

2016

Hamedani NS, Rühl H, Zimmermann JJ, Heiseler T, Oldenburg J, Mayer G, Pöttsch B, Müller J. *In Vitro Evaluation of Aptamer-Based Reversible Inhibition of Anticoagulant Activated Protein C as a Novel Supportive Hemostatic Approach*. *Nucleic Acid Ther*. 2016 Dec; 26(6):355-362.

Ambrozak A, Steinebach C, Gardner ER, Beedie SL, Schnakenburg G, Figg WD, Gütschow M. *Synthesis and Antiangiogenic Properties of Tetrafluorophthalimido and Tetrafluorobenzamido Barbituric Acids*. *ChemMedChem*. 2016 Dec 6; 11(23):2621-2629.

Brunschweiger A, Koch P, Schlenk M, Rafahi M, Radjainia H, Küppers P, Hinz S, Pineda F, Wiese M, Hockemeyer J, Heer J, Denonne F, Müller CE. *8-Substituted 1,3-dimethyltetrahydropyrazino[2,1-f]purinediones: Water-soluble adenosine receptor antagonists and monoamine oxidase B inhibitors*. *Bioorg Med Chem*. 2016 Nov 1; 24(21):5462-5480.

López-Cruz L, Dan-Miguel N, Bayarri P, Baqi Y, Müller CE, Salamone JD, Correa M. *Ethanol and caffeine effects on social interaction and recognition in mice; involvement of adenosine A_{2A} and A₁ Receptors*. *Frontiers Behav. Neurosci*. 2016 Nov 10; 1-15.

Wißbrock A, Kühl T, Silbermann K, Becker AJ, Ohlenschläger O, Imhof D. *Synthesis and evaluation of Abeta-derived and Abeta-independent enhancers of the peroxidase-like activity of heme*. *J. Med. Chem.*, 2017, 60 (1), pp 373–385.

Burbiel JC, Ghattas W, Küppers P, Köse M, Lacher S, Herzner AM, Kombu RS, Akkinepally RR, Hockemeyer J, Müller CE. *2-Amino[1,2,4]triazolo[1,5-c]quinazolines and derived novel heterocycles: Synthesis and structure-activity relationships of potent adenosine receptor antagonists*. *ChemMedChem* 2016 Oct 11; 2272-2286.

Goradia N, Wißbrock A, Wiedemann C, Bordusa F, Ramachandran R, Imhof D, Ohlenschläger O. *¹H, ¹³C, and ¹⁵N resonance assignments for the pro-inflammatory cytokine interleukin-36 α . Biomolecular NMR assignments*. 2016 Oct 10: 329-333.

Joerger M, von Pawel J, Kraff S, Fischer JR, Eberhardt W, Gauler TC, Mueller L, Reinmuth N, Reck M, Kimmich M, Mayer F, Kopp HG, Behringer DM, Ko YD, Hilger RA, Roessler M, Kloft C, Henrich A, Moritz B, Miller MC, Salamone SJ, Jaehde U. *Open-label, randomized study of individualized, pharmacokinetically (PK)-guided dosing of paclitaxel combined with carboplatin or cisplatin in patients with advanced non-small-cell lung cancer (NSCLC)*. *Ann Oncol*. 2016 Oct; 27:1895-1902

Mir Mohseni M, Höver T, Barra L, Kaiser M, Dorrestein PC, Dickschat JS, Schäberle TF. *Discovery of a Mosaic-Like Biosynthetic Assembly Line with a Decarboxylative Off-Loading Mechanism through a Combination of Genome Mining and Imaging*. *Angew Chem Int Ed Engl*. 2016 Oct 17; 55(43):13611-13614.

Rafahi M, Burbiel JC, Attah IY, Abdelrahman A, Müller CE. *Synthesis, characterization, and in vitro evaluation of the selective P2Y₂ receptor antagonist AR-C118925*. *Purinergic Signal*. 2016 Oct 20. [Epub ahead of print]

Braune A, Engst W, Elsinghorst PW, Furtmann N, Bajorath J, Gütschow M, Blaut M. *Chalcone Isomerase from Eubacterium ramulus Catalyzes the Ring Contraction of Flavanonols*. J Bacteriol. 2016 Oct 7; 198(21):2965-2974.

Fiene A, Baqi Y, Malik EM, Newton P, Li W, Lee SY, Hartland EL, Müller CE. *Inhibitors for the bacterial Ectonucleotidase Lp1NTPDase from Legionella pneumophila*. Bioorg. Med. Chem. 2016 Sep 24; 4363-4371.

Hagelstein V, Ortland I, Wilmer A, Mitchell SA, Jaehde U. *Validation of the German patient-reported outcomes of the common terminology criteria for adverse events (PRO-CTCAE)*. Ann Oncol. 2016 Sep 28; [Epub ahead of print]

Sathanoori R, Bryl-Gorecka P, Müller CE, Erb L, Weisman GA, Olde B, Erlinge D. *P2Y₂ receptor modulates shear stress-induced cell alignment and actin stress fibers in human umbilical vein endothelial cells*. Cell Mol Life Sci. 2017 Feb;74(4):731-746.

Tietze D, Leipold E, Heimer P, Böhm M, Winschel W, Imhof D, Heinemann SH, Tietze AA. *Molecular interaction of δ -conopeptide EVIA with voltage-gated Na⁺ channels*. Biochim. Biophys. Acta - General Subjects, 2016 Sep, 1860, 2053-2063.

Thiede S, Wosniok P, Herkommer D, Schulz-Fincke AC, Gütschow M, Menche D. *Total Synthesis of Leupyrrin B1: a Potent Inhibitor of Human Leukocyte Elastase*. Org Lett. 2016 Aug 19; 18(16):3964-7.

Beckmann AM, Gilberg E, Gattner S, Huang TL, Vanden Eynde JJ, Mayence A, Bajorath J, Stirnberg M, Gütschow M. *Evaluation of Bisbenzamidines as Inhibitors for Matriptase-2*. Bioorg Med Chem Lett. 2016 Aug 1; 26(15):3741-5.

Beckmann AM, Glebov K, Walter J, Merkel O, Mangold M, Schmidt F, Becker-Pauly C, Gütschow M, Stirnberg M. *The intact Kunitz Domain Protects the Amyloid Precursor Protein from Being Processed by Matriptase-2*. Biol Chem. 2016 Aug 1; 397(8):777-90.

Batalha VL, Ferreira DG, Coelho JE, Valadas JS, Gomes R, Temido-Ferreira M, Shmidt T, Baqi Y, Buée L, Müller CE, Hamdane M, Outeiro TF, Bader M, Meijsing SH, Sadri-Vakili G, Blum D, Lopes LV. *The caffeine-binding adenosine A_{2A} receptor induces age-like HPA-axis dysfunction by targeting glucocorticoid receptor function*. Nature Scientific Reports 2016 Aug; 6: 31493.

Flegel C, Vogel F, Hofreuter A, Wojcik S, Schoeder CT, Kieć-Kononowicz K, Brockmeyer NH, Müller CE, Becker C, Altmüller J, Hatt H, Gisselmann G. *Characterization of non-olfactory GPCRs in human sperm with a focus on GPR18*. Nature Scientific reports 2016 Aug; 6: 32255.

Malik EM, Rashed M, Wingen L, Baqi Y, Müller CE. *Ullmann reactions of 1-amino-4-bromoanthraquinones bearing various 2-substituents furnishing novel dyes*. Dyes and Pigments. 2016 Aug; 131, 33-40.

Park JH, Williams DR, Lee JH, Lee SD, Lee JH, Ko H, Lee GE, Kim S, Lee JM, Abdelrahman A, Müller CE, Jung DW, Kim YC. *Potent suppressive effects of 1-piperidinylimidaole based novel P2X7 receptor antagonists on cancer cell migration and invasion*. J. Med. Chem. 2016 Aug, 59, 7410-7430.

- Gupta S, Biswas A, Akhter MS, Krettler C, Reinhart C, Dodt J, Reuter A, Philippou H, Ivaskevicius V, Oldenburg J. *Revisiting the mechanism of coagulation factor XIII activation and regulation from a structure/functional perspective*. Sci Rep. 2016 Jul 25; 6:30105.
- Pezeshkpoor B, Castoldi E, Mahler A, Hanel D, Müller J, Hamedani NS, Biswas A, Oldenburg J, Pavlova A. *Identification and functional characterization of a novel F5 mutation (Ala512Val, FVB onn) associated with activated protein C resistance*. J Thromb Haemost. 2016 Jul; 14(7):1353-63.
- Lee SY, Perotti A, De Jonghe S, Herdewijn P, Hanck T, Müller CE. *Thiazolo[3,2-a]benzimidazol-3(2H)-one derivatives: structure-activity relationships of selective nucleotide pyrophosphatase/phosphodiesterase1 (NPP1) inhibitors*. Bioorg. Med. Chem. 2016 Jul, 24, 3157-3165.
- Küppers J, Schulz-Fincke AC, Palus J, Giurg M, Skarzewski J, Gütschow M. *Convergent Synthesis of two Fluorescent Ebselen-Coumarin Heterodimers*. Pharmaceuticals (Basel). 2016 Jul 8;9(3). pii: E43.
- Salar S, Lapilover E, Müller J, Hollnagel JO, Lippmann K, Friedman A, Heinemann U. *Synaptic plasticity in area CA1 of rat hippocampal slices following intraventricular application of albumin*. Neurobiol Dis. 2016 Jul;91:155-65.
- Häußler D, Mangold M, Furtmann N, Braune A, Blaut M, Bajorath J, Stirnberg M, Gütschow M. *Phosphono Bisbenzguanidines as Irreversible Dipeptidomimetic Inhibitors and Activity-based Probes of Matriptase-2*. Chemistry. 2016 Jun 13;22(25):8525-35.
- Steinebach C, Schulz-Fincke AC, Schnakenburg G, Gütschow M. *In Situ Generation and Trapping of Thioimidates: An Intermolecular Tandem Reaction to 4-Acylimino-4H-3,1-benzothiazines*. RSC Adv. 2016, 6, 15430-40.
- Brewitz HH, Goradia N, Schubert E, Galler K, Kühl T, Syllwasschy B, Popp J, Neugebauer U, Hagelueken G, Schiemann O, Ohlenschläger O, Imhof D. *Heme interacts with histidine- and tyrosine-based protein motifs and inhibits enzymatic activity of chloramphenicol acetyltransferase from Escherichia coli*. Biochim. Biophys. Acta - General Subjects, 2016 Jun, 1860, 1343-1353.
- De Filippo E, Namasivayam V, Zappe L, El-Tayeb A, Schiedel AC, Müller CE. *Role of extracellular cysteine residues in the adenosine A_{2A} receptor*. Purinergic Signal. 2016 Jun, 12, 313-329.
- Grizić D, Heimer P, Vranić E, Imhof D, Lamprecht A. *From propylene carbonate to 3,5-diacetyl-1,4-dihydro-2,6-lutidine: a novel quantification approach*. Talanta, 2016, May, 151, 75-82.
- Hess C, Schoeder CT, Pillaiyar T, Madea B, Müller CE. *Pharmacological evaluation of synthesis cannabinoids identified as constituents of spice*. Forensic Toxicol. 2016 May; 34, 329-343.

Jacobson KA, Müller CE. *Medicinal chemistry of adenosine, P2Y and P2X receptors*. Neuropharmacol. 2016 May; 104, 31-49.

Mann PA, Müller A, Wolff KA, Fischmann T, Wang H, Reed P, Hou Y, Li W, Müller CE, Xiao J, Murgolo N, Sher X, Mayhood T, Sheth PR, Mirza A, Labroli M, Xiao L, McCoy M, Gill CJ, Pinho MG, Schneider T, Romer T. *Chemical genetic analysis and functional characterization of staphylococcal wall teichoic acid 2-epimerases reveals unconventional antibiotic drug targets*. PLoS Pathog. 2016 May, 12(5), e1005585.

Wilhelm M, Mueller L, Miller MC, Link K, Holdenrieder S, Bertsch T, Kunzmann V, Stoetzer OJ, Suttmann I, Braess J, Birkmann J, Roessler M, Moritz B, Kraff S, Salamone SJ, Jaehde U. *Prospective, Multicenter Study of 5-Fluorouracil Therapeutic Drug Monitoring in Metastatic Colorectal Cancer Treated in Routine Clinical Practice*. Clin Colorectal Cancer. 2016 May 7 [Epub ahead of print]

Chen Y, Buyel JJ, Hanssen MJ, Siegel F, Pan R, Naumann J, Schell M, van der Lans A, Schlein C, Froehlich H, Heeren J, Virtanen KA, van Marken Lichtenbelt W, Pfeifer A. *Exosomal microRNA miR-92a concentration in serum reflects human brown fat activity*. Nat Commun. 2016 Apr 27; 7:11420.

Canton J, Schlam D, Breuer C, Gütschow M, Glogauer M, Grinstein S. *Calcium-sensing Receptors Signal Constitutive Macropinocytosis and Facilitate the Uptake of NOD2 Ligands in Macrophages*. Nat Commun. 2016 Apr 6;7:11284.

Beckmann AM, Maurer E, Lülldorff V, Wilms A, Furtmann N, Bajorath J, Gütschow M, Stirnberg M. *En Route to New Therapeutic Options for Iron Overload Diseases: Matriptase-2 as a target for Kunitz-type inhibitors*. Chembiochem. 2016 Apr 1;17(7):595-604.

Klepac K, Kilić A, Gnad T, Brown LM, Herrmann B, Wilderman A, Balkow A, Glöde A, Simon K, Lidell ME, Betz MJ, Enerbäck S, Wess J, Freichel M, Blüher M, König G, Kostenis E, Insel PA, Pfeifer A. *The Gq signalling pathway inhibits brown and beige adipose tissue*. Nat Commun. 2016 Mar 9; 7:10895.

Moghaddam AJ, Boehringer N, Burdziak A, Kunte HJ, Galinski EA; Schäberle TF. Different strategies of osmoadaptation in the closely related marine Myxobacteria *Enhygromyxa salina* SWB007 and *Plesiocystis pacifica* SIR-1. Microbiolgy. 2016 Feb. 03

Mertens MD, Bierwisch A, Li T, Gütschow M, Thiermann H, Wille T, Elsinghorst PW. *A Novel Fluorogenic Probe for the Investigation of Free Thiols: Application to Kinetic Measurements of Acetylcholinesterase Activity*. Toxicol Lett. 2016 Feb 26;244:161-6.

Häußler D, Gütschow M. *Fluorescently Labeled Amino Acids as Building Blocks for Bioactive Molecules*. Synthesis 2016, 48 (2), 245-55.

Engelhardt B, Fröhlich H, Kschischo M. Learning (from) the errors of a systems biology model. SciRep. 2016 Feb 11;6:20772.

Laurent C, Burnouf S, Ferry B, Batalha VL, Coelho JE, Baqi Y, Malik E, Marciniak E, Parrot S,

Van der Jeugd A, Faivre E, Flaten V, Ledent C, D'Hooge R, Sergeant N, Hamdane M, Humez S, Müller CE, Lopes LV, Buée L, Blum D. *A_{2A} adenosine receptor deletion is protective in a mouse model of tauopathy*. Mol. Psychiatry 2016 Jan, 21, 97-107.

Roydeva PG, Beckmann AM, Stirnberg M, Cesar J, Kikelj D, Ilaš J, Gütschow M. *3,1-Benzothiazines, 1,4-Benzodioxines and 1,4-Benzoxazines as Inhibitors of Matriptase-2: Outcome of a Focused Screening Approach*. Pharmaceuticals (Basel). 2016 Jan 13;9(1). pii: E2.

Podurgiel SJ, Spencer T, Kovner R, Baqi Y, Müller CE, Correa M, Salamone JD. *Induction of oral tremor in mice by the acetylcholinesterase inhibitor galantamine: reversal with adenosine A_{2A} antagonism*. Pharmacol. Biochem. Behav. 2016 Jan, 140, 62-67.

Schmitz J, Li T, Bartz U, Gütschow M. *Cathepsin B Inhibitors: Combining Dipeptide Nitriles with an Occluding Loop Recognition Element by Click Chemistry*. ACS Med Chem Lett. 2016 7(3):211-6.

Furtmann N, Häußler D, Scheidt T, Stirnberg M, Steinmetzer T, Bajorath J, Gütschow M. *Limiting the Number of Potential Binding Modes by Introducing Symmetry into Ligands: Structure-Based Design of Inhibitors for Trypsin-Like Serine Proteases*. Chemistry. 2016 Jan 11;22(2):610-25.

Simon K, Hennen S, Merten N, Blättermann S, Gillard M, Kostenis E, Gomeza J. *The Orphan G Protein-coupled Receptor GPR17 Negatively Regulates Oligodendrocyte Differentiation via Gai/o and Its Downstream Effector Molecules*. J Biol Chem. 2016 Jan 8;291(2):705-18.

Hamedani NS, Müller J. *Capillary Electrophoresis for the Selection of DNA Aptamers Recognizing Activated Protein C*. Methods Mol Biol. 2016; 1380:61-75.