubstituted Pyrazole Derivates: Regioisomerism Switches Activity from p38MAP Kinase to Important Cancer Kinases. *J. Med. Chem.* 2012, 55, 961-965.
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25. Abu Thaher, B., **Koch, P.**, Schollmeyer, D., Laufer, S. 4-(4-Fluorophenyl)-3-(pyridin-4-yl)-1-(2,4,6-trichlorophenyl)-1H-pyrazol-5-amine. *Acta Crystallogr., Sect. E: Struct. Rep. Online* 2012, E68, o2603.

2011

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