

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

Research articles, reviews:

2025

85. Sellmer, A., Able, M., Spiekermann, K., Reinecke, M., Kuster, B., Utpatel, K., Wirth, L., Pongratz, H., Plank, N., **Koch, P.**, Elz, S., Fischer, A., Tizazu, B., Fiebig, H.-H., Dove, S., Mahboobi, S. *Novel water-soluble and highly efficient dual type I/II next generation inhibitors of FMS-like tyrosine kinase 3 (FLT3). *Eur. J. Med. Chem.* 2025, 296, 117849.
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, 68, 12004-12028.
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.

2024

82. Martorelli, M., Dengler, M., Laux, J., Fischer, T., Vaiceliunaite, A., Hahn, U., Cruces, S., Pokoj, C., de Oliveira de Cunha, L., Wohlbald, 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]-1H-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., Weinhardt, 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 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]triselenocin-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.

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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.

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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.

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59. Elgokha, A., Ansideri, F., Andreev, S., Schollmeyer, D., Laufer, S. A., **Koch, P.*** N¹-{4-[2-(Methylthio)-1H-imidazol-5-yl]pyridin-2-yl}benzene-1,4-diamine. *Molbank* 2019, 2019, M1048.

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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.
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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.

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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.
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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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44. Brunschweiler, A., **Koch, P.**, Schlenk, M., Rafahi, 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.
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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.
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27. Abu Thaher, B., Koch, P., Schollmeyer, D., Laufer, S. 4-(4-Fluorophenyl)-1-(4-nitrophenyl)-3-(pyridin-4-yl)-1H-pyrazol-5-amine. *Acta Crystallogr., Sect. E: Struct. Rep. Online* 2012, E68, o366.
26. Abu Thaher, B., Koch, P., Schollmeyer, D., Laufer, S. 4-(4-Fluorophenyl)-1-phenyl-3-(pyridin-4-yl)-1H-pyrazol-5-amine. *Acta Crystallogr., Sect. E: Struct. Rep. Online* 2012, E68, o365.
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